Fredholm indices and the phase diagram of quantum Hall systems

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The quantized Hall conductance in a plateau is related to the index of a Fredholm operator. In this paper we describe the generic ''phase diagram'' of Fredholm indices associated with bounded and Toeplitz operators. We discuss the possible relevance of our results to the phase diagram of disordered integer quantum Hall systems. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1331317]

The Hall conductance of integer quantum Hall systems is described mathematically by the index of Fredholm operators. (For precise definitions, see below.) In this paper we investigate the phase diagram of the Fredholm index for a few classes of operators. For the algebra of bounded operators, little can be said beyond the fact that the phase diagrams can be arbitrarily complicated. But for the algebra of Toeplitz operators, and other related classes of operators, we establish a kind of a Gibbs phase rule.[1] Typical of our results is the statement that if the system is governed by two parameters, then one should expect jumps by one at phase boundaries and jumps by up to 2 at triple points, while jumps by more than two should never be observed.

We relate this behavior to experimental results, conjectures and open problems that arise in the context of the quantum Hall effect (QHE).[2]

In Sec. I we define Fredholm operators and their indices, and explore the different sorts of phase diagrams that can arise. In Sec. II we recall how Fredholm indices are related to the conductance of Quantum Hall systems. In Sec. III we consider phase diagrams for general bounded operators. In Sec. IV we describe the phase diagram for linear combination of shift operators, and in Sec. V we consider general Toeplitz operators. In Sec. VI we discuss the phase diagrams of soluble models related to the quantum Hall effect, and how they might be modified by disorder. We also discuss the relevance of Toeplitz operators to the quantum Hall effect and present some open problems.

I. FREDHOLM INDICES

A. Basic notions

The following is a brief description of Fredholm operators. For more details, see Refs. 3–5.

Definition 1: A bounded operator F on a separable Hilbert space is Fredholm if there exists a bounded operator B such that $1-FB$ and $1-BF$ are compact. The Fredholm index is defined by

$$\mathrm{Index}(F)=\dim \mathrm{Ker}(F)-\dim \mathrm{Ker}(F^{\dagger}). \tag{1}$$

The simplest example of a Fredholm operator with nonzero index is the unilateral shift operator: Let $e_0,e_1,e_2,\ldots$ be the canonical basis for the Hilbert space $l^2(\mathbb{N})$, and let the operator a act by

$$a(e_n)=\begin{cases} e_{n-1} & \text{if } n>0, \\ 0 & \text{if } n=0. \end{cases} \tag{2}$$

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The reason for denoting the unilateral shift operator by a is its similarity to the harmonic oscillator lowering operator. The adjoint of a acts by

$$a^\dagger(e_n)=e_{n+1}. \tag{3}$$

Since $1=aa^\dagger=a^\dagger a+|e_0\rangle\langle e_0|$, a is Fredholm. The kernel of a is one dimensional and the kernel of $a^\dagger$ is zero dimensional. Thus $\mathrm{Index}(a)=1$ and $\mathrm{Index}(a^\dagger)=-1$.

Although neither the dimension of $\mathrm{Ker}\,F$ nor that of $\mathrm{Ker}\,F^\dagger$ is stable under deformations of F, the index *is* stable. For any compact operator C, for any bounded operator B, and for ϵ sufficiently small:[4,5]

$$\mathrm{Index}(F)=\mathrm{Index}(F+\epsilon B+C). \tag{4}$$

The following theorem is standard.

Theorem 1: If $A_1,\ldots A_n$ are Fredholm operators, then the product $A_1A_2\cdots A_n$ is also Fredholm, and $\mathrm{Index}\,(A_1\cdots A_n)=\Sigma_{i=1}^n\mathrm{Index}(A_i)$.

If F and F' are Fredholm operators on the same Hilbert space, then there is a continuous path of Fredholm operators from F to F' if and only if $\mathrm{Index}(F)=\mathrm{Index}(F')$. (By continuous, we mean relative to the operator norm.) Put another way, the path components of $\mathrm{Fred}(H)$, the space of Fredholm operators on H, are indexed by the integers. The nth path component is precisely the set of Fredholm operators of index n.[4]

B. Phase diagrams

Our main concern in this paper is the following problem: Suppose one interpolates between Fredholm operators with different indices. What can one say about the way the indices change? Another way of phrasing this is: What is the phase diagram of Fredholm indices?

The answer to this question depends on the choice of the embedding space. In the space of bounded operators, the ''phases''—each labeled by its index—are open sets. But the boundary between phases, as we shall explain, is rather wild: A point on the boundary of one phase is also on the boundary of *every other* phase. This behavior is difficult to visualize.

Another class of embedding spaces that we consider is associated with Toeplitz operators with various regularity assumptions on a class of functions. Here, at least if the functions are sufficiently smooth, the boundaries between phases have a simple structure and the phase diagrams satisfy simple rules that have the flavor of Gibbs' phase rule.[1] Typical of our results is the statement that under appropriate conditions, phases whose indices differ by one have a common boundary whose codimension is one, and phases whose indices differ by two meet on a set of codimension two, etc. Figure 1 is an example of one of the phase diagrams we obtain.

II. THE HALL CONDUCTANCE AS A FREDHOLM INDEX

Theories of the quantum Hall effect are roughly of two kinds: those that focus on the bulk of the Hall and those that focus on the edge.[2] It was pointed out by Ref. 6 that the bulk-edge duality is an illustration of the *holographic principle*. In either approach, the quantized Hall conductance can be related to a Fredholm index.

A. Theories of the bulk

It is common knowledge that the Hall conductance can be identified with a Chern number.[7] For noninteracting electrons in two dimensions, this result is a special case of the fact that the Hall conductance is a Fredholm index. Since this is not common knowledge, we recall how Chern numbers and Fredholm indices are related.

For noninteracting electrons in two dimensions with the Fermi energy in a gap, TKN[2], showed that the Hall conductance for Landau Hamiltonians with *periodic* potential, is related to a Chern number.[8] The (magnetic) Brillouin zone associated with the periodicity plays a role in this theory. Because of this, the interpretation of the Hall conductance as a Chern number does not

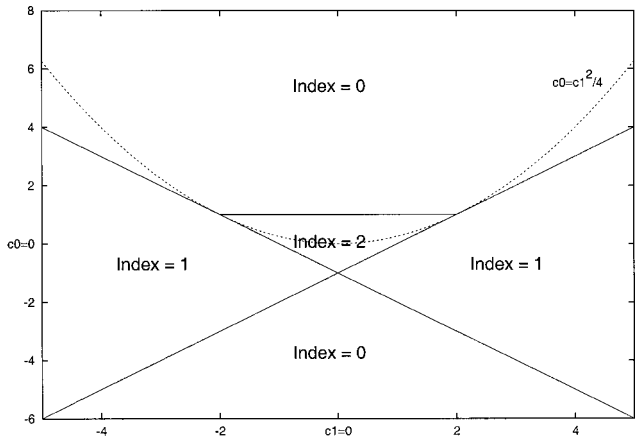

FIG. 1. A phase diagram for the Fredholm index of $F=a^2+c_1a+c_0$.

carry over to random or even quasiperiodic potentials nor to ''irrational magnetic fields,'' all of which have no (classical) Brillouin zone. Although the quantization of the Hall conductance can be established in these cases by a limiting argument,[9,7] the interpretation as a Chern number does not survive.

Bellissard,[10] in a work that had impact on noncommutative geometry,[11,12] showed that the Hall conductance with *ergodic* potential, be it periodic, quasiperiodic or random, and real magnetic field, rational or not, is a Fredholm index. This result was derived in Ref. 13 without using noncommutative geometry.

More precisely, consider the (infinite dimensional) spectral projection P on the states below the Fermi energy E_F for the one particle Hamiltonian in the plane. Let U be the multiplication operator $e^{i\theta}$, where θ is the usual polar angle in the plane. U is a singular gauge transformation that introduces an Aharonov–Bohm flux tube at the origin of the Euclidean plane. The Hall conductance is the Fredholm index of PUP thought of as an operator on the range of P.[14] Since the Fredholm index does not need a Brillouin zone, this approach offers a natural framework that accounts for the quantization and stability of the Hall conductance.

B. Theories of the edge

Finite quantum Hall systems have chiral edge currents.[15,16] Consider the case that the boundary is a circle of circumference L. The dispersion relation of the edge states is approximately linear in a small neighborhood of the Fermi energy and the Hamiltonian for a single edge channel, with velocity v_F, is

$$H=-i\frac{v_F}{L}\partial_\theta. \tag{5}$$

Now, the projection P is associated with the occupied edge states, $e^{-im\theta}$ with $m\geqslant m_0$. Introducing a flux tube into the system is associated with the unitary $U=e^{i\theta}$ and sends $H\to UHU^\dagger$. This leads to the spectral flow of the edge states. PUP is the unilateral shift operator a and the number of edge states that cross the Fermi energy is Index $PUP=1$. By an argument of Halperin[15] this is also the Hall conductance.

An extension of this idea to Harper models with an edge is described in Ref. 17.

III. THE PHASE DIAGRAM FOR BOUNDED OPERATORS

We begin with the space of bounded operators with the topology defined by the operator norm, and we wish to understand the phase diagram of a generic family of such operators. As we shall explain, the phase diagram in the entire space is quite wild: Any point on the boundary of the ''index=k'' phase is also on the boundary of every other phase.

To understand this bizarre behavior, recall that the zero operator (which is *not* a Fredholm operator) is on the boundary of every phase: Zero is the limit, as $\varepsilon \to 0$, of εa^n, with a of Eq. (2), for any n. The point of the theorem is that similar behavior occurs at all boundary points.

Theorem 2: Let U_n be the set of Fredholm operators of index n. Every point on the boundary of U_n is also on the boundary of U_m, for every integer m.

Proof: Let A be a (not Fredholm) operator on the boundary of U_n. Given $\epsilon > 0$, we must find an operator in U_m within a distance ϵ of A.

Suppose that the kernel and cokernel of A are infinite dimensional, and that there is a gap in the spectrum of $A^\dagger A$ at zero. (If this is not the case, we may perturb A by an arbitrarily small amount to make it so.) Now let B be a unitary map from the kernel of A to the cokernel. Let P (P'), be the orthogonal projection onto $\ker(A)$ [$\mathrm{coker}(A)$], and let a be a shift operator on $\ker(A)$. For each $m \geqslant 0$, $A(\epsilon) = A + \epsilon B a^m P$ has a bounded right inverse

$$A^\dagger \frac{1}{P' + AA^\dagger} P'_\perp + \frac{1}{\epsilon} (a^\dagger)^m B^\dagger P'. \tag{6}$$

It follows that the cokernel of $A(\epsilon)$ is empty. It is easy to see that the kernel of $A(\epsilon)$ is m dimensional hence $\mathrm{Index}(A(\epsilon)) = m$. Similarly, $A + \epsilon B (a^\dagger)^m P$ has index $-m$. ■

IV. LINEAR COMBINATIONS OF SHIFTS

In this section and the next we show that there are interesting and simple ''generic'' phase diagrams of Fredholm indices in some finite-dimensional spaces, and in some infinite-dimensional spaces with sufficiently fine topologies. We shall also see how control is lost as the space is enlarged and the topology is coarsened.

A. Shift by one

We begin by considering linear combinations of the shift operator a and the identity operator 1. That is, we consider the operator

$$A = c_1 a + c_0,$$

where c_1 and c_0 are constants.

Theorem 3: If $|c_1| \neq |c_0|$, then A is Fredholm. The index of A is 1 if $|c_1| > |c_0|$ and zero if $|c_1| < |c_0|$. If $|c_1| = |c_0|$, then A is not Fredholm.

Proof: First suppose $|c_0| > |c_1|$. Then A is invertible:

$$A^{-1} = c_0^{-1}(1 + (c_1/c_0)a)^{-1} = \sum_{n=0}^{\infty} \frac{(-1)^n c_1^n}{c_0^{n+1}} a^n,$$

as the sum converges absolutely. Thus A has neither kernel nor cokernel, and has index zero.

If $|c_1| > |c_0|$, then the kernel of A is one dimensional, namely all multiples of $|\psi\rangle = \Sigma_{n=0}^{\infty} z_0^n e_n$, where $z_0 = -c_0/c_1$. Notice how the norm of $|\psi\rangle$ goes to infinity as $|z_0| \to 1$. However, $A^\dagger$ has no kernel, since for any unit vector $|\phi\rangle$, $\|A^\dagger|\phi\rangle\| = \|\overline{c_1} a^\dagger |\phi\rangle + \overline{c_0}|\phi\rangle\| \geqslant \|\overline{c_1} a^\dagger |\phi\rangle\| - \|\overline{c_0}|\phi\rangle\| = |c_1| - |c_0|$. Thus the index of A is 1.

If $|c_1| = |c_0|$, then A is at the boundary between index 1 and index 0, and so cannot be Fredholm. ■

B. Finite linear combinations of shifts

Next we consider linear combinations of $1,a,a^2,\ldots$ up to some fixed a^n. That is, we consider operators of the form

$$A=c_n a^n+c_{n-1}a^{n-1}+\cdots+c_0. \tag{7}$$

This is closely related to the polynomial

$$p(z)=c_n z^n+\cdots+c_0. \tag{8}$$

Theorem 4: If none of the roots of p lie on the unit circle, then A is Fredholm, and the index of A equals the number of roots of p inside the unit circle, counted with multiplicity. If any of the roots of p lie on the unit circle, then A is not Fredholm.

Proof: The polynomial $p(z)$ factorizes as $p(z)=c_k\Pi_{i=1}^{k}(z-\zeta_i)$, where k is the degree of p (typically $k=n$, but it may happen that $c_n=0$). But then $A=c_k\Pi_{i=1}^{k}(a-\zeta_i)$. If none of the roots ζ_i lie on the unit circle, then each term in the product is Fredholm, so the product is Fredholm, and the index of the product is the sum of the indices of the factors. By Theorem 3, this exactly equals the number of roots ζ_i inside the unit circle.

If any of the roots lie on the unit circle, then a small perturbation can push those roots in or out, yielding Fredholm operators with different indices. This borderline operator therefore cannot be Fredholm. ■

The last theorem easily generalizes to linear combination of left shifts and right shifts. The index of an operator

$$A=c_n a^n+\cdots+c_1 a+c_0+c_{-1}a^\dagger+\cdots+c_{-m}(a^\dagger)^m \tag{9}$$

equals the number of roots of

$$p(z)=\sum_{i=-m}^{n} c_i z^i \tag{10}$$

inside the unit circle, minus the degree of the pole at $z=0$ (that is m, unless $c_{-m}=0$). This follows from the fact that

$$A=\left(\sum_{i=-m}^{n} c_i a^{i+m}\right)(a^\dagger)^m. \tag{11}$$

Since there is no qualitative difference between combinations of left shifts and combinations of both left and right shifts, we restrict our attention to left shifts only, and consider families of operators of the form (7).

Theorem 5: In the space of complex linear combinations of $1,a,\ldots,a^n$, almost every operator is Fredholm. For every $k\leqslant n$, the points where the index can jump by k (by which we mean the common boundaries of regions of Fredholm operators whose indices differ by k) is a set of real codimension k.

In the space of real linear combinations of $1,a,\ldots,a^n$, almost every operator is Fredholm. For every $k\leqslant n$, the points where the index jumps by k is a stratified space, the largest stratum of which has real codimension $\lfloor (k+1)/2\rfloor$, where $\lfloor x\rfloor$ denotes the integer part of x.

Proof: Our parameter space is the space of coefficients c_i, or equivalently the space of polynomials of degree $\leqslant n$. This is either $\mathbb{R}^{n+1}$ or $\mathbb{C}^{n+1}$, depending on whether we allow real or complex coefficients. In either case, the set U_k of Fredholm operators of index k is identical to the set of polynomials with k roots inside the unit circle and the remaining $n-k$ roots outside. (If $c_n=0$, we say there is a root at infinity; if $c_n=c_{n-1}=0$, there is a double root at infinity, and so on. Counting these roots at infinity, there are always exactly n roots in all.) The boundary of U_k is the set of polynomials with at most k roots inside the unit circle, at most $n-k$ outside the unit

circle, and at least one root on the unit circle. (Strictly speaking, the zero polynomial is also on this boundary. This is of such high codimension that it has no effect on the phase portrait we are developing.) We consider the common boundary of U_k and $U_{k'}$. If $k<k'$, a nonvanishing polynomial is on the boundary of both U_k and $U_{k'}$ if it has at most k roots inside the unit circle and at most $n-k'$ roots outside. It must therefore have at least $k'-k$ roots on the unit circle.

If we are working with complex coefficients, this is a set of codimension $k'-k$. The roots themselves, together with an overall scale c_n, can be used to parametrize the space of polynomials. For each root, being on the unit circle is codimension 1, while being inside or outside are open conditions. Since the roots are independent, placing $k'-k$ roots on the unit circle is codimension $k'-k$.

If we are working with real coefficients, the roots are not independent, as nonreal roots come in complex conjugate pairs. Thus, the common boundary of U_k and $U_{k'}$ breaks into several strata, depending on how many real roots and how many complex conjugate pairs lie on the unit circle. If $k'-k$ is even, the biggest stratum consists of having $(k'-k)/2$ pairs, and has codimension $(k'-k)/2$. If $k'-k$ is odd, the biggest stratum consists of having $(k'-k-1)/2$ pairs and one real root on the unit circle, and has codimension $(k'+1-k)/2$. ■

Theorem 5 is illustrated in Fig. 1, where the phase portrait is shown for $n=2$ with real coefficients, with c_2 fixed to equal 1. The points above the parabola $c_0=c_1^2/4$ have complex conjugate roots, while points below have real roots. Notice that the transition from index 2 to index 0 occurs at an isolated point when the roots are real, but on an interval when the roots come in complex-conjugate pairs.

It is clear that an almost identical theorem applies to linear combinations of left shifts up to a^n and right shifts up to $(a^\dagger)^m$. The results are essentially independent of n and m (their only effect being to limit the size of possible jumps to $n+m$). We can therefore extend the results to the space of all (finite) linear combinations of left and right shifts, which is topologized as the union over all n and m of the spaces considered above. Our result, restated for that space, is

Theorem 6: In the space of finite complex linear combinations of left and right shifts of arbitrary degree, almost every operator is Fredholm. For every integer $k\geqslant 1$, the points where the index can jump by k (by which we mean the common boundaries of regions of Fredholm operators whose indices differ by k) is a set of real codimension k.

If we restrict the coefficients to be real, then, for every $k\leqslant n$, the points where the index jumps by k is a stratified space, the largest stratum of which has real codimension $\lfloor (k+1)/2 \rfloor$.

V. TOEPLITZ OPERATORS

Although Theorem 6 refers to an infinite-dimensional space, this space is still extremely small—each point is a *finite* linear combination of shifts. In this section we consider *infinite* linear combinations of shifts. This is equivalent to studying Toeplitz operators.

Definition 2: The Hardy space H is the subspace of $L^2(S^1)$ consisting of functions whose Fourier transforms have no negative frequency terms. Equivalently, if we give $L^2(S^1)$ a basis of Fourier modes $e_n=e^{in\theta}$, where the integer n ranges from $-\infty$ to ∞, then H is the closed linear span of $e_0, e_1, e_2, \ldots$.

We think of S^1 as sitting in the complex plane, with $z=e^{i\theta}$. Now let $f(z)$ be a bounded, measurable function on S^1, and let P be the orthogonal projection from $L^2(S^1)$ to H. If $|\psi\rangle \in H$, then $|f\psi\rangle$ (pointwise product) is in $L^2(S^1)$, and $P|f\psi\rangle \in H$. We define the operator T_f by

$$T_f|\psi\rangle = P|f\psi\rangle. \tag{12}$$

Definition 3: An operator of the form (12) is called a Toeplitz operator. We call a Toeplitz operator T_f continuous if the underlying function f is continuous, and apply the terms ''differentiable,'' ''smooth,'' and ''analytic'' similarly.

Remark: Toeplitz operators can be represented by semi-infinite matrices that have constant entries on diagonals, and the various classes we have defined correspond to the decay away from the main diagonal.

Notice that

$$T_{e_m} e_n = \begin{cases} e_{n+m} & \text{if } n+m \geqslant 0, \\ 0 & \text{otherwise,} \end{cases} \tag{13}$$

so T_{e_m} is simply a shift by m, a right shift if $m>0$ and a left shift if $m<0$. All our results about shifts can therefore be understood in the context of Toeplitz operators. Theorem 5 refers to operators T_f, where f is a polynomial in z^{-1} of limited degree. Theorem 6 considers polynomials or arbitrary degree in z and z^{-1}. We will see that the results carry over to analytic functions on an annulus around S^1, and to a lesser extent to C^k Toeplitz operators, but with results that weaken as k is decreased.

Here are some standard results about Toeplitz operators. For details, see Ref. 4.

Theorem 7: A C^1 Toeplitz operator T_f is Fredholm if and only if f is everywhere nonzero on the unit circle. In that case the index of T_f is minus the winding number of f around the origin, namely

$$\text{Index}(T_f) = -\text{Winding}(f) = \frac{-1}{2\pi i} \int_{S^1} \frac{df}{f}. \tag{14}$$

Given the first half of the theorem, the equality of index and winding number is easy to understand. We simply deform f to a function of the form $f(z)=z^n$, while keeping f nonzero on all of S^1 throughout the deformation (this is always possible, see e.g., Ref. 18). In the process of deformation, neither the index of T_f nor the winding number of f can change, as they are topological invariants. Since the winding number of z^n is n, and since $T_{z^n}=(a^\dagger)^n$ (if $n\geqslant 0$, a^{-n} otherwise), which has index $-n$, the result follows.

We now consider functions f on S^1 that can be analytically continued (without singularities) to an annulus $r_0 \leqslant |z| \leqslant r_1$, where the radii $r_0<1$ and $r_1>1$ are fixed. This is equivalent to requiring that the Fourier coefficients $\hat{f}_n$ decay exponentially fast, i.e., that the sum

$$\sum_{n=-\infty}^{\infty} |\hat{f}_n|(r_0^n + r_1^n) \tag{15}$$

converges. For now we do not impose any reality constraints or other symmetries on the coefficients $\hat{f}_n$. This space of functions is a Banach space, with norm given by the sup norm on the annulus. This norm is stronger than any Sobolev norm on the circle itself.

The analysis of the corresponding Toeplitz operators is straightforward and similar to the proof of Theorem 5. Since f has no poles in the annulus, we just have to keep track of the zeroes of f. For the index of T_f to change, a zero of f must cross the unit circle. For the index to jump from k to k', $|k-k'|$ zeroes must cross simultaneously. In the absence of symmetry, the locations of the zeroes are independent and can be freely varied, so this is a codimension-$|k-k'|$ event.

If we impose a reality condition: $f(\overline{z})=\overline{f(z)}$, then zeroes appear only on the real axis or in complex conjugate pairs. In that case, changing the index by 2 is merely a codimension-1 event. Combining these observations we obtain the following theorem.

Theorem 8: In the space of Toeplitz operators that are analytic in a (fixed) annulus containing S^1, almost every operator is Fredholm. For every integer $k\geqslant 1$, the points where the index can jump by k is a set of real codimension k.

If we impose a reality condition $f(\overline{z})=\overline{f(z)}$ then, for every $k\leqslant n$, the points where the index jumps by k is a stratified space, the largest stratum of which has real codimension $\lfloor (k+1)/2 \rfloor$.

Finally we consider Toeplitz operators that are not necessarily analytic, but are merely l times differentiable, and we use the C^l norm. Our result is the following.

Theorem 9: In the space of Toeplitz C^l operators, almost every operator is Fredholm. For every integer k with $1 \leqslant k \leqslant 2l+1$, the points where the index can jump by k is a set of real codimension k. For every integer $k \geqslant 2l+1$, the points where the index can jump by k is a set of real codimension $2l+1$.

In other words, our familiar results hold up to codimension $2l+1$, at which point we lose all control of the change in index.

Proof: As long as f is everywhere nonzero, T_f is Fredholm. To get a change in index, therefore, we need one or more points where f, and possibly some derivatives of f with respect to θ, vanish. Suppose then that for some angle θ_0, $f(\theta_0)=f'(\theta_0)=\cdots=f^{(n-1)}(\theta_0)=0$ for some $n \leqslant l$, but that the nth derivative $f^{(n)}(\theta_0) \neq 0$. This is a codimension $2n-1$ event, since we are setting the real and imaginary parts of n variables to zero, but have a 1-parameter choice of points where this can occur. Without loss of generality, we suppose that this nth derivative is real and positive. By making a C^l-small perturbation of f, we can make the value of f highly oscillatory near θ_0, thereby wrapping around the origin a number of times. However, since a C^l-small perturbation does not change the nth derivative by much, the sign of the real part of f can change at most n times near θ_0, so the argument of f can only increase or decrease by $n\pi$ or less. The difference between these two extremes is $2n\pi$, or a change in winding number of n.

To change the index by an integer m, therefore, we must have the function vanish to various orders at several points, with the sum of the orders of vanishing adding to m. The generic event is for f (but not f') to vanish at m different points—this is a codimension m event, analogous to having m zeroes of a polynomial cross the unit circle simultaneously at m different points. All other scenarios have higher codimension and are analogous to having two or more zeroes of the m zeroes crossing the unit circle at the same point.

The situation is different, however, when the function f and the first l derivatives all vanish at a point θ_0. Then the higher-order derivatives are not protected from C^l-small perturbations and, by making such a perturbation, we can change f into a function that is identically zero on a small neighborhood of $\theta=\theta_0$. By making a further small perturbation, we can make f wrap around the origin as many times as we like near $\theta=\theta_0$. More specifically, if f is zero on an interval of size δ, then, for small ϵ, $\tilde{f}(\theta)=f(\theta)+\epsilon e^{iN\theta}$ will wrap around the origin approximately $N\delta/2\pi$ times near θ_0. By picking N as large (positive or negative) as we wish, we can obtain arbitrarily positive or negative indices. As long as we take $\epsilon \ll N^{-l}$, this perturbation will remain small in the C^l norm. ■

The results of this section can be extended, with minor modifications, to the algebra of matrix valued Toeplitz operators[4] where the index is related to the winding of the determinant of a matrix.

VI. QUANTUM HALL SYSTEMS

A. Phase diagrams of soluble models

Phase diagrams of the quantum Hall system describe the dependence of the Hall conductance on parameters such as the magnetic field B and the Fermi energy E. There are three idealized models where the phase diagram can be computed explicitly: The Landau Hamiltonian in the Euclidean plane, whose phase diagram is shown in Fig. 2; The Landau Hamiltonian for the hyperbolic plane, whose phase diagram is shown in Fig. 3 and Harper models in the plane,[19,8] whose phase diagram is associated with the Hofstadter butterfly, shown in Fig. 4 for the case of a tight binding model on a square lattice.

These are not models of Toeplitz operators, and none of these models are generic, especially insofar as all of them have symmetries. However, we consider the extent to which they follow the generic phase rules of (smooth, complex) Toeplitz operators anyway. Where these rules are not followed, we consider how a small generic perturbation might restore the rules.

The phase diagram for the Euclidean plane, Fig. 2 satisfies the generic phase rules away from the line $B=0$. On the line $B=0$, however, the index takes an infinitely large jump, while at the origin infinitely many phases meet. Both are forbidden by the phase rules.

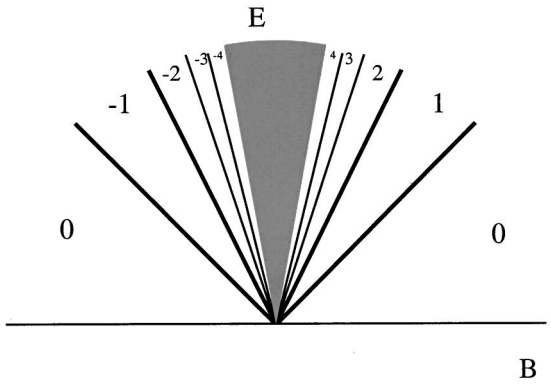

FIG. 2. The phase diagram for the Landau Hamiltonian in the Euclidean plane. The shaded wedge contains infinitely many, thinner and thinner, wedges, with indices that go to $\pm\infty$ and accumulate at the B axis.

The phase diagram in the hyperbolic plane, Fig. 3, satisfies the generic phase rules outside the shaded parabolic region. In the shaded region, the operator is not Fredholm and the index is not defined. This is contrary to the phase rules since not being Fredholm is expected to be a codimension 1 event.

The phase diagram of the Harper model, Fig. 4, is in serious conflict with the phase rule for (smooth, complex) Toeplitz operators: It is known,[20] that for a full measure of values of the magnetic field (irrational, of course), the spectrum is a Cantor set. Since the boundary between phases is contained in the spectrum, this suggests that any point on the boundary between any two phases can also be on the boundary between infinitely many other phases. This is the sort of behavior we observed for bounded operators with no restrictions. However, even in this wildness there is some regularity. For example, the center of the figure is on the boundary of all phases with *odd* indices while Theorem 2 allows for even indices as well.

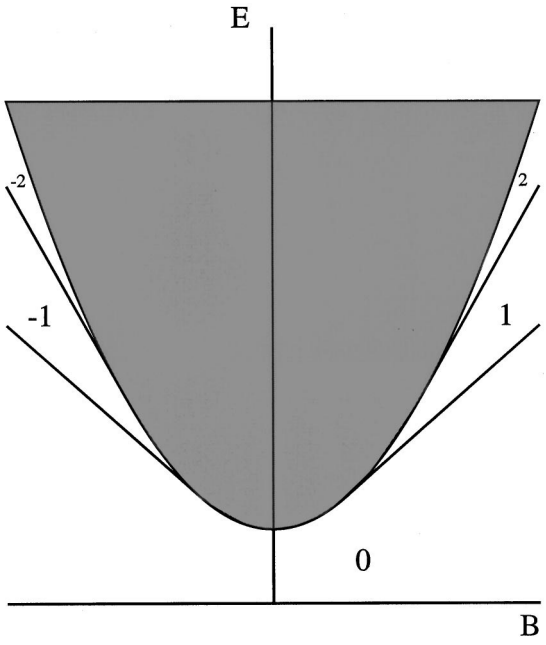

FIG. 3. The phase diagram for the Landau Hamiltonian in the hyperbolic plane. In the shaded parabolic region the operator is not Fredholm and the index is not defined.

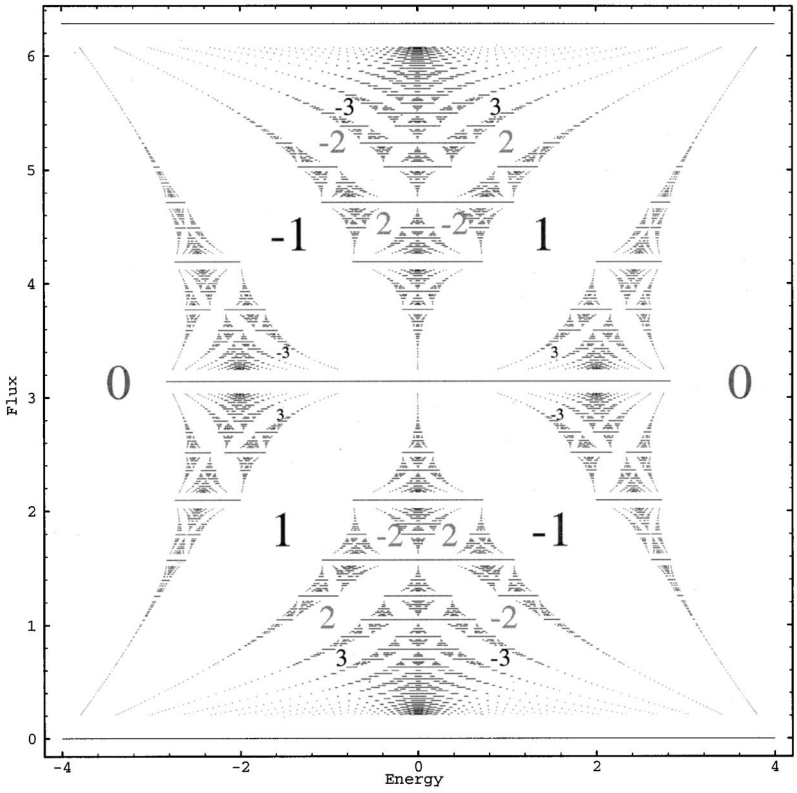

FIG. 4. The phase diagram for the Harper model associated with tight binding model on a square lattice the plane. Every point on the boundary between two phases appears to be a point of accumulation of infinitely many phases. Figure taken, with permission, from Ref. 31.

Remark: To see how Fig. 4 is obtained, we recall that for a tight-binding model with flux p/q through a unit cell, the Hall conductance, σ_j associated with the jth gap, (provided all gaps below it are open) satisfies the diophantine equation[8,21]

$$p\sigma_j = j \bmod q. \tag{16}$$

A similar equation holds for gaps counted from above. In the Harper model it is known[22] that all gaps except possibly for the central gap, are open.

Finally, consider the phase diagram of the Harper model with a disordered potential. This is not soluble in the same sense that the previous models are, but there are numerical results for it. Figure 5, which we borrowed from Ref. 23, shows the phase diagram for a split Landau level in the Harper model with disorder. More precisely, the diagram describes a Harper model with fractional flux $\frac{8}{5}$ through a unit cell.

Without disorder the conductance σ of each isolated band satisfies the Diophantine equation similar to Eq. (16), except that for a split Landau band p and q are interchanged. For flux $\frac{8}{5}$ the Diophantine equation fixes the conductances $(2,-3,2)$ of the bands at the flanks and -1 at the center. Zero disorder is, of course, not generic, and, indeed, there are bands on the E axis where the index is not defined, something that the phase rules for Toeplitz forbid. Under perturbation the diagram should deform so that these bands where the index is not defined disappear. This is indeed the case. The diagram in Ref. 23 is obtained by drawing n lines emanating from each band where n is its Hall conductance.

In summary, the wild character of the phase diagram of the Harper model is tamed by disorder and one finds, remarkably, a phase diagram compatible with the phase rules for Toeplitz operators.

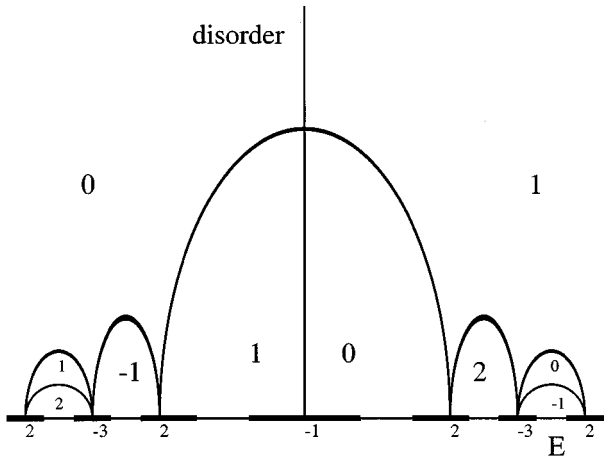

FIG. 5. The phase diagram for the Hall conductance of a split Landau level in Harper model with disorder after Ref. 23.

B. Perturbations of Landau Hamiltonians

Motivated by the effect of disorder on the Harper model phase portrait, we next consider the effect of perturbations on the phase portraits of Landau Hamiltonians. Such perturbations will modify the phase diagram near phase boundaries. As a consequence one expects a phase diagram to be qualitatively modified near points of accumulation of phases, even if the perturbation is small.

Figures 2 and 3 satisfy the phase rules in the region of large magnetic fields, but fail to do so for small magnetic fields. We now examine how the two figures might be modified to satisfy the phase rules everywhere.

The phase diagram of the Landau Hamiltonian in the plane, Fig. 2, will be significantly modified near the line $B=0$ which, by symmetry, must lie in a region with index 0. A schematic phase diagram that is generic and close to the Landau phase diagram is shown in Fig. 6.

The phase diagram in Fig. 3 has a region of full measure, the shaded parabola, where the operator is not Fredholm. This is nongeneric, and unstable. A perturbation might produce a phase diagram like Fig. 7. Note that the two perturbed diagrams, Figs. 6 and 7 are topologically identical.

How do the phase diagrams, Figs. 6 and 7, compare with what one finds in experiments on the quantum Hall effect? For large magnetic fields one finds phase diagrams that resemble both Figs.

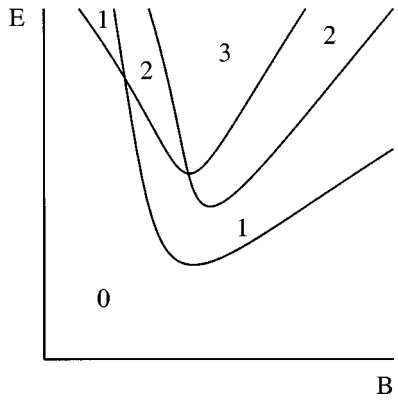

FIG. 6. A phase diagram that satisfies the phase rules of Toeplitz operators and is a perturbation of the phase diagram of Landau Hamiltonian in the plane.

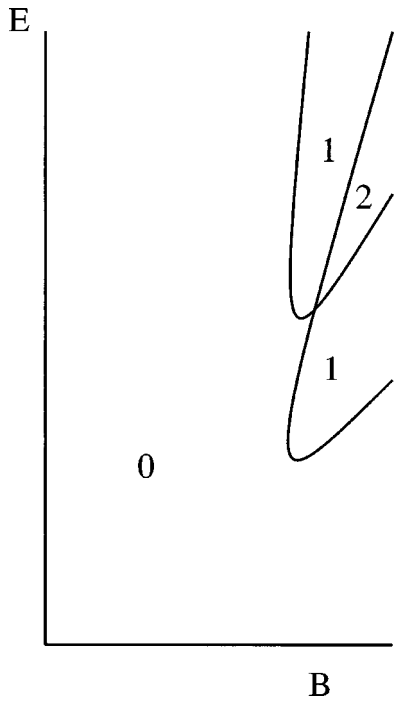

FIG. 7. A phase diagram that satisfies the rules of Toeplitz operators and is a perturbation of the phase diagram of Landau Hamiltonian in the hyperbolic plane.

2 and 6 and satisfy the phase rules. For weak magnetic fields one observes a transition to an insulating phase. The emergence of an insulating phase (with index 0) for small magnetic fields is in agreement with the phase rule and Fig. 6. However, some experiments[24] and numerical simulations[25] have been interpreted as giving evidence to direct transitions from a Hall conductance of 2 and 3 to the insulating phase. Taken literally, such transitions would violate the phase rule. However, these results may merely indicate that, for B small, the phase boundaries of Fig. 6 are too closely spaced to be distinguished numerically and experimentally.

C. Toeplitz operators

The main gap in our analysis is that we have not established a direct relation between the algebra of Toeplitz operators, where our phase rules are proven, and the class of operators relevant to (disordered) quantum Hall systems.

At the minimum, Toeplitz operators serve as a natural mathematical laboratory. However, there is a more direct justification for considering Toeplitz operators. The most elementary paradigm for a quantum Hall system is the Landau Hamiltonian, in which case one has the following.

Theorem 10: Let P be a projection on the lowest Landau level in $\mathbb{R}^2$, and let U be the gauge transformation associated with an Aharonov–Bohm flux tube at the origin. Then PUP, acting on the range of P, differs from a Toeplitz operator by a compact operator.

Proof: A basis for the lowest Landau level is

$$|n\rangle = \frac{1}{\sqrt{\pi\, n!}} z^n\, e^{-|z|^2/2}, \quad n \geqslant 0. \tag{17}$$

As a consequence

$$\langle n|U|m\rangle = \delta_{n,m+1}\frac{(m+1/2)!}{m!\sqrt{m+1}} \approx \delta_{n,m+1}\left(1-\frac{1}{8m}\right). \tag{18}$$

■

In this case, a compact perturbation of PUP is not only a Toeplitz operator; it is a simple shift. However, if the flux tube is placed at a different point, or if the magnetic field is spread out over a finite region, then we obtain a more general Toeplitz operator. If P is a projection on a higher Landau level, the same results hold but the calculation is more involved. If P is a projection onto multiple Landau levels, then PUP is a compact perturbation of a direct sum of Toeplitz operators, one for each Landau level.

This is not to say that Toeplitz operators apply directly to all systems, only that they apply to many. There are basic models where PUP fails to be Toeplitz. Indeed, an elementary model for localization is a random multiplication operator, i.e., $H=V_\omega$ on $l(\mathbb{Z}^d)$. This is a caricature of strong disorder. The eigenfunctions are now concentrated at lattice points. The projection P (below a Fermi energy) is

$$P=\sum |n\rangle\langle n|, \tag{19}$$

where the sum is over a random set of lattice points with, $V_\omega(n)<E$, in $\mathbb{Z}^d$. PUP is now a multiplication by a phase. It is an invertible operator and has Fredholm index zero. It is, however, not Toeplitz.

D. Open problems

It is tempting to directly study the index of PUP, for spectral projections P and unitary operators U, rather than rely on generic results based on Toeplitz operators. There are, however, several technical obstacles. The first is that PUP is thought of as acting on Range P, which is a Hilbert space in its own right. This means that a deformation of the parameters of the system leads to a deformation of the space Range P. In contrast, our strategy so far is formulated on a fixed space. The second obstacle is that our results depend on continuity properties while spectral projections tend to have bad continuity properties that come from a discontinuity at the Fermi energy.

To overcome the first problem one can replace PUP by an operator F defined on the entire Hilbert space with coinciding index. There is large arbitrariness in choosing F, but a natural choice is

$$F=PUP+P_\perp=PUP+P_\perp^2=1+P(U-1)P, \tag{20}$$

where $P_\perp=1-P$.

To overcome the second problem one may want to replace P by a Fermi function. That is, replace P by a smooth version

$$P(\beta,B,E_F)=\frac{1}{\exp(\beta(H(B)-E_F))+1}. \tag{21}$$

In that case, however, P^2 is no longer equal to P, and the different expressions for F in Eq. (20) are no longer equivalent. For each choice, it would be interesting to derive a phase portrait for index (F) as the temperature, Fermi energy, magnetic field and degree of randomness are varied.

E. Concluding remark

In this paper we explored what can be said about generic phase diagrams of indices of Fredholm operators. We did not use the fact that the Fredholm operators relevant to the quantum

Hall effect are of the form PUP, with P a spectral projection of an ergodic Schrödinger operator. Rather, we considered the index of several natural classes (and algebras) of operators. The weakness of this strategy is that we cannot say much that is definitive about quantum Hall systems. In its defense, we recall that replacing the particular by the generic proved to be useful in quantum physics in the hands of Wigner, von Neuman, and Dyson.[26–28] Whether it will turn out to be useful for quantum Hall effect remains to be seen.

ACKNOWLEDGMENTS

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One-dimensional crystal with a complex periodic potential

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A one-dimensional crystal model is constructed with a complex periodic potential. A wave function solution for the crystal model is derived without relying on Bloch functions. The new wave function solution of this model is shown to correspond to the solution for the probability amplitude of a two-level system. The energy discriminant is evaluated using an analytic formula derived from the probability amplitude solution, and based on an expansion parameter related to the energy and potential amplitude. From the wave function energy discriminant the crystal band structure is derived and related to standard energy bands and gaps. It is also shown that several of the properties of the two-level system apply to the one-dimensional crystal model. The two-level system solution which evolves in time is shown to manifest as a spatial configuration of the one-dimensional crystal model. The sensitivity of the wave function probability density is interpreted in the context of the new solution. The spatial configuration of the wave function, and the appearance of a long wavelength in the wave function probability density is explained in terms of the properties of Bessel functions. [DOI: 10.1063/1.1326458]

I. INTRODUCTION

In solid-state physics one-dimensional systems can be realized in several ways. First, a geometric shaping of a material may be fabricated to restrict the width in the perpendicular direction, and elongate the size in the longitudinal direction. This is the wire or strand model of a one-dimensional system, and such configurations have been observed experimentally.[1] Nearly one-dimensional electronic systems can be produced from silicon or gallium arsenide by lithographic techniques.[2] There are also materials that tend to naturally have a one-dimensional structure, such as polycarbyne[3] or cumulene.[4,5] Second, the anisotropy of a material can result in one-dimensional behavior. An example would be a Krogmann salt or a KCP compound.[6] There is also an abundance of research on quasione-dimensional crystals for x-ray emission,[7] sound propagation,[8] and various kinds of flow.[9] The experimentation on one-dimensional systems is widespread and the theoretical understanding of one-dimensional systems has great practical importance.

Typically, analysis of one-dimensional systems relies on the use of Bloch functions.[10] This is a result of the fact that to a very good approximation, crystals have potentials that are nearly invariant under translation and thus periodic. In practice, impurities and surfaces can alter the periodicity. The Bloch function solution can be obtained from Floquet's theorem, which has been previously applied to many areas[11,12] of research, including transition state dynamics.[13–17]

In this work, a complex potential[18–23] is permitted, and the wave function needed to determine the energy band structure is derived, from the Schrödinger equation, without using Bloch functions. The form of the wave function solution is expressed as a sine or cosine of a new dependent variable, and two related functions. In Sec. III, a transformation is used to obtain a new perspective on the wave function solution. An exact analytic expression for the wave function is obtained for a one-dimensional crystal in terms of two functions which are determined in several limits. In one limit the two functions are derived for the case of small potential compared to energy. The wave function solution based on this limit is used to obtain the energy discriminant. The energy discriminant is then used to study the crystal band structure. In the other limit when the potential

amplitude is large the form of the wave function solution is used to explain the expected occurrence of wave number harmonics.

The crystal energy band spectrum, is investigated in Sec. IV. The form of the wave function solution for this application is shown to manifest coefficients that are integer order Bessel functions. The zeros of the Bessel functions point to parameter values where the wave function solution can be substantially altered. The parameter values relate to the energy, potential amplitude, and the wave number periodicity associated with the potential. Regions around several zeros are numerically studied to show the dependence of the wave function probability density on the selection of parameter values near Bessel function zeros.

II. THEORETICAL BASIS FOR THE ONE-DIMENSIONAL CRYSTAL MODEL

The derivation of the equation governing the one-dimensional crystal uses a change of variables to make contact with the two-level system solution. An equivalence between the Schrödinger equation for the crystal, and the transition amplitude equation for a two-level system is demonstrated. As a result of the correspondence, the wave function solution can be derived from the two-level solution.

A. General time dependent wave equation

The basic time dependent wave equation is discussed to clarify the physical significance of a potential with a real and imaginary part. However, only the time independent wave equation derived in Sec. II B is needed for the one-dimensional crystal model. The derivation of the time independent wave equation begins with the statement of the time dependent Schrödinger equation,

$$i\hbar\frac{\partial\Phi}{\partial t}=-\frac{\hbar^2}{2m}\nabla^2\Phi+V\Phi, \tag{1}$$

where $i\cdot i=-1$, m is the electron mass, and $2\pi\hbar$ is Planck's constant. Typically the potential, V, is real to permit a correspondence of the dynamics of a wave packet with the motion of a particle described by classical mechanics. However, in this derivation a more general complex V is allowed. To interpret the imaginary part of the potential, decompose the potential $V=V_r+iV_i$, and take the time derivative of the probability density $\mathcal{P}=\Phi\Phi^*$.

$$\begin{aligned}\frac{\partial\mathcal{P}}{\partial t}&=\Phi^*\frac{\partial\Phi}{\partial t}+\frac{\partial\Phi^*}{\partial t}\Phi\\&=\Phi^*\left[-\frac{\hbar}{2im}\nabla^2\Phi+\frac{V}{i\hbar}\Phi\right]+\left[\frac{\hbar}{2im}\nabla^2\Phi^*-\frac{V^*}{i\hbar}\Phi^*\right]\Phi.\end{aligned} \tag{2}$$

A volume integral of Eq. (2) followed by an application of the divergence theorem gives

$$\frac{\partial\mathcal{P}}{\partial t}+\nabla\cdot S_{\mathrm{cur}}=\frac{2}{\hbar}V_i\mathcal{P}, \tag{3}$$

where probability current density $S_{\mathrm{cur}}=\hbar[\Phi^*\nabla\Phi-(\nabla\Phi^*)\Phi]/(2im)$. From Eq. (3), it is clear that the right side acts as a probability source when V_i is positive, and as a probability sink when it is negative. A complex potential has been used in the past to model neutron absorption[24,25] and thus the imaginary potential represents emission or absorption. Thus, in the crystal model the complex potential is viewed as representing a ''prepared'' material. The material is assumed to be capable of absorption or emission.

B. Time independent wave equation

Assuming an exponential time variation, the wave function $\Phi=\Psi(x)e^{-iEt/\hbar}$ for the one-dimensional crystal, is substituted into Eq. (1) to obtain the time independent Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2}+V(x)\Psi=E\Psi. \tag{4}$$

The energy is written as $E=\hbar^2K^2/(2m)$ and the chosen form of the potential function is

$$V(x)=\frac{\hbar^2}{2m}\left[-\frac{\beta^2}{4}\cos^2\alpha x+\frac{i\alpha\beta}{2}\sin\alpha x\right], \tag{5}$$

with variable parameters α and β and thus,

$$\frac{d^2\Psi}{dx^2}+\left[K^2+\frac{\beta^2}{4}\cos^2\alpha x-\frac{i\alpha\beta}{2}\sin\alpha x\right]\Psi=0. \tag{6}$$

The real part of the potential has amplitude $-\hbar^2\beta^2/(8m)$, and the imaginary part has amplitude $\hbar^2\alpha\beta/(4m)$. Thus, the amplitude of the real and imaginary part are related. Furthermore, the amplitude of the imaginary part of the potential is linearly related to the inverse of the period of the potential $\omega=2\pi/\alpha$. Note also that $V(x)=[V(-x)]^*$, and consequently the potential has parity and time reversal symmetry.

To facilitate the solution for Ψ, an exponential variation is factored, $\Psi=c_+e^{-i(\beta/2\alpha)\sin\alpha x}$ and after substituting into Eq. (6),

$$\frac{d^2c_+}{dx^2}-i\beta\frac{dc_+}{dx}\cos\alpha x+K^2c_+=0. \tag{7}$$

The following two coupled first-order differential equations can also be used to derive Eq. (7),

$$\frac{dc_+}{dx}=-iKc_-e^{i(\beta/\alpha)\sin\alpha x}, \tag{8a}$$

$$\frac{dc_-}{dx}=-iKc_+e^{-i(\beta/\alpha)\sin\alpha x}, \tag{8b}$$

since the derivative of Eq. (8a) with respect to x results in Eq. (7). Comparing with previous work[26] it can be seen that c_+ is closely related to the coupled equations governing the two-level probability amplitude dynamics. When K is set to one in Eq. (8) the equations are identical to the governing equations for the probability amplitude of a two-level system. A direct correspondence is obtained if distance x is scaled by K in Eq. (6), however this normalization is not convenient for the later energy band discussion.

III. FORMULATION OF THE WAVE FUNCTION SOLUTION WITH A NEW DEPENDENT VARIABLE

The x variable used in Eq. (8) is replaced with a new variable s, in order to gain insight into the wave function solution dependence on the α and β parameters, and to avoid the need for the use of Bloch functions. The objective is to use a variable that is more natural to Eq. (8) and also contains as much of the characteristic behavior as possible.

A. The wave function solution based on variable *s*

The previously derived solution[26] of the two-level probability amplitude problem relied on the introduction of a new variable s. In the crystal model wave function solution the variable s is modified by a scale factor, K. The s coordinate originally was proposed as a generalization to arbitrary wave number of a variable used previously for a strictly resonance solution.[27] In this work, for the purpose of deriving the crystal solution,

$$s = K\int_0^x dy\, e^{i\,(\beta/\alpha)\,\sin\alpha y}$$

$$= Kx\mathcal{J}_0 + \frac{K}{\alpha}\sum_{n=1}^{\infty}\mathcal{J}_{2n}\frac{\sin(2n\alpha x)}{n} - \frac{2iK}{\alpha}\sum_{n=0}^{\infty}\mathcal{J}_{2n+1}\frac{\cos[(2n+1)\alpha x]-1}{2n+1}, \tag{9}$$

where $\mathcal{J}_n = J_n(\beta/\alpha)$ is the order n Bessel function evaluated at β/α. The integral required to determine the s variable is obtained using the Eq. (A1a) and Eq. (A1b) Bessel generating function relations[28] written in the appendix.

Starting with the unscaled c_+, the K scaled solution for c_+, needed for the wave function can be readily derived from a Riccati equation as previously detailed:[26]

$$\Psi = \left\{ C_{11}\cos\left[\frac{(s+s^*)}{2}+p\right]e^{Q} + C_{12}\sin\left[\frac{(s+s^*)}{2}+p^*\right]e^{Q^*}\right\} e^{-i(\beta/2\alpha)\sin\alpha x}, \tag{10}$$

where C_{11} and C_{12} are constants depending on initial conditions and the p and Q functions are both the solution of a first-order differential equation,

$$\frac{dp}{dx} = -iK\sin\left[\left(\frac{\beta}{\alpha}\right)\sin(\alpha x)\right]\cos(s+s^*+2p), \tag{11}$$

$$\frac{dQ}{dx} = -iK\sin\left[\left(\frac{\beta}{\alpha}\right)\sin(\alpha x)\right]\sin(s+s^*+2p). \tag{12}$$

For the time independent wave function solution the time variable of the two-level probability amplitude solution has been switched to the spatial coordinate x. The complete time history of the two-level probability amplitude solution is simultaneously manifested in the spatial configuration of the time independent wave function solution.

As can be seen from Eq. (9) for s and Eqs. (10)–(12), the ratio β/α has a substantial influence on the solution of c_+ and thus Ψ, since β/α is fundamental to the variable s and the solution of the p and Q functions. Any wave number content that enters p appears in the argument of the Eq. (10) solution and any wave number content entering Q appears in the exponential. The strong β/α influence is a result of dp/dx and dQ/dx, having a factor of $K\sin[(\beta/\alpha)\sin(\alpha x)]$. This factor common to both Eqs. (11) and (12) can also be written in terms of s,

$$\frac{1}{2i}\frac{d(s-s^*)}{dx} = K\sin[(\beta/\alpha)\sin(\alpha x)]. \tag{13}$$

In selecting the potential, the choice of β/α may be large or small. When it is small corresponding to a weak potential, the maximum value of $\sin[(\beta/\alpha)\sin\alpha x]$ only achieves a value less than the possible maximum of one. However, under this condition it reflects the wave number selected by the choice of α. At small values $\sin[(\beta/\alpha)\sin\alpha x]\approx(\beta/\alpha)\sin\alpha x$, and α has the character of a wave number. The parameter β has the character of an amplitude, which is consistent with the relationship of β to the potential amplitude. When $\beta/\alpha=\pi/2$, the outer sinusoid achieves its maximum value of one and the inner and outer sinusoids closely track each other as shown in Fig. 1(a). The curve in Fig. 1(a) is calculated with $\alpha=2$. For β/α somewhat greater than $\pi/2$, a new phenom-

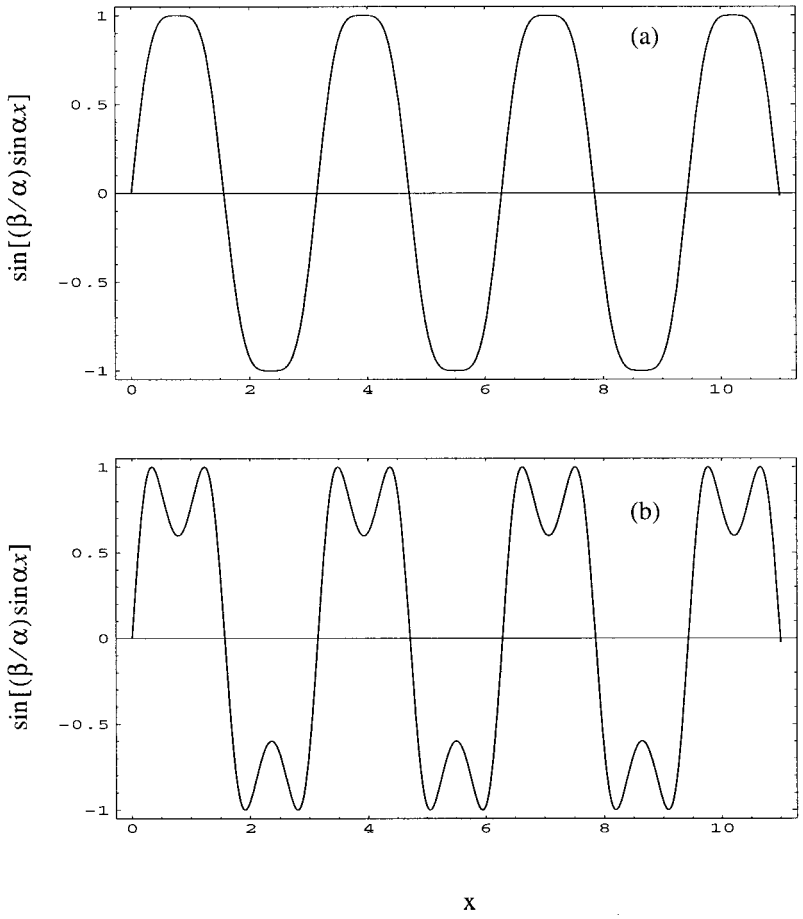

FIG. 1. The function $\sin[(\beta/\alpha)\sin \alpha x]$ is compared for $\alpha=2$ with two values: (a) $\beta/\alpha=\pi/2$, (b) $\beta/\alpha=5$.

enon begins to occur. This is illustrated in Fig. 1(b) where now $\beta/\alpha=5$ and $\alpha=2$. The outer sinusoid achieves its maximum before $\alpha x=\pi/2$, and at the peak value of one for the inner sinusoid, the outer sinusoid has an argument beyond $\pi/2$ and thus it has a value less than one. The effect is to begin to cause a ripple structure on the peaks of $\sin[(\beta/\alpha)\sin \alpha x]$. The ripple is a new wave number related to the magnitude of β/α, and thus β/α takes on the character of a wave number that is greater than α. This behavior causes harmonics of the fundamental wave number to enter the solution.

An advantage of the Eq. (10) solution compared to Bloch functions is that it is completely determined once the p and Q functions are specified. Additionally, the form of the solution provides considerable information about the spatial nature of the wave function. The key point is that the Bessel functions of integer order evident in the s variable are all oscillatory. The zero-order Bessel function is one at zero and all other orders vanish at zero. The arguments of the Bessel functions scale like the ratio of the amplitude of the real part of the potential to the imaginary part. This ratio can be small and then the solution is described in the region near zero by the approximate expression,

$$\Psi=(C_{11}\cos[\mathcal{J}_0 Kx]+C_{12}\sin[\mathcal{J}_0 Kx])e^{-i(\beta/2\alpha)\sin \alpha x}. \tag{14}$$

Equation (14) result shows in the small β/α limit that the coefficient of Kx is the zero-order Bessel function. Because $\mathcal{J}_0 Kx$ is the first term of the real part of s, it persists as the β/α argument is increased. At $\beta/\alpha=2.4048$ the zero-order Bessel function has its first zero. This

means that the character of the spatial variation contributed by $s+s^*$ dramatically changes at this location in parameter space. In other words, selecting $\beta/\alpha=2.4048$ switches off the linear spatial variation contribution of $s+s^*$. There are an infinite number of zero-order Bessel function nodes where this occurs. The other terms of $s+s^*$ are even harmonic sines with even-order Bessel functions as coefficients. Thus, it is equally possible to switch off any particular even harmonic contribution from $s+s^*$, and this may be done at any of the infinite set of available zeros. Because the nodes of the integer-order Bessel functions are interlaced, the selection of the term to switch on or off can be done while leaving all other terms at a finite value. Another interesting feature is that as the order of the Bessel function increases the first zero appears at a larger value. For large β/α, the asymptotic form

$$\mathcal{J}_n \approx \left(\frac{2\alpha}{\pi\beta}\right)^{1/2} \cos\left[\frac{\beta}{\alpha} - \frac{\pi n}{2} - \frac{\pi}{4}\right], \tag{15}$$

shows an increasing density of nodes contributed by ever larger Bessel function orders. The spacing between nodes is approximately π.

From Eqs. (11) and (12) it is clear each of these functions is similar since a $\pi/4$ shift in the p function in the argument of the sine on the right side of dQ/dx gives $dQ/dx(p+\pi/4)=dp/dx$. Additionally, both dp/dx and dQ/dx are proportional to $\sin[(\beta/\alpha)\sin(\alpha x)]$, which by using Eq. (A1b), can be expanded as

$$\sin\left[\frac{\beta}{\alpha}\sin(\alpha x)\right] = 2\sum_{n=0}^{\infty} \mathcal{J}_{2n+1} \sin[(2n+1)\alpha x]. \tag{16}$$

The form of this result reveals that p and Q can be controlled to some degree by selecting β/α to coincide with a zero of any odd integer-order Bessel function. For example, to eliminate the $\sin(\alpha x)$ term, β/α could be set to the first zero, 3.832, of $\mathcal{J}_1$ or a zero at a larger value of β/α. The odd-order Bessel functions, as also in the case of the even-order Bessel functions, are nearly zero until the argument is comparable or greater than the order. Thus, it should be expected that the higher-order harmonics of Eq. (16) have a minuscule effect unless the β/α argument is comparable or greater than the order. In the vicinity of the first peak, there is dominance over the magnitude of all other Bessel functions.

Each integer-order Bessel function has an infinite number of nodes. The primary parameter, β/α is a ratio and thus, there are two ways to select any particular Bessel zero. First, the potential period which corresponds to α can be set, and then the real potential amplitude which corresponds to β can be scanned. Second, β can be set and then α can be scanned. As α gets small, the ratio β/α can be made large. The method of selecting β/α determines the weighting between the real and imaginary part of the potential. It is also possible to diminish the influence of a Bessel function, and consequently its associated harmonic by setting β/α less than the order. The oscillatory behavior of a Bessel function with an approximate π period does not begin to be significant until the argument of the Bessel function exceeds the order.

B. Analytic solutions for the *p* and *Q* functions

The function p has a nonlinear dependence since p appears as an argument of the cosine in Eq. (11). However, an analytic solution can be obtained for this equation assuming $K\beta/\alpha \ll 1$. This is possible because dp/dx scales like $K\beta/\alpha$ when $K\beta/\alpha \ll 1$. From Eq. (9) at small β/α, it is found $s+s^* \approx 2Kx\mathcal{J}_0$. Under these conditions, Eq. (11) becomes

$$\frac{dp}{dx} = -iK \sin\left[\left(\frac{\beta}{\alpha}\right)\sin(\alpha x)\right] \cos(2Kx\mathcal{J}_0). \tag{17}$$

If α is chosen such that $\alpha=2K\mathcal{J}_0$, then Eq. (17) is a perfect derivative and

$$p=\frac{iK}{\beta}\cos\left[\left(\frac{\beta}{2K\mathcal{J}_0}\right)\sin(2Kx\mathcal{J}_0)\right]-\frac{iK}{\beta}. \tag{18}$$

For the situation where $\alpha\neq 2K\mathcal{J}_0$,

$$p=iK\mathcal{J}_1\left[\frac{\cos(\alpha+2K\mathcal{J}_0)x-1}{\alpha+2K\mathcal{J}_0}+\frac{\cos(\alpha-2K\mathcal{J}_0)x-1}{\alpha-2K\mathcal{J}_0}\right]. \tag{19}$$

Also, to lowest order in β/α, Eq. (12) becomes for $\alpha=2K\mathcal{J}_0$,

$$\begin{aligned}Q&=-2iK\mathcal{J}_1\int \sin(2Kx\mathcal{J}_0)\sin(2Kx\mathcal{J}_0)dx\\&=-iK\mathcal{J}_1\left[x-\frac{\sin(4Kx\mathcal{J}_0)}{4K\mathcal{J}_0}\right],\end{aligned} \tag{20}$$

and for $\alpha\neq 2K\mathcal{J}_0$,

$$\begin{aligned}Q&=-2iK\mathcal{J}_1\int \sin(\alpha x)\sin(2Kx\mathcal{J}_0)dx\\&=-iK\mathcal{J}_1\left[\frac{\sin(\alpha-2K\mathcal{J}_0)x}{\alpha-2K\mathcal{J}_0}-\frac{\sin(\alpha+2K\mathcal{J}_0)x}{\alpha+2K\mathcal{J}_0}\right].\end{aligned} \tag{21}$$

IV. RESULTS AND DISCUSSION

An interesting aspect of a periodic potential is the advent of forbidden energy regions. The approximate p and Q functions of Sec. III B are used to determine the energy band structure with a fully complex potential. A numerical solution is calculated and the formula of Eq. (10) is used to explain the observed wave number behavior of the probability density.

A. Energy band structure results from the analytic solution

In past research where the Schrödinger equation potential is periodic, energy band conditions have been derived from wave function boundary conditions[29] or the properties of the wave equation solutions.[30] In this work the energy discriminant, based on properties of the wave equation, as described by Bender[31] is used:

$$\Delta E=\Psi_1(\omega)+\Psi_2'(\omega), \tag{22}$$

where ω is the period of the potential. For allowed energy regions (energy bands) the constraint satisfied by the discriminant is $|\Delta E|\leqslant 2$, and for disallowed regions (energy gaps) $|\Delta E|>2$. The wave functions in the energy discriminant formula must satisfy specific conditions. For Ψ_1, at $x=0$, $\Psi_1(0)=1$, $d\Psi_1/dx(0)=0$, and applying these conditions to the Eq. (10) solution,

$$\Psi_1=\left\{\cos\left[\frac{(s+s^*)}{2}+p\right]e^{Q}+\frac{i\beta}{2K}\sin\left[\frac{(s+s^*)}{2}+p^*\right]e^{Q^*}\right\}e^{-i(\beta/(2\alpha))\sin\alpha x}, \tag{23}$$

and for Ψ_2, at $x=0$ the conditions are $\Psi_2(0)=0$, $d\Psi_2/dx(0)=1$,

$$\Psi_2=\frac{1}{K}\sin\left[\frac{(s+s^*)}{2}+p^*\right]e^{Q^*}e^{-i(\beta/(2\alpha))\sin\alpha x}. \tag{24}$$

Substituting the Eqs. (23)–(24) wave functions into the Eq. (22) formula for the discriminant,

$$\Delta E = 2\ \mathrm{Re}[\cos(K\omega\mathcal{J}_0 + p(\omega))e^{Q(\omega)}]. \tag{25}$$

The final form of the energy discriminant is intended to use the strictly imaginary Sec. III B formulas and in that case Eq. (25) becomes

$$\Delta E = 2\cos(K\omega\mathcal{J}_0)\cosh[p_i(\omega)]\cos[Q_i(\omega)] - 2\sin(K\omega\mathcal{J}_0)\sinh[p_i(\omega)]\sin[Q_i(\omega)], \tag{26}$$

where subscript ''i'' denotes the imaginary part. The restriction on the application of Eq. (26) is that $K\beta/\alpha \ll 1$.

As an example, consider the discriminant plotted in Fig. 2(a) for $\alpha = 4.$ and $\beta = 0.01$. The dashed lines are placed for reference at the critical values of ± 2. The regions where $|\Delta E| > 2$ are forbidden and this condition defines the energy gaps. As can be seen there is a local minimum around $K = 2,6,10$ and local maximum around $K = 4,8,12$. This is expected since $\mathcal{J}_0 \approx 1$ when $\beta/\alpha \ll 1$ and the argument of the cosine in Eq. (25) is nearly $K2\pi/4$. The local maximums are greater than 2 and the local minimums are less than -2. This means the solution Ψ has both periodic $\Psi(x) = \Psi(x+\omega)$ and antiperiodic solutions $\Psi(x) = -\Psi(x+\omega)$. This behavior is quite different than a potential such as $i\sin^{2N+1}(x)$ $(N = 0,1,2\ldots)$, where Bender[31] found no antiperiodic solutions existed.

Since the discriminant variation near 2 is difficult to see in the full plot of Fig. 2(a), an additional two enlarged plots are shown in Figs. 2(b) and 2(c). In Fig. 2(b) the abscissa is restricted to $3.7 < K < 4.1$ and the energy gap region of $3.8 < K < 4$ is clearly visible. The maximum value is $\Delta E = 2.027\,82$ at $K = 3.897$. In Fig. 2(c) the abscissa is restricted to $7.7 < K < 8.1$ and the energy gap region is $7.855 < K < 8$. The maximum value is $\Delta E = 2.0100$ at $K = 7.937$. These two gaps illustrate the diminishing gap width as K or energy increases and also the diminishing amplitude of $\Delta E - 2$. To go to larger K using the approximate Sec. III B formulas it is necessary to reduce β or increase α, in order to maintain $K\beta/\alpha \ll 1$. In the limit the Eq. (25) result indicates that the ΔE function oscillates between ± 2.

B. Numerical results

It is not apparent from Eq. (7) that there are any special values of α and β which would cause substantial changes to the solution. However, when the wave function is written in the form of Eq. (10), it is clear the s variable is fundamental to the solution. As discussed earlier the s variable has drastically different behavior which depends on the properties of Bessel functions. The same situation is also true of the p and Q functions. The first place a very different behavior occurs is at the first zero of $\mathcal{J}_0$ where $\beta/\alpha = 2.4048$. At this value the linear term of s, $Kx\mathcal{J}_0$ vanishes and s becomes a bounded function. For this condition the results of Sec. III B are still valid if $K \ll 1/2.4048$,

$$p = 2iK\mathcal{J}_1(\cos\alpha x - 1)/\alpha, \tag{27a}$$

$$Q = 0. \tag{27b}$$

To recover a finite value for Q, a somewhat less restrictive requirement of small K/α can be imposed. The differential equation for Q, Eq. (12) can be directly integrated if p is known. The differential equation for p, Eq. (11) can be viewed as

$$\frac{dp}{d(s^* - s)} = \frac{1}{2}\cos(s + s^* + 2p), \tag{28}$$

which may be formally written

$$\int \frac{dp}{\cos(s + s^* + 2p)} = \frac{s^* - s}{2}. \tag{29}$$

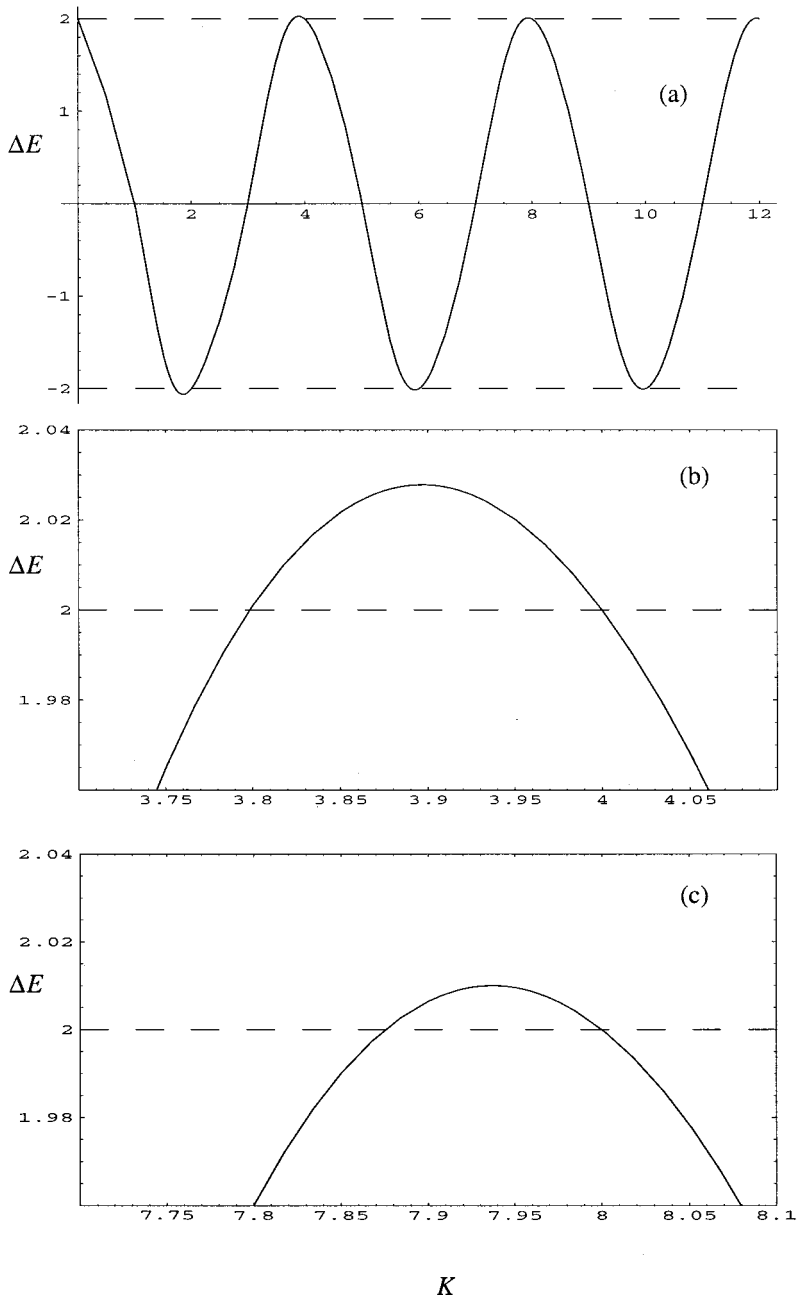

FIG. 2. The energy discriminant is displayed for $\alpha=4$, and $\beta=0.01$ with three energy parameter ranges: (a) $0<K<12$, (b) $3.7<K<4.1$, (c) $7.7<K<8.1$.

In the event $s+s^*$ is precisely constant, Eq. (29) can be immediately integrated without approximation. When $K/\alpha \ll 1$ and β/α is set to the value of a $\mathcal{J}_0$ zero, then $s+s^*$ is small and nearly constant. On the basis of these properties of the s variable an analytic solution, referred to in past work as the dwell point solution,[26] has been derived. It is most accurate when α is large and β/α is near a zero of $\mathcal{J}_0$. The dwell point solution gives the expectation that the wave function is very different, depending on whether or not $s+s^*$ is approximately constant.

For general values of K/α and β/α needed to explore the implications of the constancy of $s+s^*$, it is necessary to resort to numerical calculations to obtain the wave function. A useful function to illustrate the spatial behavior is the probability density. Using Eq. (10) it follows the probability density can be expressed in terms of c_+ as $\mathcal{P}=c_+c_+^*$, and thus it is only necessary to calculate c_+. Applying the boundary conditions, $\Psi_1(0)=1$, $d\Psi_1/dx(0)=0$, to the Eq. (10) solution,

$$c_+=\cos\left[\frac{(s+s^*)}{2}+p\right]e^Q+\frac{i\beta}{2K}\sin\left[\frac{(s+s^*)}{2}+p^*\right]e^{Q^*}. \tag{30}$$

From Eq. (7) it is clear that the $\cos\alpha x$ coefficient of dc_+/dx is expected to result in harmonics of wave number α in the solution. The source of other wave numbers unrelated to α are revealed by the form of Eq. (30). As an illustration the probability density (for a convenient ordinate scale the normalized Ψ has been multiplied by 100) is plotted in Fig. 3 for $\alpha=2$ and $K=0.4$, which adequately satisfies the $K/\alpha\ll 1$ criteria. In Fig. 3(a), $\beta=16.9$ and it is seen that there is a dominant small wave number evidenced. The probability density plot is observed to have a period of approximately 153, which is far greater than the expected fundamental length of $2\pi/(2\alpha)=1.57$. This can be understood by considering the formula for variable s. In Eq. (9) the formula shows that the argument $(s+s^*)/2$ in Eq. (30) has a linear term of $K\mathcal{J}_0x=0.022\,23x$. There is also a linear contribution from $p_r\approx-0.002\,254x$. The associated wavelength $2\pi/(2(K\mathcal{J}_0+p_r))=157$ which is very close to the period of 153 plotted in Fig. 3(a). The wavelength is almost completely determined by s, since $|p_r/x|\ll K\mathcal{J}_0$. The period is about half the wavelength associated with the smallest wave number in the solution since it appears as a square in $\mathcal{P}$. The large thickness of the curve in Fig. 3(a) is due to the comparatively rapid oscillations related to the expected α wave number and its harmonics. In Fig. 3(b), $\beta=17.1$ and $K\mathcal{J}_0x=0.011\,31x$. There is also a linear contribution from $p_r\approx-0.002\,136x$. The associated wavelength is $2\pi/(2(K\mathcal{J}_0+p_r))=342$ which agrees well with the plotted result of 340. Again the large curve thickness is due to the expected α wave number and its harmonics. For a modest change in β the long wavelength evident in $\Psi\Psi^*$ is changed by approximately a factor of two. The large change is caused by the dependence of the sinusoids in Eq. (30) on $(s+s^*)/2$ and the linear contribution from p_r. In Fig. 3(c), $\beta=17.307$ to emphasize the role of the Bessel functions in the probability density. For this value $\beta/\alpha=8.653\,73$, which results in $\mathcal{J}_0\approx 0$. As a consequence the wavelength associated with $K\mathcal{J}_0=0$ becomes infinite, and it may be assumed that a flat probability function would result. However, as shown by Fig. 3(c) there is still a very long wavelength present. Referring back to Eq. (30) this feature is explained by the presence of the real part p_r in the argument of the sinusoids. The equation for p_r,

$$\frac{dp_r}{dx}=-K\sin[(\beta/\alpha)\sin\alpha x]\sin(s+s^*+2p_r)\sinh(2p_i), \tag{31}$$

includes the factor $\sin[(\beta/\alpha)\sin\alpha x]$ which can be expanded in odd harmonics, $\sin(2n+1)\alpha x$, as shown in Eq. (16). The presence of $\sin(s+s^*+2p_r)$ on the right side of Eq. (31) causes wave number feedback in a nonlinear manner. Because of the product rules of trigonometric functions,

$$\begin{aligned}
2\sin\theta_1\sin\theta_2&=\cos(\theta_1-\theta_2)-\cos(\theta_1+\theta_2),\\
2\sin\theta_1\cos\theta_2&=\sin(\theta_1+\theta_2)+\sin(\theta_1-\theta_2),\\
2\cos\theta_1\cos\theta_2&=\cos(\theta_1-\theta_2)+\cos(\theta_1+\theta_2),
\end{aligned} \tag{32}$$

the right side of Eq. (31) contains sum and difference wave numbers. The result is that p_r attains a linear term. For the example of Fig. 3(c), the linear term of p_r is $-0.0021x$ which corresponds

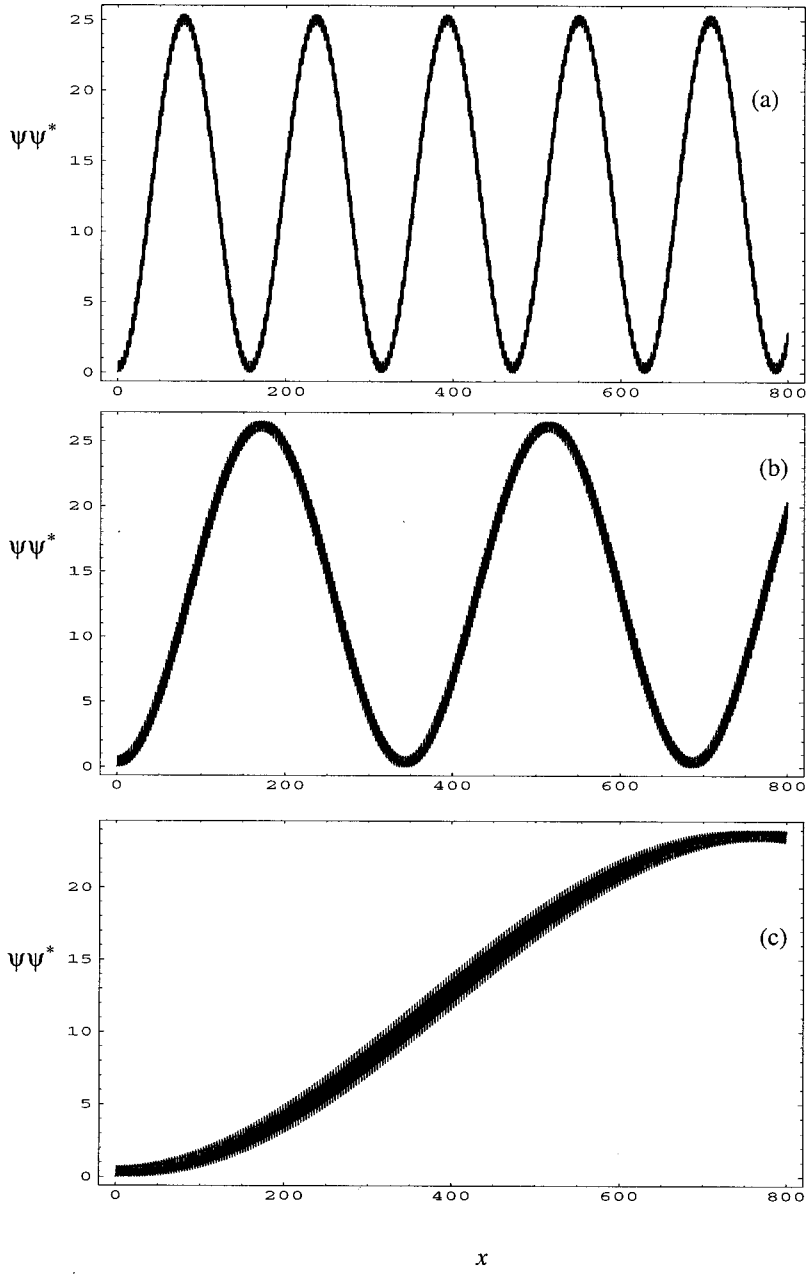

FIG. 3. The probability density for $\alpha=2$, $K=0.4$, and three β values: (a) $\beta=16.9$, (b) $\beta=17.1$, (c) $\beta=17.307$.

to a wavelength of $2\pi/(2\times 0.0021)=1495$. This agrees with the half wavelength of 750 plotted in Fig. 3(c). Thus, even though there is no linear contribution from $s+s^*$ the linear part of p_r causes a very small wave number in the probability density.

In the example of Fig. 3, β varied from 16.9 to 17.3 and the change of $\mathcal{P}$ was observed with K constant. In most instances of a physical system the potential is given and the energy can be varied. This amounts to a fixed α and β, with a variable K. The Q function is obtained from Eq. (12) and does not appear on the right side. Thus, the differential equation for Q is not nonlinear

and therefore Q is known as soon as p is determined. The most important consideration is then the dependence of p on K. To assess in a qualitative manner how K influences p, introduce a variable $u=Kx$. The s variable then becomes

$$s(u)=u\mathcal{J}_0+\frac{K}{\alpha}\sum_{n=1}^{\infty}\mathcal{J}_{2n}\frac{\sin(2n\alpha u/K)}{n}-\frac{2iK}{\alpha}\sum_{n=0}^{\infty}\mathcal{J}_{2n+1}\frac{\cos[(2n+1)\alpha u/K]-1}{2n+1}. \tag{33}$$

Now K does not appear in the linear term, however it behaves as a scale factor for α. The p_r differential equation is no longer proportional to K, though K scales α in the sine argument, and appears in $s(u)$

$$\frac{dp_r}{du}=-\sin[(\beta/\alpha)\sin(\alpha u/K)]\sin(s(u)+s^*(u)+2p_r)\sinh(2p_i). \tag{34}$$

As K increases the effective wave numbers, α/K decrease in the $s(u)$ variable and also in the $\sin[(\beta/\alpha)\sin(\alpha u/K)]$ term. The net effect is that at larger K the linear part of p_r gets larger. As an example, consider the probability density at $\alpha=2$, and $\beta=16.9$. In this example there is no concern for smallness of any parameter as required in Sec. III B or the dwell point solution. In Fig. 4(a), the probability density (for a convenient ordinate scale the normalized Ψ has been multiplied by 100) is plotted for $K=1.1$, showing the probability density is rich in structure at the α wave number and its harmonics. There is also a much longer wavelength visible. For this example $K\mathcal{J}_0=0.061\,1352$ and $p_r\approx-0.044\,2756x$. Combining these two contributions produces a wavelength $2\pi/2(0.061\,1352-0.044\,2756)=186$, which is in good agreement with the wavelength of 185 displayed in Fig. 4(a). Likewise in Fig. 4(b), for $K=1.2$, $K\mathcal{J}_0=0.066\,6929$ and $p_r\approx-0.057\,0173x$. Combining these two linear contributions produces a wavelength $2\pi/2(0.066\,6929-0.057\,0173)=325$. This is within 5% of the wavelength of 343 in Fig. 4(b). A small 9% change of K from 1.1 to 1.2 causes about a factor of two wavelength change. Note that as K increases $|p_r/x|$ increases more rapidly than $K\mathcal{J}_0$. This phenomenon admits the possibility that the linear contribution from p_r can, at a particular K value, equal $K\mathcal{J}_0$. Because the signs of these terms are opposite in this example, at $K=1.3005$ they cancel, and as shown in Fig. 4(c), there is no longer a long wavelength evidenced. Actually, $K\mathcal{J}_0=0.072\,2785$ and $p_r\approx-0.072\,2661x$ which results in a wavelength of 2.5×10^5, which is only visible after calculating out to about $x=25\,000$. At higher $K>1.3005$ the long wavelength returns. The abscissa in Fig. 4(c) is only plotted out to 100 to keep the short wavelength from producing a black rectangle filling the plot area. The curve shows a set of periodic major peaks with three minor peaks in the top third of the amplitude.

V. SUMMARY AND CONCLUSIONS

The wave function for a one-dimensional system, having a complex periodic potential has been analytically derived in terms of a variable c_+ which is the weighted sum of the familiar two-level system probability amplitude. The analytic solution has the form displayed in Eq. (10) with a dependence on complex variable s, and functions p and Q. The formulation of the analytic solution relied on the use of the variable s, which contains a substantial portion of the trigonometric argument of the solution. The variable s has a linear term in x with Bessel function coefficient $\mathcal{J}_0$, and a sum of even harmonics of the potential wave number with even integer-order $\mathcal{J}_{2n}$ Bessel coefficients and a complex sum of odd harmonics with odd-order $\mathcal{J}_{2n+1}$ Bessel coefficients. The solution in Eq. (10) is exact when p is known precisely and Q can be precisely determined from p analytically or determined to high accuracy through numerical integration. In general, the number of terms used to specify s and the degree of approximation of p and Q determines the precision of Ψ. The wave function solution was shown to correspond to a medium which exhibits absorption or emission. This is viewed as a prepared medium and thus is a special material or state.

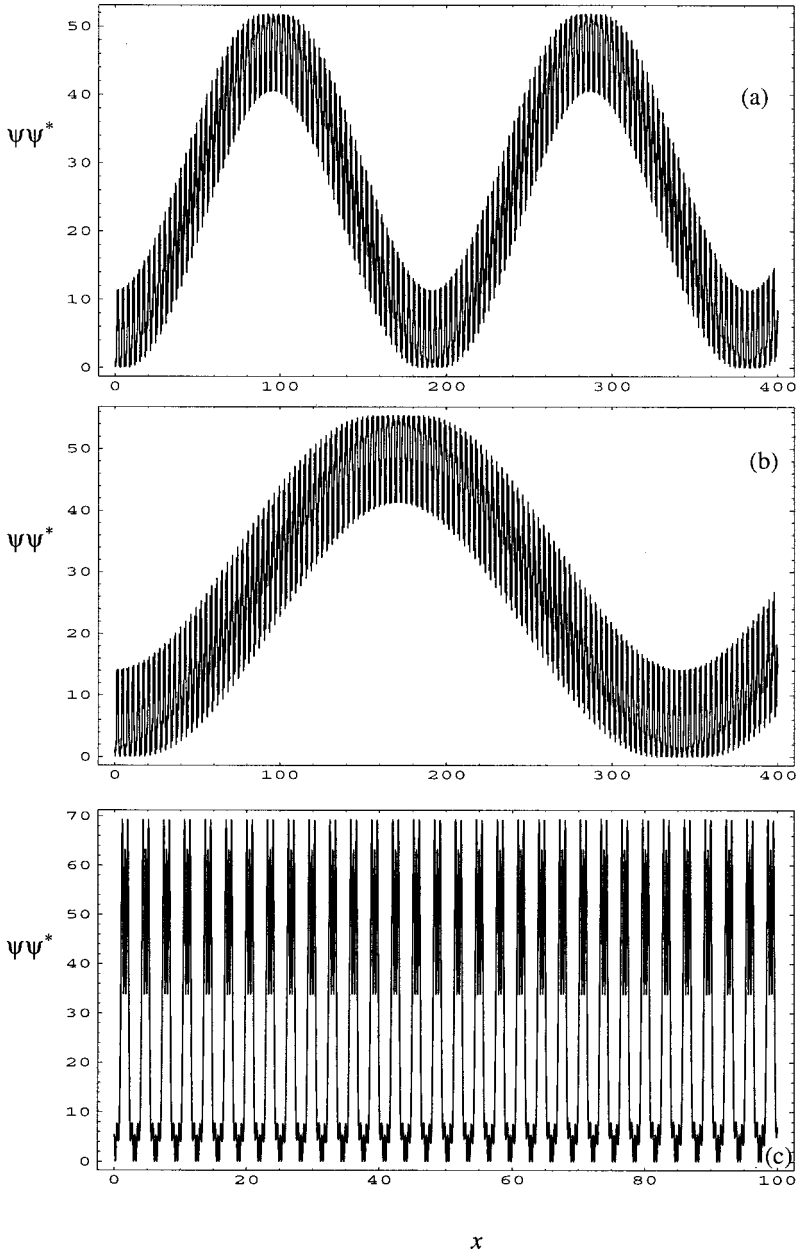

FIG. 4. The probability density for $\alpha=2$, $\beta=16.9$, and three K values: (a) $K=1.1000$, (b) $K=1.2000$, (c) $K=1.3005$.

The equation solved by Ψ in Eq. (6) has also been solved in the past using series of Bloch functions. Obviously the Bloch function solution contains all the same information of the Eq. (10) solution, however the Bloch function solution does not provide a method of understanding the dependence of the solution on α and β parameters. On the other hand the role of α and β is clear in the s variable. The s variable also points out the importance of zeros in the Bessel functions with respect to selecting interesting values of α and β. In addition the basic functions p and Q each have a differential equation with a factor of $\sin[(\beta/\alpha)\sin\alpha x]$. It was shown that for $\beta/\alpha < \pi/2$ the ratio β/α has the character of an amplitude. However, for $\beta/\alpha > \pi/2$, the ratio β/α has the character of a wave number. Consequently, as β/α is increased there is harmonic generation of the fundamental wave number contained in the solution.

The new wave function solution requires the determination of just two functions, p and Q. The form of the solution based on these two functions displays integer-order Bessel functions. The Bloch function series solves the same equation and thus it is possible to expand the Eq. (10) solution and derive the Bloch function series. The expansion procedure uses the Eq. (32) relations and the Eq. (A1) relations in the appendix. The resulting procedure produces a series with coefficients that are products of Bessel functions. Thus, the coefficients of the Bloch function series must also be products of Bessel functions that depend on α and β.

For $\beta/\alpha \ll 1$, $\mathcal{J}_{2n} \approx 0$, $\mathcal{J}_{2n+1} \approx 0$ and then s is real and $s \approx xK\mathcal{J}_0$. Using this approximation and restricting $K\beta/\alpha \ll 1$, analytic solutions for p and Q were derived. The analytic solutions were then applied to form wave functions used to determine the energy discriminant. The energy discriminant, which becomes a completely analytic function in this limit, was used to map the energy bands and gaps. The diminishing amplitude of $\Delta E - 2$ was illustrated as well as the reduction in the energy gap width as K increases.

As discussed earlier, the solution derived for p and Q in Sec. III B requires $K\beta/\alpha \ll 1$. This restriction must be imposed on the solution because as $\beta/\alpha \sim 1$ the couplings between p_r and p_i cannot be ignored and the solution requires the calculation of several difficult integrals. This difficulty can be overcome for a restricted parameter range. The solution can be extended based on an analysis of the behavior of the s variable. The main property of s that is useful in the construction of a large β/α solution is the highly nonuniform behavior of $ds/dx(\alpha,\beta)$. As x changes uniformly, s only changes uniformly when β/α is small. As β/α is increased beyond 1, ds/dx can be positive, negative, or very small. When it is very small the c_+ function tends to be approximately constant. Consequently, the solution under this condition is referred to as the dwell point solution. The dwell point solution relies on the validity of the issue of locality of $s+s^*$. For the circumstance of precisely constant $s+s^*$, Eq. (29) can be immediately integrated. Over a spatial region in which the s-plane trajectory is localized, $s+s^*$ is approximately constant, and thus separability of Eq. (28) is a good approximation. The best locality is attained near a zero of $\mathcal{J}_0$ with α large.

An interesting property of the integer-order Bessel functions is the oscillatory nature with regularly spaced zeros. The zeros of the Bessel functions point out interesting values of α and β where the character of the solution can be substantially altered. Regions around several zeros were numerically studied in Sec. IV B to show the dependence of the probability density on the selection of parameter values near Bessel function zeros. At fixed K, with $\alpha = 2$, the potential amplitude β was scanned from 16.9 to 17.3. It was shown that the appearance of the long wavelength in the probability density depends on the size of $\mathcal{J}_0$ and any low frequency contribution from p_r. Furthermore, even when $\mathcal{J}_0$ was identically zero there remained a long wavelength. The long wavelength in $\mathcal{P}$ for this case was demonstrated to be caused by the part of p_r linear in x.

Normally in a physical system the potential is given and the energy can be varied. To study the probability density under this condition β was set to 16.9 with $\alpha = 2$ and then K was varied from 1.1 to 1.3. It was found as in the previous example that the long wavelength in the probability density depends on the size of $\mathcal{J}_0$ and any low frequency contribution from p_r, except at $K = 1.3005$. At this particular value the linear part of p_r is equal and opposite to the linear part of $(s+s^*)/2$ and consequently the probability density does not have a long wavelength. Instead it is spatially distributed in very short wavelength peaks. The great difference between the spatial configuration with and without a long wavelength present hints at the possibility of a new semiconductor device. The switching action between the two modes occurs for a specific energy at fixed α and β.

ACKNOWLEDGMENTS

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APPENDIX: BESSEL GENERATING FUNCTION RELATIONS

$$\cos\left(\frac{\beta}{\alpha}\sin\theta\right)=\mathcal{J}_0+2\sum_{n=1}^{\infty}\mathcal{J}_{2n}\cos(2n\theta), \tag{A1a}$$

$$\sin\left(\frac{\beta}{\alpha}\sin\theta\right)=2\sum_{n=0}^{\infty}\mathcal{J}_{2n+1}\sin[(2n+1)\theta], \tag{A1b}$$

$$\cos\left(\frac{\beta}{\alpha}\cos\theta\right)=\mathcal{J}_0+2\sum_{n=1}^{\infty}(-1)^n\mathcal{J}_{2n}\cos(2n\theta), \tag{A1c}$$

$$\sin\left(\frac{\beta}{\alpha}\cos\theta\right)=2\sum_{n=0}^{\infty}(-1)^n\mathcal{J}_{2n+1}\sin[(2n+1)\theta]. \tag{A1d}$$

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Spectral and resonance properties of δ- and δ'-type interactions in relativistic quantum mechanics

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We discuss spectral and resonance properties of exactly solvable Dirac Hamiltonians corresponding to a surface δ and δ' interactions. First, we study spectral properties for δ-sphere and δ'-sphere models. Next, we analyze the resonance phenomena for the same models with specific boundary conditions. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1316060]

I. INTRODUCTION

The solvable models play a fundamental role in many areas of physics as they are simple and lead to much insight into the structure and properties of more complicated phenomena. Popular examples of such models are represented by the δ and δ'-sphere interactions which have been used in the recent past to describe various physical properties related as well to scattering theory as to spectral properties (see Ref. 1 and the references therein).

While these interactions have been deeper studied in nonrelativistic quantum mechanics, their profound analysis in relativistic theory was still missing. Some recent works[2–7] aim at extending our knowledge to δ and δ' interactions in relativistic quantum mechanics.

We pursue here the same objective and provide a systematic analysis of spectral and resonance properties of δ and δ'-type interactions for the Dirac operator with boundary conditions of the first and second type.[5]

The paper is organized as follows. In Sec. II, basic spectral properties are presented and analyzed. In Sec. III, we discuss the resonance properties. Section IV is devoted to some final remarks.

II. BASIC SPECTRAL PROPERTIES OF δ- AND δ'-SPHERE INTERACTIONS

A. The models

The expressions describing formally the models are of the type[2–7]

$$H = H_{\mathrm{D}} + V(|\underline{x}|), \quad \underline{x} \in \mathbb{R}^3, \tag{2.1}$$

where H_{D} is the free Dirac Hamiltonian:

$$H_{\mathrm{D}} \equiv -ic\alpha\nabla + \beta Mc^2, \tag{2.2}$$

M being the Dirac particle mass, i the complex imaginary ($i^2 = -1$), c the velocity of the light, ∇ the standard nabla operator while α and β are the Dirac matrices,

$$\alpha = \begin{pmatrix} \mathbf{0} & \sigma \\ \sigma & \mathbf{0} \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}, \tag{2.3}$$

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$\sigma \equiv \sigma^{\iota}$ ($\iota = 1,2,3$) are the 2×2 Pauli matrices:

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.4}$$

$V(|\underline{x}|)$ represents the potential that could be expressed as

$$V(|\underline{x}|) = \begin{cases} \sum_{m=1}^{N} \alpha_m \delta(|\underline{x}| - R_m), \\ \qquad \text{or} \\ \sum_{m=1}^{N} \beta_m \delta'(|\underline{x}| - R_m), \quad N \in \mathbb{N}^*, \quad N < \infty; \end{cases} \tag{2.5}$$

$\alpha_m, \beta_m \in \mathbb{R}$ and m stands for the number of concentric spheres of radii R_m.
The method adopted for the study of these singular interactions is based on the von Neumann theory of self-adjoint extensions of closed symmetric operators in Hilbert spaces.[8–11]

Let us consider the closed symmetric operator,

$$\dot{H} \equiv H_{\mathrm{D}}, \tag{2.6}$$

with the domain

$$\mathcal{D}(\dot{H}) = \{\psi \in H^{1,2}(\mathbb{R}^3) \otimes \mathbb{C}^4, \ \ \psi(S_{R_m}) = 0\}, \tag{2.7}$$

where $S_{R_m} = \{x \in \mathbb{R}^3, |x| = R_m\}$ is the closed ball of radius R_m centered at the origin in $\mathbb{R}^3$, and $H^{k,p}(\Omega)$ is the Sobolev space of indices (k,p).
The state Hilbert space $\mathcal{H}$ is decomposed as follows.[2–7]

$$\mathcal{H} = \bigoplus_{j=(1/2)}^{\infty} \bigoplus_{l=j-(1/2)}^{j+(1/2)} \bigoplus_{\mu=-j}^{j} \mathcal{H}_{jl\mu} = \bigoplus_{j=(1/2)}^{\infty} \bigoplus_{l=j-(1/2)}^{j+(1/2)} \mathcal{H}_{jl} \otimes [\Omega_{jl\mu}], \tag{2.8}$$

$\mathcal{H}_{jl}$ is the radial space:

$$\mathcal{H}_{jl} = \left\{ \psi(r) \in L^2((0,\infty)) \otimes \mathbb{C}^2; \ \ \psi(r) = \begin{pmatrix} f(r) \\ g(r) \end{pmatrix}; \ \ f,g \in L^2((0,\infty), r^2\, dr) \right\}, \tag{2.9}$$

and $[\Omega_{jl\mu}(\theta,\varphi)]$ is a space generated by the spherical spinors,

$$\Omega_{jl\mu}(\theta,\varphi) = \begin{pmatrix} \sqrt{\dfrac{j+\mu}{2l+1}} & Y_{l,\mu-(1/2)}(\theta,\varphi) \\ \sqrt{\dfrac{j-\mu}{2l+1}} & Y_{l,\mu+(1/2)}(\theta,\varphi) \end{pmatrix}, \quad \text{for } \ l = j - \frac{1}{2}, \tag{2.10}$$

$$\Omega_{jl\mu}(\theta,\varphi) = \begin{pmatrix} -\sqrt{\dfrac{j-\mu+1}{2l+1}} & Y_{l,\mu-(1/2)}(\theta,\varphi) \\ \sqrt{\dfrac{j+\mu+1}{2l+1}} & Y_{l,\mu+(1/2)}(\theta,\varphi) \end{pmatrix}, \quad \text{for } \ l = j + \frac{1}{2}, \tag{2.11}$$

where the spherical harmonics provide a basis for $L^2(S^2)$ (S^2 is the unit sphere in $\mathbb{R}^3$) and denote the linear span of vectors in $L^2(S^2)$. j,l,μ are the quantum numbers that characterize the total

angular momentum, its orbital and third (magnetic) components, respectively. Next, the following isomorphism is introduced in order to separate in each subspace $\mathcal{H}_{jl\mu}$, the radial part of the operator H and to remove the weight factor r^2 from the measure:[3,4]

$$\begin{aligned} U_{jl}:\quad & \mathcal{H}_{jl}\to L^2((0,\infty),dr)\otimes\mathbb{C}^2, \\ \psi\mapsto(U_{jl}\psi)(r)=&\begin{pmatrix} rf(r) \\ (-1)^{j-l-(1/2)}rg(r)\end{pmatrix}. \end{aligned} \tag{2.12}$$

This yields the following decomposition of $\mathcal{H}$:

$$\mathcal{H}=\bigoplus_{j=(1/2)}^{\infty}\bigoplus_{l=j-(1/2)}^{j+(1/2)}U_{jl}^{-1}[L^2((0,\infty),dr)\otimes\mathbb{C}^2]\bigotimes[\Omega_{jl-j},\ldots,\Omega_{jlj}]. \tag{2.13}$$

Provided the decomposition (2.13), one defines $\dot{H}$ as

$$\dot{H}=\bigoplus_{j=(1/2)}^{\infty}\bigoplus_{l=j-(1/2)}^{j+(1/2)}U_{jl}^{-1}\dot{h}_{jl}U_{jl}\bigotimes\mathbf{1}, \tag{2.14}$$

where ''the component operator'' $\dot{h}_{jl}$ is self-adjoint and represents the radial quantum Hamiltonian,

$$\dot{h}_{jl}=\begin{pmatrix} Mc^2 & c\left(-\dfrac{d}{dr}+\dfrac{K_{jl}}{r}\right) \\ c\left(\dfrac{d}{dr}+\dfrac{K_{jl}}{r}\right) & -Mc^2 \end{pmatrix}:=\tau, \tag{2.15}$$

with the domain

$$\begin{aligned} \mathcal{D}(\dot{h}_{jl})=&\{\psi\in L^2((0,\infty))\otimes\mathbb{C}^2;\ \ \psi,\psi'\in AC_{\mathrm{loc}}((0,\infty)-\{R\});\dot{h}_{jl}\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\}, \\ &\{R\}:=\{R_1,R_2,\ldots,R_N\} \end{aligned} \tag{2.16}$$

and the physical constant $K_{jl}=(-1)^{j-l+(1/2)}(j+\frac{1}{2})$.

From this point, it remains only to characterize the deficiency subspace which should lead to a rigorous mathematical definition of the formal expression (2.1). Indeed,[4–7] one can easily show that $\mathrm{def}(\dot{h}_{jl})=(2N,2N)$ and that all self-adjoint extensions are characterized by a $4N^2$- parameter family. However, two special families of restricted number of parameters must be considered in accordance with the boundary conditions. An account of the method of obtaining the two families of boundary conditions can be found in Refs. 5, 6.

B. Basic spectral properties with boundary conditions of the first type

1. The δ-sphere models

We analyze the spectral properties for the δ-sphere interaction, for a finitely many δ-sphere interactions and for a δ-sphere coupled with a Coulomb type potential, respectively.

(i) The formal expression describing the one δ-sphere model is[7]

$$H=H_{\mathrm{D}}+\alpha\delta(|\underline{x}|-R),\quad \alpha\in\mathbb{R},\quad \underline{x}\in\mathbb{R}^3. \tag{2.17}$$

The boundary conditions which characterize each of the two special one-parameter families of self-adjoint extensions (s.a.e.) of the free Dirac Hamiltonian H_{D} are

$$g(k,R_+)-g(k,R_-)=\frac{\alpha}{c}f(k,R)+A,$$
$$f(k,R_+)=f(k,R_-)\equiv f(k,R), \tag{2.18}$$

or

$$f(k,R_+)-f(k,R_-)=-\frac{\theta}{c}g(k,R)+B,$$
$$g(k,R_+)=g(k,R_-)\equiv g(k,R); \tag{2.19}$$

$f(k,r)$ and $g(k,r)$ are the first and second components of the wave function, respectively; k, α, θ, A and B are nonvanishing constants; c is the velocity of the light.

The first family of s.a.e. labeled by α reads as

$$h_{jl,\alpha_{jl}}\equiv\tau,$$
$$\mathcal{D}(h_{jl,\alpha_{jl}})=\{\psi(r)\in L^2((0,\infty))\otimes\mathbb{C}^2;\ \ f_{jl}\in AC_{\mathrm{loc}}((0,\infty));$$
$$g_{jl}\in AC_{\mathrm{loc}}((0,\infty)-\{R\});\ \ g_{jl}(R_+)-g_{jl}(R_-)=\frac{\alpha}{c}f_{jl}(R)+A;$$
$$h_{jl,\alpha_{jl}}\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\}. \tag{2.20}$$

The second family of s.a.e. is defined by

$$h_{jl,\theta_{jl}}\equiv\tau,$$
$$\mathcal{D}(h_{jl,\theta_{jl}})=\{\psi(r)\in L^2((0,\infty))\otimes\mathbb{C}^2;\ \ f_{jl}\in AC_{\mathrm{loc}}((0,\infty)-\{R\});$$
$$g_{jl}\in AC_{\mathrm{loc}}((0,\infty));\ \ f_{jl}(R_+)-f_{jl}(R_-)=-\frac{\theta}{c}g_{jl}(R)+B;$$
$$h_{jl,\theta_{jl}}\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\}. \tag{2.21}$$

The resolvent is of a great help for the deduction of relevant physical properties as the scattering elements, the resonances and the spectra. The resolvent of $h_{jl,\alpha_{jl}}$ and H_α are given by the following Theorem.

Theorem II.1: *If $\alpha_{jl}\neq 0$, then the following holds.*

(i) The resolvent of $h_{jl,\alpha_{jl}}$ is given by

$$(h_{jl,\alpha_{jl}}-k^2)^{-1}=(h_{jl,0}-k^2)^{-1}+\frac{-\alpha_{jl}/c}{1+(\alpha_{jl}/c)[F_{jl}^{(0)}(k,R)G_{jl}^{(0)}(k,R)]}$$
$$\times\begin{pmatrix}1&0\\0&1\end{pmatrix}(\psi_{jl}(-\overline{k}),.)\psi_{jl}(k);\ \ k^2\in\rho(h_{jl,\alpha_{jl}}),\ \ \mathrm{Im}\,k>0. \tag{2.22}$$

$G_{jl,0}=(h_{jl,0}-k^2)^{-1}$, $\mathrm{Im}\,k>0$, *is the free resolvent kernel:*

$$G_{jl,0}(k',r,r')=\begin{bmatrix}\tilde{g}_{jl0}^{(I)}(k',r,r')&\tilde{g}_{jl0}^{(I)}(k',r,r')\\ \tilde{g}_{jl0}^{(II)}(k',r,r')&\tilde{g}_{jl0}^{(II)}(k',r,r')\end{bmatrix}, \tag{2.23}$$

where

$$\tilde{g}^{(I)}_{jl0}(k',r,r')=\begin{cases} G^{(0)}_{jl}(k',r)F^{(0)}_{jl}(k',r'); & r'<r,\\ F^{(0)}_{jl}(k',r)G^{(0)}_{jl}(k',r'); & r'>r, \end{cases} \tag{2.24}$$

and

$$\tilde{g}^{(II)}_{jl0}(k',r,r')=\begin{cases} \tilde{G}^{(0)}_{jl}(k',r)\tilde{F}^{(0)}_{jl}(k',r'); & r'<r,\\ \tilde{F}^{(0)}_{jl}(k',r)\tilde{G}^{(0)}_{jl}(k',r'); & r'>r. \end{cases} \tag{2.25}$$

$F^{(0)}_{jl}$, $\tilde{F}^{(0)}_{jl}$, $G^{(0)}_{jl}$ *and* $\tilde{G}^{(0)}_{jl}$ *are given by*

$$\begin{aligned} F^{(0)}_{jl}(k',r)&=\left(\frac{k'}{2}\right)^{-K_{jl}-(1/2)}\Gamma\left(K_{jl}+\frac{3}{2}\right)r^{1/2}J_{K_{jl}+(1/2)}(k'r),\\ G^{(0)}_{jl}(k',r)&=-\frac{i\pi}{2}\frac{1}{\Gamma(K_{jl}+(3/2))}\left(\frac{k'}{2}\right)^{K_{jl}+(1/2)}r^{1/2}H^{(2)}_{K_{jl}+(1/2)}(k'r),\\ \tilde{F}^{(0)}_{jl}(k',r)&=\left(\frac{k'}{2}\right)^{-K_{jl}+(1/2)}\Gamma\left(K_{jl}+\frac{1}{2}\right)r^{1/2}J_{K_{jl}-(1/2)}(k'r),\\ \tilde{G}^{(0)}_{jl}(k',r)&=-\frac{i\pi}{2}\frac{1}{\Gamma(K_{jl}+(1/2))}\left(\frac{k'}{2}\right)^{K_{jl}-(1/2)}r^{1/2}H^{(2)}_{K_{jl}-(1/2)}(k'r), \end{aligned} \tag{2.26}$$

where $k'^2=c^{-2}(k^4-M^2c^4)$, $J_\nu(z)$ *and* $H^{(2)}_\nu(z)$ *are*[13,14] *the Bessel function and the Hankel function of the second type of order* ν, *respectively.* $\psi_{jl}(k',r)$ *is given by*

$$\psi_{jl}(k',r)=\begin{pmatrix} F^{(0)}_{jl}(k',r)G^{(0)}_{jl}(k',R)+F^{(0)}_{jl}(k',R)G^{(0)}_{jl}(k',r)\\ \tilde{F}^{(0)}_{jl}(k',r)G^{(0)}_{jl}(k',R)+F^{(0)}_{jl}(k',R)\tilde{G}^{(0)}_{jl}(k',r)\end{pmatrix}. \tag{2.27}$$

(ii) The resolvent of H_α *is given by*

$$\begin{aligned}(H_\alpha-k^2)^{-1}=(H_0-k^2)^{-1}+\bigoplus_{j=1/2}^{\infty}\bigoplus_{l=j-1/2}^{j+1/2}\bigoplus_{m=-l}^{+l}\frac{-\alpha_{jl}/c}{1+(\alpha_{jl}/c)[F^{(0)}_{jl}(k,R)G^{(0)}_{jl}(k,R)]}\\ \times[|\cdot|^{-1}(\psi_{jl}(-\overline{k})\otimes\Omega_{jlm}),.]|\cdot|^{-1}\psi_{jl}(k)\otimes\Omega_{jlm},\ \ k^2\in\rho(H_\alpha),\end{aligned} \tag{2.28}$$

with the notation

$$\psi_{jl}(k)\otimes\Omega_{jlm}=\begin{pmatrix}\psi_{(jl)_1}\Omega_{(jlm)_1}\\ \psi_{(jl)_2}\Omega_{(jlm)_2}\end{pmatrix},\quad \psi_{jl}=\begin{pmatrix}\psi_{(jl)_1}\\ \psi_{(jl)_2}\end{pmatrix},\ \ \Omega_{(jlm)}=\begin{pmatrix}\Omega_{(jlm)_1}\\ \Omega_{(jlm)_2}\end{pmatrix},$$

$\rho(\cdot)$ *is the resolvent set,* H_α:=H [*see Eq. (2.1)*].

Proof: By means of Krein's formula[10] and after a straightforward computation performed as in Ref. 4, the resolvent (2.22) is deduced. Expression (2.28) follows from the decomposition (2.13). ■

Theorem II.2: *All self-adjoint extensions of the extended Dirac operator* $H=H_D+V(|\underline{x}|)$ *with deficiency indices* (2,2) *have the same continuous spectrum as that of the free Dirac operator* H_D; *this spectrum is purely and absolutely continuous and equals* $]-\infty,-Mc^2]\cup[Mc^2,+\infty[$.

Proof: The first part of this statement follows immediately from the fact that all s.a.e. of an operator with equal and finite deficiency indices have the same continuous spectrum (see Ref. 10, Theorem 1, p. 365).

Next, in Refs. 2, 12, it has been proved that the continuous spectrum of the free Dirac operator is known to be purely and absolutely continuous and equals $]-\infty,-Mc^2]\cup[Mc^2,+\infty[$ taking into account the following radial equation (in Ref. 2, $c=1$):

$$Mc^2 f - c\frac{d}{dr}g + c\frac{K_{jl}}{r}g = \lambda f,$$

$$c\frac{d}{dr}f + c\frac{K_{jl}}{r}f - Mc^2 = \lambda g, \quad \lambda \in \mathbb{R}. \tag{2.29}$$

Finally, the spectral kernel of the extended Dirac operator coincides with the spectrum of this operator. Moreover, the spectral kernel of $h_{jl,\alpha_{jl}}$ contains the spectral kernel of $h_{jl,0}$ as the former stands for the s.a.e. of the latter. So, each part of the spectral kernel of $h_{jl,\alpha_{jl}}$ contains the corresponding part of the spectral kernel of $h_{jl,0}$. As the deficiency indices of the operator $h_{jl,0}$ is finite $(\mathrm{def}(h_{jl,0})=(2,2))$, the continuous part of its spectral kernel is invariant for its symmetric extensions.[10] Hence, the free Dirac operator $h_{jl,0}$ and its s.a.e. have the same continuous spectrum.

Besides, by the von Neumann formula,[10] the manifold $(h_{jl,\alpha_{jl}}-k^2)\mathcal{D}(h_{jl,\alpha_{jl}})$ contains the manifold $(h_{jl,0}-k^2)\mathcal{D}(h_{jl,0})$ and the difference in dimensions is finite. Therefore, the operator $(h_{jl,\alpha_{jl}}-k^2)^{-1}$ is bounded along with the operator $(h_{jl,0}-k^2)^{-1}$.

Theorem II.3: *The singularly continuous and residual spectra of the extended Dirac operator $h_{jl,\alpha_{jl}}$ are empty.*

Proof: One can follow step by step the development given in Ref. 2 to show that the singularly continuous spectrum is empty. The fact that the residual spectrum is empty results from the self-adjointness of the operator. ■

The above development trivially generalizes for $N>2$ $(\mathrm{def}(h_{jl,0})=(N,N))$. Henceforth, we shall restrict ourselves to the study of the bound state equations that are different for different models as the boundary conditions characterizing these models change.

The bound state equations for the model (2.17) provide elements for its point spectrum and their solutions are the negative eigenvalues of the singular radial Hamiltonian $h_{jl,\alpha_{jl}}$. These equations are obtained from the following Theorem.

Theorem II.4: *The bound state equations relative to the first and second families of s.a.e. read as*

$$\frac{\alpha_{jl}}{c} = \frac{\pm \tilde{T}^{(0)}_{jl}(\tilde{E},R)\tilde{L}^{(0)}_{jl}(\tilde{E},R)}{T^{(0)}_{jl}(\tilde{E},R)L^{(0)}_{jl}(\tilde{E},R)+A_1}, \quad A=\frac{\alpha_{jl}}{c}A_1 \tag{2.30}$$

and

$$\frac{\theta_{jl}}{c} = \frac{\pm T^{(0)}_{jl}(\tilde{E},R)L^{(0)}_{jl}(\tilde{E},R)}{\tilde{T}^{(0)}_{jl}(\tilde{E},R)\tilde{L}^{(0)}_{jl}(\tilde{E},R)-B_1}, \quad B=\frac{\theta_{jl}}{c}B_1, \tag{2.31}$$

respectively, where

$$
\begin{aligned}
L_{jl}^{(0)}(\tilde{E},r) &= \Gamma\left(K_{jl}+\frac{3}{2}\right)\left(\frac{\sqrt{-\tilde{E}}}{2}\right)^{-K_{jl}-(1/2)} r^{1/2} I_{K_{jl}+(1/2)}(\sqrt{-\tilde{E}}r),\\
T_{jl}^{(0)}(\tilde{E},r) &= \frac{2}{\Gamma(K_{jl}+(3/2))}\left(\frac{\sqrt{-\tilde{E}}}{2}\right)^{K_{jl}+(1/2)} r^{1/2} K_{K_{jl}+(1/2)}(\sqrt{-\tilde{E}}r),\\
\tilde{L}_{jl}^{(0)}(\tilde{E},r) &= \Gamma\left(K_{jl}+\frac{1}{2}\right)\left(\frac{\sqrt{-\tilde{E}}}{2}\right)^{-K_{jl}+(1/2)} r^{1/2} I_{K_{jl}-(1/2)}(\sqrt{-\tilde{E}}r),\\
\tilde{T}_{jl}^{(0)}(\tilde{E},r) &= \frac{2}{\Gamma(K_{jl}+(1/2))}\left(\frac{\sqrt{-\tilde{E}}}{2}\right)^{K_{jl}-(1/2)} r^{1/2} K_{K_{jl}-(1/2)}(\sqrt{-\tilde{E}}r).
\end{aligned}
\tag{2.32}
$$

I_ν and K_ν are the modified Bessel functions of the first and second type of order ν, respectively.[13]

Proof: These equations stem from the following eigenvalue equations:

$$
\begin{pmatrix} Mc^2 & c\left(-\frac{d}{dr}+\frac{K_{jl}}{r}\right) \\ c\left(\frac{d}{dr}+\frac{K_{jl}}{r}\right) & -Mc^2 \end{pmatrix}
\begin{pmatrix} f_{jl}(E,r) \\ g_{jl}(E,r) \end{pmatrix} = E\begin{pmatrix} f_{jl}(E,r) \\ g_{jl}(E,r) \end{pmatrix}, \quad E<0, \tag{2.33}
$$

that split into

$$
f''(E,r)+\left[\frac{E^2-M^2c^4}{c^2}-\frac{1}{r^2}K_{jl}(K_{jl}+1)\right]f(E,r)=0, \tag{2.34}
$$

$$
g''(E,r)+\left[\frac{E^2-M^2c^4}{c^2}-\frac{1}{r^2}K_{jl}(K_{jl}-1)\right]g(E,r)=0. \tag{2.35}
$$

A supplementary condition (physically admitted) is $E^2<M^2c^4$. This yields $\tilde{E}=(E^2-M^2c^4)/c^2<0$ and the corresponding separated equations provide the solutions (2.32). Besides, using the modified Bessel functions (2.32), the implementation of the boundary conditions (2.18) and (2.19) gives the bound state equations (2.30) and (2.31). ■

Let us discuss some solutions.

Using relations (2.32), Eq. (2.30) reduces to the equation

$$
1+\bar{\alpha}_{jl}RK_{K_{jl}+(1/2)}(\sqrt{-\tilde{E}}R)I_{K_{jl}+(1/2)}(\sqrt{-\tilde{E}}R)=0, \tag{2.36}
$$

with $\bar{\alpha}_{jl}=(2/A)(\alpha_{jl}/c\pm b)$, $\alpha_{jl}\in\mathbb{R}$, $b\in\mathbb{R}$, for the first family characterized by the parameters α_{jl}; an analogous equation with adequate parameters is obtained for the second family from (2.31).

This equation is similar to that analyzed in Ref. 1 [Eq. 2.39)], using the monotonicity properties of $K(\cdot)I(\cdot)$. For each family of s.a.e., we have two solutions $\tilde{E}_{1,2}<0$ for $\bar{\alpha}_{jl}R<-(K_{jl}+1/2)$ and no solution for $\bar{\alpha}_{jl}R\geqslant-(K_{jl}+1/2)$. Obviously, the two solutions stem from the two possibilities $\pm b$ in the expression of $\bar{\alpha}_{jl}$ occurring in Eq. (2.36).

This result is in good accordance with the wording of Proposition 6.1 given in Ref. 2. Compared with the nonrelativistic case,[1] this result is predictable since two special one parameter families of s.a.e. are defined in the relativistic case instead of one in the nonrelativistic case because of the matrix structure of the Dirac equation.

(ii) Concerning the finitely many δ-sphere interactions case, the model is formally expressed as[5]

$$H_{\{R\}}=H_{\mathrm{D}}+\sum_{m=1}^{N}\alpha_m\delta(|\underline{x}|-R_m);\quad \underline{x}\in\mathbb{R}^3, \tag{2.37}$$

where H_{D} is the free Dirac operator; $\alpha_m\neq 0$, $1\leqslant m\leqslant N$. Two special N-parameter families of s.a.e. are defined. The first family characterized by the parameters α_m, $m=1,\ldots,N$ reads as

$$h_{jl,\alpha_{jl}\{R\}}\equiv\begin{pmatrix} Mc^2 & c\left(-\dfrac{d}{dr}+\dfrac{K_{jl}}{r}\right)\\ c\left(\dfrac{d}{dr}+\dfrac{K_{jl}}{r}\right) & -Mc^2\end{pmatrix},$$

$$\mathcal{D}(h_{jl,\alpha_{jl}\{R\}})=\{\psi(r)\in L^2((0,\infty))\otimes\mathbb{C}^2;\ \ f_{jl}\in AC_{\mathrm{loc}}((0,\infty));$$

$$g_{jl}\in AC_{\mathrm{loc}}((0,\infty)-\{R\});g_{jl}(R_{m+})-g_{jl}(R_{m-})=\frac{\alpha_m}{c}f_{jl}(R_m)+A_m;$$

$$h_{jl,\alpha_{jl}\{R\}}\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\},\{R\}:=\{R_1,R_2,\ldots,R_N\}. \tag{2.38}$$

So, for all $m=1,\ldots,N$, assuming $\alpha_{jl}\in\mathbb{R}$, the negative eigenvalues of the radial extended Hamiltonian are given by the bound state equations

$$\frac{\alpha_m}{c}=\frac{\pm\tilde{T}_{jl}^{(0)}(\tilde{E},R_m)\tilde{L}_{jl}^{(0)}(\tilde{E},R_m)}{T_{jl}^{(0)}(\tilde{E},R_m)L_{jl}^{(0)}(\tilde{E},R_m)+A_1^m},\quad A_1^m=\frac{\alpha_m}{c}A_m. \tag{2.39}$$

The second family is defined by

$$\mathcal{D}(h_{jl,\theta_{jl}\{R\}})=\{\psi(r)\in L^2((0,\infty))\otimes\mathbb{C}^2;\ \ g_{jl}\in AC_{\mathrm{loc}}((0,\infty));$$

$$f_{jl}\in AC_{\mathrm{loc}}((0,\infty)\backslash\{R\});\ \ f_{jl}(R_{m+})-f_{jl}(R_{m-})=-\frac{\theta_m}{c}g_{jl}(R_m)+B_m;$$

$$h_{jl,\gamma_{jl}\{R\}}\psi\in L^2((0,\infty))\otimes\mathbb{C}^2\},\{R\}:=\{R_1,R_2,\ldots,R_N\}. \tag{2.40}$$

The corresponding bound state equations are

$$\frac{\theta_{jl}}{c}=\frac{\pm T_{jl}^{(0)}(\tilde{E},R_m)L_{jl}^{(0)}(\tilde{E},R_m)}{\tilde{T}_{jl}^{(0)}(\tilde{E},R_m)\tilde{L}_{jl}^{(0)}(\tilde{E},R_m)-B_1^m},\quad \text{with}\quad B_m=\frac{\theta_{jl}}{c}B_1^m. \tag{2.41}$$

The discussion is similar to that of the one δ-sphere model. Thus, if for each equation we get n solutions, we can hope to obtain for each family at most $2nN$ negative eigenvalues by analogy to the δ-sphere case replacing R by R_m.

(iii) In the model of one δ-sphere interaction coupled with a Coulomb potential, the formal expression describing the interaction Hamiltonian reads as[4,6,7,11]

$$H=H_{\mathrm{D}}+\frac{\gamma_0}{r}+\alpha\delta(r-R), \tag{2.42}$$

where H_{D} represents the free Dirac Hamiltonian, γ_0 and α are nonvanishing physical constants. We can define two special one-parameter families of s.a.e. according to the boundary conditions (2.18) and (2.19). For the bound state equations, we state the following Theorem.

Theorem II.5: *The negative eigenvalues $\tilde{E}$ are solutions of the equations*

$$\frac{\alpha_{jl\gamma_0}}{c}=\frac{\pm\tilde{T}^{(0)}_{jl\gamma_0}(\tilde{E},R)\tilde{L}^{(0)}_{jl\gamma_0}(\tilde{E},R)}{T^{(0)}_{jl\gamma_0}(\tilde{E},R)L^{(0)}_{jl\gamma_0}(\tilde{E},R)+A_{\gamma_0 1}},\quad A_{\gamma_0}=\frac{\alpha_{jl\gamma_0}}{c}A_{\gamma_0 1},\tag{2.43}$$

for the first family and

$$\frac{\theta_{jl\gamma_0}}{c}=\frac{\pm T^{(0)}_{jl\gamma_0}(\tilde{E},R)L^{(0)}_{jl\gamma_0}(\tilde{E},R)}{\tilde{T}^{(0)}_{jl\gamma_0}(\tilde{E},R)\tilde{L}^{(0)}_{jl\gamma_0}(\tilde{E},R)-B_{\gamma_0 1}},\quad B_{\gamma_0}=\frac{\theta_{jl\gamma_0}}{c}B_{\gamma_0 1},\tag{2.44}$$

for the second family, respectively, where

$$\begin{aligned}L_{jl\gamma_0}(\tilde{E},r)&=\left(\frac{\gamma_0}{2\epsilon(K_{jl}-\epsilon)}p_1-\frac{1}{2\epsilon}q_1\right);\ r<R,\\ T_{jl\gamma_0}(\tilde{E},r)&=\left(\frac{\gamma_0}{2\epsilon(K_{jl}-\epsilon)}p_2-\frac{1}{2\epsilon}q_2\right);\ r>R,\end{aligned}\tag{2.45}$$

and

$$\begin{aligned}\tilde{L}^{(0)}_{jl\gamma_0}(\tilde{E},r)&=\left(-\frac{1}{2\epsilon}p_1+\frac{\gamma_0}{2\epsilon(K_{jl}-\epsilon)}q_1\right);\ r<R\\ \tilde{T}^{(0)}_{jl\gamma_0}(\tilde{E},r)&=\left(-\frac{1}{2\epsilon}p_2+\frac{\gamma_0}{2\epsilon(K_{jl}-\epsilon)}q_2\right);\ r>R,\end{aligned}\tag{2.46}$$

with

$$p_1(\tilde{E},r)=r^{\mu+1}\exp(\sqrt{-\tilde{E}}r)\,{}_1F_1\left(1+\mu-\frac{\gamma_0 E}{c^2\sqrt{-\tilde{E}}};2(\mu+1);-2\sqrt{-\tilde{E}}r\right),\tag{2.47}$$

$$p_2(\tilde{E},r)=\Gamma[2(\mu+1)]^{-1}\Gamma\left[\left(1+\mu-\frac{\gamma_0 E}{c^2\sqrt{-\tilde{E}}}\right)\right](-2\sqrt{-\tilde{E}})^{2\mu+1}r^{\mu+1}\exp(\sqrt{-\tilde{E}}r)$$

$$\times U\left(1+\mu-\frac{\gamma_0 E}{c^2\sqrt{-\tilde{E}}};2(\mu+1);-2\sqrt{-\tilde{E}}r\right),$$

$$q_1(\tilde{E},r)=r^{\mu}\exp(\sqrt{-\tilde{E}}r)\,{}_1F_1\left(\mu-\frac{\gamma_0 E}{c^2\sqrt{-\tilde{E}}};2\mu;-2\sqrt{-\tilde{E}}r\right),\tag{2.48}$$

$$q_2(\tilde{E},r)=\Gamma(2\mu)^{-1}\Gamma\left(\mu-\frac{\gamma_0 E}{c^2\sqrt{-\tilde{E}}}\right)(-2\sqrt{-\tilde{E}})^{2\mu-1}r^{\mu}\exp(\sqrt{-\tilde{E}}r)$$

$$\times U\left(\mu-\frac{\gamma_0 E}{c^2\sqrt{-\tilde{E}}};2\mu;-2\sqrt{-\tilde{E}}r\right),$$

$\tilde{E}=c^{-2}(E^2-M^2c^4)<0$, $\epsilon=\sqrt{c^2K_{jl}^2-\gamma_0^2}$, $\mu=\epsilon/c$. ${}_1F_1(z)$ *and* $U(z)$ *are the hypergeometric functions of the first and second type, respectively.*[13,14]

Proof: The method of solving the bound state equations [a matrix differential equation analogous of Eq. (2.33)] can be found in Ref. 14. Besides, the implementation of the boundary conditions (2.18) and (2.19) using the obtained solutions, gives the equations (2.43) and (2.44). ■

Next, one can easily apply the technique previously used to carry out a systematic study of this model.

2. The δ'-sphere models

Here, we only sketch some important facts and merely provide a collection of relevant formulas without explicit proofs, since the whole analysis can be carried through as in the previous subsection.

For the one δ'-sphere model, we have[6]

$$H=H_{\mathrm{D}}+\tilde{\alpha}\,\delta'(|\underline{x}|-R),\quad \tilde{\alpha}\in\mathbb{R},\quad \underline{x}\in\mathbb{R}^3. \tag{2.49}$$

The boundary conditions of the first type which characterize each of the two special one-parameter families of s.a.e. of the free Dirac Hamiltonian H_{D} are given by

$$\begin{aligned} g(k,R_+)-g(k,R_-)&=-\frac{\tilde{\alpha}}{c}\frac{1}{2}[f'(k,R_+)+f'(k,R_-)]+\tilde{A},\\ f(k,R_+)&=f(k,R_-)\equiv f(k,R), \end{aligned} \tag{2.50}$$

or

$$\begin{aligned} f(k,R_+)-f(k,R_-)&=\frac{\tilde{\theta}}{c}\frac{1}{2}[g'(k,R_+)+g'(k,R_-)]-\tilde{B},\\ g(k,R_+)&=g(k,R_-)\equiv g(k,R), \end{aligned} \tag{2.51}$$

where $f(k,r)$ and $g(k,r)$ are as usual the components of the wave function; k, $\tilde{\alpha}$, $\tilde{\theta}$, $\tilde{A}$ and $\tilde{B}$ are nonvanishing constants. We can easily define two families of s.a.e. accordingly with the above boundary conditions (see Ref. 7).

The bound state equations for the first family are

$$\frac{\tilde{\alpha}_{jl}}{c}=\frac{\pm 2\tilde{T}_{jl}^{(0)}(\tilde{E},R)\tilde{L}_{jl}^{(0)}(\tilde{E},R)}{T_{jl}^{(0)}(\tilde{E},R)L_{jl}^{(0)}(\tilde{E},R)-2\tilde{A}_1},\quad \tilde{A}=\frac{\tilde{\alpha}_{jl}}{c}\tilde{A}_1. \tag{2.52}$$

For the second family of s.a.e., we have

$$\frac{\tilde{\theta}_{jl}}{2c}=\frac{\pm T_{jl}^{(0)}(\tilde{E},R)L_{jl}^{(0)}(\tilde{E},R)}{\tilde{T}_{jl}^{(0)}(\tilde{E},R)\tilde{L}_{jl}^{(0)}(\tilde{E},R)-2\tilde{B}_1},\quad \text{with}\quad \tilde{B}=\frac{\tilde{\theta}_{jl}}{c}\tilde{B}_1. \tag{2.53}$$

The same procedure as that of the previous subsection applied here, yields

$$1+\bar{\tilde{\alpha}}_{jl}RK_{K_{jl}+(1/2)}(\sqrt{-\tilde{E}}R)I_{K_{jl}+(1/2)}(\sqrt{-\tilde{E}}R)=0, \tag{2.54}$$

with $\bar{\tilde{\alpha}}_{jl}=(1/2\tilde{A})(\tilde{\alpha}_{jl}/c\pm 2\tilde{b})$, $\tilde{\beta}_{jl}\in\mathbb{R}$, $\tilde{b}\in\mathbb{R}$, for the first family characterized by the parameters $\tilde{\alpha}_{jl}$ and an analogous equation with appropriate parameters for the second family.

From this, two solutions are possible for each family of s.a.e.: For $\tilde{\bar{\alpha}}_{jl}R<-(2K_{jl}+1)$, we have one solution with $\tilde{\bar{\alpha}}_{jl}=(\tilde{\alpha}_{jl}/c+2\tilde{b})$ and another with $\tilde{\bar{\alpha}}_{jl}=(\tilde{\alpha}_{jl}/c-2\tilde{b})$, while for $\tilde{\bar{\alpha}}_{jl}R \geqslant -(2K_{jl}+1)$ there is no solution in the both cases.

Concerning the finitely many sphere case, we hope at most $2N$ eigenvalues of the above types for each extended radial operator.

Finally, for the case of one δ'-sphere interaction coupled with a Coulomb potential, the formal model is[6,7]

$$H=H_{\mathrm{D}}+\frac{\gamma_0}{r}+\tilde{\alpha}\,\delta'(r-R). \tag{2.55}$$

The corresponding extended radial operators are

$$h_{jl\gamma_0,\tilde{\alpha}_{jl}}\equiv\begin{pmatrix} Mc^2+\dfrac{\gamma_0}{r} & c\left(-\dfrac{d}{dr}+\dfrac{K_{jl}}{r}\right) \\ c\left(\dfrac{d}{dr}+\dfrac{K_{jl}}{r}\right) & -Mc^2+\dfrac{\gamma_0}{r}\end{pmatrix}:=\tau_{\gamma_0}, \tag{2.56}$$

$$\begin{aligned}\mathcal{D}(h_{jl\gamma_0,\tilde{\alpha}_{jl}})=\Big\{ & \psi(r)\in L^2((0,\infty))\otimes\mathbb{C}^2;\ ;f_{jl}\in AC_{\mathrm{loc}}((0,\infty));\\ & f'_{jl}\in AC_{\mathrm{loc}}((0,\infty)\backslash\{R\});\ g_{jl},g'_{jl}\in AC_{\mathrm{loc}}((0,\infty)\backslash\{R\});\\ & g_{jl}(k,R_+)-g_{jl}(k,R_-)=-\frac{1}{2}\frac{\tilde{\alpha}_{jl}}{c}[f'_{jl}(k,R_+)+f'_{jl}(k,R_-)]+\tilde{A};\\ & h_{jl\gamma_0,\tilde{\alpha}_{jl}}\psi\in L^2((0,\infty))\otimes\mathbb{C}^2;\ \tilde{A}\neq 0;\ -\infty<\tilde{\alpha}_{jl}<+\infty\Big\},\end{aligned} \tag{2.57}$$

for the first family and

$$h_{jl\gamma_0,\tilde{\theta}_{jl}}\equiv\tau_{\gamma_0},$$

$$\begin{aligned}\mathcal{D}(h_{jl\gamma_0,\tilde{\theta}_{jl}})=\Big\{ & \psi(r)\in L^2((0,\infty))\otimes\mathbb{C}^2;\ g_{jl},g'_{jl}\in AC_{\mathrm{loc}}((0,\infty)\backslash\{R\});\\ & f_{jl},f'_{jl}\in AC_{\mathrm{loc}}((0,\infty)\backslash\{R\});\ g_{jl}(k,R_+)=g_{jl}(k,R_-);\\ & f_{jl}(k,R_+)-f_{jl}(k,R_-)=\frac{\tilde{\gamma}_{jl}}{c}\frac{1}{2}[g'_{jl}(k,R_+)+g'_{jl}(k,R_-)]-\tilde{B};\\ & h_{jl\gamma_0,\tilde{\theta}_{jl}}\psi\in L^2((0,\infty))\otimes\mathbb{C}^2;\\ & \tilde{B}\neq 0;\ -\infty<\tilde{\theta}_{jl}<+\infty\Big\},\end{aligned} \tag{2.58}$$

for the second family.

The negative eigenvalues are solutions of the equations

$$\frac{\tilde{\alpha}_{jl\gamma_0}}{2c}=\frac{\pm\tilde{T}^{(0)}_{jl\gamma_0}(\tilde{E},R)\tilde{L}^{(0)}_{jl\gamma_0}(\tilde{E},R)}{T^{(0)}_{jl\gamma_0}(\tilde{E},R)L^{(0)}_{jl\gamma_0}(\tilde{E},R)-2\tilde{A}_{\gamma_0 1}},\quad \tilde{A}_{\gamma_0}=\frac{\alpha_{jl\gamma_0}}{c}\tilde{A}_{\gamma_0 1}, \tag{2.59}$$

for the first family and

$$\frac{\tilde{\theta}_{jl\gamma_0}}{2c}=\frac{\pm T^{(0)}_{jl\gamma_0}(\tilde{E},R)L^{(0)}_{jl\gamma_0}(\tilde{E},R)}{\tilde{T}^{(0)}_{jl\gamma_0}(\tilde{E},R)\tilde{L}^{(0)}_{jl\gamma_0}(\tilde{E},R)-2\tilde{B}_{\gamma_0 1}},\quad \tilde{B}_{\gamma_0}=\frac{\theta_{jl\gamma_0}}{c}\tilde{B}_{\gamma_0 1}, \tag{2.60}$$

for the second family.

C. Basic spectral properties with boundary conditions of second type

1. The δ-sphere models

Turning back to the one-sphere interaction, the second type boundary conditions are obtained from (2.18) and (2.19) by interchanging formally f and f' (g and g'). We have[4]

$$\begin{aligned} g'(k,R_+)-g'(k,R_-)&=\frac{\beta}{c}f'(k,R)+A,\\ f'(k,R_+)&=f'(k,R_-)\equiv f'(k,R), \end{aligned} \tag{2.61}$$

or

$$\begin{aligned} f'(k,R_+)-f'(k,R_-)&=-\frac{\gamma}{c}g'(k,R)+B,\\ g'(k,R_+)&=g'(k,R_-)\equiv g'(k,R). \end{aligned} \tag{2.62}$$

Following Ref. 4, two special one-parameter families of s.a.e. have been defined accordingly with the above boundary conditions and the bound state equations read, respectively, for the first and second families,

$$\frac{\beta_{jl}}{c}=\frac{\pm\tilde{T}^{(0)'}_{jl}(\tilde{E},R)\tilde{L}^{(0)'}_{jl}(\tilde{E},R)}{T^{(0)'}_{jl}(\tilde{E},R)L^{(0)'}_{jl}(\tilde{E},R)+A_1},\quad A=\frac{\beta_{jl}}{c}A_1, \tag{2.63}$$

$$\frac{\gamma_{jl}}{c}=\frac{\pm T^{(0)'}_{jl}(\tilde{E},R)L^{(0)'}_{jl}(\tilde{E},R)}{\tilde{T}^{(0)'}_{jl}(\tilde{E},R)\tilde{L}^{(0)'}_{jl}(\tilde{E},R)-B_1},\quad B=\frac{\gamma_{jl}}{c}B_1. \tag{2.64}$$

The generalization to finitely many concentric sphere interactions and to the one-sphere coupled with a Coulomb potential follows the same way as previously and the equations express with the derivatives of the special functions (2.32), (2.45) and (2.46).

2. The δ'-sphere models

The one-sphere model is formally expressed by Eq. (2.49). Here again, the boundary conditions of the second type are obtained from (2.50) and (2.51) by interchanging formally f and f', g and g' with the labels $\tilde{\beta}$ and $\tilde{\gamma}$ instead of β and γ in (2.61) and (2.62), that explicitly writes

$$\begin{aligned} g'(k,R_+)-g'(k,R_-)&=-\frac{\tilde{\beta}}{c}\frac{1}{2}[f(k,R_+)+f(k,R_-)]+\tilde{A},\\ f'(k,R_+)&=f'(k,R_-)\equiv f'(k,R), \end{aligned} \tag{2.65}$$

and

$$f'(k,R_+)-f'(k,R_-)=\frac{\tilde{\gamma}}{c}\frac{1}{2}[g(k,R_+)+g(k,R_-)]-\tilde{B},$$

$$g'(k,R_+)=g'(k,R_-)\equiv g'(k,R), \tag{2.66}$$

where $f(k,r)$ and $g(k,r)$ are as usual the components of the wave function; k, $\tilde{\beta}$, $\tilde{\gamma}$, $\tilde{A}$ and $\tilde{B}$ are nonvanishing constants.

The eigenvalues of the bound states are solutions of the equations

$$\frac{\tilde{\beta}_{jl}}{2c}=\frac{\pm\tilde{T}_{jl}^{(0)'}(\tilde{E},R)\tilde{L}_{jl}^{(0)'}(\tilde{E},R)}{T_{jl}^{(0)'}(\tilde{E},R)L_{jl}^{(0)'}(\tilde{E},R)-2\tilde{A}_1}, \quad \tilde{A}=\frac{\tilde{\beta}_{jl}}{c}\tilde{A}_1, \tag{2.67}$$

$$\frac{\tilde{\gamma}_{jl}}{2c}=\frac{\pm T_{jl}^{(0)'}(\tilde{E},R)L_{jl}^{(0)'}(\tilde{E},R)}{\tilde{T}_{jl}^{(0)'}(\tilde{E},R)\tilde{L}_{jl}^{(0)'}(\tilde{E},R)-2\tilde{B}_1}, \quad \tilde{B}=\frac{\tilde{\gamma}_{jl}}{c}\tilde{B}_1. \tag{2.68}$$

The generalization is now standard and we omit it since the technique is the same.

III. ANALYSIS OF RESONANCE PHENOMENA

A. The δ-sphere models

We deal now with the resonance phenomena for the extended operators. As usual,[15] resonances are defined as poles of the resolvents in the unphysical sheet $\mathrm{Im}\,k'<0$. The resolvent of $h_{jl,\beta_{jl}}$ using the boundary conditions of the second type (2.61) for a one δ-sphere interaction is given by[4]

$$(h_{jl,\beta_{jl}}-k^2)^{-1}=(h_{jl,0}-k^2)^{-1}+\frac{\beta_{jl}/c}{1-(\beta_{jl}/c)F_{jl}^{(0)'}(k,R)G_{jl}^{(0)'}(k,R)} \times\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}(\psi_{jl}(-\overline{k}),.)\psi_{jl}(k); \quad k^2\in\rho(h_{jl,\beta_{jl}}), \quad \mathrm{Im}\,k>0. \tag{3.1}$$

$G_{jl,0}=(h_{jl,0}-k^2)^{-1}$, $\mathrm{Im}\,k>0$, is the free resolvent kernel,

$$G_{jl,0}(k',r,r')=\begin{bmatrix}\tilde{g}_{jl0}^{(I)}(k',r,r') & \tilde{g}_{jl0}^{(I)}(k',r,r')\\ \tilde{g}_{jl0}^{(II)}(k',r,r') & \tilde{g}_{jl0}^{(II)}(k',r,r')\end{bmatrix}, \tag{3.2}$$

where $\tilde{g}_{jl0}^{(I)}(k',r,r')$ and $\tilde{g}_{jl0}^{(II)}(k',r,r')$ were previously defined by (2.24) and (2.25). $\psi_{jl}(k',r)$ is given by

$$\psi_{jl}(k',r)=\begin{pmatrix}F_{jl}^{(0)}(k',r)G_{jl}^{(0)'}(k',R)+F_{jl}^{(0)'}(k',R)G_{jl}^{(0)}(k',r)\\ \tilde{F}_{jl}^{(0)}(k',r)G_{jl}^{(0)'}(k',R)+F_{jl}^{(0)'}(k',R)\tilde{G}_{jl}^{(0)}(k',r)\end{pmatrix}. \tag{3.3}$$

The resonance equation is then

$$1-\frac{\beta_{jl}}{c}F_{jl}^{(0)'}(k',R)G_{jl}^{(0)'}(k',R)=0, \quad \mathrm{Im}\,k'<0, \tag{3.4}$$

i.e.,

$$1-\frac{\beta_{jl}}{c}\left[\frac{d}{dr}F_{jl}^{(0)}(k',r)\right]_{r=R}\times\left[\frac{d}{dr}G_{jl}^{(0)}(k',r)\right]_{r=R}=0, \quad \mathrm{Im}\,k'<0. \tag{3.5}$$

For the boundary conditions of the first type and for the same interaction, we obtain [see the resolvent equation (2.22)]

$$1+\frac{\alpha_{jl}}{c}F_{jl}^{(0)}(k',R)G_{jl}^{(0)}(k',R)=0, \quad \mathrm{Im}\,k'<0, \tag{3.6}$$

that is similar to the result obtained in Ref. 1. In this case, for the poles located on the negative imaginary k' axis, let $k'=-ix$, $x>0$. Then using analytic continuation of Bessel functions, the equation (3.6) transforms as follows:

$$1+\frac{\alpha_{jl}}{c}RI_{K_{jl}+(1/2)}(xR)K_{K_{jl}+(1/2)}(xR)=0. \tag{3.7}$$

Next,[1] using as usual the monotonicity properties of the modified Bessel functions and the bound

$$I_\nu(x)K_\nu(x)\leqslant(2\nu)^{-1}, \quad \nu>0, \quad x\geqslant 0, \tag{3.8}$$

in each partial wave (jl), the equation (3.7) has exactly one solution $x_1>0$ if $(\alpha_{jl}/c)R>-(2K_{jl}+1)$. The case $(\alpha_{jl}/c)R=-(2K_{jl}+1)$ gives a zero energy resonance $x_0=0$.

Let us now investigate the solutions located off the imaginary axis.

To make clear our analysis in this context, let us illustrate our study on the first partial waves corresponding to $j=1/2$, $l=0$ or 1. In the particular case of $j=1/2$ and $l=0$, $K_{jl}=-1$ and the special functions $F_{jl}^{(0)}$ and $G_{jl}^{(0)}$ in (2.26) expressed in terms of Bessel and Hankel functions of index $-1/2$. So, the resonance equation (3.6) becomes

$$1-\frac{i\pi\alpha_0 R}{2c}J_{-1/2}(k'R)H_{-1/2}^{(2)}(k'R)=0, \tag{3.9}$$

that reduces to

$$1-i\frac{\alpha_0}{ck'}\cos(k'R)\exp(-ik'R)=0, \tag{3.10}$$

using[13]

$$J_{-1/2}(k'R)=\sqrt{\frac{2}{\pi k'R}}\cos(k'R), \quad H_{-1/2}^{(2)}(k'R)=\sqrt{\frac{2}{\pi k'R}}\exp(-ik'R).$$

Here, α_0 stands for $\alpha_{jl}\,(j=1/2,\, l=0)$. Setting $k'=y-ix$, $x>0$ and $c=R=1$ for simplicity, we get

$$2y-\alpha_0\exp(-2x)\sin 2y-i[2x+\alpha_0+\alpha_0\exp(-2x)\cos 2y=0], \tag{3.11}$$

that splits into the following system:

$$\begin{aligned} 2y-\alpha_0\exp(-2x)\sin 2y&=0,\\ -2x-\alpha_0-\alpha_0\exp(-2x)\cos 2y&=0, \end{aligned} \tag{3.12}$$

or, equivalently,

$$\begin{aligned} -2x&=\ln\left[\frac{2y}{\alpha_0\sin 2y}\right],\\ \ln\left[\frac{2y}{\alpha_0\sin 2y}\right]-\alpha_0-\frac{2y\cos 2y}{\sin 2y}&=0, \quad 2\alpha_0 y\sin 2y>0. \end{aligned} \tag{3.13}$$

Theorem III.1: *The equation (3.13) has an infinity of solutions. Hence, for the partial waves corresponding to* $jl(j=1/2,\ l=0)$, $h_{jl,\alpha_{jl}}$ *has an infinite number of resonances off the imaginary axis characterized by their energies.*

Proof: To prove the first part of this Theorem, it suffices to show that the function

$$Z(y)=\ln\left[\frac{2y}{\alpha_0\sin 2y}\right]-\alpha_0-\frac{2y\cos 2y}{\sin 2y} \tag{3.14}$$

is continuous and changes signs on each part of its domain. First of all, remark that the function $Z(y)$ is even and, consequently, its graphic representation is symmetric with respect to the Z axis. So, we restrict our analysis to the positive part of the y axis, the whole picture being symmetric with respect to the Z axis for a given α_0. This domain reads as

$$\mathcal{D}_Z=\begin{cases}\cup_{n\in\mathbb{Z}_+}]n\pi,(2n+1)\dfrac{\pi}{2}[, & \forall\,\alpha_0>0, y>0,\\[2ex] \cup_{n\in\mathbb{Z}_+}](2n+1)\dfrac{\pi}{2},(n+1)\pi[, & \forall\,\alpha_0<0, y>0.\end{cases} \tag{3.15}$$

First, let us consider the case $\alpha_0>0$. The continuity property is evident. A straightforward treatment shows that

$$\lim_{\substack{y\to 0\\ y>0}} Z(y)=-\alpha_0-1<0,\quad \lim_{\substack{y\to \pi/2\\ y<\pi/2}} Z(y)=+\infty,\ \ \forall\,\alpha_0>0, \tag{3.16}$$

$$\lim_{\substack{y\to n\pi\\ y>n\pi\\ n\in\mathbb{Z}_+^\star}} Z(y)=-\infty,\qquad \lim_{\substack{y\to (2n+1)\,\pi/2\\ y<(2n+1)\,\pi/2\\ n\in\mathbb{Z}_+^\star}} Z(y)=+\infty,\ \ \forall\,\alpha_0>0. \tag{3.17}$$

A similar analysis can be easily conducted for the case $\alpha_0<0$. We have

$$\lim_{\substack{y\to (2n+1)\,\pi/2\\ y>(2n+1)\,\pi/2\\ n\in\mathbb{Z}_+}} Z(y)=-\infty,\qquad \lim_{\substack{y\to (n+1)\pi\\ y<(n+1)\pi\\ n\in\mathbb{Z}_+}} Z(y)=+\infty,\ \ \forall\,\alpha_0<0. \tag{3.18}$$

Hence, the first part of the Theorem results.

The second part of the Theorem is a consequence of the former. ■

The statements of the Theorem III.1 are well illustrated by numerical explorations. Figures 1(a)–1(d) show the function $Z(y)$ versus y for $\alpha_0>0$. The case $\alpha_0<0$ is represented in Figs. 2(a)–2(d).

The wording of Theorem III.1 can be extended to the general equation (3.6) with the same conclusion on the infinite set of resonances off the imaginary axis for $h_{jl,\alpha_{jl}}$, whatever the partial wave characterized by the quantum numbers j, l and α_{jl}. So doing, the only difficulties one encounters arise from the complexity of mathematical expressions that appear more and more less treatable analytically as the quantum numbers j and l raise. Taking just $j=1/2$ and $l=1$ leads to an intricate nonlinear system in x and y. Numerical computations allow us to go around these difficulties.

The generalization to finitely many δ-sphere interactions using for example the boundary conditions (2.61) provide the following resolvent equation:[5]

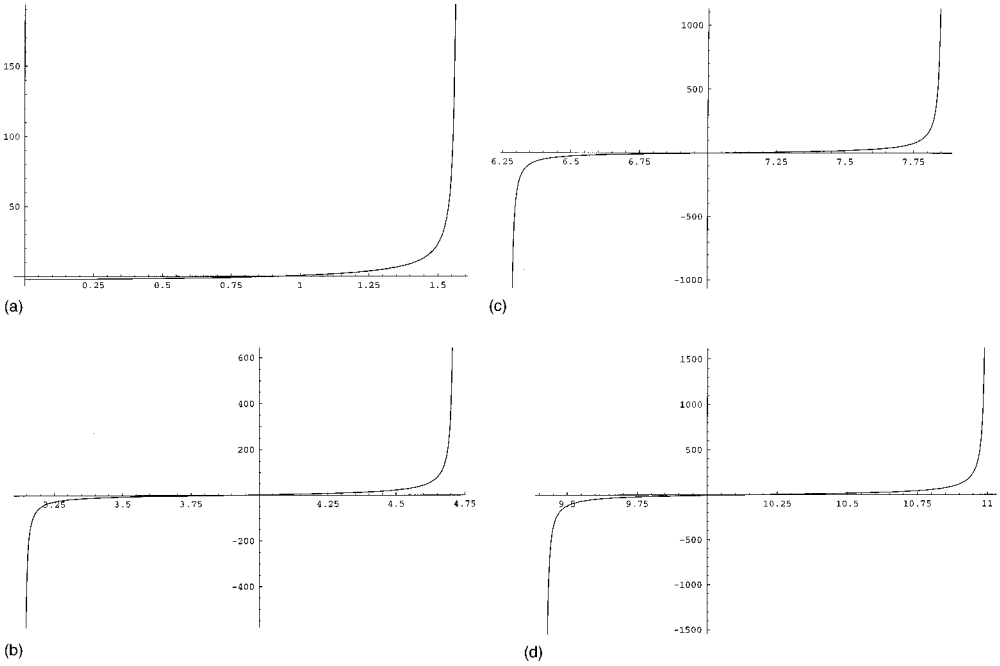

FIG. 1. (a) Curve $Z(y)$ versus $y \in]0,\pi/2[$, $\alpha_0 = 1$. (b) Curve $Z(y)$ versus $y \in]\pi,3\pi/2[$, $\alpha_0 = 1$. (c) Curve $Z(y)$ versus $y \in]2\pi,5\pi/2[$, $\alpha_0 = 1$. (d) Curve $Z(y)$ versus $y \in]3\pi,7\pi/2[$, $\alpha_0 = 1$.

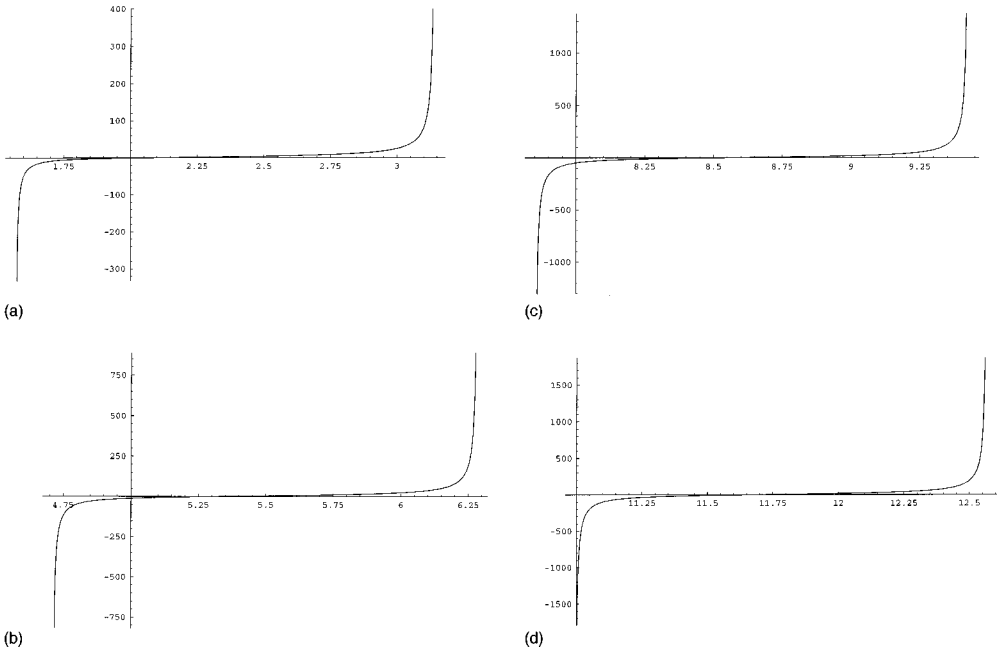

FIG. 2. (a) Curve $Z(y)$ versus $y \in]\pi/2,\pi[$, $\alpha_0 = -1$. (b) Curve $Z(y)$ versus $y \in]3\pi/2,2\pi[$, $\alpha_0 = -1$. (c) Curve $Z(y)$ versus $y \in]5\pi/2,3\pi[$, $\alpha_0 = -1$. (d) Curve $Z(y)$ versus $y \in]7\pi/2,4\pi[$, $\alpha_0 = -1$.

$$(h_{jl,\beta_{jl}\{R\}}-k^2)^{-1}=(h_{jlo}-k^2)^{-1}+\sum_{m,m'=1}^{N}\kappa_{jl}^{mm'}(k)(\psi_{jl}^{(m)}(-\overline{k}),.)\psi_{jl}^{(m')}(k),$$
$$k^2\in\rho(h_{jl,\beta_{jl}\{R\}});\quad \mathrm{Im}\,k>0, \tag{3.19}$$

with

$$\kappa_{jl}^{mm'}(k)=\frac{\beta_{jl}^{m}/c}{\delta_{mm'}-(\beta_{jl}^{m}/c)\tilde{g}_{jl}^{(I)'}(k,R_m,R_{m'})}\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \delta_{mm'}=\begin{cases}0; & m\neq m',\\ 1; & m=m',\end{cases}$$

$$\psi_{jl}^{(m)}(k)=\begin{pmatrix}F_{jl}^{(o)}(k,r)G_{jl}^{(o)'}(k,R_m)+F_{jl}^{(o)'}(k,R_m)G_{jl}^{(o)}(k,r)\\ \tilde{F}_{jl}^{(o)}(k,r)G_{jl}^{(o)'}(k,R_m)+F_{jl}^{(o)'}(k,R_m)\tilde{G}_{jl}^{(o)}(k,r)\end{pmatrix}, \tag{3.20}$$

$$\tilde{g}_{jl}^{(I)'}(k,R_m,R_{m'})=F_{jl}^{(o)'}(k,R_m)G_{jl}^{(o)'}(k,R'_m).$$

For this model, the resonance phenomena could be more complicated, mixing the resonances of a specific sphere with the resonance arising from the whole system.

Concerning the Dirac–Coulomb case, Krein's formula provides us with the following resolvent equation:

$$(h_{jl\gamma_0,\alpha_{jl}}-k^2)^{-1}=(h_{jl\gamma_0,0}-k^2)^{-1}-\frac{\alpha_{jl}}{cD}\begin{pmatrix}1&0\\0&1\end{pmatrix}(\psi_{jl\gamma_0}(-\overline{k}),.)\psi_{jl\gamma_0}(k); \tag{3.21}$$

$$k^2\in\rho(h_{jl\gamma_0,\alpha_{jl}}),\quad \mathrm{Im}\,k>0,$$

$$D=F_{jl\gamma_0}^{(0)}(k',R)\tilde{G}_{jl\gamma_0}^{(0)}(k',R)-\tilde{F}_{jl\gamma_0}^{(0)}(k',R)G_{jl\gamma_0}^{(0)}(k',R)+\frac{\alpha_{jl}}{c}F_{jl\gamma_0}^{(0)}(k',R)G_{jl\gamma_0}^{(0)}(k',R), \tag{3.22}$$

$G_{jl\gamma_0}=(h_{jl\gamma_0,0}-k^2)^{-1}$, $\mathrm{Im}\,k>0$, is the free resolvent kernel:

$$G_{jl\gamma_0}(k',r,r')=\begin{bmatrix}\tilde{g}_{jl\gamma_0}^{(I)}(k',r,r') & \tilde{g}_{jl\gamma_0}^{(I)}(k',r,r')\\ \tilde{g}_{jl\gamma_0}^{(II)}(k',r,r') & \tilde{g}_{jl\gamma_0}^{(II)}(k',r,r')\end{bmatrix}, \tag{3.23}$$

where

$$\tilde{g}_{jl\gamma_0}^{(I)}(k',r,r')=\begin{cases}G_{jl\gamma_0}^{(0)}(k',r)F_{jl\gamma_0}^{(0)}(k',r'); & r'<r,\\ F_{jl\gamma_0}^{(0)}(k',r)G_{jl\gamma_0}^{(0)}(k',r'); & r'>r,\end{cases} \tag{3.24}$$

and

$$\tilde{g}_{jl0}^{(II)}(k',r,r')=\begin{cases}\tilde{G}_{jl\gamma_0}^{(0)}(k',r)\tilde{F}_{jl\gamma_0}^{(0)}(k',r'); & r'<r,\\ \tilde{F}_{jl\gamma_0}^{(0)}(k',r)\tilde{G}_{jl\gamma_0}^{(0)}(k',r'); & r'>r,\end{cases} \tag{3.25}$$

with

$$F_{jl\gamma_0}^{(0)}(k',r)=\frac{\gamma_0}{2\epsilon(K_{jl}-\epsilon)}u_1-\frac{1}{2\epsilon}v_1;\quad r<R,$$

$$G^{(0)}_{jl\gamma_0}(k',r)=\frac{\gamma_0}{2\epsilon(K_{jl}-\epsilon)}u_2-\frac{1}{2\epsilon}v_2;\quad r>R, \tag{3.26}$$

$$\tilde{F}^{(0)}_{jl\gamma_0}(k',r)=-\frac{1}{2\epsilon}u_1+\frac{\gamma_0}{2\epsilon(K_{jl}-\epsilon)}v_1;\quad r<R,$$

$$\tilde{G}^{(0)}_{jl\gamma_0}(k',r)=-\frac{1}{2\epsilon}u_2+\frac{\gamma_0}{2\epsilon(K_{jl}-\epsilon)}v_2;\quad r>R, \tag{3.27}$$

and

$$u_1(k',r)=r^{\mu+1}\exp(-ik'r)\,{}_1F_1\left(1+\mu-i\frac{k^2\gamma_0}{c^2k'};2(\mu+1);2ik'r\right),$$

$$u_2(k',r)=\Gamma[2(\mu+1)]^{-1}\Gamma\left[\left(1+\mu-i\frac{k^2\gamma_0}{c^2k'}\right)\right](2ik')^{2\mu+1}r^{\mu+1}\exp(-ik'r) \tag{3.28}$$

$$\times U\left(1+\mu-i\frac{k^2\gamma_0}{c^2k'};2(\mu+1);2ik'r\right),$$

$$v_1(k',r)=r^{\mu}\exp(-ik'r)\,{}_1F_1\left(\mu-i\frac{k^2\gamma_0}{c^2k'};2\mu;2ik'r\right), \tag{3.29}$$

$$v_2(k',r)=\Gamma(2\mu)^{-1}\Gamma\left(\mu-i\frac{k^2\gamma_0}{c^2k'}\right)(2ik')^{2\mu-1}r^{\mu}\exp(-ik'r)U\left(\mu-i\frac{k^2\gamma_0}{c^2k'};2\mu;2ik'r\right),$$

where $k'^2=(k^4-M^2c^4)/c^2$, $\epsilon=\sqrt{c^2K_{jl}^2-\gamma_0^2}$, $\mu=\epsilon/c=\sqrt{K_{jl}^2-(\gamma_0/c)^2}$, ${}_1F_1(z)$ and $U(z)$ are the hypergeometric functions of the first and second type, respectively.

$\psi_{jl\gamma_0}(k',r)$ is given by

$$\psi_{jl\gamma_0}(k',r)=\begin{pmatrix} F^{(0)}_{jl\gamma_0}(k',r)G^{(0)}_{jl\gamma_0}(k',R)+F^{(0)}_{jl\gamma_0}(k',R)G^{(0)}_{jl\gamma_0}(k',r)\\ \tilde{F}^{(0)}_{jl\gamma_0}(k',r)G^{(0)}_{jl\gamma_0}(k',R)+F^{(0)}_{jl\gamma_0}(k',R)\tilde{G}^{(0)}_{jl\gamma_0}(k',r)\end{pmatrix}. \tag{3.30}$$

The resonance equation is then

$$F^{(0)}_{jl\gamma_0}(k',R)\tilde{G}^{(0)}_{jl\gamma_0}(k',R)-\tilde{F}^{(0)}_{jl\gamma_0}(k',R)G^{(0)}_{jl\gamma_0}(k',R)+\frac{\alpha_{jl}}{c}F^{(0)}_{jl\gamma_0}(k',R)G^{(0)}_{jl\gamma_0}(k',R)=0,\ \ \mathrm{Im}\,k'<0. \tag{3.31}$$

Using the boundary conditions of the second type the resonances could be obtained from the resolvent equation computed in Ref. 4. We have

$$F^{(0)'}_{jl\gamma_0}(k',R)\tilde{G}^{(0)'}_{jl\gamma_0}(k',R)-\tilde{F}^{(0)'}_{jl\gamma_0}(k',R)G^{(0)'}_{jl\gamma_0}(k',R)-\frac{\beta_{jl}}{c}F^{(0)'}_{jl\gamma_0}(k',R)G^{(0)'}_{jl\gamma_0}(k',R)=0,\ \ \mathrm{Im}\,k'<0. \tag{3.32}$$

A systematic study of this model can be conducted using the same machinery. The physics being the same, the only difficulties are of a technical order related to the mathematical expressions that present here a more complicated form.

B. The δ' models

We analyze the one-sphere case, its generalization to finitely many concentric spheres and the δ'-Coulomb case with the boundary conditions of the second type.

The resolvent of the δ'-sphere model is[6]

$$(h_{jl,\tilde{\beta}_{jl}\{R\}}-k^2)^{-1}=(h_{jlo}-k^2)^{-1}+\Theta_{jl}(k)(\psi_{jl}(-\overline{k}),.)\psi_{jl}^{(\Delta)}(k),$$

$$k^2\in\rho(h_{jl,\tilde{\beta}_{jl}});\ \ \mathrm{Im}\,k>0, \tag{3.33}$$

with

$$\Theta_{jl}(k')=\frac{-2(\tilde{\beta}_{jl}/c)}{2+(\tilde{\beta}_{jl}/c)g'_{jl}(k',R,R)}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \tag{3.34}$$

$$\psi_{jl}(k')=\begin{pmatrix}F_{jl}^{(o)}(k',r)G_{jl}^{(o)}(k',R)+F_{jl}^{(o)}(k',R)G_{jl}^{(o)}(k',r)\\ \tilde{F}_{jl}^{(o)}(k',r)G_{jl}^{(o)}(k',R)+F_{jl}^{(o)}(k',R)\tilde{G}_{jl}^{(o)}(k',r)\end{pmatrix}, \tag{3.35}$$

$$\psi_{jl}^{(\Delta)}(k')=\begin{pmatrix}F_{jl}^{(o)}(k',r)G_{jl}^{(o)'}(k',R)+F_{jl}^{(o)'}(k',R)G_{jl}^{(o)}(k',r)\\ \tilde{F}_{jl}^{(o)}(k',r)G_{jl}^{(o)'}(k',R)+F_{jl}^{(o)'}(k',R)\tilde{G}_{jl}^{(o)}(k',r)\end{pmatrix}, \tag{3.36}$$

$$g'_{jl}(k',R,R)=F_{jl}^{(o)}(k',R)G_{jl}^{(o)'}(k',R)+G_{jl}^{(o)}(k',R)F_{jl}^{(o)'}(k',R)=\frac{d}{dr}[F_{jl}^{(o)}(k',r)G_{jl}^{(o)}(k',r)]_{r=R}. \tag{3.37}$$

The resulting resonance energies are given by

$$2+\frac{\tilde{\beta}_{jl}}{c}g'_{jl}(k',R,R)=0,\ \ \mathrm{Im}\,k'<0. \tag{3.38}$$

Setting $k'=-ix$, this equation transforms as follows:

$$-\frac{2c}{\tilde{\beta}_{jl}}=\frac{d}{dr}[rI_{K_{jl}+1/2}(xr)K_{K_{jl}+1/2}(xr)]_{r=R}. \tag{3.39}$$

In each partial wave (jl), the Eq. (3.39) has one solution $x>0$ if $\tilde{\beta}_{jl}/c<2(2K_{jl}+1)$. The case $\tilde{\beta}_{jl}/c=2(2K_{jl}+1)$ gives a zero energy resonance, i.e., $x_0=0$ and there is an infinite number of resonances off the imaginary axis.

The generalization to finitely many spheres cases is immediate.

Concerning the δ'-Coulomb case, the resolvent is[6]

$$(h_{jl\gamma_0,\tilde{\beta}_{jl}}-k^2)^{-1}=(h_{jl\gamma_0,0}-k^2)^{-1}+-2\frac{\tilde{\beta}_{jl}}{cD}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}(\psi_{jl\gamma_0}(-\overline{k}),.)\psi_{jl\gamma_0}^{(\triangle)}(k); \tag{3.40}$$

$$k^2\in\rho(h_{jl\gamma_0,\tilde{\beta}_{jl}}),\ \ \mathrm{Im}\,k>0,$$

$$D=2[F_{jl\gamma_0}^{(0)'}(k',R)\tilde{G}_{jl\gamma_0}^{(0)'}(k',R)-\tilde{F}_{jl\gamma_0}^{(0)'}(k',R)G_{jl\gamma_0}^{(0)'}(k',R)]$$

$$+\frac{\tilde{\beta}_{jl}}{c}[F_{jl\gamma_0}^{(0)'}(k',R)G_{jl\gamma_0}^{(0)}(k',R)+F_{jl\gamma_0}^{(0)}(k',R)G_{jl\gamma_0}^{(0)'}(k',R)]. \tag{3.41}$$

The following equation gives the resonance energies:

$$0=2[F^{(0)'}_{jl\gamma_0}(k',R)\tilde{G}^{(0)'}_{jl\gamma_0}(k',R)-\tilde{F}^{(0)'}_{jl\gamma_0}(k',R)G^{(0)'}_{jl\gamma_0}(k',R)]$$

$$+\frac{\tilde{\beta}_{jl}}{c}[F^{(0)'}_{jl\gamma_0}(k',R)G^{(0)}_{jl\gamma_0}(k',R)+F^{(0)}_{jl\gamma_0}(k',R)G^{(0)'}_{jl\gamma_0}(k',R)],\quad \mathrm{Im}\,k'<0. \tag{3.42}$$

IV. FINAL REMARKS

Our results are very similar to those obtained with singular Schrödinger Hamiltonians[1] for the same interactions; the only difference lies in the interchanging between the free Schrödinger Hamiltonian $H_0=-\Delta$ and the free Dirac one H_{D}.

Moreover, as in the nonrelativistic case where the results for δ-sphere and δ-point interactions are similar,[1,8] the results of our study compared with those obtained for point interactions in relativistic quantum mechanics studied by Gesztesy and Šeba are the same.[4,16] That is the most interesting information we get from this study. This is predictable since it has been shown that the δ-sphere interaction H_α converges to the δ-point interaction H_η of strength η centered at the origin, as the radius of the sphere shrinks to zero with adequate normalization of the coupling constant α (Ref. 1, Lemma 2.2). The results concerning a systematic study of δ- and δ'-point interactions including the scattering theory in relativistic quantum mechanics is thus predictable.

Let us now discuss briefly the nonrelativistic limit $c\to\infty$. Following Ref. 14 (Chap. V, Sec. 25, 3), the spinors

$$\psi(k,r)=\begin{pmatrix} f(k,r)\\ g(k,r)\end{pmatrix},$$

the solution of the indicial equation $\dot{h}_{jl}\psi=k^2\psi$, $\mathrm{Im}\,k>0$, reduce to $f(k,r)$ as $c\to\infty$, i.e., $|g(k,r)|\ll|f(k,r)|$. This latter coincides exactly with the special functions which span the deficiency subspace in the Schrödinger case with respect to the same normalization. On the other hand, the strategy used in Ref. 16 and the references therein for point interactions using the resolvents to discuss the nonrelativistic limit applies here since the results are the same.

Finally, let us point out the fact (so far implicit) that the Hamiltonians perturbed by singular δ and δ' interactions are in fact local interactions both in nonrelativistic and relativistic mechanics. This gives us some additional information on the domains of the radial extended Hamiltonians.

Using the resolvent equation, the proof is easy. The δ- and δ'-sphere interactions in nonrelativistic quantum mechanics are treated in Refs. 1, 17. For the relativistic case, we restrict our study with an explicit proof to the δ- and δ'-sphere models using the boundary conditions of the second type, by stating the following Theorem.

Theorem IV.1: *For $\psi_{jl,o}(k,r)$ belonging to $\mathcal{D}(h_{jl,o})$ which is the domain of the free radial Dirac Hamiltonian, the domain $\mathcal{D}(h_{jl,\beta_{jl}})$ of the extended radial operator consists of spinors of the type*

$$\psi_{jl,\beta_{jl}}(k,r)=\psi_{jl,o}(k,r)+K(k,R)\begin{pmatrix}1&0\\0&1\end{pmatrix}\Phi_{jl}(k,r,R), \tag{4.1}$$

with

$$K(k,R)=\frac{(\beta_{jl}/c)[F^{(o)'}_{jl}(k,R)+A_1]}{1-(\beta_{jl}/c)F^{(o)'}_{jl}(k,R)G^{(o)'}_{jl}(k,R)}, \tag{4.2}$$

$$A_1 = G_{jl}^{(o)'}(k',R)\int_0^R [\tilde{F}_{jl}^{(o)}(k',r') - F_{jl}^{(o)}(k',r')]\tilde{F}_{jl}^{(o)}(k',r')dr'$$

$$+ F_{jl}^{(o)'}(k',R)\int_R^\infty [\tilde{G}_{jl}^{(o)}(k',r') - G_{jl}^{(o)}(k',r')]\tilde{G}_{jl}^{(o)}(k',r')dr', \tag{4.3}$$

$$\Phi_{jl}(k,r,R) = \begin{pmatrix} F_{jl}^{(o)}(k,r)G_{jl}^{(o)'}(k,R) + F_{jl}^{(o)'}(k,R)G_{jl}^{(o)}(k,r) \\ \tilde{F}_{jl}^{(o)}(k,r)G_{jl}^{(o)'}(k,R) + F_{jl}^{(o)'}(k,R)\tilde{G}_{jl}^{(o)}(k,r) \end{pmatrix}, \tag{4.4}$$

$k^2 \in \rho(h_{jl,\beta_{jl}})$, $\rho(\cdot)$ *is the resolvent set.*

Furthermore, the decomposition (4.1) is unique and we are allowed to write

$$(h_{jl,\beta_{jl}} - k^2)^{-1}\psi_{jl,\beta_{jl}}(k,r) = (h_{jl,o} - k^2)^{-1}\psi_{jl,o}(k,r). \tag{4.5}$$

Besides, if $\psi_{jl,\beta_{jl}}(k,r) \in \mathcal{D}(h_{jl,\beta_{jl}})$ *and* $\psi_{jl,\beta_{jl}} = 0$ *in an open subset of* $(0,\infty)$, *then* $h_{jl,\beta_{jl}}\psi_{jl,\beta_{jl}} = 0$ *in this subset.*

Proof: One may follow step by step Ref. 8, where a similar result has been obtained for point interactions. However, using the resolvent equation we can show how (4.1) is obtained.
We know that

$$(h_{jl,o} - k^2)^{-1}: \; L^2((0,\infty)) \otimes \mathbb{C}^2 \to \mathcal{D}(h_{jl,o}),$$

$$(h_{jl,\beta_{jl}} - k^2)^{-1}: \; L^2((0,\infty)) \otimes \mathbb{C}^2 \to \mathcal{D}(h_{jl,\beta_{jl}})$$

and

$$\mathcal{D}(h_{jl,\beta_{jl}}) = (h_{jl,\beta_{jl}} - k^2)^{-1}(h_{jl,o} - k^2)\mathcal{D}(h_{jl,o}). \tag{4.6}$$

Then for

$$\psi_{jl,o}(k,r) = \begin{pmatrix} F_{jl}^{(o)}(k,r) \\ \tilde{F}_{jl}^{(o)}(k,r) \end{pmatrix} \in \mathcal{D}(h_{jl,o}),$$

we have

$$\psi_{jl,\beta_{jl}}(k,r) = (h_{jl,\beta_{jl}} - k^2)^{-1}(h_{jl,o} - k^2)\psi_{jl,o}(k,r); \quad \psi_{jl,\beta_{jl}}(k,r) \in \mathcal{D}(h_{jl,\beta_{jl}}). \tag{4.7}$$

Inserting the resolvent equation (3.1) into (4.7), we obtain

$$\psi_{jl,\beta_{jl}}(k,r) = \begin{pmatrix} F_{jl}^{(o)}(k,r) \\ \tilde{F}_{jl}^{(o)}(k,r) \end{pmatrix} + \begin{pmatrix} K & 0 \\ 0 & K \end{pmatrix} \begin{pmatrix} F_{jl}^{(o)}(k,r)G_{jl}^{(o)'}(k,R) + F_{jl}^{(o)'}(k,R)G_{jl}^{(o)}(k,r) \\ \tilde{F}_{jl}^{(o)}(k,r)G_{jl}^{(o)'}(k,R) + F_{jl}^{(o)'}(k,R)\tilde{G}_{jl}^{(o)}(k,r) \end{pmatrix}. \tag{4.8}$$

The implementation of the boundary conditions (2.61) gives the value of the coefficient K. Thus (4.1) results. ■

Turning to the δ'-sphere case and using (3.33), the elements of the first family of s.a.e. satisfy the following decomposition:

$$\psi_{jl,\tilde{\beta}_{jl}}(k,r) = \psi_{jl,o}(k,r) + \tilde{K}(k,R)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\Phi_{jl}(k,r,R), \tag{4.9}$$

with

$$\tilde{K}(k,R)=\frac{-2(\tilde{\beta}_{jl}/c)[F_{jl}^{(o)\prime}(k,R)+A_1]}{2+(\tilde{\beta}_{jl}/c)[F_{jl}^{(o)}(k,R)G_{jl}^{(o)\prime}(k,R)+F_{jl}^{(o)\prime}(k,R)G_{jl}^{(o)}(k,R)]}, \tag{4.10}$$

$$A_1=G_{jl}^{(o)\prime}(k',R)\int_0^R[F_{jl}^{(o)}(k',r')-\tilde{F}_{jl}^{(o)}(k',r')]\tilde{F}_{jl}^{(o)}(k',r')dr'$$

$$+F_{jl}^{(o)\prime}(k',R)\int_R^\infty[G_{jl}^{(o)}(k',r')-\tilde{G}_{jl}^{(o)}(k',r')]\tilde{G}_{jl}^{(o)}(k',r')dr', \tag{4.11}$$

$$\Phi_{jl}(k,r,R)=\begin{pmatrix} F_{jl}^{(o)}(k,r)G_{jl}^{(o)\prime}(k,R)+F_{jl}^{(o)\prime}(k,R)G_{jl}^{(o)}(k,r) \\ \tilde{F}_{jl}^{(o)}(k,r)G_{jl}^{(o)\prime}(k,R)+F_{jl}^{(o)\prime}(k,R)\tilde{G}_{jl}^{(o)}(k,r)\end{pmatrix}, \tag{4.12}$$

$k^2\in\rho(h_{jl,\tilde{\beta}_{jl}})$. (4.9) is also unique and if $\psi_{jl,\tilde{\beta}_{jl}}\in\mathcal{D}(h_{jl,\tilde{\beta}_{jl}})$ and $\psi_{jl,\tilde{\beta}_{jl}}=0$ in an open set $\mathcal{O}\subset(0,\infty)$, then $h_{jl,\tilde{\beta}_{jl}}\psi_{jl,\tilde{\beta}_{jl}}=0$ in $\mathcal{O}$ which means that the δ'-sphere interaction is a local interaction in relativistic quantum mechanics.

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Fast-convergent resummation algorithm and critical exponents of ϕ^4-theory in three dimensions

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We develop an efficient algorithm for evaluating divergent perturbation expansions of field theories in the bare coupling constant g_B for which we possess a finite number L of expansion coefficients plus two more information: the knowledge of the large-order behavior proportional to $(-\alpha)^k k! k^\beta g_B^k$, with a known growth parameter α, and the knowledge of the approach to scaling of the type $c+c'/g_B^\omega$, with constants c,c' and a critical exponent of approach ω. The latter information leads to an increase in the speed of convergence and a high accuracy of the results. The algorithm is applied to the six- and seven-loop expansions for the critical exponents of $O(N)$-symmetric ϕ^4-theories, and the result for the critical exponent α is compared with a recent satellite experiment. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1289377]

I. INTRODUCTION

The field-theoretic approach to critical phenomena provides us with power series expansions for the critical exponents of a wide variety of universality classes. For ϕ^4-theories with $O(N)$ symmetry in three dimensions, these expansions have been calculated numerically as power series in the renormalized coupling constant up to seven loops for[1] the critical exponents ν and η and up to six loops for the exponent ω governing the approach to scaling. In 4-ϵ dimensions, exact ϵ-expansions are available up to five loops for all critical exponents with $O(N)$ symmetry,[2] cubic symmetry, and mixtures of these.[3] When inserted into the renormalization group equations, these expansions are supposed to determine the critical exponents via their values at an infrared-stable fixed point $g=g^*$. The latter step is nontrivial since the expansions are divergent and require resummation, for which sophisticated methods have been developed, summarized and applied most recently in Ref. 4. The resummation methods use the information from the known large-order behavior $(-\alpha)^k k! k^\beta g_B^k$ of the expansions and analytic mapping techniques to obtain quite accurate results.

A completely different resummation procedure was developed recently on the basis of variational perturbation theory[5] to the expansions in powers of the *bare coupling constant*, which goes to infinity at the critical point. The resulting *strong-coupling theory*[6] was successfully applied in three[8,9] and $4-\epsilon$ dimensions,[10] and rendered for the first time an interpolation between expansions of $4-\epsilon$ and $2+\epsilon$-dimensional theories. This method converges as fast as the previous ones, even though it does not take into account the information on the large-order behavior of the expansions. Instead, it uses the fact that the power series for the critical exponents approach their constant critical value in the form $c+c'/g_B^\omega$, where c,c' are constants, and ω is the critical exponent of the approach to scaling. The results show that the latter information is just as efficient in increasing the speed of convergence as the information on the large-order behavior.

We may therefore expect that a resummation method which incorporates both informations should lead to results with an even higher accuracy, and it is the purpose of this paper to present such a method in the form of a simple algorithm.

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II. STRONG-COUPLING

The development of our resummation algorithm is based on an improvement of the problem formulated in Refs. 6 and 7 and solved via variational perturbation theory.[5] Mathematically, the problem we want to solve is the following: Let

$$f_L(g_B)=\sum_{k=0}^{L} f_k g_B^k \tag{1}$$

be the first L terms of a divergent asymptotic expansion

$$f(g_B)=\sum_{k=0}^{\infty} f_k g_B^k \tag{2}$$

of a function $f(g_B)$, which possesses a strong-coupling expansion of the type

$$f(g_B)=g_B^s\sum_{k=0}^{\infty} b_k g_B^{-k\omega}, \tag{3}$$

which is assumed to have some finite convergence radius $|g_B|\geqslant g_B^{\mathrm{conv}}$. Suppose that the function is analytic in the complex g_B-plane with a cut along the negative real axis, with a discontinuity known from instanton calculations[11,12] to have near the tip of the cut the generic form

$$\mathrm{disc}\, f(-g_B)\equiv 2\pi i\ \gamma\,(\alpha|g_B|)^{-\beta-1}e^{-1/\alpha|g_B|}. \tag{4}$$

Via a dispersion relation,

$$f(g_B)=\frac{1}{2\pi i}\int_0^{\infty} dg_B'\,\frac{\mathrm{disc}\, f(-g_B)}{g_B'+g_B}, \tag{5}$$

or a sufficiently subtracted version of it, this discontinuity corresponds to the large-order behavior of the expansion coefficients f_k

$$f_k \overset{k\to\infty}{=} \gamma k!(-\alpha)^k k^{\beta}[1+\mathcal{O}(1/k)]. \tag{6}$$

The constant α is given by the inverse action of the radially symmetric solution to the classical field equations. The parameter β counts the number of zero modes in the fluctuation determinant around this solution. The absolute normalization γ of the large-order behavior requires the calculation of the fluctuation determinant.[11]

As far as the leading strong-coupling coefficient b_0 is concerned, this problem has been attacked before by Parisi[13] using a resummation method based on Borel transformations in combination with analytic mapping techniques. However, when applied to the asymptotic expansions of the ground state energy of the anharmonic oscillator, his method converges very slowly, too slow to lead to reliable critical exponents, where only five to seven expansion coefficients f_k known. The reason is that in Parisi's approach, the corrections to the leading power behavior fail to match the true irrational powers of the strong-coupling expansion (3).

This deficiency was cured by the strong-coupling theory of one of the authors (H.K.) in Ref. 6, and the subsequent application to critical exponents in Refs. 8, 9, and 10, which showed a surprisingly rapid convergence. However, that theory did not take advantage of the knowledge of the large-order behavior (6), which can lead to an increase in the speed of convergence and thus of the accuracy of theoretical values for the critical exponents. This will be achieved in the present improved resummation method.

III. BOREL METHODS

Basis for this method is the development of a more general Borel-type transformation which will automatically guarantee the form of the strong-coupling expansion (3) for each approximant $f_L(g_B)$. Let us first recall briefly the important properties of an ordinary Borel transformation: it is a function $B(t)$ associated with $f(g_B)$ which is defined by the Taylor series

$$B(t)=\sum_{k=0}^{\infty} B_k t^k \equiv \sum_{k=0}^{\infty} \frac{f_k}{k!} t^k. \tag{7}$$

By dividing the expansion coefficients f_k by $k!$, the factorial growth of f_k is reduced to a power growth, thus giving $B(t)$ a finite convergence radius.

An alternative definition of the Borel transform is given by the contour integral

$$B(t)\equiv \frac{1}{2\pi i} \oint_C \frac{dz}{z} e^z f(t/z), \tag{8}$$

where the contour C encloses anticlockwise the negative real axis. Indeed, inserting (1) and performing the integral we obtain (7).

If $f(g_B)$ is an analytic function in the sector

$$S^R_{\pi/2+\delta} \equiv \{g_B \mid |g_B|<R, |\arg(g_B)|<\pi/2+\delta\} \tag{9}$$

of a circle, and satisfies the so-called strong asymptotic condition

$$\left| f(g_B) - \sum_{k=0}^{L} f_k g_B^k \right| < A g_B^{L+1} \alpha^{L+1} (L+1)! \quad \text{with} \quad \alpha, A>0, \tag{10}$$

then $B(t)$ is analytic in S^{∞}_{δ}, with a finite radius of convergence $t<1/\alpha$. The original function $f(g_B)$ can be recovered from $B(t)$ by the inverse Borel transformation

$$f(g_B)=\int_0^{\infty} e^{-t} B(t g_B) dt. \tag{11}$$

Obviously, the inverse transformation can only be performed if $B(t)$ is known on the entire positive real t-axis. The Taylor series (7) for $B(t)$, however, converges only inside the circle of radius $1/\alpha$. Before we can do the integral in (11), we must therefore perform a suitable analytic continuation of (7).[14] This can be done by re-expanding $B(t)$ in powers of the function $\kappa(t)$ defined implicitly by

$$t=\frac{1}{\sigma} \frac{\kappa(t)}{[1-\kappa(t)]^p}. \tag{12}$$

This function maps the interval $[0,\infty]$ of the t-axis to the interval $[0,1]$ of the κ-plane. By a proper choice of σ it is possible to make the unit circle free of singularities. Then we may use the re-expansion $B(t)$ in powers of $\kappa(t)$ truncated after κ^L,

$$B_L(t)\equiv \sum_{k=0}^{L} v_k \kappa^k(t), \tag{13}$$

as an approximation to $B_L(t)$ on the entire positive real t axis. Inserting this into the inverse transformation formula (11), we obtain an approximation $f^a_L(g_B)$ for $f(g_B)$, which has the same first L expansion coefficients as $f_L(g_B)$ and, in addition, the correct large-order behavior (6).

How can we incorporate the strong-coupling expansion (3) of $f(g_B)$ into the approximation $f_L^a(g_B)$? In the Borel transform $B(t)$, the strong-coupling expansion (3) amounts to a large-t expansion

$$B(t)=t^s\sum_{k=0}^{\infty}\frac{\sin\pi(k\omega-s)}{\pi}\Gamma(k\omega-s)b_k t^{-k\omega}. \tag{14}$$

This follows directly by inserting (3) into (8) and integrating each term. Here and in the sequel, C denotes a path of integration which encloses anticlockwise the negative real axis in the complex plane.

If the series (3) has a finite radius of convergence, the large-t expansion of $B(t)$ is a divergent asymptotic one, because of the factor $\Gamma(k\omega-s)$ in the kth expansion coefficient.

It should be stressed, that the relation between the coefficients of the strong-coupling expansion (3) and the coefficients of expansion (14) is not generally invertible, because of the factor $\sin\pi(k\omega-s)$ which causes the coefficients of negative integer powers of t to vanish.

Note that, in general, an expansion in the Borel-plane with a power sequence in t as in (14) is not sufficient to ensure an expansion in the same powers in the g_B-plane as in (3), because of the appearance of extra integer powers in g_B. This is illustrated by the simple function $B(t)=(1+t)^s$, which possesses a strong-coupling expansion in the powers t^{s-k}. If s is noninteger the expansion of the corresponding function $f(g_B)$ reads

$$f(g_B)=\int_0^{\infty}dt\,e^{-t}(1+g_B t)^s=e^{1/g_B}\Gamma(s+1)g_B^s+e^{1/g_B}\sum_{k=0}^{\infty}\frac{(-1)^k}{(k+s+1)k!}g_B^{-k-1}, \tag{15}$$

and expanding the exponential we see that the sum contains integer powers which are not contained in the strong-coupling expansion of $B(t)$.

It is advantageous to perform a further analytic continuation of the re-expansion (13) which enforces automatically the leading power behavior t^s of $B(t)$. For this we change (13) to

$$B_L(t)\equiv[1-\kappa(t)]^{-ps}\sum_{k=0}^{L}h_k\kappa^k(t). \tag{16}$$

The coefficients h_k are determined by using (12) to expand $\kappa(t)$ in powers of t, inserting this into (16), re-expanding in powers of t, and comparing the final coefficients with those in (7). When the approximation (16) is inserted into (11), we obtain $f_L^a(g_B)$ with the correct leading power behavior g_B^s for large g_B.

Unfortunately, the simple prefactor does not produce the correct subleading powers $(g_B)^{s-k\omega}$ of the strong-coupling expansion (3), and we have not been able to find another simple analytic continuation of $B(t)$ which would achieve this.

IV. HYPER-BOREL TRANSFORMATION

A solution of this problem is, however, possible with the help of a generalization of the Borel–Leroy transformation to what we shall call a *hyper-Borel transformation*[15]

$$\tilde{B}(y)=\sum_{k=0}^{\infty}\tilde{B}_k y^k, \tag{17}$$

with coefficients

$$\tilde{B}_k\equiv\omega\frac{\Gamma(k(1/\omega-1)+\beta_0)}{\Gamma(k/\omega-s/\omega)\Gamma(\beta_0)}f_k. \tag{18}$$

A. General properties

The inverse transformation is given by the double integral

$$f(g_B)=\frac{\Gamma(\beta_0)}{2\pi i}\oint_C dt\, e^t t^{-\beta_0}\int_0^\infty \frac{dy}{y}\left[\frac{g_B}{yt^{(1-\omega)/\omega}}\right]^s \exp\left[\frac{yt^{(1-\omega)/\omega}}{g_B}\right]^\omega \tilde{B}(y), \tag{19}$$

as can easily be shown with the help of the integral representation of the inverse Gamma function

$$\frac{1}{\Gamma(z)}=\frac{1}{2\pi i}\int_C dt\, e^t t^{-z}. \tag{20}$$

The transformation possesses a free parameter β_0 which will be used to optimize the approximation $f_L(g_B)$ at each order L. The power ω of the strong-coupling expansion is assumed to lie in the interval $0<\omega<1$, as it does in the upcoming physical applications.

The hyper-Borel transformation has the desired property of allowing for a resummation of $f_L(g_B)$ with the full sequence of powers of g_B in the strong-coupling expansion (3). To show this we first observe that as in the ordinary Borel transform (7), the large-argument behavior of the gamma function known from Stirling's formula

$$\Gamma(pk+q)\overset{k\to\infty}{=}\sqrt{2\pi}^{1-p}p^{q-1/2}k^{-1/2+q-p/2}p^{pk}(k!)^p[1+\mathcal{O}(1/k)], \tag{21}$$

removes the factorial growth (6) from the expansion coefficients f_k, and leads to a simple power behavior of the coefficients $\tilde{B}_k$:

$$\tilde{B}_k\overset{k\to\infty}{=}\text{const}\times[\alpha\omega(1-\omega)^{1/\omega-1}]^k k^{\beta+\beta_0+1/2+s/\omega}[1+\mathcal{O}(1/k)]. \tag{22}$$

Thus our transform $\tilde{B}(y)$ shares with the ordinary Borel transform $B(t)$ the property of being analytic at the origin. Its radius of convergence is determined by the singularity on the negative real axis at

$$y_s=-\frac{1}{\sigma}\equiv-\frac{1}{\alpha}\frac{1}{\omega(1-\omega)^{1/\omega-1}}. \tag{23}$$

B. Resummation procedure

A resummation procedure can now be set up on the basis of the transform $\tilde{B}(y)$ as before. The inverse transformation (19) contains an integral over the entire positive axis, requiring again an analytic continuation of the Taylor expansion of $\tilde{B}(y)$ beyond the convergence radius.

The reason for introducing the transform $\tilde{B}(y)$ was to allow us to reproduce the complete power sequence in the strong-coupling expansion (3), with a leading power g_B^s and a subleading sequence of powers $g_B^{s-k\omega}$, $k=1,2,3,\ldots$. This is achieved by removing a factor $e^{-\rho\sigma y}$ with $\rho,\sigma>0$ from the truncated series (18) of our transform $\tilde{B}(y)$. Furthermore by removing a second simple prefactor of the form $(1+\sigma y)^{-\delta}$ we weaken the leading singularity in the hyper-Borel complex y-plane, which determines the large order behavior (6). The remaining series has still a finite radius of convergence. To achieve convergence on the entire positive y axis for which we must do the integral (19), we re-expand the remaining series of y in powers of $\kappa(y)$ which is related to y by an equation like Eq. (12). For simplicity we choose the parameter $p=1$, i.e.,

$$y=\frac{1}{\sigma}\frac{\kappa(y)}{1-\kappa(y)}, \tag{24}$$

which maps a shifted right half of the complex y-plane with $\mathrm{Re}[y] \geqslant -1/2\sigma$ onto the unit circle in the complex κ-plane. Thus we re-expand $\tilde{B}(y)$ in the following way:

$$\tilde{B}(y) \equiv \sum_{k=0}^{\infty} \tilde{B}_k y^k = e^{-\rho\sigma y}[1+\sigma y]^{-\delta} \sum_{k=0}^{\infty} h_k \kappa^k(y) = e^{-\rho\sigma y} \sum_{k=0}^{\infty} h_k \frac{(\sigma y)^k}{(1+\sigma y)^{k+\delta}}. \tag{25}$$

The inverse hyper-Borel transform of $\tilde{B}(y)$ is now found by forming the integrals of the expansion functions in (25):

$$I_n(g_B) = \frac{\Gamma(\beta_0)}{2\pi i} \oint_C dt\, e^t t^{-\beta_0} \int_0^{\infty} \frac{dy}{y} \left[\frac{g_B}{y t^{1/\omega - 1}} \right]^s \exp\left[\frac{y t^{1/\omega - 1}}{g_B} \right]^{\omega} e^{-\rho\sigma y} \frac{(\sigma y)^n}{(1+\sigma y)^{n+\delta}}, \tag{26}$$

so that the approximants $f_L^a(g_B)$ may be written as

$$f_L^a(g_B) = \sum_{n=0}^{L} h_n I_n(g_B). \tag{27}$$

The same functions $I_n(g_B)$ may be used as basis functions for a wide variety of divergent truncated perturbation expansions $f_L(g_B)$. The complete list of parameters on which they depend reads as follows:

$$I_n(g_B) = I_n(g_B, \omega, s, \rho, \sigma, \delta, \beta_0) = I_n(\sigma g_B, \omega, s, \rho, 1, \delta, \beta_0), \tag{28}$$

but in the following we shall mostly use the shorter notation $I_n(g_B)$. The integral representation of $I_n(g_B)$ breaks down at $s=n$, requiring an analytical continuation. For the upcoming applications in the large-g_B regime it will be sufficient to perform this continuation only in the convergent strong-coupling expansion of $I_n(g_B)$. This is obtained by performing a Taylor series expansion of the exponential function in (26), which is an expansion in powers of $1/g_B^{\omega}$. After integrating over t and y using (20), we obtain an expansion

$$I_n(g_B) = g_B^s \sum_{k=0}^{\infty} b_k^{(n)} g_B^{-k\omega}, \tag{29}$$

which has indeed the same power sequence as the strong-coupling expansion (3) of the function $f(g_B)$ to be resummed.

The expansion coefficients are

$$b_k^{(n)} = \frac{(-1)^k}{k!} \frac{\sigma^{s-k\omega}\Gamma(\beta_0)}{\Gamma[(\omega-1)k + \beta_0 + (1/\omega - 1)s]} i_k^{(n)}, \tag{30}$$

where $i_k^{(n)}$ denotes the integral

$$i_k^{(n)} = \int_0^{\infty} dy\, e^{-\rho y} (1+y)^{-\delta-n} y^{k\omega+n-s-1}. \tag{31}$$

This integral is seen to coincide with the Kummer function

$$U(\alpha, \gamma, z) \equiv \frac{1}{\Gamma(\alpha)} \int_0^{\infty} dy\, e^{-zy} y^{\alpha-1} (1+y)^{\gamma-\alpha-1}, \tag{32}$$

in terms of which we can write

$$i_k^{(n)} = \Gamma(k\omega + n - s) U(k\omega + n - s, k\omega - s - \delta + 1, \rho). \tag{33}$$

The latter expression is useful since in some applications the integral (31) may diverge, and requires an analytic continuation by deforming the contour of integration. Such deformations are automatically supplied by choosing other representations for the Kummer function, for instance,

$$U(\alpha,\gamma,z)=\frac{\pi}{\sin\pi\gamma}\left[\frac{M(\alpha,\gamma,z)}{\Gamma(1+\alpha-\gamma)\Gamma(\gamma)}-z^{1-\gamma}\frac{M(1+\alpha-\gamma,2-\gamma,z)}{\Gamma(\alpha)\Gamma(2-\gamma)}\right], \tag{34}$$

where $M(\alpha,\gamma,z)$ is the confluent hypergeometric function with a Taylor expansion

$$M(\alpha,\gamma,z)=1+\frac{\alpha}{\gamma}\frac{z}{1!}+\frac{\alpha(\alpha-1)}{\gamma(\gamma-1)}\frac{z^2}{2!}+\cdots. \tag{35}$$

The alternative expression (33) for $i_k^{(n)}$, with (34) and (35), is useful for resumming various asymptotic expansions, for example, that of the ground state energy of the anharmonic oscillator, in which case the leading strong-coupling power s has the value 1/3. There, the integral representation (31) would have to be evaluated for values $n=0, k=0$, where the integral does not exist, whereas formula (33) with (34) and (35) is well defined.

For large k, the integral on the right-hand side of (31) can be estimated with the help of the saddle point approximation. The saddle point lies at

$$y_s\approx\frac{k\omega}{\rho}, \tag{36}$$

leading to the asymptotic estimate

$$\begin{aligned} i_k^{(n)} &\overset{k\to\infty}{=} \left(\frac{k\omega}{\rho}\right)^{-\delta-n}\int_0^\infty dy\, e^{-\rho y}y^{\omega k+n-s-1}[1+\mathcal{O}(1/k)] \\ &= \left(\frac{\omega k}{\rho}\right)^{-\delta-n}\rho^{-k\omega-n+s}\Gamma(k\omega+n-s)[1+\mathcal{O}(1/k)]. \end{aligned} \tag{37}$$

The behavior of the strong-coupling coefficients $b_k^{(n)}$ for large k is obtained with the help of the identity

$$\Gamma(z)\Gamma(1-z)=\frac{\pi}{\sin\pi z} \tag{38}$$

and Stirling's formula (21), yielding

$$b_k^{(n)} \overset{k\to\infty}{=} \gamma\sin\pi[k(\omega-1)+\beta_0+(1/\omega-1)s]\left[-\frac{(1-\omega)^{(1-\omega)}}{(\sigma\rho)^\omega}\right]^k k^{\gamma_1}[1+\mathcal{O}(1/k)]. \tag{39}$$

The values of the real constants γ, γ_1 will not be needed in the upcoming discussions, and are therefore not calculated explicitly.

Equation (39) shows that the strong-coupling expansion (3) has a convergence radius

$$|g_B|\geqslant\frac{(\rho\sigma)^\omega}{(1-\omega)^{1-\omega}}, \tag{40}$$

which means that the basis functions $I_n(g_B)$, and certainly also $f(g_B)$ itself, possess additional singularities beside $g_B=0$. The parameter ρ will be optimally adjusted to match the positions of these singularities.

C. Taylor series of basis functions

For re-expanding $f_L(g_B)$ in terms of the basis functions $I_n(g_B)$, we must know their Taylor series. These are obtained by substituting into (26) the variable y by $g_B y'$, and expanding the integrand of (26) in powers of g_B. After performing the integrals over y' and t, we find

$$I_n(g_B)=\sum_{k=n}^{\infty} f_k^{(n)} g_B^k, \tag{41}$$

with the coefficients

$$f_k^{(n)}=\frac{1}{\omega}\frac{\Gamma(\beta_0)\Gamma(k/\omega-s/\omega)}{\Gamma(k(1/\omega-1)+\beta_0)}\sum_{j=0}^{k-n}\binom{-\delta-n}{j}\frac{(-\rho)^{k-n-j}}{(k-n-j)!}\sigma^k. \tag{42}$$

The coefficients in the last sum arise from the t-integral:

$$\sum_{j=0}^{k-n}\binom{-n-\delta}{j}\frac{(-\rho)^{k-n-j}}{(k-n-j)!}=\frac{(-1)^{k-n}}{\Gamma(k-n+1)\Gamma(n+\delta)}\int_0^\infty dt\, e^{-t}t^{\delta+n-1}(\rho+t)^{k-n}. \tag{43}$$

For large k, the integral may be evaluated with the help of the saddle-point approximation. Using this and Stirling's formula (21), we find

$$\sum_{j=0}^{k-n}\binom{-n-\delta}{j}\frac{(-\rho)^{k-n-j}}{(k-n-j)!}\overset{k\to\infty}{=}\frac{(-1)^{k-n}e^{\rho}}{\Gamma(\delta+n)}k^{\delta+n-1}[1+\mathcal{O}(1/k)]. \tag{44}$$

Inserting this into (42) and using once more Stirling's formula, we obtain for the expansion coefficients $f_k^{(n)}$ the following factorial growth

$$f_k^{(n)}\overset{k\to\infty}{=}\frac{(-1)^n e^{\rho}\Gamma(\beta_0)}{\sqrt{2\pi}\Gamma(\delta+n)}(1-\omega)^{1/2-\beta_0}\omega^{\beta_0-1+s/\omega}k^{\delta-\beta_0+n-3/2-s/\omega}$$
$$\times\left[\frac{\sigma}{\omega(1-\omega)^{1/\omega-1}}\right]^k k![1+\mathcal{O}(1/k)]. \tag{45}$$

For an optimal re-expansion (27), we shall choose the free parameters of the basis functions $I_n(g_B,\omega,s,\rho,\sigma,\delta,\beta_0)$ to match the large-order behavior of the coefficients f_k in (6).

D. Convergence properties of resummed series

We shall now discuss the speed of convergence of the resummation procedure. For this it will be sufficient to estimate the convergence of the strong-coupling coefficients b_k^L of the approximations $f_L(g_B)$ against the true strong-coupling coefficients b_k in (3). The convergence for arbitrary values of g_B will always be better than that. Such an estimate is possible by looking at the large-n behavior of the expansion coefficients $b_k^{(n)}$ in the strong-coupling expansion of $I_n(g_B)$ in (29). This is determined by the saddle point approximation to the integral $i_k^{(n)}$ in Eq. (31), which we rewrite as

$$i_k^{(n)}=\int_0^\infty dy\, e^{-\rho y-n\ln(1+1/y)}(1+y)^{-\delta}y^{k\omega-s-1}. \tag{46}$$

The saddle point lies at

$$y_s=\sqrt{\frac{n}{\rho}}\,[1+\mathcal{O}(1/\sqrt{n})]. \tag{47}$$

At this point, the total exponent in the integrand is

$$-\rho y_s - n \ln\left(1+\frac{1}{y_s}\right) = -2\sqrt{\rho n}[1+\mathcal{O}(1/\sqrt{n})], \tag{48}$$

implying the large-n behavior

$$b_k^{(n)} \overset{n\to\infty}{=} \text{const}\times n^{k\omega-s-1-\delta} e^{-2\sqrt{\rho n}}[1+\mathcal{O}(1/\sqrt{n})]. \tag{49}$$

The strong-coupling coefficients b_k^L of the approximations $f_L^a(g_B)$ are linear combinations of the coefficients $b_k^{(n)}$ of the basis functions $I_n(g_B)$:

$$b_k^L = \sum_{n=0}^{L} b_k^{(n)} h_n . \tag{50}$$

The speed of convergence with which the b_k^L's approach b_k as the number L goes to infinity is governed by the growth with n of the re-expansion coefficients h_n and of the coefficients $b_k^{(n)}$ in Eq. (49). We shall see that for the series to be resummed, the re-expansion coefficients h_n will grow at most like some power n^r, implying that the approximations b_k^L approach their $L\to\infty$ -limit b_k with an error proportional to

$$b_k^L - b_k \sim L^{r+k\omega-s-\delta-1/2}\times e^{-2\sqrt{\rho L}}. \tag{51}$$

The leading exponential falloff of the error $e^{-2\sqrt{\rho L}}$ is independent of the other parameters in the basis functions $I_n(g_B,\omega,p,\rho,\sigma,\delta,\beta_0)$ which still need adjustment. This is the important advantage of the present resummation method with respect to variational perturbation theory[5,8] where the error decreases merely like $e^{-\text{const}\times L^{1-\omega}}$ with $1-\omega$ close to 1/4.

The nonexponential prefactor in Eq. (51) depends on the parameters in $I_n(g_B,\omega,p,\rho,\sigma,\delta,\beta_0)$. Some of them are related to observables, others are free and may be chosen to optimize the convergence.

1. Parameters s and ω

The perturbation expansions for the critical exponents are power series in the bare coupling constant g_B whose strong-coupling limit is a constant.[8,9] The same is true for the series expressing the renormalized coupling constant g in powers of the bare coupling constant. This implies that the growth parameter s for the basis functions $I_n(g_B)$ is equal to zero in all cases. The constant asymptotic values are approached with the subleading powers $1/g_B^{k\omega-s}$, where ω is a universal experimentally measurable critical exponent.

2. Parameter σ

In the ordinary Borel transformation, the parameter α in the large-order behavior of the expansion coefficients f_k in Eq. (6), which is determined directly by the inverse value of the reduced action of the classical solution to the field equations, specifies also the position of the singularity on the negative t axis in $B(t)$. In our transform $\tilde{B}(y)$, the singularity position of the singularity is proportional to α, with an ω-dependent prefactor. It lies at [see Eq. (23)]

$$\sigma = \alpha\omega(1-\omega)^{1/\omega-1}. \tag{52}$$

This value of σ ensures that the expansion coefficients f_k^n of the basis functions $I_n(g_B)$ in Eq. (45) grow for large k with the same factor $(-\alpha)^k$ as the expansion coefficients for $f(g_B)$ in Eq. (6).

The conformal mapping (24) maps the singularity at $t=-1/\sigma$ to $\kappa=\infty$, and converts the cut along the negative into a cut in the κ-plane from 1 to ∞. The growth of the re-expansion coefficients h_n with n is therefore determined by the nature of the singularity of $\tilde{B}(y)$ at ∞.

In the upcoming applications to critical exponents it will turn out that the value (52) following from the inverse action of the solution to the classical field equations and ω will not yield the fastest convergence of the approximations $f^L(g_B)$ towards $f(g_B)$, but that a slightly smaller value gives better results. This seems to be due to the fact that the classical solution gives only the nearest singularity in the hyper-Borel transform $\tilde{B}(y)$ of $f(g_B)$. In reality, there are many additional cuts from other fluctuating field configurations which determine the size of the expansion coefficients f_k at pre-asymptotic orders k. Since the few known f_k's are always pre-asymptotic, they are best accounted for by an effective shift of the position of the singularity into the direction of the additional cuts at larger negative y, corresponding to a smaller σ.

3. Parameter ρ

According to Eq. (40), the parameter ρ determines the radius of convergence of the strong-coupling expansion of the basis functions $I_n(g_B)$. It should therefore be adjusted to fit optimally the corresponding radius of the original function $f(g_B)$. Since we do not know this radius, this adjustment will be done phenomenologically by varying ρ to optimize the speed of convergence. Specifically, we shall search at each order L for a vanishing highest re-expansion coefficient h_L or, if it does not vanish anywhere, for a vanishing derivative with respect to ρ:

$$h_L(\rho)=0 \quad \text{or} \quad \frac{dh_L(\rho)}{d\rho}=0. \tag{53}$$

4. Parameter δ

From Eq. (45) we see that the parameter δ influences the power k^β in the large-order behavior (6). By comparing the two equations, we identify the growth parameter β of $I_n(g_B)$ as being

$$\beta=\delta-\beta_0-3/2-s/\omega+n. \tag{54}$$

At first it appears to be impossible to give *all* basis functions $I_n(g_B)$ the same growth power β in (45) by simply letting δ depend on the order n as required by (54). If we were to do this, we would have to assign to δ the value

$$\delta=\delta_n\equiv\beta+\beta_0+3/2+s/\omega-n, \tag{55}$$

which depends on the index n of the function $I_n(g_B)$, and this means that we perform an analytical continuation of the power series expansion of $\tilde{B}(y)$ by re-expanding it as follows:

$$\tilde{B}(y)=\sum_{k=0}^{\infty}\tilde{B}_k y^k=e^{-\rho\sigma y}(1+\sigma y)^{-\delta}\sum_{k=0}^{\infty}h_k(\sigma y)^k. \tag{56}$$

But the series in this formula which is obtained from the series of $\tilde{B}(y)$ by removing a simple factor still has the same finite radius of convergence and could not be used to estimate $\tilde{B}(y)$ for large values of y needed to perform the back transform (19). It is, however, possible to sidetrack this problem by letting ρ grow linearly with the order L. Then the exponential factor of (56) suppresses the integrals over y for large y sufficiently to make the divergence of the re-expanded series (56) at large y irrelevant. If we determine ρ from the condition (53), the growth of ρ with L turns out to emerge by itself.

5. Parameter β_0

The parameter β_0 has two effects. From Eq. (30) we see that for

$$k>k_c\equiv\frac{\beta_0+(1/\omega-1)s}{1-\omega} \tag{57}$$

the signs of the strong-coupling expansion coefficients start to alternate irregularly. This irregularity weakens the convergence of the higher strong-coupling coefficients b_k^L with $k>k_c$ against b_k. The convergence can therefore be improved by choosing a β_0 which grows proportionally to the order L of the approximation.

In addition, β_0 appears in the power of k in (45), which is a consequence of the fact that it determines the nature of the cut in $\widetilde{B}(y)$ in the complex y-plane starting at $y=-1/\sigma$ [see Eq. (25)].

If we expand both sides of (25) in powers of $\kappa=\sigma y/(1+\sigma y)$ and compare the coefficients of powers of κ, it is easy to write down an explicit formula for the re-expansion coefficients h_n in terms of the coefficients $\widetilde{B}_j$ of $\widetilde{B}(y)$ by

$$h_n=\sum_{k=0}^{n}\sum_{j=0}^{k}\frac{\widetilde{B}_j\sigma^{-j}\rho^{k-j}}{(k-j)!}\binom{\delta+n-1}{n-k}, \tag{58}$$

where $\widetilde{B}_j$ are obtained from the original expansion coefficients f_k of $f(g_B)$ by relation (18).

Before beginning with the resummation of the perturbation expansions for the critical exponents of ϕ^4-field theories, it will be useful to obtain a feeling for the quality of the above-developed resummation procedure, in particular for the significance of the parameters upon the speed of convergence. We do this by resumming the often-used example of an asymptotic series, the perturbation expansion of the ground state energy of the anharmonic oscillator.

E. Resummation of ground state energy of anharmonic oscillator

Consider the one-dimensional anharmonic oscillator with the Hamiltonian

$$H=\frac{p^2}{2}+m^2\frac{x^2}{2}+g_Bx^4. \tag{59}$$

In this quantum mechanical system, there is no need to distinguish bare and renormalized coupling constants, but since the previous resummation formulas were all formulated in terms of g_B we shall keep this notation also here. The ground state energy has a perturbation expansion

$$E^{(0)}(g_B)=\sum_{k}^{\infty} f_kg_B^k, \tag{60}$$

whose coefficients can be calculated via the Bender–Wu recursion relation[16] to arbitrarily high orders, with a large-order behavior

$$f_k=-\sqrt{\frac{6}{\pi^3}}k!(-3)^kk^{-1/2}[1+\mathcal{O}(1/k)]. \tag{61}$$

By comparison with (6) we identify the growth parameters

$$\alpha=3,\quad \beta=-1/2. \tag{62}$$

A scale transformation $x\to g^{1/6}x$ applied to the Hamiltonian (59) reveals the scaling property[17] for the energy as a function of g_B and m^2:

$$E(m^2,g_B)=g_B^{1/3}E(g_B^{-2/3}m^2,1). \tag{63}$$

Combining this with the knowledge[17] that $E(m^2,1)$ is an analytic function at $m^2=0$, we see that $E(1,g_B)$ possesses a power series expansion of the form (3), with the parameters

$$s=1/3,\quad \omega=2/3. \tag{64}$$

Inserting the latter number together with α from Eq. (62) into (52), we identify

$$\sigma = \frac{2}{\sqrt{3}}. \tag{65}$$

The ground state energy $E^{(0)}(g_B)$ obeys a once-subtracted dispersion relation:[17]

$$E^{(0)}(g_B) = \frac{1}{2} + \frac{g_B}{\pi}\int_0^\infty \frac{dg_B'}{g_B'}\,\frac{\mathrm{Im}\,E^{(0)}(-g_B')}{g_B'+g_B}. \tag{66}$$

The perturbation expansion (60) is obtained from this by expanding $1/(g_B'+g_B)$ in powers of g_B, and performing the integral term by term. This shows explicitly that the large-order behavior (61) is caused by an imaginary part

$$\mathrm{Im}\,E^{(0)}(-|g_B|) = \sqrt{\frac{6}{\pi}}\sqrt{\frac{1}{3|g_B|}}e^{-1/3|g_B|}[1+\mathcal{O}(|g_B|)] \tag{67}$$

near the tip of the left-hand cut in the complex g_B-plane, in agreement with the general form (5) associated with the large-order behavior (6).

Let us now specify the parameter δ. We shall do this here in an n-dependent way using Eq. (55), which now reads with (64):

$$\delta = \delta_n \equiv \beta_0 + 3/2 - n. \tag{68}$$

The corresponding basis functions

$$I_n(g_B, 2/3, 1/3, \rho, 2/\sqrt{3}, \beta_0 + 3/2 - n, \beta_0), \tag{69}$$

have then all the same large-order growth parameter β in (6).

The two parameters ρ and β_0 are still arbitrary. The first is determined by an order-dependent optimization of the approximations via the conditions (53). The best choice of β_0 will be made differently depending on the regions of g_B.

Let us test the convergence of our algorithm at small negative coupling constants g_B, i.e., near the tip of the left-hand cut in the complex g_B-plane. We do this by calculating the prefactor γ in the large-order behavior (6). In this case the convergence turns out to be fastest by giving the parameter β_0 a small value, i.e., $\beta_0 = 2$. With the large-order behavior (45) of the basis functions $I_n(g_B)$, we find the resummed functions $f_L(g_B)$ of Lth order $\Sigma_{n=0}^L h_n I_n(g_B)$ to have a large-order behavior (6) with a prefactor

$$\gamma_L = \frac{e^\rho \Gamma(\beta_0)}{\sqrt{2\pi}\Gamma(\delta)}\sum_{k=0}^{L}(-1)^k h_k. \tag{70}$$

The values of these sums for increasing L are shown in Fig. 1. They converge exponentially fast against the exact limiting value

$$\gamma = \sqrt{\frac{6}{\pi^3}}, \tag{71}$$

with superimposed oscillations. The oscillations are of the same kind as those observed in variational perturbation theory for the convergence of the approximations to the strong-coupling coefficients b_k (see Figs. 5.19 and 5.20 in Ref. 5) Also here, the strong-coupling coefficients b_k^L

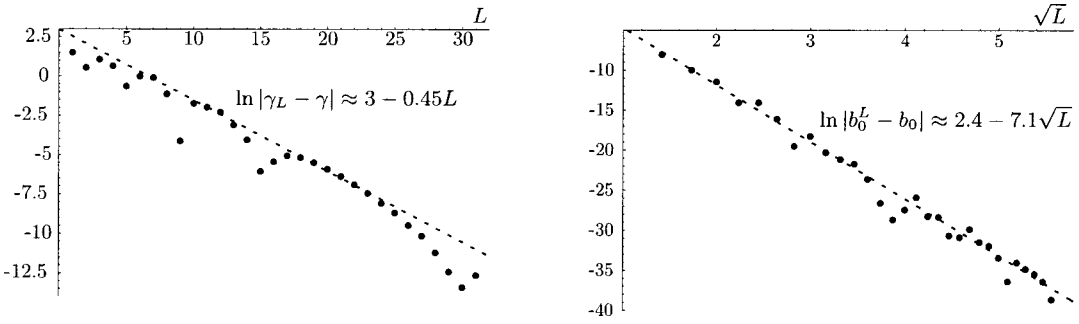

FIG. 1. Logarithmic plot of the convergence behavior of the successive approximations to the prefactor γ^L in the large-order behavior (87), and of the leading strong-coupling coefficient b_0^L.

converge exponentially fast towards b_k, but with a larger power of L in the exponent of the last term $\approx e^{-\text{const}\times\sqrt{L}}$ [see Eq. (51)], rather than $\approx e^{-\text{const}\times L^{1/3}}$ for variational perturbation theory [see Eq. (5.199) in Ref. 5]. This is seen on the right-hand side of Fig. 1.

We have applied our resummation method to the first 10 strong-coupling coefficients using the expansion coefficients f_k up to order 70. The results are shown in Table I. Comparison with a similar table in Refs. 18 and 5 shows that the new resummation method yields in 70th order the same accuracy as variational perturbation theory did in 251st order. In all cases the optimal parameter ρ turns out to be a slowly growing function with L.

In the strong-coupling regime, the convergence is fastest by choosing for β_0 an L-dependent value

$$\beta_0 = L. \tag{72}$$

Note that this choice of β_0 ruins the convergence to the imaginary part for small negative g_B which was resummed best with $\beta_0 = 2$.

F. Resummation of critical exponents

Having convinced ourselves of the fast convergence of our new resummation method, let us now turn to the perturbation expansions of the $O(N)$-symmetric ϕ^4 theories in powers of the bare coupling constant $\overline{g_B}$, defined by the Euclidean action

TABLE I. Strong-coupling coefficients b_n of the 70th order approximants $E^0_{70}(g)=\Sigma_{n=0}^{70}h_nI_n(g)$ to the ground state energy $E^0(g)$ of the anharmonic oscillator. They have the same accuracy as the variational perturbation–theoretic calculations up to order 251 in Refs. 18 and 5.

n	b_n
0	0.667 986 259 155 777 108 270 962 02
1	0.143 668 783 380 864 910 020 319
2	0.008 627 565 680 802 279 127 963
3	0.000 818 208 905 756 349 542 41
4	0.000 082 429 217 130 077 219 91
5	0.000 008 069 494 235 040 964 75
6	0.000 000 727 977 005 945 772 63
7	0.000 000 056 145 997 222 351 17
8	0.000 000 002 949 562 732 709 36
9	0.000 000 000 064 215 331 956 97
10	0.000 000 000 048 214 263 789 07

$$\mathcal{A}=\int d^D x\{\tfrac{1}{2}[\partial\phi_0(x)]^2+\tfrac{1}{2}m_0^2\phi_0^2(x)+2\pi\lambda_B[\phi_0^2(x)]^2\} \tag{73}$$

in $D=3$ dimensions. The field ϕ_0 is an N-component vector $\phi_0=(\phi_0^1,\phi_0^2,\ldots,\phi_0^N)$, and the action is $O(N)$-symmetric. We define renormalized mass m and field strength by parametrizing the behavior of the connected two point function $G^{(2)}$ in momentum space near zero momentum as

$$G^{(2)}(p,\alpha;-p,\beta)=Z_\phi\frac{\delta_{\alpha\beta}}{m^2+p^2+\mathcal{O}(p^4)}. \tag{74}$$

The renormalized coupling constant g is defined by the value of the connected four-point function at zero momenta:

$$G^{(4)}(0,\alpha;0,\beta;0,\gamma;0,\delta)=m^{-4-D}Z_\phi^2 g(\delta_{\alpha\beta}\delta_{\gamma\delta}+\delta_{\alpha\gamma}\delta_{\beta\delta}+\delta_{\alpha\delta}\delta_{\beta\gamma}). \tag{75}$$

If we introduce the dimensionless bare coupling constant $g_B\equiv\lambda_B/m$, the critical exponents are defined by

$$\begin{aligned}\eta(g_B)&=g_B\frac{d}{dg_B}\log Z_\phi,\\ 2-\nu(g_B)^{-1}&=g_B\frac{d}{dg_B}\log\frac{m_0^2}{m^2}.\end{aligned} \tag{76}$$

The following expansions for the critical indices in the bare dimensionless coupling constant are available[19] in the literature for all $O(N)$:

$$\begin{aligned}\eta(g_B)=&(16/27+8N/27)g_B^2+(-9.086\,537\,459-5.679\,085\,912N-0.567\,908\,591\,2N^2)g_B^3\\ &+(127.491\,6153+94.773\,205\,34N+17.134\,775\,5N^2+0.810\,538\,322\,1N^3)g_B^4\\ &+(-1843.491\,99-1576.466\,76N-395.267\,835\,8N^2-36.006\,602\,42N^3\\ &-1.026\,437\,849N^4)g_B^5+(28\,108.603\,98+26\,995.879\,62N+8461.481\,806N^2\\ &+1116.246\,863N^3+62.887\,906\,8N^4+1.218\,861\,532N^5)g_B^6,\end{aligned} \tag{77}$$

$$\begin{aligned}2-\nu^{-1}(g_B)=&g_B(2+N)+(523/27+316N/27+N^2)g_B^2+(229.374\,4544+162.847\,4234N\\ &+26.080\,098\,09N^2+N^3)g_B^3+(-309\,099\,6037-2520.848\,751N\\ &-572.328\,2893N^2-44.326\,461\,41N^3-N^4)g_B^4+(45\,970.718\,39\\ &+42\,170.327\,07N+12\,152.706\,75N^2+1408.064\,008N^3+65.976\,301\,08N^4+N^5)g_B^5\\ &+(-740\,843.1985-751\,333.064N-258\,945.0037N^2-39\,575.570\,37N^3\\ &-2842.8966N^4-90.714\,5582N^5-N^6)g_B^6.\end{aligned} \tag{78}$$

In addition, seventh order coefficients have been calculated for $N=0,1,2,3$:[1]

$$\eta^{(7)}=\left\{\begin{array}{r}-45\,387.489\,27\\-114\,574.4876\\-241\,0424.7646\\-454\,761.4731\end{array}\right\}g_B^7,\ \nu^{-1(7)}=\left\{\begin{array}{r}-127\,922\,69.773\\-337\,114\,16.972\\-737\,808\,09.849\\-143\,831\,857.01\end{array}\right\}g_B^7\ \text{for}\left\{\begin{array}{l}N=0\\N=1\\N=2\\N=3\end{array}\right\}. \tag{79}$$

When approaching the critical point, the renormalized mass m tends to zero, so that the problem is to find the strong-coupling limit of these expansions. In order to have the critical exponents approach a constant value, the power s in Eq. (3) must be set equal to zero.

In contrast to the quantum-mechanical discussion in the last section, the exponent ω governing the approach to the scaling limit is now unknown, and must also be determined from the available perturbation expansions. As in Refs. 8 and 9, we solve this problem by using the fact that the existence of a critical point implies the renormalized coupling constant g in powers of g_B to converge against a constant renormalized coupling g^* for $m\to 0$. The expansion of $g(g_B)$ is known up to six loops[19] for all $O(N)$:

$$\begin{aligned}g(g_B)=&\,g_B+(-8-N)g_B^2+(2108/27+514/27N+N^2)g_B^3\\&+(-878.793\,7193-312.634\,446\,71N-32.548\,413\,03N^2-N^3)g_B^4\\&+(11\,068.061\,83+5100.403\,285N+786.366\,569\,9N^2+48.213\,867\,44N^3+N^4)g_B^5\\&+(-153\,102.850\,23-85\,611.919\,96N-17\,317.7025N^2-1585.114\,189N^3\\&-65.820\,362\,03N^4-N^5)g_B^6\\&+(2297\,647.148+149\,5703.313N+371\,103.0896N^2+44\,914.04\,8\,18N^3\\&+2797.291\,579N^4+85.213\,105\,01N^5+N^6)g_B^7.\end{aligned} \tag{80}$$

The convergence against a fixed coupling g^* occurs only for the correct value of ω in the resummation functions $I_n(g_B,\omega,s,\rho,\sigma,\delta,\beta_0)$. At different values, $g(g_B)$ has some strong-coupling power behavior g_B^s with $s\neq 0$. We may therefore determine ω by forming from (80) a series for the power s,

$$s=\frac{d\log g(g_B)}{d\log g_B}=\frac{g_B}{g}g'(g_B), \tag{81}$$

resumming this for various values of ω in the basis functions, and finding the critical exponent ω from the zero of s. Alternatively, since $g(g_B)\to g^*$, we can just as well resum the series for $-gs$, which coincides with the β-function of renormalization group theory [not to be confused with the growth parameter β in (6)]

$$\beta(g_B)\equiv -g_B\frac{dg(g_B)}{dg_B}. \tag{82}$$

If we denote its strong-coupling limit by β^*,

$$\beta^*\equiv\beta(g_B)\big|_{g_B\to\infty}, \tag{83}$$

we resum the expansion for $\beta(g_B)$ to form the approximations

$$\beta_L(g_B)=\sum_{n=0}^{L}h_nI_n(g_B,\omega), \tag{84}$$

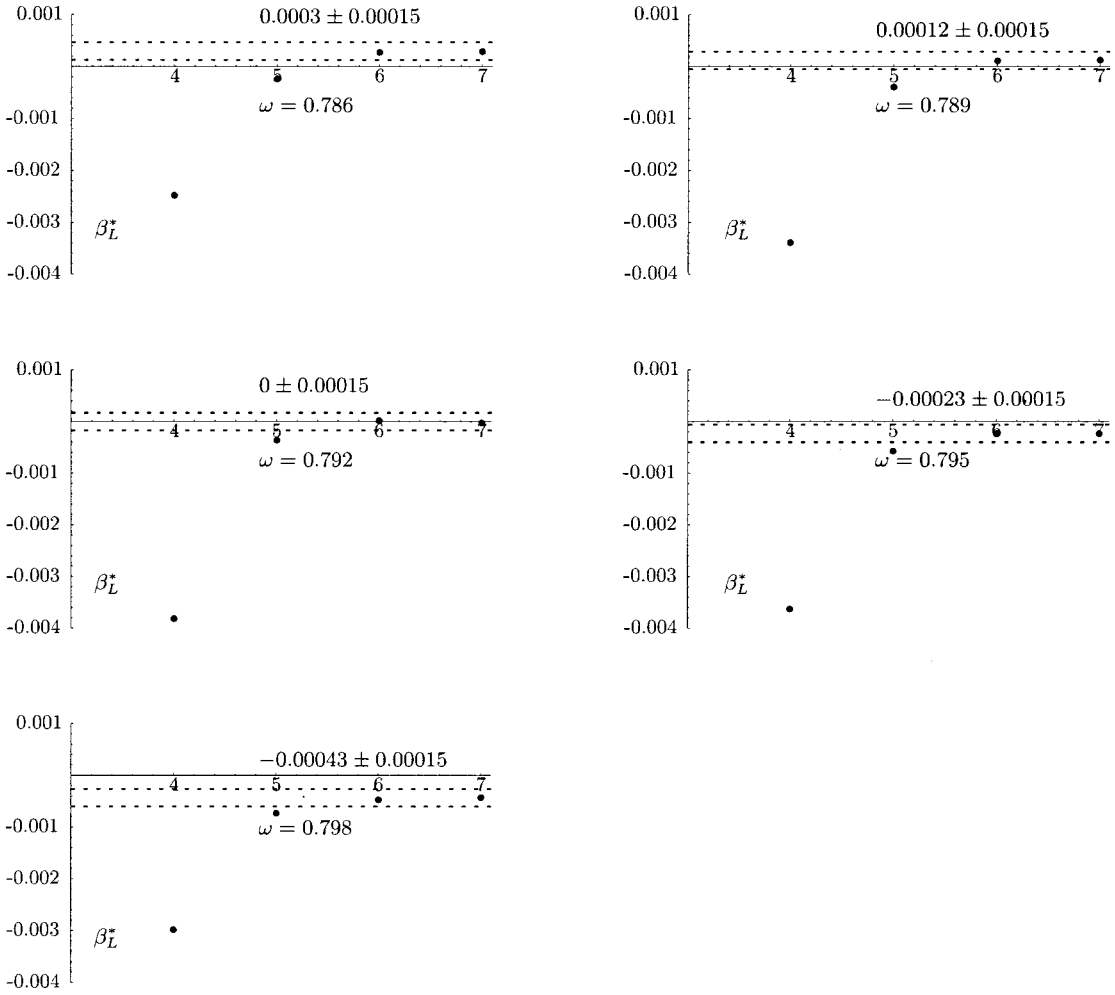

FIG. 2. Convergence of strong-coupling limits of the β-function (82) for $N=1$ and different values of ω. The upper and lower dashed lines denote the range of the $L\to\infty$ limit of β_L^* from which the value of ω is deduced in Fig. 3.

and plot the strong-coupling limits of the Lth approximations β_L^* for various values of ω. This is shown in Fig. 2. From these plots we extract the critical exponent ω by finding the ω-value for which the approximations β_L^* extrapolate best to zero for $L\to\infty$, taking into account that the convergence is exponentially fast with superimposed oscillations. These ω-values are called ω_L.

For these resummations, we must of course specify the remaining parameters in the basis functions $I_n(g_B,\omega,0,\rho,\sigma,\delta,\beta_0)$. This can, in principle, proceed as in the case of the anharmonic oscillator. The parameter α is determined from the action of a classical instanton solution $\phi_c(x)$ of the field equations, and has for all expansions the N-independent value[11]

$$\alpha=\frac{32\pi}{I_4}=1.329\,97, \tag{85}$$

where $I_p\equiv\int d^Dx[\phi_c(x)]^p$ are integrals over powers of $\phi_c(x)$.

To determine the parameter δ, we recall the remaining growth parameters β and γ of the large-order behavior (6) of the perturbative series for the critical exponents. The growth parameter β is given by the number of zero modes in the fluctuation spectrum around this classical solution:

TABLE II. First six perturbative coefficients in the expansions of the β-function in powers of the bare coupling constant g_B, divided by their asymptotic large-order estimates $(-\alpha)^k k! k^{\beta_\beta}$. The ratios increase quite slowly towards the theoretically predicted normalization constant γ_β in the asymptotic regime given in the lowest row.

N	0	1	2	3
k	$f_k^\beta / f_k^{\beta\,\mathrm{as}}$	$f_k^\beta / f_k^{\beta\,\mathrm{as}}$	$f_k^\beta / f_k^{\beta\,\mathrm{as}}$	$f_k^\beta / f_k^{\beta\,\mathrm{as}}$
2	0.57	0.45	0.35	0.27
3	0.61	0.45	0.32	0.22
4	0.73	0.51	0.34	0.22
5	0.89	0.61	0.40	0.25
6	1.07	0.73	0.47	0.29
7	1.26	0.88	0.56	0.34
⋮	⋮	⋮	⋮	⋮
γ_β	110.0	97.0	75.5	53.2

$$\begin{Bmatrix} \beta_\eta \\ \beta_{\nu^{-1}} \\ \beta_\beta \end{Bmatrix} = \begin{Bmatrix} 3+N/2 \\ 4+N/2 \\ 4+N/2 \end{Bmatrix}. \tag{86}$$

The prefactors γ in (6) requires the calculation of the fluctuation determinants around the classical solution, which yields in the case of the β-function

$$\gamma_\beta = \frac{2^{N/2+2} 3^{-3/2} \pi^{-2}}{\Gamma(N/2+2)} \left(\frac{I_1^2}{I_4}\right)^2 \left(\frac{I_6}{I_4} - 1\right)^{3/2} D_L^{-1/2} D_T^{-(N-1)/2}, \tag{87}$$

where D_L and D_T are characteristic quantities of the longitudinal and transverse parts of the fluctuation determinant, respectively. Their numerical values are[11]

D_L	D_T	I_1	I_4	I_6	H_3
10.544 ± 0.004	1.4571 ± 0.0001	31.691 522	75.589 005	659.868 352	13.563 312

(88)

The parameters γ_η, $\gamma_{\nu^{-1}}$ are obtained from γ_β by

$$\gamma_\eta = \gamma_\beta \frac{2H_3}{I_1 D(4-D)}, \quad \gamma_{\nu^{-1}} = \gamma_\beta \frac{N+2}{N+8} (D-1) 4\pi \frac{I_2}{I_1^2}, \tag{89}$$

where $I_2 = (1 - D/4) I_4$ and H_3 is listed in (88). Note that the expansions in powers of the renormalized coupling constant g have the same parameters α and β, but different parameters γ_R. These differ from the above α's by a common factor:

$$\gamma_R = \gamma e^{-(N+8)/\alpha}. \tag{90}$$

From Eq. (85), the parameter σ is found using relation (52). It turns out, however, that this value does not lead to an optimal convergence. This can be understood qualitatively by observing that the large-order behavior of the expansion coefficients of the critical exponents and of the β-function in powers of the bare coupling constant g_B is not nearly as precocious in reaching the large-order form (6) as the corresponding expansions in powers of the renormalized coupling constant g (see Fig. 1 in Ref. 9). The lack of precocity here is illustrated for the expansion coefficients f_k^β of the β-function in Table II, which gives the ratios of f_k^β and their leading asymptotic estimates $f_k^{\beta\,\mathrm{as}}$:

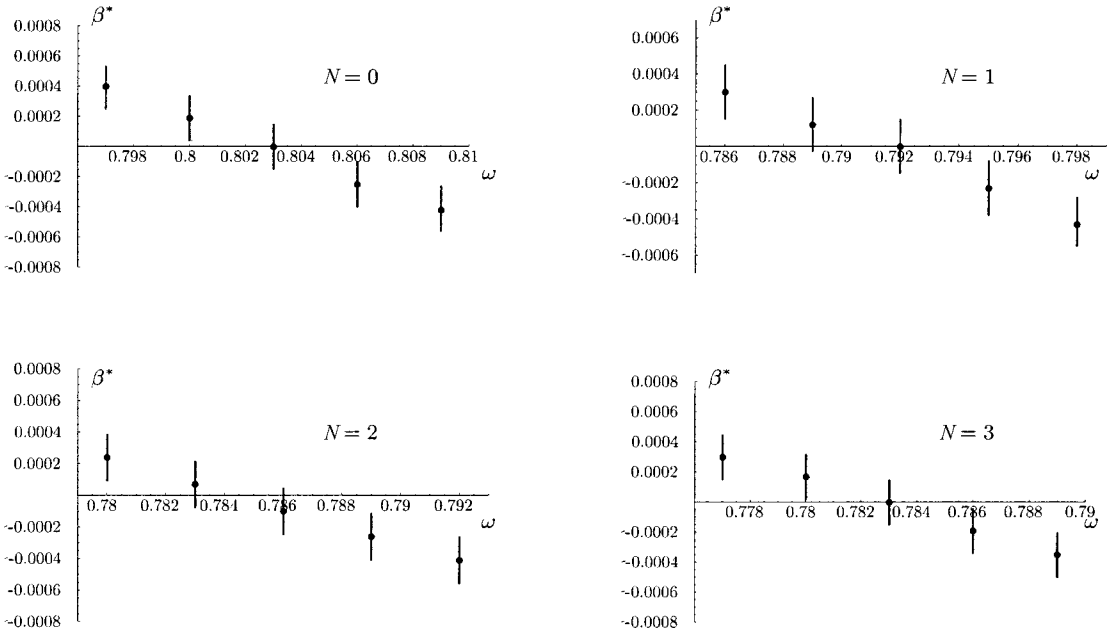

FIG. 3. Plot of resummed values of β^* against ω. The true value of ω is deduced from the condition $\beta^*=0$ and the errors are determined from the range of ω where the error bars from the resummation of β^* intersect with the x-axis.

$$f_k^\beta / f_k^{\beta\,\mathrm{as}} \equiv f_k^\beta / k!(-\alpha)^k k^\beta. \tag{91}$$

The first six approach their large-order limits quite slowly. For this reason we prefer to adapt σ not from α by Eq. (52), but by an optimization of the convergence. Since the re-expanded series converges for fixed values of δ and σ it is reasonable to determine these parameters by searching for a point of least dependence in largest available order L. This is done by imposing the conditions

$$\frac{d\kappa_L}{d\sigma}=0 \quad \text{and} \quad \frac{d^2\kappa_L}{d\sigma^2}=0 \tag{92}$$

to determine *both* parameters δ, σ, where κ_L denotes the Lth approximation to any exponent γ, ν or η. In accordance with the discussions in Sec. II A 2 this procedure provides a value of σ which is smaller than that given by (52).

After trying out a few choices, we have given the parameters β and ρ the fixed values 1 and 10, respectively, to accelerate the convergence.

The results for the critical exponents of all $O(N)$-symmetries are shown in Figs. 2–6 and Table III.

The total error is indicated in the square brackets. It is deduced from the error of resummation of the critical exponent at a fixed value of ω indicated in the parentheses, and from the error $\Delta\omega$ of ω, using the derivative of the exponent with respect to ω given in curly brackets. Symbolically, the relation between these errors is

$$[\cdots]=(\cdots)+\Delta\omega\{\cdots\}. \tag{93}$$

The accuracy of our results can be judged by comparison with the most accurately measured critical exponent α parametrizing the divergence of the specific heat of superfluid helium at the λ-transition by $|T_c-T|^{-\alpha}$. By going into a vicinity of the critical temperature with $\Delta T\approx 10^{-8}$ K, a recent satellite experiment has provided us with the value[20]

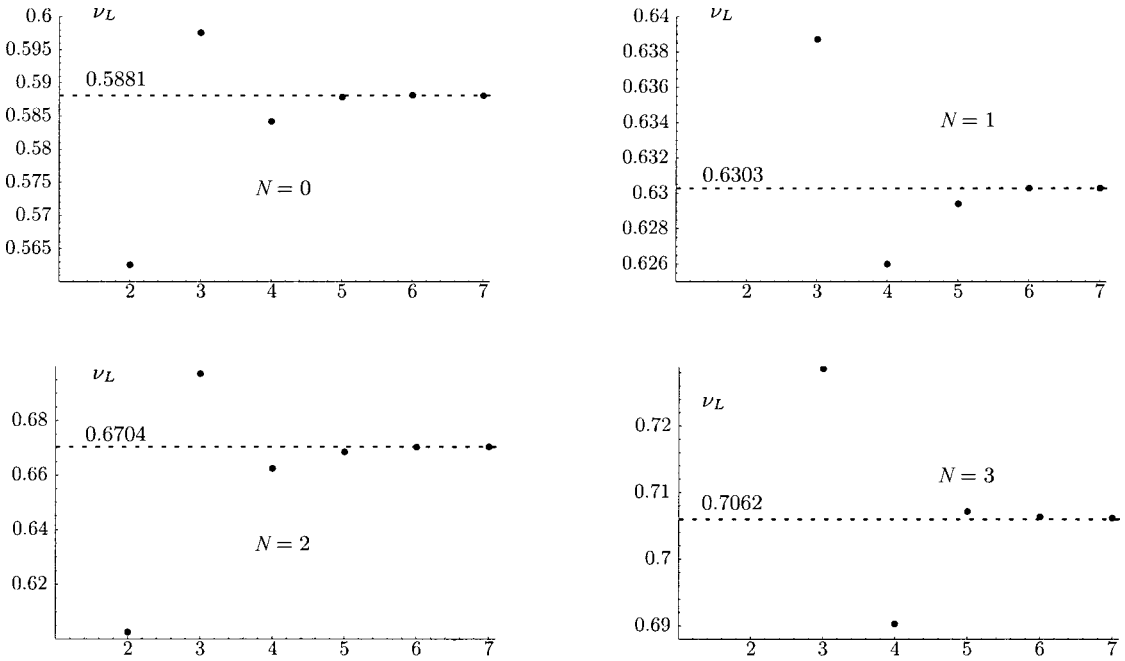

FIG. 4. Convergence of the approximations ν_L to the critical exponent ν for different values of N.

$$\alpha = -0.010\,56 \pm 0.000\,38. \tag{94}$$

Our value for ν in Table III is

$$\nu = -0.6704 \pm 0.007. \tag{95}$$

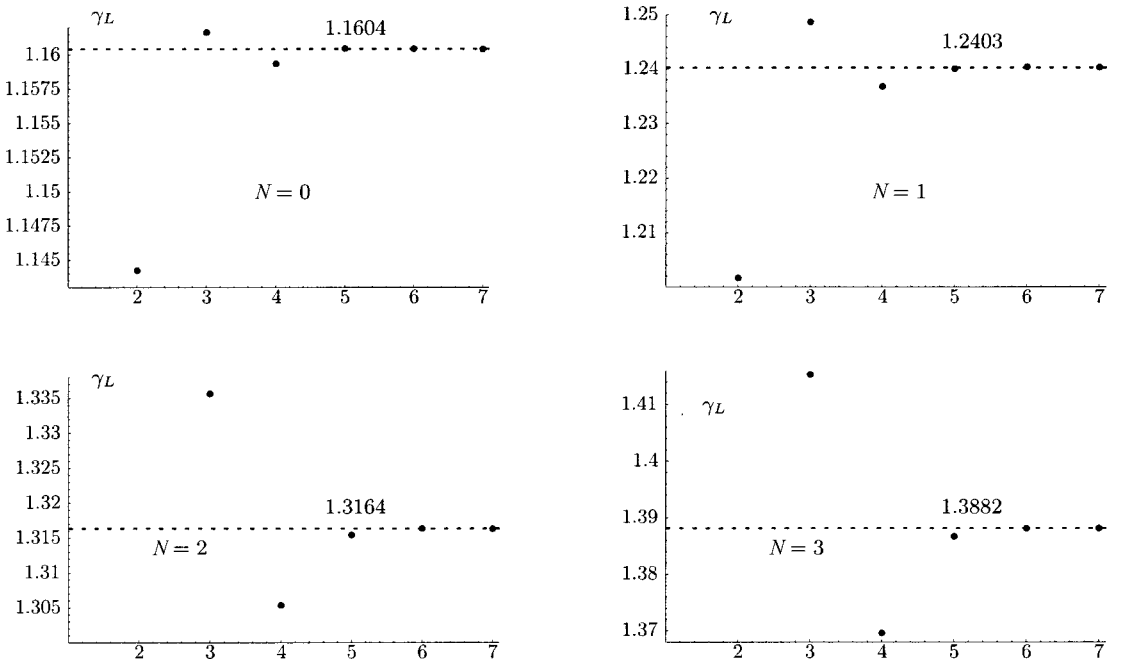

FIG. 5. Convergence of the approximations γ_L to the critical exponent γ for different values of N.

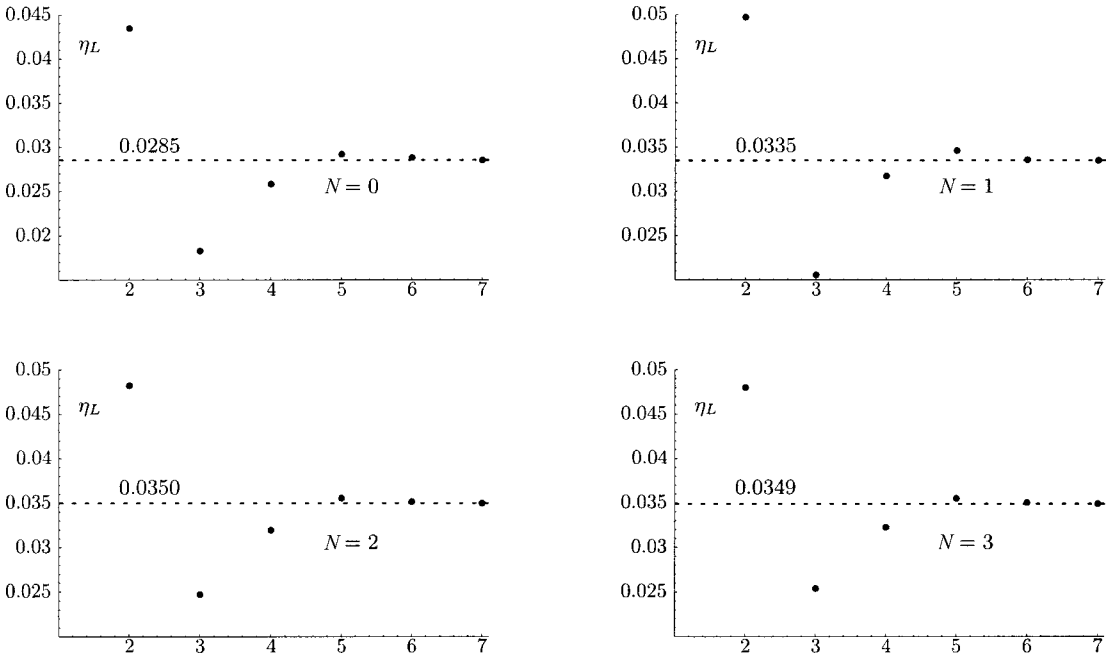

FIG. 6. Convergence of the approximations η_L to the critical exponent η for different values of N.

TABLE III. Critical exponents of the $O(N)$-symmetric ϕ^4-theory from our new resummation method. The numbers in square brackets indicate the total errors. They arise from the error of the resummation at fixed values of ω indicated in parentheses, and the errors coming from the inaccurate knowledge of ω. The former are estimated from the scattering of the approximants around the graphically determined large-L limit, the latter follow from the errors in ω and the derivatives of the critical exponents with respect to changes of ω indicated in the curly brackets.

N	γ	η	ν	ω
0	1.1604[8] (4) {0.075}	0.0285[6] (4) {0.037}	0.5881[8] (4) {0.075}	0.803[3] {1}
1	1.2403[8] (4) {0.110}	0.0335[6] (3) {0.043}	0.6303[8] (4) {0.065}	0.792[3] {1}
2	1.3164[8] (5) {0.033}	0.0349[8] (5) {0.042}	0.6704[7] (4) {0.098}	0.784[3] {1}
3	1.3882[10] (7) {0.210}	0.0350[8] (5) {0.043}	0.7062[7] (4) {0.110}	0.783[3] {1}

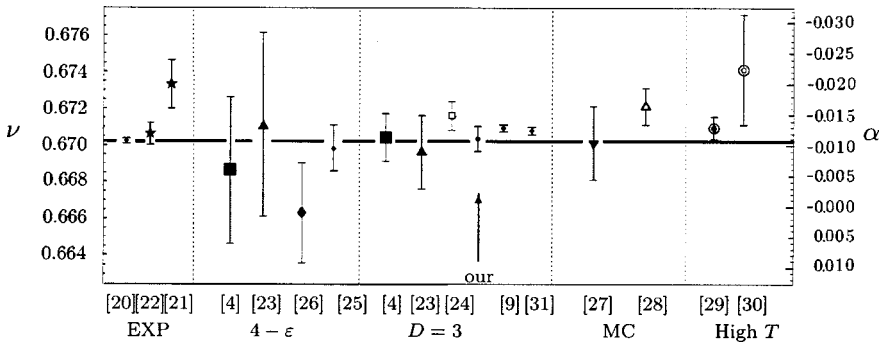

FIG. 7. Comparison of our result (96) for critical exponents α of superfluid helium with experiments and other theories.

and yields via the scaling relation $\alpha = 2 - 3\nu$:

$$\alpha = -0.0112 \pm 0.0021, \tag{96}$$

in good agreement with the experimental number (94). A comparison with other experiments and theories is shown in Fig. 7, showing that our result is among the more accurate ones.

A remark is necessary concerning the errors quoted in this paper. We do not know how to estimate precisely the errors which can appear in an involved numerical approximation scheme such as the one presented here. Our estimates are based on the range of critical exponents which can be reached by reasonably modifying the parameters in the calculations. What may be considered as reasonable is a somewhat subjective procedure. As such, our error estimates follow the rule of maximal optimism, and are probably underestimated. This is, however, not uncommon in resummations of divergent power series of critical exponents.[21–31]

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Modular theory and the reconstruction of four-dimensional quantum field theories

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In this letter we construct a representation of the 3+1-dimensional Poincaré group by modular groups of von Neumann algebras lying in a specified modular position with respect to each other. Combining this new result with an old one of Bisognano–Wichmann [J. Math. Phys. **16**, 985 (1975)] we obtain a net of local observables of a 3+1-dimensional quantum field theory out of a finite set of algebras. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1327597]

I. INTRODUCTION

In this article we continue our investigation on classifying quantum field theories by a finite set of algebras lying in a specified modular position relative to each other, see Ref. 1.

Our framework will be the algebraic approach to quantum field theory, in which the physical system is described by a net of bounded operators, see Ref. 2. As a fundamental feature we have the Reeh–Schlieder property of the vacuum.[3] Intuitively speaking this property reflects the vacuum fluctuations of local quantum field theories. Mathematically it enables one to apply the modular theory of operator algebras as developed by Tomita and Takesaki[4] to each local algebra. As has been realized by Bisognano and Wichmann[5] this rather general structure has a very beautiful interpretation in terms of space–time symmetries of the underlying quantum field theory. We will subsequently review some of these results in Sec. II.

In 1992 Borchers[6] gave an abstract version of this observation which motivated one of the authors (Wiesbrock) to investigate a special type of inclusions of algebras, so called modular inclusions.[7]

They show a rich symmetry structure. Out of such inclusions he constructed a net of algebras fulfilling the assumptions of algebraic quantum field theory in $1+1$ dimensions.[8]

In order to generalize this result to higher dimensions he introduced the notion of modular intersections of von Neumann algebras.[9] Starting with a set of 3 modular intersections and one additional modular inclusion he constructed a representation of the Poincaré group in $2+1$ dimensions. Exploiting the result of Ref. 5 these data give rise to a $2+1$-dimensional quantum field theory.[1]

In this article we will generalize this result to $3+1$ dimensions.

II. PRELIMINARIES

For the convenience of the reader we recall the notion of modular inclusion and modular intersection.

Definition 1 (Ref. 7):

(a) Let $\mathcal{N}\subset\mathcal{M}$ be von Neumann algebras acting on a Hilbert space $\mathcal{H}$, and let $\Omega\in\mathcal{H}$ be a common cyclic and separating vector. $(\mathcal{N}\subset\mathcal{M},\Omega)$ is called a $\pm$ **half-sided modular inclusion** (abbreviated by $\pm$hsm), if $\Delta_{\mathcal{M}}^{it}\mathcal{N}\Delta_{\mathcal{M}}^{-it}\subset\mathcal{N}$ for all $\pm t>0$.

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(b) Let $\mathcal{N}$ and $\mathcal{M}$ be von Neumann algebras acting on a Hilbert space $\mathcal{H}$, which have a common cyclic and separating vector $\Omega\in\mathcal{H}$. In addition let Ω also be cyclic for $\mathcal{N}\cap\mathcal{M}$. If

I. $((\mathcal{N}\cap\mathcal{M})\subset\mathcal{N},\Omega)$ and $((\mathcal{N}\cap\mathcal{M})\subset\mathcal{M},\Omega)$ are $\pm$hsm inclusions,

II. $J_{\mathcal{N}}(s-\lim_{t\to\mp\infty}\Delta_{\mathcal{N}}^{it}\Delta_{\mathcal{M}}^{-it})J_{\mathcal{N}}=s-\lim_{t\to\mp\infty}\Delta_{\mathcal{M}}^{it}\Delta_{\mathcal{N}}^{-it}$, then the triple $(\mathcal{N},\mathcal{M},\Omega)$ is called a $\pm$ **modular intersection** (abbreviated by $\pm$mi).

The fundamental Theorem in this context is:

Theorem 1 (Ref. 1): *Let $\mathcal{N}$ and $\mathcal{M}$ fulfill one of the conditions (a) or (b) in Definition 1. Then*

(a) $\ln(\Delta_{\mathcal{N}})-\ln(\Delta_{\mathcal{M}})$ *is essentially self-adjoint (for modular inclusions even positive).*

Denote by $U_{\mathcal{M},\mathcal{N}}(a),a\in\mathbf{R}$ *the unitary group on* $\mathcal{H}$ *with the generator* $\mp(1/2\pi)(\ln(\Delta_{\mathcal{N}})-\ln(\Delta_{\mathcal{M}}))$. *Then,*

(b) $\Delta_{\mathcal{M}}^{it}U_{\mathcal{M},\mathcal{N}}(a)\Delta_{\mathcal{M}}^{-it}=\Delta_{\mathcal{N}}^{it}U_{\mathcal{M},\mathcal{N}}(a)\Delta_{\mathcal{N}}^{-it}=U_{\mathcal{M},\mathcal{N}}(e^{\pm 2\pi t}a)$ *for* $t,a\in\mathbf{R}$,

(c) $J_{\mathcal{M}}U_{\mathcal{M},\mathcal{N}}(a)J_{\mathcal{M}}=J_{\mathcal{N}}U_{\mathcal{M},\mathcal{N}}(a)J_{\mathcal{N}}=U_{\mathcal{M},\mathcal{N}}(-a)$ *for all* $a\in\mathbf{R}$,

(d) $\Delta_{\mathcal{N}}^{it}\mathcal{M}\Delta_{\mathcal{N}}^{-it}\subset\mathcal{M}$ *for all* $\mp t>0$,

(e) $\mathcal{N}=U_{\mathcal{M},\mathcal{N}}(1)\mathcal{M}U_{\mathcal{M},\mathcal{N}}(-1)$,

(f) $\Delta_{\mathcal{M}}^{it}\Delta_{\mathcal{N}}^{-it}=U_{\mathcal{M},\mathcal{N}}(-1+e^{\pm 2\pi t})$,

(g) $J_{\mathcal{M}}J_{\mathcal{N}}=U_{\mathcal{M},\mathcal{N}}(-2)$,

(h) $(\mathcal{N},\mathcal{M},\Omega)$ *is* $\pm$mi (hsm)$\Leftrightarrow(\mathcal{N}',\mathcal{M}',\Omega)$ *is* $\mp$mi(hsm),

(i) $U_{\mathcal{M}',\mathcal{N}'}(a)=U_{\mathcal{M},\mathcal{N}}(a)$ *for all* $a\in\mathbf{R}$.

(There was an error in the original proof of statement (a) for the case of hsm-inclusions, which was noticed by Araki and Zsido. They also provided a way of filling the gap.[10] For an alternate proof, see Ref. 11.) It is convenient to sign the various algebras occurring in the following by two integers, f. e. by $\mathcal{M}_{12}$. (This notation is closely related to the labeling of wedge regions by two light vectors, see Sec. III.) Further Δ_{12} and J_{12} will denote the modular objects belonging to $(\mathcal{M}_{12},\Omega)$ and $U_{12,13}(a)$ is the one-parameter group mapping $\mathcal{M}_{12}$ onto $\mathcal{M}_{13}$ (see Theorem 1).

Starting with a set of 3 algebras with $\pm$mi properties, Theorem 1 provides commutation relations between their modular groups. One finds that these groups build a three-dimensional Lie group (3 generators, 3 commutation relations). It turns out to be a representation of the Lorentz group in 2+1 dimensions (for details see Ref. 9):

Theorem 2: (Ref. 9): *Let $\mathcal{M}_{12}$, $\mathcal{M}_{13}$, and $\mathcal{M}_{23}$ be von Neumann algebras acting on a Hilbert space $\mathcal{H}$ and let $\Omega\in\mathcal{H}$ be a common cyclic and separating vector. Further assume the following modular intersection properties:*

$$(\mathcal{M}_{12},\mathcal{M}_{13},\Omega)\ \text{has the}-\text{mi-property},$$

$$(\mathcal{M}_{23},\mathcal{M}_{13},\Omega)\ \text{has the}+\text{mi-property},$$

$$(\mathcal{M}_{23},\mathcal{M}_{12}',\Omega)\ \text{has the}-\text{mi-property}.$$

Then the one-parameter groups

$$\Delta_{12}^{ir},\Delta_{13}^{is},\Delta_{23}^{it}\quad for\ r,s,t\in\mathbf{R}$$

generate a representation of the group SO(2,1).

The main problem in proving this Theorem is to show that the representation of the rotation by an angle of 2π equals 1, see Ref. 9. A relation obtained in this investigation and needed in the following, is given by

Lemma 1 (Ref. 9): Let the assumptions of Theorem 2 be fulfilled. Then the following relations hold:

$$(a)\quad Ad\,U_{13,12}(1)J_{13}(\mathcal{M}_{23})=\mathcal{M}_{23},$$

$$(b)\quad Ad\,U_{12,32}(1)J_{12}(\mathcal{M}_{31})=\mathcal{M}_{31}.$$

At this point it is reasonable to ask how translations arise in this context. For this we assume the existence of another modular inclusion. Applying the symmetry on it we get several unitary groups. To achieve commutativity some more assumptions have to be satisfied. Finally, one obtains a representation of the whole Poincaré group in $2+1$ dimensions.

Theorem 3 (Ref. 1): *Let $\mathcal{M}_{12}$, $\mathcal{M}_{13}$ and $\mathcal{M}_{23}$ be von Neumann algebras fulfilling the assumptions of Theorem 2. Further let $\mathcal{N}$ be another von Neumann algebra with the following properties:*

(a) $(\mathcal{N}\subset\mathcal{M}_{12},\Omega)$ *is* $-hsm$ *inclusion,*

(b) $\mathrm{Ad}\, J_{13}(J_{\mathcal{N}}J_{12})=J_{12}J_{\mathcal{N}}$,

(c) $[\mathrm{Ad}\, J_{23}(J_{\mathcal{N}}J_{12}),J_{\mathcal{N}}J_{12}]=0$. *Then one obtains a faithful, unitary representation $\mathcal{U}_{Trans}$ of the translation group $\mathbf{R}^{2,1}$. If*

(d) for all $\alpha\in\mathbf{R}^{2,1}$ there exists a $\beta\in\mathbf{R}^{2,1}$, so that the relation

$$\mathrm{Ad}\, J_{12}(\mathcal{U}_{\mathrm{Trans}}(\alpha))=\mathcal{U}_{\mathrm{Trans}}(\beta)$$

holds, then the modular groups $\Delta_{12}^{ir},\Delta_{13}^{is},\Delta_{23}^{it}$ and $\Delta_{\mathcal{N}}^{iu}$ generate a representation of the Poincaré group in $2+1$ dimensions. This representation fulfills the spectrum condition.

One explicit commutation relation obtained in the proof of this Theorem (see lemma 12 in Ref. 1) is

$$\mathrm{Ad}\, U_{12,13}(1)(U_{\mathcal{N},12}(a))=U_{\mathcal{N},12}(a)\quad \text{for } a\in\mathbf{R}. \tag{1}$$

We will need this result several times later on.

One might think that the assumptions of Theorem 3 are rather artificial. But using the result of Ref. 12 one finds that 2 wedge-algebras with one lightray in common fulfill the requirement for having a modular intersection with respect to the vacuum (for more details, see Ref. 1, and Sec. III). Furthermore, a wedge algebra and its translation in lightray direction provide an example of a half-sided modular inclusion. We will elaborate on this in the next section.

The topic of this article is an extension of Theorem 2 and Theorem 3 to $3+1$ dimensions. In order to do this let us first review some important facts concerning $3+1$-dimensional quantum field theory.

III. MODULAR INTERSECTIONS OF von NEUMANN ALGEBRAS IN 3+1 DIMENSIONAL QUANTUM FIELD THEORY

Our framework will be the description of quantum field theory in terms of nets of local algebras, see Ref. 2. In this algebraic approach the physical system is characterized by algebras of bounded operators acting on a Hilbert space $\mathcal{H}$, indexed by space–time regions,

$$\mathcal{O}\subset\mathbf{R}^{3,1}\mapsto\mathcal{A}(\mathcal{O}).$$

They might be interpreted as bounded functions of the observables localized in that region. This net is assumed to fulfill the following physically motivated assumptions:[2]

(A) $\mathcal{A}(\mathcal{O}_1)\subset\mathcal{A}(\mathcal{O}_2)$ if $\mathcal{O}_1\subset\mathcal{O}_2$ (isotony),

(B) $\mathcal{A}(\mathcal{O}_1)\subset\mathcal{A}(\mathcal{O}_2)'$ if $\mathcal{O}_1\subset\mathcal{O}_2'$, where $\mathcal{A}(\mathcal{O})'$ denotes the commutant of $\mathcal{A}(\mathcal{O})$, $\mathcal{O}'\in\mathbf{R}^{3,1}$ the causal complement of $\mathcal{O}$ (locality),

(C) There exists a unitary representation of the Poincaré group,

$$\mathcal{U}:\mathcal{P}^{\uparrow}\mapsto\mathcal{B}(\mathcal{H})$$

acting covariantly on the net (Poincaré covariance).

(D) There exists a unique vector $\Omega\in\mathcal{H}$, which is invariant under this representation (vacuum).

Such a net describes a $3+1$-dimensional quantum field theory in the algebraic approach.

The famous Reeh–Schlieder[3] property of the vacuum now states that due to locality and vacuum fluctuations any local algebra is cyclic and separating with respect to the vacuum vector.

This enables one to apply the modular theory to each $(\mathcal{A}(\mathcal{O}),\Omega)$. For some special regions in Minkowski space, namely, wedge regions, these abstract mathematical structures have a direct physically interpretation.

A wedge region is determined by two linearly independent lightlike vectors l_1 and l_2 belonging to the forward lightcone. With a convenient notation introduced by Borchers,[12] it is defined by

$$\mathcal{W}[l_1,l_2] := \{\alpha l_1+\beta l_2+L^{\perp} \mid \alpha>0,\beta<0, l\in L^{\perp}\}.$$

$L^{\perp}$ denotes the set of all vectors lying orthogonal to l_1 and l_2 with respect to the Minkowski metric.

Bisognano and Wichmann[5] showed that if the net is generated by bounded functions of Wightman fields, then the modular groups associated with algebras of wedge regions act as Lorentz boosts. More precisely one obtains the one parameter group of boosts $\Lambda_{l_1,l_2}(t)$ leaving the set $\mathcal{W}[l_1,l_2]$ invariant,

$$\Delta^{it}_{\mathcal{A}(\mathcal{W}[l_1,l_2])}=\mathcal{U}(\Lambda_{l_1,l_2}(-2\pi t)).$$

The reader may consult Ref. 13 for an excellent review about recent results obtained in the application of modular theory in quantum field theory.

For the following we will consider such a net and fix four lightlike vectors:

$$l_1=(1,1,0,0),$$

$$l_2=(1,-(1/3),2\sqrt{2}/3,0),$$

$$l_3=(1,-(1/3),-(\sqrt{2}/3),-(\sqrt{6}/3)),$$

$$l_4=(1,-(1/3),-(\sqrt{2}/3),(\sqrt{6}/3)).$$

The spacelike components of these vectors build a tetrahedron (we thank Schmidt for the idea to this choice). Lemmas 2, 3, and 4 do not depend on the special choice of vectors, as long as they are linearly independent and belong to the forward lightcone. But in this very symmetric case the combination of some special Lorentz transformations implementing some permutations of the four vectors is much simpler than for the general case. The subgroup of $S(4)$, the permutation group of 4 elements, we have in mind, is built by elements of the form $(i)(jkl)=(jkl)(i)$ and $(ij)\times(kl)$ for pairwise different $i,j,k,l\in\{1,2,3,4\}$. Its representation by modular objects will be important in the next section.

These lightlike vectors define wedge regions $\mathcal{W}[l_i,l_j]$ for $i\neq j\in\{1,2,3,4\}$. Let the associated algebras be denoted by $\mathcal{A}(\mathcal{W}[l_i,l_j])$. Now, as already mentioned in the last section, modular intersections occur in a natural way. Analogously to Ref. 12, Lemma 6 and Ref. 1, Proposition 7, one shows

Lemma 2: Let $\mathcal{A}(\mathcal{O})$, $\mathcal{O}\subset\mathbf{R}^{3,1}$, be a net fulfilling the assumptions of the Theorem of Bisognano and Wichmann.[1] Then,

$$(\mathcal{A}(\mathcal{W}[l_i,l_j]),\mathcal{A}(\mathcal{W}[l_i,l_k]),\Omega) \textit{has the} -\text{mi property}$$

for pairwise different i,j,k $\in\{1,2,3,4\}$.

To see how $\pm$hsm-inclusions arise in this context we have to look at wedge regions translated by vectors $a\in\mathbf{R}^{3,1}$,

$$\mathcal{W}[l_i,l_j,a] := \{x\in\mathbf{R}^{3,1} \mid (x-a)\in\mathcal{W}[l_i,l_j]\}.$$

Then we have (analogously to Refs. 12 and 1),

Lemma 3: Let the assumptions be the same as in lemma 2. Then for all $\alpha>0$ and $i\neq j\in\{1,2,3,4\}$,

$$(\mathcal{A}(\mathcal{W}[l_i,l_j,\alpha l_i])\subset\mathcal{A}(\mathcal{W}[l_i,l_j]),\Omega) \text{is a } -\text{hsm}-\text{inclusion.}$$

In particular the one-parameter group that belongs to this inclusion (see Theorem 1) is equal to the representation of the translation in l_i-direction.

Furthermore in a given basis of $\mathbf{R}^{3,1}$ one easily verifies

Lemma 4: Let the assumptions be the same as in lemma 2. Then the 6 modular groups $\Delta^{it}_{\mathcal{A}(\mathcal{W}[l_i,l_j])}$ *generate a representation of the group* SO(3,1).

It is not surprising that the modular groups in Lemma 4 and another ''lightlike'' translated group together generate a representation of the whole Poincaré group.

In the next sections we will in a way invert this observation. Starting with a set of 7 algebras lying in a specific modular position we will construct a unitary representation of the Poincaré group in 3+1 dimensions.

IV. REPRESENTATION OF SO(3,1)

First we will focus our attention to the Lorentz group. Motivated by Lemma 2 we want to construct a representation of it by 6 modular groups of von Neumann algebras.

From our experience in algebraic quantum field theory the simplest Ansatz in this context is:

Assumption I: Let $\mathcal{M}_{ij}$, $1\leqslant i<j\leqslant 4$, be von Neumann algebras acting on a Hilbert space $\mathcal{H}$ with a common cyclic and separating vector $\Omega\in\mathcal{H}$. Further assume that the triple $(\mathcal{M}_{ij},\mathcal{M}_{ik},\Omega)$ has the $-$mi property for pairwise different $i,j,k\in\{1,2,3,4\}$.

In analogy to the case of ''Bisognano–Wichmann''-nets, in this abstract situation we also denote the commutants of $\mathcal{M}_{ij}$ by $\mathcal{M}_{ji}:=\mathcal{M}'_{ij}$. (Notice that Lemma 1h) states that $(\mathcal{M}_{ji},\mathcal{M}_{ki},\Omega)=(\mathcal{M}'_{ij},\mathcal{M}'_{ik},\Omega)$ has the $+$mi property.) Assumption I already fixes two subgroups of the group SO(3,1). (The authors thank Schroer for the remark of relation B):

Lemma 5: (A) The one parameter groups $\Delta^{ia}_{12},\Delta^{ib}_{13}$, *and* Δ^{ic}_{23} *for* $a,b,c\in\mathbf{R}$, *generate a representation of* SO(2,1).

(B) $[U_{14,24}(a),U_{14,34}(b)]=0$ *for all a,b in* $\mathbf{R}$.

(C) The one parameter groups Δ^{ia}_{14}, Δ^{ib}_{24} *and* Δ^{ic}_{34} *for* $a,b,c\in\mathbf{R}$, *span a three-dimensional Lie group.*

Proof: Property (A) follows directly from Theorem 2. For (B) notice that Theorem 1 implies

$$\begin{aligned}
&U_{14,24}(-1+e^{2\pi a})U_{14,34}(-1+e^{2\pi b})\\
&\quad=\Delta^{ia}_{14}(\Delta^{-ia}_{24}\Delta^{ib}_{14})\Delta^{-ib}_{34}\\
&\quad=\Delta^{i(b+(1/2\pi)\,(\ln(e^{-2\pi b}(-1+e^{2\pi a})+1)}_{14}\Delta^{-i(1/2\pi)\,\ln(e^{-2\pi b}(-1+e^{2\pi a})+1)}_{24}\Delta^{-ib}_{34}.
\end{aligned}$$

We used (1f) in the first step and then (1b) to pull the Δ_{14}-factor in front. Commuting the factors Δ_{34} and Δ_{14} as well as Δ_{24} and Δ_{34} and also using the abbreviation $c=-(1/2\pi)\ln(e^{-2\pi a}(e^{2\pi b}-1)+1)$ one similarly gets

$$\begin{aligned}
&U_{14,34}(-1+e^{2\pi b})U_{14,24}(-1+e^{2\pi a})\\
&\quad=\Delta^{i(a+(1/2\pi)\,ln(e^{-2\pi a}(-1+e^{2\pi b})+1)}_{14}\Delta^{i(c-a+(1/2\pi)\ln(e^{2\pi a}(-1+e^{-2\pi c})+1))}_{24}\\
&\qquad\times\Delta^{-i(1/2\pi)\ln(e^{2\pi a}(-1+e^{-2\pi c})+1)}_{34}.
\end{aligned}$$

An easy algebraic transformation shows that the exponents of the modular groups in both equations are equal.

Property (C) follows from property (B). □

Notice that the two commuting groups in (B) are isomorphic to the translations belonging to the isotropy group of the lightray l_4, see Sec. III. The Lie group in (C) consists of these translations and the dilatation in the l_4-direction.

Simple combinatorics show that we obtain 12 commutation relations out of Assumption I. In order to fix a group generated by 6 one-parameter groups one needs 15 relations. As it turns out the Jacobi identities will roughly lead to the three missing ones.

Let us first assume that the algebras are chosen symmetrically. For this we define

Definition 2:

$$\Gamma_{(132)(4)} := U_{21,23}(1)J_{12}U_{13,12}(1)J_{13} = U_{21,23}(1)U_{13,12}(1)$$

and those equations obtained from this by permuting the indices. Using Theorem (1i) one can also write $\Gamma_{(132)(4)} := U_{12,32}(1)J_{12}U_{13,12}(1)J_{13}$. We now state

Assumption II:

$$\text{(a) } \mathrm{Ad}\,\Gamma_{(132)(4)}(\mathcal{M}_{14}) = \mathcal{M}_{34},\ \mathrm{Ad}\,\Gamma_{(132)(4)}(\mathcal{M}_{24}) = \mathcal{M}_{14},$$

$$\text{(b) } \mathrm{Ad}\,\Gamma_{(134)(2)}(\mathcal{M}_{12}) = \mathcal{M}_{32},\ \mathrm{Ad}\,\Gamma_{(134)(2)}(\mathcal{M}_{42}) = \mathcal{M}_{12}.$$

This situation is given in Sec. III (due to the symmetric choice of the vectors $l_1,\ldots,l_4$ and the result of Bisognano and Wichmann[5]).

Lemma 6: Products of $\Gamma_{(132)(4)}$ *and* $\Gamma_{(134)(2)}$ *generate a representation of a subgroup of* S(4)*, the permutation group of 4 elements. This subgroup is built by elements of the form (ijk)(l),(ij)(kl) with pairwise different* $i,j,k,l \in \{1,2,3,4.\}$ The representation acts on the algebras by permuting their indices in the denoted way.

Proof: Using Theorem 1 and Lemma 1 it is an easy exercise to show that $\Gamma_{(132)(4)}$ and $\Gamma_{(134)(2)}$ act in the right way on the algebras $\mathcal{M}_{ij}$ for $i,j \in \{1,2,3\}, i \neq j$, since it is the same situation as in the three-dimensional case.

We will sketch the proof for $\Gamma_{(132)(4)}$ and $\mathcal{M}_{13}$,

$$\begin{aligned}\mathrm{Ad}\,\Gamma_{(132)(4)}(\mathcal{M}_{13}) &= \mathrm{Ad}\,U_{21,23}(1)J_{12}U_{13,12}(1)J_{13}(\mathcal{M}_{13})\\ &= \mathrm{Ad}\,U_{21,23}(1)J_{12}(\mathcal{M}_{21})\\ &= \mathrm{Ad}\,U_{21,23}(1)(\mathcal{M}_{12}) = \mathcal{M}_{32}.\end{aligned}$$

Therefore this is also true for their modular objects. For algebras with indices i or $j = 4$ we need the following observations:

$$\begin{aligned}\Gamma_{(132)(4)} &= \mathrm{Ad}\,\Gamma_{(132)(4)}(\Gamma_{(132)(4)})\\ &= \mathrm{Ad}\,\Gamma_{(132)(4)}(U_{21,23}(1)J_{12}U_{13,12}(1)J_{13})\\ &= U_{13,12}(1)J_{31}U_{32,31}(1)J_{32}. \qquad (2)\end{aligned}$$

Analogously one gets

$$\Gamma_{(132)(4)} = U_{32,31}(1)J_{23}U_{21,23}(1)J_{21}.$$

Combined with (2) and Theorem (1c) this leads to the relation

$$\begin{aligned}\Gamma^3_{(132)(4)} &= (U_{21,23}(1)J_{12}U_{13,12}(1)J_{13})(U_{13,12}(1)J_{31}U_{32,31}(1)J_{32})U_{32,31}(1)J_{23}U_{21,23}(1)J_{21}\\ &= U_{21,23}(1)J_{12}(U_{13,12}(1)U_{13,12}(-1))(U_{32,31}(1)U_{32,31}(-1))U_{21,23}(1)J_{21}\\ &= U_{21,23}(1)(J_{12}U_{21,23}(1)J_{12}) = 1.\end{aligned}$$

Using Assumption (IIa) this implies

$$\mathrm{Ad}\,\Gamma_{(132)(4)}(\mathcal{M}_{34}) = \mathrm{Ad}\,\Gamma^2_{(132)(4)}(\mathcal{M}_{14}) = \mathrm{Ad}\,\Gamma^{-1}_{(132)(4)}(\mathcal{M}_{14}) = \mathcal{M}_{24}.$$

Analogous relations hold for $\Gamma_{(134)(2)}$. Taking products of $\Gamma_{(134)(2)}$ and $\Gamma_{(132)(4)}$ one obtains all permutations of the form $(ijk)(l)$ and $(ij)(kl)$ for pairwise different $i,j,k,l \in \{1,2,3,4\}$. □

Assuming that the modular groups generate a 6 dimensional Lie group we use these symmetries and the Jacobi identities to obtain the missing commutation relations. At the end of this section we will give a formulation of this additional Assumption using only modular data (see Assumption III and Propositon 2).

Proposition 1: Let Assumptions I and II be fulfilled. Further assume that the modular groups Δ_{kl}^{ia} *for* $k,l \in \{1,2,3,4\}$ *generate a six-dimensional Lie group. Then this Lie group is a representation of the group* SO(3,1).

Proof: Let $\lambda_{kl} := (i/2\pi)(d/dt)\Delta_{kl}^{it}|_{t=0}$ denote the generators. Theorem (1b) and $\Delta_{kl}^{it} = \Delta_{lk}^{-it}$ give the relations

$$[\lambda_{ij},\lambda_{ik}] = \lambda_{ij} - \lambda_{ik}, \tag{3}$$

$$\lambda_{ij} = -\lambda_{ji}. \tag{4}$$

It remains to prove the right commutation relations $[\lambda_{ij},\lambda_{kl}]$ for pairwise different indices. Starting with linear combinations summing to zero and taking Lie-products according to (3) it is a lengthy but easy exercise to show the linear independence of 5 generators assuming that the algebras $\mathcal{M}_{ij}$ are not identic. We further need the following observation:

Lemma 7: The real linear subspace formed by the elements λ_{ij} *commuting with* λ_{12} *is at least two-dimensional.*

Proof: Rewriting the Jacobi identity one obtains

$$[\lambda_{12},[\lambda_{12}-\lambda_{14},\lambda_{12}-\lambda_{32}]] = 0.$$

Assume

$$[\lambda_{12}-\lambda_{14},\lambda_{12}-\lambda_{32}] = \alpha\lambda_{12}$$

for $\alpha \in \mathbf{R}$. By (3) this is equivalent to

$$[\lambda_{14},\lambda_{32}] = (\alpha-2)\lambda_{12} + \lambda_{32} + \lambda_{14}. \tag{5}$$

Applying on both sides the ''permutation'' $\Gamma_{(14)(32)}$ gives

$$[\lambda_{41},\lambda_{23}] = [\lambda_{14},\lambda_{32}] = (\alpha-2)\lambda_{43} + \lambda_{23} + \lambda_{41}. \tag{6}$$

But (5) and (6) imply

$$(\alpha-2)(\lambda_{43}-\lambda_{12}) + 2\lambda_{23} + 2\lambda_{41} = 0,$$

leading to a contradiction to the linear independence of 4 generators. □

We now take such a commuting element

$$\lambda = \left(\sum_{j=2}^{4} \alpha_{1j}\lambda_{1j}\right) + \left(\sum_{j=3}^{4} \alpha_{j2}\lambda_{j2}\right) + \alpha_{34}\lambda_{34}$$

with real α_{ij}. According to the linear independence and the commutation relation (3) it is easy to see that $\alpha_{34} \neq 0$ holds. The relation $[\lambda_{12},\lambda] = 0$ implies

$$-\alpha_{34}[\lambda_{12},\lambda_{34}] = \sum_{j=3}^{4} (\alpha_{1j}-\alpha_{j2})\lambda_{12} - \alpha_{13}\lambda_{13} - \alpha_{14}\lambda_{14} + \alpha_{32}\lambda_{32} + \alpha_{42}\lambda_{42}. \tag{7}$$

Applying $\mathrm{Ad}\,\Gamma_{(12)(34)}$ to this equation the left-hand side is invariant and the right-hand side gives $\Sigma_{j=3}^{4}(\alpha_{1j}-\alpha_{j2})\lambda_{21}-\alpha_{13}\lambda_{24}-\alpha_{14}\lambda_{23}+\alpha_{32}\lambda_{41}+\alpha_{42}\lambda_{31}$. A subtraction of these two equations gives

$$0=2(\alpha_{13}-\alpha_{32}+\alpha_{14}-\alpha_{42})\lambda_{12}+(\alpha_{42}-\alpha_{13})\lambda_{13}+(\alpha_{32}-\alpha_{14})\lambda_{14}+(\alpha_{14}-\alpha_{32})\lambda_{23}$$
$$+(\alpha_{13}-\alpha_{42})\lambda_{24}$$

and the linear independence of the generators implies $\alpha_{42}=\alpha_{13}$ and $\alpha_{14}=\alpha_{32}$. Hence (7) may be rewritten as

$$[\lambda_{12},\lambda_{34}]=\alpha(\lambda_{13}-\lambda_{42})+\beta(\lambda_{14}-\lambda_{32}) \tag{8}$$

with $\alpha:=\alpha_{13}/\alpha_{34}$ and $\beta:=\alpha_{14}/\alpha_{34}$. Using a second time the Jacobi identity we obtain

$$[[\lambda_{12},\lambda_{34}],\lambda_{14}]=\lambda_{12}-\lambda_{34}. \tag{9}$$

Next we insert relation (8) into (9) and ''permute'' the result by $\Gamma_{(1)(234)}$. This leads to

$$\beta[\lambda_{12},\lambda_{34}]=-(\lambda_{13}-\lambda_{42})+\alpha(\lambda_{14}-\lambda_{32}). \tag{10}$$

The comparison of the coefficients in (8) and (10) gives the missing relation

$$[\lambda_{12},\lambda_{34}]=\lambda_{13}-\lambda_{42}-\lambda_{14}+\lambda_{32}. \tag{11}$$

The rest follows from symmetry.

Now all 15 commutations relations are fixed. In order to make sure that the modular groups $\Delta_{14}^{it_{14}},\ldots,\Delta_{34}^{it_{34}}$ generate a representation of SO(3,1) one has to investigate the effect of the rotation by an angle 2π. But this is the identity, as shown in the proof of Theorem 2 and Lemma 1 (for details, see Ref. 9). □

Let us next propose an assumption leading to the premise of Proposition 1:

Assumption III: There exists an $\epsilon'>0$ and two strict monotone, continuous mappings $\delta:]0,\epsilon'[\mapsto R^{+}$ and $\delta':]0,\epsilon'[\mapsto R^{+}$ so that for all $0<\epsilon<\epsilon'$ the relation

$$\mathrm{Ad}\,J_{12}(\mathcal{P}_{\epsilon})\subset\mathcal{P}_{\delta(\epsilon)}\mathcal{S}_{\delta'(\epsilon)}$$

holds, where

$$\mathcal{P}_{\epsilon}:=\{\Delta_{14}^{ir}\Delta_{24}^{is}\Delta_{34}^{it}\,|\,|(r,s,t)|:=\sqrt{r^2+s^2+t^2}<\epsilon\},$$

and

$$\mathcal{S}_{\epsilon}:=\{\Delta_{12}^{ir}\Delta_{13}^{is}\Delta_{23}^{it}\,|\,|(r,s,t)|<\epsilon\}$$

denote neighborhoods of the Lie groups introduced in Lemma 5.

Proposition 2: Assumptions I, II, and III imply that the 6 modular groups $\Delta_{12}^{it_{12}},\ldots,\Delta_{34}^{it_{34}}$ *for* $t_{12},\ldots,t_{34}\in\mathbf{R}$ *generate a six-dimensional Lie group.*

Proof: We show that products of the modular groups $\Delta_{12}^{it_{12}},\ldots,\Delta_{34}^{it_{34}}$ can be commuted into a determined order in a neighborhood of the identity. For this notice that Assumption III and the symmetry imply that $\mathrm{Ad}\,J_{ij}(\mathcal{P}_{\epsilon})\subset\mathcal{P}_{\delta(\epsilon)}\mathcal{S}_{\delta(\epsilon)}$ holds for $i,j\in\{1,2,3\}$. (For convenience we choose a sloppy notation in this proof using the same δ for all functions of type δ, δ'.) Now Theorem (1g) states

$$\mathrm{Ad}\,U_{13,12}(2)(\mathcal{P}_{\epsilon})=\mathrm{Ad}\,J_{12}J_{13}(\mathcal{P}_{\epsilon})\subset\mathcal{P}_{\delta(\epsilon)}\mathcal{S}_{\delta(\epsilon)}. \tag{12}$$

With help of Theorem 1 one further shows for all $r\in\mathbf{R}$,

$$U_{13,12}(2)\Delta_{14}^{ir}=\Delta_{14}^{ir}U_{13,12}(2e^{2\pi r}).$$

Together with relation (12) this implies

$$\mathrm{Ad}\, U_{13,12}(2-2e^{2\pi r})(\mathcal{P}_\epsilon)\subset\mathcal{P}_{\delta(\epsilon)}\mathcal{S}_{\delta(\epsilon)}$$

for r in a neighborhood of zero. Due to the permutation symmetry $\Gamma_{(123)(4)}$ this also holds for $U_{12,32}, U_{13,23}$. For $U_{14,24}$, $U_{14,34}$, and $U_{24,34}$ analogous relations follow directly from Lemma 5, because they are elements of the Lie group $\mathcal{P}$. Now Theorem (1f) finishes the proof. □

Combining Proposition 1 and 2, we finally arrive at

Theorem 4: *Let* $\mathcal{M}_{ij}$, $1\leqslant i<j\leqslant 4$ *be 6 von Neumann algebras fulfilling Assumptions I, II, and III. Then their modular groups generate a representation of* SO(3,1).

A model fulfilling the assumptions of Theorem 4 was given in Sec. III. In that case the 6 algebras are realized by algebras belonging to wedge-regions in 3+1-dimensional Minkowski space.

V. REPRESENTATION OF THE TRANSLATIONS

In this section we extend the representation given by Theorem 4 to a representation of the whole Poincaré group in 3+1 dimensions. Motivated by Lemma 3 we make the following assumption (in addition to the assumptions I to III):

Assumption (A): Let $\mathcal{N}$ be another von Neumann algebra, so that the triple $(\mathcal{N}\subset\mathcal{M}_{12},\Omega)$ is a $-$hsm inclusion.

As a candidate for the translation in direction of l_1 we take

$$\mathcal{U}_{l_1}(a):=U_{12,\mathcal{N}}(a).$$

Choosing a basis in $\mathbf{R}^{3,1}$, see Sec. III, one easily verifies

$$\Lambda_{l_1,l_3}(-\ln 2)\Lambda_{l_2,l_3}(\ln 2)l_1=l_2.$$

Therefore a candidate to define the translations in l_2-direction is given by

$$\mathcal{U}_{l_2}(a):=\mathrm{Ad}\,\mathcal{U}_{Lor}(\Lambda_{l_1,l_3}(-\ln 2)\Lambda_{l_2,l_3}(\ln 2))(\mathcal{U}_{l_1}(a))=\mathrm{Ad}\, U_{13,23}(1)(\mathcal{U}_{l_1}(a)),$$

and analogously,

$$\mathcal{U}_{l_3}(a):=\mathrm{Ad}\, U_{12,32}(1)(\mathcal{U}_{l_1}(a)),$$

$$\mathcal{U}_{l_4}(a)=\mathrm{Ad}\, U_{12,42}(1)(\mathcal{U}_{l_1}(a)),$$

for all $a\in\mathbf{R}$. But there is an alternative way to these choices. We also have

$$\Lambda_{l_1,l_4}(-\ln 2)\Lambda_{l_2,l_4}(\ln 2)l_1=l_2. \tag{13}$$

Hence it is also reasonable to set

$$\tilde{\mathcal{U}}_{l_2}(a)=\mathrm{Ad}\, U_{14,24}(1)(\mathcal{U}_{l_1}(a))$$

and similarly for the others. The following assumption implies the equivalence of both definitions. Furthermore it makes sure that they are compatible with respect to the permutations defined in the last section.

Assumption (B): $\mathrm{Ad}\,\Gamma_{(1)(234)}(J_{\mathcal{N}}J_{12})=J_{\mathcal{N}}J_{12}$.

This is motivated by the observations made in Sec. III. Because of Theorem (1g) $J_{\mathcal{N}}J_{12}$ can be interpreted as a discrete translation in l_1-direction. So it should be left invariant by $\Gamma_{(1)(234)}$.

Notice that Assumption (b) of Theorem 3 can now be derived from Assumptions (A) and (B):

$$\mathrm{Ad}\, J_{13}(J_{12}J_{\mathcal{N}}) = \mathrm{Ad}\, \Gamma_{(1)(234)} J_{12}(J_{12}J_{\mathcal{N}}) = J_{\mathcal{N}}J_{12}\,. \tag{14}$$

Analogously one obtains

$$\mathrm{Ad}\, J_{14}(J_{12}J_{\mathcal{N}}) = J_{\mathcal{N}}J_{12}\,. \tag{15}$$

Next we prove the equivalence of both definitions:

Lemma 8: Assume (A) and (B). Then,

$$\mathcal{U}_{l_i}(a) = \tilde{\mathcal{U}}_{l_i}(a)$$

for all $a \in \mathbf{R}$ *and* $i \in \{2,3,4\}$.

Proof: Using (1) and Assumption B, then

$$[U_{12,14}(1), U_{12,\mathcal{N}}(2)] = [U_{12,14}(1), J_{\mathcal{N}}J_{12}] = 0 \tag{16}$$

holds. Combining this with Assumption B one gets

$$[\Gamma_{(1)(234)} U_{12,14}(1), J_{\mathcal{N}}J_{12}] = 0. \tag{17}$$

Using Theorem (1c) it is easy to see, that

$$[\Gamma_{(1)(234)} U_{12,14}(1), J_{12}] = 0 \tag{18}$$

is fulfilled. Together with (17) we have

$$[\Gamma_{(1)(234)} U_{12,14}(1), J_{\mathcal{N}}] = 0. \tag{19}$$

This implies that the modular conjugation to $(\mathrm{Ad}\, \Gamma_{(1)(234)} U_{12,14}(1)(\mathcal{N}), \Omega)$ is the modular conjugation $J_{\mathcal{N}}$ of $\mathcal{N}$. Furthermore,

$$\mathrm{Ad}\, \Gamma_{(1)(234)} U_{12,14}(1)(\mathcal{N}) \subset \mathcal{M}_{12}$$

holds, which shows that Ω is separating for

$$(\mathcal{N} \cup \mathrm{Ad}\, \Gamma_{(1)(234)} U_{12,14}(1)(\mathcal{N})) \subset \mathcal{M}_{12}$$

again with the same conjugation. So modular theory tells us

$$\mathcal{N} = \mathrm{Ad}\, \Gamma_{(1)(234)} U_{12,14}(1)(\mathcal{N}).$$

In particular we have

$$[\Delta_{\mathcal{N}}^{it}, \Gamma_{(1)(234)} U_{12,14}(1)] = 0 \tag{20}$$

for all $t \in \mathbf{R}$. Completely analogous to (1) the relation

$$[U_{12,14}(a), \mathcal{U}_{l_1}(b)] = [U_{12,14}(a), U_{12,\mathcal{N}}(b)] \quad \text{for all} \quad a,b \in \mathbf{R} \tag{21}$$

holds (for details see Lemma 12 in Ref. 1). Now using (20) and Theorem (1f) this gives

$$\mathrm{Ad}\, \Gamma_{(1)(234)}(\mathcal{U}_{l_1}(a)) = \mathcal{U}_{l_1}(a). \tag{22}$$

With $\Gamma_{(1)(234)} = \Gamma_{(123)(4)}\Gamma_{(134)(2)}$ it follows that

$$\mathrm{Ad}\, \Gamma_{(123)(4)}^{-1}(\mathcal{U}_{l_1}(a)) = \mathrm{Ad}\, \Gamma_{(134)(2)}(\mathcal{U}_{l_1}(a)) \tag{23}$$

holds. Definition 2 and Theorem 1 imply

$$\Gamma_{(134)(2)} = U_{14,34}(1)U_{13,14}(1), \tag{24}$$

$$\Gamma_{(132)(4)} = \Gamma^{-1}_{(123)(4)} = U_{12,32}(1)U_{13,12}(1). \tag{25}$$

Using relations (1) and (22) we obtain

$$\mathrm{Ad}\, U_{13,14}(1)(\mathcal{U}_{l_1}(a)) = \mathrm{Ad}\, \Gamma_{(1)(234)} U_{12,13}(1)(\mathcal{U}_{l_1}(a)) = \mathcal{U}_{l_1}(a). \tag{26}$$

Inserting (1) and (26) into (23), one finally sees

$$\tilde{\mathcal{U}}_{l_3}(a) = \mathrm{Ad}\, U_{14,34}(1)(\mathcal{U}_{l_1}(a)) = \mathrm{Ad}\, U_{12,32}(1)(\mathcal{U}_{l_1}(a)) = \mathcal{U}_{l_3}(a).$$

The remaining relations follow by symmetry. □

So finally we get the following ''candidates'' for the representators of translations in $\mathbf{R}^{3,1}$:

Definition 3:

$$\text{(a)}\ \mathcal{U}_{l_1}(a) := U_{12,\mathcal{N}}(a),$$

$$\text{(b)}\ \mathcal{U}_{l_2}(a) := \mathrm{Ad}\, U_{13,23}(1)(\mathcal{U}_{l_1}(a)) = \mathrm{Ad}\, U_{14,24}(1)(\mathcal{U}_{l_1}(a)),$$

$$\text{(c)}\ \mathcal{U}_{l_3}(a) := \mathrm{Ad}\, U_{12,32}(1)(\mathcal{U}_{l_1}(a)) = \mathrm{Ad}\, U_{14,34}(1)(\mathcal{U}_{l_1}(a)),$$

$$\text{(d)}\ \mathcal{U}_{l_4}(a) := \mathrm{Ad}\, U_{12,42}(1)(\mathcal{U}_{l_1}(a)) = \mathrm{Ad}\, U_{13,43}(1)(\mathcal{U}_{l_1}(a)),$$

for all $a \in \mathbf{R}$.

Using relations (1), (22), Definition 2 and Theorem 1 it is a straightforward calculation to verify that this definition respects the symmetries introduced in the last section. To make sure that these unitary groups commute, we state analogously to Theorem (3c):

Assumption (C): $[\mathrm{Ad}\, J_{23}(J_{\mathcal{N}} J_{12}), J_{\mathcal{N}} J_{12}] = 0$.

This is again motivated by the discussion in Sec. III. In the case of Bisognano–Wichmann-fields J_{23} acts, up to a spatial rotation, like CTP. So it maps $J_{\mathcal{N}} J_{12}$ upon another translation.

From relation (14) and Assumption (C) it follows that the groups $\mathcal{U}_{l_i}$ commute and that they fulfill the spectrum condition. For details the reader may consult the proof of Proposition 11 in Ref. 1. Hence,

Definition 4: $\mathcal{U}_{\mathrm{Trans}} : \mathbf{R}^{3,1} \to \mathcal{U}(H)$ with

$$\alpha = \left(\sum_{i=1}^{4} \alpha_i l_i \right) \to \mathcal{U}_{\mathrm{Trans}}(\alpha) := \mathcal{U}_{l_1}(\alpha_1)\mathcal{U}_{l_2}(\alpha_2)\mathcal{U}_{l_3}(\alpha_3)\mathcal{U}_{l_4}(\alpha_4)$$

defines a representation of $\mathbf{R}^{3,1}$. It remains to show that these translations have the right commutation relations with the representation $\mathcal{U}_{\mathrm{Lor}}$ of the Lorentz group. As in Theorem (3d) we need

Assumption (D): For all $\alpha \in \mathbf{R}^{3,1}$, there exists a $\beta \in \mathbf{R}^{3,1}$, so that

$$\mathrm{Ad}\, J_{12}(\mathcal{U}_{\mathrm{Trans}}(\alpha)) = \mathcal{U}_{\mathrm{Trans}}(\beta).$$

This is very similar to Assumption III. It makes sure that the whole representation $\mathcal{U}_{\mathrm{Lor}}$ maps translations upon translations. To see this, notice that the relation

$$\mathrm{Ad}\, \mathcal{U}_{\mathrm{Lor}}(\Lambda_{l_i, l_j}(2\pi t))(\mathcal{U}_{l_i}(a)) = \mathcal{U}_{l_i}(e^{2\pi t} a) \tag{27}$$

holds. Using Theorem 1 and Definition 2 one finds that $\mathcal{U}_{\mathrm{Lor}}(\Lambda_{l_i, l_j}(z \ln 2))$ maps translations upon translations for all $z \in \mathbf{Z}$. But these elements form a dense subset of SO(3,1) and so the claim follows from continuity.

So together $\mathcal{U}_{\mathrm{Lor}}$ and $\mathcal{U}_{\mathrm{Trans}}$ form a Lie group. The next Proposition states, that they have the correct commutation relations with each other.

Proposition 3: Assume (A)–(D). Then $\mathcal{U}_{\mathrm{Lor}}$ and $\mathcal{U}_{\mathrm{Trans}}$ generate a representation of the Poincaré group in 3+1 dimensions satisfying the spectrum condition.

Proof: Denote by $t_i := -(d/da)\mathcal{U}_{l_i}(a)_{|a=0}$ the generators of the translations. Relation (27) implies

$$[\lambda_{ij}, t_i] = -t_i . \tag{28}$$

With help of the Jacobi identities, one finds

$$[\lambda_{12}, [t_1, \lambda_{32}]] = -t_1 , \tag{29}$$

$$[\lambda_{13}, [t_1, \lambda_{32}]] = t_1 . \tag{30}$$

As already mentioned above $\mathcal{U}_{\mathrm{Lor}}$ maps translations upon translations, so

$$[t_1, \lambda_{32}] = \sum_{i=1}^{4} \alpha_i t_i \quad \text{with} \quad \alpha_i \in \mathbf{R} \tag{31}$$

holds. Inserting relation (31) into (29) one gets

$$-\alpha_1 t_1 + \alpha_2 t_2 + \alpha_3 [\lambda_{12}, t_3] + \alpha_4 [\lambda_{12}, t_4] = -t_1 .$$

Analogously the substitution of (31) into (30) gives

$$-\alpha_1 t_1 + \alpha_2 [\lambda_{13}, t_2] + \alpha_3 t_3 + \alpha_4 [\lambda_{13}, t_4] = t_1 .$$

Using the symmetries a summation of these two equations leads to

$$(\alpha_2 - \alpha_3)[t_3, \lambda_{12}] = (1 + \alpha_1 - \alpha_2) t_2 + (\alpha_1 - \alpha_3 - 1) t_1 . \tag{32}$$

$\alpha_2 - \alpha_3 \neq 0$ holds because of the linear independence of t_1 and t_2 (which is easy to see by commutation of $\alpha t_1 + \beta t_2 = 0$ with λ_{12}). So we obtain

$$[\lambda_{12}, t_3] = -\frac{(\alpha_1 - \alpha_3 - 1)}{(\alpha_2 - \alpha_3)} t_1 - \frac{(1 + \alpha_1 - \alpha_2)}{(\alpha_2 - \alpha_3)} t_2 =: \xi_1 t_1 + \xi_2 t_2 . \tag{33}$$

$t_1, \ldots, t_4$ are linearly independent. This can be shown analogously to the linear independence of the boost-generators and it is an easy but lengthy computation of the same type. For details one may look at Ref. 14.

Applying $\mathrm{Ad}\,\Gamma_{(123)(4)}$ to (33) the comparison with (31) gives two sets of solutions for α_2 and α_3,

$$\{\alpha_2 = -1; \alpha_3 = 1\} \quad \text{and} \quad \{\alpha_2 = \alpha_3 + 1\}.$$

Using the Jacobi identities another time the second case again leads to contradiction. See Ref. 14 for more details. Therefore we obtain the remaining relation

$$[\lambda_{12}, t_3] = t_2 - t_1$$

and again the rest follows from symmetry. □

Combining Theorem 4 and Proposition 3 we finally arrive at

Theorem 5: *Let $\mathcal{M}_{ij}, i<j \in \{1,2,3,4\}$ be von Neumann algebras fulfilling Assumptions I, II, III and A to D. Then their modular groups generate a representation of the Poincaré group in 3+1 dimensions, which fulfills the spectrum condition.*

We can use Theorem 5 in order to construct a $3+1$-dimensional quantum field theory starting from a set of seven algebras $\mathcal{M}_{ij}$ for $i,j<\{1,2,3,4\}$ and $\mathcal{N}$ fulfilling Assumptions I, II, III and A to D. For this one further needs the assumption that Ω is also cyclic for the local algebras to be constructed. We start by interpreting $\mathcal{M}_{ij}$ as the local algebras associated with the wedge regions $\mathcal{W}[l_i,l_j]$. But this is not unique due to the invariance of the wedge regions under special Poincaré group elements. Therefore we use the minimal definition by taking the intersection of all possible choices. Analogously we define local algebras associated to double cone. As already mentioned above Ω is assumed to be cyclic for these algebras and therefore modular theory implies

$$\mathcal{A}(\mathcal{W}[l_i,l_j])=\mathcal{M}_{ij}.$$

For details one may look up,[5] where the construction sketched here is carried out in detail.

VI. OPEN QUESTIONS

We conclude this article by mentioning some problems that are left open.

Looking at the requirements we assumed a symmetric situation, see Assumption II. But it seems plausible that the assumption of a special symmetric situation is not fundamental. Such a situation may be achieved by applying suitable unitary transformations on more general sets of algebras. So we expect that this assumption might be omitted.

Furthermore Assumption III, used to be able to apply the Jacobi identity, calls for nicer criteria. In the given form it is hard to verify. Therefore, it is desirable to have a formulation which is manageable. The presented one was only made for technical purposes and should be formulated in a less technical way.

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Capacity of quantum channels using product measurements[a)]

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The capacity of a quantum channel for transmission of classical information depends in principle on whether product states or entangled states are used at the input, and whether product or entangled measurements are used at the output. We show that when *product measurements* are used, the capacity of the channel is achieved with *product input states*, so that entangled inputs do not increase capacity. We show that this result continues to hold if sequential measurements are allowed, whereby the choice of successive measurements may depend on the results of previous measurements. We also present a new simplified expression which gives an upper bound for the Shannon capacity of a channel, and which bears a striking resemblance to the well-known Holevo bound. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1327598]

I. INTRODUCTION

A. Overview

Bennett and Shor[1] note that there are, in principle, four basic types of channel capacities for ''classical'' communication using quantum signals, i.e., communications in which signals are sent using an ''alphabet'' of pure states of quantum systems and decoded using measurements on the (possibly mixed state) signals which arrive. The mixed states are the result of noise which is represented by a *stochastic* or completely positive, trace-preserving map Φ. The four possible capacities correspond to using product or entangled states at the input, and using product or entangled measurements at the output. These are denoted as follows: C_{PP}, product signals and product measurements; C_{PE}, product signals and entangled measurements; C_{EP}, entangled signals and product measurements; C_{EE}, entangled signals and entangled measurements. In more precise language ''using product'' means restricting to products and ''using entangled'' means using arbitrary (product or entangled) states or measurements. Hence, it is evident that $C_{\mathrm{PP}} \leqslant \{C_{\mathrm{EP}}, C_{\mathrm{PE}}\} \leqslant C_{\mathrm{EE}}$. The main purpose of this note is to show that $C_{\mathrm{PP}} = C_{\mathrm{EP}}$, i.e., that if one is restricted to using product measurements, then using entangled inputs does not increase the capacity. Thus $C_{\mathrm{PP}} = C_{\mathrm{EP}} \leqslant C_{\mathrm{PE}} \leqslant C_{\mathrm{EE}}$. It is known[2–4] that one can have strict inequality in $C_{\mathrm{PP}} < C_{\mathrm{PE}}$ for certain non-unital channels. The question of whether or not one can have strict inequality in $C_{\mathrm{PE}} \leqslant C_{\mathrm{EE}}$ is open, although numerical evidence[5,6] suggests equality.

B. Notation and definitions

To give precise definitions, we use relatively standard notation[7,8] in which $\mathcal{M} = \{E_b\}$ denotes a ''positive operator valued measurement'' (POVM) i.e., $E_b \geqslant 0$ and $\Sigma_b E_b = I$. Let ρ_j denote a set (or alphabet) of pure state density matrices, π_j a discrete probability vector, and $\rho = \Sigma_j \pi_j \rho_j$. We

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let $\mathcal{E}=\{\pi_j,\rho_j\}$ denote this ensemble of input states. Both E_b and ρ_j are operators on a Hilbert space $\mathcal{H}$, so that the stochastic map Φ (representing the noise in the channel) acts on $B(\mathcal{H})$, the algebra of bounded operators on $\mathcal{H}$. We will write $\tilde{\mathcal{E}}=\{\pi_j,\Phi(\rho_j)\}$ for the ensemble of output states emerging from the channel.

We write the dual of Φ (or adjoint with respect to the Hilbert–Schmidt inner product) as $\widehat{\Phi}$ so that $\mathrm{Tr}[\Phi(\rho)\,E]=\mathrm{Tr}[\rho\,\widehat{\Phi}(E)]$. The adjoint of a stochastic map takes a POVM $\mathcal{M}=\{E_b\}$ to another POVM $\hat{\mathcal{M}}=\{\hat{E}_b\}$ since the trace-preserving condition on Φ is equivalent to $\widehat{\Phi}(I)=I$.

The information content of a noiseless quantum channel with a fixed input ensemble and a fixed POVM can be described using the standard Shannon formula of classical information theory.

Definition 1: For a fixed ensemble $\mathcal{E}=\{\pi_j,\rho_j\}$ and a POVM $\mathcal{M}=\{E_b\}$ on a Hilbert space $\mathcal{H}$, the quantum mutual information is given by

$$I^q(\mathcal{E};\mathcal{M})=S(\mathrm{Tr}[\rho E_b])-\sum_j \pi_j S(\mathrm{Tr}[\rho_j E_b]), \tag{1}$$

where $S(\mathrm{Tr}[\rho E_b])$ denotes the Shannon entropy $-\Sigma_b p_b\log p_b$ of the probability vector with elements $p_b=\mathrm{Tr}[\rho E_b]$ [and similarly for $S(\mathrm{Tr}[\rho_j E_b])$].

The information content of a noisy channel defined by the stochastic map Φ is obtained from (1) by replacing $\mathcal{E}$ by the output ensemble $\tilde{\mathcal{E}}=\{\pi_j,\Phi(\rho_j)\}$. Alternatively, since $\mathrm{Tr}[\Phi(\rho_j)\,E]=\mathrm{Tr}[\rho_j\,\widehat{\Phi}(E)]$, we could instead choose to regard the ''noise'' as acting on the POVM, and obtain the capacity from (1) by replacing $\mathcal{M}$ by $\hat{\mathcal{M}}$. Although this viewpoint is atypical, it can be useful, as we will see in Sec. IV.

Definition 2: For a stochastic map Φ, an input ensemble $\mathcal{E}=\{\pi_j,\rho_j\}$ and a POVM $\mathcal{M}=\{E_b\}$, the quantum information content is given by

$$I^q_\Phi(\mathcal{E};\mathcal{M})=I^q(\tilde{\mathcal{E}};\mathcal{M})=I^q(\mathcal{E};\hat{\mathcal{M}})=S(\mathrm{Tr}[\Phi(\rho)E_b])-\sum_j \pi_j S(\mathrm{Tr}[\Phi(\rho_j)E_b]). \tag{2}$$

We consider memoryless channels in which multiple uses of the channel are described by the n-fold tensor product $\Phi\otimes\Phi\cdots\otimes\Phi$ acting on the tensor product Hilbert space $\mathcal{H}\otimes\mathcal{H}\cdots\otimes\mathcal{H}$ which we denote by $\Phi^{\otimes n}$ and $\mathcal{H}^{\otimes n}$, respectively. This allows us to define the ''ultimate'' information capacity of the channel as the asymptotic rate achievable when entangled inputs and measurements are used.

Definition 3: The entangled signals/entangled measurements capacity of a quantum channel is defined as

$$C_{\mathrm{EE}}(\Phi)=\lim_{n\to\infty}\frac{1}{n}\sup_{\mathcal{E},\mathcal{M}} I^q_{\Phi^{\otimes n}}(\mathcal{E};\mathcal{M}), \tag{3}$$

where the supremum is taken over all possible (product or entangled) signals and measurements on $\mathcal{H}^{\otimes n}$.

To define capacity restricted to product measurements, we write $\mathcal{M}^{\otimes n}$ for a product POVM of the form $\{E_{b_1}\otimes E_{b_2}\cdots\otimes E_{b_n}\}$.

Definition 4: The entangled signals/product measurements capacity of a quantum channel is defined as

$$C_{\mathrm{EP}}(\Phi)=\lim_{n\to\infty}\frac{1}{n}\sup_{\mathcal{E},\mathcal{M}^{\otimes n}} I^q_{\Phi^{\otimes n}}(\mathcal{E};\mathcal{M}^{\otimes n}). \tag{4}$$

Note that the existence of the limits follows from superadditivity of the classical capacity.

The capacities C_{PP} and C_{PE} can be similarly defined. We write $\mathcal{E}^{\otimes n}$ to denote an ensemble of the form $\{\pi_{j_1,\ldots,j_n},\rho_{j_1}\otimes\cdots\otimes\rho_{j_n}\}$, where $\{\rho_j\}$ is a fixed collection of states, and $\{\pi_{j_1,\ldots,j_n}\}$ is some joint probability distribution.

Definition 5: The product signals/entangled measurements capacity of a quantum channel is defined as

$$C_{\mathrm{PE}}(\Phi)=\lim_{n\to\infty}\frac{1}{n}\sup_{\mathcal{E}^{\otimes n},\mathcal{M}} I^q_{\Phi^{\otimes n}}(\mathcal{E}^{\otimes n};\mathcal{M}). \tag{5}$$

Definition 6: The product signals/product measurements capacity of a quantum channel is defined as

$$C_{\mathrm{PP}}(\Phi)=\lim_{n\to\infty}\frac{1}{n}\sup_{\mathcal{E}^{\otimes n},\mathcal{M}^{\otimes n}} I^q_{\Phi^{\otimes n}}(\mathcal{E}^{\otimes n};\mathcal{M}^{\otimes n}). \tag{6}$$

The additivity of classical information capacity immediately implies the following result.

Theorem 7: *The product signals/product measurements capacity of a quantum channel is given by*

$$C_{\mathrm{PP}}(\Phi)=C_{\mathrm{Shan}}(\Phi)=\sup_{\mathcal{E},\mathcal{M}} I^q_{\Phi}(\mathcal{E};\mathcal{M}), \tag{7}$$

which we call the Shannon capacity.

A far deeper result is that $C_{\mathrm{PE}}(\Phi)$ can be re-expressed in terms of the well-known Holevo bound.[9,3,10] This result was proved independently in Refs. 3 and 11, building on earlier work in Refs. 4 and 12.

Theorem 8: *(Holevo–Schumacher–Westmoreland): The product signals/entangled measurements capacity of a quantum channel is given by*

$$C_{\mathrm{PE}}(\Phi)=C_{\mathrm{Holv}}(\Phi)=\sup_{\mathcal{E}}\left(S[\Phi(\rho)]-\sum_j \pi_j S[\Phi(\rho_j)]\right), \tag{8}$$

where $S(P)=-\mathrm{Tr}(P\log P)$ denotes the von Neumann entropy of the density matrix P. We call this the Holevo capacity of the channel.

C. Summary of results

Our main result, that using entangled inputs with product measurements does not increase the capacity of a channel, can be stated as

Theorem 9: *For any stochastic map, $C_{EP}(\Phi)=C_{\mathrm{Shan}}(\Phi)$.*

There is another implementation of product measurements which has the potential for a greater capacity. It involves a sequence of POVM's on the product spaces $\mathcal{H}^{\otimes n}$, whereby the POVM for the second measurement depends on the result of the first measurement, the POVM for the third measurement depends on the results of the first two measurements, and so on. The idea is that ''Bob'' can choose his successive POVM's based on the results of previous measurements. We write $C^{\mathrm{cond}}_{\mathrm{EP}}(\Phi)$ for the maximum asymptotic rate achievable for such a sequence of conditional POVM's, with entangled inputs allowed. [The precise definition of a conditional POVM is postponed to Sec. IV and the capacity is given by (34).] Our next result shows that using such conditional POVM's with entangled inputs again does not increase the channel capacity.

Theorem 10: *For any stochastic map, $C^{\mathrm{cond}}_{EP}(\Phi)=C_{\mathrm{Shan}}(\Phi)$.*

Theorem 10 was proved independently (and simultaneously), using different methods, by Shor,[13] and also later proved independently by Holevo.[14] A conditional POVM is not the most

general situation involving product measurements, which would be a POVM in which each measurement can be written as a tensor product. Except for the obvious bounds, we know of no results for the capacity associated with such POVM's.

The capacity of a classical channel can be written as the (suitably restricted) supremum of the classical mutual information. We extend this observation to the quantum case, using a tensor product formulation whereby the first two (and possibly all four) of these basic capacities are realized using mutual information in the form of the relative entropy of a density matrix and the product of its reduced density matrices. This leads to the following upper bound:

Theorem 11: *For any stochastic map,*

$$C_{\mathrm{EP}}(\Phi) \leqslant \sup_{\mathcal{M},\rho} \left[S(\rho) - \sum_b S(\sqrt{\rho}\,\hat{\Phi}(E_b)\sqrt{\rho}) + S(\tau) \right],$$

where $\tau_b = \mathrm{Tr}\,\Phi(\rho)E_b = \mathrm{Tr}\,\rho\widehat{\Phi}(E_b)$.

We call the quantity on the right U_{EP}, and we conjecture that it is equal to C_{EP}, i.e., that equality holds in Theorem 11 above. We motivate and study U_{EP} in Sec. II C, where we show that it can be rewritten in a form similar to the Holevo capacity. Combined with Theorem I C above, this conjectured equality would provide a simplified expression for the Shannon capacity of any channel, whereby the sup over both input ensemble and POVM is replaced by a sup over *one* average input state and the POVM.

Although the proof of Theorem 10 does not depend on our tensor product reformulation, we present this material first, in the following section, because we feel it gives some useful insights. Section II is largely pedagogical and provides the motivation for our conjectured expression for C_{EP}. Section III is also primarily pedagogical; it introduces the reader to Holevo's $C-Q$ and $Q-C$ channels.[3] This leads to a short proof of both the well-known Holevo bound and the new bound in Theorem 11. Moreover, the additivity of $Q-C$ channels implies Theorem 9 and motivates our proof of Theorem 10. The reader primarily interested in this proof can skip directly to Sec. IV.

II. CAPACITY FROM MUTUAL INFORMATION

A. Classical background

The *classical mutual information of two* random variables X and Y measures how much information they have in common and is given by

$$I^c(X;Y) \equiv \sum_{x,y} p(x,y)\log\frac{p(x,y)}{p(x)p(y)}. \tag{9}$$

If X and Y represent the input and output distributions of a channel, then the classical Shannon capacity is the supremum of $I^c(X;Y)$ taken over all possible joint distributions allowed by the channel.

The Shannon capacity of a quantum channel can also be obtained in this way provided that the joint distribution arises from a quantum communication process $(\Phi,\mathcal{E},\mathcal{M})$ as

$$p(j,b) = \pi_j\,\mathrm{Tr}[\Phi(\rho_j)E_b] = \pi_j\,\mathrm{Tr}[\rho_j\widehat{\Phi}(E_b)]. \tag{10}$$

Although the stochastic map Φ is usually regarded as noise acting on the signals ρ_j, it is important to recognize that it has another interpretation corresponding to the second expression for $p(j,b)$ in (10) above. In the second case, the channel transmits signals faithfully, but the ''noise'' distorts the measurement process by converting the POVM $\{E_b\}$ to a modified POVM $\{\hat{E}_b = \widehat{\Phi}(E_b)\}$ implemented by the action of the dual of Φ.

In order to make the transition from classical to quantum communication, it is sometimes useful to consider a classical probability vector $p(x)$ as the diagonal of a matrix P. We can then write the *relative entropy*,

$$H(P,Q)=\mathrm{Tr}[P\log P-P\log Q] \tag{11}$$

in a form which reduces to the usual classical expression when P and Q are diagonal, but is also valid when P and Q are density matrices representing mixed quantum states. In this notation (9) becomes

$$I^c(X;Y)=H[P_{12},P_1\otimes P_2], \tag{12}$$

where P_{12},P_1, and P_2 are diagonal matrices with nonzero entries $p(x,y),p(x)$ and $p(y)$, respectively.

B. Tensor product reformulation

A reformulation and generalization of mutual information and capacity can be made using *formal* tensor products. It should be emphasized that this is done for convenience of notation and is *distinct* from the tensor products used in describing multiple uses of the channel. Let $\mathcal{H}_{ABQR}=\mathbf{C}^J\otimes\mathbf{C}^M\otimes\mathcal{H}\otimes\mathcal{H}$, where $j=1...J$, $b=1...M$, and $\mathcal{H}_Q=\mathcal{H}_R=\mathcal{H}$ is the original Hilbert space on which ρ and E_b act. The partial traces then correspond to $T_A=\Sigma_j$, $T_B=\Sigma_b$, $T_Q=\mathrm{Tr}$, and $T_R=\mathrm{Tr}$.

Let P_{ABQ} be the block diagonal matrix with blocks $\pi_j\sqrt{\Phi(\rho_j)}E_b\sqrt{\Phi(\rho_j)}$ and $\hat{P}_{ABQ}$ the block diagonal matrix with blocks $\pi_j\sqrt{\rho_j}\,\widehat{\Phi}\,(E_b)\sqrt{\rho_j}$.

Then $P_{AB}\equiv T_QP_{ABQ}=T_Q\hat{P}_{ABQ}\equiv\hat{P}_{AB}$ and P_{AB} is a diagonal matrix with (nonzero) elements $p(j,b)=\pi_j\,\mathrm{Tr}[\Phi(\rho_j)\,E_b]$, $P_A\equiv T_{BC}P_{ABQ}=T_BP_{AB}$ is a diagonal matrix with elements $\delta_{ij}\pi_j$, $P_B\equiv T_{AQ}P_{ABQ}=T_AP_{AB}$ is a diagonal matrix with elements $\delta_{ab}\tau_b$ where $\tau_b=\mathrm{Tr}\,\Phi(\rho)E_b=\mathrm{Tr}\,\rho\widehat{\Phi}(E_b)$ as in Theorem 11.

It is straightforward to verify that

$$\begin{aligned}C_{\mathrm{PP}}\equiv C_{\mathrm{Shan}}(\Phi)&=\sup_{\mathcal{E},\mathcal{M}}[S(P_B)-S(P_{AB})+S(P_A)] &(13)\\&=\sup_{\mathcal{E},\mathcal{M}}H(P_{AB},P_A\otimes P_B)=\sup_{\mathcal{E},\mathcal{M}}I^q_\Phi(\mathcal{E};\mathcal{M})\\&=\sup_{\mathcal{E},\mathcal{M}}I^q(\tilde{\mathcal{E}};\mathcal{M})=\sup_{\mathcal{E},\mathcal{M}}I^q(\mathcal{E};\hat{\mathcal{M}}), &(14)\end{aligned}$$

where the last line in (14), although redundant is included to emphasize the fact that we can suppress the explicit dependence on Φ by using either a restricted ensemble with $\tilde{\rho}_j=\Phi(\rho_j)$ or a restricted POVM of the form $\widehat{\Phi}(E_b)$.

Note that all the matrices in (13) above are diagonal and could be replaced by probability vectors. The quantum character of the channel is hidden in the fact that P_{AB} must be the reduced density matrix of a P_{ABQ} of the form above with quantum blocks. Thus we might have replaced $\sup_{\mathcal{E},\mathcal{M}}$ above by either $\sup_{P_{ABQ}}H(P_{AB},P_A\otimes P_B)$ or $\sup_{\hat{P}_{ABQ}}H(P_{AB},P_A\otimes P_B)$ with the understanding that the supremum was to be taken over those P_{ABQ} or $\hat{P}_{ABQ}$ with the block diagonal form given above.

We can find a similar expression for the Holevo capacity by noting that $P_{AQ}\equiv T_BP_{ABQ}$ is a block diagonal matrix with blocks $\pi_j\Phi(\rho_j)$, and $P_Q\equiv T_{AB}P_{ABQ}=T_AP_{AQ}=\Phi(\rho)$.

It is again straightforward to verify that

$$C_{\mathrm{PE}}\equiv C_{\mathrm{Holv}}(\Phi)=\sup_{\mathcal{E}}[S(P_Q)-S(P_{AQ})+S(P_A)]=\sup_{\mathcal{E}}H(P_{AQ},P_A\otimes P_Q). \tag{15}$$

We can interpret this as a classical to quantum mutual information between the classical probability distribution π_j of the input alphabet and the average quantum distribution $\Phi(\rho)$ which emerges from the channel.

We conclude by observing that the entanglement assisted capacity of Ref. 15 can be written in a similar way as

$$\sup\{H(\rho_{QR},\rho_Q\otimes\rho_R):\rho_{QR}=(\Phi\otimes I)(|\Psi\rangle\langle\Psi|)\} \tag{16}$$

with $\Psi\in\mathbf{C}^2\otimes\mathbf{C}^2$. This differs slightly from Eq. (4) of Ref. 15. However, because $|\Psi\rangle\langle\Psi|$ is pure, their $S(\rho)=S[T_2(|\Psi\rangle\langle\Psi|)]=S[T_1(|\Psi\rangle\langle\Psi|)]=S(\rho_R)$ in our notation. Thus the expression in (16) above is equivalent to Eq. (4) of Ref. 15. This is a form of quantum to quantum mutual information between the subsystems of an entangled pair, one of which is subjected to noise via transmission through the channel.

We also expect that the capacity C_{EE} can be expressed as a (different) quantum to quantum mutual information. Unfortunately the precise form has eluded us. This approach does, however, lead in a natural way to a new expression related to C_{EP}.

C. Proposed expression for C_{EP}

To motivate our new candidate for C_{EP}, we let P_{BR} be the block diagonal matrix with blocks $\sqrt{\rho}\,\widehat{\Phi}(E_b)\sqrt{\rho}$. Then, $P_B\equiv T_R P_{BR}$ is a diagonal matrix with elements τ_b, $P_R\equiv T_B P_{BR}=\rho$, and define

$$U_{\mathrm{EP}}(\Phi)=\sup_{\mathcal{M},\rho}[S(P_R)+S(P_B)-S(P_{BR})]=\sup_{\mathcal{M},\rho}H(P_{BR},P_R\otimes P_B) \tag{17}$$

$$=\sup_{\mathcal{M},\rho}\left[S(\rho)-\sum_b\, S(\sqrt{\rho}\,\widehat{\Phi}(E_b)\sqrt{\rho})+S(\tau)\right]=\sup_{\tau_b,\gamma_b}\left[S(\gamma)-\sum_b\,\tau_b S(\gamma_b)\right], \tag{18}$$

where $\gamma_b=(1/\tau_b)\sqrt{\rho}\,\widehat{\Phi}(E_b)\sqrt{\rho}$ and $\gamma=\Sigma_b\tau_b\gamma_b=\rho$. The last form (18), looks like the Holevo capacity with the input ensemble $\mathcal{E}=\{\pi_j,\rho_j\}$ replaced by a new ''output measurement ensemble'' $\{\tau_b,\gamma_b\}$. How can we characterize this ensemble? Using Kraus operators we can write $\Phi(\rho)=\Sigma_k A_k^\dagger\rho A_k$, where $\Sigma_k A_k A_k^\dagger=I$. It follows that $\gamma_b=(1/\tau_b)\,\Sigma_k B_k^\dagger E_b B_k$ with $B_k=A_k^\dagger\sqrt{\rho}$. Hence γ_b is a density matrix in the range of a completely positive map which, rather than being trace-preserving or unital, satisfies $\Sigma_k B_k B_k^\dagger=\Phi(\rho)$. If we define $\Gamma_\rho(P)=\sqrt{\rho}\,\widehat{\Phi}(P)\sqrt{\rho}$ we can write

$$U_{\mathrm{EP}}(\Phi)=\sup_{\mathcal{M},\rho}\left(S[\Gamma_\rho(I)]-\sum_b\,S[\Gamma_\rho(E_b)]\right). \tag{19}$$

A different characterization is given in the next section as a condition on P_{BR}.

We can interpret (17) as a quantum to classical mutual information between the average input ρ and the classical probability vector τ_b associated with the correspondingly averaged output measurements $\mathrm{Tr}\,\rho\widehat{\Phi}(E_b)$.

We conjecture that $U_{\mathrm{EP}}=C_{\mathrm{EP}}$ although we can only show $U_{\mathrm{EP}}\geqslant C_{\mathrm{EP}}$, which is proved in the next section. Note if Φ is the completely noisy channel which maps every density matrix to the identity, then $P_{BR}=P_B\otimes P_R$ so that $H(P_{BR},P_B\otimes P_R)=0$ as expected. This also holds if ρ is a one-dimensional projection.

D. Optimization constraints

We can rewrite all of these expressions for capacity as the suitably constrained supremum of an ''Input–Output'' mutual information, $H(\rho_{\mathcal{IO}},\rho_{\mathcal{I}}\otimes\rho_{\mathcal{O}})$, i.e.,

$$\sup\{H(\rho_{\mathcal{IO}},\rho_{\mathcal{I}}\otimes\rho_{\mathcal{O}}):\rho_{\mathcal{IO}}\ \text{is a density matrix in}\ X_{\mathcal{IO}}\}, \tag{20}$$

where the subset $X_{\mathcal{IO}}$ lies in $\mathcal{A}_{\mathcal{I}}\otimes\mathcal{A}_{\mathcal{O}}$ and the algebra $\mathcal{A}$ is either $\mathbf{C}^{n\times n}$ or $\mathbf{D}^n$, the algebra of diagonal $n\times n$ matrices. We will let $\mathcal{G}=\{E:0\leqslant E\leqslant I\}$ denote the set of positive semidefinite operators less than or equal to the identity, $\mathcal{D}$ the set of density matrices, and $\leqslant\mathcal{D}$ the set of positive semi-definite matrices with trace $\leqslant 1$, i.e., the set of matrices λP, where P is a density matrix and $0\leqslant\lambda\leqslant 1$,

$$C_{\mathrm{PP}}:\ X_{\mathcal{IO}}=\{\rho_{AB}=\mathrm{Tr}_Q\,\rho_{ABQ}:\rho_{AQ}^{-1/2}\,\rho_{ABQ}\,\rho_{AQ}^{-1/2}\in\mathbf{D}^n\otimes\mathbf{D}^n\otimes\widehat{\Phi}(\mathcal{G})\}.$$

In the case of maps on $\mathbf{C}^{2\times 2}$ we expect this to be a subset of $\mathbf{D}^2\otimes\mathbf{D}^2$ although, in principle, it could be a subset of $\mathbf{D}^4\otimes\mathbf{D}^4$,

$$C_{\mathrm{PE}}:\ X_{\mathcal{IO}}=\{\rho_{AQ}:\rho_{AQ}\in\mathbf{D}^n\otimes\Phi(\leqslant\mathcal{D})\},$$

$$U_{\mathrm{EP}}:\ X_{\mathcal{IO}}=\{\rho_{BR}:\rho_B^{-1/2}\,\rho_{BR}\,\rho_B^{-1/2}\in\mathbf{D}^n\otimes\widehat{\Phi}(\mathcal{G})\},$$

$$C_{\mathrm{EE}}:\ \text{We know only that } X_{\mathcal{IO}}\subset\mathbf{C}^{n\times n}\otimes\mathbf{C}^{n\times n}.$$

In order to conclude that these expressions are equivalent to those given previously, we need to verify that when $\rho_{\mathcal{IO}}$ is in the indicated set, one can always find a corresponding ensemble $\mathcal{E}$ and/or POVM $\mathcal{M}$. The block diagonal conditions implicit in the notation above and the fact that Φ and $\widehat{\Phi}$ are trace-preserving and identity preserving respectively, makes this quite straightforward.

When $n=2$, we can describe $\mathcal{G}$ explictly by writing $E=w_0I+\mathbf{w}\cdot\sigma$ where $\sigma=(\sigma_x,\sigma_y,\sigma_z)$ denotes the formal vector of Pauli matrices and $\mathbf{w}$ in $\mathbf{R}^3$. Then $0\leqslant E\leqslant I$ if and only if $|\mathbf{w}|\leqslant\min\{w_0,1-w_0\}$ so that

$$\mathcal{G}=\bigcup_{w_0\in[0,1]}\{E=w_0I+\mathbf{w}\cdot\sigma:|\mathbf{w}|\leqslant\min\{w_0,1-w_0\}\}.$$

III. BOUNDS VIA $Q-C$ CHANNELS

Holevo[16] introduced an extremely useful family of stochastic maps of the form,

$$\Omega(P)=\sum_k R_k\,\mathrm{Tr}(PX_k),\tag{21}$$

where R_k is a family of density matrices, X_k is a POVM. He also distinguished two important subclasses of these channels

Ω_{QC}: Quantum-classical channels in which $R_k=|e_k\rangle\langle e_k|$ so that each density matrix is a one-dimensional projection from an orthonormal basis $\{e_k\}$;

Ω_{CQ}: Classical-quantum channels in which $X_k=|e_k\rangle\langle e_k|$ so that the POVM is a partition of unity arising from an orthonormal basis $\{e_k\}$.

Holevo[16] showed that the quantum capacity of such channels is additive, i.e.,

$$C_{\mathrm{PE}}(\Phi_{\mathrm{QC}}\otimes\Phi_{\mathrm{QC}}\cdots\otimes\Phi_{\mathrm{QC}})=C_{\mathrm{PE}}(\Phi_{\mathrm{QC}}^{\otimes n})=n\,C_{\mathrm{PE}}(\Phi_{\mathrm{QC}}),$$

and similarly for $C_{\mathrm{PE}}(\Phi_{\mathrm{CQ}}^{\otimes n})=n\,C_{\mathrm{PE}}(\Phi_{\mathrm{CQ}})$. In the next section, we use Holevo's strategy for proving additivity for Φ_{CQ} to prove Theorem 10.

We now show that both the celebrated ''Holevo bound'' $C_{\mathrm{PP}}(\Phi)\leqslant C_{\mathrm{PE}}(\Phi)$ and the new bound $C_{\mathrm{PP}}(\Phi)\leqslant U_{\mathrm{EP}}(\Phi)$ follow easily from the monotonicity of relative entropy under Ω_{QC} channels. Our strategy is similar to one used earlier by Yuen and Ozawa.[17]

In the first case, we let Ω_{QB} be a $Q-C$ map of the form (21) with $X_b=E_b$ and $R_b=|e_b\rangle\langle e_b|$. Then,

$$H(P_{AB},P_A\otimes P_B)=H[\Omega_{QB}(P_{AQ}),\Omega_{QB}(P_A\otimes P_Q)]\leqslant H(P_{AQ},P_A\otimes P_Q),\tag{22}$$

where P_{AQ} and P_{AB} are as in Sec. II and we have suppressed the identity in $I\otimes\Omega_{QB}$. Taking the supremum over $\mathcal{E}$ yields $C_{\mathrm{PP}}(\Phi)\leqslant C_{\mathrm{PE}}(\Phi)$.

For the new bound, let Ω_{RA} be a $Q-C$ map of the form (21) with $X_j=\pi_j\rho^{-1/2}\rho_j\,\rho^{-1/2}$ and $R_j=|e_j\rangle\langle e_j|$, so that $\Omega_{RA}(P_{BR})=P_{AB}$. Then,

$$H(P_{AB},P_A\otimes P_B)=H[\Omega_{RA}(P_{BR}),\Omega_{RA}(P_B\otimes P_R)]\leqslant H(P_{BR},P_B\otimes P_R)$$

from which it follows that $C_{\mathrm{PP}}(\Phi)\leqslant U_{\mathrm{EP}}(\Phi)$.

Remark: It may appear that the argument in (22) above yields a simple proof of the Holevo bound without using the strong subadditivity (SSA) of relative entropy[18] as in Ref. 19. However, Lindblad[20] made the useful observation that any stochastic map can be represented as the partial trace after interaction with an auxiliary system, i.e., $\Phi(P)=T_B[U_{AB}P\otimes E_BU_{AB}^\dagger]$. In fact, he used this representation to obtain monotonicity as a corollary of SSA. Thus, the arguments used to obtain the Holevo bound via monotonicity (as above or in Ref. 17) and via SSA (as in Ref. 19) are essentially equivalent. In the latter approach, an auxiliary system is added explicitly and then discarded; in the former, this is done implicitly via Lindblad's representation theorem. Further discussion of the history of the closely connected properties of SSA, monotonicity of relative entropy and the joint convexity of relative entropy is given in Refs. 21–23.

IV. PROOF OF ADDITIVITY USING $Q-C$ CHANNELS

Theorem 9 can be obtained from Holevo's result[16] that $C_{\mathrm{Holv}}(\Omega_{\mathrm{QC}})$ is additive, i.e., if Γ is a $Q-C$ channel of the form following (21), then $C_{\mathrm{Holv}}(\Gamma)$ is additive. To show how this follows, we define

$$\Gamma_{\Phi,\mathcal{M}}(P)=\sum_b\ |e_b\rangle\langle e_b|\ \mathrm{Tr}[P\widehat{\Phi}(E_b)]. \tag{23}$$

Then $\Gamma_{\Phi,\mathcal{M}}(P)$ is a $Q-C$ channel with $X_n=\widehat{\Phi}(E_b)$. Moreover, $\sup_{\mathcal{E}}I_\Phi^q(\mathcal{E};\mathcal{M})=C_{\mathrm{Holv}}(\Gamma_{\Phi,\mathcal{M}})$, and the additivity of $C_{\mathrm{Holv}}(\Gamma_{\Phi,\mathcal{M}})$ implies $\sup_{\mathcal{E}}I_{\Phi^{\otimes n}}^q(\mathcal{E};\mathcal{M}^{\otimes n})=C_{\mathrm{Holv}}(\Gamma_{\Phi,\mathcal{M}}^{\otimes n})=nC_{\mathrm{Holv}}(\Gamma_{\Phi,\mathcal{M}})$. Then Theorem 9 follows from

$$C_{\mathrm{Shan}}(\Phi)=\sup_{\mathcal{E},\mathcal{M}}I_\Phi^q(\mathcal{E};\mathcal{M})=\sup_{\mathcal{M}}C_{\mathrm{Holv}}(\Gamma_{\Phi,\mathcal{M}})=C_{\mathrm{EP}}(\Phi).$$

In order to prove Theorem 10, we will need to extend Holevo's result. Our extension, which we present below, follows Holevo's strategy[16] with the identity (27) replacing subadditivity. This also provides a self-contained proof of Theorem 9, since a product measurement is a special case of a conditional measurement.

First consider a product channel with Hilbert space $\mathcal{H}_1\otimes\mathcal{H}_2$ and noise operator $\Phi_1\otimes\Phi_2$. Let $\mathcal{E}_{12}=\{\pi_j,\rho_j\}$ be an ensemble of possibly entangled input states on $\mathcal{H}_1\otimes\mathcal{H}_2$. Let $\mathcal{M}_1=\{E_b\}$ denote the POVM on $\mathcal{H}_1$ which implements the first measurement, and for each b let $\mathcal{M}_2(b)=\{E_c^{(b)}\}$ denote the POVM on $\mathcal{H}_2$ which implements the second measurement. We then define a joint POVM $\mathcal{M}_{12}$ on $\mathcal{H}_1\otimes\mathcal{H}_2$, namely $\{E_b\otimes E_c^{(b)}\}$. Note that although each element of $\mathcal{M}_{12}$ is a product, the joint measurement need not be the product of independent measurements $\mathcal{M}_1\otimes\mathcal{M}_2$. This is the result of the fact that the second measurement may be conditioned on the results of the first. Nevertheless, it is easy to verify that $\mathcal{M}_{12}$ is a POVM since

$$\sum_{b,c}\ E_b\otimes E_c^{(b)}=\sum_b\ E_b\otimes\left(\sum_c\ E_c^{(b)}\right)=\sum_b\ E_b\otimes I.$$

The information content of a channel using such conditioned measurements is

$$I_{\Phi_1\otimes\Phi_2}^q(\mathcal{E}_{12};\mathcal{M}_{12})=I^q(\mathcal{E}_{12};\hat{\mathcal{M}}_{12})=I^q(\tilde{\mathcal{E}}_{12};\mathcal{M}_{12}), \tag{24}$$

where $\hat{\mathcal{M}}_1, \hat{\mathcal{M}}_2(b)$, and $\hat{\mathcal{M}}_{12}$ denote the POVM's in which E_b is replaced by $F_b = \widehat{\Phi_1}(E_b)$ and $E_c^{(b)}$ is replaced by $F_c^{(b)} = \widehat{\Phi_2}(E_c^{(b)})$, and we have used the notation defined in (1) and (2). Because we are interested in studying the capacity for a fixed set of POVM's, we use the form $I^q(\mathcal{E}_{12}; \hat{\mathcal{M}}_{12})$ and proceed as if we were considering a noiseless channel with a restricted POVM of the above form. Although this viewpoint is useful, it is not essential. The argument would work equally well if we explicitly included the stochastic maps or used the form $I^q(\tilde{\mathcal{E}}_{12}; \mathcal{M}_{12})$ and defined reduced density matrices using partial traces acting on, e.g., $(\Phi_1 \otimes \Phi_2)(\rho_j)$.

For any input ensemble $\mathcal{E}_{12}$ we now define a pair of associated input ensembles on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. For this purpose it is useful to let T_j denote the partial trace over $\mathcal{H}_j$. First, let $\rho_j^{(1)} = T_2[\rho_j]$ be the indicated reduced density matrix and $\mathcal{E}_1 = \{\pi_j, \rho_j^{(1)}\}$. This is our ensemble on $\mathcal{H}_1$. Second, for each j and b, define a state on $\mathcal{H}_2$ by

$$\rho_{j,b}^{(2)} = p(b|j)^{-1} T_1[(\rho_j)(F_b \otimes I)], \tag{25}$$

where $p(b|j) = \mathrm{Tr}[\rho_j (F_b \otimes I)]$. Then the corresponding input ensemble on $\mathcal{H}_2$ is $\mathcal{E}_2(b) = \{p(j|b), \rho_{j,b}^{(2)}\}$, where $p(j|b) = p(b|j)\pi_j / p(b)$ and

$$p(b) = \sum_j \pi_j p(b|j) = \mathrm{Tr}\left[\left(\sum_j \pi_j \rho_j\right)(F_b \otimes I)\right]. \tag{26}$$

We claim that

$$I^q(\mathcal{E}_{12}; \hat{\mathcal{M}}_{12}) = I^q(\mathcal{E}_1; \hat{\mathcal{M}}_1) + \sum_b p(b)\, I^q[\mathcal{E}_2(b); \hat{\mathcal{M}}_2(b)]. \tag{27}$$

Since

$$I^q[\mathcal{E}_2(b); \hat{\mathcal{M}}_2(b)] = I^q_{\Phi_2}[\mathcal{E}_2(b); \mathcal{M}_2(b)] \leqslant C_{\mathrm{Shan}}(\Phi_2), \tag{28}$$

it follows immediately from (27) that

$$I^q(\mathcal{E}_{12}; \hat{\mathcal{M}}_{12}) \leqslant I^q(\mathcal{E}_1; \hat{\mathcal{M}}_1) + \sum_b p(b)\, C_{\mathrm{Shan}}(\Phi_2) = I^q(\mathcal{E}_1; \hat{\mathcal{M}}_1) + C_{\mathrm{Shan}}(\Phi_2). \tag{29}$$

Taking the supremum over channels of this type, which we now emphasize by writing $\mathcal{M}_{12}^{\mathrm{cond}}$, gives

$$\sup_{\mathcal{E}_{12}, \mathcal{M}_{12}^{\mathrm{cond}}} I^q_{\Phi_1 \otimes \Phi_2}(\mathcal{E}_{12}; \mathcal{M}_{12}^{\mathrm{cond}}) = \sup_{\mathcal{E}_{12}, \hat{\mathcal{M}}_{12}^{\mathrm{cond}}} I^q(\mathcal{E}_{12}; \hat{\mathcal{M}}_{12}^{\mathrm{cond}}) \leqslant C_{\mathrm{Shan}}(\Phi_1) + C_{\mathrm{Shan}}(\Phi_2). \tag{30}$$

However by restricting to product ensembles and product POVM's in the sup on the left-hand side of (30), and using additivity of the classical capacity (7), we deduce

$$\sup_{\mathcal{E}_{12}, \mathcal{M}_{12}^{\mathrm{cond}}} I^q_{\Phi_1 \otimes \Phi_2}(\mathcal{E}_{12}; \mathcal{M}_{12}^{\mathrm{cond}}) \geqslant C_{\mathrm{Shan}}(\Phi_1) + C_{\mathrm{Shan}}(\Phi_2). \tag{31}$$

Hence we have an equality in (30).

Now consider the n-fold product channel $\Phi_1 \otimes \cdots \otimes \Phi_n$. Let $\mathcal{M}^{\mathrm{cond}}$ be a conditional POVM on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$. By assumption, every operator in this POVM has the form $E_b \otimes E_c^{(b)}$, where $\{E_b\}$ is a conditional POVM $\mathcal{N}^{\mathrm{cond}}$ on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_{n-1}$, and for each b, $E_c^{(b)}$ constitute a POVM on $\mathcal{H}_n$. Also, for any input ensemble $\mathcal{E}$ on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$, let $\mathcal{E}'$ be the ensemble of reduced density matrices on $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_{n-1}$. Then (29) implies

$$\sup_{\mathcal{E},\mathcal{M}^{\rm cond}} I^q_{\Phi_1\otimes\Phi_2\otimes\cdots\otimes\Phi_n}(\mathcal{E};\mathcal{M}^{\rm cond}) \leq \sup_{\mathcal{E}',\mathcal{N}^{\rm cond}} I^q_{\Phi_1\otimes\Phi_2\otimes\cdots\otimes\Phi_{n-1}}(\mathcal{E}';\mathcal{N}^{\rm cond}) + C_{\rm Shan}(\Phi_n). \quad (32)$$

Iterating (32) gives

$$\sup_{\mathcal{E},\mathcal{M}^{\rm cond}} I^q_{\Phi_1\otimes\Phi_2\otimes\cdots\otimes\Phi_n}(\mathcal{E};\mathcal{M}^{\rm cond}) \leq \sum_{k=1}^{n} C_{\rm Shan}(\Phi_k). \quad (33)$$

The definition of conditional capacity is

$$C^{\rm cond}_{\rm EP}(\Phi) = \lim_{n\to\infty}\frac{1}{n}\sup_{\mathcal{E},\mathcal{M}^{\rm cond}} I^q_{\Phi^{\otimes n}}(\mathcal{E};\mathcal{M}^{\rm cond}). \quad (34)$$

Hence if we let $\Phi_k=\Phi$, $(k=1,2,\ldots)$ it follows immediately from (33) that

$$C^{\rm cond}_{\rm EP}(\Phi) \leq C_{\rm Shan}(\Phi). \quad (35)$$

Since the capacity of the product channel is never less than the sum of the channel capacities, i.e, $C^{\rm cond}_{EP}(\Phi)\geq C_{\rm Shan}(\Phi)$ we must have equality in (35) which proves Theorem 10.

It is worth noting that our argument can be used to prove a somewhat stronger result, namely, that $\sup_{\mathcal{E}} I^q_{\Phi}(\mathcal{E};\mathcal{M}^{\rm cond})$ is additive in Φ for any fixed conditional measurement $\mathcal{M}^{\rm cond}$.

All that remains is to verify (27) which is, except for notation, equivalent to the following result from classical information theory: for any random variables J,B,C,

$$I^c(J;B,C) = I^c(J;B) + I^c(J;C|B). \quad (36)$$

Although the derivation of (36) is quite elementary (see, for example, Refs. 24 and 10), for completeness we include it in the Appendix, where we also show its equivalence to (27).

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APPENDIX: A USEFUL INFORMATION IDENTITY

First we relate (27) to an expression involving classical mutual information. The input alphabet of the product channel can be described by a classical discrete random variable J, whose distribution is given by the input ensemble $\mathcal{E}_{12}$, that is, $P(J=j)=\pi_j$. The output alphabet can be described similarly by a pair of random variables B,C, corresponding to the joint POVM $\hat{\mathcal{M}}_{12}$. The joint distribution of J,B,C is given by application of formula (10), namely,

$$P(J=j,B=b,C=c) = p(j,b,c) = \pi_j \,{\rm Tr}[\,(\rho_j)\, F_b\otimes F^{(b)}_c]. \quad (A1)$$

Applying the definitions in (1), (9), and (10) gives directly

$$I^c(J;B,C) = I^q(\mathcal{E}_{12};\hat{\mathcal{M}}_{12}). \quad (A2)$$

Furthermore, by summing over c in (A1) and conditioning on j, it follows that

$$p(b|j)=\mathrm{Tr}[\,(\rho_j)\,F_b\otimes I\,]=\mathrm{Tr}[\,(\rho_j)^{(1)}\,F_b]. \tag{A3}$$

Comparing with the definition of the ensemble $\mathcal{E}_1$, it follows that

$$I^c(J;B)=I^q(\mathcal{E}_1;\hat{\mathcal{M}}_1). \tag{A4}$$

For the second term on the right-hand side of (36), recall that by definition,

$$I^c(J;C\,|\,B)=\sum_b\, p(b)I^c(J;C\,|\,\{B=b\}). \tag{A5}$$

Also,

$$p(c|j,b)=\frac{p(j,b,c)}{p(j,b)}=\mathrm{Tr}[\,(\rho_{j,b})^{(2)}\,F_c^{(b)}\,] \tag{A6}$$

and $p(j|b)=p(j,b)/p(b)=p(b|j)\pi_j/p(b)$, so therefore

$$I^c(J;C\,|\,\{B=b\})=I^q(\mathcal{E}_2(b);\hat{\mathcal{M}}_2(b)). \tag{A7}$$

Hence Eqs. (27) and (36) are identical.

As noted before, (36) is a standard result in information theory. We include its derivation for completeness. The left-hand side can be rewritten as

$$I(J;B,C)=H(J)+H(B,C)-H(J,B,C), \tag{A8}$$

where $H(X)$ is the classical entropy of the random variable X. The two terms on the right-hand side are, respectively,

$$I(J;B)=H(J)+H(B)-H(J,B), \tag{A9}$$

$$I(J;C\,|\,B)=H(J|B)+H(C|B)-H(J,C|B). \tag{A10}$$

Further, for any random variables X and Y,

$$H(X|Y)=H(X,Y)-H(Y), \tag{A11}$$

and therefore (A10) can be written as

$$I(J;C\,|\,B)=H(J,B)-H(B)+H(C,B)-H(B)-H(J,C,B)+H(B). \tag{A12}$$

Adding (A9) and (A12) gives the right-hand side of (A8), which proves the result.

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Hyperfunction quantum field theory: Analytic structure, modular aspects, and local observable algebras

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This paper addresses the following problem of relativistic quantum field theory: Given a relativistic quantum field, construct a net of local observable algebras over space–time with ''natural'' properties. A few years ago we started a project which suggests to look at this problem in the framework of relativistic quantum field theory in terms of Fourier hyperfunctions. Accordingly we present the relevant analyticity results, some modular aspects of our theory for the Bisognano–Wichman argument, and a concrete suggestion for the definition of the local observable algebras. Finally, we construct a class of models of hyperfunction quantum fields for which the algebras of bounded operators assigned to nonempty regions in space–time are not trivial. It is remarkable that our models are not tempered quantum fields and do not admit ''test functions'' of compact support.
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I. INTRODUCTION

The problem of defining and of constructing a causal net of operator algebras for general relativistic quantum field theory has attracted considerable attention in the last 15 years (see Refs. 1–6). Typically additional (mainly technical) assumptions are involved to define causal nets of operators algebras for a standard quantum field theory, i.e., a relativistic quantum field theory in the sense of Gårding and Wightman.[7] Ultimately the goal is to construct an algebraic quantum field theory in the sense of Haag and Kastler.[4] However, at the moment it is still open what the most appropriate way of defining these local algebras is though there have been a number of promising suggestions.[1,6] And the problem of nontriviality of the operator *-algebras assigned to an open nonempty region of space–time is also not settled in these suggestions.

Accordingly we found it attractive to look for another framework to address these problems. Here we suggest to use the framework of Fourier hyperfunctions which is weaker than that of tempered distributions. Thus we have to choose quite a different route to proceed.

Our attempt is also motivated by the fact that the question of which type of generalized functions one should use in the formulation of relativistic quantum field theory, has not yet found a final answer. From the construction of models[8] and from general considerations there are strong indications that in the framework of hyperfunction quantum field theory (HFQFT for short), i.e., relativistic quantum field theory in terms of Fourier hyperfunctions,[9,10] one can do better with regard to these problems in so far that the additional assumptions can be dropped (or at least be weakened considerably). Other reasons for why it is attractive to study quantum field theory in terms of Fourier hyperfunctions are given in Refs. 11 and 12.

For the convenience of readers who are not too familiar with HFQFT and its motivation we

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recall the main points. (1) The fact that in four-dimensional space–time no nontrivial standard quantum fields have been constructed indicates that the axioms of QFT in terms of tempered distributions might be too strong. (2) On p. 425 of Ref. 11 one finds the following:

In conclusion we remark that Jaffe's formulation of the problem is not the most general. One might try [in the spirit of the work of Martineau (1963), for example] to define local properties of generalized functions (in particular the notion of support of a generalized function) even when the space of test functions does not include functions of compact support. The hope is that in this general framework one might arrive at a class of generalized functions satisfying weaker conditions than (15.53)–(15.54); in particular, the generalized functions which increase at infinity no faster than any linear exponential $|f(p)| \leqslant C_\epsilon \exp \epsilon|p|$ *for all* $\epsilon > 0$ *might be included.*

We point out that all this is realized in HFQFT. (3) In HFQFT there is a more natural relation between Wightman distributions and Schwinger functions.[13] (4) The two point function $D_m^{(-)}(x-y) = \langle \phi(x)\phi(y) \rangle$ has a local singularity of the form

$$\frac{1}{[(x-y)^2]^{(s-1)/2}}$$

in $s > 1$ space dimension. Thus an infinite power series in this quantity will have an essential singularity at the origin, and therefore not be tempered. But if $s = 1$ the local singularity in $D_m^{(-)}(x-y)$ is $\log(x-y)^2$ and so an infinite sum can define a tempered distribution. This is the reason why in the case of $s = 1$ Wick power series can converge in a framework of tempered fields, whereas in the case of $s > 1$ only Wick polynomials are defined in the framework of tempered fields. Thus (Wick ordered) entire functions of free fields find a natural formulation in HFQFT and thus provide a huge class of additional explicit models of quantum fields which are far more complex than the class of explicit models in standard QFT. (5) Certain ''formally interacting'' models can be treated rigorously in HFQFT but not in standard QFT.[8]

Since the system of axioms for HFQFT is weaker than that of standard QFT, the construction of a causal net is more difficult in HFQFT. In fact, if we look at the works quoted above we see that the existence of compactly supported test functions plays a fundamental role in all approaches to this problem in the framework of standard QFT. Thus at first it seems very questionable whether this problem can be addressed in HFQFT at all where there are no test functions of compact support available. But these doubts are based on the understanding that localization can only be achieved through localized test functions. In HFQFT localization is achieved through the main objects of the theory, namely through the fields (as operator-valued Fourier hyperfunctions) and their localization properties. Naturally, the concept of localization is more subtle in the theory of (Fourier) hyperfunctions than in Schwartz' distribution theory. (Localization of Fourier hyperfunctions is for instance explained in Sec. 2 of Ref. 10 and for hyperfunctions in Secs. 9.1 and 9.2 of Ref. 14).

In this paper we intend to show that it is sensible and promising to address the problem of defining and constructing local nets of operator algebras in the framework of Fourier hyperfunction quantum field theory by providing the following: (1) The basic ingredients for the Bisognano–Wichmann approach to this problem [existence and standard properties of the CPT-operator; HFQFT version of the Reeh–Schlieder theorem; analytic continuation over spatial wedges $W_\pm$; identification of the concrete action of the operator J of Eq. (24) and its main properties] and (2) A concrete proposal for the assignment of *-algebras of bounded operators to open nonempty domains of space–time (which is shown to be local for double cones). (3) A construction of a simple class of models of hyperfunction quantum fields (which are not standard quantum fields) for which the local algebras according to our suggestion are not trivial.

Standard quantum field theory uses the space $\mathcal{S}(\mathbf{R}^4)$ of rapidly decreasing C^∞-functions as a test function space, i.e., the field Φ is an operator-valued tempered distribution, more precisely $\Phi(f)$ is an unbounded operator defined on a dense subset $\mathcal{D}$ of a Hilbert space $\mathcal{H}$ for all $f \in \mathcal{S}(\mathbf{R}^4)$. On the other hand hyperfunction quantum field theory uses as a test function space the space $\mathcal{Q}(\mathbf{D}^4)$ of rapidly decreasing analytic functions defined below.

An element μ of the dual space $\mathcal{Q}(\mathbf{D}^n)'$ of $\mathcal{Q}(\mathbf{D}^n)$ is called a Fourier hyperfunction and an element ν of the space $\mathcal{L}(\mathcal{Q}(\mathbf{D}^n),\mathcal{H})$ of continuous linear mappings from $\mathcal{Q}(\mathbf{D}^n)$ to $\mathcal{H}$ is called a vector-valued Fourier hyperfunction. Though there are no functions of compact support in $\mathcal{Q}(\mathbf{D}^n)$, we can define the support of a Fourier hyperfunction as follows:

Let S_∞^{n-1} be the $(n-1)$-dimensional sphere at infinity, which is homeomorphic to the unit sphere $S^{n-1}=\{x\in\mathbf{R}^n;|x|=1\}$ by the mapping $x\to x_\infty$, where the point $x_\infty\in S_\infty^{n-1}$ lies on the ray connecting the origin with the point $x\in S^{n-1}$. The set $\mathbf{R}^n\cup S_\infty^{n-1}$, equipped with its natural topology [a fundamental system of neighborhoods of x_∞ is the set of all the sets $O_{\Omega,R}(x_\infty)$ given by

$$O_{\Omega,R}(x_\infty)=\{\xi\in\mathbf{R}^n;\xi/|\xi|\in\Omega,\ \ |\xi|>R\}\cup\{\xi_\infty;\xi\in\Omega\}$$

for every neighborhood Ω of x in S^{n-1} and $R>0$], is denoted by $\mathbf{D}^n$, called the radial compactification of $\mathbf{R}^n$. Let $Q^n=\mathbf{D}^n\times i\mathbf{R}^n$ and give it the product topology. Naturally, $\mathbf{C}^n=\mathbf{R}^n\times i\mathbf{R}^n$ is embedded in Q^n. Let K be a compact set in $\mathbf{D}^n$, $\{U_m\}$ a fundamental system of neighborhoods of K in Q^n and $\mathcal{O}_c^m(U_m)$ the Banach space of functions f analytic in $U_m\cap\mathbf{C}^n$ and continuous on $\overline{U_m}\cap\mathbf{C}^n$ which satisfy

$$\|f\|_m=\sup_{z\in U_m\cap\mathbf{C}^n}|f(z)|e^{|z|/m}<\infty.$$

Next we introduce the space

$$\mathcal{Q}(K)=\operatorname{ind}\lim_{m\to\infty}\mathcal{O}_c^m(U_m).$$

Observe that $\mathcal{Q}(\mathbf{D}^n)$ is dense in $\mathcal{Q}(K)$ (see for instance Ref. 15). Therefore continuous extensions are unique if they exist at all. We say that the *support* of $\mu\in\mathcal{Q}(\mathbf{D}^n)'$ is contained in K if μ has a continuous extension to $\mathcal{Q}(K)$. The localization of Fourier hyperfunctions can be summarized by recalling that Fourier hyperfunctions form a (flabby) sheaf over space–time.[16]

There are two main approaches to construct a net of local algebras from tempered quantum fields (see Refs. 1, 6, 17 for a survey of these and other attempts). One way to define local algebras $\{\mathcal{M}(O)\}$ for bounded open sets O in $\mathbf{R}^4$ is to define $\mathcal{M}(O)$ as the set of all 'bounded functions' of $\Phi(f)$ for $f\in\mathcal{S}(\mathbf{R}^4)$ with $\operatorname{supp}f\subset O$. Since the test functions of the Fourier hyperfunctions are analytic functions, there are no nonzero functions with compact supports. Therefore we cannot define local algebras for hyperfunction quantum fields by this method. Another definition of local algebras is that $\mathcal{M}(O)$ is the set of all bounded operators which commute weakly with all field operators $\Phi(f)$ with $\operatorname{supp}f\subset O'$ where $O'=\operatorname{int}\{x\in\mathbf{R}^4;(x-y)^2<0,\ \forall y\in O\}$. This definition has a counterpart in hyperfunction quantum field theory as we indicate now. Let $\mathcal{D}$ be a dense subset of the Hilbert space $\mathcal{H}$ such that $\Phi(f)\mathcal{D}\subset\mathcal{D}$ for all test functions $f\in\mathcal{Q}(\mathbf{D}^4)$. Then the mapping $(f_1,\ldots,f_n)\to\Phi(f_1)\cdots\Phi(f_n)u$ for $u\in\mathcal{D}$ defines a vector-valued Fourier hyperfunction $\Phi(x_1)\cdots\Phi(x_n)u$ (see Ref. 15). Since there are no nontrivial test functions with compact supports, we do not use smeared quantities $\Phi(f_1)\cdots\Phi(f_n)u$ but instead we use the vector-valued Fourier hyperfunctions $\Phi(x_1)\cdots\Phi(x_n)u$ directly. Since we can define the supports of Fourier hyperfunctions, we define the following set:

$$\mathcal{L}_w'(O)=\{X\in\mathcal{B}(\mathcal{H});\ \ \forall n\in\mathbb{N},\forall u\in\mathcal{D},\forall v\in\mathcal{D},$$

$$\operatorname{supp}[(X^*u,\Phi(x_1)\cdots\Phi(x_n)v)-(\Phi(x_n)^*\cdots\Phi(x_1)^*u,Xv)]\subset\mathbf{D}^{4n}\setminus O^n\}.$$

$\mathcal{L}_w'(O)$ is the set of all bounded operators which commute weakly with $\Phi(x_1)\cdots\Phi(x_n)$ for all $x_k\in O$. Since $\mathcal{L}_w'(O)$ is not necessarily an algebra, we propose to define an algebra $\mathcal{M}(O)$, for double cones O, as a subset of $\mathcal{L}_w'(O')$.

Questions of prime importance are: Is the net $\{\mathcal{M}(O)\}$ is local? Is $\{\mathcal{M}(O)\}$ not trivial? In this paper we give an affirmative answer to the first question for the family of double cones using the Bisognano–Wichmann argument (see Refs. 1, 5, 17).

In Sec. II, we study the vector-valued Fourier hyperfunctions $\Phi(x_1)\cdots\Phi(x_n)\Phi_0$, where Φ_0 is the vacuum vector, especially the analytic properties of these Fourier hyperfunctions. As a counter part of the well-known Reeh–Schlieder theorem of standard QFT we prove Proposition II.1. In Sec. II B we study the analytic properties of n-point functions $\mathcal{W}_n(x_1,\ldots,x_n) = (\Phi_0,\Phi(x_1)\cdots\Phi(x_n)\Phi_0)$ and prove the existence of the CPT-operator θ in hyperfunction quantum field theory. Next, in Sec. II C we study again analytic properties of

$$\Phi(x_1)\cdots\Phi(x_n)\Phi_0.$$

In particular we prove Proposition II.7 which is the crucial tool for the following development. As a preparation, in Sec. III, modular aspects of the theory for sets of operators over the spatial wedges $W_{\pm}$ are considered. Compared to standard QFT an additional domain problem has to be addressed (Sec. III B). This then allows us in Sec. IV to derive suitable characterizations of weak commutants of field operators localized on wedges. Then, besides a domain problem, we have prepared the ground for the Bisognano–Wichman route to causality for weak commutants over wedges and then over double-cones (Sec. V).

We want to stress that all the results and proofs are valid also in tempered quantum field theory because tempered quantum fields can be considered to be (Fourier) hyperfunction quantum fields.

As it is well known in the case of tempered quantum fields[1,3,2] the nontriviality of the local observable algebras is a difficult problem which has not yet found a general solution. Our above remarks indicate considerable additional difficulties in the case of hyperfunction quantum fields. So, instead of proving the existence of nontrivial local observable algebras in the general case, we present in Sec. VI a class of examples of hyperfunction quantum fields which have nontrivial local observable algebras. We proceed as follows.

We construct a hyperfunction quantum field as a Wick power series of a free field which is not a standard quantum field. We construct the local algebras for this field according to our suggestion. The nontriviality of these local algebras is shown as follows: A standard construction gives the local algebras for this free field. And it is shown that these local algebras for the free field are contained in the corresponding local algebras constructed for the hyperfunction quantum field. This amounts to the statement that the free field we start with and the hyperfunction quantum field constructed out of it are local relative to each other, in some sense. (We think that these hyperfunction quantum fields are in Borchers class of the free field, in the sense of HFQFT; but the Borchers class, in the sense of HFQFT, of a free field has not yet been determined.)

II. HYPERFUNCTION QUANTUM FIELD THEORY: ANALYTICITY RESULTS

Naturally we begin by specifying the framework in which we will be working.

By definition hyperfunction quantum fields are (relativistic) quantum fields over the test function space $E=\mathcal{Q}(\mathbf{D}^4)$ as discussed in Ref. 10. Here we address only the theory of a neutral scalar hyperfunction quantum field. For convenience we recall the basic defining assumptions $H_1,\ldots,H_5$. A quadruple $(\mathcal{H},U,\mathcal{D},\Phi)$ is called a *hyperfunction quantum field theory* iff the following conditions are satisfied:

H_1 *Quantum fields as operator valued Fourier hyperfunctions:* The field Φ is a linear map from $\mathcal{Q}(\mathbf{D}^4)$ into the algebra $L(\mathcal{D},\mathcal{D})$ of linear operators defined on the dense subset $\mathcal{D}$ of a separable complex Hilbert space $\mathcal{H}$. For all $u,v\in\mathcal{D}$, $f\to(u,\Phi(f)v)$ is a Fourier hyperfunction and one has $\Phi(f^*)\subset\Phi(f)^*$, where $\Phi(f)^*$ is the adjoint of the densely defined linear operator $\Phi(f)$ and $f^*(z)=\overline{f(\bar{z})}$ (Φ is Hermitian).

H_2 *Relativistic covariance:* U is a unitary representation of (the universal covering group of) the proper Poincaré group G on $\mathcal{H}$ which satisfies

$$U(g)\mathcal{D}=\mathcal{D},\ \ U(g)\Phi(f)U(g)^{-1}=\Phi(f_g),$$

for all $g\in G$ and all $f\in\mathcal{Q}(\mathbf{D}^4)$, where $f_g(x)=f(g^{-1}x)$.

H_3 *Spectral condition:* The spectrum of the energy-momentum operator P (i.e., the generator of the time–space translations in the representation U) is contained in the closed forward light cone $\overline{V}_+$, where

$$V_\pm=\{(p^0,\mathbf{p});\ \ \pm p^0>|\mathbf{p}|\}.$$

H_4 *Causality or local commutativity:* If x_1 and x_2 are spacelike separated then $\Phi(x_1)\Phi(x_2)u=\Phi(x_2)\Phi(x_1)u$ for every $u\in\mathcal{D}$.

H_5 *Uniqueness of the vacuum:* The subspace $\mathcal{H}_0$ of translation invariant vectors in $\mathcal{H}$ is one-dimensional and generated by a unit vector $\Phi_0\in\mathcal{D}$. This vacuum vector Φ_0 is also invariant under the Lorentz transformations $U(\Lambda)$ and cyclic for the field operators $\Phi(f)$, $f\in\mathcal{Q}(\mathbf{D}^4)$, i.e.,

$$\mathcal{D}_0=\text{lin span}\{\Phi_0,\ \ \Phi(f_1)\cdots\Phi(f_n)\Phi_0;f_k\in\mathcal{Q}(\mathbf{D}^4),\ \ n=1,2,\ldots\}$$

is dense in $\mathcal{H}$.

Remark: It follows from the first axiom that for every $u\in\mathcal{D}$ the mapping

$$\mathcal{Q}(\mathbf{D}^4)^n\ni(f_1,\ldots,f_n)\to\Phi(f_1)\cdots\Phi(f_n)u\in\mathcal{D} \tag{1}$$

defines a unique vector-valued Fourier hyperfunction $\Phi(x_1)\cdots\Phi(x_n)u$ (see Ref. 15). Therefore we are dealing with well defined vector valued Fourier hyperfunctions in condition H_4.

A. Basic analyticity results

Introduce the vector-valued Fourier hyperfunction

$$\Phi_n(x_1,\ldots,x_n)=\Phi(x_1)\cdots\Phi(x_n)\Phi_0 \tag{2}$$

and denote the Fourier transform of $\Phi_n(x_1,\ldots,x_n)$ by $\tilde{\Phi}_n(p_1,\ldots,p_n)$. Now, in appropriately chosen variables

$$(q_1,\ldots,q_n)=\chi^{-1}(p_1,\ldots,p_n),\ \ q_k=\sum_{j=k}^{n}p_j,$$

the Fourier hyperfunction $\tilde{\Phi}_n$ has convenient support properties. Consider

$$\tilde{Z}_n=\tilde{\Phi}_n\circ\chi_n. \tag{3}$$

Then we have (see Ref. 10)

$$\text{supp}\,\tilde{Z}_n(q_1,\ldots,q_n)\subset\overline{V}_+^n. \tag{4}$$

If $\text{Im}\,\zeta_k\in V_+$, then

$$q\to\exp\left(i\sum_{k=1}^{n}\langle\zeta_k,q_k\rangle\right)=\psi_{\zeta_1,\ldots,\zeta_n}(q_1,\ldots,q_n)$$

belongs to the space $\mathcal{Q}(\overline{V}_+^n)$ and therefore

$$Z_n(\zeta_1,\ldots,\zeta_n)=\tilde{Z}_n(\psi_{\zeta_1,\ldots,\zeta_n}) \tag{5}$$

is holomorphic in $\mathcal{T}_+^n$, where $\mathcal{T}_+^n=\{(\zeta_1,\ldots,\zeta_n);\ \text{Im}\,\zeta_k\in V_+,\ \text{for}\ \ k=1,\ldots,n\}$ and

$$\Phi_n(x_1,\ldots,x_n)=Z_n(x_1,x_2-x_1,\ldots,x_n-x_{n-1})=Z_n(\xi_1,\ldots,\xi_n). \tag{6}$$

$Z_n(\xi_1,\ldots,\xi_n)$ is the Fourier hyperfunction which is defined as the boundary value of $Z_n(\zeta_1,\ldots,\zeta_n)$ on $\mathcal{T}_+^n$. It is also the Fourier transform of the Fourier hyperfunction $\tilde{Z}_n$ introduced above. It follows that the Fourier hyperfunction (2) is the boundary value of the analytic function,

$$\Phi_n(z_1,\ldots,z_n)=Z_n(z_1,z_2-z_1,\ldots,z_n-z_{n-1})=Z_n(\zeta_1,\ldots,\zeta_n) \tag{7}$$

in $\{(z_1,\ldots,z_n)\in\mathbf{C}^{4n};(z_1,z_2-z_1,\ldots,z_n-z_{n-1})\in\mathcal{T}_+^n\}$. The condition H_2 of Lorentz covariance implies for any Lorentz transformation Λ,

$$U(\Lambda)\Phi_n(z_1,\ldots,z_n)=\Phi_n(\Lambda z_1,\ldots,\Lambda z_n)=Z_n(\Lambda\zeta_1,\ldots,\Lambda\zeta_n) \tag{8}$$

for all $(z_1,\ldots,z_n)$ such that $(z_1,z_2-z_1,\ldots,z_n-z_{n-1})\in\mathcal{T}_+^n$.

Remark: For $z=(z^0,\ldots,z^3)\in(\mathbf{C}\backslash\mathbf{R})^4$ introduce the function $h_z\in\mathcal{Q}(\mathbf{D}^4)$ defined by $h_z(t)=\Pi_{k=0}^3 e^{-(t^k-z^k)^2}/2\pi i(t^k-z^k)$. Then we have

$$f(t)=\int_{\Gamma^4}h_z(t)f(z)dz$$

for $f\in\mathcal{Q}(\mathbf{D}^4)$, where $\Gamma=\Gamma^+-\Gamma^-$, $\Gamma^\pm=\{z;z=\pm x\pm i\delta,-\infty<x<\infty\}$ is a suitable path in $(\mathbf{C}\backslash\mathbf{R})$.

For $u\in\mathcal{D}$ define a function F by $F(z_1,\ldots,z_n)=\Phi(h_{z_1})\cdots\Phi(h_{z_n})u$. Then $F(z_1,\ldots,z_n)$ is holomorphic in $(\mathbf{C}\backslash\mathbf{R})^{4n}$ and represents the vector-valued Fourier hyperfunction $\Phi(x_1)\cdots\Phi(x_n)u$ as follows:

$$\Phi(f_1)\cdots\Phi(f_n)u=\int_{\Gamma^{4n}}F(z_1,\ldots,z_n)f_1(z_1)\cdots f_n(z_n)\prod_{j=1}^{n}\prod_{k=0}^{3}dz_j^k. \tag{9}$$

And we say that $\Phi(x_1)\cdots\Phi(x_n)u$ is the boundary value of $\underline{F(z_1,\ldots,z_n)}$. Since $\Phi(h_{z_1})^*\cdots\Phi(h_{z_n})^*u=\Phi(h_{z_1}^*)\cdots\Phi(h_{z_n}^*)u=F(\overline{z_1},\ldots,\overline{z_n})$ [where $h_z^*(t)=h_z(\overline{t})=h_{\overline{z}}(t)$], hence $F(\overline{z_1},\ldots,\overline{z_n})$ represents the vector-valued Fourier hyperfunction $\Phi(x_1)^*\cdots\Phi(x_n)^*u$, we write

$$\Phi(x_1)^*\cdots\Phi(x_n)^*u=\Phi(\overline{x_1})\cdots\Phi(\overline{x_n})u \tag{10}$$

and have

$$\int_{\overline{\Gamma}^{4n}}F(\overline{z_1},\ldots,\overline{z_n})\overline{f_1(z_1)}\cdots\overline{f_n(z_n)}dz_1\cdots dz_n=\int_{\Gamma^{4n}}F(w_1,\ldots,w_n)f_1^*(w_1)\cdots f_n^*(w_n)dw_1\cdots dw_n.$$

In this notation we have in particular

$$\Phi(x_1)^*\cdots\Phi(x_n)^*\Phi_0=\Phi(\overline{x_1})\cdots\Phi(\overline{x_n})\Phi_0=\Phi(\overline{x_1},\ldots,\overline{x_n}). \tag{11}$$

With these basic analyticity properties we are well prepared to derive the main result of this section, an analogue of the much used Reeh–Schlieder theorem of standard QFT.

Proposition II.1 (HFQFT Reeh–Schlieder): Let U_n $(n=1,2,\ldots)$ be open nonempty sets in $\mathbf{R}^{4n}$ and u a vector of $\mathcal{H}$. If $(u,Z_n(\xi_1,\ldots,\xi_n))=0$ [respectively $(Z_n(\overline{\xi_1},\ldots,\overline{\xi_n}),u)=0$] in U_n as Fourier hyperfunctions for $n=0,1,2,\ldots$ (we use here $Z_0=\Phi_0$), then $u=0$.

Proof: Since $(u,Z_n(\zeta_1,\ldots,\zeta_n))$ [resp. $(Z_n(\overline{\zeta_1},\ldots,\overline{\zeta_n}),u)$] is holomorphic in $\mathcal{T}_+^n$ (respectively, in $\mathcal{T}_-^n$) and U_n is open in $\mathbf{R}^{4n}$ we get $(u,Z_n(\zeta_1,\ldots,\zeta_n))=0$ [respectively $(Z_n(\overline{\zeta_1},\ldots,\overline{\zeta_n}),u)=0$] in $\mathcal{T}_+^n$ (respectively, in $\mathcal{T}_-^n$) by edge of the wedge theorem (see Theorem 5.1 of Nagamachi and Nishimura[18]). Therefore $(u,\Phi(f_1)\cdots\Phi(f_n)\Phi_0)=0$ (respectively, $(\Phi(f_1)\cdots\Phi(f_n)\Phi_0,u)=0$) for any $f_k\in\mathcal{Q}(\mathbf{D}^4)$ for $n=0,1,2,\ldots$. By condition H_5 this implies $u=0$. □

B. Existence of a CPT-operator

There are several useful representations of the n-point functions $\mathcal{W}_n$ of the theory,

$$\mathcal{W}_n(z_1,\ldots,z_n)=(\Phi_k(\overline{z_k},\ldots,\overline{z_1}),\Phi_{n-k}(z_{k+1},\ldots,z_n))$$
$$=(\Phi_0,\Phi_n(z_1,\ldots,z_n)). \tag{12}$$

By translation invariance expressed in the form (7) the last term is equal to

$$(\Phi_0,Z_n(z_1,z_2-z_1,\ldots,z_n-z_{n-1}))$$

and thus it follows from the translation invariance of the vector Φ_0 that this quantity does not depend on z_1 when $\zeta_k=z_k-z_{k-1}$ is fixed for $k=2,\ldots,n$, and is denoted by W_{n-1}, i.e.,

$$\mathcal{W}_n(z_1,\ldots,z_n)=W_{n-1}(\zeta_2,\ldots,\zeta_n). \tag{13}$$

The function W_{n-1} is holomorphic in $\mathcal{T}_+^{n-1}$ and invariant under the proper Lorentz group $L_+^{\uparrow}$ since the vector Φ_0 is invariant under this group. We recall now some well-known results from standard QFT about the analytic continuation of the n-point functions. Since these results are based purely on analyticity arguments they apply in our context too. Accordingly the function W_{n-1} is analytically continued to a single valued $L_+(\mathbf{C})$-invariant function $\hat{W}_{n-1}$ which is analytic in the extended tube

$$\mathcal{T}'_{n-1}=\cup_{A\in L_+(\mathbf{C})}A\mathcal{T}_+^{n-1}$$

by the Bargmann–Hall–Wightman theorem.[19] $\mathcal{T}'_{n-1}$ contains real points called Jost points.[19] The Jost theorem[19] says that a real point $(\rho_2,\ldots,\rho_n)$ belongs to $\mathcal{T}'_{n-1}$ if, and only if, the convex cone $C(\rho_2,\ldots,\rho_n)$ generated by $\rho_2,\ldots,\rho_n$ contains only spacelike points. According to these results the n-point function $\mathcal{W}_n$ is analytically continued to a function $\hat{\mathcal{W}}_n$ which is analytic in

$$\mathcal{S}'_n=\{(z_1,\ldots,z_n)\in\mathbf{C}^{4n};z_k-z_{k-1}=\zeta_k\in\mathcal{T}'_{n-1}\}.$$

Condition H_4 (local commutativity) implies that $\hat{\mathcal{W}}_n$ is analytically continued to a function $\mathcal{W}_n^P$ which is symmetric and analytic in $\mathcal{S}_n^P$, the union of all domains generated from $\mathcal{S}'_n$ by arbitrary permutation of variables $z_1,\ldots,z_n$.

A certain weaker version of the locality condition H_4 called weak locality has found a number of successful applications in standard QFT because it can be characterized by a simple symmetry property (14) of the n-point functions. Since the proof of this characterization relies on analyticity arguments only it applies to HFQFT too, as we are going to show. First we recall that a hyperfunction quantum field is called *weakly local* iff for all n and all real points $(r_1,\ldots,r_n)$ in $\mathcal{S}'_n$ the relation $\hat{\mathcal{W}}_n(r_1,\ldots,r_n)=\hat{\mathcal{W}}_n(r_n,\ldots,r_1)$ holds. The announced characterization of weak locality is given by the following theorem:

Theorem II.2: *In a theory characterized by conditions H_1-H_3 and H_5 weak locality is equivalent to the following symmetry* (14) *for the n-point hyperfunctions $\mathcal{W}_n$, for all $n=2,3,\ldots$,*

$$\mathcal{W}_n(x_1,\ldots,x_n)=\mathcal{W}_n(-x_n,\ldots,-x_1)=\overline{\mathcal{W}_n(-x_1,\ldots,-x_n)}. \tag{14}$$

Proof: The arguments of Chap. V of Ref. 19 apply. □

Corollary II.3: The n-point functions of a hyperfunction quantum field theory satisfy the symmetry relations (14).

Proof: The condition H_4 of local commutativity implies weak locality. □

Theorem II.4 (TCP-Theorem): *A theory $(\mathcal{H},U,\mathcal{D},\Phi)$ characterized by conditions H_1-H_3 and H_5 is weakly local if, and only if, there is an antiunitary operator θ on $\mathcal{H}$ with the properties*

$$\theta\Phi_0=\Phi_0,\quad \theta\Phi(f_1)\cdots\Phi(f_n)\Phi_0=\Phi(f_1^-)\cdots\Phi(f_n^-)\Phi_0, \tag{15}$$

where $f_k^-(z)=\overline{f_k(-\bar{z})}$. *This antiunitary operator* θ *is called TCP-operator. It satisfies*

$$\theta^2=I,\quad \theta U(a,\Lambda)\theta=U(-a,\Lambda)\ \text{ on }\ \mathcal{H}, \tag{16}$$

$$\theta\Phi(f)\theta=\Phi(f^-)\ \text{ on }\ \mathcal{D}. \tag{17}$$

Proof: Since Theorem II.2 is established, the standard proof[19] applies. □

Corollary II.5: A hyperfunction quantum field theory has a TCP-operator θ.

Proof: Use Corollary II.3 and Theorem II.4. □

C. Analytic continuation over spatial wedges (Bisognano–Wichmann analyticity)

In the following we assume that a hyperfunction quantum field theory $(\mathcal{H},U,\mathcal{D},\Phi)$ is given as specified at the beginning of this section. We use the notation and the results from the previous sections without referring to them explicitly. Consider the following 1-parameter subgroup of the Lorentz group

$$v_t=\begin{pmatrix}\cosh t & \sinh t & 0 & 0\\ \sinh t & \cosh t & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}\in G$$

and

$$g_-=v_{i\pi}=v_{-i\pi}=\begin{pmatrix}-1 & 0 & 0 & 0\\ 0 & -1 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}.$$

Then

$$V(t)=U(v_t)$$

is a 1-parameter group of unitary operators in the Hilbert space $\mathcal{H}$ which has a self-adjoint generator L. Thus, by functional calculus, we have an analytic continuation of $V(t)$ to $V(\tau)$, $\tau\in\mathbf{C}$. Clearly, when τ does not belong to $\mathbf{R}$, the linear operators $V(\tau)$ are unbounded. Following Bisognano–Wichmann[17] we will be able to give suitable domains for these unbounded operators and to identify their action. Relation (8) implies

$$V(t)Z_n(\zeta_1,\ldots,\zeta_n)=Z_n(\zeta_1(t),\ldots,\zeta_n(t)), \tag{18}$$

where $\zeta(t)=v_t\zeta$, for all $t\in\mathbf{R}$ and all $(\zeta_1,\ldots,\zeta_n)\in\mathcal{T}_+^n$. Recall that Z_n is holomorphic on $\mathcal{T}_+^n$. For $\tau=i\lambda,\lambda\in\mathbf{R}$ we calculate

$$\operatorname{Im}\zeta(i\lambda)^0=\operatorname{Im}\zeta^0\cos\lambda+\operatorname{Re}\zeta^1\sin\lambda,$$

$$\operatorname{Im}\zeta(i\lambda)^1=\operatorname{Im}\zeta^1\cos\lambda+\operatorname{Re}\zeta^0\sin\lambda,$$

and introduce the spatial wedges

$$W_\pm=\{x\in\mathbf{R}^4;\pm x^1>|x^0|\}, \tag{19}$$

and the following subcone of the forward light-cone V_+,

$$V_+^0=\{(\eta^0,\eta^1,\eta^2,\eta^3)\in V_+;\ \ \eta^2=\eta^3=0\}.$$

Then, for $\zeta_k=\xi_k+i\eta_k$ such that $\mathrm{Re}\,\zeta_k\in W_\pm$ and $\mathrm{Im}\,\zeta_k\in V_+^0$ we have $\mathrm{Im}\,\zeta_k(i\lambda)\in V_+^0\subset V_+$ for $\pm\lambda\in[0,\pi/2]$ and thus $Z_n(\zeta_1(i\lambda),\ldots,\zeta_n(i\lambda))$ is well defined. This allows to deduce the following lemma.

Lemma II.6: (a) Let $\zeta_k\in\mathcal{T}_+$ be such that $\zeta_k(i\lambda)\in\mathcal{T}_+$ for $\pm\lambda\in[0,\pi/2]$ and $k=1,...,n$, then $Z_n(\zeta_1,\ldots,\zeta_n)\in\mathrm{dom}\,V(i\lambda)$ and

$$V(i\lambda)Z_n(\zeta_1,\ldots,\zeta_n)=Z_n(\zeta_1(i\lambda),\ldots,\zeta_n(i\lambda)) \tag{20}$$

as an identity between vector-valued analytic functions.

(b) When $\mathrm{Im}\,\zeta_k\in V_+^0$ and $\mathrm{Re}\,\zeta_k\in W_\pm$, then $\zeta_k(i\lambda)\in\mathcal{T}_+$ for $\pm\lambda\in[0,\pi/2]$ and the conclusion of (a) applies.

Proof: The proof of the Lemma 8 of Ref. 17 works without modification. □

Now, the main results of this subsection are given in the following proposition.

Proposition II.7: As identities between analytic functions in $\xi=(\xi_1,\ldots,\xi_n)\in W_\pm^n$ the following holds:

(a) If $\Phi\in\mathrm{dom}\,\mathrm{V}(\pm i\pi/2)$, then

$$(V(\pm i\pi/2)\Phi,Z_n(\xi_1,\ldots,\xi_n))=(\Phi,Z_n(\xi_1(\pm i\pi/2),\ldots,\xi_n(\pm i\pi/2)), \tag{21}$$

and

$$(\Phi,Z_n(g_-\xi_1,\ldots,g_-\xi_n))=(V(\pm i\pi/2)\Phi,Z_n(\xi_1(\pm i\pi/2),\ldots,\xi_n(\pm i\pi/2)). \tag{22}$$

(b) If $\Psi\in\mathrm{dom}\,V(\pm i\pi)$, then

$$(V(\pm i\pi)\Psi,Z_n(\xi_1,\ldots,\xi_n))=(\Psi,Z_n(g_-\xi_1,\ldots,g_-\xi_n)). \tag{23}$$

(c) Define

$$J=U(0,R)\theta, \tag{24}$$

where θ is the CPT-operator of Theorem II.4 and R the Euclidean rotation by π around the x^1-axis. If $\Psi\in\mathrm{dom}\,V(\pm i\pi)$, then

$$(V(\pm i\pi)\Psi,Z_n(\xi_1,\ldots,\xi_n))=(\Psi,JZ_n(\overline{\xi_1},\ldots,\overline{\xi_n})). \tag{25}$$

Proof: For $\mathrm{Im}\,\zeta_k\in V_+^0$ and $\xi_k=\mathrm{Re}\,\zeta_k\in W_\pm$ we know by Lemma II.6,

$$(V(\pm i\pi/2)\Phi,Z_n(\zeta_1,\ldots,\zeta_n))=(\Phi,Z_n(\zeta_1(\pm i\pi/2),\ldots,\zeta_n(\pm i\pi/2)). \tag{26}$$

The left-hand side of (26) is holomorphic in $\mathbf{R}^{4n}+iV_+^n$ and it defines a hyperfunction on $\mathbf{R}^{4n}$. There exists a neighborhood U of $\xi=(\xi_1,\ldots,\xi_n)$ in $W_\pm^n$ and $\delta>0$ such that the right-hand side of (26) is holomorphic in $U+iV_{+,\delta}^n$ and $U-iV_{+,\delta}^n$, where $V_{+,\delta}=\{\eta\in V_+;\eta^0<\delta\}$, and it defines a hyperfunction on U (see Theorem 4.4 of Ref. 18). Since both sides of (26) coincide in $U+iV_{+,\delta}^n$, they define the same hyperfunction in U. Since $\xi\in W_\pm^n$ is arbitrary, by the localization (sheaf) property of hyperfunctions, Eq. (21) holds in $W_\pm^n$ as an identity for hyperfunctions.

The left-hand side of (21) is a boundary value from $\mathbf{R}^{4n}+iV_+^n$, and the right-hand side a boundary value from both $U+iV_{+,\delta}^n$ and $U-iV_{+,\delta}^n$. Hence, by the edge of the wedge theorem, both sides are analytic in U. Again, since $\xi\in W_\pm^n$ is arbitrary, we deduce that Eq. (21) holds as an identity for analytic functions.

Now Eq. (22) follows from (21) and the following chain of identities:

$$(\Phi, Z_n(g_-\xi_1,\ldots,g_-\xi_n)) = (V(\pm i\pi/2)\Phi, Z_n(g_-\xi_1(\mp i\pi/2),\ldots,g_-\xi_n(\mp i\pi/2))$$
$$= (V(\pm i\pi/2)\Phi, Z_n(\xi_1(\pm i\pi/2),\ldots,\xi_n(\pm i\pi/2)).$$

From spectral calculus we know that if $\Psi \in \operatorname{dom} V(\pm i\pi)$ then $V(\pm i\pi/2)\Psi \in \operatorname{dom} V(\pm i\pi/2)$ and $V(\pm i\pi/2)V(\pm i\pi/2)\Psi = V(\pm i\pi)\Psi$. Thus Eqs. (21) and (22) apply and yield

$$(V(\pm i\pi)\Psi, Z_n(\xi_1,\ldots,\xi_n)) = (V(\pm i\pi/2)\Psi, Z_n(\xi_1(\pm i\pi/2),\ldots,\xi_n(\pm i\pi/2))$$
$$= (\Psi, Z_n(g_-\xi_1,\ldots,g_-\xi_n)).$$

Thus part (b) follows.

According to Sec. II B, the operator $J = U(0,R)\theta$ has the following properties:

$$J^2 = I, \quad J\Phi_0 = \Phi_0, \quad J\Phi(\overline{x})J = \Phi(g_-x), \tag{27}$$

$$JU(a,\Lambda)J = U(g_-a, g_-\Lambda g_-), \quad JV(t)J = V(t) \tag{28}$$

for all $t \in \mathbf{R}$. Now it follows from (23), for all $(\xi_1,\ldots,\xi_n) \in W_\pm^n$,

$$(V(\pm i\pi)\Psi, Z_n(\xi_1,\ldots,\xi_n)) = (\Psi, Z_n(g_-\xi_1,\ldots,g_-\xi_n))$$
$$= (\Psi, J\Phi(\overline{x_1})\cdots\Phi(\overline{x_n})\Phi_0) = (\Psi, JZ_n(\overline{\xi_1},\ldots,\overline{\xi_n})),$$

and we conclude (c). □

III. MODULAR ASPECTS

In standard QFT the modular theory for the O^*-algebra $\mathcal{P}(W_\pm)$ on $\mathcal{D}$ generated by the field operators $\Phi(f)$, $f \in \mathcal{S}(\mathbf{R}^4)$, $\operatorname{supp} f \subset W_\pm$, is fully developed. The maps

$$X\Phi_0 \to X^*\Phi_0, \quad X \in \mathcal{P}(W_\pm)$$

are closable and their closures $S_\pm$ satisfy

$$S_+ = S_-^* = JV(i\pi)$$

(see Theorem 4.52 in Inoue[20]).

Here, in HFQFT we develop certain aspects of this theory, needed for the proof of locality of our assignment of *-algebras of bounded operators to the wedges $W_\pm$. We are going to show that in our case too these maps are implemented as above.

A. Modular relation

For $\lambda \in \mathbf{R}$ introduce the subspace

$$\mathcal{D}_V(\lambda) = (1 + V(i\lambda))^{-1}\mathcal{H}$$

and observe that for $\lambda > 0$ (resp. $\lambda < 0$), $\mathcal{D}_V(\lambda)$ is a core for all $V(\tau)$ with $0 \leqslant \operatorname{Im}\tau \leqslant \lambda$ (resp. $0 \geqslant \operatorname{Im}\tau \geqslant \lambda$). For all $u \in \mathcal{D}_V(\lambda)$ the function $\tau \to V(\tau)u$ is strongly continuous and bounded in $0 \leqslant \operatorname{Im}\tau \leqslant \lambda$ (resp. $0 \geqslant \operatorname{Im}\tau \geqslant \lambda$) and analytic in the interior of this set. The operators $V(\tau)$, τ as above, are transformed under the operator J of Eq. (28) as follows:

$$J\mathcal{D}_V(\lambda) = \mathcal{D}_V(-\lambda), \quad JV(\tau)J = V(\overline{\tau}),$$

and

$$J\mathcal{V}(W_\pm)J = \mathcal{V}(W_\mp).$$

Denote $\mathcal{D}_\pm = \mathcal{D}_V(\pm\pi)$ and define

$$\mathcal{A}_\pm = \{X \in \mathcal{B}(\mathcal{H});\ \ X\Phi_0 \in \mathcal{D}_\pm\},$$

$$\mathcal{V}(W_\pm) = \{X \in \mathcal{A}_\pm;\ \ V(\pm i\pi)X\Phi_0 = JX^*\Phi_0\}. \tag{29}$$

The following two propositions provide important details about these sets of operators.

Proposition III.1: (a) $\mathcal{V}(W_\pm)\Phi_0 = \mathcal{D}_\pm$.

(b) Whenever $X_1, X_2 \in \mathcal{V}(W_\pm)$ *satisfy the condition* $X_1 V(t) X_2^* V(t)^* \in \mathcal{V}(W_\pm)$ *for all* $t \in \mathbf{R}$, *then*

$$X_1(JX_2J)\Phi_0 = (JX_2J)X_1\Phi_0. \tag{30}$$

Proof: For $u \in \mathcal{D}_\pm$ define, for all $v \in \mathcal{H}$,

$$Z_\pm(u)v = u(\Phi_0, v) + \Phi_0(JV(\pm i\pi)u, v) - (\Phi_0, u)(\Phi_0, v)\Phi_0.$$

Clearly, $Z_\pm(u)$ are bounded linear operators on $\mathcal{H}$, and for $v = \Phi_0$ we have

$$Z_\pm(u)\Phi_0 = u(\Phi_0, \Phi_0) + \Phi_0(JV(\pm i\pi)u, \Phi_0) - (\Phi_0, u)(\Phi_0, \Phi_0)\Phi_0 = u.$$

In order to determine the adjoints of the operators $Z_\pm(u)$ we calculate for all $w,\ v \in \mathcal{H}$,

$$\begin{aligned}(Z_\pm(u)^*w, v) &= (w, Z_\pm(u)v)\\ &= (w, u(\Phi_0, v) + \Phi_0(JV(\pm i\pi)u, v) - (\Phi_0, u)(\Phi_0, v)\Phi_0)\\ &= (w, u)(\Phi_0, v) + (w, \Phi_0)(JV(\pm i\pi)u, v) - (w, \Phi_0)(\Phi_0, u)(\Phi_0, v)\\ &= (\overline{(w, u)}\Phi_0, v) + (\overline{(w, \Phi_0)}JV(\pm i\pi)u, v) - (\overline{(w, \Phi_0)(\Phi_0, u)}\Phi_0, v)\end{aligned}$$

It follows, for all $w \in \mathcal{H}$,

$$Z_\pm(u)^*w = \overline{(w, u)}\Phi_0 + \overline{(w, \Phi_0)}JV(\pm i\pi)u - \overline{(w, \Phi_0)(\Phi_0, u)}\Phi_0,$$

and therefore

$$Z_\pm(u)^*\Phi_0 = \overline{(\Phi_0, u)}\Phi_0 + \overline{(\Phi_0, \Phi_0)}JV(\pm i\pi)u - \overline{(\Phi_0, \Phi_0)(\Phi_0, u)}\Phi_0 = JV(\pm i\pi)u.$$

This shows that $Z_\pm(u) \in \mathcal{V}(W_\pm)$ and $\mathcal{V}(W_\pm)\Phi_0 = \mathcal{D}_\pm$ and thus proves part (a).

In order to prove part (b) let $X_1,\ X_2 \in \mathcal{V}(W_\pm)$ be given which satisfy the hypothesis of part (b). Then we know, with $X = X_1 V(t) X_2^* V(t)^*,\ t \in \mathbf{R}$, that $V(\pm i\pi)X\Phi_0 = JX^*\Phi_0$ holds. Thus we have

$$V(\pm i\pi)X_1 V(t)X_2^*\Phi_0 = JV(t)X_2 V(t)^* X_1^*\Phi_0.$$

By the same argument for $X = X_1$ and $X = X_2$ we deduce

$$V(\pm i\pi)X_1 V(t)JV(\pm i\pi)X_2\Phi_0 = JV(t)X_2 V(t)^* JV(\pm i\pi)X_1\Phi_0.$$

Finally we employ the relations of Sec. II C between J and $V(t)$ and the group properties of $V(\tau)$ for complex τ and get

$$V(\pm i\pi)X_1 JV(t \pm i\pi)X_2 J\Phi_0 = V(t)JX_2 JV(\pm i\pi - t)X_1\Phi_0$$

and

$$V(\pm i\pi - t)X_1 JV(t \pm i\pi)X_2\Phi_0 = JX_2 JV(\pm i\pi - t)X_1\Phi_0. \tag{31}$$

Now take any $\Psi \in \mathcal{H}$ and a cutoff function $c \in \mathcal{D}(\mathbf{R})$ and consider the three vector-valued functions with complex variable τ,

$$X_1 JV(\overline{\tau} \pm i\pi) X_2 \Phi_0, \quad JX_2 JV(\pm i\pi - \tau) X_1 \Phi_0, \quad V(\overline{\tau} \pm i\pi) c(L)\Psi.$$

These functions are strongly continuous on the closed strip $0 \leqslant \pm \operatorname{Im} \tau \leqslant \pi$. The first two functions are analytic in $0 < \pm \operatorname{Im} \tau < \pi$ and the third is entire analytic in $\overline{\tau}$. Therefore the function

$$f(\tau) = (V(\overline{\tau} \pm i\pi) c(L)\Psi, \quad X_1 JV(\overline{\tau} \pm i\pi) X_2 \Phi_0) - (c(L)\Psi, JX_2 JV(\pm i\pi - \tau) X_1 \Phi_0)$$

is continuous in $0 \leqslant \pm \operatorname{Im} \tau \leqslant \pi$ and analytic in $0 < \pm \operatorname{Im} \tau < \pi$. By Eq. (31) we know $f(\tau) = 0$ for all real τ; it follows $f(\pm i\pi) = 0$, i.e.,

$$(c(L)\Psi, \quad X_1 JX_2 \Phi_0) = (c(L)\Psi, JX_2 JX_1 \Phi_0).$$

Since $\Psi \in \mathcal{H}$ and $c \in \mathcal{D}(\mathbf{R})$ are arbitrary, we have $X_1 JX_2 J\Phi_0 = JX_2 JX_1 \Phi_0$. This proves part (b). □

Proposition III.2: An operator $X \in \mathcal{A}_\pm$ belongs to the set $\mathcal{V}(W_\pm)$, i.e., it satisfies the equation

$$V(\pm i\pi) X\Phi_0 = JX^*\Phi_0$$

if, and only if, for all $n = 1,2,\ldots$,

$$(X^*\Phi_0, Z_n(\xi_1, \ldots, \xi_n))_{|W^n_\mp} = (Z_n(\overline{\xi_1}, \ldots, \overline{\xi_n}), X\Phi_0)_{|W^n_\mp}. \tag{32}$$

Proof: Assume first that $X \in \mathcal{V}(W_\pm)$ is given. For all $\xi = (\xi_1, \ldots, \xi_n) \in W^n_\mp$ we obtain, using $V(\pm i\pi) X\Phi_0 = JX^*\Phi_0$, and the relations for J from above,

$$(X^*\Phi_0, Z_n(\xi)) = (JV(\pm i\pi) X\Phi_0, Z_n(\xi)) = (V(\mp i\pi) JX\Phi_0, Z_n(\xi)).$$

Now Eq. (25) implies that this equals

$$(JX\Phi_0, JZ_n(\overline{\xi})) = (Z_n(\overline{\xi}), \quad X\Phi_0).$$

Hence relation (32) is necessary.

Conversely assume that X is a bounded linear operator on $\mathcal{H}$ for which relation (32) holds. Since $X\Phi_0 \in \mathcal{D}_\pm$ we can use (25) and get from relation (32)

$$\begin{aligned}(X^*\Phi_0, Z_n(\xi_1, \ldots, \xi_n))_{|W^n_\mp} &= (Z_n(\overline{\xi_1}, \ldots, \overline{\xi_n}), X\Phi_0)_{W^n_\mp} \\ &= (JX\Phi_0, JZ_n(\overline{\xi}))_{|W^n_\mp} = (V(\mp i\pi) JX\Phi_0, Z_n(\xi))_{|W^n_\mp}.\end{aligned}$$

Hence Proposition II.1 implies

$$X^*\Phi_0 = V(\mp i\pi) JX\Phi_0 = JV(\pm i\pi) X\Phi_0.$$

Therefore condition (32) is sufficient. □

B. Growth restriction and the domain problem

The temperedness of the distributions allows to show in standard QFT that the condition $X\Phi_0 \in \operatorname{dom} V(\pm i\pi)$ follows from condition (32). The proof relies on the fact that compactly supported testfunctions are available.

Compared to tempered distributions Fourier hyperfunctions can grow much stronger. Accordingly we impose a (mild) growth restriction on our theory. This growth condition [see Eq. (37)]

allows us to control the domains of the operators $V(\pm i\pi)$ and then we are able to prove $\mathcal{L}'_w(W_\mp)\subset\mathcal{A}_\pm$. This control of the domain is achieved by using a suitable rapidly decreasing cut-off function,

$$f(t)=c\exp(-\cosh t), \tag{33}$$

where $c>0$ is a number such that

$$\int_{-\infty}^{\infty} f(t)dt=1.$$

For $\mu>0$ denote

$$f_\mu(t)=\mu f(\mu t).$$

Lemma III.3: Let $0<\epsilon<\pi/2\mu$. Then the Fourier transform

$$\tilde{f}_\mu(p)=\int e^{ipt}f_\mu(t)dt$$

of f_μ is an entire function which satisfies the estimate

$$|\tilde{f}_\mu(p)|\leqslant M(\epsilon,\mu)e^{-\epsilon|p|} \tag{34}$$

for some $M(\epsilon,\mu)>0$, and

$$\tilde{f}_\mu(p)\to 1$$

as $\mu\to\infty$ for every p.

Proof: The identity

$$|f_\mu(t+is)|=c\mu\exp(-\cosh\mu t\cos\mu s)$$

follows from the equality

$$f_\mu(t+is)=c\mu\exp(-\cosh\mu t\cos\mu s-i\sinh\mu t\sin\mu s).$$

If $|s|<\pi/2\mu$ then $f_\mu(t+is)\to 0$ decays faster than exponentially as $t\to\pm\infty$. Therefore $\tilde{f}_\mu(p)$ is an entire function of p. Since $f_\mu(t)\to\delta(t)$ as $\mu\to\infty$,

$$\tilde{f}_\mu(p)\to 1$$

as $\mu\to\infty$ for every p.

Let $0<\epsilon<\pi/2\mu$. Then

$$\begin{aligned}|e^{\pm\epsilon p}\tilde{f}_\mu(p)|&=(2\pi)^{-1/2}\left|\int e^{ip(t\pm i\epsilon)}f_\mu(t)dt\right|\\&=(2\pi)^{-1/2}\left|\int e^{ipt}f_\mu(t\mp i\epsilon)dt\right|<\infty\end{aligned}$$

and we have

$$|\tilde{f}_\mu(p)|\leqslant M(\epsilon,\mu)e^{-\epsilon|p|}$$

for some $M(\epsilon,\mu)>0$. □

Lemma III.4: Let $V(t)=e^{itL}$. *Then, for all* $\mu>0$, $V(\pm i\epsilon)\tilde{f}_\mu(L)$ *is a bounded operator for* $\epsilon<\pi/2\mu$.

Proof: It follows from (34) that $|e^{\pm\epsilon p}\tilde{f}_\mu(p)|\leqslant M(\epsilon,\mu)$. Therefore, by spectral calculus, $\tilde{f}_\mu(L)$ maps $\mathcal{H}$ into the domain of $V(\pm i\epsilon)$ and

$$V(\pm i\epsilon)\tilde{f}_\mu(L)=\int_{-\infty}^{\infty}e^{\pm\epsilon p}\tilde{f}_\mu(p)dE(p)$$

is a bounded operator, where $E(p)$ is the spectral measure of the self-adjoint operator L. □

Recall the definition of the vector-valued Fourier hyperfunctions,

$$Z_n(\xi_1,\ldots,\xi_n)=\Phi(x_0)\Phi(x_1)\cdots\Phi(x_n)\Phi_0$$

with $\xi_j=x_j-x_{j-1}$ for $j=1,\ldots,n$. It is the boundary value of a slowly increasing vector-valued holomorphic function $Z_n(\zeta)$ in the forward tube, $\zeta=(\zeta_1,\ldots,\zeta_n)\in\mathcal{T}_+^n$ which, by Lorentz covariance, satisfies the relation

$$V(t)Z_n(\zeta)=Z_n(\zeta(t)) \tag{35}$$

for $\zeta\in\mathcal{T}_+^n$ and $\zeta(t)=v_t\zeta$. Both sides of Eq. (35) are holomorphic functions on $\mathcal{T}_+^n$, thus they define the same Fourier hyperfunctions. So, we denote

$$V(t)Z_n(\xi)=Z_n(\xi(t))$$

with $\zeta(t)=v_t\zeta$.

Lemma III.5: Suppose X *is a bounded operator on* $\mathcal{H}$ *for which the two Fourier hyperfunctions* $(X^*\Phi_0,Z_n(\xi))$ *and* $(Z_n(\overline{\xi}),X\Phi_0)$ *coincide on some open nonempty set* O *in* $\mathbf{R}^{4n}$. *Then both Fourier hyperfunctions are actually analytic functions in* O *and coincide there as analytic functions.*

Proof: $Z_n(\overline{\zeta})$ is a vector-valued slowly increasing holomorphic function in the backward tube $\mathcal{T}_-^n$ and defines a Fourier hyperfunction $Z_n(\overline{\xi})$ on $\mathbf{R}^{4n}$. From our assumption it follows that the two Fourier hyperfunctions $(X^*\Phi_0,Z_n(\xi))$ and $(Z(\overline{\xi}),X\Phi_0)$ coincide in O. By the Edge of the Wedge theorem for Fourier hyperfunction[18] we conclude. □

With the notation introduced in Sec. III A we define

$$\mathcal{V}(W_\pm)=\{X\in\mathcal{B}(\mathcal{H});X\Phi_0\in\mathcal{D}_\pm \text{ and } V(\pm i\pi)X\Phi_0=JX^*\Phi_0\}$$

and formulate the main result of this section.

Theorem III.6: *If for a bounded operator* X *on* $\mathcal{H}$ *one knows for all* n,

$$(X^*\Phi_0,Z_n(\xi))_{|W_\mp^n}=(Z_n(\overline{\xi}),X\Phi_0)_{|W_\mp^n}, \tag{36}$$

and if for every n *there are non-negative constants* M_n *and* K_n *such that*

$$|(X^*\Phi_0,Z_n(\xi(t)))|=|(Z_n(\overline{\xi}(t)),X\Phi_0)|\leqslant M_ne^{K_n\cosh t}, \tag{37}$$

then $X\in\mathcal{V}(W_\pm)$.

Proof: According to the preceding lemma we know that the growth restriction (37) for analytic functions is meaningful even if the coincidence relation (36) is originally assumed in the sense of Fourier hyperfunctions.

We employ the cut-off functions f_μ introduced above and show in a first step

$$(\tilde{f}_\mu(L)X^*\Phi_0,Z_n(\xi))_{|W_\mp^n}=(Z_n(\overline{\xi}),\tilde{f}_\mu(L)X\Phi_0)_{|W_\mp^n}$$

for large μ. To begin, observe that the properties of the cut-off function and the growth restriction (37) imply that the integrals

$$\int f_\mu(t)(X^*\Phi_0, Z_n(\xi(t)))dt \quad \text{and} \quad \int f_\mu(t)(Z_n(\overline{\xi}(t)), X\Phi_0)dt$$

exist if $\mu > 1$, and we have

$$\begin{aligned}(\tilde{f}_\mu(L)X^*\Phi_0, Z_n(\xi)) &= \int f_\mu(t)(V(t)X^*\Phi_0, Z_n(\xi))dt \\ &= \int f_\mu(t)(X^*\Phi_0, Z_n(\xi(t)))dt \\ &= \int f_\mu(t)(Z(\overline{\xi}(t)), X\Phi_0)dt \\ &= \int f_\mu(t)(Z(\overline{\xi}), V(t)X\Phi_0)dt = (Z_n(\overline{\xi}), \tilde{f}_\mu(L)X\Phi_0),\end{aligned}$$

where we used the coincidence relation (36) in the third equation.

In a second step we show that

$$(\tilde{f}_\mu(L)X^*\Phi_0, Z_n(\xi(t))) \quad \text{and} \quad (Z_n(\overline{\xi}(t)), \tilde{f}_\mu(L)X\Phi_0)$$

are bounded functions of $t \in \mathbf{R}$: It follows from Lemma III.4 that the vectors $\tilde{f}_\mu(L)X^*\Phi_0$ and $\tilde{f}_\mu(L)X\Phi_0$ belong to the domain of the operators $V(\pm i\epsilon)$ for $0 < \epsilon < \pi/2\mu$. Since $\xi(\mp i\epsilon) \in \mathcal{T}_+^n$ if $\xi \in W_\mp^n$, $Z_n(\xi(\mp i\epsilon))$ is a well defined vector in $\mathcal{H}$. By part (b) of Lemma II.6 the following is known: If $\zeta_j = \xi_j + i\eta_j \in W_\pm + iV_+^0$ for $j = 1,...,n$ then, for all $t \in \mathbf{R}$, $Z_n(\zeta(t)) \in \operatorname{dom} V(\mp i\epsilon)$ and $V(\mp i\epsilon)Z_n(\zeta(t)) = Z_n(\zeta(t \mp i\epsilon)) = V(t)Z_n(\zeta(\mp i\epsilon))$. Thus it follows

$$\begin{aligned}(V(\pm i\epsilon)\tilde{f}_\mu(L)X^*\Phi_0, V(t)Z_n(\zeta(\mp i\epsilon))) &= (V(\pm i\epsilon)\tilde{f}_\mu(L)X^*\Phi_0, V(\mp i\epsilon)Z_n(\zeta(t))) \\ &= (\tilde{f}_\mu(L)X^*\Phi_0, Z_n(\zeta(t))).\end{aligned}$$

Observing Lemma III.5 we can take the limit $\eta \to 0$ and get the identity

$$(\tilde{f}_\mu(L)X^*\Phi_0, Z_n(\xi(t))) = (V(\pm i\epsilon)\tilde{f}_\mu(L)X^*\Phi_0, V(t)Z_n(\xi(\mp i\epsilon)))$$

and hence

$$|(\tilde{f}_\mu(L)X^*\Phi_0, Z_n(\xi(t))| \leq \|V(\pm i\epsilon)\tilde{f}_\mu(L)X^*\Phi_0\| \|Z_n(\xi(\mp i\epsilon)\|$$

for all $t \in \mathbf{R}$. Similarly one proves the boundedness of the second function $(Z_n(\overline{\xi}(t)), \tilde{f}_\mu(L)X\Phi_0)$.

In a third step we use another cut-off function $c(p) \in \mathcal{D}_{\mathbf{R}}(\mathbf{R})$, i.e., a real valued C^∞-function with compact support, and show

$$(c(L)\tilde{f}_\mu(L)X^*\Phi_0, Z_n(\xi)) = (JV(\pm i\pi)c(-L)J\tilde{f}_\mu(L)X\Phi_0, Z_n(\xi)).$$

Let

$$\check{c}(t) = (2\pi)^{-1}\int_{\mathbf{R}} e^{-itp}c(p)dp \in \mathcal{S}(\mathbf{R})$$

be the inverse Fourier transform of $c(p)$. Then $c(L)J\tilde{f}_\mu(L)X\Phi_0 \in \mathrm{dom}\, V(\mp i\pi)$ and, by the previous step, the integrals

$$\int_{\mathbf{R}} \check{c}(t)(\tilde{f}_\mu(L)X^*\Phi_0, Z_n(\xi(t))dt \quad \text{and} \quad \int_{\mathbf{R}} \check{c}(t)(Z_n(\overline{\xi}(t)), \tilde{f}_\mu(L)X\Phi_0)dt$$

exist. Thus we have for all $\xi \in W^n_{\mp}$,

$$\begin{aligned}
(c(L)\tilde{f}_\mu(L)X^*\Phi_0, Z_n(\xi)) &= \int_{\mathbf{R}} (\check{c}(-t)V(-t)\tilde{f}_\mu(L)X^*\Phi_0, Z_n(\xi))dt \\
&= \int_{\mathbf{R}} \check{c}(t)(\tilde{f}_\mu(L)X^*\Phi_0, V(t)Z_n(\xi))dt \\
&= \int_{\mathbf{R}} \check{c}(t)(\tilde{f}_\mu(L)X^*\Phi_0, Z_n(\xi(t))dt \\
&= \int_{\mathbf{R}} \check{c}(t)(Z_n(\overline{\xi}(t)), \tilde{f}_\mu(L)X\Phi_0)dt \\
&= \int_{\mathbf{R}} \check{c}(t)(Z_n(\overline{\xi}), V(-t)\tilde{f}_\mu(L)X\Phi_0)dt \\
&= (Z_n(\overline{\xi}), c(-L)\tilde{f}_\mu(L)X\Phi_0) = (Jc(-L)\tilde{f}_\mu(L)X\Phi_0, JZ_n(\overline{\xi})) \\
&= (V(\mp i\pi)Jc(-L)\tilde{f}_\mu(L)X\Phi_0, Z_n(\xi)) \\
&= (JV(\pm i\pi)c(-L)\tilde{f}_\mu(L)X\Phi_0, Z_n(\xi)),
\end{aligned}$$

where we used the relations $V(\mp i\pi)J = JV(\pm i\pi)$ and

$$(\Psi, JZ_n(\overline{\xi})) = (V(\mp i\pi)\Psi, Z_n(\xi))$$

for $\Psi \in \mathrm{dom}\, V(\mp i\pi)$ (see Proposition II.7). By the Reeh–Schlieder theorem for hyperfunction quantum fields (Proposition II.1) we have

$$c(L)\tilde{f}_\mu(L)X^*\Phi_0 = JV(\pm i\pi)c(-L)\tilde{f}_\mu(L)X\Phi_0.$$

The final step removes the cut-offs. Let $c(p) \in \mathcal{D}_{\mathbf{R}}(\mathbf{R})$ such that $c(p)=1$ for $|p| \leqslant 1$ and introduce $c_\mu(p) = c(p/\mu)$ for $\mu > 0$. Then we have, as $\mu \to \infty$,

$$c_\mu(L)\tilde{f}_\mu(L)X^*\Phi_0 \to X^*\Phi_0, \quad c_\mu(-L)\tilde{f}_\mu(L)X\Phi_0 \to X\Phi_0.$$

Thus the relation

$$Jc_\mu(L)\tilde{f}_\mu(L)X^*\Phi_0 = V(\pm i\pi)c_\mu(-L)\tilde{f}_\mu(L)X\Phi_0$$

for all sufficiently large μ and the closedness of the self-adjoint operators $V(\pm i\pi)$ imply $X\Phi_0 \in \mathrm{dom}\, V(\pm i\pi)$ and $V(\pm i\pi)X\Phi_0 = JX^*\Phi_0$. □

IV. WEAK COMMUTANTS OF FIELD OPERATORS

Let $(\mathcal{H}, U, \mathcal{D}, \Phi)$ be a hyperfunction quantum field theory. For $u, v \in \mathcal{D}_0$, $n = 1,2,\ldots$, and $X \in \mathcal{B}(\mathcal{H})$ define the Fourier hyperfunction

$$\Psi_{X;n,u,v}(x_1,\ldots,x_n) = (X^*u, \Phi(x_1)\cdots\Phi(x_n)v) - (\Phi(\overline{x_n})\cdots\Phi(\overline{x_1})u, Xv). \tag{38}$$

If this Fourier hyperfunction vanishes on an open set O^n, $O\subset\mathbf{D}^4$, i.e., if $\Psi_{X;n,u,v}|O^n=0$, then this means intuitively that the operator X commutes weakly with the field operators localized on O.

To any open nonempty set O in $\mathbf{D}^4$ we assign the following set of bounded linear operators on the state space $\mathcal{H}$:

$$\begin{aligned}\mathcal{L}'_w(O)&=\{X\in\mathcal{B}(\mathcal{H});\ \ \Psi_{X;n,u,v}|O^n=0,\ \ \forall u,v\in\mathcal{D}_0,\ \ \forall n\in\mathbb{N}\}\\&=\{X\in\mathcal{B}(\mathcal{H});\ \ \operatorname{supp}\Psi_{X;n,u,v}\subset\mathbf{D}^{4n}\setminus O^n,\ \ \forall n\in\mathbb{N},\ \ \forall u,v\in\mathcal{D}_0\}.\end{aligned}\tag{39}$$

These sets $\mathcal{L}'_w(O)$ will be our starting point for the assignment of algebras $\mathcal{M}(O)$ to nonempty sets of space–time. In case O is a wedge $W_{\pm}$ or a double cone we will be able to show the locality of this assignment.

Clearly, a much simpler and more natural definition would be to consider all those bounded operators on $\mathcal{H}$ which commute weakly with $\Phi(x)$, $x\in O$ as it is done in standard QFT. In this section, by relying on some recent progress in the theory of Fourier hyperfunctions we show that actually the two definitions agree. To this end we introduce

$$\begin{aligned}L'(O)=\{&X\in\mathcal{B}(\mathcal{H});\forall u\in\mathcal{D}_0,\forall v\in\mathcal{D}_0,\\&\operatorname{supp}[(X^*u,\Phi(x)v)-(\Phi(x)^*u,Xv)]\subset\mathbf{D}^4\setminus O\}\end{aligned}$$

and show $\mathcal{L}'_w(O)=L'(O)$.

Recall the following general form of Schwartz' kernel theorem for Fourier hyperfunctions (Theorem 3.2 of Ref. 21):

Theorem IV.1: *Let K_i be a closed subset of $\mathbf{D}^{k_i}$ for $i=1,2,\ldots,N$. Then, for every separately continuous N-linear form B on $G=\mathcal{Q}(K_1)\times\cdots\times\mathcal{Q}(K_N)$ there is a unique Fourier hyperfunction F_B on $K_1\times\cdots\times K_N$, i.e., $F_B\in\mathcal{Q}(K_1\times\cdots\times K_N)'$ such that for all $(g_1,\ldots,g_N)\in G$,*

$$B(g_1,\ldots,g_N)=F_B(g_1\otimes\cdots\otimes g_N).$$

We have to comment on this result. $K_1\times\cdots\times K_N$ is a subset of $\mathbf{D}^{k_1}\times\cdots\times\mathbf{D}^{k_N}$, but not of $\mathbf{D}^n$, $n=\Sigma_{i=1}^N k_i$, in general. Accordingly elements $\mu\in\mathcal{Q}(K_1\times\cdots\times K_N)'$ have to be considered as elements of $\mathcal{Q}(\Pi_{i=1}^N\mathbf{D}^{k_i})'$ with support in $K_1\times\cdots\times K_N$. But hyperfunctions in n variables are defined on $\mathbf{D}^n$, the radial compactification of $\mathbf{R}^n$; and in this sense we need the above result. However we can choose a fundamental sequence of neighborhoods $\{U_m\}$ (resp. $\{V_m\}$) of $\mathbf{D}^n$ (resp. $\Pi_{i=1}^N\mathbf{D}^{k_i}$) such that $U_m\cap\mathbf{C}^n=V_m\cap\mathbf{C}^n=\{z\in\mathbf{C}^n;|\operatorname{Im}z|<1/m\}$. Thus we deduce $\mathcal{Q}(\mathbf{D}^n)=\mathcal{Q}(\Pi_{i=1}^N\mathbf{D}^{k_i})$ and consequently, $\mathcal{Q}(\mathbf{D}^n)'=\mathcal{Q}(\Pi_{i=1}^N\mathbf{D}^{k_i})'$ though $\mathbf{D}^n\neq\Pi_{i=1}^N\mathbf{D}^{k_i}$.

As a further preparation we prove

Lemma IV.2: Let O be an open set in $\mathbf{R}^4$. Then,

$$\mathcal{Q}(\mathbf{D}^{4n}\setminus O^n)=\mathcal{Q}((\mathbf{D}^4)^n\setminus O^n).\tag{40}$$

Proof: Let

$$O_m=\{x\in O;\operatorname{dist}(x,\partial O)>1/m\}.$$

Then $\mathbf{R}^{4n}\setminus O_m^n$ $(m=1,\ldots)$ is a fundamental system of neighborhoods of $\mathbf{R}^{4n}\setminus O^n$ in $\mathbf{R}^{4n}$. Since $\mathbf{D}^{4n}\setminus\mathbf{R}^{4n}=S_\infty^{4n-1}$, we can choose a fundamental system of neighborhoods U_m $(m=1,\ldots)$ of $\mathbf{D}^{4n}\setminus O^n$ in $\mathbf{Q}^{4n}$ such that

$$U_m\cap\mathbf{C}^{4n}=\{x\in\mathbf{R}^{4n};\|x\|>m\}\cup\mathbf{R}^{4n}\setminus O_m^n+i\{y\in\mathbf{R}^{4n};\|y\|<1/m\}.$$

Since $(\mathbf{D}^4)^n\setminus\mathbf{R}^{4n}=\cup_{j=1}^n(\mathbf{D}^4)^{j-1}\times S_\infty^3\times(\mathbf{D}^4)^{n-j}$, we can choose a fundamental system of neighborhoods V_m $(m=1,\ldots)$ of $(\mathbf{D}^4)^n\setminus O^n$ in $(\mathbf{Q}^4)^n$ such that

$$V_m\cap\mathbf{C}^{4n}=\cup_{j=1}^n\mathbf{R}^{4(j-1)}\times\{x\in\mathbf{R}^4;\|x\|>m\}\times\mathbf{R}^{4(n-j)}\cup\mathbf{R}^{4n}\setminus O_m^n+i\{y\in\mathbf{R}^4;\|y\|<1/m\}^n.$$

Since for any m_1 there exists m_2 such that $U_{m_1}\supset V_{m_2}$ (resp. $V_{m_1}\supset U_{m_2}$), we have (40). □

Corollary IV.3: A Fourier hyperfunction $\mu(\in\mathcal{Q}(\mathbf{D}^{4n})'=\mathcal{Q}((\mathbf{D}^4)^n)')$ *which vanishes in* O^n *belongs to* $\mathcal{Q}(\mathbf{D}^{4n}\setminus O^n)'=\mathcal{Q}((\mathbf{D}^4)^n\setminus O^n)'$. *Thus we have the following interpretation of the support of* μ*:*

$$\operatorname{supp}\mu\subset\mathbf{D}^{4n}\setminus O^n \quad\text{and}\quad \operatorname{supp}\mu\subset(\mathbf{D}^4)^n\setminus O^n.$$

Proposition IV.4: Suppose $j\in\{1,\ldots,n\}$ *and* t_j *is a separately continuous n-linear form on* $\mathcal{Q}(\mathbf{D}^4)^{(j-1)}\times\mathcal{Q}(\mathbf{D}^4)\times\mathcal{Q}(\mathbf{D}^4)^{(n-j)}$ *which, for fixed* $f_i\in\mathcal{Q}(\mathbf{D}^4)$, $i\neq j$ *has a continuous linear extension* $T_{\{f_i;i\neq j\}}(f_j)$ *to* $f_j\in\mathcal{Q}(K_j)$, $K_j\subset\mathbf{D}^4$ *closed. Then* t_j *has an extension to a separately continuous n-linear form* T_j *on* $\mathcal{Q}(\mathbf{D}^4)^{(j-1)}\times\mathcal{Q}(K_j)\times\mathcal{Q}(\mathbf{D}^4)^{(n-j)}$.

Proof: We have to show that for fixed $f_j\in\mathcal{Q}(K_j)$,

$$\{f_i;i\neq j\}\to T_{\{f_i;i\neq j\}}(f_j)$$

is a separately continuous $(n-1)$-linear form on $\mathcal{Q}(\mathbf{D}^4)^{(n-1)}$. By Theorem 2.7 of Ref. 10, $f_j\in\mathcal{Q}(K_j)$ is the limit in $\mathcal{Q}(K_j)$ of a sequence $\{g_k\}_{k\in\mathbb{N}}$ in $\mathcal{Q}(\mathbf{D}^4)$. Thus we get the following limit representation of the above functional,

$$T_{\{f_i;i\neq j\}}(f_j)=\lim_{k\to\infty}t_j(f_1\otimes\cdots\otimes f_{j-1}\otimes g_k\otimes f_{j+1}\otimes\cdots\otimes f_n).$$

For each k, by assumption, $t_j(f_1\otimes\cdots\otimes f_{j-1}\otimes g_k\otimes f_{j+1}\otimes\cdots\otimes f_n)$ depends continuously on $f_i\in\mathcal{Q}(\mathbf{D}^4)$ for each $i\neq j$; and $\mathcal{Q}(\mathbf{D}^4)$ is known to be a barreled space, hence by the Banach–Steinhaus theorem the above limit depends continuously on $f_i\in\mathcal{Q}(\mathbf{D}^4)$, $i\neq j$. □

Now we are prepared to prove the main result of this section.

Theorem IV.5: *If* O *is an open nonempty set of* $\mathbf{R}^4$, *then* $\mathcal{L}'_w(O)=L'(O)$.

Proof: In the notation introduced in (38) the set $L'(O)$ is characterized by

$$\begin{aligned}L'(O)&=\{X\in\mathcal{B}(\mathcal{H});\ \ \Psi_{X;1,u,v}|O=0,\ \ \forall u,v\in\mathcal{D}_0\}\\&=\{X\in\mathcal{B}(\mathcal{H});\ \ \operatorname{supp}\Psi_{X;1,u,v}\subset\mathbf{D}^4\setminus O,\ \ \forall u,v\in\mathcal{D}_0\}.\end{aligned}\tag{41}$$

Thus it suffices to show for a bounded operator X on $\mathcal{H}$: If

$$\operatorname{supp}\Psi_{X;1,u,v}\subset\mathbf{D}^4\setminus O,\ \ \forall u,v\in\mathcal{D}_0,$$

then

$$\operatorname{supp}\Psi_{X;n,u,v}\subset\mathbf{D}^{4n}\setminus O^n,\ \ \forall n\in\mathbb{N},\ \ \forall u,v\in\mathcal{D}_0.$$

Observe first that for all $f_j\in\mathcal{Q}(\mathbf{D}^4)$ the following relation holds:

$$\begin{aligned}\Psi_{X;n,u,v}(f_1\otimes\cdots\otimes f_n)&=\Psi_{X;1,u,\Phi(f_2)\cdots\Phi(f_n)v}(f_1)+\Psi_{X;1,\Phi(f_{n-1})*\cdots\Phi(f_1)*u,v}(f_n)\\&\quad+\sum_{j=2}^{n-1}\Psi_{X;1,\Phi(f_{j-1})*\cdots\Phi(f_1)*u,\Phi(f_{j+1})\cdots\Phi(f_n)v}(f_j).\end{aligned}\tag{42}$$

Clearly, the summands of this relation are separately continuous n-linear forms on $\mathcal{Q}(\mathbf{D}^4)^{(j-1)}\times\mathcal{Q}(\mathbf{D}^4)\times\mathcal{Q}(\mathbf{D}^4)^{(n-j)}$ and by Proposition IV.4, if $X\in L'(O)$, have extensions to separately continuous n-linear forms on $\mathcal{Q}(\mathbf{D}^4)^{(j-1)}\times\mathcal{Q}(K_j)\times\mathcal{Q}(\mathbf{D}^4)^{(n-j)}$, where $K_j=\mathbf{D}^4\setminus O$. Now we can apply the kernel theorem to conclude

$$\Psi_{X;n,u,v}(f_1\otimes\cdots\otimes f_n)=\sum_{j=1}^{n}T_j(f_1\otimes\cdots\otimes f_n)\tag{43}$$

with

$$T_j \in \mathcal{Q}(\mathbf{D}^{4n})' \quad \text{and} \quad \operatorname{supp} T_j \subset \mathbf{D}^{4(j-1)} \times K_j \times \mathbf{D}^{4(n-j)}. \tag{44}$$

It follows

$$\operatorname{supp} \Psi_{X;n,u,v}(x_1,\ldots,x_n) \subset \bigcup_{j=1}^{n} (\mathbf{D}^4)^{j-1} \times (\mathbf{D}^4 \backslash O) \times (\mathbf{D}^4)^{n-j}$$

$$= (\mathbf{D}^4)^n \backslash \bigcap_{j=1}^{n} (\mathbf{D}^4)^{j-1} \times O \times (\mathbf{D}^4)^{n-j} = (\mathbf{D}^4)^n \backslash O^n.$$

Finally we apply Corollary IV.3 to conclude

$$\operatorname{supp} \Psi_{X;n,u,v}(x_1,\ldots,x_n) \subset \mathbf{D}^{4n} \backslash O^n,$$

and thus $X \in \mathcal{L}'_w(O)$. □

*Corollary IV.6: (a) For any open nonempty subset O in $\mathbf{D}^4$, $\mathcal{L}'_w(O)$ is a *-invariant linear subspace of the *-algebra $\mathcal{B}(\mathcal{H})$ of bounded linear operators on the Hilbert space $\mathcal{H}$. It contains the identity of $\mathcal{B}(\mathcal{H})$.*

(b) The assignment $O \to \mathcal{L}'_w(O)$ is antimonotone, i.e., if $O_1 \subset O_2$ then $\mathcal{L}'_w(O_2) \subset \mathcal{L}'_w(O_1)$, and it is

(c) Poincaré covariant, i.e.,

$$U(g)\mathcal{L}'_w(O)U(g)^* = \mathcal{L}'_w(g \cdot O),$$

for all $g \in G$ and all open nonempty subsets $O \subset \mathbf{D}^4$.

(d) For any open nonempty subsets O_j of $\mathbf{D}^4$ one has $\mathcal{L}'_w(O_1) \cap \mathcal{L}'_w(O_2) = \mathcal{L}'_w(O_1 \cup O_2)$.

Proof: The Fourier hyperfunction $\Psi_{X;n,u,v}$ depends linearly on $X \in \mathcal{B}(\mathcal{H})$, therefore $\mathcal{L}'_w(O)$ is a linear subspace. By Hermiticity of the field we know $\Psi_{I;n,u,v} = 0$, hence this subspace contains the identity $I \in \mathcal{B}(\mathcal{H})$. A straightforward calculation shows $\Psi_{X^*;n,u,v}(x_1,\ldots,x_n) = \overline{\Psi_{X;n,u,v}(\overline{x_1},\ldots,\overline{x_n})}$. Since a Fourier hyperfunction μ and its complex conjugate $\overline{\mu}$, defined by $\overline{\mu}(f) = \overline{\mu(f^*)}$, have the same support it follows that $\Psi_{X^*;n,u,v}$ vanishes on O^n whenever $\Psi_{X;n,u,v}$ does. This proves part (a).

Part (b) is obvious from the definition.

Concerning Poincaré covariance we observe first

$$\Psi_{U(g)XU(g)^*;n,u,v}(x_1,\ldots,x_n) = \Psi_{X;n,u_g,v_g}(g^{-1}x_1,\ldots,g^{-1}x_n)$$

and note that with u, v also $u_g = U(g^{-1})u$ and $v_g = U(g^{-1})v$ belong to $\mathcal{D}_0$.

Part (d) follows from the identity $\mathcal{L}'_w(O) = L'(O)$ and the relation $L'(O_1) \cap L'(O_2) = L'(O_1 \cup O_2)$ which is obvious from the definition. Thus we conclude. □

V. CAUSALITY FOR WEDGES AND DOUBLE-CONES

As the above corollary shows the weak commutants $\mathcal{L}'_w(O)$ are known to be just *-invariant linear subspaces of the *-algebra $\mathcal{B}(\mathcal{H})$ of bounded linear operators on the Hilbert space $\mathcal{H}$ of our theory. For the wedges $W_\pm$ we will introduce a certain class of ''admissible'' *-algebras $\mathcal{M}(W_\pm)$ on $\mathcal{H}$ and for a certain subclass, relying on the results concerning modular aspects, we will be able to show locality. This then is used in the second subsection to derive locality for double cones.

A. Causality for wedges

At first we study in some detail the sets $\mathcal{L}'_w(W_\mp)$, and relate them in particular to the sets $\mathcal{V}(W_\pm)$ of Sec. III. If the growth restriction (37) of Theorem III.6 is taken into account we get results which are analogous to standard QFT.

Proposition V.1: In a hyperfunction quantum field theory $(\mathcal{H},U,\mathcal{D},\Phi)$ *the following relations hold for the spaces introduced above:*

(a) $\mathcal{L}'_w(W_\mp)\cap\mathcal{A}_\pm\subset\mathcal{V}(W_\pm)$,

(b) $J\mathcal{L}'_w(W_\pm)J=\mathcal{L}'_w(W_\mp)$,

(c) $V(t)\mathcal{L}'_w(W_\pm)V(t)^*=\mathcal{L}'_w(W_\pm)$ *for all* $t\in\mathbf{R}$,

(d) Under the assumption of the growth condition (37) of Theorem III.6, (a) can be sharpened to $\mathcal{L}'_w(W_\mp)\subset\mathcal{V}(W_\pm)$.

Proof: We denote $O_\mp=\{(x_1,\ldots,x_n)\in W^n_\mp\,;\,\xi_k=x_{k+1}-x_k\in W_\mp\}$. Observe the fact that $x_k-x_j=\Sigma_{i=j+1}^k\xi_i\in W_\mp$ for $k>j$ and that x_k and x_j are spacelike separated. For any $X\in\mathcal{L}'_w(W_\mp)$ one has

$$\begin{aligned}(X^*\Phi_0,Z_n(\xi_1,\ldots,\xi_n))_{|W^n_\mp}&=(X^*\Phi_0,\Phi(x_1)\cdots\Phi(x_n)\Phi_0)_{|O_\mp}\\&=(\Phi(x_n)^*\cdots\Phi(x_1)^*\Phi_0,X\Phi_0)_{|O_\mp}\\&=(\Phi(\overline{x_1})\cdots\Phi(\overline{x_n})\Phi_0,X\Phi_0)_{|O_\mp}\\&=(Z_n(\overline{\xi_1},\ldots,\overline{\xi_n}),X\Phi_0)_{|W^n_\mp}.\end{aligned}$$

By Proposition III.2 we deduce $X\in\mathcal{V}(W_\pm)$. This proves part (a).

Antiunitarity of the operator J implies $(JXJ)^*=JX^*J$ and thus, using the known transformation properties of the field under the operator J we calculate

$$\Psi_{JXJ;n,u,v}(x_1,\ldots,x_n)=-\Psi_{X^*;n,Jv,Ju}(g_-x_1,\ldots,g_-x_n).$$

Since the domain $\mathcal{D}_0$ is invariant under the TCP-operator θ it follows that this domain is also invariant under the operator $J=U(0,R)\theta$. Since $g_-W_\pm=W_\mp$ we see that $\Psi_{JXJ;n,u,v}$ vanishes on $W^n_\mp$ for all $u,v\in\mathcal{D}_0$ and $n=1,2,\ldots$ whenever $X\in\mathcal{L}'_w(W_\pm)$. We conclude $J\mathcal{L}'_w(W_\pm)J\subset\mathcal{L}'_w(W_\mp)$, and therefore $\mathcal{L}'_w(W_\pm)\subset J\mathcal{L}'_w(W_\mp)J$. This implies the identity stated in part (b).

In a similar way we prove part (c). Using the covariance properties of the field we calculate

$$\Psi_{V(t)XV(t)^*;n,u,v}(x_1,\ldots,x_n)=\Psi_{X;n,V(-t)u,V(-t)v}(v_{-t}x_1,\ldots,v_{-t}x_n).$$

Since $v_tW_\pm=W_\pm$ and since the domain $\mathcal{D}_0$ is invariant under $V(t)$, $t\in\mathbf{R}$, it follows, for all $t\in\mathbf{R}$, $V(t)\mathcal{L}'_w(W_\pm)V(t)^*\subset\mathcal{L}'_w(W_\pm)$, and therefore $\mathcal{L}'_w(W_\pm)\subset V(-t)\mathcal{L}'_w(W_\pm)V(-t)^*$. This proves the identity of part (c).

If the growth condition is assumed then by Theorem III.6 we know $\mathcal{L}'_w(W_\mp)\subset\mathcal{A}_\pm$ and thus (d) follows from (a). □

In general, $\mathcal{L}'_w(O)\cap\mathcal{A}_\pm\cap\mathcal{A}^*_\pm$ is only a *-invariant subspace but not a *-algebra of bounded operators on the state space $\mathcal{H}$. For the special case $O=W_\pm$ we will propose some choices for such a *-algebra which will finally enable us to assign *-algebras of bounded operators $\mathcal{M}(O)$ on $\mathcal{H}$ to all double cones O and this assignment will satisfy the condition of locality.

For $O=W_\pm$ we proceed as follows. First we introduce a certain class of *-algebras on $\mathcal{H}$ which we call ''admissible.'' Then for a certain subclass of these admissible *-algebras assigned to $W_\pm$ the locality condition will be shown.

Definition V.2: Let $(\mathcal{H},U,\mathcal{D},\Phi)$ *be a hyperfunction quantum field theory. A pair* $\mathcal{M}(W_\pm)$ *of* *-*algebras of bounded operators on the state space* $\mathcal{H}$ *is called* **admissible** *if it has the following properties:*

(A_1) $\mathcal{M}(W_\pm)\subset\mathcal{L}'_w(W_\mp)\cap\mathcal{A}_\pm\cap\mathcal{A}^*_\pm$,

(A_2) $J\mathcal{M}(W_\pm)J=\mathcal{M}(W_\mp)$,

(A_3) $V(t)\mathcal{M}(W_\pm)V(t)^*=\mathcal{M}(W_\pm)$ *for all* $t\in\mathbf{R}$.

Under the growth condition (37) *the right-hand side of* (A_1) *is* $\mathcal{L}'_w(W_\mp)$.

Since the identity operator belongs to $\mathcal{L}'_w(W_\mp)\cap\mathcal{A}_\pm\cap\mathcal{A}_\pm^*$ the trivial *-algebra is always admissible in this sense. We will see later (Proposition V.5) there is another construction to obtain admissible *-algebras.

As the following theorem shows an admissible pair of *-algebras satisfies the condition of locality, under the assumption of a strong technical condition, as in standard QFT.

Theorem V.3: *If in a hyperfunction quantum field theory* $(\mathcal{H},U,\mathcal{D},\Phi)$ *the space* $\mathcal{M}(W_\pm)\Phi_0$ *is dense in the state space* $\mathcal{H}$*, then the following assignment*

$$W_\pm\to\mathcal{M}(W_\pm)$$

is local, i.e.,

$$\mathcal{M}(W_\pm)\subset\mathcal{M}(W_\mp)'.$$

Proof: Because of property A_3 and since $\mathcal{M}(W_\pm)$ are *-algebras we know for any triple X_1, X_2, X_3 of its elements and for all $t\in\mathbf{R}$,

$$X_2V(t)X_3^*V(t)^*\in\mathcal{M}(W_\pm)\quad\text{and}\quad X_1X_3V(t)X_2^*V(t)^*\in\mathcal{M}(W_\pm).$$

By Property A_1 we know $\mathcal{M}(W_\pm)\subset\mathcal{V}(W_\mp)$ and thus Proposition III.1 applies. Part (b) of this proposition therefore implies the following chain of identities:

$$JX_2JX_1X_3\Phi_0=X_1X_3JX_2\Phi_0=(X_1J)JX_3JX_2\Phi_0=X_1JX_2JX_3\Phi_0.$$

Since $\{X_3\Phi_0;\ X_3\in\mathcal{M}(W_\pm)\}$ is dense, this equation implies $[X_1,JX_2J]=0$ for any X_1, $X_2\in\mathcal{M}(W_\pm)$, thus $\mathcal{M}(W_\pm)\subset(J\mathcal{M}(W_\pm)J)'$. Now we conclude by Property A_2. □

We prepare our discussion of a special way to obtain an admissible pair *-algebra $\mathcal{M}_0(W_\pm)$ by proving some properties of the set $\mathcal{A}_\pm=\{X\in\mathcal{B}(\mathcal{H});\ X\Phi_0\in\mathcal{D}_\pm\}$ introduced earlier.

Lemma V.4: (a) $J\mathcal{A}_\pm J=\mathcal{A}_\mp$ *and* $J\mathcal{A}_\pm^*J=\mathcal{A}_\mp^*$.

(b) $V(t)\mathcal{A}_\pm V(t)^*=\mathcal{A}_\pm$ *and* $V(t)\mathcal{A}_\pm^*V(t)^*=\mathcal{A}_\pm^*$ *for all* $t\in\mathbf{R}$.

Proof: (a) For $X\in\mathcal{A}_\pm$ we know $X\Phi_0\in\mathcal{D}_\pm$. Since $J\mathcal{D}_\pm=\mathcal{D}_\mp$ it follows $JXJ\Phi_0=JX\Phi_0\in J\mathcal{D}_\pm=\mathcal{D}_\mp$, hence $JXJ\in\mathcal{A}_\mp$, and therefore $J\mathcal{A}_\pm J\subset\mathcal{A}_\mp$; $JJ=I$ implies $\mathcal{A}_\pm\subset J\mathcal{A}_\pm J\subset\mathcal{A}_\pm$, and we get the first identity. The relation $JX^*J=(JXJ)^*$ implies now the second identity: $J\mathcal{A}_\pm J=(J\mathcal{A}_\pm J)^*=\mathcal{A}_\pm^*$.

For (b) we observe that the self-adjoint operators $V(\pm i\pi)$ commute with the unitary operators $V(t)$, $t\in\mathbf{R}$, therefore $V(t)\mathcal{D}_\pm=\mathcal{D}_\pm$. Since $V(t)\Phi_0=\Phi_0$ it follows easily $V(t)\mathcal{A}_\pm V(t)^*\subset\mathcal{A}_\pm$ for all $t\in\mathbf{R}$. Using the group properties of $V(t)$ we deduce $\mathcal{A}_\pm\subset V(-t)\mathcal{A}_\pm V(-t)^*$ for all $t\in\mathbf{R}$ and we conclude that the first identity holds. Taking adjoints the second identity follows. □

Proposition V.5: Introduce the *-*subspace,*

$$\mathcal{K}_\pm=\mathcal{K}(W_\pm)=\mathcal{L}'_w(W_\mp)\cap\mathcal{A}_\pm\cap\mathcal{A}_\pm^*,$$

respectively,

$$\mathcal{K}_\pm=\mathcal{K}(W_\pm)=\mathcal{L}'_w(W_\mp)$$

if the growth condition (37) is assumed and define

$$\mathcal{M}_0(W_\pm)=\mathcal{K}_{\text{alg}}(W_\pm)=\{C\in\mathcal{K}_\pm;C\mathcal{K}_\pm\subset\mathcal{K}_\pm,\mathcal{K}_\pm C\subset\mathcal{K}_\pm\}.\tag{45}$$

Then $\mathcal{M}_0(W_\pm)$ *are a pair of admissible* *-*algebras of bounded operators on the state space* $\mathcal{H}$.

Proof: By definition $\mathcal{M}_0(W_\pm)$ are *-algebras of bounded operators on $\mathcal{H}$ which are contained in $\mathcal{K}_\pm$. Hence condition A_1 is satisfied.

Next, by part (b) of Proposition V.1 and part (a) of Lemma V.4 we know $J\mathcal{K}_\pm J\subset\mathcal{K}_\mp$. Now, for any $Y\in\mathcal{M}_0(W_\pm)$ one has by definition, $Y\mathcal{K}_\pm\subset\mathcal{K}_\pm$ and $\mathcal{K}_\pm Y\subset\mathcal{K}_\pm$. It follows $JYJ\mathcal{K}_\pm$

$=JYJ\mathcal{K}_{\pm}JJ\subset JY\mathcal{K}_{\mp}J\subset J\mathcal{K}_{\mp}J\subset\mathcal{K}_{\pm}$ and similarly $\mathcal{K}_{\pm}JYJ\subset\mathcal{K}_{\pm}$, hence $J\mathcal{M}_0(W_{\pm})J\subset\mathcal{M}_0(W_{\mp})$ and thus, by $JJ=I$, $J\mathcal{M}_0(W_{\pm})J=\mathcal{M}_0(W_{\mp})$; therefore condition A_2 is satisfied.

Finally, by part (c) of Proposition V.1 and part (b) of Lemma V.4, $V(t)\mathcal{K}_{\mp}V(t)^*=\mathcal{K}_{\mp}$ is known for all $t\in\mathbf{R}$. Then we can proceed as for the second condition and conclude that condition A_3 is satisfied too. □

B. Causality for double-cones

Let G be the proper Poincaré group. We define

$$G_{\pm}=\{g\in G;g\cdot W_{+}=W_{\pm}\}$$

as the subset of G consisting of those elements which leave the wedge W_{+} invariant, respectively map it onto the wedge W_{-}. The following lemma determines the general form of an element in G_{+} explicitly and provides an elementary property of $G_{\pm}$. We omit the straight forward proof.

Lemma V.6: (a) G_{+} is the subgroup of G consisting of elements g of the Poincaré group G of the form $g=(a,\Lambda)$ with $a=(0,0,a^2,a^3)$ and

$$\Lambda=\begin{pmatrix}\cosh t & \sinh t & 0 & 0\\ \sinh t & \cosh t & 0 & 0\\ 0 & 0 & \cos\theta & -\sin\theta\\ 0 & 0 & \sin\theta & \cos\theta\end{pmatrix} \tag{46}$$

with $t\in\mathbf{R}$ and $\theta\in\mathbf{R}$.

(b) For $g\in G_{\pm}$ and v_t as introduced in Sec. II C, the following relation holds:

$$gv_tg^{-1}=v_{\pm t}. \tag{47}$$

Lemma V.7: For the set $G_{\pm}=\{g\in G;g\cdot W_{+}=W_{\pm}\}$ the following holds:
(a) $U(g)\mathcal{A}_{\pm}U(g)^{-1}=\mathcal{A}_{\pm}$ for all $g\in G_{+}$.
(b) $U(g)\mathcal{A}_{\pm}U(g)^{-1}=\mathcal{A}_{\mp}$ for all $g\in G_{-}$.

Proof: Lemma V.6 implies $U(g)V(t)U(g)^{-1}=V(t)$ for all $g\in G_{+}$ and all $t\in\mathbf{R}$. Using functional calculus we deduce by analytic continuation $U(g)V(\pm i\pi)=V(\pm i\pi)U(g)$ for all $g\in G_{+}$, in particular $U(g)\mathcal{D}_{\pm}=\mathcal{D}_{\pm}$. Now, since $U(g)\Phi_0=\Phi_0$ for all $g\in G$, statement (a) follows easily.

For $g\in G_{-}$ we know $g\cdot W_{+}=W_{-}$ and by Lemma V.6, for all $t\in\mathbf{R}$, $U(g)V(t)=V(-t)U(g)$. Again using functional calculus and analytic continuation we deduce $U(g)V(\pm i\pi)=V(\mp i\pi)U(g)$, in particular, $U(g)\mathcal{D}_{\pm}=\mathcal{D}_{\mp}$ for all $g\in G_{-}$. Now statement (b) follows as in the previous case. □

*Definition V.8: A pair $\mathcal{M}(W_{\pm})$ of admissible *-algebras of bounded operators on $\mathcal{H}$ is called covariant if, and only if, it satisfies the following identity:*

$$U(g)\mathcal{M}(W_{+})U(g)^{-1}=\mathcal{M}(W_{\pm})\ \forall g\in G_{\pm}. \tag{48}$$

The following lemma shows that there is at least one pair of covariant admissible *-algebras.

*Lemma V.9: The special pair $\mathcal{M}_0(W_{\pm})$ $\mathcal{H}$ of admissible *-algebras of bounded operators on $\mathcal{H}$ which was introduced in Proposition V.5 is covariant, i.e.,*

$$U(g)\mathcal{M}_0(W_{+})U(g)^{-1}=\mathcal{M}_0(W_{\pm})\ \forall g\in G_{\pm}. \tag{49}$$

Proof: On the basis of Lemma V.6–V.7 we can proceed in more or less the same way as in the proof of Proposition V.5 starting with the observation

$$U(g)\mathcal{L}'_w(W_{-})\cap\mathcal{A}_{+}\cap\mathcal{A}_{+}^{*}U(g)^{-1}=\mathcal{L}'_w(W_{\mp})\cap\mathcal{A}_{\pm}\cap\mathcal{A}_{\pm}^{*}\ \forall g\in G_{\pm}$$

which follows from part (c) of Corollary IV.6 and part (a) of Lemma V.7. □

Next consider the set of all wedgelike regions,

$$\mathcal{W}=\{W\subset\mathbf{R}^4;\ \ W=g\cdot W_+,\ \ g\in G\}=G\cdot W_+.$$

Clearly, two elements $g_1, g_2\in G$ define the same wedge, i.e., $g_1\cdot W_+=g_2\cdot W_+$, if, and only if, $g_1^{-1}g_2\in G_+$. Thus the elements of $\mathcal{W}$ are distinguished by the elements $[g]$ of the quotient G/G_+.

Now, given any pair of admissible *-algebras $\mathcal{M}(W_\pm)$ which are covariant in the sense of the identities (48), we assign to the wedge $W\in\mathcal{W}$ the set of operators $\mathcal{M}(W)$ defined by

$$\mathcal{M}(W)=U(g)\mathcal{M}(W_+)U(g)^{-1} \tag{50}$$

with any representative $g\in G$ of the equivalence class $[g]$ which characterizes W. $\mathcal{M}(W)$ is well defined: Whenever $W=g_1\cdot W_+=g_2\cdot W_+$ there is $g_0\in G_+$ such that $g_2=g_1\cdot g_0$ and therefore, by Lemma V.9, $U(g_2)\mathcal{M}(W_+)U(g_2)^{-1}=U(g_1)U(g_0)\mathcal{M}(W_+)U(g_0)^{-1}U(g_1)^{-1}$ $=U(g_1)\mathcal{M}(W_+)U(g_1)^{-1}$. This lemma also shows that for $W=W_\pm$ the above definition of $\mathcal{M}(W)$ is consistent, in particular $U(R)\mathcal{M}(W_+)U(R)^{-1}=\mathcal{M}(W_-)$ since $R\cdot W_+=W_-$, where R is the Euclidean rotation by π around the x^3-axis.

*Proposition V.10: The assignment of operator *-algebras $\mathcal{M}(W)$ to wedges $W\in\mathcal{W}$ is causal in the sense that*

$$\mathcal{M}(W)\subset\mathcal{M}(W')' \tag{51}$$

for all wedges $W\in\mathcal{W}$.

Proof: The causal complement W' of a wedge $W=g\cdot W_+\in\mathcal{W}$ again belongs to $\mathcal{W}$ since $W'=g\cdot(W_+)'=g\cdot W_-=g\cdot R\cdot W_+\in\mathcal{W}$. Now consider any pair of operators $X_1\in\mathcal{M}(W)$ and $X_2\in\mathcal{M}(W')$. There exists $Y_1\in\mathcal{M}(W_+)$ and $Y_3\in\mathcal{M}(W_+)$ such that $X_1=U(g)Y_1U(g)^{-1}$ and $X_2=U(gR)Y_3U(gR)^{-1}=U(g)U(R)Y_3U(R)^{-1}U(g)^{-1}=U(g)Y_2U(g)^{-1}$ with Y_2 $Y_2=U(R)Y_3U(R)^{-1}\in\mathcal{M}(W_-)$. By Theorem V.3 we know that the operators Y_1 and Y_2 commute. Therefore the operators X_1 and X_2 commute since

$$[X_1,X_2]=U(g)[Y_1,Y_2]U(g)^{-1}=0.$$

Thus we conclude. □

Finally recall that a double cone in Minkowski space is the intersection of all wedges that contain it. Accordingly we assign a *-algebra $\mathcal{M}(D)$ of bounded operators on $\mathcal{H}$ to a double cone D and a *-algebra $\mathcal{M}(D')$ to the spacelike complement D' of D according to the following formulas:

$$\mathcal{M}(D)=\bigcap_{D\subset W\in\mathcal{W}}\mathcal{M}(W),\quad \mathcal{M}(D')=\Big\{\bigcup_{D'\supset W\in\mathcal{W}}\mathcal{M}(W)\Big\}''. \tag{52}$$

Then by definition we have

$$\mathcal{M}(D_1)\subset\mathcal{M}(W)\subset\mathcal{M}(D_2') \tag{53}$$

for any triplet (D_1,D_2,W), with $W\in\mathcal{W}$ and where D_1, D_2 are double cones such that $D_1\subset W\subset D_2'$.

Theorem V.11: *Let a hyperfunction quantum field theory $(\mathcal{H},U,\mathcal{D},\Phi)$ be given. If $\mathcal{M}(W_+)\Phi_0$ is dense in the state space $\mathcal{H}$, then the net $\{\mathcal{M}(D)\}$ assigned to double cones D satisfies the condition of causality (local commutativity) in the sense that for any pair of double cones D_1, D_2 with $D_1\subset D_2'$ the operator algebra $\mathcal{M}(D_1)$ is contained in the commutant of the operator algebra $\mathcal{M}(D_2)$,*

$$\mathcal{M}(D_1)\subset\mathcal{M}(D_2)'. \tag{54}$$

Proof: Though we are not in the setting of standard QFT the proofs of Theorem 13.3.7 of Ref. 1 and/or Theorem 5 of Ref. 17 apply since the necessary background has been provided. □

VI. NONTRIVIALITY OF LOCAL ALGEBRAS

In this section we show that our suggestion for the assignment of local *-algebras $\mathcal{M}(O)$ to open nonempty subsets O of space–time is not vacuous by constructing a simple class of models of hyperfunction quantum fields (which are not standard quantum fields) for which it is easy to show that the algebras $\mathcal{M}(O)$ of our construction are not trivial. The first subsection gives the construction of this model while the second proves the nontriviality of these algebras.

A. Power series of free fields

A class of hyperfunction quantum fields $\rho(x)$ will be constructed as Wick power series of a free field $\phi(x)$. We begin with a brief discussion of power series of two-point functions.

The two-point Wightman function of a free neutral scalar field in four-dimensional space–time is

$$D_m^{(-)}(x)=(2\pi)^{-3}\int_{\mathbf{R}^4} e^{-ik\cdot x}\delta(k\cdot k-m^2)\,\theta(k^0)\,dk$$

$$=(2\pi)^{-3}\int_{\mathbf{R}^3}[2\omega(\mathbf{k})]^{-1}e^{-i\omega(\mathbf{k})x^0}e^{i\mathbf{k}\cdot\mathbf{x}}d\mathbf{k}, \tag{55}$$

where $k\cdot x=k^0x^0-\mathbf{k}\cdot\mathbf{x}$, $\omega(\mathbf{k})=\sqrt{\mathbf{k}^2+m^2}$.

The identity (55) shows that $D_m^{(-)}(x)$ is the Fourier transform of a distribution whose support is contained in the forward light cone. Therefore $D_m^{(-)}(x)$ is the boundary value of the function $D_m^{(-)}(z)$ which is holomorphic in the backward tube $\mathcal{T}_-=\{x+iy\in\mathbf{C}^4; y\in V_-\}$, where $V_-=\{y\in\mathbf{R}^4; y^0<-|\mathbf{y}|\}$ is a backward light cone. Moreover, we have, for any $\epsilon>0$,

$$|D_m^{(-)}(x^0-i\epsilon,\mathbf{x})|\leqslant\frac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\frac{e^{-\omega(\mathbf{k})\epsilon}}{2\omega(\mathbf{k})}d\mathbf{k}=D_m^{(-)}(-i\epsilon,\mathbf{0})=g(\epsilon), \tag{56}$$

where $g(\epsilon)$ is a decreasing function of $\epsilon>0$ [$g(\epsilon_1)\geqslant g(\epsilon_2)$ for $\epsilon_1<\epsilon_2$] and $\epsilon^2 g(\epsilon)\to(2\pi)^{-1}$ as $\epsilon\to 0$. By Lorentz invariance, $D_m^{(-)}(z)$ can be analytically continued to a function which is analytic in the extended tube $\mathcal{T}_1=\{\zeta\in\mathbf{C}^4;\zeta\cdot\zeta\notin\mathbf{R}_+\}$ and invariant under complex Lorentz transformations.

Since $D_m^{(-)}(x)$ is a boundary value of $D_m^{(-)}(z)$ which is holomorphic in the backward tube, the n-fold product $D_m^{(-)}(x)^n$ of $D_m^{(-)}(x)$ is also a boundary value of the holomorphic function $D_m^{(-)}(z)^n$ and defines a hyperfunction; moreover it is a distribution since the order of growth is ϵ^{-2n} when the boundary is approached. But

$$\sum_{n=0}^{\infty} b_n D_m^{(-)}(x)^n \tag{57}$$

is a distribution if, and only if, all except finitely many of the coefficients b_n's vanish (see Ref. 22). On the other hand, if

$$F(z)=\sum_{n=0}^{\infty} b_n z^n \tag{58}$$

is not a polynomial but an entire function, then (57) is a hyperfunction. Moreover it is a Fourier hyperfunction because $D_m^{(-)}(x-i\epsilon,x)$ for ϵ fixed is a bounded function by (56). The power series (58) determines an entire function if, and only if, its coefficients b_n satisfy the condition

$$\limsup_{n\to\infty}|b_n|^{1/n}=0.$$

If the entire function (58) is not too rapidly increasing, i.e., $F(z)=\exp z$, then (57) defines an ultradistribution of Gevrey class but if (58) is rapidly increasing, e.g., $F(z)=\exp\exp z$, then (57) does not define even an ultradistribution of Gevrey class. It defines a generalized function whose test-function space has no nontrivial functions with compact supports since it consists of quasi-analytic functions. The above statement is proved by similar arguments to those in Refs. 23 and 24. We will prove it in a forthcoming paper.

The Wick monomials $:\phi^l:(x)$ of a free field ϕ are defined by Wightman and Gårding in Ref. 25.

Now let $\{a_n^{(i)}\}$ be sequences satisfying $\lim_{n\to\infty}[|a_n^{(i)}|^2/n!]^{1/n}=0$ and define $\rho^{(i)}(x)$ by

$$\rho^{(i)}(x)=\sum_{n=0}^{\infty}a_n^{(i)}\frac{:\phi(x)^n:}{n!}. \tag{59}$$

Then Nagamachi and Mugibayashi have shown in Ref. 8 that the above series converges and defines a hyperfunction quantum field defined in the Fock space of $\phi(x)$ using the basic relation between Schwinger functions and Wightman functions for a hyperfunction quantum field which was established in Ref. 13. We give here a new direct proof which does not rely on the relation between Wightman and Schwinger functions.

To begin we recall:

Theorem VI.1 (Theorem A.1 of Ref. 26): *As a formal power series we have*

$$(\Omega,\rho^{(1)}(x_1)\cdots\rho^{(n)}(x_n)\Omega)=\sum_{r_{ij}=0;1\leqslant i<j\leqslant n}^{\infty}\frac{A(R)T^R}{R!}, \tag{60}$$

where

$$r_{ij}=r_{ji},\ \ r_{ii}=0,\ \ R_i=\sum_{j=1}^{n}r_{ij},\ \ t_{ij}=D_m^{(-)}(x_i-x_j),$$

$$R!=\prod_{1\leqslant i<j\leqslant n}(r_{ij})!,\quad T^R=\prod_{1\leqslant i<j\leqslant n}(t_{ij})^{r_{ij}},\ \ A(R)=\prod_{j=1}^{n}a_{R_j}^{(j)}.$$

From the above theorem one easily gets

Theorem VI.2 (Theorem 3.3 of Ref. 8): *If*

$$\lim_{n\to\infty}[|a_n^{(i)}|^2/n!]^{1/n}=0, \tag{61}$$

then the right-hand side of (60) is an entire function of the variables t_{ij}.

Now, if the coefficients $a_n^{(i)}$ of $\rho^{(i)}(x)$ according to (59) satisfy the condition (61), then, by the above results, the right-hand side of (59) defines a (Fourier) hyperfunction quantum field (of type I).

We indicate briefly the proof of this observation. In fact, if $z_j-z_i\in\mathcal{T}_+=\mathbf{R}^4+iV_+$ (V_+ denotes the forward light cone), then $D_m^{(-)}(z_i-z_j)$ is holomorphic there and $D_m^{(-)}(x_i-x_j)$ is the boundary value of $D_m^{(-)}(z_i-z_j)$. Therefore, if $\mathrm{Im}(z_{i+1}-z_i)\in V_+$ $(i=1,2,\ldots,n-1)$, then $(\Omega,\rho^{(1)}(z_1)\cdots\rho^{(n)}(z_n)\Omega)$ is holomorphic and $(\Omega,\rho^{(1)}(x_1)\cdots\rho^{(n)}(x_n)\Omega)$ is the boundary value of $(\Omega,\rho^{(1)}(z_1)\cdots\rho^{(n)}(z_n)\Omega)$. Since

$$|D_m^{(-)}(x^0-i\epsilon,\mathbf{x})|\leqslant[2(2\pi)^3]^{-1}\int\omega(\mathbf{k})^{-1}e^{-\omega(\mathbf{k})\epsilon}d\mathbf{k}$$

(60) defines a Fourier hyperfunction.

In order to show that (59) defines a hyperfunction quantum field (see Refs. 10, 27, 28, 9, and 13), we show that the system of Fourier hyperfunctions $\mathcal{W}_n$ of (60) satisfies the (modified) Wightman axioms, as formulated by Nagamachi and Mugibayashi in Ref. 9:

R_0 Fourier hyperfunction property:

$$\mathcal{W}_n \in \mathcal{Q}(\mathbf{D}^{4n})', \quad \mathcal{W}_n(f) = \mathcal{W}_n(\overline{f}),$$

where $\overline{f}(x_1,\ldots,x_n) = \overline{f(x_n,\ldots,x_1)}$.

R_1 Relativistic covariance: For every $(\Lambda,a) \in G$ and $n=1,2,\ldots$ we have

$$\mathcal{W}_n(\Lambda x_1 + a,\ldots,\Lambda x_n + a) = \mathcal{W}_n(x_1,\ldots,x_n)$$

as an identity for Fourier hyperfunctions on $\mathbf{R}^{4n}$. Here G denotes the proper Poincaré group.

R_2 Positivity:

$$\sum_{m,n=0}^{k} \mathcal{W}_{m+n}(\overline{f}_m \otimes f_n) \geqslant 0,$$

for any choice of $f_n \in \mathcal{Q}(\mathbf{D}^{4n})$ and any k.

R_3 Local commutativity:

$$\mathcal{W}_n(x_1,\ldots,x_j,x_{j+1},\ldots,x_n) = \mathcal{W}_n(x_1,\ldots,x_{j+1},x_j,\ldots,x_n)$$

if $(x_j - x_{j+1})^2 < 0$ as an identity for Fourier hyperfunctions on $\mathbf{R}^{4n}$, for $n=2,3,\ldots$.

R_4 Spectral condition: For $n=2,3,\ldots$ there exists a $\mu_{n-1} \in \mathcal{Q}(\overline{V_+^{n-1}})'$ such that

$$\mathcal{W}_n(x_1,\ldots,x_n) = W_{n-1}(x_2 - x_1,\ldots,x_n - x_{n-1}),$$

where W_{n-1} is the Fourier transform of μ_{n-1}.

R_5 Cluster property: If a is spacelike,

$$\mathcal{W}_n(x_1,\ldots,x_j,x_{j+1}+\lambda a,\ldots,x_n+\lambda a) \to \mathcal{W}_n(x_1,\ldots,x_j)\mathcal{W}_n(x_{j+1},\ldots,x_n)$$

as $\lambda \to \infty$.

R_1 is obviously satisfied. R_5 follows from the fact that $D_m^{(-)}(z-\lambda a) \to 0$ Im $z \in V_+$, $a^2 < 0$ and $\lambda \to \infty$. In fact, let $y_i = z_i$ for $i \leqslant k$ and $y_i = z_i + \lambda a$ for $k < i$. Then $t_{ij} = D_m^{(-)}(y_i - y_j)$, $1 \leqslant i \leqslant k < j \leqslant n$ vanishes as $\lambda \to \infty$. Therefore,

$$T^R = \prod_{1 \leqslant i < j \leqslant n} (t_{ij})^{r_{ij}} \to 0$$

unless all r_{ij} for $1 \leqslant i \leqslant k < j \leqslant n$ are zero. Thus we have

$$T^R \to \left[\prod_{1 \leqslant i < j \leqslant k} (t_{ij})^{r_{ij}} \right] \left[\prod_{k < i < j \leqslant n} (t_{ij})^{r_{ij}} \right]$$

which shows the cluster property.

In order to show R_0 and R_2, a Wick polynomial $\rho_N^{(i)}(x)$ is introduced as a truncation of $\rho^{(i)}(x)$,

$$\rho_N^{(i)}(x) = \sum_{n=0}^{N} a_n^{(i)} : \phi(x)^n : /n!.$$

Then the Wightman functions for $\rho_N^{(i)}(x)$ satisfy all the (unmodified) Wightman axioms (see Ref. 25). Since the right-hand side of (60) is an absolutely convergent series of the variables t_{ij}, $(\Omega,\rho_N^{(1)}(x_1)\cdots\rho_N^{(n)}(x_n)\Omega)$ converges to $(\Omega,\rho^{(1)}(x_1)\cdots\rho^{(n)}(x_n)\Omega)$ as $N\to\infty$ in the sense of Fourier hyperfunctions. Thus we easily see Hermiticity and the positivity. However, such limit does not necessarily preserve the support (see Theorem 4.1.14 of Ref. 16), and it is unknown whether the spectral condition and the local commutativity can be verified in this manner. But as written in Note 4.1 of Ref. 16, ''if you want to use topology, use it at the level of holomorphic functions.''

In order to simplify notations we denote here and in the remainder of this section the analytic function whose boundary value is the vacuum expectation value $(\Omega,\rho^{(1)}(x_1)\cdots\rho^{(n)}(x_n)\Omega)$ of the fields $\rho^{(i)}$ with $(\Omega,\rho^{(1)}(z_1)\cdots\rho^{(n)}(z_n)\Omega)$ and similarly for the fields $\rho_N^{(i)}$. Then the holomorphic function $(\Omega,\rho^{(1)}(z_1)\cdots\rho^{(n)}(z_n)\Omega)$ is the limit of the holomorphic functions $(\Omega,\rho_N^{(1)}(z_1)\cdots\rho_N^{(n)}(z_n)\Omega)$, and this will give us the necessary information. Our proof of the spectral condition relies the following two results from the general theory of Fourier hyperfunctions.

Theorem VI.3 (Theorem 3.3.1 of Ref. 29): *Let Γ be a closed and strictly convex cone with vertex at the origin and satisfy $\Gamma\setminus\{0\}\subset\{x_1>0\}$ and K be its closure in $\mathbf{D}^n$. Let $\Gamma^0=\{\xi;\langle x,\xi\rangle\geqslant 0,\forall x\in\Gamma\}$. Then every $\mu\in\mathcal{O}(K)'$ has the following properties: The Fourier transform $\langle\mu,e^{i\langle\cdot,\zeta\rangle}\rangle$ of μ is holomorphic in $\mathbf{R}^n\times i(\Gamma^0)^i$ and satisfies the following growth condition. For every $\Gamma'\subset\subset\Gamma^0$ (the closure of Γ' has a compact neighborhood in the closure of Γ^0 with respect to the topology of $\mathbf{D}^n$) and $\epsilon>0$,*

$$|\langle\mu,e^{i\langle\cdot,\zeta\rangle}\rangle|\leqslant C_\epsilon\exp(\epsilon|\mathrm{Re}\,\zeta|+\chi_{\Gamma,\epsilon}(\mathrm{Im}\,\zeta)),\quad \zeta\in\mathbf{R}^n\times i\Gamma', \tag{$*$}$$

where

$$\chi_{\Gamma,\epsilon}(\eta)=\sup_{x\in\Gamma-\epsilon(1,0,\ldots,0)}(-\langle x,\eta\rangle+\epsilon|x|).$$

Theorem VI.4 (Theorem 3.3.2 of Ref. 29): *Let $F(\zeta)$ be holomorphic in $\mathbf{R}^n\times i(\Gamma^0)^i$ and satisfies the growth condition (*). Then there exists a unique $\mu\in\mathcal{O}(K)'$ such that $F(\zeta)=\langle\mu,e^{i\langle\cdot,\zeta\rangle}\rangle$.*

Since $D_m^{(-)}(z)$ is a bounded holomorphic function in $\mathbf{R}^4\times i\Gamma'$ for any $\Gamma'\subset\subset V_-$, $(\Omega,\rho^{(1)}(z_1)\cdots\rho^{(n)}(z_n)\Omega)$ satisfies the estimate (*) for $\zeta_j=z_{j+1}-z_j$ and $\Gamma=\overline{V_+^{n-1}}$. Thus we deduce the spectral condition R_4. For the proof of the local commutativity, we use the following theorem on p. 83 of Ref. 19.

Theorem VI.5: *If $\mathcal{W}_n(z_1,\ldots,z_n)$ has all the properties of a Wightman function except the ones derived from locality and if in addition $\mathcal{W}_n(z_1,\ldots,z_n)$ is symmetric in $z_1,\ldots,z_n$, then it satisfies also the requirements of locality.*

This theorem is proved for hyperfunction quantum field theory in the same way as in standard tempered quantum field theory. Since $(\Omega,\rho_N^{(1)}(z_1)\cdots\rho_N^{(n)}(z_n)\Omega)$ is symmetric in $z_1,\ldots,z_n$ in the extended tube, the function $(\Omega,\rho^{(1)}(z_1)\cdots\rho^{(n)}(z_n)\Omega)$ is also symmetric there. Thus we deduce the locality condition R_3.

By the reconstruction theorem (see Ref. 9), we have a Hilbert space $\mathcal{H}$, field operators $\rho^i(f)$ for $f\in\mathcal{O}(\mathbf{D}^4)$, and a unitary representation of the Poincaré group $U(a,\Lambda)$ on $\mathcal{H}$.

The Hilbert space $\mathcal{H}$ can be assumed to be contained in the Fock space $\mathcal{H}_F$ of the free field. In fact, the vectors $\Phi_N=\rho_N^{(1)}(f_1)\cdots\rho_N^{(n)}(f_n)\Omega$ for $f_j\in\mathcal{O}(\mathbf{D}^4)$ are contained in $\mathcal{H}_F$ and

$$\|\Phi_N-\Phi_M\|^2=(\Phi_N,\Phi_N)-(\Phi_N,\Phi_M)-(\Phi_M,\Phi_N)+(\Phi_M,\Phi_M)\to 0$$

as $N,M\to\infty$. Thus $\rho^{(1)}(f_1)\cdots\rho^{(n)}(f_n)\Omega=\lim_{N\to\infty}\rho_N^{(1)}(f_1)\cdots\rho_N^{(n)}(f_n)\Omega$ belongs to $\mathcal{H}_F$.

Let $\{a_n\}_{n\in\mathbb{N}}$ be a sequence satisfying

$$\lim_{n\to\infty}[|a_n|^2/n!]^{1/n}=0$$

and define $\rho(x)$ by

$$\rho(x)=\sum_{n=0}^{\infty} a_n \frac{:\phi(x)^n:}{n!}.$$

Let $\rho^{(i)}(x)$ of (59) be either $\phi(x)$ or $\rho(x)$. Then we have the system

$$(\mathcal{H},\Omega,\phi(x),\rho(x),U(a,\Lambda)),$$

which satisfies the defining conditions $H_1,\ldots,H_5$ of a hyperfunction quantum field (see Ref. 10). Since the vectors $\phi(f_1)\cdots\phi(f_n)\Omega$ span the Fock space $\mathcal{H}_F$ we have $\mathcal{H}=\mathcal{H}_F$.

Thus we arrive at the main result of this section.

Theorem VI.6: *Let ϕ be a free massive neutral scalar field and $\{a_n\}_{n\in\mathbb{N}}$ a sequence of real numbers satisfying* $\lim_{n\to\infty}[|a_n|^2/n!]^{1/n}=0$. *Then the (Wick) power series ρ of ϕ formed with the coefficients a_n according to Eq. (59) is a hyperfunction quantum field (but not a standard quantum field if infinitely many of the coefficients a_n are nonzero*).

B. A Model with nontrivial local algebras

The power series ρ of a free scalar field ϕ provide a class of hyperfunctions quantum fields (under technical restrictions discussed in the previous section).

The main focus of our discussion now is to show, for the class of models ρ constructed above, that $\mathcal{L}'_w(O)=L'(O)$ contains indeed a nontrivial *-algebra of observables. Clearly in the proof of this statement we will use the explicit definition of the hyperfunction quantum fields ρ in an essential way.

For a free neutral scalar field $\phi(x)$ of mass m the field operators $\phi(f)$, for real $f\in\mathcal{S}(\mathbf{R}^4)$, are known to be essentially self-adjoint on

$$\mathcal{D}_0=\text{lin span}\{\Omega,\phi(f_1)\cdots\phi(f_n)\Omega;\ \ f_k\in\mathcal{S}(\mathbf{R}^4),n=1,2,\ldots\}.$$

Denote the self-adjoint closure of $\phi(f)$ by $\Phi(f)$. Then,

$$e^{i\Phi(f)}\psi=\sum_{n=0}^{\infty}\frac{i^n\phi(f)^n}{n!}\psi$$

converges for $\psi\in\mathcal{D}_0$, and defines a unitary operator $e^{i\Phi(f)}$ (see Theorem X.41 of Ref. 30).

To an open set O in $\mathbf{R}^4$ assign the *-algebra $\mathcal{M}(O)$ generated by elements $e^{i\Phi(f)}$ for $f\in\mathcal{S}(\mathbf{R}^4)$ with $\text{supp}\, f\subset O$. This defines a net of nontrivial *-algebras of bounded operators on $\mathcal{H}$. Using the relation

$$e^{i\Phi(f)}e^{i\Phi(g)}=e^{D_m^{(-)}(f,g)/2}e^{i\Phi(f+g)}, \tag{62}$$

we have $e^{i\Phi(f_1)}\cdots e^{i\Phi(f_n)}=ce^{i\Phi(f_1+\cdots+f_n)}$ for some $c\in\mathbf{C}$. Thus, locality of the net $\{\mathcal{M}(O)\}$ is evident from (62) since $D_m^{(-)}(f,g)=D_m^{(-)}(g,f)$ if the supports of f and g are spacelike separated. Define $\Psi(g)$ by

$$\Psi(g)=:\exp i\phi(g):=\sum_{n=0}^{\infty} i^n\frac{:\phi(g)^n:}{n!}.$$

Let S be a subset of $\{1,2,\ldots,n\}$ and $\psi^{(i)}=\Psi(g)$ if $i\in S$ otherwise $\psi^{(i)}=\rho(x_i)$. Then we have

$$(\Omega,\psi^{(1)}\cdots\psi^{(n)}\Omega)=\sum_{r_{ij}=0,1\leqslant i<j\leqslant n}^{\infty}\frac{A(R)T^R}{R!}, \tag{63}$$

where

$$t_{ij}=D_m^{(-)}(x_i-x_j) \quad \text{if } i,j\notin S,$$

$$t_{ij}=\int D_m^{(-)}(x_i-x_j)g_i(x_i)g_j(x_j)dx_i dx_j\in\mathbf{C} \quad \text{if } i,j\in S,$$

$$t_{ij}=D_m^{(-)}(x_i,g_j)=\int D_m^{(-)}(x_i-x_j)g_j(x_j)dx_j \quad \text{if } i\notin S \text{ and } j\in S,$$

$$t_{ij}=D_m^{(-)}(g_i,x_j)=\int D_m^{(-)}(x_i-x_j)g_i(x_i)dx_i \quad \text{if } i\in S \text{ and } j\notin S.$$

Fix $j\in\{1,\ldots,n\}$ and consider points $z_i\in\mathbf{C}^4$ which satisfy the following conditions: $\mathrm{Im}(z_{i+1}-z_i)\in V_+$, $i=1,\ldots,j-1$ and $i=j+2,\ldots,n-1$; $\mathrm{Im}\,z_{j+2}\in V_+$, $\mathrm{Im}\,z_j=0$.

Now we apply the identity (63) to

$$(\Omega,\rho(z_1)\cdots\rho(z_{j-1})\rho(x_j)\Psi(g)\rho(z_{j+2})\cdots\rho(z_n)\Omega)$$

and look at the effect of the exchange of j and $j+1$, e.g., of $t_{i,j}\to t_{i,j+1}$. We find

$$(\Omega,\rho(z_1)\cdots\rho(z_{j-1})\Psi(g)\rho(x_j)\rho(z_{j+2})\cdots\rho(z_n)\Omega).$$

If x_j and $\mathrm{supp}\,g$ are spacelike separated, then $t_{j,j+1}=D_m^{(-)}(x_j,g)=D_m^{(-)}(g,x_j)=t_{j+1,j}$. Thus we get

$$\begin{aligned}&(\Omega,\rho(z_1)\cdots\rho(z_{j-1})\rho(x_j)\Psi(g)\rho(z_{j+2})\cdots\rho(z_n)\Omega)\\&\quad=(\Omega,\rho(z_1)\cdots\rho(z_{j-1})\Psi(g)\rho(x_j)\rho(z_{j+2})\cdots\rho(z_n)\Omega)\end{aligned}$$

and therefore

$$\begin{aligned}&(\Omega,\rho(x_1)\cdots\rho(x_{j-1})\rho(x_j)\Psi(g)\rho(x_{j+1})\cdots\rho(x_n)\Omega)\\&\quad=(\Omega,\rho(x_1)\cdots\rho(x_{j-1})\Psi(g)\rho(x_j)\rho(x_{j+1})\cdots\rho(x_n)\Omega)\end{aligned}\tag{64}$$

as an identity between Fourier hyperfunctions.

Now assume that O is an open bounded nonempty subset of space–time and that $g\in\mathcal{S}(\mathbf{R}^4)$ has its support in O. Then, for all x_j in the causal complement O' of O we deduce from (64)

$$(\Psi(g)^*u,\rho(x_j)v)=(\rho(x_j)u,\Psi(g)v)\tag{65}$$

for all $u=\rho(\overline{f}_{j-1})\cdots\rho(\overline{f}_1)\Omega$ and all $v=\rho(f_{j+2})\cdots\rho(f_n)\Omega$ in $\mathcal{D}_0$, where

$$\mathcal{D}_0=\mathrm{lin\,span}\{\Omega,\rho(f_1)\cdots\rho(f_n)\Omega;\ f_j\in\mathcal{Q}(\mathbf{D}^4),\ n=1,2,\ldots\}.$$

For the hyperfunction quantum field ρ recall the definition of the set of bounded operators localized in an open set $O\subset\mathbf{R}^4$ according to Sec. IV,

$$L'(O')=\{X\in\mathcal{B}(\mathcal{H});\mathrm{supp}[(X^*u,\rho(x)v)-(\rho(x)^*u,Xv)]\subset\mathbf{D}^4\setminus O',\forall u,v\in\mathcal{D}_0\},$$

where $\mathcal{D}_0=\mathrm{lin\,span}\{\Omega,\rho(f_1)\cdots\rho(f_n)\Omega;\ f_j\in\mathcal{Q}(\mathbf{D}^4),\ n=1,2,\ldots\}$. Hence Eq. (65) shows

$$\Psi(g)\in L'(O')$$

if $\mathrm{supp}\,g\subset O$. Since

$$:\exp i\phi(g):=e^{-D_m^{(-)}(g,g)/2}\exp i\Phi(g),$$

we have $\exp i\Phi(g)\in L'(O')$, and therefore

$$\mathcal{M}(O)\subset L'(O').$$

This shows

Theorem VI.7: *Consider a free neutral scalar field ϕ and assign to open bounded nonempty sets $O\subset\mathbf{R}^4$ the *-algebras $\mathcal{M}(O)$ introduced above. For the power series ρ of ϕ according to Theorem VI.6 form the spaces $L'(O')$ of bounded operators on the state space of ρ which are localized in open bounded nonempty sets $O\subset\mathbf{R}^4$ according to Sec. III. Then,*

$$\mathcal{M}(O)\subset L'(O')=\mathcal{L}'_w(O').$$

VII. CONCLUSION

In this paper the old problem of how to assign, in a relativistic quantum field theory, local *-algebras of observables to open bounded nonempty subsets $O\subset\mathbf{R}^4$ has been addressed in the context of hyperfunction quantum field theory. Since the localization properties of hyperfunction quantum fields are considerably more subtle than standard (Wightman) quantum fields the established routes to this problem do not apply. Thus a major step in addressing this problem ''correctly'' is our suggestion of the sets $\mathcal{L}'_w(O)$ of the set of those bounded operators on the state space of the field Φ which commute weakly with all products of fields $\Phi(x_1)\cdots\Phi(x_n)$ for all $x_k\in O$, $n=1,2,\ldots$. The local *-algebras of observables $\mathcal{M}(O)$ are then defined as suitable subspaces of $\mathcal{L}'_w(O')$.

In order to enable this construction, the proof of three important structural results in hyperfunction quantum field theory which are all well known in standard QFT: existence of a CPT-operator, Reeh–Schlieder theorem, Bisognano–Wichmann analyticity had to be given. This then prepares the ground for the proof of some structural results for the weak commutants $\mathcal{L}'_w(O)$ and a suggestion for $\mathcal{M}(O)\subset\mathcal{L}'_w(O')$. Following basically a modification of the Bisognano–Wichmann strategy the locality of the net $\{\mathcal{M}(O)\}$ is established for double cones. We conclude that the Bisognano–Wichmann theory does not really rely on the existence of compactly supported test functions.

Since hyperfunctions can grow much faster than tempered distributions, a domain problem in the definition of $\mathcal{L}'_w(O)$ (which does not occur in standard QFT) has to be addressed, and a mild growth restriction for the hyperfunction quantum field is offered which allows us to solve the domain problem. Then, relying on recent results in the theory of Fourier hyperfunctions (the kernel theorem in full generality) a simplifying and more intuitive characterization of the weak commutants $\mathcal{L}'_w(O)$ is derived in

$$\mathcal{L}'_w(O)=L'(O),$$

where $L'(O)$ is the space of all bounded operators on the state space of the field which commute weakly with the field $\Phi(x)$ for $x\in O$.

It seems to us that it is expected too much to be able to prove the nontriviality of the suggested *-algebras in full generality without any further specification of the hyperfunction quantum field under consideration (as in the case of standard quantum fields). Thus we address the problem of the existence of nontrivial *-algebras $\mathcal{M}(O)$ in the context of a class of concrete models: Wick powers series of free fields (in general they are hyperfunction quantum fields but not standard quantum fields). For this class of models the existence of a nontrivial *-algebra $\mathcal{M}(O)\subset L'(O')$ is shown explicitly. It is remarkable that these models of hyperfunction quantum fields do not admit test-functions with compact support.

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Euler number of instanton moduli space and Seiberg–Witten invariants

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We show that a partition function of topological twisted $N=4$ Yang–Mills theory is given by Seiberg–Witten invariants on a Riemannian four manifolds under the condition that the sum of the Euler number and the signature of the four manifolds vanishes. The partition function is the sum of the Euler number of instanton moduli space when it is possible to apply the vanishing theorem. Also we obtain a relation of the Euler number labeled by the instanton number k with Seiberg–Witten invariants. All calculations in this article are done without assuming duality. [DOI: 10.1063/1.1331319]

I. INTRODUCTION

The aim of this article is to obtain a relation of the partition function of topological twisted $N=4$ gauge theory with Seiberg–Witten invariants in four manifolds. The partition function is given by the Euler number of instanton moduli space in some conditions. We will show that the Euler number labeled by instanton number k is expressed by Seiberg–Witten invariants when the sum of the Euler number and the signature of the base four manifolds vanishes. This result gives us the formulas to obtain the partition function of the twisted $N=4$ gauge theory by Seiberg–Witten invariants.

The partition functions of the $N=4$ Yang–Mills theories on some four manifolds are calculated by Vafa and Witten with topological field theory.[1,2] It is an SL(2,Z) modular form. SL(2,Z) transformation is understood as an extension of Montonen–Olive duality.[3] So the duality relation is apparent in that partition function.

This duality is deeply connected with the Hilbert scheme picture of instanton moduli space.[4] However, in general, instanton moduli space has variety compactification and the sum of the Euler number of any compactified moduli space is not necessarily a modular form. Actually, in our calculus, the partition function is not a modular form with no contrivance. On the other hand, $N=4$ gauge theory is given by the toroidal compactification of 10-dim $N=1$ gauge theory on a 4-dim manifold. (Note that ''compactification'' is used two ways.) So the theory is interpreted as a low-energy theory of the heterotic or type I string theory. Recent developments in string theory show us much evidence of duality relation in field theory. In our case, Vafa shows us one method to link the compactified instanton moduli space with the Hilbert scheme.[5] This fact implies that a choice of compactification is understood in string theory better than field theory. We discuss the problem of compactification and duality later.

For our purpose we use a tool similar to topological QCD constructed by S. Hyun, J. Park, and J-S. Park (H-P-P).[6] They used the non-Abelian monopole theory and related the Donaldson invariants to Seiberg–Witten invariants without using duality.[7,8] We also calculate the partition function in the low-energy limit of cohomological field theory[9] and there is no request of S-duality. This is the most different point from Dijkgraaf, Park, and Schroers.[10] They have deter-

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mined the partition function of $N=4$ supersymmetric Yang–Mills theory on a Kähler surface, using S-duality. Their result is given by Seiberg–Witten invariants, too. So, it is interesting to compare our results with theirs.

What we do first is to extend the instanton moduli space to non-Abelian monopole moduli. In usual cohomological field theory, it was done by H-P-P[11] and Labastida and Mariño.[12] Vafa–Witten theory is constructed as a balanced topological field theory (we denote it as BTFT in the following).[13] BTFT has no ghost number anomaly, and its partition function is a sum of the Euler numbers of given zero-section space under the vanishing theorem. In Sec. II, we will construct the non-Abelian monopole theory as BTFT and investigate some characteristics of the theory. The vanishing theorem is an obstruction to constructing the partition function as the sum of the Euler numbers of the monopole moduli, and to get a relation with Vafa–Witten theory. We do not study this case closer in this article.

In Sec. III, we obtain the formulas between the partition function of a twisted $N=4$ Yang–Mills theory and Seiberg–Witten invariants. To obtain them, we break the balance of topological charge. The tools in this article were used in obtaining a relation of Donaldson invariants and Seiberg–Witten invariants.[6] We use a model which has a gauge multiplet that is balanced and a hypermultiplet that is not balanced. We call the model unbalanced topological QCD. The vacuum expectation value (VEV) of an observable is calculated and the relation between the Euler number of instanton moduli space and Seiberg-Witten invariants is obtained if the vanishing theorem is applicable and the sum of the Euler number and the signature of the four manifolds vanishes. The comparison with the papers of Vafa and Witten[1] and Dijkgraaf, Park, and Schroers[10] is also made in this section. In the last section, we discuss some remaining problems and the possibility of extension.

II. BALANCED TOPOLOGICAL QCD

In this section, we construct a balanced topological QCD (BTQCD), which is a twisted $N=4$ Yang–Mills theory coupled with massive hypermultiplets in the fundamental representation.[10,11,6]

A. Balanced topological QCD

Let X be a compact Riemannian four manifold and E be an SU(2)-bundle over X. The bundle E is classified by the instanton number

$$k=\frac{1}{8\pi^2}\int_X \mathrm{Tr}\, F\wedge F, \tag{2.1}$$

where Tr is the trace in the fundamental representation of SU(2) and $F\in\Omega^2_X(\mathcal{G}_E)$ is the adjoint valued curvature two-form on X. We denote the group of gauge transformation by $\mathcal{G}$, i.e., elements of $\mathcal{G}$ are sections of P, where P is the associated principal SU(2)-bundle over X. We pick a spin^c structure c on X and consider the associated spin^c bundle $W_c^{\pm}$. Let $\mathcal{A}$ be the space of all connections on P and $\Gamma(W_c^+\otimes E)(\Gamma(W_c^-\otimes E))$ be the space of the sections of the spin^c bundle twisted by the vector bundle E. After twisting, the complex boson in the hypermultiplet becomes a section of $\Gamma(W_c^+\otimes E)(\Gamma(W_c^-\otimes E))$:

$$\begin{aligned} &q\in\Gamma(W_c^+\otimes E), \quad q^\dagger\in\Gamma(\overline{W}_c^+\otimes\tilde{E}),\\ &B\in\Gamma(W_c^-\otimes E), \quad B^\dagger\in\Gamma(\overline{W}_c^-\otimes\tilde{E}), \end{aligned} \tag{2.2}$$

where $\tilde{E}$ denotes the vector bundle conjugate to E. The spin^c Dirac operator

$$\sigma^\mu D_\mu:\Gamma(W_c^+\otimes E)\to\Gamma(W_c^-\otimes E) \tag{2.3}$$

is the Dirac operator for the spin^c bundle twisted by E. We will sometimes denote $\sigma^\mu D_\mu$ by $\not{D}$ or $\not{D}_c^E$.

Throughout this article, we restrict our attention to the case that the gauge group is SU(2) and the theory is coupled with hypermultiplets in the fundamental representation.

1. Algebra of BTQCD

In this section, the algebra of BTQCD is given.

We introduce two global supercharges $Q_\pm$ carrying an additive quantum number (ghost number) $U=\pm 1$. When they act on fields in the adjoint representation, they satisfy the following commutation relations:

$$Q_+^2=\delta_\theta^g,\ \{Q_+,Q_-\}=-\delta_c^g,\quad Q_-^2=-\delta_{\bar\theta}^g, \tag{2.4}$$

where δ_θ^g denotes the gauge transformation generated by adjoint scalar field $\theta\in\Omega_\chi^0(\mathcal{G}_E)$ and we adopt $\delta_\theta^g A_\mu=D_\mu\theta$, $\delta_\theta^g B_{+\mu\nu}=i[B_{+\mu\nu},\theta]$, and $\delta_\theta^g c=i[c,\theta]$. When they act on fields in the fundamental representation, they satisfy the following commutation relations:

$$Q_+^2=-\delta_\theta^g,\quad \{Q_+,Q_-\}=\delta_c^g,\quad Q_-^2=\delta_{\bar\theta}^g, \tag{2.5}$$

where we also introduce U(1) global transformation generated by $m\in iR$ and we adopt $\delta_\theta^g q=(i\theta+m)q$, $\delta_\theta^g q^\dagger=q^\dagger(-i\theta-m)$, $\delta_\theta^g B=(i\theta+m)B$, and $\delta_\theta^g B^\dagger=B^\dagger(-i\theta-m)$. The relative sign difference between (2.4) and (2.5) is simply the difference of representations. A simple explanation is the following. One can construct a field J^a in the adjoint representation with a pair of fields $q,q^\dagger$ in the fundamental representation,

$$J^a\equiv q^\dagger T^a q. \tag{2.6}$$

Using the above transformations, one can check (2.4) follows from (2.5):

$$Q_+^2 J^a=Q_+^2(q^\dagger T^a q)=(-\delta_\theta^g q^\dagger)T^a q+q^\dagger T^a(-\delta_\theta^g q)=i[q^\dagger Tq,\theta]^a=\delta_\theta^g J^a. \tag{2.7}$$

Note that the relative sign difference between (2.4) and (2.5) is consistent with this derivation. The recipe for giving mass to fields in the fundamental representation by global symmetry is considered by H-P-P.[6]

We define $\delta_\pm$ transformations $\delta_\pm\equiv[Q_\pm,*\}$. $\delta_\pm$ transformations are given in Appendix A. See also Refs. 13 and 6.

2. Action of BTQCD

Using the previous fields and transformations, we define the action of BTQCD as

$$h^2 S=\int\sqrt{g}\mathcal{L}, \tag{2.8}$$

where

$$\mathcal{L}=\delta_+\delta_-\mathcal{F}. \tag{2.9}$$

Here $\mathcal{F}$ is described with fields in the previous paragraph and has ghost number 0. The general recipe for constructing a balanced topological field theory is given by Moore *et al.*[13]

Here $\mathcal{F}$ is explicitly given by

$$\mathcal{F}=(B_+^{\mu\nu a}s^a_{+\mu\nu})-(\chi_+^{I\mu\nu a}\psi^a_{B\mu\nu})-(\chi^{IIa}_{B\mu}\psi^{\mu a})+(-i\tfrac{1}{3}B_+^{\mu\nu a}[B_{+\mu\rho},B_{+\nu\sigma}]^a g^{\rho\sigma})$$
$$+(B^{\dagger\alpha}s_\alpha)-(\chi_q^{I\dagger\alpha}\psi_{B\alpha})-(\chi^{II\dagger}_{B\dot\alpha}\psi_q^{\dot\alpha})+(s^{\dagger\alpha}B_\alpha)+(\psi_B^{\dagger\alpha}\chi^1_{q\alpha})+(\psi^\dagger_{q\dot\alpha}\chi_B^{II\dot\alpha})+(\xi^a\eta^a), \tag{2.10}$$

where

$$s_+^{\mu\nu}=F_+^{\mu\nu}+q^\dagger\bar\sigma^{\mu\nu}q, \tag{2.11}$$

$$s_\alpha=(\not{D}q)_\alpha. \tag{2.12}$$

Finally, the full Lagrangian is given by

$$\mathcal{L}^{\text{full}}=\delta_+\delta_-\mathcal{F}. \tag{2.13}$$

Explicit expression of this Lagrangian is given in Appendix A. This Lagrangian [(A18)] is different from Vafa–Witten[1] in matter fields (q, B, etc.) and also different from H-P-P[6] in dual fields ($B_+^{\mu\nu}$, c, B, etc.). However, due to its construction, it is balanced.

B. Fixed point

In this subsection, we study the nature of the action given in Sec. II A. Here in particular we investigate the fixed points and vanishing theorem.[1]

1. Fixed point

To check the nature of the Lagrangian, we decompose the bosonic part of Lagrangian (A18)

$$\mathcal{L}^{\text{full}}_{\text{boson}}=\mathcal{L}^{\text{eq}}_{\text{boson}}+\mathcal{L}^{\text{pro}}_{\text{boson}}, \tag{2.14}$$

where

$$\begin{aligned}\mathcal{L}^{\text{eq}}_{\text{boson}}=&-H_+^{I\mu\nu a}\{H^a_{+\mu\nu}-(s^a_{+\mu\nu}-i[B_{+\mu\rho},B_{+\nu\sigma}]^a g^{\rho\sigma}-i[B_{+\mu\nu},c]^a)\}\\&-H_B^{II\rho a}\{H^{IIa}_{B\rho}-(-2D^\mu B^a_{+\mu\rho}+iB^\dagger\sigma_\rho T^a q-iq^\dagger\bar\sigma_\rho T^aB-D_\rho c^a)\}\\&-H_q^{I\dagger\alpha}\{H^I_{q\alpha}-(s_\alpha+icB_\alpha+m_cB_\alpha)\}+(\text{h.c.})\\&-H^{II\dagger}_{B\dot\alpha}\{H_B^{II\dot\alpha}-(-(\not{D}B)^{\dot\alpha}+(\bar\sigma^{\mu\nu}B_{+\mu\nu}q)^{\dot\alpha}+icq^{\dot\alpha}+m_cq^{\dot\alpha})\}+(\text{h.c.})\end{aligned} \tag{2.15}$$

and

$$\begin{aligned}\mathcal{L}^{\text{pro}}_{\text{boson}}=&-\{[\theta,\bar\theta]^a[\bar\theta,\theta]^a-[c,\theta]^a[c,\bar\theta]^a+[B_+^{\mu\nu},\bar\theta]^a[B_{+\mu\nu},\theta]^a\}+D_\mu\bar\theta^aD^\mu\theta^a\\&+(-iq^\dagger\bar\theta-q^\dagger\bar m)(i\theta q+mq)+(-iq^\dagger\theta-q^\dagger m)(i\bar\theta q+\bar mq)\\&+(-iB^\dagger\bar\theta-B^\dagger\bar m)(i\theta B+mB)+(-iB^\dagger\theta-B^\dagger m)(i\bar\theta B+\bar mB).\end{aligned} \tag{2.16}$$

Here $\mathcal{L}^{\text{eq}}_{\text{boson}}$ is defining the moduli space that we want to consider and $\mathcal{L}^{\text{pro}}_{\text{boson}}$ is induced for the projection to gauge normal direction. Lagrangian (2.15) is rewritten as

$$\begin{aligned}\mathcal{L}^{\text{eq}}_{\text{boson}}=&H\ \text{ square terms}+\tfrac{1}{4}(s^a_{+\mu\nu}-i[B_{+\mu\rho},B_{+\nu\sigma}]^a g^{\rho\sigma})^2-\tfrac{1}{4}([B_{+\mu\nu},c]^a)^2\\&+\tfrac{1}{4}(-2D^\mu B^a_{+\mu\rho}+iB^\dagger\sigma_\rho T^aq-iq^\dagger\bar\sigma_\rho T^aB)^2+\tfrac{1}{4}(D_\rho c^a)^2+\tfrac{1}{2}|s|^2\\&+\tfrac{1}{2}|icB+m_cB|^2+\tfrac{1}{2}|-(\not{D}^\dagger B)^{\dot\alpha}+(\bar\sigma^{\mu\nu}B_{+\mu\nu}q)^{\dot\alpha}|^2+\tfrac{1}{2}|icq+m_cq|^2.\end{aligned} \tag{2.17}$$

Thus we have the following fixed point equations:

$$
\begin{gathered}
F_{+\mu\nu}+q^{\dagger}\bar{\sigma}_{\mu\nu}q-i[B_{+\mu\rho},B_{+\nu\sigma}]g^{\rho\sigma}=0,\\
-2D_{\mu}B_{+}^{\mu\nu}+iB^{\dagger}\sigma^{\nu}q-iq^{\dagger}\bar{\sigma}^{\nu}B=0,\\
s=\not{D}q=0,\\
-\not{D}^{\dagger}B+\bar{\sigma}_{\mu\nu}B_{+}^{\mu\nu}q=0,\\
D_{\nu}\theta=D_{\nu}c=D_{\nu}\bar{\theta}=0,\\
[\theta,\bar{\theta}]=[c,\theta]=[c,\bar{\theta}]=[B_{+}^{\mu\nu},\theta]=[B_{+}^{\mu\nu},\bar{\theta}]=[B_{+}^{\mu\nu},c]=0,\\
(i\theta+m)q=(i\bar{\theta}+\bar{m})q=(ic+m_{c})q=0,\\
q^{\dagger}(-i\theta-m)=q^{\dagger}(-i\bar{\theta}-\bar{m})=q^{\dagger}(-ic-m_{c})=0,\\
(i\theta+m)B=(i\bar{\theta}+\bar{m})B=(ic+m_{c})B=0,\\
B^{\dagger}(-i\theta-m)=B^{\dagger}(-i\bar{\theta}-\bar{m})=B^{\dagger}(-ic-m_{c})=0.
\end{gathered}
\tag{2.18}
$$

If hypermultiplet fields are set to zero ($q=q^{\dagger}=B=B^{\dagger}=0$), then the above equations are Vafa–Witten equations.[1,10] Thus we call the above equations extended Vafa–Witten equations.

2. Problem

In the previous paragraph, we have obtained fixed point equations of BTQCD. The equations for fermionic zero-modes are just the linearization of the fixed point equation and the condition that they are orthogonal to gauge orbits. Due to the balanced structure each fermionic zero-mode has a partner with the opposite U number. Thus there is no ghost number anomaly and the partition function is well defined, i.e., there is no need to insert observables. We want to compute the partition function of BTQCD. According to Vafa–Witten, if an appropriate vanishing theorem holds, the partition function becomes the sum of the Euler numbers of moduli space which we want to calculate. Roughly speaking, the vanishing theorem is understood as the condition that dual fields ($B_{+\mu\nu},c,B,B^{\dagger}$, etc.) are to be zero and the dimensions of their moduli space become zero, when we choose an appropriate metric.[1] However, we could not verify that the vanishing theorem holds in this model. To compare the result of this section to that of the next section, we give the only result to compute the partition function of BTQCD on the condition that the vanishing theorem holds.

C. Result

In this subsection, we give the result of computing the path integral of BTQCD. We define partition function of BTQCD as

$$
Z=\frac{1}{\mathrm{Vol}\,\mathcal{G}(2\pi)^{\Omega}}\int \mathcal{D}W\mathcal{D}\psi_{W}\mathcal{D}Q^{\dagger}\mathcal{D}\psi_{Q}^{\dagger}\mathcal{D}Q\mathcal{D}\psi_{Q}e^{-S},
\tag{2.19}
$$

where

$$
\begin{gathered}
W=A_{\mu},B_{+}^{\mu\nu},H_{B}^{\mu},H_{+}^{\mu\nu},\theta,c,\bar{\theta},\\
\psi_{W}=\psi_{\mu},\psi_{B}^{\mu\nu},\chi_{B}^{II\mu},\chi_{+}^{I\mu\nu},\xi,\eta,\\
Q=q,B,H_{q}^{I},H_{B}^{II},
\end{gathered}
\tag{2.20}
$$

$$\psi_Q = \psi_q, \psi_B, \chi_q^I, \chi_B^{II},$$

$$\Omega = \text{dim of } H\text{'s}.$$

Here we denote auxiliary fields as $H_B^\mu, H_+^{\mu\nu}, H_q^I, H_B^{II}$, and we call auxiliary fields for Y as H's of Y in the following, dim of H's is the number of the auxiliary fields.

After path integrations of the transverse part we get the partition function as the sum of two branches, according to the methods of the next section,

$$Z = Z^{\mathrm{V-W}} + Z^{B-U(1)S-W}. \tag{2.21}$$

$Z^{\mathrm{V-W}}$ is a contribution from branch 1 (gauge symmetry is unbroken), and corresponds to a Vafa–Witten partition function. $Z^{B-U(1)S-W}$ is a contribution from branch 2 [gauge symmetry is broken to U(1)], and corresponds to balanced U(1) monopole theory. The fixed point equations of the balanced U(1) monopole theory are

$$\begin{gathered} F^3_{+\mu\nu} + \tfrac{1}{2} q_1^\dagger \overline{\sigma}_{\mu\nu} q_1 = 0, \\ -2\nabla_\mu B_+^{\mu\nu 3} + i\,\tfrac{1}{2} B_1^\dagger \sigma^\nu q_1 - i\,\tfrac{1}{2} q_1^\dagger \overline{\sigma}^\nu B_1 = 0, \\ \not{D}^3 q_1 = 0, \\ -\not{D}^{\dagger 3} B_1 + \tfrac{1}{2}\,\overline{\sigma}_{\mu\nu} B_+^{\mu\nu 3} q_1 = 0, \end{gathered} \tag{2.22}$$

where $F^3_{+\mu\nu}$ is a curvature of U(1) left symmetry after breaking SU(2) and the labels of q_1 and B_1 are the ones of color. Since we do not know the vanishing theorem for dual fields $(B^3_{+\mu\nu}, B_1, B_1^\dagger)$ from (2.22), we stop to investigate this model further in this article.

III. UNBALANCED TOPOLOGICAL QCD

In this section, we compute a correlation function of an appropriate BRS exact operator (the BRS operator is defined in Appendix A) in the unbalanced topological QCD. As a result, we can describe the Euler number of instanton moduli space with Seiberg–Witten invariants. We have a similar but not the same expression to Dijkgraaf *et al.*,[10] because we treat a different theory from theirs. We discuss this point at the end of this section.

A. Unbalanced topological QCD

Here we construct the unbalanced topological QCD, which is a twisted $N=4$ Yang–Mills theory coupled with only one massive hypermultiplet in the fundamental representation (we denote it as UBTQCD in the following). Alternatively, one obtains a UBTQCD, when one sets one massive hypermultiplet $(B, \psi_B, \chi_B^{II}, H_B^{II})$ of BTQCD in the previous section to zero (we call this process breaking balanced structure).

1. Algebra of UBTQCD

The algebra of UBTQCD is given as a part of the BTQCD algebra. Contrary to the previous section, we only consider the global supercharge Q_+. When it acts on adjoint (fundamental) fields, it satisfies the following commutation relation:

$$Q_+^2 = \delta_\theta^g(-\delta_\theta^g). \tag{3.1}$$

We adopt the same δ_+ transformations as in the previous section and in Appendix A (A7)–(A14).

2. Action of UBTQCD

We define the action of UBTQCD as

$$h^2 S = \int d^4x \sqrt{g}\mathcal{L}, \tag{3.2}$$

where

$$\mathcal{L} = \delta_+ \Psi. \tag{3.3}$$

We explicitly give Ψ as

$$\begin{aligned}
\Psi = & -\chi_+^{I\mu\nu a}\{H_{+\mu\nu}^{Ia} - (s_{+\mu\nu}^a - i[B_{+\mu\rho}, B_{+\nu\sigma}]^a g^{\rho\sigma} - i[B_{+\mu\nu}, c]^a)\} \\
& - \chi^{II\rho a}\{H_{B\rho}^{IIa} - (-2D^\mu B_{+\mu\rho}^a - D_\rho c^a)\} - \chi_q^{I\dagger\alpha}\{H_{q\alpha}^I - s_\alpha\} - \{H_q^{I\dagger\alpha} - s^{\dagger\alpha}\}\chi_{q\alpha}^I \\
& + \{i[\theta, \overline{\theta}]^a \eta^a - i\xi^a [c, \overline{\theta}]^a\} + i[B_+^{\mu\nu}, \overline{\theta}]^a \psi_{B\mu\nu}^a + D_\mu \overline{\theta}^a \psi^{\mu a} \\
& - (-iq_{\dot\alpha}^\dagger \overline{\theta} - \overline{m} q_{\dot\alpha}^\dagger)\psi_q^{\dot\alpha} - \psi_{q\dot\alpha}^\dagger (i\overline{\theta} q^{\dot\alpha} + \overline{m} q^{\dot\alpha}),
\end{aligned} \tag{3.4}$$

where

$$s_+^{\mu\nu a} = F_+^{\mu\nu a} + q^\dagger \overline{\sigma}^{\mu\nu} T^a q, \tag{3.5}$$

$$s^\alpha = (\not{D} q)^\alpha. \tag{3.6}$$

Finally, the full Lagrangian is given by

$$\mathcal{L}^{\text{full}} = \delta_+ \Psi \tag{3.7}$$

$$\begin{aligned}
= & -H_+^{I\mu\nu a}\{H_{+\mu\nu}^{Ia} - (s_{+\mu\nu}^a - i[B_{+\mu\rho}, B_{+\nu\sigma}]^a g^{\rho\sigma} - i[B_{+\mu\nu}, c]^a)\} \\
& - \chi_+^{I\mu\nu a}\{-i[\chi_{+\mu\nu}^I, \theta]^a + 2D_\mu \psi_\nu^a + \psi_q^\dagger \overline{\sigma}_{\mu\nu} T^a q + q^\dagger \overline{\sigma}_{\mu\nu} T^a \psi_q - 2i[B_{+\mu\rho}, \psi_{B\nu\sigma}]^a g^{\rho\sigma} \\
& - i[\psi_{B\mu\nu}, c]^a - i[B_{+\mu\nu}, \xi]^a\} - H_B^{II\rho a}\{H_{B\rho}^{IIa} - (-2D^\mu B_{+\mu\rho}^a - D_\rho c^a)\} \\
& - \chi_B^{II\rho a}\{-i[\chi_{B\rho}^{II}, \theta]^a - 2D^\mu \psi_{B\mu\rho}^a - 2i[\psi^\mu, B_{+\mu\rho}]^a - D_\rho \xi^a - i[\psi_\rho, c]^a\} \\
& - H_q^{I\dagger\alpha}\{H_{q\alpha}^I - s_\alpha\} - \chi_q^{I\dagger}\{\not{D}\psi_q + \sigma_\rho i\psi^\rho q\} + (\text{h.c. previous two terms}) \\
& - \{[\theta, \overline{\theta}]^a [\overline{\theta}, \theta]^a - [c, \theta]^a [c, \overline{\theta}]^a + [B_+^{\mu\nu}, \overline{\theta}]^a [B_{+\mu\nu}, \theta]^a\} + D_\mu \overline{\theta}^\alpha D^\mu \theta^\alpha i[\theta, \eta]^a \eta^a \\
& + i\xi^a [\xi, \overline{\theta}]^a + i\xi^a [c, \eta]^a + i[\psi_B^{\mu\nu}, \overline{\theta}]^a \psi_{B\mu\nu}^a + i[B_+^{\mu\nu}, \eta]^a \psi_{B\mu\nu}^a + D_\mu \eta^a \psi^{\mu a} \\
& + i[\psi_\mu, \overline{\theta}]^a \psi^{\mu a} + (-iq^\dagger \overline{\theta} - q^\dagger \overline{m})(i\theta q + mq) + (-iq^\dagger \theta - q^\dagger m)(i\overline{\theta} q + \overline{m} q) \\
& + 2\psi_q^\dagger (i\overline{\theta} + \overline{m})\psi_q - 2\chi_q^{I\dagger}(i\theta + m)\chi_q^I - (-iq^\dagger \eta - q^\dagger \eta_m)\psi_q + \psi_q^\dagger (i\eta q + \eta_m q).
\end{aligned} \tag{3.8}$$

Notice that Lagrangian (3.8) is given by Lagrangian (A18) of the previous section if $(B, \psi_B, H_B^{II}, \chi_B^{II})$ is set to zero.

B. Fixed point

In this subsection, we study the nature of the action given in Sec. III A. Here in particular we investigate the fixed points and some observables to insert.

1. Fixed point

To check the nature of the Lagrangian, we decompose the bosonic part of Lagrangian (3.8):

$$\mathcal{L}^{\text{full}}_{\text{boson}}=\mathcal{L}^{\text{eq}}_{\text{boson}}+\mathcal{L}^{\text{pro}}_{\text{boson}}, \tag{3.9}$$

where

$$\begin{aligned}\mathcal{L}^{\text{eq}}_{\text{boson}}=&-H_{+}^{I\mu\nu a}\{H^{Ia}_{+\mu\nu}-(s^{a}_{+\mu\nu}-i[B_{+\mu\rho},B_{+\nu\sigma}]^{a}g^{\rho\sigma}-i[B_{+\mu\nu},c]^{a})\}\\&-H_{B}^{II\rho a}\{H^{IIa}_{B\rho}-(-2D^{\mu}B^{a}_{+\mu\rho}-D_{\rho}c^{a})\}-H_{q}^{I\dagger\alpha}\{H^{I}_{q\alpha}-s_{\alpha}\}+(\text{h.c.})\end{aligned} \tag{3.10}$$

and

$$\begin{aligned}\mathcal{L}^{\text{pro}}_{\text{boson}}=&-\{[\theta,\overline{\theta}]^{a}[\overline{\theta},\theta]^{a}-[c,\theta]^{a}+[B_{+}^{\mu\nu},\overline{\theta}]^{a}[B_{+\mu\nu},\theta]^{a}\}+D_{\mu}\overline{\theta}^{a}D^{\mu}\theta^{a}+(-iq^{\dagger}\overline{\theta}-q^{\dagger}\overline{m})\\&+(i\theta q+mq)+(-iq^{\dagger}\theta-q^{\dagger}m)(i\overline{\theta}q+\overline{m}q).\end{aligned} \tag{3.11}$$

Here $\mathcal{L}^{\text{eq}}_{\text{boson}}$ is defining the moduli space that we want to consider and $\mathcal{L}^{\text{pro}}_{\text{boson}}$ is induced for the projection to gauge normal direction. Lagrangian (3.10) is transformed into

$$\begin{aligned}\mathcal{L}^{\text{eq}}_{\text{boson}}=&-\{H^{Ia}_{+\mu\nu}-\tfrac{1}{2}(s^{a}_{+\mu\nu}-i[B_{+\mu\rho},B_{+\nu\sigma}]^{a}g^{\rho\sigma}-i[B_{+\mu\nu},c]^{a})\}^{2}\\&-\{H^{IIa}_{B\rho}-\tfrac{1}{2}(-2D^{\mu}B^{a}_{+\mu\rho}-D_{\rho}c^{a})\}^{2}-2|H^{I}_{q\alpha}-\tfrac{1}{2}s_{\alpha}|^{2}\\&+\tfrac{1}{4}(s^{a}_{+\mu\nu}-i[B_{+\mu\rho},B_{+\nu\sigma}]^{a}g^{\rho\sigma}-i[B_{+\mu\nu},c]^{a})^{2}+\tfrac{1}{4}(-2D^{\mu}B^{a}_{+\mu\rho}-D_{\rho}c^{a})^{2}+\tfrac{1}{2}|s_{\alpha}|^{2}.\end{aligned} \tag{3.12}$$

Thus we have the following fixed point equations:

$$\begin{gathered}F_{+\mu\nu}+q^{\dagger}\overline{\sigma}_{\mu\nu}q-i[B_{+\mu\rho},B_{+\nu\sigma}]g^{\rho\sigma}-i[B_{+\mu\nu},c]=0,\\-2D_{\mu}B_{+}^{\mu\nu}-D^{\nu}c=0,\\s=\not{D}q=0,\\D_{\nu}\theta=D_{\nu}\overline{\theta}=0,\\[\theta,\overline{\theta}]=[c,\theta]=[c,\overline{\theta}]=[B_{+}^{\mu\nu},\theta]=[B_{+}^{\mu\nu},\overline{\theta}]=0,\\(i\theta+m)q=(i\overline{\theta}+\overline{m})q=0,\\q^{\dagger}(-i\theta-m)=q^{\dagger}(-i\overline{\theta}-\overline{m})=0.\end{gathered} \tag{3.13}$$

2. Problem

In the previous paragraph, we have obtained the fixed point equations of UBTQCD. In the same way as in the previous section, the equations for fermionic zero-modes are just the linearization of the fixed point equations and the conditions that they are orthogonal to gauge orbits. Compared with the previous section, UBTQCD does not have balanced structure. In particular, the hypermultiplet does not have balanced structure, while adjoint representation fields still have balanced structure. The partition function of unbalanced theory becomes zero due to its ghost number anomaly when the moduli space dimension of the matter field is nonzero. Thus to get a well-defined path integral, we have to insert some observables. One can think of an observable

$$I=\int d^4x\,(q^\dagger(i\theta+m)q+\psi_q^\dagger\psi_q). \tag{3.14}$$

Note that this observable itself is BRS exact, i.e.,

$$I=\delta_+\frac{1}{2}\int d^4x\,(-\psi_q^\dagger q+q^\dagger\psi_q). \tag{3.15}$$

Thus the expectation value of I is zero according to the Ward–Takahashi identity, and the expectation value of e^I becomes zero when this theory has a ghost number anomaly. However, as we will see, we obtain nontrivial results.

C. Branch

In this subsection, we will show that the fixed point equations are decomposed to two branches. We cite H-P-P.[6]

Equations

$$D_\nu\theta=D_\nu\overline{\theta}=0,\quad [\theta,\overline{\theta}]=0 \tag{3.16}$$

imply that θ, $\overline{\theta}$ can be diagonalized in the fixed points. If connections A_μ are irreducible, θ, $\overline{\theta}$ should be zero (the gauge symmetry is unbroken). If connections A_μ are reducible, θ, $\overline{\theta}$ can be nonzero [the gauge symmetry is broken down to U(1)]. When these solutions are applied to

$$\begin{gathered}(i\theta+m)q=(i\overline{\theta}+\overline{m})q=0,\\ q^\dagger(-i\theta-m)=q^\dagger(-i\overline{\theta})-\overline{m})=0,\end{gathered} \tag{3.17}$$

we have two branches:

branch 1 $\theta=\overline{\theta}=0$ and $q=q^\dagger=0$

or

branch 2 $\theta=\theta^3T^3\neq 0$, $\overline{\theta}=\overline{\theta}^3T^3\neq 0$ and $q\neq 0$, $q^\dagger\neq 0$.

Note that in branch 2 we choose unbroken U(1) as T^3 direction without a loss of generality.

Branch 1: $\theta=\overline{\theta}=0$ and $q=q^\dagger=0$, i.e., the gauge symmetry is unbroken. The remaining fixed point equations are

$$\begin{gathered}F_+^{\mu\nu}-i[B_{+\mu\rho},B_{+\nu\sigma}]g^{\rho\sigma}=0,\quad -2D_\mu B_+^{\mu\nu}=0,\quad D_\mu c=0,\\ [B_+^{\mu\nu},c]=0.\end{gathered} \tag{3.18}$$

Here one may apply the same condition as Vafa–Witten[1] to induce the vanishing theorem, and obtain the moduli space of

$$F_+^{\mu\nu}=0. \tag{3.19}$$

Branch 2: $\theta=\theta^3T^3\neq 0$, $\overline{\theta}=\overline{\theta}^3T^3\neq 0$ and $q\neq 0$, $q^\dagger\neq 0$, i.e., the gauge symmetry is broken to U(1). Thus the bundle E splits into line bundles, $E=L\oplus L^{-1}$ with $L\cdot L=-k$. Then Eqs. (3.17) are

$$(i\theta^3T^3+m)q=\begin{pmatrix}\frac{i}{2}\theta^3+m & 0\\ 0 & -\frac{i}{2}\theta^3+m\end{pmatrix}\begin{pmatrix}q_1\\ q_2\end{pmatrix}=0,$$

$$
\begin{aligned}
(i\overline{\theta^3}T^3+\overline{m})q&=\begin{pmatrix}\frac{i}{2}\overline{\theta^3}+\overline{m} & 0\\ 0 & -\frac{i}{2}\overline{\theta^3}+\overline{m}\end{pmatrix}\begin{pmatrix}q_1\\ q_2\end{pmatrix}=0,\\
q^\dagger(-i\theta^3T^3-m)&=(q_1^\dagger \quad q_2^\dagger)\begin{pmatrix}-\frac{i}{2}\theta^3-m & 0\\ 0 & \frac{i}{2}\theta^3+m\end{pmatrix}=0,\\
q^\dagger(-i\overline{\theta^3}T^3-\overline{m})&=(q_1^\dagger \quad q_2^\dagger)\begin{pmatrix}-\frac{i}{2}\overline{\theta^3}-\overline{m} & 0\\ 0 & \frac{i}{2}\overline{\theta^3}+\overline{m}\end{pmatrix}=0.
\end{aligned}
\tag{3.20}
$$

Thus the only nontrivial solutions for q are either

$$
q=\begin{pmatrix}q_1\\ 0\end{pmatrix},\quad q^\dagger=(q_1^\dagger \quad 0),\quad \text{and}\quad \frac{i}{2}\theta^3+m=\frac{i}{2}\overline{\theta^3}+\overline{m}=0 \tag{3.21}
$$

or

$$
q=\begin{pmatrix}0\\ q_2\end{pmatrix},\quad q^\dagger=(0 \quad q_2^\dagger),\quad \text{and}\quad -\frac{i}{2}\theta^3+m=-\frac{i}{2}\overline{\theta^3}+\overline{m}=0. \tag{3.22}
$$

Throughout this article we pick the nontrivial solutions for q as $q_1\neq 0$ and $\theta^3=2im$. In this branch the equations

$$
[c,\theta]=[c,\overline{\theta}]=[B_+^{\mu\nu},\theta]=[B_+^{\mu\nu},\overline{\theta}]=0 \tag{3.23}
$$

imply that nonzero solutions of $B_+^{\mu\nu}$, c have the same direction T^3 as θ. Finally, we obtain the remaining equations

$$
\begin{aligned}
&F^3_{+\mu\nu}+\tfrac{1}{2}q_1^\dagger\overline{\sigma}_{\mu\nu}q_1=0,\\
&-2\nabla^\mu B^3_{+\mu\nu}=\partial^\mu c^3=0,\\
&\sigma^\mu\mathcal{D}_\mu q_1=0,
\end{aligned}
\tag{3.24}
$$

where ∇^μ is the covariant derivative with respect to the Levi-Civita connection of background metric $g^{\mu\nu}$. Here we reinterpret U(1)⊗U(1) [gauge U(1) and spin^{c}U(1)] as a new U(1) [spin$^{c'}$U(1)], or alternately we redefine $W_c^+\otimes\zeta=W_{c'}^+$ as a different spin^c structure $c'=c+2\zeta$, i.e., $\det(W_c^+\otimes\zeta)=L_c\otimes\zeta^2$. As a result, (3.24) can be interpreted as a perturbed Seiberg–Witten monopole equation for the spin^c structure c' as well as H-P-P[6] and B_+, c equations for the T^3 direction.

D. Gaussian integral

In this subsection we compute the path integral of UBTQCD. According to Appendix B, we could evaluate the exact path integral of this theory. In this subsection, we only denote the diagonal part of the big matrix (see Appendix B) to read the right contribution easily. As we have

already mentioned in Sec. III B, we have to insert some observables of fundamental fields to get a well-defined path integral. Thus we define the expectation value of e^I as

$$\langle e^I \rangle_{m,c,k} = \frac{1}{\mathrm{Vol}\,\mathcal{G}(2\pi)^\Omega} \int \mathcal{D}W \mathcal{D}\psi_W \mathcal{D}Q^\dagger \mathcal{D}\psi_Q^\dagger \mathcal{D}Q \mathcal{D}\psi_Q e^{-S+I}, \tag{3.25}$$

where

$$\begin{aligned} W &= A_\mu, B_+^{\mu\nu}, H_B^\mu, H_+^{\mu\nu}, \theta, c, \overline{\theta}, \\ \psi_W &= \psi_\mu, \psi_B^{\mu\nu}, \chi_B^{II\mu}, \chi_+^{I\mu\nu}, \xi, \eta, \\ Q &= q, H_q^I, \\ \psi_Q &= \psi_q, \chi_q^I, \\ I &= \int d^4x (q^\dagger (i\theta + m) q + \psi_q^\dagger \psi_q), \\ \Omega &= \text{dim of } H's. \end{aligned} \tag{3.26}$$

In a general computation of the path integral of topological field theory (TFT), it is sufficient to keep only quadratic terms for the transverse degrees and compute the one-loop approximations which give a result exactly.[9] Now let us see what are transverse degrees of freedom in each branch. Picking a Riemannian metric g, we rescale $g \to tg$ and take the $t \to \infty$ limit. In branch 1, the gauge symmetry is unbroken and the matter fields decouple as the transverse degrees of freedom. In branch 2, the gauge symmetry is broken down to U(1) and the hypermultiplet reduces to one of its color. The suppressed color degrees of freedom for the hypermultiplet and the components of the $N=4$ vector multiplet which do not belong to the Cartan subalgebra part become the transverse degrees of freedom.

On the other hand, the path integrals for the nontransverse degrees should be computed exactly. These path integrals correspond to the path integral of Vafa–Witten theory in branch 1 and the path integral of U(1) monopole theory and U(1)B_+, c theory in branch 2.

We will use the notation $\langle O \rangle_{m,c,k}$ for the VEV evaluated in the massive UBTQCD for a given spin^c and instanton number k.

1. Result of branch 1

In this branch, the degrees of freedom for the hypermultiplet become the transverse degrees of freedom. One can decompose the Lagrangian (3.8) into two parts:

$$\mathcal{L} \approx \mathcal{L}^{\mathrm{V-W}}(1) + \mathcal{L}^t(1), \tag{3.27}$$

where the Vafa–Witten part is

$$\begin{aligned} \mathcal{L}^{\mathrm{V-W}}(1) = & -H_+^{I\mu\nu a}\{H_{+\mu\nu}^{Ia} - (F_{+\mu\nu}^a - i[B_{+\mu\rho}, B_{+\nu\sigma}]^a g^{\rho\sigma} - i[B_{+\mu\nu}, c]^a)\} \\ & - \chi_+^{I\mu\nu a}\{-i[\chi_{+\mu\nu}^I, \theta]^a + 2D_\mu \psi_\nu^\sigma - 2i[B_{+\mu\rho}, \psi_{B\nu\sigma}]^a g^{\rho\sigma} - i[\psi_{B\mu\nu}, c]^a \\ & - i[B_{+\mu\nu}, \xi]^a\} - H_B^{II\rho a}\{H_{B\rho}^{IIa} - (-2D^\mu B_{+\mu\rho}^a - D_\rho c^a)\} \\ & - \chi_B^{II\rho a}\{-i[\chi_{B\rho}^{II}, \theta]^a - 2D^\mu \psi_{B\mu\rho}^a - 2i[\psi^\mu, B_{+\mu\rho}]^a - D_\rho \xi^a - i[\psi_\rho, c]^a\} \\ & - \{[\theta, \overline{\theta}]^a [\overline{\theta}, \theta]^a - [c, \theta]^a [c, \overline{\theta}]^a + [B_+^{\mu\nu}, \overline{\theta}]^a [B_{+\mu\nu}, \theta]^a\} \\ & + D_\mu \overline{\theta}^a D^\mu \theta^a + i[\theta, \eta]^a \eta^a + i\xi^a [\xi, \overline{\theta}]^a + i\xi^a [c, \eta]^a \end{aligned}$$

$$+i[\psi_B^{\mu\nu},\overline{\theta}]^a\psi^a_{B\mu\nu}+i[B_+^{\mu\nu},\eta]^a\psi^a_{V\mu\nu}+D_\mu\eta^a\psi^{\mu a}+i[\psi_\mu,\overline{\theta}]^a\psi^{\mu a} \tag{3.28}$$

and a quadratic Lagrangian due to the transverse degrees is

$$\begin{aligned}\mathcal{L}^t(1)&=-H_q^{I\dagger\alpha}\{H^I_{q\alpha}-s_\alpha\}-\chi_q^{I\dagger}\not{D}\psi_q+(\text{h.c. previous two terms})-2q^\dagger\overline{m}mq+2\psi_1^\dagger\overline{m}\psi_q-2\chi_q^{I\dagger}m\chi_q^I\\&=-2|H_q^I+\cdots|^2-2m|\chi_q^I+\cdots|^2-\frac{1}{2}q^\dagger(\not{D}^\dagger\not{D}+4m\overline{m})q+\frac{1}{2m}\psi_q^\dagger(\not{D}^\dagger\not{D}+4m\overline{m})\psi_q.\end{aligned} \tag{3.29}$$

One can rewrite the path integral (3.25) in this branch as

$$\langle e^I\rangle_{m,c,k}(1)=\underbrace{\frac{1}{Vol\mathcal{G}(2\pi)^{\Omega'}}\int\mathcal{D}W\mathcal{D}\psi_W e^{-S^{V-W}(1)}}_{\equiv Z^{V-W}_{m,c,k}(1)}\cdot\underbrace{\frac{1}{(2\pi)^{\Omega''}}\int\mathcal{D}Q^\dagger\mathcal{D}\psi_Q^\dagger\mathcal{D}Q\mathcal{D}\psi_Q e^{-S^t(1)+I(1)}}_{\equiv Z^t_{m,c,k}(1)}, \tag{3.30}$$

where

$$\begin{aligned}h^2S^{\mathrm{V-W}}(1)&=\int d^4x\,\sqrt{g}\mathcal{L}^{\mathrm{V-M}}(1),\\h^2S^t(1)&=\int d^4x\,\sqrt{g}\mathcal{L}^t(1),\\I(1)&=\int d^4x\,\sqrt{g}(q^\dagger mq+\psi_q^\dagger\psi_q),\\\Omega'&=\dim\ \text{of adjoint}\ H's,\\\Omega''&=\dim\ \text{of fundamental}\ H's.\end{aligned} \tag{3.31}$$

For the Vafa–Witten part $Z^{\mathrm{V-W}}_{m,c,k}(1)$, we completely follow Vafa–Witten.[1] Thus we have

$$Z^{\mathrm{V-M}}_{m,c,k}(1)\doteq\chi_k, \tag{3.32}$$

where χ_k stands for the Euler number of instanton moduli space with instanton number k and $\doteq$ means equality under keeping the vanishing theorem as shown in Vafa–Witten. Note that the existence of the vanishing theorem in the previous section is unknown, but, in this case, we have some examples to which we apply the vanishing theorem.[1] When the vanishing theorem is not applicable, we denote this part as $Z^{\mathrm{V-W}}_{m,c,k}(1)$ itself. We discuss the problem of compactification of moduli space later.

For the transverse part $Z^t_{m,c,k}(1)$, we first perform H_q^I,χ_q^I integral and obtain

$$\frac{1}{(2\pi)^{\Omega''}}\frac{[\det(-2m)]_{(\chi_q^{I\dagger},\chi_q^I)}}{[\det(-1/\pi)]_{(H_q^{I\dagger},H_q^I)}}=\left[\det\left(\frac{m}{2\pi}\right)\right]_{\Gamma^-}=\left(\frac{m}{2\pi}\right)^{\dim(\Gamma^-_{\lambda>0}\oplus\mathrm{Ker}(\not{D}^\dagger))}. \tag{3.33}$$

Second, we perform q,ψ_q integral for zero and nonzero modes, respectively, and obtain

$$\frac{[\det(-\not{D}^2/2m)]_{(\psi_q^\dagger,\psi_q)\text{non }0}}{[\det(-\not{D}^2/4\pi)]_{(q^\dagger,q)\text{non }0}}\cdot\frac{[\det(-1)]_{(\psi_q^\dagger,\psi_q)0}}{[\det(-m/2\pi)]_{(q^\dagger,q)0}}=\left(\frac{2\pi}{m}\right)^{\dim(\Gamma^+_{\lambda>0}\oplus\mathrm{Ker}\not{D})}. \tag{3.34}$$

Note that this expression is not exact, but is sufficient to get the right contribution (see Appendix B).

Collecting (3.33) and (3.34), one can obtain

$$Z^t_{m,c,k}(1)=\left(\frac{m}{2\pi}\right)^{\dim((\Gamma^-_{\lambda>0}\oplus\mathrm{Ker}\,\not{D}^\dagger))}\left(\frac{2\pi}{m}\right)^{\dim(\Gamma^+_{\lambda>0}\oplus\mathrm{Ker}(\not{D}))}=\left(\frac{2\pi}{m}\right)^{\mathrm{index}\,(\not{D}^E_c)}. \tag{3.35}$$

Finally, for $\langle e^{\hat{v}}\rangle_{m,c,k}(1)$, one can obtain

$$\langle e^{\hat{v}}\rangle_{m,c,k}(1)=Z^{\mathrm{V-W}}_{m,c,k}(1)\cdot Z^t_{m,c,k}(1)=Z^{\mathrm{V-W}}_{m,c,k}(1)\cdot\left(\frac{2\pi}{m}\right)^{\mathrm{index}\,(\not{D}^E_c)}\doteq\chi_k\cdot\left(\frac{2\pi}{m}\right)^{\mathrm{index}\,(\not{D}^E_c)}, \tag{3.36}$$

where $\doteq$ stands for results in the vanishing theorem case.

2. Result of branch 2

In this branch, the gauge symmetry is broken down to U(1). The components of any field which do not belong to the Cartan subalgebra part become the transverse variables, that is, the $\pm$ components of adjoint fields, i.e., $T_\pm=T_1\pm iT_2$, and the components of the hypermultiplet with the suppressed color index become the transverse variable. One can decompose the Lagrangian (3.8) into two parts

$$\mathcal{L}\approx\mathcal{L}^{U(1)}(2)+\mathcal{L}^t(2), \tag{3.37}$$

where $\mathcal{L}^{U(1)}(2)$ is the Lagrangian of U(1) UBTQCD, and $\mathcal{L}^t(2)$ is the quadratic Lagrangian due to the transverse degrees.

The U(1) part $\mathcal{L}^{U(1)}(2)$ can be further decomposed into two parts,

$$\mathcal{L}^{U(1)}(2)=\mathcal{L}^{U(1)}_{\mathrm{mono}}(2)+\mathcal{L}^{U(1)}_{B_+,c}(2), \tag{3.38}$$

$$\begin{aligned}\mathcal{L}^{U(1)}_{\mathrm{mono}}(2)=&-H^{I3\mu\nu}_+\{H^{I3}_{+\mu\nu}-(F^3_{+\mu\nu}+\tfrac{1}{2}q_1^\dagger\overline{\sigma}_{\mu\nu}q_1)\}-\chi^{I3\mu\nu}_+\{2\nabla_\mu\psi^3_\nu+\tfrac{1}{2}\psi^\dagger_{q_1}\overline{\sigma}_{\mu\nu}q_1+\tfrac{1}{2}q_1^\dagger\overline{\sigma}_{\mu\nu}\psi_{q_1}\}\\&-H^{I\dagger}_q\{H^I_{q_1}-\not{D}q_1\}-\chi^{I\dagger}_{q_1}\not{D}\psi_{q_1}+(\text{h.c. previous two terms})+\partial_\mu\overline{\theta^3}\partial^\mu\theta^3+\partial_\mu\eta^3\psi^{3\mu}\\&+2(-i\tfrac{1}{2}q_1^\dagger\overline{\theta^3}-q_1^\dagger\overline{m})(i\tfrac{1}{2}\theta^3_{q_1}+mq_1)+2\psi^\dagger_{q_1}(i\tfrac{1}{2}\overline{\theta^3}+\overline{m})\psi_{q_1}-2\chi^{I\dagger}_{q_1}(i\tfrac{1}{2}\theta^3+m)\chi^I_{q_1}\\&-(-i\tfrac{1}{2}q_1^\dagger\eta^3-q_1^\dagger\eta_m)\psi_{q_1}+\psi^\dagger_{q_1}(i\tfrac{1}{2}\eta^3q_1+\eta_mq_1),\end{aligned} \tag{3.39}$$

and

$$\mathcal{L}^{U(1)}_{B_+,c}(2)=-H^{II3\rho}_B\{H^{II3}_{B\rho}-(-2\nabla^\mu B^3_{+\mu\rho}-\partial_\rho c^3)\}-\chi^{II3\rho}_B\{-2\nabla^\mu\psi^3_{B\mu\rho}-\partial_\rho\xi^3\}, \tag{3.40}$$

where the first part $\mathcal{L}^{U(1)}_{\mathrm{mono}}(2)$ is $U(1)$ monopole theory, and the second part $\mathcal{L}^{U(1)}_{B_+,c}(2)$ is $U(1)B_+,c$ theory.

The quadratic Lagrangian due to the transverse degrees $\mathcal{L}^t(2)$ is

$$\begin{aligned}\mathcal{L}^t(2)=&-4|H^{I+}_{+\mu\nu}+\cdots|^2-8m|\chi^{I+}_{+\mu\nu}+\cdots|^2+16m^2|\overline{\theta}^+\cdots|^2-8m|\eta^+\cdots|^2\\&-A^+_\mu\Big\{(D^{3+}{*}D^{3+})^{\mu\nu}+(D^3D^{3*})^{\mu\nu}-\widetilde{B}^{3\mu\rho}_+\widetilde{B}^{3\nu}_{+\rho}-\frac{1}{2}\widetilde{q}_1^\dagger\overline{\sigma}^\mu\sigma^\nu\widetilde{q}_1+(-(\widetilde{c}^3)^2\\&+16m\overline{m})g^{\mu\nu}\Big\}A^-_\nu+\frac{1}{2m}\psi^+_\mu\Big\{(D^{3+}{*}D^{3+})^{\mu\nu}+(D^3D^{3*})^{\mu\nu}-\widetilde{B}^{3\mu\rho}_+\widetilde{B}^{3\nu}_{+\rho}\\&-\frac{1}{2}\widetilde{q}_1^\dagger\overline{\sigma}^\mu\sigma^\nu\widetilde{q}_1+(-(\widetilde{c}^3)^2+16m\overline{m})g^{\mu\nu}\Big\}\psi^-_\nu-4|H^{II+}_B+\cdots|^2-8m|\chi^{II+}_B+\cdots|^2\end{aligned}$$

$$
\begin{aligned}
&-B_{+\mu\nu}\{(D^{3+}D^{3+}*)^{\mu\rho}g^{\nu\sigma}-4\tilde{B}_{+}^{3\mu\nu}\tilde{B}_{+}^{3\rho\sigma}+(-(\tilde{c}^{3})^{2}+16m\bar{m})g^{\mu\rho}g^{\nu\sigma}\}B_{+\rho\sigma}\\
&+\frac{1}{2m}\psi_{B\mu\nu}\{(D^{3+}D^{3+}*)^{\mu\rho}g^{\nu\sigma}-4\tilde{B}_{+}^{3\mu\nu}\tilde{B}_{+}^{3\rho\sigma}+(-(\tilde{c}^{3})^{2}+16m\bar{m})g^{\mu\rho}g^{\nu\sigma}\}\psi_{B\rho\sigma}\\
&-c^{+}\{D^{3}*D^{3}-\tilde{B}_{+}^{3\mu\nu}\tilde{B}_{+\mu\nu}^{3}-(\tilde{c}^{3})^{2}-16m\bar{m}\}c^{-}+\frac{1}{2m}\xi^{+}\{D^{3}*D^{3}-\tilde{B}_{+}^{3\mu\nu}\tilde{B}_{+\mu\nu}^{3}\\
&-(\tilde{c}^{3})^{2}-16m\bar{m}\}\xi^{-}-2|H_{q_2}^{I}+\cdots|^{2}-4m|\chi_{q_2}^{I}+\cdots|^{2}-\tfrac{1}{2}q_{2}^{\dagger}\{\not{D}^{3\dagger}\not{D}^{3}-2\bar{\sigma}_{\mu\nu}\tilde{q}_{1}\tilde{q}_{1}^{\dagger}\bar{\sigma}^{\mu\nu}\\
&+16m\bar{m}\}q_{2}+\frac{1}{4m}\psi_{q_2}^{\dagger}\{\not{D}^{3\dagger}\not{D}^{3}+2\bar{\sigma}_{\mu\nu}\tilde{q}_{1}\tilde{q}_{1}^{\dagger}\bar{\sigma}^{\mu\nu}+16m\bar{m}\}\psi_{q_2}+(\text{cross terms}). \qquad (3.41)
\end{aligned}
$$

One can rewrite the path integral (3.25) in this branch as

$$
\begin{aligned}
\langle e^{I}\rangle_{m,c,k}(2)=&\underbrace{\frac{1}{Vol\mathcal{G}^{3}(2\pi)^{\Omega'}}\int \mathcal{D}W^{3}\mathcal{D}\psi_{W}^{3}\mathcal{D}Q_{1}^{\dagger}\mathcal{D}\psi_{Q1}^{\dagger}\mathcal{D}Q_{1}\mathcal{D}\psi_{Q1}e^{-S^{U(1)}(2)}}_{\equiv Z_{m,c,k}^{U(1)}(2)}\\
&\cdot\underbrace{\frac{1}{Vol\mathcal{G}^{\pm}(2\pi)^{\Omega''}}\int \mathcal{D}W^{\pm}\mathcal{D}\psi_{W}^{\pm}\mathcal{D}Q_{2}^{\dagger}\mathcal{D}\psi_{Q2}^{\dagger}\mathcal{D}Q_{2}\mathcal{D}\psi_{Q2}e^{-S^{t}(2)+J(2)}}_{\equiv Z_{m,c,k}^{t}(2)}
\end{aligned}
\qquad (3.42)
$$

where

$$
\begin{aligned}
h^{2}S^{\mathrm{U}(1)}(2)&=\int d^{4}x\,\sqrt{g}\mathcal{L}^{\mathrm{U}(1)}(2),\\
h^{2}S^{t}(2)&=\int d^{4}x\,\sqrt{g}\mathcal{L}^{t}(2),\\
I(2)&=\int d^{4}x\,\sqrt{g}(q_{2}^{\dagger}2mq_{2}+\psi_{q_2}^{\dagger}\psi_{q_2}),
\end{aligned}
\qquad (3.43)
$$

$\Omega'=$ dim of H's of nontransverse degrees,

$\Omega''=$ dim of H's of transverse degrees.

For the U(1) monopole part, we have

$$
Z_{\mathrm{mono}}^{\mathrm{U}(1)}=\frac{1}{\mathrm{Vol}\,\mathcal{G}^{3}(2\pi)^{\Omega'''}}\int \mathcal{D}W_{A}^{3}\mathcal{D}\psi_{W_A^3}\mathcal{D}Q_{1}^{\dagger}\mathcal{D}\psi_{Q1}^{\dagger}\mathcal{D}Q_{1}\mathcal{D}\psi_{Q1}e^{-S_{\mathrm{mono}}^{\mathrm{U}(1)}(2)}, \qquad (3.44)
$$

where

$$
\begin{aligned}
&W_{A}^{3}=A^{\mu 3},H_{+\mu\nu}^{3},\theta^{3},\bar{\theta^{3}},q_{1},H_{q1}^{I},\\
&\psi_{W_A}^{3}=\psi_{A}^{\mu 3},\chi_{+\mu\nu}^{3},\eta^{3},\psi_{q1},\chi_{q1}^{I},\\
&h^{2}S_{\mathrm{mono}}^{\mathrm{U}(1)}(2)=\int d^{4}x\,\sqrt{g}\mathcal{L}_{\mathrm{mono}}^{\mathrm{U}(1)}(2)
\end{aligned}
\qquad (3.45)
$$

$$\Omega''' = \text{dim of } H\text{'s of U(1) S}-\text{W part.}$$

For this part we follow H-P-P.[6] In a simple type manifold we only need to consider the zero-dimensional moduli space of the Seiberg–Witten monopoles [we call them $\mathcal{M}(x)$]. Here we denote spin^c structure c' that we have already mentioned in Sec. III C by $2x$ if c' satisfies the condition of the zero-dimensional moduli space [$\dim \mathcal{M}(c') = (c' \cdot c')/4 - (2\chi + 3\sigma)/4 = 0$], and we call this spin^c structure x the Seiberg–Witten basic class. The moduli space $\mathcal{M}(x)$ consists of a finite set of points. First, for the contributions of the zero-dimensional moduli space $\mathcal{M}(x)$, we have

$$\mathcal{N} n_x, \tag{3.46}$$

where $\mathcal{N}$ is the standard renormalization due to the local operators constructed from metric and depends only on χ and σ.[8] n_x is the sum of the number of points counted with a sign and is called the Seiberg–Witten invariant. For the total contribution to U(1) monopole part (3.44), we have to sum (3.46) with all basic classes x and obtain

$$Z^{\mathrm{U}(1)}_{\mathrm{mono}} = \mathcal{N} \sum_x n_x. \tag{3.47}$$

For U(1) B_+, c part we have

$$Z^{\mathrm{U}(1)}_{B_+} = \frac{1}{(2\pi)^{\Omega'''}} \int \mathcal{D} W^3_{B_+,c} \mathcal{D} \psi^3_{W_{B_+,c}} e^{-S^1_{B_+,c}(2)}, \tag{3.48}$$

where

$$\begin{aligned} W^3_{B_+,c} &= B^{\mu\nu 3}_+, H^{\mu 3}_B, c^3, \\ \psi^3_{W_{B_+,c}} &= \psi^{\mu\nu 3}_B, \chi^{II\mu 3}_B, \xi^3, \\ h^2 S^{U(1)\, B_+,c}(2) &= \int d^4x \sqrt{g} \mathcal{L}^{U(1) B_+,c}(2), \\ \Omega'''' &= \text{dim of } H\text{'s of U(1) } B_+, c \text{ part.} \end{aligned} \tag{3.49}$$

$Z^{\mathrm{U}(1)}_{B_+}$ is the partition function of the cohomological field theory with the fixed point

$$\nabla^\mu B^3_{+\mu\nu} = 0, \quad \partial_\nu c^3 = 0. \tag{3.50}$$

This partition function is sum of the ± 1 when there are only isolated solutions as usual. The condition that the $Z^{\mathrm{U}(1)}_{B_+}$ is nonzero is that the dimensions of the moduli space of the 0 section defined by (3.50) become zero. In fact, the virtual dimension of this moduli space is calculated to be

$$\Delta = \mathrm{index}\,(d^{*+} + d) = \tfrac{1}{2}(\chi + \sigma), \tag{3.51}$$

where χ and σ are the Euler number and signature of X, respectively. Thus $\Delta = 0$ is a condition that we get nontrivial results. We discuss this point later.

Finally, we obtain

$$Z^{\mathrm{U}(1)}_{m,c,k}(2) = \mathcal{N} Z^{\mathrm{U}(1)}_{B_+} \sum_x n_x. \tag{3.52}$$

Now we evaluate the transverse integral $Z^t_{m,c,k}(2)$. Following H-P-P,[6] we choose a unitary gauge in which

$$\theta_{\pm}=0, \tag{3.53}$$

where

$$\theta=\theta^3T^3+\theta^+T^++\theta^-T^-. \tag{3.54}$$

In this gauge θ has values on the maximal torus (Cartan subalgebra). By following the standard Faddeev–Povov gauge fixing procedure, we introduce a new nilpotent BRST operator δ with the algebra

$$\delta\theta_{\pm}=\pm iC_{\pm}\theta_3, \quad \delta C_{\pm}=0, \quad \delta\theta_3=0, \quad \delta\overline{C}_{\pm}=b_{\pm}, \quad \delta b_{\pm}=0, \tag{3.55}$$

where $C_{\pm}$ and $\overline{C}_{\pm}$ are anticommuting ghosts and antighosts, respectively, and $b_{\pm}$ are commuting auxiliary fields. The action for gauge fixing terms reads

$$\begin{aligned} S_{m,\text{gauge}}(2)&=\delta\frac{1}{mh^2}\int d^4x\,\sqrt{g}(\theta_+\overline{C}_-+\overline{C}_+\theta_-)\\ &=\frac{1}{mh^2}\int d^4x\,\sqrt{g}\{\theta_+b_-+b_+\theta_-+iC_+\theta_3\overline{C}_-+i\overline{C}_+\theta_3C_-\}\\ &=\frac{1}{mh^2}\int d^4x\,\sqrt{g}\{\theta_+b_-+b_+\theta_--C_+2m\overline{C}_--\overline{C}_+2mC_-\}. \end{aligned} \tag{3.56}$$

From the second line to the third line, we take a weak coupling limit and replace θ^3 with $2im$. Note that this action has ghost number 0.

Now consider the transverse part involving adjoint fields. We perform $b_{\pm},C_{\pm},\overline{C}_{\pm},\overline{\theta^{\pm}},\eta^{\pm}$ integral and obtain

$$\begin{aligned} &[\det(im)]^{(1/2)2}_{\Omega^0}[\det(-2)]^{(1/2)2}_{\Omega^0}\left[\det\left(\frac{16m^2}{\pi}\right)\right]^{-1/2}_{\Omega^0}[\det(-8m)]^{1/2}_{\Omega^0}\\ &=[\det(2\pi m)]^{1/2}_{\Omega^0}=(2\pi m)^{(1/2)\,\dim\,(\Omega^0_{\lambda>0}\oplus\mathrm{Ker}\,(D^3))}. \end{aligned} \tag{3.57}$$

(i) $H^{\pm}_+,\chi^{\pm}_+$ integral:

$$[\det(2\pi m)]^{1/2}_{\Omega^{2+}}=(2\pi m)^{(1/2)\,\dim\,(\Omega^{2+}_{\lambda>0}\oplus\mathrm{Ker}\,(D^{3+}*))}. \tag{3.58}$$

(ii) $H^{\pm}_B,\chi^{\pm}_B$ integral:

$$[\det(2\pi m)]^{1/2}_{\Omega^1}=(2\pi m)^{(1/2)\,\dim\,(\Omega^1_{\lambda>0}\oplus\mathrm{Ker}\,(D^{3+}+D^3*))}. \tag{3.59}$$

(iii) $A^{\pm},\psi^{\pm}$ integral for nonzero mode:

$$\frac{[\det(-(D^3D^3*+D^{3+}*D^{3+})/m)]^{1/2}_{\psi^{\pm}_{\text{non }0}}}{[\det(-(D^3D^3*+D^{3+}*D^{3+})/2\pi)]^{1/2}_{A^{\pm}_{\text{non }0}}}=\left[\det\left(\frac{2\pi}{m}\right)\right]^{1/2}_{\Omega^1_{\text{non }0}}=\left(\frac{2\pi}{m}\right)^{(1/2)\,\dim\,(\Omega^1_{\lambda>0})}. \tag{3.60}$$

(iv) $B^{\pm}_+,\psi^{\pm}_B$ integral for nonzero mode:

$$\frac{[\det(-(D^{3+}D^{3+}*)/m)]^{1/2}_{\chi^{\pm}_{B\text{non }0}}}{[\det(-(D^{3+}D^{3+}*)/2\pi)]^{1/2}_{B^{\pm}_{+\text{non }0}}}=\left[\det\left(\frac{2\pi}{m}\right)\right]^{1/2}_{\Omega^{2+}_{\text{non }0}}=\left(\frac{2\pi}{m}\right)^{(1/2)\dim(\Omega^{2+}_{\lambda>0})}. \tag{3.61}$$

(v) $c^{\pm},\xi^{\pm}$ integral for nonzero mode:

$$\frac{[\det(-(D^{3}*D^{3})/m)]^{1/2}_{\xi^{\pm}_{\text{non }0}}}{[\det(-(D^{3}*D^{3})/2\pi)]^{1/2}_{c^{\pm}_{\text{non }0}}}=\left[\det\left(\frac{2\pi}{m}\right)\right]^{1/2}_{\Omega^{0}_{\text{non }0}}=\left(\frac{2\pi}{m}\right)^{(1/2)\dim(\Omega^{0}_{\lambda>0})}. \tag{3.62}$$

Now we collect all the contributions of the adjoint transverse part and obtain

$$\begin{aligned}&\frac{1}{(2\pi)^{\Omega''_{\text{ado}}}}(2\pi m)^{(1/2)\dim(\Omega^{0}_{\lambda>0}\oplus\mathrm{Ker}\,(D^{3}))}(2\pi m)^{(1/2)\dim(\Omega^{2+}_{\lambda>0}\oplus\mathrm{Ker}\,(D^{3+}*))}\\&\quad\times(2\pi m)^{(1/2)\dim(\Omega^{1}_{\lambda>o}\oplus\mathrm{Ker}\,(D^{3+}+D^{3}*))}\cdot\left(\frac{2\pi}{m}\right)^{(1/2)\dim(\Omega^{1}_{\lambda>0})}\left(\frac{2\pi}{m}\right)^{(1/2)\dim(\Omega^{2+}_{\lambda>0})}\\&\quad\times\left(\frac{2\pi}{m}\right)^{(1/2)\dim(\Omega^{0}_{\lambda>0})}=1.\end{aligned} \tag{3.63}$$

The remaining transverse integral is a fundamental part. First we perform the H^{I}_{q2},χ^{I}_{q2} integral and obtain

$$\frac{1}{(2\pi)^{\Omega''_{\text{fun}}}}\frac{[\det(-4m)]_{(\chi^{\dagger}_{q2},\chi_{q2})}}{[\det(-1/\pi)]_{(H^{\dagger}_{q2},H^{2}_{q})}}=\left[\det\left(\frac{m}{\pi}\right)\right]_{\Gamma^{-}}=\left(\frac{m}{\pi}\right)^{\dim(\Gamma^{-}_{\lambda>0}\oplus\mathrm{Ker}\,((\not{D}^{3})^{\dagger}))}. \tag{3.64}$$

Next we perform the q_2,ψ_{q_2} integral for nonzero and zero modes, respectively, and obtain

$$\frac{[\det(-\not{D}^{\dagger}\not{D}/4m)]_{(\psi^{\dagger}_{q_2},\psi_{q_2})_{\text{non }0}}}{[\det(-\not{D}^{\dagger}\not{D}/4\pi)]_{(q^{\dagger}_{2},q_2)_{\text{non }0}}}\frac{[\det(-1)]_{(\psi^{\dagger}_{q_2},\psi_{q_2})_{0}}}{[\det(-m/\pi)]_{(q^{\dagger}_{2},q_2)_{0}}}=\left[\det\left(\frac{\pi}{m}\right)\right]_{\Gamma^{+}}=\left(\frac{\pi}{m}\right)^{\dim(\Gamma^{+}_{\lambda>0}\oplus\mathrm{Ker}\,(\not{D}^{3}))}. \tag{3.65}$$

Collecting (3.64) and (3.65), one can obtain

$$\left(\frac{m}{\pi}\right)^{\dim(\Gamma^{-}_{\lambda>0}\oplus\mathrm{Ker}((\not{D}^{3})^{\dagger}))}\left(\frac{\pi}{m}\right)^{\dim(\Gamma^{+}_{\lambda>0}\oplus\mathrm{Ker}\,(\not{D}^{3}))}=\left(\frac{\pi}{m}\right)^{\text{index}\,(\not{D}^{3})} \tag{3.66}$$

From (3.63) and (3.66) we obtain

$$Z^{t}_{m,c,k}(2)=\left(\frac{\pi}{m}\right)^{\text{index}\,(\not{D}^{3})}. \tag{3.67}$$

Finally for $\langle e^{I}\rangle_{m,c,k}$ (2) we obtain

$$\langle e^{I}\rangle_{m,c,k}(2)=Z^{U(1)}_{m,c,k}(2)\cdot Z^{2}_{m,c,k}(2)=\mathcal{N}\left(\frac{\pi}{m}\right)^{\text{index}\,(\not{D}^{3})}Z^{U(1)}_{B_{+}}\sum_{x}n_{x}. \tag{3.68}$$

3. Synthesis

As we have already mentioned, $\langle e^{I}\rangle_{m,c,k}$ itself is zero. However, from the previous two paragraphs, each branch has nontrivial contributions. Thus we have finally

$$0 = Z^{\mathrm{V-W}}_{m,c,k} \cdot \left(\frac{2\pi}{m}\right)^{\text{index } \not{D}_c^E} + \mathcal{N} Z_{B_+} \sum_x n_x \cdot \left(\frac{\pi}{m}\right)^{\text{index } \not{D}^3} \doteq \chi_k \cdot \left(\frac{2\pi}{m}\right)^{\text{index } \not{D}_c^E} + \mathcal{N} Z_{B_+} \sum_x n_x \cdot \left(\frac{\pi}{m}\right)^{\text{index } \not{D}^3}, \tag{3.69}$$

where the last expression is valid in the vanishing theorem case.

In general index $\not{D}_c^E$ is calculated to be

$$\text{index } \not{D}_c^E = -k + \frac{\text{rank}\,(E)}{8}(c\cdot c - \sigma). \tag{3.70}$$

In this case,

$$c\cdot\zeta = -\text{index } \not{D}_c^E + 2\Delta. \tag{3.71}$$

The Dirac operator $\not{D}^3$, which operates on q_2, ψ_{q_2}, and so on is necessary to be understood as the Dirac operator with the connection given by $c-2\zeta$. Then,

$$\text{index } \not{D}_c^3 = 0 + \tfrac{1}{8}((c-2\zeta)\cdot(c-2\zeta) - \sigma) \tag{3.72}$$

$$= \tfrac{1}{8}(c\cdot c - 4k + 4\ \text{index } \not{D}_c^E - 8\Delta - \sigma). \tag{3.73}$$

Thus we obtain a relation

$$\text{index } \not{D}^3 = \text{index } \not{D}_c^E - \Delta. \tag{3.74}$$

Inserting (3.74) into (3.69), since m is a free parameter, we get a nontrivial result only in the case $\Delta = 0$. Remember that Δ is also the dimension of the moduli space of U(1) B_+, c theory. Thus the condition $\Delta = 0$ is consistent with defining $Z^{\mathrm{U}(1)}_{B_+}$ in (3.48). $\Delta = 0$ is also consistent with geographic condition, for example, simple type condition ($b_2^+ \geqslant 3$), Furuta theory ($b_2 \geqslant 5/4|\sigma| + 2$) and 11/8 conjecture ($b_2 \geqslant 11/8|\sigma|$).[14,15]

Finally, under the condition $\Delta = 0$, from (3.69) we have

$$\chi_k \doteq Z^{\mathrm{V-W}}_{m,c,k} = -\mathcal{N} Z_{B_+} \sum_x n_x \left(\frac{1}{2}\right)^{\text{index } \not{D}_c^E}. \tag{3.75}$$

Note that above x satisfies that $x\cdot x = (2\chi + 3\sigma)/4$ and $x = (c + 2\zeta)/2$.

We think of the Vafa–Witten partition as the sum of (3.75) with weight $e^{\tau k}$, where τ is a parameter. But the sum of this partition function does not clarify modular invariance since $\Delta = 0$ is a special case which does not depend on the coupling τ in the topological twisted model.[1] Additionally, we do not assume duality. Then there is no guarantee that our partition function has modular invariance and is the same as Vafa–Witten's. We suppose that the difference comes from compactification of the moduli space. We do not use the duality relation and our model is not an asymptotic-free theory. So, there is a possibility that compactification in our theory is not the same as the one in the Hilbert scheme. Thus we can describe the twisted $N = 4$ Yang–Mills partition function that may not be the same as Vafa–Witten's partition function with Seiberg–Witten invariants. Our expression is similar to Dijkgraaf *et al.*[10] The most significant difference is τ dependence. Theirs is τ dependent, while ours is τ independent. The reason why their partition function depends on τ is that they treat the physical $N = 4$ Yang–Mills theory itself. According to Labastida,[13] the $N = 4$ Yang–Mills theory depends on τ. On the other hand, we treat UBTQCD, which is the twisted $N = 4$ Yang–Mills theory coupled with a fundamental hypermultiplet. As we mention earlier, this difference may cause breaking of the modular invariance. In other words, our theory is not conformal invariant, and τ is not possible to be a good parameter. However, our

computation is done without an assumption like duality relation. If there is a difference we have to interpret that the origin of the difference occurred from compactification.[16]

IV. CONCLUSION

We have studied the balanced topological QCD and its broken balance theory and obtained relations of the partition function of twisted $N=4$ SU(2) Yang–Mills theory with the partition function of twisted Abelian QCD. This relation is understood in several ways. For example, the sum of Euler numbers of instanton moduli space, which is invariant under SL(2,Z) transformation, is described by Seiberg–Witten invariants when $\Delta=0$ and the vanishing theorem is valid. In other cases there is no vanishing theorem like §5.4 in Ref. 1; we obtained similar but not the same formulas under the condition of $\Delta=0$. There is no other reason to understand the difference from the result of Vafa, Witten and Dijkgraaf *et al.*[1,10] than the difference of compactification.

Some problems are left for our future work. When $\Delta\neq 0$, can we obtain any similar nontrivial results without assumption of duality relation? We may obtain them by simple reformation. However, it is difficult to expect that the partition function has the nature of modular invariance in naive reformation. We are interested in a connection with the duality and a compactification. How can we obtain the modular invariant partition function with no assumption of duality? We have some hints of this question but no answer.

As we saw in Sec. II, the vanishing theorem of BTQCD is not studied in this article. If the theorem exists, we get the sum of Euler numbers of non-Abelian monopole moduli space as the partition function of the BTQCD. It is interesting work to investigate the nature of the partition function because the theory has the branches that contain both Vafa–Witten theory and Seiberg–Witten theory.

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APPENDIX A: THE BRS ALGEBRA AND THE BTQCD ACTION

We give the BRS algebra and the Lagrangian of BTQCD explicitly in this appendix.

1. Algebra

The δ_+ transformations are as follows:

$$\begin{aligned}
\delta_- A_\mu &= \chi^{\mathrm{II}}_\mu,\\
\delta_- \chi^{\mathrm{II}}_\mu &= -\delta^{\bar\theta}_g A_\mu = -D_\mu \bar\theta,\\
\delta_- \psi_\mu &= -\delta^c_g A_\mu - H^{\mathrm{II}}_{B_\mu} = -D_\mu c - H^{\mathrm{II}}_{B_\mu},\\
\delta_- H^{\mathrm{II}}_{B_\mu} &= -\delta^c_g \chi^{II}_{B_\mu} + \delta_+ \delta^{\bar\theta}_g A_\mu = -i[\chi^{\mathrm{II}}_{B_\mu}, c] + \delta_+ \delta^{\bar\theta}_g A_\mu;
\end{aligned} \tag{A1}$$

$$\begin{aligned}
\delta_- B^{\mu\nu}_+ &= \chi^{I\mu\nu}_+,\\
\delta_- \chi^{I\mu\nu}_+ &= -\delta^{\bar\theta}_g B^{\mu\nu}_+ = -i[B^{\mu\nu}_+, \bar\theta],\\
\delta_- \psi^{\mu\nu}_B &= -\delta^c_g B^{\mu\nu}_+ - H^{\mathrm{I}\mu\nu}_+ = -i[B^{\mu\nu}_+, c] - H^{\mathrm{I}\mu\nu}_+,\\
\delta_- H^{\mathrm{I}\mu\nu} &= -\delta^c_g \chi^{\mathrm{I}\mu\nu}_+ + \delta_+ \delta^{\bar\theta}_g B^{\mu\nu}_+ = -i[\chi^{\mathrm{I}\mu\nu}_+, c] + \delta_+ \delta^{\bar\theta}_g B^{\mu\nu}_+;
\end{aligned} \tag{A2}$$

$$\begin{aligned}
&\delta_- q^{\dot\alpha} = \chi_B^{\mathrm{II}\dot\alpha},\\
&\delta_- \chi_B^{\mathrm{II}\dot\alpha} = \delta_g^{\theta} q^{\dot\alpha} = i\bar\theta q^{\dot\alpha} + \bar m q^{\dot\alpha},\\
&\delta_- \psi_q^{\dot\alpha} = \delta_g^c q^{\dot\alpha} - H_B^{II\dot\alpha} = icq^{\dot\alpha} + m_c q^{\dot\alpha} - H_B^{\mathrm{II}\dot\alpha},\\
&\delta_- H_B^{\mathrm{II}\dot\alpha} = \delta_g^c \chi_B^{\mathrm{II}\dot\alpha} - \delta_+ \delta_g^{\theta} q^{\dot\alpha} = ic\chi_B^{\mathrm{II}\dot\alpha} + m_c - \delta_+ \delta_g^{\theta} q^{\dot\alpha};
\end{aligned} \tag{A3}$$

$$\begin{aligned}
&\delta_- B_\alpha = \chi_{q\alpha}^I,\\
&\delta_- \chi_{q\alpha}^{\mathrm{I}} = \delta_g^{\theta} B_\alpha = i\bar\theta B_\alpha + \bar m B_\alpha,\\
&\delta_- \psi_{B\alpha} = \delta_g^c B_\alpha - H_{q\alpha}^{\mathrm{I}} = icB_\alpha + m_c B_\alpha - H_{q\alpha}^{\mathrm{I}},\\
&\delta_- H_{q\alpha}^{\mathrm{I}} = \delta_g^c \chi_{q\alpha}^I - \delta_+ \delta_g^{\theta} B_\alpha = ic\chi_{q\alpha}^I + m_c \chi_{q\alpha}^{\mathrm{I}} - \delta_+ \delta_g^{\theta} B_\alpha;
\end{aligned} \tag{A4}$$

$$\begin{aligned}
&\delta_- q_{\dot\alpha}^\dagger = \chi_{B\dot\alpha}^{II\dagger},\\
&\delta_- \chi_{B\dot\alpha}^{II\dagger} = \delta_g^{\theta} q_{\dot\alpha}^\dagger = iq_{\dot\alpha}^\dagger \bar\theta - \bar m q_{\dot\alpha}^\dagger,\\
&\delta_- \psi_{q\dot\alpha}^\dagger = \delta_g^c q_{\dot\alpha}^\dagger - H_{B\dot\alpha}^{II\dagger} = iq_{\dot\alpha}^\dagger c - m_c q_{\dot\alpha}^\dagger - H_{B\dot\alpha}^{II\dagger},\\
&\delta_- H_{B\dot\alpha}^{II\dagger} = \delta_g^c \chi_{B\dot\alpha}^{II\dagger} - \delta_+ \delta_g^{\theta} q_{\dot\alpha}^\dagger = -i\chi_{B\dot\alpha}^{I\dagger} c - m_c \chi_{B\dot\alpha}^{I\dagger} - \delta_+ \delta_g^{\theta} q_{\dot\alpha}^\dagger;
\end{aligned} \tag{A5}$$

$$\begin{aligned}
&\delta_- B^{\dagger\alpha} = \chi_q^{I\dagger\alpha},\\
&\delta_- \chi_q^{I\dagger\alpha} = \delta_g^{\theta} B^{\dagger\alpha} = -iB^{\dagger\alpha}\bar\theta - \bar m B^{\dagger\alpha},\\
&\delta_- \psi_B^{\dagger\alpha} = \delta_g^c B^{\dagger\alpha} - H_q^{I\dagger\alpha} = -iB^{\dagger\alpha} c - m_c B^{\dagger\alpha} - H_q^{I\dagger\alpha},\\
&\delta_- H_q^{I\dagger\alpha} = \delta_g^c \chi_q^{I\dagger\alpha} - \delta_+ \delta_g^{\theta} B^{\dagger\alpha} = i\chi_q^{I\dagger\alpha} c - m_c \chi_q^{I\dagger\alpha} - \delta_+ \delta_g^{\theta} B^{\dagger\alpha}.
\end{aligned} \tag{A6}$$

The δ_+ transformations are given by

$$\begin{aligned}
&\delta_+ A_\mu = \psi_\mu,\\
&\delta_+ \psi_\mu = \delta_g^{\theta} A_\mu = D_\mu \theta,\\
&\delta_+ \chi_{B\mu}^{II} = H_{B\mu}^{II},\\
&\delta_+ H_{B\mu}^{II} = \delta_g^{\theta} \chi_{B\mu}^{II} = i[\chi_{B\mu}^{II}, \theta];
\end{aligned} \tag{A7}$$

$$\begin{aligned}
\delta_+ B_+^{\mu\nu} &= \psi_B^{\mu\nu}, \\
\delta_+ \psi_B^{\mu\nu} &= \delta_g^\theta B_+^{\mu\nu} = i[B_+^{\mu\nu}, \theta], \\
\delta_+ \chi_+^{I\mu\nu} &= H_+^{I\mu\nu}, \\
\delta_+ H_+^{I\mu\nu} &= \delta_g^\theta \chi_+^{I\mu\nu} = i[\chi_+^{I\mu\nu}, \theta];
\end{aligned} \tag{A8}$$

$$\begin{aligned}
\delta_+ q^{\dot\alpha} &= \psi_q^{\dot\alpha}, \\
\delta_+ \psi_q^{\dot\alpha} &= -\delta_g^\theta q_q^{\dot\alpha} = -(i\theta q_q^{\dot\alpha} + m q_q^{\dot\alpha}), \\
\delta_+ \chi_B^{II\dot\alpha} &= H_B^{II\dot\alpha}, \\
\delta_+ H_B^{II\dot\alpha} &= -\delta_g^\theta \chi_B^{II\dot\alpha} = -(i\theta \chi_B^{II\dot\alpha} + m \chi_B^{II\dot\alpha});
\end{aligned} \tag{A9}$$

$$\begin{aligned}
\delta_+ B_\alpha &= \psi_{B\alpha}, \\
\delta_+ \psi_{B\alpha} &= -\delta_g^\theta B_\alpha = -(i\theta B_\alpha + m B_\alpha), \\
\delta_+ \chi_{q\alpha}^I &= H_{q\alpha}^I, \\
\delta_+ H_{q\alpha}^I &= -\delta_g^\theta \chi_{q\alpha}^I = -(i\theta \chi_{q\alpha}^I + m \chi_{q\alpha}^I);
\end{aligned} \tag{A10}$$

$$\begin{aligned}
\delta_+ q_{\dot\alpha}^\dagger &= \psi_{q\dot\alpha}^\dagger, \\
\delta_+ \psi_{q\dot\alpha}^\dagger &= -\delta_g^\theta q_{\dot\alpha}^\dagger = -(-i q_{\dot\alpha}^\dagger \theta - m q_{\dot\alpha}^\dagger), \\
\delta_+ \chi_{B\dot\alpha}^{II\dagger} &= H_{B\dot\alpha}^{II\dagger}, \\
\delta_+ H_{B\dot\alpha}^{II\dagger} &= -\delta_g^\theta \chi_{B\dot\alpha}^{II\dagger} = -(-i \chi_{B\dot\alpha}^{II\dagger} \theta - m \chi_{B\dot\alpha}^{II\dagger});
\end{aligned} \tag{A11}$$

$$\begin{aligned}
\delta_+ B^{\dagger\alpha} &= \psi_B^{\dagger\alpha}, \\
\delta_+ \psi_B^{\dagger\alpha} &= -\delta_g^\theta B^{\dagger\alpha} = -(-iB^{\dagger\alpha}\theta - m B^{\dagger\alpha}), \\
\delta_+ \chi_q^{I\dagger\alpha} &= H_q^{I\dagger\alpha}, \\
\delta_+ H_q^{I\dagger\alpha} &= -\delta_g^\theta \chi_q^{I\dagger\alpha} = -(-i\chi_q^{I\dagger\alpha}\theta - m\chi_q^{I\dagger\alpha}).
\end{aligned} \tag{A12}$$

Transformations for $c, \theta, \overline{\theta}, m, m_c, \overline{m}$ are given by

$$
\begin{aligned}
&\delta_+\theta=0,\\
\delta_-\theta=\xi,\quad &\delta_+\xi=\delta_g^\theta c=i[c,\theta],\\
\delta_+c=\xi,\quad &\delta_-\xi=\delta_g^\theta\theta=i[\theta,\overline{\theta}],\\
\delta_-c=\eta,\quad &\delta_+\eta=\delta_g^\theta\overline{\theta}=i[\overline{\theta},\theta],\\
\delta_+\overline{\theta}=\eta,\quad &\delta_-\eta=\delta_g^{\overline{\theta}}c=i[c,\overline{\theta}],\\
&\delta_-\overline{\theta}=0;
\end{aligned}
\tag{A13}
$$

$$
\begin{aligned}
&\delta_+m=0,\\
\delta_-m=\xi_m,\quad &\delta_+\xi_m=0,\\
\delta_+m_c=\xi_m,\quad &\delta_-\xi_m=0,\\
\delta_-m_c=\eta_m,\quad &\delta_+\eta_m=0,\\
\delta_+\overline{m}=\eta_m,\quad &\delta_-\eta_m=0,\\
&\delta_-\overline{m}=0.
\end{aligned}
\tag{A14}
$$

2. Action of BTQCD

We write down the Lagrangian of BTQCD explicitly in this paragraph. Here $\delta_-\mathcal{F}$ is given as

$$
\begin{aligned}
\delta_-\mathcal{F}=&\delta_-(B_+^{\mu\nu a}s_{+\mu\nu}^a)-\delta_-(\chi_+^{I\mu\nu a}\psi_{B\mu\nu}^a)-\delta_-(\chi_{B\mu}^{IIa}\psi^{\mu a})+\delta_-(-i\tfrac{1}{3}B_+^{\mu\nu a}[B_{+\mu\rho},B_{+\nu\sigma}]^a g^{\rho\sigma})\\
&+\delta_-(B^{\dagger\alpha}s_\alpha)-\delta_-(\chi_q^{I\dagger\alpha}\psi_{B\alpha})-\delta_-(\chi_{B\dot\alpha}^{II\dagger}\psi_q^{\dot\alpha})+\delta_-(s^{\dagger\alpha}B_\alpha)+\delta_-(\psi_B^{\dagger\alpha}\chi_{q\alpha}^I)\\
&+\delta_-(\psi_{q\dot\alpha}^\dagger\chi_B^{II\dot\alpha})+\delta_-(\xi^a\eta^a)
\end{aligned}
\tag{A15}
$$

$$
\begin{aligned}
=&-\chi_+^{I\mu\nu a}\{H_{+\mu\nu}^{Ia}-(s_{+\mu\nu}^a-i[B_{+\mu\rho},B_{+\nu\sigma}]^a g^{\rho\sigma}-i[B_{+\mu\nu},c]^a)\}\\
&-\chi_+^{II\rho a}\{H_{B\rho}^{IIa}-(2D^\mu B_{+\mu\rho}^a+iB^\dagger\sigma_\rho T^a q-iq^\dagger\overline{\sigma}_\rho T^a B-D_\rho c^a)\}\\
&-\chi^{I\dagger\alpha}\{H_{q\alpha}^I-(s_\alpha+icB_\alpha+m_cB_\alpha)\}-\chi_{B\dot\alpha}^{II\dagger}\{H_B^{II\dot\alpha}-(-(\not{D}^\dagger B)^{\dot\alpha}+(\overline{\sigma}^{\mu\nu}B_{+\mu\nu}q)^{\dot\alpha}\\
&+icq^{\dot\alpha}+m_cq^{\dot\alpha})\}-\{H_q^{I\dagger\alpha}-(s^{\dagger\alpha}-iB^{\dagger\alpha}c-m_cB^{\dagger\alpha})\}\chi_{q\alpha}^I-\{H_{B\dot\alpha}^{II\dagger}-(-(\not{D}^\dagger B)_\alpha^\dagger\\
&+(q^\dagger B_{+\mu\nu}\overline{\sigma}^{\mu\nu})_{\dot\alpha}-iq_{\dot\alpha}^\dagger c-m_cq_{\dot\alpha}^\dagger)\}\chi_B^{II\dot\alpha}+\{i[\theta,\overline{\theta}]^a\eta^a-i\xi^a[c,\overline{\theta}]^a\}+i[B_+^{\mu\nu},\overline{\theta}]^a\psi_{B\mu\nu}^a\\
&+D_\mu\overline{\theta}^a\psi^{\mu a}-(-iB^{\dagger\alpha}\overline{\theta}-\overline{m}B^{\dagger\alpha})\psi_{B\alpha}-(-iq_{\dot\alpha}^\dagger\overline{\theta}-\overline{m}q_{\dot\alpha}^\dagger)\psi_q^{\dot\alpha}\\
&-\psi_B^{\dagger\alpha}(i\overline{\theta}B_\alpha+\overline{m}B_\alpha)-\psi_{a\dot\alpha}^\dagger(i\overline{\theta}q^{\dot\alpha}+\overline{m}q^{\dot\alpha}).
\end{aligned}
\tag{A16}
$$

The full Lagrangian is given as

$$\mathcal{L}^{\text{full}}=\delta_+\delta_-\mathcal{F} \tag{A17}$$

$$\begin{aligned}
&=-H_+^{I\mu\nu a}\{H_{+\mu\nu}^{Ia}-(s_{+\mu\nu}^a-i[B_{+\mu\rho},B_{+\nu\sigma}]^a g^{\rho\sigma}-i[B_{+\mu\nu},c]^a)\}-\chi_+^{I\mu\nu a}\{-i[\chi_{+\mu\nu}^I,\theta]^a\\
&\quad+2D_\mu\psi_\nu^a+\psi_q^\dagger\overline{\sigma}_{\mu\nu}T^a q+q^\dagger\overline{\sigma}_{\mu\nu}T^a\psi_q-2i[B_{+\mu\rho},\psi_{B\nu\sigma}]^a g^{\rho\sigma}-i[\psi_{B\mu\nu},c]^a-i[B_{+\mu\nu},\xi]^a\}\\
&\quad-H_B^{II\rho a}\{H_{B\rho}^{IIa}-(-2D^\mu B_{+\mu\rho}^a+iB^\dagger\sigma_\rho T^a q-iq^\dagger\overline{\sigma}_\rho T^a B-D_\rho c^a)\}\\
&\quad-\chi_B^{II\rho a}\{-i[\chi_{B\rho}^{II},\theta]^a-2D^\mu\psi_{B\mu\rho}^a-2i[\psi^\mu,B_{+\mu\rho}]^a+i\psi_B^\dagger\sigma_\rho T^a q+iB^\dagger\sigma_\rho T^a\psi_q-i\psi_q^\dagger\overline{\sigma}_\rho T^a B\\
&\quad-iq^\dagger\overline{\sigma}_\rho T^a\psi_B-D_\rho\xi^a-i[\psi_\rho,c]^a\}-H_q^{I\dagger\alpha}\{H_{q\alpha}^I-(s_\alpha+icB_\alpha+m_cB_\alpha)\}\\
&\quad-\chi_q^{I\dagger}\{\not{D}\psi_q+\sigma_\rho i\psi^\rho q+i\xi B+ic\psi_B+\xi_m B+m_c\psi_B\}+(\text{h.c. previous two terms})\\
&\quad-H_{B\dot\alpha}^{II\dagger}\{H_B^{II\dot\alpha}-(-(\not{D}^\dagger B)^{\dot\alpha}+(\overline{\sigma}^{\mu\nu}B_{+\mu\nu}q)^{\dot\alpha}+icq^{\dot\alpha}+m_cq^{\dot\alpha})\}\\
&\quad-\chi_B^{II\dagger}\{-\not{D}^\dagger\psi_B-\overline{\sigma}_\rho i\psi^\rho B+(\overline{\sigma}^{\mu\nu}\psi_{B\mu\nu}q)+(\overline{\sigma}^{\mu\nu}B_{+\mu\nu}\psi_q)+i\xi q+ic\psi_q+\xi_m q+m_c\psi_q\}\\
&\quad+(\text{h.c. previous two terms})-\{[\theta,\overline{\theta}]^a[\overline{\theta},\theta]^a-[c,\theta]^a[c,\overline{\theta}]^a+[B_+^{\mu\nu},\overline{\theta}]^a[B_{+\mu\nu},\theta]^a\}\\
&\quad+D_\mu\overline{\theta}^aD^\mu\theta^a+i[\theta,\eta]^a\eta^a+i\xi^a[\xi,\overline{\theta}]^a+i\xi^a[c,\eta]^a+i[\psi_B^{\mu\nu},\overline{\theta}]^a\psi_{B\mu\nu}^a+i[B_+^{\mu\nu},\eta]^a\psi_{B\mu\nu}^a\\
&\quad+D_\mu\eta^a\psi^{\mu a}+i[\psi_\mu,\overline{\theta}]^a\psi^{\mu a}+(-iq^\dagger\overline{\theta}-q^\dagger\overline{m})(i\theta q+mq)+(-iq^\dagger\theta-q^\dagger m)(i\overline{\theta}q+\overline{m}q)\\
&\quad+2\psi_q^\dagger(i\overline{\theta}+\overline{m})\psi_q-2\chi_1^{I\dagger}(i\theta+m)\chi_q^I-(-iq^\dagger\eta-q^\dagger\eta_m)\psi_q+\psi_q^\dagger(i\eta q+\eta_m q)\\
&\quad+(-B^\dagger\overline{\theta}-B^\dagger\overline{m})(i\theta B+mB)+(-iB^\dagger\theta-B^\dagger m)(i\overline{\theta}B+\overline{m}B)+2\psi_B^\dagger(i\overline{\theta}+\overline{m})\psi_B\\
&\quad-2\chi_B^{II\dagger}(i\theta+m)\chi_B^{II}-(-iB^\dagger\eta-B^\dagger\eta_m)\psi_B+\psi_B^\dagger(i\eta B+\eta_m B).
\end{aligned} \tag{A18}$$

APPENDIX B: THE PATH INTEGRAL OF THE TRANSVERSE PART

As we have mentioned in the first part of Sec. III D, the path integral in Sec. III D is not exact, but it amounts to the right result that we will derive in this section. In computation, we take the weak coupling limit. When we replace the nontransverse fields with the fixed point values, we denote Y_{nontrans} by $\tilde{Y}_{\text{nontrans}}$. In particular, the fixed points of θ, $\overline{\theta}$ are given as $\theta=\overline{\theta}=0$ in branch 1 and $\theta^3=2im$, $\overline{\theta}=2i\overline{m}$ in branch 2. We also discuss the different treatment of the path integral in III D at the end of this section. See Ref. 17, too.

1. Branch 1 and its big matrix

In branch 1, the path integral of the transverse part is

$$Z_{m,c,k}^t(1)=\frac{1}{(2\pi)^{\Omega''}}\int\mathcal{D}Q^\dagger\mathcal{D}\psi_Q^\dagger\mathcal{D}Q\mathcal{D}\psi_Q e^{-S^t(1)+I(1)}, \tag{B1}$$

where

$$h^2S^t(1)=\int d^4x\,\sqrt{g}\mathcal{L}^t(1),$$

$$I(1)=\int d^4x\,\sqrt{g}(q^\dagger mq+\psi_q^\dagger\psi_q).$$

$$\Omega''=\text{dim of fundamental } H's. \tag{B2}$$

For $\mathcal{L}^t(1)(3.29)$, we denote

$$\mathcal{L}^t(1) = -2|H_q^I + \cdots|^2 - 2m|\chi_q^I + \cdots|^2 - \frac{1}{2} q^\dagger M^b(1) q + \frac{1}{2m} \psi_q^\dagger M^f(1) \psi_q, \tag{B3}$$

where

$$M^b(1) = M^f(1) = \not{D}^\dagger \not{D} + 4m\overline{m}. \tag{B4}$$

In general, $M^b(M^f)$ is a matrix and is not necessarily diagonalized. M^b and M^f may not be the same as we will see soon. We call $M^b(1)$ the big matrix of branch 1.

Before computing (B1), we briefly review the notion of index $\not{D}$.

One can decompose $q \in \Gamma^+$, $H_q^I \in \Gamma^-$ into

$$\begin{aligned} \not{D}^\dagger \not{D} q^\lambda &= \lambda q^\lambda, \\ \not{D} \not{D}^\dagger H_q^{I^\lambda} &= \lambda H_q^{I^\lambda}. \end{aligned} \tag{B5}$$

This decomposition is called spectra decomposition. Note that if $\lambda > 0$, then q^λ and $H_q^{I^\lambda}$ are isomorphic. However, if $\lambda = 0$, then q^λ and $H_q^{I^\lambda}$ are not isomorphic. The index $\not{D}$ measures the difference between $\Gamma^+_{\lambda=0}$ and $\Gamma^-_{\lambda=0}$, and is defined as

$$\begin{aligned} \text{index}\, \not{D} &= \dim\ \Gamma^+_{\lambda=0} - \dim\ \Gamma^-_{\lambda=0} \\ &= \dim\ \text{Ker}\, \not{D} - \dim\ \text{Ker}\, \not{D}^\dagger, \end{aligned} \tag{B6}$$

where we denote $\Gamma^+_{\lambda=0} = \text{Ker}\, \not{D}$, $\Gamma^+_{\lambda=0} = \text{Ker}\, \not{D}^\dagger$.

In computing (B1), (B6) emerges when the nonkinetic part and the off-diagonal part of M are able to be ignored [in this branch, simply $m\overline{m}$ terms in (B4)]. This process is achieved by diagonalization and field redefinition. Then we obtain the expression (B1) as index $\not{D}$. Conversely, it is enough to obtain this expression that we consider only the kinetic diagonal part of M in the path integral.

Now we perform the path integral of the transverse part of branch 1 explicitly. First, for the H_q^I, χ_q^I integral,

$$\frac{1}{(2\pi)^{\Omega''}} \frac{[\det(-2m)]_{(\chi_q^{I\dagger}, \chi_q^I)}}{\left[\det\left(-\frac{1}{\pi}\right)\right]_{(H_q^{I\dagger}, H_q^I)}} = \left[\det\left(\frac{m}{2\pi}\right)\right]_{\Gamma^-} = \left(\frac{m}{2\pi}\right)^{\dim(\Gamma^-_{\lambda>0} \oplus \text{Ker}(\not{D}^\dagger))}. \tag{B7}$$

Note that the transformation at the second equality is necessary to derive index $\not{D}$.

For the q, ψ_q integral for nonzero-mode,

$$\frac{[\det(-\not{D}^2/2m)]_{(\psi_q^\dagger, \psi_q)_{\text{non } 0}}}{[\det(-\not{D}^2/4\pi)]_{(q^\dagger, q)_{\text{non } 0}}} = \left(\frac{2\pi}{m}\right)^{\dim(\Gamma^+_{\lambda>0})}. \tag{B8}$$

For the q, ψ_q integral for zero-mode, we consider that the integrant of this path integral comes only from observable $I(1)$ and we obtain

$$\frac{[\det(-1)]_{(\psi_q^\dagger, \psi_q)_0}}{[\det(-m/2\pi)]_{(q^\dagger, q)_0}} = \left(\frac{2\pi}{m}\right)^{\dim\ \text{Ker}\,(\not{D})}. \tag{B9}$$

From (B8) and (B9)

$$\left(\frac{2\pi}{m}\right)^{\dim(\Gamma^{+}_{\lambda>0}\oplus \mathrm{Ker}\,(\not{D}))}. \tag{B10}$$

Collecting (B7) and (B10),

$$Z^{t}_{m,c,k}=\left(\frac{m}{2\pi}\right)^{\dim(\Gamma^{-}_{\lambda>0}\oplus \mathrm{Ker}\,(\not{D}^{\dagger}))}\left(\frac{2\pi}{m}\right)^{\dim(\Gamma^{+}_{\lambda>0}\oplus \mathrm{Ker}\,(\not{D}))}=\left(\frac{2\pi}{m}\right)^{\mathrm{index}\,\not{D}}. \tag{B11}$$

Note that $\dim(\Gamma^{+}_{\lambda>0})$ and $\dim(\Gamma^{-}_{\lambda>0})$ cancel each other.

2. Branch 2 and its big matrix

In branch 2, the path integral of the transverse part is

$$Z^{t}_{m,c,k}(2)=\frac{1}{\mathrm{Vol}\;\mathcal{G}^{\pm}(2\pi)^{\Omega''}}\int \mathcal{D}W^{\pm}\mathcal{D}\psi^{\pm}_{W}\mathcal{D}Q^{\dagger}_{2}\mathcal{D}\psi^{\dagger}_{Q2}\mathcal{D}Q_{2}\mathcal{D}\psi_{Q2}e^{-S^{t}(2)+I(2)}, \tag{B12}$$

where

$$\begin{aligned} h^{2}S^{t}(2)&=\int d^{4}x\,\sqrt{g}\,\mathcal{L}^{t}(2),\\ I(2)&=\int d^{4}x\sqrt{g}(q^{\dagger}_{2}2mq_{2}+\psi^{\dagger}_{q_{2}}\psi_{q_{2}}),\\ \Omega''&=\text{dim of } H\text{'s of transverse degrees.}\end{aligned} \tag{B13}$$

For $\mathcal{L}^{t}(2)$ in (3.41), we denote

$$\begin{aligned}\mathcal{L}^{t}(2)=&-4|H^{I+}_{+\mu\nu}+\cdots|^{2}-8m|\chi^{I+}_{+\mu\nu}+\cdots|^{2}+16m^{2}|\overline{\theta}^{+}+\cdots|^{2}-8m|\eta^{+}+\cdots|^{2}-4|H^{II+}_{B}+\cdots|^{2}\\&-8m|\chi^{II+}_{B}+\cdots|^{2}-2|H^{I}_{q2}+\cdots|^{2}-4m|\chi^{I}_{q_{2}}+\cdots|^{2}-Y^{T}M^{b}(2)Y+\frac{1}{2m}\Psi^{T}_{Y}M^{f}(2)\Psi_{Y},\end{aligned} \tag{B14}$$

where Y^{T} and Ψ^{T}_{Y} are raw vectors,

$$Y^{T}=(A^{+}_{\mu},B^{+}_{+\nu\rho},c^{+},q^{\dagger}_{2}), \tag{B15}$$

$$\Psi^{T}_{Y}=(\psi^{+}_{\mu},\psi^{+}_{B\nu\rho},\xi^{+},\psi^{\dagger}_{q_{2}}), \tag{B16}$$

and Y and Ψ_{Y} are column vectors,

$$Y=(A^{-}_{\sigma},B^{-}_{+\gamma\delta},c^{-},q_{2}), \tag{B17}$$

$$\Psi_{Y}=(\psi^{-}_{\sigma},\psi^{-}_{B\gamma\delta},\xi^{-},\psi_{q_{2}}). \tag{B18}$$

To derive the result (3.67) from (B12) and (B14), we can neglect the nonkinetic terms and off-diagonal part of $M(2)$ (we will give these explicitly later). There is the contribution from the Faddeev–Popov determinant of $\theta^{\pm}=0$ gauge and it is possible to discard the path integral of $Y^{\pm}$ for zero-mode according to the balanced structure of adjoint fields.

In this remaining subsection, we concentrate on giving $M(2)$ explicitly. $M^{b}(2)(M^{f}(2))$ can be decomposed into

$$M^b(2)=\begin{pmatrix} M^b_{AA} & M^b_{Aq} \\ M^b_{q^\dagger A} & M^b_{q^\dagger q}\end{pmatrix}. \tag{B19}$$

We denote the matrix element of $M^b(2)$ (or $M^b_{AA},M^b_{Aq},M^b_{q^\dagger A},M^b_{q^\dagger q}$) by $\{M^b(2)\}^{A^+\mu B^-_+\gamma\delta}$,$\{M^b_{Aq}\}^{A^+\mu}{}_q$, etc.

a. Diagonal part of $M^b(2)(M^f(2))$

$$\begin{aligned}\{M^b_{AA}\}^{A^+\mu A^-\sigma}&=\{M^f_{AA}\}^{A^+\mu A^-\sigma}\\ &=(D^{3+}{*}D^{3+})^{\mu\sigma}+(D^3D^3{*})^{\mu\sigma}-\tilde B^{3\mu\rho}_+\tilde B^{3\sigma}_{+\rho}\\ &\quad-\tfrac12\tilde q_1^\dagger\bar\sigma^\mu\sigma^\sigma\tilde q_1+(-(\tilde c^3)^2+16m\bar m)g^{\mu\sigma}.\end{aligned} \tag{B20}$$

$$\begin{aligned}\{M^b_{AA}\}^{B^+_+\nu\rho B^-_+\gamma\delta}&=\{M^f_{AA}\}^{B^+_+\nu\rho B^-_+\gamma\delta}\\ &=(D^{3+}D^{3+}{*})^{\nu\rho}g^{\gamma\delta}-4\tilde B^{3\nu\rho}_+\tilde B^{3\gamma\delta}_+ +(-(\tilde c^3)^2+16m\bar m)g^{\nu\rho}g^{\gamma\delta}.\end{aligned} \tag{B21}$$

$$\{M^b_{AA}\}^{c^+c^-}=\{M^f_{AA}\}^{c^+c^-}=D^3{*}D^3-\tilde B^{3\mu\nu}_+\tilde B^3_{+\mu\nu}-(\tilde c^3)^2-16m\bar m. \tag{B22}$$

$$\{M^b_{q^\dagger q}\}^{q^\dagger q}=\not D^{3\dagger}\not D^3-2\bar\sigma_{\mu\nu}\tilde q_1\tilde q_1^\dagger\bar\sigma^{\mu\nu}+16m\bar m. \tag{B23}$$

$$\{M^f_{q^\dagger q}\}^{q^\dagger q}=\not D^{3\dagger}\not D^3+2\bar\sigma_{\mu\nu}\tilde q_1\tilde q_1^\dagger\bar\sigma^{\mu\nu}+16m\bar m. \tag{B24}$$

Note that $\{M^b_{q^\dagger q}\}^{q^\dagger q}$ and $\{M^f_{q^\dagger q}\}^{q^\dagger q}$ are different.

b. Off-diagonal part of $M^b_{AA}(M^f_{AA})$

$$\begin{aligned}\{M^b_{AA}\}^{A^+\mu B^-_+\rho\sigma}&=\{M^b_{AA}\}^{A^+\mu B^-_+\rho\sigma}\\ &=i(\overleftarrow{D^{3+}})_\nu\tilde c^3g^{\mu\rho}g^{\nu\sigma}-2i\tilde B^{3\mu\rho}_+(D^{3+}{*})^\rho\\ &\quad-i(\overleftarrow{D^{3*}})^\mu\tilde B^{3\rho\sigma}_+-2i(\overleftarrow{D^{3+}})_\nu\tilde B^{3\mu\rho}_+g^{\nu\sigma}.\end{aligned} \tag{B25}$$

$$\{M^b_{AA}\}^{A^+\mu c^-}=\{M^b_{AA}\}^{A^+\mu}{}_{c^-}=-i(\overleftarrow{D^{3+}})_\nu\tilde B^{3\mu\nu}_+-2i\tilde B^{3\mu\rho}_+(D^3)_\rho+i(\overleftarrow{D^{3*}})^\mu\tilde c^3. \tag{B26}$$

$$\{M^b_{AA}\}^{B^+_+\nu\rho c^-}=\{M^b_{AA}\}^{B^+_+\nu\rho}{}_{c^-}=(\overleftarrow{D^{3+}{*}})^\nu(D^3)^\rho-2\tilde c^3\tilde B^{3\nu\rho}_+. \tag{B27}$$

c. Off-diagonal part of $M^b_{Aq}(M^f_{Aq})$

Here using

$$Y^\pm=\tfrac12(Y^1\mp iY^2), \tag{B28}$$

we denote $\{M^b_{Aq}\}^{Y^1q}$,$\{M^b_{Aq}\}^{Y^2q}$ and $\{M^f_{Aq}\}^{Y^1q}$,$\{M^f_{Aq}\}^{Y^2q}$ instead of $\{M^b_{Aq}\}^{Y^+q}$,$\{M^f_{Aq}\}^{Y^+q}$. The reason why we cannot denote $\{M^b_{Aq}\}^{Y^+q}$,$\{M^f_{Aq}\}^{Y^+q}$ is that there are terms $(D^3_\mu A^+_\nu-D^3_\nu A^+_\mu)_+q_2^\dagger\bar\sigma^{\mu\nu}\tilde q_1$ and $i(\not D^3q_2)^\dagger\not A^-\tilde q_1$ that exist simultaneously in $\mathcal{L}^t(2)$ in (B14). The remaining elements of this matrix are

$$\{M^b_{Aq}\}^{A^1\mu}{}_q=-\tfrac12(\overleftarrow{D^{3+}})^\nu\tilde q_1^\dagger\bar\sigma_{\mu\nu}-i\tfrac14\tilde q_1^\dagger\bar\sigma_\mu\not D^3-i\tfrac14(\overleftarrow{D^{3+}})^\mu\tilde q_1^\dagger, \tag{B29}$$

$$\{M_{Aq}^{b}\}^{A^2\mu_q} = -i\,\tfrac{1}{2}(\overleftarrow{D^{3+}})^{\nu}\tilde{q}_1^{\dagger}\overline{\sigma}_{\mu\nu} - \tfrac{1}{4}\tilde{q}_1^{\dagger}\overline{\sigma}_{\mu}\not{D}^3 - \tfrac{1}{4}(\overleftarrow{D^{3+}})^{\mu}\tilde{q}_1^{\dagger}, \tag{B30}$$

$$\{M_{Aq}^{f}\}^{A^1\mu_q} = \tfrac{1}{2}(\overleftarrow{D^{3+}})^{\nu}\tilde{q}_1^{\dagger}\overline{\sigma}_{\mu\nu} - i\,\tfrac{1}{4}\tilde{q}_1^{\dagger}\overline{\sigma}_{\mu}\not{D}^3 - i\,\tfrac{1}{4}(\overleftarrow{D^{3+}})^{\mu}\tilde{q}_1^{\dagger}, \tag{B31}$$

$$\{M_{Aq}^{b}\}^{A^2\mu_q} = i\,\tfrac{1}{2}(\overleftarrow{D^{3+}})^{\nu}\tilde{q}_1^{\dagger}\overline{\sigma}_{\mu\nu} - \tfrac{1}{4}\tilde{q}_1^{\dagger}\overline{\sigma}_{\mu}\not{D}^3 - \tfrac{1}{4}(\overleftarrow{D^{3+}})^{\mu}\tilde{q}_1^{\dagger}, \tag{B32}$$

$$\{M_{Aq}^{b}\}^{B^1\nu\rho_q} = -i\,\tfrac{1}{2}\tilde{c}^3\tilde{q}_1^{\dagger}\overline{\sigma}^{\nu\rho} + \tfrac{1}{4}\tilde{B}^{3\nu\rho}\tilde{q}_1^{\dagger} + \tilde{B}^{3\rho}_{+\mu}\overline{\sigma}^{\mu\nu}\tilde{q}_1^{\dagger}, \tag{B33}$$

$$\{M_{Aq}^{b}\}^{B^2\nu\rho_q} = \tfrac{1}{2}\tilde{c}^3\tilde{q}_1^{\dagger}\overline{\sigma}^{\nu\rho} - i\,\tfrac{1}{4}\tilde{B}^{3\nu\rho}\tilde{q}_1^{\dagger} - \tilde{B}^{3}_{+\mu}{}^{\rho}\overline{\sigma}^{\mu\nu}\tilde{q}_1^{\dagger}, \tag{B34}$$

$$\{M_{Aq}^{f}\}^{B^1\nu\rho_q} = i\,\tfrac{1}{2}\tilde{c}^3\tilde{q}_1^{\dagger}\overline{\sigma}^{\nu\rho} + \tfrac{1}{4}\tilde{B}^{3\nu\rho}\tilde{q}_1^{\dagger} - i\tilde{B}^{3}_{+\mu}{}^{\rho}\overline{\sigma}^{\mu\nu}\tilde{q}_1^{\dagger}, \tag{B35}$$

$$\{M_{Aq}^{f}\}^{B^2\nu\rho_q} = -\tfrac{1}{2}\tilde{c}^3\tilde{q}_1^{\dagger}\overline{\sigma}^{\nu\rho} - i\,\tfrac{1}{4}\tilde{B}^{3\nu\rho}\tilde{q}_1^{\dagger} + \tilde{B}^{3}_{+\mu}{}^{\rho}\overline{\sigma}^{\mu\nu}\tilde{q}_1^{\dagger}, \tag{B36}$$

$$\{M_{Aq}^{b}\}^{c^1q} = i\,\tfrac{1}{2}\tilde{B}^{3\mu\nu}_{+}\overline{\sigma}_{\mu\nu}\tilde{q}_1^{\dagger} - \tfrac{1}{4}\tilde{c}^3\tilde{q}_1^{\dagger}, \tag{B37}$$

$$\{M_{Aq}^{b}\}^{c^2q} = -\tfrac{1}{2}\tilde{B}^{3\mu\nu}_{+}\overline{\sigma}_{\mu\nu}\tilde{q}_1^{\dagger} + i\,\tfrac{1}{4}\tilde{c}^3\tilde{q}_1^{\dagger}, \tag{B38}$$

$$\{M_{Aq}^{f}\}^{c^1q} = -i\,\tfrac{1}{2}\tilde{B}^{3\mu\nu}_{+}\overline{\sigma}_{\mu\nu}\tilde{q}_1^{\dagger} - \tfrac{1}{4}\tilde{c}^3\tilde{q}_1^{\dagger}, \tag{B39}$$

$$\{M_{Aq}^{f}\}^{c^2q} = \tfrac{1}{2}\tilde{B}^{3\mu\nu}_{+}\overline{\sigma}_{\mu\nu}\tilde{q}_1^{\dagger} + i\,\tfrac{1}{4}\tilde{c}^3\tilde{q}_1^{\dagger}. \tag{B40}$$

For (B29)–(B40), one can find the relation

$$\begin{pmatrix}\{M_{Aq}^{f}\}^{Y^1q}\\ \{M_{Aq}^{f}\}^{Y^2q}\end{pmatrix} = \begin{pmatrix}0 & i\\ -i & 0\end{pmatrix}\begin{pmatrix}\{M_{Aq}^{b}\}^{Y^1q}\\ \{M_{Aq}^{b}\}^{Y^2q}\end{pmatrix}. \tag{B41}$$

Using the explicit matrix elements (B20)–(B40), we can perform the path integral (B12) directly, instead of neglecting the nonkinetic off-diagonal part of $M^b(2)(M^f(2))$. Then we have a crucial obstacle from the difference between (B23) and (B24), while the obstacle from (B29)–(B40) is resolved by the relation (B41). This obstacle tells us that the contributions from (B23) and (B24) is not 1 and that the result (3.67) is effective up to order of square of $\tilde{q}_1$. (In fact, this problem does not appear when we treat adjoint matter instead of fundamental matter. Thus we think that this problem comes from the choice of the representation of matter fields.) However, the contributions from (B23) and (B24) becomes 1 in the $\tilde{q}_1 \to 0$ limit after path integration. Thus we estimate the contributions from (B23) and (B24) to be 1 in the case that the result $Z^t_{m,c,k}(2)$ in (3.67) is topological. This is why it is enough to estimate the path integral with the indices that only the kinetic terms in the diagonal block are counted from the big matrices in Sec. III.

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Inverse scattering for a Schrödinger equation with energy dependent potential

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In this article the inverse scattering problem of reconstructing the energy dependent potential $i\sqrt{E^2-m^2}\,P(x)+Q(x)$ of a Schrödinger equation on the line from its reflection coefficients and bound state data (i.e., poles of the transmission coefficients and associated norming constants) is solved using the Marchenko integral equation approach. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In this article we study the inverse scattering problem for the generalized 1-D Schrödinger equation,

$$\psi''(k,x)+[k^2+m^2]\psi(k,x)=[ikP(x)+Q(x)]\psi(k,x), \quad x\in\mathbb{R}, \tag{1.1}$$

where the prime denotes the derivative with respect to the spatial coordinate x, k is the wavenumber, m is a positive mass parameter, $P(x)$ describes the energy absorption or generation, and $Q(x)$ represents the restoring force density. The quantity $E=\sqrt{k^2+m^2}$ stands for the energy.

Letting $\mathbb{C}^+$ and $\mathbb{C}^-$ stand for the open upper and lower complex half-planes and defining the regions $\Omega^+=\mathbb{C}^+\backslash i\,[0,m]$ and $\Omega^-=\mathbb{C}^-\backslash i\,[-m,0]$, for a suitable choice of the square root one can use the mapping $E=\sqrt{k^2+m^2}$ to transform either of the regions $\Omega^\pm$ conformally and bijectively into either of the regions $\mathbb{C}^\pm$, thus yielding four transformations. Using the inverse transformation $k(E)=\sqrt{E^2-m^2}$ we obtain the two-fold Riemann surface with branch cuts along the real line from m to $+\infty$ and from $-m$ to $-\infty$. As we are interested primarily in the domain $E\in\mathbb{C}^+\cup\mathbb{R}$, it is natural to define $k(E)=\sqrt{E^2-m^2}$ as a single-valued continuous function of $E\in\mathbb{C}^+\cup\mathbb{R}$ with $(k(E)/E)>0$ for $E\in\mathbb{R}\backslash[-m,m]$, so that $\mathrm{Im}\,k(E)>0$ for $E\in(-m,m)$. We then write (1.1) in the equivalent form

$$\psi^\pm{}''(E,x)+E^2\psi^\pm(E,x)=[\pm i\,k(E)P(x)+Q(x)]\psi^\pm(E,x), \tag{1.2}$$

where $x\in\mathbb{R}$ and $E\in\overline{\mathbb{C}^+}$.

Let us define the Jost solutions $f_l^\pm(E,x)$ and $f_r^\pm(E,x)$ as the solutions of (1.2) with the $\pm$ sign in the first term of the right-hand side that satisfy the boundary conditions

$$\begin{aligned} f_l^\pm(E,x)&=e^{iEx}+o(1), \quad x\to+\infty,\\ f_r^\pm(E,x)&=e^{-iEx}+o(1), \quad x\to-\infty. \end{aligned} \tag{1.3}$$

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In terms of the Jost solutions, the scattering coefficients $a_l^{\pm}(E)$, $a_r^{\pm}(E)$, $b_l^{\pm}(E)$, and $b_r^{\pm}(E)$ are defined by

$$\begin{aligned} f_l^{\pm}(E,x) &= a_l^{\pm}(E)e^{iEx} + b_l^{\pm}(E)e^{-iEx} + o(1), \quad x \to -\infty, \\ f_r^{\pm}(E,x) &= a_r^{\pm}(E)e^{-iEx} + b_r^{\pm}(E)e^{iEx} + o(1), \quad x \to +\infty. \end{aligned} \tag{1.4}$$

In this article a fundamental role is played by the transformation

$$g_1(E) = \frac{g^+(E) + g^-(E)}{2}, \quad g_2(E) = \frac{g^+(E) - g^-(E)}{2ik(E)}, \tag{1.5}$$

between pairs of functions of E. This transformation allows one to convert the pair of uncoupled differential equations (1.2) into the coupled system of differential equations,

$$\begin{bmatrix} \psi_1''(E,x) \\ \psi_2''(E,x) \end{bmatrix} + E^2 \begin{bmatrix} \psi_1(E,x) \\ \psi_2(E,x) \end{bmatrix} = \Xi(E,x) \begin{bmatrix} \psi_1(E,x) \\ \psi_2(E,x) \end{bmatrix}, \tag{1.6}$$

where

$$\Xi(E,x) = \begin{bmatrix} Q(x) & -k(E)^2 P(x) \\ P(x) & Q(x) \end{bmatrix} \tag{1.7}$$

and $k(E)^2 = E^2 - m^2$. Transforming the Jost solutions as in (1.5), we obtain from (1.3) and (1.4),

$$\begin{aligned} f_{l1}(E,x) &= e^{iEx} + o(1), \quad f_{l2}(E,x) = o(1), \quad x \to +\infty, \\ f_{r1}(E,x) &= e^{-iEx} + o(1), \quad f_{r2}(E,x) = o(1), \quad x \to -\infty, \end{aligned} \tag{1.8}$$

$$\begin{aligned} f_{ls}(E,x) &= a_{ls}(E)e^{iEx} + b_{ls}(E)e^{-iEx} + o(1), \quad x \to -\infty, \\ f_{rs}(E,x) &= a_{rs}(E)e^{-iEx} + b_{rs}(E)e^{iEx} + o(1), \quad x \to +\infty, \end{aligned} \tag{1.9}$$

where $s = 1,2$.

The direct and inverse scattering problems for Schrödinger equations of the type (1.1) have been studied extensively. Jaulent and Jean[1–3] studied (1.1) with $m = 0$, imaginary $P(x)$ and real $Q(x)$, both on the half-line and on the full line (problems leading to unitary scattering data), and established the unique solvability of their Marchenko equations. Jaulent[4] derived Marchenko integral equations leading to the solution of the inverse problem for (1.1) with $m = 0$ and real potentials $P(x)$ and $Q(x)$. Sattinger and Szmigielski[5] studied (1.1) with $m = 0$, imaginary $P(x)$ and real $Q(x)$ and applied the results to solve a nonlinear evolution equation. Aktosun *et al.*[6,7] studied in detail the direct and inverse scattering problems for (1.2) for $m = 0$, obtained many results on the discrete eigenvalues, and gave sufficient conditions for the unique solvability of the Marchenko equations.

The more interesting case where $m > 0$, was taken up by Kaup[8,9] in connection with a nonlinear evolution equation (a long-wave water equation resembling the Boussinesq equation). In Ref. 9 a pair of coupled Marchenko integral equations was given to solve the inverse scattering problem. Under the assumption that $\int_{-\infty}^{\infty} dx\, P(x) = 0$, Sattinger and Szmigielski[10] considered the direct and inverse problems for (1.1) with $m = 1$ and C^{∞} potentials and applied their results to a nonlinear evolution equation. Equation (1.1), with $k^2 + m^2$ and $ikP(x)$ replaced by $k^2 - m^2$ and $kP(x)$, respectively, for real potentials $P(x)$ and $Q(x)$, is the 1-D Klein–Gordon equation. For this equation and on the half-line, Corinaldesi,[11] Degasperis,[12] and Weiss and Scharf[13] studied the inverse scattering problem and Pivovarchik[14] studied the number of bound states.

When $P,Q\in L^1(\mathbb{R})$, the Schrödinger operators in (1.2) have very different properties depending on whether $m=0$ or $m>0$, since for $m=0$ their essential spectrum is the set of $k\in\mathbb{R}$ whereas for $m>0$ it is the set of $k\in\mathbb{R}\cup i[-m,m]$. Moreover, as observed in Refs. 8 and 9, the $m>0$ equation is important for solving a certain system of nonlinear evolution equations by the inverse scattering transform, whereas no such connection is apparent for $m=0$.

In this article we analyze the inverse scattering problem for (1.2) by the Marchenko method. Essentially, although most of the scattering solutions and scattering coefficients are defined as in Refs. 6 and 7 where the $m=0$ case was treated, we differ from these papers in one important aspect: We also define the scattering solutions and scattering coefficients as if (1.6) were the equation of interest rather than (1.2). The Riemann–Hilbert problem relating the usual Faddeev solutions, as studied since the seminal papers by Faddeev[15] and Deift and Trubowitz,[16] and the Marchenko integral equations obtained by Fourier transformation are derived for quantities that are primarily connected with (1.6). The relationships between the two approaches are explained in detail. The advantage of the new approach lies in the behavior as $E\to\pm m$. In this case, (1.2) approaches two copies of the 1-D Schrödinger equation on the line with real potential $Q(x)$, whereas (1.6) tends to a nonselfadjoint matrix Schrödinger equation that also involves $P(x)$. In principle, this new approach could also have been applied to the case $m=0$, a possibility not observed before. It might then be comparatively easy to study the behavior of the solutions of (1.2) as $m\to 0^+$.

Let us discuss briefly some of the differences between Ref. 10 and the present paper. In Refs. 9 and 10 the E and k variables are transformed into the complex z variable by the conformal mapping $z=E+k=m^2/(E-k)$, where $m=1$ in Ref. 10. The complex z-plane is then divided into the regions $\mathcal{U}_+=\{z\in\mathbb{C}:|z|>m$ and $\mathrm{Im}\,z>0\}\cup\{z\in C:|z|<m$ and $\mathrm{Im}\,z<0\}$ and $\mathcal{U}_-=\{z\in\mathbb{C}:|z|>m$ and $\mathrm{Im}\,z<0\}\cup\{z\in C:|z|<m$ and $\mathrm{Im}\,z>0\}$, separated by $\Sigma=\{z\in\mathbb{C}:|z|=m\}\cup(\mathbb{R}\backslash\{0\})$. The inverse scattering problem is then posed as a vector Riemann–Hilbert problem on the curve Σ that relates vector functions analytic in $\mathcal{U}_-$ to vector functions analytic in $\mathcal{U}_+$. The unfamiliarity of the curve Σ, however, makes it hard to replace these Riemann–Hilbert problems by equivalent integral equations. For this reason we have decided not to use the z variable.

Let us now discuss the contents of this article. In Sec. II we introduce and study the scattering solutions and their asymptotic properties as $|E|\to\infty$. We also derive the continuity of the scattering solutions for (1.6) as $E\to\pm m$. In Sec. III we introduce and study the scattering coefficients and their asymptotics as $|E|\to\infty$. Their behavior as $E\to\pm m$ is also obtained. Their asymptotics as $E\to 0$ is found using the recent results in Ref. 17. It follows in particular that the scattering matrix is unitary if $E\in[-m,m]$, something that can also be derived from results in Ref. 10, and has certain contractivity and expansivity properties if $E\in\mathbb{R}\backslash[-m,m]$ and $P(x)$ does not change sign. In Sec. IV an idea by Weiss and Scharf[13] is employed to derive Marchenko integral equations for (1.6), both in the absence and in the presence of (finitely many) discrete eigenvalues. Any solution of one of the two coupled systems of two Marchenko integral equations allows one to uniquely determine the potentials $P(x)$ and $Q(x)$, provided the second one of the pair of functions being a solution has its values in $(-1,1)$. In Sec. V we relate, as in Ref. 7, the unique solvability of either of the systems of Marchenko equations to the existence of a canonical Wiener–Hopf factorization of a 2×2 matrix function on the line.

II. JOST SOLUTIONS AND FADDEEV FUNCTIONS

In this section we introduce various scattering solutions for (1.2) and (1.6) and study their symmetry and asymptotic properties.

A. Analyticity and symmetry properties

Let $P,Q\in L^1(\mathbb{R})$. Then the Jost solutions $f_l^{\pm}(E,x)$ and $f_r^{\pm}(E,x)$ satisfy the integral equations

$$f_l^{\pm}(E,x)=e^{iEx}+\frac{1}{E}\int_x^{\infty}dy\,\sin\{E(y-x)\}[\pm i\,k(E)P(y)+Q(y)]f_l^{\pm}(E,x); \tag{2.1}$$

$$f_r^{\pm}(E,x)=e^{-iEx}+\frac{1}{E}\int_{-\infty}^{x}dy\,\sin\{E(x-y)\}[\pm i\,k(E)P(y)+Q(y)]f_r^{\pm}(E,x). \tag{2.2}$$

Using the 2×2 matrix $\Xi(E,x)$ introduced in (1.7), these integral equations are easily transformed into the pairs of coupled integral equations,

$$\begin{bmatrix} f_{l1}(E,x)\\ f_{l2}(E,x)\end{bmatrix}=\begin{bmatrix}\cos(Ex)\\ \dfrac{\sin(Ex)}{k(E)}\end{bmatrix}+\int_x^{\infty}dy\,\frac{\sin\{E(y-x)\}}{E}\,\Xi(E,y)\begin{bmatrix} f_{l1}(E,y)\\ f_{l2}(E,y)\end{bmatrix};$$

$$\begin{bmatrix} f_{r1}(E,x)\\ f_{r2}(E,x)\end{bmatrix}=\begin{bmatrix}\cos(Ex)\\ \dfrac{\sin(Ex)}{k(E)}\end{bmatrix}+\int_{-\infty}^{x}dy\,\frac{\sin\{E(x-y)\}}{E}\,\Xi(E,y)\begin{bmatrix} f_{r1}(E,y)\\ f_{r2}(E,y)\end{bmatrix}.$$

Defining the Faddeev functions $m_l^{\pm}(E,x)$ and $m_r^{\pm}(E,x)$ by

$$m_l^{\pm}(E,x)=e^{-iEx}f_l^{\pm}(E,x),\quad m_r^{\pm}(E,x)=e^{iEx}f_r^{\pm}(E,x), \tag{2.3}$$

we get from (2.1) and (2.2) the Volterra integral equations,

$$m_l^{\pm}(E,x)=1+\int_x^{\infty}dy\,\frac{e^{2iE(y-x)}-1}{2iE}[\pm i\,k(E)P(y)+Q(y)]m_l^{\pm}(E,y); \tag{2.4}$$

$$m_r^{\pm}(E,x)=1+\int_{-\infty}^{x}dy\,\frac{e^{2iE(x-y)}-1}{2iE}[\pm i\,k(E)P(y)+Q(y)]m_r^{\pm}(E,y). \tag{2.5}$$

Using (1.5), these are transformed into the pairs of coupled integral equations:

$$\begin{bmatrix} m_{l1}(E,x)\\ m_{l2}(E,x)\end{bmatrix}=\begin{bmatrix}1\\0\end{bmatrix}+\int_x^{\infty}dy\,\frac{e^{2iE(y-x)}-1}{2iE}\,\Xi(E,y)\begin{bmatrix} m_{l1}(E,y)\\ m_{l2}(E,y)\end{bmatrix}; \tag{2.6}$$

$$\begin{bmatrix} m_{r1}(E,x)\\ m_{r2}(E,x)\end{bmatrix}=\begin{bmatrix}1\\0\end{bmatrix}+\int_{-\infty}^{x}dy\,\frac{e^{2iE(x-y)}-1}{2iE}\,\Xi(E,y)\begin{bmatrix} m_{r1}(E,y)\\ m_{r2}(E,y)\end{bmatrix}. \tag{2.7}$$

By differentiation with respect to x we obtain

$$\begin{bmatrix} m'_{l1}(E,x)\\ m'_{l2}(E,x)\end{bmatrix}=-\int_x^{\infty}dy\,e^{2iE(y-x)}\,\Xi(E,y)\begin{bmatrix} m_{l1}(E,y)\\ m_{l2}(E,y)\end{bmatrix}; \tag{2.8}$$

$$\begin{bmatrix} m'_{r1}(E,x)\\ m'_{r2}(E,x)\end{bmatrix}=\int_{-\infty}^{x}dy\,e^{2iE(x-y)}\,\Xi(E,y)\begin{bmatrix} m_{r1}(E,y)\\ m_{r2}(E,y)\end{bmatrix}. \tag{2.9}$$

In the next theorem we state the analyticity and continuity properties of $m_{ls}(E,x)$, $m_{rs}(E,x)$, $f_{ls}(E,x)$, $f_{rs}(E,s)$ and their derivatives ($s=1,2$). Such results will then also hold for $m_l^{\pm}(E,x)$, $m_r^{\pm}(E,x)$, $f_l^{\pm}(E,x)$, $f_r^{\pm}(E,x)$ and their derivatives.

Theorem 2.1: *Assume $P,Q\in L^1(\mathbb{R})$. Then the following is true.*

(1) For $x\in\mathbb{R}$ and $s=1,2$, the functions $m_{ls}(E,x)$, $m_{rs}(E,x)$, $m'_{ls}(E,x)$ and $m'_{rs}(E,x)$ are analytic in $\mathbb{C}^+$ and continuous in $\overline{\mathbb{C}^+}\backslash\{0\}$. Consequently, for each $x\in\mathbb{R}$ and $s=1,2$ the transformed Jost solutions $f_{ls}(E,x)$ and $f_{rs}(E,x)$ and their derivatives $f'_{ls}(E,x)$ and $f'_{rs}(E,x)$ are analytic in $\mathbb{C}^+$ and continuous in $\overline{\mathbb{C}^+}\backslash\{0\}$.

(2) If $P,Q\in L^1_1(\mathbb{R})$, the continuity of the functions in (i) *extends to $\overline{\mathbb{C}^+}$.*

Proof: Let $E \in \overline{\mathbb{C}^+}$. For large $|E|$ it is expedient to iterate the four integral equations (2.4) and (2.5) for $m_l^{\pm}(E,x)$ and $m_r^{\pm}(E,x)$, while it is more convenient to iterate the two systems (2.6) and (2.7) as $E \to \pm m$.

First, using the estimate

$$\sqrt{||E|^2-m^2|} \leqslant |k(E)| \leqslant \sqrt{|E|^2+m^2},$$

one obtains the auxiliary upper bounds:

$$\left|\frac{e^{2iE|y-x|}-1}{2iE}[\pm i\,k(E)P(y)+Q(y)]\right| \leqslant \begin{cases} 2|P(y)|+\dfrac{1}{m}|Q(y)|, & |E| \geqslant m, \\ (m\sqrt{2}\,|P(y)|+|Q(y)|)/|E|, & |E| \leqslant m, \\ |y-x|[m\sqrt{2}\,|P(y)|+|Q(y)|], & |E| \leqslant m. \end{cases}$$

In analogy with Refs. 15 and 16 we obtain the estimates

$$|m_l^{\pm}(E,x)| \leqslant \begin{cases} \exp\left(2\|P\|_1+\dfrac{1}{m}\|Q\|_1\right), & |E| \geqslant m, \\ \exp((m\sqrt{2}\,\|P\|_1+\|Q\|_1)/|E|), & |E| \leqslant m, \\ [1+\max(0,-x)]\exp(m\sqrt{2}\,\|P\|_{1,1}+\|Q\|_{1,1}), & |E| \leqslant m, \end{cases}$$

and hence

$$\max(|m_l^{\pm}(E,x)|,|m_r^{\pm}(E,x)) \leqslant c_2;$$

$$\max(|m_l^{\pm\prime}(E,x)|,|m_r^{\pm\prime}(E,x)|) \leqslant c_1c_2(\|P\|_1+\|Q\|_1)[1+|E|],$$

where $c_2 = e^{c_1(\|P\|_1+\|Q\|_1)/\min(1,|E|)}$ and $c_1 = \max(2,m\sqrt{2},1/m)$, as well as

$$|m_l^{\pm}(E,x)| \leqslant [1+\max(0,-x)]e^{c_1(\|P\|_{1,1}+\|Q\|_{1,1})}; \tag{2.10}$$

$$|m_l^{\pm\prime}(E,x)| \leqslant c_1c_3(\|P\|_1+\|Q\|_1)[1+|E|][1+\max(0,-x)], \tag{2.11}$$

where $c_3 = e^{c_1(\|P\|_{1,1}+\|Q\|_{1,1})}$. The proof for $m_r^{\pm}(E,x)$ and $m_r^{\pm\prime}(E,x)$, where (2.10) and (2.11) hold with $\max(0,-x)$ replaced by $\max(0,x)$, is similar.

Next, the derivation of the analyticity of $m_{ls}(E,x)$ and $m_{rs}(E,x)$ and their derivatives in a neighborhood of $\pm m$ in $\overline{\mathbb{C}^+}$ for $s=1,2$ is analogous. Here one employs the following estimate for the Euclidean norm of the matrix $\Xi(E,x)$:

$$\|\Xi(E,x)\| \leqslant 2|Q(x)|+(1+|k(E)|^2)|P(x)|,$$

which completes the proof. □

When $P,Q \in L_1^1(\mathbb{R})$, we find as $E \to 0$,

$$m_l^{\pm}(0,x) = 1+\int_x^{\infty} dy\,(y-x)[Q(y)\mp mP(y)]m_l^{\pm}(0,y); \tag{2.12}$$

$$m_r^{\pm}(0,x) = 1+\int_{-\infty}^{x} dy\,(x-y)[Q(y)\mp mP(y)]m_r^{\pm}(0,y). \tag{2.13}$$

Then (2.12) and (2.13) are the integral equations for the zero energy Jost functions of the usual 1-D Schrödinger equation with potential $Q(x)\mp mP(x)$. We will call $Q\mp mP$ an *exceptional* potential (for the usual Schrödinger equation) if there exists a nonzero (real) constant $\gamma^{\pm}$ such that

$$\gamma^{\pm}=\frac{m_l^{\pm}(0,x)}{m_r^{\pm}(0,x)}=\frac{f_l^{\pm}(0,x)}{f_r^{\pm}(0,x)}. \tag{2.14}$$

Otherwise $Q\mp mP$ is called a *generic* potential. Obviously, (2.12) and (2.13) can be transformed into the pairs of coupled integral equations

$$\begin{bmatrix} m_{l1}(0,x) \\ m_{l2}(0,x) \end{bmatrix}=\begin{bmatrix} 1 \\ 0 \end{bmatrix}+\int_x^{\infty} dy\,(y-x)\begin{bmatrix} Q(y) & m^2P(y) \\ P(y) & Q(y) \end{bmatrix}\begin{bmatrix} m_{l1}(0,y) \\ m_{l2}(0,y) \end{bmatrix};$$

$$\begin{bmatrix} m_{r1}(0,x) \\ m_{r2}(0,x) \end{bmatrix}=\begin{bmatrix} 1 \\ 0 \end{bmatrix}+\int_{-\infty}^{x} dy\,(x-y)\begin{bmatrix} Q(y) & m^2P(y) \\ P(y) & Q(y) \end{bmatrix}\begin{bmatrix} m_{r1}(0,y) \\ m_{r2}(0,y) \end{bmatrix}.$$

The complicated conjugation symmetry properties of $k(E)$ make it hazardous to state conjugation symmetry properties for $f_l^{\pm}(E,x)$, $f_r^{\pm}(E,x)$, $m_l^{\pm}(E,x)$, and $m_r^{\pm}(E,x)$ directly. However, since $k(-\overline{E})^2=\overline{k(E)^2}$, we immediately have for $s=1,2$,

$$\overline{f_{ls}(-\overline{E},x)}=f_{ls}(E,x), \quad \overline{f_{rs}(-\overline{E},x)}=f_{rs}(E,x), \tag{2.15}$$

and similarly for $m_{ls}(E,x)$ and $m_{rs}(E,x)$ where $s=1,2$. Now note that $(k(E)/E)>0$ for $E\in\mathbb{R}\backslash[-m,m]$ and $k(E)$ is positive imaginary for $E\in(-m,m)$. Thus $\overline{k(-\overline{E})}=-k(E)$ for $E\in\overline{\mathbb{C}^+}$. Using the identities $f_l^{\pm}(E,x)=f_{l1}(E,x)\pm ik(E)f_{l2}(E,x)$ and similarly for $f_r^{\pm}(E,x)$, we obtain

$$\overline{f_l^{\pm}(-\overline{E},x)}=f_l^{\pm}(E,x), \quad \overline{f_r^{\pm}(-\overline{E},x)}=f_r^{\pm}(E,x). \tag{2.16}$$

Similar relations hold for $m_l^{\pm}(E,x)$ and $m_r^{\pm}(E,x)$.

B. Large-*E* asymptotics

To study the large-E asymptotics of the Jost solutions, we define

$$\eta_l^{\pm}(E,x)=e^{\pm\zeta(x)}m_l^{\pm}(E,x)=e^{-iEx\pm\zeta(x)}f_l^{\pm}(E,x); \tag{2.17}$$

$$\eta_r^{\pm}(E,x)=e^{\pm p\mp\zeta(x)}m_l^{\pm}(E,x)=e^{iEx\pm p\mp\zeta(x)}f_r^{\pm}(E,x), \tag{2.18}$$

where

$$\zeta(x)=\frac{1}{2}\int_x^{\infty} dz\,P(z), \quad p=\frac{1}{2}\int_{-\infty}^{\infty} dz\,P(z). \tag{2.19}$$

Theorem 2.2: *Let $P,Q\in L^1(\mathbb{R})$. Then the following statements are true.*

(i) For each $x\in\mathbb{R}$, the functions $\eta_l^{\pm}(E,x)$ and $\eta_r^{\pm}(E,x)$ are analytic in $\mathbb{C}^+$, are continuous in $\overline{\mathbb{C}^+}\backslash\{0\}$, and we have for some constant C not depending on k and x,

$$|\eta_l^{\pm}(E,x)|\leq Ce^{C/|E|}, \quad |\eta_r^{\pm}(E,x)|\leq Ce^{C/|E|}, \quad E\in\overline{\mathbb{C}^+}\backslash\{0\}. \tag{2.20}$$

Further, as $|E|\to\infty$ in $\overline{\mathbb{C}^+}$ we have

$$\eta_l^{\pm}(E,x)=1+o(1), \quad \eta_r^{\pm}(E,x)=1+o(1); \tag{2.21}$$

$$\eta_l^{\pm\prime}(E,x)=o(E), \quad \eta_r^{\pm\prime}(E,x)=o(E). \tag{2.22}$$

(ii) If $P,Q\in L_1^1(\mathbb{R})$, the continuity of the functions in (i) *extends to $\overline{\mathbb{C}^+}$. Moreover, for $E\in\overline{\mathbb{C}^+}$ we have*

$$|\eta_l^{\pm}(E,x)|\leqslant C[1+\max(0,-x)],\quad |\eta_r^{\pm}(E,x)|\leqslant C[1+\max(0,x)].$$

Proof: Letting $z(E,x)=\eta_l^{\pm}(E,x)-1$, we obtain

$$z(E,x)=z_0(E,x)+\int_x^{\infty}dy\,\frac{e^{2iE(y-x)}-1}{2iE}e^{\pm[\zeta(x)-\zeta(y)]}[\pm i\,k(E)P(y)+Q(y)]z(E,y), \tag{2.23}$$

where

$$z_0(E,x)=\int_x^{\infty}dy\,\frac{e^{2iE(y-x)}-1}{2iE}e^{\pm[\zeta(x)-\zeta(y)]}Q(y)$$
$$\pm\frac{k(E)}{2E}\int_x^{\infty}dy\,e^{2iE(y-x)}e^{\pm[\zeta(x)-\zeta(y)]}P(y)+\left(1-\frac{k(E)}{E}\right)[e^{\pm\zeta(x)}-1].$$

Then the Riemann–Lebesgue lemma implies that $\sup_{t\geqslant x}|z_0(E,t)|$ vanishes as $E\to\pm\infty$. Iterating (2.23) we now see that $z(E,x)$ is uniformly bounded in $\overline{\mathbb{C}^+}$ for $|E|\geqslant a>0$ for each $x\in\mathbb{R}$ and $a>0$. Using a Phragmen–Lindelöf theorem (cf. Ref. 18) we conclude that $z(E,x)$ vanishes as $E\to\infty$ in $\overline{\mathbb{C}^+}$.

To prove (2.22) we introduce the function

$$\xi_l^{\pm}(E,x)=\frac{1}{iE}m_l^{\pm\prime}(E,x)e^{\pm\zeta(x)}=\frac{1}{2iE}[\pm P(x)\,\eta_l^{\pm}(E,x)+2\,\eta_l^{\pm\prime}(E,x)].$$

From (2.8) and (2.17) we get

$$\xi_l^{\pm}(E,x)=\int_x^{\infty}dy\,e^{2iE(y-x)}\left[\mp\frac{k(E)}{E}P(y)+\frac{i}{E}Q(y)\right]e^{\pm[\zeta(x)-\zeta(y)]}\eta_l^{\pm}(E,y). \tag{2.24}$$

Thus, using (2.20), we see that the integrand on the right-hand side of (2.24) is bounded by the integrable function $C_a[|P(y)|+|Q(y)|]$, uniformly in $x\in\mathbb{R}$ and $E\in\overline{\mathbb{C}^+}$ for $|E|\geqslant a>0$ and each $a>0$, where the constant C_a does not depend on x and E. By the Riemann–Lebesgue lemma, we conclude that the right-hand side of (2.24) is $o(1)$ as $E\to\pm\infty$, so that by a Phragmen–Lindelöf theorem (cf. Ref. 18) we see that the left-hand side of (2.24) is $o(1)$ as $E\to\infty$ in $\overline{\mathbb{C}^+}$. Consequently, $\xi_l^{\pm}(E,x)=o(1)$ as $E\to\infty$ in $\overline{\mathbb{C}^+}$, which implies (2.22) for $\eta_l^{\pm\prime}(E,x)$. The proof for $\eta_r^{\pm}(E,x)$ and $\eta_r^{\pm\prime}(E,x)$ is similar. □

To study the inverse scattering problem for (1.2), as in Ref. 7 we strengthen Theorem 2.2 by making additional assumptions on P and Q. In fact, we assume that P is absolutely continuous, and define the two auxiliary potential functions,

$$W^{\pm}(x)=Q(x)\mp\tfrac{1}{2}P'(x)-\tfrac{1}{4}P(x)^2. \tag{2.25}$$

Using (1.2)–(1.4) we obtain for $x\in\mathbb{R}$,

$$\eta_l^{\pm\prime\prime}(E,x)+[2iE\pm P(x)]\eta_l^{\pm\prime}(E,x)=[W^{\pm}(x)\mp i(E-k(E))P(x)]\eta_l^{\pm}(E,x), \tag{2.26}$$

$$\eta_l^{\pm}(E,+\infty)=1,\quad \eta_l^{\pm\prime}(E,+\infty)=0, \tag{2.27}$$

where $W^{\pm}(x)$ is given by (2.25). Multiplying (2.26) by $\mu_l^{\pm}(E,x)=e^{2iEx\mp 2\zeta(x)}$, we obtain for $x\in\mathbb{R}$,

$$[\mu_l^{\pm}(E,x)\ \eta_l^{\pm\prime}(E,x)]'=\mu_l^{\pm}(E,x)\,[W^{\pm}(x)\mp i(E-k(E))P(x)]\,\eta_l^{\pm}(E,x). \tag{2.28}$$

Integrating (2.28) and using (2.27) we get

$$\eta_l^{\pm\prime}(E,x)=-\int_x^{\infty}dy\,e^{2iE(y-x)\pm\int_x^y d\hat{z}\,P(\hat{z})}[W^{\pm}(y)\mp i(E-k(E))P(y)]\,\eta_l^{\pm}(E,y). \tag{2.29}$$

Integrating (2.29), using (2.27) once again and changing the order of integration, we find

$$\eta_l^{\pm}(E,x)=1+\int_x^{\infty}dy\,G_l^{\pm}(E;x,y)[W^{\pm}(y)\mp i(E-k(E))P(y)]\,\eta_l^{\pm}(E,y), \tag{2.30}$$

where we have defined

$$\begin{aligned}G_l^{\pm}(E;x,y)&=\int_x^y dz\,e^{2iE(y-z)\pm\int_z^y d\hat{z}\,P(\hat{z})}\\&=\frac{1}{2iE}[e^{2iE(y-x)\pm\int_x^y d\hat{z}\,P(\hat{z})}-1]\mp\frac{1}{2iE}\int_x^y dz\,P(z)\,e^{2iE(y-z)\pm\int_z^y d\hat{z}\,P(\hat{z})}.\end{aligned} \tag{2.31}$$

Similarly, using (1.2)–(1.4), (2.17)–(2.19), and (2.25) we obtain

$$\eta_r^{\pm\prime\prime}(E,x)-[2iE\pm P(x)]\,\eta_r^{\pm\prime}(E,x)=[W^{\mp}(x)\pm i(E-k(E))P(x)]\,\eta_r^{\pm}(E,x), \tag{2.32}$$

$$\eta_r^{\pm}(E,-\infty)=1,\quad \eta_r^{\pm\prime}(E,-\infty)=0. \tag{2.33}$$

Integrating (2.32) twice and using (2.33) we first get

$$\eta_r^{\pm\prime}(E,x)=\int_{-\infty}^x dy\,e^{2iE(x-y)\pm\int_y^x d\hat{z}\,P(\hat{z})}[W^{\mp}(y)\pm i(E-k(E))P(y)]\,\eta_r^{\pm}(E,y),$$

and subsequently

$$\eta_r^{\pm}(E,x)=1+\int_{-\infty}^x dy\,G_r^{\pm}(E;x,y)\,[W^{\mp}(y)\pm i(E-k(E))P(y)]\,\eta_r^{\pm}(E,y), \tag{2.34}$$

where we have defined

$$\begin{aligned}G_r^{\pm}(E;x,y)&=\int_y^x dz\,e^{2iE(z-y)\pm\int_y^z d\hat{z}\,P(\hat{z})}\\&=\frac{1}{2iE}[e^{2iE(x-y)\pm\int_y^x P(z)dz}-1]\pm\frac{1}{2iE}\int_y^x dz\,P(z)\,e^{2iE(z-y)\pm\int_y^z d\hat{z}\,P(\hat{z})}.\end{aligned}$$

Let us now employ the integral equations (2.30) and (2.34) to derive asymptotic expressions for $\eta_l^{\pm}(E,x)$ and $\eta_r^{\pm}(E,x)$ as $E\to\infty$ in $\overline{\mathbb{C}^+}$.

Theorem 2.3: *(1) Assume $P\in L^1(\mathbb{R})$ and $Q\in L_1^1(\mathbb{R})$. Then, for each fixed $x\in\mathbb{R}$, the functions $\eta_l^{\pm}(E,x)$ and $\eta_r^{\pm}(E,x)$ are analytic in $\mathbb{C}^+$ and continuous in $\overline{\mathbb{C}^+}$, and*

$$\eta_l^{\pm}(E,x)=1+o(1),\quad \eta_r^{\pm}(E,x)=1+o(1),\quad E\to\infty \text{ in } \overline{\mathbb{C}^+}.$$

(2) Assume that $W^+,W^-\in L^1(\mathbb{R})$. Then as $E\to\infty$ in $\overline{\mathbb{C}^+}$ we have

$$\eta_l^{\pm}(E,x)=1+O(1/|E|),\quad \eta_r^{\pm}(E,x)=1+O(1/|E|). \tag{2.35}$$

(3) If further we assume $P \in L_1^1(\mathbb{R})$, $Q \in L_2^1(\mathbb{R})$ *and* $W^{\pm} \in L_1^1(\mathbb{R})$, *then*

$$\eta_l^{\pm}(E,x) = 1 - \frac{\int_x^{\infty} dz\, W^{\pm}(z)}{2iE} + O(1/|E|^2), \quad E \to \infty \text{ in } \overline{\mathbb{C}^+}, \tag{2.36}$$

$$\eta_r^{\pm}(E,x) = 1 - \frac{\int_{-\infty}^{x} dz\, W^{\mp}(z)}{2iE} + O(1/|E|^2), \quad E \to \infty \text{ in } \overline{\mathbb{C}^+}. \tag{2.37}$$

Proof: We only prove (2.35), (2.36) and (2.37), because the rest of the proof is given in Theorem 3.1 of Ref. 6. Note that (2.31) implies for $y \geqslant x$,

$$|G_l^{\pm}(E;x,y)| \leqslant \frac{C}{|E|}, \quad E \in \overline{\mathbb{C}^+} \backslash \{0\}, \tag{2.38}$$

where $C = \frac{1}{2}(1 + (1 + ||P||_1)e^{||P||_1})$. Thus, iterating (2.30) and using (2.38) we obtain

$$|\eta_l^{\pm}(E,x) - 1| \leqslant \frac{C}{|E|}\left[\int_x^{\infty} dt\, (|W^{\pm}(t)| + m|P(t)|)\right] \exp\left(\int_x^{\infty} dz\, (|W^{\pm}(z)| + m|P(z)|)\right),$$

where $E \in \overline{\mathbb{C}^+} \backslash \{0\}$ and $|E| \geqslant m$. This implies (2.35) for $\eta_l^{\pm}(E,x)$ whenever $W^{\pm} \in L^1(\mathbb{R})$. The proof of (2.35) for $\eta_r^{\pm}(E,x)$ is obtained in a similar manner. To prove (2.36) we obtain from (2.30),

$$\begin{aligned}\eta_l^{\pm}(E,x) = 1 &+ \int_x^{\infty} dy\, G_l^{\pm}(E;x,y)[W^{\pm}(y) \mp i(E - k(E))P(y)] \\ &+ \int_x^{\infty} dy\, G_l^{\pm}(E;x,y)[W^{\pm}(y) \mp i(E - k(E))P(y)] \\ &\times \int_y^{\infty} dz\, G_l^{\pm}(E;y,z)[W^{\pm}(z) \mp i(E - k(E))P(z)]\eta_l^{\pm}(E,z).\end{aligned} \tag{2.39}$$

Using (2.36) and the inequality

$$|E - k(E)| \leqslant \frac{m^2}{|E|}, \quad |E| \geqslant m,$$

we obtain from (2.39),

$$\eta_l^{\pm}(E,x) = 1 + \int_x^{\infty} dy\, G_l^{\pm}(E;x,y)W^{\pm}(y) + O\left(\frac{1}{|E|^2}\right), \tag{2.40}$$

as $E \to \infty$ in $\overline{\mathbb{C}^+}$. Substituting (2.31) into (2.40) and integrating by parts we obtain (2.36). The proof of (2.37) is analogous. □

III. SCATTERING COEFFICIENTS

In this section we introduce various scattering coefficients as well as the scattering matrix for (1.2) and (1.6) and study their symmetry, asymptotic and unitarity and contractivity properties.

A. Wronskian relations and symmetry properties

Let $[f;g] = fg' - f'g$ denote the Wronskian. Then from (1.3) and (1.4) as $x \to \pm\infty$ we get

$$[f_l^{\pm}(E,x); f_r^{\pm}(E,x)] = -2iEa_l^{\pm}(E) = -2iEa_r^{\pm}(E), \tag{3.1}$$

where (3.1) holds for $E\in\overline{\mathbb{C}^+}$. Consequently, $a_l^{\pm}(E)=a_r^{\pm}(E)$, which we now denote by $a^{\pm}(E)$. From (1.8) and (1.9) we now easily obtain

$$\overline{a_s(-\overline{E})}=a_s(E),\quad E\in\overline{\mathbb{C}^+};\tag{3.2}$$

$$\overline{b_{ls}(-E)}=b_{ls}(E),\quad \overline{b_{rs}(-E)}=b_{rs}(E),\quad E\in\mathbb{R},\tag{3.3}$$

where $s=1,2$. Using (1.3), (1.4), and (2.16) we easily obtain

$$\overline{a^{\pm}(-\overline{E})}=a^{\pm}(E),\quad E\in\overline{\mathbb{C}^+};\tag{3.4}$$

$$\overline{b_l^{\pm}(-E)}=b_l^{\pm}(E),\quad \overline{b_r^{\pm}(-E)}=b_r^{\pm}(E),\quad E\in\mathbb{R}.\tag{3.5}$$

Next, if one assumes that $a^{\pm}(E)\neq 0$ and defines the transmission coefficients by $T^{\pm}(E)=a^{\pm}(E)^{-1}$, the reflection coefficients from the left by $L^{\pm}(E)=b_l^{\pm}(E)/a^{\pm}(E)$, and the reflection coefficients from the right by $R^{\pm}(E)=b_r^{\pm}(E)/a^{\pm}(E)$, then, if $P,Q\in L^1(\mathbb{R})$ [$P,Q\in L_1^1(\mathbb{R})$, respectively], the function $Ea^{\pm}(E)=E/T^{\pm}(E)$ is analytic in $\mathbb{C}^+$ and continuous in $\overline{\mathbb{C}^+}\backslash\{0\}$ [$\overline{\mathbb{C}^+}$, respectively] and the functions $Eb_l^{\pm}(E)=EL^{\pm}(E)/T^{\pm}(E)$ and $Eb_r^{\pm}(E)=ER^{\pm}(E)/T^{\pm}(E)$ are continuous in $\mathbb{R}\backslash\{0\}$ [$\mathbb{R}$, respectively]. In terms of the reflection and transmission coefficients we define the scattering matrix by

$$\mathbf{S}^{\pm}(E)=\begin{bmatrix}T^{\pm}(E) & R^{\pm}(E)\\ L^{\pm}(E) & T^{\pm}(E)\end{bmatrix}.\tag{3.6}$$

Let $E\in\mathbb{R}\backslash[-m,m]$. Then $k(-E)=-k(E)$ is real. Thus $f_l^{\pm}(E,x)$, $f_r^{\pm}(E,x)$, $f_l^{\mp}(-E,x)$ and $f_r^{\mp}(-E,x)$ all satisfy (1.2) and hence their Wronskians are independent of x. Using (1.3) and (1.4) we get

$$[f_l^{\pm}(E,x);f_l^{\mp}(-E,x)]=-2iE=-2iE[a_l^{\pm}(E)a_l^{\mp}(-E)-b_l^{\pm}(E)b_l^{\mp}(-E)],$$

$$[f_l^{\pm}(E,x);f_r^{\mp}(-E,x)]=-2iEb_r^{\mp}(-E)=2iEb_l^{\pm}(E),$$

$$[f_r^{\pm}(E,x);f_l^{\mp}(-E,x)]=-2iEb_r^{\pm}(E)=2iEb_l^{\mp}(-E),$$

$$[f_r^{\pm}(E,x);f_r^{\mp}(-E,x)]=2iE[a_r^{\pm}(E)a_r^{\mp}(-E)-b_r^{\pm}(E)b_r^{\mp}(-E)]=2iE,$$

where the behavior as $x\to+\infty$ is given first and then the behavior as $x\to-\infty$. As a result, we get

$$\mathbf{S}^{\pm}(E)^{-1}=\mathbf{S}^{\mp}(-E).\tag{3.7}$$

From (1.3), (1.4), and (3.6) we obtain

$$\begin{bmatrix}f_l^{\mp}(-E,x)\\ -f_r^{\mp}(-E,x)\end{bmatrix}=\mathbf{S}^{\pm}(E)\begin{bmatrix}f_r^{\pm}(E,x)\\ -f_l^{\pm}(E,x)\end{bmatrix}.\tag{3.8}$$

Let $E\in(-m,m)$. Then $k(-E)=k(E)$ is positive imaginary. Thus $f_l^{\pm}(E,x)$, $f_r^{\pm}(E,x)$, $f_l^{\pm}(-E,x)$ and $f_r^{\pm}(-E,x)$ all satisfy (1.2) and hence their Wronskians are independent of x. Using (1.3) and (1.4) we get

$$[f_l^{\pm}(E,x);f_l^{\pm}(-E,x)]=-2iE=-2iE[a_l^{\pm}(E)a_l^{\pm}(-E)-b_l^{\pm}(E)b_l^{\pm}(-E)],$$

$$[f_l^{\pm}(E,x);f_r^{\pm}(-E,x)]=-2iEb_r^{\pm}(-E)=2iEb_l^{\pm}(E),$$

$$[f_r^{\pm}(E,x);f_l^{\pm}(-E,x)]=-2iEb_r^{\pm}(E)=2iEb_l^{\pm}(-E),$$

$$[f_r^{\pm}(E,x);f_r^{\pm}(-E,x)]=2iE[a_r^{\pm}(E)a_r^{\pm}(-E)-b_r^{\pm}(E)b_r^{\pm}(-E)]=2iE,$$

where the behavior as $x\to+\infty$ is given first and then the behavior as $x\to-\infty$. As a result, we get

$$\mathbf{S}^{\pm}(E)^{-1}=\mathbf{S}^{\pm}(-E). \tag{3.9}$$

From (1.3), (1.4), and (3.6) we obtain

$$\begin{bmatrix} f_l^{\pm}(-E,x) \\ -f_r^{\pm}(-E,x) \end{bmatrix}=\mathbf{S}^{\pm}(E)\begin{bmatrix} f_r^{\pm}(E,x) \\ -f_l^{\pm}(E,x) \end{bmatrix}. \tag{3.10}$$

When $E\in\{-m,m\}$, the $\pm$ equations (1.2) are identical and the boundary conditions (1.3) do not distinguish between the $\pm$ versions of (1.2). It then follows that

$$f_{l1}(m,x)=f_l^{+}(m,x)=f_l^{-}(m,x),\quad f_{l1}(-m,x)=f_l^{+}(-m,x)=f_l^{-}(-m,x),$$

$$f_{r1}(m,x)=f_r^{+}(m,x)=f_r^{-}(m,x),\quad f_{r1}(-m,x)=f_r^{+}(-m,x)=f_r^{-}(-m,x),$$

which implies

$$a_1(m)=a^{+}(m)=a^{-}(m),\quad a_1(-m)=a^{+}(-m)=a^{-}(-m),$$

$$b_{l1}(m)=b_l^{+}(m)=b_l^{-}(m),\quad b_{l1}(-m)=b_l^{+}(-m)=b_l^{-}(-m),$$

$$b_{r1}(m)=b_r^{+}(m)=b_r^{-}(m),\quad b_{r1}(-m)=b_r^{+}(-m)=b_r^{-}(-m).$$

Hence, $\mathbf{S}^{+}(m)=\mathbf{S}^{-}(m)$ and $\mathbf{S}^{+}(-m)=\mathbf{S}^{-}(-m)$ are both unitary matrices, provided $a_1(m)=\overline{a_1(-m)}\neq 0$. The behavior of $a_2(E)$, $b_{l2}(E)$, and $b_{r2}(E)$ as $E\to\pm m$ will be given by (3.20).

Finally, for $E\in\mathbb{R}\backslash\{-m,m\}$ and under the assumption that $a^{\pm}(E)\neq 0$ for every $E\in\mathbb{R}$, we introduce the modified scattering matrix,

$$\tilde{\mathbf{S}}(E)=\tilde{\mathbf{M}}(E)[\mathbf{S}^{+}(E)\oplus\mathbf{S}^{-}(E)]\tilde{\mathbf{M}}(E)^{-1}, \tag{3.11}$$

where

$$\tilde{\mathbf{M}}(E)=\frac{1}{2ik(E)}\begin{bmatrix} ik(E) & 0 & ik(E) & 0 \\ 0 & ik(E) & 0 & ik(E) \\ 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix};$$

$$\tilde{\mathbf{M}}(E)^{-1}=\begin{bmatrix} 1 & 0 & ik(E) & 0 \\ 0 & 1 & 0 & ik(E) \\ 1 & 0 & -ik(E) & 0 \\ 0 & 1 & 0 & -ik(E) \end{bmatrix}.$$

Using that

$$\tilde{\mathbf{S}}(E)=\begin{bmatrix} T_1(E) & R_1(E) & -k(E)^2T_2(E) & -k(E)^2R_2(E) \\ L_1(E) & T_1(E) & -k(E)^2L_2(E) & -k(E)^2T_2(E) \\ T_2(E) & R_2(E) & T_1(E) & R_1(E) \\ L_2(E) & T_2(E) & L_1(E) & T_1(E) \end{bmatrix}, \tag{3.12}$$

we obtain from (3.8) and (3.10) the following Riemann–Hilbert problem valid for both $E\in\mathbb{R}\backslash[-m,m]$ and $E\in(-m,m)$:

$$\begin{bmatrix} f_{l1}(-E,x) \\ -f_{r1}(-E,x) \\ f_{l2}(-E,x) \\ -f_{r2}(-E,x) \end{bmatrix} = \tilde{\mathbf{S}}(E) \begin{bmatrix} f_{r1}(E,x) \\ -f_{l1}(E,x) \\ f_{r2}(E,x) \\ -f_{l2}(E,x) \end{bmatrix}. \tag{3.13}$$

One easily proves that $\tilde{\mathbf{S}}(E)^{-1} = \tilde{\mathbf{S}}(-E)$, both for $E \in (-m,m)$ and for $E \in \mathbb{R}\backslash[-m,m]$.

B. Various asymptotic properties

Theorem 3.1: *Let $P,Q \in L^1(\mathbb{R})$. Then*

$$a^{\pm}(E)e^{\pm p} = 1 + O\left(\frac{1}{|E|}\right), \quad E \to \infty \ \text{ in } \ \overline{\mathbb{C}^+}; \tag{3.14}$$

$$b_r^{\pm}(E) = O\left(\frac{1}{|E|}\right), \quad b_l^{\pm}(E) = O\left(\frac{1}{|E|}\right), \quad E \to \pm\infty, \tag{3.15}$$

where p is defined by (2.19).

Proof: From (3.1) we obtain

$$2iEa^{\pm}(E)e^{\pm p} = [2iE \pm P(x)]\eta_l^{\pm}(E,x)\eta_r^{\pm}(E,x) + \eta_l^{\pm\prime}(E,x)\eta_r^{\pm}(E,x) - \eta_l^{\pm}(E,x)\eta_r^{\pm\prime}(E,x). \tag{3.16}$$

Now (3.14) follows from (2.21), (2.22), and (3.16). Similarly, (3.15) follows with the help of

$$-2iEb_r^{\pm}(E) = e^{-2iEx \mp p \pm 2\zeta(x)}[\eta_l^{\pm}(E,x); \eta_l^{\mp}(-E,x)], \tag{3.17}$$

and the analogous expression involving $b_l^{\pm}(E)$. □

Let us now consider the low energy asymptotics of the scattering coefficients. From Ref. 17 we get the following result, depending on whether we are in the generic or in the exceptional case. We let $f_l^{\pm}(0,x)$ and $f_r^{\pm}(0,x)$ stand for the zero energy Jost functions of the usual 1-D Schrödinger equation with potential $Q(x) \mp mP(x)$ and $\gamma^{\pm}$ for the quantity given by (2.14).

Using Theorem 2.2 of Ref. 17, with $F(k) = k^2 + m^2$, $k_0 = im$, $\mathcal{S} = \{k \in \overline{\mathbb{C}^+} : |k - im| \leqslant m\}$ and $\mathcal{P}(k_0) = i[0,m]$, we easily obtain the following result.

Proposition 3.2: Suppose $P,Q \in L_1^1(\mathbb{R})$.

(i) In the generic case we have

$$\begin{aligned} T^{\pm}(E) &= -\frac{2iE}{[f_l^{\pm}(0,\cdot); f_r^{\pm}(0,\cdot)]} + o(E), \quad E \to 0 \ \text{ in } \ \overline{\mathbb{C}^+}, \\ L^{\pm}(E) &= -1 + o(1), \ R^{\pm}(E) = -1 + o(1), \quad E \to 0 \ \text{ in } \ \mathbb{R}. \end{aligned} \tag{3.18}$$

(ii) In the exceptional case we have

$$T^{\pm}(0) = \frac{2\gamma^{\pm}}{\gamma^{\pm 2} + 1}, \quad L^{\pm}(0) = \frac{\gamma^{\pm 2} - 1}{\gamma^{\pm 2} + 1}, \quad R^{\pm}(0) = \frac{1 - \gamma^{\pm 2}}{\gamma^{\pm 2} + 1}. \tag{3.19}$$

Finally, we consider the behavior of the scattering coefficients as $E \to \pm m$ in $\overline{\mathbb{C}^+}$.

Propositon 3.3: Let $P \in L_1^1(\mathbb{R})$ and $Q \in L_2^1(\mathbb{R})$. Then the expressions

$$\frac{a^+(E) - a^-(E)}{k(E)}, \quad \frac{b_l^+(E) - b_l^-(E)}{k(E)}, \quad \frac{b_r^+(E) - b_r^-(E)}{k(E)}, \tag{3.20}$$

have finite limits as $E\to\pm m$, $E\in\overline{\mathbb{C}^+}$.

Proof: From (1.4), (2.3), (2.6), and (2.7) we have

$$\begin{bmatrix}a_1(E)\\ a_2(E)\end{bmatrix}=\begin{bmatrix}1\\0\end{bmatrix}-\frac{1}{2iE}\int_{-\infty}^{\infty}dy\,\Xi(E,y)\begin{bmatrix}m_{l1}(E,y)\\ m_{l2}(E,y)\end{bmatrix}$$

$$=\begin{bmatrix}1\\0\end{bmatrix}-\frac{1}{2iE}\int_{-\infty}^{\infty}dy\,\Xi(E,y)\begin{bmatrix}m_{r1}(E,y)\\ m_{r2}(E,y)\end{bmatrix};$$

$$\begin{bmatrix}b_{l1}(E)\\ b_{l2}(E)\end{bmatrix}=\frac{1}{2iE}\int_{-\infty}^{\infty}dy\,e^{2iEy}\Xi(E,y)\begin{bmatrix}m_{l1}(E,y)\\ m_{l2}(E,y)\end{bmatrix};$$

$$\begin{bmatrix}b_{r1}(E)\\ b_{r2}(E)\end{bmatrix}=\frac{1}{2iE}\int_{-\infty}^{\infty}dy\,e^{-2iEy}\Xi(E,y)\begin{bmatrix}m_{r1}(E,y)\\ m_{r2}(E,y)\end{bmatrix},$$

where the limits as $E\to\pm m$ from $\overline{\mathbb{C}^+}$ exist. □

When $1/T^+(E)$ and $1/T^-(E)$ have a (necessarily common) nonzero limit as $E\to\pm m$, the next corollary is a restatement of Proposition 3.3.

Corollary 3.4: Let $P\in L_1^1(\mathbb{R})$ *and* $Q\in L_2^1(\mathbb{R})$ *and suppose* $1/T^+(E)$ *and* $1/T^-(E)$ *have a nonzero limit as* $E\to\pm m$ *in* $\overline{\mathbb{C}^+}$. *Then the expressions*

$$\frac{T^+(E)-T^-(E)}{k(E)},\quad \frac{L^+(E)-L^-(E)}{k(E)},\quad \frac{R^+(E)-R^-(E)}{k(E)},$$

have finite limits. Hence, $T_2(E)=[T^+(E)-T^-(E)]/2ik(E)$ *and the analogous quantities* $R_2(E)$ *and* $L_2(E)$ *are continuous in* $E\in\mathbb{R}$ *if* $T^\pm(E)$ *is continuous in* $E\in\mathbb{R}$.

Proposition 3.5: Assume $P\in L_1^1(\mathbb{R})$, $Q\in L_2^1(\mathbb{R})$, *and* $W^\pm\in L_1^1(\mathbb{R})$, *and let* $T^+(E)$ *and* $T^-(E)$ *be continuous in* $E\in\mathbb{R}$. *Then the functions* $L_1(E)$, $L_2(E)$, $k(E)^2L_2(E)$, $R_1(E)$, $R_2(E)$, *and* $k(E)^2R_2(E)$ *belong to* $L^2(\mathbb{R})$.

Proof: In view of Corollary 3.4 and the continuity of $T^\pm(E)$ in $E\in\mathbb{R}$, it suffices to study the asymptotic behavior of the above functions as $E\to\pm\infty$. From (2.36) and (2.37) we have as $E\to\pm\infty$,

$$\eta_l^{\pm\prime}(E,x)=\frac{W^\pm(x)}{2iE}+O\left(\frac{1}{|E|^2}\right),\quad \eta_r^{\pm\prime}(E,x)=-\frac{W^\mp(x)}{2iE}+O\left(\frac{1}{|E|^2}\right).$$

Using (3.17) we find

$$b_r^\pm(E)=\frac{R^\pm(E)}{T^\pm(E)}=O\left(\frac{1}{|E|^2}\right),$$

and similarly for $L^\pm(E)/T^\pm(E)$. On the other hand, using (3.16) we get

$$T^\pm(E)=e^{\pm p}\left\{1+\frac{\int_{-\infty}^{\infty}dz\,W^\pm(z)}{2iE}+O\left(\frac{1}{|E|^2}\right)\right\},$$

whence

$$R^\pm(E)=O\left(\frac{1}{|E|^2}\right).$$

A similar asymptotic expression can be derived for $L^\pm(E)$. This expression implies that $L_1(E)$, $L_2(E)$, and $k(E)^2L_2(E)$ belong to $L^2(\mathbb{R})$. □

C. Unitarity and contractivity properties

Let $E\in(-m,m)$. Then (1.2) is a pair of 1-D Schrödinger equations with real potentials and hence the scattering matrix $\mathbf{S}^{\pm}(E)$ is unitary (cf. Refs. 15 and 16). As a result, the reflection and transmission coefficients $R^{\pm}(E)$, $L^{\pm}(E)$, and $T^{\pm}(E)$ are continuous in $E\in(-m,m)$.

Let $E\in\mathbb{R}\backslash[-m,m]$. Observe that if $\psi(E,x)$ is a solution of the $\pm$ version of (1.2) and $\varphi(E,x)$ of the $\mp$ version of (1.2), then

$$\frac{d}{dx}[\psi(E,x);\varphi(E,x)]=\mp 2ik(E)P(x)\psi(E,x)\varphi(E,x). \tag{3.21}$$

Hence two expressions of the Wronskian of $\psi(E,x)$ and $\varphi(E,x)$ can be found by examining their value as $x\to\pm\infty$ and integrating with respect to x. Using (2.16), (3.4), (3.5), and (3.21) we get

$$[f_l^{\pm}(E,x);f_l^{\pm}(-E,x)] =\begin{cases} -2iE\pm 2ik(E)\displaystyle\int_x^{\infty} dy\, P(y)|f_l^{\pm}(E,y)|^2; \\ -2iE[|a^{\pm}(E)|^2-|b_l^{\pm}(E)|^2]\mp 2ik(E)\displaystyle\int_{-\infty}^{x} dy\, P(y)|f_l^{\pm}(E,y)|^2, \end{cases} \tag{3.22}$$

$$[f_l^{\pm}(E,x);f_r^{\pm}(-E,x)]=\begin{cases} 2iEb_l^{\pm}(E)\mp 2ik(E)\displaystyle\int_{-\infty}^{x} dy\, P(y)f_l^{\pm}(E,y)\overline{f_r^{\pm}(E,y)}; \\ -2iE\overline{b_r^{\pm}(E)}\pm 2ik(E)\displaystyle\int_x^{\infty} dy\, P(y)f_l^{\pm}(E,y)\overline{f_r^{\pm}(E,y)}, \end{cases} \tag{3.23}$$

$$[f_r^{\pm}(E,x);f_r^{\pm}(-E,x)] =\begin{cases} 2iE\mp 2ik(E)\displaystyle\int_{-\infty}^{x} dy\, P(y)|f_r^{\pm}(E,y)|^2; \\ 2iE[|a^{\pm}(E)|^2-|b_r^{\pm}(E)|^2]\pm 2ik(E)\displaystyle\int_x^{\infty} dy\, P(y)|f_r^{\pm}(E,y)|^2. \end{cases} \tag{3.24}$$

Subtracting the two right-hand sides of each of (3.22)–(3.24), we get

$$-1+|a^{\pm}(E)|^2-|b_l^{\pm}(E)|^2=\mp\frac{k(E)}{E}\int_{-\infty}^{\infty} dy\, P(y)|f_l^{\pm}(E,y)|^2; \tag{3.25}$$

$$-b_l^{\pm}(E)-\overline{b_r^{\pm}(E)}=\mp\frac{k(E)}{E}\int_{-\infty}^{\infty} dy\, P(y)f_l^{\pm}(E,y)\overline{f_r^{\pm}(E,y)}, \tag{3.26}$$

$$-1+|a^{\pm}(E)|^2-|b_r^{\pm}(E)|^2=\mp\frac{k(E)}{E}\int_{-\infty}^{\infty} dy\, P(y)|f_r^{\pm}(E,y)|^2. \tag{3.27}$$

From (3.25) and (3.27) it is clear that $a^{\pm}(E)\neq 0$ when $(\mp P(x))\geqslant 0$. In that case we define the matrix

$$\mathbf{W}^{\pm}(E)=\mp\begin{bmatrix} \displaystyle\int_{-\infty}^{\infty} dyP(y)|f_l^{\pm}(E,y)|^2 & \displaystyle\int_{-\infty}^{\infty} dyP(y)f_r^{\pm}(E,y)\overline{f_l^{\pm}(E,y)} \\ \displaystyle\int_{-\infty}^{\infty} dyP(y)\overline{f_r^{\pm}(E,y)}f_l^{\pm}(E,y) & \displaystyle\int_{-\infty}^{\infty} dyP(y)|f_r^{\pm}(E,y)|^2 \end{bmatrix},$$

and, provided $a^{\pm}(E)\neq 0$, derive the identity

$$\frac{k(E)}{E}|T^{\pm}(E)|^2\mathbf{W}^{\pm}(E)=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}-\mathbf{S}^{\pm}(E)^{\dagger}\mathbf{S}^{\pm}(E),$$

which is nonnegative selfadjoint if $(\mp P(x))\geqslant 0$. Here $\dagger$ denotes the conjugate transpose. Similarly, one proves that if $(\mp P(x))\leqslant 0$ and the transmission coefficient $T^{\pm}(E)$ is well-defined, the scattering matrix $\mathbf{S}^{\pm}(E)$ has a contractive inverse.

D. Discrete eigenvalues

The discrete eigenvalues of the pair of modified Schrödinger equations (1.2) coincide with those of the system (1.6). They form a finite or countably infinite subset of $\mathbb{C}^+$ of eigenvalues of finite algebraic multiplicity. The geometric multiplicity of the eigenvalues of either of the equations (1.2) is one, while that of (1.6) is at most two. They can only accumulate in a bounded interval of the real line, but not at points of $(-m,m)$. Accumulation as $E\to\infty$ is impossible because of (3.14). Accumulation at points of $(-m,m)$ is impossible, because the scattering matrix $\mathbf{S}^{\pm}(E)$ is unitary if $E\in(-m,m)$.

The discrete eigenvalues are symmetrically located with respect to the imaginary axis, where the geometric and algebraic multiplicities of an eigenvalue at E_0 coincide with those at $-\overline{E_0}$. This follows directly from (3.4)–(3.5). The net result is that the residues of $iT^{\pm}(E)$ at E_0 and $-\overline{E_0}$ are complex conjugates.

For the problem (1.2) with $m=0$, the properties of the discrete spectrum have been discussed in detail in Ref. 6. Many of these results also follow from spectral properties of certain operator pencils (cf. Ref. 19). If $m>0$, most of those results are expected to go through, albeit in a slightly different form.

IV. MARCHENKO EQUATIONS

In this section we derive the Marchenko integral equations leading to the solution of the inverse scattering problem.

A. Fourier transformation properties

Let us apply the method of Ref. 13 to derive Marchenko integral equations to solve the inverse scattering problem. We begin by deriving some integral representations for the (transformed) Jost solutions.

Theorem 4.1: *Assume* $P\in L^1_1(\mathbb{R})$, $Q\in L^1_2(\mathbb{R})$, *and* $W^{\pm}\in L^1_1(\mathbb{R})$. *Then the Jost solutions* $f_{rs}(E,x)$ *and* $f_{ls}(E,s)$ $(s=1,2)$ *can be represented as follows:*

$$f_{r1}(E,x)=e^{-iEx}\cosh(p-\zeta(x))+\int_{-\infty}^{x}dt\,K_{r1}(x,t)e^{-iEt},\tag{4.1}$$

$$f_{r2}(E,x)=\int_{-\infty}^{x}dt\,K_{r2}(x,t)e^{-iEt},\tag{4.2}$$

$$f_{l1}(E,x)=e^{iEx}\cosh(\zeta(x))+\int_{x}^{\infty}dt\,K_{l1}(x,t)e^{iEt},\tag{4.3}$$

$$f_{l2}(E,x)=\int_{x}^{\infty}dt\,K_{l2}(x,t)e^{iEt},\tag{4.4}$$

where $K^{\pm}_{rs}(x,t)$ *and* $K^{\pm}_{ls}(x,t)$ $(s=1,2)$ *are independent of* E *and belong to* $L^2(\mathbb{R})$ *as functions of* t *when* $x\in\mathbb{R}$ *is fixed.*

Proof: Using (2.17), (2.18), (2.36), and (2.37) it follows that $\tilde{f}_{l1}(E,x)=f_{l1}(E,x)-e^{iEx}\cosh(\zeta(x))$ and $\tilde{f}_{r1}(E,x)=f_{r1}(E,x)-e^{-iEx}\cosh(p-\zeta(x))$, as well as $\tilde{f}_{l2}(E,x)=f_{l2}(E,x)$ and $\tilde{f}_{r2}(E,x)=f_{r2}(E,x)$ belong to $L^2(\mathbb{R})$ as functions of E for fixed $x\in\mathbb{R}$. Further, these functions multiplied by $(\log(|E|+2))^{1/2}$ belong to $L^2(\mathbb{R})$. So Plancherel's theorem (cf. Ref. 20, Theorems 48 and 63) implies the existence of the integrals,

$$K_{rs}(x,t)\overset{l.i.m.}{=\!=\!=}_{a\to+\infty}\frac{1}{2\pi}\int_{-a}^{a}dE\,\tilde{f}_{rs}(E,x)e^{iEt},\quad s=1,2,$$

$$K_{ls}(x,t)\overset{l.i.m.}{=\!=\!=}_{a\to+\infty}\frac{1}{2\pi}\int_{-a}^{a}dE\,\tilde{f}_{ls}(E,x)e^{-iEt},\quad s=1,2.$$

It is clear that $K_{rs}(x,t)$ and $K_{ls}(x,t)$ $(s=1,2)$ belong to $L^2(\mathbb{R})$ as functions of t for every $x\in\mathbb{R}$ (cf. Ref. 20, Theorems 48 and 63).

Due to (1.7) and Theorem 2.1, the functions $f_{rs}(E,x)$ and $f_{ls}(E,x)$ $(s=1,2)$ are analytic in $E\in\mathbb{C}^+$. Moreover, there exists $C>0$ (depending on $x\in\mathbb{R}$) such that for $s=1,2$,

$$|f_{rs}(E,x)|\leqslant Ce^{x\,\mathrm{Im}\,E},\quad |f_{ls}(E,x)|\leqslant Ce^{-x\,\mathrm{Im}\,E},$$

for all $x\in\mathbb{R}$. From (2.37) we obtain

$$\int_{-\infty}^{\infty}dt\,|\tilde{f}_{r1}(t+i\,\mathrm{Im}\,E,x)|^2=O(e^{-2x\,\mathrm{Im}\,E}).$$

Similar estimates hold for $K_{r2}(E,x)$ and for $K_{ls}(E,x)$ $(s=1,2)$. Hence we may apply Titchmarsh's theorem (cf. Ref. 20, Theorem 96) and obtain

$$K_{r1}(x,t)=K_{r2}(x,t)=0,\quad t>x,$$

$$K_{l1}(x,t)=K_{l2}(x,t)=0,\quad t<x.$$

This proves the representations (4.1)–(4.4). □

Using (2.18), (2.19), and (2.37), we obtain

$$\begin{aligned}\tilde{f}_{r1}(E,x)&=\frac{ie^{-iEx}}{4E}\left(e^{-p+\zeta(x)}\int_{-\infty}^{x}dz\,W^+(z)+e^{p-\zeta(x)}\int_{-\infty}^{x}dz\,W^-(z)\right)+O\left(\frac{1}{|E|^2}\right)\\&=\frac{ie^{-iEx}}{4(E+i\chi)}\left(e^{-p+\zeta(x)}\int_{-\infty}^{x}dz\,W^+(z)+e^{p-\zeta(x)}\int_{-\infty}^{x}dz\,W^-(z)\right)+O\left(\frac{1}{|E|^2}\right),\end{aligned}$$

where χ is an arbitrary positive number. Its Fourier transform is of the form

$$K_{r1}(x,t)=\left[\frac{e^{-p+\zeta(x)}}{4}\int_{-\infty}^{x}dz\,W^+(z)+\frac{e^{p-\zeta(x)}}{4}\int_{-\infty}^{x}dz\,W^-(z)\right]e^{-\chi(x-t)}\theta(x-t)+M_{r1}(x,t),$$

where $\theta(z)$ is the Heaviside function given by

$$\theta(z)=\begin{cases}0, & \text{for } z<0,\\ 1, & \text{for } z>0,\end{cases}$$

$M_{r1}(x,t)$ is continuous in $t\in\mathbb{R}$ for fixed $x\in\mathbb{R}$ and there exists the partial derivative $(\partial M_{r1}(x,t)/\partial t)\in L^2(\mathbb{R})$ (cf. Ref. 20, the beginning of Sec. 6.13, before Theorem 128). Hence, $K_{r1}(x,t)$ has a jump discontinuity at $x=t$. Taking into account the identity $K_{r1}(x,x+0)=0$, we obtain

$$K_{r1}(x,x-0)=\frac{1}{4}\left(e^{-p+\zeta(x)}\int_{-\infty}^{x}dz\,W^{+}(z)+e^{p-\zeta(x)}\int_{-\infty}^{x}dz\,W^{-}(z)\right). \tag{4.5}$$

In the same way we obtain

$$K_{r2}(x,x-0)=\sinh(p-\zeta(x)). \tag{4.6}$$

Using (4.5) and (4.6) we now compute $Q(x)$ and $P(x)$ from $K_{r1}(x,x-0)$ and $K_{r2}(x,x-0)$. In fact, we obtain

$$P(x)=2\frac{d}{dx}\log(K_{r2}(x,x-0)+(K_{r2}(x,x-0)^2+1)^{1/2}), \tag{4.7}$$

$$Q(x)=2\frac{d}{dx}\left(\frac{K_{r1}(x,x-0)}{\cosh\frac{1}{2}\int_{-\infty}^{x}dz\,P(z)}-\frac{P(x)}{4}\tanh\left(\frac{1}{2}\int_{-\infty}^{x}dz\,P(z)\right)\right)+\frac{P(x)^2}{4}. \tag{4.8}$$

In the same way we derive

$$K_{l2}(x,x+0)=\sinh(\zeta(x)),$$

$$P(x)=-2\frac{d}{dx}\log(K_{l2}(x,x-0)+(K_{l2}(x,x-0)^2+1)^{1/2}), \tag{4.9}$$

$$Q(x)=-2\frac{d}{dx}\left(\frac{K_{l1}(x,x+0)}{\cosh\frac{1}{2}\int_{x}^{\infty}dz\,P(z)}-\frac{P(x)}{4}\tanh\left(\frac{1}{2}\int_{x}^{\infty}dz\,P(z)\right)\right)+\frac{P(x)^2}{4}. \tag{4.10}$$

B. Marchenko equations without bound states

Let us assume that $T^{+}(E)$ and $T^{-}(E)$ are both continuous in $E\in\mathbb{R}$. Before deriving the two pairs of Marchenko integral equations, we introduce the two sets of integral kernels as follows:

$$F_{l1}(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dE\,L_1(E)e^{iEx}=\int_{-\infty}^{\infty}\frac{dE}{4\pi}[L^{+}(E)+L^{-}(E)]e^{iEx}, \tag{4.11}$$

$$F_{l2}(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dE\,L_2(E)e^{iEx}=\int_{-\infty}^{\infty}\frac{dE}{4\pi}\frac{L^{+}(E)-L^{-}(E)}{i\,k(E)}e^{iEx}, \tag{4.12}$$

$$\begin{aligned}F_{l3}(x)&=-\frac{1}{2\pi}\int_{-\infty}^{\infty}dE\,k(E)^2L_2(E)e^{iEx}\\&=i\int_{-\infty}^{\infty}\frac{dE}{4\pi}k(E)[L^{+}(E)-L^{-}(E)]e^{iEx},\end{aligned} \tag{4.13}$$

as well as

$$F_{r1}(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dE\,R_1(E)e^{iEx}=\int_{-\infty}^{\infty}\frac{dE}{4\pi}[R^{+}(E)+R^{-}(E)]e^{iEx}, \tag{4.14}$$

$$F_{r2}(x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}dE\,R_2(E)e^{iEx}=\int_{-\infty}^{\infty}\frac{dE}{4\pi}\,\frac{R^+(E)-R^-(E)}{i\,k(E)}e^{iEx}, \tag{4.15}$$

$$\begin{aligned}F_{r3}(x)&=-\frac{1}{2\pi}\int_{-\infty}^{\infty}dE\,k(E)^2R_2(E)e^{iEx}\\&=i\int_{-\infty}^{\infty}\frac{dE}{4\pi}k(E)[R^+(E)-R^-(E)]e^{iEx}.\end{aligned} \tag{4.16}$$

Then the integrals (4.11)–(4.13) and (4.14)–(4.16) exist as a result of Proposition 3.5 and the continuity of $T^+(E)$ and $T^-(E)$ in $E\in\mathbb{R}$.

Next, we introduce the unknown functions $B_{rs}(x,y)$ and $B_{ls}(x,y)$ $(x\in\mathbb{R},\ y>0,\ s=1,2)$ by

$$B_{rs}(x,y)=\frac{K_{rs}(x,x-y)}{\cosh(p-\zeta(x))},\quad B_{ls}(x,y)=\frac{K_{ls}(x,x+y)}{\cosh(\zeta(x))}, \tag{4.17}$$

and write (4.1)–(4.4) in the form

$$f_{rs}(E,x)=e^{-iEx}\cosh(p-\zeta(x))\left[\delta_{s,1}+\int_0^{\infty}dy\,e^{iEy}B_{rs}(x,y)\right],$$

$$f_{ls}(E,x)=e^{iEx}\cosh(\zeta(x))\left[\delta_{s,1}+\int_0^{\infty}dy\,e^{iEy}B_{ls}(x,y)\right],$$

where $s=1,2$.

Starting from the two pairs of equations [cf. (3.13)],

$$\begin{aligned}&f_{r1}(-E,x)+L_1(E)f_{r1}(E,x)-k(E)^2L_2(E)f_{r2}(E,x)\\&\quad=T_1(E)f_{l1}(E,x)-k(E)^2T_2(E)f_{l2}(E,x),\end{aligned} \tag{4.18}$$

$$\begin{aligned}&f_{r2}(-E,x)+L_2(E)f_{r1}(E,x)+L_1(E)f_{r2}(E,x)\\&\quad=T_2(E)f_{l1}(E,x)+T_1(E)f_{l2}(E,x),\end{aligned} \tag{4.19}$$

and

$$\begin{aligned}&f_{l1}(-E,x)+R_1(E)f_{l1}(E,x)-k(E)^2R_2(E)f_{l2}(E,x)\\&\quad=T_1(E)f_{r1}(E,x)-k(E)^2T_2(E)f_{r2}(E,x),\end{aligned} \tag{4.20}$$

$$\begin{aligned}&f_{l2}(-E,x)+R_2(E)f_{l1}(E,x)+R_1(E)f_{l2}(E,x)\\&\quad=T_2(E)f_{r1}(E,x)+T_1(E)f_{r2}(E,x),\end{aligned} \tag{4.21}$$

and Fourier transforming the contributions to these equations that are analytic in $\mathbb{C}^-$ and vanish at infinity while taking into account (4.11)–(4.17), we obtain the two pairs of coupled Marchenko equations,

$$\begin{aligned}&B_{r1}(x,y)+\int_0^{\infty}dz\,[F_{l1}(y+z-2x)B_{r1}(x,z)+F_{l3}(y+z-2x)B_{r2}(x,z)]\\&\quad=-F_{l1}(y-2x),\end{aligned} \tag{4.22}$$

$$B_{r2}(x,y)+\int_0^\infty dz\,[F_{l2}(y+z-2x)B_{r1}(x,z)+F_{l1}(y+z-2x)B_{r2}(x,z)]$$
$$=-F_{l2}(y-2x), \tag{4.23}$$

and

$$B_{l1}(x,y)+\int_0^\infty dz\,[F_{r1}(y+z+2x)B_{l1}(x,z)+F_{r3}(y+z+2x)B_{l2}(x,z)]$$
$$=-F_{l1}(y+2x), \tag{4.24}$$

$$B_{l2}(x,y)+\int_0^\infty dz\,[F_{r2}(y+z+2x)B_{l1}(x,z)+F_{r1}(y+z+2x)B_{l2}(x,z)]$$
$$=-F_{r2}(y+2x). \tag{4.25}$$

In deriving (4.22)–(4.25), we have assumed the absence of the discrete spectrum of the two equations (1.2) and hence the analyticity of $T_1(E)$ and $T_2(E)$ in $\mathbb{C}^+$.

C. Marchenko equations with bound states

When one of the two equations (1.2) has a discrete spectrum, the derivation of the Marchenko equations (4.22)–(4.25) should be modified, since the right-hand sides of (4.18)–(4.21) may no longer vanish. To simplify the discussion, we make the following assumptions.

(1) $T^+(E)$ and $T^-(E)$ are continuous in $E\in\mathbb{R}$.
(2) The number of poles of $T^+(E)$ and $T^-(E)$ in $\mathbb{C}^+$ is finite [denote the poles of either of $T^\pm(E)$ in $\mathbb{C}^+$ by E_j, where $j=1,\ldots,\mathcal{N}$].
(3) The poles of $T^+(E)$ and $T^-(E)$ in $\mathbb{C}^+$ are simple; we write $it_j^\pm$ for the residue of $T^\pm(E)$ at $E=E_j$ ($j=1,\ldots,\mathcal{N}$). We put $t_{j1}=[t_j^+ + t_j^-]/2$ and $t_{j2}=[t_j^+ - t_j^-]/2ik(E_j)$.
(4) We remark that $t_j^\pm$, t_{j1}, t_{j2}, and $ik(E_j)$ are real if E_j is imaginary. Quantities $t_j^\pm$, t_{j1}, t_{j2}, and $ik(E_j)$ corresponding to eigenvalues symmetrically located with respect to the imaginary axis are complex conjugates. These properties are immediate from the observations made in Sec. III D.
(5) Using the terminology of Ref. 16 and recalling that the eigenvalues of either of (1.2) have geometric multiplicity one, we first introduce the norming constants,

$$C_j^\pm=\frac{f_l^\pm(E_j,x)}{f_r^\pm(E_j,x)},\quad j=1,\ldots,\mathcal{N}_j^\pm.$$

Then one easily verifies that

$$f_{l1}(E_j,x)=C_{j1}f_{r1}(E_j,x)-k_j^2C_{j2}f_{r2}(E_j,x),$$
$$f_{l2}(E_j,x)=C_{j2}f_{r1}(E_j,x)+C_{j1}f_{r2}(E_j,x),$$

where $k_j=k(E_j)$ and

$$C_{j1}=\frac{C_j^+ + C_j^-}{2},\quad C_{j2}=\frac{C_j^+ - C_j^-}{2ik_j}.$$

Calculating the residues of the expressions on the right-hand sides of (4.18)–(4.21) at $E=E_j$ in $\mathbb{C}^+$, we obtain

$$[t_{j1}C_{j1}-k_j^2 t_{j2}C_{j2}]f_{r1}(E_j,x)-k_j^2[t_{j1}C_{j2}+t_{j2}C_{j1}]f_{r2}(E_j,x), \tag{4.26}$$

$$[t_{j2}C_{j1}+t_{j1}C_{j2}]f_{r1}(E_j,x)+[-k_j^2 t_{j2}C_{j2}+t_{j1}C_{j1}]f_{r2}(E_j,x), \tag{4.27}$$

$$[t_{j1}D_{j1}-k_j^2 t_{j2}D_{j2}]f_{r1}(E_j,x)-k_j^2[t_{j1}D_{j2}+t_{j2}D_{j1}]f_{r2}(E_j,x), \tag{4.28}$$

$$[t_{j2}D_{j1}+t_{j1}D_{j2}]f_{r1}(E_j,x)+[-k_j^2 t_{j2}D_{j2}+t_{j1}D_{j1}]f_{r2}(E_j,x), \tag{4.29}$$

multiplied by the imaginary unit i. Here

$$f_{r1}(E_j,x)=D_{j1}f_{l1}(E_j,x)-k_j^2 D_{j2}f_{l2}(E_j,x),$$

$$f_{r2}(E_j,x)=D_{j2}f_{l1}(E_j,x)+D_{j1}f_{l2}(E_j,x),$$

where we note that

$$\begin{bmatrix} D_{j1} & -k_j^2 D_{j2} \\ D_{j2} & D_{j1} \end{bmatrix}=\begin{bmatrix} C_{j1} & -k_j^2 C_{j2} \\ C_{j2} & C_{j1} \end{bmatrix}^{-1}.$$

We remark that $C_j^{\pm}$, C_{j1}, C_{j2}, D_{j1}, D_{j2} and ik_j are real if E_j is imaginary. Quantities $t_j^{\pm}$, C_{j1}, C_{j2}, D_{j1}, D_{j2}, and ik_j corresponding to eigenvalues symmetrically located with respect to the imaginary axis are complex conjugates. These properties are immediate from (2.16).

We now recall that in order to compute the left-hand side minus the right-hand side of (4.22) and (4.23), we have to single out the contributions to (4.18) and (4.19) that are analytic in $\mathbb{C}^-$ and vanish at infinity and apply the operation $1/2\pi\int_{-\infty}^{\infty}dE\,e^{iE(y-x)}[\cosh(p-\zeta(x))]^{-1}$ to them. Applying the same procedure to the right-hand sides of (4.18) and (4.19) and using (4.17), (4.26), and (4.27), we obtain

$$-\sum_{j=1}^{\mathcal{N}} e^{iE_j(y-2x)}\left(A_{lj1}+\int_0^{\infty}dz\,e^{iE_j z}[A_{lj1}B_{r1}(x,z)-k_j^2 A_{lj2}B_{r2}(x,z)]\right),$$

$$-\sum_{j=1}^{\mathcal{N}} e^{iE_j(y-2x)}\left(A_{lj2}+\int_0^{\infty}dz\,e^{iE_j z}[A_{lj2}B_{r1}(x,z)-k_j^2 A_{lj1}B_{r2}(x,z)]\right),$$

where

$$A_{lj1}=t_{j1}C_{j1}-k_j^2 t_{j2}C_{j2},\quad A_{lj2}=t_{j1}C_{j2}+t_{j2}C_{j1}.$$

Introducing the modified Marchenko kernel functions,

$$\tilde{F}_{ls}(x)=F_{ls}(x)+\sum_{j=1}^{\mathcal{N}} A_{ljs}e^{iE_j x},\quad s=1,2,3,$$

where $A_{lj3}=-k_j^2 A_{lj2}$, we arrive at the coupled Marchenko integral equations,

$$B_{r1}(x,y)+\int_0^{\infty}dz\,[\tilde{F}_{l1}(y+z-2x)B_{r1}(x,z)+\tilde{F}_{l3}(y+z-2x)B_{r2}(x,z)]$$

$$=-\tilde{F}_{l1}(y-2x), \tag{4.30}$$

$$B_{r2}(x,y)+\int_0^\infty dz\,[\tilde{F}_{l2}(y+z-2x)B_{r1}(x,z)+\tilde{F}_{l1}(y+z-2x)B_{r2}(x,z)]$$
$$=-\tilde{F}_{l2}(y-2x). \tag{4.31}$$

In an analogous way we obtain the coupled Marchenko integral equations

$$B_{l1}(x,y)+\int_0^\infty dz\,[\tilde{F}_{r1}(y+z+2x)B_{l1}(x,z)+\tilde{F}_{r3}(y+z+2x)B_{l2}(x,z)]$$
$$=-\tilde{F}_{r1}(y+2x), \tag{4.32}$$

$$B_{l2}(x,y)+\int_0^\infty dz\,[\tilde{F}_{r2}(y+z+2x)B_{l1}(x,z)+\tilde{F}_{r1}(y+z+2x)B_{l2}(x,z)]$$
$$=-\tilde{F}_{r2}(y+2x), \tag{4.33}$$

where

$$\tilde{F}_{rs}(x)=F_{rs}(x)+\sum_{j=1}^{\mathcal{N}} A_{rjs}e^{iE_jx},\quad s=1,2,3,$$

$$A_{rj1}=t_{j1}D_{j1}-k_j^2t_{j2}D_{j2},\quad A_{rj2}=t_{j1}D_{j2}+t_{j2}D_{j1},$$

and $A_{rj3}=-k_j^2A_{rj2}$. Using the symmetry statements made before in this subsection, one easily proves that $\tilde{F}_{ls}(x)$ and $\tilde{F}_{rs}(x)$ $(s=1,2,3)$ are real functions.

When $T^+(E)$ and $T^-(E)$ both have a finite number of poles and some of them are multiple poles (but otherwise the first assumption is fulfilled), (4.30)–(4.33) can be derived using a generalization of the notion of norming constant given in Ref. 7, but with more complicated auxiliary kernel functions $\tilde{F}_{ls}(y)$ and $\tilde{F}_{rs}(y)$ $(s=1,2,3)$.

We now state the main result. The first part is immediate from (4.7)–(4.8) and (4.17). The second part follows from the second (4.17) and expressions involving $K_{ls}(x,t)$ and $B_{ls}(x,y)$ $(s=1,2)$ analogous to (4.7)–(4.8).

Theorem 4.2: *Suppose* $P\in L_1^1(\mathbb{R})$, $Q\in L_2^1(\mathbb{R})$, *and* $W^\pm\in L_1^1(\mathbb{R})$, *and let conditions (1)–(3) stated at the beginning of Sec. IV C be fulfilled. Then if* $B_{rs}(x,\cdot)$ $(s=1,2)$ *are the solutions of the Marchenko equations (4.30) and (4.31) and* $B_{r2}(x,0^+)\in(-1,1)$, *the potentials* $Q(x)$ *and* $P(x)$ *are given by*

$$P(x)=\frac{d}{dx}\log\frac{1+B_{r2}(x,0^+)}{1-B_{r2}(x,0^+)}; \tag{4.34}$$

$$Q(x)=2\frac{d}{dx}\left[B_{r1}(x,0^+)-\frac{P(x)}{4}\tanh\left(\frac{1}{2}\int_{-\infty}^x dz\,P(z)\right)\right]+\frac{P(x)^2}{4}. \tag{4.35}$$

Similarly, if $B_{ls}(x,\cdot)$ $(s=1,2)$ *are the solutions of the Marchenko equations (4.32) and (4.33) and* $B_{l2}(x,0^+)\in(-1,1)$, *then the potentials* $Q(x)$ *and* $P(x)$ *are given by*

$$P(x)=\frac{d}{dx}\log\frac{1-B_{l2}(x,0^+)}{1+B_{l2}(x,0^+)}; \tag{4.36}$$

$$Q(x)=-2\frac{d}{dx}\left[B_{l1}(x,0^+)-\frac{P(x)}{4}\tanh\left(\frac{1}{2}\int_x^\infty dz\,P(z)\right)\right]+\frac{P(x)^2}{4}. \tag{4.37}$$

V. SOLVABILITY OF THE MARCHENKO EQUATIONS

In this section we establish the compactness of the Marchenko integral operators and relate the unique solvability of the (pairs of) Marchenko integral equations to the canonical factorizability of a matrix function.

Theorem 5.1: *Suppose* $P \in L_1^1(\mathbb{R})$, $Q \in L_2^1(\mathbb{R})$, *and* $W^{\pm} \in L_1^1(\mathbb{R})$, *and let conditions (1)–(3) stated at the beginning of Sec. IV C be fulfilled. Then the integral operators arising from the Marchenko integral equations (4.30)–(4.33) are compact on* $L^2(\mathbb{R}^+)$.

Proof: All of these integral operators have the form

$$(Kg)(y) = \int_0^\infty dz\, F(y+z)g(z), \quad y>0,$$

where

$$F(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dE\, \Phi(E)e^{iEx},$$

for some function $\Phi(E)$ that is continuous in $E \in \mathbb{R}$ and vanishes as $E \to \pm\infty$. Such integral operators are Hankel operators with continuous symbol and as such compact on $L^2(\mathbb{R})$ (cf. Refs. 21 and 22). □

In order to derive sufficient conditions for the unique solvability of the Marchenko equations (4.30)–(4.31) or the Marchenko equations (4.32)–(4.33), we define the quantities

$$\hat{R}_s(E) = \int_{-\infty}^{\infty} dz\, e^{-iEz}\tilde{F}_{rs}(z), \quad \hat{L}_s(E) = \int_{-\infty}^{\infty} dz\, e^{-iEz}\tilde{F}_{ls}(z),$$

where $s=1,2,3$. If neither of (1.2) has any eigenvalues, we have

$$\hat{R}_1(E) = R_1(E), \quad \hat{R}_2(E) = R_2(E), \quad \hat{R}_3(E) = -k(E)^2 R_2(E),$$

$$\hat{L}_1(E) = L_1(E), \quad \hat{L}_2(E) = L_2(E), \quad \hat{L}_3(E) = -k(E)^2 L_2(E).$$

Introducing the functions

$$B_{rs}^{\pm}(E,x) = \pm\int_0^{\pm\infty} dy\, B_{rs}(x,y)e^{iEy}, \quad B_{ls}^{\pm}(E,x) = \pm\int_0^{\pm\infty} dy\, B_{ls}(x,y)e^{iEy},$$

where $s=1,2$, by Fourier transformation we obtain from (4.30)–(4.31) the Riemann–Hilbert problem,

$$\begin{bmatrix} I & 0 \\ \mathbf{F}_l(-E,x) & I \end{bmatrix}\begin{bmatrix} \mathbf{X}^+(E,x) \\ \mathbf{X}^-(-E,x) \end{bmatrix} + \begin{bmatrix} I & \mathbf{F}_l(E,x) \\ 0 & I \end{bmatrix}\begin{bmatrix} \mathbf{X}^-(E,x) \\ \mathbf{X}^+(-E,x) \end{bmatrix} = \begin{bmatrix} \mathbf{Y}(-E,x) \\ \mathbf{Y}(E,x) \end{bmatrix}, \tag{5.1}$$

where I denotes the 2×2 identity matrix and

$$\mathbf{X}^{\pm}(E,x) = \begin{bmatrix} B_{r1}^{\pm}(E,x) \\ B_{r2}^{\pm}(E,x) \end{bmatrix}, \quad \mathbf{Y}(E,x) = -e^{-2iEx}\begin{bmatrix} \hat{L}_1(E) \\ \hat{L}_2(E) \end{bmatrix},$$

$$\mathbf{F}_l(E,x) = e^{-2iEx}\begin{bmatrix} \hat{L}_1(E) & \hat{L}_3(E) \\ \hat{L}_2(E) & \hat{L}_1(E) \end{bmatrix}.$$

In the same way we define

$$\mathbf{F}_r(E,x)=e^{2iEx}\begin{bmatrix}\hat{R}_1(E) & \hat{R}_3(E)\\ \hat{R}_2(E) & \hat{R}_1(E)\end{bmatrix}.$$

In analogy with (5.1), we derive the Riemann–Hilbert problem,

$$\begin{bmatrix} I & 0\\ \mathbf{F}_l(-E,x) & I\end{bmatrix}\begin{bmatrix}\mathbf{X}^+(E,x)\\ -\mathbf{X}^-(-E,x)\end{bmatrix}+\begin{bmatrix} I & \mathbf{F}_l(E,x)\\ 0 & I\end{bmatrix}\begin{bmatrix}\mathbf{X}^-(E,x)\\ -\mathbf{X}^+(-E,x)\end{bmatrix}=\begin{bmatrix}\mathbf{Y}(-E,x)\\ -\mathbf{Y}(E,x)\end{bmatrix},$$

from the system of integral equations obtained from (4.30) and (4.31) by replacing the kernels $\hat{F}_{ls}$ with $-\hat{F}_{ls}$.

Next, by a (right) *canonical factorization* of a matrix function $W(E)$ defined for $E\in\mathbb{R}$ we mean a factorization of the form

$$W(E)=W^-(E)W^+(E), \tag{5.2}$$

where both $W^{\pm}(E)$ and $W^{\pm}(E)^{-1}$ are continuous in $E\in\overline{\mathbb{C}^{\pm}}$, are analytic in $E\in\mathbb{C}^{\pm}$, and have a limit as $E\to\infty$ in $\overline{\mathbb{C}^{\pm}}$. Replacing (5.2) with $W(E)=W^+(E)W^-(E)$, we get the definition of a left canonical factorization.

The following theorem easily follows using the methods employed in Refs. 23 and 24. Such methods were applied to inverse scattering before in Ref. 7.

Theorem 5.2: *Suppose $P\in L^1_1(\mathbb{R})$, $Q\in L^1_2(\mathbb{R})$ and $W^{\pm}\in L^1_1(\mathbb{R})$, and let conditions (1)–(3) stated at the beginning of Sec. IV C be fulfilled. Then, for fixed $x\in\mathbb{R}$, the system of Marchenko integral equations (4.30) and (4.31) and the system of integral equations obtained from them by replacing the kernels $\tilde{F}_{ls}$ with $-\tilde{F}_{ls}$ both have a unique solution if and only if the 4×4 matrix function*

$$\begin{bmatrix} I-\mathbf{F}_l(E,x)\mathbf{F}_l(-E,x) & -\mathbf{F}_l(E,x)\\ \mathbf{F}_l(-E,x) & I\end{bmatrix} \tag{5.3}$$

has a (right) canonical factorization. Similarly, for fixed $x\in\mathbb{R}$, the system of Marchenko integral equations (4.32) and (4.33) and the system of integral equations obtained from them by replacing the kernels $\tilde{F}_{rs}$ with $-\tilde{F}_{rs}$ both have a unique solution if and only if the 4×4 matrix function

$$\begin{bmatrix} I-\mathbf{F}_r(E,x)\mathbf{F}_r(-E,x) & -\mathbf{F}_r(E,x)\\ \mathbf{F}_r(-E,x) & I\end{bmatrix} \tag{5.4}$$

has a (right) canonical factorization.

In Ref. 7 the Marchenko equations are simple enough to allow for a representation of the 4×4 matrix functions in (5.3) and (5.4) as the direct sum of two 2×2 matrix functions (one being the adjoint of the other) multiplied on either side by constant nonsingular matrices. As a result, in Ref. 7 the analog of the present Theorem 5.2 involves the equivalence of the simultaneous unique solvability of two pairs of Marchenko equations to the existence of both a left and a right canonical factorization of a 2×2 matrix function. No such simplification has been found for the present problem.

We conclude this article by giving a sufficient condition for the canonical factorizability of the matrix function in (5.3) and hence of the unique solvability of the solution of the Marchenko equations (4.30)–(4.31).

Corollary 5.3: Suppose $P\in L^1_1(\mathbb{R})$, $Q\in L^1_2(\mathbb{R})$ and $W^{\pm}\in L^1_1(\mathbb{R})$, and let conditions (1)–(3) stated at the beginning of Sec. IV C be fulfilled. Then, for fixed $x\in\mathbb{R}$, the system of Marchenko integral equations (4.30) and (4.31) are uniquely solvable if

$$\sup_{E\in\mathbb{R}}\|\mathbf{F}_l(E,x)\|<1. \tag{5.5}$$

Analogously, for fixed $x \in \mathbb{R}$, the system of Marchenko integral equations (4.32) and (4.33) are uniquely solvable if

$$\sup_{E \in \mathbb{R}} \|\mathbf{F}_r(E,x)\| < 1. \tag{5.6}$$

In (5.5) and (5.6) the norm is defined as the largest singular value of the matrix.

Proof: This corollary is immediate from Theorem 5.2 by observing that (5.5) implies that $\mathbf{F}_l(E,x)$ has a canonical factorization (cf. Ref. 25, Sec. III A). □

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Expansion in the distance parameter for two vortices close together

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Static vortices close together are studied for two different models in two-dimensional Euclidean space. In a simple model for one complex field, an expansion in the parameters describing the relative position of two vortices can be given in terms of trigonometric and exponential functions. The results are then compared to those of the Ginzburg–Landau theory of a superconductor in a magnetic field at the point between type-I and type-II superconductivity. For the angular dependence a similar pattern emerges in both models. The differences for the radial functions are studied up to third order. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Ever since t'Hooft[1] and Polyakov[2] found a monopole solution in the SU(2) Yang–Mills–Higgs theory, solitons in field theories have been studied extensively. Our understanding of monopole solutions has been greatly enhanced by an existence proof for static solutions by Taubes[3] and the construction of monopole solutions started by Ward.[4] This process was not matched by quite the same progress in our understanding of the Abrikosov solutions of the Ginzburg–Landau theory, although one might have expected that the Abelian Higgs theory in $2+1$ dimensions is actually simpler than the SU(2) Yang–Mills–Higgs theory in $3+1$ dimensions. Again an existence proof was given by Taubes.[5] However, only superimposed vortices can be described explicitly and no explicit construction of separated vortices is known. In this article, we want to give the solution for two vortices close together in terms of an expansion in the parameters which describe the relative location.

In Secs. II and III, we study a model for one complex field. Here the calculations are simpler than in the Ginzburg–Landau theory which is our second model. The first model has, however, some peculiar (unphysical) features. Assuming the most symmetric form in terms of angular dependence, only two smooth vortices can be superimposed, and when ''pulled apart,'' they develop a singularity at third order. In the Ginzburg–Landau model this does not happen. In fact, delicate cancellations take place to make the expansion smooth, at least up to third order. In this model the radial functions are given as solutions of certain linear ordinary differential equations. This is discussed in Sec. IV.

II. VORTEX SOLUTIONS AND ZERO MODES IN A SIMPLE MODEL

Our first model is a model[6,7] for a pair of real fields $\phi^a(\vec{x})$, $a,b=1,2$, or equivalently, for a complex field $\phi=\phi_1+\imath\phi_2$. The Lagrangian density of the model reads

$$\mathcal{L}=\partial_{[i}\phi^a\partial_{j]}\phi^b\partial^{[i}\phi_a\partial^{j]}\phi_b+(1-|\phi|^2)^2|\phi|^2, \tag{2.1}$$

where $a,b=1,2$ labels the components of the Higgs field and $i,j=1,2$ are the space indices. The square brackets mean antisymmetrization,

$$\partial_{[i}\phi^a\partial_{j]}\phi^b=(\partial_i\phi^a)(\partial_j\phi^b)-(\partial_j\phi^a)(\partial_i\phi^b). \tag{2.2}$$

We are working in two-dimensional Euclidean space, i.e., the space indices can be raised and lowered without any change in the formulas. The indices which label the components of the Higgs field can also be raised and lowered without any change. In terms of the complex field ϕ, the Euler–Lagrange equation reads

$$\partial_i\phi^*\partial_j(\partial^{[i}\phi\partial^{j]}\phi^*)=(1-|\phi|^2)|\phi|\frac{\partial}{\partial\phi}(1-|\phi|^2)|\phi|. \tag{2.3}$$

Any solution of the equation,

$$2\det\left(\frac{\partial\phi^a}{\partial x^i}\right)=\pm(1-|\phi|^2)|\phi|, \tag{2.4}$$

solves the equation of motion (2.3). Note that Eq. (2.4) is a first-order equation whereas Eq. (2.3) is of second order. So we would expect that (2.4) is somewhat easier to solve than (2.3). For different types of models, this reduction of order was first introduced by Bogomolnyi.[8] That is why we call Eq. (2.4) the Bogomolnyi equation here. Any solution of (2.4) also attains the lower bound in the following inequality:

$$A=\int_{\mathbf{R}^2}\mathcal{L}\ \ d^2x\geqslant\frac{16\pi}{15}|Q|, \tag{2.5}$$

where

$$Q=\frac{15}{8\pi}\int_{\mathbf{R}^2}\imath\epsilon_{ij}(1-|\phi|^2)|\phi|(\partial^i\phi)(\partial^j\phi^*)d^2x \tag{2.6}$$

is the winding number. Finally, all finite-action solutions actually solve the Bogomolnyi equation, so we do not miss out on any by concentrating on the first-order equation.

We now seek to attain a smooth finite-action solution of Eq. (2.4). For

$$\phi=f(r)e^{\imath n\theta}, \tag{2.7}$$

Eq. (2.4) reduces to

$$\frac{nf(r)f'(r)}{r}=\frac{1}{2}(1-f^2)f. \tag{2.8}$$

Since $f\to 0$ as $r\to 0$ [otherwise ϕ in (2.7) is not defined at the origin], we have

$$f=\tanh\frac{r^2}{4n}. \tag{2.9}$$

The solution ϕ in (2.7) with $f(r)$ given by (2.9) is defined in the whole of $\mathbf{R}^2$ and is clearly a C^∞ function in $\mathbf{R}^2\backslash\{0\}$. Since

$$f\approx 1-2\exp\frac{r^2}{2n}\ \text{as}\ r\to\infty, \tag{2.10}$$

ϕ has the right asymptotic behavior for a solution with winding number n. We still have to ensure that ϕ is C^∞ at the origin. There we use the Taylor expansion of f,

$$f=\sum_{K=1}^{\infty}\frac{2^{2k}(2^{2k}-1)B_{2k}}{(2k)!}\left(\frac{r^2}{4n}\right)^{2k-1}=\frac{r^2}{4n}-\frac{1}{3}\left(\frac{r^2}{4n}\right)^3+\ldots\ , \tag{2.11}$$

where B_k is the kth Bernoulli number. We see that for $n=2$ and only for $n=2$, ϕ is a polynomial in x^i. In this model, we have the (somewhat peculiar) situation that within the most natural ansatz (2.7), smooth finite action solutions exist only for $n=2$, i.e., we only have a solution of the form (2.7) for two vortices.

We have found the solution for two vortices sitting on top of each other, which we now denote by $\hat{\phi}$. To extend our study to two vortices slightly apart we consider $\phi=\hat{\phi}+\gamma$, where γ is very small, and we solve the Bogomolyni equation, linearized in γ. Equation (2.4) becomes

$$\begin{aligned}&\left(f'\cos\theta\cos2\theta+\frac{2}{r}f\sin\theta\sin2\theta\right)\frac{\partial\gamma^2}{\partial x^2}+\left(f'\sin\theta\sin2\theta+\frac{2}{r}f\cos\theta\cos2\theta\right)\frac{\partial\gamma^1}{\partial x^1}\\&-\left(f'\sin\theta\cos2\theta-\frac{2}{r}f\cos\theta\sin2\theta\right)\frac{\partial\gamma^2}{\partial x^1}-\left(f'\cos\theta\sin2\theta-\frac{2}{r}f\sin\theta\cos2\theta\right)\frac{\partial\gamma^1}{\partial x^2}\\&=\frac{1}{2}(1-3f^2)(\gamma^1\cos2\theta+\gamma^2\sin2\theta).\end{aligned} \tag{2.12}$$

We find a two-parameter family of zero modes,

$$\gamma(r)=[\alpha+\beta+\imath(\alpha-\beta)]h(r)\quad\text{with}\ \ h(r)=\frac{\sinh\frac{r^2}{8}}{\cosh^3\frac{r^2}{8}}. \tag{2.13}$$

These zero modes are C^∞ functions which vanish exponentially at infinity. By a rotation, one of the parameters could be removed and the vortices could be positioned, say, on the x-axis. Since this does not simplify the calculations significantly, we will retain both parameters. Retaining the two parameters would also be necessary for a study of vortex scattering in the slow-motion approximation. This study is not done in this work.

III. THE QUADRATIC AND CUBIC TERMS

We now consider $\phi=\hat{\phi}+\gamma+\delta$, and equate the second-order terms in the Bogomolyni Eq. (2.4). This leads to the equation,

$$\begin{aligned}&\frac{2}{r}\left(f'\cos2\theta\frac{\partial\delta^2}{\partial\theta}+2f\sin2\theta\frac{\partial\delta^2}{\partial r}-f'\sin2\theta\frac{\partial\delta^1}{\partial\theta}+2f\cos2\theta\frac{\partial\delta^1}{\partial r}\right)=(\alpha^2+\beta^2)fh^2\left(\frac{1}{f^2}-3\right)\\&-\frac{1}{2}fh^2\left(3+\frac{1}{f^2}\right)\ [\alpha^2(\cos2\theta+\sin2\theta)^2+2\alpha\beta(\cos^22\theta-\sin^22\theta)+\beta^2(\cos2\theta-\sin2\theta)^2]\\&+(1-3f^2)(\delta^1\cos2\theta+\delta^2\sin2\theta),\end{aligned} \tag{3.1}$$

with $f(r)$ given in (2.9) and $h(r)$ given in (2.13).

With δ of the form

$$\delta=\alpha^2F(r,\theta)+2\alpha\beta G(r,\theta)+\beta^2H(r,\theta), \tag{3.2}$$

we obtain the following equation for $F(r,\theta)$:

$$\frac{2}{r}\left(f'\cos 2\theta\frac{\partial F^2}{\partial\theta}+2f\sin 2\theta\frac{\partial F^2}{\partial r}-f'\sin 2\theta\frac{\partial F^1}{\partial\theta}+2f\cos 2\theta\frac{\partial F^1}{\partial r}\right)$$
$$=h^2\left(\frac{1}{f}-3f\right)-\frac{h^2}{2}\left(3f+\frac{1}{f}\right)(\cos 2\theta+\sin 2\theta)^2+(1-3f^2)(F^1\cos 2\theta+F^2\sin 2\theta). \tag{3.3}$$

To solve this equation we seek a solution of the form

$$F=f_1(r)\exp^{\imath 2\theta}-\imath f_2(r)\exp^{-\imath 2\theta}. \tag{3.4}$$

The ansatz (3.4) leads to two decoupled equations for f_1 and f_2. In terms of the variable $\xi=r^2/8$, they read

$$\frac{df_1}{d\xi}+\frac{1}{f}\left(3f^2-1-\frac{df}{d\xi}\right)f_1=\frac{h^2}{2f^2}(1-9f^2), \tag{3.5}$$

$$\frac{df_2}{d\xi}+\frac{1}{f}\left(3f^2-1+\frac{df}{d\xi}\right)f_2=-\frac{h^2}{2f}(1+3f^2). \tag{3.6}$$

The general solution to Eq. (3.5) is

$$f_1=\frac{1}{\cosh^2\xi}\left(\frac{3\sinh\xi}{2\cosh^3\xi}-\frac{\sinh\xi}{\cosh\xi}+C_1\right). \tag{3.7}$$

The function f_1 is a C^∞ function for $0<\xi<\infty$. For $\xi\to 0$, $f_1\to C_1$ holds. This implies that $C_1=0$; otherwise F in (3.4) is not defined at the origin. Therefore, f_1 reads

$$f_1=\frac{3\sinh\xi}{2\cosh^5\xi}-\frac{\sinh\xi}{\cosh^3\xi}. \tag{3.8}$$

The expansion of f_1 near the origin is of the form

$$f_1=\sum_{k=1}^{\infty}a_k\xi^k=\sum_{k=1}^{\infty}a_k\left(\frac{r^2}{8}\right)^k. \tag{3.9}$$

Hence, the first term in (3.4) is a C^∞ function of x^1 and x^2 at the origin. We also see that f_1 vanishes exponentially at infinity. So its contribution to ϕ does not change the winding number (2.6) which is a multiple of the action.

A similar calculation yields a one-parameter family of solutions to Eq. (3.6), namely

$$f_2=\frac{\sinh\xi}{2\cosh^3\xi}-\frac{3\sinh^3\xi}{2\cosh^5\xi}+C_2\frac{\sinh^2\xi}{\cosh^4\xi}. \tag{3.10}$$

In contrast to f_1, all the solutions f_2 are acceptable. In fact, for all C_2, f_2 is of the form

$$f_2=\sum_{k=1}^{\infty}b_k\xi^k=\sum_{k=1}^{\infty}b_k\left(\frac{r^2}{8}\right)^k \tag{3.11}$$

near the origin, and therefore the second term in (3.4) is in $C^\infty(\mathbf{R}^2)$. The winding number and the action are also not altered because f_2 decays exponentially at infinity.

The functions G and H in (3.2) can be found in the same way. If we put all results together, we obtain the second-order terms,

$$\delta=(\alpha^2+\beta^2)f_1(r)\exp^{\imath 2\theta}+\imath(\alpha-\imath\beta)^2 f_2(r)\exp^{-\imath 2\theta}, \tag{3.12}$$

where f_1 and f_2 are given by (3.8) and (3.10), respectively.

To find the cubic terms, we consider $\phi=\hat{\phi}+\gamma+\delta+\epsilon$, with γ given in (2.13) and δ given by (3.12). We set $\beta=0$ and concentrate on

$$\epsilon=\alpha^3 I(r,\theta). \tag{3.13}$$

For the Bogomolnyi equation to hold, I must satisfy

$$\begin{aligned}
&\frac{2}{r}\Bigg(f'\cos 2\theta\frac{\partial I^2}{\partial\theta}+2f\sin 2\theta\frac{\partial I^2}{\partial r}-f'\sin 2\theta\frac{\partial I^1}{\partial\theta}+2f\cos 2\theta\frac{\partial I^1}{\partial r}\\
&\quad+h'(2f_1\cos 2\theta+2f_2\sin 2\theta)+h'(2f_1\sin 2\theta+2f_2\cos 2\theta)\Bigg)\\
&=-3f^2(I^1\cos 2\theta+I^2\sin 2\theta)-3hf(f_1-f_2)(\cos 2\theta+\sin 2\theta)\\
&\quad-3fh(\cos 2\theta+\sin 2\theta)(2f_1-f_2-2f_2\cos 2\theta\sin 2\theta)-3(\cos 2\theta+\sin 2\theta)h^3\\
&\quad+I^1\cos 2\theta+I^2\sin 2\theta+\frac{h}{2}[f_1(\cos 2\theta+\sin 2\theta)-f_2(\cos 2\theta+\sin 2\theta)]\\
&\quad+\frac{h^3}{2}(\cos 2\theta+\sin 2\theta)^3-\frac{h^3}{f^2}(\cos 2\theta+\sin 2\theta)\\
&\quad-\frac{h}{f}(\cos 2\theta+\sin 2\theta)(f_1-2f_2\cos 2\theta\sin 2\theta)+\frac{h}{2f^2}(\cos 2\theta+\sin 2\theta)^3.
\end{aligned} \tag{3.14}$$

To solve Eq. (3.14) we seek a solution of the form

$$\begin{aligned}
I^1&=g_1(\xi)+g_2(\xi)(\cos 4\theta-\sin 4\theta),\\
I^2&=g_1(\xi)-g_2(\xi)(\cos 4\theta+\sin 4\theta).
\end{aligned} \tag{3.15}$$

This implies that g_1 and g_2 must satisfy the equations

$$\frac{dg_1}{d\xi}+\left(3f-\frac{1}{f}\right)g_1=-\frac{f_1+f_2}{f}\frac{dh}{d\xi}-6hf_1+\frac{9}{2}hf_2-\frac{hf_2}{2f^2}-\frac{h^3}{4f^3}-\frac{9h^3}{4f}, \tag{3.16}$$

$$\frac{dg_2}{d\xi}-\left(\frac{1}{f}-3f+\frac{2}{f}\frac{df}{d\xi}\right)g_2=-\frac{hf_2}{2f^2}-\frac{3hf_2}{2}-\frac{h^3}{4f^3}-\frac{h^3}{4f}. \tag{3.17}$$

The general solution to Eq. (3.17) is

$$g_2=\frac{\sinh\xi}{4\cosh^5\xi}-\frac{5\sinh^3\xi}{4\cosh^7\xi}+C_2\left(\frac{\sinh^2\xi}{2\cosh^4\xi}-\frac{3\sinh^4\xi}{2\cosh^6\xi}\right)+C_3\frac{\sinh^3\xi}{\cosh^5\xi}. \tag{3.18}$$

All solutions (3.18) decay exponentially at infinity. For $r\to 0$, however,

$$g_2(r)=\frac{1}{24}r^2+\ldots\ . \tag{3.19}$$

Hence, I in (3.15) is not a C^∞ function on $\mathbf{R}^2$. Our expansion gets singular at third order for the ansatz (3.15). In the next section we will discuss a realistic model in which a similar pattern emerges but no singularities occur.

IV. ABRIKOSOV VORTICES

The Ginzburg–Landau theory of a superconductor in a magnetic field in direction z is given by the Lagrangian density

$$\mathcal{L}=\frac{1}{4}F_{ij}F^{ij}+\frac{1}{2}(D_i\phi)(D^i\phi)^*+\frac{\lambda}{8}(|\phi|^2-1)^2, \tag{4.1}$$

where ϕ is the complex Higgs field, and $D_i\phi=\partial_i\phi-\imath A_i\phi$ and $F_{ij}=\partial_iA_j-\partial_jA_i$ in terms of the gauge potentials A_i, $i=1,2$. The Euler–Lagrange equations are

$$D_iD^i\phi=\frac{\lambda}{2}\phi(1-|\phi|^2),\quad \partial_iF^{ij}=\frac{\imath}{2}[\phi(D^j\phi)^*-\phi^*D^j\phi]. \tag{4.2}$$

In the special case $\lambda=1$, it can be shown[9] that all finite action solutions of Eq. (4.2) satisfy the first-order Bogmolnyi equations,[8]

$$F_{12}=\tfrac{1}{2}(1-|\phi|^2),\quad D_1\phi=-iD_2\phi. \tag{4.3}$$

It has also been shown[9] that a $2n$-parameter family of solution of (4.3) exists with winding number

$$n=\frac{1}{2\pi}\int_{\mathbf{R}^2}F_{12}\ d^2x. \tag{4.4}$$

This family describes n vortices sitting at n position in space.

Even for n vortices sitting on top of each other, the solution is not known explicitly in terms of elementary functions. It is known,[10] however, that this solution is of the form

$$\phi=f(r)e^{\imath n\theta},\quad A_i=-\frac{na(r)}{r^2}\varepsilon_{ij}x^j, \tag{4.5}$$

where f and a satisfy

$$rf'-n(1-a)f=(2n/r)a'+f^2-1=0 \tag{4.6}$$

and

$$f(0)=a(0)=0,\quad \lim_{r\to\infty}f(r)=\lim_{r\to\infty}a(r)=1. \tag{4.7}$$

In the following, we restrict our attention to $n=2$ and use the solution (4.5) as the zero-order term in an expansion in the separation parameters. The first-order terms are given by the two zero modes describing the separation of the vortices. These were found by Weinberg.[11] Using his results we can write, up to quadratic terms,

$$\phi=fe^{2\imath\theta}+2(\alpha+\imath\beta)kf+\alpha^2\psi+\alpha\beta\phi+\beta^2\chi+\cdots, \tag{4.8}$$

$$A_1+\imath A_2=\imath\frac{2a}{r}e^{\imath\theta}-2\imath(\alpha+\imath\beta)\left(k'+\frac{2k}{r}\right)e^{-\imath\theta}$$
$$+\alpha^2(B_1+\imath B_2)+\alpha\beta(C_1+\imath C_2)+\beta^2(D_1+\imath D_2)+\cdots . \tag{4.9}$$

Here the radial function $k(r)$ satisfies

$$k''+\frac{1}{r}k'-\left(f^2+\frac{4}{r^2}\right)k=0, \tag{4.10}$$

with

$$\lim_{r\to 0} r^2k=1, \quad \lim_{r\to\infty} k(r)=0. \tag{4.11}$$

Our task is to determine $\psi,\phi,\chi,B_i,C_i,D_i$, which are functions of r and θ.

Equating the α^2-terms in the Bogomolnyi Eqs. (4.3), we obtain

$$(\partial_1+\imath\partial_2)\psi+\frac{2a}{r}\psi e^{\imath\theta}-\imath f(B_1+\imath B_2)e^{2\imath\theta}=4kf\left(k'+\frac{2k}{r}\right)e^{-\imath\theta}, \tag{4.12}$$

$$\partial_1B_2-\partial_2B_1+\tfrac{1}{2}(f\psi e^{-2\imath\theta}+f\psi e^{2\imath\theta})=-2k^2f^2. \tag{4.13}$$

A Fourier expansion with the minimal number of nonzero terms leads to the ansatz

$$\psi=g(r)f(r)e^{2\imath\theta}+\tilde{g}(r)e^{-2\imath\theta},$$
$$B_1+\imath B_2=\tilde{b}(r)e^{\imath\theta}+\imath b(r)f(r)e^{-3\imath\theta}, \tag{4.14}$$

and to equations for $g(r),\tilde{g}(r),b(r)$, and $\tilde{b}(r)$. The equations for $\tilde{g}(r)$ and $\tilde{b}(r)$ read

$$\tilde{g}=\frac{1+2a}{r}b-b', \quad \tilde{b}=-\imath h'. \tag{4.15}$$

The functions $g(r)$ and $b(r)$ must satisfy the equations

$$g''+\frac{1}{r}g'-f^2g=2k^2f^2, \tag{4.16}$$

$$b''+\frac{1}{r}b'-\left(\frac{1+f^2}{2}+\frac{1+4a+4a^2}{r^2}\right)b=-4kf\left(k'+\frac{2k}{r}\right). \tag{4.17}$$

Equating the $\alpha\beta$-terms and the β^2-terms in the Bogonolnyi Eq. (4.3), we obtain equations for ϕ and C_i, and for χ and D_i, respectively. These equations, which are very similar to Eqs. (4.12) and (4.13), can again be solved by functions with the same θ-dependence as in (4.14) but with slightly different radial functions. Collecting all results, we can write the solution, up to quadratic terms, in the form

$$\phi=fe^{2\imath\theta}+2(\alpha+\imath\beta)kf+(\alpha^2+\beta^2)gfe^{2\imath\theta}+(\alpha+\imath\beta)^2\left(\frac{1+2a}{r}b-b'\right)e^{-2\imath\theta}+\cdots,$$
$$A_1+\imath A_2=\imath\frac{2a}{r}e^{\imath\theta}-2\imath(\alpha+\imath\beta)\left(k'+\frac{2k}{r}\right)e^{-\imath\theta}-\imath(\alpha^2+\beta^2)g'e^{\imath\theta}+\imath(\alpha+\imath\beta)^2bfe^{-3\imath\theta}+\ldots . \tag{4.18}$$

It remains to be shown that the quadratic terms in (4.18) are C^∞ functions on $\mathbf{R}^2$ which do not change the action (and the winding number). To this end we use the power series expansions of $f, a,$ and r^2k at the origin (where the series converge),[12]

$$f(r)=f_1r^2+\tfrac{1}{8}f_1r^4+\ldots, \quad a(r)=\tfrac{1}{8}r^2-\tfrac{1}{24}f_1^2r^6+\ldots,$$
$$k(r)=r^{-2}+k_1r^2+\ldots \quad . \tag{4.19}$$

Here $f_1=0.236$ and $k_1=-0.025$ from the numerical analysis. We find that the solutions of (4.16) and (4.17) have the following expansions at the origin:

$$g(r)=g_{-1}\log r+g_1+\tfrac{1}{2}f_1^2r^2+\cdots,$$
$$b(r)=b_{-1}r^{-1}+b_1r+(\tfrac{1}{8}b_1-2f_1k_1)r^3+\ldots \quad . \tag{4.20}$$

The higher-order terms in $g(r)$ are even powers of r, whereas the higher-order terms in $b(r)$ are odd powers of r. Hence, the quadratic terms in (4.18) are C^∞ near the origin if and only if $h_{-1}=b_{-1}=0$. So far, the constants g_1 and b_1 are arbitrary.

For large r the functions $f, a,$ and k can be written as convergent series whose leading terms are[12]

$$f(r)=1+\tilde{f}_1(r)e^{-r}+\cdots,$$
$$a(r)=1+\tilde{a}_1(r)e^{-r}+\cdots, \tag{4.21}$$
$$k(r)=\tilde{k}_1(r)e^{-r}+\cdots,$$

with coefficient functions which are polynomially bounded. This leads to the existence of exponentially decaying solutions which asymptotically are of the form

$$g(r)=\tilde{g}_1(r)e^{-r}+\cdots, \quad b(r)=\tilde{b}_1(r)e^{-r}+\cdots. \tag{4.22}$$

Here $\tilde{g}_1$ and $\tilde{b}_1$ are polynomially bounded.

By numerical integration, the coefficients g_1 and b_1 which lead to an exponential falloff at infinity, are found to be $g_1=-0.144$ and $b_1=-0.026$. The existence of such functions can be explained analytically as follows: Eq. (4.16) shows that for positive g_1, g cannot have a maximum for any r. So the function diverges exponentially. For very small g_1, the term on the right-hand side of (4.16) will force the function to cross the r-axis, and then, as before, diverge exponentially. For very large negative g_1, the third term in (4.16) will force g to go through a maximum for large r. After that, the function cannot have a minimum and must go to minus infinity. Because of the continuous dependence on the initial data, we have an open set of data for which g crosses the r-axis, and an open set of data for which g goes through a maximum below the r-axis. Therefore, we have at least one value of g_1 for which the function does neither. This function must converge and does so to zero, exponentially.

A similar argument explains the existence of an acceptable solution $b(r)$ to Eq. (4.17). The right-hand side of that equation is positive. So again b cannot have a maximum above the r-axis. Also, for very small negative b_1, the right-hand side will force b to go through a minimum and then cross the r-axis. For very large negative b_1, the third term in (4.17) prevents b from going through a minimum. In between these two possibilities we find the desired solution which goes through a minimum but does not cross the r-axis. Such a solution must decay exponentially.

The cubic terms can be calculated in the same manner. We find, at third order,

$$\begin{aligned}\phi &= \ldots + (\alpha+\imath\beta)(\alpha^2+\beta^2)fh + (\alpha+\imath\beta)^3\left(-c' + \frac{3+2a}{r}c\right)e^{-4\imath\theta} + \cdots,\\ A_1 + \imath A_2 &= \cdots + \imath(\alpha+\imath\beta)(\alpha^2+\beta^2)\left[-h' - \frac{2}{r}h + 2g\left(k' + \frac{2k}{r}\right) + 2kg'\right]e^{-\imath\theta}\\ &\quad + \imath(\alpha+\imath\beta)^3 fc e^{-5\imath\theta} + \cdots.\end{aligned} \tag{4.23}$$

The new radial functions, $h(r)$ and $c(r)$, satisfy the equations,

$$h'' + \frac{1}{r}h' - \left(f^2 + \frac{4}{r^2}\right)h = 4k'g' + 2fk\left(2fk^2 + 3fg + \frac{1+2a}{r}b - b'\right), \tag{4.24}$$

$$c'' + \frac{1}{r}c' - \left(\frac{1+f^2}{2} + \frac{9+12a+4a^2}{r^2}\right)c = 2kf^2 b - 2\left(k' + \frac{2k}{r}\right)\left(\frac{1+2a}{r}b - b'\right). \tag{4.25}$$

Near the origin, Eq. (4.25) has a series solution in powers of r^2 of the form

$$h(r) = f_1^2 + h_1 r^2 + h_2 r^4 + \cdots. \tag{4.26}$$

The constant term is given in terms of the coefficient f_1 of the leading term in the expansion (4.19) of $f(r)$. The form of this term leads to the cancellation of the r^{-1}-terms in the radial function multiplying $e^{-\imath\theta}$ in (4.23), and thus ensures that this term in (4.23) is C^∞ on $\mathbf{R}^2$. The series in odd powers of r for $c(r)$ which solves Eq. (4.25) near the origin, is

$$c(r) = c_1 r^3 + c_2 r^5 + \cdots. \tag{4.27}$$

The form of the series solutions at the origin guarantees that the cubic terms in (4.23) are C^∞ functions on $\mathbf{R}^2$. For large r, Eqs. (4.24) and (4.25) have exponentially decaying solutions.

V. CONCLUSIONS

Our expansions show a simple θ-dependence in terms of trigonometric functions. In both models, the expansion of ϕ exhibits the following pattern:

$$\begin{array}{cccccccc}
 & & & & & & e^{2\imath\theta} & \\
 & & & & & e^{0\imath\theta} & & \\
 & & & & e^{-2\imath\theta} & & e^{2\imath\theta} & \\
 & & & e^{-4\imath\theta} & & e^{0\imath\theta} & & \\
 & & e^{-6\imath\theta} & & e^{-2\imath\theta} & & e^{2\imath\theta} & \\
 & e^{-8\imath\theta} & & e^{-4\imath\theta} & & e^{0\imath\theta} & & \\
\ldots & & \ldots & & \ldots & & \ldots &
\end{array}$$

Here the first line gives the θ dependence of the zero order term; the second line gives the first order term, and so on. We get a similar triangular pattern for the θ dependence of $A_1 + \imath A_2$ at any order. For the radial functions we find differences between the two models. In the model for one complex field, the radial functions can be given explicitly in terms of exponential functions. However, for the angular dependence (3.15), a singularity occurs at the origin. [We have found no solution to (3.14) which is not of the form (3.15); we have no proof that there is none.]

For the Ginzburg–Landau theory on the other hand, the expansion is smooth, at least up to the order to which we carried out our calculations. In this model the radial functions are not given in terms of well-known functions. Having used the technique to calculate the terms up to third order,

it is quite clear how to proceed to any order, and also how to proceed in the case of more than two vortices. We expect these expansions to converge for small separation parameters in the physical Ginzburg–Landau model. However, we do not have an estimate of the radius of convergence.

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Energy estimates for the von Kármán model of thin-film blistering

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We consider the behavior of buckling driven thin-film blisterings using von Kármán's plate theory. Our focus is on the setting where the blistered region is the unit square with clamped boundary conditions at the vertical sides and periodic ones along the horizontal sides. In this setting, we prove rigorous upper and lower bounds for the elastic energy which are of the same order as the film thickness. We also present a convincing argument for the necessity of branching of folds near the boundary as has been observed in experiments. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1316058]

I. INTRODUCTION

In this sequel to Ref. 1, we continue our investigation of thin-film blistering via the von Kármán model. These blisters are formed when a thin film in a state of residual compression decoheres and buckles away from its substrate. The goal is to better understand the nature of the complex folding and branching patterns observed in experiments.[2–7] Our focus here is on the incorporation of in-plane displacements in the model.

Given a blistered region Ω, we shall denote by u the out-of-plane displacement of the film and let (w_1,w_2) denote the in-plane displacements. Then in our scaling, the von Kármán model takes the form

$$\min_{\substack{w=0,u=0,\\ \partial u/\partial n=0, \text{ at } \partial\Omega}} \int_\Omega [(w_{\alpha,\beta}+w_{\beta,\alpha})/2+u_{,\alpha}u_{,\beta}/2-\delta_{\alpha\beta}]^2+\varepsilon^2|\nabla\nabla u|^2, \tag{1}$$

where ε is the normalized film thickness. The formulation above corresponds to the choice of zero Poisson's ratio, though we note that this choice does not affect the essential features of the problem. See Ref. 1 for a more detailed discussion of the model and, for example, Refs. 8–11 for a derivation.

In this article, we choose to study the setting where Ω is the unit square. What is more, we will take clamped boundary conditions at $x=0$ and $x=1$, but replace the clamped conditions by periodic ones along $y=0$ and $y=1$. To be more specific, our problem is formulated as

$$\min_{\substack{u=0,u_x=0, \text{ at } x=0,1\\ w_1=0,w_2=0, \text{ at } x=0,1\\ w_1,w_2,u,\nabla u, \text{ periodic in } y}} \int_0^1\int_0^1 [(w_{\alpha,\beta}+w_{\beta,\alpha})/2+u_{,\alpha}u_{,\beta}/2-\delta_{\alpha\beta}]^2+\varepsilon^2|\nabla\nabla u|^2\,dx\,dy. \tag{2}$$

Here α and β run between 1 and 2. We will henceforth refer to the first term above as the membrane energy and we refer to the singular perturbation term as the bending energy.

A primary motivation in our choice of boundary conditions is to focus our attention on perhaps the simplest geometry in which the behavior of the film near the clamped boundary can be successfully analyzed. A secondary rationale is our belief that through a local curvilinear coordi-

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nate change, the folding patterns of an arbitary smooth blistered domain might be understood through a study of the annular setting. Physically, our choice of domains is also motivated by earlier studies of instabilities of straight delamination blisters (Refs. 4, 12). By analyzing carefully the structure of solutions for a straight blister, our hope here is to gain insight into the nature of the stress distribution near the boundary which is ultimately responsible for the observed instabilities of such a blister region.

Various simplifications have been carried out on (1). If one completely ignores all in-plane displacements ($w_1=w_2=0$), then one is left with an energy of the form

$$|\Omega|+\int_\Omega\left(1-\frac{1}{2}|\nabla u|^2\right)^2+\varepsilon^2|\nabla\nabla u|^2$$

whose infimum is clearly $\mathcal{O}(1)$. This functional has been studied extensively; see, e.g., Refs. 13–17.

Another possible simplication of (1) comes from assuming a one-dimensional folding pattern, sometimes referred to as an ''Euler column.''[4] That is, one takes $u=u(x)$, $w_1=w_1(x)$ and $w_2\equiv 0$. This again yields an order 1 infimum to the energy.

In Ref. 1 we took a less drastic simplication by only assuming a one-dimensional in-plane displacement [i.e., $w_1=w_1(x)$, $w_2\equiv 0$] while allowing u to depend on x and y. Within this class of deformations, we obtained rigorous upper and lower bounds on the energy of order $\varepsilon^{2/3}$. The construction of a minimizing sequence achieving the asymptotic upper bound involved complicated branching patterns near the clamped boundaries of the unit square. This construction was reminiscent of branching sequences used in Ref. 18.

In this paper, we do not impose any restrictions on (w_1,w_2,u) and we then prove rigorous upper and lower bounds for the full von Kármán energy (1) which are of order ε. In light of these bounds, one obtains a convincing argument for the necessity of branching near the boundary. We make this argument formally at the outset of the next section. The folding patterns we obtain lend rigorous support to earlier observations made in the physics literature (Refs. 12, 19). In Ref. 19 one finds a prediction of branching near the boundary based on energetic scaling arguments while Ref. 12 contains a stability analysis of the von Kármán equations linearized about the one-dimensional ''Euler column'' solution for a straight-edged blister—an analysis which predicts the instability of this solution. Our assertion here is that the oscillatory profile near the boundary predicted by our construction imposes nonuniform stresses along the boundary which in turn indicate the instability of the delamination front as is depicted, for example, in Ref. 12, Fig. 4. The resultant wavy boundary of the blistered region would then resemble the often observed ''telephone cord'' pattern for such films.

Finally, we should note that our formulation (1) arose through a choice of eigenstrain $e^*_{\alpha\beta}=\delta_{\alpha\beta}$. In reality, the eigenstrains involved are much smaller. Alternatively, one could have taken, say, $e^*_{\alpha\beta}=k\delta_{\alpha\beta}$, with k a second small parameter (in addition to the thickness ε). Then, with a rescaling of $u\to\sqrt{k}u$ and $(w_1,w_2)\to k(w_1,w_2)$, one would arrive at an energy of order $k^{3/2}\varepsilon$. (See Remark 2.)

Note: After submission of this paper, we learned of a similar result for arbitrary smooth domains just completed in Ref. 20.

II. MAIN RESULTS

Before presenting the main theorem and its proof, we wish to give a feel for the ingredients leading to the lower and upper bounds on the minimal energy. Thus, for the moment, we proceed formally.

Much of the argument relies on the obvious requirement to keep the membrane energy as small as possible. In particular, one would expect a minimizer (or minimizing sequence) to satisfy the condition

$$\int_0^1 \left(w_{2,y}(x,y) + \frac{1}{2} u_y^2(x,y) - 1 \right)^2 dy \approx 0,$$

for x away from $x=0$ or $x=1$. In light of the periodicity of w_2 in y, this suggests that

$$\int_0^1 \frac{1}{2} u_y^2(x,y)\, dy \approx 1, \tag{3}$$

for such x. However, the boundary conditions for u imply that $\int_0^1 u_y^2(0,y)dy = \int_0^1 u_y^2(1,y)dy = 0$, necessitating a boundary layer along the two vertical sides of the unit square. Let us introduce a boundary layer width δ and note that in light of (3), the integrand in the membrane energy will be $\mathcal{O}(1)$ within this layer, yielding a contribution to the total energy of order $\mathcal{O}(\delta)$.

On the other hand, turning to the bending energy in such a boundary layer, we see that since u_y must make an $\mathcal{O}(1)$ change over an x-interval of size δ, we find

$$\varepsilon^2 \int \int_{\text{boundary layer}} u_{xy}^2 dx\, dy \sim \frac{\varepsilon^2}{\delta}. \tag{4}$$

Hence, the total energy is at least of order $\mathcal{O}(\delta + \varepsilon^2/\delta)$, which immediately indicates the lower bound of ε and a boundary layer width $\delta \sim \varepsilon$.

To motivate our construction leading to an upper bound of order ε, we must look at the other terms in the bending energy. To analyze these, we formally introduce a quantity $\gamma(x)$ representing the wavelength of oscillations of u in the y-direction for x away from the boundary. In view of (3), however, one can equivalently think of $\gamma(x)$ as measuring the amplitude of u along vertical segments. For example, one might think of $\gamma(x) = (\int_0^1 u^2(x,y)dy)^{1/2}$.

With this notion in hand, we can estimate

$$\varepsilon^2 \int \int_{\text{boundary layer}} u_{xx}^2 dx\, dy \sim \varepsilon^2 \left(\frac{\gamma(\delta)}{\delta^2} \right)^2 \delta = \frac{\varepsilon^2 \gamma(\delta)^2}{\delta^3}.$$

Since we previously found that $\delta \sim \varepsilon$, the above estimate shows that $\gamma(\delta) \sim \varepsilon$ as well if we are to achieve the upper bound of order ε. On the other hand, using the standard inequality

$$\int_0^1 u^2 dy \int_0^1 u_{yy}^2 dy \geqslant \left(\int_0^1 u_y^2 dy \right)^2,$$

we see through (3) that

$$\int_0^1 u_{yy}^2(x,y)dy \geqslant \frac{1}{\gamma(x)^2},$$

for x in the interior of the square. Consequently, the total bending energy behaves like $\varepsilon^2 \int [1/\gamma(x)^2]\, dx$. This suggests that we must increase $\gamma(x)$ from $\mathcal{O}(\varepsilon)$ to at least $\mathcal{O}(\sqrt{\varepsilon})$ as we move into the interior of the square.

In our particular construction, we achieve this transition incrementally by successively doubling the wavelengths as we move towards the interior of the square.

So far we have neglected the contribution from the membrane energy in the interior. Ideally, one might seek to eliminate this contribution entirely, leading to the conditions

$$w_{1,x} + \tfrac{1}{2} u_x^2 - 1 = 0, \tag{5}$$

$$w_{2,y} + \tfrac{1}{2} u_y^2 - 1 = 0, \tag{6}$$

$$w_{2,x}+w_{1,y}+u_x u_y=0. \tag{7}$$

Taking the sum of the second y-derivative of (5) and the second x-derivative of (6) and then subtracting the mixed second derivative of (7), one arrives at a consistency condition,

$$u_{xx}u_{yy}-u_{xy}^2=0. \tag{8}$$

That is, ideally, the graph of u should be a developable surface (see Ref. 21). In particular, one can satisfy this condition by taking $u=u(x+y)$. Our particular choice for u below involving cosine functions is motivated by these considerations and by the exact solution in the one-dimensional example found in Ref. 1.

These heuristics are now made rigorous through the following theorem.

Theorem 1: *There exist positive constants C_1 and C_2 independent of ε such that the minimal energy E_ε of (2) satisfies the bounds*

$$C_1\varepsilon\leqslant E_\varepsilon\leqslant C_2\varepsilon,$$

for ε sufficiently small.

Proof: (i) Lower bound. Suppressing the ε-dependence, we denote a minimizer to (2) by (u,w_1,w_2). Then denote by δ the positive number satisfying

$$\delta=\max_{x\in[0,1]}\left\{x:\int_0^1 u_y(x',y)^2dy\leqslant 1,\quad \forall x'\in[0,x]\right\}.$$

Certainly $0<\delta\leqslant 1$ since the boundary conditions imply that $u_y(0,y)=0$ for $y\in[0,1]$.

Then, using the periodicity of w_2 in y, we estimate the membrane energy on $[0,\delta]\times[0,1]$ as follows:

$$\int_0^\delta\int_0^1\left(w_{2,y}+\frac{1}{2}u_y^2-1\right)^2dydx\geqslant\int_0^\delta\left(\int_0^1 w_{2,y}+\frac{1}{2}u_y^2-1dy\right)^2dx=\int_0^\delta\left(\int_0^1\frac{1}{2}u_y^2-1dy\right)^2dx\geqslant\frac{1}{4}\delta. \tag{9}$$

If $\delta=1$, then the desired lower bound is immediate. If, on the other hand, $\delta<1$, then $\int_0^1 u_y(\delta,y)^2dy=1$ and one can estimate the bending energy in this strip from below by

$$\varepsilon^2\int_0^1\int_0^\delta u_{xy}^2dx\,dy\geqslant\varepsilon^2\int_0^1\frac{1}{\delta}\left(\int_0^\delta u_{xy}dx\right)^2dy=\frac{\varepsilon^2}{\delta}. \tag{10}$$

Hence, we find

$$E_\varepsilon\geqslant\frac{1}{4}\delta+\frac{\varepsilon^2}{\delta}\geqslant\varepsilon. \tag{11}$$

(ii) Upper bound. We begin by constructing a sequence of functions (u,w_1,w_2) on the unit square which will satisfy the boundary conditions at $x=0$. Again, we will suppress the ε-dependence in referring to our constructed sequence. Then through some straight-forward reflections and rescalings, we will modify the construction to satisfy the boundary conditions at $x=1$ as well.

Making the definition

$$b_n=\left(\frac{1}{2^{3/2}}\right)^n, \tag{12}$$

we will denote the strip $[b_{n+1},b_n]\times[0,1]$ by I_n for $n=0,1,2,\ldots,N$ where N will be specified later. Then for any $\varepsilon>0$ we define a positive number $a<1$ by the condition

$$\frac{1}{a\varepsilon^{1/3}} = 2k\pi, \text{ for some integer } k, \tag{13}$$

and we let

$$a_n = \frac{a\varepsilon^{1/3}}{2^n}. \tag{14}$$

We also introduce $f:[0,1]\to\mathbf{R}$ and $g:[0,1]\to\mathbf{R}$ as any two functions satisfying the conditions

$$0\leqslant f(x)\leqslant 1,\ 0\leqslant g(x)\leqslant 1, \text{ for } x\in[0,1], \tag{15}$$

$$f(1)=1,\ f'(1)=f(0)=f'(0)=0, \tag{16}$$

$$g(0)=1,\ g'(0)=g(1)=g'(1)=0, \tag{17}$$

$$f(x)^2+g(x)^2=1, \text{ for } x\in[0,1]. \tag{18}$$

We are now prepared to define the function u in our construction via the formula

$$u(x,y)=2a_n\left[\cos\left(\frac{x+y}{a_n}\right)+1\right]f_n(x)+2a_{n+1}\left[\cos\left(\frac{x+y}{a_{n+1}}\right)+1\right]g_n(x), \tag{19}$$

for $x\in I_n$ and $y\in[0,1]$, $n=0,1,2,\ldots,N$ where we have introduced

$$f_n(x)=f\left(\frac{x-b_{n+1}}{b_n-b_{n+1}}\right) \tag{20}$$

and

$$g_n(x)=g\left(\frac{x-b_{n+1}}{b_n-b_{n+1}}\right). \tag{21}$$

Note that u so defined will satisfy the periodic boundary conditions at $y=0$ and $y=1$ in light of (13) and will be sufficiently smooth in light of (16)–(17).

Next we turn to the definition of w_2. In order to eliminate one of the terms in the membrane energy completely, we will choose this function so that

$$w_{2,y}=1-\frac{u_y^2}{2}. \tag{22}$$

This leads after an integration and a use of (18) to the formula

$$\begin{aligned} w_2(x,y)=&\frac{a_n}{2}f_n(x)^2\sin\left[2\left(\frac{x+y}{a_n}\right)\right]+\frac{a_{n+1}}{2}g_n(x)^2\sin\left[2\left(\frac{x+y}{a_{n+1}}\right)\right]-2a_nf_n(x)g_n(x)\sin\left[\left(\frac{x+y}{a_n}\right)\right]\\ &+\frac{2}{3}a_nf_n(x)g_n(x)\sin\left[3\left(\frac{x+y}{a_n}\right)\right]+h_2(x), \end{aligned} \tag{23}$$

where h_2 will be specified shortly.

We turn now to the definition of w_1, where one goal will be to completely eliminate the contribution to the membrane energy from the cross-term

$$(\tfrac{1}{2}w_{1,y}+\tfrac{1}{2}w_{2,x}+\tfrac{1}{2}u_xu_y)^2.$$

This can be accomplished by choosing $h_2(x)=-2x$ and then seeking w_1 of the form

$$w_1(x,y)=w_2(x,y)+h_1(x,y)+2x,$$

where, in order to kill the cross-term, we are led to take

$$\begin{aligned}h_{1,y}(x,y)=&-a_n f_n(x)f_n'(x)\sin\left[2\left(\frac{x+y}{a_n}\right)\right]-a_{n+1}g_n(x)g_n'(x)\sin\left[2\left(\frac{x+y}{a_{n+1}}\right)\right]\\&+(f_n(x)g_n'(x)+f_n'(x)g_n(x))\left(2a_n\sin\left[\left(\frac{x+y}{a_n}\right)\right]-\frac{2}{3}a_n\sin\left[3\left(\frac{x+y}{a_n}\right)\right]\right)\\&-2u_y(x,y)\left(a_n f_n'(x)\left[\cos\left(\frac{x+y}{a_n}\right)+1\right]+a_{n+1}g_n'(x)\left[\cos\left(\frac{x+y}{a_{n+1}}\right)+1\right]\right).\end{aligned}\tag{24}$$

Integrating in y we see that each term in h_1 is a product of functions of $x+y$ and either f_nf_n', g_ng_n', f_ng_n' or g_nf_n', along with a factor that is quadratic in a_n and a_{n+1}. We take the arbitrary function of x arising through the integration to be zero.

With this choice, one can compute $h_{1,x}$ to find that $h_{1,x}=h_{1,y}$ plus terms involving products of quadratic expressions in a_n and a_{n+1} with expressions involving either $(f_n')^2,(g_n')^2,f_n'',g_n''$ or $f_n'g_n'$ multiplied against $\mathcal{O}(1)$ quantitites. Hence,

$$h_{1,x}=h_{1,y}+\mathcal{O}\left(\frac{a_n^2}{b_n^2}\right).\tag{25}$$

To clarify our construction, note from (19) that $u_x=u_y+A$ where $|A|$ is of order $\mathcal{O}(a_n/b_n)$ while $w_{2,x}$ takes the form $w_{2,x}=w_{2,y}+B-2$ where our choice of h_1 yields the condition

$$h_{1,y}+B+Au_y=0.\tag{26}$$

Turning then to the remaining term in the membrane energy, we find through (22), (25), and (26) that

$$\begin{aligned}w_{1,x}+\tfrac{1}{2}u_x^2-1&=w_{2,y}+B+h_{1,x}+\tfrac{1}{2}(u_y+A)^2-1\\&=\left(w_{2,y}+\frac{1}{2}u_y^2-1\right)+B+h_{1,y}+Au_y+\mathcal{O}\left(\frac{a_n^2}{b_n^2}\right)=\mathcal{O}\left(\frac{a_n^2}{b_n^2}\right).\end{aligned}\tag{27}$$

Estimating the bending energy is much simpler. Indeed, a view of (19), along with the fact that $a_n\leqslant b_n$, immediately yields the estimate

$$|\nabla\nabla u|=\mathcal{O}\left(\frac{1}{a_n}\right),\ \text{ in }\ I_n.\tag{28}$$

Consequently, recalling (12) and (14), we arrive at the estimate

$$\begin{aligned}\int\int_{I_n}&\left\{\left[\left(w_{1,x}+\frac{1}{2}u_x^2-1\right)^2+\left(w_{2,y}+\frac{1}{2}u_y^2-1\right)^2\right.\right.\\&\left.\left.+2\left(\frac{1}{2}(w_{1,y}+w_{2,x})+\frac{1}{2}u_xu_y\right)^2\right]+\varepsilon^2|\nabla\nabla u|^2\right\}dxdy\\&=\mathcal{O}\left(\frac{a_n^4}{b_n^3}\right)+\varepsilon^2\mathcal{O}\left(\frac{b_n}{a_n^2}\right)\leqslant C\varepsilon^{4/3}(\sqrt{2})^n,\end{aligned}\tag{29}$$

where C is a positive constant independent of ε and n.

We wish to continue the iteration on n until the function u is decreased to $\mathcal{O}(\varepsilon)$, leading us to select N so that

$$\frac{1}{2^N} \sim \varepsilon^{2/3} \quad \text{and} \quad b_{N+1} = \varepsilon. \tag{30}$$

We should point out here that this choice of N is consistent with our condition that $a_n \leqslant b_n$. Summing over n we that find that the total energy over the set $[\varepsilon,1]\times[0,1]$ is bounded from above by

$$\varepsilon^{4/3} \sum_{n=0}^{N} (\sqrt{2})^n \sim \varepsilon^{4/3} (\sqrt{2})^N = \mathcal{O}(\varepsilon). \tag{31}$$

Our next task is to match the clamped boundary conditions at $x=0$. To accomplish this, we will interpolate as was done in Ref. 1. For completeness, we present the construction below. In the strip $[0,\varepsilon]\times[0,1]$, we set $u=P$ where

$$P(x,y) = \left(\frac{u_x}{\varepsilon^2} - \frac{2u}{\varepsilon^3} \right) x^3 + \left(\frac{3u}{\varepsilon^2} - \frac{u_x}{\varepsilon} \right) x^2. \tag{32}$$

Here u and u_x are evaluated at (ε,y). Note that P and ∇P so defined agree with u and ∇u at $x=\varepsilon$ while $P(0,y)=0$ and $\nabla P(0,y)=(0,0)$.

For the functions w_1 and w_2 in this strip $[0,\varepsilon]\times[0,1]$, we simply linearly interpolate in x between the functions $w_\alpha(\varepsilon,y)$ and 0 for $\alpha=1,2$.

To estimate the energy in this boundary layer, we first note that $|\nabla P| = \mathcal{O}(1)$ while $|\nabla\nabla P| = \mathcal{O}(1/\varepsilon)$ and $|\nabla w_\alpha| = \mathcal{O}(1)$ since $|w_\alpha(\varepsilon,y)| = \mathcal{O}(\varepsilon)$ for $\alpha=1,2$ and $y\in[0,1]$. Hence, the total energy in the layer $[0,\varepsilon]\times[0,1]$ is $\mathcal{O}(\varepsilon)$.

It remains to alter our construction so as to satisfy the boundary conditions at $x=1$ as well. At first glance, one might be tempted to simply compress our construction to the interval $[0,1/2]\times[0,1]$ and then reflect u evenly in x. However, in view of the term

$$\left(w_{1,x} + \frac{1}{2} u_x^2 - 1 \right)^2$$

in the membrane energy, this would require an odd reflection in w_1 leading to a discontinuity since $w_1(1,y)\neq 0$. What is more, such an even reflection of u would lead to a jump in u_x since $u_x(1,y)\neq 0$.

Instead we will take a different tack. Using almost the same construction as we used on $[0,1]\times[0,1]$, we can work on the strips $[2-b_n,2-b_{n+1}]\times[0,1]$ for $n=0,1,2,\ldots,N$ and an interpolation layer $[2-\varepsilon,2]\times[0,1]$ to obtain the boundary values

$$u(2,y) = u_x(2,y) = w_1(2,y) = 0, \quad \text{for } y\in[0,1]. \tag{33}$$

Noticing that w_2 is the sum of $-2x$ and an oscillatory function [cf. (23)], we use the interpolation layer to eliminate the oscillation, leaving the boundary values

$$w_2(2,y) = -4.$$

In light of (33), we can now take an odd reflection in x for w_1 and even reflections for u and w_2 so as to obtain a construction on $[0,4]\times[0,1]$ whose energy is $\mathcal{O}(\varepsilon)$. Rescaling $x\to x/4$, $y\to y/4$ and $(u,w_1,w_2)\to 1/4(u,w_1,w_2)$, and using the periodicity of our original construction in y, we obtain the desired construction on the unit square. □

Remark 1: In our heuristics preceeding the proof we indicated that an interior lengthscale for oscillations in u of order $\varepsilon^{1/2}$ would suffice. In fact, there is some freedom, in that any scale between $\varepsilon^{1/2}$ and $\varepsilon^{1/3}$ will do, and we have chosen the latter in our construction.

Remark 2: When the von Kármán model is derived, it is assumed that the derivatives of the in-plane displacements (w_1, w_2) are small and, therefore, quadratic terms in these derivatives can be neglected; see, e.g., Refs. 8–11. We note that in our construction, the first derivatives of (w_1, w_2) are of order $\mathcal{O}(1)$. However, in reality, for thin-film blistering problems, the eigenstrains are smaller, e.g., $e^*_{\alpha\beta} = k\delta_{\alpha\beta}$, where $k = o(1)$. Had we taken such eigenstrains, then, with a rescaling of $u \to \sqrt{k}u$ and $(w_1, w_2) \to k(w_1, w_2)$, it is obvious that the derivatives of (w_1, w_2) would have been of order $\mathcal{O}(k)$. Consequently, our construction is consistent with the assumption in the von Kármán model.

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Fractional Fokker–Planck equation for nonlinear stochastic differential equations driven by non-Gaussian Lévy stable noises

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The Fokker–Planck equation has been very useful for studying dynamic behavior of stochastic differential equations driven by Gaussian noises. However, there are both theoretical and empirical reasons to consider similar equations driven by strongly non-Gaussian noises. In particular, they yield strongly non-Gaussian anomalous diffusion which seems to be relevant in different domains of Physics. In this paper, we therefore derive a fractional Fokker–Planck equation for the probability distribution of particles whose motion is governed by a *nonlinear* Langevin-type equation, which is driven by a Lévy stable noise rather than a Gaussian. We obtain in fact a general result for a Markovian forcing. We also discuss the existence and uniqueness of the solution of the fractional Fokker–Planck equation. [DOI: 10.1063/1.1318734]

I. INTRODUCTION AND MOTIVATION

The Fokker–Planck equation is one of the most celebrated equations in Physics, since it has been very useful for studying[1] the dynamic behavior of stochastic differential equations driven by Gaussian noises. However, it turns out that many physical phenomena are outside of this framework. For instance, it has been argued that diffusion by geophysical turbulence[2–7] corresponds, loosely speaking, to a series of sticking (pauses), when the particle is trapped by a coherent structure, and (fast) flights, when the particle moves in the jet flow. A similar phenomenology is observed for zoo plankton grazing.[8,9]

Although there have been some attempts[6] to analyze and quantify this behavior with the help of the classical Fokker–Planck equation, i.e., assuming finite moments of all orders, some laboratory experiments[3–5] or numerical simulations of geostrophic turbulence[10] show that this phenomenology could be rather a consequence of the presence of heavy tails (i.e., power law falloff) for the probability distribution and a strong anisotropy with a clearly preferred direction of diffusion. One can conclude[11] that if the processes are additive, the corresponding walks are Lévy motions.

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Let us recall that indeed stable Lévy motions $L(t)$ generalize the Brownian motion $B(t)$ in the sense that first they are also motions (e.g., Refs. 12 and 13) whose increments $\Delta L(t,\Delta t)=L(t+\Delta t)-L(t)$ are stationary (therefore ΔL has no statistical dependence on t) and independent for any nonoverlapping time lags Δt. Therefore, $L(t)$ corresponds to the sum of independent, identically distributed Lévy stable variables.[14–18] The second common property is that these increments satisfy a ''stability property:'' up to a rescaling and recentring, the sum of different steps has the same probability distribution as one of the steps. Lévy stable variables are precisely defined by this property. The stability property implies in both cases a property of attraction: under rather general conditions a renormalized sum of independent identically distributed variables converge to a stable law. Furthermore, there are no other attractive laws. This explains why the stable property is so important. The attraction property corresponds to a broad generalization of the central limit theorem, with the important difference that whereas the classical theorem (Gaussian case) is satisfied with the condition that the variance is finite, the convergence towards a Lévy law is obtained with the condition that *not only* the variance of the summands X_i is infinite, but also that all their moments of order q equal to or larger than a critical order α $(0<\alpha<2)$ are infinite. This critical order α is called the Lévy stability index and corresponds to the exponent of the power law of probability distribution tails:

$$\text{any } s\gg 1\text{: } \Pr(|\Delta L|>s)\approx s^{-\alpha}\Leftrightarrow\text{any } q\geqslant\alpha\text{: } E(|X|^q)=\infty, \tag{1}$$

where Pr denotes the probability, $E(\,)$ is the mathematical expectation, and s is a given (large) non-negative threshold. This statistical divergence of a Lévy motion is due to jumps, whereas a Brownian motion is almost surely continuous.

This index is the most important of the four parameters defining a Lévy stable law. The second one is the skewness β $(-1\leqslant\beta\leqslant 1)$ which defines the degree of asymmetry of the law, which is maximal for $\beta=-1$ or $\beta=+1$, and the law is symmetric when $\beta=0$. In spite of its name and some common properties, β nevertheless does not correspond to the classical skewness of a quasi-Gaussian law. The latter is indeed undefined for a stable Lévy law due to the above-mentioned statistical divergences. The center γ corresponds to the statistical mean when defined (i.e., $\alpha>1$) and/or to the median when symmetric (i.e., $\beta=0$). The scale parameter $D(D\geqslant 0)$ corresponds to a generalization of the variance of the Gaussian case. More precisely, as discussed below, it corresponds to the intensity scale of the cumulant of (possibly noninteger) order α. It yields an anomalous[19] generalization of the classical Einstein relation: $\mathrm{Var}[X(t)-X(t_0)]=2D(t-t_0)$, where Var( ) denotes the variance. Finally, let us emphasize that the Gaussian case corresponds to the limit case $\alpha=2$, which also implies $\beta=0$, i.e., no asymmetry.

Further comments are now in order on the relevance of Lévy motions in Physics. On the one hand, claims in favor of the relevance of Lévy motions have been made on many physical phenomena ranging from subrecoil laser cooling[20,21] to diffusion by flows in porous media,[22,23] including finance fluctuations,[24,25] see Refs. 26 and 27 for other examples. Many systems indeed display a phenomenology rather similar to that we reported above on geostrophic turbulence.

On the other hand, important questions have been raised. In particular, Ref. 28 questioned the resulting infinite variance of the advecting field for porous media. Indeed, it turns out that recent estimates[29] of the power law of the probability distributions of the hydraulic conductivity yields an exponent $\alpha\approx 3.5$. The question of finite variance might apply to other examples, in particular for atmospheric turbulence where different studies[30] yield a critical exponent $\alpha\approx 7$ for the wind field. Therefore, in spite of their clear phenomenological interest, the relevance of pure Lévy motions could be questioned.

The main goal of this paper is to clarify and define a framework adequate for handling motions more general than pure Lévy motions and which are nevertheless generated by the latter. We will do it by building upon a series of rather recent works[31–37,19,38] which show that the probability density of particles moving with a Lévy motion satisfies a generalized Fokker–Planck equation involving fractional orders of differentiation. Indeed, it could be first argued in a ''very formal and phenomenological'' manner[31] that a fractional power of the Laplacian yields an anomalous scaling for the corresponding diffusion.

A fractional Fokker–Planck equation was obtained in a less formal manner by Refs. 32 and 35 in the framework of the continuous time random walks (CTRWs) model of anomalous diffusion.[33] However, this method does not involve directly a stable Lévy process, but a walk sharing some behavior common with the latter, without being equivalent to it. A different fractional Fokker–Planck equation was introduced[37] with the help of a phenomenological and interesting transformation of the classical Fick law into a fractional Fick law. However, it is not clear that its solution corresponds to a (non-negative) probability distribution. A rather distinct approach was followed by Refs. 34 and 19 since it starts with a *linear* Langevin-type equation with random forces which are *exact* stable Lévy processes, which can be symmetric as well as asymmetric, and with no limitation on the possible values of the Lévy index α. The fundamental mathematical tool which is used is the second characteristic (or cumulant generating) function of the motion defined by this Langevin-type equation. The particular case of symmetric processes correspond to what was previously inferred by Refs. 31, 32, 35, and 37. However, it was shown that in the more general case of asymmetric processes, a new nontrivial advective–diffusive term appears. This is confirmed with the help of a reinterpretation of the characteristic function of a Lévy motion.[38]

We already discussed that theoretically and empirically the nonfiniteness of the variance could be questioned. There are two more general questions: the inhomogeneities of the medium, which are first emphasized for the introduction of the Lévy motions, are finally reduced to a (homogeneous) distribution of times when the particle is strongly kicked. As soon as this representation is granted, the medium (and its properties) does not intervene any longer. This is very restrictive and for instance incompatible with the multifractality of the medium[39,8] (or of the diffusion) when observed. The second reason is that the underlying processes are thought to be strongly nonlinear, whereas the transport is modeled with the help of a (stochastic) linear equation.

Both the successes and limitations of the previous results plead in favor of investigating a local and nonlinear modeling with the help of Lévy motions. This is the reason that we investigate the properties of *nonlinear* Langevin-type equation forced by a Lévy stable motion.

II. STATEMENT OF THE PROBLEM

Further to our above discussion, we consider the following *nonlinear* Langevin-type equation for a stochastic (real) quantity $X(t)$ (e.g., location of a particle):

$$dX(t)=m(X(t),t)dt+\sigma(X(t),t)dL, \tag{2}$$

where the driving source is a Lévy stable motion $L(t)$ instead of Brownian motion $B(t)$. The latter case corresponds to the basis of stochastic calculus (e.g., Ref. 40) and the corresponding differential equation is often called the Ito–Skorokhod equation. The extension to Lévy stable motion $L(t)$ is rather natural and straightforward (e.g., Ref. 41) due to the common properties of $L(t)$ and $B(t)$ that we discussed in Sec. I, i.e., their infinitesimal increments are independent identically distributed and furthermore stable.

More precisely the Ito stochastic calculus corresponds to consider that the dL is, similarly to dB, a forward increment in time [it should be understood as $dL(t,dt)=L(t+dt)-L(t)$]. This means that the value of X at time t is determined by events prior to the application of the stochastic force $dL(t)$, which acts only from time t to $t+dt$.

The Eq. (2) can also be understood under its integral form

$$X(t)=X(t_0)+\int m(X(t),t)dt+\int \sigma(X(t),t)dL, \tag{3}$$

where the last term corresponds to a stochastic integration of a stochastic process. The integration of a stochastic process $\Phi(t)$ [in the case of Eq. (2): $\Phi(t)=\sigma(X(t),t)$] with respect to the Lévy motion L, is rather straightforward in the case of step processes:[42]

$$\Phi(t)=\Phi_n, \quad \text{for } t\in(t_n,t_{n+1}),\ n=0,1,...,N-1; \int \Phi(t)dL=\sum_{n=0}^{N-1}\Phi_n(L(t_{n+1})-L(t_n)) \tag{4}$$

and this rather suggestive definition is naturally extended to functional spaces in which the step processes are dense.

In order to establish local properties, for instance the time evolution of the probability of the particles, we will use the differential form [Eq. (2)], whereas Refs. 34 and 19 rather used the integral form [Eq. (4)] which becomes cumbersome in the nonlinear case and is in fact useful only to establish global properties (Sec. IX).

After having emphasized the similarities between $L(t)$ and $B(t)$, it is important to underline the nontrivial consequences due to the fact, contrary to the Gaussian case which has all its moments finite, Lévy motions have a finite critical order of divergence of statistical moments $(0<\alpha<2)$. These include the fact that the mathematical techniques which could be used can be rather distinct. For instance, our derivation will rely on the use of the second characteristic function of the increments, Sec. III, instead of probabilities of the increments as done usually for the derivation of the classical Fokker–Planck equation. An obvious reason is that the former are relatively simple (see Sec. VII), while the latter are not, with the only exception of the three following cases: $\alpha=2$, $\beta=0$; $\alpha=1$, $\beta=0$; $\alpha=1/2$, $\beta=1$. The fundamental reason is that both the stability property and the divergence of moments are related to the presence of a cumulant of noninteger order α. In relation to this problem, the convenient L^2 Hilbert structure of Gaussian processes is reduced to a L^α Banach structure for stable Lévy processes. This is particularly important for the integral equation (3), when defining functional spaces where step processes are dense.

The linear case, which is the hitherto studied case, corresponds to

$$m(X(t),t)\equiv m=\text{const}; \quad \sigma(X(t),t)\equiv\sigma=\text{const}. \tag{5}$$

$X(t)-X(t_0)$ is also a Lévy motion which has the same Lévy stability index α as its increments, but with a different center or trend and scale or amplitude.

In the nonlinear case, $m(X(t),t)$ and $\sigma(X(t),t)$ are (possibly nonlinear) functions of $X(t)$ and t, which satisfy certain regularity constraints to be discussed later (Sec. IX). They correspond to inhomogeneities of the medium, which were ignored in the linear case. As a possibly important, but simple example, let us mention the Lévy extension of the so-called geometric Brownian motion, which is rather ubiquitous and for instance is at the core of the Black–Scholes model for option pricing: $m(X(t),t)=mX(t)$ and $\sigma(X(t),t)=\sigma X(t)$, where σ is the votality constant of the price $X(t)$ of a given stock share.

We will demonstrate the following proposition:

Proposition 1: The transition probability density:

$$\forall t\geqslant t_0: \;\; p(x,t|x_0,t_0)=\Pr(X(t)=x|X(t_0)=x_0) \tag{6}$$

corresponding to the nonlinear stochastic differential equation (2), with a Lévy forcing of parameters $\alpha\neq 1$ or $\beta=0$, γ, $D\geqslant 0$, is solution of the following fractional Fokker–Planck equation:

$$\begin{aligned}\frac{\partial}{\partial t}p(x,t|x_0,t_0)=&-\frac{\partial}{\partial x}(\gamma\sigma(x,t)+m(x,t))p(x,t|x_0,t_0)\\&-D\Big[(-\Delta)^{\alpha/2}(|\sigma(x,t)|^\alpha p(x,t|x_0,t_0))\\&+\beta\omega(\alpha)\frac{\partial}{\partial x}(-\Delta)^{(\alpha-1)/2}(|\sigma(x,t)|^{\alpha-1}\sigma(x,t)p(x,t|x_0,t_0))\Big]\end{aligned} \tag{7}$$

with the initial condition

$$p(x,t_0|x_0,t_0)=\delta(x-x_0), \tag{8}$$

where $\delta(x-x_0)$ is the degenerate Dirac measure in x_0 and $\omega(\alpha)$ is defined by

$$\alpha \neq 1: \quad \omega(\alpha) = \tan \frac{\pi \alpha}{2} \tag{9}$$

and where the fractional powers of the Laplacian Δ will be discussed in Sec. VI. Proposition 1 and Eq. (7) are for scalar processes (i.e., $\Delta \equiv \partial^2/\partial x^2$) and their extension to vector processes will be discussed and presented in Sec. VIII. One may note that the fractional diffusive isotropic operator $-(-\Delta)^{\alpha/2}$ applies via a fractional diffusivity $|\sigma(x,t)|^{\alpha}$, whereas the advective–diffusive term corresponds to a conjugate action of a fractional diffusive term $-(-\Delta)^{(\alpha-1)/2}|\sigma(x,t)|^{\alpha-1}$ and a convective term $(\partial/\partial x)\sigma(x,t)$ on the transition probability.

This fractional Fokker–Planck equation will be established with the help of the much more general proposition.

Proposition 2: The inverse Fourier transform of the second characteristic function or cumulant generating function of the increments of a Markov process $X(t)$ generates by convolution the Fokker–Planck equation of evolution of its transition probability $p(x,t|x_0,t_0)$.

We will demonstrate this proposition in a straightforward, yet rigorous way. More precisely, we will establish the following:

$$\frac{\partial p}{\partial t}(x,t|x_0,t_0) = \int dy \, \frac{\partial \tilde{K}}{\partial t}(x-y|y,t) p(y,t|x_0,t_0), \tag{10}$$

where $\tilde{K}$ is the inverse Fourier transform of the cumulant generating function of the increments. The $\tilde{K}$ arguments will become explicit in Sec. III.

Equation (10) not only holds for processes with stationary and independent increments, as in the linear case [Eq. (5)] but also for any Markov process, including those defined by the nonlinear Langevin-type equation [Eq. (2) with $m \neq \text{const}$, $\sigma \neq \text{const}$]. As a consequence of Eq. (10), we will demonstrate the following.

Proposition 3: When the increment's cumulant generating function of a Markov process $X(t)$ is defined by its expansion in cumulants C_n, its Fokker–Planck equation is

$$\frac{\partial p}{\partial t}(x,t|x_0,t_0) = \sum_{n \in J} \frac{(-1)^n}{n!} \frac{\partial^n}{\partial x^n}[C_n(x,t) p(x,t|x_0,t_0)]. \tag{11}$$

An obviously sufficient condition of convergence is obtained when the set J of the orders of differentiation n is finite. This is true in particular for Gaussian forcing: $J=\{1,2\}$. It corresponds to the classical Fokker–Planck equation. On the other hand, $J=\mathbf{N}$ would correspond to an analytic expansion of cumulants. In spite of its interest, we will not discuss the latter case in this paper, nor its relationship to the classical Kramers–Moyal expansion (e.g., Ref. 43).

Below, we concentrate on the case of a finite, but nonanalytic expansion: $J=\{1,\alpha\}$ (noninteger α, $0<\alpha<2$), since it corresponds to the Lévy extension (Sec. VII and yields Proposition 1 with the help of fractional derivatives, as discussed in Sec. VI.

III. THE CUMULANT GENERATING FUNCTION OF THE INCREMENTS

The first and second (conditional) characteristic functions are, respectively, the moment generating function $Z_X(k,t-t_0|x_0,t_0)$ and the cumulant generating function $K_X(k,t-t_0|x_0,t_0)$, associated with the transition probability $p(x,t|x_0,t_0)$ of a process $X(t)$. These are defined by the Fourier transform of the latter, with k being the conjugate variable of $x-x_0$:

$$F[p(x,t|x_0,t_0)] \equiv Z_X(k,t-t_0|x_0,t_0) \tag{12}$$

$$\equiv \exp(K_X(k,t-t_0|x_0,t_0)) \tag{13}$$

$$\equiv E[\exp(ik(X(t)-X(t_0))|X(t_0)=x_0], \tag{14}$$

where $E[\cdot|\cdot]$ denote the conditional mathematical expectation, F and F^{-1}, respectively, the Fourier transform and its inverse:

$$F[f]=\hat{f}(k)=\int_{-\infty}^{\infty} dx \exp(ikx)f(x), \tag{15}$$

$$F^{-1}[\hat{f}]=f(x)=\int_{-\infty}^{\infty}\frac{dk}{2\pi}\exp(-ikx)\hat{f}(k). \tag{16}$$

The corresponding quantities for increments $\delta X(\delta t)=X(t+\delta t)-X(t)$, corresponding to a given time lag $\delta t>0$, are defined in a similar way:

$$F[p(x+\delta x,t+\delta t|x,t)]=\delta Z_X(k,\delta t|x,t) \tag{17}$$

$$\equiv \exp(\delta K_X(k,\delta t|x,t)) \tag{18}$$

$$=E[\exp(ik(X(t+\delta t)-X(t))|X(t)=x], \tag{19}$$

where k is the conjugate variable of δx. The cumulants of the increments C_n are the coefficients of the Taylor expansion of δK_X:

$$\delta K_X(k,\delta t|x,t)=\delta t\sum_{n\in J}\frac{(ik)^n}{n!}C_n(x,t)+o(\delta t). \tag{20}$$

As already mentioned, the classical case corresponds to an analytic expansion of δK_X, i.e., $J\subseteq\mathbf{N}$, whereas we will be interested by a finite but nonanalytic expansion $J=\{1,\alpha\}$ (noninteger α, $0<\alpha<2$).

IV. PROCESSES WITH STATIONARY AND INDEPENDENT INCREMENTS

Let us first consider the simple subcase of a process with stationary and independent increments. It corresponds to $C_n(x,t)\equiv C_n=\text{const}$ in Eqs. (11) and (20) and as already discussed in Sec. I, it includes the linear case [Eq. (5)] of the Langevin-type equation (2).

However, we believe that the following derivation is not only somewhat pedagogical on the role of the characteristic functions for the nonlinear case, but also terser than derivations previously presented for the linear case.

The stationarity of the increments implies that the transition probability depends only on the time and space lags, i.e.,

$$p(x,t|x_0,t_0)=p(x-x_0,t-t_0) \tag{21}$$

and similarly, the characteristic functions of the increments are no longer conditioned, for instance,

$$Z_X(k,t-t_0|x_0,t_0)\equiv Z_X(k,t-t_0), \tag{22}$$

$$K_X(k,t-t_0|x_0,t_0)\equiv K_X(k,t-t_0). \tag{23}$$

On the other hand, the independence of the increments implies that the transition probabilities satisfy a convolution (over any possible intermediate position y) for any given time lag δt:

$$\forall\,\delta t>0:\ \ p(x-x_0,t+\delta t-t_0)=\int dy\, p(x-y,\delta t)(y-x_0,t-t_0) \tag{24}$$

and the corresponding characteristic functions merely factor (respectively, add). Therefore, we have,

$$Z_X(k,t+\delta t-t_0)-Z_X(k,t-t_0)=Z_X(k,t-t_0)(\delta Z_X(k,\delta t)-1). \tag{25}$$

This in turn leads to

$$Z_X(k,t+\delta t-t_0)-Z_X(k,t-t_0)=Z_X(k,t-t_0)\,\delta K_X(k,\delta t)+o(\delta t). \tag{26}$$

Its inverse Fourier transform yields

$$p(x,t+\delta t|x_0,t_0)-p(x,t|x_0,t_0)=\int dy\, F^{-1}[\,\delta K_X(k,\delta t)]p(y-x_0,t-t_0)+o(\delta t). \tag{27}$$

This demonstrates (in the limit $\delta t\to 0$) Proposition 2 and Eq. (10), as well as Proposition 3, since Eq. (27) corresponds, with the help of Eq. (20), to

$$p(x,t+\delta t|x_0,t_0)-p(x,t|x_0,t_0)=\delta t\sum_{n\in J}\frac{(-1)^n}{n!}\left[C_n\int dy\,\delta^{(n)}_{x-y}p(y,t|x_0,t_0)\right]+o(\delta t), \tag{28}$$

where δ^n_x denotes the nth derivative of the Dirac function. Therefore, we obtain

$$\frac{\partial}{\partial t}p(x,t|x_0,t_0)=\sum_{n\in J}\frac{(-1)^n}{n!}C_n\frac{\partial^n}{\partial x^n}p(x,t|x_0,t_0) \tag{29}$$

which corresponds to the linear case of Eq. (11).

V. MORE GENERAL MARKOV PROCESSES

In the case of a Markov process which does not have stationary and independent increments, there is no longer a simple convolution equation [Eq. (24)] of the transition probabilities, nor a simple factorization of characteristic functions [Eq. (25)]. However, the former satisfies a generalized convolution equation which corresponds to the Chapman–Kolmogorov identity[17] valid for any Markov process $X(t)$:

$$\forall\,\delta t>0:\ \ p(x,t+\delta t|x_0,t_0))=\int dy\,p(x,t+\delta t|y,t)p(y,t|x_0,t_0) \tag{30}$$

which indeed reduces to a mere convolution [Eq. (24)] in the case of processes with stationary and independent increments. This identity can be written under the equivalent form:

$$p(x,t+\delta t|x_0,t_0)=\int dy\int\frac{dk}{2\pi}e^{-iky+\delta K_X(k,\delta t|y,t)}p(y,t|x_0,t_0). \tag{31}$$

Noting that we have

$$p(x,t|x_0,t_0)=\int dy\,p(y,t|x_0,t_0)\int\frac{dk}{2\pi}e^{-iky}, \tag{32}$$

we obtain

$$p(x,t+\delta t|x_0,t_0)-p(x,t|x_0,t_0)=\delta t\int dy\,F^{-1}[\,\delta K_X(k,\delta t|y,t)]p(y,t|x_0,t_0)+o(\delta t). \tag{33}$$

In the limit $\delta t\to 0$, this corresponds to Proposition 2 and Eq. (10). When $J\subseteq\mathbf{N}$, it yields with the help of Eq. (20):

$$\delta p(x,t|x_0,t_0)=\delta t\sum_{n\in J}\int dy\ \delta^{(n)}_{x-y}\left[\frac{(-1)^n}{n!}C_n(y,t)p(y,t|x_0,t_0)\right]+o(\delta t). \tag{34}$$

The limit $\delta t\to 0$ corresponds to Eq. (11) and demonstrates Proposition 3 for a Markow process.

VI. EXTENSION TO FRACTIONAL ORDERS

In the two preceding sections (Secs. IV and V), the fact that the indices $n\in J$ should be integers intervened at best only in the correspondence between (integer order) differentiation $\partial^n/\partial x^n$ [in Eq. (11)] and powers of the conjugate variable k^n [in Eq. (20)]. However, by the very definition of fractional differentiation (e.g., Ref. 44), this correspondence holds also for noninteger orders. However, there is not a unique definition of fractional differentiation and therefore, as discussed in some details in Ref. 19, we cannot expect to have a unique expression of the fractional Fokker–Planck equation.

Since in the following it will be sufficient to consider an expansion of the characteristic function involving fractional powers of only the wave number $|k|$, it is interesting to consider Riesz's definition of a fractional differentiation. Indeed, the latter corresponds to consider fractional powers of the Laplacian:

$$-(-\Delta)^{\alpha/2}f(x)=F^{-1}[|k|^{\alpha}\hat{f}(k)] \tag{35}$$

which has furthermore the advantage of being valid for the vector cases. However, we will see in Sec. VIII that in general it does not apply in a straightforward manner for vector stable Lévy motions. Indeed the latter introduces rather (one-dimensional) directional Laplacians, i.e., (one-dimensional) Laplacians along a given direction $\underline{u}(|\underline{u}|=1)$:

$$-(-\Delta_{\underline{u}})^{\alpha/2}f(x)=F^{-1}[|(\underline{k},\underline{u})|^{\alpha}\hat{f}(k)], \tag{36}$$

where (.,.) denotes the scalar product. On the other hand, it will be useful to consider the fractional power of the contraction of the Laplacian tensor $\underline{\underline{\Delta}}$:

$$\Delta_{i,j}=\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j} \tag{37}$$

by a tensor $\underline{\underline{\sigma}}$ ($\underline{\underline{\sigma}}^*$ denotes its transpose), with the following definition:

$$-(-\underline{\underline{\Delta}}:\underline{\underline{\sigma}}.\underline{\underline{\sigma}}^*)^{\alpha/2}\equiv F^{-1}[|(\underline{k},\underline{\underline{\sigma}}.\underline{\underline{\sigma}}^*.\underline{k}|^{\alpha/2}]=F^{-1}[|\underline{\underline{\sigma}}^*.\underline{k}|^{\alpha}]. \tag{38}$$

VII. LÉVY CASE

The second characteristic function of the increments δL of the (scalar) Lévy forcing is the following:

$$\delta K_L(k,\delta t)=\delta t\left[ik\gamma-D|k|^{\alpha}\left(1-i\beta\frac{k}{|k|}\right)\omega(k,\alpha)\right]+o(\delta t), \tag{39}$$

where $\omega(k,\alpha)$ is defined by

$$\alpha\neq 1:\quad \omega(k,\alpha)\equiv\omega(\alpha)=\tan\frac{\pi\alpha}{2},\quad \alpha=1:\quad \omega(k,\alpha)=\frac{\pi}{2}\log|k|. \tag{40}$$

Considering an Ito-type forward integration of Eq. (2), the increments δL generates the following (first) characteristic function for the increments δX of the motion $X(t)$:

$$\delta Z_X(k,\delta t|x-\delta x,t)=E(e^{ikm(X,t)})\,\delta Z_{\sigma L}(k,\delta t|x,t)+o(\delta t) \tag{41}$$

which yields the following elementary cumulant generating function δK_X:

$$\delta K_X(k,\delta t|x,t)=\delta t\left[ikm(x,t)+ik\gamma\sigma(x,t)-D|k|^{\alpha}|\sigma(x,t)|^{\alpha}\left(1-i\beta\frac{k\sigma(x,t)}{|k||\sigma(x,t)|}\omega(k,\alpha)\right)\right]+o(\delta t) \tag{42}$$

and which is of the same type as Eq. (20), with $J=\{1,\alpha\}$. Therefore, as discussed in Sec. VI, we have fractional differentiations in the corresponding Eq. (11), which will precisely correspond to Eq. (7), and therefore establishes Proposition 1.

VIII. EXTENSION TO VECTOR PROCESSES

With but one important exception, the extension of the previous results to higher dimensions is rather straightforward. The starting point of this extension is the following nonlinear stochastic equation ($\underline{X}(t)\in R^d$):

$$d\underline{X}(t)=\underline{m}(\underline{X}(t),t)dt+\underline{\underline{\sigma}}(\underline{X}(t),t).d\underline{L}, \tag{43}$$

where $\underline{m}$ is the natural d-dimensional vector extension of the deterministic-like trend, $\underline{\underline{\sigma}}$ is the $d\times d'$-dimensional tensor extension of the modulation of the random driving force, and $\underline{L}$ is a d'-dimensional Lévy stable motion. As discussed below, the expression of the characteristic function of the latter corresponds to the source of the difficulty in extending the scalar results to higher dimensions. On the contrary, it is straightforward to check that Propositions 2 and 3 are valid in the vector case, with the following extensions ($\underline{x}\in R^d$) for Eq. (10):

$$\frac{\partial p}{\partial t}(\underline{x},t|\underline{x}_0,t_0)=\int d\underline{y}\frac{\partial\tilde{K}}{\partial t}(\underline{x}-\underline{y}|\underline{y},t)p(\underline{y},t|\underline{x}_0,t_0) \tag{44}$$

and for Eq. (11) ($\underline{n}\in J\subseteq\mathbf{N}^d,|\underline{n}|=\Sigma_{i=1}^d n_i$):

$$\frac{\partial p}{\partial t}(\underline{x},t|\underline{x}_0,t_0)=\sum_{\underline{n}\in J}\frac{(-1)^{|\underline{n}|}}{(n_1)!(n_2)!..(n_d)!}\frac{\partial^{|\underline{n}|}}{\partial x_1^{n_1}\partial x_2^{n_2}..\partial x_d^{n_d}}[C_{\underline{n}}(\underline{x},t)p(\underline{x},t|\underline{x}_0,t_0)]. \tag{45}$$

On the other hand, Eq. (43) yields the following extension to Eq. (41):

$$\delta Z_{\underline{X}}(\underline{k},\delta t|\underline{x},t)=e^{i\,\underline{k}.\underline{m}(\underline{x},t)}\,\delta Z_{\underline{\underline{\sigma}}.\underline{L}}(\underline{k},\delta t|\underline{x},t) \tag{46}$$

and therefore we have

$$\delta K_{\underline{X}}(\underline{k},\delta t|\underline{x},t)=i\,\underline{k}.\underline{m}(\underline{x},t)+\delta K_{\underline{L}}(\underline{\underline{\sigma}}^*.\underline{k},\delta t|\underline{x},t)+o(\delta t). \tag{47}$$

Let us recall that a stable Lévy vector in the classical sense[14,45,46] (see Ref. 47 for a discussion on a rather straightforward generalization, or Refs. 48, 49, and 50 for a more abstract generalization) corresponds to the limit of a sum of jumps, with a power-law distribution, along random directions $\underline{u}\in\partial B_1$, B_1 being the unit ball, distributed according to a (positive) measure $d\Sigma(\underline{u})$. The latter, which generalizes the scale parameter D of the scalar case, is the source of the difficulty since in general the probability distribution of a stable Lévy vector depends on this measure, and therefore is a nonparametric distribution. However, as discussed below, there is at least a trivial exception: the case of isotropic stable Lévy vectors.

Corresponding to our previous remarks, a (classical) stable Lévy vector has the following (Fourier) cumulant generating function:

$$K_{\underline{L}}(\underline{k})=\delta t\left[i(\underline{k},\underline{\gamma})-\int_{\underline{u}\in\partial B_1}(i\underline{k},\underline{u})^{\alpha}\,d\Sigma(\underline{u})\right]+o(\delta t) \tag{48}$$

which yields with the help of Eq. (47):

$$\frac{\partial}{\partial t}\tilde{K}_{\underline{X}}(\underline{k})=-\operatorname{div}(\underline{m}+\underline{\underline{\sigma}}.\underline{\gamma})-F^{-1}\left[\int_{\underline{u}\in\partial B_1}(i\underline{\underline{\sigma}}^{*}(\underline{x},t).\underline{k},\underline{u})^{\alpha}\,d\Sigma(\underline{u})\right]. \tag{49}$$

The scalar case [Eq. (39)] corresponds to

$$0\leqslant p\leqslant 1:\ \ \beta=2p-1,\ \ d\Sigma(u)=D\cos\left(\frac{\pi\alpha}{2}\right)[p\,\delta_{(u-1)}+(1-p)\,\delta_{(u+1)}]. \tag{50}$$

For any dimension d, the second term on the right-hand side of Eq. (49) corresponds to a fractional differentiation operator of order α. This operator can be slightly rearranged. With the help of the odd $d\Sigma^{-}(\underline{u})$ and even $d\Sigma^{+}(\underline{u})$ parts of the measure $d\Sigma(\underline{u})$:

$$2\,d\Sigma^{+}(\underline{u})=d\Sigma(\underline{u})+d\Sigma(-\underline{u}),\quad 2\,d\Sigma^{-}(\underline{u})=d\Sigma(\underline{u})-d\Sigma(-\underline{u}) \tag{51}$$

and the identity (θ being the Heaviside function):

$$(ik)^{\alpha}=|k|^{\alpha}[\,\theta(k)e^{i(\alpha\pi/2)}+\theta(-k)e^{-i(\alpha\pi/2)}] \tag{52}$$

one can write the extension of Eq. (7) under the following form:

$$\begin{aligned}\frac{\partial}{\partial t}p(\underline{x},t|\underline{x}_0,t_0)=&-\operatorname{div}[\underline{m}(\underline{x},t)+\underline{\underline{\sigma}}(\underline{x},t).\underline{\gamma})]p(\underline{x},t|\underline{x}_0,t_0)\\&-[\langle(-\underline{\underline{\Delta}}:\underline{\underline{\sigma}}.\underline{\underline{\sigma}}^{*})^{\alpha/2}\rangle_{\Sigma^{+}}-\langle(\underline{\nabla}.\underline{\underline{\sigma}}^{*}).(-\underline{\underline{\Delta}}:\underline{\underline{\sigma}}.\underline{\underline{\sigma}}^{*})^{\alpha-1/2}\rangle_{\Sigma^{-}}]\\&\times p(\underline{x},t|\underline{x}_0,t_0),\end{aligned} \tag{53}$$

where the symmetric fractional diffusive and, respectively, the antisymmetric advective–diffusive terms are defined, similarly to Eq. (38), in the following manner:

$$-\langle(-\underline{\underline{\Delta}}:\underline{\underline{\sigma}}.\underline{\underline{\sigma}}^{*})^{\alpha/2}\rangle_{\Sigma^{+}}=\int_{\underline{u}\in\partial B_1}d\Sigma^{+}(\underline{u})F^{-1}[|(\underline{\underline{\sigma}}^{*}(\underline{x},t).\underline{k},\underline{u})|^{\alpha}] \tag{54}$$

$$-\langle(\underline{\nabla}.\underline{\underline{\sigma}}^{*}).(-\underline{\underline{\Delta}}:\underline{\underline{\sigma}}.\underline{\underline{\sigma}}^{*})^{\alpha-1/2}\rangle_{\Sigma^{-}}=\int_{\underline{u}\in\partial B_1}d\Sigma^{-}(\underline{u})F^{-1}[(-i\underline{\underline{\sigma}}^{*}(\underline{x},t).\underline{k},\underline{u})|(\underline{\underline{\sigma}}^{*}(\underline{x},t).\underline{k},\overline{u})|^{\alpha-1}]. \tag{55}$$

In general, each term corresponds to a rather complex integration (which is indicated by the symbol $\langle.\rangle_{\Sigma}$) by the measure $d\Sigma$ of directional fractional Laplacians [Eq. (36)]. However, the symmetric term becomes simpler as soon as the even part $d\Sigma^{+}$ of the measure $d\Sigma$ is isotropic. Indeed, the integration over directions yields only a prefactor D:

$$\langle-(\underline{\underline{\Delta}}:\underline{\underline{\sigma}}.\underline{\underline{\sigma}}^{*})^{\alpha/2}\rangle_{\Sigma^{+}}=D(-\underline{\underline{\Delta}}:\underline{\underline{\sigma}}.\underline{\underline{\sigma}}^{*})^{\alpha/2}D=\int_{\underline{u}\in\partial B_1}d\Sigma^{+}(\underline{u})|(\underline{u}_1,\underline{u})|^{\alpha} \tag{56}$$

and for $\alpha=2$ this corresponds to the classical term $(\underline{\underline{\Delta}}:\underline{\underline{\sigma}}.\underline{\underline{\sigma}}^{*})$ of the standard d-dimensional Fokker–Planck equation. If $d\Sigma$ itself is rotation invariant, then the asymmetric operator vanishes, since $d\Sigma^{-}=0$. If furthermore, $\underline{\underline{\sigma}}$ is scalar, i.e., $\underline{\underline{\sigma}}=\sigma\underline{\underline{1}}$, then one obtains the following Fractional Fokker–Planck equation:

$$\frac{\partial}{\partial t}p(\underline{x},t|\underline{x}_0,t_0)=-\mathrm{div}[\underline{\underline{\sigma}}.\underline{\gamma}(\underline{x},t)+\underline{m}(\underline{x},t)]p(\underline{x},t|\underline{x}_0,t_0) \tag{57}$$

$$-D[(-\Delta)^{\alpha/2}]|\sigma(x,t)|^{\alpha}p(\underline{x},t|\underline{x}_0,t_0). \tag{58}$$

Therefore, as one might expect the rotation symmetries yield a rather trivial extension of the standard Gaussian case: a fractional power α of the d-dimensional Laplacian, as in the pure scalar case [Eq. (7)]. Obviously, the integration performed in Eq. (53) is also greatly simplified as soon as $d\Sigma(\underline{u})$ is discrete, i.e. its support corresponds to a discrete set of directions $\underline{u}_i$.

On the other hand, let us note that the framework of generalized stable Lévy vectors,[47–50] allows one to introduce a much stronger anisotropy than the measure $d\Sigma$ allows for classical stable Lévy vectors. This therefore diminishes the importance of the asymmetry of the latter. Indeed, the components of a generalized stable Lévy vector do not necessarily have the same Lévy stability index, the latter being generalized into a second rank tensor. Similarly, the differential operators involved in the corresponding fractional Fokker–Planck equation no longer have a unique order of differentiation. This is rather easy to check in case of a discrete measure $d\Sigma(\underline{u})$ and we will explore the general case elsewhere.

IX. EXISTENCE AND UNIQUENESS OF THE SOLUTION

The preceding sections established a generalization of the Fokker–Planck equation for the evolution of the probability distribution of nonlinear stochastic differential equations driven by Lévy stable noises. This is the main goal of this paper. Naturally, one would also like to have if possible a theorem of existence and uniqueness of the solution of this equation. Due to its origin, such a theorem will also imply that the solution will remain positive and normalized, as required for a transition probability. In this section we argue that the general results obtained[51] in the classical Gaussian case ($\alpha=2$) are also relevant for the Lévy extension, whereas up until now existence and uniqueness conditions of partial fractional differential equations have been scarcely explored (see however Refs. 52 and 53) and therefore we cannot rely on general results.

The classical Fokker–Planck equation belongs to the well-explored domain of parabolic equations. Existence and uniqueness of the solution fundamentally result[54] from the fact that the linear operator $A=-\Delta$ is a (self-adjoint) positive generator of a semigroup of contraction operators $T(t)=e^{-tA}$, $t\geqslant 0$. In the case of constant coefficients (linear Langevin equation), the solution is directly obtained with the help of $T(t)$ and this ensures its existence, uniqueness, and positiveness. Note that in our case, the semigroup action corresponds to the equation of convolution [Eq. (24)].

Similar results hold for a Lipschitz variation of the coefficients, i.e.,

$$|m(x,t)-m(y,t)|+|\sigma(x,t)-\sigma(y,t)|\leqslant D|x-y| \tag{59}$$

as well as a condition of slow growth in time of the coefficients $m(X(t),t)$ and $\sigma(X(t),t)$, e.g.,

$$|m(x,t)|+|\sigma(x,t)|\leqslant C|1+x|, \tag{60}$$

where D and C are given positive constants.

These conditions have been extensively used for the classical Fokker–Planck equation with non constant coefficients (e.g., Ref. 43). Considering now the fractional generalization, it is important to note that the fractional power of the Laplacian $-(-\Delta)^{\alpha/2}$ remains positive, since its definition Eq. (35) corresponds to replacing the eigenvalues k^2 by eigenvalues having as real part $|k|^{\alpha}$. Therefore, we remain inside of the previous framework of contraction semigroup and the previous results should hold.

This could also be seen from the integral form of the differential equation. Indeed, in the classical case, the Lipschitz condition is classical for the Brownian forcing,[55,41] as well as for the

more general case of martingale and semimartingale forcing.[56–58] The latest case is relevant for the stable Lévy forcing. The Lipschitz condition can be rather understood as a condition of convergence of the Picard iteration method towards a fixed point:

$$X^{n+1}(t)=X(t_0)+\int m(X^n(t),t)dt+\int \sigma(X^n(t),t)dL;X^0(t)=X(t_0). \tag{61}$$

On the other hand, the condition of slow growth (60) in time prevents a finite explosion time, i.e., $X(t)$ remains finite for any given finite time t: this condition is rather general, since it is already required by the deterministic part of the Langevin-type equation.

X. CONCLUSION

We have derived a fractional Fokker–Planck equation, i.e., a kinetic equation which involves fractional derivatives, for the evolution of the probability distribution of nonlinear stochastic differential equations driven by non-Gaussian Lévy stable noises. We first established this equation in the scalar case, where it has a rather compact expression with the help of fractional powers of the Laplacian, and then discussed and presented its extension to the vector case. This fractional Fokker–Planck equation generalizes broadly previous results obtained for a linear Langevin-type equation with a Lévy forcing, as well as the standard Fokker–Planck equation for a nonlinear Langevin equation with a Gaussian forcing. As suggested in Ref. 36 and in the comments of Ref. 19 on Refs. 32 and 35, we will show elsewhere, that the present results could be extended to include fractional time derivative in the Langevin equation and in the corresponding Fokker–Planck equation. This is particularly important for multifractal modeling, since the generators of dynamic universal multifractals[30] are defined by this type of equations.

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Hamiltonians and zero-curvature equations for integrable partial differential equations

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We discuss the relationship between two approaches to integrable partial differential equations, one using formal affine Lie algebras and the other Banach–Lie groups. In the first approach integrability of the equations follows from commutativity of Hamiltonian flows on the Lie algebra, while in the second it follows from commutativity of certain flows induced by an action on the Banach–Lie group. We show that these two methods are essentially equivalent since one can calculate one type of the flows from the other. The classes of solutions encompassed by the two methods, however, vary significantly. We demonstrate this relationship specifically with the nonlinear Schrödinger equation. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1312197]

I. INTRODUCTION

Integrable partial differential equations (PDE's), such as the Korteweg de Vries (KdV) equation or the cubically nonlinear Schrödinger (NLS) equation, have been studied in the context of infinite dimensional Lie groups or their Lie algebras for many years now. One approach, originated by the Kyoto school,[1] considers flows of an Abelian group on an infinite dimensional Grassmannian. The partial differential equations then arise in Hirota form as the Plücker equations for a projective embedding of the Grassmannian. On the other hand integrable PDE's are often studied in the zero-curvature form. This expression arises from modeling the Grassmannian by G/G_+ where G is a certain infinite dimensional Lie group with subgroups G_-, G_+ such that G_-G_+ is dense in G, and $G_-\cap G_+=\{I\}$. Commuting flows on G/G_+ are constructed as flows $g_-(\mathbf{t})$, $\mathbf{t}\in\mathbb{R}^n$, on G_- whose commutativity leads to matrix PDE's in the zero-curvature form which are equivalent to scalar PDE's for matrix coefficients, such as the NLS or the KdV equation. The equivalence of the Hirota approach to the zero-curvature method was given by Segal and Wilson[2] for the KP hierarchy, and was recently generalized by Bergvelt and ten Kroode.[3]

The zero-curvature equation is actually a partial differential equation on elements of $\mathfrak{g}$, the Lie algebra of G. In Ref. 4, Flaschka, Newell and Ratiu observed that this equation is also related to commutativity of certain Lax pair flows on the Lie algebra $\mathfrak{g}_-$, and that these flows have a Hamiltonian interpretation in terms of the natural Lie–Poisson structure on $\mathfrak{g}_+^*$, the dual of $\mathfrak{g}_+$. This approach leads to an understanding of the integrability of the original PDE's in terms of the Liouville integrability of the flows in $\mathfrak{g}_+^*$, as given by the Adler–Kostant–Symes theorem.

Our purpose in this paper is to describe the relation between the Lax pair flows on $\mathfrak{g}_-$ and the Abelian flows on G/G_+. The literature often treats the two approaches as equivalent but we have been unable to find a published proof of this fact. Indeed, if one takes care to distinguish which spaces of solutions are discussed in the two approaches it becomes apparent that they are not exactly equivalent. We remark in Sec. II that the Lie algebraic approach provides all regular solutions for the the NLS equation, while it is generally known that the Lie group approach leads to rather obscure subspaces of solutions due to the necessity of a Banach–Lie group structure of G (see Refs. 2 and 5). In Sec. III we describe how to construct the Banach–Lie group G and the

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Abelian flows on G/G_+ whose commutativity gives rise to integrable PDE's. This is illustrated with the NLS example.

In Sec. IV we provide a computational proof of the equivalence of the two approaches to integrable PDE's. If one begins with a suitable Abelian flow $g(\mathbf{t})$ in G, then one obtains $g_-(\mathbf{t}) \in G_-$ by a Riemann–Hilbert type splitting on G, and the solution $X(\mathbf{t})$ to the Lax equations on the Lie algebra $\mathfrak{g}_-$ is given by conjugating $X(0)$ with $g_-(\mathbf{t})$. On the other hand if we start with a solution $X(\mathbf{t})$ to the Lax equations, then producing the solution $g_-(\mathbf{t})$ to the Riemann–Hilbert problem is a little more complicated. It involves solving a differential equation on the group G_- which is determined from the Lax equations for $X(\mathbf{t})$. The first half of this argument, presented in Proposition 1, is well known (and perhaps accounts for the general notion that the two methods are entirely equivalent), but the second half, Proposition 2, is somewhat more obscure. Examining the relationship of $g_-(\mathbf{t})$ to $X(\mathbf{t})$ helps provide an understanding of the relationship between the different classes of solutions given by these two approaches. To pass from $X(\mathbf{t})$ to $g_-(\mathbf{t})$ one must solve a differential equation in some Banach–Lie group, and this requires that $X(\mathbf{t})$ lies in a particular Banach–Lie algebra. In Sec. V we present a geometric interpretation of the relationship between the two approaches. This is basically just an application of the general setting provided by Guillemin and Sternberg in Ref. 6.

II. THE ADLER–KOSTANT–SYMES METHOD OF FLASCHKA, NEWELL AND RATIU

Let $\mathfrak{g}$ be a Lie algebra and let $\mathfrak{g}^*$ denote its dual which is (weakly) paired via $\langle\,,\rangle:\mathfrak{g}^*\times\mathfrak{g}\to\mathbb{C}$. The space $\mathfrak{g}^*$ admits the structure of a Poisson manifold with the Lie–Poisson bracket defined by

$$\{F,G\}(\alpha)=\left\langle \alpha,\left[\frac{\delta F}{\delta\alpha},\frac{\delta G}{\delta\alpha}\right]\right\rangle,\quad \alpha\in\mathfrak{g}^*,\quad F,G\in C^\infty(\mathfrak{g}^*). \tag{1}$$

Here $\delta F/\delta\alpha$ is the functional derivative of F, i.e., it is the element of $\mathfrak{g}$ satisfying

$$\left\langle \beta,\frac{\delta F}{\delta\alpha}\right\rangle=\left.\frac{d}{dt}\right|_{t=0} F(\alpha+t\beta),\quad \text{for all}\quad \beta\in\mathfrak{g}^*.$$

Bracket (1) plays an important role in the description of many finite and infinite dimensional Hamiltonian systems (see Ref. 7). We shall briefly describe this in the following. If $\mathfrak{g}$ is infinite dimensional and the pairing $\langle\,,\rangle$ is weak, we must restrict this bracket to an appropriate class of functions so that $\delta F/\delta\alpha$ makes sense, i.e., it defines an element of $\mathfrak{g}$. Details of the problems that can arise may be found in Ref. 8.

A Hamiltonian $H\in C^\infty(\mathfrak{g}^*)$ generates the vector field X_H on $\mathfrak{g}^*$ by the relation $X_H[F]=\{F,H\}$ where $X_H[F]$ is the Lie derivative of F along X_H, $X_H[F](\alpha)=dF(\alpha)X_H(\alpha)$ for any $\alpha\in\mathfrak{g}^*$. It follows from (1) that the flow of X_H satisfies the generalized Lax equation,

$$\frac{d\alpha}{dt}=-\mathrm{ad}^*\left(\frac{\delta H}{\delta\alpha}\right)\alpha,$$

where $\mathrm{ad}^*(X)$ is the dual of $\mathrm{ad}(X)$ defined by $\langle\mathrm{ad}^*(X)\alpha,Y\rangle=\langle\alpha,\mathrm{ad}(X)Y\rangle$.

Now, let $\mathrm{I}(\mathfrak{g}^*)$ denote the space of all ad*-invariant functions on $\mathfrak{g}^*$:

$$\mathrm{I}(\mathfrak{g}^*)=\{F\,|\,dF(\alpha)(\mathrm{ad}^*(X)\alpha)=0,\quad \text{for all}\quad X\in\mathfrak{g},\ \alpha\in\mathfrak{g}^*\}.$$

If the Lie algebra $\mathfrak{g}$ has a Lie group G, then functions satisfying $F\circ\mathrm{Ad}^*(g^{-1})=F$ for all $g\in G$ are ad*-invariant. Here $\mathrm{Ad}^*(g)$ is the dual of $\mathrm{Ad}(g)$, $\langle\mathrm{Ad}^*(g)\alpha,X\rangle=\langle\alpha,\mathrm{Ad}(g)X\rangle$. One easily shows from the definition of the Lie–Poisson bracket that $\mathrm{I}(\mathfrak{g}^*)$ is in the center of $C^\infty(\mathfrak{g}^*)$, i.e., if $F\in I(\mathfrak{g}^*)$ then $\{F,H\}=0$ for all $H\in C^\infty(\mathfrak{g}^*)$. Thus ad*-invariant functions are integrals of the

motion for any Hamiltonian H. Unfortunately, their vector fields vanish identically so they generate only trivial flows. In order to construct nontrivial Poisson-commuting flows, one needs an additional structure on $\mathfrak{g}$.

Suppose that $\mathfrak{g}$ splits into the vector space direct sum of subalgebras,

$$\mathfrak{g}=\mathfrak{g}_-\oplus\mathfrak{g}_+,$$

and let $\Pi_+:\mathfrak{g}\to\mathfrak{g}_+$ denote the projection with kernel $\mathfrak{g}_-$. Then its dual also splits into

$$\mathfrak{g}^*=\mathfrak{g}_-^*\oplus\mathfrak{g}_+^*,$$

where $\mathfrak{g}_\pm^*=\mathrm{Ann}(\mathfrak{g}_\mp)$ is the annihilator of $\mathfrak{g}_\mp$. Since $\mathfrak{g}_+$ is a Lie subalgebra, the space $\mathfrak{g}_+^*$ is also equipped with the Lie–Poisson structure (1). Now suppose that $H_1\in \mathrm{I}(\mathfrak{g}^*)$, and let $\tilde{H}_1$ denote the restriction of H_1 to $\mathfrak{g}_+^*$. Then $\tilde{H}_1$ is generally not in the center of $C^\infty(\mathfrak{g}_+^*)$, hence $\tilde{H}_1$ generates nontrivial flows on $\mathfrak{g}_+^*$. But if H_2 is another invariant function on $\mathfrak{g}^*$, then the celebrated result of Adler, Kostant and Symes (see Refs. 9, 10, and 11) states that $\tilde{H}_1$ and $\tilde{H}_2$ Poisson commute. More precisely, $\{\tilde{H}_1,\tilde{H}_2\}=0$ where

$$\{\tilde{H}_1,\tilde{H}_2\}(\alpha)=\left\langle \alpha,\left[\Pi_+\left(\frac{\delta H_1}{\delta\alpha}\right),\Pi_+\left(\frac{\delta H_2}{\delta\alpha}\right)\right]\right\rangle,\quad \alpha\in\mathfrak{g}_+^*.$$

Thus $\tilde{H}_1$ and $\tilde{H}_2$ generate commuting Hamiltonian flows on $\mathfrak{g}_+^*$ which are given by

$$\frac{d\alpha}{dt_i}=-\mathrm{ad}^*\left(\Pi_+\left(\frac{\delta H_i}{\delta\alpha}\right)\right)\alpha,\quad \alpha\in\mathfrak{g}_+^*. \tag{2}$$

Equation (2) takes the usual Lax form if $\mathfrak{g}$ is self-dual, i.e., if we can identify $\mathfrak{g}^*$ with $\mathfrak{g}$ by a nondegenerate symmetric bilinear form on $\mathfrak{g}$ which is ad-invariant:

$$(\mathrm{ad}(Z)X,Y)=-(X,\mathrm{ad}(Z)Y). \tag{3}$$

In this case the coadjoint representation of $\mathfrak{g}$ on $\mathfrak{g}^*$ is identified with the adjoint representation of $\mathfrak{g}$ on itself, and $\mathfrak{g}_\pm^*$ is identified with $\mathfrak{g}_\mp^\perp$, the perpendicular complement of $\mathfrak{g}_\mp$ with respect to the bilinear form (3). Equation (2) then becomes

$$\frac{\partial X}{\partial t_i}=\left[\Pi_+\left(\frac{\delta H_i}{\delta X}\right),X\right],\quad X\in\mathfrak{g}_-^\perp. \tag{4}$$

Hence the Adler–Kostant–Symes theorem provides a systematic method for searching for integrals of the motion of a system described by the Lax equation (4).

Flaschka, Newell and Ratiu[4] apply the Adler–Kostant–Symes result to the loop algebra $\widetilde{sl}(2)$ of formal series $X=\Sigma_{i=-\infty}^{m}X_iz^i$, $X_i\in sl(2,\mathbb{C})$, $m<\infty$. They show that the Ablowitz–Kaup–Newell–Segur (AKNS) equations,

$$\frac{\partial Q}{\partial t_k}=[Q^{(k)},Q],\quad k\geqslant 1, \tag{5}$$

where $Q=\Sigma_{i=0}^{\infty}Q_iz^{-i}$ and $Q^{(k)}=\Sigma_{i=0}^{k}Q_iz^{k-i}$ arise as commuting Hamiltonian flows on $\widetilde{sl}(2)_+^*$. Their theory is outlined below.

Let $\mathfrak{g}$ denote the loop algebra $\widetilde{sl}(2)$ with the commutator bracket. This algebra admits a natural splitting $\mathfrak{g}=\mathfrak{g}_-\oplus\mathfrak{g}_+$ into subalgebras where

$$\mathfrak{g}_+=\left\{X=\sum_{i\geqslant 0}X_iz^i\,\middle|\,X_i\in sl(2,\mathbb{C})\right\},$$

$$\mathfrak{g}_- = \left\{ X = \sum_{i=1}^{\infty} X_i z^{-i} \,\middle|\, X_i \in sl(2,\mathbb{C}) \right\}.$$

We can identify $\mathfrak{g}^*$ with $\mathfrak{g}$ by the nondegenerate symmetric bilinear form,

$$(X,Y) = \mathrm{res}_{z=0}\,\mathrm{Tr}(X(z)Y(z)), \tag{6}$$

which is ad-invariant. The perpendicular complement of $\mathfrak{g}_-$ is $\mathfrak{g}_-^{\perp} = \mathfrak{g}_-$, so $\mathfrak{g}_+^*$ is identified with $\mathfrak{g}_-$. Now consider a family of Hamiltonian functions on $\mathfrak{g}^* \simeq \mathfrak{g}$,

$$H_k(X) = \tfrac{1}{2}\mathrm{res}_{z=0}\,\mathrm{Tr}(z^{k+1}X^2(z)), \quad k \geqslant 1. \tag{7}$$

One easily checks that the Hamiltonians H_k are ad-invariant, hence their restrictions to $\mathfrak{g}_-$ give rise to a hierarchy of commuting flows given by Eq. (4). Furthermore, if $X = \Sigma_{i=1}^{\infty} X_i z^{-i} \in \mathfrak{g}_-$, then

$$\Pi_+\left(\frac{\delta H_k}{\delta X}\right) = \Pi_+(z^{k+1}X) = \sum_{i=0}^{k} X_{i+1} z^{k-i} = M_k.$$

Therefore, for this choice of Hamiltonian functions the system of equations (4) is equivalent with the AKNS equations (5), with X standing for Q and M_k for $Q^{(k)}$.

It is generally stated that the commutativity of the flows of type (5) gives rise to the ''zero curvature'' equation,

$$\frac{\partial M_k}{\partial t_l} - \frac{\partial M_l}{\partial t_k} + [M_k, M_l] = 0. \tag{8}$$

However, if one compares $X_{t_k t_l}$ to $X_{t_l t_k}$, it only follows that the left hand side of Eq. (8) commutes with X. To see that it is actually zero requires more work. Suppose without loss of generality that $k = l + p$ for some $p \geqslant 1$. Observing that

$$M_k = z^p M_l + \sum_{i=1}^{p} X_{l+i+1} z^{p-i}, \tag{9}$$

a lengthy but straighforward computation yields

$$\frac{\partial M_k}{\partial t_l} - \frac{\partial M_l}{\partial t_k} + [M_k, M_l] = z^l \left[z^p \sum_{i=0}^{k} \frac{\partial X_{i+1}}{\partial t_l} z^{-i} - \sum_{i=0}^{l} \frac{\partial X_{i+1}}{\partial t_k} z^{-i} - \sum_{i=0}^{l} \sum_{j=1}^{p} [X_{i+1}, X_{l+j+1}] z^{p-i-j} \right]. \tag{10}$$

Since X satisfies

$$\frac{\partial X}{\partial t_k} = [M_k, X] \quad \text{and} \quad \frac{\partial X}{\partial t_l} = [M_l, X], \tag{11}$$

substituting (9) into the first equation above and making use of the second, one obtains

$$z^p \sum_{i=0}^{\infty} \frac{\partial X_{i+1}}{\partial t_l} z^{-i} = \sum_{i=0}^{\infty} \frac{\partial X_{i+1}}{\partial t_k} z^{-i} + \sum_{i=0}^{\infty} \sum_{j=1}^{p} [X_{i+1}, X_{l+j+1}] z^{p-i-j}.$$

Multiplying this equation by z^l and taking the polynomial part of both sides yields

$$0 = z^k \sum_{i=0}^{k} \frac{\partial X_{i+1}}{\partial t_l} z^{-i} - z^l \sum_{i=0}^{l} \frac{\partial X_{i+1}}{\partial t_k} z^{-i} - \sum_{j=1}^{p} \sum_{i=0}^{k-j} [X_{i+1}, X_{l+j+1}] z^{k-i-j}. \tag{12}$$

The difference between the right hand sides of Eqs. (12) and (10) is given by

$$\sum_{j=1}^{p}\sum_{i=l+1}^{k-j}[X_{i+1},X_{l+j+1}]z^{k-i-j}=\sum_{j=1}^{p}\sum_{i=1}^{p-j}[X_{i+l+1},X_{l+j+1}]z^{p-i-j}$$

$$=\sum_{s=2}^{p}\sum_{\substack{i+j=s,\\ 1\leqslant i\leqslant p-j\\ 1\leqslant j\leqslant p-1}}[X_{i+l+1},X_{l+j+1}]z^{p-i-j}$$

$$=\sum_{s=2}^{p}\sum_{\substack{i+j=s,\\ 1\leqslant i,j\leqslant p}}[X_{i+l+1},X_{l+j+1}]z^{p-i-j},$$

which is zero by skew symmetry. Thus, if X satisfies the system of equations (11), then the matrix elements of X are solutions to a hierarchy of PDE's obtained from the zero-curvature equation (8).

To illustrate the point, let $l=1$, $k=2$, and consider the subset $\mathcal{S}\subset\mathfrak{g}_-$ which consists of all $X\in\mathfrak{g}_-$ such that the first three Fourier coefficients have the form

$$X_1=\begin{pmatrix} i & 0\\ 0 & -i\end{pmatrix},\quad X_2=2\begin{pmatrix} 0 & iu\\ -\overline{iu} & 0\end{pmatrix},\quad X_3=2\begin{pmatrix} -i|u|^2 & h\\ -\overline{h} & i|u|^2\end{pmatrix},$$

for some complex valued functions $u(t_1,t_2)$ and $h(t_1,t_2)$. One easily checks that $\mathcal{S}$ is invariant under the flows (11) (see Ref. 12 for a geometric explanation of this). Then Eq. (8) with $M_1=X_1z+X_2$ and $M_2=X_1z^2+X_2z+X_3$ implies that $h=\frac{1}{2}u_x$ and u satisfies the NLS equation

$$iu_t-\tfrac{1}{2}u_{xx}-4u|u|^2=0, \tag{13}$$

where $x=t_1$ and $t=t_2$.

One should remark that any regular solution of the NLS equation can be studied in this framework. Indeed, suppose that $u(x,t)$ satisfies (13), and form X_1,X_2 and X_3 as above with this particular u and $h=\frac{1}{2}u_x$. Then X_n, $n\geqslant 4$, can be found so that for $X=\Sigma_{i=1}^{\infty}X_iz^{-i}$ we get

$$\frac{\partial X}{\partial x}=[X_1z+X_2,X]\quad\text{and}\quad\frac{\partial X}{\partial t}=[X_1z^2+X_2z+X_3,X]. \tag{14}$$

To find X_n notice that (14) implies

$$\frac{\partial X_1}{\partial x}=0,\quad\frac{\partial X_1}{\partial t}=0,$$

$$\frac{\partial X_2}{\partial x}=[X_1,X_3],\quad\frac{\partial X_2}{\partial t}=[X_1,X_4],$$

$$\frac{\partial X_3}{\partial x}=[X_2,X_3]+[X_1,X_4],\quad\frac{\partial X_3}{\partial t}=[X_1,X_5]+[X_2,X_4],$$

and generally

$$\frac{\partial X_n}{\partial x}=[X_2,X_n]+[X_1,X_{n+1}],\quad\frac{\partial X_n}{\partial t}=[X_3,X_n]+[X_2,X_{n+1}]+[X_1,X_{n+2}].$$

Now let us notice that if we ignore the t-dependence and simply consider the system of ordinary differential equations (ODE's) given by the variable x, then we can solve recursively for X_n by noting first that the off-diagonal part of X_4 is determined from $[X_1,X_4]=(X_3)_x-[X_2,X_3]$, and

that the diagonal part is determined up to an integration constant by $(X_4)_x=[X_2,X_4]+[X_1,X_5]$. Meanwhile, this last equation determines the off-diagonal part of X_5, while the next equation will determine the diagonal part, and so on.

Since the t-equations are three term recursion it is a little more complicated to see that they are not overdetermined. First, we get the off-diagonal part of X_4 from the equation for $(X_2)_t$. Then, using the equation for $(X_3)_t$ we can write the off-diagonal part of X_5 in terms of X_4 and lower terms. Finally, the diagonal part of $(X_4)_t$ involves only the off-diagonal part of X_5, and so we get an ODE for the diagonal part of X_4. Meanwhile, the off-diagonal part of $(X_4)_t$ determines the off-diagonal part of X_6 in terms of X_5 and lower terms, and the diagonal part of $(X_5)_t$ involves only the off-diagonal part of X_6. Thus the argument continues.

Finally, in order to check that we can solve these two ODE's simultaneously in order to get $X(x,t)$, we must check that the mixed partials are equal. But this just amounts to checking that zero-curvature expression is zero for our particular M_1 and M_2. As noted above, this is guaranteed by Eq. (13).

III. THE ZERO-CURVATURE METHOD AND THE RIEMANN–HILBERT PROBLEM

In this section we describe the zero-curvature approach[13] to systems of integrable PDE's, and examine its connection with the Adler–Kostant–Symes method of Flaschka, Newell and Ratiu. In the zero-curvature method one uses commutativity of certain flows on a Banach-Lie group G to derive a hierarchy of integrable nonlinear PDE's on the Lie algebra of G. The flows are generated by an action of the translation group $\mathbb{R}^n$ on G as outlined in the following.

Suppose that G is a Banach–Lie group which contains closed subgroups G_-, G_+ such that $G_-\cap G_+=\{I\}$ and G_-G_+ is open (and usually dense) in G. Then the Lie algebra of G splits into the vector space direct sum of subalgebras $\mathfrak{g}=\mathfrak{g}_-\oplus\mathfrak{g}_+$. Consider the differentiable action $\mathbb{R}^n\times G\to G$ given by

$$\mathbf{t}g=\exp\left(\sum_{i=1}^{n} t_iP_i\right)g, \tag{15}$$

where $\{P_1,\ldots,P_n\}$ is contained in an Abelian subalgebra of $\mathfrak{g}_+$. Note that the action (15) descends to an action of $\mathbb{R}^n$ on the quotient space G/G_+ by

$$\mathbf{t}(gG_+)=(\mathbf{t}g)G_+. \tag{16}$$

Now let $g\in G_-G_+$. Then $\mathbf{t}g\in G_-G_+$ for all $\mathbf{t}$ in a neighborhood U of $0\in\mathbb{R}^n$. Hence $\mathbf{t}g$ can be written in a unique way as the product

$$\mathbf{t}g=g_-(\mathbf{t})g_+(\mathbf{t}),\quad \mathbf{t}\in U, \tag{17}$$

where $g_\pm\in G_\pm$. We shall refer to (17) as the Riemann–Hilbert factorization of $\mathbf{t}g$. Combining this with Eq. (16) it follows that the action of $\mathbb{R}^n$ on the Grassmannian G/G_+ induces the flow $g_-(\mathbf{t})G_+$ on G/G_+. Since $[P_i,P_j]=0$, the t_i and t_j flows commute. Next we will show that $g_-(\mathbf{t})$ is a ''solution'' to a hierarchy of nonlinear PDE's which live on the Lie algebra of G_+. By differentiating Eq. (17) and using (15) one obtains

$$g_-^{-1}P_ig_-=g_-^{-1}\frac{\partial g_-}{\partial t_i}+\frac{\partial g_+}{\partial t_i}g_+^{-1}.$$

By taking the projection $\Pi_+:\mathfrak{g}\to\mathfrak{g}_+$ along $\mathfrak{g}_-$ it follows that

$$\Pi_+(g_-^{-1}P_ig_-)=\frac{\partial g_+}{\partial t_i}g_+^{-1}.$$

Denote $M_i(\mathbf{t})=\Pi_+(g_-^{-1}(\mathbf{t})P_ig_-(\mathbf{t}))$. Since the flows commute, the system of equations,

$$\frac{\partial g_+}{\partial t_i} = M_i g_+, \quad i=1,\ldots,n,$$

satisfies the compatibility condition $(g_+)_{t_k t_l} = (g_+)_{t_l t_k}$ which yields the zero-curvature equation,

$$\frac{\partial M_k}{\partial t_l} - \frac{\partial M_l}{\partial t_k} + [M_k, M_l] = 0. \tag{18}$$

We can think of (18) as an abstract partial differential equation on $\mathfrak{g}_+$. In practice G is usually the loop group of a linear group, and the zero-curvature condition is equivalent to a nonlinear PDE satisfied by a matrix element $u(\mathbf{t})$ of M_k and M_l. Since $u(\mathbf{t})$ can be explicitly calculated in terms of $g_-(\mathbf{t})$ we have the mappings

$$g \mapsto g_-(\mathbf{t}) \mapsto u(\mathbf{t}).$$

The function $u(\mathbf{t})$ simultaneously solves all equations of the form (18) for different values of k and l, and the Riemann–Hilbert factorization establishes the local existence of $u(\mathbf{t})$. Moreover, it linearizes the equations for $u(\mathbf{t})$ since a multiplication of g by $\exp(\Delta t_i P_i)$ corresponds to $u(\mathbf{t})$ flowing in the t_i-direction by the amount Δt_i. Since the map $g \mapsto g_-(\mathbf{t})$ is invariant under the right multiplication of g by an element of G_+, we may assume that $g \in G_-$. Then by uniqueness of the splitting we have $g = g_-(0)$, so g encodes the initial values of $u(\mathbf{t})$.

A convenient analytical structure of G which suffices to describe a number of integrable systems can be constructed as follows (see Ref. 5). Let $\mathcal{A}$ denote the Banach algebra of functions $f: S^1 \to \mathbb{C}$, $f(z) = \Sigma_{n\in\mathbb{Z}} a_n z^n$, with pointwise addition and multiplication, relative to the norm $\|f\|_1 = \Sigma_{n\in\mathbb{Z}} |a_n|$. $\mathcal{A}$ consists of continuous functions on S^1 which have an absolutely convergent Fourier series. Consider the set $GL(n,\mathcal{A})$ of all invertible elements in $M(n,\mathcal{A})$. Here $M(n,\mathcal{A})$ is the matrix Banach algebra with the norm $\|A\| = \Sigma_{i,j=1}^n \|A_{ij}\|_1$. By Wiener's Lemma[14] $f(z)^{-1} \in \mathcal{A}$ if and only if $f(z)$ vanishes nowhere on S^1, hence $GL(n,\mathcal{A})$ is the set of all elements A such that $\det(A(z)) \neq 0$ for all $z \in S^1$. Thus $GL(n,\mathcal{A})$ is a Banach–Lie group as an open submanifold of $M(n,\mathcal{A})$. Let σ be a norm preserving involution on the algebra $M(n,\mathcal{A})$, and define

$$G = \{g \in GL(n,\mathcal{A}) \,|\, g g^\sigma = I\}. \tag{19}$$

A standard result from the theory of Banach manifolds[15] asserts that the group G is a closed submanifold of $M(n,\mathcal{A})$, and hence a Banach–Lie group with Lie algebra,

$$\mathfrak{g} = \{X \in M(n,\mathcal{A}) \,|\, X + X^\sigma = 0\}.$$

Associated with the loop group G we introduce the subgroups

$$G_+ = \left\{ g \in G \,\middle|\, g(z) = \sum_{i\geqslant 0} C_i z^i \right\}, \quad G_- = \left\{ g \in G \,\middle|\, g(z) = I + \sum_{i<0} C_i z^i \right\}.$$

The Lie algebras of G_- and G_+ are closed subalgebras of $\mathfrak{g}$ which they decompose into the direct sum of vector spaces, $\mathfrak{g} = \mathfrak{g}_- \oplus \mathfrak{g}_+$. Thus the set $G_- G_+$ is open in G. A particular choice of σ and the action of $\mathbb{R}^n$ on G determines the hierarchy of differential equations represented by (18). Note that the above construction also includes twisted loop algebras related to systems such as the mKdV equation[12] and the Neumann oscillator.[16] We emphasize that there is a major difference between this method and that of Flaschka, Newell and Ratiu: *the flows are given directly from a group action and there is no use of a Hamiltonian structure.*

To illustrate these remarks let the involution σ on $M(2,\mathcal{A})$ be given by $g^\sigma(z) = \overline{g}^\tau(z)$ where the bar conjugates the Fourier coefficients of $g(z)$, but not the parameter z. Define the action of $\mathbb{R}^2$ on G by

$$\mathbf{t}g = \exp(t_1 i\sigma_3 z + t_2 i\sigma_3 z^2)g,$$

where $\sigma_3 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$. Suppose that $g_-(\mathbf{t})$ is the solution of the Riemann–Hilbert factorization of $\mathbf{t}g$ such that $g_-(0,0) = g$. If $g_- = I + A_1 z^{-1} + A_2 z^{-2} + \cdots$ is the Fourier expansion of $g_-(\mathbf{t})$, then $g_-^{-1} = I - A_1 z^{-1} + (A_1^2 - A_2) z^{-2} + \cdots$. Substituting this into $M_k = \Pi_+(g_-^{-1} i\sigma_3 z^k g_-)$ we obtain

$$M_1 = i\sigma_3 z + [i\sigma_3, A_1],$$

$$M_2 = i\sigma_3 z^2 + [i\sigma_3, A_1]z + [i\sigma_3, A_2] - A_1[i\sigma_3, A_1].$$

Denote

$$A_1 = \begin{pmatrix} ia & u \\ -\overline{u} & ib \end{pmatrix} \quad \text{and} \quad A_2 = \begin{pmatrix} p & r \\ s & q \end{pmatrix},$$

where a and b are real-valued functions of t_1 and t_2 (note that the group law in G implies that A_1 has the form specified above). We then have

$$M_1 = i\sigma_3 z + 2\begin{pmatrix} 0 & iu \\ -\overline{iu} & 0 \end{pmatrix}, \quad M_2 = zM_1 + 2\begin{pmatrix} -i|u|^2 & h \\ -\overline{h} & i|u|^2 \end{pmatrix}$$

where $h = au + ir$. Now it is straightforward to verify that the zero-curvature condition (18) implies that $h = \frac{1}{2}u_x$ and u satisfies the NLS equation (13) where $x = t_1$ and $t = t_2$.

IV. RELATING THE TWO METHODS

In this section we give a direct proof of the equivalence of the Flaschka–Newell–Ratiu method and the zero-curvature approach. We shall consider a slightly more general type of AKNS equations of which (5) is a special case. In the following it is assumed that G is a given Banach–Lie group defined by Eq. (19) whose Lie algebra admits the ad-invariant bilinear form (6), and $\mathfrak{g}_-$ satisfies $\mathfrak{g}_-^{\perp} = \mathfrak{g}_-$.

Consider the Riemann-Hilbert splitting on G,

$$\exp\left(\sum_{i=1}^{n} t_i R^p z^i\right) g = g_-(\mathbf{t}) g_+(\mathbf{t}), \quad g \in G_-, \tag{20}$$

where we assume that $R \in GL(n,\mathbb{C})$ is chosen so that $R^p z^i \in \mathfrak{g}_+$ for some $p \in \mathbb{N}$. We associate to splitting (20) the generalized AKNS equations on the Lie algebra of G_-:

$$\frac{\partial X}{\partial t_k} = [\Pi_+(z^{k+p} X^p), X], \quad X \in \mathfrak{g}_-. \tag{21}$$

Note that (21) is equivalent with (5) when $p = 1$ because Π_+ is the projection containing only non-negative powers of z. According to Flaschka–Newell–Ratiu theory, the Lax equations (21) are commuting flows of ad-invariant Hamiltonians,

$$H_k^{(p)}(X) = \frac{1}{p+1} \operatorname{res}_{z=0} \operatorname{Tr}(z^{k+p} X^{p+1}), \quad 1 \leqslant k \leqslant n.$$

Proposition 1: *If the flow $g_-(\mathbf{t}) \in G_-$ is obtained by solving the Riemann–Hilbert problem (20), then $X(\mathbf{t}) = g_-^{-1}(\mathbf{t}) R z^{-1} g_-(\mathbf{t})$ is the integral curve of (21) with initial value $X(0) = g^{-1} R z^{-1} g$.*

Proof: Define $X(\mathbf{t}) = g_-^{-1}(\mathbf{t}) R z^{-1} g_-(\mathbf{t})$. Then it readily follows that

$$\frac{\partial X}{\partial t_k}=\left[X,g_-^{-1}\frac{\partial g_-}{\partial t_k}\right]. \tag{22}$$

On the other hand, by differentiating Eq. (20) we obtain

$$z^{k+p}X^p=g_-^{-1}\frac{\partial g_-}{\partial t_k}+\frac{\partial g_+}{\partial t_k}g_+^{-1}, \tag{23}$$

which yields

$$\frac{\partial g_+}{\partial t_k}g_+^{-1}=\Pi_+(z^{k+p}X^p).$$

Substituting this back into Eq. (23) and using Eq. (22) we conclude that $X(\mathbf{t})$ is a solution of the Lax equations (21) with initial value $X(0)=g^{-1}Rz^{-1}g$. ■

Thus, by solving the Riemann–Hilbert problem one obtains solutions of the AKNS equations. This is not surprising, but one can show that the converse is also true. Namely, if one is given a solution of the AKNS system (21), then it is possible to construct the flows $g_\pm(\mathbf{t})\in G_\pm$ without actually solving the Riemann–Hilbert problem (20).

Proposition 2: *Suppose that $X(\mathbf{t})\in\mathfrak{g}_-$ is the integral curve of (21) with initial value $X(0)=g^{-1}Rz^{-1}g$ for some $g\in G_-$. Then $X(\mathbf{t})$ induces Abelian flows $g_\pm(\mathbf{t})\in G_\pm$ which represent solutions of the Riemann–Hilbert problem (20). Furthermore, the evolution of $X(\mathbf{t})$ is given by $X(\mathbf{t})=g_-^{-1}(\mathbf{t})Rz^{-1}g_-(\mathbf{t})$.*

Proof: Define $M_k^{(p)}=\Pi_+(z^{k+p}X^p)$ and $N_k^{(p)}=\Pi_-(z^{k+p}X^p)$. For fixed k, solve the following differential equations for $g_\pm\in G_\pm$:

$$\frac{\partial g_+}{\partial t_k}=M_k^{(p)}g_+,\quad \frac{\partial g_-}{\partial t_k}=g_-N_k^{(p)}, \tag{24}$$

with $g_+(0)=I$ and $g_-(0)=g$. Using the decomposition $z^{k+p}X^p=N_k^{(p)}+M_k^{(p)}$ and Eq. (21) we have

$$\frac{\partial X}{\partial t_k}=-[N_k^{(p)},X].$$

This implies

$$\frac{\partial}{\partial t_k}(g_-Xg_-^{-1})=\left(\frac{\partial X}{\partial t_k}+[N_k^{(p)},X]\right)g_-^{-1}=0.$$

Hence $g_-(\mathbf{t})X(\mathbf{t})g_-^{-1}(\mathbf{t})$ is a constant loop. But $X(0)=g^{-1}Rz^{-1}g$ and $g_-(0)=g$, so it follows that

$$X(\mathbf{t})=g_-^{-1}(\mathbf{t})Rz^{-1}g_-(\mathbf{t}). \tag{25}$$

Furthermore, in view of Eqs. (25) and (24) the identity $z^{k+p}X^p=N_k^{(p)}+M_k^{(p)}$ implies that the product g_-g_+ satisfies

$$\frac{\partial}{\partial t_k}(g_-g_+)=R^pz^kg_-g_+,\quad k=1,2,\ldots,n.$$

This equation has a unique solution $g_-(\mathbf{t})g_+(\mathbf{t})=\exp(\Sigma_{k=1}^n t_kR^pz^k)g_-(0)\,g_+(0)$ with initial value $g_-(0)\,g_+(0)=g$. Hence the flows $g_-(\mathbf{t})$ and $g_+(\mathbf{t})$ are solutions of the Riemann–Hilbert problem (20). ■

V. THE GEOMETRIC PICTURE

In Ref. 6, Guillemin and Sternberg showed that the flows in $\mathfrak{g}_+^*$ obtained from the Adler–Kostant–Symes method are given by projecting certain flows on the cotangent bundle T^*G to T^*G_+, and then identifying T^*G_+ with $G_+\times\mathfrak{g}_+^*$ via left multiplication. This geometric description of the Adler–Kostant–Symes flows is as follows.

Let $H\in I(\mathfrak{g}^*)$. Identify T^*G with $G\times\mathfrak{g}^*$ via left multiplication, and use this identification to consider H as a Hamiltonian function on T^*G. It is shown in Ref. 6 that this generates the flow through $(g,\mu)\in G\times\mathfrak{g}^*$ given by

$$(g,\mu)\mapsto(g\exp(-tX),\mu), \tag{26}$$

where $X=dH(-\mu)$. In this section we shall identify $dH(-\mu)$ with $\delta H/\delta(-\mu)\in\mathfrak{g}$.

Notice that under this flow, the space $G\times\mathfrak{g}_+^*$ is invariant. Right multiplication by the inverse induces the action of G_- on $G\times\mathfrak{g}_+^*$ given by

$$h(g,\mu)=(gh^{-1},\mathrm{Ad}^*(h^{-1})\mu).$$

Thus, on the open dense subspace $G_+G_-\times\mathfrak{g}_+^*\subset G\times\mathfrak{g}_+^*$ we have the projection

$$\pi: G_+G_-\times\mathfrak{g}_+^*\to G_+\times\mathfrak{g}_+^*,$$

$$\pi((g_+g_-,\mu))=(g_+,\mathrm{Ad}^*(g_-^{-1})\mu),$$

given by quotienting by the action.

Guillemin and Sternberg show that the Adler–Kostant–Symes flows for $H\in I(\mathfrak{g}^*)$ in $\mathfrak{g}_+^*$ are given by the $\mathfrak{g}_+^*$ component of the projection of the flow (26). Namely, if we write

$$g\exp(-tX)=g_+(t)g_-(t),$$

then this flow is given by

$$\mu(t)=\mathrm{Ad}^*(g_-^{-1}(t))\mu_0,\quad \mu_0\in\mathfrak{g}_+^*. \tag{27}$$

Now, let H_1 and H_2 be Hamiltonians in $I(\mathfrak{g}_+^*)$ whose flows are parametrized by x and t variables, respectively. Fix $\mu_0\in\mathfrak{g}_+^*$, and let

$$P_1=dH_1(-\mu_0),\quad P_2=dH_2(-\mu_0).$$

Since x and t flows commute we can write

$$g\exp(-xP_1)\exp(-tP_2)=g_+(x,t)g_-(x,t). \tag{28}$$

Hence Eq. (27) gives the flow

$$\mu(x,t)=\mathrm{Ad}^*(g_-^{-1}(x,t))\mu_0.$$

On the other hand, identifying $\mathfrak{g}_+^*$ with $\mathfrak{g}_-^{\perp}=\mathfrak{g}_-$ we have

$$\mu(x,t)=\mathrm{Ad}(g_-(x,t))\mu_0,\quad \mu_0\in\mathfrak{g}_-. \tag{29}$$

From the Adler–Kostant–Symes theorem μ satisfies the differential equations

$$\frac{\partial\mu}{\partial x}=[\Pi_+(dH_1(-\mu)),\mu], \tag{30}$$

$$\frac{\partial \mu}{\partial t} = [\Pi_+(dH_2(-\mu)), \mu]. \tag{31}$$

As in Sec. II, the PDE follows from the commutation relation for

$$\Pi_+(dH_1(-\mu)) \text{ and } \Pi_+(dH_2(-\mu)).$$

From Eq. (28) we have

$$\exp(tP_2)\exp(xP_1)g^{-1} = g_-^{-1}(x,t)g_+^{-1}(x,t).$$

Comparing this with the Riemann–Hilbert splitting of the flow $\exp(xP_1+tP_2)g^{-1}$ we conclude that M_k in Eq. (18) is given by

$$M_k = -\Pi_+(g_- P_k g_-^{-1}) = -\Pi_+[\mathrm{Ad}(g_-)dH_k(-\mu_0)] = -\Pi_+[dH_k(\mathrm{Ad}(g_-)(-\mu_0))],$$

because H_k is ad-invariant. In view of Eq. (29) it follows that the commutation relations for M_k are equivalent to those for $\Pi_+[(dH_k(-\mu))]$. Note also that the initial conditions, exemplified by $\mathcal{S}$ for the NLS example in the Flaschka–Newell–Ratiu approach, are determined by the G_- orbit through μ_0.

Notice that in order to produce the Lax pairs (30)–(31) on $\mathfrak{g}_-$ we have reduced the flows on T^*G to $T^*G_+ \subset T^*(G/G_-)$. Hence, these flows are directly related to Hamiltonian flows on the cotangent bundle of the Grassmannian G/G_-, while the zero-curvature formalism starts with flows on G/G_+. The Grassmannian G/G_- is the ''dual Grassmannian'' to G/G_+. If one identifies G/G_+ to the Grassmannian of subspaces of vectors in $L^2(S^1)$ which are in the G orbit of the Hardy space $L^2_+(S^1)$, then the G orbit of $L^2_-(S^1)$ is the collection of dual spaces to G/G_+ because the negative frequency space $L^2_-(S^1)$ is dual to $L^2_+(S^1)$. This duality gives a map from G/G_+ to G/G_- by sending a subspace in G/G_+ to its dual in G/G_-. Since the big cell of G/G_+ is identified with G_- (and likewise the big cell of G/G_- with G_+) this map can be considered as a map from G_- to G_+. However, it is not the case that the flows g_- and g_+ are related by that map. These flows are simply related by the fact that they are projections of the flow through g in G.

We now show how this works in the NLS example. Here we choose $\mu_0 \in \mathfrak{g}_-^{\perp} = \mathfrak{g}_-$ to be

$$\mu_0 = -z^{-1} i\sigma_3, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Using H_1 and H_2 from Eq. (7) we have that $dH_k(-\mu_0) = P_k$ with $P_1 = zi\sigma_3$, $P_2 = z^2 i\sigma_3$. Finally, taking $g_- = I + z^{-1}A_1 + z^{-2}A_2 + \cdots$ yields

$$M_k = \Pi_+[dH_k(-\mathrm{Ad}(g_-)\mu_0)].$$

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Lie algebraic approach to the construction of (2+1)-dimensional lattice-field and field integrable Hamiltonian equations

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Two different methods for the construction of $(2+1)$-dimensional integrable lattice-field and field Hamiltonian dynamical systems are presented. The first method is based on the so-called central extension procedure applied to the Lie algebra of shift operators and the Lie algebra of pseudodifferential operators. The second method is the so-called operand formalism. Both methods allow a construction of some new integrable nonlinear Hamiltonian lattice-field and field equations in $(2+1)$-dimensional space. © *2001 American Institute of Physics.*
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I. INTRODUCTION

For the last 20 years algebraic tools, basically the $\mathcal{R}$-matrix approach, have been widely applied for the construction of nonlinear integrable Hamiltonian dynamical systems. This approach was proposed in pioneer works by Adler,[1] Reyman and Semenov-Tian-Shansky,[2] and also by Gelfand and Dikii[3] and led finally to the celebrated Adler–Gelfand–Dikii (AGD) scheme. On the other hand, the notion of bi-Hamiltonicity, introduced by Magri,[4] revealed an important feature of integrable Hamiltonian systems. Actually, it allows a construction of a whole hierarchy of commuting vector fields (symmetries) and related gradients (co-symmetries) of conserved quantities in involution with respect to two Poisson brackets which ''decode'' the notion of bi-Hamiltonicity. In his famous paper this notion was illustrated on the Harry–Dym, nonlinear Schrödinger, mKdV, and KdV equations, and their bi-Hamiltonian structures were found, i.e., a pair of compatible Poisson (implectic) operators, where compatibility means that a linear combination of two Poisson operators is itself a Poisson operator. On the other hand, working in a frame of the AGD scheme one can quite readily construct bi-Hamiltonian structures of the above-mentioned dynamical systems and many others. We only need to start from a suitable Lax operator which defines a specific dynamical system. This approach was successfully applied to integrable field $(1+1)$-dimensional dynamical systems. In later papers[5–7] this formalism was applied to the construction of integrable lattice dynamical systems.

The next task was to develop this formalism for $(2+1)$-dimensional dynamics. However, as shown by Zakharov and Konopelchenko,[8] the regular recursion operator Φ for symmetries (or, respectively, Ψ one for co-symmetries) which admits an implectic–symplectic factorization, i.e., can be presented in the form $\Phi=\theta_2\cdot\theta_1^{-1}$ ($\Psi=\theta_1^{-1}\cdot\theta_2$), where $(\theta_1,\ \theta_2)$ is a pair of compatible implectic operators, constructed from a bi-Hamiltonian formulation of the dynamics, is a pure one-dimensional phenomenon. Nevertheless, as was shown in Refs. 9 and 10, equations in $(2+1)$-dimensions, and in particular the Kadomtsev–Petviashvili equation, admit a new type of bi-Hamiltonian formulation and thus the result of Ref. 8 is not violated. This generalized bi-Hamiltonian formulation was given as a kernel representation by Fokas and Santini[9,11,12] and also by introducing the Lenard bi-complex scheme in Refs. 13 and 14. In later works[11,15,16] the so-

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called operand formalism was introduced, i.e., the AGD scheme over the noncommutative ring of formal integro-differential operators with respect to ∂_y. The particular realization of operator value fields is formally equivalent to the central extension approach with additional space variable y, which allows a construction of a hierarchy of symmetries and a Hamiltonian formulation (Poisson tensor) of the $(2+1)$-dimensional dynamical systems. The central extension method was considered in early works by Reiman and Semenov-Tian-Shansky[2,17] and also by Prikarpatsky.[18,19] The well-known Sato approach[20,21] also allows a construction of a hierarchy of commuting vector fields, but it does not contain a systematic way for the construction of a Hamiltonian formulation of $(2+1)$-dimensional dynamics. Magnano and Magri[22] showed how to extend the Lenard bicomplex scheme onto n-field manifold and developed a method for the construction of Poisson structures for the Sato hierarchy using n-fold Hamiltonian formalism. Thus the results of previous papers[9–13,16] were extended onto n-field manifold in the $(2+1)$-dimensional case and the problem of the extension of the AGD scheme onto $(2+1)$-dimensional space for the field dynamical systems was completely solved.

Here we would like to stress that when we work with more then one-field dynamics and apply the operand formalism, we are not able to construct a whole hierarchy of commuting vector fields which can be fully presented by the central extension approach.

The basic aim of the present paper is to apply the operand formalism for the construction of lattice-field dynamics in $(2+1)$ dimensions, i.e., dynamics with one discrete and one continuous space variable. The results of this approach were given in Ref. 23 and here we present a more detailed theory including many examples. We also present the results of the operand approach, applied to the field dynamical systems. Although this formalism is not as complete as the one proposed by Magri and Magnano, nevertheless it allows some new results which we present here. As it seems to us nowadays, the Magnano–Magri approach cannot be applied for the construction of the lattice-field two-dimensional dynamics because the Lie algebra of shift operators has specific, non-derivative-like' features of the shifts. Here we develop and generalize the results of Refs. 9–13, and 16 and work in the frames of the operand formalism. In Sec. II we recall the $\mathcal{R}$-matrix formalism and the AGD scheme. In Sec. III we formulate the central extension procedure and apply it to the Lie algebras of shift and pseudodifferential (PDO) operators, respectively. We illustrate the results of our approach by many examples of known and new $(2+1)$-dimensional systems of lattice-field and field types, putting them into one unified scheme. Section IV contains the so-called operand approach to the construction of the extended bi-Hamiltonian formalism for dynamical systems in $(2+1)$-dimensions. We recall the basic notions of the operand approach, proposed in earlier works by Magri, Morosi, and Tondo,[13] and also by Athorne and Dorfman[16] and Fokas and Santini[10] and propose some generalizations of this formalism. The examples considered coincide with those from the previous section but due to the operand formalism approach the $(2+1)$-dimensional dynamical systems are endowed now with a generalized bi-Hamiltonian structure. In conclusion we discuss basic results of this work and some open problems.

II. LIE ALGEBRAIC APPROACH TO THE HAMILTONIAN DYNAMICAL SYSTEMS: $\mathcal{R}$-MATRIX FORMALISM

As mentioned in Sec. I, integrable dynamical systems may be constructed using Lie algebra techniques, and the Lax equation $L_t=[A,L]$ itself can be considered as some Hamiltonian dynamical system on a suitable Lie algebra. Here we recall basic notions of Lie algebra construction.[24]

Let g be a Lie algebra, g^* the dual algebra related to g by the *duality map* $\langle\cdot,\cdot\rangle_g\to\mathbb{R}$,

$$g^*\times g\to\mathbb{R}: \quad (\alpha,a)\to\langle\alpha,a\rangle_g, \quad a\in g, \quad \alpha\in g^*, \tag{1}$$

and $\mathcal{D}(g^*):=C^\infty(g^*)$ be a space of C^∞-functions on g^*. Then, let

$$\mathrm{ad}:g\times g\to g: \quad (a,b)\mapsto \mathrm{ad}_a b, \quad a,b\in g, \tag{2}$$

be the adjoint action of g on g, i.e., the Lie product, and

$$\mathrm{ad}^*: g\times g^*\to g^*: \quad (a,\alpha)\mapsto \mathrm{ad}_a^*\alpha, \quad a\in g, \quad \alpha\in g^* \tag{3}$$

be the co-adjoint action of g on g^*. For arbitrary $a,b\in g$ and $\alpha\in g^*$ the following relations hold:

$$\mathrm{ad}_a b=[a,b], \quad \langle \mathrm{ad}_a^*\alpha,b\rangle_g=-\langle \alpha,\mathrm{ad}_a b\rangle_g=-\langle \alpha,[a,b]\rangle_g, \tag{4}$$

where $[\cdot,\cdot]$ is a Lie bracket on g. The Lie bracket is:

(i) skew-symmetric

$$[a,b]=-[b,a] \tag{5}$$

and

(ii) satisfies the Jacobi identity

$$[[a,b],c]+[[c,a],b]+[[b,c],a]=0. \tag{6}$$

There exists a natural *Lie–Poisson bracket* on g^*, discovered by Lie[25] and rediscovered by Kirillov,[26] Kostant,[27] Souriau,[28] and Berezin.[29] Let $L\in g^*$, functions H_i, H_j belong to the space of functions on g^*: $\mathcal{D}(g^*)$, and their gradients ∇H_i, $\nabla H_j\in g$, then the Lie–Poisson bracket reads

$$\{H_i,H_j\}(L):=\langle L,[\nabla H_j,\nabla H_i]\rangle_g. \tag{7}$$

Consider next a dynamical system defined by

$$L_t=\{H,L\}. \tag{8}$$

So according to relations (4) and (7), a Hamiltonian dynamical system on g^* can be written down in the following form:

$$L_t=-\mathrm{ad}^*_{\nabla H}L=\Theta(L)\circ\nabla H, \quad L\in g^*, \quad \nabla H\in g, \tag{9}$$

where $\Theta(L): g\to g^*$ is a Poisson tensor.

We confine our further considerations to such algebras for which g^* can be identified with g. So, we assume the existence of an invariant metric, i.e., nondegenerate symmetric product on g,

$$(a,b)_g=(b,a)_g, \quad a,b\in g, \tag{10}$$

invariant under the adjoint action

$$(\mathrm{ad}_a b,c)_g+(b,\mathrm{ad}_a c)_g=0\Leftrightarrow([a,b],c)_g=(a,[b,c])_g, \quad a,b,c\in g. \tag{11}$$

In our particular realizations it will be a *trace form* $\mathrm{tr}: g\to\mathbb{R}$,

$$(a,b)_g=\mathrm{tr}(a\cdot b)=\mathrm{tr}(b\cdot a)=(b,a)_g, \tag{12}$$

where "$\cdot$" means some multiplication of the elements $a,b\in g$. For example, if g is a Lie algebra of shift operators (17), then, for $a=\Sigma_i a_i(n)\mathcal{E}^i$ and $b=\Sigma_j b_j(n)\mathcal{E}^j$ we have $a\cdot b=\Sigma_{i,j} a_i(n)b_j(n+i)\mathcal{E}^{i+j}$. For the PDO Lie algebra (21) if $a=\Sigma_i a_i(x)\partial_x^i$ and $b=\Sigma_j b_j(x)\partial_x^j$ we have $a\cdot b=\Sigma_{i,j} a_i(x)\partial_x^i b_j(x)\partial_x^j$, where $\partial_x^i b_j(x)\partial_x^j$ can be calculated using (22). Then, we can identify g^* with g, $(g^*\cong g)$ by setting

$$\langle \alpha,b\rangle_g=(a,b)_g, \quad a,b\in g, \alpha\in g^*, \tag{13}$$

where α is identified with $a\in g$. Thus, now we can write the Lie–Poisson bracket as

$$\begin{aligned}\{H_i,H_j\}(L)&=\langle L,[\nabla H_j,\nabla H_i]\rangle_g\\&=(L,[\nabla H_j,\nabla H_i])_g\\&=(\nabla H_j,[\nabla H_i,L])_g\equiv(\nabla H_j,\Theta(L)\circ\nabla H_i)_g,\end{aligned}\tag{14}$$

where ''$\circ$'' means an action of the Poisson operator on the gradient ∇H. Hence, equation of motion (9) takes the form

$$L_t=-\mathrm{ad}^*_{\nabla H}L=\Theta(L)\circ\nabla H=[\nabla H,L]=\mathrm{ad}_{\nabla H}L.\tag{15}$$

We notice that under the above-mentioned identification $g^*\cong g$, the co-adjoint action goes over into the minus adjoint one.

Now, we can identify the dynamic equation (15) and the Lax equation with a natural Hamiltonian structure

$$L_t=[A,L]=[\nabla H,L]=\Theta(L)\circ\nabla H.\tag{16}$$

This abstract approach to integrable systems profits with a deeper understanding of the nature of integrability as well as equips us with a very general and efficient tool for the construction of multi-Hamiltonian systems from a scratch. Working with the Lie algebra formalism we will apply it to the construction of finite field dynamical systems. We pick up the Lie algebra of shift operators of the form

$$g=\left\{L=\sum\nolimits_{i\ll\infty}u_i(n)\mathcal{E}^i\right\},\tag{17}$$

where $\mathcal{E}$ is a shift operator, which satisfies the simple commutation rule

$$\mathcal{E}^iu(n)=(E^iu(n))\mathcal{E}^i=u(n+i)\mathcal{E}^i,\tag{18}$$

E acts on $u(n)$ as a unit shift: $Eu(n):=u(n+1)$, $i\in\mathbb{Z}$ and $u(n)$ are discrete functions with space variable $n\in\mathbb{Z}$. For the Lie algebra g of shift operators (18) a *trace* form (12) takes the form

$$\mathrm{tr}(a)=\mathrm{tr}\left(\sum\nolimits_i a_i(n)\mathcal{E}^i\right)=\sum\nolimits_{-\infty}^{\infty}a_0(n).\tag{19}$$

The vector fields L_t and gradients ∇H are conveniently parametrized by

$$L_t=\sum\nolimits_{i<\infty}(u_i)_t\mathcal{E}^i,\quad \nabla H=\sum\nolimits_i\mathcal{E}^{-i}\frac{\delta H}{\delta u_i},\tag{20}$$

where $\delta H/\delta u_i$ is variational derivative of a functional $H=\Sigma_{n=-\infty}^{+\infty}h[u(n)]$ and $h[u(n)]:=h(u(n),u(n\pm1),u(n\pm2),\dots)$. The PDO Lie algebra is given by

$$g=\left\{L=\sum\nolimits_{i\ll\infty}u_i(x)\partial_x^i\right\},\tag{21}$$

where ∂_x^k acts on $a(x)$ according to the general Leibniz rule

$$\partial_x^ka=\sum\nolimits_{i\geqslant0}C_i^k(D_x^ia)\partial_x^{k-i},\tag{22}$$

where $D_x=\mathrm{ad}_{\partial_x}$, $D_xa=a_x$,

$$C_i^k=\left\{\begin{array}{ll}\binom{k}{i} & \text{for} \quad k\geqslant i\geqslant 0\\ 0 & \text{for} \quad i\geqslant k\geqslant 0 \ \text{ or } \ i<0\\ \binom{|k|+i-1}{i}(-1)^i & \text{for} \quad k<0, i\geqslant 0\end{array}\right\}$$

and

$$\binom{k}{i}=\frac{k!}{i!(k-i)!}.$$

Then the trace form of g (12) is

$$\mathrm{tr}(L)=\mathrm{tr}\left(\sum\nolimits_{i\ll\infty}u_i(x)\partial_x^i\right)=\int_{\mathbb{R}}\mathrm{res}\left(\sum\nolimits_{i\ll\infty}u_i(x)\partial_x^i\right)dx=\int_{\mathbb{R}}u_{-1}(x)dx, \tag{23}$$

and allows us to identify g^* with g. As a consequence, vector fields L_t and gradients ∇H are conveniently parametrized by

$$L_t=\sum\nolimits_{i\ll\infty}(u_i)_t\partial_x^i, \quad \nabla H(L)=\sum\nolimits_{i\ll\infty}\partial_x^{-1-i}\frac{\delta H}{\delta u_i}, \tag{24}$$

where $\delta H/\delta u_i$ is the usual variational derivative of the functional $H=\int_{\mathbb{R}}h[u(x)]dx$ and $h[u]$ $:=h(u, u_x, u_{xx}, \ldots)$. Both Lie algebras contain an infinite number of fields so, because we are interested in dynamical systems with finite number of fields, we have to reduce the Lie–Poisson bracket (14) onto a suitable submanifold $\overline{M}$. This procedure can be successfully done using the $\mathcal{R}$-matrix formalism.

Although all considerations in this paper are performed on the algebraic level, one has to pay much attention to the admissible classes of functions, i.e., such that the action of all constructed objects on them do make sense. At least in one space dimension it is obvious that the basic manifold M can be considered as a topological linear space of complex-valued, C^∞-functions f of a real variable $x\in\mathbb{R}$ such that $D^{-1}f$ is well defined and $\int_\Omega f\,dx<\infty$. In the case of lattice functions, the continuous space variable $x\in\mathbb{R}$ is replaced by a discrete integer variable $n\in\mathbb{Z}$. In such a case, we assume that the series $\Sigma_{n=-\infty}^{n=+\infty}f(n)$ must be absolutely convergent. In two space dimensions the situation is even more delicate as all equations are nonlocal, but the nonlocality is of a special form. For field systems, for example, operators D_x^{-1}, D_y^{-1} never appear alone but always in pairs $D_x^{-1}D_y$ or $D_y^{-1}D_x$. That is, the hierarchies of symmetries and conservation laws belong to a field of so-called quasilocal functions.[30] Of course M should be choosen as carefully as in the one-dimensional case.

Let us consider a nonlinear dynamical system

$$u_t=K[u] \tag{25}$$

on a Poisson manifold M, i.e., a manifold endowed with a Poisson structure, $u\in M$ is n-component field ($n\geqslant 1$), $K\in TM$ is a vector field from the tangent bundle of M. Let $\tilde{g}$ be an Abelian Lie algebra of Hamiltonian symmetries of (25). Then consider another Lie algebra g such that $\tilde{g}$ is isomorphic to its some subalgebra. So, for a given $\tilde{a}\in\tilde{g}$ we denote by a its counterpart from g. Finally, we assume the existence of some ''momentum mapping'' $L:M\to g^*$ such that

$$\begin{array}{ccc} M & \overset{L}{\rightarrow} & g^* \\ \phi^{\tilde{a}} \downarrow & & \downarrow \mathrm{ad}_a^* \\ M & \overset{L}{\rightarrow} & g^* \end{array}$$

is commuting for any $\tilde{a} \in \tilde{g}$. Here $\phi^{\tilde{a}}$ denotes a Hamiltonian Poisson action with infinitesimal generator $\tilde{a}$. Additionally we assume the existence of a trace form $\mathrm{tr}: g \to \mathbb{R}$ (12) allowing us to identify g^* with g. As a result of the above assumptions one can represent the Poisson structure on the manifold M as a standard reduction on M of the canonical Lie–Poisson structure on the $g^* \cong g$:

$$\{h_i, h_j\}(u) \equiv \{H_i, H_j\}(L) := (L, [\nabla H_j, \nabla H_i])_g, \tag{27}$$

where the functionals h_i, h_j belong to the functional space $\mathcal{D}(g)$. The main reason for such a construction is that *a priori* we do not know the explicit form of the dynamics (25) and the related Poisson structure. On the other hand, choosing an appropriate algebra g, we select the admissible maps L, and for each L first we construct a respective Hamiltonian subalgebra on g and then we reconstruct the related subalgebra $\tilde{g}$ on M. Hence, as regards the integrable Poissonian flows (25) on M, we intend to construct a hierarchy of Poisson commuting functionals $H_i := h_i \in \mathcal{D}(M)$, $i \in \mathbb{Z}_+$, which can be produced first on g via the standard $\mathcal{R}$-martix approach.[25,31]

We will consider a Casimir functional C of the Lie–Poisson bracket (27), satisfying

$$[\nabla C(L), L] = 0. \tag{28}$$

The role of the Casimir functionals in the $\mathcal{R}$-matrix formalism will be cleared in the following.

As we are interested in finite field dynamical systems, we have to construct an invariant with respect to ad-operation submanifold $\overline{M}$. Assume that the Lie algebra g admits a standard $\mathcal{R}$-structure, that is the new Lie bracket[32]

$$[a,b]_{\mathcal{R}} := [a, \mathcal{R}b] + [\mathcal{R}a, b] \tag{29}$$

defined by some linear homomorphism $\mathcal{R}: g \to g$. The $\mathrm{ad}^{\mathcal{R}}$-operation must be associative with respect to this bracket, i.e.,

$$\mathrm{ad}_a^{\mathcal{R}}[b,c]_{\mathcal{R}} = [\mathrm{ad}_a^{\mathcal{R}} b, c]_{\mathcal{R}} + [b, \mathrm{ad}_c^{\mathcal{R}}]_{\mathcal{R}}, \tag{30}$$

where now

$$\mathrm{ad}_a^{\mathcal{R}} b = [a,b]_{\mathcal{R}}, \tag{31}$$

or, in other words, the new Lie bracket must satisfy the Jacobi identity or sufficiently the following modified Yang–Baxter $[\mathrm{mYB}(q)]$ equation

$$[\mathcal{R}a, \mathcal{R}b] - \mathcal{R}([a,b]_{\mathcal{R}}) = -q[a,b] \tag{32}$$

for any $a, b \in g$ and constant q.[32]

Consider the following Poisson structures on the double Lie algebra $(\mathcal{R}, g)$:[33,7]

$$\{H_i, H_j\}_1(L) := (\nabla H_j, \Theta_1(L) \circ \nabla H_i)_g, \tag{33}$$

$$\{H_i, H_j\}_2(L) := (\nabla H_j, \Theta_2(L) \circ \nabla H_i)_g, \tag{34}$$

where $L \in g^* \simeq g$ is a Hill's type (scalar) Lax operator and the respective Poisson tensors are

$$\Theta_1(L)\circ\nabla H:=[\mathcal{R}\nabla H,L]+\mathcal{R}^*[\nabla H,L], \tag{35}$$

$$\Theta_2(L)\circ\nabla H:=A_1(L\nabla H)L-LA_2(\nabla HL)+S(\nabla HL)L-LS^*(L\nabla H), \tag{36}$$

where for the second Poisson structure

$$A_1+S=A_2+S^*=\mathcal{R}, \tag{37}$$

the linear maps $A_{1,2}:g\to g$ are skew-symmetric ($A_{1,2}^*=-A_{1,2}$) with respect to the trace duality and the linear map $S:g\to g$ with the adjoint S^* satisfies

$$\begin{gathered} S[A_2(a),b]+[a,A_2(b)]=[S(a),S(b)],\\ S^*[A_1(a),b]+[a,A_1(b)]=[S^*(a),S^*(b)],\quad a,b\in g. \end{gathered} \tag{38}$$

These are the most general, linear, and quadratic in L, Poisson tensors on g which are compatible as it is not difficult to check that $\Theta_2(L+\varepsilon\mathbf{1})=\Theta_2(L)+\varepsilon\Theta_1(L)$. We recall that two Poisson tensors are called compatible if their linear combination is also a Poisson tensor. The compatibility condition is needed for the construction of recursion operator and a hierarchy of commuting vector fields. The reader can find more detailed information in Ref. 24. Besides, one can verify that for solutions of Eq. (28): $\nabla H=\nabla C(L)$, we get

$$\begin{gathered} \Theta_1(L)\circ\nabla C=[\mathcal{R}\nabla C,L],\\ \Theta_2(L)\circ\nabla C=[\mathcal{R}(L\cdot\nabla C),L], \end{gathered} \tag{39}$$

which are in the form of Lie–Poisson bracket.

Theorem 1 (Ref. 31): *Given a set of Casimir functionals $C_i\in\mathcal{D}(g^*), i\in\mathbb{Z}_+$ solving Eq. (28), all the reduced on $\overline{M}$ functionals $C_i:=c_i[u]$ $u\in\overline{M}$ are in involution with respect to the Poisson brackets*

$$\{c_i,c_j\}_{\theta_s}(u)\equiv\{C_i,C_j\}_{\Theta_s}(L)=(\nabla C_j,\Theta_s(L)\circ\nabla C_i)_g=0,\quad s=1,2, \tag{40}$$

reduced from g^* on $\overline{M}$ according to the diagram (26), where $\Theta_s(L)$ are Poisson tensors on g^* and $\theta_s(u)$ are respective Poisson tensors on $\overline{M}$. Moreover the momentum mapping $L:M\to g^*$ and Hamiltonian functionals $C_i(L)$ satisfy the following evolution equations on $g^*\cong g$:

$$L_{t_i}=\mathrm{ad}_{\mathcal{R}(L^{s-1}\cdot\nabla C_i)}L=[\mathcal{R}(L^{s-1}\cdot\nabla C_i),L]=\Theta_s(L)\circ\nabla C_i,\quad s=1,2, \tag{41}$$

which is just a Lax representation of the dynamical system (25), i.e., $A=\mathcal{R}(L^{s-1}\cdot\nabla C_i)$.

To construct the simplest $\mathcal{R}$-structure let us assume that the Lie algebra g can be split into a direct sum of Lie subalgebras g_+ and g_-, i.e.,

$$g=g_+\oplus g_-,\ [g_\pm,g_\pm]\subset g_\pm. \tag{42}$$

Denoting the projections onto these subalgebras by $P_\pm$: $P_\pm g:=g_\pm$, it is easy to verify that

$$\mathcal{R}=\tfrac{1}{2}(P_+-P_-) \tag{43}$$

solves the mYB($\frac{1}{4}$) and hence defines an $\mathcal{R}$-structure on g. For both Lie algebras considered:

$$\mathcal{R}=\tfrac{1}{2}(P_{\geqslant k}-P_{<k}), \tag{44}$$

where for the Lie algebra of shift operators

$$P_{\geqslant k}g := g_{\geqslant k} = \sum_{i\geqslant k} u_i(n)\mathcal{E}^i, \quad P_{<k}g := g_{<k} = \sum_{i<k} u_i(n)\mathcal{E}^i,$$
$$P^*_{\geqslant k} = P_{\leqslant -k}, \quad P^*_{<k} = P_{>-k}, \quad k = 0,1. \tag{45}$$

and for the PDO Lie algebra

$$P_{\geqslant k}g = g_{\geqslant k} = \left\{\sum_{i\geqslant k}(u_i)\partial_x^i\right\}, \quad P_{<k}g = g_{<k} = \left\{\sum_{i<k}(u_i)\partial_x^i\right\},$$
$$P^*_{\geqslant k} = P_{<-k}, \quad P^*_{<k} = P_{\geqslant -k}, \quad k = 0,1,2. \tag{46}$$

Notice that from (28) and the fact that $P_{\geqslant k} + P_{<k} = 1$ we have

$$[\mathcal{R}(L^{s-1}\cdot\nabla C_i), L] = [P_{\geqslant k}(L^{s-1}\cdot\nabla C_i), L], \quad s = 1,2. \tag{47}$$

Thus, the introduction of an $\mathcal{R}$-matrix on g turns the algebra into a Hamiltonian phase space. With the results of this section we have demonstrated that the $\mathcal{R}$-matrix approach is a powerful tool for constructing multi-Hamiltonian formulation (41) of dynamical systems in $(1+1)$ dimensions. The details of multi-Hamiltonian dynamics in the case $k=0$ for the Lie algebra of shift operators (17) and in the case $k=0,1$ for the PDO Lie algebra (21) the reader can find in literature (see, e.g., Refs. 7, 24, 31, 34–36). Here we will use this formalism in further considerations, i.e., for the construction of $(2+1)$ dimensional dynamics.

III. CENTRAL EXTENSION APPROACH

Assume now that the Lie algebra g (PDO or shift operators) depends effectively on an independent parameter $y \in S^1$, which naturally generates the corresponding current operator Lie algebra $C(g) = C^\infty(S^1; g)$ with the following modified Tr-operation:

$$\mathrm{Tr}\, a := \int_{S^1} \mathrm{tr}(a)\, dy, \tag{48}$$

where tr operation is defined by (19) for the Lie algebra of shift operators and by (23) for the PDO Lie algebra. The scalar product reads

$$(a,b)_{C(g)} := \mathrm{Tr}(a\cdot b) \tag{49}$$

for a and $b \in C(g)$. The current Lie algebra $C(g)$ can be naturally extended via the central extension procedure: $C(g) \to \overline{C}(g) = C(g) \oplus \mathbf{C}$ with the following Lie product:

$$[(a,\alpha),(b,\beta)] := ([a,b], \omega_2(a,b)), \tag{50}$$

where $\alpha,\beta \in \mathbf{C}$ and $\omega_2 : C(g)\times C(g) \to \mathbf{C}$ is the standard Maurer-Cartan two-cocycle on $C(g)$:

$$\omega_2(a,b) := \int_{S^1} dy\,(a, D_y b)_g = \mathrm{Tr}\left(a\cdot\frac{db}{dy}\right), \quad a,b \in C(g). \tag{51}$$

The appropriate momentum map:

$$\overline{L} : M \to \overline{C}(g^*) \tag{52}$$

is associated with the corresponding current Lie algebra action of $\overline{C}(g)$ on M.

Let us repeat the $\mathcal{R}$-matrix approach for the current Lie algebra $\overline{C}(g)$.

Casimir functionals $C \in \mathcal{D}(\overline{C}(g))$ satisfy now the so-called Novikov–Lax equation

$$[\nabla C,L]+D_y\nabla C=0, \tag{53}$$

for all $\overline{L}:=(L,1)\in\overline{C}(g^*)\cong\overline{C}(g)$. The $\mathcal{R}$-structure $\overline{\mathcal{R}}\in\mathrm{Hom}(\overline{C}(g))$ is defined as follows:

$$[(a,\alpha),(b,\beta)]_{\overline{\mathcal{R}}}:=([a,b]_{\mathcal{R}},\omega_2^{\mathcal{R}}(a,b)), \tag{54}$$

where $\omega_2^{\mathcal{R}}(a,b):=\omega_2(\mathcal{R}\,a,b)+\omega_2(a,\mathcal{R}b)$.

Theorem 2 (Ref. 17): *Given a set of Casimir functionals $C_i\in\mathcal{D}(\overline{C}(g))$ solving Eq. (53), all the reduced on M functionals $C_i:=c_i(u)$, $u\in\overline{M}$, are in involution with respect to the Poisson bracket*

$$\begin{aligned}\{c_i,c_j\}(u)&\equiv\{C_i,C_j\}_{\overline{\mathcal{R}}}(L)\\&=(L,[\nabla C_j,\nabla C_i]_{\mathcal{R}})_{C(g)}+\omega_2^{\mathcal{R}}(\nabla C_i,\nabla C_j) \qquad (55)\\&=(\nabla C_j,\Theta_1(L)\circ\nabla C_i)_{C(g)}+\omega_2^{\mathcal{R}}(\nabla C_i,\nabla C_j)=0 \qquad (56)\end{aligned}$$

reduced from $\overline{C}(g)$ on M with respect to the diagram (26). Moreover, the momentum map $\overline{L}:M\to\overline{C}(g)$ and Casimir functionals C_i, satisfy the following hierarchy of evolution equations:

$$\begin{aligned}L_{t_i}&=[\mathcal{R}\nabla C_i,L]+D_y(\mathcal{R}\nabla C_i)\\&=(\Theta_1(L)+D_y\mathcal{R})\circ\nabla C_i\\&=[\mathcal{R}\nabla C_i,L-\partial_y]:=\Theta_1(L,\partial_y)\circ\nabla C_i,\quad i\in\mathbb{Z}.\end{aligned} \tag{57}$$

The quadratic structure $\Theta_2(L,\partial_y)=\Theta_2(L)+D_y\mathcal{R}$ does not survive the central extension as it fails the property of Jacobi identity. Thus, the second Poisson structure should be essentially modified. We use in the last part of this article the so-called operand approach to derive the second Poisson structures of $(2+1)$-dimensional systems in a generalized sense. In the following section we illustrate the cental extension approach for Lie algebra of shift operators and for the PDO Lie algebra.

A. Extended Lie algebra of shift operators

Here we will consider the central extension for the Lie algebra of shift operators.[23] The restricted finite field Lax operator reads

$$k=0:L=\mathcal{E}^{n+\alpha}+u_{n+\alpha-1}\mathcal{E}^{n+\alpha-1}+\cdots+u_\alpha\mathcal{E}^\alpha,\quad -n<\alpha\leqslant 0, \tag{58}$$

and the case $\alpha=0$ is also included. Lax dynamics for $\alpha=0$ are purely $(2+1)$-dimensional effect and they cannot be reduced onto $(1+1)$-dimensional space.

The Poisson structure (57) linear with respect to the restricted Lax operator (58), related to $\mathcal{R}=\frac{1}{2}(P_{\geqslant 0}-P_{<0})$ and the relations (45), follows from the centrally extended $(L\to L-\partial_y)$ linear Poisson structure $\Theta_1(L)$ (35) for $(1+1)$-lattice systems:[23]

$$\begin{aligned}L_t&=\Theta_1(L,\partial_y)\circ\nabla H\\&=[\mathcal{R}\nabla H,L-\partial_y]+\mathcal{R}^*[\nabla H,L-\partial_y]\\&=-\mathrm{ad}_L(\nabla H)_{\geqslant 0}+(\mathrm{ad}_L\nabla H)_{>0}-(D_y\nabla H)_{>0}+D_y(\nabla H)_{\geqslant 0},\end{aligned} \tag{59}$$

when substitute $H\equiv C$ with the condition $[\nabla C,L-\partial_y]=0$ (53). On the other hand, from the relation $P_{\geqslant 0}+P_{<0}=1$ the hierarchy (57) takes the form

$$L_{t_i}=[P_{\geqslant 0}\nabla C_i,L-\partial_y]. \tag{60}$$

Equation (53) for Casimir functionals can be solved putting

$$\nabla C_i(L) := \sum_{j \leqslant i} a_j \mathcal{E}^j, \quad i = 1,2,\ldots, \tag{61}$$

where the function parameters a_j are obtained from (53) succesively via the recurrent procedure. Notice that although the solutions (61) are in the form of infinite series, in fact we need only their finite parts $P_{\geqslant 0}\nabla C_i$. In the following we present $(2+1)$-dimensional generalizations of some known lattice systems as well as some new examples of lattice-field systems.

Examples. We illustrate in detail the presented formalism on the first example.

(1) The lattice-field Benjamin–Ono equation: $n=1, \alpha = 0$.

This case does not exist in the one-dimensional lattice case. The Lax operator has the form[14,37]

$$L = \mathcal{E} + u. \tag{62}$$

Using (20) for the above Lax operator we get

$$\nabla H = \frac{\delta H}{\delta u} \tag{63}$$

and substituting it in (59) we get the Poisson tensor for this system in the form

$$\theta_1 = D_y. \tag{64}$$

To construct a hierarchy of vector fields we use (61) for $i = 1,2,3,\ldots$ and find

$$\begin{aligned} P_{\geqslant 0}\nabla C_1 &= \mathcal{E} + u, \\ P_{\geqslant 0}\nabla C_2 &= \mathcal{E}^2 + [u(n+1) + u(n)]\mathcal{E} + u^2(n) + \mathcal{H}u(n)_y, \\ P_{\geqslant 0}\nabla C_3 &= \mathcal{E}^3 + [u(n+2) + u(n+1) + u(n)]\mathcal{E}^2 \\ &\quad \times [u^2(n+1) + u(n+1)u(n) + u^2(n) + \tfrac{1}{4}(E-1)(u(n)_y + 3\mathcal{H}^2 u(n)_y)]\mathcal{E} \\ &\quad + \tfrac{1}{4}u(n)_{yy} + u(n)^3 + \tfrac{2}{4}\mathcal{H}u(n)u(n)_y + \tfrac{2}{3}u(n)\mathcal{H}u(n)_y + \tfrac{3}{4}\mathcal{H}^2 u(n)_{yy}, \ldots. \end{aligned} \tag{65}$$

Then, substituting the results to Eq. (60), we get the first equations of the hierarchy

$$\begin{aligned} u(n)_{t_1} &= u_y, \\ u(n)_{t_2} &= 2uu_y + \mathcal{H}u_{yy}, \\ u(n)_{t_3} &= \tfrac{1}{4}u_{yyy} + 3u^2 u_y + \tfrac{3}{2}\mathcal{H}(uu_y)_y + \tfrac{3}{2}(u\mathcal{H}u_y)_y + \tfrac{3}{4}\mathcal{H}^2 u_{yyy}, \\ &\vdots, \end{aligned} \tag{66}$$

where $\mathcal{H} = (E+1)/(E-1)$.

(2) The lattice-field Toda equation: $n=2, \alpha = 1$.

The Lax operator takes the form[23]

$$L = \mathcal{E} + p + v\mathcal{E}^{-1}. \tag{67}$$

Poisson tensor for the lattice-field Toda equation is given by

$$\theta_1=\begin{pmatrix} 0 & v(1-E^{-1}) \\ (E-1)v & D_y \end{pmatrix} \tag{68}$$

and the first equations from the hierarchy read:

$$\begin{pmatrix} v(n) \\ p(n) \end{pmatrix}_{t_1}=\begin{pmatrix} v(n)[p(n)-p(n-1)] \\ v(n+1)-v(n)+p(n)_y \end{pmatrix},$$

$$\begin{aligned} v(n)_{t_2}&=v(n)[p^2(n)-p^2(n-1)+v(n+1)-v(n-1)+p(n)_y+p(n-1)_y], \\ p(n)_{t_2}&=v(n+1)[p(n+1)+p(n)]-v(n)[p(n-1)+p(n)]+v(n)_y \\ &\quad +v(n+1)_y+\mathcal{H}p(n)_{yy}+2p(n)p(n)_y, \\ &\vdots . \end{aligned} \tag{69}$$

The first equation from this hierarchy was derived for the first time in a different representation by Mikhailov[38,39] and in the Lagrange form was given in Ref. 40. Here we present a Hamiltonian representation of the $(2+1)$-dimensional Toda equation and its hierarchy.

(3) The case: $n=2,\alpha=0$.

This case does not exist in the one-dimensional lattice. The Lax operator takes the form

$$L=\mathcal{E}^2+u\mathcal{E}+w. \tag{70}$$

The Poisson tensor for this case is given by

$$\theta_1=\begin{pmatrix} D_y & 0 \\ 0 & E-E^{-1} \end{pmatrix} \tag{71}$$

and the first equation from the hierarchy is

$$\begin{pmatrix} u(n) \\ w(n) \end{pmatrix}_{t_1}=\begin{pmatrix} u(n)\mathcal{H}^{-1}u(n)-w(n+1)+w(n) \\ -(E+1)^{-1}u(n)_y \end{pmatrix},\ldots . \tag{72}$$

Notice that eliminating the w variables we get

$$u(n)_{tt}=\mathcal{H}^{-1}u_y+(u\mathcal{H}^{-1}u)_t \tag{73}$$

and then interchanging the variables $y\leftrightarrow t$ and putting $\mathcal{H}^{-1}u:=v$,

$$v(n)_t=\mathcal{H}v_{yy}-(v\mathcal{H}v)_y. \tag{74}$$

This is the lattice-field equation unknown so far (at least to the knowledge of the authors).

(4) The case: $n=3,\alpha=-1$.

The Lax operator takes the form

$$L=\mathcal{E}^2+p\mathcal{E}+v+u\mathcal{E}^{-1}. \tag{75}$$

The Poisson tensor for this case is given by

$$\theta_1=\begin{pmatrix} 0 & u(1-E^{-1}) & 0 \\ (E-1)u & D_y & 0 \\ 0 & 0 & E-E^{-1} \end{pmatrix} \tag{76}$$

and the first equations from the hierarchy read

$$\begin{pmatrix} u(n) \\ v(n) \\ p(n) \end{pmatrix}_{t_1} = \begin{pmatrix} u(n)\mathcal{H}^{-1}p(n-1) \\ u(n+1)-u(n)+(E+1)^{-1}p(n)_y \\ v(n+1)-v(n)-p(n)\mathcal{H}^{-1}p(n) \end{pmatrix},$$

$$\begin{pmatrix} u(n) \\ v(n) \\ p(n) \end{pmatrix}_{t_2} = \begin{pmatrix} u(n)[v(n)-v(n-1)] \\ p(n)u(n+1)-p(n-1)u(n)+v(n)_y \\ u(n+2)-u(n)+p(n)_y \end{pmatrix}, \tag{77}$$

$$\vdots .$$

This is the lattice-field hierarchy unknown so far.

B. Extended PDO Lie algebra

The Poisson bracket on the extended current PDO Lie algebra admits only a linear Poisson structure related to

$$\mathcal{R}=\tfrac{1}{2}(P_{\geqslant k}-P_{<k}), \quad k=0,1. \tag{78}$$

The new Poisson structure coming from (46) and (35) is

$$\begin{aligned} L_t &= \Theta_1(L,\partial_y)\circ\nabla H \\ &= [\mathcal{R}\nabla H, L-\partial_y]+\mathcal{R}^*[\nabla H, L-\partial_y] \\ &= -\mathrm{ad}_L(\nabla H)_{\geqslant k}+(\mathrm{ad}_L\nabla H)_{>-k}-(D_y\nabla H)_{>-k}+D_y(\nabla H)_{\geqslant k}. \end{aligned} \tag{79}$$

The quadratic structure, as was mentioned earlier, does not survive the central extension as it fails the property of the Jacobi identity. Again Eq. (53) for Casimir functionals can be solved putting

$$\nabla C_i(L) := \sum_{j\leqslant i} a_j\partial_x^j, \quad i=1,2,\ldots, \tag{80}$$

where the function parameters a_j are obtained from (53) successively via the recurrent procedure. Here we will use restricted Lax operators,

$$k=0: L=\partial_x^N+u_{N-2}\partial_x^{N-2}+\ldots+u_1\partial_x^1+u_0, \tag{81}$$

$$k=1: L=\partial_x^N+u_{N-1}\partial_x^{N-1}+\cdots+u_0+\partial_x^{-1}u_{-1}. \tag{82}$$

Here again the choice $H\equiv C$ leads from Eq. (79) to Eq. (57) and finally to the form

$$L_{t_i}=[P_{\geqslant k}\nabla C_i, L-\partial_y] \tag{83}$$

as $P_{\geqslant k}+P_{<k}=1$ and hence $\mathcal{R}=P_{\geqslant k}-\frac{1}{2}$. We will ilustrate this formalism in a few examples.

Examples. We illustrate the above formalism for the PDO Lie algebra on the first example.

(1) The KP equation: $k=0, N=2$.

The KP equation is a $(2+1)$-dimensional extension of the KdV equation. The Lax operator for the KP equation has the form[17,37]

$$L=\partial_x^2+u. \tag{84}$$

Using (24) for this Lax operator we get

$$\nabla H=\partial_x^{-1}\frac{\delta H}{\delta u} \tag{85}$$

and subsituting this gradient and the Lax operator in (79) we derive the Poisson tensor for the KP equation

$$\theta_1=2D_x. \tag{86}$$

Applying formula (80) for $i=1,2,3,\ldots$, etc., and subsituting the respective projections of gradients $P_{\geqslant 0}\nabla C_i$ into (83), we derive the KP hierarchy

$$\begin{aligned}
u_{t_1}&=u_x,\\
u_{t_2}&=u_y,\\
u_{t_3}&=u_{xxx}+6uu_x+3D_x^{-1}u_{yy},\\
u_{t_4}&=u_{xxy}+4uu_y+2u_xD_x^{-1}u_y+D_x^{-2}u_{yyy},\\
u_{t_5}&=u_{5x}+10uu_{xxx}+20u_xu_{xx}+30u^2u_x+10u_{xyy}+10u_xD_x^{-2}u_{yy}\\
&\quad+D_x^{-1}(5D_x^{-2}u_{4y}+30u_y^2+30uu_{yy}+20u_{xy}D_x^{-1}u_y+20u_xD_x^{-1}u_{yy}),\\
&\vdots.
\end{aligned} \tag{87}$$

(2) The $(2+1)$*-Boussinesq equation:* $k=0, N=3$.
The Lax operator is given by[23]

$$L=\partial_x^3+u\partial_x+v. \tag{88}$$

Poisson tensor for the Boussinesq equation takes the form

$$\theta_1=\begin{pmatrix}0 & 3D_x\\ 3D_x & 0\end{pmatrix}. \tag{89}$$

Applying formulas (80) and (83) we get the hierarchy

$$\begin{aligned}
\begin{pmatrix}u\\ v\end{pmatrix}_{t_1}&=\begin{pmatrix}u_x\\ v_x\end{pmatrix},\\
\begin{pmatrix}u\\ v\end{pmatrix}_{t_2}&=\begin{pmatrix}u_{2x}-2v_x\\ \frac{2}{3}(u_{3x}+uu_x-u_y)-v_{xx}\end{pmatrix}.
\end{aligned} \tag{90}$$

Elliminating the field v from this equation we can derive the $(2+1)$-dimensional Boussinesq equation

$$u_{tt}=-\tfrac{1}{3}u_{4x}-\tfrac{2}{3}(u^2)_{xx}-\tfrac{4}{3}u_{xy}. \tag{91}$$

This equation coincides with the KP equation after the replacement $t\leftrightarrow y$,

$$\begin{pmatrix} u \\ v \end{pmatrix}_{t_3} = \begin{pmatrix} u_y \\ v_y \end{pmatrix}, \tag{92}$$

$$u_{t_4} = 2v_{xxx} + 4(uv)_x - u_{4x} - (u^2)_{xx} - 2u_{xy} + 4v_y,$$

$$v_{t_4} = v_{4x} + 2uv_{xx} + 2(v_2)_x - 2v_{xy} + 2u_x v_x - \tfrac{2}{3}(u_{5x} + 3uu_{xxx} + 6u_x u_{xx} + 2u^2 u_x) + \tfrac{4}{3} D_x^{-1} u_{yy} - \tfrac{2}{3} u_{xxy},$$

$$u_{t_5} = u_{5x} + 5(uu_{xx})_x + 5u^2 u_x + 5(u_x v)_x - 10vv_x + 5u_{xxy} + 5uu_y + 5u_x D_x^{-1} u_y - 5D_x^{-1} u_{yy},$$

$$v_{t_5} = v_{5x} + 5(uv)_{xxx} + 5(u_{xx} v)_x + 5(u^2 v)_x - 5(v^2)_{xx} + 5v_{xxy} + 10u_y v + 5uv_y + 5v_x D_x^{-1} u_y - 5D_x^{-1} v_{yy},$$

$$u_{t_6} = 6u_{3xy} + 4v_{xxy} - 6uu_{xy} + 4uv_y + 6u_y v - 5u_{yy} - 2D_x^{-1} v_{yy} - 2u_{xx} D_x^{-1} u_y + 4v_x D_x^{-1} u_y + 2u_x D_x^{-1} v_y,$$

$$v_{t_6} = 8u_{4xy} + 6v_{3xy} + 4uu_{xxy} + 8u_{xyy} - 12(u_x u_y)_x - 4u^2 u_y + 6uv_{xy} + 24u_y v_x + 18vv_y - 3v_{yy} - 4u_{xxx} D_x^{-1} u_y - 4uu_x D_x^{-1} u_y + 6v_{xx} D_x^{-1} u_y + 6v_x D_x^{-1} v_y - 4(uD_x^{-1} u_y)_y,$$

$$\vdots.$$

3 The case: $k=0,\ N=4$.
The Lax operator is

$$L = \partial_x^4 + u\partial_x^2 + v\partial_x + w. \tag{93}$$

The Poisson tensor is given by

$$\theta_1 = \begin{pmatrix} 0 & 0 & 4D_x \\ 0 & 4D_x & 2D_x^2 \\ 4D_x & -2D_x^2 & 2D_x^3 + uD_x + D_x u \end{pmatrix}. \tag{94}$$

Applying formulas (80) and (83) we get the hierarchy of commuting vector fields

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{t_1} = \begin{pmatrix} u_x \\ v_x \\ w_x \end{pmatrix},$$

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{t_2} = \begin{pmatrix} -2u_{xx}+2v_x \\ 2w_x+v_{xx}-2u_{xxx}-uu_x \\ w_{xx}-\frac{1}{2}(u_{4x}+uu_{xx}+vu_x+u_y) \end{pmatrix},$$

$$\begin{aligned} u_{t_3} &= 2u_{5x}-20v_{4x}+40w_{xxx}+40(uw)_x-40u_{xx}v-20uv_{xx} \\ &\quad +20(v_x)^2-45u_xv_x-10uu_{xxx}-15u^2u_x+32u_{xy}-40v_y, \end{aligned}$$

$$\begin{aligned} v_{t_3} &= 10u_{6x}-28v_{5x}+40w_{4x}+40(vw)_x-40uv_{xxx}+40(uw_x)_x \\ &\quad -100u_xv_{xx}-110u_{xx}v_x+5(u^2)_{4x}-15(u^2v)_x-20v_{xy}-40w_y+30u_{xxy}+10uu_y, \\ w_{t_3} &= 5u_{7x}-12v_{6x}+12w_{5x}+20(w_x)^2+20v_xw_x+20vw_{xx} \\ &\quad +20uw_{xxx}+12u_xw_{xx}+5uu_{5x}+5(uu_x)_{4x}-10(uv)_{4x} \\ &\quad +5u^2w_x-10u(uv)_{xx}+5v(uu_x)_x-10v(uv)_x+5u(uu_x)_{xx} \\ &\quad +2u_{xx}w_x-20w_{xy}+15u_{3xy}-10v_{xxy}+10D_x^{-1}u_{yy}+15uu_{xy}+5u_xu_y-10uv_y, \\ &\vdots . \end{aligned} \tag{95}$$

(4). The case: $k=1, N=0$.

This case does not exist in $(1+1)$-dimensions. The Lax operator reads[23]

$$L=u+\partial_x^{-1}w. \tag{96}$$

For this Lax operator we get the Poisson tensor

$$\theta_1=\begin{pmatrix} 0 & -D_y \\ -D_y & 0 \end{pmatrix} \tag{97}$$

and applying formulas (80) and (83) we find the hierarchy

$$\begin{pmatrix} u \\ w \end{pmatrix}_{t_1} = \begin{pmatrix} u_x \\ w_x \end{pmatrix},$$

$$\begin{pmatrix} u \\ w \end{pmatrix}_{t_2} = \begin{pmatrix} u_{xx}+2w_x-2u_xD_y^{-1}u_x \\ -w_{xx}-2(wD_y^{-1}u_x)_x \end{pmatrix},$$

$$\begin{aligned} u_{t_3} &= u_{xxx}-3(u_xD_y^{-1}u_x)_x-3u_xD_y^{-1}w_x-3(wD_y^{-1}u_x)_x-3w_xD_y^{-1}u_x \\ &\quad +6u_xD_y^{-1}u_xD_y^{-1}u_x, \\ w_{t_3} &= w_{xxx}+3(w_xD_y^{-1}u_x)_x-3(wD_y^{-1}w_x)_x+6(wD_y^{-1}u_xD_y^{-1}u_x)_x, \\ &\vdots . \end{aligned} \tag{98}$$

(5). The case: $k=1, N=2$.
The Lax operator has the form

$$L=\partial_x^2+u\partial_x+v+\partial_x^{-1}w. \tag{99}$$

For this Lax operator we get the Poisson tensor

$$\theta_1=\begin{pmatrix} 0 & 0 & 2D_x \\ 0 & 2D_x & D_x^2-D_y+uD_x \\ 2D_x & -D_x^2-D_y+D_xu & 0 \end{pmatrix} \tag{100}$$

and applying formulas (80) and (83) we find the hierarchy

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{t_1}=\begin{pmatrix} u_x \\ v_x \\ w_x \end{pmatrix},$$

$$\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{t_2}=\begin{pmatrix} 2v_x+u_y \\ 2w_x+v_{xx}+uv_x \\ -w_{xx}+(wu)_x \end{pmatrix},$$

$$\begin{aligned} u_{t_3}&=u_{xxx}-\tfrac{3}{2}u^2u_x+6(uv)_x+6v_{xx}+12w_x+6v_y+3D_x^{-1}u_{yy}\\ &\quad+3u_xD_x^{-1}u_y,\\ v_{t_3}&=v_{xxx}+\tfrac{3}{2}(wu)_x+\tfrac{3}{2}uv_{xx}+\tfrac{3}{2}uw_x+\tfrac{3}{4}u_xv_x+\tfrac{3}{2}vv_x+\tfrac{3}{8}u^2v_x\\ &\quad+\tfrac{3}{4}v_xD_x^{-1}u_y,\\ w_{t_3}&=w_{xxx}-\tfrac{3}{2}(wu)_{xx}+\tfrac{3}{4}(wu_x)_x+\tfrac{3}{2}(wv)_x+\tfrac{3}{8}(u^2w)_x+\tfrac{3}{4}wu_y\\ &\quad+\tfrac{3}{4}w_xD_x^{-1}u_y,\\ &\vdots. \end{aligned} \tag{101}$$

The reduction $v=w=0$ gives the mKP equation

$$u_{t_3}=u_{xxx}-\tfrac{3}{2}u^2u_x+3D_x^{-1}u_{yy}+3u_xD_x^{-1}u_y. \tag{102}$$

The Poisson tensor (100) after the Dirac reduction procedure takes the form

$$\theta_1=8(D_x-D_yD_x^{-1}+u)^{-1}D_x(u-D_x-D_x^{-1}D_y)^{-1} \tag{103}$$

and the respective symplectic operator

$$J=\theta_1^{-1}=\tfrac{1}{8}(u-D_x-D_x^{-1}D_y)D_x^{-1}(D_x-D_yD_x^{-1}+u). \tag{104}$$

IV. THE OPERAND APPROACH

In this section we implement the ideas of Magri–Morosi–Tondo[13,14] and Athorne–Dorfman–Fokas[11,15,16] of the so-called *operand approach* in the frames of the $\mathcal{R}$-matrix formalism. This gives us a powerful tool for the construction of multi-Hamiltonian bilocal for-

malism of integrable systems in $(2+1)$-dimensions.

The basic idea of the operand approach is the assumption that the element u satisfies the condition: $u \equiv \hat{u} \in \hat{M} \subset C^{(\infty)}(\mathbb{Z} \times (\mathbb{R}/2\pi\mathbb{Z}); \mathcal{B})$ with $\mathcal{B}$ being some associative algebra, for instance, the algebra of pseudodifferential operators. Thus, we pass from field variables to operator variables. All considerations for the $(1+1)$-dimensional case can be extended over the operator level with the only modification related to noncommutativity of $\hat{u}$ elements. As $\hat{M}$ is some operator manifold, we produce bi-Hamiltonian operator vector fields with two Poisson operands (operators acting in the space of operators).

To compare the results with the central extension approach let us consider the following case:

$$\hat{L} = \sum_{i \leqslant \infty} \hat{u}_i \mathcal{T}^i, \quad \mathcal{T} = \{\mathcal{E} \text{ or } \partial_x\}, \quad \hat{u}_i = u_i \ \ i \neq 0, \quad \hat{u}_0 = u_0 - \partial_y, \tag{105}$$

where the operator ∂_y is such that $\mathrm{ad}_{\partial_y} = D_y$, so we have $\hat{L} = L - \partial_y$. On the operator-field Lie algebra $\hat{g}$ we define an invariant nondegenerate scalar product

$$(\hat{a}, \hat{b})_{\hat{g}} = (\hat{b}, \hat{a}) = \mathrm{Tr}(\hat{a} \cdot \hat{b}) = \int_{-\infty}^{+\infty} \int_0^{2\pi} \hat{\mathrm{Sp}}(\hat{a} \cdot \hat{b}) dx\, dy, \quad \hat{a}, \hat{b} \in \hat{g}, \tag{106}$$

where $\hat{\mathrm{Sp}}(\hat{a} \cdot \hat{b} \cdot \hat{c}) := \mathrm{tr}(\hat{a} \cdot \hat{b} \cdot \hat{c})$, and $\hat{\mathrm{Sp}}(\hat{a} \cdot \hat{b} \cdot \hat{c}) = \hat{\mathrm{Sp}}(\hat{c} \cdot \hat{a} \cdot \hat{b}) = \hat{\mathrm{Sp}}(\hat{b} \cdot \hat{c} \cdot \hat{a})$ for any $\hat{a}, \hat{b}, \hat{c} \in \hat{g}$. The bi-Hamiltonian formalism on $\hat{M}$ produces, of course, hierarchies of commuting operator vector fields $\hat{K}[\hat{u}]$, i.e., the vector fields which are polynomials in ∂_y operator

$$\hat{K}[\hat{u}] = \sum\nolimits_{i \geqslant 0} K_i[u] \partial_y^i. \tag{107}$$

What we have to do, is to find through appropriate linear combinations, ∂_y-free vector fields, i.e., ''physical'' objects.

Here we show how to calculate gradients of operator Hamiltonians and commutator of two vector operator fields in the PDO case. Let

$$\hat{H}[\hat{u}] = \int_{-\infty}^{+\infty} \hat{h}[\hat{u}] dx = \int_{-\infty}^{+\infty} (\hat{u}^2 - (\hat{u}_x)^2) dx \tag{108}$$

and take a realization of the field $\hat{u}$ in terms of ∂_y in the form

$$\hat{u} = u + \partial_y, \tag{109}$$

where now

$$\begin{aligned}
\hat{H}[u, \partial_y] &= \int_{-\infty}^{+\infty} \int_0^{2\pi} ((u + \partial_y)^2 - (u_x)^2) dx\, dy \\
&= \int_{-\infty}^{+\infty} \int_0^{2\pi} (u^2 + u_y + 2u\partial_y + \partial_y^2 - (u_x)^2) dx\, dy \\
&= \int_{-\infty}^{+\infty} \int_0^{2\pi} (u^2 + u_y - (u_x)^2) dx\, dy + \left\{ \int_{-\infty}^{+\infty} \int_0^{2\pi} 2u\, dx\, dy \right\} \partial_y \\
&\quad + \left\{ \int_{-\infty}^{+\infty} \int_0^{2\pi} 1\, dx\, dy \right\} \partial_y^2.
\end{aligned} \tag{110}$$

The gradient of $\hat{H}[u, \partial_y]$ is given by

$$\delta\hat{H}[u,\partial_y]=\langle\nabla\hat{h}[u,\partial_y],\delta u\rangle, \tag{111}$$

$$\nabla\hat{H}[u,\partial_y]=2u+2u_{xx}+2\partial_y, \tag{112}$$

where $\langle .,. \rangle$ is a dual map on $\hat{M}$.

Let us take two vector operator fields,

$$\hat{K}_1[\hat{u}]=\hat{u}, \quad \hat{K}_2[\hat{u}]=\hat{u}\hat{u}_x \tag{113}$$

which are presented using the realization (109) in the form

$$\hat{K}_1[\hat{u}]=u+\partial_y, \quad \hat{K}_2[\hat{u}]=(u+\partial_y)u_x=uu_x+u_{xy}+u_x\partial_y$$

and their commutator

$$[\hat{K}_1[\hat{u}],\hat{K}_2[\hat{u}]]=\hat{K}_1'[\hat{u}][\hat{K}_2[\hat{u}]]-\hat{K}_2'[\hat{u}][\hat{K}_1[\hat{u}]], \tag{114}$$

where ''prim'' means a Frechet derivative which is calculated in the following way:

$$\hat{K}'[\hat{u}][\hat{V}]=\left(\sum\nolimits_{i\geqslant 0} K_i'[u]\partial_y^i\right)[\hat{V}]=\sum\nolimits_{i\geqslant 0} K_i'[u][\hat{V}]\partial_y^i=\sum\nolimits_{i\geqslant 0}\lim_{\varepsilon\to 0}\frac{dK_i[u+\epsilon\hat{V}]}{d\epsilon}\partial_y^i.$$

Calculating the commutator (114) we get

$$\begin{aligned}[\hat{K}_1[\hat{u}],\hat{K}_2[\hat{u}]]&=1\cdot[uu_x+u_{xy}+u_x\partial_y]\\&\quad-(u_x+uD_x+D_xD_y)[u+\partial_y]+D_x[u+\partial_y]\partial_y\\&=-uu_x-u_{xy}-u_x\partial_y.\end{aligned} \tag{115}$$

In a similar way one can perform these calculations for the shift operator algebra just changing the integral over x by the infinite summation over n.

Theorem 3 (Ref. 41): *Let $\hat{\theta}_1$ and $\hat{\theta}_2$ be two compatible Poisson operands such that $\hat{\theta}_1$ is f-type (i.e., ∂_y free) and $\hat{\theta}_2=\overline{\theta}-\epsilon R_{\partial_y}\hat{\theta}_1=\widetilde{\theta}-\epsilon\hat{\theta}_1 R_{\partial_y}$, where R_{∂_y} stands for the right multiplication by ∂_y, $\overline{\theta}$, $\widetilde{\theta}$ are f-type operators and $\epsilon=$ const. Let $\nabla h_0=\text{const}\in\ker\hat{\theta}_1$, then*

$$K_n:=\hat{\theta}_1\circ\sum_{k=0}^{n}\epsilon^k\binom{n}{k}\hat{\Psi}^{n-k}R_{\partial_y}^k\nabla h_0:=\hat{\theta}_1\circ\hat{Q}_n\nabla h_0, \tag{116}$$

where $\hat{\Psi}=\hat{\theta}_1^{-1}\hat{\theta}_2=\widetilde{\Psi}-\epsilon R_{\partial_y}$ is a recursion operand for covector fields on $\hat{M}$, are f-type vector fields.

Proof: From the property of binomial coefficients

$$\binom{n+1}{k}=\binom{n}{k}+\binom{n}{k-1} \tag{117}$$

it is easy to verify that

$$\begin{aligned}K_{n+1}&=\hat{\theta}_1\circ\sum_{k=0}^{n}\epsilon^k\binom{n}{k}\hat{\Psi}^{n-k+1}R_{\partial_y}^k\nabla h_0\\&\quad+\hat{\theta}_1\circ\sum_{k=0}^{n}\epsilon^{k+1}\binom{n}{k}\hat{\Psi}^{n-k}R_{\partial_y}^{k+1}\nabla h_0\end{aligned}$$

$$= \hat{\theta}_1 \circ (\hat{\Psi} \hat{Q}_n + \epsilon \hat{Q}_n R_{\partial_y}) \nabla h_0 = \hat{\theta}_1 \circ (\tilde{\Psi} \hat{Q}_n \nabla h_0 + \epsilon [\hat{Q}_n, R_{\partial_y}] \nabla h_0). \tag{118}$$

If $\tilde{\Psi}$ and $\hat{Q}_n \nabla h_0$ are f-type, then $[\hat{Q}_n, R_{\partial_y}] \nabla h_0$ and K_{n+1} are f-type too, and hence $K_n(\nabla h_0)$ are f-type vector fields.

Lemma 1: If basic operator vector fields $\hat{\theta}_2 \circ \nabla h_0 \partial_y^k$ commute

$$[\hat{\theta}_2 \circ \nabla h_0 \partial_y^k, \hat{\theta}_2 \circ \nabla h_0 \partial_y^l] = 0 \tag{119}$$

and leave the recursion operand invariant with respect to a Lie derivative $\mathcal{L}$:

$$\mathcal{L}_{\hat{\theta}_2 \circ \nabla h_0 \partial_x^k} \hat{\Phi} = 0, \tag{120}$$

where $\hat{\Phi} = \hat{\theta}_2 \hat{\theta}_1^{-1} = \overline{\Phi} - \epsilon R_{\partial_y}$, then K_n constitute a commuting hierarchy of Hamiltonian vector fields.

There are two special cases of the general formula (116):

Lemma 2: Take the assumptions from Theorem 3.

(i) *If $\nabla h_0 \partial_x^k \in \ker\ \hat{\theta}_1$, $k = 0,1,2,\ldots$, then*[16]

$$K_n := \sum_{k=0}^{n} \epsilon^k \binom{n}{k} \hat{\Phi}^{n-k} \circ \hat{\theta}_2 \nabla h_0 \partial_y^k. \tag{121}$$

(ii) *If $\nabla h_0 \in \ker\ \hat{\theta}_1, \hat{\theta}_2$ then $\hat{\theta}_2 \circ \nabla h_0 \partial_y^k \equiv \hat{\Phi} \hat{\theta}_1 \circ \nabla h_0 \partial_y^k$ and*[13,14]

$$K_n := \sum_{k=1}^{n} \epsilon^k \binom{n}{k} \hat{\Phi}^{n-k} \circ \hat{\theta}_1 \nabla h_0 \partial_y^k. \tag{122}$$

The formula (121) was derived by Athorne and Dorfman.[16] In their article they applied the operand formalism for the construction of the KP hierarchy.

Lemma 3: If $\hat{L} = L - \partial_y$ then

(i) *$\hat{\theta}_1$ is of f type,*

(ii) *and $\hat{\theta}_2 = \overline{\theta} - R_{\partial_y} \hat{\theta}_1$,* where *$\overline{\theta}$ is of f-type.*

Proof of this lemma follows immediately from the fact that $\mathrm{ad}_{\hat{L}} \Leftrightarrow f$-type operator and $\mathrm{ad}_{\hat{L}}^{+} \Leftrightarrow f$-type $-2R_{\partial_y}$. Notice that $\hat{\theta}_1$ operand when applied to the f-type covectors (i.e., when reduce to $M \subset \hat{M}$), is equal to θ_1 constructed via the central extension.

Let us consider the operand formalism for the Lie algebra of shift operators and for the PDO Lie algebra.

A. Lie algebra of shift operators with operator-valued fields

The Lax operator for operator valued variables have the following form:

$$k = 0: \hat{L} = \mathcal{E}^{n+\alpha} + \hat{u}_{n+\alpha-1} \mathcal{E}^{n+\alpha-1} + \cdots + \hat{u}_\alpha \mathcal{E}^\alpha, \quad -n < \alpha \leqslant 0, \quad \alpha \in \mathbb{Z}. \tag{123}$$

As a consequence, from (106) and (19), vector fields L_t and gradients ∇H are conveniently parametrized by

$$\hat{L}_t = \sum_i (\hat{u}_i)_t \mathcal{E}^i, \quad \widehat{\nabla H} = \sum_i \mathcal{E}^{-i} \frac{\delta \hat{H}}{\delta u_i}, \tag{124}$$

where $\delta\hat{H}/\delta u_i$ is the variational derivative of an operator-valued functional $\hat{H}[u,\partial_y]$. The linear and quadratic Poisson tensors are

$$\hat{L}_t=\hat{\Theta}_1(\hat{L})\circ\nabla\hat{H}=-\mathrm{ad}_{\hat{L}}(\nabla\hat{H})_{\geqslant 0}+(\mathrm{ad}_{\hat{L}}\nabla\hat{H})_{>0}, \tag{125}$$

$$\begin{aligned}\hat{L}_t=\hat{\Theta}_2(\hat{L})\circ\nabla\hat{H}=&-\tfrac{1}{2}\mathrm{ad}_{\hat{L}}(\mathrm{ad}^{+}_{\hat{L}}\nabla\hat{H})_{\geqslant 0}+\tfrac{1}{2}\mathrm{ad}^{+}_{\hat{L}}(\mathrm{ad}_{\hat{L}}\nabla\hat{H})_{>0}\\&+\tfrac{1}{2}\mathrm{ad}_{\hat{L}}\Pi_{n+\alpha}(\mathrm{ad}_{\hat{L}}\nabla\hat{H})_0,\end{aligned} \tag{126}$$

where

$$\Pi_{n+\alpha}=(E^{n+\alpha}+1)(E^{n+\alpha}-1)^{-1}. \tag{127}$$

The $\Theta_2(L)$ for commuting fields, derived in Ref. 7, is just the (36) one, where now

$$\begin{aligned}A_1&=P_{\geqslant 1}-P_{<0}-\Pi_{n+\alpha}P_0,\\A_2&=P_{\geqslant 1}-P_{<0}+\Pi_{n+\alpha}P_0,\\S&=P_0+\Pi_{n+\alpha}P_0,\\S^*&=P_0-\Pi_{n+\alpha}P_0.\end{aligned} \tag{128}$$

Examples. Here, with the help of the operand formalism, we reconstruct the results of central extension approach applied to the algebra of shift operators.

(1) The case of $n=1$, $\alpha=0$*:*

The Lax operator reads

$$\hat{L}=\mathcal{E}+u-\partial_y. \tag{129}$$

For this Lax operator, using (124), we get the following gradient:

$$\widehat{\nabla H}=\frac{\delta\hat{H}}{\delta u}. \tag{130}$$

Substituting this Lax operator and gradient into (125), (126), we derive the first Poisson operand

$$\hat{\theta}_1=-\mathrm{ad}_u+D_y, \tag{131}$$

and the second Poisson operand

$$\begin{aligned}\hat{\theta}_2=&-\tfrac{1}{2}\mathrm{ad}^{+}_u\mathrm{ad}_u+\tfrac{1}{2}\mathrm{ad}^{+}_u D_y+\tfrac{1}{2}D_y\mathrm{ad}_u-\tfrac{1}{2}D_y^2+\tfrac{1}{2}\mathrm{ad}_u\mathcal{H}\,\mathrm{ad}_u\\&-\tfrac{1}{2}D_y\mathcal{H}\,\mathrm{ad}_u-\tfrac{1}{2}\mathrm{ad}_u\,\mathcal{H}D_y+\tfrac{1}{2}\mathcal{H}D_x^2+R_{u_y}+(ad_u-D_y)R_{\partial_y}.\end{aligned} \tag{132}$$

The recursion operand is given by

$$\hat{\Phi}=\tfrac{1}{2}\mathrm{ad}^{+}_u-\tfrac{1}{2}D_y-\tfrac{1}{2}\mathrm{ad}_u\,\mathcal{H}+\tfrac{1}{2}\mathcal{H}D_y-R_{\partial_y}, \tag{133}$$

deduced for the first time by Morosi and Tondo[14] via a completely different approach. Taking $\nabla h_0=1\in\ker\,\hat{\theta}_1,\ \hat{\theta}_2$ and applying the reduced formula (122) we get the hierarchy

$$u(n)_{t_1}=u_y,$$

$$u(n)_{t_2}=2uu_y+\mathcal{H}u_{yy},$$
$$u(n)_{t_3}=\tfrac{1}{4}u_{yyy}+3u^2u_y+\tfrac{3}{2}\mathcal{H}(uu_y)_y+\tfrac{3}{2}(u\mathcal{H}u_y)_y+\tfrac{3}{4}\mathcal{H}^2u_{yyy}, \tag{134}$$
$$\vdots,$$

where $\mathcal{H}=(E+1)/(E-1)$.

(2) The lattice-field Toda (Ref. 41): $n=2$, $\alpha=-1$.

The Lax operator has the form

$$\hat{L}=\mathcal{E}+p-\partial_y+v\mathcal{E}^{-1}. \tag{135}$$

For this Lax operator, using (124), we get the following gradient

$$\widehat{\nabla H}=\frac{\delta\hat{H}}{\delta p}+\mathcal{E}\frac{\delta\hat{H}}{\delta v}. \tag{136}$$

Substituting this Lax operator and gradient into (125), (126), we derive the first Poisson operand

$$\hat{\theta}_1=\begin{pmatrix}0 & R_v-vE^{-1}\\ ER_v-v & -(\mathrm{ad}_p-D_y)\end{pmatrix} \tag{137}$$

and the second Poisson operand

$$\hat{\theta}_2=\overline{\theta}-R_{\partial_y}\hat{\theta}_1, \tag{138}$$

where

$$\overline{\theta}_{11}=(R_vE-vE^{-1})(E-1)^{-1}(ER_v-v),$$
$$\overline{\theta}_{12}=(R_v-vE^{-1})(E-1)^{-1}(ER_p-p+D_y)+R_{v_y},$$
$$\overline{\theta}_{21}=(R_pE-p+D_y)(E-1)^{-1}(ER_v-v),$$
$$\overline{\theta}_{22}=ER_v-vE^{-1}-(R_pE-p+D_y)(E-1)^{-1}(\mathrm{ad}_p-D_y).$$

The recursion operand is given by

$$\hat{\Phi}=\hat{\theta}_2\hat{\theta}_1^{-1}=\overline{\Phi}-R_{\partial_y}I, \tag{139}$$

where

$$\begin{aligned}\overline{\Phi}_{11}=&[R_vE^1-vE^{-1}][E^1-1]^{-1}[\mathrm{ad}_p-D_y][R_v-vE^{-1}]^{-1}\\ &+[vE^{-1}-R_v][E^1-1]^{-1}[E^1R_p-p+D_y][vE^{-1}-R_v]^{-1}\\ &-R_{v_x}[vE^{-1}-R_v]^{-1},\end{aligned}$$
$$\overline{\Phi}_{12}=[R_vE^1-vE^{-1}][E^1-1]^{-1},$$
$$\overline{\Phi}_{21}=[vE^{-1}-E^1R_v][vE^{-1}-R_v]^{-1},$$

$$\overline{\Phi}_{22}=[R_pE^1-p+D_y][E^1-1]^{-1}$$

and I is a unit matrix. Taking

$$\nabla h_0=\begin{pmatrix}0\\1\end{pmatrix}\in\ker\hat{\theta}_1,$$

the general formula (116) gives the hierarchy

$$\begin{pmatrix}v(n)\\p(n)\end{pmatrix}_{t_1}=\begin{pmatrix}v(n)[p(n)-p(n-1)]\\v(n+1)-v(n)+p(n)_y\end{pmatrix},$$

$$v(n)_{t_2}=v(n)[p^2(n)-p^2(n-1)+v(n+1)-v(n-1)+p(n)_y+p(n-1)_y]$$

$$\begin{aligned}p(n)_{t_2}=&v(n+1)[p(n+1)+p(n)]-v(n)[p(n-1)+p(n)]+v(n)_y\\&+v(n+1)_y+\mathcal{H}p(n)_{yy}+2p(n)p(n)_y,\end{aligned}\tag{140}$$

$$\vdots.$$

(3) The case of $n=2$, $\alpha=0$*:*
The Lax operator has the form

$$\hat{L}=\mathcal{E}^2+u\mathcal{E}+w-\partial_y.\tag{141}$$

For this Lax operator, using (124), we get the following gradient:

$$\widehat{\nabla H}=\mathcal{E}^{-1}\frac{\delta\hat{H}}{\delta u}+\mathcal{E}\frac{\delta\hat{H}}{\delta w}.\tag{142}$$

Substituting this Lax operator and gradient into (125), (126), we derive the first Poisson operand

$$\hat{\theta}_1=\begin{pmatrix}-(\mathrm{ad}_w-D_y) & 0\\0 & E-E^{-1}\end{pmatrix},\tag{143}$$

and the second Poissson operand

$$\hat{\theta}_2=\frac{1}{2}\overline{\theta}-R_{\partial_y}\hat{\theta}_1,\tag{144}$$

where

$$\overline{\theta}_{11}=(\mathrm{ad}_w-D_y)\Pi(\mathrm{ad}_w-D_y)-\mathrm{ad}_{(w^2-w_y)}-D_y^2+2wD_y,$$

$$\overline{\theta}_{12}=(\mathrm{ad}_w-D_y)((\Pi-1)u-(\Pi+1)E^{-1}R_u),$$

$$\overline{\theta}_{21}=(uE(\Pi-1)-R_u(\Pi+1))(\mathrm{ad}_w-D_y),$$

$$\overline{\theta}_{22}=2(ER_w-wE^{-1})+2D_yE^{-1}+uE(\Pi-1)u+R_u(\Pi+1)E^{-1}R_u$$
$$-u\Pi R_u-R_u\Pi u.$$

The recursion operand is given by

$$\hat{\Phi}=\begin{pmatrix}\overline{\Phi}_{11} & \overline{\Phi}_{12}\\ \overline{\Phi}_{21} & \overline{\Phi}_{22}\end{pmatrix}-R_{\partial_y}I, \tag{145}$$

where

$$\Phi_{11}=\mathrm{ad}_w^+-D_y-(\mathrm{ad}_w-D_x)\Pi,$$

$$\Phi_{12}=(\mathrm{ad}_w-D_y)((\Pi-1)u-(\Pi+1)E^{-1}R_u)(E-E^{-1})^{-1},$$

$$\Phi_{21}=R_u(\Pi+1)-uE(\Pi-1),$$

$$\Phi_{22}=\{2(ER_w-wE^{-1})+2D_yE^{-1}+uE(\Pi-1)u$$
$$+R_u(\Pi+1)E^{-1}R_u-u\Pi R_u-R_u\Pi u\}\times(E-E^{-1})^{-1}$$

and $\Pi\equiv\Pi_2=(E^2+1)/(E^2-1)$. Taking $\nabla h_0=\binom{0}{1}\in\ker\hat{\theta}_1$, the general formula (116) gives the hierarchy

$$\begin{pmatrix}u(n)\\ w(n)\end{pmatrix}_{t_1}=\begin{pmatrix}u(n)\mathcal{H}^{-1}u(n)-w(n+1)+w(n)\\ -(E+1)^{-1}u(n)_y\end{pmatrix},$$
$$\vdots. \tag{146}$$

(4) The case of $n=3,\alpha=-1$*:*
The Lax operator is of the form

$$\hat{L}=\mathcal{E}^2+p\mathcal{E}+v-\partial_y+u\mathcal{E}^{-1}. \tag{147}$$

For this Lax operator, using (124), we get the following gradient:

$$\widehat{\nabla H}=\mathcal{E}^{-1}\frac{\delta\hat{H}}{\delta p}+\frac{\delta\hat{H}}{\delta v}+\mathcal{E}\frac{\delta\hat{H}}{\delta u}. \tag{148}$$

Substituting this Lax operator and gradient into (125), (126), we derive the first Poisson operand

$$\hat{\theta}_1=\begin{pmatrix}0 & R_u-uE^{-1} & 0\\ ER_u-u & -\mathrm{ad}_v+D_y & 0\\ 0 & 0 & E-E^{-1}\end{pmatrix} \tag{149}$$

and the second Poisson operand is given by

$$\hat{\theta}_2=\begin{pmatrix} \overline{\theta}_{11} & \overline{\theta}_{12} & \overline{\theta}_{13} \\ \overline{\theta}_{21} & \overline{\theta}_{22} & \overline{\theta}_{23} \\ \overline{\theta}_{31} & \overline{\theta}_{32} & \overline{\theta}_{33} \end{pmatrix} - R_{\partial_y}\hat{\theta}_1, \tag{150}$$

where

$$\overline{\theta}_{11}=R_uER_u-uE^{-1}u+R_u\Pi_2[ER_u-u]+u\Pi_2[E^{-1}u-R_u],$$

$$\overline{\theta}_{12}=(v-D_y)R_u+R_uR_v-uE^{-1}(\mathrm{ad}_v^+-D_y)+(uE^{-1}-R_u)\Pi_2(\mathrm{ad}_v-D_y)+R_{u_y},$$

$$\overline{\theta}_{13}=pR_u-uE^{-2}(\Pi_2+1)R_p+uE^{-1}(\Pi_2-1)p+R_uE^{-1}(\Pi_2+1)R_p-R_u\Pi_2p,$$

$$\overline{\theta}_{21}=-uR_v-(v-D_y)u+(\mathrm{ad}_v^+-D_y)ER_u+(\mathrm{ad}_v-D_y)\Pi_2(u-ER_u)+ER_{u_y},$$

$$\overline{\theta}_{22}=2pER_u-2uE^{-1}R_p+(\mathrm{ad}_v-D_y)\Pi_2(\mathrm{ad}_v-D_y)-\mathrm{ad}_{v^2}+\mathrm{ad}_{v_y}+2vD_y-D_y^2+2R_{v_y},$$

$$\overline{\theta}_{23}=2ER_u+pR_v-(v-D_y)p-2uE^{-2}-(\mathrm{ad}_v-D_y)E^{-1}R_p+(\mathrm{ad}_v-D_y)\Pi_2(p-E^{-1}R_p),$$

$$\overline{\theta}_{31}=-uR_p+pE(ER_u-u)+R_pER_u+R_p\Pi_2(ER_u-u)+p\Pi_2E(u-ER_u),$$

$$\overline{\theta}_{32}=2E^2R_u-2uE^{-1}-pE(\mathrm{ad}_v-D_y)-(v-D_y)R_p+R_pR_v+(pE-R_p)\Pi_2(\mathrm{ad}_v-D_y)-R_{p_y},$$

$$\overline{\theta}_{33}=2ER_v-2(v-D_y)E^{-1}-pEp+R_pE^{-1}R_p+p\Pi_2(Ep-R_p)+R_p\Pi_2(E^{-1}R_p-p).$$

Taking

$$\nabla h_0=\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}\in\ker\hat{\theta}_1,$$

and applying the general formula (116) we get the first hierarchy

$$\begin{pmatrix} u(n) \\ v(n) \\ p(n) \end{pmatrix}_{t_2}=\begin{pmatrix} u(n)[v(n)-v(n-1)] \\ p(n)u(n+1)-p(n-1)u(n)+v(n)_y \\ u(n+2)-u(n)+p(n)_y \end{pmatrix}, \tag{151}$$

$$\vdots.$$

Taking

$$\nabla h_0 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \in \ker \hat{\theta}_1,$$

and applying the formula (116) we get the second hierarchy

$$\begin{pmatrix} u(n) \\ v(n) \\ p(n) \end{pmatrix}_{t_1} = \begin{pmatrix} u(n)\mathcal{H}^{-1}p(n-1) \\ u(n+1)-u(n)+(E+1)^{-1}p(n)_y \\ v(n+1)-v(n)-p(n)\mathcal{H}^{-1}p(n) \end{pmatrix}, \tag{152}$$

$$\vdots .$$

B. PDO Lie algebra with operator valued fields

Lax operators for operator valued variables have the following form:

$$k=0: \hat{L} = \partial_x^N + \hat{u}_{N-2}\partial_x^{N-2} + \cdots + \hat{u}_1\partial_x^1 + \hat{u}_0, \tag{153}$$

$$k=1: \hat{L} = \hat{u}_N\partial_x^N + \hat{u}_{N-1}\partial_x^{N-1} + \cdots + \hat{u}_0 + \partial_x^{-1}\hat{u}_{-1}. \tag{154}$$

As a consequence, from (106) and (23), vector fields $\hat{L}_t$ and gradients $\widehat{\nabla H}$ are conveniently parametrized by

$$\hat{L}_t = \sum_i (\hat{u}_i)_t \partial_x^i, \quad \widehat{\nabla H} = \sum_i \partial_x^{-1-i} \frac{\delta \hat{H}}{\delta u_i}, \tag{155}$$

where $\delta\hat{H}/\delta u_i$ is the variational derivative of an operator-valued functional $\hat{H}[u, \partial_y]$. The linear Poisson tensors are

$$\hat{L}_t = \hat{\Theta}_1(\hat{L}) \circ \widehat{\nabla H} = -\operatorname{ad}_{\hat{L}}(\widehat{\nabla H})_{\geqslant k} + (\operatorname{ad}_{\hat{L}}\widehat{\nabla H})_{\geqslant -k}, \quad k=0,1. \tag{156}$$

and quadratic Poisson tensors take the form

$$\begin{aligned} k=0: \hat{L}_t = \hat{\Theta}_2(\hat{L}) \circ \widehat{\nabla H} &= (\hat{L}\widehat{\nabla H})_{\geqslant 0}\hat{L} - \hat{L}(\widehat{\nabla H}\hat{L})_{\geqslant 0} \\ &+ \frac{1}{N}[D_x^{-1}\operatorname{res}([\widehat{\nabla H}, \hat{L}]), \hat{L}], \end{aligned} \tag{157}$$

$$\begin{aligned} k=1: \hat{L}_t = \hat{\Theta}_2(\hat{L}) \circ \widehat{\nabla H} &= (\hat{L}\widehat{\nabla H})_{\geqslant 1}\hat{L} - \hat{L}(\widehat{\nabla H}\hat{L})_{\geqslant 0} + \hat{L}(\hat{L}\widehat{\nabla H})_0 \\ &- \partial_x^{-1}\operatorname{res}([\widehat{\nabla H}, \hat{L}])\hat{L} + [D_x^{-1}\operatorname{res}([\widehat{\nabla H}, \hat{L}]), \hat{L}]. \end{aligned} \tag{158}$$

Both quadratic Poisson tensors for commuting fields were derived in Ref. 36 and are the special cases of (36), where for $k=0$,

$$\begin{aligned} A_1 &= P_{\geqslant 0} - P_{<0} - \frac{1}{N}D_x^{-1}P_{-1}, \\ A_2 &= P_{\geqslant 0} - P_{<0} + \frac{1}{N}D_x^{-1}P_{-1}, \\ S &= \frac{1}{N}D_x^{-1}P_{-1}, \end{aligned} \tag{159}$$

$$S^*=-\frac{1}{N}D_x^{-1}P_{-1},$$

and for $k=1$,

$$\begin{aligned}
A_1&=P_{\geqslant 1}-P_0+\partial_x^{-1}P_{-1}-P_{<-1}-2D_x^{-1}P_{-1},\\
A_2&=P_{\geqslant 0}-P_{<0}+2D_x^{-1}P_{-1},\\
S&=-2\partial_x^{-1}P_{-1}+2D_x^{-1}P_{-1},\\
S^*&=-2P_0-2D_x^{-1}P_{-1}.
\end{aligned}\tag{160}$$

Examples. Here, with the help of the operand formalism, we reconstruct the results of central extension approach applied to the PDO algebra.

(1) The KP equation: $k=0$, $N=2$.

The Lax operator is given by

$$\hat{L}=\partial_x^2+u-\partial_y.\tag{161}$$

For this Lax operator we get the following gradient, using (155),

$$\widehat{\nabla H}=\partial_x^{-1}\frac{\delta\hat{H}}{\delta u}.\tag{162}$$

Substituting this Lax operator and gradient into (156), (157) we get[15] the first

$$\hat{\theta}_1=2D_x,\tag{163}$$

and the second

$$\begin{aligned}
\hat{\theta}_2=\tfrac{1}{2}(&D_x^3+D_x\,\mathrm{ad}_u^+ +\mathrm{ad}_u^+\,D_x-2D_xD_y+\mathrm{ad}_u\,D_x^{-1}\,\mathrm{ad}_u\\
&-D_x^{-1}D_y\,\mathrm{ad}_u-\mathrm{ad}_uD_x^{-1}D_y+D_x^{-1}D_y^2)-R_{\partial_y}\hat{\theta}_1,
\end{aligned}\tag{164}$$

Poisson operands and recursion operand

$$\begin{aligned}
\hat{\Phi}=\hat{\theta}_2\hat{\theta}_1^{-1}=\tfrac{1}{4}(&D_x^2+D_x\,\mathrm{ad}_u^+\,D_x^{-1}+\mathrm{ad}_u^+-2D_y+\mathrm{ad}_u\,D_x^{-1}\,\mathrm{ad}_u\,D_x^{-1}\\
&-D_x^{-1}D_y\,\mathrm{ad}_u\,D_x^{-1}-\mathrm{ad}_u\,D_x^{-2}D_y+D_x^{-2}D_y^2)-R_{\partial_y}.
\end{aligned}\tag{165}$$

Taking $\nabla h_0=1\in\ker\hat{\theta}_1$, and applying formula (121) we get the KP hierarchy

$$\begin{aligned}
u_{t_1}&=u_x,\\
u_{t_3}&=u_{3x}+6uu_x+3D_x^{-1}u_{yy},\\
u_{t_5}&=u_{5x}+10uu_{3x}+20u_xu_{xx}+30u^2u_x+10u_{xyy}+10u_xD_x^{-2}u_{yy}\\
&\quad+D_x^{-1}(5D_x^{-2}u_{4y}++30u_y^2+30uu_{yy}+20u_{xy}D_x^{-1}u_y+20u_xD_x^{-1}u_{yy}),\ldots.
\end{aligned}\tag{166}$$

The central extension approach gives us additional equations for this hierarchy (87), i.e.,

$$u_{t_2}=u_y,\tag{167}$$

$$u_{t_4}=u_{xxy}+4uu_y+2u_xD_x^{-1}u_y+D_x^{-2}u_{3y},\ldots.$$

These equations are purely $(2+1)$-dimensional, because they reduce to zero by the dimension reduction from $(2+1)$ to $(1+1)$.

(2) The $(2+1)$*-Boussinesq equation:* $k=0$, $N=3$.

For the $(2+1)$-Boussinesq equation the Lax operator is

$$\hat{L}=\partial_x^3+u\partial_x+v-\partial_y. \tag{168}$$

From Eq. (155) we get the following gradient

$$\widehat{\nabla H}=\partial_x^{-2}\frac{\delta\hat{H}}{\delta u}+\partial_x^{-1}\frac{\delta\hat{H}}{\delta v}. \tag{169}$$

Substituting this Lax operator and gradient into (156), (157) we get the first Poisson operand

$$\hat{\theta}_1=\begin{pmatrix}0 & 3D_x\\ 3D_x & \mathrm{ad}_u\end{pmatrix},\quad \hat{\theta}_1^{-1}=\frac{1}{3}\begin{pmatrix}-\frac{1}{3}D_x^{-1}\,\mathrm{ad}_u\,D_x^{-1} & D_x^{-1}\\ D_x^{-1} & 0\end{pmatrix}, \tag{170}$$

and the second one

$$\hat{\theta}_2=\begin{pmatrix}\overline{\theta}_{11} & \overline{\theta}_{12}\\ \overline{\theta}_{21} & \overline{\theta}_{22}\end{pmatrix}-R_{\partial_y}\hat{\theta}_1, \tag{171}$$

where

$$\overline{\theta}_{11}=2D_x^3+D_xu+R_uD_x-\mathrm{ad}_v+D_y+\tfrac{1}{3}\mathrm{ad}_u\,D_x^{-1}\,\mathrm{ad}_u,$$

$$\begin{aligned}\overline{\theta}_{12}=&-D_x^4-D_x^2R_u+vD_x+D_x\,\mathrm{ad}_v^+-2D_xD_y\\&+\tfrac{1}{3}(\mathrm{ad}_u\,D_x^{-1}\,\mathrm{ad}_v+\mathrm{ad}_u\,D_x^2+\mathrm{ad}_u\,R_u-\mathrm{ad}_u\,D_x^{-1}D_y),\end{aligned}$$

$$\begin{aligned}\overline{\theta}_{21}=&D_x^4+uD_x^2+D_xR_v+\mathrm{ad}_v^+\,D_x-D_xD_y\\&+\tfrac{1}{3}(D_x^2\,\mathrm{ad}_u+u\,\mathrm{ad}_u-D_x^{-1}D_y\,\mathrm{ad}_u+\mathrm{ad}_vD_x^{-1}\,\mathrm{ad}_u),\end{aligned}$$

$$\begin{aligned}\overline{\theta}_{22}=&\tfrac{2}{3}(D_x^2R_v-vD_x^2-D_x^5-D_x^3R_u-uD_x^3-uD_xR_u+D_yR_u+uR_v-vR_u)\\&+\tfrac{1}{3}(D_x^2v-R_vD_x^2+D_x^2D_y+uv-uD_y-R_vR_u\\&+\mathrm{ad}_v\,D_x^{-1}\,\mathrm{ad}_v-\mathrm{ad}_v\,D_x^{-1}D_y-D_x^{-1}D_y\,\mathrm{ad}_v+D_x^{-1}D_y^2).\end{aligned}$$

Taking

$$\nabla h_0=\begin{pmatrix}1\\0\end{pmatrix}\in\ker\hat{\theta}_1,$$

and applying formula (116) we get the first hierarchy of vector fields

$$\begin{pmatrix}u\\v\end{pmatrix}_{t_1}=\begin{pmatrix}u_x\\v_x\end{pmatrix},$$

$$u_{t_3}=2v_{3x}+4(uv)_x-u_{4x}-(u^2)_{2x}-2u_{xy}+4v_y, \tag{172}$$

$$v_{t_3}=v_{4x}+2uv_{2x}+2(v^2)_x+2v_{xy}+2u_xv_x-\tfrac{2}{3}(u_{5x}+3uu_{3x}+6u_xu_{2x}$$
$$+2u^2u_x)+\tfrac{4}{3}D_x^{-1}u_{2y}-\tfrac{2}{3}u_{y2x},\ldots.$$

Taking

$$\nabla h_0\begin{pmatrix}0\\1\end{pmatrix}\in\ker\hat{\theta}_1,$$

and applying formula (116) we get the first equation from the second hierarchy

$$\begin{pmatrix}u\\v\end{pmatrix}_{t_2}=\begin{pmatrix}u_{2x}-2v_x\\ \dfrac{2}{3}(u_{3x}+uu_x-u_y)-v_{xx}\end{pmatrix},\ldots. \tag{173}$$

(3) The case: $k=0$, $N=4$.
The Lax operator has the form

$$\hat{L}=\partial_x^4+u\partial_x^2+v\partial_x+w-\partial_y. \tag{174}$$

For this Lax operator we get from (155) the following gradient:

$$\widehat{\nabla H}=\partial_x^{-3}\frac{\delta\hat{H}}{\delta u}+\partial_x^{-2}\frac{\delta\hat{H}}{\delta v}+\partial_x^{-1}\frac{\delta\hat{H}}{\delta w}. \tag{175}$$

Substituting the Lax operator and the gradient in (156), (157) we get the first Poisson operand and its inverse

$$\hat{\theta}_1=\begin{pmatrix}0&0&4D_x\\0&4D_x&2D_x^2+\mathrm{ad}_u\\4D_x&-2D_x^2+\mathrm{ad}_u&2D_x^3+uD_x+D_xR_u+\mathrm{ad}_v\end{pmatrix}, \tag{176}$$

$$\hat{\theta}_1^{-1}=-\frac{1}{64}\begin{pmatrix}\hat{\theta}_{11}&4D_x^{-1}(-2D_x^2+\mathrm{ad}_u)D_x^{-1}&-16D_x^{-1}\\4D_x^{-1}(2D_x^2+\mathrm{ad}_u)D_x^{-1}&-16D_x^{-1}&0\\-16D_x^{-1}&0&0\end{pmatrix}, \tag{177}$$

where

$$\hat{\theta}_{11}=4D_x^{-1}(2D_x^3+uD_x+D_xR_u+\mathrm{ad}_v)D_x^{-1}-D_x^{-1}(-2D_x^2+\mathrm{ad}_u)D_x^{-1}(2D_x^2+\mathrm{ad}_u)D_x^{-1}$$

and the second Poisson operand

$$\hat{\theta}_2=\begin{pmatrix}\overline{\theta}_{11}&\overline{\theta}_{12}&\overline{\theta}_{13}\\\overline{\theta}_{21}&\overline{\theta}_{22}&\overline{\theta}_{23}\\\overline{\theta}_{31}&\overline{\theta}_{32}&\overline{\theta}_{33}\end{pmatrix}-R_{\partial_y}\hat{\theta}_1, \tag{178}$$

where

$$\overline{\theta}_{11}=5D_x^3-\mathrm{ad}_v+\tfrac{1}{4}(\mathrm{ad}_u D_x^{-1}\mathrm{ad}_u+6D_xu+6R_uD_x-2uD_x-2D_xR_u),$$

$$\overline{\theta}_{12}=vD_x-\mathrm{ad}_w+D_y-5D_x^4+\mathrm{ad}_u D_x^2-2D_x^2R_u$$
$$+\tfrac{1}{4}(\mathrm{ad}_u D_x^{-1}\mathrm{ad}_v+2\,\mathrm{ad}_u R_u+2D_xR_v+6D_xv),$$

$$\overline{\theta}_{13}=wD_x+\tfrac{1}{4}(\mathrm{ad}_u D_x^{-1}\mathrm{ad}_w-\mathrm{ad}_u D_x^{-1}D_y-\mathrm{ad}_u D_x^3-\mathrm{ad}_u D_xR_u$$
$$+6D_x\,\mathrm{ad}_w^+ +\mathrm{ad}_u R_v-6D_xD_y+6D_x^5+6D_x^3R_u-6D_x^2R_v),$$

$$\overline{\theta}_{21}=D_xR_v-\mathrm{ad}_w+D_y+5D_x^4+D_x^2\,\mathrm{ad}_u+2uD_x^2$$
$$+\tfrac{1}{4}(\mathrm{ad}_v D_x^{-1}\mathrm{ad}_u+2u\,\mathrm{ad}_u+6R_vD_x+2vD_x),$$

$$\overline{\theta}_{22}=2D_xR_w+2wD_x-2D_xD_y-6D_x^5-R_vD_x^2+D_x^2v-2D_x^3R_u$$
$$-2uD_x^3-uD_xR_u+\tfrac{1}{4}(\mathrm{ad}_v D_x^{-1}\mathrm{ad}_v+2u\,\mathrm{ad}_v^+-2\,\mathrm{ad}_v^+ R_u),$$

$$\overline{\theta}_{23}=2D_x^2R_w-wD_x^2-wR_u+D_yR_u-2D_x^3R_v+2D_x^4R_u+2D_x^6$$
$$+D_x^2w+\tfrac{1}{4}(\mathrm{ad}_v D_x^{-1}\mathrm{ad}_w-\mathrm{ad}_v D_x^{-1}D_y-\mathrm{ad}_v D_x^3+2uD_x^4+2uD_x^2R_u$$
$$-\mathrm{ad}_v D_xR_u-2uD_xR_v+2u\,\mathrm{ad}_w^+-2uD_y+\mathrm{ad}_v R_v),$$

$$\overline{\theta}_{31}=D_xR_w+\tfrac{1}{4}(\mathrm{ad}_w D_x^{-1}\mathrm{ad}_u-D_x^{-1}D_y\,\mathrm{ad}_u+D_x^3\,\mathrm{ad}_u+6D_x^5+6\,\mathrm{ad}_w^+ D_x$$
$$-6D_xD_y+uD_x\,\mathrm{ad}_u+6uD_x^3+6vD_x^2+v\,\mathrm{ad}_u),$$

$$\overline{\theta}_{32}=D_x^2R_w-2D_x^6-2uD_x^4-2vD_x^3-2wD_x^2+2D_x^2D_y+uR_w-R_wD_x^2$$
$$+\tfrac{1}{4}(\mathrm{ad}_w D_x^{-1}\mathrm{ad}_v-D_x^{-1}D_y\,\mathrm{ad}_v+D_x^3\,\mathrm{ad}_v-2D_x^4R_u-2uD_x^2R_u$$
$$+uD_x\,\mathrm{ad}_v-2vD_xR_u-2\,\mathrm{ad}_w^+ R_u+2D_yR_u+v\,\mathrm{ad}_v),$$

$$\overline{\theta}_{33}=\tfrac{1}{4}(\mathrm{ad}_w D_x^{-1}\mathrm{ad}_w-D_x^{-1}D_y\,\mathrm{ad}_w-\mathrm{ad}_w D_x^{-1}D_y+D_x^{-1}D_y^2+R_wD_x^3$$
$$+D_x^3w-D_x^3D_y+R_wD_xR_u+uD_xw-uD_xD_y+3D_x^3R_w+3wD_x^3$$
$$-3D_x^3D_y+3D_x^5R_u+3uD_x^5+3D_x^7-3D_x^4R_v+3vD_x^4+3uD_x^3R_u$$
$$-3uD_x^2R_v+3vD_x^2R_u+3uD_xR_w+3wD_xR_u-3D_xD_yR_u-3vD_xR_v$$
$$+vw-vD_y-R_wR_v+3vR_w-3wR_v+3D_yR_v).$$

Taking

$$\nabla h_0=\begin{pmatrix}1\\0\\0\end{pmatrix}\in\ker\hat{\theta}_1$$

and applying formula (116) we get the first hierarchy of commuting vector fields

$$\begin{pmatrix}u\\v\\w\end{pmatrix}_{t_1}=\begin{pmatrix}u_x\\v_x\\w_x\end{pmatrix},$$

$$
\begin{aligned}
u_{t_3} &= 2u_{5x} - 20v_{4x} + 40w_{3x} + 40(uw)_x - 40u_{xx}v - 20uv_{xx} \\
&\quad + 20(v_x)^2 - 45u_xv_x - 10uu_{xxx} - 15u^2u_x + 32u_{xy} - 40v_y, \\
v_{t_3} &= 10u_{6x} - 28v_{5x} + 40w_{4x} + 40(vw)_x - 40uv_{xxx} + 40(uw_x)_x \\
&\quad - 100u_xv_{xx} - 110u_{xx}v_x + 5(u^2)_{4x} - 15(u^2v)_x - 20v_{xy} \\
&\quad - 40w_y + 30u_{xxy} + 10uu_y, \qquad (179) \\
w_{t_3} &= 5u_{7x} - 12v_{6x} + 12w_{5x} + 20(w_x)^2 + 20v_xw_x + 20vw_{xx} \\
&\quad + 20uw_{xxx} + 12u_xw_{xx} + 5uu_{5x} + 5(uu_x)_{4x} - 10(uv)_{4x} \\
&\quad + 5u^2w_x - 10u(uv)_{xx} + 5v(uu_x)_x - 10v(uv)_x + 5u(uu_x)_{xx} \\
&\quad + 2u_{xx}w_x - 20w_{xy} + 15u_{3xy} - 10v_{xxy} + 10D_x^{-1}u_{yy} + 15uu_{xy} + 5u_xu_y - 10uv_y, \\
&\quad \vdots .
\end{aligned}
$$

Taking

$$
\nabla h_0 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \in \ker \hat{\theta}_1
$$

and applying formula (116) we get the firts equation of the second hierarchy

$$
\begin{pmatrix} u \\ v \\ w \end{pmatrix}_{t_2} = \begin{pmatrix} -2u_{xx} + 2v_x \\ 2w_x + v_{xx} - 2u_{3x} - uu_x \\ w_{xx} - \frac{1}{2}(u_{4x} + uu_{xx} + vu_x + u_y) \end{pmatrix}, \qquad (180)
$$

$$
\vdots .
$$

(4) The case: $k=1$, $N=0$.
The Lax operator is of the form

$$
\hat{L} = u + \partial_x^{-1}w - \partial_y . \qquad (181)
$$

For this Lax operator we get from (155) the following gradient:

$$
\widehat{\nabla H} = \partial_x^{-2}\frac{\delta \hat{H}}{\delta w} + \partial_x^{-1}\frac{\delta \hat{H}}{\delta u}. \qquad (182)
$$

Substituting the Lax operator and the gradient in (156), (158) we get the first Poisson operand

$$
\hat{\theta}_1 = \begin{pmatrix} 0 & \mathrm{ad}_u - D_y \\ \mathrm{ad}_u - D_y & \mathrm{ad}_w \end{pmatrix}, \qquad (183)
$$

and the second Poisson operand

$$
\hat{\theta}_2 = \begin{pmatrix} \overline{\theta_{11}} & \overline{\theta_{12}} \\ \overline{\theta_{21}} & \overline{\theta_{22}} \end{pmatrix} - R_{\partial_y}\hat{\theta}_1, \qquad (184)
$$

where

$$\overline{\theta}_{11}=(\mathrm{ad}_u-D_y)D_x^{-1}(\mathrm{ad}_u-D_y),$$

$$\overline{\theta}_{12}=(u-D_y)(\mathrm{ad}_u-D_y)+(\mathrm{ad}_u-D_y)D_x^{-1}\,\mathrm{ad}_w,$$

$$\overline{\theta}_{21}=(\mathrm{ad}_u-D_y)R_u+\mathrm{ad}_w\,D_x^{-1}(\mathrm{ad}_u-D_y)+R_{u_y},$$

$$\overline{\theta}_{22}=w(u-D_y)-R_uR_w+\mathrm{ad}_w\,D_x^{-1}\,\mathrm{ad}_w.$$

The recursion operand is given by

$$\hat{\Phi}=\begin{pmatrix} u-D_y & (\mathrm{ad}_u-D_y)D_x^{-1} \\ w & R_u+\mathrm{ad}_w\,D_x^{-1}\end{pmatrix}-R_{\partial_y}I. \tag{185}$$

Taking

$$\nabla h_0=\begin{pmatrix}0\\1\end{pmatrix}\in\ker\hat{\theta}_1,\hat{\theta}_2$$

and applying formula (122) we get the hierarchy

$$\begin{pmatrix}u\\w\end{pmatrix}_{t_1}=\begin{pmatrix}u_x\\w_x\end{pmatrix},$$

$$\begin{pmatrix}u\\w\end{pmatrix}_{t_2}=\begin{pmatrix}u_{2y}-2uu_y+2D_x^{-1}w_{2y}\\ -w_{2y}-2(wu)_y\end{pmatrix},$$

$$u_{t_3}=\tfrac{1}{2}(u^2)_{2y}-u^2u_y-\tfrac{1}{3}u_{3y}+uD_x^{-1}w_{2y}+D_x^{-1}(uw)_{2y}+u_yD_x^{-1}w_y, \tag{186}$$

$$w_{t_3}=-2uwu_y-u^2w_y-uw_{2y}-u_yw_y-\tfrac{1}{3}w_{3y}+wD_x^{-1}w_{2y}+w_yD_x^{-1}w_y,\ldots.$$

Interestingly, for $N=0$ the central extension approach gives another hierarchy of commuting vector fields, i.e.,

$$\begin{pmatrix}u\\w\end{pmatrix}_{t_1}=\begin{pmatrix}u_x\\w_x\end{pmatrix},$$

$$\begin{pmatrix}u\\w\end{pmatrix}_{t_2}=\begin{pmatrix}u_{xx}+2w_x-2u_xD_y^{-1}u_x\\ -w_{xx}-2(wD_y^{-1}u_x)_x\end{pmatrix},$$

$$\begin{aligned}u_{t_3}=&u_{3x}-3(wD_y^{-1}u_x)_x-3(u_xD_y^{-1}u_x)_x-3w_xD_y^{-1}u_x\\&-3u_xD_y^{-1}w_x+6u_xD_y^{-1}u_xD_y^{-1}u_x,\end{aligned} \tag{187}$$

$$w_{t_3}=w_{3x}+3(w_xD_y^{-1}u_x)_x-3(wD_y^{-1}w_x)_x+6(wD_y^{-1}u_xD_y^{-1}u_x)_x,\ldots.$$

We can transform this hierarchy to the (186) one through the following transformation: $D_y^{-1}u_x\to u$, $w\to w$, $x\leftrightarrow y$.

(5) The case: $k=1$, $N=2$.

The Lax operator takes the form

$$\hat{L}=\partial_x^2+u\partial_x+v-\partial_y+\partial_x^{-1}w. \tag{188}$$

For this Lax operator we get from (155) the following gradient:

$$\widehat{\nabla H}=\partial_x^{-2}\frac{\delta\hat{H}}{\delta u}+\partial_x^{-1}\frac{\delta\hat{H}}{\delta v}+\frac{\delta\hat{H}}{\delta w}. \tag{189}$$

Substituting the Lax operator and the gradient in (156), (158) we get the first Poisson operand and its inverse

$$\hat{\theta}_1=\begin{pmatrix} 0 & 0 & 2D_x+\mathrm{ad}_u \\ 0 & 2D_x+\mathrm{ad}_u & D_x^2-D_y+uD_x+\mathrm{ad}_v \\ 2D_x+\mathrm{ad}_u & -D_x^2-D_y+D_xR_u+\mathrm{ad}_v & \mathrm{ad}_w \end{pmatrix}, \tag{190}$$

$$\hat{\theta}_1^{-1}=\begin{pmatrix} \hat{\theta}_{11} & \hat{\theta}_{12} & (2D_x+\mathrm{ad}_u)^{-1} \\ \hat{\theta}_{21} & (2D_x+\mathrm{ad}_u)^{-1} & 0 \\ (2D_x+\mathrm{ad}_u)^{-1} & 0 & 0 \end{pmatrix}, \tag{191}$$

where

$$\begin{aligned}\hat{\theta}_{11}=&-(2D_x+\mathrm{ad}_u)^{-1}\mathrm{ad}_w(2D_x+\mathrm{ad}_u)^{-1}\\ &+(2D_x+\mathrm{ad}_u)^{-1}(-D_x^2-D_y+D_xR_u+\mathrm{ad}_v)(2D_x+\mathrm{ad}_u)^{-1}\\ &\times(D_x^2-D_y+uD_x+\mathrm{ad}_v)(2D_x+\mathrm{ad}_u)^{-1},\end{aligned}$$

$$\hat{\theta}_{12}=-(2D_x+\mathrm{ad}_u)^{-1}(-D_x^2-D_y+D_xR_u+\mathrm{ad}_v)(2D_x+\mathrm{ad}_u)^{-1},$$

$$\hat{\theta}_{21}=-(2D_x+\mathrm{ad}_u)^{-1}(D_x^2-D_y+uD_x+\mathrm{ad}_v)(2D_x+\mathrm{ad}_u)^{-1}.$$

and the second Poisson operand

$$\hat{\theta}_2=\begin{pmatrix} \overline{\theta}_{11} & \overline{\theta}_{12} & \overline{\theta}_{13} \\ \overline{\theta}_{21} & \overline{\theta}_{22} & \overline{\theta}_{23} \\ \overline{\theta}_{31} & \overline{\theta}_{32} & \overline{\theta}_{33} \end{pmatrix}-R_{\partial_y}\hat{\theta}_1, \tag{192}$$

where

$$\overline{\theta}_{11}=6D_x+5\mathrm{ad}_u+\mathrm{ad}_u D_x^{-1}\mathrm{ad}_u,$$

$$\overline{\theta}_{12}=2D_x\,\mathrm{ad}_u^+ +2\,\mathrm{ad}_v+\mathrm{ad}_{u^2}+\mathrm{ad}_u D_x^{-1}\mathrm{ad}_v-2D_y-\mathrm{ad}_u D_x^{-1}D_y,$$

$$\begin{aligned}\overline{\theta}_{13}=&2D_x^3+\mathrm{ad}_u D_x^2+u\,\mathrm{ad}_u D_x+2D_xuD_x+2D_xv+\mathrm{ad}_u v+2\,\mathrm{ad}_w\\ &+\mathrm{ad}_u D_x^{-1}\mathrm{ad}_w-2D_xD_y-\mathrm{ad}_u D_y+R_{u_y},\end{aligned}$$

$$\overline{\theta}_{21}=2\,\mathrm{ad}_u^+ D_x+2\,\mathrm{ad}_v-2D_y+\mathrm{ad}_{u^2}+\mathrm{ad}_v D_x^{-1}\mathrm{ad}_u-D_yD_x^{-1}\mathrm{ad}_u,$$

$$\begin{aligned}\overline{\theta}_{22}=&2D_x^3+\mathrm{ad}_u D_x^2+D_x^2\,\mathrm{ad}_u+vD_x-D_yD_x+D_xR_v-\mathrm{ad}_w+uD_xu\\ &+R_uD_xR_u+v\,\mathrm{ad}_u^+ -D_y\,\mathrm{ad}_u^+ +uv-uD_y-R_vR_u-\mathrm{ad}_u^+ R_v\end{aligned}$$

$$+(\mathrm{ad}_v-D_y)D_x^{-1}(\mathrm{ad}_v-D_y)+R_{u_y},$$

$$\begin{aligned}\overline{\theta}_{23}=&D_x^4+uD_x^3+D_x^2uD_x+D_x^2v-D_x^2D_y+\mathrm{ad}_v D_x^2-D_yD_x^2+R_wD_x\\&+D_x\,\mathrm{ad}_w^+ +uD_xuD_x+vuD_x-D_yuD_x+uD_xv-uD_xD_y-uR_vD_x\\&+(v-D_y)(\mathrm{ad}_v-D_y)+uw-R_uR_w+\mathrm{ad}_v D_x^{-1}\,\mathrm{ad}_w-D_yD_x^{-1}\,\mathrm{ad}_w,\end{aligned}$$

$$\begin{aligned}\overline{\theta}_{31}=&2D_x^3+D_x^2\,\mathrm{ad}_u-D_x\,\mathrm{ad}_u R_u-2D_xR_uD_x+2R_vD_x+R_v\,\mathrm{ad}_u\\&+2\,\mathrm{ad}_w+\mathrm{ad}_w D_x^{-1}\,\mathrm{ad}_u,\end{aligned}$$

$$\begin{aligned}\overline{\theta}_{32}=&-D_x^4+D_x^3R_u+D_xR_uD_x^2-R_vD_x^2+D_x^2\,\mathrm{ad}_v-D_x^2D_y+D_xw\\&+\mathrm{ad}_w^+ D_x-D_xR_uD_xR_u+D_xR_uR_v+R_vD_xR_u-D_xvR_u\\&+D_xD_yR_u+\mathrm{ad}_v R_v-D_yR_v+wu-R_wR_u+\mathrm{ad}_w D_x^{-1}\,\mathrm{ad}_v\\&-\mathrm{ad}_w D_x^{-1}D_y-D_xR_{u_y}+R_{v_y},\end{aligned}$$

$$\overline{\theta}_{33}=wD_x^2-D_x^2R_w+wuD_x+D_xR_uR_w+wv-wD_y-R_vR_w+\mathrm{ad}_w D_x^{-1}\,\mathrm{ad}_w.$$

Taking

$$\nabla h_0=\begin{pmatrix}0\\0\\1\end{pmatrix}\in\ker\hat{\theta}_1$$

and applying formula (116) we get the hierarchy

$$\begin{pmatrix}u\\v\\w\end{pmatrix}_{t_1}=\begin{pmatrix}u_x\\v_x\\w_x\end{pmatrix},$$

$$\begin{pmatrix}u\\v\\w\end{pmatrix}_{t_2}=\begin{pmatrix}2v_x+u_y\\2w_x+v_{xx}+uv_x\\-w_{xx}+(wu)_x\end{pmatrix},$$

$$\begin{aligned}u_{t_3}&=u_{xxx}-\tfrac{3}{2}u^2u_x+6(uv)_x+6v_{xx}+12w_x+6v_y+3D_x^{-1}u_{yy}+3u_xD_x^{-1}u_y,\\v_{t_3}&=v_{xxx}+\tfrac{3}{2}(wu)_x+\tfrac{3}{2}uv_{xx}+\tfrac{3}{2}uw_x+\tfrac{3}{4}u_xv_x+\tfrac{3}{2}vv_x+\tfrac{3}{8}u^2v_x+\tfrac{3}{4}v_xD_x^{-1}u_y,\\w_{t_3}&=w_{xxx}-\tfrac{3}{2}(wu)_{xx}+\tfrac{3}{4}(wu_x)_x+\tfrac{3}{2}(wv)_x+\tfrac{3}{8}(u^2w)_x+\tfrac{3}{4}wu_y+\frac{3}{4}w_xD_x^{-1}u_y,\\&\vdots.\end{aligned}\tag{193}$$

The reduction $v=w=0$ gives the mKP equation

$$u_{t_3}=u_{xxx}-\tfrac{3}{2}u^2u_x+3D_x^{-1}u_{yy}+3u_xD_x^{-1}u_y.\tag{194}$$

V. CONCLUSIONS

In this paper we illustrated two different methods for the construction of a bi-Hamiltonian representation of the lattice-field and field dynamical system in $(2+1)$-dimension. The first method is based on the central extension approach and allows a construction of a hierarchy of commuting vector fields and a Hamiltonian representation of dynamical system. The second method is the so-called operand approach. This method allows a construction of a bi-Hamiltonian representation for dynamical systems in $(2+1)$-dimension. This bi-Hamiltonian representation is related to the so-called operand Poisson tensors. Inverting the first Poisson tensor we can construct a recursion operand and applying Theorem 3 and the Lemmas 1,2 to produce a whole hierarchy of commuting vector fields. The general idea was to extend the known methods for the construction integrable nonlinear Hamiltonian dynamical systems, which are based on the $\mathcal{R}$-matrix formalism, and to derive new dynamical systems in $(2+1)$-dimensions. We used the central extension procedure for the construction of $(2+1)$-dimensional lattice-field and field dynamical systems and their Hamiltonian formulation and derived hierarchies of vector fields of the $(2+1)$–Benjamin–Ono, $(2+1)$–Toda and some new equations. The $(2+1)$-dimensional systems which do not survive a reduction onto $(1+1)$-dimensional space are also derived. We developed operand formalism and extended theorems proposed by Magri, Morosi, and Tondo[13,14] and by Athorne, Dorfman, and Fokas,[11,15,16] unified them into one and also derived, using the proposed theorem, a bi-Hamiltonian formulation of well-known and some new dynamical systems of lattice-field and field types in $(2+1)$-dimensions. The operand formalism in the majority of the cases considered gives the same result as central extension approach, but we still do not have a general formula for the construction of hierarchies of commuting vector fields and each time we have to find a ''right'' starting symmetry. This problem is still open.

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The supersymmetric Camassa–Holm equation and geodesic flow on the superconformal group

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We study a family of fermionic extensions of the Camassa–Holm equation. Within this family we identify three interesting classes: (a) equations, which are inherently Hamiltonian, describing geodesic flow with respect to an H^1 metric on the group of superconformal transformations in two dimensions, (b) equations which are Hamiltonian with respect to a different Hamiltonian structure and (c) supersymmetric equations. Classes (a) and (b) have no intersection, but the intersection of classes (a) and (c) gives a system with interesting integrability properties. We demonstrate the Painlevé property for some simple but nontrivial reductions of this system, and also discuss peakon-type solutions. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Recently there has been substantial interest in the Camassa–Holm (CH) equation:[1,2]

$$u_t - \nu u_{xxt} = \kappa u_x - 3uu_x + \nu(uu_{xxx} + 2u_x u_{xx}). \tag{1}$$

This equation has been proposed as a model for shallow water waves. It is believed to be integrable, having a bi-Hamiltonian structure, as was first observed by Fokas and Fuchssteiner[3] 12 years prior to Camassa's and Holm's work. Due to the nonlinear dispersion term, uu_{xxx}, it exhibits more general wave phenomena than other integrable water wave equations such as KdV. In particular, when $\kappa = 0$ it admits a class of nonanalytic weak solutions known as *peakons*, as well as finite time blow-up of classical solutions.[1]

Geometrically, the relationship of CH to KdV is rather deeper: Both are regularizations of the Euler equation for a one dimensional compressible fluid (Monge or inviscid Burgers equation),

$$u_t = -3uu_x. \tag{2}$$

A solution to this equation describes a geodesic on the group of diffeomorphisms of the circle $\mathrm{Diff}(S^1)$[4] with respect to a right-invariant metric induced by an L^2 norm, $\int u^2\,dx$, on the associated Lie algebra. If the group is centrally extended to the Bott–Virasoro group, the KdV equation arises.[5–8] On the other hand, if the metric is changed to one induced by an H^1 norm, $\int(u^2 + \nu u_x^2)dx$, the CH equation arises.[9–11] Both these ''deformations'' have a regularizing effect on solutions of (2), which exhibit discontinuous shocks.

Thus KdV and CH arise in a unified geometric setting; both are geodesic flows which are integrable systems. (Here, and henceforth in this paper, when we refer to a ''geodesic flow'' we

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mean the evolutionary PDE which can be formally associated—in the manner we will see in Sec. II—with any inner product on the Lie algebra of a diffeomorphism group, and which, at least in the cases mentioned above, is known to describe geodesic flow, in the usual sense of the phrase, with respect to the correpsonding right-invariant metric on the group. In the case of a general inner product, the existence of the corresponding geodesic flow, in the usual sense of the phrase, is highly nontrivial.) The following important question arises: What features of the underlying geometry give rise to integrability? In general, geodesic flows are *not* integrable: the Euler equation for fluid flow in more than one spatial dimension is an example.[4] Indeed, for the latter, Arnold has suggested a relationship between negative sectional curvatures and nonpredictability of the flow. We feel that it ought to be possible to identify some other geometric property that ''causes'' integrability. In a remarkable recent paper,[12] Fringer and Holm have shown that certain features usually considered to be hallmarks of integrable systems, such as elastic scattering and asymptotic sorting according to height, in fact, appear in geodesic flows on $\mathrm{Diff}(S^1)$ with respect to a large class of metrics. Thus, there may well be a hierarchy of geometric structures corresponding to various degrees of integrability.

One further example of an integrable bi-Hamiltonian system arising as a geodesic flow has been discussed by Ovsienko and Khesin.[5] Using the superconformal group with an L^2 type metric, they obtained the so-called kuper-KdV system of Kupershmidt.[13] This is a fermionic extension of KdV: it describes evolution of functions valued in (the odd or even parts of) a Grassmann algebra. In fact, as we will see below, taking a general L^2 type metric on the superconformal group gives rise to a one parameter family of fermionic extensions of KdV, which includes not only kuper-KdV, but also the super-KdV system of Mathieu and Manin–Radul.[14,15] The latter is integrable: it has only a single Hamiltonian structure, but unlike kuper-KdV it is supersymmetric, a property which is widely believed to contribute to integrability. It remains a mystery as to why, of the one parameter family of geodesic flows associated with L^2 type metrics on the superconformal group, only two specific choices of the parameter give rise to integrable systems.

Our main purpose in this paper is to investigate geodesic flows obtained from H^1 type norms on the superconformal group; more generally we consider the following family of fermionic extensions of CH:

$$\begin{aligned} u_t-\nu u_{xxt}&=\kappa_1 u_x+\kappa_2 u_{xxx}+\beta_1 uu_x+\beta_2 u_x u_{xx}+\beta_3 uu_{xxx}+\gamma_1\xi\xi_{xx}+\gamma_2\xi_x\xi_{xxx}+\gamma_3\xi\xi_{xxxx}, \\ \xi_t-\mu\xi_{xxt}&=\sigma_1\xi_x+\sigma_2\xi_{xxx}+\epsilon_1 u_x\xi+\epsilon_2 u\xi_x+\rho_1 u\xi_{xxx}+\rho_2 u_x\xi_{xx}+\rho_3 u_{xx}\xi_x+\rho_4 u_{xxx}\xi. \end{aligned} \tag{3}$$

Here $u(x,t)$ and $\xi(x,t)$ are fields valued, respectively, in the even and odd parts of a Grassmann algebra, and $\{\nu,\mu,\kappa_1,\kappa_2,\beta_1,\beta_2,\beta_3,\gamma_1,\gamma_2,\gamma_3,\sigma_1,\sigma_2,\epsilon_1,\epsilon_2,\rho_1,\rho_2,\rho_3,\rho_4\}$ are parameters. By rescaling u and ξ it is possible to set $\beta_1=-3$ and $\gamma_1=2$ (assuming that they are nonzero), and we shall do this throughout. In addition it is possible to eliminate up to two further parameters by rescaling the coordinates x,t.

We derive three interesting classes of systems of the form (3). In Sec. II, we consider geodesic flows on the superconformal group with an H^1 type metric; the resulting systems have a natural Hamiltonian structure, or more precisely, since the fields are Grassmann algebra valued, a graded Hamiltonian structure. In Sec. III we identify a class of systems having a different Hamiltonian structure. Unfortunately the latter has no intersection with the class of Sec. II, so there does not seem to be a bi-Hamiltonian fermionic extension of CH. In Sec. IV we consider systems of the form (3) that are invariant under supersymmetry transformations between u and ξ. This class has nontrivial intersections with both the classes of Secs. II and III. In particular there is a unique supersymmetric geodesic flow which is a candidate for being a new integrable system. We call this equation *super-CH*. In Sec. V we show that two reductions of super-CH have the Painlevé property, which is positive evidence for integrability. In Sec. VI we look for peakon-type solutions of super-CH; as for CH, multipeakon solutions arise from the solutions of a system of ODEs, but the integrability of this unfortunately remains unclear.

Super-CH is a supersymmetric geodesic flow whose bosonic part is integrable. While in this paper we do not fully establish integrability of super-CH, we regard it as an interesting test case to determine whether in general supersymmetric geodesic flows with integrable bosonic parts must be integrable.

A trivial integrable CH system of the form (3), which is not incorporated in the classes of Secs. II, III, and IV, and which we shall not discuss further, is the odd linearization of the bosonic CH system (1):

$$\begin{aligned} u_t-\nu u_{xxt}&=\kappa u_x-3uu_x+\nu(uu_{xxx}+2u_xu_{xx}),\\ \xi_t-\nu\xi_{xxt}&=\kappa\xi_x-3(\xi u)_x+\nu(\xi u_{xxx}+u\xi_{xxx}+2(\xi_xu_x)_x). \end{aligned} \tag{4}$$

Replacing u by $u+\kappa/3$ and considering the limit $\nu\to 0$, $\kappa\to\infty$, with $\nu\kappa=3$, yields the system

$$\begin{aligned} u_t&=-3uu_x+u_{xxx},\\ \xi_t&=-3(\xi u)_x+\xi_{xxx}. \end{aligned} \tag{5}$$

This trivial fermionic extension of KdV has appeared often in the literature (see, e.g., Ref. 14).

II. GEODESIC FLOWS ON THE SUPERCONFORMAL GROUP

An inner product $\langle\cdot\,,\cdot\rangle$ on a Lie algebra $\mathfrak{g}$ determines a right- (or a left-) invariant metric on the corresponding Lie group G. The equation of geodesic motion on G with respect to this metric is determined as follows.[4] Define a bilinear operator $B\colon \mathfrak{g}\times\mathfrak{g}\to\mathfrak{g}$ by

$$\langle[V,W],U\rangle=\langle W,B(U,V)\rangle,\quad \forall\ \ W\in\mathfrak{g}. \tag{6}$$

Then geodesics are determined by solutions of the ''geodesic flow,''

$$U_t=B(U,U). \tag{7}$$

In our case, $\mathfrak{g}$ is the NSR superconformal algebra, consisting of triples $(u(x),\varphi(x),a)$, where u is a bosonic field, φ is a fermionic field and a is a constant. The Lie bracket is given by

$$\begin{aligned} [(u,\varphi,a)\,,(v,\psi,b)]=\Big(&uv_x-u_xv+\frac{1}{2}\varphi\psi\,,\,u\psi_x-\frac{1}{2}u_x\psi-\varphi_xv+\frac{1}{2}\varphi v_x\,,\\ &\int dx\Big(c_1u_xv_{xx}+c_2uv_x+c_1\varphi_x\psi_x+\frac{c_2}{4}\varphi\psi\Big)\Big), \end{aligned} \tag{8}$$

where c_1,c_2 are constants. On this algebra, an H^1 type inner product is given by

$$\begin{aligned} \langle(u,\varphi,a)\,,(v,\psi,b)\rangle&=\int dx(uv+\nu u_xv_x+\alpha\varphi\,\partial_x^{-1}\psi+\alpha\mu\varphi_x\psi)+ab\\ &=\int dx(u\Delta_0v+\varphi\Delta_1\psi)+ab, \end{aligned} \tag{9}$$

where

$$\Delta_0=1-\nu\partial_x^2,\quad \Delta_1=\alpha(\partial_x^{-1}-\mu\partial_x), \tag{10}$$

and μ,ν,α are further constants, all assumed nonzero. (See Ref. 5 for the definition of the natural fermionic extension of the standard L^2 inner product, to which the above reduces if $\mu=\nu=0$. The natural fermionic extension of the standard H^1 inner product is constructed, as for pure bosonic

systems, by taking the sum of the L^2 inner product for the functions involved with the L^2 inner product for the derivatives of the functions involved.) Writing $U=(u,\varphi,a)$, $V=(v,\psi,b)$, we find $B(U,V)=(B_0,B_1,0)$, where

$$\begin{aligned}\Delta_0 B_0(U,V)&=-(2v_x\Delta_0 u+v\,\Delta_0 u_x+\tfrac{3}{2}\psi_x\Delta_1\varphi+\tfrac{1}{2}\psi\Delta_1\varphi_x)-+a(c_1v_{xxx}-c_2v_x),\\ \Delta_1 B_1(U,V)&=-\left(\frac{3}{2}v_x\Delta_1\varphi+v\,\Delta_1\varphi_x+\frac{1}{2}\psi\Delta_0 u\right)+a\left(c_1\psi_{xx}-\frac{c_2}{4}\psi\right).\end{aligned}\tag{11}$$

The geodesic flows are therefore conveniently written in the form

$$\begin{aligned}\Delta_0 u_t&=\Delta_0 B_0(U,U),\\ \Delta_0\varphi_t&=\Delta_1 B_1(U,U),\\ a_t&=0.\end{aligned}\tag{12}$$

Writing $\varphi=\lambda\xi_x$, where λ is a constant satisfying $\lambda^2=4/3\alpha$, this yields the system

$$\begin{aligned}u_t-\nu u_{xxt}&=\kappa_1 u_x+\kappa_2 u_{xxx}-3uu_x+\nu(uu_{xxx}+2u_xu_{xx})+2\xi\xi_{xx}+\frac{2\mu}{3}\xi_x\xi_{xxx},\\ \xi_t-\mu\xi_{xxt}&=\frac{\kappa_1}{4\alpha}\xi_x+\frac{\kappa_2}{\alpha}\xi_{xxx}-\frac{3}{2}u_x\xi-\left(1+\frac{1}{2\alpha}\right)u\xi_x+\mu u\xi_{xxx}+\frac{3\mu}{2}u_x\xi_{xx}+\frac{\nu}{2\alpha}u_{xx}\xi_x.\end{aligned}\tag{13}$$

Here κ_1,κ_2 are independent parameters determined by a,c_1,c_2. This is evidently a 5 parameter class of systems of type (3).

Setting ξ to zero in (13) yields the CH result of Refs. 9–11. If instead we choose μ,ν to vanish, the H^1 norm becomes an L^2 norm; then choosing κ_1 to be zero and rescaling κ_2 to 1 we obtain the following 1 parameter fermionic extension of KdV:

$$\begin{aligned}u_t&=u_{xxx}-3uu_x+2\xi\xi_{xx},\\ \xi_t&=\frac{1}{\alpha}\xi_{xxx}-\frac{3}{2}u_x\xi-\left(1+\frac{1}{2\alpha}\right)u\xi_x.\end{aligned}\tag{14}$$

Modulo rescalings, the super-KdV of Mathieu and Manin–Radul is obtained by taking $\alpha=1$. The kuper-KdV system arises by taking $\alpha=\frac{1}{4}$, the choice made in Ref. 5. Other values of the parameters give systems which are not believed to be integrable (see however Ref. 16).

III. HAMILTONIAN EQUATIONS

Like KdV, CH has a bi-Hamiltonian structure, and this accounts for its integrability. We might hope that for some choices of parameters the system (13) should also have a bi-Hamiltonian structure. One Hamiltonian structure follows automatically from the geometric origins of the system.[4] Explicitly, introducing new variables, $m=u-\nu u_{xx}$ and $\eta=\xi-\mu\xi_{xx}$, (13) takes the form

$$\begin{pmatrix}m_t\\ \eta_t\end{pmatrix}=\mathcal{P}_2\begin{pmatrix}\dfrac{\delta\mathcal{H}_2}{\delta m}\\ \dfrac{\delta\mathcal{H}_2}{\delta\eta}\end{pmatrix},\tag{15}$$

where

$$\mathcal{P}_2=\begin{pmatrix} \kappa_2\partial_x^3+\kappa_1\partial_x-\partial_x m-m\partial_x & \frac{1}{2}\partial_x\eta+\eta\partial_x \\ -\partial_x\eta-\frac{1}{2}\eta\partial_x & \frac{3}{4\alpha}\left(\frac{\kappa_1}{4}+\kappa_2\partial_x^2\right)-\frac{3}{8\alpha}m \end{pmatrix}, \tag{16}$$

and the Hamiltonian functional is given succinctly by the H^1 inner product on the algebra,

$$\mathcal{H}_2=\tfrac{1}{2}\langle U\,,\,U\rangle=\tfrac{1}{2}\int dx(u^2+\nu u_x^2+\tfrac{4}{3}(\xi_x\xi+\mu\xi_{xx}\xi_x)). \tag{17}$$

This generalizes the so-called *second Hamiltonian structure* of KdV and its fermionic extensions.[13,14] Checking (15) is straightforward: the Euler–Lagrange derivatives $\delta\mathcal{H}_2/\delta m$, $\delta\mathcal{H}_2/\delta\eta$ are defined by

$$\delta\mathcal{H}_2=\int dx\left(\frac{\delta\mathcal{H}_2}{\delta m}\,\delta m+\frac{\delta\mathcal{H}_2}{\delta\eta}\,\delta\eta\right), \tag{18}$$

from which it follows immediately that $\delta\mathcal{H}_2/\delta m=u$ and $\delta\mathcal{H}_2/\delta\eta=\frac{4}{3}\xi_x$.

To investigate the possibility of systems amongst (13) having another Hamiltonian form, we look at systems of the form

$$\begin{pmatrix} m_t \\ \eta_t \end{pmatrix}=\mathcal{P}_1\begin{pmatrix} \dfrac{\delta\mathcal{H}_1}{\delta m} \\ \dfrac{\delta\mathcal{H}_1}{\delta\eta} \end{pmatrix}, \tag{19}$$

where

$$\mathcal{P}_1=\begin{pmatrix} \partial_x(1-\nu\partial_x^2) & 0 \\ 0 & -\dfrac{\epsilon_1}{2}(1-\mu\partial_x^2) \end{pmatrix}. \tag{20}$$

Here ϵ_1 is a constant and $\mathcal{H}_1$ is a functional generalizing the KdV *first Hamiltonian*,

$$\begin{aligned}\mathcal{H}_1=\int dx\Big(&-\frac{1}{2}u^3-\frac{\beta_3}{2}uu_x^2-\frac{\kappa_2}{2}u_x^2+\frac{\kappa_1}{2}u^2+\frac{\sigma_1}{\epsilon_1}\xi\xi_x+\frac{\sigma_2}{\epsilon_1}\xi\xi_{xxx}\\&+2u\xi\xi_x+(\gamma_2-\gamma_3)u\xi_x\xi_{xx}+\gamma_3u\xi\xi_{xxx}\Big).\end{aligned} \tag{21}$$

This is the most general functional of this type, up to rescalings of u and ξ. Since $\delta m=(1-\nu\partial_x^2)\delta u$, we have $(1-\nu\partial_x^2)(\delta\mathcal{H}_1/\delta m)=(\delta\mathcal{H}_1/\delta u)$, and similarly $(1-\mu\partial_x^2)(\delta\mathcal{H}_1/\delta\eta)=(\delta\mathcal{H}_1/\delta\xi)$. Thus Eqs. (19) take the simple form

$$\begin{aligned} u_t-\nu u_{xxt}&=\partial_x\left(\frac{\delta\mathcal{H}_1}{\delta u}\right)=\kappa_1u_x+\kappa_2u_{xxx}-3uu_x+\beta_3(2u_xu_{xx}+uu_{xxx})\\&\quad+2\xi\xi_{xx}+\gamma_2\xi_x\xi_{xxx}+\gamma_3\xi\xi_{xxxx},\\ \xi_t-\mu\xi_{xxt}&=\epsilon_1\left(\frac{\delta\mathcal{H}_1}{\delta\xi}\right)=\sigma_1\xi_x+\sigma_2\xi_{xxx}+\epsilon_1(u_x\xi+2u\xi_x)+\epsilon_1(2\gamma_3-\gamma_2)u\xi_{xxx}\\&\quad+\frac{3}{2}\epsilon_1(2\gamma_3-\gamma_2)u_x\xi_{xx}+\frac{1}{2}\epsilon_1(4\gamma_3-\gamma_2)u_{xx}\xi_x+\frac{1}{2}\epsilon_1\gamma_3u_{xxx}\xi.\end{aligned} \tag{22}$$

This is a 10 parameter class of systems of the form (3). Comparing with (13), we see that the only bi-Hamiltonian systems occur when $\{\mu=\nu=\beta_3=\gamma_2=\gamma_3=0,\ \epsilon_1=-\frac{3}{2},\ \sigma_1=\kappa_1,\ \sigma_2=4\kappa_2\}$, which is equivalent to (13) with $\{\mu=\nu=0\,,\ \alpha=\frac{1}{4}\}$, i.e., the kuper-KdV system. Thus, no new bi-Hamiltonian systems arise.

We note that the systems (22) can be obtained from a Lagrangian. Introducing a potential f defined by $u=f_x$, they are Euler–Lagrange equations for the functional

$$\mathcal{L}=\int dx\Big(\frac{1}{2}(f_x-\nu f_{xxx})f_t+\frac{1}{\epsilon_1}(\xi-\mu\xi_{xx})\xi_t+\frac{1}{2}f_x^3+\frac{\beta_3}{2}f_xf_{xx}^2+\frac{\kappa_2}{2}f_{xx}^2-\frac{\kappa_1}{2}f_x^2-\frac{\sigma_1}{\epsilon_1}\xi\xi_x$$
$$-\frac{\sigma_2}{\epsilon_1}\xi\xi_{xxx}-2\,f_x\xi\xi_x+(\gamma_3-\gamma_2)f_x\xi_x\xi_{xx}-\gamma_3f_x\xi\xi_{xxx}\Big). \tag{23}$$

IV. SUPERSYMMETRIC EQUATIONS

Define a fermionic superfield $\Phi(x,\vartheta)=s\xi+\vartheta u$ and superderivative $D=\partial/\partial\vartheta+\vartheta\partial_x$, where s is a nonzero parameter and ϑ is an odd coordinate. The most general superfield equation having a component content of the form (3) is the 8 parameter system,

$$(1-\nu D^4)\Phi_t=\kappa_1D^2\Phi+\kappa_2D^6\Phi-\frac{2}{s^2}\Phi D^3\Phi+\Big(\frac{2}{s^2}-3\Big)D\Phi D^2\Phi+\Big(\frac{\gamma_3}{s^2}+\beta_3\Big)D\Phi D^6\Phi$$
$$-\frac{\gamma_3}{s^2}\Phi D^7\Phi+\Big(\beta_3+\frac{\gamma_3-\gamma_2}{s^2}\Big)D^2\Phi D^5\Phi+\Big(\beta_2-\beta_3+\frac{\gamma_2-\gamma_3}{s^2}\Big)D^3\Phi D^4\Phi, \tag{24}$$

where $\{\nu,s,\kappa_1,\kappa_2,\beta_2,\beta_3,\gamma_2,\gamma_3\}$ are parameters. The component equations are

$$u_t-\nu u_{xxt}=\kappa_1u_x+\kappa_2u_{xxx}-3uu_x+\beta_2u_xu_{xx}+\beta_3uu_{xxx}+2\xi\xi_{xx}+\gamma_2\xi_x\xi_{xxx}+\gamma_3\xi\xi_{xxxx},$$
$$\xi_t-\nu\xi_{xxt}=\kappa_1\xi_x+\kappa_2\xi_{xxx}-\frac{2}{s^2}u_x\xi+\Big(\frac{2}{s^2}-3\Big)u\xi_x+\Big(\frac{\gamma_3}{s^2}+\beta_3\Big)u\xi_{xxx}$$
$$+\Big(\beta_2-\beta_3+\frac{\gamma_2-\gamma_3}{s^2}\Big)u_x\xi_{xx}+\Big(\frac{\gamma_3-\gamma_2}{s^2}+\beta_3\Big)u_{xx}\xi_x-\frac{\gamma_3}{s^2}u_{xxx}\xi. \tag{25}$$

These systems are by construction invariant under the supersymmetry transformations,

$$\delta u=\tau\xi_x,\quad \delta\xi=\frac{\tau u}{s^2}, \tag{26}$$

where τ is an odd parameter. The super-KdV limit, namely $\{\nu,\beta_2,\beta_3,\gamma_2,\gamma_3,\kappa_1\}$ all zero, yields, modulo rescalings, the one-parameter family of systems studied by Mathieu.[14]

By comparing (25) and (22) it is straightforward to extract systems which are both supersymmetric and have Hamiltonian form (19), (20). Taking $s^2=2$ in (25), $\{\nu=\mu,\ \sigma_1=\kappa_1,\ \sigma_2=\kappa_2,\ \epsilon=-1\}$ in (22), and $\{\beta_2=2\beta_3,\ \beta_3=\gamma_2-\frac{5}{2}\gamma_3\}$ in both, we obtain the systems,

$$u_t-\nu u_{xxt}=\kappa_1u_x+\kappa_2u_{xxx}-3uu_x+(\gamma_2-\tfrac{5}{2}\gamma_3)(2u_xu_{xx}+uu_{xxx})$$
$$+2\xi\xi_{xx}+\gamma_2\xi_x\xi_{xxx}+\gamma_3\xi\xi_{xxxx},$$
$$\xi_t-\nu\xi_{xxt}=\kappa_1\xi_x+\kappa_2\xi_{xxx}-u_x\xi-2u\xi_x+(\gamma_2-2\gamma_3)u\xi_{xxx}$$
$$+\tfrac{3}{2}(\gamma_2-2\gamma_3)u_x\xi_{xx}+\tfrac{1}{2}(\gamma_2-4\gamma_3)u_{xx}\xi_x-\tfrac{1}{2}\gamma_3u_{xxx}\xi. \tag{27}$$

These may be expressed in superfield form (24) with the above choice of parameters. The manifestly supersymmetric Hamiltonian form is given by

$$M_t=\hat{\mathcal{P}}_1\frac{\delta\hat{\mathcal{H}}_1}{\delta M},\quad M=\Phi-\nu D^4\Phi, \tag{28}$$

with

$$\hat{\mathcal{P}}_1=D(1-\nu D^4), \tag{29}$$

$$\hat{\mathcal{H}}_1=\int dx\,d\vartheta\left(\frac{\kappa_1}{2}\Phi D\Phi-\frac{\kappa_2}{2}D^2\Phi D^3\Phi-\frac{1}{2}\Phi(D\Phi)^2+\frac{1}{4}\gamma_3\Phi(D^3\Phi)^2+\frac{1}{4}(\gamma_2-2\gamma_3)(D\Phi)^2D^4\Phi\right). \tag{30}$$

Since the KdV reduction of (27) (with $\kappa_1=\gamma_2=\gamma_3=0$) is not believed to be integrable, we have not explored this class of systems further.

In a similar fashion, we may look for choices of parameter sets for which the geodesic flows of Sec. II are also supersymmetric. Comparing (13) with (25), we see that the choice $\{\mu=\nu,\ \alpha=1\ ,\ \kappa_1=0\}$ in the former and $\{s^2=\frac{4}{3},\ \beta_2=2\nu,\ \beta_3=\nu,\ \gamma_2=2\nu/3,\ \gamma_3=\kappa_1=0\}$ in the latter, yields the two-parameter system of supersymmetric geodesic flows:

$$\begin{aligned}u_t-\nu u_{xxt}&=\kappa_2u_{xxx}-3uu_x+2\xi\xi_{xx}+\nu(uu_{xxx}+2u_xu_{xx})+\frac{2\nu}{3}\xi_x\xi_{xxx},\\ \xi_t-\nu\xi_{xxt}&=\kappa_2\xi_{xxx}-\frac{3}{2}(u\xi)_x+\nu\left(u\xi_{xxx}+\frac{3}{2}u_x\xi_{xx}+\frac{1}{2}u_{xx}\xi_x\right).\end{aligned} \tag{31}$$

We shall call this system, with $\kappa_2=0$ and $\nu\neq0$, the *supersymmetric Camassa–Holm equation* (super-CH). The system (31) reduces to super-KdV, upon setting ν to zero, and to CH, upon setting ξ to zero and translating u.

Not surprisingly, the systems (31) arise as geodesic flows precisely when the metric (9) on the NSR superconformal algebra is supersymmetric. Then, the calculations of Sec. II can be performed using superfields. Specifically, writing $\mathcal{U}=u+\vartheta\phi$ and $\mathcal{V}=v+\vartheta\psi$, the bracket (8) takes the form

$$[(\mathcal{U},a)\,,(\mathcal{V},b)]=\left(\mathcal{U}D^2\mathcal{V}-\mathcal{V}D^2\mathcal{U}+\frac{1}{2}D\mathcal{U}D\mathcal{V},c_1\int dx\,d\vartheta\,D^2\mathcal{U}D^3\mathcal{V}\right), \tag{32}$$

and the inner product (9) may be written as

$$\langle(\mathcal{U},a)\,,(\mathcal{V},b)\rangle=\int dx\,d\vartheta(\mathcal{U}D^{-1}\mathcal{V}+\nu D^2\mathcal{U}D\mathcal{V})+ab. \tag{33}$$

The superspace bilinear operator $\hat{B}$ is given by $\hat{B}((\mathcal{U},a),(\mathcal{V},b))=(\hat{B}_0,0)$, where $\hat{B}_0$ satisfies

$$(1-\nu D^4)D^{-1}\hat{B}_0=c_1aD^5\mathcal{V}-\tfrac{3}{2}D^2\mathcal{V}(1-\nu D^4)D^{-1}\mathcal{U}-\tfrac{1}{2}D\mathcal{V}(1-\nu D^4)\mathcal{U}-\mathcal{V}(1-\nu D^4)D\mathcal{U}. \tag{34}$$

Writing $c_1a=\kappa_2$ and $\mathcal{U}=D\Phi$, the geodesic flows $(\mathcal{U}_t,a_t)=\hat{B}((\mathcal{U},a),(\mathcal{U},a))$ yield

$$(1-\nu D^4)\Phi_t=\kappa_2D^6\Phi-\tfrac{3}{2}(\Phi D^3\Phi+D\Phi D^2\Phi)+\nu(D\Phi D^6\Phi+\tfrac{1}{2}D^2\Phi D^5\Phi+\tfrac{3}{2}D^3\Phi D^4\Phi). \tag{35}$$

We thus recover the subsystem of (24) having component content (31). Equation (35) has a superfield Hamiltonian formulation,

$$M_t=\hat{\mathcal{P}}_2\frac{\delta\hat{\mathcal{H}}_2}{\delta M},\quad M=\Phi-\nu D^4\Phi, \tag{36}$$

with

$$\hat{\mathcal{P}}_2=\kappa_2 D^5-\tfrac{1}{2}DMD-D^2M-MD^2, \tag{37}$$

$$\hat{\mathcal{H}}_2=\frac{1}{2}\langle(D\Phi,0)\,,(D\Phi,0)\rangle=\frac{1}{2}\int dx\,d\vartheta\Phi DM. \tag{38}$$

V. PAINLEVÉ INTEGRABILITY OF SUPER-CH SYSTEMS

In this section we investigate, in more detail, the supersymmetric geodesic flow (31) with $\nu=1$ and $\kappa_2=0$,

$$\begin{aligned} m_t&=-2mu_x-um_x+2\eta\xi+\tfrac{2}{3}\eta_x\xi_x,\quad m=u-u_{xx},\\ \eta_t&=-\tfrac{3}{2}\eta u_x-\tfrac{1}{2}m\xi_x-u\eta_x,\quad \eta=\xi-\xi_{xx}. \end{aligned} \tag{39}$$

We shall consider the two simplest possible choices for the Grassmann algebra in which the fields are valued, viz. algebras with one or two odd generators. Taking the algebra to be finite dimensional is a very convenient tool for preliminary investigations of systems with Grassmann algebra-valued fields. Manton[17] recently studied some simple supersymmetric classical mechanical systems in this way and he introduced the term ''deconstruction'' to denote a component expansion in a Grassmann algebra basis. In Ref. 18 we investigate fermionic extensions of KdV in a similar fashion.

A. First deconstruction of super-CH

We first consider the super-CH system (39) with fields taking values in the simplest Grassmann algebra with basis $\{1,\tau\}$, where τ is a single fermionic generator. In this case the fermionic fields may be expressed as $\xi=\tau\xi_1$, $\eta=\tau\eta_1$, where ξ_1 and η_1 are standard (i.e., commuting, c-number) functions, as are u and m in this simple case. Since $\tau^2=0$, the fermionic bilinear terms do not contribute and we are left with the system

$$\begin{aligned} m_t&=-2mu_x-um_x,\quad m=u-u_{xx},\\ \eta_{1t}&=-\tfrac{3}{2}\eta_1u_x-\tfrac{1}{2}m\xi_{1x}-u\eta_{1x},\quad \eta_1=\xi_1-\xi_{1xx}. \end{aligned} \tag{40}$$

Further analysis is simplified by changing coordinates as described in Ref. 19. Writing $m=p^2$, the first equation of (40) takes the form $p_t=(-pu)_x$, which suggests new coordinates y_0,y_1 defined via

$$dy_0=p\,dx-pu\,dt,\quad dy_1=dt, \tag{41}$$

or dually, via

$$\frac{\partial}{\partial x}=p\frac{\partial}{\partial y_0},\quad \frac{\partial}{\partial t}=\frac{\partial}{\partial y_1}-pu\frac{\partial}{\partial y_0}. \tag{42}$$

Implementing this coordinate change and eliminating the functions u and ξ_1, the remaining equations for p and $q\equiv\eta_1$ are

$$p^2\dot{p}''-p(\dot{p}p''+\dot{p}'p')+\dot{p}p'^2-2p^3p'-\dot{p}=0, \tag{43}$$

$$\dot{q}''-\frac{3p'}{p}\dot{q}'-\frac{3\dot{p}}{2p}q''+\left(\frac{4p'^2}{p^2}-\frac{2p''}{p}-\frac{1}{p^2}\right)\dot{q}+\left(\frac{15p'\dot{p}}{2p^2}-\frac{3\dot{p}'}{p}-\frac{p}{2}\right)q'$$
$$+3\left(\frac{\dot{p}p''+2p'\dot{p}'}{p^2}-\frac{4\dot{p}p'^2}{p^3}-p'\right)q=0. \tag{44}$$

Here the dot and prime denote differentiations with respect to y_1 and y_0, respectively. We note: (a) thanks to supersymmetry (26), if p is a solution of (43), then $q=p^2$ is a solution of (44); and (b) under the substitution $q=p^{3/2}r$, (44) takes the substantially simpler form

$$\dot{r}''+\left(\frac{p'^2}{4p^2}-\frac{p''}{2p}-\frac{1}{p^2}\right)\dot{r}-\frac{p}{2}r'-\frac{3p'}{4}r=0. \tag{45}$$

The system (43), (44) passes the WTC Painlevé test.

Proof: Equation (43) is a rescaled version of the Associated Camassa–Holm equation of Ref. 19. The consideration of solutions with $p(y_0,y_1)\sim p_0(y_0,y_1)\phi(y_0,y_1)^n$ near $\phi(y_0,y_1)=0$, for some $n\neq 0$, yields $n=-2$ or $n=1$ as the possible leading orders of Laurent series solutions. We need to perform the WTC Painlevé test[20] for both these types of series. The first type, namely, Laurent series solutions exhibiting double poles on the singular manifold $\phi(y_0,y_1)=0$, have already been considered in Ref. 21. These take the form

$$p=\frac{2\phi'\dot{\phi}}{\phi^2}-\frac{\dot{\phi}'}{\phi}+p_2+p_3\phi+p_4\phi^2+\ldots, \tag{46}$$

where ϕ,p_2,p_4 are arbitrary functions of y_0,y_1, and

$$p_3=\frac{-1}{2\phi'^2\dot{\phi}^2}(\phi'^2\dot{\phi}\dot{p}_2+\phi'\dot{\phi}^2p_2'-(\phi'^2\ddot{\phi}-2\phi'\dot{\phi}\dot{\phi}'+\phi''\dot{\phi}^2)p_2$$
$$-(\phi'\dot{\phi}\ddot{\phi}''-\phi'\ddot{\phi}\dot{\phi}''-\dot{\phi}\phi''\ddot{\phi}'+\ddot{\phi}\phi''\dot{\phi}')). \tag{47}$$

We have, at present, no explanation of the remarkable symmetry of these expressions under interchange of the independent variables. The second type of solutions have a simple zero on the singular manifold $\phi(y_0,y_1)=0$. They take the form

$$p=\pm\frac{\phi}{\phi'}+p_2\phi^2+p_3\phi^3+\ldots, \tag{48}$$

where ϕ,p_2,p_3 are arbitrary functions. The verification of the consistency of both these types of expansions is straightforward. This completes the WTC test for Eq. (43).

It remains to look at Eq. (44). Although linear in q, it is *not* automatically Painlevé. The movable poles and zeros in p give rise to movable poles in the coefficient functions of the linear equation for q, and we need to examine the resulting singularities of q. If p has a pole on $\phi=0$, then near $\phi=0$ we have $p\sim 2\dot{\phi}\phi'/\phi^2$, and Eq. (44) takes the form

$$\dot{q}''+\left(\frac{6\phi'}{\phi}+\ldots\right)\dot{q}'+\left(\frac{3\dot{\phi}}{\phi}+\ldots\right)q''+\left(\frac{4\phi'^2}{\phi^2}+\ldots\right)\dot{q}+\left(\frac{11\phi'\dot{\phi}}{\phi^2}+\ldots\right)q'+\left(O\left(\frac{1}{\phi^2}\right)\right)q=0.$$

Thus the equation has a solution with $q\sim\phi^n$ if $n(n-1)(n-2)+9n(n-1)+15n=0$, giving $n=-4,-2,0$. It follows that in the case when p is given by the series (46), no inconsistencies will arise near the double poles of p if (44) has a series solution of the form

$$q=\frac{q_0}{\phi^4}+\frac{q_1}{\phi^3}+\frac{q_2}{\phi^2}+\frac{q_3}{\phi}+q_4+\ldots, \tag{49}$$

with q_0, q_2, q_4 arbitrary. The consistency of such a solution can easilly be verified using a symbolic manipulator. Using MAPLE we find that

$$q_1 = \frac{2\phi'' q_0 - \phi' q_0'}{\phi'^2}. \tag{50}$$

The explicit expression for q_3 is too lengthy to be given here.

Suppose now that p has a zero on $\phi = 0$. Near this, $p \sim \pm \phi/\phi'$ and Eq. (44) has the structure

$$\dot{q}'' - \left(\frac{3\phi'}{\phi} + \ldots\right)\dot{q}' - \left(\frac{3\dot{\phi}}{2\phi} + \ldots\right)q'' + \left(\frac{3\phi'^2}{\phi^2} + \ldots\right)\dot{q} + \left(\frac{15\phi'\dot{\phi}}{2\phi^2} + \ldots\right)q' - \left(\frac{12\phi'^2\dot{\phi}}{\phi^3} + \ldots\right)q = 0.$$

Thus (44) has a solution with $q \sim \phi^n$ if $n(n-1)(n-2) - \frac{9}{2}n(n-1) + \frac{21}{2}n - 12 = 0$, giving $n = \frac{3}{2}, 2, 4$. The appearance of a half-integer here is not considered a violation of the Painlevé test (see, e.g., Ref. 22). The half-integer value of n gives rise to a series solution of (44), near a zero of p, of the form

$$q = q_0\phi^{3/2} + q_1\phi^{5/2} + q_2\phi^{7/2} + \ldots, \tag{51}$$

with q_0 arbitrary, and $q_1, q_2, \ldots$ determined by q_0 [and the arbitrary functions arising in the series (48) for p]. The two integer values of n tell us that we need to check the consistency of solutions of (44) taking the form

$$q = Q_0\phi^2 + Q_1\phi^3 + Q_2\phi^4 + \ldots, \tag{52}$$

with two arbitrary functions Q_0 and Q_2. This is indeed consistent; using MAPLE we obtain

$$Q_1 = \pm 2\phi' Q_0 p_2 - \frac{1}{3\phi'^2\dot{\phi}}(2\phi'^2\dot{Q}_0 + 2\phi''\dot{\phi}Q_0 + \phi'\dot{\phi}Q_0' + 4\phi'\dot{\phi}'Q_0), \tag{53}$$

with the choice of $\pm$ depending on the choice in (48). The general solution of (44) near a zero of p, with three arbitrary functions, is a linear combination of the series (51) and (52). Thus the system (43), (44) passes the WTC test. □

The WTC test is evidence for the complete integrability of the system (43), (44). This in turn suggests that super-CH indeed has some integrable content.

B. Second deconstruction of super-CH

We now consider the system (39) with fields taking values in a Grassmann algebra with two anticommuting fermionic generators, τ_1, τ_2. Expanding in the basis $\{1, \tau_1, \tau_2, \tau_1\tau_2\}$,

$$\begin{aligned} u &= u_0 + \tau_1\tau_2 u_1, \quad \xi = \tau_1\xi_1 + \tau_2\xi_2, \\ m &= m_0 + \tau_1\tau_2 m_1, \quad \eta = \tau_1\eta_1 + \tau_2\eta_2, \end{aligned} \tag{54}$$

where the functions $u_0, u_1, m_0, m_1, \xi_1, \xi_2, \eta_1, \eta_2$ are all standard, we obtain the system

$$m_{0t} = -2m_0u_{0x} - u_0m_{0x}, \quad m_0 = u_0 - u_{0xx}, \tag{55}$$

$$\eta_{it} = -\tfrac{3}{2}u_{0x}\eta_i - \tfrac{1}{2}m_0\xi_{ix} - u_0\eta_{ix}, \quad \eta_i = \xi_i - \xi_{ixx}, \quad i = 1,2, \tag{56}$$

$$\begin{aligned} m_{1t} = &-2m_1u_{0x} - 2m_0u_{1x} - u_0m_{1x} - u_1m_{0x} \\ &+ 2(\eta_1\xi_2 - \eta_2\xi_1) + \tfrac{2}{3}(\eta_{1x}\xi_{2x} - \eta_{2x}\xi_{1x}), \quad m_1 = u_1 - u_{1xx}. \end{aligned} \tag{57}$$

Supersymmetry (26) tells us that given a solution u_0, m_0 of (55), we can solve the remaining equations by taking $\xi_i = \alpha_i u_0$, $\eta_i = \alpha_i m_0$ $(i=1,2)$, $u_1 = \beta u_{0x}$ and $m_1 = \beta m_{0x}$, where $\alpha_1, \alpha_2, \beta$ are arbitrary constants.

We handle the system (55)–(57) following the procedure of the previous section. Writing $m_0 = p^2$ and changing coordinates to y_0, y_1, the system can be written as

$$u_0' = \left(\frac{1}{p}\right)^{\cdot}, \quad u_0 = p^2 - p\left(\frac{\dot{p}}{p}\right)', \tag{58}$$

$$\xi_i' = \frac{3\eta_i \dot{p}}{p^4} - \frac{2\dot{\eta}_i}{p^3}, \quad \xi_i = \eta_i + p\left(\frac{3\eta_i \dot{p}}{p^3} - \frac{2\dot{\eta}_i}{p^2}\right)', \quad i=1,2, \tag{59}$$

$$\left(\frac{m_1}{p^2}\right)^{\cdot} = -(2u_1 p)' + \left(\frac{8(\dot{\eta}_1\eta_2 - \dot{\eta}_2\eta_1)}{3p^3}\right)' + \left(\frac{4(\eta_1'\eta_2 - \eta_2'\eta_1)}{3p^3}\right)^{\cdot},$$
$$m_1 = u_1 - p(pu_1')'. \tag{60}$$

Applying the WTC Painlevé test to this is a mammoth task, so instead we consider the Galilean-invariant reduction and apply the Painlevé test at this level. The Galilean-invariant reduction is obtained, as usual, by restricting all functions to depend on the single variable $z = y_0 - v y_1$ alone. Evidently the first equations of both (58) and (60) can be integrated once immediately. Then eliminating u_0 from (58), ξ_i from (59) and m_1 from (60), we obtain

$$\left(\frac{p'}{p}\right)' = -\frac{p}{v} + \frac{c_1}{p} - \frac{1}{p^2}, \tag{61}$$

$$\eta_i''' - \frac{9p'}{2p}\eta_i'' + \left(\frac{11p}{2v} - \frac{5c_1}{p} + \frac{4}{p^2} + \frac{13p'^2}{2p^2}\right)\eta_i' - \frac{3p'}{p}\left(\frac{2p}{v} - \frac{3c_1}{p} + \frac{3}{p^2} + \frac{p'^2}{p^2}\right)\eta_i = 0, \quad i=1,2, \tag{62}$$

$$u_1'' + \frac{p'}{p}u_1' + \left(\frac{2p}{v} - \frac{1}{p^2}\right)u_1 = d_1 + \frac{4}{p^3}(\eta_1\eta_2' - \eta_2\eta_1'), \tag{63}$$

where c_1, d_1 are integration constants. The equation for $p(z)$ may be integrated again after multiplying both sides by p'/p; this gives

$$p'^2 = 1 - 2c_1 p + c_2 p^2 - \frac{2}{v}p^3, \tag{64}$$

where c_2 is another integration constant. This equation is well known in KdV theory. Its general solution can be written in terms of the Weierstrass $\wp$-function,

$$p(z) = -2v\wp(z) + \tfrac{1}{6}c_2 v, \tag{65}$$

where the periods of $\wp$ are determined by the coefficients c_1, c_2, v. Using (64), the coefficients in (62) can be simplified. Further, we know from supersymmetry that this equation has a solution $\eta_i = p^2$. Substituting $\eta_i = p^2 q_i$ the equation becomes a second order equation for q_i':

$$q_i''' + \frac{3p'}{2p}q_i'' + \left(-\frac{3p}{2v} - \frac{3}{2p^2} + \frac{c_2}{2}\right)q_i' = 0, \quad i=1,2. \tag{66}$$

Supersymmetry (26) allows a reduction of the order of (63) as well. It implies that $u_1 = p'/p$, $\eta_i = p^2$ is a solution. So, writing $u_1 = rp'/p, \eta_i = p^2 q_i$ in (63) yields a first order equation for r':

$$r'' + \left(c_2 p - \frac{4p^2}{v} - \frac{1}{p}\right)\frac{r'}{p'} = \frac{p}{p'}(d_1 + 4p(q_1 q_2' - q_2 q_1')). \tag{67}$$

Multiplying by the integrating factor p'^2/p and integrating, we obtain

$$r' = \frac{p}{p'^2}\left(d_1 p + d_2 + 4\int (q_1 q_2' - q_2 q_1')pp'\, dz \right), \tag{68}$$

where d_2 is a further constant of integration.

Thus the Galilean-invariant reduction of the second deconstruction of super-CH takes the form of the three equations (64), (66), (68), to which we now apply the Painlevé test. All substitutions hitherto have been ones which do not interfere with the test. Equation (64) has movable double poles and movable simple zeros. Near a double pole at z_0, the series solution contains only even powers of $(z-z_0)$,

$$p(z) = -\frac{2v}{(z-z_0)^2} + \frac{c_2 v}{6} + \frac{12c_1 - c_2^2 v}{120}(z-z_0)^2 + \frac{\dfrac{54}{v} + c_2^3 v - 18c_1 c_2}{3024}(z-z_0)^4 + \ldots, \tag{69}$$

and near a simple zero at z_0,

$$p(z) = \pm(z-z_0) - \frac{1}{2}c_1(z-z_0)^2 \pm \frac{1}{6}c_2(z-z_0)^3 - \frac{1}{24}\left(\frac{6}{v} + c_1 c_2\right)(z-z_0)^4 + \ldots . \tag{70}$$

At both the zeros and poles of p, Eq. (66), which is just a linear third order ODE, has regular singular points. Checking the Painlevé property for this reduces to doing the necessary Frobenius–Fuchs analysis at these regular singular points to check that no logarithmic singularities in the solutions q_i arise. Finally, Eq. (68) gives an explicit formula for r involving two quadratures. Here the necessary analysis involves writing series expansions for the integrands near the zeros and poles of p, and checking for the absence of $1/(z-z_0)$ terms, which would give rise to logarithms on integration. We do not present all these calculations in detail; with the aid of a symbolic manipulator they are quite straightforward. We conclude that the Galilean-invariant reduction of the second deconstruction of super-CH has the Painlevé property.

We note, in conclusion, that two of the equations we have encountered are interesting variants of the Lamé equation: In (66), the substitution $q_i' = p^{-3/4}h_i$ yields

$$h_i'' + \frac{3}{8}\left(\frac{p}{v} - \frac{c_2}{6} + \frac{c_1}{p} - \frac{7}{2p^2}\right)h_i = 0, \tag{71}$$

and similarly, on writing $u_1 = p^{-1/2}k$, the homogeneous part of (63) takes the form

$$k'' + \left(\frac{3p}{v} - \frac{c_2}{4} - \frac{3}{4p^2}\right)k = 0. \tag{72}$$

By the arguments above, the latter is integrable by quadratures.

VI. SUPERPEAKON SOLUTIONS

As mentioned in the Introduction, one of the intriguing features of the CH equation is the existence of peakon solutions. One would hope that super-CH shares this property. However, peakon solutions are weak solutions, with a discontinuity in the first derivative; and the action of supersymmetry on such functions, for a general underlying Grassmann algebra, yields objects which are not regular enough to be considered as weak solutions. So, CH peakon solutions do not admit a general supersymmetrization. The above argument does not hold in the first deconstruction, because if there is only one fermionic generator, the supersymmetry transformation (26) does not involve an x-derivative. So such supersymmetrized peakon solutions of the super-CH system (39) do exist if the fields are restricted to take values in a Grassmann algebra with only one fermionic generator.

Consider Eqs. (40) of the first deconstruction. Supersymmetry implies that if (u,m) is a solution of the first equation in (40), then $\xi_1=cu$, $\eta_1=cm$ (where c is a constant) gives a solution of the second equation. Thus, for example, the speed v traveling-wave peakon solution of CH, $u=v\exp(-|x-vt|)$, can be supersymmetrized, as can any multipeakon solution. In fact, there also exist more general superpeakons. The superposition ansatz,

$$u(x,t)=\sum_{i=1}^{N} p_i(t)\exp(-|x-q_i(t)|), \tag{73}$$

$$\xi_1(x,t)=\sum_{i=1}^{N} r_i(t)\exp(-|x-q_i(t)|), \tag{74}$$

gives a solution of the system (40) provided the functions $q_i(t),p_i(t),r_i(t)$ $(i=1,\ldots,N)$ satisfy the ODE system,

$$q_{it}=\sum_{j=1}^{N} p_j\exp(-|q_i-q_j|), \tag{75}$$

$$p_{it}=\sum_{j=1}^{N}{}' \operatorname{sgn}(q_i-q_j)p_ip_j\exp(-|q_i-q_j|), \tag{76}$$

$$r_{it}=\frac{1}{2}\sum_{j=1}^{N}{}' \operatorname{sgn}(q_i-q_j)(p_ir_j+p_jr_i)\exp(-|q_i-q_j|), \tag{77}$$

where the primed sums range over values of $j\neq i$. Equations (75) and (76) are the conditions which determine u of the form (73) to be a multipeakon solution of CH. They describe geodesic motion on an N-dimensional surface with coordinates $q_i{}^1$ and form an integrable Hamiltonian system.[23] The further equations (77) are linear equations for the functions r_i. Clearly, taking the $r_i=cp_i$ for some constant c gives a solution, these being the supersymmetrized multipeakon solutions discussed before. *More general solutions certainly exist.* Since the system (75)–(76) is integrable, integrability of the additional N linear equations (77) depends on the existence of $N-1$ independent conserved quantities depending on the r_i. We have not settled this question in general, but we note that $\Sigma_{i=1}^{N}r_i$ is a conserved quantity, just as the total momentum $\Sigma_{i=1}^{N}p_i$ is also conserved. This suffices for integrability when $N=2$, in which case the remaining equation for r_1-r_2 can be integrated explicitly. Note that unlike the existence of the superpeakons which arise in virtue of supersymmetry transformations of CH peakons, the existence of this extra conserved quantity depends critically on the coefficients of the η_1 evolution equation in (40). Even if the full superpeakon system (77) proves not to be fully integrable, the geodesy and supersymmetry conditions have certainly picked out an equation with some integrability properties (cf. Ref. 12).

VII. OUTLOOK

In this paper we have examined fermionic extensions of the Camassa–Holm equation. In particular we have identified the super-CH system (39), which, for low dimensional Grassmann algebras displays some integrability properties and has peakon-type solutions. Further investigation is needed to determine whether the super-CH system is fully integrable.

Our work provides a further instance of integrability properties arising in the context of geodesic flows on a group manifold, and in particular provides some evidence that supersymmetric geodesic flows whose bosonic part is integrable must also be integrable.

We note in closing that the KP (and super-KP) systems have yet to be presented as geodesic flows. If such a presentation exists, it would have a bearing on the question of whether there is a KP-type higher dimensional generalization of Camassa–Holm (arising in a way similar to that in which KP generalizes KdV).

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The $A_M^{(1)}$ automata related to crystals of symmetric tensors

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A soliton cellular automaton associated with crystals of symmetric tensor representations of the quantum affine algebra $U_q'(A_M^{(1)})$ is introduced. It is a crystal theoretic formulation of the generalized box–ball system in which capacities of boxes and carriers are arbitrary and inhomogeneous. Scattering matrices of two solitons coincide with the combinatorial R matrices of $U_q'(A_{M-1}^{(1)})$. A piecewise linear evolution equation of the automaton is identified with an ultradiscrete limit of the nonautonomous discrete Kadomtsev–Petviashivili equation. A class of N soliton solutions is obtained through the ultradiscretization of soliton solutions of the latter. [DOI: 10.1063/1.1322077]

I. INTRODUCTION

The box–ball system invented by Takahashi and Satsuma[1] is an important example of soliton cellular automata. It is a discrete dynamical system in which finitely many balls move along the one-dimensional array of boxes under a certain rule. Its integrability has been proved in Ref. 2 by making a connection to the difference analog of the Lotka–Volterra equation[3] through the limiting procedure called *ultradiscretization*.

By now the original box–ball system has been generalized into several directions. First, one can introduce the balls distinguished by the index from the set $\{1,2,\ldots,M\}$. Second, one lets the box at site n accommodate up to θ_n balls, where the capacity θ_n may depend on n. Third, one can introduce a *carrier* with capacity κ_t to redefine the time evolution at time t. The carrier comes from the left and proceeds to the right, picking up the balls in a box and dropping them into another under a certain rule. While it goes through the array of boxes, the successive loading–unloading process induces the motion of balls over the boxes, hence the time evolution of the system. These generalizations of the Takahashi–Satsuma box–ball system are characterized by the parameters (M,θ_n,κ_t). ($n,\ t\in\mathbb{Z}$ play the role of space and time coordinates as in the diagram in Sec. II C.) The original one[1] corresponds to the choice $(M,\forall\,\theta_n,\forall\,\kappa_t)=(1,1,\infty)$. The case $(M,\forall\,\theta_n=1,\forall\,\kappa_t=\infty)$ was introduced in Ref. 4 and studied in Ref. 5. Similarly, the cases

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$(M=1, \forall\theta_n=\theta, \forall\kappa=\kappa)$ with $\kappa>\theta$ and $(M,\theta_n,\forall\kappa_t=\infty)$ were treated in Refs. 6 and 7, respectively. These works have been done mainly from the viewpoint of the ultradiscretization.

The purpose of this paper is to study the general (M,θ_n,κ_t) case. In Sec. II we formulate the corresponding generalization of the box–ball system in terms of the crystal theory.[8–10] The latter is a representation theory of quantum groups at $q=0$. The unexpected link between the crystals and the box–ball systems has also been exploited in Refs. 11 and 12 through a crystal theoretic interpretation of the L-operator approach.[13] The idea is to regard the box–ball system as a solvable vertex model[14] at $q=0$ under a ''ferromagnetic'' boundary condition. More concretely, the box–ball system corresponding to the data (M,θ_n,κ_t) is naturally related to the $U_q'(A_M^{(1)})$ vertex model at $q=0$ whose inhomogeneity in the quantum and auxiliary spaces is parametrized by θ_n's and κ_t's, respectively.

Let B_l be the classical crystal of $U_q'(A_M^{(1)})$ in the sense of Ref. 9 corresponding to the l-fold symmetric tensor representation of $U_q(A_M)$. Then the array of boxes and the ball configurations are identified with the elements from $\cdots\otimes B_{\theta_n}\otimes B_{\theta_{n+1}}\otimes\cdots$. The time evolution by the carrier with capacity κ_t is realized as the action of the $q=0$ row transfer matrix acting on $\cdots\otimes B_{\theta_n}\otimes B_{\theta_{n+1}}\otimes\cdots$ with the auxiliary space corresponding to B_{κ_t}. We call the resulting dynamical system the $A_M^{(1)}$ automaton. It is the most general one in the $A_M^{(1)}$ case as far as the crystals for symmetric tensors are concerned. For generalizations to other root systems, see Ref. 15 for a supersymmetric one and Ref. 11 for the nonexceptional series other than $A_M^{(1)}$.

In Sec. III we introduce solitons and study the two-soliton scattering. As in Refs. 11 and 12 we label the solitons in terms of the elements of the $U_q'(A_{M-1}^{(1)})$-crystal B_l, where l plays the role of the amplitude of a soliton. In the collisions of two solitons associated with B_l and B_k, the scattering matrix is shown to coincide with the combinatorial R matrix giving the isomorphism $B_l\otimes B_k\simeq B_k\otimes B_l$ of the $U_q'(A_{M-1}^{(1)})$ crystals. These features are essentially the same with the $\forall\theta_n=1$ case.[5,11,12] A new aspect here is that depending on the amplitudes l, k and the parameters θ_n, κ_t, the smaller soliton can overtake the larger one. This is most transparently understood by viewing the scattering from the cross channel. By interchanging θ_n and κ_t, one can swap the role of the space and time and thereby the boxes and carriers. Then the curious scattering mentioned previously reduces to the ''usual'' one in the cross channel where the larger soliton overtakes the smaller one. In Sec. III D we also give a brief sketch of the conserved quantities of our automaton following Ref. 12.

In Sec. IV we set up a piecewise linear equation for the relevant combinatorial R matrix[16] and the resulting evolution equation for the $A_M^{(1)}$ automaton. Extending the earlier result,[7] we identify the evolution equation with an ultradiscrete limit of the nonautonomous discrete Kadomtsev–Petviashivili (ndKP) equation. A class of N soliton solutions is obtained through an ultradiscretization of the τ functions. As in the previous case[7] one needs to make a fine adjustment of the fermion momenta entering the vacuum expectation value expression of the τ functions. Each soliton in the automaton is obtained by letting M solitons in the ndKP merge together in the ultradiscrete limit.

Section V is a summary. Appendices A and B contain the details of the proofs of Proposition 3.8 and Theorem 4.5, respectively.

II. AUTOMATA FROM CRYSTALS

A. $U_q'(A_M^{(1)})$ crystals

Let B_k be the classical crystal of $U_q'(A_M^{(1)})$ corresponding to the k-fold symmetric tensor representation. As a set it consists of the single row semistandard tableaux of length k on letters $\{1,2,\ldots,M+1\}$:

$$B_k=\{\boxed{m_1\cdots m_k}\mid m_i\in\{1,\ldots,M+1\}, m_1\le\cdots\le m_k\},$$

where we have omitted the $k-1$ vertical lines separating the entries. We also represent the elements by the multiplicities of their contents. Namely,

$$b = \boxed{m_1 \cdots m_k} \in B_k$$

is also denoted by $b=(x_1,x_2,\ldots,x_{M+1})$ with $x_i=\#\{l|m_l=i\}$.

Denote the Kashiwara operators of B_k by $\tilde{f}_i$ and $\tilde{e}_i$ for $i=0,1,\ldots,M$. The actions of $\tilde{e}_i$, $\tilde{f}_i$ on B_k are defined as follows: for $b=(x_1,x_2,\ldots,x_{M+1})\in B_k$,

$$\begin{cases} \tilde{e}_0 b=(x_1-1,x_2,\ldots,x_{M+1}+1), \\ \tilde{f}_0 b=(x_1+1,x_2,\ldots,x_{M+1}-1), \\ \tilde{e}_i b=(x_1,\ldots,x_i+1,x_{i+1}-1,\ldots,x_{M+1}) \quad \text{for } i=1,\ldots,M, \\ \tilde{f}_i b=(x_1,\ldots,x_i-1,x_{i+1}+1,\ldots,x_{M+1}) \quad \text{for } i=1,\ldots,M. \end{cases} \tag{1}$$

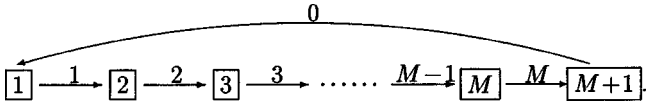
In Eq. (1), the right-hand sides are to be understood as 0 if they are not in B_k. A crystal can be regarded as a colored oriented graph called a ''crystal graph'' by defining

$$b \overset{i}{\longrightarrow} b' \leftrightarrow \tilde{f}_i b = b'.$$

Thus, for example,

$$B_1 = \{\boxed{1},\ldots,\boxed{M+1}\}$$

has the crystal graph:



Setting $\varepsilon_i(b)=\max_l\{\tilde{e}_i^{\,l}b\neq 0|l\geq 0\}$ and $\varphi_i(b)=\max_l\{\tilde{f}_i^{\,l}b\neq 0|l\geq 0\}$ for $b\in B_k$, one has

$$\varepsilon_0(b)=x_1, \quad \varepsilon_i(b)=x_{i+1} \quad \text{for } i=1,\ldots,M,$$

$$\varphi_0(b)=x_{M+1}, \quad \varphi_i(b)=x_i \quad \text{for } i=1,\ldots,M.$$

The data are necessary when we treat tensor products of the crystals. For two crystals B and B', the tensor product $B\otimes B'$ is defined. As a set,

$$B\otimes B'=\{b_1\otimes b_2|b_1\in B, b_2\in B'\}.$$

The actions of $\tilde{e}_i$ and $\tilde{f}_i$ are defined by

$$\tilde{e}_i(b_1\otimes b_2)=\begin{cases} \tilde{e}_i b_1\otimes b_2 & \text{if } \varphi_i(b_1)\geq\varepsilon_i(b_2) \\ b_1\otimes\tilde{e}_i b_2 & \text{if } \varphi_i(b_1)<\varepsilon_i(b_2) \end{cases}, \tag{2}$$

$$\tilde{f}_i(b_1\otimes b_2)=\begin{cases} \tilde{f}_i b_1\otimes b_2 & \text{if } \varphi_i(b_1)>\varepsilon_i(b_2) \\ b_1\otimes\tilde{f}_i b_2 & \text{if } \varphi_i(b_1)\leq\varepsilon_i(b_2) \end{cases}. \tag{3}$$

Here $0\otimes b$ and $b\otimes 0$ are understood to be 0. For two crystals B and B', the tensor products $B'\otimes B$ and $B\otimes B'$ constructed as shown previously are again crystals which are canonically isomorphic. The isomorphism R: $B'\otimes B\xrightarrow{\sim} B\otimes B'$ is called the combinatorial R matrix.[9,16] By the definition R commutes with $\tilde{f}_i$, $\tilde{e}_i$ for any $i=0,1,\ldots,M$. (More precisely one introduces affine crystals and the associated energy function, but in this paper we shall exclusively treat classical crystals and concern the energy function only in connection with the conserved quantities in Sec. III D).

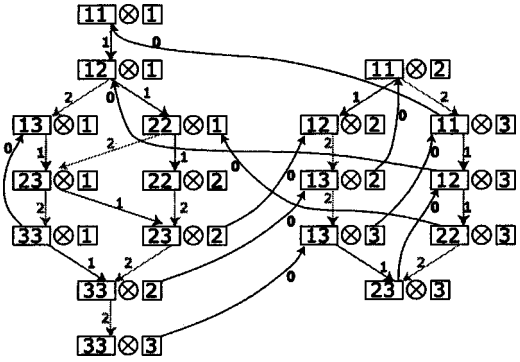


FIG. 1. Crystal graph of $U_q'(A_2^{(1)})$-crystal $B_2 \otimes B_1$.

Example 2.1: Figures 1 and 2 are the crystal graphs of $U_q'(A_2^{(1)})$-crystals $B_2 \otimes B_1$ and $B_1 \otimes B_2$, respectively.

Example 2.2: Let $B' = B_2$, $B = B_1$ of $U_q'(A_2^{(1)})$ crystals.

$$\text{(i)}\ R : \boxed{13} \otimes \boxed{2} \mapsto \boxed{1} \otimes \boxed{23},$$
$$\text{(ii)}\ R : \boxed{23} \otimes \boxed{2} \mapsto \boxed{3} \otimes \boxed{22}.$$

These are obtained by comparing the crystal graphs in Example 2.1.

We write the highest weight element in B_k with respect to $U_q(A_M)$ as u_k:

$$u_k = \overbrace{\boxed{11\ldots1}}^{k} = (k, 0, \cdots, 0) \in B_k. \tag{4}$$

B. Isomorphism

Here we give an explicit procedure to obtain the isomorphism R: $B_k \otimes B_l \to B_l \otimes B_k$ without drawing the whole crystal graphs of $B_k \otimes B_l$ and $B_l \otimes B_k$.

Let $b_1 \otimes b_2$ be an element in $B_k \otimes B_l$ such as $b_1 = (x_1, \ldots, x_{M+1})$ and $b_2 = (y_1, \ldots, y_{M+1})$. We represent $b_1 \otimes b_2$ by the two-column diagram. Each column has $M+1$ rows, enumerated as 1 to $M+1$ from the top to the bottom. We put x_i (respectively y_i) dots $\bullet$ in the ith row of the left

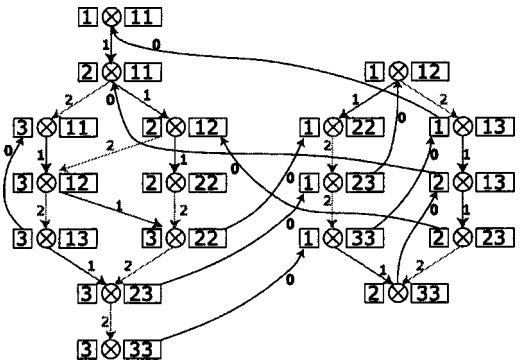
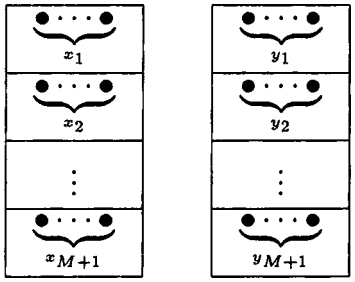


FIG. 2. Crystal graph of $U_q'(A_2^{(1)})$-crystal $B_1 \otimes B_2$.

(respectively right) column.

$b_1 \otimes b_2 =$ 

Proposition 2.3: The rule to obtain the isomorphism R is as follows.

(1) Assume $k \geqslant l$ (respectively, $k \leqslant l$). Pick any dot, say $\bullet_a$, in the right (respectively, left) column and find its partner $\bullet'_a$ in the left (respectively, right) column. The $\bullet'_a$ is chosen from the dots which are in the lowest (respectively, highest) row among all dots whose positions are higher (respectively, lower) than that of $\bullet_a$. If there is no such dot, we return to the bottom (respectively, top) and the partner $\bullet'_a$ is chosen from the dots in the lowest (respectively, highest) row among all dots. Connect $\bullet_a$ and $\bullet'_a$ by a line. We call the lines in the latter case winding and in the former case unwinding.

(2) Repeat procedure (1) for the remaining unconnected dots $(l-1)$ times [respectively, $(k-1)$ times].

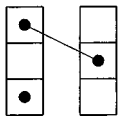
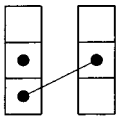
(3) The isomorphism R is obtained by sliding the remaining $(k-l)$ [respectively, $(l-k)$] unpaired dots in the left (respectively, right) column to the right (respectively, left).

The *R* obtained by this rule has the correct property as the isomorphism. This fact has been proved in Sec. III of Ref. 16. We will write the relation *R*: $u \otimes v \mapsto v' \otimes u'$ also as $u \otimes v \simeq v' \otimes u'$. Obviously one has

$$u_k \otimes u_l \simeq u_l \otimes u_k \tag{5}$$

for the element (4).

Example 2.4: Let $M=2$, $k=2$, $l=1$. Examples 2.2 (i) and 2.2 (ii) are obtained by the following diagrams:

(i)  , (ii)  .

The line in (i) is unwinding and that in (ii) is winding.

Suppose $b \otimes b' \in B \otimes B'$ is mapped to $\tilde{b}' \otimes \tilde{b} \in B' \otimes B$ under the isomorphism $B \otimes B' \simeq B' \otimes B$ of $U'_q(A_M^{(1)})$ crystals. A $\mathbb{Z}$-valued function H on $B \otimes B'$ is called an *energy function* if for any i and $b \otimes b' \in B \otimes B'$ such that $\tilde{e}_i(b \otimes b') \neq 0$, it satisfies

$$\begin{aligned} H(\tilde{e}_i(b \otimes b')) &= H(b \otimes b') + 1 \quad \text{if } i=0, \varphi_0(b) \geqslant \varepsilon_0(b'), \varphi_0(\tilde{b}') \geqslant \varepsilon_0(\tilde{b}) \\ &= H(b \otimes b') - 1 \quad \text{if } i=0, \varphi_0(b) < \varepsilon_0(b'), \varphi_0(\tilde{b}') < \varepsilon_0(\tilde{b}) \\ &= H(b \otimes b') \quad \text{otherwise.} \end{aligned} \tag{6}$$

When we want to emphasize $B \otimes B'$, we write $H_{BB'}$ for H. This definition of the energy function is due to (3. 4. e) of Ref. 16, that is a generalization of the definition for the $B=B'$ case in Ref. 9. The energy function is unique up to additive constant, since $B \otimes B'$ is connected. By definition, $H_{BB'}(b \otimes b') = H_{B'B}(\tilde{b}' \otimes \tilde{b})$. Throughout this paper we normalize it as

$$H_{B_l B_k}(u_l \otimes u_k) = 0, \tag{7}$$

irrespective of $l<k$ or $l\geqslant k$. Then it is the result of Ref. 16 that the energy function is (-1) times the number of unwinding lines in the sense of Example 2.4.

With a successive application of R's, one interchanges the order of tensor product pairwise and obtains the isomorphism of $B_{k_1}\otimes\cdots\otimes B_{k_n}$ and $B_{k_{P_1}}\otimes\cdots\otimes B_{k_{P_n}}$ for any permutation P. The compatibility of this construction is guaranteed by the Yang–Baxter equation obeyed by R. The following assertion follows easily from Proposition 2.3.

Proposition 2.5: Let $k_1,k_2,\ldots\in\mathbb{Z}_{\geqslant 1}$ be any sequence. Suppose $b\otimes u_{k_1}\otimes\cdots\otimes u_{k_n}\simeq c_1\otimes\cdots\otimes c_n\otimes b'$ is valid for some b' and c_i's under the isomorphism $B_l\otimes B_{k_1}\otimes\cdots\otimes B_{k_n}\simeq B_{k_1}\otimes\cdots\otimes B_{k_n}\otimes B_l$. For any $b\in B_l$, there exists n_0 such that $b'=u_l$ for all $n\geqslant n_0$.

This property will be needed in constructing the automation in Sec. II C.

C. Automaton

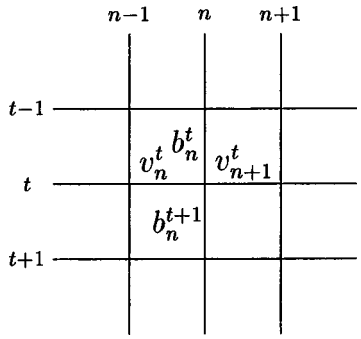
Let $\ldots,\theta_{-1},\theta_0,\theta_1,\ldots$ and $\ldots,\kappa_{-1},\kappa_0,\kappa_1,\ldots$ be two sequences of positive integers. Denote the former indices by n, and the latter indices by t. Consider the two-dimensional lattice with n and t directions,

$$n \text{ direction} \quad \cdots\otimes B_{\theta_{n-1}}\otimes B_{\theta_n}\otimes B_{\theta_{n+1}}\otimes\cdots,$$

$$t \text{ direction} \quad \cdots\otimes B_{\kappa_{t-1}}\otimes B_{\kappa_t}\otimes B_{\kappa_{t+1}}\otimes\cdots.$$

In terms of the box–ball systems, θ_n is the capacity of the nth box, and κ_t is the capacity of the tth carrier.

Draw t-constant lines horizontally, and n-constant lines vertically. Number the former downward, and the latter to the right. At any horizontal or vertical line segment of the lattice, we inscribe an element of the crystals in the following way. At the point labeled by (t, n), we put $b_n^t\in B_{\theta_n}$ on the upper line segment and $v_n^t\in B_{\kappa_t}$ on the left line segment. Thus we have $b_n^{t+1}\in B_{\theta_n}$ on the lower line segment and $v_{n+1}^t\in B_{\kappa_t}$ on the right line segment.



We impose the condition that they are related by the combinatorial R matrix,

$$R: v_n^t\otimes b_n^t\tilde{\mapsto} b_n^{t+1}\otimes v_{n+1}^t. \tag{8}$$

In the following sections, we consider the time evolution of the system downward. In view of Proposition 2.5 we can and will exclusively consider the case where for any t, $b_n^t\neq u_{\theta_n}$ only for finitely many n's and similarly for any n, $v_n^t\neq u_{\kappa_t}$ only for finitely many t's. Sometimes we ignore v_n^t's and display the time evolution of the system only with the arrays

$$\cdots\ b_{-2}^0\ b_{-1}^0\ b_0^0\ b_1^0\ b_2^0\ \cdots,$$

$$\cdots\ b_{-2}^1\ b_{-1}^1\ b_0^1\ b_1^1\ b_2^1\ \cdots,$$

$$\cdots\ b_{-2}^2\ b_{-1}^2\ b_0^2\ b_1^2\ b_2^2\ \cdots.$$

In short, the evolution of the array $\{b_n^t\}$ to $\{b_n^{t+1}\}$ is determined by

$$B_{\kappa_t}\otimes(\cdots\otimes B_{\theta_n}\otimes B_{\theta_{n+1}}\otimes\cdots)\simeq(\cdots\otimes B_{\theta_n}\otimes B_{\theta_{n+1}}\otimes\cdots)\otimes B_{\kappa_t},$$

$$u_{\kappa_t}\otimes(\cdots\otimes b_n^t\otimes b_{n+1}^t\otimes\cdots)\simeq(\cdots\otimes b_n^{t+1}\otimes b_{n+1}^{t+1}\otimes\cdots)\otimes u_{\kappa_t},$$

under the successive applications of the combinatorial R matrices R: $B_{\kappa_t}\otimes B_{\theta_j}\overset{\sim}{\mapsto}B_{\theta_j}\otimes B_{\kappa_t}$.

Setting $\mathbf{p}=\cdots\otimes b_n^t\otimes b_{n+1}^t\otimes\cdots$, we denote the time evolution induced by u_{κ_t} as above by $T_{\kappa_t}(\mathbf{p})=\cdots\otimes b_n^{t+1}\otimes b_{n+1}^{t+1}\otimes\cdots$. Obviously the time evolutions are invertible, and due to (5) they are commutative,

$$T_\kappa T_{\kappa'}=T_{\kappa'}T_\kappa. \tag{9}$$

In the rest of the paper, the two-dimensional lattice on which the automaton is defined should be appropriately understood either as large but finite or formally infinite depending on the situation.

The following observation will turn out to be useful in the sequel.

Remark 2.6: Interchanging the role of ''space'' and ''time,'' one can view (8) *as the evolution of the array* $\cdots\otimes v_{n+1}^{t+1}\otimes v_{n+1}^t\otimes v_{n+1}^{t-1}\otimes\cdots$ *to the left as*

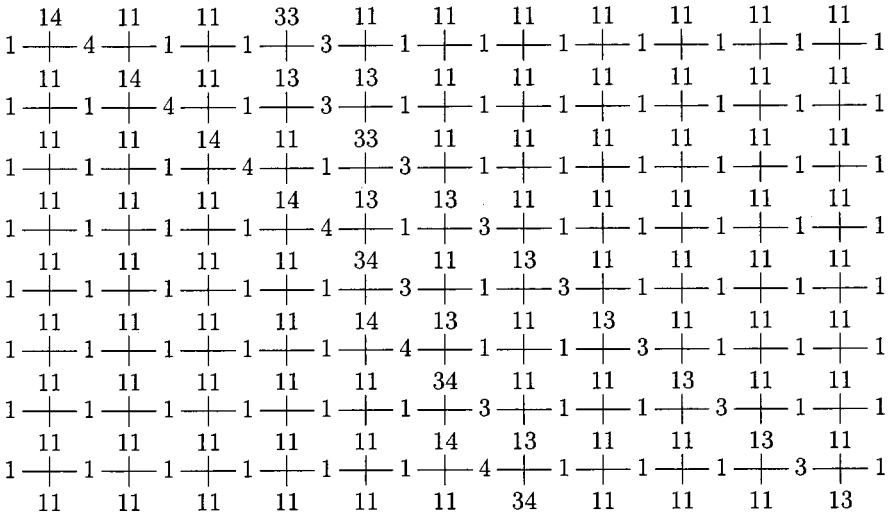
$$T_{\theta_n}(\cdots\otimes v_{n+1}^{t+1}\otimes v_{n+1}^t\otimes v_{n+1}^{t-1}\otimes\cdots)=\cdots\otimes v_n^{t+1}\otimes v_n^t\otimes v_n^{t-1}\otimes\cdots.$$

Example 2.7: Let $M=3$, $\forall\,\theta_n=1$, and $\forall\,\kappa_t=\infty$,

$$\begin{aligned}
&\cdots11114211311111111111\cdots\\
&\cdots11111142131111111111\cdots\\
&\cdots11111114231111111111\cdots\\
&\cdots11111111124311111111\cdots\\
&\cdots11111111112143111111\cdots\\
&\cdots11111111111211431111\cdots
\end{aligned}$$

where i denotes $\boxed{i}$. This is a typical two-soliton scattering. One can see that a soliton with amplitude l moves to the right with velocity l if separated sufficiently. Hence the larger solitons overtake the smaller ones. (See Sec. III A for the precise definition of the solitons and their amplitude.)

Example 2.8: Let $M=3$, $\forall\,\theta_n=2$, and $\forall\,\kappa_t=1$.



Here i and ij denote $\boxed{i}$ and $\boxed{ij}$, respectively. We have depicted both variables $\{b^t_n\}$ and $\{v^t_n\}$. This time 14 on the top left is the smaller soliton and 33 or $13\otimes 13$ is the larger soliton. Thus in terms of the $\{b^t_n\}$ variable, the smaller one overtakes the larger one as we go down the figure ending with the solitons 34 and 13. This is an opposite feature from the previous example. However in the space–time interchanged picture (Remark 2.6), it reduces to the situation similar to Example 2.7. Namely, in terms of the $\{v^t_n\}$ variable, the larger soliton overtakes the small one as $\ldots 43\ldots 3\ldots \to \ldots 4\ldots 33$, as we trace the diagram from the right to the left.

D. Equivalence with box–ball systems

Our $A^{(1)}_M$ automaton can be viewed as a generalized box–ball system. One interprets the letter 1 in the tableaux as an empty space and the other letters $2\leqslant i\leqslant M+1$ as the balls with index $M+2-i$. The element b^t_n signifies the balls contained in the nth box with capacity θ_n at time t. Similarly v^t_n stands for the carrier with capacity κ_t. Then (8) tells that through the loading–unloading process, the box and the carrier change into b^{t+1}_n and v^t_{n+1}, respectively. Sending the carrier through to the left, one has the time evolution of the box–ball state $\cdots\otimes b^t_n\otimes b^t_{n+1}\otimes\cdots$ into $\cdots\otimes b^{t+1}_n\otimes b^{t+1}_{n+1}\otimes\cdots$. For a concrete rule describing (8) in terms of the box–ball terminology, see the *BBS scattering rule* in Ref. 5. Relation (8) will also be expressed as a piecewise linear equation in Proposition 4.1.

When $\forall\,\kappa_t=\infty$ we claim that the evolution of $\{b^t_n\}$ in our $A^{(1)}_M$ automaton is equivalent to the box–ball system studied in Ref. 7 under the above-stated translation. In the latter the one-dimensional array of boxes with capacities $\ldots,\theta_{n-1},\theta_n,\theta_{n+1},\ldots$ accommodate the balls with an index from the set $\{1,\ldots,M\}$. The dynamics of the balls in each time step is governed by the following rules.[7]

(1) Move every ball only once.
(2) Move the leftmost ball with index 1 to the nearest right box with space.
(3) Move the leftmost ball with index 1 among the rest to its nearest right box with space.
(4) Repeat this procedure until all of the balls with index 1 are moved.
(5) Do the same procedure (2)–(4) for the balls with index 2.
(6) Repeat this procedure successively until all of the balls with index M are moved.

If the ball with some index is absent, one just proceeds to those with the next index. A box with space means the one that contains strictly fewer balls than its capacity. If a box contains more than one ball with the same index and they are not yet moved at an instant during the procedure, one

may pick any one of them when looking for the leftmost one. The equivalence to our automaton with $\forall \kappa_t \to \infty$ is shown by the fact that both lead to the same evolution equation, which is given from Proposition 4.1 under the said limit.

The above-mentioned rule tells that the time evolution T_∞ in our automation admits the following factorization:

$$T_\infty = \tilde{T}_M \cdots \tilde{T}_2 \tilde{T}_1, \tag{10}$$

where $\tilde{T}_j$ moves the balls with index j only, and we identify the left-hand side with the corresponding operator acting on the box–ball systems.

For later convenience we introduce the *canonical system* following Ref. 5. We keep assuming $\forall \kappa_t = \infty$ and stay in the description in terms of the box–ball system rather than crystals until the end of this section. Thus we identify $b \in B_\theta$ with the capacity θ box containing the balls as specified before. Suppose a state $\mathbf{p} = \cdots \otimes b_n \otimes b_{n+1} \otimes \cdots$ contains J balls in total. Then the action of $\tilde{T}_M \cdots \tilde{T}_2 \tilde{T}_1$ consists of J steps, each of which is to move a certain ball. To a ball to be moved in the jth step ($1 \leqslant j \leqslant J$), we assign a *signature* j. The assignment is unique up to the trivial freedom among the commonly indexed balls within the same boxes. Let $c(\mathbf{p})$ be the ball configurations obtained from $\mathbf{p}$ just by regarding the signatures as new indices. It consists of the same array of the boxes and J balls as before but with the new distinct index from 1 to J. One can still let $c(\mathbf{p})$ evolve under the previously stated rules (1)–(6) by replacing M therein with J. The resulting new box–ball system is called the canonical system. By a close inspection of rules (1)–(6), it is not difficult to confirm the commutativity:

$$c(\tilde{T}_M \cdots \tilde{T}_2 \tilde{T}_1(\mathbf{p})) = \tilde{T}_J \cdots \tilde{T}_2 \tilde{T}_1(c(\mathbf{p})). \tag{11}$$

In this sense the canonical system essentially grasps the time development pattern of the original one. This fact, first recognized in Ref. 5 for $\forall \theta_n = 1$, will be utilized in Appendix A.

III. COMBINATORIAL *R* MATRIX AS SCATTERING MATRIX OF ULTRADISCRETE SOLITONS

Here we prove Theorem 3.10, which identifies the scattering matrix of the ultradiscrete solitons with the combinatorial R matrix of $U'_q(A^{(1)}_{M-1})$.

A. Solitons

Let B'_k be the classical crystal of $U'_q(A^{(1)}_{M-1})$ corresponding to the k-fold symmetric tensor representation:

$$B'_k = \{\boxed{m_1 \cdots m_k} \mid m_i \in \{1, \ldots, M\}, m_1 \leq \cdots \leq m_k\}.$$

Denote the Kashiwara operators of B'_k by $\tilde{f}'_i$ and $\tilde{e}'_i$ for $i = 0,1, \ldots, M-1$. For distinction, from now on we use the notation $B_k, \tilde{f}_i, \tilde{e}_i$ for $U'_q(A^{(1)}_M)$ crystals and $B'_k, \tilde{f}'_i, \tilde{e}'_i$ for $U'_q(A^{(1)}_{M-1})$ crystals. Let R and R' be the combinatorial R matrices for $U'_q(A^{(1)}_M)$ and $U'_q(A^{(1)}_{M-1})$, respectively. Thus $R\tilde{f}_i = \tilde{f}_i R$ and $R'\tilde{f}'_i = \tilde{f}'_i R'$ hold when they act on the tensor product of two crystals, and similarly for $\tilde{e}_i, \tilde{e}'_i$. (We will specify the crystals that they act on each time.)

Remark 3.1: When $M = 1$ we still define B'_k as above, which is the set with the single element

$$u_k = \boxed{1 \ldots 1}.$$

We further understand that the "$U'_q(A^{(1)}_0)$" combinatorial R matrix $R' : B'_l \otimes B'_k \to B'_k \otimes B'_l$ is given by $R'(u_l \otimes u_k) = u_k \otimes u_l$.

For each $k \in \mathbb{Z}_{\geqslant 1}$ define a map $\imath_k$ by

$$\begin{array}{rccc} \imath_k: & B'_k & \longrightarrow & (B_1)^{\otimes k} \\ & \boxed{m_1 \cdots m_k} & \mapsto & \boxed{m_k+1} \otimes \cdots \otimes \boxed{m_1+1}. \end{array}$$

Let $k_1, \ldots, k_N \in \mathbb{Z}_{\geqslant 1}$ and $L_0, \ldots, L_N \in \mathbb{Z}_{\geqslant 0}$ for some $N \in \mathbb{Z}_{\geqslant 1}$. In terms of $\imath_k$ we further introduce a map

$$\imath^{(L_0,\ldots,L_N)}_{k_1,\ldots,k_N}: B'_{k_1} \otimes \cdots \otimes B'_{k_N} \to (B_1)^{\otimes L_0+\cdots+L_N+k_1+\cdots+k_N}$$

by

$$\begin{aligned} &\imath^{(L_0,\ldots,L_N)}_{k_1,\ldots,k_N}(b_1 \otimes b_2 \otimes \cdots \otimes b_N) \\ &= \boxed{1}^{\otimes L_0} \otimes \imath_{k_1}(b_1) \otimes \boxed{1}^{\otimes L_1} \otimes \imath_{k_2}(b_2) \otimes \cdots \otimes \boxed{1}^{\otimes L_{N-1}} \otimes \imath_{k_N}(b_N) \otimes \boxed{1}^{\otimes L_N}. \end{aligned}$$

In particular $\imath_k = \imath^{(0,0)}_k$. The map $\imath^{(L_0,\ldots,L_N)}_{k_1,\ldots,k_N}$ is injective. For each $k \in \mathbb{Z}_{\geqslant 1}$ let ς_k denote the map

$$\begin{array}{rccc} \varsigma_k: & (B_1)^{\otimes k} & \longrightarrow & B_k \\ & \boxed{m_1} \otimes \cdots \otimes \boxed{m_k} & \mapsto & \boxed{m'_1 \ldots m'_k} \end{array}$$

where $1 \leqslant m'_1 \leqslant \cdots \leqslant m'_k \leqslant M+1$ are just the reordering of $m_1, \ldots, m_k$ into the weakly increasing order. We assume that $\mathcal{L} := \Sigma_n \theta_n$ is sufficiently large. We set

$$\hat{\theta} = (\cdots \otimes \varsigma_{\theta_n} \otimes \varsigma_{\theta_{n+1}} \otimes \cdots): B_1^{\otimes \mathcal{L}} \to \cdots \otimes B_{\theta_n} \otimes B_{\theta_{n+1}} \otimes \cdots. \tag{12}$$

For non-negative integers $L_0, \ldots, L_N$ such that $\mathcal{L} = L_0 + \cdots + L_N + k_1 + \cdots + k_N$, denote by $\iota^{(L_0,\ldots,L_N)}_{k_1,\ldots,k_N}$ the composition $\hat{\theta} \circ \imath^{(L_0,\ldots,L_N)}_{k_1,\ldots,k_N}$, i.e.,

$$\iota^{(L_0,\ldots,L_N)}_{k_1,\ldots,k_N}: B'_{k_1} \otimes \cdots \otimes B'_{k_N} \xrightarrow{\imath^{(L_0,\ldots,L_N)}_{k_1,\ldots,k_N}} B_1^{\otimes \mathcal{L}} \xrightarrow{\hat{\theta}} \cdots \otimes B_{\theta_n} \otimes B_{\theta_{n+1}} \otimes \cdots. \tag{13}$$

Suppose that the image is obtained from the element $\cdots \otimes u_{\theta_n} \otimes u_{\theta_{n+1}} \otimes \cdots$ by replacing only the isolated segments $u_{\theta_{n_i}} \otimes u_{\theta_{n_i+1}} \otimes \cdots \otimes u_{\theta_{n'_i}} (n_i \leqslant n'_i)$ with some $b_{\theta_{n_i}} \otimes \cdots \otimes b_{\theta_{n'_i}} \in B_{\theta_{n_i}} \otimes \cdots \otimes B_{\theta_{n'_i}}$ for $1 \leqslant i \leqslant N$. Assume further that the interval is sufficiently large, namely, $n_i - n'_{i-1} \gg \max(k_1, \ldots, k_N)$ for any $2 \leqslant i \leqslant N$. In such a case we call the image of (13) an *asymptotic N soliton state*. Each soliton is essentially associated with an element in B'_k, and we call k the *amplitude* of the corresponding soliton. States obtained from an asymptotic N soliton state under arbitrary time evolutions $T_\kappa \cdots T_{\kappa'}$ will be called N soliton states. This definition will naturally be justified from the consideration on the conserved quantities in Section III D. Note that $\iota^{(L_0,\ldots,L_N)}_{k_1,\ldots,k_N}$ is not injective since $\hat{\theta}$ is not. Consequently, the result of the application of $\iota^{(L'_0,\ldots,L'_N)}_{k_1,\ldots,k_N}$ is not necessarily an ''overall translation'' of (13) in a naive sense even when $L'_i - L_i$ is i independent for $i < N$ or $i > 0$. See Example 3.2 in the following.

First we consider the $N=1$ case. As it turns out in Proposition 3.3, there is no distinction between an asymptotic one-soliton state and a one-soliton state. Moreover one can check that the definition of the one-soliton state here agrees with the one-soliton solution that will be given later in (B1). Given a one-soliton state

$$\mathbf{p} = \cdots \otimes b_{n-1} \otimes b_n \otimes b_{n+1} \otimes \cdots \in \cdots \otimes B_{\theta_{n-1}} \otimes B_{\theta_n} \otimes B_{\theta_{n+1}} \otimes \cdots,$$

one can unambiguously specify integers $n,k(\geqslant 1),s,t$ by the conditions:

$$
\begin{aligned}
&b_j = u_{\theta_j} \quad \text{if } j < n \text{ or } j > n+k,\\
&b_n = \boxed{1\cdots 1 m_1 \cdots m_t} \quad 1 \leq t \leq \theta_n,\ 2 \leq m_1 \leq \cdots \leq m_t \leq M+1,\\
&b_{n+k} = \boxed{1\cdots 1 m_1' \cdots m_s'} \quad 0 \leq s \leq \theta_{n+k}-1,\ 2 \leq m_1' \leq \cdots \leq m_s' \leq M+1,\\
&b_{n+1},\ldots,b_{n+k-1} \text{ do not contain 1 in their tableaux.}
\end{aligned}
$$

Note that ''if'' in the first condition is not ''only if'' in that $b_{n+k}=u_{\theta_{n+k}}$ is allowed as $s=0$. The amplitude of the soliton according to the above-mentioned definition equals $t+\theta_{n+1}+\cdots+\theta_{n+k-1}+s$. We set

$$
x(\mathbf{p})=\sum_{j\leqslant n}\theta_j - t, \quad y(\mathbf{p})=t+\theta_{n+1}+\cdots+\theta_{n+k-1}
$$

and call $x(\mathbf{p})$ the *coordinate* of the soliton. $y(\mathbf{p})$ should not be confused with the amplitude of the soliton.

Example 3.2: Consider $B_{\theta_1}\otimes\cdots\otimes B_{\theta_6}$ with $\theta_1=\theta_3=1$, $\theta_2=\theta_4=\theta_6=2$, and $\theta_5=3$, hence $\mathcal{L}=11$.

(i) Take

$$
b=\boxed{1}\in B_1'.
$$

Then $\iota_1^{(L_0,L_1)}(b)$ with $L_0+L_1=10$ are examples of one-soliton states with amplitude 1. One has $\iota_1^{(1,9)}(b)=\iota_1^{(2,8)}(b)$, $\iota_1^{(4,6)}(b)=\iota_1^{(5,5)}(b)$, and $\iota_1^{(6,4)}(b)=\iota_1^{(7,3)}(b)=\iota_1^{(8,2)}(b)$. For $L_0\leqslant 8$ they look as

$\boldsymbol{p}$	n	$n+k$	$x(\boldsymbol{p})$	$y(\boldsymbol{p})$
$\iota_1^{(0,10)}(b)=\boxed{2}\otimes\boxed{11}\otimes\boxed{1}\otimes\boxed{11}\otimes\boxed{111}\otimes\boxed{11}$	1	2	0	1,
$\iota_1^{(2,8)}(b)=\boxed{1}\otimes\boxed{12}\otimes\boxed{1}\otimes\boxed{11}\otimes\boxed{111}\otimes\boxed{11}$	2	3	2	1,
$\iota_1^{(3,7)}(b)=\boxed{1}\otimes\boxed{11}\otimes\boxed{2}\otimes\boxed{11}\otimes\boxed{111}\otimes\boxed{11}$	3	4	3	1,
$\iota_1^{(5,5)}(b)=\boxed{1}\otimes\boxed{11}\otimes\boxed{1}\otimes\boxed{12}\otimes\boxed{111}\otimes\boxed{11}$	4	5	5	1,
$\iota_1^{(8,2)}(b)=\boxed{1}\otimes\boxed{11}\otimes\boxed{1}\otimes\boxed{11}\otimes\boxed{112}\otimes\boxed{11}$	5	6	8	1,

where we have also listed, n, $n+k$, $x(\mathbf{p})$ and $y(\mathbf{p})$.

(ii) Take

$$
c=\boxed{11223}\in B_5'.
$$

Then $\iota_1^{(L_0,L_1)}(b)$ with $L_0+L_1=6$ are examples of one-soliton states with amplitude 5. For $L_0\leqslant 5$ they look as

$\boldsymbol{p}$	n	$n+k$	$x(\boldsymbol{p})$	$y(\boldsymbol{p})$
$\iota_5^{(0,6)}(c)=\boxed{4}\otimes\boxed{33}\otimes\boxed{2}\otimes\boxed{12}\otimes\boxed{111}\otimes\boxed{11}$	1	4	0	4,
$\iota_5^{(1,5)}(c)=\boxed{1}\otimes\boxed{34}\otimes\boxed{3}\otimes\boxed{22}\otimes\boxed{111}\otimes\boxed{11}$	2	5	1	5,
$\iota_5^{(2,4)}(c)=\boxed{1}\otimes\boxed{14}\otimes\boxed{3}\otimes\boxed{23}\otimes\boxed{112}\otimes\boxed{11}$	2	5	2	4,
$\iota_5^{(3,3)}(c)=\boxed{1}\otimes\boxed{11}\otimes\boxed{4}\otimes\boxed{33}\otimes\boxed{122}\otimes\boxed{11}$	3	5	3	3,
$\iota_5^{(4,2)}(c)=\boxed{1}\otimes\boxed{11}\otimes\boxed{1}\otimes\boxed{34}\otimes\boxed{223}\otimes\boxed{11}$	4	6	4	5,
$\iota_5^{(5,1)}(c)=\boxed{1}\otimes\boxed{11}\otimes\boxed{1}\otimes\boxed{14}\otimes\boxed{233}\otimes\boxed{12}$	4	6	5	4.

In Sec. III C we will make use of

Proposition 3.3: Let $\mathbf{p}=\iota_l^{(L_0,L_1)}(b)$ *be the one soliton of amplitude* l *associated with* $b \in B_l'$. *Then its time evolution* $T_\kappa(\mathbf{p})$ *is again one soliton and expressible as* $T_\kappa(\mathbf{p})=\iota_l^{(L_0',L_1')}(b)$ *for some* L_0', L_1' $(L_0'+L_1'=L_0+L_1)$ *but with the same* $b \in B_l'$. *The difference of their coordinates* (*velocity under* T_κ) *is given by*

$$x(T_\kappa(\mathbf{p}))-x(\mathbf{p})=\begin{cases}\kappa, & \kappa<y(\mathbf{p})\\ \min(\kappa,l)+\max(\theta_{n+k}-l,0), & \kappa\geqslant y(\mathbf{p}).\end{cases}$$

The proof is done by a cumbersome case study. When $\forall\,\theta_n=1$, the above result simplifies to $x(T_\kappa(\mathbf{p}))-x(\mathbf{p})=\min(\kappa,l)$ in agreement with Ref. 12. In general, the velocity varies locally depending on the data $\{\theta_n\}$. In Example 3.2 (i) one has $T_\kappa(\iota_1^{(0,10)}(b))=\iota_1^{(2,8)}(b)$, $T_\kappa(\iota_1^{(2,8)}(b))=\iota_1^{(3,7)}(b)$, $T_\kappa(\iota_1^{(3,7)}(b))=\iota_1^{(5,5)}(b)$, $T_\kappa(\iota_1^{(5,5)}(b))=\iota_1^{(8,2)}(b)$ for any $\kappa\geqslant 1$. Similarly in (ii) one has $T_\kappa(\iota_5^{(0,6)}(c))=\iota_5^{(\kappa',6-\kappa')}(c)$ for any $\kappa\geqslant 1$, where $\kappa'=\min(\kappa,5)$. These results agree with Proposition 3.3

Let $\iota_{k_1,\ldots,k_N}^{(L_0,\ldots,L_N)}(c_1\otimes\cdots\otimes c_N)(c_i\in B_{k_i}')$ be an asymptotic N soliton state and

$$\cdots\otimes b_n^t\otimes b_{n+1}^t\otimes\cdots=T_{\kappa_t}T_{\kappa_{t-1}}\cdots(\iota_{k_1,\ldots k_N}^{(L_0,\ldots,L_N)}(c_1\otimes\cdots\otimes c_N))$$

be its time evolution. Assume that the solitons are sufficiently separated without an interaction throughout the time interval under consideration. Let $\{v_n^t\}$ be the associated variables on the vertical edges as in (8). Then in the space–time interchanged picture, the state $\cdots\otimes v_n^{t+1}\otimes v_n^t\otimes\cdots$ is also an asymptotic N soliton state associated with the same $c_1\otimes\cdots\otimes c_N$. Namely,

$$\cdots\otimes v_n^{t+1}\otimes v_n^t\otimes\cdots=\hat\kappa\circ\iota_{k_1,\ldots,k_N}^{(L_0',\ldots,L_N')}(c_1\otimes\cdots\otimes c_N)$$

for some $L_0',\ldots,L_N'$. Here

$$\hat\kappa=(\cdots\otimes\varsigma_{\kappa_{t+1}}\otimes\varsigma_{\kappa_t}\otimes\cdots):B_1^{\otimes\mathcal{M}}\to\cdots\otimes B_{\kappa_{t+1}}\otimes B_{\kappa_t}\otimes\cdots,$$

is an analog of $\hat\theta$ in (12), and we have set $\mathcal{M}=\Sigma_t\,\kappa_t$. The figure in Example 2.8 will be of help to understand this fact. In a sense one can employ either picture to describe the scattering process. Indeed our discussion at the end of Sec. III C will rely on this observation.

B. Scattering of two solitons: A typical case

Our aim here is to show Theorem 3.9 which is valid in the ''typical'' situation (19).

Lemma 3.4: For each $i=1,\ldots,M-1$, *we have a commutative diagram:*

$$\begin{array}{ccc} B_k' & \xrightarrow{\iota_k} & (B_1)^{\otimes k} \\ {\scriptstyle\tilde e_i'}\downarrow & & \downarrow{\scriptstyle\tilde e_{i+1}} \\ B_k'\sqcup\{0\} & \xrightarrow{\iota_k} & (B_1)^{\otimes k}\sqcup\{0\}, \end{array}$$

where $\iota_k(0)=0$. *The same relation also holds between* $\tilde f_i'$ and $\tilde f_{i+1}'$.

Combining Lemma 3.4 with the realization of B_θ in $B_1^{\otimes\theta}$ as a $U_q(A_M)$ crystal (cf. Ref. 17), one can derive the following lemmas.

Lemma 3.5: In the diagram

$$\begin{array}{ccc} B'_l \otimes B'_k & \xrightarrow{\iota_{l,k}^{(L_0,L_1,L_2)}} & (\cdots \otimes B_{\theta_n} \otimes B_{\theta_{n+1}} \otimes \cdots) \\ \downarrow{\scriptstyle \tilde{e}'_i} & & \downarrow{\scriptstyle \tilde{e}_{i+1}} \\ (B'_l \otimes B'_k) \sqcup \{0\} & \xrightarrow{\iota_{l,k}^{(L_0,L_1,L_2)}} & (\cdots \otimes B_{\theta_n} \otimes B_{\theta_{n+1}} \otimes \cdots) \sqcup \{0\}, \end{array}$$

suppose that the image of $\iota_{l,k}^{(L_0,L_1,L_2)}$ *is an asymptotic two-soliton state. Then the diagram is commutative for any* $i=1,\ldots,M-1$. *The same relation holds also between* $\tilde{f}'_i$ *and* $\tilde{f}_{i+1}$

Actually, the commutativity of the above diagram holds under a milder condition than being an asymptotic two-soliton state.

Lemma 3.6: Let $p_1,\ldots,p_m$ *be the subsequence of* $a_1,\ldots,a_L (a_n \in B_{\theta_n})$ *consisting of all the elements such that* $a_n \neq u_{\theta_n}$. *Assume the same relation between* $p'_1,\ldots,p'_m$ *and* $a'_1,\ldots,a'_L$. *Then for any* $t, t' \in \mathbb{Z}_{\geqslant 0}$ *and* $\kappa \in \mathbb{Z}_{\geqslant 1}$, *the two relations*

$$\tilde{f}_{i+1}(p_1 \otimes \cdots \otimes p_m) = p'_1 \otimes \cdots \otimes p'_m,$$

$$\tilde{f}_{i+1}(u_\kappa^{\otimes t} \otimes a_1 \otimes \cdots \otimes a_L \otimes u_\kappa^{\otimes t'}) = u_\kappa^{\otimes t} \otimes a'_1 \otimes \cdots \otimes a'_L \otimes u_\kappa^{\otimes t'}$$

are equivalent for each $i=1,\ldots,M-1$. *The equivalence persists even when the right-hand sides are both 0. The same is true also for* $\tilde{e}_{i+1}$.

Proposition 3.7: Suppose an asymptotic two-soliton state has evolved into another as

$$T_k^t(\iota_{l,k}^{(L_0,L_1,L_2)}(b \otimes c)) = \iota_{k,l}^{(L'_0,L'_1,L'_2)}(c' \otimes b') \tag{14}$$

for some $\kappa, t, L_i, L'_i > 0, b, b' \in B'_l$ *and* $c, c' \in B'_k$. *Then* (14) *is also valid under the replacement of* $b \otimes c$ (*respectively,* $c' \otimes b'$) *by* $\tilde{f}'_i(b \otimes c)$ [*respectively,* $\tilde{f}'_i(c' \otimes b')$] *for any* $i=1,\ldots,M-1$ *such that* $\tilde{f}'_i(b \otimes c) \neq 0$.

Proof: (14) is equivalent to

$$u_\kappa^{\otimes t} \otimes \iota_{l,k}^{(L_0,L_1,L_2)}(b \otimes c) \simeq \iota_{k,l}^{(L'_0,L'_1,L'_2)}(c' \otimes b') \otimes u_\kappa^{\otimes t}.$$

Apply $\tilde{f}_{i+1}$ to both sides. Due to Lemmas 3.5 and 3.6, the result becomes

$$u_\kappa^{\otimes t} \otimes \iota_{l,k}^{(L_0,L_1,L_2)}(\tilde{f}'_i(b \otimes c)) \simeq \iota_{k,l}^{(L'_0,L'_1,L'_2)}(\tilde{f}'_i(c' \otimes b')) \otimes u_\kappa^{\otimes t}.$$

□

Proposition 3.8: Let $l > k$ *and assume that* $\iota_{l,k}^{(L_0,L_1,L_2)}(b_1 \otimes b_2)$ *is an asymptotic two-soliton state with*

$$b_1 = (l,0,\ldots,0) \in B'_l, \quad b_2 = (h,k-h,0,\ldots,0) \in B'_k \tag{15}$$

with $0 \leqslant h \leqslant k$ *in the notation of* (1). *Assume further that* $l > \theta_n$ *for all but finitely many n's. Then if* $\kappa \gg l$, *there exists* $t > 0$ *such that the result of the time evolution* T_κ^t *also becomes the asymptotic two-soliton state as*

$$T_\kappa^t(\iota_{l,k}^{(L_0,L_1,L_2)}(b_1 \otimes b_2)) = \iota_{k,l}^{(L'_0,L'_1,L'_2)}(c_2 \otimes c_1), \tag{16}$$

where c_1, c_2 *are given by*

$$c_2=(k,0,\ldots,0)\in B'_k, \quad c_1=(l-k+h,k-h,0,\ldots,0)\in B'_l. \tag{17}$$

The proof is given in Appendix A. In fact both $b_1\otimes b_2$ and $c_2\otimes c_1$ are $U_q(A_{M-1})$ highest element, i.e., $\tilde{e}'_i(b_1\otimes b_2)=\tilde{e}'_i(c_2\otimes c_1)=0$ for all $1\leqslant i\leqslant M-1$. Combining this property with the conservation of weights (number of the letters) and the soliton content (cf. Sec. III D), one can argue that the outgoing state should necessarily correspond to $c_2\otimes c_1$ if it is an asymptotic two-soliton state at all. However, to establish the separation into two solitons asymptotically is not a trivial task for inhomogeneous θ_n's only bounded by the condition $l\geqslant\theta_n$ for all but finitely many n's. So far we have not managed it without recourse to the actual two-soliton solution as in Appendix A.

As a $U_q(A_{M-1})$ crystal, the $U'_q(A^{(1)}_{M-1})$-crystal $B'_l\otimes B'_k$ decomposes into the connected components. Each component is parametrized with the $U_q(A_{M-1})$ highest elements $b_1\otimes b_2$ (15), and is generated by applying $\tilde{f}'_i$ operators $(1\leqslant i\leqslant M-1)$ to it. The decomposition of the same pattern takes place also for $B'_k\otimes B'_l$ according to the highest elements $c_2\otimes c_1$. Combining this fact with Propositions 3.7 and 3.8, we conclude that there exists a map S' (S matrix) uniquely defined by

$$\begin{gathered} S':B'_l\otimes B'_k\to B'_k\otimes B'_l, \\ T^t_\kappa(\iota^{(L_0,L_1,L_2)}_{l,k}(b\otimes c))=\iota^{(L'_0,L'_1,L'_2)}_{k,l}(S'(b\otimes c)), \end{gathered} \tag{18}$$

under the condition

$$\kappa\gg l>k, \quad l>\theta_n \quad \text{for all but finitely many } n\text{'s}. \tag{19}$$

It describes the two-soliton scattering.

Theorem 3.9: *Under the assumption* (19), *we have* $R'=S'$ *on the* $U'_q(A^{(1)}_{M-1})$*-crystal* $B'_l\otimes B'_k$.

Proof: By the definition and Proposition 3.7, both R' and S' commute with $\tilde{f}'_i$ for any $1\leqslant i\leqslant M-1$. Moreover, for any $U_q(A_{M-1})$ highest elements $b_1\otimes b_2$ given by (15), their actions are the same, i.e., $S'(b_1\otimes b_2)=c_2\otimes c_1=R'(b_1\otimes b_2)$, where the latter can be verified from Proposition 2.3. □

Thus in situation (19) the larger soliton overtakes the smaller soliton and the scattering matrix coincides with the combinatorial R matrix of the $U'_q(A^{(1)}_{M-1})$ crystal. For instance Example 2.7 tells that

$$S':\boxed{13}\otimes\boxed{2}\mapsto\boxed{1}\otimes\boxed{23}.$$

This agrees with Example 2.2(i).

C. Scattering of two solitons: General case

First let us consider the homogeneous case $\forall\theta_n=\theta, \forall\kappa_t=\kappa$. Fix positive integers $l>k$. We study the scattering of two solitons in $\cdots\otimes B_\theta\otimes B_\theta\otimes\cdots$ with amplitudes l and k under the time evolution T^t_κ. The qualitative feature of the scattering depends on the following cases:

(i) $l>k\geqslant\max(\theta,\kappa)$, $v_l=v_k=\kappa$,

(ii) $\min(\theta,\kappa)\geqslant l>k$, $v_l=v_k=\theta$,

(iii) $l\geqslant\kappa>k\geqslant\theta$, $v_l=\kappa>v_k=k$,

(iv) $\kappa\geqslant l>k\geqslant\theta$, $v_l=l>v_k=k$,

(v) $l\geqslant\kappa>\theta\geqslant k$, $v_l=\kappa>v_k=\theta$,

(vi) $\kappa \geqslant l > \theta \geqslant k, \quad v_l = l > v_k = \theta,$

(vii) $l \geqslant \theta > k \geqslant \kappa,$

(viii) $\theta \geqslant l > k \geqslant \kappa,$

(ix) $l \geqslant \theta > \kappa \geqslant k,$

(x) $\theta \geqslant l > \kappa \geqslant k.$

Here the classification has been done so that

$$\{(\mathrm{i}) \amalg (\mathrm{ii})\} \amalg \{(\mathrm{iii}) \cup (\mathrm{iv}) \cup (\mathrm{v}) \cup (\mathrm{vi})\} \amalg \{(\mathrm{vii}) \cup (\mathrm{viii}) \cup (\mathrm{ix}) \cup (\mathrm{x})\}.$$

For example, cases (iii) and (iv) share the $l = \kappa > k \geqslant \theta$ case. However the three groups are mutually disjoint and correspond to distinct features of the scattering as we will see in the following. The v_l and v_k are the velocities of the solitons with amplitude l and k, respectively. For each soliton it has been calculated by using Proposition 3.3 by assuming no effect from the other soliton. In cases (vi) and (x) we have excluded $l = \theta$ and $l = \kappa$, respectively, since they both lead to $v_l = v_k = \theta$ and hence no scattering. For the same reason, cases (i) and (ii) are out of question. Via the space–time interchange $\theta \leftrightarrow \kappa$, cases (vii), (viii), (ix), and (x) are mapped to (iii), (iv), (v), and (vi), respectively. [See the argument before Theorem 3.10 on the velocities in cases (vii)–(x).] Thus we are left with cases (iii)–(vi), where $l > \theta$ and $v_l > v_k$ are always valid. Following Ref. 12, we utilize the commutativity (9) and consider the two-soliton scattering under T^t_κ as

$$T^t_\kappa = T^{-t'}_\infty T^t_\kappa T^{t'}_\infty .$$

The scatterings are thus divided into three stages. In the first stage, we let solitons evolve under $T^{t'}_\infty$ for sufficiently large t'. Since $l > \theta$ matches condition (19), Theorem 3.9 tells us that the larger soliton overtakes the smaller one with the scattering rule described by $S' = R'$. In the second stage corresponding to T^t_κ, the larger soliton goes further ahead than the smaller one with no interaction because of $v_l > v_k$. Therefore in the last stage $T^{-t'}_\infty$, the two remain isolated even though they are drawn back and get relatively closer. Thus we conclude that in all the cases (iii)–(vi), the qualitative feature is the same as the one in Theorem 3.9. Namely, the larger soliton overtakes the smaller one and the scattering rule is given by the combinatorial R matrix $R' : B'_l \otimes B'_k \to B'_k \otimes B'_l$. Through the space–time interchange argument, this implies the opposite feature of scattering in cases (vii)–(x). Namely, the smaller one overtakes the larger one with the scattering rule given by the combinatorial R matrix $R' : B'_k \otimes B'_l \to B'_l \otimes B'_k$.

We note that in cases (vii)–(x) one does not necessarily have $v_l < v_k$ at any time. It actually depends on whether $\kappa \gtrless y(\mathbf{p})$ when Proposition 3.3 is applied. Nevertheless $v_l < v_k$ should be valid ''on average'' and the above-mentioned feature of the scattering should hold due to the reduction to cases (iii)–(vi) where the strict inequality $v_l > v_k$ is always valid. To summarize, we have shown

Theorem 3.10: *Let $l > k$ be the amplitude of two solitons in $\cdots \otimes B_\theta \otimes B_\theta \otimes \cdots$. Under the time evolution T_κ, the scattering matrix of the collision (if any) in the sense of (18) or $(18)_{l \leftrightarrow k}$ is given by $S' = R'$, where R' is the combinatorial R matrix of the $U'_q(A^{(1)}_{M-1})$ crystals for*

(I) $B'_l \otimes B'_k \tilde{\mapsto} B'_k \otimes B'_l \quad if \min(l, \kappa) > \max(k, \theta),$

(II) $B'_k \otimes B'_l \tilde{\mapsto} B'_l \otimes B'_k \quad if \min(l, \theta) > \max(k, \kappa),$

(III) *no scattering* (*same velocity*) *otherwise.*

Example 2.8 corresponds to the choice $l=\theta=2, k=\kappa=1$, hence to (II) in the theorem. The scattering matrix is read off the figure,

$$S' : \boxed{3} \otimes \boxed{22} \mapsto \boxed{23} \otimes \boxed{2}.$$

This agrees with the inverse of the R matrix in Example 2.2(ii).

Let us comment on the inhomogeneous case where θ_n's and κ_t's actually depend on the indices. In view of (19), the qualitative feature of the scattering remains the same as Theorem 3.10 even if we slightly relax the conditions therein. For instance the larger soliton still overtakes the smaller one with the rule $S'=R'$ if $\min(l,\kappa_t)>\max(k,\theta_n)$ holds for almost all n and t that are relevant during the scattering in question. In such cases we expect that the asymptotic N soliton state in the sense of Sec. III A undergoes the scattering which is essentially factorized into the two-body ones studied here. On the other hand, if θ_n's and κ_t's are not bounded by the condition as noted previously and indeed are far from being homogeneous, even two solitons can collide many times in general depending on the local velocities. In such a case we do not have a simple picture of the scattering.

Example 3.11: Let $M=3$.

$$\begin{aligned}
0&:\cdots 14\cdot 3\cdot 123\cdot 111\cdot 24\cdot 1\cdot 1\cdot 111\cdot 11\cdot 1\cdot 1111\cdot 1111\cdot 11111\cdot 11111\cdot 111\cdot 1111\cdots\\
1&:\cdots 11\cdot 1\cdot 114\cdot 233\cdot 11\cdot 4\cdot 2\cdot 111\cdot 11\cdot 1\cdot 1111\cdot 1111\cdot 11111\cdot 11111\cdot 111\cdot 1111\cdots\\
2&:\cdots 11\cdot 1\cdot 111\cdot 111\cdot 34\cdot 3\cdot 1\cdot 224\cdot 11\cdot 1\cdot 1111\cdot 1111\cdot 11111\cdot 11111\cdot 111\cdot 1111\cdots\\
3&:\cdots 11\cdot 1\cdot 111\cdot 111\cdot 11\cdot 1\cdot 4\cdot 113\cdot 34\cdot 2\cdot 1112\cdot 1111\cdot 11111\cdot 11111\cdot 111\cdot 1111\cdots\\
4&:\cdots 11\cdot 1\cdot 111\cdot 111\cdot 11\cdot 1\cdot 1\cdot 114\cdot 13\cdot 1\cdot 1234\cdot 1112\cdot 11111\cdot 11111\cdot 111\cdot 1111\cdots\\
5&:\cdots 11\cdot 1\cdot 111\cdot 111\cdot 11\cdot 1\cdot 1\cdot 111\cdot 14\cdot 3\cdot 1114\cdot 1223\cdot 11111\cdot 11111\cdot 111\cdot 1111\cdots\\
6&:\cdots 11\cdot 1\cdot 111\cdot 111\cdot 11\cdot 1\cdot 1\cdot 111\cdot 11\cdot 1\cdot 1134\cdot 1234\cdot 11112\cdot 11111\cdot 111\cdot 1111\cdots\\
7&:\cdots 11\cdot 1\cdot 111\cdot 111\cdot 11\cdot 1\cdot 1\cdot 111\cdot 11\cdot 1\cdot 1111\cdot 2334\cdot 11114\cdot 11112\cdot 111\cdot 1111\cdots\\
8&:\cdots 11\cdot 1\cdot 111\cdot 111\cdot 11\cdot 1\cdot 1\cdot 111\cdot 11\cdot 1\cdot 1111\cdot 1134\cdot 11123\cdot 11114\cdot 112\cdot 1111\cdots\\
9&:\cdots 11\cdot 1\cdot 111\cdot 111\cdot 11\cdot 1\cdot 1\cdot 111\cdot 11\cdot 1\cdot 1111\cdot 1111\cdot 12334\cdot 11111\cdot 114\cdot 1112\cdots
\end{aligned}$$

where $\cdot$ denotes $\otimes$, and 14 for example does

$$\boxed{14} \in B_2.$$

Not only θ_n's but also κ_t are inhomogeneous here so that the relevant time evolutions are T_5 for the process $0\to1\to2\to3\to4$, whereas they are T_2 for $4\to5\to6\to7\to8\to9$. This is an example of the double scattering of two solitons caused by the inhomogeneity. The larger soliton once overtakes the smaller one, but after the collision it gets slower due to the environmental change and is eventually passed by the smaller one again. This is easily understood from the classification (I)–(III) in Theorem 3.10 for the homogeneous case. In the first stage we have $l=4$, $\kappa=5$, $k=2$, $\theta_n\leqslant 3$ so that the larger soliton overtakes the smaller as in (I). On the other hand we have $\kappa=2$, $\theta_n\geqslant 3$ in the second stage; hence the smaller one passes the larger one as in (II). Following the time evolution downward, one finds the scattering matrices for the successive collisions:

$$\boxed{1223} \otimes \boxed{13} \mapsto \boxed{23} \otimes \boxed{1123} \mapsto \boxed{1223} \otimes \boxed{13}$$

in terms of the soliton labels with the $U_q'(A_2^{(1)})$-crystal elements. They agree with the combinatorial R matrices $B_4'\otimes B_2' \simeq B_2'\otimes B_4'$ calculated from Proposition 2.3.

D. Conserved quantities

Let us give a class of conserved quantities in the $A_M^{(1)}$ automaton. Since our construction here is based on Ref. 12 and the result is quite parallel, we will only present a brief sketch. Given an automaton state $\mathbf{p}=\cdots\otimes b_n\otimes b_{n+1}\otimes\cdots$ ($b_n=u_{\theta_n}$ for $|n|\gg 1$,), let

$$u_\kappa \otimes \mathbf{p} \simeq \cdots \otimes b'_{n-1} \otimes b'_n \otimes v_n \otimes b_{n+1} \otimes b_{n+2} \otimes \cdots$$

for some $b'_i \in B_{\theta_i}$ and $v_n \in B_\kappa$. Set

$$E_\kappa(\mathbf{p}) = -\sum_n H_{B_\kappa B_{\theta_{n+1}}}(v_n \otimes b_{n+1}),$$

which is well defined owing to the normalization (7). By the same argument as in Ref. 12 we get

$$E_\kappa(T_{\kappa'}(\mathbf{p})) = E_\kappa(\mathbf{p}) \quad \text{for any } \kappa, \kappa'.$$

Thus $E_\kappa(\mathbf{p})$, $\kappa \in \mathbb{Z}_{\geqslant 1}$ form a family of conserved quantities. If $\mathbf{p}$ is an asymptotic N soliton state in the sense of Sec. III A, it is straightforward to derive

$$E_\kappa(\mathbf{p}) = \sum_{l \geqslant 1} \min(l, \kappa) N_l, \tag{20}$$

where N_l is the number of solitons with amplitude l. Therefore if a state with the soliton content $\{N_l\}$ scatters into another state with the content $\{N'_l\}$, $N_l = N'_l$ must be valid for any l due to the conservation of all E_κ's. In both Examples 2.7 and 2.8 we have $E_1 = 2$, $E_l = 3$ for $l \geqslant 3$, in agreement with $N_1 = N_2 = 1$, $N_l = 0$ for $l \geqslant 3$. In Example 3.11, we have $E_1 = 2$, $E_2 = 4$, $E_3 = 5$, and $E_l = 6$ for $l \geqslant 4$, in agreement with $N_l = \delta_{l2} + \delta_{l4}$.

When $\forall \theta_n = 1$, (20) is obtained in proposition 4.4 in Ref. 12. An equivalent family of the conserved quantities has also been given in Ref. 5.

Another conserved quantity is the semistandard Young tableau, which can be constructed as follows. Given an automaton state $\mathbf{p} = \cdots \otimes b_n \otimes b_{n+1} \otimes \cdots$, let $c_s \cdots c_2 c_1$ be the subsequence of $\cdots b_{n-1} b_n b_{n+1} \cdots$ obtained by dropping all the b_j's such that $b_j = u_{\theta_j}$. Each c_j has the form

$$c_j = \boxed{1 \ldots 1 m_1 \ldots m_k} \quad 2 \leq m_1 \leq \cdots \leq m_k \leq M+1 \ \text{ for some } k \geq 1,$$

for which we set

$$\bar{c}_j = \boxed{m_1 - 1 \ldots m_k - 1} \in B'_k.$$

Let $\mathcal{T}(\mathbf{p}) := (((\bar{c}_1 \cdot \bar{c}_2) \cdot \bar{c}_3) \cdot \cdots \cdot \bar{c}_s)$ be the semistandard tableau constructed from the successive products of $\bar{c}_j$'s defined via the row insertion as in Ref. 18, p. 11. By virtue of the $U'_q(A_{M-1})$ invariance,[12] it is a conserved quantity under any time evolution T_κ, i.e., $\mathcal{T}(\mathbf{p}) = \mathcal{T}(T_\kappa(\mathbf{p}))$. In the context of the Robinson–Schensted–Knuth correspondence, $\mathcal{T}(\mathbf{p})$ stands for the P symbol. For any one-soliton state $\mathbf{p} = \iota_k^{(L_0, L_1)}(b)$, $b \in B'_k$, one has $\mathcal{T}(\mathbf{p}) = b$. One can also check that $\mathcal{T}(\mathbf{p})$ equals

$$\begin{array}{|c|c|}\hline 1 & 3 \\ \hline 2 \\ \cline{1-1}\end{array} \qquad \begin{array}{|c|c|c|}\hline 2 & 2 & 3 \\ \hline\end{array} \qquad \begin{array}{|c|c|c|c|c|}\hline 1 & 1 & 2 & 2 & 3 \\ \hline 3 \\ \cline{1-1}\end{array}$$

in Examples 2.7, 2.8, and 3.11, respectively, throughout the scattering.

IV. $A_M^{(1)}$ AUTOMATON AS AN ULTRADISCRETE KP EQUATION

Here we investigate the $A_M^{(1)}$ automaton constructed in Sec. II C from the viewpoint of ultradiscretization.[2,19] With the same notations as (1) we define $u_{n,j}^t$ and $v_{n,j}^t$ to be the multiplicities of the $(M+2-j)$th content of b_n^t and v_n^t, i.e.,

$$b_n^t = (u_{n,M+1}^t, u_{n,M}^t, \ldots, u_{n,1}^t),$$

$$v_n^t=(v_{n,M+1}^t v_{n,M}^t,\ldots,v_{n,1}^t),$$

Proposition 4.1: The map

$$R:v_n^t\otimes b_n^t\tilde{\mapsto}b_n^{t+1}\otimes v_{n+1}^t, \tag{21}$$

is expressed by $(1\leqslant j\leqslant M)$

$$\begin{aligned}u_{n,j}^{t+1}-v_{n,j}^t=&\max[X_1-\theta_n,X_2-\theta_n,\ldots,X_{j-1}-\theta_n,X_j-\kappa_t,\ldots,X_M-\kappa_t,0]\\&-\max[X_1-\theta_n,X_2-\theta_n,\ldots,X_j-\theta_n,X_{j+1}-\kappa_t,\ldots,X_M-\kappa_t,0],\end{aligned} \tag{22}$$

$$v_{n+1,j}^t=u_{n,j}^t+v_{n,j}^t-u_{n,j}^{t+1}, \tag{23}$$

where

$$X_\ell=X_{n;\ell}^t:=\sum_{i=\ell}^{M}u_{n,i}^t+\sum_{i=1}^{\ell}v_{n,i}^t.$$

Actually (23) is also valid for $j=M+1$.

Proof: In the present proof, we abbreviate $u_{n,j}^t$ and $v_{n,j}^t$ to u_j and v_j, respectively. We also put $u_{j+M+1}=u_j$, $v_{j+M+1}=v_j$, etc., i.e., each suffix is defined modulo $M+1$.

We define $u_j^{(k)},v_j^{(k)}$ $(j=1,2,\ldots,M+1,\ k=1,2,\ldots,M+1)$ as follows.

(1) Let $\Delta u_j=\Delta v_{j+1}:=\min[u_j,v_{j+1}]$, and $u_j^{(1)}:=u_j-\Delta u_j, v_j^{(1)}:=v_j-\Delta v_j$ for $j=1,2,\ldots,M+1$.
(2) For $\forall j$, we define $\Delta u_j^{(1)}=\Delta v_{j+2}^{(1)}:=\min[u_j^{(1)},v_{j+2}^{(1)}]$, and $u_j^{(2)}:=u_j^{(1)}-\Delta u_j^{(1)}$, $v_j^{(2)}:=v_j^{(1)}-\Delta v_j^{(1)}$.
(3) Similar to step (2), we recursively define $\Delta u_j^{(\ell-1)}=\Delta v_{j+\ell}^{(\ell-1)}:=\min[u_j^{(\ell-1)},v_{j+\ell}^{(\ell-1)}]$, $u_j^{(\ell)}:=u_j^{(\ell-1)}-\Delta u_j^{(\ell-1)}$ and $v_j^{(\ell)}:=v_j^{(\ell-1)}-\Delta v_j^{(\ell-1)}$ for $\ell=2,3,\ldots,M+1$.

From Proposition 2.3, we see that $u_j^{(M+1)}$ and $v_j^{(M+1)}$ are the number of *unconnected* dots in the $(M+2-j)$th box in the column diagrams for b_n^t and v_n^t, respectively. See Example 2.4. Noting that $\Delta u_j^{(M)}=\Delta v_j^{(M)}$ we have

$$u_{n,j}^{t+1}=v_j+u_j^{(M+1)}-v_j^{(M+1)}=v_j+u_j^{(M)}-v_j^{(M)} \tag{24}$$

for $1\leqslant j\leqslant M+1$. The following formulas are easily shown by induction:

$$\begin{aligned}u_j^{(\ell)}=&\max\left[\sum_{i=0}^{\ell-1}u_{j+i},\sum_{i=1}^{\ell-1}u_{j+i}+v_{j+1},\sum_{i=2}^{\ell-1}u_{j+i}+\sum_{i=1}^{2}v_{j+i},\ldots,u_{j+\ell-1}+\sum_{i=1}^{\ell-1}v_{j+i},\sum_{i=1}^{\ell}v_{j+i}\right]\\&-v_{j+1}-\max\left[\sum_{i=1}^{\ell-1}u_{j+i},\sum_{i=2}^{\ell-1}u_{j+i}+v_{j+2},\ldots,u_{j+\ell-1}+\sum_{i=2}^{\ell-1}v_{j+i},\sum_{i=2}^{\ell}v_{j+i}\right],\end{aligned} \tag{25}$$

$$\begin{aligned}v_j^{(\ell)}=&\max\left[\sum_{i=0}^{\ell-1}v_{j-i},\sum_{i=1}^{\ell-1}v_{j-i}+u_{j-1},\sum_{i=2}^{\ell-1}v_{j-i}+\sum_{i=1}^{2}u_{j-i},\ldots,v_{j-\ell+1}+\sum_{i=1}^{\ell-1}u_{j-i},\sum_{i=1}^{\ell}u_{j-i}\right]\\&-u_{j-1}-\max\left[\sum_{i=1}^{\ell-1}v_{j-i},\sum_{i=2}^{\ell-1}v_{j-i}+u_{j-2},\ldots,v_{j-\ell+1}+\sum_{i=2}^{\ell-1}u_{j-i},\sum_{i=2}^{\ell}u_{j-i}\right].\end{aligned} \tag{26}$$

Noticing $u_{j-1}=u_{j+M}$, $v_{j+1}=v_{j-M}$, we find

$$u_j^{(M)}-v_j^{(M)}=\max\left[\sum_{i=0}^{M}u_{j+i},\sum_{i=1}^{M}u_{j+i}+v_{j+1},\sum_{i=2}^{M}u_{j+i}+\sum_{i=1}^{2}v_{j+i},\ldots,\sum_{i=M-1}^{M}u_{j+i}+\sum_{i=1}^{M-1}v_{j+i},u_{j+M}+\sum_{i=1}^{M}v_{j+i}\right]-\max\left[\sum_{i=0}^{M}v_{j-i},\sum_{i=1}^{M}v_{j-i}+u_{j-1},\sum_{i=2}^{M}v_{j-i}+\sum_{i=1}^{2}u_{j-i},\ldots,\sum_{i=M-1}^{M}v_{j-i}+\sum_{i=1}^{M-1}u_{j-i},v_{j-M}+\sum_{i=1}^{M}u_{j-i}\right]. \tag{27}$$

Subtracting

$$\sum_{i=0}^{j-1}u_i+\sum_{i=j+1}^{M+1}v_i$$

from both max[$\cdots$] terms on the right-hand side of the equation and using the relations:

$$u_{M+1}=\theta_n-\sum_{j=1}^{M}u_j,\quad v_{M+1}=\kappa_t-\sum_{j=1}^{M}v_j,$$

we get (22) from (24). Noticing that the number of dots of two column diagrams is preserved in the rule, we obtain (23). □

Our goal in this section is to show that (22) and (23) are ultradiscrete limits of the (one-constrained) nonautonomous discrete KP equation (ndKP equation):

$$(b_{n+1}-c_{j+1})\tau(t,n,j)\tau(t+1,n+1,j+1)+(c_{j+1}-a_{t+1})\tau(t+1,n+1,j)\tau(t,n,j+1)+(a_{t+1}-b_{n+1})\tau(t,n+1,j)\tau(t+1,n,j+1)=0. \tag{28}$$

Here a_t,b_n,c_j are arbitrary complex parameters. The ndKP equation (28), which is sometimes called the (nonautonomous) Hirota–Miwa equation, is equivalent to the generating formulas of the KP hierarchy.[20,21] Its soliton solutions, Lax operators, Darboux transformations, etc., have been investigated in Ref. 22. We set $a_{t+1}=1+\delta_t$ and $b_{n+1}=1+\gamma_n$. We also assume that $c_1=1$, $c_2=c_3=\cdots=c_{M+1}=0$, and

$$\tau(t,n,j+M+1)=\tau(t,n,j). \tag{29}$$

The constraint (29) is an analog of M-reduction of the KP hierarchy which restricts the space of transformation group of τ functions to the subgroup generated by $A_M^{(1)}$.[21] Let

$$U_{n,j}^t:=\frac{\tau(t,n+1,j)\tau(t,n,j+1)}{\tau(t,n,j)\tau(t,n+1,j+1)},\qquad V_{n,j}^t:=\frac{\tau(t+1,n,j+1)\tau(t,n,j)}{\tau(t+1,n,j)\tau(t,n,j+1)}, \tag{30}$$

for $1\leqslant j\leqslant M$. We also introduce a small positive parameter ε, and put $\delta_t=\exp[-\kappa_t/\varepsilon]$ and $\gamma_n=\exp[-\theta_n/\varepsilon]$. Then we have

Theorem 4.2: Let

$$u_{n,j}^t=\lim_{\varepsilon\to+0}\varepsilon\log U_{n,j}^t,$$

$$v_{n,j}^t=\lim_{\varepsilon\to+0}\varepsilon\log V_{n,j}^t$$

be the ultradiscrete limits for $1 \leqslant j \leqslant M$, *and specify* $u^t_{n,M+1}$ *and* $v^t_{n,M+1}$ *by* $\Sigma_{j=1}^{M+1} u^t_{n,j} = \theta_n$ *and* $\Sigma_{j=1}^{M+1} v^t_{n,j} = \kappa_t$. *Then* $\{u^t_{n,j}\}$ *and* $\{v^t_{n,j}\}$ *satisfy (22) and (23).*

Proof: We use abbreviations: $\tau_j := \tau(t,n,j)$, $\tau^t_j := \tau(t+1,n,j)$, $\tau_{n,j} := \tau(t,n+1,j)$, $\tau^t_{n,j} := \tau(t+1,n+1,j)$. The ndKP equation (28) with the constraint (29) is rewritten as the following $M+1$ simultaneous equations:

$$
\begin{aligned}
&(1+\gamma_n)\tau_1\tau^t_{n,2} - (1+\delta_t)\tau^t_{n,1}\tau_2 + (\delta_t - \gamma_n)\tau_{n,1}\tau^t_2 = 0,\\
&(1+\gamma_n)\tau_2\tau^t_{n,3} - (1+\delta_t)\tau^t_{n,2}\tau_3 + (\delta_t - \gamma_n)\tau_{n,2}\tau^t_3 = 0,\\
&\cdots\\
&(1+\gamma_n)\tau_M\tau^t_{n,M+1} - (1+\delta_t)\tau^t_{n,M}\tau_{M+1} + (\delta_t - \gamma_n)\tau_{n,M}\tau^t_{M+1} = 0,\\
&\gamma_n\tau_{M+1}\tau^t_{n,1} - \delta_t\tau^t_{n,M+1}\tau_1 + (\delta_t - \gamma_n)\tau_{n,M+1}\tau^t_1 = 0.
\end{aligned}
\tag{31}
$$

Defining

$$
\begin{aligned}
&x_1 := \tau^t_{n,1}\tau_2\tau_3\cdots\tau_{M+1}, \quad y_1 := \tau_{n,1}\tau^t_2\tau_3\tau_4\cdots\tau_{M+1},\\
&x_2 := \tau_1\tau^t_{n,2}\tau_3\cdots\tau_{M+1}, \quad y_2 := \tau_1\tau_{n,2}\tau^t_3\tau_4\cdots\tau_{M+1},\\
&\cdots \quad \cdots\\
&x_{M+1} := \tau_1\tau_2\tau_3\cdots\tau^t_{n,M+1}, \quad y_{M+1} := \tau^t_1\tau_2\tau_3\tau_4\cdots\tau_{n,M+1},\\
&\vec{x} := (x_1, x_2, \ldots, x_{M+1})^T, \quad \vec{y} := (y_1, y_2, \ldots, y_{M+1})^T,
\end{aligned}
$$

we obtain

$$
\mathbf{L}\vec{x} = (\delta_t - \gamma_n)\vec{y},
$$

where

$$
\mathbf{L} = \begin{pmatrix}
(1+\delta_t) & -(1+\gamma_n) & 0 & \cdots & 0 & 0\\
0 & (1+\delta_t) & -(1+\gamma_n) & 0 & \cdots & 0\\
\vdots & \vdots & \ddots & \ddots & \ddots & \vdots\\
0 & 0 & 0 & \cdots & (1+\delta_t) & -(1+\gamma_n)\\
-\gamma_n & 0 & 0 & \cdots & 0 & \delta_t
\end{pmatrix}.
$$

Its inverse matrix is easily calculated as

$$
\mathbf{L}^{-1} = \mathbf{D}/((1+\delta_t)^M\delta_t - (1+\gamma_n)^M\gamma_n),
$$

$$
(\mathbf{D})_{i,j} = \begin{cases}
(1+\gamma_n)^{M+1-i}(1+\delta_t)^{i-1} & j = M+1\\
\delta_t(1+\delta_t)^{M+i-j-1}(1+\gamma_n)^{j-i} & j \geqslant i\ (j \neq M+1)\\
\gamma_n(1+\gamma_n)^{M-i+j}(1+\delta_t)^{i-j-1}, & j \leqslant i-1\ (j \neq M+1).
\end{cases}
$$

Thus, for $0 < \delta_t,\ \gamma_n \ll 1$, we have

$$(\delta_t-\gamma_n)\mathbf{L}^{-1}\sim\begin{pmatrix}\delta_t & \delta_t & \delta_t & \cdots & \delta_t & 1\\ \gamma_n & \delta_t & \delta_t & \cdots & \delta_t & 1\\ \gamma_n & \gamma_n & \delta_t & \cdots & \delta_t & 1\\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots\\ \gamma_n & \gamma_n & \gamma_n & \cdots & \gamma_n & 1\end{pmatrix}.$$

Precisely speaking, $A\sim B$ means $\lim_{\varepsilon\to+0}\varepsilon\log A(\varepsilon)=\lim_{\varepsilon\to+0}\varepsilon\log B(\varepsilon)$. Since

$$x_j\sim\gamma_n\sum_{i=1}^{j-1}y_i+\delta_t\sum_{i=j}^{M}y_i+y_{M+1}, \tag{32}$$

$$x_{j+1}\sim\gamma_n\sum_{i=1}^{j}y_i+\delta_t\sum_{i=j+1}^{M}y_i+y_{M+1}, \tag{33}$$

we have

$$\frac{x_j}{x_{j+1}}\sim\frac{\gamma_n\Sigma_{i=1}^{j-1}(y_i/y_{M+1})+\delta_t\Sigma_{i=j}^{M}(y_i/y_{M+1})+1}{\gamma_n\Sigma_{i=1}^{j}(y_i/y_{M+1})+\delta_t\Sigma_{i=j+1}^{M}(y_i/y_{M+1})+1}. \tag{34}$$

From the definition of $U_{n,j}^t$ and $V_{n,j}^t$, we find that the left-hand side of (34) is equal to $U_{n,j}^{t+1}/V_{n,j}^t$ and that

$$(y_j/y_{M+1})=\prod_{i=j}^{M}U_{n,i}^t\prod_{i=1}^{j}V_{n,i}^t.$$

Since it holds that

$$\lim_{\varepsilon\to+0}\varepsilon\log\left(\frac{x_j}{x_{j+1}}\right)=\lim_{\varepsilon\to+0}\varepsilon\log[\text{the right-hand side of (34)}]$$

we have (22) by putting

$$u_{n,j}^t=\lim_{\varepsilon\to+0}\varepsilon\log U_{n,j}^t,$$

$$v_{n,j}^t=\lim_{\varepsilon\to+0}\varepsilon\log V_{n,j}^t.$$

From the definitions (30), we have

$$\frac{U_{n,j}^{t+1}}{U_{n,j}^t}=\frac{V_{n,j}^t}{V_{n+1,j}^t},$$

which gives (23) in the ultradiscrete limit. □

Next, we consider soliton solutions to the $A_M^{(1)}$ automaton. It is obvious that if the limit

$$Y_{n,j}^t:=\lim_{\varepsilon\to+0}\varepsilon\log\tau(t,n,j) \tag{35}$$

exists, then from (30) we have for $1\leqslant j\leqslant M$,

$$u_{n,j}^t = Y_{n+1,j}^t + Y_{n,j+1}^t - Y_{n,j}^t - Y_{n+1,j+1}^t,$$
$$v_{n,j}^t = Y_{n,j+1}^{t+1} + Y_{n,j}^t - Y_{n,j}^{t+1} - Y_{n,j+1}^t. \tag{36}$$

From Theorem 4.2, they satisfy (22) and (23). Hence we have only to know $Y_{n,j}^t$ to get solutions to (22) and (23). We will call $Y_{n,j}^t$ an N soliton solution to the $A_M^{(1)}$ automaton when it is an ultradiscrete limit of one parameter (ε) family of certain $M\times N$ soliton solutions $\tau(t,n,j)$ to the ndKP equation (28) as explained in Appendix B. It indeed corresponds to an N soliton state in the sense of Sec. III A.

The following fact is well known.[21,22]

Proposition 4.3: The N soliton solution to (28) is given by the vacuum expectation value:

$$\tau(t,n,j) = \langle \mathrm{vac}|g(\mathbf{t})|\mathrm{vac}\rangle, \tag{37}$$

$$g(\mathbf{t}) = \prod_{k=1}^{N} (1+\alpha_k \psi(p_k,\mathbf{t})\psi^*(q_k,\mathbf{t})). \tag{38}$$

Here $\mathbf{t}=(t,n,j)$ *and* $\alpha_k (k=1,2,\ldots,N)$ *are arbitrary complex constants,*

$$\psi(p,\mathbf{t}) = \left[\prod_{t'}^{t} (a_{t'}-p)\prod_{n'}^{n} (b_{n'}-p)^{-1}\prod_{j'=1}^{j} (-c_{j'}+p)^{-1}\right]\psi(p),$$

$$\psi^*(q,\mathbf{t}) = \left[\prod_{t'}^{t} (a_{t'}-q)^{-1}\prod_{n'}^{n} (b_{n'}-q)\prod_{j'=1}^{j} (-c_{j'}+q)\right]\psi^*(q),$$

with

$$\prod_{n'}^{n} X_{n'} := \begin{cases} \Pi_{n'=1}^{n} X_{n'}, & 1\leqslant n \\ 1, & n=0 \\ \Pi_{n'=n+1}^{0} X_{n'}^{-1}, & n\leqslant -1, \end{cases}$$

and $\psi(p),\psi^*(q)$ *are fermionic field operators which satisfy*

$$\{\psi(p),\psi(p')\}_+ := \psi(p)\psi(p')+\psi(p')\psi(p)=0,$$

$$\{\psi^*(q),\psi^*(q')\}_+ = 0, \quad \{\psi(p),\psi^*(q)\}_+ = 0 \ \text{ for } \ (p\neq q),$$

$$\langle \mathrm{vac}|\psi(p_1)\psi(p_2)\cdots\psi(p_r)\psi^*(q_r)\psi^*(q_{r-1})\cdots\psi^*(q_1)|\mathrm{vac}\rangle$$
$$= \det\left(\frac{1}{p_i-q_j}\right)_{1\leqslant i,j\leqslant r} = \frac{\Pi_{i<j}(p_i-p_j)(q_j-q_i)}{\Pi_{i,j}(p_i-q_j)}.$$

The N soliton solution (38) is also a solution to (31) when it satisfies the constraint (29). We can easily show

Proposition 4.4: The constraint (29) is achieved if it holds that

$$\left(\frac{q_k}{p_k}\right)^M \left(\frac{1-q_k}{1-p_k}\right) = 1 \quad (k=1,2,\cdots,N). \tag{39}$$

Note that, for a given p_k, there are M q_k's which satisfy (39) and $q_k\neq p_k$. We use this fact to construct explicit solutions.

From Propositions 4.3 and 4.4, we can construct a class of N soliton solutions to the $A_M^{(1)}$ automaton. The result is summarized as

Theorem 4.5:

$$Y_{n+1,j+1}^{t+1}=\max_{\vec{\mu}}\left[\sum_{i=1}^{N}\mu_i K^{(i)}(t,n,j)-A(\vec{\mu};j)\right] \tag{40}$$

is an N soliton solution to the $A_M^{(1)}$ automaton. Here $\vec{\mu}=(\mu_1,\mu_2,\ldots,\mu_N)$ $(\mu_i=0,1)$ and $\max_{\vec{\mu}}[\cdots]$ denotes the maximum among the 2^N values obtained by putting $\mu_i=0$ or 1 for $i=1,2,\ldots,N$,

$$K^{(i)}(t,n,j)=K_0^{(i)}-\sum_{j'=1}^{j}\nu_{j'}^{(i)}-\sum_{t'}^{t}\min[\kappa_{t'},L^{(i)}]+\sum_{n'}^{n}\min[\theta_{n'},L^{(i)}],$$

where the sums here are generally defined by

$$\sum_{n'}^{n}X_{n'}:=\begin{cases}\Sigma_{n'=1}^{n}X_{n'}, & 1\leqslant n\\ 0, & n=0\\ -\Sigma_{n'=n+1}^{0}X_{n'}, & n\leqslant -1.\end{cases}$$

$L^{(i)}$, $\nu_j^{(i)}$ $(1\leqslant i\leqslant N,1\leqslant j\leqslant M)$ are non-negative integers which satisfy $L^{(i)}=\Sigma_{j=1}^{M}\nu_j^{(i)}$,

$$L^{(1)}\geqslant L^{(2)}\geqslant\cdots\geqslant L^{(N)},$$

$$\nu_j^{(1)}\geqslant\nu_j^{(2)}\geqslant\cdots\geqslant\nu_j^{(N)}\quad(j=1,2,\ldots,M),$$

and $K_0^{(i)}$ is an arbitrary integer. In the case:

$$\left\{\begin{array}{ll}\mu_i=1 & \text{for } i=i_1,i_2,\ldots,i_p\\ \mu_i=0 & \text{otherwise}\end{array}\right\}$$

the phase factor $A(\vec{\mu};j)$ is given by

$$A(\vec{\mu};j)=\sum_{k=1}^{p}(k-1)L^{(i_k)}+\sum_{k=1}^{p}(X^{(i_k)}(j+k-1)-X^{(i_k)}(j)),$$

where $X^{(i)}(j)=\Sigma_{j'=1}^{j}\nu_{j'}^{(i)}$ with $\nu_{j+M}^{(i)}=\nu_j^{(i)}$.

The proof of this theorem is parallel to that in Ref. 7. We give the detail in Appendix B. For $N=1$ it is the general solution, and we conjecture that it is also so for $M=1$. Except for these cases the above-mentioned result does not cover the arbitrary initial condition. There is some freedom to employ different ''phase factors'' $A(\vec{\mu};j)$ than the above-mentioned one depending on the way in taking the ultradiscrete limit.

V. SUMMARY

In this paper we have introduced the $A_M^{(1)}$ automaton, which is a crystal theoretic formulation of the generalized box–ball systems. In terms of the box–ball systems, it corresponds to the dynamics of M kinds of balls, where the carriers and boxes have arbitrary and inhomogeneous capacities. We have introduced the solitons labeled with the crystals B_k' of $U_q'(A_{M-1}^{(1)})$. Scattering matrices of two solitons are identified with the combinatorial R matrices of $U_q'(A_{M-1}^{(1)})$ crystals. Piecewise linear evolution equations are obtained and identified with an ultradiscrete limit of the nonautonomous discrete KP equation. It allowed us to construct a class of N soliton solutions. We have left the studies of phase shifts in the scattering and construction of N soliton solutions corresponding to arbitrary initial conditions for $N\geqslant 2$ as future problems. The interplay between

the ultradiscrete limit of the classical integrable systems and the $q \to 0$ limit of the quantum integrable systems elucidated in this paper deserves further investigation.

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APPENDIX A: PROOF OF PROPOSITION 3.8

First we show that it suffices to prove Proposition 3.8 for $M=1$ and $h=k$. Without a loss of generality we may set $M=2$ and consider the time evolution $T_{\kappa=\infty}$. We find it convenient to adopt the equivalent box–ball system picture explained in Sec. II D. Thus the elements in $B_1^{\otimes \mathcal{L}}$ in (13) will be represented as ... 131..2 ... for example. It stands for the array of the balls with the indices 1, 3, 1 and 2 and . denotes an empty box. (So they do *not* correspond to the letters in the semistandard tableaux in the crystal notation.) We keep the same notation $\hat{\theta}$ to denote the map corresponding to (12) in the box–ball picture. It groups the array of balls and empty boxes locally together into the boxes with capacities $\ldots, \theta_n, \theta_{n+1}, \ldots$. Then the assertion of Proposition 3.8 is that the scattering

$$\hat{\theta}(\ldots \overbrace{2\cdots 2}^{l} \ldots \overbrace{1\cdots 1}^{k-h}\overbrace{2\cdots 2}^{h}\ldots) \xrightarrow{(\tilde{T}_2\tilde{T}_1)^t} \hat{\theta}(\ldots \overbrace{2\cdots 2}^{k} \ldots \overbrace{1\cdots 1}^{k-h}\overbrace{2\cdots 2}^{l+h-k}\ldots) \tag{A1}$$

takes place for sufficiently large t. Here $\tilde{T}_1, \tilde{T}_2$ are the ball-moving operators defined in Sec. II D, and we have used $T_\infty^t = (\tilde{T}_2\tilde{T}_1)^t$ in view of (10) and the fact that the balls with index $\geqslant 3$ are absent. In (A1) the sequences ... of the empty boxes are sufficiently long since both sides are to represent the asymptotic two-soliton states in the sense of Sec. III A. Now we make use of the relation $(\tilde{T}_2\tilde{T}_1)^t = \tilde{T}_2(\tilde{T}_1\tilde{T}_2)^{t-1}\tilde{T}_1$. From the definition of the operators $\tilde{T}_i$'s and the assumption that the two solitons are sufficiently separated, (A1) is equivalent to

$$\hat{\theta}(\ldots \overbrace{2\cdots 2}^{l} \ldots \overbrace{2\cdots 2}^{h}\overbrace{1\cdots 1}^{k-h}\ldots) \xrightarrow{(\tilde{T}_1\tilde{T}_2)^{t-1}} \hat{\theta}(\ldots \overbrace{2\cdots 2}^{k} \ldots \overbrace{2\cdots 2}^{l+h-k}\overbrace{1\cdots 1}^{k-h}\ldots). \tag{A2}$$

But this is justified once one establishes

$$\hat{\theta}(\ldots \overbrace{1\cdots 1}^{l} \ldots \overbrace{1\cdots 1}^{k}\ldots) \xrightarrow{\tilde{T}_1^{t-1}} \hat{\theta}(\ldots \overbrace{1\cdots 1}^{k} \ldots \overbrace{1\cdots 1}^{l}\ldots), \tag{A3}$$

because (A2) and (A3) correspond to the same canonical system $\hat{\theta}(\ldots 12\cdots l \ldots . l+1\cdots l+k \ldots)$ in the sense of Sec. II D with respect to the relevant time evolutions and therefore they possess the parallel time evolution pattern owing to (11). In this way the proof of Proposition 3.8 is reduced to (A3), which is equivalent to the case $M=1$ and $h=k$.

Now setting $L^{(1)}=l$ and $L^{(2)}=k$, we are to show

Proposition A.1: Set $M=1$, assume that $\kappa_t \geqslant L^{(1)}(\forall t)$ and $\theta_n < L^{(1)}$ for all but finitely many n's. Then two solitons with amplitudes $L^{(1)}$ and $L^{(2)}(L^{(1)}>L^{(2)})$ scatter into two solitons with amplitudes $L^{(2)}$ and $L^{(1)}$, respectively.

Namely, the amplitudes of two solitons do not change after the collision. To prove the proposition, we need several lemmas. The following two lemmas are obvious.

Lemma A.2: For given integers K_1 and K_2, if there exists an integer n_0 such that

$$K_1+\sum_{n'}^{n_0}\ \min[\,\theta_{n'},L^{(1)}]\geqslant 0\geqslant K_2+\sum_{n'}^{n_0}\ \min[\,\theta_{n'},L^{(2)}],$$

then, for $n\geqslant n_0$,

$$K_1+\sum_{n'}^{n}\ \min[\,\theta_{n'},L^{(1)}]\geqslant K_2+\sum_{n'}^{n}\ \min[\,\theta_{n'},L^{(2)}],$$

and for $n<n_0$,

$$0>K_2+\sum_{n'}^{n}\ \min[\,\theta_{n'},L^{(2)}].$$

Lemma A.3: For given integers K_1' *and* K_2', *if there exists an integer* n_0 *such that*

$$K_2'+\sum_{n'}^{n_0}\ \min[\,\theta_{n'},L^{(2)}]\geqslant 2L^{(2)}>0\geqslant K_1'+\sum_{n'}^{n_0}\ \min[\,\theta_{n'},L^{(1)}],$$

then, for $n\geqslant n_0$,

$$K_1'+K_2'+\sum_{n'}^{n}\ \min[\,\theta_{n'},L^{(1)}]+\sum_{n'}^{n}\ \min[\,\theta_{n'},L^{(2)}]-2L^{(2)}\geqslant K_1'+\sum_{n'}^{n}\ \min[\,\theta_{n'},L^{(1)}],$$

and for $n<n_0$,

$$0>K_1'+\sum_{n'}^{n}\ \min[\,\theta_{n'},L^{(1)}].$$

Now we define an integer $N_0(t)$ for given integers K_2 and t as

$$K_2-L^{(2)}t+\sum_{n'}^{N_0(t)}\ \min[\,\theta_{n'},L^{(2)}]\geqslant 2L^{(2)}>K_2-L^{(2)}t+\sum_{n'}^{N_0(t)-1}\ \min[\,\theta_{n'},L^{(2)}].$$

With this $N_0(t)$ we can show

Lemma A.4: For any integers K_1 *and* K_2, *we have*

$$\lim_{T\to\infty}\left(K_2-L^{(2)}T+\sum_{n'}^{N_0(T)}\ \min[\,\theta_{n'},L^{(2)}]-K_1+L^{(1)}T-\sum_{n'}^{N_0(T)}\ \min[\,\theta_{n'},L^{(1)}]\right)=+\infty.$$

Proof: From the definition of $N_0(t)$, we have

$$-L^{(2)}<-tL^{(2)}+\sum_{n'=N_0(0)+1}^{N_0(t)}\ \min[\,\theta_{n'},L^{(2)}]<L^{(2)}. \tag{A4}$$

Hence we have

$$\Delta(t) := -L^{(2)}t + \sum_{n'=N_0(0)+1}^{N_0(t)} \min[\theta_{n'}, L^{(2)}] - \left(-L^{(1)}t + \sum_{n'=N_0(0)+1}^{N_0(t)} \min[\theta_{n'}, L^{(1)}] \right)$$

$$= t(L^{(1)} - L^{(2)}) - \sum_{n'=N_0(0)+1}^{N_0(t)} (\min[\theta_{n'}, L^{(1)}] - \min[\theta_{n'}, L^{(2)}]) \geqslant t(L^{(1)} - L^{(2)})$$

$$- \sum_{n'=N_0(0)+1}^{N_0(t)} (\theta_{n'} - \min[\theta_{n'}, L^{(2)}]) > tL^{(1)} - L^{(2)} - \sum_{n'=N_0(0)+1}^{N_0(t)} \theta_{n'}. \tag{A5}$$

From (A4), we obtain an inequality:

$$t > -1 + \frac{1}{L^{(2)}} \sum_{n'=N_0(0)+1}^{N_0(t)} \min[\theta_{n'}, L^{(2)}].$$

Thus, from (A5), we find

$$\Delta(t) > -(L^{(1)} + L^{(2)}) + \sum_{n'=N_0(0)+1}^{N_0(t)} \min\left[\frac{L^{(1)} - L^{(2)}}{L^{(2)}} \theta_{n'}, L^{(1)} - \theta_{n'} \right]. \tag{A6}$$

Since $L^{(1)} > L^{(2)}, L^{(1)} > \theta_n$ for all but finitely many n's and $\lim_{t \to +\infty} N_0(t) = +\infty$ which is seen from (A4), we find

$$\lim_{t \to +\infty} \Delta(t) = +\infty. \tag{A7}$$

This suffices to prove the lemma. □

Now we prove Proposition A.1. From (36) we have

$$u_n^t := u_{n,j=1}^{t+1} = Y_{n+1,1}^{t+1} - Y_{n+1,2}^{t+1} - Y_{n,1}^{t+1} + Y_{n,2}^{t+1}. \tag{A8}$$

Specializing Theorem 4.5 to a two-soliton solution with $M = 1$ and $\kappa_t = +\infty$, we have

$$Y_{n+1,1}^{t+1} = \max[0, K_1(n,t), K_2(n,t), K_1(n,t) + K_2(n,t) - 2L^{(2)}],$$

$$Y_{n+1,2}^{t+1} = \max[0, K_1(n,t) - L^{(1)}, K_2(n,t) - L^{(2)}, K_1(n,t) + K_2(n,t) - L^{(1)} - 3L^{(2)}],$$

$$K_i(n,t) = K_i + \sum_{n'}^{n} \min[\theta_{n'}, L^{(i)}] - tL^{(i)} \quad (i = 1,2).$$

Note that $Y_{n,2}^t = Y_{n,1}^{t+1}$ due to the last equation in (31) and the condition $\delta_t = \exp[-\kappa_t/\varepsilon] = 0$. Given $L^{(1)} > L^{(2)}$, there exist integers n_1, n_2, j, r_1, r_2 that satisfy

$$n_1 \leqslant n_1 + j \leqslant n_2, \quad 1 \leqslant r_1 \leqslant \min(L^{(1)}, \theta_{n_1}), \quad 1 \leqslant r_2 \leqslant \min(L^{(2)}, \theta_{n_2}),$$

$$K_1 + \sum_{n'}^{n_1} \min[\theta_{n'}, L^{(1)}] > 0 \geqslant K_2 + \sum_{n'}^{n_1} \min[\theta_{n'}, L^{(2)}],$$

$$K_1 - L^{(1)} + \sum_{n'}^{n_1+j} \min[\theta_{n'}, L^{(1)}] > 0 \geqslant K_2 - L^{(2)} + \sum_{n'}^{n_1+j} \min[\theta_{n'}, L^{(2)}],$$

where $K_i (i=1,2)$ is defined by

$$K_1 = r_1 - \sum_{n'}^{n_1} \min[\theta_{n'}, L^{(1)}],$$

$$K_2 = r_2 + 2L^{(2)} - \sum_{n'}^{n_2} \min[\theta_{n'}, L^{(2)}].$$

From Lemma A.2, we find at $t=0$ that

$$\begin{aligned} Y^1_{n+1,1} &= \max[0, K_1(n,0), K_1(n,0) + K_2(n,0) - 2L^{(2)}], \\ Y^1_{n+1,2} &= \max[0, K_1(n,0) - L^{(1)}, K_1(n,0) + K_2(n,0) - L^{(1)} - 3L^{(2)}]. \end{aligned} \tag{A9}$$

Substituting (A9) into Eq. (A8), we obtain

$$u^0_n = \begin{cases} 0 & \text{for } n < n_1 \\ r_1 & \text{for } n = n_1 \\ \theta_n & \text{for } n_1 < n < n'_1 \\ L^{(1)} - \sum_{n'=n_1+1}^{n'_1-1} \theta_{n'} - r_1 & \text{for } n = n'_1 \\ 0 & \text{for } n'_1 < n < n_2 \\ r_2 & \text{for } n = n_2 \\ \theta_n & \text{for } n_2 < n < n'_2 \\ L^{(2)} - \sum_{n'=n_2+1}^{n'_2-1} \theta_{n'} - r_2 & \text{for } n = n'_2 \\ 0 & \text{for } n'_2 < n, \end{cases} \tag{A10}$$

where $n'_i (i=1,2)$ are defined by $n'_i = n_i + 1$ if $r_i = L^{(i)}$, and otherwise by

$$L^{(i)} - \sum_{n'=n_i+1}^{n'_i} \theta_{n'} - r_i \leqslant 0 < L^{(i)} - \sum_{n'=n_i+1}^{n'_i-1} \theta_{n'} - r_i .$$

Thus we see that the two-soliton solution can correspond to any initial configuration in which $L^{(1)}$ soliton is situated to the left-hand side of $L^{(2)}$ soliton with sufficient spacing. Hence, to prove the proposition, we have only to show that the solution u^t_n describes the two-soliton state in which $L^{(2)}$ soliton is the left-hand side of $L^{(1)}$ soliton for $t \gg 1$.

From the definition of $N_0(t)$ and Lemma A.4, there exists T and j such that

$$K_2 - L^{(2)}T + \sum_{n'}^{N_0(T)} \min[\theta_{n'}, L^{(2)}] > 0 \geqslant K_1 - L^{(1)}T + \sum_{n'}^{N_0(T)} \min[\theta_{n'}, L^{(1)}],$$

$$K_2 - L^{(2)}T - L^{(2)} + \sum_{n'}^{N_0(T)+j} \min[\theta_{n'}, L^{(2)}] > 0 \geqslant K_1 - L^{(1)}T - L^{(1)} + \sum_{n'}^{N_0(T)+j} \min[\theta_{n'}, L^{(1)}].$$

Thus, from Lemma A.3, we have at $t=T$ that

$$Y_{n+1,1}^{T+1}=\max[0,K_2(n,T),K_1(n,T)+K_2(n,T)-2L^{(2)}],$$

$$Y_{n+1,2}^{T+1}=\max[0,K_2(n,T)-L^{(2)},K_1(n,T)+K_2(n,T)-L^{(1)}-3L^{(2)}].$$

Substituting these into Eq. (A8), we find that u_n^T describes a configuration in which $L^{(2)}$ soliton locates around $n=N_0(T)$ and $L^{(1)}$ soliton does around $n\gg N_0(T)$. This completes the proof.

APPENDIX B: DERIVATION OF *N* SOLITON SOLUTIONS

Here we explain the derivation of the N soliton solution in Theorem 4.5 along the simple cases $N=1$ and $N=2$. First we consider one-soliton solution. We will show that it has the form:

$$Y_{n,j}^t=\max\left[0,K_0-\sum_{i=1}^{j-1}\ell_i-\sum_{t'}^{t-1}\min[\kappa_{t'},L]+\sum_{n'}^{n-1}\min[\theta_{n'},L]\right], \tag{B1}$$

where L is the amplitude, K_0 is an integer which is related to the phase of the soliton, and ℓ_i $(i=1,2,\ldots,M)$ are the non-negative integers which correspond to the number of ith balls in the soliton and $\Sigma_{i=1}^M\ell_i=L$. We give some details of its derivation, because similar technical difficulties in obtaining multisoliton solutions are resolved in the same way.

To obtain (B1), we take $g(\mathbf{t})$ in (38) as

$$g(\mathbf{t})=\prod_{\ell=0}^{M-1}(1+c_\ell(p)\psi(p,\mathbf{t})\psi^*(q_\ell,\mathbf{t}))=1+\psi(p,\mathbf{t})\phi^*(p,\mathbf{t}),$$
$$\phi^*(p,\mathbf{t}):=\sum_{\ell=0}^{M-1}c_\ell(p)\psi^*(q_\ell,\mathbf{t}), \tag{B2}$$

where q_ℓ $(\ell=0,1,\ldots,M-1)$ are the roots of the algebraic equation:

$$\frac{x^M(1-x)-p^M(1-p)}{x-p}=0,\quad (x\neq p) \tag{B3}$$

for a given real number $p[(1+M^{-1})^{-1}<p<1]$, and $c_\ell(p)$ $(0\leqslant\ell\leqslant M-1)$ are complex coefficients which will be determined later. Since (B3) has one real positive root, we assume that q_0 is positive and we put $\eta=q_0/p$. Then p and q_0 satisfy

$$p=\frac{1-\eta^M}{1-\eta^{M+1}}, \tag{B4}$$

$$1-p=\eta^M\left(\frac{1-\eta}{1-\eta^{M+1}}\right), \tag{B5}$$

$$q_0=\eta\left(\frac{1-\eta^M}{1-\eta^{M+1}}\right). \tag{B6}$$

The τ function $\tau(t,n,j)$ is given by vacuum expectation value as

$$\tau(t,n,j)=\langle \mathrm{vac}|g(\mathbf{t})|\mathrm{vac}\rangle$$
$$=1+\sum_{\ell=0}^{M-1} c_\ell(p)\frac{1}{p-q_\ell}\left(\frac{q_\ell}{p}\right)^{j-M-1}\left(\frac{1-p/(1+\delta_0)}{1-q_\ell/(1+\delta_0)}\right)\left(\frac{1-q_\ell/(1+\gamma_0)}{1-p/(1+\gamma_0)}\right)$$
$$\times\prod_{t'}^{t-1}\left(\frac{1-p/(1+\delta_{t'})}{1-q_\ell/(1+\delta_{t'})}\right)\prod_{n'}^{n-1}\left(\frac{1-q_\ell/(1+\gamma_{n'})}{1-p/(1+\gamma_{n'})}\right). \tag{B7}$$

We introduce a small positive parameter ε and put $\eta=\exp[-L/(M\varepsilon)]$. We also put

$$\tilde{c}_\ell(p):=\frac{c_\ell(p)}{p-q_\ell}\left(\frac{q_\ell}{p}\right)^{-M-1}\left(\frac{1-p/(1+\delta_0)}{1-q_\ell/(1+\delta_0)}\right)\left(\frac{1-q_\ell/(1+\gamma_0)}{1-p/(1+\gamma_0)}\right)$$
$$\times\prod_{t'=-T_0}^{0}(1-q_\ell/(1+\delta_{t'}))\prod_{n'=1}^{N_0}(1-q_\ell/(1+\gamma_{n'})), \tag{B8}$$

$$\chi_p(s):=\sum_{\ell=0}^{M-1}\tilde{c}_\ell(p)\left(\frac{q_\ell}{p}\right)^s \quad (s\in\mathbb{Z}), \tag{B9}$$

where $T_0=T_0(\varepsilon)$ and $N_0=N_0(\varepsilon)$ are positive integers which satisfy $T_0\simeq N_0\simeq 1/\varepsilon$. Hence,

$$\lim_{\varepsilon\to+0}T_0=\lim_{\varepsilon\to+0}N_0=+\infty.$$

Since

$$\chi_p(s+M)=\sum_{\ell=0}^{M-1}\tilde{c}_\ell(p)\left(\frac{q_\ell}{p}\right)^{s+M}$$
$$=\sum_{\ell=0}^{M-1}\tilde{c}_\ell(p)\left(\frac{q_\ell}{p}\right)^{s}\left(\frac{1-p}{1-q_\ell}\right)$$
$$=(1-p)\sum_{i=0}^{\infty}p^i\sum_{\ell=0}^{M-1}\tilde{c}_\ell(p)\left(\frac{q_\ell}{p}\right)^{s+i}$$
$$=(1-p)\sum_{i=0}^{\infty}p^i\chi_p(s+i),$$

we have

$$\chi_p(s+M)=\sum_{i=0}^{M-1}\left(\sum_{\ell=0}^{\infty}(1-p)^{\ell+1}p^{M\ell}\varrho_\ell(i)\right)p^i\chi_p(s+i), \tag{B10}$$

where $\varrho_0(i)=1$, $\varrho_1(i)=i+1$, and

$$\varrho_\ell(i)=\sum_{k_1=(\ell-1)M}^{(\ell-1)M+i}\ \sum_{k_2=(\ell-2)M}^{k_1}\cdots\sum_{k_\ell=0}^{k_{\ell-1}}1$$
$$=\frac{(i+1)}{\ell!}\prod_{j=1}^{\ell-1}(\ell M+i+j+1),$$

for $\ell \geqslant 2$. Note that $\chi_p(s)$ is a real function when $\chi_p(j)$ $(0 \leqslant j \leqslant M-1)$ are real. The ratio $\varrho_{\ell+1}(i)/\varrho_\ell(i)$ $(\ell \geqslant 1, 0 \leqslant i \leqslant M-1)$ is calculated as

$$\frac{\varrho_{\ell+1}(i)}{\varrho_\ell(i)} = \frac{(\ell+1)(M+1)+i}{\ell+1} \prod_{k=2}^{\ell} \left(1+\frac{M}{\ell M+i+k}\right) < (M+1)\left(1+\frac{1}{\ell}\right)^{\ell} < (M+1)e.$$

Hence, if it holds that $(1-p)p^M < (M+1)^{-1}e^{-1}$, we obtain

$$|\chi_p(s+M)| \leqslant (1-p)\sum_{i=0}^{M-1} \left(1+(i+1)\frac{(1-p)p^M}{1-(1-p)p^M(M+1)e}\right)|\chi_p(s+i)|. \tag{B11}$$

Thus we find

$$\chi_p(s+M) \sim \eta^M \sum_{i=0}^{M-1} \chi_p(s+i)$$

for sufficiently small η.

We assume the following for $\chi_p(j)$:

$$\begin{aligned} \chi_p(1) &= \chi_0, \\ \chi_p(2) &= N_1 y^{\ell_1} \chi_p(1), \\ \chi_p(3) &= N_2 y^{\ell_2} \chi_p(2), \\ &\cdots \\ \chi_p(M) &= N_{M-1} y^{\ell_{M-1}} \chi_p(M-1). \end{aligned} \tag{B12}$$

Here χ_0 is a positive number which is related to the initial phase of soliton, $y = \exp[-1/\varepsilon]$, ℓ_j and $N_j = N_j(\varepsilon)$ $(j = 1,2,\ldots,M-1)$ are non-negative integers and positive numbers, respectively. They are also supposed to satisfy

$$\begin{aligned} &\ell_M := L - \sum_{j=1}^{M-1} \ell_j \geqslant 0, \\ &\lim_{\varepsilon \to 0} \varepsilon \log N_j(\varepsilon) = 0, \\ &N_j y^{\ell_j} \leqslant \varepsilon^{N^*}, \end{aligned} \tag{B13}$$

for a sufficiently large positive integer N^*. From these conditions, $\tilde{c}_\ell(p)$ $(0 \leqslant \ell \leqslant M-1)$ are uniquely determined by

$$\begin{pmatrix} q_0 & q_1 & \cdots & q_{M-1} \\ q_0^2 & q_1^2 & \cdots & q_{M-1}^2 \\ \vdots & \vdots & \ddots & \vdots \\ q_0^M & q_1^M & \cdots & q_{M-1}^M \end{pmatrix} \begin{pmatrix} \tilde{c}_0(p) \\ \tilde{c}_1(p) \\ \vdots \\ \tilde{c}_{M-1}(p) \end{pmatrix} = \begin{pmatrix} p\chi_p(1) \\ p^2\chi_p(2) \\ \vdots \\ p^M\chi_p(M) \end{pmatrix}. \tag{B14}$$

Note that the determinant of the $M \times M$ matrix on the left-hand side is equal to

$$\left(\prod_{i=0}^{M-1} q_i\right)\left(\prod_{j>i} (q_j - q_i)\right) \neq 0.$$

It should be also noted from (B11) to (B13) that

$$\chi_p(i) \geqslant \varepsilon^{-N^*}\chi_p(i+1) \quad \text{for } \forall i,$$
$$\chi_p(i) \geqslant C\exp[L/\varepsilon]\chi_p(i+M) \quad \text{for } \forall i \text{ and } \exists C>0. \tag{B15}$$

From (B7), we have

$$\tau(t,n,j) = 1 + \sum_{\ell=0}^{M-1} \tilde{c}_\ell(p)\left(\frac{q_\ell}{p}\right)^i \prod_{t'=-T_0}^{t-1}\left(1-\frac{q_\ell}{1+\delta_{t'}}\right)^{-1}\prod_{t'}^{t-1}\left(1-\frac{p}{1+\delta_{t'}}\right)$$
$$\times \prod_{n'}^{n-1}\left(1-\frac{p}{1+\gamma_{n'}}\right)^{-1}\prod_{n'=n}^{N_0}\left(1-\frac{q_\ell}{1+\gamma_{n'}}\right)^{-1}. \tag{B16}$$

Hereafter we restrict ourselves to the region: $|n| \leqslant N_0$ and $|t| \leqslant T_0$. Noticing that

$$\prod_{t'=T_0}^{t-1}\left(1-\frac{q_\ell}{1+\delta_{t'}}\right)^{-1}\prod_{n'=n}^{N_0}\left(1-\frac{q_\ell}{1+\gamma_{n'}}\right)^{-1}$$
$$= 1 + \left(\sum_{t=-T_0}^{t-1}\left(\frac{1}{1+\delta_{t'}}\right) + \sum_{n'=n}^{N_0}\left(\frac{1}{1+\gamma_{n'}}\right)\right)q_\ell + \cdots$$
$$=: 1 + a_1\left(\frac{q_\ell}{p}\right) + a_2\left(\frac{q_\ell}{p}\right)^2 + a_3\left(\frac{q_\ell}{p}\right)^3 + \cdots,$$

we find

$$\tau(t,n,j) = 1 + \prod_{t'}^{t-1}\left(1-\frac{p}{1+\delta_{t'}}\right)\prod_{n'}^{n-1}\left(1-\frac{p}{1+\gamma_{n'}}\right)^{-1}\sum_{i=0}^{\infty} a_i\chi_p(j+i), \tag{B17}$$

where $a_0 = 1$ and $a_{i+1}/a_i \sim \varepsilon^{-1}$. From (B15), we have

$$0 < \sum_{i=1}^{\infty} a_i\chi_p(j+i) < \chi_p(j)$$

for sufficiently small ε. Putting $\chi_0 = \exp[K_0/\varepsilon]$ and noticing the relations:

$$\lim_{\varepsilon\to+0} \varepsilon\log(1-p) = -L,$$

$$\lim_{\varepsilon\to+0} \varepsilon\log\chi_p(j) = K_0 - \sum_{i=1}^{j-1}\ell_i,$$

$$\lim_{\varepsilon\to+0} \varepsilon\log\left(1-\frac{p}{1+\gamma_n}\right)^{-1} = \min[L,\theta_n],$$

$$\lim_{\varepsilon\to+0} \varepsilon\log\left(1-\frac{p}{1+\delta_t}\right) = -\min[L,\kappa_t],$$

we obtain

$$\lim_{\varepsilon\to+0}\ \varepsilon\log\tau(t,n,j)=\max\left[0,K_0-\sum_{i=1}^{j-1}\ell_i-\sum_{t'}^{t-1}\min[\kappa_{t'},L]+\sum_{n'}^{n-1}\min[\theta_{n'},L]\right]. \tag{B18}$$

Since

$$\lim_{\varepsilon\to+0}\ N_0(\varepsilon)=\lim_{\varepsilon\to+0}\ T_0(\varepsilon)=+\infty,$$

we have shown that (B1) is a one-soliton solution to the $A_M^{(1)}$ automaton.

Next we consider two-soliton solutions. From the previous arguments about one-soliton solution, we see that the field operators $\psi(p)$ and $\phi^*(p)$ are essentially determined by L, ℓ_j $(j=1,2,\ldots,M)$ and K_0. Therefore we denote these operators by

$$\psi(p)=\psi(L:\varepsilon),\quad \phi^*(p)=\phi^*(L;\{\ell_j\};K_0:\varepsilon). \tag{B19}$$

Then we take

$$g(\mathbf{t})=(1+\psi(p_1,\mathbf{t})\phi^*(p_1,\mathbf{t}))(1+\psi(p_2,\mathbf{t})\phi^*(p_2,\mathbf{t})), \tag{B20}$$

where

$$\psi(p_i)=\psi(L^{(i)}:\varepsilon),\quad \phi^*(p_i)=\phi^*(L^{(i)};\{\ell_j^{(i)}\};K_0^{(i)}:\varepsilon)\quad (i=1,2). \tag{B21}$$

We also assume $L^{(1)}\geqslant L^{(2)}$ and $\ell_j^{(1)}\geqslant\ell_j^{(2)}$ $(j=1,2,\ldots,M)$. As we shall see in the following, the latter condition turns out to be a natural constraint for soliton solutions. Using similar notations as given previously, we have

$$\begin{aligned}\tau(t,n,j)&=\langle\mathrm{vac}|(1+\psi(p_1,\mathbf{t})\phi^*(p_1,\mathbf{t}))(1+\psi(p_2,\mathbf{t})\phi^*(p_2,\mathbf{t}))|\mathrm{vac}\rangle\\&=1+\langle\mathrm{vac}|\psi(p_1,\mathbf{t})\phi^*(p_1,\mathbf{t})|\mathrm{vac}\rangle+\langle\mathrm{vac}|\psi(p_2,\mathbf{t}))\phi^*(p_2,\mathbf{t})|\mathrm{vac}\rangle\\&\quad+\langle\mathrm{vac}|\psi(p_1,\mathbf{t})\psi^*(p_1,\mathbf{t})\psi(p_2,\mathbf{t})\phi^*(p_2,\mathbf{t})|\mathrm{vac}\rangle.\end{aligned} \tag{B22}$$

The second and third terms are calculated in the same way as above. The fourth term is evaluated as

$$\begin{aligned}&\langle\mathrm{vac}|\psi(p_1,\mathbf{t})\phi^*(p_1,\mathbf{t})\psi(p_2,\mathbf{t})\phi^*(p_2,\mathbf{t})|\mathrm{vac}\rangle\\&=\sum_{\ell_1=0}^{M-1}\sum_{\ell_2=0}^{M-1}\tilde{c}_{\ell_1}(p_1)\tilde{c}_{\ell_2}(p_2)\left(\frac{(p_1-p_2)(q_{\ell_2}^{(2)}-q_{\ell_1}^{(1)})}{(p_1-q_{\ell_2}^{(2)})(p_2-q_{\ell_1}^{(1)})}\right)\prod_{i=1,2}\left(\frac{q_{\ell_i}^{(i)}}{p_i}\right)^j\prod_{t'=-T_0}^{t-1}\\&\quad\times\left(1-\frac{q_{\ell_i}^{(i)}}{1+\delta_{t'}}\right)^{-1}\prod_{t'}^{t-1}\left(1-\frac{p_i}{1+\delta_{t'}}\right)\prod_{n'}^{n-1}\left(1-\frac{p_i}{1+\gamma_{n'}}\right)^{-1}\prod_{n'=n}^{N_0}\left(1-\frac{q_{\ell_i}^{(i)}}{1+\gamma_{n'}}\right)^{-1}.\end{aligned} \tag{B23}$$

We define $\chi_{p_i}(s)$ by

$$\chi_{p_i}(s):=\sum_{\ell=0}^{M-1}\tilde{c}_{\ell}(p_i)\left(\frac{q_{\ell}^{(i)}}{p_i}\right)^s\quad (i=1,2), \tag{B24}$$

and suppose

$$\chi_{p_i}(1)=\chi_0^{(i)},$$

$$\begin{aligned}
\chi_{p_i}(2) &= N_1^{(i)} y^{\ell_1^{(i)}} \chi_{p_i}(1), \\
\chi_{p_i}(3) &= N_2^{(i)} y^{\ell_2^{(i)}} \chi_{p_i}(2), \\
&\cdots \\
\chi_{p_i}(M) &= N_{M-1}^{(i)} y^{\ell_{M-1}^{(i)}} \chi_{p_i}(M-1),
\end{aligned} \tag{B25}$$

where positive numbers $N_j^{(i)}$ satisfy similar inequalities to (B13). From the assumption: $\ell_j^{(1)} \geqslant \ell_j^{(2)}$ $(j=1,2,\ldots,M)$, it is always possible to choose $N_j^{(i)}$ such that

$$\frac{\chi_{p_2}(j+1)}{\chi_{p_2}(j)} \gg \frac{\chi_{p_1}(j+1)}{\chi_{p_1}(j)}. \tag{B26}$$

Then (B23) is expanded as

$$\begin{aligned}
(\mathrm{B23}) = {} & \frac{(p_1-p_2)}{p_1 p_2} \prod_{k=1}^{2} \prod_{t'}^{t-1} \prod_{n'}^{n-1} \left(1-\frac{p_k}{1+\delta_{t'}}\right)\left(1-\frac{p_k}{1+\gamma_{n'}}\right)^{-1} \\
& \times \sum_{i=0}^{\infty} \sum_{i'=0}^{\infty} \left(a_{i,i'} \chi_{p_1}(j+i)\chi_{p_2}(j+1+i') - b_{i,i'} \chi_{p_2}(j+i)\chi_{p_1}(j+1+i')\right),
\end{aligned}$$

where the coefficients $a_{i,i'}$ are defined by

$$\begin{aligned}
& \left(\frac{p_1 p_2^2}{(p_1-q_{\ell_2}^{(2)})(p_2-q_{\ell_1}^{(1)})}\right) \prod_{k=1,2} \prod_{t'=-T_0}^{t-1} \left(1-\frac{q_{\ell_k}^{(k)}}{1+\delta_{t'}}\right)^{-1} \prod_{n'=n}^{N_0} \left(1-\frac{q_{\ell_k}^{(k)}}{1+\gamma_{n'}}\right)^{-1} \\
& \quad = \sum_{i=0}^{\infty} \sum_{i'=0}^{\infty} a_{i,i'} \left(\frac{q_{\ell_1}^{(1)}}{p_{\ell_1}}\right)^{i} \left(\frac{q_{\ell_2}^{(2)}}{p_{\ell_2}}\right)^{i'},
\end{aligned}$$

and

$$b_{i,i'} = \left(\frac{p_1}{p_2}\right) a_{i',i}.$$

From (B15), we evaluate

$$a_{0,0}\chi_{p_1}(j)\chi_{p_2}(j+1) \gg \sum_{i=0}^{\infty} \sum_{\substack{i'=0 \\ i+i'\neq 0}}^{\infty} a_{i,i'} \chi_{p_1}(j+i)\chi_{p_2}(j+1+i')$$

$$b_{0,0}\chi_{p_2}(j)\chi_{p_1}(j+1) \gg \sum_{i=0}^{\infty} \sum_{\substack{i'=0 \\ i+i'\neq 0}}^{\infty} b_{i,i'} \chi_{p_2}(j+i)\chi_{p_1}(j+1+i').$$

Then, noticing $a_{0,0}=p_2$, $b_{0,0}=p_1$ and using (B26), we find

$$\begin{aligned}
& \lim_{\varepsilon \to +0} \varepsilon \log \tau(t+1,n+1,j+1) \\
& \quad = \max[0, K^{(1)}(t,n,j), K^{(2)}(t,n,j), K^{(1)}(t,n,j)+K^{(2)}(t,n,j)-A(j)],
\end{aligned} \tag{B27}$$

$$K^{(i)}(t,n,j) := K_0^{(i)} - \sum_{j'=1}^{j} \mathcal{L}_{j'}^{(i)} - \sum_{t'}^{t} \min[\kappa_{t'}, L^{(i)}] + \sum_{n'}^{n} \min[\theta_{n'}, L^{(i)}] \quad (i=1,2), \tag{B28}$$

$$A(j) := L^{(2)} + \mathcal{L}_{j+1}^{(2)} \quad (0 \leqslant j \leqslant M-1). \tag{B29}$$

This gives a two-soliton solution. For the scattering where the larger soliton overtakes the smaller one like (I) in Theorem 3.10, the integer $\mathcal{L}_j^{(1)}$ $(1 \leqslant j \leqslant M)$ corresponds to the number of jth balls in the larger soliton at $t \to -\infty$, and $\mathcal{L}_j^{(2)}$ corresponds to that of the smaller soliton at $t \to +\infty$. Since the balls in the smaller soliton at $t \to +\infty$ must be included in the larger soliton at $t \to -\infty$, the condition $\mathcal{L}_j^{(1)} \geqslant \mathcal{L}_j^{(2)}$ must hold for soliton solutions. Similarly, for the scattering where the smaller soliton overtakes the larger one like (II) in Theorem 3.10, the integer $\mathcal{L}_j^{(2)}$ $(1 \leqslant j \leqslant M)$ corresponds to the number of jth balls in the smaller soliton at $t \to -\infty$, and $\mathcal{L}_j^{(1)}$ corresponds to that of the larger soliton at $t \to +\infty$. We should also note that there are several freedoms to choose the ''phase'' $A(j)$ in taking the ultradiscrete limit. However we conjecture that the above-mentioned choice will cover all the canonical systems, hence essentially all the time development patterns for $N=2$.

The N soliton solution (40) is obtained in the same way. The key in the construction is to evaluate the expansion:

$$\begin{aligned}
&\langle \mathrm{vac} | \psi(p_1)\psi^*(q_1)\psi(p_2)\psi^*(q_2)\cdots\psi(p_r)\psi^*(q_r) | \mathrm{vac} \rangle \\
&\quad = \langle \mathrm{vac} | \psi(p_1)\psi(p_2)\cdots\psi(p_r)\psi^*(q_r)\psi^*(q_{r-1})\cdots\psi^*(q_1) | \mathrm{vac} \rangle \\
&\quad = \frac{\Pi_{1 \leqslant i < j \leqslant r}(p_i - p_j)(q_j - q_i)}{\Pi_{1 \leqslant i,j \leqslant r}(p_i - q_j)} \\
&\quad = \frac{\Pi_{1 \leqslant i < j \leqslant r}(p_i - p_j)}{\Pi_{i=1}^{r} p_i^r} (q_r^{r-1} q_{r-1}^{r-2} \cdots q_2 + \text{other terms})
\end{aligned}$$

and show that this term gives the phase factor $A(\vec{\mu}; j)$ and the ''other terms'' do not contribute to the final results. This can be done in the same manner as in the case of two soliton solutions. We take

$$g(\mathbf{t}) = \prod_{i=1}^{N} (1 + \psi(p_i, \mathbf{t})\phi^*(p_i, \mathbf{t})), \tag{B30}$$

where

$$\psi(p_i) = \psi(L^{(i)}:\varepsilon), \quad \phi^*(p_i) = \phi^*(L^{(i)}; \{\mathcal{L}_j^{(i)}\}; K_0^{(i)}:\varepsilon) \quad (i=1,2,\ldots,N). \tag{B31}$$

We suppose

$$L^{(1)} \geqslant L^{(2)} \geqslant \cdots \geqslant L^{(N)},$$

and

$$\mathcal{L}_j^{(1)} \geqslant \mathcal{L}_j^{(2)} \geqslant \cdots \geqslant \mathcal{L}_j^{(N)} \quad (j=1,2,\ldots,M).$$

Note that this implies: $p_1 > p_2 > \cdots > p_N$. The latter condition is also a natural constraint for N soliton solutions as in the case of two-soliton solutions. Finally we find that the result is given by (40).

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Discontinuous trajectories of Lagrangian systems with singular hypersurface

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It is shown that a Lagrangian system whose Legendre transformation degenerates along a hypersurface behaves in a strange manner by jumping from time to time without any ''visible cause.'' In such a jump the system changes instantaneously its coordinates as well as its momenta. Necessary elements of the general theory of such systems are reported and a detailed description of a postrelativistic oscillator showing such a behavior is given. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In Lagrangian mechanics two, in a sense, extremal situations were widely studied. One of them, classical, corresponds to systems with nowhere degenerated Legendre map. In this situation the Legendre map identifies the Lagrangian dynamics with the corresponding Hamiltonian one. On the contrary, in the second case the Legendre transformation is supposed to be everywhere degenerated (and of constant rank). Such a situation is common in gauge theories and for this reason was studied in many works, starting with the pioneering paper by Dirac.[1] But in a generic, in the sense of singularity theory, situation the Legendre map $\mathcal{L}$ is almost everywhere nondegenerated except for a critical hypersurface S. Examples of this kind of Lagrangians can be found, for instance, in the literature dedicated to the motion of relativistic particles and the Einstein equations in the post-Newtonian approximation.[2–5] However, the dynamics of these systems has not been analyzed in a satisfactory way up to now, due to the difficulty of studying the behavior of trajectories near S. For reasons explained in Ref. 6 such difficulties cannot be overcome by applying the standard variational principles. Instead, a new principle is needed, which does not determine *a priori* the nature of the singularities of motion and takes into account the natural geometrical structure of the singular hypersurface. Such a prescription, the *Lagrangian transition principle*, has been proposed for the first time in Ref. 6. According to the transition principle, if a trajectory of the system reaches S at a folding point x of the Legendre map, then it makes a jump to another precisely prescribed singular point belonging to the same characteristic curve. From there the motion continues smoothly according to Euler–Lagrange equations up to a possible subsequent jump.

The Lagrangian transition principle was suggested by an analogous principle[7] describing impact and refraction phenomena for Hamiltonian discontinuous systems. We want to stress that the analogy between these two cases is purely geometrical, whereas the physical situations are *completely different*. In this sense, the Lagrangian transition principle cannot be reduced to the Hamiltonian one, and the corresponding physical context is new.

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The aim of this paper is to illustrate the Lagrangian transition principle with an example of a certain physical flavor, a relativistic oscillator in the post-Galilean approximation. This system is a special case of a class of singular Lagrangians proposed in Ref. 4 and was partially studied in Ref. 8. We have chosen it because it is ''completely integrable'' in the sense that it admits a complete analytical description. We think that its self-consistency is an argument in favor of the reasonableness of the proposed principle.

The paper is structured as follows. In Sec. II the Hamiltonian transition principle is briefly recalled, and then it is applied to deduce the classic laws of reflection and refraction in geometrical optics. This application, together with those given in Refs. 6 and 7, represents strong evidence in favor of the principle. In Sec. III we recall the Lagrangian transition principle and some of the main results on Lagrangians with folds found in Ref. 6. The last section is dedicated to a very detailed analysis of the above-mentioned relativistic oscillator.

II. TRANSITION PRINCIPLE

The transition principle is a universal, in a sense, prescription of how a physical system admitting a natural Hamiltonian (symplectic) description should react when an instant drastic change of some of its basic ''parameters'' happens. The last ones could be its Hamiltonian function, phase or configuration space, various types of constraints imposed, charge, etc. In this sense the transition principle is rather general and, for instance, describes various types of collisions between rigid bodies[6] as well as refraction and reflection phenomena in geometric optics (see the example at the end of this section). At present it seems hardly possible to derive the transition principle in its full generality from more fundamental physical laws with such commonly used tricks as the passage to the limit, conservation law arguments, etc. For instance, for Lagrangian systems with fold singularities considered in this paper the limit arguments cannot be applied because that type of singularities is stable and as such cannot be approximated by regular Lagrangians. Conservation law arguments are not, generally, sufficient for this kind of Lagrangian. Darwin's two-electron model[3] gives an example of that. By these and other similar reasons we call this prescription ''principle'' in order to stress its flavor, if not the status, of a physical law. In a subsequent paper[9] we will apply it to describe nonelastic collisions and a number of other of its particular applications are on the agenda. In last years the interest to problems of the so-called nonsmooth mechanics was growing and the recent book[10] by Brogliato gives an account of the recent developments in this field and also contains a rich bibliography. It is recommended as an alternative approach. But we would like to emphasize that the transition principle covers a larger area of physical phenomena and, in particular, those that can be mathematically interpreted as propagation of singularities of solutions of (nonlinear) PDEs, say, geometrical optics (see Refs. 11 and 12).

Below we illustrate the principle in its original and simplest version (see Refs. 6 and 7 for further details) and give in addition a remarkable application to geometrical optics.

Let (Φ,Ω) be the phase space of a dynamical system with $\Omega=\Sigma_i\, dp_i/\backslash dq_i$ being a symplectic two form on Φ. Suppose then that Φ is divided by a hypersurface Γ into two closed domains Φ_+, Φ_-, having Γ as their common boundary, i.e., $\partial\Phi_+=\Gamma=\partial\Phi_-$. Suppose also that the Hamiltonian of the system is smooth on $\Phi_\pm$. In other words, if $H_\pm=H|_{\Phi_\pm}$, then $H_\pm\in C^\infty(\Phi_\pm)$. This, in particular, means that $H_\pm|_\Gamma\in C^\infty(\Gamma)$, but it is not supposed that $H_+|_\Gamma$ coincides with $H_-|_\Gamma$. So H, and consequently the Hamiltonian field X_H associated with it, are well defined on $\Phi\backslash\Gamma$ and is bi-valued on Γ.

As is well known, the local coordinate expression of $X_{H_\pm}$ is

$$X_{H_\pm}=\sum_i\left(\frac{\partial H_\pm}{\partial p_i}\frac{\partial}{\partial q_i}-\frac{\partial H_\pm}{\partial q_i}\frac{\partial}{\partial p_i}\right).$$

The corresponding canonical equations:

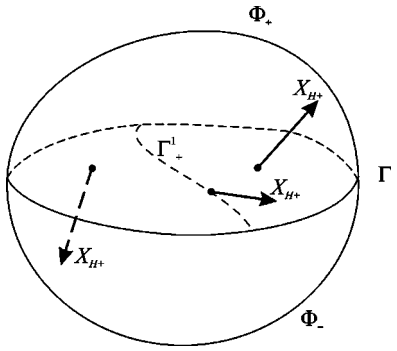

FIG. 1. In- and out-points (for H_+).

$$\dot{q}_i=\frac{\partial H_\pm}{\partial p_i}, \quad \dot{p}_i=-\frac{\partial H_\pm}{\partial q_i},$$

describe the motion of the system *inside* $\Phi_\pm$. But when the phase trajectory arrives at Γ it must ''decide'' under control of which Hamiltonian to proceed on. The *Transition Principle* prescribes how this decision should be taken.

First, recall[7] that on Γ is defined the one-dimensional *characteristic distribution* $x\mapsto l_x$, given by

$$l_x=\{\xi\in T_x(\Phi)|\Omega_x(\xi,\eta)=0 \quad \forall\,\eta\in T_x(\Gamma)\}.$$

Its integral curves are called *characteristics* of Γ.

Remark: A case of particular interest is when $\Gamma=\pi^{-1}(S)$, with $\pi:T^*(M)\to M$ being the cotangent bundle on a manifold M and $S\subset M$ being a hypersurface in the base. In this case characteristics of Γ are straight lines contained in the fibers $T^*_q(M)$, $q\in S$. In fact, if $q_n=0$ is the equation of S in a certain local chart, then the characteristic directions are given by the vector field $\partial/\partial p_n$.

Coming back to the general situation, let $x\in\Gamma$. We say that x is a $+$*-in-point* (respectively, a $+$*-out-point*) if $X_{H_+}|_x$ is directed toward Φ_+ (respectively, Φ_-). Similarly, we say that x is a $-$*-in-point* (respectively, a $-$*-out-point*) if $X_{H_-}|_x$ is directed toward Φ_- (respectively Φ_+) (see Fig. 1). In and out points of $H_\pm$ are separated by a hypersurface $\Gamma^1_\pm\subset\Gamma$ along which $X_{H_\pm}$ is tangent to Γ.

Suppose now that the phase trajectory, starting from a point inside of Φ_+ (respectively, Φ_-), reaches a point $x\in\Gamma$ at an instant $\bar{t}$, and let E be the constant value of H_+ (respectively, H_-) along the phase trajectory for $t\leqslant\bar{t}$. Denote by γ_x the characteristic curve of Γ passing through x, and by Σ^+_E (respectively, Σ^-_E) the hypersurface $\{H_+=E\}$ (respectively, $\{H_-=E\}$) of $\bar{\Phi}_+$ (respectively, $\bar{\Phi}_-$). A point $y\in\gamma_x\cap\Sigma^+_E$ (respectively, $\gamma_x\cap\Sigma^-_E$) is called *decisive* for x if it is a $+$-in-point (respectively, a $-$-in-point). Now we can state the following.

Transition principle: When a moving point reaches the separation hypersurface Γ *at a point* x *with energy* E*, then it continues its motion from all* x*-decisive points* $y\in\Sigma^\pm_E$ *simultaneously under control of corresponding Hamiltonians* $H_\pm$*. The passage of the phase point from* x *to the* y*'s is assumed to be instantaneous.*

The transition principle is illustrated in Fig. 2.

In Ref. 7 some examples illustrating this principle in mechanics and in geometrical optics are given. To these we will now add the following one.

Example (laws of reflection and refraction): Following the previous remark for notations, suppose M to be a region of the ordinary Euclidean space filled with two inhomogeneous isotropic

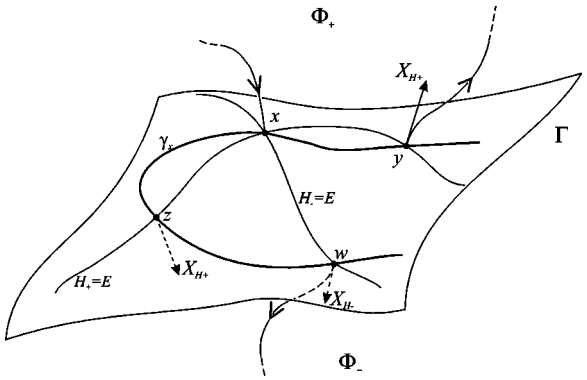

FIG. 2. The Hamiltonian transition principle (y and w are decisive for x).

optical media M_+, M_- separated by the surface S. Denote the light velocity in $M_\pm$ by $V_\pm(q)$, with (q_1,q_2,q_3) being Cartesian orthogonal coordinates in M. Then in each medium the propagation of light rays is described by the canonical system:[13]

$$\dot{q}_i=\frac{\partial H_\pm}{\partial p_i}, \quad \dot{p}_i=-\frac{\partial H_\pm}{\partial q_i}, \quad i=1,2,3$$

with

$$H_\pm(q,p)=V_\pm(q)\|p\|, \tag{1}$$

where $\|p\|=\sqrt{\Sigma_i p_i^2}$.

Suppose that a ray starting from M_+ reaches S at a point $\overline{q}\equiv(\overline{q_1},\overline{q_2},\overline{q_3})$ with an impulse $\overline{p}\equiv(\overline{p_1},\overline{p_2},\overline{p_3})$. The corresponding velocity is $\overline{v}=V_+(\overline{q})\overline{p}/\|\overline{p}\|$. In $\Phi=T^*(M)$ the phase trajectory of the ray reaches $\Gamma=\pi^{-1}(S)$ at the point $\overline{x}\equiv(\overline{q},\overline{p})$. By the previous remark the characteristic curve $\gamma_{\overline{x}}$ of Γ passing through x is a straight line contained in the fiber $T^*_{\overline{q}}(M)$. Let us choose coordinates (q_1,q_2,q_3) in such a way that S is tangent at $\overline{q}$ to the hyperplane $\{q_3=\overline{q_3}\}$ and the q_3 axis is directed toward M_-. Then the parametric equations of $\gamma_{\overline{x}}$ are

$$q_i(t)=\overline{q_i}$$

$$p_i(t)=\overline{p_i}+\delta_{i3}t, \quad t\in\mathbf{R}, \quad i=1,2,3. \tag{2}$$

If $E=H_+(\overline{q},\overline{p})$, then, in view of (2) and (1), the intersection $\gamma_{\overline{x}}\cap\Sigma_E^+$ is composed of the two points $\overline{x}$ and $x^*\equiv(\overline{q},p^*)$ with $p^*=(\overline{p_1},\overline{p_2},-\overline{p_3})$ It is easy to check that x^* is decisive for $\overline{x}$. Therefore, the transition principle tells that the reflected ray does always exist, and starts from the same point $\overline{q}\in S$ in the direction $v^*=V_+(\overline{q})p^*/\|p^*\|$ corresponding to p^*. Further, $\overline{v}$, v^* are coplanar with the normal to S at $\overline{q}$ and form with it equal angles ϕ,ψ_+, respectively (*reflection law*).

On the other hand, the intersection of $\gamma_{\overline{x}}$ with the circle $C_E^-=\Sigma_E^-\cap T^*_{\overline{q}}(M)$: (1) is empty if $\sin\phi=\sqrt{1-\overline{v_3}^2/V_+(\overline{q})^2}>\overline{n}$, with $\overline{n}=V_+(\overline{q})/V_-(\overline{q})$; (2) consists of the two points $\tilde{x}\equiv(\overline{q},\overline{p_1},\overline{p_2},\tilde{p}_3)$, $\hat{x}\equiv(\overline{q},\overline{p_1},\overline{p_2},-\tilde{p}_3)$, with $\tilde{p}_3=\|\overline{p}\|\sqrt{\overline{p_3}/\|\overline{p}\|+\overline{n}^2-1}$, if $\sin\phi\leqslant\overline{n}$. But only $\tilde{x}$ is decisive for $\overline{x}$. Hence, by the transition principle, in case (1) there is no refracted ray (*total reflection*), while in case (2) there is one refracted ray whose initial direction $\tilde{p}=(\overline{p_1},\overline{p_2},\tilde{p}_3)$ is coplanar with the incident ray and the normal to S at $\overline{q}$, and forms with this an angle ψ_- such that (*Snellius' law*):

$$\frac{\sin\phi}{\sin\psi_-}=\frac{\sqrt{1-\dfrac{\overline{p}_3^2}{\|\overline{p}\|^2}}}{\sqrt{1-\dfrac{\tilde{p}_3^2}{\|\tilde{p}\|^2}}}=\overline{n}.$$

III. LAGRANGIANS WITH SINGULAR HYPERSURFACES

In this section we briefly recall the notion of relative Hamiltonian vector field and the Lagrangian principle of transition, proposed for the first time in Ref. 6. As was mentioned in Sec. I, this principle was suggested by the *geometrical* analogy between discontinuous Hamiltonian systems considered in Sec. II and singular Lagrangians with fold-type singularities. We stress that this analogy is only geometrical, but that the two situations are totally different from the physical point of view. However, as in the Hamiltonian case, the Lagrangian transition principle allows one to completely describe discontinuities of motion that occur when the phase point of the system reaches the singular hypersurface.

A. The relative Hamiltonian vector field

As was pointed out in Ref. 6 the basic tool necessary for extending the transition principle to the Lagrangian case is the *relative Hamiltonian vector field*, whose definition we now briefly recall. Let M, $\dim M=n$, be the configuration space of a dynamical system described by a Lagrangian $L\in C^\infty(T(M))$, and let $\mathcal{L}:T(M)\to T^*(M)$ be the corresponding Legendre mapping. Recall that, in a fixed local chart $(q_1,\ldots,q_n)$ on M, $\mathcal{L}$ is represented by

$$\begin{aligned} q_i&=q_i, \quad i=1,\ldots,n,\\ p_i&=L_{v_i}(q,v), \quad i=1,\ldots,n, \end{aligned} \tag{3}$$

where (q,v), (q,p) are the natural coordinates on $T(M)$ and $T^*(M)$, respectively, associated with $(q_1,\ldots,q_n)$.

Now, one can associate with L the following vector field along $\mathcal{L}$:

$$X_L\overset{\text{def}}{=}\sum_i v_i\frac{\partial}{\partial q_i}+\sum_i L_{q_i}(q,v)\frac{\partial}{\partial p_i}. \tag{4}$$

The main properties of this operator were shown in Ref. 6. Here we limit ourselves to recalling why X_L was called Hamiltonian. In fact, it is easy to check that it satisfies the fundamental relation

$$X_L\lrcorner\Omega=-dE, \tag{5}$$

with $\Omega=\Sigma_i dp_i\wedge dq_i$ being the canonical two-form on $T^*(M)$ and

$$E(q,v)\overset{\text{def}}{=}\sum_i v_iL_{v_i}(q,v)-L(q,v)$$

being the energy function associated with L. Now, if L is regular, i.e., $\mathcal{L}$ is a diffeomorphism, then the Hamiltonian function $H=(\mathcal{L}^{-1})^*(E)$ is uniquely determined and, denoting by X_H the corresponding Hamiltonian vector field on $T^*(M)$, one immediately gets from (5) that

$$X_L=\mathcal{L}^*\circ X_H.$$

To our knowledge, the relative vector field (4) was proposed for the first time in Ref. 14. Later on some applications of it were found, especially in the study of constrained systems (see Ref. 6

for further references). However, the important role of X_L in the analysis of Lagrangian systems with singular hypersurfaces was indicated only recently in Ref. 6. In the next section we will recall briefly the main result of that work, the Lagrangian transition principle.

B. Legendre maps with folds. The Lagrangian transition principle

Referring to Sec. III A for the notations, suppose that L is non-regular and let S be the singular points locus of the Legendre map:

$$S=\{x\in T(M)|\text{rank } d_x\mathcal{L}<2n\}.$$

According to the standard-procedure, the motion of the system outside S can be described by Euler–Lagrange equations:

$$\begin{cases} \dot{q}_i=v_i, \\ \dfrac{d}{dt}(L_{v_i})-L_{q_i}=0, \end{cases} \tag{6}$$

$i=1,\ldots,n$. Equation $(6)_2$ can be rewritten in the normal form:

$$\dot{v}_i=f_i(q,v) \tag{7}$$

in a neighborhood of any point $(q,v)\in T(M)\setminus S$. So, outside of S the motions of the system coincide with the integral curves of the vector field

$$Z_L=\sum_i \left(v_i\frac{\partial}{\partial q_i}+f_i(q,v)\frac{\partial}{\partial v_i}\right).$$

On the other hand, this standard description is no longer possible if $(q,v)\in S$. Namely, accelerations become undetermined on S and velocities may have discontinuities.

As has been remarked in Sec. I for a generic Lagrangian S is a hypersurface (possibly with singularities). Its equation is

$$\mathcal{H}(q,v)=0,$$

with $\mathcal{H}:=\det\|L_{v_iv_j}\|$. We assume S to be a regular hypersurface of $T(M)$, i.e.,

$$d_x\mathcal{H}\neq 0, \quad \forall x\in S. \tag{8}$$

Further, we assume the following transversality condition

$$\text{Ker}\, d_x\mathcal{L}\cap T_x(S)=\{0\}, \quad \forall x\in S. \tag{9}$$

As was shown in Ref. 6, assumptions (8) and (9) guarantee $\mathcal{L}$ to be a *submersion with folds*.[15] Then, for any point $\overline{x}\in S$ there exist coordinates $(x_1,\ldots,x_{2n})$ on $T(M)$ and $(y_1,\ldots,y_{2n})$ on $T^*(M)$, centered at $\overline{x}$ and $\mathcal{L}(\overline{x})$, respectively, in terms of which $\mathcal{L}$ takes the form

$$\begin{aligned} y_1&=x_1\\ &\vdots\\ y_{2n-1}&=x_{2n-1}\\ y_{2n}&=x_{2n}^2. \end{aligned} \tag{10}$$

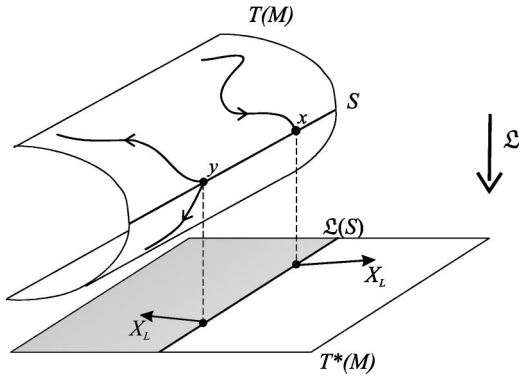

FIG. 3. The Lagrangian transition principle (y is decisive for x).

From (10) it easily follows that the range of $\mathcal{L}$ locally belongs to the half-space $y_{2n} \geqslant 0$. This allows us to extend the definition of in- and out-points and the corresponding transition principle to the Lagrangian case. Namely, a point $x \in S$ is called an *in-point* if $X_L|_x$ is directed toward the range of $\mathcal{L}$, $X_L|_x(y_{2n}) > 0$, while it is called an *out-point* if $X_L|_x$ is directed outside of it, $X_L|_x(y_{2n}) < 0$.

Let us note that the pullback $\mathcal{L}^*(\Omega)$ of the canonical symplectic form on $T^*(M)$ along the Legendre map is degenerated on S and is of rank $2n-2$ at any fold point. The restriction $\Omega_S \overset{\text{def}}{=} \mathcal{L}^*(\Omega)|_S$ continues to be of rank $2n-2$ due to (9). This means that the kernel l_x of Ω_S at a fold point $x \in S$ is one dimensional. This way one gets a one-dimensional distribution on S. *Characteristic curves* are integral curves of it. Denote by γ_x the characteristic curve passing through $x \in S$.

Now it is clear how to extend the transition principle to the Lagrangian case. Namely, calling *decisive* for $x \in S$ any in-point $y \in \gamma_x$ belonging to the same level Σ_E of energy of x, the principle can be stated as follows.

Transition Principle (Lagrangian case): When a phase point moving along Z_L reaches at an instant a point $x \in S$, it then continues its motion along all trajectories of Z_L issuing from points decisive for x. Moreover, the passage from x to a decisive point is instantaneous.

The principle is illustrated in Fig. 3.

Remark 1: According to the principle there are in general as many possible phase trajectories after the impact with S at a point x as are the points decisive for x. This is analogous to the splitting of light rays in reflection and refraction phenomena considered in Sec. II.

Remark 2: Note that, in order to define in- and out-points in the Lagrangian case, it is essential that the singularities of $\mathcal{L}$ be fold points. In Sec. IV we will see that the Lagrangian of the post-Galilean oscillator also exhibits some irregular singularities, which can be studied as well.

IV. RELATIVISTIC OSCILLATOR

In this section the behavior of a relativistic oscillator whose Lagrangian possesses fold singularities is analyzed on the basis of transition principle. We have chosen this example to show the above-mentioned theory in action mainly because of its relative simplicity: its phase trajectories and characteristics can be described analytically without difficulties. However, we will see that even in this simple case the behavior of phase trajectories with respect to the singular surface is rather interesting, at least from a geometrical point of view.

By applying the transition principle to describe the discontinuities of motion of relativistic oscillator we discover a rather remarkable phenomenon. Namely, if the energy exceeds a certain level and at the same time the velocity is not too high, the oscillator starts jumping. In other words, after a smooth motion it instantaneously changes its position (as well as velocity). In the classical

example of reflection and refraction of light, or elastic collision of bodies and particles, there is no discontinuity of position. It is worth noting that the ''jumping'' motions of the oscillator are in a good consistency with the smooth ones.

Finally, we note that the relativistic oscillator also possesses singularities of nonfold type. These are very degenerated and the phase portrait in this region is rather curious.

A. Relativistic oscillator

Recall that there were proposed various relativistic generalizations of the standard harmonic oscillator (see for instance Ref. 8). Some of them possess singularities, while others do not. In the following we study the two-dimensional post-Galilean oscillator[8] of tensor rank 2, possessing both fold and not fold type singularities:

$$L=L(r,x)=-mc^2[\sqrt{1-x}+(r/r_0)^2(1+x/2)]. \tag{11}$$

Here m,r_0 are the mass and the characteristic length of the oscillator, respectively, linked by the relation $r_0=\sqrt{m/k}\,c$ (with k being the elastic constant); r is the distance between the oscillating mass and the elastic force center; $x=v^2/c^2$ is the square of oscillator velocity, measured with respect to the light velocity c. If we fix in the plane of motion a system of orthogonal coordinates (q_1,q_2) with the origin at the center of the force, then obviously:

$$r=\sqrt{q_1^2+q_2^2}, \quad x=\frac{v_1^2+v_2^2}{c^2}.$$

Note that

$$0\leqslant x<1, \tag{12}$$

due to the fact that $v^2<c^2$. In the following we refer to $M=\mathbf{R}^2=\{(q_1,q_2)\}$ as the configuration space. So the Lagrangian (11) is defined in the domain $\mathcal{U}\subset T(M)=\{(q,v)\}=\mathbf{R}^2\times\mathbf{R}^2$, defined as

$$\mathcal{U}=\{(q,v)\in T(M)\,|\,q\in M,\|v\|<c\}.$$

However we will often not distinguish between $\mathcal{U}$ and $T(M)$. A similar convention will be adopted also for the cotangent bundle $T^*(M)$).

In the following we will systematically use in $\mathcal{U}$ the system of coordinates (r,ϕ,x,θ) [or equivalently (r,ϕ,x,u), with $u=\theta-\phi$] where ϕ and ϑ are the angle between q_1 axis and $\mathbf{r}\equiv(q_1,q_2)$, and the angle between $\mathbf{r}$ and the velocity vector $\mathbf{v}\equiv(v_1,v_2)$, respectively.

To simplify general considerations concerning Lagrangian (11) it is convenient to work with a generic Lagrangian of the form

$$L=L(r,x). \tag{13}$$

The energy function

$$E=v_1L_{v_1}+v_2L_{v_2}-L \tag{14}$$

takes the following form for Lagrangian (13):

$$E(r,x)=2xL_x-L, \tag{15}$$

which in the case of oscillator (11) becomes

$$E(r,x)=mc^2\left[\frac{1}{\sqrt{1-x}}+\left(\frac{r}{r_0}\right)^2\left(1-\frac{x}{2}\right)\right].$$

Lagrangian (13) also admits another integral of motion, namely the *angular momentum*:

$$I(r,x,u)=\frac{2}{c^2}L_x(r,x)(q_1v_2-q_2v_1)=\frac{2}{c}r\sqrt{x}L_x(r,x)\sin u. \tag{16}$$

For Lagrangian (11) it is specified as:

$$I(r,x,u)=mcr\sqrt{x}\left[\frac{1}{\sqrt{1-x}}-\left(\frac{r}{r_0}\right)^2\right]\sin u.$$

The integral I corresponds, via Noether's theorem, to the infinitesimal symmetry:

$$X=-q_2\frac{\partial}{\partial q_1}+q_1\frac{\partial}{\partial q_2}=\frac{\partial}{\partial\phi},$$

of Lagrangian (13).

B. Singular hypersurface of relativistic oscillator

The Legendre map $\mathcal{L}$ associated with Lagrangian (13) is given by

$$\begin{aligned} q_i&=q_i,\\ p_i&=L_{v_i}=\frac{2}{c^2}L_xv_i, \quad i=1,2. \end{aligned} \tag{17}$$

The corresponding Jacobian matrix in terms of standard coordinates (q,v) and (q,p) in $T(M)$ and $T^*(M)$, respectively, has the entries:

$$L_{v_iq_j}=\frac{2}{c^2}\frac{L_{xr}}{r}v_iq_j, \quad L_{v_iv_j}=\frac{2}{c^2}L_x\delta_{ij}+\frac{4}{c^4}L_{xx}v_iv_j, \quad i,j=1,2.$$

So, the corresponding Hessian is

$$\mathcal{H}(q,v)=L_{v_1v_1}L_{v_2v_2}-L_{v_1v_2}^2=\frac{4}{c^4}L_x(L_x+2xL_{xx})=\mathcal{H}(r,x)$$

It is easy to see that

$$L_x+2xL_{xx}=E_x, \tag{18}$$

and, therefore,

$$\mathcal{H}(r,x)=\frac{4}{c^4}L_xE_x.$$

Hence,

$$E_xL_x=0$$

is the equation of the singular hypersurface S. In other words

$$S=S_1\cup S_2,$$

with $S_1=\{E_x=0\},S_2=\{L_x=0\}$. Each of these hypersurfaces is fibered in tori (ϕ,θ), some of which may reduce to circles or to a point, depending on L. The bases of these ''fibrations'' are

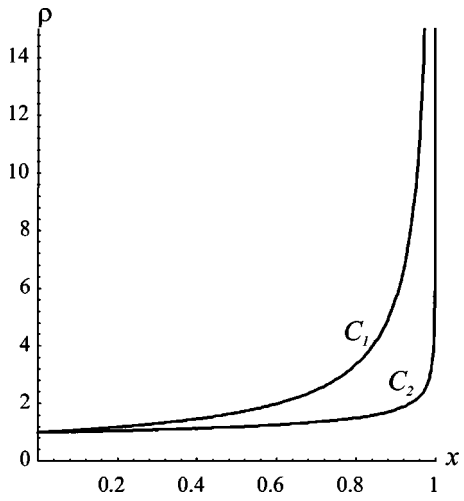

FIG. 4. Singular surface of the oscillator ($\rho = r/r_0$).

curves C_1, C_2 in the (x,r) plane, given by equations $E_x(r,x)=0$ and $L_x(r,x)=0$, respectively. These curves for the oscillator (11) are shown in Fig. 4. In this case the intersection $\gamma = S_1 \cap S_2$ is the circle $\{r=r_0, x=0\}$ included in the null section $M \subset T(M)$. γ is the locus $\operatorname{Sing} S$ of singular points of S. This follows easily from

$$\mathcal{H}_{q_i} = \frac{q_i}{r}\mathcal{H}_r = \frac{q_i}{r}(L_{xr}E_x + L_x E_{xr}),$$

$$\mathcal{H}_{v_i} = 2\frac{v_i}{c^2}\mathcal{H}_x = 2\frac{v_i}{c^2}(L_{xx}E_x + L_x E_{xx}),$$

and from the fact that $S_1 \setminus \gamma$ and $S_2 \setminus \gamma$ are regular.

Now we pass to describe how the kernel of the Legendre map behaves along the singular hypersurface S. A vector

$$\xi = \sum_{i=1}^{2}\left(a_i\frac{\partial}{\partial q_i} + b_i\frac{\partial}{\partial v_i}\right)$$

belongs to the kernel of $d\mathcal{L}$ iff

$$a_1 = a_2 = 0, \quad L_{vv}\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \tag{19}$$

In full details, the second of condition of (19) looks as

$$\left(L_x + \frac{2}{c^2}L_{xx}v_1^2\right)b_1 + \frac{2}{c^2}L_{xx}v_1v_2b_2 = 0, \tag{20}$$

$$\frac{2}{c^2}L_{xx}v_1v_2b_1 + \left(L_x + \frac{2}{c^2}L_{xx}v_2^2\right)b_2 = 0.$$

By construction these equations are linearly dependent at any point of S.

For a point $(q,v) \in S_2 \setminus S_1$ there are two possibilities: $L_{xx}(q,v)=0$ or $L_{xx}(q,v)\neq 0$. In the first case the system becomes trivial and $\operatorname{Ker} d_{(q,v)}\mathcal{L}$ is two dimensional. This never happens for the oscillator (11). In the second case system (20) reduces to the linear equation:

$$v_1 b_1 + v_2 b_2 = 0.$$

Except for the points $(v_1 = v_2 = 0)$, $\operatorname{Ker} d_{(q,v)}\mathcal{L}$ is one dimensional. It is generated by the vector

$$v_2 \frac{\partial}{\partial v_1} - v_1 \frac{\partial}{\partial v_2},$$

which coincides with $-\partial/\partial u$ in coordinates (r,ϕ,x,u). This shows that in both cases $\operatorname{Ker} d_{(q,v)}\mathcal{L}$ is tangent to S_2. So fold type singularities do not belong to S_2 and $\dim \mathcal{L}(S_2) < 3$. For the oscillator (11) $\mathcal{L}(S_2)$ is two-dimensional and coincides with the null section of $T^*(M)$.

Now we go to describe fold points belonging to $S_1 \backslash S_2$. These form an open domain $S_1^{\text{fold}} \subset S_1$ everywhere dense in S_1.

If $(q,v) \in S_1 \backslash S_2$, it follows from (18) that $L_x = -2xL_{xx}$, hence $(20)_2$ becomes

$$v_2 b_1 - v_1 b_2 = 0.$$

Therefore we have that

$$\operatorname{Ker} d_{(q,v)}\mathcal{L} = \operatorname{Span}\left(v_1 \frac{\partial}{\partial v_1} + v_2 \frac{\partial}{\partial v_2} \right) = \operatorname{Span}\left(\frac{\partial}{\partial x} \right) \quad \text{on} \quad S_1 \backslash S_2.$$

Thus, singularities of $\mathcal{L}$ along S_1 are of a substantially different nature from those along S_2. Namely, the kernel of $d\mathcal{L}$ is *transversal* to $S_1 \backslash S_2$ (due to the fact that $E_{xx} \neq 0$ on it) and is *tangent* to S_2, since $\partial L_x / \partial u = 0$ on it. Hence, $\dim \mathcal{L}(S_2) < 3$ and the transition principle cannot be applied to S_2. In the Sec. IV C we shall see that even characteristic directions are undetermined on S_2.

C. Characteristic curves on *S*

To simplify computations we will make use of coordinates (r,x,ϕ,ϑ) (or, equivalently, (r,x,u,ϕ)). Let

$$\rho = \sum_i p_i dq_i$$

be the universal one-form[7] on $T^*(M)$. Then

$$\mathcal{L}^*(\rho) = L_{v_1} dq_1 + L_{v_2} dq_2 = \frac{2}{c}\sqrt{x} L_x(r,x)(\cos u\, dr + r \sin u\, d\phi). \tag{21}$$

It follows from (21) that $\mathcal{L}^*(\rho)|_{S_2} = 0$. Hence

$$\mathcal{L}^*(\Omega)|_{S_2} = 0.$$

Therefore, $\mathcal{L}(S_2)$ is a Lagrangian submanifold in $T^*(M)$ (with possible singularities) and characteristic directions on S_2 are undetermined.

Now we pass to describe characteristics on S_1^{fold}. Since $\operatorname{grad} \mathcal{H} \neq 0$ on it, the equation $E_x(r,x) = 0$ of S_1 can be solved with respect to one of the variables, say r:

$$r = r_1(x) \quad \text{on} \quad S_1^{\text{fold}}.$$

In the case of the oscillator (11):

$$r_1(x) = \frac{r_0}{(1-x)^{3/4}}.$$

So (x,u,ϕ) can be taken as local coordinates on S_1^{fold}. Then from (21) we get:

$$\mathcal{L}^*(\rho)|_{S_1}=\frac{2}{c}\sqrt{x}L_x(r_1(x),x)[r_1'(x)\cos u\,dx+r_1(x)\sin u\,d\phi],$$

so that

$$\mathcal{L}^*(\Omega)|_{S_1}=d\mathcal{L}^*(\rho)|_{S_1}=\frac{2}{c}[\alpha(x,u)dx\wedge du+\beta(x,u)dx\wedge d\phi+\gamma(x,u)du\wedge d\phi], \tag{22}$$

with

$$\alpha(x,u)=\sqrt{x}L_x(r_1(x),x)r_1'(x)\sin u,$$

$$\beta(x,u)=\frac{d}{dx}[r_1(x)\sqrt{x}L_x(r_1(x),x)]\sin u,$$

$$\gamma(x,u)=r_1(x)\sqrt{x}L_x(r_1(x),x)\cos u.$$

Characteristic directions on S_1 are described by a characteristic vector field $X\in\mathcal{D}(S_1)$, i.e., such that

$$\mathcal{L}^*(\Omega)|_{S_1}(X,\bullet)=0. \tag{23}$$

If

$$X=a\frac{\partial}{\partial x}+b\frac{\partial}{\partial u}+c\frac{\partial}{\partial\phi},\quad a,b,c\in C^\infty(S_1),$$

then (23) is equivalent, in view of (22), to

$$\begin{pmatrix}0&-\alpha&-\beta\\ \alpha&0&-\gamma\\ \beta&\gamma&0\end{pmatrix}\begin{pmatrix}a\\b\\c\end{pmatrix}=\begin{pmatrix}0\\0\\0\end{pmatrix}.$$

This system is of rank 2 on S_1^{fold}, and its fundamental solution is

$$(a,b,c)=(\gamma,-\beta,\alpha).$$

Therefore,

$$X=\gamma\frac{\partial}{\partial x}-\beta\frac{\partial}{\partial u}+\alpha\frac{\partial}{\partial\phi}=q(x)\cos u\frac{\partial}{\partial x}-q'(x)\sin u\frac{\partial}{\partial u}+r_1'(x)\sqrt{x}L_x(r_1(x),x)\sin u\frac{\partial}{\partial\phi},$$

with $q(x)=r_1(x)\sqrt{x}L_x(r_1(x),x)$ and characteristic curves are solutions of the system:

$$\dot{x}=q(x)\cos u,$$

$$\dot{u}=-q'(x)\sin u, \tag{24}$$

$$\dot{\phi}=q(x)\frac{r_1'(x)}{r_1(x)}\sin u.$$

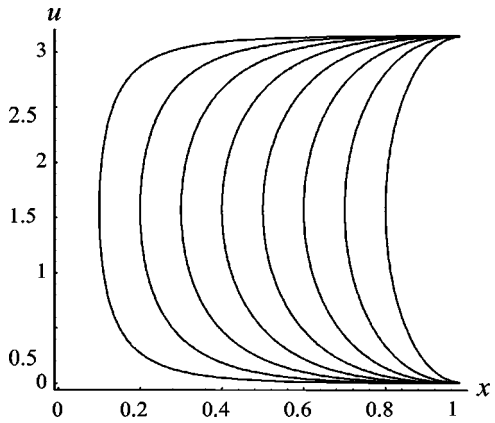

FIG. 5. Characteristic curves on S_1.

Integration of system (24) is reduced, obviously, to its subsystem $(24)_{1,2}$, whose solutions are to be described in the rectangle $[0,1[\times[-\pi,\pi]$ due to the cyclicity of u.

It follows from $(24)_{1,2}$ that

$$\frac{du}{dx}=-\frac{q'(x)}{q(x)}\tan u, \tag{25}$$

and, consequently,

$$\int \frac{du}{\tan u}=\ln|\sin u|=-\int\frac{q'(x)}{q(x)}dx=-\int\frac{dq}{q}=-\ln|q(x)|+\text{const}=\ln\frac{c}{|q(x)|},\quad c>0.$$

Hence the general integral of (25) is

$$\sin u=\frac{a}{q(x)},\quad a\in\mathbf{R}. \tag{26}$$

For the oscillator (11) it is specified as

$$\sin u=-\frac{2a}{mc^2r_0}\frac{(1-x)^{9/4}}{x^{3/2}}.$$

Let us remark that $q(x)\sin u=(c/2)\,I|_{S_1}$. So (26) shows that I is constant along characteristic curves of S_1. Therefore, by the transition principle, angular momentum (as well as energy) *does not change after the impact with* S_1.

The curves (26), denote them by γ_a, for the oscillator are shown in Fig. 5. Since the variable u is cyclic $\bmod 2\pi$ and γ_a and γ_{-a} are symmetric with respect to the x axis we can limit ourselves to dealing with the curves in the rectangle $(x,u)\in[0,1[\times[0,\pi]$.

Let $\overline{P}\equiv(\overline{x},\overline{u},\overline{\phi})\in S_1$ and let $\gamma_{\overline{a}}$ be the characteristic passing through $\overline{P}$, $\overline{E}=E(\overline{P})$. The intersection between the energy level surface $\Sigma_{\overline{E}}$ and S_1 is the torus $T_{\overline{E}}=\{r=r_1(\overline{x}),x=\overline{x}\}$. The projection of $T_{\overline{E}}$ onto the (x,u) plane is the line $x=\overline{x}$. For the oscillator (11) this is shown, together with the projection of $\gamma_{\overline{a}}$, in Fig. 6.

Therefore, assuming $\overline{u}\in[0,\pi]$, $\gamma_{\overline{a}}$ intersects $T_{\overline{E}}$ at $\overline{P}$ and at $\tilde{P}\equiv(\overline{x},\pi-\overline{u},\tilde{\phi})$. In order to determine $\tilde{\phi}$ notice that

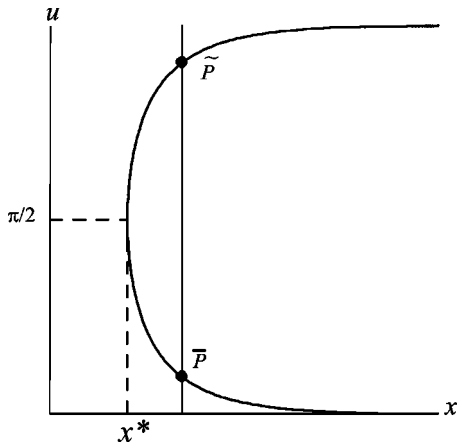

FIG. 6. Intersection between a characteristic curve and the energy level surface.

$$\frac{d\phi}{dx}=\frac{r_1'(x)}{r_1(x)}\tan u=\pm\frac{r_1'(x)}{r_1(x)}\frac{\sin u}{\sqrt{1-\sin^2 u}}=\pm|\overline{a}|\frac{r_1'(x)}{r_1(x)\sqrt{q^2(x)-\overline{a}^2}}, \tag{27}$$

as it results directly from $(24)_{1,2}$ and (26). In (27) the choice of ''+'' (respectively, ''−'') corresponds to $u\in[0,\pi/2[$ (respectively, $u\in]\pi/2,\pi]$). Hence, the possible position jump is described by

$$\tilde{\phi}-\bar{\phi}=\Delta\phi(\bar{x},\bar{u})=\pm 2|\overline{a}|\int_{x^*}^{\bar{x}}\frac{r_1'(x)}{r_1(x)\sqrt{q^2(x)-\overline{a}^2}}dx, \tag{28}$$

where x^* (see Fig. 6) is the root of

$$|q(x)|=|\overline{a}|, \tag{29}$$

and the sign + (respectively, −) corresponds to $\bar{u}\in[\pi/2,\pi]$ (respectively, $\bar{u}\in[0,\pi/2]$). In the case of the oscillator equation (29) becomes

$$x^2=\left(\frac{2|\overline{a}|}{mc^2r_0}\right)^{4/3}(1-x)^3,$$

which has only one root x^* in the interval $[0,1[$. Relation (27) remains valid also for $\bar{u}\in[-\pi,0]$. In this case the sign + (respectively, −) corresponds to $\bar{u}\in[-\pi,-\pi/2]$ (respectively, $\bar{u}\in[-\pi/2,0]$).

Since on a given characteristic only two points lie, $\bar{P}$ and $\tilde{P}$, belonging to the same energy level, a jump from $\bar{P}$ to $\tilde{P}$ or vice versa may happen only if one of these points is ''in'' while the other is ''out.'' This occurs iff the function $X_L(g)$, $g(q,p)=0$, being the equation of $\mathcal{L}(S_1)$, takes opposite signs at points $\bar{P}$, $\tilde{P}$, and we go to analyze when such is the case.

It follows from (4) that for Lagrangian (13)

$$X_L=v_1\frac{\partial}{\partial q_1}+v_2\frac{\partial}{\partial q_2}+\frac{L_r}{r}\left(q_1\frac{\partial}{\partial p_1}+q_2\frac{\partial}{\partial p_2}\right). \tag{30}$$

In the following we work with the local chart (r,ϕ,y,α), $y=(p_1^2+p_2^2)/m^2c^2$, $\alpha=\arctan p_2/p_1$, on $T^*(M)$. In terms of these coordinates the Legendre map (17) is given as follows:

$$y=\psi(r,x),\quad \alpha=\theta, \tag{31}$$

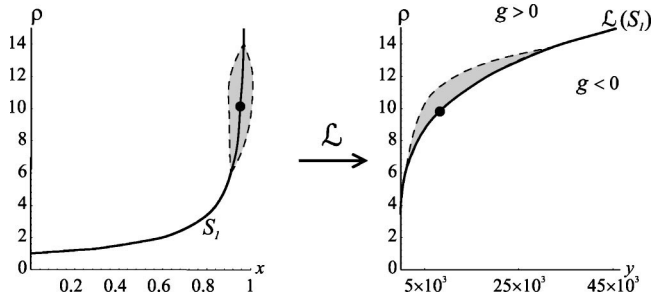

FIG. 7. Legendre map for the oscillator ($\rho = r/r_0$).

with $\psi(r,x) = (4/m^2c^4)\, xL_x^2(r,x)$, and the expression (30) takes the form

$$X_L = c\sqrt{x}\left(\cos u\,\frac{\partial}{\partial r} + \frac{\sin u}{r}\,\frac{\partial}{\partial \phi}\right) + \frac{\sqrt{\psi}}{mc} L_r\left(2\cos u\,\frac{\partial}{\partial y} - \frac{\sin u}{\psi}\,\frac{\partial}{\partial \alpha}\right). \tag{32}$$

Due to $(31)_1$ hypersurface $\mathcal{L}(S_1)$ is given by

$$g(r,y) = 0,$$

with

$$g(r,y) = \frac{4}{m^2c^4} x_1(r)\tilde{L}_x^2(r) - y, \tag{33}$$

where $x = x_1(r)$ is the function implicitly defined by equation $E_x(r,x) = 0$, and $\tilde{L}_x(r) = L_x(r,x_1(r))$. For the oscillator (11) the Legendre mapping $\mathcal{L}$ is illustrated in Fig. 7. In this case, as is easy to see from (31) and (33), the image with respect to $\mathcal{L}$ of a sufficiently small neighborhood of a point $(q,v) \in S_1$ is contained in the region $\{g > 0\}$.
From (32) we get:

$$X_L(g) = \cos u\left(c\sqrt{x} g_r + \frac{2\sqrt{\psi}}{mc} L_r g_y\right).$$

But from (18), (33) and $\mathcal{L}(S_1)$'s equation follows:

$$g_r = \frac{4}{m^2c^4}[x_1'\tilde{L}_x^2 + 2x_1\tilde{L}_x(\tilde{L}_{xr} + x_1'\tilde{L}_{xx})] = \frac{4\tilde{L}_x}{m^2c^4}(x_1'\tilde{E}_x + 2x_1\tilde{L}_{xr}) = \frac{8}{m^2c^4} x_1\tilde{L}_x\tilde{L}_{xr},$$

where, as before, $\tilde{f}(r)$ means $f(r,x_1(r))$. Hence, we obtain

$$X_L(g) = \frac{4}{m^2c^3}\sqrt{x}\cos u(2x_1\tilde{L}_x\tilde{L}_{xr} - L_xL_r). \tag{34}$$

Since $2xL_{xr} - L_r = E_r$ the restriction of (34) to S_1 is

$$\widetilde{X_L(g)} = \frac{4}{m^2c^3}\sqrt{x_1}\cos u\tilde{L}_x\tilde{E}_r. \tag{35}$$

In the case of the oscillator we have $\tilde{L}_x < 0$, $\tilde{E}_r > 0$. Therefore (35) shows that $\widetilde{X_L(g)}$ is:

(1) positive in the region S_1^+ corresponding to $u \in [\pi/2,\pi] \cup [-\pi,-\pi/2]$;
(2) negative in the region S_1^- corresponding to $u \in [-\pi/2,\pi/2]$;

(3) null on the bidimensional surface $W=S_1\cap\{u=\pm\pi/2\}$.

Hence, keeping in mind what was said previously about the range of $\mathcal{L}$ and applying the transition principle, we see the following.

(1) If $\overline{P}\in S_1^+$, then $\overline{P}$ is an in-point, while $\tilde{P}$ is an out-point. Therefore, if the phase point, starting from outside S_1, reaches it at $\tilde{P}$, its trajectory can be prolongated starting from $\overline{P}$ (jump from $\tilde{P}$ to $\overline{P}$).

(2) If $\overline{P}\in S_1^-$, then $\overline{P}$ is an out-point, while $\tilde{P}$ is an in-point. Therefore, if the phase point, starting from outside S_1, reaches it at $\overline{P}$, its trajectory can be prolongated starting from $\tilde{P}$ (jump from $\overline{P}$ to $\tilde{P}$).

(3) If $\overline{P}\in W$, i.e., if $\overline{u}=\pm\pi/2$, then $\overline{P}\equiv\tilde{P}$. In this case the jump becomes infinitesimal and its direction is indicated by the Hamiltonian vector field. In fact $\mathcal{L}(W)$ is described in terms of coordinates (r,ϕ,y,α) by

$$g(r,y)=0,$$

$$\cos u=0.$$

But it follows from (32) that on W

$$X_L(\cos u)=-\frac{L_r}{mc\sqrt{\psi}}\sin u=\pm\frac{L_r}{mc\sqrt{\psi}},$$

which is different from zero on S_1. More precisely, it is positive for $u=\pi/2$ and negative for $u=-\pi/2$; in both cases X_L is directed toward the region S_1^- in which singular trajectories end.

Finally note that, for the oscillator (11),

$$X_L(p_i)=\frac{q_i}{r}L_r\neq 0 \quad \text{on } S_2\backslash S_1.$$

Since $\mathcal{L}(S_2)$ coincides with the null section of $T^*(M)$, this shows that X_H is transversal to $\mathcal{L}(S_2)$.

D. Phase trajectories of the oscillator

In this section we will study phase trajectories of the oscillator outside S. It will be shown that their behavior depends strongly on their position with respect to the singular surface. Trajectories arriving at S have discontinuities, described by the transition principle, and together with others form a perfectly self-consistent dynamical model.

In this section coordinates (r,x,u,ϕ) are used. Let, as before,

$$Z_L=\dot{r}\frac{\partial}{\partial r}+\dot{\phi}\frac{\partial}{\partial\phi}+\dot{x}\frac{\partial}{\partial x}+\dot{u}\frac{\partial}{\partial u}$$

be the vector field on $T(M)$ corresponding to the Lagrangian L. Since I,E are first integrals, then

$$Z_L(I)=Z_L(E)=0,$$

or, equivalently

$$\begin{pmatrix} I_r & I_x & I_u \\ E_r & E_x & 0 \end{pmatrix}\begin{pmatrix} \dot{r} \\ \dot{x} \\ \dot{u} \end{pmatrix}=\begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Therefore

$$\dot{r}=-kI_uE_x, \quad \dot{x}=kI_uE_r, \quad \dot{u}=k(I_rE_x-I_xE_r). \tag{36}$$

On the other hand,

$$\dot{r}=\frac{d}{dt}(\sqrt{q_1^2+q_2^2})=\frac{q_1v_1+q_2v_2}{r}=c\sqrt{x}\cos u.$$

So that

$$k=-\frac{c\sqrt{x}\cos u}{E_xI_u}=-\frac{c\sqrt{x}\sin u}{IE_x}=-\frac{c^2}{2rL_xE_x}. \tag{37}$$

Notice also

$$I_rE_x-I_xE_r=\frac{E_x}{c\sqrt{x}}\sin u(2xL_x+rL_r), \tag{38}$$

which follows directly from (15), (18), (16), and

$$\frac{\partial}{\partial x}(\sqrt{x}L_x)=\frac{E_x}{2\sqrt{x}}.$$

This way one gets the first three Euler–Lagrange equations:

$$\dot{r}=c\sqrt{x}\cos u$$

$$\dot{x}=-c\frac{E_r}{E_x}\sqrt{x}\cos u \tag{39}$$

$$\dot{u}=-\frac{c\sin u}{2r\sqrt{x}L_x}(2xL_x+rL_r),$$

which form a closed subsystem of the whole system.

Denote by $\tilde{Z}_L$ the projection of Z_L onto the (x,r,u) space. Then, solutions of (39) are identified with trajectories of $\tilde{Z}_L$. Due to obvious symmetry with respect to the (x,r) plane it is sufficient to consider those of them for which $u\in[0,\pi]$ (i.e., counterclockwise motions around the center of the elastic force).

The fourth Euler–Lagrange equation,

$$\dot{\phi}=\frac{c\sqrt{x}}{r}\sin u, \tag{40}$$

can be found directly from

$$\tan\phi=\frac{q_2}{q_1},$$

so that

$$\phi(t)=c\int_0^t\frac{\sqrt{x(\tau)}}{r(\tau)}\sin u(\tau)d\tau+\text{const}, \tag{41}$$

with $(x(t),r(t),u(t))$ being a solution of (39).

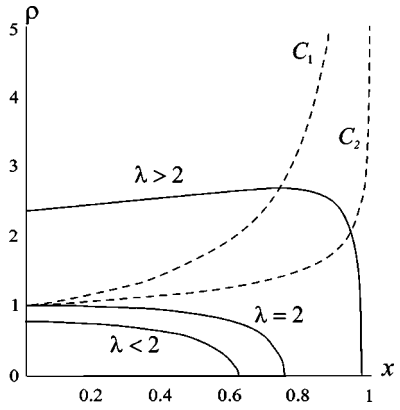

FIG. 8. Energy level surfaces of the oscillator.

Let

$$\Xi_{\lambda,\mu}=\{E=\lambda mc^2\}\cap\{I=\mu mcr_0\}. \tag{42}$$

Obviously,

$$\Xi_{\lambda,\mu}=\Gamma_{\lambda,\mu}\times S^1,$$

where $\Gamma_{\lambda,\mu}$ is the projection of $\Xi_{\lambda,\mu}$ into (r,x,u) space, while the circle S^1 corresponds to the cyclic coordinate ϕ. In their turn surfaces $\Xi_{\lambda,\mu}$ foliate the energy level three-fold,

$$\Sigma_\lambda=\{E=\lambda mc^2\}.$$

In the case of oscillator (11) Σ_λ is not empty for $\lambda\in[1,+\infty]$.
Let $\tilde{\Sigma}_\lambda$ be the projection of Σ_λ onto the (r,x,u) space. Obviously

$$\tilde{\Sigma}_\lambda=\Gamma_\lambda\times S^1,$$

where Γ_λ is the curve in (r,x) plane given by equation $E(r,x)=\lambda mc^2$ and S^1 is the circle corresponding to the cyclic coordinate u. Curves Γ_λ are shown in Fig. 8. One can see that Γ_λ intersects the projections C_1,C_2, of S_1,S_2, respectively, as follows: (i) at two different points P_1,P_2, if $\lambda>2$; (ii) at the single point Q, if $\lambda=2$; (iii) nowhere, if $1\leqslant\lambda<2$. Therefore Σ_λ intersects S_1 and S_2:

(1) along two tori $T_i=\Sigma_\lambda\cap S_i$, $i=1,2$, if $\lambda>2$. These tori project onto P_i's and have (ϕ,u) as cyclic coordinates.
(2) along the circle $\gamma=S_1\cap S_2$, with the cyclic coordinate ϕ, if $\lambda=2$.
(3) nowhere if $\lambda<2$.

Therefore, $\Sigma_\lambda\backslash S$ has three connected components, if $\lambda>2$ and is connected, if $\lambda\leqslant 2$.

In the case $\lambda>2$ the behavior of phase trajectories depends strongly on the connected component of $\Sigma_\lambda\backslash S$ they belong to. Due to (41) it is sufficient to study trajectories of (39), i.e., connected components of curves $\Gamma_{\lambda,\mu}\backslash\tilde{S}$, with $\tilde{S}$ being the projection of S onto the (r,x,u) space. In Fig. 9 the projections into the (x,u) plane of three different kinds of such trajectories contained in $\tilde{\Sigma}_\lambda$ for a fixed λ are shown. As before we limit ourselves to $0\leqslant u\leqslant\pi$. The three vertical lines correspond to the projections $\tilde{T}_i$ of tori T_i's (in fact they are circles, due to the cyclicity of coordinate u). Passing to further details, denote by $x_i=x_i(\lambda)$ the constant value of x along T_i. Connected components $\Sigma_\lambda^1,\Sigma_\lambda^2,\Sigma_\lambda^3$ of $\Sigma_\lambda\backslash S$ correspond to $x<x_1$, $x_1<x<x_2$ and $x_2<x$, respec-

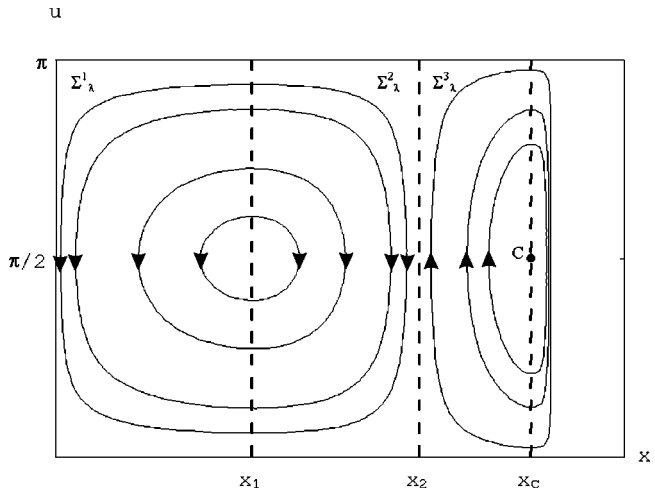

FIG. 9. Phase portrait of the oscillator for a fixed value of energy ($\lambda > 2$).

tively. The trajectories belonging to Σ^1_λ and Σ^2_λ are discontinuous in the sense that they end on S_1 and then jump, according to the transition principle, at another point of S_1. More exactly, in the situation shown in the figure, such a trajectory starts from a point of $T_1^+ = T_1 \cap \{\pi/2 \leqslant u \leqslant \pi\}$ and reaches a point in $T_1^- = T_1 \cap \{0 \leqslant u \leqslant \pi/2\}$ in a finite time. Trajectories γ_1 and γ_2, whose projections $\tilde{\gamma}_1$ and $\tilde{\gamma}_2$ are shown in Fig. 10, correspond to the same value of λ and of μ. Denote by $P_{\text{start}} \equiv (\overline{x}, \overline{r}, \pi - \overline{u}) \in \tilde{T}_1^+$ and $P_{\text{end}} \equiv (\overline{x}, \overline{r}, \overline{u}) \in \tilde{T}_1^-$ the common starting and ending points of $\tilde{\gamma}_1$ and $\tilde{\gamma}_2$. When a phase point starts from $(P_{\text{start}}, \phi_0) \equiv (\overline{x}, \overline{r}, \pi - \overline{u}, \phi_0)$ and then goes along γ_1 (or, alternatively, γ_2) it arrives at the point $(P_{\text{end}}, \overline{\phi}) \equiv (\overline{x}, \overline{r}, \overline{u}, \overline{\phi})$ with $\overline{\phi}$ given by (28) and then proceeds along the trajectory whose projection is $\tilde{\gamma}_1$ or, alternatively, $\tilde{\gamma}_2$, and so on.

In Fig. 11 the situation in the configuration space $M = \{(q_1, q_2)\} = \{(r, \phi)\}$ is shown. The oscillating particle, starting from the point $(r = \overline{r}, \phi = 0)$, moves along the projection $\hat{\gamma}_1$ of γ_1 onto

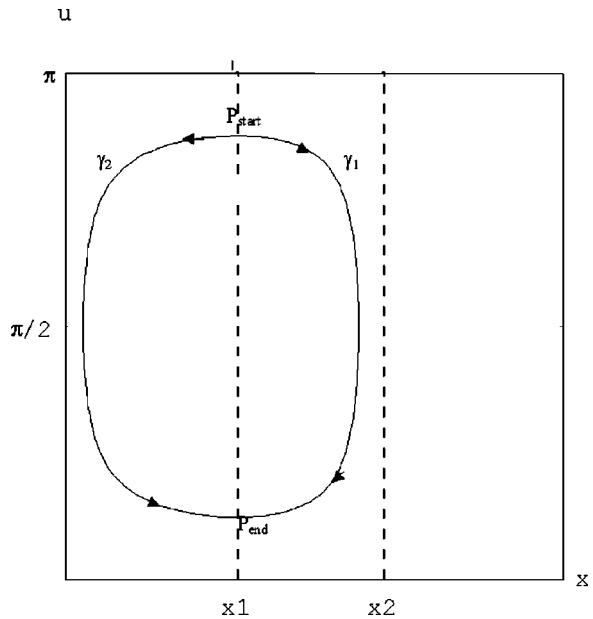

FIG. 10. Jumping phase trajectories.

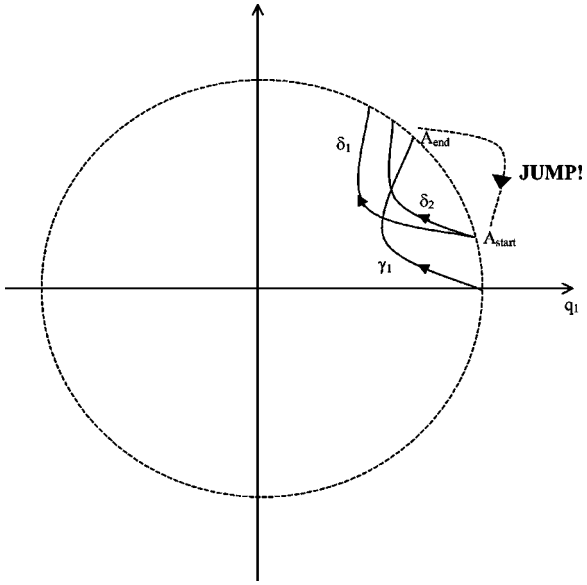

FIG. 11. Jumping oscillator.

M until it reaches the point $A_{\text{end}} \equiv (r=\overline{r}, \phi=\overline{\phi})$. From there it jumps to the point $A_{\text{start}} \equiv (r=\overline{r}, \phi=\tilde{\phi})$, where $\tilde{\phi}$ is given by (28). Then it splits into the two trajectories δ_1, δ_2, both with initial velocity

$$(x=\overline{x}, u=\tilde{u}=\pi-\overline{u}).$$

Consider now the trajectories of (39) contained in Σ^3_λ. These are regular closed trajectories winding around the center $C=C(\lambda) \equiv (x=x_C, u=\pi/2)$, where $x_C=x_C(\lambda)$ is the zero of the equation $2xL_x(r_{en}(x,\lambda),x)+rL_r(r_{en}(x,\lambda),x)=0$, and $r=r_{en}(x,\lambda)$ is implicitly defined by the equation $E(r,x)=\lambda mc^2$. The corresponding trajectories in the configuration space are shown in Fig. 12. They are precessions around the force center.

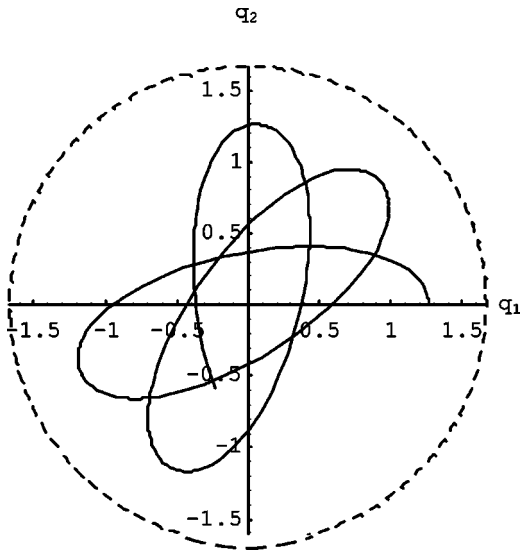

FIG. 12. Regular precessions of the oscillator.

Note that both the discontinuous trajectories in Σ^2_λ and the regular ones in Σ^3_λ near S_2 tend to be parallel to it, so that this component of the singular hypersurface is never reached by the phase point, at least for trajectories with nonzero angular momentum.

V. CONCLUSIONS

The self-consistency of the example discussed in this paper shows that the transition principle is natural not only from the geometrical but also from the dynamical point of view. The following question should, however, be answered: whether the existence of the singular hypersurface is merely due to approximation procedures or, on the contrary, it has a substantial physical meaning. So, it would be very interesting to look for singular Lagrangians which could be directly experimentally tested.

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A hierarchy of generalized AKNS equations, *N*-Hamiltonian structures and finite-dimensional involutive systems and integrable systems

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An eigenvalue problem and the associated hierarchy of nonlinear soliton equations are proposed in this paper. In particular, a representative system of generalized AKNS soliton equations in the hierarchy is given, namely, $q_t=-\frac{1}{2}q_{xx}+q^2r-2\mu q^2r_x-2\mu rqq_x+2\mu^2q^3r^2$, $r_t=\frac{1}{2}r_{xx}-qr^2-2\mu r^2q_x-2\mu qrr_x+2\mu^2q^2r^3$. *N*-Hamiltonian structures are also established for all the hirarchy of generalized AKNS soliton equations based on $N+1$ pairs of Hamiltonian pairs. And then the eigenvalue problem is nonlinear as a finite-dimensional completely integrable Hamiltonian system under the Bargmann constraint between the potentials and the eigenvalue functions, and its involutive system is also given. Finally, the involutive solutions of the hierarchy of generalized AKNS soliton equations are found, in particular, the involutive solutions of the system of generalized Schrödinger equations are given. © *2001 American Institute of Physics.*
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I. INTRODUCTION

As is well known, it plays important roles in the soliton theory and dynamical integrable system to find many new nonlinear evolution equations and to further consider their algebraic properties and geometrical structures, such as the Hamiltonian structure, conserved density, symmetry, and Liouville integrable property.[1–36] In 1983, Tu[5] developed a simple approach to Hamiltonian structures of integrable systems. The essence of the method was the use of the chain rule of variational derivatives. It was improved further by Chowdhury and Swapna.[6] Recently, Tu[9] proposed a so-called loop algebra scheme to generate the hierarchy of Liouville sense integrable evolution equations and their Hamiltonian structures from the eigenvalue problem. This approach has been applied to find many new important nonlinear evolution equations hierarchies, such as the AKNS hierarchy,[1–4] TA hierarchy,[5] TB hierarchy,[7] TC hierarchy,[8] BTP hierarchy,[10] Kaup–Newell hierarchy,[11] WKI hierarchy,[12] Benjamin–Ono hierarchy,[13] Dirac hierarchy,[14] coupled KdV hierarchy,[15] Harry-Dym hierarchy,[16] coupled Burgers hierarchy,[18,24] Kupershmidt hierarchy,[19] coupled MKdV hierarchy,[25] and AKNS–Kaup–Newell hierarchy,[20] and so on, and the associated Hamiltonian structures can also be derived by virtue of the trace identity. In addition, the bi-Hamiltonian structure[17,21,22] and tri-Hamiltonian structure[20,23] had been also presented and applied to some soliton hierarchies by using the recursion operators.

In order to find many finite-dimensional integrable Hamiltonian systems (FDIHS), Cao *et al.*[26–28] proposed an effective skill, nonlinearization technique, to find new FDIHS, in which the well-known Bargmann constraint and Neumann constraint are contained. Many FDIHS have been obtained through using the approach (see Refs. 26–30). But this method has its disadvantages. Only lower order constraint flows could be found. In order to obtain higher order constraint flows, more recently, Zeng[31,32] presented a powerful approach, which contains Cao's method, by introducing so-called Jacobi–Ostrogradsky coordinates. It can easily prove that these higher constraint

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flows are Liouville sense integrable by virtue of the r-matrix and Poisson structure.[31–34]

In this paper, we would like to introduce an eigenvalue problem

$$\phi_x = U(\lambda,u)\phi = U\phi, \quad U\begin{pmatrix} -\lambda-\mu qr & q \\ r & \lambda+\mu qr \end{pmatrix}, \quad \phi=\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}, \quad u=\begin{pmatrix} q\\ r\end{pmatrix}, \tag{1}$$

where q and r are two scalar potentials, λ being a constant spectral parameter, and μ being an arbitrary constant, which is a simple extension of the AKNS eigenvalue problem,[1–4]

$$\phi_x = U(\lambda,u)\phi = U\phi, \quad U\begin{pmatrix} -\lambda & q \\ r & \lambda \end{pmatrix}, \quad \phi=\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}. \tag{2}$$

As $\mu=0$, the eigenvalue problem (1) reduces to the AKNS eigenvalue problem (2).

This paper is organized as follows. In Sec. II, we give a generalized AKNS soliton hierarchy and its N-Hamiltonian structure by introducing the auxiliary problem of (1), trace identity and Hamiltonian pairs. As the special case of (1), the N-Hamiltonian structure of the AKNS hierarchy is about (2). In Sec. III, we first obtain $N+1$ pairs of Lennard's operators pairs. Then a system of constraint conditions are proposed; (1) is nonlinearized to a finite-dimensional completely integrable system in the Liouville sense under the first constraint condition. In Sec. IV, the involutive solutions of the hierarchy of generalized AKNS soliton equations are obtained. Finally, some summaries and conclusions are given in Sec. V.

II. THE HIERARCHY OF GENERALIZED AKNS EQUATIONS ASSOCIATED WITH EQ. (1) AND *N*-HAMILTONIAN STRUCTURES

It is clear that the adjoint equation of Eq. (1) can be written as

$$V_x=[U,V]\equiv UV-VU, \quad V=V(\lambda,u)=\begin{pmatrix} a & b\\ c & -a\end{pmatrix}=\sum_{i=0}^{\infty}\begin{pmatrix} a_i & b_i\\ c_i & -a_i\end{pmatrix}\lambda^{-i}, \tag{3}$$

where $a_i, b_i, c_i (i=0,1,2,...)$ are all functions of q and r to be determined later. Equation (3) leads to

$$a_{n,x}=qc_n-rb_n, \quad b_{n,x}=-2b_{n+1}-2qa_n-2\mu qrb_n, \quad c_{n,x}=2c_{n+1}-2ra_n+2\mu qrc_n. \tag{4}$$

The following recursion formulas are obtained from Eq. (4):

$$\begin{pmatrix} c_{n+1}\\ b_{n+1}\end{pmatrix}=L\begin{pmatrix} c_n\\ b_n\end{pmatrix}, \quad L=\begin{pmatrix} \frac{1}{2}\partial-r\partial^{-1}q-\mu qr & r\partial^{-1}r\\ -q\partial^{-1}q & -\frac{1}{2}\partial+q\partial^{-1}r-\mu qr\end{pmatrix}, \tag{5a}$$

$$a_{n+1}=\tfrac{1}{2}(rb_{n,x}+qc_{n,x})-\mu qra_{n,x}, n=1,2,..., \tag{5b}$$

where $\partial=\partial/\partial x$, $\partial\partial^{-1}=1$. If we take the values $a_0=-1$, $b_0=c_0=0$, then, Eqs. (5a) and (5b) imply the following results:

$$a_1=0, \quad b_1=q, \quad c_1=r, a_2=\tfrac{1}{2}qr, \quad b_2=-\tfrac{1}{2}qx-\mu q^2r,$$

$$c_2=\tfrac{1}{2}r_x-\mu qr^2, \quad a_3=\tfrac{1}{4}(qr_x-rq_x)-\mu q^2r^2,$$

$$b_3=\tfrac{1}{4}q_{xx}+\tfrac{1}{2}\mu(q^2r)_x-\tfrac{1}{2}q^2r+\tfrac{1}{2}\mu rqq_x+\mu^2q^3r^2,$$

$$c_3=\tfrac{1}{4}q_{xx}+\tfrac{1}{2}\mu(qr^2)_x-\tfrac{1}{2}qr^2-\tfrac{1}{2}\mu qrr_x+\mu^2q^2r^3,$$

$$a_4=\tfrac{1}{8}(rq_{xx}-qr_{xx}-q_xr_x)-\tfrac{3}{8}q^2r^2+\tfrac{3}{4}\mu(r^2qq_x-q^2rr_x).$$

In order to deduce a hierarchy of nonlinear evolution equations from Eq. (1), we introduce the auxiliary problem of Eq. (1), namely,

$$\phi_{t_n}=V^{(n)}\phi=V^{(n)}(\lambda,u)\phi, \tag{6}$$

$$V^{(n)}=(\lambda^n V)^+ +\Delta_n=\sum_{i=0}^{n}\begin{pmatrix} a_i & b_i \\ c_i & -a_i \end{pmatrix}\lambda^{n-i}+\begin{pmatrix} \delta_{1n} & 0 \\ 0 & \delta_{2n} \end{pmatrix}, \tag{7}$$

where δ_{1n},delta$_{2n}$ are functions to be determined later. Therefore it is easy to prove that the compatibility condition $\phi_{xt}=\phi_{tx}$ of Eqs. (1) and (6) generates the zero curvature equation $U_{t_n}-V^{(n)}+[U,V^{(n)}]=0$, namely,

$$\delta_{1n,x}=-\mu(qr_t+rq_t), \quad \delta_{1n}=-\delta_{2n}, \tag{8}$$

$$q_t=-2b_{n+1}+2q\delta_{1n}, \tag{9}$$

$$r_t=2c_{n+1}+2r\delta_{2n}. \tag{10}$$

From Eqs. (8)–(10), we have

$$\delta_{1n}=-\mu\partial^{-1}(qr_t+rq_t)=\mu\partial^{-1}(2rb_{n+1}-2qc_{n+1}). \tag{11}$$

Substituting Eq. (11) into Eqs. (9) and (10), we deduce the following hierarchy of nonlinear evolution equations:

$$u_t=\begin{pmatrix} q_{t_n} \\ r_{t_n} \end{pmatrix}=K_n=\begin{pmatrix} -4\mu q\partial^{-1}q & -2+4\mu q\partial^{-1}r \\ 2+4\mu r\partial^{-1}q & -4\mu r\partial r \end{pmatrix}\begin{pmatrix} c_{n+1} \\ b_{n+1} \end{pmatrix}$$

$$=M\begin{pmatrix} c_{n+1} \\ b_{n+1} \end{pmatrix}=ML^nN\begin{pmatrix} r \\ q \end{pmatrix}. \tag{12}$$

In order to consider and N-Hamiltonian structures and the integrability of Eq. (12) under the Liouville's sense. We need to introduce new variables, namely,

$$G_{n+1}=\begin{pmatrix} G_{n+1}^{(1)} \\ G_{n+1}^{(2)} \end{pmatrix}=\begin{pmatrix} c_{n+1}-2\mu ra_{n+1} \\ b_{n+1}-2\mu qa_{n+1} \end{pmatrix}. \tag{13}$$

According to Eqs. (4) and (13), we get

$$\begin{pmatrix} c_{n+1} \\ b_{n+1} \end{pmatrix}=\begin{pmatrix} 1+2\mu r\partial^{-1}q & -2\mu r\partial^{-1}r \\ 2\mu q\partial^{-1}q & 1-2\mu q\partial^{-1}r \end{pmatrix}\begin{pmatrix} c_{n+1}-2\mu ra_{n+1} \\ b_{n+1}-2\mu qa_{n+1} \end{pmatrix}=N\begin{pmatrix} c_{n+1}-2\mu ra_{n+1} \\ b_{n+1}-2\mu qa_{n+1} \end{pmatrix}. \tag{14}$$

Therefore we have the following recursion relation:

$$G_{n+1}=\begin{pmatrix} c_{n+1}-2\mu ra_{n+1} \\ b_{n+1}-2\mu qa_{n+1} \end{pmatrix}=N^{-1}LN\begin{pmatrix} c_n-2\mu ra_n \\ b_n-2\mu qa_n \end{pmatrix}=\Psi G_n, \quad n=1,2,..., \tag{15}$$

where

$$N^{-1}=\begin{pmatrix} 1-2\mu r\partial^{-1}q & 2\mu r\partial^{-1}r \\ -2\mu q\partial^{-1}q & 1+2\mu q\partial^{-1}r \end{pmatrix},$$

and $\Psi=N^{-1}LN$ is a recursion operator.

According to Eqs. (12) and (14), we easily derive

$$u_{t_n}=\begin{pmatrix} q_{t_n} \\ r_{t_n} \end{pmatrix}=K_n=J_0G_{n+1}=J_1G_n=J_2G_{n-1}=\cdots=J_nG_1=J_{n+1}G_0, \tag{16}$$

where $J_n=ML^nN=J_0(N^{-1}LN)^n$, $n=0,1,2,...$ and

$$J_0=MN=\begin{pmatrix} -8\mu q\partial^{-1}q & -2+8\mu q\partial^{-1}r \\ 2+8\mu r\partial^{-1}q & -8\mu r\partial^{-1}r \end{pmatrix}.$$

Proposition 1: The 2×2 matrix integrodifferential operator J_0 defined by the above equation is a Hamiltonian operator for the arbitrary constant μ.

Proof: Because it is a skew symmetry operator, i.e., $J_0^*=-J_0$ and it is easy to prove that J_0 satisfies the Jacobi identity, that is,

$$\langle Z,J_0'(u([J_0X]Y\rangle+\text{cycle}(X,Y,Z)\equiv0(\text{mod}\,\partial),$$

with $X=(X_1,X_2)^T$, $Y=(Y_1,Y_2)^T$, $Z=(Z_1,Z_2)^T$, and $J_0'(u)[f]$ denotes the Frechet derivative of J_0,

$$J_0'(u)[f]=\frac{d}{d\epsilon}J_0(u+\epsilon f)|_{\epsilon=0}.$$

Hence, J_0 is Hamiltonian (or symplectic) operator.

According to the same theory, we can also prove that other operators $J_i(i=1,2,...)$ are also all Hamiltonian operators.

Through using the same as the notion applied in Refs. 8 and 9, the Killing–Cartan standard form is defined by $\langle X,Y\rangle=\text{const.}\cdot\text{tr}(XY)$. In order to calculation conveniently, we take const. $=1$. Hence we have from Eqs. (1) and (3),

$$\left\langle V,\frac{\partial U}{\partial q}\right\rangle=c-2\mu ra,\quad \left\langle V,\frac{\partial U}{\partial r}\right\rangle=c-2\mu qb,\quad \left\langle V,\frac{\partial U}{\partial\lambda}\right\rangle=-2a. \tag{17}$$

According to definition of the trace identity,[8,9] yields

$$\frac{\delta}{\delta u}\left(\left\langle V,\frac{\partial U}{\partial\lambda}\right\rangle\right)=\lambda^{-\beta}\frac{\partial}{\partial\lambda}\lambda^{\beta}\left(\left\langle V,\frac{\partial U}{\partial q}\right\rangle,\left\langle V,\frac{\partial U}{\partial r}\right\rangle\right)^T, \tag{18}$$

where β is constant to be determined later. Substituting Eq. (17) into (18) and combining these conditions

$$a=\sum_{i\geqslant0}a_n\lambda^{-i},\quad b=\sum_{i\geqslant0}b_n\lambda^{-i},\quad c=\sum_{i\geqslant0}c_n\lambda^{-i},$$

we get through comparing the coefficients of λ^{-n-2} of two sides of Eq. (18), yields

$$\frac{\delta}{\delta u}(-2a_{n+2})=(\beta-n-1)(c_{n+1}-2\mu ra_{n+1},b_{n+1}-2\mu qa_{n+1})^T. \tag{19}$$

In order to get the value of β, we take $n=-1$ in Eq. (19) and obtain $\beta=0$. Therefore we have

$$G_{n+1}=\begin{pmatrix} c_{n+1}-2\mu ra_{n+1} \\ b_{n+1}-2\mu qa_{n+1} \end{pmatrix}=\frac{\delta H_{n+1}}{\delta u}=\Psi\frac{\delta H_n}{\delta u}=\Psi G_n, \tag{20}$$

with the Hamiltonian functions satisfying

$$H_0=2\mu rq, \quad H_n=\frac{2a_{n+1}}{n}, \quad n=1,2,\ldots. \tag{21}$$

Therefore the hierarchy of the nonlinear evolution Eq. (16) possesses the following formal N-Hamiltonian structures from Eqs. (16) and (20):

$$u_{t_n}=\begin{pmatrix} q_{t_n} \\ r_{t_n} \end{pmatrix}=K_n=J_0\frac{\delta H_{n+1}}{\delta u}=J_1\frac{\delta H_n}{\delta u}=J_2\frac{\delta H_{n-1}}{\delta u}=\cdots=J_{n+1}\frac{\delta H_0}{\delta u}. \tag{22}$$

In fact, we can easily show that the Hamiltonian functions $\{H_n\}_n^\infty=0$ satisfying $\delta H_{n+1}/\delta u=\Psi(\delta H_n/\delta u)$, $n\geqslant 0$ are all common conserved densities for the whole generalized AKNS hierarchy. And they are commute with each other under the $n+2$ Poisson brackets associated with the Hamiltonian operators $J_i=J_0\Psi^i$, $i=0,1,2,...$, because a direct calculation can show that

$$\begin{aligned}\{H_n,H_m\}J_i&=\int\left\langle\frac{\delta H_n}{\delta u},J_i\frac{\delta H_m}{\delta u}\right\rangle dx=\int\left\langle\frac{\delta H_n}{\delta u},J_i\Psi\frac{\delta H_{m-1}}{\delta u}\right\rangle dx\\&=\int\left\langle\frac{\delta H_n}{\delta u},\Psi^*J_i\frac{\delta H_m}{\delta u}\right\rangle dx=\int\left\langle\Psi\frac{\delta H_n}{\delta u},J_i\frac{\delta H_m}{\delta u}\right\rangle dx\\&=\{H_{n+1},H_{m-1}\}_{J_i}=\cdots=\{H_m,H_n\}_{J_i},n,m\geqslant 0.\end{aligned} \tag{23}$$

Therefore we get $\{H_n,H_m\}_{J_i}=0$. During the course of the proof of Eq. (23), we use the following formula obtained from $J_i^*=-J_i$:

$$J_i\Psi=J_0\Psi^{i+1}=J_{i+1}=-J_{i+1}^*=-(J_i\Psi)^*=-\Psi^*J_i^*=\Psi^*J_i.$$

And we can also derive

$$[K_n,K_m]=\left[J_i\frac{\delta H_n}{\delta u},J_i\frac{\delta H_m}{\delta u}\right]=J_i\frac{\delta}{\delta u}\{H_n,H_m\}=0,n,m\geqslant 0, \tag{24}$$

which shows that every system generalize AKNS equations posses infinitely many commuting symmetries $\{K_n\}_{n=0}^\infty$.

Remark 1: Taking $n=2$, Eq. (16) becomes a new system of the generalized ANKS soliton equations,

$$q_t=-\tfrac{1}{2}q_{xx}+q^2r-2\mu q^2r_x-2\mu rqq_x+2\mu^2q^3r^2, \tag{25a}$$

$$r_t=\tfrac{1}{2}r_{xx}-qr^2-2\mu r^2q_x-2\mu qrr_x+2\mu^2q^2r^3. \tag{25b}$$

If setting $\mu=0$, then Eqs. (25) reduce to the AKNS equation.[1–4] Equations (25) possess the flowing quadr-Hamiltonian structures,

$$u_t=\begin{pmatrix} q_t \\ r_t \end{pmatrix}=J_0\frac{\delta H_3}{\delta u}=J_1\frac{\delta H_2}{\delta u}=J_2\frac{\delta H_1}{\delta u}=J_3\frac{\delta H_0}{\delta u},$$

where the Hamiltonian functions H_i, $(i=0,1,2,3)$ are

$$H_0=2\mu qr, \quad H_1=qr, \quad H_2=\tfrac{1}{4}(qr_x-rq_x)-\mu q^2r^2,$$

$$H_3=\tfrac{1}{12}(rq_{xx}-qr_{xx}-q_xr_x)-\tfrac{1}{4}q^2r^2+\tfrac{1}{2}\mu(r^2qq_x-q^2rr_x).$$

Remark 2: Equation (2) is a special case of Eq. (1) with $\mu=0$, so according to the above results, we can come to some conclusions about the hierarchy of the AKNS equations,

$$u_t=\begin{pmatrix} q_{t_n} \\ r_{t_n} \end{pmatrix}=K_n=\begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix}\begin{pmatrix} c_{n+1} \\ b_{n+1} \end{pmatrix}=M\begin{pmatrix} c_{n+1} \\ b_{n+1} \end{pmatrix}=ML^nN\begin{pmatrix} r \\ q \end{pmatrix}, \tag{26}$$

where

$$L=\begin{pmatrix} \frac{1}{2}\partial-r\partial^{-1}q & r\partial^{-1}r \\ -q\partial^{-1}q & -\frac{1}{2}\partial+q\partial^{-1}r \end{pmatrix},\ M=\begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix},\ N=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Therefore, we have

$$J_0=MN=M=\begin{pmatrix} 0 & -2 \\ 2 & 0 \end{pmatrix},$$

$$J_1=MLN=ML=\begin{pmatrix} 2q\partial^{-1}q & \partial-2r\partial^{-1}q \\ \partial-2r\partial^{-1}q & 2r\partial^{-1}r \end{pmatrix},\ J_i=ML^iN=ML^i, i=2,3,\ldots.$$

It is clear that J_0 and J_1 are both Hamiltonian operators and we can also derive that J_i, $i=2,3,\ldots$ are also Hamiltonian operators. The hierarchy of the AKNS equation (23) also possesses the following N-Hamiltonian structures:

$$u_t=\begin{pmatrix} q_t \\ r_t \end{pmatrix}=K_n=J_0\frac{\delta H_{n+1}}{\delta u}=J_1\frac{\delta H_n}{\delta u}=J_2\frac{\delta H_{n-1}}{\delta u}=\cdots=J_{n+1}\frac{\delta H_0}{\delta u}$$

with the Hamiltonian functions satisfy Eq. (21). They are all common conserved densities for the hierarchy of AKNS equations and commute with each other under these Poisson brackets associated with the Hamiltonian operators J_i, $i=0,1,2,\ldots$. In addition, there exists many commuting symmetries $\{K_n=J_i\,\delta H_{n-i+1}/\delta u\}_{n=0}^{\infty}$ for every system of AKNS equations.

III. FINITE-DIMENSIONAL INVOLUTIVE SYSTEMS

Let $\lambda_i(i=1,2,\ldots,N)$ be N different eigenvalues of problem (1), and $\phi_i=(\phi_{1i},\phi_{2i})^T$ be the corresponding solutions of problem (1), then (1) can become

$$\begin{pmatrix} \phi_{1i} \\ \phi_{2i} \end{pmatrix}_x=\begin{pmatrix} -\lambda_i-\mu qr & q \\ r & \lambda_i+\mu qr \end{pmatrix}\begin{pmatrix} \phi_{1i} \\ \phi_{2i} \end{pmatrix},\ u=\begin{pmatrix} q \\ r \end{pmatrix}. \tag{27}$$

Through the direct calculation, we get the spectral gradient $\nabla\lambda_i$ of the spectral value λ_i with respect to the potentials q and r,

$$\nabla\lambda_i=\frac{\delta\lambda_i}{\delta u}=\left(\frac{\delta\lambda_i}{\delta q},\frac{\delta\lambda_i}{\delta r}\right)^T=\left(-2\int \phi_{1i}\phi_{2i}dx\right)^{-1}\begin{pmatrix} \phi_{2i}^2+2\mu r\phi_{1i}\phi_{2i} \\ -\phi_{1i}^2+2\mu r\phi_{1i}\phi_{2i} \end{pmatrix}.$$

Proposition 2: The Hamiltonian operators J_k and J_{k+1} are all the pairs of Lennard's operators for $k=0,1,2,\ldots$.

Proof: Through the direct calculation, we easily find

$$J_{k+1}\nabla\lambda_i=\lambda_iJ_k\nabla\lambda_i.\ \ k=0,1,2,\ldots, \tag{28}$$

which shows that the proposition is true. In fact, we can prove that they are also Hamiltonian pairs.[23]

Next, we consider the following formal constraint conditions:

$$\frac{\delta H_{k+1}}{\delta u}-\gamma\sum_{i=1}^{N}\frac{\delta\lambda_{k+1}}{\delta u}=\frac{\delta H_{k+1}}{\delta u}-\gamma\begin{pmatrix}\langle\Phi_2,\Phi_2\rangle+2\mu r\langle\Phi_1,\Phi_2\rangle\\-\langle\Phi_1,\Phi_1\rangle+2\mu q\langle\Phi_1,\Phi_2\rangle\end{pmatrix}=0, \tag{29}$$

where $\Phi_j=(\phi_{j1},\phi_{j2},\ldots,\phi_{jN})$, $j=1,2$ and $\langle\cdot,\cdot\rangle$ denotes the standard inner product in R^N.

Taking $k=0$, $\gamma=\frac{1}{2}$ in Eq. (29), yields the first explicit constraint condition,

$$q=-\frac{\langle\Phi_1,\Phi_1\rangle}{2(1-2-\mu\langle\Phi_1,\Phi_2\rangle)},\quad r=\frac{\langle\Phi_2,\Phi_2\rangle}{2(1-2-\mu\langle\Phi_1,\Phi_2\rangle)}. \tag{30a}$$

In fact, this being the Bargmann constraint, that is

$$G_1=\begin{pmatrix}r\\q\end{pmatrix}=\sum_{i=1}^{N}\nabla\lambda_i=\begin{pmatrix}\langle\Phi_2,\Phi_2\rangle+2-\mu r\langle\Phi_1,\Phi_2\rangle\\-\langle\Phi_1,\Phi_1\rangle+2-\mu q\langle\Phi_1,\Phi_2\rangle\end{pmatrix}. \tag{30b}$$

Hence, (27) reduces to the following finite-dimensional Hamiltonian system under the Bargmann constraint (30a),

$$\Phi_{1x}=-\Lambda\Phi_1-\frac{\Phi_2\langle\Phi_1,\Phi_1\rangle}{2(1-2-\mu\langle\Phi_1,\Phi_2\rangle)}+\frac{-\mu\Phi_1\langle\Phi_1,\Phi_1\rangle\langle\Phi_2,\Phi_2\rangle}{4(1-2-\mu\langle\Phi_1,\Phi_2\rangle)^2}=\frac{\partial H_1}{\partial\Phi_2}, \tag{31a}$$

$$\Phi_{2x}=\Lambda\Phi_2+\frac{\Phi_1\langle\Phi_2,\Phi_2\rangle}{2(1-2-\mu\langle\Phi_1,\Phi_2\rangle)}-\frac{-\mu\Phi_2\langle\Phi_1,\Phi_1\rangle\langle\Phi_2,\Phi_2\rangle}{4(1-2-\mu\langle\Phi_1,\Phi_2\rangle)^2}=-\frac{\partial H_1}{\partial\Phi_1}, \tag{31b}$$

with the Hamiltonian function H_1 being

$$H_1=-\langle\Lambda\Phi_1,\Phi_2\rangle-\frac{\langle\Phi_1,\Phi_1\rangle\langle\Phi_2,\Phi_2\rangle}{4(1+2\mu\langle\Phi_1,\Phi_2\rangle)},$$

where $\Lambda=\mathrm{diag}(\lambda_1,\lambda_2,\ldots,\lambda_N)$. For other constraint conditions ($k\geqslant 0$), we can reduce problem (27) to other finite-dimensional Hamiltonian systems.

Theorem 1: Let (Φ_1,Φ_2) satisfy Eq. (31), then

$$q=-\frac{\langle\Phi_1,\Phi_1\rangle}{2(1-2\mu\langle\Phi_1,\Phi_2\rangle)},\quad r=\frac{\langle\Phi_2,\Phi_2\rangle}{2(1-2\mu\langle\Phi_1,\Phi_2\rangle)}$$

is a solution of the stationary generalized AKNS equations,

$$K_N+d_1K_{N-1}+\cdots+d_NK_0=0. \tag{32}$$

Proof: Letting the operator $J_0^{-1}J_1$ act upon Eq. (30b) for m times and noting $G_{n+1}=J_0-1J_1G_n$ and Eq. (28), we have

$$G_m+\alpha_2G_{m-2}+\cdots+\alpha_mG_0+\alpha_{m+1}G_{-1}=\begin{pmatrix}\langle\Lambda^m\Phi_2,\Phi_2\rangle+2-\mu r\langle\Lambda^m\Phi_1,\Phi_2\rangle\\-\langle\Lambda^m\Phi_1,\Phi_1\rangle+2-\mu q\langle\Lambda^m\Phi_1,\Phi_2\rangle\end{pmatrix}, \tag{33}$$

where $\alpha_j(j=2,3,\ldots,m+1)$ are arbitrary constants and $G_{-1}\in\mathrm{Ker}\,J_0$. Introducing the following polynomial:

$$P(y):=\Pi_{i=1}^{N}(y-\lambda_i)=y^N+p_1y^{N-1}+\cdots+p_N=\sum_{k=0}^{N}p_{N-k}y^k.$$

And then let the operator $J_0\Sigma_{k=0}^{N}p_{N-k}y^k$ act upon Eq. (33) and noting $K_n=J_0G_n$, we can derive Eq. (32). Where $d_i(i=1,2,\ldots,N)$ are determined by $\alpha_i(i=2,3,\ldots,m+1)$ and $p_i(i=1,2,\ldots,N)$.

The standard Poisson bracket containing two functions in the symplectic space $(R^{2N}, d\Phi_1 \Lambda d\Phi_2)$ is defined by

$$(F,G)=\sum_{i=1}^{N}\left(\frac{\partial F}{\partial \Phi_{1i}}\frac{\partial G}{\partial \Phi_{2i}}-\frac{\partial F}{\partial \Phi_{2i}}\frac{\partial G}{\partial \Phi_{1i}}\right)=\langle F_{\Phi_1}, G_{\Phi_2}\rangle-\langle F_{\Phi_2}, G_{\Phi_1}\rangle.$$

F, G are involutive, if $(F,G)=0$. Next, we would like to construct a set of functions $\{F_n\}$ as follows:

$$\begin{aligned} F_n=&-\langle \Lambda^{n+1}\Phi_1, \Phi_2\rangle(1-2-\mu\langle \Phi_1, \Phi_2\rangle) \\ &+\frac{1}{2}\sum_{i=0}^{n}\begin{vmatrix}\langle \Lambda^{i-1}\Phi_1, \Phi_1\rangle & \langle \Lambda^{i-1}\Phi_1, \Phi_2\rangle \\ \langle \Lambda^{n-i}\Phi_1, \Phi_2\rangle & \langle \Lambda^{i-1}\Phi_2, \Phi_2\rangle\end{vmatrix} n \\ &=0,1,2,\ldots . \end{aligned} \tag{34}$$

Proposition 3: For the functions F_n defined by Eq. (34), there exist the relation for arbitrary n, $m \in Z^+$,

$$\langle F_{n,\Phi_1}, F_{m,\Phi_2}\rangle=\langle F_{m,\Phi_1}, F_{n,\Phi_2}\rangle.$$

Proposition 4: The functions $\{F_n\}$ determined by Eq. (34) are involutive, i.e., $(F_n, F_m)=0$ under the Poisson bracket in symplectic space $(R^{2N}, d\Phi_1 \Lambda d\Phi_2)$.

Proof: According to Proposition 4, it yields

$$\begin{aligned}(F_n, F_m)&=\langle F_{n,\Phi_1}, F_{m,\Phi_2}\rangle-\langle F_{n,\Phi_2}, F_{m,\Phi_1}\rangle \\ &=\langle F_{m,\Phi_1}, F_{n,\Phi_2}\rangle-\langle F_{m,\Phi_1}, F_{n,\Phi_2}\rangle=(F_m, F_n)=-(F_n, F_m).\end{aligned}$$

Hence $(F_n, F_m)=0$ and we complete the proof of the proposition.

Theorem 2: The Hamiltonian systems (F_n),

$$(F_n): \Phi_{1t_n}=\frac{\partial F_n}{\partial \Phi_2}, \quad \Phi_{2t_n}=-\frac{\partial F_n}{\partial \Phi_1}, \quad n=0,1,2,\ldots \tag{35}$$

with Hamiltonian functions F_n determined by Eq. (34) are completely integrable in the Liouville sense.

Proof: According to Proposition 4, we know that the conclusion is true.

Theorem 3: The Hamiltonian system (31) is completely integrable in Liouville sense in the symplectic manifold $(R^{2N}, d\Phi_1 \Lambda d\Phi_2)$ and its involutive system is $\{F_n\}$, i.e., $(H_1, F_n)=0$.

Proof: According to Eqs. (31) and (33) and Propositions 4–6, we can prove that H_1 and $F_n (n=0,1,2,\ldots)$ are involutive under the Poisson bracket in symplectic space $(R^{2N}, d\phi_1 \Lambda d\phi_2)$ by a direct calculation, that is

$$(H_1, F_n)=\langle H_{1,\Phi_1}, F_{n,\Phi_2}\rangle-\langle H_{1,\Phi_2}, F_{n,\Phi_1}\rangle=0, \quad n=0,1,2,\ldots .$$

Therefore we complete the proof of the theorem.

IV. THE INVOLUTIVE SOLUTIONS OF THE HIERARCHY OF THE SOLITON EQUATION (16)

Denote the solution operators of the initial-value problems of the integrable Hamiltonian systems (15) and (F_n) by f_0^x and $f_n^{t_n}$, respectively. $(H_1, F_n)=0$ implies that any two canonical systems (15) and (F_n) are compatible, then their own flows f_0^x and $f_n^{t_n}$ commute. Therefore the involutive solution of the consistent Eq. (15) and (F_n) is[35]

$$\begin{pmatrix} \Phi_1(x,t_n) \\ \Phi_2(x,t_n) \end{pmatrix} = f_0^x f_n^{t_n} \begin{pmatrix} \Phi_1(0,0) \\ \Phi_2(0,0) \end{pmatrix}$$

and a smooth function of (x,t_n).

Proposition 5: Let $(\Phi_1(x,t_n),\Phi_2(x,t_n))$ be an involutive solution of the consistent system (15) and (F_n), then the Bagmann constraints (30a),

$$q(x,t_n) = -\frac{\langle \Phi_1,\Phi_1\rangle}{2(1-2-\mu\langle \Phi_1,\Phi_2\rangle)}, \quad r(x,t_n) = \frac{\langle \Phi_2,\Phi_2\rangle}{2(1-2-\mu\langle \Phi_1,\Phi_2\rangle)} \tag{36}$$

satisfy the soliton hierarchy of the generalized AKNS equations,

$$u_{t_n} = \begin{pmatrix} q_{t_n} \\ r_{t_n} \end{pmatrix} = K_n = J_0 G_{n+1} = J_n G_1 = J_0 \Psi^n G_1. \tag{37}$$

Proof: Through a direct differential calculation with respect to t_n for Eq. (36) and combining (35), we can derive that Eq. (37) holds.

According to Proposition 5, we can derive the following conclusion:

Proposition 6: Let $(\Phi_1(x,t_2),\Phi_2(x,t_2))$ be an involutive solution of the consistent systems (15) and (F_2), then the Bagmann constraint (30a),

$$q(x,t_2) = -\frac{\langle \Phi_1(x,t_2),\Phi_1(x,t_2)\rangle}{2(1-2-\mu\langle \Phi_1(x,t_2),\Phi_2(x,t_2)\rangle)},$$

$$r(x,t_2) = \frac{\langle \Phi_2(x,t_2),\Phi_2(x,t_2)\rangle}{2(1-2-\mu\langle \Phi_1(x,t_2),\Phi_2(x,t_2)\rangle)}, \tag{38}$$

satisfy the system of generalized AKNS soliton equations (25).

V. SUMMARY AND CONCLUSION

By introducing the associated auxiliary problem of problem (1), we derive a hierarchy of the generalized AKNS soliton equations, which contains the known AKNS soliton hierarchy. Its finite-dimensional *N*-Hamiltonian structures are obtained by virtue of the trace identity and a recursion operator and are shown to be Liouville sense integrable. Here, we propose the notation, *N*-Hamiltonian structure, which is natural extension of bi-Hamiltonian structure[18,21,22] and tri-Hamiltonian structure.[20,23] In addition, for the contained condition (29), we only consider the case $k=0$, under which (27) is nonlinearized into finite-dimensional Hamiltonian system. For other cases $k \geqslant 1$, (27) can also be nonlinearized into higher order constrained flows by introducing so-called Jacobi–Ostrogradsky coordinates. If introducing the Lax matrix and *r*-matrix again,[31–34] we can study the separation of variables[31,34] for these finite-dimensional integrable Hamiltonian systems (FDIHS). Then the separability of the FDIHS will give rise to the Jacobi inverse problem for the associated soliton hierarchies. The soliton hierarchies can be solved in terms of Riemann theta function by a standard Jacobi inverse technique.[36] These problems need to be further considered.

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Unimodular relativity and cosmological constant

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Unimodular relativity is a theory of gravity and space–time with a fixed absolute space–time volume element, the *modulus*, which we suppose is proportional to the number of microscopic modules in that volume element. In general relativity an arbitrary fixed measure can be imposed as a gauge condition, while in unimodular relativity it is determined by the events in the volume. Since this seems to break general covariance, some have suggested that it permits a nonzero covariant divergence of the material stress-energy tensor and a variable cosmological ''constant.'' In Lagrangian unimodular relativity, however, even with higher derivatives of the gravitational field in the dynamics, the usual covariant continuity holds and the cosmological constant is still a constant of integration of the gravitational field equations. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1328077]

I. INTRODUCTION TO UNIMODULAR RELATIVITY

Unimodular relativity is an alternative theory of gravity considered by Einstein in 1919[1] without a Lagrangian and put into Lagrangian form by Anderson and Finkelstein.[2] The space–time of unimodular relativity is a measure manifold, a manifold provided by nature with a fixed absolute physical measure field $\mu(x)$ to be found by direct measurement, subject to no dynamical development. The sole structural variable is a conformal metric tensor $f_{\mu\nu}$, subject to dynamical equations. The measure of a space–time region may be regarded as indirectly counting the modules of which it is composed, in the way that the volume of a lake indirectly counts its water molecules. Both space–time measure and liquid measure indicate a modular structure below the limit of resolution of the present measuring instruments.

The conformal metric field $f_{\mu\nu}(x)$ is a symmetric relative tensor of weight 1/2, signature 1–3, and determinant -1 in all coordinate systems, with nine independent components, operationally defined by the system of light paths, whose tangent vectors dx^μ obey $f_{\mu\nu}\,dx^\mu dx^\nu=0$.

The unimodular space–time structure also defines a metric tensor

$$g_{\mu\nu}=\sqrt{\mu}f_{\mu\nu}(x), \tag{1}$$

but the determinant

$$-g:=\det g_{\mu\nu}=-\mu^2 \tag{2}$$

is not a dynamical variable. The conformal metric f is the sole gravitational variable of unimodular relativity.

We assume that the metric tensor field $g_{\mu\nu}$ found by measuring the proper times $d\tau^2=g_{\mu\nu}\,dx^\mu\,dx^\nu$ for a sufficiently fine network of intervals dx^μ, also determines the measure field μ by the usual relation (2).

Once the measure μ has been experimentally determined it establishes a class of admissible metrics obeying (2). Metrics violating (2) are unphysical according to unimodular relativity.

The variable of general relativity is a compound of a light-cone field f and a measure field μ, and the group of general relativity is a nonsimple group of diffeomorphisms, with an invariant subgroup of unimodular coordinate transformations, those with Jacobian $\det(\partial x'/\partial x)=1$. Unimodular relativity has a simple group and a simple variable.

Originally we proposed unimodular relativity because there is indeed an experimental atomic standard of length near each point of space–time, not built into general relativity.[2] This suggests that the macroscopic structure of space–time is a smoothed description of an underlying atomic space–time microstructure, which seems necessary for other reasons.

Since the actual value of the cosmological constant is so finely tuned, it is natural to attempt to derive its value from physical principles. A theory in which it is variable would be a useful starting point for any such attempt. Recently the difference in symmetry between unimodular and general relativity led some to hope that they might differ on the constancy of this parameter.[3]

On the other hand, many authors have already argued that the difference is only a gauge condition, which has no physical consequences.[4] However, some authors do not share this point of view. In particular, van der Bij *et al.*[5] stated very clearly the physical difference between the usual formulation of gravity and the unimodular theory. Also, an interesting and somewhat alternative approach is presented in Ref. 6.

We examine the gauge-condition argument more carefully here. In its usual form it omits several relevant features special to this problem. Usually gauge conditions are applied to Lagrangians that are already physically well defined in their absence; the unimodularity condition is not a gauge condition of this kind.

One should also take into account the possibility of higher-order derivatives in the gravitational equations, of the kind that might arise from renormalization in some hypothetical quantum field theory of gravity.

We show here that any gravitational theory of classical unimodular relativity with a Lagrangian density that is invariant under the unimodular coordinate group is equivalent in its experimental predictions to a theory of classical general relativity. Higher-order corrections do not disturb this equivalence.

II. THE METRIC TENSOR OF UNIMODULAR RELATIVITY

In deriving the field equations from a variational principle (on which our approach is based), the measure μ is not varied but is treated as if it were a fixed external field. This disturbs general covariance. The law of nature may take a simpler form in *unimodular coordinates*, where $\mu(x) \equiv 1$. Unimodular coordinate systems are related by unimodular transformations.

Let R be the Riemann scalar computed from the metric tensor $g_{\mu\nu}$ of (1). Let L_M be the Lagrangian density of the matter field in the presence of $g_{\mu\nu}=\sqrt{\mu} f_{\mu\nu}$. Then

$$S=\int d^4x\left(\frac{\Gamma}{2}R+L_M\right) \tag{3}$$

is a possible action functional for unimodular relativity in a unimodular coordinate system. The constant $\Gamma=1/4\pi G$ is the inverse rationalized gravitational constant, the reciprocal square of the rationalized Planck length, in units with $\hbar=c=1$.

In unimodular relativity, there is initially no way to vary all 10 components of $g_{\mu\nu}$ independently. The action is in principle defined only for $g=\mu^2$. Only derivatives with respect to the nine-dimensional conformal metric field f are defined.

A cosmological constant term $\Lambda\sqrt{g}$ in the action function would be an ineffectual additive constant since $\sqrt{g}=\mu$ is not varied.

This action can be transformed to any other coordinate system under the general diffeomorphism group, but is not generally invariant in functional form, since the fixed measure μ sets an absolute scale at each event.

The derivative with respect to the conformal metric f requires special care. Since infinitesimal variations δf are subject to the unimodular condition (2), they obey

$$f^{\mu\nu}\delta f_{\mu\nu}=0. \tag{4}$$

If $W:\mathcal{F}\to\mathcal{W}$, $f\mapsto W(f)$ is a functional from the function manifold $\mathcal{F}$ of conformal metrics on a region $\mathcal{R}$ to some value-manifold $\mathcal{W}$, we define the functional derivative $W_f=\delta W/\delta f$ as the linear operator

$$W_f: d\mathcal{F}\to\mathcal{W} \tag{5}$$

such that for any $\delta f\in d\mathcal{F}$ vanishing on the boundary $\partial\mathcal{R}$ the tangent space to $\mathcal{F}$ at f,

$$\delta W = W_f\cdot\delta f = \int d^4x\,\frac{\delta W}{\delta f_{\mu\nu}(x)}\,\delta f_{\mu\nu}(x). \tag{6}$$

Then the dynamical equation that follows from the action principle for any space–time region $\mathcal{R}$ is

$$\delta S(\mathcal{R}) = \int_{\partial\mathcal{R}} d\sigma_\mu\,\pi^\mu\cdot\delta f \tag{7}$$

with a boundary term that is linear in δf on the boundary $\partial\mathcal{R}$ and vanishes for variations that vanish on the boundary. The tensor field π^μ canonically conjugate to $f(x)$ is defined by these relations.

III. FIELD EQUATIONS AND THE COSMOLOGICAL CONSTANT

It is often inconvenient to work with a field variable subject to non-linear conditions like the conformal metric. One may reformulate unimodular relativity with an unconstrained variable $g_{\mu\nu}(x)$ and take the unimodular condition (2) into account through Lagrange's method of undetermined multipliers.

To do this, however, we must give values to the Lagrangian density for metric tensors that have $g\neq\mu$[22,4,7] and hence are unphysical. One way to do this is to replace μ by $\sqrt{g}$ and $f_{\mu\nu}$ by $g_{\mu\nu}/g^{1/4}$ at all their ''appearances'' in the action S, so that S is defined in a 10-dimensional neighborhood $\mathcal{F}'\supset\mathcal{F}$ in a smooth way consistent with the values on $\mathcal{F}$. Then in addition one adds a Lagrangian-multiplier term expressing the unimodular condition. We call the resulting extension of S to $\mathcal{F}'$ the *extended action function* S'.

But this prescription is ambiguous, since it depends on ''appearances,'' on how S is written, on matters of notation. The extended action S' is arbitrary up to a correction term $\Delta_M S$ depending on the matter variables and the metric $g_{\mu\nu}$, subject only to the condition that $\Delta_M L$ and its derivative with respect to λ vanish in the unimodular sector (2):

$$S' = S+\Delta_M S+\int d^4x\sqrt{g}\lambda(x)\left[\frac{\mu}{\sqrt{g(x)}}-1\right], \tag{8}$$

$\Delta_M S=\int d^4x\sqrt{g}\Delta_M L$ is the *unimodular ambiguity* in the action. No physical results may depend on the choice of $\Delta_M L$, and so no physical experiments can determine $\Delta_M L$.

In mechanical theories sometimes we impose a constraint and thereby reduce an already well-defined system to a system of lower dimensionality. For example, we reduce a free particle to a spherical pendulum by constraining it to a sphere. Then there is a well-defined unconstrained Lagrangian, found by removing the constraint, and the ambiguity $\Delta_M L$ does not arise.

But according to unimodular relativity we have no way of actually removing the unimodular condition (2). In this sense it is not a constraint, so we call it a condition. While the proper time $d\tau$ of a coordinate interval dx^μ at x depends on the gravitational field at x, each coordinate cell d^4x at x comes with its own intrinsic measure $\mu(x)d^4x$, independent of gravity. The unimodular ambiguity $\Delta_M L$ acknowledges that as a matter of principle we cannot know how the system would evolve absent the unimodular condition.

The admissible infinitesimal variations df within the neghborhood $\mathcal{F}'$ are those that obey (4) for all $x \in \mathcal{R}$. That is, they all belong to the null space of the inverse conformal metric tensor $f^{\mu\nu}$.

The action principle states that for any physical field $f=(f_{\mu\nu}(x))$, and for any variations $\delta f=(\delta f_{\mu\nu}(x))$ about f,

$$S_f \cdot \delta f := \int_{\mathcal{R}} d^4x\, S_f(x)\, \delta f(x) = \int_{\partial\mathcal{R}} S^{\mu\nu}\delta f_{\mu\nu}. \tag{9}$$

That is, any vector $\delta f(x)$ in the null space of $f^{-1}(x)$ is in the null space of $S_f(x)$. It follows that $S_f(x)$ is in the ray of $f^{-1}(x)$:

$$\frac{\delta S}{\delta f_{\mu\nu}(x)} = \lambda(x) f^{\mu\nu}(x). \tag{10}$$

The multiplier $\lambda(x)$ is then fixed by the unimodular condition.

This implies that the augmented action (8) is stationary up to boundary terms when we vary $\lambda(x)$ and the 10 components $g_{\mu\nu}(x)$ independently.

The unimodular condition makes the stress tensor ambiguous as well as the dynamical equations. In unimodular relativity the general relativistic concept of the stress tensor

$$T^{\mu\nu} = \frac{1}{\sqrt{g}} \frac{\delta(\sqrt{g} L_M)}{\delta g_{\mu\nu}} \tag{11}$$

has no principled meaning at first, since it involves breaking the unimodular condition, nor has the statement of covariant continuity, $T^{\mu\nu}{}_{;\nu}=0$.

We may suppose that $\Delta_M L$ has the form

$$\Delta_M L = \left[\frac{\mu(x)}{\sqrt{g(x)}} - 1 \right] l_M, \tag{12}$$

where l_M is any function of the matter variables and $g_{\mu\nu}$. We write $L'_M := L_M + \Delta_M L$ for the sum.

From any general-relativity action principle S we obtain in this way an ambiguous unimodular-relativity action principle

$$S' = \int \sqrt{g(x)}\, d^4x \left\{ \frac{\Gamma}{2} R(x) + \frac{\Gamma}{2} \lambda(x) \left[\frac{\mu(x)}{\sqrt{g(x)}} - 1 \right] + L_M + \Delta_M L \right\}. \tag{13}$$

The second term in S' expresses the unimodular condition and breaks general covariance. The fourth term expresses the unimodular ambiguity. We vary the 10 $g_{\mu\nu}(x)$ and the Lagrange multiplier $\lambda(x)$ independently. We have written the λ term in a form that makes λ a scalar field under the general group.

Variation of λ in S' recovers the condition

$$\sqrt{g(x)} = \mu(x). \tag{14}$$

The unimodular ambiguity $\Delta_M L$ does not affect this result, since it vanishes when the unimodular condition holds.

Variation of $g_{\mu\nu}$ gives the equation of motion

$$\delta S' = \int \sqrt{g}\, d^4x \{\Gamma(\tfrac{1}{2} g^{\mu\nu} R - R^{\mu\nu}) + \tfrac{1}{2}\Gamma\lambda g^{\mu\nu}\}\delta g_{\mu\nu} + \int \sqrt{g}\, d^4x \left\{ \frac{1}{\sqrt{g}} \frac{\delta}{\delta g_{\mu\nu}} (\sqrt{g} L_M + \sqrt{g}\Delta_M L) \right\} \delta g_{\mu\nu} = 0, \tag{15}$$

or

$$R^{\mu\nu} - \tfrac{1}{2} g^{\mu\nu} R - \tfrac{1}{2}\lambda g^{\mu\nu} = 8\pi G T'^{\mu\nu}, \tag{16}$$

where $G := 1/\Gamma$ is a rationalized gravitational coupling strength and

$$T'^{\mu\nu} := \frac{1}{\sqrt{g}} \frac{\delta}{\delta g_{\mu\nu}} (\sqrt{g} L_M + \sqrt{g}\Delta_M L). \tag{17}$$

Tracing (16) gives the Lagrange multiplier:

$$\lambda = -\tfrac{1}{2}(8\pi G T' + R). \tag{18}$$

The field equation then simplifies to

$$R^{\mu\nu} - \tfrac{1}{2} R g^{\mu\nu} = 8\pi G T'^{\mu\nu} - \tfrac{1}{4} g^{\mu\nu}(8\pi G T' + R), \tag{19}$$

or equivalently

$$R_{\mu\nu} - \tfrac{1}{4} R g_{\mu\nu} = 8\pi G T'^{\mathrm{T}}_{\mu\nu}, \tag{20}$$

where

$$T'^{\mathrm{T}}_{\mu\nu} := T'_{\mu\nu} - \tfrac{1}{4} g_{\mu\nu} T' \tag{21}$$

is the traceless (part of the) stress tensor, or the *sess tensor* (note that the tr has been removed). The covariant divergence of (19) is

$$8\pi G T'^{\mu\nu}{}_{;\nu} = \tfrac{1}{4} g^{\mu\nu}(8\pi G T' + R)_{,\nu} \equiv -\tfrac{1}{2} g^{\mu\nu}\lambda, \tag{22}$$

which was suggested as a ''modified covariant divergence law'' by Tiwari.[3]

In general relativity, general invariance of the action function implies that the covariant divergence $T'^{\mu\nu}{}_{;\nu}$ vanishes in virtue of the field equations for matter.[8,9] Then it follows that

$$-\tfrac{1}{2}(8\pi G T' + R) = \lambda = \text{constant}. \tag{23}$$

If the stress tensor of unimodular relativity were covariantly continuous too, then the undetermined multiplier λ could be identified with a cosmological constant Λ, though now a constant of the motion determined by the initial data, rather than a fixed absolute constant as supposed in general relativity.

In unimodular relativity however, $T'^{\mu\nu}$ is not covariantly continuous because the action S' is not generally covariant, which seems to justify Tiwari's suggestion. $T'^{\mu\nu}$ is ambiguous by an additive term

$$\Delta T^{\mu\nu} = -\tfrac{1}{2} g^{\mu\nu} l_M \tag{24}$$

and its trace is correspondingly ambiguous by

$$\Delta T = -2l_{\mathrm{M}}. \tag{25}$$

However substitution of these expressions into (20) immediately leads to

$$R_{\mu\nu} - \tfrac{1}{4}Rg_{\mu\nu} = 8\pi G T^{\mathrm{T}}_{\mu\nu}, \tag{26}$$

with

$$T^{\mathrm{T}}_{\mu\nu} := T_{\mu\nu} - \tfrac{1}{4}g_{\mu\nu}T, \tag{27}$$

where $T_{\mu\nu}$ is the usual covariantly continuous stress-energy tensor (11) of the matter field. The gravitational field equations *do not* depend on the ambiguity in the matter field Lagrangian. The cosmological constant again arises as a constant of integration.

Einstein's law of gravity is a second-order differential equation for the metric field. In quantum field theories higher-order derivatives arise from renormalization. One might hope that in higher-order theories, the unimodular relativity differs in content from general relativity, and allows the cosmological constant to vary. In such theories the cosmological constant may be defined as $\lambda = S(h)/\mu$ where $S(h)$ is the value of the gravitational action density for the case of the Minkowski metric.

It easily follows from the generalized (contracted) Bianchi identities of the higher order theory (see, for example, Refs. 10 and 11) that even in higher-order unimodular relativity, where the gravitational part of the action is an arbitrary generally invariant functional of the curvature scalar, the cosmological constant also arises as the constant of integration.

IV. CONCLUSIONS

We have shown that in Lagrangian unimodular relativity the usual covariant continuity equation holds for the source stress tensor, and the cosmological constant is a constant of integration of the gravitational field equations. Higher derivatives of the gravitational field may appear in the Lagrangian without disturbing these conclusions. The essential point is that the stress tensor have no covariant divergence. This follows from either unimodular or general covariance.

There are several reasons not to be quite certain that these classical conclusions will still hold in the quantum domain.

The fact remains that unimodular relativity forces us to allow many values as possibilities for the cosmologcal constant, while general relativity fixes on one value. In quantum theories, possibilities affect actualities. In a quantum theory of sufficient scope, these many possibilities for the cosmological constant of unimodular relativity might influence the actual experimental situation.[7]

Furthermore, quantum field theories often lack symmetries and conservation laws present in the classical Lagrangian from which they stem, due to divergences inherent in the limiting process used to define the quantum theory. This results in quantum anomalies, for example. Similar effects may permit the cosmological constant—the vacuum rest-energy-density—to vary in some quantum version of unimodular relativity.

Perhaps the most basic weakness in the deduction is the postulate of strong locality. This is implicit in general covariance and is required to deduce the covariant continuity of stress. If there is a fundamental quantum time, a limit to locality, as some suggest, then the cosmological constant can vary.

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Projective symmetry in null Einstein–Maxwell space-times

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A discussion of projective symmetry in general relativity is given. Techniques are developed and used to show that null Einstein–Maxwell fields in general relativity cannot admit any proper projective symmetry. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1332121]

I. INTRODUCTION

In spite of much recent interest in the study of symmetry in general relativity theory, projective symmetry seems to be ignored. This may be largely to do with the difficulties involved although, following Ref. 1, some progress was made in Ref. 2. The results of this latter paper suggested that examples of space-times admitting proper projective symmetries would not be plentiful (see also Refs. 3 and 4) and this present paper continues by demonstrating their absence in space-times of the null Einstein–Maxwell type. Non-null Einstein–Maxwell fields will be considered in a future paper.

Let M be a smooth space-time with smooth Lorentz metric g of signature $(-\ +\ +\ +)$ and associated curvature tensor components R_{abcd}. The Ricci tensor components are $R_{ab}\equiv R^{c}{}_{acb}$, the Ricci scalar is $R\equiv R_{ab}g^{ab}$ and the Weyl tensor components are C_{abcd}. A Lie (respectively, a covariant and a partial) derivative is denoted by $\mathcal{L}$ (respectively, a semicolon and a comma). A smooth vector field X on M may be decomposed uniquely in any coordinate system on M according to

$$X_{a;b}=\tfrac{1}{2}h_{ab}+F_{ab}\quad (h_{ab}=h_{ba},\quad F_{ab}=-F_{ba}), \tag{1}$$

where $h(=\mathcal{L}_X g)$ is symmetric and F (the *projective bivector*) is skew-symmetric. Such a vector field X is called *projective* if the local diffeomorphisms ψ_t (for appropriate t) associated with X map geodesics into geodesics. This is equivalent to the condition that h satisfies

$$h_{ab;c}=2g_{ab}\phi_c+g_{ac}\phi_b+g_{bc}\phi_a \tag{2}$$

for some smooth closed 1-form on M with local components ϕ_a. Thus ϕ_a is locally a gradient and will, where appropriate, be written as $\phi_a=\phi_{,a}$ for some function ϕ on some open subset of M. The function ϕ may be taken as a global function on M if M is simply connected.[5] The statement that h is covariantly constant on M is, from (2), equivalent to ϕ_a being zero on M and is, in turn, equivalent to X being an *affine* vector field on M (so that the local diffeomorphisms ψ_t preserve not only geodesics but also their affine parameters). If X is projective but not affine it is called *proper projective*. If X is affine and $h=cg(c\in\mathbb{R})$ then X is *homothetic* (otherwise proper affine). If X is homothetic and $c\neq 0$ it is *proper homothetic* while if $c=0$ it is *Killing*.

II. PROJECTIVE SYMMETRY

Let X be a projective vector field on M. Then (1) and (2) hold and also (cf. Ref. 1)

$$\mathcal{L}_X R^{a}{}_{bcd}=\delta^{a}_{d}\phi_{b;c}-\delta^{a}_{c}\phi_{b;d},\quad \mathcal{L}_X R_{ab}=-3\phi_{a;b}. \tag{3}$$

Also the Ricci identity on h gives[2]

$$h_{ae}R^{e}{}_{bcd}+h_{be}R^{e}{}_{acd}=g_{ac}\phi_{b;d}-g_{ad}\phi_{b;c}+g_{bc}\phi_{a;d}-g_{bd}\phi_{a;c}. \tag{4}$$

The difficulty with projective vector fields is the complicated relationship (2) satisfied jointly by h_{ab} and ϕ_a. However, the following result is useful in obtaining prior algebraic information on h_{ab} and $\phi_{a;b}$ and follows from (4). The first parts were given in Ref. 6 following a special case in Ref. 2 and the other part is a straightforward extension. A prior definition is required. Let $m \in M$ and let G be a (real or complex) bivector at m. Then G is called a *curvature eigenbivector* with eigenvalue $\lambda \in \mathbb{C}$ if, at m, $R^{ab}{}_{cd}G^{cd}=\lambda G^{ab}$.

Theorem 1: Let X be a projective vector field on M so that (1) and (2) hold and let G be a curvature eigenbivector at $m \in M$ with eigenvalue $\lambda \in \mathbb{C}$.

(i) If G (and hence λ) are real and G is simple (i.e., $G^{ab}=2p^{[a}q^{b]}$ for p and q in the tangent space T_mM to M at m) then each vector in the span of p and q (the *blade* of G) is an eigenvector of the symmetric tensor at m given by

$$P_{ab}=\lambda h_{ab}+2\phi_{a;b} \tag{5}$$

with the same eigenvalue α.

(ii) If G is real and non simple then G uniquely determines a timelike–spacelike orthogonal pair of two-dimensional subspaces of T_mM [i.e., there exists a real null tetrad (l,n,x,y) at m with $l^an_a=x^ax_a=y^ay_a=1$ and all other inner products of tetrad members zero such that $G^{ab}=2Al^{[a}n^{b]}+2Bx^{[a}y^{b]}$ with A and B real and nonzero]. These subspaces spanned, respectively, by the vector pairs (l,n) and (x,y) are eigenspaces of P in (5).

(iii) If G and λ are not real then similar, if a little more complicated, information is available and this is, perhaps, best discussed when it arises.

III. PROJECTIVE SYMMETRY AND NULL EINSTEIN–MAXWELL FIELDS

Let (M,g) represent a null Einstein–Maxwell field. Then it is assumed that M admits a global, nowhere zero, smooth, null vector field l such that the Ricci tensor satisfies $R_{ab}=\psi l_a l_b$ for some smooth, nowhere zero function ψ. Also, the contracted Bianchi identity shows that l is geodesic and, henceforth, l will be assumed to be affinely parametrized ($l_{a;b}l^b=0$) in each coordinate system considered. Finally the Goldberg–Sachs theorem[7,8] shows that the Petrov type at each point of M is algebraically special with l as a repeated principle null direction. In fact, M may then be decomposed as a *disjoint* union

$$M=II\cup \operatorname{int} D\cup \operatorname{int} III\cup \operatorname{int} N\cup \operatorname{int} O\cup M', \tag{6}$$

where *II*, *III*, *D*, *N*, and *O* are the subsets of M at each point of which the Petrov type is the same as the subset label (and *I* is empty), where int denotes the interior of a subset in the manifold topology of M and where M' is a closed subset of M defined by the disjointness of the decomposition and with no interior.[9] Since *I* is empty the ''rank'' theorem together with a minimal polynomial argument given in Ref. 9 shows that *II* is open and so $II=\operatorname{int} II$. The idea is to let X be a projective vector field on M and to consider the regions in the decomposition (6) separately. If m is a point in any of the open regions of constant Petrov type in (6) then one may introduce a local real null tetrad (l,n,x,y) of vector fields in some open region about m [but still within the particular chosen open subset in (6)] (see, e.g., Ref. 10). Then one constructs bivectors in this region given by (and using the abbreviation $x\wedge y=2x^{[a}y^{b]}$, etc.)

$$V=l\wedge x, \quad \overset{*}{V}=-l\wedge y, \quad M=l\wedge n, \quad \overset{*}{M}=x\wedge y,$$

$$U=n\wedge x, \quad \overset{*}{U}=n\wedge y, \tag{7}$$

where $*$ denotes the usual dual. One can now choose the null tetrad so that the curvature tensor takes the form

$$R_{abcd}=A(V_{ab}V_{cd}+\overset{*}{V}_{ab}\overset{*}{V}_{cd})+C_{abcd}, \tag{8}$$

where A is some nowhere zero function on M, and the first term on the right-hand side is the Maxwell term. Thus for each Petrov type one substitutes for C an appropriate canonical form (e.g., as in Refs. 11, 12, and 8) and then one is ready to apply Theorem 1. So let X be a projective vector field on M.

Region int O. Here, the Weyl tensor is zero and so from (8) the curvature tensor, considered as a 6×6 matrix, is of rank 2 and satisfies $R_{abcd}l^d=0$. It now follows (Ref. 2, theorem 4) that, in $\operatorname{int} O$, $\phi_a=0$ and so from (2) $h_{ab;c}=0$. Thus the restriction of X to $\operatorname{int} O$ is affine on each connected and simply connected open subset of $\operatorname{int} O$. If the restriction over a particular component U is proper affine then it is easily checked that the holonomy group of U (with the latter regarded as a space-time) is of the type R_8 (see e.g. Ref. 13) and that l is covariantly constant on U. If X is not proper affine on U it is homothetic (possibly *Killing*) on U.

Region int N. Here the Petrov type is N and use of the appropriate canonical form for the Weyl tensor shows that $R_{abcd}l^d=0$ and that

$$R_{abcd}=A_1V_{ab}V_{cd}+A_2\overset{*}{V}_{ab}\overset{*}{V}_{cd} \tag{9}$$

with A_1 and A_2 functions on $\operatorname{int} N$ satisfying $A_1^2+A_2^2\neq 0$ at each point of $\operatorname{int} N$. However, one cannot guarantee that A_1 and A_2 are each nonzero at each $m\in\operatorname{int} N$ and so the Riemann rank may vary over $\operatorname{int} N$. Let $W_1\subset\operatorname{int} N$ be the (necessarily open) subset of M consisting of those points at which A_1 *and* A_2 are not zero (i.e., the open subset of $\operatorname{int} N$ where the curvature rank is 2) and let W_2 be the interior of the subset $\operatorname{int} N\backslash W_1$ (the latter subset being the subset of $\operatorname{int} N$ where exactly one of A_1 and A_2 is zero and hence where the curvature rank is 1). Then $\operatorname{int} N$ has the disjoint decomposition $\operatorname{int} N=W_1\cup W_2\cup E$ where E is defined by the disjointness. It is easily checked that E has no interior. Then over W_1 one may, as in the previous case, appeal to Theorem 4 in Ref. 2 to see that $\phi_a=0$ on W_1 and make similar remarks about when the various restrictions of X are proper affine or not. Over W_2 the curvature rank is 1 and, from (7) and (9) one sees that $V,\overset{*}{V}$, M, and $\overset{*}{M}$ are curvature eigenbivectors with eigenvalue zero. It follows from Theorem 1 that l, n, x, and y are eigenvectors of $\phi_{a;b}$ with zero eigenvalue at each point of W_2 and hence that $\phi_{a;b}=0$ on W_2. If one now appeals to holonomy considerations on each connected and simply connected open subset of W_2 then it follows from Theorem 5 in Ref. 13 and Theorems 7, 8, and 9 in Ref. 2 that on each such open subset either $\phi_a=0$ or the holonomy group is type R_{10}. But if on some such open subset ϕ_a is not identically zero (but still satisfies $\phi_{a;b}=0$) the holonomy type R_{10} conditions allow the choice of the local null tetrad (l,n,x,y) (depending on which open region of W_2 one is on, i.e., where $A_1\neq 0$ and $A_2=0$, or vice versa) such that (7) and (9) hold and such that $\phi_a=Cy_a$ for some $C\in\mathbb{R}$. Also (4) gives

$$h_{ae}R^e{}_{bcd}+h_{be}R^e{}_{acd}=0. \tag{10}$$

Now (10) implies that (Ref. 14)

$$h_{ab}=\alpha g_{ab}+\beta y_ay_b+\gamma l_al_b+2\,\delta l_{(a}y_{b)} \tag{11}$$

for appropriate functions α, β, γ, and δ. Then on substituting (11) and the relation $\phi_a=Cy_a$ into (2) and contracting with x^ax^b one finds that $\alpha_{,c}=2Cy_c$. On substituting this back into (2) and contracting with l^a one immediately finds $C=0$ and so $\phi_a=0$ on the region considered and hence on W_2. Thus $\phi_a=0$ (and $h_{ab;c}=0$) on $W_1\cup W_2$. Now put $W=W_1\cup W_2$ and note that $\operatorname{int}(\operatorname{int} N\backslash W)=\emptyset$. This follows since if $\emptyset\neq V\subseteq\operatorname{int} N\backslash W$ with V open then $V\cap W=\emptyset$ and so on

$V\cap W_1=0$ and hence $V\subseteq \text{int}\, N\backslash W_1$. Since V is open this gives $V\subseteq \text{int}(\text{int}\, N\backslash W_1)=W_2$ and hence the contradiction that $V\cap W\neq\emptyset$. From this one can see that if $m\in \text{int}\, N\backslash W$ then any open neighborhood V' of m intersects W nontrivially (otherwise $V'\cap \text{int}\, N$ would be open, nonempty and contained in $\text{int}\, N\backslash W$). Thus since $\phi_a\equiv 0$ on W, $\phi_a\equiv 0$ on $\text{int}\, N$ by continuity.

It is remarked that over connected and simply connected open subsets of $\text{int}\, N$ whose holonomy group is of type R_3, R_8 or R_{10}, X could restrict to a proper affine vector field and elsewhere only to a homothetic vector field.[13,15]

Region int III. In this case, Eq. (8) and an appeal to the Petrov canonical forms show that

$$R_{abcd}=A(V_{ab}V_{cd}+\overset{*}{V}_{ab}\overset{*}{V}_{cd})+B(V_{ab}M_{cd}+M_{ab}V_{cd}-\overset{*}{V}_{ab}\overset{*}{M}_{cd}-\overset{*}{M}_{ab}\overset{*}{V}_{cd}) \tag{12}$$

on $\text{int}\, III$ with A and B nowhere zero functions on $\text{int}\, III$. It follows from (7) (and using an obvious abbreviated notation where $R_{abcd}V^{cd}$ is written as RV, etc.) that

$$RV=0,\quad \overset{*}{R}V=0,$$

$$RM=-2BV,\quad \overset{*}{R}M=-2B\overset{*}{V},$$

$$RU=2AV+2BM,\quad \overset{*}{R}U=-2A\overset{*}{V}+2B\overset{*}{M}. \tag{13}$$

Now (13) and Theorem 1 show that on $\text{int}\, III$

$$\phi_{a;b}=\alpha g_{ab}+\beta l_a l_b \tag{14}$$

and (4) and (14) then give, on $\text{int}\, III$,

$$h_{ae}R^e{}_{bcd}+h_{be}R^e{}_{acd}=\beta(g_{ac}l_b l_d-g_{ad}l_b l_c+g_{bc}l_a l_d-g_{bd}l_a l_c). \tag{15}$$

Contracting (15) successively with M^{cd} and $\overset{*}{M}{}^{cd}$ gives

$$h_{ae}V^e{}_b+h_{bc}V^e{}_a=-2\beta B^{-1}l_a l_b,\quad h_{ae}\overset{*}{V}{}^e{}_b+h_{be}\overset{*}{V}{}^e{}_a=0 \tag{16}$$

and the second of (16) yields, by an argument similar to one used earlier[14]

$$h_{ab}=\lambda g_{ab}+\mu l_a l_b+\nu x_a x_b+2\rho l_{(a}x_{b)}. \tag{17}$$

A substitution of (17) into the first of (16) shows that $\nu\equiv 0$ on $\text{int}\, III$.

Next, substitute (17) with $\nu=0$ into (15) and contract first with U^{cd} and then with $\overset{*}{U}{}^{cd}$, using (13). The resulting equations show (since A and B are nowhere zero on $\text{int}\, III$) that $\rho=\mu=\beta=0$ on $\text{int}\, III$. Hence $h_{ab}=\lambda g_{ab}$ and on substituting this into (2) and contracting at each $m\in \text{int}\, III$ with $k\in T_m M$ satisfying $\phi_a k^a=0$, $k_a k^a\neq 0$, one finds that $\lambda_{,a}=2\phi_a$. A back substitution into (2) and a further contraction with k^a then shows that $\phi_a=0$ at m and hence that $\phi_a\equiv 0$ and $\lambda=$ constant on $\text{int}\, III$. Thus the restriction of X to any component of $\text{int}III$ is affine and, since the curvature tensor has rank 4 [from (13)], the restriction of X to any component of $\text{int}\, III$ is homothetic.[15]

Region II. In this case, Eq. (8) and the canonical Petrov type *II* form allow the null tetrad to be chosen locally in this region so that

$$R_{abcd}=A_1(V_{ab}V_{cd})+A_2(\overset{*}{V}_{ab}\overset{*}{V}_{cd})+C(U_{ab}V_{cd}+V_{ab}U_{cd}-\overset{*}{U}_{ab}\overset{*}{V}_{cd}$$
$$-\overset{*}{V}_{ab}\overset{*}{U}_{cd}+2M_{ab}M_{cd}-2\overset{*}{M}_{ab}\overset{*}{M}_{cd})-D(U_{ab}\overset{*}{V}_{cd}+\overset{*}{U}_{ab}V_{cd}$$
$$+V_{ab}\overset{*}{U}_{cd}+\overset{*}{V}_{ab}U_{cd}+2M_{ab}\overset{*}{M}_{cd}+2\overset{*}{M}_{ab}M_{cd}), \tag{18}$$

where A_1, A_2, C, and D are real functions and $A_1^2+A_2^2$ is nowhere zero on II. It is convenient to disjointly decompose II as $II=W_1\cup W_2\cup E$ where W_1 is the necessarily open subset of II consisting of exactly those points of II where D is not zero and where $W_2=\mathrm{int}(II\backslash W_1)$. Then E is well defined by disjointness and has no interior.

One finds from (18), using the same abbreviated notation, that

$$RV=2CV-2D\overset{*}{V},\quad \overset{*}{R}V=2C\overset{*}{V}+2DV,$$
$$RM=-4CM+4D\overset{*}{M},\quad \overset{*}{R}M=-4C\overset{*}{M}-4DM, \tag{19}$$
$$RU=2CU-2D\overset{*}{U}+2A_1V,\quad \overset{*}{R}U=2C\overset{*}{U}+2DU-2A_2\overset{*}{V}.$$

From this it is easily checked that $V+i\overset{*}{V}$ and $M+i\overset{*}{M}$ are complex curvature eigenbivectors with eigenvalues $2(C+iD)$ and $-4(C+iD)$ and so the region W_1 is that part of II where these eigenvalues are not real. Then the appropriate contractions of (4) and use of (19) gives the equations

$$P_{ad}V^d{}_b+P_{bd}V^d{}_a-Q_{ad}\overset{*}{V}{}^d{}_b-Q_{bd}\overset{*}{V}{}^d{}_a=0,$$
$$P_{ad}\overset{*}{V}{}^d{}_b+P_{bd}\overset{*}{V}{}^d{}_a+Q_{ad}V^d{}_b+Q_{bd}V^d{}_a=0, \tag{20}$$
$$(P_{ab}=2Ch_{ab}+2\phi_{a;b,}\quad Q_{ab}=2Dh_{ab})$$

and

$$P'_{ad}M^d{}_b+P'_{bd}M^d{}_a-Q'_{ad}\overset{*}{M}{}^d{}_b-Q'_{bd}\overset{*}{M}{}^d{}_a=0,$$
$$P'_{ad}\overset{*}{M}{}^d{}_b+P'_{bd}\overset{*}{M}{}^d{}_a+Q'_{ad}M^d{}_a+Q'_{bd}M^d{}_a=0, \tag{21}$$
$$(P'_{ab}=-4Ch_{ab}+2\phi_{a;b,}\quad Q'_{ab}=-4Dh_{ab}).$$

First consider the subset W_1 on which D is nowhere zero. Then (20) holds and algebraic information on h_{ab} and $\phi_{a;b}$ can be obtained by substituting for V and $\overset{*}{V}$ into each of (20) from (7). If one performs these substitutions and then contracts over the indices a and b with all combinations of the basis vectors l, n, x and y one finds [using the abbreviation $P(l,n)$ for $P_{ab}l^an^b$, etc.] that

$$
\begin{gathered}
P(l,l)=Q(l,l)=P(l,x)=P(l,y)=Q(l,x)=Q(l,y)=0,\\
P(n,x)=-Q(n,y)\quad P(n,y)=Q(n,x),\\
Q(l,n)=Q(x,x)-P(x,y)=Q(y,y)+P(x,y),\\
P(l,n)=P(x,x)+Q(x,y)=P(y,y)-Q(x,y).
\end{gathered}
\tag{22}
$$

A similar procedure using (21) yields

$$
\begin{gathered}
P'(l,l)=P'(n,n)=Q'(l,l)=Q'(n,n)=P'(x,y)=Q'(x,y)=0,\\
P'(x,x)=P'(y,y)\quad Q'(x,x)=Q'(y,y),\\
P'(l,x)=-Q'(l,y)\quad P'(l,y)=Q'(l,x),\\
P'(n,x)=Q'(n,y)\quad P'(n,y)=-Q'(n,x).
\end{gathered}
\tag{23}
$$

Since D is nowhere zero on W_1, h_{ab} is a multiple of Q and Q' (and $Q'=-2Q$). Then (22) and (23) show that $Q(x,x)=Q(y,y)$ and then $P(x,y)=0$. This implies that $Q(l,n)=Q(x,x)=Q(y,y)$ and the information accumulated on h in the above null tetrad shows that

$$
h_{ab}=\alpha g_{ab}+2\lambda l_{(a}x_{b)}+2\mu l_{(a}y_{b)} \tag{24}
$$

for functions α, λ, and μ on W_1. The information on h in (24) gives rise to similar information on Q and Q' which can then be transmitted to P and P' through (22) and (23), respectively. One finds that $P(l,l)=P(l,x)=P(l,y)=P(x,y)=0$, $P(l,n)=P(x,x)=P(y,y)$ and that $P'(l,l)=P'(n,n)=P'(l,x)=P'(l,y)=P'(x,y)=0$, $P'(x,x)=P'(y,y)$. Thus

$$
P_{ab}=\beta g_{ab}+\gamma l_a l_b+2\delta l_{(a}x_{b)}+2\epsilon l_{(a}y_{b)}, \tag{25}
$$

$$
P'_{ab}=\beta' g_{ab}+2\gamma' l_{(a}n_{b)}+2\delta' l_{(a}x_{b)}+2\epsilon' l_{(a}y_{b)} \tag{26}
$$

for functions $\beta,\gamma,\ldots,\epsilon'$ on W_1. But the defining Eqs. (20) and (21) for P and P' show that $P-P'=6Ch$ and then (24)–(26) show that $\gamma\equiv\gamma'\equiv 0$ on W_1. Thus, on W_1,

$$
\phi_{a;b}=\sigma g_{ab}+2\nu l_{(a}x_{b)}+2\rho l_{(a}y_{b)} \tag{27}
$$

for functions σ, ν, and ρ on W_1. Now one substitutes (24) and (27) into (4), noting that the terms containing α and σ immediately cancel. Then since one of A_1 and A_2 is not zero at each point of *II*, and hence W_1, suppose that at $m\in W_1$, $A_1(m)\neq 0$. A contraction of (4) with U^{cd} (after making the above substitutions and cancellations) and comparison of the independent symmetric tensors on either side of the resulting equation yields $\lambda=\mu=\nu=\rho=0$ at m. If $A_2(m)\neq 0$ a contraction with $\overset{*}{U}{}^{cd}$ (or an appeal to symmetry) gives the same conclusion. So $\lambda\equiv\mu\equiv\nu\equiv\rho\equiv 0$ and $h_{ab}=\alpha g_{ab}$ and $\phi_{a;b}=\sigma g_{ab}$ on W_1. Finally, just as in the conclusion of the type *III* discussion, one then finds from (2) that $\phi_a\equiv 0$ on W_1 and λ is constant on each component of U. Hence any restriction of X to some connected open subset of W_1 is homothetic.

Now consider the subset W_2 of *II*. Here, D is zero and the curvature eigenbivectors and eigenvalues introduced earlier are real and from (19) are V and $\overset{*}{V}$ (with eigenvalue $2C$) and M and $\overset{*}{M}$ (with eigenvalue $-4C$). Also, the given Petrov type shows that C is nowhere zero on W_2. Then Theorem 1 shows that in this case

$$2Ch_{ab}+2\phi_{a;b}=\mu g_{ab}+\nu l_a l_b$$
$$-4Ch_{ab}+2\phi_{a;b}=\mu' g_{ab}+2\nu' l_{(a}n_{b)} \tag{28}$$

for functions μ, ν, μ', and ν' on W_2. From this one finds

$$h_{ab}=\alpha g_{ab}+\beta l_a l_b+2\gamma l_{(a}n_{b)},$$
$$\phi_{a;b}=\alpha' g_{ab}+\beta' l_a l_b+2\gamma' l_{(a}n_{b)} \tag{29}$$

for functions $\alpha,\beta,\ldots,\gamma'$ on W_2. Now return to the second equation in (3) and recall the expression $R_{ab}=\psi l_a l_b$ for a nowhere zero function ψ on W_2. First note that from (1) and the first of (29),

$$\mathcal{L}_X(l^a)=l^a{}_{;b}X^b-X^a{}_{;b}l^b \Rightarrow l_a(\mathcal{L}_X l^a)=0$$
$$\Rightarrow(\text{since}\ \ \mathcal{L}_X(l^a l_a)=0)\ \ l^a(\mathcal{L}_X l_a)=0. \tag{30}$$

So (3) and the second equation of (29) gives

$$\mathcal{L}_X(\psi l_a l_b)=-3\alpha' g_{ab}-3\beta' l_a l_b-6\gamma' l_{(a}n_{b)}. \tag{31}$$

On expanding the left-hand side of (31) and contracting with $x^a x^b$ one finds $\alpha'\equiv 0$ on W_2 and a back substitution of this result into (31) and a contraction with l^a, using (30), gives $\gamma'\equiv 0$ on W_2. Thus $\phi_{a;b}=\beta' l_a l_b$. The Ricci identity $\phi_{a;[bc]}=\phi^d R_{dabc}$ on contraction with l^a then gives

$$R_{abcd}H^{cd}=0, \quad H_{ab}=2l_{[a}\phi_{b]}. \tag{32}$$

But from (19) the curvature tensor has rank 6 and so no nonzero bivector H could satisfy (32). Hence $H\equiv 0$ and so $\phi_a=\chi l_a$ for some function χ on W_2. Then the second equation of (29) with $\alpha'\equiv\gamma'\equiv 0$ shows that $\chi l_{a;b}=l_a r_b$ for some covector field r on W_2 and hence that l is recurrent on any open subset of W_2 on which χ does not vanish. But this recurrency of l would force a curvature rank of 4 or less on that subset[13,15] and thus $\chi\equiv 0$ and $\phi_a\equiv 0$ on W_2. Hence $\phi_a\equiv 0$ on $W_1\cup W_2$ and hence (by a similar argument to that in the type N case) $\phi_a\equiv 0$ on II.

Region D. In this case the curvature tensor takes the form (18) with $A_1=A_2=A$ and with A nowhere zero on D and the argument is essentially identical to that on region II. Thus one finds that $\phi_a\equiv 0$ on $\text{int}\,D$.

In summary the above analysis has shown that if X is a projective vector field on a null Einstein–Maxwell space-time M then $\phi_a\equiv 0$ on $\text{int}\,O$, $\text{int}\,N$, $\text{int}\,III$, $\text{int}\,D$ and II and hence, from (6), on $M\backslash M'$. Since $\text{int}\,M'=\emptyset$ it then follows by continuity that $\phi_a\equiv 0$ on M. Thus X is not proper projective. The following theorem has been established.

Theorem 2: If M is a null Einstein–Maxwell space-time and if X is a projective vector field on M then X is not proper.

It should be remarked that one could have considered separate null Einstein–Maxwell space-times of the constant Petrov types O, N, III, D, and II and established the lack of proper projective vector fields in each case. These results, of course, follow from the above although not conversely, since there is an extra patching procedure to be considered. Also one can add a little more to the theorem by noting from (8), (9), (13), and (19) that the curvature tensor has rank$\geqslant 4$ for Petrov types III, D, and II. Hence from Refs. 3 and 15 and the above theorem any projective vector field X on a null Einstein–Maxwell space-time of one of these Petrov types (or a region of one of these types in such a space-time where the Petrov type is not constant) cannot be proper affine and so must be homothetic. However, X could be proper affine for a null Einstein–Maxwell space-time (or a region of such a space-time) of Petrov type N or O.

The situation for non-null Einstein–Maxwell and other fields will be considered elsewhere.

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Rotating Bianchi type *V* dust models generalizing the $k=-1$ Friedmann model

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The Einstein equations are investigated for a rotating Bianchi type *V* dust model in which one of the Killing fields is spanned on velocity and rotation (case 1.2.2.2 in the classification scheme of the earlier papers). A first integral of the field equations is found, and with a special value of this integral coordinate transformations are used to eliminate two components of the metric. The $k=-1$ Friedmann model is shown to be contained among the solutions in the limit of zero rotation. The field equations for the simplified metric are reduced to 3 second-order ordinary differential equations that determine 3 metric components plus a first integral that algebraically determines the fourth component. First derivatives of the metric components are subject to a constraint (a second-degree polynomial with coefficients depending on the functions). It is shown that the set does not follow from a Lagrangian of the Hilbert type. The group of Lie point-symmetries of the set is found, it is two-dimensional noncommutative. Finally, a method of searching for first integrals (for sets of differential equations) that are polynomials of degree 1 or 2 in the first derivatives is applied. No such first integrals exist. The method is used to find a constraint (of degree 1 in first derivatives) that could be imposed on the metric, but it leads to a vacuum solution, and so is of no interest for cosmology.
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I. STATEMENT OF THE PROBLEM AND SUMMARY OF THE PAPER

This paper is a continuation of a series of papers on rotating dust models in relativity.[1–3] The initial motivation for this research was the desire to find a rotating generalization of the Friedmann models. In spite of much effort spent on investigating solutions of Einstein equations with a rotating matter source, no such generalization has been found so far; see literature surveys in Refs. 3 and 4. References 1, 2 and 3 provided a complete classification scheme for hypersurface–homogeneous rotating perfect fluid models with zero acceleration. Unlike previous approaches, the classification includes also timelike and null symmetry orbits, and so it is the farthest-reaching application of the Bianchi classification to rotating and nonaccelerating perfect fluid models in relativity. The models split into 3 general classes: I, in which two of the Killing fields are everywhere spanned on the vector fields of velocity u^α and rotation w^α (Ref. 1); II, in which only one Killing field is spanned on u^α and w^α (Ref. 2); and III, in which all Killing fields are linearly independent of u^α and w^α (Ref. 3). The many particular cases arise because of several possible alignments or misalignments among the 3 Killing fields and u^α and w^α.

By the Bianchi type of the symmetry algebra and by the relation of the velocity field to the symmetry orbits it can be recognized in which cases generalizations of the Friedmann models can be expected. Two such candidate cases were found in class II, and five more in class III. Those of class III were prohibitively complicated, but one of the cases of class II allowed for some progress, and this one is presented in the present paper. It is the Bianchi type *V* subcase of the case 1.2.2.2, given by Eq. (5.19) in Ref. 2. For the other candidate case found in class II, Eq. (5.10) in Ref. 2,

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the $k=0$ Friedmann limit is calculated in a much more complicated way, this will be a subject of another paper.

In Sec. II, the metric is simplified by a coordinate transformation, and a first integral of the Einstein equations is found. With a zero value of this integral, coordinate transformations can be used to eliminate two components of the metric tensor, and the number of nontrivial Einstein equations is reduced to 7. Although there are only 4 functions+matter density to be determined by these 7 equations, the set later turns out to be self-consistent. In Sec. III, it is shown that the $k=-1$ Friedmann models are contained among the metrics that result in the limit of zero rotation. In Sec. IV, the Einstein equations are reduced to a set S of 3 second-order equations to determine 3 metric components+a quadrature Q to determine the fourth component (g_{33}). Of the Einstein equations derived in Sec. II, one is fulfilled identically in consequence of the set $\{S\cup Q\}$, one turns out to be a constraint imposed on the initial data, and the one that determines the matter-density turns out to provide a first integral. The first integral determines g_{33} algebraically in terms of the other components, and so it is a replacement for the quadrature Q. It is also shown that the set S cannot be obtained as the Euler–Lagrange equations from a variational principle of the Hilbert type. Finally, it is shown in Sec. IV how the set $\{S\cup Q\}$ reproduces the Friedmann equations in the limit of zero rotation and zero shear. In Sec. V, the two-dimensional (non-Abelian) group of Lie point-symmetries of the set is found. In Sec. VI, a method of systematic search for polynomial first-order first integrals of a set of ordinary differential equations is applied to the set S of Sec. IV. It is shown that no first integrals that are polynomials of degree 1 or 2 in the first derivatives exist. The same method is used to reveal the existence of a possible constraint on initial data, which is of degree 1 in first derivatives, that is preserved by the set S. However, the constraint necessarily implies zero matter-density, and so it is not interesting for cosmology.

Equations that are of secondary importance for the main text, but are difficult to reproduce, can be found in the preprint version of this paper.[5] They have been deleted from this text at the request of the referee.

II. THE EINSTEIN EQUATIONS, THEIR FIRST INTEGRAL AND IMPLICATIONS OF THE ZERO VALUE OF THIS INTEGRAL

The subject of the present paper are the Einstein equations for the Bianchi type V subcase of case 1.2.2.2 of Ref. 2. For reference, the initial formulas are recalled in their original notation.

The Bianchi type V symmetry results when $c=0$ in Eqs. (5.19) of Ref. 2 and when, in addition, $j=-a$ in Eqs. (5.16). Hence, the metric is

$$\begin{aligned} ds^2 = {} & dt^2 + 2y\,dt\,dx + y^2 h_{11}\,dx^2 + 2h_{12}\,dx\,dy + 2y^2 h_{13}\,dx\,dz \\ & + (h_{22}/y^2)dy^2 + 2h_{23}\,dy\,dz + y^2 h_{33}\,dz^2, \end{aligned} \tag{2.1}$$

where the coordinates are $\{x^\alpha\}=\{x^0,x^1,x^2,x^3\}=\{t,x,y,z\}$, and $h_{ij}, i,j=1,2,3$ are unknown functions of the variable

$$v = e^t y^{C_2/a}, \tag{2.2}$$

a and C_2 being arbitrary constants. The velocity field u^α, the rotation field w^α and the Killing fields $k_{(i)}{}^\alpha$, $i=1,2,3$ are given by

$$\begin{gathered} u^\alpha = \delta^\alpha{}_0, \quad w^\alpha = (\rho/y)\,\delta^\alpha{}_0, \quad k_{(1)}{}^\alpha = \delta^\alpha{}_1, \quad k_{(3)}{}^\alpha = \delta^\alpha{}_3, \\ k_{(2)}{}^\alpha = C_2\,\delta^\alpha{}_0 + a(x\,\delta^\alpha{}_1 - y\,\delta^\alpha{}_2 + z\,\delta^\alpha{}_3), \end{gathered} \tag{2.3}$$

where ρ is the matter-density of dust. The rotation tensor $\omega_{\alpha\beta}$ has only one algebraically independent nonzero component:

$$\omega_{12} = \tfrac{1}{2}, \tag{2.4}$$

and therefore the coordinates used here are ill-suited for considering the limit $\omega\to 0$.

As shown in Ref. 1, it follows from the equations of motion and from the equation of conservation of the number of particles that

$$g:=\det(g_{\alpha\beta})=-(y/\rho)^2. \tag{2.5}$$

This is the form in which the metric resulted from the Killing equations in Ref. 2. It is advantageous to transform the coordinates as follows:

$$t=t'-(C_2/a)\ln y', \quad x=x'-C_2/(ay'), \quad (y,z)=(y',z'). \tag{2.6}$$

The result is equivalent to substituting $C_2=0$ and $a=1$ in Eqs. (2.1)–(2.4), i.e., the forms of the metric (2.1), of the vector fields u^α, w^α, ${k_{(1)}}^\alpha$ and ${k_{(3)}}^\alpha$ in (2.3) and of the rotation tensor $\omega_{\alpha\beta}$ in (2.4) do not change [although the new h'_{ij} in (2.1) will be linear combinations of the old h_{ij}], while the new ${k_{(2)}}^\alpha$ basis vector will be

$${k_{(2)}}^\alpha=x\,{\delta^\alpha}_1-y\,{\delta^\alpha}_2+z\,{\delta^\alpha}_3, \tag{2.7}$$

and the argument of h_{ij} will now be $v=\mathrm{e}^{t'}$, i.e., the h_{ij} are from now on unknown functions of the time-coordinate t.

It is convenient to parametrize the metric as follows:

$$\mathrm{d}s^2=(\mathrm{d}t+y\,\mathrm{d}x)^2-(yK_{11}\,\mathrm{d}x)^2-(K/y)^2(\mathrm{d}y+y^2h\,\mathrm{d}x)^2-{K_{33}}^2[yg\,\mathrm{d}x+(f/y)\mathrm{d}y+y\,\mathrm{d}z]^2, \tag{2.8}$$

where K_{11}, K, K_{33}, h, f and g are unknown functions of t. The components of the Einstein tensor referred to below are tetrad components $G_{IJ}={e^\alpha}_I{e^\beta}_J G_{\alpha\beta}$, i.e., projections of the coordinate components $G_{\alpha\beta}$ onto the orthonormal tetrad $e^I:={e^I}_\alpha\,\mathrm{d}x^\alpha$ implied by (2.8):

$$e^0=\mathrm{d}t+y\,\mathrm{d}x, \quad e^1=yK_{11}\,\mathrm{d}x, \quad e^2=(K/y)(\mathrm{d}y+y^2h\,\mathrm{d}x),$$

$$e^3=K_{33}[yg\,\mathrm{d}x+(f/y)\mathrm{d}y+y\,\mathrm{d}z], \tag{2.9}$$

where ${e^\alpha}_I$ is the inverse matrix to ${e^I}_\alpha$, i.e., ${e^\alpha}_I{e^I}_\beta={\delta^\alpha}_\beta$, ${e^\alpha}_J{e^I}_\alpha={\delta^I}_J$. In the parametrization (2.8), the determinant of the metric is

$$g=-(yK_{11}KK_{33})^2. \tag{2.10}$$

The tetrad components of the Einstein tensor corresponding to the metric (2.8) are given in Appendix A of Ref. 5. As seen from there, two combinations of those equations are of first order, they are $K_{11}G_{03}+G_{13}=0$, i.e.,

$$\left(\tfrac{3}{2}K_{33}/K_{11}\right)[({K_{11}}^2-1)K^{-2}f_{,t}+h(hf_{,t}-g_{,t})]=0, \tag{2.11}$$

and $K_{11}G_{02}+G_{12}=0$, i.e.,

$$(K_{11}K)^{-1}[-\tfrac{3}{2}K^2hh_{,t}+\tfrac{1}{2}h-K_{11}K_{11,t}+({K_{11}}^2-1)(2K_{,t}/K-K_{33,t}/K_{33})]=0. \tag{2.12}$$

As shown in Appendix B of Ref. 5, the case $h=0$ does not lead to interesting developments, so we shall proceed further under the assumption

$$h\neq 0. \tag{2.13}$$

Then, Eq. (2.11) implies

$$g_{,t}=[h+(K_{11}{}^2-1)/(hK^2)]f_{,t}. \tag{2.14}$$

With this, the equations $G_{03}=G_{13}=G_{23}=0$ turn out to be equivalent, and they can be written as follows:

$$-\frac{1}{2}\left(\frac{K_{11}{}^2-1}{h}\cdot\frac{K_{33}{}^3 f_{,t}}{K_{11}K}\right)_{,t}+\frac{K_{33}{}^3 f_{,t}}{K_{11}K}=0. \tag{2.15}$$

This invites the introduction of the new variable $u(t)$ by $u_{,t}=h/(K_{11}{}^2-1)$, and then (2.15) becomes

$$\left(\frac{K_{33}{}^3 f_{,u}}{K_{11}K}\right)_{,u}-2\frac{K_{33}{}^3 f_{,u}}{K_{11}K}=0, \tag{2.16}$$

which has the first integral $K_{33}{}^3 f_{,u}/(K_{11}K)=C\mathrm{e}^{2u}$, $C=\text{const}$, i.e.,

$$f_{,t}=C\mathrm{e}^{2u}hK_{11}K/[K_{33}{}^3(K_{11}{}^2-1)]. \tag{2.17}$$

From here on, we shall follow only the special case $C=0$, which is a solution of the Einstein equations, but not a general one: it is a subcase chosen *ad hoc* for further progress with integration. Then, from (2.17) and (2.14) $f=\text{const}$, $g=\text{const}$, and from (2.9) the coordinate transformation $z'=z+f/y+gx$ leads to

$$f=g=0, \tag{2.18}$$

without changing any of the other formulas for $g_{\alpha\beta}$, u^α, w^α, $\omega_{\alpha\beta}$ or $k_{(i)}{}^\alpha$.

The Einstein equations $G_{03}=G_{13}=G_{23}=0$ are now fulfilled identically. We are left with 7 equations that should determine the 4 functions K_{11}, K, K_{33} and h, and the matter density ρ in addition. It will turn out in Sec. IV that the 7 equations are dependent just in the way needed to make the problem self-consistent and determinate.

III. THE FRIEDMANN LIMIT OF THE METRIC

As already stated, the coordinates used in Sec. II are ill-suited for considering the limit $\omega\to 0$. This limit can be calculated after a coordinate transformation and a reparametrization of the metric.

Since $\omega_{12}=-\omega_{21}=\frac{1}{2}$ are the only nonzero components of the rotation tensor, a natural coordinate transformation to consider is

$$y=\omega_0 y', \tag{3.1}$$

where ω_0 is a constant. After the transformation

$$\omega'_{12}=\tfrac{1}{2}\omega_0=-\omega'_{21} \tag{3.2}$$

(all other $\omega_{\alpha\beta}=0$), and the limit of zero rotation is $\omega_0\to 0$. However, before this limit is taken, the metric functions in (2.8) must be reparametrized or else the limit will be singular. The following reparametrizations will do the job:

$$K_{11}=\tilde{K}_{11}/\omega_0,\quad K_{33}=\tilde{K}_{33}/\omega_0,\quad f=\tilde{f}\omega_0. \tag{3.3}$$

The transformation (3.1) and the reparatmetrization (3.3) result in a metric whose limit $\omega_0\to 0$ (with primes and tildes omitted) is

$$\mathrm{d}s^2=\mathrm{d}t^2-(yK_{11}\,\mathrm{d}x)^2-(K/y)^2\,\mathrm{d}y^2-K_{33}{}^2[yg\,\mathrm{d}x+(f/y)\mathrm{d}y+y\,\mathrm{d}z]^2. \tag{3.4}$$

The $k=-1$ Friedmann model results when $g=f=0$ and $K_{11}=K=K_{33}:=R(t)$, where $R(t)$ is the Friedmann scale factor. The resulting coordinates are none of the standard ones, but are related by $y=e^u$ to one of the sets used in the literature [see Eq. (1.3.15) in Ref. 6].

The fact that (3.4), the limit $\omega_0\to 0$ of (2.8), is still more general than the Friedmann metric means that shear survives the transition $\omega\to 0$.

It will be shown at the end of Sec. IV that the explicitly written out Einstein equations do allow a continuous limiting transition $\omega\to 0$, $\sigma\to 0$, and in the limit they reproduce exactly the Friedmann equations.

IV. THE INDEPENDENT EINSTEIN EQUATIONS

We shall now proceed with the subcase (2.18). Equation (2.11) is then fulfilled identically. Equation (2.12) does not change, and it can be more conveniently rewritten if K_{11} is parametrized as follows:

$$K_{11}=\cosh(F). \tag{4.1}$$

Then, from (2.12),

$$K_{33},_t=K_{33}[-\tfrac{3}{2}K^2hh,_t/\sinh^2(F)+\tfrac{1}{2}h/\sinh^2(F)+2K,_t/K-\cosh(F)F,_t/\sinh(F)]. \tag{4.2}$$

When this is substituted into the remaining Einstein equations [(A.1)–(A.10) in Ref. 5], the function K_{33} disappears from the set completely, i.e., we are left with 6 equations to determine h, K, F and the matter-density plus the quadrature implied by (4.2) that allows one to calculate K_{33} once $h(t)$, $K(t)$ and $F(t)$ are known.

Since (2.12) is now satisfied, the equations $G_{02}=0$ and $G_{12}=0$ are equivalent, and they can be written as

$$\begin{aligned} h,_{tt}=&\tfrac{3}{2}K^2hh,_t^2/\sinh^2(F)-5K,_th,_t/K+(2\cosh^2(F)-1)F,_th,_t/\sinh(F)\cosh(F)\\ &+hh,_t/\sinh^2(F)+K,_t/K^3+F,_t/K^2\cosh(F)\sinh(F)-\tfrac{1}{2}h/(K\sinh(F))^2. \end{aligned} \tag{4.3}$$

This is used to eliminate $h,_{tt}$ from the other Einstein equations. The equation $G_{01}=0$ can then be solved for $F,_{tt}$ (see Appendix C in Ref. 5) and this is used to eliminate $F,_{tt}$ from the diagonal components of the Einstein tensor (all the nondiagonal Einstein equations have been used up at this point). After such a substitution, the following identity is fulfilled:

$$G_{11}+G_{33}-2G_{22}\equiv 0, \tag{4.4}$$

i.e., one of the three equations $G_{11}=G_{22}=G_{33}=\Lambda$ can be discarded because it is a consequence of the remaining two. We choose to discard $G_{33}=\Lambda$.

Then, $K,_{tt}$ can be calculated from $G_{22}-G_{11}=0$. The result is

$$\begin{aligned} K,_{tt}=&\tfrac{1}{4}K^3\sinh^{-2}(F)h,_t^2-\tfrac{3}{2}K^3h\cosh(F)\sinh^{-3}(F)F,_th,_t\\ &-\cosh^{-1}(F)\sinh^{-1}(F)K,_tF,_t+2\cosh(F)\sinh^{-1}(F)K,_tF,_t-K\cosh^2(F)\sinh^{-2}(F)F,_t^2\\ &-\tfrac{3}{4}Kh,_t+\tfrac{3}{2}K^3h^2\sinh^{-4}(F)h,_t+\tfrac{3}{4}K^3h^2\sinh^{-2}(F)h,_t\\ &-\tfrac{3}{2}hK,_t-h\sinh^{-2}(F)K,_t-Kh\cosh^{-1}(F)\sinh^{-1}(F)F,_t+\tfrac{3}{2}Kh\cosh^3(F)\sinh^{-3}(F)F,_t\\ &-\tfrac{1}{4}K^{-1}\cosh^2(F)\sinh^{-2}(F)-\tfrac{1}{2}Kh^2\sinh^{-4}(F)-\tfrac{1}{4}Kh^2\sinh^{-2}(F). \end{aligned} \tag{4.5}$$

This is used to eliminate $K,_{tt}$ from the right-hand side of the equation determining $F,_{tt}$ (see Appendix C in Ref. 5), and the result is

$$
\begin{aligned}
F_{,tt} = &-\tfrac{3}{4}K^2\cosh^{-1}(F)\sinh^{-1}(F)h_{,t}^2-\tfrac{3}{2}Kh\cosh^{-1}(F)\sinh^{-1}(F)K_{,t}h_{,t}\\
&+2K^{-2}\cosh^{-1}(F)\sinh(F)K_{,t}^2-K^{-1}K_{,t}F_{,t}-\cosh(F)\sinh^{-1}(F)F_{,t}^2\\
&+\tfrac{3}{4}K^2h^2\cosh^{-1}(F)\sinh^{-1}(F)h_{,t}+\tfrac{3}{2}K^2h^2\cosh^{-1}(F)\sinh^{-3}(F)h_{,t}\\
&+\tfrac{1}{2}\cosh^{-1}(F)\sinh^{-1}(F)h_{,t}-\tfrac{3}{4}\cosh^{-1}(F)\sinh(F)h_{,t}-\tfrac{3}{2}K^{-1}h\cosh^{-1}(F)\sinh^{-1}(F)K_{,t}\\
&-\tfrac{3}{2}K^{-1}h\cosh^{-1}(F)\sinh(F)K_{,t}+h\sinh^{-2}(F)F_{,t}+\tfrac{5}{2}hF_{,t}-\tfrac{1}{4}K^{-2}\cosh^{-1}(F)\sinh(F)\\
&-\tfrac{3}{4}K^{-2}\cosh^{-1}(F)\sinh^{-1}(F)-\tfrac{1}{2}h^2\cosh^{-1}(F)\sinh^{-3}(F)-\tfrac{1}{4}h^2\cosh^{-1}(F)\sinh^{-1}(F).
\end{aligned}
\tag{4.6}
$$

With (4.2), (4.3), (4.5) and (4.6) all substituted, the equation $G_{11}=\Lambda$ reduces to the following form:

$$
\begin{aligned}
G_{11} = &\tfrac{1}{4}K^2\cosh^{-2}(F)h_{,t}^2+\tfrac{3}{2}Kh\cosh^{-2}(F)K_{,t}h_{,t}+\tfrac{3}{2}K^2h\cosh^{-1}(F)\sinh^{-1}(F)F_{,t}h_{,t}\\
&-2K^{-2}\cosh^{-2}(F)\sinh^2(F)K_{,t}^2-2K^{-1}\cosh^{-1}(F)\sinh(F)F_{,t}K_{,t}+F_{,t}^2\\
&+\tfrac{3}{2}K^2h^2\cosh^{-2}(F)h_{,t}-3K^2h^2\sinh^{-2}(F)h_{,t}-\tfrac{1}{2}\cosh^{-2}(F)h_{,t}+\tfrac{3}{2}h_{,t}\\
&+\tfrac{5}{2}K^{-1}h\cosh^{-2}(F)K_{,t}+3K^{-1}hK_{,t}-\tfrac{5}{2}h\cosh^{-1}(F)\sinh^{-1}(F)F_{,t}\\
&-3h\cosh^{-1}(F)\sinh(F)F_{,t}+\tfrac{1}{4}K^{-2}\cosh^{-2}(F)+\tfrac{3}{2}K^{-2}+\tfrac{1}{2}h^2\cosh^{-2}(F)+h^2\sinh^{-2}(F)\\
=&\,\Lambda.
\end{aligned}
\tag{4.7}
$$

Now it may be verified that $G_{11}=\text{const}$ is preserved by Eqs. (4.3), (4.5) and (4.6). This is done as follows. The derivative $(\mathrm{d}/\mathrm{d}t)\,G_{11}$ is calculated, and $h_{,tt}$, $K_{,tt}$ and F_{tt} that reappear are eliminated using (4.3), (4.5) and (4.6). Then, $K_{,t}^2$ is found from (4.7) and used to eliminate $K_{,t}^3$ and $K_{,t}^2$ from $(\mathrm{d}/\mathrm{d}t)\,G_{11}$. The result is the identity $(\mathrm{d}/\mathrm{d}t)\,G_{11}\equiv 0$. This means that, in virtue of the other field equations, if $G_{11}=\Lambda$ holds at any given time, it will remain constant at all other times. Hence, $G_{11}=\Lambda$ is a limitation imposed by the Einstein equations on the initial data for Eqs. (4.3), (4.5), (4.6), and it defines the cosmological constant in terms of the other constants that will appear after (4.3), (4.5) and (4.6) are solved. If $\Lambda=0$, then $G_{11}=0$ reduces the number of arbitrary constants by 1.

Hence, with (4.4), we are left with only four equations: (4.2), (4.7) and any two equations from the set $S=\{(4.3),(4.5),(4.6)\}$, to determine the four functions K_{33}, h, K and F. The third equation in S is implied by the remaining two together with (4.7). The only field equation that has not yet been used up is

$$G_{00}=(8\pi G/c^4)\rho-\Lambda. \tag{4.8}$$

This may be expected to simply define the matter-density in terms of the metric functions. However, in the formulation used in this paper, matter-density enters the equations in two ways: as a source term in G_{00} above, and also through (2.5). From (2.5) and (2.10) it follows that ρ must be related to the other functions by

$$\rho=(K_{11}KK_{33})^{-1}. \tag{4.9}$$

Together with (4.8) and (4.1) this implies that the following must hold:

$$[(G_{00}+\Lambda)\cosh(F)KK_{33}]_{,t}\equiv 0. \tag{4.10}$$

Indeed, this is an identity. This is verified as follows. First, (4.1), (4.2), (4.3), (4.5) and (4.6) are substituted into G_{00} (with $f=g=0$) to eliminate all second derivatives. Then, (4.10) is calculated, and (4.2), (4.3), (4.5) and (4.6) are used to eliminate $K_{33},_t$ and all second derivatives again. Finally, (4.7) is used to eliminate $K,_t^3$ and $K,_t^2$ from the left-hand side of (4.10). In the end, the identity (4.10) results. Hence, (2.5) and (4.8) are consistent in virtue of the other field equations, and moreover $(G_{00}+\Lambda)\cosh(F)KK_{33}=C=\text{const}$ [with second derivatives of h, K and F eliminated by (4.3), (4.5) and (4.6) and with $K,_t^2$ eliminated by (4.7)] is the following first integral of the Einstein equations:

$$K_{33}\Big[-3Kh\sinh(F)F,_t-\frac{3}{2}Kh^2\cosh^{-1}(F)+\frac{3}{2}K\cosh^{-1}(F)\sinh^2(F)h,_t$$
$$+3h\cosh^{-1}(F)\sinh^2(F)K,_t-\frac{3}{2}K^{-1}\sinh^2(F)\cosh^{-1}(F)-\frac{3}{2}K^3h^2\cosh^{-1}(F)h,_t\Big]=C. \tag{4.11}$$

Note that, from (4.8) and (4.9), $C=8\pi G/c^4\neq 0$, and so (4.11) determines K_{33} algebraically. Hence, (4.11) can replace (4.2) as the definition of K_{33}. Thereby, the problem of this paper was reduced to the following procedure.

(1) Find the most general solution of the set $\{(4.3),(4.5),(4.6)\}$. It will contain 6 arbitrary constants $\{C_1,\ldots,C_6\}$.

(2) Impose (4.7) on the $\{h,K,F\}$ found in the previous step. This will be just a definition of Λ in terms of $\{C_1,\ldots,C_6\}$ or, when $\Lambda=0$, an additional constraint imposed on $\{C_1,\ldots,C_6\}$.

(3) Calculate K_{33} from (4.11), with $C=8\pi G/c^4$.

(4) Calculate the matter-density from (4.9).

As shown in Ref. 7, an efficient method to find first integrals of a set of equations exists if the set can be obtained from a Lagrangian. Unfortunately, the problem of determining whether a given set of equations is derivable from a Lagrangian is rather complicated and unsolved in general.[8] It is known that the Einstein equations for class B Bianchi metrics may not admit a Lagrangian, even though the general Einstein equations do (see Ref. 9 for an explanation). It is shown in Appendix A that Eqs. (4.3), (4.5), (4.6) do not follow from the most natural Lagrangian conceivable in this case: a second-degree polynomial in the first derivatives of h, K and F, with coefficients being functions of h, K and F.

For further reference, let us consider the limit of zero rotation in (4.2)–(4.3) and (4.5)–(4.7). After the reparametrization (3.3) we have

$$\cosh(F)=\tilde{K}_{11}/\omega_0,\quad \sinh(F)=\sqrt{\tilde{K}_{11}{}^2/\omega_0^2-1},$$
$$F,_t=\tilde{K}_{11,t}/\sqrt{\tilde{K}_{11}{}^2-\omega_0^2}, \tag{4.12}$$

and then (4.2) in the limit $\omega_0\to 0$ becomes

$$\tilde{K}_{33,t}=\tilde{K}_{33}(2K,_t/K-\tilde{K}_{11,t}/\tilde{K}_{11}), \tag{4.13}$$

which is an identity in the Friedmann limit $\tilde{K}_{11}=K=\tilde{K}_{33}=R(t)$.

The limiting form of (4.3) is

$$h,_{tt}=-5h,_tK,_t/K+2\tilde{K}_{11,t}h,_t/\tilde{K}_{11}+K,_t/K^3. \tag{4.14}$$

The limit $\omega_0\to 0$ of (4.5) is

$$K_{,tt}=-K\tilde{K}_{11,t}{}^2/\tilde{K}_{11}{}^2-\tfrac{3}{4}Kh_{,t}-\tfrac{3}{2}hK_{,t}$$
$$+\tfrac{3}{2}Kh\tilde{K}_{11,t}/\tilde{K}_{11}-1/(4K)+2K_{,t}\tilde{K}_{11,t}/\tilde{K}_{11}. \tag{4.15}$$

The same limit of (4.6) is

$$\tilde{K}_{11,tt}/\tilde{K}_{11}=2K_{,t}^2/K^2-K_{,t}\tilde{K}_{11,t}/(K\tilde{K}_{11})+\tfrac{3}{2}h\tilde{K}_{11,t}/\tilde{K}_{11}-\tfrac{3}{2}h_{,t}-\tfrac{3}{2}hK_{,t}/K-1/(4K^2). \tag{4.16}$$

In the Friedmann limit $\tilde{K}_{11}=K=R(t)$, Eqs. (4.15) and (4.16) become identical:

$$R_{,tt}/R=R_{,t}^2/R^2-\tfrac{3}{4}h_{,t}-1/(4R^2). \tag{4.17}$$

Finally, the limit $\omega_0\to 0$ of (4.7) is

$$-2K_{,t}^2/K^2-2K_{,t}\tilde{K}_{11,t}/(K\tilde{K}_{11})+\tilde{K}_{11,t}{}^2/\tilde{K}_{11}{}^2+\tfrac{3}{2}h_{,t}+3hK_{,t}/K-3h\tilde{K}_{11,t}/\tilde{K}_{11}+3/(2K^2)=\Lambda. \tag{4.18}$$

The Friedmann limit of this is

$$-3R_{,t}^2/R^2+\tfrac{3}{2}h_{,t}+3/(2R^2)=\Lambda. \tag{4.19}$$

Finding $h_{,t}$ from (4.19) and substituting it in (4.17) we obtain

$$R_{,tt}/R=-R_{,t}^2/(2R^2)+1/(2R^2)-\Lambda/2, \tag{4.20}$$

which is exactly one of the Friedmann equations. Incidentally, the $h_{,t}$ found from (4.19), if substituted in (4.14), leads to (4.20) again. Hence, in the Friedmann limit, (4.14) follows from (4.19) and (4.17). The function h, as seen from (3.4), does not enter the limiting metric $\omega\to 0$ at all because, after the reparametrization (3.3), it is multiplied by ω_0.

Note that also (4.11) has a meaningful Friedmann limit. In order to make this limit finite, it must be assumed that

$$C=\tilde{C}/\omega_0^2, \tag{4.21}$$

and then the limit $\omega_0\to 0$ of (4.11) is

$$K_{33}[\Lambda K\tilde{K}_{11}+2K_{,t}^2\tilde{K}_{11}/K+2K_{,t}\tilde{K}_{11,t}-K\tilde{K}_{11,t}{}^2/\tilde{K}_{11}-3\tilde{K}_{11}/K]=\tilde{C}. \tag{4.22}$$

In the Friedmann limit this becomes

$$R(\Lambda R^2+3R_{,t}^2-3)=\tilde{C}. \tag{4.23}$$

Recalling the Friedmann formula for the mass-density, with $k=-1$:

$$3R_{,t}^2/R^2-3/R^2+\Lambda=(8\pi G/c^2)\rho, \tag{4.24}$$

we recognize in (4.23) the familiar mass-conservation formula of the Friedmann model, $\rho R^3=c^2\tilde{C}/(8\pi G)=\text{const}$.

V. THE LIE POINT-SYMMETRIES OF THE EQUATIONS (4.3), (4.5) AND (4.6)

The basic definitions and theorems concerning point-symmetries are presented in detail in Refs. 7 and 8.

Equations (4.3), (4.5) and (4.6) are of the following form:

$$\frac{d^2z^i}{dt^2}=W^i{}_{jk}\frac{dz^j}{dt}\frac{dz^k}{dt}+V^i{}_j\frac{dz^j}{dt}+U^i, \tag{5.1}$$

where $i=0,1,2$; $(z^0,z^1,z^2)=(h,K,F)$ and $W^i{}_{jk}$, $V^i{}_j$ and U^i are functions of the z^i, but not of t. (Incidentally, the independence of t of all these coefficients immediately implies one group of symmetries, $t\to t'=t+s$, where s is the group parameter.) Let the following be a one-dimensional group of point transformations:

$$t'=t'(t,\{z^j\},\tau),\quad z'^i=z'^i(t,\{z^j\},\tau), \tag{5.2}$$

where τ is the group parameter and $\tau=\tau_0$ corresponds to the identity [so that $t'(t,\{z^j\},\tau_0)\equiv t$, etc.]. The generators of this group [the field of vectors tangent to the orbits of the group (5.2)] are then

$$X=\xi\frac{\partial}{\partial t}+\eta^j\frac{\partial}{\partial z^j}, \tag{5.3}$$

where

$$\begin{bmatrix}\xi\\ \eta^j\end{bmatrix}=\frac{d}{d\tau}\begin{bmatrix}t'\\ z'^j\end{bmatrix}_{\tau=\tau_0}. \tag{5.4}$$

The generator X is extended to arbitrary derivatives $d^kz/dt^k:=\overset{(k)}{z}$ by the recursive formulas

$$\overset{(0)j}{\eta}=\eta^j,\qquad \overset{(k)j}{\eta}=\frac{d\overset{(k-1)j}{\eta}}{dt}-\frac{d^kz^j}{dt^k}\frac{d\xi}{dt}, \tag{5.5}$$

$$\overset{(k)}{X}=\xi\frac{\partial}{\partial t}+\eta^j\frac{\partial}{\partial z^j}+\overset{(1)j}{\eta}\frac{\partial}{\partial\overset{(1)j}{z}}+\cdots+\overset{(k)j}{\eta}\frac{\partial}{\partial\overset{(k)j}{z}}. \tag{5.6}$$

The derivatives d/dt in (5.5) are total derivatives, i.e.,

$$\frac{d}{dt}f(t,\{z^i\},\{\overset{(1)i}{z}\},\ldots,\{\overset{(k)i}{z}\})=\frac{\partial f}{\partial t}+\frac{dz^j}{dt}\frac{\partial f}{\partial z^j}+\sum_{p=1}^{k}\overset{(p+1)j}{z}\frac{\partial}{\partial\overset{(p)j}{z}},$$

and the order n to which the generator X has to be extended is equal to the highest order of derivatives in the set (5.1) ($n=2$ in our case). A generator of a point-symmetry obeys then

$$\overset{(n-1)}{X}\ \Omega^i=\frac{d\overset{(n-1)i}{\eta}}{dt}-\Omega^i\frac{d\xi}{dt}, \tag{5.7}$$

where Ω^i is the right-hand side of (5.1). Equations (5.7) must be identities in all the derivatives $\overset{(1)i}{z},\ldots,\overset{(n-1)i}{z}$, and so they imply several separate equations to be obeyed by the ξ and η^i.

For our equations (5.1), Eqs. (5.7) imply the following four relations:

$$\xi_{,kl}+W^j{}_{kl}\xi_{,j}=0, \tag{5.8}$$

$$\eta^i{}_{,kl}=W^i{}_{kl,s}\eta^s+2W^i{}_{s(l}\eta^s{}_{,k)}-W^s{}_{kl}\eta^i{}_{,s}+\delta^i{}_{(l}V^s{}_{k)}\xi_{,s}+V^i{}_{,(l}\xi_{,k)}+2\frac{\partial^2\xi}{\partial t\,\partial z^{(k}}\delta^i{}_{l)}, \tag{5.9}$$

where parentheses on indices denote symmetrization,

$$\frac{\partial^2 \eta^i}{\partial t\,\partial z^k} = W^i{}_{ks}\frac{\partial \eta^s}{\partial t} + \frac{1}{2}V^i{}_{k,s}\eta^s + \frac{1}{2}V^i{}_s\eta^s{}_{,k} - \frac{1}{2}V^s{}_k\eta^i{}_{,s} + \frac{1}{2}V^i{}_k\frac{\partial \xi}{\partial t} + U^i\xi_{,k} + \frac{1}{2}\delta^i{}_k U^s\xi_{,s} + \frac{1}{2}\delta^i{}_k\frac{\partial^2 \xi}{\partial t^2}, \tag{5.10}$$

$$\frac{\partial^2 \eta^i}{\partial t^2} = V^i{}_s\frac{\partial \eta^s}{\partial t} + U^i{}_{,s}\eta^s - U^s\eta^i{}_{,s} + 2U^i\frac{\partial \xi}{\partial t}. \tag{5.11}$$

The general solution of these equations [with $W^i{}_{kl}$, $V^i{}_k$ and U^i read off from (4.3), (4.5) and (4.6)] is

$$X = A\frac{\partial}{\partial t} + B\left(t\frac{\partial}{\partial t} - h\frac{\partial}{\partial h} + K\frac{\partial}{\partial K}\right), \tag{5.12}$$

where A and B are arbitrary constants. The proof that this is the most general solution is laborious but straightforward, it is given in Appendix E of Ref. 5. Hence, our set of equations has a two-dimensional symmetry group whose generators are

$$X_{(1)} = \frac{\partial}{\partial t}, \quad X_{(2)} = t\frac{\partial}{\partial t} - h\frac{\partial}{\partial h} + K\frac{\partial}{\partial K}, \tag{5.13}$$

and the corresponding finite symmetry transformations are

$$t' = t + \tau_1, \quad (h', K', F') = (h, K, F);$$

$$t' = \mathrm{e}^{\tau_2}t, \quad h' = \mathrm{e}^{-\tau_2}h, \quad K' = \mathrm{e}^{\tau_2}K, \quad F' = F, \tag{5.14}$$

where τ_1 and τ_2 are the group parameters.

Unfortunately, these symmetries do not lead to any discernible simplification of the set $S = \{(4.3),(4.5),(4.6)\}$. In variables adapted to the generator $X_{(1)}$, the independent variable is K, and $t(K)$ is one of the functions. The set (5.1) thus transformed is of first order in $\phi(K) := dt/dK$, but the first-order equation is still a member of a complicated set and none of the equations separate out. Moreover, after the transformed set is algebraically solved for $t_{,KK}$, $h_{,KK}$ and $F_{,KK}$, the right-hand sides become polynomials of *third* degree in $t_{,K}$, $h_{,K}$ and $F_{,K}$.

The variables adapted to the generator $X_{(2)}$ are (t', h', K'), where

$$t = \mathrm{e}^{K'}t', \quad K = \mathrm{e}^{K'}, \quad h = \mathrm{e}^{-K'}h'. \tag{5.15}$$

In these variables, the set (5.1) becomes of first order in $\psi(t') = K'_{,t'}$. However, after it is solved for $h'_{,t't'}$, $K'_{,t't'}$ and $F_{,t't'}$, the right-hand sides of $h'_{,t't'}$ and $F_{,t't'}$ contain rational functions of the form $W/(1 + t'K'_{,t'})$, where W is a monomial of second degree in some of the $h'_{,t'}$, $K'_{,t'}$ and $F_{,t'}$. Neither equation separates out. It is not possible to adapt the variables to both the generators simultaneously because the group is nonabelian. This author was not able to make any use of the new variables.

VI. FIRST INTEGRALS THAT ARE POLYNOMIALS IN $(h_{,t}, K_{,t}, F_{,t})$

Suppose that the set $\tilde{S} = \{(4.3),(4.5),(4.6),(4.7)\}$ has a first integral of the form

$$I := Q_{ij}\dot{z}^i\dot{z}^j + L_i\dot{z}^i + E = C = \text{const}, \tag{6.1}$$

where C is an arbitrary constant, $Q_{ij} = Q_{ji}$, L_i and E are unknown functions of (h, K, F), $i, j = 1,2,3$, $z^1 = h, z^2 = K, z^3 = F$. Then $\mathrm{d}I/\mathrm{d}t \equiv 0$ in virtue of $\tilde{S}$, i.e., using (5.1) to eliminate $\dot{z}^i$:

$$(2Q_{ij}\dot{z}^j+L_i)(W^i{}_{kl}\dot{z}^k\dot{z}^l+V^i{}_k\dot{z}^k+U^i)+Q_{ij,k}\dot{z}^i\dot{z}^j\dot{z}^k+L_{i,j}\dot{z}^i\dot{z}^j+E_{,i}\dot{z}^i\equiv 0. \tag{6.2}$$

It can be verified that first integrals of the form (6.1) do not exist for our set $\tilde{S}$. The calculations are conceptually straightforward, but lead through horrible intermediate expressions, so they are not reported here. The hypothesis that (6.1) is a first integral uniquely leads to an equation that is equivalent to (4.7).

The same method may be used to test whether our set of equations admits a constraint that would be a polynomial of degree 1 or 2 in the first derivatives. The only difference with respect to the procedure of looking for a first integral is that in verifying whether (6.2) is zero, Eq. (6.1) is used, too. If a nontrivial solution of (6.2) with this additional simplification is found, then it means that the derivative of (6.1) by t is zero if (6.1) holds for any fixed t. Then, such (6.1) is a constraint preserved by the set $\tilde{S}$. However, even this attempt has not led to useful results. Constraints of degree 2, i.e., those with $Q_{ij}\neq 0$, lead to prohibitively complicated equations and could not be investigated. One constraint of the form (6.1) with $Q_{ij}=0$ was found, but it is equivalent to the square bracket in (4.11) being zero, and so implies zero matter density. Again, the details are not reported because they contain complicated equations, but no ingenious ideas. This result proves the usefulness of the method—a sensible constraint was revealed—but the solution with zero density is not interesting for cosmology, and thus not necessarily worth investigating.

The zero-density constraint was found without using Eq. (4.7). Equation (4.7) would reduce the number of unknown functions by one, but the resulting set of equations is prohibitively complicated and no progress was achieved.

VII. SUMMARY OF RESULTS

It was shown that the Einstein equations for the metric (2.8) with $f=g=0$ are self-consistent and solvable. They reduce to the set $S=\{(4.3),(4.5),(4.6)\}$ to determine h, K and $K_{11}=\cosh(F)$, and (4.11) to determine K_{33} (where $C=8\pi G/c^4$). The matter density is found from (4.9). The first derivatives of the functions obeying the set S must obey (4.7).

The Friedmann solution with $k=-1$ is contained among the solutions of this set, as shown in Eqs. (4.12)–(4.24). Unfortunately, no explicit example of a more general solution could be found. Attempts to follow *ad hoc* Ansatzes produced uninteresting results. The Ansatz $K=K_{33}$ led to the deSitter solution in disguise, in which the t-lines had nonzero rotation. The Ansatz $K_{11}=K/C$ ($C=\text{const}$), which is consistent with the Friedmann limit, led to such complicated equations that it could not even be verified if they are not contradictory. The assumption of zero shear implies zero expansion, in virtue of the theorem $(\sigma=0)\Rightarrow(\omega\theta=0)$ that holds for dust (see Ref. 10).

The set S was shown to have a two-dimensional group of point-symmetries, given by (5.14), and to admit no Lagrangian of the Hilbert type. It was also verified that no first integrals of the form (6.1) exist.

The progress achieved in this paper was the reduction of the problem of existence of a rotating generalization of the $k=-1$ Friedmann model to the technical problem of finding an explicit solution of the set S. The solvability of the set S may be taken for granted because the Friedmann model itself was shown to be one of its solutions. It is still unknown, though, whether a continuous family of solutions exists labeled by the parameter ω (rotation) such that the limit $\omega\to 0$ taken in the explicit solution leads to the $k=-1$ Friedmann model.

A similar analysis as done here should be done for the other promising cases identified in Ref. 3.

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APPENDIX A: NONEXISTENCE OF A HILBERT-TYPE LAGRANGIAN FOR THE SET {(4.3), (4.5), (4.6)}

Equations (4.3), (4.5) and (4.6) can be written in the form

$$\frac{\mathrm{d}^2 z^i}{\mathrm{d}t^2} = W^i{}_{jk}\frac{\mathrm{d}z^j}{\mathrm{d}t}\frac{\mathrm{d}z^k}{\mathrm{d}t} + V^i{}_j\frac{\mathrm{d}z^j}{\mathrm{d}t} + U^i, \tag{A1}$$

where $i=0,1,2$; $z^0=h$, $z^1=K$, $z^2=F$ and $W^i{}_{jk}$, $V^i{}_j$ and U^i are functions of (h,K,F) (but not of t). Note that the set (A.1) is covariant with respect to arbitrary transformations $z^i \to z'^i = f^i(\{z^j\})$: the first derivatives $\mathrm{d}z^j/\mathrm{d}t$ transform then like a contravariant vector, and so do the terms U^i, the coefficients $V^i{}_j$ transform like a mixed tensor, and the coefficients $(-W^i{}_{jk})$ transform like components of an affine connection. [The nontensorial terms in the transformed $(-W^i{}_{jk})$ arise from $\mathrm{d}^2 z^i/\mathrm{d}t^2$.] The most natural Ansatz for a Lagrangian for (A1) is

$$L = Q_{ij}\frac{\mathrm{d}z^i}{\mathrm{d}t}\frac{\mathrm{d}z^j}{\mathrm{d}t} + L_i\frac{\mathrm{d}z^i}{\mathrm{d}t} + \Phi, \tag{A2}$$

where Q_{ij}, L_i and Φ are functions of (h,K,F). Such a Lagrangian would result from the Hilbert Lagrangian by taking out a complete divergence and integrating the result with respect to the spatial variables. The Euler–Lagrange equations implied by (A2) are

$$Q_{is}\frac{\mathrm{d}^2 z^s}{\mathrm{d}t^2} = -\left(Q_{ki,l} - \frac{1}{2}Q_{kl,i}\right)\frac{\mathrm{d}z^k}{\mathrm{d}t}\frac{\mathrm{d}z^l}{\mathrm{d}t} + \frac{1}{2}(L_{k,i} - L_{i,k})\frac{\mathrm{d}z^k}{\mathrm{d}t} + \frac{1}{2}\Phi_{,i}. \tag{A3}$$

If these are to be equivalent to (A1), then the following must hold:

$$Q_{is}W^s{}_{kl} = -\tfrac{1}{2}(Q_{ki,l} + Q_{li,k} - Q_{kl,i}), \tag{A4}$$

$$Q_{is}V^s{}_k = \tfrac{1}{2}(L_{k,i} - L_{i,k}), \tag{A5}$$

$$Q_{is}U^s = \tfrac{1}{2}\Phi_{,i}. \tag{A6}$$

Equation (A4) implies that $(-W^i{}_{jk})$ must be Christoffel symbols constructed from the metric Q_{ij}, Eq. (A5) implies that $\frac{1}{2}L_i$ must be a vector potential for the tensor field $Q_{is}V^s{}_k$, and Eq. (A6) implies that $\Phi/2$ must be a scalar potential for the vector field $Q_{is}U^s$. All of these are strong conditions and they may be impossible to fulfill in many cases.

Indeed, for our equations (4.3), (4.5), (4.6), the solution of (A4) turns out to be $Q_{ij} \equiv 0$, i.e., the Lagrangian (A2) does not exist. An outline of the proof is given in Appendix D of Ref. 5.

Since the Euler–Lagrange equations (A4) are covariant with respect to arbitrary transformations of the Lagrangian variables [in our case $h \to h'(h,K,F)$, etc.], and equations of the form (A1) are covariant, too, the conclusion that a Lagrangian of the form (A2) exists (or does not exist) is coordinate-independent, i.e., having shown that Eqs. (4.3),(4.5),(4.6) do not follow from a Lagrangian (A2) in our variables $\{h,K,F\}$, we know that no such Lagrangian will exist in any other variables.

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The method of adjoint operators and a symmetry operator for the Maxwell equations in type-D vacuum backgrounds

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Since in all the type-D solutions of the Einstein vacuum field equations with a cosmological term each maximal spin-weighted component of the electromagnetic spinor field satisfies a decoupled equation and there exists a two-index Killing spinor field; we show, via the adjoint operators method, that a symmetry operator for the Maxwell equations can be constructed. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1319515]

I. INTRODUCTION

In a recent paper[1] we showed that the symmetry operator for the Maxwell equations obtained when the space–time is a type-D solution of the Einstein vacuum field equations with a cosmological constant in Ref. 2 (without an explicit derivation) can be obtained under the conditions that the background space–time admits an algebraically general two-index Killing spinor field and that *each component* of the electromagnetic spinor field satisfies a decoupled equation. Our aim in the present paper is to obtain, via the method of adjoint operators, the same result but under the condition that *each maximal spin-weighted* component satisfies a decoupled equation. We think that the approach described in this work, to obtain the main result, offers hope of an improved understanding of the analogous problem for the gravitational perturbation equations. Thus, in Sec. II we review the adjoint operators method originally introduced by Wald[3] and in Sec. III we apply it to the Maxwell equations in order to obtain the symmetry operator for the Maxwell equations. In this work, the spinor formalism and the Newman–Penrose notation are used throughout; see Refs. 4, 5 for all relevant notation and definitions.

II. THE METHOD OF ADJOINT OPERATORS

Let f be a tensor or spinor field (its components representing unknown variables) that satisfies a coupled system of homogeneous linear partial differential equations given by

$$\mathcal{E}(f)=0, \tag{1}$$

where $\mathcal{E}$ is a linear differential operator that maps tensor or spinor fields like f into tensor or spinor fields, possibly of a type different from that of f. If by performing linear combinations of Eqs. (1) and their derivatives, one can obtain a decoupled equation of the form

$$\mathcal{O}(\chi)=0, \tag{2}$$

where χ is a function made out (linearly) of the components of f and their derivatives and $\mathcal{O}$ is a linear differential operator that maps scalar fields into scalar fields. Then, there exists a linear operator $\mathcal{T}$ such that $\chi=\mathcal{T}(f)$ and the fact that Eq. (2) is obtained by linear combinations of Eqs.

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(1) and their derivatives means that there must exist a linear differential operator $\mathcal{S}$ [representing the manipulations that one must perform on Eq. (1) to derive Eq. (2)] such that $\mathcal{SE}(f)=\mathcal{O}(\chi)=\mathcal{OT}(f)$. Hence

$$\mathcal{SE}=\mathcal{OT}, \tag{3}$$

must hold as an operator identity, so that when both sides of Eq. (3) are applied to a solution f of Eq. (1) one gets the decoupled equation (2).

By defining the adjoint, $\mathcal{A}^\dagger$, of a linear differential operator $\mathcal{A}$ in such a way that $\mathcal{A}^\dagger$ is also a linear operator and

$$(\mathcal{AB})^\dagger=\mathcal{B}^\dagger\mathcal{A}^\dagger, \tag{4}$$

for any pair of linear operators $\mathcal{A}$ and $\mathcal{B}$ whose composition is well defined, then using this property one can establish the (main result of the adjoint operators method) following.

Theorem 1: Suppose the identity $\mathcal{SE}=\mathcal{OT}$ holds for the linear partial differential operators $\mathcal{S}$, $\mathcal{E}$, $\mathcal{O}$ and $\mathcal{T}$ and that ψ satisfies $\mathcal{O}^\dagger(\psi)=0$. Then $\mathcal{S}^\dagger(\psi)$ satisfies $\mathcal{E}^\dagger(\mathcal{S}^\dagger(\psi))=0$.

Proof: Taking the adjoint of $\mathcal{SE}=\mathcal{OT}$ we have $\mathcal{E}^\dagger\mathcal{S}^\dagger=\mathcal{T}^\dagger\mathcal{O}^\dagger$, applying these operators to ψ, we obtain

$$\mathcal{E}^\dagger(\mathcal{S}^\dagger(\psi))=0, \tag{5}$$

which is the desired result. Thus, in particular, if $\mathcal{E}^\dagger=\pm\mathcal{E}$, then $\mathcal{S}^\dagger(\psi)$ is a solution of $\mathcal{E}(f)=0$.

Remark 1: If ψ satisfies $\mathcal{O}^\dagger(\psi)=0$ then, $\mathcal{E}^\dagger\mathcal{S}^\dagger(\psi)=0$, and hence if $\mathcal{E}^\dagger=\pm\mathcal{E}$, then $0=\mathcal{SES}^\dagger(\psi)=\mathcal{OTS}^\dagger(\psi)$. *Therefore, if $\mathcal{E}^\dagger=\pm\mathcal{E}$, the operator $\mathcal{TS}^\dagger$ maps solutions of the adjoint equation $\mathcal{O}^\dagger(\psi)=0$ into solutions of the equation $\mathcal{O}(\chi)=0$.*

Observe that to prove Theorem 1 the important property is that given by Eq. (4). In particular if the adjoint of a linear operator $\mathcal{A}$, that maps tensor or spinor fields into tensor or spinor fields, is defined as that linear operator $\mathcal{A}^\dagger$ such that

$$g\cdot\mathcal{A}(f)-[\mathcal{A}^\dagger(g)]\cdot f=\nabla_\alpha s^\alpha, \tag{6}$$

for every pair of tensor or spinor fields f and g for which the full contraction of g and $\mathcal{A}(f)$ denoted by $g\cdot\mathcal{A}(f)$, yields a scalar field, where s^α is some vector field (which depends on f and g), then it follows that Eq. (4) holds. For example for the derivative operators $(D,\Delta,\delta,\overline{\delta})$ one finds that[6]

$$\begin{aligned}
D^\dagger&=-(D+\varepsilon+\overline{\varepsilon}-\rho-\overline{\rho}),\\
\Delta^\dagger&=-(\Delta-\gamma-\overline{\gamma}+\mu+\overline{\mu}),\\
\delta^\dagger&=-(\delta+\beta-\overline{\alpha}-\tau+\overline{\pi}),\\
\overline{\delta}^\dagger&=-(\overline{\delta}-\alpha+\overline{\beta}+\pi-\overline{\tau}).
\end{aligned} \tag{7}$$

III. THE SOLUTION OF THE MAXWELL EQUATIONS AND THE SYMMETRY OPERATOR

It is well-known that the (source-free) Maxwell equations in a space–time solution of the Einstein vacuum field equations in terms of the electromagnetic potential are given by

$$\nabla^{\dot{A}}{}_{B}\nabla^{\dot{C}(A}\epsilon^{B)C}\Phi_{\dot{C}C}=0. \tag{8}$$

Comparing Eqs. (1) and (8) we see that for the electromagnetic case, the components of the spinor field f are $\Phi^{B}{}_{\dot{C}}$, while the components of the operator $\mathcal{E}$ are given by

$$[\mathcal{E}]^{\dot{A}A\dot{C}C}=\nabla^{\dot{A}}{}_{B}\nabla^{\dot{C}(A}\epsilon^{B)C}. \tag{9}$$

If $H_{A\dot{A}}$ and $W_{A\dot{A}}$ are two complex vector fields, then from the above expression we have

$$H\cdot\mathcal{E}(W)\equiv H_{A\dot{A}}\nabla^{\dot{A}}{}_{B}\nabla^{\dot{C}(A}W^{B)}{}_{\dot{C}}=\nabla^{\dot{A}}{}_{B}[H_{A\dot{A}}\nabla^{\dot{C}(A}W^{B)}{}_{\dot{C}}]-[\nabla^{\dot{C}(A}W^{B)}{}_{\dot{C}}][\nabla^{\dot{A}}{}_{B}H_{A\dot{A}}], \tag{10}$$

from this follows that

$$H\cdot\mathcal{E}(W)-[\mathcal{E}(H)]\cdot W=\nabla_{A\dot{A}}s^{A\dot{A}}, \tag{11}$$

where

$$s_{A}{}^{\dot{B}}=H_{A\dot{A}}\nabla^{\dot{C}(A}W^{B)}{}_{\dot{C}}-W_{A\dot{A}}\nabla^{\dot{C}(A}H^{B)}{}_{\dot{C}}. \tag{12}$$

Therefore, $\mathcal{E}^{\dagger}=\mathcal{E}$.

Since the Maxwell equations in terms of the electromagnetic spinor field can be written in the following form:

$$\nabla^{\dot{A}}{}_{B}\varphi^{AB}=0, \tag{13}$$

where

$$\varphi^{AB}=\nabla^{\dot{C}(A}\Phi^{B)}{}_{\dot{C}}, \tag{14}$$

then from these equations we obtain that, in this case, the components of the field χ are given by φ^{AB} and the components of the operator $\mathcal{T}$ are given by

$$[\mathcal{T}]^{AB\dot{C}C}=\nabla^{\dot{C}(A}\epsilon^{B)C}. \tag{15}$$

The hardest part in applying the method of adjoint operators to solve a coupled system of homogeneous linear partial differential equations is to obtain one decoupled equation. For the electromagnetic case, it is well-known that when the space–time is a type-D solution of the Einstein vacuum field equations with a possible nonvanishing cosmological term, each component of the electromagnetic spinor field φ_{AB} satisfies a decoupled equation. This means that there must exist three different operators $\mathcal{S}_{(i)}$ (with $i=0,1,2$) such that when they are applied to the Maxwell equations one obtains the decoupled equations for the components of the electromagnetic spinor field. Here we present one way of obtaining these three operators which is useful in writing the decoupled equations in a covariant way. For this end we write the Maxwell equations with sources in terms of the electromagnetic spinor field, i.e.,

$$J_{B\dot{M}}=\nabla_{\dot{M}}{}^{A}\varphi_{AB}, \tag{16}$$

and we assume that the operators $\mathcal{S}_{(i)}$ are first-order differential operators that can be written as

$$\mathcal{S}_{(i)}^{B\dot{M}}=gH_{(i)}^{AB}\nabla_{A}^{\dot{M}}f, \tag{17}$$

where g and f are scalar fields and $H_{(i)}^{AB}$, for each value of i, is a two-index symmetric spinor field, which will be determined from the condition that when $\mathcal{S}_{(i)}$ is applied to the Maxwell equations one obtains a decoupled equation for the φ_i component of the electromagnetic spinor field. (i.e., for $\varphi_0=o_Ao_B\varphi^{AB}$, $\varphi_1=o_{(A}\iota_{B)}\varphi^{AB}$ or $\varphi_2=\iota_A\iota_B\varphi^{AB}$; where $\{o^A,\iota^A\}$ is a spin frame such that $o_A\iota^A=1$.) In other words, we require that

$$\mathcal{S}_{(i)}^{B\dot{M}}J_{B\dot{M}}=\mathcal{O}_i\varphi_i \tag{18}$$

(here and in what follows the repeated index i does not mean summation convention) where $\mathcal{O}_i$, for each value of i, is a second-order differential operator that maps scalar fields into scalar fields. Observe that Eq. (18) is Eq. (3) for the electromagnetic case applied to the electromagnetic potential vector field. This means that in this way we not only are going to obtain the operators $\mathcal{S}_{(i)}$ but also the operators $\mathcal{O}_i$, which is equivalent to obtain the decoupled equations.

Using the Newman–Penrose notation we have that Eq. (18) is equivalent to

$$\begin{aligned}\mathcal{S}^{B\dot{M}}_{(i)}J_{B\dot{M}} = fg\{&H^{00}_{(i)}[(\delta-\overline{\alpha}-\beta+\overline{\pi}+\delta\ln f)J_{0\dot{0}}-(D-\varepsilon+\overline{\varepsilon}-\overline{\rho}+D\ln f)J_{0\dot{1}}+\sigma J_{1\dot{0}}-\kappa J_{1\dot{1}}]\\&+H^{10}_{(i)}[(\delta+\beta-\overline{\alpha}+\overline{\pi}+\tau+\delta\ln f)J_{1\dot{0}}-(D+\varepsilon+\overline{\varepsilon}-\overline{\rho}+\rho+D\ln f)J_{1\dot{1}}\\&+(\Delta-\gamma-\overline{\gamma}-\mu+\overline{\mu}+\Delta\ln f)J_{0\dot{0}}-(\overline{\delta}-\alpha+\overline{\beta}-\overline{\tau}-\pi+\overline{\delta}\ln f)J_{0\dot{1}}]\\&+H^{11}_{(i)}[(\Delta+\gamma-\overline{\gamma}+\overline{\mu}+\Delta\ln f)J_{1\dot{0}}-(\overline{\delta}+\alpha+\overline{\beta}-\overline{\tau}+\overline{\delta}\ln f)J_{1\dot{1}}-\nu J_{0\dot{0}}+\lambda J_{0\dot{1}}]\},\end{aligned} \tag{19}$$

where

$$\begin{aligned}J_{0\dot{0}}&=[(\overline{\delta}-2\alpha+\pi)\varphi_0-(D-2\rho)\varphi_1-\kappa\varphi_2],\\J_{0\dot{1}}&=[(\Delta-2\gamma+\mu)\varphi_0-(\delta-2\tau)\varphi_1-\sigma\varphi_2],\\J_{1\dot{0}}&=[(\overline{\delta}+2\pi)\varphi_1-(D+2\varepsilon-\rho)\varphi_2-\lambda\varphi_0],\\J_{1\dot{1}}&=[(\Delta+2\mu)\varphi_1-(\delta+2\beta-\tau)\varphi_2-\nu\varphi_0].\end{aligned} \tag{20}$$

Now we impose the conditions that $i=0$ and that the only component different from zero of $H^{AB}_{(0)}$ is $H^{00}_{(0)}$. Under these conditions Eq. (19) can be written in the following form $\mathcal{S}^{B\dot{M}}_{(0)}J_{B\dot{M}}=\mathcal{O}_0\varphi_0+\mathcal{P}_1\varphi_1+\mathcal{P}_2\varphi_2$, where $\mathcal{P}_1$ and $\mathcal{P}_2$ are differential operators such that when the commutator between D and δ and the Ricci identities are used they can be rewritten in the following form:

$$\begin{aligned}&[(\Delta-3\gamma-\overline{\gamma}+\overline{\mu})(-2\kappa)+(\overline{\delta}-3\alpha+\overline{\beta}-\overline{\tau})(2\sigma)+2\rho\delta\ln f-2\tau D\ln f\\&\quad+(2\rho+D\ln f)\delta-(2\tau+\delta\ln f)D-4\Psi_1],\end{aligned} \tag{21}$$

and

$$[(2\rho+D\ln f)\sigma-(2\tau+\delta\ln f)\kappa+\Psi_0], \tag{22}$$

respectively. From these expressions we observe that $\mathcal{P}_1$ and $\mathcal{P}_2$ are identically to the zero operator if

$$\kappa=\sigma=\Psi_0=\Psi_1=0,\quad \delta\ln f=-2\tau \text{ and } D\ln f=-2\rho. \tag{23}$$

It is important to remark that the integrability conditions on these equations are identically satisfied. Actually they are the conditions such that the background space-time admits a shear-free congruence of null geodesics, i.e., the space-time is algebraically special. In this case one can choose the spin frame $\{o^A,\iota^A\}$ with o^A being the repeated principal null spinor of the conformal curvature. From Eq. (23) we have that Eq. (19) reduces to

$$\mathcal{S}^{B\dot{M}}_{(0)}J_{B\dot{M}}=gfH^{00}_{(0)}[(\delta-\beta-\overline{\alpha}+\overline{\pi}-2\tau)(\overline{\delta}-2\alpha+\pi)-(D-\varepsilon+\overline{\epsilon}-\overline{\rho}-2\rho)(\Delta-2\gamma+\mu)]\varphi_0. \tag{24}$$

Therefore, we observe that when $\Phi_A{}^{\dot{B}}$ satisfies the Maxwell equations without sources and the space-time is algebraically special then the operator $\mathcal{S}_{(0)}$ engenders a decoupled equation for φ_0 (with $H^{AB}_{(0)}=o^A o^B$ and $g=f^{-1}$) given by

$$\mathcal{O}_0\varphi_0\equiv[(\delta-\beta-\overline{\alpha}+\overline{\pi}-2\tau)(\overline{\delta}-2\alpha+\pi)-(D-\varepsilon+\overline{\varepsilon}-\overline{\rho}-2\rho)(\Delta-2\gamma+\mu)]\varphi_0=0. \quad (25)$$

If now we impose the conditions that $i=2$ and that the only component different from zero of $H^{AB}_{(2)}$ is $H^{11}_{(2)}$, then after using the commutator of Δ and $\overline{\delta}$ and the Ricci identities we obtain that the differential operators acting on φ_0 and φ_1 can be rewritten in the following form:

$$[(D+3\varepsilon+\overline{\varepsilon}-\overline{\rho})(2\nu)-(\delta+3\beta-\overline{\alpha}+\overline{\pi})(2\lambda)-2\mu\overline{\delta}\ln f$$
$$+2\pi\Delta\ln f+(\Delta\ln f-2\mu)\overline{\delta}-(\overline{\delta}\ln f-2\pi)\Delta-4\Psi_3], \quad (26)$$

and

$$[(2\mu-\Delta\ln f)\lambda-(2\pi-\overline{\delta}\ln f)\nu+\Psi_4], \quad (27)$$

respectively. Therefore, in this case the conditions to obtain a decoupled equation for φ_2 are

$$\lambda=\nu=\Psi_3=\Psi_4=0, \quad \Delta\ln f=2\mu \ \text{ and } \ \overline{\delta}\ln f=2\pi. \quad (28)$$

The integrability conditions on these equations are identically satisfied. As in the previous case they are equivalent to say that the space-time admits a shear-free congruence of null geodesics. Therefore, if in addition to the decoupled equation for φ_0 we want to obtain a decoupled equation for φ_2, then the background space–time must be of type-D. With $H^{AB}_{(2)}=\iota^A\iota^B$, where ι^A is the other repeated principal null spinor field of the conformal curvature, and using Eq. (28) we find that when $J_{B\dot{M}}=0$ Eq. (19) reduces to

$$\mathcal{O}_2\varphi_2\equiv[(\Delta+\gamma-\overline{\gamma}+\overline{\mu}+2\mu)(D+2\varepsilon-\rho)-(\overline{\delta}+\alpha+\overline{\beta}-\overline{\tau}+2\pi)(\delta+2\beta-\tau)]\varphi_2=0. \quad (29)$$

Finally, assuming that $i=1$ and that the only component different from zero of the spinor field $H^{AB}_{(1)}$ is $H^{10}_{(1)}$, then using the commutators between D and δ, Δ and $\overline{\delta}$ and the Ricci identities we find that the differential operators acting on φ_0 and φ_2, can be rewritten in a such a way that they are identically to the zero operator under the conditions (23) and (28). In this case the decoupled equation for φ_1 is given by

$$\mathcal{O}_1\varphi_1\equiv[(\delta+\beta-\overline{\alpha}+\overline{\pi}-\tau)(\overline{\delta}+2\pi)-(D+\varepsilon+\overline{\varepsilon}-\overline{\rho}-\rho)(\Delta+2\mu)$$
$$-(\Delta-\gamma-\overline{\gamma}+\overline{\mu}+\mu)(D-2\rho)+(\overline{\delta}-\alpha+\overline{\beta}-\overline{\tau}+\pi)(\delta-2\tau)]\varphi_1=0. \quad (30)$$

Remark 2: The conditions given by Eqs. (23) and (28) are equivalent to say that the background space–time admits a two-index Killing spinor field. That is, a symmetric spinor field L_{AB} that satisfies $\nabla_{\dot{A}(B}L_{CD)}=0$,[7] in this case $L_{AB}=-2\phi^{-1}o_{(A}\iota_{B)}$, where $\phi=\sqrt{f}$. This means that the existence of decoupled equations for the components of the electromagnetic spinor field is very close related to the two-index Killing spinor field admitted by all the type-D metrics. We will see that the Killing spinor is also crucial for the construction of a differential operator that maps the space of solutions of the Maxwell equations without sources into itself.

From the computations presented above we have that the expressions for the $\mathcal{S}_{(i)}$ operators are given by

$$\mathcal{S}^{B\dot{M}}_{(0)}=\phi^2 o^A o^B\nabla_A{}^{\dot{M}}\phi^{-2}, \quad \mathcal{S}^{B\dot{M}}_{(1)}=\phi^2 o^{(A}\iota^{B)}\nabla_A{}^{\dot{M}}\phi^{-2}, \quad \mathcal{S}^{B\dot{M}}_{(2)}=\phi^2\iota^A\iota^B\nabla_A{}^{\dot{M}}\phi^{-2}. \quad (31)$$

Therefore, the decoupled equations in a covariant way can be written as

$$\phi^2\nabla_{(A}{}^{\dot{M}}\phi^{-2}\nabla_{|\dot{M}|}{}^{C}\varphi_{B)C}=0. \tag{32}$$

(Parentheses denote symmetrization on the indices enclosed and the indices between bars are excluded from the symmetrization.) Observe that Eq. (32) is equivalent to $\mathcal{O}_i\varphi_i=0$. Using Eq. (7), from Eqs. (25), (29) and (30) we obtain $\mathcal{O}_i^\dagger$. The corresponding adjoint equations are given by

$$\begin{aligned}
\mathcal{O}_0^\dagger\psi_2 &\equiv [(\overline{\delta}+\alpha+\overline{\beta}-\overline{\tau})(\delta+2\beta+\tau)-(\Delta+\gamma-\overline{\gamma}+\overline{\mu})(D+2\varepsilon+\rho)]\psi_2=0,\\
\mathcal{O}_1^\dagger\psi_1 &\equiv [(\overline{\delta}+\overline{\beta}-\alpha-\overline{\tau})\delta-(\Delta-\gamma-\overline{\gamma}-\mu+\overline{\mu})D+(\delta+\beta-\overline{\alpha}+\tau+\overline{\pi})\overline{\delta}\\
&\quad -(D+\varepsilon+\overline{\varepsilon}-\overline{\rho}+\rho)\Delta]\psi_1=0,\\
\mathcal{O}_2^\dagger\psi_0 &\equiv [(D+\varepsilon+\overline{\varepsilon}-\overline{\rho})(\Delta-2\gamma-\mu)-(\delta-\beta-\overline{\alpha}+\overline{\pi})(\overline{\delta}-2\alpha-\pi)]\psi_0=0.
\end{aligned} \tag{33}$$

The covariant version of these equations is obtained from Eq. (32) by applying property (4) to the differential operator appearing in Eq. (32). Thus Eqs. (33) are equivalent to

$$\nabla_{\dot{R}(A}\phi^{-2}\nabla^{S\dot{R}}\phi^2\psi_{C)S}=0. \tag{34}$$

Since in this case we have a decoupled equation for each component of the electromagnetic spinor field then, in accordance with Theorem 1, we can construct three solutions to the Maxwell equations without sources. Using property (4) to obtain $\mathcal{S}_{(i)}^\dagger$ from Eqs. (31), we find that these three solutions are given by

$$\Phi_{(0)}^{B\dot{M}}=\phi^{-2}\nabla_A{}^{\dot{M}}\phi^2 o^A o^B\psi_2, \tag{35}$$

$$\Phi_{(1)}^{B\dot{M}}=\phi^{-2}\nabla_A{}^{\dot{M}}\phi^2 o^{(A}\iota^{B)}\psi_1, \tag{36}$$

$$\Phi_{(2)}^{B\dot{M}}=\phi^{-2}\nabla_A{}^{\dot{M}}\phi^2 \iota^A\iota^B\psi_0. \tag{37}$$

After some computations one can show that these solutions are equivalent each other. Since the $\Phi_{(i)}$'s are solutions of the Maxwell equations then

$$\Phi^{B\dot{M}}=\phi^{-2}\nabla_A{}^{\dot{M}}\phi^2\psi^{AB}, \tag{38}$$

where ψ_{AB} is a solution of Eq. (34), is also a solution of the Maxwell equations. It is important to remark that if the background space-time is not of type-D, but algebraically special, then we only can obtain a decoupled equation (for φ_1 or φ_2) and in this case the solution to the Maxwell equations without sources is given by Eq. (35) or Eq. (37) and therefore, we cannot write it in a covariant way.

That $\Phi^{B\dot{M}}$ given by Eq. (38) satisfies the Maxwell equations is guaranteed by Theorem 1. Then this means that

$$\varphi_{AB}=\nabla^{\dot{C}}{}_{(A}\Phi_{B)\dot{C}}, \tag{39}$$

and

$$G_{\dot{A}\dot{B}}=\nabla^B{}_{(\dot{R}}\Phi_{\dot{S})B}, \tag{40}$$

are solutions of the Maxwell equations. From Remark 1 we have that if ψ_i is a solution of $\mathcal{O}_i^\dagger\psi_i=0$ then $\varphi_i=[\mathcal{T}\mathcal{S}^\dagger(\psi)]_i$ is a solution of $\mathcal{O}_i\varphi_i=0$. Using $\mathcal{T}$ given by Eq. (15) and computing

$\mathcal{S}^{\dagger}_{(i)}$ from Eqs. (31) and (4), one finds that the statement of Remark 1, in a covariant way, is equivalent to $\varphi_i=\varphi_{AB}=0$, the last equality is obtained from the fact that ψ_{AB} satisfies Eq. (34). Therefore, the operator $\mathcal{TS}^{\dagger}$ maps solutions of Eqs. (33), into the trivial solution of Eqs. (25), (29) and (30). This is equivalent to say that the vector potential given by Eq. (38) is a vector potential of a self-dual electromagnetic field given by $G_{A\dot{A}}$ in Eq. (40).

Remark 3: A straightforward computation shows that if φ_0,φ_1 and φ_2 satisfy Eqs. (25), (30) and (29), respectively, then $\psi_0=\phi^{-2}\varphi_0,\psi_1=-\phi^{-2}\varphi_1$ and $\psi=\phi^{-2}\psi_2$ satisfy Eqs. (33), recall that $\phi=\sqrt{f}$. In a covariant way this means that if φ_{AB} is a solution of Eq. (32) then $\psi_{AB}=L_{AC}L_{BD}\varphi^{CD}$ is a solution of Eq. (34). Using this fact and Eqs. (38) and (40) one finds that if φ_{AB} is a solution of the Maxwell equations without sources in a type-D solution of the Einstein vacuum field equations with a cosmological term then $G_{\dot{R}\dot{S}}=\nabla^{B}{}_{(\dot{R}}\phi^{-2}\nabla^{S}{}_{\dot{S})}\phi^{2}L_{BD}L_{SE}\varphi^{DE}$ is also a solution of the Maxwell equations.[1,2,8]

Observe that the result established in the previous remark was obtained analyzing the relationship between the solutions to the scalar equations $\mathcal{O}_i\varphi_i=0$ and $\mathcal{O}_i^{\dagger}\psi_i=0$. It turns out that the connection between the two sets of solutions is given by the two-index Killing spinor admitted by all the type-D metrics. It seems that this result is also a direct consequence of the existence of decoupled equations for *each component* of the electromagnetic spinor field, but in what follows we are going to show that we can obtain the same result without assuming a decoupled equation for φ_1. For this end, we rewrite $G_{A\dot{B}}$ in the following form:

$$
\begin{aligned}
G_{\dot{0}}&=2\phi^{-2}[(\overline{\delta}-\alpha-\overline{\beta}+3\pi)(\overline{\delta}-2\alpha+\pi)\varphi_0+(D+\varepsilon-\overline{\varepsilon}-3\rho)(D+2\varepsilon-\rho)\varphi_2],\\
G_{\dot{1}}&=\phi^{-2}\{[(\Delta-\gamma-\overline{\gamma}+3\mu-\overline{\mu})(\overline{\delta}-2\alpha+\pi)+(\overline{\delta}-\alpha+\overline{\beta}+3\pi+\overline{\tau})(\Delta-2\gamma+\mu)]\varphi_0\\
&\quad+[(D+\varepsilon+\overline{\varepsilon}-3\rho+\overline{\rho})(\delta+2\beta-\tau)+(\delta+\beta-\overline{\alpha}-3\tau-\overline{\pi})(D+2\varepsilon-\rho)]\varphi_2\},\\
G_{\dot{2}}&=2\phi^{-2}[(\Delta-\gamma+\overline{\gamma}+3\mu)(\Delta-2\gamma+\mu)\varphi_0+(\delta+\beta+\overline{\alpha}-3\tau)(\delta+2\beta-\tau)\varphi_2].
\end{aligned}
\tag{41}
$$

In doing this we only have used the Maxwell equations and the facts that when the background space-time is of type-D the following commutation relations hold[9] (in a spin frame such that the only non-vanishing component of the Weyl spinor is Ψ_2):

$$
\begin{aligned}
&[D+(p+1)\varepsilon+\overline{\varepsilon}+q\rho-\overline{\rho}](\delta+p\beta+q\tau)=[\delta+(p-1)\beta-\overline{\alpha}+q\tau+\overline{\pi}](D+p\varepsilon+q\rho),\\
&[\Delta-(p-1)\gamma-\overline{\gamma}-q\mu+\overline{\mu}](\overline{\delta}-p\alpha-q\pi)=[\overline{\delta}-(p-1)\alpha+\overline{\beta}-q\pi-\overline{\tau}](\Delta-p\gamma-q\mu),
\end{aligned}
\tag{42}
$$

where p and q are arbitrary constants.

The remarkable thing is that Eqs. (41) can be written in a covariant way using the two-index Killing spinor admitted by all the type-D space–times, which was our desired aim. In fact one direct computation, using a spin frame such that Ψ_2 is the only component different from zero of the Weyl spinor curvature, shows that Eqs. (41) are equivalent to

$$
T_{\dot{R}\dot{S}}=\nabla^{B}{}_{(\dot{R}}\phi^{-2}\nabla^{S}{}_{\dot{S})}\phi^{2}Y_{BS},
\tag{43}
$$

where

$$
Y_{AB}=\tfrac{1}{2}[L_{AC}L_{BD}\varphi^{CD}+L^{D}{}_{C}L^{C}{}_{(A}\varphi_{B)D}].
\tag{44}
$$

Observe that since $\varphi_{AB}=0$, this operator maps solutions with indices without dots of the Maxwell equations into solutions with dotted indices of the Maxwell equations.

IV. CONCLUDING REMARKS

Remember that Eqs. (41) were obtained using the Maxwell equations, in a spin frame such that the only component different from zero of the Weyl spinor curvature is Ψ_2 and the identities

(42), which are equivalent to the Teukolsky–Starobinsky identities[8,9] for the electromagnetic case. From this, it seems that the fact that Eqs. (41) can be rewritten in a covariant way by using the two-index Killing spinor is because there exist some kind of ''equivalence'' between the Teukolsky-Starobinsky identities and the two-index Killing spinor admitted by all the type-D space-times.

From the result obtained above we hope that an analogous program can be applied to the Weyl spinor perturbations of type-D vacuum backgrounds where one can only obtain decoupled equations for the maximal spin-weighted components of the Weyl spinor perturbations. In this case there exist also the Teukolsky-Starobinsky identities.[10,11]

Finally we point out that it could be interesting to study in detail the relationship between the result obtained here and the result obtained from a generalization of the Killing-Yano equation point of view.[12]

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Initial-value problems for evolutionary partial differential equations and higher-order conditional symmetries

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We suggest a new approach to the problem of dimensional reduction of initial/boundary value problems for evolution equations in one spatial variable. The approach is based on higher-order (generalized) conditional symmetries of the equations involved. It is shown that reducibility of an initial value problem for an evolution equation to a Cauchy problem for a system of ordinary differential equations can be fully characterized in terms of conditional symmetries which leave invariant the equation in question. We also give some examples of the solution of initial value problems for second- and third-order nonlinear differential equations by reduction by their conditional symmetries. We give a systematic classification of general second-order partial differential equations admitting second-order conditional symmetries, based on Lie's classification of invariant second-order ordinary differential equations. This yields five classes of principally new initial value problems for nonlinear evolution equations which admit no Lie symmetries and are reducible via second-order conditional symmetries. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1330199]

I. INTRODUCTION

As is well-known, the basic idea of the classical Lie approach to solving partial differential equations (PDEs) is to use symmetries to reduce the number of independent variables in order to get an ordinary differential equation. If one can then solve the resulting ordinary differential equation, the whole procedure yields particular solutions of the initial PDE. This procedure of dimensional reduction is referred to in the literature as symmetry reduction, and it has proved to be a very efficient tool for constructing exact solutions of many linear and nonlinear differential equations arising in different areas of applied mathematics (see, e.g., Refs. 1–3 and the references therein).

On the other hand, the problem of the application of the symmetry approach to the analysis of boundary and initial value problems still remains a great challenge for mathematicians. The main difficulty is that the symmetry groups admitted by boundary and initial value problems arising in applications are not sufficiently rich to allow for the effective use of the technique of symmetry reduction. It would be natural to attempt to exploit conditional (nonclassical) symmetries of PDEs in order to extend the range of the initial/boundary value problems that can be handled within the framework of the symmetry approach.

Our aim in the present paper is to present our view of the problem of dimensional reduction of initial value problems for evolution equations in two independent variables t, x:

$$u_t = F(t,x,u,u_1,u_2,\ldots,u_n), \tag{1}$$

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where $u \in C^n(\mathbf{R^2},\mathbf{R^1})$, $u_k=\partial^k u/\partial x^k$, $1\leqslant k\leqslant n$. The approach we give below is based on higher-order conditional symmetries of PDEs of the form (1). The concept of higher-order conditional symmetry was introduced by Fushchych and Zhdanov,[4] and independently by Fokas and Liu.[5] It was proved in Ref. 4 that it is higher-order conditional symmetries that are responsible for the ''nonlinear separation of variables'' introduced by Galaktionov[6] (see also the related papers addressing this problem[7–9]).

The structure of the paper is as follows. In Sec. II we give some necessary notations, definitions and theorems. In Sec. III, we formulate the principal theorem on the reduction of the initial value problem for a PDE of the form (1) to a Cauchy problem for some system of ordinary differential equations. In addition, we give two illustrative examples of applications of the theorem to the reduction of initial value problems for the second- and third-order nonlinear evolution equations. Section IV is devoted to the systematic classification of second-order evolutionary PDEs using their second-order conditional symmetries. The results of this classification are used to describe the initial value problems for second-order PDEs that admit dimensional reductions to Cauchy problems for some systems of ordinary differential equations.

II. BASIC NOTATIONS AND DEFINITIONS

It is known that reducibility of any PDE in two variables to a single ordinary differential equation is in one-to-one correspondence with its Q-conditional symmetry[10,11] (see also Refs. 12–17). We have proved in Ref. 18 that reducibility of (1) to a system of several ordinary differential equations is in one-to-one correspondence with its invariance under a nonpoint group of infinitesimal transformations,

$$\begin{aligned} u' &= u+\epsilon\eta(t,x,u,u_1,\ldots,u_N),\\ u_1' &= u_1+\epsilon D_x\eta(t,x,u,u_1,\ldots,u_N),\ldots, \end{aligned} \tag{2}$$

provided some smoothness requirements are satisfied. The above group is generated by the Lie–Bäcklund vector field,

$$Q=\sum_{k=0}^{\infty}(D_x^k\eta)\frac{\partial}{\partial u_k}\equiv\eta\frac{\partial}{\partial u}+(D_x\eta)\frac{\partial}{\partial u_1}+(D_x^2\eta)\frac{\partial}{\partial u_2}+\cdots. \tag{3}$$

In formulas (1), (3) we use the following notation:

$$D_x=\frac{\partial}{\partial x}+\sum_{k=0}^{\infty}u_{k+1}\frac{\partial}{\partial u_k},\quad D_x^{j+1}=D_x(D_x^j),\quad D_x^0=1.$$

Remark 1: In general, the function η in (3) may also depend on derivatives of the function u with respect to t. However, on the solution manifold of PDE (1) we can express all the derivatives of u with respect to t in terms of $t,x,u,u_1,u_2,\ldots$, and thus eliminate derivatives with respect to the variable t.

Remark 2: If the function η has the structure

$$\eta=\tilde{\eta}(t,x,u)-\xi_0(t,x,u)u_t-\xi_1(t,x,u)u_1, \tag{4}$$

then the Lie–Bäcklund vector field (3) is equivalent to a Lie vector field and can be represented in the standard form (*see, e.g., Refs. 2, 19*):

$$Q=\xi_0(t,x,u)\frac{\partial}{\partial t}+\xi_1(t,x,u)\frac{\partial}{\partial x}+\tilde{\eta}(t,x,u)\frac{\partial}{\partial u}.$$

As the form of a Lie–Bäcklund vector field is fully defined by the form of the coefficient η of $\partial/\partial u$ we will use the notation

$$Q=\eta\frac{\partial}{\partial u}+\ldots,$$

instead of (3).

Definition 1: PDE (1) is invariant under the Lie–Bäcklund vector field (3) if the condition

$$Q(u_t-F)\big|_M=0 \tag{5}$$

holds, where M is the set of all differential consequences of the equation $u_t-F=0$, that is $D_x^jD_t^k(u_t-F)=0, j,k=0,1,2,\ldots$.

Definition 2: PDE (1) is conditionally-invariant under the Lie–Bäcklund vector field (3) if the following condition holds:

$$Q(u_t-F)\big|_{M\cap L_x}=0. \tag{6}$$

Here the symbol L_x stands for the set of all differential consequences of the equation $\eta=0$ with respect to x, that is $D_x^j\eta=0, j=0,1,2,\ldots,$.

The procedure for constructing Lie–Bäcklund vector fields is, in fact, encoded in the above definitions. If one considers the problem of finding Lie–Bäcklund symmetries in the sense of Definition 1, then the first thing to do is to act with the operator Q on the expression u_t-F, considered as a function of the independent variables $t,x,u,u_t,u_1,\ldots,u_n$. The next step is to eliminate the derivatives $u_{tj}, j=0,1,2,\ldots,$ with the use of the equation $u_t-F=0$ and its differential consequences $D_x^j(u_t-F)=0, j=1,2,\ldots,$. Equating the resulting expression to zero yields a system of linear PDEs called the system of determining equations. Solving this system yields the most general form of the Lie–Bäcklund vector field (3) admitted by Eq. (1). Further details about the procedure for calculating higher symmetries of PDEs and numerous examples of equations possessing these symmetries can be found in Refs. 2, 19, 20. The procedure for calculating higher conditional symmetries is essentially the same. The only difference is the necessity of taking into account not only the differential consequences of Eq. (1) but also the differential consequences $D_x^j\eta=0, j=1,2,\ldots,$ of the invariance condition $\eta=0$. This additional restriction, on the one hand, extends considerably the scope of invariant equations (as the number of variables to be split, decreases) but, on the other hand, yields a nonlinear system of determining equations.

Clearly, if PDE (1) is invariant under the Lie–Bäcklund vector field (3), then it is conditionally invariant under it; however, the converse is not true. Consequently, this means that Definition 2 is a generalization of the standard definition of invariance of a partial differential equation with respect to the Lie–Bäcklund vector field.

If we consider the nonlinear PDE,

$$\eta(t,x,u,u_1,\ldots,u_N)=0, \tag{7}$$

as an N-th-order ordinary differential equation with respect to variable x, then its general integral can be given (locally) in the form

$$u(t,x)=U(t,x,\varphi_1(t),\varphi_2(t),\ldots,\varphi_N(t)), \tag{8}$$

where $\varphi_j(t)$, $(j=1,\ldots,N)$ are arbitrary smooth functions. In the following, we call expression (8) the *ansatz* invariant under the Lie–Bäcklund vector field (3). The following result (see Ref. 18) establishes the connection between reducibility of a given PDE (1) to ordinary differential equations and its higher-order conditional symmetry.

Theorem 1: *Let Eq. (1) with $F\in C^{N+1}(\mathcal{D})$, where $\mathcal{D}$ is an open domain in $\mathbf{R}^{n+3}$, be conditionally invariant under Lie–Bäcklund vector field (3) with $\eta\in C^2(\mathcal{D}')$, where $\mathcal{D}'$ is an open*

domain in $\mathbf{R}^{N+3}$ *and* $\partial\eta/\partial u_N \neq 0$ *on* $\mathcal{D}'$. *Then ansatz (8) invariant under the Lie–Bäcklund vector field (3) reduces PDE (1) to a system of N ordinary differential equations for some functions* $\varphi_j(t)$ $(j=1,\ldots,N)$,

$$\dot{\varphi}_j = F_j(t,\varphi_1,\ldots,\varphi_N), \quad j=1,\ldots,N. \tag{9}$$

Now suppose the converse. Namely, that ansatz (8), where the function U and its derivatives $\partial U^{k+1}/\partial\varphi_j\partial x^k$, $(j=1,\ldots,N,\ k=0,\ldots,N)$ *exist and are continuous on an open domain* $\mathcal{D}_1$ *in* $\mathbf{R}^{N+2}$, *reduces (1) to a system of ordinary differential equations (9) with* $F_i \in C^1(\mathcal{D}_1')$, *where* $\mathcal{D}_1'$ *is an open domain in* $\mathbf{R}^{N+2}$. *Then there exists a Lie–Bäcklund vector field (3) such that Eq. (1) is conditionally-invariant with respect to it.*

The principal reason for the existence of the phenomenon of nonlinear separation of variables in nonintegrable evolution equations is their higher-order conditional symmetry. Of course, the usual Lie and higher-order Lie symmetries can be also used to reduce nonlinear PDEs that have the necessary algebraic properties, but there exist equations that admit no Lie symmetries but are nonetheless reducible to one or several ordinary differential equations due to their (first- or higher-order) conditional symmetry. As an example we give the following nonlinear PDE:

$$u_t = u_{xx} + f_1(t, r(u_x)-x)u_x + f_2(t, r(u_x)-x) - \frac{1}{r'(u_x)}, \tag{10}$$

where f_1, f_2, r are arbitrary smooth functions of their arguments with $r'(u_x)\neq 0$. This equation admits neither first- nor higher-order Lie symmetries (except for the trivial one-parameter translation group by u). However, it can be reduced to a system of two ordinary differential equations due to the fact that Eq. (10) is conditionally invariant with respect to the Lie–Bäcklund field,

$$Q = (r'(u_x)u_{xx} - 1)\frac{\partial}{\partial u} + \cdots.$$

III. REDUCTION OF INITIAL VALUES PROBLEMS FOR EVOLUTION PDES

Consider the following initial value problem for the evolution equation (1):

$$\begin{aligned} u_t &= F(t,x,u,u_1,u_2,\ldots,u_n), \\ (\alpha(x)u_1 + \beta(x)u)\big|_{t=t_0} &= \gamma(x), \end{aligned} \tag{11}$$

where $\alpha(x)$, $\beta(x)$, $\gamma(x)$ are smooth functions.

If the problem (11) is invariant under a one-parameter transformation group, then it is possible to reduce it by symmetry reduction. However, this approach is too restrictive, since a choice of initial conditions that are invariant with respect to a Lie group can be very limited. Indeed, the transformation group in question must leave invariant the initial surface at $t=t_0$, and this imposes rather strong limitations on the exploitation of symmetry reduction in its classical setting. For instance, even such a simple symmetry as invariance under t-translations violates the symmetry of problem (11).

We will show that using higher-order conditional symmetries enables us to overcome this difficulty. The principal idea is to rewrite the generator of a one-parameter transformation group,

$$Q = \xi_0(t,x,u)\frac{\partial}{\partial t} + \xi_1(t,x,u)\frac{\partial}{\partial x} + \tilde{\eta}(t,x,u)\frac{\partial}{\partial u},$$

as a canonical generator of a Lie–Bäcklund field of the form (3), with $\eta = \tilde{\eta}(t,x,u) - \xi_0(t,x,u)u_t - \xi_1(t,x,u)u_1$, and then to eliminate all t derivatives with the use of Eq. (1). Since the vector field (3) generates an infinitesimal transformation group of the form (2), the initial

surface at $t=t_0$, as well as any boundary surface $X(x)=0$, is invariant with respect to it, and an *arbitrary* Lie symmetry can, in principle, be used for dimensional reduction of the initial value problem (11)! However, the price for this is that the order of the symmetry operator is no longer equal to one, and the standard procedure of symmetry reduction has to be modified in order to be applicable to the case under investigation. To this end we will use Theorem 1.

One of the immediate conclusions is that higher-order conditional symmetry is not just one more exotic concept, but the natural and efficient tool for handling initial value problems (11) within the framework of the symmetry approach.

It is natural to expect that, provided PDE (1) admits higher-order conditional symmetry (and some reasonable restrictions are satisfied), there exist functions $\alpha(x)$, $\beta(x)$, $\gamma(x)$ such that the initial value problem (11) reduces [by virtue of the ansatz (8)] to the Cauchy problem for the functions $\varphi_j(t)$, $(j=1,\ldots,N)$. This means that PDE (1) should reduce to a system of ordinary differential equations (9), and the initial condition given in (11) should reduce to a set of algebraic relations prescribing the values of the functions $\varphi_j(t)$, $(j=1,\ldots,N)$ at $t=t_0$.

To make the above procedure meaningful one has to give a formal definition of what is meant by a reduction of the initial-value problem,

$$(\alpha(x)u_1+\beta(x)u)\big|_{t=t_0}=\gamma(x). \tag{12}$$

Definition 3: We say that ansatz (8) reduces the initial-value condition (12) if substituting it into (12) yields an expression that vanishes identically when

$$\varphi_i(t_0)=C_i, \quad i=1,2,\ldots,N,$$

where $C_1,\ldots,C_N$ are some constants.

We prove the following assertion.

Theorem 2: *Ansatz (8), invariant with respect to the Lie–Bäcklund field (3), reduces the initial-value condition (12) if and only if*

(a) the system of two PDEs,

$$\eta(t,x,u,u_1,\ldots,u_N)=0, \;\; a(t,x)u_1+b(t,x)u-c(t,x)=0, \tag{13}$$

is compatible, and

(b) its solution is obtained from the general integral (8) of equation $\eta=0$ considered as an ordinary differential equation with respect to x.

Proof: The implication *reduction* $\Rightarrow$ *compatibility* is evident. We prove the converse assertion.

Suppose that conditions *a* and *b* of the theorem hold. Then, substituting ansatz (8) into the left-hand side of the second equation of (13) yields an expression of the form $R(t,x,\varphi_1(t),\varphi_1(t),\ldots,\varphi_N(t))$.

As the solution of system (13) exists (by assumption) and belongs to the family (8), there are constants $C_1,C_2,\ldots,C_N$ such that the relation

$$R(t,x,C_1,C_2,\ldots,C_N)=0$$

holds. This means that ansatz (8) reduces the initial-value condition. This establishes the theorem.

Definition 4: We say that the equation

$$\eta(t,x,u,u_1,\ldots,u_N)=0, \tag{14}$$

considered as an ordinary differential equation with respect to x, is conditionally invariant under the operator

$$X=\xi(t,x,u)\frac{\partial}{\partial x}+\zeta(t,x,u)\frac{\partial}{\partial u}, \tag{15}$$

with $\xi \neq 0$ *if the following relation holds:*

$$\tilde{X}\,\eta|_{\mathcal{M}} = 0. \tag{16}$$

Here, $\tilde{X}$ *is the* N*th prolongation of the operator* X*. The symbol* $\mathcal{M}$ *stands for the intersection of the surface defined in the space* $\mathbf{R}^{N+3}$ *of the variables* t, x, u, u_t, u_x,..., u_N *by the equation* $\eta = 0$ *and differential consequences* (*with respect to* x) *of the equation* $\xi(t,x,u)u_1 - \zeta(t,x,u) = 0$ *up to the order* $N-1$*. When* $\xi = 0$*, we say that (14) is conditionally invariant under the operator (15), if solving the relation* $\zeta(t,x,u) = 0$ *with respect to* u *yields an exact solution of (14).*

Theorem 3: *Ansatz (8), invariant with respect to the Lie–Bäcklund field (3), reduces the initial value condition (12) if and only if*

(a) Eq. (9) is conditionally invariant under the operator (15) with $\xi = \alpha(x)$, $\zeta = -\beta(x)u + \gamma(x)$, *and*

(b) the solution of the corresponding system (13) exists and is obtained from the general integral (8) of the equation $\eta = 0$*, considered as an ordinary differential equation with respect to* x.

Proof: To prove the theorem it is sufficient to show that, given condition b, then condition a of Theorem 3 is equivalent to condition a of Theorem 2.

Since the assertion to be proved is evident for the case $\alpha = 0$, we will concentrate on the case when $\alpha \neq 0$.

When $\alpha \neq 0$, we can make a change of variables,

$$\tilde{x} = X(t,x), \quad \tilde{u} = U_1(t,x)u + U_2(t,x),$$

so that the operator (15) takes the form $\tilde{X} = \partial/\partial\tilde{x}$ (to simplify notations, we omit the tilde in the sequel). Now, system (13) reads as follows:

$$\tilde{\eta}(t,x,u,u_1,\ldots,u_N) = 0, \;\; u_1 = 0. \tag{17}$$

Compatibility of this system means that the function $\tilde{\eta}(t,x,u,0,\ldots,0)$ is independent of x, whence we find that there exist smooth functions

$$a_0(t,u,u_1,\ldots,u_N), \;\; a_i(t,x,u,u_1,\ldots,u_N), \;\; i = 1,2,\ldots,N,$$

such that

$$\tilde{\eta}(t,x,u,u_1,\ldots,u_N) = a_0(t,u,u_1,\ldots,u_N) + \sum_{i=1}^{N} a_i(t,x,u,u_1,\ldots,u_N)u_i\,.$$

Hence, we conclude that the equation $\tilde{\eta} = 0$ is conditionally invariant with respect to the operator $\partial/\partial x$. Reversing this argument completes the proof of the equivalence of conditions a of Theorems 2 and 3. This proves Theorem 3.

As an immediate consequence of Theorem 3, we see that a necessary condition for the reducibility of a Cauchy problem by solutions invariant under some Lie–Bäcklund field (3) is the conditional invariance of the equation $\eta = 0$ with respect to the operator (15) with $\xi = \alpha(x)$, $\zeta = -\beta(x)u + \gamma(x)$. In view of this fact, we can formulate the following symmetry approach to the reduction of initial value problems (11) for the case when the corresponding evolution equation admits first- or higher-order conditional symmetry:

(i) rewrite the symmetry operator in the canonical form (3),

(ii) calculate the classical or conditional symmetry of the equation $\eta = 0$ within the class of operators,

$$X = \alpha(x)\frac{\partial}{\partial x} + (-\beta(x)u + \gamma(x))\frac{\partial}{\partial u}, \tag{18}$$

(iii) carry out the reduction of the initial value problem (11) to a Cauchy problem for a system of ordinary differential equations using ansatz (8), invariant with respect to the Lie–Bäcklund vector field (3).

Note that condition b of Theorem 3 cannot be neglected, since conditional invariance alone cannot guarantee reducibility of the corresponding initial value problem. As an example, consider the Lie–Bäcklund vector field,

$$Q=(u_x+u^2-1)\frac{\partial}{\partial u}+\dots .$$

The equation $u_x+u^2-1=0$ is evidently invariant under translations by x. Furthermore, system

$$u_x+u^2-1=0,\ \ u_1=0$$

is compatible [it has the solution $u(t,x)=1$]. However, the ansatz,

$$u(t,x)=\tanh(x+\varphi(t)), \tag{19}$$

which is invariant under Q, does not reduce the initial condition $u_1|_{t=t_0}=0$. The reason for this is that the function $u(t,x)=1$ does not belong to the family (19), and thus the condition b of Theorem 3 fails to hold.

Let us now proceed to giving examples which illustrate the main features of the whole procedure. As the first example, we consider the nonlinear heat-conduction equation,

$$u_t=u_x^{-1}u_{xx},\ \ u_x\neq 0. \tag{20}$$

It is evidently invariant with respect to the one-parameter transformation group having the generator $Q=\partial/\partial t+a\,(\partial/\partial u)$ with a being an arbitrary constant. Our aim is to describe the initial value problems,

$$\begin{gathered} u_t=u_x^{-1}u_{xx}, \\ (\alpha(x)u_x+\beta(x)u)|_{t=t_0}=\gamma(x), \end{gathered} \tag{21}$$

that are reducible to Cauchy problems for some first-order systems of ordinary differential equations. First we note that, since the initial surface at $t=t_0$ is not invariant with respect to the group generated by the operator Q, we cannot apply the symmetry reduction method in its standard form. However, if we rewrite Q in the canonical form (3) and eliminate the t derivative on the solution manifold of PDE (20), then the resulting Lie–Bäcklund vector field,

$$\tilde{Q}=(u_x^{-1}u_{xx}-a)\frac{\partial}{\partial u}+\dots,$$

generates an infinitesimal transformation group leaving invariant the initial surface $t=t_0$. Consequently, we can apply the procedure developed above and based on Theorem 3. Solving the invariance condition $u_x^{-1}u_{xx}-a=0$ gives the ansatz for $u=u(t,x)$,

$$u(t,x)=\varphi_1(t)\exp(ax)+\varphi_2(t), \tag{22}$$

which reduces the initial PDE (20) to a system of two ordinary differential equations for φ_1, φ_2 (Theorem 1).

In order to exploit Theorem 3, we calculate the Lie symmetry of equation $u_{xx}-au_x=0$ and obtain the five-dimensional invariance algebra with basis elements,

$$e_1=\frac{\partial}{\partial x},\quad e_2=\exp(ax)\left(\frac{\partial}{\partial x}+au\frac{\partial}{\partial u}\right),$$

$$e_3=u\frac{\partial}{\partial u},\quad e_4=\exp(ax)\frac{\partial}{\partial u},\quad \frac{\partial}{\partial u}.$$

In other words, the most general form of the Lie vector field admitted by PDE $u_{xx}-au_x=0$ reads as

$$C_1\frac{\partial}{\partial x}+C_2\exp(ax)\left(\frac{\partial}{\partial x}+au\frac{\partial}{\partial u}\right)+C_3u\frac{\partial}{\partial u}+C_4\exp(ax)\frac{\partial}{\partial u}+C_5\frac{\partial}{\partial u},$$

where C_1, C_2,..., C_5 are arbitrary real constants. Hence, using Theorem 3, we find the form of the unknown functions $\alpha(x)$, $\beta(x)$, $\gamma(x)$ to be

$$\alpha(x)=(C_1+C_2\exp(ax)),\quad \beta(x)=-C_3-aC_2\exp(ax),$$

$$\gamma(x)=C_4+C_5\exp(ax).$$

Direct verification shows that the initial value problem,

$$\begin{gathered}u_t=u_x^{-1}u_{xx},\\ ((C_1+C_2\exp(ax))u_x-(C_3+aC_2\exp(ax))u)|_{t=t_0}=C_4+C_5\exp(ax),\end{gathered}\tag{23}$$

under $C_2(aC_1-C_3)\neq 0$ fulfills the conditions of Theorem 3 and, consequently, can be reduced to a Cauchy problem for a system of ordinary differential equations. Indeed, inserting ansatz (22) into (23) yields

$$\varphi_1'(t)=0,\quad \varphi_2'(t)=a,$$

$$\varphi_1(t_0)=\frac{aC_5+C_4}{aC_1-C_3},\quad \varphi_2(t_0)=\frac{C_5}{C_2},\quad C_2(aC_1-C_3)\neq 0.$$

Finally, solving the above Cauchy problem gives the following unique solution of the initial value problem (23):

$$u(t,x)=\frac{aC_5+C_4}{aC_1-C_3}\exp(ax)+a(t-t_0)+\frac{C_5}{C_2}.$$

Next, we apply the above scheme for reduction of the initial value problem for the third-order nonlinear PDE,

$$u_t=u_{xxx}+u_x^2-4auu_x+4a^2u^2,\tag{24}$$

where a is an arbitrary real parameter. Note that when $a\neq 0$, Eq. (24) cannot be solved by the methods of soliton theory, and in this sense it is nonintegrable. When $a=0$, (24) is reduced to the KdV equation by the (nonpoint) change of dependent variable $v(t,x)=u_x(t,x)$. In what follows we suppose that $a\neq 0$.

Direct calculation shows that Eq. (24) is conditionally invariant with respect to the Lie–Bäcklund vector field (3) with $\eta=u_{xxx}-3au_{xx}+2a^2u_x$. On calculating the Lie symmetry of the equation $\eta=u_{xxx}-3au_{xx}+2a^2u_x=0$, and taking into account Theorem 3, we get the following initial value problem for PDE (24):

$$
\begin{aligned}
&u_t = u_{xxx} + u_x^2 - 4auu_x + 4a^2u^2,\\
&((C_1 + C_2\exp(ax) + C_3\exp(-ax))u_x + (C_4 - 2aC_2\exp(ax))u)\big|_{t=t_0}\\
&\quad = C_5 + C_6\exp(ax) + C_7\exp(2ax).
\end{aligned}
\tag{25}
$$

Integrating the equation $\eta = 0$ and substituting its general solution,

$$
u(t,x) = \varphi(t) + \varphi_2(t)\exp(ax) + \varphi_3(t)\exp(2ax) \tag{26}
$$

into (25) give the following Cauchy problem:

$$
\vec{\varphi}\,'(t) = \mathcal{F}(\vec{\varphi}(t)),
$$

$$
\mathcal{C}\vec{\varphi}(t_0) = \vec{C},
$$

where

$$
\vec{\varphi}(t) = \begin{pmatrix} \varphi_1(t) \\ \varphi_2(t) \\ \varphi_3(t) \end{pmatrix}, \quad \mathcal{F}(\vec{\varphi}) = \begin{pmatrix} 4a^2\varphi_1^2 \\ a^3\varphi_2 + 4a^2\varphi_1\varphi_2 \\ 8a^3\varphi_3 + a^2\varphi_2^2 \end{pmatrix},
$$

$$
\mathcal{C} = \begin{pmatrix} C_4 & aC_3 & 0 \\ -2aC_2 & aC_1 + C_4 & 2aC_3 \\ 0 & -aC_2 & C_4 + 2aC_1 \end{pmatrix}, \quad \vec{C} = \begin{pmatrix} C_5 \\ C_6 \\ C_7 \end{pmatrix}.
$$

Thus, using higher-order conditional symmetries of the nonlinear PDE (24), we reduce the initial value problem (25) to the Cauchy problem for a system of three first-order ordinary differential equations for the functions $\varphi_1(t), \varphi_2(t), \varphi_3(t)$. The general solution of the system in question reads as

$$
\varphi_1(t) = (\kappa_1 - 4a^2t)^{-1},
$$

$$
\varphi_2(t) = \kappa_2\exp(a^3t)(\kappa_1 - 4a^2t)^{-1},
$$

$$
\varphi_3(t) = \exp(8a^3t)\left(\kappa_3 + a^2\kappa_2^2\int_{t_0}^{t}\exp(-6a^3z)(\kappa_1 - 4a^2z)^{-2}dz\right),
$$

where $\kappa_1, \kappa_2, \kappa_3$ are arbitrary real parameters (integration constants).

We emphasize that the exact analytic solution of the nonlinear PDE (24) that is obtained via substitution of the corresponding expressions for the functions $\varphi_1(t), \varphi_2(t), \varphi_3(t)$ into (26) cannot be constructed within the standard symmetry reduction approach. The reason for this is that the solution is not invariant with respect to the two-parameter displacement group defined by $\partial/\partial t$, $\partial/\partial x$, which is the maximal Lie symmetry algebra of (24).

Specifying $\kappa_1, \kappa_2, \kappa_3$ appropriately, we can solve any representative of the seven-parameter family of initial value problems given in (25). Consider, for example, the case $C_1 = C_2 = C_3 = C_7 = 0$ and $C_4 = 1$, $C_5 = k_1$, $C_6 = k_2$. Then the unique solution of the corresponding initial value problem,

$$
u_t = u_{xxx} + u_x^2 - 4auu_x + 4a^2u^2,
$$

$$
u(t_0,x) = k_1 + k_2\exp(ax),
$$

is given by

TABLE I. Lie's classification of invariant second-order ordinary differential equations.

No.	Equation	Symmetry algebra
1	$y''=f(y,y')$	$\frac{\partial}{\partial x}$
2	$y''=f(y')$	$\frac{\partial}{\partial x}, \frac{\partial}{\partial y}$
3	$y''=x^{-1}f(y')$	$\frac{\partial}{\partial x}, x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}$
4	$y''=2(y-x)^{-1}((y')^2+ay'\sqrt{y'}+y')$	$\frac{\partial}{\partial x}+\frac{\partial}{\partial y}, x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}, x^2\frac{\partial}{\partial x}+y^2\frac{\partial}{\partial y}$
5	$y''=ay^{-3}$	$\frac{\partial}{\partial x}, 2x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}, x^2\frac{\partial}{\partial x}+xy\frac{\partial}{\partial y}$
6	$y''=a\exp(-y')$	$\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, x\frac{\partial}{\partial x}+(x+y)\frac{\partial}{\partial y}$
7	$y''=a(y')^{(k-2)/(k-1)},\ k\neq 1,2$	$\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, x\frac{\partial}{\partial x}+ky\frac{\partial}{\partial y}$
8	$y''=a(1+(y')^2)^{3/2}\exp(k\arctan y')$	$\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, (kx+y)\frac{\partial}{\partial x}+(ky-x)\frac{\partial}{\partial y}$
9	$y''=0$	$\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, x\frac{\partial}{\partial y}, x\frac{\partial}{\partial x}, y\frac{\partial}{\partial x}, y\frac{\partial}{\partial y}, x^2\frac{\partial}{\partial x}+xy\frac{\partial}{\partial y}, xy\frac{\partial}{\partial x}+y^2\frac{\partial}{\partial y}$

$$u(t,x)=(k_1+k_2\exp(ax+a^3(t-t_0)))(1-4k_1a^2(t-t_0))^{-1}$$
$$+a^2k_2^2\exp(2ax+8a^3t-2a^3t_0)\int_{t_0}^{t}\exp(-6a^3z)(1-4k_1a^2z)^{-2}\,dz.$$

IV. CONDITIONALLY-INVARIANT SECOND-ORDER PDES

An analysis of the examples given in the previous section reveals an evident restriction on the scope of applicability of the reduction techniques based on higher conditional symmetries. It comes from a necessity to integrate a nonlinear high-order ordinary differential equation (7). Moreover, in order to use Theorem 3, we need to ensure that the ordinary differential equation $\eta=0$ has a nontrivial Lie symmetry. These observations suggest the idea of using Lie's classification of invariant second-order ordinary differential equations as the source of the functions η. With this choice of the conditional symmetry we are guaranteed that differential equation $\eta=0$ admits two-, three- or eight-parameter transformation group and, consequently, is integrable by quadratures. Surprisingly, it is possible to implement this approach to classifying second-order PDEs (1) by their second-order conditional symmetries in full generality.

In Table I we present the complete list of invariant real second-order ordinary differential equations together with their maximal invariance algebras, obtained by Lie (Refs. 21, 22). Note that a,k are arbitrary real parameters and f is an arbitrary function. As classification has been done

to within an arbitrary reversible transformation of the variables x,y, the equations given in Table I are representatives of the conjugacy classes of invariant ordinary differential equations.

We exclude from further consideration case 1 of Table I, since the corresponding ordinary differential equation is not integrable by quadratures. Next, since our final aim is to exploit conditional symmetries for the description and reduction of initial value problems, it makes no sense to consider case 4. This is because the symmetry group admitted by the corresponding ordinary differential equation within the class (18) is the same as that of the more general equation given in case 3 of Table I. The same argument applies to case 8. Consequently, we will deal only with the remaining cases 2, 3, 5–7, 9.

We take as the function η in operator (3) the expressions $y''-f(x,y,y')$, where f is one of the right-hand sides of equations listed in the second column of Table I and make the replacements $y\to u$, $y'\to u_x$ and $y''\to u_{xx}$. We classify PDEs of the form

$$u_t=u_{xx}+F(t,x,u,u_x), \tag{27}$$

admitting the corresponding Lie–Bäcklund vector fields. As we have already mentioned, this program can be realized in full generality. Indeed, given the above choice of higher conditional symmetry operators, we are able to describe the most general PDEs (27) admitting these symmetries. The form of the function F is the same for all the cases, namely,

$$F(t,x,u,u_x)=rF_1(t,\omega_1,\omega_2)+pF_2(t,\omega_1,\omega_2)+q.$$

Here F_1,F_2 are arbitrary smooth functions of the indicated variables and the forms of the coefficients r,p,q and of the ''invariants'' ω_1,ω_2 are presented in Table II.

As an example, we consider the case of the Lie–Bäcklund field $Q=(u_{xx}-a\exp(-u_x))(\partial/\partial u)+\cdots$. Inserting this operator into the invariance condition (6) yields the second-order PDE for the function $F=F(t,x,u,u_x)$ (we have generated it using MATHEMATICA),

$$a^3\exp(-3u_x)+a^2\exp(-2u_x)F_{u_xu_x}+a\exp(-u_x)(u_x+1)F_u+2au_x\exp(-u_x)F_{uu_x}$$
$$+u_x^2F_{uu}+a\exp(-u_x)F_x+2a\exp(-u_x)F_{xu_x}+2u_xF_{xu}+F_{xx}=0.$$

The equation obtained looks rather fearsome. However, it simplifies radically with the change of variables $F=\tilde F(t,x,\omega_1,\omega_2)$, where ω_1,ω_2 are the integrals of the ordinary differential equation $u_{xx}-a\exp(-u_x)=0$. As a result, we find that the function $\tilde F$ satisfies the following PDE:

$$a^3\exp(-3u_x)+a\exp(-u_x)\tilde F_x+\tilde F_{xx}=0.$$

Now, we eliminate u_x, using the second invariant $\omega_2=-ax+\exp(u_x)$, and thus get an ordinary differential equation with respect to x. Solving it yields formulas 6 from Table II. The other cases are dealt with in an analogous way.

Now we proceed to calculating the initial conditions (12) such that the initial value problems for conditionally invariant PDEs (27) given in Table II are reducible to Cauchy problems for systems of two ordinary differential equations. To this end we exploit Theorem 3. First of all we note that for Eqs. 2, 3 of Table II, the condition b of Theorem 3 fails to hold. For this reason, the corresponding initial value problem is not reduced to a Cauchy problem within the framework of our approach. For the remaining cases 5, 6, 7.1, 7.2 and 9 we get the following initial conditions.

Case 5: $(C_1+2C_2x+C_3x^2)u_x(t_0,x)-(C_2+C_3x)u(t_0,x)=0$,
$C_3\neq 0$, $C_1C_3\neq C_2^2$;

Case 6: $(C_1+C_3x)u_x(t_0,x)-C_3u(t_0,x)=C_2+C_3x$, $C_3\neq 0$;

Case 7.1: $(C_1+C_3x)u_x(t_0,x)-kC_3u(t_0,x)=C_2$, $C_3\neq 0$;

Case 7.2: $(C_1+C_3x)u_x(t_0,x)=C_2$, $C_2\neq 0$;

TABLE II. Conditionally-invariant PDEs (27).

No.	Coefficients r,p,q	Functions ω_1,ω_2
2	$r=1$ $p=u_x$ $q=-(f'(u_x))^{-1}$	$\omega_1=u-\int^{f(u_x)} g(z)dz$ $\omega_2=f(u_x)-x$
3	$r=1$ $p=xu_x-u$ $q=-(xf'(u_x))^{-1}$	$\omega_1=u-x\exp(-f(u_x))\times\int^{f(u_x)} g(z)\exp(z)dz$ $\omega_2=f(u_x)-\ln x$
5	$r=u^{-1}u_x(a+u^2u_x^2)^{1/2}$ $p=u^3(2xu_x-u)(a+u^2u_x^2)^{-3/2}$ $q=-au^{-3}$	$\omega_1=2u^3u_x(a+u^2u_x^2)^{-1}-2x$ $\omega_2=u^{-2}(u_x^2u^2-a)$
6	$r=1$ $p=u_x$ $q=-a\exp(-u_x)$	$\omega_1=au+(1-u_x)\exp(u_x)$ $\omega_2=-ax+\exp(u_x)$
7.1	$r=1$ $p=u_x$ $q=-au_x^{(k-2)/(k-1)},\ k\neq 0,1,2$	$\omega_1=u+\dfrac{1-k}{ak}u_x^{k/(k-1)}$ $\omega_2=\dfrac{ax}{1-k}+u_x^{1/(k-1)}$
7.2	$r=1$ $p=u_x$ $q=-au_x^2$	$\omega_1=u-a^{-1}\ln(u_x)$ $\omega_2=ax+(u_x)^{-1}$
9	$r=1$ $p=x$ $q=0$	$\omega_1=xu_x-u$ $\omega_2=u_x$

Case 9: $(C_1+C_4x+C_6x^2)u_x(t_0,x)-(C_5+C_6x)u(t_0,x)=C_2+C_3x$,
$\Delta=C_1C_6+C_5(C_5-C_4)\neq 0$, $\Delta_1=C_2(C_4-C_5)-C_1C_3$,
$\Delta_2=C_2C_6-C_3C_5$.

In the above formulas $C_1,C_2,\ldots,C_6$ are arbitrary real constants satisfying the given constraints. These constraints ensure that the corresponding initial value problem fulfills both the conditions of Theorem 3.

The last step of the reduction algorithm is the construction of ansatzes for the function $u(t,x)$ and the reduction of both the invariant equation and initial conditions to systems of ordinary differential equations and algebraic equations, correspondingly. We present the list of obtained results in Table III, where $F_i=F_i(t,\varphi_1(t),\varphi_2(t)),i=1,2$, the functions $\varphi_1(t),\varphi_2(t)$ are new dependent variables and the symbol g stands for the converse of the function $f(u_x)$, i.e., $g(f(u_x))\equiv u_x$.

Let us emphasize that the nonlinear evolution equations constructed above, for arbitrary functions F_1,F_2, admit no Lie symmetry. Consequently, the symmetry reduction algorithm cannot be applied to perform dimensional reductions of these equations. This means that the reductions obtained in this section (both for PDEs and initial value problems) are purely non-Lie reductions and cannot be obtained within the framework of the standard Lie's approach.

V. CONCLUSIONS

In our work we show that higher-order conditional symmetry is a useful and efficient concept in handling initial-value problems. In fact, in view of Theorem 3, one may claim that the method of conditional symmetries is the most appropriate tool for reductions of initial-value problems for evolution type equations. It extends the scope of applicability of symmetry methods to the analysis of initial value problems via dimensional reductions.

TABLE III. Ansatzes and reduced equations.

No.	Ansatz for $u(t,x)$	ODEs	Cauchy data
2	$\varphi_1(t)+g(x+\varphi_2(t))$	$\varphi_1'=F_1$ $\varphi_1'=F_2$	No reduction
3	$\varphi_1(t)+\exp(-\varphi_2(t))$ $\times\int^{\ln(x)+\varphi_2(t)}\exp(y)g(y)dy$	$\varphi_1'=F_1$ $-\varphi_1F_2$ $\varphi_2'=F_2$	No reduction
5	$\frac{1}{2\sqrt{\varphi_2(t)}}(4a+\varphi_2^2(t)$ $\times(2x+\varphi_1(t))^2)^{1/2}$	$\varphi_1'=2\varphi_1^{1/2}F_1$ $-2\varphi_1\varphi_2^{1/2}F_2$ $\varphi_2'=2\varphi_2^{1/2}F_2$	$\varphi_1(t_0)=\frac{2C_2}{C_3}$ $\varphi_2(t_0)=\frac{C_3\sqrt{a}}{\sqrt{C_1C_3-C_2^2}}$
6	$\varphi_1(t)+a^{-1}(ax+\varphi_2(t))$ $\times(\ln(ax+\varphi_2(t))-1)$	$\varphi_1'=F_1$ $\varphi_2'=aF_2$	$\varphi_1(t_0)=\frac{C_2-C_1}{C_3}$ $\varphi_2(t_0)=\frac{aC_1}{C_3}$
7.1	$\varphi_1(t)+\frac{k-1}{ak}\left(\frac{ax}{k-1}+\varphi_2(t)\right)^k$	$\varphi_1'=F_1$ $\varphi_2'=\frac{a}{k-1}F_2$	$\varphi_1(t_0)=\frac{C_2}{kC_3}$ $\varphi_2(t_0)=\frac{aC_1}{(k-1)C_3}$
7.2	$\varphi_1(t)-a^{-1}\ln(\varphi_2(t)-ax)$	$\varphi_1'=F_1$ $\varphi_2'=-aF_2$	$C_3=-aC_2$ $\varphi_2(t_0)=\frac{C_1}{C_2}$
9	$\varphi_1(t)+\varphi_2(t)x$	$\varphi_1'=F_1$ $\varphi_1'=F_2$	$\varphi_1(t_0)=\frac{\Delta_1}{\Delta}$ $\varphi_2(t_0)=\frac{\Delta_2}{\Delta}$

Furthermore, the technique developed in this paper can be applied to boundary value problems as well, provided the PDE under study admits some higher-order Lie–Bäcklund vector field. Indeed, inserting ansatz (8) into the boundary condition,

$$U(t,u,u_1,\ldots,u_M)|_{x=x_0}=0,\quad M<N,$$

yields an algebraic relation for the functions $\varphi_i, i=1,2,\ldots,N$. This means that, if we are given a reducible initial value problem, then we can add *any* boundary condition, so that the resulting problem remains reducible. However, the problem of compatibility of initial and boundary conditions must be investigated separately (see also the paper in Ref. 23 and the references therein).

We consider in the present paper the case of one dependent variable. However, all our arguments can be directly applied to the analysis of systems of evolution equations in one spatial dimension. One final point is that it seems to be possible to apply the same technique for the reduction of multi-dimensional evolution equations admitting classical or nonclassical symmetries. These and related problems are under study now and will be reported on in future publications.

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Symmetry group methods for heat kernels

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We apply methods of symmetry groups to heat equations on $\mathbb{R}$ with drift terms and to heat equations for Lie groups. In particular, we are able to characterize those functions f for which equations of the form $(\partial^2 u/\partial x^2)+f(x)u_x=u_t$ have a point symmetry which takes a constant solution to the fundamental solution. Further, we apply symmetry methods to the heat equation of the $ax+b$ group. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1316763]

I. INTRODUCTION

From the point of view of harmonic analysis, one of the more intriguing remarks to be found in Olver's book[1] is that the fundamental solution of the one-dimensional heat equation may be obtained from the constant solution by acting with an element of the symmetry group. It is the purpose of this paper to explore some extensions and ramifications of this remark.

We will discuss three aspects of the problem. In Sec. II we introduce the basic techniques involved with symmetry group calculations, and their application to heat kernels. We then use ideas from Refs. 2 and 3, applying the method of group representations to the problem of exponentiating generalized symmetries. Although, at the level of generalized vector fields, this can be a forbiddingly difficult process, the technique of introducing a suitable group representation, exponentiating in the appropriate representation space, and transforming back, often yields rather simple formulas.

The essential observation is that at the level of group representations, the difference between point symmetries and generalized symmetries disappears. As the culmination of this section, we are able to show that for any simply connected nilpotent Lie group, the heat equation corresponding to any sub-Laplacian satisfying the Hörmander condition has a generalized symmetry taking a constant solution to the heat kernel. In Sec. III we show how symmetry calculations yield the fundamental solutions for certain equations on the real line.

In Sec. IV, we are able to characterize those functions $f(x)$ for which the equation

$$\frac{\partial^2 u}{\partial x^2}+f(x)\frac{\partial u}{\partial x}=\frac{\partial u}{\partial t}$$

has an ordinary symmetry taking a constant solution to the fundamental solution. It turns out that f must satisfy one of several Ricatti equations. We are able also to give some explicit formulas for the heat kernel in these cases. Section V extends the results of Sec. IV to the two other finite-dimensional Lie algebras of vector fields on $\mathbb{R}$, viz. those spanned by $\partial/\partial x$ and $x(\partial/\partial x)$ and by $\partial/\partial x$, $x(\partial/\partial x)$, and $x^2(\partial/\partial x)$, respectively.

In the final section, a different approach is considered. We apply symmetry methods to the heat kernel on the $ax+b$ group, obtaining new information about its behavior.

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We believe that the idea of applying the symmetry methods of Lie to the study of heat kernels on Lie groups to be a novel one which will require further investigation.

II. SYMMETRIES: GENERALIZED SYMMETRIES

Let us recall the notion of a symmetry of a system of differential equations.

Consider the system

$$P_\nu(x,D^\alpha u)=0, \quad \nu=1,...p, \tag{2.1}$$

α a multi-index, $D^\alpha=\partial^{|\alpha|}/\partial x_1^{\alpha_1}\cdots\partial x_n^{\alpha_n}$.

A symmetry of (2.1) is a mapping defined on the space of solutions, $\mathcal{H}$, i.e.,

$$B:\ \mathcal{H}\to\mathcal{H}.$$

So if u is a solution of (2.1) then Bu is also a solution. That is, symmetries map solutions to new solutions. Symmetry methods are important because they allow us to construct complex solutions to a differential equation from simple solutions. (See the heat equation example below.) Lie developed a technique for computing *groups* of symmetries. An excellent modern account is contained in Ref. 1.

We consider P to be an operator on the manifold $X\times U$ where the independent variables are elements of X and the dependent variables elements of U. The first-order differential operator

$$v=\sum_{i=1}^{n}\xi_i(a,u)\frac{\partial}{\partial x_i}+\sum_{j=1}^{p}\phi^j(x,u)\frac{\partial}{\partial u^j} \tag{2.2}$$

generates a local group of transformations on $X\times U$. The n jet bundle of $X\times U$, is denoted by $J^n(X,U)$. $J^n(X,U)$ is a C^∞ manifold which may be thought of as consisting of $X\times U$ together with the derivatives of the u variables up to order n.

The theory of jet bundles is developed extensively in Ref. 4. Briefly, the construction involves considering $C^\infty(X,U)$ and taking the equivalence relation defined by *$f\sim g$ if f and g have identical Taylor polynomial to nth order*.

In Ref. 4 it is shown that under this equivalence relation $C^\infty(X,U)$ can be given the structure of a smooth manifold, denoted $J^n(X,U)$. Local coordinates on $J^n(X,U)$ are viewed as consisting of the x variables, the u variables, and the derivatives of u up to order n. We may then consider (2.1) as an algebraic equation on $J^n(X,U)$.

The flow generated by v is a symmetry group of (2.1) if the extension of v to $J^n(X,U)$ (called the nth prolongation of v, denoted $\mathrm{pr}^n v$), satisfies Lie's condition (see Theorem 2.1). $\mathrm{pr}^n v$ may be calculated from v by essentially requiring that the chain rule hold. An explicit formula for $\mathrm{pr}^n v$ was found by Olver and is given in Ref. 1 (pp. 108–117).

Lie's condition that v generate a symmetry of (2.1) may be stated as follows.

Theorem 2.1 (Lie): *A vector field v of the form (2.2) generates a local group of symmetries of (2.1) if and only if*

$$\mathrm{pr}^n v[P_\nu(x,D^\alpha)u]=0,$$

whenever u is a solution of (2.1).

Proof: See Ref. 1, Chap. 2.

Remark: In Craddock's thesis and in Refs. 2, 3 and 5, a new approach to the study of group symmetries was developed. This approach demonstrates that the local groups of symmetries which Lie's prolongation method yields may often be extended to global group actions by methods of representation theory.

Calculation of the flow associated with v is called exponentiating v; v generates a transformation that moves x and u to $\tilde{x}(x,u,\epsilon)$ and $\tilde{u}(x,u,\epsilon)$, respectively. The process of exponentiating v is straightforward. Given v of the form (2.2), we solve the first-order system of differential equations

$$\frac{d\tilde{x}_i}{d\epsilon}=\xi_i(\tilde{x},\tilde{u}),\quad \tilde{x}_i(0)=x_i,\quad i=1,2,...,n,$$

$$\frac{d\tilde{u}_j}{d\epsilon}=\phi^j(\tilde{x},\tilde{u}),\quad \tilde{u}^j(0)=u^j,\quad j=1,...,p.$$

Then the new solution is $\tilde{u}(\tilde{x})$. A convenient shorthand for this notation is to write

$$\rho(\exp \epsilon v)(u(x))=\tilde{u}(\tilde{x}).$$

Example 1: The one-dimensional heat equation

$$u_t=u_{xx} \tag{2.3}$$

was shown by Lie to have a six-dimensional Lie algebra of symmetries (cf. Ref. 1, p. 120ff).

A basis for this Lie algebra is

$$v_1=\frac{\partial}{\partial x},\quad v_2=\frac{\partial}{\partial t},\quad v_3=u\frac{\partial}{\partial u},\quad v_4=x\frac{\partial}{\partial x}+2t\frac{\partial}{\partial t}-\frac{1}{2}u\frac{\partial}{\partial u},$$

$$v_5=2t\frac{\partial}{\partial x}-xu\frac{\partial}{\partial u},\quad v_6=4xt\frac{\partial}{\partial x}+4t^2\frac{\partial}{\partial t}-(x^2+2t)u\frac{\partial}{\partial u}.$$

It is easy to show that v_6 exponentiates to produce an action on solutions given by

$$\rho(\exp \epsilon v_6)u(x,t)=\frac{1}{\sqrt{1+4\epsilon t}}\exp\left\{\frac{-\epsilon x^2}{1+4\epsilon t}\right\}u\left(\frac{x}{1+4\epsilon t},\frac{t}{1+4\epsilon t}\right).$$

Thus if u solves (2.3), so does $\rho(\exp \epsilon v_6)u$, at least for ϵ sufficiently small.

Note that $u=1$ solves (2.3). Therefore by symmetry so does

$$u=\frac{1}{\sqrt{1+4\epsilon t}}\exp\left\{\frac{-\epsilon x^2}{1+4\epsilon t}\right\}.$$

Translating t by $-(1/4\epsilon)$ and choosing $\epsilon=\pi$ gives the new solution

$$k_t(x)=\frac{1}{\sqrt{4\pi t}}\exp\left\{\frac{-x^2}{4t}\right\}.$$

Thus we have found the heat kernel for (2.3) by using a group transformation applied to the trivial solution $u=1$. This leads to an obvious question: Can we use symmetries to construct fundamental solutions from trivial solutions in some systematic manner for other equations? This question motivates the rest of this paper.

Symmetries generated by a vector field of the form (2.2) are known as point symmetries. We may also study generalized symmetries by considering generalized vector fields of the form

$$v=\sum_{i=1}^{n}\xi_i(x,u,D^\alpha u)\frac{\partial}{\partial x_i}+\sum_j \phi^J(x,u,D^\alpha u)\frac{\partial^{|J|}}{\partial u_{x_j}}, \tag{2.4}$$

where J ranges over a set of multi-indices and the derivatives in the second sum are with respect to u and with respect to the partial derivatives of u with respect to the x variables. The order of a generalized symmetry is the order of the highest derivative appearing in (2.4). For example,

$$v = xu_x \frac{\partial}{\partial x} + u_{xx} \frac{\partial}{\partial u} \tag{2.5}$$

is a generalized vector field of the second order.

When dealing with generalized symmetries it is convenient to employ the so-called evolutionary form of (2.4). One can replace v by a vector field of the form

$$v_Q = \sum_J Q_J(x, D^\alpha u) \frac{\partial}{\partial u_J}, \tag{2.6}$$

where

$$Q_J(x, D^\alpha) = \phi^J(x, u, D^\alpha u) - \sum_{i=1}^{n} \xi_i(x, u, D^\alpha u) u_i^J \tag{2.7}$$

in which $u_i^J = \partial u^J / \partial x_i$.

For example,

$$v = x \frac{\partial}{\partial x} + 2t \frac{\partial}{\partial t} \tag{2.8}$$

is equivalent to the evolutionary form

$$v_Q = -(xu_x + 2tu_t) \frac{\partial}{\partial u}. \tag{2.9}$$

Chapter 5 of Ref. 1 contains a detailed analysis of such symmetries. The *infinite* prolongation of v (denoted pr$v$) to an infinite jet bundle may be defined and a group of transformations associated with v constructed. The following theorem holds.

Theorem 2.2: *Let v be a generalized vector field of the form (2.4). Then the group of transformations associated with (2.4) is a local group of symmetries of (2.1) if and only if*

$$\mathrm{pr}v[P_\nu(x, D^\alpha u)] = 0,$$

whenever

$$P_\nu(x, D^\alpha) u = 0.$$

Proof: See Ref. 1, Chap. 5.

For the remainder of this work we restrict to the case where there is only one dependent variable u.

A major difficulty with generalized symmetries is that the group action arising from a generalized vector field may be very hard to calculate. Theoretically, one solves the initial value problem

$$\frac{\partial \tilde{u}}{\partial \epsilon} = Q(\tilde{x}, D^\alpha \tilde{u}) \tag{2.10}$$

with $\tilde{u}(\tilde{x}, 0) = u(x)$. For example, to determine the group action associated with $-u_x \partial / \partial u$, we solve

$$\frac{\partial \tilde{u}}{\partial \epsilon} = -\tilde{u}_{\tilde{x}} \tag{2.11}$$

with $\tilde{u}(\tilde{x},0)=u(x)$. In this instance we have $\tilde{u}(\tilde{x},\epsilon)=u(x-\epsilon)$.

However, the initial value problem (2.10) may be ill posed. Consequently many results on generalized symmetries are of a rather theoretical nature. One aim of this paper is to promote interest in such symmetries and introduce an approach to dealing with certain of these problems. We make the blanket assumption that (2.10) is well posed.

Computation of generalized symmetries, by which we shall mean vector fields satisfying the Lie condition of Theorem 2.2, is itself a rather difficult task. Techniques involving, for example, recursion operators are available. In addition if the order of the generalized symmetry is predetermined, one can find all generalized symmetries of that order for a given equation, though this may be computationally intensive. Nevertheless the general problem remains unsolved.

In Refs. 2 and 3, a new method of studying group symmetries was introduced and applied *inter alia* to the heat equation on $\mathbb{R}^n$, and to a number of other examples. The essence of this method is to observe that the groups determined by Lie's prolongation algorithm are very often equivalent to the action of a representation of the corresponding Lie group on some space of functions (or possibly distributions).

To explain this remark, consider an evolution equation of the form

$$Pu = \frac{\partial u}{\partial t}, \tag{2.12}$$

where u is a function on $\mathbb{R}^n \times \mathbb{R}$ and P is a polynomial in $\{\partial/\partial x_i : i=1\cdots n\}$. Suppose that we can find a heat kernel for such an equation, that is a kernel K on $\mathbb{R}^n \times \mathbb{R}$ so that the integral

$$u(x,t) = \int_{\mathbb{R}^n} f(y)K(x-y,t)dy = (Af)(x,t)$$

converges for all $f \in L^2(\mathbb{R}^n)$ to a solution of (2.12). Then given any group S which admits a continuous representation π on $L^2(\mathbb{R}^n)$, the equation

$$\begin{aligned}(\sigma(s)u)(x,t) &= \int_{\mathbb{R}^n} (\pi(s)f)(y)K(x-y,t)dy \\ &= A(\pi(s)f)(x,t) \quad (s \in S)\end{aligned} \tag{2.13}$$

defines a symmetry of (2.12).

The content of Refs. 2 and 3 is essentially that the symmetries one computes by Lie's method are very often equivalent to representations of the underlying Lie group via the equivalence relation (2.13). That is, Lie's prolongation algorithm in a fundamental sense, constructs representations of a Lie group on some vector space of solutions of a (linear) PDE. Precisely how far the relation between Lie's method and representations of the underlying group goes will be the subject of a forthcoming paper.

A part of the value in using (2.13) to study symmetries lies in the fact that properties which may be somewhat difficult to understand on the left-hand side of (2.13) may be utterly transparent on the right-hand side. See the comments following Theorem 2.3 for an example.

In Ref. 2 it is shown that the group $G=H_3 \times \mathrm{SL}(2,\mathbb{R})$ is a global group of symmetries for the one-dimensional heat equation $u_{xx}=u_t$, and that the symmetries generated by the vector fields $\{v_1,\ldots,v_6\}$ of example 1 are intertwined by this method with an analytic continuation of the Segal–Shale–Weil representation of G. In this case, every Segal–Shale–Weil induced symmetry is a point symmetry. (The one arising from the Weyl element maps the constant solution of the heat equation to the fundamental solution.)

However, for other equations and for other representations on $L^2(\mathbb{R}^n)$, the symmetries induced in this way will typically be generalized symmetries. We also remark that since they are presented in ''exponentiated form,'' this suggests an approach to finding the exponentials of generalized symmetries.

Before considering the case of a general Lie group, let us exemplify the concluding remarks of the previous paragraph. Consider the linearized KdV equation

$$u_{xxx}=u_t. \tag{2.14}$$

Lie's prolongation algorithm may be applied to find a basis of four vector fields for the Lie algebra of point symmetries; $v_1=\partial/\partial x$, $v_2=\partial/\partial t$, $v_3=x(\partial/\partial x)+3(\partial/\partial t)$, $v_4=u(\partial/\partial u)$. Thus, if u solves (2.2), so do $u(x-\epsilon,t),u(x,t-\epsilon),u(e^{\epsilon},e^{3\epsilon}t),e^{\epsilon}u(x,t)$.

Standard Fourier transform methods allow us to write the solution of (2.14) as

$$Af(x,t)=\frac{1}{2\pi}\int_{-\infty}^{\infty} f(\xi)\exp\{-i\xi^3t+i\xi x\}d\xi.$$

This integral can be shown to converge for $f\in L^1(\mathbb{R})$ and can also be extended by a density argument to $L^2(\mathbb{R})$.

We now construct the symmetry that translation on $L^2(\mathbb{R})$ yields. Let $(\pi(\epsilon)f)(y)=f(y-\epsilon)$. Then

$$(\sigma(\epsilon)u)(x,t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}(\pi(\epsilon))f(y)\exp\{-iy^3t+iyx\}dy$$

$$=\frac{1}{2\pi}e^{i\epsilon x-i\epsilon^3t}\int_{-\infty}^{\infty}(f(s)e^{3it\epsilon s^2-is^3t})e^{isz}\,ds,$$

where $z=x-3\epsilon^2t$. Thus

$$(\sigma(\epsilon)u)(x,t)=e^{i\epsilon x-i\epsilon^3t}\int_{-\infty}^{\infty}u(x-3\epsilon^2t-y,t)K_{3i\epsilon t}(y)dy,$$

where

$$\int_{-\infty}^{\infty}e^{3it\epsilon s^2+ix}\,ds=\frac{1}{\sqrt{12\epsilon it}}\exp\left\{\frac{ix^2}{12\epsilon t}\right\}=K_{3\epsilon it}(x).$$

Differentiating with respect to ϵ and setting $\epsilon=0$, gives the characteristic for the evolutionary form of the vector field, v_Q generating this symmetry,

$$\left.\frac{d}{d\epsilon}(\sigma(\epsilon)u)(x,t)\right|_{\epsilon=0}=ixu+3it\frac{\partial^2u}{\partial x^2}.$$

Thus, the vector field generating the symmetry $\sigma(\epsilon)$ has evolutionary form $v_Q=i(xu+3tu_{xx})\times(\partial/\partial u)$. This does not reduce to a standard vector field. It is therefore a generalized symmetry.

This example suggests two things. First, at the level of group representations, there seems to be no difference between a point symmetry and a generalized symmetry. Second, since the group representation method gives us symmetries in exponentiated form, we may hope to use it to exponentiate generalized symmetries. As an example take the heat equation $u_t=u_{xx}$. We have a generalized symmetry

$$v_Q = u_{xxx}\frac{\partial}{\partial u}.$$

If

$$u(x,t) = \int_{-\infty}^{\infty} \phi(y) e^{-y^2 t + iyx}\, dy \quad \text{for } \phi \in L^2(\mathbb{R}),$$

then

$$\frac{\partial^3 u}{\partial x^3} = -i \int_{-\infty}^{\infty} y^3 \phi(y) e^{-y^2 t + iyx}\, dy.$$

Now if

$$\rho(\exp \epsilon v_Q) u(x,t) = \int_{-\infty}^{\infty} (R(\epsilon)\phi)(y) e^{-y^2 t + iyx}\, dy,$$

where $R(\epsilon)$ is a representation of a one parameter group, and v_Q generates this one parameter group, then we have

$$u_{xxx} = \frac{d}{d\epsilon}\rho(\epsilon)u(x,t)\bigg|_{\epsilon=0} = \int_{-\infty}^{\infty} \left(\frac{dR(\epsilon)}{d\epsilon}\phi\right)(y) e^{-y^2 t + iyx}\, dy \bigg|_{\epsilon=0}$$

$$= -i \int_{-\infty}^{\infty} y^3 \phi(y) e^{-y^2 t + iyx}\, dy.$$

If we take $(R(\epsilon)\phi)(y) = e^{-i\epsilon y^3}\phi(y)$, then we have effectively exponentiated v_Q:

$$\rho(\exp \epsilon v_Q) u(x,t) = \int_{-\infty}^{\infty} e^{-i\epsilon y^3} \phi(y) e^{-y^2 t + iyx}\, dy$$

$$= \frac{1}{(3\epsilon)^{1/3}} \int_{-\infty}^{\infty} u(x-y,t)\, \mathrm{Ai}\left(\frac{y}{(3\epsilon)^{1/3}}\right) dy,$$

where Ai is an Airy function of the first kind.

Obviously one might have obtained this result by standard techniques, and our method is certainly not completely rigorous or general, but it offers an interesting way to study the problem.

We now set up a version of the group representation approach which holds for equations more general than the heat equation on $\mathbb{R}$, and in particular applies to a range of sub-Laplacians on Lie groups.

Theorem 2.3: *Let X and U be manifolds, and suppose that*

$$P(x, u, u_{x_1}, \ldots, u_{x_1 x_1}, \ldots) = 0 \tag{2.15}$$

is a differential equation on $J^n(X,U)$. Suppose further that there exists a connected submanifold $X_1 \subset X$ a measure μ on X_1 and a kernel function $K(x,y)$ so that for all $f \in L^2(X_1, \mu)$, the integral $Af(x) = \int_{X_1} K(x,y) f(y)\, d\mu(y)$ converges to a solution of (2.15).

Let G be a Lie group which possesses a representation $\{\pi, L^2(X_1, \mu)\}$. Then G is a global group of symmetries for (2.15).

Proof: The proof is little more than an observation. Since $(\pi(g)f)(y) \in L^2(X_1, \mu)$ whenever $f \in L^2(X_1, \mu)$, then we may define a symmetry of (2.15) as we did above, i.e.,

$$(\sigma(g)u)(y)=(A\pi(g)f)(y).$$

■

Remark: This result immediately implies that any equation for which we may compute solutions by $u(x)=Af(x)$, $f\in L^2(\mu)$, $A\in\mathcal{B}(L^2(\mu))$ must have infinitely many group symmetries, since there are obviously infinitely many group actions on $L^2(\mu)$ which can be used to construct symmetries. In practice, usually all but finitely many are generalized symmetries, though equations with infinitely many point symmetries exist. The two-dimensional Laplace equation is the best known example (see Ref. 3). We remark that the existence of an infinite-dimensional symmetry group is closely related to the linearization of a partial differential equation. See Ref. 6, Chap. 6, for more on this important topic. In fact this result is more general. Any PDE which is integrable in the sense that it possesses a mapping from some vector space of functions (or distributions) into its solution space, will have infinitely many symmetries by the above construction. Conversely, any equation which does not have infinitely many symmetries cannot be integrable in this particular sense. These symmetries, generalized and otherwise can be explicitly constructed by Lie's prolongation algorithm. This illustrates how the group representation approach can make certain symmetry properties transparent. The existence of infinitely many group symmetries for a PDE satisfying the given conditions is far from clear with the prolongation approach, but it is obvious if we use the representation theory method.

We now let G be a Lie group with Lie algebra $\mathfrak{g}$. Suppose that $X_1,\ldots,X_n\in\mathfrak{g}$ are left invariant vector fields which generate the Lie algebra in the sense that their successive brackets span $\mathfrak{g}$. The operator $\mathcal{L}=\Sigma_{i=1}^n X_i^2$ is then a sub-Laplacian and satisfies the Hörmander condition on G. The associated heat equation

$$\left(\frac{\partial}{\partial t}-\mathcal{L}\right)u(x,t)=0,\quad (x,t)\in G\times(0,\infty) \tag{2.16}$$

has been the object of intensive study, starting from Hunt's paper[7]—see also Refs. 8, 9, and 10. In fact, Folland[11] shows that there exists a unique function $h\in C^\infty(G\times(0,\infty))$ such that

$$\text{(a)}\quad \int_G h_t(x)dx=1,\quad \text{(b)}\quad h(x,t)\geqslant 0,\quad \text{(c)}\quad h(x,t)=h(x^{-1},t),$$

and (d) for all $f\in L^p(1\leqslant p<\infty)$, the function $u(x,t)=h_t*f(x)$ solves (2.16) with initial condition $u(x,0)=f(x)$. As usual, $h_t(x)=h(x,t)$; we shall refer to h_t as the heat kernel for $\mathcal{L}$.

Now consider the group acting by the left regular representations on say $\mathcal{S}(G)$ (assuming G has a well-defined Schwartz space and the left regular action preserves it). Since the left regular action commutes with convolution, we see that if $u(x,t)=(h_t*f)(x)$ is a solution, then so is $(\sigma(g)u)$ given by $h_t*\lambda(g)f(x)=\Delta(g)^{-1}u(g^{-1}x,t)$ where Δ is the modular function of G. Obviously many interesting symmetries may be constructed in this way as the example of the linearized KdV equation, presented above, demonstrates. Since $h_t\in C^\infty$, we may also obtain distributional solutions of (2.16) by allowing u to be defined by $h_t*\phi$, where ϕ is a distribution of compact support. Substituting in the Dirac delta for ϕ gives us h_t as a distributional solution. On the other hand, any continuous mapping $\mathcal{S}'(G)\to\mathcal{S}'(G)$ gives a (possibly generalized) symmetry of (2.16). Thus, if there is a continuous invertible mapping ψ: $\mathcal{S}'(G)\to\mathcal{S}'(G)$ so that $\psi(\delta_a)=1$, the symmetry $\sigma_{\psi^{-1}}$ necessarily maps the constant to the fundamental solution. In the case where $G=\mathbb{R}^n$, the Fourier transform provides such a transformation.

In fact, since the topology of $S(G)$ is defined only by the topological nature of G and not by its group structure, such an operator will exist whenever G is homeomorphic to $\mathbb{R}^n$. In particular, this holds if G is a simply connected nilpotent Lie group: in this case, the exponential map is a bijection of $\mathfrak{g}$ onto G. Thus, we can state

Theorem 2.4: *Let G be a simply connected nilpotent Lie group, and let $\mathcal{L}$ be a sub-Laplacian on G satisfying the Hörmander condition. Then there exists a generalized vector field v generating a symmetry of $\mathcal{L}-(\partial/\partial t)$ which carries the constant solution to the heat kernel.*

Proof: The preceding remarks clearly justify the result. However, let us explicitly exhibit such a generalized vector field arising from a specific action of $\mathrm{SL}_2(\mathbb{R})$. The calculation will be useful in what follows. Let H be a simply connected nilpotent Lie group homeomorphic to $\mathbb{R}^n$ and let the heat kernel be $h_t(x)$. Set

$$u(x,t)=\int_H f(y)h_t(y^{-1}x)dy. \tag{2.17}$$

Now consider a basis for the Lie algebra $\mathfrak{sl}_2$

$$k_1=\begin{pmatrix}0 & 2\\ 0 & 0\end{pmatrix},\quad k_2=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},\quad k_3=\begin{pmatrix}0 & 0\\ -2 & 0\end{pmatrix}$$

and a representation of $\mathrm{SL}_2(\mathbb{R})$ on $L^2(H)$ identified with $L^2(\mathbb{R}^n)$ defined by

$$R\begin{pmatrix}1 & b\\ 0 & 1\end{pmatrix}f(y)=e^{-ib|y|^2}f(y), \tag{2.18}$$

$$R\begin{pmatrix}a & 0\\ 0 & a^{-1}\end{pmatrix}f(y)=a^{n/2}f(ay), \tag{2.19}$$

$$R\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}f(y)=\hat{f}(y), \tag{2.20}$$

where $a>0$ and $\hat{f}$ is the Fourier transform of f. [In (2.19) we are assuming that there is a well-defined action of $\mathbb{R}^+$ on H.] R defines the so-called Segal–Shale–Weil representation of $\mathrm{SL}_2(\mathbb{R})$. In fact it is a projective representation if n is odd. Usually one thinks of it as a representation of the *double cover* of $\mathrm{SL}_2(\mathbb{R})$. See Ref. 2 for more details.

Consider the one parameter subgroup of $\mathrm{SL}_2(\mathbb{R})$ generated by (k_1+k_3). This is actually the subgroup of rotations about the origin. We define a symmetry of the heat equation by

$$\sigma\begin{pmatrix}\cos 2\epsilon & \sin 2\epsilon\\ -\sin 2\epsilon & \cos 2\epsilon\end{pmatrix}u(x,t)=\int_H R(\exp(\epsilon(k_1+k_3))f(y)h_t(y^{-1}x)dy. \tag{2.21}$$

Setting $\epsilon=\pi/4$, we obtain

$$\sigma\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}u(x,t)=\int_H \hat{f}(y)h_t(y^{-1}x)dy. \tag{2.22}$$

Thus if we take the solution with initial condition $u(x,0)=1$ this symmetry ''rotates'' (in some sense) the solution to one with initial condition $u(x,0)=\delta(x)$. That is, it takes the constant solution to the fundamental solution. If we assume suitable smoothness properties for f and differentiate both sides of (2.21) with respect to ϵ and set $\epsilon=0$ we obtain

$$v(u)=\int_H (k_1+k_3)(f)(y)h_t(y^{-1}x)dy \tag{2.23}$$

in which v is an operator acting on u which corresponds to k_1+k_3 acting on f. In local coordinates we may write

$$v(u)=Q(x,D^{\alpha}u)\frac{\partial}{\partial u}u \tag{2.24}$$

for some function Q. v is then the evolutionary representative of a generalized symmetry which maps the constant solution to the fundamental solution for $\epsilon=\pi/4$.

The question of when there is a point symmetry with this property has motivated the remainder of the paper.

Remark 1: Theorem 2.4 guarantees for a large class of equations the existence of a symmetry that maps the constant solution of some heat equation to the heat kernel. Obviously it would be useful to know what the particular symmetry is for a given equation. Then one could identify the heat kernel by a group transformation of the constant solution. Unfortunately this result does not tell us whether or not the symmetry is a point symmetry, as is the case for the heat equation on $\mathbb{R}$, or whether it is a generalized symmetry.

Remark 2: Theorem 2.4 may be extended to equations other than the heat equation. All that is required is a suitable integral kernel for an operator $Pu=0$. We will not however consider such equations.

The proof of Theorem 2.4 suggests that if we wish to obtain the heat kernel from the constant solution by symmetry we should try to find an element of the Lie algebra of symmetries which corresponds to the element k_1+k_3 in $\mathfrak{sl}_2$. Below we will do precisely this for a class of heat equations with drift on the real line, and we will show that for these equations, the element corresponding to k_1+k_3 of $\mathfrak{sl}_2$ does indeed produce the heat kernel. The symmetries accomplishing the transformation will turn out to be point symmetries.

III. HEAT KERNELS ON $\mathbb{R}^n$

Let us now present some examples of how the heat kernel may sometimes be obtained by the method described above. We study the following equations.

(1) The heat equation

$$\frac{\partial u}{\partial t}=\Delta u \quad \text{on } \mathbb{R}^n.$$

(2) The Fokker–Planck equation

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+\frac{\partial}{\partial x}(xu).$$

(3) The harmonic oscillator

$$-\frac{\partial u}{\partial t}=-\frac{1}{2}\frac{\partial^2 u}{\partial x^2}+\frac{1}{2}(x^2-1)u.$$

The heat kernel for the harmonic oscillator is given by Mehler's formula.[12] We will derive Mehler's formula by an elegant symmetry group calculation which should illustrate how effective Lie group techniques can be for determining fundamental solutions.

(1) The heat equation

$$\frac{\partial u}{\partial t}=\Delta u$$

has symmetry group $G=H_{2n+1}\rtimes(\mathrm{SL}(2,\mathbb{R})\times\mathrm{SO}(n))$ (see Craddock[2]). A basis for the Lie algebra of symmetries was found by Goff.[13] Details of the calculation of symmetries in the $n=1$ case may be found in Ref. 1. It can be shown that the vector fields

$$v_1=\frac{\partial}{\partial t} \quad \text{and} \quad v_2=4\sum_{i=1}^{n} x_i t\frac{\partial}{\partial x_i}+4t^2\frac{\partial}{\partial t}-\left(\sum_{i=1}^{n} x_i^2+2nt\right)u\frac{\partial}{\partial u}$$

generate symmetries, and further, by examining the commutator tables we establish the existence of a Lie algebra isomorphism taking k_1+k_3 to v_1+v_2. Thus exponentiating v_1+v_2 and setting $\epsilon=\pi/4$ should produce a symmetry which maps the solution of the heat equation with $u(x,0)=f(x)$ to the solution with $u(x,0)=\hat{f}(x)$.

Let us exhibit the $n=1$ case, and leave the general case to the interested reader. We need to exponentiate

$$v=4xt\frac{\partial}{\partial x}+(1+4t^2)\frac{\partial}{\partial t}-(x^2+2t)u\frac{\partial}{\partial u}.$$

Elementary calculations show that the action generated by the above vector field is

$$\sigma(\exp \epsilon v)u(x,t)=\sqrt{\frac{\sec(\tan^{-1}(2t)-2\epsilon)}{\sec(\tan^{-1}(2t))}}\exp\left[-\frac{x^2(2t-\tan(\tan^{-1}(2t)-2\epsilon))}{2(1+4t^2)}\right]$$
$$\times u\left(\frac{x\sec(\tan^{-1}(2t)-2\epsilon)}{\sqrt{1+4t^2}},\frac{1}{2}\tan(\tan^{-1}(2t)-2\epsilon)\right). \tag{3.1}$$

To obtain the solution of the one-dimensional heat equation with initial data $u(x,0)=\hat{f}(x)$ from the solution with $u(x,0)=f(x)$ we must set $\epsilon=\pi/4$. This gives

$$\sigma\left(\exp\frac{\pi}{4}v\right)u(x,t)=\frac{1}{\sqrt{2t}}\exp\left(-\frac{x^2}{4t}\right)u\left(\frac{x}{2t},-\frac{1}{4t}\right). \tag{3.2}$$

Using (3.2) and taking $u(x,t)=1/\sqrt{2\pi}$ we find the solution with initial data $u(x,0)=\delta(x)$ to be

$$k(x,t)=\frac{1}{\sqrt{4\pi t}}e^{-(x^2/4t)},$$

which is of course the fundamental solution of the heat equation.

It is not difficult to see that this result may also be obtained by applying first the group action arising from v_2 and then the group action arising from v_1 as described in the introduction. In fact it is frequently computationally easier to do this. With experience, one can often see from the form of the vector fields and their corresponding group actions, which ones will lead to the fundamental solution. To determine the heat kernel we simply perform the group translation $x\to x-y$ which arises from the vector field $\partial/\partial x$.

(2) Next we consider the Fokker–Planck equation

$$\frac{\partial u}{\partial t}=\frac{\partial^2}{\partial x^2}+x\frac{\partial u}{\partial x}+u. \tag{3.3}$$

Bluman and Cole[14] calculated the group of symmetries for the Fokker–Planck equation. This equation, and the harmonic oscillator equation which follow, lie somewhat outside the methodology which we have so far described. This is because they do not possess constant solutions. Nevertheless, we can perform the symmetry analysis and obtain the fundamental solution and heat kernel from ''time independent'' solutions. We may once more obtain the heat kernel by identifying an element of the Lie algebra of symmetries corresponding to the element k_1+k_3 of $\mathfrak{sl}_2$. However, it is quicker to use successive transformations by appropriate symmetries.

We use the fact that

$$v_1 = e^{-t}\partial/\partial x \quad \text{and} \quad v_5 = -xe^{-2t}\frac{\partial}{\partial x} + e^{-2t}\frac{\partial}{\partial y} + e^{-2t}u\frac{\partial}{\partial u}$$

generate symmetries. So if $u(x,t)$ is a solution of the Fokker–Planck equation then so are

$$\rho(\exp \epsilon v_1)u(x,t) = u(x - \epsilon e^{-t}, t)$$

and

$$\rho(\exp \epsilon v_5)u(x,t) = \frac{e^t}{\sqrt{e^{2t} - 2\epsilon}} u\left(\frac{x}{1 - 2\epsilon e^{-2t}}, \frac{1}{2}\log(e^{2t} - 2\epsilon) \right).$$

A solution of

$$\frac{\partial^2}{\partial x^2} + x\frac{\partial u}{\partial x} + u = 0$$

is $u_0(x) = e^{-x/2}$. Thus

$$\rho(\exp \epsilon v_5)u_0 = \frac{e^t}{\sqrt{e^{2t} - 2\epsilon}} \exp\left\{ \frac{-x^2}{2(1 - 2\epsilon e^{-2t})} \right\}$$

$$= \frac{e^t}{\sqrt{e^{2t} - 2\epsilon}} \exp\left\{ \frac{-x^2 e^{2t}}{2(e^{2t} - 2\epsilon)} \right\}$$

is also a solution of the Fokker–Planck equation. Setting $\epsilon = 1/2$, we obtain the solution

$$K(t,x,0) = \frac{e^t}{\sqrt{e^{2t} - 1}} \exp\left\{ \frac{-x^2 e^{2t}}{2(e^{2t} - 1)} \right\}.$$

We now wish to obtain the full heat kernel. Below we will explain how this is done in more detail. For now, we remark that letting $x \to x - ye^{-t}$ yields the new solution

$$K(t,x,y) = \frac{e^t}{\sqrt{e^{2t} - 1}} \exp\left\{ \frac{-(x - ye^{-t})^2 e^{2t}}{2(e^{2t} - 1)} \right\}.$$

This is, up to a multiplicative constant, the desired heat kernel. A fact which may be readily checked by a Fourier transform calculation, which converts the Fokker–Plank equation into a simple first-order linear PDE.

(3) As our final example, we show how to derive Mehler's formula for the harmonic oscillator. The equation

$$-\frac{\partial u}{\partial t} = -\frac{1}{2}\frac{\partial^2 u}{\partial x^2} + \frac{1}{2}(x^2 - 1)u \tag{3.4}$$

is known to have heat kernel given by Mehler's formula (see Ref. 12, p. 113):

$$K(t,x,y) = \{\pi(1 - e^{-2t})\}^{-1/2} \exp\left\{ \frac{4xye^{-t} - (x^2 + y^2)(1 + e^{-2t})}{2(1 - e^{-2t})} \right\}.$$

Equation (3.4) does not have a constant solution. Nevertheless it has the stationary solution $u_0(x)=e^{-(x^2/2)}$. We will show that there exists a point symmetry taking $u_0(x)$ to $K(t,x,0)$.

Following the usual procedure for computing symmetry groups, we find that if

$$v=\xi(x,t,u)\partial/\partial x+\tau(x,t,u)\partial/\partial t+\phi(x,t,u)\partial/\partial u$$

generates a symmetry then

$$\begin{aligned}-(\phi_t-\xi_t)u_x+(\phi_u-\tau_t)(-\tfrac{1}{2}u_{xx}+\tfrac{1}{2}(x^2-1)u)\\ =-\tfrac{1}{2}(\phi_{xx}+(2\phi_{xu}-\xi_{xx})u_x-\tau_{xx}u_t+(\phi_{uu}-2\xi_{xu})u\\ -2\tau_x u_{xt}+(\phi_u-2\xi_x)u_{xx})+\tfrac{1}{2}(x^2-1)\phi+xu\xi,\end{aligned}$$

where we may take $\tau_u=\xi_u=0$ since (3.4) is linear.

A straightforward calculation shows that a basis for the Lie algebra of symmetries is

$$v_1=xe^{2t}\partial/\partial x+e^{-2t}\partial/\partial t+(x^2-1)e^{-2t}u\partial/\partial u,$$

$$v_2=-xe^{2t}\frac{\partial}{\partial x}+e^{2t}\frac{\partial}{\partial t}+x^2e^{2t}u\frac{\partial}{\partial u},$$

$$v_3=\frac{\partial}{\partial t},$$

$$v_4=e^{-t}\frac{\partial}{\partial x}+xe^{-t}u\frac{\partial}{\partial u},$$

$$v_5=e^{t}\frac{\partial}{\partial x}-xe^{t}u\frac{\partial}{\partial u},$$

$$v_6=u\frac{\partial}{\partial u}.$$

It is not hard to show that these vector fields form a basis for the Lie algebra $\mathfrak{h}_3\oplus\mathfrak{sl}_2$, where $\mathfrak{h}_3$ is the Lie algebra of the three-dimensional Heisenberg group. Exponentiating $\{v_1,\ldots,v_6\}$ we find that if $u(x,t)$ is a solution of (3.3) then so are

$$\rho(\exp\epsilon v_1)u(x,t)=\frac{1}{\sqrt{1+2\epsilon e^{-2t}}}\exp\left\{\frac{\epsilon e^{-2t}x^2}{1+2\epsilon e^{-2t}}\right\}u\left(\frac{x}{\sqrt{1+2\epsilon e^{-2t}}},\frac{1}{2}\ln\left(\frac{e^{-2t}}{1+2\epsilon e^{-2t}}\right)\right),$$

$$\rho(\exp\epsilon v_2)u(x,t)=\exp\left\{\frac{\epsilon x^2}{e^{-2t}-2\epsilon}\right\}u\left(\frac{xe^t}{\sqrt{e^{-2t}-2\epsilon}},\frac{1}{2}\ln(e^{-2t}-2\epsilon)\right),$$

$$\rho(\exp\epsilon v_3)u(x,t)=u(x,t-\epsilon),$$

$$\rho(\exp\epsilon v_4)u(x,t)=\exp\left\{\epsilon xe^{-t}-\frac{\epsilon^2}{2}e^{-2t}\right\}u(x,\epsilon e^{-t},t),$$

$$\rho(\exp\epsilon v_5)u(x,t)=\exp\left\{-\epsilon xe^{t}+\frac{\epsilon^2}{2}e^{2t}\right\}u(x-\epsilon e^{t},t),$$

$$\rho(\exp\epsilon v_6)u(x,t)=e^{\epsilon}u(x,t).$$

The element of the Lie algebra of symmetries which corresponds to k_1+k_3 is v_2+v_1. However we really only need the action of v_1. Observe that

$$\rho(\exp \epsilon v_1)u_0=\frac{1}{\sqrt{1+2\epsilon e^{-2t}}}\exp\left\{\frac{\epsilon e^{-2t}x^2}{1+2\epsilon e^{-2t}}\right\}\exp\left(\frac{-x^2}{2(1+2\epsilon e^{-2t})}\right)$$

$$=\frac{1}{\sqrt{1+2\epsilon e^{-2t}}}\exp\left\{\frac{-x^2(1-2\epsilon e^{-2t})}{2(1+2\epsilon e^{-2t})}\right\}, \quad \text{put } 2\epsilon=-1$$

$$=\frac{1}{\sqrt{1-e^{-2t}}}\exp\left\{\frac{-x^2(1+e^{-2t})}{2(1-e^{-2t})}\right\}$$

which is Mehler's formula for $y=0$.

The question remains as to how we translate $K(t,x,0)$ to give $K(t,x,y)$. Let us look at the problem in a more general setting. Consider an elliptic operator H, such that the semigroup e^{-tH} has a convolution kernel $K(t,x,y)$. If $f\in L^2(\mathbb{R}^n)$, then

$$u(x,t)=\int_{\mathbb{R}^n} f(y)K(t,x,y)dy$$

is a solution of

$$\frac{\partial u}{\partial t}=-Hu \tag{3.5}$$

with $u(x,0)=f(x)$.

We know that we can define symmetries of (3.5) by considering a group G with a continuous representation $\{\pi,L^2(\mathbb{R}^n)\}$, and setting

$$(\rho(g)u)(x,t)=\int_{\mathbb{R}^n}(\pi(g)f)(y)K(t,x,y)dy.$$

Let us assume that we have a symmetry $\rho(g)$ such that if u_0 is a solution of

$$Hu=0,$$

then

$$(\rho(g)u_0)(x,t)=K(t,x,0).$$

Now consider the representation of $\mathbb{R}^n$ on $L^2(\mathbb{R}^n)$ given by

$$(\sigma(a)f)(y)=f(y-a).$$

If

$$u_0(x)=\int_{\mathbb{R}^n} f(y)K(t,x,y)dy,$$

and

$$(\rho(g)u_0)(x)=\int_{\mathbb{R}^n}(\pi(g)f)(y)K(t,x,y)dy=K(t,x,0),$$

then

$$(\pi(g)f)(y)=\delta(y).$$

Then, if we apply σ to $\rho(g)u$ we have

$$\begin{aligned}(\sigma(a)\rho(g)u_0)(x,t)&=\int_{\mathbb{R}^n}(\sigma(a)\delta)(y)K(t,x,y)dy\\&=\int_{\mathbb{R}^n}\delta(y-a)K(t,x,y)dy\\&=K(t,x,a).\end{aligned}$$

Clearly, the symmetry that takes $K(t,x,0)$ to $K(t,x,y)$ is the one that is equivalent to the translation representation σ of $\mathbb{R}^n$.

If we look at the heat equation on $\mathbb{R}$ we see that the constant solution is mapped to $K(t,x)=(1/\sqrt{4\pi t})\exp\{-x^2/4t\}$ and that the convolution kernel is given by translating x by y. That is

$$K(t,x,y)=\rho(\exp yv_1)K(t,x,0),$$

where $v_1=\partial/\partial x$ generates the translational symmetry of the heat equation.

For the Fokker–Planck equation we see that a solution of $Hu=0$ can be mapped to $K(t,x,0)$ and

$$\rho(\exp yv_1)K(t,x,0)=K(t,x,y),$$

where $v_1=e^{-t}\partial/\partial x$ generates the symmetry $x\to x-\epsilon e^{-t}$. Now the Lie algebra of point symmetries of the heat equation and the Fokker–Planck equation are isomorphic (see Ref. 2). At the level of the Lie algebra $e^{-t}\partial/\partial x$ is equivalent to $\partial/\partial x$. That is $v_1=e^{-t}\partial/\partial x$, generates the symmetry which is equivalent to translation on $\mathbb{R}$.

We now need to determine which element of the symmetry algebra for the harmonic oscillator is equivalent to translation. The easiest way to do this is to compute the commutator table and compare with the table for the Lie algebra $\mathfrak{h}_3\oplus\mathfrak{sl}_2$. In this way it can be shown that the desired element of the symmetry algebra is $\frac{1}{2}(v_5-v_4)=v$. If we use ρ to denote the action of v on solutions then

$$\rho(\exp yv)u(x,t)=\exp\left\{\frac{-yxe^{t}+yxe^{-t}}{2}-\frac{y^2}{8}(e^{2t}-e^{-2t})\right\}u\left(x-\frac{1}{2}y(e^{t}+e^{-t}),t\right).$$

Applying $\rho(\exp yv)$ to the function $K(t,x,0)$ calculated above must give $K(t,x,y)$. A straightforward calculation yields

$$\rho(\exp yv)K(t,x,0)=\frac{1}{\sqrt{1-e^{-2t}}}\exp\left(\frac{4xye^{-t}-(x^2+y^2)(1+e^{-2t})}{2(1-e^{-2t})}\right).\tag{3.6}$$

Up to a multiplicative constant, this is indeed the heat kernel. Thus we have obtained Mehler's formula for the harmonic oscillator by group translation of a stationary solution.

The process of computing the heat kernel for $\partial u/\partial t=Hu$ from a point symmetry calculation should now be clear. We begin by finding solutions of

$$Hu=0.\tag{3.7}$$

We determine the symmetry which takes a solution u_0 of (3.7) to $K(t,x,0)$. $K(t,x,0)$ is then shifted to $K(t,x,y)$ by an appropriate group translation. We encapsulate this result in the following.

Theorem 3.5: *Let*

$$\frac{\partial u}{\partial t} = Hu \tag{3.8}$$

have heat kernel $K(t,x,y)$ such that for $f \in L^2(\mathbb{R}^n)$,

$$u(x,t) = \int_{\mathbb{R}^n} f(y)K(t,x,y)dy$$

solves (3.8) with $u(x,0) = f(x)$.

Assume that there exists a symmetry group G of (3.8) acting by ρ, such that if $u_0(x)$ is a solution of

$$Hu_0 = 0$$

then $\rho(g)u_0 = K(t,x,0)$.

Then $K(t,x,y)$ may be obtained by a further symmetry operation where the symmetry is defined by

$$\pi(a)u(x,t) = \int_{\mathbb{R}^n} f(y-a)K(t,x,y)dy$$

$$= \int_{\mathbb{R}^n} (\sigma(a)f)(y)K(t,x,y)dy.$$

So

$$(\pi(y)\rho(g)u_0)(x,t) = K(t,x,y).$$

Comment: We may of course relax the condition that $f \in L^2(\mathbb{R}^n)$. In fact it is frequently *necessary* to do so. The heat equation is an example of this, as described in Ref. 2.

Proof: If

$$(\rho(g)u_0)(x,t) = \int_{\mathbb{R}^n} f(y)K(t,x,y)dy$$

$$= K(t,x,0).$$

Then

$$(\pi(a)\rho(g)u)(x,t) = \int_{\mathbb{R}^n} f(y-a)K(t,x,y)dy$$

$$= \int_{\mathbb{R}^n} f(y)K(t,x,y+a)dy$$

$$= K(t,x,a).$$

Hence $(\pi(y)\rho(g)u)(x,t) = K(t,x,y)$. ■

Obviously the most important aspect of this problem is the existence of a symmetry taking a solution of $Hu=0$ to $K(t,x,0)$. Equations where this may be effected with a point symmetry are clearly of interest.

In the next section we will characterize the functions $f(x)$ so that there exists a point symmetry of

$$\frac{\partial u}{\partial t}=\frac{\partial^2 u}{\partial x^2}+f(x)\frac{\partial u}{\partial x}$$

taking the constant solution of $u_{xx}+f(x)u_x=0$ to $K(t,x,0)$.

IV. ONE-DIMENSIONAL HEAT KERNELS WITH DRIFT

In this section, we will give a characterization of one-dimensional heat equations with a drift term for which there exists a point symmetry taking the constant solution **1** to the fundamental solution. The equations we shall consider have the form

$$\frac{\partial^2 u}{\partial x^2}+f(x)\frac{\partial u}{\partial x}=\frac{\partial u}{\partial t}. \tag{4.1}$$

In the preceding sections we made use of the construction (2.13). If u is a solution of (4.1) and $K(t,x,y)$ is a kernel function such that for all $f\in L^2(\mathbb{R})\int_{\mathbb{R}}f(y)K(t,x,y)dy$ defines a solution of (4.1) then the relation

$$\sigma(g)u(x,t)=\int_{\mathbb{R}}\pi(g)f(y)K\,dy \tag{4.2}$$

with g in some appropriate locally compact group, defines symmetries of (4.1). $K(t,x,y)$ will typically be the heat kernel. We shall characterize those equations of the form (4.1) such that the kernel function $K(t,x,y)$ or at least $K(t,x,0)$ may be obtained by a point symmetry acting on the constant solution. To be clear, by ''heat kernel,'' we mean the kernel function K of (4.2). We should note that it is possible that the technique we develop here may work for similar equations. For example, those of the form $u_t=\mathcal{H}(u)$, where $\mathcal{H}$ is a formally self-adjoint differential operator.

We shall prove the following theorem.

Theorem 4.1: *There exists a point symmetry of (4.1) taking* **1** *to the fundamental solution if and only if f satisfies one of the following Ricatti equations:*

$$\text{(i)}\quad f'+\frac{1}{2}f^2=\frac{A}{x^2}-\frac{a}{2},$$

$$\text{(ii)}\quad f'+\frac{1}{2}f^2=\frac{1}{8}x^2+\frac{C}{x^2},$$

$$\text{(iii)}\quad f'+\frac{1}{2}f^2=\frac{C}{(x+2)^2},$$

$$\text{(iv)}\quad f'+\tfrac{1}{2}f^2=\tfrac{2}{3}Cx,$$

$$\text{(v)}\quad f'+\tfrac{1}{2}f^2=\tfrac{1}{2}Cx^2+D,$$

where A, C, D, a are arbitrary real numbers.

Before proving the result let us make the observation that these Ricatti equations have arisen in other contexts. Bluman derived conditions under which the fundamental solutions of certain Fokker–Plank equations on a finite interval may be obtained as *group invariant* solutions of

related boundary value problems, and obtained Ricatti equations similar to those listed in Theorem 4.1. The details may be found in Ref. 14. The interested reader may wish to compare our results with his.

Proof of the theorem: The point symmetry algebra of (4.1) is generated by

$$v=\xi\frac{\partial}{\partial x}+\tau\frac{\partial}{\partial t}+\phi\frac{\partial}{\partial u},$$

where

$$\mathrm{pr}^2 v[u_{xx}+f(x)u_x-u_t]=0.$$

This gives immediately, using the prolongation formula, the defining equations for ϕ, ξ, τ:

$$\phi^{xx}+f(x)\phi^x+f'(x)u_x\xi-\phi^t=0.$$

Now (4.1) is linear, so $\xi_u=\tau_u=0$. Hence we find

$$\begin{aligned}&\phi_{xx}+(2\phi_{xu}-\xi_{xx})u_x-\tau_{xx}(u_{xx}+f(x)u_x)+\phi_{uu}u_x^2+(\phi_u-2\xi_x)u_{xx}-2\tau_x u_{xt}\\&\quad+f(x)(\phi_x+(\phi_u-\xi_x)u_x-\tau_x(u_{xx}+f(x)u_x))+f'(x)u_x\xi\\&\quad=\phi_t-\xi_t u_x+(\phi_u-\tau_t)(u_{xx}+f(x)u_x),\end{aligned}$$

where we have used $u_t=u_{xx}+f(x)u_x$.

Thus we have the system of defining equations

$$\phi_{xx}+f(x)\phi_x=\phi_t,$$

$$2\phi_{xu}-\xi_{xx}-f(x)\tau_{xx}+f(x)(\phi_u-\xi_x)-f^2(x)\tau_x+f'(x)\xi=-\xi_t+f'(x)(\phi_u-\tau_t),$$

$$-\tau_{xx}+(\phi_u-2\xi_x)-f(x)\tau_x=(\phi_u-\tau_t),$$

$$-2\tau_x=0,$$

$$\phi_{uu}=0.$$

Now, if τ is constant, it is clear that the fundamental solution cannot arise from exponentiation of v. If τ is constant the symmetry only generates translations in time, so it clearly cannot map a constant, time independent solution to a time dependent solution. Hence, we seek conditions of f which yield a nontrivial τ.

From the equation $\phi_{uu}=0$, we see that $\phi=\alpha u+\beta$ where α and β both satisfy (4.1). Furthermore, the fact that $\tau_x=0$ tells us that $2\xi_x=\tau_t$, and hence we deduce that

$$\xi=\frac{x}{2}\tau_t+\rho(t)\quad\text{for some function}\quad\rho.$$

Now $\phi_{xu}=\alpha_x$, so we obtain from the second equation

$$2\alpha_x-f(x)\xi_x+f'(x)\xi=-\xi_t-f(x)\tau_t,$$

and substituting $\xi_x=\frac{1}{2}\tau_t$, we obtain

$$\begin{aligned}2\alpha_x&=\tfrac{1}{2}f(x)\tau_t-f'(x)(\tfrac{1}{2}x\tau_t+\rho(t))-\tfrac{1}{2}x\tau_{tt}-\rho'(t)-f(x)\tau_t\\&=-\tfrac{1}{2}f(x)\tau_t-\tfrac{1}{2}xf'(x)\tau_t-f'(x)\rho(t)-\tfrac{1}{2}x\tau_{tt}-\rho'(t).\end{aligned}$$

From this it follows that

$$2\alpha = -\tfrac{1}{2}xf(x)\tau_t - f(x)\rho(t) - \tfrac{1}{4}x^2\tau_{tt} - x\rho'(t) + \sigma(t)$$

for a suitable function σ, and hence

$$2\alpha_t = -\tfrac{1}{2}xf(x)\tau_{tt} - f(x)\rho'(t) - \tfrac{1}{4}x^2\tau_{ttt} - x\rho''(t) + \sigma'(t).$$

Since $2\alpha_{xx} + 2f(x)\alpha_x = 2\alpha_t$, and

$$2\alpha_{xx} = -\frac{1}{2}\frac{d^2}{dx^2}(xf(x))\tau_t - f''(x)\rho - \frac{1}{2}\tau_{tt}.$$

We must therefore have

$$-\frac{\tau_t}{2}(xf(x))'' - f''(x)\rho - \frac{1}{2}\tau_{tt} + f(x)\left(-\frac{1}{2}f(x)\tau_t - \frac{1}{2}xf'(x)\tau_t - f'(x)\rho(t) - \frac{1}{2}x\tau_{tt} - \rho'(t)\right)$$
$$= -\frac{1}{2}xf(x)\tau_{tt} - f(x)\rho'(t) - \frac{1}{4}x^2\tau_{ttt} - x\rho''(t) + \sigma'(t).$$

This equation gives a limited number of possibilities for f if we wish to have τ nontrivial. In fact, collecting terms in τ_t gives the coefficient

$$-\tfrac{1}{2}(xf)'' - \tfrac{1}{2}f^2 - \tfrac{1}{2}xff'(x)$$

since we can eliminate the $-\tfrac{1}{2}xf(x)\tau_{tt}$ from each side of the equation.

Careful examination shows that, τ will only be nontrivial if one of the following five cases occur: Clearly either (i) $\tau_{ttt}=0$ or (ii) $\tau_{ttt}\neq 0$. There are several subcases in (ii) viz: (a) $\rho=0$; (b) $\tau_t=\rho$, $\rho\neq 0$; (c) $\rho_{tt}=C\tau_t$; (d) $\tau_{ttt}=C\tau_t$, $\rho_{tt}=C\rho$, $\sigma_t=-D\tau_t-\tfrac{1}{2}\tau_{tt}$. Here C and D are constants. Determining the admissible equations for f is now straightforward. See the following cases for example.

Case (i) leads to the condition

$$-\tfrac{1}{2}(xf)'' - \tfrac{1}{2}f^2(x) - \tfrac{1}{2}xff' = a, \quad a \text{ constant.} \tag{4.3}$$

Case (ii)(a) gives

$$-\tfrac{1}{2}(xf)'' - \tfrac{1}{2}f^2 - \tfrac{1}{2}xff' = -\tfrac{1}{4}x^2. \tag{4.4}$$

We will analyze these two cases. Let us deal first with Eq. (4.3), which we may rewrite as

$$xf'' + xf'f + 2f' + f^2 = -2a.$$

Substituting $u = f' + \tfrac{1}{2}f^2$ we have $u' = f'' + f'f$, and the equation becomes $x(du/dx) + 2u = -2a$, which has solution $u = (A/x^2) - a$. Thus we obtain the Ricatti equation for f

$$f' + \frac{1}{2}f^2 = \frac{A}{x^2} - a.$$

In the case of Eq. (4.4), the substitution $u = f' + \tfrac{1}{2}f^2$ reduces the equation to $(d/dx)(x^2u) = x^3$, which has solution $u = \tfrac{1}{4}x^2 + (C/x^2)$, and so f satisfies

$$f' + \frac{1}{2}f^2 = \frac{1}{8}x^2 + \frac{C}{x^2}.$$

The remaining three cases may be dealt with similarly and are left to the reader. This completes the ''only if'' part of the proof.

We now proceed to prove the other direction. In order to achieve this, we need to show that if f satisfies the given Ricatti equations, then a point symmetry exists taking a constant solution to the fundamental solution. Detailing all possible cases would be a lengthy procedure. For brevity, we treat equation (i); the details of Eqs. (ii)–(v) are essentially identical and are left to the reader.

In case (i) we have $\tau_{ttt}=0$. So $\tau(t)$ has the form $\tau=c_2+2c_4t+4c_6t^2$. We thus have $\sigma_t'=-\frac{1}{2}\tau_{tt}+a\tau_t$ giving $\sigma=-4c_6(t-at^2)+2ac_4t$.

We need to determine ξ and ρ. If $f''+ff'=x$ then we must have $\rho=0$. Hence

$$\xi=\tfrac{1}{2}x(2c_4+8c_6t)=c_4x+4c_6xt$$

and

$$\begin{aligned}\alpha&=-\tfrac{1}{4}(xf)\tau_t-\tfrac{1}{8}\tau_{tt}+\tfrac{1}{2}\sigma\\&=-\tfrac{1}{4}(xf)(2c_4+8c_0t)-\tfrac{1}{8}x^2(8c_6)+ac_4t-2c_6(t-at^2)+c_3.\end{aligned}$$

Thus a basis for the Lie algebra of symmetries is

$$v_2=\partial/\partial t,\quad v_3=u\partial/\partial u,\quad v_4=x\partial/\partial x+2t\partial/\partial t-(\tfrac{1}{2}xf+at)u\partial/\partial u,$$

$$v_6=4xt\partial/\partial x+4t^2\partial/\partial t-(2xft+x^2+2t+2at^2)u\partial/\partial u.$$

It can easily be shown that v_2, v_4, v_6 generate a copy of $\mathfrak{sl}_2$ and that v_2+v_6 corresponds to the action of the subgroup of rotations about the origin. We will show that exponentiating v_2+v_6 gives the ''heat kernel'' at $y=0$ for (4.1), i.e., takes $u=1$ to $K_t(x,0)$.

To exponentiate v_2+v_6 we solve

$$\frac{d\tilde{x}}{d\epsilon}=4xt,\quad \frac{d\tilde{t}}{d\epsilon}=1+4\tilde{t}^2,\quad \frac{d\tilde{u}}{d\epsilon}=-(2xft+x^2+2t+2at^2)\tilde{u},$$

$$\tilde{x}(0)=x,\quad \tilde{t}(0)=t,\quad \tilde{u}(0)=u.$$

We obtain immediately

$$\tilde{x}=\frac{x\sec(2\epsilon+\tan^{-1}(2t))}{\sqrt{1+4t^2}},\quad \tilde{t}=\frac{1}{2}\tan(2\epsilon+\tan^{-1}(2t)).$$

Hence

$$\begin{aligned}\frac{d\tilde{u}}{\tilde{u}}=-\Bigg(&\frac{x\sec(2\epsilon+\tan^{-1}(2t))}{\sqrt{1+4t^2}}f\Bigg(\frac{x\sec(2\epsilon+\tan^{-1}(2t))}{\sqrt{1+4t^2}}\Bigg)\tan(2\epsilon+\tan^{-1}(2t))\\&+\frac{x^2\sec^2(2\epsilon+\tan^{-1}(2t))}{1+4t^2}+\tan(2\epsilon+\tan^{-1}(2t))+\frac{a}{2}\tan^2(2\epsilon+\tan^{-1}(2t))\Bigg)d\epsilon.\end{aligned}$$

Introduce the function F, such that $F'=f$. Elementary integration produces the function $\tilde{u}$ in terms of x, t, u, and ϵ. We rewrite this function in terms of $\tilde{x}$ and $\tilde{t}$ to conclude that if u is a solution of (4.1) for the given f, then so is

$$\tilde{u}=\exp\left(-\frac{1}{2}\left(F(x)-F\left(\frac{x\sec(\tan^{-1}(2t)-2\epsilon)}{\sqrt{1+4t^2}}\right)\right)-\frac{x^2[2t-\tan(\tan^{-1}(2t)-2\epsilon)]}{2(1+4t^2)}\right.$$
$$\left.-\frac{1}{2}\ln\left(\frac{\sqrt{1+4t^2}}{\sec(\tan^{-1}(2t)-2\epsilon)}\right)-\frac{a}{4}(2t-\tan(\tan^{-1}(2t)-2\epsilon)-2\epsilon)\right)$$
$$\times u\left(\frac{x\sec(\tan^{-1}(2t)-2\epsilon)}{\sqrt{1+4t^2}},\frac{1}{2}\tan(\tan^{-1}(2t)-2\epsilon)\right).$$

We now put $\epsilon=\pi/4$ and set $u=1/\sqrt{2\pi}$. We use the identities

$$\sec\left(\tan^{-1}(2t)-\frac{\pi}{2}\right)=\frac{\sqrt{1+4t^2}}{2t},\quad \tan\left(\tan^{-1}(2t)-\frac{\pi}{2}\right)=-\frac{1}{2t}.$$

The solution $u=1/\sqrt{2\pi}$ is mapped to the new solution

$$K_t(x)=\frac{1}{\sqrt{4\pi t}}\exp\left\{-\frac{1}{2}\left(F(x)-F\left(\frac{x}{2t}\right)\right)-\frac{x^2}{4t}-\frac{a(1+4t^2)}{8t}+\frac{a\pi}{8}\right\}.$$

The function $K_t(x)$ is the heat kernel at $y=0$ as may be readily checked. The case $\rho\neq 0$ is similar.

This proves the theorem for (i). The other cases proceed in a similar way. ■

The Ricatti equations of Theorem 4.1 may be linearized by introducing the substitution $f=2y'/y$. This allows the general solutions to be determined.

The Ricatti equations of Theorem 4.1 may be rewritten as

$$\text{(i)}\quad y''=\frac{1}{2}\left(\frac{A}{x^2}-\frac{a}{2}\right)y,$$

$$\text{(ii)}\quad y''=\frac{1}{2}\left(\frac{1}{8}x^2+\frac{C}{x^2}\right)y,$$

$$\text{(iii)}\quad y''=\frac{1}{2}\left(\frac{C}{(x+2)^2}\right)y,$$

$$\text{(iv)}\quad y''=\tfrac{1}{3}Cxy,$$

$$\text{(v)}\quad y''=\tfrac{1}{2}(\tfrac{1}{2}Cx^2+D)y.$$

We now list the general solutions:

$$\text{(i)}\quad y=B_1\sqrt{x}J_{-\sqrt{4+8A}/4}\left(\frac{\sqrt{\alpha}x}{2}\right)+B_2\sqrt{x}J_{\sqrt{4+8A}/4}\left(\frac{\sqrt{\alpha}x}{2}\right),$$

$$\text{(ii)}\quad y=B_1\sqrt{x}I_{-\frac{1}{8}\sqrt{4+8C}}\left(\frac{x^2}{8}\right)+B_2\sqrt{x}I_{\frac{1}{8}\sqrt{4+8C}}\left(\frac{x^2}{8}\right),$$

$$\text{(iii)}\quad y=B_1(8+8x+2x^2)^{1-\sqrt{1+2C}/4}+B_2(8+8x+2x^2)^{1+\sqrt{1+2C}/4},$$

$$\text{(iv)}\quad y=B_1\,\mathrm{Ai}\left(\frac{x}{(3C)^{\frac{1}{3}}}\right)+D_1B_i\left(\frac{x}{(3C)^{\frac{1}{3}}}\right),$$

$$\begin{aligned}\text{(v)}\quad y=\exp\Bigg\{&-\frac{1}{4}\Bigg(\frac{D+\sqrt{D^2-C(-2Dx^2-Cx^4)}}{\sqrt{C}}-\ln(-16C^2D\\&-16C^2\sqrt{D^2-C(-2Cx^2-Cx^4)})\Bigg)\Bigg\}(D\\&+\sqrt{D^2-C(-2Dx^2-Cx^4)})^{1/4}\\&\times\Bigg(B_1M\left(\frac{3}{4}-\frac{D}{4\sqrt{C}},\frac{3}{2},\frac{1}{2\sqrt{C}}(D+\sqrt{D^2-C(-2Cx-Cx^4)})\right)\\&+B_2U\left(\frac{3}{4}-\frac{D}{4\sqrt{C}},\frac{3}{2},\frac{1}{2\sqrt{C}}(D+\sqrt{D^2-C(-2Cx-Cx^4)})\right)\Bigg).\end{aligned}$$

Here, B_1, B_2, D_1 are constants. $J_a(z)$ and $I_a(z)$ are Bessel functions of the first kind; Ai and Bi are Airy functions; and $M(a,b,z)$, $U(a,b,z)$ are the hypergeometric functions as described in Abramowitz and Stegun (Ref. 15, Chap. 15). From these solutions we may determine all possible forms for f. An exhaustive analysis of these functions and the heat kernels to which they give rise is beyond the scope of this paper.

In fact we may solve the Ricatti equations in (i) through (v) for various cases to obtain easy derivations for heat kernels of many interesting equations of the form (4.1).

Consider (i) with $a=0$.

Then

$$f'+\frac{1}{2}f^2=\frac{A}{x^2}.$$

If $A=0$ then $f(x)=2/(x+c)$, $c=$constant. In this case $\tau_{tt}=0$ and in addition to $\{v_2,v_3,v_4,v_6\}$ given in the proof of the theorem we also have

$$v_1=\frac{\partial}{\partial x}-\frac{u}{x+c}\frac{\partial}{\partial u},$$

$$v_5=2t\frac{\partial}{\partial x}-\left(x+\frac{2t}{x+c}\right)u\frac{\partial}{\partial u}.$$

We can also solve for $A\neq 0$, provided $A=\frac{1}{2}a^2-a$, a is a constant. We obtain the following possibilities for f:

$$\text{(i)}\quad f=\frac{2}{x+c},$$

$$\text{(ii)}\quad f=\frac{a}{x},$$

$$\text{(iii)}\quad f=\frac{a}{x}+\frac{2(1-a)}{x+2c(1-a)x^{a}},\quad a\neq 1,\quad c \text{ constant},$$

$$\text{(iv)}\quad f=\frac{1}{x}+\frac{2}{2cx+x\ln x},\quad c \text{ constant}.$$

Let us collect some results together.

Corollary 4.2: For equation (4.1) and for each given $f(x)$, we have the following heat kernels:

$$\text{(i)}\quad f=\frac{2}{x+c},\quad K(t,x,0)=\frac{x}{(x+c)(4\pi t)^{3/2}}\exp\left\{\frac{-x^2}{4t}\right\},$$

$$\text{(ii)}\quad f=\frac{a}{x},\quad K(t,x,0)=\frac{1}{(4\pi t)^{(a+1)/2}}\exp\left\{\frac{-x^2}{4t}\right\},$$

$$\text{(iii)}\quad f=\frac{a}{x}+\frac{2(1-a)}{x(1+2c(1-a)x^{a-1})},\quad a\neq 1,$$

$$K(t,x,0)=\frac{1}{(4\pi t)^{(a+1)/2}}\left[1+\frac{x^{1-a}}{2x(1-a)}\right]\exp\left\{\frac{-x^2}{4t}\right\},$$

$$\text{(iv)}\quad f=\frac{1}{x}+\frac{2}{2cx+x\ln x},\quad K(t,x,0)=\frac{1}{4\pi t}\left[1-\frac{\ln(4\pi t)}{2c+\ln x}\right]\exp\left\{\frac{-x^2}{4t}\right\},$$

$$\text{(v)}\quad f=\frac{-\sqrt{\alpha}(1-Ae^{\sqrt{\alpha}x})}{1+Ae^{\sqrt{\alpha}x}},\quad \alpha>0,\quad A \text{ constant},$$

$$K(t,x,0)=\frac{1}{\sqrt{4\pi t}}\left(\frac{1+A\exp\sqrt{\alpha}x}{1+A\exp\left(\dfrac{\sqrt{\alpha}x}{4\pi t}\right)}\right)\exp\left\{\frac{-x^2}{4t}+\frac{\sqrt{\alpha}x}{2}-\frac{\sqrt{\alpha}x}{8\pi t}-\frac{\alpha\left(t-\dfrac{1}{4\pi}\right)^2}{2t}\right\}.$$

In some cases we can translate $K(t,x,0)$ to obtain $K(t,x,y)$ by picking an appropriate group translation. For example, for $f=2/(x+c)$,

$$K(t,x,y)=\left(1-\frac{y}{x+c}\right)K(t,x-y,0).$$

So, for example, $u_{xx}+(2/x)u_x=u_t$ has ''heat kernel''

$$K(t,x,y)=\frac{1}{(4\pi t)^{3/2}}(1-y/x)\exp\left\{\frac{-(x-y)^2}{4t}\right\}.$$

For $f=[-\sqrt{\alpha}(1-Ae^{\sqrt{\alpha}x})/(1+Ae^{\sqrt{\alpha}x})]$,

$$K(t,x,y)=e^{-\sqrt{\alpha}y/2}\left(\frac{1+Ae^{\sqrt{\alpha}x}}{1+Ae^{\sqrt{\alpha}(x-y)}}\right)K(t,x-y,0).$$

In cases where no such simple group translation exists as a point symmetry, we would need to seek a generalized symmetry to translate $K(t,x,0)$ to $K(t,x,y)$. We have not attempted to do this.

The interested reader may attempt to find other heat kernels by finding different solutions to (i) through (v).

V. HEAT KERNELS FOR OTHER FINITE-DIMENSIONAL LIE ALGEBRAS ON $\mathbb{R}$

In the preceding section, we considered those drift terms for which $(\partial^2/\partial x^2)+f(x)(\partial/\partial x)$ had a fundamental solution obtained from a point symmetry.

Notice that $\partial^2/\partial x^2$ may be thought of as the Laplacian generated by the one-dimensional Lie algebra of differential operators on $\mathbb{R}$ generated by $\partial/\partial x$. Recall that this is one of three finite-dimensional Lie algebras of first-order differential operators on $\mathbb{R}$. The other two are spanned by $\partial/\partial x$ together with $x(\partial/\partial x)$, and by $\partial/\partial x$, $x(\partial/\partial x)$, and $x^2(\partial/\partial x)$.

These generate the Lie algebra of the $ax+b$ group and of SL $(2,\mathbb{R})$, respectively. In this section, we consider sums-of-squares Laplacians, with drift terms, for these two algebras.

The Laplacian generated by $\partial/\partial x$ together with $x(\partial/\partial x)$ has the form $\Delta=(1+x^2)(\partial^2/\partial x^2)+x(\partial/\partial x)$.

We study equations of the form

$$\Delta u+f(x)\frac{\partial u}{\partial x}=\frac{\partial u}{\partial t},$$

which may be written

$$(1+x^2)\frac{\partial^2 u}{\partial x^2}+(x+f(x))\frac{\partial u}{\partial x}=\frac{\partial u}{\partial t}.$$

Observe that if we put $x=\sinh\xi$ in this equation, we have $\partial u/\partial x=(1/(\partial/\cosh\xi)\partial\xi)$ and $\partial^2 u/\partial x^2=(1/\cosh^2\xi)(\partial^2/\partial\xi^2)-(\sinh\xi/\cosh\xi)(\partial/\partial\xi)$. Hence, the equation is transformed into

$$\frac{\partial^2 u}{\partial\xi^2}+h(\xi)\frac{\partial u}{\partial\xi}=\frac{\partial u}{\partial t}, \tag{5.1}$$

where $h(\xi)=\tanh\xi f(\sinh\xi)$.

This is exactly of the form (4.1). We find again that (5.1) has a point symmetry generating the fundamental solution if and only if h satisfies one of the Ricatti equations of Theorem 4.1.

Thus, for example, applying Corollary 4.2, we see that when

$$h(\xi)=\left(\frac{a}{\xi}+\frac{2(1-a)c}{\xi+2(1-a)c\xi^a}\right),$$

$$f(\sinh\xi)=\frac{1}{\tanh\xi}\left(\frac{a}{\xi}+\frac{2(1-a)c}{\xi+2(1-a)c\xi^a}\right),\quad a\neq 1.$$

Putting $x=\sinh\xi$ gives

$$f(x)=\frac{\sqrt{1+x^2}}{x}\left(\frac{a}{\sinh^{-1}x}+\frac{2(1-a)c}{\sinh^{-1}x+2(1-a)c(\sinh^{-1}x)^a}\right).$$

Thus, we obtain the following.

Corollary 5.1:

$$(1+x^2)\frac{\partial^2 u}{\partial x^2}+\left(x+\frac{\sqrt{1+x^2}}{x}\left(\frac{a}{\sinh^{-1}x}+\frac{2(1-a)c}{\sinh^{-1}\xi+2(1-a)c(\sinh^{-1}x)^a}\right)\right)\frac{\partial u}{\partial x}=\frac{\partial u}{\partial t},$$

$a\neq 1$, *has heat kernel*

$$k(t,x,0)=\frac{1}{(4\pi)^{(a+1)/2}}\left[1+\frac{(\sinh^{-1}x)^{1-a}}{2c(1-a)}\right]\exp\left\{-\frac{(\sinh^{-1}x)^2}{4t}\right\}.$$

The other case we want to consider here is the Lie algebra spanned by $\partial/\partial x$, $x(\partial/\partial x)$, and $x^2(\partial/\partial x)$.

The appropriate sums-of-squares Laplacian for this basis is

$$\Delta=(1+x^2+x^4)\frac{\partial^2}{\partial x^2}+(x+2x^3)\frac{\partial}{\partial x},$$

and we consider the equation

$$\Delta u+f(x)\frac{\partial u}{\partial x}=\frac{\partial u}{\partial t},$$

which we may rewrite as

$$(1+x^2+x^4)\frac{\partial^2 u}{\partial x^2}+(x+2x^3+f(x))\frac{\partial u}{\partial x}=\frac{\partial u}{\partial t}.$$

If we put $k^{-1}(x)=\int dx/\sqrt{1+x^2+x^4}$, which is a higher analogue of the inverse tanh function, then the substitution $x=k(\xi)$ reduces the equation to

$$\frac{\partial^2 u}{\partial^2 \xi}+\frac{k(\xi)}{k'(\xi)}f(k(\xi))\frac{\partial u}{\partial \xi}=\frac{\partial u}{\partial t}.$$

Putting $[k(\xi)/k'(\xi)]f(k(\xi))=h(\xi)$, there are a limited number of possibilities for f, and using Corollary 4.2 we see, for example, that the heat kernel for

$$\frac{\partial u}{\partial t}=(1+x^2+x^4)\frac{\partial^2 u}{\partial x^2}+\left(x+2x^2+\frac{\sqrt{1+x+x^2}}{x}\left(\frac{a}{k^{-1}(x)}+\frac{2(1-c)a}{k^{-1}(x)+2(1-c)a(k^{-1}(x))^a}\right)\right)\frac{\partial u}{\partial x}$$

is

$$k(t,x,0)=\frac{1}{(4\pi t)^{(a+1)/2}}\left[1+\frac{(k^{-1}x)^{1-a}}{2c(1-a)}\right]\exp\left\{\frac{-k^{-1}(x)^2}{4t}\right\}.$$

Similar formulas may be found whenever we have an explicit solution for the Ricatti equations of Theorem 4.1.

VI. THE $ax+b$ GROUP

In this section we apply another aspect of group symmetry techniques to the study of properties heat kernels. The study of the asymptotic behavior of heat kernels is an important area of harmonic analysis. In this final section we will illustrate how quite simple group symmetry methods may be used to derive some new and unusual integrals of the heat kernel of the $ax+b$ group. Such integrals may be useful in studying the heat kernel's asymptotics, as well as having intrinsic interest. We believe that further investigation of these ideas will be useful for other equations.

In the remainder of this section, we consider the $ax+b$ group, given in matrix presentation by

$$G=\left\{\begin{pmatrix} a & b \\ 0 & 1 \end{pmatrix}: a>0, b\in\mathbb{R}\right\}.$$

It is known[9,16] that the heat equation for G may be written as

$$y^2\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 y}{\partial y^2}\right)+y\frac{\partial u}{\partial y}=\frac{\partial u}{\partial t} \tag{6.1}$$

with $y>0$, $x\in\mathbb{R}$. Further, the heat kernel is

$$\rho_t(y,x)=\frac{\sqrt{y}}{\sqrt{4\pi^3 t}}\int_0^\infty \frac{e^{-[(r^2/2t)-\pi^2]}\sinh r\sin\dfrac{\pi r}{t}}{(1+x^2+y^2+2y\cosh r)^{1/2}}dr,$$

where $r=(x^2+y^2)^{1/2}$. This integral cannot be done explicitly, and a great deal of effort has gone into estimating its asymptotics—see, for example, Ref. 9.

A basis for the symmetry algebra of point symmetries is easily shown to consist of

$$v_1=\frac{\partial}{\partial x},\quad v_2=\frac{\partial}{\partial t},\quad v_3=u\frac{\partial}{\partial u},\quad v_4=x\frac{\partial}{\partial x}+y\frac{\partial}{\partial y}-\frac{1}{2}u\frac{\partial}{\partial u},$$

$$v_5=(x^2-y^2)\frac{\partial}{\partial x}+2xy\frac{\partial}{\partial y}-ux\frac{\partial}{\partial u}.$$

Calculation of the commutator table shows that these vector fields generate the Lie algebra of $\mathrm{SL}(2,\mathbb{R})\oplus\mathbb{R}^2$.

We wish to determine solutions of (6.1) which are invariant under the symmetries generated by one of the vector fields above. We shall see that different choices of vector field give different information about the heat kernel.

Let us first use v_4, which generates the scaling symmetry

$$\sigma(\exp\epsilon v_4)u(x,y,t)=e^{1/2\epsilon}u(e^\epsilon y,e^\epsilon x,t).$$

Since scalar multiplication of u is also a symmetry, we may drop the factor of $e^{1/2\epsilon}$. According to the method of Ref. 1, Chap. 3, we now note that $r=x/y$ is an invariant of v_4 and hence we may obtain a group invariant solution of (6.1) by solving the reduced equation.

$$(1+r^2)\frac{\partial u^2}{\partial r^2}+r\frac{\partial u}{\partial r}=\frac{\partial u}{\partial t}.$$

As in Sec. V, this may be solved by setting $r=\sinh\xi$ to obtain

$$\frac{\partial^2 u}{\partial \xi^2}=\frac{\partial u}{\partial t},$$

the heat equation on $\mathbb{R}$. Thus, Eq. (6.1), with an initial condition of the form $u(y,x,0)=h(x/y)$, has a solution

$$u(u,x,t)=\int_{-\infty}^{\infty}h(\sinh\xi)K_t(\sinh^{-1}(x/y)-\xi)d\xi,$$

where K_t is the heat kernel on $\mathbb{R}$. Replacing ξ by $\sinh^{-1}\omega$, this becomes

$$u(y,x,t)=\int_{-\infty}^{\infty}h(\omega)K_t(\sinh^{-1}(x/y)-\sinh^{-1}/\omega)\,\frac{d\omega}{\sqrt{1+\omega^2}}.$$

It is amusing to compare this with the solution found via the usual heat kernel p_t, viz.

$$u(y,x,t)=\int_{-\infty}^{\infty}\int_{0}^{\infty}h(\xi/\eta)p_t((\eta,\xi)^{-1}(y,x))\,\frac{d\eta}{\eta}d\xi.$$

Putting $\omega=\xi/\eta$ and $z=\eta$, this becomes

$$u(y,x,t)=\int_{-\infty}^{\infty}h(\omega)\left(\int_{0}^{\infty}p_t\left(\frac{y}{z},\frac{x-z\omega}{z}\right)dz\right)d\omega,$$

whence we obtain

$$\int_{0}^{\infty}p_t\left(\frac{y}{z},\frac{x-z\omega}{z}\right)dz=\frac{K_t\left(\sinh^{-1}\left(\frac{x}{y}\right)-\sinh^{-1}\omega\right)}{\sqrt{1+\omega^2}}.$$

This may be regarded as some kind of new estimate on the asymptotic behavior of p_t.

In fact, using the machinery developed in Sec. V, we may use the preceding sequence of changes of variables to solve the heat equation with drift on the $ax+b$ group provided that the drift term is of the form $f(x/y)$, where f is one of the functions of the form in Theorem (4.1). The result is as follows. We leave the detailed verification to the reader.

Proposition 6.1: Consider the equation

$$y^2\left(\frac{\partial^2u}{\partial x^2}+\frac{\partial^2u}{\partial y^2}\right)+y\frac{\partial u}{\partial y}+\frac{y}{\cosh\left(\frac{x}{y}\right)}f\left(\sinh\left(\frac{x}{y}\right)\right)\frac{\partial u}{\partial x}=\frac{\partial u}{\partial t},$$

$$u(x,y,0)=h\left(\frac{x}{y}\right),$$

where f is given by one of the functions of Corollary 4.2. This equation has solution

$$u(y,x,t)=\int_{-\infty}^{\infty}h(\omega)K\left(\sinh^{-1}\frac{x}{y}-\sinh^{-1}\omega,t\right)\frac{d\omega}{\sqrt{1+\omega^2}},$$

where $K(x,t)$ is the given heat kernel for $(\partial^2u/\partial x^2)+f(x)(\partial u/\partial x)=\partial u/\partial t$.

In the preceding section we used the v_4 symmetry reduction to obtain an integral of the heat kernel p_t. We now repeat the exercise using the v_1 symmetry and the v_5 symmetry. The results are contained in the following theorem. Our methods may be applied to heat kernels of other Lie groups as well.

Proposition 6.2: Let p_t be the heat kernel on G and K_t the heat kernel of $\mathbb{R}$. Then

$$\text{(i)}\quad \int_0^\infty p_t\left(\frac{y}{z}, \frac{x-z\omega}{z}\right)dz = \frac{K_t\left(\sinh^{-1}\frac{x}{y} - \sinh^{-1}\omega\right)}{\sqrt{1+\omega^2}}$$

$$\text{(ii)}\quad \int_{-\infty}^\infty p_t((\eta,\xi)^{-1}(y,x))d\xi = K_t(\log y - \log \eta),$$

$$\text{(iii)}\quad \int_0^\infty p_t(ye^{-z}(e^{2z}+s^2), e^{-z}x(e^{2z}+s^2) - e^{-z}s)e^{-z/2}\frac{ds}{\sqrt{e^{2z+s}}} = \frac{e^{t/4}}{\sqrt{y}}K_t\left(\log\frac{y}{x^2+y^2} - t - z\right).$$

Proof: (i) was proved above.

For the proof of (ii), note that $v_1 = \partial/\partial x$ generates the symmetry

$$\sigma(\exp \epsilon v_1)u(x,y,t) = u(y, x-\epsilon, t);$$

an invariant of this is $r = y$. This yields the reduced equation

$$y^2 u_{yy} + y u_y = u_t, \quad y > 0.$$

Putting $y = e^s$, we find the equation

$$u_{ss} = u_t, \quad -\infty < s < \infty$$

and hence, as above, the boundary value problem

$$y^2(u_{yy} + u_{xx}) + y u_y = u_t,$$

$$u(y,x,0) = f(y)$$

has the solution

$$u(y,x,t) = \int_0^\infty f(\eta)K_t(\log y - \log \eta)\frac{d\eta}{\eta}.$$

Comparing as above with the solution coming directly from p_t, we obtain (ii).

To prove (iii) note that v_5 generates the symmetry

$$\sigma(\exp \epsilon v_5)u(x,y,t) = \frac{1}{\sqrt{(1+\epsilon x)^2 + \epsilon^2 y^2}}u\left(\frac{y}{(1+\epsilon x)^2+\epsilon^2 y^2}, \frac{x+\epsilon(x^2+y^2)}{(1+\epsilon x)^2+\epsilon^2 y^2}, t\right),$$

invariants being $r = \log[y/(x^2+y^2)]$ and $v = \sqrt{y}u$.

Substituting these new parameters into our equation, it reduces to

$$v_{rr} - v_r + \tfrac{1}{4}v = v_t, \quad -\infty < r < \infty.$$

This may be solved by standard Fourier transform techniques to obtain

$$v(r,t) = e^{t/4}\int_{-\infty}^\infty f(\lambda)K_t(r - t - \lambda)d\lambda.$$

Thus, the solution of the initial value problem

$$y^2(u_{xx}+u_{yy})+yu_y=u_t,$$

$$u(y,x,0)=\frac{1}{\sqrt{y}}h\left(\frac{y}{x^2+y^2}\right)$$

is

$$u(y,x,t)=\frac{e^{t/4}}{\sqrt{y}}\int_{-\infty}^{\infty}f(\xi)K_t\left(\log\frac{y}{x^2+y^2}-t-\xi\right)d\xi. \tag{6.2}$$

In order to compare this with the solution coming directly from p_t, viz,

$$u(y,x,t)=\int_{-\infty}^{\infty}\int_0^{\infty}\frac{1}{\eta}f\left(\log\frac{\eta}{\xi^2+\eta^2}\right)p_t((\eta,\xi)^{-1}(y,x))\frac{d\eta}{\eta}d\xi,$$

we set $r=\eta/(\xi^2+\eta^2)$, $s=\xi/(\xi^2+\eta^2)$, to obtain

$$u(y,x,t)=\int_{-\infty}^{\infty}\int_0^{r}f(\log r)p_t\left(y\frac{(r^2+s^2)}{r},\frac{x(r^2+s^2)-s}{r}\right)\frac{dr\,ds}{r^{3/2}\sqrt{r^2+s^2}}.$$

Finally, substituting $z=\log r$ and comparing this expression with (6.2), we obtain (iii). ■

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Optimally defined Racah–Casimir operators for su(n) and their eigenvalues for various classes of representations

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This paper deals with the striking fact that there is an essentially canonical path from the ith Lie algebra cohomology cocycle, $i=1,2,\ldots,l$, of a simple compact Lie algebra $\mathfrak{g}$ of rank l to the definition of its primitive Casimir operators $C^{(i)}$ of order m_i. Thus one obtains a complete set of Racah–Casimir operators $C^{(i)}$ for each $\mathfrak{g}$ and nothing else. The paper then goes on to develop a general formula for the eigenvalue $c^{(i)}$ of each $C^{(i)}$ valid for any representation of $\mathfrak{g}$, and thereby to relate $c^{(i)}$ to a suitably defined generalized Dynkin index. The form of the formula for $c^{(i)}$ for su(n) is known sufficiently explicitly to make clear some interesting and important features. For the purposes of illustration, detailed results are displayed for some classes of representation of su(n), including all the fundamental ones and the adjoint representation. © *2001 American Institute of Physics.*
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I. INTRODUCTION

It is well-known (see, e.g., Refs. 1–3 for lists of references and further details) that the l basis elements of the Lie algebra cohomology of a simple compact Lie algebra $\mathfrak{g}$ define, up to a constant, l totally antisymmetric tensors. In fact, these may also be understood as the coordinates of the different invariant $(2m-1)$-forms on the manifold of the compact group G associated with $\mathfrak{g}$ that, in the Chevalley–Eilenberg version of the Lie algebra cohomology,[4] characterize the $(2m-1)$-cocycles. Given a simple compact $\mathfrak{g}$, we shall refer to these l tensors as the Omega tensors $\Omega^{(2m_s-1)}$ of $\mathfrak{g}$. They have orders $2m_s-1$, $s=1,2,\ldots,l$, where m_s are the orders of the primitive Casimir–Racah operators of $\mathfrak{g}$ (see also Refs. 1–3 for lists of references). For su(n), $m_s\in\{2,3,\ldots,n\}$, and hence the Omega tensors are of orders $3,5,\ldots(2l+1)$. There is an essentially canonical path from the Omega tensors of a given $\mathfrak{g}$ that leads to the set of its l *primitive* Racah–Casimir operators $C^{(m_s)}$. Following this path,[2] the resulting set of Racah–Casimir operators $C^{(m_s)}$ [represented by invariant symmetric tensors $t^{(m_s)}$ of order m_s] is optimally defined in the sense that it contains one member for each required order m_s and nothing else. The procedure allows for the appearance of no $C^{(m_s)}$ other the l primitive ones; any formal attempt to define $C^{(m)}$ for, say, su(n) for $m>n$ simply produces a vanishing result. Since this paper concentrates on su(n), we shall not worry about the refinements that are needed to deal explicitly with all the invariants of the even orthogonal algebras $\mathfrak{g}=D_l$, where the Pfaffian enters the picture. Nor will the subsequent discussion make explicit the qualifications that may be needed to cover the exceptional algebras.

The paper proceeds from the definition of a complete set of primitive Racah–Casimir operators for $\mathfrak{g}$ to a new general result for the eigenvalues $c^{(m_s)}(D)$ of $C^{(m_s)}(D)$ for a generic representation D,

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$$X_i \mapsto D(X_i) \tag{1}$$

of the Lie algebra

$$[X_i, X_j] = i f_{ijk} X_k \tag{2}$$

of $\mathfrak{g}$. We have here written f_{ijk} for the structure constants of $\mathfrak{g}=\mathrm{su}(n)$. For this algebra, almost all of the technical machinery is at hand[2,5] to enable us to display explicitly the key features of our general result for $c^{(m)}(D)$. Obvious analogues of these results are applicable to all other $\mathfrak{g}$.

Our main result states that, for any representation D,

$$(\dim D)\, c^{(m_s)}(D) = 2^{1-m_s} (gdi)^{(m_s)}(D) \Omega^{(2m_s-1)^2}, \tag{3}$$

where

$$\Omega^{(2m_s-1)^2} \equiv \Omega_{i_1 \cdots i_{2m_s-1}} \Omega_{i_1 \cdots i_{2m_s-1}}, \tag{4}$$

and $(gdi)^{(m_s)}(D)$ is a number dependent on the order m_s of the Racah–Casimir operators, the representation D considered and $\mathfrak{g}$, or rather in the case of $\mathrm{su}(n)$, on n. For the representation considered, $(gdi)^{(m_s)}(D)$, $s=1,\ldots,l$, is an acronym for the sth *generalized Dynkin index* for the representation D considered and its use in (3) is discussed below. What is special about $\mathrm{su}(n)$ is that $\Omega^{(2m_s-1)^2}$ is known explicitly for all n and for all $2 \leqslant m \leqslant n$ (from now on, we drop the subindex $s=1,\ldots,l$ in m_s). From Ref. 5 we quote

$$\Omega^{(2m-1)^2} = \frac{2^{2m-3}}{(2m-2)!}\, n \prod_{r=1}^{m-1} (n^2 - r^2) \tag{5}$$

$$= \frac{4}{(2m-2)(2m-3)}\, \Omega^{(2m-3)^2}. \tag{6}$$

Equation (5) exhibits features of (3) which we believe apply equally well to all other $\mathfrak{g}$. Equation (5) shows that $\Omega^{(2m-1)^2} \neq 0$ and hence $\Omega^{(2m-1)}$ is nonvanishing only of $m \leqslant n$. In other words the primitive $(2m-1)$-cocycle exists only for $m \leqslant n$ as known from Lie algebra cohomology, and (3) gives a null result for $c^{(m)}(D)$ only when $n < m$. The power of two in (3) has been chosen, as far as we know it to be necessary, to ensure that, as is customary for an index, $(gdi)^{(m)}(D)$ takes on only integral values. In the case of $m=2$ and the familiar Dynkin index itself,[6] (3) takes on its standard form (see, e.g., Ref. 7),

$$(gdi)^{(2)}(D) = \frac{2 \dim D}{n \dim \mathfrak{g}}\, c^{(2)}(D), \tag{7}$$

using $f_{ijk} f_{ijk} = \Omega^{(3)^2} = n(n^2-1) = n.\dim(\mathrm{su}(n))$. The factor n in the denominator of (7) reflects the fact that for uniformity (in m) of our definitions of the various $C^{(m)}$ for $\mathrm{su}(n)$, we have defined the quadratic Casimir operator of $\mathrm{su}(n)$ as

$$C^{(2)} = n X_i X_i, \quad i = 1, \ldots, n-1, \tag{8}$$

see Sec. II C. For higher values of m there is less agreement as to how the Casimir operators $C^{(m)}$, and hence the $(gdi)^{(m)}(D)$, should be defined. We have argued that our definition of the former is optimal, featuring as it does t-tensors[2] and Omega tensors that are in one-to-one correspondence with the cohomology cocycles of $\mathrm{su}(n)$. This is tantamount to asserting that the Omega tensors are the fundamental entities (in fact, Ω^3 is given by the structure constants of the algebra themselves), and our definition of Casimir operators follows from this and reflects it too. A good recent account

of the role of, and of one way of defining, generalized Dynkin indices, which were originally introduced in Ref. 8, is Ref. 9, which refers to earlier papers.[10,11] The paper[9] also emphasizes the role of ''orthogonal'' tensors—in essence our t-tensors—making reference to Ref. 2 in this context, and attributing the recognition of the importance of orthogonality to the definition of generalized Dynkin indices to Ref. 8. Reference 9 contains extensive tabulations of generalized Dynkin indices, as does Ref. 12. Another useful discussion of indices is contained in Ref. 13, which aims, as we do here, at getting results for all su(n) valid for all n, using procedures—Cvitanovic's bird-track methods—that are there also applied to other $\mathfrak{g}$. Our work differs from that of the papers just cited in that it emphasizes the central role of the Omega-tensors, and employs a definition of indices that follows from this viewpoint. In view of (5) we believe that a significant amount of new information is contained in our work. We would further wish to advocate that (3)—the formula for the eigenvualue $c^{(m)}(D)$ of the Racah–Casimir operator of order m—be seen as the result of primary importance. The $(gdi)^{(m)}(D)$ are merely numbers, knowledge of which is required to complete the determination of the $c^{(m)}(D)$. Thus while the number $(gdi)^{(m)}(D)$ in some sense characterizes the eigenvalue $c^{(m)}(D)$, general su(n) formulas for $(gdi)^{(m)}(D)$ do not automatically exhibit the restrictions on n necessary for their applicability. Thus, for the adjoint represention ad, see below, of su(n),

$$(gdi)^{(4)}(\mathrm{ad}) = 2n. \tag{9}$$

But this applies *only* when $n \geqslant 4$, since (3)–(5) show that $c^{(4)}(D)$ equals zero for any D for $n = 2,3$, as it should do, since $\mathcal{C}^{(4)}$ is absent for these n-values. See also comments following (70) and (103) below.

The paper turns next to providing some illustrations of the results that are contained within (3). We wish to deduce the values of $(gdi)^{(m)}(D)$ for various m and representations D, obtaining results from a single computation that are valid for all n. For this purpose we consider the following classes of representations of su(n). We will use the notation $\mathcal{F}^s$ for $s = 1,2 \ldots, l$, for the fundamental representations of su(n) of rank $l = n-1$ (writing also $\mathcal{F} \equiv \mathcal{F}^1$ for the defining representation), and denote the adjoint representation of the algebra by ad.

A. The defining representation of su(n), $\mathcal{F}$

$\mathcal{F} = (1,0,\ldots,0)$ and is given by

$$X_i \mapsto \tfrac{1}{2}\lambda_i \equiv \mathcal{F}_i, \tag{10}$$

where the λ_i are the standard Gell–Mann matrices of su(n).[14] Using results from Ref. 5, we can show by a single calculation that

$$(gdi)^{(m)}(\mathcal{F}) = 1 \tag{11}$$

for all n and for all $m \leqslant n$. This simple general result offers some indication of the appropriateness of our definition of $(gdi)^{(m)}$.

B. The adjoint representation ad of su(n)

In Dynkin coordinates $\mathrm{ad} = (1,0,\ldots,1)$ (see, e.g., Ref. 7) and it is given by

$$X_i \mapsto \mathrm{ad}(X_i) \equiv \mathrm{ad}_i, \quad (\mathrm{ad}_i)_{jk} = -if_{ijk}. \tag{12}$$

We show that $(gdi)^{(m)}(\mathcal{F}) = 0$ for all odd m for all n, and give results for $m = 2,4$ and 6, on the basis of one calculation for each of these three m values.

C. The representation $\mathcal{D}$ of $\mathfrak{g} = $ su(n)

Let $\mathcal{D}$ denote the representation of $\mathfrak{g}$ built[15,16] using the set of Hermitian Dirac matrices of a euclidean space of dimension $\dim \mathfrak{g} = r$. The representation $\mathcal{D}$ is defined by means of

$$X_i \mapsto \mathcal{D}(X_i) \equiv S_i = -\tfrac{1}{4} i f_{ijk} \gamma_j \gamma_k , \tag{13}$$

in terms of Dirac matrices such that

$$\{\gamma_i , \gamma_j\} = 2\delta_{ij} ; \tag{14}$$

hence, $\mathcal{D}$ has dimension $2^{[r/2]}$ ($[x]$ denotes the integral part of x). Unlike all the other representations that we treat $\mathcal{D}$ is reducible; it describes the direct sum of a number of copies of the irreducible representation of $\mathfrak{g}$ whose highest weight is the principal Weyl vector $\delta = \frac{1}{2}\Sigma_{\alpha>0}\alpha$, i.e., half the sum of the positive roots of su(n), given by $\delta = (1, \ldots, 1)$ in Dynkin coordinates. This representation has dimension $2^{(r-l)/2}$. The actual number of copies of δ in $\mathcal{D}$ is $2^{[l/2]}$. It follows that $\dim \mathcal{D} = 2^{[l/2]} 2^{(r-l)/2} = 2^{[r/2]}$. We restrict to $\mathfrak{g} = \mathrm{su}(n)$, for which $l = n-1$ and $r = n^2 - 1$. We show that $(gdi)^{(m)}(\mathcal{D})$ is zero for all odd m for all su(n), and give explicit results for $m = 2$ and $m = 4$ only.

D. The *l* fundamental representations $\mathcal{F}^s$ and the irrep $\mathcal{S}_p = (p,0,\ldots,0)$

By dealing with the completely symmetrized and also the completely antisymmetrized direct products of p copies of the defining representation $\mathcal{F}$, we derive results for the representations of su(n) with Dynkin coordinates $(p,0,\ldots,0)$, and for the fundamental representations $\mathcal{F}^s$, $s = 1,2,\ldots,n-1$. For the latter, we give all indices for all $\mathcal{F}^s$ for $n = 3,4,5$, and 6. Bird-track methods[13] are employed here.

The material of this paper is organized as follows. Section II gives a brief description of the various families of su(n) tensors, including the Omega tensors, that are involved in the build up to the definition of Casimir operators. To some extent this reviews our earlier paper,[2] where detailed references to previous studies of Casimir operators may be found. In Sec. III, we derive and discuss the key result (3). In Sec. IV, we turn to the illustration of (3) for the classes of su(n) representations just listed.

The interest of this paper in the eigenvalues of Casimir operators has been in the context of generalized Dynkin indices, because our approach brings these in completely naturally. There are however other sources of information on the subject. There is Ref. 17 where valuable explicit formulas are given for all Casimir operators of all classical algebras and also for g_2, while Ref. 18 addresses the problem for other exceptional algebras.

II. DEFINITIONS OF TENSORS AND RACAH–CASIMIR OPERATORS

A. The *d*-tensors

This is a family of symmetric tensors first defined by Sudbery.[19] The definition sets out from the standard Gell–Mann totally symmetric third order tensor d_{ijk} that exists for all $n \geqslant 3$ and is traceless $d_{ijk}\delta_{ij} = 0$. Higher order tensors in the family

$$d^{(r)}_{(i_1,\ldots,i_r)} , \tag{15}$$

are defined recursively by symmetrizing

$$d^{(r)}_{i_1,\ldots,i_r} = d^{(r-1)}_{i_1,\ldots,i_{r-2}j} d^{(3)}_{ji_{r-1}i_r} , \tag{16}$$

over all its $i_1, \ldots, i_r$ indices. Round brackets here denote symmetrization with unit weight. Thus

$$d^{(3)}_{(ijk)} = d_{ijk} ,$$

$$d^{(4)}_{(ijkl)} = \tfrac{1}{3}(d_{ijp}d_{pkl} + d_{jkp}d_{pil} + d_{kip}d_{pjl}). \tag{17}$$

Sometimes it is useful to refer to $d^{(2)}_{ij} = \delta_{ij}$ as the rank two member of the family.

B. The Omega tensors

Using the mentioned correspondence between $(2m-1)$-cocycles and $\Omega^{(2m-1)}$ tensors, we have (see, e.g., Refs. 1, 2 for the structure of these expressions)

$$\Omega^{(3)}_{ijk}=f_{ijk}=f_{aij}d^{(2)}_{(ak)}, \tag{18}$$

$$\Omega^{(5)}_{ijkpq}=f_{a[ij}f^{b}{}_{kp]}d^{(3)}_{(abq)}, \tag{19}$$

$$\Omega^{(7)}_{ijkpqrs}=f_{a[ij}f^{b}{}_{kp}f^{c}{}_{qr]}d^{(4)}_{(abcs)}, \tag{20}$$

and in general

$$\Omega^{(2m-1)}_{i_1j_i\cdots\, i_{m-1}j_{m-1}k}=f^{k_1}{}_{[i_1j_1}\cdots\ f^{k_{m-1}}{}_{i_{m-1}j_{m-1}]}d^{(m)}_{(k_1\cdots\ k_m)}. \tag{21}$$

Here square brackets indicate unit weight antisymmetrization over all the surrounded indices. The structure of $\Omega^{(2m-1)}$ above is general for any $\mathfrak{g}$; what makes it specific to su(n) are the orders $(3,5,\ldots,(2l+1))$, and of course the fact that the f's are the su(n) ones. One may check explicitly that $\Omega^{(2m-1)}$ tensor is fully antisymmetric in all its $(2m-1)$ indices $(i_1j_1i_2j_2\cdots\ i_{m-1}j_{m-1}k)$, even if only the first $(2m-2)$ indices are antisymmetrized by actual square brackets. The position of the indices in this paper is without metric significance. Since $\mathfrak{g}$ is compact and its generators are Hermitian, we may take the Killing metric as the unit matrix, and so the raising of indices may just serve to remove them from the sets of indices that are subject to antisymmetrization (or symmetrization).

A detailed account of the properties of Omega tensors has recently been prepared.[5] The extensive compilation of results contained in Ref. 5 includes the important formula (5), together with its derivation. As noted above, (5) makes clear that $\Omega^{(2m-1)}$ is absent for su(n) whenever $m>n$.

C. The *t*-tensors

Following Ref. 2 we review some properties of this family of totally symmetric and totally tracelsss tensors $t^{(m)}$ for su(n). The definitions are

$$t^{(2)}_{ak}=\Omega^{(3)}_{ijk}f_{ija}, \tag{22}$$

$$t^{(3)}_{abm}=\Omega^{(5)}_{ijklm}f_{ija}f_{klb}, \tag{23}$$

$$t^{(4)}_{abcq}=\Omega^{(7)}_{ijklmpq}f_{ija}f_{klb}f_{mpc}, \tag{24}$$

$$t^{(5)}_{abcds}=\Omega^{(9)}_{ijklmpqrs}f_{ija}f_{klb}f_{mpc}f_{qrd}, \tag{25}$$

and in general

$$t^{(m)}_{k_1\cdots\ k_m}=\Omega^{(2m-1)}_{i_1j_1\cdots\, i_{m-1}j_{m-1}k}f_{i_1j_1k_1}\cdots\ f_{i_{m-1}j_{m-1}k_{m-1}}. \tag{26}$$

It follows from definition (26) that the tensor $t^{(m)}$ is fully symmetric (Ref. 2, lemma 3.2).

We do not make extensive use of explicit expressions for the t-tensors, but it is useful to note results from[2,5]

$$t^{(2)}_{ij}=n\,\delta_{ij}, \tag{27}$$

$$t^{(3)}_{ijk}=\tfrac{1}{3}n^2d_{ijk}, \tag{28}$$

$$t^{(4)}_{ijkl}=\tfrac{1}{15}(n(n^2+1)d^{(4)}_{(ijkl)}-2(n^2-4)\,\delta_{(ij}\delta_{kl)}), \tag{29}$$

$$t^{(5)}_{ijklm}=\frac{n}{105}((n(n^2+5)d^{(5)}_{(ijklm)}-2(3n^2-20)d_{(ijk}\delta_{lm)}). \tag{30}$$

We have adjusted the normalizations in (27)–(30) by excluding some powers of two present in (6.12)–(6.14) of Ref. 2. The t-tensors are ''orthogonal'' among themselves, which means that the maximal contraction of a $t^{(m)}$ with a tensor $t^{(m')}$ of different order yields zero. This implies, in particular, that $t^{(m)}$ is traceless with respect any two indices. In the simplest, third order case, Eq. (28), this is just the well known property $d_{ikk}=0$. For order four, $t^{(4)}$, this means that

$$t^{(4)}_{ijkl}\delta_{ij}=0, \quad t^{(4)}_{ijkl}d_{ijk}=0. \tag{31}$$

But, since the trace formulas for d-tensors give

$$d^{(4)}_{(ijkl)}d_{ijm}=\frac{2}{3}\,\frac{(n^2-8)}{n}d_{klm}, \tag{32}$$

we learn that the nontrivial result for the nonmaximal contraction

$$t^{(4)}_{ijkl}d_{ijm}=\tfrac{2}{45}n^2(n^2-9)d_{klm}, \tag{33}$$

holds, although it collapses to zero, as it ought, for $n=3$. Also (33) yields the second part of (31) when one makes the contraction $k=m$. For order five, the orthogonality of the t-tensors means that

$$t^{(5)}_{ijklm}t^{(2)}{}_{ij}=0, \quad t^{(5)}_{ijklm}t^{(3)}_{ijk}=0, \quad t^{(5)}_{ijklm}t^{(4)}{}_{ijkl}=0, \tag{34}$$

and so on.

One way to see that the t-tensors, like the Omega tensors, are absent for $m>n$ is to consider the fully contracted square of a generic t-tensor,

$$t^{(m)^2}=t^{(m)}_{k_1\cdots\ k_m}t^{(m)}_{k_1\cdots\ k_m}. \tag{35}$$

This scalar quantity can be seen to contain the same product of factors as is seen in (5). Thus it is a polynomial in n that has factors which vanish whenever $n<m$. Actually the proof of this claim for the t-tensors was achieved for $m\leqslant 5$ in Ref. 2, whereas (5) is proved in full generality in Ref. 5, relatively speaking rather easily.

The d-tensors are less convenient than the t-tensors in that for su(n) they are well-defined for any order m, but are present as nonprimitive tensors for $m>n$. However,[19,2,20] the unwanted or rather inessential d-tensors of higher orders can always be expressed in terms of the primitive set with $m\leqslant n$. For example, for su(3) we have

$$d^{(4)}_{(ijkl)}=\tfrac{1}{3}\,\delta_{(ij}\delta_{kl)}, \tag{36}$$

$$d^{(5)}_{(ijklm)}=\tfrac{1}{3}\,\delta_{(ij}d_{klm)}, \tag{37}$$

and, for su(4),

$$d^{(5)}_{(ijklm)}=\tfrac{2}{3}\,\delta_{(ij}d_{klm)}. \tag{38}$$

The above expressions exhibit the nonprimitive character of the symmetric tensors on their left-hand sides. It becomes increasingly hard to supply such results for su(n) at higher n. Fortunately this is unnecessary. Further, as Ref. 5 shows, the d-tensors serve perfectly well for the definition of Omega tensors. If non-primitive d-tensors like (36)–(38) are employed in the definition of

tensors like those of Sec. II B, when we know that no Omega tensor is allowed (Ref. 2, Corollary 3.1), a vanishing result is obtained.[5] It follows that symmetric invariant tensors differing in nonprimitive parts lead to the same Omega tensors.

D. The Racah–Casimir operators

Given the t-tensor of Eq. (26), we define, for su(n), the generalized Casimir operator of rank m by means of

$$C^{(m)}=t^{(m)}_{i_1 i_2 \cdots\ i_m} X_{i_i} X_{i_2} \cdots\ X_{i_m}, \tag{39}$$

where the X_i are the generators of the Lie algebra (2) of su(n). The definition (39) produces each of the primitive su(n) Casimir operators of orders $m \in \{2,3,\ldots,n\}$, and nothing else. This is so because the l su(n) Lie algebra cohomology cocycles and their associated Omega tensors are in one-to-one correspondence with the t-tensors and hence with the $C^{(m)}$. Had we used the d-tensors in (39) instead of the t-tensors, we would always thereby obtain commuting su(n) invariant operators, but of all orders for all su(n) so that all but l of them are nonprimitive. For low enough n, we can derive results which show explicitly how some of the nonprimitive operators so obtained can be written in terms of primitive ones. But, in the context of the present work, this is not important; use of (39) bypasses the problem entirely.

We should point out one consequence of the uniformity in m of the definitions (27)–(30) of t-tensors. Equation (27) implies

$$C^{(2)}=t^{(2)}_{ij} X_i X_j = n X_i X_i\,, \tag{40}$$

with a possibly unexpected, but harmless, factor n. For example, for the su(3) representation (λ,μ) in Dynkin coordinates, Eq. (40) gives the eigenvalue

$$c^{(2)}(\lambda,\mu)=(\lambda^2+\lambda\mu+\mu^2+3\lambda+3\mu), \tag{41}$$

and, for the representation (λ,μ,ν) (cf. Ref. 7) of su(4),

$$c^{(2)}(\lambda,\mu,\nu)=\tfrac{1}{2}(3\lambda^2+4\mu^2+3\nu^2+4\lambda\mu+2\lambda\nu+4\mu\nu+12\lambda+6\mu+12\nu). \tag{42}$$

It may also be worth mentioning the result[21] for the eigenvalue of the cubic Casimir operator of su(3),

$$c^{(3)}(\lambda,\mu)=\tfrac{1}{6}(\lambda+2\mu+3)(2\lambda+\mu+3)(\lambda-\mu). \tag{43}$$

One may use the defining representations of su(3) and su(4) to check that the normalizations of (41)–(43) give agreement with (39), (27), and (28).

III. THE EIGENVALUES OF THE HIGHER CASIMIR OPERATORS

For su(n) for large enough n, $n \geqslant m$, we defined the mth order Casimir operator by means of (39), where the X_i are the su(n) generators. This yields an invariant operator $C^{(m)}(D)$ with eigenvalue $c^{(m)}(D)$ in any representation $X_i \mapsto D_i$ so that

$$C^{(m)}(D)=c^{(m)}(D)\, I_{\dim D}\,. \tag{44}$$

Then, using (26), we find

$$
\begin{aligned}
c^{(m)}(D)\dim D &= \mathrm{Tr}\, C^{(m)}(D) \\
&= \Omega^{(2m-1)}_{i_1 j_1 \cdots\, i_{m-1} j_{m-1} k_m} f_{i_1 j_1 k_1} \cdots\; f_{i_{m-1} j_{m-1} k_{m-1}}\, \mathrm{Tr}\, D_{k_1 \cdots\, k_m} \\
&= (-i)^{m-1}\, \Omega^{(2m-1)}_{i_1 j_1 \cdots\, i_{m-1} j_{m-1} k_m}\, \mathrm{Tr}\,([D_{i_1}, D_{j_1}] \cdots\; [D_{i_{m-1}}, D_{j_{m-1}}] D_{k_m}) \\
&= (-2i)^{m-1}\, \Omega^{(2m-1)}_{i_1 j_1 \cdots\, i_{m-1} j_{m-1} k_m}\, \mathrm{Tr}\, D_{[i_1 j_1 \cdots\, i_{m-1} j_{m-1} k_m]}\,. \qquad (45)
\end{aligned}
$$

The first trace in (45), $\mathrm{Tr}\, D_{k_1 \cdots\, k_m}$ is in practice a unit weight symmetric trace $\mathrm{Tr}\, D_{(k_1} \cdots\; D_{k_m)}$ since $t^{(m)}$ is symmetric and $C^{(m)}(D)$ is given by (39) with $X = D$. For the last one we have written

$$
D_{[ij \cdots\, s]} = D_{[i} D_j \cdots\; D_{s]}\,. \qquad (46)
$$

We note here the transfer of the total antisymmetry from the Omega tensor to the trace of a product of $(2m-1)$ D's. This enables a crucial development since, as stated, $\mathrm{Tr}(D_{[i_1 j_1 \cdots\, i_{m-1} j_{m-1} k_m]})$ must belong to the $(2m-1)$-cocycle space and, hence, has to be proportional to the only primitive, SU(n)-invariant, skew symmetric, $(2m-1)$-Omega tensor.

Hence (see also Sec. III A) for any representation D, we may write

$$
\mathrm{Tr}\, D_{[i_1 j_1 \cdots\, i_{m-1} j_{m-1} k_m]} = \left(\frac{1}{4} i\right)^{m-1} (gdi)^{(m)}(D)\, \Omega^{(2m-1)}_{i_1 j_i \cdots\, i_{m-1} j_{m-1} k_m}\,, \qquad (47)
$$

thereby defining a quantity $(gdi)^{(m)}(D)$ which depends on m and D and in general on the Lie algebra $\mathfrak{g}$ in question. Since $\mathfrak{g} = \mathrm{su}(n)$ here, $(gdi)^{(m)}(D)$ depends also on n. As noted above (gdi) is an acronym for generalized Dynkin index. Insertion of (47) into (45) immediately gives rise to one of the main results of this paper,

$$
\dim D\, c^{(m)}(D) = 2^{(1-m)} (gdi)^{(m)}(D)\, \Omega^{(2m-1)2}. \qquad (48)
$$

The importance of (48) is enhanced for su(n) by the availability of the explicit result (5), valid for all n and for all m relevant to that n value, $m \leqslant n$. The relationship of our discussion of $c^{(m)}(D)$ and $(gdi)^{(m)}(D)$ to the work of previous authors is reviewed in the introduction. Our presentation conforms fully to this for $m = 2$. Otherwise our approach differs from that of others in view of the primary role in it that is played by the Omega tensors. This feature is inherited from Ref. 2, but (5) was not known when Ref. 2 was written.

We believe the analysis described here for the A_l family of Lie algebras extends to other classical compact simple algebras, exhibiting similar attractive features, and in some fashion to the exceptional algebras. For example, the crucial property of ''orthogonality'' among two t-tensors of different order follows from their general definition in terms of their respective Ω cocycle tensors, and does not depend on the specific simple $\mathfrak{g}$ being considered.[2] However the corresponding tensor calculus, and the analogue of the su(n) λ-matrix machinery is not yet developed sufficiently to produce simple expressions and formulas for all simple algebras.

A. Another approach to (47)

We sketch here another means of justifying our use of (47).

We have by now familiar steps

$$
\mathrm{Tr}\, D_{[i_1 j_1 \cdots\, i_{m-1} j_{m-1} k_m]} = \left(\frac{1}{2} i\right)^{m-1} f^{k_1}{}_{[i_1 j_1} \cdots\; f^{k_{m-1}}{}_{i_{m-1} j_{m-1}]}\, \mathrm{Tr}\, D_{k_1 \cdots\, k_m}. \qquad (49)
$$

It is legitimate to insert round brackets first to enclose the set $k_1 \cdots\, k_{m-1}$ of indices, and then by use of the cyclic property of the trace to extend them to enclose the full set $k_1 \cdots\, k_m$. Now we may refer to the discussion in Ref. 2 for the construction of a basis for the vector space of su(n)-invariant symmetric tensors like $\mathrm{Tr}\, D_{(k_1 \cdots\, k_m)}$. The term in the expansion of $\mathrm{Tr}\, D_{(k_1 \cdots\, k_m)}$ with respect to this basis which involves $d^{(m)}_{(k_1 \cdots\, k_m)}$ is the significant one for our argument. Use of it immediately gives rise to a result for $\mathrm{Tr}\, D_{[i_1 j_1 \cdots\, i_{m-1} j_{m-1} k_m]}$ of the form (47). All the other

terms of the expansion are made up of symmetrized products of lower order d-tensors, and give rise to vanishing contributions to (47) in view of Jacobi identities, as shown in Ref. 5.

IV. APPLICATION TO CERTAIN CLASSES OF REPRESENTATIONS OF su(n)

We consider here several important classes of representations of su(n), including the fundamental ones, for which one may provide a definition that applies uniformly for all n.

A. The fundamental defining representation $\mathcal{F}$ of su(n)

The representation $\mathcal{F}$ is defined by (10) where the Gell–Mann lambda-matrices[14] are subject to

$$\mathrm{Tr}\,\lambda_i=0, \quad \mathrm{Tr}\,\lambda_i\lambda_j=2\delta_{ij}, \quad \lambda_i^\dagger=\lambda_i, \tag{50}$$

$$\lambda_i\lambda_j=\frac{2}{n}\delta_{ij}+(d+if)_{ijk}\lambda_k, \tag{51}$$

valid for all su(n), $n\geqslant 3$.

Using notation like that defined by (46), we quote from Ref. 5 the result for the trace of the fully antisymmetric product of an *odd* number of $(2m-1)$ lambda matrices,

$$\mathrm{Tr}\,\lambda_{[i_1j_1\cdots\, i_{m-1}j_{m-1}k]}=2i^{m-1}\Omega_{[i_1j_1\cdots\, i_{m-1}j_{m-1}k]}. \tag{52}$$

We may now use (10) to substitute $\mathcal{F}_i$ for λ_i in (52), and deduce from (45), that

$$nc^{(m)}(\mathcal{F})=2^{(-m+1)}\Omega^{(2m-1)2}, \tag{53}$$

so that (48) gives

$$(gdi)^{(m)}(\mathcal{F})=1, \tag{54}$$

which also follows by comparing (52) and (47).

This result applies to all su(n) and for any $m\leqslant n$. Equation (53) and the explicit expression (5) for $\Omega^{(2m-1)^2}$ show that $(gdi)^{(m)}(\mathcal{F})$ is zero otherwise. Equation (54) does not itself provide new information (see Table II in Ref. 9) but (53) presents its information in a way that perhaps is. In this context, it may be worthwhile to display some formulas for eigenvalues in full detail,

$$c^{(2)}(\mathcal{F})=\tfrac{1}{2}(n^2-1), \tag{55}$$

$$c^{(3)}(\mathcal{F})=\tfrac{1}{12}(n^2-1)(n^2-4), \tag{56}$$

$$c^{(4)}(\mathcal{F})=\tfrac{1}{180}(n^2-1)(n^2-4)(n^2-9), \tag{57}$$

$$c^{(5)}(\mathcal{F})=\tfrac{1}{1680}(n^2-1)(n^2-4)(n^2-9)(n^2-16). \tag{58}$$

The factors that make $c^{(m)}(\mathcal{F})$ vanish when $m>n$ are visible here; the last factor above is $(n^2-(m-1)^2)$, and a nonzero result requires $n\geqslant m$.

B. The adjoint representation ad of su(n)

The adjoint representation ad of the su(n) algebra is defined by means of

$$X_i\mapsto ad_i, \quad (\mathrm{ad}_i)_{jk}=-if_{ijk}. \tag{59}$$

We do not possess a general formula for the factor μ that occurs in

$$\mathrm{Tr}\,\mathrm{ad}_{[i_1\cdots\ i_{2m-1}]}=\mu\,\Omega_{[i_1\cdots\ i_{2m-1}]}. \tag{60}$$

However it is easy to prove that for *m odd* the trace in (60) vanishes, so that $c^{(m)}(\mathrm{ad})=0$ for all odd m. Since the matrices of the adjoint representation of any simple Lie algebra are antisymmetric, we find, e.g., that

$$\mathrm{Tr}\,\mathrm{ad}_{[ijkpq]}=\mathrm{Tr}\,(\mathrm{ad}_{[ijkpq]})^T=-\mathrm{Tr}\,\mathrm{ad}_{[qpkji]}=-\mathrm{Tr}\,\mathrm{ad}_{[ijkpq]}=0. \tag{61}$$

For *m even* no such conclusion follows: the same steps applied to, say, the sevenfold trace do not give zero, because now an odd permutation is required at the last step to restore the indices to their original order.

It remains to look at the even cases $m=2,4$ and $m=6$, each by a separate calculation to get explicit formulas for $c^{(m)}(\mathrm{ad})$ for su(n). The results are

$$c^{(2)}(\mathrm{ad})=n^2, \tag{62}$$

$$c^{(4)}(\mathrm{ad})=\frac{2^3}{6!}n^2(n^2-4)(n^2-9), \tag{63}$$

$$c^{(6)}(\mathrm{ad})=\frac{2^5}{10!}n^2\prod_{k=2}^{5}(n^2-k^2), \tag{64}$$

from which we may conjecture that, for arbitrary *even* p,

$$c^{(p)}(\mathrm{ad})=\frac{2^{p-1}}{[2(p-1)]!}n^2\prod_{k=2}^{p-1}(n^2-k^2), \tag{65}$$

whereas $c^{(\mathrm{odd})}(\mathrm{ad})=0$.

The generalized Dynkin indices are then

$$(gdi)^{(2)}(\mathrm{ad})=2n, \tag{66}$$

$$(gdi)^{(3)}(\mathrm{ad})=0, \tag{67}$$

$$(gdi)^{(4)}(\mathrm{ad})=2n, \tag{68}$$

$$(gdi)^{(5)}(\mathrm{ad})=0, \tag{69}$$

$$(gdi)^{(6)}(\mathrm{ad})=2n, \tag{70}$$

etc. We recall that $\mathcal{C}^{(6)}$ is absent for $n<6$ [Eq. (64) contains explicit factors that reflect this], and hence note that (70) really only applies when $n\geqslant 6$. See also remarks that follow (103). Results (66) and (68) agree with results in Ref. 13.

The proof of (62) is easy. To obtain (63) we use

$$\mathrm{Tr}\,\mathrm{ad}_{[ijklpqr]}=\left(\frac{1}{2}i\right)^3 f^a{}_{[ij}f^b{}_{kl}f^c{}_{pq]}\,\mathrm{Tr}(\mathrm{ad}_r\,\mathrm{ad}_{(abc)})=\left(\frac{1}{4}i\right)^3 2n\,\Omega_{ijklpqr}. \tag{71}$$

To perform the last step, a result from Ref. 2 is employed,

$$\mathrm{Tr}\,(\mathrm{ad}_r\,\mathrm{ad}_{(abc)})=\frac{n}{4}d^{(4)}_{(abcr)}+2\,\delta_{(ab}\delta_{cr)}. \tag{72}$$

In fact the second term of (72) does not contribute to (71) because it is nonprimitive.

The proof of (64) similarly requires the formula

$$\mathrm{Tr}\,\mathrm{ad}_{(abcder)}=\frac{n}{16}d^{(6)}_{(abcder)}+\cdots\ , \tag{73}$$

where the dots denote terms which do not contribute to (64). One obtains this result by a method similar to that sketched in Ref. 2 to derive (A21) there. This requires a preliminary result,

$$\mathrm{Tr}\,\mathrm{ad}_{(abcd}D_{e)}=\frac{n}{8}d^{(5)}_{(abcde)}+\delta_{(ab}d_{cde)}\,, \tag{74}$$

where $(D_i)_{jk}=d_{ijk}$. The deduction of each of the last two results entails a considerable amount of effort, making liberal use of identities found in the Appendix to Ref. 2.

C. The reducible representation $\mathcal{D}$

The representation $\mathcal{D}$ of $\mathfrak{g}=\mathrm{su}(n)$, of dimension $2^{[\dim \mathfrak{g}/2]}=2^{[(n^2-1)/2]}$, has been described in the Introduction. However in this case again, we lack an explicit analog of (52). Again too the odd order Casimir operators have zero eigenvalues. To show this is true, we note there exists a matrix C such that

$$C\gamma_iC^{-1}=\pm\gamma_i^T\,, \tag{75}$$

with the sign depending on $\dim \mathfrak{g}$. Hence in general ($S_i\equiv\mathcal{D}(X_i)$),

$$S_i=-\tfrac{1}{4}i\,f_{ijk}\gamma_j\gamma_k\,,\quad [S_i\,,S_j]=if_{ijk}S_k\,, \tag{76}$$

obeys

$$S_i^T=-CS_iC^{-1}. \tag{77}$$

This is sufficient to allow steps like those used in (60) to complete the demonstration, since the matrix C is invisible within the trace. To get nonvanishing results we look at m even, this time confining ourselves to the cases $m=2$ and $m=4$. We have

$$c^{(2)}(\mathcal{D})=\frac{n}{8}\Omega^{(3)^2}, \tag{78}$$

$$c^{(3)}(\mathcal{D})=0, \tag{79}$$

$$c^{(4)}(\mathcal{D})=-\frac{n}{64}\Omega^{(7)^2}, \tag{80}$$

and hence

$$(gdi)^{(2)}(\mathcal{D})=\frac{n}{4}(\dim\mathcal{D}), \tag{81}$$

$$(gdi)^{(3)}(\mathcal{D})=0, \tag{82}$$

$$(gdi)^{(4)}(\mathcal{D})=-\frac{n}{8}(\dim\mathcal{D}). \tag{83}$$

We have already noted that $\mathcal{D}$ is a direct sum of $2^{[(n-1)/2]}$ copies of the irreducible representation $\delta=(1,\ldots,1)$ of su(n),[16] and that $\dim \mathcal{D}=2^{[(n^2-1)/2]}$. It follows that the indices given by (81) and (83) are in all cases integers.

We remark also that the results (78)–(80) apply also to the representation δ of su(n) since $\mathcal{D}$ is a direct sum of copies of δ.

For su(3), for which δ coincides with the adjoint representation, $\mathcal{D}$ comprises two copies of ad, $c^{(2)}(\mathcal{D})=c^{(2)}(\delta)=c^{(2)}(\mathrm{ad})=9$ [Eq. (62)], but

$$(gdi)^{(2)}(\mathcal{D})=2(gdi)^{(2)}(\mathrm{ad}), \tag{84}$$

as is to be expected since by Eq. (47) the dimension of the representation enters into the definition of the Dynkin index.

The easier of the proofs known to us for (80) follows the same lines as the proof of (62). It therefore requires the result

$$\mathrm{Tr}\,(S_d S_{(abc)})=-\frac{n}{64}d^{(4)}_{(abcd)}(\dim \mathcal{D})+\frac{3n^2-8}{64}\delta_{(ab}\delta_{cd)}(\dim \mathcal{D}), \tag{85}$$

which is proven in much the same way as (A11) in Ref. 2 is proven. Some nontrivial work on traces of gamma matrices is involved. Also, as for (72), the second term of (85) does not contribute to the derivation of (83). The minus sign in (83) may be noted. It is not exceptional: the tables of Ref. 9 have plenty of negative entries.

D. The representations $\mathcal{S}_p$ of highest weight $(p,0,\ldots,0)$

The representations $\mathcal{S}_p$ carried by totally symmetric su(n) tensors of rank p, the defining representation $\mathcal{F}$ being the case with $p=1$, i.e., $\mathcal{S}_1=\mathcal{F}=\mathcal{F}^1$. We can extend the results obtained for $\mathcal{F}=(1,0,\ldots,0)$ easily to $\mathcal{S}_2$ for which we define matrices

$$(M_i)_{a_1a_2,b_1b_2}=\delta_{(a_1}{}^{(b_1}\lambda_{i_{a_2})}{}^{b_2)}. \tag{86}$$

It is easy to check that (86) satisfies (2). As previous sections indicate, what one needs for the calculation of generalized Dynkin indices in our approach is the evaluation of traces

$$\mathrm{Tr}\,D_{(a}D_b\cdots D_{s)}. \tag{87}$$

It is easy to use (86) to compute

$$\mathrm{Tr}\,M_iM_j=\tfrac{1}{2}(n+2)\,\delta_{ij}, \tag{88}$$

$$\mathrm{Tr}\,M_{(i}M_jM_{k)}=\tfrac{1}{4}(n+4)d_{ijk}, \tag{89}$$

$$\mathrm{Tr}\,M_{(i}M_jM_kM_{l)}=\tfrac{1}{8}(n+8)d^{(4)}_{(ijkl)}+\cdots, \tag{90}$$

where the dots indicate lower order terms known but known also, because of Jacobi identities, not to contribute to the calculation of the eigenvalues $c^{(4)}(\mathcal{S}_2)$. Thus we find that all results agree with

$$(gdi)^{(m)}(\mathcal{S}_2)=n+2^{m-1}. \tag{91}$$

To proceed further it is advisable to use heavier duty methods. Bird-track methods allow us to subsume the calculations just done into the treatment of the general p case, by dealing with the totally symmetrized p-fold direct products of defining representations.

Our results include the following:

$$(gdi)^{(m)}(\mathcal{S}_p)=\frac{(n+p)!}{(p-1)!(n+1)!},\quad m=2; \tag{92}$$

$$=\frac{(n+p)!}{(p-1)!(n+2)!}(n+2p),\quad m=3; \tag{93}$$

$$=\frac{(n+p)!}{(p-1)!(n+3)!}(n^2-n+6pn+6p^2),\quad m=4. \tag{94}$$

The result (91) for $\mathcal{S}_2$ of course conforms to these results. To derive these expressions, we employ results for totally symmetrized traces that appear in Ref. 13 as Eqs. (12.69)–(12.71). We note also from Ref. 13 the diagram (12.64) used to define the matrices of $(p,0,\ldots,0)$, and the essential results (5.19) and (5.23) given in the valuable chapter in Ref. 13 on permutations.

E. The *l* fundamental representations $\mathcal{F}^s$ of su(n)

The representation $\mathcal{F}^2=(0,1,0,\ldots,0)$ of su(n) is the antisymmetric part of the direct product $\mathcal{F}\otimes\mathcal{F}$, where $\mathcal{F}=\mathcal{F}^1$ is the defining representation of su(n). Thus we define for $\mathcal{F}^2$ the matrices,

$$(N_i)_{a_1a_2,b_1b_2}=\delta_{[a_1}{}^{[b_1}\lambda_{i\,a_2]}{}^{b_2]}. \tag{95}$$

This differs from (86) only in that round symmetrization brackets are replaced by square antisymmetrization brackets. We find the following results:

$$\mathrm{Tr}\,N_iN_j=\tfrac{1}{2}(n-2)\,\delta_{ij}, \tag{96}$$

$$\mathrm{Tr}\,N_{(i}N_jN_{k)}=\tfrac{1}{4}(n-4)d_{ijk}, \tag{97}$$

$$\mathrm{Tr}\,N_{(i}N_jN_kN_{l)}=\tfrac{1}{8}(n-8)d^{(4)}_{(ijkl)}+\cdots\ . \tag{98}$$

Again all these results agree with the general statement

$$(gdi)^{(m)}(\mathcal{F}^2)=n-2^{m-1}. \tag{99}$$

It is of clear interest to proceed further down the antisymmetrization path. For su(n), the totally antisymmetrized parts of the s-fold products of defining representations correspond to the fundamental representations $\mathcal{F}^s$ of su(n) for $s=1,2,\ldots,l=(n-1)$, i.e., $\mathcal{F}^s$ has a one in the sth place of its Dynkin coordinate description and zeros elsewhere; its highest weight is the sth fundamental dominant weight.

Using bird-track methods, we find

$$(gdi)^{(m)}(\mathcal{F}^s)=\frac{(n-2)!}{(s-1)!(n-s-1)!},\quad m=2; \tag{100}$$

$$=\frac{(n-3)!}{(s-1)!(n-s-1)!}(n-2s),\quad m=3; \tag{101}$$

$$=\frac{(n-4)!}{(s-1)!(n-s-1)!}(n^2+n-6sn+6s^2),\quad m=4. \tag{102}$$

The result (99) for $s=2$ conforms to these results; for $s=1$ we get $(gdi)^{(m)}(\mathcal{F}^1)=1$, which also follows from (92)–(94) for $p=1$ as it should. Results analogous to (100)–(102) for $m=5$ and $m=6$ have also been computed. For $s=2$ they each agree with (99). When $s=3$ we have

$$(gdi)^{(5)}(\mathcal{F}_3)=\tfrac{1}{2}(n-6)(n-27). \tag{103}$$

Since su(n) has a fifth order Casimir operator only for $n \geqslant 5$, (103) applies only for such n. It gives 11 for $n=5$ and vanishes for $n=6$, but is nonzero for all larger n except $n=27$. In other words $c^{(5)}(\mathcal{F}_3)$ vanishes when $n=6$ in virtue of its (gdi) factor rather than its Ω factor.

To obtain these results we have followed methods for the antisymmetric case analogous to those of the previous section for the symmetric case. Permutation lemmas (5.19) and (5.23) of Ref. 13 expedite the work.

The results of this section permit the evaluation of all the indices of all the fundamental representations of su(n) for all $n \leqslant 6$. These are presented in Tables I–IV in Sec. V.

The results of (92)–(94) are very closely related to results to be found in Chap. 16 of Ref. 13. Although no such statement holds for (100)–(102), all the tools needed to derive them were found in Ref. 13 polished and ready for use.

V. TABLES OF INDICES FOR su(n) FOR $n \leqslant 6$

The (gdi) indices presented in Tables I–IV that follow have been deduced from (99)–(103), where one easy check is available. If $X_i \mapsto D_i$ defines the representation D of su(n), then

$$X_i \mapsto \overline{D}_i = -D_i^T \tag{104}$$

defines the representation $\overline{D}$ of su(n). It then follows that

$$c^{(m)}(D) = \pm c^{(m)}(\overline{D}), \tag{105}$$

where the plus applies to even m and the minus to m odd. The data in the accompanying tables conforms to this. Further some entries for su(4) and su(6) agree with the consequence of (105) that odd Casimir operators have zero eigenvalues for self-conjugate representations.

TABLE I. Indices for su(3).

	Generalized Dynkin indices of su(3)	
su(3)	$s=1$ or (1,0)	$s=2$ or (0,1)
$m=2$	1	1
$m=3$	1	−1

TABLE II. Indices for su(4).

	Generalized Dynkin indices of su(4)		
su(4)	$s=1$ or (1,0,0)	$s=2$ or (0,1,0)	$s=3$ or (0,0,1)
$m=2$	1	2	1
$m=3$	1	0	−1
$m=4$	1	−4	1

TABLE III. Indices for su(5).

	Generalized Dynkin indices of su(5)			
su(5)	$s=1$ or (1,0,0,0)	$s=2$ or (0,1,0,0)	$s=3$ or (0,0,1,0)	$s=4$ or (0,0,0,1)
$m=2$	1	3	3	1
$m=3$	1	1	−1	−1
$m=4$	1	−3	−3	1
$m=5$	1	−11	11	−1

TABLE IV. Indices for su(6).

su(6)	Generalized Dynkin indices of su(6) (1,0,0,0,0)	(0,1,0,0,0)	(0,0,1,0,0)	(0,0,0,1,0)	(0,0,0,0,1)
$m=2$	1	4	6	4	1
$m=3$	1	2	0	−2	−1
$m=4$	1	−2	−6	−2	1
$m=5$	1	−10	0	10	−1
$m=6$	1	−26	66	−26	1

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Smeared heat-kernel coefficients on the ball and generalized cone

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We consider smeared zeta functions and heat-kernel coefficients on the bounded, generalized cone in arbitrary dimensions. The specific case of a ball is analyzed in detail and used to restrict the form of the heat-kernel coefficients A_n on smooth manifolds with boundary. Supplemented by conformal transformation techniques, it is used to provide an effective scheme for the calculation of the A_n. As an application, the complete $A_{5/2}$ coefficient is given. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1285969]

I. INTRODUCTION

The coefficients A_n in the small-time asymptotic expansion of the heat-kernel corresponding to a Laplacian-like operator on smooth manifolds (possibly with a boundary) play important roles both in quantum field theory and pure mathematics.

Many schemes for their evaluation have been developed, which may be divided roughly into ''direct''[1–7] and ''indirect.''[8–12] For manifolds without boundary, the A_n are determined by algebraic equations and their computation can be, and has been, done by computer. In principle, the only things needed are the coincidence limits of the geodesic distance and of its derivatives at two points. Methods employing one or another variation on this scheme can be termed direct. The ''indirect'' method has been developed most systematically by Branson and Gilkey.[8] Conformal transformation techniques give relations between the numerical multipliers in the heat-kernel coefficients. However, on its own, this method is unable to determine the coefficients fully. Additional information is needed, coming from other functorial relations or special case calculations.[8] Given a subset of numerical coefficients, the method then provides all required information with relative ease. Our aim in the present article is to give a special case calculation containing enough information, which, when supplemented by the methods of Ref. 8, leads to a very effective scheme for the evaluation of at least a substantial part of any A_n.

In a previous article[13] (see also Ref. 14) we considered the nonsmeared heat kernel of the Laplacian with Dirichlet or Robin boundary conditions on the $(d+1)$-dimensional bounded cone. Here we generalize this work to include a smearing function. This is an essential step in elucidating the form of the coefficients in the presence of boundaries and is also vital when conformal properties are being analyzed, particularly those of the functional determinant.

The resulting restrictions are more informative than others available and are used to determine the first few heat-kernel coefficients on an arbitrary smooth manifold with a boundary. The complete pure boundary coefficient $A_{5/2}$ is given, showing the practicability of our approach for high orders.[15]

The paper is organized as follows. In Sec. II a method is developed for the calculation of the smeared heat-kernel coefficients on the generalized cone. Both Dirichlet and Robin boundary

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conditions are treated. This information is used in Sec. III to put restrictions on the general form of the coefficients. Supplemented by additional relations,[8] the coefficients $A_0,\ldots,A_{5/2}$, are (re)considered and fully determined. In the Conclusion we summarize our main results and suggest extensions.

II. SMEARED ζ FUNCTION ON THE GENERALIZED CONE

Our immediate objective is the determination of the smeared heat-kernel coefficients on the $(d+1)$-dimensional bounded generalized cone $\mathcal{M}=I\times\mathcal{N}$ with the hyperspherical metric, cf. Ref. 16,

$$ds^2=dr^2+r^2d\Sigma^2, \tag{1}$$

where $d\Sigma^2$ is the metric on the manifold $\mathcal{N}$, and r runs from 0 to 1. $\mathcal{N}$ will be referred to as the base of the cone. If it has no boundary, then it is the boundary of $\mathcal{M}$ with extrinsic curvature $K^a_b=\delta^a_b$.

We consider the Laplacian on $\mathcal{M}$,

$$\Delta_{\mathcal{M}}=\frac{\partial^2}{\partial r^2}+\frac{d}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\Delta_{\mathcal{N}}, \tag{2}$$

with Dirichlet or Robin boundary conditions. The nonzero eigenmodes of $\Delta_{\mathcal{M}}$ that are finite at the origin have eigenvalues $-\alpha^2$ and are of the form

$$\frac{J_\nu(\alpha r)}{r^{(d-1)/2}}Y(\Omega), \tag{3}$$

where the harmonics on $\mathcal{N}$ satisfy

$$\Delta_{\mathcal{N}}Y(\Omega)=-\lambda^2Y(\Omega) \tag{4}$$

and

$$\nu^2=\lambda^2+(d-1)^2/4. \tag{5}$$

One can also add the coupling $-\xi R$ to $\Delta_{\mathcal{M}}$, changing the following analysis slightly.[13]

In order to deal with the smeared ζ function, we parallel the analysis presented in Ref. 13 and refer to it for further details. We consider both Dirichlet,

$$J_\nu(\alpha)=0, \tag{6}$$

and Robin boundary conditions,

$$\left(1-\frac{D}{2}-S\right)J_\nu(\alpha)+\alpha J'_\nu(\alpha)=0, \tag{7}$$

where $D=d+1$. Pure Neumann conditions correspond to $S=0$.

Our main interest is in the calculation of the boundary terms of the heat-kernel expansion. A convenient way of handling these is to introduce smeared, integrated quantities, e.g., the heat kernel,

$$K(F;\tau)=\int dx\,F(x)K(x,x,\tau), \tag{8}$$

and its Mellin transform, the ζ function,

$$\zeta(F;s)=\sum_{\alpha}\int dx\,F(x)\phi(x)\phi^{*}(x)\frac{1}{\alpha^{2s}}, \tag{9}$$

in terms of eigenfunctions, ϕ, and eigenvalues, $-\alpha^2$. In addition, the base ζ function,

$$\zeta_{\mathcal{N}}(s)=\sum_{\nu}d(\nu)\nu^{-2s}, \tag{10}$$

will turn out to be very useful. Here, $d(\nu)$ is the (''angular'') degeneracy.

On the generalized cone, the eigenfunctions (3) are products of Bessel functions and ''spherical,'' i.e., base, harmonics. If we smear in the radial coordinate only, then in (9) the integration over the base yields exactly the same degeneracies as in the unsmeared case, i.e., the $d(\nu)$, and the contour expression for the ζ function on $\mathcal{M}$ reads (we treat Dirichlet scalars first) as

$$\zeta(F;s)=\sum\int_{\gamma}\frac{dk}{2\pi i}k^{-2s}\int_0^1 dr\,F(r)\overline{J}_{\nu}^2(kr)rd(\nu)\frac{\partial}{\partial k}\ln J_{\nu}(k), \tag{11}$$

where the overbar stands for normalized, $\overline{J}_{\nu}(\alpha r)=\sqrt{2}J_{\nu}(\alpha r)/J_{\nu}'(\alpha)$.

The boundary parts of the coefficients contain normal derivatives, $F_{r\cdots r}$, of F and we choose for F a polynomial in r^2 (why r^2 will be clear soon) that contains sufficient independent derivatives to pick out the relevant contributions. For example, in A_1, since there is only one normal derivative F_r, it is sufficient to take

$$F(r)=f_0+f_1r^2 \tag{12}$$

and to use

$$F(1)=f_0+f_1,\quad F_r(1)=2f_1, \tag{13}$$

in order to identify the boundary terms.

To explain our method more precisely, we continue with this simple example, (12), and afterward generalize to an arbitrary polynomial. Using

$$\int_0^1 dr\,r^3\overline{J}_{\nu}^2(\alpha r)=\frac{2}{3}\frac{\nu^2-1}{\alpha^2}+\frac{1}{3}, \tag{14}$$

and substituting (12) into (11), we obtain two contributions:

$$\zeta_{\mathcal{M}}(F;s)=(f_0+\tfrac{1}{3}f_1)\zeta_{\mathcal{M}}(s)+\frac{2}{3}f_1\sum(\nu^2-1)d(\nu)\int_{\gamma}\frac{dk}{2\pi i}k^{-2(s+1)}\frac{\partial}{\partial k}\ln J_{\nu}(k). \tag{15}$$

Here, $\zeta_{\mathcal{M}}(s)$ is defined to be $\zeta_{\mathcal{M}}(1;s)$ and is known from our previous analysis.[13] Also, the second line in (15) may be immediately given by direct comparison with our previous calculation. The contour integral is the same as previously apart from replacing $s\to s+1$. For the second term this is already all we need. The first term contains a factor ν^2, raising the argument of the base zeta function by one. [See Eq. (20)].

In order to describe the method further, it is necessary to use some notation introduced in Ref. 13. For the calculation of the heat-kernel coefficients, a split of the zeta function into two parts is very useful. One part contains all the relevant contributions and comes from the uniform asymptotic expansion of the Bessel function $I_{\nu}(k)$. As has been shown in Ref. 13, these are the only contributions to the heat-kernel coefficients. Explicitly, for $\nu\to\infty$ with $z=k/\nu$ fixed, one has

$$I_\nu(\nu z)\sim\frac{1}{\sqrt{2\pi\nu}}\frac{e^{\nu\eta}}{(1+z^2)^{1/4}}\left[1+\sum_{k=1}^{\infty}\frac{u_k(t)}{\nu^k}\right], \tag{16}$$

with $t=1/\sqrt{1+z^2}$ and $\eta=\sqrt{1+z^2}+\ln(z/(1+\sqrt{1+z^2}))$. Any required number of $u_k(t)$ polynomials can be obtained via the recursion relation given in Ref. 17 and 18. In addition, we need the cumulant expansion

$$\ln\left[1+\sum_{k=1}^{\infty}\frac{u_k(t)}{\nu^k}\right]\sim\sum_{n=1}^{\infty}\frac{D_n(t)}{\nu^n}, \tag{17}$$

where the D_n have the polynomial structure

$$D_n(t)=\sum_{b=0}^{n}x_{n,b}t^{n+2b}. \tag{18}$$

The second part of the split, named $Z(s)$ in Ref. 13 and accordingly $Z(F;s)$ here, is analytic and is of no relevance to the construction of the coefficients.

By adding and subtracting L leading terms of the asymptotic expansion, (17), and performing the same steps as described in Ref. 13 one finds the aforementioned split,

$$\zeta_{\mathcal{M}}(F;s)=Z(F;s)+\sum_{i=-1}^{L}A_i(F;s), \tag{19}$$

with the definitions

$$A_{-1}(F;s)=\frac{1}{4\sqrt{\pi}}\frac{\Gamma\left(s-\frac{1}{2}\right)}{\Gamma(s+1)}\zeta_{\mathcal{N}}(s-1/2)\left[f_0+\frac{1}{3}f_1+\frac{2}{3}f_1\frac{s-1/2}{s+1}\right]$$
$$-\frac{2}{3}f_1\frac{1}{4\sqrt{\pi}}\frac{\Gamma\left(s+\frac{1}{2}\right)}{\Gamma(s+2)}\zeta_{\mathcal{N}}(s+1/2),$$

$$A_0(F;s)=-\tfrac{1}{4}\zeta_{\mathcal{N}}(s)[f_0+f_1]-\tfrac{1}{4}\zeta_{\mathcal{N}}(s+1)f_1, \tag{20}$$

$$A_i(F;s)=-\frac{1}{\Gamma(s)}\zeta_{\mathcal{N}}(s+i/2)\sum_{b=0}^{i}x_{i,b}\frac{\Gamma(s+b+i/2)}{\Gamma(b+i/2)}\left[f_0+\frac{1}{3}f_1+\frac{2}{3}f_1\frac{s+b+i/2}{s}\right]$$
$$-\frac{2}{3}f_1\zeta_{\mathcal{N}}(s+1+i/2)\sum_{b=0}^{i}x_{i,b}\frac{\Gamma(s+1+b+i/2)}{\Gamma(s+1)\Gamma(b+i/2)}.$$

As is apparent in (20), base contributions are separated from radial ones. This enables the heat-kernel coefficients of the Laplacian on the manifold $\mathcal{M}$ to be written in terms of those on $\mathcal{N}$.

In the next section we discuss the restrictions our calculation places on the general form of the heat-kernel coefficients. It is known, for example, that the coefficient A_2 contains the third normal derivative of the smearing function F and the higher coefficients involve correspondingly higher derivatives. It is thus obvious that the $F(r)$ employed earlier (12) will not be general enough to discuss coefficients beyond $A_{3/2}$. In order to apply our technique to all higher coefficients, at least in principle, we consider the polynomial

$$F(r)=\sum_{n=0}^{N} f_n r^{2n}. \tag{21}$$

This leads to normalization integrals of the type

$$S[1+2p]=\int_0^1 dr\, \overline{J}_\nu^2(\alpha r) r^{1+2p}, \tag{22}$$

which can be treated using Schafheitlin's reduction formula.[19] Writing this formula for the case when α is a zero of the Bessel function, $J_\nu(\alpha)=0$, one has

$$\int_0^1 dr\, \overline{J}_\nu^2(\alpha r) r^{\mu+2}=\frac{\mu+1}{\mu+2}\,\frac{(\nu^2-(\mu+1)^2/4)}{\alpha^2}\int_0^1 dr\, \overline{J}_\nu^2(\alpha r) r^{\mu}+\frac{1}{\mu+2}. \tag{23}$$

This can be iterated down to the standard normalization value, $\mu=1$, and is the origin of (14). In order to use this formula, which is our essential technical novelty, we see that it is necessary to have a polynomial in r^2.

Schafheitlin's formula gives the recursion for the normalization integrals (22),

$$S[1+2p]=\frac{2p}{2p+1}\,\frac{\nu^2-p^2}{\alpha^2}S[2p-1]+\frac{1}{2p+1}, \tag{24}$$

so that $S[1+2p]$ has the following form:

$$S[1+2p]=\sum_{m=0}^{p}\left(\frac{\nu}{\alpha}\right)^{2m}\sum_{l=0}^{m}\gamma_{ml}^{p}\nu^{-2l}, \tag{25}$$

with the numerical coefficients γ_{ml}^{p} being easily determined recursively.

As seen in the treatment of the function $F(r)$ in Eq. (12), using the same rules of replacement, the $A_i(s)$ read, after some rearrangement, as

$$A_{-1}(F;s)=\frac{1}{4\sqrt{\pi}}\sum_{l=0}^{N}\left[\sum_{m=l}^{N}L_{m,l}^{(N)}\frac{\Gamma(s-1/2+m)}{\Gamma(s+1+m)}\right]\zeta_{\mathcal{N}}(s-1/2+l),$$

$$A_0(F;s)=-\frac{1}{4}\sum_{l=0}^{N}\left[\sum_{m=l}^{N}L_{m,l}^{(N)}\right]\zeta_{\mathcal{N}}(s+l), \tag{26}$$

$$A_i(F;s)=-\sum_{l=0}^{N}\left[\sum_{m=l}^{N}L_{m,l}^{(N)}\sum_{b=0}^{i}x_{i,b}\frac{\Gamma(s+b+i/2+m)}{\Gamma(s+m)\Gamma(b+i/2)}\right]\zeta_{\mathcal{N}}(s+l+i/2),$$

where the linear form in the f_p is defined by

$$L_{m,l}^{(N)}=\sum_{p=m}^{N}\gamma_{ml}^{p}f_p.$$

For Dirichlet boundary conditions, these formulas provide the generalization of our formalism[13] to the radially smeared case. This is enough for our purposes because the general forms of the heat-kernel coefficients contain only normal derivatives, and these are radial derivatives on the generalized cone.

In the special case of the D ball, the residues of the poles of the base (i.e., sphere) ζ function are given in terms of Bernoulli polynomials and the ball coefficients are then efficiently evaluated by machine.[13] One could equally well take the torus as the base manifold, but the information obtained differs only slightly.

We now turn to Robin boundary conditions. It is possible to proceed in the same way as for Dirichlet, but complications arise and the situation is sufficiently different so as to warrant a separate treatment.

Write the Robin condition (7) as

$$G_\nu(\alpha)=\alpha J'_\nu(\alpha)+uJ_\nu(\alpha)=0.$$

The normalization is

$$\int_0^1 J_\nu^2(\alpha r)r\,dr=\frac{1}{2\alpha^2}(\alpha^2-\nu^2+u^2)J_\nu^2(\alpha), \tag{27}$$

and the normalized Schafheitlin formula reads as

$$\int_0^1 dr\overline{J}_\nu^2(\alpha r)r^{\mu+2}=\frac{\mu+1}{\mu+2}\,\frac{(\nu^2-(\mu+1)^2/4)}{\alpha^2}\int_0^1 dr\,\overline{J}_\nu^2(\alpha r)r^\mu + \frac{1}{\mu+2}\left(1+\frac{(\mu+1)\left(u+\frac{1}{2}(\mu+1)\right)}{\alpha^2-\nu^2+u^2}\right). \tag{28}$$

Continuing as in the Dirichlet case, and defining $S[1+2p]$ as in (22), we find the reduction formula,

$$S[1+2p]=\frac{2p}{2p+1}\,\frac{\nu^2-p^2}{\alpha^2}S[2p-1]+\frac{1}{2p+1}\left(1+\frac{2p(u+p)}{\alpha^2+u^2-\nu^2}\right). \tag{29}$$

Explicitly, this gives the following form:

$$S[1+2p]=\sum_{m=0}^{p}\left(\frac{\nu}{\alpha}\right)^{2m}\sum_{l=0}^{m}\gamma_{ml}^p\nu^{-2l}+\frac{1}{\alpha^2+u^2-\nu^2}\sum_{m=0}^{p-1}\left(\frac{\nu}{\alpha}\right)^{2m}\sum_{l=0}^{n}\delta_{ml}^p\nu^{-2l}, \tag{30}$$

where the γ_{ml}^p are the same as in (25) and the δ_{ml}^p are also easily determined by machine.

For the ζ function we have

$$\zeta^{\mathrm{Rob}}(F;s)=\sum\int_\gamma\frac{dk}{2\pi i}k^{-2s}\int_0^1 dr\,F(r)\overline{J}_\nu^2(kr)rd(\nu)\,\frac{\partial}{\partial k}\ln G_\nu(k), \tag{31}$$

where the contour γ has to be chosen so as to enclose the zeros of *only* $G_\nu(k)$. Thus the poles of $S[1+2p]$, located at $k=\pm\sqrt{\nu^2-u^2}$ must be outside the contour. It is important to locate the contour properly because, when deforming it to the imaginary axis, contributions from the pole at $k=\sqrt{\nu^2-u^2}$ arise.

As a result, apart from contributions identical to (26), with the usual changes between Dirichlet and Robin boundary conditions,[13] we have the extra pieces

$$\zeta^p_\delta(F;s)=\frac{\sin\pi s}{\pi}\sum\ d(\nu)\sum_{m=0}^{p-1}\sum_{l=0}^{m}\delta^p_{ml}\nu^{-2l}$$
$$\times\int_{m/\nu}^{\infty}dz\,\frac{[(z\nu)^2-m^2]^{-s}}{u^2-\nu^2(1+z^2)}z^{-2m}\frac{\partial}{\partial z}\ln(uI_\nu(z\nu)+z\nu I'_\nu(\nu z)), \tag{32}$$

$$\zeta^p_{\rm shift}(F;s)=-\frac{1}{2}\sum_{m=0}^{p-1}\sum_{l=0}^{m}\delta^p_{ml}\sum\ d(\nu)\,\nu^{2m-2l}(\nu^2-u^2)^{-s-m-1/2}$$
$$\times\frac{\partial}{\partial k}\ln(kJ'_\nu(k)+uJ_\nu(k))|_{k=\sqrt{\nu^2-u^2}}, \tag{33}$$

the last one arising on moving the contour over the pole at $k=\sqrt{\nu^2-u^2}$. These are the contributions additional to those in the Dirichlet case. The index p refers to the fact that these are the contributions coming from the power r^p in (21). In order to obtain the full zeta function, the $\Sigma_{p=0}^{N}f_p\zeta^p$ has to be done.

Looking at (32), we first define the asymptotic contributions $A^p_{i,\delta}(F;s)$ in the same manner as before by taking the different terms in the asymptotic expansion of the argument of the logarithm. We illustrate the calculation by dealing with

$$A^p_{-1,\delta}(F;s)=\frac{\sin\pi s}{\pi}\sum\ d(\nu)\sum_{m=0}^{p-1}\sum_{l=0}^{m}(-1)^m\delta^p_{ml}\nu^{1-2l}$$
$$\times\int_{m/\nu}^{\infty}dz\,\frac{[(z\nu)^2-m^2]^{-s}}{u^2-\nu^2(1+z^2)z^{2m+1}}(1+z^2)^{1/2}. \tag{34}$$

Using the expansion for small u,

$$\frac{1}{u^2-\nu^2(1+z^2)}=-\sum_{i=0}^{\infty}\frac{u^{2i}}{(\nu^2)^{i+1}(1+z^2)^{i+1}},$$

one arrives at

$$A^p_{-1,\delta}(F;s)=-\frac{\sin\pi s}{\pi}\sum_{i=0}^{\infty}u^{2i}\sum\ d(\nu)\sum_{m=0}^{p-1}\sum_{l=0}^{m}(-1)^m\delta^p_{ml}\nu^{-1-2i-2l}$$
$$\times\int_{m/\nu}^{\infty}dz\,\frac{[(z\nu)^2-m^2]^{-s}}{(1+z^2)^{i+1/2}z^{2m+1}}. \tag{35}$$

At this point we can continue as in previous articles by realizing that the above integrals are representations of a hypergeometric function.[20] With the help of their Mellin–Barnes representation,[20] the ν summation can be done, yielding the base ζ function, and in the massless case our final result reads as

$$A^p_{-1,\delta}(F;s)=\frac{1}{2\Gamma(s)}\sum_{i=0}^{\infty}u^{2i}\sum_{m=0}^{p-1}\sum_{l=0}^{m}\delta^p_{ml}$$
$$\times\frac{\Gamma(-s-m)\Gamma(s+i+m+1/2)}{\Gamma(-s+1)\Gamma(i+1/2)}\zeta_{\mathcal{M}}(s+l+i+1/2). \tag{36}$$

In the same way one obtains for the other $A^p_{i,\delta}(s)$,

$$A^p_{0,\delta}(F;s) = -\frac{1}{4\Gamma(s)}\sum_{i=0}^{\infty}\frac{u^{2i}}{\Gamma(i+2)}\sum_{m=0}^{p-1}\sum_{l=0}^{m}(-1)^m\delta^p_{ml} \times\frac{\Gamma(s+i+m+1)\Gamma(1-s-m)}{\Gamma(1-s)}\zeta_{\mathcal{N}}(s+i+l+1), \tag{37}$$

$$A^p_{n,\delta}(F;s) = \frac{1}{2\Gamma(s)}\sum_{i=0}^{\infty}u^{2i}\sum_{m=0}^{n-1}\sum_{l=0}^{m}(-1)^m\delta^p_{ml}\sum_{b=0}^{n}x_{n,b}(n+2b) \times\frac{\Gamma(1-s-m)\Gamma(s+i+n/2+b+m+1)}{\Gamma(1-s)\Gamma(i+n/2+b+2)}\zeta_{\mathcal{N}}(s+i+l+1+n/2). \tag{38}$$

These forms are well suited for machine evaluation and the residues relevant for the heat-kernel expansion are thereby quickly determined.

The remaining task is to deal with $\zeta^p_{\text{shift}}(F;s)$ defined in (33). To get the relevant residues we need the asymptotic behavior of J_ν, information that can be found in Abramowitz and Stegun.[17] Ultimately, as a practical application, we want to restrict the general form of the $A_{5/2}$ coefficient, and so, restricting the calculation to the order necessary for this coefficient, we arrive at

$$\zeta^p_{\text{shift}}(F;s) = -\frac{1}{2}\sum_{m=0}^{p-1}\sum_{l=0}^{m}\delta^p_{ml} \times(u\zeta_{\mathcal{N}}(s+l+1)+u^3(s+m+1)\zeta_{\mathcal{N}}(s+l+2)+\cdots), \tag{39}$$

after some algebra. As mentioned, the dots indicate contributions having their rightmost pole to the left of $s=(D-5)/2$.

All the relevant results for the calculation up to the $A_{5/2}$ coefficient are now on hand. It would be possible to go further, if desired. (But see our cautionary note at the end.)

III. HEAT-KERNEL COEFFICIENTS ON GENERAL MANIFOLDS

In this section we describe the restrictions placed on the general form of the heat-kernel coefficients by our special case evaluation. Because the case we treat has a vanishing Riemann tensor and constant extrinsic curvature, it cannot, in general, determine the complete coefficient. However, supplemented by a lemma on product manifolds and using relations of the heat-kernel coefficients under conformal rescalings,[8] we will develop a very effective scheme for their calculation. Although for Dirichlet and Robin conditions the coefficients are already completely known up to A_2, we will describe our procedure by starting with these low coefficients. We will see that the lower the coefficient the more restrictive is the special case; a ball calculation. This opens up for future applications the possibility of applying our approach to spectral boundary conditions[21–23] and to boundary conditions involving tangential derivatives discussed recently in the context of the quantization of gauge fields in the presence of boundaries.[24–27]

In what follows we will take the standpoint that the volume part of the coefficients is known. This is motivated by the fact that its calculation is purely algebraic and very effective schemes already exist.[1,2,7] In contrast, the boundary contributions are not determined purely algebraically, and their evaluation turns out to be much more involved. It is here that our special case evaluation of the smeared coefficients on the ball gives the additional information necessary for the complete calculation of the coefficients. We will show the effectiveness of the scheme by giving all of $A_{5/2}$, but we first explain things in detail, starting from the lower coefficients.

Some notation is needed. Here and in the following $F[\mathcal{M}]=\int_{\mathcal{M}}dx\,F(x)$ and $F[\partial\mathcal{M}]=\int_{\partial\mathcal{M}}dy\,F(y)$, with dx and dy being the Riemannian volume elements of $\mathcal{M}$ and $\partial\mathcal{M}$. In addition, '';'' denotes differentiation with respect to the Levi-Civita connection of $\mathcal{M}$ and '':'' covariant differentiation tangentially with respect to the Levi-Civita connection of the boundary.

Finally, our sign convention is $R^i_{jkl}=-\Gamma^i_{jk,l}+\Gamma^i_{jl,k}+\Gamma^i_{nk}\Gamma^n_{jl}-\Gamma^i_{nl}\Gamma^n_{jk}$ (see, for example Ref. 28). To state the general form of the coefficients define the partial differential operator,

$$P=-\Delta-E,$$

together with Dirichlet or Robin boundary conditions,

$$\mathcal{B}^-\phi\equiv\phi|_{\partial\mathcal{M}} \quad \text{and} \quad \mathcal{B}^+_S\phi\equiv(\phi_{;m}-S\phi)|_{\partial\mathcal{M}}.$$

To have a uniform notation we set $S=0$ for Dirichlet boundary conditions and write $B^{\mp}_S$. Let $D_{\mathcal{B}}$ be the operator defined by the appropriate boundary conditions.

If F is a smooth function on $\mathcal{M}$, there is an asymptotic series as $t\to 0$ of the form

$$\mathrm{Tr}_{L^2}(Fe^{-tP_{\mathcal{B}}})\approx\sum_{n\geqslant 0} t^{(n-D)/2}a_n(F,P_{\mathcal{B}}),$$

where the $a_n(F,P_{\mathcal{B}})$ are locally computable.[29]

We now state, one by one, the general form of the coefficients and compare them with our special case evaluation. For convenience we will drop the index $\mathcal{B}$ of the operator P. The coefficient A_0 is, by normalization,

$$A_0(F,P)=(4\pi)^{-D/2}F[\mathcal{M}].$$

The next one is

$$A_{1/2}(F,P)=\delta(4\pi)^{-d/2}F[\partial\mathcal{M}].$$

For the ball this means

$$A_{1/2}(F,P)=\delta(4\pi)^{-d/2}F(1)\mathrm{vol}(S^d).$$

Using the relations (26) and (36)–(39) we can immediately determine δ,

$$\delta=\left(-\frac{1^-}{4},\frac{1^+}{4}\right).$$

The coefficient $A_{1/2}$ is thus given for a general manifold from the result on the ball (which was clear, of course). Passing on to A_1, the general form is

$$A_1(F,P)=(4\pi)^{-D/2}6^{-1}\{(6FE+FR)[\mathcal{M}]+(b_0FK+b_1F_{;m}+b_2FS)[\partial\mathcal{M}]\}.$$

In our special case on the ball, $K^b_a=\delta^b_a$, and thus

$$A_1(F,P)=(4\pi)^{-D/2}6^{-1}\,\mathrm{vol}(S^d)\{b_0F(1)d+b_1F'(1)+b_2F(1)S\}.$$

Comparing with the results given in the previous section, one finds

$$b_0=2;\quad b_1=(3^-,-3^+);\quad b_2=12.$$

Thus, our special case also gives the entire A_1 coefficient without any further information being needed. It is very important that the calculation can be performed for an arbitrary ball dimension, D, and also for a smearing function $F(r)$. This allows one just to compare polynomials in d with the associated extrinsic curvature terms in the general expression and simply to read off the universal constants in this expression.

The idea is now clear and in the following we will state only the general expression and the restrictions found from the special case presented in the previous section. We continue with the next higher coefficient, with the general form

$$A_{3/2}(F,P)=\frac{\delta}{96(4\pi)^{d/2}}(F(c_0E+c_1R+c_2R_{mm}+c_3K^2+c_4K_{ab}K^{ab}+c_7SK+c_8S^2)$$
$$+F_{;m}(c_5K+c_9S)+c_6F_{;mm})[\partial\mathcal{M}].$$

The ball calculation immediately gives seven of the ten unknowns,

$$c_3=(7^-,13^+),\quad c_4=(-10^-,2^+),\quad c_5=(30^-,-6^+),$$

$$c_6=24,\quad c_7=96,\quad c_8=192,\quad c_9=-96.$$

We next apply the lemma on product manifolds mentioned above.[8] Let $N^\nu(F)=F_{;m\ldots}$ be the νth normal covariant derivative. There exist local formulas $a_n(x,P)$ and $a_{n,\nu}(y,D)$, so that

$$A_n(F,P,\mathcal{B}_S^{\mp})=\{FA_n(x,P)\}[\mathcal{M}]+\left\{\sum_{\nu=0}^{2n-1}N^\nu(F)A_{n,\nu}(y,P,\mathcal{B}_S^{\mp})\right\}[\partial\mathcal{M}].$$

Let $\mathcal{M}=\mathcal{M}_1\times\mathcal{M}_2$ and $P=P_1\otimes 1+1\otimes P_2$ and $\partial\mathcal{M}_2=\varnothing$. Then

$$A_{n,\nu}(y,P,\mathcal{B}_S^{\mp})=\sum_{p+q=n}A_{p,\nu}(y_1,P_1,\mathcal{B}_S^{\mp})A_q(x_2,P_2).$$

For $A_{3/2}$ this means

$$A_{3/2}(y,P)=A_{3/2}(y_1,P_1)A_0(x_2,P_2)+A_{1/2}(y_1,P_1)A_1(x_2,P_2).$$

We will choose $P_1=-\Delta_1$ and $P_2=-\Delta_2-E(x_2)$ with obvious notation to obtain

$$\delta 96^{-1}(c_0E+c_1R(\mathcal{M}_2))=\delta 6^{-1}(6E+R(\mathcal{M}_2)),$$

where we used, in addition, $R(\mathcal{M}_1\times\mathcal{M}_2)=R(\mathcal{M}_1)+R(\mathcal{M}_2)$. This gives

$$c_0=96,\quad c_1=16.$$

It is seen that the determination of $A_{3/2}$ is relatively simple, once the ball result is on hand. The lemma on product manifolds is also very easily applied and already only one of the universal constants c_i, namely c_2, is missing.

The remaining information is obtained using the relations between the heat-kernel coefficients under conformal rescaling,[8]

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0}a_n(1,e^{-2\epsilon F}P)-(D-2n)a_n(F,P)=0. \tag{40}$$

Setting to zero the coefficients of all terms in (40) gives several relations between the universal constant c_i. We will need only one of them. Thus, setting to zero the coefficient of $F_{;mm}$ gives

$$\tfrac{1}{2}(D-2)c_0-2(D-1)c_1-(D-1)c_2-(D-3)c_6=0,$$

and so $c_2=-8$ for Dirichlet and Robin boundary conditions. This completes the calculation of $A_{3/2}$.

We continue with the treatment of A_2. Its general form is[8]

$$
\begin{aligned}
A_2(F,P)=(4\pi)^{-D/2}360^{-1}\{&F(60\Delta E+60RE+180E^2+12\Delta R+5R^2-2R_{ij}R^{ij}\\
&+2R_{ijkl}R^{ijkl})[\mathcal{M}]+[F(d_1E_{;m}+d_2R_{;m}+d_3K^a_{:a}+d_4K_{ab:}{}^{ab}+d_5EK\\
&+d_6RK+d_7R_{mm}K+d_8R_{ambm}K^{ab}+d_9R_{abc}{}^bK^{ac}+d_{10}K^3\\
&+d_{11}K_{ab}K^{ab}K+d_{12}K_{ab}K^b_cK^{ac}+d_{13}SE+d_{14}SR+d_{15}SR_{mm}\\
&+d_{16}SK^2+d_{17}SK_{ab}K^{ab}+d_{18}KS^2+d_{19}S^3+d_{20}S^a_{:a})\\
&+F_{;m}(e_1E+e_2R+e_3R_{mm}+e_4K^2+e_5K_{ab}K^{ab}+e_8SK+e_9S^2)\\
&+F_{;mm}(e_6K+e_{10}S)+e_7(\Delta F)_{;m}][\partial\mathcal{M}]\}. \qquad (41)
\end{aligned}
$$

The ball calculation gives

$$
\begin{gathered}
d_{10}=(40/21^-,40/3^+),\quad d_{11}=(-88/7^-,8^+),\quad d_{12}=(320/21^-,32/3^+),\\
d_{16}=144,\quad d_{17}=48,\quad d_{18}=480,\quad d_{19}=480,\\
e_4=(180/7^-,-12^+),\quad e_5=(-60/7^-,-12^+),\quad e_6=24,\\
e_7=(30^-,-30^+),\quad e_8=-72,\quad e_9=-240,\quad e_{10}=120. \qquad (42)
\end{gathered}
$$

The product formula here reads as

$$
A_2(y,P)=A_2(y_1,P_1)A_0(x_2,P_2)-A_0(y_1,P_1)A_2(x_2,P_2)+A_1(y_1,P_1)A_1(x_2,P_2),
$$

and leads to the universal constants,

$$
\begin{gathered}
d_5=120,\quad d_6=20,\quad d_{13}=720,\quad d_{14}=120,\\
e_1=(180^-,-180^+)\quad e_2=(30^-,-30^+). \qquad (43)
\end{gathered}
$$

These two inputs already give 20 of the 30 unknowns; the remaining 10 are determined by the conformal rescaling (40),

$$
\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} a_2(1,e^{-2\epsilon F}P)-(D-4)a_2(F,P)=0. \qquad (44)
$$

Having already evaluated many of the constants only a few more relations are required to fix the remaining ones. In the following list, we give, on the left, the term in (44) whose coefficient is equated to zero.

Term	Coefficient
$EF_{;m}$	$0=-2d_1+60(D-6)+d_5(D-1)-(D-4)e_1-\frac{1}{2}(D-2)d_{13}$
$(\Delta F)_{;m}$	$0=6(D-6)+\frac{1}{2}(D-2)d_1-2(D-1)d_2-(D-4)e_7$
$F_{:a}K^a_:$	$0=-4(D-6)+(D-4)d_3-\frac{1}{2}(D-2)d_5+2(D-1)d_6+d_7+d_9$
$KF_{;mm}$	$0=\frac{1}{2}(D-2)d_5-2(D-1)d_6-(D-1)d_7-d_8-(D-4)e_6$
$K_{ab:}{}^bF^a_:$	$0=(D-4)d_4+d_8+(D-3)d_9+4(D-6)$
$R_{mm}F_{;m}$	$0=(D-1)d_7+d_8-2d_9+e_3+4(D-6)-\frac{1}{2}(D-2)d_{15}$

$$F_{:a}S^{a}_{:} \qquad 0=-\tfrac{1}{2}(D-2)d_{13}+2(D-1)d_{14}+d_{15}+(D-4)d_{20}. \tag{45}$$

From here one finds the universal constants,

$$\begin{gathered} d_1=(120^-,-240^+), \quad d_2=(18^-,-42^+), \quad d_3=24, \quad d_4=0, \\ d_7=-4, \quad d_8=12, \quad d_9=-4, \quad d_{15}=0, \quad d_{20}=120, \quad e_3=0. \end{gathered} \tag{46}$$

This completes the evaluation of A_2 and we finally come to the calculation of $A_{5/2}$, which, for an arbitrary smearing function F, has been calculated only for a totally geodesic boundary $\partial\mathcal{M}$. When $F=1$, it has been determined for $\mathcal{M}$ a domain of $\mathbb{R}^m$.

It has been shown that for a smooth, but not necessarily totally geodesic, boundary there exist universal constants such that

$$\begin{aligned} A_{5/2}(F,P)=&\mp 5760^{-1}(4\pi)^{-d/2}\{F\{g_1E_{;mm}+g_2E_{;m}S+g_3E^2+g_4E_{:a}{}^{a}+g_5RE+120\Omega_{ab}\Omega^{ab} \\ &+g_6\Delta R+g_7R^2+g_8R_{ij}R^{ij}+g_9R_{ijkl}R^{ijkl}+g_{10}R_{mm}E+g_{11}R_{mm}R+g_{12}RS^2 \\ &+(-360^-,90^+)\Omega_{am}\Omega^{a}{}_{m}+g_{13}R_{;mm}+g_{14}R_{mm:a}{}^{a}+g_{15}R_{mm;mm}+g_{16}R_{;m}S \\ &+g_{17}R_{mm}S^2+g_{18}SS_{:a}{}^{a}+g_{19}S_{:a}S^{a}_{:}+g_{20}R_{ammb}R^{ab}+g_{21}R_{mm}R_{mm}+g_{22}R_{ammb}R^{a}{}_{mb}{}^{a} \\ &+g_{23}ES^2+g_{24}S^4\}+F_{;m}\{g_{25}R_{;m}+g_{26}RS+g_{27}R_{mm}S+g_{28}S_{:a}{}^{a}+g_{29}E_{;m}+g_{30}ES \\ &+g_{31}S^3\}+F_{;mm}\{g_{32}R+g_{33}R_{mm}+g_{34}E+g_{35}S^2\}+g_{36}SF_{;mmm}+g_{37}F_{;mmmm} \\ &+F\{d_1KE_{;m}+d_2KR_{;m}+d_3K^{ab}R_{ammb;m}+d_4KS_{:b}{}^{b}+d_5K_{ab}S^{ab}_{:}+d_6K_{:b}S^{b}_{:} \\ &+d_7K_{ab:}{}^{a}S^{b}_{:}+d_8K_{:b}{}^{b}S+d_9K_{ab:}{}^{ab}S+d_{10}K_{:b}K^{b}_{:}+d_{11}K_{ab:}{}^{a}K^{b}_{:}+d_{12}K_{ab:}{}^{a}K^{bc}{}_{:c} \\ &+d_{13}K_{ab:c}K^{ab}{}_{:}{}^{c}+d_{14}K_{ab:c}K^{ac}{}_{:}{}^{b}+d_{15}K_{:b}{}^{b}K+d_{16}K_{ab:}{}^{ab}K+d_{17}K_{ab:}{}^{a}{}_{c}K^{bc} \\ &+d_{18}K_{:bc}K^{bc}+d_{19}K_{bc:a}{}^{a}K^{bc}+g_{38}KSE+d_{20}KSR_{mm}+g_{39}KSR+d_{21}K_{ab}R^{ab}S \\ &+d_{22}K^{ab}SR_{ammb}+g_{40}K^2E+g_{41}K_{ab}K^{ab}E+g_{42}K^2R+g_{43}K_{ab}K^{ab}R+d_{23}K^2R_{mm} \\ &+d_{24}K_{ab}K^{ab}R_{mm}+d_{25}KK_{ab}R^{ab}+d_{26}KK^{ab}R_{ammb}+d_{27}K_{ab}K^{ac}R^{b}_{c}+d_{28}K^{b}_{a}K^{ac}R_{bmmc} \\ &+d_{29}K_{ab}K_{cd}R^{acbd}+d_{30}KS^3+d_{31}K^2S^2+d_{32}K_{ab}K^{ab}S^2+d_{33}K^3S+d_{34}KK_{ab}K^{ab}S \\ &+d_{35}K_{ab}K^{bc}K^{a}_{c}S+d_{36}K^4+d_{37}K^2K_{ab}K^{ab}+d_{38}K_{ab}K^{ab}K_{cd}K^{cd}+d_{39}KK_{ab}K^{bc}K^{a}_{c} \\ &+d_{40}K_{ab}K^{bc}K_{cd}K^{da}\}+F_{;m}\{g_{44}KE+d_{41}KR_{mm}+g_{45}KR+d_{42}KS^2+d_{43}K_{:b}{}^{b} \\ &+d_{44}K_{ab:}{}^{ab}+d_{45}K_{ab}R^{ab}+d_{46}K^{ab}R_{ammb}+d_{47}K^2S+d_{48}K_{ab}K^{ab}S+d_{49}K^3 \\ &+d_{50}KK_{ab}K^{ab}+d_{51}K_{ab}K^{bc}K^{a}_{c}\}+F_{;mm}\{d_{52}KS+d_{53}K^2+d_{54}K_{ab}K^{ab}\}+d_{55}KF_{;mmm}\} \\ &[\partial\mathcal{M}]. \end{aligned} \tag{47}$$

In this case, specializing to the ball gives

$$g_{24}=1440,\quad g_{31}=-720,$$
$$g_{35}=360,\quad g_{36}=-180,$$
$$g_{37}=45,\quad d_{30}=2160,$$
$$d_{31}=1080,\quad d_{32}=360,$$
$$d_{33}=885/4,\quad d_{34}=315/2,$$
$$d_{35}=150,\quad d_{36}=(-65/128^{-},2041/128^{+}),$$
$$d_{37}=(-141/32^{-},417/32^{+}),\quad d_{40}=(-327/8^{-},231/8^{+}),$$
$$d_{42}=-600,\quad d_{47}=-705/4,$$
$$d_{48}=75/2,\quad d_{49}=(495/32^{-},-459/32^{+}),$$
$$d_{50}=(-1485/16^{-},-267/16^{+}),\quad d_{51}=(225/2^{-},54^{+}),$$
$$d_{52}=30,\quad d_{53}=(1215/16^{-},315/16^{+}),$$
$$d_{54}=(-954/8^{-},-645/8^{+}),\quad d_{55}=(105^{-},30^{+}),$$

and $d_{38}+d_{39}=(1049/32^{-},1175/32^{+})$.

The product formula explicitly reads as

$$A_{5/2}(y,P)=A_{5/2}(y_1,P_1)A_0(x_2,P_2)+A_{3/2}(y_1,P_1)A_1(x_2,P_2)+A_{1/2}(y_1,P_1)A_2(x_2,P_2),$$

which gives the 22 universal constants,

$$g_3=720,\quad g_5=240,\quad g_6=48,\quad g_7=20,$$
$$g_8=-8,\quad g_9=8,\quad g_{10}=-120,\quad g_{11}=-20,$$
$$g_{12}=480,\quad g_{23}=2880,\quad g_{26}=-240,\quad g_{30}=-1440,$$
$$g_{32}=60,\quad g_{34}=360,\quad g_{38}=1440,\quad g_{39}=240,$$
$$g_{40}=(105^{-},195^{+}),\quad g_{41}=(-150^{-},30^{+}),\quad g_{42}=(105/6^{-},195/6^{+}),$$
$$g_{43}=(-25^{-},5^{+}),\quad g_{44}=(450^{-},-90^{+}),\quad g_{45}=(75^{-},-15^{+})$$

All this information puts us in a very good position to use the relations between the heat-kernel coefficients that result from conformal rescalings. The relevant relation reads as

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} A_{5/2}(1,e^{-2\epsilon F}P)-(D-5)A_{5/2}(F,P)=0. \tag{48}$$

Setting to zero the coefficients of all terms in (48), we obtain the equations given in (50). (They are ordered in such a way that nearly every equation immediately yields a universal constant. This was the main motivation for the given ordering.) Using the relation (50), we find

$$g_1=360,\quad g_2=-1440,\quad g_4=240,$$
$$g_{13}=12,\quad g_{14}=24,\quad g_{15}=15,$$
$$g_{16}=-270,\quad g_{17}=120,\quad g_{18}=960,$$
$$g_{19}=600,\quad g_{20}=-16,\quad g_{21}=-17,$$
$$g_{22}=-10,\quad g_{25}=(60^{-},195/2^{+}),\quad g_{27}=90,$$

$$g_{28}=-270, \quad g_{29}=(450^{-},630^{+}), \quad g_{33}=-90,$$

$$d_1=(450^{-},-90^{+}), \quad d_2=(42^{-},-111/2^{+}), \quad d_3=(0^{-},30^{+}),$$

$$d_4=240, \quad d_5=420, \quad d_6=390,$$

$$d_7=480, \quad d_8=420, \quad d_9=60,$$

$$d_{20}=30, \quad d_{21}=-60, \quad d_{22}=-180.$$

Thus, the equations given up to this point allow for the determination of the universal constants apart from two groups. The first group is $d_{23},\ldots,d_{29},d_{38},d_{39},d_{41},d_{45},d_{46}$ and the second one, $d_{10},\ldots,d_{19},d_{43},d_{44}$. The first group is completely determined using the relations given in (51). One finds

$$d_{23}=(-215/16^{-},-275/16^{+}), \quad d_{24}=(-215/8^{-},-275/8^{+}),$$

$$d_{25}=(14^{-},-1^{+}), \quad d_{26}=(-49/4^{-},-109/4^{+}),$$

$$d_{27}=16, \quad d_{28}=(47/2^{-},-133/2^{+}),$$

$$d_{29}=32, \quad d_{38}=(777/32^{-},375/32^{+}),$$

$$d_{39}=(17/2^{-},25^{+}), \quad d_{41}=(-255/8^{-},165/8^{+}),$$

$$d_{45}=(-30^{-},-15^{+}), \quad d_{46}=(-465/4^{-},-165/4^{+}).$$

Finally, we consider the second group mentioned above. As we will see, one needs just one more relation in addition to those obtained from Eq. (48), which are presented in (52). They yield

$$d_{11}=(58^{-},238^{+}), \quad d_{15}=(6^{-},111^{+}),$$

$$d_{16}=(-30^{-},-15^{+}), \quad d_{19}=(54^{-},114^{+}),$$

together with the relations

$$2d_{10}+d_{43}=-91, \quad 2d_{10}-d_{18}=(-983/8^{-},-1403/8^{+}),$$

$$2d_{14}-3d_{18}=(-913/4^{-},-2533/4^{+}), \quad d_{13}+d_{14}=(297/8^{-},837/8^{+}),$$

$$d_{18}-d_{44}=(60^{-},225^{+}), \quad 2d_{12}-2d_{17}-d_{18}=(-7/4^{-},-787/4^{+}),$$

$$2d_{12}-d_{17}=32.$$

This is all we can get with the relation (48). It is seen that, given d_{43} or d_{44}, for example, the remaining constants can be determined. This is achieved with the equation (8)

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} A_{5/2}(e^{-2\epsilon f}F,e^{-2\epsilon f}P)=0, \quad \text{for } D=7. \tag{49}$$

Thus, finally, one gets

$$d_{10}=(-413/16^{-},487/16^{+}), \quad d_{12}=(-11/4^{-},49/4^{+}),$$

$$d_{13}=(355/8^{-},535/8^{+}), \quad d_{14}=(-29/4^{-},151/4^{+}),$$

$$d_{17}=(-75/2^{-},-15/2^{+}),\quad d_{18}=(285/4^{-},945/4^{+}),$$

$$d_{43}=(-315/8^{-},-1215/8^{+}),\quad d_{44}=45/4,$$

which concludes the calculation of the complete $A_{5/2}$ coefficient on a smooth manifold with a boundary. All terms not displayed in the above lists have been used as checks on the computed universal constants.

IV. CONCLUSIONS

In this article we have developed a technique for the calculation of smeared heat-kernel coefficients on the generalized cone. This is a generalization of our previous work,[13] where we treated the $F=1$ case only. All technical and aesthetic advantages emphasized previously are still present for arbitrary F. Namely, by restricting attention to the ball, and using a function F as general as needed, the coefficients can be found as polynomials in the dimension of the ball. This has the advantage that the special case evaluation can easily be used to put restrictions on the general form of the heat-kernel coefficients. This idea was applied to the coefficients $A_0,\ldots,A_{5/2}$ for Dirichlet and Robin boundary conditions. Supplemented by a lemma on product manifolds and relations from conformal rescalings, we have shown that starting with the results of the special case, treated here for the first time, the complete coefficients are obtained very effectively.

The method is clearly capable of being applied to other situations. An example of even more complexity is the generalized boundary condition involving tangential derivatives of the field.[24–27] Up to now, for this case, we have applied the technique of special case evaluation only to the four-dimensional ball.[30] The treatment of the D-dimensional ball is under consideration with the aim of finding the general form of the coefficients using the ideas presented here. Another situation of interest is the spectral boundary condition applied to spinor fields. These conditions are nonlocal and it is known that the relations obtained with conformal techniques are not sufficient for the determination of the entire coefficient.[31] However, supplemented by the ball calculation, it is possible to find at least the lower coefficients in this case too. We reserve exposition of these extensions for later.

A general word of caution, however. The evaluation of higher and higher coefficients quickly becomes prodigiously complicated, even for just the volume terms, and there is the danger of it becoming an end in itself. The question is whether there is any value in displaying an impenetrable profusion of terms, without some strong motivation. As far as the boundary terms go, we feel that with $A_{5/2}$ we probably have reached the limit of what can sensibly be calculated and displayed. Already the expressions are becoming unwieldy. Further progress in this area should, we think, be limited to extending the class of manifolds, say to those with nonsmooth boundaries, and to the consideration of other fields and boundary conditions as indicated in the preceding paragraph.

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APPENDIX

In this appendix we list the relations resulting from the conformal property (48).
The first group of relations is

Term	Coefficient
$EF_{;mm}$	$0=-2g_1+(D-2)g_3-2(D-1)g_5-(D-1)g_{10}-(D-5)g_{34}$

$$ESF_{;m} \quad 0=-2g_2-(D-2)g_{23}+(D-1)g_{38}-(D-5)g_{30}$$

$$SF_{;mmm} \quad 0=\tfrac{1}{2}(D-2)g_2-2(D-1)g_{16}-(D-5)g_{36}$$

$$KSF_{;mm} \quad 0=\tfrac{1}{2}(D-2)g_2-2(D-1)g_{16}+\tfrac{1}{2}(D-2)g_{38}-(D-1)d_{20}-2(D-1)g_{39}$$
$$-d_{21}+d_{22}-(D-5)d_{52}$$

$$FE_{:a}{}^{a} \quad 0=-g_1+(D-2)g_3-(D-5)g_4-2(D-1)g_5-g_{10}$$

$$F_{;mmmm} \quad 0=\tfrac{1}{2}(D-2)g_1-2(D-1)g_6-2(D-1)g_{13}-(D-1)g_{15}-(D-5)g_{37}$$

$$F\Delta R \quad 0=\tfrac{1}{2}(D-2)g_5-(D-4)g_6-4(D-1)g_7-Dg_8-4g_9-g_{11}-g_{13}+\tfrac{1}{2}g_{20}$$

$$FR_{;mm} \quad 0=-\tfrac{1}{2}(D-2)g_5+(D-4)g_6+4(D-1)g_7+2(D-1)g_8+8g_9+g_{11}+g_{13}$$
$$-2g_{15}-\frac{D}{2}g_{20}+g_{22}$$

$$FR_{mm:a}{}^{a} \quad 0=\tfrac{1}{2}(D-2)g_1-2(D-1)g_6+\tfrac{1}{2}(D-2)g_{10}-2(D-1)g_{11}-2(D-1)g_{13}$$
$$-(D-5)g_{14}-2g_{15}+(D-1)g_{20}-2g_{21}-2g_{22}$$

$$F_{;mm}S^2 \quad 0=-2(D-1)g_{12}-(D-1)g_{17}+\tfrac{1}{2}(D-2)g_{23}-(D-5)g_{35}$$

$$FS_{:a}S^{a}_{:} \quad 0=-4(D-1)g_{12}-2g_{17}-(D-3)g_{18}+2g_{19}+(D-2)g_{23}$$

$$F_{;m}E_{;m} \quad 0=-5g_1-\tfrac{1}{2}(D-2)g_2+(D-1)d_1-(D-5)g_{29}$$

$$F_{;mmm}K \quad 0=\tfrac{1}{2}(D-2)g_1-4(D-1)g_6-2(D-1)g_{13}-g_{15}+\tfrac{1}{2}(D-2)d_1$$
$$-2(D-1)d_2+d_3-(D-5)d_{55}$$

$$F_{;m}R_{;m} \quad 0=-\tfrac{1}{4}(D-2)g_1+(2D-7)g_6+(D-6)g_{13}-2g_{15}-\tfrac{1}{2}(D-2)g_{16}$$
$$+(D-1)d_2-\tfrac{1}{2}d_3-(D-5)g_{25}$$

$$F_{;mm}R_{mm} \quad 0=-(D-2)g_1+4(D-1)g_6-2(D-2)g_8-8g_9+\tfrac{1}{2}(D-2)g_{10}$$
$$-2(D-1)g_{11}+4(D-1)g_{13}-2(D-1)g_{21}-2g_{22}-(D-5)g_{33}$$

$$F_{;m}R_{mm}S \quad 0=-\tfrac{1}{2}(D-2)g_2+2(D-1)g_{16}-(D-2)g_{17}+(D-1)d_{20}$$
$$-d_{21}-d_{22}-(D-5)g_{27}$$

$$FKS_{:a}{}^{a} \quad 0=-(D-4)d_4-d_5+d_6+d_7-d_8-d_9+\tfrac{1}{2}(D-2)g_{38}$$
$$-d_{20}-2(D-1)g_{39}-d_{21}$$

$$FK_{:a}{}^{a}S \quad 0=\tfrac{1}{2}(D-2)g_2+2(D-1)g_{16}-d_4+d_6-(D-4)d_8$$
$$+\tfrac{1}{2}(D-2)g_{38}-d_{20}-2(D-1)g_{39}-d_{21}$$

$$FK_{ab}S^{ab}_{:} \quad 0=-(D-2)g_2+4(D-1)g_{16}+3d_5-(D-2)d_7+(D-2)d_9$$
$$-(D-2)d_{21}+d_{22}$$

$$FK_{ab:}{}^{ab}S \quad 0=-d_5+d_7-(D-4)d_9-(D-2)d_{21}+d_{22}$$

$$F_{;m}S_{:a}{}^{a} \quad 0=\tfrac{1}{2}(D-2)g_2-2(D-1)g_{16}-(D-2)g_{18}+(D-2)g_{19}+(D-1)d_4 +d_5-(D-1)d_6-d_7+(D-1)d_8+d_9-(D-5)g_{28}. \tag{A1}$$

For the second one we have the following.

Term	Coefficient
$F_{;mm}K_{ab}K^{ab}$	$0=-(D-2)g_1+4(D-1)g_6+4(D-1)g_{13}+2g_{15}+d_3+\tfrac{1}{2}(D-2)g_{41} -2(D-1)g_{43}-(D-1)d_{24}-d_{27}+d_{28}-(D-5)d_{54}$
$F_{;mm}K^2$	$0=-2(D-1)g_6+\tfrac{1}{2}(D-2)d_1-2(D-1)d_2+(D-2)g_{40} -2(D-1)g_{42}-(D-1)d_{23}-d_{25}+d_{26}-(D-5)d_{53}$
$F_{;m}KR$	$0=\tfrac{1}{2}(D-2)g_5-2g_6-4(D-1)g_7-2g_8-g_{11}-2d_2-\tfrac{1}{2}(m-2)g_{39} +2(D-1)g_{42}+2g_{43}+d_{25}-(D-5)g_{45}$
$F_{;m}KR_{mm}$	$0=\tfrac{1}{2}(D-2)g_1+\tfrac{1}{2}(D-2)g_{10}-2(D-1)g_{11}-2(D-1)g_{13}+4g_{15} +g_{20}-2g_{21}-\tfrac{1}{2}(D-2)d_1+2(D-1)d_2+d_3-\tfrac{1}{2}(D-2)d_{20} +2(D-1)d_{23}+2d_{24}-d_{25}-d_{26}-(D-5)d_{41}$
$F_{;m}K_{ab}R^{ab}$	$0=-\tfrac{1}{2}(D-2)g_1+2(D-1)g_6-2(D-2)g_8-8g_9+2(D-1)g_{13} -4g_{15}+g_{20}-d_3-\tfrac{1}{2}(D-2)d_{21}+(D-1)d_{25}+2d_{27}+2d_{29}-(D-5)d_{45}$
$F_{;m}K^{ab}R_{ammb}$	$0=-(D-2)g_1+4(D-1)g_6+4(D-1)g_{13}+2g_{15}-(D-2)g_{20} +2g_{22}-d_3-\tfrac{1}{2}(D-2)d_{22}+(D-1)d_{26}+2d_{28}+2d_{29}-(D-5)d_{46}$
$F_{;m}K_{ab}K^{bc}K_c^a$	$0=(D-2)g_1-4(D-1)g_6-4(D-1)g_{13}-2g_{15}-d_3-(D-2)d_{27} +d_{28}+2d_{29}-\tfrac{1}{2}(D-2)d_{35}+(D-1)d_{39}+4d_{40}-(D-5)d_{51}$
$FR_{ac}K_b^cK^{ab}$	$0=-2(D-2)g_8-8g_9+4g_{15}+g_{20}+2d_3+4d_{13}+4d_{14}-4d_{19} -(D-2)d_{27}+d_{28}+2d_{29}.$

(A2)

Finally, the third group:

Term	Cofficient
$FK_{:b}K^{:b}$	$0=2(D-1)g_6-4g_{15}-(D-2)g_{20}+2g_{22}-\tfrac{1}{2}(D-2)d_1 +2(D-1)d_2+2d_{10}+d_{11}-(D-3)d_{15}-d_{16}-d_{18}+(D-2)g_{40} -4(D-1)g_{42}-2d_{23}-2d_{25}$
$FK_{ab:}{}^{a}K_{:}^{b}$	$0=2(D-2)g_1-4(D-1)g_6-8(D-1)g_{13}+(4D-6)g_{20}-8g_{22} -(D-2)d_1+4(D-1)d_2-(D-3)d_{11}+2d_{12}-2d_{14}+2d_{16} -2d_{17}+2d_{18}-2(D-2)d_{25}+2d_{26}-4d_{29}$

$$
\begin{aligned}
FK_{ab:c}K^{ab\ c}_{\ :} \quad 0 &= (D-2)g_1 - 4(D-1)g_6 - 4(D-1)g_{13} - 2g_{15} + (D-2)g_{20} \\
&\quad - 2g_{22} - 3d_3 + 2d_{13} + 2d_{14} - (D-3)d_{19} + (D-2)g_{41} \\
&\quad - 4(D-1)g_{43} - 2d_{24} - 2d_{27} \\
FKK_{ab:}^{\ \ ab} \quad 0 &= 4(D-2)g_8 + 16g_9 - 4g_{15} - Dg_{20} + 2g_{22} + d_{11} + 2d_{12} - (D-4)d_{16} \\
&\quad - 2d_{17} - d_{18} - (D-2)d_{25} + d_{26} - 2d_{29} \\
F_{:m}K_{:a}^{\ \ a} \quad 0 &= -\tfrac{3}{2}(D-2)g_1 + 4(D-1)g_6 - 4(D-2)g_8 - 16g_9 + 6(D-1)g_{13} \\
&\quad + \tfrac{1}{2}(D-2)d_1 - 2(D-1)d_2 - d_3 - \tfrac{1}{2}(D-2)d_4 + \tfrac{1}{2}(D-2)d_6 \\
&\quad - \tfrac{1}{2}(D-2)d_8 - 2(D-1)d_{10} \\
&\quad - d_{11} - 2d_{13} + 2(D-1)d_{15} + d_{16} + d_{18} + 2d_{19} - (D-5)d_{43} \\
F_{:m}K_{ab:}^{\ \ \ ab} \quad 0 &= \tfrac{1}{2}(D-2)g_1 - 2(D-1)g_6 + 4(D-2)g_8 + 16g_9 - 2(D-1)g_{13} \\
&\quad + 2g_{15} + 2d_3 - \tfrac{1}{2}(D-2)d_5 + \tfrac{1}{2}(D-2)d_7 - \tfrac{1}{2}(D-2)d_9 \\
&\quad - (D-1)d_{11} - 2d_{12} - 2d_{14} + (D-1)d_{16} + 2d_{17} + (D-1)d_{18} \\
&\quad - (D-5)d_{44} \\
FK_{ab:}^{\ \ \ a}K^{bc}_{\ \ :c} \quad 0 &= (4-3D)g_{20} + 6g_{22} - 2d_3 - 2(D-2)d_{12} - 4d_{13} - 2d_{14} \\
&\quad + (D+1)d_{17} + 4d_{19} - (D-2)d_{27} + d_{28} + 2d_{29} \\
FK_{:ab}K^{ab} \quad 0 &= 2(D-2)g_1 - 4(D-1)g_6 - 2(D-2)g_8 - 8g_9 - 8(D-1)g_{13} \\
&\quad + (4D-5)g_{20} - 8g_{22} - (D-2)d_1 + 4(D-1)d_2 - (D-2)d_{11} \\
&\quad - 2d_{14} + (D-2)d_{16} + 3d_{18} - (D-2)d_{25} + d_{26} - 2d_{29}.
\end{aligned} \tag{A3}
$$

This completes the list of relations used for the calculation of the $A_{5/2}$ coefficient.

Note added in proof. As suggested in the Conclusions the method has now been applied to generalized boundary conditions involving tangential derivatives and to spectral boundary conditions. Details can be found in Refs. 32 and 33.

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The complex Bateman equation in a space of arbitrary dimension

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The general solution to the complex Bateman equation in a space of arbitrary dimensions is constructed.
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I. INTRODUCTION

We define the complex Bateman equation in n-dimensional space by analogy with the so-called universal field equation[1] as

$$\det\begin{vmatrix} 0 & \frac{\partial\phi}{\partial\bar{y}_1} & \cdots & \frac{\partial\phi}{\partial\bar{y}_n} \\ \frac{\partial\phi}{\partial y_1} & \frac{\partial^2\phi}{\partial y_1\partial\bar{y}_1} & \cdots & \frac{\partial^2\phi}{\partial x_1\partial\bar{y}_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial\phi}{\partial y_n} & \frac{\partial^2\phi}{\partial y_n\partial\bar{y}_1} & \cdots & \frac{\partial^2\phi}{\partial y_n\partial\bar{y}_n} \end{vmatrix} = 0. \tag{1}$$

Recently it was shown that the general solution to this equation, in the case where $n=2$ is given implicitly, by equating two arbitrary functions of three variables, $F(\phi,y_1,y_2)$ and $G(\phi,\bar{y}_1,\bar{y}_2)$ and solving the resulting equation

$$F(\phi,y_1,y_2)=G(\phi,\bar{y}_1,\bar{y}_2) \tag{2}$$

for $\phi(y_1,y_2,\bar{y}_1,\bar{y}_2)$.[2] After we found this solution, we were astonished to find it set as an exercise as Problem (8) (ii) on page 328 of Chaundy's *The Differential Calculus*, Oxford University Press (1935)![3] This assertion may be readily verified by partial differentiation. The corresponding result for (1) is the subject of this article.

II. EQUIVALENT FIRST-ORDER EQUATIONS

The complex Bateman equation, (1), is the eliminant of $(n+1)$ linear equations which may be written as

$$\sum_{i=1}^{n}\alpha^i\phi_{\bar{y}_i}=0, \quad \phi_{y_s}=\sum_{1}^{n}\alpha^i_{y_s}\phi_{\bar{y}_i}, \tag{3}$$

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where ϕ_{y_i} denotes $\partial\phi/\partial y_i$, etc. Similarly, it is also the eliminant of the equations

$$\sum_{i=1}^{n} \beta^i \phi_{y_i} = 0, \quad \phi_{\bar{y}_s} = \sum_{1}^{n} \beta^i_{\bar{y}_s} \phi_{y_i}. \tag{4}$$

From (3) and (4) it follows that

$$\sum_{s} \alpha^s_{y_i} \beta^k_{\bar{y}_s} = \delta^k_i, \tag{5}$$

or in other words, the above-introduced Jacobian matrices $\alpha^s_{y_i}$ and $\beta^k_{\bar{y}_s}$ are inverses of one another. Let us multiply and sum each equation of the first system (3) by β^s [and carry out a similar operation for system (4)]. We obtain

$$\sum_{i=1}^{n} \beta^s \alpha^i_{y_s} \phi_{\bar{y}_i} = 0, \quad \sum_{1}^{n} \alpha^s \beta^i_{\bar{y}_s} \phi_{y_i} = 0. \tag{6}$$

Now we come to a crucial step; Eq. (6) cannot contain any new information, but will only repeat those equations already quoted. In other words,

$$\sum_{i} \beta^i \alpha^s_{y_i} = \theta \alpha^s \tag{7}$$

for some θ. It follows immediately (taking into account the inverse properties of the above-introduced matrices) in symmetrical fashion that

$$\sum_{i} \alpha^i \beta^s_{\bar{y}_i} = \theta^{-1} \beta^s, \tag{8}$$

which is consistent with the other set of equations. We shall show that in fact θ is unity, as a requirement that this linear system is equivalent to the complex Bateman equation Sec. III.

Dividing these last equations, respectively, by α^s, β^s and introducing the notation $v^\nu = \alpha^\nu/\alpha^n$, $u^\mu = \beta^\mu/\beta^n$ with the convention that Greek indices take values from 1 up to $n-1$ we can eliminate θ by subtracting the last equation to arrive at the following system:

$$-v^\nu_{y_n} = \sum u^\mu v^\nu_{y_\mu}, \quad -u^\mu_{\bar{y}_n} = \sum v^\nu u^\mu_{\bar{y}_\nu}. \tag{9}$$

In the familiar case of two-dimensional space this system takes the form

$$-v_{y_1} = u v_{y_2}, \quad -u_{\bar{y}_1} = v u_{\bar{y}_2}, \tag{10}$$

the general solution of which is connected with

$$G(\phi; y_1, y_2) = F(\phi; \bar{y}_1, \bar{y}_2). \tag{11}$$

We therefore expect that in the general case of n dimensions the general solution of the complex Bateman equation (1) is connected in some way to a system of $n-1$ equations for $n-1$ unknown functions ψ^μ:

$$Q^\nu(\psi^\mu; y_1, \ldots, y_n) = P^\nu(\psi^\mu; \bar{y}_1, \ldots, \bar{y}_n), \quad \nu = 1 \cdots n-1. \tag{12}$$

III. CONDITIONS OF SELF-CONSISTENCY

As a direct corollary of (3) and (4) it follows that the functions ψ can be thought of as either dependent upon the set of variables $(u^\mu;y_i)$, or else $(v^\nu;\overline{y_j})$,

$$\psi(v^\nu;\overline{y_i})=\psi(u^\mu;y_j). \tag{13}$$

This result is equivalent to using two equations from (3) and (4). The remaining $2n$ equations, taking into account (13), may be transformed in the following way:

$$\psi_{y_s}=\sum\ \alpha^i_{y_s}\sum\ \psi_{u^\mu}u^\mu_{\overline{y_i}}=\sum\ \psi_{u^\mu}\sum\ \alpha^i_{y_s}\left(\frac{\beta^\mu_{\overline{y_i}}}{\beta^n}-\frac{\beta^\mu\beta^n_{\overline{y_i}}}{(\beta^n)^2}\right)=\frac{1}{\beta^n}\sum\ \psi_{u^\mu}(\delta_{s\mu}-u^\mu\delta_{sn}). \tag{14}$$

Or finally,

$$\psi_{y_\mu}=\frac{1}{\beta^n}\psi_{u^\mu}(u^\mu;y_i),\quad \psi_{y_n}=-\frac{1}{\beta^n}\sum\ u^\mu\psi_{u^\mu}, \tag{15}$$

$$\psi_{\overline{y_\nu}}=\frac{1}{\alpha^n}\psi_{v^\nu}(v^\nu;\overline{y_i}),\quad \psi_{\overline{y_n}}=-\frac{1}{\alpha^n}\sum\ v^\nu\psi_{v^\nu}. \tag{16}$$

(The reader can compare these equations with the analogous equations in the paper on the real universal equation.) Now let us use the integrability conditions of self-consistency of the second-order mixed derivatives. Using the conditions of self-consistency for Greek barred and unbarred indices, which read

$$\left(\frac{\psi_{v^\nu}}{\alpha^n}\right)_{y_\mu}=\left(\frac{\psi_{u^\mu}}{\beta^n}\right)_{\overline{y}_\nu}, \tag{17}$$

we consider what follows from the conditions of self-consistency for the other pairs $(y_\mu,\overline{y_n})$, $(\overline{y}_\nu,y_n)$, and $(y_n,\overline{y_n})$. We have in consequence (for the first pair of variables)

$$\frac{\partial}{\partial y_\mu}\frac{\partial\psi}{\partial\overline{y_n}}=-\frac{\partial}{\partial y_\mu}\sum\ v^\nu\frac{\psi_{v^\nu}}{\alpha^n}=-\frac{\psi_{y_\mu}}{\alpha^n}-\sum\ v^\nu\left(\frac{\psi_{v^\nu}}{\alpha^n}\right)_{y_\mu}=-\frac{\psi_{y_\mu}}{\alpha^n}-\sum\ v^\nu\left(\frac{\psi_{u^\mu}}{\beta^n}\right)_{\overline{y}_\nu}=\frac{\partial}{\partial\overline{y}_n}\left(\frac{\psi_{u^\mu}}{\beta^n}\right). \tag{18}$$

The last row of this equality can been transformed into

$$\sum_\alpha\ \psi_{u^\mu,u^\alpha}\left(u^\alpha_{\overline{y}_n}+\sum\ v^\nu u^\alpha_{\overline{y}_\nu}\right)+\left(\frac{\psi_{u^\mu}}{\alpha^n}\right)\left(1-\frac{\Sigma_i\alpha^i\beta^n_{\overline{y}_i}}{\beta^n}\right)=0. \tag{19}$$

Rewriting the previous equality,

$$\psi_{\overline{y_n}}+\sum\ v^\nu\psi_{\overline{y}_\nu}=0, \tag{20}$$

in terms of the variables (u,y) to give

$$\sum\ \psi_{u^\alpha}\left(u^\alpha_{\overline{y}_n}+\sum\ v^\nu u^\alpha_{\overline{y}_\nu}\right)=0, \tag{21}$$

we arrive at a linear system of n equations for the n unknowns:

$$\left(u^{\alpha}_{\overline{y}_n}+\sum v^{\nu}u^{\alpha}_{\overline{y}_\nu}\right),\quad \alpha^n\left(1-\frac{\Sigma_i\alpha^i\beta^n_{\overline{y}_i}}{\beta^n}\right),$$

and assuming that the determinant of the corresponding universal equation in the $(n-1)$ dimensional space u^{α} is different from zero (the degenerate case, when it is equal to zero demands special consideration):

$$\sum_i \alpha^i\beta^n_{\overline{y}_i}=\beta^n,\quad u^{\mu}_{\overline{y}_n}+\sum v^{\nu}u^{\mu}_{\overline{y}_\nu}=0, \tag{22}$$

$$\sum_i \beta^i\alpha^n_{y_i}=\alpha^n,\quad v^{\nu}_{y_n}+\sum u^{\mu}v^{\nu}_{y_\mu}=0, \tag{23}$$

which proves that $\theta=1$ in (8) and (9) and shows that the hydrodynamical system (9) is the direct corollary of the main equations. The equivalence of the second mixed partial derivatives $(\psi_{\overline{y}_n})_{y_n}$ in both orders leads to equivalent expressions. They are not essential for what follows and are omitted here.

IV. THE SYSTEM OF HYDRODYNAMIC TYPE

We understand by a system of hydrodynamic type the system (9) rewritten in the following:

$$v^{\nu}_{y_n}+\sum u^{\mu}v^{\nu}_{y_\mu}=0,\quad u^{\mu}_{\overline{y}_n}+\sum v^{\nu}u^{\mu}_{\overline{y}_\nu}=0. \tag{24}$$

Two propositions with respect to this system will be required in the following.[3]

Proposition 1: The conditions that the pair of operators

$$D=\frac{\partial}{\partial y_n}+\sum u^{\mu}\frac{\partial}{\partial y_\mu},\quad \overline{D}=\frac{\partial}{\partial\overline{y}_n}+\sum v^{\nu}\frac{\partial}{\partial\overline{y}_\nu} \tag{25}$$

are commutative are that the functions (u^{μ},v^{ν}) are solutions of system (24).

Acting with the help of operators $(D,\overline{D})$ on the second and the first equations of (24), respectively, we further conclude that the $2(n-1)$ functions

$$\overline{D}(v^{\nu})=v^{\nu}_{\overline{y}_n}+\sum v^{\mu}v^{\nu}_{\overline{y}_\mu},\quad D(u^{\mu})=u^{\mu}_{y_n}+\sum u^{\nu}u^{\mu}_{y_\nu} \tag{26}$$

are also solutions of the first and the second system of Eq. (24).

As a corollary we obtain the following

Proposition 2: Suppose the following notation for the above-mentioned expressions is introduced:

$$v^{\nu}_{\overline{y}_n}+\sum v^{\mu}v^{\nu}_{\overline{y}_\mu}=Q^{\nu}(v;\overline{y}),\quad u^{\mu}_{y_n}+\sum u^{\nu}u^{\mu}_{y_\nu}=P^{\mu}(u;y). \tag{27}$$

Then, as has been anticipated in the notation, Q^{μ} depends upon y_j, $\overline{y_j}$ through the variables v^j and $\overline{y_j}$, and P^{μ} through u^j, y_j. Indeed, the n sets of variables $(1,u)$, satisfy a linear system of $n-1$ matrix equations arising from the first equation of (24) and the fact that Q^{μ} is a solution, for each $\mu=1\cdots n-1$, namely

$$\begin{pmatrix} v^1_{y_1} & \cdots & v^1_{y_{n-1}} & v^1_{y_n} \\ \vdots & \ddots & \vdots & \vdots \\ v^{n-1}_{y_1} & \cdots & v^{n-1}_{y_n} & v^{n-1}_{y_n} \\ Q^\nu_{y_1} & \cdots & Q^\nu_{y_{n-1}} & Q^\nu_{y_n} \end{pmatrix} \begin{pmatrix} u^1 \\ \vdots \\ u^{n-1} \\ 1 \end{pmatrix} = 0. \tag{28}$$

The condition for the existence of a solution is that the determinant of the Jacobian matrix should vanish, which implies that each Q^μ is a function of the variables y only through the functions v. The corresponding result holds for P^μ in a similar manner, so Proposition 2 is proved.

Compared with (24) and (27) is an inhomogeneous system of hydrodynamic equations separated into functions (u,v). Now we are able to find solutions of the primary equations (22) and (23). To this end, let us rewrite them in the terms of operators D, $\overline{D}$:

$$\overline{D}\left(\frac{1}{\beta^n}\right) = -\frac{1}{\alpha^n\beta^n} = D\left(\frac{1}{\alpha^n}\right). \tag{29}$$

We have in consequence the result that there must exist a function Θ such that

$$\frac{1}{\beta^n} = D\Theta, \quad \frac{1}{\alpha^n} = \overline{D}\Theta, \quad (\overline{D}\Theta)(D\Theta) = -\overline{D}D\Theta. \tag{30}$$

The solution of Eq. (30) follows the pattern for the solution to the complex variable equation $f_z f_{\bar{z}} + f_{z\bar{z}} = 0$ and takes the form

$$\exp\Theta = -g(u;y) + \overline{g}(v;\overline{y}). \tag{31}$$

V. GENERAL SOLUTION OF THE HYDRODYNAMIC SYSTEM

Suppose we have the following system of equations defining implicitly $(n-1)$ unknown functions (ψ) in $(2n)$ dimensional space $(y,\overline{y})$:

$$Q^\nu(\psi;y) = P^\nu(\psi;\overline{y}) \tag{32}$$

with the convention that all Greek indices take values between 1 and $(n-1)$. The number of equations in (32) coincides with the number of unknown functions ψ^α.

With the help of the usual rules of differentiation of implicit functions we find from (32):

$$\psi_y = (P_\psi - Q_\psi)^{-1} Q_y, \quad \psi_{\overline{y}} = -(P_\psi - Q_\psi)^{-1} P_{\overline{y}}. \tag{33}$$

Let us assume that between n derivatives with respect to barred and unbarred variables the following linear dependencies obtain:

$$\sum_1^n c_i \psi^\alpha_{y_i} = 0, \quad \sum_1^n d_i \psi^\alpha_{\overline{y}_i} = 0 \tag{34}$$

and analyze the consequences of these facts.

Assuming that $c_n \neq 0$, $d_n \neq 0$, dividing them into each equation of the left and right systems, respectively, and introducing the notation $u^\alpha = c_\alpha / c_n$, $v^\alpha = d_\alpha / d_n$ we may rewrite the last set in the following form:

$$\psi^\alpha_{y_n} + \sum_1^{n-1} u^\nu \psi^\alpha_{y_\nu} = 0, \quad \psi^\alpha_{\overline{y}_n} + \sum_1^{n-1} v^\nu \psi^\alpha_{\overline{y}_\nu} = 0. \tag{35}$$

Substituting values of the derivatives from (33) and multiplying the result by the matrix $(P_\psi - Q_\psi)$ from the left we obtain

$$Q^\alpha_{y_n} + \sum_1^{n-1} u^\nu Q^\alpha_{y_\nu} = 0, \quad P^\alpha_{\bar{y}_n} + \sum_1^{n-1} v^\nu P^\alpha_{\bar{y}_\nu} = 0. \tag{36}$$

From these last equations it immediately follows that

$$u^\nu = -(Q_{y_\nu})^{-1} Q_{y_n}, \quad v^\nu = -(P_{\bar{y}_\nu})^{-1} P_{\bar{y}_n}. \tag{37}$$

We see that if we augment the initial system (32) by $(n-1)$ vector functions (u,v) defined by (37), then the differential operators D, $\bar{D}$ defined by (5) in connection with (35) annihilate each ψ either as a Q or a P function:

$$D\psi = \bar{D}\psi = DQ = DP = \bar{D}Q = \bar{D}P = 0. \tag{38}$$

This means that $D\bar{f}(\psi,\bar{y}) = \bar{D}f(\psi,y) = 0$. As a direct corollary of this fact, $Dv = \bar{D}u = 0$ and the generators D, $\bar{D}$ constructed in this way mutually commute. Thus we have found the general solution of the hydrodynamic system and a concrete realization of the manifold with the properties of Sec. IV.

With respect to the generators D, $\bar{D}$ all functions of $2n$ dimensional space may be divided into the following subclasses: functions of general position F, $DF \neq 0$, $\bar{D}F \neq 0$, holomorphic functions f, $\bar{D}f = 0$, $Df \neq 0$, antiholomorphic ones $\bar{f}$, $D\bar{f} = 0$, $\bar{D}\bar{f} \neq 0$, and f^0 ''central'' functions, both holomorphic and antiholomorphic simultaneously; $\bar{D}f^0 = Df^0 = 0$. Each central function may be represented in the following form:

$$f^0 = f^0(Q) = f^0(P) = g^0(\phi).$$

VI. EQUATIONS FOLLOWING FROM THE OTHER RESTRICTIONS

Formula (37) together with (32) give the general solution of the hydrodynamic system (24). Indeed this solution depends upon $2(n-1)$ arbitrary functions (32) each of $(2n-1)$ independent arguments, which are sufficient for the statement of Cauchy or Goursat initial value problems. The general solution of the complex Bateman equation (1) depends upon only two arbitrary functions each of $(2n-1)$ arguments. Thus all other restrictions arising on the way must reduce the $2(n-1)$ arbitrary functions of (32) to only two.

For this purpose it is necessary to calculate derivatives of the functions u,v defined by (37). We have in consequence, suppressing the index ν,

$$\begin{aligned} u_{y_\alpha} &= -Q_y^{-1}\left(Q_{y_n,y_\alpha} + \sum Q_{y_n,\psi^\beta}\psi^\beta_{y_\alpha} - Q_{y,y_\alpha}Q_y^{-1}Q_{y_n} - \sum Q_{y,\psi^\beta}\phi^\beta_{y_\alpha}Q_y^{-1}Q_{y_n}\right) \\ &\equiv -Q_y^{-1}(DQ_{y_\alpha}) + Q_y^{-1}(DQ_\psi)(P_\psi - Q_\psi)^{-1}Q_{y_\alpha}. \end{aligned} \tag{39}$$

By the same technique we can calculate $u_{\bar{y}}, v_y$ using

$$u_{\bar{y}} = Q_y^{-1}(DQ_\psi)(P_\psi - Q_\psi)^{-1}P_{\bar{y}}, \quad v_y = -P_{\bar{y}}^{-1}(DP_\psi)(P_\psi - Q_\psi)^{-1}Q_y. \tag{40}$$

Comparing (13) with results of Sec. V we conclude that the function ψ is central and so depends only on $(n-1)$ arguments. For us it will be more convenient to go back directly to the linear systems (3) and (4) and investigate their properties. We have in consequence

$$\sum \phi_{\psi^\alpha}\psi^\alpha_{y_s} = \sum \phi_{\psi^\alpha} \sum \psi^\alpha_{\bar{y}_i}\alpha^i_{y_s}.$$

Further evaluation of the last equality is connected with the substitution of the explicit expressions for the derivatives of the functions ψ (33). The results of the further calculations we present in the form of multiplication of the row ϕ_ψ by the corresponding matrix:

$$\phi_\psi(P_\psi-Q_\psi)^{-1}\left(Q_{y_s}+\sum\ \alpha^i_{y_s}Q_{\bar{y}_i}\right)=\phi_\psi(P_\psi-Q_\psi)^{-1}\left(Q_{y_s}+\sum\ v^\nu_{y_s}Q_{\bar{y}_\nu}\right)$$
$$=\phi_\psi(I-\alpha^n(P_\psi-Q_\psi)^{-1}\bar{D}P_\psi)(P_\psi-Q_\psi)^{-1}Q_{y_s}=0. \tag{41}$$

In the process of the above evaluation we have used the equalities $\bar{D}Q=0$ and the explicit expression for the derivatives of the functions v with respect to the unbarred coordinates (40).

Equation (41) for $s=n$ is a direct corollary of the equations with Greek indices as a consequence of the equality $DQ=0$. Assuming that $\det Q^\mu_{y_\nu}\neq 0$, $\det(P_\psi-Q_\psi)\neq 0$, we may rewrite Eq. (41) with Greek indices in the final form:

$$\sum\ \phi_{\psi^\alpha}(I-\alpha^n(P_\psi-Q_\psi)^{-1}\bar{D}P_\psi)^\alpha_\nu=0. \tag{42}$$

A similar equation follows from (4):

$$\sum\ \phi_{\psi^\alpha}(I-\beta^n(P_\psi-Q_\psi)^{-1}DQ_\psi)^\alpha_\nu=0. \tag{43}$$

Now we assume that only one from the set of the functions ψ^α satisfies the complex Bateman equation. Suppose it is ψ^1 and that the solution may be chosen in the form $\phi(\psi^1)$. Of course, this suggestion must be confirmed by the detailed investigations of all results following from (42) and (43). We omit here this consideration, replacing it by checking the final result. Under this assumption, Eqs. (42) and (43) are equivalent to the following $2(n-1)$ equalities:

$$(I-\beta^n(P_\psi-Q_\psi)^{-1}DQ_\psi)^1_\nu=0,\quad (I-\alpha^n(P_\psi-Q_\psi)^{-1}\bar{D}P_\psi)^1_\nu=0,$$

which after substituting into them the explicit expressions for $1/\alpha^n=\bar{D}\Theta$, $1/\beta^n=D\Theta$ from (31) it will be convenient to rewrite in the form of multiplication of the row by the matrix $(P_\psi-Q_\psi)=\delta$:

$$(\bar{D}\Theta,0\cdots0)=(1,0\cdots0)\delta^{-1}\bar{D}\delta,$$

multiplying the last equality with the matrix δ^{-1} on the right we obtain

$$(D\Theta,0\cdots0)\delta^{-1}=-(1,0\cdots0)D\delta^{-1},\quad (\bar{D}\Theta,0\cdots0)\delta^{-1}=-(1,0\cdots0)\bar{D}\delta^{-1}. \tag{44}$$

The integration of the last system is straightforward with the following result:

$$(\delta^{-1})_{1,\beta}=\rho(\psi)_\beta\exp\Theta=\rho(\psi)_\beta(\bar{g}-g). \tag{45}$$

We consider in the following the simplest examples of solutions of the last system for functions Q,P from which the situation in the general case of arbitrary n will be clarified.

A. The case $n=2$

In this case there is only one Greek index and two scalar equations (44) lead to the result

$$\exp\Theta=\rho(\psi^1)(P_{\psi^1}-Q_{\psi^1})=\bar{g}-g.$$

The last equality may be considered as the definition of the functions $g,\bar{g}$ in terms of P,Q:

$$\overline{g}=\rho(\psi^1)P_{\psi^1}(\psi^1;\overline{y_1},\overline{y_2}),\quad g=\rho(\psi^1)Q_{\psi^1}(\psi^1,y_1,y_2)$$

with the correct dependence upon their independent arguments.

B. The case $n=3$

This case is more illustrative of the general situation. Using the explicit form of the matrix δ,

$$\delta=\begin{pmatrix}\Delta^1_{\psi^1} & \Delta^2_{\psi^1}\\ \Delta^1_{\psi^2} & \Delta^1_{\psi^1}\end{pmatrix},$$

we can invert it explicitly and after substitution into (45) it leads to

$$\begin{aligned}(P^1_{\psi^2}-Q^1_{\psi^2})+\frac{\rho_2}{\rho_1}(P^2_{\psi^2}-Q^2_{\psi^2})=0,\\ (P^1_{\psi^1}-Q^1_{\psi^1})+\frac{\rho_2}{\rho_1}(P^2_{\psi^1}-Q^2_{\psi^1})=\overline{g}-g.\end{aligned}\tag{46}$$

Taking into account the explicit dependence of P,Q functions upon their arguments we separate the last system into two systems of equations for Q,P, respectively ($\rho_2/\rho_1=\rho$):

$$Q^1_{\psi^1}+\rho Q^2_{\psi^1}=g,\quad Q^1_{\psi^2}+\rho Q^2_{\psi^2}=0.$$

The condition of self-consistency of the last two equations (equality of second mixed derivatives of the function Q^1) leads to

$$\rho_{\psi^2}Q^2_{\psi^1}-\rho_{\psi^1}Q^2_{\psi^2}=g_{\psi^2},$$

a single equation for the determination of the function Q^2. Let us consider in the last equation Q^1 as an arbitrary given function $p=p(\psi;y)$. Then the equation for it may be considered as a definition of the function g, which for what follows it is better to rewrite in the form

$$\rho p_{\psi^1}-\left(\int d\psi^2\,\rho p_{\psi^2}\right)_{\psi^1}=g.$$

Substituting this expression into the first initial equation we obtain for Q^1:

$$Q^1=\int d\psi^2\,\rho p_{\psi^2}=\rho p-\int d\psi^2\,p\rho_{\psi^2}.$$

Introducing the new function $F=\int d\psi^2 p\nu_{\psi^2}$ we are now able with its help to represent both functions Q^1,Q^2 in a local form:

$$Q^2=\frac{F_{\psi^2}}{\rho_{\psi^2}},\quad Q^1=\rho Q^2-F.$$

The same procedure may be used with a similar result for the functions P^1,P^2:

$$P^2=\frac{\overline{F}_{\psi^2}}{\rho_{\psi^2}},\quad P^1=\rho P^2-\overline{F}.$$

Equating $P^{1,2}=Q^{1,2}$ and taking into account that all factors depending upon functions ψ may be canceled, we arrive at the following system:

$$F=\overline{F},\quad F_{\psi^2}=\overline{F}_{\psi^2}, \tag{47}$$

which determine implicitly two functions ψ, one of which, ψ^1, is the solution of the complex Bateman equation in three dimensions.

C. The general case of arbitrary *n*

Let us denote the minors of $(n-2)$th order of the first column of the matrix δ, $\Delta^1_{\psi^\beta}$ by M^β and introduce the notation $\rho^\beta=M^\beta/M^1$. Then the systems (44) and (45) may be solved in the following way:

$$\sum \rho^\alpha \Delta^\alpha_{\psi^1}=\overline{g}-g,\quad \rho^\alpha=\rho^\alpha(\psi) \tag{48}$$

and rewrite the definition of the functions ρ^α in the form

$$M^\alpha=\rho^\alpha M^1.$$

Multiplying the last equalities by elements of each (given) column (except for the first one) with further summation of the results we always obtain zero on the left-hand sides of the equalities arising (determinants with equal columns). Thus we may rewrite (48) in the equivalent form

$$\sum \rho^\alpha \Delta^\alpha_{\psi^1}=\overline{q}-q,\quad \sum \rho^\alpha \Delta^\alpha_{\psi^A}=0,\quad 2\neq A\neq(n-1).$$

Keeping in mind that $\Delta^\alpha_{\psi^\beta}=P^\alpha_{\psi^\beta}-Q^\alpha_{\psi^\beta}$ and recalling the definition of (anti) holomorphic functions of Sec. V, we separate the last system into two independent ones:

$$\sum \rho^\alpha Q^\alpha_{\psi^1}=g,\quad \sum \rho^\alpha Q^\alpha_{\psi^A}=0,\quad \sum \rho^\alpha P^\alpha_{\psi^1}=\overline{g},\quad \sum \rho^\alpha P^\alpha_{\psi^A}=0.$$

Further transformations of both barred and unbarred systems are similar and so we will follow through the evaluation of the first one.

Introducing a new function $F=\Sigma\rho^\alpha Q^\alpha$ we obtain

$$\sum \rho^\alpha_{\psi^1} Q^\alpha=-g+F_{\psi^A},\quad \sum \rho^\alpha_{\psi^A} Q^\alpha=F_{\psi^A}. \tag{49}$$

In particular, we recall that $\rho^1=1$ and so each equation on its left-hand side contains only $(n-2)$ terms. Thus between $(n-1)$ equations above at least one linear dependence exists. Denoting the coefficients of it by $d^A=D^A(\psi)$ we rewrite the condition of self-consistency of the last system in the form of a single equation relating the function F in terms of the function g:

$$g=F_{\psi^1}+\sum d^A F_{\psi^A}.$$

Inverting the problem we can consider the last equality as a definition of the function g in terms of the given F. Solving the last $(n-2)$ equations of the system (49) and adding to them Q^1 obtained from the definition of the function F, we obtain finally

$$Q^B=\sum (\rho^{-1}_\psi)^B_A F_{\psi^A},\quad Q^1=F-\sum \rho^A Q^A.$$

Completely similar calculations lead to the following expressions for the functions P:

$$P^B=\sum\ (\rho_{\psi}^{-1})^B_A\overline{F}_{\psi^A},\quad P^1=\overline{F}-\sum\ \rho^A P^A.$$

We especially emphasize that all coefficient functions in the above-mentioned expressions determining functions Q,P in terms of two arbitrary functions $F,\overline{F}$ are functions only of the arguments ψ (central functions) and are the same in both cases.

Equating $P^\beta=Q^\beta$ after the obvious cancellation of all (scalar, matrix) factors depending only upon the functions ψ we reach the final system of equations implicitly determining all functions ψ:

$$F=\overline{F},\quad F_{\psi^A}=\overline{F}_{\psi^A}. \tag{50}$$

The function ψ^1 is the solution of the Complex Bateman equation (1) in the space of n dimensions.

VII. THE MAIN THEOREM

Theorem: The general solution of the complex Bateman equation (1) is defined by the function ψ^1, which is implicitly determined from the following system of $(n-1)$ equations for $(n-1)$ functions ψ^ν:

$$F(\psi;y)=\overline{F}(\psi;\overline{y}),\quad F_{\psi^A}=\overline{F}_{\psi^A},\quad 2\leqslant A\leqslant(n-1).$$

VIII. OUTLOOK

The principal concrete results of the present paper are concentrated in the theorem of Sec. VII, giving the explicit general solution (in implicit form) of the complex Bateman equation (1) in n dimensional space.

But a no less important hydrodynamic type system with two times $(y_n,\overline{y_n})$ was discovered and solved. A reduction of its general solution leads to the general solution of complex Bateman equation. We cannot exclude the possibility that there exist other reductions leading to no less interesting systems and equations.[4]

Nevertheless, the majority of these results were obtained more on the basis of intuitive calculations. We think that the algebraic-geometrical form of the answer tells us of the necessity to consider the group of motions (the symmetry structure) of the manifold (32) determining the general solution of hydrodynamic system (24). The properties of the group of inner symmetry of it must explain more precisely and directly the proposed way of integration of the systems under consideration (hydrodynamic and complex Bateman) as the uniquely possible one.

We have a feeling that in these problems algebraic-geometrical methods are more appropriate and effective. Unfortunately, they are not within our area of expertise.

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Differential calculuses on the quantized braided groups

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Braided differential calculuses on the quantized braided groups are constructed and their braided bialgebra (Hopf algebra) structures are demonstrated. These are a kind of generalization and unification of the differential calculuses on quantum groups, braided groups, quantum supergroups, etc., and contain the latter ones as special cases. Moreover, it is shown that some quantum differential (co)vector algebras are covariant under the braided ''local'' coactions of the obtained braided differential bialgebras (Hopf algebras). Some examples are also given. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1328742]

I. INTRODUCTION

In the last few years the differential calculuses on the quantum groups, braided groups, and other quantum spaces have attracted increasing attention owing to their great importance in mathematics and physics (see, e.g., Refs. 1–7, and references therein). In this paper we construct differential calculuses on some more general algebraic systems: the quantized braided groups (QBGs). The QBGs were proposed by Hlavaty years ago,[8] and contain the usual quantum groups,[9,10] braided groups,[11] quantum supergroups,[12] quantum anyonic groups,[13] μ-braided GL_q,[14] etc., as special cases. Thus, the theory of QBGs has, among other features, a remarkable advantage that enables us to study the two quite different kinds of noncommutativities (associated, respectively, with quantization and general braid statistics) in a unified way. Some properties and applications of the QBGs have been discussed recently.[15,16]

The main aim of the present paper is to construct quantized braided differential calculuses on the QBGs. Then the braided ''local'' coactions of the obtained quantized braided differential bialgebras (Hopf algebras) on some quantum differential (co)vector spaces are also considered. These are a kind of generalization and unification of the differential calculuses and coactions for the usual quantum groups, braided groups, quantum supergroups, etc., and the latter ones can be obtained as special cases.

In Sec. II, we recall some related results of QBGs, which are useful for later discussions. In Sec. III, differential calculuses on the QBGs are constructed and their braided bialgebra (Hopf algebra) structures are demonstrated in some detail. Some examples are also given for illustrating the formulas obtained. Section IV shows the covariance of some quantum differential vector algebras under braided ''local'' coactions of the braided differential bialgebras (Hopf algebras) given in Sec. III. Finally, Sec. V contains some conclusions and discussions.

II. QUANTIZED BRAIDED GROUPS

For later use, here we recall some related results of the QBGs.[8,16] Let $T=\{T^i_j\}^N_{i,j=1}$ be a matrix of N^2 elements T^i_j and $R,Z\in M_N(\mathbf{C})\otimes M_N(\mathbf{C})$ be an R-matrix pair satisfying the following set of quantum Yang–Baxter-type equations:[8]

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$$R_{12}R_{13}R_{23}=R_{23}R_{13}R_{12},\quad Z_{12}Z_{13}Z_{23}=Z_{23}Z_{13}Z_{12},$$
$$R_{12}Z_{13}Z_{23}=Z_{23}Z_{13}R_{12},\quad Z_{12}Z_{13}R_{23}=R_{23}Z_{13}Z_{12}. \tag{2.1}$$

Then the quantized braided (matrix) group $A(R,Z)$ is defined as follows.

(i) $A(R,Z)$ is generated by $\{T_j^i, 1\}$ with the algebra relations

$$R_{12}Z_{12}^{-1}T_1Z_{12}T_2=Z_{21}^{-1}T_2Z_{21}T_1R_{12}, \tag{2.2}$$

the coproduct and counit

$$\Delta(T_j^i)=T_k^i\otimes T_j^k,\quad \varepsilon(T_j^i)=\delta_j^i, \tag{2.3}$$

and the braiding

$$\Psi(Z_{12}^{-1}T_1\otimes Z_{12}T_2)=T_2Z_{12}^{-1}\otimes T_1Z_{12}. \tag{2.4}$$

(ii) There is an antipode S obeying usual axioms such as

$$S(T)T=TS(T)=I,\quad S(1)=1 \tag{2.5}$$

and extending to the whole algebra by the rule

$$S\cdot=\cdot\Psi(S\otimes S). \tag{2.6}$$

If $A(R,Z)$ satisfies condition (i) only, we call it a quantized braided (matrix) bialgebra. Moreover, for $a\otimes b$, $c\otimes d\in A(R,Z)\otimes A(R,Z)$, the product in the (braided) tensor product algebra is given by (as in Ref. 11)

$$(a\otimes b)(c\otimes d)=a\Psi(b\otimes c)d. \tag{2.7}$$

Similar to Ref. 11, sometimes we also use the notations with a prime ($'$) to denote the second factor of $A(R,Z)\otimes A(R,Z)$ and omit writing the tensor product $\otimes$. Thus the braiding relation (2.4) can also be written simply as $Z_{12}^{-1}T_1'Z_{12}T_2=T_2Z_{12}^{-1}T_1'Z_{12}$.

We mention some special cases of QBGs: When $Z=R$ or $Z=I$ while R is any regular solution of the quantum Yang–Baxter equation (QYBE), then $A(R,Z)$ is reduced to the ordinary braided group[11] or quantum group,[9,10] respectively. If Z is diagonal and R is some specified $R(q)$,[14] then $A(R(q),Z)$ gives the μ-braided GL_q considered in Ref. 14, etc.

In this paper, R, Z are always assumed to be invertible. A matrix solution R of QYBE is being called Hecke type if it satisfies

$$(PR-q)(PR+q^{-1})=0,$$

or

$$PRPR=1+\lambda PR \tag{2.8}$$

for a suitable q and $\lambda=q-q^{-1}$, where P is the usual permutation matrix.

Proposition 2.1:[16] Defining $R^{(n)}\equiv(ZP)^nR(Z^{-1}P)^n$, if (R,Z) is an R-matrix pair satisfying (2.1), then $(R^{(n)},Z)$ satisfies (2.1), too, for each integer $n=0,\pm1,\pm2,\ldots$. Moreover, if R is Hecke type, then so is $R^{(n)}$.

III. DIFFERENTIAL CALCULUSES ON THE QBGS

In this section, we construct quantized braided differential (matrix) bialgebras on the QBGs and show that if some suitable braided antipode is introduced, we can obtain braided differential Hopf algebras.

Consider $\{T^i_j\}$ and their differential forms $\{dT^i_j\}$, and let the external differentiation d obey $d^2=0$ and the usual (graded) Leibnitz rule, then we have the following.

Theorem 3.1: Let (R,Z) obey (2.1), R be Hecke type, and Z have the second inverse $\tilde{Z} \equiv((Z^{t_2})^{-1})^{t_2}$ (t_2 denotes transposition in the second factor). Then the element set $\{T^i_j, dT^i_j, 1\}$ generates a braided differential bialgebra, denoted by $\Omega_{A(R,Z)}$, with the following algebra relations:

$$R_{12}Z^{-1}_{12}T_1Z_{12}T_2=Z^{-1}_{21}T_2Z_{21}T_1R_{12}, \tag{3.1a}$$

$$R^{-1}_{21}Z^{-1}_{12}T_1Z_{12}dT_2=Z^{-1}_{21}dT_2Z_{21}T_1R_{12}, \tag{3.1b}$$

$$R^{-1}_{21}Z^{-1}_{12}dT_1Z_{12}dT_2=-Z^{-1}_{21}dT_2Z_{21}dT_1R_{12}, \tag{3.1c}$$

coproduct and counit

$$\Delta T=T\otimes T\equiv TT', \quad \Delta(dT)=dTT'+TdT', \qquad \varepsilon(T)=I, \quad \varepsilon(dT)=0, \tag{3.2}$$

and braidings

$$\begin{aligned} &Z^{-1}_{12}T'_1Z_{12}T_2=T_2Z^{-1}_{12}T'_1Z_{12}, \quad Z^{-1}_{12}dT'_1Z_{12}T_2=T_2Z^{-1}_{12}dT'_1Z_{12},\\ &Z^{-1}_{12}T'_1Z_{12}dT_2=dT_2Z^{-1}_{12}T'_1Z_{12}, \quad Z^{-1}_{12}dT'_1Z_{12}dT_2=-dT_2Z^{-1}_{12}dT'_1Z_{12}. \end{aligned} \tag{3.3}$$

If we also introduce a braided antipode S: $S(T)\equiv T^{-1}$ as in (2.5) and $S(dT)\equiv dT^{-1}=-T^{-1}TT^{-1}$, then $\Omega_{A(R,Z)}$ forms a braided Hopf algebra.

Proof: By definition, $\Omega_{A(R,Z)}$ is an associative algebra. For simplifying notations, we denote $\hat{R}_{12}=Z_{12}R_{21}Z^{-1}_{21}$ in the following. Consider, e.g., the expression containing triples of the generators as

$$T_1Z_{12}dT_2Z_{13}Z_{23}T_3. \tag{3.4}$$

We involve Z in (3.4) in order that the algebra relations (3.1) can be conveniently used, and this does not lose the generality because of the existence of $\tilde{Z}$. Transposing (3.4) in two ways, from (3.1) we obtain

$$\begin{aligned} \underline{T_1Z_{12}dT_2}Z_{13}Z_{23}T_3&=\hat{R}_{12}dT_2Z_{21}\underline{T_1R_{12}Z_{13}Z_{23}T_3}\\ &=\hat{R}_{12}\underline{dT_2Z_{21}Z_{23}\hat{R}^{-1}_{31}T_3}Z_{31}T_1R_{13}R_{12}\\ &=\hat{R}_{12}\hat{R}^{-1}_{31}\hat{R}^{-1}_{32}T_3Z_{32}dT_2R^{-1}_{32}Z_{21}Z_{31}T_1R_{13}R_{12}, \end{aligned}$$

$$\begin{aligned} T_1Z_{12}\underline{dT_2Z_{13}Z_{23}T_3}&=\underline{T_1Z_{12}Z_{13}\hat{R}^{-1}_{32}T_3}Z_{32}dT_2R^{-1}_{32}\\ &=\hat{R}^{-1}_{32}\hat{R}^{-1}_{31}T_3Z_{31}\underline{T_1R_{13}Z_{12}Z_{32}dT_2}R^{-1}_{32}\\ &=\hat{R}^{-1}_{32}\hat{R}^{-1}_{31}T_3Z_{31}Z_{32}\hat{R}_{12}dT_2Z_{21}T_1R_{12}R_{13}R^{-1}_{32}. \end{aligned}$$

The two right-hand side results are equal from (2.1) and Proposition 2.1. In the above-given calculations we have used (2.1) and (3.1) many times to the underlined parts in each expression to obtain the next expression. For other triples of generators, the calculations are similar. So these do not impose any additional relation on T, dT.

Now we check that Ψ, Δ, S are well defined when extended to products. First, we calculate that, e.g., from (3.1b),

$$\begin{aligned}
&\Psi(R_{21}^{-1}Z_{12}^{-1}T_1Z_{12}dT_2\otimes Z_{13}Z_{23}dT_3)\\
&\quad=(\mathrm{id}\otimes\cdot)\Psi[(R_{21}^{-1}Z_{12}^{-1}T_1\otimes Z_{12}dT_2)\otimes Z_{13}Z_{23}dT_3]\\
&\quad=-R_{21}^{-1}Z_{12}^{-1}Z_{23}Z_{13}dT_3\otimes Z_{13}^{-1}T_1Z_{13}Z_{12}Z_{23}^{-1}dT_2Z_{23}\\
&\quad=-Z_{23}Z_{13}R_{21}^{-1}Z_{12}^{-1}dT_3\otimes Z_{13}^{-1}Z_{23}^{-1}T_1Z_{12}dT_2Z_{13}Z_{23}\\
&\quad=-Z_{23}Z_{13}dT_3\otimes Z_{13}^{-1}Z_{23}^{-1}R_{21}^{-1}Z_{12}^{-1}T_1Z_{12}dT_2Z_{13}Z_{23}.
\end{aligned}$$

On the other hand,

$$\begin{aligned}
&\Psi(Z_{21}^{-1}dT_2Z_{21}T_1R_{12}\otimes Z_{13}Z_{23}dT_3)\\
&\quad=(\mathrm{id}\otimes\cdot)\Psi[(Z_{21}^{-1}dT_2\otimes Z_{21}T_1R_{12})\otimes Z_{13}Z_{23}dT_3]\\
&\quad=-Z_{21}^{-1}Z_{13}Z_{23}dT_3\otimes Z_{23}^{-1}dT_2Z_{23}Z_{21}Z_{13}^{-1}T_1Z_{13}R_{12}\\
&\quad=-Z_{23}Z_{13}dT_3\otimes Z_{21}^{-1}Z_{23}^{-1}Z_{13}^{-1}dT_2Z_{21}T_1Z_{23}Z_{13}R_{12}\\
&\quad=-Z_{23}Z_{13}dT_3\otimes Z_{13}^{-1}Z_{23}^{-1}Z_{21}^{-1}dT_2Z_{21}T_1R_{12}Z_{13}Z_{23}.
\end{aligned}$$

These two results are equal by using (3.1b) once again. The consistency of Ψ with other algebra relations and with high order products of generators T, dT can be verified similarly. Hence the braiding Ψ is well defined on $\Omega_{A(R,Z)}$ and is functorial with respect to the product.

Next we extend Δ to products in such a way that it is a homomorphism to the braided tensor product (2.7), this is consistent because, e.g., for (3.1c), from (3.1) to (3.3) we have

$$\begin{aligned}
&\Delta(R_{21}^{-1}Z_{12}^{-1}dT_1Z_{12}dT_2)\\
&\quad=R_{21}^{-1}Z_{12}^{-1}(dT_1T_1'+T_1dT_1')Z_{12}(dT_2T_2'+T_2dT_2')\\
&\quad=R_{21}^{-1}Z_{12}^{-1}dT_1\underline{T_1'Z_{12}dT_2}T_2'+R_{21}^{-1}Z_{12}^{-1}dT_1\underline{T_1'Z_{12}T_2}dT_2'+R_{21}^{-1}Z_{12}^{-1}T_1\underline{dT_1'Z_{12}dT_2}T_2'\\
&\qquad+R_{21}^{-1}Z_{12}^{-1}T_1\underline{dT_1'Z_{12}T_2}dT_2'\\
&\quad=\underline{R_{21}^{-1}Z_{12}^{-1}dT_1Z_{12}dT_2}Z_{12}^{-1}T_1'Z_{12}T_2'+R_{21}^{-1}\underline{Z_{12}^{-1}dT_1Z_{12}T_2}Z_{12}^{-1}T_1'Z_{12}dT_2'\\
&\qquad-\underline{R_{21}^{-1}Z_{12}^{-1}T_1Z_{12}dT_2}Z_{12}^{-1}dT_1'Z_{12}T_2'+\underline{R_{21}^{-1}Z_{12}^{-1}T_1Z_{12}T_2}Z_{12}^{-1}dT_1'Z_{12}dT_2'\\
&\quad=-Z_{21}^{-1}dT_2Z_{21}dT_1\underline{R_{12}Z_{12}^{-1}T_1'Z_{12}T_2'}+R_{21}^{-1}R_{12}^{-1}Z_{21}^{-1}T_2Z_{21}dT_1\underline{R_{21}^{-1}Z_{12}^{-1}T_1'Z_{12}dT_2'}\\
&\qquad-Z_{21}^{-1}dT_2Z_{21}T_1\underline{R_{12}Z_{12}^{-1}dT_1'Z_{12}T_2'}+Z_{21}^{-1}T_2Z_{21}T_1\underline{R_{21}^{-1}Z_{12}^{-1}dT_1'Z_{12}dT_2'}\\
&\quad=-Z_{21}^{-1}dT_2Z_{21}dT_1Z_{21}^{-1}T_2'Z_{21}T_1'R_{12}+R_{21}^{-1}R_{12}^{-1}Z_{21}^{-1}T_2Z_{21}dT_1Z_{21}^{-1}dT_2'Z_{21}T_1'R_{12}\\
&\qquad-Z_{21}^{-1}dT_2Z_{21}T_1Z_{21}^{-1}T_2'Z_{21}dT_1'R_{21}^{-1}-Z_{21}^{-1}T_2Z_{21}T_1Z_{21}^{-1}dT_2'Z_{21}dT_1'R_{12},\\
&\qquad\Delta(-Z_{21}^{-1}dT_2Z_{21}dT_1R_{12})=-Z_{21}^{-1}(dT_2T_2'+T_2dT_2')Z_{21}(dT_1T_1'+T_1dT_1')R_{12}\\
&\quad=-Z_{21}^{-1}dT_2\underline{T_2'Z_{21}dT_1}T_1'R_{12}-Z_{21}^{-1}dT_2\underline{T_2'Z_{21}T_1}dT_1'R_{12}-Z_{21}^{-1}T_2\underline{dT_2'Z_{21}dT_1}T_1'R_{12}\\
&\qquad-Z_{21}^{-1}T_2\underline{dT_2'Z_{21}T_1}dT_1'R_{12}\\
&\quad=-Z_{21}^{-1}dT_2Z_{21}dT_1Z_{21}^{-1}T_2'Z_{21}T_1'R_{12}-Z_{21}^{-1}dT_2Z_{21}T_1Z_{21}^{-1}T_2'Z_{21}dT_1'R_{21}^{-1}R_{21}R_{12}\\
&\qquad+Z_{21}^{-1}T_2Z_{21}dT_1Z_{21}^{-1}dT_2'Z_{21}T_1'R_{12}-Z_{21}^{-1}T_2Z_{21}T_1Z_{21}^{-1}dT_2'Z_{21}dT_1'R_{12}.
\end{aligned}$$

The two results are equal because of the Hecke property of R and relation (3.1). For relations (3.1b) and (3.1a), the calculations are similar. So the coproduct Δ is well-defined. The functoriality of Ψ with respect to Δ can also be easily verified.

Finally, for the antipode S, from (2.6), (3.3), and the functoriality of Ψ we have, e.g., for (3.1b),

$$\begin{aligned} S(R_{21}^{-1}Z_{12}^{-1}T_1Z_{12}dT_2) &= R_{21}^{-1}dT_2^{-1}Z_{12}^{-1}T_1^{-1}Z_{12} \\ &= -R_{21}^{-1}T_2^{-1}dT_2\underline{T_2^{-1}Z_{12}^{-1}T_1^{-1}Z_{12}} \\ &= -R_{21}^{-1}T_2^{-1}\underline{dT_2R_{12}^{-1}T_1^{-1}Z_{21}^{-1}}T_2^{-1}Z_{21}R_{12} \\ &= -\underline{R_{21}^{-1}T_2^{-1}Z_{12}^{-1}T_1^{-1}Z_{12}R_{21}Z_{21}^{-1}}dT_2T_2^{-1}Z_{21}R_{12} \\ &= -T_1^{-1}Z_{21}^{-1}T_2^{-1}dT_2T_2^{-1}Z_{21}R_{12}, \end{aligned}$$

$$S(Z_{21}^{-1}dT_2Z_{21}T_1R_{12}) = T_1^{-1}Z_{21}^{-1}dT_2^{-1}Z_{21}R_{12}.$$

So $S(R_{21}^{-1}Z_{12}^{-1}T_1Z_{12}dT_2)=S(Z_{21}^{-1}dT_2Z_{21}T_1R_{12})$. For the other relations in (3.1) and high orders of products the calculations are similar. Thus S is well defined.

Other braided Hopf algebra axioms such as $\cdot(S\otimes\mathrm{id})\Delta=\cdot(\mathrm{id}\otimes S)\Delta=\eta\varepsilon$, etc., can be easily verified. □

When $Z=I$, while R is any solution of QYBE with Hecke property, the $\Omega_{A(R,Z)}$ reduces to $\Omega_{A(R)}$, the differential bialgebra (or Hopf algebra) on the quantum group $A(R)$.[2,3,5] When $Z=R$, the $\Omega_{A(R,Z)}$ reduces to $\Omega_{B(R)}$, the braided differential bialgebra (or Hopf algebra) on the braided group $B(R)$.[6] Moreover, the $\Omega_{A(R,Z)}$ also contains the differential calculuses on the quantum supergroups, on the quantum anionic groups, etc., as special cases provided that the R-matrix pair (R,Z) is suitably chosen.

To illustrate the above-mentioned formulas, we give a simple example. Taking

$$R=\begin{pmatrix} q & 0 & 0 & 0 \\ 0 & 1 & \lambda & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & q \end{pmatrix}, \quad Z=\begin{pmatrix} r & 0 & 0 & 0 \\ 0 & u & 0 & 0 \\ 0 & 0 & v & 0 \\ 0 & 0 & 0 & w \end{pmatrix}, \qquad T=\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \quad q\neq\pm i, \quad ruvw\neq 0, \tag{3.5}$$

then from (3.1), the corresponding braided differential bialgebra (Hopf algebra), denoted by $\Omega_{A_2(R,Z)}$, has the following algebra relations:

$$v\beta\alpha=qr\alpha\beta, \quad r\gamma\alpha=qv\alpha\gamma, \quad ur\gamma\beta=vw\beta\gamma, \quad u\delta\beta=qw\beta\delta,$$

$$w\delta\gamma=qu\gamma\delta, \quad \delta\alpha=\alpha\delta+\lambda v^{-1}r\gamma\beta, \quad \alpha d\alpha=q^2d\alpha\alpha, \quad r\alpha d\beta=qvd\beta\alpha,$$

$$v\beta d\alpha=qrd\alpha\beta+q\lambda vd\beta\alpha, \quad \beta d\beta=q^2d\beta\beta, \quad v\alpha d\gamma=qrd\gamma\alpha, \quad \alpha d\delta=d\delta\alpha,$$

$$wv\beta d\gamma=urd\gamma\beta+\lambda uvd\delta\alpha, \quad w\beta d\delta=qud\delta\beta, \quad r\gamma d\alpha-\lambda v\alpha d\gamma=qvd\alpha\gamma,$$

$$u\delta d\beta-\lambda w\beta d\delta=qwd\beta\delta, \quad \gamma d\gamma=q^2d\gamma\gamma, \quad u\gamma d\delta=qwd\delta\gamma, \quad w\delta d\gamma=qud\gamma\delta+\lambda qwd\delta\gamma,$$

$$\delta d\delta=q^2d\delta\delta, \quad (d\alpha)^2=0, \quad (d\beta)^2=0, \quad (d\gamma)^2=0, \quad (d\delta)^2=0,$$

$$rd\alpha d\beta=-qvd\beta d\alpha, \quad vd\beta d\alpha=-qrd\alpha d\beta-q\lambda vd\beta d\alpha, \quad vd\alpha d\gamma=-qrd\gamma d\alpha,$$

$$d\alpha d\delta=-d\delta d\alpha,\quad wvd\beta d\gamma=-urd\gamma d\beta-\lambda uvd\delta d\alpha,\quad wd\beta d\delta=-qud\delta d\beta,$$

$$rd\gamma d\alpha-\lambda vd\alpha d\gamma=-qvd\alpha d\gamma,\quad rud\gamma d\beta-\lambda uvd\alpha d\delta=-vwd\beta d\gamma,$$

$$ud\delta d\alpha-\lambda wd\beta d\gamma=-ud\alpha d\delta-\lambda wd\beta d\gamma,\quad ud\delta d\beta-\lambda wd\beta d\delta=-qwd\beta d\delta,$$

$$ud\gamma d\delta=-qwd\delta d\gamma,\quad wd\delta d\gamma=-qud\gamma d\delta-\lambda qwd\delta d\gamma.$$

Defining the degree of the generators of $\Omega_{A_2(R,Z)}$ as $|\alpha|=|\beta|=|\gamma|=|\delta|=0$, $|d\alpha|=|d\beta|=|d\gamma|=|d\delta|=1$; $|ab|=|a|+|b| \bmod 2$, $a, b\in\Omega_{A_2(R,Z)}$, then from (3.3) the braiding relations are

$$\Psi(\mu\otimes\nu)=(-1)^{|\mu||\nu|}\nu\otimes\mu,\qquad \Psi(\nu\otimes\mu)=(-1)^{|\nu||\mu|}\mu\otimes\nu,$$
$$\text{if } \mu\in\{\alpha,\delta,d\alpha,d\delta\},\ \nu\in\{\alpha,\beta,\gamma,\delta,d\alpha,d\beta,d\gamma,d\delta\}$$

$$\Psi(\beta\otimes\beta)=\frac{rw}{uv}\beta\otimes\beta,\quad \Psi(\beta\otimes\gamma)=\frac{uv}{rw}\gamma\otimes\beta,\quad \Psi(\gamma\otimes\beta)=\frac{uv}{rw}\beta\otimes\gamma,$$

$$\Psi(\gamma\otimes\gamma)=\frac{rw}{uv}\gamma\otimes\gamma,\quad \Psi(d\beta\otimes\beta)=\frac{rw}{uv}\beta\otimes d\beta,\quad \Psi(d\beta\otimes\gamma)=\frac{uv}{rw}\gamma\otimes d\beta,$$

$$\Psi(d\gamma\otimes\beta)=\frac{uv}{rw}\beta\otimes d\gamma,\quad \Psi(d\gamma\otimes\gamma)=\frac{rw}{uv}\gamma\otimes d\gamma,\quad \Psi(\beta\otimes d\beta)=\frac{rw}{uv}d\beta\otimes\beta,$$

$$\Psi(\beta\otimes d\gamma)=\frac{uv}{rw}d\gamma\otimes\beta,\quad \Psi(\gamma\otimes d\beta)=\frac{uv}{rw}d\beta\otimes\gamma,\quad \Psi(\gamma\otimes d\gamma)=\frac{rw}{uv}d\gamma\otimes\gamma,$$

$$\Psi(d\beta\otimes d\beta)=-\frac{rw}{uv}d\beta\otimes d\beta,\quad \Psi(d\beta\otimes d\gamma)=-\frac{uv}{rw}d\gamma\otimes d\beta,\quad \Psi(d\gamma\otimes d\beta)=-\frac{uv}{rw}d\beta\otimes d\gamma,$$

$$\Psi(d\gamma\otimes d\gamma)=-\frac{rw}{uv}d\gamma\otimes d\gamma.$$

IV. BRAIDED ''LOCAL'' COACTIONS ON SOME QUANTUM DIFFERENTIAL ALGEBRAS

In this section, we show that the braided differential Hopf algebra $\Omega_{A(R,Z)}$ given in Theorem 3.1 can coact on some quantum differential algebras covariantly. Since the calculations involve the differentials and braidings, we call the coaction braided ''local'' coaction. Here are two typical examples.

Proposition 4.1: Let $\Omega_{V^*(R)}$ denote the quantum differential algebra on the quantum (co)vector space $V^*(R)$. $\Omega_{V^*(R)}$ is generated by $\{x=(x_i),\ dx=(dx_i),$ (written as row vectors), $1\}$ with the relations[4] (use the tensor notation)

$$x_2x_1R_{12}=qx_1x_2,\quad qdx_2x_1R_{12}=x_1dx_2,\quad qdx_2dx_1R_{12}=-dx_1dx_2. \tag{4.1}$$

Then $\Omega_{V^*(R)}$ is covariant under the braided ''local'' coaction β of the braided differential bialgebras $\Omega_{A(R,Z)}$,

$$\beta: x\mapsto xT,\quad dx\mapsto dxT+xdT \tag{4.2}$$

with the braidings

$$T_1'x_2=x_2Z_{12}^{-1}T_1'Z_{12},\quad T_1'dx_2=dx_2Z_{12}^{-1}T_1'Z_{12},$$
$$dT_1'x_2=x_2Z_{12}^{-1}dT_1'Z_{12},\quad dT_1'dx_2=-dx_2Z_{12}^{-1}dT_1'Z_{12}. \tag{4.3}$$

Proof: For simplifying the notations, in (4.2) we have omitted writing the tensor product $\otimes$. Moreover, since $x, dx \in \Omega_{V^*(R)}$ and $T, dT \in \Omega_{A(R,Z)}$ live in different algebras, in the following calculations, we shall also omit the primes on T, dT when using braidings such as (4.3).

The covariance properties of the first relation in (4.1) have been pointed out in Refs. 8 and 16, here we consider the second and third. For the second relation, we have

$$\begin{aligned} q(dx_2T_2+x_2dT_2)x_1T_1R_{12} &= q\underline{dx_2T_2x_1}T_1R_{12}+qx_2\underline{dT_2x_1}T_1R_{12} \\ &= qdx_2x_1\underline{Z_{21}^{-1}T_2Z_{21}T_1R_{12}}+qx_2x_1\underline{Z_{21}^{-1}dT_2Z_{21}T_1R_{12}} \\ &= \underline{qdx_2x_1R_{12}}Z_{12}^{-1}T_1Z_{12}T_2+\underline{qx_2x_1R_{21}^{-1}}Z_{12}^{-1}T_1Z_{12}dT_2 \\ &= x_1\underline{dx_2Z_{12}^{-1}T_1Z_{12}}T_2+x_1\underline{x_2Z_{12}^{-1}T_1Z_{12}}dT_2 \\ &= x_1T_1dx_2T_2+x_1T_1x_2dT_2=x_1T_1(dx_2T_2+x_2dT_2), \end{aligned}$$

where we have used relations (3.1), (4.1), and (4.3). Similarly, for the third relation we have

$$\begin{aligned} &q(dx_2T_2+x_2dT_2)(dx_1T_1+x_1dT_1)R_{12} \\ &\quad= qdx_2dx_1\underline{Z_{21}^{-1}T_2Z_{21}T_1R_{12}}-qx_2dx_1Z_{21}^{-1}dT_2Z_{21}T_1R_{12} \\ &\qquad+qdx_2x_1\underline{Z_{21}^{-1}T_2Z_{21}dT_1}R_{12}+qx_2x_1\underline{Z_{21}^{-1}dT_2Z_{21}dT_1R_{12}} \\ &\quad= \underline{qdx_2dx_1R_{12}}Z_{12}^{-1}T_1Z_{12}T_2-qx_2dx_1Z_{21}^{-1}dT_2Z_{21}T_1R_{12} \\ &\qquad+\underline{qdx_2x_1R_{12}}Z_{12}^{-1}dT_1Z_{12}T_2(1+\lambda R_{21}P_{12})-\underline{qx_2x_1R_{21}^{-1}}Z_{12}^{-1}dT_1Z_{12}dT_2 \\ &\quad= -dx_1\underline{dx_2Z_{12}^{-1}T_1Z_{12}}T_2+x_1\underline{dx_2Z_{12}^{-1}dT_1Z_{12}}T_2-\underline{q^{-1}x_2dx_1R_{21}^{-1}Z_{12}^{-1}T_1Z_{12}}dT_2 \\ &\qquad-x_1\underline{x_2Z_{12}^{-1}dT_1Z_{12}}dT_2 \\ &\quad= -dx_1T_1dx_2T_2-x_1dT_1dx_2T_2-dx_1T_1x_2dT_2-x_1dT_1x_2dT_2 \\ &\quad= -(dx_1T_1+x_1dT_1)(dx_2T_2+x_2dT_2). \end{aligned}$$

So the transformed quantum covectors and their differentials obey the same relations as that of the original quantities. Here we have used (3.1), (4.1), (4.3) and the Hecke property of R. □

Proposition 4.2: Let $\Omega_{V(R)}$ denote the quantum differential algebra on the quantum vector algebra $V(R)$. $\Omega_{V(R)}$ is generated by $\{v=(v^i), dv=(dv^i)$, (written as column vectors), $1\}$ with the relations[5]

$$R_{12}v_2v_1=qv_1v_2, \quad qR_{21}v_1dv_2=dv_2v_1, \quad qR_{12}dv_2dv_1=-dv_1dv_2. \tag{4.4}$$

Then $\Omega_{V(R)}$ is covariant under the braided ''local'' coaction β of the braided differential Hopf algebra $\Omega_{A(R,Z)}$,

$$\beta: v\mapsto T^{-1}v, \quad dv\mapsto dT^{-1}v+T^{-1}dv \tag{4.5}$$

with the braidings

$$\begin{gathered} Z_{12}^{-1}T_1'^{-1}Z_{12}v_2=v_2T_1'^{-1}, \quad Z_{12}^{-1}dT_1'^{-1}Z_{12}v_2=v_2dT_1'^{-1}, \\ Z_{12}^{-1}T_1'^{-1}Z_{12}dv_2=dv_2T_1'^{-1}, \quad Z_{12}^{-1}dT_1'^{-1}Z_{12}dv_2=-dv_2dT_1'^{-1}. \end{gathered} \tag{4.6}$$

Proof: Similar to the explanations in Refs. 17 and 16, here the meanings of $T^{-1}v$ and $dT^{-1}v+T^{-1}dv$ are precisely $\Psi(T^{-1}v)$ and $\Psi(dT^{-1}v)+\Psi(T^{-1}dv)$ by definition as elements of the braided tensor-product algebra $\Omega_{V(R)}\otimes\Omega_{A(R,Z)}$. We write $T^{-1}v$, etc., with T^{-1}, etc., on the left for convenience with regard to their matrix structure. In practice, it is convenient to write the braiding relations in the implicit forms as in (4.6). Moreover, we omit the primes on T^{-1} and dT^{-1} as in the proof of Proposition 4.1. The covariance of the first relation in (4.4) has been pointed out in Refs. 8 and 16, now we consider the second and the third relations. For the second, we have

$$
\begin{aligned}
&qR_{21}T_1^{-1}v_1(dT_2^{-1}v_2+T_2^{-1}dv_2)\\
&\quad=qR_{21}T_1^{-1}\underline{v_1dT_2^{-1}}v_2+qR_{21}T_1^{-1}\underline{v_1T_2^{-1}}dv_2\\
&\quad=q\underline{R_{21}T_1^{-1}Z_{21}^{-1}dT_2^{-1}Z_{21}}v_1v_2+q\underline{R_{21}T_1^{-1}Z_{21}^{-1}T_2^{-1}Z_{21}}v_1dv_2\\
&\quad=dT_2^{-1}Z_{12}^{-1}T_1^{-1}Z_{12}\underline{qR_{12}^{-1}v_1v_2}+T_2^{-1}Z_{12}^{-1}T_1^{-1}Z_{12}\underline{qR_{21}v_1dv_2}\\
&\quad=dT_2^{-1}\underline{Z_{12}^{-1}T_1^{-1}Z_{12}v_2}v_1+T_2^{-1}\underline{Z_{12}^{-1}T_1^{-1}Z_{12}dv_2}v_1\\
&\quad=dT_2^{-1}v_2T_1^{-1}v_1+T_2^{-1}dv_2T_1^{-1}v_1\\
&\quad=(dT_2^{-1}v_2+T_2^{-1}dv_2)T_1^{-1}v_1.
\end{aligned}
$$

Similarly, for the third relation we have

$$
\begin{aligned}
&qR_{12}(dT_2^{-1}v_2+T_2^{-1}dv_2)(dT_1^{-1}v_1+T_1^{-1}dv_1)\\
&\quad=qR_{12}dT_2^{-1}\underline{v_2dT_1^{-1}}v_1+qR_{12}dT_2^{-1}\underline{v_2T_1^{-1}}dv_1+qR_{12}T_2^{-1}\underline{dv_2dT_1^{-1}}v_1+qR_{12}T_2^{-1}\underline{dv_2T_1^{-1}}dv_1\\
&\quad=q\underline{R_{12}dT_2^{-1}Z_{12}^{-1}dT_1^{-1}Z_{12}}v_2v_1+qR_{12}\underline{dT_2^{-1}Z_{12}^{-1}T_1^{-1}Z_{12}}v_2dv_1-qR_{12}T_2^{-1}Z_{12}^{-1}dT_1^{-1}Z_{12}dv_2v_1\\
&\qquad+q\underline{R_{12}T_2^{-1}Z_{12}^{-1}T_1^{-1}Z_{12}}dv_2dv_1\\
&\quad=-dT_1^{-1}Z_{21}^{-1}dT_2^{-1}Z_{21}\underline{qR_{21}^{-1}v_2v_1}+(1+\lambda P_{12}R_{21})T^{-1}Z_{21}^{-1}dT_2^{-1}Z_{21}\underline{qR_{12}v_2dv_1}\\
&\qquad-qR_{12}T_2^{-1}Z_{12}^{-1}dT_1^{-1}Z_{12}dv_2v_1+T_1^{-1}Z_{21}^{-1}T_2^{-1}Z_{21}\underline{qR_{12}dv_2dv_1}\\
&\quad=-dT_1^{-1}\underline{Z_{21}^{-1}dT_2^{-1}Z_{21}v_1}v_2+T_1^{-1}\underline{Z_{21}^{-1}dT_2^{-1}Z_{21}dv_1}v_2-dT_1^{-1}\underline{Z_{21}^{-1}T_2^{-1}Z_{21}q^{-1}R_{21}^{-1}dv_2v_1}\\
&\qquad-T_1^{-1}\underline{Z_{21}^{-1}T_2^{-1}Z_{21}dv_1}dv_2\\
&\quad=-dT_1^{-1}v_1dT_2^{-1}v_2-T_1^{-1}dv_1dT_2^{-1}v_2-dT_1^{-1}v_1T_2^{-1}dv_2-T_1^{-1}dv_1T_2^{-1}dv_2\\
&\quad=-(dT_1^{-1}v_1+T_1^{-1}dv_1)(dT_2^{-1}v_2+T_2^{-1}dv_2).
\end{aligned}
$$

In the above-mentioned calculations, we have used the relations for $\Omega_{A(R,Z)}$ in a form obtained by applying the braided antipode S to (3.1), and also used (4.4), (4.6) and the Hecke property of R.□

As some important special cases of Propositions 4.1 and 4.2, we mention that, when $Z=I$, R is a regular solution of QYBE, we obtain the braided ''locally'' covariant coactions of $\Omega_{A(R)}$ on $\Omega_{V^*(R)}$ and $\Omega_{V(R)}$, which were given in Refs. 2 and 5 for different purposes. When $Z=R$, we obtain the braided ''local'' coactions of $\Omega_{B(R)}$ on $\Omega_{V^*(R)}$ and $\Omega_{V(R)}$, etc. However, here we use the ''right-hand'' notations.

V. CONCLUSIONS AND DISCUSSIONS

We have constructed the braided differential bialgebras (Hopf algebras) $\Omega_{A(R,Z)}$ on the quantized braided groups $A(R,Z)$. The $\Omega_{A(R,Z)}$ is a kind of generalization of the differential calculuses on the quantum groups, braided groups, quantum supergroups, etc., and unifies them into a single

algebraic system. When some further restrictions are imposed on the R-matrix pair (R,Z), the quantum differential bialgebras (Hopf algebras) $\Omega_{A(R)}$,[2,3,5] the braided differential bialgebras (Hopf algebras) $\Omega_{B(R)}$,[6] etc., can be obtained as special cases of $\Omega_{A(R,Z)}$.

The covariance properties of the quantum differential (co)vector algebras $\Omega_{V^*(R)}$ and $\Omega_{V(R)}$ under the braided ''local'' coactions of $\Omega_{A(R,Z)}$ are also considered. These can be taken as the bases of $A(R,Z)$ gauge theories, which will be discussed in further work.

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On the classification of irreducible finite-dimensional representations of $U_q'(so_3)$ algebra

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In an earlier work [M. Havlíček *et al.*, J. Math. Phys. **40**, 2135 (1999)] we defined for any finite dimension five nonequivalent irreducible representations of the nonstandard deformation $U_q'(so_3)$ of the Lie algebra so_3 where q is not a root of unity [for each dimension only one of them (called classical) admits limit $q\to 1$]. In the first part of this paper we show that any finite-dimensional irreducible representation is equivalent to some of these representations. In the case $q^n=1$ we derive new Casimir elements of $U_q'(so_3)$ and show that a dimension of any irreducible representation is not higher than n. These elements are Casimir elements of $U_q'(so_m)$ for all m and even of $U_q'(iso_{m+1})$ due to Inönu–Wigner contraction. According to the spectrum of one of the generators, the representations are found to belong to two main disjoint sets. We give full classification and explicit formulas for all representations from the first set (we call them nonsingular representations). If n is odd, we have full classification also for the remaining singular case with the exception of a finite number of representations. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Quantum orthogonal and Lorentz groups and their corresponding q-deformed algebras are of special interest for modern physics. M. Jimbo and V. Drinfeld defined q-deformations $U_q(g)$ for all simple complex Lie algebras g by means of Cartan subalgebras and root subspaces. Reshetikhin, Takhtajan, and Faddeev defined quantum algebras $U_q(g)$ in terms of the universal R-matrix. These approaches do not give a satisfactory presentation of the quantum algebra $U_q(so(n,\mathbb{C}))$ because these definitions of algebras do not allow inclusions $U_q(so(n+1,\mathbb{C}))\supset U_q(so(n,\mathbb{C}))$. These reductions are easy to explore if we take q-deformations of the Lie algebra $so(n,\mathbb{C})$ defined in terms of the generators $I_{k,k-1}=E_{k,k-1}-E_{k-1,k}$ [where E_{is} is the matrix with elements $(E_{is})_{rt}=\delta_{ir}\delta_{st}$] rather than by means of Cartan subalgebras and root elements [for definition see Ref. 1 or (81)–(83)]. As a result we obtain the associative algebra denoted by $U_q'(so(n,\mathbb{C}))$.

In this article we are interested in algebra $U_q'(so(3,\mathbb{C}))$ [for convenience we write $U_q'(so_3)$]. This algebra turns out to be of great importance for quantum gravity when considering the quantum algebra of gauge invariant quantities (see Ref. 2). This article is a prolongation of Ref. 3 where we presented for any finite dimension five nonequivalent irreducible representations of the algebra $U_q'(so_3)$.

The first main result of this article is a proof that any finite-dimensional irreducible representation of $U_q'(so_3)$ is equivalent to some of the described ones when q is not a root of unity [Secs. III and IV]. The considerations are based on an important fact that number $2\varepsilon(q-q^{-1})^{-1}$, $\varepsilon=\pm 1$, can never be an eigenvalue of generators of $U_q'(so_3)$ in irreducible finite-dimensional representation if q is not a root of unity (see Theorem 2). This simply formulated assertion is a consequence of Lemma 14, which represents deep insight in the algebraical structure of $U_q'(so_3)$.

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As a corollary we obtain that the generators are diagonalizable in any finite-dimensional irreducible representation when q is not a root of unity (the same situation as in classical case $q=1$). If the dimension of irreducible representation is greater than one, there exist two weight vectors—analogs of highest and lowest weight in the classical case $q=1$.

Irreducible finite-dimensional representations in the case $q^n=1$ are studied in Secs. V–VII. The basic tools are three new Casimir elements (Lemma 2) in the polynomial form in one of the generators. The proof that these Casimir elements commute is based on nontrivial combinatorial identities (see Lemma 12 in Appendix A). First we show that any irreducible representation of $U_q'(so_3)$ is finite-dimensional. According to the spectrum of one choosen generator (say I_3) we define two types of representations: nonsingular and singular ones (spectrum of I_3 contains value $-i[\nu]_q$ with $q^\nu=i\varepsilon q^{-k/2}$ for some $k\in\mathbb{Z}$, $\varepsilon\in\{-1,1\}$).

For nonsingular irreducible representations we give their full classification with explicit form for any n. It consists of a three-parameter set of n-dimensional nonequivalent irreducible representations presented earlier in Ref. 3 and one k-dimensional irreducible representation, where $k=1,2,...,n-1$ if n is odd, $k=1,2,...,n/2$ if n is even. If n is even, there is, moreover, one one-parameter set of nonequivalent $n/2$-dimensional irreducible representations (see Table II).

The structure of singular representations is much more complicated and we give a final result only for the case where n is odd. There are four nonequivalent irreducible representations for dimensions $1,2,...,(n+1)/2$ and two families of n-dimensional nonequivalent irreducible representations: one- and two-parameter ones. With the exception of the mentioned one-parameter family we also give explicit formulas. As to dimensions $(n+3)/2,...,n-1$ we have uncertainty: there are at most four irreducible representations for each dimension, but we did not prove their existence for $n\geqq 7$ (see Table III).

The simple consequence of our considerations is the assertion that singular n-dimensional irreducible representation generator I_3 is diagonalizable iff Casimir C has a special value (Note 12). With only one exception, the explicit forms of all irreducible representations having I_3 diagonalizable are presented. The systematic study of representations and corresponding problems of $U_q'(so_3)$ in full detail presented in this article could be useful as illustrations of possible complications considering deformations of Lie algebras. We hope that similar techniques can be applied in the other cases of various deformations.

II. BASIC DEFINITIONS AND FACTS

We suppose through the whole article that q is fixed complex number, $q\notin\{0,1,-1\}$.

Definition 1: $U_q'(so_3)$ is a complex associative algebra generated by three elements I_1, I_2, I_3 and relations (square roots of q is convention only)

$$q^{1/2}I_1I_2-q^{-1/2}I_2I_1=I_3, \tag{1}$$

$$q^{1/2}I_2I_3-q^{-1/2}I_3I_2=I_1, \tag{2}$$

$$q^{1/2}I_3I_1-q^{-1/2}I_1I_3=I_2. \tag{3}$$

Theorem 1: The set $\{I_1^kI_2^mI_3^n|k,m,n\in\mathbb{N}\cup\{0\}\}$ forms a basis of the linear space $U_q'(so_3)$.

Proof: Theorem 1 is proven by means of the diamond lemma (see Ref. 4, subsection 4.1.5).

Note 1: The algebra defined by the relations (1)–(3) is distinctive among others in the following sense: although we can assume more general deformation of the Lie algebra o(3) defined by relations

$$\alpha_1I_1I_2-\alpha_2I_2I_1=\alpha_3I_3,$$

$$\alpha_4I_2I_3-\alpha_5I_3I_2=\alpha_6I_1,$$

$$\alpha_7I_3I_1-\alpha_8I_1I_3=\alpha_9I_2$$

$(\alpha_1,\ldots,\alpha_9\in\mathbb{C}-\{0\})$, it can be proven that (very important) Theorem 1 is valid if and only if the deformation has the form (1)–(3) (up to an isomorphism).

Lemma 1: An element

$$C=q^2I_1^2+I_2^2+q^2I_3^2-(q^{5/2}-q^{1/2})I_1I_2I_3 \tag{4}$$

is a Casimir element of $U_q'(\mathrm{so}_3)$.

Proof: Clearly from the defining relations $[C,I_1]=[C,I_2]=[C,I_3]=0$ (the brackets denote the usual commutator $[x,y]=xy-yx$).

Lemma 2: Let $q^n=1$. Then the element

$$C^{(n)}(I_1)=\sum_{j=0}^{[(n-1)/2]}\binom{n-j}{j}\frac{1}{n-j}\left(\frac{i}{q-q^{-1}}\right)^{2j}I_1^{n-2j} \tag{5}$$

is a Casimir element of $U_q'(\mathrm{so}_3)$; $[x]$ for $x\in\mathbb{R}$ denotes the integral part of x.

Proof: Because $C^{(n)}(I_1)$ is a polynomial in I_1 and because of (3) it is sufficient to show $[C^{(n)}(I_1),I_3]=0$, i.e. (see Lemma 13),

$$\sum_{j=0}^{[(n-1)/2]}\binom{n-j}{j}\frac{1}{n-j}\left(\frac{i}{q-q^{-1}}\right)^{2j}(p_{n-2j}(I_1)I_2+q_{n-2j}(I_1)I_3-I_1^{n-2j}I_3)=0.$$

Thus we have to prove that two polynomials with complex coefficients

$$P_n(x):=\sum_{j=0}^{[(n-1)/2]}\binom{n-j}{j}\frac{1}{n-j}\left(\frac{i}{q-q^{-1}}\right)^{2j}p_{n-2j}(x),$$

$$Q_n(x):=\sum_{j=0}^{[(n-1)/2]}\binom{n-j}{j}\frac{1}{n-j}\left(\frac{i}{q-q^{-1}}\right)^{2j}(q_{n-2j}(x)-x^{n-2j})$$

are zero polynomials. Let us consider first polynomial P_n. Using Lemma 13 [we use the property $\binom{u}{v}=0$ for $u,v\in\mathbb{Z}$, $v<0$ or $0\leqq u<v$ to change bounds of various sums advantageously, for example to make inner summations independent] we have

$$P_n(x)=q^{-1/2}\sum_{c=0}^{[(n-1)/2]}\left(\frac{q+q^{-1}}{q-q^{-1}}\right)^{-2[(n-1)/2]+2c}(-1)^c\pi_{n,c}(q)\left(\frac{x(q+q^{-1})}{2}\right)^{n-1-2c},$$

where

$$\pi_{n,c}(q)=p_{n,c}((q-q^{-1})^{-2}),$$

$$p_{n,c}(y)=\sum_{j=0}^{[(n-1)/2]}\sum_{t=0}^{[(n-1)/2]-j}\binom{n-j}{j}\frac{1}{n-j}\binom{n-2j}{2t+1}\binom{t}{c-j}y^j(1+4y)^{[(n-1)/2]-(t+j)}.$$

Then we find a better form for polynomial $p_{n,c}$:

$$p_{n,c}(y)=\sum_{d=0}^{[(n-1)/2]}p_{n,c,d}y^d,$$

where

$$p_{n,c,d}=4^d\sum_{j=0}^{[(n-1)/2]}\binom{n-j}{j}\frac{1}{4^j(n-j)}\sum_{t=0}^{[(n-1)/2]-j}\binom{n-2j}{2t+1}\binom{t}{c-j}\binom{\left[\frac{n-1}{2}\right]-j-t}{d-j}.$$

Now we use formula (A1) (see Lemma 12; we take $N=n-2j$, $M=c-j$, $H=[(n-1)/2]-d$ and fact that it is sufficient to compute outer sum over $j=0...\min\{c,d\}$):

$$p_{n,c,d}=\sum_{j=0}^{\min\{c,d\}}\binom{n-j}{j}\frac{4^{[(n-1)/2]-c}}{n-j}\binom{\left[\frac{n-1}{2}\right]-d}{c-j}(-2j+2d+1+(n-2d-1)^{n'})$$

$$\cdot\frac{(2[n/2]-2j)!(n-1-c-d)!([n/2]-c)!}{([n/2]-j)!(d-j+1-n')!(2[n/2]-2c)!(n-2d+n'-1)!},$$

where $n'=n \bmod 2$. Now we can apply directly (A2) and have

$$p_{n,c,d}=\frac{4^{[(n-1)/2]-c}\binom{n-1-d}{d}\binom{n-1-c}{c}}{(n/2)^{1-n'}(n-2d)^{n'}}.$$

We come back to polynomial $p_{n,c}$:

$$p_{n,c}(y)=\frac{4^{[(n-1)/2]-c}\binom{n-1-c}{c}}{(n/2)^{1-n'}}\sum_{d=0}^{[(n-1)/2]}\frac{\binom{n-1-d}{d}}{(n-2d)^{n'}}y^d.$$

If n is even, then $n'=0$ and we can apply the formula [see Ref. 5, (5.74)]

$$\sum_{k=0}^{[n/2]}\binom{n-k}{k}z^k=\frac{1}{\sqrt{1+4z}}\left(\left(\frac{1+\sqrt{1+4z}}{2}\right)^{n+1}-\left(\frac{1-\sqrt{1+4z}}{2}\right)^{n+1}\right),$$

$$n\in\mathbb{N},\quad z\in\mathbb{C}-\{-\tfrac{1}{4}\}. \tag{6}$$

Then, after returning to $y\to(q-q^{-1})^{-2}$, we have directly $p_{n,c}((q-q^{-1})^{-2})=0$ using the fact $q^n=1$ for all $c\leqq n/2-1$.

If n is odd, then $n'=1$ and we apply the formula [see Ref. 5, (5.75)]

$$\sum_{k=0}^{[n/2]}\binom{n-k}{k}\frac{n}{n-k}z^k=\left(\frac{1+\sqrt{1+4z}}{2}\right)^n+\left(\frac{1-\sqrt{1+4z}}{2}\right)^n,\quad n\in\mathbb{N},\quad z\in\mathbb{C}. \tag{7}$$

Again we have directly $p_{n,c}((q-q^{-1})^{-2})=0$ using the fact $q^n=1$ for all $c\leqq(n-1)/2$.

Let us now examine the polynomial Q_n. Using (B3) we can transform Q_n into two parts. The first part is zero because it is a multiple of P_n. Using (7) and the fact that $q^n=1$ we get directly that the second part is equal to zero, too.

Corollary 1: The same assertion as in Lemma 2 is valid for the generators I_2 and I_3.

Proof: Use the automorphism $\rho:U_q'(so_3)\to U_q'(so_3)$ defined by relations

$$\rho(I_1)=I_2,\quad \rho(I_2)=I_3,\quad \rho(I_3)=I_1. \tag{8}$$

□

Definition 2: Let $\nu\in\mathbb{C}$. We denote by O_ν and R_ν these special linear combinations:

$$O_\nu:=iI_2+q^{-\nu+1/2}I_1,$$

$$R_\nu := iI_2 - q^{\nu+1/2} I_1 .$$

Lemma 3: Let $R: U_q'(\mathrm{so}_3) \to L(V)$ be a linear representation of $U_q'(\mathrm{so}_3)$ on (not necessarily finite-dimensional) vector space V [through the whole article we will usually denote the operators $R(I_1)$, $R(I_2)$ and $R(I_3)$ acting on vectors from the representation space V by the same symbols I_1, I_2, I_3, so there can be no misunderstanding]. Let $x \in \mathrm{Ker}\,(I_3 + i[\nu+k]_q)$ for some fixed $k \in \mathbb{Z}$ and $\nu \in \mathbb{C}$ [we denote $\mathrm{Ker} A = \{v \in V | Av = 0\}$ and $[a]_q := (q^a - q^{-a})/(q - q^{-1})$ for $a \in \mathbb{C}$]. Then

$$I_3(O_{\nu+k} x) = -i[\nu+k+1]_q (O_{\nu+k} x), \tag{9}$$

$$I_3(R_{\nu+k} x) = -i[\nu+k-1]_q (R_{\nu+k} x), \tag{10}$$

$$O_{\nu+k-1} R_{\nu+k} x = -(C + q[\nu+k-1]_q [\nu+k]_q) x, \tag{11}$$

$$R_{\nu+k+1} O_{\nu+k} x = -(C + q[\nu+k]_q [\nu+k+1]_q) x, \tag{12}$$

where C denotes Casimir element (4).

Proof: By inspection using the defining relations (1)–(3).

Note 2: The system of linear equations ($x, y, z \in V$)

$$O_\nu x = y, \quad \text{i.e.,} \quad iI_2 x + q^{-\nu+1/2} I_1 x = y,$$

$$R_\nu x = z, \quad \text{i.e.,} \quad iI_2 x - q^{\nu+1/2} I_1 x = z$$

has a unique solution for the vectors $I_1 x$ and $I_2 x$ for given y, z if and only if $q^\nu \neq i\varepsilon$ for both $\varepsilon \in \{-1, 1\}$.

Note 3: Let $R^{(1,1)}$ be a representation of $U_q'(\mathrm{so}_3)$. Then $R^{(\eta_1, \eta_2)}$, $\eta_1, \eta_2 \in \{1, -1\}$, where

$$R^{(1,-1)}(I_1) = -R^{(1,1)}(I_1), \quad R^{(1,-1)}(I_2) = -R^{(1,1)}(I_2), \quad R^{(1,-1)}(I_3) = R^{(1,1)}(I_3),$$

$$R^{(-1,1)}(I_1) = -R^{(1,1)}(I_1), \quad R^{(-1,1)}(I_2) = R^{(1,1)}(I_2), \quad R^{(-1,1)}(I_3) = -R^{(1,1)}(I_3),$$

$$R^{(-1,-1)}(I_1) = R^{(1,1)}(I_1), \quad R^{(-1,-1)}(I_2) = -R^{(1,1)}(I_2), \quad R^{(-1,-1)}(I_3) = -R^{(1,1)}(I_3)$$

form four representations of $U_q'(\mathrm{so}_3)$. If the dimension of representation is odd and at least two of the three operators $R^{(1,1)}(I_j)$, $j = 1,2,3$, are bijective, these four representations are nonequivalent (the determinants of the operators have different signs).

III. BASIS CONSTRUCTION AND SPECTRAL PROPERTIES WHEN q IS NOT A ROOT OF UNITY

The following theorem plays an important simplifying role in our considerations.

Theorem 2: If q is not a root of unity, then $\mathrm{Ker}\,(I_3 - (2\varepsilon/(q - q^{-1}))) = \{0\}$ for both $\varepsilon \in \{-1, 1\}$ in any irreducible finite-dimensional representation of $U_q'(\mathrm{so}_3)$.

Proof: See Appendix B.

Corollary 2: The same assertion as in Theorem 2 is valid for generators I_2 and I_1.

Proof: Use the automorphism (8).

Theorem 3: Let R be an irreducible representation of $U_q'(\mathrm{so}_3)$ on vector space V, $\dim V = r$, and let q not be a root of unity. Then there exist $\nu \in \mathbb{C}$ and vector $0 \neq x_0 \in \mathrm{Ker}\,(I_3 + i[\nu]_q)$ such that $O_\nu x_0 = 0$ and

$$V = \mathbb{C}\{x_0, x_{-1,\ldots}, x_{-r+1}\}_{\mathrm{lin}}, \quad x_{-j-1} := R_{\nu-j} x_{-j}, \quad j = 0,1,\ldots,r-2.$$

Proof: Let $0 \neq y_0 \in \mathrm{Ker}\,(I_3 + i[\mu]_q)$ for some $[\mu]_q$, where q^μ is choosen such that numbers $-i[\mu]_q, -i[\mu+1]_q, \ldots$ are mutually different (see Lemma 10). Let us define vectors

$$y_{j+1} := O_{\mu+j} y_j, \quad j \geqq 0 \tag{13}$$

and let $l \in \mathbb{N}$ such that vectors $y_0,\ldots,y_{l-1}$ are linearly independent and $y_l \in \mathbb{C}\{y_0,\ldots,y_{l-1}\}_{\text{lin}}$ (such l exists, it is the consequence of the finite dimension of V). Equation (9) shows that all vectors $y_0,\ldots,y_{l-1},y_l$ fulfill eigenequation $I_3 y_j = -i[\mu+j]_q y_j$ with different eigenvalues and, therefore, the only possibility for y_l is

$$y_l = 0. \tag{14}$$

Denote $x_0 := y_{l-1}$, $\nu := \mu + l - 1$ and define similarly vectors

$$x_{-j-1} := R_{\nu-j} x_{-j}, \quad j \geqq 0.$$

Again from (10) follows

$$I_3 x_{-j} = -i[\nu - j]_q x_{-j}, \quad j \geqq 0. \tag{15}$$

Let $k \in \mathbb{N}$ be such that vectors $x_0,\ldots,x_{-k+1}$ are linearly independent and $x_{-k} \in \mathbb{C}\{x_0,\ldots,x_{-k+1}\}_{\text{lin}}$. Equation (11) then implies for $j = 1,2,\ldots,k-1$

$$O_{\nu-j} x_{-j} = O_{\nu-j} R_{\nu-j+1} x_{-j+i} = -(C + q[\nu-j+1]_q[\nu-j]_q) x_{-j+1},$$

and for Eqs. (13) and (14)

$$O_\nu x_0 = 0. \tag{16}$$

Since representation R is irreducible, Casimir operator C [see (4)] equals a multiple of the identity and we will denote this complex constant by the same symbol $C \in \mathbb{C}$. Equation (16) together with (12) implies $0 = R_{\nu+1} O_\nu x_0 = -(C + q[\nu+1]_q[\nu]_q) x_0$, which gives for C value $C = -q[\nu+1]_q[\nu]_q$. We have (put $x_1 := 0$) for all $j \in \{0,\ldots,k-1\}$

$$R_{\nu-j} x_{-j} = x_{-j-1}, \tag{17}$$

$$O_{\nu-j} x_{-j} = -(C + q[\nu-j+1]_q[\nu-j]_q) x_{-j+1}. \tag{18}$$

According to Note 2 this system has solution $I_1 x_{-j}$ and $I_2 x_{-j}$ iff $q^{\nu-j} \neq i\varepsilon$ for both $\varepsilon \in \{-1,1\}$. This condition is fulfilled: in the opposite case $-i[\nu-j]_q = 2\varepsilon/(q-q^{-1})$ and it is an eigenvalue of the vector x_{-j}. Theorem 2 excludes such eigenvalues for I_3 in finite-dimensional representation if q is not a root of unity. Vectors $I_1 x_{-j}$ and $I_2 x_{-j}$ are expressed by means of $x_0,\ldots,x_{-k+1}$; therefore $\mathbb{C}\{x_0,x_{-1},\ldots,x_{-k+1}\}_{\text{lin}}$ is an invariant subspace and, due to the irreducibility of R, this subspace equals to V, i.e., $k = r$. □

Corollary 3: If q is not a root of unity, then in any irreducible representation generator I_3 is diagonalizable. The same assertion holds for the generators I_1 and I_2.

Proof: Vectors $x_0,\ldots,x_{-r+1}$ are eigenvectors of generator I_3. The second assertion follows from Corollary 2. □

IV. EXPLICIT FORMULAS WHEN *q* IS NOT A ROOT OF UNITY

Let us prolongate considerations of Theorem 3. Solving (17) and (18) we obtain

$$I_1 x_{-j} = \frac{-q^{-1/2}}{q^{\nu-j} + q^{-\nu+j}} (D_j x_{-j+1} + x_{-j-1}), \quad 0 \leqq j \leqq r-1, \tag{19}$$

$$I_2 x_{-j} = \frac{i}{q^{\nu-j}+q^{-\nu+j}}(q^{\nu-j}D_j x_{-j+1} - q^{-\nu+j}x_{-j-1}),$$
$$D_j := C + q[\nu-j+1]_q[\nu-j]_q = -q[j]_q[2\nu-j+1]_q, \tag{20}$$

where $x_1 := 0$ and x_{-r} is some vector from V. As $x_{-r} \in \mathrm{Ker}\,(I_3 + i[\nu-r]_q)$ [see (15)] and q-number $-i[\nu-r]_q$ can be equal to at most one of the numbers $-i[\nu]_q, \ldots, -i[\nu-r+1]_q$, say $-i[\nu-p]_q$, $0 \leqq p \leqq r-1$ (see Lemma 10), there exists $\alpha \in \mathbb{C}$ such that $x_{-r} = \alpha x_{-p}$ (reason: linear-dependent vectors have the same eigenvalue) and $\alpha = 0$ or $\alpha \neq 0$ covers both cases.

Calculating $(q^{1/2}I_1I_2 - q^{-1/2}I_2I_1 - I_3)x_{-r+1} = 0$ [see (1)] we obtain

$$\frac{-iq^{-1}D_r}{q^{\nu-r+1}+q^{-\nu+r-1}}x_{-r+1} + \frac{\alpha i D_p(q^{-\nu+r-1}+q^{-\nu-p-1})}{(q^{\nu-r+1}+q^{-\nu+r-1})(q^{\nu-p}+q^{-\nu+p})}x_{-p+1}$$
$$+ \frac{i\alpha q^{-\nu-1}(q^r - q^p)}{(q^{\nu-r+1}+q^{-\nu+r-1})(q^{\nu-p}+q^{-\nu+p})}x_{-p-1} = 0. \tag{21}$$

Now we distinguish two cases $\alpha = 0$ and $\alpha \neq 0$.

A. Classical case $\alpha = 0$

Equation (21) gives now $D_r = 0$, i.e., $q^{2r} = 1$ or $q^{4\nu} = q^{2r-2}$. Because q is not a root of unity, thus $q^\nu = \varepsilon q^{(r-1)/2}$ or $q^\nu = i\varepsilon q^{(r-1)/2}$ for some $\varepsilon \in \{-1,1\}$.

If r is odd, then the case $q^\nu = i\varepsilon q^{(r-1)/2}$ is not allowed: we have $-i[\nu-(r-1)/2]_q = 2\varepsilon/(q - q^{-1})$ in the spectrum of I_3, which contradicts Theorem 2. It can be directly verified that in all remaining cases relations (1)–(3) are fulfilled and relations (19) and (20) take the following form:

$$I_3 x_{-j} = -i\frac{c_1 q^{-j+(r-1)/2} - c_1^{-1}q^{j-(r-1)/2}}{q-q^{-1}}x_{-j}, \quad 0 = \leqq j \leqq r-1, \quad x_1 = x_{-r} = 0, \tag{22}$$

$$I_1 x_{-j} = \frac{-q^{-1/2}}{c_1 q^{-j+(r-1)/2} + c_1^{-1}q^{j-(r-1)/2}}(c_1^2 q[j]_q[j-r]_q x_{-j+1} + x_{-j-1}), \tag{23}$$

$$I_2 x_{-j} = \frac{ic_1^3 q^{1/2}}{c_1 q^{-j+(r-1)/2} + c_1^{-1}q^{j-(r-1)/2}}(q^{r/2-j}[j]_q[j-r]_q x_{-j+1} - q^{-r/2+j}x_{-j-1}), \tag{24}$$

$c_1 = \varepsilon$ or $c_1 = i\varepsilon$. Possibility $c_1 = i\varepsilon$ is excluded also in the case when r is even: in Ref. 3 (Sec. IV) reducible representations $R_l^{(\pm i)}$, $l = (r-1)/2$, were defined on r-dimensional space $V = \mathbb{C}\{|m\rangle | m = -l, \ldots, l\}_{\mathrm{lin}}$ and representations (22)–(24) are equivalent to $R_l^{(-\varepsilon i)}$ through mapping

$$Tx_{-j} = \prod_{k=1}^{j} q^{1/2}[r-k]_q |-l+j\rangle, \quad j = 0,\ldots,2l = r-1.$$

In the only allowed case $c_1 = \varepsilon$ the representations are equivalent to irreducible representations $R_l^{(\varepsilon)}$ defined in Ref. 3 on the same space V through mapping

$$Tx_{-j} = \prod_{k=1}^{j} (-q^{1/2})[r-k]_q |-l+j\rangle, \quad j = 0,\ldots,2l = r-1.$$

It is shown in Ref. 3 that representations $R_l^{(1)}$ and $R_l^{(-1)}$ are equivalent. We see that formulas (22)–(24) admit limit $q \to 1$ and pass to usual formulas for irreducible representation of the Lie algebra o(3).

Note 4: Formulas (22)–(24) (from now we always assume $c_1=1$) define irreducible representation also for some roots of unity. If $q^k=-1$ for some $k\in\{r-1,r-3,...\}$, matrix I_1 is not defined. If $q^k=-1$ for some $k\in\{r-2,r-4,...\}$ or $q^k=1$ for some $k\in\{r-1,r-2,...\}$, representations (22)–(24) are reducible (some element of I_1 below diagonal is equal to zero). Therefore, we have the following.

(a) Let $q^n=1$, n odd. Then $q^j\neq -1$ for any $j\in\mathbb{N}$ (see Note 6) and (22)–(24) form irreducible representation for $n\geqq r$.
(b) Let $q^n=1$, n even (this implies $q^{n/2}=-1$). Then
  (i) we have irreducible representation if $n/2\geqq r$; and
  (ii) formulas lead to irreducible representation also for $n/2=r-1$. If $q^{r-1}\neq -1$, the diagonal matrix T,

$$Tx_0=(q^{(r-1)/2}+q^{-(r-1)/2})x_0,\quad Tx_{-j}=x_{-j},\quad j=1,2,...,r-1,$$

  is bijective, and equivalent representation TI_iT^{-1}, $i=1,2,3$, does not have singularity at $q^{r-1}=-1$ after continuous prolongation.

B. Nonclassical case $\alpha\neq 0$

In this case $q^\nu=i\varepsilon q^{(r+p)/2}$ for some $p\in\{0,1,...,r-1\}$ and $x_{-r}=\alpha x_{-p}$. Equation (21) has now the form

$$\frac{\varepsilon q^{-1}D_r}{q^{(r-p)/2-1}-q^{-(r-p)/2+1}}x_{-r+1}+\frac{\alpha\varepsilon q^{-1}}{q^{(r-p)/2-1}-q^{-(r-p)/2+1}}x_{-p-1}=0. \tag{25}$$

This equation can be satisfied only in two cases:

(a) $p+1=r-1$ but now $q^\nu=i\varepsilon q^{r-1}$, and again $2\varepsilon/(q-q^{-1})=-i[\nu-r+1]_q$ would be in the spectrum of generator I_3 which contradicts Theorem 2.
(b) $p+1=r$, which implies $x_{-p-1}=x_{-r}=\alpha x_{-r+1}$. Substituting into (25) we obtain

$$\alpha=i\varepsilon' q^{1/2}[r]_q \quad \text{for some} \quad \varepsilon'\in\{-1,1\}.$$

The final form of relations (19) and (20) in this case is

$$I_3x_{-j}=\varepsilon\frac{q^{1/2-r+j}+q^{-1/2+r-j}}{q-q^{-1}}x_{-j},\quad 0\leqq j\leqq r-1,\quad x_1=0,\quad x_{-r}=i\varepsilon' q^{1/2}[r]_q x_{-r+1}, \tag{26}$$

$$I_1x_{-j}=\frac{-i\varepsilon q^{-1/2}}{q^{1/2-r+j}-q^{-1/2+r-j}}(q[j]_q[2r-j]_q x_{-j+1}+x_{-j-1}), \tag{27}$$

$$I_2x_{-j}=\frac{-iq^{1/2}}{q^{1/2-r+j}-q^{-1/2+r-j}}([j]_q[2r-j]_q q^{r-j}x_{-j+1}+q^{-r+j}x_{-j-1}). \tag{28}$$

Similarly, these four representations are equivalent to irreducible representations $R_r^{(-i\varepsilon,\varepsilon')}$ from Ref. 3 acting on the space $V=\mathbb{C}\{|k\rangle|k=1,...,r\}_{\text{lin}}$ through mapping

$$Tx_{-j}=\prod_{k=1}^{j}(-q^{1/2})[2r-k]_q|r-j\rangle,\quad j=0,...,r-1.$$

All five constructed representations were described in Ref. 3 where their mutual nonequivalence and irreducibility were proved. So we have the following.

TABLE I. Finite-dimensional representations when q is not a root of unity.

Representation characteristic	Corresponding formulas	Dimension	No./each dimension
Classical (admit limit $q\to 1$)	(22)–(24), $c_1=1$	any	1
Nonclassical (does not admit limit $q\to 1$)	(26)–(28), $\epsilon,\epsilon'\in\{-1,1\}$	any	4

Theorem 4 (Main result): Any r-dimensional irreducible representation of $U_q'(\mathrm{so}_3)$ when q is not a root of unity is equivalent to one of five nonequivalent irreducible representations defined either by (22)–(24) where $c_1=1$ or by (26)–(28) where ε, $\varepsilon'\in\{-1,1\}$ (see Table I).

Note 5: If $q^k=1$, $k\in\{3,5,...,2r-1\}$, then matrix I_1 given by (27) is not defined. If $q^k=-1$ and $k\in\{2,...,r-1,r+1,...,2r-1\}$ or $q^k=1$ and $k\in\{4,6,...,2r-2\}$, matrices (26)–(28) form reducible representation. Therefore we have the following.

(a) Let $q^n=1$, n odd. Then $q^j\neq -1$ for any $j\in\mathbb{N}$ and
  (i) for $n>2r-1$ we have irreducible representation, and
  (ii) similarly as in Note 4, formulas lead to irreducible representation also in the case $n=2r-1$. The equivalence matrix T which removes singularity from I_1 now has form

$$Tx_0=(q^{1/2-r}-q^{-1/2+r})x_0;\quad Tx_{-j}=x_{-j},\quad j=1,2,...,r-1.$$

(b) Let $q^n=1$, n even ($\Rightarrow q^{n/2}=-1$). Then (26)–(28) define representation which is irreducible only if $n\subset\{4,6,...,2r-2,2r+2,...,2(2r-1)\}$, i.e., if $n\geqq 4r$ or $n=2r$.

V. REPRESENTATIONS WHEN q IS A ROOT OF UNITY

Note 6: Through Secs. V–VII we assume that q is a root of unity, i.e., $q^n=1$ for some fixed $n\in\mathbb{N}$, $q^j\neq 1$ for $j<n$.

Lemma 4: $U_q'(\mathrm{so}_3)$ is at most a $3n(n-1)+1$-dimensional module over the center.

Proof: Because the Casimir elements $C^{(n)}(I_j)$, $j\in\{1,2,3\}$ [see (5)], belong to the center of $U_q'(\mathrm{so}_3)$, any element $A=I_1^{j_0}I_2^{k_0}I_3^{l_0}\in U_q'(\mathrm{so}_3)$, where $j_0,k_0,l_0\geqq 0$, can be expressed as linear combination

$$A=\sum_{j,k,l=0}^{n-1} Z_{j,k,l}I_1^jI_2^kI_3^l, \tag{29}$$

where $Z_{j,k,l}$ belong to the center. Similarly, due to Casimir element C [see (4)] we can remove from sum (29) all operators $I_1^jI_2^kI_3^l$ where product $jkl>0$ because all such operators can be expressed as a linear combination with coefficients from the center of elements $I_1^jI_2^k$, $I_2^jI_3^k$ and $I_1^jI_3^k$, $0\leqq j,k\leqq n-1$. Therefore, we have

$$A=\sum_{j,k=1}^{n-1} Z_{j,k}^{(1)}I_1^jI_2^k+\sum_{j,k=1}^{n-1} Z_{j,k}^{(2)}I_1^jI_3^k+\sum_{j,k=1}^{n-1} Z_{j,k}^{(3)}I_2^jI_3^k+\sum_{j=1}^{n-1} Z_j^{(4)}I_1^j+\sum_{j=1}^{n-1} Z_j^{(5)}I_2^j+\sum_{j=1}^{n-1} Z_j^{(6)}I_3^j+Z^{(7)}I,$$

where I denotes identity element and $Z_{\cdots}^{(\cdot)}$ are from center. The number of elements on right-hand side is $3(n-1)^2+3(n-1)+1=3n(n-1)+1$. □

Corollary 4: When q is a root of unity, any irreducible representation of $U_q'(\mathrm{so}_3)$ has finite dimension $\leqq[\sqrt{3n(n-1)+1}]$.

Proof: Let $\rho:U_q'(\mathrm{so}_3)\to L(V)$ be any nontrivial irreducible representation. Choose any $0\neq x\in V$. Then $V'=\mathbb{C}\{\rho(I_1^jI_2^kI_3^l)x|j,k,l\geqq 0\}_{\mathrm{lin}}$ is clearly an invariant subspace with at most countable basis. Because ρ is irreducible, we have $V'=V$. Now we can use Schur's lemma (see Ref. 6, section 8.2), which states that Casimir operators (4) and (5) are equal to a multiple of the identity. A previous lemma says that $\dim\mathbb{C}\{\rho(I_1^jI_2^kI_3^l)|j,k,l\geqq 0\}_{\mathrm{lin}}\leqq 3n(n-1)+1$. From the Burnside theo-

rem (see Ref. 7) follows that $\mathbb{C}\{\rho(I_1^j I_2^k I_3^l)|j,k,l\geqq 0\}_{\text{lin}}=L(V)$, i.e., $\dim L(V)\leqq 3n(n-1)+1$, which means that irreducible representation has finite dimension $\dim V\leqq[\sqrt{3n(n-1)+1}]$.

Definition 3: Representation is called having *weight vector* x_0 if there exist $x_0\neq 0$ and $\nu,\mu\in\mathbb{C}$ such that

$$I_3x_0=-i[\nu]_q x_0 \quad \text{and} \quad (O_\nu x_0=\mu x_0 \ \text{ or } \ R_\nu x_0=\mu x_0).$$

Note 7: It can be easily seen [taking $\nu'=-\nu+\pi i(\ln q)^{-1}$] that we can always assume $O_\nu x_0=\mu x_0$ in previous definition, i.e., representation has weight vector x_0 if there exist $x_0\neq 0$ and $\nu,\mu\in\mathbb{C}$ such that

$$I_3x_0=-i[\nu]_q x_0 \quad \text{and} \quad O_\nu x_0=\mu x_0. \tag{30}$$

Lemma 5: Let us assume (30). Then

$$q^\nu=i\varepsilon q^{-1/2} \ \text{ for some } \ \varepsilon\in\{-1,1\} \quad \text{and} \quad \mu^2=-C+q\left(\frac{q^{1/2}+q^{-1/2}}{q-q^{-1}}\right)^2 \tag{31}$$

or

$$\mu=0 \quad \text{and} \quad C=-q[\nu]_q[\nu+1]_q. \tag{32}$$

Proof: Applying I_3 on (30) [see (9)] we have $-i[\nu+1]_q O_\nu x_0=-i[\nu+1]_q\mu x_0=\mu(-i[\nu]_q)x_0$, so that either $\mu=0$ or $-i[\nu+1]_q=-i[\nu]_q\Rightarrow q^\nu=i\varepsilon q^{-1/2}$. Using (12) we obtain $-(C+q[\nu]_q[\nu+1]_q)x_0=\mu R_{\nu+1}x_0$. If $\mu=0$, we have $C=-q[\nu]_q[\nu+1]_q$. If $\mu\neq 0$, then $R_{\nu+1}=O_\nu$ (due to $q^\nu=i\varepsilon q^{-1/2}$) and therefore $-(C+q[\nu]_q[\nu+1]_q)x_0=\mu(\mu x_0)\Rightarrow\mu^2=-C+q((q^{1/2}+q^{-1/2})(q-q^{-1})^{-1})^2$. □

Note 8: Sign convention. Assume (31) in (30). Then we have

$$I_3x_0=\varepsilon\frac{q^{1/2}+q^{-1/2}}{q-q^{-1}}x_0, \quad O_\nu x_0=\tilde{\varepsilon}\sqrt{-C+q\left(\frac{q^{1/2}+q^{-1/2}}{q-q^{-1}}\right)^2}\,x_0,$$

where $\varepsilon,\tilde{\varepsilon}\in\{-1,1\}$. Turning to representation

$$I_1\to\varepsilon\tilde{\varepsilon}I_1, \quad I_2\to\tilde{\varepsilon}I_2, \quad I_3\to\varepsilon I_3,$$

we can, without loss of generality, assume $\varepsilon=\tilde{\varepsilon}=1$ and obtain three other possibilities using Note 3.

Lemma 6: Let us have irreducible representation with weight vector x_0 on a vector space V. Then $V=\mathbb{C}\{I_1^m x_0|m=0,1,...,n-1\}_{\text{lin}}$ and therefore $\dim V\leqq n$.

Proof: Let us assume (30). We use the formula $I_3I_1^m=p_m(I_1)I_2+q_m(I_1)I_3$ from Lemma 13. We have $I_2x_0=-i\mu x_0+q^{-\nu+1/2}I_1x_0$ so that

$$I_3(I_1^m x_0)=p_m(I_1)(-i\mu x_0+q^{-\nu+1/2}I_1x_0)+-i[\nu]_q q_m(I_1)x_0.$$

Therefore subspace $\mathbb{C}\{x_0,I_1x_0,I_1^2x_0,...\}_{\text{lin}}$ is invariant not only with respect to I_1, but also with respect to I_3 and, due to (3), also with respect to I_2.

Because $q^n=1$, we have an irreducible representation [see (5)]

$$I_1^n=\alpha_{n-2}I_1^{n-2}+\alpha_{n-4}I_1^{n-4}+\cdots,$$

where α_j are some complex constants [they depend on q and can be read out from (5) but we do not need it here]. Thus $\mathbb{C}\{x_0,I_1x_0,I_1^2x_0,...\}_{\text{lin}}=\mathbb{C}\{x_0,I_1x_0,...,I_1^{n-1}x_0\}_{\text{lin}}=V$. □

Definition 4: Representation is called *nonsingular* if there exist $x_0\neq 0$ and $\nu\in\mathbb{C}$ such that

$$I_3 x_0 = -i[\nu]_q x_0 \quad \text{and} \quad q^{\nu} \notin \{i\varepsilon q^{-k/2} | k=0,...,n-1; \varepsilon = \pm 1\}. \tag{33}$$

Otherwise, i.e., if x_0 has eigenvalue $-i[\nu]_q$ such that

$$q^{\nu} = i\varepsilon q^{-k/2} \quad \text{for some} \quad k \in \{0,...,n-1\} \quad \text{and} \quad \varepsilon \in \{-1,1\}, \tag{34}$$

we call the representation *singular*.

Note 9: In the nonsingular case the sequence $[\nu]_q, [\nu+1]_q, \ldots, [\nu+n-1]_q$ contains mutually different numbers (see Lemma 11) and it does not contain $2i\varepsilon/(q-q^{-1}), \varepsilon = \pm 1$; equations from Note 2 are therefore solvable.

Lemma 7: Consider the nonsingular irreducible representation of $U_q'(\mathrm{so}_3)$ on the vector space V [i.e., assume (33)]. Then either it is a representation having weight vector or

$$V = \mathbb{C}\{x_0, O_{\nu} x_0, O_{\nu+1} O_{\nu} x_0, \ldots, O_{\nu+n-2} \ldots O_{\nu} x_0\}_{\mathrm{lin}}, \quad \dim V = n.$$

Proof: Take x_0 from (33) and consider the set

$$\{x_0, x_1, \ldots, x_{m-1}\}, \quad x_i := O_{\nu+i-1} x_{i-1}, \quad i = 1,...,m-1,$$

where m is chosen such that this set consists of linear-independent vectors, $\dim \mathbb{C}\{x_0, x_1, \ldots, x_{m-1}\}_{\mathrm{lin}} = m$, and simultaneously, $x_m = O_{\nu+m-1} x_{m-1} \in \mathbb{C}\{x_0, x_1, \ldots, x_{m-1}\}_{\mathrm{lin}}$.

If $m = 1,...,n-1$, then the last condition is equivalent (due to the nondegeneracy of the spectrum of I_3) to the equality $O_{\nu+m-1} x_{m-1} = 0$ and we have representation with weight vector x_{m-1}.

If $m = n, \ldots, 2n-1$, the mentioned condition is equivalent to the equality $O_{\nu+m-1} x_{m-1} = \alpha x_{m-n}$. For $m > n$ we have $x_{m-n} = O_{\nu+m-n-1} x_{m-n-1} = O_{\nu+m-1} x_{m-n-1}$ so that $O_{\nu+m-1}(x_{m-1} - \alpha x_{m-n-1}) = 0$ and we have again representation with weight vector.

If $m = n$, then this argument cannot be used and we proceed as follows. Consider the vectors $x_{-1}, x_{-2}, \ldots, x_{-m'+1}$ defined by $x_{-i} := R_{\nu-i+1} x_{-i+1}$, where m' is chosen such that the set $\{x_{-m'+1}, x_{-m'+2}, \ldots, x_{-1}, x_0, x_1, \ldots, x_{n-1}\}$ is linear independent and $x_{-m'} = R_{\nu-m'+1} x_{-m'+1} \in \mathbb{C}\{x_{-m'+1}, \ldots, x_{n-1}\}_{\mathrm{lin}}$.

Due to Corollary 4, $m' < n-1$ and therefore there exists $\beta \in \mathbb{C}$ such that

$$x_{-m'} = R_{\nu-m'+1} x_{-m'+1} = \beta x_{n-m'}. \tag{35}$$

Now, if $m' \in \{2,3,...,n-2\}$, then [see (12)]

$$R_{\nu-m'+1} O_{\nu+n-m'} x_{n-m'} = R_{\nu-m'+1} x_{n-m'+1} = -(C + q[\nu-m'][\nu-m'+1]_q) x_{n-m'}. \tag{36}$$

For $C \neq -q[\nu-m'][\nu-m'+1]_q$ we may calculate $x_{n-m'}$ and, substituting into (35), we again have

$$R_{\nu-m'+1}\left(x_{-m'+1} + \frac{\beta}{(C + [\nu-m'][\nu-m'+1]_q)} x_{n-m'+1} \right) = 0,$$

i.e., representation has a weight vector.

If $C = -q[\nu-m'][\nu-m'+1]_q$, we have representation with weight vector $x_{n-m'+1}$ [see (36)]. The only open case is $m' = 1$, i.e.,

$$O_{\nu+n-1} x_{n-1} = \alpha x_0, \quad R_{\nu} x_0 = \beta x_{n-1} \tag{37}$$

(where $\alpha, \beta \in \mathbb{C}$) and $\dim \mathbb{C}\{x_0, \ldots, x_{n-1}\}_{\mathrm{lin}} = n$. The subspace $\mathbb{C}\{x_0, \ldots, x_{n-1}\}_{\mathrm{lin}}$ is invariant with respect to $2n$ operators $O_{\nu}, O_{\nu+1}, \ldots, O_{\nu+n-1}, R_{\nu}, R_{\nu+1}, \ldots, R_{\nu+n-1}$ [see (9)–(12) and (37)]:

$$(iI_2 + q^{-\nu-k+1/2} I_1) x_k = O_{\nu+k} x_k = x_{k+1}, \quad 0 \leqq k \leqq n-2, \tag{38}$$

$$(iI_2+q^{-\nu-n+k/2}I_1)x_{n-1}=O_{\nu+n-1}x_{n-1}=\alpha x_0, \tag{39}$$

$$(iI_2-q^{\nu+k+3/2}I_1)x_k=R_{\nu+k}x_k=-(C+q[\nu+k-1]_q[\nu+k]_q)x_{k-1}, \quad 1\leqq k\leqq n-1, \tag{40}$$

$$(iI_2-q^{\nu+1/2}I_1)x_0=R_\nu x_0=\beta x_{n-1}. \tag{41}$$

This system can be solved for the vectors I_1x_k and I_2x_k (see Note 9). For I_3 we have $I_3x_k=-i[\nu+k]_qx_k$, $k=0,...,n-1$. Thus invariance of $\mathbb{C}\{x_0,\ldots,x_{n-1}\}_{\text{lin}}$ is proved and, due to assumed irreducibility, the proof is finished. □

Lemma 8: Any irreducible representation of $U_q'(so_3)$ such that $\text{Ker}\,(I_3-\varepsilon\,(q^{1/2}+q^{-1/2})/(q-q^{-1}))\neq\{0\}$ for some $\varepsilon\in\{1,-1\}$ has a weight vector from this subspace.

Proof: Let ν fulfill the equation $q^\nu=i\varepsilon q^{-1/2}$. Consider vectors $0\neq x_0\in\text{Ker}\,(I_3-\varepsilon(q^{1/2}+q^{-1/2})/(q-q^{-1}))$ and $x_1:=O_\nu x_0$. If $O_\nu x_0=\alpha x_0$ for some $\alpha\in\mathbb{C}$, the representation has a weight vector, so let x_1 and x_0 be linearly independent. Equation (9) shows that x_1 has the same eigenvalue as x_0. Following (12) we have

$$R_{\nu+1}x_1=R_{\nu+1}O_\nu x_0=-(C+q[\nu]_q[\nu+1]_q)x_0,$$

but $R_{\nu+1}=O_\nu$ so that subspace $\mathbb{C}\{x_0,x_1\}_{\text{lin}}$ is invariant with respect to O_ν. The weight vector is therefore any eigenvector of restriction O_ν to the subspace $\mathbb{C}\{x_0,x_1\}_{\text{lin}}$. □

Lemma 9: A singular irreducible representation has a weight vector with the exception that n is even and vectors $x_0,O_\nu x_0,\ldots,O_{\nu+n/2}O_{\nu+n/2-1},\ldots,O_\nu x_0$, where $0\neq x_0\in\text{Ker}\,(I_3-2\varepsilon/(q-q^{-1}))$ for some $\varepsilon\in\{1,-1\}$, are linear independent.

Proof: Let $0\neq x_0\in\text{Ker}\,(I_3+i[\nu]_q)$ and $q^\nu\in\{i\varepsilon q^{-k/2}|k=0,1,...,n-1\}$ if n is odd and $q^\nu\in\{i\varepsilon q^{-k/2}|k=1,3,...,n-1\}$ if n is even. In these cases the sequence $[\nu]_q,\ldots,[\nu+n-1]_q$ contains value $i\varepsilon(q^{1/2}+q^{-1/2})/(q-q^{-1})$. Consider the vectors

$$x_0,O_\nu x_0,\ldots,O_{\nu+n-2},\ldots,O_\nu x_0 \tag{42}$$

for which we have $O_{\nu+j},\ldots,O_\nu x_0\in\text{Ker}\,(I_3+i[\nu+j+1]_q)$. If any of these vectors is equal to zero, then the representation has a weight vector; if all vectors are nonzero, then $\text{Ker}\,(I_3+\varepsilon(q^{1/2}+q^{-1/2})/(q-q^{-1}))\neq\{0\}$ and we use Lemma 8.

In the remaining case (i.e., $q^\nu\in\{i\varepsilon q^{-k/2}|k=0,2,...,n-2\}$, n is even) we have

$$\{[\nu]_q,\ldots,[\nu+n-1]_q\}=\left\{\pm\frac{2i}{q-q^{-1}},\pm i\,\frac{q+q^{-1}}{q-q^{-1}},\ldots,\pm i\,\frac{q^{[n/4]}+q^{-[n/4]}}{q-q^{-1}}\right\},$$

and if all vectors (42) are nonzero, then they are eigenvectors of I_3 with $n/2+1$ different eigenvalues

$$\frac{2\varepsilon}{q-q^{-1}},\varepsilon\,\frac{q+q^{-1}}{q-q^{-1}},\ldots,\varepsilon\,\frac{q^{[n/4]}+q^{-[n/4]}}{q-q^{-1}},-\varepsilon\,\frac{q^{[n/4]}+q^{-[n/4]}}{q-q^{-1}},\ldots,-\frac{2\varepsilon}{q-q^{-1}}.$$

Taking vector $\tilde{x}_0\in\text{Ker}\,(I_3-2\varepsilon/(q-q^{-1}))$ instead of x_0 we obtain the set $\{\tilde{x}_0,O_\nu\tilde{x}_0,\ldots,O_{\nu+n/2-1},\ldots O_\nu\tilde{x}_0\}$ of $n/2+1$ linear-independent vectors. □

Thus we can now state the following theorem.

Theorem 5: Let n be odd and R be any irreducible representation of $U_q'(so_3)$. Then either (a) or (b) is true, where we have the following.

(a) Representation R has weight vector x_0 [see Definition 3, Eq. (30)] and for representation space V we have

$$V=\mathbb{C}\{I_1^mx_0|m=0,1,...,n-1\}_{\text{lin}}, \quad \dim V\leqq n. \tag{43}$$

(b) The representation is nonsingular [see (33) for definition of vector x_0] and for representation space V we have

$$V=\mathbb{C}\{x_i|i=0,...,n-1\}_{\rm lin},\quad x_i:=O_{\nu+i-1}x_{i-1},\quad i=1,...,n-1,\quad \dim V=n. \tag{44}$$

Now it remains to consider the last case when n is even, the representation does not have any weight vector, and I_3 has an eigenvector with eigenvalue $2\varepsilon/(q-q^{-1})$.

Theorem 6: Let n be even and R be any irreducible representation of $U_q'(\mathrm{so}_3)$. Then either (a), (b), or (c) is true, where (a) and (b) are from Theorem 5 and (c) is as follows.

(c) For the representation space V we have

$$V=\mathbb{C}\{x_0,\ldots,x_{n/2},I_1x_0,\ldots,I_1^{n/2-1}x_0\}_{\rm lin},\quad 0\neq x_0\in\mathrm{Ker}\left(I_3-\frac{2\varepsilon}{(q-q^{-1})}\right),$$

$$x_i:=O_{\nu+i-1}x_{i-1},\quad \dim V=n.$$

Proof: Let us suppose that neither case (a) nor (b) takes place. Then we have (see Lemma 9) $0\neq x_0\in\mathrm{Ker}\,(I_3-2\varepsilon/(q-q^{-1}))$ for some $\epsilon\in\{-1,1\}$ and vectors $x_0,x_1,\ldots,x_{n/2}$, where $x_i:=O_{\nu+i-1}x_{i-1}$, $i=1,...,n/2$, are linear-independent eigenvectors of I_3. Therefore, Corollary 5 $(v_0\to x_0,\eta\to\varepsilon)$ implies linear independence of the set $\{w_1,\ldots,w_{n/2-1},x_0,x_1,\ldots,x_{n/2}\}$, because vector w_s is the principal vector corresponding to the eigenvalue $\varepsilon\,(q^s+q^{-s})/(q-q^{-1})$.

Since $b_{n/2}^{(n/2)}=0$, the vector $w_{n/2}$ fulfills eigenvalue equation $(I_3-\varepsilon(q^{n/2}+q^{-n/2})/(q-q^{-1}))w_{n/2}=0$. Because n is even, we have $q^{n/2}=-1$ (see Note 6) and therefore $\varepsilon\,(q^{n/2}+q^{-n/2})/(q-q^{-1})=-2\varepsilon/(q-q^{-1})$ (vector $x_{n/2}$ has the same eigenvalue). We distinguish two cases:

(a) the vectors $w_{n/2}$ and $x_{n/2}$ are linearly independent, and
(b) $w_{n/2}=\gamma x_{n/2}$ for some $\gamma\in\mathbb{C}$.

Let us consider the case (a). We will show that it is not possible. Consider the vectors

$$\tilde{x}_{n/2}=w_{n/2},\tilde{x}_{n/2-1},\ldots,\tilde{x}_0,\quad \tilde{x}_i:=R_{\tilde{\nu}+i+1}\tilde{x}_{i+1},\quad i=0,...,n/2-1,\quad q^{\tilde{\nu}}=-i\varepsilon.$$

Since the representation does not have a weight vector, the above vectors are (nonzero) eigenvectors with mutually different eigenvalues; $\tilde{x}_k$ and x_k belong to the same eigenvalue $\varepsilon(q^k+q^{-k})/(q-q^{-1})$.

Let us show now that the set of vectors $\{\tilde{x}_{n/2},\ldots,\tilde{x}_0,w_1,\ldots,w_{n/2-1},x_{n/2},\ldots,x_0\}$ is linearly independent. First define the following projective operators,

$$P_0=c_0\prod_{l=1}^{n/2-1}\left(I_3-\varepsilon\frac{q^l+q^{-l}}{q-q^{-1}}\right)^2\left(I_3-\frac{-2\varepsilon}{q-q^{-1}}\right),$$

$$P_k=c_k\left(I_3-\frac{2\varepsilon}{q-q^{-1}}\right)\prod_{\substack{l=1\\ l\neq k}}^{n/2-1}\left(I_3-\varepsilon\frac{q^l+q^{-l}}{q-q^{-1}}\right)^2\left(I_3-\frac{-2\varepsilon}{q-q^{-1}}\right),\quad 0<k<\frac{n}{2},$$

$$P_{n/2}=c_{n/2}\left(I_3-\frac{2\varepsilon}{q-q^{-1}}\right)\prod_{l=1}^{n/2-1}\left(I_3-\varepsilon\frac{q^l+q^{-l}}{q-q^{-1}}\right)^2,$$

where

$$c_0^{-1}=\prod_{l=1}^{n/2-1}\left(\frac{2\varepsilon}{q-q^{-1}}-\varepsilon\frac{q^l+q^{-l}}{q-q^{-1}}\right)^2\left(\frac{2\varepsilon}{q-q^{-1}}-\frac{2\varepsilon}{q-q^{-l}}\right),$$

$$c_k^{-1}=\left(\varepsilon\frac{q^k+q^{-k}}{q-q^{-1}}-\frac{2\varepsilon}{q-q^{-1}}\right)\prod_{\substack{l=1\\ l\neq k}}^{n/2-1}\left(\varepsilon\frac{q^k+q^{-k}}{q-q^{-1}}-\varepsilon\frac{q^l+q^{-l}}{q-q^{-1}}\right)^2\left(\varepsilon\frac{q^k+q^{-k}}{q-q^{-1}}-\frac{2\varepsilon}{q-q^{-1}}\right),$$

$$0<k<\frac{n}{2},$$

$$c_{n/2}^{-1}=\left(\frac{-2\varepsilon}{q-q^{-1}}-\frac{2\varepsilon}{q-q^{-1}}\right)\prod_{l=1}^{n/2-1}\left(\frac{-2\varepsilon}{q-q^{-1}}-\varepsilon\frac{q^l+q^{-l}}{q-q^{-1}}\right)^2.$$

Assume, on the contrary, that

$$\tilde{x}_k=\alpha_{k-1}\tilde{x}_{k-1}+\cdots+\alpha_0\tilde{x}_0+\beta_1 w_1+\cdots+\beta_{n/2-1}+\omega_{n/2-1}+\gamma_{n/2}x_{n/2}+\cdots+\gamma_0 x_0. \tag{45}$$

If $k=0$ or $k=n/2$, we apply P_0 or $P_{n/2}$, respectively, and we obtain

$$\tilde{x}_0=\gamma_0 x_0, \quad (\text{resp.} \quad \tilde{x}_{n/2}=\gamma_{n/2}x_{n/2}).$$

Application of the operator $O_{\nu+n/2-1}\cdots O_{\nu+1}O_\nu$ to the first equation leads to linear dependence

$$\text{const}(\tilde{x}_{n/2}-\gamma_0 x_{n/2})=0,$$

where const$\neq 0$ [see (11)]. Thus both cases are in contradiction with the assumption.

If $0<k<n/2$, we use the operator $(I_3-\varepsilon(q^k+q^{-k})/(q-q^{-1}))P_k$ and we have $b_k^{(k)}w_k=0$, i.e., $b_k^{(k)}=0$. Then, using operator P_k acting on Eq. (45) we come to linear dependence,

$$\tilde{x}_k=\gamma_k x_k,$$

and, using further operator $O_{\nu+n/2-1}\cdots O_{\nu+k+1}O_{\nu+k}$, we come to the linear dependence of vectors $x_{n/2}$ and $\tilde{x}_{n/2}$ (contradiction).

Let us now construct principal vectors $\tilde{w}_1,\ldots,\tilde{w}_{n/2-1}$ using eigenvectors $\tilde{x}_0,\ldots,\tilde{x}_{n/2}$ in the same way as the vectors $w_1,\ldots,w_{n/2-1}$ were constructed by means of the vectors $x_0,\ldots,x_{n/2}$. Due to Lemma 4 we have

$$\begin{aligned}\tilde{w}_k=&\alpha_{k-1}\tilde{w}_{k-1}+\cdots+\alpha_1\tilde{w}_1+\beta_{n/2}\tilde{x}_{n/2}+\cdots+\beta_0\tilde{x}_0\\&+\gamma_{n/2-1}w_{n/2-1}+\cdots+\gamma_1 w_1+\delta_0 x_0+\cdots+\delta_{n/2}x_{n/2}\end{aligned}$$

for some $k<n/2-1$. Using again the operator $(I_3-\epsilon(q^k+q^{-k})/(q-q^{-1}))P_k$ we come to the linear dependence of eigenvectors $\tilde{x}_k$ and x_k, which is the contradiction. Thus the case (a) is not possible.

The case (b) therefore takes place, thus we have an n-dimensional subspace, spanned by vectors $x_0,\ldots,x_{n/2},w_1,\ldots,w_{n/2-1}$ in the representation space of the considered irreducible representation. This subspace is invariant with respect to the operator I_3, but it may not be invariant with respect to the operator I_1: we have no information about the vector $I_1x_{n/2}$. However, assertion of Lemma 14 is valid if we use it for vector $x_{n/2}$, i.e., we can put $v_0\to x_{n/2}$ and $\eta\to-\epsilon$ and construct similarly vectors $\tilde{w}_s$ for $s\in\{1,...,n/2-1\}$ fulfilling modified (B18), and we obtain $\tilde{w}_{n/2}=\tilde{\gamma}x_0$ for some $\tilde{\gamma}\in\mathbb{C}$.

Therefore, the subspace

$$\mathbb{C}\{\tilde{w}_{n/2-1},\ldots,\tilde{w}_1,x_0,\ldots,x_{n/2},w_1,\ldots,w_{n/2-1}\}_{\text{lin}}$$

is invariant with respect to the operators I_3 and I_1 (and therefore it is invariant with respect to the operator I_2, too).

Lemma 17 used on the characteristic polynomial of operator I_3 [because the representation is n-dimensional we know its explicit form (5)] implies that each eigenvalue has multiplicity at most equal to 2, i.e., principal vectors w_k and $\tilde{w}_k$ may differ at most by an eigenvector corresponding to the eigenvalue $\varepsilon(q^k+q^{-k})/(q-q^{-1})$, which, in our case, means $\tilde{w}_k-w_k=\text{const}\,x_k$. □

VI. EXPLICIT FORMULAS FOR NONSINGULAR IRREDUCIBLE REPRESENTATIONS WHEN $q^n=1$

When q is a root of unity, $q^n=1$ with n odd or even, according to Theorems 5 and 6 we must distinguish two, resp. three, cases: (a), (b), and (c). This section covers for all n the case (b) (the representation is nonsingular) and partly the case (a) (the representation has a weight vector and is in addition nonsingular). The following section finishes the case (a) (a singular representation having a weight vector) for odd n.

(1) Let us first assume the case (b) [see (44)]. From (38)–(41) we have

$$I_3x_j=-i[\nu+j]_qx_j,\quad 0\leqq j\leqq n-1, x_n=\alpha x_0, \tag{46}$$

$$I_1x_0=\frac{q^{-1/2}}{q^{\nu}+q^{-\nu}}x_1-\frac{\beta q^{-1/2}}{q^{\nu}+q^{-\nu}}x_{n-1}, \tag{47}$$

$$I_1x_j=\frac{q^{-1/2}(C+q[\nu+j-1]_q[\nu+j]_q)}{q^{\nu+j}+q^{-(\nu+j)}}x_{j-1}+\frac{q^{-1/2}}{q^{\nu+j}+q^{-(\nu+j)}}x_{j+1},\quad 1\leqq j\leqq n-1, \tag{48}$$

$$I_2x_0=\frac{-iq^{\nu}}{q^{\nu}+q^{-\nu}}x_1-\frac{i\beta q^{-\nu}}{q^{\nu}+q^{-\nu}}x_{n-1}, \tag{49}$$

$$I_2x_j=\frac{iq^{-\nu-j}(C+q[\nu+j-1]_q[\nu+j]_q)}{q^{\nu+j}+q^{-(\nu+j)}}x_{j-1}-\frac{iq^{\nu+j}}{q^{\nu+j}+q^{-(\nu+j)}}x_{j+1},\quad 1\leqq j\leqq n-1. \tag{50}$$

From $(q^{1/2}I_1I_2-q^{-1/2}I_2I_1-I_3)x_0=0$ we obtain the value of Casimir element $C=-\alpha\beta-q[\nu]_q[\nu-1]_q$. After substituting into (46)–(50) we easily check that these relations form representation of $U_q'(\mathrm{so}_3)$. Let us put

$$T|j\rangle=q^{-j/2}(-1)^jx_j,\quad j=0,...,n-1,\quad \lambda=-iq^{-\nu},\quad a=\beta(-1)^{n-1}q^{n/2-1},\quad b=\alpha(-1)^nq^{-n/2}.$$

Using this equivalence matrix T, representation $R_{ab\lambda}$ defined in Ref. 3 by (46)–(49) is found to be equivalent with our considered representation. In Ref. 3 it is proven that this representation is irreducible if $q^{\nu}\neq\pm iq^{-n/2+1}$; however, this is fulfilled in our case.

Note 10: (*i*) Equations (46)–(50) form an irreducible representation also if $\alpha=0$ or $\beta=0$. In this case it is a representation with one or two weight vectors.

(*ii*) Equations (46)–(50) form an irreducible representation also in the case $q^{2n}=1$ (which implies $q^n=-1$, see Note 6), $\alpha=\beta=0$. This can be immediately verified.

(2) Let us now assume that the representation is nonsingular and fulfills the case (a), [see (43)]. Consider the set of vectors in representation space

$$\{x_0,x_{-1},...,x_{-k+1}\},\quad x_{-j-1}:=R_{\nu-j}x_{-j}, \tag{51}$$

such that

$$\dim\mathbb{C}\{x_0,x_{-1},...,x_{-k+1}\}_{\mathrm{lin}}=k\quad\text{and}\quad x_{-k}\equiv R_{\nu-k+1}x_{-k+1}\in\mathbb{C}\{x_0,x_{-1},...,x_{-k+1}\}_{\mathrm{lin}}. \tag{52}$$

Because the representation is nonsingular, Lemma 5 gives

$$O_{\nu}x_0=0,\quad C=-q[\nu+1]_q[\nu]_q. \tag{53}$$

If $k=1$, we obtain a trivial one-dimensional representation.

If $k=n$, then $x_{-k}=\alpha x_0$ for some $\alpha\in\mathbb{C}$ and we obtain the special case of nonsingular representation (46)–(50) studied above.

If $1<k<n$, then $x_{-k}=0$ (different eigenvalues) and, using (11), we obtain another condition for *C:*

TABLE II. Nonsingular representations, $q^n=1$.

Corresponding formulas	Dimension	No.
(46)–(50), $\alpha,\beta,\nu\in\mathbb{C},\nu$ fulfilling (33)	n	3 parameters
(22)–(24) (see Note 4)	$1\leqq$dimension$<n$ if n is odd $1\leqq$dimension$\leqq n/2$ if n is even	1/each dimension
(46)–(50), $\alpha,\beta=0$, $\nu\in\mathbb{C}$, ν fulfilling (33), $n\to n/2$ (this possibility can take place only if n is even)	$n/2$	1 parameter

$$0=O_{\nu-k}x_{-k}=O_{\nu-k}R_{\nu-k+1}x_{-k+1}=-(C+q[\nu-k]_q[\nu-k+1]_q)x_{-k+1}. \tag{54}$$

Comparing with (53) we obtain $C=-q[\nu+1]_q[\nu]_q=-q[\nu-k]_q[\nu-k+1]_q$, thus $q^{2k}=1$ or $q^\nu=\varepsilon\sqrt{\varepsilon'}q^{(k-1)/2}$ for some $\varepsilon,\varepsilon'\in\{-1,1\}$.

(i) If $q^\nu=\varepsilon\sqrt{\varepsilon'}q^{(k-1)/2}$, then $\varepsilon'=1$ because the representation is assumed to be nonsingular. Solving (51) and (11) we obtain explicit forms of matrices I_1 and I_2. This representation is equivalent to the one defined by (22)–(24). Representations with $\varepsilon=\pm1$ are equivalent. According to Note 4 we have if n is odd, the representation is irreducible. If n is even, we have an irreducible representation if $1<k\leqq n/2$ and a reducible representation if $n/2<k<n$.

(ii) If $q^{2k}=1$, then $n=2k$ (because $1<k<n$), $q^k=-1$, and ν is independent. We obtain again formulas (46)–(50), which give an irreducible representation (see Note 10). Furthermore, for special $\nu=n/2-1$ we obtain an equivalent representation to the $n/2$-dimensional representation from (*i*).

Theorem 7: Let $q^n=1$ and let R be an irreducible nonsingular representation. Then R is equivalent to one of the representations given in Table II.

VII. EXPLICIT FORMULAS FOR SINGULAR IRREDUCIBLE REPRESENTATIONS WHEN $q^n=1$, n ODD

To obtain explicit formulas of singular representations, let us write first $\{i\varepsilon q^{-k/2}|k=0,\ldots,n-1;\varepsilon=\pm1\}=M_n\cup M_n'$, where $M_n=\{i\varepsilon q^{-1/2-m}|m=0,1,\ldots,(n-1)/2;\varepsilon=\pm1\}$, and $M_n'=\{i\varepsilon q^{-m}|m=1,2,\ldots,(n-1)/2;\varepsilon=\pm1\}$.

Possible eigenvalues of generator I_3 in singular representation are

$$\varepsilon\frac{q^{1/2}+q^{-1/2}}{q-q^{-1}},\varepsilon\frac{q^{3/2}+q^{-3/2}}{q-q^{-1}},\ldots,\varepsilon\frac{q^{n/2-1}+q^{-n/2+1}}{q-q^{-1}},\frac{2\varepsilon\tilde{\varepsilon}}{q-q^{-1}},$$

where $\tilde{\varepsilon}\equiv q^{n/2}\in\{-1,1\}$ (we use this abbreviation through the whole section).

Let $q^\nu\in M_n\cup M_n'$ and let

$$I_3x_0=-i[\nu]_qx_0,\quad O_\nu x_0=\mu x_0. \tag{55}$$

We distinguish five cases.

Case 1: $q^\nu\in M_n'$, i.e., $q^\nu=i\varepsilon q^{-m}$ for some $m\in\{1,2,\ldots,(n-1)/2\}$. Take the set (51) such that (52) holds. If $1\leqq k\leqq(n-1)/2-m$, then $x_{-k}=0$ (reason: mutually different eigenvalues) and similarly as in (53) and (54) we have

$$C=-q[\nu+1]_q[\nu]_q=-q[\nu-k]_q[\nu-k+1]_q. \tag{56}$$

This condition implies $q^{2k}=1$ or $q^{2(k+2m-1)})=1$. However, none of these possibilities can be fulfilled (see Note 6).

If $k>(n-1)/2-m$, then there exist nonzero vector $x_{-(n-1)/2+m}$ with eigenvalue $\varepsilon\tilde{\varepsilon}(q^{1/2}+q^{-1/2})/(q-q^{-1})$. According to Lemma 8, there exists a new weight vector x_0' with this eigenvalue and the rest of this case is covered by case 3, resp. 5.

Case 2: $\mathrm{Ker}(I_3-2\varepsilon\tilde{\varepsilon}/(q-q^{-1}))=\{0\}$ and $q^\nu\in M_n$, $q^\nu\neq\pm iq^{-1/2}$. Let $q^\nu=i\varepsilon q^{-1/2-m}$, $m\in\{1,2,\ldots,(n-3)/2\}$ and take the set (51) such that (52) and $k\leqq(n-1)/2-m$. Similarly as in (54) we have again (56), which cannot be satisfied.

Case 3: $\mathrm{Ker}(I_3-2\varepsilon\tilde{\varepsilon}/(q-q^{-1}))=\{0\}$ and $q^\nu=i\varepsilon q^{-1/2}$ for some $\varepsilon\in\{-1,1\}$. Take $q^\nu=i\varepsilon q^{-1/2}$ and consider (51) and (52). We now have $1\leqq k\leqq(n-1)/2$ and from (54)

$$C=-q[\nu-k+1]_q[\nu-k]_q=q\frac{(q^{1/2-k}+q^{-1/2+k})(q^{-1/2-k}+q^{1/2+k})}{(q-q^{-1})^2}.$$

Similarly as in Lemma 5 we have

$$\mu=i\tilde{\tilde{\varepsilon}}q^{1/2}[k]_q,\quad \tilde{\tilde{\varepsilon}}\in\{-1,1\}.$$

We have the same situation as in Sec. IV, nonclassical case B. Therefore we obtain formulas (26)–(28) [see Note 5(a)(i)].

Case 4: $\mathrm{Ker}\,(I_3-2\epsilon\tilde{\epsilon}/(q-q^{-1}))\neq\{0\}$ and $q^\nu\in M_n$, $q^\nu\neq\pm iq^{-1/2}$. In this case $q^\nu=i\varepsilon q^{-1/2-m}$, $m\in\{1,2,...,(n-1)/2\}$. For C we have

$$C=-q[\nu]_q[\nu+1]_q=q\frac{(q^{1/2-m}+q^{-1/2+m})(q^{-1/2-m}+q^{1/2+m})}{(q-q^{-1})^2}. \tag{57}$$

Value m can be assumed the lowest one in the sense that no weight vector with eigenvalue $\varepsilon(q^{-1/2-m'}+q^{1/2+m'})/(q-q^{-1}),m'<m$ exists. In the set

$$\{x_0,x_{-1,\ldots},x_{-(n-1)/2+m}\},\quad x_{-j-1}:=R_{\nu-j}x_{-j}$$

the vector $y_0\equiv x_{-(n-1)/2+m}\in\mathrm{Ker}\,(I_3-2\epsilon\tilde{\epsilon}/(q-q^{-1}))\neq\{0\}$ and we can use it as v_0 in Lemma 14 and Corollary 5 ($\epsilon\tilde{\epsilon}\to\eta$). Let us define vectors w_s, $s=1,...,n$, as in (B18).

For $y_j=O_{\tilde{\nu}+j-1}y_{j-1}=O_{\tilde{\nu}+j-1}O_{\tilde{\nu}+j-2}\cdots O_{\tilde{\nu}}y_0$, $j=1,2,...,q^{\tilde{\nu}}=i\epsilon\tilde{\epsilon}$ we have [using (11)]

$$y_j=\prod_{l=0}^{j-1}(-(C+q[\nu-(n-1)/2+m+l]_q[\nu-(n-1)/2+m+l+1]_q))x_{-(n-1)/2+m+j}. \tag{58}$$

Due to fixed value of Casimir operator (57), $y_j=0$ for all $j\geqq(n-1)/2-m+1$ while $y_0,\ldots,y_{(n-1)/2-m}$ are eigenvectors of generator I_3. Corollary 5 then implies the following.

(i) The set

$$\{x_0,x_{-1},\ldots,x_{-(n-1)/2+m}\equiv y_0,w_1,\ldots,w_{(n-1)/2-m}\}$$

contains $n-2m$ linear-independent vectors, and vector w_k is principal vector to eigenvector $x_{(n-1)/2+m+k}$.

(ii) Since $y_{(n-1)/2-m+1}=y_{(n-1)/2-m+2}=0,w_{(n-1)/2-m+1}\in\mathrm{Ker}\,(I_3-\varepsilon q^{-1/2-m+1}+q^{1/2+m-1}/q-q^{-1})=\{0\}$ and $w_{(n-1)/2-m+2}\in\mathrm{Ker}\,(I_3-\varepsilon q^{-1/2-m+2}+q^{1/2+m-2}/q-q^{-1})=\{0\}$, i.e.,

$$I_1^s y_0+\cdots+\frac{2\varepsilon\tilde{\varepsilon}b_s^{(s)}[s-2]_q^2}{q^{s-1}-q^{-s+1}}\tilde{D}_1y_{s-2}=0, \tag{59}$$

$$I_1^{s+1}y_0+\cdots+\frac{2\varepsilon\tilde{\varepsilon}b_{s+1}^{(s+1)}[s-1]_q^2}{q^s-q^{-s}}\tilde{D}_1y_{s-1}=0, \tag{60}$$

$s=(n-1)/2-m+1$. Vectors y_{s-2} and y_{s-1} are multiples of x_{-1} and x_0, respectively, and relations

$$R_{\nu-1}x_{-1}=x_{-2}, \quad O_{\nu-1}x_{-1}=-(C+q[\nu-1]_q[\nu]_q)x_0$$

give

$$I_1x_{-1}=\frac{i\varepsilon\tilde{\varepsilon}q^{-1/2}}{q^{s-2}-q^{-s+2}}(x_{-2}+(C+q[\nu-1]_q[\nu]_q)x_0).$$

Subtracting the I_1 ''multiple'' of (59) from (60) and comparing the coefficient by vector x_0 we obtain the relation

$$\frac{2\varepsilon\tilde{\varepsilon}b_s^{(s)}[s-2]_q^2\tilde{D}_1}{q^{s-1}-q^{-s+1}}\cdot\frac{i\varepsilon\tilde{\varepsilon}q^{-1/2}}{q^{s-2}-q^{-s+2}}+\frac{2\varepsilon\tilde{\varepsilon}b_{s+1}^{(s+1)}[s-1]_q^2\tilde{D}_1}{q^s-q^{-s}}=0,$$

which leads to condition $q^{4m}=1$. Because $4\leqq 4m\leqq 2n-2$, we must have $4m=n$, but this is a contradiction (n is odd).

Case 5: $\mathrm{Ker}\,(I_3-2\varepsilon\tilde{\varepsilon}/(q-q^{-1}))\neq\{0\}$ and $q^\nu=i\varepsilon q^{-1/2}$ for some $\varepsilon\in\{-1,1\}$. According to Note 8, put $\varepsilon=1$ and, in Lemma 5, assume

$$\mu=+\sqrt{-C+q\left(\frac{q^{1/2}+q^{-1/2}}{q-q^{-1}}\right)^2}. \tag{61}$$

Consider (51) where $k=(n+1)/2$. Again, we can use $y_0\equiv x_{-(n-1)/2}$ as v_0 in Lemma 14 and Corollary 5. Let us again put $y_j=O_{\tilde{\nu}+j-1}y_{j-1}=O_{\tilde{\nu}+j-1}O_{\tilde{\nu}+j-2}\cdots O_{\tilde{\nu}}y_0$ for $j=1,2,...,q^{\tilde{\nu}}=i\tilde{\varepsilon}$ and let us define vectors w_s, $s=1,...,n$, as in (B18). We have

$$y_j=\prod_{l=0}^{j-1}\left(-\left(C-q\frac{(q^l+q^{-l})(q^{l+1}+q^{-l-1})}{(q-q^{-1})^2}\right)\right)x_{-(n-1)/2+j}. \tag{62}$$

Consider the set

$$V'=\mathbb{C}\{x_0,x_{-1},...,x_{-(n-3)/2},x_{-(n-1)/2},w_1,...,w_{m-1}\}_{\mathrm{lin}}, \tag{63}$$

such that $\dim V'=(n+1)/2+m-1$, $w_m\in V'$ and $m\leqq(n+1)/2$ (such m exists because $\dim V'\leqq n$). V' is invariant with respect to I_3 and also I_1.

We distinguish two cases:

(i) $m\leqq(n-1)/2$. Assumption $w_m\in V'$ and (B17) give

$$w_m=\alpha x_{-(n-1)/2+m} \quad \text{for some} \quad \alpha\in\mathbb{C}, \tag{64}$$

$$\prod_{l=0}^{m-1}\left(-\left(C-q\frac{(q^l+q^{-l})(q^{l+1}+q^{-l-1})}{(q-q^{-1})^2}\right)\right)=0 \tag{65}$$

[see (62)]. Because $w_{m+1}\in V'$, the last equation (giving $y_{m+1}=0$) implies further ($x_1:=x_0$)

$$w_{m+1}=\beta x_{-(n-1)/2+m+1} \quad \text{for some} \quad \beta\in\mathbb{C}. \tag{66}$$

Explicit forms of (64) and (66) are

$$I_1^m y_0+\frac{a_{m-2}^{(m)}}{q^{m-1}-q^{-m+1}}I_1^{m-2}y_0+\cdots+\frac{2b_m^{(m)}[m-2]_q^2\tilde{D}_1}{q^{m-1}-q^{-m+1}}y_{m-2}=\alpha x_{-(n-1)/2+m},$$

$$I_1^{m+1}y_0+\frac{a_{m-1}^{(m+1)}}{q^m-q^{-m}}I_1^{m-1}y_0+\cdots+\frac{2b_{m+1}^{(m+1)}[m-1]_q^2\tilde{D}_1}{q^m-q^{-m}}y_{m-1}=\beta x_{-(n-1)/2+m+1}.$$

Subtracting the I_1 multiple of the first equation from the second, we obtain the relation among linearly independent vectors which can be fulfilled only if

$$\frac{a_{m-2}^{(m)}}{q^{m-1}-q^{-m+1}}=\frac{a_{m-1}^{(m+1)}}{q^m-q^{-m}},$$

which fixes the value of the Casimir operator

$$C=q\frac{(q^{m-1}+q^{-m+1})(q^m+q^{-m})}{(q-q^{-1})^2}.$$

It shows that vectors $y_1,\ldots,y_{m-1}$ are nonzero, i.e., $w_1,\ldots,w_{m-1}$ are principal vectors.

Further, using relations (19) with $q^\nu=i\varepsilon q^{-1/2}$ and $j=(n-1)/2-m$, $j=(n-1)/2-m+2$ and comparing coefficients of vector $x_{-(n-1)/2+m-1}$ we obtain the equation determining $\alpha\in\mathbb{C}$.

Note that for $m=1$ it is clear (because there is no other such representation with that dimension) that we must obtain the same representation as in Sec. IV, nonclassical case B, formulas (26)–(28) [see Note 5(a)(ii)].

(ii) $m=(n+1)/2$: from (B17) we have

$$\left(I_3-\tilde{\varepsilon}\frac{q^{1/2}+q^{-1/2}}{q-q^{-1}}\right)w_{(n+1)/2}=\text{const}\,x_0, \tag{67}$$

thus vector $w_{(n+1)/2}$ fulfills the same principal equation as $w_{(n-1)/2}$ [const can be read out from (62) and (67)]. Because the dimension of Jordan blocks in matrix I_3 is at most 2, there exists $\alpha\in\mathbb{C}$ such that

$$w_{(n+1)/2}=\alpha x_0+\text{const}'\,w_{(n-1)/2} \tag{68}$$

(again, const′ can be easily computed, α is unknown).

Therefore we get two-parameter set of operators

$$\{(I_3^{(C,\alpha)},I_1^{(C,\alpha)})\,|\,(C,\alpha)\in\mathbb{C}\times\mathbb{C}\}. \tag{69}$$

Matrix I_1 is defined through Eqs. (19), (55), (B18), and (68), matrix I_3 through Eqs. (15), (B17), and (62).

We will now show that matrices (69) form representation of $U_q'(\mathrm{so}_3)$ for all $(C,\alpha)\in\mathbb{C}^2$ and that almost all are irreducible.

We can easily prove that for each $(C,\alpha)\in\mathbb{C}^2$

$$(q^2I_1^{(C,\alpha)^2}+I_2^{(C,\alpha)^2}+q^2I_3^{(C,\alpha)^2}-(q^{5/2}-q^{1/2})I_1^{(C,\alpha)}I_2^{(C,\alpha)}I_3^{(C,\alpha)})e_1=Ce_1,$$

where $I_2^{(C,\alpha)}:=q^{1/2}I_3^{(C,\alpha)}I_1^{(C,\alpha)}-q^{-1/2}I_1^{(C,\alpha)}I_3^{(C,\alpha)}$ and $e_1=(1,0,\ldots,0)\in\mathbb{C}^n$. This means that the value of parameter C is really the value of the Casimir operator.

Further, rewriting operator $I_1^{(C,\alpha)}$ in basis

$$V'=\mathbb{C}\{x_0,x_{-1},\ldots,x_{-(n-3)/2},y_0=x_{-(n-1)/2},I_1y_0,\ldots,I_1^{m-1}y_0\}_{\text{lin}}, \tag{70}$$

we can achieve the result

$$\det I_1^{(C,\alpha)}=\det I_1^{(C,0)}+\alpha\prod_{j=0}^{(n-3)/2}\frac{iq^{-1/2}}{q^{-j+1/2}-q^{j-1/2}}, \tag{71}$$

i.e., $\det I_1^{(C,\alpha)}$ depends on α so that parameter α cannot be removed by change of basis.

Let $M=\{(C,\alpha)\in\mathbb{C}^2|\text{matrices } I_3^{(C,\alpha)}, I_1^{(C,\alpha)} \text{ define an irreducible representation of } U_q'(so_3)\}$. Let us show now that there exists $M_1\subset\mathbb{C}^2$ of Lebesgue measure zero such that $M=\mathbb{C}-M_1$.

Consider irreducible n-dimensional representation (46)–(50) after automorphism ρ from Corollary 1:

$$I_1x_j=-i[\nu+j]_qx_j,\quad 0\leqq j\leqq n-1,\ x_n=\tilde{\alpha}x_0, \tag{72}$$

$$I_3x_0=\frac{-iq^{\nu}}{q^{\nu}+q^{-\nu}}x_1-\frac{i\tilde{\beta}q^{-\nu}}{q^{\nu}+q^{-\nu}}x_{n-1}, \tag{73}$$

$$I_3x_j=\frac{iq^{-\nu-j}(C+q[\nu+j-1]_q[\nu+j]_q)}{q^{\nu+j}+q^{-(\nu+j)}}x_{j-1}-\frac{iq^{\nu+j}}{q^{\nu+j}+q^{-(\nu+j)}}x_{j+1},\quad 1\leqq j\leqq n-1, \tag{74}$$

where

$$C=-\tilde{\alpha}\tilde{\beta}-q[\nu]_q[\nu-1]_q \quad\text{and}\quad (\tilde{\alpha},\tilde{\beta},q^{\nu})\in\mathbb{C}^2\times(\mathbb{C}-\{i\varepsilon q^{-i}|j=0,\ldots,n-1,\varepsilon=\pm1\}). \tag{75}$$

Due to irreducibility, Casimir element $C^{(n)}$ in this representation is equal to a multiple of the identity:

$$C^{(n)}(I_3)=-\det I_3=-\tilde{\alpha}\prod_{k=0}^{n-1}\frac{q^{-1/2}}{q^{\nu+k}+q^{-\nu-k}}+\tilde{\beta}\frac{q^{-1/2}}{q^{\nu}+q^{-\nu}}\prod_{k=0}^{n-2}\frac{q^{-1/2}(C+q[\nu+k]_q[\nu+k-1]_q)}{q^{\nu+k+1}+q^{-\nu-k-1}}.$$

If we choose constants $\tilde{\alpha}$ and $\tilde{\beta}$ such that

$$\det I_3=\frac{2\tilde{\varepsilon}}{n(q-q^{-1})^n}, \tag{76}$$

representation (72)–(74) is singular. Condition (76) is equivalent to

$$\tilde{\alpha}-\tilde{\beta}\prod_{k=0}^{n-2}(C+q[\nu+k]_q[\nu+k+1]_q)=\frac{2}{(q-q^{-1})^n}\prod_{k=0}^{n-1}(q^{\nu+k}+q^{-\nu-k}). \tag{77}$$

Using (75) we have

$$\tilde{\beta}^2\prod_{k=0}^{n-2}(C+q[\nu+k]_q[\nu+k+1]_q)-\tilde{\beta}\frac{2}{(q-q^{-1})^n}\prod_{k=0}^{n-1}(q^{\nu+k}+q^{-\nu-k})+C+q[\nu-1]_q[\nu]_q=0$$

having at least one solution $\tilde{\beta}$ for any pair $(C,q^{\nu})\in\mathbb{C}\times(\mathbb{C}-\{i\varepsilon q^{-j}|j=0,\ldots,n-1,\varepsilon=\pm1\})$. For given $\alpha\in\mathbb{C}$ we choose $q^{\nu}\in\mathbb{C}$ such that $\det I_1^{(C,\alpha)}=\det I_1$, i.e.,

$$\prod_{j=0}^{n-1}(-i[\nu+j]_q)=\det I_1^{(C,0)}+\alpha\prod_{j=0}^{(n-3)/2}\frac{iq^{-1/2}}{q^{-j+1/2}-q^{j-1/2}}. \tag{78}$$

If q^{ν} is a solution of (78), then this equation is solved also by $q^{\nu+1},\ldots,q^{\nu+n-1}$. However, if constants (C,α) fulfill the condition

$$\varepsilon\prod_{j=0}^{n-1}\frac{q^j+q^{-j}}{q-q^{-1}}=\det I_1^{(C,0)}+\alpha\prod_{j=0}^{(n-3)/2}\frac{iq^{-1/2}}{q^{-j+1/2}-q^{j-1/2}} \tag{79}$$

solutions q^{ν} of (78) are bad—they belong to the set $\{i\varepsilon q^{-j}|j=0,\ldots,n-1,\varepsilon=\pm1\}$.

TABLE III. Singular representations, $q^n=1$, n odd.

Corresponding formulas	Dimension	No./each dimension
(26)–(28) (I_3 diagonal)	$1\leqq k\leqq(n+1)/2$	4
explicit formulas not computed, I_3 not diagonalizable	$(n+1)/2<k\leqq n-1$	at most 4
(72)–(74), $C,\tilde{\alpha},\tilde{\beta},\nu\in C$, fulfilling (75) and (77)	n	2 parameters
(69), $(C,\alpha)\in M_1$ (see Theorem 8)	n	1 parameter

Therefore we can state the following.

Theorem 8: Let n be odd. Then the following assertions are true:

(i) If R is a singular n-dimensional irreducible representation of $U_q'(\mathrm{so}_3)$, then there exists at most one pair $(C,\alpha)\in\mathbb{C}^2$ and $\eta_1,\eta_2\in\{-1,1\}$ such that R is equivalent to some of the four representations generated from representation (69) using Note 3.

(ii) If M_1 is the set of all pairs (C,α) satisfying condition (79), then the Lebesgue measure of M_1 is equal to zero. If $(C,\alpha)\in\mathbb{C}^2-M_1$, then matrices (69) form a representation equivalent to some of four representations generated from representation (72)–(74) using Note 3.

Note 11: Matrices (69) form a representation for all $(C,\alpha)\in\mathbb{C}^2$. When $(C,\alpha)\in\mathbb{C}^2-M_1$ it follows from the previous theorem. When $(C,\alpha)\in M_1$, then we have $(C,\alpha_1)\notin M_1$ for all $\alpha_1\neq\alpha$ [condition (79) is linear in α]. Clearly

$$\lim_{\alpha_1\to\alpha} I_j^{(C,\alpha_1)}=I_j^{(C,\alpha)},\quad j=1,2,3,$$

which follows from the fact that only one of the n^2 matrix coefficients of $I_1^{(C,\alpha)}$ [see (68)] depends (linearly) on α, and matrix coefficients of $I_3^{(C,\alpha)}$ do not depend on α at all. Using this continuity argument on relations (1)–(3) we obtain the desired result. Note we do not know if representations from M_1 are irreducible.

Theorem 9: Let $q^n=1$ for n odd. If R is an irreducible singular representation, then R is equivalent to one of the representations given in Table III.

Note 12: In the two last cases described in Table III we know also matrix I_3 is written in basis (63) $[m=(n+1)/2]$. Relations (62) and (B17) show that this matrix is diagonalizable iff

$$C=C_{\mathrm{diag}}\equiv\frac{2q(q+q^{-1})}{(q-q^{-1})^2}. \tag{80}$$

Comparing Tables II [see also (46)] and III we see that in the case n odd we have full classification and explicit formulas of all irreducible representations with diagonalizable I_3 with only one exception—point $(C_{\mathrm{diag}},\alpha)\in M_1$ [Theorem 8 (ii)].

VIII. CONCLUSION AND REMARKS

(i) In Lemma 2 we give a proof that $C^{(n)}(I_1)$ is a Casimir element of $U_q'(\mathrm{so}_3)$ when q is a root of unity, $q^n=1$. This interesting polynomial seems to be of great importance for algebras $U_q'(\mathrm{so}_m)$, $m\geqq 3$.

Let us recall that $U_q'(\mathrm{so}_m)$ is an associative algebra generated by elements $I_{i,i-1}$, $i\in\{2,\ldots,m\}$ and relations

$$I_{i,i-1}I_{i-1,i-2}^2-(q+q^{-1})I_{i-1,i-2}I_{i,i-1}I_{i-1,i-2}+I_{i-1,i-2}^2I_{i,i-1}=-I_{i,i-1}, \tag{81}$$

$$I_{i,i-1}^2I_{i-1,i-2}-(q+q^{-1})I_{i,i-1}I_{i-1,i-2}I_{i,i-1}+I_{i-1,i-2}I_{i,i-1}^2=-I_{i-1,i-2}, \tag{82}$$

$$[I_{i,i-1},I_{j,j-1}]=0, \quad |i-j|>1, \tag{83}$$

where $[\cdot,\cdot]$ denotes the usual commutator. One can also give an equivalent definition of $U'_q(\mathrm{so}_m)$ in terms of generators I_{ij}, $i\in\{2,...,m\}$, $j\in\{1,...,i-1\}$, fulfilling these commutation relations:

$$I_{ij}=[I_{j+1,j},I_{i,j+1}]_q\equiv q^{1/2}I_{j+1,j}I_{i,j+1}-q^{-1/2}I_{i,j+1}I_{j+1,j} \quad \text{for } i>j+1,$$

$$[I_{jk},I_{ij}]_q=I_{ik}, \quad [I_{ij},I_{ik}]_q=I_{jk}, \quad [I_{ik},I_{jk}]_q=I_{ij} \quad \text{for } i>j>k,$$

$$[I_{ij},I_{kl}]=0, \quad \text{for } i>j>k>l \text{ and } i>k>l>j,$$

$$[I_{ij},I_{kl}]_q=(q-q^{-1})(I_{jl}I_{ik}-I_{il}I_{kj}) \quad \text{for } i>k>j>l.$$

Using this definition we can formulate the following statement:

Theorem 10: $C^{(n)}(I_{ij})$, $i\in\{2,...,m\}$, $j\in\{1,...,i-1\}$ is a Casimir element of $U'_q(\mathrm{so}_m)$ when $q^n=1$.

Proof: Let us give the proof for $m=4$. One can find a more detailed proof in Ref. 8. We can consider generator I_{21} as an element of $U'_q(\mathrm{so}_3)$ subalgebra of $U'_q(\mathrm{so}_4)$ generated by two elements I_{21} and I_{32}. It implies $[C^{(n)}(I_{21}),I_{32}]=0$. The second commutator $[C^{(n)}(I_{21}),I_{43}]=0$ follows from (83). The commutators with elements I_{31}, I_{41}, and I_{42} are then trivially equal to zero because these three elements can be expressed in terms of I_{21}, I_{32}, and I_{43}. The same arguments can be used for $C^{(n)}(I_{32})$ with generator I_{41} used instead of I_{43}. □

As algebra $U_q(\mathrm{iso}_{m+1})$ can be obtained from $U'_q(\mathrm{so}_{m+1})$ by Inönu–Wigner contraction $[I_{m+1,i}\to\varepsilon I_{m+1,i}, U'_q(\mathrm{so}_m)$ fixed]; polynoms $C^{(n)}(I_{ij})$ with $I_{ij}\in U'_q(\mathrm{so}_m)$ remain Casimir operators also for $U_q(\mathrm{iso}_{m+1})$.

(ii) By doing classification of singular irreducible representations in the first nontrivial case when n is even, i.e., $q^4=1$, one can see that it is richer in comparison with cases when n is odd. The same result can be assumed in other cases $n=6,8,...$.

(iii) In Ref. 9 irreducible star representations (that is, such that $I_1^*=-I_1$ and $I_3^*=-I_3$) with diagonal generator I_3 are presented. These irreducible representations are equivalent to irreducible representations described by formulas (72)–(74) with $C=C_{\mathrm{diag}}$ [see (80)] and suitable $\nu\in\mathbb{C}$.

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APPENDIX A: COMBINATORIAL IDENTITIES

Here we present basic properties of q-numbers and some combinatorial identities.

Lemma 10: Let q be not root of unity (i.e., $q^j\neq 1$ for all $j\in\mathbb{N}$).

(a) For given $\lambda\in\mathbb{C}$ we can choose $\nu\in\mathbb{C}$ such that $\lambda=[\nu]_q$, $[\nu+1]_q$, $[\nu+2]_q,\ldots$ are mutually different.

(b) if $q^\nu=i\varepsilon q^{-k/2}$ for some $k\in\mathbb{Z},\varepsilon\in\{-1,1\}$, then (1) $[\nu+k-j]_q=[\nu+j]_q$ for all $j\in\mathbb{Z}$, and (2) the equation $[\nu+j_1]_q=[\nu+j_2]_q$ for some $j_1,j_2\in\mathbb{Z},j_1\neq j_2$ implies $j_1=k-j_2$.

(c) If $[\nu]_q\notin\{i\varepsilon(q^{k/2}+q^{-k/2})/(q-q^{-1})|k=0,1,...,\varepsilon=\pm 1\}$, then q-numbers $[\nu]_q,[\nu\pm 1]_q,\ldots$ are mutually different. □

Proof: Straightforward.

Lemma 11: Let $q^n=1$ for some $n\in\mathbb{N},q^j\neq 1$ for $j\in\mathbb{N},j<n$. Then

(a) $q^\nu\notin\{i\varepsilon q^{-k/2}|k=0,1,...,n-1;\varepsilon=\pm 1\}$ implies q-numbers $[\nu]_q,[\nu+1]_q,\ldots,[\nu+n-1]_q$ are mutually different.

(b) If $q^\nu=i\varepsilon q^{-k/2}$ for some $k\in\{0,1,...,n-1\}$, $\varepsilon\in\{1,-1\}$, then

$$[\nu+j]_q=[\nu+k-j]_q, \quad j=0,1,...,[k/2],$$

$$[\nu+k+j]_q=[\nu+n-j]_q, \quad j=1,...,[(n-k)/2],$$

and no other equalities of the numbers $[\nu]_q,\ldots,[\nu+n-1]_q$ can be found.

Proof: Straightforward. □

Lemma 12: Some useful combinatorial identities. The following formulas hold (we take $0^0=1$):

(1) Let $N\in\mathbb{N}$, $0\leqq H\leqq[(N-1)/2]$, $0\leqq M\leqq[(N-1)/2]$. Let us denote $N'=N \bmod 2$, i.e., $N'=1$ when N is odd and zero otherwise. Then

$$\sum_{t=0}^{[(N-1)/2]}\binom{N}{2t+1}\binom{\left[\frac{N-1}{2}\right]-t}{\left[\frac{N-1}{2}\right]-H}\binom{t}{M}$$
$$=4^{H-M}\binom{H}{M}(N-2H(1-N'))\frac{(2[N/2])!([N/2]+H-M)!([N/2]-M)!}{[N/2]!(2H+1)!(2[N/2]-2M)!([N/2]-H)!}. \tag{A1}$$

(2) Let $n\in\mathbb{N}$, $0\leqq c\leqq[(n-1)/2]$, $0\leqq d\leqq[(n-1)/2]$. Put $n'=n \bmod 2$. Then

$$\sum_{j=0}^{d}\binom{n-j}{j}\frac{2d-2j+1+(n-2d-1)^{n'}}{n-j}$$
$$\times\binom{\left[\frac{n-1}{2}\right]-d}{c-j}\cdot\frac{(2[n/2]-2j)!(n-1-c-d)!([n/2]-c)!}{([n/2]-j)!(d-j+1-n')!(2[n/2]-2c)!(n-2d+n'-1)!}$$
$$=\frac{\binom{n-1-d}{d}\binom{n-1-c}{c}}{(n/2)^{1-n'}(n-2d)^{n'}}. \tag{A2}$$

Proof: We prove both formulas for odd and even N (resp. n) separately.

(1) Let N be even, $N=2K$, $K\in N$. Then we have

$$\sum_{t=0}^{K-1}\binom{2K}{2t+1}\binom{K-1-t}{K-1-H}\binom{t}{M}=\frac{\mathrm{d}^M}{\mathrm{d}z^M}\left(\frac{1}{M!}\sum_{t=0}^{K-1}\binom{2K}{2t+1}\binom{K-1-t}{K-1-H}z^t\right)\Bigg|_{z=1}.$$

To compute the inner sum we express it in terms of hypergeometric functions and use M times formula [see Ref. 5, (5.106)]

$$\frac{\mathrm{d}}{\mathrm{d}z}F(a,b;c;z)=\frac{ab}{c}F(a+1,b+1;c+1;z). \tag{A3}$$

Then, using formula [see Ref. 5, (5.92)]

$$F(a,-n;c;1)=\frac{\Gamma(c-a+n)\Gamma(c)}{\Gamma(c-a)\Gamma(c+n)}, \quad n\in\mathbb{N}\cup\{0\}, \quad \mathrm{Re}(c-a)\geqq 0, \quad \mathrm{Re}\,c\geqq 0, \tag{A4}$$

we find the closed form of the sum:

$$\sum_{t=0}^{K-1}\binom{2K}{2t+1}\binom{K-1-t}{K-1-H}\binom{t}{M}=4^{H-M}\binom{H}{M}(2K-2H)\frac{(2K)!(K+H-M)!(K-M)!}{K!(2H+1)!(2K-2M)!(K-H)!},$$

$$K\in\mathbb{N},\quad 0\leqq M\leqq K,\quad 0\leqq H\leqq K.$$

We use exactly the same approach to find the closed form for N odd, $N=2K-1$:

$$\sum_{t=0}^{K-1}\binom{2K-1}{2t+1}\binom{K-1-t}{K-1-H}\binom{t}{M}$$

$$=4^{H-M}\binom{H}{M}(2K-1)\frac{(2K-2)!(K+H-M-1)!(K-M-1)!}{(K-1)!(2H+1)!(2K-2M-2)!(K-1-H)!},$$

$$K\in\mathbb{N},\quad 0\leqq M\leqq K-1,\quad 0\leqq H\leqq K-1.$$

(2) Let n be even, $n=2k$. First express the sum in terms of hypergeometric functions and then use the formula [see Ref. 5, (5.97)]:

$$F(a,b,-n;c,a+b-c-n+1;1)=\frac{\Gamma(c-a+n)\Gamma(c-b+n)\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)\Gamma(c+n)\Gamma(c-a-b+n)},\tag{A5}$$

$$n\in\mathbb{N}\cup\{0\},\quad \mathrm{Re}\,c\geqq 0,\quad \mathrm{Re}\,(c-a)\geqq 0,\quad \mathrm{Re}(c-b)\geqq 0,\quad \mathrm{Re}\,(c-a-b)\geqq 0$$

to obtain the closed form:

$$\sum_{j=0}^{d}\binom{2k-j}{j}\frac{2d+2-2j}{2k-j}\binom{k-1-d}{c-j}\frac{(2k-2j)!(2k-1-c-d)!(k-c)!}{(k-j)!(1+d-j)!(2k-2c)!(2k-2d-1)!}$$

$$=\frac{1}{k}\binom{2k-1-d}{d}\binom{2k-1-c}{d},$$

$$k\in\mathbb{N},\quad 0\leqq c\leqq k-1,\quad 0\leqq d\leqq k-1.$$

For odd $n=2k-1$ we have

$$\sum_{j=0}^{d}\binom{2k-1-j}{j}\frac{2k-2j-1}{2k-j-1}\binom{k-1-d}{c-j}\frac{(2k-2j-2)!(2k-2-c-d)!(k-c-1)!}{(k-j-1)!(d-j)!(2k-2c-2)!(2k-2d-1)!}$$

$$=\frac{1}{2k-2d-1}\binom{2k-2-d}{d}\binom{2k-2-c}{c},\quad k\in\mathbb{N},\quad 0\leqq c\leqq k-1,\quad 0\leqq d\leqq k-1.$$

Composing the results we obtain the required formulas. □

APPENDIX B: PROOF OF THE THEOREM 2

Here we present necessary theorems and lemmas used in the proof of Theorem 2.

Lemma 13: Let $n\in\mathbb{N}$. Then

$$I_3I_1^n=p_n(I_1)I_2+q_n(I_1)I_3,$$

where

$$p_n(x)=q^{-1/2}\left(\frac{x(q+q^{-1})}{2}\right)^{n-1}\sum_{t=0}^{[(n-1)/2]}\binom{n}{2t+1}\left(\left(\frac{q-q^{-1}}{q+q^{-1}}\right)^2-\left(\frac{2}{x(q+q^{-})}\right)^2\right)^t,\tag{B1}$$

$$q_n(x)=-q^{1/2}\frac{x(q-q^{-1})}{2}p_n(x)+\left(\frac{x(q+q^{-1})}{2}\right)^{n}\sum_{t=0}^{[n/2]}\binom{n}{2t}\left(\left(\frac{q-q^{-1}}{q+q^{-1}}\right)^2-\left(\frac{2}{x(q+q^{-})}\right)^2\right)^t. \tag{B2}$$

Furthermore, we have

$$q_n(x)=-q^{1/2}\frac{x(q+q^{-1})}{2}\left(\frac{q-q^{-1}}{q+q^{-1}}+\sqrt{\left(\frac{q-q^{-1}}{q+q^{-1}}\right)^2-\left(\frac{2}{x(q+q^{-1})}\right)^2}\right)p_n(x)$$
$$+\left(\frac{x(q+q^{-1})}{2}\right)^{n}\left(1+\sqrt{\left(\frac{q-q^{-1}}{q+q^{-1}}\right)^2-\left(\frac{2}{x(q+q^{-1})}\right)^2}\right)^{n}. \tag{B3}$$

Proof: Equations (1)–(3) give us system of difference equations

$$p_{n+1}(x)=qxp_n(x)+q^{-1/2}q_n(x),$$

$$q_{n+1}(x)=q^{1/2}p_n(x)+q^{-1}xq_n(x),$$

which can be separated to the form

$$p_{n+2}(x)=(q+q^{-1})xp_{n+1}(x)-(x^2+1)p_n(x), \tag{B4}$$

$$q_{n+2}(x)=(q+q^{-1})xq_{n+1}(x)-(x^2+1)q_n(x). \tag{B5}$$

The initial conditions are

$$p_1(x)=q^{-1/2},\quad p_2(x)=(q^{1/2}+q^{-3/2})x,\quad q_1(x)=q^{-1}x,\quad q_2(x)=q^{-2}x^2-1.$$

We find the solution of (B4) and (B5) in the form $q_n(x)=C_1\lambda_1^n+C_2\lambda_2^n$ (and similarly for p_n) where C_i are constants easily derived from initial conditions and λ_i are roots of characteristic polynomial

$$\lambda^2-(q+q^{-1})x\lambda+(x^2+1)=0.$$

Note 13: Let us remark that formulas (B1) [resp. (B2)] are of course easily summable using formulas

$$\sum_{t=0}^{[(n-1)/2]}\binom{n}{2t+1}z^t=\frac{1}{2}z^{-1/2}((1+z^{1/2})^n-(1-z^{1/2})^n),\quad \sum_{t=0}^{[n/2]}\binom{n}{2t}z^t=\frac{1}{2}((1+z^{1/2})^n+(1-z^{1/2})^n).$$

Lemma 14: Let us have some irreducible representation of $U_q'(\mathrm{so}_3)$, let $\eta\in\{-1,1\}$, $q^{\xi}=i\eta$, $0\neq v_0\in\mathrm{Ker}(I_3+i[\xi]_q)$. Define vectors

$$v_{j+1}:=O_{\xi+j}v_j,\quad j\geqq 0. \tag{B6}$$

Then for each $s,1\geqq s<s_q+2$, there exist unique complex constants (depending on q and C) $a_s^{(s)},a_{s-2}^{(s)},a_{s-4}^{(s)},\ldots,a_2^{(s)}$ (resp. $a_1^{(s)}$ if s is odd) and $b_s^{(s)},b_{s-2}^{(s)},\ldots,b_0^{(s)}$ (resp $b_1^{(s)}$) such that

$$I_3I_1^sv_0=a_s^{(s)}I_1^sv_0+a_{s-2}^{(s)}I_1^{s-2}v_0+a_{s-4}^{(s)}I_1^{s-4}v_0+\cdots+\cdots+b_{s-4}^{(s)}v_{s-4}+b_{s-2}^{(s)}v_{s-2}+b_s^{(s)}v_s, \tag{B7}$$

and for each $s,1\geqq s<s_q+1$, there exist constants $c_{s+1}^{(s)},c_{s-1}^{(s)},c_{s-3}^{(s)},\ldots,c_1^{(s)}$ (resp. $c_2^{(s)}$ if s is odd) and $d_{s+1}^{(s)},d_{s-1}^{(s)},\ldots,d_1^{(s)}$ (resp. $d_0^{(s)}$) such that

$$I_2I_1^sv_0=c_{s+1}^{(s)}I_1^{s+1}v_0+c_{s-1}^{(s)}I_1^{s-1}v_0+c_{s-3}^{(s)}I_1^{s-3}v_0+\cdots+\cdots+d_{s-3}^{(s)}v_{s-3}+d_{s-1}^{(s)}v_{s-1}+d_{s+1}^{(s)}v_{s+1}, \tag{B8}$$

where $s_q=+\infty$ if q is not the root of unity, $s_q=n-1$ if $q^n=1$ and n is odd, and $s_q=n/2-1$ if $q^n=1$ and n is even.

Furthermore, we have

$$a_s^{(s)}=\eta\frac{q^s+q^{-s}}{q-q^{-1}},\quad c_{s+1}^{(s)}=\eta q^{s+1/2},\quad d_{s+1}^{(s)}=-i\left(\frac{-i\eta q^{1/2}}{q-q^{-1}}\right)^s([s]_q!)^{-1}, \tag{B9}$$

$$b_s^{(s)}=\eta\left(\frac{-i\eta q^{-1/2}}{q-q^{-1}}\right)^s([s-1]_q!)^{-1}(q^s-q^{-s}),\quad c_{s-1}^{(s)}=\frac{-\eta q^{-1/2}}{q-q^{-1}}([s-1]_q+q^s(1+s+\tilde{D}_1)), \tag{B10}$$

$$a_{s-2}^{(s)}=\frac{-\eta q^{-1}}{(q-q^{-1})^2}((q^s-q^{-s})\tilde{D}_1+sq(q^{s-1}-q^{-s+1})), \tag{B11}$$

$$b_0^{(2)}=\frac{-\eta(-8+Cq^{-1}(q-q^{-1})^2(q+q^{-1}))}{(q-q^{-1})^3}, \tag{B12}$$

$$b_{s-2}^{(s)}=\eta\left(\frac{-i\eta q^{-1/2}}{q-q^{-1}}\right)^s\frac{[s-2]_q^2}{[s-1]_q!}\left((q^s-q^{-s})C+\frac{q^{1-s}}{(q-q^{-1})}F_s\right),\quad s>2, \tag{B13}$$

$$d_0^{(1)}=\frac{-\eta(2-6q^2+Cq^2(q-q^{-1})^2)}{q^{3/2}(q-q^{-1})^3}, \tag{B14}$$

$$d_{s-1}^{(s)}=\frac{b_{s-1}^{(s-1)}}{(q-q^{-1})(q^s-q^{-s})}\left(-Cq^{s-1/2}+\frac{q^{1/2}}{(q-q^{-1})^2(q^{s-1}-q^{-s+1})}G_s\right),\quad s>1, \tag{B15}$$

$$\tilde{D}_1:=C-q\frac{2(q+q^{-1})}{(q-q^{-1})^2},$$

$$F_s:=-sq^s(q-q^{-1})(q^{s-1}-q^{-s+1})-2q^s[s]_q(q+q^{-1}),$$

$$G_s:=-s-sq^{-4}+(2s-1)q^{-2}-3q^2+(2+s+sq^{-4}-2(s-1)q^{-2})q^{2s}+q^{-2s}(q-q^{-1})^2,$$

where we denote $[j]_q!:=[j]_q\cdot[j-1]_q\cdot\cdots\cdot[1]_q$.

Proof: From the definition of vectors v_j and from (12) we have

$$O_{\xi+j}v_j=v_{j+1},\quad j\geqq 0,$$

$$R_{\xi+j}v_j=R_{\xi+j}O_{\xi+j-1}v_{j-1}=-(C+q[\xi+j-1]_q[\xi+j]_q)v_{j-1},\quad j\geqq 1. \tag{B16}$$

Since $O_{\xi+j}=iI_2-i\eta q^{1/2-j}I_1$ and $R_{\xi+j}=iI_2-i\eta q^{j+1/2}I_1$ we can find vectors I_1v_j and I_2v_j, $j=1,\ldots,s_q$ from these equations:

$$I_1v_j=\frac{-i\eta q^{-1/2}}{q^j-q^{-j}}(\tilde{D}_jv_{j-1}+v_{j+1}),\quad I_2v_j=\frac{-i}{q^j-q^{-j}}(\tilde{D}_jq^{-j}v_{j-1}+q^jv_{j+1}),$$

$$\tilde{D}_j:=C-q\frac{(q^{j-1}+q^{-j+1})(q^j+q^{-j})}{(q-q^{-1})^2}.$$

Lemma can be proved by induction using these relations. □

Note 14: Consider all coefficients from Lemma 14 as functions of complex variable $C\in\mathbb{C}$ (q fixed):

$$a_j^{(i)}=a_j^{(i)}(C),\quad b_j^{(i)}=b_j^{(i)}(C),\ldots,\text{etc.}$$

Then it can be easily proved by induction that for each $C_0\in\mathbb{C}$ we have

$$\lim_{C\to C_0} a_j^{(i)}(C)=a_j^{(i)}(C_0),\ldots,$$

i.e., that they are continuous functions on $\mathbb{C}$.

Corollary 5: Let us assume the same as in Lemma 14. Then for all $s\in\{1,...,s_q+1\}$ there exist unique complex constants (depending on q and C) $\hat{a}_{s-4}^{(s)},\ldots,\hat{a}_2^{(s)}$ (or $\hat{a}_1^{(s)}$ if s is odd) and $\hat{b}_{s-4}^{(s)},\hat{b}_{s-6}^{(s)},\ldots,\hat{b}_0^{(s)}$ (or $\hat{b}_1^{(s)}$) such that

$$\left(I_3-\eta\frac{q^s+q^{-s}}{q-q^{-1}}\right)w_s=b_s^{(s)}v_s, \tag{B17}$$

where

$$w_2=I_1^2v_0+\frac{\eta b_0^{(2)}}{q-q^{-1}}v_0,$$

$$w_s=I_1^sv_0+\frac{\eta a_{s-2}^{(s)}}{q^{s-1}-q^{-s+1}}I_1^{s-2}v_0+\hat{a}_{s-4}^{(s)}I_1^{s-4}v_0+\cdots+\hat{b}_{s-4}^{(s)}v_{s-4}+\frac{2\eta b_s^{(s)}[s-2]_q^2}{q^{s-1}-q^{-s+1}}\tilde{D}_1v_{s-2},$$

$$s>2. \tag{B18}$$

Proof: Assume $s>2$. Taking (B7) for s and $s-2$,

$$(I_3-a_s^{(s)})(I_1^sv_0)=a_{s-2}^{(s)}I_1^{s-2}v_0+a_{s-4}^{(s)}I_1^{s-4}v_0+\cdots+b_{s-2}^{(s)}v_{s-2}+b_s^{(s)}v_s,$$

$$(I_3-a_{s-2}^{(s-2)})(I_1^{s-2}v_0)=a_{s-4}^{(s-2)}I_1^{s-4}v_0+\cdots+b_{s-2}^{(s-2)}v_{s-2},$$

we obtain

$$(I_3-a_s^{(s)})\left(I_1^sv_0+\frac{a_{s-2}^{(s)}}{a_{s-2}^{(s-2)}-a_s^{(s)}}I_1^{s-2}v_0-\frac{b_{s-2}^{(s)}(a_{s-2}^{(s-2)}-a_s^{(s)})-a_{s-2}^{(s)}b_{s-2}^{(s-2)}}{(a_{s-2}^{(s-2)}-a_s^{(s)})^2}v_{s-2}\right)=w_{s-4}+b_s^{(s)}v_s,$$

where $w_{s-4}\in W_{s-4}\equiv\mathbb{C}\{I_1^{s-4}v_0,I_1^{s-6}v_0,\ldots,v_{s-6},v_{s-4}\}_{\text{lin}}$.

Using (B7) for $s-4$, $s-6$, ..., 2 (or 1 if s is odd) we easily show that

$$w_{s-4}=(I_3-a_s^{(s)})w'_{s-4}$$

for some $w_{s-4}^l\in W_{s-4}$. □

Note 15: As in Note 14 coefficients $\hat{a}_j^{(i)},\hat{b}_j^{(i)}$ are continuous functions of $C\in\mathbb{C}$.

Lemma 15: Same assumptions as in Lemma 14. Let vectors $v_0,v_1,\ldots$ are nonzero and $v_m=0$ for some $m\in\{0,...,s_q\}$. Then the vectors $v_0,\ldots,v_{m-1}$ are linear-independent eigenvectors of I_3 with different eigenvalues. Equation (B17) shows that $w_1,\ldots,w_{m-1}$ [see (B18)] are their principal vectors to the eigenvalues $\eta(q^s+q^{-s})/(q-q^{-1}),s\in\{1,...,m-1\}$. From (B17) we also have that if $w_m\neq0$, then w_m is an eigenvector of I_3 with eigenvalue $\eta(q^m+q^{-m})/(q-q^{-1})$.

Proof: Clear.

Lemma 16: Let q not be a root of unity. Let us have some finite-dimensional irreducible representation of $U_q'(\text{so}_3)$, and let $\eta\in\{-1,1\}$, $q^\xi=i\eta$, $\text{Ker}(I_3+i[\xi]_q)\neq\{0\}$. Then for each $v_0\in\text{Ker}(I_3+i[\xi]_q)$ there exists $m\in\mathbb{N}$ such that $w_m=0$ [for definition of w_j, see (B18)].

Proof: For each $v_0\in\text{Ker}(I_3+i[\xi]_q)$ consider (B6). Since the representation is finite-dimensional and the vectors $v_0,v_1,\ldots$ belong to different eigenvalues, there exists $m(v_0)\in\mathbb{N}$ such

that $v_{m(v_0)-1}\neq 0$ and $v_{m(v_0)}=0$. Since $v_{m(v_0)}\equiv O_{\xi+m(v_0)-1}v_{m(v_0)-1}$, (12) fixes the value of the Casimir operator: $C+q[\xi+m(v_0)-1]_q[\xi+m(v_0)]_q=0$. We will show that $w_{m\equiv m(v_0)}=0$.

Assume, on the contrary, that $w_m\neq 0$. Then w_m is eigenvector of I_3 with eigenvalue $\eta(q^m+q^{-m})/(q-q^{-1})$. Consider the vectors

$$\tilde{v}_m\equiv w_m,\quad \tilde{v}_{m+1}=O_{\xi+m}\tilde{v}_m,\quad \ldots,\quad \tilde{v}_{m+k}=O_{\xi+m+k-1}\tilde{v}_{\xi+m+k-1},\quad \ldots.$$

All these vectors are nonzero {in the opposite case, i.e., if $\tilde{v}_{m+k}=0$, (12) would give for the Casimir operator another value $C+q[\xi+m+k-1]_q[\xi+m+k]_q=0$} and therefore eigenvectors of operator I_3 with mutually different eigenvalues. It is in contradiction with assumed finite dimension of representation. □

Proof of Theorem 2: Let us assume the opposite case: let ν fulfill the equation $q^\nu=i\varepsilon$ for some $\varepsilon\in\{-1,1\}$ and let $x_0\in V$ such that $I_3x_0=-i[\nu]_qx_0=2\varepsilon(q-q^{-1})^{-1}x_0$. Let us define vectors

$$x_{j+1}:=O_{\nu+j}x_j,\quad j\geqq 0. \tag{B19}$$

Then from Lemma 16 ($v_i\to x_i$) it follows that there exists $m\in\mathbb{N}$ such that $w_m=0$ [see (B18)] from which we have

$$I_1^mx_0=-\frac{\eta\alpha_{m-2}^{(m)}}{q^{m-1}-q^{-m+1}}I_1^{m-2}x_0-\hat{a}_{m-4}^{(m)}I_1^{m-4}v_0-\cdots-\hat{b}_{m-4}^{(m)}v_{m-4}-\frac{2\eta b_m^{(m)}[m-2]_q^2}{q^{m-1}-q^{-m+1}}\tilde{D}_1x_{m-2}.$$

Applying $q^{1/2}I_1$ to Eq. (B8) (with $s\to m-1, v_i\to x_i$) and subtracting the $q^{-1/2}I_2$-multiple of this equation we obtain vector $I_3I_1^{m-1}x_0$ [see (1)]. Comparing with Eq. (B7), especially the coefficient by vector x_{m-1}, we obtain the condition which can be fulfilled only if q is a root of unity. □

Lemma 17: (a) Let $q^{2m}=1$, $q^j\neq 1$ for $j<2m$ and $\varepsilon\in\{-1,1\}$. Then

$$\begin{aligned}\sum_{j=0}^{m}\binom{2m-j}{j}\frac{2m}{2m-j}\frac{(-1)^j}{(q-q^{-1})^{2j}}x^{2m-2j}-\frac{2}{(q-q^{-1})^{2m}}&\\ =\prod_{j=0}^{2m-1}\left(x-\varepsilon\frac{q^j+q^{-j}}{q-q^{-1}}\right)&\\ =\left(x-\frac{2\varepsilon}{q-q^{-1}}\right)\left(x-\frac{-2\varepsilon}{q-q^{-1}}\right)\prod_{j=1}^{m-1}\left(x-\varepsilon\frac{q^j+q^{-j}}{q-q^{-1}}\right)^2.&\end{aligned}$$

(b) Let $q^{2m+1}=1$, $q^j\neq 1$ for $j<2m+1$ and $\varepsilon\in\{-1,1\}$. Put $q^{m+1/2}\equiv\tilde{\varepsilon}$. Then

$$\begin{aligned}\sum_{j=0}^{m}\binom{2m+1-j}{j}\frac{2m+1}{2m+1-j}\frac{(-1)^j}{(q-q^{-1})^{2j}}x^{2m+1-2j}-\frac{2\varepsilon\tilde{\varepsilon}}{(q-q^{-1})^{2m+1}}&\\ =\left(x-\frac{2\varepsilon\tilde{\varepsilon}}{q-q^{-1}}\right)\prod_{j=0}^{m-1}\left(x-\varepsilon\frac{q^{1/2+j}+q^{-1/2-j}}{q-q^{-1}}\right)^2.&\end{aligned}$$

Proof: (a) We will use the formula (7). Let

$$p(x)=\sum_{j=0}^{m}\binom{2m-j}{j}\frac{2m}{2m-j}\frac{(-1)^j}{(q-q^{-1})^{2j}}x^{2m-2j}-\frac{2}{(q-q^{-1})^{2m}}. \tag{B20}$$

Then we have directly $p(\varepsilon(q^j+q^{-j})/(q-q^{-1}))=0$. It means that numbers $\varepsilon(q^j+q^{-j})/(q-q^{-1}), j\in\{0,\ldots,m\}$, are roots of polynomial p. However, not all of these roots are mutually different:

$$\varepsilon\frac{q^k+q^{-k}}{q-q^{-1}}=\varepsilon\frac{q^j+q^{-j}}{q-q^{-1}}\Leftrightarrow k+j=2m,$$

so we have to prove that p' (the first derivative of the polynomial p) has as roots the numbers $\varepsilon(q^j+q^{-j})/(q-q^{-1}), j\in\{1,...,m-1\}$. If $\varepsilon(q^j+q^{-j})/(q-q^{-1})=0$ we see immediately from the left-hand side of (7) that $p'(0)=0$. Otherwise we compute $p'(x)$ by differentiating the right-hand side of (7) and see that $p'(\varepsilon(q^j+q^{-j})/(q-q^{-1}))=0$.

Thus the roots $\varepsilon(q^k+q^{-k})/(q-q^{-1}), k\in\{1,...,m-1\}$, have multiplicity 2 and the theorem holds.

Formula (b) is proved similarly. □

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Convergence of the exponential Lie series

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Improved results on convergence of the Magnus expansion are reported. Consequences are discussed for exponential perturbation theory, construction of numerical methods, control theory or, in general, for problems where time-ordered integrals are involved. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Consider the linear differential equation,

$$\frac{\mathrm{d}}{\mathrm{d}t}Z(t)=A(t)Z(t), \quad Z(0)=I, \tag{1}$$

where $A(t)$ is a bounded family of operators in some Banach space equipped with the norm $\|\cdot\|$. Time-ordered integrals are central when dealing with such initial value problems. One instance in physics is provided by the so-called Dyson time-ordered exponential widely used in both quantum mechanics and high energy physics. Most systems of interest have some small parameter, ϵ, such that $Z'=\epsilon A(t)Z$, and the traditional way of approximating the solution of these is some perturbative expansion of the solution $Z(t)$ in powers of ϵ.

Less known, and used, are nonlinear methods of approximation of linear systems. At first sight it may sound complicated to treat a linear system by nonlinear means, but in some cases such an approach has some clear advantages over the standard approaches. A particular consequence is that certain constants of motion and other geometric features of the exact solution can be preserved exactly in approximate solutions.

One such approach which has become increasingly more popular is the Magnus expansion[1] whose applications are expanding continuously, and accordingly it has been reinvented an extraordinary number of times with new names.[2–7] Sometimes referred to as *exponential perturbation theory* in quantum mechanics,[8] *exponential Lie series associated with the Chen–Fliess expansion* in control theory,[2,4,9] or just *Lie integral*,[6] the Magnus expansion has been found useful in a large variety of problems. A formulation of the expansion in terms of Lie operators can also be applied to nonlinear systems of ODEs.[5,10] Even more general, it has been applied in the analysis of noncommutative stochastic differential equations.[11–13] Examples of a different nature are encountered in numerical analysis with the development of geometric integration.[14,15] It has also been used in a variety of time-dependent problems in physics: infrared divergences in QED,[16] spectral line broadening,[17] high-resolution NMR spectroscopy in terms of average Hamiltonians,[18–20] Coulomb excitations in nuclei,[21] multi-photon excitation of molecules,[22] multilevel Landau–Zener effect[23] and neutrino oscillations in matter,[24] to quote just a few. Recently the Magnus expansion has been used as a tool to show the exponential smallness of effects in relation to conservative numerical integration algorithms. In that case the radius of convergence for a bounded operator

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equation relates directly with the smallness of the unremovable remainder in the averaging procedure. The crucial property of the Magnus expansion is that truncations provide asymptotic approximations to differential equations.

In essence, Magnus expansion yields the solution of the linear operator equation (1) in exponential form,

$$Z(t)=\exp[\Omega(t)]Z(0). \tag{2}$$

It is now worth mentioning two ways of viewing (2) that motivate most of the applications of the Magnus expansion. First, (2) gives the solution of (1) at time t. Second, and more importantly, one can view (2) as the solution of the differential equation,

$$\frac{\mathrm{d}}{\mathrm{d}s}X(s)=\Omega(t)X(s),\quad X(0)=Z(0), \tag{3}$$

at $s=1$. The latter way can be utilized as a means to *average* out rapid oscillations in $A(t)$ making the problem more suited for, e.g., numerical calculations. Such approaches have led to particularly efficient methods for stochastic differential equations.[11]

Of course, if $A(t)$ commutes with itself at different times then the solution is well known, and $\Omega(t)$ collapses into $\int_0^t A(s)\mathrm{d}s$. Otherwise, the Magnus operator $\Omega(t)$ can be obtained by solving[1,25]

$$\dot{\Omega}=\frac{\mathrm{ad}_\Omega}{\exp(\mathrm{ad}_\Omega)-1}A=\sum_{j=0}^{\infty}\frac{B_j}{j!}\mathrm{ad}_\Omega^j A,\quad \mathrm{ad}_\Omega^0 A=A, \tag{4}$$

as a series expansion,

$$\Omega(t)=\sum_{k=1}^{\infty}\Omega_k(t),\quad \Omega_k(0)=0. \tag{5}$$

Equation (4) is written in terms of the adjoint operator $\mathrm{ad}_\Omega A\equiv[\Omega,A]\equiv\Omega A-A\Omega$, and Bernoulli numbers[26] $\{B_j\}$. Clearly this construction leads to Ω_k's that are elements in the Lie algebra determined by the family $A(t)$. More importantly, an approximate solution $\tilde{\Omega}(t)$ residing in the same Lie algebra is obtained by truncating (5). Magnus approximations, $\tilde{\Omega}(t)=\Sigma_{k=1}^{n}\Omega_k(t)$, are then written in terms of multiple integrals of nested commutators of A evaluated at different times. Thus, replacing the linear equation (1) with the nonlinear one (4) is the crux of this approach, and leads directly to the aforementioned favorable properties for the approximate solution $\tilde{Z}(t)=\exp[\tilde{\Omega}(t)]$, at the cost of the finite radius of convergence of the expansion which has caused problems in some applications.[27–30] The re-summation of the fundamental solution is also concomitant with the amount of work needed to obtain a given order of approximation. It is therefore central to understand as fully as possible the causes of the observed divergences, and give conditions when one safely can apply the Magnus expansion to obtain meaningful approximations.

In the present paper we present results on the convergence properties of the Magnus expansion on which two studies may be found in recent issues of this journal.[7,31] Due to the many possible ways of writing down the expansion, it becomes central in a convergence analysis to find a form of the expansion that is simple to state and has as few redundancies or nontrivial cancellations as possible. The expansion found by solving (4) iteratively does not have a structure malleable enough for a very good bound. Explicitly stated the question we address is therefore the following: *For a given $A(t)$ what is the maximum value of t such that Magnus series (5) converges*?

In the original paper by Magnus no explicit result for convergence in terms of $A(t)$ is stated, though it is mentioned that the expansion converges provided t is sufficiently small. Some lower

bounds for the absolute convergence of Magnus expansion may be found in the literature.[8,14,31] The largest one to date[32,33] states that the convergence is guaranteed provided

$$\int_0^t \|A(s)\| \mathrm{d}s \leqslant 1.086869. \tag{6}$$

Since the goal of providing the bound is to explain practical applications of Magnus series we choose to continue to work with norms of A in our statements, even though more refined bounds involving eigenvalues of Ω could tighten our results somewhat. It is noteworthy that the result above has been obtained in two different ways albeit both strategies are based on the Magnus operator equation (4). Arguably one may deduce from this coincidence that the bounding procedures underpinning both procedures has reached some natural barrier.

In the present work we develop a new method showing that as a matter of fact the domain of convergence of Magnus expansion can be further enlarged. It is the Lie algebraic nature of (4) that gives rise to complications, mainly due to the rather intricate nature of Lie algebra bases. More specifically, it is not clear at this moment how to simplify Ω_k generated by (4) to a form amenable to good bounds due to the complexity of the algebra of iterated integrals and commutators.[34]

We shall resort to a form of the expansion that avoids dealing explicitly with commutators since the bound $\|[\Omega,A]\| \leqslant 2\|\Omega\|\|A\|$ induces a geometrically growing factor when applied to nested commutators, which together with the complications of Lie algebra bases is hard to reduce. Certainly the absence of multiple commutators might surprise the reader acquainted with the subject. However from Dynkin's theorem[35] the nested commutator structure is readily recovered. We shall base our computations on a particular combinatorial approach to Magnus series given in Refs. 3 and 36, later rediscovered in Ref. 5. In Sec. II we collect these formulas and outline our approach for estimating the convergence domain. Furthermore the material related to absolute convergence of the series is developed. Section II A contains a proof of the convergence result, while Sec. II B contains numerical evidence of the sharpness of the bound in Sec. II A. The final Sec. III contains our conclusions.

II. THE METHOD

The usual ways of solving (4) with (5) results in the expressions

$$\Omega_1 = \int_0^t \mathrm{d}t_1 A(t_1), \quad \Omega_2 = \frac{1}{2}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 [A(t_1),A(t_2)], \tag{7}$$

$$\Omega_3 = \frac{1}{4}\int_0^t \left[\int_0^\kappa \left[\int_0^\xi A(\nu)\,d\nu, A(\xi) \right] d\xi, A(\kappa) \right] d\kappa + \frac{1}{12}\int_0^t \left[\int_0^\kappa A(\nu)\,d\nu, \left[\int_0^\kappa A(\xi)\,d\xi, A(\kappa) \right] \right] d\kappa, \tag{8}$$

$$= \frac{1}{6}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_3 ([A(t_1),[A(t_2),A(t_3)]] + [A(t_3),[A(t_2),A(t_1)]]). \tag{9}$$

Higher order terms may be obtained, for instance, from either recurrence relations[37] or binary trees techniques.[14] Equations (7)–(9) illustrate the structure of nested commutators and time-ordered integrals in Ω_n of increasing complexity, as well as the nonuniqueness of explicit formulas due to Jacobi identity.

Mielnik and Plebański[36] devised an algorithm for direct formal construction of $\Sigma_{k=1}^{\infty}\Omega_k$. According to them,

$$\Omega(t) = \sum_{n=1}^{\infty} \int_0^t \cdots \int_0^t \mathrm{d}t_n \cdots \mathrm{d}t_1 L_n(t_n,\cdots,t_1) A(t_n)\cdots A(t_1). \tag{10}$$

The point to notice is that $L_n(t_n,\ldots,t_1)$ admits the representation

$$L_n(t_n,\ldots,t_1)=\frac{\Theta_n!(n-1-\Theta_n)!}{n!}(-1)^{n-1-\Theta_n}, \tag{11}$$

with the definition $\Theta_n:=\theta_{n-1,n-2}+\cdots+\theta_{2,1}$, where the step function $\theta_{b,a}=1$ if $t_b>t_a$ and 0 otherwise.

Accordingly we have $n!$ sectors defined by inequalities $t_{i_n}>t_{i_{n-1}}\cdots>t_{i_1}$. For the proper chronological sector $(i_n=n,i_{n-1}=n-1,\ldots,i_1=1)$ we get the maximal value $\Theta_n=n-1$, while the anti-chronological sector $(i_n=1,i_{n-1}=2,\ldots,i_1=n)$ gives the minimal $\Theta_n=0$. For mixed sectors $0<\Theta_n<n-1$. Thus, the main result of Refs. 3, 36 is that

$$\Omega(t)=\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t \mathrm{d}t_n\cdots\mathrm{d}t_1\frac{\Theta_n!(n-1-\Theta_n)!}{n!}(-1)^{n-1-\Theta_n}A(t_n)\cdots A(t_1). \tag{12}$$

Every monomial $A(t_n)\cdots A(t_1)$ in (12) may be replaced by the fully nested commutator $(1/n)\,[A(t_n),\ldots,[A(t_2),A(t_1)]]$ in order to recover the commutator structure[35] giving an expansion in a Lie algebra. However, as already pointed out above, such a structure will be avoided in the following and we will stay with (12).

Now, consider

$$\left\|\int_0^t\cdots\int_0^t \mathrm{d}t_n\cdots\mathrm{d}t_1 L_n A(t_n)\cdots A(t_1)\right\|\leqslant(\|A\|^*)^n\int_0^t\cdots\int_0^t \mathrm{d}t_n\cdots\mathrm{d}t_1|L_n|, \tag{13}$$

where $\|A\|^*=\sup_{s\in[0,t]}\|A(s)\|$. Hence the convergence of the series (12) follows from an appropriate bound on $\int_0^t\cdots\int_0^t \mathrm{d}t_n\cdots\mathrm{d}t_1|L_n|$. Observe that L_n has the same constant value on sections of the n-cube $[0,t]^n$ corresponding to constant $\Theta_n=:k$. Thus by computing the fraction of the volume of $[0,1]^n$ corresponding to a given k $(0\leqslant k\leqslant n-1)$ we arrive at a bound for the terms of the expansion. Denote this fraction V_n^k; then

$$\|\Omega_n\|\leqslant(t\|A\|^*)^n\sum_{k=0}^{n-1}V_n^k\frac{k!(n-1-k)!}{n!}, \tag{14}$$

after using (12) and the fact that the fraction of the n-cube $[0,t]^n$ scales as t^n times the same fraction of the n-cube $[0,1]^n$. Now to compute the fraction V_n^k we consider the representation

$$V_n^k=\sum_{k_1+k_2+\cdots+k_{n-1}=k}\int_0^1\int_{\gamma_{k_1}}\int_{\gamma_{k_2}}\cdots\int_{\gamma_{k_{n-1}}}\mathrm{d}t_n\cdots\mathrm{d}t_2\mathrm{d}t_1, \tag{15}$$

where $\int_{\gamma_{k_i}}=\int_0^{t_i}$ if $k_i=1$, $\int_{\gamma_{k_i}}=\int_{t_i}^1$ when $k_i=0$ and the sum is taken over all combinations with $k_i=1$ or 0. For example, the chronological ordering corresponds to $k_i=1$ for $i=1,\ldots,n-1$ with $V_n^{n-1}=1/n!$, whereas the anti-chronological ordering has $k_i=0$ for $i=1,\ldots,n-1$ with $V_n^0=1/n!$. In order to find V_n^k for all n and k we introduce instead the functions $P_n^k(x)$ given by

$$P_n^k(t_1)=\sum_{k_1+k_2+\cdots+k_{n-1}=k}\int_{\gamma_{k_1}}\int_{\gamma_{k_2}}\cdots\int_{\gamma_{k_{n-1}}}dt_n\cdots dt_2. \tag{16}$$

Clearly we have $V_n^k=\int_0^1 P_n^k(x)dx$, and it is straightforward to see that the following two-index recurrence relation holds:

$$P_n^k(x)=\int_0^x P_{n-1}^k(s)\mathrm{d}s+\int_x^1 P_{n-1}^{k-1}(s)\mathrm{d}s,\quad (n\geqslant 1,\ k=1,\ldots,n-1),$$
$$P_n^0(x)=\frac{x^{n-1}}{(n-1)!},\quad P_n^{n-1}(x)=\frac{(1-x)^{n-1}}{(n-1)!},\tag{17}$$

and $P_n^k(x)=0$ for any other value of the indices. By multiplying $P_n^k(x)$ by $a^n b^k$ and summing over the appropriate domain we have

$$G(a,b,x):=\sum_{n=3}^{\infty}\sum_{k=1}^{n-2} a^n b^k P_n^k(x)=\sum_{n=3}^{\infty}\sum_{k=1}^{n-2} a^n b^k\int_0^x P_{n-1}^k(s)\mathrm{d}s+\sum_{n=3}^{\infty}\sum_{k=1}^{n-2} a^n b^k\int_x^1 P_{n-1}^{k-1}(s)\mathrm{d}s.\tag{18}$$

Taking the boundary values into account we find that the generating function G satisfies

$$\frac{\partial G}{\partial x}=(a-ab)G+a^2(\mathbf{e}^{ab(1-x)}-1)-a^2b(\mathbf{e}^{ax}-1),\tag{19}$$

whose solution is easily found to be

$$G(a,b,x)=\frac{1}{b-1}[(ab-a)\mathbf{e}^{(ab(1-x))}+a+ab(\mathbf{e}^{ax}-1)+\mathbf{e}^{ax(b-1)}(1-b)G(a,b,0)].\tag{20}$$

From this, and the fact that $G(a,b,0)=ab\int_0^1 G(a,b,x)dx+ab(\mathbf{e}^a-a)$ it follows that

$$\sum_{n=1}^{\infty}\sum_{k=0}^{n} a^n b^k V_n^k=\frac{1-\exp(a(1-b))}{b\exp(a(1-b))-1}.\tag{21}$$

By differentiating (21) we find the recursion

$$V_n^k=\frac{(n-k)}{n}V_{n-1}^{k-1}+\frac{(k+1)}{n}V_{n-1}^k\quad (n\geqslant 1,\ k=0,\ldots,n-1),\tag{22}$$

which together with the values $V_n^{n-1}=1/n!$ and $V_n^0=1/n!$ greatly facilitates the computation of V_n^k when numerical values are sought.

A. Analytic estimate of the convergence radius

In order to give a rigorous bound on the convergence domain let us introduce the related value,

$$U_n^k:=\frac{(n-k-1)!k!}{n!}V_n^k;\tag{23}$$

hence the bound (14) becomes

$$\|\Omega_n\|\leqslant(t\|A\|^*)^n\sum_{k=0}^{n-1} V_n^k\frac{k!(n-1-k)!}{n!}=(t\|A\|^*)^n\sum_{k=0}^{n-1} U_n^k.\tag{24}$$

Using the recursion (22) we find that

$$\sum_{k=0}^{n-1} U_n^k=2\sum_{k=0}^{n-2}\frac{(n-k-1)(k+1)}{n^2}U_{n-1}^k\leqslant\frac{1}{2}\sum_{k=0}^{n-2} U_{n-1}^k,\tag{25}$$

since $(n-k-1)(k+1)\leqslant n^2/4$ for $k=0,\ldots,n-2$; thus $\Sigma_{k=0}^{n-1}U_n^k\leqslant C2^{-n}$ where an easy calculation shows that we can choose $C=2$. From this it follows that the expansion (5) converges provided

$$\|A\|^*t<2. \tag{26}$$

Recall that $\|A\|^*$ denotes the maximum value of $\|A(s)\|$ for $s\in[0,t]$. Hence, a comparison with (6) is only pertinent provided $A(t)$ does not vary very much so as

$$\int_0^t\|A(s)\|\mathrm{d}s\sim\|A(s)\|^*t \tag{27}$$

can be allowed, in which case one can argue that the new domain of convergence defined by (26) is almost twice the preceding one (6).

B. Numerical estimate of the convergence radius

Our determination of absolute convergence of $\Sigma_{k=1}^{\infty}\Omega_k(t)$ was based on the bound (14), i.e.,

$$\|\Omega(t)\|\leqslant\sum_{n=1}^{\infty}\|\Omega_n(t)\|\leqslant\sum_{n=1}^{\infty}\|A\|^{*n}t^n\sum_{k=0}^{n-1}\frac{(n-1-k)!k!}{n!}V_n^k=:\sum_{n=1}^{\infty}\|A\|^{*n}t^nc_n. \tag{28}$$

D'Alembert's criterium for convergence applied to the above series leads to a lower bound estimate for absolute convergence of Magnus expansion. Let $r_n:=c_{n+1}/c_n$ with $n>1$; thus the domain of convergence is given by the value $\lim_{n\to\infty}r_n$.

In order to test the tightness of the inequality (25) we will carry out some numerical experiments. Numerical evaluation of $\{r_n\}$ shows slow convergence of the sequence, thus some procedure of convergence acceleration is in order. Since the growth of $\{r_n\}$ is seemingly monotonous beyond the first few values we choose to fit r_n in some range $n=n_0\cdots N$ with $n_0>1$ and N sufficiently large. An accurate way of extrapolating to the value at the limit $n\to+\infty$ is by rational Padé approximants. A direct fit of a rational function to a set of points can be performed iteratively as a linear problem,[38] but is in general a delicate task, highly sensitive to numerical errors. Instead, we choose to use a *Thiele continued fraction*[26,39] which provides us with a simple and efficient algorithm. The calculation is carried out using the stable reciprocal difference method, with a recursive formula for the needed coefficients.

The values obtained using the Thiele extrapolation show a rapid convergence to the rational value $r_\infty=1/2$. Consequently, our analytic bound (26) agrees with the numerical one and no accuracy was lost in the bound (25).

III. CONCLUSIONS

We have seen that, apart form the bounding procedure, the ordering of the elements in the Magnus expansion is critical with regards to the radius of convergence one can prove for the series. It is worth mentioning which effects could be taken into account in order to further improve the bound. The only inequality applied to find the bound was (13), hence any improvement in this can enlarge the bound (26). Inequality (13) subsumes the effect of different ordering of Ω_n and any relation between products like $A(t_1)A(t_2)\cdots A(t_n)$ when integrated over a chronological sector. We now believe it is the latter effect that is most significant if one seeks to further improve upon the convergence result.

The result in (26) may be of particular significance for numerical integrators based on Magnus expansion, since the approximation (27) is most likely accurate. Together with bounds on other discretization errors our result can give improved error bounds for such methods.

Also, this result is significant in the context of nonlinear ODE where Magnus expansion considered as an exponential Lie series allows one to study the effects of nonautonomous, periodic perturbations to, e.g., Hamiltonian systems. It indicates that the constants of bounds found in the literature are rather pessimistic. To transfer the result developed here to the nonlinear case it is

sufficient to endow our procedure with norms of vector fields and their compositions. This gives rise to a *Gevrey*-1 asymptotic sum whose optimal truncation gives rise to approximations that are exponentially accurate in the period of the perturbation.

With regards to applications of the Magnus expansion to quantum problems some particular results on convergence are known[27–30] albeit they are different in nature to that reported here. They refer to the situation when the Hermitian Hamiltonian $H=-i\hbar A$, is split into two parts, namely $H(t)=H_0+\epsilon H_1(t)$, with $0\leqslant\epsilon\ll 1$, and state the domain of convergence after a unitary transformation leading to the Dirac interaction picture. In this case the Hamiltonian is given by $H_{\mathrm{Int}}(t)=\epsilon\exp(i\hbar H_0 t)H_1(t)\exp(-i\hbar H_0 t)$, hence our bound on the convergence domain becomes $\|H_{\mathrm{Int}}\|^* t=\epsilon\|H_1\|^* t<2$, provided the operator norm $\|\cdot\|^*$ is unitary invariant. Thus the convergence domain in the interaction picture is significantly enlarged.

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Nonstandard comodules for quantum matrix bialgebras

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We carry out a construction of nonstandard matrix quantum groups comodules through a generalization of the coaction on tensor powers of a comodule. This generalization amounts to consider the situation where quantum space coordinates and its endomorphism matrix entries belong to a noncommutative quadratic algebra. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1285814]

I. INTRODUCTION

Quantum Groups arise as the abstract structure underlying the symmetries of integrable systems in $(1+1)$ dimensions.[1] There, the theory of quantum inverse scattering give rise to some deformed algebraic structures which were first explained by Drinfel'd as deformations of classical Lie algebras.[2,3] An analog structure was obtained by Woronowicz in the context of noncommutative C^*-algebras.[4] There is a third approach, due to Manin, where Quantum Groups are interpreted as the endomorphisms of certain non commutative algebraic varieties defined by quadratic algebras, called quantum linear spaces (QLS).[5] Faddeev *et al.* had also interpreted the Quantum Groups from the point of view of corepresentations and quantum spaces, furnishing a connection with the quantum deformations of the universal enveloping algebras and the quantum double of Hopf algebras.[6,7]

From the algebraic point of view, quantum groups are Hopf algebras and the relation with the endomorphism algebra of QLS come from their corepresentations on tensor product spaces. The usual construction of the coaction on the tensor product space involves the flip operator interchanging factors of the tensor product of the QLS with the bialgebra. This fact implies the commutativity between the matrix elements of a representation of the endomorphism and the coordinates of the QLS. Moreover, the flip operator for the tensor product is also involved in many steps of the construction of Quantum Groups. In the braided approach to q-deformations, the flip operator is replaced by a braiding giving rise to the quasitensor category of k-modules, where a natural braided coaction appears.[8]

In the present work, we introduce a deformed coaction over the tensor product space, thus admitting noncommutative relations between endomorphism matrix entries and quantum linear space coordinates, however this has nothing to do with the braided approach mentioned above. We find the conditions under which the general algebraic framework of multiplicative quantum groups still holds. It is also shown that the bialgebras arising from this context may be regarded as a partial twisting of usual quantum groups and the connections with integrable systems is analyzed after the introduction of the spectral parameter. This twisted coaction allow us to introduce new deformation parameters in the endomorphism bialgebra of the QLS, as it is shown in the quantum plane example where a four parameters deformation is obtained, although the Yang–Baxter condition is relaxed. Also, we find a noncentral object playing the role of (q,p,r,s)-deformed deter-

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minant. In the undeformed limit for the parameters (r,s) we recover the biparametric deformation $GL_{q,p}(2)$ described in Ref. 13.

We present a brief description of the corepresentations of bialgebras in Sec. II and develop our approach to nonstandard comodules in Sec. III. In Sec. IV we present the result of the previous section as twisted bialgebras. The connection with integrable systems is discussed in Sec. V and, finally, we work out the quantum plane example in Sec. VII.

II. QUANTUM ALGEBRAS AND COREPRESENTATIONS

Let V be a vector space of dimension n, $\{e_i\}$ a basis for V and H_0 the trivial bialgebra of functions over $GL(n,\mathbf{C})$. This bialgebra is freely generated by the identity and the coordinates functions T_i^j, in the basis $\{e_i\}$, defined by

$$T_i^j : GL(n,C) \to C,$$

$$T_i^j : g \to g_i^j$$

for $g \in GL(n,\mathbf{C})$. The T_i^j are group like, hence their coproduct and counit are given by

$$\Delta T_i^j = T_i^k \otimes T_k^i, \tag{1}$$

$$\varepsilon(T_i^j) = \delta_j^i. \tag{2}$$

From now on, summation over the repeated index is assumed. The comodule (δ,V), with

$$\begin{aligned} &\delta : V \to H_0 \otimes V, \\ &\delta(e_i) = T_i^j \otimes e_j, \end{aligned} \tag{3}$$

provides a representation of $GL(n,\mathbf{C})$ in V, through the g_i^j in the basis b of V. It has the coassociativity property and preserves the counit, which is expressed by the relations

$$(I_{H_0} \otimes \delta_V)\delta_V = (\Delta \otimes I_V), \tag{4}$$

$$(\epsilon \otimes I_{H_0})\delta_V = I_V. \tag{5}$$

In order to extend the comodule to the tensor product algebra $V^{\otimes}$, one can introduce the coaction on $V \otimes V$,

$$\begin{aligned} &\delta_{V\otimes V} : V \otimes V \to H_0 \otimes V \otimes V, \\ &\delta_{V\otimes V} = (m \otimes I_{V\otimes V})(I_{H_0} \otimes \tau \otimes I_V)(\delta_V \otimes \delta_V). \end{aligned} \tag{6}$$

The extension to $V^{\otimes N}$ is achieved via the recursive relations

$$\begin{aligned} &\delta_{V^{\otimes N}} : V^{\otimes N} \to H_0 \otimes V^{\otimes N}, \\ &\delta_{V^{\otimes N}} = (m \otimes I_{V^{\otimes N}})(I_{H_0} \otimes \tau_{V^{\otimes N},H_0} \otimes I_V)(\delta_{V^{\otimes (N-1)}} \otimes \delta_V), \end{aligned} \tag{7}$$

where $\tau_{V^{\otimes N},H_0}$ is the flip operator mapping $\tau_{V^{\otimes N},H_0} : V^{\otimes N} \otimes H_0 \to H_0 \otimes V^{\otimes N}$. This definition satisfies the coassociativity and counit properties described in relations (4) and (5). It is also worth to remark that the appearance of the flip operator in (7) leads to the commutativity between the coordinates of the quantum space and its endomorphism matrix entries, as it is assumed for the quantum plane and $GL_q(2)$.[5]

Building up corepresentations for objects with more structure than $V^{\otimes}$, as quadratic algebras for example, requires some extra conditions that we sketch below.

Let A denote the quadratic algebra generated by the ideal $I(\mathfrak{B})$, where $\mathfrak{B}: V\otimes V\rightarrow V\otimes V$, then

$$A(\mathfrak{B})=\frac{V^{\otimes}}{I(\mathfrak{B})}, \tag{8}$$

and $V^{\otimes}$ is a tensor algebra on V. In general we consider $\mathfrak{B}$ with the form

$$\mathfrak{B}=(I_{V\otimes V}-B), \tag{9}$$

$$e_i e_j - B_{ij}^{kl} e_k e_l . \tag{10}$$

$\delta_{V\otimes V}$ must be an homomorphism of quadratic algebra, i.e.,

$$(I_{H_0}\otimes\mathfrak{B})\,\delta_{V\otimes V}=\delta_{V\otimes V}\mathfrak{B}. \tag{11}$$

This is satisfied if H is the bialgebra arising from the quotient of the free algebra generated by the objects T_i^j and the ideal $I(\mathfrak{B},H_0)$ generated by the quadratic relation

$$B_{ij}^{kl}T_k^r T_l^a - T_i^k T_j^l B_{kl}^{rs}, \tag{12}$$

i.e.,

$$H=\frac{H_0}{I(\mathfrak{B},H_0)}. \tag{13}$$

Since $I(\mathfrak{B},H_0)$ is a coideal with relation to Δ, H becomes a bialgebra, namely an *FRT bialgebra*. Equation (12) is a central object in the so-called FRT construction.[6] In this way, $A(\mathfrak{B})$ becomes in a H-algebra comodule.

Indeed, in the strict context of Quantum Groups additional conditions are imposed on the bitensor B. These constraints stem from the categorical setting of these structures; quantum linear spaces belongs to the monoidal category of $A(\mathfrak{B})$-comodules. In fact, if the coaction defined in (6) can be extended to the module $V\otimes W$, for W another $A(\mathfrak{B})$-comodule, so that $V\otimes W$ is also an $A(\mathfrak{B})$-comodule, then the category is monoidal. Moreover, it is relevant to supply this category with an additional structure on the monoidal product, namely, a representation of the braid group. This turns the category into a quasitensor or braided category, where its main property is the existence of a natural isomorphism Ψ: $V\otimes W\rightarrow W\otimes V$, for V and W two arbitrary $A(\mathfrak{B})$-comodules, satisfying the McLane's hexagon conditions. For the kind of quadratic bialgebras we are concerned, this is achieved by requiring $A(\mathfrak{B})$ be dual-quasitriangular[2,8] (see Sec. IV) from which arises the celebrated Quantum Yang–Baxter equation,

$$B_{12}B_{23}B_{12}=B_{23}B_{12}B_{23}.$$

However, it is worth remarking that in the case of general bialgebras or Hopf algebras the $A(\mathfrak{B})$-comodules $V\otimes W$ and $W\otimes V$ may be quite unrelated.

III. GENERALIZED FRT COMODULES

The main aim of this section is to build up the mathematical framework encoding the situation in which entries of the endomorphism matrix may not commute with the coordinates of the quantum linear space defined in (8). We will reach it by means of a modification in the corepresentation theory, obtained by substituting the flip map τ in the standard definition of the coaction on $V\otimes V$ by a nontrivial map γ.

As described in the previous section, supplying the quantum linear space with a comodule structure requires a right definition of a coaction on the tensor product space, and the standard definition of $\delta_{V\otimes V}$, Eq. (6), provides both $V\otimes V$ with a H_0-comodule structure and $A=V^{\otimes}/I(\mathfrak{B})$ with an H-comodule structure.

Then, let us introduce the map γ, defined by

$$\gamma: V\otimes H\to H\otimes V, \tag{14}$$

$$\gamma(e_i\otimes T_j^k)=\gamma_{ijn}^{klm}T_l^n\otimes e_m, \tag{15}$$

and our proposal of generalized or noncommutative coaction on tensor product space is

$$\delta_{V\otimes V}^{\gamma}=(m\otimes I_{V\otimes V})(I_{H_\gamma}\otimes\gamma\otimes I_V)(\delta_V\otimes\delta_V). \tag{16}$$

Then, we shall see that a H_γ-comodule structure there it is possible, for some H_γ to be constructed and provided γ satisfying some requirements. The first question is finding the condition under which $\delta_{V\otimes V}^{\gamma}$ is actually a coaction. It is addressed in the following proposition:

Proposition 1: The map $\delta_{V\otimes V}^{\gamma}: V\otimes V\to H_0\otimes V\otimes V$ *is a coaction turning* $V\otimes V$ *into a* H_0*-comodule iff* $\gamma: V\otimes H_0\to H_0\otimes V$ *satisfies the following conditions:*

$$\gamma_{ijn}^{klm}=\delta_i^m\theta_{jn}^{kl}, \tag{17}$$

$$\theta_{ij}^{pl}\theta_{pk}^{rs}-\delta_j^s\theta_{ik}^{rl}=0, \tag{18}$$

$$\theta_{jn}^{kn}=\delta_j^k. \tag{19}$$

Proof: These properties for γ are readily derived from the coassociativity and counit conditions,

$$\begin{gathered}(\Delta\otimes I_{V\otimes V})\circ\delta_{V\otimes V}^{\gamma}=(I_{H_\gamma}\otimes\delta_{V\otimes V}^{\gamma})\circ\delta_{V\otimes V}^{\gamma},\\ (\epsilon\otimes I_{V\otimes V})\circ\delta_{V\otimes}^{\gamma}=I_{V\otimes V}.\end{gathered} \tag{20}$$

□

A mapping γ satisfying the conditions (17)–(19) leads to a comodule over $V^{\otimes N}$ as stated in the following proposition.

Proposition 2: Let $\delta_{V^{\otimes N}}: V^{\otimes N}\to H_0\otimes V^{\otimes N}$ *be defined by,*

$$\begin{gathered}\delta_V^{\gamma}e_i=\delta_V\ \ e_i=T_i^k\otimes e_k,\\ \delta_{V^{\otimes N}}^{\gamma}=(m_{H_0}\otimes I_{V^{\otimes N}})(I_{H_0}\otimes\gamma_{V^{\otimes(N-1)},H_0}\otimes I_V)(\delta_{V^{\otimes(N-1)}}\otimes\delta_V),\end{gathered} \tag{21}$$

for $N\geqslant 1$, *where*

$$\gamma V^{\otimes N},H_0(e_{i_1}\otimes\ldots e_{i_N}\otimes T_j^k)=\gamma_{V,H_0}\otimes I_{V\otimes(N-1)}(e_{i_1}\otimes\gamma_{V\otimes(N-1),H_0}(e_{i_2}\otimes\cdots\otimes e_{i_N}\otimes T_j^k))$$

and

$$\gamma_{V,H_0}=\gamma,$$

then $(V^{\otimes},\{\delta_{V\otimes N}^{\gamma}\})$ *is a left* H_o*-comodule.*

The proof runs as the previous one, just with a more complicated algebra.

Recalling the bijection between comodules and multiplicative matrices,[5] let us consider the multiplicative matrix M in $V\otimes V$ with coefficients in H_o corresponding to the comodule $\delta_{V\otimes V}^{\gamma}$, i.e.,

$$\delta^{\gamma}_{V\otimes V}\equiv M\in \mathrm{End}(V\otimes V,H_0),$$
$$\delta^{\gamma}_{\otimes V}(e_i\otimes e_j)=M^{rs}_{ij}\otimes e_r\otimes e_s, \tag{22}$$

hence M is

$$M^{kl}_{ij}=T^k_i\theta^{lm}_{jn}T^n_m. \tag{23}$$

Let us adopt the following convention: for A^{kl}_{ij} and D^{kl}_{ij} being any pair of four-tensors, we write $(A\times B)^{rs}_{ij}=A^{kl}_{ij}\times D^{rs}_{kl}$, where $\times$ stands for any kind of product (tensor, algebraic, etc.), and sum over repeated index is also assumed.

With this notation, conditions (18) and (19) are

$$\Delta M=M\otimes M,$$
$$\epsilon(M)=I. \tag{24}$$

The next step is to consider a quadratic structure on $V\otimes V$ giving rise to a QLS. Now, the bialgebra H_o is no longer in the endomorphism algebra of the QLS. Let us consider a QLS generated by the quotient algebra

$$A(\mathfrak{B})=\frac{V^{\otimes}}{I(\mathfrak{B})}, \tag{25}$$

where $\mathfrak{B}$ means the relations defining the quadratic algebra. Associated with it we now introduce a new bialgebra structure on the free algebra generated by the $\{T^k_i\}$.

Proposition 3: Let H_0 the free algebra generated by the $\{T^k_i\}$, γ as in the previous proposition and $I(\mathfrak{B}M-M\mathfrak{B})$ is the ideal generated by the quadratic relation,

$$(\mathfrak{B}M-M\mathfrak{B})^{kl}_{ij}\equiv B^{ab}_{ij}T^k_a\theta^{lm}_{bn}T^n_m-T^a_i\theta^{bm}_{jn}T^n_mB^{kl}_{ab}, \tag{26}$$

then, the quotient algebra H_γ defined as

$$H_\gamma=\frac{H_0}{I(\mathfrak{B}M-M\mathfrak{B})} \tag{27}$$

is a bialgebra.

Proof: A necessary and sufficient condition for H_γ to be a bialgebra is that $I(\mathfrak{B}M-M\mathfrak{B})$ be a coideal, i.e.,

$$\Delta I\subset I\otimes H_0+H_0\otimes I.$$

Then, taking into account the relation (24), one gets

$$\Delta(\mathfrak{B}M-M\mathfrak{B})=\mathfrak{B}\Delta M-\Delta M\mathfrak{B}=\mathfrak{B}(M\otimes M)-(M\otimes M)\mathfrak{B}$$
$$=(\mathfrak{B}M-M\mathfrak{B})\otimes M-M\otimes(\mathfrak{B}M-M\mathfrak{B})$$

and

$$\epsilon(\mathfrak{B}M-M\mathfrak{B})=\mathfrak{B}\epsilon(M)-\epsilon(M)\mathfrak{B}=0,$$

hence H_γ is a bialgebra. □

The main result of this section is expressed in the following proposition:

Proposition 4: $\{\delta^{\gamma}_{V\otimes N}\}$ *supplies* $A(\mathfrak{B})=V^{\otimes}/I(\mathfrak{B})$ *with a left* H_{γ}*-comodule structure. Moreover, if* H' *is another bialgebra coacting on* $A(\mathfrak{B})$ *via the coaction* $\{\delta'^{\gamma}_{V\otimes N}\}$*, with the same* γ*, then there exists a unique map* $f:H_{\gamma}\rightarrow H'$ *such that* $\delta'^{\gamma}_{V\otimes N}=(f\otimes id_{V\otimes N})\delta^{\gamma}_{V\otimes N}$*. Then,* H_{γ} *is unique up to isomorphism.*

Proof: This assertion means the map $\delta^{\gamma}_{V\otimes V}:A(\mathfrak{B})\rightarrow H^{\gamma}\otimes A(\mathfrak{B})$ is an homomorphism of quadratic algebras, as in Eq. (11). This fact is realized by the communication relation

$$(I_{H_{\gamma}}\otimes\mathfrak{B})\circ\delta^{\gamma}_{V\otimes V}=\gamma^{\gamma}_{V\otimes V}\circ\mathfrak{B},$$

which is immediately satisfied by virtue of the ideal defining H_{γ}, i.e., the condition

$$\mathfrak{B}M=M\mathfrak{B}.$$

The universality property follows on the same steps as in Proposition VIII.6.1 of Ref. 7, just taking into account the coaction (16) and (21), and that θ is a linear map. □

Resuming, we can make the following assertion: given a quadratic algebra $A(\mathfrak{B})$ and a map γ satisfying the relations (17)–(19), then $H_{\gamma}=H_0/I(\mathfrak{B}M-M\mathfrak{B})$ is a bialgebra and $\{\delta^{\gamma}_{V\otimes N}\}$ renders $A(\mathfrak{B})$ into a H_{γ}-comodule (a similar quadratic algebra arise in the context of quantum braided group[9]). This may be understood because of the bijection between all the structures of left comodule on $V=\mathbf{C}^n$ and the multiplicative matrix $\mathbf{M}(n,H_{\gamma})$,[5] since $M\in H_{\gamma}$ satisfy $\Delta M=M\otimes M$ and $\epsilon(M)=I_{V\otimes V}$, for $M\in H_{\gamma}$.

In some physical applications of Quantum Groups comodules are also equipped with an algebra structure, i.e., they are QG comodules-algebras. Let us analyze how this works in the framework of the $\{\delta^{\gamma}_{V\otimes N}\}$ coaction. A *H_{γ}-comodule algebra* $(V^{\otimes}(m_V,\eta_V),\{\delta^{\gamma}_{V\otimes N}\})$ is a *H_{γ}-comodule* $(V^{\otimes},\{\delta^{\gamma}_{V\otimes N}\})$ such that the product in V extended to $V^{\otimes}$, $m_V:V\otimes V\rightarrow V$, and the unit $\eta_V:k\rightarrow V$ are H_{γ}-comodule homomorphisms. Equivalently, it can be shown that $V^{\otimes}(m_V,\eta_V)$ is a *H_{γ}-comodule algebra* iff $\{\delta^{\gamma}_{V\otimes N}\}$ are algebra homomorphisms. It means that the following constraint must hold:

$$(I_{H_{\gamma}}\otimes m_V)\circ\delta^{\gamma}_{V\otimes V}=\delta_V\circ m_V, \tag{28}$$

$$\delta^{\gamma}_{V\otimes N}\circ\eta_{V\otimes N}=\eta_{H_{\gamma}}\otimes\eta_{V\otimes N}. \tag{29}$$

Observe that the first relation can be written as

$$(I_{H_{\gamma}}\otimes m_V)\circ\delta^{\gamma}_{V\otimes V}=m_{H_{\gamma}\otimes V}\circ(\delta_V\otimes\delta_V), \tag{30}$$

so, in order to compensate the γ appearing in the left hand side we must redefine $m_{H_{\gamma}\otimes V}$. Thus we get now

$$m_{H_{\gamma}\otimes V}=(m_{H_{\gamma}}\otimes m_V)(I_{H_{\gamma}}\otimes\gamma\otimes I_V). \tag{31}$$

The question now is if $m_{H_{\gamma\otimes V}}$ is an associative product. Due to Proposition 2, $\gamma=(\theta\otimes I_V)\circ\tau$. There are two possibilities to fulfill this constraint:

(1) $\theta:H_{\gamma}\rightarrow H_{\gamma}$ is an algebra homomorphism.
(2) $\theta\circ m=m\circ(\theta\otimes I_V)$.

On the other side, the unit constraint, Eq. (29) imposes that

$$\theta\circ\eta_{H_{\gamma}}=\eta_{H_{\gamma}}. \tag{32}$$

The existence of an antipode is not involved in the comodule structure, so the above construction still holds when H_γ is a Hopf algebra, giving rise to nonstandard comodules of Quantum Groups.

As it was remarked at the end of the previous section, without the quasintriangularity constraints, $\otimes$ stands just for a monoidal product, i.e., the $A(\mathfrak{B})$-comodules $V\otimes W$ and $W\otimes V$ may be quite unrelated. In the next section we discuss the question of quasitriangularity and the Yang–Baxter constraint on the bialgebra H_γ.

In the last section, we describe an explicit example enjoying all these properties presented above, namely a multiparameter deformed version of the endomorphism of the quantum plane. In this example the first possibility for fulfilling the associativity of the $m_{H_\gamma\otimes V}$ product is realized.

IV. RELATION WITH TWISTED BIALGEBRAS

Let us introduce a bialgebra structure on $\mathrm{Hom}(H_0^{\otimes 2},k)$ by means the convolution product $*$ of linear forms, defined as $(f*g)(T)=(f\otimes g)(\Delta T)$ for $f,g\in \mathrm{Hom}(H_0^{\otimes 2},k)$ and $T\in H_0^{\otimes 2}$. The coproduct is $(\Delta h)(T\otimes T')=(h\circ m)(T\otimes T')$ for $h\in \mathrm{Hom}(H_0^{\otimes 2},k)$ and $T,T'\in H_0$. The unit is ϵ, the counit of the H_0, namely, $(\epsilon * f)(T)=f(T)$.

In this framework,[2,8,7] H defined in Eq. (13) can be presented as the bialgebra $H(m,\Delta,\eta,\epsilon,R)$, with $R:H_0^{\otimes 2}\to k$ being an invertible linear form, related to $\mathfrak{B}$ of the previous section by

$$R(T_i^k\otimes T_j^l)=R_{ij}^{kl}\equiv B_{ji}^{kl}, \tag{33}$$

and defined by the quadratic ideal generated by the relation

$$m^{0p}=R*m*\overline{R}. \tag{34}$$

Here, $m^{op}=m\circ\tau$ and $R*\overline{R}=\overline{R}*R=\epsilon$. Moreover, H is said to be *dual quasitriangular*[8] provided R satisfies

$$R\circ(I_H\otimes m)=R_{13}*R_{12}\quad R\circ(m\otimes I_H)=R_{13}*R_{23}. \tag{35}$$

Here, $R_{12}=R\otimes\epsilon$, $R_{23}=\epsilon\otimes R$, $R_{13}=(\epsilon\otimes R)\circ R)\otimes(\tau\otimes I_H)$. This last relations implies R is a solution of the *Quantum Yang–Baxter equation*,

$$R_{12}*R_{13}*R_{23}=R_{23}*R_{13}*R_{12}. \tag{36}$$

Coming back to our problem, let us work out the bialgebra structure H_γ, Eq.(27), derived from noncommutative corepresentations of the previous section. The following characterization of the γ map drives to a different interpretation of the bialgebra H_γ.

Let θ be the linear map,

$$\begin{gathered}\theta:H_0\to H_0,\\ \theta(T_i^j)=\theta_{im}^{jn}T_n^m=\tilde{T}_i^j,\end{gathered} \tag{37}$$

with the properties

$$\begin{gathered}\theta_{ij}^{pl}\theta_{pk}^{rs}-\delta_j^s\theta_{ik}^{rl}=0,\\ \theta_{jn}^{kn}=\delta_j^k.\end{gathered} \tag{38}$$

Proposition 5: θ is a coalgebra homomorphism, such that

$$\Delta \tilde{T}_i^j = \tilde{T}_i^k \otimes \tilde{T}_k^j ,$$
$$\epsilon(\tilde{T}_i^j) = \delta_i^j . \tag{39}$$

Proof: The properties (38) implies that $\tilde{T}$ are group like elements, then satisfying the coassociativity and counit properties.

With this notation, the twisting γ, Eq. (14) can now be expressed as

$$\gamma(e_i \otimes T_j^k) = \theta(T_j^k) \otimes e_i = \tilde{T}_j^k \otimes e_i$$

and the quadratic relation (26) can be written more explicitly as

$$R_{ij}^{ab} T_a^k \tilde{T}_b^l = T_j^a \tilde{T}_i^b R_{ba}^{kl} . \tag{40}$$

This relation generates the ideal which give rise to the quadratic algebra $H_\gamma(m, \Delta, \eta, \epsilon)$.

Now we address the question of quasitriangularity. Let us introduce the deformed product

$$m_\theta = m \circ (I_H \otimes \theta) \tag{41}$$

with θ such that m_θ is a well defined product. Hence, in addition to Eqs. (35), the relation

$$R * m_\theta = m_\theta^{0p} * R \tag{42}$$

allows us to cast the bialgebra $H_\gamma(m, \Delta, \eta, \epsilon)$ into a standard FRT bialgebra $H(m_\theta, \Delta, \eta, \epsilon, R)$, with deformed product m_θ and supplied with the two-form R. This form is close to dual-quasitriangularity. To get a well defined m_θ, i.e., θ such that m_θ satisfies $m_\theta(m_\theta \otimes I_H) = m_\theta(I_H \otimes m_\theta)$ and $m_\theta(\eta \otimes I_H) = m_\theta(I_H \otimes \eta) = I_H$, one may choose for instance $\theta \circ m = m \otimes (\theta \otimes I_H)$.

An easy way to construct a product m_θ satisfying the requirements of Proposition 1 is to consider it as the twisting of the usual product by a 2-cocycle. This will also allow to relate the above construction with twisted bialgebras. The twisting by 2-cocyles of quasitriangular Hopf algebras is due to Drinfel'd[10] who has shown that starting from a quasitriangular Hopf algebra, a new quasitriangular Hopf algebra is obtained twisting by a 2-cocycle the coproduct and the quasitriangular structure $\mathcal{R}$. In our case, we shall use in a partial twisting; we shall need just a twisting of the product or a twisting of the dual-quasitriangular structure. We shall show that the deformation introduced by the noncommutative coaction boils down to a partial twisting of the usual FRT bialgebras, which in general do not preserves dual-quasitriangularity. To this end, we extract some dual results from the Drinfeld analysis.

Following Ref. 8, we introduce a 2-cocycle on the bialgebra $\mathrm{Hom}(H^{\otimes 2}, k)$ as being an invertible element of $H^{\otimes 2}$, in the sense of the product $*$, satisfying the condition $\phi_{23} * ((I_H \otimes \Delta) \circ \phi) = \phi_{12} * ((\Delta \otimes I_H) \circ \phi)$.

The maps $\phi : H^{\otimes 2} \to k$ being a 2-cocycle give rise to a new bialgebra structure on H_0, namely $H_\phi(m_\phi, \Delta, \eta, \epsilon)$, with a twisted product m_ϕ,

$$m_\phi : H_0^{\otimes 2} \to H_0 ,$$
$$m_\phi = \phi * m * \overline{\phi}. \tag{43}$$

Moreover, if ϕ is a bialgebra bicharacter, i.e.,

$$\phi(m \otimes I_H) = \phi_{13} * \phi_{23} ,$$
$$\phi(I_H \otimes m) = \phi_{13} * \phi_{12} , \tag{44}$$

then the 2-cocycle condition leads to the Quantum Yang–Baxter equation,

$$\phi_{12}*\phi_{13}*\phi_{23}=\phi_{23}*\phi_{13}*\phi_{12}. \tag{45}$$

The above proposition provides the framework to interpret the bialgebra H_γ as a twisted one. In fact, let us assume the map θ, introduced in Eq. (37), can be written as

$$\theta(T_j^k)=\theta_{jn}^{km}T_m^n=\rho_j^m T_m^n\overline{\rho}_n^k, \tag{46}$$

i.e., the map θ admits the factorization,

$$\theta_{ij}^{kl}=\rho_i^l\overline{\rho}_j^k. \tag{47}$$

Then, we may introduce the bialgebra bicharacter $\phi:H_0^{\otimes 2}\to k$, inherited from the associativity constraint, defined by the relations

$$\begin{gathered}\phi(T_i^k\otimes T_j^l)=(\epsilon\otimes\rho)(T_i^k\otimes T_j^l),\\ \rho(T_i^k)=\rho_i^k,\\ \phi(T_i^k\otimes e)=\phi(e\otimes T_i^k)=1,\\ \phi(m\otimes I_H)=\phi_{13}*\phi_{23},\\ \phi(I_H\otimes m)=\phi_{13}*\phi_{12},\end{gathered} \tag{48}$$

with $\rho:H_0\to k$ an invertible map, i.e., there exist $\overline{\rho}$ such that $\overline{\rho}*\rho=\rho*\overline{\rho}=\epsilon$, and e is unit of the algebra H_0. Then ϕ is a 2-cocycle, giving rise to the twisted product on H_0,

$$\begin{gathered}m_\phi(T_i^k\otimes T_j^l)=T_i^k\tilde{T}_j^l,\\ \tilde{T}_i^j=\rho_i^m T_m^n\overline{\rho}_n^j.\end{gathered} \tag{49}$$

Observe that condition (18) is trivially fulfilled. Then, the bialgebra $H_\gamma(m,\Delta,\eta,\epsilon,R)$, Eq. (27), is isomorphic to a partial twisting by the 2-cocycle ϕ, (48), of the standard FRT bialgebra $H(m,\Delta,\eta,\epsilon,R)$, (40). The twisting can be performed on the product, thus obtaining the bialgebra isomorphism $H_\gamma(m,\Delta,\eta,\epsilon,R)=H(m_\phi,\Delta,\eta,\epsilon,R)$, with the quadratic ideal $\mathfrak{B}M-M\mathfrak{B}$ being expressed as

$$m_\phi^{op}(T_i^k\otimes T_j^l)=(R*m_\phi*\overline{R})(T_i^k\otimes T_j^l), \tag{50}$$

or, alternatively, one may leaves the product untwisted, but applying the twisting onto the R map,

$$R^\phi=\overline{\phi}_{21}*R*\phi$$

and, again, $H_\gamma(m,\Delta,\eta,\epsilon,R)=H(m,\Delta,\eta,\epsilon,R^\phi)$ with the ideal of Eq. (40), expressed as

$$m^{op}(T_i^k\otimes T_j^l)=(R^\phi*m*\overline{R}^\phi)(T_i^k\otimes T_j^l). \tag{51}$$

In general, both schemes may spoil out dual-quasitriangularity. However, it is important to recover the strict context of Quantum Groups, i.e., the quasitensor structure on the monoidal category of $H_\gamma(m,\Delta,\eta,\epsilon,R)$-comodules. This leaves open the connection with statistical systems. In fact, in these systems the R^ϕ matrix plays the role of Boltzmann weight, and the monodromy matrix are the T_i^k. All this works if R^ϕ provides a representation of the bialgebra H_γ, as it happens with dual-quasitriangular bialgebras. This is achieved if R^ϕ satisfy the relations

$$R^{\phi}(m\otimes I_H)=R^{\phi}_{13}*R^{\phi}_{23},$$
$$R^{\phi}(I_H\otimes m)=R^{\phi}_{13}*R^{\phi}_{12}, \tag{52}$$

so that R^{ϕ} is a solution of the Quantum Yang–Baxter equation. In this way, those quantum bialgebras arising from noncommutative corepresentations with factorizable θ-map, can be mapped into standard FRT bialgebras by a twisting of the original R. In this way, independently of whether the original R is quasitriangular or not, the quasitriangularity of R^{ϕ} means that it is a solution of the quantum Yang–Baxter equation,

$$R^{\phi}_{12}*R^{\phi}_{13}*R^{\phi}_{23}=R^{\phi}_{23}*R^{\phi}_{13}*R^{\phi}_{12},$$

and the monoidal category of H_{γ}-comodules, with $\delta^{\gamma}_{V\otimes V}$, becomes into a quasitensorial one.

V. INTEGRABILITY

The deep relation between Hopf algebras and two dimensional physical systems stems from the integrability condition. As we saw in the previous section, for bialgebras arising from noncommutative corepresentations with a factorizable θ-map it is possible to arrive to dual quasitriangularity structure, then connection goes as usual. We shall see in this section in which way a general bialgebra H_{γ} may be associated to some integrable systems. The main question is the introduction of the spectral parameter, which is related to the coupling constant of the physical system. In doing so, we proceed as in Ref. 2 by regarding a collection of vector spaces $V(\lambda)=\mathbf{C}^n$ for every $\lambda\in\mathbf{C}$, with basis $b(\lambda)=\{e_i(\lambda), i=1,...,n\}$.

For each value of the spectral parameter λ the coordinate functions T^j_i generates a bialgebra $H_0(\lambda)$ with coproduct $\Delta T^j_i(\lambda)=T^k_i(\lambda)\otimes T^j_k(\lambda)$ and counit $\epsilon(T^j_i(\lambda))=\delta^j_i$. Furthermore, the union of the $H_0(\lambda)$ of these bialgebras for all values of λ, i.e., $\mathcal{H}_0=U_{\lambda}H_0(\lambda)$, is also a bialgebra with the same coproduct and counit. Also, a $\mathcal{H}_0$-comodule structure on $V(\lambda)$ is obtained by the coaction $\delta_{V(\lambda)}e_i(\lambda)=T^k_i(\lambda)\otimes e_i(\lambda)$.

Now, let us consider the map

$$\mathfrak{B}(\lambda,\mu): V(\lambda)\otimes V(\mu)\to V(\mu)\otimes V(\lambda),$$
$$e_i(\lambda)\otimes e_j(\mu)\to B^{kl}_{ij}(\lambda,\mu)e_k(\mu)\otimes e_l(\lambda), \tag{53}$$

and the QLS defined by the quadratic algebra,

$$A=\frac{\oplus_{\lambda}V^{\otimes}(\lambda)}{R}, \tag{54}$$

where

$$\mathcal{R}=U_{\lambda,\mu}[1\otimes 1-B(\lambda,\mu)]V(\lambda)\otimes V(\mu).$$

In order to obtain a structure of $\mathcal{H}_0$ comodule on A, we define, following the previous section, the map γ as

$$\gamma: V(\lambda)\otimes\mathcal{H}_0\to\mathcal{H}_0\otimes V(\lambda),$$
$$\gamma(e_i(\lambda)\otimes T^k_j(\mu))=\gamma^{klm}_{ijn}(\lambda,\mu)T^n_l(\mu)\otimes e_m(\lambda), \tag{55}$$

and the coaction on the tensor product space $V(\lambda)\otimes V(\mu)$,

$$\delta^{\gamma}_{V\otimes V}=(m\otimes I_{V(\mu)})(I_{H_{\gamma}}\otimes\gamma(\lambda,\mu)\otimes I_{V(\mu)})(\delta_{V(\lambda)}\otimes\delta_{V(\mu)}). \tag{56}$$

In analogy with Proposition 2, this can be extended to a map,

$$\delta^{\gamma}: A \to \mathcal{H}_0 \otimes A$$

supplying A with a left $\mathcal{H}_0$-comodule structure.

The results analogous to those ones of Propositions 1–3 of Sec. II are still valid provided the replacements

$$\gamma_{ijn}^{klm}(\lambda,\mu) = \delta_i^m \theta_{jn}^{kl}(\lambda,\mu),$$

$$\theta_{ij}^{pl}(\lambda,\mu)\,\theta_{pk}^{rs}(\lambda,\mu) - \delta_j^s \theta_{ik}^{rl}(\lambda,\mu) = 0, \tag{57}$$

$$\theta_{jn}^{kn}(\lambda,\mu) = \delta_j^k,$$

and

$$M_{ij}^{kl}(\lambda,\mu) = T_i^k(\lambda)\,\theta_{jn}^{km}(\lambda,\mu)\,T_m^n(\mu). \tag{58}$$

So that, the ideal $\mathfrak{B}M - M\mathfrak{B}$ of Proposition 2 becomes in

$$B_{ij}^{mn}(\lambda,\mu)M_{mn}^{kl}(\lambda,\mu) - M_{ij}^{mn}(\mu,\lambda)B_{mn}^{kl}(\lambda,\mu). \tag{59}$$

In order to study integrability, we analyze this equation, Eq. (59). In general, a γ map just satisfying the condition of Proposition 1, does not lead to integrability making it necessary to impose additional conditions on it. In the following we study some options.

Our first ansatz is to require that

$$\gamma_{imj}^{mkl}(\lambda,\mu) \equiv \delta_i^l \theta_{mj}^{mk} = \delta_i^l \delta_j^k. \tag{60}$$

In this way, assuming B to be invertible, one can multiply (59) by the inverse of B and then make the contraction of the free index of both B and B^{-1}, thus reaching the integrability condition,

$$T(\lambda)T(\mu) = T(\mu)T(\lambda). \tag{61}$$

Here, $T(\lambda)$ means the trace $T_m^m(\lambda)$.

There is a less obvious way to recover integrability. Condition (59) in terms of θ is

$$B_{ij}^{kl}(\lambda,\mu)T_k^m(\lambda)\,\theta_{lv}^{nu}(\lambda,\mu)T_u^v(\mu) = T_i^k(\lambda)\,\theta_{jv}^{lu}(\lambda,\mu)T_u^v(\mu)B_{kl}^{mn}(\lambda,\mu). \tag{62}$$

If the following nontrivial commutation holds,

$$B_{ij}^{rk}(\lambda,\mu)\,\theta_{sr}^{sl}(\lambda,\mu) = \theta_{si}^{sr}(\lambda,\mu)B_{rj}^{lk}(\lambda,\mu), \tag{63}$$

we may now contract (62) with $\theta_{ar}^{ai}(\lambda,\mu)$ and, after using (63), we get

$$B_{rj}^{il}(\lambda,\mu)\,\theta_{si}^{sk}(\lambda,\mu)T_k^m(\lambda)\,\theta_{lv}^{nu}(\lambda,\mu)T_u^v(\mu) = \theta_{sr}^{si}(\lambda,\mu)T_i^k(\lambda)\,\theta_{jv}^{lu}(\lambda,\mu)T_u^v(\mu)B_{kl}^{mn}(\lambda,\mu), \tag{64}$$

and now we proceed as in the previous case; multiplying by $(B^{-1})_{ab}^{rj}$, and then performing the contractions (a,m), (b,n), thus getting

$$\theta_{sa}^{sk}(\lambda,\mu)T_k^a(\lambda)\,\theta_{bv}^{bu}(\lambda,\mu)T_u^v(\mu) = \theta_{sk}^{si}(\lambda,\mu)T_i^k(\lambda)\,\theta_{lv}^{lu}(\lambda,\mu)T_u^v(\mu). \tag{65}$$

Introducing the quantum matrix $\tilde{T}$ of the final of the previous section, the new integrability condition is written as

$$\tilde{T}(\lambda)\tilde{T}(\mu) = \tilde{T}(\mu)\tilde{T}(\lambda). \tag{66}$$

This last approach to integrability may have an interpretation in the framework of statistical models through their monodromy matrices $T_i^k(\lambda)$. In those models, periodic boundary conditions drive to the transfer matrix by taking the trace over the auxiliary space of the monodromy matrix, which means a sum over all the edge states (see, for example Ref. 11). The objects $\tilde{T}(\lambda)$ means a weighted sum over these edge states, so that θ seems to behave as a twisting factor on the boundary conditions. The periodic ones correspond to the trivial choice $\theta_{ij}^{kl}=\delta_i^l\delta_j^k$. Also, we speculate that many other kind of boundary conditions would be reached by a suitable choice of θ.[14]

As a matter of fact, in Ref. 15, a spin chain model was constructed from the R-matrix of the twisted version of $GL_q(2)$, namely $GL_{p,q}(2)$ (we shall see in the next section that this biparametric deformation of $GL(2)$ coacts also on the standard quantum plane through a twisted coaction). There one may observe that the local twist of the Boltzmann weight can be regarded as some operators coacting through δ^γ on some QLS associated to the inner space at each site, also showing that the effect on the full chain boils down to a twist of the boundary conditions.

We would also like to emphasize that the present construction of nonstandard corepresentationes could be nontrivially realized in conformal field theories. In this respect it is noteworthy that the vertex operators in these theories satisfy a QLS algebra and therefore transform covariantly under the action of a QG. For example, in the WZW model the algebra of vertex operators transforms covariantly under $U_q(\mathrm{sl}(2))$.

In the next section we present a multiparametric example constructed from the quantum plane and fulfilling the first integrability condition.

VI. THE QUANTUM PLANE

Let us consider the quantum plane $A_q^{2|0}$ described by

$$e_1e_2=qe_2e_1. \tag{67}$$

In the basis $\{e_1\otimes e_1, e_1\otimes e_2, e_2\otimes e_1, e_2\otimes e_1\}$, this relation can be expressed by means of the quadratic form B as

$$B=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & q & 0 \\ 0 & q & 1-q^2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{68}$$

which is a solution of the Yang–Baxter equation,

$$B_{12}B_{23}B_{12}=B_{23}B_{12}B_{23}. \tag{69}$$

It is worth remarking that the following construction leads to the same structure for other choice of B, as the symmetric and idempotent B',

$$B'=\frac{1}{q+q^{-1}}\begin{bmatrix} q+q^{-1} & 0 & 0 & 0 \\ 0 & q-q^{-1} & 2 & 0 \\ 0 & 2 & q^{-1}-q & 0 \\ 0 & 0 & 0 & q+q^{-1} \end{bmatrix}. \tag{70}$$

This B' is not a solution of the Yang–Baxter equation but, in the Manin construction for pseudo-symmetric quantum space,[5] it enables us to characterize all the endomorphisms of the quantum plane by the relation $B'M-MB'$ as the only solution to the master relation $(I-B')M(I+B')$.

The endomorphism matrix T is

$$T=\begin{bmatrix} a & b \\ c & d \end{bmatrix}. \tag{71}$$

We find a multiparametric $\theta(r,p,s)$, solution of the coassociativity, counity, and the integrability condition, Eqs. (18), (19), (60), that it is factorizable

$$\theta_{ij}^{kl}=\rho_i^l\overline{\rho}_j^k, \tag{72}$$

with

$$\rho=\begin{bmatrix} 1 & r/s \\ -s/p & (1-r)/p \end{bmatrix}, \tag{73}$$

and $\overline{\rho}$ is it inverse.

This means that the induced map $\phi=\epsilon\otimes\rho$ is a 2-cocycle whenever $s\neq 0$, hence there is an obstruction in to obtain the undeformed limit $s\to 0$. In this sense, this $\phi(r,p,s)$ is not a 2-cocycle for the whole spectrum of its parameters and the twisting arising from it does not yields a continuous deformation of the algebra H_0.

From this matrix we obtain the rules to commute e and T,

$$\gamma(e_i\otimes T_j^k)=\theta_{jp}^{ks}T_s^p\otimes e_i. \tag{74}$$

As we see, there are now three new deformation parameters (p,r,s) besides q, which was introduced by the quadratic algebra of the quantum plane (67).

The relations $BM-MB$ can be written in a compact form by introducing the objects $\tilde{T}_i^j=\theta_{ir}^{js}T_s^r$, such that

$$\tilde{T}=\begin{bmatrix} \tilde{a} & \tilde{b} \\ \tilde{c} & \tilde{d} \end{bmatrix}, \tag{75}$$

so that we get

$$\begin{gathered} a\tilde{c}-qc\tilde{a}=0, \\ a\tilde{b}-qb\tilde{a}=0, \\ b\tilde{c}-c\tilde{b}=0, \\ c\tilde{d}-qd\tilde{c}=0, \\ b\tilde{d}-qd\tilde{b}=0, \\ a\tilde{d}-d\tilde{a}+(q^{-1}-q)c\tilde{b}=0, \end{gathered} \tag{76}$$

and

$$\begin{gathered} \gamma(e_i\otimes\tilde{a})=\tilde{a}\otimes e_i, \\ \gamma(e_i\otimes\tilde{d})=\tilde{d}\otimes e_i, \\ \gamma(e_i\otimes\tilde{b})=p\tilde{b}\otimes e_i, \\ \gamma(e_i\otimes\tilde{c})=p^{-1}\tilde{c}\otimes e_i. \end{gathered} \tag{77}$$

Relations (76) acquire a highly nontrivial form in terms of the T_i^k. In this way, one can define a four parameter deformation of the $M(2)$, namely, $M_{q,p,r,s}(2)$,

$$M_{q,p,r,s}(2)=\frac{k[T_i^j]}{I(BM-MB)}. \tag{78}$$

Also, the Grassmannian plane $A_q^{0/2}(\xi_1,\xi_2)$, defined by the relation

$$\xi_1\xi_2=-\frac{1}{q}\xi_2\xi_1$$

is naturally a $M_{q,p,r,s}(2)$-comodule.[12] This allows us to define a determinant for this $M_{q,p,r,s}(2)$ from the coaction $\delta^{\gamma}_{V\otimes V}$ on the object $\xi_1\xi_2$,

$$\delta^{\gamma}_{V\otimes V}(\xi_1\xi_2)=D\otimes\xi_1\xi_2. \tag{79}$$

Thus we get

$$D=M_{12}^{12}-qM_{12}^{21}=a\tilde{d}-qb\tilde{c}=ad-\frac{q}{p}(1-r)bc-\frac{r}{s}ac-q\frac{s}{p}bd. \tag{80}$$

As was explained above, this is a nonperturbative deformation; the limit to the undeformed case cannot be taken simultaneously. However, there is a sequential limit leading to another 3 and 2 parameters deformation. In fact, if we take first the limit $r\to 0$ we get $M_{q,p,s}(2)$ and now the remaining $\phi(p,s)$ is now a genuine 2-cocycle, so that the twisting is well defined in the whole spectrum of p and s. Taking now a second undeformed limit, we set $s\to 0$, then we recover the biparametric $M_{q,p}(2)$ obtained by Manin *et al.*,[13] as nonstandard quantum groups. In these limits θ becomes

$$\theta(p)=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & p & 0 \\ 0 & \frac{1}{p} & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{81}$$

and now, the 2-cocycle $\phi=\epsilon\otimes\rho$ becomes

$$\rho=\begin{bmatrix} 1 & 0 \\ 0 & 1/p \end{bmatrix}, \tag{82}$$

and the relations $BM-MB$, or $R^{\phi}*m=m^{op}*R^{\phi}$, reduce to

$$\begin{gathered} ac-pqca=0, \\ ab-p^{-1}qba=0, \\ bc-p^2cb=0, \\ cd-p^{-1}qdc=0, \\ bd-pqdb=0, \\ ad-da+p(q^{-1}-q)cb=0, \end{gathered} \tag{83}$$

which define a two parametric $M_{q,p}(2)$ as the quotient algebra,[13]

$$M_{q,p}(2)=\frac{k[T_i^j]}{I(BM-MB)} \tag{84}$$

for i and j from 1 to 2. It is worth remarking that $R^{\phi}(q,p)=\overline{\phi}_{21}(p)*R(q)*R(q)*\phi(p)$ is a solution of the Quantum Yang–Baxter equation, and assuming R^{ϕ} is a bialgebra bicharacter, it supplies $M_{q,p}(2)$ with a dual-quasitriangular structure.

This γ gives rise to the following relations between matrix entries and the coordinates of the quantum plane:

$$\begin{aligned}
\gamma(e_i\otimes a)&=a\otimes e_i,\\
\gamma(e_i\otimes d)&=d\otimes e_i,\\
\gamma(e_i\otimes b)&=pb\otimes e_i,\\
\gamma(e_i\otimes c)&=p^{-1}c\otimes e_i.
\end{aligned} \tag{85}$$

Defining $\tilde{T}_i^j=\theta_{il}^{jk}T_k^l$ we get

$$\tilde{T}=\begin{bmatrix} a & pc \\ \dfrac{b}{p} & d \end{bmatrix}, \tag{86}$$

and with the coproduct

$$\Delta\tilde{T}_i^j=\tilde{T}_i^k\otimes\tilde{T}_k^j. \tag{87}$$

The determinant becomes in

$$D=\det{}_{q,p}=ad-p^{-1}qbc,$$

that satisfy the following commutation relations:

$$\begin{aligned}
Da\mp aD&=0,\\
Db-p^{-2}bD&=0,\\
Dc-p^{2}cD&=0,\\
Dd-dD&=0.
\end{aligned}$$

With these properties, and assuming that D is an invertible element of $M_{q,p}(2)$, the antipode can be defined

$$S\begin{bmatrix} a & b \\ c & d \end{bmatrix}=D^{-1}\begin{bmatrix} d & -(pq)^{-1}b \\ -pqc & a \end{bmatrix}, \tag{88}$$

and, consequently, the quasitriangular Hopf algebra $GL_{qp}(2)$ is obtained.[13] This means that through the noncommutative coaction,

$$\delta^{\gamma}(e_1\otimes e_1)=aa\otimes e_1\otimes e_1+pab\otimes e_1\otimes e_2+ba\otimes e_2\otimes e_1+pbb\otimes e_2\otimes e_2,$$

$$\delta^{\gamma}(e_1\otimes e_2)=\frac{1}{p}ac\otimes e_1\otimes e_1+ac\otimes e_1\otimes e_2+\frac{1}{p}bc\otimes e_2\otimes e_1+cd\otimes e_2\otimes e,$$

$$\delta^{\gamma}(e_2\otimes e_1)=ca\otimes e_1\otimes e_1+pcb\otimes e_1\otimes e_2+da\otimes e_2\otimes e_1+pdb\otimes e_2\otimes e_2,$$

$$\delta^{\gamma}(e_1\otimes e_2)=\frac{1}{p}cc\otimes e_1\otimes e_1+cd\otimes e_1\otimes e_2+\frac{1}{p}dc\otimes e_2\otimes e_1+dd\otimes e_2\otimes e,$$

with $\gamma(e_k\otimes T^l_j)$ defined in Eq. (85), the standard Quantum Planes $A_q^{2/0}$ and $A_q^{0/2}$ appears also as $GL_{p,q}(2)$-comodules, this result can be obtained by completely different means as in Ref. 16.

VII. CONCLUDING REMARKS

We have introduced a new ingredient in the construction of comodules of Quantum (semi) Groups admitting noncommutativity between endomorphism matrix entries and quantum space coordinates. This feature give rise to an extra deformation of all the involved structures. Our approach is not a full braiding as those obtained from the quasitensor category of *k*-modules.[8] In a less ambitious project, we have just redefined the coaction showing that it is possible to introduce a nontrivial map $\gamma: V\otimes H_\gamma\rightarrow H_\gamma\otimes V$ without spoiling out the Hopf algebra and the comodule structures provided that γ turns H_γ into a Quantum Matrix Group. No additional modification were introduced in the usual structure of bialgebras, preserving the product and coproduct untouched. However, provided a factorizable γ, this generalization of the coaction boils down to a twisting of the algebra structure or a twist of the *R*-matrix, and in some cases it is possible to recover a quasitriangular FRT bialgebra.

Although the map γ seems too constrained, we have found nontrivial solutions introducing many new deformation parameters, still under the additional condition of integrability. This last point was also analyzed, showing that integrability can be reached at least in two independent ways. Working on the Quantum Planes as examples, it was shown that the biparametric deformation of $GL(2,\mathbf{C})$, namely, $GL_{p,q}(2)$, can be regarded as coacting in a twisted way over the standard quantum plane.

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A spinor-like representation of the contact superconformal algebra $K'(4)$

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In this work we construct an embedding of a nontrivial central extension of the contact superconformal algebra $K'(4)$ into the Lie superalgebra of pseudodifferential symbols on the supercircle $S^{1/2}$. Associated with this embedding is a one-parameter family of spinor-like tiny irreducible representations of $K'(4)$ realized just on 4 fields instead of the usual 16. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1326920]

I. INTRODUCTION

Recall that a *superconformal algebra* is a simple complex Lie superalgebra such that it contains the centerless Virasoro algebra (i.e., the Witt algebra) $\mathrm{Witt}=\oplus_{n\in\mathbb{Z}}\mathbb{C}L_n$ as a subalgebra, and has growth 1. The $\mathbb{Z}$-graded superconformal algebras are ones for which $\mathrm{ad}L_0$ is diagonalizable with finite-dimensional eigenspaces; see Ref. 1. In general, a superconformal algebra is a subalgebra of the Lie superalgebra of all derivations of $\mathbb{C}[t,t^{-1}]\otimes\Lambda(N)$, where $\Lambda(N)$ is the Grassmann algebra in N odd variables.

The Lie superalgebra $K(N)$ of contact vector fields with Laurent polynomials as coefficients is characterized by its action on a contact 1-form (Refs. 1, 2 and 3); it is isomorphic to the $SO(N)$ *superconformal algebra* (Ref. 4). $K(N)$ is simple except when $N=4$. In this case $K'(4)=[K(4),K(4)]$ is simple. Note that $K'(N)$ is spanned by 2^N fields. It was discovered in Refs. 5, 6 and 7 that the Lie superalgebra of contact vector fields with polynomial coefficients in 1 even and 6 odd variables contains an exceptional simple Lie superalgebra (see also Refs. 2 and 3). It was shown in Ref. 3 that the derived Lie superalgebra of divergence-free derivations of $\mathbb{C}[t,t^{-1}]\otimes\Lambda(2)$, which is spanned by 8 fields, can be realized inside $K(4)$ using the construction of the exceptional superconformal algebra inside $K(6)$.

Note that a Lie algebra of contact vector fields can be realized as a subalgebra of Poisson algebra; see Ref. 8. The Poisson algebra of formal Laurent series on $\dot{T}^*S^1=T^*S^1\backslash S^1$ has a well-known deformation, that is the Lie algebra R of pseudodifferential symbols on the circle. The Poisson algebra can be considered to be the semiclassical limit of R; see Refs. 9, 10, 11 and 12.

In this work we define a family $R_h(N)$ of Lie superalgebras of pseudodifferential symbols on the supercircle $S^{1/N}$, where $h\in]0,1]$, which contracts to the Poisson superalgebra.

For each h we construct an embedding of a central extension $\hat{K}'(4)$ into $R_h(2)$. These central extensions are isomorphic to one of 3 independent central extensions, which are known for $K'(4)$ (Refs. 1, 2, 13 and 14). The corresponding central element is $h\in R_h(2)$. The elements of embeddings of $\hat{K}'(4)$ are power series in h; considering their limits as $h\to 0$, we obtain an embedding of $K'(4)$ into the Poisson superalgebra.

The idea of our construction is as follows. We consider the Schwimmer–Seiberg's deformation $S(2,\alpha)$ of the Lie superalgebra of divergence-free derivations of $\mathbb{C}[t,t^{-1}]\otimes\Lambda(2)$ (Refs. 15 and 1) and observe that the exterior derivations of $S'(2,\alpha)$ form an $\mathfrak{sl}(2)$ if $\alpha\in\mathbb{Z}$. The exterior derivations of $S'(2,\alpha)$ for all $\alpha\in\mathbb{Z}$ generate a subalgebra of the Poisson superalgebra isomorphic

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to the loop algebra $\tilde{\mathfrak{sl}}(2)$ [$\mathfrak{sl}(2)$ corresponds to $\alpha=1$]. We prove that the family $S'(2,\alpha)$ for all $\alpha\in\mathbb{Z}$ and $\tilde{\mathfrak{sl}}(2)$ generate a Lie superalgebra isomorphic to $K'(4)$. The similar construction for each $h\in]0,1]$ gives an embedding of a nontrivial central extension of $K'(4)$:

$$\hat{K}'(4)\subset R_h(2). \tag{1.1}$$

It is known that the Lie algebra R has two independent central extensions; see Refs. 9, 10 and 11. Accordingly, there exist, up to equivalence, two nontrivial 2-cocycles on its superanalog $R_{h=1}(N)$. The 2-cocycle on $K'(4)$, which corresponds to the central extension $\hat{K}'(4)$ is equivalent to the restriction of one of the 2-cocycles on $R_{h=1}(2)$.

Finally, the embedding (1.1) for $h=1$ allows us to define a new one-parameter family of tiny irreducible representations of $\hat{K}'(4)$. Recall that there exists a two-parameter family of representations of $K'(N)$ in the superspace spanned by 2^N fields. These representations are defined by the natural action of $K'(N)$ in the spaces of ''densities;'' see Ref. 1.

We obtain representations of $\hat{K}'(4)$, where the value of the central charge is equal to 1, realized on just 4 fields, instead of the usual 16.

II. SUPERCONFORMAL ALGEBRAS

In this section we review the notion of a superconformal algebra and give the necessary definitions.

A *superconformal algebra* is a complex Lie superalgebra $\mathfrak{g}$ such that

(1) $\mathfrak{g}$ is simple,
(2) $\mathfrak{g}$ contains the Witt algebra $\mathrm{Witt}=\mathrm{der}\,\mathbb{C}[t,t^{-1}]=\oplus_{n\in\mathbb{Z}}\mathbb{C}L_n$ with the well-known commutation relations

$$[L_n,L_m]=(n-m)L_{n+m} \tag{2.1}$$

as a subalgebra,
(3) adL_0 is diagonalizable with finite-dimensional eigenspaces:

$$\mathfrak{g}=\oplus_j\mathfrak{g}_j,\mathfrak{g}_j=\{x\in\mathfrak{g}|[L_0,x]=jx\}, \tag{2.2}$$

so that $\dim\mathfrak{g}_j<C$, where C is a constant independent of j; see Ref. 1. The main series of superconformal algebras are $W(N)(N\geqslant 0)$, $S'(N,\alpha)(N\geqslant 2)$ and $K'(N)$ $(N\geqslant 1)$. The corresponding central extensions were classified in Ref. 1; see also Refs. 2, 13, 14 and 16.

The superalgebras $W(N)$. Consider the superalgebra $\mathbb{C}[t,t^{-1}]\otimes\Lambda(N)$, where $\Lambda(N)$ is the Grassmann algebra in N variables $\theta_1,\ldots,\theta_N$. Let p be the parity of the homogeneous element. Let $p(t)=\overline{0}$ and $p(\theta_i)=\overline{1}$ for $i=1,...,N$. By definition $W(N)$ is the Lie superalgebra of all derivations of $\mathbb{C}[t,t^{-1}]\otimes\Lambda(N)$. Let ∂_i stand for $\partial/\partial\theta_i$ and ∂_t stand for $\partial/\partial t$. Every $D\in W(N)$ is represented by a differential operator,

$$D=f\partial_t+\sum_{i=1}^{N} f_i\partial_i, \tag{2.3}$$

where f, $f_i\in\mathbb{C}[t,t^{-1}]\otimes\Lambda(N)$. $W(N)$ has no nontrivial 2-cocycles if $N>2$. If $N=1$ or 2, then there exists, up to equivalence, one nontrivial 2-cocycle on $W(N)$.

The superalgebras $S(N,\alpha)$. The Lie superalgebra $W(N)$ contains a one-parameter family of Lie superalgebras $S(N,\alpha)$; see Refs. 15 and 1. By definition

$$S(N,\alpha)=\{D\in W(N)|\mathrm{Div}(t^\alpha D)=0\},\quad \text{for } \alpha\in\mathbb{C}. \tag{2.4}$$

Recall that

$$\mathrm{Div}(D)=\partial_t f+\sum_{i=1}^{N}(-1)^{p(f_i)}\partial_i(f_i) \tag{2.5}$$

and

$$\mathrm{Div}(fD)=Df+f\,\mathrm{Div}\,D, \tag{2.6}$$

where f is an even function. Let $S'(N,\alpha)=[S(N,\alpha),S(N,\alpha)]$ be the derived superalgebra. Assume that $N>1$. If $\alpha\notin\mathbb{Z}$, then $S(N,\alpha)$ is simple, and if $\alpha\in\mathbb{Z}$, then $S'(N,\alpha)$ is a simple ideal of $S(N,\alpha)$ of codimension one defined from the exact sequence,

$$0\to S'(N,\alpha)\to S(N,\alpha)\to\mathbb{C}t^{-\alpha}\theta_1\cdots\theta_N\partial_t\to 0. \tag{2.7}$$

Notice that

$$S(N,\alpha)\cong S(N,\alpha+n),\quad \text{for } n\in\mathbb{Z}. \tag{2.8}$$

There exists, up to equivalence, one nontrivial 2-cocycle on $S'(N,\alpha)$ if and only if $N=2$; see Ref. 1. Let $\hat{S}'(2,\alpha)$ be the corresponding central extension of $S'(2,\alpha)$. Note that $S'(2,\alpha)$ is spanned by 4 even fields and 4 odd fields. Sometimes the name ''$N=4$ superconformal algebra'' is used for $\hat{S}'(2,0)$; see Refs. 4 and 3.

The superalgebras $K(N)$. By definition,

$$K(N)=\{D\in W(N)\,|\,D\Omega=f\Omega,\quad \text{for some } f\in\mathbb{C}[t,t^{-1}]\otimes\Lambda(N)\}, \tag{2.9}$$

where

$$\Omega=dt-\sum_{i=1}^{N}\theta_i\,d\theta_i \tag{2.10}$$

is a contact 1-form; see Refs. 1, 2 and 3. Every differential operator $D\in K(N)$ can be represented by a single function,

$$f\in\mathbb{C}[t,t^{-1}]\otimes\Lambda(N): f\to D_f. \tag{2.11}$$

Let

$$\Delta(f)=2f-\sum_{i=1}^{N}\theta_i\partial_i(f). \tag{2.12}$$

Then

$$D_f=\Delta(f)\partial_t+\partial_t(f)\sum_{i=1}^{N}\theta_i\partial_i+(-1)^{p(f)}\sum_{i=1}^{N}\partial_i(f)\partial_i. \tag{2.13}$$

Notice that

$$\begin{aligned} D_{f+g}&=D_f+D_g,\\ [D_f,D_g]&=D_{\{f,g\}}, \end{aligned} \tag{2.14}$$

where

$$\{f,g\}=\Delta(f)\partial_t(g)-\partial_t(f)\Delta(g)+(-1)^{p(f)}\sum_{i=1}^{N}\partial_i(f)\partial_i(g). \tag{2.15}$$

The superalgebras $K(N)$ are simple, except when $N=4$. If $N=4$, then the derived superalgebra $K'(4)=[K(4),K(4)]$ is a simple ideal in $K(4)$ of codimension one defined from the exact sequence

$$0\to K'(4)\to K(4)\to \mathbb{C}D_{t^{-1}\theta_1\theta_2\theta_3\theta_4}\to 0. \tag{2.16}$$

There exists no nontrivial 2-cocycles on $K(N)$ if $N>4$. If $N\leqslant 3$, then there exists, up to equivalence, one nontrivial 2-cocycle. Let $\hat{K}(N)$ be the corresponding central extension of $K(N)$. Notice that $\hat{K}(1)$ is isomorphic to the Neveu–Schwarz algebra (Ref. 17), and $\hat{K}(2)\cong\hat{W}(1)$ is isomorphic to the so-called $N=2$ superconformal algebra; see Ref. 18. The superalgebra $K'(4)$ has 3 independent central extensions (Refs. 1, 2, 13 and 14), which is important for our task.

III. LIE SUPERALGEBRAS OF PSEUDODIFFERENTIAL SYMBOLS

Recall that the ring R of pseudodifferential symbols is the ring of the formal series,

$$A(t,\xi)=\sum_{-\infty}^{n}a_i(t)\xi^i, \tag{3.1}$$

where $a_i(t)\in\mathbb{C}[t,t^{-1}]$, and the variable ξ corresponds to $\partial/\partial t$; see Refs. 9, 10, 11 and 12. The multiplication rule in R is determined as follows:

$$A(t,\xi)\circ B(t,\xi)=\sum_{n\geqslant 0}\frac{1}{n!}\partial_\xi^n A(t,\xi)\partial_t^n B(t,\xi). \tag{3.2}$$

Notice that R is a generalization of the associative algebra of the regular differential operators on the circle, and the multiplication rule in R, when restricted to the polynomials in ξ, coincides with the multiplication rule for the differential operators. The Lie algebra structure on R is given by

$$[A,B]=A\circ B-B\circ A, \tag{3.3}$$

where $A,\ B\in R$.

The Poisson algebra P of pseudodifferential symbols has the same underlying vector space. The multiplication in P is naturally defined. The Poisson bracket is defined as follows:

$$\{A(t,\xi),B(t,\xi)\}=\partial_\xi A(t,\xi)\partial_t B(t,\xi)-\partial_t A(t,\xi)\partial_\xi B(t,\xi) \tag{3.4}$$

(Refs. 12 and 19). One can construct the contraction of the Lie algebra R to P using the linear isomorphisms:

$$\varphi_h: R\to R, \tag{3.5}$$

defined by

$$\varphi_h(a_i(t)\xi^i)=a_i(t)h^i\xi^i,\ \text{ where }\ h\in\,]0,1]; \tag{3.6}$$

see Ref. 12. The new multiplication in R is defined by

$$A\circ_h B=\varphi_h^{-1}(\varphi_h(A)\circ\varphi_h(B)). \tag{3.7}$$

Correspondingly, the commutator is

$$[A,B]_h = A\circ_h B - B\circ_h A. \tag{3.8}$$

Thus

$$[A,B]_h = h\{A,B\} + hO(h). \tag{3.9}$$

Hence

$$\lim_{h\to 0}\frac{1}{h}[A,B]_h = \{A,B\}. \tag{3.10}$$

To construct a superanalog of R, consider an associative superalgebra $\Theta_h(N)$ with generators $\theta_1,\dots,\theta_N,\partial_1,\dots,\partial_N$ and relations

$$\begin{aligned} \theta_i\theta_j &= -\theta_j\theta_i, \\ \partial_i\partial_j &= -\partial_j\partial_i, \\ \partial_i\theta_j &= h\delta_{i,j} - \theta_j\partial_i, \end{aligned} \tag{3.11}$$

where $h\in\,]0,1]$. Define an associative superalgebra,

$$R_h(N) = R\otimes\Theta_h(N), \tag{3.12}$$

such that

$$(A\otimes X)(B\otimes Y) = \frac{1}{h}(A\circ_h B)\otimes(XY), \tag{3.13}$$

where $A, B\in R$, and $X, Y\in\Theta_h(N)$. The product in $R_h(N)$ determines the natural Lie superalgebra structure on this space:

$$[(A\otimes X),(B\otimes Y)]_h = \frac{1}{h}(A\circ_h B)\otimes(XY) - (-1)^{p(X)p(Y)}\frac{1}{h}(B\circ_h A)\otimes(YX). \tag{3.14}$$

For each $h\in\,]0,1]$ there exists an embedding,

$$W(N)\subset R_h(N), \tag{3.15}$$

such that the commutation relations in $R_h(N)$, when restricted to $W(N)$, coincide with the commutation relations in $W(N)$. In particular, when $h=1$, we obtain the superanalog $R(N) := R_{h=1}(N)$ of the Lie algebra of pseudodifferential symbols on the circle.

The Poisson superalgebra $P(N)$ has the underlying vector space $P\otimes\Theta(N)$, where $\Theta(N) := \Theta_{h=0}(N)$ is the Grassman algebra with generators $\theta_1,\dots,\theta_N,\overline{\theta_1},\dots,\overline{\theta_N}$, where $\overline{\theta_i}=\partial_i$ for $i=1,\dots,N$. The Poisson bracket is defined as follows:

$$\{A,B\} = \partial_\xi A\partial_t B - \partial_t A\partial_\xi B - (-1)^{p(A)}\left(\sum_{i=1}^{N}\partial_{\theta_i}A\partial_{\overline{\theta_i}}B + \partial_{\overline{\theta_i}}A\partial_{\theta_i}B\right), \tag{3.16}$$

where $A, B\in P(N)$; cf. Refs. 2, 5. Thus

$$\lim_{h\to 0}[A,B]_h = \{A,B\}. \tag{3.17}$$

Correspondingly, we have the embedding

$$W(N)\subset P(N). \tag{3.18}$$

Remark 3.1: Recall that there exist, up to equivalence, two nontrivial 2-cocycles on R (Refs. 9, 10 and 11). Analogously, one can define two 2-cocycles, c_ξ and c_t, on $R(N)$; cf. Ref. 20. Let $A, B \in R$, and $X, Y \in \Theta_{h=1}(N)$. Then

$$c_\xi(A\otimes X, B\otimes Y) = \text{the coefficient of } t^{-1}\xi^{-1}\theta_1\dots\theta_N\partial_1\dots\partial_N \text{ in } ([\log\xi, A]\circ B)\otimes(XY), \tag{3.19}$$

where

$$[\log\xi, A(t,\xi)] = \Sigma_{k\geq 1}\frac{(-1)^{k+1}}{k}\partial_t^k A(t,\xi)\xi^{-k}, \tag{3.20}$$

and

$$c_t(A\otimes X, B\otimes Y) = \text{the coefficient of } t^{-1}\xi^{-1}\theta_1\dots\theta_N\partial_1\dots\partial_N \text{ in } ([\log t, A]\circ B)\otimes(XY), \tag{3.21}$$

where

$$[\log t, A(t,\xi)] = \Sigma_{k\geq 1}\frac{(-1)^{k+1}}{k}t^{-k}\partial_\xi^k A(t,\xi). \tag{3.22}$$

IV. THE CONSTRUCTION OF EMBEDDING

Let $\mathrm{Der}\, S'(2,\alpha)$ be the Lie superalgebra of all derivations of $S'(2,\alpha)$.

Lemma 4.1: The exterior derivations $\mathrm{Der}_{\mathrm{ext}} S'(2,\alpha)$ for all $\alpha\in\mathbb{Z}$ generate the loop algebra,

$$\tilde{\mathfrak{sl}}(2)\subset P(2). \tag{4.1}$$

Proof: In Ref. 21 we observed that the exterior derivations of $S'(2,0)$ form an $\mathfrak{sl}(2)$. Let

$$\{\mathcal{L}_n^\alpha, E_n, H_n, F_n, h_n^\alpha, p_n^0, x_n^0, y_n^\alpha\}_{n\in\mathbb{Z}} \tag{4.2}$$

be a basis of $S'(2,\alpha)$ defined as follows:

$$\begin{aligned}
\mathcal{L}_n^\alpha &= -t^n(t\xi + \tfrac{1}{2}(n+\alpha+1)(\theta_1\partial_1+\theta_2\partial_2)),\\
E_n &= t^n\theta_2\partial_1,\\
H_n &= t^n(\theta_2\partial_2-\theta_1\partial_1),\\
F_n &= t^n\theta_1\partial_2,\\
h_n^\alpha &= t^n\xi\theta_2-(n+\alpha)t^{n-1}\theta_1\theta_2\partial_1,\\
p_n^0 &= -t^{n+1}\partial_2,\\
x_n^0 &= t^{n+1}\partial_1,\\
y_n^\alpha &= t^n\xi\theta_1+(n+\alpha)t^{n-1}\theta_1\theta_2\partial_2.
\end{aligned} \tag{4.3}$$

Let us show that if $\alpha\in\mathbb{Z}$, then $\mathrm{Der}_{\mathrm{ext}} S'(2,\alpha)\cong\mathfrak{sl}(2)=\langle \boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{H}}, \boldsymbol{\mathcal{F}}\rangle$, where

$$[\boldsymbol{\mathcal{H}}, \boldsymbol{\mathcal{E}}] = 2\boldsymbol{\mathcal{E}}, \quad [\boldsymbol{\mathcal{H}}, \boldsymbol{\mathcal{F}}] = -2\boldsymbol{\mathcal{F}}, \quad [\boldsymbol{\mathcal{E}}, \boldsymbol{\mathcal{F}}] = \boldsymbol{\mathcal{H}}, \tag{4.4}$$

and the action of $\mathfrak{sl}(2)$ is given as follows:

$$[\boldsymbol{\mathcal{E}}, h_n^\alpha] = x_{n-1+\alpha}, \quad [\boldsymbol{\mathcal{E}}, y_n^\alpha] = p^0_{n-1+\alpha}, \quad [\boldsymbol{\mathcal{F}}, x_n] = h^\alpha_{n+1-\alpha}, \quad [\boldsymbol{\mathcal{F}}, p_n^0] = y^\alpha_{n+1-\alpha},$$
$$[\boldsymbol{\mathcal{H}}, x_n^0] = x_n^0, \quad [\boldsymbol{\mathcal{H}}, h_n^\alpha] = -h_n^\alpha, \quad [\boldsymbol{\mathcal{H}}, p_n^0] = p_n^0, \quad [\boldsymbol{\mathcal{H}}, y_n^\alpha] = -y_n^\alpha. \tag{4.5}$$

Notice that

$$\mathrm{Der}_{\mathrm{ext}} S'(2,\alpha) \cong H^1(S'(2,\alpha), S'(2,\alpha)); \tag{4.6}$$

see Ref. 22. Consider the following $\mathbb{Z}$-grading deg of $S'(2,\alpha)$:

$$\deg \mathcal{L}_n^\alpha = n, \quad \deg E_n = n+1-\alpha, \quad \deg F_n = n-1+\alpha, \quad \deg H_n = n,$$
$$\deg h_n^\alpha = n, \quad \deg p_n = n, \quad \deg x_n = n+1-\alpha, \quad \deg y_n^\alpha = n-1+\alpha. \tag{4.7}$$

Let

$$L_0^\alpha = -\mathcal{L}_0^\alpha + \tfrac{1}{2}(1-\alpha)H_0. \tag{4.8}$$

Then

$$[L_0^\alpha, s] = (\deg s)s, \tag{4.9}$$

for a homogeneous $s \in S'(2,\alpha)$. Accordingly,

$$[L_0^\alpha, D] = (\deg D)D, \tag{4.10}$$

for a homogeneous $D \in \mathrm{Der}_{\mathrm{ext}} S'(2,\alpha)$. On the other hand, since the action of a Lie superalgebra on its cohomology is trivial, then one must have

$$[L_0^\alpha, D] = 0. \tag{4.11}$$

Hence the nonzero elements of $\mathrm{Der}_{\mathrm{ext}} S'(2,\alpha)$ have deg=0, and they preserve the superalgebra $S'(2,\alpha)_{\deg=0}$. One can check that the exterior derivations of $S'(2,\alpha)_{\deg=0}$ form an $\mathfrak{sl}(2)$, and extend them to the exterior derivations of $S'(2,\alpha)$ as in (4.5). One should also note that if the restriction of a derivation of $S'(2,\alpha)$ to $S'(2,\alpha)_{\deg=0}$ is zero, then this derivation is inner. We can identify the exterior derivation $t^{-\alpha}\xi\theta_1\theta_2$ [see (2.7)] with $-\boldsymbol{\mathcal{F}}$. We cannot realize all the exterior derivations as regular differential operators on the supercircle, but can do this using the symbols of pseudodifferential operators. In fact, let $\alpha = 1$. Then

$$\mathrm{Der}_{\mathrm{ext}} S'(2,1) = \mathfrak{sl}(2) = \langle \boldsymbol{\mathcal{F}}, \boldsymbol{\mathcal{H}}, \boldsymbol{\mathcal{E}} \rangle \subset P(2), \tag{4.12}$$

where

$$\boldsymbol{\mathcal{F}} = -t^{-1}\xi\theta_1\theta_2, \quad \boldsymbol{\mathcal{H}} = -\theta_1\partial_1 - \theta_2\partial_2, \quad \boldsymbol{\mathcal{E}} = t\xi^{-1}\partial_1\partial_2. \tag{4.13}$$

One can then construct the loop algebra of $\mathfrak{sl}(2)$ as follows:

$$\tilde{\mathfrak{sl}}(2) = \langle \boldsymbol{\mathcal{F}}_n, \boldsymbol{\mathcal{H}}_n, \boldsymbol{\mathcal{E}}_n \rangle_{n \in \mathbb{Z}}, \tag{4.14}$$

where

$$\boldsymbol{\mathcal{F}}_n = -t^{n-1}\xi\theta_1\theta_2,$$
$$\boldsymbol{\mathcal{H}}_n = nt^{n-1}\xi^{-1}\theta_1\theta_2\partial_1\partial_2 - t^n(\theta_1\partial_1 + \theta_2\partial_2), \tag{4.15}$$

$$\boldsymbol{\mathcal{E}}_n = t^{n+1}\xi^{-1}\partial_1\partial_2 .$$

The nonvanishing commutation relations are

$$[\boldsymbol{\mathcal{H}}_n, \boldsymbol{\mathcal{E}}_k] = 2\boldsymbol{\mathcal{E}}_{n+k}, \quad [\boldsymbol{\mathcal{H}}_n, \boldsymbol{\mathcal{F}}_k] = -2\boldsymbol{\mathcal{F}}_{n+k}, \quad [\boldsymbol{\mathcal{E}}_n, \boldsymbol{\mathcal{F}}_k] = \boldsymbol{\mathcal{H}}_{n+k}. \tag{4.16}$$

Let $\alpha \in \mathbb{Z}$. Then

$$\mathrm{Der}_{\mathrm{ext}} S'(2,\alpha) \cong \langle \boldsymbol{\mathcal{F}}_{-\alpha+1}, \boldsymbol{\mathcal{H}}_0, \boldsymbol{\mathcal{E}}_{\alpha-1} \rangle. \tag{4.17}$$

□

Theorem 4.1: The superalgebras $S'(2,\alpha)$ for all $\alpha \in \mathbb{Z}$ together with $\tilde{\mathfrak{sl}}(2)$ generate a Lie superalgebra isomorphic to $K'(4)$.

Proof: Let

$$\begin{aligned} I_n^0 &= t^n(\theta_1\partial_1 + \theta_2\partial_2), \\ \mathfrak{r}_n &= t^{n-1}\theta_1\theta_2\partial_1, \\ \mathfrak{s}_n &= t^{n-1}\theta_1\theta_2\partial_2 . \end{aligned} \tag{4.18}$$

Then according to (4.3),

$$\begin{aligned} \mathcal{L}_n^\alpha &= \mathcal{L}_n^0 - \tfrac{1}{2}\alpha I_n^0, \\ h_n^\alpha &= h_n^0 - \alpha\mathfrak{r}_n, \\ y_n^\alpha &= y_n^0 + \alpha\mathfrak{s}_n . \end{aligned} \tag{4.19}$$

One can easily check that the superalgebras $S'(2,\alpha)$, where $\alpha \in \mathbb{Z}$, generate $W(2) \subset P(2)$. In fact, $W(2)$ is spanned by 8 fields defined in Eq. (4.3), where $\alpha = 0$, together with 3 fields defined in Eq. (4.18) and the field $\boldsymbol{\mathcal{F}}_n$. If we include two even fields, $\boldsymbol{\mathcal{E}}_n$ and $\boldsymbol{\mathcal{H}}_n$, into the picture, then from the commutation relations, we obtain two additional odd fields:

$$\begin{aligned} \mathfrak{q}_n &= t^n\xi^{-1}\theta_2\partial_1\partial_2, \\ \mathfrak{t}_n &= -t^n\xi^{-1}\theta_1\partial_1\partial_2 . \end{aligned} \tag{4.20}$$

Let $\mathfrak{g} \subset P(2)$ be the Lie superalgebra generated by the superalgebras $S'(2,\alpha)$ for all $\alpha \in \mathbb{Z}$ and $\tilde{\mathfrak{sl}}(2)$. We will show that there exists an isomorphism:

$$\psi : K'(4) \to \mathfrak{g}. \tag{4.21}$$

Let

$$\begin{aligned} \mathcal{L}_n &= \mathcal{L}_n^0 + \boldsymbol{\mathcal{H}}_n + \tfrac{1}{2} I_n^0, \\ I_n &= I_n^0 + \boldsymbol{\mathcal{H}}_n, \\ p_n &= p_n^0 + \mathfrak{t}_n, \\ x_n &= x_n^0 - \mathfrak{q}_n . \end{aligned} \tag{4.22}$$

Set

$$h_n = h_n^0, \quad y_n = y_n^0. \tag{4.23}$$

Then $\mathfrak{g} = \mathfrak{g}_0^- \oplus \mathfrak{g}_1^-$, where

$$\begin{gathered}\mathfrak{g}_0^- = \langle \mathcal{L}_n, I_n, E_n, H_n, F_n, \boldsymbol{\mathcal{E}}_n, \boldsymbol{\mathcal{H}}_n, \boldsymbol{\mathcal{F}}_n \rangle, \\ \mathfrak{g}_1^- = \langle h_n, p_n, x_n, y_n, \mathfrak{r}_n, \mathfrak{s}_n, \mathfrak{q}_n, \mathfrak{t}_n \rangle.\end{gathered} \tag{4.24}$$

We will describe the nonvanishing commutation relations in $\mathfrak{g}$ with respect to this basis.

For $[\mathfrak{g}_0^-, \mathfrak{g}_0^-]$ the relations are

$$\begin{gathered}[\mathcal{L}_n, \mathcal{L}_k] = (n-k)\mathcal{L}_{n+k}; \\ [H_n, E_k] = 2E_{n+k}, [H_n, F_k] = -2F_{n+k}, \quad [E_n, F_k] = H_{n+k}; \\ [\boldsymbol{\mathcal{H}}_n, \boldsymbol{\mathcal{E}}_k] = 2\boldsymbol{\mathcal{E}}_{n+k}, [\boldsymbol{\mathcal{H}}_n, \boldsymbol{\mathcal{F}}_k] = -2\boldsymbol{\mathcal{F}}_{n+k}, \quad [\boldsymbol{\mathcal{E}}_n, \boldsymbol{\mathcal{F}}_k] = \boldsymbol{\mathcal{H}}_{n+k}; \\ [\mathcal{L}_n, X_k] = -kX_{n+k}, \quad \text{where } X_k = I_k, E_k, H_k, F_k, \boldsymbol{\mathcal{E}}_k, \boldsymbol{\mathcal{H}}_k, \boldsymbol{\mathcal{F}}_k.\end{gathered} \tag{4.25}$$

For $[\mathfrak{g}_0^-, \mathfrak{g}_1^-]$ the relations are

$$[\mathcal{L}_n, X_k] = \left(-k + \frac{n}{2}\right) X_{n+k}, \quad \text{where } X_k = h_k, p_k, x_k, y_k;$$

$$[\mathcal{L}_n, X_k] = \left(-k - \frac{n}{2}\right) X_{n+k}, \quad \text{where } X_k = \mathfrak{r}_k, \mathfrak{s}_k, \mathfrak{q}_k, \mathfrak{t}_k;$$

$$[I_n, X_k] = nY_{n+k}, \quad \text{where } X_k = h_k, p_k, x_k, y_k, \quad \text{and } Y_k = \mathfrak{r}_k, \mathfrak{t}_k, -\mathfrak{q}_k, -\mathfrak{s}_k, \quad \text{respectively;}$$

$$[H_n, X_k] = X_{n+k}, \quad \text{where } X_k = h_k, x_k, \mathfrak{q}_k, \mathfrak{r}_k;$$

$$[H_n, X_k] = -X_{n+k}, \quad \text{where } X_k = y_k, p_k, \mathfrak{s}_k, \mathfrak{t}_k; \tag{4.26}$$

$$[E_n, X_k] = Y_{n+k}, [F_n, Y_k] = X_{n+k}, \quad \text{where } X_k = y_k, p_k, \mathfrak{s}_k, \mathfrak{t}_k,$$
$$\text{and } Y_k = h_k, x_k, -\mathfrak{r}_k, -\mathfrak{q}_k, \quad \text{respectively;}$$

$$[\boldsymbol{\mathcal{H}}_n, X_k] = X_{n+k} + nY_{n+k}, \quad \text{where } X_k = p_k, x_k, \mathfrak{q}_k, \mathfrak{t}_k \quad \text{and } Y_k = \mathfrak{t}_k, -\mathfrak{q}_k, 0, 0, \quad \text{respectively;}$$

$$[\boldsymbol{\mathcal{H}}_n, X_k] = -X_{n+k} - nY_{n+k}, \quad \text{where } X_k = h_k, y_k, \mathfrak{r}_k, \mathfrak{s}_k, \quad \text{and } Y_k = \mathfrak{r}_k, -\mathfrak{s}_k, 0, 0, \quad \text{respectively;}$$

$$[\boldsymbol{\mathcal{E}}_n, X_k] = Y_{n+k} - nZ_{n+k}, \quad [\boldsymbol{\mathcal{F}}_n, Y_k] = X_{n+k} - n\overline{Z}_{n+k}, \quad \text{where } X_k = h_k, y_k, \mathfrak{r}_k, \mathfrak{s}_k,$$

$$Y_k = x_k, p_k, -\mathfrak{q}_k, -\mathfrak{t}_k, Z_k = \mathfrak{q}_k, -\mathfrak{t}_k, 0, 0, \quad \text{and } \overline{Z}_k = -\mathfrak{r}_k, \mathfrak{s}_k, 0, 0, \quad \text{respectively.}$$

Finally, for $[\mathfrak{g}_1^-, \mathfrak{g}_1^-]$ the relations are

$$\begin{gathered}[h_n, x_k] = (k-n)E_{n+k}, [p_n, y_k] = (k-n)F_{n+k}, \\ [h_n, p_k] = \mathcal{L}_{n+k} - \tfrac{1}{2}(k-n)H_{n+k}, [x_n, y_k] = -\mathcal{L}_{n+k} + \tfrac{1}{2}(k-n)H_{n+k}, \\ [h_n, \mathfrak{q}_k] = E_{n+k}, [x_n, \mathfrak{r}_k] = E_{n+k}, [p_n, \mathfrak{s}_k] = F_{n+k}, [y_n, \mathfrak{t}_k] = F_{n+k}, \\ [p_n, \mathfrak{q}_k] = -\boldsymbol{\mathcal{E}}_{n+k}, [x_n, \mathfrak{t}_k] = -\boldsymbol{\mathcal{E}}_{n+k}, [h_n, \mathfrak{s}_k] = -\boldsymbol{\mathcal{F}}_{n+k}, [y_n, \mathfrak{r}_k] = -\boldsymbol{\mathcal{F}}_{n+k},\end{gathered} \tag{4.27}$$

$$[p_n,\mathfrak{r}_k]=\tfrac{1}{2}I_{n+k}-\tfrac{1}{2}(H_{n+k}+\boldsymbol{\mathcal{H}}_{n+k}),[x_n,\mathfrak{s}_k]=\tfrac{1}{2}I_{n+k}+\tfrac{1}{2}(H_{n+k}-\boldsymbol{\mathcal{H}}_{n+k}),$$

$$[h_n,\mathfrak{t}_k]=\tfrac{1}{2}I_{n+k}+\tfrac{1}{2}(H_{n+k}+\boldsymbol{\mathcal{H}}_{n+k}),[y_n,\mathfrak{q}_k]=\tfrac{1}{2}I_{n+k}-\tfrac{1}{2}(H_{n+k}-\boldsymbol{\mathcal{H}}_{n+k}).$$

Recall that the elements of $K(4)$ can be identified with the functions from $\mathbb{C}[t,t^{-1}]\otimes\Lambda(4)$. Let

$$\breve{\theta}_1=\theta_2\theta_3\theta_4,\quad \breve{\theta}_2=\theta_1\theta_3\theta_4,\quad \breve{\theta}_3=\theta_1\theta_2\theta_4,\quad \breve{\theta}_4=\theta_1\theta_2\theta_3. \tag{4.28}$$

The following 16 series of functions together with $t^{-1}\theta_1\theta_2\theta_3\theta_4$ span $\mathbb{C}[t,t^{-1}]\otimes\Lambda(4)$:

$$\begin{gathered}
f_n^1=2nt^{n-1}\theta_1\theta_2\theta_3\theta_4,\\
f_n^2=-\tfrac{1}{2}t^{n+1}+\tfrac{1}{2}it^n(\theta_2\theta_3-\theta_1\theta_4)-\tfrac{1}{2}n(n+1)t^{n-1}\theta_1\theta_2\theta_3\theta_4,\\
f_n^k=\tfrac{1}{2}t^{n\mp1}(\pm\theta_1\theta_2\mp\theta_3\theta_4-i\theta_1\theta_3-i\theta_2\theta_4),\quad k=3,4,\\
f_n^5=it^n(\theta_1\theta_4-\theta_2\theta_3),\\
f_n^k=\tfrac{1}{2}t^n(\mp\theta_1\theta_4\mp\theta_2\theta_3+i\theta_2\theta_4-i\theta_1\theta_3),\quad k=6,7,\\
f_n^8=-it^n(\theta_1\theta_2+\theta_3\theta_4),\\
f_n^k=\frac{(i)^{p(k)}}{\sqrt{8}}(t^n(\theta_1\mp i\theta_2\mp\theta_3+i\theta_4)-nt^{n-1}(\breve{\theta}_1\pm i\breve{\theta}_2\mp\breve{\theta}_3-i\breve{\theta}_4)),\quad k=9,10,\\
f_n^k=\frac{(i)^{p(k)}}{\sqrt{8}}(t^{n+1}(\theta_1\pm i\theta_2\mp\theta_3-i\theta_4)-(n+1)t^n(\breve{\theta}_1\mp i\breve{\theta}_2\mp\breve{\theta}_3+i\breve{\theta}_4)),\quad k=11,12,\\
f_n^k=\frac{(-i)^{p(k)}}{\sqrt{2}}t^{n-1}(\breve{\theta}_1\pm i\breve{\theta}_2\mp\breve{\theta}_3-i\breve{\theta}_4),\quad k=13,14,\\
f_n^k=\frac{(-i)^{p(k)}}{\sqrt{2}}t^n(\breve{\theta}_1\mp i\breve{\theta}_2\mp\breve{\theta}_3+i\breve{\theta}_4),\quad k=15,16,
\end{gathered} \tag{4.29}$$

where $p(k)=0$ if k is even, and $p(k)=1$ if k is odd.

The 16 series of the corresponding differential operators $\{D_{f_n^i}\}_{i=1,\ldots,16}$ span $K'(4)$. Set

$$\begin{gathered}
\psi(D_{f_n^1})=I_n,\quad \psi(D_{f_n^2})=\mathcal{L}_n,\\
\psi(D_{f_n^3})=E_n,\quad \psi(D_{f_n^4})=F_n,\quad \psi(D_{f_n^5})=H_n,\\
\psi(D_{f_n^6})=\boldsymbol{\mathcal{E}}_n,\quad \psi(D_{f_n^7})=\boldsymbol{\mathcal{F}}_n,\quad \psi(D_{f_n^8})=\boldsymbol{\mathcal{H}}_n,\\
\psi(D_{f_n^9})=x_n,\quad \psi(D_{f_n^{10}})=h_n,\quad \psi(D_{f_n^{11}})=y_n,\quad \psi(D_{f_n^{12}})=p_n,\\
\psi(D_{f_n^{13}})=\mathfrak{q}_n,\quad \psi(D_{f_n^{14}})=\mathfrak{r}_n,\quad \psi(D_{f_n^{15}})=\mathfrak{s}_n,\quad \psi(D_{f_n^{16}})=\mathfrak{t}_n.
\end{gathered} \tag{4.30}$$

Notice that $f_n^1=0$, if $n=0$. This corresponds to the fact that $D_{t^{-1}\theta_1\theta_2\theta_3\theta_4}\notin K'(4)$. One can verify that ψ is an isomorphism from $K'(4)$ onto $\mathfrak{g}$. □

Remark 4.2: We have obtained an embedding,

$$K'(4)\subset P(2). \tag{4.31}$$

In general, a Lie algebra of contact vector fields can be realized as a subalgebra of Poisson algebra; see Ref. 8. We will explain this from the geometrical point of view in application to our case. Recall that the Lie algebra Vect(S^1) of smooth vector fields on the circle has a natural embedding into the Poisson algebra of functions on the cylinder $\dot{T}^*S^1=T^*S^1\backslash S^1$ with the removed zero section; see Refs. 11, 12 and 19. One can introduce the Darboux coordinates $(q,p)=(t,\xi)$ on this manifold. The symbols of differential operators are functions on $\dot{T}^*S^1$ which are formal Laurent series in p with coefficients periodic in q. Correspondingly, they define Hamiltonian vector fields on $\dot{T}^*S^1$:

$$A(q,p)\to H_A=\partial_p A\partial_q-\partial_q A\partial_p. \tag{4.32}$$

The embedding of Vect(S^1) into the Lie algebra of Hamiltonian vector fields on $\dot{T}^*S^1$ is given by

$$f(q)\partial_q\to H_{f(q)p}. \tag{4.33}$$

Notice that we obtain a subalgebra of Hamiltonian vector fields with Hamiltonians which are homogeneous of degree 1. (This condition holds in general, if one considers the *symplectification* of a contact manifold; see Ref. 8.) In other words, we obtain a subalgebra of Hamiltonian vector fields, which commute with the (semi-) Euler vector field:

$$[H_A,p\partial_p]=0. \tag{4.34}$$

We will show that for $N\geqslant 0$ there exists the analogous embedding:

$$K(2N)\subset P(N). \tag{4.35}$$

The analog of the formula (4.32) in the supercase is as follows (Refs. 2, 5):

$$A(q,p,\theta_i,\overline{\theta_i})\to H_A=\partial_p A\partial_q-\partial_q A\partial_p-(-1)^{p(A)}\sum_{i=1}^{N}(\partial_{\theta_i}A\partial_{\overline{\theta_i}}+\partial_{\overline{\theta_i}}A\partial_{\theta_i}). \tag{4.36}$$

Then $K(2N)$ is defined as the set of all (Hamiltonian) functions $A(q,p,\theta_i,\overline{\theta_i})\in P(N)$ such that

$$\left[H_A,p\partial_p+\sum_{i=1}^{N}\overline{\theta_i}\partial_{\overline{\theta_i}}\right]=0. \tag{4.37}$$

Equivalently, we have the following characterization of the embedding (4.35). Consider a $\mathbb{Z}$-grading of the (associative) superalgebra $P(N)=\oplus_{j\in\mathbb{Z}}P_j(N)$ defined by

$$\begin{aligned}&\deg p=\deg\overline{\theta_i}=1,\quad \text{for } i=1,...,N,\\ &\deg q=\deg\theta_i=0,\quad \text{for } i=1,...,N.\end{aligned} \tag{4.38}$$

Thus with respect to the Poisson bracket,

$$\{P_j(N),P_k(N)\}\subset P_{j+k-1}(N). \tag{4.39}$$

Then

$$K(2N)=P_1(N). \tag{4.40}$$

Theorem 4.2: There exists an embedding,

$$\hat{K}'(4)\subset R_h(2), \tag{4.41}$$

for each $h\in]0,1]$, such that the central element in $\hat{K}'(4)$ is $h\in R_h(2)$, and

$$\lim_{h\to 0}\hat{K}'(4)=K'(4)\subset P(2). \tag{4.42}$$

Proof: For each $h\in]0,1]$ and $\alpha\in\mathbb{Z}$ we have an embedding,

$$\mathrm{Der}\,S'(2,\alpha)\subset R_h(2). \tag{4.43}$$

The exterior derivations $\mathrm{Der}_{\mathrm{ext}}S'(2,\alpha)$ for all $\alpha\in\mathbb{Z}$ generate the loop algebra,

$$\tilde{\mathfrak{sl}}(2)=\langle \boldsymbol{\mathcal{F}}_n,\boldsymbol{\mathcal{H}}_n,\boldsymbol{\mathcal{E}}_n\rangle_{n\in\mathbb{Z}}\subset R_h(2), \tag{4.44}$$

where

$$\boldsymbol{\mathcal{F}}_n=-t^{n-1}\xi\theta_1\theta_2,$$

$$\boldsymbol{\mathcal{H}}_n=\frac{1}{h}((\xi^{-1}\circ_h t^n\xi)(h^2-h\theta_1\partial_1-h\theta_2\partial_2-\theta_1\theta_2\partial_1\partial_2)+t^n\theta_1\theta_2\partial_1\partial_2), \tag{4.45}$$

$$\boldsymbol{\mathcal{E}}_n=(\xi^{-1}\circ_h t^{n+1})\partial_1\partial_2,$$

so that Eqs. (4.16)–(4.17) hold. Let $\mathfrak{g}\subset R_h(2)$ be the Lie superalgebra generated by $S'(2,\alpha)$ for all $\alpha\in\mathbb{Z}$ and $\tilde{\mathfrak{sl}}(2)$. Set

$$\begin{aligned}\mathfrak{q}_n&=(\xi^{-1}\circ_h t^n)(h\partial_1+\theta_2\partial_1\partial_2),\\ \mathfrak{t}_n&=(\xi^{-1}\circ_h t^n)(h\partial_2-\theta_1\partial_1\partial_2).\end{aligned} \tag{4.46}$$

The basis (4.24) in $\mathfrak{g}$ is defined by Eqs. (4.3), (4.18), (4.22)–(4.23) and (4.45)–(4.46). The commutation relations in $\mathfrak{g}$ with respect to this basis are given by Eqs. (4.25)–(4.27). The Lie superalgebra $\mathfrak{g}$ is isomorphic to a central extension,

$$\hat{K}'(4)=K'(4)\oplus\mathbb{C}C, \tag{4.47}$$

of $K'(4)$. The corresponding 2-cocycle (up to equivalence) is

$$\begin{aligned}c(t^{n+1},t^{k+1}\theta_1\theta_2\theta_3\theta_4)&=\delta_{n+k+2,0},\\ c(t^{n+1}\theta_i,t^{k+1}\partial_i(\theta_1\theta_2\theta_3\theta_4))&=\tfrac{1}{2}\,\delta_{n+k+2,0},\quad \text{for } i=1,\ldots,4.\end{aligned} \tag{4.48}$$

The isomorphism,

$$\psi:\hat{K}'(4)\to\mathfrak{g}, \tag{4.49}$$

is defined by Eq. (4.30) and the equation

$$\psi(C)=I_0=h\in R_h(2). \tag{4.50}$$

The corresponding 2-cocycle in the basis (4.24) is

$$c(p_n,\mathfrak{r}_k)=\tfrac{1}{2}\,\delta_{n,-k},$$

$$
\begin{aligned}
c(x_n,\mathfrak{s}_k)&=\tfrac{1}{2}\,\delta_{n,-k},\\
c(h_n,\mathfrak{t}_k)&=\tfrac{1}{2}\,\delta_{n,-k},\\
c(y_n,\mathfrak{q}_k)&=\tfrac{1}{2}\,\delta_{n,-k},\\
c(\mathcal{L}_n,I_k)&=n\,\delta_{n,-k}.
\end{aligned}
\tag{4.51}
$$

Note that in the realization of $K'(4)$ inside $P(2)$, obtained in Theorem 4.1, we have $I_0=0$. □

Remark 4.3: The 2-cocycle c is one of three nontrivial 2-cocycles on $K'(4)$; see Refs. 1 and 2. [In Ref. 1 this cocycle is defined by Eq. (4.22), where $d=0$, $e=1$]. Note that the cocycle c is equivalent to the restriction of the 2-cocycle c_t on $R(2)$; see Eqs. (3.21), (3.22).

V. ONE-PARAMETER FAMILY OF REPRESENTATIONS OF $\hat{K}'(4)$

Theorem 5.1: There exists a one-parameter family of irreducible representations of $\hat{K}'(4)$ depending on parameter $\mu\in\mathbb{C}$ in the superspace spanned by 2 even fields and 2 odd fields where the value of the central charge is equal to one.

Proof: Let $g\in t^{\mu}\mathbb{C}[t,t^{-1}]$, where $\mu\in\mathbb{R}\backslash\mathbb{Z}$. One can think of ξ^{-1} as the anti-derivative,

$$
\xi^{-1}g(t)=\int g(t)dt. \tag{5.1}
$$

Let $f(t)\in\mathbb{C}[t,t^{-1}]$. According to (3.2),

$$
\xi^{-1}\circ f=\sum_{n=0}^{\infty}(-1)^n(\xi^n f)\xi^{-n-1}. \tag{5.2}
$$

Notice that this formula, when applied to a function g, corresponds to the formula of integration by parts. Let

$$
V^{\mu}=t^{\mu}\mathbb{C}[t,t^{-1}]\otimes\Lambda(2)=t^{\mu}\mathbb{C}[t,t^{-1}]\otimes\langle 1,\theta_1,\theta_2,\theta_1\theta_2\rangle,\mu\in\mathbb{R}\backslash\mathbb{Z}. \tag{5.3}
$$

Using the realization of $\hat{K}'(4)$ inside $R(2)$ (see Theorem 4.2 for $h=1$) we obtain a representation of $\hat{K}'(4)$ in V^{μ}. A central element in $\hat{K}'(4)$ is $I_0=1\in R(2)$; the 2-cocycle is defined by Eq. (4.51). Let $\{v_m^i\}$, where $m\in\mathbb{Z}$ and $i=0,1,2,3$, be the following basis in V^{μ}:

$$
\begin{aligned}
v_m^0&=\frac{1}{m+\mu}\,t^{m+\mu},\\
v_m^1&=t^{m+\mu}\theta_1,\\
v_m^2&=t^{m+\mu}\theta_2,\\
v_m^3&=t^{m+\mu}\theta_1\theta_2.
\end{aligned}
\tag{5.4}
$$

The action of $\hat{K}'(4)$ is given as follows:

$$
\mathcal{L}_n(v_m^0)=-(m+n+\mu-1)v_{m+n}^0,
$$

$$
\mathcal{L}_n(v_m^i)=-(m+\tfrac{1}{2}n+\mu)v_{m+n}^i,\quad i=1,2,
$$

$$
\begin{gathered}
\mathcal{L}_n(v^3_m)=-(m+n+\mu+1)v^3_{m+n},\\
E_n(v^1_m)=v^2_{m+n},\quad F_n(v^2_m)=v^1_{m+n},\\
\boldsymbol{\mathcal{E}}_n(v^3_m)=v^0_{m+n+2},\quad \boldsymbol{\mathcal{F}}_n(v^0_m)=-v^3_{m+n-2},\\
H_n(v^i_m)=\mp v^i_{m+n},\quad i=1,2,\\
\boldsymbol{\mathcal{H}}_n(v^i_m)=\pm v^i_{m+n},\quad i=0,3,\\
h_n(v^1_m)=-(m+n+\mu)v^3_{m+n-1},\quad y_n(v^2_m)=(m+n+\mu)v^3_{m+n-1},\\
h_n(v^0_m)=v^2_{m+n-1},\quad y_n(v^0_m)=v^1_{m+n-1},\\
x_n(v^1_m)=(m+n+\mu)v^0_{m+n+1},\quad p_n(v^2_m)=-(m+n+\mu)v^0_{m+n+1},\\
x_n(v^3_m)=v^2_{m+n+1},\quad p_n(v^3_m)=v^1_{m+n+1},\\
\mathfrak{r}_n(v^1_m)=v^3_{m+n-1},\quad \mathfrak{s}_n(v^2_m)=v^3_{m+n-1},\\
\mathfrak{q}_n(v^1_m)=v^0_{m+n+1},\quad \mathfrak{t}_n(v^2_m)=v^0_{m+n+1},\\
I_n(v^i_m)=v^i_{m+n},\quad i=0,1,2,3.
\end{gathered}
\tag{5.5}
$$

Note that I_0 acts by the identity operator. One can then define a one-parameter family of representations of $\hat{K}'(4)$ depending on parameter $\mu\in\mathbb{C}$ in the superspace $V=\langle v^0_m,v^3_m,v^1_m,v^2_m\rangle_{m\in\mathbb{Z}}$, where $p(v^i_m)=\overline{0}$, for $i=0$, 3, and $p(v^i_m)=\overline{1}$ for $i=1$, 2, according to the formulas (5.5).

□

Remark 5.1: The elements $\{\mathcal{L}_n,H_n,h_n,p_n\}_{n\in\mathbb{Z}}$ span a subalgebra of $K'(4)$ isomorphic to $K(2)$. Note that V decomposes into the direct sum of two submodules over this superalgebra:

$$
V=\langle v^0_m,v^2_m\rangle_{m\in\mathbb{Z}}\oplus\langle v^3_m,v^1_m\rangle_{m\in\mathbb{Z}}. \tag{5.6}
$$

Remark 5.2: We conjecture that there exists a *two*-parameter family of representations of $\hat{K}'(4)$ in the superspace spanned by 4 fields. In order to define it, instead of the superspace of functions, V^μ, one should consider the superspace of ''densities.''

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On solvable potentials related to SO(2,2)

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Scattering problems in one dimension associated with the SO(2,2) group are studied. The *S* matrices for the systems under consideration are calculated by using the theory of intertwining operators for semisimple Lie groups. The wave functions are expressed in terms of matrix elements of principal series representation of the SO(2,1) group. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The group theoretical studies of dynamical systems in nonrelativistic quantum mechanics has a long history. The first study in this direction was made by Pauli,[1] before Schrödinger's equation was published. In that pioneering work, Pauli showed that the bound-state spectrum of the quantum-mechanical nonrelativistic Coulomb problem could be obtained by studying the abstract algebra generated by angular momentum and the Runge–Lenz vector. Following that, Fock and Bargmann[2,3] have recognized that this algebra is isomorphic to the $\mathfrak{so}(4)$ Lie algebra. Moreover, it was realized that the ''accidental'' degeneracies, i.e., degeneracies not connected with geometrical SO(3) symmetries of the Hamiltonian, are due to the dynamical invariance group SO(4). Ever since dynamical invariance groups have been determined for many quantum mechanical systems. This is a situation in which the Hamiltonian H of the system belongs to the center of the enveloping algebra of some group G, i.e., $H=f(C)$, where C is the Casimir operator of dynamical symmetry group G. For example, in the Coulomb bound-state problem, $H=\alpha/2(C-1)$, where C is the second-order Casimir operator of symmetric tensor representations of SO(4).

Since the work of Zwanzinger[4] it has become clear that group theoretical methods can be successfully applied to the solution of scattering problems. In that paper Zwanzinger showed how the symmetry group SO(3.1) allows for an algebraic determination of the Coulomb *S* matrix. However, this method, which at the beginning has been developed only for Coulomb problem, cannot be generalized to other scattering problems and for this reason, the Coulomb problem was the only known example for a long time.

Important results have been obtained in this respect by the Yale group and others.[5–10] It appears that knowledge of the interrelation between dynamical algebra, which describes the scattering problem, and an Euclidean algebra, which describes the problem in the absence of interactions, allow in principle, pure algebraic calculation of *S* matrices. This technique, which is called the Euclidean connection, essentially uses the theory of group expansions or deformations.[11] However, due to the absence of a general procedure for the descriptions of such connection formulas, it is rather difficult to derive the *S* matrix using the above-mentioned method. (Note that the general expansion problem is not yet solved.)

Since knowledge of the dynamic group is sufficient to solve the bound state problems, it is quite suggestive to ask whether or not one can use information on the dynamic group directly to obtain stringent restrictions upon the structure of the scattering matrices, or even to determine it completely. The answer is in the affirmative.[12] It has been discovered that the *S* matrices for systems under consideration are related to intertwining operators between Weyl equivalent principal series representations of the dynamical group *G*. In other words, *S* matrices for systems under consideration are constrained to satisfy

$$\mathrm{SU}^{\chi}(g)=U^{\tilde{\chi}}(g)S \quad \text{for all} \quad g\in G \tag{1.1}$$

or

$$SdU^{\chi}(b)=dU^{\tilde{\chi}}(b)S \quad \text{for all} \quad b\in \mathfrak{g}, \tag{1.2}$$

where U^{χ} and $U^{\tilde{\chi}}$ are the Weyl equivalent unitary irreducible representations (UIRs) of principal series of G, while dU^{χ} and $dU^{\tilde{\chi}}$ are the corresponding representations of the algebra $\mathfrak{g}$ of G. Thus, one can in principle evaluate the S matrix from (1.1) or (1.2) without ever writing a Shrödinger equation, or wave functions, or ever mentioning the concepts of space and time.

Moreover, it follows from Eq. (1.1) or (1.2) that if the matrix of representation operator U is diagonal in some basis then the matrix of the intertwining operator is also diagonal. This fact leads to the suggestion that there might exist a class of one-dimensional potentials for which the scattering matrix is determined by diagonal elements of the intertwining operator. This is exactly what happens in the Olshanetsky–Perelomov approach[13] to one-dimensional many-body problems related to Lie algebras (where the Hamiltonians of systems are described in terms of the ''radial part'' of the Casimir operator) or in the ''potential group'' approach to scattering problems.[5–10] Thus, the number of subgroup chains provided by representation theory necessarily correspond to the number of class of quantum-mechanical systems. Therefore the problem of classification of all one-dimensional many-body systems with dynamic group G may be reduced to the more tractable problem of the enumeration of all subgroup chains of G. Moreover the well-developed theory of intertwining operators for the semisimple Lie group[14,15] led to the hope that one may determine explicitly the scattering matrices for all systems related to semisimple Lie groups.

This paper is the first of two devoted to the study of scattering problems for solvable potentials related to the SO(2.2) group. In the present paper we consider one-dimensional potential scattering of a system with a SO(2.2) ''potential group.'' [5] We hence illustrated the method in the simple case of the most degenerate representation of SO(2.2). Our other purpose here is to prepare all the necessary background for the second paper in the series, devoted to the Natanzon-type potentials. The content of the paper is arranged as follows. In Sec. II, we describe the construction of S matrices corresponding to the $\mathrm{SO(2,2)}\supset\mathrm{SO(2)}\times\mathrm{SO(2)}$, $\mathrm{SO(2,2)}\supset\mathrm{SO(2)}\times\mathrm{E(1)}$, $\mathrm{SO(2,2)}\supset\mathrm{SO(2)}\times\mathrm{SO(1,1)}$, $\mathrm{SO(2,2)}\supset\mathrm{SO(1,1)}\times\mathrm{E(1)}$, and $\mathrm{SO(2,2)}\supset\mathrm{E(1)}\times\mathrm{E(1)}$ reductions. The reason for the restriction to these reductions is that the basis functions on the symmetric space SO(2,2)/SO(2.1) are expressed in terms of matrix elements of the SO(2,1) group for all these reductions. In Sec. III we discuss a class of quantum scattering problems governed by Hamiltonian $H=-(C+1)/8$. Finally, we have included in Appendices A and B some technical of the calculation that for clarity were omitted from the main text.

II. GROUP THEORETICAL CONSTRUCTION OF THE *S* MATRIX

Let $R^{2,2}$ be a four-dimensional pseudo-Euclidean space with the bilinear form

$$[x,y]=x_1y_1+x_2y_2-x_3y_3-x_4y_4. \tag{2.1}$$

By SO(2,2) we denote the connected component of the group of linear transformation of $R^{2,2}$ preserving the form (2.1). We consider SO(2,2) as acting on $R^{2,2}$ on the right. In accordance with this we shall write the vector in the row form $x=(x_1,x_2,x_3,x_4)$

Let us denote $\{g_{ij}(\theta)\}$ $i<j$, $i,j=1,2,3,4$ the one-parameter subgroups of SO(2,2) consisting of rotations or pseudorotations in the x_i-x_j planes, that is, of transformations of the form

$$x_k'=x_k, \quad k\neq i,j, \quad x_i'=x_i\cos\theta+x_j\sin\theta, \quad x_j'=-x_i\sin\theta+x_j\cos\theta \tag{2.2}$$

or

$$x_k'=x_k, \quad k\neq i,j, \quad x_i'=x_i\cosh\theta+x_j\sinh\theta, \quad x_j'=x_i\sinh\theta+x_j\cosh\theta, \tag{2.3}$$

respectively. The matrices

$$a_{ij}=\frac{\mathrm{d}}{\mathrm{d}\theta}g_{ij}(\theta)\big|_{\theta=0},\quad i<j \tag{2.4}$$

form a basis of the Lie algebra $\mathfrak{so}(2,2)$ of the group SO(2,2). Defining

$$\begin{aligned} a_1&=(a_{13}+a_{24})/2,\quad b_1=(a_{13}-a_{24})/2,\\ a_2&=(a_{23}-a_{14})/2,\quad b_2=(a_{23}+a_{14})/2,\\ a_3&=(a_{34}-a_{12})/2,\quad b_3=-(a_{12}+a_{34})/2, \end{aligned} \tag{2.5}$$

one has

$$\begin{aligned} &[a_1,a_2]=a_3,\quad [b_1,b_2]=b_3,\\ &[a_2,a_3]=-a_1,\quad [b_2,b_3]=-b_1,\\ &[a_3,a_1]=-a_2,\quad [b_3,b_1]=-b_2. \end{aligned} \tag{2.6}$$

The generators a_i and b_i separately form a Lie algebra of SO(2,1). In other words SO(2,2) is the product group of two SO(2,1) groups, i.e., SO(2,2)=SO(2,1)×SO(2,1).

Let us note at this point that the group SO(2,1) has three subgroups SO(2), SO(1,1), and E(1) generated, for example, by a_3, a_1 and a_2+a_3, respectively, where E(1) is an Euclidean group in one dimension. It is also worth noting that each UIR of SO(1.1) is doubly degenerate in principal series of UIR of SO(2.1).

We want to deal only with single particle scattering by one-dimensional potential related to the SO(2,2) group. For this case the theory of most degenerate (or, class I) representations[16–18] of SO(2,2) is helpful.

The most degenerate representations of SO(2,2) are known to form three series: principal, supplementary, and discrete. It is also known that only the principal series of SO(2,2) describe scattering states. Consequently, the relevant unitary representations will be the principal series and we restrict the discussion to it.

The principal series of the most degenerate representation of SO(2,2) are characterized by the pair $\chi=(\rho,\epsilon)$, where ϵ is equal to 0 or 1, while $0\leqslant\rho<\infty$. The representations specified by labels $\chi=(\rho,\epsilon)$ and $\tilde{\chi}=(-\rho,\epsilon)$ are equivalent. For the sake of simplicity, we consider the representations with $\epsilon=0$, although the case $\epsilon=1$ can also be easily treated. Hence, we are interested in examining the intertwining operator of U^{χ}, $\chi=(\rho,0)$, in different subgroup bases.

The calculation of these can be performed by two different methods. If the principal series of the algebra $\mathfrak{so}(2,2)$ in some basis is known, we can get recurrence relations for the intertwining operator by applying both sides of Eq. (1.2) to the basis vectors. By solving the recurrence relations, one can find its explicit form. An alternative way employs Eq. (1.1). By realizing the principal series of SO(2,2) on suitable Hilbert spaces of some functions we can derive from Eq. (1.1) the functional relations for the kernel of the intertwining operator. This global approach, which is complimentary to the infinitesimal treatment, allows one to obtain integral representations for the matrix elements of the intertwining operator.

In Appendix A, we calculate the matrix form of the intertwining operator in the basis corresponding to the reductions with respect to SO(2)×SO(2), SO(2)×E(1), SO(2)×SO(1,1), SO(1,1)×E(1), and E(1)×E(1). As a result we come to following conclusion: The S matrices of the one-dimensional system described by $(\rho,0)$ representation of SO(2,2) in the above-mentioned subgroup basis have the following form.

(i) The SO(2,2)⊃SO(2)×SO(2) reduction. The S matrix for this class of potentials is given by

$$S=\begin{pmatrix} R(m,k) & 0 \\ 0 & R(m,k) \end{pmatrix}, \tag{2.7}$$

where

$$R(m,k)=c\,\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+k\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+k\right)}$$

with the notation as in Appendix A. The energy-dependent parameter ρ is determined by the relation between the Hamiltonian and the Casimir invariant.

(ii) The SO(2,2)⊃SO(2)×E(1) reduction. In this case

$$S=\begin{pmatrix} R(\lambda,m) & 0 \\ 0 & R(\lambda,m) \end{pmatrix}, \tag{2.8}$$

where

$$R(\lambda,m)=c\lambda^{-i\rho}\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)}.$$

(iii) The SO(2,2)⊃SO(2)×SO(1,1) reduction. Now, we have

$$S=\begin{pmatrix} R(\mu,m) & T(\mu,m) \\ T(\mu,m) & R(\mu,m) \end{pmatrix}, \tag{2.9}$$

$$R(\mu,m)=\frac{c}{\pi}\cosh\pi\mu\,\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+i\mu\right)\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}-i\mu\right)\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)},$$

$$T(\mu,m)=i\,\frac{c}{\pi}\sinh\frac{\pi\rho}{2}\,\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+i\mu\right)\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}-i\mu\right)\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)}.$$

(iv) The SO(2,2)⊃SO(1,1)×E(1) reduction. The corresponding S matrix is given by

$$S=\begin{pmatrix} R(\mu,\lambda) & T(\mu,\lambda) \\ T(\mu,\lambda) & R(\mu,\lambda) \end{pmatrix}, \tag{2.10}$$

$$R(\mu,\lambda)=\frac{c}{\pi}\lambda^{-i\rho}\cosh\pi\mu\,\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+i\mu\right)\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}-i\mu\right),$$

$$T(\mu,\lambda)=i\,\frac{c}{\pi}\lambda^{-i\rho}\sinh\pi\frac{\rho}{2}\,\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+i\mu\right)\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}-i\mu\right).$$

(v) The SO(2,2)⊃E(1)×E(1) reduction. For this class of the potentials

$$S=\begin{pmatrix} R(\lambda,\mu) & 0 \\ 0 & R(\lambda,\mu) \end{pmatrix}, \tag{2.11}$$

where $R(\lambda,\mu)=c|\lambda\mu|^{-i\rho}$.

It should be noted that the potential functions of the third and fourth classes admit a double degeneracy of the wave function for every positive value of energy. [The twofold degeneracy corresponds to the fact that each UIR of SO(1,1) is twofold degenerate in principal series of UIR of SO(2,1).] Therefore, one may construct wave packets which are partly transmitted and partly reflected by the potential. According to (2.9) and (2.10), in both cases, the reflection and transmission coefficients are

$$|R|^2=\frac{\cosh^2 \pi\mu}{\cosh^2 \pi\mu+\sinh^2 \pi\dfrac{\rho}{2}},$$

$$|T|^2=\frac{\sinh^2 \pi\dfrac{\rho}{2}}{\cosh^2 \pi\mu+\sinh^2 \pi\dfrac{\rho}{2}},$$

respectively. It is also worth nothing that the reflection coefficient $|R|^2=1$ for all potentials of first, second, and fifth classes; hence the reflection is total. This is a result of very general properties, shared by all one-dimensional Hamiltonians which have continuous nondegenerate spectrum.

III. CLASS OF POTENTIALS RELATED TO THE SO(2,2) GROUP

In this section we give a simple example of how the inverse problem can be solved. By the inverse problem we mean the determination of potentials from a given dynamical group. For the sake of simplicity, we suppose that the Hamiltonian of a quantum-mechanical system is a linear function of the Casimir operator. In this study of such a system, we can, without loss of generality, limit ourselves to the case where $H=-(C+1)/8$.

Let us consider a reducible representation of SO(2,2), which contains the irreducible subrepresentation $(\rho,0)$. For example, let $T(g)$ be a quasiregular representation of SO(2,2). This representation can be realized in the Hilbert space of square-integrable functions $f(x)$ on hyperboloid X,

$$x_1^2+x_2^2-x_3^2-x_4^2=1, \tag{3.1}$$

with an invariant measure $dx=dx_1\,dx_2\,dx_3/|x_4|$. The representation $T(g)$ is defined by

$$T(g)f(x)=f(xg). \tag{3.2}$$

The (Hermitian) infinitesimal operators $A_{ij}=-i(d/d\theta)T(g_{ij}(\theta))|_{\theta=0}$ of the representation $T(g)$ corresponding to the one-parameter subgroups $g_{ij}(\theta)$ are given by

$$\begin{aligned} A_{12}&=-i\left(x_2\frac{\partial}{\partial x_1}-x_1\frac{\partial}{\partial x_2}\right), \quad A_{23}=-i\left(x_3\frac{\partial}{\partial x_2}+x_2\frac{\partial}{\partial x_3}\right), \\ A_{13}&=-i\left(x_3\frac{\partial}{\partial x_1}-x_1\frac{\partial}{\partial x_3}\right), \quad A_{24}=-ix_4\frac{\partial}{\partial x_2}. \end{aligned} \tag{3.3}$$

Then, the Casimir operator $C=A_{12}^2+A_{34}^2-A_{13}^2-A_{14}^2-A_{23}^2-A_{24}^2$ has the form

$$C=-\frac{\partial^2}{\partial x_1^2}-\frac{\partial^2}{\partial x_2^2}-\frac{\partial^2}{\partial x_3^2}+I(I+2), \tag{3.4}$$

where $I=x_1\partial/\partial x_1+x_2\partial/\partial x_2+x_3\partial/\partial x_3$.

We now require the representation space to be irreducible. [We note that representation (3.2) is decomposed onto principal and discrete series representations.][17,19] Such a restriction is obtained if all functions are eigenfunctions of the Casimir operator

$$Cf=j(j+2)f. \tag{3.5}$$

Since we are interested only in continuous spectrum, we will put $j=-1-i\rho$.

The coordinate independent solutions to this equation are given by

$$e_{p,n}(x)=|[x,n]|^{-2-j} \tag{3.6}$$

with

$$\int\int\int_X |[x,n]|^{-1+i\rho}\overline{|[x,n']|^{-1+i\rho'}}\,\mathrm{d}x=\frac{16\pi^2}{\rho^2\tanh^2\pi\rho/2}\,\delta(\rho-\rho')\,\delta(n-n'),$$

where $x\in X$, n, $n'\in\Gamma$ and Γ is a contour on the cone $C=\{n\in R^{2,2}|n_1^2+n_2^2-n_3^2-n_4^2=0\}$ intersecting each generator. The case when Γ is the section of the cone by the Euclidean sphere of radius $\sqrt{2}$ with center at origin is described in Refs. 16 and 17. In this case Γ is the direct product of two circles of unit radius (see Appendix A).

The structure (3.3) of A_{ij} has the consequence that the two commuting SO(2,1) subgroups generated by a_i and b_i share the same Casimir operator. In fact, we have

$$C_a=C_b=\tfrac{1}{4}C,$$

where $C_a=A_1^2+A_2^2-A_3^2$, $C_b=B_1^2+B_2^2-B_3^2$ and $\dot{A}_i,B_i$ are infinitesimal operators corresponding to generators a_i,b_i, respectively. In other words, the operator C is essentially the Casimir operator of regular representation of $\mathrm{SO}(2,1)\simeq\mathrm{SL}(2,R)$. For this reason, the solution to Eq. (3.5) is related to matrix elements of $\mathrm{SL}(2,R)$. This should be no surprise because the group $\mathrm{SL}(2,R)\simeq\mathrm{SO}(2,1)$ can be realized as the hyperboloid X,

$$\mathrm{SL}(2,R)\ni g(x)=\begin{pmatrix} x_1+x_3 & x_4+x_2 \\ x_4-x_2 & x_1-x_3 \end{pmatrix},\quad x\in R^{2,2}, x_1^2+x_2^2-x_3^2-x_4^2=1. \tag{3.7}$$

We are now prepared to obtain the explicit form of Hamiltonians $H=-(C+1)/8$ for all subgroup reductions mentioned in Sec. II.

(i) The reduction $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\times\mathrm{SO}(2)$. We want to diagonalize the $\mathrm{SO}(2)\times\mathrm{SO}(2)$ subgroup. Then, the reduction conditions are

$$A_3f_{mk}^{(1)}=mf_{mk}^{(1)},\quad B_3f_{mk}^{(1)}=kf_{mk}^{(1)}.$$

The parametrization that we have seen for hyperboloid (3.1) must be such as to make A_3,B_3 particularly simple. The appropriate parametrization of $\mathrm{SL}(2,R)$ will be the Cartan parametrization

$$g=\begin{pmatrix} \cos\frac{\varphi}{2} & \sin\frac{\varphi}{2} \\ -\sin\frac{\varphi}{2} & \cos\frac{\varphi}{2} \end{pmatrix}\begin{pmatrix} e^{\alpha/2} & 0 \\ 0 & e^{-\alpha/2} \end{pmatrix}\begin{pmatrix} \cos\frac{\psi}{2} & \sin\frac{\psi}{2} \\ -\sin\frac{\psi}{2} & \cos\frac{\psi}{2} \end{pmatrix}, \tag{3.8}$$

$$0\leqslant\varphi\leqslant2\pi,\quad 0\leqslant\psi\leqslant2\pi,\quad 0<\alpha<\infty.$$

By equating the element $g(x)$ to (3.8), we get the equations relating $x_i, i=1,...,4$, to new variables φ, α, ψ,

$$x_1=\cosh\frac{\alpha}{2}\cos\frac{\psi+\varphi}{2},\quad x_3=\sinh\frac{\alpha}{2}\cos\frac{\psi-\varphi}{2},$$
$$x_2=\cosh\frac{\alpha}{2}\sin\frac{\psi+\varphi}{2},\quad x_4=\sinh\frac{\alpha}{2}\sin\frac{\psi-\varphi}{2}. \tag{3.9}$$

Then $A_3=-i(\partial/\partial\varphi)$ and $B_3=-i(\partial/\partial\psi)$ as we expected. If we compute the Casimir operator C for this parametrization, it becomes

$$\frac{1}{4}C=\frac{\partial^2}{\partial\alpha^2}+\coth\alpha\frac{\partial}{\partial\alpha}+\frac{1}{\sinh^2\alpha}\left(\frac{\partial^2}{\partial\varphi^2}-2\cosh\alpha\frac{\partial^2}{\partial\varphi\partial\psi}+\frac{\partial^2}{\partial\psi^2}\right). \tag{3.10}$$

Thus, the basis functions $f^{(1)}_{mk}$ corresponding to the considered reduction can be written as $\Phi(\alpha)e^{im\varphi}e^{in\psi}$, where $\Phi(\alpha)$ satisfies

$$4\left(-\frac{\mathrm{d}^2}{\mathrm{d}\alpha^2}-\coth\alpha\frac{\mathrm{d}}{\mathrm{d}\alpha}+\frac{m^2-2mk\cosh\alpha+k^2}{\sinh^2\alpha}\right)\Phi(\alpha)=-j(j+2)\Phi(\alpha).$$

Now we redefine the function $\Phi(\alpha)$ to absorb the weight function in the hyperboloid measure $\mathrm{d}x=\sinh\alpha\,\mathrm{d}\varphi\,\mathrm{d}\psi$, $\Phi(\alpha)=[\sinh\alpha]^{-1/2}\Psi(\alpha)$. Then this equation reduces to the Schrödinger one,

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\alpha^2}+\frac{(m-k)^2-\frac{1}{4}}{4\sinh^2\alpha/2}-\frac{(m+k)^2-\frac{1}{4}}{4\cosh^2\alpha/2}\right)\Psi(\alpha)=2E\Psi(\alpha), \tag{3.11}$$

where $E=\rho^2/8$.

Thus, the knowledge of the interwining operator in SO(2)×SO(2) basis solves the scattering problem for the Pöschl–Teller potential. Among other, things the group structure provides the integral representation of the basis function

$$f^{(1)}_{mk}(x)=\varkappa\int_0^{2\pi}\int_0^{2\pi}|[x,n]|^{-2-j}\exp(im\varphi'+ik\psi')\mathrm{d}\varphi'\,\mathrm{d}\psi', \tag{3.12}$$

where x and n are given by Eqs. (3.9) and (A3), respectively. The normalization constant $\varkappa$ is chosen as in Appendix A, i.e.,

$$\varkappa=2^j\pi^{-1}\Gamma^2\left(\frac{2+j}{2}\right)\Gamma^{-2}\left(\frac{-1-j}{2}\right).$$

The explicit expression for $f^{(1)}_{mk}$ is given in Appendix A. As a result, for the scattering solutions of the Schrödinger equation with the Poschl–Teller potential we have

$$\Phi(\alpha)=\frac{2^{j+2}\pi^{1/2}\Gamma\left(\frac{2+j}{2}\right)\Gamma\left(\frac{j}{2}+m+1\right)}{\Gamma\left(\frac{-1-j}{2}\right)\Gamma\left(-\frac{j}{2}+m\right)}(\sinh\alpha)^{1/2}\mathfrak{P}^{(-2-j)/2}_{km}(\cosh\alpha), \tag{3.13}$$

where $\mathfrak{P}^j_{mn}(z)$ is the generalized Legendre function (of the first kind) as defined by Vilenkin.[20]

(ii) The reduction SO(2,2)⊃SO(2)×E(1). It is easy to see that geometrically the Iwasawa decomposition of SL(2,R),

$$g=\begin{pmatrix} \cos\varphi/2 & \sin\varphi/2 \\ -\sin\varphi/2 & \cos\varphi/2 \end{pmatrix}\begin{pmatrix} e^{\alpha/2} & 0 \\ 0 & e^{-\alpha/2} \end{pmatrix}\begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix}, \tag{3.14}$$

$$0<\alpha<\infty, \quad 0<\varphi<2\pi, \quad -\infty<t<\infty,$$

is merely telling us that the appropriate parametrization of hyperboloid (3.1) is given by

$$x_1=\cosh\frac{\alpha}{2}\cos\frac{\varphi}{2}-\frac{t}{2}e^{\alpha/2}\sin\frac{\varphi}{2}, \quad x_3=\sinh\frac{\alpha}{2}\cos\frac{\varphi}{2}+\frac{t}{2}e^{\alpha/2}\sin\frac{\varphi}{2},$$

$$x_2=\cosh\frac{\alpha}{2}\sin\frac{\varphi}{2}+\frac{t}{2}e^{\alpha/2}\cos\frac{\varphi}{2}, \quad x_4=-\sinh\frac{\alpha}{2}\sin\frac{\varphi}{2}+\frac{t}{2}e^{\alpha/2}\cos\frac{\varphi}{2}$$

with $\mathrm{d}x=\frac{1}{8}e^{\alpha}\mathrm{d}\alpha\,\mathrm{d}\varphi\,\mathrm{d}t$. Then $A_3=i(\partial/\partial\varphi)$, $B_2+B_3=-i(\partial/\partial t)$, and

$$C=4\frac{d\partial^2}{\partial\alpha^2}+4\frac{\partial}{\partial\alpha}-8e^{-\alpha}\frac{\partial^2}{\partial\varphi\partial t}+4e^{-2\alpha}\frac{\partial^2}{\partial t^2}. \tag{3.15}$$

The basis functions in this reduction are the eigenfunctions of the set of operators C, A_3, and B_2+B_3, with

$$A_3 f^{(2)}_{m\lambda}=m f^{(2)}_{m\lambda} \quad (B_2+B_3)f^{(2)}_{m\lambda}=\lambda f^{(2)}_{m\lambda}.$$

Substitution of $f^{(2)}_{m\lambda}(x)$ by $e^{-\alpha/2}\Psi(\alpha)\exp(im\varphi+i\lambda t)$ transforms the Casimir equation into the Schrödinger equation

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\alpha^2}+\lambda^2e^{-2\alpha}-2m\lambda e^{-\alpha}\right)\Psi(\alpha)=2E\Psi(\alpha) \tag{3.16}$$

with $E=\rho^2/8$. Thus, the S matrix for the scattering on the Morse potential is given by (2.8), where $\rho=2\sqrt{2E}$. Finally, for the scattering solutions of the Schrödinger equation we obtain

$$\Psi(\alpha)=\begin{cases} \dfrac{2^{1+j}\Gamma\left(\dfrac{j}{2}-m+1\right)}{\Gamma(-1-j)}(2\lambda)^{1/2}\exp(\alpha/2)W_{m,-(1+j)/2}(2e^{-\alpha}\lambda) & \text{if } \lambda>0 \\ \dfrac{2^{1+j}\Gamma\left(\dfrac{j}{2}+m+1\right)}{\Gamma(-1-j)}(-2\lambda)^{1/2}\exp(\alpha/2)W_{-m,-(1+j)/2}(-2e^{-\alpha}\lambda) & \text{if } \lambda<0 \end{cases}.$$

(iii) The reduction $\mathrm{SO}(2,2)\supset\mathrm{SO}(2)\times\mathrm{SO}(1,1)$. The basis functions corresponding to the considered reduction are the eigenfunctions of C, A_1, and B_3 with

$$A_1 f^{(3)}_{m\mu\tau}=\mu f^{(3)}_{m\mu\tau}, \quad B_3 f^{(3)}_{m\mu\tau}=m f^{(3)}_{m\mu\tau},$$

where $\tau=\pm1$ is the multiplicity label. Since the operators B_3 and A_1 generate rotations and pseudorotations, respectively, the appropriate parametrization for $\mathrm{SL}(2,R)$ in these circumstances is

$$g=\begin{pmatrix} e^{\beta/2} & 0 \\ 0 & e^{-\beta/2} \end{pmatrix}\begin{pmatrix} \cosh\dfrac{\alpha}{2} & \sinh\dfrac{\alpha}{2} \\ \sinh\dfrac{\alpha}{2} & \cosh\dfrac{\alpha}{2} \end{pmatrix}\begin{pmatrix} \cos\dfrac{\varphi}{2} & \sin\dfrac{\varphi}{2} \\ -\sin\dfrac{\varphi}{2} & \cos\dfrac{\varphi}{2} \end{pmatrix},$$

$$-\infty<\beta<\infty, \quad -\infty<\alpha<\infty, \quad -2\pi<\beta<2\pi.$$

According to this, we choose the following coordinate systems on the hyperboloid:

$$\begin{aligned}
x_1&=\cosh\frac{\alpha}{2}\cosh\frac{\beta}{2}\cos\frac{\varphi}{2}-\sinh\frac{\alpha}{2}\sinh\frac{\beta}{2}\sin\frac{\varphi}{2},\\
x_2&=\sinh\frac{\alpha}{2}\sinh\frac{\beta}{2}\cos\frac{\varphi}{2}+\cosh\frac{\alpha}{2}\cosh\frac{\beta}{2}\sin\frac{\varphi}{2},\\
x_3&=\cosh\frac{\alpha}{2}\sinh\frac{\beta}{2}\cos\frac{\varphi}{2}-\sinh\frac{\alpha}{2}\cosh\frac{\beta}{2}\sin\frac{\varphi}{2},\\
x_4&=\sinh\frac{\alpha}{2}\cosh\frac{\beta}{2}\cos\frac{\varphi}{2}+\cosh\frac{\alpha}{2}\sinh\frac{\beta}{2}\sin\frac{\varphi}{2}
\end{aligned} \tag{3.17}$$

with $\mathrm{d}x=\frac{1}{8}\cosh\alpha\mathrm{d}\alpha\,\mathrm{d}\beta\,\mathrm{d}\varphi$. Then $A_1=-i(\partial/\partial\beta)$, $B_3=-i(\partial/\partial\varphi)$, and

$$C=4\frac{\partial^2}{\partial\alpha^2}+4\frac{\sinh\alpha}{\cosh\alpha}\frac{\partial}{\partial\alpha}-8\frac{\sinh\alpha}{\cosh^2\alpha}\frac{\partial^2}{\partial\beta\partial\varphi}+\frac{1}{\cosh^2\alpha}\left(\frac{\partial^2}{\partial\beta^2}-\frac{\partial^2}{\partial\varphi^2}\right). \tag{3.18}$$

Now, the Casimir equation in these coordinates after substitution of the $f^{(3)}_{m\mu\tau}(x)$ by $(\cosh\alpha)^{-1/2}\Psi_\tau(\alpha)e^{i\mu\beta+im\varphi}$ is transformed into the Schrödinger equation

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\alpha^2}+\frac{\mu^2-m^2-2m\mu\sinh\alpha}{\cosh^2\alpha}\right)\Psi_\tau(\alpha)=2E\Psi_\tau(\alpha) \tag{3.19}$$

with $E=\rho^2/8$.

Thus, knowing the intertwining operator for the SO(2,2) group in the SO(2)×SO(1.1) basis solves the scattering problem for the Pöschl–Teller type potential

$$2V(\alpha)=\frac{\mu^2-m^2-2m\mu\sinh\alpha}{\cosh^2\alpha}. \tag{3.20}$$

Moreover, we have (see Appendix B)

$$\begin{aligned}
\Psi_\tau(\alpha)=&\frac{\Gamma\left(1+\frac{j}{2}+m\right)\Gamma\left(1+\frac{j}{2}-i\tau\mu\right)\exp[i\pi(m+1)(\tau+1)/2]}{\pi\Gamma(-1-j)}\\
&\times(\cosh\alpha)^{1/2}\mathfrak{Q}^{j/2}_{i\tau\mu,m}(i\tau\sinh\alpha),
\end{aligned} \tag{3.21}$$

where $\mathfrak{Q}^j_{\mu\nu}(z)$ is the generalized Legendre function of the second kind as defined by Azimov.[21]

The two functions Ψ_{+1} and Ψ_{-1} are finite everywhere, both are admissible solutions. The first of these represents a wave incident from the left. Reflection occurs at the potential barrier (3.20), but there is also transmission to the right. A similar interpretation of Ψ_{-1} can be made. It represents a wave incident from the right, and transmitted through the barrier to the left. According to (2.9), the reflection and transmission coefficients are

$$|R|^2=\frac{\cosh^2 \pi\mu}{\cosh^2 \pi\mu+\sinh^2 \pi\sqrt{2E}},$$
$$|T|^2=\frac{\sinh^2 \pi\sqrt{2E}}{\cosh^2 \pi\mu+\sinh^2 \pi\sqrt{2E}}, \tag{3.22}$$

respectively.

(iv) The reduction $SO(2,2)\supset SO(1,1)\times E(1)$. The reduction conditions are

$$A_2 f^{(4)}_{\lambda\mu\tau}=\mu f^{(4)}_{\lambda\mu\tau}, \quad (B_2+B_3) f^{(4)}_{\lambda\mu\tau}=\lambda f^{(4)}_{\lambda\mu\tau},$$

where $\tau=\pm 1$ is the multiplicity label. The corresponding parametrization of $SL(2,R)$ is then of the form

$$g=\begin{pmatrix} \cosh\frac{\beta}{2} & \sinh\frac{\beta}{2} \\ \sinh\frac{\beta}{2} & \cosh\frac{\beta}{2} \end{pmatrix} \begin{pmatrix} e^{\alpha/2} & 0 \\ 0 & e^{-\alpha/2} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^{\sigma} \begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix},$$

where $\sigma=0,1$. Now, on the basis of the above-mentioned parametrization for $SL(2,R)$, we have divided the hyperboloid X into two subregions. So then the passage from x_i to new variables β,α,t gives the following:

$$X^+: \quad (\sigma=0),$$

$$x_1=\cosh\frac{\alpha}{2}\cosh\frac{\beta}{2}+\frac{t}{2}e^{\alpha/2}\sinh\frac{\beta}{2}, \quad x_3=\sinh\frac{\alpha}{2}\cosh\frac{\beta}{2}-\frac{t}{2}e^{\alpha/2}\sinh\frac{\beta}{2},$$

$$x_2=-\sinh\frac{\alpha}{2}\sinh\frac{\beta}{2}+\frac{t}{2}e^{\alpha/2}\cosh\frac{\beta}{2}, \quad x_4=\cosh\frac{\alpha}{2}\sinh\frac{\beta}{2}+\frac{t}{2}e^{\alpha/2}\cosh\frac{\beta}{2}$$

with $dx=\frac{1}{8}e^{\alpha}d\alpha\, d\beta\, dt$ and

$$X^-: \quad (\sigma=1),$$

$$x_1=\sinh\frac{\alpha}{2}\sinh\frac{\beta}{2}-\frac{t}{2}e^{-\alpha/2}\cosh\frac{\beta}{2}, \quad x_3=-\cosh\frac{\alpha}{2}\sinh\frac{\beta}{2}+\frac{t}{2}e^{-\alpha/2}\cosh\frac{\beta}{2},$$

$$x_2=\cosh\frac{\alpha}{2}\cosh\frac{\beta}{2}-\frac{t}{2}e^{-\alpha/2}\sinh\frac{\beta}{2}, \quad x_4=\sinh\frac{\alpha}{2}\cosh\frac{\beta}{2}-\frac{t}{2}e^{-\alpha/2}\sinh\frac{\beta}{2}$$

with $dx=\frac{1}{8}e^{\alpha}d\alpha\, d\beta\, dt$.

Now the expressions for A_2 and B_2+B_3 are uniformly given in both regions by $A_2=-i(\partial/\partial\beta)$, $B_2+B_3=-i(\partial/\partial t)$ while C is given as

$$C=+4\frac{\partial^2}{\partial\alpha^2}+4\frac{\partial}{\partial\alpha}+8e^{-\alpha}\frac{\partial^2}{\partial\beta\partial t}-4e^{-2\alpha}\frac{\partial^2}{\partial t^2} \tag{3.23}$$

and

$$C=4\frac{\partial^2}{\partial\alpha^2}-4\frac{\partial}{\partial\alpha}-8e^{\alpha}\frac{\partial^2}{\partial\beta\partial t}-4e^{2\alpha}\frac{\partial^2}{\partial t^2} \tag{3.24}$$

in X^+ and X^-, respectively. The potentials gained for $\mathrm{SO}(2,2)\supset\mathrm{SO}(1,1)\times\mathrm{E}(1)$ reduction is

$$2V(\alpha)=\begin{cases}\lambda^2 e^{-2\alpha}-2\lambda\mu e^{-\alpha} & \text{if } \alpha>0\\ \lambda^2 e^{2\alpha}+2\lambda\mu e^{\alpha} & \text{if } \alpha<0\end{cases}. \tag{3.25}$$

Hence formula (2.50) with $\rho=2\sqrt{2E}$ is determined as the S matrix for this potential.

(v) The reduction $\mathrm{SO}(2,2)\supset\mathrm{E}(1)\times\mathrm{E}(1)$. The basis functions in this reduction will be the eigenfunctions of C, A_2+A_3 and B_2+B_3 with

$$(A_2+A_3)f^{(5)}_{\lambda\mu}=\mu f^{(5)}_{\lambda\mu},\quad (B_2+B_3)f^{(5)}_{\lambda\mu}=\lambda f^{(5)}_{\lambda\mu}.$$

Therefore, we choose Gauss parametrization for $\mathrm{SL}(2,R)$

$$g=\begin{pmatrix}1 & 0\\ t & 1\end{pmatrix}\begin{pmatrix}e^{\alpha/2} & 0\\ 0 & e^{-\alpha/2}\end{pmatrix}\begin{pmatrix}1 & y\\ 0 & 1\end{pmatrix},$$

$$-\infty<t<\infty,\quad 0<\alpha<\infty,\quad -\infty<y<\infty.$$

According to this, one has to choose the following coordinate system on hyperboloid X:

$$x_1=\cosh\frac{\alpha}{2}+\frac{yt}{2}e^{\alpha/2},\quad x_3=\sinh\frac{\alpha}{2}-\frac{yt}{2}e^{\alpha/2},$$

$$x_2=\tfrac{1}{2}e^{\alpha/2}(y-t),\quad x_4=\tfrac{1}{2}e^{\alpha/2}(y+t)$$

with $dx=\frac{1}{4}e^{\alpha}\mathrm{d}\alpha\,\mathrm{d}t\,\mathrm{d}y$. Then $A_2+A_3=-i(\partial/\partial t)$ and $B_2+B_3=-i(\partial/\partial y)$. The Casimir operator in these coordinates is

$$C=4\left(\frac{\partial^2}{\partial\alpha^2}+\frac{\partial}{\partial\alpha}+e^{-\alpha}\frac{\partial^2}{\partial t\,\partial y}\right). \tag{3.26}$$

By arguments very similar to those used to obtain (3.11) we can show that the Casimir invariant is related to the group Hamiltonian $H=(-\mathrm{d}^2/\mathrm{d}\alpha^2+\mu\lambda e^{-\alpha})/2$ by $H=-(C+1)/8$. Therefore, formula (2.11) at $\rho=2\sqrt{2E}$ determines the scattering matrices for the system with Toda potential $V=\mu\lambda e^{-\alpha}/2$. Moreover, one has

$$\Psi(\alpha)=\frac{2^{-1-j}}{\Gamma\left(\dfrac{-1-j}{2}\right)}(\lambda\mu)^{(i+j)/2}K_{-1-j}(e^{-\alpha/2}\sqrt{\lambda\mu}),\quad \text{if } \lambda\mu>0, \tag{3.27}$$

where $K_j(z)$ is the modified Bessel function of the third kind.

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APPENDIX A: THE INTERTWINING OPERATORS OF SO(2,2)

The principal series of the most degenerate representation of SO(2,2) is characterized by the pair $\chi=(\rho,\epsilon)$ where ϵ is equal to 0 or 1, while $0\leqslant\rho<\infty$ can be realized in the space of infinitely differentiable functions $f(\zeta)$ on the cone $[\zeta,\zeta]=0$, homogeneous of degree $j=-1-i\rho$ and with parity ϵ,

$$f(t\zeta)=|t|^j\,\mathrm{sign}^{\epsilon}t\,f(\zeta). \tag{A1}$$

A representation operator U^χ of the group SO(2,2) is defined by

$$U^\chi(g)f(\zeta)=f(\zeta g). \tag{A2}$$

For the purposes of this paper, we are interested in examining the interwining operator of $U^\chi, \chi=(\rho,0)$, in different bases.

Generally we may choose a large number of different coordinate systems on the cone. The different choices of separable orthogonal coordinate systems lead to different subgroup reductions.

(i) The $SO(2,2)\supset SO(2)\times SO(2)$ reduction. This chain of group reduction corresponds to an introduction of spherical coordinates on the cone, so that

$$\zeta=\omega n, \quad n=\left(\cos\frac{\psi+\varphi}{2},\ \sin\frac{\psi+\varphi}{2},\ \cos\frac{\psi-\varphi}{2},\ \sin\frac{\psi-\varphi}{2}\right), \tag{A3}$$

$$0\leqslant\omega<\infty, \quad 0<\psi\leqslant 2\pi, \quad 0<\varphi\leqslant 2\pi.$$

Indeed, in these coordinates the infinitesimal operators A_3 and B_3 of the representation (A2) are diagonal

$$A_3=-i\frac{\partial}{\partial\varphi}, \quad B_3=-i\frac{\partial}{\partial\psi}. \tag{A4}$$

Here and in the following infinitesimal operators corresponding to generators a_i, b_i are denoted by A_i, B_i respectively.

Due to homogeneity condition (A1) we obtain the following realization of U^χ:

$$U^\chi(g)f(n)=\left(\frac{\omega}{\omega_g}\right)^j f(n_g), \tag{A5}$$

where ω_g and n_g are determined from the parametrization (A3) of $\zeta_g=\zeta g$. Consequently, the representation $U^\chi, \chi=(\rho,0)$ of SO(2,2) can be realized on the Hilbert space $L^2(S^1\times S^1)$ of even functions $f(n)$ on the direct product of two circles $S^1\times S^1$, with inner product

$$(f,f')=\frac{1}{(2\pi)^2}\int_{S^1\times S^1}\int \overline{f(n)}f'(n)\mathrm{d}n, \tag{A6}$$

where $\mathrm{d}n=\mathrm{d}\varphi\,\mathrm{d}\psi$ is the invariant measure on $S^1\times S^1$. The intertwining operator A between the representations U^χ and $U^{\tilde\chi}$ is defined by

$$(Af)(n)=\int_{S^1\times S^1}\int K(n,n')f(n')\mathrm{d}n' \tag{A7}$$

with

$$AU^\chi(g)=U^{\tilde\chi}(g)A. \tag{A8}$$

Thus, Eq. (A8) will serve to fix the dependence of the kernel $K(n,n')$ on n and n'. Equality (A8) implies that

$$(AU^\chi(g)f)(n)=(U^{\tilde\chi}(g)Af)(n). \tag{A9}$$

So the kernel $K(n,n')$ is constrained to satisfy the functional equation

$$K(n_g,n'_g)=\left(\frac{\omega_g}{\omega}\right)^{2+j}\left(\frac{\omega'_g}{\omega}\right)^{2+j}K(n,n'). \tag{A10}$$

The kernel K is, up to a constant $\varkappa(j)$ uniquely determined and is given by

$$K(n,n')=\varkappa(j)|[n,n']|^{-2-j}. \tag{A11}$$

The verification of Eq. (A11) is based on the relation

$$[n_g,n'_g]=\left(\frac{\omega_g}{\omega}\right)^{-1}\left(\frac{\omega'_g}{\omega}\right)^{-1}[n,n'], \tag{A12}$$

which is an obvious consequence of the relation $[\zeta g,\zeta' g]=[\zeta,\zeta']$ where $[.,.]$ is defined by (2.1). The module of constant $\varkappa$ is fixed by the normalization, which gives

$$|\varkappa|^2=\pi^{-2}2^{-4}\rho^2\tan^2(\pi\rho/2). \tag{A13}$$

Therefore, we put

$$\varkappa=\frac{2^j}{\pi}\frac{\Gamma^2\left(\frac{2+j}{2}\right)}{\Gamma^2\left(\frac{-1-j}{2}\right)}c, \tag{A14}$$

where c is the phase factor. Thus we obtain

$$Af(\varphi,\psi)=\varkappa\int_0^{2\pi}\int_0^{2\pi}\left|\sin\frac{\varphi-\varphi'}{2}\sin\frac{\psi-\psi'}{2}\right|^{-2-j}f(\varphi',\psi')\mathrm{d}\varphi'\,\mathrm{d}\psi. \tag{A15}$$

For the sake of brevity the value of function f at n is denoted by $f(\varphi,\psi)$. Taking into account the fact that the function $|mn\rangle=\exp(im\varphi+ik\psi)$ forms SO(2)×SO(2) bases in $L^2(S^1\times S^1)$, we have

$$\langle m'k'|A|mk\rangle=\delta_{mm'}\delta_{kk'}S(m,k), \tag{A16}$$

where

$$\begin{aligned}S(m,k)&=\varkappa\int_0^{2\pi}\int_0^{2\pi}\left|\sin\frac{\varphi}{2}\sin\frac{\psi}{2}\right|^{-2-j}\exp(im\varphi+ik\psi)\mathrm{d}\varphi\,\mathrm{d}\psi\\&=c\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+k\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+k\right)}.\end{aligned} \tag{A17}$$

(ii) The SO(2,2)⊃SO(2)×E(1) reduction. Since A_3 and B_2+B_3 are sought to be diagonal, we introduce new coordinates in cone as follows $\zeta=\omega n,\ \omega>0$, where now

$$n=\left(\cos\frac{\varphi}{2}-t\sin\frac{\varphi}{2},\sin\frac{\varphi}{2}+t\cos\frac{\varphi}{2},\cos\frac{\varphi}{2}+t\sin\frac{\varphi}{2},-\sin\frac{\varphi}{2}+t\cos\frac{\varphi}{2}\right), \tag{A18}$$

$$0<\varphi\leqslant 2\pi,\quad -\infty<t<\infty.$$

Then the operators A_3 *and* B_2+B_3 have the forms

$$A_3=-i\frac{\partial}{\partial\varphi},\quad B_2+B_3=-i\frac{\partial}{\partial t}. \tag{A19}$$

The intertwining operator A in this realization is given by

$$Af(\varphi,t)=\varkappa\int_0^{2\pi}\int_{-\infty}^{+\infty}\left|(t-t')\sin\frac{\varphi-\varphi'}{2}\right|^{-2-j}f(\varphi',t')\mathrm{d}\varphi'\,\mathrm{d}t', \tag{A20}$$

where $f(\varphi,t)\equiv f(n)$. Taking into account that $|m\lambda\rangle=\exp(im\varphi+i\lambda t)$, we have

$$\langle m'\lambda'|A|m\lambda\rangle=\delta_{mm'}\delta(\lambda-\lambda')S(m,\lambda), \tag{A21}$$

where

$$S(m,\lambda)=c|\lambda|^{-i\rho}\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)}. \tag{A22}$$

(iii) The $SO(2,2)\supset SO(2)\times SO(1,1)$ reduction. This case is somewhat more complicated than the previous one. We find that the parametrization $\zeta=\omega n$, $n>0$ covers only with two choices of n,

$$n^\tau=\Big(\cosh\frac{\beta}{2}\cos\frac{\varphi}{2}-\tau\sinh\frac{\beta}{2}\sin\frac{\varphi}{2},\tau\sinh\frac{\beta}{2}\cos\frac{\varphi}{2}+\cosh\frac{\beta}{2}\sin\frac{\varphi}{2},$$
$$\sinh\frac{\beta}{2}\cos\frac{\varphi}{2}-\tau\cosh\frac{\beta}{2}\sin\frac{\varphi}{2},\tau\cosh\frac{\beta}{2}\cos\frac{\varphi}{2}+\sinh\frac{\beta}{2}\sin\frac{\varphi}{2}\Big), \tag{A23}$$

where $\tau=\pm1$, $-\infty<\beta<\infty$, $0<\varphi\leqslant2\pi$. Observe that the operators A_1 and B_3 are diagonal,

$$A_1=-i\frac{\partial}{\partial\beta},\quad B_3=-i\frac{\partial}{\partial\varphi}. \tag{A24}$$

Then, a function $f(x)$ on the cone has to be thought of as a pair, expressed by $f(x)=\{f(\omega n^+),f(\omega n^-)\}$, and we have

$$Af^\tau(\beta,\varphi)=\varkappa\sum_{\tau'=\pm1}\int_0^{2\pi}\int_{-\infty}^{+\infty}|[1-\tau\tau'\cos(\varphi-\varphi')]$$
$$\times[1-\tau\tau' ch(\beta-\beta')]|^{-2-j}f(\beta,\varphi)\mathrm{d}\varphi'\,\mathrm{d}\beta', \tag{A25}$$

where $f^\tau(\beta,\varphi)\equiv f(n^\tau)$. This then gives the integral representation of the matrix elements of S in the $SO(2)\times SO_0(1,1)$ basis. Taking into account that

$$|m\mu+\rangle=\begin{pmatrix}1\\0\end{pmatrix}\exp(im\varphi+i\mu\beta),\quad |m\mu+\rangle=\begin{pmatrix}0\\1\end{pmatrix}\exp(im\varphi+i\mu\beta), \tag{A26}$$

we have

$$\langle m'\mu'\tau'|A|m\mu\tau\rangle=\delta(\mu-\mu')\delta_{mm'}S_{\tau\tau'}(\mu,m), \tag{A27}$$

where

$$S_{++}=S_{+-}=\frac{c}{\pi}\cos\pi\mu\,\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+i\mu\right)\Gamma\left(\frac{1}{2}-i\frac{\rho}{2}-i\mu\right)\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)},$$

$$S_{-+}=S_{+-}=i\frac{c}{\pi}\sinh\pi\frac{\rho}{2}\,\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+i\mu\right)\Gamma\left(\frac{1}{2}-i\frac{\rho}{2}-i\mu\right)\frac{\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+m\right)}{\Gamma\left(\frac{1}{2}+\frac{i\rho}{2}+m\right)}.$$

(iv) The $SO(2,2)\supset SO(1,1)\times E(1)$ reduction. This subgroup reduction corresponds to a coordinate system on the cone, in which $\zeta=\omega n^{\tau},\omega>0,\tau=\pm1$, where

$$n^{-}=\left(\cosh\frac{\beta}{2}+t\sinh\frac{\beta}{2},-\sinh\frac{\beta}{2}+t\cosh\frac{\beta}{2},\cosh\frac{\beta}{2}-t\sinh\frac{\beta}{2},\sinh\frac{\beta}{2}+t\cosh\frac{\beta}{2}\right) \quad \text{(A28)}$$

and

$$n^{+}=\left(-\sinh\frac{\beta}{2}-t\cosh\frac{\beta}{2},\cosh\frac{\beta}{2}-t\sinh\frac{\beta}{2},-\sinh\frac{\beta}{2}+t\cosh\frac{\beta}{2},-\cosh\frac{\beta}{2}-t\sinh\frac{\beta}{2}\right) \quad \text{(A29)}$$

with $-\infty<\beta<\infty$, $-\infty<t<\infty$. Observe that, in this case, operators A_2 and B_2+B_3 are diagonal

$$A_2=-i\frac{\partial}{\partial\beta},\quad B_2+B_3=-i\frac{\partial}{\partial t}. \quad \text{(A30)}$$

Thus we obtain

$$Af^{\tau}(\beta,t)=\varkappa\sum_{\tau'=\pm1}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}|[\cosh(\beta-\beta')-\tau\tau'](t-t')|^{-2-j}f^{\tau}(\beta',t')\mathrm{d}\beta'\,\mathrm{d}t', \quad \text{(A31)}$$

where we have taken $f^{\tau}(\beta,t)=f(n^{\tau})$ for n^{τ} given by (A28) and (A29). This then gives the integral representation of the matrix element of A in the $SO_0(1,1)\times E(1)$ basis. As a result

$$\langle\lambda'\mu'\tau'|A|\lambda\mu\tau\rangle=\delta(\mu-\mu')\,\delta(\lambda-\lambda')S_{\tau\tau'}(\mu,\lambda), \quad \text{(A32)}$$

where

$$S_{++}=S_{--}=\frac{c}{\pi}|\lambda|^{-i\rho}\cosh\pi\mu\,\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+i\mu\right)\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}-i\mu\right),$$

$$S_{-+}=S_{+-}=i\frac{c}{\pi}|\lambda|^{-i\rho}\sinh\pi\frac{\rho}{2}\,\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}+i\mu\right)\Gamma\left(\frac{1}{2}-\frac{i\rho}{2}-i\mu\right).$$

(v) The $SO(2,2)\supset E(1)\times E(1)$ reduction. Let us now introduce coordinates on the cone by putting

$$\zeta=\omega n,\quad n=(1+yt,y-t,1-yt,y+t),$$

where $\omega>0,-\infty<t<\infty,-\infty<y<\infty$. Clearly we have diagonalized the operators A_2+A_3 and B_2+B_3:

$$A_2+A_3=-i\frac{\partial}{\partial t},\quad B_2+B_3=-i\frac{\partial}{\partial y}. \tag{A33}$$

In this realization the intertwining operator A is given by

$$Af(t,y)=\varkappa\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}|(t-t')(y-y')|^{-2-j}f(t',y')\mathrm{d}t'\,\mathrm{d}y'. \tag{A34}$$

Therefore, the matrix element of A in the E(1)×E(1) basis $|\mu,\lambda\rangle$ is given by

$$\langle\mu'\lambda'|A|\mu\lambda\rangle=\delta(\mu-\mu')\,\delta(\lambda-\lambda')S(\mu,\lambda), \tag{A35}$$

where $S(\mu,\lambda)=c(\mu\lambda)^{-i\rho},\ \mu\lambda>0$.

APPENDIX B: BASIS FUNCTIONS ON THE HYPERBOLOID *X*

In this section we calculate basis functions corresponding to the reduction considered in Sec. III.

(i) The SO(2,2)⊃SO(2)×SO(2) reduction. The basis functions in this reduction are defined as (3.12)

$$f^{(1)}_{mk}(x)=\varkappa\int_0^{2\pi}\int_0^{2\pi}\left|\cosh\frac{\alpha}{2}\cos\frac{\psi'-\psi+\varphi'-\varphi}{2}-\sinh\frac{\alpha}{2}\cos\frac{\psi'-\psi-\varphi'+\varphi}{2}\right|^{-2-j}$$
$$\times\exp(im\varphi'+ik\psi')\mathrm{d}\psi'\,\mathrm{d}\varphi'. \tag{B1}$$

For the explicit calculation we rewrite (B1) in the following form:

$$f^{(1)}_{mk}(x)=\varkappa\exp(im\varphi+ik\psi)\int_0^{2\pi}\int_0^{2\pi}(\cosh\alpha-\sinh\alpha\cos\psi')^{-(2+j)/2}\left|\cos\left(\frac{\varphi'+\varphi_0}{2}\right)\right|^{-2-j}$$
$$\times\exp(im\varphi'+ik\psi')\mathrm{d}\psi'\,\mathrm{d}\varphi', \tag{B2}$$

where

$$\cos\varphi_0=\frac{\cosh\alpha\cos\psi'-\sinh\alpha}{\cosh\alpha-\sinh\alpha\cos\psi'},\quad \sin\varphi_0=\frac{\sin\psi'}{\cosh\alpha-\sinh\alpha\cos\psi'}.$$

After integration over the angle φ' expression (B2) reduces to the well-known integral representation for the matrix elements of the SO(2,1) group in the SO(2) basis.[20] As a result we find

$$f^{(1)}_{mk}(x)=\frac{2^{j+2}\pi^{1/2}\Gamma\left(\frac{2+j}{2}\right)\Gamma\left(\frac{j}{2}+m+1\right)}{\Gamma\left(\frac{-1-j}{2}\right)\Gamma\left(\frac{-j}{2}+m\right)}\exp(im\varphi+ik\psi)\mathfrak{P}^{-(2+j)/2}_{k,m}(\cosh\alpha), \tag{B3}$$

where $\mathfrak{P}^{j}_{mn}(z)$ is the generalized Legendre function as defined by Vilenkin.[20]

(ii) SO(2,2)⊃SO(2)×E(1). The basis functions in this reduction are defined as

$$f^{(2)}_{m\lambda}(x)=\varkappa\int_0^{2\pi}\int_{-\infty}^{+\infty}\left|e^{-\alpha/2}\cos\frac{\varphi'-\varphi}{2}-e^{-\alpha/2}(t'-t)\sin\frac{\varphi'-\varphi}{2}\right|^{-2-j}e^{im\varphi'+i\lambda t'}\mathrm{d}\varphi'\,\mathrm{d}t'. \tag{B4}$$

The explicit calculation is achieved by writing (B4) in the form

$$f^{(2)}_{m\lambda}(x)=\varkappa\exp(im\varphi+i\lambda t)\int_0^{2\pi}\int_{-\infty}^{+\infty}(e^{-\alpha}+e^{\alpha}t'^2)^{-(2+j)/2}\left|\cos\frac{\varphi'-\varphi_0}{2}\right|^{-2-j}$$
$$\times\exp(im\varphi'+i\lambda t')\mathrm{d}\varphi'\,\mathrm{d}t', \tag{B5}$$

where

$$\cos\varphi_0=\frac{e^{-\alpha}-e^{\alpha}t'^2}{e^{-\alpha}+e^{\alpha}t'^2},\quad \sin\varphi_0=\frac{2t'}{e^{-\alpha}+e^{\alpha}t'^2}.$$

We then have that

$$f^{(2)}_{m\lambda}(x)=\begin{cases}\dfrac{2^{1+j}\Gamma\left(\dfrac{j}{2}-m+1\right)}{\Gamma(-1-j)}(2\lambda)^{j/2}\exp(im\varphi+i\lambda t)W_{m,-(1+j)/2}(2e^{-\alpha}\lambda) & \text{if } \lambda>0\\ \dfrac{-2^{1+j}\Gamma\left(\dfrac{j}{2}+m+1\right)}{\Gamma(-1-j)}(-2\lambda)^{j/2}\exp(im\varphi+i\lambda t)W_{-m,-(1+j)/2}(-2e^{-\alpha}\lambda) & \text{if } \lambda<0,\end{cases} \tag{B6}$$

where $W_{\mu\nu}(z)$ is the Whittaker function.[22] Furthermore we can check that the basis function $f^{(2)}_{m\lambda}$ is indeed related to the SO(2)−E(1) mixed basis matrix elements of the principal series representation of SO(2,1).[23]

(iii) SO(2,2)⊃SO(2)×SO(1,1). The basis function $f^{(3)}_{m\mu\tau}$ may be calculated from the formula

$$f^{(3)}_{m\mu\tau}(x)=\varkappa\int_0^{2\pi}\int_{-\infty}^{+\infty}\left|e^{-\alpha\tau/2}\cosh\frac{\beta'-\beta}{2}\cos\frac{\varphi'-\varphi}{2}-\tau e^{\alpha\tau/2}\sinh\frac{\beta'-\beta}{2}\right.$$
$$\left.\times\sin\frac{\varphi'-\varphi}{2}\right|^{-2-j}\exp(i\mu\beta'+im\varphi')\mathrm{d}\varphi'\,\mathrm{d}\beta'. \tag{B7}$$

The explicit calculation is achieved by writing (B7) in the form

$$f^{(3)}_{m\mu\tau}(\beta,\alpha,\varphi)=\exp(i\mu\beta+im\varphi)\int_0^{2\pi}\int_{-\infty}^{+\infty}|\cosh\alpha\cosh\beta'-\tau\sinh\alpha|^{(-2-j)/2}$$
$$\times[1-\tau\cos(\varphi'-\varphi_0)]^{(-2-j)/2}\exp(i\mu\beta'+im\varphi')\mathrm{d}\varphi'\,\mathrm{d}\beta',$$

where

$$\cos\varphi_0=\frac{\sinh\alpha\cosh\beta'-\tau\cosh\alpha}{\cosh\alpha\cosh\beta'-\tau\sinh\alpha},\quad \sin\varphi_0=\frac{\sinh\beta'}{\cosh\alpha\cosh\beta'-\tau\sinh\alpha}.$$

We then obtain

$$f^{(3)}_{m\mu\tau}(\beta,\alpha,\varphi)=\frac{\Gamma\left(1+\dfrac{j}{2}+m\right)\Gamma\left(1+\dfrac{j}{2}-i\tau\mu\right)\exp[i\pi(m+1)(\tau+1)/2]}{\pi\Gamma(-1-j)}$$
$$\times\exp(i\mu\beta+im\varphi-\pi\tau\mu)\mathfrak{Q}^{j/2}_{i\tau\mu,m}(i\tau\sinh\alpha), \tag{B8}$$

where $\mathfrak{Q}^{j}_{\mu\nu}(z)$ is the generalized Legendre function of the second kind as defined by Azimov.[21] Observe that the basis function $f^{(3)}_{m\mu\tau}$ is related to SO(2)–SO(1,1) mixed basis matrix elements of SO(2,1).[23]

(iv) The SO(2,2)⊃SO(1,1)×E(1) reduction. The basis functions in this reduction are given by

$$f^{(4)}_{\lambda\mu\tau}(x)=\varkappa\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}|[x,n^{\tau}]|^{-2-j}\exp(i\mu\beta'+i\lambda t')\mathrm{d}\beta'\,\mathrm{d}t', \tag{B9}$$

where n^{τ} are given by (A28) and (A29). After integration over t', expression (B9) reduces to the integral representations for SO(1,1)−E(1) mixed basis matrix elements of SO(2,1).[23] As result

$$f^{(4)}_{\lambda\mu+}(x)=\pi^{1/2}(2\lambda)^{1+j}\frac{\Gamma\left(\frac{2+j}{2}\right)}{\Gamma\left(\frac{-1-j}{2}\right)}e^{i\mu\beta+i\lambda t}\left[\Gamma\left(\frac{j}{2}-i\mu+1\right)(-2i\lambda)^{-(2+j)/2}\right.$$

$$\left.\times W_{i\mu,(1+j)/2}(-2i\lambda e^{\alpha})+\Gamma\left(\frac{j}{2}+i\mu+1\right)(2i\lambda)^{-(2+j)/2}W_{-i\mu,(1+j)/2}(2i\lambda e^{\alpha})\right],$$

$$f^{(4)}_{\lambda\mu-}(x)=\pi^{1/2}(2\lambda)^{1+j}e^{-i\lambda e^{\alpha}}\frac{\Gamma\left(\frac{2+j}{2}\right)}{\Gamma\left(\frac{-1-j}{2}\right)}e^{\alpha(2+j)/2}$$

$$\times B\left(\frac{j}{2}-i\mu+1,\frac{j}{2}+i\mu+1\right)e^{i\mu\beta+i\lambda t}\,{}_1F_1\left(\frac{j}{2}+i\mu+1,2+j;2i\lambda e^{\alpha}\right)$$

with $x\in X^{-}$, $B(a,b)=\Gamma(a)\Gamma(b)/\Gamma(a+b)$ and

$$f^{(4)}_{\lambda\mu+}(x)=\pi^{1/2}(2\lambda)^{1+j}e^{i\lambda e^{-\alpha}}\frac{\Gamma\left(\frac{2+j}{2}\right)}{\Gamma\left(\frac{-1-j}{2}\right)}e^{-\alpha(2+j)/2}$$

$$\times B\left(\frac{j}{2}-i\mu+1,\frac{j}{2}+i\mu+1\right)e^{i\mu\beta+i\lambda t}\,{}_1F_1\left(\frac{j}{2}+i\mu+1,2+j;-2i\lambda e^{-\alpha}\right)$$

$$f^{(4)}_{\lambda\mu-}(x)=\pi^{1/2}(2\lambda)^{1+j}\frac{\Gamma\left(\frac{2+j}{2}\right)}{\Gamma\left(\frac{-1-j}{2}\right)}e^{i\mu\beta+i\lambda t}\left[\Gamma\left(\frac{j}{2}+i\mu+1\right)(-2i\lambda)^{(-2-j)/2}\right.$$

$$\left.\times W_{-i\mu,(1+j)/2}(-2i\lambda e^{-\alpha})+\Gamma\left(\frac{j}{2}-i\mu+1\right)(2i\lambda)^{(-2-j)/2}W_{i\mu,(1+j)/2}(2i\lambda e^{-\alpha})\right]$$

with $x\in X^{+}$.

(v) The SO(2,2)⊃E(1)×E(1) reduction. The basis function in this reduction may be calculated from

$$f^{(5)}_{\lambda\mu}(x)=\varkappa\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}|e^{-\alpha/2}+(y'-y)(t'-t)e^{\alpha/2}|^{-2-j}\exp(i\lambda\xi'+i\mu t')\mathrm{d}y'\,\mathrm{d}t'.$$

We obtain

$$f^{(5)}_{\lambda\mu}(x)=\frac{2^{-1-j}}{\Gamma(-1-j)}(\lambda\mu)^{(1+j)/2}\exp\left(i\lambda y+i\mu t-\frac{\alpha}{2}\right)K_{-1-j}(e^{-\alpha/2}\sqrt{\lambda\mu}),\lambda\mu>0,$$

where $K_j(z)$ is the modified Bessel function of the third kind.

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Ground state energy of massive scalar field inside a spherical region in the global monopole background

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Using the zeta function regularization method we calculate the ground state energy of scalar massive field inside a spherical region in the space–time of a pointlike global monopole. Two cases are investigated: (i) First, we calculate the Casimir energy inside a sphere of radius R and analyze the obtained result. We observe that this energy may be positive or negative depending on metric coefficient α and nonconformal coupling ξ. In the limit $R\to\infty$, this energy vanishes: (ii) In the second model, we surround the monopole by an additional sphere of radius $r_0 < R$ and consider the scalar field confined in the region between these two spheres. In this case, the ground state energy presents an additional contribution due to boundary at r_0 which is divergent for small radius. Additional comments about renormalization are considered. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Different types of topological objects may have been formed during Universe expansion, among them we have domain walls, cosmic strings and monopoles.[1] These topological defects appear as a consequence of breakdown of local or global gauge symmetries of a system composed by self-coupling iso-scalar Higgs fields Φ^a. Global monopoles are created due to phase transition when a global gauge symmetry is spontaneously broken and they may have an important role in cosmology and astrophysics. The process of global monopole creation is accompanied by particle production.[2] Grand unified theory predicts great number of these objects in the Universe,[3] but this problem can be avoided using inflationary models. From an astrophysical point of view, there is at most one global monopole in the local group of galaxies.[4]

The space–time of a global monopole in an $O(3)$ broken symmetry model has been investigated by Barriola and Vilenkin.[5] They have shown that far from the compact monopole's core the space–time is approximately described by a spherical symmetric metric with an additional deficit solid angle. It is also possible to find solution for the Einstein equation coupled with an energy-momentum tensor associated with a pointlike global monopole. For simplicity we shall consider in this article this singular configuration. In Ref. 6 a simplified model is presented in order to consider some internal structure for the global monopole.

The analysis of quantum fields on the global monopole background has been considered in Refs. 7–9. It was shown, taking into account only dimensional and conformal considerations,[7] that the vacuum expectation value of the energy-momentum tensor associated with a collection of conformal massless quantum fields of arbitrary spin in this background has the following general structure,

$$\langle T_k^i \rangle = S_k^i \frac{\hbar c}{r^4},$$

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where the quantities S_k^i depend only on the solid angle deficit and spin of the fields. For a scalar field this tensor was investigated more carefully by Mazzitelli and Lousto[8] and for a massless spinor field by the authors of Ref. 9 in detail.

The above energy-momentum tensor has nonintegrable singularity at the origin, therefore the ground state energy cannot be found by integrating the energy density. The same problem also appears for cosmic string space–time[10] and in the Minkowski one with a boundary condition on the dihedral angle.[11] The calculation of ground state energy for the cosmic string space–time was considered in Refs. 12 and 13, using different approaches. For an infinitely thin cosmic string, a specific global effect appears which leads to additional surface renormalization.[12] The ground state energy of the massive scalar field in the background of a cosmic string with internal nonsingular structure has been considered in Ref. 13. It has been found that it is zero, independently of the transverse diameter of the string.

The nontrivial topology of space–time, as well as its curvature, leads to a number of interesting effects which are not presented in a flat space. For example, there appear self-interacting forces on massive pointlike particles at rest. These forces have been investigated in Refs. 14 and 15 for cosmic string and global monopole space–times.

In the framework of the zeta function regularization method[16] (see also Ref. 17), the ground state energy of a scalar massive field can be obtained from

$$E(s)=\tfrac{1}{2}M^{2s}\zeta_A(s-\tfrac{1}{2}), \tag{1}$$

which is expressed in terms of the zeta function ζ_A associated with the Laplace operator $\hat{A}=-\Delta+\xi\mathcal{R}+m^2$ defined in the three-dimensional spatial section of the space–time. Here, the parameter M, with dimension of mass, has been introduced in order to have the correct dimension for the energy. In order to calculate the renormalized ground state energy we shall use the approach which was suggested and developed in Refs. 18–21.

In this article we would like to discuss the ground state energy of a scalar massive field in the background of a pointlike global monopole space–time inside a spherical region, considering an arbitrary nonminimal coupling of this field with the geometry. Because the energy-momentum tensor has nonintegrable singularity at the origin we would like to investigate two cases: (i) In the first we consider a pointlike global monopole and calculate the ground state energy using the zeta function approach; and (ii) in the second one, we consider a sphere surrounding the monopole and cut out internal part of it by an appropriate boundary condition for the radial functions. This procedure permits us to show up the role of the singularity. In the limit of zero radius of the inner sphere, this model corresponds to a topological defect, because, in this case, there is no internal structure.

The zeta function of the Laplace operator on the pointlike global monopole background has been considered by Bordag, Kirsten and Dowker in Ref. 22, using the method given in Refs. 18–21. There, the general mathematical structure of the zeta function and the heat kernel coefficients on the generalized cone have been obtained. Because the main emphasis of the present article is on the ground state energy, we shall rederive in Sec. III some specific formulas for our case which was not considered in Ref. 22.

The organization of this article is as follows. In Sec. II we briefly review some geometrical properties about global monopole space–time which will be needed. In Sec. III, the zeta function of the Laplace operator on the three-dimensional section of a pointlike global monopole space–time is given. In Sec. IV we consider the zeta function for global monopole space–time, cutting out the interior of the sphere around the origin. In Sec. V, the ground state energy of the massive scalar field with arbitrary nonconformal coupling on the global monopole background is considered for both cases. In Sec. VI, we discuss our results. The signature of the space–time, the sign of the Riemann and Ricci tensors, is the same as in Christensen's paper.[23] We use units $\hbar=c=G=1$.

II. THE GEOMETRY

Global monopoles are heavy objects probably formed in the early Universe by a phase transition which occurred in a system composed by a scalar self-coupling triplet field ϕ^a whose original global symmetry $O(3)$ is spontaneously broken to $U(1)$.

The simplest model which gives rise a global monopole is described by the Lagrangian density

$$L=\frac{1}{2}(\partial_l\phi^a)(\partial^l\phi^a)-\frac{\lambda}{4}(\phi^a\phi^a-\eta^2)^2.$$

Coupling this matter field with Einstein equations, Barriola and Vilenkin[5] have shown that the effect produced by this configuration, from the geometrical point of view, can be approximately represented by a deficit solid angle in the $(3+1)$-dimensional space–time, whose line element is given by

$$ds^2=-dt^2+\alpha^{-2}dr^2+r^2(d\theta^2+\sin^2\theta d\varphi^2), \tag{2}$$

where the parameter $\alpha^2=1-8\pi\eta^2$ is smaller than unity and depends on the symmetry breaking energy scale η. The solid angle in the geometry defined by (2) is $4\pi\alpha^2$, consequently smaller than 4π. So this space–time presents a deficit solid angle given by $\delta\Omega=32\pi^2\eta^2$. We also can note that it is not flat. The nonzero components of the Riemann and Ricci tensors, and the scalar curvature are given by

$$\mathcal{R}^{\theta\varphi}_{\ .\theta\varphi}=\mathcal{R}^{\theta}_{\ \theta}=\mathcal{R}^{\varphi}_{\ \varphi}=\frac{1-\alpha^2}{r^2},\quad \mathcal{R}=\frac{2(1-\alpha^2)}{r^2}.$$

For further application, let us consider an extrinsic curvature tensor on the sphere of radius R around the origin:

$$K_{ij}=\nabla_i N_j.$$

Here N_j is the outward unit normal vector with coordinates $N_j=(0,\alpha,0,0)$. This tensor has two nonzero components,

$$K^{\theta}_{\theta}=K^{\varphi}_{\varphi}=\frac{\alpha}{R}.$$

III. ZETA FUNCTION FOR POINTLIKE GLOBAL MONOPOLE SPACE–TIME

In order to calculate the ground state energy given by Eq. (1) we have to obtain the zeta function of the operator $\hat{A}$ in the neighborhood of the point $s=-\frac{1}{2}$. To do the calculation of the zeta function we follow Refs. 19, 20, and 22. The zeta function of the operator $\hat{A}=-\triangle+\xi\mathcal{R}+m^2$ is defined in terms of the sum over all eigenvalues of this operator by

$$\zeta_A\left(s-\frac{1}{2}\right)=\sum_{(n)}(\lambda^2_{(n)}+m^2)^{1/2-s}.$$

Here $\lambda^2_{(n)}$ is the eigenvalue of the operator $\hat{B}=\hat{A}-m^2$. The eigenfunctions of the operator $\hat{A}$ defined on the background (2), which are regular at the origin, have the form

$$\Phi(\mathbf{r})=\sqrt{\frac{\lambda}{\alpha r}}Y_{lm}(\theta,\varphi)J_{\mu}\left(\frac{\lambda}{\alpha}r\right), \tag{3}$$

where Y_{lm} are the spherical harmonics and J_{μ} is the Bessel function of the first kind with index

$$\mu=\frac{1}{\alpha}\sqrt{\left(l+\frac{1}{2}\right)^2+2(1-\alpha^2)\left(\xi-\frac{1}{8}\right)}. \tag{4}$$

A discrete set of eigenvalues $\lambda_{l,j}$ can be found by imposing some boundary condition on this function. Let us consider the Dirichlet boundary condition at the surface of a sphere of radius R concentric with the pointlike monopole:

$$\sqrt{\lambda_{l,j}}J_\mu\left(\frac{\lambda_{l,j}}{\alpha}R\right)=0. \tag{5}$$

Then, the zeta function reads

$$\zeta_A^R\left(s-\frac{1}{2}\right)=\sum_{l=0}^{\infty}\sum_{j=0}^{\infty}(2l+1)(\lambda_{l,j}^2+m^2)^{1/2-s},$$

where the label R in the zeta function was introduced to indicate this kind of boundary condition. The solutions $\lambda_{l,j}$ of Eq. (5) cannot be found in closed form. For this reason we use the method suggested in Refs. 18–20, which allows us to express the zeta function in terms of the eigenfunctions. According to this approach, the sum over j may be converted into a contour integral in a complex λ-plane using the principal of argument, namely

$$\zeta_A^R\left(s-\frac{1}{2}\right)=\sum_{l=0}^{\infty}(2l+1)\int_\gamma d\lambda^2(\lambda^2+m^2)^{1/2-s}\frac{\partial}{\partial\lambda}\ln\lambda^{-\mu}J_\mu\left(\frac{\lambda}{\alpha}R\right),$$

where the contour γ runs counterclockwise and must enclose all solutions of Eq. (5) on the positive real axis. Shifting the contour to the imaginary axis, we obtain the following formula for the zeta function (see Ref. 19 for details):

$$\zeta_A^R\left(s-\frac{1}{2}\right)=-\frac{\cos\pi s}{\pi}\sum_{l=0}^{\infty}(2l+1)\int_m^\infty dk(k^2-m^2)^{1/2-s}\frac{\partial}{\partial k}\ln k^{-\mu}I_\mu\left(\frac{k}{\alpha}R\right). \tag{6}$$

Here I_μ is the modified Bessel function. In what follows, we will use the uniform expansion for the Bessel function $I_\mu(\mu z)$ as

$$I_\mu(\mu z)=\sqrt{\frac{t}{2\pi\mu}}e^{\mu\eta(z)}\left\{1+\sum_{k=1}^{\infty}\frac{u_k(t)}{\mu^k}\right\}, \tag{7}$$

where $t=1/\sqrt{1+z^2}$, $\eta(z)=\sqrt{1+z^2}+\ln(z/(1+\sqrt{1+z^2}))$ and $z=kR/\mu\alpha$. The first coefficients $u_k(t)$ and the recursion relations for the higher ones are listed in Ref. 24 This uniform expansion leads to the power series in m, and the term u_N gives the contribution $\sim 1/m^{3-N}$. We shall make the calculations up to $N=3$. In this case we obtain the following formula for uniform expansion of the logarithm of Bessel function:

$$\ln\left(k^{-\mu}I_\mu\left(\frac{k}{\alpha}R\right)\right)=\mu(\eta(z)-z)-\frac{1}{4}\ln(1+z^2)+\frac{1}{\mu}D_1(t)+\frac{1}{\mu^2}D_2(t)+\frac{1}{\mu^3}D_3(t), \tag{8}$$

where

$$D_1(t)=\sum_{a=0}^{1} x_{1,a}t^{1+2a}=\frac{1}{8}t-\frac{5}{24}t^3,$$

$$D_2(t)=\sum_{a=0}^{2} x_{2,a}t^{2+2a}=\frac{1}{16}t^2-\frac{3}{8}t^4+\frac{5}{16}t^6, \tag{9}$$

$$D_3(t)=\sum_{a=0}^{3} x_{3,a}t^{3+2a}=\frac{25}{384}t^3-\frac{531}{640}t^5+\frac{221}{128}t^7-\frac{1105}{1152}t^9.$$

In the above expression we omit all constants which are not important for calculation of the zeta function. Adding and subtracting uniform expansion (8) in the integrand of formula (6), we may represent the zeta function in the form

$$\zeta_A^R\left(s-\frac{1}{2}\right)=N^R(s)+\frac{m^{-2s}}{(4\pi)^{3/2}\Gamma(s-\frac{1}{2})}\sum_{k=-1}^{3} A_k(s,R), \tag{10}$$

where

$$N^R(s)=-\frac{\cos\pi s}{\pi R}\sum_{l=0}^{\infty}(2l+1)\mu\alpha\int_{\beta/\mu\alpha}^{\infty}dx\left\{x^2-\left(\frac{\beta}{\mu\alpha}\right)^2\right\}^{1/2-s}$$
$$\times\frac{\partial}{\partial x}\left\{\ln I_\mu(\mu x)-\mu\eta(x)+\frac{1}{4}\ln(1+x^2)-\frac{1}{\mu}D_1(t)-\frac{1}{\mu^2}D_2(t)-\frac{1}{\mu^3}D_3(t)\right\}, \tag{11}$$

$$A_{-1}(s,R)=\frac{4\pi^{3/2}m\beta}{\alpha}\sum_{l=0}^{\infty}(2l+1)\left[\frac{\Gamma(s-1)}{\sqrt{\pi}}{}_2F_1-\frac{\alpha\mu}{\beta}\Gamma\left(s-\frac{1}{2}\right)\right], \tag{12}$$

$$A_0(s,R)=-2\pi^{3/2}m\mathcal{Z}(0,s-\tfrac{1}{2}), \tag{13}$$

$$A_1(s,R)=-\frac{\pi m\alpha}{\beta}\left[\mathcal{Z}(0,s)-\frac{10}{3}\mathcal{Z}(2,s+1)\right], \tag{14}$$

$$A_2(s,R)=-\frac{\pi^{3/2}m\alpha^2}{2\beta^2}\left[\mathcal{Z}\left(0,s+\frac{1}{2}\right)-6\mathcal{Z}\left(2,s+\frac{3}{2}\right)+\frac{5}{2}\mathcal{Z}\left(4,s+\frac{5}{2}\right)\right], \tag{15}$$

$$A_3(s,R)=-\frac{\pi m\alpha^3}{24\beta^3}\left[25\mathcal{Z}(0,s+1)-\frac{1062}{5}\mathcal{Z}(2,s+2)\right.$$
$$\left.+\frac{884}{5}\mathcal{Z}(4,s+3)-\frac{1768}{63}\mathcal{Z}(6,s+4)\right]. \tag{16}$$

Here ${}_2F_1={}_2F_1(-\frac{1}{2},s-1;\frac{1}{2};-(\mu\alpha/\beta))^2$ is the hypergeometric function, $\beta=mR$ and

$$\mathcal{Z}(p,s)=\Gamma(q)\sum_{l=0}^{\infty}\frac{2l+1}{(1+\alpha^2\mu^2/\beta^2)^s}\left(\frac{\alpha\mu}{\beta}\right)^p. \tag{17}$$

The series in Eq. (12),

$$T(s)=\sum_{l=0}^{\infty}(2l+1)\left[\frac{\Gamma(s-1)}{\sqrt{\pi}}{}_2F_1-\frac{\alpha\mu}{\beta}\Gamma\left(s-\frac{1}{2}\right)\right], \tag{18}$$

can be expressed in terms of the same function given in Eq. (17). Indeed, one can use analytical continuation of the hypergeometrical function [24]

$$
{}_2F_1\left(-\frac{1}{2},s-1;\frac{1}{2};-\left(\frac{\alpha\mu}{\beta}\right)^2\right)=\frac{\alpha\mu}{\beta}\frac{\Gamma\frac{1}{2}\Gamma(s-\frac{1}{2})}{\Gamma(s-1)}+\frac{\Gamma(\frac{1}{2})\Gamma(\frac{1}{2}-s)}{\Gamma(-\frac{1}{2})\Gamma(\frac{3}{2}-s)}
$$

$$
\times\left(1+\left(\frac{\alpha\mu}{\beta}\right)^2\right)^{1-s}{}_2F_1\left(1,s-1;s+\frac{1}{2};\frac{1}{1+(\alpha\mu/\beta)^2}\right).
$$

So, the first term on the rhs of the above equation cancels the second divergent term in the sum (18) which is due to term $k^{-\mu}$ in (6) (see Ref. 13). Now, one can use power series expansion for the hypergeometric function because its argument $1/(1+(\alpha\mu/\beta)^2)$ is always smaller than unity. Then, we get

$$
T(s)=\frac{1}{2\sqrt{\pi}}\Gamma\left(s-\frac{1}{2}\right)\sum_{l=0}^{\infty}\frac{\mathcal{Z}(0,n+s-1)}{\Gamma(n+s+\frac{1}{2})}. \tag{19}
$$

Therefore, in order to calculate the zeta function, we have to obtain an analytical continuation of the series $\mathcal{Z}(p,q)$. In fact, we may consider just

$$
\mathcal{Z}(0,s)=\Gamma(q)\sum_{l=0}^{\infty}\frac{2l+1}{(1+\alpha^2\mu^2/\beta^2)^s}, \tag{20}
$$

because the other functions with $p=2,4,6,...$ can be expressed in terms of $\mathcal{Z}(0,q)$. Substituting the value for μ given in Eq. (4) into Eq. (20), we obtain

$$
\mathcal{Z}(0,s)=2\Gamma(q)\beta^{2s}\sum_{l=0}^{\infty}\frac{l+\frac{1}{2}}{((l+\frac{1}{2})^2+b^2)^s}, \tag{21}
$$

where $b^2=\beta^2+2(1-\alpha^2)(\xi-1/8)$. This series is convergent for $\Re q>1$. It is not difficult to obtain the analytical continuation of this series for a small value of parameter b. Indeed, expanding $\mathcal{Z}$ in powers of b we have

$$
\mathcal{Z}(0,s)=2\beta^{2s}\sum_{k=0}^{\infty}\frac{(-1)^k}{k!}\Gamma(k+s)b^{2k}\zeta_H\left(2k+2s-1,\frac{1}{2}\right). \tag{22}
$$

In order to consider the analytical continuation of this function in the domain $\Re q\leqslant 1$ and for a large value of b, let us take the series

$$
F(s,a,b^2)=\sum_{l=0}^{\infty}\frac{1}{((l+a)^2+b^2)^s}.
$$

This series, which has been considered in great detail by Elizalde,[25] presents the following analytical continuation for great b:

$$
F(s,a,b^2)\simeq\frac{b^{-2s}}{\Gamma(s)}\sum_{l=0}^{\infty}\frac{(-1)^l\Gamma(l+s)}{l!}b^{-2l}\zeta_H(-2l,a)+\frac{\sqrt{\pi}\Gamma(s-\frac{1}{2})}{2\Gamma(s)}b^{1-2s}
$$

$$
-\frac{2\pi b^{-1/2-s}}{\Gamma(s)}\sum_{n=1}^{\infty}n^{s-1/2}\cos(2\pi na)K_{s-1/2}(2\pi nb).
$$

Here ζ_H is the Hurwitz zeta function and K_n is the modified Bessel function. Differentiating this series with respect to a and putting $a=1/2$ we obtain the analytical continuation that we need, which is the following:

$$\sum_{l=0}^{\infty}\frac{l+\frac{1}{2}}{((l+\frac{1}{2})^2+b^2)^s}\simeq\frac{b^{2-2s}}{2(s-1)}+\sum_{l=0}^{\infty}\frac{(-1)^l\Gamma(l+s)}{l!\Gamma(s)}b^{-2s-2l}\zeta_H(-1-2l,\tfrac{1}{2}).$$

Taking into account this expression we obtain the analytical continuation for $\mathcal{Z}(0,q)$, which is given by the expression

$$\mathcal{Z}(0,s)\simeq\left(\frac{b^2}{\beta^2}\right)^{-s}\left\{b^2\Gamma(s-1)+2\sum_{l=0}^{\infty}\frac{(-1)^l}{l!}\Gamma(l+s)b^{-2l}\zeta_H(-1-2l,\tfrac{1}{2})\right\},\tag{23}$$

where $b^2/\beta^2=1+2(1-\alpha^2)(\xi-\frac{1}{8})/\beta^2$. This function has simple poles for integer numbers $q=1,0,-1,-2,\ldots$. In order to obtain a renormalized value for the ground state energy we have to extract from our expression for zeta function (10) the part which survives in the limit $m\to\infty$. Moreover, to calculate the zeta function up to degree m^0 we need only two terms from series (23) in which $\zeta_H(-1,\frac{1}{2})=\frac{1}{24}$, and $\zeta_H(-3,\frac{1}{2})=-7/960$, and three terms of $T(s)$ which are obtained from Eq. (19).

Putting this expression into Eqs. (19) and (12)–(16), expanding in powers of $1/\beta=1/mR\ll 1$ and s, and collecting terms with similar degree on the mass m up to m^0 (here we cannot collect terms with higher orders in m because we used uniform expansion up to this power), we obtain

$$\begin{aligned}\zeta_A^R\left(s-\frac{1}{2}\right)=\frac{m^{-2s}}{(4\pi)^{3/2}}\Bigg\{&\left[\frac{4\pi R^3}{3\alpha}\right]m^4\frac{\Gamma(s-2)}{\Gamma(s-\frac{1}{2})}+[-2\pi^{3/2}R^2]m^3\frac{\Gamma(s-\frac{3}{2})}{\Gamma(s-\frac{1}{2})}\\&+\left[\frac{7}{3}\pi\alpha R-\frac{4\pi R}{\alpha}\left(\Delta-\frac{1}{12}\right)\right]m^2\frac{\Gamma(s-1)}{\Gamma(s-\frac{1}{2})}+\left[2\pi^{3/2}\left(\Delta-\frac{1}{12}\right)\right]m\\&+\left[\frac{\pi\alpha}{R}\left(\Delta-\frac{1}{12}+\frac{229}{2520}\alpha^2\right)-\frac{2\pi}{\alpha R}\left(\Delta^2-\frac{1}{6}\Delta+\frac{7}{240}\right)\right]\frac{\Gamma(s)}{\Gamma(s-\frac{1}{2})}+\ldots\Bigg\},\end{aligned}\tag{24}$$

where $\Delta=2(1-\alpha^2)(\xi-\frac{1}{8})$. All these terms are pole contributions to the zeta function and all next terms will be finite for $s\to 0$. Comparing the above expression with that obtained by the Mellin transformation taking the trace of heat kernel (in three dimensions),

$$\begin{aligned}\zeta_A^R\left(s-\frac{1}{2}\right)&=\frac{1}{\Gamma(s-\frac{1}{2})}\int_0^{\infty}dt\,t^{s-3/2}K(t)\\&=\frac{m^{-2s}}{(4\pi)^{3/2}}\Bigg\{B_0^Rm^4\frac{\Gamma(s-2)}{\Gamma(s-\frac{1}{2})}+B_{1/2}^Rm^3\frac{\Gamma(s-\frac{3}{2})}{\Gamma(s-\frac{1}{2})}\\&\quad+B_1^Rm^2\frac{\Gamma(s-1)}{\Gamma(s-\frac{1}{2})}+B_{3/2}^Rm+B_2^R\frac{\Gamma(s)}{\Gamma(s-\frac{1}{2})}+\ldots\Bigg\},\end{aligned}\tag{25}$$

we obtain the heat kernel coefficients:

$$B_0^R=\frac{4\pi R^3}{3\alpha},\quad B_{1/2}^R=-2\pi^{3/2}R^2,\quad B_1^R=\frac{7}{3}\pi\alpha R-\frac{4\pi R}{\alpha}\left(\Delta-\frac{1}{12}\right),$$

$$B_{3/2}^R=2\pi^{3/2}\left(\Delta-\frac{1}{12}\right),\quad B_2^R=\frac{\pi\alpha}{R}\left(\Delta-\frac{1}{12}+\frac{229}{2520}\alpha^2\right)-\frac{2\pi}{\alpha R}\left(\Delta^2-\frac{1}{6}\Delta+\frac{7}{240}\right). \tag{26}$$

Those terms which are proportional to the inverse degree of α come from the exponential part of the uniform expansion given by (7), which gives $T(s)$ (19). The terms which are linear in α^1 or α^0 come from the series $\Sigma u_k/\mu^k$ in (7).

Now we may compare our results with well-known formulas given in Refs. 26, 22, 17, and 27. The coefficients B_0^R, $B_{1/2}^R$, B_1^R, $B_{3/2}^R$ coincide with general formulas in three dimensions (note the necessary geometrical quantities to perform the calculations are given at the end of Sec. II):

$$\begin{aligned}
B_0^R&=\frac{4\pi R^3}{3\alpha}=\int_V dV,\\
B_{1/2}^R&=-2\pi^{3/2}R^2=-\frac{\sqrt{\pi}}{2}\int_{\partial V}dS,\\
B_1^R&=\frac{7}{3}\pi\alpha R-\frac{4\pi R}{\alpha}\left(\Delta-\frac{1}{12}\right)=\left(\frac{1}{6}-\xi\right)\int_V\mathcal{R}\,dV+\frac{1}{3}\int_{\partial V}(\mathrm{tr}\,K)dS,\\
B_{3/2}^R&=2\pi^{3/2}\left(\Delta-\frac{1}{12}\right)\\
&=-\frac{\sqrt{\pi}}{192}\int_{\partial V}(-96\xi\mathcal{R}+16\mathcal{R}+8\mathcal{R}_{ik}N^iN^k+7(\mathrm{tr}\,K)^2-10(\mathrm{tr}\,K)^2)dS.
\end{aligned} \tag{27}$$

As we will see, there are some problems connected with the term B_2. The general structure of this term is the following (see Refs. 23 and 27):

$$B_2^R=\int_V b_2\,dV+\int_{\partial V}c_2\,dS, \tag{28}$$

where

$$b_2=-\tfrac{1}{180}\mathcal{R}^{ik}\mathcal{R}_{ik}+\tfrac{1}{180}\mathcal{R}^{iklj}\mathcal{R}_{iklj}+\tfrac{1}{6}(\tfrac{1}{5}-\xi)\Box\mathcal{R}+\tfrac{1}{2}(\tfrac{1}{6}-\xi)^2\mathcal{R}^2 \tag{29}$$

is the volume part, and

$$\begin{aligned}
c_2=&\tfrac{1}{3}(\tfrac{1}{6}-\xi)\mathcal{R}(\mathrm{tr}\,K)+\tfrac{1}{3}(3/20-\xi)\mathcal{R}_{;l}N^l-\tfrac{1}{90}\mathcal{R}_{lk}N^lN^k(\mathrm{tr}\,K)+\tfrac{1}{30}\mathcal{R}_{iljk}N^lN^kK^{ij}\\
&-\tfrac{1}{90}\mathcal{R}_{il}K^{il}+\tfrac{1}{315}[\tfrac{5}{3}(\mathrm{tr}\,K)^3-11(\mathrm{tr}\,K)(\mathrm{tr}\,K^2)+\tfrac{40}{3}(\mathrm{tr}\,K^3)]+\tfrac{1}{15}\Box(\mathrm{tr}\,K)
\end{aligned} \tag{30}$$

is the boundary contribution. Taking into account the results obtained in Sec. II we have

$$b_2=-\frac{1}{r^4}\frac{\alpha}{4\pi}\left\{\pi\alpha\left(\Delta-\frac{1}{12}+\frac{17}{120}\alpha^2\right)-\frac{2\pi}{\alpha}\left(\Delta^2-\frac{1}{6}\Delta+\frac{7}{240}\right)\right\}, \tag{31}$$

$$c_2=-\frac{4\alpha^3}{315R^3}. \tag{32}$$

We observe that b_2 is proportional to $1/r^4$ and the integral over volume in Eq. (28) will diverge at the origin. This problem has already been discussed by Cheeger,[28] Brüning and Seeley,[29] and Bordag, Kirsten and Dowker[22] using *partie finite* of the integral. We regularize the expression for B_2 by restricting the domain of radial integration:

$$B_2=-\int_{\varepsilon}^{R}\frac{dr}{r^2}\left\{\pi\alpha\left(\Delta-\frac{1}{12}+\frac{17}{120}\alpha^2\right)-\frac{2\pi}{\alpha}\left(\Delta^2-\frac{1}{6}\Delta+\frac{7}{240}\right)\right\}-\frac{16\pi\alpha^3}{315R}. \tag{33}$$

After integration we take its finite remainder parts as $\varepsilon\to 0$, and the expression obtained in this way coincides with that given in Eq. (26).

Our expressions for the heat kernel coefficients also agree with those obtained in Ref. 22. In that article the heat kernel coefficients have been calculated for the conformal case ($\xi=1/8$, in three dimensions). In order to compare both results we have to set $\xi=1/8(\triangle=0)$ in Eq. (26) and use the formulas of Appendix A from Ref. 22 for the three-dimensional case $d=2$.

To proceed with the renormalization, which we shall discuss later, we have to subtract from zeta function (10) the asymptotic expansion (24). Because all divergences at $s\to 0$ are contained in (24), we set $s=0$ in the remained part. After a long calculation we arrive at the following formula for the zeta function:

$$\zeta_A^R\left(s-\frac{1}{2}\right)=-\frac{m}{16\pi^2\beta}\{B^R(\beta)\ln\beta^2+\Omega^R(\beta)\}+\frac{m^{-2s}}{(4\pi)^{3/2}}\left\{B_0^R m^4\frac{\Gamma(s-2)}{\Gamma(s-\frac{1}{2})}\right.$$
$$\left.+B_{1/2}^R m^3\frac{\Gamma(s-\frac{3}{2})}{\Gamma(s-\frac{1}{2})}+B_1^R m^2\frac{\Gamma(s-1)}{\Gamma(s-\frac{1}{2})}+B_{3/2}^R m+B_2^R\frac{\Gamma(s)}{\Gamma(s-\frac{1}{2})}\right\}, \tag{34}$$

where

$$B^R(\beta)=\tfrac{1}{2}Rm^4B_0^R-Rm^2B_1^R+RB_2^R=\tfrac{1}{2}\beta^4b_0^R-\beta^2b_1^R+b_2^R. \tag{35}$$

In order to exhibit the dependence on the mass m and on the radius of sphere R, we have introduced in the formula above the dimensionless heat kernel coefficients, which are given by relations

$$b_0^R=B_0^R/R^3=\frac{4\pi}{3\alpha},\quad b_1^R=B_1^R/R=\frac{7}{3}\pi\alpha-\frac{4\pi}{\alpha}\left(\Delta-\frac{1}{12}\right), \tag{36}$$

$$b_2^R=B_2^RR=\pi\alpha\left(\Delta-\frac{1}{12}+\frac{229}{2520}\alpha^2\right)-\frac{2\pi}{\alpha}\left(\Delta^2-\frac{1}{6}\Delta+\frac{7}{240}\right). \tag{37}$$

The function $\Omega^R(\beta)$ tends to a constant for $\beta\to 0$ and $\Omega^R(\beta)=-B^R(\beta)\ln\beta^2+\sqrt{\pi}b_{5/2}^R/\beta+O(1/\beta^2)$ for $\beta\to\infty$. The details of calculation and a closed form for $\Omega^R(\beta)$ are outlined in the Appendix.

At this point we would like to make a comment. The origin of the term $B^R\ln\beta^2$ is the following: In the limit $m\to\infty$ the singular part of the zeta function has the structure given by Eq. (25). For a small value of m it has the same pole structure multiplied by β^{2s}. This is because all functions $\mathcal{Z}(p,s)$ are proportional to this degree of β as it may be seen from Eq. (22). The difference between them in the limit $s\to 0$ is $s\ln\beta^2$ multiplied by Eq. (25). Obviously, in this limit, only B_0^R, B_1^R, B_2^R survive and give the logarithm contribution to Eq. (34).

IV. THE MODEL

Because the geometrical characteristics of global monopole space–time are divergent at the origin we consider the following model: The center of the monopole is surrounded by a sphere

with radius r_0 whose interior region is cut out. It means that in our model there is no internal structure for the global monopole. The present model reflects this peculiarity of a topological defect.

In the context of this model, we have to take into account both solutions of the radial equation of the Laplace operator, instead of only that given in Eq. (3), which is regular at the origin. The eigenfunctions now have the following form:

$$\Phi(\mathbf{r})=\sqrt{\frac{\lambda}{\alpha r}}Y_{lm}(\theta,\varphi)\left\{C_1 J_\mu\left(\frac{\lambda}{\alpha}r\right)+C_2 N_\mu\left(\frac{\lambda}{\alpha}r\right)\right\}, \tag{38}$$

where N_μ is the Bessel function of the second kind.

In this case we have two boundaries and one has to impose two boundary conditions. Let us again choose the Dirichlet boundary condition for the radial functions at spheres of radii R and r_0, which implies the following relations:

$$C_1 J_\mu\left(\frac{\lambda}{\alpha}R\right)+C_2 N_\mu\left(\frac{\lambda}{\alpha}R\right)=0 \tag{39}$$

and

$$C_1 J_\mu\left(\frac{\lambda}{\alpha}r_0\right)+C_2 N_\mu\left(\frac{\lambda}{\alpha}r_0\right)=0. \tag{40}$$

The set of discrete eigenvalues $\lambda_{l,j}$ can be found from the equation

$$J_\mu\left(\frac{\lambda_{l,j}}{\alpha}r_0\right)N_\mu\left(\frac{\lambda_{l,j}}{\alpha}R\right)-N_\mu\left(\frac{\lambda_{l,j}}{\alpha}r_0\right)J_\mu\left(\frac{\lambda_{l,j}}{\alpha}R\right)=0, \tag{41}$$

which is, in fact, the condition for existence of the solution (38). Therefore, instead of Eq. (6) we obtain the following formula for the zeta function:

$$\zeta_A\left(s-\frac{1}{2}\right)=-\frac{\cos\pi s}{\pi}\sum_{l=0}^{\infty}(2l+1)\int_m^\infty dk(k^2-m^2)^{1/2-s} \times\frac{\partial}{\partial k}\ln\left(I_\mu\left(\frac{kR}{\alpha}\right)K_\mu\left(\frac{kr_0}{\alpha}\right)-K_\mu\left(\frac{kR}{\alpha}\right)I_\mu\left(\frac{kr_0}{\alpha}\right)\right). \tag{42}$$

This general expression may be essentially simplified in the limit $R/r_0\to\infty$ which we are interested in. Taking into account that in this limit the ratio $K_\mu(kR/\alpha)/I_\mu(kR/\alpha)<\pi\exp(-2mR/\alpha)$ is exponentially small, we may divide the expression for zeta function (42) in two parts,

$$\zeta_A(s-\tfrac{1}{2})=\zeta_A^R(s-\tfrac{1}{2})+\zeta_A^{r_0}(s-\tfrac{1}{2}), \tag{43}$$

where

$$\zeta_A^R\left(s-\frac{1}{2}\right)=-\frac{\cos\pi s}{\pi}\sum_{l=0}^{\infty}(2l+1)\int_m^\infty dk(k^2-m^2)^{1/2-s}\frac{\partial}{\partial k}\ln\left(k^{-\mu}I_\mu\left(\frac{k}{\alpha}R\right)\right) \tag{44}$$

and

$$\zeta_A^{r_0}\left(s-\frac{1}{2}\right)=-\frac{\cos\pi s}{\pi}\sum_{l=0}^{\infty}(2l+1)\int_m^\infty dk(k^2-m^2)^{1/2-s}\frac{\partial}{\partial k}\ln\left(k^{\mu}K_\mu\left(\frac{k}{\alpha}r_0\right)\right). \tag{45}$$

The first part is the zeta function for a pointlike global monopole which we have already calculated in the previous section. It depends only on the boundary condition on the sphere of radius R. The second part depends on the boundary condition on the inner sphere of radius r_0. This kind of division of the zeta function has been used in the case of thick cosmic strings in Ref. 13. It is also in qualitative agreement with Ref. 20. Indeed, according with Ref. 20, the internal solution gives Bessel function I_μ and the external solution gives the function K_μ in the expression for the zeta function. The first part of zeta function (44) depends on the solutions inside the sphere of radius R, and the second part of zeta function (45) depends on the solutions outside the sphere of radius r_0.

Let us consider now the second expression (45). To calculate $\zeta_A^{r_0}$ we use the same approach which we have used in the previous section. We have to take into account the uniform expansion for the modified Bessel function of second kind $K_\mu(\mu x)$ which has the form

$$K_\mu(\mu z)=\sqrt{\frac{\pi t}{2\mu}}e^{-\mu\eta(z)}\left\{1+\sum_{k=1}^{\infty}(-1)^k\frac{u_k(t)}{\mu^k}\right\}. \tag{46}$$

Different from the uniform expansion of the Bessel function of the first kind given by Eq. (7), the odd degrees of μ in the above formula have the opposite sign. This fact leads to the change of sign of the heat kernel coefficients with integer index, also with respect of the heat kernel coefficients which were considered in last section. Using this uniform expansion we arrive at the following formulas for the zeta function $\zeta_A^{r_0}$:

$$\zeta_A^{r_0}\left(s-\frac{1}{2}\right)=N^{r_0}(s)+\frac{m^{-2s}}{(4\pi)^{3/2}\Gamma(s-\frac{1}{2})}\sum_{k=-1}^{3}(-1)^k A_k(s,r_0), \tag{47}$$

where

$$N^{r_0}(s)=-\frac{\cos\pi s}{\pi R}\sum_{l=0}^{\infty}(2l+1)\mu\alpha\int_{\beta/\mu\alpha}^{\infty}dx\left\{x^2-\left(\frac{\beta}{\mu\alpha}\right)^2\right\}^{1/2-s}$$
$$\times\frac{\partial}{\partial x}\left\{\ln(K_\mu(\mu x))+\mu\eta(x)+\frac{1}{4}\ln(1+x^2)+\frac{1}{\mu}D_1(t)-\frac{1}{\mu^2}D_2(t)+\frac{1}{\mu^3}D_3(t)\right\}, \tag{48}$$

and the functions $A_k(s,r_0)$ are the same as in Eqs. (12)–(16), but now they depend on the radius r_0. Proceeding in the same way as it was done in the previous section, we obtain the following expression for the second part of zeta function $\zeta_A^{r_0}$:

$$\zeta_A^{r_0}\left(s-\frac{1}{2}\right)=-\frac{m}{16\pi^2\beta_0}\{B^{r_0}(\beta_0)\ln\beta_0^2+\Omega^{r_0}(\beta_0)\}+\frac{m^{-2s}}{(4\pi)^{3/2}}\left\{B_0^{r_0}m^4\frac{\Gamma(s-2)}{\Gamma(s-\frac{1}{2})}\right.$$
$$\left.+B_{1/2}^{r_0}m^3\frac{\Gamma(s-\frac{3}{2})}{\Gamma(s-\frac{1}{2})}+B_1^{r_0}m^2\frac{\Gamma(s-1)}{\Gamma(s-\frac{1}{2})}+B_{3/2}^{r_0}m+B_2^{r_0}\frac{\Gamma(s)}{\Gamma(s-\frac{1}{2})}\right\}, \tag{49}$$

where $\beta_0=mr_0$ and

$$B^{r_0}(\beta_0)=\tfrac{1}{2}r_0m^4B_0^{r_0}-r_0m^2B_1^{r_0}+r_0B_2^{r_0}=\tfrac{1}{2}\beta_0^4b_0^{r_0}-\beta_0^2b_1^{r_0}+b_2^{r_0}. \tag{50}$$

Contrary to the previous section, the heat kernel coefficients with integer number have changed sign and they are

$$b_0^{r_0}=B_0^{r_0}/r_0^3=-\frac{4\pi}{3\alpha},\quad b_1^{r_0}=r_0/B_1^{r_0}=-\frac{7}{3}\pi\alpha+\frac{4\pi}{\alpha}\left(\Delta-\frac{1}{12}\right), \tag{51}$$

$$b_2^{r_0}=B_2^{r_0}r_0=-\pi\alpha\left(\Delta-\frac{1}{12}+\frac{229}{2520}\alpha^2\right)+\frac{2\pi}{\alpha}\left(\Delta^2-\frac{1}{6}\Delta+\frac{7}{240}\right). \tag{52}$$

The heat kernel coefficients, according to Eq. (43), are the sum of B_n^R and $B_n^{r_0}$ and they are in agreement with general formulas. We have to take into account that normal vectors for spheres of radius R and r_0 have opposite directions and that the boundaries consist now of two spheres. It is easy to understand the division of the zeta function in two parts given by Eq. (43), and the opposite sign of the heat kernel coefficients B^R and B^{r_0} with integer indexes, by calculating B_0 and $B_{1/2}$. For the space between two spheres we have

$$B_0=\int_V dV=\frac{4\pi}{\alpha}\int_{r_0}^{R}r^2\,dr=\frac{4\pi}{3\alpha}R^3-\frac{4\pi}{3\alpha}r_0^3=B_0^R+B_0^{r_0}, \tag{53}$$

$$B_{1/2}=-\frac{\sqrt{\pi}}{2}\int_R dS-\frac{\sqrt{\pi}}{2}\int_{r_0}dS=-2\pi^{3/2}R^2-2\pi^{3/2}r_0^2=B_{1/2}^R+B_{1/2}^{r_0}. \tag{54}$$

Therefore, the full zeta function in this case has the following form:

$$\begin{aligned}\zeta_A\left(s-\frac{1}{2}\right)=&-\frac{m}{16\pi^2\beta_0}\{B^{r_0}(\beta_0)\ln\beta_0^2+\Omega^{r_0}(\beta_0)\}-\frac{m}{16\pi^2\beta}\{B^R(\beta)\ln\beta^2+\Omega^R(\beta)\}\\&+\frac{m^{-2s}}{(4\pi)^{3/2}}\left\{B_0m^4\frac{\Gamma(s-2)}{\Gamma(s-\frac{1}{2})}+B_{1/2}m^3\frac{\Gamma(s-\frac{3}{2})}{\Gamma(s-\frac{1}{2})}+B_1m^2\frac{\Gamma(s-1)}{\Gamma(s-\frac{1}{2})}\right.\\&\left.+B_{3/2}m+B_2\frac{\Gamma(s)}{\Gamma(s-\frac{1}{2})}\right\}.\end{aligned} \tag{55}$$

The close expression for Ω^{r_0} is given in the Appendix.

V. THE GROUND STATE ENERGY

In the framework of the zeta function approach the ground state energy is proportional to the zeta function of the Laplace operator and is given by Eq. (1). In order to analyze this energy, let us first of all consider the ground state energy for a pointlike global monopole. The full energy of the system consists of two parts, namely, the classical part due to the boundary and monopole background, and the quantum one due to loop corrections. The general expression for boundary contributions has been considered in Refs. 16 and 20 and it has the following form:

$$E_{cl}^R=p_RV_R+\sigma_RS_R+F_RR+\Lambda_R+\frac{h_R}{R}. \tag{56}$$

Here $V_R=4\pi R^3/3\alpha$ and $S_R=4\pi R^2$ are the volume and area of the spherical surface. Parameters p_R and σ_R have simple physical means as pressure and surface tension. The constant contribution described by parameter Λ_R may be explained by the cosmological constant.[30] The other two parameters, F_R, and h_R, do not have special names.

The energy in the monopole background can be obtained by integrating the (t,t) component of the energy-momentum tensor:[7]

$$E_{cl}^{gm}=-\int_0^R \frac{\eta^2\alpha^2}{r^2}dV=-4\pi\eta^2\alpha R. \tag{57}$$

The quantum correction, using Eq. (34), is

$$E_q^R=\frac{1}{2}M^{2s}\zeta_A^R\left(s-\frac{1}{2}\right)_{s\to 0}=-\frac{m}{32\pi^2\beta}\{B^R(\beta)\ln\beta^2+\Omega^R(\beta)\}+\left(\frac{M}{m}\right)^{2s}\frac{1}{16\pi^{3/2}}$$
$$\times\left\{B_0^R m^4\frac{\Gamma(s-2)}{\Gamma(s-\frac{1}{2})}-\frac{2}{3}B_{1/2}^R m^3+B_1^R m^2\frac{\Gamma(s-1)}{\Gamma(s-\frac{1}{2})}+B_{3/2}^R m+B_2^R\frac{\Gamma(s)}{\Gamma(s-\frac{1}{2})}\right\}_{s\to 0}, \tag{58}$$

where the heat kernel coefficients B_k^R and B^R are given by Eqs. (26) and (35), respectively.

In order to obtain a well defined result for the full energy, we have to renormalize the parameters of the classical part (56) according to the rules

$$p_R\to p_R-\left(\frac{M}{m}\right)^{2s}\frac{3m^4b_0^R}{64\pi^{5/2}}\frac{\Gamma(s-2)}{\Gamma(s-\frac{1}{2})},\quad \sigma_R\to\sigma_R+\frac{m^3b_{1/2}^R}{96\pi^{5/2}},$$

$$F_R\to F_R-\left(\frac{M}{m}\right)^{2s}\frac{m^2b_1^R}{16\pi^{3/2}}\frac{\Gamma(s-1)}{\Gamma(s-\frac{1}{2})},\quad \Lambda_R\to\Lambda_R-\frac{mb_{3/2}^B}{16\pi^{3/2}}, \tag{59}$$

$$h_R\to h_R-\left(\frac{M}{m}\right)^{2s}\frac{b_2^R}{16\pi^{3/2}}\frac{\Gamma(s)}{\Gamma(s-\frac{1}{2})}.$$

After this procedure we obtain the following expression for ground state energy:

$$E_q^R=-\frac{m}{32\pi^2\beta}\{B^R(\beta)\ln\beta^2+\Omega^R(\beta)\}. \tag{60}$$

A similar general structure for the ground state energy in the massless case has been obtained by Blau, Visser and Wipf[16] using dimensional considerations only. For the massive case we find the same structure. If we used another scale for mass as, for example, like $M\to M/\chi$, in renormalization rules (59), the above logarithmic term $\ln\beta^2$ would be replaced by $\ln(\chi\beta)^2$.

The expression (60) is, in fact, the Casimir energy for the internal part of the spherical bag in the global monopole background. For the small radius of the bag, this energy tends to infinity as $\ln R/R$:

$$E_q^R\sim-\frac{m}{16\pi^2\beta}b_2^R\ln\beta, \tag{61}$$

and for the large radius of the bag $R\to\infty$ it tends to zero:

$$E_q^R\sim-\frac{mb_{5/2}^R}{16\pi^{3/2}\beta^2}. \tag{62}$$

Using these two limits we may analyze qualitatively the dependence of the Casimir energy of the internal part of the bag on its radius. The behavior of energy is defined by two heat kernel coefficients b_2^R and $b_{5/2}^R$. Both of these coefficients are the functions of nonminimal coupling parameter ξ and metric coefficient α. In general, three kinds of different behaviors exist, which are plotted in Fig. 1. It is possible to analyze the energy in the general case, however we shall discuss only the cases $\xi=\frac{1}{6}, \frac{1}{8}, 0$.

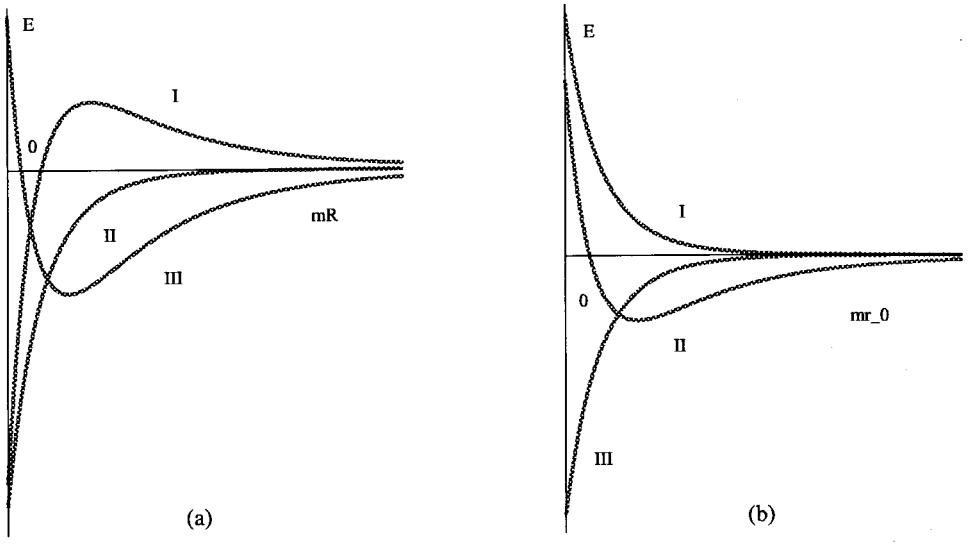

FIG. 1. Three types of dependence of the ground state energy for the field (a) inside the sphere of radius R and (b) outside the sphere of radius r_0.

(1) $\xi=\frac{1}{6}$. In this case the behavior may be of kinds I and II, namely, the first kind for $\alpha<1.24$ and the second one for $\alpha>1.24$. The coefficient b_2^R does not change its sign, but $b_{5/2}^R$ does for $\alpha=1.24$.
(2) $\xi=\frac{1}{8}$. The behavior of energy may be of kinds I, II and III. The first kind is for $\alpha<1.045$; the second kind is in the region $1.045<\alpha<1.17$ and the third one is for $\alpha>1.17$. At the point $\alpha=1.045$ the coefficient $b_{5/2}^R$ changes the sign, but b_2^R does not up to $\alpha=1.17$ where it changes the sign, too.
(3) $\xi=0$. This case is similar to the previous one: it is of the first kind for $\alpha<1.016$, of the second for region $1.016<\alpha<1.054$, and of the third for $\alpha>1.054$.

For $\alpha\leqslant 1$ and $\xi=\frac{1}{6},\frac{1}{8},0$, only the first kind of behavior is possible. In the case when $\alpha=1$, the energy was calculated numerically in Ref. 20 and our results are in agreement with that calculation. In this case $b_2^R=-\pi^2 16/315$, $b_{5/2}^R=-\pi^{3/2}/120$ and the dependence may be of the first kind only.

In the limit $R\to\infty$, the quantum correction tends to zero and the full energy contains only the classical part which is due to boundary and background.

Let us now proceed in our model. We surround the monopole origin by spheres of radii r_0 and $R>r_0$ and consider the bosonic matter field in the space between them. We do not take into account the interior of the sphere of radius r_0 because there is nothing inside it. We impose the Dirichlet boundary condition on this sphere which means that there is no flux into this region. The full energy in this case consists of five parts,

$$E=E_{cl}^R+E_{cl}^{r_0}+E_{cl}^{gm}+E_q^R+E_q^{r_0}, \tag{63}$$

where

$$E_{cl}^R=p_R V_R+\sigma_R S_R+F_R R+\Lambda_R+\frac{h_R}{R}, \tag{64}$$

$$E_{cl}^{r_0}=p_{r_0} V_{r_0}+\sigma_{r_0} S_{r_0}+F_{r_0} r_0+\Lambda_{r_0}+\frac{h_{r_0}}{r_0}, \tag{65}$$

$$E_{cl}^{gm}=-4\pi\eta^2\alpha(R-r_0) \tag{66}$$

are the classical parts of energy due to the boundaries and global monopole background, and

$$E_q^R=\frac{1}{2}M^{2s}\zeta_A^R\left(s-\frac{1}{2}\right)_{s\to 0}=-\frac{m}{32\pi^2\beta}\{B^R(\beta)\ln\beta^2+\Omega^R(\beta)\}+\left(\frac{M}{m}\right)^{2s}\frac{1}{16\pi^{3/2}}$$
$$\times\left\{B_0^R m^4\frac{\Gamma(s-2)}{\Gamma(s-\frac{1}{2})}-\frac{2}{3}B_{1/2}^R m^3+B_1^R m^2\frac{\Gamma(s-1)}{\Gamma(s-\frac{1}{2})}+B_{3/2}^R m+B_2^R\frac{\Gamma(s)}{\Gamma(s-\frac{1}{2})}\right\}_{s\to 0}, \tag{67}$$

$$E_q^{r_0}=\frac{1}{2}M^{2s}\zeta_A^{r_0}\left(s-\frac{1}{2}\right)_{s\to 0}=-\frac{m}{32\pi^2\beta_0}\{B^{r_0}(\beta_0)\ln\beta_0^2+\Omega^{r_0}(\beta_0)\}+\left(\frac{M}{m}\right)^{2s}\frac{1}{16\pi^{3/2}}$$
$$\times\left\{B_0^{r_0} m^4\frac{\Gamma(s-2)}{\Gamma(s-\frac{1}{2})}-\frac{2}{3}B_{1/2}^{r_0} m^3+B_1^{r_0} m^2\frac{\Gamma(s-1)}{\Gamma(s-\frac{1}{2})}+B_{3/2}^{r_0} m+B_2^{r_0}\frac{\Gamma(s)}{\Gamma(s-\frac{1}{2})}\right\}_{s\to 0} \tag{68}$$

are the quantum corrections. Adopting the same renormalization prescription for parameters in E_{cl}^R and $E_{cl}^{r_0}$ as in Eq. (59), one arrives at the following expressions for renormalized quantum corrections:

$$E_q^R=-\frac{m}{32\pi^2\beta}\{B^R(\beta)\ln\beta^2+\Omega^R(\beta)\} \tag{69}$$

and

$$E_q^{r_0}=-\frac{m}{32\pi^2\beta_0}\{B^{r_0}(\beta_0)\ln\beta_0^2+\Omega^{r_0}(\beta_0)\}. \tag{70}$$

The sum of these terms gives the Casimir energy of the field in space between the two spheres in the global monopole background. The first part we have already discussed. We may consider the second part in the same way. For the small radius of the sphere, $r_0\to 0$, it tends to infinity,

$$E_q^{r_0}\sim-\frac{m}{16\pi^2\beta_0}b_2^{r_0}\ln\beta_0, \tag{71}$$

and for the large radius of the sphere $r_0\to\infty$ it tends to zero,

$$E_q^{r_0}\sim-\frac{m b_{5/2}^{r_0}}{16\pi^{3/2}\beta_0^2}. \tag{72}$$

Due to the fact that $b_2^{r_0}=-b_2^R$ and $b_{5/2}^{r_0}=b_{5/2}^R$, the energy $E_q^{r_0}$ has different behavior at small radius r_0. The sum of b_n^R and $b_n^{r_0}$ constitutes the whole heat kernel coefficients for this space. For this reason three kinds of dependence of $E_q^{r_0}$ on the radius are possible, and these are displayed in Fig. 1. The same results are available for $E_q^{r_0}$ as it was obtained above for E_q^R for $\xi=\frac{1}{6},\frac{1}{8},0$; we have to change only the left plot to the right one in Fig. 1. The case $b_2=0$ has to be analyzed numerically; however, this discussion is out of the scope of the present article.

For any nonzero radius of the inner cavity r_0 we have a finite result. In this case the Casimir energy may be positive or negative, depending on the parameters of the theory. The main problem now is with the limit $r_0\to 0$, which has to reproduce the topological defect itself. The energy $E_q^{r_0}$ presents divergence in this limit as $\ln r_0/r_0$. This is in contradiction with earlier considerations about the pointlike monopole. If we set the radius $r_0=0$ at the beginning, as it was done in Sec.

III, we obtain zero ground state energy for $R\to\infty$. From the point of view of heat kernel coefficients we have already thrown away the divergent part of B_2 using *partie finite* of integral (33). In the framework of our model this part is divergent at the origin and the additional renormalization is needed.

In order to do the renormalization we may use the last term h_{r_0}/r_0 in the classical part of the energy which is due to the boundary (65). We define a parameter M_0 with dimension of mass by the relation $h_{r_0}=GM_0^2$, where G is gravitational constant. With this definition, the divergent contribution for small radius r_0 may be canceled by the renormalization rule

$$M_0^2\to M_0^2+\frac{m_{\mathrm{Pl}}^2}{32\pi^2}\{2B^{r_0}\ln(mr_0)+\Omega^{r_0}(mr_0)\}, \tag{73}$$

where m_{Pl}^2 is the Plank mass, and then ground state energy is zero.

VI. CONCLUSION

In this article we have considered the ground state energy of a quantum scalar field in the background of global monopole space–time, with a line element given by Eq. (2), in the framework of zeta function approach. In order to point out the role of singularity, we investigated two cases: In the first, we calculated the ground state energy for a pointlike global monopole. We surrounded the origin by a sphere of radius R and obtained the ground state energy of the field inside. It has the form (60) and tends to zero in the limit $R\to\infty$ and to infinity when $R\to 0$. The behavior of this Casimir energy in these cases is determined by the heat kernel coefficients b_2^R and $b_{5/2}^R$. The qualitative plots of the ground state energy for different values of the parameters $\xi=\frac{1}{6},\ \frac{1}{8},0$ and α are given in Fig. 1(a). For these values of ξ and $\alpha\leqslant 1$ it is of the first kind only.

In order to avoid the problem with singularity at origin, we investigated as a second case, in Sec. IV, the following model: We surrounded the origin by a sphere of radius $r_0<R$ and considered the scalar field in the region between these two spheres using the Dirichlet boundary condition on the wave function associated with the massive scalar field on these surfaces. This boundary condition guarantees that there is no flux of particles through the spherical surfaces. The Casimir energy in this case consists of two parts given in Eqs. (69) and (70). The first part is the same as for the pointlike monopole case and the second one is due to the inner sphere of radius r_0 around the origin. The structure of the second part of the ground state energy (70) is similar: there is a logarithmic divergence at origin which tends to zero for infinite radius. The sign of energy for a small distance is opposite. For this reason we have the three kinds of dependence of energy displayed in Fig. 1(b).

In the limit $R\to\infty$ and finite $r_0\neq 0$ only one contribution to the ground state energy survives (69). In the limit $r_0\to 0$, it is divergent and additional renormalization is needed which is given by Eq. (73). After this renormalization, the ground state energy of a global monopole will be zero. This is in agreement with the ground state energy of a pointlike global monopole.

If one fills up this cavity around the origin with matter, the situation becomes different. We may expect the same kind of divergence for additional energy from the interior of the monopole but with opposite sign. We have already seen that the internal and external contributions have opposite signs: $b_2^R=-b_2^{r_0}$. For this reason we may expect that this kind of divergence will cancel. However, we cannot say anything analytically about the divergence of $\Omega(mr_0)/r_0$. In flat space-time[20] it cancels, too, because the ground state energy is zero for zero radius of the bag. The same cancellation takes place in the case of a thick cosmic string background considered in Ref. 13. All of these aspects will be discussed in a separate paper.

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APPENDIX: FORMULAS FOR ZETA-FUNCTION

In this appendix we want to give a brief explanation about the most important results we found. First of all, we represent the expressions for A_k as a series in powers of $\beta=mr_0$, regarding for a moment $b,\beta<1$ and $\Delta>-\frac{1}{4}$ in order to have convergence of series. They are

$$A_{-1}(s,R)=\frac{m}{\beta}\beta^{2s}\frac{4\pi}{\alpha}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\beta^{2n}\frac{\Gamma(s-1+n)}{s+n-\frac{1}{2}}\sum_{l=0}^{\infty}\frac{\nu_l}{(\nu_l^2+\Delta)^{s+n-1}}, \tag{A1}$$

$$A_0(s,R)=-\frac{m}{\beta}\beta^{2s}4\pi^{3/2}\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}b^{2n}\Gamma\left(s+n-\frac{1}{2}\right)\zeta_H\left(2s+2n-2,\frac{1}{2}\right), \tag{A2}$$

$$A_k(s,R)=-\frac{m}{\beta}\beta^{2s}16\pi^{3/2}\alpha^k\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}b^{2n}\sum_{a=0}^{k}x_{k,a}\frac{\Gamma(s+k/2+a+n-\frac{1}{2})}{\Gamma(k/2+a)}\times\sum_{l=0}^{\infty}\frac{(\nu_l^2+\Delta)^a}{\nu_l^{2s+k+2a+2n-2}}. \tag{A3}$$

In the above formulas we have used the following notations: $\nu_l=l+\frac{1}{2}$, $\Delta=2(1-\alpha^2)(\xi-\frac{1}{8})$ and $b^2=\beta^2+\Delta$. As we can see, only the first three terms in the expression for A_{-1}, with $n=0,1,2$, two terms in A_0, A_1, A_2, and one term in A_3 are divergent in the limit $s\to 0$. Extracting these terms we may set $s=0$ in the remaining series and we get the following result:

$$\begin{aligned}\zeta_A^R\left(s-\frac{1}{2}\right)&=N^R(s,\beta)+\frac{m^{-2s}}{(4\pi)^{3/2}\Gamma(s-\frac{1}{2})}\sum_{k=-1}^{3}A_k(s,R)\\&=\frac{m^{-2s}}{(4\pi)^{3/2}\Gamma\left(s-\frac{1}{2}\right)}\beta^{2s}\left\{m^4B_0^R\Gamma(s-2)+m^3B_{1/2}^R\Gamma\left(s-\frac{3}{2}\right)+m^2B_1^R\Gamma(s-1)\right.\\&\quad\left.+mB_{3/2}^R\Gamma\left(s-\frac{1}{2}\right)+B_2^R\Gamma(s)\right\}-\frac{1}{16\pi^2R}\left\{\sum_{k=-1}^{3}\omega_k(\beta)+\omega_f^R(\beta)\right\},\end{aligned} \tag{A4}$$

where

$$\begin{aligned}\omega_f^R(\beta)&=32\pi\sum_{l=0}^{\infty}\nu_l\sqrt{\nu_l^2+\Delta}\int_{\beta/\sqrt{\nu_l^2+\Delta}}^{\infty}dx\sqrt{x^2-\frac{\beta^2}{\nu_l^2+\Delta}}\\&\quad\times\frac{\partial}{\partial x}\left\{\ln I_\mu(\mu x)-\mu\eta(x)+\frac{1}{4}\ln(1+x^2)-\frac{1}{\mu}D_1-\frac{1}{\mu^2}D_2-\frac{1}{\mu^3}D_3\right\},\end{aligned} \tag{A5}$$

$$\begin{aligned}\omega_{-1}(\beta)&=-\frac{4\pi}{\alpha}\left\{\left[-\frac{7}{2}\zeta'(-3)-\frac{7}{160}+\frac{1}{240}\ln 2+\Delta\left(-2\zeta'(-1)+\frac{1}{6}-\frac{1}{6}\ln 2\right)\right]\right.\\&\quad+\beta^2\left[2\zeta'(-1)+\frac{1}{4}+\frac{1}{6}\ln 2+\Delta(2\gamma+4\ln 2-3)\right]+\beta^4\left[\frac{1}{3}\gamma+\frac{2}{3}\ln 2-\frac{13}{36}\right]\\&\quad\left.-\sum_{n=3}^{\infty}\frac{(-1)^n}{n!}\Gamma(n-1)\Delta^n\zeta_H\left(2n-3,\frac{1}{2}\right)-2\beta^2\sum_{n=2}^{\infty}\frac{(-1)^n}{n!}\Delta^n\Gamma(n)\zeta(2n-1)\right\}\end{aligned}$$

$$+\frac{1}{3}\beta^4 Y_{1,1}(\Delta)+\sum_{n=3}^{\infty}\frac{(-1)^n}{n!}\frac{\Gamma(n-1)}{n-\frac{1}{2}}\beta^{2n}\sum_{l=0}^{\infty}\frac{\nu_l}{(\nu_l^2+\Delta)^{n-1}}\Bigg\}, \tag{A6}$$

$$\omega_0(\beta)=-2\pi^2\sum_{n=2}^{\infty}\frac{(-1)^n}{n!}\frac{\Gamma(n-\frac{1}{2})}{\Gamma(\frac{3}{2})}b^{2n}\zeta_H\left(2n-2,\frac{1}{2}\right), \tag{A7}$$

$$\omega_1(\beta)=-2\pi\alpha\Bigg\{\left[-\zeta'(-1)-\frac{5}{36}-\frac{1}{12}\ln 2+\Delta\left(-\gamma-2\ln 2+\frac{5}{3}\right)\right]+\beta^2\left[\frac{7}{3}\gamma+\frac{1}{2}+\frac{14}{3}\ln 2\right]$$
$$+\sum_{n=2}^{\infty}\frac{(-1)^n}{n!}\left(\Gamma(n)-\frac{10}{3}\Gamma(n+1)\right)b^{2n}\zeta_H\left(2n-1,\frac{1}{2}\right)-\frac{10}{3}\Delta Y_{1,1}(b)\Bigg\}, \tag{A8}$$

$$\omega_2(\beta)=-2\pi^2\alpha^2\Bigg\{\frac{3}{16}\pi^2\Delta+\frac{5}{32}\pi^2\Delta^2+\frac{1}{2}Y_{1/2,0}(b)-\frac{3}{2}Y_{3/2,0}(b)+\frac{15}{16}Y_{5/2,0}(b)$$
$$+\Delta\left[-\frac{3}{2}Y_{3/2,2}(b)+\frac{15}{8}Y_{5/2,2}(b)\right]+\Delta^2\frac{15}{16}Y_{5/2,4}(b)\Bigg\}, \tag{A9}$$

$$\omega_3(\beta)=-2\pi\alpha^3\Bigg\{\frac{293}{1512}-\frac{22}{2520}\gamma-\frac{229}{1260}\ln 2+\left[\frac{25}{24}X_{1,1}(b)-\frac{177}{20}X_{2,1}(b)\right.$$
$$\left.+\frac{221}{15}X_{3,1}(b)-\frac{442}{63}X_{4,1}(b)\right]+\Delta\left[-\frac{177}{20}Y_{2,3}(b)+\frac{442}{15}Y_{3,3}(b)-\frac{442}{21}Y_{4,3}(b)\right]$$
$$+\Delta^2\left[\frac{221}{15}Y_{3,5}(b)-\frac{442}{21}Y_{4,5}(b)\right]-\Delta^3\frac{442}{63}Y_{4,7}(b)\Bigg\}, \tag{A10}$$

$$X_{p,q}(b)=\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\frac{\Gamma(n+p)}{\Gamma(p)}b^{2n}\zeta_H\left(2n+q,\frac{1}{2}\right), \tag{A11}$$

$$Y_{p,q}(b)=\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\frac{\Gamma(n+p)}{\Gamma(p)}b^{2n}\zeta_H\left(2n+q,\frac{1}{2}\right). \tag{A12}$$

Each of the above series may be analytically continued in terms of digamma function Ψ for arbitrary values of b and Δ. For example,

$$\sum_{n=3}^{\infty}\frac{(-1)^n}{n!}\frac{\Gamma(n-1)}{n-\frac{1}{2}}\beta^{2n}\sum_{l=0}^{\infty}\frac{\nu_l}{(\nu_l^2+\Delta)^{n-1}}=-2\beta^4\int_0^1 dx x(1-x)^2$$
$$\times\left\{\Psi\left[\frac{1}{2}-i\sqrt{\Delta+\beta^2x^2}\right]+\Psi\left[\frac{1}{2}+i\sqrt{\Delta+\beta^2x^2}\right]-\Psi\left[\frac{1}{2}-i\sqrt{\Delta}\right]-\Psi\left[\frac{1}{2}+i\sqrt{\Delta}\right]\right\}, \tag{A13}$$

$$\sum_{n=3}^{\infty}\frac{(-1)^n}{n!}\Gamma(n-1)\Delta^n\zeta_H\left(2n-3,\frac{1}{2}\right)$$
$$=-\Delta^2\int_0^1 dx x(1-x^2)\left\{\Psi\left[\frac{1}{2}-i\sqrt{\Delta}\right]+\Psi\left[\frac{1}{2}+i\sqrt{\Delta}\right]-2\Psi\left[\frac{1}{2}\right]\right\}. \tag{A14}$$

This kind of representation is suitable for numerical calculations.

Adding and subtracting the asymptotic expansion of zeta function (25) we obtain the following formula:

$$\zeta_A^R\left(s-\frac{1}{2}\right)=-\frac{m}{16\pi^2\beta}\{B^R(\beta)\ln\beta^2+\Omega^B(\beta)\}+\frac{m^{-2s}}{(4\pi)^{3/2}}\left\{B_0^R m^4\frac{\Gamma(s-2)}{\Gamma(s-\frac{1}{2})}\right.$$
$$\left.+B_{1/2}^R m^3\frac{\Gamma(s-\frac{3}{2})}{\Gamma(s-\frac{1}{2})}+B_1^R m^2\frac{\Gamma(s-1)}{\Gamma(s-\frac{1}{2})}+B_{3/2}^R m+B_2^R\frac{\Gamma(s)}{\Gamma(s-\frac{1}{2})}\right\},\qquad\text{(A15)}$$

where $\Omega^B(\beta)=\Sigma_{k=-1}^3\omega_k(\beta)+\omega_f^R(\beta)$. It is easy to see that the function $\Omega^B(\beta)$ tends to a constant which may be calculated using the above formulas. Indeed, in the limit $\beta\to\infty$ we have to obtain asymptotic expansion of zeta function. Because one has already extracted the first five terms, the next will be $B_{5/2}$. For this reason we get the following behavior for great β: $\Omega^B(\beta)\sim -B^R\ln\beta^2+\sqrt{\pi}b_{5/2}^R/\beta+\cdots$. The coefficient $b_{5/2}^R$ may be found in the same way and it has the following form:

$$b_{5/2}^R=\frac{R}{m}B_{5/2}^R=\pi^{3/2}\{\tfrac{1}{16}\alpha^4+\tfrac{1}{2}(\Delta-\tfrac{1}{12})\alpha^2-(\Delta^2-\tfrac{1}{6}\Delta+\tfrac{7}{240})\}.\qquad\text{(A16)}$$

It is not difficult to obtain the formulas for zeta function $\zeta_A^{r_0}$ from the above expressions. The index k in A_k corresponds to a term which is proportional to μ^{-k} in uniform expansion of the Bessel function in Eq. (8). The uniform expansion of the modified Bessel function of the second kind given in Eq. (46) may be obtained from uniform expansion of the modified Bessel function of the first kind in (7) by replacing the index μ by $-\mu$. For this reason, in order to obtain the formulas for the zeta function $\zeta_A^{r_0}$, we must do the replacements $R\to r_0$, $\beta\to\beta_0$ and $A_k(s,R)\to(-1)^kA_k(s,r_0)$ in the above formulas for zeta function ζ_A^R. As the odd degrees of μ give contributions to heat kernel coefficients with integer index, they will change the sign. Therefore we have the following formula for zeta function $\zeta_A^{r_0}$:

$$\zeta_A^{r_0}\left(s-\frac{1}{2}\right)=-\frac{m}{16\pi^2\beta_0}\{B^{r_0}(\beta_0)\ln\beta_0^2+\Omega^{r_0}(\beta_0)\}+\frac{m^{-2s}}{(4\pi)^{3/2}}\left\{B_0^{r_0}m^4\frac{\Gamma(s-2)}{\Gamma(s-\frac{1}{2})}\right.$$
$$\left.+B_{1/2}^{r_0}m^3\frac{\Gamma(s-\frac{3}{2})}{\Gamma(s-\frac{1}{2})}+B_1^{r_0}m^2\frac{\Gamma(s-1)}{\Gamma(s-\frac{1}{2})}+B_{3/2}^{r_0}m+B_2^{r_0}\frac{\Gamma(s)}{\Gamma(s-\frac{1}{2})}\right\},\qquad\text{(A17)}$$

where $\Omega^{r_0}(\beta_0)=\Sigma_{k=-1}^3(-1)^k\omega_k(\beta_0)+\omega_f^{r_0}(\beta_0)$ and

$$\omega_f^R(\beta)=32\pi\sum_{l=0}^{\infty}\nu_l\sqrt{\nu_l^2+\Delta}\int_{\beta/\sqrt{\nu_l^2+\Delta}}^{\infty}dx\sqrt{x^2-\frac{\beta^2}{\nu_l^2+\Delta}}$$
$$\times\frac{\partial}{\partial x}\left\{\ln K_\mu(\mu x)+\mu\eta(x)+\frac{1}{4}\ln(1+x^2)+\frac{1}{\mu}D_1-\frac{1}{\mu^2}D_2+\frac{1}{\mu^3}D_3\right\}.\qquad\text{(A18)}$$

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Maximal subalgebras of vector fields for equivariant quantizations

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The elaboration of new quantization methods has recently developed the interest in the study of subalgebras of the Lie algebra of polynomial vector fields over a Euclidean space. In this framework, these subalgebras define maximal equivariance conditions that one can impose on a linear bijection between observables that are polynomial in the momenta and differential operators. Here, we determine which finite dimensional graded Lie subalgebras are maximal. In order to characterize these, we make use of results of Guillemin, Singer, and Sternberg and Kobayashi and Nagano. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1332782]

I. INTRODUCTION

Our interest in the present study comes from recent works about new equivariant quantizations (Refs. 1 and 2).

One can define quantization maps as linear bijections $\mathcal{Q}$ from the space $\mathrm{Pol}(T^*M)$ of functions on the cotangent bundle of a smooth manifold M, that are polynomial on the fibre, to a space $D_\lambda(M)$ of differential operators acting on tensor densities of weight λ over M.

It is known that a quantization map $\mathcal{Q}$ cannot be equivariant with respect to all diffeomorphisms of M. From the infinitesimal point of view, this means that such a map does not commute with the action on these spaces of the Lie algebra $\mathrm{Vect}(M)$ of vector fields over M. In other words, differential operators and polynomials are inequivalent modules of $\mathrm{Vect}(M)$.

However, when M is endowed with an additional structure, some particular subalgebras of $\mathrm{Vect}(M)$ naturally deserve consideration, because they are made up of infinitesimal transformations preserving the structure.

The authors of Refs. 1 and 2 considered the case of infinitesimal projective or conformal transformations of M. In suitable charts, these can be realized in polynomial vector fields over a Euclidean space. For instance, if M is endowed with a projective structure (i.e., M is locally identified with a real projective space, say of dimension n) then in appropriate charts, the Lie algebra of infinitesimal projective transformations—isomorphic to $\mathrm{sl}(n+1,\mathbb{R})$—is generated by the vector fields,

$$\frac{d}{dx^j}, x^j\frac{d}{dx^k}, x^j\sum_{l=1}^{n} x^l\frac{d}{dx^l}, \quad \forall j,k\leqslant n. \tag{1}$$

In this setting, those conformal and projective subalgebras share the property of being maximal in the algebra of polynomial vector fields: they are not contained in any larger proper subalgebra. The reader may refer to Refs. 2 and 3 for proofs.

Now, it was proved in Refs. 1 and 2 that one could construct a quantization map equivariant with respect to those subalgebras. This quantization is unique up to normalization.

In this framework, our concern in the present paper is to determine all finite dimensional graded subalgebras of polynomial vector fields over a given Euclidean space that are maximal.

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Independently of quantization purposes, other maximality conditions have also been studied.

In Ref. 4, Kantor classified irreducible transitively differential groups. This notion gives rise, from the Lie algebraic point of view, to the class of finite dimensional graded Lie subalgebras of polynomial vector fields containing all constant vector fields. The author then seeks for irreducible (see Ref. 4, p. 1405 or below) subalgebras being maximal in this class.

Another more recent study is that of Post (Ref. 5). In this paper, a stronger grading requirement is imposed in order to define a class of finite dimensional Lie algebras containing all constant vector fields. All maximal subalgebras of this class are then identified.

We point out two differences between the maximality conditions examined here and in these studies.

On the one hand, we impose fewer conditions on the subalgebras we consider, keeping only the requirements for a subalgebra to be graded and finite dimensional. On the other hand, the maximality property is not investigated inside a particular class of subalgebras, but in the general class of all subalgebras of polynomial vector fields.

Before giving our main result and a brief description of the tools we shall use, let us fix some notations.

Throughout this note, we assume that E is an n-dimensional vector space over $\mathbb{K}$, which is taken to be $\mathbb{R}$ or $\mathbb{C}$. We shall deal with polynomial vector fields over E.

We denote by $\mathrm{Vect}_*(E)$ the space of these vector fields, i.e., the space of polynomial maps from E to E. It is worth noticing that the vector fields considered when E is complex are thus holomorphic. Let $\{e_j, j=1,...,n\}$ be a basis of E. Assume that $X, Y \in \mathrm{Vect}_*(E)$ are written $X=\Sigma_{j=1}^n X^j e_j$ and $Y=\Sigma_{j=1}^n Y^j e_j$. We denote as usual by $[X, Y]$ the Lie bracket

$$\sum_{j,k} X^j \partial_j Y^k e_k - Y^j \partial_j X^k e_k,$$

where ∂_j represents the derivation d/dx^j along the jth axis. For the sake of convenience, we shall also use this notation to designate the jth vector of a basis of E. We denote by $\mathrm{ad}(X)$ the map $Y \mapsto [X,Y]$.

We name Euler vector field the identity transformation of E. In a basis $\{\partial_j\}$, it reads

$$\mathcal{E}(x)=\sum x^j \partial_j .$$

It defines a natural grading on $\mathrm{Vect}_*(E)$,

$$\mathrm{Vect}_*(E)=\bigoplus_{p \geqslant -1} \mathrm{Vect}_p(E),$$

where $\mathrm{Vect}_p(E)$ denotes the space of eigenvectors of $\mathrm{ad}(\mathcal{E})$ associated with the eigenvalue p, i.e., vector fields with homogeneous coefficients of degree $p+1$.

We are interested in these graded subalgebras L,

$$L=\bigoplus_{-1 \leqslant p \leqslant r} L_p \quad \text{with} \quad L_p=\mathrm{Vect}_p(E) \cap L,$$

which are maximal in $\mathrm{Vect}_*(E)$. As mentioned above, the notion of maximality has been used in various senses. Therefore, it is worth emphasizing the following definition.

Definition 1: A subalgebra L of $\mathrm{Vect}_*(E)$ is maximal if

$$L \subset L' \Rightarrow L'=L \quad \text{or} \quad L'=\mathrm{Vect}_*(E),$$

whenever L' is a subalgebra of $\mathrm{Vect}_*(E)$.

II. MAIN RESULT

Definition 2: (See, for instance, Ref. 6, p. 682.) A graded subalgebra $L=L_{-1}\oplus\cdots\oplus L_k$ of $\mathrm{Vect}_*(E)$ is said to be irreducible if the representation $(L_{-1},\mathrm{ad}_{|L_0})$ is irreducible.

Theorem 1: *Let $L=L_{-1}\oplus\cdots\oplus L_k$ be a graded subalgebra of $\mathrm{Vect}_*(E)$. Then L is maximal if and only if*

(1) $L_{-1}=\mathrm{Vect}_{-1}(E)$;

(2) L is irreducible;

(3) $L_1\neq 0$;

(4) when $\mathbb{K}=\mathbb{R}$, the representation $(L_{-1},\mathrm{ad}_{|L_0})$ admits no complex structure.

The text below is organized as follows. In Sec. III, we prove the necessity of the first three conditions above. Then, in Sec. IV, we consider polynomial vector fields from a slightly modified point of view, in order to prove, in Sec. V, the fourth condition given above. We expose in Sec. VI how the graded maximal subalgebras relate to the irreducible filtered Lie algebras of finite type, which were classified in Ref. 7. Using the classification of all irreducible infinite dimensional subalgebras of polynomial vector fields (see, for instance, Refs. 8, 9, 10, 6, and references therein), we show in Sec. VII that all these algebras give rise to a canonical graded maximal subalgebra of polynomial vector fields.

III. CONSTANT VECTOR FIELDS AND IRREDUCIBILITY

Lemma 1: Let L be a maximal subalgebra of $\mathrm{Vect}_*(E)$. Then $\mathcal{E}\in L$ if and only if L is graded.

Proof: The sufficiency of the condition follows from the fact that

$$\mathbb{K}\mathcal{E}+L$$

is a Lie subalgebra when L is graded. In order to check the necessity of the condition, notice that

$$\mathrm{ad}(\mathcal{E})^k L\subset L,\quad \forall k\in\mathbb{N},$$

gives a Vandermonde system allowing to compute the homogeneous components of a vector field $X\in L$. □

This proof is similar to the proof by Koecher (see Ref. 11, p. 354) that any ideal of $\mathrm{Vect}_*(E)$ is graded. We therefore state the following remark:

Remark 1: If L is a subalgebra of $\mathrm{Vect}_*(E)$ that contains $\mathcal{E}$, then any ideal of L is graded.

Lemma 2: Let L_{-1}, L_0, and L_+ be vector subspaces of $\mathrm{Vect}_{-1}(E)$, $\mathrm{Vect}_0(E)$, and $\oplus_{i\geqslant 1}\mathrm{Vect}_i(E)$, respectively, such that

(1) $L_{-1}\oplus L_0$ is a Lie subalgebra;

(2) $[L_{-1},L_+]\subset L_0\oplus L_+$, and $[L_0,L_+]\subset L_+$.

Set $c^0(L_+)=L_+$ and $c^{k+1}(L_+)=[L_+,c^k(L_+)]$, $(k\in\mathbb{N})$.

Then the smallest Lie subalgebra containing

$$L_{-1}\oplus L_0\oplus L_+$$

is

$$L_{-1}\oplus L_0\oplus\sum_{k\in\mathbb{N}} c^k(L_+).$$

In particular, if $L_+\subset\mathrm{Vect}_1(E)$, the latter subalgebra is graded.

Proof: Using Jacobi identity, we check that $[L_0,c^k(L_+)]\subset c^k(L_+)$ and consequently $[L_{-1},c^k(L_+)]\subset\Sigma_{i=0}^k c^k(L_+)$ by induction on $k\geqslant 1$. By definition, $[c^0(L_+),c^k(L_+)]=c^{k+1}(L_+)$ for all $k\in\mathbb{N}$. Then, we check, by induction on $j\geqslant 0$, that $[c^j(L_+),c^k(L_+)]\subset c^{j+k+1}(L_+)$.

Therefore, $L_{-1}\oplus L_0\oplus\Sigma_{k\in\mathbb{N}}c^k(L_+)$ is a Lie subalgebra. It is trivially the smallest one to contain the subspaces L_{-1}, L_0 and L_+. □

Definition 3: Let F be a vector subspace of $\mathrm{Vect}_{-1}(E)$. We set

$$\mathcal{N}^i(F)=\{X\in\mathrm{Vect}_i(E):\mathrm{ad}(F)^{i+1}X\subset F\}$$

and

$$\mathcal{N}(F)=\oplus_{i\geqslant -1}\mathcal{N}^i(F).$$

Notice that $\mathcal{N}^{-1}(F)=F$ and that $\mathcal{N}^0(F)$ is the intersection of the normalizer of F and the subspace of linear vector fields.

Proposition 2: Let $L=\oplus_{i\geqslant -1}L_i$ be a graded subalgebra of $\mathrm{Vect}_*(E)$. Then $\mathcal{N}(L_{-1})$ is an infinite dimensional graded subalgebra containing L. Moreover, $\mathcal{N}(L_{-1})=\mathrm{Vect}_*(E)$ if and only if $L_{-1}=\mathrm{Vect}_{-1}(E)$.

Proof: It is obvious that $[\mathcal{N}^i(L_{-1}),\mathcal{N}^j(L_{-1})]\subset\mathcal{N}^{i+j}(L_{-1})$. Furthermore, if $L_{-1}=0$ or $L_{-1}=\mathrm{Vect}_{-1}(E)$,

$$\mathcal{N}(L_{-1})=L_{-1}\oplus\bigoplus_{i\geqslant 0}\mathrm{Vect}_i(E).$$

Now, if $h\in L_{-1}$, then, for every polynomial function $p:E\to\mathbb{K}$, the field $x\mapsto p(x)h$ belongs to $\mathcal{N}(L_{-1})$. □

Corollary 3: Let L be a finite dimensional graded maximal subalgebra of $\mathrm{Vect}_*(E)$. Then $\mathrm{Vect}_{-1}(E)\subset L$.

Corollary 4: Let L be a finite dimensional graded maximalsubalgebra of $\mathrm{Vect}_*(E)$. Then $L_1\neq 0$.

Proof: Notice that L cannot be made only of constant and linear vector fields. Indeed, it would then be included in the maximal subalgebra (1) presented in the introduction, for instance. Therefore, $L_k\neq 0$ for some $k>0$. The conclusion follows from Corollary 3. □

Proposition 5: Let L be a finite dimensional graded maximal subalgebra of $\mathrm{Vect}_*(E)$. Then

$$(L_{-1}=\mathrm{Vect}_{-1}(E),\mathrm{ad}_{|L_0})$$

is an irreducible representation of L_0. It follows that any nontrivial ideal of L contains every constant vector field.

Proof: Let $F\neq\{0\}$ be a stable subspace of L_{-1} under the action of L_0.

The space

$$L_{-1}\oplus\mathcal{N}^0(F)\oplus\bigoplus_{i\geqslant 1}\{X\in\mathrm{Vect}_i(E):\mathrm{ad}(L_{-1})^iX\subset\mathcal{N}^0(F)\}$$

satisfies the hypotheses of Lemma 2. Its algebraic closure is an infinite dimensional proper subalgebra containg L properly, hence a contradiction.

Let now I be a nontrivial ideal of L. It contains at least one constant vector field since $[\mathrm{Vect}_{-1}(E),I]\subset I$. It contains all of them since $I\cap L_{-1}$ is a stable subspace of L_{-1}. □

IV. A CONVENIENT MODEL FOR POLYNOMIAL VECTOR FIELDS

It will be useful to consider the spaces of multilinear symmetric mappings from $E\times\cdots\times E$ to E instead of those of homogeneous polynomial vector fields. We shall write

$$\mathcal{T}_i(E)=S^{i+1}E^*\otimes E,\quad\text{and}\quad\mathcal{T}_*(E)=\bigoplus_{i\geqslant -1}\mathcal{T}_i(E).$$

To turn $\mathcal{T}_*(E)$ into a Lie algebra, we define as in Ref. 6 the following bracket operation. If $t\in\mathcal{T}_p(E)$ and $t'\in\mathcal{T}_q(E)$ then $[t,t']\in\mathcal{T}_{p+q}(E)$ and

$$[t,t'](x_0,x_1,\ldots,x_{p+q})=\frac{1}{p!(q+1)!}\sum_j t(t'(x_{j_0},x_{j_1},\ldots,x_{j_q}),x_{j_{q+1}},\ldots,x_{j_{p+q}})$$
$$-\frac{1}{(p+1)!q!}\sum_k t'(t(x_{k_0},x_{k_1},\ldots,x_{k_p}),x_{k_{p+1}},\ldots,x_{k_{p+q}}),$$

where both j and k run over all possible permutations of the $p+q+1$ first natural numbers.

Proposition 6: The map $T:\mathcal{T}_*(E)\to\mathrm{Vect}_*(E)$ *defined by*

$$T(M):x\in E\mapsto-\frac{1}{(p+1)!}M(x,\ldots,x),\quad\forall M\in\mathcal{T}_p(E)$$

is an isomorphism of Lie algebras.

V. ABSENCE OF COMPLEX STRUCTURE

We now assume $\mathbb{K}=\mathbb{R}$ and prove, in Lemma 3, the fourth condition of maximality of our main result.

Let E be a real vector space of even dimension and J a complex structure of E, i.e., an endomorphism of E such that $J^2=-id$. We denote by E_J the complex vector space defined by E with the structure of $\mathbb{C}$-module defined by

$$(a+ib)e:=ae+bJe,\quad\forall a,b\in\mathbb{R},\quad\forall e\in E.$$

Define

$$\mathcal{T}_p^J(E)=\{M\in\mathcal{T}_p(E)\,|\,J(M(x_0,\ldots,x_p))=M(Jx_0,x_1\ldots,x_p),\forall x_0,\ldots,x_p\in E\}$$

for all $p\geqslant-1$. Then the subalgebra $\mathcal{T}_*^J(E)=\oplus_{i\geqslant-1}\mathcal{T}_p^J(E)$ of $\mathcal{T}_*(E)$ is isomorphic to $\mathcal{T}_*(E_J)$ as a real Lie algebra. Indeed, the condition defining $\mathcal{T}_*^J(E)$ means that an application $M\in\mathcal{T}_*(E)$ is $\mathbb{C}$-multilinear on E_J.

Lemma 3: Let E be a real vector space and $L=\mathcal{T}_{-1}(E)\oplus\oplus_{j=0}^k L_j$ *a graded subalgebra of* $\mathcal{T}_*(E)$. *Assume that J is a complex structure of* $(L_{-1},ad_{|L_0})$, *i.e.,*

$$[x_0,Jx_{-1}]=J[x_0,x_{-1}],\quad\forall x_0\in L_0,\forall x_{-1}\in L_{-1}$$

and

$$J^2=-id.$$

Then,

$$L\subset\mathcal{T}_*^J(L_{-1})\subset\mathcal{T}_*(L_{-1}),$$

where both inclusions are strict.

Proof: Indeed, $L_{-1}=\mathcal{T}_{-1}^J(E)=\mathcal{T}_{-1}(E)$. The requirement for J to intertwine the action of L_0 on L_{-1} precisely means that $L_0\subset\mathcal{T}_0^J(E)$. If $L_{k-1}\subset\mathcal{T}_{k-1}^J(E)$ and $M\in L_k$, the equalities

$$J\circ M(x_0,\ldots,x_k)=J([M,x_1](x_0,x_2,\ldots,x_k))=M(x_1,Jx_0,x_2,\ldots,x_k)=M(Jx_0,x_1,\ldots,x_k)$$

show that $M\in\mathcal{T}_k^J(E)$.

The inclusions are strict because the dimension of $\mathcal{T}_*^J(L_{-1})$ is infinite and because the dimension of $\mathcal{T}_p^J(L_{-1})$, for all $p\geqslant0$, is strictly less than that of $\mathcal{T}_p(L_{-1})$. □

This lemma generalizes the construction used in Ref. 3 to show that a subalgebra of infinitesimal conformal transformations, isomorphic to so(3, 1, $\mathbb{R}$), is not maximal in $\mathrm{Vect}_*(\mathbb{R}^2)$.

VI. IRREDUCIBLE FILTERED ALGEBRAS OF FINITE TYPE

Let $L=\oplus_{j=-1}^{k}L_j$ be a graded maximal subalgebra of polynomial vector fields. In the last section, we have shown that L possesses interesting properties. It actually belongs to a broader class of Lie algebras studied in Ref. 7, Theorem 1, p. 875.

This theorem describes the structure of some filtered finite dimensional Lie algebras together with a group of automorphisms.

We shall only associate the trivial group $\{id\}$ to such an algebra. Furthermore, the reader may find worth noticing that the algebras we consider carry the filtration which is naturally associated to their grading and that the other hypotheses of the theorem are satisfied in view of the first three conditions required in our main result for a subalgebra to be maximal.

For the sake of simplicity, we shall name algebras described by this theorem *Irreducible filtered algebras of finite type*, as it was done in Ref. 6, or simply write IFFT-algebras.

As a consequence of the mentioned result, we know that L is simple and is of order two, i.e., $L=L_{-1}\oplus L_0\oplus L_1$. Moreover, there exists a unique element $e\in L$ such that L_p is the eigenspace of $\mathrm{ad}(e)$ associated with the eigenvalue p. This element is thus in the center of L_0. We shall name it the Euler element of L. Finally, L_{-1} and L_1 are dual to each other as modules over L_0 with respect to the Killing form of L.

On the one hand, Kobayashi and Nagano gave a list of the admissible algebras and detailed in each case the associated grading. The pairs (L,e) where L is a real IFFT-algebra and e its Euler element are classified in Ref. 7, pp. 892–895. On the other hand, to any graded algebra $L=\oplus_{k\geqslant -1}L_k$, they associated in a natural way a graded subalgebra of $\mathcal{T}_*(L_{-1})$ (see Ref. 6, p. 683). The reader may compare this construction with that of Gradl (Ref. 12). In the case of $L=L_{-1}\oplus L_0\oplus L_1$, this is done by the following monomorphism $\phi: L\to\mathcal{T}_*(L_{-1})$,

$$\begin{cases}\phi_{|L_{-1}}=id,\\ \phi_{|L_0}=\mathrm{ad}_{|L_0},\\ \phi(M)=(x,y)\mapsto[[M,x],y]. \quad \forall M\in L_1,\forall x,y\in L_{-1}.\end{cases}$$

Notice that this is the only way to proceed provided the value of ϕ on L_{-1} is set to *id.*

VII. IFFT-ALGEBRAS ARE MAXIMAL

In this section, we prove the sufficiency of the conditions given in our main result for a subalgebra of polynomial vector fields to be maximal.

We first assume that E is a complex vector space and $L=L_{-1}\oplus L_0\oplus L_1$ an irreducible graded subalgebra of $\mathcal{T}_*(E)$ such that $L_{-1}=\mathcal{T}_{-1}(E)$ and $L_1\neq 0$. Then we shall show how the proof adapts to the real case.

Let L' be a subalgebra of $\mathcal{T}_*(E)$ such that $L'\supset L$. Then L' is graded and irreducible, since L is.

If L' is finite dimensional, one sees, by using the description of the IFFT-algebras (see Sec. VI), that $L'_1=L_1$, that L' is simple and eventually that $L=L'$, since $[L'_{-1},L'_1]=L_0$.

Therefore, if L' contains properly L, then it must be infinite dimensional. It possesses two additional properties, consequences of the following result.

Proposition 7 (Ref. 6, p. 688): *Let $\oplus_{p\geqslant -1}G_p$ be an irreducible graded Lie algebra of infinite type or finite type of order $\geqslant 2$ over a field of characteristic 0. Then G_0 is reductive and $[G_{-1},G_1]$ contains the semisimple part of G_0.*

(a) L'_0 is reductive and has a nontrivial center (the multiples of the identity transformation of L_{-1});

(b) L' is still simple. Indeed, if I is an ideal of L' then $I \supset L$ (see Proposition 5), which implies that I contains the multiples of the identity transformation of L_{-1} and in turn that $I \supset L'_j$ for all $j \neq 0$. Since $[L'_{-1}, L'_1]$ contains the semisimple part of L'_0, the conclusion follows.

In order to prove the maximality of L, the remaining point is to ensure that $L' = \mathcal{T}_*(E)$. The key result is due to Cartan. We refer the reader to the works of Guillemin, Quillen, Singer, Sternberg, Kobayashi, and Nagano (Refs. 8, 9, 10, 6).

This result states that the only irreducible infinite dimensional graded subalgebras of $\mathrm{Vect}_*(E)$ are

(1) $\mathrm{Vect}_*(E)$ itself;
(2) the divergence-free vector fields;
(3) the Hamiltonian vector fields with respect to a symplectic form given on E, provided E is even dimensional;
(4) the last two subalgebras supplemented with the multiples of the Euler vector field.

But the subalgebras described in (4) are not simple, and those in (2) and (3) have a simple linear part.

Hence the proof.

Now, when E is a real vector space and L and L' as above, one proceeds in the same way to prove the simplicity of L', noticing that both L_0 and L'_0 still have a one dimensional center.

Indeed, if x_0 is central in one of these two subalgebras, then $\mathrm{ad}(x_0)$ intertwines the action of L_0 on L_{-1}. Since the representation $(L_{-1}, \mathrm{ad}_{|L_0})$ admits no complex structure, Schur's lemma ensures that $\mathrm{ad}(x_0)_{|L_{-1}}$ is a multiple of the identity transformation of L_{-1}. Therefore, $\dim Z(L_0) = 1$.

The description of irreducible infinite dimensional graded subalgebras of $\mathrm{Vect}_*(E)$ is essentially due to Matsushima. It can be found in Refs. 6 and 13.

Two cases arise whether $L'_0 \otimes \mathbb{C}$ acts irreducibly on $E \otimes \mathbb{C}$ or not. In the first case, L' should be one of the real analogs of the Cartan algebras listed above. But in the second, E admits a complex structure as a L_0 module, which contradicts the hypotheses.

Theorem 1 is proved.

In order to complete our search for maximal subalgebras of polynomial vector fields over a given *real* vector space, we need to be able to identify in the tables given in Ref. 7, pp. 892–895, the algebras such that the representation $(L_{-1}, \mathrm{ad}_{|L_0})$ admits a complex structure.

Proposition 8: Let L_{-1} be a real vector space and $L = L_{-1} \oplus L_0 \oplus L_1$ an IFFT-algebra. Then $(L_{-1}, \mathrm{ad}_{|L_0})$ admits a complex structure if and only if the algebra L admits a complex structure.

Proof: The sufficiency of the condition is obvious. Notice that a complex structure on L stabilizes the eigenspaces of e.

Let J_{-1} be a complex structure on $(L_{-1}, \mathrm{ad}_{|L_0})$. Let $J_1 : L_1 \to L_1$ be the adjoint of J_{-1} with respect to the Killing form β of L, i.e.,

$$\beta(J_1 x_1, x_{-1}) = \beta(x_1, J_{-1} x_{-1}), \quad \forall x_{-1} \in L_{-1}, \forall x_1 \in L_1.$$

The so defined J_1 intertwines the action of L_0 on L_1. Moreover,

$$[J_1 x_1, x_{-1}] = [x_1, J_{-1} x_{-1}], \quad \forall x_{-1} \in L_{-1}, \forall x_1 \in L_1.$$

Indeed, for all $x_{-1}, y_{-1} \in L_{-1}$ and $x_1, y_1 \in L_1$,

$$\begin{aligned} \beta([[x_1, J_{-1} x_{-1}], y_{-1}], y_1) &= \beta(J_{-1} x_{-1}, [x_1, [y_1, y_{-1}]]) \\ &= \beta(x_{-1}, [J_1 x_1, [y_1, y_{-1}]]) \\ &= \beta([[J_1 x_1, x_{-1}], y_{-1}], y_1). \end{aligned}$$

Define

$$J_0: L_0 \to \mathcal{T}_0(L_{-1}): A \mapsto A \circ J_{-1}.$$

This map is actually valued in L_0 since

$$\begin{aligned}(J_0[x_1, x_{-1}])y_{-1} &= [[x_1, x_{-1}], J_{-1}y_{-1}] = [[x_1, J_{-1}y_{-1}], x_{-1}] \\ &= [[J_1 x_1, y_{-1}], x_{-1}] = [J_1 x_1, x_{-1}]y_{-1}\end{aligned}$$

for all $y_{-1} \in L_{-1}$.

The map $J: L \to L$ defined by its restrictions J_i to $L_i (i = -1, ..., 1)$ is then a complex structure of L as a Lie algebra. □

The statement ''IFFT-algebras are maximal'' should be taken in the following sense. In the tables given in Ref. 7, one can distinguish complex algebras from real ones admitting no complex structure. The latter give rise to maximal subalgebras of the real algebra $\mathcal{T}_*(L_{-1})$. One may consider the former as Lie subalgebras of the real Lie algebra $\mathcal{T}_*(L_{-1})$, in which case Lemma 3 shows that they are not maximal. They are maximal when regarded in their natural position of complex subalgebras of the complex Lie algebra $\mathcal{T}_*(L_{-1})$.

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Integrable Schrödinger operators with magnetic fields: Factorization method on curved surfaces

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The factorization method for Schrödinger operators with magnetic fields on a two-dimensional surface M^2 with nontrivial metric is investigated. This leads to the new integrable examples of such operators and brings a new look at some classical problems such as the Dirac magnetic monopole and the Landau problem. The global geometric aspects and related spectral properties of the operators from the factorization chains are discussed in detail. We also consider the Laplace transformations on a curved surface and extend the class of Schrödinger operators with two integrable levels introduced in the flat case by S. P. Novikov and one of the authors.
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I. INTRODUCTION

In spite of the fact that some important examples of integrable Schrödinger equations with magnetic fields were known since the 1930s (Landau problem, Dirac magnetic monopole), the general problem of integrability for such equations is still far from being understood.

In two dimensions probably the first important step in this direction has been taken by Dubrovin, Krichever and Novikov in 1976, who introduced a very important class of Schrödinger operators with magnetic fields integrable (''finite-gap'') on one energy level.[1] The coefficients of the corresponding operators are periodic (or quasiperiodic) so that the total magnetic flux is zero.

The case of periodic magnetic fields with nonzero flux has been considered by Dubrovin and Novikov[2] following the Aharonov–Casher observation[3] that the Pauli operators for spin $\frac{1}{2}$ particles in a magnetic field are related to the factorizable Schrödinger operators. This allowed one to describe explicitly the ground states of the corresponding operators (see Refs. 4 and 5 for the details).

In Ref. 6 Novikov and one of the authors found a class of operators with magnetic fields which are integrable on two different energy levels including the ground state. In Sec. V of this article we present some generalizations of this result, but our main goal here is to investigate what the factorization method can give for the theory of Schrödinger operators L with magnetic fields on a curved two-dimensional surface M^2.

Although some ideas have been developed already in the 19th century by Darboux, and Moutard *et al.* (see, e.g., Ref. 7), it was probably Schrödinger who first used the factorization method in quantum mechanics[8] (see also Ref. 9). The idea of this method is very simple: if a given operator L can be factorized as

$$L = D_1 D_2,$$

then the new operator

$$\tilde{L} = D_2 D_1$$

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has the same spectrum as L (provided the operators are good enough), except possibly $\lambda=0$, and if one knows the eigenfunctions ψ of L, then the formula

$$\tilde{\psi}=D_2\psi$$

gives the eigenfunctions of $\tilde{L}$. One can obviously include a shift into the factorization scheme:

$$L=D_1D_2+c\rightarrow\tilde{L}=D_2D_1+c,$$

where c is a constant. In one dimension it is always possible to factorize the Schrödinger operator and continue this procedure to construct an infinite chain of operators related by this transformation usually called the *factorization chain* (or dressing chain). In the case when this chain is periodic with an odd period the spectrum and eigenfunctions of all these operators can be described explicitly (see Ref. 10). The classical example is a harmonic oscillator when $\tilde{L}=L+\text{const}$.

In two dimensions the factorization of the general Schrödinger operator L with magnetic field on a curved surface M^2 is possible only in the special case when the potential is equal up to a sign to the magnetic field (see Theorem 1). A simple but important calculation shows that the transformation

$$L=D^*D\rightarrow\tilde{L}=DD^*$$

changes the magnetic field B by the Gaussian curvature K of M^2:

$$\tilde{B}=B+K.$$

In contrast to the one-dimensional, case in two dimensions one cannot, in general, continue the factorization procedure. We give a complete classification of all possible factorization chains on a curved surface M^2 (Theorem 2), which in particular says that infinite factorization chain exists only on the surfaces with constant Gaussian curvature. The magnetic field and the potential of the corresponding operators must also be constant.

In Sec. III we discuss the global geometric aspects of the factorization chains. The index theorem and the classical Gauss–Bonnet formula play a crucial role here. They explain a big difference between positive and negative curvature cases. In the positive constant curvature case, when $M^2=S^2$ is the standard round sphere, we have the *Dirac magnetic monopole*.[11–13] We show how the factorization method leads to the complete description of the spectrum of the corresponding Schrödinger operator L in the same way as Schrödinger did for the harmonic oscillator in Ref. 8. For the flat torus we have the standard *Landau problem*.[14] We also discuss what the factorization method gives for the analog of the Landau problem on a surface of constant negative curvature with genus more than 1.

In Sec. IV we present some new examples of integrable Schrödinger operators with magnetic fields related to the two-term factorization chains on the surfaces with nonconstant curvature. The main observation here is that if the Laplace–Beltrami operator on M^2 is integrable, then the same is true for the operator with the additional magnetic field $B=\pm K$ and the potential $U=K$, K being the Gaussian curvature.

In the last section we consider the quasi-cyclic chains of the Schrödinger operators with magnetic fields on a curved surface related by Laplace transformations generalizing the constructions from Ref. 6. This leads to a class of operators with two known energy levels, one of which is the ground state.

II. FACTORIZATION METHOD ON CURVED SURFACES: LOCAL THEORY

Consider an oriented analytic surface M^2 with a Riemannian metric ds^2. It is known that M^2 has a complex structure such that the metric is conformal. In any complex chart $z=x+iy$, $\overline{z}=x-iy$ the metric has the form

$$ds^2=\frac{dzd\overline{z}}{h^2(z,\overline{z})}=\frac{dx^2+dy^2}{h^2(z,\overline{z})}.$$

The Laplace–Beltrami operator Δ_h can be defined locally as

$$\Delta_h=4h^2\partial\overline{\partial}=h^2(\partial_x^2+\partial_y^2),$$

where $\partial=\partial_z=\frac{1}{2}(\partial_x-i\partial_y)$ and $\overline{\partial}=\partial_{\overline{z}}=\frac{1}{2}(\partial_x+i\partial_y)$. To introduce the magnetic field one should replace the usual derivatives by their covariant counterparts:

$$\begin{gathered}\nabla_x=\partial_x-ia, \quad \nabla_y=\partial_y-ib,\\ \nabla=\partial-iA, \quad \overline{\nabla}=\overline{\partial}-i\overline{A},\\ A=\tfrac{1}{2}(a-ib), \quad \overline{A}=\tfrac{1}{2}(a+ib).\end{gathered} \tag{1}$$

The corresponding Schrödinger operator

$$L_A=-h^2[(\partial_x-ia)^2+(\partial_y-ib)^2]$$

can be rewritten as

$$L_A=-4h^2\nabla\overline{\nabla}+h^2H=-4h^2\overline{\nabla}\nabla-h^2H=-2h^2(\nabla\overline{\nabla}+\overline{\nabla}\nabla), \tag{2}$$

where

$$H=\partial_x b-\partial_y a=i[\nabla_x,\nabla y]=2[\nabla,\overline{\nabla}].$$

Geometrically, we have a complex $U(1)$-bundle over M^2 with the connection form

$$\alpha=i(adx+bdy) \tag{3}$$

and the curvature

$$\Omega=d\alpha=iHdx\wedge dy=-\frac{H}{2}dz\wedge d\overline{z} \tag{4}$$

(see the next section for further discussion of the geometric aspects). Let us define magnetic field B by the relation

$$\Omega=iBd\sigma, \tag{5}$$

where $d\sigma=(1/h^2)\,dx\wedge dy$ is the area element of the surface. By definition we have

$$B=h^2H. \tag{6}$$

The most general Schrödinger operator on M^2 has the form

$$L=-h^2[(\partial_x-ia)^2+(\partial_y-ib)^2]+U, \tag{7}$$

where the potential $U(x,y)$ is a real function on M^2.

Consider the following *factorization problem* for (7): when L can be represented locally as

$$L=(\alpha_1\partial+\alpha_0)(\alpha_1^*\overline{\partial}+\alpha_0^*) \tag{8}$$

(α-factorization) or

$$L=(\beta_1\overline{\partial}+\beta_0)(\beta_1^*\partial+\beta_0^*) \tag{9}$$

(β-factorization) for some functions α, α^*, β, β^* ? In the Euclidean case such factorizations appeared in the theory of Pauli operators for spin 1/2 particles (see Refs. 3 and 4). On a curved surface the situation is pretty similar.

Theorem 1: *The α-factorization for the Schrödinger operator (7) exists iff $U=-B$. Similarly, the necessary and sufficient condition for the β-factorization is $U=B$.*

The sufficiency readily follows from formulas (2):

$$\text{If } U=-B, \text{ then } L=-4h^2\nabla\overline{\nabla}.$$

$$\text{If } U=B, \text{ then } L=-4h^2\overline{\nabla}\nabla.$$

The factorization is not unique: if $L=D_1D_2$ is any factorization, then $L=(D_1f^{-1})(fD_2)$ is another one for an arbitrary function f. This actually gives all such factorizations.

Having a factorized operator $L=D_1D_2$ one can consider the new operator

$$\tilde{L}=D_2D_1.$$

Notice that the change of factorization $D_1\to D_1f^{-1}$ and $D_2\to fD_2$ corresponds to the gauge transformation of $\tilde{L}$:

$$\tilde{L}\to fD_2D_1f^{-1}=f\tilde{L}f^{-1}.$$

The magnetic field and the potential do not depend on the gauge and are defined correctly. Let us compute them for α-factorized L. We can assume that $D_2=\overline{\nabla}$ and $D_1=-4h^2\nabla$, so that

$$\tilde{L}=D_2D_1=-4\overline{\nabla}(h^2\nabla)=-4h^2\overline{\nabla}\nabla-2h_{\bar{z}}h\nabla=-4h^2(\overline{\nabla}+2h_{\bar{z}}h^{-1})\nabla=-4h^2\tilde{\overline{\nabla}}\tilde{\nabla}, \tag{10}$$

where $\tilde{\overline{\nabla}}=\overline{\nabla}+2h_{\bar{z}}h^{-1}$, $\tilde{\nabla}=\nabla$.

Remark: The nonsymmetry between $\tilde{\nabla}$ and $\tilde{\overline{\nabla}}$ can be easily corrected by a suitable gauge transformation: $\tilde{\nabla}\to h\tilde{\nabla}h^{-1}=\nabla-h_zh^{-1}$ and $\tilde{\overline{\nabla}}\to h\tilde{\overline{\nabla}}h^{-1}=\overline{\nabla}+h_{\bar{z}}h^{-1}$. In the future we will not worry about such a nonsymmetry provided the corresponding magnetic field is real.

The new magnetic field is

$$\begin{aligned}\tilde{B}&=2h^2[\tilde{\nabla},\tilde{\overline{\nabla}}]=2h^2[\nabla,\overline{\nabla}+2h_{\bar{z}}h^{-1}]=B+4h^2(h_{\bar{z}}h^{-1})_z\\&=B+4h^2(\ln h)_{z\bar{z}}=B+h^2\triangle\ln h=B+K,\end{aligned}$$

where K is the *Gaussian curvature* of the surface. Here we have used the standard formula for K in the conformal coordinates

$$K=h^2\triangle\ln h \tag{11}$$

(see, e.g., Ref. 15). Thus the new magnetic field is

$$\tilde{B}=B+K. \tag{12}$$

According to Theorem 1 the new potential is

$$\tilde{U}=\tilde{B}=B+K. \tag{13}$$

Similarly, for β-factorization the new magnetic field and the new potential are

$$\tilde{B}=B-K, \quad \tilde{U}=K-B.$$

Let us introduce the notation (B,U) for the gauge class of Schrödinger operators (7) with given magnetic field B and potential U. Then we have the following two-term factorization chains:

$$(B,-B)\overset{\alpha}{\to}(B+K,B+K) \tag{14}$$

and

$$(B,B)\overset{\beta}{\to}(B-K,K-B). \tag{15}$$

Notice that $\alpha\circ\beta=\beta\circ\alpha=Id$:

$$(B,-B)\overset{\alpha}{\to}(B+K,B+K)\overset{\beta}{\to}(B,-B),$$

$$(B,B)\overset{\beta}{\to}(B-K,K-B)\overset{\alpha}{\to}(B,B).$$

The question is: can we continue the α-chain allowing a shift by a constant? The answer is simple: in order to have α-factorization for an operator from the class $(B+K,B+K-2c)$, $c=\text{const}$ we should require $B+K-2c=-(B+K)$ or $B+K=c$. In this case we have the following three-term chains with an arbitrary constant c:

$$(c-K,K-c)\overset{\alpha}{\to}(c,c)=(c,-c)+2c\overset{\alpha}{\to}(c+K,c+K)+2c=(c+K,3c+K) \tag{16}$$

and similarly

$$(c+K,c+K)\overset{\beta}{\to}(c,-c)=(c,c)-2c\overset{\beta}{\to}(c-K,K-c)-2c=(c-K,K-3c). \tag{17}$$

Here by $(B,U)+c$ with constant c we denote the class of operators $L+c$ with $L\in(B,U)$. Of course $(B,U)+c=(B,U+c)$, but it is convenient for us to use this notation to explain the procedure. Notice that the operators with constant magnetic field and constant potential can be considered as the natural analog of the *Landau operators* on a curved surface M^2. One more step in the factorization procedure is possible only if the Gaussian curvature is constant: $K=K_0$. In that case we actually can perform infinitely many steps:

$$(c-K_0,\ K_0-c)\overset{\alpha}{\to}(c,c)\overset{\alpha}{\to}(c+K_0,\ 3c+K_0)\overset{\alpha}{\to}\ldots\overset{\alpha}{\to}(c+mK_0,\ (2m+1)c+m^2K_0)\overset{\alpha}{\to}\ldots \tag{18}$$

for any $m\in\mathbf{Z}_+$ and similarly

$$(c+K_0,\ c+K_0)\overset{\beta}{\to}(c,-c)\overset{\beta}{\to}(c-K_0,\ K_0-3c)$$

$$\overset{\beta}{\to}\ldots\overset{\beta}{\to}(c-mK_0,-(2m+1)c+m^2K_0)\overset{\beta}{\to}\ldots \tag{19}$$

Summarizing all this we have the following.

Theorem 2: *All possible factorization chains on a surface M^2 with Gaussian curvature K are given by*

(1) two-term chains (14) and (15) with an arbitrary magnetic field B;

(2) three-term chains (16) and (17) of the operators on M^2 with constant magnetic fields. If a surface M^2 has a constant Gaussian curvature then we have also

(3) infinite chains (18) and (19) with constant magnetic fields.

III. GLOBAL GEOMETRY AND SPECTRAL PROPERTIES OF *L*

Let us assume now that M^2 is a closed surface of genus g with given Riemannian metric, ξ is a complex $U(1)$-bundle over M^2, α is a connection on ξ, and $\Omega=iBd\sigma$ is its curvature form. Here as above $d\sigma$ is the area element of the surface determined by the metric and B is a function on M^2 called magnetic field.

Remark: We should mention that for a given magnetic field B the corresponding connection α is defined uniquely modulo natural gauge transformations only when M^2 is a topological sphere. For a surface of genus g one can always add to α a closed one-form without changing B. Modulo exact forms corresponding to the gauge transformations the connections form the first cohomology group $H^1(M^2,\mathbf{R})\simeq\mathbf{R}^{2g}$. These additional $2g$ parameters are called the *Aharonov–Bohm* fluxes (see Refs. 16 and 17). All the spectra we consider in general depend not only on the magnetic field B but also on the choice of the connection α and therefore on these parameters. When $g=1$ (i.e., when M^2 is a torus) this corresponds to the choice of two *Bloch quasi-momenta*.

Notice that the total magnetic flux is an integer multiple of 2π:

$$\frac{1}{2\pi}\int_{M^2}Bd\sigma=b,\quad b\in\mathbf{Z}. \tag{20}$$

The integer b is actually the first Chern class of ξ:

$$b=c_1(\xi)\in H^2(M^2,\mathbf{Z})\simeq\mathbf{Z} \tag{21}$$

(see, e.g., Ref. 15). Having all this plus a potential U which is a function on M^2 one can define the Schrödinger operator L in (7) as explained in the previous section. This operator is acting on the sections $S(\xi)$ of the bundle ξ and is self-adjoint with respect to the natural Hermitian structure with the norm

$$\|\psi\|^2=\int_{M^2}|\psi|^2d\sigma.$$

Let us analyze now what happens when we apply the factorization procedure. Consider first the two-term chain (14):

$$(B,-B)\overset{\alpha}{\to}(B+K,B+K)$$

or, in the local coordinates,

$$L=D^*D\to DD^*=\tilde{L},$$

where $D=2\overline{\nabla}$ and $D^*=-2h^2\nabla$. Here we have used the complex structure on M^2 uniquely determined by the Riemannian metric, which exists according to the classical results (see, e.g., Ref. 15).

Notice, first of all, that the operator D maps the sections $S(\xi)$ of ξ into the sections $S(\eta)$ of the bundle $\eta=\xi\otimes T^{0,1}(M^2)$ which are the antiholomorphic one-forms on M^2 with the values in ξ of the form $\psi d\overline{z},\psi\in S(\xi)$. This space also has the natural Hermitian structure induced by the Hermitian structure on ξ and the metric on M^2. It is easy to check that $D^*=-2h^2\nabla$ is indeed operator adjoint to $D=2\overline{\nabla}$ with respect to these structures, so the operator $L=D^*D$ is nonnegative and $\mathrm{Ker}\,L=\mathrm{Ker}\,D$.

The new operator $\tilde{L}=DD^*$ is acting on the sections $S(\eta)$ of the bundle η and in the local coordinates has the form (10):

$$\tilde{L}=-4\overline{\nabla}(h^2\nabla)=-4h^2(\overline{\nabla}+2h_{\bar{z}}h^{-1})\nabla.$$

The new covariant derivatives $\tilde{\overline{\nabla}}=\overline{\nabla}+2h_{\bar{z}}h^{-1}$, $\tilde{\nabla}=\nabla$, correspond to the natural connection on η induced by the connection α on ξ and the natural Hermitian connection on the antiholomorphic cotangent bundle $T^{0,1}(M^2)$ (see Ref. 18). The curvature of this connection is

$$\tilde{\Omega}=i(B+K)d\sigma,$$

where K is the Gaussian curvature of the metric. Notice that the total flux of the new magnetic field $\tilde{B}=B+K$ (or, equivalently, the first Chern class of the bundle η) is

$$c_1(\eta)=\tilde{b}=\frac{1}{2\pi}\int_{M^2}\tilde{B}d\sigma=b+\chi=b+(2-2g), \tag{22}$$

where $\chi=2-2g$ is the *Euler characteristics* of M^2 because of the *Gauss–Bonnet formula*:

$$\int_{M^2}Kd\sigma=2\pi\chi. \tag{23}$$

The operator D is an elliptic operator from $S(\xi)$ into $S(\eta)$. Its index can be determined by the index theorem and is given by the Riemann–Roch formula

$$\mathrm{ind}\,D=\dim\mathrm{Ker}\,D-\dim\mathrm{Ker}\,D^*=b-g+1. \tag{24}$$

When the magnetic field is large enough, more precisely when $b>2g-2$, we have

$$\dim\mathrm{Ker}\,D^*=0,\quad \dim\mathrm{Ker}\,D=b-g+1. \tag{25}$$

In that case the ground state of the operator L is degenerate:

$$\dim\mathrm{Ker}L=\dim\mathrm{Ker}\,D=b-g+1,$$

while $\tilde{L}$ is positive operator:

$$\dim\mathrm{Ker}\tilde{L}=\dim\mathrm{Ker}\,D^*=0.$$

The rest of the spectrum (which is discrete according to general theory) is the same for L and $\tilde{L}$: the intertwining operators D and D^* establish the isomorphism of the corresponding eigenspaces. Notice that if $b=g-1$, then, according to the Riemann–Roch formula (24), $\dim\mathrm{Ker}\,L=\dim\mathrm{Ker}\,\tilde{L}$ so that L and $\tilde{L}$ are isospectral everywhere (not just for $\lambda>0$). Now for the general factorization chain one should only take into account the additional shift of the spectrum.

For the β-factorization chains (15) the analysis is similar, one should simply replace the holomorphic structure by the antiholomorphic one.

Let us consider now some examples.

Example 1: Dirac magnetic monopole on a sphere. Let M^2 be a sphere $S^2 \subset R^3$ with the standard metric of constant Gaussian curvature K. The Hamiltonian of the Dirac monopole with a charge $q \in \mathbf{Z}$ in our notations is a Schrödinger operator H_q from the gauge class $(B,0)$, where B is a constant satisfying the quantization relation

$$\frac{1}{2\pi}\int_{S^2} B d\sigma = \frac{B}{2\pi}\int_{S^2} d\sigma = 2B = q,$$

i.e., $B = q/2$ must be integer or half-integer. It is acting on the sections of the U(1)-bundle with the first Chern class q. As we have seen earlier, such an operator can be included in the infinite factorization chain:

$$\begin{aligned}(B,0) &= (B,-B)+B \to (B+K,\ B+K)+B \\ &= (B+K,\ 2B+K) \\ &= (B+K,\ -(B+K))+3B+2K \to (B+2K,B+2K)+3B+2K \\ &= (B+2K,4B+4K) \to \ldots \to (B+mK,\ 2mB+m^2K) \to \ldots, \end{aligned} \tag{26}$$

$m \in \mathbf{Z}_+$. If $B = q/2 > 0$, then the operator $(B,-B)$ is positive and, according to index theorem (25),

$$\dim \mathrm{Ker}(B,-B) = q - g + 1 = q + 1$$

since $g = 0$ and $q \geqslant 2g - 1 = -1$. Therefore the ground state of H_q has the energy $\lambda = B = q/2$ and the corresponding eigenspace has dimension $q + 1 = 2B + 1$. The second operator $(B+K,2B+K)$ in the chain has the same spectrum as $(B,0)$, except the ground state. By the same reasons its ground state has energy $\lambda = 3B + 2K$ which is degenerate:

$$\dim \mathrm{Ker}[(B+K,2B+K)-(3B+2K)] = \dim \mathrm{Ker}[B+K,-(B+K)] = 2B+2+1 = 2B+3.$$

Thus the second eigenvalue of H_q is $\lambda_2 = 3B + 2K$ with degeneracy $2B + 3$. On the mth step we will have the operator $(B+mK,2mB+m^2K) = (B+mK,-B-mK)+(2m+1)B+(m^2+m)K$ which leads to the eigenvalue

$$\lambda_m = (2m+1)B + m(m+1)K$$

with degeneracy $2B + 2m + 1$. Thus we arrived at the well-known result about the spectrum of the Dirac monopole (see, e.g., Ref. 13):

$$\mathrm{Spec} H_q = \left\{ \lambda_n = (2m+1)\frac{q}{2} + m(m+1)K \text{ with degeneracy } \quad q + 2m + 1 \right\},$$

$m = 0,1,2,\ldots$.

We can make all this explicit (including the calculation of the corresponding eigenfunctions) using the stereographic coordinate $z = x + iy$. Assume for simplicity that the radius of the sphere $R = 1$, so that the Gaussian curvature $K = 1/R^2 = 1$. The metric has the form

$$ds^2 = \frac{4}{(1+z\overline{z})^2} dz d\overline{z}.$$

The corresponding chain of operators in a suitable gauge has the form

$$L_N = -(1+z\bar{z})^2\partial\bar{\partial} - Nz(1+z\bar{z})\partial + N\bar{z}(1+z\bar{z})\bar{\partial} + N^2(1+z\bar{z})$$
$$= D_N^* D_N + N(N+1) = D_{N-1}D_{N-1}^* + N(N-1), \tag{27}$$

$$D_N = (1+z\bar{z})\bar{\partial} + Nz; \quad D_N^* = -(1+z\bar{z})\partial + (N+1)\bar{z}.$$

Here $L_N = H_{2N} + N^2$, where H_{2N} is the Dirac monopole operator with the charge $q=2N$, $B=N$. We obviously have the intertwining relations

$$L_{N+1}D_N = D_N L_N, \quad L_N D_N^* = D_N^* L_{N+1}. \tag{28}$$

To find the ground state of $L_N : L_N\psi = N(N+1)\psi$ one should solve the equation $D_N\psi = 0$:

$$(1+z\bar{z})\bar{\partial}\psi + Nz\psi = 0, \quad \text{or} \quad \bar{\partial}\ln\psi = -\frac{Nz}{1+z\bar{z}}.$$

The solutions are easy to find:

$$\psi = \frac{f(z)}{(1+z\bar{z})^N},$$

where f is any holomorphic function of z. Because of the condition

$$\int |\psi|^2 d\sigma = \int\int_{R^2} \frac{|\psi|^2 dz d\bar{z}}{(1+z\bar{z})^2} < \infty,$$

the function $f(z)$ must be a polynomial of order $\leqslant 2N$. This gives us the space of dimension $2N+1$. Applying to this space the ''lowering'' operators $D_{N-1}^*, D_{N-2}^*, \ldots$ we will construct all eigenfunctions of the operators $L_{N-1}, L_{N-2}, \ldots$ with the eigenvalue $\lambda = N(N+1)$. This gives the following description of the eigenfunctions of the Dirac monopole operator H_q.

Theorem 3: *The eigenfunctions of the Dirac magnetic monopole operator with the charge q on a unit sphere corresponding to the eigenvalue*

$$\lambda = (2m+1)\frac{q}{2} + m(m+1), \quad m \in Z_+, \tag{29}$$

form the space of dimension $q+2m+1$ *which can be described as*

$$\psi = D_{N-m}^* \ldots D_{N-2}^* D_{N-1}^* \frac{f(z)}{(1+z\bar{z})^N}, \tag{30}$$

where $N = m + q/2$ *and* $f(z)$ *is an arbitrary polynomial of degree* $\deg f \leqslant 2N = 2m+q$.

One can check that the formulas for ψ we have given actually determine the smooth sections of the corresponding line bundles over the sphere S^2.

The eigenfunctions of the Dirac magnetic monopole are known as *monopole harmonics* and have been investigated by Wu and Yang,[13] who were probably the first to identify them explicitly as the sections. Our derivation is different and closer to the one of the paper[19] by D'Hoker and Vinet who discovered the supersymmetry of the corresponding Pauli equation in the presence of a magnetic monopole (see also Ref. 20).

Remark: If $q=2N$ is an even integer, then $H_{2N} = L_N - N^2$ can be intertwined with the shifted standard Laplace–Beltrami operator $L_0 = -\Delta_g$ on the sphere S^2:

$$H_{2N}D = D(L_0 - N^2), \quad D = D_{N-1}\cdots D_1 D_0,$$

so that one can use the well-known eigenfunctions of L_0 (spherical harmonics) to construct the eigenfunctions of H_q. Notice that we have given an alternative description of spherical harmonics using the factorization chain. The explicit form of the intertwining operator D is

$$D=\frac{1}{(1+z\overline{z})^{N-2}}\overline{\partial}(1+z\overline{z})^2\overline{\partial}(1+z\overline{z})^2\overline{\partial}\cdots\overline{\partial}(1+z\overline{z})^2\overline{\partial},$$

which is of the order N in $\overline{\partial}$.

It is interesting to compare the Dirac monopole problem on a sphere with the Landau problem on the surfaces of genus $g\geqslant 2$ with the constant negative Gaussian curvature $K<0$ which we analyze later. The corresponding classical problems behave very differently so one should expect the same for the quantum problems as well.

For the investigation of the intermediate case of flat torus which is the classical Landau problem we refer to Refs. 14 and 5. In that case $K=0$ and our formula (26) leads to the usual Landau spectrum

$$\lambda_m=\{(2m+1)B,\quad m=0,1,\dots\},$$

where B is assumed positive and quantized. The corresponding eigenfunctions can be expressed in terms of the classical elliptic σ-functions (see Refs. 5 and 2 for the details).

Example 2: Landau problem on a surface of genus $g\geqslant 2$. Let M^2 be any analytic surface with the metric ds^2 of constant curvature $K=-1$. Such surface M^2 can be considered as a quotient of the Lobachevsky plane $\mathcal{L}$ by an infinite discrete group G:

$$M^2=\mathcal{L}/G.$$

Here $\mathcal{L}$ can be realized as an open disc $|z|<1$ with the metric

$$ds^2=\frac{4}{(1-z\overline{z})^2}dzd\overline{z}.$$

The Schrödinger operator on $\mathcal{L}$ with constant magnetic field B (Landau operator) can be written as $L_B^{\mathcal{L}}=-(1-z\overline{z})^2(\nabla\overline{\nabla}+\overline{\nabla}\nabla)$, where

$$\nabla=\partial-B\frac{\overline{z}}{1-z\overline{z}},\quad \overline{\nabla}=\overline{\partial}+B\frac{z}{1-z\overline{z}},$$

or, explicitly,

$$L_B^{\mathcal{L}}=-(1-z\overline{z})^2\partial\overline{\partial}+B\overline{z}(1-z\overline{z})\overline{\partial}-Bz(1-z\overline{z})\partial+B^2z\overline{z}. \tag{31}$$

In order to define the corresponding operator L_B acting on the sections of some $U(1)$-bundle over M^2 one needs the quantization condition

$$\frac{1}{2\pi}\int_{M^2}Bd\sigma=\frac{1}{2\pi}B\int_{M^2}d\sigma=(2g-2)B\in\mathbf{Z} \tag{32}$$

to be satisfied. Here we have again used the Gauss–Bonnet formula

$$\frac{1}{2\pi}\int_{M^2}Kd\sigma=-\frac{1}{2\pi}\int_{M^2}d\sigma=\chi=2-2g.$$

Notice that to define L_B one also needs to choose a connection α which depends on $2g$ Aharonov–Bohm fluxes (see the remark at the beginning of this section).

Let us see what the factorization chain (18) gives us for the calculation of the spectrum of L_B. We have the chain (26) with $K=-1$:

$$\begin{aligned}(B,0)&\to(B,-B)+B\to(B-1,B-1)+B\\&=(B-1,2B-1)\to\ldots\to(B-m,2mB-m^2)\\&=(B-m,m-B)+(2m+1)B-(m^2+m).\end{aligned}$$

Let us assume that $B>0$. By Riemann–Roch formula (24) the index of the operator $(B-m,m-B)$ is $(2g-2)(B-m)-g+1=(2g-2)(B-m-\frac{1}{2})$, so it is positive if

$$m<B-\tfrac{1}{2}.$$

Using the same arguments as in the previous example we can claim that the first $[B-\frac{1}{2}]+1$ eigenvalues of the operator L_B have the form

$$\lambda_m=(2m+1)B-m(m+1),\quad m=0,1,2,\ldots,[B-\tfrac{1}{2}]. \tag{33}$$

Let us remember that B has the form $k/(2g-2)$ for some positive integer k. Moreover, we can say that if $(2g-2)(B-m)>2g-2$, i.e., if

$$m<B-1,$$

then the corresponding eigenspace has the dimension

$$\dim \mathrm{Ker}(L_B-\lambda_m)=(2g-2)(B-m-\tfrac{1}{2}). \tag{34}$$

Notice that the spectrum (33) depends only on the magnetic field B but not on the Aharonov–Bohm fluxes. It is related to the discrete part of the spectrum of the Landau operator $L_B^{\mathcal{L}}$ on the whole Lobachevsky plane (see, e.g. Ref. 21). It would be interesting to find an effective representation for the corresponding eigenfunctions on a surface M^2 given explicitly as an algebraic curve in $\mathbf{C}^2$.

From these considerations we have nothing to say about the rest of the spectrum of L_B [which in fact depends both on Aharonov–Bohm fluxes and on $(3g-3)$ complex parameters (*moduli*) determining the conformal structure on M^2]. In particular, we can not say anything about the spectrum of the pure Laplace–Beltrami operator L_0 on M^2. This is a reflection of the fact that the corresponding classical geodesics problem on M^2 is nonintegrable. In this relation we would like to mention an interesting paper[22] where the both classical and quantum problems with a constant magnetic field are considered on a surface which is a (noncompact) quotient of the Lobachevsky plane by a subgroup of the modular group.

IV. NEW EXAMPLES OF THE INTEGRABLE QUANTUM PROBLEMS WITH MAGNETIC FIELD

Let us consider any surface M^2 with integrable quantum geodesic problem

$$L\psi=\lambda\psi,$$

where $L=-\Delta_h$ and Δ_h is the Laplace–Beltrami operator on M^2. By definition the integrability means that there exists an integral, which is another differential operator F commuting with L: $[F,L]=0$ and having an independent highest symbol. We have shown [see (16)] that L can be factorized $L=D^*D$ and the new operator $\tilde{L}=DD^*$ has the magnetic field $B=\pm K$ (K is the Gaussian curvature) and the potential $U=K$. We claim that this new operator is also integrable. Indeed, consider the differential operator

$$\tilde{F}=DFD^*, \tag{35}$$

Then

$$\tilde{L}\tilde{F}=DD^*DFD^*=DLFD^*=DFLD^*=DFD^*DD^*=\tilde{F}\tilde{L},$$

i.e., $\tilde{F}$ commutes with $\tilde{L}$. It is easy to check that if the highest symbol of F is independent of the highest symbol of L, then the same is true for $\tilde{F}$ and $\tilde{L}$. The intertwining relations

$$\tilde{L}D=DL \quad \text{and} \quad D^*\tilde{L}=LD^*$$

establish isomorphism between the two spectral problems

$$L\psi=\lambda\psi \quad \text{and} \quad \tilde{L}\tilde{\psi}=\lambda\tilde{\psi}$$

for any $\lambda\neq 0$: $\tilde{\psi}=D\psi$, $\psi=D^*\tilde{\psi}$. For $\lambda=0$ the situation is described by the Riemann–Roch formula:

$$\dim \mathrm{Ker}\, L-\dim \mathrm{Ker}\ \tilde{L}=1-g. \tag{36}$$

In particular, for the sphere S^2 we have $g=0$,

$$\dim \mathrm{Ker}\, L=1, \quad \dim \mathrm{Ker}\, \tilde{L}=0.$$

This means that the ground state of $\tilde{L}$ has the energy which is equal to the minimal positive eigenvalue of L: if Spec $L=\{\lambda_0=0, \lambda_1,\lambda_2,\dots\}$, then Spec $\tilde{L}=\{\lambda_1,\lambda_2,\dots\}$.

For the torus T^2 we have $g=1$ and

$$\dim \mathrm{Ker}\, L=\dim \mathrm{Ker}\, \tilde{L}=1$$

so that

$$\mathrm{Spec\,L}=\mathrm{Spec}\,\tilde{L}.$$

This is true for all the values of quasi-momenta, i.e., for the whole Bloch spectrum. Notice for the torus the total magnetic flux of $\tilde{L}$ is zero.

We do not know any integrable Laplace–Beltrami operators on a surface of genus $g\geqslant 2$. For the corresponding classical problem about geodesics on M^2 there exists a rigorous proof that there are no such metrics (see Ref. 23).

Theorem 4: *Let M^2 be any surface such that the corresponding quantum geodesic problem $-\Delta_h\psi=\lambda\psi$ is integrable. Then the Schrödinger operator $\tilde{L}$ on M^2 with magnetic field $B=\pm K$ and potential $U=K$, K is the Gaussian curvature of M^2, is integrable, too, and has the same spectrum as $L=-\Delta_h$ with the only possible exception at $\lambda=0$.*

Example: Consider an ellipsoid M^2,

$$\frac{x^2}{a^2}+\frac{y^2}{b^2}+\frac{z^2}{c^2}=1,$$

with the metric induced from $\mathbf{R}^3$. The geodesic problem on M^2 has been solved by Jacobi who showed that it can be integrated by separation of variables. The same is true for the corresponding quantum problem. Gaussian curvature of M^2 has the form

$$K=(abc)^{-2}\left(\frac{x^2}{a^4}+\frac{y^2}{b^4}+\frac{z^2}{c^4}\right)^{-2},$$

so we can claim that the Schrödinger operator $\tilde{L}$ on M^2 with the magnetic field

$$B=(abc)^{-2}\left(\frac{x^2}{a^4}+\frac{y^2}{b^4}+\frac{z^2}{c^4}\right)^{-2}$$

and the potential

$$U=-(abc)^{-2}\left(\frac{x^2}{a^4}+\frac{y^2}{b^4}+\frac{z^2}{c^4}\right)^{-2}$$

is integrable and $\mathrm{Spec}\, L=\mathrm{Spec}\,\tilde{L}\cup\{0\}$. Notice that the order of the additional quantum integral $\tilde{F}=DFD^*$ is 4, since the order of F is known to be 2.

Remark: We do not claim that that the minimal order of the additional integral is 4. On the contrary, in this case one can show that there exists an additional integral of order 2. It would be interesting to investigate the corresponding classical mechanical problem of motion on the ellipsoid in this special magnetic field. We conjecture that it is nonintegrable.

This example can be generalized in the following way. Consider any surface M^2 with the Liouville metric

$$ds^2=g_{11}du^2+g_{22}dv^2,\quad g_{11}=\frac{u-v}{f},\quad g_{22}=\frac{v-u}{g},$$

where $f(u)$ and $g(v)$ are arbitrary functions of the specified arguments. Its Gaussian curvature is expressed by the formula

$$K=\frac{f-g}{2(u-v)^3}-\frac{f'+g'}{4(u-v)^2}.$$

The corresponding Laplace–Beltrami operator

$$\Delta_h=\sqrt{g^{11}g^{22}}\partial_u\frac{g^{11}}{\sqrt{g^{11}g^{22}}}\partial_u+\sqrt{g^{11}g^{22}}\partial_v\frac{g^{22}}{\sqrt{g^{11}g^{22}}}\partial_v$$

commutes with the second-order operator

$$F=v\sqrt{g^{11}g^{22}}\partial_u\frac{g^{11}}{\sqrt{g^{11}g^{22}}}\partial_u+u\sqrt{g^{11}g^{22}}\partial_v\frac{g^{22}}{\sqrt{g^{11}g^{22}}}\partial_v,$$

so that variables can be separated both in the classical and quantum cases. So, we can claim that the Schrödinger operator with magnetic field $B=\pm K$ and the potential $U=K$ is integrable on any Liouville surface.

As a degenerate case of this construction one can get the surfaces of revolution in R^3 with the metric

$$ds^2=\rho(z)^2d\varphi^2+(1+\rho'(z)^2)dz^2.$$

In that case the Gaussian curvature is given by the formula

$$K=\frac{\rho'\rho''}{\rho(1+(\rho')^2)^2}.$$

We would like to mention that there exist the intertwining relations between two Schrödinger operators which are not related to any factorization of the operators (see Ref. 24 for some examples). We will present here another example of this type modifying the previous analysis ofthe Dirac monopole. Recall that the operator L_N of the Dirac monopole on the unit sphere given by (27),

$$L_N=-(1+z\overline{z})^2\partial\overline{\partial}-Nz(1+z\overline{z})\partial+N\overline{z}(1+z\overline{z})\overline{\partial}+N^2(1+z\overline{z}),$$

satisfies the interwining relations (28),

$$L_{N+1}D_N=D_NL_N,$$

where

$$D_N=(1+z\overline{z})\overline{\partial}+Nz.$$

It can be readily verified that the modified operators $\tilde{L}_N$ given by

$$\tilde{L}_N=L_N-\tfrac{1}{4}P^2-(N+1)P,\quad \tilde{L}_{N+1}=L_{N+1}-\tfrac{1}{4}P^2-NP$$

satisfy the same intertwining relations

$$\tilde{L}_{N+1}\tilde{D}_N=\tilde{D}_N\tilde{L}_N,$$

where the modified intertwining operator $\tilde{D}_N$ is of the form

$$\tilde{D}_N=D_N+\frac{\varphi}{1+z\overline{z}},$$

Here φ is a quadratic polynomial in z:

$$\varphi=q+pz-\overline{q}z^2,\quad p\in R,\quad q,\overline{q}\in C,$$

and P is given by the formula

$$P=\varphi'-\frac{2\overline{z}\varphi}{1+z\overline{z}}=p\frac{1-z\overline{z}}{1+z\overline{z}}-2\frac{\overline{q}z+q\overline{z}}{1+z\overline{z}}.$$

Geometrically, P represents the restriction to the sphere S^2 of an arbitrary linear function from the ambient space R^3. Without any loss of generality we may assume $q=\overline{q}=0$ (by appropriately choosing the axis of stereographic projection), so $P=p\,(1-z\overline{z})/(1+z\overline{z})$.

In particular, for $N=-1$ we have the intertwining relation between the Dirac monopole operator with charge 2 in the potential $U=-\frac{1}{4}P^2$ and the usual Laplace–Beltrami operator with the additional potential $V=-\frac{1}{4}P^2+P$.

One can show that this construction actually gives all the potential deformations of the intertwining relations (28).

V. LAPLACE TRANSFORMATIONS ON A CURVED SURFACE AND QUASI-CYCLIC CHAINS

Let L be any Schrödinger operator with magnetic field B and potential U:

$$L=-4h^2\nabla\overline{\nabla}+(U+B)=-4h^2\overline{\nabla}\nabla+(U-B).$$

In general none of these forms is pure factorizable but on the level $\lambda=0$: $L\psi=0$ we still can do the transformation

$$\tilde{\psi}=\nabla\psi \quad \text{or} \quad \tilde{\psi}=\overline{\nabla}\psi.$$

In particular, if

$$L\psi=[-4h^2\overline{\nabla}\nabla+(U-B)]\psi=0$$

and $\tilde{\psi}=\nabla\psi$, we have

$$\overline{\nabla}\tilde{\psi}=\frac{U-B}{4h^2}\psi$$

and therefore

$$\tilde{\nabla}\overline{\nabla}\tilde{\psi}=\frac{U-B}{4h^2}\tilde{\psi},$$

where $\tilde{\nabla}$ satisfies the relation

$$\tilde{\nabla}\frac{U-B}{4h^2}=\frac{U-B}{4h^2}\nabla$$

implying

$$\tilde{\nabla}=\nabla-\ln(U-B)_z+(\ln h^2)_z. \tag{37}$$

Thus $\tilde{\psi}=\nabla\psi$ satisfies the new Schrödinger equation $\tilde{L}\tilde{\psi}=0$, where

$$\tilde{L}=-4h^2\tilde{\nabla}\overline{\nabla}+(U-B)=-4h^2\tilde{\nabla}\overline{\nabla}+(\tilde{U}+\tilde{B}). \tag{38}$$

The new magnetic field is

$$\tilde{B}=2h^2[\tilde{\nabla},\overline{\nabla}]=B+2h^2(\ln(U-B))_{z\bar{z}}-4h^2(\ln h)_{z\bar{z}}=B+\tfrac{1}{2}\Delta_h(\ln(U-B))-K, \tag{39}$$

where $\Delta_h=4h^2\partial\overline{\partial}$ is the Laplace–Beltrami operator on M^2, and K is the Gaussian curvature. The new potential is

$$\tilde{U}=U-B-\tilde{B}=U-[2B+\tfrac{1}{2}\Delta_h(\ln(U-B))-K]. \tag{40}$$

The formulas (37)–(40) define correctly the Laplace transformation for the Schrödinger operators on a curved surface. The only difference with the standard formulas in the flat case (see, e.g., Ref. 6) is the additional Gaussian curvature term.

Following Ref. 6 let us call the chain of Laplace transformations

$$\begin{aligned} B_{k+1}&=B_k+\tfrac{1}{2}\Delta_h(\ln(U_k-B_k))-K,\\ U_{k+1}&=U_k-B_k-B_{k+1}=U_k-\Big[2B_k+\tfrac{1}{2}\Delta_h(\ln(U_k-B_k))-K\Big], \end{aligned} \tag{41}$$

$k=0,\ldots,N$, *quasi-cyclic* if both the initial and final Schrödinger operators are factorizable, possibly at the different energy levels:

$$U_0+B_0=0, \quad U_N+B_N=U_{N-1}-B_{N-1}=-c, \tag{42}$$

where $c>0$ is a constant.

As well as in the flat case,[6] the last operator L_N has two ''integrable'' levels: $L_N\psi_0=0$ and $L_N\psi_c=-c\psi_c$. Indeed, ψ_0 can be found as the result

$$\psi_0=\nabla_{N-1}\nabla_{N-2}\ldots\nabla_0\psi$$

of the Laplace transformations applied to the solutions of the initial equation $L_0\psi=0$, which is equivalent to

$$\overline{\nabla}_0\psi=0, \tag{43}$$

while ψ_c are the ground states of the operator $L_N=-4h^2\nabla_N\overline{\nabla}_N-c$ satisfying the equation

$$\overline{\nabla}_N\psi=0. \tag{44}$$

Obviously we should assume that solutions of both (43) and (44) do exist, which imposes some global assumptions on the magnetic field. Let us discuss these assumptions.

First of all, let us notice that the magnetic charge $b=(1/2\pi)\int_{M^2}Bd\sigma$ (which should be integer because of the quantization condition) changes under Laplace transformations according to the formula

$$\tilde{b}=b+2g-2$$

as it follows from (39) and the Gauss–Bonnet formula. After N steps we have $b_N=b_0+2N(g-1)$. Also from (41) we have

$$\int_{M^2}(U_k+B_k)d\sigma=\int_{M^2}(U_{k-1}-B_{k-1})d\sigma=\int_{M^2}(U_{k-1}+B_{k-1})d\sigma-4\pi b_{k-1}.$$

Since $U_0+B_0=0$ it follows that

$$\frac{1}{2\pi}\int_{M^2}(U_N+B_N)d\sigma=-\frac{1}{2\pi}\int_{M^2}cd\sigma=-2Nb-N(N-1)(2g-2),$$

so we have the relation

$$c\frac{A(M^2)}{2\pi}=2Nb_0+N(N-1)(2g-2), \tag{45}$$

where $A(M^2)=\int_{M^2}d\sigma$ is the area of M^2. For the sphere we have $c=Nb_0-N(N-1)$, for the torus $cA(M^2)=4\pi Nb_0$, and for a surface of genus $g>1$ the relation $c(2g-2)=2Nb_0+N(N-1)(2g-2)$.

This determines the constant c in the quasi-cyclic chain if we know the magnetic charge b_0 of the first operator and therefore imposes a quantization condition on c since b_0 is an integer. In terms of this integer b_0 the sufficient conditions for the equations (43) and (44) to have a solution have the form (see Sec. III)

$$b_0>g-1, \quad b_0+2N(g-1)>g-1.$$

For the topological sphere S^2 this is equivalent to the inequality $b_0>2N-1$, for the torus this simply means that b_0 is positive, and for a surface of genus $g>1$ we have just the first inequality $b_0>g-1$.

Theorem 5: *Let $U_k, B_k, k=0,1,\ldots,N$, satisfy the quasi-cyclic chain (41) on a curved surface M^2 and let the magnetic charge of the first operator b_0 satisfy the conditions described above. Then the last operator of the chain L_N has two known energy levels independent of the Aharonov–*

Bohm fluxes: the ground state $\lambda=-c$ *and* $\lambda=0$. *The corresponding eigenfunctions can be found from the solutions of the first order equations (43) and (44) and for a large* b_0 *form the spaces of the dimensions* $b_0+(2N-1)(g-1)$ *for* $\lambda=-c$ *and* b_0-g+1 *for* $\lambda=0$ *respectively*.

Example 1: Quasi-cyclic chains of length $N=1$:

$$U_0+B_0=0,$$

$$U_1+B_1=U_0-B_0=-c$$

implies that $U_0=-B_0=-c/2$ are constants, so that L_0 is the Landau operator on a curved surface M^2. Notice that

$$B_1=B_0+\tfrac{1}{2}\Delta_h(\ln(-c))-K=B_0-K,$$

$$U_1=U_0-2B_0+K=K-3B_0,$$

so that in this case the Laplace transformation coincides with one step of the factorization procedure (17): $(B_0,-B_0)\to(B_0-K,K-3B_0),B_0=c/2$. Thus in this case we claim that the Schrödinger operator with the magnetic field $B=c/2-K$ and the potential $U=K-3c/2$ has two lowest energy levels known: $\lambda=-c$ and $\lambda=0$ provided the quantization and positivity conditions for c are satisfied.

Example 2: Quasi-cyclic chains with $N=2$:

$$U_0+B_0=0\Leftrightarrow U_0=-B_0;$$

$$B_1=B_0+\tfrac{1}{2}\Delta_h(\ln B_0)-K,\quad U_1=U_0-B_0-B_1=-2B_0-B_1;$$

$$U_2+B_2=U_1-B_1=-2B_0-2B_1=-c.$$

Thus we have the following relation for the magnetic field B_0:

$$2B_0+\frac{1}{2}\Delta_h(\ln B_0)-K=\frac{c}{2}$$

or

$$\Delta_h(\ln B_0)=c+2K-4B_0,$$

which, after introducing $\varphi=\ln B_0$, takes the form

$$\Delta_h\varphi=c+2K-4e^{\varphi}. \tag{46}$$

When $K=0$ this reduces to the equation from Ref. 6.

As well as in the flat case, any solution of (46) determines a Schrödinger operator in the magnetic field with two integrable levels.

Remark: When $c=0$, Eq. (46) reduces to

$$\Delta_h\varphi=2K-4e^{\varphi},$$

which is a natural analog of the well-known Liouville equation for a curved surface. It can be transformed into the standard Liouville equation $\tilde{\varphi}_{z\bar{z}}=-e^{\tilde{\varphi}}$ by a substitution $\varphi=\tilde{\varphi}+2\ln h$. When $c\neq 0$ the equation (46) is probably nonintegrable already in the flat case.

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Borel summable solutions to one-dimensional Schrödinger equation

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It is shown that so called fundamental solutions the semiclassical expansions of which have been established earlier to be Borel summable to the solutions themselves appear also to be the unique solutions to the one-dimensional (1D) Schrödinger equation having this property. Namely, it is shown in this paper that for the polynomial potentials the Borel function defined by the fundamental solutions can be considered as the canonical one. The latter means that any Borel summable solution can be obtained by the Borel transformation of this unique canonical Borel function multiplied by some $\hbar$-dependent and Borel summable constant. This justifies the exceptional role the fundamental solutions play in 1D quantum mechanics and completes the relevant semiclassical theory relied on the Borel resummation technique and developed in our other papers. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1331099]

I. INTRODUCTION

The semiclassical approximation is one of the most widely used approximate methods in physics, particularly, in quantum mechanics. In fact it is not limited only to pure power series expansions in the Planck constant $\hbar$ but it is used also in all problems which can be formulated semiclassically. The method can be applied in this way to, say, the quartic oscillator perturbation theory from the one hand[1,2] and to a variety of problems with so called large-N expansions from the other.[3–5] Therefore, independently of the expansion parameter we shall consider all such asymptotic series expansions as semiclassical.

The method can be stated in the Schrödinger wave function formulation of quantum mechanics[6,7] as well as in the Feynman path inegral form of the latter.[8,9] Its main ingredient as the approximation method is to represent considered quantities by a limited number of first terms of the corresponding infinite series expansions, knowing usually that the series is typically asymptotic, i.e., divergent. Therefore, contrary to the case of convergent series, such a representation of the expanded quantities is of a rather limited value.

First, it cannot be done arbitrarily accurate by enlarging a number of kept terms, i.e., such an approximation can be only the best one in which the case a finite rest is exponentially small (in the parameter of the expansion) in comparison with the main contribution.

Second, it is just these exponentially small differences which can become dominating in other domains of the expansion parameter being arbitrarily close to the original one, i.e., such a finite representation of quantities by their corresponding asymptotic series are strongly limited to the original domain and it cannot give any information about the analytic properties of the quantities considered as functions of the expansion parameter. In particular this finite sum cannot be continued analytically outside the original domain of obtaining it.

The latter means that the considered quantities cannot be recovered in some simple way by the knowledge of a finite number of terms of their semiclassical expansions even if the series are

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abbreviated at their least terms. (In the latter case the approximation is considered to be best.) In fact these analytic properties are determined rather by the behavior of so called large order terms of the series. It is just the properties of these large order terms (considered as functions of their order) which allow us actually to reconstruct quantities represented by such semiclassical series. In particular if these terms grow with their order not faster than factorially then the Borel method of summation of the diverging series can be used in such cases. We shall call such semiclassical series Borel summable.

In the case of the Borel summable semiclassical expansions the Borel method of summation can be used in the following way.

First the Borel function is determined approximately after the knowledge of a limited number of first terms of the asymptotic series expansion of the considered quantity. Namely, by its definition the approximate Borel function is obtained as a sum of these known first terms divided by the corresponding factorials. The sum represents in this way the abbreviated Taylor series expansion corresponding to the exact Borel function. (The latter is obtained if all the terms of the asymptotic series are used to construct the Taylor series in the above way.) The last series has a finite radius of convergence and therefore an additional knowledge even approximate of the singularity structure of the corresponding Borel function is still necessary for an approximate recovery of this function from its abbreviated Taylor series. This knowledge can be extracted to the known extent from the detailed knowledge of the large order behavior of the considered semiclassical series. Having (or assuming) however this knowledge a function with the desired singularity structure can be constructed and its Taylor series expansion can be compared with the known abbreviated Taylor series so that the free parameters of the assumed singularities can be determined. Finally by the Borel transformation of the Borel function the original quantity is reproduced approximately in this way.[4]

The above reproduction can still be performed in the spirit of asymptotic expansions and on different levels of accuracy. The lowest level is obtained when the Borel integral is substituted by its best asymptotics. It means that the quantity considered is represented again by a finite sum a definite number of first terms of which coincide exactly with the original terms used to construct the (approximate) Borel function. However this sum can now contain many more terms since it ends on the least term of the asymptotic series corresponding to the Borel integral. Therefore it can approximate the considered quantity much better than the sum of the original terms with which the method has started.

However, since the method contains still additional information about the singularity structure of the Borel function then one step further can be done in getting a still better level of accuracy by extracting from the Borel integral so called exponentially small contributions. Such computations are known as the hyperasymptotic ones.[10,11] The finite semiclassical sum is then completed by the exponentially small contributions the forms and numbers of which are determined by the known (assumed) singularity structure of the Borel function.[12] The latter means that the Borel summability allows us to realize the *principle of resurgence*, i.e., to recover the information contained in the divergent tails of the semiclassical series.[10,12–17]

It should be noted also, however, that the exponentially small contributions are of their own importance since in many cases of quantities considered these contributions are dominant. Among the latter cases the most well known one is the difference between the energy levels of different parities in the symmetric double well.[6] But these are also the cases of transition probabilities in the tunnelling phenomena[6] or their adiabatic limits in the time-dependent problem of transitions between two (or more) energy levels (see Refs. 18, 19 and references cited therein) or the exponential decaying of resonances in the weak electric field (see Refs. 20, 21 and references cited therein).

The applicability of the Borel resummation to the semiclassical expansions in quantum mechanics has been proved by many authors.[22–24] Particularly, the 1D quantum mechanics offers a possibility of constructing a full semiclassical theory relied on the Borel resummation.[1,12,25] Namely, several years ago one of the authors of the present paper discovered[1] that for a large family of analytical potentials including all the polynomial ones there are solutions to a 1D

stationary Schrödinger equation for which their well defined semiclassical expansions are Borel summable to the solutions themselves. These solutions appearing for polynomial potentials in a finite number were called fundamental because of their completeness for solving any one-dimensional problem.[5] Their Borel summability property played an essential role in many of their applications.[1] In particular this property allowed us to prove the Borel summability of energy levels for most of the polynomial potentials.

On the other hand it is easy to construct solutions to the Schrödinger equation (in fact, infinitely many of them) with well defined Borel summable semiclassical expansions but with results of such Borel resummations not coinciding with the initial solutions generating the series. However the results of the Borel resummations are again solutions to the Schrödinger equation since in general each successful Borel resummation of any semiclassical series always leads to some solution to the Schrödinger equation.

In this paper we want to demonstrate an exceptional role the fundamental solutions mentioned above play with respect to the Borel summability property showing that they provide a general scheme for a construction of Borel summable solutions to the 1D stationary Schrödinger equation at least for polynomial potentials. A main ingredient of such a scheme is an observation that the Borel function of some fundamental solution is not only such a function for any other fundamental solution but it is also a Borel function allowing us to construct any Borel summable solution to a given 1D Schrödinger equation with polynomial potential.

The latter conclusion means that in all the semiclassical problems in 1D quantum mechanics in which the Borel resummation method is to be applied the fundamental solutions should be used preferably.

Our way of considering the problem of the Borel summability in 1D quantum mechanics makes use of the global features of the fundamental solutions and the Stokes graphs related to them and as such is to some extent complementary to the way utilized by Delabaere *et al.*[13,14] making use of rather local properties of the considered quantities.

Our method can be also used to analyze the adiabatic limits considered by Joye *et al.*[18] at least in the case of two energy levels.[26] The cases of several levels need, however, a generalization of our method since these cases are described by systems of the linear equations in numbers larger than two.

To make the original results of our paper more transparent we have formulated them in many places in the forms of theorems or lemmas equipped with the corresponding proofs. However we do not consider our paper to pretend to a full formal mathematical rigor supposing most of the presented ideas to be sufficiently obvious and clear by presented proofs or when confronted with our earlier papers or with the papers of other authors mentioned.

The paper is organized as follows.

In the next section we remind a construction and basic properties of the fundamental solutions and Borel functions corresponding to them as well.

In Sec. III we show that the Borel functions corresponding to different fundamental solutions are only different branches of the same unique Borel function and can be recovered by the Borel transformations performed along suitably chosen paths on the ''Borel plane.'' We show also here that there are two ways of integrations in the Borel plane providing us with the Borel summable solutions to the Schrödinger equation which, on their own, coincide each, up to $\hbar$-dependent multiplicative constants, with the corresponding fundamental solutions.

In Sec. IV we consider in some detail a general expression for the semiclassical expansions to the Schrödinger equation and introduce there also their standardized forms. We point out in this section an essential difference between the forms of the latter for the Borel summable and non-summable quantities.

In Sec. V we show the existence almost at each point of the x-plane two pairs of the base solutions to the Schrödinger equation with well defined Borel summable semiclassical asymptotic but not summed to the solutions themselves. The semiclassical expansions of the solutions considered in this section and their Borel resummations are a particular illustration of our main thesis that a result of any such a resummation is always some fundamental solution.

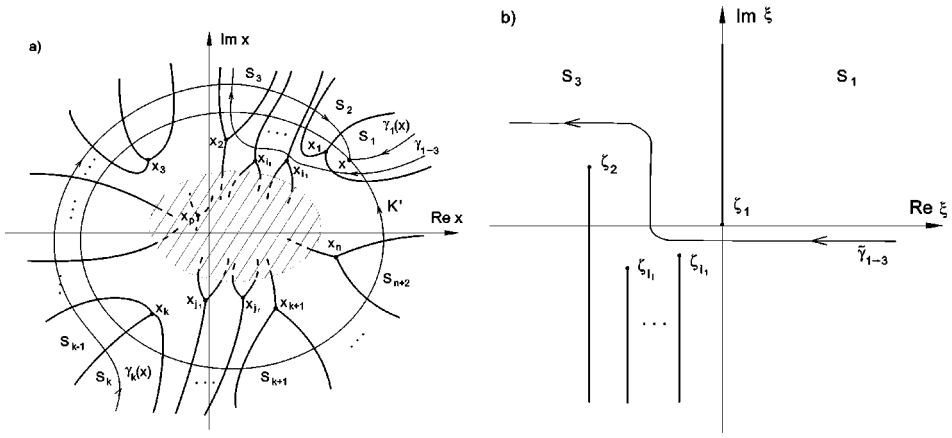

FIG. 1. (a) A general form of the Stokes graph for the polynomial potential discussed in Sec. II. (b) The ξ-variable map of the Stokes graph of (a) containing the sectors S_1 and S_3.

In Sec. VI we generalize the results of Sec. IV and show that the Borel function defined by the fundamental solutions can be considered as canonical in a sense that up to a multiplicative $\hbar$-dependent constant any Borel summable solution to the Schrödinger equation can be obtained by the Borel transformation of this canonical Borel function. This means that each Borel summable solution has to be essentially some of the fundamental solutions.

Section VII is a discussion of the results of the paper.

II. FUNDAMENTAL SOLUTIONS TO 1D STATIONARY SCHRÖDINGER EQUATION

Let us remind shortly basic lines in defining fundamental solutions.[1,5]

A set of fundamental solutions is attached in a unique way to a so called Stokes graph corresponding to a given polynomial potential $V(x)$ of the nth degree. Each Stokes graph is a collection of lines (Stokes lines) in the complex x-plane which are a loci of points where the real parts of action functions defined by the following n integrals:

$$W_i(x,E)=\int_{x_i}^{x}\sqrt{q(y,E)}dy,$$
$$q(x,E)=2V(x)-2E, \tag{1}$$

vanish. In (1) E is the energy of the system and x_i, $i=1,2,\ldots,n$, are roots of $q(x)$.

The fundamental solutions are defined in infinite connected domains called sectors with boundaries of the latter consisting of Stokes lines and x_i's; see Fig. 1(a).

In a sector S_k a corresponding fundamental solution ψ_k to the Schrödinger equation:

$$\psi''(x)-\hbar^{-2}q(x)\psi(x)=0, \tag{2}$$

has Dirac's form

$$\psi_k(x)=q^{-1/4}(x)\cdot e^{(\sigma_k/\hbar)\,W_k(x)}\cdot\chi_k(x), \tag{3}$$

with x_k lying at the boundary of S_k and with a sign $\sigma_k(=\pm 1)$ [which we shall call a *signature* of the solution (3)], chosen in such a way as to have

$$\Re(\sigma_k W_k(x))<0. \tag{4}$$

The amplitude factor $\chi_k(x,\hbar)$ in (3) has the following Fröman and Fröman's form:[27]

$$\chi_k(x,\hbar)=1+\sum_{n\geqslant 1}\left(\frac{\sigma_k\hbar}{2}\right)^n\int_{\infty_k}^{x}dy_1\int_{\infty_k}^{y_1}dy_2\ldots\int_{\infty_k}^{y_{n-1}}dy_n\omega(y_1)\omega(y_2)\ldots\omega(y_n)$$
$$\times(1-e^{-(2\sigma_k/\hbar)(W_k(x)-W_k(y_1))})(1-e^{(-2\sigma_k/\hbar)(W_k(y_1)-W_k(y_2))})$$
$$\cdots(1-e^{(-2\sigma_k/\hbar)(W_k(y_{n-1})-W_k(y_n))}), \tag{5}$$

with

$$\omega(x)=\frac{1}{4}\frac{q''(x)}{q^{3/2}(x)}-\frac{5}{16}\frac{q'^2(x)}{q^{5/2}(x)}=-q^{-1/4}(x)(q^{-1/4}(x))'', \tag{6}$$

and with integration paths in (5) chosen to be canonical,[1,5] i.e., on such paths the following condition is satisfied:

$$\sigma_k\Re(W_k(y_j)-W_k(y_{j+1}))\geqslant 0, \tag{7}$$

for any ordered pair of integration variables (with $y_0=x$). The condition (7) ensures the solution (3) to vanish at the infinity ∞_k of the sector S_k.

A domain $D_k(\supset S_k)$ where $\chi_k(x)$ can be represented by (5) with the canonical integration paths is called canonical. In each D_k the following semiclassical expansion for $\chi_k(x)$ can be deduced from (5) by standard methods (see also the next section):

$$\chi_k(x,\hbar)\sim\chi_k^{\mathrm{as}}(x,\hbar)=\sum_{n\geqslant 0}\left(\frac{\sigma_k\hbar}{2}\right)^n\chi_{k,n}(x),$$

$$\chi_{k,n}(x)=\int_{\infty_k}^{x}dy\,q^{-1/4}(y)(q^{(-1/4)(y)}\chi_{k,n-1}(y))''$$
$$=\int_{\infty_k}^{x}dy_n\,q^{-1/4}(y_n)\times\left(q^{-1/4}(y_n)\int_{\infty_k}^{y_n}dy_{n-1}\,q^{-1/4}(y_{n-1})\right.$$
$$\left.\times\left(\ldots q^{-1/4}(y_2)\int_{\infty_k}^{y_2}dy_1\,q^{-1/4}(y_1)(q^{-1/4}(y_1))''\ldots\right)''\right)'', \tag{8}$$

$$n=1,2,\ldots,\quad \chi_{k,0}(x)\equiv 1.$$

What has been said above assumed a real and positive value of $\lambda\equiv\hbar^{-1}$ (we prefer to use rather λ as a more convenient variable). However when considering Borel summability properties of $\chi_k(x,\lambda)$ it is unavoidable to complexify λ. If it is done the only change in the above descriptions of properties of Fröman and Fröman solutions to the Schrödinger equation is to substitute $W(x,E)$ in the conditions (4) and (7) by $e^{i\phi}W(x,E)$ where $\phi=\arg\lambda$. Of course, the domains D_k as well as the Stokes graph itself depend then on ϕ. In particular, all the Stokes lines rotate then around the corresponding turning points x_i, $i=1,2,\ldots,n$, they emanate from by the angle $-2\phi/3$. For $\phi=\pm\pi$ the Stokes graph comes back to its initial position, i.e., a dependence of the Stokes graph on ϕ is periodic with π as its period. Such a full rotation of Stokes graph we shall call *cyclic*. We can use the cyclic rotations to enumerate all the sectors according to the order they come into each other by the subsequent cyclic rotations starting from the one chosen arbitrarily. We shall assume from now on such a convention for the sector ordering with the numbers attached to sectors increasing anticlockwise.

By a cyclic rotation a solution $\psi_k(x,\lambda)$ from a sector S_k transforms into a solution $\psi_{k-1}(x,\lambda)$ or $\psi_{k+1}(x,\lambda)$ (modulo $n+2$, the last number being the total number of sectors for a polynomial potential of the nth degree) according to whether the rotation of the Stokes graph is clockwise or anticlockwise, respectively. Of course, for a fixed x after at most two subsequent cyclic rotations

(in the same direction) the path of integration in (5) stops to be canonical if it was as such before the rotation operations. Let us note also that making, say clockwise, $n+2$ subsequent cyclic rotations a solution $\psi_k(x,\lambda)$ does not come back exactly to its initial form (3) but acquires rather an additional phase factor which in the case of even n is equal to $(-\imath)^n \exp(\lambda \sigma_k \oint_{K'} \sqrt{q(x,E)}dx)$ where the (closed) contour K' encloses (anticlockwise) all n roots of the potential $V(x)$ [see Fig. 1(a)]. In the case of odd n one needs to surround all the roots twice as much to close the corresponding path of analytical continuation of $\chi_k(x,\lambda)$ in the x-plane with the result analogous with the even case. It means of course that as a function of λ a solution $\psi_k(x,\lambda)$ branches infinitely around the points $\lambda=0,\infty$ of the λ-plane.[1]

As we have mentioned earlier it was shown in Ref. 1 that in sector S_k the series (8) can be Borel summed to $\chi_k(x,\lambda)$ itself. To be a little bit detailed it was shown in Ref. 1 that when $x \in S_k$,

(1) the size of a sector in the λ-plane where the expansion (8) is valid is larger than 2π; and

(2) the rate of grow of $\chi_{k,n}(x)$ in (8) with n is factorial.

The last property which was established by an application of the Bender–Wu formula[2] ensured that the following Borel series:

$$\sum_{n\geqslant 0} \chi_{k,n}(x) \frac{(-s)^n}{n!}, \tag{9}$$

was convergent in a circle: $|s|<|W_k(x,E)|$.

On its turn the property (1) above ensured that the series (9) define Borel functions $\tilde{\chi}_k(x,s)$ holomorphic in the half-plane: $\Re s<-\sigma_k \Re W_k(x,E)$ allowing us to recover $\chi_k(x,\lambda)$ from the series (8) by the following Borel transformation of $\tilde{\chi}_k(x,s)$:

$$\chi_k(x,\lambda)=2\lambda \int_{C_\phi} e^{2\lambda s}\tilde{\chi}_k(x,s)ds, \tag{10}$$

where C_ϕ is a half-line in the Borel half-plane $\Re s<-\sigma_k \Re W_k(x,E)$ starting at infinity and ending at $s=0$ with ϕ as its declination angle ($\pi/2\leqslant\phi\leqslant 3\pi/2$).

However, for the latter transformations to exist it is neccessary for the functions $\tilde{\chi}_k(x,s)$ to be holomorphic only in some vicinity of a ray $\arg s=\phi_0$ along which the transformation (10) can be taken.[28] Such a limiting situation appears when $\chi_k(x,\lambda)$ is continued from the sector S_k to other domains of the Stokes graph so that such a continuation generates singularities of $\tilde{\chi}_k(x,s)$ in the half-plane $\Re s<0$ close to the ray $\arg s=\phi_0$. A mechanism of such singularity generations has been described by one of the present authors.[12] Some of these singularities are fixed and the others are moving with their positions in the s-plane depending on x. The possibility to perform the Borel transformation (10) of $\tilde{\chi}_k(x,s)$ along the ray $\arg s=\phi_0$ to get $\chi_k(x,\lambda)$ disappears at the moment when two of the moving singularities which are localized close to the ray $\arg s=\phi_0$ pinch the latter. It is clear that such cases depend continuously on x, i.e., for a given ϕ_0 in the domain $D_k(\phi_0)$ of the x-plane there is a maximal domain $B_k(\phi_0)$ $(D_k(\phi_0)\supset B_k(\phi_0)\supset S_k(\phi_0))$ inside which the series (8) for $\chi_k(x,\lambda)$ is Borel summable along C_{ϕ_0} to $\chi_k(x,\lambda)$ itself. To find a boundary of $B_k(\phi_0)$ one can use Voros' technique[24] of rotating of the reduced Stokes graph (i.e., the one obtained in the limit $|\lambda|\to\infty$) with changing of $\arg\lambda$ (see also Ref. 1): when $x \in \partial B_k(\phi_0)$ the total change of $\arg\lambda$ preserving the canonicness of the integration path in (5) running from $\infty_k(\phi_0)$ to x cannot be greater than π. Let us note also that for $x\in B_k(\phi_0)$ but close to $x_0\in\partial B_k(\phi_0)$ the Borel transformation of $\tilde{\chi}_k(x,s)$ along the ray $\arg s=\phi_0$ provides us with $\chi_k(x,\lambda)$ defined for $\pi/2-\phi_0\leqslant\arg\lambda\leqslant 3\pi/2-\phi_0$.

III. PROPERTIES OF THE BOREL FUNCTIONS $\tilde{\chi}_K(x,s)$

In this section we shall establish properties of the fundamental solutions and their corresponding Borel functions not discussed in our papers quoted in the previous sections.

First let us note that we can drop the subscribe k at the Borel functions $\tilde{\chi}_k(x,s)$ because in fact all these functions define one and the same Borel function. This property is the subject of the following theorem.

Theorem 1: *Let* $\tilde{\chi}(x,s)$ *coincide with* $\tilde{\chi}_1(x,s)$ *when* $x \in S_1$ *and* $|s|<|\xi(x)|$ *and where* $\xi(x) \equiv -\sigma_1 W_1(x,E)$. *Then*

(a) $\tilde{\chi}(x,s)$ *coincides with the Borel functions* $\tilde{\chi}_k(x,s)$, $k=2,\ldots,n+2$, *corresponding to the remaining fundamental solutions*;

(b) each fundamental solution can be obtained from $\tilde{\chi}(x,s)$ *when* $x \in S_1$ *by the Borel transformation with the integration path obtained by a suitable homotopic deformation of the path* C_1 *used to recover* $\chi_1(x,\lambda)$.

Proof: The part (a) of the theorem follows directly from the definitions of the Borel functions $\tilde{\chi}_k(x,s)$ by (9). Namely, for $x \in K' \cap S_1$ while $|s|<|\xi(x)|$, we can transform the coefficients $\chi_{1,n}(x)$ defining $\tilde{\chi}(x,s)$ by the series (9) into the corresponding coefficients $\chi_{k,n}(x)$. To do it, it is enough to continue analytically the infinite limit ∞_1 of all the integrations in (8) from the sector S_1 to the sector S_k to achieve the infinity ∞_k of the sector S_k. Of course this is a deformation of the integration path $\gamma_1(x)$ in (8) into the $\gamma_k(x)$ one but this does not affect the integrations if *none* of the turning points is touched by the deformed path which is assumed and seen in Fig. 1(a). In other words such a deformation should be homotopic. Due to this operation we have, of course, $\chi_{1,n}(x) \equiv \chi_{k,n}(x), n \geqslant 1$ and, by (9) $\tilde{\chi}_k(x,s) \equiv \tilde{\chi}(x,s)$, $k=2,\ldots,n+2$.

Before going to the proof of the part (b) of the theorem let us make the following comments to the proof done so far.

First let us call as the standard paths the integration paths $\gamma_k(x)$ which appear in this way in (8) linking the infinity ∞_k, $k=2,\ldots,n+2$, with the point x, $x \in K' \cap S_1$.

Let us note further that continuing the infinite tail of the standard path by moving by the subsequent sectors around the *closed* contour K' (to close the contour K' in the case of the odd n it is necessary to round the infinity point two times) we have to come back again to the sector S_1 when crossing the ''last'' S_{n+2} one. The consistency condition which follows then from (8) demands that the integral $\oint_{K'} q^{-1/4}(x)(q^{-1/4}(x)\chi_{1,n}(x))'' dx$ should then vanish for each $n \geqslant 0$. One can easily check that it happens indeed for all the polynomial potentials.

For the factor $\chi_k(x,\lambda)$, however, as given by (5) if $k \neq 2, n+2$ the standard path is of course noncanonical [see Fig. 1(a)]. But this means merely that $\chi_k(x,\lambda)$ obtained in this way is an effect of its analytical continuation along K' from the sector S_k, where it could be initially defined, to the sector S_1. This of course means also that $\chi_k(x,\lambda)$ cannot be obtained from (10) by the integration along a half-line but rather by the corresponding integration along some more complicated path described below.

To restore, however, the Borel function corresponding to $\chi_k(x,\lambda)$ when $x \in S_k$ it is necessary only to continue $\tilde{\chi}(x,s)$ analytically by moving the point x from the sector S_1 to S_k along the contour K'. Of course at the end of this continuation the standard path linking ∞_k with the continued x is then found completely in the sector S_k being there a typical canonical path for the integrations in (5) and (8).

On the Borel plane the latter analytical continuation of $\tilde{\chi}(x,s)$ corresponds to a motion of the branch point of at $s=\xi(x)=-\sigma_1 \int_{x_1}^{x} \sqrt{q(y,E)}\,dy$ shown in Fig. 3 along the line $\tilde{K}'$ which is the image of K' on the s-Riemann surface given by the map $s=\xi(x)$. During this motion the argument of this branch point changes by $(k-1)\pi$.

Let us finish these comments of the part (a) of the theorem by noticing that this part can be proved also using the results of the discussion performed in Appendix A and Theorem 6.

The validity of the part (b) follows easily just from Theorem 6 of Appendix A. Namely, to prove this part consider first $\tilde{\chi}(x,s)$ when x is continued from the sector S_1 to the sector S_3 along the contour K' shown in Fig. 1(a) while s is kept fixed. A pattern of the first sheet of the s-Riemann surface is then shown in Fig. 10(b). To recover $\chi_3(x,\lambda)$ by (10) we have to integrate $\tilde{\chi}(x,s)$ over the negative real half-axis. Let us now move all the branch points shown in Fig. 10(b) back according to moving back the point x on the contour K' to its original position in the sector S_1. The point $s=0$ of this sheet is then left from the right. This motion causes the integration path

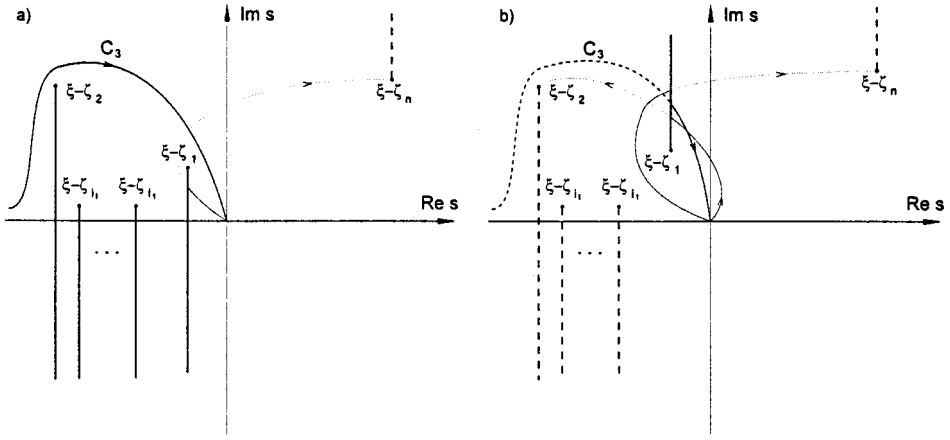

FIG. 2. (a) The position of the branch points at $\xi-\zeta_1,\ldots,\xi-\zeta_2$ and of the contour C_3 for $\tilde{\chi}(x,s)$ when $x\in K'\cap S_2$. (b) The same as in (a) after uprighting the cut emerging from the point $\xi-\zeta_1$.

just mentioned to be deformed into the one shown in Fig. 2(a). If we apply now to the cut emerging from the branch point $\xi-\zeta_1$ an operation of rotating it clockwise by π which is reversed to the unscreening operation described in Theorem 6 of Appendix A we obtain the situation drawn in Fig. 2(b). This figure shows in detail why in these positions of the considered cuts the integration in (10) along the path C_3 provides us with the factor $\chi_3(x,\lambda)$ which corresponds to the sector S_3 [i.e., the infinite integration limit in (5) coincides with ∞_3], but is continued on the x-plane to the sector S_1 along the contour K'.

Let us note further that in the positions of the cuts shown in Fig. 2(b) we can obtain the factors $\chi_1(x,\lambda)$ and $\chi_2(x,\lambda)$ as well integrating along the left and right real half-axes.

We can repeat the above analysis starting from the cut pattern shown in Fig. 11(b) and corresponding to the Borel function $\tilde{\Phi}(\xi(x),s)(\equiv\tilde{\chi}(x,s))$ continued to the sector S_k along the contour K'. In this position of ξ the factor $\chi_k(x,\lambda)$ is recovered by (10) by integrating $\tilde{\Phi}(\xi,s)$ along, say, the negative real half-axis (assuming k is odd). Next, moving the point x back to its original position in the sector S_1 and applying to the consecutive cuts emerging from the branch points at $\xi-\zeta_{i_{k-1}}$, $\xi-\zeta_{i_{k-2}},\ldots,\ \xi-\zeta_2,\ \xi-\zeta_1$ the operations reversed to the uprighting ones described in Theorem 6 of Appendix A we achieve the pattern of Fig. 3. It follows from the figure that the above operations deform merely homotopically the integration contour C_k from its original position when it coincides with the negative real half-axis to the one shown in this figure where it has a spiral form allows it to avoid all the branch points.

Let us note that as it follows from the analysis performed in Appendix A the *fixed* branch points lie on the lower sheets of the s-Riemann surface beeing *always* screened by the moving ones and therefore *not* participating in the deformation of the contour C_k.

Note also that this deformation of the contour C_k does not affect the convergence of the integral (10) since as we have shown in Ref. 12 and mentioned in Appendix A on *each* sheet of the s-Riemann surface the divergence of $\tilde{\Phi}(\xi,s)$ at infinity is at most exponential.

In this way we have however completed the proof of the theorem. QED.

It is certainly worth stressing that a net result which follows from Theorem 1 is that to obtain the subsequent $\chi_k(x,\lambda)$'s, $k=2,3,\ldots,n+2$ it is enough (according to our enumeration convention) to deform C_1 homotopically anticlockwise by making its infinite tail to rotate by the angles $\pi,2\pi,\ldots,(n+1)\pi$ so that to coincide eventually with the real half-axes, positive or negative, on the corresponding sheets, see Fig. 3. We get in this way the sequence of paths $C_2,\ C_3,\ldots,\ C_{n+2}$ integrations on which according to the formula (10) provide us with the corresponding $\chi_k(x,\lambda)$'s, $k=2,\ldots,n+2$. But these latter χ-factors are exactly the ones which were obtained in Sec. II by applying to $\chi_1(x,\lambda)$ the subsequent cyclic rotations since the latter correspond to (opposite) rotations on the λ-Riemann surface by the angles $-\pi,-2\pi,\ldots,-(n+1)\pi$. It follows however

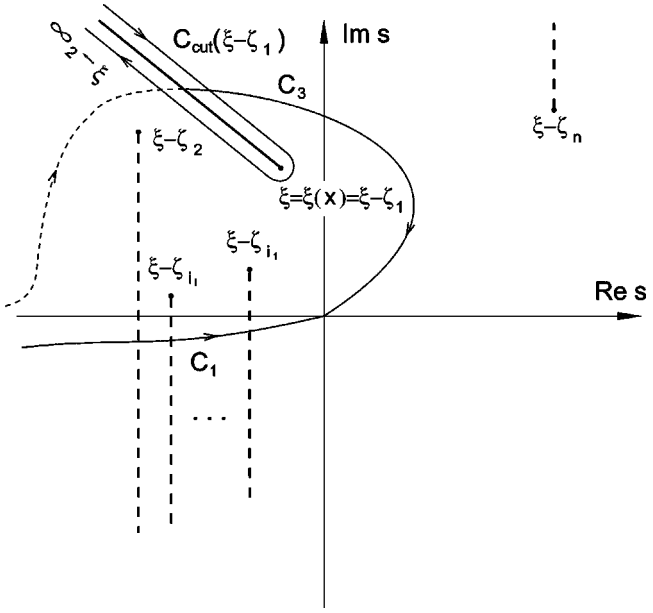

FIG. 3. The corresponding integration paths C_1, $C_2,\ldots,C_k$ in the formula (10) when $x\in K'\cap S_2$.

from the formula (10) that such cyclic rotations have to be accompanied then by the compensating rotations of the integration path on the s-Riemann surface to maintain the convergence of the formula.

We see therefore that the cyclic rotation property of transforming the fundamental solution $\psi_1(x,\lambda)$ into $\psi_k(x,\lambda)$ can be realized in the following two equivalent ways.

(1) On the x-plane by deforming the integration path $\gamma_1(x)$ in the formula (5) [when it defines the solution $\psi_1(x,\lambda)$, with $x\in S_1$] into the corresponding standard path linking the sector S_1 with the sector S_k.
(2) On the Borel plane by deforming the the path C_1 in the way described above.

We know however that after such $n+2$ cyclic rotations we do not come back to exactly the same factor $\chi_1(x,\lambda)$ but the latter acquires rather an additional phase factor which for the even degree polynomials is equal to $(-\imath)^n\exp(-\lambda\sigma_1\oint_{K'}\sqrt{q(x,E)}dx)$. Therefore deforming the path C_{n+2} once more in the above way to a path C_{n+3} and integrating $\tilde{\Phi}(\xi,s)$ along this path we get as a result again $\chi_1(x,\lambda)$ but multiplied by the phase factor just mentioned, i.e., for the even degree polynomials we have

$$\int_{C_{n+3}} e^{2\lambda s}\tilde{\chi}(x,s)ds = e^{-\lambda\sigma_1\oint_{K'}\sqrt{q(y,E)}dy-\imath n(\pi/2)}\int_{C_1} e^{2\lambda s}\tilde{\chi}(x,s)ds. \tag{11}$$

Deforming C_1 appropriately clockwise we obtain of course the corresponding integration paths $C'_{k'}$, $k'=2,3,\ldots$, providing us with $\chi_k(x,\lambda)$'s ordered in the opposite way, i.e., with $k=n-k'+4=n+2,n+1,\ldots,2$. For the path C'_{n+3} we get an identity similar to (11) but with the opposite sign at the exponent of the proportionality coefficient. This confirms that the s-Riemann surface of $\tilde{\chi}(x,s)$ is in general infinitely sheeted. The only obvious case with the finite six sheeted s-Riemann surface is provided by the linear potential.[12]

Let us discuss still in some detail the deformation procedure of the path C_1 described above.

The singularity pattern of Fig. 3 which corresponds to $x\in S_1$ shows that to fall on the corresponding sheets in order to approach eventually the chosen direction of the real axis the paths C_k

have to avoid in general the existing singularities of $\tilde{\chi}(x,s)$ on its s-Riemann surface. According to Fig. 3 such necessary deformations have to be applied for example to the path C_3 and to the subsequent ones but not to C_2.

The integration in (10) along C_3 provides us with $\chi_3(x,\lambda)$ but since $x \in S_1$ the corresponding integration path in (5) cannot then be canonical, i.e., if $|\lambda| \to \infty$ then $\psi_3(x,\lambda)$ does not behave according to its JWKB factor in (3). The obvious reason for that is just the (branch point) singularity of $\tilde{\chi}(x,s)$ at $s=\xi$ (with $\Re\xi>0$) which causes $\chi_3(x,\lambda)$ calculated in this way to diverge as $e^{2\lambda\xi}$ in the semiclassical limit.

To restore, therefore, the proper canonical behavior of $\chi_3(x,\lambda)$ in this limit given by (8) we would have to move the singularity at $s=\xi$ to the left half-plane of Fig. 3, i.e., to move the corresponding variable x from the sector S_1 to S_2 along the contour K'. This is just the procedure described in the course of the proof of the theorem.

Earlier we have distinguished the canonical paths of integrations in (5) as the ones which ensured that the χ-factors in (3) had well defined semiclassical expansions given by (8). A part of these paths penetrating the domains B_k's mentioned in the previous section ensured also that the fundamental solutions defined by them were Borel summable and these resummations were achieved by the Borel transforms of the Borel function $\tilde{\chi}(x,s)$ along half-lines running from the infinity of the Borel ''plane'' and ending at its center. Let us call *canonical* also these latter paths on the Borel ''plane.''

However we could notice above that it is possible to generalize substantially the notion of the Borel transformation by integrating in the Borel ''plane'' along the paths C_k described above and recovering in this way the fundamental solutions obtained by the deformations of the canonical paths in the formulas (5) due to the cyclic rotations of the Stokes graph.

It is therefore worthwhile distinguishing also these new types of the Borel transformation paths and these noncanonical paths in the x-''plane'' as well which appear as a result of the homotopic deformations of the canonical paths by the cyclic rotations. Namely, we shall call further such paths both on the s- and on the x-''plane'' as the *standard* paths in common.

Although it should be obvious that the Borel transformation of the Borel function $\tilde{\chi}(x,s)$ along any standard path should always provide us with the corresponding χ-factor of the Dirac form (3) of the fundamental solutions we show this fact explicitly in Appendix B.

It is a good moment of our discussion to mention an old problem of the semiclassical theory known as the connection problem.[29–32] In the context of our considerations it arises when we are interested in the semiclassical behavior of $\psi_3(x,\lambda)$ while x is kept in S_1 (i.e., $x \in S_1$). In such a case we can deform the standard path C_3 into two paths, a path C_3' surrounding the cut generated by the singularity at $s=\xi$ (see Fig. 4) and again the canonical path C_1. By multiplying (10) (with C_3 as the integration path) by $q^{-1/4}e^{-\lambda\xi}$ we obtain $\psi_3(x,\lambda)$ to be represented in this way by the following linear combination of two solutions to the Schrödinger equation (2):

$$\psi_3(x,\lambda)=\psi_1(x,\lambda)+C(\lambda)\psi_2(x,\lambda). \tag{12}$$

Of course, $\psi_1(x,\lambda)$ is generated by the C_1 part of C_3. The fact that the cut integration part of $\psi_3(x,\lambda)$ is just proportional to $\psi_2(x,\lambda)$ can be easily seen by pushing ξ to infinity along the cut which corresponds to approaching by $x(\xi)$ the infinity of the sector S_2. The cut integral (multiplied by $q^{-1/4}e^{-\lambda\xi}$) vanishes however in this limit (since $\Re\xi \to -\infty$) which proves our assertion. In other words we have

$$q^{-1/4}(x,E)e^{-\lambda\int_{x_1}^{x}\sqrt{q(y,E)}dy}2\lambda\int_{C_{\mathrm{cut}}(\xi)}e^{2\lambda s}\tilde{\chi}(x,s)ds=C(\lambda)\psi_2(x,\lambda). \tag{13}$$

It is easily seen that the last relation is independent of such critical forms of the Stokes graph as the ones corresponding to the coinciding of two (or more) turning points. However, when the

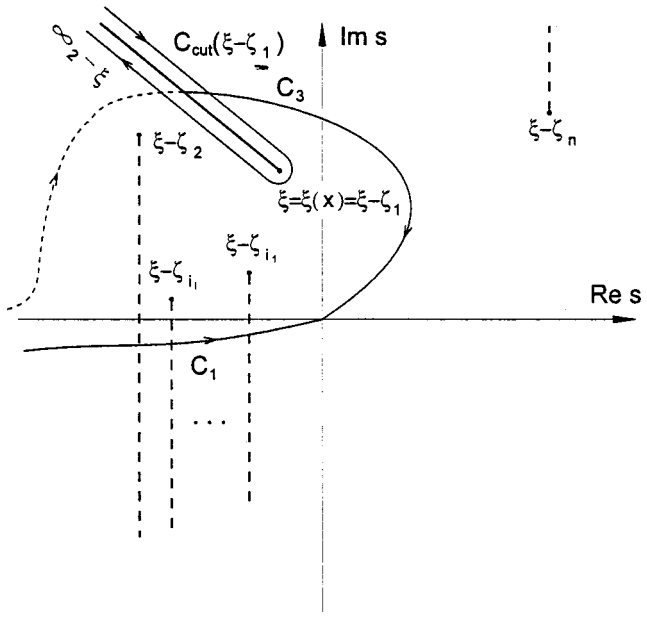

FIG. 4. The path C_3 splitted into the paths C_1 and $C_{\text{cut}}(\xi-\zeta_1)$.

Stokes graph is built only by the simple turning points then this relation can be established by the standard methods, i.e., by continuing the fundamental solutions along the canonical paths on the x-''plane,'' which gives[1,5]

$$C(\lambda)=-\imath\chi_{3\to 1}(\lambda), \tag{14}$$

where $\chi_{3\to 1}(\lambda)=\lim_{x\to\infty_1}\chi_3(x,\lambda)=\chi_{1\to 3}(\lambda)$ is calculated by (5) along the canonical path $\gamma_{1\to 3}$ [see Fig. 1(b)].

Writing further $\psi_2(x,\lambda)$ in Dirac's form (3) we get

$$\begin{aligned}\chi_2(x,\lambda)&=\imath\chi_{3\to 1}^{-1}(\lambda)e^{-2\lambda\xi}2\lambda\int_{C_{\text{cut}}(\xi)}e^{2\lambda s}\tilde{\chi}(x,s)ds\\&=\imath\chi_{3\to 1}^{-1}(\lambda)2\lambda\int_{C_{\text{cut}}(0)}e^{2\lambda s}\tilde{\chi}(x,s+\xi)ds.\end{aligned} \tag{15}$$

Taking now into account that $\chi_2(x,\lambda)$ is given by the Borel transformation along the canonical path C_2 in Fig. 4 while $\chi_{3\to 1}(\lambda)[\equiv\chi_{1\to 3}(\lambda)]$ can be obtained analogously by the integration $\tilde{\chi}_{\text{can}}(\infty_3,s)[\equiv\lim_{x\to\infty_3}\tilde{\chi}(x,s)]$ along C_1 when $\xi(x)$ in Fig. 1(b) goes from the sector S_1 to ∞_3 of the sector S_3 along the canonical path we get the following relation for $\tilde{\chi}(x,s)$ and its jump $\Delta_{s_0}\tilde{\chi}(x,s)$ through the cut emerging from the branch point $s=s_0=\xi(x)$:

$$\tilde{\chi}(x,s)=\imath\tilde{\chi}_{\text{can}}{}^{*-1}(\infty_3,s)*\Delta_0\tilde{\chi}(x,-s+\xi(x)). \tag{16}$$

The ''*'' symbols in (16) denote the convolution operations [see Appendix C, formula (56)].

One easily recognizes in (16) the fundamental solution version of the analytical bootstrap property of the Borel function $\tilde{\chi}(x,s)$ discovered by Voros.[24] It is our aim in this paper, however, to show that in the case of the polynomial potentials there are *no* other versions of the realization of the analytical bootstrap idea since in this case the Borel function $\tilde{\chi}(x,s)$ is unique (up to an irrelevant constant) being uniquely defined by the fundamental solutions.

The same comments as above are valid of course with respect to the results of the integrations along the subsequent standard paths C_k, $k=4,5,\ldots$, i.e., these paths provide us with the corresponding $\chi_k(x,\lambda)$'s calculated along the noncanonical standard paths on the x-''plane'' obtained by the continuation of the variable x from S_k to S_1 along the contour K'. Such a form does not allow us to estimate easily its semiclassical limit. To recover this limit properly we have to deform C_k's keeping its infinite tail along the appropriate real half-axis. This deformation splits C_k into C_1 or C_2 (the latter choice depends on a sign of $\Re\lambda$) and into a number of paths surrounding some cuts (the cuts have to run to the left half-planes for $\Re\lambda>0$ or to the right ones in the opposite case). Each such cut contribution represents a solution to the Schrödinger equation (see Appendix B) being proportional to some fundamental solution. The identification of these solutions can be performed by considering the limit of the latter when $\xi\to\infty$ along the appropriate cuts (or their elongations) (the solutions have to vanish in this limit) and following parallelly the corresponding paths drawn by $x(\xi)$ on the Stokes graph. Again, if the Stokes graph considered is determined only by simple turning points then a total number of the fundamental solutions engaged in the above splitting operation is limited only to those of them which can contact canonically with the sector S_1 where the variable x/ξ ($\xi=\xi(x)$) actually is and the proportionality coefficients of the cut contributions to appropriate fundamental solutions can be calculated by the standard methods.[1,5]

Let x be fixed somewhere on K' [see Fig. 1(a)].

We shall call a cut path each path surrounding a half-line cut of the s-Riemann surface running from its infinity and ending at some of its moving or fixed branch points.

Together with the result of Appendix B the net results of the above discussion can be summarized as the following two theorems.

Theorem 2: *(a) The Borel function $\tilde{\chi}(x,s)$ when Borel transformed along a standard or a cut path and multiplied by the JWKB factor always provides us with a solution to the Schrödinger equation (2) having the Dirac form (3).*

(b) The solutions we get in this way are always proportional to fundamental solutions.

(c) If a solution defined by a cut path is generated by the deformation of the standard path then if it is proportional to the fundamental solution $\psi_k(x,\lambda)$ with a proportionality constant $C_k(\lambda)$ then a jump $\Delta_{s_0}\tilde{\Phi}(\xi(x),s)$ of $\tilde{\Phi}(\xi(x),s)(\equiv\tilde{\chi}(x,s))$ through the cut generated by the branch point at $s=s_0$ is related in the following way with $\tilde{\Phi}(\xi,s)$ itself (a case of the analytic bootstrap of Voros[24]):

$$\tilde{\Phi}((-1)^{k-1}\xi(x'),s)=\tilde{C}_k(s,s_0)*\Delta_{s_0}\tilde{\Phi}(\xi,\pm s+s_0), \tag{17}$$

where the rhs of (17) is the convolution of $\tilde{C}_k(s,s_0)$ which is the Borel function corresponding to the inverse of the constant $C_k(\lambda)$ multiplied by $e^{2\lambda s_0}$ and of $\tilde{\Phi}(\xi,s)$ shifted, respectively, while $\tilde{\Phi}((-1)^{k-1}\xi(x'),s)$ denotes $\tilde{\chi}(x,s)$ continued analytically along K' from the point $x\in K'\cap S_1$ to the point $x'\in K'\cap S_k$ such that $\xi(x)=(-1)^{k-1}\xi(x')$. The ''$\pm$'' signs at the variable s in (17) takes into account that Borel integrations along the cut and the canonical path C_k^{can} to recover $\chi_k(x,\lambda)$ can go to the same (''$+$'' sign) or to the opposite (''$-$'' sign) infinities of $\Re$'s.

The existence of $\tilde{C}_k(s,s_0)$ and the holomorphicity of $\Delta_{s_0}\tilde{\Phi}(\xi(x),\pm s+s_0)$, at $s=0$, is assumed.

Proof of the theorem: The part (a) of the theorem is obvious by noticing that any Borel transformation along the standard/cut path with the Borel function $\tilde{\chi}(x,\lambda)$ defined by (9) satisfies the linear differential equation defining $\chi(x,\lambda)$'s (see Appendix B).

The part (b) of the theorem when concerning the standard paths is a repetition of the corresponding result of Theorem 1. With respect, however, to the cut paths it follows as a conclusion summarizing the discussion preceding the formulation of this theorem.

The part (c) is the direct consequence of the hypothesis of this part of the theorem written explicitly as

$$q^{-1/4}(x')e^{\sigma_k\lambda\xi(x')}2\lambda\int_{C_{\mathrm{cut}}(s_0)}e^{2\sigma\lambda s}\tilde{\Phi}(\xi(x),s)ds$$
$$=C(\lambda)q^{-1/4}(x')e^{\sigma_k\lambda\xi(x')}\chi_k(x',\lambda)$$
$$=C(\lambda)q^{-1/4}(x')e^{\sigma_k\lambda\xi(x')}2\lambda\int_{C_k^{\mathrm{can}}}e^{-2\sigma_k\lambda s}\tilde{\Phi}(\xi,s)ds, \tag{18}$$

where C_k^{can} denotes the canonical path on the Borel ''plane'' used for recovering $\chi_k(x,\lambda)$, σ_k is a signature of the latter and $\sigma=\pm 1$ is taken as $+1$ for the integration along the cut $C_{\mathrm{cut}}(s_0)$ to $-\infty$ of $\Re s$ and as -1 in the opposite case.

Since $\chi_k(x',\lambda)$ in (18) is recovered by the integration $\tilde{\Phi}(\xi(x'),s)$ along the *canonical* path C_k^{can} then it means that this latter function results as its analytical continuation from the first sheet where it determines $\chi_1(x,\lambda)$ (by the integration along a canonical path C_1 on this sheet) to the sheet considered. This continuation has to be performed along the path $\tilde{K}'$, the image of K' on the Borel ''plane,'' as long as ξ acquires the argument equal to $(k-1)\pi$ which put ξ in the position $(-1)^{k-1}\xi$ on the final sheet. This corresponds of course to a point x' on K' such that $\xi(x)=(-1)^{k-1}\xi(x')$.

Now, if $\sigma_k=\sigma$ (this case is the only one possible when s_0 is the fixed branch point) then we get the relation (17) with ''+'' at the variable s and with ''−'' in the opposite case.

This latter conclusion ends, however, the proof of the theorem. QED.

Let us note, as a comment to the part (b) of the above theorem, that the proportionality constants can be always calculated independently when all turning points of considered polynomial problems are simple. We can use then the powerful method of analytical continuation of the fundamental solutions along the canonical paths which guarantees the full control of the semiclassical properties of calculated quantities at each stage of such calculations. The considerations preceding the above theorem are the good illustration of the possibilities of the method.

Theorem 3: *The connection problem, i.e., the analytical continuation of the fundamental solutions throughout the x-plane along the contour K′ of Fig. 1(a) can be solved by performing this continuation on the Borel plane. By such a continuation the original Borel integration along the deformed path has to be split into integrations along standard and cut paths the latter emerging from the branch points of $\tilde{\chi}(x,s)$ pinching the deformed path.*

Proof: The validity of the theorem follows directly from the preceding discussion.

Another important property of the fundamental solutions which distinguishes these solutions among other possible Borel summable solutions can be formulated as the following theorem.

Theorem 4: *Let x_0 $[=x(\xi_0)]$ be an arbitrary point of the x-plane not coinciding with a root of $q(x,E)$. Then there is a (nonempty) subset $N(x_0)$ of fundamental solutions of both signatures with the following properties.*

(1) The point x_0 is canonical for every member of $N(x_0)$.
(2) Every element of $N(x_0)$ can be obtained by the formula (10) integrating along a corresponding standard path.

We shall assume $N(x_0)$ to collect all such fundamental solutions.

Proof of the theorem: The validity of this theorem can be easily seen by considering the topology of sectors with respect to the chosen x on the Riemann surface of the action variable $\xi(\equiv\xi(x))$ substituting the variable x (see Fig. 5 and Ref. 1). For real λ the Stokes lines on the surface are now parallel to imaginary axes and the sectors are left and right half-planes not containing (the images of) turning points on each sheet of the surface.[1] The λ-rotations of the Stokes graph make Stokes lines on the ξ-Riemann surface rotating around the images of the turning points preserving their parallelness.

We shall distinguish the following four cases for the position of x_0 for real λ.

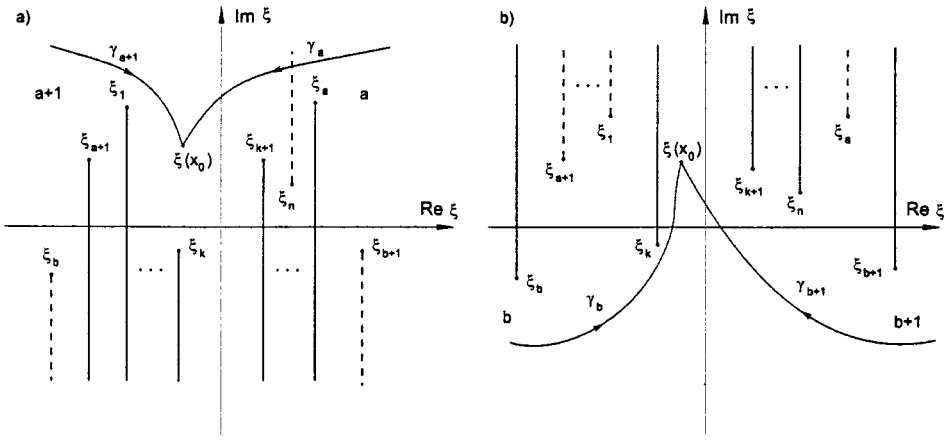

FIG. 5. (a) The sectors S_{a+1} and S_a the fundamental solutions of which communicate canonically with the point $\xi(x_0)$. (b) The sectors S_b and S_{b+1} the fundamental solutions of which communicate canonically with the *same* point $\xi(x_0)$.

(1) x_0 does not lie on any Stokes line but
   (a) x_0 belongs to some sector,
   (b) x_0 does not belong to any sector;
(2) x_0 lies on some Stokes line and
   (c) this Stokes line is finite, i.e., it emerges from some turning point and ends on the other,
   (d) this Stokes line is infinite, i.e., it emerges from some turning point and runs to infinity of the $x(\xi)$-plane.

The above possibilities exhaust of course all the possible positions of x_0 with respect to the Stokes lines.

Consider case (a) of (1).

First let us note that for real λ the Stokes lines are parallel to the imaginary axis as it is shown in Fig. 5. If x_0 is in some sector, say S_a, then obviously the fundamental solution ψ_a defined in this sector belongs to $N(x_0)$. There are however another two fundamental solutions which belong to $N(x_0)$ too. Namely, these are the two neighbors of ψ_a, i.e., ψ_{a+1} and ψ_{a-1} (according to our enumeration convention). Both of them have their signatures opposite to ψ_a. Depending on a position of x_0 in S_a there is always one of these two neighbor solutions which is Borel summable at x_0 simultaneously with ψ_a and at the same time can communicate with it canonically.

Consider next case (b) of (1).

In this case x_0 is in some infinite vertical strip on the ξ-Riemann surface (see Fig. 5) bounded from each side by two chains of Stokes lines parallel to each other. Following each of these chains of lines while keeping on the strip we find on them their extremal turning points, i.e., the ones from which Stokes lines emerge running to imaginary infinities, positive or negative. Consider such a Stokes line which bounds the strip from the right and runs to positive imaginary infinity. This Stokes line bounds simultaneously from the left a strip neighbor to the one just considered. This new strip is again bounded from the right by a chain of Stokes lines whose structure is similar to the Stokes line chains already considered. So there is again in this chain a Stokes line ending it and running to positive imaginary infinity. We can repeat this procedure of moving to the right of the ξ-''plane'' to finish eventually with a ''strip'' which is a right half-plane of the ξ-plane sheet considered. This procedure has to be finite since there is a finite number of extremal turning points met in this way due to the polynomial potential. It is clear also that this half-plane corresponds to a sector, say S_a, of the Stokes graph. The way of its finding proves that the fundamental solution ψ_a defined in it belongs to the set $N(x_0)$. Mutatis mutandis to this set belongs also the solution ψ_{a+1} corresponding to the sector S_{a+1}, the next one to S_a and having an opposite signature. By the same reasoning but moving down the ξ-sheet we find two others sectors, call them S_b and S_{b+1}, the fundamental solutions of which are both Borel summable at x_0 having of course

opposite signatures. Therefore there are at least four fundamental solutions in $N(x_0)$ for this case. Besides, within the pairs ψ_a, ψ_b and ψ_{a+1}, ψ_{b+1} both the fundamental solutions can communicate with themselves canonically and can be simultaneously Borel summable. This last result is a conclusion from the fact that these pairs of fundamental solutions are related by the cyclic rotations.

Consider now the case (c) of (2).

In this case we can consider both the sides of the Stokes line on which x_0 is placed as pieces of two strips for which this line is their bound. The strips can be identified as the wholes by the procedure similar to the one used previously. Namely, we move along a chain of Stokes lines directing to, say, the positive imaginary infinity choosing the most right Stokes line each time we meet some turning point. Continuing this motion we meet finally the last such turning point from which the most right Stokes line emerges running directly to the positive imaginary infinity. From this moment we can repeat the arguments of the previous point when concluding that we can find in the right half-plane on a certain ξ-sheet a sector, call it S_a again, a fundamental solution of which is Borel summable at x_0, i.e., this solution belongs to $N(x_0)$.

However, this case differs a little bit from the previous one by the fact that the neighbor sector ψ_{a+1} is *not* Borel summable at x_0 in the actual position of this variable. Nevertheless, if we rotate the variable λ anticlockwise by an arbitrary small angle we immediately satisfy the Watson–Sokal–Nevanlinna conditions for the Borel resummation of ψ_{a+1}. Making a cyclic rotation in the same direction we transform the last solution into ψ_a and this rotation can still be continued a little bit further. This proves that ψ_a indeed satisfies the conditions mentioned above to be Borel summable at x_0 in its actual position.

Again mutatis mutandis we can prove moving down the ξ-sheet the existence of another fundamental solution in the right half of the sheet which is Borel summable at x_0. Let us call it ψ_b.

Repeating the procedure and keeping the most left Stokes lines while moving to the imaginary infinities in both directions, positive and negative, we find still another two respective solutions ψ_d and ψ_c. Collecting them into the following pairs ψ_a, ψ_c and ψ_b, ψ_d we find that the solutions in each pair communicate canonically with each other and are Borel summable simultaneously at x_0.

In this way we have proved however our theorem. QED.

Theorem 4 is, to some extent, a generalization of Theorem 1. Namely, we have the following.

Corollary: In the assertion (b) *of Theorem 1 we can take any regular point of the* x*-plane in which we want to obtain any fundamental solution continued to this point by the cyclic rotation operations defined in Sec. II.*

Proof: Our reasoning is the following.

Theorem 4 tells us that for a given (regular) x_0 there is *always* a fundamental solution, say $\psi_a(x,\lambda)$, Borel summable at this point. This means however that the χ-factor of this solution is recovered from the Borel function $\tilde{\chi}(x,s)$ by the Borel transformation along the path C_a coinciding with the left/right real half-axis of the Borel plane. The latter plane is of course a sheet of the s-Riemann surface obtained from the one in Fig. 7 by the unscreening operation. Depending on the actual position of x_0 the representation of branch points on this sheet can be richer than in the cases considered in Theorem 1 because of the closest environment of x_0 which can be richer in turning points. This structure can be analyzed in a way similar to that in Appendix A giving a typical branch point pattern with both moving and fixed branch points on this sheet lying above or below the path C_a but allowing us to perfom the Borel transformation along the path.

We can now start to deform homotopically the path C_a exactly in the same way as we did with the path C_1 in Theorem 1 taking its infinite end and rotating it by the angles $\pm\pi$, $\pm 2\pi, \ldots,$ to appropriate positions along the left/right half-axis on the sheets corresponding to subsequent fundamental solutions starting from $\psi_{a+1}(x,\lambda)$ in the clockwise direction of the deformation or from $\psi_{a-1}(x,\lambda)$ in the opposite case. This procedure could be disturbed only when the deformed path C_a met on its way a chain of branch points elongating to infinity. This is *not* possible however since such possible chains of branch points are always screened by the moving

cuts. A good illustration of the described situation is provided by the harmonic oscillator case (see Ref. 12).

We have already mentioned in the course of the proof of Theorem 1 that the suitable deformations of the path C_1 to $C_2,\ldots,C_{n+2}$ described in this theorem restore all the fundamental solutions when $x\in S_1$ strictly corresponded to the recovering these solutions from $\psi_1(x,\lambda)$ defined in S_1 by the cyclic rotations. Exactly the same relation connects the above deformations of the path C_a with the cyclic rotations of the Stokes graph from its position just considered.

The last conclusion finishes the proof of the corollary. QED.

IV. GENERAL FORM OF SEMICLASSICAL EXPANSION FOR χ-FACTORS

Let us note that the χ-factors entering the Dirac forms (3) are the solutions of the following two second order linear differential equations obtained by the substitution (3) into the Schrödinger equation:

$$-q^{-1/4}(x)(q^{-1/4}(x)\chi(x))''+2\sigma\lambda\chi'(x)=0. \tag{19}$$

The equations (19) provide us with a general form of semiclassical expansions for the χ-factors if such expansions exists. Namely, assuming the latter we can substitute into (19) the semiclassical expansion for χ:

$$\chi(x,\lambda)\sim\sum_{n\geqslant 0}\left(\frac{\sigma}{2\lambda}\right)^n\chi_n(x), \tag{20}$$

to get the following recurrent relations for $\chi_n(x)$:

$$\begin{gathered}\chi_n(x)=C_n+\int_{x_n}^{x}q^{-1/4}(y)(q^{-1/4}(y)\chi_{n-1}(y))''dy,\quad n\geqslant 1,\\ \chi_0(x)\equiv C_0,\end{gathered} \tag{21}$$

where x_n, $n\geqslant 1$, are arbitrary chosen regular points of $\omega(x)$ and C_n, $n\geqslant 0$, are arbitrary constants. It is, however, easy to show that choosing all the points x_n to be the same, say x_0, merely redefines the constants C_n. Assuming this we get for $\chi_n(x)$,

$$\begin{gathered}\chi_n(x)=\sum_{k=0}^{n}C_{n-k}I_k(x,x_0),\\ I_0(x,x_0)\equiv 1,\\ I_k(x,x_0)=\int_{x_0}^{x}d\xi_k\,q^{-1/4}(\xi_k)\Bigg(q^{-1/4}(\xi_k)\int_{x_0}^{\xi_k}d\xi_{k-1}\,q^{-1/4}(\xi_{k-1})\\ \times\Bigg(q^{-1/4}(\xi_{k-1})\int_{x_0}^{\xi_{k-2}}d\xi_{k-2}\cdots\Bigg(q^{-1/4}(\xi_2)\int_{x_0}^{\xi_2}d\xi_1\,q^{-1/4}(\xi_1)(q^{-1/4}(\xi_1))''\Bigg)''\cdots\Bigg)''\Bigg)'',\\ k=1,2,\ldots.\end{gathered} \tag{22}$$

Substituting (22) into (20) we get finally for the expansion:

$$\chi(x,\lambda)\sim\sum_{n\geqslant 0}\left(\frac{\sigma}{2\lambda}\right)^n C_n\sum_{k\geqslant 0}\left(\frac{\sigma}{2\lambda}\right)^k I_k(x,x_0). \tag{23}$$

In this way we have proven the following lemma.

Lemma 1: An arbitrary semiclassical expansion (20) which follows from (19) can be given the form (23) with an arbitrarily chosen regular point x_0 *and arbitrary constants* C_n, $n \geqslant 0$.

We shall call (23) the standard form of the expansion (20).

Of course, for a given χ the choice of x_0 determines the constants, i.e., the latter depend on it. However, if such a χ is given a choice of x_0 cannot be arbitrary. The reasons for that are that if χ considered can be semiclassically expanded then a domain of the x-plane for such an expansion is strictly determined. Good examples of the latter statement are provided just by the fundamental solutions. Each of the latter possesses as we have discussed it in Sec. II its allowed canonical domain of the semiclassical expansion (23). Therefore each χ possesses its own domain D_χ of the existence of the corresponding semiclassical expansion χ^{as}. Such a domain can however also be empty.

Suppose D_χ is not empty and let $x, x_0 \in D_\chi$. Then we can expand χ semiclassically and this expansion has the form (23). Let us assume a little bit more about χ, namely that there is a domain $B_\chi \subset D_\chi$ in which χ is Borel summable and let $x, x_0 \in B_\chi$. Then both $\chi(x,\lambda)$ and $\chi(x_0,\lambda)$ can be restored by the Borel transformation of the corresponding Borel functions and, respectively, along the negative real half-axis (by assumption) of the Borel plane. Their semiclassical expansions (23) can be obtained then by substituting simply into the Borel integral the Borel series (9) with the respective arguments x and x_0. But it means, of course, that we can obtain $\chi^{\mathrm{as}}(x_0,\lambda)$ simply from $\chi^{\mathrm{as}}(x,\lambda)$ by putting $x = x_0$ in the latter. Doing this in (23) we see that it takes in this case the following form:

$$\chi(x,\lambda) \sim \chi^{\mathrm{as}}(x,\lambda) = \chi^{\mathrm{as}}(x_0,\lambda) \sum_{k \geqslant 0} \left(\frac{\sigma}{2\lambda} \right)^k I_k(x,x_0). \tag{24}$$

Therefore the following lemma has been proven.

Lemma 2: If $\psi(x,\lambda)$ *is a solution to the Schrödinger equation (2) given in some domain B in the Dirac form (3) with the corresponding factor* $\chi(x,\lambda)$ *having in B the standard semiclassical expansion (23) which is Borel summable in B to the factor* $\chi(x,\lambda)$ *itself then this semiclassical expansions takes in B the form (24) where* $x_0 \in B$.

The above formula shows explicitly the way of determining the series of the constants C_n in the case just discussed. However, we shall show below that in general the form (24) can not be valid, i.e., the series of constants in (23) *is not* a semiclassical expansion of $\chi(x,\lambda)$ at $x = x_0$ even if the corresponding semiclassical expansions exist in both of the points.

Nevertheless, the formula (24) can be certainly applied to the fundamental solution χ-factors $\chi_k(x,\lambda)$ with $\chi_k^{\mathrm{as}}(x,\lambda)$ and $\chi_k^{\mathrm{as}}(x_0,\lambda)$ defined by (8) when $x, x_0 \in B_k \subset D_k$, with D_k being the canonical domain of $\chi_k(x,\lambda)$. In these latter cases the formula (24) can be derived directly from (8) by noticing that

$$\chi_{k,n}(x) = \sum_{p=0}^{n} \chi_{k,p}(x_0) I_{n-p}(x,x_0), \tag{25}$$

and by multiplying both sides of (25) by $(2\sigma\lambda)^{-n}$ and summing over n (from 0 to ∞).

V. OTHER SOLUTIONS WITH WELL DEFINED BOREL SUMMABLE SEMICLASSICAL ASYMPTOTICS

In this section we shall show that at each point of the x-plane not coinciding with the root of $q(x,E)$ there are two pairs of base solutions to (19) each of which can be expanded semiclassically in some well defined domain. These expansions are Borel summable in corresponding domains although not to the solutions themselves.

A. Fröman and Fröman construction of solutions to Schrödinger equation

A construction of the solutions just mentioned is the following.[27,25]

In the x-plane we choose any point x_0 [not being a root of $q(x)$ however]. The point distinguishes a line $\Re W_k(x,E)=\Re W_k(x_0,E)$ (it is independent of $k=1,2,\ldots,n$) on which it lies so that $\Re W_k(x,E)$ increases on one side of the line and decreases on the other. On each side of the line we can define two independent solutions each having the form (3) with the following formulas for the χ-factors:[27,25]

$$\chi_1^{\sigma}(x,x_0)=1+\sum_{n\geqslant 1}\left(\frac{\sigma}{2\lambda}\right)^n\int_{x_0}^{x}d\xi_1\int_{x_0}^{\xi_1}d\xi_2\ldots\int_{x_0}^{\xi_{n-1}}d\xi_n\,\omega(\xi_1)\omega(\xi_2)\ldots\omega(\xi_n)$$
$$\times(1-e^{-2\sigma\lambda(W_k(x)-W_k(\xi_1))})(1-e^{-2\sigma\lambda(W_k(\xi_1)-W_k(\xi_2))})\cdots(1-e^{-2\sigma\lambda(W_k(\xi_{n-1})-W_k(\xi_n))}) \tag{26}$$

and

$$\chi_2^{\sigma}(x,x_0)=\frac{\sigma}{2\lambda}\frac{1}{q^{1/2}(x_0)}\Bigg[1-e^{-2\sigma\lambda(W_k(x)-W_k(x_0))}+\sum_{n\geqslant 1}\left(\frac{\sigma}{2\lambda}\right)^n\int_{x_0}^{x}d\xi_1\int_{x_0}^{\xi_1}d\xi_2$$
$$\ldots\int_{x_0}^{\xi_{n-1}}d\xi_n\,\omega(\xi_1)\omega(\xi_2)\ldots\omega(\xi_n)(1-e^{-2\sigma\lambda(W_k(x)-W_k(\xi_1))})$$
$$\times(1-e^{-2\sigma\lambda(\mathbf{W}_k(\xi_1)-W_k(\xi_2))})\ldots(1-e^{-2\sigma\lambda(W_k(\xi_n)-W_k(x_0))})\Bigg], \tag{27}$$

where $\sigma=+1$ for x on the side of increasing $\Re W_k(x,E)$ and $\sigma=-1$ in the opposite case so that all integrations in (26) and (27) run from x_0 to x along the canonical paths, finite this time. Due to that both the solutions to the Schrödinger equation obtained by multiplying the χ-factors (26) and (27) by the corresponding WKB-factors increase exponentially in the semiclassical limit.

The χ-factors of (26) and (27) satisfy the following ''initial'' conditions:

$$\chi_1^{\sigma}(x_0,x_0)=\chi_2^{\sigma'}(x_0,x_0)=1 \quad \text{and} \quad \chi_1^{\sigma'}(x_0,x_0)=\chi_2^{\sigma}(x_0,x_0)=0. \tag{28}$$

B. Semiclassical expansions for $\chi_1(x,\lambda)$ and $\chi_2(x,\lambda)$

Consider now the solutions (26) and (27) defined at a vicinity of some point x_0. We shall show below that if x can be linked with x_0 by a canonical path the solutions can be expanded semiclassically having the corresponding forms (23) where x_0 means now the ''initial'' point for the solutions.

To formulate the corresponding lemma let us first invoke Theorem 4 of the previous section to note that when x_0 is chosen then there are always at least two fundamental solutions of opposite signatures belonging to $N(x_0)$ which are Borel summable at the point x_0 and communicate with themselves canonically. Let us choose these two fundamental solutions to be $\psi_a(x,\lambda)$ and $\psi_b(x,\lambda)$.

For the solution $\psi_1(x,\lambda)$ to the Schrödinger equation (2) defined by $\chi_1(x,\lambda)$ and the fundamental solutions $\psi_a(x,\lambda)$ and $\psi_b(x,\lambda)$ we have

$$\psi_1(x,\lambda)=\alpha(x_0,\lambda)\psi_a(x,\lambda)+\beta(x_0,\lambda)\psi_b(x,\lambda), \tag{29}$$

due to the linear independence of the latter. For definiteness we shall assume further that $\sigma_{1,2}=\sigma_a=-\sigma_b=-1$ in the corresponding formulas for the solutions so that $\Re\xi(x)<\Re\xi(x_0)$ if x can be linked with x_0 by a canonical path. The coefficients α and β in (29) can be easily calculated according to the general rules described in Refs. 1 and 5, for example. We have

$$\alpha(x_0,\lambda)=\frac{\chi_b(x_0,\lambda)}{\chi_{a\to b}(\lambda)}\exp\left(\lambda\int_{x_a}^{x_0}\sqrt{q(x,E)}dx\right),$$
$$\beta(x_0,\lambda)=\frac{1}{\chi_b(x_0,\lambda)}\left(1-\frac{\chi_a(x_0,\lambda)\chi_b(x_0,\lambda)}{\chi_{a\to b}(\lambda)}\right)\exp\left(-\lambda\int_{x_b}^{x_0}\sqrt{q(x,E)}dx\right), \tag{30}$$

where the condition (28) for $\chi_1(x,\lambda)$ has been used as well as the following relation:

$$\chi_1(\infty_b,\lambda)=\chi_b(x_0,\lambda). \tag{31}$$

The last relation generalizes a little bit a relation $\chi_{i\to j}=\chi_{j\to i}$ valid for any pair of fundamental solutions communicating canonically.[5]

We shall prove the following lemma.

Lemma 3: (a) The factors $\chi_{1,2}$ given by (26) and (27), respectively, can be expanded in corresponding domains $D_{1,2}=\{x:\Re\xi(x)<\Re\xi(x_0)\}$ into the semiclassical series determined by the following formulas:

$$\chi_1^{\mathrm{as}}(x,\lambda)=\frac{\chi_b^{\mathrm{as}}(x_0,\lambda)\chi_a^{\mathrm{as}}(x,\lambda)}{\chi_{a\to b}^{\mathrm{as}}(\lambda)}=\frac{\chi_a^{\mathrm{as}}(x_0,\lambda)\chi_b^{\mathrm{as}}(x_0,\lambda)}{\chi_{a\to b}^{\mathrm{as}}(\lambda)}\sum_{n\geqslant 0}\left(\frac{\sigma}{2\lambda}\right)^n I_n(x,x_0) \tag{32}$$

and

$$\chi_2^{\mathrm{as}}(x,\lambda)=\left(1-\frac{\chi_a^{\mathrm{as}}(x_0,\lambda)\chi_b^{\mathrm{as}}(x_0,\lambda)}{\chi_{a\to b}^{\mathrm{as}}(\lambda)}\right)\frac{\chi_a^{\mathrm{as}}(x_0,\lambda)}{\chi_a'^{\mathrm{as}}(x_0,\lambda)}\sum_{n\geqslant 0}\left(\frac{\sigma}{2\lambda}\right)^n I_n(x,x_0). \tag{33}$$

(b) The domains $D_{1,2}$ are maximal for the above expansions to be valid and are contained in the canonical domain D_a of the fundamental solution χ_a.

(c) The asymptotic series (32) and (33) can be Borel summed with the following results:

$$[\chi_1^{\mathrm{as}}(x,x_0,\lambda)]_a^{\mathrm{BS}}=C_a(x_0,\lambda)\frac{\chi_a(x,\lambda)}{\chi_a(x_0,\lambda)} \tag{34}$$

and

$$[\chi_2^{\mathrm{as}}(x,x_0,\lambda)]_a^{\mathrm{BS}}=(1-C_a(x_0,\lambda))\frac{\chi_a(x,\lambda)}{\chi_a'(x_0,\lambda)}, \tag{35}$$

where the Borel sum $C_a(x_0,\lambda)\equiv[\chi_a^{\mathrm{as}}(x_0,\lambda)\chi_b^{\mathrm{as}}(x_0,\lambda)/\chi_{a\to b}^{\mathrm{as}}(\lambda)]^{\mathrm{BS}}$ is defined below.

(d) The representations (34) and (35) are not unique.

Proof of the lemma: To prove the part (a) of the lemma let us first divide both the sides of (29) by $q^{-1/4}(x)\exp(-\lambda\int_{x_a}^{x}\sqrt{q(y)}dy)$ to get

$$\chi_1(x,\lambda)=\frac{\chi_b(x_0,\lambda)}{\chi_{a\to b}(\lambda)}\chi_a(x,\lambda)+\left(1-\frac{\chi_a(x_0,\lambda)\chi_b(x_0,\lambda)}{\chi_{a\to b}(\lambda)}\right)\exp\left(2\lambda\int_{x_0}^{x}\sqrt{q(y)}dy\right)\frac{\chi_b(x,\lambda)}{\chi_b(x_0,\lambda)}. \tag{36}$$

Next we note that the term in (36) proportional to $\chi_b(x,\lambda)$ is exponentially small in the semiclassical limit when compared with the first one. Therefore pushing λ to infinity in (36) we get (32).

It is now easy to find the semiclassical series (33) for $\chi_1(x,\lambda)$. To this end let us note that $\chi_{1,2}(x,x_0)$ are linear independent solutions of (19) satisfying the conditions (28) so that we can write for $\chi_a(x,\lambda)$:

$$\chi_a(x,\lambda)=\chi_a(x_0,\lambda)\chi_1(x,x_0,\lambda)+\chi_a'(x_0,\lambda)\chi_2(x,x_0,\lambda). \tag{37}$$

Getting asymptotics of both the sides of (37) and solving the obtained equation with respect to $\chi_2^{\mathrm{as}}(x,\lambda)$ we obtain (33).

The thesis (b) of the lemma follows from the fact that both the solutions $\chi_{1,2}(x,\lambda)$ diverge exponentially for $\Re x>\Re x_0$ when $\lambda\to\infty$ [the property which follows directly when the considered pair of solutions is expressed by the second pair of them defined by (26) and (27) with the opposite signature] and from the fact that the condition $\Re x<\Re x_0$ defines also a (proper) part of the canonical domain D_a of the fundamental solution χ_a.

To prove the part (c) of the lemma it is necessary to invoke the exponential representation of the fundamental solution χ-factors.[5] By this representation the following is meant:

$$\chi_{a,b}(x,\lambda)=\exp\left(\mp\int_{\infty_{a,b}}^{x}\rho^{-}(y,\lambda)dy+\int_{\infty}^{x}\rho^{+}(y,\lambda)dy\right),$$

$$\chi_{a,b}^{\mathrm{as}}(x,\lambda)=\exp\left(\mp\int_{\infty_{a,b}}^{x}\rho_{\mathrm{as}}^{-}(y,\lambda)dy+\int_{\infty}^{x}\rho_{\mathrm{as}}^{+}(y,\lambda)dy\right), \tag{38}$$

$$\rho_{\mathrm{as}}^{-}(y,\lambda)=\sum_{n\geqslant 0}\frac{\rho_{2n}^{-}(y)}{\lambda^{2n+1}},\quad \rho_{\mathrm{as}}^{+}(y,\lambda)=\sum_{n\geqslant 0}\frac{\rho_{2n+1}^{+}(y)}{\lambda^{2n+2}},$$

where the coefficients $\rho_n^{\pm}(y)$, $n\geqslant 0$, have been calculated explicitly in Ref. 5 [see Sec. 2.3 of this reference, where the roles of $\rho^{\pm}(x,\lambda)$ are played by the corresponding $\chi^{\pm}(x,E,\lambda)$-functions]. The important properties of the coefficients as well as of the asymptotic series in (38) they constitute are in Refs. 1, 5 (see Appendix 2 in Ref. 5).

(a) They are point (path-independent) functions of y, i.e., they are universal, sector independent functions.
(b) $\rho_n^{-}(y)$ have square root singularities at every turning point.
(c) $\rho_n^{+}(y)$ are meromorphic at each turning point with vanishing residues at the points [i.e., $\oint\rho_n^{+}(y)dy=0$ around any turning point].
(d) Both the series in (38) are Borel summable.

This is the property (c) which causes the ρ_{as}^{+}-integral in (38) to be again the point function of y, i.e., it is sector independent.

The property (d) which follows from the corresponding property of fundamental solutions[1] generates two Borel functions $\rho^{\pm}(x,s)$:

$$\tilde{\rho}^{-}(x,s)=\sum_{n\geqslant 0}\frac{\rho_n^{-}(x)}{(2n)!}s^{2n},\quad \tilde{\rho}^{+}(x,s)=-\sum_{n\geqslant 0}\frac{\rho_n^{+}(x)}{(2n+1)!}s^{2n+1}, \tag{39}$$

which can be Borel transformed along any standard path $\tilde{C}$ in the Borel plane providing us each time with the corresponding Borel sums $\rho_{\tilde{C}}^{\pm}(x,\lambda)$ of the series in (39). If we performed a Borel resummation of the first formula in (39) along such a path $\tilde{C}$ we get

$$\chi_C(x,\lambda)=e^{\int_{\infty_C}^{x}(-\rho_C^{-}(y,\lambda)+\rho_C^{+}(y,\lambda))dy}, \tag{40}$$

where $\chi_C(x,\lambda)$ is a χ-function of some fundamental solution, rotated possibly in the λ-plane. The minus sign in (40) has been chosen for definiteness.

Noticing further, that

$$\chi_b^{\mathrm{as}}(x_0,\lambda)\chi_a^{\mathrm{as}}(x_0,\lambda)=e^{2\int_{\infty}^{x_0}\rho_{\mathrm{as}}^{+}(x,\lambda)dx}\chi_{a\to b}^{\mathrm{as}}(\lambda), \tag{41}$$

we can sum à là Borel both the equations (32) and (33) along the path $\tilde{C}_a$ recovering the factor $\chi_a(x,\lambda)$ to obtain the formulas (34) and (35). In these formulas $C_a(x_0,\lambda)$ is therefore the following Borel sum:

$$C_a(x_0,\lambda)=\exp\left(2\int_{\infty_a}^{x_0}\rho_a^+(y,\lambda)dy\right). \tag{42}$$

The representations (34) and (35) are not unique since, in general, there can be other fundamental solutions in $N(x_0)$ with the same signature as the solutions $\chi_{1,2}$ have which can substitute the solution χ_a in our considerations. However, having the same signatures these other fundamental solutions can provide us with the representations (34) and (35) which, in this case, differ between themselves only by exponentially small contributions.

The last statements end our proof of Lemma 3. QED.

One can easily identify the coefficients in front of the sum on the rhs' of (32) and (33) as the corresponding series of constants in the standard expansions (23). It is important to note that *none* of them is equal to the asymptotic series corresponding to $\chi_1(x_0,\lambda)\equiv 1$ and $\chi_2(x_0,\lambda)\equiv 0$, respectively. This confirms of course our earlier statement that the semiclassical series (32) and (33) cannot be Borel summed to the respective factors $\chi_1(x,\lambda)$ and $\chi_2(x,\lambda)$. A reason for that is the presence of exponential terms $e^{-2\lambda\sigma(W_k(x)-W_k(x_0))}$ in the asymptotic formulas for (26) and (27) [when $\Re(W_k(x)-W_k(x_0))=0$] which breaks the necessary conditions for the Watson–Sokal theorem[28] to be applied. Note that these exponential terms are absent in the case of fundamental solutions which are obtained in the limit $x_0\to\infty_k$ taken along a canonical path, for any $k=1,2,\ldots,2n+2$.

VI. UNIQUENESS OF FUNDAMENTAL SOLUTIONS AS BOREL SUMMABLE SOLUTIONS

Let $\psi(x,\lambda)$ be any solution to the Schrödinger equation (2) given at some domain D of the x-plane. Let us choose in D a point x_0 which is not a root of $q(x,E)$ [i.e., which is regular for $\omega(x)$ as given by (6)]. The solution $\psi(x,\lambda)$ can always be given each of the two Dirac forms (3) with the corresponding χ-factors satisfying the equation (19). Let us write these forms in the following way:

$$\psi(x,\lambda)=C_\pm(\lambda)q^{-1/4}(x)e^{\pm\lambda\int_{x_0}^{x}\sqrt{q(y)}dy}\chi_\pm(x,\lambda). \tag{43}$$

We shall say that $\psi(x,\lambda)$ has *well defined* semiclassical expansion in D if there is a choice of a sign in (43) and an accompanied constant $C_\pm(\lambda)$ such that the χ-factor $\chi_\pm(x,\lambda)$ corresponding to this choice can be expanded semiclassically in the standard way given by (23).

It follows directly from the above definition that only one of the two possible choices can satisfy it.

We shall also say that $\psi(x,\lambda)$ is Borel summable in D if it has well defined semiclassical expansion there and the corresponding series (23) is Borel summable to the uniquely chosen χ-factor $\chi(x,\lambda)$ of $\psi(x,\lambda)$.

We shall prove below the following main theorem of this paper.

Theorem 5: *Let a solution $\psi(x,\lambda)$ given at some vicinity D of x_0 (x_0 does not coincide with any turning point) be Borel summable in D. Then this solution must coincide with one of the fundamental solutions up to some λ-dependent constant.*

Proof: To prove the theorem we could utilize the solutions (26) and (27) and all their properties which we have established in Lemma 3 of the previous section. It can however be quite instructive to prove the theorem not invoking for the latter solutions since it makes the main arguments supporting the theorem (which have worked implicitly also in proving Lemma 3 of the previous section) to be more transparent.

According to Theorem 4 of Sec. III, for x_0 chosen we can always find in the set $N(x_0)$ a number of fundamental solutions of the same signatures as the respective $\chi(x,\lambda)$ corresponding to $\psi(x,\lambda)$ has. Let $\chi_a(x,\lambda)$ be one of them. It is Borel summable at x_0 and in some of its vicinity. Then using (24) both for $\chi(x,\lambda)$ and $\chi_a(x,\lambda)$ we have

$$\frac{\chi^{\mathrm{as}}(x,\lambda)}{\chi^{\mathrm{as}}(x_0,\lambda)}=\sum_{n\geqslant 0}\left(\frac{\sigma}{2\lambda}\right)^n I_n(x,x_0)=\frac{\chi_a^{\mathrm{as}}(x,\lambda)}{\chi_a^{\mathrm{as}}(x_0,\lambda)}. \tag{44}$$

It follows from (44) that the outer parts of this equality having the same semiclassical expansions have to have also the same Borel function. Since $\chi^{\mathrm{as}}(x,\lambda)$ and $\chi^{\mathrm{as}}(x_0,\lambda)$ are both Borel summable in D they can be summed along the same standard path $\tilde{C}$ on their corresponding Borel planes if x is chosen to be sufficiently close to x_0. It is, however, easy to check (see Appendix C) that under the latter condition the same standard path $\tilde{C}$ can be chosen to sum the quotient on the lhs of (44) since its corresponding Borel function is holomorphic around this path. However, the same must be true for the rhs quotient, i.e., the corresponding Borel functions of its two factors can be integrated also along $\tilde{C}$ lying in their Borel planes. Let us sum therefore à là Borel both the outer sides of (44) along this path. We get

$$\chi(x,\lambda)=\chi(x_0,\lambda)\frac{2\lambda\int_{\tilde{C}}e^{2\lambda s}\tilde{\chi}_a(x,s)ds}{2\lambda\int_{\tilde{C}}e^{2\lambda s}\tilde{\chi}_a(x_0,s)ds}. \tag{45}$$

The last equation, however, ends the proof of the theorem. QED.

As a comment to the last theorem we would like to stress that it summarizes a particular property of the semiclassical theory of the 1D Schrödinger equation with the polynomial potentials. Namely, this is that the standard semiclassical expansion (23) is constructed basically by the series $\Sigma_{n\geqslant 0}(\sigma/2\lambda)^n I_n(x,x_0)$ which can be Borel summable and the Borel function of which, by (44), coincides up to a λ-dependent multiplicative constant with the one of the fundamental solutions and, also by (44), with the Borel function of any Borel summable solution. This means that we can consider the Borel function of the fundamental solutions as the canonical one. The latter can be uniquely defined by the condition of being equal to unity at $s=0$ on the ''first sheet'' of the corresponding Riemann surface which the condition actually satisfies.

VII. CONCLUSIONS AND DISCUSSION

Theorem 5 of the previous section shows that in the case of the Schrödinger equation with the polynomial potentials its Borel summable solutions are the fundamental ones. The Borel function generated by these solutions is, up to analytical continuation, the unique one. This property justifies our earlier use of the fundamental solutions to investigate the problem of the Borel summability of energy levels and matrix elements in 1D quantum mechanics.[1] It also shows that only the fundamental solutions can be invoked when *any* problem connected with the Borel resummation is considered and conditions for such resummations are satisfied.[28]

The latter objection is important since not all the results we obtain for the case of polynomial potentials can be immediately extended to other cases of potentials. These are, for example, the rational potentials being the next class of potentials of modeling importance. In particular, the universality of the Borel function in the later case of potentials seems not to be satisfied.[33]

Nevertheless, the role of the corresponding fundamental solutions as the unique Borel summable ones seems to be maintained not only in the case of rational potentials but also in the case of other meromorphic potentials such as the Pöschl–Teller one, for example.

The fundamental solutions we have discussed in Sec. II can be given another form when each of the factors in (3) becomes a complicated function of λ.[34] These generalized representations however preserve all the Borel summing features of the original fundamental solutions being only a partial Borel resummation of the latter.[25]

Finally, we would like to note that the result obtained in the present paper completes the ones obtained in our other papers.[1,12,25] Namely, all these results show that the semiclassical theory in 1D quantum mechanics can be completely formulated on the basis of the Borel method of resummation. This is certainly true in the case of the polynomial potentials and it seems to be true with some modifications for meromorphic potentials as well.[33] In the formulation of such a theory the essential role as we have shown in the present paper is played by the fundamental solutions (see also Refs. 1, 12, 25). The theory allows us to construct the simplest semiclassical approximations as well as to complete the latter by the exponentially small contributions up to a desired level of accuracy.[12] In such a theory even a change of variable in the Schrödinger equation the procedure which is used very frequently as a way of improving the semiclassical approximations is also a result of the proper Borel resummation operation.[25,34]

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APPENDIX A

Here we would like to draw some basic conclusions which follow for the Borel function $\tilde{\chi}(x,s)$ from its representation given by the topological expansion developed in our recent paper (see Ref. 12) and not dicussed there.

First of all let us recapitulate shortly basic elements of this representation. Namely, we have shown in Ref. 12 that the Borel function defined originally in some sector, say can be represented in this sector as the following series $[\xi=\xi(x)=\int_{x_1}^{x}\sqrt{q(y,E)}dy]$:

$$\tilde{\Phi}_1(\xi,s)=\sum_{q\geqslant 0}\tilde{\Phi}_1^{(q)}(\xi,s), \tag{A1}$$

where $\tilde{\Phi}_1(\xi(x),s)\equiv\tilde{\chi}(x,s)$ and the terms $\tilde{\Phi}^{(q)}(\xi,s),q\geqslant 0$ of the series are given by the formulas

$$\tilde{\Phi}_1^{(0)}(\xi,s)=I_0(\sqrt{4s\Omega(\xi)}),$$

$$\tilde{\Phi}_1^{(2q)}(\xi,s)=\int_{\tilde{C}(s)}d\eta_1\int_{\tilde{C}(\eta_1)}d\eta_2\ldots\int_{\tilde{C}(\eta_{q-1})}d\eta_q\int_{\infty_1}^{\xi-\eta_1}d\xi_1\int_{\infty_1}^{\xi_1}d\xi_2\ldots\int_{\infty_1}^{\xi_{q-1}}d\xi_q,$$

$$\tilde{\omega}(\xi_1+\eta_1)\tilde{\omega}(\xi_1+\eta_2)\cdot\ldots\cdot\tilde{\omega}(\xi_q+\eta_q)\tilde{\omega}(\xi_q)(2s-2\eta_1)^{2q}\frac{I_{2q}(z_{2q}^{1/2})}{z_{2q}^{q}},$$

$$z_{2q}=4(s-\eta_1)\Omega(\xi)+8(s-\eta_1)\sum_{p=1}^{q}(\Omega(\xi_p+\eta_{p+1})-\Omega(\xi_q+\eta_p)),$$

$$\eta_{q+1}\equiv 0,\quad q=1,2,\ldots, \tag{A2}$$

$$\tilde{\Phi}_1^{(2q+1)}(\xi,s)=\int_{\tilde{C}(s)}d\eta_1\ldots\int_{\tilde{C}(\eta_q)}d\eta_{q+1}\,\tilde{\omega}(\xi-\eta_1+\eta_2)\int_{\infty_1}^{\xi-\eta_1}d\xi_1\ldots\int_{\infty_1}^{\xi_{q-1}}d\xi_q\tilde{\omega}(\xi_1+\eta_2)$$

$$\times\tilde{\omega}(\xi_1+\eta_3)\cdot\cdots\cdot\tilde{\omega}(\xi_q+\eta_{q+1})\tilde{\omega}(\xi_q)(2s-2\eta_1)^{2q+1}\frac{I_{2q+1}(z_{2q+1}^{1/2})}{z_{2q+1}^{(2q+1/2)}},$$

$$z_{2q+1}=4(s-\eta_1)\Omega(\xi)+8(s-\eta_1)\sum_{p=0}^{q}(\Omega(\xi_p+\eta_{p+2})-\Omega(\xi_p+\eta_{p+1})),$$

$$\xi_0\equiv\xi,\quad \eta_{q+2}\equiv 0,\quad q=0,1,2,\ldots,$$

where $\tilde{\omega}(\xi(x))\equiv\omega(x)q^{-1/2}(x),\Omega=\int_{\infty_1}^{\xi}\tilde{\omega}(\eta)d\eta$ and the functions $I_q(x),q\geqslant 0$, in (A2) are the modified Bessel functions [of the first kind, Ref. 35, p. 5, formula (12)].

The formulas (A2) can be obtained from the following recurrences:

$$\tilde{\Phi}_1^{(2q+2)}(\xi,s)=-\int_{\tilde{C}(s)}d\eta\int_{\tilde{C}(\eta)}d\eta'\int_{\infty_1}^{\xi}d\xi_1\,\tilde{\omega}(\xi_1)\tilde{\omega}(\xi_1-\eta')(2s-2\eta)$$
$$\times\tilde{\Phi}_1^{(2q)}(\xi_1-\eta',\eta-\eta')\frac{I_1(\sqrt{4(s-\eta)(\Omega(\xi)-2\Omega(\xi_1)+\Omega(\xi_1-\eta'))})}{\sqrt{4(s-\eta)(\Omega(\xi)-2\Omega(\xi_1)+\Omega(\xi_1-\eta'))}},\tag{A3}$$

$$\tilde{\Phi}_1^{(2q+1)}(\xi,s)=-\int_{\tilde{C}(s)}d\eta\int_{\tilde{C}(\eta)}d\eta'\,\tilde{\omega}(\xi-\eta')$$
$$\times\tilde{\Phi}_1^{(2q)}(\xi-\eta',\eta-\eta')I_0(\sqrt{-4(s-\eta)(\Omega(\xi)-\Omega(\xi-\eta'))}),$$
$$q=0,1,2,\ldots,$$

where $\tilde{\Phi}_1^{(0)}(\xi,s)$ is given by (A2).

Note that (A3) can be obtained from (A2) and vice versa by applying the following relations:

$$\int_0^1 dx\,I_m(\sqrt{\alpha x})I_m(\sqrt{\beta(1-x)})(\alpha x)^{1/2\,m}(\beta(1-x))^{(1/2)\,n}$$
$$=2\alpha^m\beta^n\frac{I_{m+n+1}(\sqrt{\alpha+\beta})}{(\sqrt{\alpha+\beta})^{m+n+1}}\frac{1}{(k-1)!(n-k)!}\int_\eta^s d\eta'(s-\eta')^{k-1}(\eta'-\eta)^{n-k}=\frac{(s-\eta)^n}{n!}.\tag{A4}$$

The ξ-integrations in (A2) and (A3) run over some ξ-Riemann surfaces of the subintegral functions starting from the infinite points of these surfaces which are the corresponding images of the infinite point of the sector S_1. The η-integrations, contrary to the ξ-ones, are finite and run over the s-Riemann surfaces. All the latter integrations end at $s=0$.

For these integrations the most important are the branch point structures of the Riemann surfaces corresponding to the functions $\tilde{\omega}(\xi)$ and $\Omega(\xi)$ and the shifts of these surfaces by some complex number η. The two latter surfaces corresponds to the functions $\tilde{\omega}(\xi-\eta)$ and $\Omega(\xi-\eta)$.

Since every of these four surfaces has complicated topology (defined by its branch points) we decided not trying to sew them suitably together when these functions are integrated simultaneously but rather to consider them, for safeness, separately. These topologies are determined, of course, by the singularities of the respective functions $\tilde{\omega}(\xi)$ and $\Omega(\xi)$. Besides, since the latter of these two functions is defined as the integral over the former then the corresponding Riemann surface on which $\Omega(\xi)$ is defined is a map of the surface corresponding to $\tilde{\omega}(\xi)$, i.e., there is a well defined relation between these two surfaces.

For the polynomial potentials with simple roots all singularities of $\tilde{\omega}(\xi)$ and $\Omega(\xi)$ are cubic root branch points corresponding to turning points. Therefore, the four surfaces discussed above acquires a suitable cut pattern each. The corresponding ξ-integration runs over the sheets of these

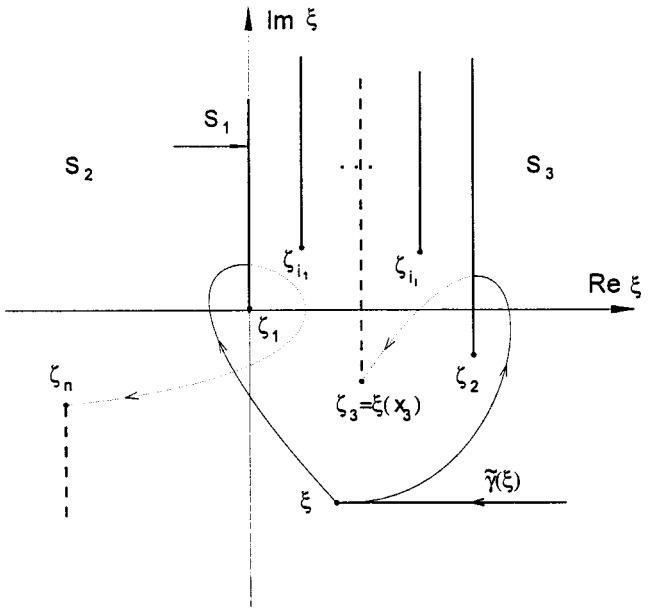

FIG. 6. The branch point structure of the ξ-Riemann surface sheet for $\tilde{\Phi}(\xi,s)$ containing the sectors S_2 and S_3 when $x \in K' \cap S_3$.

surfaces which are unambiguously related to each others (by the above shift or by a map) so that the integration paths on this sheets look the *same* running from ∞_1 to some finite point, the *same* on each sheet.

It is necessary to stress that every subsequent integration in (A2) or every subsequent step in the recurrent formulas (A3) changes the structure of the Riemann surfaces corresponding to functions resulting from these integrations. Namely, these surfaces become still more complicated preserving all the branch points of the previous stage and acquiring new ones as a result of the last integration(s).

Nevertheless, these structures look relatively simple if we consider them on definite sheets of the Riemann surfaces we want to stay considering the properties of the Borel functions $\tilde{\Phi}(\xi,s)$. Namely, starting from the sheets corresponding to the sector S_1 we shall keep the variable x [or $\xi(x)$] changing along the contour K' of Fig. 1(a). This corresponds to a path $\gamma_1(x)$ on the x-plane which begins in the sector S_1 and crosses on its way all the Stokes lines running to the infinity of the plane (but each line only once) penetrating subsequent sectors in their cyclic (clockwise or anticlockwise) ordering introduced in Sec. II. We shall call such a path the outer path.

Under the above condition the final pattern of the branch points of $\tilde{\Phi}(\xi,s)$ viewed from the relevant sheets is quite simple. First let us note that, as it follows from (A2) and (A3), under the above circumstances we can deform homotopically the infinite end of the outer path γ from the sector S_1 to any of the subsequent sectors $S_2,\ldots,S_{n+1}$ (in this or in the reversed orders). This is the consequence of the fact that the initial condition (7) put on the path γ to make it canonical is no longer valid since all the dangerous exponentials in the formula (5) enforcing this condition disappeared on the way of passing to the formulas (A2) and (A3). Figure 6 shows the corresponding result of such an operation for $x \in K' \cap S_3$. This proves that under the above condition (A2) and (A3) define the *same* unique Borel function $\tilde{\Phi}(\xi,s)$ for all the $n+1$ fundamental solutions (3). This deformation can be done keeping the end point x $(\xi(x))$ of the outer path γ in *any* of the sectors $S_1,\ldots,S_{n+1}$. The latter property means, of course, that if ξ is in S_k and the infinite end of γ is in S_l then $\tilde{\Phi}(\xi,s)$ represents the Borel function of the fundamental solution ψ_k (defined in S_k) analytically continued to the sector S_l and the formulas (A2) and (A3) define then this continuation explicitly.

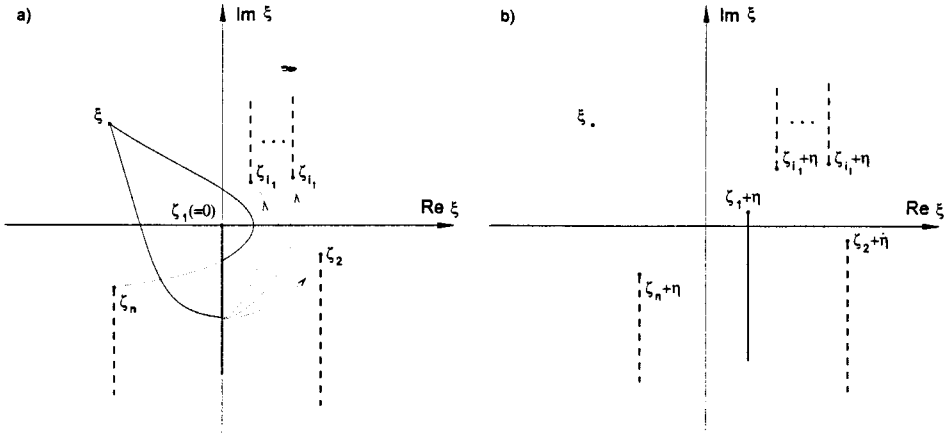

FIG. 7. (a) The 'first' sheet of the ξ-Riemann surface corresponding to $\tilde{\Phi}^{(0)}(\xi,s)$ when $x\in K'\cap S_3$. (b) The 'first' sheet of the ξ-Riemann surface corresponding to $\tilde{\Phi}^{(0)}(\xi-\eta,s)$ when $x\in K'\cap S_3$.

Theorem 6: *Let the end point x go around the contour K' of Fig. 1(a) starting from the sector S_1 and passing consecutively by the sectors $S_2,\ldots,S_{n+1}$. Then the sheets from which the χ-factors corresponding to the subsequent sectors are recovered by the Borel transformations over the Borel function $\tilde{\chi}(x,s)$ along the suitable real half-axes have the branch point structures shown in Fig. 11.*

Proof: Let us consider first a sheet of the s-Riemann surface corresponding to the sector S_1 and let the point x be then on K' in the sector S_1 so that $\Re\xi(x)>0$.

Consider $\tilde{\Phi}^{(0)}(\xi,s)$. Since $I_0(\sqrt{4s\Omega(\xi)})$ is the holomorphic function of its argument then $\tilde{\Phi}^{(0)}(\xi,s)$ is an entire function of s (i.e., holomorphic in the whole s-plane) so that its corresponding s-Riemann surface coincides with the s-plane. What concerns its ξ-Riemann surface structure it coincides with the one of $\Omega(\xi)$ since for each natural power of the latter its ξ-Riemann structure is the same and $I_0(\sqrt{4s\Omega(\xi)})$ determines $\tilde{\Phi}^{(0)}(\xi,s)$ as the holomorphic function of ξ in each nonsingular point of $\Omega(\xi)$. Therefore $\tilde{\Phi}^{(0)}(\xi,s)$ has on the corresponding first sheet in the ξ-plane a unique branch point at ζ_1, as it is shown in Fig. 7(a), if the corresponding cut emerges from this branch point vertically down. There are no other branch points visible then on the sheet. These other branch points, however, are on the sheets lying *below* the first sheet and the closest ones at $\zeta_2,\zeta_{i_1},\ldots,\zeta_{i_l}$ and ζ_n are shown in Fig. 7(a) with the dashed lines of cuts emerging from them. The full thin paths on the figure emerging from the point ξ show us how to approach these last branch points starting from ξ. We shall adopt this convention for the remaining figures too.

Figure 7(b) shows the ξ-Riemann surface for the shifted function $\tilde{\Phi}^{(0)}(\xi-\eta,s)$.

Next consider $\tilde{\Phi}^{(1)}(\xi,s)$. It is given by the second of the formulas (A3) for $q=0$. In this formula we have to integrate first over the variable η'. As it follows from the formula the branch point structure of the η'-Riemann surface is determined by the functions $\tilde{\omega}(\xi-\eta')$, $\Omega(\xi-\eta')$ and $\tilde{\Phi}^{(0)}(\xi-\eta',\eta'-\eta)$ and its first and second sheets are shown in Fig. 8(a).

The integration over η' leads us to a function defined on the ξ-Riemann surface shown in Fig. 7(b). The cuts shown there are a result of the end point (EP) mechanism of the singularity produced (Ref. 12, see also Ref. 36). Namely, the η'-integration is perturbed if the moving branch points of Fig. 8(a) can approach the fixed end points $\eta'=0$ and $\eta'=\eta$ of the integration path $C(\eta)$. For example, to generate the branch point at $\zeta_1(=0)$ we simply move the branch point $\xi-\zeta_1$ against the end point $\eta'=0$ of $C(\eta)$ to touch it finally. To produce the branch point at ζ_2 in Fig. 8(b) we have to move $\xi-\zeta_1$ down avoiding the end point η' from the left and below and next moving it to the right in such a way as to make the screened branch point at $\xi-\zeta_2$ coinciding with the end point η'.

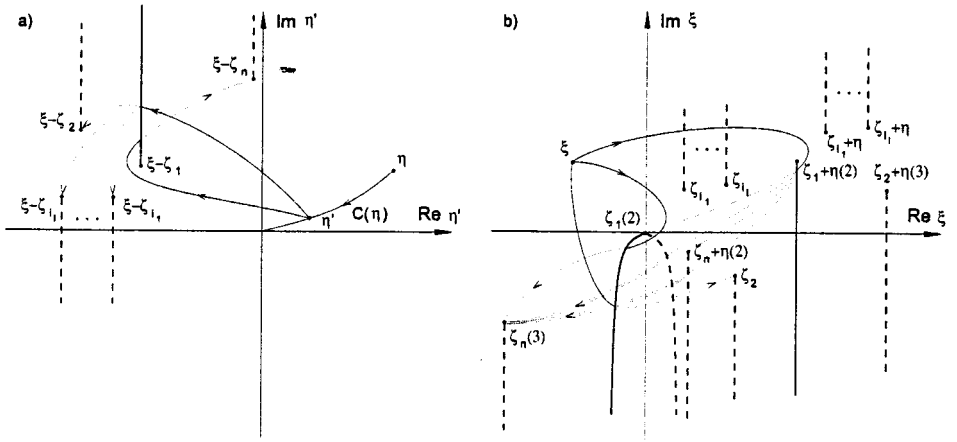

FIG. 8. (a) The singularity structure of the integrand in the second formula (48) for $q=0$ and the integration path $C(\eta)$. (b) The resulting ξ-singularity structure of $\tilde{\Phi}^{(1)}(\xi,s)$.

In the way described above we can generate the branch points at the position shown in Fig. 8(b). A convention adopted in this figure for the cut designing is to draw a full thin path emerging from the point ξ and if the path crosses a cut it becomes dotted. If it crosses the next appropriate cut it is doubly dotted and so on. This way of designing cuts allows us to establish the sheets on which they are distributed. The figure in parentheses at the different branch points indicates the multiplicity of the latter, i.e., their appearing on *different* sheets at the *same* positions. However, for the sake of transparency of the figures not all paths showing the distributions of the branch points on the sheets have been shown.

It is worth noting that this multiplication of branch points with the same coordinates but lying on different sheets in this figure is necessary to keep fixed the relative distribution of the branch points Fig. 8(a) when the moving ones in Fig. 8(b) change their positions. In fact the branch points in this figure with the same coordinate substitute each other during such a motion. This is because the branch point $\xi-\zeta_1$ in Fig. 8(a) has to be always accompanied by the branch points at $\xi-\zeta_2$ and $\xi-\zeta_n$ lying on the next two lower sheets. For example, if the branch points $\zeta_1+\eta$ and $\zeta_2+\eta$ move to the left so that they pass the branch point at $\zeta_1(=0)$ having it between themselves then the point $\zeta_2+\eta$ on the sheet opened by the first of these moving points is screened in some moment by the cut emerging from $\zeta_1=0$ lying on the first sheet in Fig. 8(b). But then the branch point at $\zeta_2+\eta$ on the sheet opened just by this latter cut becomes unscreened substituting its copy on the sheet we started with. Of course, all three copies of the branch points at $\zeta_2+\eta$ are mapped by the relation $\xi-\eta=\zeta_k$, $k=1,2,3$, into the one copy of them at $\xi-\zeta_2$ on the η'-plane of Fig. 8(a).

The final integration over η repeats only the steps done earlier introducing nothing new to the distribution of the branch ponts on the first sheet not modifying the lower sheets as well so that the final branch point structures of the first sheets look again as in Figs. 8(a) and 8(b) where we have to substitute η' and η by s on both the figures.

Consider next $\tilde{\Phi}^{(2)}(\xi,s)$. It is given by the first of the formulas (A3) for $q=0$. The initial ξ-Riemann surface structure is similar to that shown in Fig. 7 and look as in Figs. 9(a) and 9(b). The first ξ_1-integration in the corresponding formula (A3) provides us this time with both the types of singularities on the η'-Riemann surface, i.e., generated by the E-mechanism, which makes a replica of the branch point structures of Fig. 8(a), and by the pinch (P) mechanisms (discussed in Ref. 12; see also Ref. 36). A singularity generated by the second mechanism arises when, for example, the branch point at $\zeta_1+\eta'$ in Fig. 9(b) moves against the one at $\zeta_1=0$ of Fig. 9(a) pinching the integration path $\tilde{\gamma}(\xi)$. It can be done by making a tour around the end ξ of the path $\tilde{\gamma}(\xi)$ in both the directions, i.e., clockwise or anticlockwise. In this example we will produce branch point singularities on both the lower sheets of the η'-Riemann surface shown if Fig. 9(c)

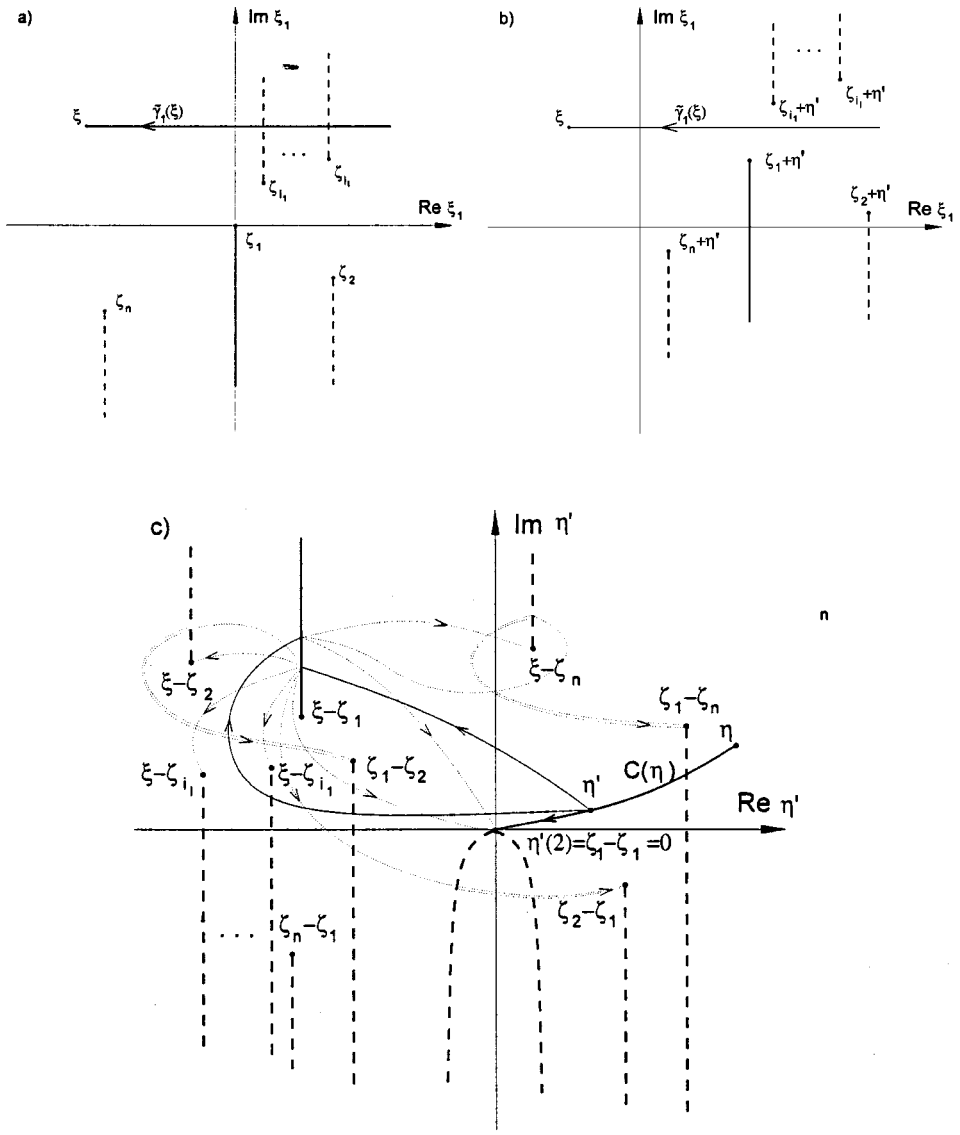

FIG. 9. (a) The ξ_1-singularity structure of the only ξ_1-dependent factors of the integrand in the first formula (48) for $q=0$. (b) The ξ_1-singularity structure of the η'-dependent factors of the integrand in the first formula (48) for $q=0$. (c) The η'-singularity structure of the first formula (48) for $q=0$ after the ξ_1-integration.

at $\eta'=0$. We can pinch the path $\tilde{\gamma}(\xi)$ by $\xi_1+\eta'$ also in this way but against the branch points at ζ_2 and ζ_n. This needs only to cross the cut emerging from $\zeta_1(=0)$ to reach the points mentioned, i.e., the first one by crossing this cut from the left while the second—from the right. It means that η' itself has to do the same in Fig. 9(c) crossing the cuts emerging from $\eta'=0$ on the corresponding sheets. The positions of the branch points generated in this way are shown in Fig. 9(c) where only a closest part of them is shown. It follows from the figure that some of the closest fixed branch points are at η' on the two sheets opened by the branch point at $\xi-\zeta_1$. The other ones lie on the sheets opened by the the branch points at $\xi-\zeta_2,\xi-\zeta_{i_1},\ldots,\xi-\zeta_{i_l}$ and $\xi-\zeta_n$ and by the fixed branch points generated in this way, i.e., still on the lower sheets.

A discussion of the remaining two η'- and η-inegrations goes along the same lines as in the previous discussion on calculating $\tilde{\Phi}^{(1)}(\xi,s)$ with the similar results obtained accordingly to Fig. 9(c). The only appearing difference is that in both these integrations the P-mechanism of the

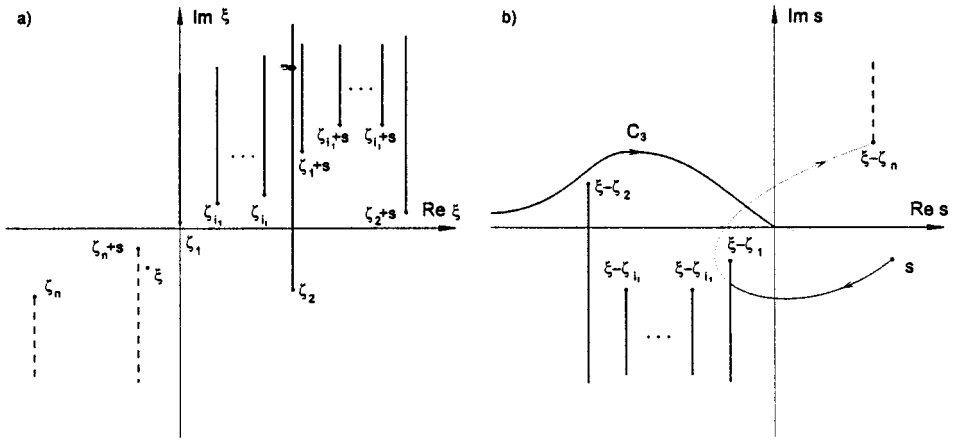

FIG. 10. (a) The ξ-singulalrity structure of $\tilde{\Phi}(\xi,s)$ for $x\in K'\cap S_3$. (b) The s-singularity structure of $\tilde{\Phi}(\xi,s)$ for $x\in K'\cap S_3$.

moving branch point singularity generation on the ξ-Riemann surface becomes active since, except for the moving singularities, there are also the fixed ones on the corresponding sheets of the η'- and η-Riemann surfaces [see Fig. 9(c)]. Therefore, the final first sheet structures are again a replica of those shown in Fig. 8(b) for the ξ-Riemann surface and in Fig. 9(c) for the s-Riemann one (with the η-, η'-variables substituted suitably by the s-one). Of course, because of the reason of transparency only the branch points on the first three sheets are shown in the figures. A comment made previously on the proliferation of the moving branch points with the same coordinates but lying on different sheets is also still valid and Fig. 8(b) reproduces this fact correctly.

Now consider the cases $\tilde{\Phi}^{(2q+1)}(\xi,s)$ and $\tilde{\Phi}^{(2q+2)}(\xi,s)$ assuming that the first sheets of the ξ-, s-Riemann surface structure of $\tilde{\Phi}^{(2q)}(\xi,s)$ is given by Fig. 8(b) and Fig. 9(c) (with the suitable $\eta,\ \eta'\to s$ substitutions on the figures). It is clear that we can repeat all the previous analyses and conclusions without any changes if the considered structure is limited only to the sheets defined by the formulas (A3) and the branch points shown in Figs. 8(a) and 9(c), i.e., the structure in these figures is reproduced also for the functions $\tilde{\Phi}^{(2q+1)}(\xi,s)$ and $\tilde{\Phi}^{(2q+2)}(\xi,s)$. Since the series (A2) is convergent this structure is the same also for $\tilde{\Phi}(\xi,s)$ itself.

It is important to note that the *fixed* branch points on the s-Riemann surface are generated in the scheme of the topological expansion (A2) on *lower* sheets.

Having $\tilde{\Phi}(\xi,s)$ defined in the above way we can restore the χ-factors defined in the sectors S_1 or S_2 by the Borel transformations of $\tilde{\Phi}(\xi,s)$ along the left half-axis to get $\chi_1(x,\lambda)$ or along the right one to get $\chi_2(x,\lambda)$. Clearly, the signs of λ in both these integrations are different.

To prove the assertion of the theorem about the structure of the ξ-, s-Riemann surface for $\tilde{\Phi}(\xi,s)$ continued to the sector S_k along the contour K' in Fig. 1(a) we should perform this continuation on the ξ-, s-Riemann surface corresponding to $\tilde{\Phi}(\xi,s)$ changing ξ, respectively, and drawing cuts properly. Such an operation, however, needs the detailed knowledge of the structure of many lower sheets of the ξ-, s-Riemann surface, a task which seems to be in general hopeless. However, we have already noticed that such a continuation can be easily performed with the help of the formulas (A2)–(A3) by changing the infinite ends of the ξ-integrations in these formulas, i.e., moving them to the appropriate sectors when the variable $\xi(=\xi(x))$ itself is continued to these sectors when x changes along the contour K'. For definitness let ξ be continued to the sector S_3. Then we can continue the mentioned infinite ends to the same sector. According to the Stokes graph in Fig. 1(a) the corresponding pattern of the sheets on which $\tilde{\omega}(\xi)$ and $\Omega(\xi)$ are defined are shown in Fig. 6. Therefore, taking this figure as the original one and using again the formulas (A3) we can repeat once again the analyses done above. The only difference are introduced by addi-

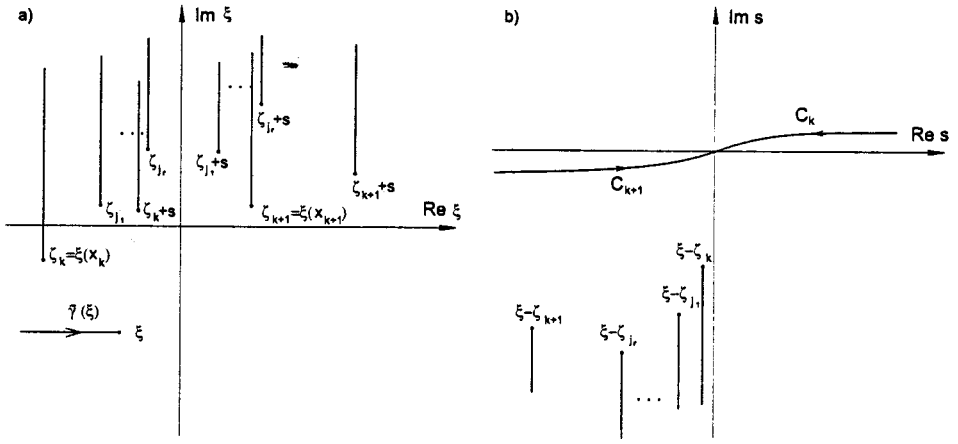

FIG. 11. (a) The ξ-singularity structure of $\tilde{\Phi}(\xi,s)$ for $x\in K'\cap S_k$. (b) The s-singularity structure of $\tilde{\Phi}(\xi,s)$ for $x\in K'\cap S_k$.

tional branch points which can appear according to the Stokes graph in Fig. 1(a). Then forgetting about the branch points which lie on the lower sheets in Fig. 6 (such as ζ_3) we get as the final structure of the first sheets for $\tilde{\Phi}(\xi,s)$ the one shown in Fig. 10.

The pattern in Fig. 10 is the one which has also to follow if we would continue the pattern of Fig. 8(b) (with the $\eta\to s$ substitution) by moving anticlockwise the variable ξ around the branch point ζ_1 and uprighting the cut emerging from this point by rotating it in the same anticlockwise direction. Then the cut emerging from ζ_2 on the figure is unscreened and uprighting it again anticlockwise as well as all the other consecutive cuts met by ξ on its way to the sector S_3 we have to reveal by these *uprighting operations* of the cuts the pattern of Fig. 10(a). Compairing the latter with Fig. 8(b) we see that these operations do their job properly. The proliferation of the branch points with the same coordinates on different sheets plays an essential role in this operation allowing us to recover the cuts which are screened by the uprighting operations made over the cuts emerging from $\xi=\zeta_1$ and $\xi=\zeta_2$.

On the s-Riemann surface of $\tilde{\Phi}(\xi,s)$ shown in Fig. 9(c) (with $\eta'\to s$ on the axes) the corresponding operation with cuts are of course reversed, i.e., each consecutive cut which is unscreened by the anticlockwise upside-down rotation of its predecessor originating by the cut emerging from the branch point $\xi-\zeta_1$ in Fig. 9(c) has also to be rotated in the same way. This process stops on the cut emerging from the last branch point at $\xi-\zeta_2$ being unscreened. We can then move this new pattern first down leaving the origin of the first sheet to the right and next move to the right leaving the origin of the sheet above all the moved branch points. The final position has to coincide then with that shown in Fig. 10(b).

We shall call the above operations with cuts leadind us to uncovering the desired sheets of the ξ-, s-Riemann surface the *unscreening operations*.

It is now clear that we can follow the above way considering the ξ-, s-Riemann surface structure corresponding to $\tilde{\Phi}(\xi,s)$ when ξ is in S_k being continued along the contour K' in Fig. 1(a). The tour along the contour K' is mapped properly on the ξ-Riemann surface of $\tilde{\Phi}(\xi,s)$ where ξ moves anticlockwise avoiding all met branch points from the left and putting upside-down the crossed cuts emerging from them realizing in this way the unscreening operation. The same unscreening operations of putting the properly chosen cuts upside-down are applied on the s-Riemann surface. We start from the pattern of Fig. 9(b) and repeat the procedure described above k times. The final pattern has to have the form shown in Figs. 11(a) and 11(b). Its detailed structure shown in the figure can be obtained from the formulas (A3) by the analyses described above.

Borel transforming along the left half-axis of Fig. 11(b) we recover the χ-factor corresponding to the sector S_k (if k is odd) or the one corresponding to the sector S_{k+1} when the Borel transformation is performed along the right half-axis. QED.

To finish the above discussion let us note yet that as it follows from our estimation of the convergence of the series (A2) made in Ref. 12 (see Appendix A.3 there) its *divergence* on each sheet of its s-Riemann surface (when ξ is fixed) is no faster than the exponential one.

APPENDIX B

We shall show here that the Borel transformation (10) of $\tilde{\chi}(x,s)$ [as given by (9) with $\chi_{k,n}(x)$ in the latter satisfying the reccurent relations (21) (in its differential form)] along any standard path satisfies the differential equation (19).

To this end write (21) in its differential form:

$$\chi'_{n+1}(x)=q^{-1/4}(x)(q^{-1/4}(x)\chi_n(x))'', \quad n\geqslant 0. \tag{B1}$$

Next multiply both the sides of (B1) by $(-s)^n/n!$ and sum them over n $(n\geqslant 0)$ to get

$$\frac{\partial^2\tilde{\chi}(x,s)}{\partial s\,\partial x}+q^{-1/4}(x)\frac{\partial^2}{\partial x^2}(q^{-1/4}(x)\tilde{\chi}(x,s))=0. \tag{B2}$$

Finally, multiply (B2) by $2\lambda e^{2\sigma\lambda s}$ and integrate (by parts) along a standard/cut path C to have

$$2\sigma\lambda\left(2\lambda\int_C ds\, e^{2\sigma\lambda s}\tilde{\chi}(x,s)\right)'+q^{-1/4}(x)\left(q^{-1/4}(x)2\lambda\int_C ds\, e^{2\sigma\lambda s}\tilde{\chi}(x,s)\right)''=0,$$

$$\lambda>0,\ \sigma=\begin{cases}+1, & \text{for infinity of } \Re C<0\\ -1, & \text{for infinity of } \Re C>0.\end{cases} \tag{B3}$$

According to (10) the equation (B3) coincides with (19).

APPENDIX C

We shall show here that if x is sufficiently close to x_0 then the Borel function of the quotient of $\chi^{as}(x,\lambda)$ and $\chi^{as}(x_0,\lambda)$ [with its factors corresponding to $\chi(x,\lambda)$ and $\chi(x_0,\lambda)$, respectively] can be integrated along the same standard path $\tilde{C}$ along which both the factors of the quotient can be summed too. It means that all the three Borel functions, the quotient and its two factors, are holomorphic in a common strip containing $\tilde{C}$.

To show this let us note that it is certainly true for the Borel fuctions $\tilde{\chi}(x,s)$ and $\tilde{\chi}(x_0,s)$ of the two quotient factors considered separately from the Borel function of the quotient itself. This is the result of the analytical dependence on x of singularities of the Borel functions of both these factors.[12] Therefore there is a strip $\tilde{S}$ on the Borel planes of $\tilde{\chi}(x,s)$ and $\tilde{\chi}(x_0,s)$ containing a standard path $\tilde{C}$ along which these functions can be integrated to reproduce the corresponding χ-factors $\chi(x,\lambda)$ and $\chi(x_0,\lambda)$. It is now elementary to show that if $\tilde{\chi}(x_0,s)$ is holomorphic in $\tilde{S}$ then the Borel function of $\chi^{-1}(x_0,\lambda)$ is also. This latter conclusion follows from the semiclassical expansion of $\chi^{-1}(x_0,\lambda)$. Namely, we have for this expansion,

$$\left(\frac{1}{\chi(x_0,\lambda)}\right)^{as}=\frac{1}{\chi^{as}(x_0,\lambda)}=\sum_{n\geqslant 0}\frac{1}{C_0^{n+1}}(C_0-\chi^{as}(x_0,\lambda))^n, \tag{C1}$$

where for $\chi^{as}(x_0,\lambda)$ we have assumed

$$\chi^{as}(x_0,\lambda)=\sum_{n\geqslant 0}\frac{C_n}{(2\lambda)^n}. \tag{C2}$$

The expansion (C1) follows of course from the identical (in form) expansion of $\chi^{-1}(x_0,\lambda)$ itself valid for $|\arg|\leqslant\pi/2$ when λ is sufficiently large.

The Borel function corresponding to the expansion (C1) is therefore

$$\begin{aligned}\frac{\tilde{1}}{\chi(x,\lambda)} &= C_0+\sum_{n\geqslant 1}\frac{(C_0-\tilde{\chi}(x,\lambda))^n}{C_0^{n+1}}\\ &= C_0+\sum_{n\geqslant 1}\frac{(C_0-\tilde{\chi})^{*n}(x,s)}{C_0^{n+1}}\\ &= C_0+\sum_{n\geqslant 1}\frac{(-1)^{n+1}}{C_0^{n+1}}\int_0^s ds_1(C_0-\tilde{\chi}(x,s-s_1))\\ &\quad\times\int_0^{s_1} ds_2\,\tilde{\chi}'(x,s_1-s_2)\cdots\int_0^{s_{n-3}} ds_{n-2}\,\tilde{\chi}'(x,s_{n-3}-s_{n-2})\\ &\quad\times\int_0^{s_{n-2}} ds_{n-1}\,\tilde{\chi}'(x,s_{n-2}-s_{n-1}),\end{aligned}\tag{C3}$$

where the prime at $\tilde{\chi}'(x,s)$ means the differentiation over s and where the following definition of the star (convolution) operation has been used:

$$(\tilde{f}*\tilde{g})(s)=\frac{d}{ds}\int_0^s\tilde{f}(s)\tilde{g}(s-s')ds'.\tag{C4}$$

From the representation (C4) it follows easily that the strip $\tilde{S}$ of the holomorphicity of $\tilde{\chi}(x,s)$ is also such a strip for the Borel function of $\chi^{-1}(x,\lambda)$ since the series in (C4) is uniformly convergent in $\tilde{S}$.

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Quantization of solitons in coset space

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The perturbation theory around the soliton fields of the sin-Gordon model is developed in the coset space. It is shown by explicit calculations that all corrections to the topological soliton contribution are canceled exactly. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1337613]

I. INTRODUCTION

The problem of quantization of the extended objects was formulated mainly in the middle of the 1970s, see the review paper[1] and references cited therein. One starts from the classical Lagrange equation:

$$\frac{\delta S(u)}{\delta u(x,t)}=0, \tag{1}$$

where, for simplicity, $u(x,t)$ is the real scalar field.[2] If this equation has nontrivial solution $u_c(x,t)$ then the problem of its quantization will arise. One of the first attempts to construct the perturbation theory was based on the WKB expansion in the vicinity of u_c.[3,4]

The Born–Oppenheimer method was adopted also.[5,6] First of all, to construct the quantum mechanics, the structure of Hilbert space $\mathcal{H}$ is postulated. So, it is assumed that the Fock column consists from the vacuum state $|0\rangle$ and from the multiple meson states $|p_1,p_2,\ldots,p_n\rangle$, $n\geqslant 1$. The ordinary perturbation theory operates just with this meson sector only. The *anzats* $|P_1,P_2,\ldots,P_l\rangle$[5] for the l-soliton state, $l\geqslant 1$, is introduced also.

It is postulated that the quantum excitations in the soliton sector are described by the excitation of the meson field.[5] Therefore, to construct the perturbation theory, there should also be the mixed states:

$$|P_1,\ldots,P_l;p_1,\ldots,p_n\rangle,\quad l\geqslant 1,\ n\geqslant 1, \tag{2}$$

but, at the same time,

$$\langle P_1,\ldots,P_l;p_1,\ldots,p_n|p_1,\ldots,p_{n'}\rangle\equiv 0,\ l\geqslant 1,\ n+n'\geqslant 0, \tag{3}$$

i.e., it is assumed that the solitons are the absolutely stable field configurations.[1]

The present paper in a definite sense completes the picture in Refs. 5 and 6, The $(1+1)$-dimensional exactly integrable sin-Gordon model will be considered to illustrate our result. We will investigate the multiple production of mesons by soliton and the truth of (3) will be shown at the end of explicit calculations. In other words, it will be shown that the postulate in

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Refs. 5 and 6 concerning orthogonality of the meson $\mathcal{H}_m$ and soliton $\mathcal{H}_s$ Hilbert spaces can be proved. We will see that this conclusion follows from exactness of the semiclassical approximation for the sin-Gordon model.

It should be noted that the exactness of the semiclassical approximation in the topological soliton sector of the sin-Gordon model is not beyond the realm.[3] It is well known also that the integrable Coulomb problem is exactly semiclassical. We have the same for the quantum rigid rotator,[7] which is the isomorphic to the Poshle–Teller model. The general discussion of the exactness of the semiclassical approximation from a geometrical point of view was given in Ref. 8.

It will be crucial for us in many respects to follow the WKB ideology. So, we will consider the meson production amplitudes

$$a_{nm}(p,q)=\langle p_1,\ldots,p_n|q_1,\ldots,q_m\rangle_c, \quad n,m=1,2,\ldots. \tag{4}$$

The index c means that the calculations are performed in the soliton sector and p_i and q_i are the meson momenta. By definition,

$$p_i^2=q_i^2=m^2, \tag{5}$$

since the quantum uncertainty principle leads to the impossibility of mass-shell observation of the field.[9] The ordinary reduction formalism will be used to calculate a_{nm}. This means that we will construct the *phenomenological S*-matrix of the meson interaction through the soliton fields, i.e., we will start from the assumption that the states (2) exist, and it will be shown at the end of the calculations that such *S*-matrix is trivial:

$$a_{nm}(p,q)\equiv 0, \quad n+m>0. \tag{6}$$

The formalism allows to prove (6). For this purpose we will build the perturbation theory expansion over $1/g$, where g is the interaction constant.[10] This perturbation theory is dual to the theory described in Ref. 1, over g, i.e., one cannot decompose the definite order over g contribution in terms of the $1/g$ expansion, and vice versa. So, only the summary results of both expansion may be compared.

Following to WKB ideology, to find the corrections to the semiclassical approximation in the vicinity of the extremum $u_c(x,t)$, one should find the solution of the equation for the Green function:

$$(\partial^2+v''(u_c))G(x,t;x',t')=\delta(x-x')\,\delta(t-t'),$$

where $v''(u)$ is the second derivative of the potential function $v(u)$. This Green function describes propagation of a particle in the time dependent inhomogeneous and anisotropic external field $u_c(x,t)$. Generally, this problem has no closed solution. So, for instance, the attempt to solve the problem using the momentum decomposition[11] leads to the hardly handling double-parametric perturbation theory. To avoid this problem we will build a new perturbation theory over $1/g$.

Imagining particle coordinates as the elements of the Lee group, the classical particle motion may be described mapping the trajectory on group manifold. Roughly speaking, this means that the group combination law creates the particles classical trajectory.[12]

Moreover, this program was realized for description of the particle quantum motion.[13] It was shown for essentially nonlinear Lagrangian $L=\frac{1}{2}g_{\mu\nu}(x)\dot{x}^\mu\dot{x}^\nu$ that the semiclassical approximation is exact on the (semi)simple Lee group manifold. But this slender solution of quantum problems is destructed in presence of the interaction potential $v(x)=O(x^n)$, $n>2$, since the last one breaks the isotropy and homogeneity of the Lee group manifolds.[10] The developed perturbation theory will describe the quantum perturbations breaking isotropy and homogeneity of the group manifold.

Developed formalism contains the following steps.[10,14] (i) We will introduce the manifold W_G of trajectories u_c, solving the Eq. (1). The manifold W_G will be labeled by the local coordinates

(ξ,η), i.e., we will consider $u_c=u_c(x;\xi,\eta)$ since u_c should belong to W_G *completely*. (ii) The numbers (ξ,η) are interpreted as the generalized coordinates of the particle. Then $u_c(x;\xi,\eta)$ will define the external potential for it. The quantum motion of the particle may be described noting that W_G is the homogeneous and isotropic manifold, since this case is a rather quantum mechanical problem in the flat space.

It was shown in Ref. 14 that the WKB model,[5] where the field excitations in vicinity of u_c are decomposed over the meson states, and our model quantum mechanics of the particle in the external potential defined by u_c, are isomorphic. In other words, we know that the quantum trajectory of the particle covers the phase space $(\xi,\eta)\in W_G$ densely. But it should be noted also that the model described in Ref. 5 presents the expansion over the interaction constant λ and our perturbation theory describes expansion over the $(1/\lambda)$.

In the classical limit (labeled by the index 0) the motion of our particle must be free,[14] i.e., its velocity should be a constant,

$$\dot{\xi}_0=\text{const}, \quad \dot{\eta}_0=0. \tag{7}$$

This may be achieved expressing the set $\{\eta\}$ through the set of generators of the subgroup broken by u_c.[15] It is evident, such choice of the particles coordinate gives the same effect as in the above discussed transformation to the homogeneous and isotropic (semi)simple Lee group manifold,[10] see also Ref. 16. Moreover, we will see that even in the case of nontrivial potential function, one can get to the free particles motion, rescaling the quantum sources.[10,14]

Thus, the necessary invariant subspace W_G would be chosen equal to the coset space G/G_c:

$$W_G=G/G_c, \tag{8}$$

where G is the symmetry group and $G_c\subset G$ is the classical solutions u_c symmetry group. The problem of quantization of the coset space have a reach history, see, e.g., Ref. 17. As described in Refs. 10 and 14, the formalism presents one possible realization of the coset spaces quantization scheme.

The last one means that we will realize the transformation generated by the classical trajectory:[14]

$$u_c:\ (u,p)(x,t)\rightarrow(\xi,\eta). \tag{9}$$

Such construction of perturbation theory in the W_G space requires the additional effort noting that the dimension of the original phase space $(u,p)\in T^*V$ is infinite. Therefore, Eq. (9) assumes the infinite reduction since the dimension of coset space W_G is finite.[18] The crucial reduction scheme was formulated in Ref. 14.

In other words, quantizing the sin-Gordon soliton fields, the space coordinate would be an irrelevant variable. This is the well-known fact, e.g., Ref. 4, and it leads to the Lorentz noncovariant perturbation theory. It is the consequence of the solitary profile of considered field configurations and its absolute stability, i.e., of conservation of the topological charge. The necessary information concerning this question will be given in Sec. III.

Having the complete theory, one can analyze the perturbations. The crucial point of the new perturbation theory is the statement[10] that the quantum corrections are accumulated strictly on the boundaries ∂W_G (bifurcation manifolds[19,20,15]) of the W_G space. Therefore, if

$$\partial u_c\cap\partial W_G=\varnothing, \tag{10}$$

then the problem is exactly semiclassical. On other hand, Eq. (10) means conservation of the topological charge: ∂u_c is the flow induced by the quantum perturbations in W_G and if (10) is not satisfied, then one should exist a flow into the forbidden, separated by the bifurcation boundary, domain with other topological charge. So, Eq. (10) is the topological charge conservation.

On the other hand, Eq. (10) leads to (6) since particle production is the pure quantum effect. This will be shown in Sec. IV.

The paper is organized as follows. In Sec. II we will (i) formulate the necessary boundary conditions to derive the LSZ reduction formula, (ii) find the explicit expression for a_{nm}, (iii) formulate the mapping into the coset space W_G. In Sec. III we (i) consider the sin-Gordon model, (ii) discuss the coset space boundary condition, (iii) remind the structure of the new perturbation theory,[14] (iv) describe meson multiple production to show (6).

II. DENSITY MATRIX ON THE DIRAC MEASURE

The main point of this section is the attempt to generalize the ordinary for field theory boundary condition

$$u(x\in\sigma_\infty)=0,$$

where σ_∞ is the remote hypersurface. This boundary condition is used to remove the surface term, and it is necessary to formulate the reduction formalism. We would like to introduce the new boundary condition to have a possibility to include the nonvanishing on σ_∞ field configurations and, at the same time, throw off the surface term.

The $(n+m)$-point Green functions G_{nm} are introduced through the generating functional Z_j:[21]

$$G_{nm}(x,y)=(-i)^{n+m}\prod_{k=1}^{n}\hat{j}(x_k)\prod_{k=1}^{m}\hat{j}(y_k)Z_j, \tag{11}$$

where $\hat{j}(x)=\delta/\delta j(x)$ and the generating functional

$$Z_j=\int Du\, e^{iS_j(u)}. \tag{12}$$

The action

$$S_j(u)=S(u)-V(u)+\int \mathrm{d}x\,\mathrm{d}t\, j(x,t)u(x,t), \tag{13}$$

where

$$S(u)=\int \mathrm{d}x\,\mathrm{d}t\left(\tfrac{1}{2}(\partial u)^2-m^2u^2\right),\quad m^2\geqslant 0, \tag{14}$$

is the free part and $V(u)$ describes the interactions. At the end of the calculations one should put $j=0$.

To provide convergence, the integral (12) will be defined on the Mills complex time contour C_+.[22] For example,

$$C_\pm:\quad t\to t+i\varepsilon,\varepsilon\to+0,\ -\infty\leqslant t\leqslant+\infty \tag{15}$$

and after all calculations, one should return the time contour on the real axis putting $\varepsilon=0$.

In a 'meson' sector the integration in (12) is performed over all field configurations with standard vacuum boundary condition:

$$\int \mathrm{d}^2x\,\partial_\mu(u\partial^\mu u)=\int_{\sigma_\infty}\mathrm{d}\sigma_\mu\, u\partial^\mu u=0. \tag{16}$$

It follows from this conditions that

$$u(x\in\sigma_\infty)=0,\quad pa_\mu u(x\in\sigma_\infty)=0. \tag{17}$$

It excludes a contribution from the surface term, since it assumes that field disappeared on the remote hypersurface σ_∞. Considering the soliton sector this boundary condition requires the modification since there is in the $(x-t)$ space such direction along which the soliton field does not disappear. The integral (12) would have a formal meaning until this boundary condition will not be specified.

Let us introduce now the field φ through the equation

$$-\frac{\delta S(\varphi)}{\delta\varphi(x,t)}=j(x,t). \tag{18}$$

It is assumed that we can formulate such boundary condition that the surface term may be neglected calculating the variational derivative in (18). Then we perform the ordinary shift $u\to u+\varphi$ in integral (12). Considering φ as the probe field created by the source:

$$\varphi(x)=\int \mathrm{d}^2x'\, G_0(x-x')j(x'),\quad (\partial^2+m^2)G_0(x-x')=\delta(x-x'), \tag{19}$$

the connected Green function G^c_{nm} will only be interesting for us,

$$G^c_{nm}(x,y)=(-i)^{n+m}\prod_{k=1}^{n}\hat{j}(x_k)\prod_{k=1}^{m}\hat{j}(y_k)Z(\varphi), \tag{20}$$

where

$$Z(\varphi)=\int Du\, e^{iS(u)-iV(u+\varphi)} \tag{21}$$

is the new generating functional.

To calculate the nontrivial elements of the S matrix we must put the external particles on the mass shell. Formally this procedure means amputation of the external legs of G^c_{nm} and further multiplication on the free particle wave functions. In result the amplitude of n into m particle transition a_{nm} in the momentum representation has the form

$$a_{nm}(q,p)=(-i)^{n+m}\prod_{k=1}^{n}\hat{\varphi}(q_k)\prod_{k=1}^{m}\hat{\varphi}^*(p_k)Z(\varphi). \tag{22}$$

Here the particles creation operator

$$\hat{\phi}^*(q)=\int \mathrm{d}^2x\, e^{iqx}\hat{\phi}(x),\quad \hat{\phi}(x)=\frac{\delta}{\delta\phi(x)}. \tag{23}$$

was introduced. The Eq. (22) is the ordinary LSZ reduction formulas. But one should remember that the boundary condition (16) should be generalized to have permission for inclusion of the soliton contributions calculating $Z(\varphi)$.

Describing the particles multiple production it is enough to consider the generating functional

$$\rho(\alpha,z)=\exp\Big\{-\int \mathrm{d}\Omega_1(p)(\hat{\varphi}^*_+(p)\hat{\varphi}_-(p)e^{i\alpha_+p}z_+(p) + \hat{\varphi}^*_-(p)\hat{\varphi}_+(p)e^{i\alpha_-p}z_-(p))\Big\}Z(\varphi_+)Z^*(\varphi_-), \tag{24}$$

where

$$d\Omega_n(p)=\prod_{k=1}^{n}\frac{d^1p_k}{(2\pi)2\epsilon(p_k)}=\prod_{k=1}^{n}d\Omega_1(p_k),\quad \epsilon(p)=(p^2+m^2)^{1/2}.$$

Let us calculate

$$\int\frac{d^2\alpha_+}{(2\pi)^2}e^{-iP\alpha_+}\frac{d^2\alpha_-}{(2\pi)^2}e^{-iP\alpha_-}\prod_{k=1}^{n}\frac{\delta}{\delta z_+(p_k)}\prod_{k=1}^{m}\frac{\delta}{\delta z_-(q_k)}\rho(\alpha,z)|_{z_+=z_-=0}.$$

Inserting here the definition (24), one can find that this expression gives

$$\delta\left(P-\sum_{k=1}^{n}p_k\right)\delta\left(P-\sum_{k=1}^{m}q_k\right)|a_{nm}(p,q)|^2,$$

where the δ functions are the result of integration over $\alpha_\pm$. So, the factors $e^{i\alpha_\pm p}$ in (24) permit to introduce the energy-momentum shell and the δ function defines the restriction on the shell. Both restrictions

$$P=\sum_{k=1}^{m}q_k,\quad P=\sum_{k=1}^{n}p_k$$

are compatible since the amplitude a_{nm} is translationally invariant. The integration over P gives energy-momentum conservation law.

Notice now that $\rho(\alpha,z)$ is defined through the generating functional

$$\rho_0(\varphi)=Z(\varphi_+)Z^*(-\varphi_-)=\int Du_+\,Du_-\,e^{iS_+(u_+)-iS_-(u_-)}e^{-iV_+(u_++\varphi_+)+iV_-(u_--\varphi_-)}. \quad (25)$$

Then, we can consider the closed-path boundary condition

$$\int_{\sigma_\infty}d\sigma_\mu\,u_+\partial^\mu u_+=\int_{\sigma_\infty}d\sigma_\mu\,u_-\partial^\mu u_-, \quad (26)$$

instead of (16) and (17). The natural solution of this boundary condition is

$$u_+(x\in\sigma_\infty)=u_-(x\in\sigma_\infty)=u(x\in\sigma_\infty). \quad (27)$$

It provides cancellation of the surface term on the remote hypersurface σ_∞ independently on the value of the field $u(x\in\sigma_\infty)$.

Considering the system with the large number of particles, we can simplify calculations choosing the center-of-mass (c.m.) frame $P=(P_0=E,\vec{0})$. It is useful also[23] to rotate the contours of integration over

$$\alpha_{0,k}:\ \alpha_{0,k}=-i\beta_k,\ \mathrm{Im}\,\beta_k=0,\quad k=1,2.$$

Then $\rho(\beta,z)$ have a meaning of the density matrix, where β would have, in the some definite case,[24] meaning of the inverse temperature and z is the activity.[25]

It was shown in Ref. 14 that the unitarity condition unambiguously determines contributions in the path integrals for ρ. Exist the statement:

S1. The density matrix $\rho(\alpha,z)$ has the following representation:

$$\rho(\alpha,z)=e^{-i\hat{K}(je)}\int DM(u)e^{iS_O(u)-iU(u,e)}e^{N(\alpha,z;u)}\equiv\mathcal{O}(u)e^{N(\alpha,z;u)}. \quad (28)$$

It should be underlined that this representation is strict and is valid for arbitrary Lagrange theory of arbitrary dimensions. The derivation of (28) is given in the Appendix.

Expansion over the operator

$$\hat{K}(je)=\frac{1}{2}\,\mathrm{Re}\int_{C_+}\mathrm{d}x\,\mathrm{d}t\,\frac{\delta}{\delta j(x,t)}\,\frac{\delta}{\delta e(x,t)}\equiv\frac{1}{2}\,\mathrm{Re}\int_{C_+}\mathrm{d}x\,\mathrm{d}t\,\hat{j}(x,t)\hat{e}(x,t) \tag{29}$$

generates the perturbation series. We will assume that this series exist (at least in the Borel sense). The variational derivatives in (29) are defined as follows:

$$\frac{\delta\phi(x,t\in C_i)}{\delta\phi(x',t'\in C_j)}=\delta_{ij}\delta(x-x')\,\delta(t-t')\quad i,j=+,-,$$

where C_i is the Mills time contour. The auxiliary variables (j,e) must be taken equal to zero at the very end of the calculations.

The functionals $U(u,e)$ and $S_O(u)$ are defined by the equalities

$$S_O(u)=(S(u+e)-S(u-e))+2\ \mathrm{Re}\int_{C_+}\mathrm{d}x\,\mathrm{d}t\,e(x,t)(\partial^2+m^2)u(x,t), \tag{30}$$

$$U(u,e)=V(u+e)-V(u-e)-2\ \mathrm{Re}\int_{C_+}\mathrm{d}x\,\mathrm{d}t\,e(x,t)v'(u), \tag{31}$$

where $S(u)$ is the free part of the Lagrangian and $V(u)$ describes interactions. The phase $S_O(u)$ is not equal to zero if u have the nontrivial topological charge.[14] We will discuss carefully this question later.

The measure $DM(u,p)$ has the form

$$DM(u)=\prod_{x,t}\mathrm{d}u(x,t)\,\delta\left(\frac{\delta(S(u)-V(u))}{\delta u(x,t)}+j(x,t)\right). \tag{32}$$

The functional δ function in the measure means that the necessary and sufficient set of contributions in the integral over $u(x,t)$ is defined by the classical equation

$$-\frac{\delta(S(u)-V(u))}{\delta u(x,t)}=j(x,t), \tag{33}$$

disturbed by the quantum source $j(x,t)$.

For further calculation another representation will be useful. If we insert into the integral (28)

$$1=\int\prod_{x,t}\mathrm{d}p(x,t)\,\delta(p(x,t)-\dot{u}(x,t))$$

then the measure DM takes the form

$$DM(u,p)=\prod_{x,t}\mathrm{d}u(x,t)\mathrm{d}p(x,t)\,\delta\left(\dot{u}(x,t)-\frac{\delta H_j(u,p)}{\delta p(x,t)}\right)\delta\left(\dot{p}(x,t)+\frac{\delta H_j(u,p)}{\delta u(x,t)}\right) \tag{34}$$

with the total Hamiltonian

$$H_j(u,p)=\int\mathrm{d}x\left\{\frac{1}{2}p^2+\frac{1}{2}\,(\nabla u)^2+v(u)-ju\right\}. \tag{35}$$

The last one includes the energy ju of quantum fluctuations. The measure (34) describes motion in the symplectic space $(u,p)\in V$. But it should be underlined that the used expansion is not the Lagrange transformation. So, generally, it is quite possible, considering x as the index of the space shell, that not all of $p(x,t)$ are the independent variables. For this reason the measure (34) has mostly a Lagrange meaning.

The measure (34) contains the following information.[10,14]

(a) *Only the strict solutions of equations*

$$\dot{u}-\frac{\delta H_j(u,p)}{\delta p}=0,\quad \dot{p}+\frac{\delta H_j(u;p)}{\delta u}=0 \tag{36}$$

at $j=0$ *should be taken into account*. This rigidness means absence in the formalism of the pseudo-solution (similar to multi-instanton, or multikink) contributions.

(b) $\rho(\alpha,z)$ *is described by the sum of all solutions of Eq. (36), independently from their nearness in the functional space*.

(c) *The field disturbed by* $j(x)$ *belongs to the same manifold (topology class) as the classical field defined by (36).*[10]

(d) *The consequence of properties b. and c. is the selection rule: quantum dynamics is realized in the coset space of highest dimension.*[10] This, excluding from consideration the pure meson sector.

The particle density

$$N(\alpha,z;u)=N_+(\alpha_+,z_+;u)+N_-(\alpha_-,z_-;u), \tag{37}$$

where

$$N_\pm(\alpha_\pm,z_\pm;u)=\int \mathrm{d}\Omega_1(q)e^{i\alpha_\pm q}z_\pm(q)|\Gamma(q;u)|^2. \tag{38}$$

The vertex $\Gamma(q;u)$ is the function of the external particle momentum q and is the linear functional of $u(x)$:

$$\Gamma(q;u)=-\int \mathrm{d}x\, e^{iqx}\frac{\delta S(u)}{\delta u(x)}=\int \mathrm{d}x\, e^{iqx}(\partial^2+m^2)u(x),\quad q^2=m^2, \tag{39}$$

for the mass m field. This parameter presents the momentum distribution of the interacting field $u(x)$ on the remote hypersurface σ_∞ *if* $u(x)$ is the regular function. Notice, the operator cancels the mass-shell states of $u(x)$.

Generally $\Gamma(q;u)$ is connected directly with *external* particles properties and sensitive to the symmetry of the interacting fields system.[26]

The construction (39) means, because of the operator (∂^2+m^2) and remembering that the external states should be mass shell by definition,[9] the solution $\rho(\alpha,z)=0$ is actually possible for particular topology (compactness and analytic properties) of *quantum* field $u(x)$. So, $\Gamma(q;u)$ carry remarkable properties: (i) it directly defines the observables, (ii) is defined by the topology of $u(x)$. Notice that the space-time topology of $u(x,t)$ becomes important calculating integral (39) by parts. This procedure is available if $u(x,t)$ is the regular function. But the *quantum* fields are always singular. Therefore, the solution $\Gamma(q;u)=0$ is valid iff the semiclassical approximation is exact, i.e., the particle production is the pure quantum effect. Just this situation is realized in the soliton sector of the sin-Gordon model.

Let G be the symmetry of the problem and let G_c be the symmetry of the solution u_c. Then

S2. The measure (34) admits the transformation:

$$u_c:(u,p)\to(\xi,\eta)\in W=G/G_c \tag{40}$$

and transformed measure has the form

$$DM(u,p)=\prod_{x,tC} \mathrm{d}\xi(t)\mathrm{d}\eta(t)\,\delta\left(\dot{\xi}-\frac{\delta h_j(\xi,\eta)}{\delta\eta}\right)\delta\left(\dot{\eta}+\frac{\delta h_j(\xi,\eta)}{\delta\xi}\right), \tag{41}$$

where $h_j(\xi,\eta)=H_j(u_c,p_c)$ *is the transformed Hamiltonian*

$$h_j(\xi,\eta;t)=h(\eta)-\int \mathrm{d}x\, j(x,t)u_c(x;\xi,\eta) \tag{42}$$

and $u_c(x;\xi,\eta)$ *is the soliton solution parametrized by* (ξ,η).

The proof of Eq. (41) is the same as for the Coulomb problem considered in Ref. 14. But the case of the $(1+1)$-dimensional model needs the additional explanations. First of all, one must introduce the functional

$$\Delta(u,p)=\int \prod_t \mathrm{d}^N\xi(t)\mathrm{d}^N\eta(t)\prod_{x,t}\delta(u(x,t)-u_c(x;\xi,\eta))\,\delta(p(x,t)-p_c(x;\xi,\eta)). \tag{43}$$

The equalities

$$u(x,t)=u_c(x;\xi,\eta),\quad p(x,t)=p_c(x;\xi,\eta) \tag{44}$$

assume that for given $u(x,t)$ and $p(x,t)$ one can hide the t dependence into the N functions $\xi=\xi(t)$ and $\eta=\eta(t)$. It is assumed that this procedure can be done for arbitrary x. In other respects, functions $u(x,t)$ and $p(x,t)$, and therefore, $u_c(x;\xi,\eta)$ and $p(x;\xi,\eta)$, are arbitrary.

For more confidence, one may divide the space onto the N cells and to each $(u,p)_x$ we may adjust $(\xi,\eta)_x$. It is possible that (ξ,η) are x independent. In this degenerate case $\Delta\sim(\delta(0))^k$, where $k\leqslant N$ is the degree of the degeneracy. We will omit the index x considering $(\xi,\eta)_x$ as the vector of the necessary dimension.

If (ξ,η) are the solutions of (44), then

$$\Delta(u,p)=\int \prod_t \mathrm{d}\xi'(t)\mathrm{d}\eta'(t)\,\delta(u_c^{\xi}\xi'+u_c^{\eta}\eta')\,\delta(p_c^{\xi}\xi'+p_c^{\eta}\eta')=\Delta_c(\xi,\eta)\neq 0, \tag{45}$$

where, for instance, $u_c^X=\partial u_c(x;\xi,\eta)/\partial X$, $X=\xi,\eta$. Notice the importance of the last condition. If it is fulfilled, then one may insert into (28), with measure (41),

$$1=\frac{\Delta(u,p)}{\Delta_c(\xi,\eta)} \tag{46}$$

and integrate over $u(x,t)$ and $p(x,t)$. Notice that the possible infinite factor $(\delta(0))^k$ would be canceled in the ratio (46).

The Jacobian of transformation

$$J=\int \frac{Du\,Dp}{\Delta_c(\xi,\eta)}\prod_{x,t}\delta\left(\dot{u}-\frac{\delta H_j(u,p)}{\delta p}\right)\delta\left(\dot{p}+\frac{\delta H_j(u,p)}{\delta u}\right)$$
$$\times\,\delta(u(x,t)-u_c(x;\xi,\eta))\,\delta(p(x,t)-p_c(x;\xi,\eta)), \tag{47}$$

is proportional to functional δ-functions again. To have the transformation, we should use the last two δ functions. Notice, if the first two δ functions are used to calculate J, then the last two δ functions realize the constraints. In result,

$$J=\frac{1}{\Delta_c(\xi,\eta)}\prod_{x,t}\delta\left(\dot{u}_c-\frac{\delta H_j(u_c,p_c)}{\delta p_c}\right)\delta\left(\dot{p}_c+\frac{\delta H_j(u_c,p_c)}{\delta u_c}\right). \tag{48}$$

It should be underlined that u_c and p_c are *arbitrary* functions of ξ and η, i.e., on this stage we make the transformation of arbitrary functions $u(x,t)$ and $p(x,t)$ on the new arbitrary functions $u_c(x;\xi,\eta)$ and $p_c(x;\xi,\eta)$, where, generally speaking, $\xi=\xi(x,t)$ and $\eta=\eta(x,t)$. Then Δ_c is the corresponding determinant.

The expression (48) can be rewritten identically to the form

$$J=\frac{1}{\Delta_c(\xi,\eta)}\int\prod_{x,t}\mathrm{d}\xi'(t)\mathrm{d}\eta'(t)\,\delta\left(\dot\xi'-\left(\dot\xi-\frac{\delta h_j(\xi,\eta;t)}{\delta\eta}\right)\right)\delta\left(\dot\eta'-\left(\dot\eta+\frac{\delta h_j(\xi,\eta;t)}{\delta\xi}\right)\right)$$
$$\times\,\delta\left(u_c^\xi\xi'+u_c^\eta\eta'+\{u_c,h_j\}-\frac{\delta H_j}{\delta p_c(x,t)}\right)\delta\left(p_c^\xi\xi'+p_c^\eta\eta'-\{p_c,h_j\}+\frac{\delta H_j}{\delta u_c(x,t)}\right),\qquad(49)$$

where $\{,\}$ is the Poisson bracket.

Let us assume now that the auxiliary function $h_j(\xi,\eta;t)$ is chosen so that the equalities

$$\{u_c,h_j\}=\frac{\delta H_j}{\delta p_c(x,t)},\quad \{p_c,h_j\}=-\frac{\delta H_j}{\delta u_c(x,t)}\qquad(50)$$

are satisfied identically. Then, taking into account the condition (45), one can find

$$J=\delta\left(\dot\xi-\frac{\delta h_j(\xi,\eta;t)}{\delta\eta}\right)\delta\left(\dot\eta+\frac{\delta h_j(\xi,\eta;t)}{\delta\xi}\right).\qquad(51)$$

This ends the transformation. Notice that the determinant Δ_c was canceled identically.

The transformation specify by the Eqs. (50) the function h_j. It assumes that one can find such functions $u_c=u_c(x;\xi,\eta)$ and $p_c=p_c(x;\xi,\eta)$, with property (45), that (50) has unique solution $h_j(\xi,\eta;t)$.

Let us convert the problem assuming that just h_j is known. It is natural to assume that

$$h_j(\xi,\eta;t)=H_j(u_c,p_c),\qquad(52)$$

then u_c and p_c are defined by Eqs. (50) and

$$\dot\xi=\frac{\delta h_j(\xi,\eta;t)}{\delta\eta},\quad \dot\eta=-\frac{\delta h_j(\xi,\eta;t)}{\delta\xi}.\qquad(53)$$

It is not hard to see that (50) together with (53) are equivalent to incident equations (36). This is seen from the following chain of equalities:

$$\dot u_c(x;\xi\eta)=u_c^\xi\dot\xi+u_c^\eta\dot\eta=u_c^\xi\frac{\partial h_j(\xi,\eta;t)}{\partial\eta}-u_c^\eta\frac{\partial h_j(\xi,\eta;t)}{\partial\xi}$$
$$=\{u_c,h_j\}=\frac{\delta H_j}{\delta p_c(x,t)}$$

and the same we have for p_c. Therefore (u_c,p_c) is the classical phase space flow and the space W_G, labeled by (ξ,η), is the coset space G/G_c.

In result, the new measure takes the form (41), i.e., ξ and η should obey the equations (53):

$$\dot\xi=\omega(\eta)-\int\mathrm{d}x\,j(x,t)\frac{\partial u_N(x;\xi,\eta)}{\partial\eta},\quad \dot\eta=\int\mathrm{d}x\,j(x,t)\frac{\partial u_N(\xi,\eta)}{\partial\xi},\qquad(54)$$

where $\omega(\eta)\equiv\partial h(\eta)/\partial\eta$. Hence the source of quantum perturbations are proportional to the time-local tangent vectors

$$\int \mathrm{d}x\, \partial u_N(x;\xi,\eta)/\partial\eta, \quad \int \mathrm{d}x\, \partial u_N(x;\xi,\eta)/\partial\xi$$

to the soliton configurations. It suggests the idea in Ref. 14 to split the Lagrange sources

$$j(x,t)\to(j_\xi,j_\eta)(t).$$

The mechanism of splitting was described in Ref. 10. The resulting operator $\mathcal{O}(u_c)$, defined in (28), has the same structure. But new perturbations of the generating operator

$$\hat{K}(e_\xi,e_\eta;j_\xi,j_\eta)=\tfrac{1}{2}\mathrm{Re}\int_{C_+}\mathrm{d}t\{\hat{j}_\xi(t)\cdot\hat{e}_\xi(t)+\hat{j}_\eta(t)\cdot\hat{e}_\eta(t)\}. \tag{55}$$

The measure takes the form

$$DM(\xi,\eta)=\prod_t \mathrm{d}\xi(t)\mathrm{d}\eta(t)\,\delta(\dot{\xi}-\omega(\eta)-j_\xi(t))\,\delta(\dot{\eta}-j_\eta(t)). \tag{56}$$

The effective potential $U=U(u_c;e_c)$ with

$$e_c(x,t)=e_\xi(t)\cdot\frac{\partial u_N(x;\xi,\eta)}{\partial\eta(t)}-e_\eta(t)\cdot\frac{\partial u_N(x;\xi,\eta)}{\partial\xi(t)}. \tag{57}$$

Notice that the space degree of freedom is disappeared from our consideration.

III. MULTIPLE PRODUCTION IN SIN-GORDON MODEL

We would consider the theory with the Lagrangian

$$L=\frac{1}{2}(\partial_\mu u)^2+\frac{m^2}{\lambda^2}[\cos(\lambda u)-1]. \tag{58}$$

It is well known that this field model possesses the soliton excitations in the $(1+1)$ dimension.

Formally nothing prevents to linearize partly our problem considering the Lagrangian

$$L=\frac{1}{2}[(\partial_\mu u)^2-\alpha m^2u^2]+\frac{m^2}{\lambda^2}\left[\cos(\lambda u)-1+\alpha\frac{\lambda^2}{2}u^2\right]\equiv S(u)-v(u). \tag{59}$$

The last term $v(u)=O(u^4)$ describes interactions. The corresponding vertex function is

$$\Gamma(q;u)=\int \mathrm{d}x\,\mathrm{d}t\, e^{iqx}(\partial^2+m^2)u(x,t), \quad q^2=m^2. \tag{60}$$

It should be noted here that the division chosen in (59) onto the free and interaction parts did not affect the equation of motion, see (33), and effective potential, see (31), i.e., in this sense α may be chosen arbitrary. But α will arise in the definition of the mass: one should change $m^2\to\alpha m^2$ in (60). This means that our S-matrix approach requires additional, external, normalization condition for the mass shell. We will choose $\alpha=1$ assuming that m is the measured mass of the meson.

We assume that $u(x,t)$ belongs to Schwarz space:

$$u(x,t)|_{|x|=\infty}=0\left(\mathrm{mod}\frac{2\pi}{\lambda}\right). \tag{61}$$

This means that $u(x,t)$ tends to zero $[\mathrm{mod}\,(2\pi/\lambda)]$ at $|x|\to\infty$ faster then any power of $1/|x|$.

The ν-soliton classical Hamiltonian h_ν is the sum

$$h_\nu(\eta)=\int \mathrm{d}r\ \sigma(r)\sqrt{r^2+m^2}+\sum_{i=1}^{\nu} h(\eta_i), \tag{62}$$

where $\sigma(r)$ is the continuous spectrum and $h(\eta)$ is the soliton energy. Notice absence of the energy of soliton interactions.

The ν-soliton solution u_ν depends on the 2ν parameters. Half of the ν can be considered as the position of the solitons and the other ν as the solitons momentum. Generally, at $|t|\to\infty$ the u_ν solution decomposed on the single solitons u_s and on the double soliton bound states u_b:

$$u_\nu(x,t)=\sum_{j=1}^{n_1} u_{s,j}(x,t)+\sum_{k=1}^{n_2} u_{b,k}(x,t)+O(e^{-|t|}). \tag{63}$$

For this reason the one soliton u_s and two-soliton bound state u_b would be the main elements of our formalism. Its (ξ,η) parametrizations, i.e., the solution of Eq. (50), has the form:[27]

$$u_s(x;\xi,\eta)=-\frac{4}{\lambda}\arctan\{\exp(mx\cosh\beta\eta-\xi)\},\quad \beta=\frac{\lambda^2}{8} \tag{64}$$

and

$$u_b(x;\xi,\eta)=-\frac{4}{\lambda}\arctan\left\{\tan\frac{\beta\eta_2}{2}\,\frac{mx\sinh\dfrac{\beta\eta_1}{2}\cos\dfrac{\beta\eta_2}{2}-\xi_2}{mx\cosh\dfrac{\beta\eta_1}{2}\sin\dfrac{\beta\eta_2}{2}-\xi_1}\right\}. \tag{65}$$

The (ξ,η) parametrization of soliton individual energies $h(\eta)$ takes the form

$$h_s(\eta)=\frac{m}{\beta}\cosh\beta\eta,\quad h_b(\eta)=\frac{2m}{\beta}\cosh\frac{\beta\eta_1}{2}\sin\frac{\beta\eta_2}{2}\geqslant 0.$$

The bound-state energy h_b depends on η_2 amd η_1. First one defines the inner motion of two bounded solitons and the second one defines the bound states center of mass motion. Correspondingly we will call these parameters as the internal and external ones. Note that the inner motion is periodic, see (65).

Following the definition of the Dirac measure one should sum over all solutions of the Lagrange equation, see the property (b). In Sec. II. As follows from the equality:

$$\sum_{\{u_c\}}=\int_{W_G}\mathrm{d}\xi_0\,\mathrm{d}\eta_0\sigma(u;\xi_0,\eta_0),$$

we should define the density $\sigma(u;\xi_0,\eta_0)$ of states in the element of the coset space W_G. The Faddeev–Popov *ansatz* is used for this purpose.[4]

In our approach, performing the transformation into the coset space W_G, we define the density $\sigma(u;\xi_0,\eta_0)$. Indeed, using the definition

$$\int Dx\prod_t \delta(\dot{x})=\int \mathrm{d}x(0)=\int \mathrm{d}x_0$$

the functional integrals with measure (56) are reduced to the ordinary ones over the initial data $(\xi,\eta)_0$.

But it is important here to trace on the following question. One can note that, at first glance, integration over $(\xi,\eta)_0$ may only give $\rho\sim V_0^1$, where V_0 is the zero modes volume, i.e., is a volume of the W_G space. On other hand, as follows from definition of $\rho\sim|a_{nm}|^2$, one may expect that $\rho\sim V_0^2$. This discrepancy should have an explanation.

Remembering definition of ρ as the square of the amplitudes, we should define the contributions on the whole time contour $C=C_+ + C_-$, see (15), to take into account the input condition that the trajectories $u_+(t\in C_+)$ and $u_-(t\in C_-)$ are absolutely independent in the frame of the closed-path boundary condition (27):

$$u_c(x,t\in\partial C_+)=u_c(x,t\in\partial C_-), \tag{66}$$

where $\partial C_\pm$ is the boundary of $C_\pm$. Other directions to the $\sigma_{|}infty$ are not important here.

Then, if we introduce $(\xi,\eta)(t\in C_\pm)|_0\equiv(\xi_0,\eta_0)_\pm$, one should have in mind that, generally speaking, $(\xi_0,\eta_0)_+\neq(\xi_0,\eta_0)_-$ and the integration over them should be performed independently. This may explain the above discrepancy and one should have $\rho\sim V_0^2$.

It is not hard to see that for our topological solitons the condition (66) leads to the equalities

$$(\xi_0,\eta_0)_+=(\xi_0,\eta_0)_-=(\xi_0,\eta_0). \tag{67}$$

To see this it is enough to insert (64), or (65), into (66) and take into account that at $t\in\partial C_\pm$ the estimation (63) is right.

Solution (67) means that, for arbitrary functional $F(\xi,\eta)$,

$$\int\prod_{t\in C_++C_-}\mathrm{d}\xi\mathrm{d}\eta\,\delta(\dot\xi)\delta(\dot\eta)F(\xi,\eta)=\int\mathrm{d}\xi_{0+}\mathrm{d}\eta_{0+}\int\mathrm{d}\xi_0 d\,\eta_0F(\xi_0,\eta_0). \tag{68}$$

Therefore, $\rho\sim V_0^2$. We will put out the integrals over inessential variables ξ_{0+} and η_{0+}.

It should be underlined that (67) is the consequence of the conservation of the topological charge: the solitons by this reason are the stable formation and, therefore, to satisfy the closed path boundary condition, one should have (67).

Performing the shifts

$$\xi_i(t)\to\xi_i(t)+\int\mathrm{d}t'\,g(t-t')j_{\xi,i}(t')\equiv\xi_i(t)+\xi_i'(t),$$

$$\eta_i(t)\to\eta_i(t)+\int\mathrm{d}t'\,g(t-t')j_{\eta,i}(t')\equiv\eta_i(t)+\eta_i'(t),$$

we can get the Green function $g(t-t')$ into the operator exponent

$$\hat K(ej)=\frac{1}{2}\int\mathrm{d}t\,\mathrm{d}t'\Theta(t-t')\{\hat\xi'(t')\cdot\hat e_\xi(t)+\hat\eta'(t')\cdot\hat e_\eta(t)\}, \tag{69}$$

since the Green function $g(t-t')$ of the transformed theory is the step function[10]

$$g(t-t')=\Theta(t-t'). \tag{70}$$

Such Green function allows to shift $C_\pm$ on the real-time axis. This, noting (67), excludes doubling of the degrees of freedom.

Notice the Lorentz noncovariantness of our perturbation theory with Green function (70).

The measure takes the form

$$D^\nu M(\xi,\eta)=\prod_{i=1}^{\nu}\prod_t\mathrm{d}\xi_i(t)\mathrm{d}\eta_i(t)\,\delta(\dot\xi_i-\omega(\eta+\eta'))\delta(\dot\eta_i). \tag{71}$$

The interactions are described by

$$U(u_\nu;e_c)=-\frac{2m^2}{\lambda^2}\int \mathrm{d}x\,\mathrm{d}t\,\sin\lambda u_\nu(\sin\lambda e_c-\lambda e_c) \tag{72}$$

with

$$u_\nu=u_\nu(x;\xi+\xi',\eta+\eta') \tag{73}$$

and e_c was defined in (57).

The equation

$$\dot{\xi}_i=\omega(\eta_i+\eta_i') \tag{74}$$

is trivially integrable. In the quantum case $\eta_i'\neq 0$ this equation describes motion in the nonhomogeneous and anisotropic manifold. So, the expansion over $(\hat{\xi}',\hat{e}_\xi,\hat{\eta}',\hat{e}_\eta)$ generates the local in time fluctuations of W_G manifold. The weight of these fluctuations is defined by $U(u_\nu;e_c)$.

Expansion of $\exp\{\hat{K}(je)\}$ gives the strong coupling perturbation series. The analyses show that[14]

S3. Action of the integro-differential operator $\hat{\mathcal{O}}$ leads to the following representation:

$$\rho(\alpha,z)=\int_{W_G}\left\{\mathrm{d}\xi(o)\cdot\frac{\partial}{\partial\xi(0)}R^\xi(\alpha,z)+\mathrm{d}\eta(0)\cdot\frac{\partial}{\partial\eta(0)}R^\eta(\alpha,z)\right\}. \tag{75}$$

This means that the contributions into ρ are accumulated strictly on the boundary bifurcation manifold ∂W_G. The proof of this important result was given in Refs. 10 and 14 and we will use it without comments.

We would divide calculations on two parts. First of all, we would consider the semiclassical approximation and then we will show that this approximation is exact.

Performing the last integration we find

$$\rho(\alpha,z)=\int\prod_{i=1}^{\nu}\{\mathrm{d}\xi_0\,\mathrm{d}\eta_0\}_i e^{-i\hat{K}}e^{iS_O(u_\nu)}e^{-iU(u_\nu;e_c)}e^{N(\alpha,z;u_\nu)}, \tag{76}$$

where

$$u_\nu=u_\nu(\eta_0+\eta',\xi_0+\omega(t)+\xi') \tag{77}$$

and

$$\omega(t)=\int \mathrm{d}t'\,\Theta(t-t')\omega(\eta_0+\eta')(t'). \tag{78}$$

In the semiclassical approximation $\xi'=\eta'=0$ we have

$$u_\nu=u_\nu(x;\eta_0,\xi_0+\omega(\eta_0)t). \tag{79}$$

Notice that the surface term

$$\int \mathrm{d}x^\mu\,\partial_\mu(e^{iqx}u_\nu)=0. \tag{80}$$

Then

$$\int \mathrm{d}^2x\, e^{iqx}(\partial^2+m^2)u_\nu(x,t)=-(q^2-m^2)\int \mathrm{d}^2x\, e^{iqx}u_\nu(x,t)=0, \tag{81}$$

since q^2 belongs to the mass shell by definition. The condition (80) is satisfied for all $q_\mu\neq 0$ since u_ν belongs to the Schwarz space. Therefore, in the semiclassical approximation $R^c(\alpha,z)$ is the trivial function of z: $\partial R^c(\alpha,z)/\partial z=0$.

Expending the operator exponent in (76), we find that action of the operators $\hat{\xi}'$, $\hat{\eta}'$ create the terms

$$\sim \int \mathrm{d}^2x\, e^{iqx}\theta(t-t')(\partial^2+m^2)u_\nu(x,t)\neq 0. \tag{82}$$

So, generally $R(\alpha,z)$ is the nontrivial function of z.

Now we will show that the semiclassical approximation is exact in the soliton sector of the sin-Gordon model. The structure of the perturbation theory is readily seen in the normal-product form

$$R(\alpha,z)=\sum_\nu \int \prod_{i=1}^{N}\{\mathrm{d}\xi_0\mathrm{d}\eta_0\}_i :e^{-iU(u_\nu;\hat{J}/2i)}e^{iS_O(u_\nu)}e^{N(\alpha,z;u_\nu)}:, \tag{83}$$

where

$$\hat{J}=\hat{J}_\xi\cdot\frac{\partial u_\nu}{\partial\eta}-\hat{J}_\eta\cdot\frac{\partial u_\nu}{\partial\xi}=\Omega\hat{J}_X\frac{\partial u_\nu}{\partial X} \tag{84}$$

and

$$\hat{J}_X=\int \mathrm{d}t'\,\Theta(t-t')\hat{X}(t') \tag{85}$$

with the $2N$-dimensional vector $X=(\xi,\eta)$. In Eq. (84) Ω is the ordinary symplectic matrix.

The colons in (83) mean that the operator $\hat{J}$ should stay to the left of all functions. The structure (84) shows that each order over $\hat{J}_{X_i}$ is proportional at least to the first order derivative of u_ν over conjugate to X_i variable.

The expansion of (83) over $\hat{J}_X$ can be written using the form

$$\rho(\alpha,z)=\sum_\nu \int \prod_{i=1}^{\nu}\{\mathrm{d}\xi_0\,\mathrm{d}\eta_0\}_i\left\{\sum_{i=1}^{2\nu}\frac{\partial}{\partial X_{0i}}P_{X_i}(u_\nu)\right\}, \tag{86}$$

where $P_{X_i}(u_\nu)$ is the infinite sum of the time-ordered polynomial over u_ν and its derivatives.[14] The explicit form of $P_{X_i}(u_\nu)$ is unimportant, it is enough to know, see (84), that

$$P_{X_i}(u_\nu)\sim\Omega_{ij}\frac{\partial u_\nu}{\partial X_{0j}}. \tag{87}$$

Therefore,

$$\frac{\partial}{\partial z}R(\alpha,z)=0 \tag{88}$$

since (i) each term in (86) is the total derivative, (ii) we have (87), and (iii) u_ν belongs to Schwarz space.

IV. CONCLUSION

We would like to conclude this paper noting the role of the coset space G/G_c topology. It was shown that if

(i) $W_G=G/G_c\neq\varnothing$,
(ii) $W_G=T^*V$ is the simplectic manifold,
(iii) ∂u_c is the phase space flow [see (87)],
(iv) $\partial u_c\cap\partial W_G=\varnothing$,

then the semiclassical approximation is exact.

For this reason, being absolutely stable, topological solitons are unable to describe the multiple production processes. This property of the exactly integrable models was formulated also as the absence of stochastization in the integrable systems.[28] The $O(4)\times O(2)$-invariant solution of $O(4,2)$-invariant theories[29] is noticeably more interesting from this point of view.[30]

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APPENDIX: DERIVATION OF EQ. (29)

The generating functional (24) can be written in the form

$$\rho(\beta,z)=e^{-\overline{n}(s)(\beta,z;\varphi)}\rho_0(\varphi), \tag{A1}$$

where the particles number operator

$$\overline{n}(s)(\beta,z;\varphi)=\overline{n}(s)(\beta_+,z_+;\varphi)+\overline{n}(s)^*(\beta_-,z_-;\varphi) \tag{A2}$$

and

$$\overline{n}(s)(\beta_+,z_+;\varphi_+)=\int \mathrm{d}\Omega_1(q)\hat{\varphi}_+^*(q)\hat{\varphi}_-(q)e^{-\beta_+\epsilon(q)}z_+(q) \tag{A3}$$

is the produced particle number operator.

The functional ρ_0 was introduced in (25):

$$\begin{aligned}\rho_0(\varphi)&=Z(\varphi_+)Z^*(-\varphi_-)\\&=\int Du_+\,Du_-e^{iS_+(u_+)-iS_-(u_-)}e^{-iV_+(u_++\varphi_+)+iV_-(u_--\varphi_-)}.\end{aligned} \tag{A4}$$

So, the integration over u_+ and u_- is not performed independently: one should take into account the boundary condition (27). We can perform in this integral the linear transformation

$$u_\pm(x)=u(x)\pm\phi(x). \tag{A5}$$

Then the boundary condition (27) leads to the equality

$$\phi(x\in\sigma_\infty)=0, \tag{A6}$$

leaving $u(x\in\sigma_\infty)$ arbitrary. Last one means that the integration over this turning-point field $u(x\in\sigma_\infty)$ should be performed, see Sec. III.

Let us extract in the exponents (A4) the linear term over $(\phi+\varphi)$:

$$V_+(u+(\phi+\varphi))-V_-(u-(\phi+\varphi))$$
$$=U(u,\phi+\varphi)+2\,\mathrm{Re}\int_{C_+}\mathrm{d}x(\phi(x)+\varphi(x))v'(u) \tag{A7}$$

and

$$S_+(u+\varphi)-S_-(u-\varphi)=S_O(u)-2i\,\mathrm{Re}\int_{C_+}\mathrm{d}x\,\varphi(x)(\partial_\mu^2+m^2)u(x), \tag{A8}$$

where

$$2\,\mathrm{Re}\int_{C_+}=\int_{C_+}+\int_{C_-}.$$

Notice that generally speaking, $S_O(u)\neq 0$, if the topology of the field $u(x)$ is nontrivial, see Sec. III.

The expansion over $(\phi+\varphi)$ can be written in the form

$$e^{-iU(u,\phi+\varphi)}=e^{(1/2i)\,\mathrm{Re}\int_{C_+}\mathrm{d}x\,\hat{j}(x)\widehat{\varphi'}(x)}e^{i2\,\mathrm{Re}\int_{C_+}\mathrm{d}x\,\mathrm{d}t\,j(x)(\phi(x)+\varphi(x))}e^{-iU(u,\varphi')}, \tag{A9}$$

where $\hat{j}(x)$, $\widehat{\varphi'}(x)$ are the variational derivatives. The auxiliary variables (j,φ') must be taken equal to zero at the very end of the calculations.

In result,

$$\rho_0(\phi)=e^{(1/2i)\mathrm{Re}\int_{C_+}\mathrm{d}x\,\hat{j}(x)\hat{\varphi}(x)}\int Du\,e^{is_0(u)}e^{-iU(u,\varphi)}e^{i2\,\mathrm{Re}\int_{C_+}\mathrm{d}x(j(x)-v'(u))\phi(x)}$$
$$\times\prod_x\,\delta(\partial_\mu^2u+m^2u+v'(u)-j), \tag{A10}$$

where the functional δ function was defined by the equality

$$\prod_x\,\delta(\partial_\mu^2u+m^2u+v'(u)-j)=\int D'\phi\,e^{-2i\,\mathrm{Re}\int_{C_+}\mathrm{d}x(\partial_\mu^2u+m^2u+v'(u)-j)\varphi(x)}, \tag{A11}$$

where the prime means that $D'\phi$ does not includes the integration over $\phi(x\in\sigma_\infty)$. This condition is not seen in the functional δ function because of the definition

$$\int\,\prod_x\,\mathrm{d}u(x)\,\delta(\partial_\mu u(x))=\int\mathrm{d}u(x_\mu\in\sigma_\infty).$$

Equation (A10) can be rewritten in the equivalent form

$$\rho_0(\phi)=e^{-i\hat{K}(j,\varphi)}\int DM(u)e^{is_0(u)-iU(u,\varphi)}e^{i2\,\mathrm{Re}\int_{C_+}\mathrm{d}x\,\phi(x)(\partial_\mu^2+m^2)u(x)} \tag{A12}$$

because of the δ functional measure

$$DM(u)=\prod_x\,\mathrm{d}u(x)\,\delta(\partial_\mu^2u+m^2u+v'(u)-j), \tag{A13}$$

with

$$\hat{K}(j\varphi)=\frac{1}{2}\mathrm{Re}\int_{C_+}\mathrm{d}x\hat{j}(x)\hat{\varphi}(x). \tag{A14}$$

Notice at the end that the contour C_+ in (A14) cannot be shifted on the real time axis since the Green function of the equation

$$\partial_\mu^2 u + m^2 u + v'(u) = j$$

is singular on the light cone.

The action of operator $\mathbf{N}(\beta, z; \hat{\phi})$ maps the interacting fields system on the physical states. Last ones are marked by $z_\pm$ and $\beta_\pm$. The operator exponent is the linear functional over ϕ and this allows easily find (28).

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Superintegrable systems in quantum mechanics and classical Lie theory

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The relation is established between some concepts of quantum mechanics and those of soliton theory. In particular, superintegrable systems in two-dimensional quantum mechanics are shown to be invariant under generalized Lie symmetries and to allow recursion operators. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In classical mechanics a Hamiltonian system with n degrees of freedom is called ''integrable,'' or ''Liouville integrable,'' if it allows n functionally independent integrals of motion in involution that are well-defined functions on phase space.[1] The same concept is used in nonrelativistic quantum mechanics. There a system is integrable if it allows a set of n pairwise commuting linearly independent linear operators, including the Hamiltonian.

A system in classical, or quantum, mechanics is ''superintegrable'' if it allows more than n integrals of motion. A classical system with n degrees of freedom can allow up to $2n-1$ functionally independent integrals of motion. We shall call such a system ''maximally superintegrable.'' The best known maximally superintegrable systems in an n-dimensional Euclidean space E_n correspond to two spherically symmetric potentials, namely the Kepler (or Coulomb) potential $V=\alpha r^{-1}$ and the harmonic oscillator $V=\omega^2 r^2$. These are also the only spherically symmetric potentials in E_3 in which all finite trajectories are closed.[1,2] It is well known[3–5] that in quantum mechanics the corresponding operators, commuting with the Hamiltonian, form an $o(4)$ algebra for the hydrogen atom and a $su(3)$ algebra for the harmonic oscillator.

A systematic search for superintegrable systems in classical and quantum mechanics was started some time ago[6–8] and by now a sizable literature on this topic exists (see, e.g., Refs. 3–31 and references therein).

In quantum mechanics, the usual restriction is to consider linear operators that are polynomials in the momenta and require that they should commute with the Hamiltonian. Thus, in Euclidean space $E_n$we write the stationary Schrödinger equation as

$$H\psi=E\psi, \quad H=-\tfrac{1}{2}\Delta+V(\vec{r}) \tag{1.1}$$

and require

$$[H,\hat{X}_i]=0, \tag{1.2}$$

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where $\hat{X}_i$ are some polynomials in the momenta.

In a two-dimensional space E_2 it was shown[6,7] that one first-order operator $\hat{X}$ satisfying Eq. (1.2) implies that the potential has a geometric symmetry. This means that it is invariant either under rotations, $V(x,y)=V(r)$, or under translations, $V=V(x)$.

One second-order operator $\hat{X}$ implies that the Schrödinger equation (1.1) allows the separation of variables in one of the following coordinate systems: Cartesian, polar, parabolic, or elliptic. If two linearly independent operators commute with H, then H is (maximally) superintegrable. All finite classical trajectories are closed, the quantum energy levels are degenerate, and the Schrödinger equation can be solved in terms of known special functions.

The purpose of this article is to consider the problem of the integrability and superintegrability of the Schrödinger equation from a different point of view. Namely, we relate integrability and superintegrability to similar concepts in soliton theory.[32] There one is dealing with infinite dimensional Hamiltonian systems, with infinitely many integrals of motion. An indication of integrability is the existence of infinitely many ''generalized'' symmetries,[33] sometimes called ''Lie-Bäcklund'' symmetries,[34] i.e., symmetries depending on derivatives of the dependent variables. Another basic feature of soliton systems is the existence of a recursion operator that generates higher symmetries from lower ones.

Thus, we shall consider the Schrödinger equation (1.1) in two dimensions and establish conditions on the potential $V(x,y)$ for it to have one or more symmetries depending on first and second derivatives of the wave function ψ. We shall show that the same conditions imply the existence of a recursion operator.

In Sec. II we formulate the problem of finding Lie point symmetries and generalized symmetries of the linear Schrödinger equation in E_2 with an arbitrary potential. We use the formalism of evolutionary vector fields[33] and their prolongations. Section III is devoted to first-order symmetries, i.e., Lie transformations depending only on x,y,u,u_x,u_y. They turn out to be point symmetries and exist only if the potential is invariant under rotations about some point, or translations in some direction. In Sec. IV we find all second-order generalized symmetries. Generalized symmetries in classical and quantum mechanics were already introduced by Anderson *et al.*[31,34] and Fokas *et al.*[28–30] Here we perform a systematic study and in particular show that second-order symmetries exist if and only if the Schrödinger equation allows the separation of variables. The simplest superintegrable systems are introduced in Sec. V. They are required to have one first-order and one second-order symmetry. It turns out that four such systems exist with potential $\alpha r^{-1}, \omega^2 r^2, \alpha x^{-2}$, and αx, respectively. The study of superintegrable systems is completed in Sec. VI, where all potentials allowing two second-order symmetries are obtained. Four classes of such Schrödinger equations exist, each allowing separation of variables in at least two coordinate systems. Finally, in Sec. VII we show that a recursion operator, generating new symmetries from known ones can be identified with a linear operator commuting with the Hamiltonian.

II. FORMULATION OF THE PROBLEM

Our aim is to study the Lie point symmetries and generalized symmetries of the two-dimensional Schrödinger equation (1.1). First of all we notice that the stationary Schrödinger equation can be treated as a real equation since the real and imaginary parts of the wave function ψ satisfy the same equation. On the other hand, it is sometimes convenient to use complex independent variables. Thus, we rewrite Eq. (1.1) as

$$-\tfrac{1}{2}(u_{xx}+u_{yy})+(V-E)u=0, \quad \psi=u=u_1+iu_2, \tag{2.1}$$

or

$$S=u_{z\bar{z}}-Ru=0, \quad R=\tfrac{1}{2}(V(z,\bar{z})-E)$$
$$z=x+iy, \quad \bar{z}=x-iy. \tag{2.2}$$

The function $u(z,\bar{z})=\overline{u(z,\bar{z})}$ represents both the real and imaginary parts of ψ.

To find symmetries we shall use the formalism of evolutionary vector fields.[33] This allows us to treat Lie point symmetries, and generalized symmetries, on the same footing. An nth order symmetry is given by a vector field

$$\hat{W}=Q(z,\bar{z},u,u_z,u_{\bar{z}},u_{zz},u_{z\bar{z}},u_{\bar{z}\bar{z}},\ldots)\partial_u, \tag{2.3}$$

where the characteristic Q of the symmetry depends on derivatives up to order n. The condition for $\hat{W}$ to generate a symmetry of the equation, i.e., generate transformations taking solutions into solutions, is

$$pr^{(2)}\hat{W}S|_{S=0}=0 \tag{2.4}$$

with S given in Eq. (2.2). The vector field $\hat{W}$ acts only on functions of u, its second prolongation acts on functions of $u,u_z,u_{\bar{z}},u_{zz},u_{z\bar{z}}$ and $u_{\bar{z}\bar{z}}$. The part of the prolongation needed to act on Eq. (2.2) is

$$pr^{(2)}\hat{W}=\hat{W}+D_zD_{\bar{z}}Q\partial_{u_{z\bar{z}}}, \tag{2.5}$$

where D_z is the total derivative. The vector field $\hat{W}$ will generate point symmetries if it is of first order and moreover satisfies

$$Q=\phi(z,\bar{z},u)-\xi(z,\bar{z},u)u_z-\overline{\xi}(z,\bar{z},u)u_{\bar{z}},\quad \phi(z,\bar{z},u)=\overline{\phi}(z,\bar{z},u). \tag{2.6}$$

Equation (2.4) provides a set of determining equations for the function Q. Indeed, Q depends on derivatives up to order n. The prolongations introduce derivatives of order $n+1$ and $n+2$. All mixed derivatives like $u_{z\bar{z}},u_{zz\bar{z}},u_{z\bar{z}\bar{z}},\ldots$ must be eliminated, using Eq. (2.2) and its differential consequences. The coefficients of terms involving $u_{(n+1)z},u_{(n+1)\bar{z}},u_{(n+2)z},u_{(n+2)\bar{z}}$ must vanish separately. This will determine the dependence of Q on the highest derivatives. Proceeding in this manner we obtain an overdetermined system of linear partial differential equations for the function Q. Once Q is determined we obtain a flow

$$\frac{d}{d\lambda}\begin{pmatrix}u_1\\u_2\end{pmatrix}=\begin{pmatrix}Q_1\\Q_2\end{pmatrix} \tag{2.7}$$

that is compatible with the Schrödinger equation. In Eq. (2.7) λ is a group parameter and Q_1 and Q_2 are general solutions of the same determining equations, i.e., they differ only by possibly different choices of integration constants. The condition $Q_1=Q_2=0$ will provide us with invariant solutions of the Schrödinger equation. More generally, we can solve Eq. (2.7) together with the Schrödinger equation. Each flow (2.7) will provide us with a one-parameter family of solutions of the Schrödinger equation.

Some obvious symmetries exist for any (real) potential $V(x,y)$. They are

$$\begin{pmatrix}Q_1\\Q_2\end{pmatrix}=\begin{pmatrix}a&b\\c&d\end{pmatrix}\begin{pmatrix}u_1\\u_2\end{pmatrix}+\begin{pmatrix}h_1(x,y)\\h_2(x,y)\end{pmatrix}, \tag{2.8}$$

where a, b, c and d are arbitrary constants and h_1 and h_2 are real solutions of the Schrödinger equation. The constant matrix expresses the fact that u_1 and u_2 solve the same linear homogeneous equation, the functions $h_{1,2}$ express the linear superposition formula.

Our aim in this article is to find all first- and second-order Lie symmetries and the potentials that allow them. We shall classify the potentials under the Euclidean group $E(2)$, which leaves the Schrödinger equation form invariant. We shall need the Euclidean Lie algebra $e(2)$ with basis

$$L_3=y\partial_x-x\partial_y,\quad P_1=\partial_x,\quad P_2=\partial_y. \tag{2.9}$$

At an intermediate stage we shall use complex variables, in which the Schrödinger equation is Eq. (2.2). The determining equation (2.4) can be rewritten as

$$D_{z\bar{z}}Q - RQ|_{u_{z\bar{z}}=Ru} = 0. \tag{2.10}$$

The type of Lie symmetries that we obtain from Eq. (2.10) depends on the restrictions we impose on the characteristic functions Q_1 and Q_2. In this article we impose the following restrictions:

(1) Q_1 and Q_2 depend on derivatives up to second order only.
(2) The symmetries are energy independent, i.e., Q_1 and Q_2 are the same for all energies E.

The second condition is in keeping with the general philosophy of quantum mechanics. The Schrödinger equation is viewed as an eigenvalue problem and symmetries depend on the Hamiltonian, but not on the individual energy level.

We shall see in the following, that the functions Q_1 and Q_2 are linear in u_1 and u_2 and their derivatives. This makes it possible to write

$$\begin{pmatrix} Q_1 \\ Q_2 \end{pmatrix} = M_1 \hat{X} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + M_2 \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} + \begin{pmatrix} h_1(x,y) \\ h_2(x,y) \end{pmatrix}, \tag{2.11}$$

where M_1 and M_2 are arbitrary constant matrices, h_1 and h_2 are arbitrary real solutions of the Schrödinger equation, and $\hat{X}$ is a differential operator (to be determined in the following). Moreover, we shall show that the operator $\hat{X}$ commutes with the Hamiltonian

$$[H, \hat{X}] = 0. \tag{2.12}$$

III. FIRST-ORDER SYMMETRIES

Let us now consider the determining equation (2.10) with

$$Q = Q(z, \bar{z}, u, u_z, u_{\bar{z}}). \tag{3.1}$$

The expression $D_{z\bar{z}}Q$ will involve third-order terms $u_{zz\bar{z}}$ and $u_{z\bar{z}\bar{z}}$, but those are reduced to first-order ones, using the Schrödinger equation (2.2). From the coefficients of u_{zz} $u_{\bar{z}\bar{z}}$, u_{zz} and $u_{\bar{z}\bar{z}}$ we obtain

$$Q = \alpha(z) u_z + \bar{\alpha}(\bar{z}) u_{\bar{z}} + \phi(z, \bar{z}, u) \tag{3.2}$$

with ϕ real. The dependence on the first derivatives is thus linear. From the coefficients of u_z $u_{\bar{z}}$, u_z and $u_{\bar{z}}$ in Eq. (2.10) we now obtain

$$Q = \alpha(z) u_z + \bar{\alpha}(\bar{z}) u_{\bar{z}} + \gamma u + h(z, \bar{z}), \tag{3.3}$$

where $\gamma = \bar{\gamma}$ is a constant and h is a real function. Putting (3.3) back into Eq. (2.10) we obtain

$$\alpha_z R + \alpha R_z + \bar{\alpha}_{\bar{z}} R + \bar{\alpha} R_{\bar{z}} = 0, \tag{3.4}$$

$$h_{z\bar{z}} - Rh = 0. \tag{3.5}$$

Thus, $h(z, \bar{z}) = h(x,y)$ is an arbitrary (real) solution of the Schrödinger equation [see Eq. (2.11)].

In real variables Eq. (3.4) with the analyticity conditions $\alpha_{\bar{z}} = 0$, $\bar{\alpha}_z = 0$ implies

$$(\alpha_{1x} + \alpha_{2y})(V - E) + \alpha_1 V_x + \alpha_2 V_y = 0, \tag{3.6}$$

$$\alpha_{1x} - \alpha_{2y} = 0, \quad \alpha_{2x} + \alpha_{1y} = 0, \tag{3.7}$$

where

$$\alpha_1(x,y)=\mathrm{Re}\,\alpha, \quad \alpha_2(x,y)=\mathrm{Im}\,\alpha.$$

Up to now the symmetry Q and hence the functions α_1 and α_2 were allowed to depend on the energy E. Now, in keeping with the philosophy of quantum mechanics, we request that the symmetries be the same for all energies. This implies

$$\alpha_{1x}+\alpha_{2y}=0 \tag{3.8}$$

in Eq. (3.6). Together with the Cauchy–Riemann equations (3.7) this allows us to solve the system (3.6)–(3.8) completely. We obtain

$$\alpha_1=\alpha y+\beta, \quad \alpha_2=-\alpha x+\gamma, \tag{3.9}$$

where α, β, and γ are real constants and the potential $V(x,y)$ satisfies

$$[\alpha(y\partial_x-x\partial_y)+\beta\partial_x+\gamma\partial_y]V(x,y)=0. \tag{3.10}$$

The solution of Eq. (3.10) is

$$V=V(\xi), \quad \xi=\tfrac{1}{2}\alpha(x^2+y^2)-\gamma x+\beta y. \tag{3.11}$$

For $\alpha\neq 0$ we use a translation to annul β and γ. For $\alpha=0$ we rotate to put $\beta=0$.

We can sum up the results as a theorem.

Theorem 1: *First-order energy independent Lie symmetries of the Schrödinger equation (1.1) exist if and only if the potential allows a geometric symmetry, i.e., satisfies Eq. (3.10). The flow corresponding to this symmetry is*

$$\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}_\lambda = (M_1\hat{X}+M_2)\begin{pmatrix} u_1 \\ u_2 \end{pmatrix}+\begin{pmatrix} h_1(x,y) \\ h_2(x,y) \end{pmatrix} \tag{3.12}$$

with

$$\hat{X}=\alpha L_3+\beta P_1+\gamma P_2, \quad \psi=u_1+iu_2. \tag{3.13}$$

$\alpha,\beta,\gamma\in R$, $M_1,M_2\in R^{(2\times 2)}$, and h_1, h_2 are real solutions of the Schrödinger equation.

Theorem 1 states that all first-order symmetries are hydrodynamic type[35,36] symmetries. It gives the precise relation between Lie symmetries of the Schrödinger equation and first-order operators, commuting with the Hamiltonian. Both are just manifestations of rotational, or translational symmetry of the potential. Equations (3.12) and (3.13) define Lie point symmetries if M_1 and M_2 are diagonal.

IV. SECOND-ORDER SYMMETRIES

A. The determining equations and general form of the symmetry

We again start from Eq. (2.10), this time with

$$Q=Q(z,\bar{z},u,u_z,u_{\bar{z}},u_{zz},u_{\bar{z}\bar{z}}) \tag{4.1}$$

[the term $u_{z\bar{z}}$ can be eliminated using the Schrödinger equation (2.2)]. The vanishing of the coefficients of $u_{zzz}u_{\bar{z}\bar{z}\bar{z}}$, u_{zzz}, and $u_{\bar{z}\bar{z}\bar{z}}$ implies that Q must be linear in u_{zz} and $u_{\bar{z}\bar{z}}$. The coefficients of $u_{zz}u_{\bar{z}\bar{z}}$, u_{zz}, and $u_{\bar{z}\bar{z}}$ must also vanish and we obtain that Q is linear in all derivatives. Substituting back into (2.10) we require that the coefficients of $u_zu_{\bar{z}}$, u_z, $u_{\bar{z}}$ and 1 must vanish separately. Finally, we obtain

$$Q=A(z)u_{zz}+\overline{A}(\overline{z})u_{\overline{z}\overline{z}}+B(z)u_z+\overline{B}(\overline{z})u_{\overline{z}}+C(z,\overline{z})u+h(z,\overline{z}),$$
$$C(z,\overline{z})=\overline{C(z,\overline{z})},\quad h(z,\overline{z})=\overline{h(z,\overline{z})} \tag{4.2}$$

with

$$RA_z+2AR_z+C_{\overline{z}}=0,$$
$$R\overline{A}_{\overline{z}}+2\overline{A}R_{\overline{z}}+C_z=0, \tag{4.3}$$

$$C_{z\overline{z}}+(B_z+\overline{B}_{\overline{z}})R+BR_z+\overline{B}R_{\overline{z}}+A_zR_z+\overline{A}_{\overline{z}}R_{\overline{z}}+AR_{zz}+\overline{A}R_{\overline{z}\overline{z}}=0, \tag{4.4}$$

$$h_{z\overline{z}}-Rh=0. \tag{4.5}$$

The function h just represents the linear superposition principle. Equations (4.3) and (4.4) must be solved. To do this we return to real variables, putting

$$\mathrm{Re}\,A=2a_1,\quad \mathrm{Im}\,A=2a_2,\quad \mathrm{Re}\,B=b_1,\quad \mathrm{Im}\,B=b_2.$$

We now have

$$Q=a_1(u_{xx}-u_{yy})+2a_2u_{xy}+b_1u_x+b_2u_y+C(x,y)u+h(x,y). \tag{4.6}$$

Analyticity imposes the Cauchy–Riemann conditions on the functions (a_1,a_2) and (b_1,b_2), i.e.,

$$a_{1,x}=a_{2,y},\quad a_{1y}=-a_{2,x}, \tag{4.7}$$

$$b_{1,x}=b_{2,y},\quad b_{1y}=-b_{2,x}. \tag{4.8}$$

The function $C(x,y)$ is determined by Eq. (4.3),

$$C_x=-(V-E)(a_{1x}+a_{2y})-2a_1V_x-2a_2V_y,$$
$$C_y=-(V-E)(a_{1y}-a_{2x})-2a_2V_x+2a_1V_y. \tag{4.9}$$

The compatibility condition for Eq. (4.9) is

$$2[(V-E)a_1]_{xy}-(a_2V_x)_x+(a_2V_y)_y=0. \tag{4.10}$$

We now request that a_1 and a_2 be energy independent. This implies

$$a_{1,x\,y}=0. \tag{4.11}$$

Combining Eqs. (4.11) and (4.7), we obtain

$$a_1=-\tfrac{1}{2}a(x^2-y^2)+by+cx+d,$$
$$a_2=-axy-bx+cy+e, \tag{4.12}$$

where $a,\ldots,e$ are real constants.

In Eq. (4.4) we eliminate $C_{z\overline{z}}$ using Eq. (4.3). We set the energy-dependent and energy-independent parts equal to zero separately and obtain

$$b_1=-ax+\alpha y+\beta+c,$$
$$b_2=-ay-\alpha x+\gamma-b, \tag{4.13}$$

where α, β, and γ are constants and

$$[\alpha(y\partial_x - x\partial_y) + \beta\partial_x + \gamma\partial_y]V = 0. \tag{4.14}$$

Equation (4.14) is precisely the condition (3.10) for a first-order symmetry to exist. We are interested in the most general potential for which one second-order symmetry exists. Hence, we require Eq. (4.14) to be satisfied trivially, and put

$$\alpha = \beta = \gamma = 0. \tag{4.15}$$

We now rewrite Eq. (4.2) for Q as

$$\begin{aligned} Q = \{&aL_3^2 + b(L_3P_1 + P_1L_3) + c(L_3P_2 + P_2L_3) + d(P_1^2 - P_2^2) \\ &+ 2eP_1P_2 + \phi(x,y)\}u + h(x,y) \end{aligned} \tag{4.16}$$

with

$$\begin{aligned} \phi_x &= -2(ay^2 + 2by + d)V_x + 2(axy + bx - cy - e)V_y, \\ \phi_y &= 2(axy + bx - cy - e)V_x + 2(-ax^2 + 2cx + d)V_y. \end{aligned} \tag{4.17}$$

The compatibility condition for Eq. (4.17) gives us the condition on the potential, necessary and sufficient for a second-order symmetry to exist, namely

$$\begin{aligned} &(-axy - bx + cy + e)(V_{xx} - V_{yy}) + [a(x^2 - y^2) - 2by - 2cx - 2d]V_{xy} \\ &\quad - 3(ay + b)V_x + 3(ax - c)V_y = 0. \end{aligned} \tag{4.18}$$

Now let us consider a second-order operator $\hat{X}$, the differential part of which lies in the enveloping algebra of the Euclidean Lie algebra $e(2)$:

$$\begin{aligned} \hat{X} = &aL_3^2 + b(L_3P_1 + P_1L_3) + c(L_3P_2 + P_2L_3) + d(P_1^2 - P_2^2) \\ &+ 2eP_1P_2 + \alpha L_3 + \beta P_1 + \gamma P_2 + \phi(x,y). \end{aligned} \tag{4.19}$$

Let us require that it should commute with the Hamiltonian:

$$[H, \hat{X}] = 0. \tag{4.20}$$

This will be the case if and only if the function ϕ and the potential are related by Eq. (4.17) and the potential satisfies Eq. (4.14) [and the compatibility condition (4.18)].

We have obtained the following theorem.

Theorem 2: *A second-order Lie symmetry (4.1) of the Schrödinger equation (2.1) exists if and only if there exists a second-order operator $\hat{X}$ of the form (4.19) that commutes with the Hamiltonian.*

Finding the operator $\hat{X}$ and the symmetry characteristic Q is thus reduced to solving Eq. (4.18) for the potential and (4.17) for $\phi(x,y)$. This task was already solved in Refs. 6 and 7. For completeness, we review the results in the following.

B. Classification of second-order symmetries

In Sec. IV A we have reduced the set of determining equations for the characteristic Q of a second-order symmetry to Eq. (4.18) for the potential $V(x,y)$.

To solve this equation, we first classify the operators $\hat{X}$ into orbits under the action of the Euclidean group $E(2)$. We also allow linear combinations of $\hat{X}$ with H to ensure that only $P_1^2 - P_2^2$ enters in $\hat{X}$, not P_1^2 and P_2^2 separately.

The result is that the operator $\hat{X}$ can be transformed into precisely one of the following operators.

(1) $a=0$, $b=0$, $c=0$, $d^2+e^2\neq 0$:

$$\hat{X}_C=-\tfrac{1}{2}(P_1^2-P_2^2)+\phi_C(x,y). \tag{4.21}$$

(2) $a\neq 0$, $l^2=(1/a^3)[(2a^2d+b^2-c^2)^2+4(a^2e+bc)^2]^{1/2}=0$:

$$\hat{X}_R=L_3^2+\phi_R(x,y). \tag{4.22}$$

(3) $a=0$, $b^2+c^2\neq 0$:

$$\hat{X}_P=L_3P_2+P_2L_3+\phi_P(x,y). \tag{4.23}$$

(4) $a\neq 0$, $l^2\neq 0$:

$$\hat{X}_E=L_3^2+\frac{l^2}{2}(P_1^2-P_2^2)+\phi_E(x,y), \tag{4.24}$$

where l^2 is given above Eq. (4.22).

We shall call $\hat{X}_C$, $\hat{X}_R$, $\hat{X}_P$ and $\hat{X}_E$ Cartesian, polar, parabolic, and elliptic operators, respectively.

C. Solution of the determining equations

Let us now run through the four representative cases (4.21)–(4.24).

(1) *The Cartesian operator* $\hat{X}_C$. We have $a=b=c=e=0$ in Eqs. (4.16)–(4.19), and also $\alpha=\beta=\gamma=0$. Equation (4.18) reduces to $V_{xy}=0$ and we obtain

$$V=f(x)+g(y), \quad \phi_C=f(x)-g(y), \tag{4.25}$$

where $f(x)$ and $g(y)$ are arbitrary functions.

This is the most general potential that allows the separation of variables in Cartesian coordinates.

(2) *The polar operator* $\hat{X}_R$. We have $a=1$, $b=c=d=e=\alpha=\beta=\gamma=0$. Equation (4.18) simplifies greatly in polar coordinates

$$x=r\cos\vartheta, \quad y=r\sin\vartheta \tag{4.26}$$

and we obtain

$$V=f(r)+\frac{1}{r^2}g(\vartheta), \quad \phi_R=-2g(\vartheta). \tag{4.27}$$

This is the most general potential that allows the separation of variables in polar coordinates.

(3) *The parabolic operator* $\hat{X}_P$. We have $a=b=d=e=\alpha=\beta=\gamma=0, c=1$ in Eqs. (4.16)–(4.19). Equation (4.18) simplifies in parabolic coordinates

$$x=\tfrac{1}{2}(\xi^2-\eta^2), \quad y=\xi\eta \tag{4.28}$$

and we can solve to obtain

$$V=\frac{f(\xi)+g(\eta)}{\xi^2+\eta^2}, \quad \phi_P=\frac{g(\eta)\xi^2-f(\xi)\eta^2}{\xi^2+\eta^2}. \tag{4.29}$$

This is the most general potential that allows separation in parabolic coordinates.

(4) *The elliptic operator* $\hat{X}_E$. We have $a=1, b=c=\alpha=\beta=\gamma=0, d=l^2/2$.

To solve Eq. (4.18) in this case we introduce elliptic coordinates

$$x=l\cosh\rho\cos\sigma, \quad y=l\sinh\rho\sin\sigma \tag{4.30}$$

and obtain

$$V=\frac{f(\sigma)+g(\rho)}{\cos^2\sigma-\cosh^2\rho},$$
$$\phi_E=-l^2\frac{\cosh 2\rho f(\sigma)+\cos 2\sigma g(\rho)}{\cos^2\sigma-\cosh^2\rho}. \tag{4.31}$$

This is the most general potential that allows separation of variables in elliptic coordinates, where l is one half of the interfocal distance.

We have again obtained a general result.

Theorem 3: *A second-order Lie symmetry exists if and only if the potential V(x,y) is such that the Schrödinger equation (1.1) allows the separation of variables in Cartesian, polar, parabolic, or elliptic coordinates.*

The flow corresponding to such a symmetry has the form (2.11) with $\hat{X}$ as in (4.19) with $\alpha=\beta=\gamma=0$. The presence of the constant matrix M_1 in (2.11) indicates that we can choose separation constants differently for the real and imaginary part of the wave function ψ.

V. SUPERINTEGRABLE SYSTEMS WITH ONE FIRST-ORDER AND ONE SECOND-ORDER LIE SYMMETRY

In Sec. III we showed that a first-order symmetry exists if the potential allows a geometric symmetry: rotations or translations. Let us consider the two cases separately and request that a further symmetry, a second-order one, should exist.

A. Potentials invariant under rotations

The potential has the form $V=V(r)$. The first-order symmetry is given by Eq. (3.12), with $\hat{X}=L_3$, i.e., angular momentum. To find a second-order symmetry we must find a nontrivial and independent solution of Eq. (4.18). For $V=V(r)$ Eq. (4.18) reduces to

$$(-cy-bx)\left[V_{rr}+\frac{2}{r}V_r\right]+[-2dxy+e(x^2-y^2)]\frac{1}{r^2}\left(V_{rr}-\frac{1}{r}V_r\right)=0. \tag{5.1}$$

Since V depends only on r and the coefficients in Eq. (5.1) are not rotationally invariant, only two solutions exist, namely

$$\text{(i)} \quad d=e=0, \quad V=\frac{\alpha}{r}, \tag{5.2}$$

$$\text{(ii)} \quad b=c=0, \quad V=\omega^2 r^2. \tag{5.3}$$

For the Coulomb potential we obtain two second-order symmetries, given by

$$\hat{X}_1^C=P_1L_3+L_3P_1-\frac{2\alpha y}{r}, \tag{5.4}$$

$$\hat{X}_2^C=P_2L_3+L_3P_2+\frac{2\alpha x}{r}. \tag{5.5}$$

We have

$$[\hat{X}_1^C,\hat{X}_2^C]=8HL_3,\quad [L_3,\hat{X}_1^C]=\hat{X}_2^C,\quad [L_3,\hat{X}_2^C]=-\hat{X}_1^C. \tag{5.6}$$

The operators (5.4) and (5.5) correspond to the fact that the Schrödinger equation separates in parabolic coordinates with an arbitrary orientation of the axes. Moreover, $\hat{X}_1$ and $\hat{X}_2$ are simply the two components of the Laplace–Runge–Lenz vector.

For the harmonic oscillator we also obtain two second-order symmetries. The corresponding operators are

$$\hat{X}_1^h=-\tfrac{1}{2}P_1^2+\omega^2x^2+\tfrac{1}{2}P_2^2-\omega^2y^2, \tag{5.7}$$

$$\hat{X}_2^h=-P_1P_2+2\omega^2xy, \tag{5.8}$$

satisfying

$$[\hat{X}_1^h,\hat{X}_2^h]=-4\omega^2L_3,\quad [L_3,\hat{X}_1^h]=-2\hat{X}_2^h,\quad [L_3,\hat{X}_2^h]=-2\hat{X}_1^h. \tag{5.9}$$

This result is in full agreement with the Bertrand theorem: The only rotationally invariant potentials in which all finite trajectories are closed are precisely $V=\alpha/r$ and $V=\omega^2r^2$.

B. Potentials invariant under a translation

We have $V=V(x)$ and the first-order Lie symmetry is given by taking $\hat{X}=P_2$. Equation (4.18) for a second-order symmetry reduces to

$$y[-a(xV_{xx}+3V_x)+cV_{xx}]+[-b(xV_{xx}+3V_x)+eV_{xx}]=0. \tag{5.10}$$

The term proportional to y must vanish separately, since V depends only on x.

For $a\neq 0$ we translate x to annul c and obtain

$$V=\frac{\alpha}{x^2},\quad c=e=0. \tag{5.11}$$

The second-order symmetries correspond to a, b, and d and are given by

$$\begin{gathered}\hat{X}_1=L_3^2-2\alpha\frac{y^2}{x^2},\quad \hat{X}_2=L_3P_1+P_1L_3-4\alpha\frac{y}{x^2},\\ \hat{X}_3=-\frac{1}{2}\,P_1^2+\frac{\alpha}{x^2}=H+\frac{1}{2}\,P_2^2.\end{gathered} \tag{5.12}$$

We have the following commutation relations:

$$[P_2,\hat{X}_1]=\hat{X}_2,\quad [P_2,\hat{X}_2]=-4\hat{X}_3,\quad [P_2,\hat{X}_3]=0. \tag{5.13}$$

However, $[\hat{X}_2,\hat{X}_3]=Y$, where Y is a third-order operator. Commuting $\hat{X}_2$ and $\hat{X}_3$ with Y we obtain higher order operators and the Lie algebra is infinite dimensional.

For $a=0$, $c\neq 0$ we obtain

$$V=\alpha x,\quad a=b=0. \tag{5.14}$$

The second-order symmetries correspond to c, d, and e. They are given by the operators

$$\begin{gathered}\hat{X}_1=L_3P_2+P_2L_3+\alpha y^2,\quad \hat{X}_2=P_1P_2+\alpha y,\\ \hat{X}_3=-\tfrac{1}{2}P_1^2+\alpha x=H+\tfrac{1}{2}P_2^2.\end{gathered} \tag{5.15}$$

The commutation relations are

$$[P_2,\hat{X}_1]=2\hat{X}_2,\quad [P_2,\hat{X}_2]=\alpha I,\quad [P_2,\hat{X}_3]=0. \tag{5.16}$$

However $[\hat{X}_1,\hat{X}_3]$ is again a third-order operator and the Lie algebra is infinite dimensional. Let us sum up the results.

Theorem 4: *Precisely four $E(2)$ classes of potentials exist, allowing one first-order Lie symmetry and at least one second-order one. For $V=\omega^2 r^2$ the symmetries $\{L_3,\hat{X}_1,\hat{X}_2,H\}$ form a $u(2)$ algebra. For $V(r)=\alpha/r$, L_3, $\hat{X}_1$ and $\hat{X}_2$ form an $o(3)$, $o(2,1)$ or $e(2)$ algebra for a fixed energy $E<0$, $E>0$, and $E=0$, respectively. For $V=\alpha x^{-2}$ and $V=\alpha x$ the second-order Lie symmetries generate infinite-dimensional Lie algebras.*

VI. SUPERINTEGRABLE SYSTEMS WITH TWO SECOND-ORDER LIE SYMMETRIES

Our starting point will be Theorem 3 of Sec. IV. We will assume that one second-order Lie symmetry is already known. The potential $V(x,y)$ is thus specified up to two functions of one variable each. A second-order operator $\hat{X}_1$ is also specified. We must solve Eq. (4.18) to find a second operator $\hat{X}_2$. The operator $\hat{X}_2$ can be simplified by linear combinations with $\hat{X}_1$ and H. We assume that no first-order symmetry exists, i.e., we have $\alpha=\beta=\gamma=0$ in Eq. (4.19).

We have four cases to consider.

A. A Cartesian operator $\hat{X}_1$

We have $\hat{X}_1=\hat{X}_c$ as in Eq. (4.21). We substitute $V(x,y)=f(x)+g(y)$ into Eq. (4.18) and obtain an equation for X_2, namely:

$$\begin{aligned} &a[xy(f_{xx}-g_{yy})+3(yf_x-xg_y)]+b[x(f_{xx}-g_{yy})+3f_x]\\ &\quad+c[-y(f_{xx}-g_{yy})+3g_y]-e(f_{xx}-g_{yy})=0. \end{aligned} \tag{6.1}$$

Translations do not change the form of $\hat{X}_1$, nor of the potential, so we can use them to simplify Eq. (6.1). Two cases must be distinguished.

(a) $a\neq 0$. We normalize a to $a=1$ and transform $b\to 0, c\to 0$ by translations. The general solution of Eq. (6.1) then yields (for $e=0$)

$$\begin{aligned} V_I&=\omega^2(x^2+y^2)+\frac{\alpha}{x^2}+\frac{\beta}{y^2},\\ \hat{X}_2&=\hat{X}_R=L_3^2-2\left(\frac{\alpha}{\cos^2\phi}+\frac{\beta}{\sin^2\phi}\right). \end{aligned} \tag{6.2}$$

For $e\neq 0$ we would have $\alpha=\beta=0$ in (6.2) and a first-order symmetry exists. The potential V_{I} is the most general one that allows separation of variables in Cartesian and polar coordinates. Moreover, the operator $\hat{X}_2+(l^2/2)\hat{X}_1$ also provides a second-order symmetry. Hence the potential V_{I} also allows separation of variables in elliptic coordinates with an arbitrary focal distance.

(b) $a=0, b^2+c^2\neq 0$. By a translation we set $e=0$. The remaining equation is

$$b[x(f_{xx}-g_{yy})+3f_x]+c[-y(f_{xx}-g_{yy})+3g_y]=0. \tag{6.3}$$

For $b\neq 0, c\neq 0$ the potential V must be linear and hence allows a first-order symmetry.

For $b=0$, $c=1$ we obtain

$$V_{\mathrm{II}}=\omega^2(4x^2+y^2)+\frac{\alpha}{y^2}+\beta x,$$
$$\hat{X}_2=L_3P_2+P_2L_3-4\omega^2xy^2+4\frac{\alpha x}{y^2}-\beta y^2. \tag{6.4}$$

For $b=1$, $c=0$ we obtain an equivalent result [i.e., (6.4)] with x and y interchanged). The potential V_{II} is the most general one that allows separation in Cartesian and (properly oriented) parabolic coordinates.

B. A polar operator $\hat{X}_1$

We have $\hat{X}_1=\hat{X}_R$ as in Eq. (4.22). We substitute the potential (4.27) into Eq. (4.18) and obtain, in polar coordinates,

$$\begin{aligned}&(b\cos\vartheta+c\sin\vartheta)\left[-r^4\left(f_{rr}+\frac{2}{r}f_r\right)+g_{\vartheta\vartheta}-2g\right]+[-b\sin\vartheta+c\cos\vartheta]3g_\vartheta\\&+[-d\sin 2\vartheta+e\cos 2\vartheta]\frac{1}{r}\left[r^4\left(f_{rr}-\frac{1}{r}f_r\right)-(g_{\vartheta\vartheta}-8g)\right]\\&+[d\cos 2\vartheta+e\sin 2\vartheta]\frac{6}{r}g_\vartheta=0.\end{aligned} \tag{6.5}$$

For $b=c=0$ we reobtain the result of Eq. (6.2). Hence we take $b^2+c^2\neq 0$.

The form of the potential and operator X_R is invariant under rotations, so we use them to simplify Eq. (6.5), i.e., to arrange $b=0$, $c=1$.

For $d^2+e^2\neq 0$ we obtain only $V=\mathrm{const}$, so we put $d=e=0$. In this case we obtain

$$V_{\mathrm{III}}=\frac{\alpha}{r}+\frac{1}{r^2}\left(\frac{\beta+\gamma\cos\vartheta}{\sin^2\vartheta}\right)$$
$$\hat{X}_2=L_3P_2+P_2L_3+2\alpha(\cos\vartheta)+2\frac{\gamma(\cos^2\vartheta+1)+2\beta\cos\vartheta}{r\sin^2\vartheta}. \tag{6.6}$$

The potential V_{III} is the most general one for which the Schrödinger equation separates in polar and parabolic coordinates.

C. A parabolic operator $\hat{X}_1$

We have $\hat{X}_1=\hat{X}_P$ as in Eq. (4.23) and the potential is as in Eq. (4.29). Substituting into Eq. (4.18) we obtain an equation for $\hat{X}_2$, namely

$$\begin{aligned}&(\xi^2+\eta^2)^4\{-a[\xi\eta(f''-g'')+3(\eta f'-\xi g')]-2b(f''-g'')\}\\&-8d\{(\xi^2+\eta^2)[+\xi\eta(\xi^2+\eta^2)(f''-g'')-3\eta(3\xi^2-\eta^2)f'-3\xi(\xi^2-3\eta^2)g']\\&-24\xi\eta(\xi^2-\eta^2)(f+g)\}+4e\{(\xi^2+\eta^2)[(\xi^4-\eta^4)(f''-g'')\\&-6\xi(\xi^2-3\eta^2)f'+6\eta(3\xi^2-\eta^2)g']+12(\xi^4-6\xi^2\eta^2+\eta^4)(f+g)\}=0.\end{aligned} \tag{6.7}$$

For $a\neq 0$, or $b\neq 0$ we differentiate Eq. (6.7) nine times with respect to both ξ and η. We find that both f and g must be polynomials of at most order 9.

Substituting back into Eq. (6.7) we find that for $a\neq 0$, $b\neq 0$, we obtain a new potential and invariant

$$V_{\mathrm{IV}}=\frac{2\alpha+\beta\xi+\gamma\eta}{\xi^2+\eta^2}=\frac{\alpha}{r}+\frac{1}{\sqrt{2r}}\left(\beta\cos\frac{\vartheta}{2}+\gamma\sin\frac{\vartheta}{2}\right),$$
$$\hat{X}_2=P_1L_3+L_3P_1+\frac{\beta\eta(\eta^2-\xi^2)+\gamma\xi(\xi^2-\eta^2)-4\alpha\eta\xi}{(\eta^2+\xi^2)}. \tag{6.8}$$

For $a=0$, $b=0$, $(d,e)\neq(0,0)$ we reobtain the result of Eq. (6.4).

D. An elliptic operator X_1

The potential has the form of Eq. (4.31) and $\hat{X}_1=\hat{X}_E$ is given in Eq. (4.24). The second operator $\hat{X}_2$ must also be of elliptic type, otherwise we would have obtained the corresponding system in Secs. VI A, VI B, or VI C. However, if $\hat{X}_1$ and $\hat{X}_2$ are of elliptic type, their difference is of Cartesian type and we reobtain the potential V_{I}. So this case need not be considered.

We have obtained the following result.

Theorem 5: *Precisely four superintegrable systems with two second-order Lie symmetries exist in the Euclidean space E_2. Each of them corresponds to a Schrödinger equation allowing the separation of variables in at least two coordinate systems. They are*

(1)

$$V_{\mathrm{I}}=\omega^2(x^2+y^2)+\frac{\alpha}{x^2}+\frac{\beta}{y^2},$$
$$\hat{X}_1=P_1^2-P_2^2-2\left[\omega^2(x^2-y^2)+\frac{\alpha}{x^2}-\frac{\beta}{y^2}\right],$$
$$\hat{X}_2=L_3^2-2\left(\frac{\alpha}{\cos^2\phi}+\frac{\beta}{\sin^2\phi}\right).$$

The equation separates in Cartesian, polar, and also elliptic coordinates.

(2)

$$V_{\mathrm{II}}=\omega^2(4x^2+y^2)+\frac{\alpha}{y^2}+\beta x,$$
$$\hat{X}_1=P_1^2-P_2^2-2\left[\omega^2(4x^2-y^2)+\beta x-\frac{\alpha}{y^2}\right],$$
$$\hat{X}_2=L_3P_2+P_2L_3-4\,\omega^2 x y^2+\frac{4\alpha x}{y^2}-\beta y^2.$$

The equation separates in Cartesian and parabolic coordinates.

(3)

$$V_{\mathrm{III}}=\frac{\alpha}{r}+\frac{1}{r^2}\left(\frac{\beta+\gamma\cos\vartheta}{\sin^2\vartheta}\right),$$
$$\hat{X}_1=L_3^2-2\left(\frac{\beta+\gamma\cos\vartheta}{\sin^2\vartheta}\right),$$
$$\hat{X}_2=L_3P_2+P_2L_3+2\alpha\cos\vartheta+2\frac{\gamma(\cos^2\vartheta+1)+2\beta\cos\vartheta}{r\sin^2\vartheta}.$$

The equation separates in polar and parabolic coordinates.

(4)

$$V_{\mathrm{IV}}=\frac{2\alpha+\beta\xi+\gamma\eta}{\xi^2+\eta^2}=\frac{\alpha}{r}+\frac{1}{\sqrt{2r}}\left(\beta\cos\frac{\vartheta}{2}+\gamma\sin\frac{\vartheta}{2}\right),$$

$$\hat{X}_1=L_3P_1+P_1L_3+\frac{\beta\eta(\eta^2-\xi^2)+\gamma\xi(\xi^2-\eta^2)-4\alpha\eta\xi}{(\xi^2+\eta^2)},$$

$$\hat{X}_2=L_3P_2+P_2L_3+2\frac{\alpha(\xi^2-\eta^2)+\eta\xi(\gamma\xi-\beta\eta)}{(\xi^2+\eta^2)}.$$

The equation separates in two different parabolic coordinate systems (and in any parabolic system of coordinates).

In other words, a consistent application of second-order Lie symmetries leads to the same result as was obtained 35 years ago in Ref. 6.

VII. RECURSION OPERATORS

In soliton theory, recursion operators are used to obtain infinitely many higher symmetries from one known symmetry. Generally speaking, they exist only for integrable, or linearizable nonlinear equations. A recursion operator L for a differential equation can be defined as a linear operator that takes evolutionary symmetries into new evolutionary symmetries.[33] Thus, consider an equation and an evolutionary symmetry

$$\hat{W}=Q\partial_u. \tag{7.1}$$

The operator L is a recursion operator if

$$\hat{\tilde{W}}=(LQ)\partial_u \tag{7.2}$$

is also a symmetry of the same equation for any given symmetry characteristic Q.

In general, for nonlinear equations, recursion operators are very useful, but are hard to find.

Now let us consider the case of the Schrödinger equation (2.2) and let Q be a characteristic of a symmetry. The operator L will be a recursion operator if we have

$$D_{z\bar{z}}(LQ)-R(LQ)|_{u_{z\bar{z}}=Ru}=0. \tag{7.3}$$

Any linear operator L satisfying the commutation relation

$$[\Sigma,L]=\lambda\Sigma,\quad \Sigma=\partial_{z\bar{z}}-R \tag{7.4}$$

will also satisfy Eq. (7.3) and vice versa. Here λ can be a function of z and $\bar{z}$, or a linear operator.

In order to determine the operator L from Eq. (7.4), we must impose some restrictions, in particular as to the order of the linear operator L.

Let us first consider first-order recursion operators

$$L=A(z,\bar{z})D_z+\bar{A}(z,\bar{z})D_{\bar{z}}+C(z,\bar{z}). \tag{7.5}$$

In keeping with the spirit of this article, we must require that L be the same for all energies E. This implies $\lambda=0$ in Eq. (7.4). But this simply means that L commutes with the Hamiltonian and we find that the recursion operator L coincides with the linear operator $\hat{X}$ of Eqs. (2.11), (2.12) and more specifically (3.13).

A second-order recursion operator will have the form

$$L=A(z,\bar{z})D_z^2+2B(z,\bar{z})D_zD_{\bar{z}}+\bar{A}(z,\bar{z})D_{\bar{z}}^2+C(z,\bar{z})D_z+\bar{C}(z,\bar{z})D_{\bar{z}}+F(z,\bar{z}). \tag{7.6}$$

Condition (7.4), combined with the requirement that L be energy independent, requires $\lambda=0$. Thus, we again find that the recursion operator L satisfies $[H,L]=0$, i.e, coincides with the operator $\hat{X}$ of Eq. (4.19).

VIII. CONCLUSIONS

We have established the exact relation between generalized Lie symmetries of the Schrödinger equation in the Euclidian plane E_2, separability of the Schrödinger equation in configuration space, superintegrable systems in quantum mechanics, and recursion operators in quantum mechanics. More specifically, in this article we have restricted ourselves to second-order symmetries. Work is in progress on nth order energy independent symmetries and on the integrability properties of Schrödinger equation with higher order Lie symmetries. We are also investigating the possibility of obtaining and utilizing symmetries that do depend on the energy.

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Three formulas for the off-diagonal density matrix of a dirac spinor, with an application[a)]

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Expressions for the off-diagonal density matrix of a Dirac spinor in space–time dimensions 2, 3, and 4 are derived. They are used to obtain formulas for the dual potential of a free Dirac current in two, three, and four dimensions of space–time.
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I. INTRODUCTION

In 1954, Louis Michel and I, seeking to describe massive, polarized, spin-$\frac{1}{2}$ particles in terms of solutions of the Dirac equation, derived the following formula for the diagonal density matrix:[1]

$$u(p,s)\otimes u(p,s)^{+}=\tfrac{1}{4}[1+\gamma^5\not{s}][m+\not{p}]\operatorname{sgn}p^0. \tag{1.1}$$

Here, $u(p,s)$ is the solution of the Dirac equation

$$(\not{p}-m)u(p,s)=0 \tag{1.2}$$

of energy momentum, p, and polarization, s, normalized so that

$$u(p,s)^{+}u(p,s)=m\ \operatorname{sgn}p^0. \tag{1.3}$$

The energy momentum, p, satisfies

$$p^2=p\cdot p=(p^0)^2-\vec{p}^2=m^2, \tag{1.4}$$

and the polarization, s, satisfies

$$s\cdot p=0,\quad s^2=-1. \tag{1.5}$$

The notation for the 4×4 Dirac matrices, γ^μ, $\mu=0,1,2,3$, is such that

$$\gamma^\mu\gamma^\nu+\gamma^\nu\gamma^\mu=2g^{\mu\nu};\quad g^{00}=1=-g^{ii},\quad i=1,2,3;\quad g^{ij}=0,\quad i\neq j, \tag{1.6}$$

and

$$\not{a}=a^0\gamma^0-\vec{a}\cdot\vec{\gamma};\quad \gamma^5=i\gamma^0\gamma^1\gamma^2\gamma^3, \tag{1.7}$$

$$(u(p,s)^{+})_\alpha=\sum_{\beta=1}^{4}\overline{(u(p,s))_\beta}A_{\beta\alpha}, \tag{1.8}$$

where A is a Hermitian matrix satisfying

$$A\gamma^\mu A^{-1}=(\gamma^\mu)^*. \tag{1.9}$$

[a)]In memoriam Louis Michel (1923–1999).

An overbar means complex conjugate, and a star means Hermitian adjoint. In the following, specific representations of the γ's will sometimes be used for space–times of dimensions 2, 3, and 4, but the results are independent of the choice of γ's.

Michel and I were attempting to express all physically significant matrix elements of the $u(p,s)$ in terms of the momenta and polarization observables of the particles. For such purposes, it is natural to ask for an off-diagonal version of (1.1), an expression for $u(q,t)\otimes u(p,s)^+$ in terms of the momenta p and q and the corresponding polarization vectors s and t. We found such a formula:

$$u(q,t)\oplus u(p,s)^+ = x\left|\mathrm{tr}\, P(q,t)P(p,s)\right|^{-1/2} P(q,t)P(p,s), \tag{1.10}$$

where

$$P(p,s) = \mathrm{sgn}\, p^0 [1+\gamma^5 \not{s}][m+\not{p}] \tag{1.11}$$

and x is a phase factor. This formula implies immediately

$$u(p,s)^+ u(q,t) = x\left|\mathrm{tr}\, P(q,t)P(p,s)\right|^{-1/2} \mathrm{tr}\,(P(q,t)(P(p,s)) \tag{1.12}$$

and consequently

$$u(q,t)\otimes u(p,s)^+ = u(p,s)^+ u(q,t)[\mathrm{tr}\,[P(q,t)P(p,s)]]^{-1} P(q,t)P(p,s). \tag{1.13}$$

What follows in this article can be regarded as an extended discussion of this formula, (1.13), together with an application arising in quantum field theory. A different line was taken by Jean Nuyts.[2] He fixed the phase of $u(q,t)$ by writing it as a Lorentz transform of $u(p,s)$. His Appendix D contains many of the formulas used in Sec. IV of the present article.

II. TWO-DIMENSIONAL SPACE–TIME

In two-dimensional space–time, the Dirac matrices are 2×2 matrices satisfying

$$\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2g^{\mu\nu}, \quad \mu,\nu = 0,1; \quad g^{00} = +1 = -g^{11}, \quad g^{01} = 0, \tag{2.1}$$

and the Dirac equation reads

$$(-\not{p}+m)u(p) = 0, \tag{2.2}$$

where m is positive and

$$\not{p} = p^0\gamma^0 - p^1\gamma^1. \tag{2.3}$$

The adjoint

$$u(p)^+ = \overline{u(p)}A$$

satisfies

$$u(p)^+(\not{p}+m) = 0. \tag{2.4}$$

To compute $u(q)\otimes u(p)^+$, consider first the special choice of Dirac matrices

$$\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma^1 = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \gamma^5 = \gamma^0\gamma^1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.5}$$

The Dirac equation then says that $u(p)$ lies in the null space of the matrix

$$\begin{Bmatrix} m & -(p^0+p^1) \\ -(p^0-p^1) & m \end{Bmatrix} \tag{2.6}$$

and $u(p)$ is proportional to

$$\begin{pmatrix} p^0+p^1 \\ m \end{pmatrix}. \tag{2.7}$$

A may be chosen as γ^0. The relation $(p^0-p^1)(p^0+p^1)=m^2$ implies that $u(p)$, normalized so that $u(p)^+\gamma^0 u(p)=|p^0|$, may be chosen as

$$u(p)=\frac{1}{\sqrt{2}}\begin{pmatrix} |p^0+p^1|^{1/2} \\ |p^0-p^1|^{1/2}\operatorname{sgn} p^0 \end{pmatrix}. \tag{2.8}$$

Consequently,

$$\begin{aligned} u(q)\otimes u(p)^+ &= \frac{1}{2}\begin{Bmatrix} |(q^0+q^1)(p^0-p^1)^{1/2}\operatorname{sgn} p^0 & |(p^0+p^1)(q^0+q^1)|^{1/2} \\ |(q^0-q^1)(p^0-p^1)|^{1/2}\operatorname{sgn} p^0\operatorname{sgn} q^0 & |(q^0-q^1)(p^0+p^1)|^{1/2}\operatorname{sgn} q^0 \end{Bmatrix} \\ &= \frac{1}{2}\left\{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} u(p)^+u(q)+\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} u(p)^+\gamma^5 u(q)+\gamma^0 u(p)^+\gamma^0 u(q)\right. \\ &\quad \left. -\gamma^1 u(p)^+\gamma^1 u(q)\right\}, \end{aligned} \tag{2.9}$$

where

$$\begin{aligned} u(p)^+u(q) &= \tfrac{1}{2}[|(q^0+q^1)(p^0-p^1)|^{1/2}\operatorname{sgn} p^0+|(q^0-q^1)(p^0+p^1)|^{1/2}\operatorname{sgn} q^0], \\ u(p)^+\gamma^5 u(q) &= \tfrac{1}{2}[|(q^0+q^1)(p^0-p^1)|^{1/2}\operatorname{sgn} p^0-|(q^0-q^1)(p^0+p^1)|^{1/2}\operatorname{sgn} q^0], \\ u(p)^+\gamma^0 u(q) &= \tfrac{1}{2}[|(q^0+q^1)(p^0+p^1)|^{1/2}+|(q^0-q^1)(p^0-p^1)|^{1/2}\operatorname{sgn} p^0\operatorname{sgn} q^0], \\ u(p)^+\gamma^1 u(q) &= \tfrac{1}{2}[|(q^0+q^1)(p^0+p^1)|^{1/2}-|(q^0-q^1)(p^0-p^1)|^{1/2}\operatorname{sgn} p^0\operatorname{sgn} q^0]. \end{aligned}$$

Notice that $u(p)^+u(q)$ is invariant under restricted Lorentz transformations because

$$\begin{aligned} (q^0+q^1)(p^0-p^1) &= q\cdot p+\det\{p,q\}, \\ (q^0-q^1)(p^0+p^1) &= q\cdot p-\det\{p,q\}. \end{aligned} \tag{2.10}$$

This is evident for $u(p)^+u(q)$, up to a sign, because

$$(u(p)^+u(q))^2=\tfrac{1}{4}\operatorname{sgn} p^0\operatorname{sgn} q^0[(p+q)\cdot(p+q)].$$

From (2.9), one gets expressions for the ratios

$$\left[\frac{u(p)^+\gamma^5 u(q)}{u(p)^+u(q)}\right], \quad \left[\frac{u(p)^+\gamma^0 u(q)}{u(p)^+u(q)}\right], \quad \left[\frac{u(p)^+\gamma^1 u(q)}{u(p)^+u(q)}\right],$$

which reduce to tensors in p and q. Consider first

$$\frac{u(p)^+\gamma^5 u(q)}{u(p)^+u(q)}=\frac{[|(q^0+q^1)(p^0-p^1)|^{1/2}\operatorname{sgn}p^0-|(q^0-q^1)(p^0+p^1)|^{1/2}\operatorname{sgn}q^0]}{[|(q^0+q^0)(p^0-p^1)|^{1/2}\operatorname{sgn}p^0+|(q^0-q^1)(p^0+p^1)|^{1/2}\operatorname{sgn}q_0]}.$$

Multiplying numerator and denominator by the numerator one gets for the denominator

$$2\operatorname{sgn}p^0\operatorname{sgn}q^0(q^1p^0-q^0p^1)$$

and for the numerator

$$2\operatorname{sgn}p^0\operatorname{sgn}q^0(p\cdot q-m^2),$$

so

$$\frac{u(p)^+\gamma^5 u(q)}{u(p)^+u(q)}=\frac{(p\cdot q-m^2)}{q^1p^0-q^0p^1}=\frac{(q^1p^0-q^0p^1)}{(p\cdot q+m^2)}. \tag{2.11}$$

The last identity is most easily derived by recognizing that $\det\{p,q\}=q^1p^0-q^0p^1$ and using the multiplication law for determinants. Similar manipulations yield

$$\frac{u(p)^+\gamma^\mu u(q)}{u(p)^+u(q)}=\frac{2m(p+q)^\mu}{(p+q)^2}, \tag{2.12}$$

and hence the desired analog of (1.13) is

$$u(q)\otimes u(p)^+=\frac{u(p)^+u(q)}{2}\left[1+\gamma^5\frac{2\det\{p,q\}}{(p+q)^2}+(\not{p}+\not{q})\frac{2m}{(p+q)^2}\right]. \tag{2.13}$$

When $p=q$, the coefficient of γ^5 vanishes and the formula reduces to the following analog of (1.1):

$$u(p)\otimes u(p)^+=\tfrac{1}{2}[m+\not{p}]\operatorname{sgn}p^0.$$

Equation (2.13) is the main result of this section.

It is easy to see that if one had chosen a different irreducible set of γ^μ, say $\hat{\gamma}^\mu$, and the appropriate corresponding $\hat{A}$, the result (2.13) would have been the same. The argument is standard. Any two irreducible sets of γ's satisfying (2.1) are related by a nonsingular matrix T:

$$\hat{\gamma}^\mu=T^{-1}\gamma^\mu T.$$

Then

$$(\hat{\gamma}^\mu)^*=\hat{A}\hat{\gamma}^\mu\hat{A}^{-1},$$

if $\hat{A}$ is chosen as

$$\hat{A}=T^*AT.$$

The quantity

$$\hat{\mu}(p)=Tu(p)$$

satisfies the Dirac equation in the hatted γ's, and the formula for $\hat{u}(q)\otimes\hat{u}(p)^+$ in the hatted γ's is a consequence of that in the unhatted γ's.

Of course, (2.13) can also be derived directly from the analog of (1.13):

$$u(q)\otimes u(p)^+=u(p)^+u(q)[\operatorname{tr}(P(q)P(p))]^{-1}P(q)P(p) \tag{2.14}$$

where

$$P(p)=[m+\not{p}],$$

because

$$P(q)P(p)=[m^2+m(\not{p}+\not{q})+\not{q}\not{p}]$$

and

$$\not{q}\not{p}=q\cdot p+\gamma^5\det\{p,q\}.$$

There is an additional useful formula for the axial vector, which connects it with the pseudoscalar

$$\begin{aligned} u(p)^+\gamma^5\gamma^\mu u(q)&=\varepsilon^{\mu\nu}u(p)^+\gamma_\nu u(q)\\ &=-\begin{Bmatrix}u(p)^+\gamma^1u(q)\\ u(p)^+\gamma^0u(q)\end{Bmatrix}\\ &=\frac{-2m}{(p-q)^2}u(p)^+\gamma^5u(q)(p^\mu-q^\mu). \end{aligned}\tag{2.15}$$

The proof can be based on (2.9):

$$\frac{u(p)^+\gamma^1u(q)}{u(p)^+\gamma^5u(q)}=\frac{[|(p^0+p^1)(q^0+q^1)|^{1/2}-|(p^0-p^1)(q^0-q^1)|^{1/2}\operatorname{sgn}p^0\operatorname{sgn}q^0]}{[|(q^0+q^1)(p^0-p^1)|^{1/2}\operatorname{sgn}p^0-|(q^0-q^1)(p^0+p^1)|^{1/2}\operatorname{sgn}q^0]}.$$

Multiplying numerator and denominator by

$$[|(q^0+q^1)(p^0-p^1)|^{1/2}\operatorname{sgn}p^0+|(q^0-q^1)p^0-p^1|^{1/2}\operatorname{sgn}q^0],$$

one gets for the denominator

$$2\operatorname{sgn}p^0\operatorname{sgn}q^0(q^1p^0-q^0p^1),$$

while the numerator turns out to be

$$2m\operatorname{sgn}p^0\operatorname{sgn}q^0(p^1+q^1).$$

When the numerator and denominator are multiplied by p^0-q^0, the denominator produces a factor p^1+q^1, leaving

$$\frac{u(p)^+\gamma^1u(q)}{u(p)^+\gamma^5u(q)}=\frac{2m(p^0-q^0)}{(p-q)^2}$$

as required. The argument for

$$\frac{u(p)^+\gamma^0u(q)}{u(p)^+\gamma^5u(q)}=\frac{2m(p^1-q^1)}{(p-q)^2}$$

is similar.

III. THREE-DIMENSIONAL SPACE–TIME

In three-dimensional space–time, as in all linear spaces of odd dimension, the Clifford algebra has two inequivalent irreducible representations. They can be taken as

$$\gamma^0=\begin{Bmatrix}0 & 1\\ 1 & 0\end{Bmatrix},\quad \gamma^1=\begin{Bmatrix}0 & -1\\ 1 & 0\end{Bmatrix},\quad \gamma^2=\begin{Bmatrix}i & 0\\ 0 & -i\end{Bmatrix} \tag{3.1}$$

and the negatives of these. The analog of γ^5 distinguishes these two representations,

$$\tilde{\gamma}^5=-i\gamma^0\gamma^1\gamma^2=\pm 1, \tag{3.2}$$

respectively. In the following, I will work with (3.1) but will indicate the effect of using $-\gamma^\mu$ instead of γ^μ by inserting $\tilde{\gamma}^5$ in appropriate places in the final result.

The solution of the Dirac equation, $u(p)$, lies in the null space of the matrix

$$(-\not{p}+m)=\begin{pmatrix} m+ip^2 & -(p^0+p^1)\\ -(p^0-p^1) & m-ip^2\end{pmatrix}, \tag{3.3}$$

so $u(p)$ is proportional to

$$\begin{pmatrix} p^0+p^1\\ m+ip^2\end{pmatrix}. \tag{3.4}$$

Since

$$|p^0+p^1|^2+|m+ip^2|^2=2p^0(p^0+p^1)=2|p^0||p^0+p^1|,$$

the normalization of (3.3) goes as before, and yields

$$u(p)=\frac{1}{\sqrt{2}}\begin{Bmatrix} |p^0+p^1|^{1/2}\\ |p^0-p^1|^{1/2}\dfrac{(m+ip^2)}{|m+ip^2|}\operatorname{sgn}p^0\end{Bmatrix}. \tag{3.5}$$

The definition of the adjoint spinor is the same as in two dimensions, so

$$\begin{aligned} u(q)\otimes u(p)^+=\frac{1}{2}\Bigg[&\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}u(p)^+u(q)+\gamma^0u(p)^+\gamma^0u(q)\\ &-\gamma^1u(p)^+\gamma^1u(q)-\gamma^2u(p)^+\gamma^2u(q)\Bigg],\end{aligned} \tag{3.6}$$

where

$$\begin{aligned} u(p)^+u(q)=\frac{1}{2}\Bigg[&|(q^0+q^1)(p^0-p^1)|^{1/2}\frac{(m-ip^2)}{|m-ip^2|}\operatorname{sgn}p^0\\ &+|(q^0-q^1)(p^0+p^1)|^{1/2}\frac{(m+iq^2)}{|m+iq^2|}\operatorname{sgn}q^0\Bigg],\end{aligned}$$

$$\begin{aligned} u(p)^+\gamma^0u(q)=\frac{1}{2}\Bigg[&|(q^0+q^1)(p^0+p^1)|^{1/2}\\ &+|(q^0-q^1)|^{1/2}\frac{(m-ip^2)}{|m-ip^2|}\,\frac{(m+iq^2)}{|m+iq^2|}\operatorname{sgn}p^0\operatorname{sgn}q^0\Bigg],\end{aligned} \tag{3.7}$$

$$u(p)^+\gamma^1 u(q)=\frac{1}{2}\Bigg[|(q^0+q^1)(p^0+p^1)|^{1/2} -|(q^0-q^1)(p^0-p^1)|^{1/2}\frac{(m-ip^2)}{|m-ip^2|}\,\frac{(m+iq^2)}{|m+iq^2|}\operatorname{sgn}p^0\operatorname{sgn}q^0\Bigg],$$

$$u(p)^+\gamma^2 u(q)=\frac{i}{2}\Bigg[|(q^0+q^1)(p^0-p^1)|^{1/2}\frac{(m-ip^2)}{|m-ip^2|}\operatorname{sgn}p^0 -|(q^0-q^1)(p^0+p^1)|^{1/2}\frac{(m+iq^2)}{|m+iq^2|}\operatorname{sgn}q^0\Bigg].$$

Since

$$|u(p)^+u(q)|^2=\frac{|(p+q)^2|}{4}, \tag{3.8}$$

$u(p)^+u(q)$ is Lorentz invariant in absolute value, but its phase is not, in contrast to the situation in two dimensions.

The computation of the ratios $u(p)^+\gamma^\mu u(q)[u(p)^+u(q)]^{-1}$ is rather tedious in this special choice of basis, but eventually yields the simple result

$$\frac{u(p)^+\gamma^\mu u(q)}{u(p)^+u(q)}=\frac{2m[p^\mu+q^\mu+(i/m)\tilde{\gamma}^5\epsilon^{\mu\kappa\lambda}q_\kappa p_\lambda]}{(p+q)^2}, \tag{3.9}$$

so

$$u(q)\otimes u(p)^+=\frac{u(p)^+u(q)}{2}\left[1+\frac{2m}{(p+q)^2}\,\gamma_\mu\left(p^\mu+q^\mu+\frac{i}{m}\tilde{\gamma}^5\epsilon^{\mu\kappa\lambda}q_\kappa p_\lambda\right)\right]. \tag{3.10}$$

Here $\epsilon^{\kappa\lambda\mu}$ is totally antisymmetric under permutation of indices and $\epsilon^{012}=1$. Equation (3.9) is the main result of this section.

This result can also be obtained directly from (2.14) with the altered definition $\not{p}=p^0\gamma^0-p^1\gamma^1-p^2\gamma^2$, since,

$$[m+\not{q}][m+\not{p}]=m^2+m(\not{q}+\not{p})+\not{q}\not{p}$$

and

$$\operatorname{tr}P(q)P(p)=2(q\cdot p+m^2)=(p+q)^2$$

as before, but now

$$\not{q}\not{p}=q\cdot p+i\tilde{\gamma}^5\gamma_\mu\epsilon^{\mu\kappa\lambda}q_\kappa p_\lambda\,.$$

IV. FOUR-DIMENSIONAL SPACE–TIME

Here there is only one irreducible representation of the Clifford algebra,

$$\gamma^\mu\gamma^\nu+\gamma^\mu\gamma^\mu=2g^{\mu\nu},\quad \mu,\nu=0,1,2,3,$$

up to equivalence. A standard choice of the γ's is the set of 4×4 matrices:

$$\gamma^0=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \vec{\gamma}=\begin{pmatrix}0&-\vec{\tau}\\\vec{\tau}&0\end{pmatrix},\quad \gamma^5=i\gamma^0\gamma^1\gamma^2\gamma^3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}. \tag{4.1}$$

Then the matrix A that appears in Eq. (1.4) may be taken to be γ^0.

The desired expansion of $u(q,t)\otimes u(p,s)^+$ may be written

$$u(q,t)\otimes u(p,s)^+ = \tfrac{1}{4}[\mathbf{1}u(p,s)^+u(q,t)+\gamma^5 u(p,s)^+\gamma^5 u(q,t)+\gamma_\mu u(p,s)^+\gamma^\mu u(q,t) - \gamma^5\gamma_\mu u(p,s)^+\gamma^5\gamma^\mu u(q,t)+\tfrac{1}{2}\sigma_{\kappa\lambda}u(p,s)^+\sigma^{\kappa\lambda}u(q,t)], \tag{4.2}$$

and, according to Eq. (1.7), the ratios of the coefficients to the first coefficient may be obtained by multiplying out the matrix product $P(q,t)P(p,s)$ and dividing by $\mathrm{tr}(P(q,t)P(p,s))$. This requires a number of identities. For example,

$$P(q,t)=[1+\gamma^5\not{t}][m+\not{q}]=[m+\not{q}+m\gamma^5\not{t}-i\gamma^5\sigma_{\kappa\lambda}t^\kappa q^\lambda] \tag{4.3}$$

because

$$\not{a}\not{b}=a\cdot b-i\sigma_{\mu\nu}a^\mu b^\nu, \tag{4.4}$$

where

$$\sigma_{\mu\nu}=\frac{i}{2}(\gamma_\mu\gamma_\nu-\gamma_\mu\gamma_\nu).$$

On the other hand, to get the product

$$\begin{aligned}P(q,t)P(p,s)=[&m^2+m\not{p}+m^2\gamma^5\not{s}-im\gamma^5\sigma_{\kappa\lambda}s^\mu p^\nu\\ &+m\not{q}+\not{q}\not{p}-\gamma^5\not{q}\not{s}m+i\gamma^5\not{q}\sigma_{\mu\nu}s^\mu p^\nu+m^2\gamma^5\not{t}+m\gamma^5\not{t}\not{p}-m^2\not{t}\not{s}\\ &+im\not{t}\sigma_{\mu\nu}s^\mu p^\nu-im\gamma^5\sigma_{\kappa\lambda}t^\kappa q^\lambda-i\gamma^5\sigma_{\kappa\lambda}\not{p}t^\kappa q^\lambda\\ &-im\sigma_{\kappa\lambda}\not{s}t^\kappa q^\lambda-\sigma_{\kappa\lambda}\sigma_{\mu\nu}t^\kappa q^\lambda s^\mu p^\nu]\end{aligned} \tag{4.5}$$

into the form (4.2) we need the identities

$$\begin{aligned}\gamma_\lambda\sigma_{\mu\nu}&=ig_{\lambda\mu}\gamma_\nu-ig_{\lambda\nu}\gamma_\mu+\epsilon_{\lambda\mu\nu\rho}\gamma^5\gamma^\rho,\\ \sigma_{\kappa\lambda}\gamma_\mu&=ig_{\lambda\mu}\gamma_\kappa-ig_{\kappa\mu}\gamma_\lambda+\epsilon_{\kappa\lambda\mu\rho}\gamma^5\gamma^\rho,\\ \sigma_{\kappa\lambda}\sigma_{\mu\nu}&=g_{\kappa\mu}g_{\lambda\nu}-g_{\kappa\nu}g_{\lambda\mu}+i\epsilon_{\kappa\lambda\mu\nu}\gamma^5-i(g_{\kappa\mu}\sigma_{\lambda\nu}+g_{\lambda\nu}\sigma_{\kappa\mu}-g_{\kappa\nu}\sigma_{\lambda\mu}-g_{\lambda\mu}\sigma_{\kappa\nu}),\\ \gamma^5\sigma_{\kappa\lambda}&=\frac{i}{2}\epsilon_{\kappa\lambda\mu\nu}\sigma^{\mu\nu}.\end{aligned} \tag{4.6}$$

They imply

$$\begin{aligned}i\gamma^5\not{q}\sigma_{\mu\nu}s^\mu p^\nu&=(q\cdot p)\gamma^5\not{s}-(q\cdot s)\gamma^5\not{p}+iq^\lambda s^\mu p^\nu\epsilon_{\lambda\mu\nu\rho}\gamma^\rho,\\ im\not{t}\sigma_{\mu\nu}s^\mu p^\nu&=m[(t\cdot p)\not{s}-(t\cdot s)\not{p}+it^\lambda s^\mu p^\nu\epsilon_{\lambda\mu\nu\rho}\gamma^5\gamma^\rho],\\ -i\gamma^5\sigma_{\kappa\lambda}\not{p}t^\kappa q^\lambda&=(q\cdot p)\gamma^5\not{t}-(t\cdot p)\gamma^5\not{q}-it^\kappa q^\lambda p^\mu\epsilon_{\kappa\lambda\mu\rho}\gamma^\rho,\\ -imt^\kappa q^\lambda s^\mu\sigma_{\kappa\lambda}\gamma_\mu&=m[(s\cdot q)\not{t}-(s\cdot t)\not{q}-it^\kappa q^\lambda s^\mu\epsilon_{\kappa\lambda\mu\rho}\gamma^5\gamma^\rho],\\ \sigma_{\kappa\lambda}\sigma_{\mu\nu}t^\kappa q^\lambda s^\mu p^\nu&=(s\cdot t)(p\cdot q)-(p\cdot t)(s\cdot q)+i\gamma^5\epsilon_{\kappa\lambda\mu\nu}t^\kappa q^\lambda s^\mu p^\nu-i(s\cdot t)\sigma_{\lambda\nu}q^\lambda p^\nu\\ &\quad-i(q\cdot p)\sigma_{\kappa\mu}t^\kappa s^\mu+i(p\cdot t)\sigma_{\lambda\mu}q^\lambda s^\mu+i(q\cdot s)\sigma_{\kappa\nu}t^\kappa p^\nu,\end{aligned} \tag{4.7}$$

so

$$P(q,t)P(p,s)=[(m^2+q\cdot p)(1-s\cdot t)+(t\cdot p)(q\cdot s)]+\gamma^5[-m(q\cdot s)+m(p\cdot t)-i\epsilon_{\kappa\lambda\mu\nu}t^\kappa q^\lambda s^\mu p^\nu]$$
$$+\gamma_\mu[m(p^\mu+q^\mu)(1-s\cdot t)+m((t\cdot p)s^\mu+(s\cdot q)t^\mu)+i\epsilon^\mu_{\rho\sigma\tau}(s+t)^\rho q^\sigma p^\tau]$$
$$+\gamma^5\gamma_\mu[(m^2+(q\cdot p))(s^\mu+t^\mu)-(q\cdot s)p^\mu-(t\cdot p)q^\mu-i\epsilon^\mu_{\rho\sigma\tau}(p+q)^\rho t^\sigma s^\tau]$$
$$+\tfrac{1}{2}\sigma_{\mu\nu}[m\epsilon^{\mu\nu}_{\kappa\lambda}(s^\kappa+t^\kappa)(p^\lambda+q^\lambda)+2i((s\cdot t)q^\mu p^\nu+(m^2+q\cdot p)t^\mu s^\nu-(t\cdot p)q^\mu s^\nu$$
$$+(q\cdot s)p^\mu t^\nu)]. \tag{4.8}$$

Thus

$$u(q,t)\otimes u(p,s)^+=u(p,s)^+u(q,t)\{1+[4((m^2+q\cdot p)(1-s\cdot t)+(t\cdot p)(q\cdot s))]^{-1}$$
$$\times[\gamma^5[-m((q\cdot s)-(p\cdot t))-i\epsilon_{\kappa\lambda\mu\nu}t^\kappa q^\lambda s^\mu p^\nu]+\gamma_\mu[m[(1-s\cdot t)(p^\mu+q^\mu)$$
$$+(t\cdot p)s^\mu+(s\cdot q)t^\mu]+(i\epsilon^\mu_{\rho\sigma\tau}(s+t)^\rho q^\sigma p^\tau)]+\gamma^5\gamma_\mu[(m^2+q\cdot p)(s^\mu+t^\mu)$$
$$-(q\cdot s)p^\mu-(t\cdot p)q^\mu-i(\epsilon^\mu_{\rho\sigma\tau}(s^\rho+t^\rho)q^\sigma p^\tau)]+\tfrac{1}{2}\sigma_{\mu\nu}[m\epsilon^{\mu\nu}_{\kappa\lambda}(s^\kappa+t^\kappa)(p^\lambda+q^\lambda)$$
$$+2i((s\cdot t)q^\mu p^\nu+(m^2+q\cdot p)t^\mu s^\nu-(p\cdot t)q^\mu s^\nu+(q\cdot s)p^\mu t^\nu)]]\}. \tag{4.9}$$

This rather formidable expression, the analog in four dimensions of (2.13) in two-dimensional space–time and (3.9) in three-dimensional space-time, is the main result of this section.

V. AN APPLICATION TO QUANTUM FIELD THEORY

A current, j, in a space–time of n dimensions has a dual, J, which is a totally antisymmetric tensor of rank $n-1$:

$$J_{\mu_1\cdots\mu_{n-1}}=\epsilon_{\mu_1\cdots\mu_n}j^{\mu_n}.$$

In turn, such a J has a dual which is the first rank tensor j:

$$j^{\mu_1}=\frac{1}{(n-1)!}\epsilon^{\mu_1\cdots\mu_n}J_{\mu_2\cdots\mu_n}.$$

When j is conserved

$$\partial_\mu j^\mu=0,$$

J satisfies the differential equation

$$\partial_{\mu_1}\epsilon^{\mu_1\cdots\mu_n}J_{\mu_2\cdots\mu_n}=0. \tag{5.1}$$

In the language of differential forms $J_{\mu_1\cdots\mu_{n-1}}$ defines a differential form

$$J=\sum_{\mu_1\cdots\mu_{n-1}}J_{\mu_1\cdots\mu_{n-1}}dx^{\mu_1}\wedge\cdots\wedge dx^{\mu_{n-1}},$$

and the differential equation (5.1) says that

$$dJ=0, \tag{5.2}$$

i.e., the differential form J is closed. If it happens that $J=dK$, where K is a monomial $n-2$ form, J is then said to be exact. If J is exact, it is automatically closed since $d^2=0$. For brevity, such a form K will be referred to as a dual potential.

In quantum field theory, it is of interest to prove the existence and determine the properties of dual potentials for Dirac currents.[3] Such currents have Fourier representations in which the factor $\exp i(p-q)\cdot x$ is accompanied by the matrix element

$$u(p)^+\gamma^\mu u(q)$$

in two- or three-dimensional space–time and

$$u(p,s)^+\gamma^\mu u(q,t)$$

in four dimensions. The duals of these currents have similar Fourier representations in which the matrix elements

$$\epsilon_{\kappa\mu}u(p)^+\gamma^\mu u(q), \quad \epsilon_{\kappa\lambda\mu}u(p)^+\gamma^\mu u(q),$$

and

$$\epsilon_{\kappa\lambda\mu\nu}u(p,s)^+\gamma^\nu u(q,t)$$

appear, respectively.

For two dimensions, from (2.15) we get

$$\epsilon_{\kappa\lambda}u(p)^+\gamma^\lambda u(q)=-2m[(p-q)^2]^{-1}u(p)^+\gamma^5 u(q)(p-q)_\kappa=K(p,q)i(p-q)_\kappa \tag{5.3}$$

with

$$K(p,q)=2mi[(p-q)^2]^{-1}u(p)^+\gamma^5 u(q).$$

In three dimensions, using (3.10) we get

$$\epsilon_{\kappa\lambda\mu}u(p)^+\gamma^\mu u(q)=2mu(p)^+u(q)[(p+q)^2]^{-1}\left[\epsilon_{\kappa\lambda\mu}(p^\mu+q^\mu)+\frac{i}{m}\tilde{\gamma}^5\epsilon_{\kappa\lambda\mu}\epsilon^\mu_{\rho\sigma}q^\rho p^\sigma\right]. \tag{5.4}$$

Since

$$\epsilon_{\kappa\lambda\mu}\epsilon^\mu_{\rho\sigma}=g_{\kappa\rho}g_{\sigma\lambda}-g_{\kappa\sigma}g_{\lambda\rho} \tag{5.5}$$

and

$$(p^\rho q^\sigma-q^\rho p^\sigma)=\tfrac{1}{2}[(p^\rho-q^\rho)(p^\sigma+q^\sigma)-(p^\sigma-q^\sigma)(p^\rho+q^\rho)], \tag{5.6}$$

the second term in the square brackets can be written as the monomial

$$-\frac{i\tilde{\gamma}^5}{2m}[(p-q)_\kappa(p+q)_\lambda-(p-q)_\lambda(p+q)_\kappa],$$

which is of the form required to make

$$\epsilon_{\kappa\lambda\mu}u(p)^+\gamma^\mu u(q)=(p-q)_\kappa K_\lambda(p,q)-(p-q)_\lambda K_\kappa(p,q). \tag{5.7}$$

The first term, $\epsilon_{\kappa\lambda\mu}(p+q)^\mu$, is the dual of vector $p+q$; it is a bivector describing the two planes perpendicular to $p+q$. [The dual of any monomial p-vector is a monomial $(m-p)$-vector,

if n is the dimension of the vector space.] Since $(p-q)$ is orthogonal to $(p+q)$, because $p^2=q^2=m^2$, we can pick any vector, r, orthogonal to $p+q$ and linearly independent of $p-q$ and write

$$\epsilon_{\kappa\lambda\mu}(p+q)^{\mu}\propto(p-q)_{\kappa}r_{\lambda}-(p-q)_{\lambda}r_{\kappa}.$$

To fix the normalization of r, set the two sides equal and form the scalar product with $(p-q)^{\lambda}$. The result is

$$r_{\kappa}=-\frac{\epsilon_{\kappa\lambda\mu}(p-q)^{\lambda}(p+q)^{\mu}}{(p-q)^2}+b(p-q)_{\kappa}, \tag{5.8}$$

where b is any real-valued function of p and q. The choice $b=0$ makes r orthogonal to both $(p+q)$ and $(p-q)$. Thus

$$K_{\lambda}(p,q)=\frac{i}{(p+q)^2}u(p)^{+}u(q)\left[-\tilde{\gamma}^5(p+q)_{\lambda}+\frac{2mi}{(p-q)^2}\epsilon_{\lambda\rho\sigma}(p-q)^{\rho}(p+q)^{\sigma}\right] \tag{5.9}$$

with the square bracket determined uniquely up to the addition of an arbitrary multiple of $(p-q)$.

In four dimensions we have from (4.9)

$$\epsilon_{\kappa\lambda\mu\nu}u(p,s)^{+}\gamma^{\nu}u(q,t)=\frac{u(p,s)^{+}u(q,t)}{4[(m^2+q\cdot p)(1-s\cdot t)+(t\cdot p)(q\cdot s)]}[m\epsilon_{\kappa\lambda\mu\nu}(1-s\cdot t)(p^{\nu}+q^{\nu})$$
$$+(t\cdot p)s^{\nu}+(s\cdot q)t^{\nu}+i\epsilon_{\kappa\lambda\mu\nu}\epsilon^{\nu}_{\rho\sigma\tau}(s+t)^{\rho}q^{\sigma}p^{\tau}]. \tag{5.10}$$

The last term may be written with the use of the identity

$$\epsilon_{\kappa\lambda\mu\nu}\epsilon^{\nu}_{\rho\sigma\tau}=g_{\kappa\rho}g_{\lambda\sigma}g_{\mu\tau}-g_{\kappa\rho}g_{\lambda\tau}g_{\mu\sigma}$$
$$+g_{\kappa\sigma}g_{\lambda\tau}g_{\mu\rho}-g_{\kappa\sigma}g_{\lambda\rho}g_{\mu\tau}+g_{\kappa\tau}g_{\lambda\rho}g_{\mu\sigma}-g_{\kappa\tau}g_{\lambda\sigma}g_{\mu\rho} \tag{5.11}$$

as

$$i[(s+t)_{\kappa}q_{\lambda}p_{\mu}-(s+t)_{\kappa}q_{\mu}p_{\lambda}+(s+t)_{\lambda}q_{\mu}p_{\kappa}-(s+t)_{\lambda}q_{\kappa}p_{\mu}+(s+t)_{\mu}q_{\kappa}p_{\lambda}-(s+t)_{\mu}q_{\lambda}p_{\kappa}],$$

which is just the trivector $i(s+t)\wedge q\wedge p$ written in components. Since, by (5.6), $q\wedge p=\frac{1}{2}(p+q)\wedge(p-q)$, we have the result that the last term of the square bracket in (5.10) is

$$\frac{i}{2}(p-q)\wedge(s+t)\wedge(p+q).$$

The simplification of the remaining term in (5.10) proceeds analogously to that for (5.4). Note first that $(p-q)$ is orthogonal to $v=(1-s\cdot t)(p+q)+(t\cdot p)s+(s\cdot q)t$. Thus, the trivector $m\epsilon_{\kappa\lambda\mu\nu}[(1-s\cdot t)(p^{\nu}+q^{\nu})+(s\cdot t)^{\nu}+(q\cdot s)t^{\nu}]$ is of the form $(p-q)\wedge r_1\wedge r_2$ where r_1 and r_2 are orthogonal to $(p-q)$ and to $(1-s\cdot t)(p+q)+(t\cdot p)s+(s\cdot q)t$. The bivector $r_1\wedge r_2$ is up to a constant factor just the dual of the bivector $(p-q)\wedge[(1-s\cdot t)(p+q)+(t\cdot p)s+(s\cdot q)t]$ uniquely determined up to the addition of a multiple of that bivector. The constant of proportionality, a, is fixed by contracting the two sides of the identity

$$m\epsilon_{\kappa\lambda\mu\nu}v^{\nu}=a[(p-q)_{\kappa}\tfrac{1}{2}\epsilon_{\lambda\mu\rho\sigma}(p-q)^{\rho}v^{\sigma}$$
$$+(p-q)_{\lambda}\tfrac{1}{2}\epsilon_{\mu\kappa\rho\sigma}(p-q)^{\rho}v^{\sigma}+(p-q)_{\mu}\tfrac{1}{2}\epsilon_{\kappa\lambda p\sigma}(p-q)^{\rho}v^{\sigma}]$$

with $(p-q)^{\kappa}$. The result is

$$a=\frac{2m}{(p-q)^2},$$

so, finally, we have

$$\epsilon_{\kappa\lambda\mu\nu}u(p)^{+}\lambda^{\nu}u(q)=(p-q)_{\kappa}K_{\lambda\mu}+(p-q)_{\lambda}K_{\mu\kappa}+(p-q)_{\mu}K_{\kappa\lambda},$$

where

$$K_{\kappa\lambda}=\frac{u(p,s)^{+}u(q,t)}{4[(m^2+q\cdot p)(1-s\cdot t)+(t\cdot p)(q\cdot s)]}$$
$$\times\left[\frac{i}{2}((s+t)_{\kappa}(p+q)_{\lambda}-(s+t)_{\lambda}(p+q)_{\kappa})+\frac{m}{(p-q)^2}\right.$$
$$\left.\times\epsilon_{\kappa\lambda\rho\sigma}(p-q)^{\rho}((1-s\cdot t)(p+q)+(t\cdot p)s+(s\cdot q)t)^{\sigma}\right]. \tag{5.12}$$

Equations (5.3), (5.9), and (5.12) are the basic input for the quantum field theories described in Ref. 3.

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An expansion of general validity for the diffusive parameters of a charged particle in a zero-point field

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The following calculations provide expressions for the drift velocity and the average diffusion coefficient, applying to diffusion in configuration space of a nonrelativistic charged particle interacting with the zero-point field of stochastic electrodynamics. The particle is assumed to evolve according to a widely popular reduced form of the Braffort–Marshall equation, which is free from runaway solutions, and supposed to be found in stationary conditions, with regard to the average values of physical quantities. The results show an interesting similarity with the equations of quantum mechanics. © *2001 American Institute of Physics.*
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I. INTRODUCTION

This work attempts to find a general expression for the diffusion coefficient of a particle interacting with a zero-point field (ZPF), following a procedure, which has been applied previously to a quasi-free particle in a ZPF.[1] It has been found that the results can be easily extended to cover more general cases of a particle acted upon by a static potential field, if one only wants to calculate the averaged diffusion coefficient in steady conditions. This modified procedure makes use of a representation of the response functions involved by a Fourier integral.

The position of the problem will be recalled very briefly in the following, since it has been displayed more extensively elsewhere.[1–5]

A charged particle in an electromagnetic (em) ZPF is considered, although a ZPF of different nature could also be taken into consideration,[6] embedded in a three-dimensional configuration space. The particle has mass m, electromagnetic charge e (or $-e$), and coordinate $\vec{x}$. Canonical coordinates and conjugated momenta are denoted by q_i, p_i $(i=1,2,3)$, and, since the static potential field $\nu(q_1,q_2,q_3)$ is assumed separable, the subscripts will be omitted throughout, thus reducing the problem to a one-dimensional one.

The full relativistic problem has been treated by Dirac, and Abraham and Lorentz (see Ref. 7 for a review). Here a nonrelativistic limit is taken, so that the following equation of motion results in each coordinate (the dots denoting time derivatives, and the prime derivatives with respect to the spatial coordinate in the argument)

$$-\tau_c\ddot{p}+\dot{p}+\nu'(q)=k(t) \tag{1.1}$$

with $p=m\dot{q}$, τ_c the interaction time related to the classical radius of the particle through the velocity of light c in vacuo,

$$\tau_c=\frac{2}{3}\frac{e^2}{mc^3}=\frac{2}{3}\left(\frac{1}{137}\right)^3 \quad \text{in a.u.,} \tag{1.2}$$

the numbers referring to the electron, $k(t)$ is the electric component of the force from ZPF. Equation (1.1) has often been called the Braffort–Marshall equation.

The stochastic properties of the random electric force $\vec{k}(t)=-e\vec{E}(t)$ have been analyzed in detail by numerous authors.[8–12] The spectrum is given by

$$\phi_{ij}(\omega)=m\hbar\,\tau_c|\omega|^3\delta_{ij}\,, \tag{1.3}$$

where $\hbar$ is Planck constant divided by 2π, ω the frequency, and δ_{ij} denoting the Kronecker symbols. Then the autocorrelation function of the electric force results

$$\phi_{ij}(t-s)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\omega\;\phi_{ij}(\omega)e^{-i\omega(t-s)-\varepsilon|t-s|} \tag{1.4}$$

with $\varepsilon>0$ arbitrarily small.

The next step consists of splitting the velocity into a Eulerian plus a Lagrangian component, in the following manner:[3]

$$p(q,t)=p(q)+\tilde{p}(t) \tag{1.5}$$

with $p(q)$ verifying a differential equation

$$-\frac{\tau_c}{m^2}[p(q)^2p''(q)+p(q)p'(q)^2]+\frac{1}{m}p(q)p'(q)+\nu'(q)=g(q), \tag{1.6}$$

$g(q)$ being an arbitrary smooth function, and $\tilde{p}(t)$ verifying the following system of first-order ordinary differential equations, valid to $O(\tau_c^2)$,

$$\left.\begin{aligned}\dot{q}&=\frac{1}{m}[p(q)+\tilde{p}(t)],\\ \dot{\tilde{p}}&=-\left[\frac{1}{m}p'(q)+\beta(q)+\frac{\tau_c^2}{m}\frac{\mathrm{d}}{\mathrm{d}t}\nu''(q)\right]\tilde{p}(t)\\ &\quad-\overline{g}(q)+\left[1-\frac{\tau_c^2}{m}\nu''(q)\right]mb(t).\end{aligned}\right\} \tag{1.7}$$

The symbols are explained in the following equations:

$$\beta(q)=\frac{\tau_c}{m}\nu''(q)+\frac{\tau_c^2}{m^2}p(q)\nu'''(q), \tag{1.8}$$

$$\overline{g}(q)=g(q)+\frac{\tau_c}{m}p(q)g'(q)+O(\tau_c^2), \tag{1.8$'$}$$

$$b(t)=\frac{1}{m\tau_c}\int_t^{+\infty}k(\alpha)\exp\left\{\frac{t-\alpha}{\tau_c}\right\}\mathrm{d}\alpha, \tag{1.8$''$}$$

Now, the splitting (1.5) without further specification is quite arbitrary and meaningless, because both terms on the right-hand side depend, besides their arguments, also upon initial conditions, as pointed out in Refs. 3, 5, and 13–15. However, the explicitation of the dependence upon q and t, respectively, allows to compute their averages by different means, as a function of coordinate q times the average density or as a function of the derivatives of the average density at the point q. This was shown in the quoted references (see especially Ref. 15), where the nonuniqueness of the diffusion operator for a given set of initial conditions was pointed out. It was shown moreover in a specific example that for a given $p(q)$ a precise relation among initial conditions is required in order that the diffusion equation may be attributed with a physical significance, as an equation for the two-time transition probabilities, at arbitrary times.

By substitution of Eq. (1.5) into Eq. (1.1) and considering that $q(t)$ is a function of initial conditions and time, it is possible to obtain a closed equation for $p(q)$, not involving the time nor the random force explicity, by introducing an appropriate separating function $g(q)$ (see Ref. 3 for details).

Then, after an integration with respect to time, the original equation (1.1) has been transformed into the system of coupled first-order differential equations (1.7) for the variables $q(t)$ and $\tilde{p}(t)$. Equations (1.7) look like characteristic equations, and actually they may be reobtained up to $O(\tau_c)$ as characteristic equations from the dissipative Hamilton–Jacobi equation relative to Eq. (1.13) below, which consequently might as well be considered the starting point of this paper, in the place of (1.1).

It will be found convenient to use Refs. 3 and 5, in order to cancel out the memory term in the averaged equation of continuity for the density of particles in configuration space

$$\overline{g}(q) = -mD_0\left[\frac{1}{m}p''(q)+\beta'(q)\right]+O(\tau_c^2), \tag{1.8'''}$$

where D_0 is the averaged diffusion coefficient. More generally, an operator $\hat{D}_q^{\mathrm{tr}}$ acting upon the variable q may be substituted for D_0. System (1.7) can be solved in terms of the function[1,4]

$$\begin{aligned} g(t,s) &= \exp\left\{-\frac{1}{m}\int_s^t p'(q(\alpha))\mathrm{d}\alpha - \int_s^t \beta(q(\alpha))\mathrm{d}\alpha\right\} \\ &\cong \exp\left\{-\frac{1}{m}\int_s^t p'(q(\alpha))\mathrm{d}\alpha - \overline{\beta}(t-s)\right\} \end{aligned} \tag{1.9}$$

the approximate expression being sufficiently accurate for the purposes of this work. The existence of $\overline{\beta}$ is guaranteed under the hypothesis of Birkhoff theorem for the extended system, particle plus ZPF. Thus $\overline{\beta}$ is given by the phase average over the metrically indecomposable invariant set in which the trajectory evolves.[16] For a mixing system, in which correlations vanish for sufficiently large time, $\overline{\beta}$ can be given by Kubo's[17] cumulant expansion in this limit $|t-s|\to\infty$. To $O(\tau_c)$,

$$\overline{\beta} = \frac{\tau_c}{m}\langle \nu''(q)\rangle + O(\tau_c^2). \tag{1.10}$$

From (1.6) and (1.8‴) follows

$$\frac{1}{2m}p(q)^2+\nu(q)+D_0p'(q) = E - \int p(q)\beta(q)\mathrm{d}q - mD_0\beta(q) \tag{1.11}$$

and, therefore, upon differentiating, averaging, and making use of stationarity there follows[1,5]

$$\frac{1}{m}\langle p'(q)^2\rangle + \langle \nu''(q)\rangle = O(\tau_c), \tag{1.12}$$

where $O(\tau_c)$ consists of the smaller terms in (1.11) and of the corrections to the leading constant term D_0—the averaged diffusion coefficient.[1] This assumption will be proved to be self-consistent [see Eqs. (2.8″) and (2.9)]. From (1.12) follows that the system has positive dissipation and therefore is stable given that $\langle[\Re\mathrm{e}p'(q)]^2\rangle < \langle[\Im\mathrm{m}p'(q)]^2\rangle$, and, in particular, for purely imaginary $p(q)$, which entails that the right-hand side (rhs) of (1.10) be real and positive.

Equations (1.7) do not constitute a complete solution for the third-order differential equation (1.1). By computing the derivative of the first equation (1.7), substituting from the second-one and from (1.8″), (1.11) there follows

$$\mathring{\mathring{q}}+\beta(q)\mathring{q}+\frac{1}{m}\nu'(q)=b(t)+O(\tau_c^2) \tag{1.13}$$

which shows that the solutions which are being considered satisfy simultaneously Eqs. (1.1) and (1.13). They also satisfy a fourth order equation proposed by Caldirola [see Ref. 2 Eqs. (1.11a) and (1.11b)], and are exempt from runaway effects, because of the particular choice of boundary conditions.

Equation (1.11) above can be interpreted as the Hamilton–Jacobi equation satisfied by the average motion, augmented with the term [see Ref. 4 Eq. (2.7)], which is proportional to the average density of that part of kinetic energy which depends bilinearly on both components of velocity

$$\int_{-\infty}^{\infty} D_0 p'(q)\langle\delta(q(t)-q)\rangle \mathrm{d}q \approx \int_{-\infty}^{+\infty}\frac{1}{m}\langle p(q(t))\tilde{p}(t)\delta(q(t)-q)\rangle \mathrm{d}q. \tag{1.14}$$

The dissipative terms also can be interpreted as the potential of the average density of dissipative forces, since

$$\int_{-\infty}^{+\infty} m D_0\beta'(q)\langle\delta(q(t)-q)\rangle \mathrm{d}q \approx \int_{-\infty}^{\infty}\langle\beta(q(t))\tilde{p}(t)\delta(q(t)-q)\rangle \mathrm{d}q. \tag{1.15}$$

In the above expressions and in the following the Heaviside function $h(\alpha)$ and the Dirac $\delta(\alpha)$ function of argument α are used.

II. THE DIFFUSION COEFFICIENT

The diffusion coefficient can thus be obtained from the expression in terms of functional integrals over the realizations of the stochastic electric field $\{E(s);-\infty<s\leqslant t\}$.[1–3]

The boundary conditions for the driven process $q(t)$ have been adjusted in such a way that the particle has a fixed coordinate q_0 at the time t_0, while the velocity is supposed to be equilibrated with the stochastic random field.[1–4] There follows the general expression for the diffusion coefficient in the frozen-trajectory approximation (FTA), see Ref. 1,

$$\hat{D}_q(t,t_0)^{\mathrm{FTA}}\langle\delta(q(t)-q)\rangle=\int_0^t \mathrm{d}\tau\left\langle \delta(q(t)-q)e^{-\bar{\beta}(t-\tau)}\int_{-\infty}^{\tau}\mathrm{d}\sigma\int_{-\infty}^{t}\mathrm{d}s\, g(\tau,\sigma)g(\tau,s)\right\rangle \phi_b(s-\sigma), \tag{2.1}$$

the brackets denoting stochastic averages taken over the realizations of the random process $\{k(t');-\infty<t'\leqslant t\}$, and ϕ_b the autocorrelation function of the renormalized random force $b(t)$. The hat stands for an operator notation over the variable q. Averaging both sides of Eq. (2.1) by integration over $\mathrm{d}q$, there results

$$D_0(t,t_0)^{\mathrm{FTA}}=\int_{t_0}^{t}\mathrm{d}\tau\, e^{-\bar{\beta}(t-\tau)}\int_{-\infty}^{\tau}\mathrm{d}\sigma\int_{-\infty}^{t}\mathrm{d}s\langle g(\tau,\sigma)g(\tau,s)\rangle\phi_b(s-\sigma). \tag{2.2}$$

Higher-order terms containing higher derivatives of $\langle\delta(q(t)-q)\rangle$ could be added to this expression, which represents the first term of an expansion of the rhs of (2.1) in powers of the autocorrelation function ϕ_b.[18] In the following the averaged expression (2.2) will be analyzed, although the similar methods could equally be applied to the more refined expression (2.1), as shown in Ref. 1.

To this end it is convenient to represent the function

$$\Phi\langle\tau-\sigma,\tau-s\rangle=\left\langle \exp\left\{-\frac{1}{m}\int_{\sigma}^{\tau}p'(q(\alpha))\mathrm{d}\alpha-\frac{1}{m}\int_{s}^{\tau}p'(q(\alpha))\mathrm{d}\alpha\right\}\right\rangle e^{-\overline{\beta}(\tau-\sigma)h(\tau-\sigma)-\overline{\beta}(\tau-s)h(\tau-s)} \tag{2.3}$$

as a double Fourier integral in the variables $\tau-\sigma$, $\tau-s$. Having assumed stationarity of the physical state of the system, it is defined

$$\begin{aligned}
\Phi(\omega,\tau-s)=&\int_{-\infty}^{0}\mathrm{d}(\tau-\sigma)\left\langle \exp\left\{-\frac{1}{m}\int_{\sigma}^{\tau}p'(q(\alpha))\mathrm{d}\alpha-\frac{1}{m}\int_{s}^{\tau}p'(q(\alpha))\mathrm{d}\alpha\right\}\right\rangle\\
&\times e^{-\overline{\beta}(\tau-s)h(\tau-s)+\iota\omega(\tau-\sigma)}+\int_{0}^{+\infty}\mathrm{d}(\tau-\sigma)\left\langle \exp\left\{-\frac{1}{m}\int_{\sigma}^{\tau}p'(q(\alpha))\mathrm{d}\alpha\right.\right.\\
&\left.\left.-\frac{1}{m}\int_{s}^{\tau}p'(q(\alpha))\mathrm{d}\alpha\right\}\right\rangle e^{-\overline{\beta}(\tau-\sigma)-\overline{\beta}(\tau-s)h((\tau-s)+i\omega(\tau-\sigma)}\\
=&\int_{-\infty}^{0}\mathrm{d}(\tau-\sigma)\left\langle m\frac{\delta q(\sigma)}{\delta\tilde{p}(\tau)}\exp\left\{-\frac{1}{m}\int_{s}^{\tau}p'(q(\alpha))\mathrm{d}\alpha\right\}\right\rangle e^{-\overline{\beta}(\tau-s)h(\tau-s)+\iota\omega(\tau-\sigma)}\\
&+\int_{0}^{+\infty}\mathrm{d}(\tau-\sigma)\left\langle\left(\frac{\delta\tilde{p}(\tau)}{\delta k(\sigma)}\right)^{\mathrm{FTA}}\exp\left\{-\frac{1}{m}\int_{s}^{\tau}p'(q(\alpha))\mathrm{d}\alpha\right\}\right\rangle e^{-\overline{\beta}(\tau-s)h(\tau-s)+\iota\omega(\tau-\sigma)}\\
=&\left\langle m\left(\frac{\delta q}{\delta\tilde{p}}\right)_{-\omega}\exp\left\{-\frac{1}{m}\int_{s}^{\tau}p'(q(\alpha))\mathrm{d}\alpha\right\}\right\rangle e^{-\overline{\beta}(\tau-s)h(\tau-s)}\\
&+\left\langle\left(\frac{\delta\tilde{p}}{\delta k}\right)_{\omega}^{\mathrm{FTA}}\exp\left\{-\frac{1}{m}\int_{s}^{\tau}p'(q(\alpha))\mathrm{d}\alpha\right\}\right\rangle e^{-\overline{\beta}(\tau-s)h(\tau-s)}\\
=&\left\langle m\frac{(\delta q/\delta k)_{-\omega}^{\mathrm{FTA}}}{(\delta\tilde{p}/\delta k)_{-\omega}^{\mathrm{FTA}}}\exp\left\{-\frac{1}{m}\int_{s}^{\tau}p'(q(\alpha))\mathrm{d}\alpha\right\}\right\rangle e^{-\overline{\beta}(\tau-s)h(\tau-s)}\\
&+\left\langle\left(\frac{\delta\tilde{p}}{\delta k}\right)_{\omega}^{\mathrm{FTA}}\exp\left\{-\frac{1}{m}\int_{s}^{\tau}p'(q(\alpha))\mathrm{d}\alpha\right\}\right\rangle e^{-\overline{\beta}(\tau-s)h(\tau-s)}.
\end{aligned} \tag{2.4}$$

Consequently, the Fourier transform $\Phi(\omega,\omega')$ exists if the Fourier transform of the response functions in the FTA exists for position and velocity. $\Phi(\omega,\omega')$ is of course a symmetric function of ω and ω'. The results of the explicit calculations are

$$\begin{aligned}
&\int_{-\infty}^{\tau}\mathrm{d}\sigma\int_{-\infty}^{t}\mathrm{d}s\langle g(\tau,\sigma)g(\tau,s)\rangle\phi_b(s-\sigma)\\
&=-\frac{\hbar\tau_c}{8\pi^3 m}\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_{-\infty}^{+\infty}\mathrm{d}\omega'\int_{0}^{+\infty}\mathrm{d}u\,\frac{u^3}{1+\tau_c^2u^2}\Phi(\omega,\omega')\left\{\frac{1}{\omega+\omega'-\iota\varepsilon}\right.\\
&\times\left(\frac{1}{\omega'-u-\iota\varepsilon}+\frac{1}{\omega'+u-\iota\varepsilon}\right)-\frac{1}{\omega+\omega'-\iota\overline{\beta}}\left(\frac{1}{\omega'-u-\iota\overline{\beta}}+\frac{1}{\omega'+u-\iota\overline{\beta}}\right)\\
&+\frac{1}{\omega+\omega'-\iota\varepsilon}\left(\frac{1}{\omega+u-\iota\varepsilon}+\frac{1}{\omega-u-\iota\varepsilon}\right)-\frac{1}{\omega+\omega'-\iota\overline{\beta}}\left(\frac{1}{\omega+u-\iota\varepsilon}+\frac{1}{\omega-u-\iota\varepsilon}\right)
\end{aligned}$$

$$+\frac{e^{(\iota\omega'-\iota u+\overline{\beta})(t-\tau)}}{\omega+\omega'-\iota\overline{\beta}}\left(\frac{1}{\omega'-u-\iota\overline{\beta}}+\frac{1}{\omega+u-\iota\varepsilon}\right)$$
$$+\frac{e^{(\iota\omega'+\iota u+\overline{\beta})(t-\tau)}}{\omega+\omega'-\iota\overline{\beta}}\left(\frac{1}{\omega'+u-\iota\overline{\beta}}+\frac{1}{\omega-u-\iota\varepsilon}\right)\Bigg\}. \tag{2.5}$$

Since the integral over du in this expression is (for $\varepsilon\to 0$) convergent, using (2.2), there follows, by shifting the path of integration over du from the real to the imaginary axis

$$D_0(t,t_0)^{\mathrm{FTA}}=-\frac{\iota\hbar\tau_c}{4\pi^3 m}\int_{-\infty}^{0}\mathrm{d}\eta\,\frac{\eta^3}{1-\tau_c^2\eta^2}\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_{-\infty}^{+\infty}\mathrm{d}\omega'\,\frac{\Phi(\omega,\omega')}{\omega+\omega'-\iota\overline{\beta}}\,\frac{1-e^{(\iota\omega'+\eta)(t-t_0)}}{\iota\omega'+\eta}$$
$$\times\left(\frac{1}{\iota\omega'+\eta+\overline{\beta}}+\frac{1}{\iota\omega-\eta}\right)-(1-e^{-\overline{\beta}(t-t_0)})\,\frac{\iota\hbar\tau_c}{4\pi^2 m}$$
$$\times\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_{-\infty}^{+\infty}\mathrm{d}\omega'\frac{\Phi(\omega,\omega')|\omega'|^3}{\overline{\beta}(1+\tau_c^2\omega'^2)(\omega+\omega'-\iota\varepsilon)}+O(\overline{\beta}\tau_c). \tag{2.6}$$

Now, the first term is easily proved to be equivalent to that which has been calculated in Ref. 3, Eq. (20). It yields corrections to the diffusion coefficient which produce, by first-order perturbation theory applied to the Hamilton–Jacobi–Yasue–Riccati (HJYR) Eq. (1.11), energy shifts which are the same functional form as the Lamb shifts.[1,3,5]

Using the symmetry properties of the function $\Phi(\omega,\omega')$, the pole term can be rewritten in the following manner, so as to recast the whole expression for $D_0(t,t_0)^{\mathrm{FTA}}$ into the form (see Ref. 1)

$$D_0(t,t_0)^{\mathrm{FTA}}\cong-\langle\Re(t,t_0)\rangle+(1-e^{-\overline{\beta}(t-t_0)})\,\frac{\hbar\tau_c\iota}{8\pi^2 m}\Bigg\{\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_{-\infty}^{+\infty}\mathrm{d}\omega'\frac{\Phi(\omega,\omega')}{\overline{\beta}(\omega+\omega'-\iota\varepsilon)}$$
$$\times\left(\frac{\omega^3}{1+\tau_c^2\omega^2}+\frac{\omega'^3}{1+\tau_c^2\omega'^2}\right)-2\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_{0}^{+\infty}\mathrm{d}\omega'\frac{\Phi(\omega,\omega')}{\overline{\beta}(\omega+\omega'-\iota\varepsilon)}\,\frac{2\omega'^3}{1+\tau_c^2\omega'^2}\Bigg\}$$
$$=-\langle\Re(t,t_0)\rangle+(1-e^{-\overline{\beta}(t-t_0)})\,\frac{\hbar\tau_c\iota}{8\pi^2 m}\Bigg\{\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_{-\infty}^{+\infty}\mathrm{d}\omega'\frac{\Phi(\omega,\omega')}{\overline{\beta}(1-\tau_c^2\omega\omega')}$$
$$\times\left(\frac{\omega^2}{1+\tau_c^2\omega^2}+\frac{\omega'^2}{1+\tau_c^2\omega'^2}-\omega\omega'\right)$$
$$-2\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_{0}^{+\infty}\mathrm{d}\omega'\frac{2\Phi(\omega,\omega')\omega'^3}{\overline{\beta}(\omega+\omega')(1+\tau_c^2\omega'^2)}-2\iota\pi\int_{0}^{+\infty}\mathrm{d}\omega\,\frac{2\Phi(-\omega,\omega)\omega^3}{\overline{\beta}(1+\tau_c^2\omega^2)}\Bigg\}. \tag{2.7}$$

Now, using stationarity, Eqs. (1.10), (1.12), and (2.3), there follows:

$$D_0(t,t_0)^{\mathrm{FTA}} \cong -\langle \Re(t,t_0)\rangle + (1-e^{-\overline{\beta}(t-t_0)})\frac{\hbar\tau_c\iota}{2m}\left\{ -\frac{\frac{1}{m^2}\langle p'(q)^2\rangle}{\frac{\tau_c}{m}\langle \nu''(q)\rangle} - \frac{1}{2\pi^2}\int_{-\infty}^{+\infty} d\omega \right.$$

$$\left. \times 2\int_0^{+\infty} d\omega' \frac{\Phi(\omega,\omega')\omega'^3}{\overline{\beta}(\omega+\omega')(1+\tau_c^2\omega'^2)} - \frac{1}{2\pi} 2\int_0^{+\infty} d\omega \frac{\Phi(-\omega,\omega)\omega^3}{\overline{\beta}(1+\tau_c^2\omega^2)} \right\}$$

$$= -\langle \Re(t,t_0)\rangle + (1-e^{-\overline{\beta}(t-t_0)})\frac{\iota\hbar}{2m} - (1-e^{-\overline{\beta}(t-t_0)})\frac{\iota\hbar}{2\pi^2\langle \nu''(q)\rangle}$$

$$\times \left\{ \int_{-\infty}^{+\infty} d\omega \int_0^{+\infty} d\omega' \, \frac{\Phi(\omega,\omega')\omega'^3}{(\omega+\omega')(1+\tau_c^2\omega'^2)} + \iota\pi \int_0^{+\infty} d\omega \frac{\Phi(-\omega,\omega)\omega^3}{(1+\tau_c^2\omega^2)} \right\}. \tag{2.8}$$

The justification for the substitution

$$\frac{1}{4\pi^2}\int_{-\infty}^{+\infty} d\omega \int_{-\infty}^{+\infty} d\omega' \frac{\Phi(\omega,\omega')}{(1-\tau_c^2\omega\omega')}\left(\frac{\omega^2}{1+\tau_c^2\omega^2} + \frac{\omega'^2}{1+\tau_c^2\omega'^2} - \omega\omega' \right) \to -\frac{1}{m^2}\langle p'(q)^2\rangle \tag{2.8'}$$

is obvious in the limit $\tau_c \to 0$, hence $\overline{\beta}\to 0$. It is only necessary to prove that the left-hand side (lhs) is continuous for $\tau_c \to 0$, so that the limiting value equals the second derivative in the origin of the function (2.3), multiplied by (-1). For $\overline{\beta}$ finite, the second derivative diverges, but nevertheless (2.8′) is valid because the lhs is a continuous function of τ_c. Equation (2.8) has been obtained by dropping all the terms originating from the step function in the definition (2.3).

Thus, two different procedures may be followed.

(a) If $\Phi(\omega,\omega')$ exists in the limit $\tau_c \to 0$, then it is allowed to put $\overline{\beta}=0$ in Eqs. (2.3) and (2.4), thus making $\Phi(\tau-\sigma,\tau-s)$ a smooth function of the arguments. This leads to (2.7) and (2.8) whose range of validity is, strictly speaking

$$\overline{\beta}\tau_\Phi \ll 1 \ll \overline{\beta}(t-t_0),$$

where τ_Φ is the correlation time of $\Phi(\tau-\sigma,\tau-s)$.

Equation (2.8) has been proved under the assumption $\tau_c \to 0$. Therefore, in this limit, three terms survive in the expression for the diffusion coefficient, which are written extensively in the rhs of (2.8).

(b) The discontinuity of the derivatives of $\Phi(\tau-\sigma,\tau-s)$ introduced by (2.3) can be handled by making use of the theory of distributions, thus yielding an equivalent result, as shown below through Eqs. (3.2)–(3.4).

If the support of the spectral function $\Phi(\omega,\omega')$ is entirely contained in the region comprised between the negative semiaxes, then D_0 is purely imaginary positive, because[1,5]

$$D_0(t,t_0)^{\mathrm{FTA}} = -\langle \Re(t,t_0)\rangle + (1-e^{-\overline{\beta}(t-t_0)})\frac{\iota\hbar}{2m} + O(\tau_c). \tag{2.8''}$$

Then every stationary probability distribution can be chosen as a real function of coordinate $P_{\rm st}(q)$. Consequently, $p(q)$ results to be purely imaginary for real q. The average of $(1/m)p'(q)$ then is given by

$$\left\langle \frac{1}{m}p'(q)\right\rangle = D_0\left\langle \frac{\mathrm{d}^2}{\mathrm{d}q^2}\ln P_{\rm st}(q)\right\rangle$$
$$= D_0\int_{-\infty}^{+\infty}\mathrm{d}q\left(\frac{P''_{\rm st}(q)}{P_{\rm st}(q)}-\frac{P'_{\rm st}(q)^2}{P_{\rm st}(q)^2}\right)P_{\rm st}(q)$$
$$= D_0P'_{\rm st}(q)\big|_{-\infty}^{+\infty}-D_0\int_{-\infty}^{+\infty}\mathrm{d}q\,\frac{P'_{\rm st}(q)^2}{P_{\rm st}(q)}. \tag{2.9}$$

Since $P'_{\rm st}(q)$ must vanish in both limits, there follows that $\langle(1/m)p'(q)\rangle$ is purely imaginary with the sign opposite to that of D_0.

Consequently, $\Phi(\omega,\omega')$ is centered inside the region comprised between the negative semiaxes ω, ω', and if it is assumed Gaussian sharply peaked around its center, it can be inferred that with high accuracy

$$\Phi(\omega,\omega')=0 \quad \text{for } \omega \text{ or } \omega'>0. \tag{2.10}$$

Thus, loosely speaking, the remaining terms in Eq. (2.8) can only produce small corrections to the main value represented by (2.8″), since they remain bounded in the limit $\tau_c\to 0$, being proportional to $\hbar/m$.

III. COMMENTS

The averaged diffusion coefficient for a classical Newtonian particle interacting with a ZPF through the Braffort–Marshall equation,[11] which is the nonrelativistic limit of the Dirac equation for a point particle,[7] has been calculated under the assumption of stationarity of the system, making use of a Fourier representation of the response functions involved. These are evaluated in the frozen-trajectory approximation. The present approach, although restricted by the stationarity assumption, is however in some respect more general than the developments followed in Refs. 1 and 5, because the asymptotic expansion of the ZPF correlation function has been avoided, consequently, the results do not suffer from the restriction that the particle oscillation frequencies should be smaller than $1/\tau_c$. Of course, this does not allow to extend the present treatment to the higher frequencies, although the equations that are used are, like Newton's equations, still meaningful beyond that frequency. In fact, the contribution of the pole term to the diffusion coefficient is here evaluated exactly and is given by the second term in the rhs of (2.6), by summing over the whole spectrum of the response functions of the particle.

The main result which has been obtained by the present developments is that, for systems whose response functions have only a narrow frequency band centered around the main frequency, the diffusion coefficient, averaged in configuration space over a stationary state probability density distribution, has the same value independently of the system, *viz.* $i\hbar/2m$ (see Ref. 2). The leading corrections for a small interaction constant τ_c produce corrections to the ''energy'' of the stationary states of the same functional form as the Lamb shifts of quantum electrodynamics.[1,19]

If the wings of the frequency spectrum include the region of positive frequencies ω, ω', they produce small corrections to the main value, which remain bounded and small in the limit $\tau_c\to 0$. This follows readily if the wings have a Lorentzian shape for τ_c and $\overline{\beta}\neq 0$, but they have finite right and left second moments as $\tau_c\to 0$, hence $\overline{\beta}\to 0$.

We proceed now to examine the conditions under which the main term on the rhs of (2.6) is bounded.

(a) Generally speaking, $\Phi(\omega,\omega')$ is the Fourier transform of a linear combination of products of response functions or FTA response functions, therefore it is licit to assume that it is a meromorphic function of both arguments, falling off to zero at infinity. Divergences might occur in the limits $\omega'\to\pm\infty$, because

$$\lim_{\omega'\to\pm\infty}\frac{\Phi(\omega,\omega')|\omega'|^3}{(1+\tau_c^2\omega'^2)(\omega+\omega'-\iota\varepsilon)}=\pm\frac{\Phi(\omega,\omega')}{\tau_c^2}, \tag{3.1}$$

$$\lim_{\omega'\to\pm\infty}\frac{\Phi(\omega,\omega')|\omega'|^3}{\omega+\omega'-\iota\varepsilon}=\pm\Phi(\omega,\omega')\omega'^2. \tag{3.1'}$$

Now, if ω is not a pole

$$\left|\frac{1}{2\pi}\int_{-\infty}^{+\infty}\Phi(\omega,\omega')\mathrm{d}\omega'\right|=|\Phi(\omega,\tau=s)|<+\infty. \tag{3.2}$$

Putting

$$\Phi(\omega,\omega')=\frac{c(\omega)}{\omega'}+\Phi^R(\omega,\omega') \tag{3.3}$$

results in

$$\begin{aligned}\Phi(\omega,t)&=\frac{c(\omega)}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\omega'\frac{e^{-i\omega' t}}{\omega'}+\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\omega'\,\Phi^R(\omega,\omega')e^{-i\omega' t}\\&=-\frac{c(\omega)}{2\pi}\int_{0}^{+\infty}\mathrm{d}\omega'\frac{2\iota\sin\omega' t}{\omega'}+\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}\omega'\,e^{-i\omega' t}\Phi^R(\omega,\omega')\end{aligned} \tag{3.4}$$

with

$$\Phi^R(\omega,\omega')=O\left(\frac{1}{\omega'^2}\right) \tag{3.5}$$

for $\omega'\to\infty$.

Since the first term is discontinuous for $t=0$, while $\Phi(\omega,t)$ is continuous, there follows

$$c(\omega)=0 \tag{3.6}$$

and consequently the integral of (3.1) converges absolutely in both limits $\omega'\to\pm\infty$. However, there appears a proportionality coefficient $(1/\tau_c)^2$ which would allow the integral, though bounded for every τ_c, to diverge as $\tau_c\to 0$.

Now the same argument shows that for $\tau_c=0$, $\omega'\to\pm\infty$,

$$\Phi_0(\omega,\omega')=O\left(\frac{1}{\omega'^4}\right), \tag{3.7}$$

where $\Phi_0(\omega,\omega')$ is the limit of $\Phi(\omega,\omega')$ as $\tau_c\to 0$, hence $\overline{\beta}\to 0$ everywhere in (2.3). There follows that the expression on the rhs of (3.1′) which contains $\Phi_0(\omega,\omega')$ in the place of $\Phi(\omega,\omega')$ converges absolutely in both limits $\omega'\to\pm\infty$, when integrated over $\mathrm{d}\omega'$. There follows that the main integral in the rhs of (2.6) converges absolutely $\forall\tau_c$ in a suitable closed interval $0\leqslant\tau_c\leqslant a$ of the real axis.

Now, if the function $\Phi(\omega,\omega')\to\Phi_0(\omega,\omega')$ uniformly with respect to ω, ω', the integral in question results to be a continuous function of τ_c in the closed interval, and therefore is bounded inside that interval by a quantity independent of τ_c. The continuity is certainly uniform if the support of $\Phi(\omega,\omega';\tau_c)$ is a compact subset of the plane ω, ω'. This compactification can be obtained by introducing a large cutoff maximum frequency, the limiting results for $\tau_c\to 0$ being however independent of that value. For $\tau_c\neq 0$, however, the cutoff dependence may become effective, in the form of a logarithmic divergence (see below).

(b) The introduction of a cutoff maximum frequency can be avoided by defining as before $\Phi_0(\omega,\tau-s)$ as the limiting value of the function $\Phi(\omega,\tau-s,\tau_c)$ as $\beta(q)\to 0$ in Eqs. (1.9) and (1.11) and consequently in (2.3). Then, by assuming $\Phi_0(\omega,\tau-s)$ to be a smooth function of the arguments, it is convenient to evidence the singularity in the second derivative introduced by definition (2.3), by the following ansatz, where the equality must be intended in the sense of distribution theory:[20]

$$\frac{\partial^2}{\partial s^2}\Phi(\omega,\tau-s;\tau_c)=\frac{\partial^2}{\partial s^2}\Phi_0(\omega,\tau-s)+\overline{\beta}\delta(\tau-s)\int_{-\infty}^{+\infty}\Phi_0(\omega,\omega')\frac{\mathrm{d}\omega'}{2\pi} \tag{3.8}$$

which implies

$$\Phi(\omega,\omega';\tau_c)=\Phi_0(\omega,\omega')-\frac{\overline{\beta}}{\omega'^2}\int_{-\infty}^{+\infty}\Phi_0(\omega,\omega'')\frac{\mathrm{d}\omega''}{2\pi}. \tag{3.9}$$

This accounts for terms which are not absolutely integrable at infinity in $-\omega'^2\Phi(\omega,\omega';\tau_c)$, which is the Fourier transform of the second derivative with respect to t of (3.4). By this substitution into Eq. (2.6), taking into account the term denoted by $O(\overline{\beta}\tau_c)$ on the rhs of this equation, there follows:

$$\begin{aligned}D_0(t,t_0)^{\mathrm{FTA}}=(1-e^{-\overline{\beta}(t-t_0)})&\left(\frac{\iota\hbar}{2m}-\frac{\iota\hbar}{2\pi^2\langle\nu''(q)\rangle}\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_0^{+\infty}\mathrm{d}\omega'\frac{\Phi_0(\omega,\omega')\omega'^3}{(1+\tau_c^2\omega'^2)(\omega+\omega'-\iota\varepsilon)}\right.\\&\left.+\frac{\iota\hbar\tau_c}{4\pi^3 m}\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_{-\infty}^{+\infty}\mathrm{d}\omega'\,\Phi_0(\omega,\omega')\frac{\omega\ln|\tau_c\omega|+\frac{\iota\pi}{2}|\omega|}{1+\tau_c^2\omega^2}\right)+\frac{\hbar\tau_c}{4\pi^3 m}\\&\times\int_{-\infty}^{0}\mathrm{d}\eta\frac{\eta^3}{1-\tau_c^2\eta^2}\int_{-\infty}^{+\infty}\mathrm{d}\omega\int_{-\infty}^{+\infty}\mathrm{d}\omega'\,\Phi_0(\omega,\omega')\frac{e^{(i\omega'+\eta)(t-t_0)}-e^{-\overline{\beta}(t-t_0)}}{(\eta+\iota\omega')(\eta+\iota\omega'+\overline{\beta})(\eta-\iota\omega)},\end{aligned} \tag{3.10}$$

which is the same as Eq. (2.8) to $O(\tau_c\ln\tau_c)$ (see Ref. 1), higher order terms having not been thoroughly considered here. The notation $O(\overline{\beta}\tau_c)$ results from taking the limit $\overline{\beta}\to 0$ everywhere in the last term of (2.6): this is appropriate because this term must exactly cancel the equivalent term of the main integral [see Eq. (3.8)], which has therefore consistently been neglected in (2.8). If a cutoff frequency $\omega_m\ll 1/\tau_c$ were introduced as explained in (a), then $\ln 1/\omega_m$ would appear in Eq. (3.10) in the place of $\ln\tau_c$.

The present developments strongly suggest that wavelike properties could be attributed to material particles interacting with a ZPF, beyond the special case of a harmonic oscillator in the ground state (see Ref. 2 and references therein), inasmuch as the diffusing behavior of these particles could be satisfactorily described by equations surprisingly similar to the equations describing quantum mechanical particles in stationary states, provided the detailed spatial dependence of the diffusion coefficient would be neglected.[21] Notice that this dependence can be handled by the same methods, by redefining the various averaged quantities according to Ref. 1

[see Eq. (3.10) therein]. In this paper the basic formulas for the diffusion coefficient have been evaluated using the Fourier transforms of the response functions, thereby taking advantage of their well-known analytical properties.[20]

It may be recalled that similar results were obtained in Refs. 22 and 23 by considering a stochastic process in which the coordinate is driven by a Wiener process through a complex coupling constant, whose value is adjusted ''*ad hoc*.'' The equations of motion are thus obtained from a stationary principle for expectation values of appropriate functionals. The interest in the present developments results from the fact that the equations of motion can be deduced from the Newtonian equation (1.13), which after all, is not in contradiction with electrodynamics.[7,10,11,24–39]

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Computation of Lie transfer maps for perturbed Hamiltonian systems

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Time evolution of a Hamiltonian system can be viewed as a canonical transformation; therefore perturbations, giving rise to near-identity deviations from an unperturbed solution, can be represented by products of Lie transformations, or, together with the unperturbed solution, *Lie transfer maps*. In this paper I broaden the applicability to all perturbed Hamiltonian systems the method of Dragt and Finn and subsequent co-workers, who developed a representation using a product of Lie transformations factored by phase space variable order. In the present paper, perturbation parameters are no longer necessarily associated with the phase space variables; this method treats both ''internal'' and ''external'' perturbations on an equal footing, and a *rank* is assigned to each variable to reflect the degree of perturbation it represents. With the companion program PGLT, analytic development of the Lie transfer maps is relatively easy for many systems.
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I. INTRODUCTION

From a perturbation Hamiltonian, a known unperturbed solution, and a sequence of Lie transformations factored by rank, it is possible to compute a *transfer map* through a particular order in perturbation parameters. This can be viewed as a function giving positions and momenta (generalized coordinates) at the final time as a function of those at the initial time. Upon combining the unperturbed solutions with the Lie transformations, one may call this a *Lie transfer map*. From the map, this function can then be evaluated numerically to propagate the system. Propagation in this way is unlike the two prevalent methods: numerical integration and normal form. Numerical integration requires iterative computation of the right-hand sides of a differential equation over a number of short time steps. Normal form propagation, common in celestial mechanics, requires the derivation of an analytic Hamiltonian that is in some sense close to the original, that is purely secular (independent of coordinates) and thereby represents an averaged motion. Then propagation involves multiplying the time rate of change of the coordinates by the time interval. In contrast to the normal form method, the transfer map method uses the actual Hamiltonian, and does not compute an averaged Hamiltonian. It should be noted that Deprit's[1] application of Lie transformations, widely used in celestial mechanics, was in the context of the computation of the normal form. Although some of his general mathematical results—properties of Lie transformations—are applicable here, our use of these transformations is different.

Dragt and Finn[2] showed that an analytic symplectic map can be written as a product of Lie transformations. Later, Steinberg[3] showed that one need not assume a Hamiltonian system; the solution of any system of ordinary differential equations may be given as a factored product expansion of partial differential operators. A method for computing the transfer maps using Lie transformations for some kinds of perturbations was described by Dragt and Forest.[4] This was expanded to treat Hamiltonian terms linear in the phase space variables by the author.[5,6] The present paper continues in this tradition; like the foregoing papers, it is an example of a *regular perturbation* theory (Ref. 7 Chap. 132; Ref. 8). (This class of methods is called ''naive perturba-

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tion theory'' in Ref. 9, but ''regular perturbation'' is more common, and less pejorative.) It describes a method for computing perturbations of any system for which the unperturbed solution is known, not just linear.

Anticipating the developments of this paper, it is worthwhile to jump to the end and see what results we can expect for a simple problem, that of the perturbed simple harmonic oscillator in one degree of freedom. The Hamiltonian will be

$$\mathcal{H}=(\tfrac{1}{2}\omega_0^2x^2+\tfrac{1}{2}X^2)-\tfrac{1}{4}x^4\mu, \tag{1}$$

with x the coordinate and X its conjugate momentum. The quantity $0<\mu\ll 1$ is the perturbation parameter. In action-angle variables,

$$J=\frac{1}{2\omega_0}(\omega_0^2x^2+X^2), \quad \theta=\arctan\left(\frac{\omega_0 x}{X}\right), \tag{2}$$

$$x=\sqrt{\frac{2J}{\omega_0}}\sin\theta, \quad X=\sqrt{2\omega_0 J}\cos\theta, \tag{3}$$

so that the Hamiltonian is

$$\mathcal{H}=\omega_0 J+\mu J^2\frac{1}{\omega_0^2}\left(\frac{3}{8}-\frac{1}{2}\cos 2\theta+\frac{1}{8}\cos 4\theta\right). \tag{4}$$

For a particle evolving under this Hamiltonian, the position and momentum after some time t may be computed,

$$\begin{aligned}\theta\leftarrow\theta+\phi_0+\mu J\left(\frac{3}{4}\frac{t}{\omega_0^2}+\frac{1}{\omega_0^3}\left(\frac{1}{2}\sin 2\theta-\frac{1}{2}\sin(2\theta+2\phi_0)-\frac{1}{16}\sin 4\theta+\frac{1}{16}\sin(4\theta+4\phi_0)\right)\right),\\ J\leftarrow J+\mu J^2\frac{1}{\omega_0^3}\left(-\frac{1}{2}\cos 2\theta+\frac{1}{2}\cos(2\theta+2\phi_0)+\frac{1}{8}\cos 4\theta-\frac{1}{8}\cos(4\theta+4\phi_0)\right),\end{aligned} \tag{5}$$

with $\phi_0=\omega_0 t$, to first order in the perturbation μ. The details of computing with the Lie transfer maps are addressed in another paper.[10]

Clearly, the quartic harmonic oscillator is not our ultimate goal. More realistic, and complicated problems, such as a satellite orbit, pendulum motion, charged-particle motion through a magnet in a particle accelerator, ray paths of light through a lens in light optics, or a satellite orbit are solvable by this method.

II. LIE TRANSFORMATIONS

With f and g functions on phase space, let the *Lie operator* $:f:$ be defined by the Poisson bracket $:f:g=[f,g]$. A *Lie transformation* is defined as the exponential of a Lie operator:

$$e^{:f:}=\sum_{i=0}^{\infty}\frac{:f:^i}{i!}, \tag{6}$$

and thus

$$e^{:f:}g=g+[f,g]+\tfrac{1}{2}[f,[f,g]]+\cdots. \tag{7}$$

Lie transformations have several interesting properties. For ease of reference, some are repeated here; for details, proofs and other theorems, consult Dragt[11] or Steinberg,[12] which both provide a comprehensive overview of the field. First, each of the Lie transformations is *symplectic*:

if M is the Jacobian matrix of the transformation, $M_{ij}=\partial e^{:f:}\zeta_i/\partial\zeta_j$ in phase space ζ, then $M^TJM=J$, with $J_{ij}=[\zeta_i,\zeta_j]$, a matrix of ones and zeros. When considering numeric calculations, however, the truncation of the Taylor series in (6) or (7) will produce a nonsymplectic transformation. Second, a similarity transformation on a Lie transformation has the effect of transforming the argument of the function,

$$e^{:f:}e^{:g:}e^{:-f:}=e^{:e^{:f:}g:}. \tag{8}$$

The goal of this paper is to show that any perturbed symplectic map can be represented as a factored product of Lie transformations. Dragt[11] showed a similar fact for arbitrary symplectic maps factored by order of phase space variables, and later with Forest[4] how to construct the Lie expressions. In the present paper, the factorization is by order of perturbation; the exact meaning of this will be provided. I will show that the full map of a perturbed system can be written in terms of Lie expressions f and the solution to the unperturbed problem $\mathcal{U}$,

$$\mathcal{M}=\ldots e^{:f_{\Delta+2}:}e^{:f_{\Delta+1}:}e^{:f_{\Delta}:}\mathcal{U}, \tag{9}$$

and describe a method for computing the f_i from the unperturbed $\mathcal{U}$ and Hamiltonian $\mathcal{H}$.

Once the Lie expressions f_i are known, computation of the map for a fixed time interval, including perturbations, is straightforward. One may extend this calculation to any order for which the map has been computed.

III. GRADING: COUNTING PERTURBATIONS

A. Rank

Traditionally, in a perturbation of Taylor series analysis, we use a small quantity, say ϵ, to regulate the consistent computation of terms. By expanding each computation in ϵ properly, we may cutoff the series at a particular order. In this section, we shall make this more rigorous. In particular, we need to generalize to multiple perturbations of different order, and to phase space variables that are themselves perturbations.

Any variable may be assigned a non-negative integer *rank* based on the exponent of the perturbation parameter. This parameter δ accompanies all perturbation quantities; these quantities have a defined rank, a non-negative integer that represents the exponent of the parameter associated with the variable. For example, suppose the variables x and y exist in a system, and have ranks 1 and 3, respectively. Then every instance of x may be viewed as being δx and every instance of y may be viewed as being $\delta^3 y$. This rank will follow the algebra of exponents, e.g., if x is rank 1, then x^2 is rank 2. The rank of a term (product of a constant and variables) is the sum of the individual ranks of the variables.

It needs to be emphasized that, subject to the constraints outlined above, the grading is arbitrary—a given physical system could have several different gradings. However, one would typically give a grade of one to each power of the most significant perturbation(s), two to terms that were approximately their square, etc.

B. Bracket grade

A polynomial that is the sum of terms of different rank does not have a defined rank. However, the space of polynomials may be divided into subspaces according to the the minimum of the ranks of their terms. By this definition, the rank *grades* the space of polynomials, that is, divides it into subspaces S_m for m a non-negative integer, such that $[S_m,S_n]\subseteq S_{m+n}$ for m, $n\geqslant 0$ (see Healy and Dragt,[13] Sec. 4.2.1) provided a particular condition is met: If f and g have defined ranks, then the rank of their Poisson bracket $r([f,g])$ is

$$r([f,g])=r(f)+r(g)-\Delta. \tag{10}$$

The quantity Δ will be called the *bracket grade*; it is a constant non-negative integer, characteristic of the algebra. The bracket grade constraint (10) is equivalent to the statement that the sum of the ranks of the two conjugate phase space variables x_i, X_i are equal for all degrees of freedom i:

$$r(x_i)+r(X_i)=\Delta. \tag{11}$$

To see this, note that $[x_i,X_i]=1$ which has a rank of zero (being a constant), $0=r([x_i,X_i])=r(x_i)+r(X_i)-\Delta$, so $r(x_i)+r(X_i)=\Delta$.

The grading function $\mathcal{G}(f)$ gives the maximum i for which the function f is a member of S_i. It is equal to the rank r for functions in which r has a value (i.e., individual terms). Without ambiguity, one may speak of the rank of a polynomial or function, meaning this grading function. For analytic functions other than polynomials, we can assign a subspace on the basis of the Taylor series approximation to it. In general though, the functions we shall use will be polynomials in the perturbation quantities; any other functions (like sine and cosine) will have nonperturbation variables as arguments. Thus the Lie expressions discussed in Sec. II can be thought of as polynomials representing the perturbation.

We shall need to be able to select terms of a certain rank; let the symbol P_k denote the *projection operator* at rank k; that is, $P_k(x)$ consists of all terms of x at rank k.

A *grading* implies a *percolation* that forms an ideal structure for the Lie algebra which allows us to do perturbation theory; see Ref. 13 for more details. There it is shown that one need not have a grading in order to do perturbation, just a percolation. In fact, the method described there for dealing with inhomogeneous terms in particle accelerator beamline elements is a percolation with no grading. However, with a grading, the symbolic computations are a great deal simpler. The method described in this paper can be used to solve these types of problems (as well as perturbations for many other physical systems) in an easier way.

C. Perturbation operators and Lie transformations

In order to compute the result of a Lie transformation, the Taylor series for the exponential must be stopped at some order. Stopping is permissible if the perturbations become too insignificant to worry about, or the series is finite. Thus we may make the following definition: A Lie operator $\mathcal{O}$ is a *perturbation operator* if for all phase space functions g,

$$\mathcal{G}(\mathcal{O}g)>\mathcal{G}(g), \tag{12}$$

or there is an integer n such that

$$\mathcal{O}^n g=0. \tag{13}$$

The only terms that satisfy the latter condition are those that are linear in the phase space variables. Closely related, a *perturbation transformation* is a Lie transformation that is the exponential of a perturbation operator. These will be used to define perturbations.

Define the *rank raising* of a function, Lie operator or transformation as the amount by which the corresponding Lie operator $:f:$, when applied to another function g, raises the rank, i.e., $\mathcal{G}(\{f,g\})-\mathcal{G}(g)$. According to (10), this means that the rank raising for f is $\mathcal{G}(f)-\Delta$.

The conditions above state that a perturbation transformation $e^{:f:}$ has either positive rank raising or terminates. In the former and more common case, each term in the Taylor series of the exponential (6) becomes less significant or ''higher order,'' and can be safely neglected at some rank. In formal language, we pick an integer n, do our computations in a subspace S_n, and drop terms that are not in S_n, but rather in S_m for $m>n$. In the latter case the Taylor series of the exponential actually terminates; there is some n for which $:f:^n=0$. It has special applications; for example, handling placement errors in a particle accelerator. This requirement means that one of the Poisson brackets in the Taylor series is known to be zero for all arguments to the Lie transformation. There is one way that this can happen: if the function f is linear in the phase-space variables, the series for $e^{:f:}$ will terminate at the second term:

$$e^{:f:} = I + :f: , \tag{14}$$

because a Poisson bracket's action on first-order polynomials is to produce a constant.

In the terminating series case, if the grade of the function is less than the bracket grade $\mathcal{G}(f) < \Delta$, the second term in the Taylor series of the exponential would produce terms of lower rank than the first. While this is mathematically sensible, it corresponds to no physically realistic system and makes computer implementation harder, so it is excluded. Similarly, f could have no perturbations, $\mathcal{G}(f) = 0$ if $\Delta = 0$ and it was linear in the phase space variables. As we are after a perturbation development, however, we shall insist that the grade of f is positive, $\mathcal{G}(f) > 0$.

Thus Lie transformations $e^{:f:}$ acceptable to perturbation theory may be easily summarized. One of these conditions must hold:

(i) The rank raising of f is positive, $\mathcal{G}(f) > \Delta$,
(ii) f is first order in the phase space variables, and $\mathcal{G}(f) \geqslant \Delta > 0$.

D. Internal and external perturbations

For some applications, it is possible to view the perturbations as *internal*, that is, the generalized coordinates themselves represent the perturbation: the deviation of a particle in a magnet from a reference trajectory subjects it to forces unaccounted for in that trajectory (the unperturbed solution); these forces are small if the deviation is. For some applications, such as celestial mechanics, it is possible to view the perturbations as *external*, that is, some parameter(s) (not a generalized coordinate) represent the perturbation: a satellite's orbit around the earth deviates from the Keplerian ellipse (the unperturbed solution) due to the earth's deviation from perfectly spherical mass distribution, a fixed property of the earth. The perturbed harmonic Hamiltonian (1), has an external perturbation, μ, but may also be written with an internal perturbation.

A more precise definition of internal and external perturbation is that if one or more phase space variables have positive rank, then the system has an internal perturbation. If one or more nonphase space variables have positive rank, then it has an external perturbation. A perturbed system may have internal perturbations, external perturbations, or both. A phase space variable with a positive rank represents an internal perturbation; a nonphase space variable with a positive rank represents an external perturbation.

If the perturbation is purely internal and the rank is a count of the phase space variables, that is, each phase space variable has a rank of one, then the rank is merely the *order* of the phase space variables. This is the perturbation counting used in the program MARYLIE.[14]

IV. REPRESENTATIONS OF TRANSFORMATIONS

A. Perturbation transformations

There are a number of representations of a map $\mathcal{M}$ possible. First, any map, not necessarily symplectic, may be described as an explicit list of the transformations of each of the phase space variables. Second, as a Lie transformation $e^{:f:}$; it will always be symplectic. A subclass of this is the *homogeneous Lie transformation*, represented by $e^{:f_n:}$, where n indicates a polynomial homogeneous in rank n.

We now broaden the concept of perturbation transformation in Sec. III C to any representation. Let a map $\mathcal{M}$ be a function of external perturbation(s) $\epsilon_1, \ldots, \epsilon_n$, and acting on phase space, $\mathcal{M}(\epsilon_1, \ldots, \epsilon_n)\zeta$. This map is a perturbation transformation if it is the displaced identity at the rank of each phase space variable with no external perturbations,

$$c_i + \zeta_i = P_{r_i}\mathcal{M}(0,0,\ldots)\zeta_i , \tag{15}$$

where P_n is projection of terms of rank n, for all phase space variables z_i, and c_i is a constant independent of the phase space variables and perturbations.

A Lie transformation that is a perturbation transformation by the definition of Sec. III C is one under this definition as well. If the rank raising of f is positive, the projection of $e^{:f:}$ is the identity. If the rank raising is zero, and f is first order in the phase space variables, this produces the displacement term c_i. Normally, we would only consider a perturbation-dependent displacement, so c_i would be zero.

B. Map factorization

It is possible to represent the perturbations of any analytic symplectic perturbation transformation as the product of homogeneous Lie transformations:

Theorem 1 (Map factorization): Let $\mathcal{M}$ be a perturbation transformation that is analytic and symplectic. Then it may be represented by successive homogeneous Lie transformations

$$\mathcal{M}\zeta=\cdots e^{:f_{\Delta+1}:}e^{:f_{\Delta}:}\zeta \tag{16}$$

or

$$\mathcal{M}\zeta=e^{:g_{\Delta}:}e^{:g_{\Delta+1}:}\cdots\zeta, \tag{17}$$

where Δ is the bracket grade.

Proof: The proof will be for ascending factorization (17); the proof of the descending factorization (16) is similar. Because $\mathcal{M}$ is analytic, it has an explicit representation, a Taylor series in the perturbation parameter(s):

$$\mathcal{M}\zeta_i=P_r(\mathcal{M}\zeta_i)+P_{r_i+1}(\mathcal{M}\zeta_i)+\cdots. \tag{18}$$

The first term on the right-hand side may be removed with the appropriate g_{Δ}. We require

$$e^{:g_{\Delta}:}\zeta_i=P_{r_i}(\mathcal{M}\zeta_i); \tag{19}$$

this is easily solved for g_{Δ} because it is linear in phase space, so $e^{:g_{\Delta}:}\zeta_i=c_i+\zeta_i$ for some constant c_i. With this quantity, we can say

$$e^{:-g_{\Delta}:}\mathcal{M}\zeta_i=c_i+\zeta_i+P_{r_i+1}(\mathcal{M}'\zeta_i)+P_{r_i+2}(\mathcal{M}'\zeta_i)+\cdots, \tag{20}$$

with $\mathcal{M}'=e^{:-g_{\Delta}:}\mathcal{M}$. Call this $\overline{\zeta_i}$, the transformed phase space variable. The Poisson bracket is

$$[\overline{\zeta_i},\overline{\zeta_j}]=[\zeta_i,\zeta_j]+[\zeta_i,P_{r_j+1}(\mathcal{M}'\zeta_j)]+[P_{r_i+1}(\mathcal{M}'\zeta_i),\zeta_j]+\mathcal{O}(\delta^{r_i+r_j-\Delta+2}). \tag{21}$$

By virtue of $\mathcal{M}$ and $e^{:g_{\Delta}:}$ being symplectic, the two Poisson brackets $[\overline{\zeta_i},\overline{\zeta_j}]=[\zeta_i,\zeta_j]=J_{ij}$ are the same. The two remaining Poisson brackets are of equal rank, $r_i+r_j-\Delta+1$. Thus at rank $r_i+r_j-\Delta+1$, $[\zeta_i,P_{r_j+1}(\mathcal{M}'\zeta_j)]=[\zeta_j,P_{r_i+1}(\mathcal{M}'\zeta_i)]$ for all i, j. The individual coefficients $\{M_k^1,\ldots,M_k^{2d}\}$, where d is the number of degrees of freedom, must be related in order that the map be symplectic. By Lemma 1 of Dragt and Finn[2] there is a function g such that

$$P_{r_i+1}(\mathcal{M}'\zeta_i)=[g,\zeta_i]. \tag{22}$$

Applying this transformation, we eliminate the terms of (20) at rank r_i+1,

$$e^{:-g_{\Delta+1}:}e^{:-g_{\Delta}:}\mathcal{M}\zeta_i=c_i+\zeta_i+P_{r_i+2}(\mathcal{M}''\zeta_i)+\cdots, \tag{23}$$

with $\mathcal{M}''=e^{:-g_{\Delta+1}:}\mathcal{M}'\zeta_i=e^{:-g_{\Delta+1}:}e^{:-g_{\Delta}:}\mathcal{M}\zeta_i$.

The process described can continue at successively higher ranks, so that continuing to rank k gives

$$\mathcal{M}\zeta_i = e^{:g_\Delta:} e^{:g_{\Delta+1}:} \cdots e^{:g_k:} \zeta_i + \mathcal{O}(\delta^{r_i+k-\Delta+1}). \tag{24}$$

Since this is true for all i and k was arbitrary, we have (17). □

While this proof is not constructive, there is an algorithm described in Ref. 15 that shows how to compute the homogeneous polynomials f and g. In general terms, the function g_n is computed by integrating the M^i_{n-1} with respect to the conjugate variable, but any given i will produce only ζ_i-dependent terms, and any terms dependent on more than one phase space variable will show up in more than one integration. Thus the algorithm must be careful to get all terms and not duplicate.

In an ascending series, the highest rank is applied first and then successively lower ones, whereas in a descending series the lowest rank is applied first and then successively higher ones. The names, while they appear reversed, are a reference to how the ranks read left-to-right, rather than how they are applied mathematically. It is possible to represent any symplectic map either way, but of course the polynomials are different. It turns out that for some contexts, one form is ''natural,'' while for others, the other one is. In particular, the Hamiltonian factorization algorithm (Sec. V) produces descending factorizations, while in numerical application of maps for propagation, the ascending form is more convenient. It is thus useful to be able to transform between the two, along with transformation to and from explicit maps; both these topics are covered in Ref. 15.

The concept of rank introduced above provides a convenient method of factorization, but factorization may also be done by order, the total exponent of phase space variables. If there is an external perturbation, one must then keep an entirely separate expansion. This is less convenient because expression of a full perturbed transformation can be more complicated, but it has been done in the context of accelerator physics problems.[6] The two forms may be converted by concatenating the factored transformations together, and then map factoring by order or rank as appropriate. Two Lie transformations can be *concatenated*, that is, combined into a single Lie transformation, by means of the Baker–Campbell–Hausdorff formula. More details on this and related manipulations are given in Ref. 15.

We shall call the sequence of maps (16) or (17) a *factored Lie product*. When combined with the unperturbed solution, we have the complete Lie transfer map.

V. HAMILTONIAN FACTORIZATION

The map factorization theorem, while useful for calculating the polynomials if the map is given, is not helpful in a constructive sense when we seek to solve a Hamiltonian problem. This section shows a method for computing the factored Lie product for time evolution of a perturbed Hamiltonian, knowing

(i) the full Hamiltonian,
(ii) the solution for the unperturbed Hamiltonian,
(iii) how to do Poisson brackets,
(iv) how to do time integration.

The method presented in this section will produce a factored Lie product of the descending form (16). In Sec. V E an example worked step-by-step is given.

The method of Hamiltonian factorization was developed in the context of what we are calling here internal perturbations by Dragt and Forest.[4] The method described here is a generalization, primarily in the following ways: the map under the unperturbed Hamiltonian is arbitrarily labeled $\mathcal{U}$ instead of presuming that it will be a linear function of the generalized coordinates, and the bracket grade is an arbitrary non-negative integer (Δ) instead of two. These result in a subtle difference in the development of the solution; here we need to include ''at bracket grade'' terms not present in the previous analysis. Nevertheless, where the details are unclear here, the reader should consult their paper.

In this method, there is a constraint which has no meaningful implication to real physics problems, and that is the assumption that time (the independent variable) must be rank zero, so that differentiation and integration with respect to time will not change rank.

A. Hamiltonian evolution

Using properties of Lie transformations, it can be shown that evolution of a map $\mathcal{M}$ on phase space under a Hamiltonian satisfies Hamilton's equations,

$$\dot{\mathcal{M}} = \mathcal{M} : -\mathcal{H}(\zeta^{\text{in}}, t) : , \tag{25}$$

with initial generalized coordinates ζ^{in}, which means that for an arbitrary function on phase space $g(\zeta)$, for ζ at an arbitrary time,

$$\dot{\mathcal{M}}(g(\zeta^{\text{in}})) = \mathcal{M} : -\mathcal{H}(\zeta^{\text{in}}, t) : (g(\zeta^{\text{in}})). \tag{26}$$

B. The interaction picture

We say that evolution under a Hamiltonian $\mathcal{H}$ gives rise to a map $\mathcal{M}$ over some time period if $\mathcal{M}$ is the function that gives the generalized coordinates at the final time ζ^f after evolving under $\mathcal{H}$ from the generalized coordinates at the initial time ζ^i,

$$\zeta^f = \mathcal{M}\zeta^i. \tag{27}$$

Let the $\mathcal{M}$ be defined as the composition of two other maps, called the unperturbed map $\mathcal{U}$ and the perturbation $\mathcal{P}$:

$$\mathcal{M} = \mathcal{P}\mathcal{U}. \tag{28}$$

The terminology will be justified shortly. Differentiating the map product

$$\dot{\mathcal{M}} = \dot{\mathcal{P}}\mathcal{U} + \mathcal{P}\dot{\mathcal{U}} \tag{29}$$

and substituting the map evolution equation (25) gives

$$\mathcal{P}\mathcal{U} : -\mathcal{H} := \dot{\mathcal{P}}\mathcal{U} + \mathcal{P}\dot{\mathcal{U}}. \tag{30}$$

The Hamiltonian may be expanded by rank,

$$\mathcal{H} = \mathcal{H}^u_\Delta + \mathcal{H}^p_\Delta + \mathcal{H}_{\Delta+1} + \mathcal{H}_{\Delta+2} + \cdots . \tag{31}$$

The Hamiltonian is free of phase-space dependent terms of rank lower than Δ. The terms of the Hamiltonian at rank Δ are split into two, $\mathcal{H}^u_\Delta$ and $\mathcal{H}^p_\Delta$. $\mathcal{H}^u_\Delta$ is meant to be the unperturbed part, and $\mathcal{H}^p_\Delta$, together with $\mathcal{H}_i$ $(i > \Delta)$ is meant to capture the perturbations. According to the definitions of Sec. III C, if $\Delta = 0$, there are no perturbation terms at bracket grade, i.e., $\mathcal{H}^p_\Delta = 0$. If $\Delta > 0$, however, then $\mathcal{H}^p_\Delta$ consists of those terms at bracket grade that are linear in phase space. $\mathcal{H}_n = P_n(\mathcal{H})$ for $n > 0$ are terms of the Hamiltonian with rank n, which are all perturbations.

There is a known solution $\mathcal{U}$ to the equation of motion for the Hamiltonian $\mathcal{H}^u_\Delta$,

$$\dot{\mathcal{U}} = \mathcal{U} : -\mathcal{H}^u_\Delta :, \tag{32}$$

which may be substituted in (30) to obtain an equation of motion for $\mathcal{P}$:

$$\dot{\mathcal{P}}\mathcal{U} = \mathcal{P}\mathcal{U} : -\mathcal{H}_R : \quad \text{with} \quad \mathcal{H}_R = \mathcal{H} - \mathcal{H}^u_\Delta \tag{33}$$

or

$$\dot{\mathcal{P}}=\mathcal{P}\mathcal{U}:-\mathcal{H}_R:\mathcal{U}^{-1}=\mathcal{P}:-\mathcal{H}_R^{\text{int}}:, \tag{34}$$

where $\mathcal{H}_R^{\text{int}}(\zeta)=\mathcal{H}_R(\mathcal{U}\zeta)$ is the perturbed interaction Hamiltonian.

The known solution to the unperturbed problem $\mathcal{U}$, though denoted analogously to the perturbation map $\mathcal{P}$ being solved, will not usually be represented the same way. The solution $\mathcal{U}$ will usually be written as an explicit transformation, that is, as expressions for the final phase space variables as function(s) of the initial phase space variables. For example, if the unperturbed problem is a linear system, $\mathcal{U}$ may be written as a matrix. On the other hand, the perturbation map $\mathcal{P}$ is being developed as a sequence of Lie transformations.

The goal of the next two sections is to derive an algorithm for computing $\mathcal{P}$ using factored Lie products (16).

C. The map in the interaction picture

Since $\mathcal{P}$ is a perturbation transformation, it can be factored (Sec. IV B); for convenience let the homogeneous Lie transformations be designated $\mathcal{M}_\Delta^p=e^{:f_\Delta:}$ and $\mathcal{M}_n=e^{:f_n:}$ for $n>\Delta$; the perturbation map is

$$\mathcal{P}=\cdots\mathcal{M}_{\Delta+2}\mathcal{M}_{\Delta+1}\mathcal{M}_\Delta^p. \tag{35}$$

The time derivative of this map may be computed using (34)

$$\begin{aligned}\dot{\mathcal{P}}&=\cdots+\cdots\dot{\mathcal{M}}_{\Delta+2}\mathcal{M}_{\Delta+1}\mathcal{M}_\Delta^p+\cdots\mathcal{M}_{\Delta+2}\dot{\mathcal{M}}_{\Delta+1}\mathcal{M}_\Delta^p+\cdots\mathcal{M}_{\Delta+2}\mathcal{M}_{\Delta+1}\dot{\mathcal{M}}_\Delta^p\\&=\cdots\mathcal{M}_{\Delta+2}\mathcal{M}_{\Delta+1}\mathcal{M}_\Delta^p:-\mathcal{H}_R^{\text{int}}:.\end{aligned} \tag{36}$$

We may apply $\mathcal{P}^{-1}$ on the left to obtain a relation between the interaction Hamiltonian and the perturbation transformations,

$$\begin{aligned}&\cdots+\cdots\mathcal{M}_\Delta^{p-1}\mathcal{M}_{\Delta+1}^{-1}\mathcal{M}_{\Delta+2}^{-1}\dot{\mathcal{M}}_{\Delta+2}\mathcal{M}_{\Delta+1}\mathcal{M}_\Delta^p+\cdots\mathcal{M}_\Delta^{p-1}\mathcal{M}_{\Delta+1}^{-1}\dot{\mathcal{M}}_{\Delta+1}\mathcal{M}_\Delta^p\\&\quad+\cdots\mathcal{M}_\Delta^{p-1}\dot{\mathcal{M}}_\Delta^p=:-\mathcal{H}_R^{\text{int}}:.\end{aligned} \tag{37}$$

This may look complicated, but we can reduce it to something usable by taking the ''adjoint of the adjoint;'' we define the operator # # by analogy to : :, so that $\#f\#:g:=\{:f:,:g:\}$, where the braces indicate the commutator. The exponential of this operator is defined with the customary Taylor series, and, as a Lie transformation, possesses all the identities such as the similarity relationship (8). We may take each term in (37) and rewrite the similarity transformation using this adjoint, for example,

$$\mathcal{M}_\Delta^{p-1}\mathcal{M}_{\Delta+1}^{-1}\mathcal{M}_{\Delta+2}^{-1}\dot{\mathcal{M}}_{\Delta+2}\mathcal{M}_{\Delta+1}\mathcal{M}_\Delta^p=e^{\#-f_\Delta\#}e^{\#-f_{\Delta+1}\#}\mathcal{M}_{\Delta+2}^{-1}\dot{\mathcal{M}}_{\Delta+2}. \tag{38}$$

With the integrated exponential function iex defined as

$$\text{iex}(w)=\int_0^1 e^{tw}\,dt=\sum_{m=0}^{\infty}\frac{w^m}{(m+1)!}, \tag{39}$$

then

$$\mathcal{M}_n^{-1}\dot{\mathcal{M}}_n=\text{iex}(-\#f_n\#):\dot{f}_n: \tag{40}$$

(see Ref. 4); we find that we have labored fruitfully to simplify (37)

$$\cdots e^{\#-f_\Delta\#}e^{\#-f_{\Delta+1}\#}\,\mathrm{iex}(-\#f_{\Delta+2}\#):\dot{f}_{\Delta+2}:+e^{\#-f_\Delta\#}\,\mathrm{iex}(-\#f_{\Delta+1}\#):\dot{f}_{\Delta+1}:$$
$$+\mathrm{iex}(-\#f_\Delta\#):\dot{f}_\Delta:=:-\mathcal{H}_R^{\mathrm{int}}:. \tag{41}$$

Using the technique of ''decolonizing,'' [4] we may demote each expression on the adjoint scale $-\#\ \#$ to : : and : : to simple phase space expressions:

$$\cdots e^{:-f_\Delta:}e^{:-f_{\Delta+1}:}\,\mathrm{iex}(-:f_{\Delta+2}:)\dot{f}_{\Delta+2}+e^{:-f_\Delta:}\,\mathrm{iex}(-:f_{\Delta+1}:)\dot{f}_{\Delta+1}$$
$$+\mathrm{iex}(-:f_\Delta:)\dot{f}_\Delta=-\mathcal{H}_R^{\mathrm{int}}, \tag{42}$$

which may be rewritten more compactly in terms of summation and products:

$$\sum_{i=\Delta}^{\infty}\left(\prod_{j=\Delta}^{i-1}e^{:-f_j:}\right)\mathrm{iex}(-:f_i:)\dot{f}_i=-\mathcal{H}_R^{\mathrm{int}}. \tag{43}$$

We may now begin to see our destination: from this formula, we can compute each of the polynomials f_n. We can compute $-\mathcal{H}_R^{\mathrm{int}}$ from the original Hamiltonian and the solution to the unperturbed problem. Then rank by rank, we can compute each of the polynomials in order $f_\Delta,\ldots,f_{n-1}$ to get f_n.

D. Sequential computation of polynomials

Explicitly, this procedure is as follows. Let the ''rest map'' C_k be defined as the difference of the two sides of (43) with the summation truncated

$$C_k(t)=-\mathcal{H}_R^{\mathrm{int}}(t)-\sum_{i=\Delta}^{k}\left(\prod_{j=\Delta}^{i-1}e^{:-f_j:}\right)\mathrm{iex}(-:f_i:)\dot{f}_i. \tag{44}$$

If the upper limit is lower than the lower limit for the summation or product, the term is to be ignored, i.e., $\Sigma_A^B=0$ and $\Pi_A^B=1$ if $B<A$. We can express (44) inductively:

$$C_{\Delta-1}=-\mathcal{H}_R^{\mathrm{int}} \tag{45a}$$

and

$$C_k=C_{k-1}-\left(\prod_{j=\Delta}^{k-1}e^{:-f_j:}\right)\mathrm{iex}(-:f_k:)\dot{f}_k \tag{45b}$$

for $k\geqslant\Delta$.

Note that the rest map is seen to be zero at a rank below the step k, $P_l(C_k)=0$ for $l\leqslant k$, because the Lie operator $:f_k:$ raises the rank for $k>\Delta$. Thus we apply the projection P_k to both sides of (45b) to find

$$P_k(C_{k-1})=e^{:-f_\Delta:}\dot{f}_k; \tag{46}$$

the right-hand side is purely rank k. The product of Lie transformations reduces to just the Lie transformation in f_Δ because all other transformation are the identity at rank-raise zero. Similarly, $\mathrm{iex}(-:f_k:)$ is the identity at rank-raise zero. Since $\dot{f}_k$ is rank k, we care only about rank-raise zero in the transformations.

Solving for f_Δ, Eq. (46) with $k=\Delta$ becomes

$$P_\Delta(-\mathcal{H}_R^{\mathrm{int}})=e^{:-f_\Delta:}\dot{f}_\Delta. \tag{47}$$

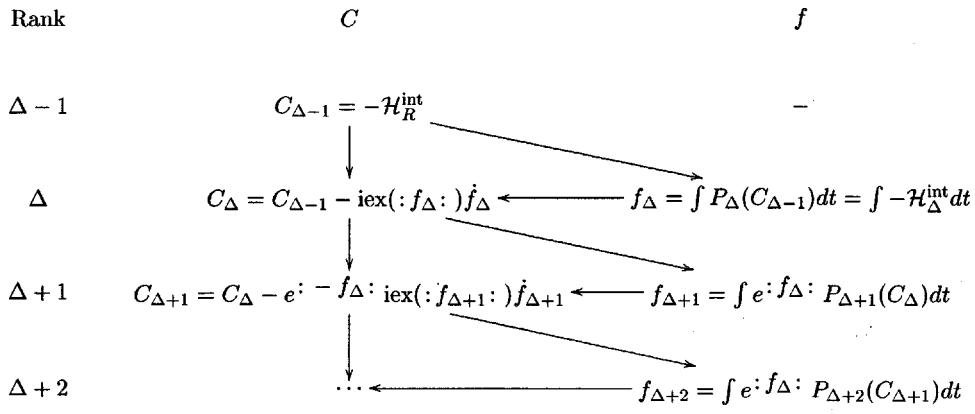

FIG. 1. Factoring the Hamiltonian rank by rank. Each f_n is computed using prior values of C; each C_n is computed using current and prior values of f.

As stated in Sec. III B, f_Δ must be first order in the phase space variables. Therefore, $:f_\Delta:\dot{f}_\Delta$ is a constant, and there are no subsequent terms. We can thus truncate the series at the first term

$$P_\Delta(-\mathcal{H}_R^{\text{int}}) = \dot{f}_\Delta, \tag{48}$$

which is easily solved,

$$f_\Delta = \int P_\Delta(C_{\Delta-1})dt = \int -\mathcal{H}_\Delta^{\text{int}}dt, \tag{49}$$

where $\mathcal{H}_\Delta^{\text{int}}$ is the rank-Δ term of $\mathcal{H}_R^{\text{int}}$. For $k>\Delta$ the solution is straightforward. Solving for $\dot{f}_k$ in (46),

$$\dot{f}_k = e^{:f_\Delta:}P_k(C_{k-1}) \tag{50}$$

or

$$f_k = \int e^{:f_\Delta:}P_k(C_{k-1})dt. \tag{51}$$

The factorization (35) that this algorithm produces is the descending form (16).

E. Summary and example of the computation

The Lie polynomials and transfer map are computed with the following steps: compute

(1) the interaction Hamiltonian according to $\mathcal{H}_R^{\text{int}}(\zeta) = -\mathcal{H}_R(\mathcal{U}\zeta)$, and $C_{\Delta-1}$ by (45a),
(2) f_Δ from $C_{\Delta-1}$ according to (49),
(3) for $k \geqslant \Delta$, C_k from C_{k-1} and $f_\Delta, \ldots, f_{k-1}$, according to (45b),
(4) f_k from C_{k-1} for $k>\Delta$ according to (51),
(5) repeat at step 3 as desired.

This procedure is diagrammed in Fig. 1. With it, we may iteratively find all the polynomials up to the rank we desire.

We may now use these steps to compute the Lie transfer map for the quartic harmonic oscillator introduced in Sec. I, with action-angle Hamiltonian (4). First, assume that the unperturbed solution,

$$\mathcal{U}=\begin{cases}\theta\leftarrow\theta+\omega_0 t,\\ J\leftarrow J,\end{cases} \tag{52}$$

is known. In this formulation, the bracket grade is zero, $\Delta=0$. As before, we will use ϕ for $\omega_0 t$; then the transformed Hamiltonian is obtained by substituting $\theta+\phi$ for θ in the action-angle Hamiltonian (4),

$$\mathcal{H}^{\text{int}}=\omega_0 J+\delta\mu J^2\frac{1}{\omega_0^2}\left(\frac{3}{8}-\frac{1}{2}\cos(2\theta+2\phi_0)+\frac{1}{8}\cos(4\theta+4\phi_0)\right). \tag{53}$$

We can split this into the unperturbed part, $\omega_0 J$, and the perturbation part,

$$\mathcal{H}_R^{\text{int}}=\delta\mu J^2\frac{1}{\omega_0^2}\left(\frac{3}{8}-\frac{1}{2}\cos(2\theta+2\phi)+\frac{1}{8}\cos(4\theta+4\phi)\right). \tag{54}$$

The first rest-map is, according to (45a), just the negative of the interaction Hamiltonian

$$C_{-1}=-\mathcal{H}_R^{\text{int}}=-\delta\mu J^2\frac{1}{\omega_0^2}\left(\frac{3}{8}-\frac{1}{2}\cos(2\theta+2\phi)+\frac{1}{8}\cos(4\theta+4\phi)\right). \tag{55}$$

Thus, the first polynomial, at the bracket grade $\Delta=0$, is zero, $f_0=\int P_0(C_{-1})dt=0$. Using (45b) and this fact, we find $C_0=C_{-1}$.

So far, this is not really interesting. At $k=1$ though, we start getting nonzero results; using (51),

$$\begin{aligned}f_1&=\int e^{:f_0:}P_1(C_0)dt\\&=\int-\delta\mu J^2\frac{1}{\omega_0^2}\left(\frac{3}{8}-\frac{1}{2}\cos(2\theta+2\phi)+\frac{1}{8}\cos(4\theta+4\phi)\right)dt\\&=\delta\mu J^2\left(-\frac{3}{8}\frac{t}{\omega_0^2}+\frac{1}{\omega_0^3}\left(-\frac{1}{4}\sin 2\theta+\frac{1}{4}\sin(2\theta+2\phi_0)+\frac{1}{32}\sin 4\theta-\frac{1}{32}\sin(4\theta+4\phi_0)\right)\right).\end{aligned} \tag{56}$$

At the next rank, the rest map is more complicated, because we now must apply f_1 as a transformation:

$$\begin{aligned}C_1=\exp:\delta\mu J^2\frac{1}{\omega_0^2}&\left(-\frac{3}{8}+\frac{1}{2}\cos(2\theta+2\phi_0)-\frac{1}{8}\cos(4\theta+4\phi_0)\right)+\delta^2\mu^2J^3\left(\frac{t}{\omega_0^4}\left(-\frac{3}{8}\sin(2\theta\right.\right.\\&+2\phi_0)+\frac{3}{16}\sin(4\theta+4\phi_0)\Big)+\frac{1}{\omega_0^5}\left(\frac{17}{64}-\frac{1}{4}\cos 2\phi_0-\frac{1}{64}\cos 4\phi_0+\frac{3}{64}\cos(2\theta-2\phi_0)\right.\\&+\frac{3}{16}\cos 2\theta-\frac{21}{64}\cos(2\theta+2\phi_0)+\frac{3}{32}\cos(2\theta+4\phi_0)-\frac{3}{64}\cos 4\theta+\frac{3}{64}\cos(4\theta+4\phi_0)\\&\left.\left.+\frac{1}{64}\cos(6\theta+2\phi_0)-\frac{1}{32}\cos(6\theta+4\phi_0)+\frac{1}{64}\cos(6\theta+6\phi_0)\right)\right)+\mathcal{O}(\delta^3):.\end{aligned} \tag{57}$$

Note that the rest map is now an infinite series in δ; we must cut it off at order 2, because that is all that is necessary for calculating the next polynomial:

$$f_2=\exp:\delta^2\mu^2J^2\Bigg(\frac{t}{\omega_0^5}\Bigg(\frac{17}{64}+\frac{3}{16}\cos 2\theta+\frac{3}{16}\cos(2\theta+2\phi_0)-\frac{3}{64}\cos 4\theta-\frac{3}{64}\cos(4\theta+4\phi_0)\Bigg)$$
$$+\frac{1}{\omega_0^6}\Bigg(-\frac{1}{8}\sin 2\phi_0-\frac{1}{256}\sin 4\phi_0-\frac{3}{128}\sin(2\theta-2\phi_0)+\frac{33}{128}\sin 2\theta-\frac{33}{128}\sin(2\theta+2\phi_0)$$
$$+\frac{3}{128}\sin(2\theta+4\phi_0)-\frac{3}{128}\sin 4\theta+\frac{3}{128}\sin(4\theta+4\phi_0)-\frac{1}{384}\sin 6\theta+\frac{1}{128}\sin(6\theta+2\phi_0)$$
$$-\frac{1}{128}\sin(6\theta+4\phi_0)+\frac{1}{384}\sin(6\theta+6\phi_0)\Bigg)\Bigg):. \tag{58}$$

When applied to the phase space variables θ and J, the factored Lie product to this rank $e^{:f_2:}e^{:f_1:}$ will give us the explicit map (5); this is done in Ref. 10.

The above example has no f_Δ term. Consider then another example, with $\Delta=2$ and a nonzero f_Δ term. It is a simple harmonic oscillator in Cartesian coordinates with a quartic perturbation as above, but in addition it has a bracket-grade perturbation $X\nu$,

$$\mathcal{H}=\delta^2(\tfrac{1}{2}X\nu+\tfrac{1}{2}\omega_0^2x^2+\tfrac{1}{2}X^2)-\tfrac{1}{4}\delta^4x^4\mu. \tag{59}$$

Here, the Cartesian phase space variable x and its conjugate momentum X each have rank one, as does the external perturbation ν. The unperturbed solution is simply the harmonic oscillator solution,

$$\mathcal{U}=\begin{cases} x\leftarrow & x\cos\phi_0+X\dfrac{1}{\omega_0}\sin\phi_0 \\ X\leftarrow & -x\omega_0\sin\phi_0+X\cos\phi_0 \end{cases}. \tag{60}$$

The interaction Hamiltonian is

$$\mathcal{H}_R^{\text{int}}=\delta^2\Bigg(\nu\Bigg(-\frac{1}{2}x\omega_0\sin\phi_0+\frac{1}{2}X\cos\phi_0\Bigg)+\frac{1}{2}\omega_0^2x^2+\frac{1}{2}X^2\Bigg)+\delta^4\mu\Bigg(x^4\Bigg(-\frac{3}{32}-\frac{1}{8}\cos 2\phi_0$$
$$-\frac{1}{32}\cos 4\phi_0\Bigg)+x^3X\frac{1}{\omega_0}\Bigg(-\frac{1}{4}\sin 2\phi_0-\frac{1}{8}\sin 4\phi_0\Bigg)+x^2X^2\frac{1}{\omega_0^2}\Bigg(-\frac{3}{16}+\frac{3}{16}\cos 4\phi_0\Bigg)$$
$$+xX^3\frac{1}{\omega_0^3}\Bigg(-\frac{1}{4}\sin 2\phi_0+\frac{1}{8}\sin 4\phi_0\Bigg)+X^4\frac{1}{\omega_0^4}\Bigg(-\frac{3}{32}+\frac{1}{8}\cos 2\phi_0-\frac{1}{32}\cos 4\phi_0\Bigg)\Bigg)+\mathcal{O}(\delta^5). \tag{61}$$

Because $\Delta=2$, the first rest map computed is C_1,

$$C_1=\exp:\delta^2\nu(\tfrac{1}{2}x\omega_0\sin\phi_0-\tfrac{1}{2}X\cos\phi_0)+\mathcal{O}(\delta^3):\ . \tag{62}$$

In contrast to the previous example, at the bracket grade two, this is nonzero, so that the first Lie polynomial f_2 is nonzero,

$$f_2=\exp:\mathcal{O}(\delta^3):\exp:\delta^2\nu\Bigg(x\Bigg(\frac{1}{2}-\frac{1}{2}\cos\phi_0\Bigg)-\frac{1}{2}X\frac{1}{\omega_0}\sin\phi_0\Bigg):\ . \tag{63}$$

The next rest map C_3 is the same as the last one (62); however, at rank 4,

$$C_4=\exp{:}\,\delta^2\nu\left(\frac{1}{2}x\omega_0\sin\phi_0-\frac{1}{2}X\cos\phi_0\right)+\delta^4\mu\left(x^4\left(\frac{3}{32}+\frac{1}{8}\cos 2\phi_0+\frac{1}{32}\cos 4\phi_0\right)\right.$$
$$+x^3X\frac{1}{\omega_0}\left(\frac{1}{4}\sin 2\phi_0+\frac{1}{8}\sin 4\phi_0\right)+x^2X^2\frac{1}{\omega_0^2}\left(\frac{3}{16}-\frac{3}{16}\cos 4\phi_0\right)+xX^3\frac{1}{\omega_0^3}\left(\frac{1}{4}\sin 2\phi_0\right.$$
$$\left.\left.-\frac{1}{8}\sin 4\phi_0\right)+X^4\frac{1}{\omega_0^4}\left(\frac{3}{32}-\frac{1}{8}\cos 2\phi_0+\frac{1}{32}\cos 4\phi_0\right)\right)+\mathcal{O}(\delta^5){:}\ \ , \tag{64}$$

and the corresponding Lie polynomial is

$$f_4=\exp{:}\,\mathcal{O}(\delta^5){:}\exp{:}\,\delta^4\left(\mu\nu^{24}\left(\frac{3}{512}\frac{t}{\omega_0^4}+\frac{1}{\omega_0^5}\left(-\frac{1}{256}\sin 2\phi_0+\frac{1}{2048}4\phi_0\right)\right)+\mu\nu^3\left(x\frac{1}{\omega_0^4}\left(\frac{3}{256}\right.\right.\right.$$
$$\left.-\frac{1}{64}\cos 2\phi_0+\frac{1}{256}\cos 4\phi_0\right)+X\left(\frac{3}{64}\frac{t}{\omega_0^4}+\frac{1}{\omega_0^5}\left(-\frac{1}{32}\sin 2\phi_0+\frac{1}{256}\sin 4\phi_0\right)\right)\Big)$$
$$+\mu\nu^2\left(x^2\left(\frac{3}{64}\frac{t}{\omega_0^2}-\frac{3}{256}\frac{1}{\omega_0^3}\sin 4\phi_0\right)+xX\frac{1}{\omega_0^4}\left(\frac{9}{128}-\frac{3}{32}\cos 2\phi_0+\frac{3}{128}\cos 4\phi_0\right)\right.$$
$$\left.+X^2\left(\frac{9}{64}\frac{t}{\omega_0^4}+\frac{1}{\omega_0^5}\left(-\frac{3}{32}\sin 2\phi_0+\frac{3}{256}\sin 4\phi_0\right)\right)\right)+\mu\nu\left(x^3\frac{1}{\omega_0^2}\left(\frac{5}{64}-\frac{1}{16}\cos 2\phi_0\right.\right.$$
$$\left.-\frac{1}{64}\cos 4\phi_0\right)+x^2X\left(\frac{3}{16}\frac{t}{\omega_0^2}-\frac{3}{64}\frac{1}{\omega_0^3}\sin 4\phi_0\right)+xX^2\frac{1}{\omega_0^4}\left(\frac{9}{64}-\frac{3}{16}\cos 2\phi_0+\frac{3}{64}\cos 4\phi_0\right)$$
$$\left.+X^3\left(\frac{3}{16}\frac{t}{\omega_0^4}+\frac{1}{\omega_0^5}\left(-\frac{1}{8}\sin 2\phi_0+\frac{1}{64}\sin 4\phi_0\right)\right)\right)+\mu\left(x^4\left(\frac{3}{32}t+\frac{1}{\omega_0}\left(\frac{1}{16}\sin 2\phi_0\right.\right.\right.$$
$$\left.\left.+\frac{1}{128}\sin 4\phi_0\right)\right)+x^3X\frac{1}{\omega_0^2}\left(\frac{5}{32}-\frac{1}{8}\cos 2\phi_0-\frac{1}{32}\cos 4\phi_0\right)+x^2X^2\left(\frac{3}{16}\frac{t}{\omega_0^2}-\frac{3}{64}\frac{1}{\omega_0^3}\sin 4\phi_0\right)$$
$$+xX^3\frac{1}{\omega_0^4}\left(\frac{3}{32}-\frac{1}{8}\cos 2\phi_0+\frac{1}{32}\cos 4\phi_0\right)+X^4\left(\frac{3}{32}\frac{t}{\omega_0^4}+\frac{1}{\omega_0^5}\left(-\frac{1}{16}\sin 2\phi_0\right.\right.$$
$$\left.\left.\left.\left.+\frac{1}{128}\sin 4\phi_0\right)\right)\right)\right){:}\exp{:}\,\delta^2\nu\left(x\left(\frac{1}{2}-\frac{1}{2}\cos\phi_0\right)-\frac{1}{2}X\frac{1}{\omega_0}\sin\phi_0\right){:}\,. \tag{65}$$

VI. CONCLUSION

For a particular perturbation problem where each perturbation has a positive integer rank, knowledge of its Hamiltonian, a map for the unperturbed solution, and a method for doing time integrals and Poisson brackets is sufficient to calculate a transfer map represented in Lie polynomials to a desired rank of perturbation. Such a map is a regular perturbation solution to the problem.

For propagation of a given system once the map has been computed, it is necessary to turn the Lie transfer map into an explicit function of the coordinates and time (and parameters, of course). Once such an explicit map is obtained, it is possible to check its validity by seeing that it satisfies the map form of Hamilton's equations. In some cases the difficulty in computing the map of a full Hamiltonian dictates the combination of this method with numerical integration. A paper is in preparation by the author addressing these topics.

The perturbed harmonic oscillator in one degree of freedom used to illustrate the method has pedagogical value but limited practical value. Real applications can be as diverse as celestial mechanics and accelerator physics. Applications to celestial mechanics and astrodynamics are

worthy of separate papers in themselves; a paper is in preparation by the author on the application of this technique to the perturbed Kepler problem of a satellite orbiting a body with zonal perturbations. In this case, the perturbation is external, the phase space variables are not perturbation variables.

Potential application to accelerator beam dynamics problems might take the form of phase space as deviations from a *design trajectory* through a beamline element as in Dragt's formulation. One expects that the deviations are small, thus, there is an internal perturbation, with each phase space variable having rank one. External perturbations may arise from lattice parameter errors, such as powering or placement errors. It is possible to handle these problems by keeping two separate hierarchies of perturbations,[5] but the unified approach described here greatly simplifies the management of the computation.

Readers interested in results from computing maps for these or other nontrivial physical systems should contact the author.

For any application, the computation and manipulation of maps and associated expressions can become cumbersome quite quickly. For this reason, the author has developed a computer algebra program PGLT (perturbations with graded lie transformations) to automate the algebra involved in using Lie expressions, transformations and related objects. It is described in more detail in another paper.[15] All of the Lie algebraic calculations described in this paper (as well as a good deal more) become a matter of calling a single function, once an appropriate algebra hierarchy and integration rules have been defined.

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Exactly calculable field components of electric dipoles in planar boundary

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The Sommerfeld integrals for the electromagnetic fields in the planar boundary between air and a homogeneous, isotropic medium, due to a horizontal and a vertical electric dipole each lying along the interface, are examined in detail. In the case of the horizontal dipole, the tangential electric field is given in terms of series that involve confluent hypergeometric functions, namely, the Fresnel and exponential integrals. A similar exposition is presented for the magnetic and vertical electric fields of the vertical dipole. When the index of refraction of the adjacent space is of a sufficiently large magnitude, the derived series converge rapidly and uniformly with the distance from the source. Specifically, their rates of convergence are shown to be independent of distance. It is pointed out that the corresponding formulas of King *et al.* are valid down to any distance close to the source, where they smoothly connect to known ''quasi-static'' approximations. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1330731]

I. INTRODUCTION

Almost a century ago, Sommerfeld[1] first formulated the problem of the radiating vertical electric dipole located in the planar boundary between two homogeneous and isotropic half spaces by invoking the Hertz vector $\mathbf{\Pi}$ rather than the electromagnetic fields $\mathbf{E}$ and $\mathbf{B}$. With the use of the Fourier–Bessel representations in cylindrical coordinates, Sommerfeld proposed approximate formulas for $\mathbf{\Pi}$ for distances of many wavelengths in air away from the source. Soon after, his student Hörschelman[2] applied the same method to the case of the horizontal electric dipole in air. Other authors revisited these problems aiming at alternative representations for $\mathbf{\Pi}$ that could be amenable to asymptotic evaluations for sufficiently large distances. A historical account and extensive list of references can be found in the monograph by Baños.[3]

Serious efforts to derive accurate expressions for the $\mathbf{\Pi}$ of electric or magnetic dipoles were often made under the simplifying yet practically significant assumption that both the source and the observation point lie at the interface.[3–10] Some of the components of $\mathbf{\Pi}$ then involve the Fourier–Bessel integrals,[3]

$$U(\rho)=\int_0^\infty d\lambda\lambda\,\frac{1}{\sqrt{\lambda^2-k_1^2}+\sqrt{\lambda^2-k_2^2}}J_0(\lambda\rho), \tag{1.1}$$

$$V(\rho)=\int_0^\infty d\lambda\lambda\,\frac{1}{k_2^2\sqrt{\lambda^2-k_1^2}+k_1^2\sqrt{\lambda^2-k_2^2}}J_0(\lambda\rho), \tag{1.2}$$

where k_j $(j=1,2)$ is the complex wave number in medium j, ρ is the polar distance from the source, and J_0 is the Bessel function of order 0. Van der Pol[6] showed that $U(\rho)$ is given in terms of elementary functions, while $V(\rho)$ can be converted to a finite, one-dimensional integral of an elementary function that readily yields Sommerfeld's approximate result. On the basis of Van der

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Pol's formula for $V(\rho)$, Rice[10] derived exact series expansions that, although credited as being ''uniform'' in the distance ρ,[11] become impractical when $|k_j\rho| \gg 1$. He also proposed disparate asymptotic expansions for these distances when the refraction index k_1/k_2 is close to 1, k_2 being the wave number in air. Along the same lines is the exposition by Wise.[7] Noteworthy is Fock's[9] expansion for $V(\rho)$ in terms of products of Bessel functions with half-integer indices, where the expansion parameter $(k_1^2-k_2^2)/(k_1^2+k_2^2)$ is assumed to be of magnitude less than 1. Baños[3] re-derived the Sommerfeld–Van der Pol formula by applying a version of the steepest descent method, where a simple pole is extracted from the vicinity of a saddle point, and neglecting high orders in k_2/k_1. However, the issue of connecting this formula, which is valid in the range $k_2^3\rho/|k_1^2| \geqslant O(1)$, to the respective approximation for $|k_1\rho| \ll 1$ was not essentially addressed.

In a series of works,[12] Wait gave asymptotic formulas for the Sommerfeld integrals in different ranges of polar distances and source heights. Consider, for example, the ranges $k_2\rho \ll 1$, $k_2\rho = O(1)$, and $k_2\rho \gg 1$ when the dipole and the observation point both lie in the boundary;[13] even in this simplest nontrivial case, Wait's approximations seem to be based on intuitive arguments. In particular, in the ''quasi-static approach,''[13] the fields in air are regarded as solutions of Laplace's or Poisson's equation with no practical restriction on $k_1\rho$, but there is no clear indication, for instance, about the convergence or the magnitude of the remainder of the underlying expansion when $k_1 = O(k_2)$ with $k_2 < |k_1|$. In the spirit of the quasi-static approach, the computation of the Hertz vector is carried out in Refs. 14–16 for low frequencies via a convenient resummation of the λ-Maclaurin expansion for the radical under the integral sign. The ensuing simple expressions are interpreted as superpositions of primary and reflected fields, where the earth is replaced by a perfectly conducting medium with the boundary being shifted by the distance $1/k_1$.[16] Notably, the electric and magnetic fields are obtained through direct differentiations of the approximate formulas for $\mathbf{\Pi}$.

Recently, integrated formulas were derived by King *et al.*[17] for the electromagnetic field in air over an imperfectly conducting or dielectric earth when the source is a horizontal or vertical electric dipole. Their major simplifying conditions are $k_2^2 \ll |k_1^2|$ and $k_2 r > O(1)$, r being the radial distance from the source. Some of the novelties of their approach can be outlined as follows. First, these authors deal directly and systematically with the field itself and not the Hertz vector; their set of formulas satisfy Maxwell's equations and the required boundary conditions consistently to the desired order in k_2^2/k_1^2. Second, in their sequence of approximation steps, the direct and the ideal-image fields are singled out, some of the remaining integrals are computed exactly by analytical means, and large-argument approximations for the Bessel functions are only applied to the remainders that involve the Sommerfeld pole. The results advance the works of Baños[3] and others both quantitatively, with the retainment of a larger number of terms, and qualitatively, with the notions of the surface and lateral waves being dissociated in the mathematical treatment from that of a saddle-point in the vicinity of a pole.

In a recent paper,[18] King and Wu make use of the approximate formulas of Ref. 17 for the horizontal dipole to calculate the electromagnetic field in air of infinitely long transmission lines above the earth. However, as pointed out in Ref. 18, the violation of the condition $|k_1 r| > 1$ at extremely low frequencies introduces an inaccuracy for the axial component of the electric field. A formula for this component that is uniform in distance was later derived in a more elaborate analysis by Margetis.[19] The inaccuracy mentioned above signifies one of the instances where approximate formulas that are known to hold sufficiently far from the source are forced to be extended to distances too close to the source. An interesting question is whether it is possible, and if so in what sense, to connect the lateral-wave formulas of King *et al.*[17] to known near-field expressions, such as those given by Wait for $k_2\rho \ll 1$,[13] so that the final formulas adequately describe the field for all reasonable distances when $k_2^2 \ll |k_1^2|$.[20] Various interesting references and formulas for the evaluation of Sommerfeld-type integrals are provided in Ref. 21. Noteworthy among these formulas are the representations in terms of incomplete cylindrical functions.

The purpose of this paper is twofold. The first is to evaluate exactly, in terms of series that are uniform in ρ, those Sommerfeld integrals that are given by integrals of elementary functions, by relaxing the condition $k_2^2 \ll |k_1^2|$. This task is carried out in Secs. III and IV for the electromagnetic

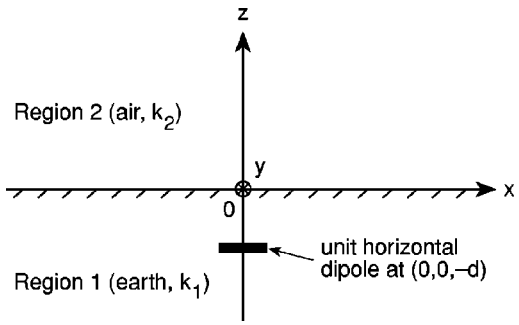

FIG. 1. The geometry and Cartesian coordinate system for a unit horizontal dipole in the earth. The height d is allowed to approach zero ($d\to 0^+$).

field of electric dipoles lying in the planar interface; the use of the Hertz vector is entirely avoided, in the spirit of Ref. 17. The expansion parameter is the inverse of the refraction index, k_2/k_1, which is assumed to be of magnitude less than 1, and the coefficients are known transcendental functions, namely, the exponential and Fresnel integrals. These series are believed to be new. In particular, the rates of convergence of the derived series are shown to depend only on the ratio k_2^2/k_1^2.[11] Emphasis is also placed on obtaining bounds and estimates for the remainders when a finite number of terms are summed. As a consequence, stringent conditions for the validity of simplifications under $k_2^2 \ll |k_1^2|$ can follow. All derivations are subject to routine mathematical rigor, and comparisons with numerical computations are beyond the scope of this paper.[22] A discussion on the merits of the present analysis for numerical evaluations is provided in Sec. VI.

The second purpose is to demonstrate that the corresponding lateral-wave formulas in Ref. 17 may indeed be extended to distances from the source that are short compared to the wavelength in air. In Sec. V we deal precisely with this task via the step-by-step approximations of the exact series. Finally, in Appendix A we calculate analytically a class of integrals involving Bessel functions through a generalized Schwinger–Feynman representation; Van der Pol's formula[6] essentially follows as a special case. The nature of the field asymptotic expansions for $k_2\rho \gg 1$ is analyzed in Appendix B on the basis of the derived series, while in Appendix C we revisit the simplifications of the original integrals in the limiting cases $k_2\rho \ll 1$ and $k_2\rho \gg 1$. The time dependence $e^{-i\omega t}$ is suppressed throughout the analysis.

II. FORMAL REPRESENTATIONS

A. Horizontal electric dipole

The geometry and Cartesian coordinate system are shown in Fig. 1. As the source and the observation point approach the boundary from below ($d\to 0^+$) and from above ($z\to 0^+$), respectively, the Fourier–Bessel representation for the electromagnetic field in the cylindrical coordinates (ρ,ϕ,z) with $x=\rho\cos\phi$ and $y=\rho\sin\phi$ $(0\leqslant\phi<2\pi)$ is[17]

$$E_{2z}=\frac{k_1^2}{k_2^2}E_{1z}=\frac{i\omega\mu_0}{4\pi k_2^2}\int_0^\infty d\lambda\lambda^2\frac{k_2^2\sqrt{k_1^2-\lambda^2}-k_1^2\sqrt{k_2^2-\lambda^2}}{k_2^2\sqrt{k_1^2-\lambda^2}+k_1^2\sqrt{k_2^2-\lambda^2}}J_1(\lambda\rho)\cos\phi, \tag{2.1}$$

$$E_{2\phi}=E_{1\phi}=\frac{\omega\mu_0}{4\pi}\int_0^\infty d\lambda\,\lambda\left\{\frac{\sqrt{k_1^2-\lambda^2}\,\sqrt{k_2^2-\lambda^2}}{k_1^2\sqrt{k_2^2-\lambda^2}+k_2^2\sqrt{k_1^2-\lambda^2}}[J_0(\lambda\rho)+J_2(\lambda\rho)]\right.$$
$$\left.+\frac{1}{\sqrt{k_1^2-\lambda^2}+\sqrt{k_2^2-\lambda^2}}[J_0(\lambda\rho)-J_2(\lambda\rho)]\right\}\sin\phi, \tag{2.2}$$

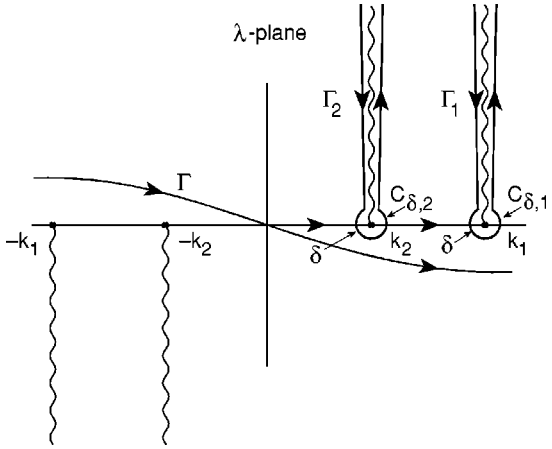

FIG. 2. Branch-cut configuration and integration paths pertaining to the Sommerfeld integrals (2.1)–(2.6) for the horizontal electric dipole and (2.10)–(2.12) for the vertical electric dipole. The original integration path is shown with arrows in the positive real axis. The contours Γ and Γ_j $(j=1,2)$ serve the asymptotic evaluations for $k_2\rho \gg 1$ carried out in Appendix C.

$$E_{2\rho}=E_{1\rho}=-\frac{\omega\mu_0}{4\pi}\int_0^\infty d\lambda\lambda\left\{\frac{\sqrt{k_1^2-\lambda^2}\sqrt{k_2^2-\lambda^2}}{k_1^2\sqrt{k_2^2-\lambda^2}+k_2^2\sqrt{k_1^2-\lambda^2}}[J_0(\lambda\rho)-J_2(\lambda\rho)]\right.$$
$$\left.+\frac{1}{\sqrt{k_1^2-\lambda^2}+\sqrt{k_2^2-\lambda^2}}[J_0(\lambda\rho)+J_2(\lambda\rho)]\right\}\cos\phi, \tag{2.3}$$

$$B_{2z}=B_{1z}=i\frac{\mu_0}{2\pi}\int_0^\infty d\lambda\lambda^2\frac{1}{\sqrt{k_1^2-\lambda^2}+\sqrt{k_2^2-\lambda^2}}J_1(\lambda\rho)\sin\phi, \tag{2.4}$$

$$B_{2\phi}=B_{1\phi}=-\frac{\mu_0}{8\pi}\int_0^\infty d\lambda\lambda\left\{\frac{\sqrt{k_2^2-\lambda^2}-\sqrt{k_1^2-\lambda^2}}{\sqrt{k_2^2-\lambda^2}+\sqrt{k_1^2-\lambda^2}}[J_0(\lambda\rho)+J_2(\lambda\rho)]\right.$$
$$\left.+\frac{k_2^2\sqrt{k_1^2-\lambda^2}-k_1^2\sqrt{k_2^2-\lambda^2}}{k_2^2\sqrt{k_1^2-\lambda^2}+k_1^2\sqrt{k_2^2-\lambda^2}}[J_0(\lambda\rho)-J_2(\lambda\rho)]\right\}\cos\phi, \tag{2.5}$$

$$B_{2\rho}=B_{1\rho}=-\frac{\mu_0}{8\pi}\int_0^\infty d\lambda\lambda\left\{\frac{\sqrt{k_2^2-\lambda^2}-\sqrt{k_1^2-\lambda^2}}{\sqrt{k_2^2-\lambda^2}+\sqrt{k_1^2-\lambda^2}}[J_0(\lambda\rho)-J_2(\lambda\rho)]\right.$$
$$\left.+\frac{k_2^2\sqrt{k_1^2-\lambda^2}-k_1^2\sqrt{k_2^2-\lambda^2}}{k_2^2\sqrt{k_1^2-\lambda^2}+k_1^2\sqrt{k_2^2-\lambda^2}}[J_0(\lambda\rho)+J_2(\lambda\rho)]\right\}\sin\phi, \tag{2.6}$$

the first subscript in each component referring to the region (1 for $z<0$ and 2 for $z>0$).

These integrals are divergent in the conventional sense. The procedure implied by allowing $d\to 0^+$ and $z\to 0^+$ in Fig. 1 dictates that they be interpreted in the sense of Abel.[23] The first Riemann sheet is such that $(j=1,2)$

$$\mathrm{Im}\,\sqrt{k_j^2-\lambda^2}\geqslant 0,\quad \lambda>0, \tag{2.7}$$

with the branch-cut configuration of Fig. 2 where k_1 is taken to be real and $k_2<k_1$. Note that each $\sqrt{k_j^2-\lambda^2}$ is even in λ and the denominator,

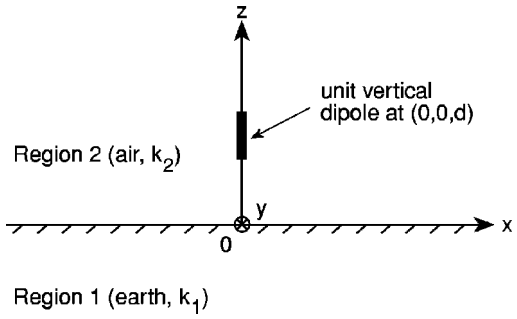

FIG. 3. The geometry and Cartesian coordinate system for a unit vertical dipole in air. The height d is allowed to approach zero ($d\to 0^+$).

$$D(\lambda)=k_1^2\sqrt{k_2^2-\lambda^2}+k_2^2\sqrt{k_1^2-\lambda^2}, \tag{2.8}$$

has four simple zeros in the Riemann surface. These are located at

$$\lambda=\pm k_S=\pm\frac{k_1k_2}{\sqrt{k_1^2+k_2^2}}, \tag{2.9}$$

and are not present in the first Riemann sheet.

B. Vertical electric dipole

The $\hat{\mathbf{z}}$-directed unit dipole is immersed in air (region 2, $z>0$), as depicted in Fig. 3. In the limit $d\to 0^+$ and $z\to 0^+$ the field is[17]

$$B_{2\phi}=B_{1\phi}=i\frac{\mu_0k_1^2}{2\pi}\int_0^\infty d\lambda\lambda^2\frac{1}{k_2^2\sqrt{k_1^2-\lambda^2}+k_1^2\sqrt{k_2^2-\lambda^2}}J_1(\lambda\rho), \tag{2.10}$$

$$E_{2z}=\frac{k_1^2}{k_2^2}E_{1z}=-\frac{\omega\mu_0k_1^2}{2\pi k_2^2}\int_0^\infty d\lambda\lambda^3\frac{1}{k_2^2\sqrt{k_1^2-\lambda^2}+k_1^2\sqrt{k_2^2-\lambda^2}}J_0(\lambda\rho)=\frac{i\omega}{k_2^2}\frac{1}{\rho}\frac{d}{d\rho}\rho B_{2\phi}, \tag{2.11}$$

$$E_{2\rho}=E_{1\rho}=-\frac{i\omega\mu_0}{4\pi k_2^2}\int_0^\infty d\lambda\lambda^2\frac{k_2^2\sqrt{k_1^2-\lambda^2}-k_1^2\sqrt{k_2^2-\lambda^2}}{k_2^2\sqrt{k_1^2-\lambda^2}+k_1^2\sqrt{k_2^2-\lambda^2}}J_1(\lambda\rho). \tag{2.12}$$

The first Riemann sheet along with the branch-cut configuration, and the integration path are chosen as described in Sec. II A and shown in Fig. 2. Throughout the following analysis, it is assumed that

$$0<k_2<|k_1|,\quad 0\leqslant \mathrm{Arg}\ k_1<\pi/4. \tag{2.13}$$

III. EXACT B_{2z}, $E_{2\phi}$, AND $E_{2\rho}$ OF HORIZONTAL ELECTRIC DIPOLE

For mathematical convenience, consider the replacements

$$k_j=iq_j,\quad \sqrt{k_j^2-\lambda^2}=i\sqrt{\lambda^2+q_j^2}\quad (j=1,2). \tag{3.1}$$

The Sommerfeld pole corresponds to $q_S=-ik_S$. For the purpose of carrying out the requisite integrations, q_1 and q_2 are thought of as positive with $q_2<q_1$, unless it is stated or implied otherwise. The final formulas are continued analytically to complex $q_j=-ik_j$ $(j=1,2)$ in view of restrictions (2.13).

A. The *z*-component of the magnetic field

It is verified that B_{2z} is expressed in terms of elementary functions.[13] The requisite integral equals

$$B_{2z}=\frac{\mu_0}{2\pi}\frac{1}{q_1^2-q_2^2}\frac{1}{\rho^4}[\mathcal{I}_m(q_1\rho)-\mathcal{I}_m(q_2\rho)]\sin\phi, \tag{3.2}$$

where

$$\mathcal{I}_m(\alpha)=\int_0^\infty dx\, x^2\sqrt{x^2+\alpha^2}J_1(x)=\frac{\alpha^{5/2}}{2^{-3/2}\Gamma\left(-\frac{1}{2}\right)}K_{5/2}(\alpha), \tag{3.3}$$

via the analytic continuation to $\mu=-3/2$ of the right-hand side of the equation,[24]

$$\int_0^\infty dx\frac{x^2J_1(x)}{(x^2+\alpha^2)^{\mu+1}}=\frac{\alpha^{1-\mu}}{2^\mu\Gamma(\mu+1)}K_{1-\mu}(\alpha).$$

$K_\nu(\alpha)$ is the modified Bessel function of the third kind.[25] Hence,

$$\mathcal{I}_m(\alpha)=-\alpha^2\left(1+\frac{3}{\alpha}+\frac{3}{\alpha^2}\right)e^{-\alpha}. \tag{3.4}$$

It follows that

$$B_{2z}=-\frac{\mu_0}{2\pi}\frac{1}{(k_1^2-k_2^2)\rho^2}\left[e^{ik_1\rho}k_1^2\left(1+\frac{3i}{k_1\rho}-\frac{3}{k_1^2\rho^2}\right)-e^{ik_2\rho}k_2^2\left(1+\frac{3i}{k_2\rho}-\frac{3}{k_2^2\rho^2}\right)\right]\sin\phi. \tag{3.5}$$

This result is also derived by Wait through differentiation of the Hertz vector.[13] Discussions on a similar integral appearing in the problem of the radiating vertical magnetic dipole can be found in the books by Baños[3] and Kong.[26]

B. The ϕ-component of the electric field

With the definition $q_S=-ik_S$, consider the decomposition

$$\frac{\sqrt{\lambda^2+q_1^2}\sqrt{\lambda^2+q_2^2}}{q_1^2\sqrt{\lambda^2+q_2^2}+q_2^2\sqrt{\lambda^2+q_1^2}}=\frac{1}{q_1^4-q_2^4}[q_1^2\sqrt{\lambda^2+q_1^2}-q_2^2\sqrt{\lambda^2+q_2^2}]+\frac{q_1^3q_2^3}{q_1^4-q_2^4}\times\frac{1}{q_1^2+q_2^2}\left[\frac{q_2}{q_1}\frac{\sqrt{\lambda^2+q_1^2}}{\lambda^2+q_S^2}-\frac{q_1}{q_2}\frac{\sqrt{\lambda^2+q_2^2}}{\lambda^2+q_S^2}\right]. \tag{3.6}$$

Accordingly, Eq. (2.2) reads as

$$E_{2\phi}=-\frac{i\omega\mu_0}{2\pi}\frac{1}{q_1^2-q_2^2}\left\{\frac{d}{d\rho}\left[\frac{\mathcal{I}_e(q_1\rho)-\mathcal{I}_e(q_2\rho)}{\rho^2}\right]+\frac{1}{q_1^2+q_2^2}\frac{1}{\rho}\left[\frac{q_1^2\mathcal{I}_e(q_1\rho)-q_2^2\mathcal{I}_e(q_2\rho)}{\rho^2}\right]\right.$$
$$\left.+\frac{q_1^3q_2^3}{(q_1^2+q_2^2)^2}\frac{1}{\rho}\mathcal{W}(\rho)\right\}\sin\phi, \tag{3.7}$$

where

$$\mathcal{I}_e(\alpha)=\int_0^\infty dx\sqrt{x^2+\alpha^2}J_1(x)=\alpha+e^{-\alpha}, \tag{3.8}$$

with recourse to Ref. 24, and

$$\mathcal{W}(\rho)=\int_0^\infty d\lambda\left[\frac{q_2}{q_1}\frac{\sqrt{\lambda^2+q_1^2}}{\lambda^2+q_S^2}-\frac{q_1}{q_2}\frac{\sqrt{\lambda^2+q_2^2}}{\lambda^2+q_S^2}\right]J_1(\lambda\rho). \tag{3.9}$$

The task is to express $\mathcal{W}(\rho)$ in terms of known transcendental functions.

Following Van der Pol,[6] a first step is to convert the representation (3.9) into an integral of elementary functions. The radical in the integrand reads as follows:

$$\frac{q_2}{q_1}\frac{\sqrt{\lambda^2+q_1^2}}{\lambda^2+q_S^2}-\frac{q_1}{q_2}\frac{\sqrt{\lambda^2+q_2^2}}{\lambda^2+q_S^2}=\frac{1}{\lambda^2+q_S^2}\frac{\sqrt{\lambda^2+q_s^2x^2}}{\sqrt{x^2-1}}\Bigg|_{x=q_2/q_S}^{q_1/q_S}$$
$$=\int_{q_2/q_S}^{q_1/q_S}d[(x^2-1)^{-1/2}]\frac{1}{\sqrt{\lambda^2+q_S^2x^2}}. \tag{3.10}$$

The interchange of the order of integration yields

$$\mathcal{W}(\rho)=\int_{q_2/q_S}^{q_1/q_S}d\left(\frac{1}{\sqrt{x^2-1}}\right)\int_0^\infty d\lambda\frac{J_1(\lambda\rho)}{\sqrt{\lambda^2+q_S^2x^2}}, \tag{3.11}$$

where, from Ref. 24 or Eq. (A6) of Appendix A,

$$\int_0^\infty d\lambda\frac{J_1(\lambda\rho)}{\sqrt{\lambda^2+q_S^2x^2}}=\frac{1}{q_S\rho x}(1-e^{-q_S\rho x}). \tag{3.12}$$

Therefore, through integration by parts,

$$\mathcal{W}(\rho)=-\frac{1}{q_S\rho}\left[\frac{q_1-q_2}{q_S}-\frac{q_1e^{-q_2\rho}-q_2e^{-q_1\rho}}{q_S}+\rho W(\rho)\right], \tag{3.13}$$

where

$$W(\rho)=W(\rho;q_1,q_2,q_S),\quad W(\rho;\xi_1,\xi_2,\xi_3)=\int_{\xi_2}^{\xi_1}d\upsilon\frac{\upsilon}{\sqrt{\upsilon^2-\xi_3^2}}e^{-\upsilon\rho},\quad \xi_3\leqslant\xi_2<\xi_1. \tag{3.14}$$

The procedure described hitherto is not different from the one in Ref. 27 for the Hertz vector of a vertical dipole. An alternative derivation of the last equation, that is amenable to generalizations, is provided in Appendix A. It is noted that $W(\rho)$ can be expressed in terms of incomplete cylindrical functions as further discussed in Sec. VI. Despite this fact, it is more advantageous to rewrite $W(\rho)$ as

$$W(\rho)=W(\rho;\infty,q_S,q_S)-W(\rho;\infty,q_1,q_S)-W(\rho;q_2,q_S,q_S). \tag{3.15}$$

The first term is calculated explicitly:[25]

$$W(\rho;\infty,q_S,q_S)=q_S\int_0^\infty dy\,\cosh y e^{-q_S\rho\cosh y}=q_S K_1(q_S\rho). \tag{3.16}$$

1. Integral $W(\rho;\infty,q_1,q_S)$

By invoking the identity

$$(1-u)^{-1/2}=\sum_{m=0}^{M-1}\frac{(\frac{1}{2})_m}{m!}u^m+\frac{(\frac{1}{2})_M}{(M-1)!}u^M\int_0^1 dt(1-t)^{M-1}(1-ut)^{-M-1/2}, \tag{3.17}$$

with $u=q_S^2\nu^{-2}$ and a positive integer M, the second term in Eq. (3.15) reads as

$$W(\rho;\infty,q_1,q_S)=\frac{e^{-q_1\rho}}{\rho}\left[\sum_{m=0}^{M-1}U_m(\rho)+R_{1M}(\rho)\right], \tag{3.18}$$

where

$$U_m(\rho)=\frac{(\frac{1}{2})_m}{m!}(q_S\rho)^{2m}g_{2m}(q_1\rho), \tag{3.19}$$

$$g_n(z)=\int_z^\infty d\tau\tau^{-n}e^{-\tau+z}, \tag{3.20}$$

$$R_{1M}(\rho)=q_1\rho\frac{(\frac{1}{2})_M}{(M-1)!}\left(\frac{q_S}{q_1}\right)^{2M}\int_1^\infty d\eta\eta^{-2M}e^{-q_1\rho(\eta-1)}$$

$$\times\int_0^1 dt(1-t)^{M-1}(1-q_S^2q_1^{-2}\eta^{-2}t)^{-M-1/2} \tag{3.21a}$$

$$=q_1\rho\frac{(\frac{1}{2})_M}{M!}\left(\frac{q_S}{q_1}\right)^{2M}\int_1^\infty d\eta\eta^{-2M}{}_2F_1(M+\tfrac{1}{2},1;M+1;q_S^2q_1^{-2}\eta^{-2})e^{-q_1\rho(\eta-1)}. \tag{3.21b}$$

In the above, ${}_2F_1$ is the hypergeometric function[28] and $(a)_m$ is Pochhammer's symbol.[28]

By bearing in mind that $1-t\leqslant|1-wt|$ for $0\leqslant t\leqslant 1$ and $|w|\leqslant 1$, it is inferred that for admissible complex q_1 and q_2 ($\mathrm{Re}\,q_1\geqslant 0$),

$$|R_{1M}(\rho)|<|q_1\rho|(1-|q_S^2|/|q_1^2|)^{-3/2}\frac{(\frac{1}{2})_M}{M!}\left|\frac{q_S^2}{q_1^2}\right|^M,\quad M=1,2,\ldots, \tag{3.22a}$$

which can be used to prove the convergence of the corresponding series as $M\to\infty$. This relation must be supplemented with the formula

$$R_{1M}(\rho)\sim\frac{(\frac{1}{2})_M}{M!}{}_2F_1(M+\tfrac{1}{2},1;M+1;q_S^2/q_1^2)\frac{q_1\rho}{2M+q_1\rho}\left(\frac{q_S}{q_1}\right)^{2M},\quad |q_1\rho|\gg 1, \tag{3.22b}$$

in order to show that $|R_{1M}(\rho)|$ remains bounded as $|q_1\rho|\to\infty$. It is noted in passing that for $m=0,1,2,\ldots,$

$$ {}_2F_1(m+\tfrac{3}{2},1;m+2;z)=(-1)^m\frac{m+1}{(\tfrac{1}{2})_{m+1}}(1-z)^{-1/2}\frac{d^m}{dz^m}\left[\frac{(1-z)^m}{1+\sqrt{1-z}}\right]. $$

Use of the asymptotic formula ($\eta\gg 1$),

$$ \int_0^1 dt(1-t)^{M-1}(1-q_S^2q_1^{-2}\eta^{-2}t)^{-M-1/2} $$

$$ \sim\frac{1}{M-1-(M+1/2)q_S^2q_1^{-2}\eta^{-2}},\quad M\gg 1, \tag{3.23} $$

in Eq. (3.21a) leads to

$$ R_{1M}(\rho)\sim\frac{(\tfrac{1}{2})_M}{M!}\left(\frac{q_S^2}{q_1^2}\right)^M(1-q_S^2/q_1^2)^{-1}\frac{q_1\rho}{2M+q_1\rho},\quad M\gg 1. \tag{3.24} $$

By inspection of Eq. (3.14), the rate of convergence of the series from Eq. (3.18) is essentially independent of ρ. In particular, $U_m(\rho)$ is approximated by

$$ U_m(\rho)\sim\frac{q_1\rho}{2m+q_1\rho}\frac{(\tfrac{1}{2})_m}{m!}\left(\frac{q_S^2}{q_1^2}\right)^m,\quad m\gg 1. \tag{3.25} $$

This formula also holds when $m=O(1)$ and $|q_1\rho|\gg 1$ with $\mathrm{Re}\,q_1\geqslant 0$, and becomes exact when $m=0$ for any $q_1\rho$. Hence,

$$ \frac{U_{m+1}(\rho)}{U_m(\rho)}\sim\frac{m+1/2}{m+1}\frac{2m+q_1\rho}{2m+2+q_1\rho}\frac{q_S^2}{q_1^2},\quad |2m+q_1\rho|\gg 1. \tag{3.26} $$

In the sense of Cauchy for convergence,

$$ W(\rho;\infty,q_1,q_S)=\frac{e^{-q_1\rho}}{\rho}\sum_{m=0}^{\infty}\frac{(\tfrac{1}{2})_m}{m!}(q_S\rho)^{2m}g_{2m}(q_1\rho). \tag{3.27} $$

The coefficients $g_n(q_1\rho)$ are partial derivatives in x of the generating function,

$$ \sum_{n=1}^{\infty}g_n(z)x^{n-1}=-e^{z-x}\,\mathrm{Ei}(x-z), \tag{3.28} $$

where $\mathrm{Ei}(-z)$ is the exponential integral.[28] Finally,

$$ g_n(z)=\begin{cases}1, & n=0,\\ \dfrac{(-1)^n}{(n-1)!}\dfrac{d^{n-1}}{dz^{n-1}}[e^z\mathrm{Ei}(-z)], & n=1,2,\ldots.\end{cases} \tag{3.29} $$

An asymptotic expansion for $W(\rho;\infty,q_1,q_S)$ when $|q_1\rho|\gg 1$ is derived in Appendix B.

2. Integral $W(\rho;q_2,q_S,q_S)$

With the change of variable $\xi=v-q_S$ in the original integral from Eqs. (3.14) and use of the identity

$$(1+2u)(1+u)^{-1/2}=\sum_{m=0}^{M-1}(-1)^{m+1}\frac{(\frac{1}{2})_m}{m!}\frac{m+1/2}{m-1/2}u^m+(-1)^{M-1}\frac{(\frac{1}{2})_{M-1}}{(M-1)!}u^M$$
$$\times\int_0^1 dt(1-t)^{M-1}(M+1/2+ut)(1+ut)^{-M-1/2}, \tag{3.30}$$

where now $u=(2q_S)^{-1}\xi$, it is straightforward to get

$$W(\rho;q_2,q_S,q_S)=\frac{e^{-q_S\rho}}{\sqrt{2q_S}}\int_0^{q_2-q_S}\frac{d\xi}{\sqrt{\xi}}(\xi+q_S)\left(1+\frac{\xi}{2q_S}\right)^{-1/2}e^{-\xi\rho}, \tag{3.31a}$$

$$=-q_Se^{-q_2\rho}\left[\sum_{m=0}^{M-1}V_m(\rho)+R_{2M}(\rho)\right]. \tag{3.31b}$$

In the above,

$$V_m(\rho)=-e^{i\pi/4}i^{m+1}\frac{(\frac{1}{2})_m}{m!}\frac{m+1/2}{m-1/2}(2q_S\rho)^{-m-1/2}f_m(i(q_2-q_S)\rho), \tag{3.32}$$

$$f_m(z)=\int_0^z d\tau\tau^{m-1/2}e^{-i(z-\tau)}, \tag{3.33}$$

$$R_{2M}(\rho)=(-1)^M\frac{(\frac{1}{2})_{M-1}}{(M-1)!}\left(\frac{q_2-q_S}{2q_S}\right)^{M+1/2}\int_0^1 d\eta\eta^{M-1/2}e^{(q_2-q_S)\rho(1-\eta)}$$
$$\times\int_0^1 dt(1-t)^{M-1}\left(M+\frac{1}{2}+\frac{q_2-q_S}{2q_S}\eta t\right)\left(1+\frac{q_2-q_S}{2q_S}\eta t\right)^{-M-1/2}. \tag{3.34}$$

Because

$$\mathrm{Re}\frac{q_2-q_S}{2q_S}=\mathrm{Re}\frac{k_2-k_S}{2k_S}>0, \tag{3.35}$$

one may employ the inequality $|1+wt|\geqslant 1$ for $t\geqslant 0$ and $\mathrm{Re}\,w>0$, to show that for complex q_1 and q_2 with $\mathrm{Re}\,(q_2-q_S)\leqslant 0$,

$$|R_{2M}(\rho)|<\frac{(\frac{1}{2})_M}{M!}\frac{M+1}{M^2-1/4}\left|\frac{q_2-q_S}{2q_S}\right|^{M+1/2}, \quad M=1,2,\ldots. \tag{3.36a}$$

The convergence of the right-hand side of Eq. (3.31b) as $M\to\infty$ follows. Furthermore,

$$R_{2M}(\rho)\sim(-1)^M\frac{(\frac{1}{2})_M}{M!}\Bigg[{}_2F_1(M+\tfrac{1}{2},1;M+1;-w)$$
$$+\frac{1}{M-1/2}{}_2F_1(M-\tfrac{1}{2},1;M+1;-w)\Bigg]_{w=(q_2-q_S)/(2q_S)}$$
$$\times\frac{1}{M-1/2-(q_2-q_S)\rho}\left(\frac{q_2-q_S}{2q_S}\right)^{M+1/2}, \quad |(q_2-q_S)\rho|\gg 1. \tag{3.36b}$$

M is any positive integer. In the above, the hypergeometric functions reduce to elementary functions. For instance, by setting $M=1$ in the second line,

$$ {}_2F_1(\tfrac{1}{2},1;2;z)=\frac{2}{1+\sqrt{1-z}}. $$

On the other hand, by virtue of formula (3.23),

$$ R_{2M}(\rho)\sim(-1)^M\frac{(\frac{1}{2})_{M-1}}{M!}\left(\frac{q_2-q_S}{2q_S}\right)^{M+1/2}\int_0^1 d\eta\,\frac{M+1/2}{1+\dfrac{q_2-q_S}{2q_S}\,\eta}\,e^{(M-1/2)\ln\,\eta+(q_2-q_S)\rho(1-\eta)} $$

$$ \sim\frac{2q_S}{q_2+q_S}(-1)^M\frac{(\frac{1}{2})_M}{M!}\,\frac{M+1/2}{M-1/2}\,\frac{1}{M-1/2-(q_2-q_S)\rho}\left(\frac{q_2-q_S}{2q_S}\right)^{M+1/2},\quad M\gg 1. \tag{3.37} $$

When $|q_2\rho|\gg 1$, the corresponding sum needs to be combined with the asymptotic expansion for the modified Hankel function of Eq. (3.16), as discussed in Appendix B. In some analogy with expressions (3.25) and (3.26),

$$ V_m(\rho)\sim\frac{(-1)^m}{m-1/2-(q_2-q_S)\rho}\,\frac{(\frac{1}{2})_m}{m!}\,\frac{m+1/2}{m-1/2}\left(\frac{q_2-q_S}{2q_S}\right)^{m+1/2}, \tag{3.38} $$

which in turn leads to

$$ \frac{V_{m+1}(\rho)}{V_m(\rho)}\sim-\frac{m-\frac{1}{2}}{m+\frac{1}{2}}\,\frac{m+\frac{3}{2}}{m+1}\,\frac{m-\frac{1}{2}-(q_2-q_S)\rho}{m+\frac{1}{2}-(q_2-q_S)\rho}\,\frac{q_2-q_S}{2q_S},\quad |m-(q_2-q_S)\rho|\gg 1, \tag{3.39} $$

provided that m is a positive integer.

The aforementioned considerations indicate some rather attractive convergence properties of the series expansions when $|q_2^2|\ll|q_1^2|$. Their termwise differentiation with respect to ρ is legitimate and preserves the uniform-in-ρ convergence. The series from Eq. (3.31b) is

$$ W(\rho;q_2,q_S,q_S)=e^{i\pi/4}\frac{q_S e^{-q_2\rho}}{\sqrt{2q_S\rho}}\sum_{m=0}^{\infty}\,i^{m+1}\frac{(\frac{1}{2})_m}{m!}\,\frac{m+1/2}{m-1/2}(2q_S\rho)^{-m}f_m(i(q_2-q_S)\rho). \tag{3.40} $$

The generating function for $f_m(z)$ is

$$ \sum_{m=0}^{\infty}\frac{f_m(z)}{m!}(ix)^m=\sqrt{2\pi}e^{-iz}(1+x)^{-1/2}F_0((1+x)z), \tag{3.41} $$

where

$$ F_0(z)=\int_0^z dt\,\frac{e^{it}}{\sqrt{2\pi t}}=C(z)+iS(z), \tag{3.42} $$

and $C(z)$ and $S(z)$ are the Fresnel integrals,[28]

$$ C(z)=\int_0^z dx\,\frac{\cos x}{\sqrt{2\pi x}},\quad S(z)=\int_0^z dx\,\frac{\sin x}{\sqrt{2\pi x}}. \tag{3.43} $$

Hence,

$$f_m(z)=\sqrt{2\pi}(-i)^m e^{-iz} z^{1/2+m}\frac{d^m}{dz^m}[z^{-1/2}F_0(z)]. \tag{3.44}$$

3. Exact formula for $E_{2\phi}$

The combination of Eqs. (3.15), (3.16), (3.27), and (3.40), with Eqs. (3.19) and (3.32), furnishes the desired expression for $W(\rho)$, viz.,

$$W(\rho)=q_S K_1(q_S\rho)+q_S e^{-q_2\rho}\sum_{m=0}^{\infty} V_m(\rho)-\frac{e^{-q_1\rho}}{\rho}\sum_{m=0}^{\infty} U_m(\rho). \tag{3.45}$$

From Eq. (3.13),

$$\mathcal{W}(\rho)=-i\frac{k_1-k_2}{k_S^2\rho}+i\frac{k_1 e^{ik_2\rho}-k_2 e^{ik_1\rho}}{k_S^2\rho}+\frac{\pi}{2}H_1^{(1)}(k_S\rho)-e^{ik_2\rho}\sum_{m=0}^{\infty} V_m(\rho)-\frac{e^{ik_1\rho}}{ik_S\rho}\sum_{m=0}^{\infty} U_m(\rho), \tag{3.46}$$

where

$$U_m(\rho)=\begin{cases} 1, & m=0,\\ \dfrac{(\frac{1}{2})_m}{m!(2m-1)!}(-k_S^2\rho^2)^m\dfrac{d^{2m-1}}{dz^{2m-1}}[e^z\ \mathrm{Ei}(-z)]_{z=-ik_1\rho}, & m=1,2,\ldots, \end{cases} \tag{3.47}$$

$$V_m(\rho)=\sqrt{2\pi}i^m\frac{(\frac{1}{2})_m}{m!}\frac{m+1/2}{m-1/2}\left(\frac{k_2-k_S}{2k_S}\right)^{m+1/2}\left\{e^{-iz}\frac{d^m}{dz^m}[z^{-1/2}F_0(z)]\right\}_{z=(k_2-k_S)\rho}. \tag{3.48}$$

The substitution of Eqs. (3.8) and (3.46) into (3.7) gives

$$\begin{aligned} E_{2\phi}=-\frac{i\omega\mu_0}{2\pi}\frac{k_2^2}{k_1^4-k_2^4}\Bigg\{ & -ie^{ik_1\rho}k_1\left[\frac{k_1^2+k_2^2(2-k_S/k_2)}{k_2^2\rho^2}+i\frac{k_1^2+2k_2^2}{k_1k_2^2\rho^3}\right]\\ & +ie^{ik_2\rho}\frac{2k_1^2+k_2^2}{k_2\rho^2}\left(1+\frac{i}{k_2\rho}\right)-i\frac{k_1k_S^2}{k_2\rho}\Bigg[\frac{i\pi}{2}H_1^{(1)}(k_S\rho)-ie^{ik_2\rho}\sum_{m=0}^{\infty} V_m(\rho)\\ & -\frac{e^{ik_1\rho}}{k_S\rho}\sum_{m=0}^{\infty} U_{m+1}(\rho)\Bigg]\Bigg\}\sin\phi. \end{aligned} \tag{3.49}$$

Note that when $k_2^2\ll|k_1^2|$, the argument of each Fresnel integral becomes

$$(k_2-k_S)\rho=k_2\left[1-\left(1+\frac{k_2^2}{k_1^2}\right)^{-1/2}\right]\rho\sim\frac{k_2^3\rho}{2k_1^2}=\wp, \tag{3.50}$$

where $|(k_2-k_S)\rho|$ is the Sommerfeld ''numerical distance.''[29]

For $k_2\rho\gg 1$, the Hankel function in Eq. (3.49) is approximated by an expansion with the phase factor $e^{ik_S\rho}$. This expansion exactly cancels terms produced by the Fresnel integrals, so that the final expression describes only waves traveling with the phase velocity of medium 1 or 2 (terms $\propto e^{ik_j\rho}$, $j=1,2$), as shown in Appendix B.

C. The ρ-component of the electric field

The integral for $E_{2\rho}$ is evaluated via the interchange of $1/\rho$ and the operator $(d/d\rho)$ in Eq. (3.7). The series that result through the term-by-term differentiation of expansions (3.27) and (3.40) also exhibit rapid convergence for $k_2^2 \ll |k_1^2|$, with a rate which is essentially independent of the distance ρ. Without further ado,

$$E_{2\rho}=\frac{i\omega\mu_0}{2\pi}\frac{k_2^2}{k_1^4-k_2^4}\left\{e^{ik_1\rho}\left(\frac{k_1^2-k_2^2}{k_2^2\rho^3}-ik_1\frac{k_1^2-k_2^2}{k_2^2\rho^2}+\frac{k_1^2}{\rho}\right)\right.$$
$$\left.+e^{ik_2\rho}\left(\frac{k_1^2-k_2^2}{k_2^2\rho^3}-i\frac{k_1^2-k_2^2}{k_2\rho^2}-\frac{k_1^2}{\rho}\right)-i\frac{k_1}{k_2}k_S W'(\rho)\right\}\cos\phi, \tag{3.51a}$$

$$=\frac{i\omega\mu_0}{2\pi}\frac{k_2^2}{k_1^4-k_2^4}\left\{e^{ik_1\rho}\left(\frac{k_1^2-k_2^2}{k_2^2\rho^3}-ik_1\frac{k_1^2-k_2^2}{k_2^2\rho^2}+\frac{k_1^2}{\rho}\right)\right.$$
$$+e^{ik_2\rho}\left(\frac{k_1^2-k_2^2}{k_2^2\rho^3}-i\frac{k_1^2-k_2^2}{k_2\rho^2}-\frac{k_1^2}{\rho}\right)+\frac{\pi}{2}\frac{k_1}{k_2}k_S^3 H_1^{(1)'}(k_S\rho)$$
$$\left.-\frac{k_1}{k_2}k_S^2\frac{d}{d\rho}\left[\frac{e^{ik_1\rho}}{ik_S\rho}\sum_{m=0}^{\infty}U_m(\rho)+e^{ik_2\rho}\sum_{m=0}^{\infty}V_m(\rho)\right]\right\}\cos\phi, \tag{3.51b}$$

where $W(\rho)$ is defined by Eq. (3.14) and the prime here denotes differentiation with respect to the argument.

It is desirable to further manipulate this formula. Decomposition (3.15) entails

$$W'(\rho)=ik_S^2\frac{\pi}{2}H_1^{(1)'}(k_S\rho)+\tilde{W}(\rho;\infty,-ik_1,-ik_S)+\tilde{W}(\rho;-ik_2,-ik_S,-ik_S), \tag{3.52a}$$

where

$$\tilde{W}(\rho;\xi_1,\xi_2,\xi_3)=\int_{\xi_2}^{\xi_1}d\nu\frac{\nu^2}{\sqrt{\nu^2-\xi_3^2}}e^{-\nu\rho},\quad \xi_3\leqslant\xi_2<\xi_1. \tag{3.52b}$$

1. Integral $\tilde{W}(\rho;\infty,q_1,q_S)$

With the steps of Sec. III B and for $M=1,2,\ldots,$

$$\tilde{W}(\rho;\infty,q_1,q_S)=\frac{e^{-q_1\rho}}{\rho^2}(1+q_1\rho)-q_S^2e^{-q_1\rho}\left[\sum_{m=0}^{M-1}\tilde{U}_m(\rho)+\tilde{R}_{1M}(\rho)\right], \tag{3.53}$$

where

$$\tilde{U}_m(\rho)=-\frac{(\frac{1}{2})_{m+1}}{(m+1)!}(q_S\rho)^{2m}g_{2m+1}(q_1\rho),\quad m=0,1,2,\ldots, \tag{3.54}$$

with $g_n(z)$ defined by Eq. (3.20), and

$$\tilde{R}_{1M}(\rho)=-\frac{(\frac{1}{2})_{M+1}}{M!}\left(\frac{q_S}{q_1}\right)^{2M}\int_1^{\infty}d\eta\,\eta^{-2M-1}e^{-q_1\rho(\eta-1)}$$
$$\times\int_0^1 dt(1-t)^M(1-q_S^2q_1^{-2}\eta^{-2}t)^{-M-3/2}. \tag{3.55}$$

It is easily verified that

$$|\tilde{R}_{1M}(\rho)|<(1-|k_S^2|/|k_1^2|)^{-3/2}\frac{(\frac{1}{2})_{M+1}}{(M+1)!}\left|\frac{k_S^2}{k_1^2}\right|^M, \quad M=1,2,\ldots, \tag{3.56a}$$

$$\tilde{R}_{1M}(\rho)\sim-\frac{(\frac{1}{2})_{M+1}}{(M+1)!}{}_2F_1(M+\tfrac{3}{2},1;M+2;k_S^2/k_1^2)\frac{1}{2M+1-ik_1\rho}\left(\frac{k_S^2}{k_1^2}\right)^M, \quad |k_1\rho|\gg 1, \tag{3.56b}$$

$$\tilde{R}_{1M}(\rho)\sim-(1-k_S^2/k_1^2)^{-1}\frac{(\frac{1}{2})_{M+1}}{(M+1)!}\frac{1}{2M+1-ik_1\rho}\left(\frac{k_S^2}{k_1^2}\right)^M, \quad M\gg 1, \tag{3.56c}$$

while, for $|2m+1-ik_1\rho|\gg 1$,

$$\tilde{U}_m(\rho)\sim-\frac{(\frac{1}{2})_{m+1}}{(m+1)!}\frac{1}{2m+1-ik_1\rho}\left(\frac{k_S^2}{k_1^2}\right)^m, \tag{3.57a}$$

$$\frac{\tilde{U}_{m+1}(\rho)}{\tilde{U}_m(\rho)}\sim\frac{m+3/2}{m+2}\frac{2m+1-ik_1\rho}{2m+3-ik_1\rho}\frac{k_S^2}{k_1^2}. \tag{3.57b}$$

2. Integral $\tilde{W}(\rho;q_2,q_S,q_S)$

Likewise,

$$\tilde{W}(\rho;q_2,q_S,q_S)=q_S^2e^{-q_2\rho}\left[\sum_{m=0}^{M-1}\tilde{V}_m(\rho)+\tilde{R}_{2M}(\rho)\right], \tag{3.58}$$

where, for $m=0,1,2,\ldots,$

$$\tilde{V}_m(\rho)=-e^{i\pi/4}i^{m+1}\frac{(\frac{1}{2})_m}{m!}\frac{m^2+3/4}{(m-1/2)(m-3/2)}(2q_S\rho)^{-m-1/2}f_m(i(q_2-q_S)\rho), \tag{3.59}$$

with $f_m(z)$ defined by Eq. (3.44), and

$$\begin{aligned}\tilde{R}_{2M}(\rho)=(-1)^M&\frac{(\frac{1}{2})_{M-1}}{(M-1)!}\frac{1}{M-3/2}\left(\frac{q_2-q_S}{2q_S}\right)^{M+1/2}\int_0^1 d\eta\,\eta^{M-1/2}e^{(q_2-q_S)\rho(1-\eta)}\\&\times\int_0^1 dt(1-t)^{M-1}\left[M^2+\frac{3}{4}+\left(2M+3+3\frac{q_2-q_S}{2q_S}\eta t\right)\frac{q_2-q_S}{2q_S}\eta t\right]\\&\times\left(1+\frac{q_2-q_S}{2q_S}\eta t\right)^{-M-1/2}.\end{aligned} \tag{3.60}$$

It is of interest to note the relations

$$|\tilde{R}_{2M}(\rho)|<\frac{(\frac{1}{2})_M}{M!}\frac{M^2+M+3}{|M-3/2|(M^2-1/4)}\left|\frac{k_2-k_S}{2k_S}\right|^{M+1/2}, \quad M=1,2,\ldots, \tag{3.61a}$$

$$\tilde{R}_{2M}(\rho)\sim(-1)^M\frac{(\frac{1}{2})_M}{M!}\Bigg[{}_2F_1(M+\tfrac{1}{2},1;M+1;-w)+\frac{2}{M-1/2}\,{}_2F_1(M-\tfrac{1}{2},1;M+1;-w)$$
$$+\frac{3}{(M-1/2)(M-3/2)}\,{}_2F_1(M-\tfrac{3}{2},1;M+1;-w)\Bigg]_{w=(k_2-k_S)/(2k_S)}$$
$$\times\frac{1}{M-1/2+i(k_2-k_S)\rho}\left(\frac{k_2-k_S}{2k_S}\right)^{M+1/2},\quad |(k_2-k_S)\rho|\gg 1, \tag{3.61b}$$

$$\tilde{R}_{2M}(\rho)\sim\frac{2k_S}{k_2+k_S}(-1)^M\frac{(\frac{1}{2})_M}{M!}\,\frac{M^2+3/4}{(M-1/2)(M-3/2)}\,\frac{1}{M-1/2+i(k_2-k_S)\rho}$$
$$\times\left(\frac{k_2-k_S}{2k_S}\right)^{M+1/2},\quad M\gg 1. \tag{3.61c}$$

Again, the hypergeometric functions here are calculable in terms of elementary functions. For $m\gg 1$ and $|m+i(k_2-k_S)\rho|\gg 1$,

$$\tilde{V}_m(\rho)\sim(-1)^m\frac{(\frac{1}{2})_m}{m!}\,\frac{m^2+3/4}{(m-1/2)(m-3/2)}\,\frac{1}{m-1/2+i(k_2-k_S)\rho}\left(\frac{k_2-k_S}{2k_S}\right)^{m+1/2}, \tag{3.62a}$$

$$\frac{\tilde{V}_{m+1}(\rho)}{\tilde{V}_m(\rho)}\sim-\frac{m+1/2}{m+1}\,\frac{m-3/2}{m+1/2}\,\frac{(m+1)^2+3/4}{m^2+3/4}\,\frac{m-1/2+i(k_2-k_S)\rho}{m+1/2+i(k_2-k_S)\rho}\,\frac{k_2-k_S}{2k_S}. \tag{3.62b}$$

3. Exact formula for $E_{2\rho}$

It follows that in the limit $M\to\infty$ all series converge uniformly in ρ. $W'(\rho)$ from Eq. (3.52) reads as

$$W'(\rho)=e^{ik_1\rho}\left(\frac{1}{\rho^2}-\frac{ik_1}{\rho}\right)+k_S^2\left[\frac{i\pi}{2}H_1^{(1)'}(k_S\rho)-e^{ik_2\rho}\sum_{m=0}^{\infty}\tilde{V}_m(\rho)+e^{ik_1\rho}\sum_{m=0}^{\infty}\tilde{U}_m(\rho)\right]. \tag{3.63}$$

Finally, substituting $W'(\rho)$ in Eq. (3.51a) yields

$$E_{2\rho}=\frac{i\omega\mu_0}{2\pi}\,\frac{k_2^2}{k_1^4-k_2^4}\Bigg\{e^{ik_1\rho}\left[\frac{k_1^2-k_2^2}{k_2^2\rho^3}-ik_1\frac{k_1^2-k_2^2(1-k_S/k_2)}{k_2^2\rho^2}+\frac{k_1^2(1-k_S/k_2)}{\rho}\right]$$
$$+e^{ik_2\rho}\left(\frac{k_1^2-k_2^2}{k_2^2\rho^3}-i\,\frac{k_1^2-k_2^2}{k_2\rho^2}-\frac{k_1^2}{\rho}\right)$$
$$-i\,\frac{k_1}{k_2}k_S^3\left[\frac{i\pi}{2}H_1^{(1)'}(k_S\rho)-e^{ik_2\rho}\sum_{m=0}^{\infty}\tilde{V}_m(\rho)+e^{ik_1\rho}\sum_{m=0}^{\infty}\tilde{U}_m(\rho)\right]\Bigg\}\cos\phi, \tag{3.64}$$

where $\tilde{U}_m(\rho)$ and $\tilde{V}_m(\rho)$ are given by Eqs. (3.54) and (3.59). An asymptotic formula for $k_2\rho\gg 1$ can be derived along the lines of Appendix B.

IV. EXACT $B_{2\phi}$ AND E_{2z} OF VERTICAL ELECTRIC DIPOLE

A. Magnetic field

In consideration of Eq. (3.1) with $q_S=-ik_S$ and the decomposition,

$$\frac{1}{q_1^2\sqrt{\lambda^2+q_2^2}+q_2^2\sqrt{\lambda^2+q_1^2}}=\frac{q_1q_2}{q_1^4-q_2^4}\left[\frac{q_1}{q_2}\frac{\sqrt{\lambda^2+q_2^2}}{\lambda^2+q_S^2}-\frac{q_2}{q_1}\frac{\sqrt{\lambda^2+q_1^2}}{\lambda^2+q_S^2}\right], \tag{4.1}$$

Eq. (2.10) becomes

$$B_{2\phi}=-\frac{\mu_0}{2\pi}\frac{q_1^3q_2}{q_1^4-q_2^4}\int_0^\infty d\lambda\lambda^2\left[\frac{q_2}{q_1}\frac{\sqrt{\lambda^2+q_1^2}}{\lambda^2+q_S^2}-\frac{q_1}{q_2}\frac{\sqrt{\lambda^2+q_2^2}}{\lambda^2+q_S^2}\right]J_1(\lambda\rho). \tag{4.2}$$

From Eq. (3.10), one gets

$$B_{2\phi}=-\frac{\mu_0}{2\pi}\frac{q_1^3q_2}{q_1^4-q_2^4}\int_{q_2/q_S}^{q_1/q_S}d[(x^2-1)^{-1/2}]\int_0^\infty d\lambda\lambda^2\frac{J_1(\lambda\rho)}{\sqrt{\lambda^2+q_S^2x^2}}, \tag{4.3}$$

where

$$\int_0^\infty d\lambda\lambda^2\frac{J_1(\lambda\rho)}{\sqrt{\lambda^2+q_S^2x^2}}=\sqrt{\frac{2}{\pi\rho}}(q_Sx)^{3/2}K_{3/2}(q_S\rho x)=\frac{1}{\rho^2}(1+q_S\rho x)e^{-q_S\rho x}, \tag{4.4}$$

via the analytic continuation to $\nu=1$ of the right-hand side of the formula[24]

$$\int_0^\infty dx\frac{x^{\nu+1}J_\nu(ax)}{\sqrt{x^2+k^2}}=\frac{a^{-1/2}k^{\nu+1/2}}{2^{-1/2}\sqrt{\pi}}K_{\nu+1/2}(ka).$$

Alternatively,

$$B_{2\phi}=-\frac{\mu_0}{2\pi}\frac{q_1^3q_2}{q_1^4-q_2^4}\left\{\frac{1}{\rho^2}\left[\frac{q_2}{q_1}\mathcal{I}_e(q_1\rho)-\frac{q_1}{q_2}\mathcal{I}_e(q_2\rho)\right]-q_S^2\mathcal{W}(\rho)\right\}, \tag{4.5}$$

where $\mathcal{I}_e(\alpha)$ is given by Eq. (3.8) and $\mathcal{W}(\rho)$ is defined by Eq. (3.9). $B_{2\phi}$ can be expressed in terms of incomplete cylindrical functions.[27]

With the $W(\rho)$ introduced in Eq. (3.13), the exact $B_{2\phi}$ from Eq. (4.3) reads as

$$\begin{aligned}B_{2\phi}&=-\frac{\mu_0}{2\pi}\frac{q_1^3q_2}{q_1^4-q_2^4}\left\{\frac{1}{\rho^2}\left[e^{-q_1\rho}\frac{q_2}{q_1}(1+q_1\rho)-e^{-q_2\rho}\frac{q_1}{q_2}(1+q_2\rho)\right]+q_SW(\rho)\right\}\\&=-\frac{\mu_0}{2\pi}\frac{k_1^3k_2}{k_1^4-k_2^4}\left\{e^{ik_1\rho}\frac{k_2}{k_1}\left[-\frac{ik_1(1-k_S/k_2)}{\rho}+\frac{1}{\rho^2}\right]-e^{ik_2\rho}\frac{k_1}{k_2}\left(-\frac{ik_2}{\rho}+\frac{1}{\rho^2}\right)\right.\\&\quad\left.-ik_S^2\left[\frac{i\pi}{2}H_1^{(1)}(k_S\rho)-ie^{ik_2\rho}\sum_{m=0}^\infty V_m(\rho)-\frac{e^{ik_1\rho}}{k_S\rho}\sum_{m=0}^\infty U_{m+1}(\rho)\right]\right\}.\end{aligned} \tag{4.6}$$

U_m and V_m $(m=0,1,2,\ldots)$ are given by Eqs. (3.47) and (3.48). For obtaining an asymptotic formula for $B_{2\phi}$ when $k_2\rho\gg1$, one may follow the steps of Appendix B.

B. The *z*-component of the electric field

By use of Eqs. (4.1) and (3.10), Eq. (2.11) becomes

$$E_{2z}=\frac{i\omega\mu_0 q_1^3}{2\pi q_2}\frac{1}{q_1^4-q_2^4}\int_{q_2/q_S}^{q_1/q_S} d[(x^2-1)^{-1/2}]$$
$$\times\left[\int_0^\infty d\lambda\lambda\sqrt{\lambda^2+q_S^2x^2}J_0(\lambda\rho)-q_S^2x^2\int_0^\infty d\lambda\frac{\lambda J_0(\lambda\rho)}{\sqrt{\lambda^2+q_S^2x^2}}\right]. \tag{4.7}$$

After some straightforward algebra,[24]

$$E_{2z}=-\frac{i\omega\mu_0 k_1^3}{2\pi k_2}\frac{1}{k_1^4-k_2^4}\left\{e^{ik_1\rho}k_2\left[\frac{k_1(1-k_S^2/k_2^2)}{\rho}+\frac{i}{\rho^2}-\frac{1}{k_1\rho^3}\right]\right.$$
$$\left.-e^{ik_2\rho}k_1\left[\frac{k_2(1-k_S^2/k_1^2)}{\rho}+\frac{i}{\rho^2}-\frac{1}{k_2\rho^3}\right]-ik_S^3\check{W}(\rho)\right\}, \tag{4.8}$$

where

$$\check{W}(\rho)=\check{W}(\rho;-ik_1,-ik_2,-ik_S),\quad \check{W}(\rho;\xi_1,\xi_2,\xi_3)=\int_{\xi_2}^{\xi_1}\frac{d\upsilon}{\sqrt{\upsilon^2-\xi_3^2}}e^{-\upsilon\rho},\quad \xi_3\leqslant\xi_2<\xi_1. \tag{4.9}$$

Similar to Eq. (3.15),

$$\check{W}(\rho;q_1,q_2,q_S)=\check{W}(\rho;\infty,q_S,q_S)-\check{W}(\rho;\infty,q_1,q_S)-\check{W}(\rho;q_2,q_S,q_S), \tag{4.10}$$

the first term of which is calculated as[25]

$$\check{W}(\rho;\infty,q_S,q_S)=\int_0^\infty dt e^{-q_S\rho\cosh t}=K_0(q_S\rho). \tag{4.11}$$

1. Integral $\check{W}(\rho;\infty,q_1,q_S)$

On the basis of a term-by-term integration of Eq. (3.17),

$$\check{W}(\rho;\infty,q_1,q_S)=e^{-q_1\rho}\left[\sum_{m=0}^{M-1}\check{U}_m(\rho)+\check{R}_{1M}(\rho)\right],\quad M=1,2,\ldots, \tag{4.12}$$

where

$$\check{U}_m(\rho)=\frac{(\frac{1}{2})_m}{m!}(q_S\rho)^{2m}g_{2m+1}(q_1\rho)=-\frac{(\frac{1}{2})_m}{m!(2m)!}(-k_S^2\rho^2)^m\frac{d^{2m}}{dz^{2m}}[e^z\,\mathrm{Ei}(-z)]_{z=-ik_1\rho}, \tag{4.13}$$

$$\check{R}_{1M}(\rho)=\frac{(\frac{1}{2})_M}{(M-1)!}\left(\frac{q_S}{q_1}\right)^{2M}\int_1^\infty d\eta\,\eta^{-2M-1}e^{-q_1\rho(\eta-1)}$$
$$\times\int_0^1 dt(1-t)^{M-1}(1-q_S^2q_1^{-2}\eta^{-2}t)^{-M-1/2}$$
$$=\frac{(\frac{1}{2})_M}{M!}\left(\frac{q_S}{q_1}\right)^{2M}\int_1^\infty d\eta\,\eta^{-2M-1}{}_2F_1(M+\tfrac{1}{2},1;M+1;q_S^2q_1^{-2}\eta^{-2})e^{-q_1\rho(\eta-1)}. \tag{4.14}$$

Appealing properties of the series expansion ensue from the relations

$$|\check{R}_{1M}(\rho)|<\frac{1}{2}(1-|k_S^2|/|k_1^2|)^{-3/2}\frac{(\frac{1}{2})_M}{M!}\left|\frac{k_S^2}{k_1^2}\right|^M, \quad M=1,2,\ldots, \tag{4.15a}$$

$$\check{R}_{1M}(\rho)\sim\frac{(\frac{1}{2})_M}{M!}{}_2F_1(M+\tfrac{1}{2},1;M+1;k_S^2/k_1^2)\,\frac{1}{2M+1-ik_1\rho}\left(\frac{k_S^2}{k_1^2}\right)^M, \quad |k_1\rho|\gg 1, \tag{4.15b}$$

$$\check{R}_{1M}(\rho)\sim(1-k_S^2/k_1^2)^{-1}\frac{(\frac{1}{2})_M}{M!}\,\frac{1}{2M+1-ik_1\rho}\left(\frac{k_S^2}{k_1^2}\right)^M, \quad M\gg 1, \tag{4.15c}$$

and, with $|2m+1-ik_1\rho|\gg 1$,

$$\check{U}_m(\rho)\sim\frac{(\frac{1}{2})_m}{m!}\,\frac{1}{2m+1-ik_1\rho}\left(\frac{k_S^2}{k_1^2}\right)^m, \tag{4.16a}$$

$$\frac{\check{U}_{m+1}(\rho)}{\check{U}_m(\rho)}\sim\frac{m+1/2}{m+1}\,\frac{2m+1-ik_1\rho}{2m+3-ik_1\rho}\,\frac{k_S^2}{k_1^2}. \tag{4.16b}$$

As $M\to\infty$, the remainder $\check{R}_{1M}(\rho)$ approaches zero while being bounded uniformly in distance. The rate of convergence of the exact series is independent of ρ.

2. Integral $\check{W}(\rho;q_2,q_S,q_S)$

By use of Eq. (3.17),

$$\check{W}(\rho;q_2,q_S,q_S)=e^{-q_2\rho}\left[\sum_{m=0}^{M-1}\check{V}_m(\rho)+\check{R}_{2M}(\rho)\right], \tag{4.17}$$

where

$$\begin{aligned}\check{V}_m(\rho)&=-e^{i\pi/4}i^{m+1}\frac{(\frac{1}{2})_m}{m!}(2q_S\rho)^{-m-1/2}f_m(i(q_2-q_S)\rho)\\&=\sqrt{2\pi}i^m\frac{(\frac{1}{2})_m}{m!}\left(\frac{k_2-k_S}{2k_S}\right)^{m+1/2}\left\{e^{-iz}\frac{d^m}{dz^m}[z^{-1/2}F_0(z)]\right\}_{z=(k_2-k_S)\rho},\end{aligned} \tag{4.18}$$

$$\begin{aligned}\check{R}_{2M}(\rho)&=(-1)^M\frac{(\frac{1}{2})_M}{(M-1)!}\left(\frac{q_2-q_S}{2q_S}\right)^{M+1/2}\int_0^1 d\eta\,\eta^{M-1/2}e^{(q_2-q_S)\rho(1-\eta)}\\&\quad\times\int_0^1 dt(1-t)^{M-1}\left(1+\frac{q_2-q_S}{2q_S}\,\eta t\right)^{-M-1/2}\\&=(-1)^M\frac{(\frac{1}{2})_M}{M!}\left(\frac{q_2-q_S}{2q_S}\right)^{M+1/2}\\&\quad\times\int_1^\infty d\eta\,\eta^{M-1/2}{}_2F_1\left(M+\tfrac{1}{2},1;M+1;-\frac{q_2-q_S}{2q_S}\,\eta\right)e^{(q_2-q_S)\rho(1-\eta)}.\end{aligned} \tag{4.19}$$

$F_0(z)$ is defined by Eq. (3.42).

In analogy with expressions (4.15) and (4.16),

$$|\check{R}_{2M}(\rho)|<\frac{(\frac{1}{2})_M}{M!}\frac{1}{M+1/2}\left|\frac{k_2-k_S}{2k_S}\right|^{M+1/2}, \quad M=1,2,\ldots, \tag{4.20a}$$

$$\check{R}_{2M}(\rho)\sim(-1)^M\frac{(\frac{1}{2})_M}{M!}{}_2F_1\left(M+\tfrac{1}{2},1;M+1;-\frac{k_2-k_S}{2k_S}\right)$$
$$\times\frac{1}{M-1/2+i(k_2-k_S)\rho}\left(\frac{k_2-k_S}{2k_S}\right)^{M+1/2}, \quad |(k_2-k_S)\rho|\gg 1, \tag{4.20b}$$

$$\check{R}_{2M}(\rho)\sim\frac{2k_S}{k_2+k_S}(-1)^M\frac{(\frac{1}{2})_M}{M!}\frac{1}{M-1/2+i(k_2-k_S)\rho}\left(\frac{k_2-k_S}{2k_S}\right)^{M+1/2}, \quad M\gg 1, \tag{4.20c}$$

while for $|m+i(k_2-k_S)\rho|\gg 1$ and $m=1,2,\ldots,$

$$\check{V}_m(\rho)\sim(-1)^m\frac{(\frac{1}{2})_m}{m!}\frac{1}{m-1/2+i(k_2-k_S)\rho}\left(\frac{k_2-k_S}{2k_S}\right)^{m+1/2}, \tag{4.21a}$$

$$\frac{\check{V}_{m+1}(\rho)}{\check{V}_m(\rho)}\sim-\frac{m+1/2}{m+1}\frac{m-1/2+i(k_2-k_S)\rho}{m+1/2+i(k_2-k_S)\rho}\frac{k_2-k_S}{2k_S}. \tag{4.21b}$$

3. Exact formula for E_{2z}

By virtue of Eqs. (4.8)–(4.10),

$$E_{2z}=-\frac{i\omega\mu_0k_1^3}{2\pi k_2}\frac{1}{k_1^4-k_2^4}\left\{e^{ik_1\rho}k_2\left[\frac{k_1(1-k_S^2/k_2^2)}{\rho}+\frac{i}{\rho^2}-\frac{1}{k_1\rho^3}\right]\right.$$
$$-e^{ik_2\rho}k_1\left[\frac{k_2(1-k_S^2/k_1^2)}{\rho}+\frac{i}{\rho^2}-\frac{1}{k_2\rho^3}\right]$$
$$\left.-ik_S^3\left[\frac{i\pi}{2}H_0^{(1)}(k_S\rho)-e^{ik_2\rho}\sum_{m=0}^{\infty}\check{V}_m(\rho)-e^{ik_1\rho}\sum_{m=0}^{\infty}\check{U}_m(\rho)\right]\right\}. \tag{4.22}$$

$\check{U}_m(\rho)$ and $\check{V}_m(\rho)$ are defined by Eqs. (4.13) and (4.18).

V. SIMPLIFIED FORMULAS FOR $k_2\ll|k_1|$

The exact results of Secs. III and IV are simplified considerably under the condition

$$k_2\ll|k_1|, \tag{5.1}$$

which holds in many cases of practical interest. In this section, connection formulas for the approximations of Appendix C are recovered to the leading order in k_2/k_1.

A. Horizontal electric dipole

1. The z-component of the magnetic field

Equation (3.5) for B_{2z} becomes

$$B_{2z}\sim\frac{\mu_0}{2\pi k_1^2}\left[e^{ik_2\rho}\left(\frac{k_2^2}{\rho^2}+\frac{3ik_2}{\rho^3}-\frac{3}{\rho^4}\right)-e^{ik_1\rho}\left(\frac{k_1^2}{\rho^2}+\frac{3ik_1}{\rho^3}-\frac{3}{\rho^4}\right)\right]\sin\phi, \tag{5.2}$$

which is identical to the result given in Ref. 17 and agrees with formulas (C4), (C20), and (C21) of Appendix C. Note that condition (5.1) is redundant for establishing a smooth connection to formula (C4).

2. Tangential electric field

With

$$U_1(\rho)=-\frac{k_S^2\rho^2}{2}\left[e^{-ik_1\rho}\,\mathrm{Ei}(ik_1\rho)-\frac{1}{ik_1\rho}\right], \tag{5.3}$$

$$V_0(\rho)=-e^{i\pi/4}e^{-i(k_2-k_S)\rho}\sqrt{\frac{\pi}{2k_S\rho}}+\sqrt{\frac{\pi}{k_S\rho}}F((k_2-k_S)\rho), \tag{5.4}$$

$E_{2\phi}$ of Eq. (3.49) becomes

$$\begin{aligned}E_{2\phi}\sim-\frac{i\omega\mu_0}{2\pi k_1^2}\Bigg\{&e^{ik_2\rho}k_2\left[\frac{2i}{\rho^2}\left(1+\frac{k_2^2}{2k_1^2}\right)-\frac{2}{k_2\rho^3}\left(1+\frac{k_2^2}{2k_1^2}\right)-\frac{k_S^2}{k_1\rho}\sqrt{\frac{\pi}{k_S\rho}}F((k_2-k_S)\rho)\right.\\&+\frac{\pi k_S^2}{2k_1\rho}e^{-i(k_2-k_S)\rho}\left(e^{-ik_S\rho}H_1^{(1)}(k_S\rho)+e^{i\pi/4}\sqrt{\frac{2}{\pi k_S\rho}}\right)\Bigg]-e^{ik_1\rho}k_1\Bigg[\frac{i}{\rho^2}\left(1+\frac{k_2^2}{k_1^2}\right)\\&\left.-\frac{1}{k_1\rho^3}\left(1+\frac{2k_2^2}{k_1^2}\right)+\frac{ik_2^4}{2k_1^2}\left(e^{-ik_1\rho}\,\mathrm{Ei}(ik_1\rho)-\frac{1}{ik_1\rho}\right)\Bigg]\Bigg\}\sin\phi.\end{aligned} \tag{5.5}$$

A close inspection of the terms inside the parentheses containing the exponential integral Ei shows that these contribute to higher orders in k_2^2/k_1^2. On the other hand, the Hankel function and its accompanying term are negligible for $k_2\rho\leqslant O(1)$ under condition (5.1), while they are cancelled by the V_m's when $k_2\rho\gg 1$, as outlined in Appendix B. A moment's reflection leads to the uniform formula

$$E_{2\phi}\sim-\frac{i\omega\mu_0}{2\pi k_1^2}\left\{e^{ik_2\rho}\left[\frac{2ik_2}{\rho^2}-\frac{2}{\rho^3}-\frac{k_S^2k_2}{k_1\rho}\sqrt{\frac{\pi}{k_S\rho}}F((k_2-k_S)\rho)\right]-e^{ik_1\rho}\left(\frac{ik_1}{\rho^2}-\frac{1}{\rho^3}\right)\right\}\sin\phi, \tag{5.6}$$

valid for all distances that are consistent with the planar-earth model. This formula yields approximation (C6) as well as (C24) and (C25) of Appendix C when $k_2\rho\ll 1$ and $k_2\rho\gg 1$, respectively.

Similar steps can be taken for $E_{2\rho}$ of Eq. (3.64), to obtain

$$\begin{aligned}E_{2\rho}\sim-\frac{i\omega\mu_0}{2\pi}\frac{k_2^2}{k_1^2}\Bigg\{&e^{ik_2\rho}\left[-\frac{1-k_2^2/k_1^2}{k_2^2\rho^3}+i\frac{1-k_2^2/k_1^2}{k_2\rho^2}+\frac{1}{\rho}+\frac{ik_S^3}{k_1k_2}\sqrt{\frac{\pi}{k_S\rho}}F((k_2-k_S)\rho)\right.\\&\left.-\frac{\pi k_S^3}{2k_1k_2}e^{-i(k_2-k_S)\rho}\left(e^{-ik_S\rho}H_1^{(1)\prime}(k_S\rho)-e^{-i\pi/4}\sqrt{\frac{2}{\pi k_S\rho}}\right)\right]\\&-e^{ik_1\rho}\left[\frac{1-k_2^2/k_1^2}{k_2^2\rho^3}-\frac{ik_1}{k_2^2\rho^2}-\frac{ik_S^3}{2k_1k_2}\left(e^{-ik_1\rho}\,\mathrm{Ei}(ik_1\rho)-\frac{k_2^3}{k_S^3}\frac{1}{ik_1\rho}\right)\right]\Bigg\}\cos\phi.\end{aligned} \tag{5.7}$$

In consideration of the asymptotic expansion (B18) of Appendix B, it is inferred that

$$E_{2\rho}\sim-\frac{i\omega\mu_0}{2\pi k_1^2}\left\{e^{ik_2\rho}k_2\left[\frac{k_2}{\rho}+\frac{i}{\rho^2}-\frac{1}{k_2\rho^3}+\frac{ik_S^3}{k_1k_2}\sqrt{\frac{\pi}{k_S\rho}}F((k_2-k_S)\rho)\right]\right.$$
$$\left.-e^{ik_1\rho}k_1\left(\frac{1}{k_1\rho^3}-\frac{i}{\rho^2}\right)\right\}\cos\phi. \tag{5.8}$$

This formula is useful for all reasonable purposes yet it assumes that

$$k_2\rho\ll|k_1^5/k_2^5|, \tag{5.9}$$

which poses no practical restriction. The formula agrees with approximations (C5), (C22), and (C23) of Appendix C.

B. Vertical electric dipole

1. Magnetic field

Equation (4.6) for $B_{2\phi}$ furnishes

$$B_{2\phi}\sim-\frac{\mu_0}{2\pi}\left\{e^{ik_2\rho}\left[\frac{ik_2}{\rho}-\frac{1}{\rho^2}-\frac{k_2k_S^2}{k_1}\sqrt{\frac{\pi}{k_S\rho}}F((k_2-k_S)\rho)\right.\right.$$
$$\left.+\frac{\pi k_S^2k_2}{2k_1}e^{-i(k_2-k_S)\rho}\left(e^{-ik_S\rho}H_1^{(1)}(k_S\rho)+e^{i\pi/4}\sqrt{\frac{2}{\pi k_S\rho}}\right)\right]+e^{ik_1\rho}\frac{k_2^2}{k_1^2}$$
$$\left.\times\left[-\frac{ik_2^2}{2k_1\rho}\left(1-\frac{3}{4}\frac{k_2^2}{k_1^2}\right)+\frac{1}{\rho^2}-\frac{ik_1k_S^3\rho}{2k_2}\left(e^{-ik_1\rho}\,\mathrm{Ei}(ik_1\rho)-\frac{1}{ik_1\rho}\right)\right]\right\}. \tag{5.10}$$

Under the sensible condition

$$k_2\rho\ll|k_1^3/k_2^3|, \tag{5.11}$$

the exponential integral and its accompanying term can be neglected. Consequently,

$$B_{2\phi}\sim-\frac{\mu_0}{2\pi}\left\{e^{ik_2\rho}\left[\frac{ik_2}{\rho}-\frac{1}{\rho^2}-\frac{k_2k_S^2}{k_1}\sqrt{\frac{\pi}{k_S\rho}}F((k_2-k_S)\rho)\right]+e^{ik_1\rho}\frac{k_2^2}{k_1^2}\frac{1}{\rho^2}\right\}, \tag{5.12}$$

which connects smoothly to expressions (C10), and (C32) and (C33) of Appendix C.

2. The z-component of the electric field

The retainment of the first term in each series of Eq. (4.22) for E_{2z} yields

$$E_{2z}\sim-\frac{i\omega\mu_0}{2\pi k_2}\left\{-e^{ik_2\rho}\left[\frac{k_2(1-k_2^2/k_1^2)}{\rho}+\frac{i}{\rho^2}-\frac{1}{k_2\rho^3}+\frac{ik_S^3}{k_1}\sqrt{\frac{\pi}{k_S\rho}}F((k_2-k_S)\rho)\right.\right.$$
$$\left.-\frac{\pi k_S^3}{2k_1}e^{-i(k_2-k_S)\rho}\left(e^{-ik_S\rho}H_0^{(1)}(k_S\rho)-e^{-i\pi/4}\sqrt{\frac{2}{\pi k_S\rho}}\right)\right]$$
$$\left.+e^{ik_1\rho}\frac{k_2}{k_1}\left[-\frac{k_1}{\rho}\frac{k_2^4}{k_1^4}+\frac{i}{\rho^2}-\frac{1}{k_1\rho^3}-\frac{ik_S^3}{k_2}\left(e^{-ik_1\rho}\,\mathrm{Ei}(ik_1\rho)-\frac{k_2^3}{k_S^3}\frac{1}{ik_1\rho}\right)\right]\right\}. \tag{5.13}$$

With condition (5.11), the preceding expression becomes

$$E_{2z}\sim -\frac{i\omega\mu_0}{2\pi k_2}\left\{-e^{ik_2\rho}\left[\frac{k_2}{\rho}+\frac{i}{\rho^2}-\frac{1}{k_2\rho^3}+\frac{ik_S^3}{k_1}\sqrt{\frac{\pi}{k_S\rho}}F((k_2-k_S)\rho)\right]\right.$$
$$\left.+e^{ik_1\rho}\frac{k_2}{k_1}\left(\frac{i}{\rho^2}-\frac{1}{k_1\rho^3}\right)\right\}, \tag{5.14}$$

in agreement with approximations (C11), and (C34) and (C35) of Appendix C.

Approximations (5.6), (5.8), (5.12), and (5.14) are in full agreement with the formulas of King *et al.*,[17] provided that the replacement of $(k_2-k_S)\rho$ by $\wp$ is made according to (3.50).

VI. CONCLUSIONS AND DISCUSSION

We start this paper with the Fourier–Bessel integral representations for the fields in the planar boundary between air and a homogeneous half space of infinitesimal electric dipoles lying in the interface. The focus is on the components E_ρ and E_ϕ of the horizontal dipole and B_ϕ and E_z of the vertical dipole in the cylindrical coordinates of Figs. 1 and 3. These components can be given by one-dimensional integrals of elementary functions, as is known from previous works on the Hertz vector.[4–10] The present analysis is believed to go a step further by relaxing the condition $k_2^2 \ll |k_1^2|$ and replacing the integrals by simple, exact integrated series which are usable for any distance from the source. It is verified that the B_z component of a horizontal dipole is described by simple elementary functions.

The exposition bears two appealing features. The first feature is that the ratio of any successive terms in each series is shown to be proportional to k_2^2/k_1^2, i.e., the inverse of the diffraction index squared, while it remains bounded uniformly in ρ. The relative errors due to the retainment of a finite number of terms in the series, say M, are essentially of the order of $(k_2^2/k_1^2)^M$ regardless of $k_2\rho$ and $k_1\rho$. In most cases of practical interest where $|k_1|\geqslant 3k_2$, at most three or four terms of each expansion suffice for reasonable accuracy.

The second feature is that the summands are expressed in simple closed form as the well-known exponential and Fresnel integrals. These functions explicitly reveal the dependence on the physical parameters such as the $k_1\rho$ and the Sommerfeld numerical distance. They also provide a natural connection to the recently obtained, approximate formulas of King *et al.* that distinguish between the direct and ideal-image fields and the lateral-wave or surface-wave contributions when $k_2^2 \ll |k_1^2|$.[17] The present treatment not only verifies the results of these authors by different, exact means, but also extends their validity to distances close to the source.

The two features mentioned above illustrate the advantages of the proposed formulas over representations of the incomplete Hankel function used for the same purpose.[27] The price that one seems to pay for this simplicity, however, is the limitation in the choice of possible configurations or field components that can be treated exactly in a similar fashion.[21] Obtaining integrated series of analogous properties for the remaining components of Eqs. (2.1)–(2.6) and (2.10)–(2.12) is an open problem for future work.

Higher-order terms of the derived series may become of importance for radiowave propagation over a very dry earth; another example of applications could perhaps be related to the so-called ''low-k'' dielectric insulators.[30] As in Ref. 19, the present model is restricted in its applicability due to the assumption of a planar boundary. Lowest-order correction formulas to take into account the effect of a finite yet sufficiently large radius of curvature are given elsewhere.[31–34]

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APPENDIX A: GENERALIZED FORMULA FOR INTEGRAL $\mathcal{W}(\boldsymbol{\rho})$

In this appendix, a generalized integration procedure is described which leads to Eq. (3.13) as a special case. More precisely, with the decomposition

$$\mathcal{W}(\rho)=\frac{q_2}{q_1}I(q_1\rho,q_S\rho;-1/2)-\frac{q_1}{q_2}I(q_2\rho,q_S\rho;-1/2), \tag{A1}$$

attention is focused on the integral

$$I(\alpha,\beta;\zeta)=\int_0^\infty dx\,\frac{(x^2+\alpha^2)^{-\zeta}}{x^2+\beta^2}J_1(x),\quad \alpha\geqslant\beta>0. \tag{A2}$$

Of course, I is understood as Abel summable in $x\to\infty$. Without loss of generality, α and β are assumed to be positive. The inequality $\alpha\geqslant\beta$ is imposed for definiteness.

1. Case $\alpha=\beta$

With $\alpha=\beta$,

$$I(\alpha,\alpha;\zeta)=\int_0^\infty dx(x^2+\alpha^2)^{-\zeta-1}J_1(x). \tag{A3}$$

The starting point is the known formula[24]

$$\int_0^\infty dx\,x^{\nu+1}\frac{J_\nu(x)}{(x^2+\alpha^2)^{1+\zeta}}=\frac{2^{-\zeta}\alpha^{\nu-\zeta}}{\Gamma(1+\zeta)}K_{\nu-\zeta}(\alpha),\quad -1<\mathrm{Re}\,\nu<2\,\mathrm{Re}\,\zeta+3/2, \tag{A4}$$

where $K_{\nu-\zeta}$ is the modified Bessel function of the third kind. Note that one may not set $\nu=-1$ on both sides of this equation simultaneously. Caution needs to be exercised because allowing $\nu\to-1^+$ in

$$x^{\nu+1}J_\nu(x)=O(x^{2\nu+1})\ \text{ as }\ x\to0^+,$$

results in a nonintegrable singularity at $x=0$ with a vanishing numerical coefficient.

A remedy is to employ the integral

$$\int_0^\infty dx\,x^{\nu+1}J_\nu(x)=0,\ \ \mathrm{Re}\,\nu>-1, \tag{A5}$$

and rewrite $I(\alpha,\alpha;\zeta)$ as

$$\begin{aligned}I(\alpha,\alpha;\zeta)=&-\lim_{\nu\to-1^+}\left\{\int_0^\infty dx\,x^{\nu+1}[(x^2+\alpha^2)^{-1-\zeta}-\alpha^{-2(1+\zeta)}]J_\nu(x)\right\}\\&+\alpha^{-2(1+\zeta)}\int_0^\infty dx\,J_1(x)\\=&-\frac{2^{-\zeta}\alpha^{-(1+\zeta)}}{\Gamma(1+\zeta)}K_{1+\zeta}(\alpha)+\alpha^{-2(1+\zeta)}.\end{aligned} \tag{A6}$$

Because $K_{n+1/2}(\alpha)$ is elementary if n is any integer, the conclusion is reached that $I(\alpha,\alpha;\zeta)$ is an elementary function if $\zeta=n-1/2$. Explicitly, one gets[25]

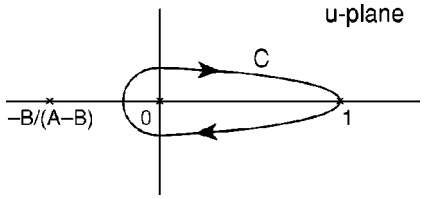

FIG. 4. Contour of integration C for the integral of Eq. (A11).

$$I(\alpha,\alpha;n-1/2)=\begin{cases}\alpha^{-2n-1}+\dfrac{(-1)^{n+1}}{(2n-1)!!}\left(\dfrac{d}{\alpha\,d\alpha}\right)^{n}\dfrac{e^{-\alpha}}{\alpha}, & n=1,2,\ldots,\\ \alpha^{-1}(1-e^{-\alpha}), & n=0,\\ \alpha^{-2n-1}\left[1+\{(2|n|-1)!!\}\left(\dfrac{d}{\alpha\,d\alpha}\right)^{|n|-1}\dfrac{e^{-\alpha}}{\alpha}\right], & -n=1,2,\ldots,\end{cases} \tag{A7}$$

where, in the usual notation, $(2m-1)!!=1\cdot 3\cdots(2m-1)$ for positive integer m.

2. Case $\alpha>\beta$

Let

$$A=x^2+\alpha^2, \quad B=x^2+\beta^2, \tag{A8}$$

and consider the integral representations

$$A^{-\zeta}=\frac{1}{\Gamma(\zeta)}\int_0^\infty d\xi\,\xi^{-1+\zeta}e^{-A\xi}, \quad \mathrm{Re}\,\zeta>0,$$

$$B^{-1}=\int_0^\infty d\eta\,e^{-B\eta}. \tag{A9}$$

The radical in Eq. (A2) is recast in the form

$$A^{-\zeta}B^{-1}=\frac{1}{\Gamma(\zeta)}\int_0^\infty\int_0^\infty d\xi\,d\eta\,\xi^{-1+\zeta}e^{-(A\xi+B\eta)} \quad [\xi=uv,\eta=(1-u)v]$$

$$=\zeta\int_0^1 du\,u^{-1+\zeta}[Au+B(1-u)]^{-1-\zeta}, \quad \mathrm{Re}\,\zeta>0. \tag{A10}$$

Analytic continuation to complex ζ with $\mathrm{Re}\,\zeta<0$ is brought about via the integral

$$A^{-\zeta}B^{-1}=\frac{\zeta}{1-e^{i2\pi\zeta}}\int_C du\,u^{-1+\zeta}[Au+B(1-u)]^{-1-\zeta}, \tag{A11}$$

where C is a closed contour in the u-plane. C originates from $u=1$ in the first Riemann sheet and encircles the origin in the clockwise sense, as shown in Fig. 4. The first Riemann sheet is defined so that

$$u^{-1+\zeta}>0 \quad \text{and} \quad [Au+B(1-u)]^{-1-\zeta}>0, \ 0<u<1, \tag{A12}$$

with the associated branch cuts lying along the positive and negative real axis. Note that in addition to the branch point at $u=0$ another branch point exists in the negative axis at $u=-B/(A-B)$.

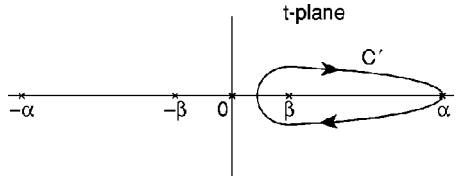

FIG. 5. Map of C of Fig. 4 in the t-plane via $t^2=\alpha^2u+\beta^2(1-u)$.

With Eq. (A6), it follows that

$$I(\alpha,\beta;\zeta)=\frac{\zeta}{1-e^{i2\pi\zeta}}\int_C du\,u^{-1+\zeta}\int_0^\infty dx\{x^2+[\alpha^2u+\beta^2(1-u)]\}^{-1-\zeta}J_1(x)$$

$$=-\frac{\zeta e^{-i\pi\zeta}}{2i\sin\pi\zeta}\int_C du\,u^{-1+\zeta}[\alpha^2u+\beta^2(1-u)]^{-(1+\zeta)}$$

$$\times\left\{1-\frac{2^{-\zeta}}{\Gamma(1+\zeta)}[\alpha^2u+\beta^2(1-u)]^{(1+\zeta)/2}K_{1+\zeta}(\sqrt{\alpha^2u+\beta^2(1-u)})\right\}. \quad \text{(A13)}$$

Hence, $I(\alpha,\beta;\zeta)$ is an integral of an elementary function if $\zeta=n-1/2$, n: integer.

Let

$$t=t(u)=\sqrt{\alpha^2u+\beta^2(1-u)}, \quad t(1)=\alpha, \ \ t(0)=\beta. \quad \text{(A14)}$$

This transformation maps C onto C' (Fig. 5):

$$I(\alpha,\beta;\zeta)=-\frac{\zeta e^{-i\pi\zeta}}{i\sin\pi\zeta}\frac{1}{(\alpha^2-\beta^2)^\zeta}\int_{C'}dt\,t^{-1-2\zeta}(t^2-\beta^2)^{-1+\zeta}$$

$$\times\left\{1-\frac{2^{-\zeta}}{\Gamma(1+\zeta)}t^{1+\zeta}K_{1+\zeta}(t)\right\}. \quad \text{(A15)}$$

By virtue of the identity

$$\frac{d}{dt}[t^{-2\zeta}(t^2-\beta^2)^\zeta]=2\beta^2\zeta t^{-1-2\zeta}(t^2-\beta^2)^{-1+\zeta}, \quad \text{(A16)}$$

application of integration by parts to Eq. (A15) furnishes

$$I(\alpha,\beta;\zeta)=\alpha^{-2\zeta}\beta^{-2}\left[1-\frac{2^{-\zeta}\alpha^{1+\zeta}}{\Gamma(1+\zeta)}K_{1+\zeta}(\alpha)\right]$$

$$-\frac{e^{-i\pi\zeta}}{2i\sin\pi\zeta}\frac{2^{-\zeta}}{\Gamma(1+\zeta)}\frac{1}{\beta^2(\alpha^2-\beta^2)^\zeta}\int_{C'}dt\,t^{-2\zeta}(t^2-\beta^2)^\zeta\frac{d}{dt}[t^{1+\zeta}K_{1+\zeta}(t)]. \quad \text{(A17)}$$

It is of some interest to write down recursive formulas that are particularly useful for $\zeta=n-1/2$, where n is any integer. Clearly, from Eq. (A2),

$$I(\alpha,\beta;\zeta+1)=-\frac{1}{2\alpha}\frac{1}{\zeta}\frac{\partial}{\partial\alpha}I(\alpha,\beta;\zeta), \quad \text{(A18)}$$

while

$$I(\alpha,\beta;\zeta-1)=(\alpha^2-\beta^2)I(\alpha,\beta;\zeta)+I(\alpha,\alpha;\zeta-1)$$
$$=(\alpha^2-\beta^2)I(\alpha,\beta;\zeta)+\alpha^{-2\zeta}-\frac{2^{-\zeta+1}\alpha^{-\zeta}}{\Gamma(\zeta)}K_{-\zeta}(\alpha). \tag{A19}$$

Therefore, it suffices to evaluate $I(\alpha,\beta;\zeta)$ for $\zeta=-1/2$. Equation (A18) can be employed for $\zeta=-1/2, 1/2, 3/2, \ldots$, and Eq. (A19) is adequate for $\zeta=-1/2, -3/2, -5/2, \ldots$.

The substitution $\zeta=-1/2$ in Eq. (A17) gives

$$I(\alpha,\beta;-1/2)=\frac{\alpha}{\beta^2}(1-e^{-\alpha})-\frac{\sqrt{\alpha^2-\beta^2}}{2\beta^2}\int_{C'}dt\,\frac{t}{\sqrt{t^2-\beta^2}}e^{-t}. \tag{A20}$$

Since the integrand has now an integrable singularity at $t=\beta$, the path can be indented back to the positive real axis:

$$I(\alpha,\beta;-1/2)=\frac{\alpha}{\beta^2}(1-e^{-\alpha})-\frac{\sqrt{\alpha^2-\beta^2}}{\beta^2}\int_{\beta}^{\alpha}dt\,\frac{t}{\sqrt{t^2-\beta^2}}e^{-t}. \tag{A21}$$

This result agrees with Eqs. (3.13) and (3.14). Evidently, applying Eq. (A18) does not produce any new integrals of elementary functions.

APPENDIX B: AN ASYMPTOTIC EXPANSION FOR $E_{2\phi}$

In this appendix, an asymptotic formula is derived for the $E_{2\phi}$ of Sec. III when $k_2\rho\gg 1$ and $k_2<|k_1|$ on the basis of its exact series expansion. Consider the $W(\rho)$ of Eq. (3.14). The combination of the first and third terms in Eq. (3.15) yields

$$W(\rho)=W(\rho;\infty,-ik_2,-ik_S)-W(\rho;\infty,-ik_1,-ik_S), \tag{B1}$$

where the second term here is given by Eq. (3.27) and

$$W(\rho;\infty,q_2,q_S)=e^{-q_S\rho}q_S\int_{(q_2-q_S)/q_S}^{\infty}\frac{d\eta}{\sqrt{\eta}}(1+\eta)(2+\eta)^{-1/2}e^{-q_S\rho\eta}. \tag{B2}$$

1. Wave through region 2

When $|q_S\rho|\gg 1$, the major contribution to integral (B2) arises from the vicinity of the lower endpoint of width $O[(q_S\rho)^{-1}]$. If in addition $|(q_2-q_S)\rho|\leqslant O(1)$, $\eta=0$ falls inside the critical region and the radical can be replaced by a Maclaurin expansion. Accordingly,

$$W(\rho;\infty,q_2,q_S)=-e^{-q_2\rho}q_S\left[\sum_{m=0}^{M-1}\mathcal{V}_m(\rho)-e^{(q_2-q_S)\rho}\Upsilon_M(\rho)-R_{2M}(\rho)\right],\quad M\geqslant 1, \tag{B3}$$

where

$$\mathcal{V}_m(\rho)=-e^{i\pi/4}i^{m+1}\frac{(\frac{1}{2})_m}{m!}\frac{m+1/2}{m-1/2}(2q_S\rho)^{-m-1/2}\varphi_m(i(q_2-q_S)\rho), \tag{B4}$$

$$\varphi_m(z)=\sqrt{2\pi}(-i)^m e^{-iz}z^{1/2+m}\frac{d^m}{dz^m}[z^{-1/2}e^{iz}F(z)], \tag{B5}$$

$$F(z)=e^{-iz}\int_z^{\infty}dx\,\frac{e^{ix}}{\sqrt{2\pi x}}=e^{-iz}\left[\frac{1}{2}(1+i)-F_0(z)\right]. \tag{B6}$$

$F_0(z)$ is introduced in Eqs. (3.41) and (3.42), $R_{2M}(\rho)$ is given by Eq. (3.34), and $\Upsilon_M(\rho)$ is the remainder in the sense of Poincaré[35] of an asymptotic expansion for $e^{q_S\rho}K_1(q_S\rho)$ when M terms are summed,[25] i.e., $\Upsilon_M(\rho)=O[(k_S\rho)^{-M-1/2}]$ as $|k_S\rho|\to\infty$ for $M=O(1)$, uniformly in $\mathrm{Arg}(k_S\rho)$. Compare with Eqs. (3.31).

For $1\leqslant M=O(1)$ and $|(k_2-k_S)/(2k_S)|\ll 1$,

$$R_{2M}(\rho)=O\left[\left(\frac{k_2-k_S}{2k_S}\right)^{M+1/2}\right],\quad |(k_2-k_S)\rho|\leqslant O(1), \tag{B7}$$

leading to

$$\frac{e^{-i(k_2-k_S)\rho}\Upsilon_M(\rho)+R_{2M}(\rho)}{\mathcal{V}_{M-1}(\rho)}=O\left(\frac{1}{k_2\rho}\right). \tag{B8}$$

When $|(k_2-k_S)\rho|\gg 1$, the remainder $R_{2M}(\rho)$ dominates over the $\Upsilon_M(\rho)$ in Eq. (B3). It follows that

$$R_{2M}(\rho)=O\left[\left(\frac{k_2-k_S}{2k_S}\right)^{M+1/2}\frac{1}{(k_2-k_S)\rho}\right],\quad |(k_2-k_S)\rho|\gg 1,\ M=O(1), \tag{B9}$$

by inspection of Eq. (3.36b), and

$$\frac{e^{-i(k_2-k_S)\rho}\Upsilon_M(\rho)+R_{2M}(\rho)}{-\mathcal{V}_{M-1}(\rho)}=O\left(\frac{k_2-k_S}{2k_S}\right). \tag{B10}$$

Of course, in the limit $M\to\infty$ the remainder $\Upsilon_M(\rho)$ is unbounded and the series from Eq. (B3) diverges. In the sense implied by Eq. (B3),

$$W(\rho;\infty,q_2,q_S)\sim -e^{-q_2\rho}q_S\sum_{m=0}^{\infty}\mathcal{V}_m(\rho). \tag{B11}$$

This asymptotic expansion can be attained somewhat heuristically from the exact series (3.40) combined with the asymptotic expansion for $H_1^{(1)}(k_S\rho)$. Notice that

$$\frac{d^m}{dz^m}[z^{-1/2}F_0(z)]=\frac{e^{i\pi/4}}{\sqrt{2}}(-1)^m\left(\frac{1}{2}\right)_m z^{-1/2-m}-\frac{d^m}{dz^m}[z^{-1/2}e^{iz}F(z)]. \tag{B12}$$

2. Wave through region 1

From Eq. (B1), consider the integral

$$W(\rho;\infty,q_1,q_S)=q_1\int_1^{\infty}d\eta\,\frac{\eta}{\sqrt{\eta^2-\overline{q}}}e^{-q_1\rho\eta},\quad \overline{q}=q_S^2/q_1^2,\ |\overline{q}|<1. \tag{B13}$$

When $|q_1\rho|\gg 1$, the principal contribution to integration comes from the vicinity of $\eta=1$. Accordingly, expand the radical as

$$\frac{\eta}{\sqrt{\eta^2-\overline{q}}}-1=\sum_{n=0}^{N-1}\frac{(-1)^n}{n!}\mathcal{A}_n(\overline{q})(\eta-1)^n+O[(\eta-1)^N],\quad N\geqslant 1, \tag{B14}$$

where

$$\mathcal{A}_0(\overline{q})=\frac{\overline{q}}{\sqrt{1-\overline{q}}(1+\sqrt{1-\overline{q}})}, \tag{B15}$$

and, for $n=1,2,\ldots,$[28]

$$\begin{aligned}\mathcal{A}_n(\overline{q})&=(-1)^n\frac{d^n}{d\eta^n}\frac{\eta}{\sqrt{\eta^2-\overline{q}}}\bigg|_{\eta=1}\\&=\overline{q}\frac{2^n}{\sqrt{\pi}}\Gamma\left(\frac{n+3}{2}\right)\Gamma\left(1+\frac{n}{2}\right){}_2F_1\left(\frac{n+3}{2},\frac{n}{2}+1;2;\overline{q}\right)\\&=2^{[(n-1)/2]}\{(2[n/2]+1)!!\}\frac{d^{[(n-1)/2]}}{d\overline{q}^{[(n-1)/2]}}\{\overline{q}^{[(n-1)/2]+1}(1-\overline{q})^{-(2[n/2]+3)/2}\}.\end{aligned} \tag{B16}$$

$[x]$ denotes the integral part of x. Note that the second line of Eq. (B16) holds even for $n=0$.

It follows that

$$W(\rho;\infty,q_1,q_S)=\frac{e^{-q_1\rho}}{\rho}\left\{1+\sum_{n=0}^{N-1}\frac{\mathcal{A}_n(\overline{q})}{(-q_1\rho)^n}+O[(q_1\rho)^{-N}]\right\},\quad N\geqslant 1. \tag{B17}$$

The first term inside the braces is the $U_0(\rho)$ from Eq. (3.19). This expansion can be verified directly from Eq. (3.18) by invoking the formula[28]

$$e^z\mathrm{Ei}(-z)=\sum_{n=0}^{N-1}(-1)^{n+1}n!\,z^{-1-n}+O(|z|^{-N-1})\ \text{ as }\ z\to\infty,\quad \begin{cases}N=1,2,\ldots,\\ |\mathrm{Arg}\ z|<3\pi/2,\end{cases} \tag{B18}$$

which holds uniformly in Arg z, interchanging the order of summation and subsequently allowing $M\to\infty$.

3. Asymptotic formula for $E_{2\phi}$

The resulting asymptotic expansion for $E_{2\phi}$ reads as

$$\begin{aligned}E_{2\phi}\sim&-\frac{i\omega\mu_0}{2\pi}\frac{k_2^2}{k_1^4-k_2^4}\left\{-ie^{ik_1\rho}k_1\left[\frac{k_1^2+k_2^2(2-k_S/k_2)}{k_2^2\rho^2}+i\frac{k_1^2+2k_2^2}{k_1k_2^2\rho^3}\right]\right.\\&\left.+ie^{ik_2\rho}\frac{2k_1^2+k_2^2}{k_2\rho^2}\left(1+\frac{i}{k_2\rho}\right)-\frac{k_1k_S^2}{k_2\rho}\left[\frac{e^{ik_1\rho}}{ik_S\rho}\sum_{n=0}^{\infty}\frac{\mathcal{A}_n(k_S^2/k_1^2)}{(ik_1\rho)^n}-e^{ik_2\rho}\sum_{m=0}^{\infty}\mathcal{V}_m(\rho)\right]\right\}\sin\phi.\end{aligned} \tag{B19}$$

Similar expressions can be written down by inspection for the other components of Secs. III and IV.

APPENDIX C: ASYMPTOTIC FORMULAS FOR $k_2\rho\ll 1$ AND $k_2\rho\gg 1$

In this appendix, simple approximations are applied directly to the integrals (2.1)–(2.6) and (2.10)–(2.12) when $k_2^2\ll|k_1^2|$ under the conditions $k_1\rho=O(1)$ and $k_2\rho\gg 1$.

1. Case $k_2^2\ll|k_1^2|$, $k_1\rho=O(1)$

In terms of the q_j $(j=1,2)$ of Eqs. (3.1), $|q_2\rho|\ll 1$ while $q_1\rho$ is kept fixed and $|q_2^2|\ll|q_1^2|$. Then the principal contribution to integration arises from a range where $\lambda=O(1/\rho)\gg|q_2|$. Accordingly, the following approximation becomes effective:

$$\sqrt{k_2^2-\lambda^2}\sim i\lambda$$

A. Horizontal electric dipole

With these approximations, B_{2z} becomes

$$B_{2z}\sim \frac{\mu_0}{2\pi}\int_0^\infty d\lambda\ \lambda^2\frac{J_1(\lambda\rho)}{\sqrt{\lambda^2+q_1^2}+\lambda}\sin\phi=\frac{\mu_0}{2\pi q_1^2}\left\{\frac{1}{\rho^4}\mathcal{I}_m(q_1\rho)-\int_0^\infty d\lambda\ \lambda^3 J_1(\lambda\rho)\right\}\sin\phi, \tag{C2}$$

where

$$\int_0^\infty d\lambda\ \lambda^3 J_1(\lambda\rho)=-\frac{3}{\rho^4}, \tag{C3}$$

while the integral $\mathcal{I}_m$ is given by Eq. (3.4). Hence,

$$B_{2z}\sim \frac{\mu_0 k_1^2}{2\pi}\left[e^{ik_1\rho}\left(\frac{3}{k_1^4\rho^4}-\frac{3i}{k_1^3\rho^3}-\frac{1}{k_1^2\rho^2}\right)-\frac{3}{k_1^4\rho^4}\right]\sin\phi. \tag{C4}$$

In the same vein, by virtue of Eq. (3.8) for $\mathcal{I}_e$,

$$\begin{aligned}E_{2\rho}&\sim \frac{i\omega\mu_0}{2\pi q_1^2}\left\{\left(\frac{1}{\rho}+\frac{d}{d\rho}\right)\left[\frac{1}{\rho^2}\mathcal{I}_e(q_1\rho)\right]-\frac{1}{\rho}\int_0^\infty d\lambda\ \lambda J_1(\lambda\rho)\right\}\cos\phi\\&=\frac{i\omega\mu_0 k_1}{2\pi}\left\{e^{ik_1\rho}\left(\frac{1}{k_1^3\rho^3}-\frac{i}{k_1^2\rho^2}\right)+\frac{1}{k_1^3\rho^3}\right\}\cos\phi,\end{aligned} \tag{C5}$$

$$\begin{aligned}E_{2\phi}&\sim -\frac{i\omega\mu_0}{2\pi q_1^2}\left\{\left(\frac{1}{\rho}+\frac{d}{d\rho}\right)\left[\frac{1}{\rho^2}\mathcal{I}_e(q_1\rho)\right]-\frac{d}{d\rho}\int_0^\infty d\lambda\ \lambda J_1(\lambda\rho)\right\}\sin\phi\\&=\frac{i\omega\mu_0 k_1}{2\pi}\left\{e^{ik_1\rho}\left(-\frac{1}{k_1^3\rho^3}+\frac{i}{k_1^2\rho^2}\right)+\frac{2}{k_1^3\rho^3}\right\}\sin\phi.\end{aligned} \tag{C6}$$

The computation of the limiting forms of E_{2z}, $B_{2\rho}$ and $B_{2\phi}$ is more involved:

$$\begin{aligned}E_{2z}&\sim \frac{i\omega\mu_0}{2\pi q_1^2}\lim_{\epsilon\to 0^+}\frac{\partial}{\partial\rho}\int_0^\infty d\lambda\ \sqrt{\lambda^2+q_1^2}e^{-\epsilon\sqrt{\lambda^2+q_1^2}}J_0(\lambda\rho)\cos\phi\\&=\frac{i\omega\mu_0}{2\pi q_1^2}\lim_{\epsilon\to 0^+}\frac{\partial}{\partial\rho}\frac{\partial^2}{\partial\epsilon^2}\left\{I_0\left[\frac{q_1}{2}(\sqrt{\epsilon^2+\rho^2}-\epsilon)\right]K_0\left[\frac{q_1}{2}(\sqrt{\epsilon^2+\rho^2}+\epsilon)\right]\right\}\cos\phi\\&=\frac{\omega\mu_0}{4\rho}J_1(k_1\rho/2)H_1^{(1)}(k_1\rho/2)\cos\phi,\end{aligned} \tag{C7}$$

$$B_{2\rho}\sim -\frac{i\mu_0}{4}\frac{d}{d\rho}\left[\frac{1}{\rho}J_1(k_1\rho/2)H_1^{(1)}(k_1\rho/2)\right]\sin\phi, \tag{C8}$$

where use is made of Ref. 36, and

$$B_{2\phi}\sim -\frac{i\mu_0}{4\rho^2}\frac{k_1}{k_2}J_1(k_1\rho/2)H_1^{(1)}(k_1\rho/2)\cos\phi. \tag{C9}$$

Compare with the exposition in Ref. 13. In principle, the behavior of the z-component of the electric field depends on the limit path. For instance, if the observation point is forced to approach the source along a straight line from region 1 ($z<0$), this component behaves as $\sim 1/\rho^3$. [The divergence can ensue from taking $\epsilon=\rho$ in the second line of Eq. (C7).]

B. Vertical electric dipole

From the Fourier–Bessel integral (2.10),

$$B_{2\phi}\sim \frac{\mu_0}{2\pi q_1^2}\left[q_1^2\int_0^\infty d\lambda\,\lambda J_1(\lambda\rho)-\frac{q_2^2}{\rho^2}\mathcal{I}_e(q_1\rho)\right]$$
$$=-\frac{\mu_0}{2\pi\rho^2}\left[e^{ik_1\rho}\frac{k_2^2}{k_1^2}-\left(1+\frac{k_2}{k_1}ik_2\rho\right)\right]\sim-\frac{\mu_0}{2\pi\rho^2}\left(e^{ik_1\rho}\frac{k_2^2}{k_1^2}-1\right). \tag{C10}$$

Likewise, starting with Eq. (2.11) gives

$$E_{2z}\sim\frac{i\omega\mu_0}{2\pi\rho}\left[e^{ik_1\rho}\left(\frac{1}{k_1^2\rho^2}-\frac{i}{k_1\rho}\right)-\frac{1}{k_2^2\rho^2}\right]. \tag{C11}$$

The formula for $E_{2\rho}$ is more involved, in analogy with Eqs. (C7)–(C9). It is

$$E_{2\rho}\sim\frac{i\omega\mu_0}{2\pi\rho}\left[\frac{i\pi}{2}J_1(k_1\rho/2)H_1^{(1)}(k_1\rho/2)-\frac{k_2^2}{k_1^2}\right]. \tag{C12}$$

2. Case $k_2^2\ll|k_1^2|$, $k_2\rho\gg 1$

When $|k_j\rho|\gg 1$ $(j=1,2)$, the oscillations of the Bessel functions in Eqs. (2.1)–(2.6) and (2.10)–(2.12) force the major contributions to integration to arise from the vicinities of the branch points at $\lambda=k_j$ with widths $O(1/\rho)$. The condition $k_2^2\ll|k_1^2|$ permits considerable simplification because, heuristically speaking, the two contributing regions separate.

Following Sommerfeld,[29] one may replace each J_n $(n=0,1,2)$ by $(1/2)[H_n^{(1)}+H_n^{(2)}]$. The contour Γ can be chosen symmetric under inversion through the origin, as shown in Fig. 2. Use is made of the analytic continuation formula

$$H_n^{(2)}(ze^{-i\pi})=(-1)^{n+1}H_n^{(1)}(z),\quad n:\ \text{integer}. \tag{C13}$$

For notational convenience, let $\mathcal{F}_{2\kappa,j}$ ($\mathcal{F}=E,\ B;\ \kappa=\rho,\ \phi,\ z;\ j=1,2$) denote the part of the field component that corresponds to the contour integral along Γ_j. Each $\mathcal{F}_{2\kappa,j}$ follows upon the replacements

$$\mathcal{F}_{2\kappa}\to\mathcal{F}_{2\kappa,j}\ \text{ under }\ \int_0^\infty d\lambda(\cdots)J_n(\lambda\rho)\to\frac{1}{2}\int_{\Gamma_j}d\lambda(\cdots)H_n^{(1)}(\lambda\rho). \tag{C14}$$

Each $\mathcal{F}_{2\kappa,j}$ amounts to a wave traveling with the phase velocity of medium j.

With

$$H_0^{(1)}(\lambda\rho)+H_2^{(1)}(\lambda\rho)=\frac{2}{\lambda\rho}H_1^{(1)}(\lambda\rho), \tag{C15}$$

the Hankel functions in each $\mathcal{F}_{2\kappa,j}$ are approximated according to

$$H_n^{(1)}(k_j\rho(1+it))\sim e^{ik_j\rho-in\pi/2-i\pi/4}\sqrt{\frac{2}{\pi k_j\rho}}e^{-k_j\rho t},\quad |k_j\rho|\gg 1,\ t\to 0^+. \tag{C16}$$

Due to the rapid exponential decrease here, the major contribution to integration on each side of the branch cut (positive t-axis) originates from the corresponding branch point ($t=0$).[37]

Upon the change of variable $\lambda=k_j(1+it)$, it is recognized that for $\lambda\sim k_j$,

$$\sqrt{1-(\lambda/k_j)^2}=\pm e^{-i\pi/4}\sqrt{2t}\sqrt{1+it/2}\sim\pm e^{-i\pi/4}\sqrt{2t},\quad t\to 0^+,\quad \sqrt{t}\geqslant 0, \tag{C17}$$

where the upper sign holds along the left-hand side and the lower sign along the right-hand side of each branch cut. For instance, $D(\lambda)$ of Eq. (2.8) becomes

$$D(\lambda)\sim\pm e^{-i\pi/4}\sqrt{2t}+k_2/k_1,\quad \lambda\sim k_2, \tag{C18}$$

$$D(\lambda)\sim ik_1/k_2\pm(k_2/k_1)e^{-i\pi/4}\sqrt{2t}\sim ik_1/k_2,\quad \lambda\sim k_1. \tag{C19}$$

In each $\mathcal{F}_{2\kappa,j}$, the contribution from the circle $C_{\delta,j}$ of radius δ vanishes in the limit $\delta\to 0^+$.

A. Horizontal electric dipole

The integrals for the z-component of the magnetic field are

$$B_{2z,2}\sim e^{ik_2\rho}\frac{\mu_0}{2\pi}\frac{k_2^4}{k_1^2}\sqrt{\frac{2}{\pi k_2\rho}}\int_0^\infty dt\sqrt{2t}e^{-k_2\rho t}\sin\phi=e^{ik_2\rho}\frac{\mu_0}{2\pi}\frac{k_2^2}{k_1^2\rho^2}\sin\phi, \tag{C20}$$

$$B_{2z,1}\sim -e^{ik_1\rho}\frac{\mu_0}{2\pi}\frac{1}{\rho^2}\sin\phi. \tag{C21}$$

The integrals pertaining to the ρ-component of the electric field become

$$\begin{aligned}E_{2\rho,2}&\sim\frac{\omega\mu_0k_2^3}{2\pi k_1^2}\frac{e^{ik_2\rho}}{\sqrt{\pi k_2\rho}}\left[\int_0^\infty dt\frac{\sqrt{t}}{it+(1/2)k_2^2/k_1^2}e^{-k_2\rho t}+\frac{2i}{k_2\rho}\int_0^\infty dt\sqrt{t}e^{-k_2\rho t}\right]\cos\phi\\&\sim e^{ik_2\rho}\frac{\omega\mu_0k_2^4}{2\pi k_1^3}\sqrt{\frac{\pi}{k_2\rho}}[F(\wp)-i(2\pi\wp)^{-1/2}]\cos\phi,\end{aligned} \tag{C22}$$

$$E_{2\rho,1}\sim e^{ik_1\rho}\frac{\omega\mu_0}{2\pi k_1\rho^2}\cos\phi. \tag{C23}$$

$\wp$ and $F(z)$ are defined by Eqs. (3.50) and (B6), respectively.

By a comparison of Eqs. (2.2) and (2.3), no further calculations need to be done for $E_{2\phi,j}$.

$$\begin{aligned}E_{2\phi,2}&\sim-\frac{\omega\mu_0k_2^3}{2\pi k_1^2}\frac{e^{ik_2\rho}}{\sqrt{\pi k_2\rho}}\left\{\frac{1}{ik_2\rho}\left(\frac{\pi k_2}{k_1}[F(\wp)-i(2\pi\wp)^{-1/2}]\right)+ik_2\rho\left(\frac{i}{k_2^2\rho^2}\sqrt{\frac{\pi}{k_2\rho}}\right)\right\}\sin\phi\\&=e^{ik_2\rho}\frac{i\omega\mu_0k_2^3}{2\pi k_1^3\rho}\sqrt{\frac{\pi}{k_2\rho}}[F(\wp)-2i(2\pi\wp)^{-1/2}]\sin\phi,\end{aligned} \tag{C24}$$

$$E_{2\phi,1}\sim -e^{ik_1\rho}\frac{\omega\mu_0}{2\pi k_1\rho^2}\sin\phi. \tag{C25}$$

The rest of the components are calculated under similar approximations as follows:

$$E_{2z,2}\sim e^{ik_2\rho}\frac{\omega\mu_0 k_2^2}{2\pi k_1}\frac{1}{\sqrt{\pi k_2\rho}}\int_0^\infty dt\,\frac{\sqrt{t}}{it+(1/2)k_2^2/k_1^2}e^{-k_2\rho t}\cos\phi$$

$$=e^{ik_2\rho}\frac{\omega\mu_0 k_2^3}{2\pi k_1^2}\sqrt{\frac{\pi}{k_2\rho}}[F(\wp)-i(2\pi\wp)^{-1/2}]\cos\phi, \tag{C26}$$

$$E_{2z,1}\sim e^{ik_1\rho}\frac{i\omega\mu_0}{2\pi k_1\rho^2}\cos\phi, \tag{C27}$$

$$B_{2\rho,2}\sim e^{ik_2\rho}\frac{i\mu_0 k_2^3}{2\pi k_1^2\rho}\sqrt{\frac{\pi}{k_2\rho}}[F(\wp)-2i(2\pi\wp)^{-1/2}]\sin\phi, \tag{C28}$$

$$B_{2\rho,1}\sim e^{ik_1\rho}\frac{i\mu_0}{2\pi\rho^2}\sin\phi, \tag{C29}$$

and, in analogy with formulas (C24) and (C25),

$$B_{2\phi,2}\sim -e^{ik_2\rho}\frac{\mu_0 k_2^4}{2\pi k_1^2}\sqrt{\frac{\pi}{k_2\rho}}[F(\wp)-i(2\pi\wp)^{-1/2}]\cos\phi, \tag{C30}$$

$$B_{2\phi,1}\sim -e^{ik_1\rho}\frac{\mu_0 k_2}{2\pi k_1\rho^2}\left(i\frac{k_2}{k_1}-\frac{1}{k_2\rho}\right)\cos\phi. \tag{C31}$$

Compare with Ref. 17.

B. Vertical electric dipole

In the same vein, the field of a vertical electric dipole can be calculated with recourse to Eqs. (2.10)–(2.12). See also Ref. 32. Without further ado,

$$B_{2\phi,2}\sim e^{ik_2\rho}\frac{\mu_0 k_2^3}{2\pi k_1}\sqrt{\frac{\pi}{k_2\rho}}[F(\wp)-i(2\pi\wp)^{-1/2}], \tag{C32}$$

$$B_{2\phi,1}\sim -e^{ik_1\rho}\frac{\mu_0}{2\pi}\frac{k_2^2}{k_1^2\rho^2}, \tag{C33}$$

$$E_{2z,2}\sim -e^{ik_2\rho}\frac{\omega\mu_0 k_2^2}{2\pi k_1}\sqrt{\frac{\pi}{k_2\rho}}[F(\wp)-i(2\pi\wp)^{-1/2}], \tag{C34}$$

$$E_{2z,1}\sim e^{ik_1\rho}\frac{\omega\mu_0}{2\pi k_1\rho^2}, \tag{C35}$$

$$E_{2\rho,2}\sim -e^{ik_2\rho}\frac{\omega\mu_0 k_2^3}{2\pi k_1^2}\sqrt{\frac{\pi}{k_2\rho}}[F(\wp)-i(2\pi\wp)^{-1/2}], \tag{C36}$$

$$E_{2\rho,1}\sim -e^{ik_1\rho}\frac{i\omega\mu_0}{2\pi k_1\rho^2}. \tag{C37}$$

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The harmony in the Kepler and related problems

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The technique of reduction of order developed by Nucci [J. Math. Phys. **37**, 1772–1775 (1996)] is used to produce nonlocal symmetries in addition to those reported by Krause [J. Math. Phys. **35**, 5734–5748 (1994)] in his study of the complete symmetry group of the Kepler problem. The technique is shown to be applicable to related problems containing a drag term which have been used to model the motion of low altitude satellites in the Earth's atmosphere and further generalizations. A consequence of the application of this technique is the demonstration of the group theoretical relationship between the simple harmonic oscillator and the Kepler and related problems. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In a paper of a few years ago Krause[1] introduced a new concept into the study of the symmetries of ordinary differential equations. He called this a complete symmetry group and defined it by adding two properties to the definition of a Lie symmetry group. These were that the manifold of solutions is an homogeneous space of the group and the group is specific to the system, i.e., no other system admits it. This definition required the introduction of a new type of symmetry defined by

$$Y=\left[\int \xi(t,x_1,\ldots,x_N)\mathrm{d}t\right]\partial_t+\sum_{i=1}^{N}\eta_i(t,x_1,\ldots,x_N)\partial_{x_i}. \tag{1.1}$$

This definition of a symmetry differs from that of a Lie point symmetry due to the presence of the integral as the coefficient function of ∂_t.

As an illustration of the concept of a complete symmetry group Krause used the Kepler problem and obtained three symmetries of the type of (1.1). He claimed that these three symmetries could not be obtained by means of the standard Lie point symmetry analysis. Naturally it was not long before this claim was shown by Nucci[2] to be incorrect in the case of an autonomous system. In the case of the Kepler problem, an autonomous system, one of the dependent variables can be taken to be the new independent variable and the order of the system be reduced by one. An analysis of the reduced system for Lie point symmetries leads to results different from the analysis of the original system. In particular the three additional nonlocal symmetries obtained by Krause followed from point symmetries of the reduced system.

One of the fundamental problems of mechanics is that of the Kepler problem which describes the interaction of two point particles with an inverse square law of attraction. It is well known that this problem possesses the first integrals of the conservation of the scalar energy, the vector of angular momentum and vectors in the plane of the orbit known as Hamilton's vector[3] and the

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Laplace–Runge–Lenz vector.[4–9] The invariance Lie algebra of the first integrals under the operation of taking the Poisson bracket is so(4) (in the case of negative energy) and the Lie algebra of the five Lie point symmetries of the equation of motion $A_2 \oplus \mathrm{so}(3)$. The algebra of the complete symmetry group has not been given. The elements of the five-dimensional algebra are

$$X_1 = \partial_t, \quad X_3 = x_2 \partial_{x_3} - x_3 \partial_{x_2},$$

$$X_2 = t\partial_t + \tfrac{2}{3} r \partial_r, \quad X_4 = x_3 \partial_{x_1} - x_1 \partial_{x_3}, \tag{1.2}$$

$$X_5 = x_1 \partial_{x_2} - x_2 \partial_{x_1}.$$

The additional three nonlocal symmetries provided by Krause are

$$Y_1 = 2\left(\int x_1 \, \mathrm{d}t \right) \partial_t + x_1 r \partial_r,$$

$$Y_2 = 2\left(\int x_2 \, \mathrm{d}t \right) \partial_t + x_2 r \partial_r, \tag{1.3}$$

$$Y_1 = 2\left(\int x_3 \, \mathrm{d}t \right) \partial_t + x_3 r \partial_r$$

in which $r^2 = x_1^2 + x_2^2 + x_3^2$.

There have been several other systems, generalizations of the Kepler problem, which have been shown to have a similar set of conserved quantities.[10–13] Just as the Laplace–Runge–Lenz vector provides a direct route to the equation of the orbit of the classical Kepler problem, the corresponding vectors of the generalized Kepler problems provide the same direct route to the equations of their orbits. The Lie point symmetry associated with the Laplace–Runge–Lenz vector of the classical Kepler problem is the rescaling symmetry, X_2. The generalizations of the Laplace–Runge–Lenz vector do not always have such an associated Lie point symmetry. In the case of the equation of motion

$$\ddot{\mathbf{r}} - \left(\frac{\dot{g}}{2g} + \frac{3\dot{r}}{2r} \right) \dot{\mathbf{r}} + \mu g \mathbf{r} = 0, \tag{1.4}$$

which is a variation of the model proposed by Danby[14–17] for the motion of a satellite in a low altitude orbit subject to atmospheric drag, *viz*.

$$\ddot{\mathbf{r}} + \frac{\alpha \dot{\mathbf{r}}}{r^2} + \frac{\mu \mathbf{r}}{r^3} = 0, \tag{1.5}$$

and for which the generalization of the Laplace–Runge–Lenz vector is

$$\mathbf{J} = \frac{\dot{\mathbf{r}} \times \hat{\mathbf{L}}}{L} + \frac{\mu}{A^2} \hat{\mathbf{r}}, \tag{1.6}$$

where L is the magnitude of the angular momentum, $\mathbf{L}$, and A is a constant of the motion defined through

$$L = A(gr^3)^{1/2}, \tag{1.7}$$

Pillay *et al.*[18] showed that, instead of the Lie point symmetry for the classical Kepler problem, X_2, the nonlocal symmetry

$$G=-\frac{1}{2}\left[\int \frac{g'r}{g}\mathrm{d}t\right]\partial_t+r\partial_r \tag{1.8}$$

was the corresponding associated Lie symmetry.

In this paper we intend to demonstrate the existence of far more nonlocal symmetries for the classical Kepler problem than were reported by Krause. We derive them as Lie point symmetries of a reduced system using the method of Nucci.[19] By deriving these additional nonlocal symmetries in this way we are able to say something definite about the expanded symmetry group. The essence of the method of Nucci is to reduce the order of the system by using the symmetry, X_1, which is a statement of the autonomy of the system. We recall that in a reduction of order the symmetry Z which does not have the property $[X_1,Z]=\lambda X_1$ becomes an exponential nonlocal symmetry.[20] By an exponential nonlocal symmetry we mean one of the form

$$G=\exp\left[\int f\,\mathrm{d}t\right](\tau\partial_t+\eta_i\partial_{x_i}) \tag{1.9}$$

in which without a knowledge of the solution of the differential equation f is not an exact derivative and τ and the η_i are functions only of t, the x_i and their derivatives. In this case we have nonlocal symmetries becoming local on the reduction of order. Consequently we know that the symmetries of the reduced equation quite possibly have zero Lie bracket with X_1 and this will enable us to construct the algebra. Further we shall show that these considerations which are applicable to the classical Kepler problem can be extended to the generalizations such as the one in (1.4).

In the next section we review the reduction procedure of Nucci[2] and in Sec. III we apply it to the classical Kepler problem and see that there is a certain delicacy in the choice of the new independent variable. For the sake of simplicity we work in two dimensions. In Sec. IV we make some observations about these symmetries, the route to further simplification and the algebra. In Sec. V we obtain the results for Danby problem,[14] in Sec. VI those for the generalized problem represented by (1.4), in Sec. VII the symmetries for another generalization in which the force is not only not central but is also angle dependent and in Sec. VIII we present our conclusions and make some pertinent observations about going to the full three dimensions.

II. THE METHOD OF REDUCTION OF ORDER

Consider the system of N second order ordinary differential equations given by

$$\ddot{x}_i=f_i(x,\dot{x}),\quad i=1,N \tag{2.1}$$

in which t is the independent variable and $x_i, i=1,N$ the N dependent variables. These equations may be considered as equations from Newtonian mechanics, which was Krause's approach, but there is no necessity for that to be the case. There is also no necessity for the dependent variables to represent Cartesian coordinates. Indeed there is no need for the system to be of the second order. It just so happens that many of the equations which arise in practice have their origins in Newton's second law and so are second order equations. There is no requirement that the system be autonomous. In the case of a nonautonomous system we can apply the standard procedure of introducing a new variable $x_{N+1}=t$ and an additional first order equation $\dot{x}_{N+1}=1$ so that the system becomes formally autonomous. In our discussion we confine our attention to autonomous systems. We reduce the system (2.1) to a $2N$-dimensional first order system by means of the change of variables

$$\begin{aligned} w_1 &= x_1 & w_{N+1} &= \dot{x}_1 \\ w_2 &= x_2 & w_{N+2} &= \dot{x}_2 \\ &\vdots & &\vdots \\ w_{N-1} &= x_{N-1} & w_{2N-1} &= \dot{x}_{N-1} \\ w_N &= x_N & w_{2N} &= \dot{x}_N \end{aligned} \tag{2.2}$$

so that the system (2.1) becomes

$$\dot{w}_i = g_i(x,w), \quad i = 1,2N, \tag{2.3}$$

where $g_i = w_{N+i}$ for $i = 1,N$ and $g_i = f_i$ for $i = N+1,2N$.

In the first step of the reduction of the original system (2.1) we simply follow the conventional method used to reduce a higher order system to a first order system. Any optimization is performed in the further selection of the final variables. This selection may be motivated by the existence of a known first integral, such as angular momentum, or some specific symmetry in the original system (2.1).

We choose one of the variables w_i to be the new independent variable y. For the purpose of the development here we can make the identification $w_N = y$. By taking the quotients of the first order equations of the remaining members of the set (2.2) with (2.3N) we obtain the $(2N-1)$-dimensional system

$$\frac{\mathrm{d}w_i}{\mathrm{d}w_N} = \frac{g_i}{g_N} = \frac{g_i}{w_{2N}}, \quad i = 1,\ldots,N-1,N+1,\ldots,2N. \tag{2.4}$$

We do not attempt to calculate the Lie point symmetries of the system (2.4) because the Lie point symmetries of a first order system are generalized symmetries and one has to impose some *Ansatz* on the form of the symmetry. Rather we select $n \leqslant N-1$ of the variables to be the new dependent variables and rewrite the system (2.4) as a system of n second order equations plus $2(N-n) - 1$ first order equations. The selection of the new dependent variables is dictated by a number of considerations. The first and foremost is that we must be able to eliminate the unwanted variables from the system (2.4). After this condition has been satisfied we may look to seek variables which reflect some symmetry of the system, for example, an ignorable coordinate such as the azimuthal angle in a central force problem.

After the symmetries have been calculated, they can now be translated back to symmetries of the original system as follows. Suppose that the symmetry in the original variables is given by

$$G = \tau\partial_t + \eta_i\partial_{x_i}. \tag{2.5}$$

The symmetry G is first extended and then rewritten in terms of the new coordinates as follows:

$$G^{[1]} = \tau\partial_t + \eta_i\partial_{x_i} + (\dot{\eta}_i - \dot{x}_i\dot{\tau})\partial_{\dot{x}_i} = \tau\partial_t + \zeta_i\partial_{w_i} = \sigma\partial_y + \xi_i\partial_{u_i}, \tag{2.6}$$

where in the first line the summation is from 1 to N, in the second from 1 to $N-1$ and $N+1$ to $2N$, and in the third over the number of dependent variables u_i (the number cannot be fixed in advance without a knowledge of the specific system); $\zeta_i = \eta_i$ for $i = 1,N-1$ and $\zeta_i = \dot{\eta}_i - \dot{g}_i\dot{\tau}$ for $i = N+1,2N$; $\sigma = \eta_N$; $\xi_i = \zeta_j \partial u_i / \partial w_j$. The only way that τ appears in the symmetries of the reduced system is through its derivative with respect to time. If the nonlocality in the original system occurs as a simple integral in τ of a function of the original dependent variables, x_i, this will be passed to the reduced system as a function of the new variables. When the point symmetries of the reduced system are computed, the form which the symmetries take in the original system can be determined from (2.6). Since τ is determined as its derivative with respect to time, the symmetry of the original system must necessarily be nonlocal unless the derivative is an exact differential. We note in passing that there is no inherent restriction on the nature of the symme-

tries. They could equally be contact or generalized symmetries and the same considerations would apply. The only requirement is that τ be a simple integral, not that the integrand be a point function. However, for the purposes of this paper we confine our attention to point symmetries and the integrand in τ to a point function.

In addition to the nonlocal symmetries which may be collected by this procedure the reduced system will have as point symmetries those symmetries of the original system which have the correct Lie bracket with the symmetry ∂_t which is at the basis of the reduction of order outlined above. Thus, if G is a symmetry of the original system and

$$[G,\partial_t]=\lambda\partial_t, \tag{2.7}$$

G will, when expressed in the appropriate coordinates, be a point symmetry of the reduced system whereas, if

$$[G,\partial_t]\neq\lambda\partial_t, \tag{2.8}$$

G will not be a point symmetry of the original system but an exponential nonlocal symmetry.[20] Consequently there is the potential for a loss of symmetry in the reduction process just as there is the hope of an increase in the total number of symmetries, both point and nonlocal, known for the original system.

III. LIE POINT SYMMETRIES OF THE REDUCED KEPLER PROBLEM

The Lagrangian for the two-dimensional Kepler problem is

$$L=\frac{1}{2}(\dot r^2+r^2\dot\theta^2)+\frac{\mu}{r} \tag{3.1}$$

in plane polar coordinates, and the two equations of motion are

$$\ddot r-r\dot\theta^2=-\frac{\mu}{r^2}, \tag{3.2}$$

$$r\ddot\theta+2\dot r\dot\theta=0. \tag{3.3}$$

We introduce the new variables and their time derivatives

$$w_1=r,\quad \dot w_1=w_3,$$

$$w_2=\theta,\quad \dot w_2=w_4,$$

$$w_3=\dot r,\quad \dot w_3=w_1w_4^2-\frac{\mu}{w_1^2}, \tag{3.4}$$

$$w_4=\dot\theta,\quad \dot w_4=-\frac{2w_3w_4}{w_1}.$$

In accordance with the development in the preceding section we select w_2 to be the new independent variable y. The left-hand side of (3.4) leads to the reduced system

$$\frac{\mathrm{d}w_1}{\mathrm{d}y}=\frac{w_3}{w_4}, \tag{3.5}$$

$$\frac{dw_3}{dy} = w_1 w_4 - \frac{\mu}{w_1^2 w_4} \tag{3.6}$$

$$\frac{dw_4}{dy} = -\frac{2w_3}{w_1}. \tag{3.7}$$

From (3.5) we have $w_3 = w_4 w_1'$, where the prime denotes differentiation with respect to the new independent variable, y, and we replace (3.7) by

$$\frac{dw_4}{dy} = -\frac{2w_4 w_1'}{w_1}. \tag{3.8}$$

In (3.6) we replace w_3 by $w_4 w_1'$ to obtain

$$w_4 w_1'' - \frac{w_4 w_1'^2}{w_1} = w_1 w_4 - \frac{\mu}{w_1^2 w_4}. \tag{3.9}$$

By our replacement of w_3 we have not precisely decided that the variables u_1 and u_2 are to be w_1 and w_4. If we do make this identification, we obtain a system of two equations, one of the second order and one of the first order, *viz*.

$$u_1'' = 2\frac{u_1'^2}{u_1} + u_1 - \frac{\mu}{u_1^2 u_2^2}, \tag{3.10}$$

$$u_2' = -2\frac{u_1' u_2}{u_1}. \tag{3.11}$$

We observe that (3.11) is trivially integrated to give $u_1^2 u_2$ as a constant. [This is a consequence, naturally, of the symmetry ∂_θ of the original system (3.2) and (3.3) which is a reflection of the fact that θ is an ignorable coordinate.] Consequently we may just as well define our new variables to be

$$u_1 = w_1 \quad \text{and} \quad \tilde{u}_2 = u_1^2 u_2 \tag{3.12}$$

so that the system of equations we are to consider is

$$\begin{aligned} u_1'' &= 2\frac{u_1'^2}{u_1} + u_1 - \frac{\mu u_1^2}{\tilde{u}_2^2}, \\ \tilde{u}_2' &= 0. \end{aligned} \tag{3.13}$$

Hereafter we drop the tilde.

We calculate the Lie point symmetries of the system (3.13) using the well-known interactive program developed by Nucci[19] and obtain the symmetries

$$
\begin{aligned}
X_1 &= \partial_y, \\
X_2 &= 2u_1\partial_{u_1} + u_2\partial_{u_2}, \\
X_3 &= u_1(\mu u_1 - u_2^2)\partial_{u_1}, \\
X_4 &= u_1^2 \cos y\, \partial_{u_1}, \\
X_5 &= -u_1^2 \sin y\, \partial_{u_1}, \\
X_6 &= (\mu u_1 - u_2^2)\cos y\, \partial_y + u_1(2\mu u_1 - u_2^2)\sin y\, \partial_{u_1}, \\
X_7 &= -(\mu u_1 - u_2^2)\sin y\, \partial_y + u_1(2\mu u_1 - u_2^2)\cos y\, \partial_{u_1}, \\
X_8 &= u_2^2 \cos 2y\, \partial_y - u_1(\mu u_1 - u_2^2)\sin 2y\, \partial_{u_1}, \\
X_9 &= u_2^2 \sin 2y\, \partial_y + u_1(\mu u_1 - u_2^2)\cos 2y\, \partial_{u_1}.
\end{aligned}
\tag{3.14}
$$

Some of these symmetries are readily identified, but not many of them. Clearly X_1 represents the rotational invariance of the system and constitutes the subalgebra, so(2), of the original system of equations. In X_2 we recognize the rescaling symmetry closely associated with the Laplace–Runge–Lenz vector.

The other symmetries are not so easy to identify without making some calculation. To obtain the form of the symmetries in the original coordinates we must make use of (2.6). If we write the symmetry in the original coordinates as

$$
G = \tau\partial_t + \eta\partial_r + \zeta\partial_\theta, \tag{3.15}
$$

in terms of the new variables, the symmetry has the form

$$
\tilde{G} = \zeta\partial_y + \eta\partial_{u_1} + \left[\dot{\zeta} + \left(\frac{2\eta}{r} - \dot{\tau}\right)\dot{\theta}\right] r^2\partial_{u_2}, \tag{3.16}
$$

where the coefficient functions are all expressed in terms of the original variables. The calculations are not particularly interesting and we simply list the symmetries. They are

$$X_1=\partial_\theta,$$

$$X_2=3t\partial_t+2r\partial_r,$$

$$X_3=2\left[\mu\int r^2\,\mathrm{d}t-L^2t\right]\partial_t+\mu r(r^2-L^2)\partial_r,$$

$$X_4=2\int r\cos\theta\,\mathrm{d}t\partial_t+r^2\cos\theta\partial_r,$$

$$X_5=2\int r\sin\theta\,\mathrm{d}t\partial_t+r^2\sin\theta\partial_r, \tag{3.17}$$

$$X_6=\int\left[(3\mu r-L^2)\sin\theta+\mu\frac{\dot r}{\dot\theta}\cos\theta\right]\mathrm{d}t\,\partial_t+r\sin\theta(2\mu r-L^2)\partial_r+\cos\theta(\mu r-L^2)\partial_\theta,$$

$$X_7=\int\left[(3\mu r-L^2)\cos\theta-\mu\frac{\dot r}{\dot\theta}\sin\theta\right]\mathrm{d}t\,\partial_t+r\cos\theta(2\mu r-L^2)\partial_r-\sin\theta(\mu r-L^2)\partial_\theta,$$

$$X_8=2\mu\int r\sin 2\theta\,\mathrm{d}t\partial_t+r(\mu r-L^2)\sin 2\theta\partial_r-L^2\cos 2\theta\partial_\theta,$$

$$X_9=2\mu\int r\cos 2\theta\,\mathrm{d}t\,\partial_t+r(\mu r-L^2)\cos 2\theta\partial_r+L^2\sin 2\theta\partial_\theta,$$

so that we see that we lost only the time translation symmetry in the reduction of order and therefore gained six additional symmetries.

IV. THE LIE POINT SYMMETRIES OF THE REDUCED KEPLER PROBLEM: FURTHER CONSIDERATIONS

Further interpretation of the Lie point symmetries of the reduced generalized Kepler problem is facilitated by the redefinition of the symmetries given in (3.14). We do not alter the definitions of the first three symmetries, but we shall include them in this new listing for the sake of completeness. We now have the set of symmetries

$$\begin{aligned}
X_1&=\partial_y,\\
X_2&=2u_1\partial_{u_1}+u_2\partial_{u_2},\\
X_3&=u_1(\mu u_1-u_2^2)\partial_{u_1},\\
X_{4\pm}&=X_4\pm iX_5=e^{\pm iy}u_1^2\partial_{u_1},\\
X_{5\pm}&=X_6\mp iX_7=e^{\pm iy}[(\mu u_1-u_2^2)\partial_y\mp u_1(2\mu u_1-u_2^2)\partial_{u_1}],\\
X_{6\pm}&=X_8\pm iX_9=e^{\pm 2iy}[u_2^2\partial_y\pm u_1(\mu u_1-u_2^2)\partial_{u_1}].
\end{aligned} \tag{4.1}$$

We may search for the first integrals/invariants associated with each of these symmetries in the usual way. By way of concrete example we take X_{4+}. The invariants of the first extension of X_{4+}, *viz.*

$$X_{4+}^{[1]}=e^{iy}[u_1^2\partial_{u_1}+(2u_1u_1'+iu_1^2)\partial_{u_1'}], \tag{4.2}$$

are found from the associated Lagrange's system

$$\frac{\mathrm{d}y}{0}=\frac{\mathrm{d}u_1}{u_1^2}=\frac{\mathrm{d}u_2}{0}=\frac{\mathrm{d}u_1'}{2u_1u_1'+iu_1^2} \tag{4.3}$$

and are

$$\alpha=y,\quad \beta=u_2,\quad \text{and}\quad \gamma=\frac{u_1'+iu_1}{u_1^2}, \tag{4.4}$$

where the first two are by inspection and the third comes from the solution of the second and fourth of (4.3). The integral/invariant is a function of these three arguments and is found by demanding that the total derivative with respect to y be zero when the differential equations (3.13) are taken into account. We obtain the associated Lagrange system

$$\frac{\mathrm{d}\alpha}{1}=\frac{\mathrm{d}\beta}{0}=\frac{\mathrm{d}\gamma}{-i\gamma-\mu/\beta^2} \tag{4.5}$$

which gives β as one of the characteristics and

$$\omega_+=e^{iy}\left(\frac{u_1'+iu_1}{u_1^2}-\frac{i\mu}{u_2^2}\right) \tag{4.6}$$

as the second characteristic. Both β and ω are first integrals/invariants of the system (3.13). Naturally we recognize the former as the angular momentum.

If we perform the same calculation with X_{4-}, we obtain a similar result, *viz.*

$$\omega_-=e^{-iy}\left(\frac{u_1'-iu_1}{u_1^2}+\frac{i\mu}{u_2^2}\right). \tag{4.7}$$

The two can be combined into one convenient expression given by

$$J_\pm=e^{\pm iy}(v'\mp iv),\quad v=\mu-\frac{u_2^2}{u_1}, \tag{4.8}$$

where we have made use of the constancy of u_2 to write $J_\pm=u_2^2\omega_\pm$. For the system (3.13) $J_\pm$ are two invariants and for the original system (3.1) and (3.2), the two components of the first integral known as the Laplace–Runge–Lenz vector, written in complex form.

In (4.8) we introduced a new variable v. If we use this variable instead of u_1 in the system (3.13), we obtain the system

$$\begin{aligned} v''+v&=0,\\ u_2'&=0 \end{aligned} \tag{4.9}$$

so that the natural variable which arises from the invariants of $X_{4\pm}$ is a variable which further simplifies the reduced system. This is an interesting phenomenon for we are obtaining natural variables as we progress through the process of determining the symmetries of the reduced equation. It behooves us to rewrite the symmetries in terms of this new variable. We find that

$$
\begin{aligned}
X_1 &= \partial_{u_2}, \\
X_2 &= \partial_y, \\
X_3 &= v\,\partial_v \bmod(u_2^2), \\
X_{4\pm} &= e^{\pm iy}\partial_v \bmod(u_2^2), \\
X_{6\pm} &= e^{\pm 2iy}[\partial_y \pm iv\,\partial_v] \bmod(u_2^2), \\
X_{8\pm} &= e^{\pm iy}[v\,\partial_y \pm iv^2\partial_v] \bmod(u_2^2)
\end{aligned}
\tag{4.10}
$$

which is certainly a simpler appearance.

In the simpler form presented in (4.10) we see that the calculation of the integrals/invariants is simpler. For example, if we take $X_{6\pm}$, the first set of characteristics comes from the solutions of the associated Lagrange system

$$
\frac{dy}{1} = \frac{dv}{iv} = \frac{dv'}{-iv' - 2v}. \tag{4.11}
$$

The characteristics are

$$
\alpha = ve^{\mp iy} \quad \text{and} \quad \beta = vv' \mp iv^2. \tag{4.12}
$$

The condition for the function to be an invariant (in this case not a first integral of the reduced system since the independent variable is explicitly present) is that these two characteristics satisfy the first order equation

$$
\frac{d\alpha}{\alpha} = \frac{d\beta}{\beta}, \tag{4.13}
$$

whence the invariants are given by

$$
I_\pm = \frac{\beta}{\alpha} = (v' \mp iv)e^{\pm iy} \tag{4.14}
$$

which are, of course, the two components of the Laplace–Runge–Lenz vector. We note that there is also a first integral associated with each of $X_{6\pm}$ and this is the angular momentum which, in these coordinates, is an ignorable coordinate.

For the sake of completeness we list the first integrals/invariants associated with the symmetries listed in (4.10). They are given in the same order and with the same subscripts as the symmetries are listed:

$$
\begin{aligned}
&G_1 \quad I_1 = L, \quad I_2 = J_+J_- = 2L^2E + \mu^2, \\
&G_2 \quad I_1 = L, \quad I_2 = \frac{J_+}{J_-}, \\
&G_3 \quad I_1 = L, \quad I_2 = \frac{J_+}{J_-}, \\
&G_{4\pm} \quad I_1 = L, \quad I_{2\pm} = J_\pm, \\
&G_{5\pm} \quad I_1 = L, \quad I_{2\pm} = \frac{J_\pm}{J_\mp}, \\
&G_{6\pm} \quad I_1 = L, \quad I_{2\pm} = J_\pm.
\end{aligned}
\tag{4.15}
$$

We note that in the second integral associated with G_1 we have expanded the product into the standard expression relating the square of the magnitude of the Laplace–Runge–Lenz vector with the energy and the angular momentum. For the second integral of $G_{5\pm}$ we could have equally written $I_2=J_+/J_-$, but we chose to maintain the pattern of $\pm$.

V. THE KEPLER PROBLEM WITH DRAG

In the introduction we referred to the model proposed by Danby[14] for the motion of a low altitude satellite subjected to a resistive force due to the Earth's atmosphere described by the equation of motion

$$\ddot{\mathbf{r}}+\frac{\alpha\dot{\mathbf{r}}}{r^2}+\frac{\mu\mathbf{r}}{r^3}=0, \tag{5.1}$$

where α and μ are constants. Since the direction of the angular momentum is a constant, we may analyze the problem in two dimensions using plane polar coordinates (r,θ). The two equations of motion are

$$\ddot{r}-r\dot{\theta}^2+\frac{\alpha\dot{r}}{r^2}+\frac{\mu}{r^2}=0, \tag{5.2}$$

$$r\ddot{\theta}+2\dot{r}\dot{\theta}+\frac{\alpha\dot{\theta}}{r}=0. \tag{5.3}$$

We introduce the new variables and their time derivatives

$$\begin{gathered} w_1=r, \quad \dot{w}_1=w_3, \\ w_2=\theta, \quad \dot{w}_2=w_4, \\ w_3=\dot{r}, \quad \dot{w}_3=w_1w_4^2-\frac{\alpha w_3}{w_1^2}-\frac{\mu}{w_1^2}, \\ w_4=\dot{\theta}, \quad \dot{w}_4=-\frac{2w_3w_4}{w_1}-\frac{\alpha w_4}{w_1^2}. \end{gathered} \tag{5.4}$$

We again select w_2 to be the new independent variable y. The right-hand side of (5.4) becomes

$$\frac{\mathrm{d}w_1}{\mathrm{d}y}=\frac{w_3}{w_4}, \tag{5.5}$$

$$\frac{\mathrm{d}w_3}{\mathrm{d}y}=w_1w_4-\frac{\alpha w_3}{w_1^2w_4}-\frac{\mu}{w_1^2w_4}, \tag{5.6}$$

$$\frac{\mathrm{d}w_4}{\mathrm{d}y}=-\frac{2w_3}{w_1}-\frac{\alpha w_4}{w_1^2}. \tag{5.7}$$

In this case the choice of (5.5) to eliminate w_3 is obvious and we obtain the two-dimensional system

$$w_1''w_4+w_1'w_4'=w_1w_4-\frac{\alpha w_1'}{w_1^2}-\frac{\mu}{w_1^2w_4}, \tag{5.8}$$

$$w_4' = -\frac{2w_1' w_4}{w_1} - \frac{\alpha}{w_1^2}. \tag{5.9}$$

In the case of (5.9) we can easily manipulate it to obtain

$$(w_1^2 w_4)' = \alpha \Leftrightarrow w_1^2 w_4 = -\alpha y + \beta, \tag{5.10}$$

where β is a constant of integration, which indicates that the angular momentum is not conserved. We have a choice of defining the new variable u_2 as either $w_1^2 w_4$, which is not conserved but is a convenient variable for manipulations, or $w_1^2 w_4 + \alpha y$, which is conserved but is not a convenient variable for manipulation. For the present we make the former choice. In Eq. (5.8) we make use of (5.10) to eliminate w_4 and w_4' to obtain

$$\left(-\frac{1}{w_1}\right)''(\alpha y+\beta)^2 + 2\alpha\left(-\frac{1}{w_1}\right)'(\alpha y+\beta) + \left(-\frac{1}{w_1}\right)(\alpha y+\beta)^2 + \mu = 0. \tag{5.11}$$

We introduce the second new variable as

$$u_1 = -\frac{\alpha y+\beta}{w_1} \tag{5.12}$$

so that (5.11) becomes

$$u_1'' + u_1 = -\frac{\mu}{\alpha y+\beta}. \tag{5.13}$$

Clearly we could regain the equation of a simple harmonic oscillator by means of the further change of variable $v = u_1 - u_{1ps}$, where u_{1ps} is a particular solution of (5.13). Consequently the Kepler problem with drag differs from the standard Kepler problem in that the second equation of the reduced system, *viz.*

$$u_2' = -\alpha, \tag{5.14}$$

has a nonzero right-hand side. This could be eliminated by now making the second choice mentioned above. Consequently we make a final change of variables

$$\begin{aligned} v_1 &= u_1 - \int \frac{\mu \sin(y-s)\,ds}{\alpha s - \beta}, \\ v_2 &= u_2 + \alpha \end{aligned} \tag{5.15}$$

to obtain the same reduced system (4.9), as we had for the Kepler problem when we introduced the sensible coordinates. Naturally we obtain the same set of symmetries as given in (4.10).

The Lie point symmetries of the reduced system translate into the symmetries

$$\Gamma_1=\left(\int\frac{\mathrm{d}t}{r^2\dot\theta}\right)\partial_t,$$

$$\Gamma_2=2\left[\int\frac{(\alpha r+I')\mathrm{d}t}{r(\alpha\theta-\beta)}\right]\partial_t+\left[\frac{\alpha r+I'}{\alpha\theta-\beta}\right]\partial_r-\partial_\theta,$$

$$\Gamma_3=\left[2t+\int\frac{I\,\mathrm{d}t}{r(\alpha\theta-\beta)}\right]\partial_t+\left(r+\frac{I}{\alpha\theta-\beta}\right)\partial_r,$$

$$\Gamma_{4\pm}=2\left[\int\frac{e^{\pm i\theta}\,\mathrm{d}t}{r(\alpha\theta-\beta)}\right]\partial_t+\left[\frac{e^{\pm i\theta}}{\alpha\theta-\beta}\right]\partial_r, \tag{5.16}$$

$$\Gamma_{5\pm}=2\left\{\int e^{\pm i\theta}\left[\frac{\alpha r+I}{r(\alpha\theta-\beta)}\mp\left(2+\frac{I}{r(\alpha\theta-\beta)}\right)\right]\mathrm{d}t\right\}\partial_t+e^{\pm 2i\theta}\left[\frac{\alpha r+I'}{\alpha\theta-\beta}\mp i\left(r+\frac{I}{\alpha\theta-\beta}\right)\right]\partial_r$$
$$-e^{\pm 2i\theta}\partial_\theta,$$

$$\Gamma_{6\pm}=\left\{\int e^{\pm i\theta}\left[(r(\alpha\theta-\beta)+I)\left(\frac{\alpha r+I'}{r(\alpha\theta-\beta)}\mp i\left(3+\frac{2I}{r(\alpha\theta-\beta)}\right)\right)+\alpha r+I'+\frac{\dot r}{\dot\theta}(\alpha\theta-\beta)\right]\mathrm{d}t\right\}\partial_t$$
$$+e^{\pm i\theta}(r(\alpha\theta-\beta)+I)\left[\frac{\alpha r+I'}{\alpha\beta-\beta}\mp i\left(r+\frac{I}{\alpha\theta-\beta}\right)\right]\partial_r-e^{\pm i\theta}[r(\alpha\theta-\beta)+I]\partial_\theta,$$

where I stands for the integral introduced in (5.15a) and I' its derivative with respect to θ, for the original system (5.1).

In addition to the symmetries listed in (5.16) Eq. (5.1) has the point symmetry ∂_t which was the symmetry used for the reduction of order. Consequently we can conclude that algebraically the Kepler problem and the Kepler problem with drag are identical.

In the above derivation we have followed a line of development in which observation and experience play major roles in reducing the system (5.4) to the simplest possible form. The need for both are considerably obviated when the interactive Lie symmetry solver devised by Nucci[19] is used. The equations to be solved suggest the appropriate variables since they are the characteristics of the partial differential equations to be solved. We illustrate this in the case of the variable related to angular momentum with the following tableau:

$$w_2=y,$$

$$w_3=\frac{\mathrm{d}w_1}{\mathrm{d}y}w_4,$$

$w_4=u_1,\quad w_1=u_2,$

$$\dot u_1=-2\frac{\dot u_2u_1}{u_2}-\frac{\alpha}{u_2^2},$$

$$\ddot u_2=\frac{(u_2^2+2\dot u_2^2)u_1^2u_2-\mu}{u_1^2u_2^2},$$

$$w_4=\frac{w_5}{w_1^2},$$

$w_5=u_1, \quad w_1=u_2,$

$$\dot{u}_1=-\alpha,$$

$$\ddot{u}_2=\frac{-\mu u_2^3+u_1^2u_2^2+2u_1^2\dot{u}_2^2}{u_1^2u_2},$$

$$w_5=w_6-\alpha y,$$

$w_6=u_1, \quad w_1=u_2,$

$$\dot{u}_1=0,$$

$$\ddot{u}_2=\frac{(\alpha y-u_1)^2(u_2^2+2\dot{u}_2^2)-\mu u_2^3}{(\alpha y-u_1)^2u_2}.$$

(We have used w_4, w_5, and w_6 to successively define a new variable which is a candidate for selection as u_1. We are not introducing additional variables.)

VI. THE GENERALIZATION OF THE KEPLER PROBLEM WITH DRAG

Equation (1.4) has, in two dimensions, the two components of the equation of motion

$$\begin{aligned}\ddot{r}&=r\dot{\theta}^2+\frac{1}{2}\left(\frac{g'}{g}+\frac{3}{r}\right)\dot{r}^2-\mu g r,\\ \ddot{\theta}&=\frac{\dot{r}\dot{\theta}}{2r}\left(\frac{g'}{g}-\frac{1}{r}\right).\end{aligned} \tag{6.1}$$

We introduce the variables w_i, $i=1,4$ as above. Now the system of first order equations in these variables is

$$\begin{aligned}\dot{w}_1&=w_3,\\ \dot{w}_2&=w_4,\\ \dot{w}_3&=w_1w_4^2+\frac{1}{2}\left(\frac{g'}{g}+\frac{3}{r}\right)w_3^2-\mu g w_1,\\ \dot{w}_4&=\frac{w_3w_4}{2w_1}\left(\frac{g'}{g}-\frac{1}{w_1}\right).\end{aligned} \tag{6.2}$$

As the new independent variable we take again $y=w_2$. The system (6.2) becomes

$$\begin{aligned}\frac{dw_1}{dy}&=\frac{w_3}{w_4}\Leftrightarrow w_3=w_4w_1',\\ \frac{dw_3}{dy}&=w_1w_4+\frac{1}{2}\left(\frac{g'}{g}+\frac{3}{r}\right)w_4w'^2_1-\mu g\frac{w_1}{w_4},\\ \frac{dw_4}{dy}&=\frac{w_3}{2w_1}\left(\frac{g'}{g}w_1-1\right).\end{aligned} \tag{6.3}$$

When we substitute for w_3, the third of (6.3) is easily integrated to give

$$A=\left(\frac{w_1}{g}\right)^{1/2} w_4, \tag{6.4}$$

where A is an arbitrary constant of integration. The right-hand side is the same function as the characteristic of the parabolic partial differential equation produced when the system (6.3) is analyzed using the code developed by Nucci[19] and this is an appropriate choice for one of the variables. We take $u_1=w_1=r$ and $u_2=\dot{\theta}(r/g)^{1/2}$ so that with the elimination of w_3 from (6.3) we have, after a certain amount of simplification, the system of two equations

$$\begin{gathered} u_2u_1''=u_1u_2+2\frac{u_2u_1'^2}{u_1}-\frac{\mu u_1^2}{u_2}, \\ u_2'=0. \end{gathered} \tag{6.5}$$

We observe that (6.5) is precisely the system (3.13) and so we immediately introduce the new variable $v=\mu-u_2^2/u_1$ to obtain the simpler system (4.9) which has the symmetries listed in (4.10). In terms of the original variables these symmetries are

$$\begin{gathered} X_1=\partial_\theta, \\ X_2=-\left(\int \frac{g'r}{g}\,\mathrm{d}t\right)\partial_t+2r\partial_r, \\ X_3=\frac{1}{2}\left[\int (\mu rg-r\dot{\theta}^2)\left(\frac{1}{r}-\frac{g'}{g}\right)\mathrm{d}t\right]\partial_t+(\mu rg-r\dot{\theta}^2)\partial_r, \\ X_{4\pm}=\frac{1}{2}\left[\int e^{\pm i\theta}(g-rg')\mathrm{d}t\right]\partial_t+[e^{\pm i\theta}rg]\partial_r, \\ X_{5\pm}=\frac{1}{2}\left\{\int e^{\pm i\theta}\left[\frac{gr}{\dot{\theta}^2}\left(\mu-\frac{\dot{\theta}^2}{g}\right)^2\left(\frac{1}{r}-\frac{g'}{g}\right)\pm 2i\left(\mu-\frac{\dot{\theta}^2}{g}\right)+\frac{2\dot{r}\dot{\theta}}{gr}\right]\mathrm{d}t\right\}\partial_t \\ +\left\{e^{\pm i\theta}\frac{gr}{\dot{\theta}^2}\left(\mu-\frac{\dot{\theta}^2}{g}\right)^2\right\}\partial_r+\left\{e^{\pm i\theta}\left(\mu-\frac{\dot{\theta}^2}{g}\right)\right\}\partial_\theta, \\ X_{6\pm}=\pm\frac{1}{2}i\left\{\int e^{\pm 2i\theta}\left(3+\frac{rg'}{g}+\frac{\mu(g-rg')}{\dot{\theta}^2}\right)\mathrm{d}t\right\}\partial_t\pm i\left\{e^{\pm 2i\theta}r\left(\frac{\mu g}{\dot{\theta}^2}-1\right)\right\}\partial_r+e^{\pm 2i\theta}\partial_\theta. \end{gathered} \tag{6.6}$$

VII. AN EXAMPLE WITH AN ANGLE-DEPENDENT FORCE

Sen[21] obtained conserved quantities similar to those of the Kepler problem for the Hamiltonian

$$H=\frac{1}{2}\left(p_r^2+\frac{p_\theta}{r^2}\right)-\frac{\mu}{r}-\frac{\alpha\sin[\frac{1}{2}(\theta-\beta)]}{r^{1/2}} \tag{7.1}$$

in which the potential depends upon the azimuthal angle and μ, α, and β are constants. Subsequently Gorringe and Leach[22] showed that the equation of motion

$$\ddot{\mathbf{r}}+g\hat{\mathbf{r}}+h\hat{\boldsymbol{\theta}}=0, \tag{7.2}$$

where

$$g=\frac{U''(\theta)+U(\theta)}{r^2}+2\frac{V'(\theta)}{r^{3/2}} \quad \text{and} \quad h=\frac{V(\theta)}{r^{3/2}}, \tag{7.3}$$

or

$$\ddot{r}-r\dot{\theta}^2+g=0, \tag{7.4}$$

$$r\ddot{\theta}+2\dot{r}\dot{\theta}+h=0 \tag{7.5}$$

in plane polar coordinates, could be solved for the orbit equation in a manner similar to that of the Kepler problem since it also possessed a Laplace–Runge–Lenz vector. The only restrictions on the functions $U(\theta)$ and $V(\theta)$ are that they be differentiable.

We make the same reduction as in the previous cases to arrive at the two- dimensional system

$$w_1w_1''w_4^2-2w_1'^2w_4^2-w_1^2w_4^2=w_1'h-gw_1, \tag{7.6}$$

$$w_1w_4w_4'+2w_1'w_4^2=-h, \tag{7.7}$$

where $w_1=r$ and $w_4=\dot{\theta}$ as before.

The Laplace–Runge–Lenz vector for Eq. (7.2) is[22]

$$\mathbf{J}=\dot{\mathbf{r}}\times\mathbf{L}-U\hat{\mathbf{r}}-[U'+2r^{1/2}V]\hat{\boldsymbol{\theta}}, \tag{7.8}$$

where $\mathbf{L}:=\mathbf{r}\times\dot{\mathbf{r}}$ is the angular momentum. If we take the two Cartesian components of $\mathbf{J}$, *viz*, J_x and J_y, and combine them, we obtain

$$\begin{aligned}J_\pm&=-J_x\pm iJ_y=[(r^3\dot{\theta}^2-U)\pm i(-r^2\dot{r}\dot{\theta}-U'-2r^{1/2}V)]e^{\pm i\theta}\\&=[(w_1^3w_4^2-U)\pm i(-w_1^2w_4w_3-U'-2w_1^{1/2}V)]e^{\pm iy}\\&=\left[\left(\frac{L^2}{w_1}-U\right)\pm i\left(\frac{L^2}{w_1}-U\right)'\right]e^{\pm iy}.\end{aligned} \tag{7.9}$$

We see that, when we write the components of the Laplace–Runge–Lenz vector in this form, we have the same structure as for the standard Kepler problem. (One could call the components the Ermanno–Bernoulli constants in honor of the original discoverers of these conserved quantities.) Immediately we have the clue to the identification of one of the new variables and we let

$$u_1=w_1^3w_4^2-U=\frac{L^2}{w_1}-U, \tag{7.10}$$

so that the Ermanno–Bernoulli constants for (7.2) are

$$J_\pm=(u_1\pm iu_1')e^{\pm iy}. \tag{7.11}$$

The identification of the second variable is more delicate. Equation (7.7) can be written in terms of the magnitude of the angular momentum, L, as

$$LL'=-w_1^{3/2}V(y) \tag{7.12}$$

and, when (7.10) is taken into account, this becomes

$$0=\frac{L'}{L^2}+\frac{V(y)}{(u_1+U(y))^{3/2}}. \tag{7.13}$$

From (7.11) we have

$$u_1=\tfrac{1}{2}(J_+e^{-iy}+J_-e^{+iy})=J\cos y, \tag{7.14}$$

since $J_-=J_+^*$ and we have written $J=|J_+|=|J_-|$. Then we can use (7.13) to define a new variable

$$u_2=\frac{1}{L}-\int\frac{V(y)\mathrm{d}y}{(J\cos y+U(y))^{3/2}}. \tag{7.15}$$

The reduced system of equations is

$$\begin{aligned} &u_1''+u_1=0,\\ &u_2'=0 \end{aligned} \tag{7.16}$$

which is just the reduced system we obtained for the standard Kepler problem and so it has the symmetries given in (7.10). These translate to

$$\begin{aligned}
\Gamma_1&=3\left(\int r^2\dot\theta\,\mathrm{d}t\right)\partial_t+2r^3\dot\theta\partial_r,\\
\Gamma_2&=\left[\int\left(\frac{2U'}{r^2\dot\theta^2}+\frac{3Vr^2\dot\theta}{U+J\cos\theta}\right)\mathrm{d}t\right]\partial_t+\left[\frac{U'}{r^2\dot\theta^2}+\frac{2Vr^3\dot\theta}{U+J\cos\theta}\right]\partial_r-\partial_\theta,\\
\Gamma_3&=2\left[t-\int\frac{U\mathrm{d}t}{r^3\dot\theta^2}\right]\partial_t+\left[r-\frac{U}{r^2\dot\theta^2}\right]\partial_r,\\
\Gamma_{4\pm}&=2\left(\int\frac{e^{\pm i\theta}}{r^3\dot\theta^2}\mathrm{d}t\right)\partial_t+\frac{e^{\pm i\theta}}{r^2\dot\theta^2}\partial_r,\\
\Gamma_{5\pm}&=\left\{\int e^{\pm 2i\theta}\left[\frac{3Vr^2\dot\theta}{U+J\cos\theta}+\frac{2(U'\mp iU)}{r^3\dot\theta^2}\right]\mathrm{d}t\right\}\partial_t\\
&\quad-e^{\pm 2i\theta}\left[\frac{2Vr^3\dot\theta}{U+J\cos\theta}\pm ir+\frac{U'\mp iU}{r^2\dot\theta}\right]\partial_r+e^{\pm 2i\theta}\partial_\theta,\\
\Gamma_{6\pm}&=\left\{\int e^{\pm i\theta}\left[2U'\left(1-\frac{U}{r^3\dot\theta^2}\right)-3(r^2\dot r\dot\theta\pm ir^3\dot\theta^2-2r^{1/2}V\mp iU)\right]\mathrm{d}t\right\}\partial_t\\
&\quad-e^{\pm i\theta}\left[\frac{2Vr^2\dot\theta}{U+J\cos\theta}(U'\pm i(r^3\dot\theta^2-U))\left(1-\frac{U}{r^3\dot\theta^2}\right)\right]\partial_r+e^{\pm i\theta}[r^3\dot\theta^2-U]\partial_\theta,
\end{aligned} \tag{7.17}$$

for the original system (7.2). In addition there is the symmetry, ∂_t, which was used for the reduction of order.

Again we see the very close connection between the structure of the Ermanno–Bernoulli constants and the appropriate variables for the reduction of order.

VIII. CONCLUSIONS AND OBSERVATIONS

For the Kepler problem in three dimensions we obtain the same symmetries as in (3.14) with the addition of

$$X_{10}=\partial_{u_3}, \tag{8.1}$$

where u_3 is the azimuthal angle, ϕ. Consequently our analysis in the lower dimensional configurational space is justified by the result that the additional dimension simply adds another ignorable coordinate to the original system and so a trivial first order ordinary differential equation to the reduced system.

In this paper we have examined the process of reduction of order introduced by Nucci[2] to derive the additional nonlocal symmetries required for the complete specification of the Kepler problem in the context not only of the Kepler problem but also in some generalizations which have appeared in the literature and which possess certain characteristics in common with the Kepler problem. In particular we have found that the possession of a conserved vector similar to that of the Laplace–Runge–Lenz vector, whether or not the magnitude of the angular momentum is conserved, leads in all cases to a reduced system consisting of the simple harmonic oscillator and a trivial first order ordinary differential equation. In the reduced system the Lie point symmetries can be written in a fairly simple fashion. When translated to the original system, they are not so simple in appearance. However, one can determine the algebraic properties of the several systems studied from those of the reduced system provided one adds the Lie point symmetry used in the reduction of order, *viz.* ∂_t. The Lie algebra of Lie point symmetries of the reduced system is $A_1 \oplus \mathrm{sl}(3,R)$ and consequently the original systems each have the algebra $2A_1 \oplus \mathrm{sl}(3,R)$ since the symmetry used in the reduction of order has a zero Lie bracket with the other symmetries.

Considering the results obtained in this paper we can envisage a reversal of the procedure. Instead of taking a system which has a vector of the type of a Laplace–Runge–Lenz vector we could simply commence with the reduced system and introduce some transformation of the two ''reduced'' variables and an *Ansatz* on the relationship defining the variable we have been denoting by w_3. One could expect to obtain many ''lame ducks.'' However, there is one aspect which has the potential for some application. Many of the systems for which Laplace–Runge–Lenz vectors have been obtained do not have a known Hamiltonian representation. By the procedures of transformations treated in this paper one could seek to commence with the Hamiltonian of the Kepler problem and find Hamiltonians for the other systems. In the case of the system (7.3) the existence of a Hamiltonian has been shown only in the restricted case treated by Sen. The attractions for the applications in quantum mechanics are obvious.

In the reduced system the components of the Laplace–Runge–Lenz vector, the Ermanno–Bernoulli constants, are simply the two linearly independent first order invariants of the simple harmonic oscillator. In fact, in the reduced system we have a separation in the new variables of the Ermanno–Bernoulli constants in the second order equation and the conservation of a generalized angular momentum in the first order equation. We recall that for higher dimensional oscillators there exist the conserved components of the Jauch–Hill–Fradkin tensor[23,24] which play an important role in the description of the orbit and their time-dependent counterparts which give the actual trajectory of the particle.[25–27] Naturally these tensors have no role to play in the type of problem considered in this paper. However, it is intriguing to ponder the identity that the corresponding problem of Kepler type would have. (For a recent contribution to this more general problem see Ref. 28.)

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Thermodynamics of trapped interacting bosons in one dimension

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On the basis of Bethe ansatz solution of bosons with δ-function interaction in a one-dimensional potential well, the thermodynamics equilibrium of the system in finite temperature is studied by using the strategy of Yang and Yang. The thermodynamics quantities, such as specific heat, etc., are obtained for the cases of the strong coupling and weak coupling limits respectively. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1331562]

I. INTRODUCTION

There has been much interest recently in the study of strongly correlated electronic systems in one dimension. This is because not only various nonperturbative methods[1–10] are applicable to models in one dimension but also several photoemission experiments for one-dimensional compounds of alkali-metal copper oxides[11–13] are carried out. Bosons with δ-function interaction in one dimension is a simple but interesting model. It was solved in Ref. 14 under the periodic boundary condition, in Refs. 15 and 16 under the boundary condition of potential well of infinite depth, and in Ref. 17 under that of potential well of finite depth. A strategy for studying the thermodynamics of exactly solvable models was proposed in Ref. 18 when discussing the solution of Ref. 14. In the present paper, using the strategy of Ref. 18 we study the thermodynamics on the basis of the Bethe-ansatz solution of Ref. 17. After we recall the model Hamiltonian and the Bethe-ansatz equation we study the thermal equilibrium in Sec. II. The formal expressions of free energy and pressure are obtained. In Sec. III we consider the strong coupling limit and obtain the quasimomentum distribution and specific heat explicitly. In Sec. IV the case of weak coupling limit is discussed extensively.

II. THERMAL EQUILIBRIUM AT FINITE TEMPERATURE

The Hamiltonian of bosons in a one-dimensional potential well of finite depth with δ interaction reads

$$H=-\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2}+\sum_{i=1}^{N}V(x_i)+2c\sum_{i>j=1}^{N}\delta(x_i-x_j), \tag{1}$$

where

$$V(x_i)=\begin{cases}0 & |x|<L/2,\\ V_0^2 & |x|>L/2.\end{cases} \tag{2}$$

Eq. (1) is the first quantization version of the Gross–Pitaevski[19] equation, which was widely used to study the Bose–Einstein condensation[20] in recent years. The model Hamiltonian (1) was solved by means of Bethe-ansatz method.[17] The logarithm of the Bethe-ansatz equation reads

$$\frac{2\pi}{L}I_j = k_j + \frac{2}{L}\sin^{-1}\left(\frac{k_j}{V_0}\right) + \frac{1}{L}\sum_{l\neq j}\left[\tan^{-1}\left(\frac{k_j+k_l}{c}\right)+\tan^{-1}\left(\frac{k_j-k_l}{c}\right)\right], \tag{3}$$

where the integers I_j play the role of the quantum numbers. Equation (3) is the secular equation to determine the spectrum. Moreover the transcendental equation (3) is difficult to solve directly. Now, we consider the problem in the thermodynamic limit: $N\gg 1$ and $L\gg 1$ with a fixed concentration $D=N/L$ by introducing a ''smooth'' positive-defined density $\overline{\rho}(k)$ describing the distribution of roots and holes[21]

$$\overline{\rho}(k)=\frac{1}{L}\frac{dI(k)}{dk}.$$

Treating k_j as a continuous variable k and differentiating Eq. (3) with respect to k, we get an integral equation

$$2\pi\overline{\rho}(k)=1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}+\int dk'\,\overline{\rho}(k')\left[\frac{c}{c^2+(k-k')^2}+\frac{c}{c^2+(k+k')^2}\right]$$
$$-\frac{1}{L}\sum_m\left[\frac{c}{c^2+(k-h_m)^2}+\frac{c}{c^2+(k+h_m)^2}\right], \tag{4}$$

where we have used the replacement

$$\lim_{N,L\to\infty}\frac{1}{L}\sum_{l\neq j}f(k_l)=\int\overline{\rho}(k)f(k)dk-\frac{1}{L}\sum_m f(h_m),$$

in the thermodynamics limit. The summation in the right-hand side runs over ''holes'' (including k_j) which can be written formally as an integral $\int\rho_h(k)f(k)dk$ with $\rho_h(k)=(1/L)\Sigma_m\delta(k-h_m)$. Furthermore, Eq. (4) is written as an integral equation for the density of holes $\rho_h(k)$ and the density of roots $\rho(k)=\overline{\rho}(k)-\rho_h(k)$,

$$2\pi(\rho+\rho_h)=1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}+\int dk'\,\rho(k')\left[\frac{c}{c^2+(k-k')^2}+\frac{c}{c^2+(k+k')^2}\right]. \tag{5}$$

The Bethe-ansatz solution is obtained for the case of bounded states (i.e., $\mathrm{Im}\,k_j=0$), so the range of the integration is $[-V_0,V_0]$. In terms of the distribution function of roots, we can write out the energy per particle

$$E/N=D^{-1}\int\rho(k)k^2\,dk, \tag{6}$$

where

$$D=N/L=\int\rho(k)dk. \tag{7}$$

On the basis of the strategy of Ref. 18, the total entropy of the system is obtained

$$S/N=D^{-1}\int[(\rho+\rho_h)\ln(\rho+\rho_h)-\rho\ln\rho-\rho_h\ln\rho_h]dk, \tag{8}$$

where the Boltzmann constant is set to unit.

In the thermal equilibrium, the free energy $\Omega=(E-TS-\mu N)$ should be in minimum. Writing

$$\frac{\rho_h(k)}{\rho(k)}=\exp[\epsilon(k)/T], \tag{9}$$

we obtain from the minimizing requirements, $\delta\Omega=0$, the following equations:

$$\epsilon(k)=-\mu+k^2-\frac{T}{2\pi}\int\left[\frac{c}{c^2+(k-k')^2}+\frac{c}{c^2+(k+k')^2}\right]\ln(1+e^{-\epsilon(k')/T})dk'. \tag{10}$$

Equation (5) is readily written as

$$2\pi(1+e^{\epsilon/T})\rho(k)=1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}+\int dk'\,\rho(k')\left[\frac{c}{c^2+(k-k')^2}+\frac{c}{c^2+(k+k')^2}\right]. \tag{11}$$

Principally, Eq. (10) can be solved by iteration and then Eq. (5) can be a Fredholm-type equation for $\rho(k)$.

We would like to mention some points about the parameter μ. If minimizing the Helmholtz free energy $F=E-TS$ under the condition that the concentration D in (7) is a constant, one will have a Lagrangian multiplier. The multiplier function is just the same as the chemical potential μ when considering a grand assemble. So both procedures are equivalent.

Multiplying Eq. (10) with ρD^{-1} and integrating over k, we obtain

$$\mu=D^{-1}\int(k^2-\epsilon)\rho\,dk-\frac{T}{2\pi D}\int\left[2\pi(\rho+\rho_h)-1-\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}\right]\ln(1+e^{-\epsilon/T})dk. \tag{12}$$

The argument k of ρ and ϵ are always omitted in our notions as long as it does not bring about confusion. With the help of Eq. (9), the entropy (8) is rewritten as

$$\frac{S}{N}=D^{-1}\int[(\rho+\rho_h)\ln(1+e^{-\epsilon/T})+\rho\epsilon/T]dk. \tag{13}$$

The Helmholtz free energy per particle is

$$\frac{F}{N}=\frac{1}{D}\int(k^2-\epsilon)\rho\,dk-\frac{T}{D}\int[(\rho+\rho_h)\ln(1+e^{-\epsilon/T})]dk. \tag{14}$$

Comparison of Eq. (12) and Eq. (14) gives rise to

$$F=\mu N-\frac{TL}{2\pi}\int\left[1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}\right]\ln(1+e^{-\epsilon/T})dk. \tag{15}$$

Thus the free energy will be obtained once the $\epsilon(k)$ is solved from Eq. (10). As in thermodynamics $F=-PL+\mu N$, the pressure is $P=-(\partial F/\partial L)_T$. It was shown[22] that if ϵ, μ are implicit functions of some thermodynamic quantities x (such as T, L), the derivative of Eq. (15) with respect to x is the same as the partial derivative of Eq. (15) with respect to the explicit variable x. Then it is easy to calculate the pressure in terms of the ϵ, namely,

$$P=\frac{T}{2\pi}\int\left[1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}\right]\ln(1+e^{-\epsilon/T})dk. \tag{16}$$

It is formally similar to the results of Ref. 18 except that one more term arising from the boundary condition is involved. Likewise, the entropy is

$$S=\frac{L}{2\pi}\int\left[1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}\right]\left[\ln(1+e^{-\epsilon/T})+\frac{\epsilon/T}{1+e^{\epsilon/T}}\right]dk. \tag{17}$$

The other thermal quantities such as specific heat, etc., are also obtainable if one is able to solve $\epsilon(k)$ from Eq. (10). We will calculate them in some special cases in the following sections.

III. STRONG COUPLING LIMIT

It is difficult to obtain an explicit expression of $\epsilon(k)$ from Eq. (10). However, in some special cases, we are able to obtain some plausible results. In the strong coupling limit $c\gg V_0$, Eq. (10) becomes

$$\epsilon(k)=-\mu+k^2-\frac{T}{2\pi}\int\ln[1+e^{(\mu-k'^2)/T}]\frac{d}{dk'}\left[\tan^{-1}\left(\frac{k'-k}{c}\right)+\tan^{-1}\left(\frac{k'+k}{c}\right)\right]dk'. \tag{18}$$

Integrating by part under the consideration of the approximation that $\tan^{-1}(k/c)\simeq k/c$ for $c\gg V_0$, we have

$$\epsilon=-\mu'+k^2, \tag{19}$$

where

$$\mu'=\mu+\frac{2}{\pi c}\int\frac{k'^2}{1+e^{(-\mu+k'^2)/T}}dk'. \tag{20}$$

Because of $(2/L)\sqrt{V_0^2-k^2}\ll 1$ and $c\gg V_0$, we obtain up to the first order that

$$2\pi(\rho+\rho_h)=1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}+\frac{4V_0}{c}. \tag{21}$$

From Eqs. (9), (19), and (21), we obtain an analytic expression of $\rho(k)$:

$$2\pi\rho(k)=\left[1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}+\frac{4V_0}{c}\right][1+e^{(-\mu'+k^2)/T}]^{-1}. \tag{22}$$

Obviously, the $\rho(k)$ is a Fermi-type distribution. When c, $L\to\infty$,

$$2\pi\rho(k)=\frac{1}{1+e^{(-\mu+k^2)/T}}, \tag{23}$$

which is just the distribution of free Fermi gas. The chemical potential μ should be positive–definite for the positive–definite density of roots.

As all particles are bounded in the potential well, i.e., $\mathrm{Max}(k)\sim V_\theta$, $\rho(k)$ should vanish almost for $k>V_0^{1/2}$. This requirement together with Eq. (22) gives

$$(V_0^2-\mu')/T\gg 1.$$

The system being thermal equilibrium exhibits a simple dependence on the large momentum cutoff $T_0(T_0=V_0^2-\mu')$, due to boundary effects. Therefore, the system can be in a state of

thermal equilibrium only when $T \ll T_0$. Otherwise some particles may overcome the potential energy at the boundary and escape out of the well. Substituting the obtained ϵ into Eq. (15), we obtain

$$F = \mu N - \frac{TL}{2\pi} \int \ln[1 + e^{(\mu' - k^2)/T}] \frac{d}{dk} \left[k + \frac{2}{L} \sin^{-1}\left(\frac{k}{V_0} \right) \right] dk. \tag{24}$$

As $k \ll V_0$, we can replace $\sin^{-1}(k/V_0)$ by k/V_0, then

$$F = \mu N - \frac{2L}{\pi} \left(1 + \frac{2}{LV_0} \right) \int_0^{V_0} \frac{k^2}{1 + e^{(-\mu' + k^2)/T}} dk. \tag{25}$$

In the low-temperature condition, the free energy becomes

$$F = \mu N - \frac{2L}{\pi} \left(1 + \frac{2}{LV_0} \right) \left(\frac{1}{3} \mu'^{3/2} + \frac{T^2 \pi^2}{24 \mu'^{1/2}} \right), \tag{26}$$

where

$$\mu' = \mu + \frac{1}{c} \left(\frac{4}{3\pi} \mu^{3/2} + \frac{T^2 \pi}{6 \mu^{1/2}} \right). \tag{27}$$

The μ' is regarded as a mandation of chemical potential according to Eq. (22). However, we are not able to get an explicit result for the specific heat by partial derivative of Eq. (26), because the chemical potential μ might be temperature dependent. In order to observe some properties of specific heat at low temperature, we let $c \to \infty$ and let μ_0 denote chemical potential at zero temperature. The μ_0 is determined by

$$D = \frac{1}{2\pi} \int_{-\sqrt{\mu_0}}^{\sqrt{\mu_0}} \left(1 + \frac{1}{L} \frac{2}{\sqrt{V_0^2 - k^2}} \right) dk. \tag{28}$$

Considering $\lim_{T \to 0} \mu(T)/\mu_0 = 1$, we have

$$F = \mu_0 N - \frac{2L}{\pi} \left(1 + \frac{2}{LV_0} \right) \left(\frac{1}{3} \mu_0^{3/2} + \frac{T^2 \pi^2}{24 \mu_0^{1/2}} \right). \tag{29}$$

We find that the specific heat at low temperature is Fermi-liquid-like,

$$C_V = \frac{\pi L}{6 \mu_0^{1/2}} \left(1 + \frac{2}{LV_0} \right) T. \tag{30}$$

Thus the interaction between the particles plays an important role to their statistical properties though the system we considered is a boson system. This is a model belonging to the class of Haldane's exclusion statistics.[23]

IV. WEAK COUPLING LIMIT

Obviously, Eq. (10) can be written as

$$\epsilon = -\mu + k^2 - \frac{T}{2\pi} \int e^{-c|\omega|} e^{ik\omega} \cos(k'\omega) \ln(1 + e^{-\epsilon/T}) dk'\, d\omega. \tag{31}$$

Because in the weak coupling limit $c \ll 1$, we have

$$\epsilon(k) = -\mu + k^2 - T \ln(1 + e^{-\epsilon/T}) - f(k,c), \tag{32}$$

where

$$f(k,c)=\frac{T}{2\pi}\sum_{n=1}^{\infty}\int\frac{(-1)^n c^n|\omega|^n}{n!}e^{ik\omega}\cos(k'\omega)\ln(1+e^{(\mu-k^2)/T})dk'\,d\omega.$$

This leads to

$$e^{-\epsilon/T}=[e^{(-\mu+k^2-f(k,c))/T}-1]^{-1}. \tag{33}$$

Likewise, Eq. (5) gives rise to

$$2\pi\rho_h(k)=1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}+g(k,c), \tag{34}$$

where

$$g(k,c)=\sum_{n=1}^{\infty}\int\frac{(-1)^n c^n|\omega|^n}{n!}e^{ik\omega}\cos(k'\omega)dk'\,d\omega.$$

With the help of (33), we obtain the distribution function of roots

$$2\pi\rho(k)=\left[1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}+g(k,c)\right]\frac{1}{e^{[-\mu+k^2-f(k,c)]/T}-1}. \tag{35}$$

Physically, it represents the distribution of quasimomenta of the system as a collection. Because the density of root should be positive–definite, $\mu+f(k,c)$ must be always smaller than the corresponding k^2, particularly, $\mu+f(0,c)\leqslant 0$. So Eq. (35) is a bosonlike distribution. If considering the boundary effects so that $\rho(V_0)\simeq 0$ we have $V_0^2-\mu-f(V_0,c)\gg T$. There is a large-momentum cutoff $T_0=V_0^2-f(V_0,c)-\mu$ such that the system can be in a thermal equilibrium only when $T\ll T_0$.

Now we consider the free energy, and only take account of the leading terms for $c\ll 1$,

$$2\pi\rho(k)=\left[1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}\right]\frac{1}{e^{(k^2-\mu)/T}-1}. \tag{36}$$

The free energy (15) becomes

$$F=\mu N+T\frac{L}{2\pi}\int\left[1+\frac{1}{L}\frac{2}{\sqrt{V_0^2-k^2}}\right]\ln[1-e^{(\mu-k^2)/T}]dk. \tag{37}$$

Since $k\ll V_0$, $\sin^{-1}(k/V_0)\simeq k/V_0$, we have

$$F=\mu N-\frac{L}{\pi}\left(1+\frac{2}{LV_0}\right)\int\frac{k^2}{e^{(k^2-\mu)/T}-1}dk. \tag{38}$$

As for free bosons (i.e., $c=0$), the chemical potential should be nonpositive–definite and smaller than the energy of any particles. Moreover, for a fixed concentration ($D=N/L$), it is a function of temperature decreasing as the temperature increases according to Eq. (36). Hence when temperature goes to zero, the chemical potential will approach to zero from a negative value.

At low temperature, Eq. (38) becomes

$$F=\mu N-\frac{LT^{3/2}}{2\sqrt{\pi}}\left(1+\frac{2}{LV_0}\right)Li_{3/2}(e^{\mu/T}), \tag{39}$$

where $Li_n(z)$ is polylogarithm function with $Li_{3/2}(1)=\zeta(3/2)$ and $\zeta(x)$ is Riemann's Zeta function. Since $Li_n(z)$ can be expanded into series of z and the chemical potential μ should be zero at zero temperature, we neglect the $Li_{3/2}(e^{\mu/T})$'s dependence on T. Then the entropy has the form

$$S=\frac{3LT^{1/2}}{4\sqrt{\pi}}\left(1+\frac{2}{LV_0}\right)Li_{3/2}(e^{\mu/T}), \tag{40}$$

and the specific heat

$$C_V=\frac{3LT^{1/2}}{8\sqrt{\pi}}\left(1+\frac{2}{LV_0}\right)Li_{3/2}(e^{\mu/T}), \tag{41}$$

which has boson-gas-like behaviors.

V. CONCLUSIONS AND REMARKS

In the above, we discussed the thermodynamics of bosons in a one-dimensional potential well on the basis of the exact solution of the model. Using the strategy of Yang and Yang,[18] we studied the general thermodynamic properties of the system. We considered the problem in the strong coupling limit and found that the behavior of the system at low temperature is Fermi liquidlike even though it is a boson system. Therefore, the interaction plays an important role. Meanwhile we obtained the specific heat which is linearly dependent on the temperature T. For the weak coupling limit, we found that the system behaves like boson gas at low temperature.

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Logarithmic bounds for infinite Prandtl number rotating convection

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I. INTRODUCTION

Convection refers to fluid motion that is induced by buoyancy. In thermal convection buoyancy is due to temperature differences and one of the interesting questions is how much of the total heat transfer is due to convection. The natural measure of this quantity is the Nusselt number, N, and many experiments and numerical simulations have been performed to discern the relationship between N and the various parameters which describe the system. Much of this research has focused on the forcing parameter,[1–6] although it has been observed that rotation plays a nontrivial role as well.[7]

The standard mathematical description of a convective system in a rotating frame of reference is based on the rotating Boussinesq equations for Rayleigh–Bénard convection (see, for example, Chandrasekhar[8]). This is a system of equations coupling the three dimensional Navier–Stokes equations to a heat advection-diffusion equation. The parameters in this system are the Rayleigh number R which captures the forcing, and the Ekman number E which is inversly proportional to the rate of rotation. The only known rigorous upper bound for N at large values of the Rayleigh number is of the order $R^{1/2}$. This bound was first derived by Howard using variational methods.[9] More recently, a background method[10] has been used to obtain this bound as well.[11] This bound is also valid in the presence of rotation.[12] Experimental and numerical findings, however, indicate a bound of the form

$$N \sim R^q,$$

where the reported values for q belong approximately to the interval $[2/7,1/3]$ for large R. The exponents 2/7 and 1/3 have been discussed by several authors.[13–21]

A third parameter in the system is the Prandtl number, a parameter determined by the physical characteristics of the fluid. The Prandtl number is the ratio of the kinematic viscocity to the heat conduction coefficient. A simplified set of equations can be derived by taking the limit as the Prandtl number goes to infinity. These equations are easier to analyze than the Boussinesq equations; in particular one can prove global existence and uniqueness of smooth solutions.[12] The known rigorous bounds for the rotating infinite Prandtl number system are the uniform bound

$$N \leqslant 1 + C_1 R^{2/5},$$

and the rotation dependent bound

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$$N \leqslant 1 + C_2 E R^2$$

(with constants independent of E and R). The latter bound is most useful for strong rotation. These upper bounds were both obtained using the background field method.[12,22–24] In the absence of rotation ($E=\infty$) a bound of the form

$$N \leqslant 1 + cR^{1/3}(1+\log_+ R)^{2/3},$$

has been obtained.[25] The 1/3 exponent is physical and close to the experimentally observed exponents. The goal of this paper is to provide a similar bound in the rotating case, allowing for finite values of E. As we shall see the correction due to rotation vanishes as $E \to \infty$, and we recover the above logarithmic bound even for rather strong rotation [$E \geqslant R^{-1/6}(\log R)^{-5/6}$]. However, as rotation is increased even further the logarithmic bound deteriorates, allowing for the observed increase of Nusselt number at intermediate rotation rates.[7] The $R^{2/5}$ bound may take over for a range of E. As $E \to 0$ the ER^2 bound takes over and accounts for the decrease of the Nusselt number due to very strong stratification.

The paper is organized as follows. In the next section we recall the equations, basic facts about the Nusselt number and some uniform estimates that hold for all Ekman numbers. In the third section we describe the method for bounding the heat flux and the results. The fourth section is devoted to proofs of the estimates of the nonrotation terms and the fifth section to the proofs of the estimates due to rotation.

II. INFINITE PRANDTL NUMBER EQUATIONS

We begin with the equations of motion for infinite Prandtl number Rayleigh–Bénard convection in a rotating reference frame, where the Boussinesq approximation is used for the buoyancy force. These form a system of five equations for velocities (u,v,w), pressure p and temperature T in three spatial dimensions. The components of the velocity vector $\mathbf{u}=(u,v,w)$ satisfy the equations

$$-\Delta u - E^{-1} v + p_x = 0, \tag{1}$$

$$-\Delta v + E^{-1} u + p_y = 0, \tag{2}$$

$$-\Delta w + p_z = RT, \tag{3}$$

and the divergence-free condition

$$u_x + v_y + w_z = 0. \tag{4}$$

The temperature, T, is advected according to the active scalar equation

$$(\partial_t + \mathbf{u}\cdot\nabla) T = \Delta T. \tag{5}$$

The two nondimensional parameters are the Rayleigh number, R, which describes the forcing due to the heat difference, and the Ekman number E which is inversely proportional to the rate of rotation.

We will consider a rectangular domain, with the vertical height scaled to 1 and the horizontal lengths scaled to the aspect ratio L. The horizontal independent variables (x,y) belong to a square $Q \subset \mathbf{R}^2$ of side length L. The vertical variable z belongs to the interval $[0,1]$. The non-negative variable t represents time. For boundary conditions we will consider all the functions u, v, w, p, T periodic in x and y with period L. The velocity components u, v, and w vanish for $z=0$ and 1 while the temperature T obeys $T=0$ at $z=1$ and $T=1$ at $z=0$. By taking a function $\tau(z)$ that satisfies $\tau(0)=1$ and $\tau(1)=0$, we will express the temperature as

$$T(x,y,z,t) = \tau(z) + \theta(x,y,z,t). \tag{6}$$

The role of τ is that of a convenient background which carries the inhomogeneous boundary conditions; thus θ obeys the same homogeneous boundary conditions as the velocity. The equation obeyed by θ is

$$(\partial_t + \mathbf{u}\cdot\nabla - \Delta)\,\theta = \tau'' - w\tau', \tag{7}$$

where we have used $\tau' = d\tau/dz$. We will use a normalized L^2 norm

$$\|f\|^2 = \frac{1}{L^2}\int_0^1\int_0^L\int_0^L |f(x,y,z)|^2\,dxdydz.$$

We denote by Δ_D^{-1} the inverse of the Laplacian with periodic-Dirichlet boundary conditions and the Laplacian in the horizontal directions x and y is denoted by Δ_h. We will use $\langle\cdot\rangle$ for the long time average

$$\langle f\rangle = \lim\sup_{t\to\infty}\frac{1}{t}\int_0^t f(s)ds.$$

The total heat transport is quantified by the Nusselt number which is defined in terms of a long time average of the vertical heat flux

$$N = 1 + \left\langle \int_0^1 b(z)dz \right\rangle, \tag{8}$$

where

$$b(z) = \frac{1}{L^2}\int_0^L\int_0^L w(x,y,z)T(x,y,z)dx\,dy. \tag{9}$$

we note that by using (6) the quantity $b(z)$ can be written

$$b(z) = \frac{1}{L^2}\int_0^L\int_0^L w(x,y,z)\,\theta(x,y,z)dx\,dy. \tag{10}$$

One can verify that the Nusselt number is also expressed as

$$N = \langle\|\nabla T\|^2\rangle. \tag{11}$$

From the velocity equations it follows that

$$\|\nabla\mathbf{u}\|^2 = \frac{R}{L^2}\int_0^L\int_0^L\int_0^1 w(x,y,z,t)T(x,y,z,t)dxdydz, \tag{12}$$

holds at each instant of time and thus

$$\langle\|\nabla\mathbf{u}\|^2\rangle = R(N-1). \tag{13}$$

The temperature equation obeys a maximum principle so that

$$0 \leqslant T \leqslant 1,$$

holds pointwise in space and time and consequently from (12) it follows that

$$\|\nabla\mathbf{u}\|^2 \leqslant R^2, \tag{14}$$

at each instance of time. One can easily derive from the rotating infinite Prandtl number system (see, for example, Ref. 23) two coupled equations for the vertical velocity w and the vertical component of vorticity $\zeta = v_x - u_y$

$$\Delta^2 w - E^{-1}\zeta_z = -R\Delta_h T, \tag{15}$$

$$-\Delta\zeta - E^{-1}w_z = 0. \tag{16}$$

Multiplying the first equation by w, the second one by ζ, adding and integrating we deduce that

$$\|\Delta w\|^2 + 2\|\nabla\zeta\|^2 \leqslant R^2, \tag{17}$$

holds pointwise in time. We used the fact, due to incompressibility, that w together with w_z and ζ vanish at the vertical boundaries.

III. BOUNDING THE HEAT FLUX

From the definition of the Nusselt number (11), given in terms of the temperature, we can derive an equivalent expression in terms of the background profile and fluctuations using (6) to replace T with its decomposition into τ and θ in the quantity $|\nabla T|^2$. This gives us the expression

$$N = \langle \|\nabla\theta|^2\rangle + \int_0^1 (\tau')^2\, dz + 2\left\langle \int_0^L\int_0^L\int_0^1 \theta_z \tau'\, dz dy dx \right\rangle.$$

The last term may be replaced by multiplying the evolution equation for θ (7) by θ and integrating. Upon taking a long time average, we have

$$\left\langle \int_0^L\int_0^L\int_0^1 \tau'\,\theta_z dz dy dx \right\rangle = \langle \|\nabla\theta\|^2\rangle - \left\langle \int_0^L\int_0^L\int_0^1 w\tau'\, dz dy dx \right\rangle,$$

where we have made use of the boundary conditions and the incompressibility condition. Combining these, we have the following form for the Nusselt number:

$$N + \langle \|\nabla\theta\|^2\rangle = 2\left\langle -\int_0^1 \tau'(z) b(z) dz \right\rangle + \int_0^1 (\tau'(z))^2 dz. \tag{18}$$

Let us now write

$$b(z,t) = \frac{1}{L^2}\int_0^L\int_0^L\int_0^z\int_0^{z_1} w_{zz}(x,y,z_2,t)\,\theta(x,z) dx\, dy\, dz\, dz_2\, dz_1.$$

It follows that:

$$|b(z,t)| \leqslant \tfrac{1}{2} z^2 (1 + \|\tau\|_{L^\infty}) \|w_{zz}\|_{L^\infty(dz;L^1(dx))}. \tag{19}$$

Restricting ourselves to bounded profiles, $\|\tau\|_{L^\infty} \leqslant 1$, and relaxing the supnorm we have simply

$$|b(z,t)| \leqslant z^2 \|w_{zz}(\cdot,t)\|_{L^\infty}. \tag{20}$$

Consequently we obtain the inequality

$$N \leqslant \int_0^1 (\tau'(z))^2 dz + 2\int_0^1 z^2 |\tau'(z)| \langle \|w_{zz}(\cdot,t)\|_{L^\infty}\rangle dz. \tag{21}$$

Up to this point, the background profile τ has not been specified. We will choose for simplicity a smooth approximation of a profile concentrated in a boundary layer of width δ, for example $\tau(z)=1-z/\delta$ for $0\leqslant z\leqslant\delta$ and 0 for $z>\delta$. We will assume thus that the function $\tau(z)$ obeys

$$|\tau'(z)|\leqslant C\frac{1}{\delta},$$

$$|\tau''(z)|\leqslant C\frac{1}{\delta^2},$$

$|\tau(z)|\leqslant 1$ and $\tau'(z)=0$ for $z>\delta$. We will adjust δ to optimize the bounds but we will require at least

$$\delta\geqslant\frac{C}{R^p}.$$

We will not attempt to optimize prefactors in this paper; we will simply denote Rayleigh and Ekman number independent constants by C. The power p is not specified (this assumption will only be used inside a logarithmic bound). Before optimizing in δ we deduce from (21) the inequality

$$N\leqslant\frac{C}{\delta}+C\delta^2\langle\|w_{zz}(\cdot,t)\|_{L^\infty}\rangle. \tag{22}$$

We will use now the two equations (15) and (16) to derive a single expression for w_{zz}, the quantity relevant to calculations of the heat flux. Noting that ζ vanishes on the vertical boundaries, solving for ζ in the second equation and substituting into the first equation, we obtain

$$\Delta^2 w+E^{-2}(\partial_z\Delta_D^{-1}\partial_z)w=-R\Delta_h T. \tag{23}$$

Moving the rotation term to the right-hand side and applying the inverse bilaplacian, we deduce

$$w=-R(\Delta_{\mathrm{DN}}^2)^{-1}\Delta_h T-E^{-2}(\Delta_{\mathrm{DN}}^2)^{-1}(\partial_z\Delta_D^{-1}\partial_z)w. \tag{24}$$

Here $(\Delta_{\mathrm{DN}}^2)^{-1}$ is the inverse bilaplacian with homogeneous Dirichlet and Neumann (DN) boundary conditions. Notice that $\Delta_h T=\Delta_h\theta$ since the background temperature profile τ depends on z only. Taking two z derivatives then gives

$$w_{zz}=-RB_1\theta-E^{-2}B_2 w, \tag{25}$$

where

$$B_1=\partial_{zz}(\Delta_{\mathrm{DN}}^2)^{-1}\Delta_h \tag{26}$$

and

$$B_2=\partial_{zz}(\Delta_{\mathrm{DN}}^2)^{-1}(\partial_z\Delta_D^{-1}\partial_z). \tag{27}$$

We will estimate the quantity of interest to us $\|w_{zz}\|_{L^\infty}$ using the decomposition above. Obviously

$$\langle\|w_{zz}(\cdot,t)\|_{L^\infty}\rangle\leqslant R\langle\|B_1\theta(\cdot,t)\|_{L^\infty}\rangle+E^{-2}\langle\|B_2 w(\cdot,t)\|_{L^\infty}\rangle, \tag{28}$$

holds.

In the following sections, we prove the two key estimates

$$\langle\|B_1\theta(\cdot,t)\|_{L^\infty}\rangle\leqslant C\{1+C\log_+ R\}^2 \tag{29}$$

and

$$\langle \|B_2 w(\cdot,t)\|_{L^\infty} \rangle \leqslant C\sqrt{R(N-1)}. \tag{30}$$

Using these two inequalities, and the combination of (28) and (22), we can optimize with respect to δ we obtain our main result

Theorem 1: *There exists a constant C such that the Nusselt number for the infinite Prandtl number equation with rotation is bounded by*

$$N \leqslant 1 + CR^{1/3}\{1+\log_+ R\}^{2/3},$$

when

$$E \geqslant R^{-1/6}\{1+\log_+ R\}^{-5/6}.$$

When $E \leqslant R^{-1/6}\{1+\log_+ R\}^{-5/6}$ *then the Nusselt number obeys*

$$N \leqslant CE^{-4/5}R^{1/5}.$$

Indeed, using the bounds (29) and (30) together with (28) in (22) and optimizing with respect to δ we obtain

$$N \leqslant 1 + C\{R(1+\log_+ R)^2\}^{1/3} + CE^{-2/3}R^{1/6}(N-1)^{1/6}, \tag{31}$$

which implies the statement of the theorem. From inequality (31) and the previously obtained bounds

$$N \leqslant 1 + CR^{2/5},$$

$$N \leqslant 1 + CER^2,$$

the following picture emerges. For rotations ranging from very weak to rather strong, ($E \geqslant R^{-1/6}\{1+\log_+ R\}^{-5/6}$), the bound $R^{1/3}\{1+\log_+ R\}^{2/3}$ applies. For stronger rotation, $R^{-1/4} \leqslant E \leqslant R^{-1/6}\{1+\log_+ R\}^{-5/6}$, the bound $N \leqslant 1 + CE^{-4/5}R^{1/5}$ is optimal. For stronger rotation yet, $R^{-2} \leqslant E \leqslant R^{-1/4}$, the bound $N \leqslant 1 + CR^{2/5}$ operates, and finally at exceedingly large rotation $E \leqslant R^{-2}$ the Nusselt number becomes bounded and then identically one. If instead of varying rotation at fixed Rayleigh numbers one varies the Rayleigh numbers and fixes the Ekman number, then the logarithmic one-third power law bound emerges for any fixed rotation, no matter how strong, provided the Rayleigh number is high enough.

IV. SINGULAR INTEGRALS AND THE B_1 TERM

In this section, we outline the estimates and results for the nonrotating case. Consider the operator

$$B_1 = \frac{\partial^2}{\partial z^2}(\Delta_{\mathrm{DN}}^2)^{-1}\Delta_h,$$

where $w = (\Delta_{\mathrm{DN}}^2)^{-1} f$ is the solution of

$$\Delta^2 w = f,$$

with horizontally periodic and vertically Dirichlet and Neumann boundary conditions $w = w' = 0$. Logarithmic L^∞ estimates for B_1 were obtained in Ref. 25). They are recalled in the following:

Theorem 2: *For any* $\alpha \in (0,1)$ *there exists a positive constant* C_α *such that every Hölder continuous function* θ *that is horizontally periodic and vanishes at the vertical boundaries satisfies*

$$\|B_1\theta\|_{L^\infty} \leqslant C_\alpha \|\theta\|_{L^\infty}\{1+\log(1+\|\theta\|_{C^{0,\alpha}})\}^2. \tag{32}$$

The spatial $C^{0,\alpha}$ norm is defined as

$$\|\theta\|_{C^{0,\alpha}} = \sup_{X=(x,y,z)\in Q\times[0,1]} |\theta(X,t)| + \sup_{X\neq Y} \frac{|\theta(X,t)-\theta(Y,t)|}{|X-Y|^\alpha}.$$

The proof decomposes $B_1\theta$ into the sum

$$B_1\theta = (I - B_3 + B_4 + B_5)B_3\theta,$$

where

$$B_3(\theta) = (\Delta_D)^{-1}\Delta_h\theta.$$

B_3 is an integral operator with kernel K given by

$$B_3(\theta)(x,y,z) = L^{-2}\int_0^L\int_0^L\int_0^1 K(x-\xi,y-\eta,z,\zeta)(\theta(\xi,\eta,\zeta)-\theta(x,y,z))d\xi\, d\eta\, d\zeta. \tag{33}$$

B_4 and B_5 are singular layer integral operators with kernels that are singular at the boundary. The operator B_4 can be written as

$$B_4(\theta)(x,y,z) = L^{-2}\int_0^L\int_0^L\int_0^1 J(x-\xi,y-\eta,z,\zeta)(\theta(\xi,\eta,\zeta)-\theta(\xi,\eta,1))d\xi\, d\eta\, d\zeta \tag{34}$$

and

$$B_5(\theta)(x,y,z) = L^{-2}\int_0^L\int_0^L\int_0^1 S(x-\xi,y-\eta,z,\zeta)(\theta(\xi,\eta,\zeta)-\theta(\xi,\eta,0))d\xi\, d\eta\, d\zeta, \tag{35}$$

for any continuous function θ that obeys the homogeneous boundary conditions [so that $\theta(\xi,\eta,0)=\theta(\xi,\eta,1)=0$]. It was shown in Ref. 25 that there exist constants such that

$$|K(x-\xi,y-\eta,z,\zeta)| \leqslant C(|x-\xi|^2+|y-\eta|^2+|z-\zeta|^2)^{-3/2}, \tag{36}$$

$$|J(x-\xi,y-\eta,z,\zeta)| \leqslant C(|x-\xi|^2+|y-\eta|^2+|1-\zeta|^2)^{-3/2}, \tag{37}$$

$$|S(x-\xi,y-\eta,z,\zeta)| \leqslant C(|x-\xi|^2+|y-\eta|^2+|\zeta|^2)^{-3/2}. \tag{38}$$

Once these inequalities are established it is not difficult to derive for all B_j, $j=3,4,5$ the estimates

$$\|B_j\theta\|_{L^\infty} \leqslant C_\alpha \|\theta\|_{L^\infty}[1+\log(1+\|\theta\|_{C^{0,\alpha}})], \tag{39}$$

for which the bound in (32) follows by composition. We will make now contact with the dynamical evolution of θ given by (7) by establishing two inequalities. The first

$$\|\nabla\theta\|_{L^4}^2 \leqslant C\|\theta\|_{L^\infty}\|\Delta\theta\|_{L^2},$$

is obtained by integration by parts and hold for all functions that are smooth enough and obey the homogeneous boundary conditions. The second inequality,

$$\frac{1}{L^2}\int_0^L\int_0^L |w(x,y,z,t)|^2 \leqslant z\|\nabla\mathbf{u}(\cdot,t)\|^2,$$

follows from the boundary conditions, the fundamental theorem of calculus and the Schwartz inequality. Multiplying (7) by $-\Delta\theta$ and integrating one obtains, after using these last two inequalities

$$\frac{1}{2}\frac{d}{dt}\|\nabla\theta\|^2+\|\Delta\theta\|^2\leqslant C\|\nabla\mathbf{u}\|^2\left\{1+\int_0^1[(\tau''(z))^2+z(\tau'(z))^2]dz\right\}. \tag{40}$$

Now using the bound on $\|\nabla\mathbf{u}\|$, (14), and taking a long time average we see that there exists a positive constant C such that

$$\langle\|\Delta\theta\|^2\rangle\leqslant CR^2\left\{1+\int_0^1[(\tau''(z))^2+z(\tau'(z))^2]dz\right\}. \tag{41}$$

By Sobolev embedding it follows that averages of squares of spatial $C^{0,\alpha}$ norms of θ are bounded by the same right-hand side

$$\langle\|\theta\|_{C^{0,\alpha}}^2\rangle\leqslant CR^2\left\{1+\int_0^1[(\tau''(z))^2+z(\tau'(z))^2]dz\right\}. \tag{42}$$

Taking long time averages in the estimate (32) and using the concavity of the logarithm and the bound (42) we deduce the bound

$$\langle\|B_1\theta(\cdot,t)\|_{L^\infty}\rangle\leqslant C\left\{1+\log\left[1+CR^2\left\{1+\int_0^1[(\tau''(z))^2+z(\tau'(z))^2]dz\right\}\right]\right\}^2. \tag{43}$$

Using the general conditions on τ that make the integrals of gradients of τ not larger than powers of R we obtain (29).

V. ESTIMATES FOR THE ROTATION TERM

The goal of this section is to derive inequality (30), the estimate which appears in the rotating term. This is done using the bound on $\|\nabla\mathbf{u}\|$ (13), the lemma below, and taking long time averages.

Lemma: For the operator B_2 defined by (27), there exists a constant C such that

$$\|B_2w\|_{L^\infty}^2\leqslant C\|w_z\|^2. \tag{44}$$

To prove the lemma we will use Sobolev embedding to obtain pointwise bounds from bounds in H^2; in other words we will use

$$\|B_2w\|_{L^\infty}\leqslant C\|(1-\Delta)B_2w\|. \tag{45}$$

By showing that

$$\|B_2w\|\leqslant\tfrac{1}{2}\|w_z\| \tag{46}$$

and that

$$\|\Delta B_2w\|\leqslant\frac{\sqrt{2}+1}{\sqrt{2}}\|w_z\|, \tag{47}$$

the lemma will follow. We derive first the inequality (46). Recalling that B_2 is defined as $[\partial_{zz}(\Delta_{\mathrm{DN}}^2)^{-1}\partial_z\Delta_D^{-1}\partial_z]$, it is clear that the inequality follows from a corresponding bound of the norm of the operator $[\partial_{zz}(\Delta_{\mathrm{DN}}^2)^{-1}\partial_z\Delta_D^{-1}]$ in L^2. We accomplish this by showing that $\partial_{zz}(\Delta_{\mathrm{DN}}^2)^{-1}$

and $\partial_z \Delta_D^{-1}$ are both bounded in L^2. For the first of these, let ϕ be the solution of the bilaplacian equation $\Delta_{\mathrm{DN}}^2 \phi = f$. Multiplying this equation by ϕ and integrating over the whole domain gives

$$(\Delta^2 \phi, \phi) = (f, \phi), \tag{48}$$

where

$$(f,g) = \frac{1}{L^2} \int_0^1 \int_0^L \int_0^L f(x,y,z) g(x,y,z) dx dy dz.$$

Expressing the bilaplacian as

$$\Delta^2 = \partial_{zzzz} + 2\partial_{zz}\Delta_h + \Delta_h^2, \tag{49}$$

it follows after integrating by parts that

$$(\Delta^2 \phi, \phi) = \|\phi_{zz}\|^2 + 2\|\phi_{xz}\|^2 + 2\|\phi_{yz}\|^2 + \|\Delta_h \phi\|^2. \tag{50}$$

The boundary terms obtained by integrating by parts all vanish because of the boundary conditions. Equations (48) and (50) imply that

$$\|\phi_{zz}\|^2 \leqslant \|f\| \|\phi\|. \tag{51}$$

We now note from the fundamental theorem of calculus applied twice and the boundary conditions that

$$\|\phi\| \leqslant \frac{1}{\sqrt{2}} \|\phi_{zz}\|, \tag{52}$$

and therefore, from (51) we have

$$\|\phi_{zz}\| \leqslant \frac{1}{\sqrt{2}} \|f\|.$$

Since ϕ is by definition the solution to the bilaplacian equation, we can rewrite this inequality as

$$\|\partial_{zz} (\Delta_{\mathrm{DN}}^2)^{-1} f\| \leqslant \frac{1}{\sqrt{2}} \|f\|. \tag{53}$$

We bound the operator $\partial_z \Delta^{-1}$ in the same way. Let ψ represent the solution to the Poisson equation $\Delta \psi = f$ with Dirichlet boundary conditions. Multiplying by ψ and integrating over the domain yields

$$\|\partial_z \Delta_D^{-1} f\| \leqslant \frac{1}{\sqrt{2}} \|f\|. \tag{54}$$

Now the L^2 bounds given by Eqs. (53) and (54) can be used to obtain the estimate (46) on the operator B_2.

For (47) we need to show that

$$\|\Delta \partial_{zz} (\Delta_{\mathrm{DN}}^2)^{-1} \partial_z \Delta_D^{-1} \partial_z w\| \leqslant \frac{\sqrt{2}+1}{\sqrt{2}} \|\partial_z w\|. \tag{55}$$

Noticing that $\partial_z \Delta_D^{-1}$ may be written

$$\Delta\Delta(\Delta_{\mathrm{DN}}^2)^{-1}\partial_z\Delta_D^{-1},$$

and by expressing $\Delta=\partial_{zz}+\Delta_h$, we obtain the following form for the operator in (55):

$$\Delta\partial_{zz}(\Delta_{\mathrm{DN}}^2)^{-1}\partial_z\Delta_D^{-1}=[I-\partial_{zz}\Delta_h(\Delta_{\mathrm{DN}}^2)^{-1}-\Delta_h^2(\Delta_{\mathrm{DN}}^2)^{-1}]\partial_z\Delta_D^{-1}. \tag{56}$$

We have already shown that $\partial_z\Delta_D^{-1}$ is bounded in L^2, so we need only concern ourselves with the other two operators. Let φ be the solution to the bilaplacian equation $\Delta^2\varphi=f$ with Dirichlet and Neumann boundary conditions. Multiplying by $\Delta_h^2\varphi$ and integrating over the domain, we obtain

$$(\Delta^2\varphi,\Delta_h^2\varphi)=(f,\Delta_h^2\varphi). \tag{57}$$

Noting that we can separate the bilaplacian into vertical and horizontal derivatives, we have

$$(\Delta^2\varphi,\Delta_h^2\varphi)=(\partial_{zzzz}\varphi,\Delta_h^2\varphi)+2(\Delta_h\partial_{zz}\varphi,\Delta_h^2\varphi)+\|\Delta_h^2\varphi\|^2. \tag{58}$$

Integrating by parts, the first term gives

$$(\partial_{zzzz}\varphi,\Delta_h^2\varphi)=\|\partial_{zz}\Delta_h\varphi\|^2.$$

The boundary terms disappear due to boundary conditions. Similarly, the second term in (58) becomes, after integrating by parts

$$(\Delta_h\partial_{zz}\varphi,\Delta_h^2\varphi)=\|\Delta_h\partial_{xz}\varphi\|^2+\|\Delta_h\partial_{yz}\varphi\|^2.$$

Again, because of the boundary conditions, the boundary terms vanish. Equations (57) and (58) together with the Schwartz inequality, yield

$$\|\partial_{zz}\Delta_h\varphi\|^2+2\|\Delta_h\partial_{xz}\varphi\|^2+2\|\Delta_h\partial_{yz}\varphi\|^2+\tfrac{1}{2}\|\Delta_h^2\varphi\|^2\leqslant\tfrac{1}{2}\|f\|^2.$$

This inequality implies both that

$$\|\partial_{zz}\Delta_h(\Delta_{\mathrm{DN}}^2)^{-1}w\|^2\leqslant\tfrac{1}{2}\|f\|^2$$

and also that

$$\|\Delta_h^2(\Delta_{\mathrm{DN}}^2)^{-1}w\|^2\leqslant\|f\|^2.$$

Now by using (56) we obtain the estimate stated in (55) and proof of the lemma is completed.

VI. DISCUSSION

For infinite Prandtl number convection without rotation, there exists a rigorous upper bound on the heat transfer which is of the order $R^{1/3}(\log R)^{2/3}$. In the presence of rotation, however, a low-order perturbation to the bilaplacian operator is introduced. This has the effect of an additional term in the upper bound for the heat transfer, as seen in (31). As the rotation is increased the bound deteriorates slowly but holds as long as $E\geqslant R^{-1/6}(\log R)^{-5/6}$. For a region $R^{-1/4}\leqslant E\leqslant R^{-1/6}(\log R)^{-5/6}$ a bound of the type $N\leqslant E^{-4/5}R^{1/5}$ is the best known bound, for stronger rotation $R^{-2}\leqslant E\leqslant R^{-1/4}$ the uniform bound $N\leqslant R^{2/5}$ applies and if rotation is increased further the Nusselt number becomes bounded and then equal to one. On the other hand, suppose the rotation is arbitrary but fixed and the Rayleigh number is increased; for sufficiently large Rayleigh numbers the logarithmic $R^{1/3}(\log R)^{2/3}$ bound applies.

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On upper bounds for infinite Prandtl number convection with or without rotation

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Bounds for the bulk heat transport in Rayleigh–Benard convection for an infinite Prandtl number fluid are derived from the primitive equations. The enhancement of heat transport beyond the minimal conduction value (the Nusselt number Nu) is bounded in terms of the nondimensional temperature difference across the layer (the Rayleigh number Ra) according to $\mathrm{Nu} \leqslant c\mathrm{Ra}^{2/5}$, where $c<1$ is an absolute constant. This rigorous upper limit is uniform in the rotation rate when a Coriolis force, corresponding to the rotating convection problem, is included. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1336157]

I. INTRODUCTION

Rayleigh–Benard convection, where a fluid layer heated from below produces an instability leading to convective fluid motions, has played a central role in both the experimental and theoretical development of the modern sciences of nonlinear dynamics and physical pattern formation. Driven far beyond the instability, thermal convection becomes turbulent. Heat transport by convective turbulence is an important component of a wide variety of problems in applied physics ranging from stellar structure in astrophysics,[1] to mantle convection and plate tectonics in geophysics,[2] to transport in physical oceanography and atmospheric science.[3] One of the fundamental quantities of interest in these systems is the total heat transport across the layer, usually expressed in terms of the nondimensional Nusselt number Nu, the enhancement of heat flux beyond the minimal conductive value. This flux is a function of the buoyancy force across the layer, usually measured in units set by the layer geometry and material dissipation parameters as the Rayleigh number Ra. There are at least two other parameters in these systems: The Prandtl number Pr, a material parameter, is the ratio of diffusivities of momentum and temperature. And the aspect ratio $\mathcal{A}$, the ratio of the cross-sectional length scale(s) to the layer depth, is a geometric parameter characterizing the convection domain.

A major goal of both theory and experiment is to elucidate the Nu–Ra relationship, which is expected to take the form of a scaling law

$$\mathrm{Nu} \sim \mathrm{Ra}^{\alpha}, \tag{1.1}$$

in the high Rayleigh number limit of fully developed convective turbulence. It is generally assumed that the high Ra scaling law will be independent of the aspect ratio, and independent of the Prandtl number for finite values of Pr. Great interest centers on the asymptotic (as $\mathrm{Ra} \to \infty$) value of the scaling exponent α.

For many applications there is a relatively uncontroversial model of the phenomena, the so-called Boussinesq equations. This model consists of the heat advection-diffusion equation for the local temperature coupled to the incompressible Navier–Stokes equations via a buoyancy force proportional to the local temperature. There have been many theoretical predictions—as well

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as more than a few *a posteriori* explanations—for the numerical value of the scaling exponent α based in part on this model.[4] And while a number of laboratory experiments over the last two decades[5–9] have produced data yielding clear scaling over many orders of magnitude variation in Ra, experiments have not yet produced unambiguous measurements of α. (Directly observed values of α have varied between roughly 1/4 and 1/3.)

One of the early high-Rayleigh number theories[10] predicted, for finite Pr, an ''ultimate'' regime as $\mathrm{Ra}\to\infty$ with $\mathrm{Nu}\sim(\mathrm{Pr}\,\mathrm{Ra})^{1/2}$ (modulo logarithmic modifications). This scaling is distinguished in that the physical heat flux is then independent of the material transport coefficients,[1] and additionally in that this Rayleigh number dependence is in accord with the most general rigorous upper bounds on the heat transport derived from the Boussinesq equations[11] with at most mild statistical assumptions.[12] In particular the best high Ra rigorous bounds to date are of the form $\mathrm{Nu}\leqslant c\mathrm{Ra}^{1/2}$ uniform in the Prandtl number for $0<\mathrm{Pr}\leqslant\infty$. Several recent experimental investigations have suggested some indication of the eventual realization of this $\alpha=1/2$ limit,[6,7] but others have concluded that this regime may not be achieved.[8,9]

In this paper we focus on a specific version of the problem modeled by the infinite Prandtl number limit of the Boussinesq equations. Then the inertial terms in the momentum equations are neglected and the velocity vector field is linearly slaved to the temperature field. The infinite Prandtl number limit is the standard model for mantle convection studies[2] in terrestrial geophysics where $\mathrm{Pr}\approx 10^{24}$, and it is often taken as a reasonable description of high Prandtl number convection at moderate Rayleigh numbers. The Reynolds number is always small for infinite Prandtl number, and the expectation for the high Rayleigh number scaling of the Nusselt number is modified accordingly. The scaling $\mathrm{Nu}\sim\mathrm{Ra}^{1/3}$ was predicted on the basis of marginally stable boundary layer arguments,[13,14] and this value of α is distinguished in that it yields a finite heat flux into a semi-infinite layer. This 1/3 scaling is also predicted as an upper limit of the infinite Prandtl number limit of the Boussinesq equations on the basis of an approximate treatment of an upper bound analysis utilizing mild statistical hypothesis.[15] More recently, the suggestive high Rayleigh number bound $\mathrm{Nu}\leqslant c\mathrm{Ra}^{1/3}(\log\mathrm{Ra})^{2/3}$ was proven directly from the equations of motion.[16]

The effect of rotation on convective heat transport is an important issue in astrophysical and geophysical applications, and it has also been the subject of recent laboratory studies.[17] Rotation is modeled by the addition of a Coriolis force to the momentum balance in the Boussinesq model, and introduces another nondimensional variable into the system, the Taylor number Ta, which is proportional to the square of the rotation rate. Rotation modifies the transition from conduction to convection,[18,19] and generally rotation is observed to suppress convective heat transport in accord with the Taylor–Proudman theorem. The mathematical analysis of the effect of rotation in terms of its effect on rigorous bounds for convective heat transport is only partially successful, however, because to a great extent the existing bounding techniques utilize energy balances. The Coriolis force does no work, so it drops out of the analysis. Indeed, the $\mathrm{Nu}\leqslant c\mathrm{Ra}^{1/2}$ bound for arbitrary Prandtl number convection in Refs. 11 and 12 are uniform Ta. To date there are no rigorous estimates of the suppression of convection by rotation for arbitrary Prandtl number fluids.

There has been considerably more success for the analysis of the effect of rotation on infinite Prandtl number convection. When the Coriolis force is introduced directly into the linear slaving of the velocity field to the temperature field, it remains effective when the full momentum equation—and not just the energy balance—is utilized as a constraint in the analysis. A bound on Nu with the proper qualitative dependence on rotation was recently established,[20] $\mathrm{Nu}\leqslant c_1\,\mathrm{Ra}^2/\sqrt{\mathrm{Ta}}$ for no-slip boundaries. The Rayleigh number dependence of this estimate is overly pessimistic for moderate rotations; in Ref. 21 it is shown that for moderate rotations [$\mathrm{Ta}\leqslant c\,\mathrm{Ra}^{1/3}(\log\mathrm{Ra})^{5/3}$] an estimate of the form $\mathrm{Nu}\leqslant c\mathrm{Ra}^{1/3}(\log\mathrm{Ra})^{2/3}$ is valid.

The new results in this paper are to derive another rigorous upper bound for the Nusselt number in the infinite Prandtl number model which is effective for a range of Rayleigh and Taylor numbers. We will prove that

$$\mathrm{Nu}\leqslant c\mathrm{Ra}^{2/5}, \tag{1.2}$$

where the prefactor c is an absolute constant uniform in Ta. This is a qualitative improvement over the only other known uniform bound $\sim \mathrm{Ra}^{1/2}$, and depending on the specific values of Ra and Ta it can be a quantitative improvement of the estimates in Refs. 20 and 21. We will establish (1.2) two ways, one in the absence of rotation with the prefactor $c=0.2545\cdots$, and another in the presence of rotation[22] with a slightly larger prefactor $c=0.6635\cdots$.

The rest of this paper is organized as follows. In the next section we present a full description of the Boussinesq model of fluid convection along with the precise definitions of the dependent and independent variables, some basic identities, and a little preliminary analysis. Section III contains the upper bound computation, all the relevant estimates, and two proofs of the 2/5 bound, without and with rotation.

II. FORMULATION OF THE PROBLEM

We begin with the Boussinesq model of fluid convection in a rotating reference frame. A layer of fluid is confined between horizontal rigid planes separated by vertical distance h. The bottom plate at $z=0$ is held at constant temperature T_{bottom}, and the top one at $z=h$ is held at temperature T_{top}; both plates are no-slip as regards the fluid motion. The z axis is the vertical direction, the direction in which gravity acts and the direction of the axis of rotation. The unit vectors in the x, y, and z directions are, respectively, $\mathbf{i}$, $\mathbf{j}$, $\mathbf{k}$, and the velocity field is $\mathbf{u}(\mathbf{x},t)=\mathbf{i}u+\mathbf{j}v+\mathbf{k}w$. The temperature field is $T(\mathbf{x},t)$. Neglecting compressibility everywhere except in the buoyancy force, and scaling the density to one, the velocity field, the pressure field $p(\mathbf{x},t)$, and temperature field are governed by the Boussinesq equations

$$\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}+\nabla p+2\Omega\mathbf{k}\times\mathbf{u}=\nu\Delta\mathbf{u}+g\alpha\mathbf{k}T, \tag{2.1}$$

$$\nabla\cdot\mathbf{u}=0, \tag{2.2}$$

$$\frac{\partial T}{\partial t}+\mathbf{u}\cdot\nabla T=\kappa\Delta T. \tag{2.3}$$

In the above, Ω is the rotation rate, ν is the kinematic viscosity, g is the acceleration of gravity, α is the thermal expansion coefficient, and κ is the thermal diffusion coefficient. Incompressibility together with the no-slip boundary conditions lead to the supplementary boundary condition

$$\frac{\partial w}{\partial z}=0 \quad \text{at } z=0,h. \tag{2.4}$$

In this work we restrict attention to periodic boundary conditions on all dependent variables in the horizontal directions with periods L_x and L_y.

The standard nondimensional formulation of the problem is realized by measuring lengths in units of the layer depth h, time in units of the thermal diffusion time h^2/κ, velocity in terms of κ/h, and temperature on a scale where $T_{\mathrm{top}}=0$ and $T_{\mathrm{bottom}}=1$. The equations of motion are then transformed to

$$\frac{1}{\mathrm{Pr}}\left(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\right)+\sqrt{\mathrm{Ta}}\,\mathbf{k}\times\mathbf{u}+\nabla p=\Delta\mathbf{u}+\mathrm{Ra}\,\mathbf{k}T, \tag{2.5}$$

$$\nabla\cdot\mathbf{u}=0, \tag{2.6}$$

$$\frac{\partial T}{\partial t}+\mathbf{u}\cdot\nabla T=\Delta T, \tag{2.7}$$

with boundary conditions

$$\mathbf{u}|_{z=0}=0=\mathbf{u}|_{z=1}, \quad T|_{z=0}=1, \quad T|_{z=1}=0. \tag{2.8}$$

All the parameters of the system are thus absorbed into four pure numbers. The natural control parameter is the Rayleigh number

$$\mathrm{Ra}=\frac{g\alpha(T_{\mathrm{bottom}}-T_{\mathrm{top}})h^3}{\upsilon\kappa}, \tag{2.9}$$

a ratio of the overall buoyancy force to the damping coefficients. The rotation is measured by the Taylor number

$$\mathrm{Ta}=\left[\frac{2\Omega h^2}{\upsilon}\right]^2, \tag{2.10}$$

which is sometimes expressed in terms of the Ekman number $\mathrm{Ek}=\mathrm{Ta}^{-1/2}$. The Prandtl number

$$\mathrm{Pr}=\frac{\upsilon}{\kappa}, \tag{2.11}$$

is a material parameter. In the remainder of this paper we shall be concerned with the infinite Prandtl number model where the inertial terms in the momentum equations (2.5) are dropped so that the velocity field is linearly slaved to the temperature field

$$\sqrt{\mathrm{Ta}}\ \mathbf{k}\times\mathbf{u}+\nabla p=\Delta\mathbf{u}+\mathrm{Ra}\ \mathbf{k}T. \tag{2.12}$$

The fourth pure number characterizing the model is the aspect ratio of the system, which we define to be the nondimensional area on the layer

$$\mathcal{A}=\frac{L_xL_y}{h^2}. \tag{2.13}$$

The infinite Prandtl number model leads to direct linear relationships among the temperature, the vertical velocity w, and the vertical vorticity

$$\zeta=\frac{\partial v}{\partial x}-\frac{\partial u}{\partial y}. \tag{2.14}$$

Indeed, eliminating the pressure from (2.12) it is straightforward to see that

$$\Delta^2 w-\sqrt{\mathrm{Ta}}\,\frac{\partial\zeta}{\partial z}=-\mathrm{Ra}\ \Delta_H T, \tag{2.15}$$

where Δ_H denotes the horizontal Laplacian $\partial_x^2+\partial_y^2$, and

$$-\Delta\zeta-\sqrt{\mathrm{Ta}}\,\frac{\partial w}{\partial z}=0. \tag{2.16}$$

In view of the incompressibility and no-slip conditions on $\mathbf{u}$, the boundary conditions accompanying (2.15) and (2.16) are

$$w|_{z=0}=0=w|_{z=1}, \quad \left.\frac{\partial w}{\partial z}\right|_{z=0}=0=\left.\frac{\partial w}{\partial z}\right|_{z=1} \tag{2.17}$$

and

$$\zeta|_{z=0}=0=\zeta|_{z=1}. \tag{2.18}$$

A. Heat transport

The total heat transport is the space–time average of the vertical component of the heat current $\mathbf{k}\cdot\mathbf{J}$, where $\mathbf{J}$ is proportional to $\mathbf{u}T-\nabla T$. The standard nondimensional measure of the convective heat transport is the enhancement of the heat flux due to fluid motion, the Nusselt number Nu. The Nusselt number is defined as the ratio of the total vertical heat flux to the conductive heat flux $\kappa(T_{\text{bottom}}-T_{\text{top}})/h$.

The convection rate is a time averaged bulk property in the turbulent case, so it is helpful in defining it to introduce the notation

$$\int_V dV=\int_0^{L_x/h}dx\int_0^{L_y/h}dy\int_0^1 dz, \tag{2.19}$$

(where x, y, and z are the nondimensional coordinates) for the volume integration

$$\|f\|=\left(\int_V dV|f(x,y,z)|^2\right)^{1/2}, \tag{2.20}$$

for the L_2 norm on the domain, and

$$\langle f\rangle=\lim_{t\to\infty}\frac{1}{t}\int_0^t f(t')dt', \tag{2.21}$$

for the long time average of f. In the event the limit above does not exist (or is not unambiguously unique), we may interpret the definition in terms of the limit supremum as regards the upper bounds to be derived here.

Straightforward manipulation of the equations of motion yield a variety of expressions for the Nusselt number in terms of solutions to (2.7), (2.15), and (2.16)

$$\text{Nu}=1+\frac{1}{\mathcal{A}}\left\langle\int_V dV\,wT\right\rangle \tag{2.22}$$

$$=\frac{1}{\mathcal{A}}\langle\|\nabla T\|^2\rangle \tag{2.23}$$

$$=\frac{1}{\text{Ra}}\frac{1}{\mathcal{A}}\langle\|\nabla\mathbf{u}\|^2\rangle. \tag{2.24}$$

The goal of the analysis is to produce *a priori* bounds for the function $\text{Nu}(\text{Ra},\text{Ta},\mathcal{A})$. We will derive bounds that are uniform in the rotation rate and the aspect ratio, so for convenience we will refer to the Nusselt number as simply Nu(Ra).

B. A useful decomposition

A device that we shall use throughout is the decomposition of the temperature field into a steady ''background profile'' and a time-dependent fluctuation field

$$T(\mathbf{x},t)=\tau(z)+\theta(\mathbf{x},t). \tag{2.25}$$

The background profile $\tau(z)$ is, for the moment, arbitrary except that it satisfies the boundary conditions on $T(\mathbf{x},t)$. That is

$$\tau(0)=1 \quad \text{and} \quad \tau(1)=0. \tag{2.26}$$

Thus the fluctuation θ satisfies homogeneous boundary conditions

$$\theta|_{z=0}=0=\theta|_{z=1}, \tag{2.27}$$

together with periodicity in the horizontal. A particular background profile will be chosen later for convenience in the analysis.

We introduce the decomposition (2.25) into (2.7) to obtain

$$\frac{\partial\theta}{\partial t}+\mathbf{u}\cdot\nabla\theta=\Delta\theta-\tau' w+\tau'', \tag{2.28}$$

where $\tau'(z)$ and $\tau''(z)$ are the first and second derivatives of the $\tau(z)$. The evolution of the L_2 norm (squared) of the fluctuation field is obtained by dotting θ into Eq. (2.28) and integrating over the volume. Then upon performing some integrations by parts and invoking the boundary conditions we obtain

$$\frac{d}{dt}\frac{1}{2}\|\theta\|^2=-\|\nabla\theta\|^2-\int_V dV\,\tau'(z)\,w\,\theta-\int_V dV\,\tau'(z)\frac{\partial\theta}{\partial z}. \tag{2.29}$$

Now consider the L_2 norm (squared) of the decomposition of the gradient of the temperature field

$$\|\nabla T\|^2=\mathcal{A}\int_0^1 dz\,\tau'(z)^2+2\int_V dV\,\tau'(z)\frac{\partial\theta}{\partial z}+\|\nabla\theta\|^2. \tag{2.30}$$

Adding $2\times$(2.29) to (2.30), taking the long time average and recalling (2.23), we find the fundamental (for what follows) relation for the heat transport:

$$\mathrm{Nu}=\int_0^1 dz\,\tau'(z)^2-\frac{1}{\mathcal{A}}\left\langle\int_V dV\,(|\nabla\theta|^2+2\tau'(z)w\theta)\right\rangle. \tag{2.31}$$

III. UPPER BOUNDS

The derivation of upper bounds on the convective heat transport is based on the basic decomposition in (2.31). From this starting point we follow two distinct paths to producing effective rigorous estimates for Nu(Ra). One approach is to choose the background profile $\tau(z)$ to assure non-negativity of the quadratic form

$$Q\{\theta\}=\int_V dV\,(|\nabla\theta|^2+2\tau'(z)w\theta), \tag{3.1}$$

defined for functions $\theta(x,y,z)$ satisfying the fluctuation's boundary conditions with $w(x,y,z)$ given in terms of θ according to (2.15)—noting that $\Delta_H T=\Delta_H\theta$—and (2.16). Then the Nusselt number is bounded explicitly by $\int_0^1 dz\,\tau'(z)^2$. The other approach is to derive an *a priori* upper bound on $|\langle\int_V dV\tau'(z)w\theta\rangle|$ in terms of Ra and the functional form of τ, followed by an appropriate adjustment of τ to balance this estimate with $\int_0^1 dz\,\tau'(z)^2$. We will see that while the first approach can be carried out to derive a bound $\sim\mathrm{Ra}^{2/5}$ in the absence of rotation, i.e., for Ta=0, the second approach produces a similarly scaling bound uniform in Ta for all $-\infty<\mathrm{Ta}<\infty$, albeit with a slightly larger prefactor.

In both approaches the background profile is chosen so that the support of $\tau'(z)$ is concentrated near the boundaries where w and θ are forced to vanish due to the boundary conditions. In particular we take

$$\tau(z)=\begin{cases} 1-\dfrac{z}{2\delta} & \text{for } 0\leqslant z\leqslant\delta \\ \frac{1}{2} & \text{for } \delta\leqslant z\leqslant 1-\delta \\ \dfrac{1-z}{2\delta} & \text{for } 1-\delta\leqslant z\leqslant 1 \end{cases}, \tag{3.2}$$

where the adjustable parameter $\delta\,(0\leqslant\delta\leqslant\frac{1}{2})$ is referred to as the ''boundary layer'' thickness of the profile. Then $\tau'(z)$ vanishes in the bulk, and is the constant $-1/2\delta$ within distance δ of the isothermal boundaries. With this choice of background profile, both approaches rely on detailed local estimates for θ and w in the boundary layers near $z=0$ and $z=1$.

A. The 2/5 bound without rotation

First we treat the case of no rotation, i.e., Ta=0. Then the vertical velocity w satisfies

$$\Delta^2 w=-\mathrm{Ra}\;\Delta_H\theta, \tag{3.3}$$

together with the boundary conditions in (2.17). The procedure is now to show that we may choose the background profile's boundary layer thickness δ small enough (depending on Ra) to ensure that the quadratic form Q in (3.1) is non-negative. Then the bound will be $\mathrm{Nu}\leqslant 1/2\delta$.

We go over to the Fourier series representation to derive sufficient conditions for the non-negativity of Q. Decomposing Q mode by mode in the translation invariant horizontal directions, we observe that it will be non-negative when for each horizontal wave number $\mathbf{k}$

$$Q_{\mathbf{k}}\{\theta_{\mathbf{k}}\}=\int_0^1[|D\theta_{\mathbf{k}}|^2+k^2|\theta_{\mathbf{k}}|^2+\tau'(w_{\mathbf{k}}^*\theta_{\mathbf{k}}+w_{\mathbf{k}}\theta_{\mathbf{k}}^*)]dz, \tag{3.4}$$

is non-negative. In the above, $\theta_{\mathbf{k}}(z)$ is a complex valued function satisfying $\theta_{-\mathbf{k}}(z)=\theta_{\mathbf{k}}(z)^*$ and homogeneous Dirichlet boundary conditions

$$\theta_{\mathbf{k}}(0)=0=\theta_{\mathbf{k}}(1), \tag{3.5}$$

the z derivative is denoted by D, and the complex valued function $w_{\mathbf{k}}(z)$ is the linear functional of $\theta_{\mathbf{k}}$ defined by

$$(-D^2+k^2)^2 w_{\mathbf{k}}=\mathrm{Ra}\;k^2\theta_{\mathbf{k}}, \tag{3.6}$$

with both homogeneous Dirichlet and Neumann boundary conditions:

$$w_{\mathbf{k}}(0)=0=w_{\mathbf{k}}(1)\quad\text{and}\quad Dw_{\mathbf{k}}(0)=0=Dw_{\mathbf{k}}(1). \tag{3.7}$$

Note that $w_{\mathbf{k}}$ also satisfies $w_{-\mathbf{k}}(z)=w_{\mathbf{k}}(z)^*$. In this subsection we will also use $\|\cdot\|$ to denote the L_2 norm and $\|\cdot\|_\infty$ to denote the L_∞ norm [0,1], i.e.,

$$\|f\|=\sqrt{\int_0^1|f(z)|^2dz} \tag{3.8}$$

and

$$\|f\|_\infty=\sup_{0\leqslant z\leqslant 1}|f(z)|. \tag{3.9}$$

Consider first the temperature fluctuation component $\theta_{\mathbf{k}}(z)$. We estimate the growth of $\theta_{\mathbf{k}}(z)$ in the boundary layer according to

$$|\theta_{\mathbf{k}}(z)| = \left| \int_0^z D\theta_{\mathbf{k}}(z')dz' \right| \leq \sqrt{z} \sqrt{\int_0^{1/2} |D\theta_{\mathbf{k}}(z')|^2 dz'}, \tag{3.10}$$

for $0 \leq z \leq \frac{1}{2}$. Of course a similar estimate holds for the growth away from the boundary at $z = 1$.

We may obtain control of higher derivatives of $w_{\mathbf{k}}(z)$ in terms of the L_2 norm of $\theta_{\mathbf{k}}$ which will result in the growth of $w_{\mathbf{k}}(z)$ away from the boundaries being bounded by a higher power of the distance to the wall. Squaring (3.6) and integrating from 0 to 1, and integrating by parts where the boundary conditions permit, we have

$$\begin{aligned} \mathrm{Ra}^2 k^4 \|\theta_{\mathbf{k}}\|^2 = \|D^4 w_{\mathbf{k}}\|^2 - 2k^2 \int_0^1 [D^4 w_{\mathbf{k}}^* D^2 w_{\mathbf{k}} + D^4 w_{\mathbf{k}} D^2 w_{\mathbf{k}}^*] dz \\ + 6k^4 \|D^2 w_{\mathbf{k}}\|^2 + 4k^6 \|D w_{\mathbf{k}}\|^2 + k^8 \|w_{\mathbf{k}}\|^2. \end{aligned} \tag{3.11}$$

The indefinite term above may be estimated by its neighboring terms. For any $a > 0$

$$\left| 2k^2 \int_0^1 [D^4 w_{\mathbf{k}}^* D^2 w_{\mathbf{k}} + D^4 w_{\mathbf{k}} D^2 w_{\mathbf{k}}^*] dz \right| \leq a \|D^4 w_{\mathbf{k}}\|^2 + \frac{4k^4}{a} \|D^2 w_{\mathbf{k}}\|^2. \tag{3.12}$$

Choosing $a = \frac{1}{2}(\sqrt{41} - 5) \approx 0.7016$, then, we see that

$$\mathrm{Ra}^2 k^4 \|\theta_{\mathbf{k}}\|^2 \geq C[\|D^4 w_{\mathbf{k}}\|^2 + k^4 \|D^2 w_{\mathbf{k}}\|^2], \tag{3.13}$$

where $C = \frac{1}{2}(7 - \sqrt{41}) \approx 0.2984$. This will be enough to give us L_∞ control of $D^2 w_{\mathbf{k}}$ in light of the following:

Lemma: Let $f(z)$ be a smooth (say, $D^3 f$ is continuous) real valued function satisfying both homogeneous Dirichlet and Neumann boundary conditions on [0,1]. Then

$$\|D^2 f\|_\infty \leq \sqrt{2 \|D^4 f\| \|D^2 f\|}. \tag{3.14}$$

We note that this lemma is not true unless both sets of boundary conditions are satisfied. Counterexamples are the functions $f(z) = 2z^3 - 3z^2 + z$ and $f(z) = 2z^3 - 3z^2 + 1$ which satisfy, respectively, homogeneous Dirichlet and homogeneous Neumann boundary conditions on [0,1]. Each of these functions has $\|D^2 f\|_\infty = 6$ although $\|D^4 f\| = 0$.

To prove the lemma, first note that because of the homogeneous Dirichlet conditions, $\int_0^1 Df(z)dz = 0$, so Df must have a zero inside the interval (0,1). That is, there exists a point $z_0 \in (0,1)$ so that $Df(z_0) = 0$. Then because of the homogeneous Neumann conditions, $\int_0^{z_0} D^2 f(z)dz = 0$ and $\int_{z_0}^1 D^2 f(z)dz = 0$ so there exist points $z_1 \in (0, z_0)$ and $z_2 \in (z_0, 1)$ so that $D^2 f(z_1) = 0 = D^2 f(z_2)$.

So with $0 < z_1 < z_2 < 1$ being distinct zeros on $D^2 f$, we use the fundamental theorem of calculus to write

$$(D^2 f(z))^2 = 2 \int_{z_1}^z dz' D^2 f(z') D^3 f(z'), \tag{3.15}$$

and, for any point $\tilde{z} \in (0,1)$

$$D^3 f(z') = D^3 f(\tilde{z}) + \int_{\tilde{z}}^{z'} dz'' D^4 f(z''). \tag{3.16}$$

Inserting (3.16) into (3.15) we have

$$(D^2f(z))^2=2D^3f(\tilde z)\int_{z_1}^{z}dz'D^2f(z')+2\int_{z_1}^{z}dz'D^2f(z')\int_{\tilde z}^{z'}dz''D^4f(z''). \tag{3.17}$$

Integrating (3.17) with respect to $\tilde z$ from z_1 to z_2 and noting that the first term on the right hand side vanishes, we deduce

$$(z_2-z_1)(D^2f(z))^2=2\int_{z_1}^{z_2}d\tilde z\int_{z_1}^{z}dz'D^2f(z')\int_{\tilde z}^{z'}dz''D^4f(z''). \tag{3.18}$$

The Schwarz inequality (applied twice) then implies

$$(z_2-z_1)(D^2f(z))^2\leqslant 2(z_2-z_1)\|D^2f\|\,\|D^4f\|, \tag{3.19}$$

which proves the lemma.

Returning attention to $w_{\mathbf{k}}(z)=u(z)+iv(z)$ with u and v real (and each satisfying the boundary conditions in the lemma) and recalling (3.13), we have

$$\begin{aligned}|D^2w_{\mathbf{k}}(z)|^2&=(D^2u(z))^2+(D^2v(z))^2\\&\leqslant 2\|D^2u\|\|D^4u\|+2\|D^2v\|\,\|D^4v\|\\&\leqslant k^2\|D^2u\|^2+\frac{1}{k^2}\|D^4u\|^2+k^2\|D^2v\|^2+\frac{1}{k^2}\|D^4v\|^2\\&=k^2\|D^2w_{\mathbf{k}}\|^2+\frac{1}{k^2}\|D^4w_{\mathbf{k}}\|^2\\&\leqslant\frac{\mathrm{Ra}^2}{C}k^2\|\theta_{\mathbf{k}}\|^2.\end{aligned} \tag{3.20}$$

Hence the growth of $w_{\mathbf{k}}$ from the boundary at $z=0$ is limited by

$$\begin{aligned}|w_{\mathbf{k}}(z)|&=\left|\int_0^z dz'\int_0^{z'}dz''D^2w_{\mathbf{k}}(z'')\right|\\&\leqslant\frac{1}{2}z^2\|D^2w_{\mathbf{k}}\|_\infty\\&\leqslant\frac{1}{2}z^2\frac{\mathrm{Ra}}{\sqrt{C}}k\|\theta_{\mathbf{k}}\|.\end{aligned} \tag{3.21}$$

An analogous pointwise bound holds near the boundary at $z=1$.

The magnitude of the indefinite term in $Q_{\mathbf{k}}$ is then bounded in terms of the positive definite terms:

$$\int_0^1 \tau'(w_{\mathbf{k}}^*\theta_{\mathbf{k}}+w_{\mathbf{k}}\theta_{\mathbf{k}}^*)dz \leqslant \frac{1}{\delta}\int_0^\delta |w_{\mathbf{k}}(z)\|\theta_{\mathbf{k}}(z)|dz+\frac{1}{\delta}\int_{1-\delta}^1 |w_{\mathbf{k}}(z)\|\theta_{\mathbf{k}}(z)|dz$$

$$\leqslant \frac{1}{\delta}\int_0^\delta dz\,\frac{1}{2}z^2\left(\frac{\mathrm{Ra}}{\sqrt{C}}k\|\theta_{\mathbf{k}}\|\right)\sqrt{z}\sqrt{\int_0^{1/2}|D\theta_{\mathbf{k}}(z')|^2dz'}$$

$$+\frac{1}{\delta}\int_{1-\delta}^1 dz\,\frac{1}{2}(1-z)^2\left(\frac{\mathrm{Ra}}{\sqrt{C}}k\|\theta_{\mathbf{k}}\|\right)|\theta_{\mathbf{k}}(z)|\sqrt{1-z}\sqrt{\int_{1/2}^1|D\theta_{\mathbf{k}}(z')|^2dz'}$$

$$\leqslant \frac{1}{7}\delta^{5/2}\frac{\mathrm{Ra}}{\sqrt{C}}k\|\theta_{\mathbf{k}}\|\left(\sqrt{\int_0^{1/2}|D\theta_{\mathbf{k}}(z')|^2dz'}+\sqrt{\int_{1/2}^1|D\theta_{\mathbf{k}}(z')|^2dz'}\right)$$

$$\leqslant \frac{1}{7}\delta^{5/2}\frac{\mathrm{Ra}}{\sqrt{C}}\frac{1}{\sqrt{2}}(k^2\|\theta_{\mathbf{k}}\|^2+\|D\theta_{\mathbf{k}}\|^2). \tag{3.22}$$

Hence $Q_{\mathbf{k}}$ is non-negative for all $\mathbf{k}$ when we choose δ so that

$$1=\frac{1}{7\sqrt{2C}}\delta^{5/2}\mathrm{Ra}. \tag{3.23}$$

The heat transport is then bounded according to

$$\mathrm{Nu}\leqslant\frac{1}{2\delta}=\frac{1}{2(98C)^{1/5}}\mathrm{Ra}^{2/5}=0.2545\cdots\mathrm{Ra}^{2/5}. \tag{3.24}$$

This proof does not go through when $\mathrm{Ta}\neq 0$, however, because we cannot establish the highest derivative control in (3.13).

B. The 2/5 bound with rotation

In the presence of rotation we adopt another strategy to derive the 2/5 scaling bound, albeit with a slightly larger prefactor. When $\mathrm{Ta}\neq 0$ we cannot use the tight z^2 bound on w near the boundary because we cannot produce an effective estimate for the fourth derivative of w in L_2. We can, however, establish a $z^{3/2}$ growth. Then we do not require that the quadratic form Q be non-negative, but rather we find an *a priori* estimate for Q and then adjust the background boundary layer thickness δ to make the best of it.

Consider first the temperature field. Because $T(\mathbf{x},t)$ solves the advection-diffusion equation (2.7), it satisfies a maximum principle. That is, if the initial data $T(\mathbf{x},0)$ is bounded pointwise between the values at the boundaries, i.e., if $0\leqslant T(\mathbf{x},0)\leqslant 1$, then the solution subsequently sustains those limits: $0\leqslant T(\mathbf{x},t)\leqslant 1$. The background profile in (3.2) is also bounded pointwise in magnitude between 0 and 1, so the fluctuation θ also obeys the same limits. Hence

$$\|T\|_\infty=\|\tau\|_\infty=1 \quad \text{and} \quad \|\theta\|_\infty\leqslant 1. \tag{3.25}$$

We now establish growth limits on w near the boundaries as follows: The vertical components of velocity and vorticity are slaved to the temperature fluctuations by

$$\Delta^2 w-\sqrt{\mathrm{Ta}}\,\frac{\partial\zeta}{\partial z}=-\mathrm{Ra}\;\Delta_H\theta \tag{3.26}$$

and

$$-\Delta\zeta-\sqrt{\mathrm{Ta}}\,\frac{\partial w}{\partial z}=0. \tag{3.27}$$

Multiplying (3.26) by w and (3.27) by ζ, integrating over the full domain, and integrating by parts with the help of the boundary conditions (2.17) and (2.18)

$$\left\|\frac{\partial^2 w}{\partial z^2}\right\|^2+2\left\|\nabla_H\frac{\partial w}{\partial z}\right\|^2+\|\Delta_H w\|^2+\|\nabla\zeta\|^2=\mathrm{Ra}\int_V dV\,\theta(-\Delta_H w)\leqslant\frac{\mathrm{Ra}^2}{4}\|\theta\|^2+\|\Delta_H w\|^2, \tag{3.28}$$

where, not unexpectedly, ∇_H denotes the horizontal gradient $\mathbf{i}(\partial/\partial x)+\mathbf{j}(\partial/\partial y)$. Then thanks to (3.25), the second vertical derivative of the vertical velocity is bounded according to

$$\left\|\frac{\partial^2 w}{\partial z^2}\right\|^2\leqslant\frac{\mathrm{Ra}^2}{4}\|\theta\|^2\leqslant\frac{\mathrm{Ra}^2}{4}\mathcal{A}. \tag{3.29}$$

Then in view of w's boundary conditions, for $0\leqslant z\leqslant\frac{1}{2}$

$$|w(x,y,z)|=\left|\int_0^z dz'\int_0^{z'}dz''\frac{\partial^2 w}{\partial z^2}\right|\leqslant\frac{2}{3}z^{3/2}\sqrt{\int_0^{1/2}dz''\left(\frac{\partial^2 w}{\partial z^2}\right)^2}. \tag{3.30}$$

A similar estimate holds near the top boundary at $z=1$.

Combining (3.25), (3.29), and (3.30), the indefinite (last) term on the right-hand side of

$$\mathrm{Nu}=\int_0^1 dz\,\tau'(z)^2-\frac{1}{\mathcal{A}}\langle\|\nabla\theta\|^2\rangle-\frac{2}{\mathcal{A}}\left\langle\int_V dV\tau'(z)w\theta\right\rangle, \tag{3.31}$$

is seen to satisfy

$$\begin{aligned}\int_V dV\tau'(z)w\theta&\leqslant\frac{1}{2\delta}\int_0^{L_x/h}dx\int_0^{L_y/h}dy\int_0^{\delta}dz|w(x,y,z)|\|\theta\|_\infty\\&\quad+\frac{1}{2\delta}\int_0^{L_x/h}dx\int_0^{L_y/h}dy\int_{1-\delta}^{1}dz|w(x,y,z)|\|\theta\|_\infty\\&\leqslant\frac{1}{2\delta}\frac{2}{3}\frac{2}{5}\delta^{5/2}\sqrt{2\mathcal{A}}\left\|\frac{\partial^2 w}{\partial z^2}\right\|\\&\leqslant\frac{\sqrt{2}}{15}\delta^{3/2}\mathrm{Ra}\,\mathcal{A}.\end{aligned} \tag{3.32}$$

Hence

$$\mathrm{Nu}\leqslant\frac{1}{2\delta}+\frac{2\sqrt{2}}{15}\delta^{3/2}\mathrm{Ra}. \tag{3.33}$$

Now we minimize the right-hand side above with respect to δ by choosing

$$\delta=\frac{5^{2/5}}{2^{3/5}}\mathrm{Ra}^{-2/5} \tag{3.34}$$

to conclude that

$$\mathrm{Nu} \leqslant \frac{5^{3/5}}{3\times 2^{2/5}}\,\mathrm{Ra}^{2/5} = 0.6635\cdots\mathrm{Ra}^{2/5}. \tag{3.35}$$

This bound is independent of the rotation, i.e., uniform in Ta for $0 \leqslant \mathrm{Ta} < \infty$, and valid so long as the initial temperature data lie between the temperatures at the boundaries.

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The equivalence of the class of Rivlin–Sawyers equations and a class of stochastic models for polymer stress

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This paper establishes the precise relationship between the macroscopic class of factorized Rivlin–Sawyers equations and a class of microscopic-based stochastic models. The former is a well-established and popular class of rheological models for polymeric fluids, while the latter is a more recently introduced class of rheological models which combines aspects of network and reptation theory with aspects of continuum mechanic models. It is shown that the two models are equivalent in a defined sense under certain unrestrictive assumptions. The first part of the proof gives the functional relationship between the linear viscoelastic memory function of the Rivlin–Sawyers model and the probability density for creation times of random variables in the stochastic model. The main part of the proof establishes the relationship between the strain descriptions in each model by showing that the difference in corresponding strain expressions can be made arbitrarily small using the appropriate weighted norm from spectral approximation theory. [DOI: 10.1063/1.1332783]

I. INTRODUCTION

One of the main challenges in fields such as materials science, viscoelastic fluid mechanics, and polymer rheology and processing is the development of accurate rheological models to describe the complex stress–strain relationship in polymeric fluids. Many models have been proposed in the literature, each having varying degrees of success when applied to predict polymer flow behavior. In general, rheological models, or viscoelastic constitutive equations, are classified as macroscopic or microscopic.

Macroscopic models are closed-form phenomenological models which are formulated on the level of continuum mechanics. These models most often take the form of a differential equation, such as the Giesekus model or Phan-Thien–Tanner (PTT) model, or a Lagrangian integral of the Rivlin–Sawyers[1] or K-BKZ type.[2,3] Microscopic models are molecular-based or kinetic theory models. In these models, the macromolecules and their dynamics are modeled and the stress tensor is given by an expression which involves the polymer configurations. For dilute polymer solutions, these models include the bead-spring, or elastic dumbbell, models such as the Rouse model, the Hookean dumbbell model and the FENE model. For concentrated polymer solutions and polymer melts, they include the network theory of Lodge[4,5] and the reptation models of Doi and Edwards[6–9] and Curtiss and Bird.[10,11] Macroscopic expressions for many of these models have been formulated after (most often severe) simplifying assumptions have been made to derive the closed form. Furthermore, some of the macroscopic models, such as the PTT model, have been derived from microscopic considerations.

Among the most successful macroscopic models are those from the class of (factorized) Rivlin–Sawyers integral equations. In general, these models have performed reasonably well in describing polymer behavior in complex flow situations. However, the empirical nature of the

constitutive model limits the degree of success for these highly complicated fluids. All relevant polymer physics have not been included in these empirical models, and the lack of an underlying molecular understanding hinders further improvements.

It is widely recognized that advances in viscoelastic fluid mechanics can only come with the development of improved microscopic-based models since, unlike the macroscopic models, they allow for the inclusion of relevant polymer physics. Armed with efficient stochastic simulation methods, a molecular model can be improved on the molecular level by modifying it within the framework of stochastic processes, without sacrificing its tractability. In particular, no simplifying assumptions need to be made in order to derive a closed-form constitutive equation from the microscopic model. Moreover, advances in micro–macro simulations have allowed the coupling of finite element techniques for calculating macroscopic velocity and pressure fields with Brownian dynamics or stochastic simulation techniques for computing polymer stress from simulated molecular dynamics or coarse-grained models.[12–24]

Recently a new class of microscopic-based stochastic models has been introduced[25,26] which combines aspects of microscopic models from network and reptation theory with aspects of macroscopic models such as the Rivlin–Sawyers model. The model has been shown to provide good predictions of polymer melt rheology in shear and elongational flow. The objective of this paper is to establish the precise relationship between this class of microscopic-based models and the class of factorized Rivlin–Sawyers integral equations. In particular, it is shown that, under quite unrestrictive assumptions, the two models are equivalent in a well-defined sense. By establishing this equivalence, we thus give a precise underlying molecular understanding to the class of factorized Rivlin–Sawyers models. In principle, this then allows the Rivlin–Sawyers equation to be improved through the inclusion of physical insight within its stochastic formulation.

The remaining of the paper is organized as follows. The Rivlin–Sawyers model and the related stochastic model are described in Secs. II and III, respectively. The statement of the equivalence of the two models is presented in Sec. IV, while the main part of the equivalence proof is given in Sec. V. The paper concludes with a discussion in Sec. VI.

II. CONTINUUM MECHANICS MODEL

The incompressible flow of a polymeric fluid under isothermal conditions is governed by the usual mass and momentum conservation equations from continuum mechanics,

$$\nabla \cdot \mathbf{u} = 0,$$

$$\rho \frac{D\mathbf{u}}{Dt} = \nabla \cdot \boldsymbol{\sigma},$$

where $\mathbf{u}$ is the velocity field, ρ is the (constant) density, $D/Dt = \partial/\partial t + (\mathbf{u}\cdot\nabla)$ is the material derivative, and $\boldsymbol{\sigma}$ is the (Cauchy) stress tensor given by

$$\boldsymbol{\sigma} = -p\,\boldsymbol{\delta} + \boldsymbol{\tau}$$

in which $\boldsymbol{\delta}$ is the second-order unit tensor. The scalar field p represents an isotropic pressure and $\boldsymbol{\tau}$ is the extra-stress tensor. A constitutive equation for $\boldsymbol{\tau}$, along with appropriate boundary conditions, are needed to close the system. If the fluid is Newtonian, then $\boldsymbol{\tau}$ is the viscous stress tensor given by Newton's law, $\boldsymbol{\tau} = \mu[\nabla\mathbf{u} + (\nabla\mathbf{u})^{\dagger}]$, assuming incompressibility, where μ is the constant viscosity under constant temperature. Substitution of this $\boldsymbol{\tau}$ into the momentum equation yields the well-known Navier–Stokes equations.

For viscoelastic fluids, Newton's law does not hold and we need another constitutive equation for $\boldsymbol{\tau}$ to relate the stress to the strain, or more precisely, strain history. One of the most successful of these equations, to date, is the factorized Rivlin–Sawyers integral constitutive equation[1] whose general form is

$$\boldsymbol{\pi}(t)=\int_{-\infty}^{t}[h_1(I_1,I_2)\{\mathbf{B}(t,t')-\boldsymbol{\delta}\}+h_2(I_1,I_2)\{\mathbf{C}(t,t')-\boldsymbol{\delta}\}]m(t-t')dt'. \tag{1}$$

In this equation, t represents the present, or reference, time, while t' represents some time in the past ($t'\leqslant t$). The tensors $\mathbf{B}$ and $\mathbf{C}=\mathbf{B}^{-1}$ represent the (finite) Finger strain and (finite) Cauchy strain tensors, respectively, and are defined by

$$\mathbf{B}(t,t')=\mathbf{E}(t,t')\cdot\mathbf{E}^{\dagger}(t,t') \quad \text{and} \quad \mathbf{C}(t,t')=\boldsymbol{\Delta}^{\dagger}(t,t')\cdot\boldsymbol{\Delta}(t,t'), \tag{2}$$

where $\mathbf{E}(t,t')$ and $\boldsymbol{\Delta}(t,t')=\mathbf{E}^{-1}(t,t')$ are relative deformation gradient tensors whose components in Cartesian coordinates are

$$E_{ij}(t,t')=\frac{\partial x_i(t)}{\partial x_j(t')} \quad \text{and} \quad \Delta_{ij}(t,t')=\frac{\partial x_i(t')}{\partial x_j(t)}.$$

The tensor $\mathbf{E}(t,t')$ represents the gradient of the deformation of a fluid element at present time t relative to its configuration at time t' in the past, while $\boldsymbol{\Delta}(t,t')$ represents the gradient of the deformation at time t' relative to its configuration at time t.

The invariants of the Finger strain tensor are $I_1=\operatorname{tr}\mathbf{B}$, $I_2=\frac{1}{2}[(\operatorname{tr}\mathbf{B})^2-\operatorname{tr}(\mathbf{B}^2)]$ and $I_3=\det\mathbf{B}$, where tr and det denote the trace and determinant, respectively. Due to incompressibility, $I_3=\det\mathbf{B}=1$ and by the Cayley–Hamilton theorem,

$$\mathbf{B}^2-I_1\mathbf{B}+I_2\boldsymbol{\delta}=\mathbf{B}^{-1}\equiv\mathbf{C}$$

from which it follows that $I_2=\operatorname{tr}\mathbf{C}$. In the limit of small deformations, both I_1 and I_2 approach the value 3.

The functions h_1 and h_2 are strain-dependent functions of $I_1=\operatorname{tr}\mathbf{B}$ and $I_2=\operatorname{tr}\mathbf{C}$. Both h_1 and h_2 are continuous, positive functions with domain $[3,\infty)\times[3,\infty)$ and range $\Omega\subset\Re_+$ where Ω is a bounded set in the nonnegative real numbers $\Re_+=[0,\infty)$. For realistic strain functions (which are not identically zero), $\Omega=(0,1]$ with $h_i(3,3)=1$ and $h_i(I_1,I_2)$ decreasing to zero as $I_1,I_2\to\infty$.

The function $m(t-t')$ is the linear viscoelastic memory function. Related to this function is the relaxation modulus $G(t-t')$ through the definition $m(t-t')=\partial G(t-t')/\partial t'$. Both $m(s)$ and $G(s)$, where $s=t-t'\geqslant 0$, are continuous, positive functions which decrease monotonically to zero at $s=t-t'\to\infty$.

The tensors $\mathbf{B}$ and $\mathbf{C}$ do not depend on the material being modeled; they depend solely on the flow field. The functions h_1 and h_2, on the other hand, are material-dependent. A variety of forms for these functions have been proposed in the literature, whose parameters are determined by fitting rheological data taken from the material under defined, simple flow conditions.

The factorized K-BKZ equation constitutes a subclass of the Rivlin–Sawyers class of equations in which the strain functions h_1 and h_2 are related by

$$h_1=\frac{\partial W}{\partial I_1} \quad \text{and} \quad h_2=-\frac{\partial W}{\partial I_2},$$

for some potential function $W=W(I_1,I_2)$.[2,3]

Equation (1) is said to be *factorized* since the strain and time effects have been separated into two factors as $h_i(I_1,I_2)m(t-t')$, $i=1,2$. This is a standard assumption that is made when using these models. Another standard assumption implicit in Eq. (1) is that there is no interaction between effects at any two past times, t' and t''. Each past time contributes to the stress only through its interaction with the present time t. This assumption allows the more general, but computationally prohibitive, nested integral model to be reduced to the single-integral form of Eq. (1).

III. STOCHASTIC MODEL

In this section, we describe the microscopic-based stochastic model in which we are interested. We begin with a short review of network and reptation models on which the dynamics of the stochastic model are based. We then describe the dynamics of the stochastic model and form an expression for the extra-stress tensor $\boldsymbol{\tau}$ as a function of these dynamics.

A. Network and reptation models

The dynamics of concentrated polymer solutions and polymer melts must take into account the interactions between the macromolecules. One of the first approaches to model the interactions of polymer molecules in undiluted polymers was to modify the classical network theories of rubber elasticity. The basic idea in these theories is that the chemical crosslinks of a macromolecular solid are represented by permanent junction points in a network structure formed by the macromolecules. As the solid is deformed, the network structure is deformed, but the junction points never break and no new junction points are created. This theory has been modified for liquids by assuming that the junction points are temporary and are always being created and destroyed. In this way, the interactions of polymers are described by the temporary unified motion of macromolecular segments which are connected by the junction points.

The most well-known of the original network models for fluids is the Lodge network model for rubberlike liquids.[4,5] The Lodge model assumes that the creation rates are independent of time and the loss rates are constants. The creation and loss rates are related to the relaxation spectrum of the material (that is, the relaxation times and moduli) and can therefore be determined from the linear viscoelastic behavior of the fluid. There have been several modifications to the original Lodge network model.[27–32] The modifications of Phan-Thien and Tanner[27] and Wagner[28] produce models which allow for derivation of a closed-form expression and analytical solutions in some rheometric flows. Both contain a function which must be empirically determined. In more general network models, where the creation and loss rates are configuration dependent, analytical solutions cannot be found and numerical techniques must be utilized. Simulations of polymer network models in defined flow fields have been performed by Petruccione and Biller.[29–32]

Another class of models for undiluted polymers falls in the category of reptation. The first reptation theory to describe the rheology of undiluted polymers was introduced by Doi and Edwards[6–9] who described the motion of a single polymer represented by a Rouse chain. The main assumption behind the Doi–Edwards model is that each polymer in the highly entangled system of macromolecules moves, or reptates, in a tube formed by the other polymers. That is, the surrounding polymers form a topological constraint, represented by a tube, and allow the polymer inside to move only backwards and forwards within this tube in a reptational manner. The conformation of the polymer chain during deformation is determined by the affine deformation of the tube by the imposed flow field, the retraction of the chain within the tube, and the reptation of the chain ends out of the tube. A few years later, Curtiss and Bird[10,11] developed a kinetic theory for undiluted polymers in which the hindrance of sideway motion of polymers (here represented by Kramer chains) in a concentrated system is described by anisotropic friction tensors. These tensors represent the same physics as the constraining tube in the Doi–Edwards model.

The original Doi–Edwards model has undergone many modifications in efforts to improve its predictions.[33–49] Notable here are those related to tube diameter and tube cross section.[43–49] The original Doi–Edwards model assumes that the diameter of a tube (whose cross section is always circular) does not change during deformation or flow. The assumption of constant tube diameter was relaxed by Marrucci and de Cindio,[43] for example, who assumed that the volume of the tube segment remains constant during deformation, so that the tube diameter varies depending on the relative stretching of the tube segment. Assuming the tube segments deform affinely in the flow field, the tube diameter (as well as the force in the polymer chain) varies according to the orientation of the segment. In a further improvement, Wagner and Schaeffer[45] assumed that the tube radius is a function of the average stretch of the tube. More recently, modifications in the shape of the tube cross section have been considered. Ianniruberto and Marrucci[46] and Marrucci and Ianniruberto[47] postulated that during deformation or flow, the tube cross section does not

remain circular, but instead becomes an ellipse, given that the tube segments deform affinely in the flow field. This idea of ''anisotropic tube cross section'' was further explored by Öttinger.[48,49] Unlike the previous authors, Öttinger was able to derive a time evolution equation for the tube cross section as well as to develop a complete, thermodynamically admissible reptation model including anisotropic tube cross sections and other effects.

Unlike the original Doi–Edwards model which was simple enough to allow for analytical tractability, the modified models rely on stochastic simulation techniques for computing stress.

B. Dynamics and stress tensor

Let the 3×1 column vectors $\mathbf{Q}_1(t')$ and $\mathbf{Q}_2(t')$ denote two independent standard Gaussian (vector-valued) random variables (mean $\langle \mathbf{Q}_i(t')\rangle = \mathbf{0}$ and covariance $\langle \mathbf{Q}_i(t')\mathbf{Q}_i(t')\rangle = \boldsymbol{\delta}$, $i=1,2$), and let $\boldsymbol{\kappa}$ be the transpose of the velocity gradient tensor, $\boldsymbol{\kappa}=(\nabla \mathbf{u})^{\dagger}$. During time interval $t'<t<t'+s<\infty (s>0)$, let $\mathbf{Q}_1(t)$ and $\mathbf{Q}_2(t)$, respectively, be governed by the following deterministic equations:

$$\frac{d\mathbf{Q}_1(t)}{dt} = \boldsymbol{\kappa}(t)\cdot \mathbf{Q}_1(t), \tag{3}$$

$$\frac{d\mathbf{Q}_2(t)}{dt} = -\boldsymbol{\kappa}^{\dagger}(t)\cdot \mathbf{Q}_2(t). \tag{4}$$

These equations are based on the assumption that the vectors deform affinely in the flow field represented by $\boldsymbol{\kappa}$. At time $t'+s$, let $\mathbf{Q}_i (i=1,2)$ again be (independently) randomly generated according to the Gaussian distribution function and, using this newly generated vector as an initial condition, let $\mathbf{Q}_i$ again evolve according to Eq. (3) (for $i=1$) or Eq. (4) (for $i=2$) during a second time interval, and so forth over many time intervals. Finally, let $\mathbf{Q}(t)=[\mathbf{Q}_1^{\dagger}(t),\mathbf{Q}_2^{\dagger}(t)]^{\dagger}$. (In the following, we omit the †.)

In the framework of network theory of concentrated polymer solutions and polymer melts, $\mathbf{Q}_1$, with any distribution function ψ_0 (not necessarily Gaussian), describes the configuration of segments, or strands, defining the temporary physical entanglements of the macromolecules. This segment vector points from one junction point in the network to a neighboring junction point. During the lifetime s of the entanglement, or strand, created at time t', the configuration of $\mathbf{Q}_1$ is governed by the deterministic equation of motion, Eq. (3). The destruction of one or more entanglements can lead to new entanglements, whose initial configurations obey the distribution function ψ_0. See Lodge[4,5] for a description of the original network model for fluids, and Phan-Thien and Tanner,[27] Wagner,[28] and Petruccione and Biller[29–32] for modifications to this model.

The vector $\mathbf{Q}_2$ can be interpreted within the framework of (modified) reptation theory as a representation of the tube cross section, or area element of the strand. Hence, $\mathbf{Q}_2$ represents the same idea of anisotropic tube cross section discussed earlier. This vector points from the centerline of the constraining tube to the surface of the tube, where the tube surface represents an obstruction, such as an entanglement, caused by the presence of the surrounding macromolecules. The equation of motion for $\mathbf{Q}_2$, Eq. (4), describes the time evolution of the tube diameter or area element in the flow field during the lifetime of $\mathbf{Q}_2$. See Doi and Edwards[6–9] for a description of the original reptation model and Ianniruberto and Marrucci,[46] Marrucci and Ianniruberto,[47] and Öttinger[48,49] for modifications to this model based on anisotropic tube cross sections. Modifications based on varying tube diameter can be found in Marrucci and de Cindio,[43] Marrucci and Hermans,[44] and Wagner and Schaeffer.[45]

In general, the configuration vectors $\mathbf{Q}_1(t)$ and $\mathbf{Q}_2(t)$ are not orthogonal. However, if the initial vectors, $\mathbf{Q}_1(t')$ and $\mathbf{Q}_2(t')$, are orthogonal, then $\mathbf{Q}_1(t)$ and $\mathbf{Q}_2(t)$ remain orthogonal during their common lifetimes. In this case, $\mathbf{Q}_2(t)$ represents the orthogonal cross-sectional diameter.

The solutions to the two sets of initial-value ordinary differential equations, Eqs. (3) and (4), are

$$\hat{\mathbf{Q}}_1(t,t') = \mathbf{E}(t,t') \cdot \mathbf{Q}_1(t'), \tag{5}$$

$$\hat{\mathbf{Q}}_2(t,t') = \mathbf{\Delta}^{\dagger}(t,t') \cdot \mathbf{Q}_2(t'). \tag{6}$$

We use the notation $\hat{\mathbf{Q}}_1(t,t')$ and $\hat{\mathbf{Q}}_2(t,t')$ to represent the solutions $\mathbf{Q}_1(t)$ and $\mathbf{Q}_2(t)$ of Eqs. (3) and (4), respectively, in order to indicate the initial time t', i.e., creation time of the entanglement, and set $\hat{\mathbf{Q}}(t,t') = [\hat{\mathbf{Q}}_1(t,t'), \hat{\mathbf{Q}}_2(t,t')]$.

Since $\mathbf{Q}_i(t')$, $i=1,2$, are standard Gaussian random variables, it follows from Eqs. (2), (5), and (6) that $\hat{\mathbf{Q}}_i(t,t')$ are also Gaussian random variables with mean $\langle \hat{\mathbf{Q}}_i(t,t') \rangle = \mathbf{0}$ and covariance,

$$\langle \hat{\mathbf{Q}}_1(t,t') \hat{\mathbf{Q}}_1(t,t') \rangle = \mathbf{B}(t,t'), \tag{7}$$

$$\langle \hat{\mathbf{Q}}_2(t,t') \hat{\mathbf{Q}}_2(t,t') \rangle = \mathbf{C}(t,t'), \tag{8}$$

where $\mathbf{B}(t,t')$ and $\mathbf{C}(t,t')$ are the Finger and Cauchy strain tensors of the Rivlin–Sawyers equation. From the above equations it furthermore follows that

$$\langle \hat{Q}_1^2 \rangle = I_1 \quad \text{and} \quad \langle \hat{Q}_2^2 \rangle = I_2, \tag{9}$$

where $Q^2 = \mathbf{Q} \cdot \mathbf{Q} = \operatorname{tr} \mathbf{QQ}$ and where $I_1 = \operatorname{tr} \mathbf{B}$ and $I_2 = \operatorname{tr} \mathbf{C}$ are the invariants of the Finger strain tensor.

Equations (7)–(9) represent the first immediate relationships to the strain tensors of the Rivlin–Sawyers equation [Eq. (1)] on the continuum mechanics level.

Having introduced the model dynamics through the two random vectors $\mathbf{Q}_1$ and $\mathbf{Q}_2$, we now formulate the extra-stress tensor $\boldsymbol{\tau}$ as a function of these dynamics. For any random vector $\mathbf{Q}(t) = [\mathbf{Q}_1(t), \mathbf{Q}_2(t)]$ (not necessarily Gaussian), the expectation of an arbitrary function, $F(\mathbf{Q}(t))$, can be written in terms of conditional expectations of $F(\mathbf{Q}(t))$ as follows:

$$\langle F(\mathbf{Q}(t)) \rangle = \int_{-\infty}^{t} \mathrm{E}(F(\mathbf{Q}(t)) | \mathrm{T}_t = t') \mu^{\mathrm{T}_t}(t') dt' = \int_{-\infty}^{t} \langle F(\hat{\mathbf{Q}}(t,t')) \rangle \mu(t-t') dt', \tag{10}$$

where T_t is a random variable representing the creation time of a strand $\mathbf{Q}$ which lives at time t, and μ^{T_t} is the probability density associated with the probability measure for the random variable T_t. Therefore, $\mu^{\mathrm{T}_t}(t')dt'$ represents the probability that a strand which lives at time t was created in the interval of length dt' around t', for sufficiently small dt'. In replacing μ^{T_t} with $\mu(t-t')$ in the second integral of Eq. (10), we have adopted the assumption used in the factorized Rivlin–Sawyers equation that strain effects and time effects may be separated, or factored. Hence, the probability $\mu^{\mathrm{T}_t}(t')dt'$ depends only on the time difference $t-t'$ and not on specific values of t and t'.

The following general expression for $\mathbf{F}(\mathbf{Q}(t))$ was proposed,[25,26] thus introducing a new class of stochastic models for the extra-stress $\boldsymbol{\tau}$,

$$\boldsymbol{\tau}(t) = \langle \mathbf{F}(\mathbf{Q}(t)) \rangle = G(0) \langle f_1(Q_1^2, Q_2^2) \mathbf{Q}_1(t) \mathbf{Q}_1(t) + f_2(Q_1^2, Q_2^2) \mathbf{Q}_2(t) \mathbf{Q}_2(t) \rangle, \tag{11}$$

where $G(t-t')$ is the relaxation modulus, and f_1 and f_2 are scalar functions of $Q_i^2 = \operatorname{tr} \mathbf{Q}_i \mathbf{Q}_i$, $i=1,2$. In order for the model to predict the correct linear viscoelastic behavior, f_1 and f_2 must satisfy the constraint

$$\tfrac{1}{3} \langle Q_1^{e2} f_1^e - Q_2^{e2} f_2^e \rangle_0 + \tfrac{2}{15} \langle (Q_1^{e2})^2 f_{1,1}^e - (Q_2^{e2})^2 f_{2,2}^e \rangle_0 = 1,$$

which was derived under small deformation conditions.[25] The superscripts e represent equilibrium values and the notation $\langle\cdot\rangle_0$ indicates taking a Gaussian average in six-dimensional space with respect to the Gaussian probability density in six-dimensional space with mean $\mathbf{0}$ and square of the width $\boldsymbol{\delta}$.

The stochastic model, Eq. (11), was shown to predict well some material behavior of different polymeric melts.[25]

IV. EQUIVALENCE OF MODELS

We have described two models: The factorized Rivlin–Sawyers integral equation, which is a phenomenological model on the continuum mechanics level of description, and a class of microscopic-based stochastic models. By choosing the form of the stress tensor in Eq. (11), in particular by the inclusion of the functions f_1 and f_2, the stochastic model offers the ability to blend the physically-based molecular models from network theory and reptation theory, on which the dynamics are based, with continuum mechanics models.

In this section, we state and prove the manner in which, and conditions under which, these two models are equivalent.

The notation used in the theorem is that introduced above.

Theorem 1: Let $m(t-t')$ denote the linear viscoelastic memory function of a given incompressible fluid, where $m(0)<\infty$. Then given any pair of (continuous) functions $h_i:\mathfrak{R}_+^2\rightarrow\mathfrak{R}$, $i=1,2$, such that

$$\int_0^\infty\int_0^\infty h_i(x,y)e^{-(x+y)}dxdy<\infty, \tag{12}$$

there exists functions $f_i:\mathfrak{R}_+^2\rightarrow\mathfrak{R}$, $i=1,2$, such that the factorized Rivlin–Sawyers integral equation given by Eq. (1) can be approximated to arbitrary accuracy by the stochastic model given by Eq. (11). It also follows that the probability density for the creation time of a strand in the stochastic model, $\mu(t-t')$, is such that $\mu(0)<\infty$.

Conversely, let $\mu(t-t')$ denote the probability density for the creation time of a strand, where $\mu(0)<\infty$. Then given any pair of (continuous) functions $f_i:\mathfrak{R}_+^2\rightarrow\mathfrak{R}$, $i=1,2$, such that

$$\int_0^\infty\int_0^\infty f_i(x,y)e^{-(x+y)}dxdy<\infty, \tag{13}$$

there exists functions $h_i:\mathfrak{R}_+^2\rightarrow\mathfrak{R}$, $i=1,2$, such that the stochastic model given by Eq. (11) can be approximated to arbitrary accuracy by a Rivlin–Sawyers equation given by Eq. (1). It follows also that the linear viscoelastic memory function of the Rivlin–Sawyers model, $m(t-t')$, is such that $m(0)<\infty$.

In the manner just described, we say that the class of factorized Rivlin–Sawyers integral constitutive equations for an incompressible fluid, given by Eq. (1), is equivalent to the class of stochastic models given by Eq. (11). □

The expression for the error is a weighted average as described in the proof.

The theorem is proved by showing:

(1) Any linear viscoelastic memory function $m(t-t')$ of the Rivlin–Sawyers equation, Eq. (1), can be related to a probability density function $\mu(t-t')$ of Eq. (10), and vice versa;
(2) The expression for the strain in the Rivlin–Sawyers equation [the expression enclosed by the brackets in Eq. (1)] is equivalent to $\langle F(\hat{\mathbf{Q}}(t,t'))\rangle$ in Eq. (10), that is,

$$\begin{aligned} &h_1(I_1,I_2)[\mathbf{B}(t,t')-\boldsymbol{\delta}]+h_2(I_1,I_2)[\mathbf{C}(t,t')-\boldsymbol{\delta}] \\ &\quad=\langle f_1(\hat{Q}_1^2,\hat{Q}_2^2)\hat{\mathbf{Q}}_1(t,t')\hat{\mathbf{Q}}_1(t,t')+f_2(\hat{Q}_1^2,\hat{Q}_2^2)\hat{\mathbf{Q}}_2(t,t')\hat{\mathbf{Q}}_2(t,t')\rangle, \end{aligned} \tag{14}$$

to within an isotropic tensor. The proof of part 1 is trivial. Any $m(t-t')$ is related to a probability density function $\mu(t-t')$ via $\mu(t-t')=m(t-t')/G(0)$. By the properties of $m(s)$ and $G(s)$ given in Sec. II it can easily be verified that such a defined $\mu(s)$ satisfies the definition of probability density function, namely, $\mu(s)\geqslant 0$ and $\int_0^\infty \mu(s)ds=1$.

Although it is not necessary for the proof, we can show that both $m(s)$ and $\mu(s)$ are related to the probability of $\mathbf{Q}$ having a survival time exceeding $s=t-t'$. This is useful for the actual simulation procedure in the implementation of the stochastic model.[25] We show this in the following: If we let E_1 represent the event that an entanglement is produced in the time interval $[t',t'+dt']$ and let E_2 represent the event that an entanglement lives at time t, then $\mathrm{P}(E_1|E_2)=\mu^{\mathrm{T}_t}(t')dt'\equiv\mu(t-t')dt'$ by the definition of the probability density $\mu^{\mathrm{T}_t}(t')dt'=\mu(t-t')dt'$ in Eq. (10). Furthermore, letting S be a random variable representing the survival time of an entanglement, then $\mathrm{P}(E_2|E_1)=\int_{t-t'}^\infty p(s)ds$, where $p(s)$ is the probability density for the survival time S. Under the assumption that $\mathrm{P}(E_1)$ and $\mathrm{P}(E_2)$ are constant, which is physically reasonable, we find from the basic principle of conditional probability, $\mathrm{P}(E_1|E_2)=\mathrm{P}(E_2|E_1)\mathrm{P}(E_1)/\mathrm{P}(E_2)$, that

$$\mu(t-t')=\frac{1}{\langle S\rangle}\int_{t-t'}^\infty p(s)ds, \tag{15}$$

where $\langle S\rangle=\int_0^\infty sp(s)ds$ is the expected value of S. Equation (15) can easily be derived using the condition that $\int_{-\infty}^t \mu(t-t')dt'=1$.

From Eq. (15) it follows that $\mu(0)=1/\langle S\rangle$, so that

$$\int_{t-t'}^\infty p(s)ds=\frac{\mu(t-t')}{\mu(0)}=\frac{m(t-t')}{m(0)}. \tag{16}$$

V. PROOF OF PART 2

We now prove part 2 of the theorem. It is sufficient to show that given any functions h_1 and h_2 satisfying the conditions of the theorem, there exists functions f_1 and f_2 such that the left hand side of Eq. (14) can be approximated to arbitrary accuracy by the right-hand side of Eq. (14) in some appropriate norm.

We establish part 2 of the theorem in the following three subsections. In Sec. V A, we prove the result for the special case of polynomial strain functions. Some results from spectral approximations (polynomial approximations on unbounded domains) are given in Sec. V B. The results of these two subsections are used to extend the proof to general strain functions in Sec. V C.

A. Equivalence of models: Case of polynomial strain functions

In this subsection, we establish Theorem 1 for the case of polynomial strain functions by proving the following lemma.

Lemma 1: Let N be a finite nonnegative integer and let the strain functions h_1 and h_2 be polynomials of degree N in two variables I_1 and I_2, denoted by $h_{1,N}(I_1,I_2)$ and $h_{2,N}(I_1,I_2)$, respectively, which satisfy the conditions of Theorem 1. Then there exists a unique pair of polynomials $f_{1,N}$ and $f_{1,N}$, each of degree N, in two (random) variables $\hat{Q}_1^2$ and $\hat{Q}_2^2$ such that, to within an isotropic second order tensor,

$$h_{1,N}(I_1,I_2)[\mathbf{B}-\boldsymbol{\delta}]+h_{2,N}(I_1,I_2)[\mathbf{C}-\boldsymbol{\delta}]=\langle f_{1,N}(\hat{Q}_1^2,\hat{Q}_2^2)\hat{\mathbf{Q}}_1\hat{\mathbf{Q}}_1+f_{2,N}(\hat{Q}_1^2,\hat{Q}_2^2)\hat{\mathbf{Q}}_2\hat{\mathbf{Q}}_2\rangle. \tag{17}$$

□

Proof: Expanding the polynomials $h_{1,N}$ and $h_{2,N}$ about equilibrium, $I_1=I_2=3$, we have for the left-hand side of Eq. (17),

$$h_{1,N}(I_1,I_2)[\mathbf{B}-\boldsymbol{\delta}]+h_{2,N}(I_1,I_2)[\mathbf{C}-\boldsymbol{\delta}]$$
$$=\left[\sum_{\substack{i,j=0\\ i+j\leqslant N}}^{N} b_{ij}(I_1-3)^i(I_2-3)^j\right]\mathbf{B}+\left[\sum_{\substack{i,j=0\\ i+j\leqslant N}}^{N} c_{ij}(I_1-3)^i(I_2-3)^j\right]\mathbf{C}+\text{isotropic tensor}, \tag{18}$$

where the b_{ij} and c_{ij} are constants.

Expanding the polynomials $f_{1,N}$ and $f_{2,N}$ about $\hat{Q}_1^2=\hat{Q}_2^2=0$, and taking advantage of the independence of $\hat{\mathbf{Q}}_1$ and $\hat{\mathbf{Q}}_2$ to factor averages, yields the following for the right-hand side of Eq. (17),

$$\langle f_{1,N}(\hat{Q}_1^2,\hat{Q}_2^2)\hat{\mathbf{Q}}_1\hat{\mathbf{Q}}_1+f_{2,N}(\hat{Q}_1^2,\hat{Q}_2^2)\hat{\mathbf{Q}}_2\hat{\mathbf{Q}}_2\rangle$$
$$=\sum_{\substack{i,j=0\\ i+j\leqslant N}}^{N} f_{ij}^1\langle(\hat{Q}_2^2)^j\rangle\langle(\hat{Q}_1^2)^i\hat{\mathbf{Q}}_1\hat{\mathbf{Q}}_1\rangle+\sum_{\substack{i,j=0\\ i+j\leqslant N}}^{N} f_{ij}^2\langle(\hat{Q}_1^2)^i\rangle\langle(\hat{Q}_2^2)^j\hat{\mathbf{Q}}_2\hat{\mathbf{Q}}_2\rangle, \tag{19}$$

where the f_{ij}^1 and f_{ij}^2 are constants.

Since we take the initial values, $\mathbf{Q}_1(t')$ and $\mathbf{Q}_2(t')$, in the equations of motion, Eqs. (3) and (4), to be Gaussian random vectors, then the following relations between factors in the expansions of Eqs. (18) and (19) can be shown.

Claim 1: Let $\hat{\mathbf{Q}}_1\equiv\hat{\mathbf{Q}}_1(t,t')$ be the solution of the equation of motion given in Eq. (3), where the initial condition is set at time $t'\leqslant t$. Then for $n=0,1,2,\ldots$ we have

$$\langle\hat{\mathbf{Q}}_1\hat{\mathbf{Q}}_1(\hat{Q}_1^2)^n\rangle=p_n^0\boldsymbol{\delta}+p_n^1\mathbf{B}(t,t')+p_n^2\mathbf{C}(t,t'), \tag{20}$$

where p_n^0, p_n^1, and p_n^2 are polynomials in I_1-3 and I_2-3 which can be defined recursively by

$$p_n^0=-2n(I_2-3)p_{n-1}^1-6np_{n-1}^1+2np_{n-1}^2,$$

$$p_n^1=(2n+3)p_{n-1}^0+(2n+1)(I_1-3)p_{n-1}^1+3(2n+1)p_{n-1}^1+(I_2-3)p_{n-1}^2+3p_{n-1}^2,$$

$$p_n^2=2np_{n-1}^1,$$

and $p_0^0=0$, $p_0^1=1$, $p_0^2=0$. Furthermore, denoting $\langle(\hat{Q}_1^2)^n\rangle$ by p_n^3, it immediately follows that

$$p_n^3\equiv\langle(\hat{Q}_1^2)^n\rangle=\mathrm{tr}\langle\hat{\mathbf{Q}}_1\hat{\mathbf{Q}}_1(\hat{Q}_1^2)^{n-1}\rangle$$
$$=(I_1-3)p_{n-1}^1+(I_2-3)p_{n-1}^2+3(p_{n-1}^0+p_{n-1}^1+p_{n-1}^2) \tag{21}$$

for $n=1,2,\ldots$ and $p_0^3=1$. Note that p_n^1 and p_n^3 are polynomials of degree n, while p_n^0 and p_n^2 are polynomials of degree $n-1$. □

Claim 2: Let $\hat{\mathbf{Q}}_2\equiv\hat{\mathbf{Q}}_2(t,t')$ be the solution of the equation of motion given in Eq. (4), where the initial condition is set at time $t'\leqslant t$. Then for $n=0,1,2,\ldots$ we have

$$\langle\hat{\mathbf{Q}}_2\hat{\mathbf{Q}}_2(\hat{Q}_2^2)^n\rangle=p_n^{0'}\boldsymbol{\delta}+p_n^{1'}\mathbf{C}(t,t')+p_n^{2'}\mathbf{B}(t,t'), \tag{22}$$

where $p_n^{0'}$, $p_n^{1'}$, and $p_n^{2'}$ are polynomials in I_1-3 and I_2-3 which can be defined recursively by

$$p_n^{0'}=-2n(I_1-3)p_{n-1}^{1'}-6np_{n-1}^{1'}+2np_{n-1}^{2'},$$

$$p_n^{1'}=(2n+3)p_{n-1}^{0'}+(2n+1)(I_2-3)p_{n-1}^{1'}+3(2n+1)p_{n-1}^{1'}+(I_1-3)p_{n-1}^{2'}+3p_{n-1}^{2'},$$

$$p_n^{2'} = 2n p_{n-1}^{1'},$$

and $p_0^{0'} = 0$, $p_0^{1'} = 1$, $p_0^{2'} = 0$. Furthermore, denoting $\langle (\hat{Q}_2^2)^n \rangle$ by $p_n^{3'}$, it immediately follows that

$$\begin{aligned} p_n^{3'} \equiv \langle (\hat{Q}_2^2)^n \rangle &= \mathrm{tr} \langle \hat{\mathbf{Q}}_2 \hat{\mathbf{Q}}_2 (\hat{Q}_2^2)^{n-1} \rangle \\ &= (I_2 - 3) p_{n-1}^{1'} + (I_1 - 3) p_{n-1}^{2'} + 3(p_{n-1}^{0'} + p_{n-1}^{1'} + p_{n-1}^{2'}) \end{aligned} \tag{23}$$

for $n = 1,2,\ldots$ and $p_0^{3'} = 1$. Note that $p_n^{1'}$ and $p_n^{3'}$ are polynomials of degree n, while $p_n^{0'}$ and $p_n^{2'}$ are polynomials of degree $n-1$. □

The proof of these claims can be established solely with induction arguments and using the relations

$$\langle \hat{\mathbf{Q}}_1 \hat{\mathbf{Q}}_1 (\hat{Q}_1^2)^n \rangle = \mathbf{B} \langle (\hat{Q}_1^2)^n \rangle + 2n \mathbf{B} \cdot \langle \hat{\mathbf{Q}}_1 \hat{\mathbf{Q}}_1 (\hat{Q}_1^2)^{n-1} \rangle, \tag{24}$$

$$\langle \hat{\mathbf{Q}}_2 \hat{\mathbf{Q}}_2 (\hat{Q}_2^2)^n \rangle = \mathbf{C} \langle (\hat{Q}_2^2)^n \rangle + 2n \mathbf{C} \cdot \langle \hat{\mathbf{Q}}_2 \hat{\mathbf{Q}}_2 (\hat{Q}_2^2)^{n-1} \rangle, \tag{25}$$

which follow from Wick's theorem (which can be applied since we assume a Gaussian distribution function)[50] and

$$\mathbf{B}^2 = I_1 \mathbf{B} - I_2 \boldsymbol{\delta} + \mathbf{C},$$

which follows from the Cayley–Hamilton theorem.

The following three observations follow from Claims 1 and 2.

Observation 1: p_n^1 and $p_n^{1'}$ are identical if I_1 and I_2 are interchanged in either. More precisely, for $n = 0,1,2,\ldots$,

$$p_n^1 = (2n+1)!!(I_1 - 3)^n + \sum_{\substack{i,j=0 \\ i+j \leqslant n-1}}^{n-1} \beta_{ij}^{(n)} (I_1 - 3)^i (I_2 - 3)^j, \tag{26}$$

$$p_n^{1'} = (2n+1)!!(I_2 - 3)^n + \sum_{\substack{i,j=0 \\ i+j \leqslant n-1}}^{n-1} \beta_{ij}^{(n)} (I_1 - 3)^j (I_2 - 3)^i. \tag{27}$$

The set of coefficients $\{\beta_{ij}^{(n)}\}$ can be defined recursively in terms of the sets of coefficients $\{\beta_{ij}^{(k)}\}$, $k = n-1, n-2, n-3$ as follows:

$$\beta_{ij}^{(n)} = \begin{cases} (2n+1)[\beta_{i-1,j}^{(n-1)} + 3\beta_{ij}^{(n-1)}] \\ \quad -4(n+1)(n-1)\beta_{i,j-1}^{(n-2)}, \quad \text{if } i+j = n-1 \\ (2n+1)[\beta_{i-1,j}^{(n-1)} + 3\beta_{ij}^{(n-1)}] \\ \quad -4(n+1)(n-1)[\beta_{i,j-1}^{(n-2)} + 3\beta_{ij}^{(n-2)}], \quad \text{if } i+j = n-2 \\ (2n+1)[\beta_{i-1,j}^{(n-1)} + 3\beta_{ij}^{(n-1)}] \\ \quad -4(n+1)(n-1)[\beta_{i,j-1}^{(n-2)} + 3\beta_{ij}^{(n-2)}] \\ \quad +4(2n+3)(n-1)(n-2)\beta_{ij}^{(n-3)}, \quad \text{if } i+j \leqslant n-3 \end{cases}$$

for $n = 1,2,\ldots$, and $\beta_{00}^{(0)} = 1$. The only nonzero nth order coefficient in Eqs. (26) and (27) appears outside the summations; namely, $\beta_{n,0}^{(n)} = (2n+1)!!$ and $\beta_{n-k,k}^{(n)} = 0$ for $k = 1,\ldots,n$. [In the recursive formulas we interpret $\beta_{i-1,j}^{(n-1)} = 0$ for $i = 0$ and $\beta_{i,j-1}^{(n-2)} = 0$ for $j = 0$.] □

Observation 2: p_n^2 and $p_n^{2'}$ are identical if I_1 and I_2 are interchanged in either. More precisely, for $n = 1,2,\ldots$,

$$p_n^2 = 2n(2n-1)!!(I_1-3)^{n-1} + \sum_{\substack{i,j=0 \\ i+j\leqslant n-2}}^{n-2} 2n\beta_{ij}^{(n-1)}(I_1-3)^i(I_2-3)^j, \tag{28}$$

$$p_n^{2'} = 2n(2n-1)!!(I_2-3)^{n-1} + \sum_{\substack{i,j=0 \\ i+j\leqslant n-2}}^{n-2} 2n\beta_{ij}^{(n-1)}(I_1-3)^j(I_2-3)^i, \tag{29}$$

and $p_0^2 = p_0^{2'} = 0$. The coefficients $\beta_{ij}^{(n-1)}$ are the same as those corresponding to p_{n-1}^1 and $p_{n-1}^{1'}$ as defined in Observation 1 above. □

Observation 3: p_n^3 and $p_n^{3'}$ are identical if I_1 and I_2 are interchanged in either. More precisely, for $n = 1,2,\ldots,$

$$p_n^3 = (2n-1)!!(I_1-3)^n + \sum_{\substack{i,j=0 \\ i+j\leqslant n-1}}^{n-1} \gamma_{ij}^{(n)}(I_1-3)^i(I_2-3)^j, \tag{30}$$

$$p_n^{3'} = (2n-1)!!(I_2-3)^n + \sum_{\substack{i,j=0 \\ i+j\leqslant n-1}}^{n-1} \gamma_{ij}^{(n)}(I_1-3)^j(I_2-3)^i, \tag{31}$$

and $p_0^3 = p_0^{3'} = 1$. The set of coefficients $\{\gamma_{ij}^{(n)}\}$ can be defined recursively in terms of the sets of coefficients $\{\beta_{ij}^{(k)}\}$, $k = n-1, n-2, n-3$, of Observation 1, as follows:

$$\gamma_{ij}^{(n)} = \begin{cases} \beta_{i-1,j}^{(n-1)} + 3\beta_{ij}^{(n-1)} - 4(n-1)\beta_{i,j-1}^{(n-2)}, & \text{if } i+j = n-1 \\ \beta_{i-1,j}^{(n-1)} + 3\beta_{ij}^{(n-1)} - 4(n-1)[\beta_{i,j-1}^{(n-2)} + 3\beta_{ij}^{(n-2)}], & \text{if } i+j = n-2 \\ \beta_{i-1,j}^{(n-1)} + 3\beta_{ij}^{(n-1)} - 4(n-1)[\beta_{i,j-1}^{(n-2)} + 3\beta_{ij}^{(n-2)}] & \\ \quad + 12(n-1)(n-2)\beta_{ij}^{(n-3)}, & \text{if } i+j \leqslant n-3 \end{cases}$$

or

$$(2n+1)\gamma_{ij}^{(n)} = \begin{cases} \beta_{ij}^{(n)} - 4n(n-1)\beta_{i,j-1}^{(n-2)}, & \text{if } i+j = n-1 \\ \beta_{ij}^{(n)} - 4n(n-1)[\beta_{i,j-1}^{(n-2)} + 3\beta_{ij}^{(n-2)}], & \text{if } i+j = n-2 \\ \beta_{ij}^{(n)} - 4n(n-1)[\beta_{i,j-1}^{(n-2)} + 3\beta_{ij}^{(n-2)}] & \\ \quad + 16n(n-1)(n-2)\beta_{ij}^{(n-3)}, & \text{if } i+j \leqslant n-3 \end{cases}$$

for $n = 1,2,\ldots$ and $\gamma_{00}^{(0)} = \beta_{00}^{(0)} = 1$. The only nonzero nth order coefficient in Eqs. (30) and (31) appears outside the summations; namely, $\gamma_{n,0}^{(n)} = \beta_{n-1,0}^{(n-1)} = (2n-1)!!$ and $\gamma_{n-k,k}^{(n)} = \beta_{n-k-1,k}^{(n-1)} = 0$ for $k = 1,\ldots,n$. [As before, we interpret $\beta_{i-1,j}^{(n-1)} = 0$ for $i = 0$ and $\beta_{i,j-1}^{(n-2)} = 0$ for $j = 0$.]

(Note: $\{\gamma_{ij}^{(n)}\}$ can also be defined recursively in terms of the sets of coefficients $\{\gamma_{ij}^{(k)}\}$, $k = n-1, n-2, n-3$.) □

A similar observation can be stated for the polynomials p_n^0 and $p_n^{0'}$, but it is not needed in the proof and so is omitted.

Substituting Eqs. (20) and (22), along with $p_n^3 \equiv \langle(\hat{Q}_1^2)^n\rangle$, and $p_n^{3'} \equiv \langle(\hat{Q}_2^2)^n\rangle$, into Eq. (19) yields

$$\begin{aligned}
&\langle f_{1,N}(\hat{Q}_1^2,\hat{Q}_2^2)\hat{\mathbf{Q}}_1\hat{\mathbf{Q}}_1+f_{2,N}(\hat{Q}_1^2,\hat{Q}_2^2)\hat{\mathbf{Q}}_2\hat{\mathbf{Q}}_2\rangle\\
&\quad=\sum_{\substack{i,j=0\\ i+j\leqslant N}}^{N} f_{ij}^1[p_j^{3\prime}][p_i^0\boldsymbol{\delta}+p_i^1\mathbf{B}+p_i^2\mathbf{C}]+\sum_{\substack{i,j=0\\ i+j\leqslant N}}^{N} f_{ij}^2[p_i^3][p_j^{0\prime}\boldsymbol{\delta}+p_j^{1\prime}\mathbf{C}+p_j^{2\prime}\mathbf{B}]\\
&\quad=\sum_{\substack{i,j=0\\ i+j\leqslant N}}^{N}\{[f_{ij}^1p_i^1p_j^{3\prime}+f_{ij}^2p_i^3p_j^{2\prime}]\mathbf{B}+[f_{ij}^1p_i^2p_j^{3\prime}+f_{ij}^2p_i^3p_j^{1\prime}]\mathbf{C}+[f_{ij}^1p_j^{3\prime}p_i^0+f_{ij}^2p_i^3p_j^{0\prime}]\boldsymbol{\delta}\}\\
&\quad=F_{1,N}\mathbf{B}+F_{2,N}\mathbf{C}+\text{isotropic tensor.}
\end{aligned}\tag{32}$$

For convenience, we have denoted by $F_{1,N}$ and $F_{2,N}$ the polynomial factors of $\mathbf{B}$ and $\mathbf{C}$, respectively, in the last line of the above equation.

Equation (32) is precisely in the form we want, the terms on the right-hand side in brackets, represented by $F_{1,N}$ and $F_{2,N}$, being polynomials of I_1-3 and I_2-3. Comparing Eqs. (18) and (32), the proof is complete if we can show that for every pair of polynomials $h_{1,N}$ and $h_{2,N}$, there exists a unique pair of polynomials f_1 and f_2 such that

$$\begin{aligned}
h_{1,N}(I_1,I_2)\mathbf{B}+h_{2,N}(I_1,I_2)\mathbf{C}&=\left[\sum_{\substack{i,j=0\\ i+j\leqslant N}}^{N} b_{ij}(I_1-3)^i(I_2-3)^j\right]\mathbf{B}+\left[\sum_{\substack{i,j=0\\ i+j\leqslant N}}^{N} c_{ij}(I_1-3)^i(I_2-3)^j\right]\mathbf{C}\\
&=\sum_{\substack{i,j=0\\ i+j\leqslant N}}^{N}[f_{ij}^1p_i^1p_j^{3\prime}+f_{ij}^2p_i^3p_j^{2\prime}]\mathbf{B}+\sum_{\substack{i,j=0\\ i+j\leqslant N}}^{N}[f_{ij}^1p_i^2p_j^{3\prime}+f_{ij}^2p_i^3p_j^{1\prime}]\mathbf{C}\\
&=F_{1,N}(I_1,I_2)\mathbf{B}+F_{2,N}(I_1,I_2)\mathbf{C}.
\end{aligned}\tag{33}$$

The isotropic terms in Eqs. (18) and (32), can be neglected in the above equation since they can be combined with the other isotropic tensors in the total stress tensor $\boldsymbol{\sigma}=-p\boldsymbol{\delta}+\boldsymbol{\tau}$.

Equating the coefficients of $(I_1-3)^i(I_2-3)^j$, for $i,j=0,\ldots,N; i+j\leqslant N$, in the series expansions multiplying the tensors $\mathbf{B}$ and $\mathbf{C}$ in Eq. (33) leads respectively to the following relations between the coefficients f_{ij}^1, f_{ij}^2 and the coefficients b_{ij}, c_{ij}:

$$\mathbf{A}_{11}\mathbf{f}^1+\mathbf{A}_{12}\mathbf{f}^2=\mathbf{b},\tag{34}$$

$$\mathbf{A}_{21}\mathbf{f}^1+\mathbf{A}_{22}\mathbf{f}^2=\mathbf{c},\tag{35}$$

where $\mathbf{A}_{11}$, $\mathbf{A}_{12}$, $\mathbf{A}_{21}$, and $\mathbf{A}_{22}$ are each $[(N+1)(N+2)/2]\times[(N+1)(N+2)/2]$ matrices. The vectors $\mathbf{f}^1$ and $\mathbf{f}^2$ are $[(N+1)(N+2)/2]\times 1$ column vectors containing the coefficients f_{ij}^1 and f_{ij}^2, respectively. Likewise, $\mathbf{b}$ and $\mathbf{c}$ are $[(N+1)(N+2)/2]\times 1$ column vectors containing the coefficients b_{ij} and c_{ij}, respectively. The order of the coefficients in these four vectors leads to attractive properties of the matrices $\mathbf{A}_{ij}$, which will be exploited later. The ordering in each vector is such that the $(N+1)$ coefficients of order $i+j=N$ appear first, followed by the N coefficients of order $i+j=N-1$, and so on, the last entry in each vector being the coefficient of order $i+j=0$. Within each group of coefficients of a given order $i+j=l$, we adopt the following convention: in vectors $\mathbf{f}^1$ and $\mathbf{b}$, the coefficients appear in increasing order on the second index j ($f_{l,0}^1,f_{l-1,1}^1,\ldots,f_{0,l}^1$ and $b_{l,0}$, $b_{l-1,1},\ldots,b_{0,l}$), while in vectors $\mathbf{f}^2$ and $\mathbf{c}$ the coefficients appear in increasing order on the first index i ($f_{0,l}^2,f_{1,l-1}^2,\ldots,f_{l,0}^2$ and $c_{0,l}$, $c_{1,l-1},\ldots,c_{l,0}$). In other words, if we define $k_{ij}=[(N+1)(N+2)-(i+j+1)(i+j+2)]/2+(j+1)$ then the k_{ij}-entry of $\mathbf{f}^1$ and $\mathbf{b}$ is f_{ij}^1 and b_{ij}, respectively, and the k_{ij}-entry of $\mathbf{f}^2$ and $\mathbf{c}$ is f_{ji}^2 and c_{ji}, respectively. Observe for later use that, by the definition of k_{ij}, $i+j<i'+j'$ implies $k_{ij}>k_{i'j'}$ (although the converse is not true), and $k_{ij}=k_{i',j'}$ if and only if $i=i'$ and $j=j'$.

Claim 3: Letting $\mathbf{f}=(\mathbf{f}^1,\mathbf{f}^2)^\dagger$ and $\mathbf{d}=(\mathbf{b},\mathbf{c})^\dagger$, systems (34) and (35) can be written as

$$\mathbf{Af}=\mathbf{d}, \tag{36}$$

where

$$\mathbf{A}=\begin{pmatrix}\mathbf{L}_1 & \mathbf{L}_2\\ \mathbf{L}_2 & \mathbf{L}_1\end{pmatrix} \tag{37}$$

and $\mathbf{L}_1$ and $\mathbf{L}_2$ are lower triangular matrices. Furthermore, the diagonal entries of $\mathbf{L}_1$ are all nonzero, while the diagonal entries of $\mathbf{L}_2$ are all zero. It follows that $\det(\mathbf{A})\neq 0$ so that $\mathbf{A}:\Re^m \rightarrow \Re^m$ represents an invertible linear (matrix) operator on the space $\Re^m$, where $m=(N+1)(N+2)$. □

The proof of this claim can be found in the Appendix.

The fact that $\mathbf{A}$ is an invertible operator on $\Re^m$ means that for any set of coefficients $\mathbf{f}\in\Re^m$ of the series expansions in Eq. (19) there exists a unique set of coefficients $\mathbf{d}\in\Re^m$ of the series expansions in Eq. (18) given by $\mathbf{d}=\mathbf{Af}$. Likewise, for any $\mathbf{d}\in\Re^m$ there is a unique $\mathbf{f}\in\Re^m$ given by $\mathbf{f}=\mathbf{A}^{-1}\mathbf{d}$. Therefore, if the functions h_1 and h_2 are polynomials of degree N then there are unique polynomials f_1 and f_2 of degree N such that Eq. (17) holds.

With this, the lemma is proved. □

Remark 1: The lemma and proof still hold if h_1 and h_2 are polynomials of different degrees. In this case, N is taken to be the larger of the two degrees.

Remark 2: The proof above also establishes that for any polynomials $f_{1,N}$ and $f_{2,N}$ satisfying the conditions of Theorem 1, there exists a unique pair of polynomials $h_{1,N}$ and $h_{2,N}$ such that Eq. (17) holds to within an isotropic tensor.

We have shown that the equivalence theorem is true when the strain functions are polynomials in two variables. Before extending the proof to general strain functions satisfying the conditions of the theorem, we need some results from spectral approximations.

B. Results from spectral approximations

In this subsection, some mathematical ideas from polynomial approximations on unbounded domains are discussed. Inasmuch as possible, we restrict the discussion to those concepts necessary for our purposes. Details on this subject can be found in the literature.[51–55] Furthermore, we formulate the ideas in one dimension. The concepts and results generalize to tensorized domains.[55]

We begin by defining some weighted Sobolev spaces on the positive real numbers $\Re_+=[0,\infty)$ along with their norms. In each case, the subscript w denotes the weight function, which is $w=e^{-x}$. First we define the weighted Sobolev space,

$$L^2_w(\Re_+)=\left\{ f:\Re_+\rightarrow\Re \,\middle|\, f \text{ is measurable and } \int_0^\infty [f(x)]^2 e^{-x}dx<\infty \right\}$$

which is equipped with the norm

$$\|f\|_{L^2_w(\Re_+)}=\left(\int_0^\infty [f(x)]^2 e^{-x}dx \right)^{1/2}. \tag{38}$$

This is a Hilbert space under the inner product defined by

$$(f,g)_{L^2_w(\Re_+)}=\int_0^\infty f(x)g(x)e^{-x}dx \quad \forall f,g\in L^2_w(\Re_+).$$

Higher order weighted Sobolev spaces, $H^m_w(\Re_+)$, are defined in the usual manner. Specifically, for any non-negative integer m, the space $H^m_w(\Re_+)$ is the space of all functions in $L^2_w(\Re_+)$ whose derivatives up to and including order m are also in $L^2_w(\Re_+)$. This space is provided with the usual norm

$$\|f\|_{H_w^m(\Re_+)}=\left[\sum_{k=0}^{m}\int_0^\infty\left(\frac{d^k f(x)}{dx^k}\right)^2 e^{-x}dx\right]^{1/2},$$

for any $f\in H_w^m(\Re_+)$.

Next we recall some features of Laguerre polynomials. The family of Laguerre polynomials $\{l_n(x):n=0,1,2,\dots\}$ forms an orthonormal set of polynomials on $\Re_+=[0,\infty)$ with respect to the weight function $w(x)=e^{-x}$ and the inner product

$$(f,g)_w=\int_0^\infty f(x)g(x)w(x)dx.$$

That is, for $m, n=0,1,2,\dots,$

$$\int_0^\infty l_m(x)l_n(x)e^{-x}dx=\delta_{mn}.$$

The polynomials are defined recursively as

$$l_0(x)=1,\quad l_1(x)=1-x$$

$$l_n(x)=[(2n-1-x)l_{n-1}(x)-(n-1)l_{n-2}(x)]/n,\quad n\geqslant 2,$$

and for each n, $u=l_n$ satisfies the differential equation

$$xu''+(1-x)u'+nu=0.$$

It is known that a function f satisfying $\int_0^\infty f(x)e^{-x}dx<\infty$ can be expanded in terms of the Laguerre polynomials as follows:[56]

$$f(x)=\sum_{n=0}^{\infty}c_n l_n(x),\quad \text{where } c_n=\int_0^\infty f(x)l_n(x)e^{-x}dx\quad x>0. \tag{39}$$

Let $P_N(\Re_+)$ be the space of polynomials of degree less than or equal to N, restricted to $\Re_+$. A basis for $P_N(\Re_+)$ is the set of the first $N+1$ Laguerre polynomials, $\{l_k:k=0,\dots,N\}$. The orthogonal projection operator $\pi^N:L_w^2(\Re_+)\to P_N(\Re_+)$ from the weighted Sobolev space $L_w^2(\Re_+)$ onto $P_N(\Re_+)$ is defined by

$$\pi^N f=\sum_{n=0}^{N}c_n l_n,\quad \forall f\in L_w^2(\Re_+), \tag{40}$$

where the coefficients c_n are defined as in Eq. (39). From Eqs. (38), (39), and (40), it is easy to show that for any n and any $f\in L_w^2(\Re_+)$,

$$\|f-\pi^N f\|_{L_w^2(\Re_+)}^2=\sum_{n=N+1}^{\infty}c_n^2. \tag{41}$$

Therefore, Eq. (41) represents the error in approximating a function $f\in L_w^2(\Re_+)$ by the polynomial of degree N defined in Eq. (40).

We now state the following error estimate established by Maday, Pernaud-Thomas, and Vandeven,[53] Funaro,[51] and Bernardi and Maday.[54]

Theorem 2: (Theorem 12.6 in Bernardi and Maday[54]): For any positive integer k and any positive real number s, let $H_{wk}^s(\Re_+)$ be the Sobolev space defined by

$$H^s_{wk}(\mathfrak{R}_+)=\{f\in H^s_w(\mathfrak{R}_+)|x^{k/2}f\in H^s_w(\mathfrak{R}_+)\},$$

where $H^s_w(\mathfrak{R}_+)$ is the interpolation space between $H^m_w(\mathfrak{R}_+)$ and $L^2_w(\mathfrak{R}_+)$ with index $1-s/m$ where m is any integer such that $m\geqslant s$. The space $H^s_{wk}(\mathfrak{R}_+)$ is equipped with the norm

$$\|f\|_{H^s_{wk}(\mathfrak{R}_+)}=\|(1+x)^{k/2}f\|_{H^s_w(\mathfrak{R}_+)}$$

for any $f\in H^s_{wk}(\mathfrak{R}_+)$.

Then, for any real number $s\geqslant 0$, there exists a constant $C>0$, depending only on s, such that for any function $f\in H^s_{wk}(\mathfrak{R}_+)$, the following estimate holds:

$$\|f-\pi^N f\|_{L^2_w(\mathfrak{R}_+)}\leqslant CN^{-s/2}\|f\|_{H^s_{wk}(\mathfrak{R}_+)}, \tag{42}$$

where k is the largest integer less than $s+1$. □

Remark 1: This theorem implies that, once s is fixed, then given any $\epsilon>0$, there is an N such that

$$\|f-\pi^N f\|_{L^2_w(\mathfrak{R}_+)}\leqslant CN^{-s/2}\|f\|_{H^s_{wk}(\mathfrak{R}_+)}<\epsilon. \tag{43}$$

Remark 2: The above concepts and theorem generalize to higher dimension tensorized domains.[55] Of interest to us is the generalization to $\mathfrak{R}^2_+=[0,\infty)\times[0,\infty)$, briefly outlined below.

A function $f(x,y)$ satisfying $\int_0^\infty\int_0^\infty f(x,y)e^{-(x+y)}dxdy<\infty$ can be expanded as

$$f(x,y)=\sum_{k,l=0}^{\infty} c_{kl}l_k(x)l_l(y),$$

where

$$c_{kl}=\int_0^\infty\int_0^\infty f(x,y)l_k(x)l_l(y)e^{-(x+y)}dxdy,$$

and where $\{l_k(x)l_l(y):k,l=0,\ldots,N\}$ is a basis for the tensor space $P_N(\mathfrak{R}^2_+)\equiv P_N(\mathfrak{R}_+)\times P_N(\mathfrak{R}_+)=\{p_{ij}(x,y)|p_{ij}(x,y)=p_i(x)p_j(y)$ for $p_i(x),p_j(y)\in P_N(\mathfrak{R}_+)$ and integers $0\leqslant i,j\leqslant N\}$. The orthogonal projection operator $\Pi^N:L^2_w(\mathfrak{R}^2_+)\to P_N(\mathfrak{R}^2_+)$ from the tensor Sobolev space $L^2_w(\mathfrak{R}^2_+)$ onto $P_N(\mathfrak{R}^2_+)$ is defined by

$$\Pi^N f(x,y)=\sum_{k,l=0}^{N} c_{kl}l_k(x)l_l(y),\quad \forall f\in L^2_w(\mathfrak{R}^2_+). \tag{44}$$

It is easily shown that Π^N is the composite of the individual orthogonal projection operators, π^N_x and π^N_y, i.e., $\Pi^N=\pi^N_x\circ\pi^N_y$, where the subscripts x and y indicate the variable with which the operator π^N, defined in Eq. (40), is applied.

The generalization of Theorem 2 then tells us that given any $\epsilon>0$ there is an N such that

$$\|f(x,y)-\Pi^N f(x,y)\|_{L^2_w(\mathfrak{R}^2_+)}<\epsilon. \tag{45}$$

Equation (45) is the result we use in the following subsection to complete the proof.

C. Equivalence of models: General case

The proof of Eq. (14) for the general case of arbitrary strain functions, satisfying the conditions of Theorem 1, can now be given. It follows from the case of polynomial strain functions and the approximation of functions on unbounded domains given in the previous subsections.

Given any $\epsilon>0$, let N of Eq. (45) be fixed. By the hypothesis of Theorem 1, the functions h_1 and h_2 are in the weighted Laguerre space $L^2_w(\Re^2_+)$. Therefore, h_1 and h_2 can be approximated by polynomials $\hat{h}_{1,N}$ and $\hat{h}_{2,N}$ using Laguerre polynomial basis functions. Following the notation of the previous subsection, we have

$$\hat{h}_{1,N}(I_1,I_2)=\Pi^N h_1(I_1,I_2)=\sum_{i,j=0}^{N}\hat{b}_{ij}l_i(I_1)l_j(I_2),$$

$$\hat{h}_{2,N}(I_1,I_2)=\Pi^N h_2(I_1,I_2)=\sum_{i,j=0}^{N}\hat{c}_{ij}l_i(I_1)l_j(I_2),$$

where Π^N is the orthogonal projection operator given in Eq. (44). The approximating polynomials $\hat{h}_{1,N}$ and $\hat{h}_{2,N}$ can be rewritten in terms of the basis $\{(I_1-3)^i(I_2-3)^j\}$ as follows:

$$\hat{h}_{1,N}(I_1,I_2)=\sum_{i,j=0}^{N}b_{ij}(I_1-3)^i(I_2-3)^j=\sum_{\substack{i,j=0\\ i+j\leqslant N'}}^{N'}b_{ij}(I_1-3)^i(I_2-3)^j=h_{1,N'}(I_1,I_2),$$

$$\hat{h}_{2,N}(I_1,I_2)=\sum_{i,j=0}^{N}c_{ij}(I_1-3)^i(I_2-3)^j=\sum_{\substack{i,j=0\\ i+j\leqslant N'}}^{N'}c_{ij}(I_1-3)^i(I_2-3)^j=h_{2,N'}(I_1,I_2),$$

where $N'=2N$.

From the extension of Theorem 2 to $\Re^2_+$, i.e., Eq. (45),

$$\|h_i(I_1,I_2)-h_{i,N'}(I_1,I_2)\|_{L^2_w(\Re^2_+)}<\epsilon \tag{46}$$

for $i=1,2$.

Now, from the result for the special case of polynomial strain functions [Lemma 1, Eq. (33)], we know that for $h_{1,N'}$ and $h_{2,N'}$ there exists polynomials $f_{1,N'}$ and $f_{2,N'}$ such that

$$h_{1,N'}=\sum_{\substack{i,j=0\\ i+j\leqslant N'}}^{N'}(f^1_{ij}p^1_i p^{3\prime}_j+f^2_{ij}p^3_i p^{2\prime}_j)=F_{1,N'},$$

$$h_{2,N'}=\sum_{\substack{i,j=0\\ i+j\leqslant N'}}^{N'}(f^1_{ij}p^2_i p^{3\prime}_j+f^2_{ij}p^3_i p^{1\prime}_j)=F_{2,N'},$$

where f^1_{ij} and f^2_{ij} are the coefficients in the polynomials $f_{1,N'}$ and $f_{2,N'}$. Replacing $h_{i,N'}$ with $F_{i,N'}$ in Eq. (46) gives us the desired error estimate

$$\|h_i(I_1,I_2)-F_{i,N'}(I_1,I_2)\|_{L^2_w(\Re^2_+)}<\epsilon \tag{47}$$

for $i=1,2$.

Thus we have shown that for every $\epsilon>0$, there is an N' and polynomial functions f_1 and f_2 of degree N' such that the weighted error between h_i and the expression $F_{i,N'}$, which is uniquely defined in terms of the coefficients of f_i, is less than ϵ. This completes the proof.

□

VI. DISCUSSION

We conclude by making some additional small remarks about the conditions of Theorem 1, followed by some properties of the transformation in Eqs. (36) and (37), and finally a corollary to the theorem.

First, we remark that the conditions on the functions h_i and f_i in Eqs. (12) and (13) in Theorem 1 pose no serious restriction. In particular, the realistic forms for h_i decrease to zero as $I_1, I_2 \to \infty$, and it is reasonable to assume that realistic forms for f_i do the same.

Second, the condition on the equivalence that $\mu(0) < \infty$, or $m(0) < \infty$, is needed since the probability density $p(s)$ is not integrable when $\mu(s) \to \infty$ as $s \to 0$. Apparently, this excludes the Doi–Edwards reptation model, which can be written as a Rivlin–Sawyers integral, from having an equivalent stochastic form, Eq. (11), since, in the Doi–Edwards model, $\mu(s) \sim 1/\sqrt{s}$, for small s. However, the divergence of $\mu(s)$ in the Doi–Edwards model results from an infinite number of increasingly higher frequency modes, only a finite number of which can be physically meaningful. Therefore, one can safely truncate after a finite number of modes, without changing the essential physics, but removing the singularity.

Third, the system in Eqs. (36) and (37) results only if the degree of the polynomial approximation of all functions, h_1, h_2, f_1, and f_2, is the same. However, this is not a restriction since such a condition can always be met. The proof proceeds even if one of the functions is identically zero. The corresponding coefficient vector, in this case, is the zero vector.

From the properties of the polynomials p_n^m (or equivalently $p_n^{m'}$), $m = 1,2,3$, it can be seen that the matrices $\mathbf{L}_1$ and $\mathbf{L}_2$ have the forms,

$$\mathbf{L}_1 = \begin{pmatrix} \mathbf{D}_{N+1}^{(N)} & & & & & & & \\ \mathbf{M}_{N,N+1}^{(N)} & \mathbf{D}_N^{(N-1)} & & & & & & \\ \mathbf{M}_{N-1,N+1}^{(N)} & \mathbf{M}_{N-1,N}^{(N-1)} & \mathbf{D}_{N-1}^{(N-2)} & & & & & \\ \cdot & \cdot & \cdot & \cdot & & & & \\ \cdot & \cdot & \cdot & & \cdot & & & \\ \cdot & \cdot & \cdot & & & \cdot & & \\ \mathbf{M}_{2,N+1}^{(N)} & \mathbf{M}_{2,N}^{(N-1)} & \mathbf{M}_{2,N-1}^{(N-2)} & \cdot & \cdot & \cdot & \mathbf{D}_2^{(1)} & \\ \mathbf{M}_{1,N+1}^{(N)} & \mathbf{M}_{1,N}^{(N-1)} & \mathbf{M}_{1,N-1}^{(N-2)} & \cdot & \cdot & \cdot & \mathbf{M}_{1,2}^{(1)} & 1 \end{pmatrix}, \tag{48}$$

$$\mathbf{L}_2 = \begin{pmatrix} \mathbf{0}_{N+1,N+1}^{(N)} & & & & & & & & \\ \tilde{\mathbf{D}}_N^{(N)} | \mathbf{0}_{N,1}^{(N)} & \mathbf{0}_{N,N}^{(N-1)} & & & & & & & \\ \tilde{\mathbf{M}}_{N-1,N}^{(N)} | \mathbf{0}_{N-1,1}^{(N)} & \tilde{\mathbf{D}}_{N-1}^{(N-1)} | \mathbf{0}_{N-1,1}^{(N-1)} & \mathbf{0}_{N-1,N-1}^{(N-2)} & & & & & & \\ \tilde{\mathbf{M}}_{N-2,N}^{(N)} | \mathbf{0}_{N-2,1}^{(N)} & \tilde{\mathbf{M}}_{N-2,N-1}^{(N-1)} | \mathbf{0}_{N-2,1}^{(N-1)} & \tilde{\mathbf{D}}_{N-2}^{(N-2)} | \mathbf{0}_{N-2,1}^{(N-2)} & \mathbf{0}_{N-2,N-2}^{(N-3)} & & & & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & & & & \\ \cdot & \cdot & \cdot & \cdot & & \cdot & & & \\ \cdot & \cdot & \cdot & \cdot & & & \cdot & & \\ \tilde{\mathbf{M}}_{2,N}^{(N)} | \mathbf{0}_{2,1}^{N} & \tilde{\mathbf{M}}_{2,N-1}^{(N-1)} | \mathbf{0}_{2,1}^{(N-1)} & \tilde{\mathbf{M}}_{2,N-2}^{(N-2)} | \mathbf{0}_{2,1}^{(N-2)} & \tilde{\mathbf{M}}_{2,N-3}^{(N-3)} | \mathbf{0}_{2,1}^{(N-3)} & \cdot & \cdot & \cdot & \mathbf{0}_{2,2}^{(1)} & \\ \tilde{\mathbf{M}}_{1,N}^{(N)} | 0 & \tilde{\mathbf{M}}_{1,N-1}^{(N-1)} | 0 & \tilde{\mathbf{M}}_{1,N-2}^{(N-2)} | 0 & \tilde{\mathbf{M}}_{2,N-3}^{(N-3)} | 0 & \cdot & \cdot & \cdot & \tilde{\mathbf{D}}_1^{(1)} | 0 & 0 \end{pmatrix}. \tag{49}$$

Each $\mathbf{M}_{lm}^{(n)}$ and $\tilde{\mathbf{M}}_{lm}^{(n)}$ is an $l \times m$ matrix; $\mathbf{D}_m^{(n)}$ is an $m \times m$ diagonal matrix with all nonzero entries along the principal diagonal (i.e., $[\mathbf{D}_m^{(n)}]_{ii} \neq 0$); $\tilde{\mathbf{D}}_m^{(n)}$ is an $m \times m$ matrix which contains all zero entries except for entries along its minor diagonal which are all nonzero ($[\tilde{\mathbf{D}}_m^{(n)}]_{i,n-i+1} \neq 0$); and $\mathbf{0}_{lm}^{(n)}$ is the $l \times m$ zero matrix. In all matrices, the superscript (n) indicates that the matrix entries are coefficients of terms of order n. Columns k_{0j}, $j = 0, \ldots, N$, of $\mathbf{L}_2$ contain only zeros since $p_0^2 = p_0^{2'} = 0$.

Let $\mathbf{L}_1^{(n)}$ and $\mathbf{L}_2^{(n)}$ be the $\mathbf{L}_1$ and $\mathbf{L}_2$ matrices corresponding to polynomial approximations of degree n. We have the following relations between $\mathbf{L}_1^{(n)}$ and $\mathbf{L}_2^{(n)}$ and the matrices corresponding to polynomial approximations of degree $(n-1)$,

$$\mathbf{L}_1^{(n)}=\begin{pmatrix} \mathbf{D}_{n+1}^{(n)} & \\ \mathbf{M}_{n(n+1)/2,n+1}^{(n)} & \mathbf{L}_1^{(n-1)} \end{pmatrix},$$

$$\mathbf{L}_2^{(n)}=\begin{pmatrix} \mathbf{0}_{n+1}^{(n)} & \\ \tilde{\mathbf{M}}_{n(n+1)/2,n+1}^{(n)} & \mathbf{L}_2^{(n-1)} \end{pmatrix}.$$

Note that the addition of higher order terms with zero coefficients does not change the solution due to the form of $\mathbf{L}_1^{(n)}$ and $\mathbf{L}_2^{(n)}$ above.

The forms of $\mathbf{L}_1$ and $\mathbf{L}_2$ allow us to write directly the solution $\mathbf{f}$ of the system in Eqs. (36) and (37) as follows: For $i,j=0,\ldots,N, i+j\leqslant N$, the k_{ij} entry of $\mathbf{f}^1$ and $\mathbf{f}^2$ are

$$f_{ij}^1=\frac{1}{[\mathbf{L}_1]_{k_{ij}k_{ij}}}\left[b_{ij}-\sum_{\substack{l,m=0\\ i+j+1\leqslant l+m\leqslant N}}^{N} ([\mathbf{L}_1]_{k_{ij}k_{lm}} f_{lm}^1+[\mathbf{L}_2]_{k_{ij}k_{lm}} f_{ml}^2)\right], \tag{50}$$

$$f_{ji}^2=\frac{1}{[\mathbf{L}_1]_{k_{ij}k_{ij}}}\left[c_{ji}-\sum_{\substack{l,m=0\\ i+j+1\leqslant l+m\leqslant N}}^{N} ([\mathbf{L}_1]_{k_{ij}k_{lm}} f_{ml}^2+[\mathbf{L}_2]_{k_{ij}k_{lm}} f_{lm}^1)\right]. \tag{51}$$

Note that for each i,j the expressions defining f_{ij}^1 and f_{ji}^2 only involve variables f_{lm}^1 and f_{ml}^2 corresponding to higher-order terms, i.e., $l+m>i+j$.

From Eqs. (50) and (51) and the properties of matrices $\mathbf{L}_1$ and $\mathbf{L}_2$, a corollary to Theorem 1 results concerning the (factorized) K-BKZ class of equations. The K-BKZ constitutive equation forms a subclass of the Rivlin–Sawyers equation, Eq. (1), in which the strain functions h_1 and h_2 are defined in terms of a potential function $W=W(I_1,I_2)$ as $h_1=\partial W/\partial I_1$ and $h_2=-\partial W/\partial I_2$. Therefore, the strain functions in the K-BKZ equation satisfy the condition

$$\frac{\partial h_1(I_1,I_2)}{\partial I_2}=-\frac{\partial h_2(I_1,I_2)}{\partial I_1}. \tag{52}$$

The following corollary can be shown.

Corollary: The factorized K-BKZ subclass of factorized Rivlin–Sawyers constitutive equations, which satisfies the condition in Eq. (52), is equivalent to the subclass of equations for $\langle \mathbf{F}(\mathbf{Q}(t))\rangle$, given by Eq. (11), in which the functions f_1 and f_2 satisfy the condition

$$\frac{\partial f_1(Q_1^2,Q_2^2)}{\partial Q_2^2}=-\frac{\partial f_2(Q_1^2,Q_2^2)}{\partial Q_1^2}. \tag{53}$$

□

In other words, this corollary says that $\partial h_1/\partial I_2=-\partial h_2/\partial I_1$ if and only if $\partial f_1/\partial Q_2^2=-\partial f_2/\partial Q_1^2$.

The proof of this corollary is established as follows. If the functions h_1, h_2, f_1, and f_2 are written as polynomials of degree N as indicated in Eqs. (18) and (19), then Eqs. (52) and (53) are, respectively, equivalent to the following relationships between the polynomial coefficients:

$$c_{ij}=-\left(\frac{j+1}{i}\right) b_{i-1,j+1}, \tag{54}$$

$$f^2_{ij} = -\left(\frac{j+1}{i}\right) f^1_{i-1,j+1} \tag{55}$$

for $i=1,\ldots,N$, $j=0,\ldots,N-1$, and $i+j\leqslant N$. The corollary is proved by showing that condition (54) holds if and only if condition (55) holds. This can be seen to follow directly from Eqs. (50) and (51) and the properties of matrices $\mathbf{L}_1$ and $\mathbf{L}_2$ given above and in the Appendix.

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APPENDIX: PROOF OF CLAIM 3

To prove Claim 3 we need to show that $\mathbf{A}_{11}=\mathbf{A}_{22}=\mathbf{L}_1$ and $\mathbf{A}_{12}=\mathbf{A}_{21}=\mathbf{L}_2$ are lower triangular matrices, and $[\mathbf{L}_1]_{kk}\neq 0$ and $[\mathbf{L}_2]_{kk}=0$ for all $k=1,\ldots,(N+1)(N+2)/2$.

(1) Entry $(k_{i'j'},k_{ij})$ of matrix $\mathbf{A}_{11}$ [in Eq. (34)] contains the coefficient of $(I_1-3)^{i'}(I_2-3)^{j'}$ in the series $p^1_i p^{3'}_j$, which by Eqs. (26) and (31) is

$$\begin{aligned} p^1_i p^{3'}_j &= (2i+1)!!(2j-1)!!\,(I_1-3)^i(I_2-3)^j \\ &\quad + (2i+1)!!(I_1-3)^i \sum_{\substack{m,n=0\\ m+n\leqslant j-1}}^{j-1} \gamma^{(j)}_{nm}(I_1-3)^m(I_2-3)^n \\ &\quad + (2j-1)!!(I_2-3)^j \sum_{\substack{m,n=0\\ m+n\leqslant i-1}}^{i-1} \beta^{(i)}_{mn}(I_1-3)^m(I_2-3)^n \\ &\quad + \sum_{\substack{m,n=0\\ m+n\leqslant i-1}}^{i-1} \sum_{\substack{m',n'=0\\ m'+n'\leqslant j-1}}^{j-1} \beta^{(i)}_{mn}\gamma^{(j)}_{n'm'}(I_1-3)^{m+m'}(I_2-3)^{n+n'} \end{aligned} \tag{A1}$$

for $j=1,2,\ldots$ and all i. For $j=0$, $p^1_i p^{3'}_j$ is simply p^1_i [given in Eq. (26)] since $p^{3'}_0=1$. There is only one term of the highest possible order $i+j$, which is seen on the first line of Eq. (A1). The series on the second and third lines are each of order $i+j-1$, while the series on the fourth line is of order $i+j-2$. Since the order of Eq. (A1) is $i+j$ and given the fact that $i'+j'>i+j$ implies $k_{i'j'}<k_{ij}$ (as previously noted by our numbering convention), it follows that $[\mathbf{A}_{11}]_{k_{i'j'}k_{ij}}=0$ for $k_{i'j'}<k_{ij}$. This says that $\mathbf{A}_{11}$ is a lower triangular matrix. The fact that $\mathbf{A}_{11}$ has nonzero diagonal entries follows from the observation that $k_{ij}=k_{i'j'}$ if and only if $i=i'$ and $j=j'$, so that $[\mathbf{A}_{11}]_{k_{ij}k_{ij}}=(2i+1)!!(2j-1)!!\neq 0$ for $j=1,2,\ldots$ and $[\mathbf{A}_{11}]_{k_{ij}k_{ij}}=(2i+1)!!\neq 0$ for $j=0$.

(2) Entry $(k_{i'j'},k_{ij})$ of matrix $\mathbf{A}_{12}$ [in Eq. (34)] contains the coefficient of $(I_1-3)^{i'}(I_2-3)^{j'}$ in the series $p^3_j p^{2'}_i$, which by Eqs. (29) and (30) is

$$\begin{aligned} p^3_j p^{2'}_i &= 2i(2i-1)!!(2j-1)!!(I_1-3)^j(I_2-3)^{i-1} \\ &\quad + 2i(2j-1)!!(I_1-3)^j \sum_{\substack{m,n=0\\ m+n\leqslant i-2}}^{i-2} \beta^{(i-1)}_{nm}(I_1-3)^m(I_2-3)^n \\ &\quad + 2i(2i-1)!!(I_2-3)^{i-1} \sum_{\substack{m,n=0\\ m+n\leqslant j-1}}^{j-1} \gamma^{(j)}_{mn}(I_1-3)^m(I_2-3)^n \end{aligned}$$

$$+2i\sum_{\substack{m,n=0\\ m+n\leqslant j-1}}^{j-1}\ \sum_{\substack{m',n'=0\\ m'+n'\leqslant i-2}}^{i-2}\gamma_{mn}^{(j)}\beta_{n'm'}^{(i-1)}(I_1-3)^{m+m'}(I_2-3)^{n+n'} \tag{A2}$$

for $i,j=1,2,\ldots$. For $j=0$, $p_j^3 p_i^{2'}$ reduces to $p_i^{2'}$ [given in Eq. (29)] since $p_0^3=1$, while the series vanishes whenever $i=0$ since $p_0^{2'}=0$. The order of Eq. (A2) is only $i+j-1$, and the single term of this order appears on the first line. The series on the second and third lines are each of order $i+j-2$, while the series on the fourth line is of order $i+j-3$. The fact that $\mathbf{A}_{12}$ is a lower triangular matrix follows from the same argument given above for $\mathbf{A}_{11}$. Similarly, the diagonal entries of $\mathbf{A}_{12}$ are all zero since $[\mathbf{A}_{12}]_{k_{ij}k_{ij}}$ is the coefficient of $(I_1-3)^i(I_2-3)^j$, but $p_j^3 p_i^{2'}$ is only of order $i+j-1$, for $i\neq 0$ and is zero for $i=0$.

(3) Entry $(k_{i'j'},k_{ij})$ of matrix $\mathbf{A}_{22}$ [in Eq. (35)] contains the coefficient of $(I_1-3)^{j'}(I_2-3)^{i'}$ in the series $p_i^{1'}p_j^3$. The coefficient of $(I_1-3)^{j'}(I_2-3)^{i'}$ in $p_i^{1'}p_j^3$ equals the coefficient of $(I_1-3)^{i'}(I_2-3)^{j'}$ in $p_i^1 p_j^{3'}$, which is the $(k_{i'j'},k_{ij})$ entry of matrix $\mathbf{A}_{11}$.

The fact that $\mathbf{A}_{22}=\mathbf{A}_{11}$ follows from two observations. First, the different ordering of the coefficients in **b** and **c** is such that row k_{ij} of **b** corresponds to the coefficient of $(I_1-3)^i(I_2-3)^j$ (in the series expansion of damping function h_1) iff row k_{ij} of **c** corresponds to the coefficient of $(I_1-3)^j(I_2-3)^i$ (in the series expansion of damping function h_2). Second, $p_j^{1'}p_i^3$ and $p_i^1 p_j^{3'}$ are identical if in either one, i and j are first interchanged and then all I_1 and I_2 are interchanged (since by Observation 1 p_i^1 and $p_i^{1'}$ are identical if I_1 and I_2 are interchanged in either expression, as are p_i^3 and $p_i^{3'}$ by Observation 3).

(4) Entry $(k_{i'j'},k_{ij})$ of matrix $\mathbf{A}_{21}$ [in Eq. (35)] contains the coefficient of $(I_1-3)^{j'}(I_2-3)^{i'}$ in the series $p_i^2 p_j^{3'}$. The coefficient of $(I_1-3)^{j'}(I_2-3)^{i'}$ in $p_i^2 p_j^{3'}$ equals the coefficient of $(I_1-3)^{i'}(I_2-3)^{j'}$ in $p_i^{2'}p_j^3$, which is the $(k_{i'j'},k_{ij})$ entry of matrix $\mathbf{A}_{12}$.

$\mathbf{A}_{21}=\mathbf{A}_{12}$ by arguments similar to those given in part (3). □

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The geometry of photon surfaces

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The photon sphere concept in Schwarzschild space–time is generalized to a definition of a photon surface in an arbitrary space–time. A photon sphere is then defined as an $SO(3)\times\mathbb{R}$-invariant photon surface in a static spherically symmetric space–time. It is proved, subject to an energy condition, that a black hole in any such space–time must be surrounded by a photon sphere. Conversely, subject to an energy condition, any photon sphere must surround a black hole, a naked singularity or more than a certain amount of matter. A second order evolution equation is obtained for the area of an $SO(3)$-invariant photon surface in a general nonstatic spherically symmetric space–time. Many examples are provided. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1308507]

I. INTRODUCTION

The exterior region of the maximally extended Schwarzschild space–time is described by the metric

$$\mathbf{g}=-\left(1-\frac{2m}{r}\right)dt^2+\left(1-\frac{2m}{r}\right)^{-1}dr^2+r^2(d\theta^2+\sin^2\theta\,d\phi^2),\quad r>2m. \tag{1}$$

For any null geodesic in this exterior region the null geodesic equations give

$$\frac{d^2r}{d\lambda^2}=(r-3m)\left\{\left(\frac{d\theta}{d\lambda}\right)^2+\sin^2\theta\left(\frac{d\phi}{d\lambda}\right)^2\right\}, \tag{2}$$

where λ is an affine parameter along the geodesic. The right side here is evidently positive for $r>3m$ and negative for $r:2m<r<3m$. It follows that any future endless null geodesic in the maximally extended Schwarzschild space–time starting at some point with $r>3m$ and initially directed outwards, in the sense that $dr/d\lambda$ is initially positive, will continue outwards and escape to infinity. Any future endless null geodesic in the maximally extended Schwarzschild space–time starting at some point with $r:2m<r<3m$ and initially directed inwards, in the sense that $dr/d\lambda$ is initially negative, will continue inwards and fall into the black hole. The hypersurface $\{r=3m\}$, known as the Schwarzschild photon sphere, thus distinguishes the borderline between these two types of behavior; any null geodesic starting at some point of the photon sphere and initially tangent to the photon sphere will remain in the photon sphere. (See Darwin[1,2] for a detailed analysis of the behavior of null and timelike geodesics in Schwarzschild space–time.)

The Schwarzschild photon sphere also has physical significance for massive bodies. For any timelike geodesic in the exterior region the geodesic equations give

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$$\frac{d^2r}{ds^2} = -\frac{m}{r^2} + (r-3m)\left\{\left(\frac{d\theta}{ds}\right)^2 + \sin^2\theta\left(\frac{d\phi}{ds}\right)^2\right\}, \tag{3}$$

where s is the arc length along the geodesic. At any point with $r>3m$ one may arrange for the two terms on the right of (3) to cancel and so obtain a timelike geodesic at constant r. For $r:2m<r<3m$ the right hand side of (3) is evidently negative. Thus any future endless timelike geodesic in the maximally extended Schwarzschild space–time starting at some point between the event horizon at $r=2m$ and the photon sphere at $r=3m$ and initially directed inwards, in the sense that dr/ds is initially negative, will continue inwards and fall into the black hole. Any observer who traverses a Schwarzschild photon sphere must therefore engage some form of propulsion or else be drawn in to the black hole to meet an inevitable fate.

A photon sphere has been defined by Virbhadra and Ellis[3] as a timelike hypersurface of the form $\{r=r_0\}$ where r_0 is the closest distance of approach for which the Einstein bending angle of a light ray is unboundedly large. These authors subsequently[4] considered the Einstein deflection angle for a general static spherically symmetric metric and obtained an equation for a photon sphere. The existence of a photon sphere in a space–time has important implications for gravitational lensing. In any space–time containing a photon sphere, gravitational lensing will give rise to relativistic images.[3,4]

The Schwarzschild photon sphere may be usefully compared with the concept of a closed trapped surface. Any null geodesic originating from any point on a closed trapped surface in Schwarzschild space–time is drawn into the singularity at $r=0$. By contrast, any null geodesic originating from any point on the photon sphere will be drawn into the singularity if and only if it is initially directed inwards.

Our main objectives in the present paper are to give a geometric definition of a photon surface in a general space–time and of a photon sphere in a general static spherically symmetric space–time.

An evolution equation is obtained for the cross-sectional area of a photon surface in a dynamic spherically symmetric space–time. It is shown, subject to suitable energy conditions, that in any static spherically symmetric space–time a black hole must be surrounded by a photon sphere, and a photon sphere must surround either a black hole, a naked singularity or more than a certain amount of matter. Many examples are given of photon spheres in static spherically symmetric space–times. Photon surface evolution is considered for the dynamic space–time example of Vaidya null dust collapse to a naked singularity.

II. PHOTON SURFACES

The hypersurface $S:=\{r=3m\}$ in Schwarzschild space–time has two main properties: first that any null geodesic initially tangent S will remain tangent to S, and second that S does not evolve with time. The following general definition of a photon surface is based on only the first of these properties. A more restrictive class of photon surfaces may be defined when the space–time admits a group of symmetries (see Definition II.2).

Definition II.1: A photon surface of $(M,\mathbf{g})$ is an immersed, nowhere-spacelike hypersurface S of $(M,\mathbf{g})$ such that, for every point $p\in S$ and every null vector $\mathbf{k}\in T_pS$, there exists a null geodesic $\gamma:(-\epsilon,\epsilon)\to M$ of $(M,\mathbf{g})$ such that $\dot\gamma(0)=\mathbf{k}, |\gamma|\subset S$.

Any null hypersurface is trivially a photon surface. Photon surfaces are conformally invariant structures. If S is a photon surface of $(M,\mathbf{g})$ then S is a photon surface of $(M,\Omega^2\mathbf{g})$ for any smooth function $\Omega:M\to(0,\infty)$.

Note that Definition II.1 is entirely local. In particular, a photon surface S need contain no endless null geodesics of $(M,\mathbf{g})$. Moreover, a photon surface need only be immersed, rather than embedded in M, and so may have self-intersections. If $(M,\mathbf{g})$ is of dimension $n+1$ $(n\geqslant 2)$ then, through each point p of a photon surface S in $(M,\mathbf{g})$, there is an $(n-2)$-parameter family of null geodesics of $(M,\mathbf{g})$ that lie entirely in S.

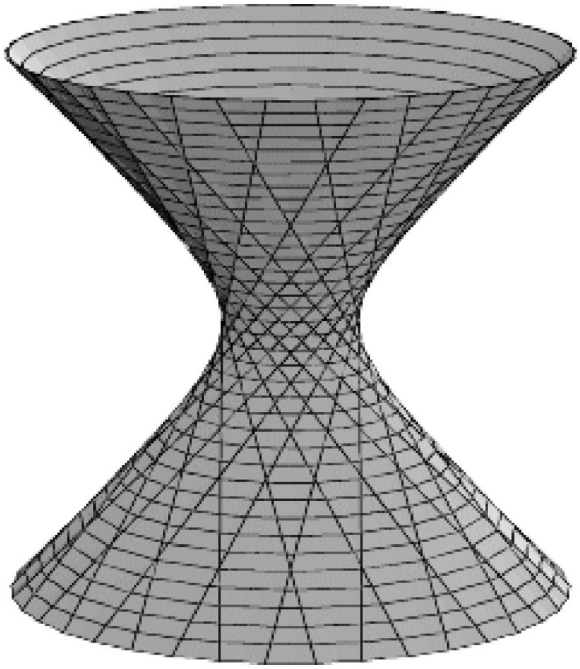

FIG. 1. A photon surface in Minkowski 3-space. The two families of ruling lines are null geodesics with respect to both the Minkowski 3-metric and the induced 2-metric. The lines may be regarded as the space–time paths of pulsed laser beams.

In this paper we will be principally concerned with photon surfaces in space–times of $3+1$ dimensions. The exceptions are Examples 1 and 3 which give photon surfaces in space–times of dimension $2+1$ and $4+1$, respectively.

Example 1 (Minkowski 3-space): In Minkowski 3-space $\mathbb{M}^3$, consider the single-sheeted hyperboloid S given by

$$-t^2+x^2+y^2=a^2, \tag{4}$$

for some constant $a>0$. This surface is doubly ruled, the rulings being given by

$$\gamma_\theta^{\pm}(t) := a(0,\cos\theta,\sin\theta)+at(1,\mp\sin\theta,\pm\cos\theta) \tag{5}$$

$(-\infty<t<\infty, 0\leqslant\theta<2\pi)$, where θ identifies the intersection points with $\{t=0\}$ and t is the parameter along the ruling lines. The tangents $\dot{\gamma}_\theta^{\pm}(t)$ to the ruling lines are null with respect to the $\mathbb{M}^3$ metric. Clearly they are geodesics in $\mathbb{M}^3$. At each point of S there can be just two null directions tangent to S. These must therefore be the directions of the two ruling lines through that point. Hence S is a photon surface in the sense of Definition II.1 (see Fig. 1).

Note that for any circle of the form

$$C=\{t_0,x_0+r\cos\theta,y_0+r\sin\theta\}, \quad r>0, \tag{6}$$

and any future-directed timelike vector field $\mathbf{X}$ along C that respects the symmetry of C, in the sense of

$$\mathbf{X}=(X^t,X^r\cos\theta,X^r\sin\theta), \tag{7}$$

for constant $X^t>0$, X^r such that $(X^t)^2>(X^r)^2$, there is a unique single-sheeted hyperboloid S through C such that $\mathbf{X}$ is tangent to S along C.

In the case $a=0$, Eq. (4) gives the null cone through the origin. The complement of p in this null cone is a null photon surface of $\mathbb{M}^3$.

Example 2 (Minkowski 4-space): One may generalize Example 1 to Minkowski 4-space $\mathbb{M}^4$ as follows. Let S be a timelike hypersurface in $\mathbb{M}^4$ of the form

$$-t^2+x^2+y^2+z^2=a^2, \tag{8}$$

for some constant $a>0$. The two-parameter family of lines,

$$\gamma^{\pm}_{\theta,\phi}(t)=a(0,\cos\theta,\sin\theta\sin\phi,\sin\theta\cos\phi)+at(1,\mp\sin\theta,\pm\cos\theta\sin\phi,\pm\cos\theta\cos\phi), \tag{9}$$

foliate S and are null geodesics with respect to the $\mathbb{M}^4$ metric. For each $p\in S$, the tangents at p to those $\gamma^{\pm}_{\theta,\phi}(t)$ that pass through p can be shown to generate the null cone of T_pS. Hence S is a photon surface in the sense of Definition II.1. In terms of the double null coordinates,

$$u:=t+r, \tag{10}$$

$$v:=t-r, \tag{11}$$

for $r:=(x^2+y^2+z^2)^{1/2}$, Eq. (8) assumes the simple form

$$uv=-a^2. \tag{12}$$

In the future direction S tends asymptotically to the null hypersurface $\{v=0\}$, while in the past direction S tends asymptotically to the null hypersurface $\{u=0\}$.

Example 3 (de Sitter space): de Sitter space–time may be regarded[5] as a single-sheeted hyperboloid in Minkowski 5-space $\mathbb{M}^5$. By analogy with Examples 1 and 2, de Sitter space–time is thus realized as a photon surface in $\mathbb{M}^5$.

Example 4 (The Robertson–Walker models): Every Robertson–Walker model is conformally flat and therefore locally conformally transformable to Minkowski space. The photon surfaces of any Robertson–Walker model may thus be obtained, at least locally, by conformal transformations of Minkowski space.

Theorem II.1: *Let S be a timelike hypersurface of $(M,\mathbf{g})$. Let $\mathbf{n}$ be a unit normal field to S and let h_{ab} be the induced metric on S. Let χ_{ab} be the second fundamental form on S and let σ_{ab} be the trace-free part of χ_{ab}. Then the following are equivalent:*

(i) *S is a photon surface;*
(ii) *$\chi_{ab}k^ak^b=0, \forall$ null $\mathbf{k}\in T_pS, \ \forall p\in S$;*
(iii) *$\sigma_{ab}=0$;*
(iv) *every affine null geodesic of $(S,\mathbf{h})$ is an affine null geodesic of $(M,\mathbf{g})$.*

Proof: (i)⇒(ii). Suppose S is a photon surface. Let $p\in S$ and let $\mathbf{k}\in T_pS$ be null. There exists an affine null geodesic $\gamma:(-\epsilon,\epsilon)\to M$ of $(M,\mathbf{g})$ such that $\dot\gamma(0)=\mathbf{k}, |\gamma|\subset S$. One has

$$\chi_{ab}\dot\gamma^a\dot\gamma^b=n_{a;b}\dot\gamma^a\dot\gamma^b=(n_a\dot\gamma^a)_{;b}\dot\gamma^b=0, \tag{13}$$

along γ. At p this gives $\chi_{ab}k^ak^b=0$.

(ii)⇒(iii). Let $p\in S$. By (ii) one has $\sigma_{ab}k^ak^b=\chi_{ab}k^ak^b=0, \ \forall$ null $\mathbf{k}\in T_pS$. Let $\{\mathbf{e}_{(0)},\mathbf{e}_{(1)},\mathbf{e}_{(2)}\}$ be an orthonormal basis for T_pS with $\mathbf{e}_{(0)}$ timelike and $\mathbf{e}_{(1)}$, $\mathbf{e}_{(2)}$ spacelike. Any null $\mathbf{k}\in T_pS$, normalized such that $g(\mathbf{k},\mathbf{e}_{(0)})=-1$, has components $k^a=(1,\cos\psi,\sin\psi)$ with respect to $\{\mathbf{e}_{(0)},\mathbf{e}_{(1)},\mathbf{e}_{(2)}\}$ for some $\psi\in[0,2\pi)$. A calculation gives

$$\sigma_{ab}k^ak^b=(\sigma_{00}+\tfrac{1}{2}\sigma_{11}+\tfrac{1}{2}\sigma_{22})+2\sigma_{01}\cos\psi+2\sigma_{02}\sin\psi+\tfrac{1}{2}(\sigma_{11}-\sigma_{22})\cos2\psi+\sigma_{12}\sin2\psi. \tag{14}$$

This must vanish for all $\psi \in [0,2\pi)$. One thus has $\sigma_{01}=\sigma_{02}=\sigma_{12}=0$ and $-\sigma_{00}=\sigma_{11}=\sigma_{22}$. Since σ_{ab} is trace-free one must also have $\sigma_{00}=\sigma_{11}+\sigma_{22}$. There follows $\sigma_{ab}=0$.

(iii)⇒(iv). For any curve in S with null tangent $\mathbf{k}$ one has

$$k^a{}_{\|b}k^b = h^a{}_c k^c{}_{;b} k^b = k^a{}_{;b}k^b + (\sigma_{bc}k^b k^c)n^a, \tag{15}$$

where $\|$ denotes covariant differentiation in S with respect to $\mathbf{h}$. The second term on the right of (15) vanishes by hypothesis. If $\mathbf{k}$ is tangent to an affine null geodesic of $(S,\mathbf{h})$ then the term on the left of (15) also vanishes and so $\mathbf{k}$ is tangent to an affine null geodesic of $(M,\mathbf{g})$.

(iv)⇒(i). Let $p \in S$ and let $\mathbf{k} \in T_pS$ be null. Let $\gamma:(-\epsilon,\epsilon)\to S$ be an affine null geodesic of $(S,\mathbf{h})$ such that $\dot\gamma(0)=\mathbf{k}$. Then, by (iv), γ is an affine null geodesic of $(M,\mathbf{g})$ such that $\dot\gamma(0)=\mathbf{k}$, $|\gamma| \subset S$. □

Condition (iii) of Theorem II.1 is equivalent to a requirement that χ_{ab} is pure trace in the sense of

$$\chi_{ab} = \tfrac{1}{3}\Theta h_{ab}, \tag{16}$$

where $\Theta := h^{cd}\chi_{cd}$ is the expansion of the unit normal to S. For Example 1 one has $\Theta = 2/a$; for Example 2 one has $\Theta = 3/a$. [Note that, by a standard abuse of notation, h_{ab} denotes both the induced metric on S and the symmetric tensor field of rank (0,2) along S in M which satisfies $h_{ab}n^b=0$ and pulls back to the induced metric on S.]

It is clear from condition (iii) of Theorem II.1 that a space–time must be specialized in some respect in order to admit any timelike photon surfaces in the sense of Definition II.1. For this reason it is helpful to restrict attention to space–times which admit groups of symmetries.

Definition II.2: Suppose $(M,\mathbf{g})$ admits a group G of isometries. A photon surface S of $(M,\mathbf{g})$ that is invariant under G, in the sense that each $g \in G$ maps S onto itself, will be called a G-invariant photon surface.

Clearly any G-invariant null hypersurface is a G-invariant photon surface. In particular, if $G=\mathbb{R}$ or $G=\mathbb{S}$, then any Killing horizon[6,7] is a G-invariant photon surface.

III. DYNAMIC SPHERICAL SYMMETRY: GENERAL THEORY

By definition, a general spherically symmetric space–time admits an $SO(3)$ isometry group for which the group orbits are spacelike 2-spheres. The following result describes the evolution of the cross-sectional area of an $SO(3)$-invariant photon surface in a spherically symmetric space–time.

Theorem III.1: *Let $(M,\mathbf{g})$ be a spherically symmetric space–time. Let S be an $SO(3)$-invariant timelike hypersurface of $(M,\mathbf{g})$ and let $\mathbf{X}$ be the $SO(3)$-invariant unit future-directed timelike tangent vector field along S orthogonal to the $SO(3)$-invariant 2-spheres in S. Let $\mathcal{T}$ be one such $SO(3)$-invariant 2-sphere in S and let $\mathcal{T}_s$ be the $SO(3)$-invariant 2-sphere in S at arc length s from $\mathcal{T}$ along the integral curves of $\mathbf{X}$. Then S is a photon surface of $(M,\mathbf{g})$ iff the area ${}^{(2)}A_s$ of $\mathcal{T}_s$ satisfies*

$$\frac{d^2}{ds^2}{}^{(2)}A_s = \frac{1}{4\,{}^{(2)}A_s}\left(\frac{d}{ds}{}^{(2)}A_s\right)^2 + {}^{(2)}A_s\left(\frac{1}{3}\Theta^2 - G_{ab}n^a n^b\right) - 4\pi, \tag{17}$$

where n^a is the unit normal to S, Θ is the expansion of n^a and $G_{ab} := R_{ab} - \frac{1}{2}Rg_{ab}$ is the Einstein tensor of $(M,\mathbf{g})$.

Proof: Let h_{ab} be the induced Lorentzian 3-metric on S and, for each s, let ${}^{(2)}h_{ab}$ be the induced Riemannian 2-metric on $\mathcal{T}_s$. The expansion of $\mathbf{X}$ in $(S,\mathbf{h})$ is given by ${}^{(2)}\Theta = {}^{(2)}h^{ab}X_{a;b}$ where the covariant derivative is that of $(M,\mathbf{g})$. Since $\mathbf{X}$ is both shear-free and vorticity-free in $(S,\mathbf{h})$, the Raychaudhuri equation for $\mathbf{X}$ in $(S,\mathbf{h})$ assumes the form

$$\frac{d}{ds}{}^{(2)}\Theta = -\frac{1}{2}({}^{(2)}\Theta)^2 - {}^{(3)}R_{ab}X^aX^b, \tag{18}$$

where ${}^{(3)}R_{ab}$ is the Ricci tensor of $(S,\mathbf{h})$.

From first principles one has

$${}^{(2)}R = {}^{(3)}R + 2\,{}^{(3)}R_{ab}X^aX^b - ({}^{(2)}\chi^a{}_a)^2 + {}^{(2)}\chi^a{}_b\,{}^{(2)}\chi^b{}_a, \tag{19}$$

$${}^{(3)}R = R - 2R_{ab}n^an^b + (\chi^a{}_a)^2 - \chi^a{}_b\chi^b{}_a, \tag{20}$$

where ${}^{(2)}\chi_{ab}$ is the second fundamental form of each $\mathcal{T}_s$ in $(S,\mathbf{h})$. Since X^a is shear-free and vorticity free in $(S,\mathbf{h})$ one has ${}^{(2)}\chi_{ab} = \frac{1}{2}\,{}^{(2)}\Theta\,{}^{(2)}h_{ab}$. The second fundamental form of S admits the canonical decomposition $\chi_{ab} = \frac{1}{3}\Theta h_{ab} + \sigma_{ab}$. Equations (19) and (20) therefore give

$${}^{(2)}R = {}^{(3)}R + 2\,{}^{(3)}R_{ab}X^aX^b - \tfrac{1}{2}{}^{(2)}\Theta^2, \tag{21}$$

$${}^{(3)}R = R - 2R_{ab}n^an^b + \tfrac{2}{3}\Theta^2 - \sigma^a{}_b\sigma^b{}_a, \tag{22}$$

which combine to yield

$$2\,{}^{(3)}R_{ab}X^aX^b = {}^{(2)}R + 2G_{ab}n^an^b - \tfrac{2}{3}\Theta^2 + \tfrac{1}{2}({}^{(2)}\Theta)^2 + \sigma^a{}_b\sigma^b{}_a. \tag{23}$$

One may now substitute for the second term on the right of (18) to obtain

$$\frac{d}{ds}{}^{(2)}\Theta = -\frac{3}{4}({}^{(2)}\Theta)^2 + \frac{1}{3}\Theta^2 - \frac{1}{2}{}^{(2)}R - G_{ab}n^an^b - \frac{1}{2}\sigma^a{}_b\sigma^b{}_a. \tag{24}$$

From first principles one has ${}^{(2)}\Theta = (d/ds)\ln {}^{(2)}A$, and the Gauss–Bonnet theorem gives ${}^{(2)}R\,{}^{(2)}A = 8\pi$. Substituting for ${}^{(2)}\Theta$ and ${}^{(2)}R$ in (24) one obtains

$$\frac{d^2}{ds^2}{}^{(2)}A_s = \frac{1}{4\,{}^{(2)}A_s}\left(\frac{d}{ds}{}^{(2)}A_s\right)^2 + {}^{(2)}A_s\left(\frac{1}{3}\Theta^2 - G_{ab}n^an^b - \frac{1}{2}\sigma^a{}_b\sigma^b{}_a\right) - 4\pi. \tag{25}$$

This agrees with (17) iff $\sigma^a{}_b\sigma^b{}_a = 0$.

Construct, for the tangent bundle TS of S, an orthonormal basis field of the form $\{\mathbf{X},\mathbf{e}_{(1)},\mathbf{e}_{(2)}\}$, with $\mathbf{e}_{(1)}$ and $\mathbf{e}_{(2)}$ unit spacelike. With respect to this basis one has

$$\sigma^a{}_b\sigma^b{}_a = (\sigma^0{}_0)^2 + (\sigma^1{}_1)^2 + (\sigma^2{}_2)^2 + 2(\sigma^1{}_2)^2 - 2(\sigma^1{}_0)^2 - 2(\sigma^2{}_0)^2. \tag{26}$$

By spherical symmetry the vector field $\sigma^a{}_bX^b$ must be proportional to X^a. Hence one has $\sigma^1{}_0 = \sigma^2{}_0 = 0$. The vanishing of $\sigma^a{}_b\sigma^b{}_a$ is thus equivalent to the vanishing of σ_{ab}. One has $\sigma_{ab} = 0$ iff S is a photon surface. □

A spherically symmetric metric is locally expressible in the form

$$g_{ab} = \begin{pmatrix} g_{00} & g_{01} & 0 & 0 \\ g_{10} & g_{11} & 0 & 0 \\ 0 & 0 & g_{\theta\theta} & 0 \\ 0 & 0 & 0 & g_{\theta\theta}\sin^2\theta \end{pmatrix}, \tag{27}$$

with respect to coordinates (x^0,x^1,θ,ϕ) adapted to the spherical symmetry, where g_{00}, $g_{01} = g_{10}$, g_{11} and $g_{\theta\theta} > 0$ depend only on x^0 and x^1. It is often convenient to introduce a radial coordinate r, depending only on x^0 and x^1, such that $g_{\theta\theta}$ is a function of r only. One is free to specify $g_{\theta\theta}$ as a function of r alone since to do so is, in effect, a definition of the coordinate r. This will be assumed to be done throughout this paper.

The following result is useful in the locating of $SO(3)$-invariant photon surfaces in dynamic spherically symmetric space–times.

Lemma III.2: Let $(M,\mathbf{g})$ *be a spherically symmetric space–time. Let S be an* $SO(3)$*-invariant timelike hypersurface of* $(M,\mathbf{g})$ *and let* $\mathbf{X}$ *be the* $SO(3)$*-invariant unit future-directed timelike tangent vector field along S that is orthogonal to the* $SO(3)$*-invariant* 2*-spheres in S. Then S is a photon surface of* $(M,\mathbf{g})$ *iff*

$$X^a{}_{;b}X^b=\tfrac{1}{2}(g^{\theta\theta}n^b\partial_b g_{\theta\theta})n^a, \tag{28}$$

holds along S, where n^a *is the unit normal field to S in* $(M,\mathbf{g})$.

Proof: By spherical symmetry, and since $\mathbf{X}$ is unit timelike, the vector field $\nabla_{\mathbf{X}}\mathbf{X}$ must be proportional to $\mathbf{n}$. Hence it suffices to show that S is a photon surface iff along S one has

$$\mathbf{n}\cdot\nabla_{\mathbf{X}}\mathbf{X}=\tfrac{1}{2}g^{\theta\theta}n^b\partial_b g_{\theta\theta}, \tag{29}$$

or equivalently,

$$\chi_{ab}X^aX^b=-\tfrac{1}{2}g^{\theta\theta}n^a\partial_a g_{\theta\theta}. \tag{30}$$

Construct for TS a local orthonormal basis field of the form $\{\mathbf{X},\mathbf{e}_{(\theta)},\mathbf{e}_{(\phi)}\}$. With respect to this basis field the components of $\chi^a{}_b$ form a diagonal matrix with

$$\chi^\theta{}_\theta=\chi^\phi{}_\phi=n^\theta{}_{;\theta}=\tfrac{1}{2}g^{\theta\theta}n^a\partial_a g_{\theta\theta}. \tag{31}$$

Equation (30) is thus equivalent to $\chi^0{}_0=\chi^\theta{}_\theta=\chi^\phi{}_\phi$ which is in turn equivalent to $\sigma^0{}_0=\sigma^\theta{}_\theta=\sigma^\phi{}_\phi$. In view of the trace-free property of $\sigma^a{}_b$, Eq. (30) is thus equivalent to $\sigma^a{}_b=0$. From Theorem II.1 one has that $\sigma^a{}_b=0$ holds along S iff S is a photon surface. □

Let us continue to work with respect to the coordinate system $\{x^0,x^1,\theta,\phi\}$ employed in (27). Let $x^a(s)$ be an integral curve of the vector field $\mathbf{X}$ in Lemma III.2. One has

$$\frac{dx^a}{ds}=X^a, \tag{32}$$

and Eq. (28) becomes

$$\frac{d^2x^a}{ds^2}+\Gamma^a_{bc}\frac{dx^b}{ds}\frac{dx^c}{ds}=\frac{1}{2}(g^{\theta\theta}n^b\partial_b g_{\theta\theta})n^a. \tag{33}$$

Since $\mathbf{X}=(dx^0/ds)\,(1,dx^1/dx^0,0,0)$ is unit timelike one has

$$\left(\frac{ds}{dx^0}\right)^2=-g_{ab}\frac{dx^a}{dx^0}\frac{dx^b}{dx^0}. \tag{34}$$

The x^0 and x^1 components of Eq. (33) thus combine to give

$$\frac{d^2x^1}{(dx^0)^2}=-\frac{1}{2}g^{\theta\theta}n^a\partial_a g_{\theta\theta}\left(n^1-\frac{dx^1}{dx^0}n^0\right)g_{bc}\frac{dx^b}{dx^0}\frac{dx^c}{dx^0}+\left(\frac{dx^1}{dx^0}\Gamma^0_{ab}-\Gamma^1_{ab}\right)\frac{dx^a}{dx^0}\frac{dx^b}{dx^0}, \tag{35}$$

where the components of $\mathbf{n}$ are given by

$$n^0=\psi g_{1a}\frac{dx^a}{dx^0};\quad n^1=-\psi g_{0a}\frac{dx^a}{dx^0}, \tag{36}$$

for

$$\psi := (-\Delta)^{-1/2}\left(-g_{ab}\frac{dx^a}{dx^0}\frac{dx^b}{dx^0}\right)^{-1/2}, \tag{37}$$

where

$$\Delta := g_{00}g_{11} - (g_{01})^2 \tag{38}$$

is the determinant of the time–space part of g_{ab} in (27). Equation (35) is the coordinate equivalent of (28) and provides for the easy determination of $SO(3)$-invariant photon surfaces (see Example 10).

IV. STATIC SPHERICAL SYMMETRY: GENERAL THEORY

By definition, a spherically symmetric space–time is static if it admits an $SO(3)\times\mathbb{R}$ group of isometries such that the $\mathbb{R}$ orbits are generated by a Killing field **K** which is both hypersurface orthogonal and orthogonal to the $SO(3)$ orbits. In the present section we will be concerned with $SO(3)\times\mathbb{R}$-invariant photon surfaces in static spherically symmetric space–times. Such surfaces may be termed photon spheres because, as will be seen, they are a natural generalization to general static spherically symmetric space–times of the Schwarzschild photon sphere concept. The term ''photon sphere'' will be regarded as applicable only in static spherically symmetric space–times. For clarity, the term ''$SO(3)\times\mathbb{R}$-invariant photon surface'' will usually be employed in preference to ''photon sphere.''

Although the space–times of Examples 1 and 2 are static and spherically symmetric, the photon surfaces in these space–times are not $SO(3)\times\mathbb{R}$-invariant and so are not photon spheres. Of the Robertson–Walker space–times of Example 4, only the Einstein cylinder is both spherically symmetric and static. None of the photon surfaces of the Einstein cylinder are $SO(3)\times\mathbb{R}$-invariant. Thus the Einstein cylinder has no photon spheres.

One may characterize an $SO(3)\times\mathbb{R}$-invariant photon surface, or photon sphere, in a static spherically symmetric space–time by means of the following special case of Theorem III.1.

Theorem IV.1: *Let* $(M,\mathbf{g})$ *be a static spherically symmetric space–time with Killing field* **K** *and let* S *be an* $SO(3)\times\mathbb{R}$*-invariant timelike hypersurface of* $(M,\mathbf{g})$*. Then* S *is an* $SO(3)\times\mathbb{R}$*-invariant photon surface of* $(M,\mathbf{g})$ *if there exists an* $SO(3)$*-invariant* 2*-sphere* $\mathcal{T}\subset S$ *satisfying*

$$A(\Theta^2 - 3G_{ab}n^a n^b) = 12\pi, \tag{39}$$

where A *is the area of* $\mathcal{T}$*,* n^a *is the unit normal to* S *and* Θ *is the trace of the second fundamental form of* S*. Conversely, if* S *is an* $SO(3)\times\mathbb{R}$*-invariant photon surface of* $(M,\mathbf{g})$ *then (39) holds for every* $SO(3)$*-invariant* 2*-sphere* $\mathcal{T}\subset S$*.*

Proof: Note that the unit future-directed timelike tangent field **X** along S in Theorem III.1 is proportional to the restriction to S of the Killing field **K**.

Suppose first that there exists an $SO(3)$-invariant 2-sphere $\mathcal{T}\subset S$ such that (39) holds. The quantities A, Θ and $G_{ab}n^a n^b$ remain constant as $\mathcal{T}$ is mapped along the flow lines of the Killing field **K**. So they also remain constant as they are mapped along the flow lines of **X**. Hence (17) holds with the term on the left and the first term on the right both zero. Thus, by Theorem III.1, S is a photon surface of $(M,\mathbf{g})$. By hypothesis S is $SO(3)\times\mathbb{R}$-invariant.

For the converse, suppose that S is an $SO(3)\times\mathbb{R}$-invariant photon surface of $(M,\mathbf{g})$. Then (17) holds for every $SO(3)$-invariant 2-sphere $\mathcal{T}_s\subset S$. Since **K** induces groups of local isometries, the area A_s of $\mathcal{T}_s$ is independent of the parameter s. Hence the term on the left and the first term on the right of (17) both vanish and one obtains (39). □

Corollary 1: If one has $G_{ab}Y^aY^b \geqslant 0$*,* $\forall$ *vectors* **Y** *and* S *is an* $SO(3)\times\mathbb{R}$*-invariant timelike photon surface of* $(M,\mathbf{g})$*, then for any* $SO(3)$*-invariant* 2*-sphere* $\mathcal{T}\subset S$ *one has*

$$A\Theta^2 \geqslant 12\pi, \tag{40}$$

with equality holding iff $G_{ab}n^a n^b = 0$ *along* S. □

For Schwarzschild space–time where (see Example 5) the only timelike photon sphere is at $r=3m$, one has $A=4\pi(3m)^2$, $\Theta = 1/(\sqrt{3}m)$ and $G_{ab}=0$ which verifies (39) and (40) for this case.

If the Einstein equations hold with a zero cosmological constant then, in the corollary to Theorem IV.1, the hypothesis $G_{ab}Y^aY^b \geqslant 0$ for all vectors $\mathbf{Y}$ is equivalent to $T_{ab}Y^aY^b \geqslant 0$ for all vectors $\mathbf{Y}$. This is a physically reasonable energy condition. In particular, for a perfect fluid with density ρ and pressure p, it is equivalent to a condition that ρ and p are both non-negative. More generally, the condition holds for an energy tensor with a single timelike eigenvector (type I in the classification of Hawking and Ellis[5]) iff each energy tensor eigenvalue is non-negative.

The characterization of timelike photon surfaces provided by Theorem IV.1 involves derivatives of the metric components up to second order. The following result (Theorem IV.2) provides an entirely different characterization of $SO(3)\times\mathbb{R}$-invariant photon surfaces in terms of derivatives of the metric components up to only first order.

Let a general static spherically symmetric metric $\mathbf{g}$ be expressed in the form (27) with $g_{\theta\theta}$ a function of r only. The Killing equation $K_{(a;b)}=0$ and the orthogonality of $\mathbf{K}$ to ∂_θ and ∂_ϕ gives $K^a\partial_a g_{\theta\theta}=0$ and hence $\nabla_{\mathbf{K}} r = 0$ where r is to be regarded as a scalar field on M. Since r is independent of θ and ϕ it follows that any $SO(3)\times\mathbb{R}$-invariant hypersurface S of $(M,\mathbf{g})$ must be of the form $\{r=\text{const}\}$. If S is also a timelike hypersurface then $r^{;a}$ is a spacelike vector field along S and $\mathbf{K}$ is a timelike vector field in a neighborhood of S.

If the coordinates x^0 and x^1 implicit in (27) are chosen such that $\mathbf{K}=\partial_{x^0}$ then the Killing equation gives that all the metric components g_{ab} in (27) are independent of x^0. Since r is constant along the integral curves of $\mathbf{K}$, the coordinate x^1 must be a function of r only. A natural choice is $x^1=r$. One may redefine x^0 according to $x^0 \to x^0 - \int (g_{01}/g_{00})dx^1$. This diagonalizes the time–space part of g_{ab} and leaves the components of g_{ab} independent of x^0. Furthermore the curves $\{x^1,\theta,\phi=\text{const}\}$ are unchanged except that they are re-parametrized. The vector field ∂_{x^0} then becomes a conformal Killing field.

Define the tensor field,

$$\epsilon^{ab} := (-\Delta)^{-1/2}\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{41}$$

on M, where the components are given with respect to the coordinate basis employed in (27) and Δ is the determinant of the time–space part of $\mathbf{g}$ in (27), as in (38).

Theorem IV.2: *Let* $(M,\mathbf{g})$ *be a static spherically symmetric space–time with* $\mathbf{g}$ *of the form (27), with* $g_{\theta\theta}$ *a function of the coordinate* r *only. Let* S *be an* $SO(3)\times\mathbb{R}$*-invariant timelike hypersurface of* $(M,\mathbf{g})$ *and suppose that* ∇r *is nowhere-zero along* S. *Then* S *is an* $SO(3)\times\mathbb{R}$*-invariant photon surface of* $(M,\mathbf{g})$ *iff*

$$2g_{\theta\theta}\epsilon^{ab}\epsilon^{cd}r_{;ac}r_{;b}r_{;d} + r^{;a}r_{;a}r^{;c}\partial_c g_{\theta\theta} = 0, \tag{42}$$

holds along S.

Proof: Since $(M,\mathbf{g})$ is both spherically symmetric and static, the surface S is of the form $\{r=\text{const}\}$. The unit spacelike normal to S is therefore given by

$$n^a = \eta r^{;a} \tag{43}$$

for

$$\eta := (r^{;a}r_{;a})^{-1/2}. \tag{44}$$

The second fundamental form of S is given by

$$\chi_{ab} := \eta h_a{}^c h_b{}^d r_{;cd}. \tag{45}$$

The vector fields,

$$\mathbf{X}^a := (-\Delta g^{bc} r_{;b} r_{;c})^{-1/2} (r_{;1}, -r_{;0}, 0, 0), \tag{46}$$

$$\mathbf{e}_{(\theta)} := (g_{\theta\theta})^{-1/2} \partial_\theta, \tag{47}$$

$$\mathbf{e}_{(\phi)} := (g_{\theta\theta} \sin^2 \theta)^{-1/2} \partial_\phi, \tag{48}$$

form an orthonormal frame field along S, with $\mathbf{e}_{(\theta)}$ and $\mathbf{e}_{(\phi)}$ unit spacelike and $\mathbf{X}$ unit timelike. One has

$$\chi_{ab} X^a \mathbf{e}^b_{(\theta)} = \chi_{ab} X^a \mathbf{e}^b_{(\phi)} = \chi_{ab} \mathbf{e}^a_{(\theta)} \mathbf{e}^b_{(\phi)} = 0, \tag{49}$$

$$\chi_{ab} \mathbf{e}^a_{(\theta)} \mathbf{e}^b_{(\theta)} = \chi_{ab} \mathbf{e}^a_{(\phi)} \mathbf{e}^b_{(\phi)} = \frac{\eta r^{;a} \partial_a g_{\theta\theta}}{2 g_{\theta\theta}}, \tag{50}$$

$$\chi_{ab} X^a X^b = \eta^3 \epsilon^{ab} \epsilon^{cd} r_{;ac} r_{;b} r_{;d}. \tag{51}$$

Condition (iii) of Theorem II.1 holds iff χ_{ab} is proportional to h_{ab} and hence iff

$$-\chi_{ab} X^a X^b = \chi_{ab} \mathbf{e}^a_{(\theta)} \mathbf{e}^b_{(\theta)} = \chi_{ab} \mathbf{e}^a_{(\phi)} \mathbf{e}^b_{(\phi)}. \tag{52}$$

This is equivalent to

$$-\eta^2 \epsilon^{ab} \epsilon^{cd} r_{;ac} r_{;b} r_{;d} = \frac{r^{;a} \partial_a g_{\theta\theta}}{2 g_{\theta\theta}}, \tag{53}$$

which is in turn equivalent to (42). □

Equation (42) can have solutions such that $\{r = \text{const}\}$ is a spacelike hypersurface and therefore not a photon surface (see, e.g., Example 7). It is therefore always necessary in the use of Theorem IV.2 to check that the hypersurface $\{r = \text{const}\}$ is in fact timelike or null.

Note that in a region of space–time where the Killing field $\mathbf{K}$ is spacelike, for example, behind the event horizon of Schwarzschild space–time, the hypersurfaces $\{r = \text{const}\}$ are necessarily spacelike and so cannot be photon spheres.

Case 1 ($x^1 := r$, components of g_{ab} independent of x^0): As discussed previously, for a static spherically symmetric metric it is possible to choose $x^1 := r$, with $g_{\theta\theta}$ depending only upon r and with all the components of g_{ab} independent of x^0. In this case (42) reduces to

$$g_{00} \partial_r g_{\theta\theta} = g_{\theta\theta} \partial_r g_{00}. \tag{54}$$

This agrees with an equation obtained by Virbhadra and Ellis[4] on the basis of a different definition[3] of a photon sphere. Note that even though the components $g_{rr}, g_{0r} = g_{r0}$ do not appear in (54), they are not assumed to vanish. A particular sub-case of interest is that of time-space coordinates, with $t := x^0$ timelike in the sense of $g^{tt} < 0$. Another sub-case of interest is that of single null (radiation) coordinates, with $u := x^0$ null in the sense of $g^{uu} = 0$.

Case 2 (double null coordinates u, v): Let $x^0 := u$, $x^1 := v$ be double null coordinates in the sense of $g^{uu} = g^{vv} = 0$. The radial coordinate r is to be regarded as a function of u and v. Then (42) assumes the form

$$g_{\theta\theta} \{ r_{;uu} (r_{;v})^2 - 2 r_{;uv} r_{;u} r_{;v} + r_{;vv} (r_{;u})^2 \} + 2 (r_{;u} r_{;v})^2 \partial_r g_{\theta\theta} = 0. \tag{55}$$

The metric components $g_{uv} = g_{vu}$ enter here through the covariant derivatives of r.

Equations (42), (54) and (55) may be referred to as photon sphere equations since they give the location of timelike photon spheres in static spherically symmetric space–times.

In order to facilitate further progress, a general static spherically symmetric metric will be written in such a form as to cast the Einstein tensor in a particularly simple and convenient form.

One has from previous remarks that a general static spherically symmetric metric is locally expressible in the form

$$\mathbf{g}=g_{tt}\,dt^2+g_{rr}\,dr^2+r^2(d\theta^2+\sin^2\theta d\phi^2), \tag{56}$$

where g_{tt} and g_{rr} are functions of r only. Let

$$m(r):=\frac{1}{2}r\left(1-\frac{1}{g_{rr}}\right) \tag{57}$$

$$\mu(r):=\ln(-g_{tt}g_{rr}). \tag{58}$$

Then the metric assumes the form

$$\mathbf{g}=-\left(1-\frac{2m(r)}{r}\right)e^{\mu(r)}\,dt^2+\left(1-\frac{2m(r)}{r}\right)^{-1}dr^2+r^2(d\theta^2+\sin^2\theta d\phi^2), \tag{59}$$

and the Einstein tensor is given by

$$G^a{}_b=8\pi\begin{pmatrix}-\rho(r) & 0 & 0 & 0\\ 0 & p_1(r) & 0 & 0\\ 0 & 0 & p_2(r) & 0\\ 0 & 0 & 0 & p_2(r)\end{pmatrix}, \tag{60}$$

for

$$8\pi\rho(r):=\frac{2m'(r)}{r^2}, \tag{61}$$

$$8\pi p_1(r):=\frac{1}{r^2}\{(r-2m(r))\mu'(r)-2m'(r)\}, \tag{62}$$

$$\begin{aligned}8\pi p_2(r):=\frac{1}{4r^2}\{&(2(r+m(r)-3rm'(r))\mu'(r)+r(r-2m(r))(\mu'(r))^2\\&-4rm''(r)+2r(r-2m(r))\mu''(r)\},\end{aligned} \tag{63}$$

where a prime denotes differentiation with respect to r. For the right sides of (61), (62) and (63) to be defined at some radius $\hat{r}>0$ one evidently needs $m(r)$ and $\mu(r)$ to be twice differentiable at $r=\hat{r}$. Equations (61) and (62) combine to give

$$\mu'(r)=\frac{8\pi r(\rho(r)+p_1(r))}{\left(1-\frac{2m(r)}{r}\right)}, \tag{64}$$

whereby one may rewrite (63) in the more convenient form

$$\frac{2}{r}(p_2(r)-p_1(r))=p_1'(r)+\frac{\left(\frac{m(r)}{r^2}+4\pi r p_1(r)\right)(\rho(r)+p_1(r))}{\left(1-\frac{2m(r)}{r}\right)}. \tag{65}$$

In the perfect fluid case $p_1(r)=p_2(r)=:p(r)$ Eq. (65) reduces to the Tolman–Oppenheimer–Volkoff equation,

$$p'(r)=-\frac{\left(\frac{m(r)}{r^2}+4\pi r p(r)\right)(\rho(r)+p(r))}{\left(1-\frac{2m(r)}{r}\right)}. \tag{66}$$

By means of Eqs. (61) and (64), the photon sphere equation (54) becomes

$$1-\frac{3m(r)}{r}-4\pi r^2 p_1(r)=0. \tag{67}$$

For r such that $2m(r)<r$, and hence such that the hypersurface $\{r=\text{const}\}$ is timelike, Eq. (67) gives the location of the $SO(3)\times\mathbb{R}$-invariant timelike photon surfaces for the metric (59).

Equation (67) is the basis for the following result which shows that, subject to a suitable energy condition, any black hole in a static spherically symmetric space–time must be surrounded by an $SO(3)\times\mathbb{R}$-invariant photon surface. For the purpose of this and subsequent results, a function $f:\mathbb{R}\supset I\to\mathbb{R}$ on an interval I will be said to be piecewise C^r if I is the disjoint union of a locally finite collection of intervals I_i such that $f|I_i$ is C^r. Each interval I_i may be open, closed or half-open.

Theorem IV.3: *Suppose the metric* $\mathbf{g}$ *has the form (59) for* $r_0<r<\infty$, *for some* $r_0>0$, *with* $m(r)$ *and* $\mu(r)$ *both* C^0, *piecewise* C^2 *functions of* $r\in(r_0,\infty)$. *Suppose the following hold:*

(1) $\rho(r)$ *and* $p_1(r)$ *are bounded functions of* $r\in(r_0,\infty)$;
(2) $2m(r)<r$, $\forall r\in(r_0,\infty)$;
(3) $\rho(r)\geqslant 0$, $p_1(r)\geqslant 0$, $\forall r\in(r_0,\infty)$;
(4) $\lim_{r\to\infty}4\pi r^2 p_1(r)=\lim_{r\to\infty}4\pi r^2\rho(r)=0$;
(5) for each value of t *the 2-surfaces* $\mathcal{T}_{t,r}:=\{t=\text{const}\}\cap\{r=\text{const}\}$, $r_0<r<\infty$, *are such that* $\mathcal{T}_t:=\lim_{r\to r_0}\mathcal{T}_{t,r}$ *exists as an embedded spacelike 2-sphere in* $(M,\mathbf{g})$ *and is marginally outer trapped.*

Then $(M,\mathbf{g})$ *admits an* $SO(3)\times\mathbb{R}$*-invariant timelike photon surface of the form* $\{r=r_1\}$ *for some* $r_1\in(r_0,\infty)$.

Proof: Fix t and let $\mathbf{k}$ be the outward future-directed null normal field along each $\mathcal{T}_{t,r}$, $r_0<r<\infty$, normalized such that $\mathbf{g}(\mathbf{k},\mathbf{n})=1$, where $\mathbf{n}=(1-2m(r)/r)^{1/2}\partial_r$ is the outward radial unit tangent to $\{t=\text{const}\}$. Since $\mathbf{k}$ is parallelly propagated along each of the geodesic integral curves of $\mathbf{n}$, one has that $\lim_{r\to r_0}\mathbf{k}$ is a well-defined, nowhere-zero null vector field along $\mathcal{T}_t:=\lim_{r\to r_0}\mathcal{T}_{t,r}$. For $r\in(r_0,\infty)$ the vector field $\mathbf{k}$ has the form $k^a=(k^t,a(r)k^t,0,0)$ for

$$a(r):=(-g_{tt}/g_{rr})^{1/2}=\left(1-\frac{2m(r)}{r}\right)e^{\mu(r)/2}. \tag{68}$$

The expansion of $\mathbf{k}$ is given by

$$\Theta_{\text{out}}={}^{(2)}h^b{}_a k^a{}_{;b}=\frac{2a(r)}{r}k^t. \tag{69}$$

The condition that $\mathcal{T}_t$ is marginally outer trapped therefore implies

$$0=\lim_{r\to r_0} a(r)=\lim_{r\to r_0}\left(1-\frac{2m(r)}{r}\right)e^{\mu(r)/2}. \tag{70}$$

The non-negativity of $\rho(r)$ and $p_1(r)$ gives, by means of (61) and (64), that $m(r)$ and $\mu(r)$ are nondecreasing functions of $r\in(r_0,\infty)$. Thus (70) holds iff at least one of

$$\lim_{r\to r_0}\left(1-\frac{2m(r)}{r}\right)=0; \quad \lim_{r\to r_0}\mu(r)=-\infty \tag{71}$$

holds.

Suppose the first of (71) fails. Then the second must hold and one has

$$\lim_{r\to r_0}\left(1-\frac{2m(r)}{r}\right)^{-1}<\infty. \tag{72}$$

From the boundedness of $\rho(r)$ and $p_1(r)$ on $r\in(0,\infty)$ one has, by means of (64) and (72), that $\limsup_{r\to r_0}\mu'(r)$ is finite. This is incompatible with the second of (71). Hence the first of (71) must hold.

Let $f:(r_0,\infty)\to\mathbb{R}$ be the left side of (67). By the non-negativity of $p_1(r)$ and the first of (71) one has $\lim_{r\to r_0}f(r)\leqslant-\frac{1}{2}$. By condition (4), Eq. (61) and l'Hôpital's rule one has $\lim_{r\to\infty}m(r)/r=\lim_{r\to\infty}r^2p_1(r)=0$ and hence $\lim_{r\to\infty}f(r)=1$. Hence there exists some $r_1\in(r_0,\infty)$ such that $f(r_1)=0$. The hypersurface $\{r=r_1\}$ is an $SO(3)\times\mathbb{R}$-invariant photon surface of $(M,\mathbf{g})$. □

Condition (3) of Theorem IV.3 may be expressed more succinctly as $G_{ab}Y^aY^b\geqslant 0$, $\forall$ vectors $\mathbf{Y}$. With regard to condition (5) of Theorem IV.3, to have required $\mathcal{T}_t$ to be contained in the hypersurface $\{t=\text{const}\}$ would have been too strong since, for Schwarzschild space–time, no spacelike hypersurface of the form $\{t=\text{const}\}$ in the exterior region contains a marginally outer trapped 2-surface.

Theorem IV.3 may be interpreted to the effect that, subject to the energy conditions expressed in condition (3), any static spherically symmetric black hole must be surrounded by an $SO(3)\times\mathbb{R}$-invariant timelike photon surface. The following result may then be regarded as a partial converse in that it shows, subject to a suitable energy condition, that if there exists an $SO(3)\times\mathbb{R}$-invariant timelike photon surface then there must be a naked singularity or a black hole, or more than a certain amount of matter.

Proposition IV.4: *Suppose the metric* $\mathbf{g}$ *has the form (59) for* $0<r<\infty$, *with* $m(r)$ *and* $\mu(r)$ *both* C^0, *piecewise* C^2 *functions of* $r\in(0,\infty)$. *If the following all hold:*

(1) $\rho(r)$ *is a nonincreasing, bounded function of* $r\in(0,\infty)$;
(2) $\lim_{r\to 0}m(r)=0$;
(3) $4m(r)<r$, $\forall r\in(0,\infty)$;
(4) $p_1(r)\leqslant\rho(r)/3$, $\forall r\in(0,\infty)$,

then $(M,\mathbf{g})$ *can contain no* $SO(3)\times\mathbb{R}$*-invariant timelike photon surfaces.*

Proof: By conditions (1) and (2) with Eq. (61) one has $m(r)\geqslant(4\pi/3)r^3\rho(r)$ $\forall r>0$. By condition (4) one therefore has $4\pi r^2p_1(r)\leqslant(4\pi/3)r^2\rho(r)\leqslant m(r)/r$, $\forall r>0$. The left side of (67) is thus bounded from below by $1-4m(r)/r$, $\forall r>0$. This is positive by condition (3). The left side of (67) is therefore nonvanishing for all $r>0$. □

Note that this result is valid even for negative $p_1(r)$ and $\rho(r)$. Condition (2) of Proposition IV.4 prohibits any curvature singularity at $r=0$. Condition (3) may be interpreted as a requirement that there is no black hole and less than a certain amount of matter. The result shows that one of these two conditions must fail if there is an $SO(3)\times\mathbb{R}$-invariant timelike photon surface and conditions (1) and (4) both hold.

When the matter is a perfect fluid it is possible to improve condition (3) of Proposition IV.4 to condition (3) of the following result.

Theorem IV.5: *Suppose the metric* **g** *has the form (59) for* $0<r<\infty$, *with* $m(r)$ *and* $\mu(r)$ *both* C^1, *piecewise* C^2 *functions of* $r\in(0,\infty)$. *If the following all hold:*

(1) *the matter is a perfect fluid with pressure* $p(r)$ *and density* $\rho(r)$;
(2) $\lim_{r\to\infty}4\pi r^2p(r)=\lim_{r\to\infty}4\pi r^2\rho(r)=0$;
(3) $(24/7)m(r)<r$, $\forall r\in(0,\infty)$;
(4) $p(r)\leqslant\rho(r)/3$, $\forall r\in(0,\infty)$,

then $(M,\mathbf{g})$ *can contain no* $SO(3)\times\mathbb{R}$*-invariant timelike photon surfaces.*

Proof: Let $f:(0,\infty)\to\mathbb{R}$ be the left side of Eq. (67). Since $m(r)$ and $\mu(r)$ are C^1, piecewise C^2 functions of $r\in(0,\infty)$, one has by Eq. (62) that $f(r)$ is a C^0, piecewise C^1 function of $r\in(0,\infty)$. The function $f'(r)$ is then a piecewise C^0 function of $r\in(0,\infty)$ which, by means of the Tolman–Oppenheimer–Volkoff Eq. (66), is given by

$$rf'(r)=3\frac{m(r)}{r}-12\pi r^2\rho(r)-8\pi r^2p(r)+\frac{\left(\frac{m(r)}{r}+4\pi r^2p(r)\right)}{\left(1-2\frac{m(r)}{r}\right)}4\pi r^2(\rho(r)+p(r)). \quad (73)$$

For $r=r_1\in(0,\infty)$ such that

$$0=f(r_1)=1-3\frac{m(r_1)}{r_1}-4\pi r_1^2p(r_1), \quad (74)$$

Eq. (73) reduces to

$$r_1f'(r_1)=1-8\pi r_1^2(\rho(r_1)+p(r_1)). \quad (75)$$

From condition (3) and Eq. (74) one has $4\pi r_1^2p(r_1)>1/8$, whence by condition (4) one has $4\pi r_1^2\rho(r_1)>3/8$. Thus (75) gives $f'(r_1)<0$.

By condition (2), Eq. (61) and l'Hôpital's rule one has $\lim_{r\to\infty}m(r)/r=\lim_{r\to\infty}4\pi r^2p(r)=0$ and hence $\lim_{r\to\infty}f(r)=1$. Since it has been established that $f'(r)$ is negative for all $r\in(0,\infty)$ such that $f(r)=0$, one must therefore have $f(r)>0$ for all $r\in(0,\infty)$. Hence the space–time can contain no $SO(3)\times\mathbb{R}$-invariant timelike photon surfaces. □

Note that, as for Proposition IV.4, Theorem IV.5 is valid even for negative pressure and density.

One would like to remove the insufficient matter parts of condition (3) of Proposition IV.4 and condition (3) of Theorem IV.5, in other words to weaken these to a no-black-hole condition $2m(r)<r$, $\forall r>0$. But no result to this effect is forthcoming. On the other hand no counterexample is known.

To conclude this section it will be shown that the physical significance of the photon sphere in Schwarzschild space–time, as discussed in the Introduction, carries over to the general static spherically symmetric case. Suppose the metric has the form (59) for $r_0<r<\infty$ and is asymptotically flat in the limit $r\to\infty$. Assume $p_1(r)\geqslant0$, $m(r)\geqslant0$, $\forall r>r_0$. The matter need not be a perfect fluid. Denote the left side of (67) by $f(r)$. The condition of asymptotic flatness gives $\lim_{r\to\infty}f(r)=1$ so, if there are any $SO(3)\times\mathbb{R}$-invariant timelike photon surfaces, there will be an outermost such surface S. For simplicity assume $f'(r)\neq0$ at S. Let $\mathcal{R}_{\text{ext}}$ be the connected component of $\{q\in M:f(q)>0\}$ that has S as its inner boundary and extends to $r=\infty$. Let $\mathcal{R}_{\text{int}}$ be the connected component of $\{q\in M:f(q)<0\}$ that has S as its outer boundary.

Consider first the case of a future endless affine null geodesic $\gamma(\lambda)$. The null geodesic equations for the metric (59) give

$$\frac{d^2r}{d\lambda^2}=rf(r)\left\{\left(\frac{d\theta}{d\lambda}\right)^2+\sin^2\theta\left(\frac{d\phi}{d\lambda}\right)^2\right\}-\frac{\mu'(r)}{2}\left(\frac{dr}{d\lambda}\right)^2. \tag{76}$$

At any point $p\in|\gamma|\cap\mathcal{R}_{\text{ext}}$ such that $dr/d\lambda=0$ one has $d^2r/d\lambda^2>0$. At any point $p\in|\gamma|\cap\mathcal{R}_{\text{int}}$ such that $dr/d\lambda=0$ one has $d^2r/d\lambda^2<0$. Thus if γ starts outside S (i.e., in $\mathcal{R}_{\text{ext}}$) and is initially directed outwards, in the sense that $dr/d\lambda$ is initially positive, then γ will continue outwards. If γ starts in $\mathcal{R}_{\text{int}}$ and is initially directed inwards, in the sense that $dr/d\lambda$ is initially negative, then γ will continue inwards until it falls either into a singularity or through an $SO(3)\times\mathbb{R}$-invariant photon surface other than S.

Consider now a unit speed timelike geodesic $\xi(s)$. The timelike geodesic equations give

$$\frac{d^2r}{ds^2}=-\frac{m(r)}{r^2}-4\pi rp_1(r)+rf(r)\left\{\left(\frac{d\theta}{ds}\right)^2+\sin^2\theta\left(\frac{d\phi}{ds}\right)^2\right\}-\frac{\mu'(r)}{2}\left(\frac{dr}{ds}\right)^2. \tag{77}$$

For any point $p\in\mathcal{R}_{\text{ext}}$ one can arrange for the first three terms on the right of (77) to cancel and so obtain a unit speed timelike geodesic $\xi(s)$ through $p\in\mathcal{R}_{\text{ext}}$ at constant r. For $p\in\mathcal{R}_{\text{int}}$ the first three terms on the right of (77) are evidently negative. For $p\in|\xi|\cap\mathcal{R}_{\text{int}}$ such that $dr/ds=0$ one has $d^2r/ds^2<0$. Thus if ξ starts in $\mathcal{R}_{\text{int}}$ and is initially directed inwards, in the sense that dr/ds is initially negative, then ξ will continue inwards until it falls either into a singularity or through an $SO(3)\times\mathbb{R}$-invariant photon surface other than S.

V. SPHERICAL SYMMETRY: EXAMPLES

The following are some examples of $SO(3)\times\mathbb{R}$-invariant and $SO(3)$-invariant photon surfaces in familiar space–times.

Example 5 (Schwarzschild space–time): The metric of Schwarzschild space–time in single null (radiation) coordinates has the form

$$\mathbf{g}=-\left(1-\frac{2m}{r}\right)du^2+2\,du\,dr+r^2(d\theta^2+\sin^2\theta d\phi^2). \tag{78}$$

In this case Eq. (54) reduces to $r=3m$. The timelike hypersurface $\{r=3m\}$ is thus an $SO(3)\times\mathbb{R}$-invariant photon surface, or photon sphere, as expected. There are no other $SO(3)\times\mathbb{R}$-invariant timelike photon surfaces.

For a nonzero cosmological constant Λ, the Schwarzschild metric (78) generalizes to the Schwarzschild–de Sitter metric,

$$\mathbf{g}=-\left(1-\frac{2m}{r}+\frac{\Lambda r^2}{3}\right)du^2+2\,du\,dr+r^2(d\theta^2+\sin^2\theta d\phi^2). \tag{79}$$

One finds that Eq. (54) reduces to $r=3m$, independent of the value of Λ. This is surprising since Schwarzschild and Schwarzschild–de Sitter space–times are not conformally related.

Example 6 (Schwarzschild interior solution): The Schwarzschild interior solution describes a spherically symmetric distribution of perfect fluid of radius R, bounded pressure p and constant density $\rho_0>0$. The solution is to have a metric of the form (59) and is to be matched at $r=R$ to a Schwarzschild vacuum solution in such a way that the pressure is a continuous function of r. One thus has $p_1(r)=p_2(r)=:p(r)$ for all $r:0\leqslant r<\infty$, $\rho(r)=\rho_0$ for all $r:0\leqslant r\leqslant R$, $\rho(r)=0$ for all $r:R<r<\infty$ and $p(r)=0$ for all $r:R\leqslant r<\infty$. The pressure $p(r)$ for $r:0\leqslant r\leqslant R$ is to be obtained by an integration of the Tolman–Oppenheimer–Volkoff equation (66) subject to the boundary condition $p(R)=0$. This yields

$$m(r)=\frac{4\pi}{3}\rho_0r^3,\quad 0\leqslant r\leqslant R, \tag{80}$$

$$e^{\mu(r)}=\frac{(3-u(r))^2}{4u^2(r)}, \quad 0\leqslant r\leqslant R, \tag{81}$$

$$p(r)=\frac{u(r)-1}{3-u(r)}\rho_0, \quad 0\leqslant r\leqslant R, \tag{82}$$

for

$$u(r):=\left(\frac{3-8\pi\rho_0 r^2}{3-8\pi\rho_0 R^2}\right)^{1/2}, \quad 0\leqslant r\leqslant R. \tag{83}$$

The spherically symmetric system described by the Schwarzschild interior solution can exist in a state of stable equilibrium iff $m(R)/R<4/9$ (see Stephani[8]). This condition is equivalent to $8\pi\rho_0 R^2<8/3$, which implies $p(r)\geqslant 0$, $\forall r\geqslant 0$, and implies that the absence of a black hole is a general feature of the Schwarzschild interior solution.

The left side of Eq. (67) now assumes the form

$$1-\frac{3m(r)}{r}-4\pi r^2 p(r)=\begin{cases} 1-\dfrac{8\pi\rho_0 r^2}{3-u(r)} & :0<r\leqslant R, \\ 1-\dfrac{3m(R)}{r} & :r\geqslant R. \end{cases} \tag{84}$$

For $m(R)/R<1/3$ one has that (84) is positive for all $r>0$, so there are no timelike photon spheres. For $m(R)/R=1/3$ there is a single timelike photon sphere which lies at the boundary $r=R$ of the matter. For $1/3<m(R)/R<4/9$ there is one timelike photon sphere outside the matter at $r=3m(R)>R$ and one timelike photon sphere inside the matter at

$$r=\left(\frac{1-3\pi\rho_0 R^2}{\pi\rho_0(3-8\pi\rho_0 R^2)}\right)^{1/2}=\frac{2R}{3}\left(\frac{1-\dfrac{9m(R)}{4R}}{\left(1-\dfrac{2m(R)}{R}\right)\dfrac{m(R)}{R}}\right)^{1/2}<R. \tag{85}$$

For fixed R the radius of the outer photon sphere is a strictly increasing function of $m(R)/R$ while the radius of the inner photon sphere is a strictly decreasing function of $m(R)/R$.

Thus a Schwarzschild interior solution matched to a Schwarzschild vacuum exterior solution contains no black hole, and contains one timelike photon sphere iff $1/3=m(R)/R$ and two timelike photon spheres iff $m(R)/R$ lies in the range $1/3<m(R)/R<4/9$. However for such values of $m(R)/R$ the space–time is unphysical in that the pressure at the center is $p(0)\geqslant\rho_0/\sqrt{3}>\rho_0/3$. Therefore under the reasonable energy condition $p(r)\leqslant\rho_0/3$, $\forall r: 0\leqslant r<\infty$ there are no photon spheres in this example.

The energy condition $0\leqslant p(r)\leqslant\rho(r)/3$, $\forall r\in[0,\infty)$ is in fact satisfied iff $m(R)/R$ lies in the range $0\leqslant m(R)/R\leqslant 5/18$. The corresponding space–times (in view of $5/18<7/24$) satisfy all of conditions (1) to (4) of Theorem IV.5, except the smoothness of $\rho(r)$ at $r=R$. Thus considering a smoothed family of solutions approximating the solution above and having it as a strict limit, but each with smooth $\rho(r)$ at $r=R$, we can apply Theorem IV.5 to show no photon spheres exist in all the cases discussed in this section where this energy condition is satisfied. On the other hand Proposition IV.4 is directly applicable without smoothing, but only applies to the subset of these cases with $0\leqslant m(R)/R<1/4$.

Example 7 (Reissner–Nordström space–time): The Reissner–Nordström solution comprises a metric $\mathbf{g}$ and an electromagnetic field F_{ab} given by

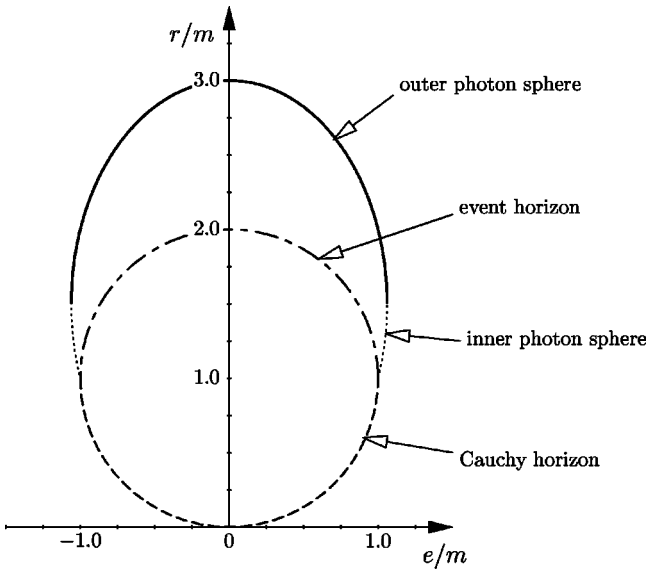

FIG. 2. The radii of the event horizon, Cauchy horizon and photon spheres for Reissner–Nordström space–time.

$$\mathbf{g}=-\left(1-\frac{2m}{r}+\frac{e^2}{r^2}\right)du^2+2\,du\,dr+r^2(d\theta^2+\sin^2\theta d\phi^2), \tag{86}$$

$$F_{tr}=-F_{rt}=\frac{e}{r^2},\ \textit{all other components vanishing,} \tag{87}$$

where m is the ADM mass and e is the electric charge. We assume $m>0$. There is an event horizon at $r=r_+:=m+\sqrt{m^2-e^2}$ and a Cauchy horizon at $r=r_-:=m-\sqrt{m^2-e^2}$. The event horizon exists for $0\leqslant(e/m)^2\leqslant 1$, and the Cauchy horizon exists for $0<(e/m)^2\leqslant 1$. For $(e/m)^2=1$ they both lie at $r=m$. There can be no timelike photon spheres between the event horizon and the Cauchy horizon because the Killing field **K** is spacelike there. Outside the event horizon the Killing field **K** is timelike, so every hypersurface of the form $\{r=\text{const}\}$ which lies outside the event horizon and satisfies the photon sphere equation (54) is necessarily a timelike photon sphere.

Equation (54) assumes the form

$$r^2-3mr+2e^2=0, \tag{88}$$

which has solutions $r_{ps}^{\pm}$ given by

$$r_{ps}^{\pm}/m=\frac{3\pm\sqrt{9-8(e/m)^2}}{2}. \tag{89}$$

The hypersurface $S^+:=\{r=r_{ps}^+\}$ exists for $0\leqslant(e/m)^2\leqslant 9/8$ and lies outside the event horizon and is therefore a timelike photon sphere. The hypersurface $S^-:=\{r=r_{ps}^-\}$ exists for $0<(e/m)^2\leqslant 9/8$ but lies outside the event horizon only for $1<(e/m)^2\leqslant 9/8$, and so is a timelike photon sphere only then. The hypersurfaces S^+ and S^- coincide for $(e/m)^2=9/8$. The Cauchy horizon and event horizon are always null photon spheres.

For $0\leqslant(e/m)^2\leqslant 1$ the curvature singularity at $r=0$ is locally naked but hidden behind an event horizon which lies strictly inside the only timelike photon sphere. For $1<(e/m)^2$ the singularity at $r=0$ is globally naked and is surrounded by two timelike photon spheres in the case $1<(e/m)^2<9/8$, one timelike photon sphere in the case $(e/m)^2=9/8$ and by no photon spheres, either timelike or null, in the case $(e/m)^2>9/8$ (see Fig. 2).

Example 8 (Janis–Newman–Winicour space–time): The most general static spherically symmetric solution to the Einstein massless scalar field equations for a scalar field Φ satisfying $\Box\Phi=0$ was obtained by Janis, Newman and Winicour.[9] The Ricci tensor has the form $R_{ab}=8\pi\Phi_{;a}\Phi_{;b}$. The solution is known[10] to be expressible in the form

$$\mathbf{g}=-\left(1-\frac{b}{r}\right)^{\nu}dt^2+\left(1-\frac{b}{r}\right)^{-\nu}dr^2+\left(1-\frac{b}{r}\right)^{1-\nu}r^2(d\theta^2+\sin^2\theta d\phi^2), \tag{90}$$

$$\Phi=\frac{q}{b\sqrt{4\pi}}\ln\left(1-\frac{b}{r}\right), \tag{91}$$

for $r:b<r<\infty$ where the constants b, ν are related to the ADM mass m and scalar charge q by

$$\nu=\frac{2m}{b},\quad b=2\sqrt{m^2+q^2}. \tag{92}$$

We assume $b>0$. There is a curvature singularity at $r=b$. In order to obtain $m\geqslant 0$ one must assume $0\leqslant\nu\leqslant 1$. For $q=0$ the solution reduces to the Schwarzschild solution.

Since all hypersurfaces of the form $\{r=\text{const}\}$ are timelike, one has from the photon sphere equation (54) that the only timelike photon sphere is at

$$r=\frac{b(2\nu+1)}{2}, \tag{93}$$

which exists only for $\nu:\frac{1}{2}<\nu\leqslant 1$, i.e., for $0\leqslant q^2<3m^2$. For $\frac{1}{2}<\nu\leqslant 1$ it is known[11] that a photon coming from infinity is deflected through an unboundedly large angle, i.e., the photon passes increasingly many times around the singularity as the closest distance of approach tends to the right side of (93).

Example 9 (Charged dilaton space–time): The static spherically symmetric charged dilaton solution[12] comprises a metric $\mathbf{g}$, a dilaton field Φ and an electromagnetic field F_{ab} given by

$$\mathbf{g}=-\left(1-\frac{r_+}{r}\right)\left(1-\frac{r_-}{r}\right)^{\omega}dt^2+\left(1-\frac{r_+}{r}\right)^{-1}\left(1-\frac{r_-}{r}\right)^{-\omega}dr^2+\left(1-\frac{r_-}{r}\right)^{1-\omega}r^2\,d\Omega^2, \tag{94}$$

$$e^{2\Phi}=\left(1-\frac{r_-}{r}\right)^{(1-\omega)/\beta}, \tag{95}$$

$$F_{tr}=-F_{rt}=\frac{e}{r^2},\quad \textit{all other components vanishing}, \tag{96}$$

where r_+ and r_- are related to the ADM mass m and electric charge e by

$$r_++\omega r_-=2m, \tag{97}$$

$$r_+r_-=e^2(1+\beta^2), \tag{98}$$

and β is a free parameter which controls the coupling strength between the dilaton and Maxwell fields, with ω defined in terms of β^2 by

$$\omega:=\frac{1-\beta^2}{1+\beta^2}. \tag{99}$$

We assume $m>0$.

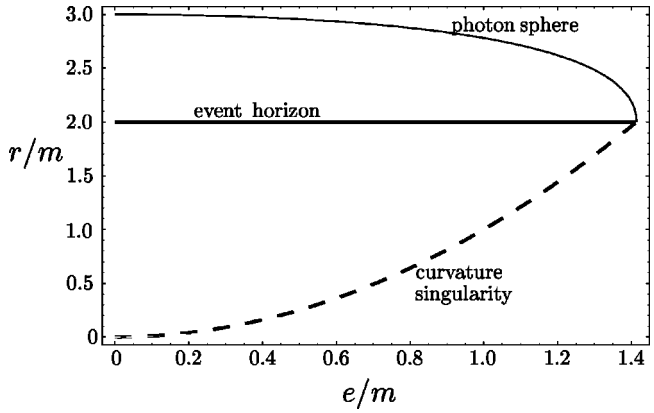

FIG. 3. The radii of the photon sphere, event horizon and curvature singularity are plotted against the electric charge for the charged dilaton solution.

For $\beta=0$ the solution reduces to the Reissner–Nordström solution considered in Example 7. For $\beta=0$ and $e=0$ the solution reduces to the Schwarzschild solution. The solution also reduces to the Schwarzschild solution for $e=r_-=0$ and arbitrary β. Here we shall consider the case $\beta^2=1$. In this case one has $(r_+,r_-)=(2m,e^2/m)$. There is an event horizon at $r=r_+=2m$ and a curvature singularity at $r=r_-=e^2/m$. For $0\leqslant(e/m)^2<2$ the singularity at $r=r_-$ lies inside a black hole while for $(e/m)^2>2$ it is globally naked.

For $\beta^2=1$ the photon sphere equation (54) reduces to

$$r_{ps}^{\pm}/m=\frac{(6+(e/m)^2)\pm\sqrt{36+(e/m)^4-20(e/m)^2}}{4}. \tag{100}$$

For $0\leqslant(e/m)^2<2$ one has $r_{ps}^-\leqslant r_-<r_+<r_{ps}^+$ so there is a single timelike photon sphere. For $(e/m)^2=2$ one has $r_{ps}^-=r_-=r_+=r_{ps}^+$ so there are no timelike photon spheres. For $2<(e/m)^2<18$ both r_{ps}^+ and r_{ps}^- are complex so there are no timelike photon spheres. For $(e/m)^2\geqslant 18$ one has $r_{ps}^-\leqslant r_{ps}^+<r_-$ so there are again no timelike photon spheres. Thus in the black hole case $0\leqslant(e/m)^2<2$ there is a single timelike photon sphere, while in the naked singularity case $(e/m)^2>2$ there are no timelike photon spheres. (See Fig. 3.)

Example 10 (Vaidya null dust collapse): The Vaidya null dust collapse model is a nonstatic, spherically symmetric space–time with a metric which, in terms of single null (radiation) coordinates (u,r,θ,ϕ), assumes the form

$$\mathbf{g}=-\left(1-\frac{2m(u)}{r}\right)du^2+2\,du\,dr+r^2(d\theta^2+\sin^2\theta d\phi^2), \tag{101}$$

where $m(u)$ is a freely specifiable function of u. Setting $x^0:=u$, $x^1:=r$ in (35) one obtains

$$\frac{d^2r}{du^2}=\frac{1}{r}\left(g_{uu}+\frac{dr}{du}\right)\left(g_{uu}+2\frac{dr}{du}\right)-\frac{3}{2}\frac{dr}{du}\partial_r g_{uu}-\frac{1}{2}(g_{uu}\partial_r g_{uu}+\partial_u g_{uu}), \tag{102}$$

$$=\frac{1}{r}\left\{\left(1-\frac{3m(u)}{r}\right)\left(1-\frac{2m(u)}{r}-3\frac{dr}{du}\right)-\frac{dm(u)}{du}+2\left(\frac{dr}{du}\right)^2\right\}. \tag{103}$$

This is the evolution equation for a spherically symmetric photon surface of the Vaidya collapse metric (101).

Consider the special case,

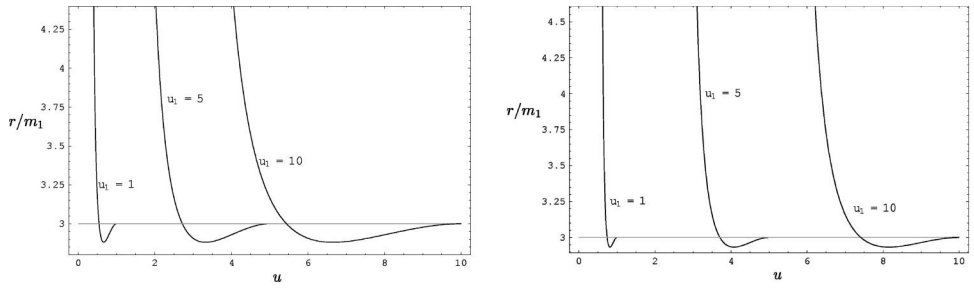

FIG. 4. The backwards evolution of the $r=3m_1$ Schwarzschild photon surface through collapsing Vaidya null dust. The space–time coordinates of the evolved surface are plotted for $m(u)=u/16$ (left) and $m(u)=u/32$ (right) for various values of the null time $u_1>0$ of the junction between the null dust and Schwarzschild regions. In each case the evolved photon surface fails to intersect the Minkowskian region $u<0$.

$$m(u)=\begin{cases} 0 & :-\infty<u<0, \\ \lambda u & :0\leqslant u\leqslant u_1, \\ m_1:=\lambda u_1 & :u_1<u<\infty, \end{cases} \tag{104}$$

for given constants $\lambda>0$, $u_1>0$. For $u<0$ the space–time is locally Minkowskian, for $u:0\leqslant u\leqslant u_1$ there is inward falling null dust, and for $u>u_1$ the space–time is locally isometric to Schwarzschild space–time with ADM mass $m_1>0$. It is well-known there is a curvature singularity at $r=0$ and that for $\lambda:0<\lambda\leqslant\frac{1}{16}$ the part of this singularity at $u=0$ is locally naked.

Fix $\lambda:0<\lambda\leqslant\frac{1}{16}$. For $u>u_1$ Eq. (103) gives, as expected, that there is a photon surface at $r=3m_1$. We seek to evolve this photon surface backwards in time, though the in-falling null dust, to obtain a maximally extended photon surface S. The boundary conditions are

$$\left.\begin{aligned} r&=3m_1 \\ \frac{dr}{du}&=0 \end{aligned}\right\} \quad \text{at } u=u_1. \tag{105}$$

The results are shown in Fig. 4 for $\lambda=1/16$ and $\lambda=1/32$ for selected values of u_1. One sees that in all cases S tends in the past direction to a null hypersurface of the form $\{u=\text{const}\}$. The conformal diagram must therefore be of the form sketched in Fig. 5.

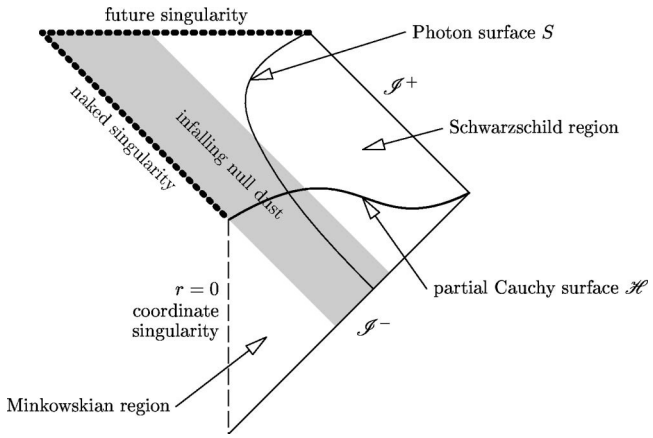

FIG. 5. The conformal diagram of the Vaidya null dust collapse model showing the photon surface S arising from the backwards evolution of the Schwarzschild photon sphere. Any partial Cauchy surface $\mathcal{H}$ which extends to spatial infinity is cut into two components by S.

It is evident from Fig. 5 that the naked central singularity is enclosed within the photon surface S in the sense that any partial Cauchy surface $\mathcal{H}$ extending to spatial infinity must intersect S in a 2-sphere. The physical significance of this may warrant further investigation.

VI. CONCLUDING REMARKS

The definition of a photon surface given in Sec. II is valid in an arbitrary space–time. However the result that a photon surface must have a second fundamental form which is pure trace indicates that a space–time must be specialized in some respect if it is to contain any photon surfaces. For spherically symmetric space–times there are always photon surfaces that respect the spherical symmetry. For space–times that are not spherically symmetric, the definitions of a photon surface and G-invariant photon surface may seem too restrictive. The problem is that, in general, one may not have orbiting null geodesics at a fixed radius. In Kerr space–time, for example, although there are orbiting null geodesics in the equatorial plane, those null geodesics which move in the direction of rotation do so at a different radius than those which move in the opposite direction. But it seems implausible that a concept which is physically important in the case of exact spherical symmetry should become invalid when even a small amount of angular momentum is introduced. A nontrivial generalization of the concepts of photon surface and G-invariant photon surface, at least to axially symmetric space–times, is thus required.

ACKNOWLEDGMENTS

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High order relativistic corrections to Keplerian motion

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The first terms of the general solution for an asymptotically flat stationary axisymmetric vacuum spacetime endowed with an equatorial symmetry plane are calculated from the corresponding Ernst potential up to seventh order in the radial pseudospherical coordinate. The metric is used to determine the influence of high order multipoles in the perihelion precession of an equatorial orbit and in the node line precession of a nonequatorial orbit with respect to a geodesic circle. Both results are written in terms of invariant quantities such as the Geroch–Hansen multipoles and the energy and angular momentum of the orbit. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1335556]

I. INTRODUCTION

The construction of new exact solutions of the Einstein vacuum field equations describing an asymptotically flat stationary axially symmetric spacetime has increased in the last decade due to the several methods of generation of solutions from a given one, such as the Bäcklund transformations, the inverse scattering method and the HKX tranformations (cf., for instance, Ref. 1 and references quoted therein). Nevertheless we are very far from being able to implement the physical behavior of an exact solution at will and in order to obtain results which could be tested experimentally we are led to use approximate expressions for the metrics with the desired physical requirements.

In this paper we study the influence of the first Geroch–Hansen multipole moments[2,3] of order higher than three in some astrophysical situations with stationary and axial symmetry. As it is well known, these moments can be calculated from the coefficients of the power expansion of the Ernst potential on the symmetry axis,[4] being linear the relation between both families of constants until the third moment, that is, the octupole. The subsequent expressions for the multipole moments of order higher than three become considerably more complicated as the order increases and there is not even a closed formula for calculating all of them. Our purpose in this paper is therefore to show to what extent these nonlinearities affect the motion of test particles tracing their orbits around a nonspherical, in principle rotating, compact mass distribution. Of course, these terms are irrelevant for our solar system calculations, but they are meaningful for highly relativistic astrophysical objects, such as pulsars, as stated in Ref. 5.

With this aim in mind we calculate in Sec. II the first seven terms of a power expansion of the Ernst potential with arbitrary values for the multipole moments and construct the corresponding approximate metric. This result is used in Sec. III to obtain an expression for the perihelion precession of an equatorial trajectory and in Sec. IV to produce the corrections to the Newtonian precession of the nodes of a slightly nonequatorial orbit with reference to a close neighboring geodesic circle. There is some previous work on this subject in Refs. 6 and 7, but these references deal only with terms up to the quadrupole moment. The results will be discussed in Sec. V.

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II. CALCULATION OF THE METRIC

The metric of a stationary axially symmetric vacuum spacetime can be written in a canonical form in terms of the Weyl coordinates,

$$ds^2=-f(dt-A\,d\phi)^2+\frac{1}{f}\{e^{2\gamma}(d\rho^2+dz^2)+\rho^2 d\phi^2\}, \tag{1}$$

where t and ϕ are the coordinates associated with the commuting Killing vectors ∂_t and ∂_ϕ, and the functions f, A and γ depend only on the coordinates ρ and z.

The whole set of Einstein equations can be shown[8] to be equivalent to the following system of partial differential equations:

$$\varepsilon=f+i\chi, \tag{2}$$

$$\varepsilon_{\rho\rho}+\frac{1}{\rho}\varepsilon_\rho+\varepsilon_{zz}=\frac{2}{\varepsilon+\bar{\varepsilon}}(\varepsilon_\rho^2+\varepsilon_z^2), \tag{3}$$

$$A_\rho=\frac{4\rho}{(\varepsilon+\bar{\varepsilon})^2}\chi_z, \tag{4}$$

$$A_z=-\frac{4\rho}{(\varepsilon+\bar{\varepsilon})^2}\chi_\rho, \tag{5}$$

$$\gamma_\rho=\frac{\rho}{(\varepsilon+\bar{\varepsilon})^2}(\varepsilon_\rho\bar{\varepsilon}_\rho-\varepsilon_z\bar{\varepsilon}_z), \tag{6}$$

$$\gamma_z=\frac{\rho}{(\varepsilon+\bar{\varepsilon})^2}(\varepsilon_\rho\bar{\varepsilon}_z+\varepsilon_z\bar{\varepsilon}_\rho). \tag{7}$$

It can be shown that the integrability of the last four equations is guaranteed if Eq. (3), the Ernst equation, is satisfied. Therefore, in order to obtain a solution of the Einstein equations with two Killing vectors, it suffices to solve the Ernst equation and then calculate the metric functions by quadratures.

It is also usual to write the Ernst equation in terms of another potential, ξ, related to the previous one by the following relation:

$$\xi=\frac{1-\varepsilon}{1+\varepsilon}, \tag{8}$$

which satisfies another partial differential equation,

$$(\xi\bar{\xi}-1)\left(\xi_{\rho\rho}+\frac{1}{\rho}\xi_\rho+\xi_{zz}\right)=2\bar{\xi}(\xi_\rho^2+\xi_z^2), \tag{9}$$

which is also satisfied by ξ^{-1}. This latter form is the one introduced originally in Ref. 8 and allows a simple integration of the Kerr metric.

This form is particularly useful for calculating the multipole moments and it will be the one we shall employ.

In order to calculate the approximate solution, we shall write the Ernst potential ξ as a function of two coordinates r and θ related to the Weyl ones by the following transformation,

$$\rho=r\sin\theta, \quad z=r\cos\theta. \tag{10}$$

We can implement the requirement of asymptotic flatness by writing ξ as a formal inverse power expansion in the pseudospherical radial coordinate r,

$$\xi=\sum_{n=1}^{\infty}\xi_n r^{-n}, \tag{11}$$

where the functions ξ_n depend only on the coordinate θ.

Since we are interested in having a solution which is symmetric with respect to the equatorial plane $\theta=\pi/2$, we shall require that the functions ξ_n of odd order be real whereas those of even order will be taken to be imaginary.

With this information at hand we can now proceed to calculate the metric functions. The function f is just the real part of ε and from our knowledge of ξ we can calculate the first eight terms of its expansion in the radial coordinate,

$$f=1+\sum_{n=1}^{\infty}f_n r^{-n}, \tag{12}$$

$$f_1=-2\,m_0, \tag{13}$$

$$f_2=2\,m_0^2, \tag{14}$$

$$f_3=m_2-\frac{4\,m_0^3}{3}-3\,m_2\cos^2\theta, \tag{15}$$

$$f_4=-2\,m_0\,m_2+\frac{2\,m_0^4}{3}+(6\,m_0 m_2+2\,m_1^2)\cos^2\theta, \tag{16}$$

$$f_5=-\frac{3\,m_4}{4}+2\,m_0^2 m_2+\frac{8\,m_0 m_1^2}{35}-\frac{4\,m_0^5}{15}+\left(\frac{15\,m_4}{2}-6\,m_0^2 m_2-\frac{44\,m_0\,m_1^2}{7}\right)\cos^2\theta-\frac{35\,m_4\cos^4\theta}{4}, \tag{17}$$

$$\begin{aligned} f_6=&\frac{3\,m_0\,m_4}{2}+\frac{m_2^2}{2}-\frac{4\,m_2\,m_0^3}{3}-\frac{16\,m_0^2 m_1^2}{35}+\frac{4\,m_0^6}{45}\\ &+\left(-15\,m_0\,m_4-6\,m_1\,m_3-3\,m_2^2+4\,m_2\,m_0^3+\frac{356\,m_0^2 m_1^2}{35}\right)\cos^2\theta\\ &+\left(\frac{35\,m_0\,m_4}{2}+10\,m_1\,m_3+\frac{9\,m_2^2}{2}\right)\cos^4\theta, \end{aligned} \tag{18}$$

$$\begin{aligned} f_7=&\frac{5\,m_6}{8}-\frac{3\,m_0^2 m_4}{2}-\frac{4\,m_0\,m_1\,m_3}{11}-m_0\,m_2^2-\frac{16\,m_1^2\,m_2}{231}+\frac{2\,m_0^4 m_2}{3}+\frac{32\,m_0^3 m_1^2}{63}-\frac{8\,m_0^7}{315}\\ &+\left(-\frac{105\,m_6}{8}+15\,m_0^2 m_4+\frac{216\,m_0\,m_1\,m_3}{11}+6\,m_0\,m_2^2+\frac{38\,m_1^2\,m_2}{11}-2\,m_0^4 m_2\right.\\ &\left.-\frac{1208\,m_0^3 m_1^2}{105}\right)\cos^2\theta+\left(\frac{315\,m_6}{8}-\frac{35\,m_0^2 m_4}{2}-\frac{340\,m_0\,m_1\,m_3}{11}-\frac{114\,m_1^2\,m_2}{11}-9\,m_0\,m_2^2\right)\cos^4\theta\\ &-\frac{231\,m_6}{8}\cos^6\theta, \end{aligned} \tag{19}$$

where the constants m_n which arise from the integration of the Ernst equation are real if n is even and otherwise imaginary.

The first six terms of the metric function A can be obtained by direct integration of the equations (4) and (5). In spite of the factor i before the expression for A, this function is obviously real since the constants m_n are imaginary for odd n,

$$A=-i\sin^2\theta\sum_{n=1}^{\infty}A_n r^{-n}, \tag{20}$$

$$A_1=-2m_1, \tag{21}$$

$$A_2=-2m_0m_1, \tag{22}$$

$$A_3=m_3-\frac{8m_0^2m_1}{5}-5m_3\cos^2\theta, \tag{23}$$

$$A_4=\frac{3m_0m_3}{2}+\frac{m_1m_2}{2}-\frac{16m_0^3m_1}{15}+\left(-\frac{15m_0m_3}{2}+\frac{3m_1m_2}{2}\right)\cos^2\theta, \tag{24}$$

$$A_5=-\frac{3m_5}{4}+\frac{4m_0^2m_3}{3}+\frac{8m_0m_1m_2}{7}-\frac{64m_0^4m_1}{105}+\left(\frac{21m_5}{2}-\frac{20m_0^2m_3}{3}\right)\cos^2\theta-\frac{63m_5}{4}\cos^4\theta, \tag{25}$$

$$\begin{aligned}A_6=&-\frac{5m_0m_5}{4}-\frac{m_1m_4}{4}-\frac{m_2m_3}{2}+\frac{8m_0^3m_3}{9}+\frac{48m_0^2m_1m_2}{35}+\frac{8m_0m_1^3}{105}-\frac{32m_0^5m_1}{105}\\&+\left(\frac{35m_0m_5}{2}-\frac{5m_1m_4}{2}+m_2m_3-\frac{40m_0^3m_3}{9}-\frac{8m_0^2m_1m_2}{5}+\frac{16m_0m_1^3}{21}\right)\cos^2\theta\\&+\left(-\frac{105m_0m_5}{4}+\frac{35m_1m_4}{4}-\frac{5m_2m_3}{2}\right)\cos^4\theta.\end{aligned} \tag{26}$$

The only function which remains to be calculated is γ and can be obtained as a quadrature from equations (6) and (7),

$$\gamma=\sum_{n=1}^{\infty}\gamma_n r^{-2n}, \tag{27}$$

$$\gamma_1=-\frac{m_0^2\sin^2\theta}{2}, \tag{28}$$

$$\gamma_2=\frac{3m_0m_2}{4}-\frac{m_1^2}{4}+\left(-\frac{9m_0m_2}{2}+\frac{5m_1^2}{2}\right)\cos^2\theta+\left(\frac{15m_0m_2}{4}-\frac{9m_1^2}{4}\right)\cos^4\theta, \tag{29}$$

$$\gamma_3 = -\frac{5\,m_0\,m_4}{8} + \frac{m_1\,m_3}{2} - \frac{3\,m_2^2}{8} + \frac{2\,m_0^2 m_1^2}{35} + \left(\frac{75\,m_0\,m_4}{8} - \frac{21\,m_1\,m_3}{2} + \frac{45\,m_2^2}{8} - \frac{2\,m_0^2 m_1^2}{35}\right)\cos^2\theta + \left(-\frac{175\,m_0\,m_4}{8} + \frac{55\,m_1\,m_3}{2} - \frac{117\,m_2^2}{8}\right)\cos^4\theta + \left(\frac{105\,m_0\,m_4}{8} - \frac{35\,m_1\,m_3}{2} + \frac{75\,m_2^2}{8}\right)\cos^6\theta, \tag{30}$$

$$\gamma_4 = \frac{35\,m_0\,m_6}{64} - \frac{15\,m_1\,m_5}{32} + \frac{45\,m_2\,m_4}{64} - \frac{9\,m_3^2}{32} - \frac{14\,m_0^2 m_1\,m_3}{165} - \frac{2\,m_0\,m_1^2 m_2}{33} + \frac{16\,m_0^4 m_1^2}{1575} + \left(-\frac{245\,m_0\,m_6}{16} + \frac{135\,m_1\,m_5}{8} - \frac{315\,m_2\,m_4}{16} + \frac{81\,m_3^2}{8} + \frac{28\,m_0^2 m_1\,m_3}{55} - \frac{4\,m_0\,m_1^2 m_2}{231} + \frac{16\,m_0^4 m_1^2}{1575}\right)\cos^2\theta + \left(\frac{2205\,m_0\,m_6}{32} - \frac{1365\,m_1\,m_5}{16} + \frac{3075\,m_2\,m_4}{32} - \frac{795\,m_3^2}{16} - \frac{14\,m_0^2 m_1\,m_3}{33} + \frac{6\,m_0\,m_1^2 m_2}{77}\right)\cos^4\theta + \left(-\frac{1617\,m_0\,m_6}{16} + \frac{1071\,m_1\,m_5}{8} - \frac{2415\,m_2\,m_4}{16} + \frac{625\,m_3^2}{8}\right)\cos^6\theta + \left(\frac{3003\,m_0\,m_6}{64} - \frac{2079\,m_1\,m_5}{32} + \frac{4725\,m_2\,m_4}{64} - \frac{1225\,m_3^2}{32}\right)\cos^8\theta. \tag{31}$$

III. PERIHELION PRECESSION OF A CLOSED ORBIT

It is well known from Bertrand's theorem (cf. for instance Ref. 9) that stable bounded orbits of particles moving under the influence of a central force which is neither Newtonian nor harmonic are not closed. Therefore whenever the source of the gravitational field is not exactly monopolar, the bounded trajectories on the equatorial plane will no longer be the elliptic orbits described by Kepler's first law but will take the form of a precessing ellipse if the deviation from spherical symmetry is small.

The situation becomes a bit more complicated in general relativity. Although it has been proven[10] that there are just two asymptotically flat static spherically symmetric spacetimes in which the stable orbits are closed, they are rather different from the classical physical situations. Therefore, when relativistic effects are taken into account, not even the motion around a spherical distribution of mass is closed. This effect has been tested in our solar system and it amounts to a slow precession of the perihelion of the orbit of Mercury. Of course other multipole moments of the mass distribution will also contribute to this effect and, in principle, these moments could be calculated by measuring the precession of a certain number of test particles orbiting at conveniently different distances from the gravitational source.

If the test particles are small enough for the tidal forces to be unimportant within the characteristic length of the particle, we can regard them as point particles. If the effects due to their intrinsic angular momentum can be taken as negligible it can be assumed that they trace out timelike geodesics in the spacetime surrounding the gravitational source. Hence, in order to study the influence of the far field multipole moments of the gravitational field, we shall have to solve the geodesic equations for the previously calculated metric. We shall restrict ourselves to the equatorial plane $\theta = \pi/2$.

Since the timelike and azimuthal coordinates are ignorable, we have two first integrals for the motion corresponding to the conserved quantities E and l, respectively, the total energy per unit of mass and the projection of the angular momentum on the z axis, also per unit of mass, of the test particle. In terms of its 4-velocity $u = (\dot{t}, \dot{r}, \dot{\theta}, \dot{\phi})$ these quantities have the following form:

$$E = -\partial_t \cdot u = f(\dot{t} - A\dot{\phi}) \tag{32}$$

$$l=\partial_\phi\cdot u=f\,A\,(\dot{t}-A\dot{\phi})+\frac{1}{f}r^2\,\dot{\phi}, \tag{33}$$

where the overhead dot stands for the derivative with respect to proper time.

Therefore the equations for t and ϕ can be written as follows:

$$\dot{\phi}=f\,\frac{l-E\,A}{r^2}, \tag{34}$$

$$\dot{t}=\frac{E}{f}+f\,A\,\frac{l-E\,A}{r^2}. \tag{35}$$

Another integral arises from the fact that the trajectory is timelike and therefore $u\cdot u=-1$. For the geodesics under consideration this means

$$-1=-f(\dot{t}-A\dot{\phi})^2+\frac{1}{f}(e^{2\gamma}\dot{r}^2+r^2\,\dot{\phi}^2). \tag{36}$$

From the previous three equations $\dot{r}$ can be obtained as a function of the nonignorable coordinates and the conserved quantities. However, since we are interested in the shape of the orbit rather than in its time evolution, we divide (36) by $\dot{\phi}$ to get the derivative of the radial coordinate with respect to the azimuthal angle,

$$r_\phi^2=e^{-2\gamma}\left\{\frac{r^4\,(E^2-f\,)}{f^2\,(l-E\,A)^2}-r^2\right\}. \tag{37}$$

It will be useful to write this equation in terms of another function $u=1/r$ as it is done in classical mechanics for solving the motion under central forces,

$$u_\phi^2=e^{-2\gamma}\left\{\frac{E^2-f}{f^2\,(l-E\,A)^2}-u^2\right\}=F(u)=\sum_{n=0}^{6}c_n\,u^n+O(u^7). \tag{38}$$

This equation can be turned into a quasilinear one by taking a derivative with respect to ϕ and cancelling the u_ϕ factors, since for the analysis of perihelion precession circular orbits are of no interest,

$$u_{\phi\phi}=\tfrac{1}{2}F'(u). \tag{39}$$

In order to solve these equations perturbatively we need expand them in powers of a small parameter. A good candidate is the inverse of the angular momentum per unit of mass, l, since according to Kepler's 1–2–3 law, which is assumed to be a good approximation at a great distance from the source, it behaves as $l\sim\sqrt{m\,r}$, where m is the mass of the particle. It can be combined with the mass of the source m_0 to yield an acceptable dimensionless small parameter for analyzing the far gravitational field. Hence we shall use $\epsilon=m_0/l$ and expand u in the following way:

$$u=\epsilon^2\sum_{n=0}^{11}u_n\,\epsilon^n+O(\epsilon^{14}). \tag{40}$$

The reason for starting the expansion at this order is that the expression for the Kepler ellipse, which is expected to be the first term, is second order in ϵ.

The energy per unit of mass of the particle is also to be expanded in ϵ. Therefore we write

$$E=1+\epsilon^2\sum_{n=0}^{n=11} E_n\,\epsilon^n+O(\epsilon^{14}). \tag{41}$$

In order to avoid the appearance of secular terms we use a coordinate ψ related to ϕ by

$$\psi=\omega\phi, \quad \omega=\sqrt{1+\sum\ \omega_i\epsilon^i}. \tag{42}$$

The coefficients c_n are all of the order ϵ^2 except c_2 which is clearly of zeroth order in ϵ and therefore Eq. (38) takes the form of a hierarchy of forced harmonic oscillators which can be solved iteratively up to the order of accuracy provided by our knowledge of the metric,

$$u_{n\ \psi\psi}+u_n=f_n(\psi). \tag{43}$$

The first terms of the expansion of the solution to the equations (38) and (39) are

$$u_0=\frac{1}{m_0}(1+\sqrt{1+2\,E_0}\cos\psi), \tag{44}$$

$$u_1=0, \tag{45}$$

$$u_2=\frac{6+4\,E_0}{m_0}, \tag{46}$$

$$u_3=(8+4\,E_0)\,\frac{i\,m_1}{m_0^3}. \tag{47}$$

Of course the term of lowest order is the Kepler ellipse if E_0 is negative.

From the information we have about the metric we can calculate ω up to the eleventh power of ϵ. These terms are just what we need to calculate the expression for the perihelion precession, so we shall focus on them. The expressions of the terms u_n are not needed and therefore we shall not enclose them here.

Instead of writing the results as a function of the integration constants m_i, it will be more useful to write them in terms of the Geroch–Hansen multipole moments, P_i, the physical interpretation of which is more appealing. Bear in mind that the odd multipole moments are imaginary and have to be multiplied by $-i$ to obtain the usual real expressions J_n. To calculate these moments we shall make use of the procedure described in Ref. 4.

If we have an expansion of the Ernst potential ξ on the symmetry axis in terms of the Weyl coordinate z, viz.,

$$\xi(\rho=0)=\sum_{n=0}^{\infty} C_n\,z^{-(n+1)}, \tag{48}$$

then the multipole moments can be calculated as follows:

$$P_n=C_n, \quad n\leqslant 3, \tag{49}$$

$$P_4=C_4+\tfrac{1}{7}\overline{C}_0(C_1^2-C_2C_0), \tag{50}$$

$$P_5=C_5+\tfrac{1}{3}\overline{C}_0(C_2\,C_1-C_3\,C_0)+\tfrac{1}{21}\overline{C}_1\,(C_1^2-C_2\,C_0). \tag{51}$$

As a function of these multipole moments the first coefficients in the expansion of the energy per unit of mass, E, read as

$$E_1=0, \tag{52}$$

$$E_2=-6-10E_0-\frac{E_0^2}{2}, \tag{53}$$

$$E_3=-(8+12E_0)\frac{iP_1}{P_0^2}, \tag{54}$$

$$E_4=-\frac{47}{4}-20E_0-13E_0^2+\frac{E_0^3}{2}+(2+3E_0)\frac{P_2}{P_0^3}, \tag{55}$$

$$E_5=-(56+104E_0+56E_0^2)\frac{iP_1}{P_0^2}, \tag{56}$$

where E_0, the Keplerian energy, is a free parameter which has $-1/2$ as a lower bound, corresponding to a circular orbit.

The frequency ω is different from one and therefore the orbit is not closed. Between two consecutives perihelion approaches the test particle traces an angle $2\pi/\omega$. Hence the perihelion has shifted an angle, $\Delta\phi$ given up to the eleventh power of ϵ by the following expression:

$$\begin{aligned}\Delta\phi&=2\pi(\omega^{-1}-1)\\&=\pi\{\Delta_0+\Delta_1+\Delta_2+\Delta_4+\Delta_8+\Delta_{16}+\Delta_{32}+\Delta_{2\times4}+\Delta_{2\times8}+\Delta_{2\times16}+\Delta_{4\times8}\},\end{aligned} \tag{57}$$

where the shift has been split into different terms according to their origin: The first one, Δ_0, comprises the Newtonian contribution to the precession, that is, the terms which remain after taking the classical limit $c\to\infty$. Of course only the gravitational moments are present since rotation has no influence whatsoever in Newtonian dynamics. Since the speed of light, c, and the gravitational coupling constant, G, have been taken to be one, the terms look rather alike in magnitude. However, if the respective factors are written (a factor G/c for each ϵ, a factor G/c^2 for each P_{2n}, a factor G/c^3 for each P_{2n+1}, a factor c^{-1} for each l and a factor G^{-2} for each E_0), the actual magnitude of every term is recovered. For instance, the first Newtonian term has a factor G^2 and the second a G^4. For oblate gravitational sources the quadrupole moment, P_2 is negative, whence it contributes to a positive shift of the perihelion in the first order. In the next order the shift contribution of the quadrupole is, however, always positive. (*n.b.*: E_0, though negative for bounded orbits, has a lower limit about $-1/2$ which does not allow it to overcome the energy-independent term.) On the other hand the sedecimpole P_4 term bears the opposite sign to the one of the quadrupole,

$$\Delta_0=-\frac{3P_2}{P_0^3}\epsilon^4+\left\{\left(\frac{105}{8}+\frac{45E_0}{4}\right)\frac{P_4}{P_0^5}+\left(\frac{105}{8}+\frac{15E_0}{4}\right)\frac{P_2^2}{P_0^6}\right\}\epsilon^8. \tag{58}$$

The second term, Δ_1, comprises the contribution to the perihelion precession due to a spherically symmetric mass distribution, i.e., the Schwarzschild effect. It can be calculated exactly in terms of elliptic functions and is of the order of G^2/c^2. The contribution of every order is always positive,

$$\begin{aligned}\Delta_1=6\epsilon^2&+\left(\frac{105}{2}+15E_0\right)\epsilon^4+\left(\frac{975}{2}+165E_0\right)\epsilon^6+\left(\frac{159105}{32}+\frac{16725E_0}{8}+\frac{705E_0^2}{8}\right)\epsilon^8\\&+\left(\frac{1701507}{32}+\frac{216375E_0}{8}+\frac{20115E_0^2}{8}\right)\epsilon^{10}.\end{aligned} \tag{59}$$

In the term Δ_2 we have included the influence of a dipole of rotation on the perihelion shift. It is of the order of G^2/c^2. Since its lower terms in ϵ are odd, it is sensitive to whether the probe rotates in the same direction as the source does or not. It is positive if the angular momentum of the source and the orbital angular momentum of the probe are antiparallel and negative otherwise. This has a qualitative explanation in the fact that the perihelion shift due to a mass monopole decreases with the angular momentum of the test particle; if the source happens to be rotating and its angular momentum is J, then l is replaced in the first order by $l+2\,J/r$ as it can be seen in Eq. (38) after substitution of P_1 by $i\,J$, whence the ''effective'' l increases if both momenta are parallel and it would be expected that the perihelion advance diminishes. In contrast, the quadratic terms in P_1 are independent of the direction of rotation and are always positive whence they induce a perihelion advance. The cubic terms in P_1 behave as the linear ones,

$$\begin{aligned}\Delta_2=&\frac{8\,i\,P_1\epsilon^3}{P_0^2}+(168+48\,E_0)\frac{i\,P_1}{P_0^2}\epsilon^5-(120+24\,E_0)\frac{P_1^2}{P_0^4}\epsilon^6+(2562+1020\,E_0+36\,E_0^2)\frac{i\,P_1}{P_0^2}\epsilon^7\\&-\left(\frac{65607}{16}+\frac{44607\,E_0}{28}+\frac{195\,E_0^2}{4}\right)\frac{P_1^2}{P_0^4}\epsilon^8+\left\{(36046+17640\,E_0+1356\,E_0^2-16\,E_0^3)\frac{i\,P_1}{P_0^2}\right.\\&\left.-(2048+672\,E_0)\frac{i\,P_1^3}{P_0^6}\right\}\epsilon^9-\left(\frac{10256685}{112}+\frac{1320387\,E_0}{28}+\frac{118305\,E_0^2}{28}\right)\frac{P_1^2}{P_0^4}\epsilon^{10}\\&+\left\{\left(\frac{3927489}{8}+\frac{569361\,E_0}{2}+\frac{70659\,E_0^2}{2}+174\,E_0^3+15\,E_0^4\right)\frac{i\,P_1}{P_0^2}\right.\\&\left.-\left(\frac{2735961}{28}+\frac{341339\,E_0}{7}+\frac{27429\,E_0^2}{7}\right)\frac{i\,P_1^3}{P_0^6}\right\}\epsilon^{11}.\end{aligned}\tag{60}$$

Under the name Δ_4 the relativistic terms depending only on the quadrupole moment, P_2, and the mass are comprised. The first correction has a factor G^4/c^2 in front of it. As it was to be expected, it does not depend on the direction of rotation and, as its Newtonian counterpart, it is positive for oblate gravitational sources. The quadratic terms as a whole are always positive,

$$\begin{aligned}\Delta_4=&-(90+42\,E_0)\frac{P_2}{P_0^3}\epsilon^6-\left(\frac{25383}{16}+\frac{28305\,E_0}{28}+\frac{375\,E_0^2}{4}\right)\frac{P_2}{P_0^3}\epsilon^8\\&+\left\{-\left(\frac{2686203}{112}+\frac{503379\,E_0}{28}+\frac{80187\,E_0^2}{28}\right)\frac{P_2}{P_0^3}+\left(\frac{12471}{16}+519\,E_0+\frac{165\,E_0^2}{4}\right)\frac{P_2^2}{P_0^6}\right\}\epsilon^{10}.\end{aligned}\tag{61}$$

The symbol Δ_8 stands for the corrections to the perihelion shift due to a rotation octupole moment P_3. The first correction is of the order of G^4/c^2. They bear the same relation to the dipole terms as the quadrupole to the monopole terms: The overall sign changes,

$$\begin{aligned}\Delta_8=&-\left\{(30+24\,E_0)\epsilon^7+(801+825\,E_0+138\,E_0^2)\epsilon^9\right.\\&\left.+\left(\frac{28671}{2}+16475\,E_0+4278\,E_0^2+102\,E_0^3\right)\epsilon^{11}\right\}\frac{i\,P_3}{P_0^4}.\end{aligned}\tag{62}$$

The influence of the sedecimpole gravitational moment, P_4, is included in Δ_{16} and does not show up until the tenth order of the small parameter. In nongeometrized units it is proportional to G^6/c^2,

$$\Delta_{16}=\left(\frac{7425}{16}+570\,E_0+\frac{495\,E_0^2}{4}\right)\frac{P_4}{P_0^5}\epsilon^{10}. \tag{63}$$

The last multipole moment to be considered is the rotational trigintaduopole moment, P_5, and it is comprised in Δ_{32}. It is of the eleventh order in ϵ,

$$\Delta_{32}=\left(\frac{945}{8}+210\,E_0+\frac{135\,E_0^2}{2}\right)\frac{iP_5}{P_0^6}\epsilon^{11}. \tag{64}$$

Now we review the couplings among the different multipole moments other than mass. Up to the order considered there is no coupling between the gravitational moments higher than the mass (except for self-couplings), but there are rotation–rotation couplings and gravitation–rotation couplings. The first one to appear is the dipole–quadrupole coupling, $\Delta_{2\times4}$. It has a factor of G^4/c^2 in the lowest order. If both angular momenta are antiparallel and the source is oblate ($P_2<0$), then the contribution of the bilinear terms is positive. The quadratic terms in the quadrupole P_2 are again positive if J and l are antiparallel. Finally the quadratic terms in the dipole are positive if the body is oblate,

$$\begin{aligned}\Delta_{2\times4}=&-(90+24\,E_0)\frac{iP_1P_2}{P_0^5}\epsilon^7-(3939+2127\,E_0+126\,E_0^2)\frac{iP_1P_2}{P_0^5}\epsilon^9\\&+(2280+900\,E_0)\frac{P_1^2P_2}{P_0^7}\epsilon^{10}+\left\{\left(\frac{1419}{2}+303\,E_0\right)\frac{iP_1P_2^2}{P_0^8}\right.\\&\left.-\left(\frac{2825301}{28}+\frac{507992\,E_0}{7}+\frac{75765\,E_0^2}{7}+90\,E_0^3\right)\frac{iP_1P_2}{P_0^5}\right\}\epsilon^{11}.\end{aligned} \tag{65}$$

The only rotation–rotation coupling up to this order is between the dipole and octupole moments. It comes under the name of $\Delta_{2\times8}$ and it is at least of the order G^6/c^4. Since it is linear on both rotational moments this term is not sensitive to the direction of rotation. It is of the tenth order in ϵ,

$$\Delta_{2\times8}=(1068+972\,E_0+120\,E_0^2)\frac{P_1P_3}{P_0^6}\epsilon^{10}. \tag{66}$$

The higher rotation–gravitation couplings involve the rotational dipole and the gravitational sedecimpole, $\Delta_{2\times16}$, and the rotational octupole and the gravitational quadrupole, $\Delta_{4\times8}$. Both appear first in the eleventh order of perturbation and are at least of the order of ϵ^{11}. The term $\Delta_{2\times16}$ is positive if P_4 is positive and the angular momenta are antiparallel,

$$\Delta_{2\times16}=\left(\frac{4005}{8}+495\,E_0+\frac{135\,E_0^2}{2}\right)\frac{iP_1P_4}{P_0^7}\epsilon^{11}, \tag{67}$$

$$\Delta_{4\times8}=\left(\frac{1383}{4}+348\,E_0+45\,E_0^2\right)\frac{iP_2P_3}{P_0^7}\epsilon^{11}. \tag{68}$$

It would be of great interest to know the range of applicability of this perturbative expansion. In an Appendix at the end of this paper a simpler case is studied: It is shown there for which values of the parameters the expansions are acceptable for the Schwarzschild metric.

IV. PRECESSION OF THE LINE OF NODES OF A NONEQUATORIAL ORBIT

Let us consider now a bounded orbit slightly departing from the equatorial plane. If the mass distribution of the source were spherically symmetric, the equatorial plane would not be at all privileged and the orbit would always intersect it at the same nodes. However, this is no longer the situation when the source is not exactly spherical, since then the nodes precess due to the perturbation generated by higher order multipoles. In classical nonrelativistic mechanics the first contribution to the precession of the nodes arises from the quadrupole moment, as it is shown in an Appendix at the end of this paper, whereas in general relativity it is the rotational dipole moment the first one to contribute.

In the approximation used in this section we consider a geodesic on the equatorial plane and calculate the evolution of small deviations from it. Since the geodesic equation reads as

$$\ddot{x}^{\mu}+\Gamma^{\mu}_{\rho\sigma}\dot{x}^{\rho}\dot{x}^{\sigma}=0, \tag{69}$$

it is straightforward that nearby geodesics which deviate from the original geodesic by a vector δ^{μ} fulfill

$$\ddot{\delta}^{\mu}+2\,\Gamma^{\mu}_{\rho\sigma}\,\dot{\delta}^{\rho}\dot{x}^{\sigma}+\Gamma^{\mu}_{\rho\sigma,\nu}\dot{x}^{\rho}\dot{x}^{\sigma}\,\delta^{\nu}=0. \tag{70}$$

Since we are interested in small deviations from the equatorial plane, we shall focus our attention on the θ coordinate. Taking into account that the reference geodesic lies on the symmetry plane $\theta=\pi/2$ and that the first derivatives of the metric with respect to θ vanish on it, the geodesic deviation equation for δ^{θ} reduces to

$$\ddot{\delta}^{\theta}-\tfrac{1}{2}g^{\theta\theta}g_{\rho\sigma,\theta\theta}\dot{x}^{\rho}\dot{x}^{\sigma}\,\delta^{\theta}=0. \tag{71}$$

Instead of considering an arbitrary bounded reference geodesic on the equatorial plane, we shall restrict ourselves to geodesic circles. Of course many interesting features will be lost, but we deem that this paper would become even longer if we take them into account.

In order to compute the evolution of the nodes with respect to the azimuthal angle on the geodesic, the previous equation needs to be divided by $\dot{\phi}^2$, which is constant on the circle. From now on we shall write δ instead of δ^{θ} to avoid cumbersome notations,

$$\delta_{\phi\phi}+\Omega^2\,\delta=0, \quad \Omega^2=-\frac{1}{2\,\dot{\phi}^2}g^{\theta\theta}g_{\rho\sigma,\theta\theta}\dot{x}^{\rho}\dot{x}^{\sigma}, \tag{72}$$

where every function is to be calculated on $\theta=\pi/2$ and $r=R$, the radius of the geodesic circle.

The previous expression states that the nodes of nearby geodesics are separated by regular intervals of the coordinate ϕ. If Ω is different from one, these nodes will travel around the geodesic circle instead of remaining at constant values of the azimuthal angle. Since it would be of interest to write down the result in a coordinate-independent expression, it will be required to make use of the geodesic equations to remove the dependence on the radius of the circle, R, and also to cast the energy, E, as a function of the angular momentum of the circular orbit, l, so that the final result will be a function of the multipole moments and l only.

As it is well known, the timelike geodesic equations can be obtained from the Lagrange equations applied to a functional $L=g_{\mu\nu}\dot{x}^{\mu}\dot{x}^{\nu}$ and the constraint $L=-1$. Two of these equations, namely (34) and (35), have already been used to remove the dependence on the derivatives of the ignorable coordinates. The equation corresponding to variations of θ is automatically satisfied. We are left just with two equations, corresponding to the constraint and the variations of r, viz.,

$$1=\frac{E^2}{f}-f\frac{(l-E\,A)^2}{r^2}, \tag{73}$$

$$\frac{E^2}{f^2}\partial_r f - 2\,E\,f\frac{l-E\,A}{R^2}\partial_r A - f^2\frac{(l-E\,A)^2}{R^4}\partial_r\left(\frac{r^2}{f}\right)=0, \tag{74}$$

where we have used $\dot{r}=0$ and $\theta=\pi/2$.

From the last equation we get E/l as a function of R,

$$\frac{E}{l}=\frac{-b\pm\sqrt{b^2-4\,a\,c}}{2\,a}, \tag{75}$$

$$\begin{aligned} a&=A^2\,f^2\,R^{-4}\,\partial_r(r^2\,f^{-1})-f^{-2}\,\partial_r f-2\,A\,f\,R^{-2}\partial_r A\\ &=-2\,P_0\,R^{-2}+O(R^{-3}), \end{aligned} \tag{76}$$

$$\begin{aligned} b&=2\,R^{-2}\,f\partial_r A-2\,A\,f^2\,R^{-4}\partial_r(r^2\,f^{-1})\\ &=-12\,i\,P_1\,R^{-4}+O(R^{-5}), \end{aligned} \tag{77}$$

$$c=f^2\,R^{-4}\partial_r(r^2\,f^{-1})=2\,R^{-3}+O(R^{-4}). \tag{78}$$

Since the energy must be positive, the solution with the minus (plus) signus in front of the square root equation corresponds to a positive (negative) l. On the other hand, Eq. (73) furnishes l in terms of E/l which has obviously the same coefficients which were obtained for E in the previous section after substitution of $E_0=-1/2$.

The frequency of the precession of the nodes can be written now independently of the choice of coordinates. As was to be expected, the first term is equal to one, corresponding to the frequency of the nodes when the mass distribution of the gravitational source is perfectly spherical.

The contributions to the precession of the line of nodes of a timelike geodesic which is slightly tilted with respect to a geodesic equatorial circle have been classified in the same way as it was done for the perihelion shift: A classical term plus the relativistic terms, divided according to their multipole content. In order to write down the expressions in nongeometrized units, factors including G and c have to be included as it was done in the previous section. The description which was made there of the necessary factors for each term in $\Delta\phi$ for the perihelion shift also applies. The information that we have of the metric allows us to calculate the coefficients up to l^{-13}.

There is, of course, no contribution from a pure mass monopole. Were the frequency equal to one, then the nodes would remain at constant ϕ. Therefore, $\Delta\phi=2\,\pi\,(\Omega^{-1}-1)$ describes the angle through which the line of nodes has precessed in one revolution of the reference circle,

$$\Delta\phi=\pi\{\Delta_0+\Delta_2+\Delta_4+\Delta_8+\Delta_{16}+\Delta_{32}+\Delta_{2\times4}+\Delta_{2\times8}+\Delta_{2\times16}+\Delta_{4\times8}\}. \tag{79}$$

For oblate objects ($P_2<0$), the influence of the mass quadrupole amounts to a delay in the precession of the line of nodes with respect to the ϕ coordinate on the circle of reference. Therefore the line of nodes does not precess in the same direction as the perihelion. This fact should not be confused with the precession of the angular momentum vector in time, which is of course positive. The contribution from the sedecimpole term is negative for positive P_4 and the one from the sexagintaduopole is positive for positive P_6. There is also a classical coupling between P_4 and P_2. The nonlinear terms in the quadrupole moment bear a positive sign,

$$\Delta_0=\frac{3\,P_0\,P_2}{l^4}+\left(-\frac{15\,P_0^3P_4}{2}+\frac{9\,P_0^2P_2^2}{4}\right)l^{-8}+\left(\frac{105\,P_0^5P_6}{8}+\frac{45\,P_0^4P_2\,P_4}{8}+\frac{81\,P_0^3P_2^3}{8}\right)l^{-12}. \tag{80}$$

Most of the dipole-dependent terms are sensitive to the direction of motion of the test particle relative to the rotation of the source. If the angular momenta are parallel (l has the same sign as

$J=-i\,P_1$), then the linear and cubic terms in P_1 induce an advance of the line of nodes. On the other hand the quadratic and quartic terms in the dipole moment are not sensitive to that relative sign and their influence always amounts to a delay,

$$\Delta_2=-\frac{4\,i\,P_0P_1}{l^3}-\frac{18\,i\,P_0^3P_1}{l^5}+\frac{18\,P_0^2P_1^2}{l^6}-\frac{243\,i\,P_0^5P_1}{2\,l^7}+\frac{4131\,P_0^4P_1^2}{14\,l^8}$$
$$+\left(196\,iP_0^3P_1^3-\frac{3861\,iP_0^7P_1}{4}\right)l^{-9}+\frac{27294\,P_0^6P_1^2}{7}l^{-10}$$
$$+\left(\frac{37983\,iP_0^5P_1^3}{7}-\frac{268515\,iP_0^9P_1}{32}\right)l^{-11}+\left(-2565\,P_0^4P_1^4+\frac{1060043\,P_0^8P_1^2}{22}\right)l^{-12}$$
$$+\left(\frac{734200\,iP_0^7P_1^3}{7}-\frac{4944807\,iP_0{}^{11}P_1}{64}\right)l^{-13}. \tag{81}$$

The relativistic contribution of the linear terms in the quadrupole moment P_2 is again negative for oblate sources. The quadratic terms furnish a negative contribution to the precession shift regardless of whether the source is oblate or prolate, whereas the classical quadratic correction is positive, as it was shown previously,

$$\Delta_4=\frac{24\,P_0^3P_2}{l^6}+\frac{2799\,P_0^5P_2}{14\,l^8}+\left(-24\,P_0^4P_2^2+\frac{12396\,P_0^7P_2}{7}\right)l^{-10}$$
$$+\left(-\frac{327223\,P_0^6P_2^2}{308}+\frac{361993\,P_0^9P_2}{22}\right)l^{-12}. \tag{82}$$

As it happened with the perihelion precession, the rotational octupole term has the opposite sign to the one of the linear dipole term and of course it is dependent on the direction in which the probe orbits,

$$\Delta_8=\frac{12\,iP_0^3P_3}{l^7}+\frac{156\,iP_0^5P_3}{l^9}+\frac{3387\,iP_0^7P_3}{2\,l^{11}}+\frac{17707\,iP_0^9P_3}{l^{13}}. \tag{83}$$

The relativistic sedecimpole term bears the same sign as its classical counterpart, although it is much smaller in magnitude. There is no relativistic term in P_6, just the classical term which has already been described,

$$\Delta_{16}=-\frac{120\,P_0^5P_4}{l^{10}}-\frac{2905\,P_0^7P_4}{2\,l^{12}}, \tag{84}$$

and again we have another permutation of sign; the term in P_5 bears the same sign as the linear dipole term,

$$\Delta_{32}=-\frac{45\,iP_0^5P_5}{2\,l^{11}}-\frac{1905\,iP_0^7P_5}{4\,l^{13}}. \tag{85}$$

Now we discuss the coupling terms between multipole moments other than the mass. The bilinear coupling between the dipole and the quadrupole moment is positive for oblate gravitational sources which rotate in the same direction as the test particle. The quadratic term in P_1 is negative for oblate objects no matter in which direction they rotate. The quadratic term in P_2 is positive when the angular momenta J and l are parallel,

$$\Delta_{2\times 4}=\frac{18\,iP_0^2P_1\,P_2}{l^7}+\frac{441\,iP_0^4P_1\,P_2}{l^9}-\frac{273\,P_0^3P_1^2P_2}{l^{10}}$$
$$+\left(-\frac{81\,iP_0^3P_1\,P_2^2}{2}+\frac{198369\,iP_0^6P_1\,P_2}{28}\right)l^{-11}-\frac{3007003\,P_0^5P_1^2P_2}{308\,l^{12}}$$
$$+\left(-\frac{10899iP_0^5P_1P_2^2}{4}-4482iP_0^4P_1^3P_2+\frac{5509583iP_0^8P_1P_2}{56}\right)l^{-13}. \tag{86}$$

The rotational bilinear coupling between the dipole and the octupole moment is independent of the direction of rotation and it is positive when $J=-i\,P_1$ and $J_3=-i\,P_3$ have the same sign. There is however a higher coupling which is quadratic in the dipole moment and contributes in the same way as does Δ_8

$$\Delta_{2\times 8}=-\frac{186\,P_0^4P_1\,P_3}{l^{10}}-\frac{100201\,P_0^6P_1\,P_3}{22\,l^{12}}-\frac{3168iP_0^5P_1^2P_3}{l^{13}}. \tag{87}$$

The last terms to be considered up to this order are the couplings between P_1 and P_4 and between P_2 and P_3, which are both sensitive to the relative directions of rotation of the source and the probe particle,

$$\Delta_{2\times 16}=-\frac{255\,iP_0^4P_1\,P_4}{2\,l^{11}}-\frac{14193\,iP_0^6P_1\,P_4}{4\,l^{13}}, \tag{88}$$

$$\Delta_{4\times 8}=-\frac{21\,iP_0^4P_2\,P_3}{l^{11}}-\frac{1971\,iP_0^6P_2\,P_3}{2\,l^{13}}. \tag{89}$$

V. CONCLUSIONS

In this paper we have displayed the approximate general asymptotically flat stationary axisymmetric metric for the vacuum spacetime surrounding a compact source possessing a symmetry plane orthogonal to the symmetry axis. The calculations have been carried out for the Ernst potential up to the term in r^{-7} in the pseudospherical radial coordinate. This has been useful to calculate relativistic corrections to the classical orbits around a compact mass distribution. In particular the perihelion precession on the symmetry plane and the precession of the nodes of a slightly tilted circular orbit have been calculated.

Concerning the perihelion shift, it has been shown that the contributions of each gravitational and rotational multipole moment follow a curious pattern of alternation of signs: The term in the mass monopole is always positive, whereas the linear quadrupole term is negative for positive P_2 (the quadratic term in P_2 is always positive) and the sedecimpole term is again positive for positive P_4. The sexagintaquattuorpole P_6 is outside the limits of our perturbative expansion. If we think for instance of an oblate source which is very close to a classical axisymmetric homogeneous ellipsoid, then we would also have alternating signs in the gravitational multipole expansion ($P_{2\,n}=3\,P_0(c^2-a^2)^n/[(2\,n+1)(2\,n+3)]$), c and a being the lengths of the ellipsoid's semiaxis parallel and orthogonal to the symmetry axis, respectively) and every term would have a positive contribution. The linear and cubic rotational dipole term is always positive for counterrotating configurations of the source and the probe (the quadratic contribution is always positive regardless of the relative rotation) whereas the octupole term is positive if $J_3=-i\,P_3$ and l bear the same sign. The trigintaduopole term has the same sign as the dipole term. It should be pointed out that the energy-dependent terms are not strong enough to affect these signs. The coupling between different multipoles preserves the sign of the product of the corresponding linear terms, that is, if there is a P_n-P_m coupling, then its sign is obtained from the product of the -1 factors multiplying the corresponding linear terms in P_n and P_m. No coupling between mass multipole

moments of order higher than the monopole appears to this order except for self-couplings. The sign-independent terms, such as the mass monopole term and the quadratic dipole and quadratic quadrupole terms, always give rise to a perihelion advance.

The influence of the different multipole moments on the precession of the line of nodes of a particle departing by a small amount from the equatorial plane is somewhat different from the behavior which has been shown for the perihelion precession: The alternating pattern of the signs of the linear terms in the multipole moments other than the mass is preserved both for gravitational and rotational moments independently up to the considered perturbation order: If the P_{2n} were all positive, then the contribution of each P_{2n} would be opposite to the one of P_{2n+2} and a similar reasoning is valid for the rotational terms. However the relativistic coupling terms bear the opposite sign to the one which would be expected from the product of the -1 factors before the corresponding linear terms: For instance, if the P_1 and P_2 linear terms are positive then the corresponding bilinear coupling is negative. On the other hand, this rule is not valid for the Newtonian self-couplings. Another difference arises from the fact that the gravitational sexagintaduopole moment P_6 does influence the precession of the line of nodes in this order of perturbation, whereas it does not affect the perihelion precession. Also, there were no couplings between the gravitational moments (self-couplings and mass-couplings excluded) in the perihelion precession, but there is one (the classical P_2-P_4-coupling) in the node precession. It is curious that, while the Newtonian sign-independent terms are always positive, the relativistic ones (the quadratic dipole and the quadratic quadrupole self-couplings) are negative.

Of course most of these corrections are meaningless for astronomical purposes in our solar system, but are very likely to be relevant for highly relativistic astrophysical objects, suchs as pulsars and blackholes, where other post-Newtonian effects[5] have been shown to be present.

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APPENDIX A: SCHWARSCHILD SPACE–TIME

In this appendix we shall study the range of applicability of the perturbation expansion for bounded orbits in Schwarschild's space–time. For this metric the geodesic equation (38) can be solved exactly in terms of elliptic functions. Instead of writing it as a differential equation for u as a function of ϕ, we are writing it as a differential equation for ϕ. In this section u is no longer the inverse of the pseudospherical radius but of the usual Boyer–Lindquist radius,

$$\phi_u=\left(2P_0u^3-u^2+\frac{2P_0}{l^2}u+\frac{E^2-1}{l^2}\right)^{-1/2}=g(u)^{-1/2}. \tag{A1}$$

We are considering that $E<1$ and therefore $g(u)$ has at least one zero. For bounded motion we need three zeros so that the orbit ranges between the apsidal points. If we call these zeros $a\geqslant b\geqslant c\geqslant 0$, then Eq. (A1) can be integrated[11] in terms of the elliptic integral of the first kind, $F(\gamma,q)$, in the region $b\geqslant u>c$,

$$(\phi-\phi_0)\sqrt{\frac{P_0(a-c)}{2}}=F(\gamma,q)=\int_0^{\gamma}d\alpha(1-q^2\sin^2\alpha)^{-1/2}, \tag{A2}$$

$$\gamma=\arcsin\sqrt{\frac{u-c}{b-c}},\quad q=\sqrt{\frac{b-c}{a-c}}. \tag{A3}$$

An expression for u in terms of ϕ is easily obtained taking into account that the elliptic sine is the sine of $F(\gamma,q)$,

$$u=c+(b-c)sn^2\left\{\sqrt{\frac{P_0(a-c)}{2}}(\phi-\phi_0)\right\}. \tag{A4}$$

Since the real period of the elliptic sine is $4K(q)=4F(\pi/2,q)$, then our u function is $2K(q)$-periodic. Therefore the exact perihelion precession of the orbit of a test particle around a spherical nonrotating compact object will be

$$\Delta\phi=\frac{2\sqrt{2}K(q)}{\sqrt{P_0(a-c)}}-2\pi, \tag{A5}$$

the perturbation expansion of which in ϵ coincides with the one of Δ_1 in Eq. (59), as it was to be expected,

$$K(q)=\frac{\pi}{2}\left\{1+\sum_{n=1}^{\infty}\left(\frac{(2n-1)!!}{2^n n!}\right)^2 q^{2n}\right\}. \tag{A6}$$

The limits of the range of applicability of the previous expansion are $q=1$ $(a=b)$ and $q=0$ $(b=c)$. For both values, there are two zeros of $g(u)$ which coalesce and the bounded motion is no longer stable. Therefore we are led to study the range of parameters for which $g(u)$ has double roots. This happens when u takes either of the values $u_\pm$ which are solutions of $g'(u)=0$,

$$u_\pm=\frac{1\pm\sqrt{1-12\epsilon^2}}{6P_0}, \tag{A7}$$

and therefore the allowed region is the one enclosed between the curves $g(u_\pm)=0$ in the E^2-q^2 parameter plane. This yields critical values for the energy per unit of mass, $E_c^2=8/9$, and the perturbation parameter, $\epsilon_c^2=1/12$. The perturbative approach is no longer valid beyond this point in the parameter plane since there are no stable bounded orbits. It is remarkable that for $\epsilon^2>1/16$ there is not only a lower limit for the energy of the bounded orbit but also an upper limit.

APPENDIX B: CLASSICAL PRECESSION OF THE LINE OF NODES

In this appendix we shall briefly derive the classical expression for the precession of the line of nodes.

The Lagrangian for the motion of a particle in a gravitational field is

$$L=\tfrac{1}{2}\dot{r}^2+\tfrac{1}{2}r^2\dot{\theta}^2+\tfrac{1}{2}r^2\sin^2\theta\dot{\phi}^2-V(r,\theta), \tag{B1}$$

$$V(r,\theta)=-\sum_{n=0}^{\infty}\frac{P_n p_n(\cos\theta)}{r^{n+1}}. \tag{B2}$$

The equations of motion and conserved quantities which can be obtained from this Lagrangian are

$$E=\tfrac{1}{2}\dot{r}^2+\tfrac{1}{2}r^2\dot{\theta}^2+\tfrac{1}{2}r^2\sin^2\theta\dot{\phi}^2+V(r,\theta), \tag{B3}$$

$$l=r^2\sin^2\theta\dot{\phi}, \tag{B4}$$

$$\ddot{r}=r\dot{\theta}^2+r\sin^2\theta\dot{\phi}^2-\partial_r V(r,\theta), \tag{B5}$$

$$r^2\ddot{\theta}+2r\dot{r}\dot{\theta}=r^2\sin\theta\cos\theta\dot{\phi}^2-\partial_\theta V(r,\theta). \tag{B6}$$

Truncating the Legendre expansion at the sexagintaquattuorpole multipole moment, P_6, we get the following expressions for the energy per unit of mass, E, and the radius, R, of a circular orbit on the plane $\theta=\pi/2$ in the far field region,

$$E=-\frac{P_0^2}{2\,l^2}+\frac{P_0^3\,P_2}{2\,l^6}-\frac{3\,P_0^5\,P_4+9\,P_0^4\,P_2^2}{8\,l^{10}}+O(l^{-14}), \tag{B7}$$

$$R^{-1}=\frac{P_0}{l^2}-\frac{3\,P_0^2\,P_2}{2\,l^6}+\frac{15\,P_0^4\,P_4+36\,P_0^3\,P_2^2}{8\,l^{10}}+O(l^{-14}). \tag{B8}$$

In order to obtain the oscillations about the equatorial plane of a slightly tilted bounded trajectory with respect to the circular orbit, we introduce a small variation in equation (B6). The result will be divided by $\dot{\phi}^2$ to yield the evolution of $\delta\theta$ as a function of ϕ,

$$(\delta\theta)_{\phi\phi}=-\Omega^2\,\delta\theta,\quad \Omega=\sqrt{1+\frac{R^2}{l^2}V_{\theta\theta}(R,\pi/2)}. \tag{B9}$$

From this expression we get the frequency of the oscillations, Ω, which can be written in terms of l and the multipole moments by inserting equation (B8) into it,

$$\Delta\phi=2\,\pi\left(\frac{1}{\Omega}-1\right)=\frac{3\,\pi\,P_0\,P_2}{l^4}+\frac{\pi\,(9\,P_0^2\,P_2^2-30\,P_0^3\,P_4)}{4\,l^8}$$
$$+\frac{\pi\,(105\,P_0^5\,P_6+45\,P_0^4\,P_2\,P_4+81\,P_0^3\,P_2^3)}{8\,l^{12}}+O(l^{-16}), \tag{B10}$$

which obviously coincides with the term Δ_0 which was calculated using the full relativistic theory in Sec. IV.

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Acoustics of early universe—Lifshitz versus gauge-invariant theories

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Appealing to classical methods of order reduction, we reduce the Lifshitz system to a second order differential equation. We demonstrate its equivalence to well known gauge-invariant results. For a radiation dominated universe we express the metric and density corrections in their exact forms and discuss their acoustic character. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1335557]

I. INTRODUCTION

The density perturbations affect the microwave background temperature. The theory of gravitational instability describes how these inhomogeneities propagate throughout the radiational era, and foresee the temperature image they ''paint'' on the last scattering surface. Classical perturbation theory formulated half a century ago by Lifshitz and Khalatnikov[1–3] has nowadays been replaced by more appropriate gauge-invariant descriptions.[4–11] These formalisms introduce some new measures of inhomogeneity. They do not appeal to the metric tensor, so they easily avoid spurious perturbations arising from an inappropriate choice of the equal time hypersurfaces. They guarantee that the space structures they describe are real physical objects.

On the other hand, the interpretation of the microwave background temperature fluctuations[12] is based on the Sach–Wolfe effect, where the metric corrections play a key role.[13] Therefore, data obtained from COBE is mostly referred to as the classical concepts of Lifshitz and Khalatnikov, and only in a minor part to gauge-invariant measures, which are more precise but difficult to observe.[14] Both theories in their original formulations differ essentially. Lifshitz theory provides the two parameter family of increasing solutions for the density contrast [Ref. 3, formula (115.19)], while all the gauge-invariant approaches foresee in concert only a single growing density mode. Thus the interpretation of the microwave temperature map as the initial data for cosmic structure formation is fairly ambiguous.

In this paper we attempt to reconcile both types of theories. We appeal to simple and classical methods of order reduction of differential equations.[15] By use of these techniques we remove the pure-gauge perturbations from Lifshitz theory in the radiation dominated universe. In consequence we reduce the Lifshitz system to a second order differential equation, exactly the same as obtained earlier on the ground of gauge-invariant formalisms. Applying well known solutions, we express corrections to the metric tensor, the density contrast and the peculiar velocity in exact form. We show that in the early universe, scalar perturbations of any length-scale form acoustic waves propagating with the velocity $1/\sqrt{3}$.

II. ORDER REDUCTION

[Most of the calculations in this paper have been done by use of MATHEMATICA (Wolfram Research Inc. Version 3.0). Appropriate notebooks are available from the authors (golda@oa.uj.edu.pl) on request.]

Relativistic perturbations of a Friedman universe, described in synchronous coordinates[1–3] form a system of two second order differential equations with variable coefficients. In contrast, the similar Newtonian problem is expressed by only one second order equation.[16–18] Obviously, the

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two additional degrees of freedom appearing in the relativistic case must correspond to pure coordinate transformations (gauge freedom),[2] and should be removed from the theory.

Removing pure-gauge modes we reduce the Lifshitz equations with pressure $p=\rho/3$ to Bessel equation. The procedure is as follows: (1) we raise the equations order to fourth, in order to separate the $\mu_n(\eta)$ and $\lambda_n(\eta)$ coefficients, and then (2) we reduce the order of each of the separated equations back by eliminating gauge degrees of freedom. The resulting equations have exact solutions in the form of Hankel functions $H_{3/2}$ and their integrals.

In the synchronous system of reference, the metric corrections $h_{\mu\nu}$ $(\mu,\nu=1,2,3)$ to the homogeneous and isotropic, spatially flat universe fulfill the partial differential equations[3] $(8\pi G=c=1)$,

$$h_\alpha^{\beta\prime\prime}+2\frac{a'}{a}h_\alpha^{\beta\prime}+(h^{\gamma;\beta}_{\alpha;\gamma}+h^{\beta;\gamma}_{\gamma;\alpha}-h^{;\beta}_{;\alpha}-h^{\beta;\gamma}_{\alpha;\gamma})=0, \tag{2.1}$$

$$2\left[1+3\frac{dp}{d\rho}\right]^{-1}\left(h''+\frac{a'}{a}\left[2+3\frac{dp}{d\rho}\right]h'\right)+(h^{\delta;\gamma}_{\gamma;\delta}-h^{;\gamma}_{;\gamma})=0. \tag{2.2}$$

These equations are usually solved by means of the Fourier transform,

$$h_{\mu\nu}=\int \mathcal{A}(\mathbf{n})\left[\lambda_n(\eta)\left(\frac{\delta_{\mu\nu}}{3}-\frac{n_\mu n_\nu}{n^2}\right)+\frac{1}{3}\mu_n(\eta)\delta_{\mu\nu}\right]e^{i\mathbf{n}\cdot\mathbf{x}}d^3\mathbf{n}+\text{c.c.} \tag{2.3}$$

The Fourier transform (2.3) is defined for absolute integrable functions (the case of least interest for cosmology), for nonintegrable functions in the framework of distribution theory, or can be understood as a stochastic integral if the initial conditions are given at random.[19,20] When the barotropic fluid $(p/\rho=\delta p/\delta\rho=w=\text{const})$ is the matter content of the universe, the functions $\lambda_n(\eta)$ and $\mu_n(\eta)$ obey ordinary, second order equations,

$$-n^2w(\lambda_n(\eta)+\mu_n(\eta))+2\frac{a'(\eta)}{a(\eta)}\lambda_n'(\eta)+\lambda_n''(\eta)=0, \tag{2.4}$$

$$-n^2w(1+3w)(\lambda_n(\eta)+\mu_n(\eta))+(2+3w)\frac{a'(\eta)}{a(\eta)}\mu_n'(\eta)+\mu_n''(\eta)=0, \tag{2.5}$$

where a prime denotes differentiation with respect to the conformal time η and a is the scale factor for the background metric tensor. In order to separate the variable $\lambda_n(\eta)$, we differentiate (2.4) twice and eliminate terms containing $\mu_n(\eta)$ or its derivatives by the help of Eq. (2.5). We obtain the fourth-order differential equation,

$$\begin{aligned}&\left(n^2w\frac{a'(\eta)}{a(\eta)}-6w\left(\frac{a'(\eta)}{a(\eta)}\right)^3+2(-1+3w)\frac{a'(\eta)}{a(\eta)}\frac{a''(\eta)}{a(\eta)}+2\frac{a^{(3)}(\eta)}{a(\eta)}\right)\lambda_n'(\eta)\\&\quad+\left(n^2w+6w\left(\frac{a'(\eta)}{a(\eta)}\right)^2+4\frac{a''(\eta)}{a(\eta)}\right)\lambda_n''(\eta)+(4+3w)\frac{a'(\eta)}{a(\eta)}\lambda_n^{(3)}(\eta)+\lambda_n^{(4)}(\eta)=0.\end{aligned} \tag{2.6}$$

In the same way one can treat (2.5) to find the equation for $\mu_n(\eta)$,

$$\begin{aligned}&\left(n^2w\frac{a'(\eta)}{a(\eta)}-(2+3w)\frac{a'(\eta)}{a(\eta)}\frac{a''(\eta)}{a(\eta)}+(2+3w)\frac{a^{(3)}(\eta)}{a(\eta)}\right)\mu_n(\eta)\\&\quad+\left(n^2w+2(2+3w)\frac{a''(\eta)}{a(\eta)}\right)\mu_n''(\eta)+(4+3w)\frac{a'(\eta)}{a(\eta)}\mu_n^{(3)}(\eta)+\mu_n^{(4)}(\eta)=0.\end{aligned} \tag{2.7}$$

In the following part of this paper we restrict ourselves to a universe filled with relativistic particles, where both $w=p_0/\rho_0=\frac{1}{3}$ and $\mathcal{M}=\rho_0 a^4$ are constants of motion, and the scale factor a is a linear function of the conformal time $a(\eta)=\sqrt{\mathcal{M}/3}\,\eta$. In the flat universe the expansion rate $\theta(\eta)=3a'(\eta)/a(\eta)^2$ and the energy density $\rho_0(\eta)$ relate to each other by $\rho_0(\eta)=\theta(\eta)^2/3$, so the equations for $\lambda_n(\eta)$ and $\mu_n(\eta)$ take fairly legible form, both prior to

$$-\frac{1}{3}n^2(\lambda_n(\eta)+\mu_n(\eta))+\frac{2}{\eta}\lambda_n'(\eta)+\lambda_n''(\eta)=0, \tag{2.8}$$

$$\frac{2}{3}n^2(\lambda_n(\eta)+\mu_n(\eta))+\frac{3}{\eta}\mu_n'(\eta)+\mu_n''(\eta)=0, \tag{2.9}$$

and after separation,

$$\left(\frac{n^2}{3\eta}-\frac{2}{\eta^3}\right)\lambda_n'(\eta)+\left(\frac{n^2}{3}+\frac{2}{\eta^2}\right)\lambda_n(\eta)+\frac{5}{\eta}\lambda_n^{(3)}(\eta)+\lambda_n^{(4)}(\eta)=0, \tag{2.10}$$

$$\frac{n^2}{3\eta}\mu_n'(\eta)+\frac{n^2}{3}\mu_n''(\eta)+\frac{5}{\eta}\mu_n^3(\eta)+\mu_n^{(4)}(\eta)=0. \tag{2.11}$$

We start with Eq. (2.10). The two well known gauge solutions[1] are (with the accuracy to multiplicative constants)

$$f_1(\eta)=1, \tag{2.12}$$

$$f_2(\eta)=-\sqrt{\mathcal{M}/3}\int\frac{1}{a(\eta)}\,d\eta=-\ln(\eta). \tag{2.13}$$

We expect to obtain solutions for (2.10) in the form[15]

$$\lambda_n(\eta)=f_1(\eta)\left(\int A(\eta)\,d\eta\right), \tag{2.14}$$

$$A(\eta)=\frac{d}{d\eta}\left(\frac{f_2(\eta)}{f_1(\eta)}\right)\left(\int\frac{B(\eta)}{\eta}\,d\eta\right), \tag{2.15}$$

where $A(\eta)$ and $B(\eta)$ are some auxiliary functions. Inserting (2.14)–(2.15) into (2.10) we obtain the Bessel equation in its canonical form,

$$\left(\frac{n^2}{3}-\frac{2}{\eta^2}\right)B(\eta)+B''(\eta)=0. \tag{2.16}$$

Equation (2.16) is already free of gauge modes, as one can see from simple heuristic considerations. Let us assume that there exist a third linearly independent solution of Eq. (2.4), which corresponds to a pure coordinate transformation. Then, the linear space of gauge modes would be 3-dimensional, leaving only a single degree of freedom for the real, physical perturbations. Such a theory has no proper Newtonian limit.

Equation (2.16) is identical to the Sakai equation [Ref. 21 formula (5.1)], the equation for density perturbations in an orthogonal gauge [Ref. 5, formula (4.9), Ref. 8, formulas (16)–(17)], the equation for gauge-invariant density gradients [Ref. 9, formula (38)] or Laplacians [Ref. 4, formulas (8)–(9), Ref. 11, formula (22)] after transforming these equations to their canonical form (see Ref. 22). It is interesting to note that Eq. (2.16) is also identical to the propagation equation for gravitational waves[23,24] (except for gravitational waves moving with the speed of light). This means that the solutions to Eq. (2.16) represent waves traveling with the phase velocity $1/\sqrt{3}$ (we

show this explicitly in the next section). This picture also is consistent with the phonon approach,[25] as the transformation $\phi(\eta)=B(\eta)/\eta+B'(\eta)$ to the Field–Shepley variable[26,27] reduces (2.16) to the harmonic oscillator $\phi''(\eta)+(n^2/3)\,\phi(\eta)=0$. (The procedure we present here may also be treated as a method to reconstruct metric corrections and hydrodynamic quantities in their explicit form, out of the Field and Shepley variables.)

III. SOLUTIONS

The general solution for (2.16) is a combination of

$$B(\eta)=e^{-i\omega\eta}\left(1+\frac{1}{i\omega\eta}\right), \tag{3.1}$$

and its complex conjugate, with the frequency $\omega=n/\sqrt{3}$. (For similar solutions in the gravitational waves theory see Ref. 24.) These solutions are proportional to Hankel functions $H_{3/2}$, but more frequently are presented as a combination of Bessel and Neumann functions $B=a_1J+a_2N$.[5] Performing integrations (2.14)–(2.15) we determine the solution for $\lambda_n(\eta)$ and find the correction $\mu_n(\eta)$ by solving Eq. (2.4) algebraically,

$$\lambda(\omega\eta)=-\frac{e^{-i\omega\eta}}{i\omega\eta}-\mathrm{Ei}(-i\omega\eta), \tag{3.2}$$

$$\mu(\omega\eta)=\left(1+\frac{1}{i\omega\eta}\right)\frac{e^{-i\omega\eta}}{i\omega\eta}+\mathrm{Ei}(-i\omega\eta). \tag{3.3}$$

Obviously, Eq. (2.11) is automatically fulfilled. As a result we obtain the metric corrections $h_{\mu\nu}$ expanded into planar waves with the frequency constant in conformal time η and with varying amplitude,

$$\begin{aligned} h_{\mu\nu}=&-\int \mathcal{A}(\mathbf{n})\left(\frac{\delta_{\mu\nu}}{3}-\frac{n_\mu n_\nu}{n^2}\right)\left(\frac{e^{i(\mathbf{n}\cdot\mathbf{x}-\omega\eta)}}{i\omega\eta}+e^{i\mathbf{n}\cdot\mathbf{x}}\,\mathrm{Ei}(-i\omega\eta)\right)d^3\mathbf{n}\\ &+\int \mathcal{A}(\mathbf{n})\frac{\delta_{\mu\nu}}{3}\left(\left(1+\frac{1}{i\omega\eta}\right)\frac{e^{i(\mathbf{n}\cdot\mathbf{x}-\omega\eta)}}{i\omega\eta}+e^{i\mathbf{n}\cdot\mathbf{x}}\,\mathrm{Ei}(-i\omega\eta)\right)d^3\mathbf{n}+\mathrm{c.c.} \end{aligned} \tag{3.4}$$

The density perturbation and peculiar velocity can be inferred from formulas (8.2)–(8.3) of Ref. 2 and expressed as

$$\frac{\delta\rho}{\rho}=\int \mathcal{A}(\mathbf{n})u_\rho(\mathbf{n}\cdot\mathbf{x},\omega\eta)d^3\mathbf{n}+\mathrm{c.c.}, \tag{3.5}$$

$$\delta v=\int \mathcal{A}(\mathbf{n})u_v(\mathbf{n}\cdot\mathbf{x},\omega\eta)d^3\mathbf{n}+\mathrm{c.c.}, \tag{3.6}$$

where the Fourier modes form traveling waves,

$$u_\rho(\mathbf{n}\cdot\mathbf{x},\omega\eta)=\frac{2}{3}\left(1+\frac{1}{i\omega\eta}+\frac{i\omega\eta}{2}\right)\frac{e^{i(\mathbf{n}\cdot\mathbf{x}-\omega\eta)}}{i\omega\eta}, \tag{3.7}$$

$$u_v(\mathbf{n}\cdot\mathbf{x},\omega\eta)=\frac{1}{2\sqrt{3}}\left(1+\frac{i\omega\eta}{2}\right)\frac{e^{i(\mathbf{n}\cdot\mathbf{x}-\omega\eta)}}{i\omega\eta}. \tag{3.8}$$

A generic scalar perturbation in the early universe is a superposition of acoustic waves. Its amplitude decreases to reach a constant and positive value at late times. This decrease is substan-

tial in the low frequency (early times) limit $\omega\eta \ll 1$. Solutions are formally divergent at $\eta=0$, nevertheless evaluating the cosmic structure backward in time beyond its stochastic initiation η_i has no well defined physical sense.

The only perturbations, which are regular at $\eta=0$, and growing near the initial singularity, consist of standing waves $u(\mathbf{n}\cdot\mathbf{x},\omega\eta)+u(-\mathbf{n}\cdot\mathbf{x},\omega\eta)$ (compare Ref. 21, 28, 29 or similar effect in the gravitational waves theory[23]). They form a one-parameter family in the 2-parameter space of all solutions, so they are nongeneric. This property has been confirmed by use of other techniques in the gauge-invariant theories.[30] In the stochastic approach nongeneric solutions are of marginal interest since they contribute with the zero probability measure.

IV. SUMMARY AND CONCLUSIONS

It is a matter of dispute whether cosmic structure was created solely by gravity forces[1] or initiated by other, nongravitational phenomena manifesting themselves as stochastic processes[19,20] in some early epochs. For the first hypothesis regular and growing solutions are indispensable, while in the second one the generic perturbations play a key role. In a radiation dominated universe these properties exclude each other.

Lifshitz theory and the gauge-invariant theories differ less than usually expected. Both types of theories, when properly written, lead to the same perturbation equation of the wave-equation form. Generic scalar perturbations are superpositions of acoustic waves. Solutions depend on the product $n\eta$ (equivalently on $\omega\eta$). Everything which concerns early epochs refers also to long waves, and *vice versa*. (This is a peculiar property of the spatially flat radiation-filled universe.) The perturbation scale does not divide solutions into different classes. Perturbations propagate with the same speed $1/\sqrt{3}$, which does not depend on the wave vector. This confirms the wave nature of scalar perturbations in the radiation dominated universe (an important property already pointed out by Lukash,[25] but hardly discussed elsewhere) and compels one to use the complete metric corrections (3.4) in the Sachs–Wolfe procedure (not only the nongeneric growing solutions) at the end of the radiational era.

The reduction technique we apply in this paper can be used for other equations of state. For $p/\rho=\text{const}\neq 1/3$ solutions can be expressed in terms of hypergeometric functions. In other cases solutions may not reduce to any known elementary or special functions, although the reduced equation (2.16) can be always found.

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APPENDIX A: LIFSHITZ ''SYNCHRONOUS'' GAUGE

The original Lifshitz approach[1–3] provides solutions which are different from (3.2)–(3.3), and also inconsistent with the gauge-invariant theories. To explain these differences in detail, we appeal to the complete solution to (2.10)–(2.11) containing both physical and spurious inhomogeneities. All the gauge freedom within the synchronous system is limited to the choice of the integral constants in (2.15). Actually each of these ''constants'' can be defined as an arbitrary function of the wave number $\mathbf{n}$ (equivalently ω). We write them explicitly as $\mathcal{A}(\mathbf{n})$ and $\mathcal{G}(\mathbf{n})$ satisfying

$$\lambda(\omega\eta)=f_1(\eta)\left(\mathcal{A}(\mathbf{n})\int A(\eta)\,d\eta-\mathcal{G}(\mathbf{n})\ln(i\omega)\right), \tag{A1}$$

$$A(\eta)=\frac{d}{d\eta}\left(\frac{f_2(\eta)}{f_1(\eta)}\right)\left(\int\frac{B(\eta)}{\eta}d\eta+\frac{\mathcal{G}(\mathbf{n})}{\mathcal{A}(\mathbf{n})}\right), \tag{A2}$$

so they are equal to the Fourier coefficients in the integral,

$$h_{\mu\nu}=\int \mathcal{A}(\mathbf{n})\left(\frac{n_\mu n_\nu}{n^2}-\frac{\delta_{\mu\nu}}{3}\right)\left(\frac{e^{i(\mathbf{n}\cdot\mathbf{x}-\omega\eta)}}{i\omega\eta}+e^{i\mathbf{n}\cdot\mathbf{x}}\,\mathrm{Ei}(-i\omega\eta)\right)d^3\mathbf{n}$$
$$+\int \mathcal{A}(\mathbf{n})\frac{\delta_{\mu\nu}}{3}\left[\left(1+\frac{1}{i\omega\eta}\right)\frac{e^{i(\mathbf{n}\cdot\mathbf{x}-\omega\eta)}}{i\omega\eta}+e^{i\mathbf{n}\cdot\mathbf{x}}\,\mathrm{Ei}(-i\omega\eta)\right]d^3\mathbf{n}$$
$$+\int \mathcal{G}(\mathbf{n})\left[\left(\frac{n_\mu n_\nu}{n^2}-\frac{\delta_{\mu\nu}}{3}\right)\ln(i\omega\eta)+\frac{\delta_{\mu\nu}}{3}\left(\ln(i\omega\eta)-\frac{1}{\omega^2\eta^2}\right)\right]e^{i\mathbf{n}\cdot\mathbf{x}}\,d^3\mathbf{n}+\text{c.c.} \quad \text{(A3)}$$

Each coefficient $\mathcal{A}(\mathbf{n})$, $\mathcal{G}(\mathbf{n})$, can be defined independently. The gauge freedom is carried by $\mathcal{G}(\mathbf{n})$ which follows directly from (2.13). Also knowing the gauge-invariant methods one can *a posteriori* check that $\mathcal{A}(\mathbf{n})$ affects the gauge-invariant inhomogeneity measures, while $\mathcal{G}(\mathbf{n})$ does not. Now, the density contrast and the peculiar velocity, as inferred from formulas (8.2)–(8.3) of Ref. 2,

$$\frac{\delta\rho}{\rho}=\int\left[\mathcal{A}(\mathbf{n})u_\rho(\mathbf{n}\cdot\mathbf{x},\omega\eta)+\mathcal{G}(\mathbf{n})\tilde{u}_\rho(\mathbf{n}\cdot\mathbf{x},\omega\eta)\right]d^3\mathbf{n}+\text{c.c.}, \quad \text{(A4)}$$

$$\delta v=\int\left[\mathcal{A}(\mathbf{n})u_v(\mathbf{n}\cdot\mathbf{x},\omega\eta)+\mathcal{G}(\mathbf{n})\tilde{u}_v(\mathbf{n}\cdot\mathbf{x},\omega\eta)\right]d^3\mathbf{n}+\text{c.c.}, \quad \text{(A5)}$$

consists of the physical modes u_ρ, u_v already found in (3.7)–(3.8) and the pure-gauge modes equal to

$$\tilde{u}_\rho(\mathbf{n}\cdot\mathbf{x},\omega\eta)=\frac{2}{3}\frac{1}{\omega^2\eta^2}e^{i\mathbf{n}\cdot\mathbf{x}}, \quad \text{(A6)}$$

$$\tilde{u}_v(\mathbf{n}\cdot\mathbf{x},\omega\eta)=\frac{i}{2\sqrt{3}}\frac{1}{\omega\eta}e^{i\mathbf{n}\cdot\mathbf{x}}. \quad \text{(A7)}$$

We expand integrals (A4) and (A5) in the early times limit (with the accuracy to η^2), to obtain

$$\frac{\delta\rho}{\rho}=\int\left[\frac{2}{3}\frac{\mathcal{A}(\mathbf{n})+\mathcal{G}(\mathbf{n})}{\omega^2\eta^2}+\left(\frac{1}{9}i\omega\eta+\frac{1}{12}\omega^2\eta^2\right)\mathcal{A}(\mathbf{n})\right]e^{i\mathbf{n}\cdot\mathbf{x}}d^3\mathbf{n}+\text{c.c.}, \quad \text{(A8)}$$

$$\delta v=\frac{1}{2\sqrt{3}}\int\left[\frac{\mathcal{A}(\mathbf{n})+\mathcal{G}(\mathbf{n})}{i\omega\eta}+\frac{1}{2}\mathcal{A}(\mathbf{n})\left(1+\frac{\omega^2\eta^2}{6}\right)\right]e^{i\mathbf{n}\cdot\mathbf{x}}d^3\mathbf{n}+\text{c.c.} \quad \text{(A9)}$$

Both physical and gauge perturbations manifest identical singular behavior at $\eta=0$. Therefore, one cannot distinguish between them solely on the grounds of their asymptotic forms. On the other hand, one is able to regularize perturbations by the gauge choice $\mathcal{G}(\mathbf{n})=-\mathcal{A}(\mathbf{n})$. Then, the equal time hypersurfaces follow the hypersurfaces of equal density at early epochs. This gauge (commonly known as the synchronous gauge) has been actually employed by Lifshitz and Khalatnikov,[1,2] where divergent terms $1/(\omega\eta)^2$ are cancelled by the exactly opposite pure-gauge corrections. (This does not refer to the metric correction where $1/\eta$-divergence is still present.) In consequence, perturbations described there form a mixture of both the physical and the gauge modes.

In the Lifshitz gauge, the mode amplitude $[u_\rho(\mathbf{n}\cdot\mathbf{x},\omega\eta)\overline{u_\rho(\mathbf{n}\cdot\mathbf{x},\omega\eta)}]^{1/2}$ grow with time, therefore, the two independent solutions for the density contrast increase. The same concerns the

peculiar velocity. In the low $\omega\eta$ limit the density contrast and peculiar velocity form the two-parameter linear spaces of growing solutions. As a consequence, a generic inhomogeneity increases, which is in conflict with the gauge-invariant theories.[4,5,9]

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Petrov type *D* Einstein space–times of embedding class two

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A space–time is of embedding class 2 if its curvature tensor can be written in terms of two symmetric tensors $a_{\alpha\beta}$ and $b_{\alpha\beta}$ which satisfy the Gauss, Codazzi, and Ricci equations. For an Einstein space–time the Ricci tensor is proportional to the metric tensor. Using the Petrov classification of the curvature tensor and canonical forms of $a_{\alpha\beta}$ and $b_{\alpha\beta}$, this paper produces a list of the embedding class 2 Petrov type *D* Einstein space–times. After a summary of the basic equations and the previous work on embedding class 2 space–times, the field equations for Einstein space–times are expressed in a canonical form and the type *D* Petrov conditions applied. The resulting equations are solved and give two sets of metrics. The first are known metrics which are products of two 2-spaces of constant curvature and the second set is a generalization of the Kottler solution. The form of the second set of solutions depends upon whether the metric depends upon one or two of the four coordinates.
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I. INTRODUCTION

The local isometric embedding of four-dimensional space–times V_4 into a flat pseudo-Euclidean space E_N of $N \leqslant 10$ dimensions has sometimes been used in general relativity as an alternative to the intrinsic curvilinear coordinates of the V_4.

Various attempts have been made to give a physical meaning to the flat embedding space. These issues are discussed in a seminar held in 1965[1] and in the references of the survey article by Goenner.[2]

In this paper the more pragmatic approach adopted by Kramer *et al.*[3] will be used. The invariance of the embedding class gives a classification scheme for all solutions of Einstein's field equations, but is mathematically different from classifications based on groups of motions or Petrov types and can, therefore, act as a refinement of these schemes and can give more information about known solutions or find new solutions.

This paper extends the results of two previous papers Hodgkinson.[4,5] The embedding equations are solved to find two sets of metric tensors. The first set of solutions contains the known metrics which are products of two 2-spaces of constant curvature called decomposable by Kramer,[3] or reducible by Petrov.[6] The second set is related to the known Kottler solution.

The method used is similar to Hodgkinson,[5] the Einstein field equations are written in terms of the first fundamental forms using the Gauss equation and by considering the Codazzi equations simplified forms of $a_{\alpha\beta}$ and $b_{\alpha\beta}$ are obtained. These specialized $a_{\alpha\beta}$ and $b_{\alpha\beta}$ are then used to create differential equations for the components of the metric tensor which are solved to produce the two sets of metric tensors.

II. CODAZZI AND RICCI EQUATIONS

The Gauss, Codazzi, and Ricci equations provide the necessary and sufficient conditions that space–times can be embedded (locally and isometrically) in a pseudo-Euclidean space. For the case of embedding class 2, the conditions are that there exist two symmetric tensors $a_{\alpha\beta}$ and $b_{\alpha\beta}$ and a vector s_α, which satisfy the following equations of Eisenhart.[7]

Gauss equation,

$$R_{\alpha\beta\gamma\delta}=\epsilon_1(a_{\alpha\gamma}a_{\beta\delta}-a_{\alpha\delta}a_{\beta\gamma})+\epsilon_2(b_{\alpha\gamma}b_{\beta\delta}-b_{\alpha\delta}a_{\beta\gamma}), \tag{1}$$

where $\epsilon_1=\pm 1$ and $\epsilon_2=\pm 1$.

Codazzi equations,

$$a_{\alpha\beta;\gamma}-a_{\alpha\gamma;\beta}=\epsilon_2(-s_\gamma b_{\alpha\beta}+s_\beta b_{\alpha\gamma}), \tag{2}$$

$$b_{\alpha\beta;\gamma}-b_{\alpha\gamma;\beta}=-\epsilon_1(-s_\gamma a_{\alpha\beta}+s_\beta a_{\alpha\gamma}). \tag{3}$$

Ricci equation,

$$s_{\alpha;\beta}-s_{\beta;\alpha}=a_{\alpha\gamma}b^{\gamma}_{\beta}-b_{\alpha\gamma}a^{\gamma}_{\beta}. \tag{4}$$

In a previous paper by Hodgkinson[4] it is shown that, for Petrov type D Weyl tensors, the vector s_α is a gradient and therefore from Eq. (4) the matrices a^{α}_{β} and b^{α}_{β} commute. The tensors $a_{\alpha\beta}$, $b_{\alpha\beta}$, and s_α are not uniquely determined, they are subject to rotations (pseudo-rotations) in the 2-space orthogonal to Riemannian V_4 in the pseudo-Euclidean embedding space E_6. The proof that s_α is a gradient depends upon $R_{\alpha\beta}=0$, but for Einstein spaces with $R_{\alpha\beta}=\Lambda g_{\alpha\beta}$ the proof is very similar and the result is the same and this means that it is possible to make the Ricci vector $s_\alpha=0$ and this condition will be used throughout this paper.

The steps followed are as follows: in Sec. III the solution of the Gauss equations for $\epsilon_1=\epsilon_2$ gives two different cases which produce the two different types of metrics. Section IV uses the Codazzi and Ricci equations to find explicit forms for the metrics. Section IV A gives the metrics for the two 2-spaces of constant curvature and Sec. IV B gives the Kottler-type metrics. Section V considers the analysis when $\epsilon_1=-\epsilon_2$ and finally Sec. VI lists the Petrov type D Einstein space–times of embedding class 2.

Throughout the analysis it is assumed that both a^{α}_{β} and b^{α}_{β} were of maximum rank. Kaigorodov and Yakupov[8] have given a list of the degenerate forms of a^{α}_{β} and b^{α}_{β}. Direct substitution of these forms shows that no new solutions are obtained.

III. THE CASE $\epsilon_1=\epsilon_2$ GAUSS AND FIELD EQUATIONS

The field equations for an Einstein space are

$$R^{\gamma}_{\alpha\gamma\beta}=R_{\alpha\beta}=\Lambda g_{\alpha\beta}, \tag{5}$$

where Λ is a constant and $g_{\alpha\beta}$ is the metric tensor. Letting $\epsilon_1=\epsilon_2=\epsilon$ and substituting for the Ricci tensor gives

$$(a^{\alpha}_{\beta}a^{\beta}_{\gamma}-aa^{\alpha}_{\gamma})+(b^{\alpha}_{\beta}b^{\beta}_{\gamma}-bb^{\alpha}_{\gamma})=-\epsilon\Lambda\,\delta^{\alpha}_{\gamma} \tag{6}$$

where $a=a^{\alpha}_{\alpha}$ and $b=b^{\alpha}_{\alpha}$ and the matrices a^{α}_{β} and b^{α}_{β} are both matrices of Segrè-type [1111] (Hodgkinson[4]). Rewriting Eq. (6) in the form

$$A^2+B^2=(\rho^2-\epsilon\Lambda)I, \tag{7}$$

where

$$A\equiv\left(a^{\alpha}_{\beta}-\frac{a}{2}\delta^{\alpha}_{\beta}\right),\quad B\equiv\left(b^{\alpha}_{\beta}-\frac{b}{2}\delta^{\alpha}_{\beta}\right),\quad I=\delta^{\alpha}_{\beta},\ \text{and}\ \rho^2=\frac{a^2+b^2}{4},$$

a^{α}_{β} and b^{α}_{β} are diagonal matrices and have the following forms (no summation on γ):

$$a^{\gamma}_{\gamma}=\rho\cos(\alpha)+r\cos(\theta_\gamma),\quad b^{\gamma}_{\gamma}=\rho\sin(\alpha)+r\sin(\theta_\gamma),$$

where

$$r^2=\rho^2-\epsilon\Lambda$$

and α, θ_γ are five dependent parameters which satisfy the relationship

$$2\epsilon\Lambda=r^2(\cos(\theta_0-\theta_1)+\cos(\theta_0-\theta_2)+\cos(\theta_0-\theta_3)+\cos(\theta_1-\theta_2)+\cos(\theta_1-\theta_3)+\cos(\theta_2-\theta_3)). \tag{8}$$

The nonzero components of the Weyl tensor $C_{\alpha\beta\gamma\delta}\equiv C_{AB}$ in the Petrov notation are

$$C_{11}=\frac{r^2}{2}(\cos(\theta_0-\theta_1)+\cos(\theta_2-\theta_3))-\frac{\epsilon\Lambda}{3}, \tag{9}$$

$$C_{22}=\frac{r^2}{2}(\cos(\theta_0-\theta_2)+\cos(\theta_1-\theta_3))-\frac{\epsilon\Lambda}{3}, \tag{10}$$

$$C_{33}=\frac{r^2}{2}(\cos(\theta_0-\theta_3)+\cos(\theta_1-\theta_2))-\frac{\epsilon\Lambda}{3}. \tag{11}$$

The Petrov classification requires $C_{11}+C_{22}+C_{33}=0$, but for Petrov type D Weyl tensors we need two of the C_{AA} to be equal, without loss of generality we take $C_{11}=C_{22}$. Then using standard trigonometric identities, Eqs. (9) and (10) give

$$\cos\left(\frac{\theta_0-\theta_1-\theta_2+\theta_3}{2}\right)\sin\left(\frac{\theta_1-\theta_2}{2}\right)\sin\left(\frac{\theta_0-\theta_3}{2}\right)=0. \tag{12}$$

Equation (12) will be satisfied if any of the three factors vanish. The consequences of the vanishing of any of the factors will be considered next and in Secs. IV A and IV B.

Considering the case of $\theta_0-\theta_1-\theta_2+\theta_3=\pi$ gives

$$C_{11}=C_{22}=-\frac{\epsilon\Lambda}{3},\quad C_{33}=\frac{2\epsilon\Lambda}{3}.$$

These solutions require

$$2\Lambda=\epsilon r^2(\cos(\theta_0-\theta_3)+\cos(\theta_1-\theta_2)) \tag{13}$$

in agreement with Eq. (8).

Reverting to the matrices $a_{\alpha\beta}$, $b_{\alpha\beta}$ and letting

$$-\lambda_0=a^0_{\ 0},\quad \lambda_1=a^1_{\ 1},\quad \lambda_2=a^2_{\ 2},\quad \lambda_3=a^3_{\ 3},$$

$$-\mu_0=b^0_{\ 0},\quad \mu_1=b^1_{\ 1},\quad \mu_2=b^2_{\ 2},\quad \mu_3=b^3_{\ 3}$$

with the raising and lowering of a zero index on $a^\alpha_{\ \beta}$ or $b^\alpha_{\ \beta}$ changing the sign, the equations for the curvature tensor with $\epsilon_1=\epsilon_2=\epsilon$ are

$$\lambda_1\lambda_3+\mu_1\mu_3=\lambda_2\lambda_3+\mu_2\mu_3=\lambda_0\lambda_1+\mu_0\mu_1=\lambda_0\lambda_2+\mu_0\mu_2=0, \tag{14}$$

$$\lambda_1\lambda_2+\mu_1\mu_2=-\lambda_0\lambda_3-\mu_0\mu_3=\epsilon\Lambda. \tag{15}$$

Using the Grobner basis algorithm to solve this set of six nonlinear equations in eight unknowns gives essentially two solutions in terms of arbitrary unknowns. For the first let λ_2,μ_2, and μ_3 be arbitrary, the remaining five are

$$\lambda_0=\frac{\mu_2\lambda_2\epsilon\Lambda}{\mu_3((\mu_2)^2+(\lambda_2)^2)},\quad \lambda_1=\frac{\lambda_2\epsilon\Lambda}{(\mu_2)^2+(\lambda_2)^2},\quad \lambda_3=-\frac{\mu_2\mu_3}{\lambda_2},\tag{16}$$

$$\mu_0=-\frac{\epsilon\Lambda(\lambda_2)^2}{\mu_3((\mu_2)^2+(\lambda_2)^2)},\quad \mu_1=\frac{\mu_2\epsilon\Lambda}{(\mu_2)^2+(\lambda_2)^2}.\tag{17}$$

The second set is found with λ_0 and μ_1 arbitrary and

$$\lambda_1=\lambda_2=\mu_0=\mu_3=0,\quad \lambda_3=-\frac{\epsilon\Lambda}{\lambda_0},\quad \mu_2=\frac{\epsilon\Lambda}{\mu_1}.\tag{18}$$

Both solutions can be analyzed in a similar manner, although the functional forms are different the same four metrics are produced. So the analysis will only be given for the first solution.

IV. THE CASE $\epsilon_1=\epsilon_2$ CODAZZI AND RICCI EQUATIONS

A. Case 1. The metrics which are products of constant curvature

For further investigation it is necessary to use the Codazzi equations as in Hodgkinson.[5] This involves writing the $a_{\alpha\beta}$ and $b_{\alpha\beta}$ in terms of four basis vectors which can be proved to be hypersurface orthogonal.

The basis vectors satisfy

$$-u_\alpha u^\alpha=v_\alpha v^\alpha=e_\alpha e^\alpha=f_\alpha f^\alpha=1\tag{19}$$

with all other scalar products zero. This gives

$$a_{\alpha\beta}=\lambda_0 u_\alpha u_\beta+\lambda_1 v_\alpha v_\beta+\lambda_2 e_\alpha e_\beta+\lambda_3 f_\alpha f_\beta,\tag{20}$$

$$b_{\alpha\beta}=\mu_0 u_\alpha u_\beta+\mu_1 v_\alpha v_\beta+\mu_2 e_\alpha e_\beta+\mu_3 f_\alpha f_\beta.\tag{21}$$

The derivatives of the tetrad vectors are

$$u_{\alpha;\beta}=v_\alpha A_\beta+e_\alpha B_\beta+f_\alpha C_\beta,\tag{22}$$

$$v_{\alpha;\beta}=u_\alpha A_\beta+e_\alpha D_\beta+f_\alpha E_\beta,\tag{23}$$

$$e_{\alpha;\beta}=u_\alpha B_\beta-v_\alpha D_\beta+f_\alpha G_\beta,\tag{24}$$

$$f_{\alpha;\beta}=u_\alpha C_\beta-v_\alpha E_\beta-e_\alpha G_\beta.\tag{25}$$

Using the Codazzi equations and contracting Eqs. (22)–(25) with the different tetrad vectors gives equations for $A_\alpha, B_\alpha, C_\alpha, D_\alpha, E_\alpha$, and G_α, more details are given in Hodgkinson.[5]

Letting a comma denote partial differentiation, the equations for A_α are

$$(\lambda_0+\lambda_1)A_\alpha=\lambda_{0,\beta}v^\beta u_\alpha-\lambda_{1,\beta}u^\beta v_\alpha+(\lambda_0+\lambda_2)B_\beta v^\beta e_\alpha+(\lambda_0+\lambda_3)C_\beta v^\beta f_\alpha,\tag{26}$$

$$(\lambda_0+\lambda_1)A_\alpha=\lambda_{0,\beta}v^\beta u_\alpha-\lambda_{1,\beta}u^\beta v_\alpha+(\lambda_1-\lambda_2)D_\beta u^\beta e_\alpha+(\lambda_1-\lambda_3)E_\beta u^\beta f_\alpha,\tag{27}$$

$$(\mu_0+\mu_1)A_\alpha=\mu_{0,\beta}v^\beta u_\alpha-\mu_{1,\beta}u^\beta v_\alpha+(\mu_0+\mu_2)B_\beta v^\beta e_\alpha+(\mu_0+\mu_3)C_\beta v^\beta f_\alpha,\tag{28}$$

$$(\mu_0+\mu_1)A_\alpha=\mu_{0,\beta}v^\beta u_\alpha-\mu_{1,\beta}u^\beta v_\alpha+(\mu_1-\mu_2)D_\beta u^\beta e_\alpha+(\mu_1-\mu_3)E_\beta u^\beta f_\alpha,\tag{29}$$

and similar ones exist for $B_\alpha, C_\alpha, D_\alpha, E_\alpha$, and G_α. Using Eqs. (16) and (17) with the linear independence of the basis vectors it is a straightforward substitution task to show that

$$\frac{((\lambda_2)^2+(\mu_2)^2)((\lambda_2)^2+(\mu_2)^2-\epsilon\Lambda)\mu_3}{(\mu_2+\mu_3)(\mu_2\mu_3-(\lambda_2)^2)\epsilon\Lambda}B_\beta v^\beta=0 \tag{30}$$

and

$$\frac{\mu_3((\lambda_2)^2+(\mu_2)^2)((\mu_3)^2((\lambda_2)^2+(\mu_2)^2)-(\lambda_2)^2\epsilon\Lambda)}{(\mu_2+\mu_3)(\mu_2\mu_3-(\lambda_2)^2)\epsilon\Lambda}C_\beta v^\beta=0. \tag{31}$$

We assume, at this stage, that there are no relationships between the arbitrary parameters λ_2,μ_2, and μ_3, which can make the coefficients of $B_\beta v^\beta=C_\beta v^\beta$ zero. The conditions that λ_2,μ_2, and μ_3 are not independent will be considered at the end of this section.

A similar analysis for D_α and E_α gives $B_\beta v^\beta=C_\beta v^\beta=D_\beta u^\beta=E_\beta u^\beta=0$ and the form of the equations for A_α becomes

$$A_\alpha=\frac{1}{\lambda_0+\lambda_1}(\lambda_{0,\beta}v^\beta u_\alpha-\lambda_{1,\beta}u^\beta v_\alpha)=\frac{1}{\mu_0+\mu_1}(\mu_{0,\beta}v^\beta u_\alpha-\mu_{1,\beta}u^\beta v_\alpha). \tag{32}$$

Similar forms for $B_\alpha, C_\alpha, D_\alpha, E_\alpha$, and G_α may be found by an analogous process. Using the fact that $u_\alpha,v_\alpha,e_\alpha$, and f_α are hypersurface orthogonal, conditions for the consistency of Eqs. (32) and those for $B_\alpha, C_\alpha, D_\alpha, E_\alpha$, and G_α can be found. Since this task is repetitive and routine only one example will be given.

Checking for C_α, E_α, and G_α gives

$$\frac{1}{\lambda_0+\lambda_3}(\lambda_{0,\beta}f^\beta)=\frac{1}{\mu_0+\mu_3}(\mu_{0,\beta}f^\beta), \tag{33}$$

$$\frac{1}{\lambda_1-\lambda_3}(\lambda_{1,\beta}f^\beta)=\frac{1}{\mu_1-\mu_3}(\mu_{1,\beta}f^\beta), \tag{34}$$

$$\frac{1}{\lambda_2-\lambda_3}(\lambda_{2,\beta}f^\beta)=\frac{1}{\mu_2-\mu_3}(\mu_{2,\beta}f^\beta). \tag{35}$$

Using the z coordinate adapted to the f_α tetrad gives a set of three partial differential equations. Substituting from Eqs. (16) and (17) gives for Eq. (33)

$$\frac{\partial\mu_2}{\partial z}\lambda_2-\frac{\partial\lambda_2}{\partial z}\mu_2=0, \tag{36}$$

this integrates to give $\mu_2=k\lambda_2$, where k is independent of z. Using this value of μ_2 together with Eqs. (16) and (17) substituted into Eqs. (34) and (35) gives

$$\mu_3(\lambda_2)^3(1+k^2)^2\frac{\partial\lambda_2}{\partial z}=0, \tag{37}$$

$$\mu_3\lambda_2(1+k^2)\frac{\partial\lambda_2}{\partial z}=0. \tag{38}$$

In order to keep the arbitrariness of the parameters these conditions require λ_2 (and μ_2) to be independent of z. Repeating the analysis for the y coordinate adapted to e_α, the x coordinate adapted to v_α gives

$$\mu_2(x,y)=k\lambda_2(x,y), \tag{39}$$

where k is a constant and μ_3 is a function of t and z only. These functional dependencies allow Eqs. (16) and (17) to be simplified to

$$\lambda_0=-\frac{k\epsilon\Lambda}{\mu_3(1+k^2)},\quad \lambda_1=-\frac{\epsilon\Lambda}{\lambda_2(1+k^2)},\quad \lambda_3=k\mu_3, \tag{40}$$

$$\mu_0=\frac{\epsilon\Lambda}{\mu_3(1+k^2)},\quad \mu_1=-\frac{k\epsilon\Lambda}{\lambda_2(1+k^2)},\quad \mu_2=k\lambda_2, \tag{41}$$

where $\lambda_2=\lambda_2(x,y)$ and $\mu_3=\mu_3(t,z)$ are arbitrary functions.

These dependencies between the λ's and the μ's reduce the equations for A_α, B_α, C_α, D_α, E_α, and G_α to

$$A_\alpha=B_\alpha=E_\alpha=G_\alpha=0 \tag{42}$$

and

$$C_\alpha=\frac{1}{\lambda_0+\lambda_3}(\lambda_{0,\beta}f^\beta u_\alpha-\lambda_{3,\beta}u^\beta f_\alpha), \tag{43}$$

$$D_\alpha=\frac{1}{\lambda_1-\lambda_2}(\lambda_{1,\beta}e^\beta v_\alpha+\lambda_{2,\beta}v^\beta e_\alpha). \tag{44}$$

In terms of coordinates adapted to the tetrad, the metric may be written in the form

$$ds^2=-T^2\,dt^2+X^2\,dx^2+Y^2\,dy^2+Z^2\,dz^2, \tag{45}$$

where $u^\alpha=T^{-1}\delta_0^\alpha$, $v^\alpha=X^{-1}\delta_1^\alpha$, $e^\alpha=Y^{-1}\delta_2^\alpha$, and $f^\alpha=Z^{-1}\delta_3^\alpha$ with $x^0=t$, $x^1=x$, $x^2=y$, and $x^3=z$.

Comparing the derivatives of the tetrad vectors obtained from the equation of the metric (45) and those from Eqs. (43) and (44) allows the metric to be written

$$ds^2=-(T(t,z))^2\,dt^2+(X(x,y))^2\,dx^2+(Y(x,y))^2\,dy^2+(Z(t,z))^2\,dz^2. \tag{46}$$

The field equations $R_{\alpha\beta}=\Lambda g_{\alpha\beta}$ give for R_{11},

$$\frac{X_{yy}}{XY^2}+\frac{Y_{xx}}{X^2Y}-\frac{X_xY_x}{X^3Y}-\frac{X_yY_y}{XY^3}=\Lambda, \tag{47}$$

where a suffix denotes partial differentiation, with similar ones for R_{00}, R_{22}, R_{33}.

Since Λ is a constant, the left-hand side of Eq. (47) is a constant, i.e., the xy space is a 2-space of constant curvature K. According to Kramer *et al.*[3] the metrics of 2-spaces of constant curvature have six distinct types

$$d\sigma^2=Q^2((dx^1)^2\pm\Sigma^2(x^1,w)(dx^2)^2),\quad K=wQ^{-2}, \tag{48}$$

where $\Sigma(x^1,w)=\sin(x^1)$ or x^1 or $\sinh(x^1)$ if $w=1$ or $=0$ or $=-1$, respectively. Examination of the values of w and Σ which preserve the signature of ds^2 and satisfy the field equations gives four solutions. When both 2-spaces have positive curvature $K=\Lambda$, the metric is

$$ds^2=-\frac{\sin^2(z)}{\Lambda}dt^2+\frac{dx^2}{\Lambda}+\frac{\sin^2(x)}{\Lambda}dy^2+\frac{dz^2}{\Lambda}. \tag{49}$$

A scaling of the coordinates $x^\alpha\to\sqrt{\Lambda}x^\alpha$ in Eq. (49) reduces it to

$$ds^2 = -\sin^2(z\sqrt{\Lambda})dt^2 + dx^2 + \sin^2(x\sqrt{\Lambda})dy^2 + dz^2.$$

This metric agrees with one of the four classified as reducible and listed by Petrov[6] or called decomposable in the terminology of Kramer *et al.*[3] The other three have similar representations and are listed in Sec. VI.

During the previous analysis any special relationships between the parameters were ignored, so it is necessary, following Eqs. (30) and (31), to consider the implication of λ_2, μ_2, μ_3 being dependent.

From Eqs. (30) and (31) it is possible that

$$(\lambda_2)^2 + (\mu_2)^2 = \epsilon\Lambda \quad \text{and/or} \quad ((\mu_3)^2((\lambda_2)^2 + (\mu_2)^2) - (\lambda_2)^2\epsilon\Lambda) = 0.$$

Using these condition in Eqs. (16) and (17) gives either $\theta_1 = \theta_2$ or $\theta_0 = \theta_1$ and in both cases the analysis would be similar to the $\theta_0 = \theta_3$ case, which follows in Sec. IV B. The denominators of Eqs. (30) and (31) would vanish if $\mu_2 = -\mu_3$ or $\mu_2\mu_3 = (\lambda_2)^2$. The first condition gives $\theta_0 = \theta_1$ considered in Sec. IV B, while the second gives $\lambda_3 = -\lambda_2$ and $\mu_0 = -\mu_1$ which again is essentially analyzed in Sec. IV B.

B. Case 2. The Kottler metrics

For Eq. (12) two other possible solutions are $\theta_0 = \theta_3$ or $\theta_1 = \theta_2$. Without loss of generality we will assume that $\theta_0 = \theta_3$ gives

$$\lambda_0 = \frac{r}{2}(\cos(\theta_1) + \cos(\theta_2)) = -\lambda_3, \tag{50}$$

$$\lambda_1 = \frac{r}{2}(\cos(\theta_1) - \cos(\theta_2) - 2\cos(\theta_0)), \tag{51}$$

$$\lambda_2 = \frac{r}{2}(\cos(\theta_2) - \cos(\theta_1) - 2\cos(\theta_0)), \tag{52}$$

$$\mu_0 = \frac{r}{2}(\sin(\theta_1) + \sin(\theta_2)) = -\mu_3, \tag{53}$$

$$\mu_1 = \frac{r}{2}(\sin(\theta_1) - \sin(\theta_2) - 2\sin(\theta_0)), \tag{54}$$

$$\mu_2 = \frac{r}{2}(\sin(\theta_2) - \sin(\theta_1) - 2\sin(\theta_0)). \tag{55}$$

Again by examining A_α, B_α, C_α, D_α, E_α, and G_α and using linear independence and Eqs. (50) to (55) we obtain

$$A_\alpha = \frac{1}{\lambda_0 + \lambda_1}(\lambda_{0,\beta}v^\beta u_\alpha - \lambda_{1,\beta}u^\beta v_\alpha) = \frac{1}{\mu_0 + \mu_1}(\mu_{0,\beta}v^\beta u_\alpha - \mu_{1,\beta}u^\beta v_\alpha) \tag{56}$$

with similar expressions for B_α, D_α, E_α, and G_α.

Let the t, x, y, and z coordinates be adapted to the tetrad vectors. The fact that C_α is indeterminate makes

$$\frac{\partial\lambda_0}{\partial z} = \frac{\partial\mu_0}{\partial z} = \frac{\partial\lambda_0}{\partial t} = \frac{\partial\mu_0}{\partial t} = 0. \tag{57}$$

Differentiating Eqs. (50) and (53) partially with respect to z gives

$$\frac{\partial r}{\partial z}(\cos(\theta_1)+\cos(\theta_2))-r\left(\sin(\theta_1)\frac{\partial\theta_1}{\partial z}+\sin(\theta_2)\frac{\partial\theta_2}{\partial z}\right)=0, \tag{58}$$

$$\frac{\partial r}{\partial z}(\sin(\theta_1)+\sin(\theta_2))+r\left(\cos(\theta_1)\frac{\partial\theta_1}{\partial z}+\cos(\theta_2)\frac{\partial\theta_2}{\partial z}\right)=0. \tag{59}$$

Eliminating $\partial\theta_2/\partial z$ from Eqs. (58) and (59) gives

$$\frac{\partial r}{\partial z}(1+\cos(\theta_1-\theta_2))-r(\sin(\theta_1-\theta_2))\frac{\partial\theta_1}{\partial z}=0, \tag{60}$$

and similarly eliminating $\partial\theta_1/\partial z$ implies

$$\frac{\partial\theta_1}{\partial z}=-\frac{\partial\theta_2}{\partial z}.$$

To find relationships between $\partial r/\partial z$, $\partial\theta_0/\partial z$, and $\partial\theta_1/\partial z$ use Eqs. (8) with $\theta_0=\theta_3$,

$$2\epsilon\Lambda=r^2(2\cos(\theta_1-\theta_0)+2\cos(\theta_2-\theta_0)+1+\cos(\theta_1-\theta_2)). \tag{61}$$

Differentiating partially with respect to z and substituting for $\partial\theta_2/\partial z$ gives

$$-2r(2\cos(\phi_1)+2\cos(\phi_2)+\cos(\phi_2-\phi_1)+1)\frac{\partial r}{\partial z}-2r^2(\sin(\phi_1)+\sin(\phi_2))\frac{\partial\theta_0}{\partial z}$$
$$+2r^2(\sin(\phi_1)-\sin(\phi_2)-\sin(\phi_2-\phi_1))\frac{\partial\theta_1}{\partial z}=0, \tag{62}$$

where $\phi_1=\theta_1-\theta_0$ and $\phi_2=\theta_2-\theta_0$.

It is possible to find two new equations in $\partial r/\partial z$, $\partial\theta_0/\partial z$, and $\partial\theta_1/\partial z$ in order to examine the z dependency of the r and θ's.

The equations for E_α and G_α require

$$\frac{1}{\lambda_1-\lambda_3}\frac{\partial\lambda_1}{\partial z}=\frac{1}{\mu_1-\mu_3}\frac{\partial\mu_1}{\partial z} \tag{63}$$

and

$$\frac{1}{\lambda_2-\lambda_3}\frac{\partial\lambda_2}{\partial z}=\frac{1}{\mu_2-\mu_3}\frac{\partial\mu_2}{\partial z}. \tag{64}$$

Substituting and simplifying gives

$$1/2r(\sin(\phi_1)+\sin(\phi_2)-\sin(-\phi_1+\phi_2))\frac{\partial r}{\partial z}+r^2(1-\cos(\phi_1))\frac{\partial\theta_0}{\partial z}$$
$$+1/2r^2(-\cos(\phi_1)-\cos(\phi_2)+\cos(-\phi_1+\phi_2)+1)\frac{\partial\theta_1}{\partial z}=0 \tag{65}$$

and

$$1/2r(\sin(\phi_1)+\sin(\phi_2)+\sin(-\phi_1+\phi_2))\frac{\partial r}{\partial z}+r^2(1-\cos(\phi_2))\frac{\partial \theta_0}{\partial z}$$

$$-1/2r^2(-\cos(\phi_1)-\cos(\phi_2)+\cos(-\phi_1+\phi_2)+1)\frac{\partial \theta_1}{\partial z}=0. \tag{66}$$

To examine the dependence of the three equations (62), (65), and (66) they are written in the form $AX=0$, where $X=[\partial r/\partial z, \partial\theta_0/\partial z, \partial\theta_1/\partial z]^T$ and A is the matrix of the coefficients. The determinant of A factors to

$$-4-4\cos(\phi_1+\phi_2)+6\cos(\phi_1)+6\cos(\phi_2)-4\cos(-\phi_1+\phi_2)+\cos(-\phi_1+2\phi_2)$$
$$+\cos(\phi_1+2\phi_2)+\cos(\phi_2-2\phi_1)+\cos(\phi_2+2\phi_1)-2\cos(2\phi_1)-2\cos(2\phi_2).$$

Using standard trigonometric substitutions this expression reduces to

$$16\cos\left(\frac{\phi_1+\phi_2}{2}\right)\cos\left(\frac{\phi_1-\phi_2}{2}\right)\sin^2\left(\frac{\phi_1}{2}\right)\sin^2\left(\frac{\phi_2}{2}\right).$$

This determinant has to vanish for the consistency of Eqs. (62), (65), and (66) which is only valid for $\theta_1=\theta_2$, $\theta_1=\theta_0$, $\theta_2=\theta_0$, $\theta_1+\theta_2-2\theta_0=\pi$ or $\theta_1-\theta_2=\pi$.

The conditions $\theta_1=\theta_2$ or $\theta_1-\theta_2=\pi$ together with the condition

$$\frac{\partial\theta_1}{\partial z}=-\frac{\partial\theta_2}{\partial z}$$

make θ_1 and θ_2 independent of z, so Eqs. (58) and (62) show that r and θ_0 are also independent of z.

The condition $\theta_1+\theta_2-2\theta_0=\pi$ and Eqs. (65) and (66) make either r and the θ's independent of z or $\sin(\phi_2-\phi_1)=0$ which also implies z independence.

The condition $\theta_1=\theta_0$ (and similarly $\theta_2=\theta_0$) reduces Eqs. (62), (65), and (66) to the equation

$$\cos\left(\frac{\phi_2}{2}\right)\frac{\partial r}{\partial z}-\frac{r}{2}\sin\left(\frac{\phi_2}{2}\right)\frac{\partial\phi_2}{\partial z}=0$$

which integrates to

$$r\cos\left(\frac{\phi_2}{2}\right)=g(t,x,y),$$

where g is an arbitrary function of t, x, and y. A similar analysis using Eq. (57) gives the t independence of g and since under these conditions $\lambda_0+\lambda_1=0$ then from Eq. (56) A_α is indeterminate making λ_0 and μ_0 independent of x. This fact reduces g to depend only on one variable y and Eq. (61) implies that all the parameters depend upon only one variable, which is considered later in this section.

Assuming that these extra conditions are not satisfied then r, θ_0, θ_1, and θ_2 are independent of z and likewise from Eq. (57) they are independent of t. The consequences for the metric coefficients are that X and Y are independent of t and z. Since C_α is indeterminate, the functional dependencies of T and Z are also indeterminate.

Since all the variables on the right-hand side of Eq. (61) are functions of x and y only then Eq. (61) is essentially a function of x and y equal to zero, i.e., x and y are dependent variables. Hence, r, θ_0, θ_1, and θ_2 are functions of a single variable say x. Then a comparison of the derivatives of the tetrad vectors for A_α, D_α, and E_α allows the metric (45) to be written

$$ds^2 = W^2(x)d\Sigma^2 + X^2(x)dx^2 + Y^2(x)dy^2, \tag{67}$$

where $d\Sigma^2$ is a two-dimensional metric dependent only on t and z.

The field equations $R_{\alpha\beta} = \Lambda g_{\alpha\beta}$ can be investigated for this metric where the equation $R_{22} = \Lambda g_{22}$ gives

$$2\frac{YW_xY_x}{WX^2} + \frac{YY_{xx}}{X^2} - \frac{YX_xY_x}{X^3} = \Lambda Y^2 \tag{68}$$

and $R_{11} = \Lambda g_{11}$ gives

$$2\frac{W_{xx}}{W} - 2\frac{W_xX_x}{WX} + \frac{Y_{xx}}{Y} - \frac{X_xY_x}{XY} = \Lambda X^2. \tag{69}$$

Eliminating Λ gives

$$\frac{Y_x}{Y} - \frac{W_{xx}}{W_x} + \frac{X_x}{X} = 0 \tag{70}$$

which integrates to

$$XY = qW_x, \tag{71}$$

where q is a constant.

The equation $R_{33}/g_{33} = \Lambda$ is

$$\frac{K}{W^2} + \frac{(W_x)^2}{W^2X^2} + \frac{W_{xx}}{WX^2} - \frac{W_xX_x}{WX^3} + \frac{W_xY_x}{WX^2Y} = \Lambda, \tag{72}$$

where K is the Gaussian curvature of $d\Sigma^2$. Partial differentiation of Eq. (72) with respect to t and z shows that K is a constant.

Substituting Eq. (71) into Eq. (68) simplifies and rearranges to give

$$\frac{d}{dx}\left(YY_x\frac{W^2}{W_x}\right) = \Lambda q^2W^2W_x \tag{73}$$

which integrates twice to give

$$Y^2 = \frac{q^2}{3}\Lambda W^2 - 2\frac{p}{W} + 2c_1, \tag{74}$$

where p and c_1 are constants of integration.

Without loss of generality the transformation $W(x) \to x$ and a rescaling gives

$$Y^2 = c - \frac{\Lambda}{3}x^2 + \frac{m}{x}. \tag{75}$$

The value of the constant c depends upon the Einstein space condition and the form of the constant curvature metric. The general form of the metrics is

$$ds^2 = x^2\,d\Sigma^2 + Y^{-2}(x)dx^2 + Y^2(x)dy^2. \tag{76}$$

These metrics are similar to the Kottler form of the Einstein space (see Kramer *et al.*[4] and Petrov.[5] A full list is provided in Sec. VI.

In this section since $\epsilon_1=\epsilon_2=\pm 1$, then the signature of the embedding pseudo-Euclidean space E_6 is either 0 if $\epsilon_1=-1$ or 4 if $\epsilon_1=1$.

V. THE CASE $\epsilon_1=-\epsilon_2$

Letting $\epsilon_1=-\epsilon_2=\epsilon$ gives the equivalent of Eq. (7) as

$$A^2-B^2=(\sigma^2-\epsilon\Lambda)I, \tag{77}$$

where

$$\sigma^2=\frac{a^2-b^2}{4}.$$

The analysis follows the same course with trigonometric terms being replaced by hyperbolic ones. The same metrics are found showing that the metrics that are products of two 2-spaces of constant curvature and the modified Kottler metrics can be embedded in a pseudo-Euclidean space E_6 with signature 2.

It is possible that when $\epsilon_1=-\epsilon_2$ then $\sigma=0$, this degeneracy means that $a=b$ or $a=-b$ in both cases the type D condition on the Weyl tensor gives a flat space solution.

VI. A SUMMARY OF THE METRICS

This section contains a list of all the Petrov type D Einstein space–times of embedding class 2.

The following list gives the reducible metrics.

(1)

$$ds^2=-\frac{\sin^2(z)}{\Lambda}dt^2+\frac{dx^2}{\Lambda}+\frac{\sin^2(x)}{\Lambda}dy^2+\frac{dz^2}{\Lambda}, \tag{78}$$

both 2-spaces have positive curvature $K=\Lambda$.

(2)

$$ds^2=-\frac{\sinh^2(z)}{\Lambda}dt^2+\frac{dx^2}{\Lambda}+\frac{\sinh^2(x)}{\Lambda}dy^2+\frac{dz^2}{\Lambda}, \tag{79}$$

both 2-spaces have negative curvature $K=-\Lambda$.

(3)

$$ds^2=-\frac{dt^2}{\Lambda}+\frac{dx^2}{\Lambda}+\frac{\sin^2(x)}{\Lambda}dy^2+\frac{\sinh^2(t)}{\Lambda}dz^2, \tag{80}$$

$$ds^2=-\frac{dt^2}{\Lambda}+\frac{dx^2}{\Lambda}+\frac{\sinh^2(x)}{\Lambda}dy^2+\frac{\sin^2(t)}{\Lambda}dz^2, \tag{81}$$

one space has positive curvature the other negative curvature.

The scaling of the coordinates given in Sec. IV A gives the agreement with Petrov.[6]

The following list gives the generalized Kottler ones based upon $\theta_0=\theta_3$ in Eq. (12).

(1) A flat $\Sigma^2(z,t)$ the resulting metric is

$$ds^2=\left(-\frac{\Lambda}{3}x^2+\frac{m}{x}\right)^{-1}dx^2+\left(-\frac{\Lambda}{3}x^2+\frac{m}{x}\right)dy^2+x^2\,dz^2-x^2\,dt^2, \tag{82}$$

with $c=0$.

(2) A two-dimensional space–time with negative curvature is

$$ds^2=\left(1-\frac{\Lambda}{3}x^2+\frac{m}{x}\right)^{-1}dx^2+\left(1-\frac{\Lambda}{3}x^2+\frac{m}{x}\right)dy^2+x^2\sinh(t)^2\,dz^2-x^2\,dt^2, \tag{83}$$

with $c=1$.

(3) A two-dimensional space–time with positive curvature is

$$ds^2=\left(1-\frac{\Lambda}{3}x^2+\frac{m}{x}\right)^{-1}dx^2+\left(1-\frac{\Lambda}{3}x^2+\frac{m}{x}\right)dy^2+x^2\,dz^2-x^2\sin(z)^2\,dt^2, \tag{84}$$

with $c=1$.

Naturally, if alternative identifications of the θ's are taken, the following metric forms or similar are obtained.

(1)

$$ds^2=\left(-\frac{\Lambda}{3}x^2+\frac{m}{x}\right)^{-1}dx^2-\left(-\frac{\Lambda}{3}x^2+\frac{m}{x}\right)dt^2+x^2\,dy^2+x^2\,dz^2. \tag{85}$$

(2)

$$ds^2=\left(\frac{\Lambda}{3}t^2+\frac{m}{t}\right)dx^2-\left(\frac{\Lambda}{3}t^2+\frac{m}{t}\right)^{-1}dt^2+t^2\,dy^2+t^2\,dz^2. \tag{86}$$

(3)

$$ds^2=\left(-1+\frac{\Lambda}{3}x^2+\frac{m}{x}\right)dy^2-\left(-1+\frac{\Lambda}{3}t^2+\frac{m}{t}\right)^{-1}dt^2+t^2\sin(z)^2\,dy^2+t^2\,dz^2. \tag{87}$$

(4)

$$ds^2=\left(1-\frac{\Lambda}{3}x^2+\frac{m}{x}\right)^{-1}dx^2-\left(1-\frac{\Lambda}{3}x^2+\frac{m}{x}\right)dt^2+x^2\sin(z)^2\,dy^2+x^2\,dz^2. \tag{88}$$

The above metrics are the only possible Einstein spaces of embedding class 2. This implies that any type *D* Einstein space–times not of these forms are at least of embedding class 3. In a set of two papers[9,10] Van den Bergh has produced a classification of the symmetric tensors for the embedding class 2 problem and one of his applications is to the vacuum Petrov type *D* space–times.

It is a useful comparison to consider the limit as $\Lambda\to 0$ of the previous solutions to those in his paper. For the metrics (70)–(81) as $\Lambda\to 0$, $K\to 0$ and the resulting limit is flat space. As $\Lambda\to 0$ in the metrics listed in (82)–(88) they become either Ehlers–Kundt class A or class B metrics as defined in Kramer *et al.*[3] These results are in agreement with the results of Van den Bergh.[10]

The tensors $a^{\alpha}{}_{\beta}$ and $b^{\alpha}{}_{\beta}$ are not uniquely determined. The previous analysis has shown that different forms can lead to essentially the same embedding. This corresponds to the freedom of rotations in the two-dimensional space orthogonal to the four-dimensional Riemannian in the six-dimensional pseudo-Euclidean embedding space. The explicit embedding equations and the forms of $a^{\alpha}{}_{\beta}$ and $b^{\alpha}{}_{\beta}$ and their representations in terms of the curvature tensor for the embeddings developed in this paper are subjects for further investigation.

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The Biot–Savart operator for application to knot theory, fluid dynamics, and plasma physics

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The *writhing number* of a curve in 3-space is the standard measure of the extent to which the curve wraps and coils around itself; it has proved its importance for molecular biologists in the study of knotted DNA and of the enzymes which affect it. The *helicity* of a vector field defined on a domain in 3-space is the standard measure of the extent to which the field lines wrap and coil around one another; it plays important roles in fluid dynamics and plasma physics. The *Biot–Savart operator* associates with each current distribution on a given domain the restriction of its magnetic field to that domain. When the domain is simply connected, the divergence-free fields which are tangent to the boundary and which minimize energy for given helicity provide models for stable force-free magnetic fields in space and laboratory plasmas; these fields appear mathematically as the extreme eigenfields for an appropriate modification of the Biot–Savart operator. Information about these fields can be converted into bounds on the writhing number of a given piece of DNA. The purpose of this paper is to reveal new properties of the Biot–Savart operator which are useful in these applications. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1329659]

I. INTRODUCTION

Let Ω be a compact domain with smooth boundary in 3-space, and let $\mathrm{VF}(\Omega)$ be the space of smooth vector fields on Ω with the L^2 inner product $\langle V,W\rangle=\int_\Omega V\cdot W d(\mathrm{vol})$. By ''smooth,'' equivalently C^∞, we mean that derivatives of all orders exist and are continuous.

If we think of the smooth vector field V on Ω as a distribution of electric current, then the Biot–Savart formula

$$\mathrm{BS}(V)(y)=(1/4\pi)\int_\Omega V(x)\times(y-x)/|y-x|^3 \ \mathrm{d}(\mathrm{vol}_x)$$

gives the resulting magnetic field $\mathrm{BS}(V)$ throughout 3-space. If we restrict this magnetic field to the domain Ω, then we get the *Biot–Savart operator*,

$$\mathrm{BS}:\mathrm{VF}(\Omega)\to\mathrm{VF}(\Omega).$$

Theorem A: *The equation* $\nabla\times\mathrm{BS}(V)=V$ *holds in* Ω *if and only if* V *is divergence-free and tangent to the boundary of* Ω.

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It is well known that curl is a left inverse to the Biot–Savart operator when the input field V is divergence-free and tangent to the boundary. The new information is that this result holds in no other cases. The impact of this is that eigenvalue problems for the Biot–Savart operator, which are central to the study of helicity, cannot in general be converted to eigenvalue problems for curl (that is, to a system of partial differential equations).

Theorem B: *The kernel of the Biot–Savart operator is precisely the space of gradient vector fields which are orthogonal to the boundary of* Ω.

Actually, somewhat more is true. If V is a smooth gradient vector field defined on Ω and orthogonal to its boundary, then its magnetic field $\mathrm{BS}(V)=0$ throughout 3-space. Conversely, if V is a smooth vector field defined on Ω whose magnetic field $\mathrm{BS}(V)=0$ in Ω, then V is a gradient field orthogonal to the boundary of Ω, and hence $\mathrm{BS}(V)=0$ throughout 3-space.

Theorem C: *The image of the Biot–Savart operator is a proper subspace of the image of curl, whose orthogonal projection into the subspace of ''fluxless knots'' is one-to-one.*

Vector fields on the domain Ω which are divergence-free and tangent to its boundary are called *fluid knots*; we explain this terminology in Sec. IV. *Fluxless knots* are fluid knots with zero flux through every cross-sectional surface $(\Sigma,\partial\Sigma)\subset(\Omega,\partial\Omega)$. The above theorems lead to several interesting examples of ''impossible'' magnetic fields. Nevertheless, Theorem *C* falls short of giving a precise characterization of the image of the Biot–Savart operator, and hence of those fields in a domain Ω which are magnetic fields of current distributions within Ω.

Theorem D: *The Biot–Savart operator is a bounded operator, and hence extends to a bounded operator on the* L^2 *completion of its domain, where it is both compact and self-adjoint.*

The eigenfields of this operator which correspond to its extreme eigenvalues turn out to be the vector fields in Ω with minimum energy for given helicity. If we start with a vector field V which is divergence-free and tangent to the boundary of its domain Ω, that is, a fluid knot, then its magnetic field $\mathrm{BS}(V)$, though divergence-free, will in general not be tangent to the boundary of Ω. In such a case, we simply modify the Biot–Savart operator BS by following it by orthogonal projection back to the subspace of fluid knots. The eigenfields of this modified Biot–Savart operator which correspond to its extreme eigenvalues are then the fluid knots in Ω with minimum energy for given helicity. When the domain Ω is simply connected, these energy-minimizers model the stable plasma fields in Ω.

II. PRELIMINARIES

A. Writhing, helicity, and the Biot–Savart operator

The *writhing number* $\mathrm{Wr}(K)$ of a smooth curve K in 3-space, defined by the formula

$$\mathrm{Wr}(K)=(1/4\pi)\int_{K\times K}(dx/ds\times dy/dt)\cdot(x-y)/|x-y|^3\ \mathrm{ds}\ \mathrm{dt}, \tag{2.1}$$

was introduced by Călugăreanu[1–3] in 1959–1961 and named by Fuller[4] in 1971, and is the standard measure of the extent to which the curve wraps and coils around itself.

The *helicity* $H(V)$ of a smooth vector field V on the domain Ω in 3-space, defined by the formula

$$H(V)=(1/4\pi)\int_{\Omega\times\Omega}V(x)\times V(y)\cdot(x-y)/|x-y|^3\ \mathrm{d}(\mathrm{vol}_x)\ \mathrm{d}(\mathrm{vol}_y), \tag{2.2}$$

was introduced by Woltjer[5] in 1958 and named by Moffatt[6] in 1969, and is the standard measure of the extent to which the field lines wrap and coil around one another.

Clearly, helicity for vector fields is the analogue of writhing number for knots.

The helicity of V is closely related to its image under the Biot–Savart operator,

$$\begin{aligned} H(V) &= (1/4\pi)\int_{\Omega\times\Omega} V(x) \times V(y)\cdot(x-y)/|x-y|^3 \ \mathrm{d}(\mathrm{vol}_x)\ \mathrm{d}(\mathrm{vol}_y) \\ &= \int_\Omega V(y)\cdot\left[(1/4\pi)\int_\Omega V(x) \times (y-x)/|y-x|^3 \ \mathrm{d}(\mathrm{vol}_x)\right]\mathrm{d}(\mathrm{vol}_y) \\ &= \int_\Omega V(y)\cdot \mathrm{BS}(V)(y)\ \mathrm{d}(\mathrm{vol}_y) \\ &= \int_\Omega V\cdot \mathrm{BS}(V)\ \mathrm{d}(\mathrm{vol}), \end{aligned}$$

so the helicity of V is just the L^2 inner product of V and $\mathrm{BS}(V)$,

$$H(V) = \langle V, \mathrm{BS}(V)\rangle. \tag{2.3}$$

It is because of this formula that the Biot–Savart operator,

$$\mathrm{BS}:\mathrm{VF}(\Omega)\to\mathrm{VF}(\Omega), \tag{2.4}$$

plays such a prominent role in the study of writhing of knots and helicity of vector fields.

B. Applications: A quick guide to the literature

For a glance at the prehistory of the writhing number, see Gauss's half-page note[7] (1833) on an integral formula for the linking number of two disjoint closed curves in 3-space. Rewrite his expression in modern notation and let the two curves coincide and you will have the formula for the writhing number.

The writhing number has proved its importance for molecular biologists in the study of knotted duplex DNA and of the enzymes which affect it; see White,[8] Fuller,[9] Bauer, Crick, and White,[10] Wang,[11] Sumners,[12–14] and Cantarella, Kusner, and Sullivan.[15]

For an overview of the connection between knot theory and electrodynamics, see Lomonaco.[16]

Woltjer's formula for the helicity of a vector field arose from his interest in force-free magnetic fields. These are magnetic fields which are everywhere parallel to the current flows which give rise to them, so that the Lorentz force on the flowing charged particles is zero. Because the gross magnetic field in the Crab Nebula appeared to be steady over a number of years, Woltjer believed it to be force-free, and studied[17] it in great detail. Two early papers on force-free magnetic fields are Lundquist[18] and Chandrasekhar–Kendall.[19] Two more recent papers are Laurence and Avellaneda[20] and Tsuji.[21] Marsh's book[22] has an extensive and up-to-date bibliography on this subject.

For a study of the connection between writhing and helicity, see Berger and Field[23] and Moffatt and Ricca.[24,25]

For the connection between helicity and the ordinary and asymptotic Hopf invariants, see Whitehead[26] and Arnold.[27]

For an introduction to the spectral theory of the Biot–Savart operator and its use in determining upper bounds for writhing and helicity, see Ref. 28. For explicit computation of extreme eigenfields, see Refs. 29 and 30. For an analysis of isoperimetric problems connected with the Biot–Savart operator, see Ref. 31. For application to the qualitative study of stable plasma flows, see Cantarella.[32] For an overview of our work, see our survey paper.[33]

For further information on related spectral problems for the curl operator, see Yoshida and Giga.[34]

For the connection between this spectral theory and plasma physics, see Yoshida.[35]

For a study of magnetic field generation in electrically conducting fluids, see the book by Moffatt.[36]

For connections with dynamo theory, see the survey article by Childress.[37]

For many papers on the connections with the dynamics of fluids and plasmas, see the books by Moffatt and Tsinober[38] and by Moffatt, Zaslavsky, Comte, and Tabor.[39]

For the connections between force-free fields, contact topology and fluid dynamics, see Etnyre and Ghrist.[40]

C. The Hodge decomposition theorem

In this section we present the Hodge Decomposition Theorem for vector fields on bounded domains in R^3, which we will use throughout the paper. Although we state it below for the space $\mathrm{VF}(\Omega)$ of smooth vector fields on Ω with the usual L^2 inner product, it holds just as well for the L^2 completions of $\mathrm{VF}(\Omega)$ and of the various subspaces described below.

The papers of Weyl[41] and Friedrichs,[42] the notes of Blank, Friedrichs, and Grad,[43] and the book of Schwarz[44] are all good references; an exposition of this theorem in the form given below appears in Ref. 45.

Hodge Decomposition Theorem: *We have a direct sum decomposition of* $VF(\Omega)$ *into five mutually orthogonal subspaces*,

$$\mathrm{VF}(\Omega) = \mathrm{FK} \oplus \mathrm{HK} \oplus \mathrm{CG} \oplus \mathrm{HG} \oplus \mathrm{GG},$$

with

$$\begin{aligned} \ker\ \mathrm{curl} &= \mathrm{HK} \oplus \mathrm{CG} \oplus \mathrm{HG} \oplus \mathrm{GG}, \\ \mathrm{image}\ \mathrm{grad} &= \mathrm{CG} \oplus \mathrm{HG} \oplus \mathrm{GG}, \\ \mathrm{image}\ \mathrm{curl} &= \mathrm{FK} \oplus \mathrm{HK} \oplus \mathrm{CG}, \\ \ker\ \mathrm{div} &= \mathrm{FK} \oplus \mathrm{HK} \oplus \mathrm{CG} \oplus \mathrm{HG}, \end{aligned}$$

where

$$\mathrm{FK} = \mathrm{Fluxless\ Knots} = \{\nabla \cdot V = 0,\ V \cdot n = 0,\ \text{all interior fluxes} = 0\},$$

$$\mathrm{HK} = \mathrm{Harmonic\ Knots} = \{\nabla \cdot V = 0,\ \nabla \times V = 0,\ V \cdot n = 0\},$$

$$\mathrm{CG} = \mathrm{Curly\ Gradients} = \{V = \nabla\varphi,\ \nabla \cdot V = 0,\ \text{all boundary fluxes} = 0\},$$

$$\mathrm{HG} = \mathrm{Harmonic\ Gradients} = \{V = \nabla\varphi,\ \nabla \cdot V = 0,\ \varphi \ \text{locally constant on } \partial\Omega\},$$

$$\mathrm{GG} = \mathrm{Grounded\ Gradients} = \{V = \nabla\varphi,\ \varphi|_{\partial\Omega} = 0\},$$

and furthermore,

$$\mathrm{HK} \cong H_1(\Omega; R) \cong H_2(\Omega, \partial\Omega; R) \cong R^{\text{genus of } \partial\Omega},$$

$$\mathrm{HG} \cong H_2(\Omega; R) \cong H_1(\Omega, \partial\Omega; R) \cong R^{(\#\text{ components of } \partial\Omega) - (\#\text{ components of } \Omega)}.$$

We need to explain the meanings of the conditions which appear in the statement of this theorem.

The outward pointing unit vector field orthogonal to $\partial\Omega$ is denoted by n, so the condition $V \cdot n = 0$ indicates that the vector field V is tangent to the boundary of Ω.

Let Σ stand generically for any smooth surface in Ω with $\partial\Sigma\subset\partial\Omega$. Earlier, when commenting on the statement of Theorem C, we indicated this by writing $(\Sigma,\partial\Sigma)\subset(\Omega,\partial\Omega)$. Now, orient Σ by picking one of its two unit normal vector fields n. Then, for any vector field V on Ω, we can define the *flux* of V through Σ to be the value of the integral $\Phi=\int_\Sigma V\cdot n \ \ \mathrm{d(area)}$.

Assume that V is divergence-free and tangent to $\partial\Omega$. Then the value of this flux depends only on the homology class of Σ in the relative homology group $H_2(\Omega,\partial\Omega;Z)$. For example, if Ω is an n-holed solid torus, then there are disjoint oriented cross-sectional disks $\Sigma_1,\ldots,\Sigma_n$, positioned so that cutting Ω along these disks will produce a simply-connected region. The fluxes $\Phi_1,\ldots,\Phi_n$ of V through these disks determine the flux of V through any other cross-sectional surface.

If the flux of V through every smooth surface Σ in Ω with $\partial\Sigma\subset\partial\Omega$ vanishes, we say ''*all interior fluxes*$=0$.'' Then,

$$\mathrm{FK}=\{V\epsilon\ \ \mathrm{VF}(\Omega):\nabla\cdot V=0,\ V\cdot n=0,\ \ \text{all interior fluxes}=0\} \tag{2.5}$$

will be the subspace of *fluxless knots*, already mentioned when explaining the statement of Theorem C.

The subspace,

$$\mathrm{HK}=\{V\epsilon\ \ \mathrm{VF}(\Omega):\nabla\cdot V=0,\ \nabla\times V=0,\ V\cdot n=0\} \tag{2.6}$$

of *harmonic knots* is isomorphic to the absolute homology group $H_1(\Omega;R)$ and also, via Poincaré duality, to the relative homology group $H_2(\Omega,\partial\Omega;R)$, and is thus a finite-dimensional vector space, with dimension equal to the genus of $\partial\Omega$.

The orthogonal direct sum of these two subspaces,

$$\mathrm{K}(\Omega)=\mathrm{FK}\oplus\mathrm{HK} \tag{2.7}$$

is the subspace of $\mathrm{VF}(\Omega)$ consisting of all divergence-free vector fields defined on Ω and tangent to its boundary. These are the vector fields that represent current flows in the standard versions of the laws of Magnetostatics.

We called these vector fields *fluid knots* in the Introduction, and pause to explain this terminology. Given a knot in 3-space, we can choose a thin tubular neighborhood of the knot to be our domain Ω, and then choose a divergence-free vector field V in Ω, for example orthogonal to the cross-sectional disks and hence tangent to the boundary. In this way, questions about the geometry of the knot can sometimes profitably be reformulated as questions about the vector field V, our ''fluid knot.'' We did exactly this in our paper[28] when deriving an upper bound for the writhing number of a knot of given length and thickness.

If V is a vector field defined on Ω, we will say that *all boundary fluxes of V are zero* if the flux of V through each component of $\partial\Omega$ is zero. Then,

$$\mathrm{CG}=\{V\epsilon\,\mathrm{VF}(\Omega):V=\nabla\varphi,\ \ \nabla\cdot V=0,\ \ \text{all boundary fluxes}=0\} \tag{2.8}$$

will be called the subspace of *curly gradients* because these are the only gradients which lie in the image of curl.

Next we define the subspace of *harmonic gradients*,

$$\mathrm{HG}=\{V\epsilon\,\mathrm{VF}(\Omega):V=\nabla\varphi,\ \ \nabla\cdot V=0,\ \varphi\ \text{locally constant on}\ \partial\Omega\}, \tag{2.9}$$

meaning that φ is constant on each component of $\partial\Omega$. This subspace is isomorphic to the absolute homology group $H_2(\Omega;R)$ and also, via Poincaré duality, to the relative homology group $H_1(\Omega,\partial\Omega;R)$, and is hence a finite-dimensional vector space, with dimension equal to the number of components of $\partial\Omega$ minus the number of components of Ω.

The definition of the subspace of *grounded gradients*,

$$\mathrm{GG}=\{V\epsilon\,\mathrm{VF}(\Omega):V=\nabla\varphi,\ \ \varphi|_{\partial\Omega}=0\}, \tag{2.10}$$

is self-explanatory.

A vector field V belongs to the subspace $\mathrm{HG} \oplus \mathrm{GG}$ of $\mathrm{VF}(\Omega)$ if and only if it is the gradient of a smooth function φ on Ω which is constant on each component of $\partial\Omega$, or equivalently, is a gradient vector field which is orthogonal to $\partial\Omega$. Theorem B asserts that these vector fields form the kernel of the Biot–Savart operator.

The five orthogonal direct summands of $\mathrm{VF}(\Omega)$ can be characterized as follows:

$$\mathrm{FK} = (\ker\ \mathrm{curl})^{\perp},$$

$$\mathrm{HK} = (\ker\ \mathrm{curl}) \cap (\mathrm{image}\ \mathrm{grad})^{\perp},$$

$$\mathrm{CG} = (\mathrm{image}\ \mathrm{grad}) \cap (\mathrm{image}\ \mathrm{curl}),$$

$$\mathrm{HG} = (\ker\ \mathrm{div}) \cap (\mathrm{image}\ \mathrm{curl})^{\perp},$$

$$\mathrm{GG} = (\ker\ \mathrm{div})^{\perp}.$$

These characterizations bear witness to the geometric and analytic significance of the summands.

We end this section with examples of vector fields from each of the five summands.

1. FK=fluxless knots

Let Ω be a round ball of radius 1, centered at the origin in 3-space. Consider the vector field

$$V = -y\hat{\imath} + x\hat{\jmath}.$$

This is the velocity field for rotation of 3-space about the z-axis at constant angular speed. It is divergence-free and tangent to the boundary of the ball Ω, and hence belongs to the subspace FK of fluxless knots, because there are no harmonic knots on a ball.

2. HK=harmonic knots

Let Ω be a solid torus of revolution about the z-axis. Using cylindrical coordinates (r,φ,z), consider the vector field

$$V = (1/r)\,\hat{\varphi},$$

which is the magnetic field due to a steady current running up the z-axis. It is divergence-free and curl-free and tangent to the boundary of the solid torus Ω, and hence belongs to the subspace HK of harmonic knots.

3. CG=curly gradients

Let Ω be a round ball of radius 1, centered at the origin. Consider the harmonic function z, and the gradient field

$$V = \nabla z = \hat{k}.$$

This vector field is divergence-free and has zero flux through the one and only component of $\partial\Omega$, hence it belongs to the subspace CG of curly gradients.

4. HG=harmonic gradients

Let Ω be the region between two concentric round spheres, say of radius 1 and 2, centered at the origin. Using spherical coordinates (r,θ,φ), consider the harmonic function $1/r$, and its gradient vector field

$$V = \nabla(1/r) = (-1/r^2)\hat{r},$$

just the inverse square central field. Since the harmonic function $1/r$ is constant on each component of $\partial\Omega$, the vector field V belongs to the subspace HG of harmonic gradients. We may think of V as the electric field between two concentric spheres held at different potentials.

5. GG=grounded gradients

Let Ω be a round ball of radius 1, centered at the origin. Consider the function given by $r^2-1=x^2+y^2+z^2-1$, and the vector field

$$V=\nabla(r^2-1)=2x\hat{i}+2y\hat{j}+2z\hat{k}.$$

Since the function r^2-1 has constant value zero on the boundary of Ω, the vector field V belongs to the subspace GG of grounded gradients. We may view V as an electric field with interior charges inside a conducting boundary.

III. STANDARD INFORMATION ABOUT THE BIOT–SAVART OPERATOR

A. The basic facts

Given a smooth vector field V on Ω, the *vector potential* $\mathrm{A}(V)$ for $\mathrm{BS}(V)$ is defined by the formula,

$$\mathrm{A}(V)(y)=(1/4\pi)\int_\Omega V(x)/|y-x|\ \ \mathrm{d}(\mathrm{vol}_x). \tag{3.1}$$

Here is the classically known information about the Biot–Savart operator and its vector potential. Note that some of the assertions below hold for any vector field $V\epsilon\mathrm{VF}(\Omega)$, while others need the more restrictive assumption that V is divergence-free and tangent to the boundary of Ω, in other words, that V lies in the subspace $\mathrm{K}(\Omega)$ of fluid knots.

Standard Information: *Let Ω be a compact domain in 3-space with smooth boundary $\partial\Omega$. Let V be a smooth vector field defined on Ω. Then*

(1) $\mathrm{BS}(V)$ *and* $\mathrm{A}(V)$ *are well-defined on all of 3-space, that is, the improper integrals defining them converge everywhere;*
(2) $\mathrm{BS}(V)$ *and* $\mathrm{A}(V)$ *are of class C^∞ on Ω, and on the closure Ω' of $R^3-\Omega$.* $\mathrm{BS}(V)$ *is continuous on R^3, but its derivatives typically suffer jump discontinuities as one crosses $\partial\Omega$.* $\mathrm{A}(V)$ *is of class C^1 on R^3, but its second derivatives typically suffer jump discontinuities as one crosses $\partial\Omega$;*
(3) $\Delta\mathrm{A}(V)=-V$ *in Ω and* $\Delta\mathrm{A}(V)=0$ *in Ω', where Δ is the vector Laplacian;*
(4) $\nabla\times\mathrm{A}(V)=\mathrm{BS}(V)$ *on R^3;*
(5) If $V\epsilon\mathrm{K}(\Omega)$, *then* $\mathrm{A}(V)$ *is divergence-free on R^3;*
(6) $\nabla\cdot\mathrm{BS}(V)=0$ *in Ω and in Ω';*
(7) If $V\epsilon\mathrm{K}(\Omega)$, *then* $\nabla\times\mathrm{BS}(V)=V$ *in Ω and* $\nabla\times\mathrm{BS}(V)=0$ *in Ω';*
(8) If $V\epsilon\mathrm{K}(\Omega)$, *then* $\int_C\mathrm{BS}(V)\cdot ds=0$ *for all closed curves C on $\partial\Omega$ which bound in $R^3-\Omega$;*
(9) In general, $\mathrm{A}(V)$ *decays at ∞ like $1/r$ and* $\mathrm{BS}(V)$ *decays at ∞ like $1/r^2$; however, if* $V\epsilon\mathrm{K}(\Omega)$, *then* $\mathrm{A}(V)$ *decays at ∞ like $1/r^2$ and* $\mathrm{BS}(V)$ *decays at ∞ like $1/r^3$.*

Proofs of most of these basic facts can be found throughout the physics literature (see, for example, Griffiths[46]), with the exception of item (9), which we prove in the Appendix. Item (7) contains the first half of Theorem A; we will prove that immediately, since it affects the rest of the paper.

B. Proof of (7)

The argument to follow begins as in Griffiths,[46] pp. 215–217, but is then modified to suit our purpose.

To prove (7), we assume that V is a fluid knot, and must show that

$$\nabla_y \times \mathrm{BS}(V)(y) = V(y), \quad \text{when } y \in \Omega,$$
$$= 0, \qquad \text{when } y \in \Omega'.$$

From now on, we will use the shorthand notation $\{V(y) \text{ in } \Omega/0 \text{ in } \Omega'\}$, or simply $\{V(y)/0\}$, to express these two outcomes.

The above assertion will follow immediately from the next proposition, which will then serve as a springboard to the rest of the paper.

Proposition 1:

$$\nabla_y \times \mathrm{BS}(V)(y) = \{V(y) \text{ in } \Omega/0 \text{ in } \Omega'\} + (1/4\pi)\nabla_y \int_\Omega (\nabla_x \cdot V(x))/|y-x| \ \mathrm{d}(\mathrm{vol}_x)$$
$$-(1/4\pi)\nabla_y \int_{\partial\Omega} V(x)\cdot n/|y-x| \ \mathrm{d}(\mathrm{area}_x).$$

If V is divergence-free, then the second term on the right-hand side vanishes; if V is tangent to the boundary of Ω, then the third term on the right-hand side vanishes. If both hold, that is, if V is a fluid knot, then we get item (7).

We can view the statement of Proposition 1 as Maxwell's equation,

$$\nabla \times B = J + \partial E/\partial t, \tag{3.2}$$

as follows.

Let V represent a current distribution throughout the domain Ω. At time $t=0$, let the volume charge density ρ throughout Ω and the surface charge density σ along $\partial\Omega$ both be zero. Then set

$$\rho = -(\nabla \cdot V)t \ \text{ throughout } \ \Omega, \tag{3.3}$$

and

$$\sigma = (V\cdot n)t \ \text{ along } \ \partial\Omega. \tag{3.4}$$

Equation (3.3) for the volume charge density ρ is forced on us by the continuity equation,

$$\nabla \cdot V = -\partial\rho/\partial t. \tag{3.5}$$

Likewise, Eq. (3.4) for the surface charge density σ is forced on us by a version of the continuity equation appropriate to the boundary of our domain. The current V is simply carrying charge from locations within Ω and on its boundary to other such locations. Thus the surface charge density given by (3.4) has a time rate of change equal to the flux density of the current V through the boundary $\partial\Omega$.

Now the volume charge throughout Ω gives rise to a time varying electric field

$$E_\rho(y,t) = \left[(1/4\pi)\nabla_y \int_\Omega (\nabla_x \cdot V(x))/|y-x| \ \mathrm{d}(\mathrm{vol}_x) \right] t, \tag{3.6}$$

and the surface charge along $\partial\Omega$ gives rise to a time varying electric field,

$$E_\sigma(y,t) = \left[-(1/4\pi)\nabla_y \int_{\partial\Omega} V(x)\cdot n(x)/|y-x| \ \mathrm{d}(\mathrm{area}_x) \right] t, \tag{3.7}$$

both fields extending throughout 3-space.

The total electric field

$$E(y,t) = E_\rho(y,t) + E_\sigma(y,t) \tag{3.8}$$

has a time rate of change

$$\partial E/\partial t = \partial E_\rho/\partial t + \partial E_\sigma/\partial t = E'_\rho + E'_\sigma. \tag{3.9}$$

With this notation, the equation of Proposition 1 condenses to

$$\nabla \times \mathrm{BS}(V) = \{V/0\} + E'_\rho + E'_\sigma, \tag{3.10}$$

which is just Maxwell's Eq. (3.2). Proving Proposition 1 confirms these interpretations.

Proof of Proposition 1: We must evaluate

$$\begin{aligned}\nabla_y \times \mathrm{BS}(V)(y) &= \nabla_y \times (1/4\pi) \int_\Omega V(x) \times (y-x)/|y-x|^3 \ \ \mathrm{d}(\mathrm{vol}_x) \\ &= (1/4\pi) \int_\Omega \nabla_y \times \{V(x) \times (y-x)/|(y-x)|^3\} \ \ \mathrm{d}(\mathrm{vol}_x).\end{aligned} \tag{3.11}$$

We will need the following formula from vector calculus:

$$\nabla \times (A \times B) = (B \cdot \nabla)A - (A \cdot \nabla)B + A(\nabla \cdot B) - B(\nabla \cdot A). \tag{3.12}$$

Applying this formula to the integrand, we get

$$\begin{aligned}&\nabla_y \times \{V(x) \times (y-x)/|y-x|^3\} \\ &\quad = ((y-x)/|y-x|^3 \cdot \nabla_y) V(x) - (V(x) \cdot \nabla_y)((y-x)/|y-x|^3) \\ &\qquad + V(x) \nabla_y \cdot ((y-x)/|y-x|^3) - ((y-x)/|y-x|^3)(\nabla_y \cdot V(x)).\end{aligned} \tag{3.13}$$

The first and last terms on the right-hand side are zero, because they involve differentiation with respect to y of $V(x)$, which depends only on x. Thus,

$$\nabla_y \times \{V(x) \times (y-x)/|y-x|^3\} = V(x) \nabla_y \cdot ((y-x)/|y-x|^3) - (V(x) \cdot \nabla_y)((y-x)/|y-x|^3). \tag{3.14}$$

In the first term on the right-hand side, the second factor

$$\nabla_y \cdot ((y-x)/|y-x|^3) \tag{3.15}$$

is the divergence of the well known ''inverse square central field.'' Using spherical coordinates centered at x, this can be written as

$$\nabla \cdot \hat{r}/r^2 = (1/r^2)(\partial/\partial r)(r^2(1/r^2)) = 0, \tag{3.16}$$

away from the origin.

But the integral of $\nabla \cdot \hat{r}/r^2$ over any ball centered at the origin, when converted to a surface integral via the divergence theorem, is clearly 4π,

$$\int_{\mathrm{ball}} \nabla \cdot \hat{r}/r^2 \ \ \mathrm{d}(\mathrm{vol}) = \int_{\mathrm{sphere}} (\hat{r}/r^2) \cdot n \ \ \mathrm{d}(\mathrm{area}) = 4\pi. \tag{3.17}$$

Thus,

$$\nabla \cdot \hat{r}/r^2 = 4\pi \delta^3(r), \tag{3.18}$$

where $\delta^3(r)$ is the three-dimensional delta function; equivalently,

$$\nabla_y \cdot ((y-x)/|y-x|^3) = 4\pi\delta^3(y-x). \tag{3.19}$$

Hence,

$$(1/4\pi)\int_\Omega V(x)\nabla_y \cdot ((y-x)/|y-x|^3)\ \ \mathrm{d}(\mathrm{vol}_x) = (1/4\pi)\int_\Omega V(x) 4\pi\delta^3(y-x)\ \ \mathrm{d}(\mathrm{vol}_x)$$
$$= V(y)\ \ \text{in}\ \ \Omega\,/\,0\ \ \text{in}\ \ \Omega'. \tag{3.20}$$

Thus far, we have proved that

$$\nabla_y \times \mathrm{BS}(V)(y) = \{V(y)\,/\,0\} - (1/4\pi)\int_\Omega (V(x)\cdot\nabla_y)((y-x)/|y-x|^3)\ \ \mathrm{d}(\mathrm{vol}_x). \tag{3.21}$$

Now we focus on the second term on the right-hand side and must show that

$$-(1/4\pi)\int_\Omega (V(x)\cdot\nabla_y)((y-x)/|y-x|^3)\ \ \mathrm{d}(\mathrm{vol}_x)$$
$$= (1/4\pi)\nabla_y \int_\Omega (\nabla_x \cdot V(x))/|y-x|\ \ \mathrm{d}(\mathrm{vol}_x)$$
$$-(1/4\pi)\nabla_y \int_{\partial\Omega} V(x)\cdot n/|y-x|\ \ \mathrm{d}(\mathrm{area}_x). \tag{3.22}$$

We begin by writing each of the three terms in (3.22) in the form

$$\pm(1/4\pi)\nabla_y \int_\Omega (\text{something})\ \ \mathrm{d}(\mathrm{vol}_x). \tag{3.23}$$

Starting with the left-hand side of (3.22), we claim that its integrand can be rewritten as

$$(V(x)\cdot\nabla_y)((y-x)/|y-x|^3) = \nabla_y(V(x)\cdot(y-x)/|y-x|^3). \tag{3.24}$$

To see this, we need the formula from vector calculus,

$$\nabla(V\cdot W) = V\times(\nabla\times W) + W\times(\nabla\times V) + (V\cdot\nabla)W + (W\cdot\nabla)V. \tag{3.25}$$

We use this with $\nabla = \nabla_y$, $V = V(x)$, and $W = (y-x)/|y-x|^3$. Three of the four terms on the right-hand side of (3.25) will then be zero; the first is zero because $\nabla_y \times W = 0$; the second is zero because $\nabla_y \times V(x) = 0$; the fourth is zero because $(W\cdot\nabla_y)V(x) = 0$. Thus $\nabla_y(V\cdot W) = (V\cdot\nabla_y)W$, which is exactly our claim.

The first term on the right-hand side of (3.22) is already in the desired form.

The second term on the right-hand side of (3.22) can be rewritten as

$$\int_{\partial\Omega} V(x)\cdot n/|y-x|\ \ \mathrm{d}(\mathrm{area}_x) = \int_\Omega \nabla_x \cdot (V(x)/|y-x|)\ \ \mathrm{d}(\mathrm{vol}_x), \tag{3.26}$$

thanks to the divergence theorem.

Now that all the terms in (3.22) have been rewritten in the desired form, we claim that the integrands on both sides are equal, namely, that

$$-V(x)\cdot(y-x)/|y-x|^3 = (\nabla_x \cdot V(x))/|y-x| - \nabla_x \cdot (V(x)/|y-x|). \tag{3.27}$$

This is an immediate consequence of the formula

$$\nabla\cdot(fA)=(\nabla f)\cdot A+f(\nabla\cdot A), \tag{3.28}$$

and the proof of Proposition 1 is complete.

C. Examples

We give three examples to illustrate Proposition 1, each in ''bare bones'' format, and invite the interested reader to carry out the supporting calculations.

Example 1: In this example, we start with the vector field

$$V=\partial/\partial z=\hat{z} \tag{3.29}$$

on the ball Ω of radius a centered at the origin. Note that $V\epsilon\ \mathrm{CG}(\Omega)$.

Switching to spherical coordinates (r,θ,φ), a straightforward computation yields

$$\begin{aligned}\mathrm{BS}(V)&=(a^3/3)(\sin\theta)/r^2\hat{\varphi}\quad \text{for}\quad r\geqslant a\\ &=(1/3)r\sin\theta\hat{\varphi}\quad \text{for}\quad r\leqslant a.\end{aligned} \tag{3.30}$$

Note that inside the ball, $\mathrm{BS}(V)$ coincides with the velocity field of a body rotating with constant angular velocity about the z-axis.

Next we compute $\nabla\times\mathrm{BS}(V)$,

$$\nabla\times\mathrm{BS}(V)=(a^3/3)\{(2\cos\theta/r^3)\hat{r}+(\sin\theta/r^3)\hat{\theta}\}\quad \text{for}\quad r\geqslant a, \tag{3.31}$$

which is a standard dipole field, while

$$\nabla\times\mathrm{BS}(V)=(2/3)\{(\cos\theta)\hat{r}-(\sin\theta)\hat{\theta}\}=(2/3)V\quad \text{for}\quad r\leqslant a. \tag{3.32}$$

We invite the reader to check Proposition 1, equivalently the Maxwell equation (3.10), inside the domain Ω by directly computing that $E'_\sigma=(-1/3)V$ there.

Example 2 (see Example 4 of Sec. II C): In this example, we start with the function $f=1/r$ on the domain Ω between the spheres of radii 1 and 2 centered at the origin, and then consider the vector field

$$V=\nabla f=-\hat{r}/r^2 \tag{3.33}$$

on this domain. Note that the function f is harmonic, and is constant on each component of $\partial\Omega$. Therefore V lies in the subspace $\mathrm{HG}(\Omega)$ of harmonic gradients inside $\mathrm{VF}(\Omega)$. Borrowing once again from the future proof of Theorem B, we note that V lies in the kernel of the Biot–Savart operator.

We invite the reader to confirm Maxwell's equation (3.10) by checking that

$$\begin{aligned}E_\sigma&=\hat{r}/r^2\quad \text{inside}\quad \Omega,\\ &=0\qquad \text{outside}\quad \Omega.\end{aligned} \tag{3.34}$$

Example 3 (see Example 5 of Sec. II C): In this example, we start with the function $f(x,y,z)=x^2+y^2+z^2-1=r^2-1$ on the unit ball Ω centered at the origin, and then consider the vector field

$$V=\nabla f=2r\hat{r} \tag{3.35}$$

on this ball. Note that V lies in the subspace $\mathrm{GG}(\Omega)$ of grounded gradients inside $\mathrm{VF}(\Omega)$, and is therefore (borrowing from the future proof of Theorem B) in the kernel of the Biot–Savart operator BS.

With this in mind, we invite the reader to confirm Maxwell's equation (3.10) in this case by computing that

$$E_\rho = -2r\hat{r} \quad \text{inside } \Omega$$
$$= -2\hat{r}/r^2 \quad \text{outside } \Omega, \tag{3.36}$$

and that

$$E_\sigma = 0 \quad \text{inside } \Omega$$
$$= 2\hat{r}/r^2 \quad \text{outside } \Omega. \tag{3.37}$$

IV. PROOF OF THEOREM A

Recall the statement:

Theorem A: *The equation* $\nabla \times BS(V) = V$ *holds in* Ω *if and only if* V *is divergence-free and tangent to the boundary of* Ω.

The condition that V be divergence-free and tangent to the boundary of Ω can also be written as $V \epsilon \mathrm{K}(\Omega) = \mathrm{FK} \oplus \mathrm{HK}$, the subspace of fluid knots. For the same effort, we will also get

Addendum to Theorem A: *The equation* $\nabla \times BS(V) = 0$ *holds in the closure* Ω' *of* $R^3 - \Omega$ *if and only if* $V \epsilon FK \oplus HK \oplus HG \oplus GG$.

This condition on V is equivalent to V being orthogonal to the subspace CG of curly gradients in $\mathrm{VF}(\Omega)$. Then we will prove.

Corollary to Theorem A: *The vector potential* $A(V)$ *is divergence-free if and only if* V *is divergence-free and tangent to the boundary of* Ω.

A. Proof of Theorem A

Half of Theorem A has already appeared as item (7) in our list of Standard Information, and was proved in Sec. III B, namely, if $V \epsilon \mathrm{K}(\Omega) = \mathrm{FK} \oplus \mathrm{HK}$, then $\nabla \times \mathrm{BS}(V) = V$ in Ω.

By contrast, if $V \epsilon$ HG$\oplus$GG, then it would be impossible for $\nabla \times \mathrm{BS}(V)$ to equal V in Ω unless $V = 0$, since we know from the Hodge Decomposition Theorem that the image of curl is FK$\oplus$HK$\oplus$CG.

It remains to show that if V is in CG, then $\nabla \times \mathrm{BS}(V)$ can never equal V in Ω unless $V = 0$.

The proof will be based on the Maxwell equation,

$$\nabla_y \times \mathrm{BS}(V)(y) = \{V(y) \text{ in } \Omega \,/\, 0 \text{ in } \Omega'\} - (1/4\pi)\nabla_y \int_{x \epsilon \partial\Omega} V(x) \cdot n(x)/|x-y| \ \mathrm{d}(\mathrm{area}_x). \tag{4.1}$$

Following our discussion in Sec. III B, we can write the second term on the right-hand side of this equation as

$$E'_\sigma(y) = -(1/4\pi)\nabla_y \int_{x \epsilon \partial\Omega} V(x) \cdot n(x)/|x-y| \ \mathrm{d}(\mathrm{area}_x). \tag{4.2}$$

Although E'_σ is the time rate of change of the electrostatic field E_σ, it is also the same as the electrostatic field due to a charge density $\sigma(x) = V(x) \cdot n(x)$ along $\partial\Omega$, and so we can treat it as though it were an electrostatic field.

We write

$$E'_\sigma(y) = -\nabla_y \psi(y), \tag{4.3}$$

where

$$\psi(y) = (1/4\pi) \int_{x \in \partial\Omega} V(x) \cdot n(x) / |x-y| \ \ \mathrm{d}(\mathrm{area}_x). \tag{4.4}$$

Although we have in general been writing our gradient fields with a plus sign, as in the equation $V = \nabla\varphi$, we write electrostatic fields with a minus sign, $E'_\sigma = -\nabla\psi$, to follow standard convention.

While the electrostatic potential function ψ for a surface charge distribution σ is continuous, the electrostatic field E'_σ will in general have a jump discontinuity as we cross the surface. Nevertheless, we have $\nabla \cdot E'_\sigma = 0$ in Ω and $\nabla \cdot E'_\sigma = 0$ in Ω'.

We claim that if V is a nonzero vector field in CG, then E'_σ cannot be identically zero in Ω.

Recall the definition of the subspace CG of curly gradients. A smooth vector field V defined on Ω is in CG if and only if $V = \nabla\varphi$, where φ is a harmonic function on Ω, and where the flux of V through each component of $\partial\Omega$ is zero. That is, for each component $\partial\Omega_i$ of $\partial\Omega$, we have

$$\int_{\partial\Omega_i} V(x) \cdot n(x) \ \ \mathrm{d}(\mathrm{area}_x) = \int_{\partial\Omega_i} \sigma(x) \ \ \mathrm{d}(\mathrm{area}_x) = 0. \tag{4.5}$$

In other words, the total charge on each component of $\partial\Omega$ is zero.

Suppose now that $E'_\sigma = 0$ in Ω. We must show that $V = 0$.

First we will show that $E'_\sigma = 0$ in Ω', the closure of $R^3 - \Omega$.

The hypothesis that $E'_\sigma = 0$ inside Ω tells us that ψ must be constant on each component $\partial\Omega_i$ of $\partial\Omega' = \partial\Omega$.

Now we consider the field $\psi E'_\sigma$ in Ω', and compute its divergence (a standard trick in electrostatics),

$$\nabla \cdot (\psi E'_\sigma) = (\nabla\psi) \cdot E'_\sigma + \psi(\nabla \cdot E'_\sigma) = -E'_\sigma \cdot E'_\sigma = -|E'_\sigma|^2. \tag{4.6}$$

Hence,

$$\int_{\Omega'} |E'_\sigma|^2 \ \ \mathrm{d}(\mathrm{vol}) = -\int_{\Omega'} \nabla \cdot (\psi E'_\sigma) \ \ \mathrm{d}(\mathrm{vol}) = -\int_{\partial\Omega'} \psi E'_\sigma \cdot n' \, \mathrm{d}(\mathrm{area}), \tag{4.7}$$

where n' is the unit outward-pointing normal vector to Ω', so that $n' = -n$.

Using the divergence theorem in Ω' requires a comment, since one of its components is unbounded. That unbounded component should really be approximated by a bounded domain with one boundary component out near infinity. The flux of $\psi E'_\sigma$ through this boundary component goes to zero as it recedes towards infinity, because the area grows like r^2, while the field E'_σ decays like $1/r^2$ and the potential ψ decays like $1/r$.

With that said, we continue,

$$\int_{\Omega'} |E'_\sigma|^2 \ \ \mathrm{d}(\mathrm{vol}) = -\int_{\partial\Omega'} \psi E'_\sigma \cdot n' \, \mathrm{d}(\mathrm{area}) = -\sum_i \ \psi_i \int_{\partial\Omega_i} E'_\sigma \cdot n' \, \mathrm{d}(\mathrm{area}), \tag{4.8}$$

since ψ is constant, say with value ψ_i, on each component $\partial\Omega_i$ of the boundary.

Now, by Gauss' Law,

$$\begin{aligned} \int_{\partial\Omega_i} E'_\sigma \cdot n' \, d(\mathrm{area}) &= \pm \,\text{total charge ``inside'' } \partial\Omega_i \\ &= \pm \sum_{\text{some } j} \int_{\partial\Omega_j} \sigma(x) \ \ \mathrm{d}(\mathrm{area}_x) = 0, \end{aligned} \tag{4.9}$$

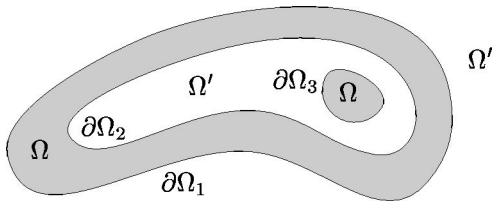

FIG. 1. Components of the domain Ω and of its complement, Ω'.

because the total charge on *each* component $\partial\Omega_j$ of $\partial\Omega$ is zero (see Fig. 1).

Thus, $\int_{\Omega'}|E'_\sigma|^2 d(\mathrm{vol})=0$, and hence $E'_\sigma\equiv 0$ in Ω'.

Now we have $E'_\sigma\equiv 0$ in Ω and also in Ω'. Then Gauss's Law, applied to the typical ''pill box'' neighborhood of a point on $\partial\Omega$, implies that the surface charge distribution σ is identically zero (see Fig. 2).

Since $\sigma(x)=V(x)\cdot n(x)$, this imples that V is tangent to the boundary of Ω, and hence $V\in \mathrm{K}(\Omega)$. But $\mathrm{K}(\Omega)\cap \mathrm{CG}=0$, so $V=0$.

This completes the proof of Theorem A.

B. Proof of Addendum to Theorem A

We know that if V lies in $\mathrm{K}(\Omega)=\mathrm{FK}\oplus\mathrm{HK}$, then $\nabla\times \mathrm{BS}(V)=0$ in Ω', according to item (7) in our list of Standard Information from Sec. III A.

Borrowing from the future, we will see in the proof of Theorem B that if $V\epsilon \mathrm{HG}\oplus\mathrm{GG}$, then $\mathrm{BS}(V)=0$ throughout 3-space, so that surely $\nabla\times \mathrm{BS}(V)=0$ in Ω'.

This gives us half of the Addendum to Theorem A.

It remains to show that if V is in CG, then $\nabla\times \mathrm{BS}(V)$ cannot be zero in Ω' unless $V=0$ in Ω.

The proof of this is based on the Maxwell equation (4.1), as was the proof of Theorem A; it is a copy of the argument given there, with the roles of Ω and Ω' reversed, so we omit further details.

C. Proof of Corollary to Theorem A

If V is divergence-free and tangent to the boundary of Ω, then we already know from item (5) in the list of Standard Information that the vector potential $A(V)$ is divergence-free.

Recall, also from that list, items

(3) $\Delta \mathrm{A}(V)=-V$, and

(4) $\nabla\times \mathrm{A}(V)=\mathrm{BS}(V)$ for all $V\epsilon$ $\mathrm{VF}(\Omega)$.

Now take the second derivative formula,

$$\nabla\times(\nabla\times W)=\nabla(\nabla\cdot W)-\Delta W \tag{4.10}$$

for any vector field W, and rewrite it with $\mathrm{A}(V)$ in place of W,

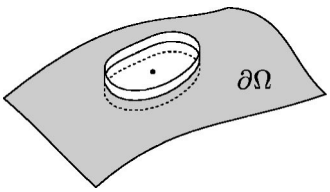

FIG. 2. A typical ''pill box'' neighborhood of a point on $\partial\Omega$.

$$\nabla\times(\nabla\times \mathrm{A}(V))=\nabla(\nabla\cdot \mathrm{A}(V))-\Delta \mathrm{A}(V). \tag{4.11}$$

Using items (3) and (4) above, substitute $\mathrm{BS}(V)$ for $\nabla\times \mathrm{A}(V)$ on the left-hand side, and V for $-\Delta \mathrm{A}(V)$ on the right-hand side, to get

$$\nabla\times \mathrm{BS}(V)=\nabla(\nabla\cdot \mathrm{A}(V))+V. \tag{4.12}$$

If $\mathrm{A}(V)$ is divergence-free, then we get

$$\nabla\times \mathrm{BS}(V)=V \quad \text{inside } \Omega, \tag{4.13}$$

which by Theorem A implies that $V\epsilon\, \mathrm{K}(\Omega)$.

We conclude that $\mathrm{A}(V)$ is divergence-free if and only if $V\epsilon\, \mathrm{K}(\Omega)$, which is exactly the assertion of the Corollary.

V. PROOF OF THEOREM B

A. Proof of Theorem B, easy direction

Recall the statement:

Theorem B: *The kernel of the Biot–Savart operator is precisely the space of gradient vector fields which are orthogonal to the boundary of* Ω.

The easy direction is to assume that V is a gradient vector field which is orthogonal to the boundary of Ω (equivalently, that $V\epsilon\, \mathrm{HG}\oplus\mathrm{GG}$), and then conclude that $\mathrm{BS}(V)=0$. We will do that here, and will actually show that $\mathrm{BS}(V)=0$ throughout all of 3-space, rather than just in Ω.

We begin with the following lemma, which is stated without proof on p. 60 of Griffiths.[46]

Lemma 1: *Let V be a smooth vector field on the domain* Ω*, and let n denote the outward pointing unit normal vector field to* $\partial\Omega$*. Then,*

$$\int_\Omega \nabla\times V\, \mathrm{d}(\mathrm{vol})=-\int_{\partial\Omega} V\times n\, \mathrm{d}(\mathrm{area}).$$

Proof: Start with the Divergence Theorem,

$$\int_\Omega \nabla\cdot V \mathrm{d}(\mathrm{vol})=\int_{\partial\Omega} V\cdot n\ \ \mathrm{d}(\mathrm{area}).$$

Then replace V by $V\times C$, where C is any constant vector,

$$\int_\Omega \nabla\cdot(V\times C)\ \ \mathrm{d}(\mathrm{vol})=\int_{\partial\Omega}(V\times C)\cdot n\ \ \mathrm{d}(\mathrm{area}).$$

Writing $\nabla\cdot(V\times C)=(\nabla\times V)\cdot C$ and moving C outside the integral, the left-hand side becomes

$$C\cdot\int_\Omega \nabla\times V\ \ \mathrm{d}(\mathrm{vol}).$$

Writing $(V\times C)\cdot n=-(V\times n)\cdot C$ and again moving C outside the integral, the right-hand side becomes

$$-C\cdot\int_{\partial\Omega} V\times n\ \ \mathrm{d}(\mathrm{area}).$$

Since the left- and right-hand sides are equal for all C, we must have

$$\int_\Omega \nabla \times V \ \ \mathrm{d}(\mathrm{vol}) = -\int_{\partial\Omega} V \times n \ \ \mathrm{d}(\mathrm{area}),$$

proving the lemma.

Suppose now that $V = \nabla\varphi$ is a gradient vector field on Ω which is orthogonal to the boundary, which means that φ is constant on each component $\partial\Omega_i$ of $\partial\Omega$. We must show that $\mathrm{BS}(V) = 0$.

Begin with the formula for the Biot–Savart operator,

$$\mathrm{BS}(V)(y) = (1/4\pi)\int_\Omega V(x) \times (y-x)/|y-x|^3 \ \ \mathrm{d}(\mathrm{vol}_x). \tag{5.1}$$

Fix y, and let $W = (y-x)/|y-x|^3$. Then,

$$\mathrm{BS}(V) = (1/4\pi)\int_\Omega (\nabla\varphi) \times W \ \ \mathrm{d}(\mathrm{vol}). \tag{5.2}$$

Now consider the vector field φW on Ω and take its curl,

$$\nabla \times (\varphi W) = (\nabla\varphi) \times W + \varphi(\nabla \times W) = (\nabla\varphi) \times W, \tag{5.3}$$

since $\nabla \times W = 0$. Thus

$$\mathrm{BS}(V) = (1/4\pi)\int_\Omega \nabla \times (\varphi W) \ \ \mathrm{d}(\mathrm{vol}). \tag{5.4}$$

We would like to use the preceding lemma to replace the right-hand side of this formula by the expression

$$-(1/4\pi)\int_{\partial\Omega} (\varphi W) \times n \ \ \mathrm{d}(\mathrm{area}). \tag{5.5}$$

But the vector field φW does not quite fit the hypothesis of the lemma, since it has an isolated singularity at the point y (which we can assume is in the interior of Ω). However, this singularity is ''radial;'' if we surround it by a small sphere, the vector field φW will be orthogonal to the sphere, and so the integral $\int (\varphi W) \times n \ \ \mathrm{d}(\mathrm{area})$ over this small sphere will be zero. It follows immediately that the lemma can be applied in this case, in spite of the singularity.

We do so, and continue

$$\begin{aligned} \mathrm{BS}(V) &= -(1/4\pi)\int_{\partial\Omega} (\varphi W) \times n \ \ \mathrm{d}(\mathrm{area}) \\ &= -(1/4\pi)\sum_i \varphi_i \int_{\partial\Omega_i} W \times n \ \ \mathrm{d}(\mathrm{area}), \end{aligned} \tag{5.6}$$

where φ_i is the constant value of φ on $\partial\Omega_i$.

Now we claim that, for each i,

$$\int_{\partial\Omega_i} W \times n \ \ \mathrm{d}(\mathrm{area}) = 0. \tag{5.7}$$

To see this, let Ω_i be the compact domain in 3-space bounded by $\partial\Omega_i$. Then, using the lemma once again,

$$\int_{\partial\Omega_i} W\times n \ \ \mathrm{d(area)} = \pm \int_{\Omega_i} \nabla\times W \ \ \mathrm{d(vol)} \tag{5.8}$$

with the + or − sign chosen according as n points into or out of Ω_i. In any case, $\nabla\times W=0$, so the integral vanishes.

Thus $\mathrm{BS}(V)=0$ throughout 3-space.

B. Proof of Theorem B, harder direction

The heart of the argument is the following energy estimate.

Proposition 2: *Let Ω be a compact domain with smooth boundary in 3-space, and V a smooth divergence-free vector field defined in Ω. Let E'_σ be the electrostatic field due to the charge distribution $\sigma(x)=V(x)\cdot n(x)$ along $\partial\Omega$. Then,*

$$\int_{3\text{-space}} |E'_\sigma|^2 \ \ \mathrm{d(vol)} \leqslant \int_\Omega |V|^2 \ \ \mathrm{d(vol)}.$$

That is, the energy of the electrostatic field E'_σ throughout all of 3-space is bounded from above by the energy of the original field V in Ω.

When V is not required to be divergence-free, the energy of the field E'_σ can be made arbitrarily large, while keeping the energy of V itself as small as desired: make $V(x)\cdot n(x)$ large along $\partial\Omega$, and then quickly taper V off to zero throughout most of Ω.

Proof of Proposition 2: Given a divergence-free vector field V, we can subtract from V its orthogonal projection into the space $\mathrm{K}(\Omega)=\mathrm{FK}\oplus\mathrm{HK}$ of fluid knots. This will leave the corresponding electrostatic field E'_σ unchanged, while at worst decreasing the energy in V.

So in proving the proposition, there is no loss in generality in assuming that V is already orthogonal to this subspace, and hence a gradient vector field...as well as being divergence-free. Thus we can write

$$V=\nabla\varphi \ \ \text{with} \ \ \Delta\varphi=0. \tag{5.9}$$

Likewise,

$$E'_\sigma(y)=-\nabla_y\psi(y), \tag{5.10}$$

where

$$\psi(y)=(1/4\pi)\int_{x\in\partial\Omega} V(x)\cdot n(x)/|x-y| \ \ \mathrm{d(area}_x). \tag{5.11}$$

Lemma 2: $$\int_{3\text{-space}} |E'_\sigma|^2 \mathrm{d(vol)} = \int_{\partial\Omega} \psi\partial\varphi/\partial n \,\mathrm{d(area)}.$$

Proof of Lemma 2: This is a standard result in electrostatics; see Griffiths[46] pp. 94–95. For convenience, we give the argument here.

Since the surface charge distribution σ along $\partial\Omega$ is given by

$$\sigma(x)=V(x)\cdot n(x)=(\nabla\varphi(x))\cdot n(x)=(\partial\varphi/\partial n)(x), \tag{5.12}$$

we can rewrite the equation to be proved as

$$\int_{3\text{-space}} |E'_\sigma|^2 \ \ \mathrm{d(vol)} = \int_{\partial\Omega} \psi\sigma \ \ \mathrm{d(area)}. \tag{5.13}$$

This more clearly displays the relation of the integrand on the right-hand side to the field E'_σ; the function σ is the surface charge distribution along $\partial\Omega$ which gives rise to the field E'_σ, while the function ψ is the electrostatic potential for E'_σ, that is, $E'_\sigma = -\nabla\psi$.

The proof is a little easier to express if we replace the surface charge distribution σ by a volume charge distribution ρ in a small neighborhood $N(\partial\Omega)$ of $\partial\Omega$, and let $E'_\rho = -\nabla\psi$ be the resulting electrostatic field, because in this situation we can write $\nabla \cdot E_\rho = \rho$.

With this understanding, we must show that

$$\int_{3\text{-space}} |E'_\rho|^2 \ \mathrm{d(vol)} = \int_{N(\partial\Omega)} \psi\rho \ \mathrm{d(vol)}. \tag{5.14}$$

To prove this, rewrite the integral on the right-hand side as

$$\int_{N(\partial\Omega)} \psi(\nabla \cdot E'_\rho) \ \mathrm{d(vol)}. \tag{5.15}$$

Next,

$$\nabla \cdot (\psi E'_\rho) = (\nabla\psi) \cdot E'_\rho + \psi(\nabla \cdot E'_\rho) = -|E'_\rho|^2 + \psi(\nabla \cdot E'_\rho). \tag{5.16}$$

Hence

$$\begin{aligned} \int_{N(\partial\Omega)} \psi\rho \ \mathrm{d(vol)} &= \int_{N(\partial\Omega)} \psi(\nabla \cdot E'_\rho) \ \mathrm{d(vol)} \\ &= \int_{N(\partial\Omega)} \nabla \cdot (\psi E'_\rho) \ \mathrm{d(vol)} + \int_{N(\partial\Omega)} |E'_\rho|^2 \ \mathrm{d(vol)}. \end{aligned} \tag{5.17}$$

If, in the integral on the left-hand side above, we replace the neighborhood $N(\partial\Omega)$ by any larger domain, call it Ω^*, the value of the integral will not change because $\rho = 0$ outside $N(\partial\Omega)$. And the equation above will still hold if we replace $N(\partial\Omega)$ by Ω^* in each of the three integrals,

$$\int_{\Omega^*} \psi\rho \ \mathrm{d(vol)} = \int_{\Omega^*} \nabla \cdot (\psi E'_\rho) \ \mathrm{d(vol)} + \int_{\Omega^*} |E'_\rho|^2 \ \mathrm{d(vol)}. \tag{5.18}$$

Apply the divergence theorem to the first integral on the right-hand side, so that we now have

$$\int_{\Omega^*} \psi\rho \ \mathrm{d(vol)} = \int_{\partial\Omega^*} (\psi E'_\rho) \cdot n \ \mathrm{d(area)} + \int_{\Omega^*} |E'_\rho|^2 \ \mathrm{d(vol)}. \tag{5.19}$$

Visualize the domain Ω^* growing larger and larger, with its boundary receding towards infinity. Then ψ decays like $1/r$, while E'_ρ decays like $1/r^2$ and the area of $\partial\Omega^*$ grows like r^2. Thus the value of the first integral on the right-hand side decays like $1/r$, and so goes to zero in the limit. Hence

$$\int_{N(\partial\Omega)} \psi\rho \ \mathrm{d(vol)} = \int_{3\text{-space}} |E'_\rho|^2 \ \mathrm{d(vol)}, \tag{5.20}$$

the desired result for volume charge distributions.

If we compress the neighborhood $N(\partial\Omega)$ towards the surface $\partial\Omega$, the above result for volume charge distributions will tend to the corresponding result for surface charge distributions,

$$\int_{\partial\Omega} \psi\sigma \ \mathrm{d(area)} = \int_{3\text{-space}} |E'_\sigma|^2 \ \mathrm{d(vol)}, \tag{5.21}$$

and the lemma is proved.

Completion of the proof of Proposition 2: Now we recall Green's first identity.

Let $A=\psi\nabla\varphi$. Then

$$\nabla\cdot A=\nabla\cdot(\psi\nabla\varphi)=\nabla\psi\cdot\nabla\varphi+\psi\Delta\varphi=\nabla\psi\cdot\nabla\varphi, \tag{5.22}$$

since $\Delta\varphi=0$.

Thus,

$$\int_\Omega -E'_\sigma\cdot V \ \ \mathrm{d(vol)}=\int_\Omega \nabla\psi\cdot\nabla\varphi \ \ \mathrm{d(vol)}=\int_\Omega \nabla\cdot A \ \ \mathrm{d(vol)}=\int_{\partial\Omega} A\cdot n \ \ \mathrm{d(area)}$$
$$=\int_{\partial\Omega}\psi\nabla\varphi\cdot n \ \ \mathrm{d(area)}=\int_{\partial\Omega}\psi\partial\varphi/\partial n \ \ \mathrm{d(area)}=\int_{3\text{-space}}|E'_\sigma|^2 \ \ \mathrm{d(vol)}, \tag{5.23}$$

by the lemma.

Hence,

$$\int_{3\text{-space}}|E'_\sigma|^2 \ \ \mathrm{d(vol)}=\int_\Omega -E'_\sigma\cdot V\mathrm{d(vol)}$$
$$\leqslant\left(\int_\Omega|E'_\sigma|^2 \ \ \mathrm{d(vol)}\right)^{1/2}\left(\int_\Omega|V|^2 \ \ \mathrm{d(vol)}\right)^{1/2}$$
$$\leqslant\left(\int_{3\text{-space}}|E'_\sigma|^2 \ \ \mathrm{d(vol)}\right)^{1/2}\left(\int_\Omega|V|^2 \ \ \mathrm{d(vol)}\right)^{1/2}, \tag{5.24}$$

and therefore

$$\int_{3\text{-space}}|E'_\sigma|^2 \ \ \mathrm{d(vol)}\leqslant\int_\Omega|V|^2 \ \ \mathrm{d(vol)}, \tag{5.25}$$

as claimed, finishing the proof of Proposition 2.

Completion of the proof of Theorem B: In the previous section, we showed that HG⊕GG, the space of gradient vector fields which are orthogonal to the boundary of Ω, lies within the kernel of the Biot–Savart operator $\mathrm{BS}:\mathrm{VF}(\Omega)\to\mathrm{VF}(\Omega)$.

Now we must show that there is nothing else in the kernel.

We will do this by assuming that V is orthogonal to GG (equivalently, is divergence-free) and that $\mathrm{BS}(V)=0$, and will show that V must lie in HG.

First we observe that, under these assumptions, V must be a gradient vector field.

To see this, consider the Maxwell equation in Ω,

$$\nabla_y\times\mathrm{BS}(V)(y)=V(y)-(1/4\pi)\nabla_y\int_{x\in\partial\Omega}V(x)\cdot n(x)/|x-y| \ \ \mathrm{d(area}_x), \tag{5.26}$$

written in the form appropriate for any divergence-free vector field V.

If V had a nonzero component in the subspace FK⊕HK of fluid knots, then that component would persist when we computed $\nabla\times\mathrm{BS}(V)$, since the Maxwell equation tells us that $\nabla\times\mathrm{BS}(V)$ differs from V by a gradient vector field. It follows that no such V could possibly be in the kernel of BS.

So we can assume that V is a gradient vector field, and write $V=\nabla\varphi$. Since V is orthogonal to GG, the function φ must be harmonic. To show that V lies in HG, we must show that the function φ is constant on each component of $\partial\Omega$.

To start on this, note that the second term on the right-hand side in the Maxwell equation above is the electrostatic field $E'_\sigma(y)$, and write that equation more succinctly as

$$\nabla \times \mathrm{BS}(V) = V + E'_\sigma. \tag{5.27}$$

Now if $\mathrm{BS}(V)=0$, then $E'_\sigma = -V$ in Ω.

It follows that E'_σ must be identically zero outside Ω because, by Proposition 2, it simply has no more energy.

This, in turn, implies that the electrostatic potential function ψ for the field E'_σ must be constant on each component of $\partial\Omega$.

But the three equations,

$$E'_\sigma = -\nabla\psi \quad (\text{everywhere}), \tag{5.28}$$

$$V = \nabla\varphi \quad (\text{inside } \Omega), \tag{5.29}$$

$$E'_\sigma = -V \quad (\text{inside } \Omega), \tag{5.30}$$

tell us that

$$\nabla\varphi = \nabla\psi \quad (\text{inside } \Omega), \tag{5.31}$$

and hence that

$$\varphi = \psi + \text{ some constant} \tag{5.32}$$

on each component of Ω, where the constant may depend on the component.

Thus φ inherits from ψ the property of being constant on each component of $\partial\Omega$, and hence $V=\nabla\varphi$ must lie in HG, the desired conclusion.

This completes the proof of Theorem B.

In fact, we have actually proved a bit more.

Theorem B′: *The kernel of $\nabla\times BS$, the composition of the curl and Biot–Savart operators, is also the space of gradient vector fields which are orthogonal to the boundary of Ω.*

This follows, with no further argument, because the only way we used the hypothesis that $\mathrm{BS}(V)=0$ in this section was to set $\nabla\times\mathrm{BS}(V)=0$ on the left-hand side of the Maxwell equation (5.27).

VI. PROOF OF THEOREM C

A. Statement and proof of Theorem C

Recall the statement:

Theorem C: *The image of the Biot–Savart operator is a proper subspace of the image of curl, whose orthogonal projection into the subspace of ''fluxless knots'' is one-to-one.*

This will follow immediately from Theorems B and B′ and (borrowing from the future) from Theorem D.

Proof:

Keep in mind the Hodge decomposition,

$$\mathrm{VF}(\Omega) = \mathrm{FK}\oplus\mathrm{HK}\oplus\mathrm{CG}\oplus\mathrm{HG}\oplus\mathrm{GG}. \tag{6.1}$$

We know from Theorem B that the kernel of the Biot–Savart operator BS is the subspace $\mathrm{HG}\oplus\mathrm{GG}$ of $\mathrm{VF}(\Omega)$.

We know from Theorem D that this operator is self-adjoint.

It follows that the image of BS lies within the orthogonal complement of its kernel, that is, within the subspace $\mathrm{FK}\oplus\mathrm{HK}\oplus\mathrm{CG}$, which is precisely the image of curl.

Alternatively, the formula $\nabla \times \mathrm{A}(V) = \mathrm{BS}(V)$, which appeared as item (4) on our list of Standard Information in Sec. III A, also tells us that the image of BS lies within the image of curl.

Now it follows from Theorems B and B′ together that

$$\mathrm{Image}(\mathrm{BS}) \cap \mathrm{Ker}(\mathrm{curl}) = \{0\}, \tag{6.2}$$

and since, by the Hodge Decomposition Theorem, the kernel of curl is $\mathrm{HK} \oplus \mathrm{CG} \oplus \mathrm{HG} \oplus \mathrm{GG}$, the orthogonal projection of the image of BS into FK must be one-to-one.

From this it also follows that the image of the BS is a proper subspace of the image of curl.

This completes the proof of Theorem C.

B. Impossible magnetic fields

We are looking for smooth vector fields U on a compact, smoothly bounded domain Ω in 3-space, for which it is impossible to find a smooth vector field V on Ω satisfying the equation $U = \mathrm{BS}(V)$. We will call such a field U an impossible magnetic field.

Of course, Eq. (6.2) tells us that any nonzero vector field U in $\mathrm{HK} \oplus \mathrm{CG} \oplus \mathrm{HG} \oplus \mathrm{GG}$ is an impossible magnetic field.

But here is a more interesting example.

Consider the velocity vector field U of a ''speeding bullet,'' as pictured below (see Fig. 3).

We visualize the unit ball Ω in 3-space as a lead bullet sitting in a cartridge which has been shot directly upwards from a rifled barrel, so that it spins as it moves forward. In cylindrical coordinates r, φ, z, the velocity vector field U is given by

$$U = r\hat{\varphi} + \hat{z}. \tag{6.3}$$

Note that the first summand $r\hat{\varphi}$ lies in FK, while the second summand $\hat{z}$ lies in CG.

Now look back to Example 1 in Sec. III C. There we started with the vector field $V = \hat{z}$ on the unit ball Ω and computed its magnetic field within the ball,

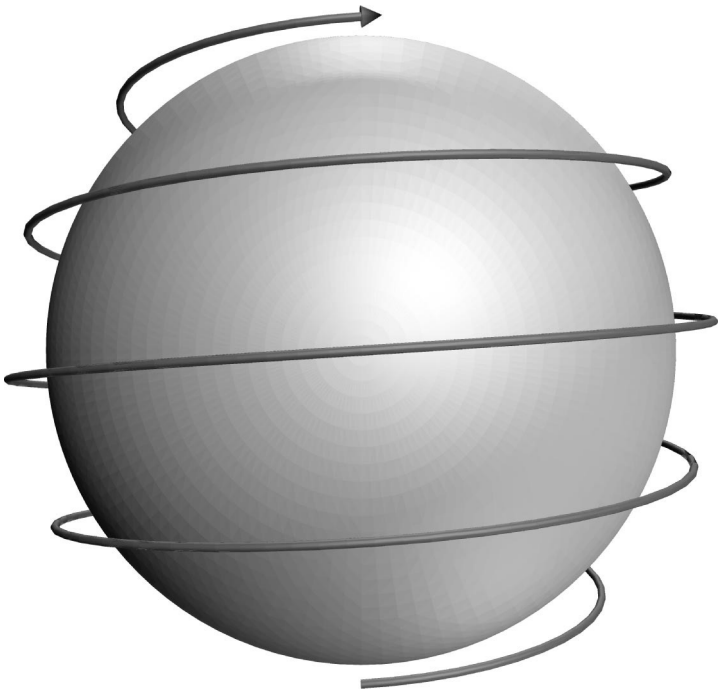

FIG. 3. An impossible magnetic field on the unit ball Ω.

$$\begin{aligned} \mathrm{BS}(V) &= (1/3) r \sin\theta \hat{\varphi} \quad \text{(spherical coordinates)} \\ &= (1/3) r \hat{\varphi} \quad \text{(cylindrical coordinates)}. \end{aligned} \tag{6.4}$$

So of course (settling back to cylindrical coordinates),

$$\mathrm{BS}(3V) = r\hat{\varphi}. \tag{6.5}$$

But this magnetic field on the unit ball ''poisons'' U as a candidate magnetic field, since U and $\mathrm{BS}(3V)$ have the same orthogonal projection into the space FK of fluxless knots. By Theorem C, the vector field U cannot possibly be the Biot–Savart transform of any smooth vector field on Ω.

VII. PROOF OF THEOREM D

It will be convenient to divide the statement and proof of Theorem D into three pieces, as follows:

(1) The Biot–Savart operator $\mathrm{BS}:\mathrm{VF}(\Omega)\to\mathrm{VF}(\Omega)$ is bounded, and hence extends to a bounded operator on the L^2 completion,

$$\mathrm{BS}:\overline{\mathrm{VF}}(\Omega)\to\overline{\mathrm{VF}}(\Omega);$$

(2) The operator $\mathrm{BS}:\overline{\mathrm{VF}}(\Omega)\to\overline{\mathrm{VF}}(\Omega)$ is compact, that is, it takes the unit ball in $\overline{\mathrm{VF}}(\Omega)$ to a set with compact closure in $\overline{\mathrm{VF}}(\Omega)$;

(3) The operator $\mathrm{BS}:\overline{\mathrm{VF}}(\Omega)\to\overline{\mathrm{VF}}(\Omega)$ is self-adjoint with respect to the L^2 inner product, that is, $\langle V_1, \mathrm{BS}(V_2)\rangle = \langle \mathrm{BS}(V_1), V_2\rangle$, for all vector fields V_1 and V_2 in $\overline{\mathrm{VF}}(\Omega)$.

A. A useful lemma

The proof that the Biot–Savart operator is bounded, as asserted in (1) above, will follow along the lines of the usual Young's inequality proof that convolution operators are bounded; see Folland,[47] p. 9, or Zimmer,[48] Proposition B.3 on p. 10. We extract this proof as a lemma, so that we can use it again in the proof of part (2).

Lemma 3: *Let $\phi(x)$ be a scalar-valued function with the property that*

$$N_\Omega(\phi) = \max_y \int_\Omega |\phi(y-x)| \ \ \mathrm{d}(\mathrm{vol}_x)$$

is finite, where the maximum is over all points $y \epsilon R^3$. Then the operator $T_\phi : \mathrm{VF}(\Omega)\to\mathrm{VF}(\Omega)$ defined by

$$T_\phi(V)(y) = \int_\Omega V(x) \times \phi(y-x) \, \frac{y-x}{|y-x|} \, \mathrm{d}(\mathrm{vol}_x)$$

is a bounded map with respect to the L^2 norm, and furthermore,

$$|T_\phi(V)| \leq N_\Omega(\phi)|V|.$$

Proof: Fix $y \epsilon \Omega$. Then, using the Cauchy–Schwarz inequality,

$$
\begin{aligned}
|T_\phi(V)(y)| &\leq \int_\Omega |V(x)||\phi(y-x)| \ \ \mathrm{d}(\mathrm{vol}_x) \\
&= \int_\Omega |V(x)\{\phi(y-x)\}^{1/2}| \ \ |\{\phi(y-x)\}^{1/2}| \ \ \mathrm{d}(\mathrm{vol}_x) \\
&\leq \left(\int_\Omega |V(x)|^2 |\phi(y-x)| \ \ \mathrm{d}(\mathrm{vol}_x) \right)^{1/2} \left(\int_\Omega |\phi(y-x)| \ \ \mathrm{d}(\mathrm{vol}_x) \right)^{1/2} \\
&\leq (N_\Omega(\phi))^{1/2} \left(\int_\Omega |\phi(y-x)| \ \ |V(x)|^2 \ \ \mathrm{d}(\mathrm{vol}_x) \right)^{1/2}. \qquad (7.1)
\end{aligned}
$$

We square both sides, integrate and use Fubini's theorem to get

$$
\begin{aligned}
\int_\Omega |T_\phi(V)(y)|^2 \ \ \mathrm{d}(\mathrm{vol}_y) &\leq N_\Omega(\phi) \int_\Omega \int_\Omega |\phi(y-x)||V(x)|^2 \ \ \mathrm{d}(\mathrm{vol}_x) \ \ \mathrm{d}(\mathrm{vol}_y) \\
&= N_\Omega(\phi) \int_\Omega |V(x)|^2 \left(\int_\Omega |\phi(y-x)| \ \ \mathrm{d}(\mathrm{vol}_y) \right) \mathrm{d}(\mathrm{vol}_x) \\
&\leq N_\Omega(\phi)^2 \int_\Omega |V(x)|^2 \ \ \mathrm{d}(\mathrm{vol}_x). \qquad (7.2)
\end{aligned}
$$

Taking square roots, we get

$$
|T_\phi(V)| \leq N_\Omega(\phi)|V|, \qquad (7.3)
$$

and conclude that T_ϕ is a bounded operator whose norm is at most $N_\Omega(\phi)$, as claimed.

B. Proof of (1)

Define the *optical size* of Ω, written $\mathrm{OS}(\Omega)$, to be the number

$$
\mathrm{OS}(\Omega) = \max_y \int_\Omega 1/|y-x|^2 \ \ \mathrm{d}(\mathrm{vol}_x), \qquad (7.4)
$$

where the maximum is taken over all points $y \in R^3$. The integral just above can be taken as a measure of the effort required to optically scan the domain Ω from the location y; the optical size of Ω is the maximum effort required to scan it from any location.

Then, in the language of Lemma 3,

$$
\begin{aligned}
\mathrm{BS}(V)(y) &= (1/4\pi) \int_\Omega V(x) \times (y-x)/|y-x|^3 \ \ \mathrm{d}(\mathrm{vol}_x) \\
&= T_{\phi_0}(V)(y), \qquad (7.5)
\end{aligned}
$$

where

$$
\phi_0(y-x) = (1/4\pi)(1/|y-x|^2). \qquad (7.6)
$$

The lemma yields immediately that, for $V \in \mathrm{VF}(\Omega)$,

$$
|\mathrm{BS}(V)| \leq (1/4\pi)\mathrm{OS}(\Omega)|V|, \qquad (7.7)
$$

and we conclude that $\mathrm{BS}:\mathrm{VF}(\Omega) \to \mathrm{VF}(\Omega)$ is a bounded operator.

Now let $\overline{\mathrm{VF}}(\Omega)$ denote the L^2 completion of the space $\mathrm{VF}(\Omega)$; we will refer to the elements of $\overline{\mathrm{VF}}(\Omega)$ as L^2 *vector fields*.

Then we can, and do, extend the Biot–Savart operator to a bounded operator,

$$\mathrm{BS}:\overline{\mathrm{VF}}(\Omega)\to\overline{\mathrm{VF}}(\Omega), \tag{7.8}$$

with the same bound as above.

This completes the proof of part (1).

C. Proof of (2)

To prove that the Biot–Savart operator is compact, we use two standard facts from functional analysis. First is the fact that for any compact domain Ω, if $\phi(x)$ is continuous on R^3, then the integral operator

$$(T_\phi f)(y)=\int_\Omega \phi(y-x)f(x)\ \ \mathrm{d}(\mathrm{vol}_x) \tag{7.9}$$

defines a compact operator on $L^2(\Omega)$; see Zimmer,[48] Theorem 3.1.5 on p. 53. It is stated there only for operators on scalar-valued functions, but the extension to vector-valued ones, using the definition given in Lemma 9.3, is trivial.

Second is the fact that the norm-limit of compact operators is compact; see Zimmer,[48] Lemma 3.1.3 on p. 52.

Now let

$$\phi_N(x)=\begin{cases} N^2/4\pi & \text{if } |x|\leqslant 1/N \\ 1/(4\pi|x|^2) & \text{if } |x|\geqslant 1/N. \end{cases} \tag{7.10}$$

Note that ϕ_N is a continuous function, and that

$$\begin{aligned} N_\Omega(\phi_0-\phi_N)&=\max_y\int_\Omega|\varphi_0(y-x)-\varphi_N(y-x)|\ \ \mathrm{d}(\mathrm{vol}_x)\\ &\leqslant(1/4\pi)\int_{|x|\leqslant 1/N}((1/|x|^2)-N^2)\ \ \mathrm{d}(\mathrm{vol}_x)\\ &\leqslant(1/4\pi)\int_{|x|\leqslant 1/N}(1/|x|^2)\ \ \mathrm{d}(\mathrm{vol}_x)=1/N. \end{aligned} \tag{7.11}$$

By the first functional analysis fact, T_{ϕ_N} is a compact operator from $\overline{\mathrm{VF}}(\Omega)$ to $\overline{\mathrm{VF}}(\Omega)$. By our Lemma, we see that as T_{ϕ_N} converges in norm to T_{ϕ_0}, the Biot–Savart operator, as $N\to\infty$. Using the second functional analysis fact, we conclude that $\mathrm{BS}:\overline{\mathrm{VF}}(\Omega)\to\overline{\mathrm{VF}}(\Omega)$ is a compact operator.

This completes the proof of part (2).

D. Proof of (3)

It is easy to see why the Biot–Savart operator is self-adjoint.

Suppose that V_1 and V_2 are smooth vector fields defined on Ω. Then

$$\begin{aligned}\langle V_1, \mathrm{BS}(V_2)\rangle &= \int_\Omega V_1(y)\cdot \mathrm{BS}(V_2)(y)\ \ \mathrm{d}(\mathrm{vol}_y)\\ &= \int_\Omega V_1(y)\cdot\left[(1/4\pi)\int_\Omega V_2(x)\times(y-x)/|y-x|^3\ \ \mathrm{d}(\mathrm{vol}_x)\right]\mathrm{d}(\mathrm{vol}_y)\\ &= (1/4\pi)\int_{\Omega\times\Omega} V_1(y)\times V_2(x)\cdot(y-x)/|y-x|^3\ \ \mathrm{d}(\mathrm{vol}_x)\ \ \mathrm{d}(\mathrm{vol}_y)\\ &= (1/4\pi)\int_{\Omega\times\Omega} V_2(x)\times V_1(y)\cdot(x-y)/|x-y|^3\ \ \mathrm{d}(\mathrm{vol}_y)\ \ \mathrm{d}(\mathrm{vol}_x)\\ &= \langle V_2, \mathrm{BS}(V_1)\rangle. \end{aligned} \tag{7.12}$$

It is a straightforward exercise to check that these improper integrals are all convergent.

Thus $\mathrm{BS}:\mathrm{VF}(\Omega)\to\mathrm{VF}(\Omega)$ is a self-adjoint operator, and therefore remains self-adjoint when extended to the L^2 completion $\overline{\mathrm{VF}}(\Omega)$ of $\mathrm{VF}(\Omega)$.

Theorem D is proved.

APPENDIX: THE DECAY RATE OF A(V) AND BS(V) AT INFINITY

In item (9) in our list of standard information from Sec. III A, we asserted that in general, $\mathrm{A}(V)$ decays at ∞ like $1/r$ and that $\mathrm{BS}(V)$ decays at ∞ like $1/r^2$. In the special case that $V\epsilon\mathrm{K}(\Omega)$, we asserted that $\mathrm{A}(V)$ decays at ∞ like $1/r^2$ and that $\mathrm{BS}(V)$ decays at ∞ like $1/r^3$.

We give the proofs here.

The defining formula for the vector potential,

$$\mathrm{A}(V)(y) = (1/4\pi)\int_\Omega V(x)/|y-x|\ \ \mathrm{d}(\mathrm{vol}_x), \tag{A1}$$

expresses an inverse first power law, with integration over a compact region Ω. It follows immediately that $\mathrm{A}(V)$ decays at infinity at least as fast as $1/r$.

When we say that $\mathrm{A}(V)$ *decays at infinity at least as fast* as $1/r$, we mean that the product $|\mathrm{A}(V)(y)||y|$ has a finite upper bound on R^3, and likewise for corresponding expressions used below.

The Biot–Savart formula,

$$\mathrm{BS}(V)(y) = (1/4\pi)\int_\Omega V(x)\times(y-x)/|y-x|^3\ \ \mathrm{d}(\mathrm{vol}_x), \tag{A2}$$

expresses an inverse square law, with integration over a compact region Ω. Again it follows immediately that $\mathrm{BS}(V)$ decays at infinity at least as fast as $1/r^2$.

The proof of the faster decay rates when $V\epsilon\ \mathrm{K}(\Omega)$ will be divided into two lemmas.

Lemma 4: *The following are equivalent:*

(1) $\mathrm{A}(V)$ *decays at infinity at least as fast as* $1/r^2$*;*
(2) $\mathrm{BS}(V)$ *decays at infinity at least as fast as* $1/r^3$*;*
(3) $\int_\Omega V\mathrm{d}(\mathrm{vol}) = 0$.

Proof:

It is an easy exercise to check that conditions (1) and (2) each imply (3). For example, when $|y|$ is very large, we have

$$|y|\mathrm{A}(V)(y)\approx(1/4\pi)\int_\Omega V(x)\ \ \mathrm{d}(\mathrm{vol}_x). \tag{A3}$$

If the integral of V is not zero, then $|y|^2|\mathrm{A}(V)(y)|$ certainly blows up at ∞. Thus condition (1) implies condition (3), and likewise, (2) implies (3).

Suppose now that condition (3) holds. Then,

$$\begin{aligned}|y|^2\mathrm{A}(V)(y)&=(1/4\pi)\int_\Omega |y|^2V(x)/|y-x|\ \ \mathrm{d}(\mathrm{vol}_x)\\ &=(1/4\pi)\int_\Omega |y|^2V(x)/|y-x|\ \ \mathrm{d}(\mathrm{vol}_x)-(1/4\pi)\int_\Omega |y|V(x)\ \ \mathrm{d}(\mathrm{vol}_x)\\ &=(1/4\pi)\int_\Omega \{(|y^2/|y-x|)-|y|\}V(x)\ \ \mathrm{d}(\mathrm{vol}_x),\end{aligned} \tag{A4}$$

where the integral added on the right-hand side is zero thanks to condition (3).

Now,

$$\{(|y|^2/|y-x|)-|y|\}=\{|y|/|y-x|\}\{|y|-|y-x|\}.$$

The first factor on the right-hand side approaches 1 as $y\to\infty$ because Ω is bounded. The second factor on the right-hand side is $\leqslant|x|$, and hence also bounded. Thus

$$\{(|y|^2/|y-x|)-|y|\}$$

is bounded as $y\to\infty$.

Since $\int_\Omega|V(x)|d(\mathrm{vol}_x)$ is certainly bounded, it follows that $|y|^2|\mathrm{A}(V)(y)|$ is bounded, and hence that $\mathrm{A}(V)$ decays at ∞ at least as fast as $1/r^2$. Thus condition (3) implies condition (1), as claimed.

Again suppose that condition (3) holds. Then

$$\begin{aligned}|y|^3\,\mathrm{BS}(V)(y)&=(1/4\pi)\int_\Omega V(x)\times(y-x)|y|^3/|y-x|^3\ \ \mathrm{d}(\mathrm{vol}_x)\\ &=(1/4\pi)\int_\Omega V(x)\times(y-x)|y|^3/|y-x|^3\ \ \mathrm{d}(\mathrm{vol}_x)-(1/4\pi)\int_\Omega V(x)\times y\ \ \mathrm{d}(\mathrm{vol}_x)\\ &=(1/4\pi)\int_\Omega V(x)\times\{((y-x)|y|^3/|y-x|^3)-y\}\ \ \mathrm{d}(\mathrm{vol}_x),\end{aligned} \tag{A5}$$

where again the integral added on the right-hand side is zero because of condition (3). Continuing,

$$\{((y-x)|y|^3/|y-x|^3)-y\}=\{y(|y|^3-|y-x|^3)/|y-x|^3\}-\{x|y|^3/|y-x|^3\}.$$

Processing the first term on the right-hand side,

$$\{y(|y|^3-|y-x|^3)/|y-x|^3\}=\{y/|y-x|\}\ \ \{|y|-|y-x|\}\ \ \{(|y|^2+|y||y-x|+|y-x|^2)/|y-x|^2\}.$$

The first factor on the right-hand side of this last equation is bounded as $y\to\infty$ because Ω is bounded. The second factor on the right-hand side is $\leqslant|x|$, and hence is also bounded. The third factor on the right-hand side approaches the value 3 as $y\to\infty$, and hence is also bounded. It follows that

$$\{y(|y|^3-|y-x|^3)/|y-x|^3\}$$

is bounded as $y\to\infty$.

Now the term

$$\{x|y|^3/|y-x|^3\}$$

is certainly bounded as $y\to\infty$, and so we conclude that

$$\{((y-x)|y|^3/|y-x|^3)-y\}$$

is also bounded as $y\to\infty$. From this it follows that

$$|y|^3\,\mathrm{BS}(V)(y)$$

is bounded for all y, and hence that $\mathrm{BS}(V)(y)$ decays at ∞ at least as fast as $1/r^3$. Thus condition (3) implies condition (2).

This completes the proof of Lemma 4.

Lemma 5: $\int_\Omega V(x)d(\mathrm{vol}_x)=0$ *for all* V *in* $\mathrm{FK}\oplus\mathrm{HK}\oplus\mathrm{HG}\oplus\mathrm{GG}$, *but this relation determines a codimension-three subspace of* CG.

Proof:

We begin with the proof that $\int_\Omega V(x)d(\mathrm{vol}_x)=0$ for all $V\epsilon\mathrm{FK}\oplus\mathrm{HK}=\mathrm{K}(\Omega)$.

The argument will be coordinate-wise, so that we can deal with scalar-valued integrals instead of vector-valued ones. So let us write the typical point of Ω as $x=(x_1,x_2,x_3)$, and then write $V(x)=(V_1(x),V_2(x),V_3(x))$.

Then

$$\nabla\cdot(x_1V)=(\nabla x_1)\cdot V+x_1(\nabla\cdot V)=(\nabla x_1)\cdot V=V_1, \tag{A6}$$

since V is divergence-free.

Hence,

$$\int_\Omega V_1(x)\ \ \mathrm{d}(\mathrm{vol}_x)=\int_\Omega\nabla\cdot(x_1V)\ \ \mathrm{d}(\mathrm{vol}_x)=\int_{\partial\Omega}x_1V\cdot n\ \ \mathrm{d}(\mathrm{area})=0, \tag{A7}$$

because V is tangent to $\partial\Omega$.

Of course the same argument holds for V_2 and V_3, so we conclude that

$$\int_\Omega V(x)\ \ \mathrm{d}(\mathrm{vol}_x)=0, \tag{A8}$$

as claimed.

Now we prove that $\int_\Omega V(x)\ \ \mathrm{d}(\mathrm{vol}_x)=0$ for all $V\epsilon\ \mathrm{HG}\oplus\mathrm{GG}$.

Write $V=\nabla\varphi$ with φ constant on each component of $\partial\Omega$.

We claim that

$$\int_\Omega V\ \ \mathrm{d}(\mathrm{vol})=\int_\Omega\nabla\varphi\ \ \mathrm{d}(\mathrm{vol})=\int_{\partial\Omega}\varphi n\ \ \mathrm{d}(\mathrm{area}). \tag{A9}$$

We see this as follows:

Let C be any constant vector. Then,

$$\nabla\cdot(\varphi C)=(\nabla\varphi)\cdot C+\varphi(\nabla\cdot C)=(\nabla\varphi)\cdot C. \tag{A10}$$

Hence

$$\left(\int_\Omega \nabla\varphi \ \ \mathrm{d(vol)}\right)\cdot C = \int_\Omega (\nabla\varphi)\cdot C \ \ \mathrm{d(vol)}$$
$$= \int_\Omega \nabla\cdot(\varphi C) \ \ \mathrm{d(vol)}$$
$$= \int_{\partial\Omega} (\varphi C)\cdot n \ \ \mathrm{d(area)}$$
$$= \left(\int_{\partial\Omega} \varphi n \ \ \mathrm{d(area)}\right)\cdot C. \tag{A11}$$

Since this is true for all constant vectors C, we must have

$$\int_\Omega \nabla\varphi \ \ \mathrm{d(vol)} = \int_{\partial\Omega} \varphi n \ \ \mathrm{d(area)}, \tag{A12}$$

as claimed.

Now suppose that

$$\partial\Omega = \partial\Omega_1 \cup \cdots \cup \partial\Omega_k \tag{A13}$$

is the decomposition of $\partial\Omega$ into its connected components, and let φ_i denote the constant value of the function φ on the boundary component $\partial\Omega_i$. Then

$$\int_\Omega V \ \ \mathrm{d(vol)} = \int_\Omega \nabla\varphi \ \ \mathrm{d(vol)} = \int_{\partial\Omega} \varphi n \ \ \mathrm{d(area)} = \sum_i \ \varphi_i \int_{\partial\Omega_i} n \ \ \mathrm{d(area)} = 0, \tag{A14}$$

because $\int n \ \ \mathrm{d(area)}$ over any closed surface in 3-space is always zero.

This completes the proof that $\int_\Omega V(x) \ \ \mathrm{d(vol}_x) = 0$ for all $V \in \mathrm{HG} \oplus \mathrm{GG}$.

The observation that this relation determines a codimension-three subspace of CG follows directly from the fact that the three constant vector fields $\hat{x}$, $\hat{y}$, and $\hat{z}$ are curly gradients, completing the proof of Lemma 5.

Clearly, Lemmas 4 and 5 imply the faster decay rates of $\mathrm{A}(V)$ and $\mathrm{BS}(V)$ when $V \in \mathrm{K}(\Omega)$, completing our argument.

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For those readers interested in the history of the Biot–Savart Law, we recommend R. A. R. Tricker's little volume, *Early Electrodynamics, The First Law of Circulation*.[49] It contains extensive translations of the works of Oerstead, Biot, Savart, and Ampere, and a detailed analysis of this fascinating period of scientific discovery and of the interactions amongst its principals.

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Finite conformal modules over $N=2,3,4$ superconformal algebras

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In this paper we continue the study of representation theory of formal distribution Lie superalgebras initiated by Cheng and Kac [Asian J. Math. **1**, 181–193 (1997); **2**, 153–156 (1998) (erratum)]. We study finite Verma-type conformal modules over the $N=2$, $N=3$ and the two $N=4$ superconformal algebras and also find explicitly all singular vectors in these modules. From our analysis of these modules we obtain a complete list of finite irreducible conformal modules over the $N=2$, $N=3$ and the two $N=4$ superconformal algebras. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1333698]

I. INTRODUCTION

Superconformal algebras have been playing an important role in the study of string theory and conformal field theory, which have been the subject of intensive study since the seminal paper.[1] Superconformal algebras may be viewed as natural superextensions of the Virasoro algebra and their roots in physics literature can be traced at least back to as early as the 1970s.[2] A mathematically rigorous definition of a superconformal algebra is as follows. It is a simple Lie superalgebra $\mathfrak{g}$ over the complex numbers $\mathbb{C}$ spanned by the modes of a finite family $\mathfrak{F}$ of mutually local fields satisfying the following two axioms:[3]

(1) $\mathfrak{F}$ contains the Virasoro field.
(2) The coefficients of the operator product expansions of members from $\mathfrak{F}$ are linear combinations of members from $\mathfrak{F}$ and their derivatives.

A Lie superalgebra $\mathfrak{g}$ satisfying the second axiom only is referred to as a *formal distribution Lie superalgebra* in Ref. 3.

In order to facilitate the study of formal distribution Lie superalgebras the notion of a *conformal superalgebra* was introduced in Ref. 3 (see Sec. II). It proves to be an effective tool for this purpose.

A natural class of representations of formal distribution Lie superalgebras to study is the class of *conformal modules*.[4] A conformal module is a pair consisting of a $\mathfrak{g}$-module V and a family $\mathcal{E}$ of fields whose modes span V such that members from $\mathfrak{F}$ and $\mathcal{E}$ are mutually local. Just as the study of formal distribution Lie superalgebras reduces to the study of conformal superalgebras, the study of conformal modules is essentially reduced to the study of modules over the corresponding conformal superalgebras.

The study of modules over the conformal superalgebra can further be reduced to the study of modules over the *extended annihilation subalgebra*, which is a semidirect sum of the subalgebra of positive modes of the corresponding formal distribution Lie superalgebra and a one-dimensional derivation. It is in this language that the problem of classifying finite irreducible

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conformal modules over the Virasoro, $N=1$ (Neveu–Schwarz) and the current superalgebra was solved in Ref. 4.

The problem of classifying conformal modules over other superconformal algebras, which is the main theme of the present article, turns out to be more subtle. The main purpose here is to give a classification of finite irreducible conformal modules over the $N=2$, $N=3$ and the two $N=4$ superconformal algebras.

We first construct finite Verma-type conformal modules for a general superconformal algebra and prove that every finite irreducible conformal module is a homomorphic image of such a module. As a consequence we obtain a bijection between finite irreducible conformal modules of a superconformal algebra and finite-dimensional irreducible modules of a certain finite-dimensional reductive Lie (super)algebra (Corollary 3.1).

We then study these Verma-type modules in detail for the four members of the family of superconformal algebras mentioned above. It turns out that, unlike for the Virasoro and the $N=1$ (Neveu–Schwarz) superconformal algebras, the Verma-type modules for these superconformal algebras are in general reducible, and thus we need to analyze their submodules. This is accomplished by finding explicit formulas for all singular vectors inside such a module and then show that the submodule generated by these singular vectors is maximal (in all but two cases). We also find an explicit basis for this maximal submodule, which then enables us to give a quite explicit description of all finite irreducible conformal modules over these superconformal algebras.

This article is organized as follows. In Sec. II basic facts of formal distribution Lie superalgebras, conformal superalgebras and extended annihilation subalgebras are recalled. Section III is devoted to the study of a class of modules over a certain class of Lie superalgebras that include the annihilation subalgebra of every superconformal algebra. This class of modules gives rise to finite Verma-type conformal modules of superconformal algebras. The results of Sec. III are then used in Secs. IV–VII, where finite irreducible conformal modules over the $N=2$, $N=3$, the ''small'' $N=4$ and the ''big'' $N=4$ superconformal algebra, respectively, are classified.

In this article all vector spaces, (super)algebras and tensor products are over taken over the complex numbers $\mathbb{C}$.

II. PRELIMINARIES

In this section we review some of the basic facts on formal distribution Lie (super)algebras and conformal modules that will be used later on. The material here is taken from Refs. 3–5, and the reader is referred to these articles for more details.

A. Formal distribution Lie superalgebras

Recall that a *formal distribution* or a *field* with coefficients in a Lie superalgebra $\mathfrak{g}=\mathfrak{g}_{\bar{0}}+\mathfrak{g}_{\bar{1}}$ is a formal series of the form

$$a(z)=\sum_{n\in\mathbb{Z}} a_{[n]}z^{-n-1},$$

where $a_{[n]}\in\mathfrak{g}$ and z is an indeterminate.

Two formal distributions $a(z)$ and $b(z)$ with coefficients in $\mathfrak{g}$ are said to be mutually *local* if there exists $N\in\mathbb{Z}_+$ such that

$$(z-w)^N[a(z),b(w)]=0. \tag{2.1}$$

Let $\delta(z-w)=z^{-1}\Sigma_{n\in\mathbb{Z}}(z/w)^n$ be the formal delta function. Then (2.1) may be written as

$$[a(z),b(w)]=\sum_{j=0}^{N-1}(a_{(j)}b)(w)\partial_w^{(j)}\delta(z-w) \tag{2.2}$$

[here $\partial_w^{(j)}$ stands for $(1/j!)\partial^j/\partial w^j$] for some uniquely determined formal distributions $(a_{(j)}b)(w)$, and thus defines a $\mathbb{C}$-bilinear product $\cdot_{(j)}\cdot$ for each $j\in\mathbb{Z}_+$ on the space of all formal distributions with coefficients in $\mathfrak{g}$. Also $\partial_z a(z)=\Sigma_n(\partial a)_{[n]}z^{-n-1}$, where $(\partial a)_{[n]}=-na_{[n-1]}$, and hence the space of all formal distributions is also a (left) $\mathbb{C}[\partial_z]$-module.

A Lie superalgebra $\mathfrak{g}$ is called a *formal distribution Lie superalgebra*, if there exists a family $\mathfrak{F}$ of mutually local formal distributions whose coefficients span $\mathfrak{g}$. We will write $(\mathfrak{g},\mathfrak{F})$ for such a Lie superalgebra.

Given a formal distribution Lie superalgebra $(\mathfrak{g},\mathfrak{F})$, we may include $\mathfrak{F}$ in the minimal family $\overline{\mathfrak{F}}$ of mutally local distributions which is closed under ∂_z and all products $\cdot_{(j)}\cdot$. Then $\overline{\mathfrak{F}}$ is a *conformal superalgebra*, i.e., it is a left $\mathbb{Z}_2$-graded $\mathbb{C}[\partial]$-module R with a $\mathbb{C}$-bilinear product $a_{(n)}b$ for each $n\in\mathbb{Z}_+$ such that the following axioms hold $[a,b,c\in R;m,n\in\mathbb{Z}_+$ and $\partial^{(j)}=(1/j!)\,\partial^j]$ (cf. Refs. 6 and 7):

(C0) $a_{(n)}b=0$, for $n>>0$,
(C1) $(\partial a)_{(n)}b=-na_{(n-1)}b$,
(C2) $a_{(n)}b=(-1)^{p(a)p(b)}\Sigma_{j=0}^{\infty}(-1)^{j+n+1}\partial^{(j)}(b_{(n+j)}a)$,
(C3) $a_{(m)}(b_{(n)}c)=\Sigma_{j=0}^{\infty}\binom{m}{j}(a_{(j)}b)_{(m+n-j)}c+(-1)^{p(a)p(b)}b_{(n)}(a_{(m)}c)$.

It is convenient to write the products of $a,b\in R$ in the generating series form

$$a_\lambda b=\sum_{n=0}^{\infty}a_{(n)}b\frac{\lambda^n}{n!},$$

where λ is a formal indeterminate. Such an expression lies in $R[\lambda]$.

Conversely, if a conformal superalgebra $R=\oplus_{i\in I}\mathbb{C}[\partial]a^i$ is free $\mathbb{C}[\partial]$-module, we may associate to R a formal distribution Lie superalgebra $(\mathfrak{g}(R),\mathfrak{F}(R))$ with Lie superalgebra $\mathfrak{g}(R)$ spanned by $\mathbb{C}$-basis $a^i_{[m]}$ $(i\in I,\ m\in\mathbb{Z})$ and fields $\mathfrak{F}(R)=\{a^i(z)=\Sigma_{n\in\mathbb{Z}}a^i_{[n]}z^{-n-1}\}_{i\in I}$ with bracket [cf. (2.2)]:

$$[a^i(z),a^j(w)]=\sum_{k\in\mathbb{Z}_+}(a^i_{(k)}a^j)(w)\partial_w^{(k)}\delta(z-w),$$

so that $\overline{\mathfrak{F}(R)}=R$, giving rise to commutation relations $(m,n\in\mathbb{Z};\ i,j\in I)$

$$[a^i_{[m]},a^j_{[n]}]=\sum_{k\in\mathbb{Z}_+}\binom{m}{k}(a^i_{(k)}a^j)_{[m+n-k]}. \tag{2.3}$$

It follows that the Lie superalgebra $\mathfrak{g}$ of a formal distribution Lie superalgebra $(\mathfrak{g},\mathfrak{F})$ is isomorphic to $\mathfrak{g}(\overline{\mathfrak{F}})$ divided by an *irregular* ideal, that is an ideal which does not contain every $a_{[n]}$ for some nonzero element $a\in\overline{\mathfrak{F}}$.

Example 2.1: The (centerless) *Virasoro algebra* $\mathfrak{V}$ has a basis L_n $(n\in\mathbb{Z})$ with commutation relations

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

It is spanned by the coefficients of the field $L(z)=\Sigma_{n\in\mathbb{Z}}L_nz^{-n-2}$ satisfying

$$[L(z),L(w)]=\partial_wL(w)\,\delta(z-w)+2L(w)\partial_w\delta(z-w). \tag{2.4}$$

The conformal algebra associated to the Virasoro algebra is the *Virasoro conformal algebra* $R(\mathfrak{V})=\mathbb{C}[\partial]\otimes L$ with products $L_\lambda L=(\partial+2\lambda)L$.

Example 2.2: Let $\mathfrak{g}$ be a finite-dimensional Lie (super)algebra. Let $\tilde{\mathfrak{g}}=\mathfrak{g}\otimes\mathbb{C}[t,t^{-1}]$ denote the corresponding *current algebra* with bracket

$$[a\otimes f(t),b\otimes g(t)]=[a,b]\otimes f(t)g(t),\quad a,b\in\mathfrak{g};f(t),g(t)\in\mathbb{C}[t,t^{-1}].$$

For each $a\in\mathfrak{g}$ define a field $a(z)=\Sigma_{n\in\mathbb{Z}}(a\otimes t^n)z^{-n-1}$. Then $\tilde{\mathfrak{g}}$ is spanned by the coefficients of $a(z)$ satisfying

$$[a(z),b(w)]=[a,b](w)\,\delta(z-w). \tag{2.5}$$

The conformal (super)algebra associated to the current algebra is the *current conformal algebra* $R(\tilde{\mathfrak{g}})=\mathbb{C}[\partial]\otimes\mathfrak{g}$ with products $a_\lambda b=[a,b]$, $a,b\in\mathfrak{g}$.

Example 2.3: The semidirect sum $\mathfrak{V}\ltimes\tilde{\mathfrak{g}}$ is another example of a formal distribution Lie (super)algebra. The collection of fields is $\{L(z),a(z)|a\in\mathfrak{g}\}$ and we have in addition to (2.4) and (2.5)

$$[L(z),a(w)]=\partial_w a(w)\,\delta(z-w)+a(w)\,\partial_w\delta(z-w). \tag{2.6}$$

The conformal algebra associated to the semidirect sum of the Virasoro algebra and the current algebra is $R(\mathfrak{V}\ltimes\tilde{\mathfrak{g}})=R(\mathfrak{V})\ltimes R(\tilde{\mathfrak{g}})$. For $a\in\mathfrak{g}$ we have $L_\lambda a=(\partial+\lambda)a$.

B. Conformal modules

Let $(\mathfrak{g},\mathfrak{F})$ be a formal distribution Lie superalgebra. Let V be a $\mathfrak{g}$-module such that V is spanned over $\mathbb{C}$ by the coefficients of a family $\mathcal{E}$ of fields. If all $a(z)\in\mathfrak{F}$ are local with respect to all $v(z)\in\mathcal{E}$, then the pair $(V,\mathcal{E})$ is called a *conformal module* over $(\mathfrak{g},\mathfrak{F})$.

Now the family $\mathcal{E}$ of a conformal module $(V,\mathcal{E})$ over $(\mathfrak{g},\mathfrak{F})$ similarly can be included in a larger family $\overline{\mathcal{E}}$, which is still local with respect to the fields from $\overline{\mathfrak{F}}$, and invariant under ∂ and $a_{(j)}$, for all $a\in\overline{\mathfrak{F}}$ and $j\in\mathbb{Z}_+$. It can be shown that for $a,b\in\overline{\mathfrak{F}}$ and $v\in\overline{\mathcal{E}}$ $(m,n\in\mathbb{Z}_+)$ one has

$$[a_{(m)},b_{(n)}]v=\sum_{j=0}^{m}\binom{m}{j}(a_{(j)}b)_{(m+n-j)}v,\quad (\partial a)_{(n)}v=[\partial,a_{(n)}]v=-na_{(n-1)}v.$$

Thus it follows that any conformal module $(V,\mathcal{E})$ over a formal distribution Lie superalgebra $(\mathfrak{g},\mathfrak{F})$ gives rise to a module $M=\overline{\mathcal{E}}$ over the *conformal superalgebra* $R=\overline{\mathfrak{F}}$, defined as follows. It is a (left) $\mathbb{Z}_2$-graded $\mathbb{C}[\partial]$-module equipped with a family of $\mathbb{C}$-linear maps $a\to a^M_{(n)}$ of R to $\mathrm{End}_{\mathbb{C}}M$, for each $n\in\mathbb{Z}_+$, such that the following properties hold for $a,b\in R$ and $m,n\in\mathbb{Z}_+$:

(M0) $a^M_{(n)}v=0$, for $v\in M$ and $n>>0$,
(M1) $[a^M_{(m)},b^M_{(n)}]=\Sigma_{j=0}^{m}\binom{m}{j}(a_{(j)}b)^M_{(m+n-j)}$,
(M2) $(\partial a)^M_{(n)}=[\partial,a^M_{(n)}]=-na^M_{(n-1)}$.

Again it is convenient to write the action of an element $a\in R$ on an element $v\in M$ in the form of a generating series in $V[\lambda]$:

$$a_\lambda v:=\sum_{n=0}^{\infty}a_{(n)}v\frac{\lambda^n}{n!}.$$

Conversely, suppose that a conformal superalgebra $R=\oplus_{i\in I}\mathbb{C}[\partial]a^i$ is a free $\mathbb{C}[\partial]$-module and consider the associated formal distribution Lie superalgebra $(\mathfrak{g}(R),\mathfrak{F}(R))$. Let M be a module over the conformal superalgebra R and suppose that M is a free $\mathbb{C}[\partial]$-module with $\mathbb{C}[\partial]$-basis $\{v^\alpha\}_{\alpha\in J}$. This gives rise to a conformal module $V(M)$ over $\mathfrak{g}(R)$ with fields $\mathcal{E}=\{v^\alpha(z)=\Sigma_{n\in\mathbb{Z}}v^\alpha_{[n]}z^{-n-1}|\alpha\in J\}$ and $\mathbb{C}$-basis $v^\alpha_{[n]}$, defined by

$$a^i(z)v^\alpha(w)=\sum_{j\in\mathbb{Z}_+}(a^i_{(j)}v^\alpha)(w)\partial_w^{(j)}\delta(z-w).$$

A conformal module $(V,\mathcal{E})$ (respectively module M) over a formal distribution Lie superalgebra $(\mathfrak{g},\mathfrak{F})$ (respectively over a conformal superalgebra R) is called *finite*, if $\overline{\mathcal{E}}$ (respectively M) is a finitely generated $\mathbb{C}[\partial]$-module. A conformal module $(V,\mathcal{E})$ over $(\mathfrak{g},\mathfrak{F})$ is called *irreducible* if

there is no nontrivial invariant subspace which contains all $v_{[n]}$, $n\in\mathbb{Z}$, for some nonzero $v\in\overline{\mathcal{E}}$. An invariant subspace that does not contain all $v_{[n]}$, for some non-zero $v\in\mathcal{E}$, is called an *irregular submodule* and conformal modules that differ by an irregular submodule are called referred to as *equivalent* in Ref. 5. Clearly a conformal module is irreducible if and only if the associated module $\overline{\mathcal{E}}$ over the conformal superalgebra $\overline{\mathfrak{F}}$ is irreducible.

Remark 2.1: It follows from (M2) that an eigenvector $v\in M$ of the linear operator ∂ is an R-invariant, i.e., $a_{(n)}v=0$, for all $n\geqslant 0$. Thus a finite irreducible module over a conformal superalgebra R is either free over $\mathbb{C}[\partial]$ or else it is one-dimensional over $\mathbb{C}$.

Suppose that $(\mathfrak{g},\mathfrak{F})$ is a formal distribution Lie superalgebra such that $\mathfrak{g}(\overline{\mathfrak{F}})\cong\mathfrak{g}$. Our discussion implies that any irreducible conformal module $(V,\mathcal{E})$ over $(\mathfrak{g},\mathfrak{F})$ is a quotient of an irreducible conformal module of the form $V(M)$ divided by an irregular submodule, where M is an irreducible module over the conformal superalgebra $\overline{\mathfrak{F}}$. Hence, in particular, if $V(M)$ is irreducible as a $\mathfrak{g}$-module for every irreducible M, then every finite irreducible conformal module over $(\mathfrak{g},\mathfrak{F})$ is isomorphic to $V(M)$, for some finite irreducible $\overline{\mathfrak{F}}$-module M.

Example 2.4: The Virasoro algebra $\mathfrak{V}$ may be identified with the Lie algebra of regular vector fields on $\mathbb{C}^\times$, where $L_n=-t^{n+1}\,d/dt$, $n\in\mathbb{Z}$. For $\alpha,\Delta\in\mathbb{C}$ let

$$F_{\mathfrak{V}}(\alpha,\Delta)=\mathbb{C}[t,t^{-1}]e^{-\alpha t}dt^{1-\Delta}.$$

The Lie algebra $\mathfrak{V}$ acts on the space $F_{\mathfrak{V}}(\alpha,\Delta)$ in a natural way:

$$\left(f(t)\frac{\partial}{\partial t}\right)g(t)dt^{1-\Delta}=(f(t)g'(t)+(1-\Delta)g(t)f'(t))dt^{1-\Delta},$$

where $f(t)\in\mathbb{C}[t,t^{-1}]$ and $g(t)\in\mathbb{C}[t,t^{-1}]e^{-\alpha t}$. Letting $v_{[n]}=t^ne^{-\alpha t}dt^{1-\Delta}$ and $v(z)=\Sigma_{n\in\mathbb{Z}}v_{[n]}z^{-n-1}$ this action is equivalent to

$$L(z)v(w)=(\partial_w+\alpha)v(w)\,\delta(z-w)+\Delta v(w)\partial_w\delta(z-w).$$

Hence we have constructed a two-parameter family of conformal modules over $\mathfrak{V}$. This gives a family of $R(\mathfrak{V})$-modules $\mathbb{C}[\partial]\otimes\mathbb{C}v_\Delta$ with products $L_\lambda v_\Delta=(\alpha+\partial+\Delta\lambda)v_\Delta$. This module is irreducible if and only if $\Delta\neq 0$, in which case it will be denoted by $L_{\mathfrak{V}}(\alpha,\Delta)$. We set $L_{\mathfrak{V}}(\alpha,0)$ to be the one-dimensional (over $\mathbb{C}$) $R(\mathfrak{V})$-module on which ∂ acts as the scalar α.

Example 2.5: Let $\mathfrak{g}$ be a finite-dimensional simple Lie algebra and U^Λ the finite-dimensional irreducible module of highest weight Λ. Then $F_{\tilde{\mathfrak{g}}}(\Lambda)=U^\Lambda\otimes\mathbb{C}[t,t^{-1}]$ is naturally a module over $\tilde{\mathfrak{g}}$ with action given by

$$(a\otimes f(t))(u\otimes g(t))=au\otimes f(t)g(t),\quad a\in\mathfrak{g},u\in U^\Lambda;f(t),g(t)\in\mathbb{C}[t,t^{-1}]. \tag{2.7}$$

For each vector $u\in U^\Lambda$ define $u(z)=\Sigma_{n\in\mathbb{Z}}(u\otimes t^n)z^{-n-1}$ so that (2.7) is equivalent to

$$a(z)u(w)=au(w)\,\delta(z-w),$$

and hence $F_{\tilde{\mathfrak{g}}}(\Lambda)$ is conformal. This gives a family of $R(\tilde{\mathfrak{g}})$-modules, which is irreducible if and only if $\Lambda\neq 0$, in which case it will be denoted by $L_{\tilde{\mathfrak{g}}}(\Lambda)$. By $L_{\tilde{\mathfrak{g}}}(0)$ we will mean the trivial $R(\tilde{\mathfrak{g}})$-module. Similarly one defines the one-dimensional module $L_{\tilde{\mathfrak{g}}}(\alpha,0)$.

Example 2.6: $\tilde{\mathfrak{g}}$ acts on $F_{\mathfrak{V}\ltimes\tilde{\mathfrak{g}}}(\alpha,\Delta,\Lambda)=U^\Lambda\otimes F_{\mathfrak{V}}(\alpha,\Delta)$ similarly as in Example 2.5. However, on $F_{\mathfrak{V}\ltimes\tilde{\mathfrak{g}}}(\alpha,\Delta,\Lambda)$ we have also an action of $\mathfrak{V}$, thus making it into a module over $\mathfrak{V}\ltimes\tilde{\mathfrak{g}}$. This module defines an $R(\mathfrak{V}\ltimes\tilde{\mathfrak{g}})$-module which is irreducible if and only if $(\Delta,\Lambda)\neq(0,0)$, and in which case it will be denoted by $L_{\mathfrak{V}\ltimes\tilde{\mathfrak{g}}}(\alpha,\Delta,\Lambda)$. By $L_{\mathfrak{V}\ltimes\tilde{\mathfrak{g}}}(\alpha,0,0)$ we will mean the one-dimensional module on which ∂ acts as the scalar α.

The following theorem was proven in Ref. 4.

Theorem 2.1: *Let $\mathfrak{g}$ stand for a finite-dimensional simple Lie algebra. Any finite irreducible module over the conformal algebras $R(\mathfrak{V})$, $R(\tilde{\mathfrak{g}})$ and $R(\mathfrak{V}\ltimes\tilde{\mathfrak{g}})$ are as follows:*

(*i*) $L_{\mathfrak{V}}(\alpha,\Delta)$,
(*ii*) $L_{\tilde{\mathfrak{g}}}(\Lambda)$ *and* $L_{\tilde{\mathfrak{g}}}(\alpha,0)$,
(*iii*) $L_{\mathfrak{V}\ltimes\tilde{\mathfrak{g}}}(\alpha,\Delta,\Lambda)$.

Remark 2.2: We note that a similar statement as Theorem 2.1 part (*iii*) holds even if $\mathfrak{g}$ is replaced by the one-dimensional Lie algebra $\mathbb{C}a$. In this case $U^{\Lambda}=\mathbb{C}u$ with $au=\Lambda u$, $\Lambda\in\mathbb{C}$. Also, part (*ii*) remains true for all but three series of finite-dimensional simple Lie superalgebras.

C. Extended annihilation subalgebras

Given a formal distribution Lie superalgebra $(\mathfrak{g},\mathfrak{F})$ we let $\mathfrak{g}_+$ denote the $\mathbb{C}$-span of all $a_{[n]}$, where $n\geqslant 0$ and $a\in\mathfrak{F}$. Due to (2.3) $\mathfrak{g}_+$ is closed under the bracket and hence forms a subalgebra of $\mathfrak{g}$, which we will call the *annihilation algebra* of $(\mathfrak{g},\mathfrak{F})$. Let ∂ be the derivation of $\mathfrak{g}_+$ defined by $[\partial,a_{[n]}]=-na_{[n-1]}$, and consider the semi-direct sum of $\mathfrak{g}^+=\mathbb{C}\partial\ltimes\mathfrak{g}_+$. Then $\mathfrak{g}^+$ is called the *extended annihilated algebra* of $(\mathfrak{g},\mathfrak{F})$. The following proposition, which follows by comparing (M1) with (2.3), is important for the theory of conformal modules.

Proposition 2.1:[4] *Let R be a conformal superalgebra and $(\mathfrak{g}(R),R(\mathfrak{F}))$ be its associated formal distribution Lie superalgebra with extended annihilation algebra $\mathfrak{g}(R)^+$. Then a module over the conformal superalgebra R is precisely a $\mathfrak{g}(R)^+$-module M satisfying $a_{[n]}v=0$, for each $v\in M$, $a\in R$ and $n>>0$.*

Remark 2.3: Let R be a conformal superalgebra with $\mathbb{C}[\partial]$-basis $\{a^i|i\in I\}$ and M a free $\mathbb{C}[\partial]$-module with basis $\{v^j|j\in J\}$. Given $a^i_{(n)}v^j\in M$ for all $i\in I$, $j\in J$, $n\in\mathbb{Z}_+$, which is 0 for $n>>0$, condition (M2) uniquely extends the action of $a^i_{(n)}$ to all of M. If in addition (M1) holds, then M is an R-module. Hence the action of an R-module M is completely determined by the action of a $\mathbb{C}[\partial]$-basis of R on a $\mathbb{C}[\partial]$-basis of M.

Example 2.7: In the case of the Virasoro algebra $\mathfrak{V}$ the annihilation algebra $\mathfrak{V}_+$ is spanned by elements L_n, $n\geqslant -1$. In the case of the current algebra $\tilde{\mathfrak{g}}_+$ is spanned by $a\otimes t^n$, where $a\in\mathfrak{g}$ and $n\geqslant 0$, while in the case of $\mathfrak{V}\ltimes\tilde{\mathfrak{g}}$ it is $\mathfrak{V}_+\ltimes\tilde{\mathfrak{g}}_+$.

The problem of classifying conformal modules over $(\mathfrak{g},\mathfrak{F})$ is thus reduced to the problem of classifying a class of modules over $\mathfrak{g}(\bar{\mathfrak{F}})^+$. It is clear that in all our examples one has $\mathfrak{g}(\bar{\mathfrak{F}})=\mathfrak{g}$, and thus we are to study modules over $\mathfrak{g}^+$. Now if in addition there exists an element L_{-1} in $\mathfrak{g}_+$ such that $L_{-1}-\partial$ is central in $\mathfrak{g}^+$, then every irreducible representation of $\mathfrak{g}^+$ is an irreducible representation of $\mathfrak{g}_+$, on which $(L_{-1}-\partial)$ acts as a scalar $\alpha\in\mathbb{C}$. In the case of the $\mathfrak{V}$ and $\mathfrak{V}\ltimes\tilde{\mathfrak{g}}$ and the $N=2,3,4$ superconformal superalgebras, which we will define later, such an L_{-1} always exists so that we only need to consider representations of $\mathfrak{g}_+$. The irreducible representations of $\mathfrak{V}_+$ and $\mathfrak{V}_+\ltimes\tilde{\mathfrak{g}}_+$ that give rise to those in Theorem 2.1 are denoted by $L_{\mathfrak{V}_+}(\Delta)$ and $L_{\mathfrak{V}_+\ltimes\tilde{\mathfrak{g}}_+}(\Delta,\Lambda)$, respectively. The corresponding actions are clear and can be found in Ref. 4.

III. FINITE VERMA-TYPE CONFORMAL MODULES

Let $\mathcal{L}$ be a Lie superalgebra over $\mathbb{C}$ with a distinguished element ∂ and a descending sequence of subspaces $\mathcal{L}=\mathcal{L}_{-1}\supset\mathcal{L}_0\supset\mathcal{L}_1\supset\mathcal{L}_2\supset\cdots\supset\mathcal{L}_n\supset\cdots$, such that $[\partial,\mathcal{L}_k]=\mathcal{L}_{k-1}$, for all $k>0$. Let W be an $\mathcal{L}$-module, which is finitely generated over $\mathbb{C}[\partial]$, such that for all $w\in W$ there exists a non-negative integer k (depending on w) with $\mathcal{L}_k w=0$. For $m\geqslant -2$ set $W_m=\{w\in W|\mathcal{L}_{m+1}w=0\}$ and let M be the minimal non-negative integer such that $W_M\neq 0$.

Lemma 3.1:[4] *Suppose that $M\geqslant 0$. Then $\mathbb{C}[\partial]W_M=\mathbb{C}[\partial]\otimes W_M$ and hence $\mathbb{C}[\partial]W_M\cap W_M=W_M$. In particular W_M is a finite-dimensional vector space.*

Let $\mathfrak{g}$ be a Lie superalgebra satisfying the following three conditions.

(L1) $\mathfrak{g}$ is $\mathbb{Z}$-graded of finite depth $d\in\mathbb{N}$, i.e., $\mathfrak{g}=\oplus_{j\geqslant -d}\mathfrak{g}_j$ with $[\mathfrak{g}_i,\mathfrak{g}_j]\subset\mathfrak{g}_{i+j}$.

(L2) There exists a semisimple element $z\in\mathfrak{g}_0$ such that its centralizer in $\mathfrak{g}$ is contained in $\mathfrak{g}_0$.

(L3) There exists an element $\partial \in \mathfrak{g}_{-d}$ such that $[\partial, \mathfrak{g}_i] = \mathfrak{g}_{i-d}$, for $i \geqslant 0$.

Remark 3.1: If $\mathfrak{g}$ contains the grading operator with respect to its gradation, then condition (L2) is automatic.

Examples of Lie superalgebras satisfying (L1)–(L3) are provided by annihilation subalgebras of superconformal algebras, which we will describe in more detail.

Let t be an even indeterminate and $\xi_1, \ldots, \xi_N$ be N odd indeterminate. Denote by $\Lambda(N)$ the Grassmann superalgebra in the indeterminates $\xi_1, \ldots, \xi_N$ and set $\Lambda(1,N) := \mathbb{C}[t, t^{-1}] \otimes \Lambda(N)$. Let $\mathrm{W}(1,N)$ be the derivation superalgebra of $\Lambda(1,N)$. Then $\mathrm{W}(1,N)$ is a formal distribution Lie superalgebra.[8] Letting $\partial/\partial t$ and $\partial/\partial \xi_i$, for $i = 1, \ldots, N$, be the usual differential operators, every element in $D \in \mathrm{W}(1,N)$ can be written as[9]

$$D = a_0 \frac{\partial}{\partial t} + \sum_{i=1}^{N} a_i \frac{\partial}{\partial \xi_i}, \quad a_0, a_i, \ldots, a_N \in \Lambda(1,N).$$

The *standard gradation* of $\mathrm{W}(1,N)$ is obtained by setting the degree of t and ξ_i to be 1. Its annihilation subalgebra is $\mathrm{W}(1,N)_+ = \oplus_{j \geqslant -1} (\mathrm{W}(1,N))_j$. $\mathrm{W}(1,N)_+$ in this gradation contains its grading operator given by $z = t\,\partial/\partial t + \Sigma_{i=1}^{N} \xi_i\,\partial/\partial \xi_i$ so that (L2) is satisfied. Also choosing ∂ to be $\partial/\partial t$ it follows that (L3) is also satisfied so that $\mathrm{W}(1,N)$ is a Lie superalgebra of the type above. Note that $\mathrm{W}(1,N)_0 \cong \mathrm{gl}(1,N)$.

The subalgebra of divergence zero vector fields in $\mathrm{W}(1,N)$ contains an ideal of codimension 1. This ideal is its derived algebra and is the superconformal algebra $\mathrm{S}(1,N)$.[8] The standard gradation of $\mathrm{W}(1,N)_+$ induces a gradation on the annihilation subalgebra $\mathrm{S}(1,N)_+$ of $\mathrm{S}(1,N)$. Choosing $z = t\,\partial/\partial t + (1/N)\,\Sigma_{i=1}^{N} \xi_i\,\partial/\partial \xi_i$ along with $\partial = \partial/\partial t$ it follows that $\mathrm{S}(1,N)_+$ in this gradation also satisfies (L1)–L(3). Observe that $\mathrm{S}(1,N)_0 \cong \mathrm{sl}(1,N)$ and also that the ''small'' $N=4$ superconformal algebra (to be defined in Sec. VI) is isomorphic to $\mathrm{S}(1,2)$.[10]

The contact superalgebra $\mathrm{K}(1,N)$ is the subalgebra of $\mathrm{W}(1,N)$ defined by

$$\mathrm{K}(1,N) := \{D \in \mathrm{W}(1,N) \,|\, D\omega = f_D \omega, \quad \text{for some} \quad f_D \in \Lambda(1,N)\},$$

where $\omega := dt - \Sigma_{i=1}^{N} \xi_i d\xi_i$ is the standard contact form. Here the action of D on ω is the usual action of vector fields on differential forms.

The map from $\Lambda(1,N)$ to $\mathrm{K}(1,N)$ given by

$$f \to 2\,f \frac{\partial}{\partial t} + (-1)^{p(f)} \sum_{i=1}^{N} \left(\xi_i \frac{\partial f}{\partial t} + \frac{\partial f}{\partial \xi_i} \right) \left(\xi_i \frac{\partial}{\partial t} + \frac{\partial}{\partial \xi_i} \right)$$

is a bijection and hence it allows us to identify $\mathrm{K}(1,N)$ with the polynomial superalgebra $\Lambda(1,N)$. The Lie bracket in $\Lambda(1,N)$, also called the contact bracket, then reads for homogeneous elements $f, g \in \Lambda(1,N)$

$$[f,g] = (2-E) f \frac{\partial g}{\partial t} - \frac{\partial f}{\partial t} (2-E) g + (-1)^{p(f)} \sum_{i=1}^{N} \frac{\partial f}{\partial \xi_i} \frac{\partial g}{\partial \xi_i},$$

where $E = \Sigma_{i=1}^{N} \xi_i\,\partial/\partial \xi_i$ is the Euler operator.

When N is even it is sometimes more convenient to make the change of basis $\xi_j^+ = (1/\sqrt{2})\,(\xi_j + i\xi_{j+N/2})$ and $\xi_j^- = (1/\sqrt{2})\,(\xi_j - i\xi_{j+N/2})$, for $j = 1, \ldots, N/2$ and $i = \sqrt{-1}$, so that the contact bracket takes the split form:

$$[f,g] = (2-E) f \frac{\partial g}{\partial t} - \frac{\partial f}{\partial t} (2-E) g + (-1)^{p(f)} \sum_{i=1}^{N/2} \left(\frac{\partial f}{\partial \xi_i^+} \frac{\partial g}{\partial \xi_i^-} + \frac{\partial f}{\partial \xi_i^-} \frac{\partial g}{\partial \xi_i^+} \right),$$

where E again is the Euler operator $\Sigma_{i=1}^{N/2} (\xi_i^+\,\partial/\partial \xi_i^+ + \xi_i^-\,\partial/\partial \xi_i^-)$.

The contact superalgebra K(1,N) is a formal distribution Lie superalgebra with fields defined as follows: Let $I=\{i_1,\ldots,i_k\}$ be an ordered subset of $\{1,\ldots,N\}$, and denote by ξ_I the monomial $\xi_{i_1}\cdots\xi_{i_k}$. Each such monomial gives rise to a field $\xi_I(z)=\Sigma_{j\in\mathbb{Z}}\xi_I t^j z^{-j-1}$. Evidently the span of the coefficients of all such $\xi_I(z)$ is K(1,N). Furthermore, it is easy to check that these fields are mutually local and form a formal distribution Lie superalgebra. This Lie superalgebra becomes $\mathbb{Z}$-graded by putting the degree of $\xi_I t^n$ to $2n+k-2$. Obviously t is the grading operator of this gradation. This gradation of K(1,N) is usually referred to as its *standard gradation.*

The annihilation subalgebra K(1,N)$_+$ of K(1,N) is spanned by the basis elements $\xi_I t^n$, where $n\geqslant 0$ and I runs over all subsets of $\{i_1,\ldots,i_k\}$ ordered in (strictly) increasing order. The $\mathbb{Z}$-gradation from K(1,N) induces a gradation on K(1,N)$_+$ making it a $\mathbb{Z}$-graded Lie superalgebra of depth 2 so that $\mathrm{K}(1,N)_+=\oplus_{j=-2}^{\infty}(K(1,N)_+)_j$ satisfies (L1) and (L2). In this gradation it is easy to check that $[1,(K(1,N)_+)_j]=(K(1,N)_+)_{j-2}$ for all $j\geqslant 0$, so that K(1,N)$_+$ also satisfies condition (L3). It is easy to see that the annihilation subalgebra of the small $N=4$ superconformal algebra, which we define in Sec. VI, also satisfies conditions (L1)–(L3). Note that $\mathrm{K}(1,N)_0\cong c\,\mathrm{so}_N$, the direct sum of the Lie algebra so_N and the one-dimensional Lie algebra.

Finally, it follows from the description of the exceptional superconformal algebra CK_6 as a subalgebra of K(1,6) in Ref. 11 that its annihilation subalgebra $(\mathrm{CK}_6)_+=\oplus_{j\geqslant -2}(\mathrm{CK}_6)_j$ is a Lie superalgebra satisfying (L1)–(L3) with $(\mathrm{CK}_6)_0\cong c\,\mathrm{so}_6$.

The modules over the annihilation subalgebras that are equivalent to modules over the corresponding conformal superalgebras are then $\mathfrak{g}$-modules V satisfying the following conditions.

(V1) For all $v\in V$ there exists an integer $k_0\geqslant -d$ (depending on v) such that $\mathfrak{g}_k v=0$, for all $k\geqslant k_0$.

(V2) V is finitely generated over $\mathbb{C}[\partial]$.

We shall call $\mathfrak{g}$-modules satisfying these two properties *finite*. Let V be a finite irreducible $\mathfrak{g}$-module. For $n\geqslant -d-1$ set $V_n=\{v\in V|\mathfrak{g}_j v=0,\forall j>n\}$. Let N be the minimal integer such that $V_N\neq 0$. Such an N exists by (V1).

Lemma 3.2: If $N\geqslant 0$, then V_N is a finite-dimensional vector space over $\mathbb{C}$.

Proof: We let $\mathcal{L}=\mathfrak{g}$ and put $\mathcal{L}_j=\oplus_{i\geqslant jd}\mathfrak{g}_i$ so that we have a filtration of subspaces

$$\mathcal{L}\supset\mathcal{L}_0\supset\mathcal{L}_1\supset\mathcal{L}_2\supset\cdots\supset\mathcal{L}_n\supset\cdots,$$

with $[\partial,\mathcal{L}_i]=\mathcal{L}_{i-1}$, for all $i\geqslant 0$ by (L3). Let $W_m:=\{v\in V|\mathcal{L}_{m+1}v=0\}$ and let M be the minimal integer such that $W_M\neq 0$. Since $N\geqslant 0$ implies that $M\geqslant 0$, this setting puts us in the situation of Lemma 3.1, from which we conclude that W_M is a finite-dimensional vector space over $\mathbb{C}$. Of course $V_N\subset W_M$ and hence it follows that V_N is finite-dimensional as well. □

We obtain the following description of finite irreducible $\mathfrak{g}$-modules.

Theorem 3.1: *Let $\mathfrak{g}=\oplus_{j\geqslant -d}\mathfrak{g}_j$ be a Lie superalgebra satisfying conditions (L1)–(L3) and V be a finite irreducible $\mathfrak{g}$-module. There exists a finite-dimensional irreducible $\mathfrak{g}_0$-module U_0, extended trivially to an $\mathcal{L}_0(=\oplus_{j\geqslant 0}\mathfrak{g}_j)$-module, and a $\mathfrak{g}$-epimorphism φ: $\mathrm{Ind}_{\mathcal{L}_0}^{\mathfrak{g}}U_0\to V$.*

Proof: We will continue to use the notation defined earlier. First we show that $N\leqslant 0$. Suppose that $N>0$. It is easy to see that V_N is invariant under $\mathcal{L}_0$. Now there exists a basis $\{x_1,\ldots,x_m\}$ of $\mathfrak{g}_N$ together with nonzero complex number $\lambda_1,\ldots,\lambda_m$ such that $[z,x_i]=\lambda_i x$, where z is the element of (L2). Since V_N is a finite-dimensional vector space it follows in particular that x_i acts nilpotently on V_N for all $1\leqslant i\leqslant m$. But $[\mathfrak{g}_N,\mathfrak{g}_N]\subset\oplus_{j\geqslant N+1}\mathfrak{g}_j$ and so the action of the x_i's on V_N commutes. Therefore there exits a nonzero $v\in V_N$ such that $\mathfrak{g}_N v=0$. But in this case $V_{N-1}\neq 0$, which contradicts the minimality of N. Thus $N\leqslant 0$.

In the case when $N=0$, there exists an epimorphism of $\mathfrak{g}$-modules $\mathrm{Ind}_{\mathcal{L}_0}^{\mathfrak{g}}V_0\to V$, with V_0 finite-dimensional due to Lemma 3.2. By irreducibility of V it follows that $V_0=U_0$ is an irreducible $\mathfrak{g}_0$-module. Now if $N<0$, then there exists a nonzero vector v invariant under the action of $\mathfrak{g}_j$, for $j\geqslant 0$. Again we have an epimorphism of $\mathfrak{g}$-modules $\mathrm{Ind}_{\mathcal{L}_0}^{\mathfrak{g}}\mathbb{C}v\to V$. □

As a corollary of Theorem 3.1 we obtain the following.

Corollary 3.1: There exists a bijection between finite irreducible conformal modules of the

superconformal algebra $\mathfrak{g}$ *and finite-dimensional irreducible representations of the Lie (super)algebra* $\mathfrak{g}_0$, *where*

(*i*) $\mathfrak{g}=\mathrm{K}(1,N)$ *and* $\mathfrak{g}_0=c\mathrm{so}_N$,
(*ii*) $\mathfrak{g}=\mathrm{W}(1,N)$ *and* $\mathfrak{g}_0=\mathrm{gl}(1,N)$,
(*iii*) $\mathfrak{g}=\mathrm{S}(1,N)$ *and* $\mathfrak{g}_0=\mathrm{sl}(1,N)$, *and*
(*iv*) $\mathfrak{g}=CK_6$ *and* $\mathfrak{g}_0=c\mathrm{so}_6$.

Proof: By Theorem 3.1 every finite irreducible $\mathfrak{g}$-module is a homomorphic image of $\mathrm{Ind}_{\mathcal{L}_0}^{\mathfrak{g}}U_0$. Now the usual argument for highest weight representations implies that given a finite-dimensional irreducible $\mathfrak{g}_0$-module U_0 the $\mathfrak{g}$-module $\mathrm{Ind}_{\mathcal{L}_0}^{\mathfrak{g}}U_0$ contains a unique maximal submodule, from which the bijection then follows. □

Remark 3.2: It is usual to put a half-integer gradation on $\mathrm{K}(1,N)$ when thinking of it as a superconformal algebra. The grading operator of $\mathrm{K}(1,N)$ with respect to this gradation is then $t/2$ rather than t. In this gradation one has $\mathrm{K}(1,N)_+=\oplus_{j\geqslant -1}\mathfrak{g}_j$, where $j\in\frac{1}{2}\mathbb{Z}$. Theorem 3.1 of course remains valid after making some obvious changes regarding gradation. For a Lie superalgebra $\mathfrak{g}=\oplus_{j\geqslant -1}\mathfrak{g}_j$ with $j\in\frac{1}{2}\mathbb{Z}$, we will make it a convention to write $\mathfrak{g}_-$ for the subalgebra $\oplus_{j<0}\mathfrak{g}_j$.

IV. FINITE IRREDUCIBLE MODULES OVER THE $N=2$ CONFORMAL SUPERALGEBRA

The $N=2$ superconformal algebra is the formal distribution Lie superalgebra $\mathrm{K}(1,2)$. Letting ξ^+,ξ^- denote the two odd indeterminates (so that we are using the split contact form), this algebra is generated by the following four fields: $L(z)=\Sigma_{n\in\mathbb{Z}}-(t^{n+1}/2)z^{-n-2}$, $G^{\pm}(z)=\Sigma_{r\in(1/2)+\mathbb{Z}}\xi^{\pm}t^{r+1/2}z^{-r-3/2}$ and $J(z)=\Sigma_{n\in\mathbb{Z}}\xi^-\xi^+t^nz^{-n-1}$. Its corresponding conformal superalgebra is then generated freely over $\mathbb{C}[\partial]$ by $\{L,J,G^{\pm}\}$ with products

$$L_\lambda L=(\partial+2\lambda)L,\quad L_\lambda J=(\partial+\lambda)J,\quad L_\lambda G^{\pm}=(\partial+\tfrac{3}{2}\lambda)G^{\pm},$$

$$J_\lambda G^{\pm}=\pm G^{\pm},\quad G^+_\lambda G^-=(\partial+2\lambda)J+2L.$$

Letting $L_n=-t^{n+1}/2$, $G^{\pm}_r=\xi^{\pm}t^{r+1/2}$ and $J_n=\xi^-\xi^+t^n$ with $n\in\mathbb{Z}$, $r\in\frac{1}{2}+\mathbb{Z}$, the non-zero brackets in $\mathrm{K}(1,2)$ are ($m,n\in\mathbb{Z}$ and $r,s\in\frac{1}{2}+\mathbb{Z}$)

$$[L_m,L_n]=(m-n)L_{m+n},\quad [L_m,G^{\pm}_r]=\left(\frac{m}{2}-r\right)G^{\pm}_{m+r},\quad [L_m,J_n]=-nJ_{n+m},$$

$$[J_m,G^{\pm}_r]=\pm G^{\pm}_{m+r},\quad [G^+_r,G^-_s]=2L_{r+s}+(r-s)J_{r+s}.$$

The annihilation subalgebra $\mathfrak{g}=\mathrm{K}(1,2)_+$ is then spanned by L_m, J_n and $G^{\pm}_r$, where $m\geqslant -1$, $n\geqslant 0$ and $r\geqslant -\frac{1}{2}$. Note that letting $\mathfrak{g}_j$ be the span of X_j, where $X=L,J,G^{\pm}$, equips $\mathfrak{g}=\oplus_{j\geqslant -1}\mathfrak{g}_j$, $j\in\frac{1}{2}\mathbb{Z}$, with a (consistent) $\frac{1}{2}\mathbb{Z}$-gradation. We denote L_{-1} by ∂ from now on.

Let $\mathbb{C}v_{\Delta,\Lambda}$, $\Delta,\Lambda\in\mathbb{C}$, be the one-dimensional module over the abelian Lie algebra $\mathfrak{g}_0=\mathbb{C}L_0+\mathbb{C}J_0$, determined by

$$L_0v_{\Delta,\Lambda}=\Delta v_{\Delta,\Lambda},\quad J_0v_{\Delta,\Lambda}=\Lambda v_{\Delta,\Lambda}.$$

We may extend $\mathbb{C}v_{\Delta,\Lambda}$ to a module over $\mathcal{L}_0=\oplus_{j\geqslant 0}\mathfrak{g}_j$ by setting $\mathfrak{g}_jv_{\Delta,\Lambda}=0$, for $j>0$. Let $M_{\mathfrak{N}^2_+}(\Delta,\Lambda):=\mathrm{Ind}_{\mathcal{L}_0}^{\mathfrak{g}}\mathbb{C}v_{\Delta,\Lambda}$. We denote by N the unique maximal submodule of $M_{\mathfrak{N}^2_+}(\Delta,\Lambda)$. The quotient $M_{\mathfrak{N}^2_+}(\Delta,\Lambda)/N$ is the irreducible highest weight module $L_{\mathfrak{N}^2_+}(\Delta,\Lambda)$ of highest weight (Δ,Λ). By Theorem 3.1 $L_{\mathfrak{N}^2_+}(\Delta,\Lambda)$ for $\Delta,\Lambda\in\mathbb{C}$ form a complete list of finite irreducible $\mathrm{K}(1,2)_+$-modules. Our next objective is to give a more explicit description of N and hence of $L_{\mathfrak{N}^2_+}(\Delta,\Lambda)$.

It is clear that $\partial^kv_{\Delta,\Lambda}$, $\partial^kG^+_{-1/2}v_{\Delta,\Lambda}$, $\partial^kG^-_{-1/2}v_{\Delta,\Lambda}$ and $\partial^kG^+_{-1/2}G^-_{-1/2}v_{\Delta,\Lambda}$, $k\geqslant 0$, is a basis consisting of (L_0,J_0)-weight vectors for $M_{\mathfrak{N}^2_+}(\Delta,\Lambda)$ of (L_0,J_0)-weights $(\Delta+k,\Lambda)$, $(\Delta+k$

$+\frac{1}{2},\Lambda+1)$, $(\Delta+k+\frac{1}{2},\Lambda-1)$ and $(\Delta+k+1,\Lambda)$, respectively. A nonzero (L_0,J_0)-weight vector $v\in M_{\mathfrak{N}_+^2}(\Delta,\Lambda)$ is called a *singular vector* if $\mathfrak{g}_j v=0$, for all $j>0$. We call a singular vector *proper* if it is not a scalar multiple of the highest weight vector $v_{\Delta,\Lambda}$. Obviously $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)$ is irreducible if and only if $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)$ contains no proper singular vector. We now analyze singular vectors inside $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)$.

Lemma 4.1: Let $k\geqslant 1$ and suppose that $w=\alpha\partial^k v_{\Delta,\Lambda}+\beta\partial^{k-1}G^+_{-1/2}G^-_{-1/2}v_{\Delta,\Lambda}$ is a singular vector of (L_0,J_0)-weight $(\Delta+k,\Lambda)$ in $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)$, where $\alpha,\beta\in\mathbb{C}$. Then $k=1$. Furthermore, any proper singular vector of this form is a scalar multiple of either $G^+_{-1/2}G^-_{-1/2}v_{\Delta,\Lambda}$, in which case $\Delta=-\frac{1}{2}$ and $\Lambda=1$, or $(-2\partial+G^+_{-1/2}G^-_{-1/2})v_{\Delta,\Lambda}$, in which case $\Delta=-\frac{1}{2}$ and $\Lambda=-1$.

Proof: Note that w is singular if and only if $J_1 w=G^{\pm}_{1/2}w=0$. We compute

$$G^+_{1/2}w=(\alpha k-\beta(2\Delta+\Lambda))\partial^{k-1}G^+_{-1/2}v_{\Delta,\Lambda}=0, \tag{4.1}$$

$$G^-_{1/2}w=(\alpha k+\beta(2\Delta-\Lambda+2k))\partial^{k-1}G^-_{-1/2}v_{\Delta,\Lambda}=0, \tag{4.2}$$

$$J_1 w=(\alpha\Lambda k+\beta(2\Delta+\Lambda))\partial^{k-1}v_{\Delta,\Lambda}+\beta(k-1)\Lambda\partial^{k-2}G^+_{-1/2}G^-_{-1/2}v_{\Delta,\Lambda}=0. \tag{4.3}$$

But then $\beta\neq 0$, since otherwise (4.1) would imply that $k=0$. However, $\beta\neq 0$ together with (4.1) and (4.2) implies that

$$2\Delta+k=0. \tag{4.4}$$

Now (4.3) gives

$$\alpha\Lambda k+\beta(2\Delta+\Lambda)=0,\quad \beta(k-1)\Lambda=0. \tag{4.5}$$

Now if $k>1$, then (4.5) gives $\Lambda=0$ and $\Delta=0$. But then $k=0$ by (4.1). Hence $k=1$ so that by (4.4) we have $\Delta=-\frac{1}{2}$.

Now if $\alpha\neq 0$, we have from (4.1) and (4.3) $\alpha(1+\Lambda)=0$ and hence $\Lambda=-1$. The first equation of (4.5) then implies that $\alpha+2\beta=0$.

On the other hand, if $\alpha=0$, the first equation of (4.5) gives $\Lambda=1$. □

Lemma 4.2: Let $k\in\mathbb{Z}_+$.

(*i*) *If $\partial^k G^+_{-1/2}v_{\Delta,\Lambda}$ is a singular vector of (L_0,J_0)-weight $(\Delta+k+\frac{1}{2},\Lambda+1)$, then $k=0$ and $2\Delta-\Lambda=0$. Furthermore, in this case $G^+_{-1/2}v_{\Delta,\Lambda}$ is a singular vector.*

(*ii*) *If $\partial^k G^-_{-1/2}v_{\Delta,\Lambda}$ is a singular vector of (L_0,J_0)-weight $(\Delta+k+\frac{1}{2},\Lambda-1)$, then $k=0$ and $2\Delta+\Lambda=0$. Furthermore, in this case $G^-_{-1/2}v_{\Delta,\Lambda}$ is a singular vector.*

Proof: The lemma follows immediately from the following two equations:

$$G^-_{1/2}\partial^k G^+_{-1/2}v_{\Delta,\Lambda}=(2\Delta-\Lambda+2k)\partial^k v_{\Delta,\Lambda}+k\partial^{k-1}G^+_{-1/2}G^-_{-1/2}v_{\Delta,\Lambda}=0,$$

$$G^+_{1/2}\partial^k G^-_{-1/2}v_{\Delta,\Lambda}=(2\Delta+\Lambda)\partial^k v_{\Delta,\Lambda}+k\partial^{k-1}G^+_{-1/2}G^-_{-1/2}v_{\Delta,\Lambda}=0.$$

□

Thus Lemmas 4.1 and 4.2 prove the following.

Proposition 4.1: Any proper singular vector in $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)$ is a scalar multiple of the following.

(*i*) *$G^+_{-1/2}v_{\Delta,\Lambda}$, in which case we have $2\Delta-\Lambda=0$. In the particular case of $\Delta=-\frac{1}{2}$ and $\Lambda=-1$ we have in addition $G^-_{-1/2}G^+_{-1/2}v_{\Delta,\Lambda}$.*

(*ii*) *$G^-_{-1/2}v_{\Delta,\Lambda}$, in which case we have $2\Delta+\Lambda=0$. In the particular case of $\Delta=-\frac{1}{2}$ and $\Lambda=1$ we have in addition $G^+_{-1/2}G^-_{-1/2}v_{\Delta,\Lambda}$.*

Let N be the subspace of $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)$ given by

$$N=\mathbb{C}[\partial]G^+_{-1/2}v_{\Delta,\Lambda}+\mathbb{C}[\partial]G^-_{-1/2}G^+_{-1/2}v_{\Delta,\Lambda}, \quad \text{if } 2\Delta-\Lambda=0 \text{ and } \Lambda\neq 0,$$

$$N=\mathbb{C}[\partial]G^-_{-1/2}v_{\Delta,\Lambda}+\mathbb{C}[\partial]G^+_{-1/2}G^-_{-1/2}v_{\Delta,\Lambda}, \quad \text{if } 2\Delta+\Lambda=0 \text{ and } \Lambda\neq 0.$$

It follows from Proposition 4.1 that in either case N is a submodule of $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)$.

Theorem 4.1: *The modules $L_{\mathfrak{N}_+^2}(\Delta,\Lambda)$, for $\Delta,\Lambda\in\mathbb{C}$, form a complete list of nonisomorphic finite (over $\mathbb{C}[\partial]$) irreducible* $\mathrm{K}(1,2)_+$*-modules. Furthermore, $L_{\mathfrak{N}_+^2}(\Delta,\Lambda)$ as a $\mathbb{C}[\partial]$-module has rank*

(*i*) 4, *in the case* $2\Delta\pm\Lambda\neq 0$,
(*ii*) 2, *in the case* $2\Delta\pm\Lambda=0$ *and* $2\Delta\mp\Lambda\neq 0$, *and*
(*iii*) 0, *in the case* $\Delta=\Lambda=0$.

Proof: If $2\Delta+\Lambda\neq 0$ and $2\Delta-\Lambda\neq 0$, then by Proposition 4.1 $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)$ contains no proper singular vector and hence is irreducible.

Suppose that $2\Delta+\Lambda=0$ and $2\Delta-\Lambda\neq 0$. In this case consider the submodule of $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)$ generated by the singular vector $G^-_{-1/2}v_{\Delta,\Lambda}$. This module is precisely N above and hence $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)/N$ is freely generated over $\mathbb{C}[\partial]$ by $v_{\Delta,\Lambda}$ and $G^+_{-1/2}v_{\Delta,\Lambda}$. We claim that $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)/N$ is irreducible. The even part of $\mathrm{K}(1,2)_+$ is isomorphic to the semi-direct sum of $\mathfrak{V}_+$ (generated by L_n) and $\tilde{\mathfrak{g}}_+$ (generated by J_n), where $\mathfrak{g}$ is the one-dimensional Lie algebra. We first consider $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)/N$ as a module over the $\mathfrak{V}_+\ltimes\tilde{\mathfrak{g}}_+$. The vectors $v_{\Delta,\Lambda}$ and $G^+_{1/2}v_{\Delta,\Lambda}$ have (L_0,J_0)-weights (Δ,Λ) and $(\Delta+\frac{1}{2},\Lambda+1)$, respectively, and, furthermore, both are annihilated by L_n and J_n, for $n\geqslant 1$. Now since $2\Delta+\Lambda=0$ and $2\Delta-\Lambda\neq 0$, we have $(\Delta,\Lambda)\neq(0,0)$ and $(\Delta+\frac{1}{2},\Lambda+1)\neq(0,0)$. From this it follows that $M_{\mathfrak{N}_+^2}(\Delta,\Lambda)/N$ as a module over $\mathfrak{V}_+\ltimes\tilde{\mathfrak{g}}_+$ is a direct sum of two non-isomorphic irreducible modules, namely $\mathbb{C}[\partial]v_{\Delta,\Lambda}\cong L_{\mathfrak{V}_+\ltimes\tilde{\mathfrak{g}}_+}(\Delta,\Lambda)$ and $\mathbb{C}[\partial]G^+_{-1/2}v_{\Delta,\Lambda}\cong L_{\mathfrak{V}_+\ltimes\tilde{\mathfrak{g}}_+}(\Delta+\frac{1}{2},\Lambda+1)$ (see Sec. II for notation). But we have

$$G^-_{1/2}G^+_{-1/2}v_{\Delta,\Lambda}=(2\Delta-\Lambda)v_{\Delta,\Lambda}\neq 0,$$

which implies that as a $\mathrm{K}(1,2)_+$-module $L_{\mathfrak{N}_+^2}(\Delta,\Lambda)$ is irreducible.

The case when $2\Delta-\Lambda=0$ and $2\Delta+\Lambda\neq 0$ is completely analogous and we leave it to the reader.

Finally, in the case when $\Delta=\Lambda=0$, both $G^+_{-1/2}v_{\Delta,\Lambda}$ and $G^-_{-1/2}v_{\Delta,\Lambda}$ are proper singular vectors. Now the submodule in $M_{\mathfrak{N}_+^2}(0,0)$ generated by these two vectors contains $[G^+_{-1/2},G^-_{-1/2}]v_{\Delta,\Lambda}=2\partial v_{\Delta,\Lambda}$, and hence has codimension 1 over $\mathbb{C}$. So the resulting quotient is the trivial module. □

It follows that every finite irreducible module over the $N=2$ conformal superalgebra is of the form $L_{\mathfrak{N}^2}(\alpha,\Delta,\Lambda)$, where $\alpha,\Delta,\Lambda\in\mathbb{C}$. We will write down explicit formulas for the action of the conformal superalgebra on such irreducible modules in the generating series form. Since we have already explained in Sec. II how such formulas can be obtained in general, we will omit the proofs.

In the case when $2\Delta\pm\Lambda\neq 0$ the module $L_{\mathfrak{N}^2}(\alpha,\Delta,\Lambda)$ is generated freely over $\mathbb{C}[\partial]$ by two even vectors v,v^{+-} and two odd vectors v^+,v^-. We have the following action on the generators:

$$L_\lambda v=(\partial+\alpha+\Delta\lambda)v, \quad L_\lambda v^\pm=(\partial+\alpha+(\Delta+\tfrac{1}{2})\lambda)v^\pm,$$

$$L_\lambda v^{+-}=(\partial+\alpha+(\Delta+1)\lambda)v^{+-}+\left(\Delta+\frac{\Lambda}{2}\right)\lambda^2 v,$$

$$J_\lambda v=\Lambda v,\quad J_\lambda v^{\pm}=(\Lambda\pm 1)v^{\pm},\quad J_\lambda v^{+-}=\Lambda v^{+-}+(2\Delta+\Lambda)\lambda v,$$

$$G^{\pm}_\lambda v=v^{\pm},\quad G^{+}_\lambda v^{+}=G^{-}_\lambda v^{-}=0,\quad G^{+}_\lambda v^{-}=v^{+-}+(2\Delta+\Lambda)\lambda v,$$

$$G^{+}_\lambda v^{+-}=-\lambda(2\Delta+\Lambda)v^{+},\quad G^{-}_\lambda v^{+}=(2\partial+2\alpha+\lambda(2\Delta-\Lambda))v-v^{+-},$$

$$G^{-}_\lambda v^{+-}=(2\partial+2\alpha+(2\Delta+2-\Lambda)\lambda)v^{-}.$$

In the case when $2\Delta+\Lambda=0$ but $2\Delta-\Lambda\neq 0$ the module $L_{\mathfrak{N}^2}(\alpha,\Delta,\Lambda)$ is generated freely over $\mathbb{C}[\partial]$ by one even vector v and one odd vector v^{+}. The action is then given by

$$L_\lambda v=(\partial+\alpha+\Delta\lambda)v,\quad L_\lambda v^{+}=(\partial+\alpha+(\Delta+\tfrac{1}{2})\lambda)v^{+},$$

$$J_\lambda v=-2\Delta v,\quad J_\lambda v^{+}=(-2\Delta+1)v^{+},\quad G^{+}_\lambda v=v^{+},\quad G^{+}_\lambda v^{+}=0,$$

$$G^{-}_\lambda v=0,\quad G^{-}_\lambda v^{+}=(2\partial+2\alpha+4\Delta\lambda)v.$$

In the case $2\Delta-\Lambda=0$ but $2\Delta+\Lambda\neq 0$ the module $L_{\mathfrak{N}^2}(\alpha,\Delta,\Lambda)$ is generated freely over $\mathbb{C}[\partial]$ by one even vector v and one odd vector v^{-} with action:

$$L_\lambda v=(\partial+\alpha+\Delta\lambda)v,\quad L_\lambda v^{-}=(\partial+\alpha+(\Delta+\tfrac{1}{2})\lambda)v^{-},$$

$$J_\lambda v=2\Delta v,\quad J_\lambda v^{-}=(2\Delta-1)v^{-},\quad G^{+}_\lambda v=0,$$

$$G^{+}_\lambda v^{-}=(2\partial+2\alpha+4\Delta\lambda)v,\quad G^{-}_\lambda v=v^{-},\quad G^{-}_\lambda v^{-}=0.$$

Finally $L_{\mathfrak{N}^2}(\alpha,0,0)$ is the one-dimensional trivial module on which ∂ acts as the scalar α.

Remark 4.1: We note that the formulas above are obtained by first putting $v=v_{\Delta,\Lambda}$, $v^{\pm}=G^{\pm}_{-1/2}v_{\Delta,\Lambda}$ and $v^{+-}=G^{+}_{-1/2}G^{-}_{-1/2}v_{\Delta,\Lambda}$ and then compute the action of the operators L_n, J_m and $G^{\pm}_r$, for $n\geqslant -1$, $m\geqslant 0$ and $r\geqslant -\frac{1}{2}$ on these vectors. Translation into the language of conformal modules is an easy task using these formulas and we will omit this. Of course the parity of the vectors $v,v^{\pm},v^{+-}$ in all the examples above can be reversed. Finally, we note that the adjoint module is isomorphic to $L_{\mathfrak{N}^2}(0,1,0)$.

V. FINITE IRREDUCIBLE MODULES OVER THE *N*=3 CONFORMAL SUPERALGEBRA

The $N=3$ superconformal algebra is the formal distribution Lie superalgebra K(1,3). Letting ξ_1,ξ_2,ξ_3 be the three odd indeterminates K(1,3) is spanned over $\mathbb{C}$ by the following basis elements ($n\in\mathbb{Z}$ and $r\in\frac{1}{2}+\mathbb{Z}$):

$$L_n=-\frac{t^{n+1}}{2},\quad H_n=2i\xi_1\xi_2t^n,\quad E_n=(-\xi_1\xi_3-i\xi_2\xi_3)t^n,\quad F_n=(\xi_1\xi_3-i\xi_2\xi_3)t^n,$$

$$\Psi_r=-\xi_1\xi_2\xi_3t^{r-1/2},\quad h_r=-2i\xi_3t^{r+1/2},\quad e_r=(i\xi_1-\xi_2)t^{r+1/2},\quad f_r=(i\xi_1+\xi_2)t^{r+1/2}.$$

Let $\{H,E,F\}$ denote the standard basis of the Lie algebra sl_2 and $\{h,e,f\}$ denote the standard basis of its adjoint module. Furthermore, we let $(\cdot|\cdot)$ denote the non-degenerate invariant symmetric bilinear form on sl_2 with $(H|H)=2$. Keeping this notation in mind the commutation relations of K(1,3) are then given as follows (where $X,Y=H,E,F$ and $x,y=h,e,f$):

$$[L_m,L_n]=(m-n)L_{m+n},\quad [L_m,X_n]=-nX_{m+n},\quad [L_m,x_r]=\left(\frac{m}{2}-r\right)x_{m+r},$$

$$[L_m,\Psi_r]=\left(-\frac{m}{2}-r\right)\Psi_{m+r},\quad [X_m,Y_n]=[X,Y]_{m+n},\quad [X_m,\Psi_r]=0,$$

$$[X_m,y_r]=[X,y]_{m+r}+2m(X|Y)\Psi_{m+r},\quad [x_r,\Psi_s]=-X_{r+s},\quad [\Psi_r,\Psi_s]=0,$$

$$[x_r,y_s]=-(r-s)[X,Y]_{r+s}-4(X|Y)L_{r+s},$$

where $m,n\in\mathbb{Z}$ and $r,s\in\frac{1}{2}+\mathbb{Z}$. Above we have written $[X,y]$ for the action of X on y. The eight formal distributions generating this algebra are given by $L(z)=\Sigma_{n\in\mathbb{Z}}L_nz^{-n-2}$, $X(z)=\Sigma_{n\in\mathbb{Z}}X_nz^{-n-1}$, $x(z)=\Sigma_{r\in 1/2+\mathbb{Z}}x_rz^{-r-3/2}$ and $\Psi(z)=\Sigma_{r\in 1/2+\mathbb{Z}}\Psi_rz^{-r-1/2}$. The corresponding operator product expansions of these fields are easily derived from (2.3), and so we will omit them.

The annihilation subalgebra $\mathrm{K}(1,3)_+$ is equipped with a $\frac{1}{2}\mathbb{Z}$-gradation of depth 1, i.e., $\mathrm{K}(1,3)_+=\mathfrak{g}=\oplus_{j\geqslant -1}\mathfrak{g}_j$, $j\in\frac{1}{2}\mathbb{Z}$, and its zeroth graded component $\mathfrak{g}_0$ is isomorphic to a copy of $\mathrm{gl}_2\cong\mathrm{sl}_2\oplus\mathbb{C}L_0$, with H_0, E_0 and F_0 providing the standard basis for the copy of sl_2.

Let $U^{\Delta,\Lambda}$ be the finite-dimensional irreducible sl_2-module of highest weight $\Lambda\in\mathbb{Z}_+$ on which L_0 acts as the scalar Δ. We let $v_{\Delta,\Lambda}$ be a highest weight vector in $U^{\Delta,\Lambda}$. We extend $U^{\Delta,\Lambda}$ to a module over the subalgebra $\mathcal{L}_0=\oplus_{j\geqslant 0}\mathfrak{g}_j$ in a trivial way and call this $\mathcal{L}_0$-module also $U^{\Delta,\Lambda}$. By Theorem 3.1 every finite irreducible $\mathfrak{g}$-module is a homomorphic image of $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)=\mathrm{Ind}_{\mathcal{L}_0}^{\mathfrak{g}}U^{\Delta,\Lambda}$ and furthermore $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)$ has a unique maximal submodule N, whose irreducible quotient we denote by $L_{\mathfrak{N}_+^3}(\Delta,\Lambda)$.

Note that $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)$ as a module over sl_2 is a direct sum of infinitely many copies of finite-dimensional irreducible representations. Since ∂ commutes with E_0, the E_0-invariant $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)^{E_0}$ is a $\mathbb{C}[\partial]$-submodule of $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)$, and hence is a free $\mathbb{C}[\partial]$-module. We can explicitly write down formulas for a $\mathbb{C}[\partial]$-basis of $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)^{E_0}$. In the case when $\Lambda\geqslant 2$ the following is a $\mathbb{C}[\partial]$-basis:

$$a_1=v_{\Delta,\Lambda},\quad a_2=e_{-1/2}v_{\Delta,\Lambda},\quad a_3=(\Lambda h_{-1/2}+2e_{-1/2}F_0)v_{\Delta,\Lambda},$$

$$a_4=((\Lambda-1)(\Lambda f_{-1/2}-h_{-1/2}F_0)-e_{-1/2}F_0^2)v_{\Delta,\Lambda},$$

$$a_5=e_{-1/2}h_{-1/2}v_{\Delta,\Lambda},\quad a_6=(\Lambda e_{-1/2}f_{-1/2}-e_{-1/2}h_{-1/2}F_0)v_{\Delta,\Lambda},$$

$$a_7=((\Lambda-1)(\Lambda h_{-1/2}f_{-1/2}+4\partial F_0+2e_{-1/2}f_{-1/2}F_0)-e_{-1/2}h_{-1/2}F_0^2)v_{\Delta,\Lambda},$$

$$a_8=(e_{-1/2}h_{-1/2}f_{-1/2}-2\partial h_{-1/2})v_{\Delta,\Lambda}.$$

The cases $\Lambda=0,1$ are similar. Namely, when $\Lambda=1$ we have $a_4=a_7=0$, and the remaining six vectors form a $\mathbb{C}[\partial]$-basis. Finally, in the case when $\Lambda=0$, the terms $a_3=a_4=a_6=a_7=0$, so that $M_{\mathfrak{N}_+^3}(\Delta,0)^{E_0}$ has rank 4 over $\mathbb{C}[\partial]$. (Actually the vectors a_i depend on Λ, so it would be more appropriate to write something like a_i^Λ instead of just a_i. However, from the context it will always be clear what Λ is, so that it is safe to adopt the simpler notation of a_i.) We denote the coefficient of $v_{\Delta,\Lambda}$ in the expression a_i by u_i^Λ so that we have $a_i=u_i^\Lambda v_{\Delta,\Lambda}$, for $i=1,\ldots,8$. For example, $u_1^\Lambda=1$, while $u_2^\Lambda=e_{-1/2}$, etc. We note that finding all vectors in $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)^{E_0}$ above amounts essentially to decomposing tensor products of irreducible representations of sl_2 and then finding the corresponding highest weight vectors of the irreducible components.

Similarly we call a nonzero (L_0,H_0)-weight vector v in $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)$ *singular* if $v\in M_{\mathfrak{N}_+^3}(\Delta,\Lambda)^{E_0}$ and $\mathfrak{g}_jv=0$, for all $j>0$. As before a singular vector is called *proper* if it is not a scalar multiple of $v_{\Delta,\Lambda}$. Evidently $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)$ is irreducible if and only if $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)$ contains no proper singular vector. Our first objective is to classify singular vectors inside $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)$.

Proposition 5.1: Any proper singular vector in $M_{\mathfrak{N}_+^3}(\Delta,\Lambda)$ *is of the form* ($\alpha\in\mathbb{C}$ *with* $\alpha\neq 0$)

(*i*) αa_2, *if* $4\Delta-\Lambda=0$,
(*ii*) αa_4, *if* $4\Delta+\Lambda+2=0$ *and* $\Lambda\geqslant 2$, *and*
(*iii*) αa_6, *if* $4\Delta+\Lambda+2=0$ *and* $\Lambda=1$.

Remark 5.1: The proof of the proposition is a straightforward, albeit a tedious, calculation. We will not give the details here, but instead just point out that a weight vector $v\in M_{\mathfrak{N}_+^3}(\Delta,\Lambda)^{E_0}$ is singular if and only if $f_{1/2}$ and $\Psi_{1/2}$ annihilate v. This fact simplifies the calculation significantly.

From Proposition 5.1 one obtains immediately the following.

Corollary 5.1: Suppose that (Δ,Λ) *does not satisfy either* $4\Delta-\Lambda=0$ *or* $4\Delta+\Lambda+2=0$ *and* $\Lambda\geqslant 1$. *Then* $L_{\mathfrak{N}_+^3}(\Delta,\Lambda)=M_{\mathfrak{N}_+^3}(\Delta,\Lambda)$ *is an irreducible* $\mathrm{K}(1,3)_+$*-module of rank* $8\Lambda+8$ *over* $\mathbb{C}[\partial]$.

Proposition 5.2: Suppose that $4\Delta-\Lambda=0$. *Then* $L_{\mathfrak{N}_+^3}(\Delta,\Lambda)$ *is a free* $\mathbb{C}[\partial]$*-module of rank* 4Λ.

Proof: By Proposition 5.1 a_2 is a singular vector in $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)$ of H_0-weight $\Lambda+2$. Consider N, the $\mathfrak{g}$-submodule generated by a_2. Then we have $N=U(\mathfrak{g}_-)V_2$, where V_2 is the irreducible sl_2-submodule generated by a_2. Note that the map $v_{\Lambda/4+1/2,\Lambda+2}\to a_2$ extends uniquely to an epimorphism of $\mathrm{K}(1,3)_+$-modules from $M_{\mathfrak{N}_+^3}(\Lambda/4+1/2,\Lambda+2)$ to N. In particular, it is an sl_2-module epimorphism. Now both modules are completely reducible sl_2-modules and hence this map sends E_0-invariants onto E_0-invariants. Since $M_{\mathfrak{N}_+^3}(\Lambda/4+1/2,\Lambda+2)^{E_0}$ is generated over $\mathbb{C}[\partial]$ by $\{u_i^{\Lambda+2}v_{\Lambda/4+1/2,\Lambda+2}|1\leqslant i\leqslant 8\}$, it follows that N^{E_0} is generated over $\mathbb{C}[\partial]$ by $\{u_i^{\Lambda+2}a_2|1\leqslant i\leqslant 8\}$. Now N^{E_0} is a $\mathbb{C}[\partial]$-submodule of $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)$, since $[\partial,E_0]=0$. Thus it is a free $\mathbb{C}[\partial]$-submodule generated by $\{u_i^{\Lambda+2}a_2|1\leqslant i\leqslant 8\}$. We compute

$$u_1^{\Lambda+2}a_2=a_2,\quad u_2^{\Lambda+2}a_2=0,\quad u_3^{\Lambda+2}a_2=-(\Lambda+4)a_5,$$

$$u_4^{\Lambda+2}a_2=-(\Lambda+3)a_6-4(\Lambda+1)(\Lambda+3)\partial a_1,\quad u_5^{\Lambda+2}a_2=0,$$

$$u_6^{\Lambda+2}a_2=-4(\Lambda+3)\partial a_2,\quad u_7^{\Lambda+2}a_2=(\Lambda+3)(\Lambda+2)a_8+2(\Lambda+3)\partial a_3,$$

$$u_8^{\Lambda+2}a_2=-2\partial a_5.$$

By inspection it is clear that the following is a set of $\mathbb{C}[\partial]$-generators for N^{E_0}:

$$S^\Lambda=\left\{a_2,a_5,a_6+4(\Lambda+1)\partial a_1,a_8+\frac{2}{\Lambda+2}\partial a_3\right\}.$$

First consider the case when $\Lambda\geqslant 2$. It follows from the description of S^Λ above that $\{a_1,a_3,a_4,a_7\}$ is a $\mathbb{C}[\partial]$-basis for the E_0-invariants of the quotient $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N$. Since a_1 and a_3 both have H_0-weight Λ, they generate two copies of the irreducible sl_2-module of dimension $\Lambda+1$. On the other hand, a_4 and a_7 both have weight $\Lambda-2$, and so they generate two copies of the irreducible sl_2-module of dimension $\Lambda-1$. Thus $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N$ is a free $\mathbb{C}[\partial]$-module of rank $2(\Lambda+1)+2(\Lambda-1)=4\Lambda$. So, in order to complete the proof it remains to show that $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N$ is irreducible.

Note that L_n, $n\geqslant -1$, together with E_0,H_0,F_0 generate a copy of $\mathfrak{V}_+\oplus\mathrm{sl}_2$ and so we may consider $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N$ as a module over $\mathfrak{V}_+\oplus\mathrm{sl}_2$. By parity consideration $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N$ is a direct sum of two $(\mathfrak{V}_+\oplus\mathrm{sl}_2)$-modules, namely $(M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N)_{\bar{0}}=\mathbb{C}[\partial]V_1+\mathbb{C}[\partial]V_7$ and $(M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N)_{\bar{1}}=\mathbb{C}[\partial]V_3+\mathbb{C}[\partial]V_4$, where V_i is the irreducible sl_2-module generated by a_i. It is subject to a direct verification that L_n, for $n\geqslant 1$, annihilates the vectors a_1,a_3,a_4,a_7 (in fact, one only needs to check that $L_1a_7=0$, others being trivial) and hence $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N$ as a $\mathfrak{V}_+$

$\oplus \mathrm{sl}_2$-module is a direct sum the following four non-isomorphic irreducible modules: $\mathbb{C}[\partial]V_3 \cong L_{\mathfrak{V}_+}(\Lambda/4+1/2)\boxtimes U^{\Lambda}$, $\mathbb{C}[\partial]V_4 \cong L_{\mathfrak{V}_+}(\Lambda/4+1/2)\boxtimes U^{\Lambda-2}$, $\mathbb{C}[\partial]V_1 \cong L_{\mathfrak{V}_+}(\Lambda/4)\boxtimes U^{\Lambda}$ and $\mathbb{C}[\partial]V_7 \cong L_{\mathfrak{V}_+}(\Lambda/4+1)\boxtimes U^{\Lambda-2}$, where we denote by U^{μ} the irreducible sl_2-module of highest weight μ. Now we compute

$$\Psi_{1/2}a_3 = -\Lambda(\Lambda+2)a_1, \quad f_{1/2}a_4 = (2\Lambda+2)F_0^2 a_1,$$
$$E_1 a_7 = 2\Lambda(\Lambda-1)(2\Lambda+2)a_1, \tag{5.1}$$

from which it follows that we may go from each irreducible $\mathfrak{V}_+ \oplus \mathrm{sl}_2$-component of $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N$ to the irreducible component containing the highest weight vectors, and hence the module $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N$ is irreducible.

Now if $\Lambda=1$, the vectors a_4 and a_7 are both zero. Therefore, the quotient $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N = \mathbb{C}[\partial]V_1 \oplus \mathbb{C}[\partial]V_3$. But then the first identity in (5.1) shows that $M_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)/N$ is irreducible. The rank of $L_{\mathfrak{N}_+^3}(\Lambda/4,\Lambda)$ is then $2(\Lambda+1)=4\Lambda$ in the case $\Lambda=1$.

Finally, when $\Lambda=0$, the vectors $a_3,a_4,a_6,a_7=0$, so that S^{Λ} reduces to $\{a_2,a_5,\partial a_1,a_8\}$. Therefore, $M_{\mathfrak{N}_+^3}(0,0)/N=\mathbb{C}a_1$ is the trivial module and so has rank 0. □

Proposition 5.3: Suppose that $4\Delta+\Lambda+2=0$ *and* $\Lambda\geq 1$. *Then* $L_{\mathfrak{N}_+^3}(\Delta,\Lambda)$ *is a free* $\mathbb{C}[\partial]$*-module of rank* $4\Lambda+8$.

Proof: By Proposition 5.1 a_4 is a singular vector of $M_{\mathfrak{N}_+^3}(-(\Lambda+2)/4,\Lambda)$ of H_0-weight $\Lambda-2$. Let N denote the $\mathfrak{g}$-submodule generated by a_4.

Consider first the case $\Lambda\geq 4$. As in the proof of Proposition 5.1, N^{E_0} is a free $\mathbb{C}[\partial]$-module generated over $\mathbb{C}[\partial]$ by $\{u_i^{\Lambda-2}a_4 | 1\leq i\leq 8\}$. We compute

$$u_1^{\Lambda-2}a_4 = a_4, \quad u_2^{\Lambda-2}a_4 = (\Lambda-1)a_6, \quad u_3^{\Lambda-2}a_4 = (\Lambda-2)a_7, \quad u_4^{\Lambda-2}a_4 = 0,$$
$$u_5^{\Lambda-2}a_4 = \Lambda(\Lambda-1)a_8 + 2(\Lambda-1)\partial a_3, \quad u_6^{\Lambda-2}a_4 = 0, \quad u_7^{\Lambda-2}a_4 = 0,$$
$$u_8^{\Lambda-2}a_4 = -2\partial a_7.$$

This implies that the set $S^{\Lambda}=\{a_4,(\Lambda-1)a_6,(\Lambda-2)a_7,\Lambda(\Lambda-1)a_8+2(\Lambda-1)\partial a_3,\partial a_7\}$ generates N^{E_0} over $\mathbb{C}[\partial]$ and so $\{a_1,a_2,a_3,a_5\}$ is a $\mathbb{C}[\partial]$-basis for $(M_{\mathfrak{N}_+^3}(-(\Lambda+2)/4,\Lambda)/N)^{E_0}$ in the case when $\Lambda\geq 4$.

Next consider the case $\Lambda=3$. In this case, letting N be as before, N^{E_0} is generated over $\mathbb{C}[\partial]$ by $\{u_i^{\Lambda-2}a_4 | 1\leq i\leq 8, i\neq 4,7\}$. Hence it follows from the above formulas that again $\{a_1,a_2,a_3,a_5\}$ is a $\mathbb{C}[\partial]$-basis for $(M_{\mathfrak{N}_+^3}(-(\Lambda+2)/4,\Lambda)/N)^{E_0}$.

In the case when $\Lambda=2$ we let N' denote the module generated by a_4. It follows that the vectors $\{u_1^{\Lambda-2}a_4, u_2^{\Lambda-2}a_4, u_5^{\Lambda-2}a_4, u_8^{\Lambda-2}a_4\}$ generate N'^{E_0} over $\mathbb{C}[\partial]$ so that $S^{\Lambda}=\{a_4,a_6,a_8+\partial a_3,\partial a_7\}$ generate N^{E_0}. Hence $(M_{\mathfrak{N}_+^3}(-(\Lambda+2)/4,\Lambda)/N')^{E_0}$ contains in addition a one-dimensional (over $\mathbb{C}$) subspace spanned by a_7. However, $\partial a_7=0$ in $M_{\mathfrak{N}_+^3}(-(\Lambda+2)/4,\Lambda)/N'$ and hence it is a $\mathfrak{g}$-invariant by Remark 2.1. In this case we set $N=N'+\mathbb{C}a_7$ so that the quotient module $(M_{\mathfrak{N}_+^3}(-(\Lambda+2)/4,\Lambda)/N)^{E_0}$ is again generated over $\mathbb{C}[\partial]$ by $\{a_1,a_2,a_3,a_5\}$.

Now a_1 and a_3 have H_0-weight Λ, while a_2 and a_5 have H_0-weight $\Lambda+2$. Thus $M_{\mathfrak{N}_+^3}(-(\Lambda+2)/4,\Lambda)/N$ has rank $2(\Lambda+1)+2(\Lambda+3)=4\Lambda+8$ over $\mathbb{C}[\partial]$. So it remains to show that $M_{\mathfrak{N}_+^3}(-(\Lambda+2)/4,\Lambda)/N$ is irreducible.

Again we consider $M_{\mathfrak{N}_+^3}(-(\Lambda+2)/4,\Lambda)/N$ as a module over $\mathfrak{V}_+\oplus\mathrm{sl}_2$. It is easy to check that L_n, $n\geq 1$, annihilates a_1,a_2,a_3,a_5. (Again one really only needs to check that $L_1a_5=0$.) Thus it follows in the case of $\Lambda\geq 3$ that $M_{\mathfrak{N}_+^3}(-(\Lambda+2)/4,\Lambda)/N$ is a direct sum of the following four non-isomorphic irreducible $\mathfrak{V}_+\oplus\mathrm{sl}_2$-modules: $\mathbb{C}[\partial]V_1 \cong L_{\mathfrak{V}_+}(-(\Lambda+2)/4)\boxtimes U^{\Lambda}$, $\mathbb{C}[\partial]V_2$

$\cong L_{\mathfrak{V}_+}(-\Lambda/4)\boxtimes U^{\Lambda+2}$, $\mathbb{C}[\partial]V_3 \cong L_{\mathfrak{V}_+}(-\Lambda/4)\boxtimes U^{\Lambda}$ and $\mathbb{C}[\partial]V_5 \cong L_{\mathfrak{V}_+}(-(\Lambda-2)/4)\boxtimes U^{\Lambda+2}$, where as before U^{μ} stands for the irreducible sl_2-module of highest weight μ and V_i is the sl_2-submodule generated by the vector a_i. Now we compute

$$f_{1/2}a_2 = 2(\Lambda+1)a_1, \quad \Psi_{1/2}a_3 = -\Lambda(\Lambda+2)a_1, \quad F_1 a_5 = -4(\Lambda+1)a_1, \tag{5.2}$$

from which again it follows that we may go from any irreducible $\mathfrak{V}_+ \oplus \mathrm{sl}_2$-component of $M_{\mathfrak{N}^3_+}(-(\Lambda+2)/4,\Lambda)/N$ to the component containing the highest weight vectors, and hence $M_{\mathfrak{N}^3_+}(-(\Lambda+2)/4,\Lambda)/N$ is irreducible.

As for the case $\Lambda=2$ we have $M_{\mathfrak{N}^3_+}(-(\Lambda+2)/4,\Lambda)/N$ as a $\mathfrak{V}_+ \oplus \mathrm{sl}_2$-module is also a direct sum of the $\mathbb{C}[\partial]V_1 \oplus \mathbb{C}[\partial]V_2 \oplus \mathbb{C}[\partial]V_3 \oplus \mathbb{C}[\partial]V_5$. The first three modules, as in the case of $\Lambda \geqslant 3$, are irreducible. However, $\mathbb{C}[\partial]V_5$ contains a unique irreducible submodule generated by the vector ∂a_5, which is isomorphic to $L_{\mathfrak{V}_+}(-1)\boxtimes U^{\Lambda+2}$. But then (5.2) together with the fact that

$$F_2 \partial a_1 = -24 a_1$$

shows that $M_{\mathfrak{N}^3_+}(-(\Lambda+2)/4,\Lambda)/N$ is irreducible in this case as well.

In the case when $\Lambda=1$ we have by Proposition 5.1 that a_6 is the unique (up to a scalar) singular vector inside $M_{\mathfrak{N}^3_+}(-\frac{3}{4},1)$. Let N denote the $\mathfrak{g}$-submodule generated by a_6. Since a_6 has H_0-weight 1, N^{E_0} is the free $\mathbb{C}[\partial]$-module generated by $\{u_i^{\Lambda}a_6 | 1 \leqslant i \leqslant 8, i \neq 4,7\}$. We have

$$u_1^{\Lambda}a_6 = a_6, \quad u_2^{\Lambda}a_6 = 0, \quad u_3^{\Lambda}a_6 = -3a_8 - 6\partial a_3,$$

$$u_5^{\Lambda}a_6 = 0, \quad u_6^{\Lambda}a_6 = -8\partial a_6, \quad u_8^{\Lambda}a_6 = -2\partial a_8 - 4\partial^2 a_3,$$

from which it follows that N^{E_0} is generated over $\mathbb{C}[\partial]$ by $S^{\Lambda} = \{a_6, a_8 + 2\partial a_3\}$. Since $a_4 = a_7 = 0$ in this situation, we see that $(M_{\mathfrak{N}^3_+}(-\frac{3}{4},1)/N)^{E_0}$ is generated over $\mathbb{C}[\partial]$ by the vectors a_1, a_2, a_3, a_5, just as in the case $\Lambda \geqslant 2$. Now the exact same argument as in the $\Lambda \geqslant 2$ case shows that $M_{\mathfrak{N}^3_+}(-\frac{3}{4},1)/N$ is irreducible and has rank $4\Lambda+8$ over $\mathbb{C}[\partial]$. □

We summarize the work in this section in the following theorem.

Theorem 5.1: *The modules $L_{\mathfrak{N}^3_+}(\Delta,\Lambda)$, for $\Delta \in \mathbb{C}$ and $\Lambda \in \mathbb{Z}_+$, form a complete list of non-isomorphic finite (over $\mathbb{C}[\partial]$) irreducible $\mathrm{K}(1,3)_+$-modules. Furthermore, $L_{\mathfrak{N}^3_+}(\Delta,\Lambda)$ as a $\mathbb{C}[\partial]$-module has rank*

(*i*) 4Λ, *in the case* $4\Delta - \Lambda = 0$,
(*ii*) $4\Lambda+8$, *the case* $4\Delta + \Lambda + 2 = 0$ *and* $\Lambda \geqslant 1$, *and*
(*iii*) $8\Lambda+8$, *in all other cases.*

Furthermore, the $\mathbb{C}[\partial]$-rank of $L_{\mathfrak{N}^3_+}(\Delta,\Lambda)_0^-$ equals the $\mathbb{C}[\partial]$-rank of $L_{\mathfrak{N}^3_+}(\Delta,\Lambda)_1^-$ in all cases.

Remark 5.2: Translating the above theorem back into the languages of modules over conformal superalgebras and of conformal modules is now a straightforward task. We thus have proved that all finite irreducible modules over the $N=3$ conformal superalgebra are of the form $L_{\mathfrak{N}^3}(\alpha,\Delta,\Lambda)$, where $\alpha,\Delta \in \mathbb{C}$ and $\Lambda \in \mathbb{Z}_+$. The definition of these modules and also the action of the $N=3$ conformal superalgebra on them are quite easy to obtain from our explicit description of a $\mathbb{C}[\partial]$-basis of these modules. To do so would, however, take up quite a significant portion of space, and thus we leave this task to the interested reader. We only remark that the adjoint module is isomorphic to $L_{\mathfrak{N}^3}(0,\frac{1}{2},0)$.

VI. FINITE IRREDUCIBLE MODULES OVER THE "SMALL" $N=4$ CONFORMAL SUPERALGEBRA

The "small" $N=4$ superconformal algebra is the following subalgebra of K(1,4): Let $\xi_1, \xi_2, \xi_3, \xi_4$ denote four odd indeterminates generating the Grassmann superalgebra $\Lambda(4)$. For a monomial ξ_I in $\Lambda(4)$ we let ξ_I^* be its Hodge dual, i.e., the unique monomial in $\Lambda(4)$ such that $\xi_I\xi_I^*=\xi_1\xi_2\xi_3\xi_4$. Then the small $N=4$ superconformal algebra is isomorphic to any of the following two subalgebras in K(1,4) spanned by the following basis elements ($n\in\mathbb{Z}$, $r\in\frac{1}{2}+\mathbb{Z}$, $\beta^2=1$):[11]

$$L_n^\beta=-\tfrac{1}{2}(t^{n+1}+\beta n(n+1)\xi_1\xi_2\xi_3\xi_4t^{n-1}),$$

$$H_n^\beta=i(\xi_1\xi_2-\beta\xi_3\xi_4)t^n,$$

$$E_n^\beta=\tfrac{1}{2}(-\xi_1\xi_3-\beta\xi_2\xi_4-i\xi_2\xi_3+i\beta\xi_1\xi_4)t^n,$$

$$F_n^\beta=\tfrac{1}{2}(\xi_1\xi_3+\beta\xi_2\xi_4-i\xi_2\xi_3+i\beta\xi_1\xi_4)t^n,$$

$$G_r^{-+\beta}=\frac{1}{\sqrt{2}}\left((\xi_3+i\xi_4)t^{r+1/2}-\beta\left(r+\frac{1}{2}\right)(\xi_3^*+i\xi_4^*)t^{r-1/2}\right),$$

$$G_r^{++\beta}=\frac{1}{\sqrt{2}}\left((\xi_1+i\xi_2)t^{r+1/2}-\beta\left(r+\frac{1}{2}\right)(\xi_1^*+i\xi_2^*)t^{r-1/2}\right),$$

$$G_r^{+-\beta}=\frac{1}{\sqrt{2}}\left((\xi_3-i\xi_4)t^{r+1/2}-\beta\left(r+\frac{1}{2}\right)(\xi_3^*-i\xi_4^*)t^{r-1/2}\right),$$

$$G_r^{--\beta}=\frac{1}{\sqrt{2}}\left((i\xi_2-\xi_1)t^{r+1/2}-\beta\left(r+\frac{1}{2}\right)(i\xi_2^*-\xi_1^*)t^{r-1/2}\right).$$

As before let $\{H,E,F\}$ denote the standard basis of the Lie algebra sl_2 and $\{G^{++},G^{-+}\}$ denote the standard basis of its standard module, i.e., $H\cdot G^{++}=G^{++}$, $H\cdot G^{-+}=-G^{-+}$, $E\cdot G^{++}=F\cdot G^{-+}=0$, $F\cdot G^{++}=G^{-+}$ and $E\cdot G^{-+}=G^{++}$. Likewise $\{G^{+-},G^{--}\}$ also denotes a copy of the standard basis of the standard sl_2-module with actions $H\cdot G^{+-}=G^{+-}$, $H\cdot G^{--}=-G^{--}$, $E\cdot G^{+-}=F\cdot G^{--}=0$, $F\cdot G^{+-}=G^{--}$ and $E\cdot G^{--}=G^{+-}$. With this notation in mind the commutation relations are then given as follows (where $X,Y=H,E,F$ and $x,y=G^{++},G^{-+},G^{+-},G^{--}$):

$$[L_m^\beta,L_n^\beta]=(m-n)L_{m+n}^\beta,\quad [L_m^\beta,X_n^\beta]=-nX_{m+n}^\beta,\quad [L_m^\beta,x_r^\beta]=\left(\frac{m}{2}-r\right)x_{m+r}^\beta,$$

$$[X_m^\beta,Y_n^\beta]=[X,Y]_{m+n}^\beta,\quad [X_m^\beta,y_r^\beta]=(X\cdot y)_{m+r}^\beta,\quad [x_r^\beta,x_s^\beta]=0,$$

$$[G_r^{++\beta},G_s^{+-\beta}]=(r-s)(1+\beta)E_{r+s}^\beta,\quad [G_r^{++\beta},G_s^{-+\beta}]=(r-s)(1-\beta)E_{r+s}^\beta,$$

$$[G_r^{++\beta},G_s^{--\beta}]=-(r-s)H_{r+s}^\beta-2L_{r+s}^\beta,\quad [G_r^{+-\beta},G_s^{-+\beta}]=(r-s)\beta H_{r+s}^\beta+2L_{r+s}^\beta,$$

$$[G_r^{+-\beta},G_s^{--\beta}]=-(r-s)(1-\beta)F_{r+s}^\beta,\quad [G_r^{-+\beta},G_s^{--\beta}]=-(r-s)(1+\beta)F_{r+s}^\beta,$$

where $m,n\in\mathbb{Z}$ and $r,s\in\frac{1}{2}+\mathbb{Z}$. The eight formal distributions generating this algebra are given by $L^\beta(z)=\Sigma_{n\in\mathbb{Z}}L_n^\beta z^{-n-2}$, $X^\beta(z)=\Sigma_{n\in\mathbb{Z}}X_n^\beta z^{-n-1}$, and $x^\beta(z)=\Sigma_{r\in(1/2)+\mathbb{Z}}x_r^\beta z^{-r-3/2}$. The operator product expansions of these fields are easily derived using (2.3).

We will denote the ''small'' $N=4$ superconformal algebra simply by SK(1,4) and assume for the rest of this section that we have chosen its realization as the subalgebra of K(1,4) with $\beta=1$ for future computational purposes. For simplicity we will drop the superscript β and write L_n for L_n^β, etc., when we mean $\beta=1$.

The annihilation subalgebra $\mathfrak{g}=\mathrm{SK}(1,4)_+$ of SK(1,4) is equipped with a $\frac{1}{2}\mathbb{Z}$-gradation of depth 1, i.e., $\mathfrak{g}=\oplus_{j\geqslant -1}\mathfrak{g}_j$, $j\in\frac{1}{2}\mathbb{Z}$, and its zeroth graded component $\mathfrak{g}_0$ is isomorphic to a copy of $\mathrm{gl}_2\cong\mathrm{sl}_2\oplus\mathbb{C}L_0$, with H_0, E_0 and F_0 providing the standard basis of the copy of sl_2. Again we let $U^{\Delta,\Lambda}$ be the finite-dimensional irreducible sl_2-module of highest weight $\Lambda\in\mathbb{Z}_+$ on which L_0 acts as the scalar Δ and $v_{\Delta,\Lambda}$ be a highest weight vector in $U^{\Delta,\Lambda}$. As in the case of $\mathrm{K}(1,3)_+$, we may extend $U^{\Delta,\Lambda}$ to a module over the subalgebra $\mathcal{L}_0=\oplus_{j\geqslant 0}\mathfrak{g}_j$ trivially and call this $\mathcal{L}_0$-module also $U^{\Delta,\Lambda}$. Again Theorem 3.1 tells us that every finite irreducible $\mathfrak{g}$-module is the quotient of $M_{\mathfrak{N}_+^4}(\Delta,\Lambda)=\mathrm{Ind}_{\mathcal{L}_0}^{\mathfrak{g}}U^{\Delta,\Lambda}$ by its unique maximal submodule, for some $\Delta\in\mathbb{C}$ and $\Lambda\in\mathbb{Z}_+$. We denote the unique irreducible quotient by $L_{\mathfrak{N}_+^4}(\Delta,\Lambda)$ so that every finite irreducible $\mathrm{SK}(1,4)_+$-module is of the form $L_{\mathfrak{N}_+^4}(\Delta,\Lambda)$, for $\Delta\in\mathbb{C}$ and $\Lambda\in\mathbb{Z}_+$.

Now $M_{\mathfrak{N}_+^4}(\Delta,\Lambda)$ is completely reducible as a module over $\mathrm{sl}_2=\mathbb{C}H_0+\mathbb{C}E_0+\mathbb{C}F_0$, and the subspace of E_0-invariants $M_{\mathfrak{N}_+^4}(\Delta,\Lambda)^{E_0}$ is a free $\mathbb{C}[\partial]$-submodule of $M_{\mathfrak{N}_+^4}(\Delta,\Lambda)$ due to $[E_0,\partial]=0$. We write down explicit formulas for a $\mathbb{C}[\partial]$-basis of $M_{\mathfrak{N}_+^4}(\Delta,\Lambda)^{E_0}$, which in the case when $\Lambda\geqslant 2$ takes the following form:

$$a_1=v_{\Delta,\Lambda},\quad a_2=G^{++}_{-1/2}v_{\Delta,\Lambda},\quad a_3=G^{+-}_{-1/2}v_{\Delta,\Lambda},\quad a_4=(\Lambda G^{-+}_{-1/2}-G^{++}_{-1/2}F_0)v_{\Delta,\Lambda},$$

$$a_5=(-\Lambda G^{--}_{-1/2}+G^{+-}_{-1/2}F_0)v_{\Delta,\Lambda},\quad a_6=G^{-+}_{-1/2}G^{++}_{-1/2}v_{\Delta,\Lambda},\quad a_7=G^{+-}_{-1/2}G^{--}_{-1/2}v_{\Delta,\Lambda},$$

$$a_8=G^{++}_{-1/2}G^{+-}_{-1/2}v_{\Delta,\Lambda},\quad a_9=(G^{-+}_{-1/2}G^{+-}_{-1/2}-G^{++}_{-1/2}G^{--}_{-1/2})v_{\Delta,\Lambda},$$

$$a_{10}=(-\Lambda G^{++}_{-1/2}G^{--}_{-1/2}+G^{++}_{-1/2}G^{+-}_{-1/2}F_0)v_{\Delta,\Lambda},$$

$$a_{11}=((\Lambda-1)(-\Lambda G^{-+}_{-1/2}G^{--}_{-1/2}+G^{-+}_{-1/2}G^{+-}_{-1/2}F_0+G^{++}_{-1/2}G^{--}_{-1/2}F_0)-G^{++}_{-1/2}G^{+-}_{-1/2}F_0^2)v_{\Delta,\Lambda},$$

$$a_{12}=G^{-+}_{-1/2}G^{++}_{-1/2}G^{+-}_{-1/2}v_{\Delta,\Lambda},\quad a_{13}=G^{++}_{-1/2}G^{+-}_{-1/2}G^{--}_{-1/2}v_{\Delta,\Lambda},$$

$$a_{14}=G^{-+}_{-1/2}G^{++}_{-1/2}(-\Lambda G^{--}_{-1/2}+G^{+-}_{-1/2}F_0)v_{\Delta,\Lambda},$$

$$a_{15}=(-\Lambda G^{-+}_{-1/2}G^{+-}_{-1/2}G^{--}_{-1/2}+G^{++}_{-1/2}G^{+-}_{-1/2}G^{--}_{-1/2}F_0)v_{\Delta,\Lambda},$$

$$a_{16}=G^{-+}_{-1/2}G^{++}_{-1/2}G^{+-}_{-1/2}G^{--}_{-1/2}v_{\Delta,\Lambda}.$$

Now in the case when $\Lambda=1$ we have $a_{11}=0$ so that the remaining 15 vectors form a $\mathbb{C}[\partial]$-basis for $M_{\mathfrak{N}_+^4}(\Delta,\Lambda)^{E_0}$, while in the case when $\Lambda=0$ we have $a_4=a_5=a_{10}=a_{11}=a_{14}=a_{15}=0$, so that $M_{\mathfrak{N}_+^4}(\Delta,0)^{E_0}$ has rank 10 over $\mathbb{C}[\partial]$. As in Sec. V, we denote the coefficient of $v_{\Delta,\Lambda}$ in the expression a_i by u_i^Λ so that we have $a_i=u_i^\Lambda v_{\Delta,\Lambda}$, for $i=1,\ldots,16$.

Singular vectors are then defined to be nonzero (L_0,H_0)-weight vectors $v\in M_{\mathfrak{N}_+^4}(\Delta,\Lambda)^{E_0}$ with $\mathfrak{g}_j v=0$, for all $j>0$. Similarly, we define *proper singular vectors*. Our approach is analogous to the one of Sec. V, that is, first to analyze singular vectors inside $M_{\mathfrak{N}_+^4}(\Delta,\Lambda)$. This is given by the following proposition, whose proof is again a straightforward calculation, which admittedly is rather tedious.

Proposition 6.1: A complete list of proper singular vectors inside $M_{\mathfrak{N}_+^4}(\Delta,\Lambda)$ is given by

(*i*) $2\Delta-\Lambda=0$.
(a) $\alpha a_2+\beta a_3$, $(\alpha,\beta)\neq(0,0)$,
(b) αa_8, $\alpha\neq 0$.

(*ii*) $2\Delta+\Lambda+2=0$ *and* $\Lambda\geqslant 2$.
(a) $\alpha a_4+\beta a_5$, $(\alpha,\beta)\neq(0,0)$,
(b) αa_{11}, $\alpha\neq 0$.
(*iii*) $2\Delta+\Lambda+2=0$ *and* $\Lambda=1$.
(a) $\alpha a_4+\beta a_5$, $(\alpha,\beta)\neq(0,0)$,
(b) $\alpha a_{14}+\beta(a_{15}-2\partial a_5)$, $(\alpha,\beta)\neq(0,0)$,
(c) $\alpha(a_{16}-2\partial a_{10})$, $\alpha\neq 0$.
(*iv*) $2\Delta+\Lambda+2=0$ and $\Lambda=0$.
(a) $\alpha a_6+\beta a_7+\gamma(a_9-2\partial a_1)$, $(\alpha,\beta,\gamma)\neq(0,0,0)$,
(b) $\alpha a_{13}+\beta(a_{12}+2\partial a_2)$, $(\alpha,\beta)\neq(0,0)$.

Remark 6.1: We note that in order to check that a weight vector $v\in M_{\mathfrak{N}_+^4}(\Delta,\Lambda)^{E_0}$ is singular, it is enough to check that v is annihilated by F_1, $G_{1/2}^{-+}$ and $G_{1/2}^{--}$.

Corollary 6.1: Suppose that (Δ,Λ) *does not satisfy either* $2\Delta-\Lambda=0$ *or* $2\Delta+\Lambda+2=0$. *Then* $L_{\mathfrak{N}_+^4}(\Delta,\Lambda)=M_{\mathfrak{N}_+^4}(\Delta,\Lambda)$ *is an irreducible* $\mathrm{SK}(1,4)_+$*-module of rank* $16\Lambda+16$ *over* $\mathbb{C}[\partial]$.

Proposition 6.2: Suppose that $2\Delta-\Lambda=0$. *Then* $L_{\mathfrak{N}_+^4}(\Delta,\Lambda)$ *is a free* $\mathbb{C}[\partial]$*-module of rank* 4Λ.

Proof: By Proposition 6.1 a_2 and a_3 are singular vectors in $M_{\mathfrak{N}_+^4}(\Lambda/2,\Lambda)$. Consider N_2 and N_3, the $\mathfrak{g}$-submodules generated by a_2 and a_3, respectively, and let $N=N_2+N_3$. Then we have $N_2=U(\mathfrak{g}_-)V_2$ and $N_3=U(\mathfrak{g}_-)V_3$, where V_2 and V_3 are the irreducible sl_2-submodules generated by a_2 and a_3, respectively. Let us first compute $N_2^{E_0}$. Since the H_0-weight of a_2 is $\Lambda+1$, we know that $N_2^{E_0}$ is a free $\mathbb{C}[\partial]$-module generated over $\mathbb{C}[\partial]$ by $\{u_i^{\Lambda+1}a_2|1\leqslant i\leqslant 16\}$. We have

$$u_1^{\Lambda+1}a_2=a_2,\quad u_2^{\Lambda+1}a_2=0,\quad u_3^{\Lambda+1}a_2=-a_8,\quad u_4^{\Lambda+1}a_2=(\Lambda+2)a_6,$$

$$u_5^{\Lambda+1}a_2=-a_9-a_{10}+2(\Lambda+2)\partial a_1,\quad u_6^{\Lambda+1}a_2=0,\quad u_7^{\Lambda+1}a_2=a_{13}-2\partial a_3,$$

$$u_8^{\Lambda+1}a_2=0,\quad u_9^{\Lambda+1}a_2=-a_{12}+2\partial a_2,\quad u_{10}^{\Lambda+1}a_2=a_{12}+2(\Lambda+2)\partial a_2,$$

$$u_{11}^{\Lambda+1}a_2=2(\Lambda+2)\partial a_4-(\Lambda+2)a_{14},\quad u_{12}^{\Lambda+1}a_2=0,\quad u_{13}^{\Lambda+1}a_2=-2\partial a_8,$$

$$u_{14}^{\Lambda+1}a_2=2(\Lambda+2)\partial a_6,\quad u_{15}^{\Lambda+1}a_2=-(\Lambda+2)a_{16}+2(\Lambda+1)\partial a_9-2\partial a_{10},\quad u_{16}^{\Lambda+1}a_2=-2\partial a_{12}.$$

Next we find $\mathbb{C}[\partial]$-generators of $N_3^{E_0}$. Similarly, $\{u_i^{\Lambda+1}a_3|1\leqslant i\leqslant 16\}$ generates $N_3^{E_0}$ over $\mathbb{C}[\partial]$:

$$u_1^{\Lambda+1}a_3=a_3,\quad u_2^{\Lambda+1}a_3=a_8,\quad u_3^{\Lambda+1}a_3=0,\quad u_4^{\Lambda+1}a_3=(\Lambda+1)a_9-a_{10},$$

$$u_5^{\Lambda+1}a_3=(\Lambda+2)a_7,\quad u_6^{\Lambda+1}a_3=a_{12},\quad u_7^{\Lambda+1}a_3=0,\quad u_8^{\Lambda+1}a_3=0,$$

$$u_9^{\Lambda+1}a_3=a_{13},\quad u_{10}^{\Lambda+1}a_3=(\Lambda+2)a_{13},\quad u_{11}^{\Lambda+1}a_3=-(\Lambda+2)a_{15},$$

$$u_{12}^{\Lambda+1}a_3=-a_{16},\quad u_{13}^{\Lambda+1}a_3=0,\quad u_{14}^{\Lambda+1}a_3=(\Lambda+2)a_{16},\quad u_{15}^{\Lambda+1}a_3=0,\quad u_{16}^{\Lambda+1}a_3=0.$$

It follows that N^{E_0} is generated over $\mathbb{C}[\partial]$ by the following set:

$$S^{\Lambda}=\{a_2,a_3,a_6,a_7,a_8,a_9-2\partial a_1,a_{10}-2(\Lambda+1)\partial a_1,a_{12},a_{13},a_{14}-2\partial a_4,a_{15},a_{16}\}.$$

Suppose that $\Lambda\geqslant 2$. From the description of S^{Λ} we see that $\{a_1,a_4,a_5,a_{11}\}$ is a $\mathbb{C}[\partial]$-basis for the E_0-invariants of the quotient $M_{\mathfrak{N}_+^4}(\Lambda/2,\Lambda)/N$. Since a_1 has H_0-weight Λ, it generates a copy of the irreducible sl_2-module of dimension $\Lambda+1$. Now a_4 and a_5 both have weight $\Lambda-1$, and so they generate two copies of the irreducible sl_2-module of dimension Λ. Finally, a_{11} has weight

$\Lambda-2$, and so it generates a copy of the irreducible sl_2-module of dimension $\Lambda-1$. Thus $M_{\mathfrak{N}_+^4}(\Lambda/2,\Lambda)/N$ is a free $\mathbb{C}[\partial]$-module of rank $(\Lambda+1)+2\Lambda+(\Lambda-1)=4\Lambda$. So we need to show that $M_{\mathfrak{N}_+^4}(\Lambda/2,\Lambda)/N$ is irreducible.

As in Sec. V L_n, $n\geqslant -1$, together with E_0,H_0,F_0 generate a copy of $(\mathfrak{V}_+\oplus\mathrm{sl}_2)$, which thus allow us to study the $(\mathfrak{V}_+\oplus\mathrm{sl}_2)$-module structure of $M_{\mathfrak{N}_+^4}(\Lambda/2,\Lambda)/N$. By parity consideration $M_{\mathfrak{N}_+^4}(\Lambda/2,\Lambda)/N$ is a direct sum of two modules, namely $(M_{\mathfrak{N}_+^4}(\Lambda/2,\Lambda)/N)_{\bar{0}}=\mathbb{C}[\partial]V_1+\mathbb{C}[\partial]V_{11}$ and $(M_{\mathfrak{N}_+^4}(\Lambda/2,\Lambda)/N)_{\bar{1}}=\mathbb{C}[\partial]V_4+\mathbb{C}[\partial]V_5$, where V_i is the irreducible sl_2-module generated by a_i. We can easily check that L_n, for $n\geqslant 1$, annihilates the vectors a_1,a_4,a_5,a_{11}. (Again the only nontrivial part is to check that $L_1a_{11}=0$.) Thus $M_{\mathfrak{N}_+^4}(\Lambda/2,\Lambda)/N$ as a $\mathfrak{V}_+\oplus\mathrm{sl}_2$-module is a direct sum of the following four irreducible modules: $\mathbb{C}[\partial]V_1\cong L_{\mathfrak{V}_+}(\Lambda/2)\boxtimes U^{\Lambda}$, $\mathbb{C}[\partial]V_4\cong L_{\mathfrak{V}_+}((\Lambda+1)/2)\boxtimes U^{\Lambda-1}$, $\mathbb{C}[\partial]V_5\cong L_{\mathfrak{V}_+}((\Lambda+1)/2)\boxtimes U^{\Lambda-1}$ and $\mathbb{C}[\partial]V_{11}\cong L_{\mathfrak{V}_+}((\Lambda+2)/2)\boxtimes U^{\Lambda-2}$, where as usual U^{μ} is the irreducible sl_2-module of highest weight μ. Note that, contrary to the $\mathrm{K}(1,3)_+$ case, the odd part here is a sum of two isomorphic modules. To conclude that $M_{\mathfrak{N}_+^4}(\Lambda/2,\Lambda)/N$ is irreducible, we show again that one may go from each irreducible $\mathfrak{V}_+\oplus\mathrm{sl}_2$-component to the irreducible component containing the $\mathfrak{g}$-highest weight vectors. But this follows from the following computation:

$$G_{1/2}^{++}(\alpha a_4+\beta a_5)=\beta\Lambda(2\Lambda+2)a_1,\quad \alpha,\beta\in\mathbb{C}, \tag{6.1}$$

$$G_{1/2}^{--}a_4=(2\Lambda+2)F_0a_1,\quad E_1a_{11}=\Lambda(\Lambda-1)(2\Lambda+2)a_1. \tag{6.2}$$

Now if $\Lambda=1$, the vector a_{11} is zero. Therefore the quotient $M_{\mathfrak{N}_+^4}(\Lambda/4,\Lambda)/N=\mathbb{C}[\partial]V_1\oplus\mathbb{C}[\partial]V_4\oplus\mathbb{C}[\partial]V_5$. But then (6.1) and the first identity in (6.2) show that $M_{\mathfrak{N}_+^4}(\Lambda/4,\Lambda)/N$ is irreducible. The rank of $L_{\mathfrak{N}_+^4}(\Lambda/4,\Lambda)$ is then $(\Lambda+1)+2\Lambda$, which equals to 4Λ, in the case $\Lambda=1$.

Finally, when $\Lambda=0$, the vectors $a_4=a_5=a_{10}=a_{11}=a_{14}=a_{15}=0$ so that S^{Λ} reduces to $\{a_2,a_3,a_6,a_7,a_8,a_9,\partial a_1,a_{12},a_{13},a_{16}\}$. Hence $M_{\mathfrak{N}_+^4}(0,0)/N=\mathbb{C}a_1$ is the trivial module and so has rank 0. □

Proposition 6.3: Suppose that $2\Delta+\Lambda+2=0$. *Then* $L_{\mathfrak{N}_+^4}(\Delta,\Lambda)$ *is a free* $\mathbb{C}[\partial]$*-module of rank* $4\Lambda+8$.

Proof: By Proposition 6.1 a_4 and a_5 are singular vectors of $M_{\mathfrak{N}_+^4}(-(\Lambda+2)2,\Lambda)$ in the case $\Lambda\geqslant 1$.

Assume first that $\Lambda\geqslant 3$. Let N_4 and N_5 be the $\mathfrak{g}$-submodules generated by a_4 and a_5, respectively. We form the $\mathfrak{g}$-submodule $N=N_4+N_5$ and consider N^{E_0}. The set $\{u_i^{\Lambda-1}a_4|1\leqslant i\leqslant 16\}$ is a set of $\mathbb{C}[\partial]$-generators for $N_4^{E_0}$, since a_4 has H_0-weight $\Lambda-1$. We have

$$u_1^{\Lambda-1}a_4=a_4,\quad u_2^{\Lambda-1}a_4=-\Lambda a_6,\quad u_3^{\Lambda-1}a_4=2\Lambda\partial a_1-\Lambda a_9+a_{10},\quad u_4^{\Lambda-1}a_4=0,$$

$$u_5^{\Lambda-1}a_4=-a_{11},\quad u_6^{\Lambda-1}a_4=0,\quad u_7^{\Lambda-1}a_4=-a_{15}+2\partial a_5,\quad u_8^{\Lambda-1}a_4=2\Lambda\partial a_2+\Lambda a_{12},$$

$$u_9^{\Lambda-1}a_4=a_{14}+2\partial a_4,\quad u_{10}^{\Lambda-1}a_4=(\Lambda-1)a_{14},\quad u_{11}^{\Lambda-1}a_4=0,\quad u_{12}^{\Lambda-1}a_4=2\Lambda\partial a_6,$$

$$u_{13}^{\Lambda-1}a_4=-\Lambda a_{16}+2\partial a_{10},\quad u_{14}^{\Lambda-1}a_4=0,\quad u_{15}^{\Lambda-1}a_4=-2\partial a_{11},\quad u_{16}^{\Lambda-1}a_4=2\partial a_{14}.$$

Similarly, the following is a set of $\mathbb{C}[\partial]$-generators for $N_5^{E_0}$:

$$u_1^{\Lambda-1}a_5=a_5,\quad u_2^{\Lambda-1}a_5=a_{10},\quad u_3^{\Lambda-1}a_5=-a_7,\quad u_4^{\Lambda-1}a_5=a_{11},\quad u_5^{\Lambda-1}a_5=0,$$

$$u_6^{\Lambda-1}a_5=a_{14},\quad u_7^{\Lambda-1}a_5=0,\quad u_8^{\Lambda-1}a_5=-\Lambda a_{13},\quad u_9^{\Lambda-1}a_5=a_{15},\quad u_{10}^{\Lambda-1}a_5=0,$$

$$u_{11}^{\Lambda-1}a_5=0,\quad u_{12}^{\Lambda-1}a_5=-a_{16},\quad u_{13}^{\Lambda-1}a_5=0,\quad u_{14}^{\Lambda-1}a_5=0,\quad u_{15}^{\Lambda-1}a_5=0,$$

$$u_{16}^{\Lambda-1}a_5=0.$$

Therefore,

$$S^{\Lambda}=\{a_4,a_5,a_6,a_7,a_9-2\partial a_1,a_{10},a_{11},a_{12}+2\partial a_2,a_{13},a_{14},a_{15},a_{16}\}$$

is a set of $\mathbb{C}[\partial]$-generators for N^{E_0}, which implies that $\{a_1,a_2,a_3,a_8\}$ is a $\mathbb{C}[\partial]$-basis for $(M_{\mathfrak{N}_+^4}(-(\Lambda+2)/2,\Lambda)/N)^{E_0}$ in the case when $\Lambda\geqslant 3$.

In the case when $\Lambda=2$ the set $\{u_i^{\Lambda-1}a_4,u_i^{\Lambda-1}a_5|1\leqslant i\leqslant 16,i\neq 11\}$ generates N^{E_0}. But $u_{11}^{\Lambda-1}a_4=u_{11}^{\Lambda-1}a_5=0$, and hence $\{a_1,a_2,a_3,a_8\}$ is also a $\mathbb{C}[\partial]$-basis for $(M_{\mathfrak{N}_+^4}(-(\Lambda+2)/2,\Lambda)/N)^{E_0}$ in this case as well.

In the case when $\Lambda=1$ we note that $a_{11}=0$ and $\{u_i^{\Lambda-1}a_4,u_i^{\Lambda-1}a_5|1\leqslant i\leqslant 16,i\neq 4,5,10,11,14,15\}$ generates N^{E_0} over $\mathbb{C}[\partial]$. From the formulas above one sees that a set of $\mathbb{C}[\partial]$-generators for N^{E_0} is given by the set S^{Λ} above, but with a_{11} removed. Hence the quotient module is again generated freely over $\mathbb{C}[\partial]$ by $\{a_1,a_2,a_3,a_8\}$.

Hence, in the case, when $\Lambda\geqslant 1$ the quotient module $(M_{\mathfrak{N}_+^4}(-(\Lambda+2)/2,\Lambda)/N)^{E_0}$ is generated freely over $\mathbb{C}[\partial]$ by $\{a_1,a_2,a_3,a_8\}$. Now a_1 has H_0-weight Λ, a_2 and a_3 both have H_0-weight $\Lambda+1$, and a_8 has H_0-weight $\Lambda+2$. Therefore $M_{\mathfrak{N}_+^4}(-(\Lambda+2)/2,\Lambda)/N$ has rank $(\Lambda+1)+2(\Lambda+2)+(\Lambda+3)=4\Lambda+8$ over $\mathbb{C}[\partial]$. So it remains to show that $M_{\mathfrak{N}_+^4}(-(\Lambda+2)/2,\Lambda)/N$ is irreducible.

We again study $M_{\mathfrak{N}_+^4}(-(\Lambda+2)/2,\Lambda)/N$ as a $\mathfrak{V}_+\oplus \mathrm{sl}_2$-module. It is easy to check that L_n, $n\geqslant 1$, annihilates a_1,a_2,a_3,a_8 and hence $M_{\mathfrak{N}_+^4}(-(\Lambda+2)/2,\Lambda)/N$ is a direct sum of the following four irreducible $\mathfrak{V}_+\oplus \mathrm{sl}_2$-modules: $\mathbb{C}[\partial]V_1\cong L_{\mathfrak{V}_+}(-(\Lambda+2)/2)\boxtimes U^{\Lambda}$, $\mathbb{C}[\partial]V_2\cong L_{\mathfrak{V}_+}(-(\Lambda+1)/2)\boxtimes U^{\Lambda+1}$, $\mathbb{C}[\partial]V_3\cong L_{\mathfrak{V}_+}(-(\Lambda+1)/2)\boxtimes U^{\Lambda+1}$ and $\mathbb{C}[\partial]V_8\cong L_{\mathfrak{V}_+}(-\Lambda/2)\boxtimes U^{\Lambda+2}$, where V_i is the sl_2-submodule generated by the vector a_i. Again $\mathbb{C}[\partial]V_2\cong\mathbb{C}[\partial]V_3$ as $\mathfrak{V}_+\oplus\mathrm{sl}_2$-modules. Now we compute

$$G_{1/2}^{--}(\alpha a_2+\beta a_3)=2\alpha(\Lambda+1)a_1,\quad \forall\,\alpha,\beta\in\mathbb{C},$$

$$G_{1/2}^{-+}a_3=-2(\Lambda+1)a_1,\quad F_1a_8=-2(\Lambda+1)a_1.$$

Therefore $M_{\mathfrak{N}_+^4}(-(\Lambda+2)/2,\Lambda)/N$ is irreducible.

Now consider the case of $\Lambda=0$. By Proposition 6.1 a_6, a_7 and $a_9-2\partial a_1$ are singular vectors inside $M_{\mathfrak{N}_+^4}(-1,0)$. Let N_6, N_7 and N_9 be the $\mathfrak{g}$-submodules generated by a_6, a_7 and $a_9-2\partial a_1$, respectively, and put $N=N_6+N_7+N_9$. We note that a_6, a_7 and $a_9-2\partial a_1$ have H_0-weight 0, hence $N_6^{E_0}$ is generated over $\mathbb{C}[\partial]$ by $\{u_i^{\Lambda}a_6|1\leqslant i\leqslant 16,i\neq 4,5,10,11,14,15\}$ and similarly for $N_7^{E_0}$ and $N_9^{E_0}$. We first compute a set of $\mathbb{C}[\partial]$-generators for $N_6^{E_0}$:

$$u_1^{\Lambda}a_6=a_6,\quad u_2^{\Lambda}a_6=0,\quad u_3^{\Lambda}a_6=2\partial a_2+a_{12},\quad u_6^{\Lambda}a_6=0,$$

$$u_7^{\Lambda}a_6=4\partial^2a_1-2\partial a_9+a_{16},\quad u_8^{\Lambda}a_6=0,\quad u_9^{\Lambda}a_6=4\partial a_6,$$

$$u_{12}^{\Lambda}a_6=0,\quad u_{13}^{\Lambda}a_6=4\partial^2a_2+2\partial a_{12},\quad u_{16}^{\Lambda}a_6=4\partial^2a_6.$$

A set of $\mathbb{C}[\partial]$-generators for $N_7^{E_0}$ is given as follows:

$$u_1^{\Lambda}a_7=a_7,\quad u_2^{\Lambda}a_7=a_{13},\quad u_3^{\Lambda}a_7=0,\quad u_6^{\Lambda}a_7=a_{16},\quad u_7^{\Lambda}a_7=0,$$

$$u_8^{\Lambda}a_7=0,\quad u_9^{\Lambda}a_7=0,\quad u_{12}^{\Lambda}a_7=0,\quad u_{13}^{\Lambda}a_7=0,\quad u_{16}^{\Lambda}a_7=0.$$

Finally, we have the following set of $\mathbb{C}[\partial]$-generators for $N_9^{E_0}$:

$$u_1^\Lambda(a_9-2\partial a_1)=a_9-2\partial a_1,\quad u_2^\Lambda(a_9-2\partial a_1)=-a_{12}-2\partial a_2,$$

$$u_3^\Lambda(a_9-2\partial a_1)=a_{13},\quad u_6^\Lambda(a_9-2\partial a_1)=-2\partial a_6,\quad u_7^\Lambda(a_9-2\partial a_1)=2\partial a_7,$$

$$u_8^\Lambda(a_9-2\partial a_1)=0,\quad u_9^\Lambda(a_9-2\partial a_1)=2a_{16},\quad u_{12}^\Lambda(a_9-2\partial a_1)=0,$$

$$u_{13}^\Lambda(a_9-2\partial a_1)=2\partial a_{13},\quad u_{16}^\Lambda(a_9-2\partial a_1)=2\partial a_{16}.$$

From this it follows that $\{a_6,a_7,a_9-2\partial a_1,a_{12}+2\partial a_2,a_{13},a_{16}\}$ generate N^{E_0} over $\mathbb{C}[\partial]$. But $a_4=a_5=a_{10}=a_{11}=a_{14}=a_{15}=0$, and thus $(M_{\mathfrak{N}_+^4}(-1,0)/N)^{E_0}$ is generated over $\mathbb{C}[\partial]$ by the vectors a_1, a_2, a_3 and a_8, which takes us back to the case when $\Lambda\geqslant 1$, except that here $\mathbb{C}[\partial]V_8$ is not irreducible. It contains a unique irreducible submodule isomorphic to $L_{\mathfrak{V}_+}(1)\boxtimes U^2$ generated by ∂a_8. But then the above calculation plus the fact that

$$F_2\partial a_8=-4(\Lambda+1)a_1$$

show that $M_{\mathfrak{N}_+^4}(-1,0)/N$ is irreducible of rank 8. □

Theorem 6.1: *The modules $L_{\mathfrak{N}_+^4}(\Delta,\Lambda)$, for $\Delta\in\mathbb{C}$ and $\Lambda\in\mathbb{Z}_+$, form a complete list of non-isomorphic finite (over $\mathbb{C}[\partial]$) irreducible* $\mathrm{SK}(1,4)_+$*-modules. Furthermore $L_{\mathfrak{N}_+^4}(\Delta,\Lambda)$ as a $\mathbb{C}[\partial]$-module has rank*

(*i*) 4Λ, *in the case* $2\Delta-\Lambda=0$,
(*ii*) $4\Lambda+8$, *in the case* $2\Delta+\Lambda+2=0$, *and*
(*iii*) $16\Lambda+16$, *in all other cases.*

Furthermore, the $\mathbb{C}[\partial]$-rank of $L_{\mathfrak{N}_+^4}(\Delta,\Lambda)_{\bar 0}$ equals the $\mathbb{C}[\partial]$-rank of $L_{\mathfrak{N}_+^4}(\Delta,\Lambda)_{\bar 1}$ in all cases.

Remark 6.2: Translating the above theorem into the languages of modules over conformal algebras and of conformal modules is again straightforward. We therefore obtain that all finite irreducible modules over the ''small'' $N=4$ conformal superalgebra are of the form $L_{\mathfrak{N}^4}(\alpha,\Delta,\Lambda)$, where $\alpha,\Delta\in\mathbb{C}$ and $\Lambda\in\mathbb{Z}_+$. The definition of these modules and also the action of the conformal superalgebra on them are easily gotten from our explicit description of a $\mathbb{C}[\partial]$-basis in this section and hence omitted, as to reproduce them would take up quite a significant amount of space. Again we only note that the adjoint module is isomorphic to $L_{\mathfrak{N}^4}(0,1,2)$.

VII. FINITE IRREDUCIBLE MODULES OVER THE ''BIG'' $N=4$ CONFORMAL SUPERALGEBRA

In this section we give a classification of finite irreducible conformal modules over the contact superalgebra K(1,4), also known as the ''big'' $N=4$ superconformal algebra. Our approach is based on our results obtained in Sec. VI.

Recall from Sec. VI that L_n^β, X_n^β and x_r^β, where $X=H,E,F$, $x=G^{++}$, G^{-+}, G^{+-}, G^{--}, $n\in\mathbb{Z}$, $r\in\frac{1}{2}+\mathbb{Z}$ and the fixed number β is either 1 or -1, provide a basis for a copy of SK(1,4) inside K(1,4). In this section it will be convenient to distinguish these two copies. We therefore denote the copy obtained by setting $\beta=1$ simply by SK(1,4), while the copy obtained by setting $\beta=-1$ we denote by $\overline{\mathrm{SK}}(1,4)$. It is easy to see from our formulas that $\mathrm{K}(1,4)=\mathrm{SK}(1,4)+\overline{\mathrm{SK}}(1,4)$. Similarly we distinguish the basis elements of SK(1,4) and $\overline{\mathrm{SK}}(1,4)$ as follows. The generators inside $\overline{\mathrm{SK}}(1,4)$ will be denoted by L_n,X_n,x_r, while generators inside $\overline{\mathrm{SK}}(1,4)$ will be denoted by $\overline{L_n},\overline{X_n},\overline{x_r}$, where again $X=H,E,F$, $x=G^{++}$, G^{-+}, G^{+-}, G^{--}. Of course we have $x_{-\frac{1}{2}}=\overline{x}_{-\frac{1}{2}}$, $L_{-1}=\overline{L}_{-1}$ and $L_0=\overline{L}_0$.

Remark 7.1: The map $\phi:\mathrm{SK}(1,4)\to\overline{\mathrm{SK}}(1,4)$ defined by $\phi(L_n)=\overline{L}_n$, $\phi(X_n)=\overline{X}_n$, $\phi(G_r^{++})=\overline{G}_r^{++}$, $\phi(G_r^{+-})=\overline{G}_r^{-+}$, $\phi(G_r^{-+})=\overline{G}_r^{+-}$ and $\phi(G_r^{--})=\overline{G}_r^{--}$, where $n\in\mathbb{Z}$ and $r\in\frac{1}{2}+\mathbb{Z}$ is an isomorphism of Lie superalgebras. Thus all formulas in Sec. VI with $\phi(L_n)$, $\phi(X_n)$ and $\phi(x_r)$ replacing L_n, X_n and x_r, respectively, remain valid.

Let $\mathfrak{g}=\mathrm{K}(1,4)_+$ be the annihilation subalgebra of K(1,4) so that we have $\mathfrak{g}=\mathrm{SK}(1,4)_+ +\overline{\mathrm{SK}}(1,4)_+$, the sum of the corresponding annihilation subalgebras. We have as before $\mathfrak{g}=\oplus_{j\geqslant -1}\mathfrak{g}_j$, where $j\in\frac{1}{2}+\mathbb{Z}$. Furthermore, $\mathfrak{g}_-=\mathrm{SK}(1,4)_-=\overline{\mathrm{SK}}(1,4)_-$ and $\mathfrak{g}_0=\mathbb{C}L_0\oplus\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2\cong c\mathrm{so}_4$, where sl_2 and $\overline{\mathrm{sl}}_2$ denote two copies of the Lie algebra sl_2, generated by H_0,E_0,F_0 and $\overline{H}_0,\overline{E}_0,\overline{F}_0$, respectively.

Let $U^{\Delta,\Lambda,\overline{\Lambda}}$ be the finite-dimensional irreducible $\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2$-module of highest weight $(\Lambda,\overline{\Lambda})\in\mathbb{Z}_+\times\mathbb{Z}_+$ on which L_0 acts as the scalar $\Delta\in\mathbb{C}$ and let $v_{\Delta,\Lambda,\overline{\Lambda}}$ denote a highest weight vector in $U^{\Delta,\Lambda,\overline{\Lambda}}$ so that $H_0v_{\Delta,\Lambda,\overline{\Lambda}}=\Lambda v_{\Delta,\Lambda,\overline{\Lambda}}$, $\overline{H}_0v_{\Delta,\Lambda,\overline{\Lambda}}=\overline{\Lambda}v_{\Delta,\Lambda,\overline{\Lambda}}$ and $L_0v_{\Delta,\Lambda,\overline{\Lambda}}=\Delta v_{\Delta,\Lambda,\overline{\Lambda}}$. Regarding $U^{\Delta,\Lambda,\overline{\Lambda}}$ as a module over $\mathcal{L}_0=\oplus_{j\geqslant 0}\mathfrak{g}_j$ it follows from Theorem 3.1 that every finite irreducible $\mathfrak{g}$-module is a quotient of $M_{\mathfrak{S}_+^4}(\Delta,\Lambda,\overline{\Lambda})=\mathrm{Ind}_{\mathcal{L}_0}^{\mathfrak{g}}U^{\Delta,\Lambda,\overline{\Lambda}}$. The unique irreducible quotient will be denoted by $L_{\mathfrak{S}_+^4}(\Delta,\Lambda,\overline{\Lambda})$.

Now $M_{\mathfrak{S}_+^4}(\Delta,\Lambda,\overline{\Lambda})$ is a completely reducible $\mathfrak{g}_0$-module, and the subspace of $\mathbb{C}E_0\oplus\mathbb{C}\overline{E}_0$-invariants, denoted by $M_{\mathfrak{S}_+^4}(\Delta,\Lambda,\overline{\Lambda})^{E_0,\overline{E}_0}$, is a free $\mathbb{C}[\partial]$-submodule of $M_{\mathfrak{S}_+^4}(\Delta,\Lambda,\overline{\Lambda})$. We write down explicit formulas for a $\mathbb{C}[\partial]$-basis for the space $M_{\mathfrak{S}_+^4}(\Delta,\Lambda,\overline{\Lambda})^{E_0,\overline{E}_0}$, which in the case when $\Lambda,\overline{\Lambda}\geqslant 2$ is as follows:

$$b_1=v_{\Delta,\Lambda,\overline{\Lambda}},\quad b_2=G_{-1/2}^{++}v_{\Delta,\Lambda,\overline{\Lambda}},$$

$$b_3=(\Lambda G_{-1/2}^{-+}-G_{-1/2}^{++}F_0)v_{\Delta,\Lambda,\overline{\Lambda}},\quad b_4=(\overline{\Lambda}G_{-1/2}^{+-}-G_{-1/2}^{++}\overline{F}_0)v_{\Delta,\Lambda,\overline{\Lambda}},$$

$$b_5=(\Lambda\overline{\Lambda}G_{-1/2}^{--}-\overline{\Lambda}G_{-1/2}^{+-}F_0-\Lambda G_{-1/2}^{-+}\overline{F}_0+G_{-1/2}^{++}F_0\overline{F}_0)v_{\Delta,\Lambda,\overline{\Lambda}},$$

$$b_6=G_{-1/2}^{++}G_{-1/2}^{+-}v_{\Delta,\Lambda,\overline{\Lambda}},\quad b_7=(\Lambda(G_{-1/2}^{-+}G_{-1/2}^{+-}+G_{-1/2}^{++}G_{-1/2}^{--})-2G_{-1/2}^{++}G_{-1/2}^{+-}F_0)v_{\Delta,\Lambda,\overline{\Lambda}},$$

$$b_8=((\Lambda-1)(-\Lambda G_{-1/2}^{-+}G_{-1/2}^{--}+G_{-1/2}^{-+}G_{-1/2}^{+-}F_0+G_{-1/2}^{++}G_{-1/2}^{--}F_0)-G_{-1/2}^{++}G_{-1/2}^{+-}F_0^2)v_{\Delta,\Lambda,\overline{\Lambda}},$$

$$b_9=G_{-1/2}^{++}G_{-1/2}^{-+}v_{\Delta,\Lambda,\overline{\Lambda}},b_{10}=(\overline{\Lambda}(G_{-1/2}^{++}G_{-1/2}^{--}-G_{-1/2}^{-+}G_{-1/2}^{+-})-2G_{-1/2}^{++}G_{-1/2}^{-+}\overline{F_0})v_{\Delta,\Lambda,\overline{\Lambda}},$$

$$b_{11}=((\overline{\Lambda}-1)(-\overline{\Lambda}G_{-1/2}^{+-}G_{-1/2}^{--}+G_{-1/2}^{+-}G_{-1/2}^{-+}\overline{F}_0+G_{-1/2}^{++}G_{-1/2}^{--}\overline{F}_0)-G_{-1/2}^{++}G_{-1/2}^{-+}\overline{F}_0^2)v_{\Delta,\Lambda,\overline{\Lambda}},$$

$$b_{12}=G_{-1/2}^{++}G_{-1/2}^{+-}G_{-1/2}^{-+}v_{\Delta,\Lambda,\overline{\Lambda}},\quad b_{13}=(\Lambda G_{-1/2}^{++}G_{-1/2}^{-+}G_{-1/2}^{--}-G_{-1/2}^{++}G_{-1/2}^{-+}G_{-1/2}^{+-})v_{\Delta,\Lambda,\overline{\Lambda}},$$

$$b_{14}=(\overline{\Lambda}G_{-1/2}^{++}G_{-1/2}^{+-}G_{-1/2}^{--}-G_{-1/2}^{++}G_{-1/2}^{+-}G_{-1/2}^{-+})v_{\Delta,\Lambda,\overline{\Lambda}},$$

$$b_{15}=(\Lambda G_{-1/2}^{-+}G_{-1/2}^{--}(\overline{\Lambda}G_{-1/2}^{+-}-G_{-1/2}^{++}\overline{F}_0)+\overline{\Lambda}G_{-1/2}^{++}G_{-1/2}^{+-}(G_{-1/2}^{--}F_0-G^{-+}F_0\overline{F}_0))v_{\Delta,\Lambda,\overline{\Lambda}},$$

$$b_{16}=(G_{-1/2}^{++}G_{-1/2}^{+-}G_{-1/2}^{-+}G_{-1/2}^{--}-\partial(G_{-1/2}^{-+}G_{-1/2}^{+-}+G_{-1/2}^{++}G_{-1/2}^{--}))v_{\Delta,\Lambda,\overline{\Lambda}}.$$

In the case when $\Lambda=\overline{\Lambda}=1$ (respectively $\Lambda=\overline{\Lambda}=0$) we have $b_8=b_{11}=0$ (respectively $b_3=b_4=b_5=b_7=b_8=b_{10}=b_{11}=b_{13}=b_{14}=b_{15}=0$), thus giving us 14 (respectively 6) generators. Other cases are easily described as well; however, we will not need them because of Proposition 7.1. Thus we will omit them.

We will, as before, denote the coefficient of $v_{\Delta,\Lambda,\overline{\Lambda}}$ in b_i by $u_i^{\Lambda,\overline{\Lambda}}$ for $1\leqslant i\leqslant 16$. In the case when $\Lambda=\overline{\Lambda}$, which is the only case we will be concerned with in what follows, we simply write u_i^{Λ} for $u_i^{\Lambda,\Lambda}$ and also $v_{\Delta,\Lambda}$ for $v_{\Delta,\Lambda,\Lambda}$.

Proposition 7.1: If $M_{\mathfrak{S}^4_+}(\Delta,\Lambda,\overline{\Lambda})$ is a reducible $\mathfrak{g}$-module, then either $2\Delta-\Lambda=2\Delta-\overline{\Lambda}=0$ or else $2\Delta+\Lambda+2=2\Delta+\overline{\Lambda}+2=0$. In particular, if $\Lambda\neq\overline{\Lambda}$, then $M_{\mathfrak{S}^4_+}(\Delta,\Lambda,\overline{\Lambda})$ is irreducible.

Proof: As a module over $\mathrm{SK}(1,4)_+$ we have $M_{\mathfrak{S}^4_+}(\Delta,\Lambda,\overline{\Lambda})=U(\mathfrak{g}_-)\otimes U^{\Delta,\Lambda,\overline{\Lambda}}$ is a direct sum of $\overline{\Lambda}+1$ copies of $M_{\mathfrak{N}^4_+}(\Delta,\Lambda)$, generated by the highest weight vectors $\overline{F}_0^j v_{\Delta,\Lambda,\overline{\Lambda}}$, where $0\leqslant j\leqslant\overline{\Lambda}$. Since the $\overline{H}_0$-weights of the $\overline{F}_0^j v_{\Delta,\Lambda,\overline{\Lambda}}$'s are all distinct for distinct j's, it follows that these modules as $\mathrm{SK}(1,4)_+\rtimes\mathbb{C}\overline{H}_0$-modules are all non-isomorphic. Therefore, if $M_{\mathfrak{N}^4_+}(\Delta,\Lambda)$ is irreducible over $\mathrm{SK}(1,4)_+$, then $M_{\mathfrak{S}^4_+}(\Delta,\Lambda,\overline{\Lambda})$ is irreducible over $\mathfrak{g}$. From this and Corollary 6.1 we thus conclude that in the case when $\Delta-2\Lambda\neq 0$ and $\Delta+2\Lambda+2\neq 0$ the $\mathfrak{g}$-module $M_{\mathfrak{S}^4_+}(\Delta,\Lambda,\overline{\Lambda})$ is irreducible.

By symmetry we conclude that if $\Delta-2\overline{\Lambda}\neq 0$ and $\Delta+2\overline{\Lambda}+2\neq 0$, then $M_{\mathfrak{S}^4_+}(\Delta,\Lambda,\overline{\Lambda})$ is irreducible over $\mathfrak{g}$ as well.

Therefore, $M_{\mathfrak{S}^4_+}(\Delta,\Lambda,\overline{\Lambda})$ is possibly reducible only if both Λ and $\overline{\Lambda}$ satisfy one of the two linear equations $\Delta-2x=0$ and $\Delta+2x+2=0$. But the case $\Delta-2\Lambda=0$ and $\Delta+2\overline{\Lambda}+2=0$ is not possible, since both Λ and $\overline{\Lambda}$ are non-negative integers. By the same token $\Delta-2\overline{\Lambda}=0$ and $\Delta+2\Lambda+2=0$ is not possible, either. Hence either we have $\Delta-2\Lambda=0$ and $\Delta-2\overline{\Lambda}=0$, or else $\Delta+2\Lambda+2=0$ and $\Delta+2\overline{\Lambda}+2=0$. In either case we must have $\Lambda=\overline{\Lambda}$. □

The next step is to analyze proper singular vectors inside $M_{\mathfrak{S}^4}(\Delta,\Lambda,\overline{\Lambda})$. (The definitions of singular vectors and proper singular vectors of $\mathfrak{g}$ are of course analogous.) By Proposition 7.1 proper singular vectors exist only if $\Lambda=\overline{\Lambda}$ with either $2\Delta+\Lambda=0$ or $2\Delta+\Lambda+2=0$.

Proposition 7.2: A complete list of proper singular vectors inside $M_{\mathfrak{S}^4_+}(\Delta,\Lambda,\Lambda)$ is given by

(*i*) αb_2, $\alpha\neq 0$, *in the case* $2\Delta-\Lambda=0$, *and*
(*ii*) αb_5, $\alpha\neq 0$, *in the case* $2\Delta+\Lambda+2=0$ *and* $\Lambda\geqslant 1$.

Proof: Since as a $\mathrm{SK}(1,4)_+$-module $M_{\mathfrak{S}^4}(\Delta,\Lambda,\Lambda)$ is a direct sum of $\Lambda+1$ copies of $M_{\mathfrak{N}^4}(\Delta,\Lambda)$ we obtain a description of the vector space spanned by all proper $\mathrm{SK}(1,4)_+$-singular vectors by virtue of Proposition 6.1. But as a $\overline{\mathrm{SK}}(1,4)_+$-module $M_{\mathfrak{S}^4}(\Delta,\Lambda,\Lambda)$ is also a direct sum of $\Lambda+1$ copies of $M_{\mathfrak{N}^4}(\Delta,\Lambda)$, from which we obtain similarly a description of the vector space spanned by all proper $\overline{\mathrm{SK}}(1,4)_+$-singular vectors (see Remark 7.1). The intersection of these two spaces is the space of proper singular vectors.

In the case when $2\Delta-\Lambda=0$ it follows from Proposition 6.1 that the space of proper $\mathrm{SK}(1,4)_+$-singular vectors is spanned by $G^{++}_{-1/2}\overline{F}_0^j v_{\Delta,\Lambda}$, $G^{+-}_{-1/2}\overline{F}_0^j v_{\Delta,\Lambda}$ and $G^{++}_{-1/2}G^{+-}_{-1/2}\overline{F}_0^j v_{\Delta,\Lambda}$, for $0\leqslant j\leqslant\Lambda$. On the other hand, the space of proper $\overline{\mathrm{SK}}(1,4)_+$-singular vectors is spanned by $G^{++}_{-1/2}F_0^j v_{\Delta,\Lambda}$, $G^{-+}_{-1/2}F_0^j v_{\Delta,\Lambda}$ and $G^{++}_{-1/2}G^{-+}_{-1/2}F_0^j v_{\Delta,\Lambda}$, for $0\leqslant j\leqslant\Lambda$. It is not hard to see that the intersection of these two spaces is the one-dimensional space spanned by $G^{++}_{-1/2}v_{\Delta,\Lambda}$, which is b_2.

Other cases are analogous and so we omit the details. □

Proposition 7.3: Suppose that $2\Delta-\Lambda=0$. Then $L_{\mathfrak{S}^4_+}(\Delta,\Lambda,\Lambda)$ is a free $\mathbb{C}[\partial]$-module of rank $8\Lambda(\Lambda+1)$.

Proof: By Proposition 7.2 b_2 is a singular vector in $M_{\mathfrak{S}^4_+}(\Lambda/2,\Lambda,\Lambda)$. Consider N, the $\mathfrak{g}$-submodule generated by b_2. Then we have $N=U(\mathfrak{g}_-)V$, where V is the irreducible $\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2$-submodule generated by b_2. Let us compute the space $N^{E_0,\overline{E}_0}$, the space of $(\mathbb{C}E_0\oplus\mathbb{C}\overline{E}_0)$-invariants inside N. Since the $(H_0,\overline{H}_0)$-weight of b_2 is $(\Lambda+1,\Lambda+1)$, we know that N^{E_0,E_0} is a free $\mathbb{C}[\partial]$-module generated over $\mathbb{C}[\partial]$ by $\{u_i^{\Lambda+1}b_2|1\leqslant i\leqslant 16\}$. We have

$$u_1^{\Lambda+1}b_2=b_2,\quad u_2^{\Lambda+1}b_2=0,\quad u_3^{\Lambda+1}b_2=-(\Lambda+2)b_9,\quad u_4^{\Lambda+1}b_2=-(\Lambda+2)b_6,$$

$$u_5^{\Lambda+1}b_2=-\frac{(\Lambda+2)}{2}(b_7+b_{10}+4(\Lambda+1)\partial b_1),\quad u_6^{\Lambda+1}b_2=0,\quad u_7^{\Lambda+1}b_2=-(\Lambda+3)b_{12},$$

$$u_8^{\Lambda+1}b_2=-(\Lambda+2)(b_{13}-2\partial b_3),\quad u_9^{\Lambda+1}b_2=0,\quad u_{10}^{\Lambda+1}b_2=(\Lambda+3)b_{12}-4(\Lambda+1)\partial b_2,$$

$$u_{11}^{\Lambda+1}b_2=-(\Lambda+2)(b_{14}-2\partial b_4),\quad u_{12}^{\Lambda+1}b_2=0,\quad u_{13}^{\Lambda+1}b_2=-2(\Lambda+2)\partial b_9,$$

$$u_{14}^{\Lambda+1}b_2=-2(\Lambda+2)\partial b_6,\quad u_{15}^{\Lambda+1}b_2=-4(\Lambda+1)\partial^2 b_1-(\Lambda+2)^2 b_{16}+(\Lambda+2)\partial b_7,$$

$$u_{16}^{\Lambda+1}b_2=-4\partial b_{12}.$$

It follows that $N^{E_0,\overline{E_0}}$ is generated over $\mathbb{C}[\partial]$ by the set

$$S^\Lambda=\Big\{b_2,b_6,b_7+b_{10}+4(\Lambda+2)\partial b_1,b_9,b_{12},b_{13}-2\partial b_3,b_{14}$$
$$-2\partial b_4,b_{16}-\left(\frac{1}{\Lambda+2}\right)\partial b_7-2\frac{(\Lambda+1)}{(\Lambda+2)^2}\partial^2 b_1\Big\}.$$

In the case when $\Lambda\geqslant 2$ it follows from the description of S^Λ that $\{b_1,b_3,b_4,b_5,b_8,b_{10}+2\Lambda\partial b_1,b_{11},b_{15}\}$ is a $\mathbb{C}[\partial]$-basis for the $(\mathbb{C}E_0\oplus\mathbb{C}\overline{E}_0)$-invariants of the quotient space $M_{\mathfrak{S}_+^4}(\Lambda/2,\Lambda,\Lambda)/N$. (The choice of $b_{10}+2\Lambda\partial b_1$ instead of just b_{10} will be explained later.)

The $(L_0,H_0,\overline{H}_0)$-weights of b_1, b_3, b_4, b_5, b_8, $b_{10}+2\Lambda\partial b_1$, b_{11}, b_{15} are (Δ,Λ,Λ), $(\Delta+\frac{1}{2},\Lambda-1,\Lambda+1)$, $(\Delta+\frac{1}{2},\Lambda+1,\Lambda-1)$, $(\Delta+\frac{1}{2},\Lambda-1,\Lambda-1)$, $(\Delta+1,\Lambda-2,\Lambda)$, $(\Delta+1,\Lambda,\Lambda)$, $(\Delta+1,\Lambda,\Lambda-2)$, and $(\Delta+\frac{3}{2},\Lambda-1,\Lambda-1)$, respectively. Hence $M_{\mathfrak{S}_+^4}(\Lambda/2,\Lambda,\Lambda)/N$ is a free $\mathbb{C}[\partial]$-module of rank $8\Lambda(\Lambda+1)$. So, we need to show that $M_{\mathfrak{S}_+^4}(\Lambda/2,\Lambda,\Lambda)/N$ is irreducible.

Now L_n, $n\geqslant -1$, together with E_0, H_0, F_0 and $\overline{E}_0$, $\overline{H}_0$, $\overline{F}_0$ generate a copy of $(\mathfrak{V}_+\oplus\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2)$, which thus allows us to study the $(\mathfrak{V}_+\oplus\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2)$-module structure of $M_{\mathfrak{S}_+^4}(\Lambda/2,\Lambda,\Lambda)/N$. We can easily check that L_n, for $n\geqslant 1$, annihilates the vectors b_1, b_3, b_4, b_5, b_8, $b_{10}+2\Lambda\partial b_1$, b_{11}, b_{15}. (We want to point out that b_{10} is not annihilated by L_n, for $n\geqslant 1$, hence the choice of $b_{10}+2\Lambda\partial b_1$.) Thus $M_{\mathfrak{S}_+^4}(\Lambda/2,\Lambda,\Lambda)/N$ as a $(\mathfrak{V}_+\oplus\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2)$-module is a direct sum of the following eight irreducible modules: $\mathbb{C}[\partial]V_1\cong L_{\mathfrak{V}_+}(\Lambda/2)\boxtimes U^{\Lambda,\Lambda}$, $\mathbb{C}[\partial]V_3\cong L_{\mathfrak{V}_+}((\Lambda+1)/2)\boxtimes U^{\Lambda-1,\Lambda+1}$, $\mathbb{C}[\partial]V_4\cong L_{\mathfrak{V}_+}((\Lambda+1)/2)\boxtimes U^{\Lambda+1,\Lambda-1}$, $\mathbb{C}[\partial]V_5\cong L_{\mathfrak{V}_+}((\Lambda+1)/2)\boxtimes U^{\Lambda-1,\Lambda-1}$, $\mathbb{C}[\partial]V_8\cong L_{\mathfrak{V}_+}((\Lambda+2)/2)\boxtimes U^{\Lambda-2,\Lambda}$, $\mathbb{C}[\partial]V_{10}\cong L_{\mathfrak{V}_+}((\Lambda+2)/2)\boxtimes U^{\Lambda,\Lambda}$, $\mathbb{C}[\partial]V_{11}\cong L_{\mathfrak{V}_+}((\Lambda+2)/2)\boxtimes U^{\Lambda,\Lambda-2}$, $\mathbb{C}[\partial]V_{15}\cong L_{\mathfrak{V}_+}((\Lambda+3)/2)\boxtimes U^{\Lambda-1,\Lambda-1}$, where V_i is the irreducible $\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2$-module generated by b_i, for $i\neq 10$, and V_{10} is generated by $b_{10}+2\Lambda\partial b_1$, and finally $U^{\mu,\mu'}$ denotes the irreducible $\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2$-module of highest weight (μ,μ'). Note that as $(\mathfrak{V}_+\oplus\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2)$-modules they are all non-isomorphic and thus to show that $M_{\mathfrak{S}_+^4}(\Lambda/2,\Lambda,\Lambda)/N$ is irreducible; it suffices to show that one may send a $(\mathfrak{V}_+\oplus\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2)$-highest weight vector in any irreducible $(\mathfrak{V}_+\oplus\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2)$-component to the irreducible component containing the $\mathfrak{g}$-highest weight vectors. This follows from the following computation:

$$G_{1/2}^{--}b_3=2(\Lambda+1)F_0b_1,\quad \overline{G}_{1/2}^{--}b_4=2(\Lambda+1)\overline{F}_0b_1,$$

$$G_{1/2}^{++}b_5=-2\Lambda^2(\Lambda+1)b_1,\quad E_1b_8=2\Lambda(\Lambda-1)(\Lambda+1)b_1,$$

$$\overline{F}_1(b_{10}+2\Lambda\partial b_1)=-2(\Lambda+2)\overline{F}_0b_1,\quad \overline{E}_1b_{11}=2\Lambda(\Lambda-1)(\Lambda+1)b_1,$$

$$\overline{G}^{++}_{3/2}\, b_{15} = -2\Lambda^2(\Lambda+1)b_1.$$

Now if $\Lambda=1$, the vectors $b_8=b_{11}=0$. Therefore, $M_{\mathfrak{S}^4_+}(\Lambda/2,\Lambda,\Lambda)/N$ is $\mathbb{C}[\partial]V_1\oplus\mathbb{C}[\partial]V_3\oplus\mathbb{C}[\partial]V_4\oplus\mathbb{C}[\partial]V_5\oplus\mathbb{C}[\partial]V_{10}\oplus\mathbb{C}[\partial]V_{15}$. But then the above calculation also shows that $M_{\mathfrak{S}^4_+}(\Lambda/2,\Lambda,\Lambda)/N$ is irreducible. The rank of $L_{\mathfrak{S}^4_+}(\Lambda/2,\Lambda,\Lambda)$ is then $4+3+3+1+4+1=16$, which is equal to $8\Lambda(\Lambda+1)$ in the case when $\Lambda=1$.

Finally, when $\Lambda=0$, the vectors $b_3=b_4=b_5=b_7=b_8=b_{10}=b_{11}=b_{13}=b_{14}=b_{15}=0$ and S^Λ reduce to $\{b_2,b_6,\partial b_1,b_9,b_{12},b_{16}\}$. Hence $M_{\mathfrak{S}^4_+}(0,0,0)/N=\mathbb{C}b_1$ is the trivial module and so has rank 0. □

Proposition 7.4: Suppose that $2\Delta+\Lambda+2=0$ *and* $\Lambda\geqslant 1$. *Then* $L_{\mathfrak{S}^4_+}(\Delta,\Lambda,\Lambda)$ *is a free* $\mathbb{C}[\partial]$*-module of rank* $8(\Lambda+1)(\Lambda+2)$.

Proof: By Proposition 7.2 b_5 is a singular vector in $M_{\mathfrak{S}^4_+}(-(\Lambda+2)/2,\Lambda,\Lambda)$. Let N be the $\mathfrak{g}$-submodule generated by b_5 so that $N=U(\mathfrak{g}_-)V$, where V is the irreducible $\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2$-submodule generated by b_5. Consider $N^{E_0,\overline{E}_0}$, the subspace in N of $\mathbb{C}E_0\oplus\mathbb{C}\overline{E}_0$-invariants. Now the $(H_0,\overline{H}_0)$-weight of b_5 is $(\Lambda-1,\Lambda-1)$ and so $N^{E_0,\overline{E}_0}$ is a free $\mathbb{C}[\partial]$-module generated over $\mathbb{C}[\partial]$ by $\{u_i^{\Lambda-1}b_5 \mid 1\leqslant i\leqslant 16\}$. We have

$$u_1^{\Lambda-1}b_5=b_5,\quad u_2^{\Lambda-1}b_5=\tfrac{1}{2}(b_7+b_{10}),\quad u_3^{\Lambda-1}b_5=-\Lambda b_8,\quad u_4^{\Lambda-1}b_5=-\Lambda b_{11},$$

$$u_5^{\Lambda-1}b_5=0,\quad u_6^{\Lambda-1}b_5=\Lambda b_{14},\quad u_7^{\Lambda-1}b_5=-(\Lambda-1)b_{15},\quad u_8^{\Lambda-1}b_5=0,$$

$$u_9^{\Lambda-1}b_5=\Lambda b_{13},\quad u_{10}^{\Lambda-1}b_5=(\Lambda-1)b_{15},\quad u_{11}^{\Lambda-1}b_5=0,$$

$$u_{12}^{\Lambda-1}b_5=\Lambda(\Lambda b_{16}+\partial b_7),\quad u_{13}^{\Lambda-1}b_5=0,\quad u_{14}^{\Lambda-1}b_5=0,\quad u_{15}^{\Lambda-1}b_5=0,$$

$$u_{16}^{\Lambda-1}b_5=\partial b_{15}.$$

It follows in the case $\Lambda\geqslant 2$ that $N^{E_0,\overline{E}_0}$ is generated over $\mathbb{C}[\partial]$ by the set

$$S^\Lambda=\{b_5,b_7+b_{10},b_8,b_{11},b_{13},b_{14},b_{15},\Lambda b_{16}+\partial b_7\}.$$

Hence in this case $\{b_1,b_2,b_3,b_4,b_6,b_9,b_{10}+2\Lambda\partial b_1,b_{12}\}$ is a $\mathbb{C}[\partial]$-basis for the $(\mathbb{C}E_0\oplus\mathbb{C}\overline{E}_0)$-invariants of $M_{\mathfrak{S}^4_+}(-(\Lambda+2)/2,\Lambda,\Lambda)/N$.

The $(L_0,H_0,\overline{H}_0)$-weights of b_1, b_2, b_3, b_4, b_6, b_9, $b_{10}+2\Lambda\partial b_1$, b_{12} are (Δ,Λ,Λ), $(\Delta+\frac{1}{2},\Lambda+1,\Lambda+1)$, $(\Delta+\frac{1}{2},\Lambda-1,\Lambda+1)$, $(\Delta+\frac{1}{2},\Lambda+1,\Lambda-1)$, $(\Delta+1,\Lambda+2,\Lambda)$, $(\Delta+1,\Lambda,\Lambda+2)$, $(\Delta+1,\Lambda,\Lambda)$, $(\Delta+\frac{3}{2},\Lambda+1,\Lambda+1)$, respectively. Hence $M_{\mathfrak{S}^4_+}(-(\Lambda+2)/2,\Lambda)/N$ is a free $\mathbb{C}[\partial]$-module of rank $8(\Lambda+1)(\Lambda+2)$. So, we need to show that $M_{\mathfrak{S}^4_+}(\Lambda/2,\Lambda,\Lambda)/N$ is irreducible.

Again we will study the $(\mathfrak{V}_+\oplus\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2)$-module structure of $M_{\mathfrak{N}^4_+}(\Lambda/2,\Lambda)/N$. We can check directly that L_n, for $n\geqslant 1$, annihilates the vectors b_1, b_2, b_3, b_4, b_6, b_9, $b_{10}+2\Lambda\partial b_1$, b_{12}. Thus $M_{\mathfrak{S}^4_+}(-(\Lambda+2)/2,\Lambda,\Lambda)/N$ as a $(\mathfrak{V}_+\oplus\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2)$-module is a direct sum of the following eight irreducible modules: $\mathbb{C}[\partial]V_1\cong L_{\mathfrak{V}_+}(-(\Lambda+2)/2)\boxtimes U^{\Lambda,\Lambda}$, $\mathbb{C}[\partial]V_2\cong L_{\mathfrak{V}_+}(-(\Lambda+1)/2)\boxtimes U^{\Lambda+1,\Lambda+1}$, $\mathbb{C}[\partial]V_3\cong L_{\mathfrak{V}_+}(-(\Lambda+1)/2)\boxtimes U^{\Lambda-1,\Lambda+1}$, $\mathbb{C}[\partial]V_4\cong L_{\mathfrak{V}_+}(-(\Lambda+1)/2)\boxtimes U^{\Lambda+1,\Lambda-1}$, $\mathbb{C}[\partial]V_6\cong L_{\mathfrak{V}_+}(-\Lambda/2)\boxtimes U^{\Lambda+2,\Lambda}$, $\mathbb{C}[\partial]V_9\cong L_{\mathfrak{V}_+}(-\Lambda/2)\boxtimes U^{\Lambda,\Lambda+2}$, $\mathbb{C}[\partial]V_{10}\cong L_{\mathfrak{V}_+}(-\Lambda/2)\boxtimes U^{\Lambda,\Lambda}$, $\mathbb{C}[\partial]V_{12}\cong L_{\mathfrak{V}_+}(-(\Lambda-1)/2)\boxtimes U^{\Lambda+1,\Lambda+1}$, where V_i is the irreducible $\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2$-module generated by b_i, for $i\neq 10$, and V_{10} is generated by $b_{10}+2\Lambda\partial b_1$, and $U^{\mu,\mu'}$ is the irreducible $\mathrm{sl}_2\oplus\overline{\mathrm{sl}}_2$-module of highest weight (μ,μ'). Note these modules are all irreducible. Note further that they are all non-isomorphic. So as before, to show that $M_{\mathfrak{S}^4_+}(-(\Lambda+2)/2,\Lambda,\Lambda)/N$ is irre-

ducible, it suffices to show that one may send a $(\mathfrak{V}_+ \oplus \mathrm{sl}_2 \oplus \overline{\mathrm{sl}}_2)$-highest weight vector in any irreducible $(\mathfrak{V}_+ \oplus \mathrm{sl}_2 \oplus \overline{\mathrm{sl}}_2)$-component to the irreducible component containing the $\mathfrak{g}$-highest weight vectors. For this purpose we compute

$$G^{--}_{1/2} b_2 = 2(\Lambda+1) b_1, \quad \overline{G}^{+-}_{1/2} b_3 = -2\Lambda(\Lambda+1) b_1,$$

$$G^{-+}_{1/2} b_4 = -2\Lambda(\Lambda+1) b_1, \quad F_1 b_6 = -2(\Lambda+1) b_1,$$

$$\overline{F}_1 b_9 = -2(\Lambda+1) b_1 \quad \overline{F}_1 (b_{10} + 2\Lambda \partial b_1) = 2\Lambda \overline{F}_0 b_1,$$

$$\overline{G}^{--}_{3/2} b_{12} = 8(\Lambda+1) b_1.$$

This settles the case when $\Lambda \geqslant 2$.

In the case when $\Lambda = 1$, $N^{E_0, \overline{E}_0}$ is generated over $\mathbb{C}[\partial]$ by

$$S^{\Lambda} = \{b_5, b_7 + b_{10}, b_{13}, b_{14}, b_{16} + \partial b_7, \partial b_{15}\}.$$

Therefore, $M_{\mathfrak{S}^4_+}(-(\Lambda+2)/2, \Lambda, \Lambda)/N$ contains a ∂-invariant (and hence $\mathfrak{g}$-invariant) vector b_{15}. Since in this case the vectors $b_8 = b_{11} = 0$, $M_{\mathfrak{S}^4_+}(-(\Lambda+2)/2, \Lambda, \Lambda)/(N + \mathbb{C}b_{15})$ as a $\mathfrak{V}_+ \oplus \mathrm{sl}_2 \oplus \overline{\mathrm{sl}}_2$-module is isomorphic to $\mathbb{C}[\partial]V_1 \oplus \mathbb{C}[\partial]V_2 \oplus \mathbb{C}[\partial]V_3 \oplus \mathbb{C}[\partial]V_4 \oplus \mathbb{C}[\partial]V_6 \oplus \mathbb{C}[\partial]V_9 \oplus \mathbb{C}[\partial]V_{10} \oplus \mathbb{C}[\partial]V_{12}$. Every component is irreducible except for $\mathbb{C}[\partial]V_{12}$, which contains a unique (irreducible) $\mathfrak{V}_+ \oplus \mathrm{sl}_2 \oplus \overline{\mathrm{sl}}_2$-submodule isomorphic to $L_{\mathfrak{V}_+}(1) \otimes U^{2,2}$ generated by the highest weight vector ∂b_{15}. But then the above calculation plus the fact that

$$\overline{G}^{--}_{5/2} \partial b_{12} = 24(\Lambda+1) \partial b_1$$

also shows that $M_{\mathfrak{S}^4_+}(-(\Lambda+2)/2, \Lambda, \Lambda)/(N + \mathbb{C}b_{15})$ is irreducible. □

We summarize the results of this section in the following theorem.

Theorem 7.1: *The modules $L_{\mathfrak{S}^4_+}(\Delta, \Lambda, \overline{\Lambda})$, for $\Delta \in \mathbb{C}$ and $\Lambda, \overline{\Lambda} \in \mathbb{Z}_+$, form a complete list of non-isomorphic finite (over $\mathbb{C}[\partial]$) irreducible $\mathrm{K}(1,4)_+$-modules. Furthermore, $L_{\mathfrak{S}^4_+}(\Delta, \Lambda, \overline{\Lambda})$ as a $\mathbb{C}[\partial]$-module has rank*

(*i*) $8\Lambda(\Lambda+1)$, *in the case* $2\Delta - \Lambda = 0$ *and* $\Lambda = \overline{\Lambda}$,
(*ii*) $8(\Lambda+1)(\Lambda+2)$, *in the case* $2\Delta + \Lambda + 2 = 0$ *and* $\Lambda = \overline{\Lambda}$, *and*
(*iii*) $16(\Lambda+1)(\overline{\Lambda}+1)$, *in all other cases.*

*Furthermore, the $\mathbb{C}[\partial]$-rank of $L_{\mathfrak{S}^4_+}(\Delta, \Lambda, \overline{\Lambda})^-_0$ equals the $\mathbb{C}[\partial]$-*rank of $L_{\mathfrak{S}^4_+}(\Delta, \Lambda, \overline{\Lambda})^-_1$ *in all cases.*

Remark 7.2: Again the translation into the languages of modules over conformal algebras and of conformal modules is straightforward and hence is omitted. We thus obtain that all finite irreducible modules over the ''big'' $N=4$ conformal superalgebra are of the form $L_{\mathfrak{S}^4}(\alpha, \Delta, \Lambda, \overline{\Lambda})$, where $\alpha, \Delta \in \mathbb{C}$ and $\Lambda, \overline{\Lambda} \in \mathbb{Z}_+$. Again the definition of these modules and the action of the conformal superalgebra on them are easily derived from our explicit description of a $\mathbb{C}[\partial]$-basis in this section. We note that the adjoint module is isomorphic to $M_{\mathfrak{S}^4}(0,0,0,0)$. This module is not simple, since K(1,4) is not a simple Lie superalgebra. Its derived algebra $\mathrm{K}(1,4)'$ (which is a simple formal distribution Lie superalgebra) is an ideal in K(1,4) of codimension 1.[10] Since the annihilation subalgebra of $\mathrm{K}(1,4)'$ and K(1,4) are identical, and hence their conformal modules are identical. Therefore the results in this section also give explicit description of irreducible conformal modules over $\mathrm{K}(1,4)'$. We finally remark that the $\mathrm{K}(1,4)'$ as a conformal module over K(1,4) corresponds to $L_{\mathfrak{S}^4}(0, \frac{1}{2}, 1, 1)$.

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Braided coaddition on the quantized braided matrices

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An additive braided coproduct (also be called braided coaddition) is introduced on the quantized braided matrices (QBMs). It gives QBMs another braided-Hopf algebra structure. The coaddition is also shown to be compatible with the existing coproduct such that they together form a so-called quantized-braided ring. And some quantized braided differential operator bialgebras (Hopf algebras) relating to this braided coaddition are constructed. These give a unification and generalization of the known results about braided and quantum matrices. Moreover, the coaddition construction and the related differential calculi on the QBMs are further extended to a kind of more general quantum matrix algebraic systems. Some examples are also given. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1326457]

I. INTRODUCTION

Quantized braided matrices (groups) [QBM(Gs)] were proposed by Hlavaty[1] years ago, they are a kind of more general algebraic structures that contain the usual quantum matrices (groups),[2–4] braided matrices (groups),[5–7] quantum supermatrices (supergroups),[8] quantum anyonic matrices (groups),[9] and μ-braided GL_q matrices (groups)[10] as special cases. Thus the theory of QBM(G)s has, among others, a remarkable advantage that enable us to study two quite different kinds of noncommutativities (associated, respectively, with quantization and general braid statistics) in a unified way. Some of properties and applications of the QBM(G)s have been discussed recently.[11–13]

In this paper, we consider some other features of QBM(G)s. We introduce an additive braided coproduct (also be called braided coaddition) on the QBMs and show that it is compatible with the existing (multiplicative) coproduct in a way obeying some quantized braided codistributivity axiom. Moreover, we construct corresponding braided differential calculi on the QBMs and discuss some related results. These are motivated by the works of Meyer[14] and Majid,[15] where the braided coadditions on braided and quantum matrices were introduced respectively. In some sense, the scheme of the present paper gives a unification and generalization of that in Refs. 14 and 15, the related results for the braided[14] and quantum[15] matrices can be obtained as special cases. Furthermore, we also find that the coaddition construction and some related results on the QBMs can even be further extended to a kind of more general algebraic systems.

We begin in Sec. II by recalling some notion and results about the QBM(G)s. In Sec. III we introduce braided coaddition on QBMs and show that it and the existing coproduct together form a so-called quantized-braided ring. The braided differential operators with respect to the coaddition are introduced in Sec. IV and their bialgebra structures are given. Section V gives some example to explain the formulations of Secs. III and IV. In Sec. VI the braided coaddition and associated differential operator algebras on QBMs are further generalized to more general algebraic systems. Finally, Sec. VII contains some conclusions and discussions.

II. QUANTIZED BRAIDED MATRICES

Here we briefly recall some related results about the QBM(G)s from Refs. 1 and 11, these are useful in the discussions later.

Let $T=\{T_j^i\}_{i,j=1}^N$ be a matrix of N^2 elements T_j^i and $R,Z\in M_N(\mathbf{C})\otimes M_N(\mathbf{C})$ be an R-matrix pair satisfying the set of quantum Yang–Baxter-type equations,[1]

$$\begin{aligned} &R_{12}R_{13}R_{23}=R_{23}R_{13}R_{12}, \quad Z_{12}Z_{13}Z_{23}=Z_{23}Z_{13}Z_{12},\\ &R_{12}Z_{13}Z_{23}=Z_{23}Z_{13}R_{12}, \quad Z_{12}Z_{13}R_{23}=R_{23}Z_{13}Z_{12}, \end{aligned} \tag{2.1}$$

then the quantized braided matrix bialgebra, denoted by $A(R,Z)$, is generated by T_j^i and 1 with the following algebra relations,

$$R_{12}Z_{12}^{-1}T_1Z_{12}T_2=Z_{21}^{-1}T_2Z_{21}T_1R_{12}, \tag{2.2}$$

the coproduct and counit

$$\Delta(T_j^i)=T_k^i\otimes T_j^k, \quad \varepsilon(T_j^i)=\delta_j^i, \tag{2.3}$$

and the braiding

$$\Psi(Z_{12}^{-1}T_1\otimes Z_{12}T_2)=T_2Z_{12}^{-1}\otimes T_1Z_{12}. \tag{2.4}$$

Throughout this paper, we always assume R, Z both to be invertible, and for $a\otimes b$, $c\otimes d\in A(R,Z)\otimes A(R,Z)$, the product in the (braided) tensor product algebra is given by

$$(a\otimes b)(c\otimes d)=a\Psi(b\otimes c)d \tag{2.5}$$

as in Ref. 15.

If we also introduce an antipode in $A(R,Z)$, then we obtain a quantized braided group.[1]

We mention some special cases of QBM(G)s: When $Z=R$ or $Z=I$ while R is any regular solution of the quantum Yang–Baxter equation (QYBE), then $A(R,Z)$ is reduced to the ordinary braided matrix (group) or quantum matrix (group), respectively; If Z is diagonal and R is some specified $R(q)$, then $A(R(q),Z)$ gives the μ-braided GL_q matrices (groups) considered in Ref. 10, etc.

Moreover, we have the following:[11]

Proposition 2.1: Defining $R^{(n)}\equiv(ZP)^nR(Z^{-1}P)^n$, if (R,Z) is an R-matrix pair satisfying (2.1), then $(R^{(n)},Z)$ satisfies (2.1), too, for each integer $n=0,\pm1,\pm2,\ldots$. Here P is the usual permutation matrix. □

Some times we need certain restricted conditions on R-matrices. A matrix solution R of the QYBE is called being Hecke-type if it satisfies

$$(PR-q)(PR+q^{-1})=0, \quad \text{or} \quad PRPR=1+\lambda PR \tag{2.6}$$

for suitable q and $\lambda=q-q^{-1}$.

Proposition 2.2: If R is Hecke-type, then so is $R^{(n)}$ for each $n=0,\pm1,\pm2,\ldots$.

Proof: The $R^{(n)}$ is defined in Proposition 2.1, thus $PR^{(n)}=(PZ)^nPR(PZ)^{-n}$. So from Eq. (2.6) we have

$$PR^{(n)}PR^{(n)}=(PZ)^nPRPR(PZ)^{-n}=(PZ)^n(1+\lambda PR)(PZ)^{-n}=1+\lambda PR^{(n)}. \quad \square$$

III. BRAIDED COADDITION ON QUANTIZED BRAIDED MATRICES

In this section we show that besides the coproduct (2.3) with the braiding (2.4), another kind of additive coproduct (or called braided coaddition) can also be introduced in $A(R,Z)$.

Theorem 3.1: Let the R-matrix pair (R,Z) obey Eqs. (2.1). Let R be Hecke type-and Z have the second inverse $\tilde{Z}\equiv((Z^{t_2})^{-1})^{t_2}$ (t_2 denotes transposition in the second factor). Then in the matrix algebra defined by (2.2), we can introduce the following additive coproduct, counit, and antipode:

$$\underline{\Delta}T\otimes 1+1\otimes T,\quad \underline{\varepsilon}T=0,\quad \underline{S}T=-T, \tag{3.1}$$

such that the relations (2.2), (3.1) give a braided-Hopf algebra with the braiding

$$\underline{\Psi}(T_1\otimes Z_{12}T_2)=Z_{12}R_{21}Z_{21}^{-1}T_2\otimes Z_{21}T_1R_{12}. \tag{3.2}$$

This braided-Hopf algebra will be denoted by $A(R,Z)$.

Proof: For the brevity of notations, we write (recall $R^{(n)}$ in Proposition 2.1)

$$\hat{R}_{12}\equiv R_{12}^{(1)}=Z_{12}R_{21}Z_{21}^{-1}, \tag{3.3}$$

thus the braiding (3.2) can be written as $\Psi(T_1\otimes Z_{12}T_2)=\hat{R}_{12}T_2\otimes Z_{21}T_1R_{12}$.

That the relation (2.2) defines an associative algebra has been pointed out by Hlavaty.[1] Here we have to check that Ψ, Δ, S, ε in (3.2), (3.1) are all well-defined when extended to products and satisfy the axioms of braided-Hopf algebra. First, we show that Ψ extends to tensor products according to the rules of braiding. In fact, from (3.2) we calculate (the meaning of Ψ_{ij} can easily be seen in the following calculations and the computations have generality because of the existence of $\tilde{Z}$)

$$\begin{aligned}
&\underline{\Psi}_{23}\underline{\Psi}_{13}\underline{\Psi}_{12}(T_1\otimes Z_{12}T_2\otimes Z_{13}Z_{23}T_3)\\
&\quad=\underline{\Psi}_{23}\underline{\Psi}_{13}(\hat{R}_{12}T_2\otimes Z_{21}T_1\otimes R_{12}Z_{13}Z_{23}T_3)\\
&\quad=\underline{\Psi}_{23}\underline{\Psi}_{13}(\hat{R}_{12}T_2\otimes Z_{21}Z_{23}T_1\otimes Z_{13}T_3R_{12})\\
&\quad=\underline{\Psi}_{23}(\hat{R}_{12}T_2\otimes Z_{21}Z_{23}\hat{R}_{13}T_3\otimes Z_{31}T_1R_{13}R_{12})\\
&\quad=\underline{\Psi}_{23}(\hat{R}_{12}\hat{R}_{13}T_2\otimes Z_{23}T_3\otimes Z_{21}Z_{31}T_1R_{13}R_{12})\\
&\quad=\hat{R}_{12}\hat{R}_{13}\hat{R}_{23}T_3\otimes Z_{32}T_2R_{23}\otimes Z_{21}Z_{31}T_1R_{13}R_{12}\\
&\quad=\hat{R}_{12}\hat{R}_{13}\hat{R}_{23}T_3\otimes Z_{32}Z_{31}T_2\otimes Z_{21}T_1R_{23}R_{13}R_{12};
\end{aligned}$$

$$\begin{aligned}
&\underline{\Psi}_{12}\underline{\Psi}_{13}\underline{\Psi}_{23}(T_1\otimes Z_{12}T_2\otimes Z_{13}Z_{23}T_3)\\
&\quad=\underline{\Psi}_{12}\underline{\Psi}_{13}(T_1\otimes Z_{12}Z_{13}\hat{R}_{23}T_3\otimes Z_{32}T_2R_{23})\\
&\quad=\underline{\Psi}_{12}\underline{\Psi}_{13}(\hat{R}_{23}T_1\otimes Z_{13}T_3\otimes Z_{12}Z_{32}T_2R_{23})\\
&\quad=\underline{\Psi}_{12}(\hat{R}_{23}\hat{R}_{13}T_3\otimes Z_{31}T_1\otimes R_{13}Z_{12}Z_{32}T_2R_{23})\\
&\quad=\underline{\Psi}_{12}(\hat{R}_{23}\hat{R}_{13}T_3\otimes Z_{31}Z_{32}T_1\otimes Z_{12}T_2R_{13}R_{23})\\
&\quad=\hat{R}_{23}\hat{R}_{13}T_3\otimes Z_{31}Z_{32}\hat{R}_{12}T_2\otimes Z_{21}T_1R_{12}R_{13}R_{23}\\
&\quad=\hat{R}_{23}\hat{R}_{13}\hat{R}_{12}T_3\otimes Z_{32}Z_{31}T_2\otimes Z_{21}T_1R_{12}R_{13}R_{23},
\end{aligned}$$

these two results are equal from relations (2.1). And in the above calculations we have used (2.1) and Proposition 2.1 many times.

Noted that in terms of $\hat{R}$, Eq. (2.2) can be written as $\hat{R}_{21}T_1Z_{12}T_2=T_2Z_{21}T_1R_{12}$, the extension of the braiding to products is then in such a way that $\underline{\Psi}$ is functorial with respect to the product, in the sense

$$\begin{aligned}\underline{\Psi}(\hat{R}_{21}T_1Z_{12}T_2\otimes Z_{13}Z_{23}T_3)&=(id\otimes\cdot)(\underline{\Psi}\otimes id)(id\otimes\underline{\Psi})(\hat{R}_{21}T_1\otimes Z_{12}T_2\otimes Z_{13}Z_{23}T_3)\\&=\hat{R}_{21}\hat{R}_{23}\hat{R}_{13}T_3\otimes Z_{31}Z_{32}T_1Z_{12}T_2R_{13}R_{23}\\&=\hat{R}_{13}\hat{R}_{23}T_3\otimes\hat{R}_{21}Z_{31}Z_{32}T_1Z_{12}T_2R_{13}R_{23}\\&=\hat{R}_{13}\hat{R}_{23}T_3\otimes Z_{32}Z_{31}\hat{R}_{21}T_1Z_{12}T_2R_{13}R_{23},\end{aligned}$$

to see that this extension is well-defined, we also calculate

$$\begin{aligned}\underline{\Psi}(T_2Z_{21}T_1R_{12}\otimes Z_{13}Z_{23}T_3)&=(id\otimes\cdot)(\underline{\Psi}\otimes id)(id\otimes\underline{\Psi})(T_2\otimes Z_{21}T_1\otimes Z_{23}Z_{13}T_3R_{12})\\&=\hat{R}_{13}\hat{R}_{23}T_3\otimes Z_{32}Z_{31}T_2Z_{21}T_1R_{23}R_{13}R_{12},\end{aligned}$$

which are consistent by the relation (2.2) and the QYBE about R. The extension to the high orders of products can then be computed in an entirely similar way. Hence, $\underline{\Psi}$ is well-defined and functorial with respect to the product.

Next we extend Δ to products in such a way that it is a homomorphism to the braided tensor product like (2.5). This is consistent because

$$\begin{aligned}\underline{\Delta}(R_{12}Z_{12}^{-1}T_1Z_{12}T_2)&=R_{12}Z_{12}^{-1}(T_1\otimes 1+1\otimes T_1)Z_{12}(T_2\otimes 1+1\otimes T_2)\\&=R_{12}Z_{12}^{-1}T_1Z_{12}T_2\otimes 1+R_{12}Z_{12}^{-1}T_1Z_{12}\otimes T_2\\&\quad+R_{12}R_{21}Z_{21}^{-1}T_2Z_{21}\otimes T_1R_{12}+1\otimes R_{12}Z_{12}^{-1}T_1Z_{12}T_2\\&=R_{12}Z_{12}^{-1}T_1Z_{12}T_2\otimes 1+R_{12}Z_{12}^{-1}T_1Z_{12}\otimes T_2\\&\quad+(1+\lambda R_{12}P_{12})Z_{21}^{-1}T_2Z_{21}\otimes T_1R_{12}+1\otimes R_{12}Z_{12}^{-1}T_1Z_{12}T_2;\end{aligned}$$

$$\begin{aligned}\underline{\Delta}(Z_{21}^{-1}T_2Z_{21}T_1R_{12})&=Z_{21}^{-1}(T_2\otimes 1+1\otimes T_2)Z_{21}(T_1\otimes 1+1\otimes T_1)R_{12}\\&=Z_{21}^{-1}T_2Z_{21}T_1R_{12}\otimes 1+Z_{21}^{-1}T_2Z_{21}\otimes T_1R_{12}\\&\quad+R_{12}Z_{21}^{-1}T_1Z_{12}\otimes T_2R_{21}R_{12}+1\otimes Z_{21}^{-1}T_2Z_{21}T_1R_{12}\\&=Z_{21}^{-1}T_2Z_{21}T_1R_{12}\otimes 1+Z_{21}^{-1}T_2Z_{21}\otimes T_1R_{12}\\&\quad+R_{12}Z_{12}^{-1}T_1Z_{12}\otimes T_2(1+\lambda P_{12}R_{12})+1\otimes Z_{21}^{-1}T_2Z_{21}T_1R_{12},\end{aligned}$$

where we have used the Hecke property (2.6) of R. These two results are equal due to the relation (2.2). Hence Δ is well-defined. It is trivial to see that the braiding $\underline{\Psi}$ is functorial with respect to the coproduct $\underline{\Delta}$.

Finally, for a braided-Hopf algebra, the antipode by definition is braided antimultiplicative in the sense $\underline{S}(ab)=\cdot\underline{\Psi}(\underline{S}a\otimes\underline{S}b)$. Then we can calculate that

$$\underline{S}(\hat{R}_{21}T_1Z_{12}T_2)=\cdot\underline{\Psi}(\hat{R}_{21}\underline{S}T_1\otimes Z_{12}\underline{S}T_2)=\hat{R}_{21}\hat{R}_{12}T_2Z_{21}T_1R_{12}=\hat{R}_{21}T_1Z_{12}T_2R_{21}R_{12},$$

where the relation (2.2) has been used. On the other hand,

$$\underline{S}(T_2Z_{21}T_1R_{12})=\cdot\underline{\Psi}(\underline{S}T_2\otimes Z_{21}\underline{S}T_1R_{12})=\hat{R}_{21}T_1Z_{12}T_2R_{21}R_{12}.$$

So we have $S(\hat{R}_{21}T_1Z_{12}T_2)=S(T_2Z_{21}T_1R_{12})$. On the high orders of products the calculations are similar. Thus S is well-defined.

Other axioms such as $\cdot(S\otimes id)\circ\Delta=\cdot(id\otimes S)\circ\Delta=\eta\circ\varepsilon$, etc. are easily verified. □

We have had two coproducts [of multiplicative one in (2.3) and additive one in (3.1)] on $A(R,Z)$. They are compatible in a way that corresponds to the usual distributivity axiom, which can be shown as follows:

Definition 3.2: If a quantized braided bialgebra (A,Δ,ε) has also a second braided Hopf algebra structure $(A,\underline{\Delta},\varepsilon,S)$ for the same algebra A and obeys the codistributivity axioms

$$(id\otimes\cdot)\circ\Delta_{A\otimes A}\circ\underline{\Delta}=(\underline{\Delta}\otimes id)\circ\Delta,\quad(\cdot\otimes id)\circ\Delta_{A\otimes A}\circ\underline{\Delta}=(id\otimes\underline{\Delta})\circ\Delta, \tag{3.4}$$

where $\Delta_{A\otimes A}=(id\otimes\Psi\otimes id)(\Delta\otimes\Delta)$ is the coproduct in the braided tensor product coalgbra related to Δ, then we call the algebraic system $(A,\Delta,\varepsilon;\underline{\Delta},\varepsilon,S)$ a quantized-braided ring. Δ and $\underline{\Delta}$ are called braided comutiplication and braided coaddition, respectively.

Proposition 3.3: The quantized braided bialgebra $[A(R,Z),\Delta,\varepsilon]$ given by (2.2)–(2.4) together with the braided Hopf algebra structure $[A(R,Z),\underline{\Delta},\varepsilon,S]$ in Theorem 3.1 forms a quantized-braided ring.

Proof: Here we have also used $A(R,Z)$ to denote the algebra defined only by (2.2). We have to prove the codistributivity conditions (3.4). They hold trivially on the generators. On the products $T_1Z_{12}T_2$, we have for the first condition

$$\begin{aligned}
&(id\otimes\cdot)\circ\Delta_{A\otimes A}\circ\underline{\Delta}(T_1Z_{12}T_2)\\
&\quad=(id\otimes\cdot)\Delta_{A\otimes A}(T_1Z_{12}T_2\otimes 1+1\otimes T_1Z_{12}T_2+T_1\otimes Z_{12}T_2+\hat{R}_{12}T_2\otimes Z_{21}T_1R_{12})\\
&\quad=(id\otimes\cdot)(id\otimes\Psi\otimes id)(T_1Z_{12}T_2\otimes Z_{12}^{-1}T_1Z_{12}T_2\otimes 1\otimes 1+1\otimes 1\otimes T_1Z_{12}T_2\otimes Z_{12}^{-1}T_1Z_{12}T_2\\
&\qquad+T_1\otimes T_1\otimes Z_{12}T_2\otimes T_2+\hat{R}_{12}T_2\otimes T_2\otimes Z_{21}T_1\otimes T_1R_{12})\\
&\quad=T_1Z_{12}T_2\otimes 1\otimes Z_{12}^{-1}T_1Z_{12}T_2+1\otimes T_1Z_{12}T_2\otimes Z_{12}^{-1}T_1Z_{12}T_2+T_1\otimes Z_{12}T_2\otimes Z_{12}^{-1}T_1Z_{12}T_2\\
&\qquad+\hat{R}_{12}T_2\otimes Z_{21}T_1\otimes Z_{21}^{-1}T_2Z_{21}T_1R_{12}\\
&\quad=(T_1Z_{12}T_2\otimes 1+1\otimes T_1Z_{12}T_2+T_1\otimes Z_{12}T_2+\hat{R}_{12}T_2\otimes Z_{21}T_1R_{12})\otimes Z_{12}^{-1}T_1Z_{12}T_2\\
&\quad=(\underline{\Delta}\otimes id)(T_1Z_{12}T_2\otimes Z_{12}^{-1}T_1Z_{12}T_2)=(\underline{\Delta}\otimes id)\circ\Delta(T_1Z_{12}T_2),
\end{aligned}$$

where we have used the relations (2.2)–(2.4) and (3.1), (3.2). The general case can be verified in a similar way duo to the consistency of the coproducts, braidings with the algebra relation (2.2), and similarly for the second codistributivity axiom. □

We conclude this section with a restatement of Theorem 3.1 in another form, which is more convenient to some discussions later.

Lemma 3.4: Let (R,Z) be an N-dimensional R-matrix pair as in Sec. II and let R be Hecke type, Z have the second inverse $\tilde{Z}$, then

$$\mathbf{R}^{AB}_{CD}=\hat{R}^{c_0\alpha}_{\beta b_0}Z^{b_1\beta}_{\gamma a_0}R^{a_1\gamma}_{\delta d_1}\tilde{Z}^{\delta d_0}_{c_1\alpha} \tag{3.5}$$

satisfies the N^2-dimensional QYBE with multi-indices $A=(a_1,a_0)$, $B=(b_1,b_0)$, etc. Moreover, if we define another matrix

$$\mathbf{R}'^{AB}_{CD}=\hat{R}^{-1\,\delta c_0}_{\quad b_0\alpha}Z^{b_1\alpha}_{\beta a_0}R^{a_1\beta}_{\gamma d_1}\tilde{Z}^{\gamma d_0}_{c_1\delta}, \tag{3.6}$$

then $\mathbf{R}$, $\mathbf{R}'$ satisfy the mixed QYBEs,

$$\mathbf{R}'_{12}\mathbf{R}_{13}\mathbf{R}_{23}=\mathbf{R}_{23}\mathbf{R}_{13}\mathbf{R}'_{12}, \quad \mathbf{R}_{12}\mathbf{R}_{13}\mathbf{R}'_{23}=\mathbf{R}'_{23}\mathbf{R}_{13}\mathbf{R}_{12} \tag{3.7}$$

and the relations

$$(\mathbf{PR}+1)(\mathbf{PR}'-1)=(\mathbf{PR}'-1)(\mathbf{PR}+1)=0. \tag{3.8}$$

Proof: Recall that $\hat{R}$ is given by (3.3), then the fact that $\mathbf{R}$ satisfies QYBE and $\{\mathbf{R},\mathbf{R}'\}$ satisfy Eqs. (3.7) can be verified directly by writing them in terms of R, Z and using relations (2.1) and Proposition 2.1 repeatedly. As for the relations (3.8), we shall equivalently show $\mathbf{PRPR}'=\mathbf{PR}'\mathbf{PR}=\mathbf{PR}-\mathbf{PR}'+1$. From (3.5), (3.6) we have

$$\begin{aligned}(\mathbf{PRPR}')^{AB}_{EF}&=\mathbf{R}^{BA}_{DC}\mathbf{R}'^{CD}_{EF}\\&=\hat{R}^{d_0\alpha}_{\beta a_0}Z^{a_1\beta}_{\gamma b_0}R^{b_1\gamma}_{\delta c_1}\tilde{Z}^{\delta c_0}_{d_1\alpha}\hat{R}^{-1}{}^{\delta' e_0}_{d_0\alpha'}Z^{d_1\alpha'}_{\beta' c_0}R^{c_1\beta'}_{\gamma' f_1}\tilde{Z}^{\gamma' f_0}_{e_1\delta'}\\&=\hat{R}^{d_0\alpha}_{\beta a_0}Z^{a_1\beta}_{\gamma b_0}R^{b_1\gamma}_{\delta c_1}\hat{R}^{-1}{}^{\delta' e_0}_{d_0\alpha}R^{c_1\delta}_{\gamma' f_1}\tilde{Z}^{\gamma' f_0}_{e_1\delta'}=\delta^{e_0}_{a_0}Z^{a_1\beta}_{\gamma b_0}R^{b_1\gamma}_{\delta c_1}R^{c_1\delta}_{\gamma' f_1}\tilde{Z}^{\gamma' f_0}_{e_1\beta},\end{aligned}$$

$$\begin{aligned}(\mathbf{PR}'\mathbf{PR})^{AB}_{EF}&=\mathbf{R}'^{BA}_{DC}\mathbf{R}^{CD}_{EF}\\&=\hat{R}^{-1}{}^{\delta d_0}_{a_0\alpha}Z^{a_1\alpha}_{\beta b_0}R^{b_1\beta}_{\gamma c_1}\tilde{Z}^{\gamma c_0}_{d_1\delta}\hat{R}^{e_0\alpha'}_{\beta' d_0}Z^{d_1\beta'}_{\gamma' c_0}R^{c_1\gamma'}_{\delta' f_1}\tilde{Z}^{\delta' f_0}_{e_1\alpha'}\\&=\hat{R}^{-1}{}^{\delta d_0}_{a_0\alpha}Z^{a_1\alpha}_{\beta b_0}R^{b_1\beta}_{\gamma c_1}\hat{R}^{e_0\alpha'}_{\delta d_0}R^{c_1\gamma}_{\delta' f_1}\tilde{Z}^{\delta' f_0}_{e_1\alpha'}=\delta^{e_0}_{a_0}Z^{a_1\alpha}_{\beta b_0}R^{b_1\beta}_{\gamma c_1}R^{c_1\gamma}_{\delta' f_1}\tilde{Z}^{\delta' f_0}_{e_1\alpha}.\end{aligned}$$

By using the Hecke property of R and Proposition 2.2, we can further have

$$(\mathbf{PRPR}')^{AB}_{EF}=\delta^{e_0}_{a_0}Z^{a_1\beta}_{\gamma b_0}(\delta^{\gamma}_{\gamma'}\delta^{b_1}_{f_1}+\lambda P^{\gamma b_1}_{c_1\delta}R^{c_1\delta}_{\gamma' f_1})\tilde{Z}^{\gamma' f_0}_{e_1\beta}=\delta^{AB}_{EF}+\lambda\,\delta^{e_0}_{a_0}Z^{a_1\beta}_{\gamma b_0}R^{b_1\gamma}_{\gamma' f_1}\tilde{Z}^{\gamma' f_0}_{e_1\beta},$$

$$\begin{aligned}(\mathbf{PR})^{AB}_{EF}-(\mathbf{PR}')^{AB}_{EF}&=(\hat{R}^{e_0\alpha}_{\beta a_0}-\hat{R}^{-1}{}^{\alpha e_0}_{a_0\beta})Z^{a_1\beta}_{\gamma b_0}R^{b_1\gamma}_{\delta f_1}\tilde{Z}^{\delta f_0}_{e_1\alpha}\\&=\lambda\,\delta^{e_0}_{a_0}\delta^{\alpha}_{\beta}Z^{a_1\beta}_{\gamma b_0}R^{b_1\gamma}_{\delta f_1}\tilde{Z}^{\delta f_0}_{e_1\alpha}=\lambda\,\delta^{e_0}_{a_0}Z^{a_1\alpha}_{\gamma b_0}R^{b_1\gamma}_{\delta f_1}\tilde{Z}^{\delta f_0}_{e_1\alpha}.\end{aligned}$$

Hence, (3.8) is satisfied. □

In terms of $\mathbf{R}$, $\mathbf{R}'$ and from Lemma 3.4, we have the following:

Proposition 3.5: Introducing the notation $T_A=T^{a_0}_{a_1}$, then the algebra relation (2.2) and braiding relation (3.2) can be rewritten, respectively, as

$$T_AT_B=T_DT_C\mathbf{R}'^{CD}_{AB}, \tag{3.9}$$

$$\underline{\Psi}(T_A\otimes T_B)=T_D\otimes T_C\mathbf{R}^{CD}_{AB}. \tag{3.10}$$

Moreover, on the algebra given by the relation (3.9) one can express the (additive) coproduct $\underline{\Delta}$, counit $\underline{\varepsilon}$ and braided-antipode $\underline{S}$ as

$$\underline{\Delta}T_A=T_A\otimes 1+1\otimes T_A, \quad \underline{\varepsilon}T_A=0, \quad \underline{S}T_A=-T_A, \tag{3.11}$$

which form a braided-Hopf algebra with braiding (3.10).

Proof: The equivalence of the algebra relation (2.2) with (3.9), the braiding (3.2) with (3.10) can be verified by direct calculations, in these processes the existence of R^{-1}, Z^{-1}, and $\tilde{Z}$ is crucial. From Lemma 3.4, the second part of the Proposition can be obtained by following the results of Majid in Ref. 16. This is a restatement of Theorem 3.1 in braided vector form. □

When some suitable restrictions are imposed on the R-matrix pair (R,Z), we can obtain some special cases of the above results. For examples, when $Z=I$, R is a regular solution of QYBE, then Theorem 3.1, Propositions 3.3, 3.5 reduce to the corresponding results for the ordinary (non-braided) quantum matrices;[15] When $Z=R$, the Proposition 3.5 gives the related results for the (nonquantized) braided matrices.[14] So the results here can be regarded as a generalization and unification of the results for quantum and braided matrices.

IV. BRAIDED DIFFERENTIALS ON THE QBM BIALGEBRAS

One of the applications of the new braided addition law in Sec. III is to introduce braided differential operators on the underlying quantized braided matrix space $A(R,Z)$. Denote $\Delta T=T\otimes 1+1\otimes T\equiv U+T$ and let $f(T)$ be a function of T, then similar to Ref. 15, the corresponding differentials

$$\partial^I\equiv\partial^{i_1}_{i_0}=\frac{\partial}{\partial T^{i_0}_{i_1}}:\quad \underline{A}(R,Z)\mapsto\underline{A}(R,Z)$$

are defined by

$$\partial^I f(T)=[T_I^{-1}(f(U+T)-f(T))]\big|_{U=0}=\text{coeff of } T_I \text{ in } f(U+T), \tag{4.1}$$

here we have the braid statistics $T_1Z_{12}U_2=\hat{R}_{12}U_2Z_{21}T_1R_{12}$ from (3.2). In terms of $\mathbf{R}$, $\mathbf{R}'$ introduced in Sec. III, the algebra of $\{\partial^I\}$ can be constructed explicitly following Ref. 17.

Proposition 4.1: The braided differential operators $\partial=\{\partial^{i_1}_{i_0}\}$ (written as a matrix) form a braided-Hopf algebra with the relations,

$$R_{21}\partial_1\tilde{Z}_{21}\partial_2=\partial_2\tilde{Z}_{12}\partial_1\hat{R}_{12},\quad \underline{\Psi}(\partial_1\otimes\tilde{Z}_{21}\partial_2)=R_{12}\partial_2\otimes\tilde{Z}_{12}\partial_1\hat{R}_{12}, \tag{4.2}$$

$$\underline{\Delta}(\partial)=\partial\otimes 1+1\otimes\partial,\quad \underline{\varepsilon}(\partial)=0,\quad \underline{S}(\partial)=-\partial. \tag{4.3}$$

Proof: Here, it is convenient to use the formula associated to the data in Lemma 3.4 and Proposition 3.5. Following Ref. 17, the braided derivatives obey the braided vector algebra relations and braidings

$$\partial^I\partial^J=\mathbf{R}'^{IJ}_{AB}\partial^B\partial^A,\quad \underline{\Psi}(\partial^I\otimes\partial^J)=\mathbf{R}^{IJ}_{AB}\partial^B\otimes\partial^A \tag{4.4}$$

for $\mathbf{R}$ and $\mathbf{R}'$ in (3.5) and (3.6). These form a braided-Hopf algebra with the operations in (4.3). Writing out (4.4) in terms of R, Z, then by some calculations we obtain explicit relations and braidings in (4.2). □

We point out that the braided-Hopf algebra given by (4.2), (4.3) as well as one given in Theorem 3.1 both are special cases of some more general braided-Hopf algebra given in Sec. VI later.

Next we mention the corresponding braided Heisenberg–Weyl algebra. the general scheme in Ref. 17 gives the relations

$$\partial^I T_J-T_A\mathbf{R}^{AI}_{JB}\partial^B=\delta^I_J, \tag{4.5}$$

in our case these are

$$\partial^{i_1}_{i_0}T^{j_0}_{j_1}-\hat{R}^{j_0\alpha}_{\beta i_0}Z^{i_1\beta}_{\gamma a_0}T^{a_0}_{a_1}R^{a_1\gamma}_{\delta b_1}\partial^{b_1}_{b_0}\tilde{Z}^{\delta b_0}_{j_1\alpha}=\delta^{i_1}_{j_1}\delta^{j_0}_{i_0}, \tag{4.6}$$

which is the algebra of (R,Z)-quantum mechanics generated by the quantized braided ''momenta'' $\partial^{i_1}_{i_0}$ acting on the quantized braided coordinate functions $T^{j_0}_{j_1}$.

For the special case $Z=I$, Proposition 4.1 and relations (4.6) are reduced to the corresponding results related (nonbraided) quantum matrices.[15]

V. EXAMPLE

To illustrate the formulas in Secs. III and IV, here we give an example.

Taking

$$R=\begin{pmatrix} q & 0 & 0 & 0 \\ 0 & 1 & \lambda & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & q \end{pmatrix}, \quad Z=\begin{pmatrix} r & 0 & 0 & 0 \\ 0 & u & 0 & 0 \\ 0 & 0 & v & 0 \\ 0 & 0 & 0 & w \end{pmatrix}, \tag{5.1}$$

$$T=\begin{pmatrix} \mathrm{a} & \mathrm{b} \\ \mathrm{c} & \mathrm{d} \end{pmatrix}, \quad \lambda=q-q^{-1}, \quad ruvw\neq 0,$$

then from (2.2) and (3.2), the corresponding $\underline{A}(R,Z)$ has the algbra relations

$$\begin{gathered} v\,\mathrm{ba}=qr\,\mathrm{ab}, \quad r\,\mathrm{ca}=qv\,\mathrm{ac}, \quad ur\,\mathrm{cb}=vw\,\mathrm{bc}, \\ u\,\mathrm{db}=qw\,\mathrm{bd}, \quad w\,\mathrm{dc}=qu\,\mathrm{cd}, \quad \mathrm{da}=\mathrm{ad}+\lambda v^{-1} r\,\mathrm{cb}, \end{gathered} \tag{5.2}$$

and the braidings

$$\begin{gathered} \underline{\Psi}(\mathrm{a}\otimes\mathrm{a})=q^2\mathrm{a}\otimes\mathrm{a}, \quad \underline{\Psi}(\mathrm{a}\otimes\mathrm{b})=q(v/r)\mathrm{b}\otimes\mathrm{a}, \quad \underline{\Psi}(\mathrm{a}\otimes\mathrm{c})=q(r/v)\mathrm{c}\otimes\mathrm{a}, \\ \underline{\Psi}(\mathrm{a}\otimes\mathrm{d})=\mathrm{d}\otimes\mathrm{a}, \quad \underline{\Psi}(\mathrm{b}\otimes\mathrm{a})=q(r/v)\mathrm{a}\otimes\mathrm{b}+q\lambda\,\mathrm{b}\otimes\mathrm{a}, \quad \underline{\Psi}(\mathrm{b}\otimes\mathrm{b})=q^2\mathrm{b}\otimes\mathrm{b}, \\ \underline{\Psi}(\mathrm{b}\otimes\mathrm{c})=(ur/vw)\mathrm{c}\otimes\mathrm{b}+\lambda(u/w)\mathrm{d}\otimes\mathrm{a}, \quad \underline{\Psi}(\mathrm{b}\otimes\mathrm{d})=q(u/w)\mathrm{d}\otimes\mathrm{b}, \\ \underline{\Psi}(\mathrm{c}\otimes\mathrm{a})=q\lambda\,\mathrm{c}\otimes\mathrm{a}+q(u/r)\mathrm{a}\otimes\mathrm{c}, \\ \underline{\Psi}(\mathrm{c}\otimes\mathrm{b})=(vw/ur)\mathrm{b}\otimes\mathrm{c}+\lambda(v/r)\mathrm{d}\otimes\mathrm{a}, \\ \underline{\Psi}(\mathrm{c}\otimes\mathrm{d})=q(w/u)\mathrm{d}\otimes\mathrm{c}, \quad \underline{\Psi}(\mathrm{d}\otimes\mathrm{a})=\mathrm{a}\otimes\mathrm{d}+\lambda^2\mathrm{d}\otimes\mathrm{a}+\lambda(w/u)\mathrm{b}\otimes\mathrm{c}+\lambda(r/v)\mathrm{c}\otimes\mathrm{b}, \\ \underline{\Psi}(\mathrm{d}\otimes\mathrm{b})=q(w/u)\mathrm{b}\otimes\mathrm{d}+q\lambda\,\mathrm{d}\otimes\mathrm{b}, \quad \underline{\Psi}(\mathrm{c}\otimes\mathrm{c})=q^2\mathrm{c}\otimes\mathrm{c}, \\ \underline{\Psi}(\mathrm{d}\otimes\mathrm{c})=q(u/w)\mathrm{c}\otimes\mathrm{d}+q\lambda\,\mathrm{d}\otimes\mathrm{c}, \quad \underline{\Psi}(\mathrm{d}\otimes\mathrm{d})=q^2\mathrm{d}\otimes\mathrm{d}. \end{gathered} \tag{5.3}$$

Then $\tilde{\mathrm{a}}=\mathrm{a}\otimes 1+1\otimes\mathrm{a}$, $\tilde{\mathrm{b}}=\mathrm{b}\otimes 1+1\otimes\mathrm{b}$, $\tilde{\mathrm{c}}=\mathrm{c}\otimes 1+1\otimes\mathrm{c}$, $\tilde{\mathrm{d}}=\mathrm{d}\otimes 1+1\otimes\mathrm{d}$ satisfy the same relations as a, b, c, d do in (5.2).

Moreover, denoting the related differential operators by

$$\partial=\begin{pmatrix} \partial_a & \partial_b \\ \partial_c & \partial_d \end{pmatrix},$$

then formulas (4.2) give the relations

$$\begin{gathered} v\,\partial_a\partial_b=qr\,\partial_b\partial_a, \quad r\,\partial_a\partial_c=qv\,\partial_c\partial_a, \quad ur\,\partial_b\partial_c=vw\,\partial_c\partial_b, \\ u\,\partial_b\partial_d=qw\,\partial_d\partial_b, \quad w\,\partial_c\partial_d=qu\,\partial_d\partial_c, \quad \partial_a\partial_d=\partial_d\partial_a+\lambda r^{-1} v\,\partial_c\partial_b \end{gathered} \tag{5.4}$$

and braidings

$$\underline{\Psi}(\partial_a\otimes\partial_a)=q^2\partial_a\otimes\partial_a,\quad \underline{\Psi}(\partial_a\otimes\partial_b)=qrv^{-1}\partial_b\otimes\partial_a+q\lambda\partial_a\otimes\partial_b,$$

$$\underline{\Psi}(\partial_a\otimes\partial_c)=qvr^{-1}\partial_c\otimes\partial_a+q\lambda\partial_a\otimes\partial_c,\quad \underline{\Psi}(\partial_b\otimes\partial_a)=q(v/r)\partial_a\otimes\partial_b,$$

$$\underline{\Psi}(\partial_a\otimes\partial_d)=\partial_d\otimes\partial_a+\lambda^2\partial_a\otimes\partial_d+\lambda(v/r)\partial_d\otimes\partial_b+\lambda(u/w)\partial_b\otimes\partial_c,$$

$$\underline{\Psi}(\partial_b\otimes\partial_b)=q^2\partial_b\otimes\partial_b,\quad \underline{\Psi}(\partial_b\otimes\partial_c)=(vw/ur)\partial_c\otimes\partial_b+\lambda(w/u)\partial_a\otimes\partial_d,$$

$$\underline{\Psi}(\partial_b\otimes\partial_d)=q(w/u)\partial_d\otimes\partial_b+q\lambda\partial_b\otimes\partial_d,\quad \underline{\Psi}(\partial_c\otimes\partial_a)=q(r/v)\partial_a\otimes\partial_c, \tag{5.5}$$

$$\underline{\Psi}(\partial_c\otimes\partial_b)=(ru/vw)\partial_b\otimes\partial_c+\lambda(r/v)\partial_a\otimes\partial_d,\quad \underline{\Psi}(\partial_c\otimes\partial_c)=q^2\partial_c\otimes\partial_c,$$

$$\underline{\Psi}(\partial_c\otimes\partial_d)=q(u/w)\partial_d\otimes\partial_c+q\lambda\partial_c\otimes\partial_d,\quad \underline{\Psi}(\partial_d\otimes\partial_a)=\partial_a\otimes\partial_d,$$

$$\underline{\Psi}(\partial_d\otimes\partial_b)=q(u/w)\partial_b\otimes\partial_d,\quad \underline{\Psi}(\partial_d\otimes\partial_c)=q(w/u)\partial_c\otimes\partial_d,$$

$$\underline{\Psi}(\partial_d\otimes\partial_d)=q^2\partial_d\otimes\partial_d.$$

The corresponding Heisenberg–Weyl algebra can also be obtained from (4.6) by some tedious but straightforward calculations which will not be given here for saving space.

The above results contain 2-dim superquantum matrices as special cases and when $r=u=v=w=1$, these reduce to the results about $M_q(2)$ in Ref. 15.

VI. SOME FURTHER GENERALIZED RESULTS

in this section we show that the braided coaddition can even be introduced on some more general quantized (matrix) algebras. For certain special case, they recover the results in Sec. III. Moreover, the braided-Hopf algebra generated by $\{\partial^{i_1}_{i_0}\}$ in Proposition 4.1 is also an example of the extended algebra in this section.

Definition 6.1: Consider an ordered sequence of three numerical matrices Q, R, $Z\in M_N\otimes M_N$, if Q, R are invertible solutions of QYBE and Z satisfies the following mixed QYBEs:

$$Z_{12}Z_{13}Q_{23}=Q_{23}Z_{13}Z_{12},\quad R_{12}Z_{13}Z_{23}=Z_{23}Z_{13}R_{12}, \tag{6.1}$$

then we call the sequence an *R-matrix triple* and denote it by (Q,R,Z).

Theorem 6.2: Let (Q,R,Z) be an R-matrix triple, let also Q, R be Hecke-type and Z have the second inverse $\tilde{Z}$. Then a braided-Hopf algebra $A(Q,R,Z)$ can be constructed as follows:

$\underline{A}(Q,R,Z)$ is generated by $T=\{T^i_j\}^N_{i,j=1}$ and $\overline{1}$ with the algebra relations

$$Q_{21}T_1Z_{12}T_2=T_2Z_{21}T_1R_{12}, \tag{6.2}$$

the (additive) coproduct, counit and braided antipode

$$\underline{\Delta}(T)=T\otimes 1+1\otimes T,\quad \underline{\varepsilon}(T)=0,\quad \underline{S}(T)=-T, \tag{6.3}$$

and the braiding

$$\underline{\Psi}(T_1\otimes Z_{12}T_2)=Q_{12}T_2\otimes Z_{21}T_1R_{12}. \tag{6.4}$$

Proof: The fact that (6.2) can consistently define an associative algebra has been pointed out by Friedel and Maillet[18] in some more general form. The remainder part of the theorem can be

verified by a way similar to the proof of Theorem 3.1. For example, the coproduct Δ in (6.3) can be consistently extended to products of generators as a algebra homomorphism with the braided tensor product, this can be shown by the following calculations:

$$\begin{aligned}\underline{\Delta}(Q_{21}T_1Z_{12}T_2)&=Q_{21}(T_1\otimes 1+1\otimes T_1)Z_{12}(T_2\otimes 1+1\otimes T_2)\\&=Q_{21}T_1Z_{12}T_2\otimes 1+Q_{21}T_1Z_{12}\otimes T_2+Q_{21}Q_{12}T_2Z_{21}\otimes T_1R_{12}+1\otimes Q_{21}T_1Z_{12}T_2\\&=Q_{21}T_1Z_{12}T_2\otimes 1+Q_{21}T_1Z_{12}\otimes T_2+(1+\lambda P_{12}Q_{12})T_2Z_{21}\otimes T_1R_{12}\\&\quad+1\otimes Q_{21}T_1Z_{12}T_2;\end{aligned}$$

$$\begin{aligned}\underline{\Delta}(T_2Z_{21}T_1R_{12})&=(T_2\otimes 1+1\otimes T_2)Z_{21}(T_1\otimes 1+1\otimes T_1)R_{12}\\&=T_2Z_{21}T_1R_{12}\otimes 1+T_2Z_{21}\otimes T_1R_{12}+Q_{21}T_1Z_{12}\otimes T_2R_{21}R_{12}+1\otimes T_2Z_{21}T_1R_{12}\\&=T_2Z_{21}T_1R_{12}\otimes 1+T_2Z_{21}\otimes T_1R_{12}+Q_{21}T_1Z_{12}\otimes T_2(1+\lambda P_{12}R_{12})\\&\quad+1\otimes T_2Z_{21}T_1R_{12},\end{aligned}$$

where we have used the braiding (6.4) and the Hecke property of Q, R. The verifications of the consistency for $\underline{\Psi}$, $\underline{S}$, $\underline{\varepsilon}$ in (6.4), (6.3) are omitted because of their similarity to that for Theorem 3.1. □

We would like to point out that the results in Lemma 3.4 and Proposition 3.5 can also be extended to $A(Q,R,Z)$. By the calculations similar to Sec. III, we have

Proposition 6.3: Let (Q,R,Z) be an R-matrix triple and satisfy the conditions in Theorem 6.2. Now defining

$$\mathbf{Q}^{AB}_{CD}=Q^{c_0\alpha}_{\beta b_0}Z^{b_1\beta}_{\gamma a_0}R^{a_1\gamma}_{\delta d_1}\tilde{Z}^{\delta d_0}_{c_1\alpha},\quad \mathbf{Q}'^{AB}_{CD}=Q^{-1\,\delta c_0}_{\quad b_0\alpha}Z^{b_1\alpha}_{\beta a_0}R^{a_1\beta}_{\gamma d_1}\tilde{Z}^{\gamma d_0}_{c_1\delta},\tag{6.5}$$

then they satisfy the following equations:

$$\begin{gathered}\mathbf{Q}_{12}\mathbf{Q}_{13}\mathbf{Q}_{23}=\mathbf{Q}_{23}\mathbf{Q}_{13}\mathbf{Q}_{12},\quad \mathbf{Q}'_{12}\mathbf{Q}_{13}\mathbf{Q}_{23}=\mathbf{Q}_{23}\mathbf{Q}_{13}\mathbf{Q}'_{12},\quad \mathbf{Q}_{12}\mathbf{Q}_{13}\mathbf{Q}'_{23}=\mathbf{Q}'_{23}\mathbf{Q}_{13}\mathbf{Q}_{12},\\(\mathbf{PQ}+1)(\mathbf{PQ}'-1)=(\mathbf{PQ}'-1)(\mathbf{PQ}+1)=0.\end{gathered}\tag{6.6}$$

Moreover, the relations

$$\begin{gathered}T_AT_B=T_DT_C\mathbf{Q}'^{CD}_{AB},\quad \underline{\Psi}(T_A\otimes T_B)=T_D\otimes T_C\mathbf{Q}^{CD}_{AB},\\\underline{\Delta}T_A=T_A\otimes 1+1\otimes T_A,\quad \underline{\varepsilon}T_A=0,\quad \underline{S}T_A=-T_A\end{gathered}\tag{6.7}$$

give a covecter braided group[16] version of $A(Q,R,Z)$.

Proof: The proof is similar to that of Lemma 3.4 and Proposition 3.5, and will be omitted. □

As done in Sec. IV, the corresponding braided differential calculus and braided Heisenberg–Weyl algebra, etc. can also be constructed. If we require Z to be a regular solution of QYBE and Q to be taken as $Q=\hat{R}=ZPRZ^{-1}P$, then the results here are reduced to the ones of Secs. III and IV. Moreover, we point out that the braided differential operator Hopf algebra in Proposition 4.1 can also be regarded as a special case of $A(Q,R,Z)$ as long as we take $T=\partial$ (as a matrix) and take the related R-matrix triple as $(R,\hat{R},P\tilde{Z}P)$. That the triple $(R,\hat{R},P\tilde{Z}P)$ is indeed an R-matrix triple as required in Theorem 6.2 can be verified from the relations obeyed by the original R, Z.

VII. CONCLUSIONS AND DISCUSSIONS

Besides the usual (multiplicative) coproduct, we have introduced another kind of (additive) coproduct on the QBMs. With this so-called braided coaddition, the QBMs acquire a braided-Hopf algebra structure. We also show that these two coproducts together make QBM a quantized-braided ring, which is an analog of the ordinary matrix ring. Motivated by Ref. 15, we then construct the corresponding differential operator bialgebras (braided Hopf algebras) acting on QBMs and the related quantized braided Heisenberg–Weyl algebras, which can be regarded as a mathematical description of some multiparameter deformed quantum systems with general braid statistics.

The discussions of this paper extend the related schemes for braided matrices[14] and quantum matrices[15] to a more general one and unify these different results into a *single* structure. Moreover, we find that the braided coaddition and differentiation operations can be introduced on some further generalized algebraic systems. When taking some special cases, the related results in Refs. 14 and 15 are recovered, respectively. In Sec. V a simple but genuine quantized braided example is given, other examples can be obtained by taking some specified R-matrix pair (R,Z), see, e.g., Refs. 12, 10, etc.

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Bounded solutions of a second order evolution equation and applications

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In this paper we study the following abstract second order differential equation with dissipation in a Hilbert space H: $u''+cu'+dA\,u+kG(u)=P(t)$, $u\in H$, $t\in\mathbb{R}$, where c, d and k are positive constants, $G:H\to H$ is a Lipschitzian function and $P:\mathbb{R}\to H$ is a continuous and bounded function. $A:D(A)\subset H\to H$ is an unbounded linear operator which is self-adjoint, positive definite and has compact resolvent. Under these conditions we prove that for some values of d, c and k this system has a bounded solution which is exponentially asymptotically stable. Moreover; if $P(t)$ is almost periodic, then this bounded solution is also almost periodic. These results are applied to a very well known second order system partial differential equations; such as the sine-Gordon equation, The suspension bridge equation proposed by Lazer and McKenna, etc. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In this paper, we study the existence and the asymptotic behavior of the bounded solutions of the following abstract second order differential equation with dissipation:

$$u''+cu'+dAu+kG(u)=P(t),\quad u\in H,\quad t\in\mathbb{R}, \tag{1.1}$$

where H is a Hilbert space, c, d and k are positive constants, $P:\mathbb{R}\to H$ is a continuous and bounded function and $G:H\to H$ is a Lipschitzian function, i.e., there exists $L>0$ such that

$$\|G(U_1)-G(U_2)\|\leqslant L\|U_1-U_2\|,\quad U_1,U_2\in H. \tag{1.2}$$

$A:D(A)\subset H\to H$ is an unbounded linear operator, self-adjoint, positive definite and has compact resolvent. Under these conditions stated on A we have the following.

The spectrum $\sigma(A)$ of A consisting of isolated eigenvalues,

$$0<\lambda_1<\lambda_2<\ldots<\lambda_n\to\infty,$$

each one with finite multiplicity γ_j equal to the dimension of the corresponding eigenspace and the following.

(a) There exists a complete orthonormal set $\{\phi_{j,k}\}$ of eigenvector of A in H.
(b) For all $x\in D(A)$ we have

$$Ax=\sum_{j=1}^{\infty}\lambda_j\sum_{k=1}^{\gamma_j}\langle x,\phi_{j,k}\rangle\phi_{j,k}=\sum_{j=1}^{\infty}\lambda_jE_jx, \tag{1.3}$$

where $\langle\cdot,\cdot\rangle$ is the inner product in H and

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$$E_j x = \sum_{k=1}^{\gamma_j} <x, \phi_{j,k}> \phi_{j,k}.$$

So, $\{E_j\}$ is a family of complete orthogonal projections in H and

$$x = \sum_{j=1}^{\infty} E_j x, \quad x \in H.$$

(c) $-A$ generates an analytic semigroup $\{e^{-At}\}$ given by

$$e^{-At}x = \sum_{j=1}^{\infty} e^{-\lambda_j t} E_j x, \quad x \in H.$$

Many very well known systems of partial differential equations can be written in the form of system (1.1).

Example 1.1: The sine-Gordon Equation with Dirichlet boundary conditions,

$$\begin{cases} U_{tt} + cU_t - dU_{xx} + k \sin U = p(t,x), \quad 0 < x < l, \quad t \in \mathbb{R}, \\ U(t,0) = U(t,l) = 0, \quad t \in \mathbb{R}, \end{cases} \tag{1.4}$$

where c and k are positive constants, $p: \mathbb{R} \times [0,l] \to \mathbb{R}$ is continuous and bounded. In this case we take: $H = L^2(0,l)$ and $A\phi = -\phi_{xx}$ with domain $D(A) = H^2 \cap H_0^1$. $G(u) = \sin u$ and $P(t) = p(t,\cdot)$

Example 1.2: The suspension bridge model proposed by Lazer and McKenna (see Refs. 1 and 2),

$$\begin{cases} U_{tt} + cU_t + dU_{xxxx} + kU^+ = p(t,x), \quad 0 < x < l, \quad t \in \mathbb{R}, \\ U(t,0) = U(t,l) = U_{xx}(t,0) = U_{xx}(t,l) = 0, \quad t \in \mathbb{R}, \end{cases} \tag{1.5}$$

where c, d and k are positive constants, $p: \mathbb{R} \times [0,l] \to \mathbb{R}$ is continuous and bounded. In this case we take $H = L^2(0,l)$ and $A\phi = -\phi_{xxxx}$ with domain

$$D(A) = \{\phi \in H : \phi_{xxxx} \in H; \phi(0) = \phi(l) = \phi_{xx}(0) = \phi_{xx}(l) = 0\}.$$

$G(U) = U^+$ and $P(t) = p(t,\cdot)$.

Example 1.3: We consider a system of sine-Gordon equations occurring in the Josephson junctions (see Levi[3]),

$$\begin{cases} U_{tt} + cU_t - d\Delta U + k \sin U + k(U - V) = p_1(t,x), \\ V_{tt} + cV_t - d\Delta V + k \sin V + k(V - U) = p_2(t,x), \\ U(t,x) = V(t,x) = 0 \quad \text{on} \quad \partial\Omega \times \mathbb{R}, \end{cases} \tag{1.6}$$

where Ω is a smooth bounded domain in $\mathbb{R}^n$. In this case we take $H = L^2(\Omega) \times L^2(\Omega)$, $A(\phi_1, \phi_2) = (-\Delta\phi_1, -\Delta\phi_2)$ with domain $D(A) = (H_0^1(\Omega) \cap H^2(\Omega))^2$.

A finite dimensional version of the system (1.1) ($H = \mathbb{R}^n$ and an $A - n \times n$ matrix) has been studied in Refs. 4, 5 and 6, where they proved the existence of a bounded solution of this equation, which is exponentially stable, and applied those results to the spatial discretization of the systems (1.4) and (1.5). For an infinite dimensional second order evolution equation we can see Ref. 7, where they study the existence of bounded solutions for the telegraph equation. Here we study the existence, the stability, the almost-periodicity and the smoothness (classic solution) of the bounded solution. Specifically, we prove the following theorem.

Theorem 1.1: *If G and P are of C^1 class and for some c, d y k we have that*

$$\mathrm{Re}\left\{\frac{c\pm\sqrt{c^2-4\,d\lambda_j}}{2}\right\}>kL,\quad j=1,2,3,\ldots, \tag{1.7}$$

then (1.1) has one and only one bounded solution $u(t)$ defined on $\mathbb{R}$, i.e.,

$$\sup_{t\in\mathbb{R}}\{\|u(t)\|^2+\|\dot{u}(t)\|^2\}<\infty.$$

Moreover, this bounded solution is the only bounded solution of the equation (1.1) and is exponentially stable, and if $P(t)$ is almost periodic, then $u(t)$ is also almost periodic.

The criterion for almost-periodicity of a **bounded** solution of first and second order Cauchy problem are given in Ref. 8, Theorems 4.3 and 4.5. But, the existence of the bounded solutions is not considered there. On the other hand, our method is very simple, we just rewrite the equation (1.1) as a first order system of abstract ordinary differential equations. Next, we prove that the linear part of this equation generates a C_0-group which decays exponentially to zero. After that, we find a formula for the **mild** bounded solution of this system. From this formula we can prove the existence, the stability and the almost-periodicity of the **mild** bounded solution easily. Finally, we prove that this mild bounded solution is a classic solution of (1.1); that is to say, we prove the smoothness of the bounded solution (see Theorem 3.2).

II. PRELIMINARY RESULTS

Before we prove the main theorems of this paper, we shall prove some preliminary results to be used in the next section. The equation (1.1) can be rewritten as a first order system of ordinary differential equations in the space $W=H\times H$ as follows:

$$w'+\mathcal{A}w+k\mathcal{G}(w)=\mathcal{P}(t),\quad w\in W,\quad t\in\mathbb{R}, \tag{2.1}$$

where $v=u'$ and

$$w=\begin{pmatrix}u\\ v\end{pmatrix},\ \mathcal{G}=\begin{pmatrix}0\\ G(u)\end{pmatrix},\ \mathcal{P}=\begin{pmatrix}0\\ P(t)\end{pmatrix}\quad\text{and}\quad \mathcal{A}=\begin{pmatrix}0 & -I_H\\ dA & cI_H\end{pmatrix}, \tag{2.2}$$

is an unbounded linear operator with domain $D(\mathcal{A})=D(A)\times H$.

In this section we shall study the linear part of the equation (2.1); that is to say, the equation

$$w'+\mathcal{A}w=0,\ w\in W,\ t\in\mathbb{R}. \tag{2.3}$$

To this end, we shall define the following family of a complete orthogonal family of projections in W:

$$\hat{E}_j=\begin{pmatrix}E_j & 0\\ 0 & E_j\end{pmatrix},\quad j=1,2,\ldots, \tag{2.4}$$

and consider the family of 2×2 matrices,

$$B_j=\begin{pmatrix}0 & -1\\ d\lambda_j & c\end{pmatrix}. \tag{2.5}$$

Then, from (1.3) we get that

$$\mathcal{A}w=\sum_{j=1}^{\infty}B_j\hat{E}_jw,\ w\in D(\mathcal{A}). \tag{2.6}$$

On the other hand, the eigenvalues of the matrix B_j are given by

$$\rho(j)=\frac{c\pm\sqrt{c^2-4\,d\lambda_j}}{2},\quad j=1,2,\ldots, \tag{2.7}$$

which are simple if $c\neq=2\sqrt{d\lambda_j},\quad j=1,2,\ldots$.

The following Theorem can be proved in a similiar way as Theorem 2.1 in the following.

Theorem 2.1: *Suppose that* $c\neq 2\sqrt{d\lambda_j}$, $j=1,2,\ldots$. *Then: we have the following.*

(a) The operator $-\mathcal{A}$ *generates a* C_0*-group* $e^{-\mathcal{A}t}$ *given by*

$$e^{-\mathcal{A}t}w=\sum_{j=1}^{\infty} e^{-B_j t}\hat{E}_j w w\in W,\ \ t\in\mathbb{R}. \tag{2.8}$$

(b) The spectrum $\sigma(-\mathcal{A})$ *of* $-\mathcal{A}$ *is given by*

$$\sigma(-\mathcal{A})=\left\{\frac{-c\pm\sqrt{c^2-4\,d\lambda_j}}{2},\quad j=1,2,\ldots\right\}.$$

(c) We have the following estimates:

$$\|e^{-\mathcal{A}t}\|\leqslant e^{-\beta t},\quad t\geqslant 0, \tag{2.9}$$

$$\|e^{-\mathcal{A}t}\|\leqslant e^{-\alpha t},\quad t\leqslant 0, \tag{2.10}$$

where α, β *are positive numbers and*

$$-\beta=-\beta(c,d)=\max\left\{\mathrm{Re}(\rho_j)=\mathrm{Re}\left(\frac{-c\pm\sqrt{c^2-4\,d\lambda_j}}{2}\right):j=1,2,\ldots,i=1,2\right\},$$

$$-\alpha=-\alpha(c,d)=\min\left\{\mathrm{Re}(\rho_j)=\mathrm{Re}\left(\frac{-c\pm\sqrt{c^2-4\,d\lambda_j}}{2}\right):j=1,2,\ldots,i=1,2\right\}.$$

Corollary 2.1: The initial value problem,

$$\begin{cases} w'+\mathcal{A}w=0,\\ w(t_0)=w_0, \qquad w_0\in D(\mathcal{A}),\end{cases}$$

has the unique solution

$$w(t)=e^{-\mathcal{A}(t-t_0)}w_0=\sum_{j=1}^{\infty}\{e^{-\rho_1(j)(t-t_0)}Q_1(j)w_0+e^{-\rho_2(j)(t-t_0)}Q_2(j)w_0\}, \tag{2.11}$$

where $\{Q_i(j):i=1,2\}_{j=1}^{\infty}$ *is a complete orthogonal system of projections in* W.

III. EXISTENCE OF MILD BOUNDED SOLUTIONS

In this section we shall prove the existence of mild bounded solutions of the system (2.1), which gives us the first part of the proof of Theorem 1.1.

Definition 3.1 (mild solution): For mild solution $w(t)$ of (2.1) with initial condition $w(t_0)=w_0\in W$, we understand a function given by

$$w(t)=e^{-\mathcal{A}(t-t_0)}w_0+\int_{t_0}^{t}e^{-\mathcal{A}(t-s)}\{-k\mathcal{G}(w(s))+\mathcal{P}(s)\}ds,\quad t\in\mathbb{R}. \tag{3.1}$$

Remark 3.1: It is easy to prove that any solution of (2.1) is a solution of (3.1). It may be thought that a solution of (3.1) is always a solution of (2.1) but this is not true in general. However, we shall prove in Theorem 3.2 that bounded solutions of (3.1) are solutions of (2.1).

We shall consider $W_b = C_b(\mathbb{R}, W)$ the space of bounded and continuous functions defined in $\mathbb{R}$ taking values in $W = H \times H$. W_b is a Banach space with suprem norm

$$\|w\|_b = \sup\{\|w(t)\|_W : t \in \mathbb{R}\}, \quad w \in W_b .$$

A ball of radio $\rho > 0$ and center zero in this space is given by

$$B_\rho^b = \{w \in W_b : \|w(t)\|_b \leqslant \rho, \quad t \in \mathbb{R}\}.$$

The proof of the following lemma is similar to Lemma 3.1 of Ref. 4.

Lemma 3.1: Let w be in W_b. Then, w is a mild solution of (2.1) if and only if w is given by

$$w(t) = \int_{-\infty}^{t} e^{-\mathcal{A}(t-s)}\{-k\mathcal{G}(w(s)) + \mathcal{P}(s)\}ds, \quad t \in \mathbb{R}. \tag{3.2}$$

The following theorem refers to mild bounded solutions of system (2.1). Even though the proof is similar to Theorem 3.2 of Ref. 4, we will give the proof.

Theorem 3.1: *If for some c, d y k we have that*

$$\mathrm{Re}\left\{\frac{c \pm \sqrt{c^2 - 4\,d\lambda_j}}{2}\right\} > kL, \quad j = 1,2,3,\ldots, \tag{3.3}$$

then Eq. (2.1) has one and only one bounded mild solution $w_b(t)$.

Moreover, this bounded solution is the only bounded solution of Eq. (3.1) and is exponentially stable.

Proof: Condition 3.3 implies that for $\rho > 0$ big enough we have the following estimate:

$$0 < L_p + k\|G(0)\| = \sup_{s \in \mathbb{R}} \|P(s)\| + k\|G(0)\| < (\beta(c,d) - kL)\rho. \tag{3.4}$$

For the existence of such a solution, we shall prove that the following operator has a unique fixed point in the ball B_ρ^b, $T : B_\rho^b \to B_\rho^b$,

$$(Tw)(t) = \int_{-\infty}^{t} e^{-\mathcal{A}(t-s)}\{-k\mathcal{G}(w(s)) + \mathcal{P}(s)\}ds, \quad t \in \mathbb{R}.$$

In fact, for $w \in B_\rho^b$ we have

$$\|Tw(t)\| \leqslant \int_{-\infty}^{t} e^{-\beta(t-s)}\{kL\|w(s)\| + k\|G(0)\| + L_p\} \leqslant \frac{(kL)\rho + k\|G(0)\| + L_p}{\beta}.$$

The condition (3.4) implies that

$$kL\rho + k\|G(0)\| + L_p < \beta\rho \Leftrightarrow \frac{kL\rho + k\|G(0)\| + L_p}{\beta} < \rho.$$

Therefore, $Tw \in B_\rho^b$ for all $w \in B_\rho^b$.

Now, we shall see that T is a contraction mapping. In fact, for all $w_1, w_2 \in B_\rho^b$ we have that

$$\|Tw_1(t) - Tw_2(t)\| \leqslant \int_{-\infty}^{t} e^{-\beta(t-s)} kL\|w_1(s) - w_2(s)\|ds \leqslant \frac{kL}{\beta}\|w_1 - w_2\|_b, \quad t \in \mathbb{R}.$$

Hence,

$$\|w_1 - Tw_2\|_b \leqslant \frac{kL}{\beta}\|Tw_1 - w_2\|_b, \quad w_1, w_2 \in B_\rho^b.$$

The condition (3.4) implies that

$$0 < \beta - kL \Leftrightarrow kL < \beta \Leftrightarrow \frac{kL}{\beta} < 1.$$

Therefore, T has a unique fixed point w_b in B_ρ^b,

$$w_b(t) = (Tw_b)(t) = \int_{-\infty}^{t} e^{-\mathcal{A}(t-s)}\{-k\mathcal{G}(w_b(s)) + \mathcal{P}(s)\}ds, \quad t \in \mathbb{R}.$$

From Lemma 3.1, w_b is a bounded solution of Eq. (3.1). Since condition (3.4) holds for any $\rho > 0$ big enough independent of $kL < \beta(c,d)$, then w_b is the unique bounded solution of Eq. (3.1).

To prove that $w_b(t)$ is exponentially stable in the large, we shall consider any other solution $w(t)$ of (3.1) and consider the following estimate:

$$\|w(t) - w_b(t)\| \leqslant \left\| e^{-\mathcal{A}t}(w(0) - w_b(0)) + \int_0^t e^{-\mathcal{A}(t-s)}\{k\mathcal{G}(w(s)) - k\mathcal{G}(w_b(s))\}ds \right\|$$

$$\leqslant e^{-\beta t}\|(w(0) - w_b(0))\| + \int_0^t e^{-\beta(t-s)}kL\|w(s) - w_b(s)\|ds.$$

Then,

$$e^{\beta t}\|w(t) - w_b(t)\| \leqslant \|(w(0) - w_b(0))\| + \int_0^t e^{\beta s}kL\|w(s) - w_b(s)\|ds.$$

Hence, applying the Gronwall's inequality we obtain

$$\|w(t) - w_b(t)\| \leqslant e^{(kL_\rho - \beta)t}\|(w(0) - w_b(0))\|, \quad t \geqslant 0.$$

From (3.4) we get that $kL - \beta < 0$ and therefore $w_b(t)$ is exponentially stable in the large. □

Corollary 3.1: The bounded solution $w_b(\cdot, P)$ of (3.1) given by Theorem 3.1 depends continuously on $P \in C_b(\mathbb{R}, H)$. Moreover,

$$\|w_b(\cdot, P_1) - w_b(\cdot, P_2)\|_b \leqslant \frac{1}{\beta - kL}\|P_1 - P_2\|_b, \quad P_1, P_2 \in C_b(\mathbb{R}, H).$$

We conclude this part with the following lemma about almost-periodicity of the bounded solutions of Eq. (3.1). Although the proof is similar to the one given in Ref. 4 for Lemma 3.2, we will give it again.

Lemma 3.2: If $P(t)$ is almost periodic, then the unique bounded solution of Eq. (3.1) given by Theorem 3.1 is also almost periodic.

Proof: To prove this lemma, we shall use the following well known fact, due to Bohr. A function $f \in C(\mathbb{R}; W)$ is almost periodic (*a.p.*; according to Bohr) if and only if the Hull $H(f)$ of f is compact in the topology of uniform convergence.

Where $H(f)$ is the closure of the set of translates of f under the topology of uniform convergence,

$$H(f) = \overline{\{f_\tau : \tau \in \mathbb{R}\}}, \quad f_\tau(t) = f(t + \tau), \quad t \in \mathbb{R}.$$

Since the limit of a uniformly convergent sequence of *a.p.* functions is *a.p.*, then the set A_ρ of *a.p.* functions in the ball B_ρ^b is closed, where ρ is given by Theorem 3.1.

Claim: The contraction mapping T given in Theorem 3.1 leaves A_ρ invariant. In fact, if $w \in A_\rho$, then $f(t)=-k\mathcal{G}(w(t))+\mathcal{P}(t)$ is also an *a.p.* function. Now, consider the function

$$F(t)=(Tw)(t)=\int_{-\infty}^{t} e^{-\mathcal{A}(t-s)}\{-k\mathcal{G}(w(s))+\mathcal{P}(s)\}ds$$

$$=\int_{-\infty}^{t} e^{-\mathcal{A}(t-s)}f(s)ds, \quad t\in\mathbb{R}.$$

Then, it is enough to establish that $H(F)$ is compact in the topology of uniform convergence. Let $\{F_{\tau_k}\}$ be any sequence in $H(F)$. Since f is *a.p.* we can select from $\{f_{\tau_k}\}$ a Cauchy subsequence $\{f_{\tau_{k_j}}\}$, and we have that

$$F_{\tau_{k_j}}(t)=F(t+\tau_{k_j})=\int_{-\infty}^{t+\tau_{k_j}} e^{-\mathcal{A}(t+\tau_{k_j}-s)}f(s)ds=\int_{-\infty}^{t} e^{-\mathcal{A}(t-s)}f(s+\tau_{k_j})ds.$$

Hence,

$$\|F_{\tau_{k_j}}(t)-F_{\tau_{k_i}}(t)\|\leqslant\int_{-\infty}^{t}\|e^{-\mathcal{A}(t+-s)}\|\|f(s+\tau_{k_j})-f(s+\tau_{k_i})\|ds$$

$$\leqslant\|f_{\tau_{k_j}}-f_{\tau_{k_i}}\|_b\int_{-\infty}^{t} e^{-\beta(t-s)}\,ds=\frac{1}{\beta}\|f_{\tau_{k_j}}-f_{\tau_{k_i}}\|_b.$$

Therefore, $\{F_{\tau_{k_j}}\}$ is a Cauchy sequence. So, $H(F)$ is compact in the topology of uniform convergence, F is *a.p.* and $TA_\rho\subset A_\rho$.

Now, the unique fixed point of T in the ball B_ρ^b lies in A_ρ. Hence, the unique bounded solution $w_b(t)$ of Eq. (3.1) given in Theorem 3.1 is also almost periodic. □

A. Proof of Theorem 1.1

In this part, we shall prove that the mild bounded solution $w_b(t)$ of Eq. (2.1) is also a classic solution of this equation; that is to say, we shall prove the smoothness of this solution. With this we conclude the proof of Theorem 1.1.

Theorem 3.2: *Under the hypotheses of Theorem 3.1. If G and P are of C^1 class, then $w_b(t)$ satisfies (2.1) and*

$$w_b(\cdot)\in C_b(\mathbb{R};D(\mathcal{A})).$$

Moreover, if $w_b(t)=(u_b(t),v_b(t))^T$, then $v_b(t)=u_b'(t)$,

$$u_b\in C_b(\mathbb{R};D(A)),\quad u_b'\in C_b(\mathbb{R};D(A^{1/2})),\quad u_b''\in C_b(\mathbb{R};H),$$

and

$$u_b''+cu_b'+dAu_b+kG(u_b)=P(t),\quad t\in\mathbb{R}.$$

Proof: Define the function $F(t)=-k\mathcal{G}(w_b(t))+\mathcal{P}(t)$. Then

$$F(t)=\begin{pmatrix}0\\ f(t)\end{pmatrix},$$

where $f(t)=-kG(u_b(t))+P(t)$, $w_b(t)=(u_b(t),v_b(t))^T$ and $f\in C_b(\mathbb{R};H)$.

Now, consider the second order equation,

$$u''+cu'+dAu=f(t),\ \ u\in H,\ \ t\in\mathbb{R}. \tag{3.5}$$

Then, from Proposition 1.3 in Ref. 9, p. 182, Eq. (3.5) admits a unique solution u which satisfies

$$u\in C_b(\mathbb{R};H),\ \ u'\in C_b(\mathbb{R};H).$$

Therefore, $w(t)=(u(t),u'(t))^T$ is a bounded solution of the integral equation,

$$w(t)=e^{-\mathcal{A}(t-t_0)}w(t_0)+\int_{t_0}^{t}e^{-\mathcal{A}(t-s)}F(s)ds,\ \ t\in\mathbb{R}.$$

Then, taking limit as t_0 goes to $-\infty$, we get that

$$w(t)=\int_{-\infty}^{t}e^{-\mathcal{A}(t-s)}F(s)ds=\int_{-\infty}^{t}e^{-\mathcal{A}(t-s)}\{-k\mathcal{G}(w(s))+\mathcal{P}(s)\}ds.$$

Hence, $w_b(t)=w(t)=(u(t),u'(t))$, so

$$f(t)=-kG(u(t))+P(t)\quad\text{and}\ \ f\in C_b^1(\mathbb{R};H).$$

Then, using the second part of Proposition 1.3 in Ref. 9, p. 182, we get that

$$u\in C_b(\mathbb{R};D(A)),\ \ u'\in C_b(\mathbb{R};D(A^{1/2}))\quad\text{and}\ \ u''\in C_b(\mathbb{R};H).$$

□

As an application of these results we can consider the sine-Gordon equation with Dirichlet boundary condition (1.4). In the same way, one can consider many other examples like (1.5) and (1.6).

Corollary 3.2: If in the system (1.4) the function $t\to p(t,\cdot)\in L^2(0,L)$ is of C^1 class, then for some values of c, d and k the system (1.4) admits a unique solution u such that

$$u\in C_b(\mathbb{R};H^2\cap H_0^1),\ \ u'\in C_b(\mathbb{R};H_0^1)\quad\text{and}\ \ u''\in C_b(\mathbb{R};L^2(0,L)).$$

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A mathematical proof of a result derived from the application of the Thompson–Lampard theorem of electrostatics

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We give an entirely mathematical demonstration and a generalization of a recent result obtained from the application of the Thompson–Lampard theorem of electrostatics, i.e., $\Sigma_{n\ \mathrm{even}}[8\sin^2(n\pi a/2)\sinh^2(n\pi a/2)]/[n\sinh(n\pi)]+\Sigma_{n\ \mathrm{odd}}[8\cos^2(n\pi a/2)\cosh^2(n\pi a/2)]/[n\sinh(n\pi)]=\ln 2$. It is shown that, as it should be, the result of the left-hand side, $\ln 2$, is independent of the value of a. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1332123]

I. INTRODUCTION

Recently, Jackson[1] has presented a beautiful and pedagogical discussion of the Thompson–Lampard theorem of electrostatics.[2–4] As a consequence of the application of the theorem to several geometries, some curious results about series and products emerged. One of these results concerns the unbelievable relation

$$S=\sum_{n\ \mathrm{even}}\frac{8\sin^2(n\pi a/2)\sinh^2(n\pi a/2)}{n\sinh(n\pi)}+\sum_{n\ \mathrm{odd}}\frac{8\cos^2(n\pi a/2)\cosh^2(n\pi a/2)}{n\sinh(n\pi)}=\ln 2, \tag{1}$$

valid for $0\leqslant a<1$. When $a=0$, Eq. (1) becomes

$$\sum_{n\ \mathrm{odd}}\frac{8}{n\sinh(n\pi)}=\ln 2, \tag{2}$$

from where the relation

$$\prod_{k=0}^{\infty}\left[\frac{1+\exp[-(2k+1)\pi]}{1-\exp[-(2k+1)\pi]}\right]^8=2 \tag{3}$$

is obtained.

Although these relations are derived from the application of the theorem, Jackson was able to give an independent, mathematical proof, only in the case of $a=0$ but was unable to provide a mathematical proof of the general case for $0\leqslant a<1$. About the general case he commented that ''its proof (for me at least) depends on the validity of the theorem.''

It is our aim in this paper to provide such a proof, showing that indeed the two terms in (1) add to $\ln 2$, independent of a, $0\leqslant a<1$. Along the way, we give a new formula, involving trigonometric functions and exponentials which is not found explicitly, in Gradshteyn and Ryzhik[5] but which is needed in our proof. We start our proof providing a generalization of (1) and showing that the generalized sum can be written in terms of Jacobi's theta functions. We then study the particular case of Eq. (1) and show that the two terms in S add to $\ln 2$, independent of a.

II. GENERALIZATION OF EQ. (1) AND ITS EXPRESSION IN TERMS OF JACOBI'S THETA FUNCTIONS

The mathematical structure of S expressed by the sum in Eq. (1) lead us to suggest the following generalization, denoted by S_g:

$$S_g=\sum_{n\ \text{even}}\frac{8\sin(n\pi a/2)\sin(n\pi b/2)\sinh(n\pi a/2)\sinh(n\pi b/2)}{n\sinh(n\pi)}+\sum_{n\ \text{odd}}\frac{8\cos(n\pi a/2)\cos(n\pi b/2)\cosh(n\pi a/2)\cosh(n\pi b/2)}{n\sinh(n\pi)} \tag{4}$$

$$\equiv S_1+S_2. \tag{5}$$

If one expresses the hyperbolic functions in (4) in terms of exponentials, S_1 can be written as

$$\begin{aligned}S_1&=4\sum_{n\ \text{even}}\frac{\sin(n\pi a/2)\sin(n\pi b/2)}{n}e^{n\pi a/2}(1-e^{-n\pi a})e^{n\pi b/2}(1-e^{-n\pi b})e^{-n\pi}(1-e^{-2n\pi})^{-1}\\&=4\sum_{n\ \text{even}}\frac{\sin(n\pi a/2)\sin(n\pi b/2)}{n}e^{-n\pi(1-a/2-b/2)}(1-e^{-n\pi a})(1-e^{-n\pi b})\sum_{k=0}^{\infty}e^{-2n\pi k}\\&=4\sum_{k=0}^{\infty}\left\{\sum_{n\ \text{even}}\frac{\sin(n\pi a/2)\sin(n\pi b/2)}{n}e^{-n\pi(1-a/2-b/2+2k)}\right.\\&\quad-\sum_{n\ \text{even}}\frac{\sin(n\pi a/2)\sin(n\pi b/2)}{n}e^{-n\pi(1+a/2-b/2+2k)}\\&\quad-\sum_{n\ \text{even}}\frac{\sin(n\pi a/2)\sin(n\pi b/2)}{n}e^{-n\pi(1-a/2+b/2+2k)}\\&\quad\left.+\sum_{n\ \text{even}}\frac{\sin(n\pi a/2)\sin(n\pi b/2)}{n}e^{-n\pi(1+a/2+b/2+2k)}\right\}.\end{aligned} \tag{6}$$

We now apply formula 1.462 of Gradshteyn and Ryzhik,[5]

$$\sum_{k=1}^{\infty}\frac{\sin kx\sin ky}{k}\exp[-2k|t|]=\frac{1}{4}\ln\left[\frac{\sin^2\frac{x+y}{2}+\sinh^2 t}{\sin^2\frac{x-y}{2}+\sinh^2 t}\right], \tag{7}$$

to evaluate the sums inside $\{\}$ in (6). For that let $n_{\text{even}}=2j$. We then obtain

$$\begin{aligned}S_1=\frac{1}{2}\sum_{k=0}^{\infty}\left\{\ln\left[\frac{\sin^2\pi(a+b)/2+\sinh^2\pi(1-a/2-b/2+2k)}{\sin^2\pi(a-b)/2+\sinh^2\pi(1-a/2-b/2+2k)}\right]\right.\\-\ln\left[\frac{\sin^2\pi(a+b)/2+\sinh^2\pi(1+a/2-b/2+2k)}{\sin^2\pi(a-b)/2+\sinh^2\pi(1+a/2-b/2+2k)}\right]\\-\ln\left[\frac{\sin^2\pi(a+b)/2+\sinh^2\pi(1-a/2+b/2+2k)}{\sin^2\pi(a-b)/2+\sinh^2\pi(1-a/2+b/2+2k)}\right]\\\left.+\ln\left[\frac{\sin^2\pi(a+b)/2+\sinh^2\pi(1+a/2+b/2+2k)}{\sin^2\pi(a-b)/2+\sinh^2\pi(1+a/2+b/2+2k)}\right]\right\}.\end{aligned} \tag{8}$$

Now, consider the sum S_2, and let us express the hyperbolic functions in terms of exponentials

$$
\begin{aligned}
S_2 &= 4\sum_{n\ \text{odd}} \frac{\cos n\pi a/2 \cos n\pi b/2}{n} e^{n\pi(a+b)/2}(1+e^{-n\pi a})(1+e^{-n\pi b})e^{-n\pi}(1-e^{-2n\pi})^{-1} \\
&= 4\sum_{n\ \text{odd}} \frac{\cos n\pi a/2 \cos n\pi b/2}{n} e^{n\pi[(a+b)/2-1]}(1+e^{-n\pi a})(1+e^{-n\pi b})\sum_{k=0}^{\infty} e^{-2n\pi k} \\
&= 4\sum_{k=0}^{\infty}\left\{\sum_{n\ \text{odd}} \frac{\cos n\pi a/2 \cos n\pi b/2}{n} e^{-n\pi[1-(a+b)/2+2k]}\right. \\
&\quad + \sum_{n\ \text{odd}} \frac{\cos n\pi a/2 \cos n\pi b/2}{n} e^{-n\pi[1-(a-b)/2+2k]} \\
&\quad + \sum_{n\ \text{odd}} \frac{\cos n\pi a/2 \cos n\pi b/2}{n} e^{-n\pi[1-(b-a)/2+2k]} \\
&\quad \left. + \sum_{n\ \text{odd}} \frac{\cos n\pi a/2 \cos n\pi b/2}{n} e^{-n\pi[1+(a+b)/2+2k]}\right\}. \qquad (9)
\end{aligned}
$$

To evaluate the sums inside $\{\}$ in (9) we will need a formula like (7) but involving cosines instead of sines. Since such a formula is not found in Gradhsteyn and Rhyzik,[5] we will derive it in Appendix A. Using now the formula (A6) we can evaluate the sums in Eq. (9). We get

$$S_2 = \sum_{n=1}^{24}\sum_{k=0}^{\infty} s_{nk}, \qquad (10)$$

where

$$s_{1k} = -\tfrac{1}{2}\ln(1-e^{-\pi[1-(a+b)/2+2k]+i\pi(a-b)/2}), \qquad (11)$$

$$s_{2k} = -\tfrac{1}{2}\ln(1-e^{-\pi[1-(a+b)/2+2k]-i\pi(a-b)/2}), \qquad (12)$$

$$s_{3k} = -\frac{1}{4}\ln\left[\frac{\sin^2\dfrac{\pi(a+b)}{4}+\sinh^2\dfrac{\pi}{2}\left[1-\dfrac{a+b}{2}+2k\right]}{\sin^2\dfrac{\pi(a-b)}{4}+\sinh^2\dfrac{\pi}{2}\left[1-\dfrac{a+b}{2}+2k\right]}\right], \qquad (13)$$

$$s_{4k} = \tfrac{1}{4}\ln(1-e^{-2\pi[1-(a+b)/2+2k]+i\pi(a-b)}), \qquad (14)$$

$$s_{5k} = \tfrac{1}{4}\ln(1-e^{-2\pi[1-(a+b)/2+2k]-i\pi(a-b)}), \qquad (15)$$

$$s_{6k} = \frac{1}{8}\ln\left[\frac{\sin^2\dfrac{\pi(a+b)}{2}+\sinh^2\pi\left[1-\dfrac{a+b}{2}+2k\right]}{\sin^2\dfrac{\pi(a-b)}{2}+\sinh^2\pi\left[1-\dfrac{a+b}{2}+2k\right]}\right], \qquad (16)$$

$$s_{7k} = -\tfrac{1}{2}\ln(1-e^{-\pi[1-(a-b)/2+2k]+i\pi(a-b)/2}), \qquad (17)$$

$$s_{8k} = -\tfrac{1}{2}\ln(1-e^{-\pi[1-(a-b)/2+2k]-i\pi(a-b)/2}), \qquad (18)$$

$$s_{9k}=-\frac{1}{4}\ln\left[\frac{\sin^2\frac{\pi(a+b)}{4}+\sinh^2\frac{\pi}{2}\left[1-\frac{a-b}{2}+2k\right]}{\sin^2\frac{\pi(a-b)}{4}+\sinh^2\frac{\pi}{2}\left[1-\frac{a-b}{2}+2k\right]}\right], \tag{19}$$

$$s_{10k}=\tfrac{1}{4}\ln(1-e^{-2\pi[1-(a-b)/2+2k]+i\pi(a-b)}), \tag{20}$$

$$s_{11k}=\tfrac{1}{4}\ln(1-e^{-2\pi[1-(a-b)/2+2k]-i\pi(a-b)}), \tag{21}$$

$$s_{12k}=\frac{1}{8}\ln\left[\frac{\sin^2\frac{\pi(a+b)}{2}+\sinh^2\pi\left[1-\frac{a-b}{2}+2k\right]}{\sin^2\frac{\pi(a-b)}{2}+\sinh^2\pi\left[1-\frac{a-b}{2}+2k\right]}\right], \tag{22}$$

$$s_{13k}=-\tfrac{1}{2}\ln(1-e^{-\pi[1-(b-a)/2+2k]+i\pi(a-b)/2}), \tag{23}$$

$$s_{14k}=-\tfrac{1}{2}\ln(1-e^{-\pi[1-(b-a)/2+2k]-i\pi(a-b)/2}), \tag{24}$$

$$s_{15k}=-\frac{1}{4}\ln\left[\frac{\sin^2\frac{\pi(a+b)}{4}+\sinh^2\frac{\pi}{2}\left[1-\frac{b-a}{2}+2k\right]}{\sin^2\frac{\pi(a-b)}{4}+\sinh^2\frac{\pi}{2}\left[1-\frac{b-a}{2}+2k\right]}\right], \tag{25}$$

$$s_{16k}=\tfrac{1}{4}\ln(1-e^{-2\pi[1-(b-a)/2+2k]+i\pi(a-b)}), \tag{26}$$

$$s_{17k}=\tfrac{1}{4}\ln(1-e^{-2\pi[1-(b-a)/2+2k]-i\pi(a-b)}), \tag{27}$$

$$s_{18k}=\frac{1}{8}\ln\left[\frac{\sin^2\frac{\pi(a+b)}{2}+\sinh^2\pi\left[1-\frac{b-a}{2}+2k\right]}{\sin^2\frac{\pi(a-b)}{2}+\sinh^2\pi\left[1-\frac{b-a}{2}+2k\right]}\right], \tag{28}$$

$$s_{19k}=-\tfrac{1}{2}\ln(1-e^{-\pi[1+(a+b)/2+2k]+i\pi(a-b)/2}), \tag{29}$$

$$s_{20k}=-\tfrac{1}{2}\ln(1-e^{-\pi[1+(a+b)/2+2k]-i\pi(a-b)/2}), \tag{30}$$

$$s_{21k}=-\frac{1}{4}\ln\left[\frac{\sin^2\frac{\pi(a+b)}{4}+\sinh^2\frac{\pi}{2}\left[1+\frac{a+b}{2}+2k\right]}{\sin^2\frac{\pi(a-b)}{4}+\sinh^2\frac{\pi}{2}\left[1+\frac{a+b}{2}+2k\right]}\right], \tag{31}$$

$$s_{22k}=\tfrac{1}{4}\ln(1-e^{-2\pi[1+(a+b)/2+2k]+i\pi(a-b)}), \tag{32}$$

$$s_{23k}=\tfrac{1}{4}\ln(1-e^{-2\pi[1+(a+b)/2+2k]-i\pi(a-b)}), \tag{33}$$

$$s_{24k}=\frac{1}{8}\ln\left[\frac{\sin^2\frac{\pi(a+b)}{2}+\sinh^2\pi\left[1+\frac{a+b}{2}+2k\right]}{\sin^2\frac{\pi(a-b)}{2}+\sinh^2\pi\left[1+\frac{a+b}{2}+2k\right]}\right]. \tag{34}$$

Now, adding Eqs. (8) and (10) and after a large number of simplifications, factorizations and use of the elementary properties of trigonometric and hyperbolic functions, we obtain

$$\begin{aligned} S_g &= S_1 + S_2 \\ &= \sum_{k=0}^{\infty} \ln \frac{N_k}{D_k} \\ &= \ln \prod_{k=0}^{\infty} \frac{N_k}{D_k} \\ &= \ln \frac{\Pi_{k=0}^{\infty} N_k}{\Pi_{k=0}^{\infty} D_k}, \end{aligned} \tag{35}$$

where

$$\begin{aligned} N_k = &(1+xy^{1+i}z^{-(1+i)})(1+xy^{1-i}z^{i-1})(1+xy^{i-1}z^{1-i})(1+xy^{-(1+i)}z^{1+i}) \\ &\times (1+xy^{1-i}z^{1-i})(1+xy^{1+i}z^{1+i})(1+xy^{i-1}z^{i-1})(1+xy^{-(1+i)}z^{-(1+i)}) \end{aligned} \tag{36}$$

and

$$\begin{aligned} D_k = &(1-xy^{1+i}z^{1-i})(1-xy^{1-i}z^{1+i})(1-xy^{i-1}z^{-(1+i)})(1-xy^{-(1+i)}z^{i-1}) \\ &\times (1-xy^{i-1}z^{1+i})(1-xy^{-(1+i)}z^{1-i})(1-xy^{1+i}z^{i-1})(1-xy^{1-i}z^{-(1+i)}) \end{aligned} \tag{37}$$

with

$$x = (e^{-\pi})^{1+2k} \equiv q^{1+2k}, \tag{38}$$

$$y = e^{\pi a/2}, \quad z = e^{\pi b/2}. \tag{39}$$

Consider now the following product[6]

$$f(t) = \prod_{k=0}^{\infty} (1 \pm q^{1+2k}t)(1 \pm q^{1+2k}t^{-1}) \tag{40}$$

and let $t = e^{2iu}$. Then, Eq. (40) can be written as

$$f(u) = \prod_{k=0}^{\infty} (1 \pm 2q^{1+2k}\cos 2u + q^{2+4k}). \tag{41}$$

We will make use now of Eqs. (40) and (41) to relate the products in Eq. (35) with ratios of Jacobi's theta functions. The numerator of the logarithm of Eq. (35) can be written as

$$\begin{aligned} \prod_{k=0}^{\infty} N_k = \prod_{k=0}^{\infty} &(1+q^{1+2k}(y/z)^{1+i})(1+q^{1+2k}(y/z)^{-(1+i)})(1+q^{1+2k}(y/z)^{1-i}) \\ &\times (1+q^{1+2k}(y/z)^{i-1})(1+q^{1+2k}(yz)^{1-i})(1+q^{1+2k}(yz)^{i-1}) \\ &\times (1+q^{1+2k}(yz)^{1+i})(1+q^{1+2k}(yz)^{-(1+i)}) \end{aligned} \tag{42}$$

with

$$y/z = e^{\pi(a-b)/2}, \tag{43}$$

$$yz = e^{\pi(a+b)/2}. \tag{44}$$

Similarly, the denominator of the logarithm of Eq. (35) can be written as

$$\begin{aligned}\prod_{k=0}^{\infty} D_k = \prod_{k=0}^{\infty} & (1-q^{1+2k}y^{1+i}z^{1-i})(1-q^{1+2k}y^{-(1+i)}z^{i-1})(1-q^{1+2k}y^{1-i}z^{1+i}) \\ & \times(1-q^{1+2k}y^{i-1}z^{-(1+i)})(1-q^{1+2k}y^{i-1}z^{1+i})(1-q^{1+2k}y^{1-i}z^{-(1+i)}) \\ & \times(1-q^{1+2k}y^{-(1+i)}z^{1-i})(1-q^{1+2k}y^{1+i}z^{i-1}).\end{aligned} \tag{45}$$

We see that each pair of terms in Eqs. (42) and (45) has the form given by Eq. (40). Thus, we can write Eqs. (42) and (45) as product of functions of the form given by Eq. (41).

Thus, Eq. (35) can be written as

$$S_g = \ln \frac{f(u_1)f(u_2)f(u_3)f(u_4)}{g(u_5)g(u_6)g(u_7)g(u_8)}, \tag{46}$$

where

$$u_1 = \frac{\pi}{4}(1-i)(a-b), \tag{47}$$

$$u_2 = -\frac{\pi}{4}(i+1)(a-b), \tag{48}$$

$$u_3 = -\frac{\pi}{4}(i+1)(a+b), \tag{49}$$

$$u_4 = \frac{\pi}{4}(1-i)(a+b), \tag{50}$$

$$u_5 = \frac{\pi}{4}(a-b) - i\frac{\pi}{4}(a+b), \tag{51}$$

$$u_6 = \frac{\pi}{4}(b-a) - i\frac{\pi}{4}(a+b), \tag{52}$$

$$u_7 = \frac{\pi}{4}(a+b) + i\frac{\pi}{4}(a-b), \tag{53}$$

$$u_8 = -\frac{\pi}{4}(a+b) + i\frac{\pi}{4}(a-b), \tag{54}$$

while $f(u_i)$ and $g(u_j)$ are the $f(u)$ functions in Eq. (41) with the plus and minus signs, respectively.

Relating the $f(u_i)$ and $g(u_j)$ to Jacobi's theta functions $\theta_3(u_i)$ and $\theta_4(u_j)$, which in their infinite product representations are given by[6–9]

$$\theta_3(u) = G\prod_{n=1}^{\infty}(1+2q^{2n-1}\cos 2u + q^{4n-2}), \tag{55}$$

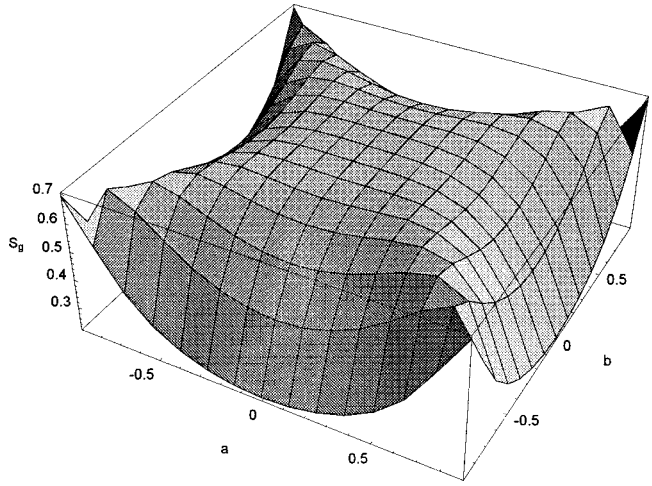

FIG. 1. Plot of the periodic function S_g as a function of the parameters a and b, in the interval $-1<a,\ b<1$.

$$\theta_4(u)=G\prod_{n=1}^{\infty}(1-2q^{2n-1}\cos 2u+q^{4n-2}), \tag{56}$$

with

$$G=\prod_{n=1}^{\infty}(1-q^{2n}), \tag{57}$$

we have, finally,

$$S_g=\ln\frac{\theta_3(u_1)\theta_3(u_2)\theta_3(u_3)\theta_3(u_4)}{\theta_4(u_5)\theta_4(u_6)\theta_4(u_7)\theta_4(u_8)}. \tag{58}$$

Figure 1 shows a plot of S_g in terms of the parameters a and b in the interval $-1<a,\ b<1$. As seen S_g is not a constant for arbitrary values of the parameters. However, in Sec. IV we provide a proof that for $a=b$, $S_g=S$ is indeed a constant and also prove, in general, the nonconstancy of S_g for arbitrary values of a and b $(a\neq b)$.

III. EQUATION (1) IN TERMS OF JACOBI'S THETA FUNCTIONS

When $a=b$ Eq. (58) becomes [recall that $\theta_3(u)$ and $\theta_4(v)$ are even functions of their arguments]

$$S=\ln\left[\frac{\theta_3\left(\frac{\pi a}{2}(1+i)\right)\theta_3\left(\frac{\pi a}{2}(1-i)\right)(\theta_3(0))^2}{\left(\theta_4\left(\frac{\pi a}{2}i\right)\right)^2\left(\theta_4\left(\frac{\pi a}{2}\right)\right)^2}\right]. \tag{59}$$

If $a=0$, use of Eqs. (55)–(57) reveals that the expression inside $\{\}$ in (59) reduces to the one given by Jackson,[1] i.e.,

$$S=\ln\prod_{k=0}^{\infty}\left(\frac{1+e^{-\pi(1+2k)}}{1-e^{-\pi(1+2k)}}\right)^8$$

$$=\ln\left(\frac{\theta_3(0)}{\theta_4(0)}\right)^4$$

$$=\ln\frac{1}{k'^2}$$

$$=\ln 2, \tag{60}$$

where k' is the complementary modulus.[6]

Our purpose now is to demonstrate that S is a constant, independent of a, and equal to $\ln 2$.

IV. PROOF THAT *S* IS A CONSTANT FOR ALL *a*

We will give two demonstrations of the proposition that S is a constant, independent of a and equal to $\ln 2$. The first proof is based on the manipulation of some relations between Jacobi's theta functions, while the second one is more formal and makes use of Liouville theorems of doubly periodic functions.

A. Demonstration 1

Let us write Eq. (59) as

$$S=\ln\left[\frac{\theta_3(z+zi)\,\theta_3(z-zi)(\theta_3(0))^2}{(\theta_4(zi))^2(\theta_4(z))^2}\right]$$

$$=\ln\left\{\left(\frac{\theta_3(0)}{\theta_4(0)}\right)^4\left(\frac{A}{B}\right)\right\}, \tag{61}$$

where

$$A=\frac{\theta_3(z+zi)\,\theta_3(z-zi)}{(\theta_3(0))^2}, \tag{62}$$

$$B=\frac{(\theta_4(z)\,\theta_4(zi))^2}{(\theta_4(0))^4}, \tag{63}$$

and $z=\pi a/2$.

Our aim now is to prove that A/B in Eq. (61) is equal to 1, that is, $A=B$. In order to do so we will use some relations among theta functions to reduce B to A. The relevant theorems for our proof are given in Appendix B to which we will be referring in the steps that follow.

First, by (B1),

$$(\theta_4(0))^4B=(\theta_4(z))^2(\theta_4(zi))^2$$

$$=(\theta_4(0))^2\theta_4(z+zi)\,\theta_4(z-zi)+(\theta_1(z))^2(\theta_1(zi))^2. \tag{64}$$

Also, by (B2),

$$(\theta_3(0))^4(\theta_4(0))^4B=(\theta_3(0))^4(\theta_4(0))^2\theta_4(z+zi)\,\theta_4(z-zi)+(\theta_3(0))^4(\theta_1(z))^2(\theta_1(zi))^2$$

$$=(\theta_3(0))^2(\theta_1(z))^2(\theta_2(zi))^2(\theta_4(0))^2+(\theta_3(0))^2(\theta_4(0))^2(\theta_3(z))^2(\theta_4(zi))^2$$

$$+(\theta_3(0))^4(\theta_1(z))^2(\theta_1(zi))^2. \tag{65}$$

On the other hand, by (B2) with $v=0$,

$$(\theta_3(0))^2(\theta_4(zi))^2=(\theta_1(zi))^2(\theta_2(0))^2+(\theta_3(zi))^2(\theta_4(0))^2. \tag{66}$$

Thus, substituting Eq. (66) into Eq. (65) we obtain

$$(\theta_3(0))^4(\theta_4(0))^4B=(\theta_3(0))^2(\theta_1(z))^2(\theta_2(zi))^2(\theta_4(0))^2+(\theta_3(z))^2(\theta_4(0))^2(\theta_1(zi))^2(\theta_2(0))^2$$
$$+(\theta_3(z))^2(\theta_4(0))^2(\theta_3(zi))^2(\theta_4(0))^2+(\theta_3(0))^4(\theta_1(z))^2(\theta_1(zi))^2. \tag{67}$$

Using (B3) and (B4) we get

$$(\theta_4(0))^2=k'(\theta_3(0))^2, \tag{68}$$

$$(\theta_2(0))^2=k(\theta_3(0))^2, \tag{69}$$

since $\theta_1(0)=0$.

Thus, substituting Eqs. (68) and (69) into Eq. (67) one obtains

$$(\theta_3(0))^4(\theta_4(0))^4B=(\theta_3(0))^4[k'(\theta_1(z))^2(\theta_2(zi))^2+k'k(\theta_3(z))^2(\theta_1(zi))^2$$
$$+k'^2(\theta_3(z))^2(\theta_3(zi))^2+(\theta_1(z))^2(\theta_1(zi))^2]. \tag{70}$$

Applying (B4) in (40) we obtain

$$(\theta_4(0))^4B=-k'^2(\theta_1(z))^2(\theta_1(zi))^2+k'k(\theta_1(z))^2(\theta_3(zi))^2+k'k(\theta_3(z))^2(\theta_1(zi))^2$$
$$+k'^2(\theta_3(z))^2(\theta_3(zi))^2+(\theta_1(z))^2(\theta_1(zi))^2. \tag{71}$$

Since $q=e^{-\pi(K'/K)}$ by definition, $K(k)$ being the complete elliptic integral of first class and k its modulus,[6] it implies, in our case where $q=e^{-\pi}$, that

$$\begin{aligned} K(k)&=K'(k)\\ &=K(k')\\ &=K(\sqrt{1-k^2}) \end{aligned} \tag{72}$$

or

$$k'=k=\frac{1}{\sqrt{2}}. \tag{73}$$

Then, it follows that Eq. (71) can be written as

$$2(\theta_4(0))^4B=(\theta_1(z))^2(\theta_1(zi))^2+(\theta_3(z))^2(\theta_3(zi))^2$$
$$+((\theta_1(z))^2(\theta_3(zi))^2+(\theta_3(z))^2(\theta_1(zi))^2). \tag{74}$$

Using the so-called Jacobi's imaginary transformations[7]

$$\theta_1(z,\tau)=\alpha\theta_1(z\tau',\tau')/i, \tag{75}$$

$$\theta_3(z,\tau)=\alpha\theta_3(z\tau',\tau'), \tag{76}$$

$$\alpha=\frac{1}{\sqrt{-i\tau}}e^{i\tau'z^2/\pi},\quad \tau'=-\frac{1}{\tau}, \tag{77}$$

and the fact that, in our case, $\tau=\tau'=i$, we can prove that the third term in (74) vanishes. Thus, Eq. (74) reduces to

$$B=\frac{(\theta_3(z))^4-(\theta_1(z))^4}{2\alpha^2(\theta_4(0))^4} \tag{78}$$

with $\alpha=e^{-z^2/\pi}$.

Second, starting from Eq. (62) and employing (B5), (68), (73), and (75)–(77) we get

$$\begin{aligned} A&=\frac{(\theta_1(z))^2(\theta_1(zi))^2+(\theta_3(z))^2(\theta_3(zi))^2}{2(\theta_4(0))^4}\\ &=\frac{(\theta_3(z))^4-(\theta_1(z))^4}{2\alpha^2(\theta_4(0))^4}\\ &=B. \end{aligned} \tag{79}$$

Consequently, we have proved that

$$S=\ln\left\{\left(\frac{\theta_3(0)}{\theta_4(0)}\right)^4\right\} \tag{80}$$

$$=\ln 2, \tag{81}$$

where (81) follows from (68) and (73).

B. Demonstration 2

Demonstration 1 can be called a *tour de force* demonstration. Here, we will give a simpler and more elegant demonstration which can be accomplished by the direct application of some general theorems about elliptic functions.

Consider the function S as given in (61). First, we will show that S is an elliptic function of periods $\pi/2$ and $(\pi/2)\,i$. This implies that the function will have the same value each time a changes by one.

Thus, changing $z\to z+(\pi/2)$ we change $S\to S'$, where

$$S'=\frac{\theta_3(z+zi+\frac{1}{2}\pi+\frac{1}{2}\pi i)\,\theta_3(z-zi+\frac{1}{2}\pi-\frac{1}{2}\pi i)\,\theta_3^2(0)}{\theta_4^2(zi+\frac{1}{2}\pi i)\,\theta_4^2(z+\frac{1}{2}\pi)}. \tag{82}$$

Now, applying the fundamental properties of these theta functions (see basic property table on p. 319 of Ref. 9), we get

$$S'=\frac{\theta_1(z+zi)\,\theta_1(zi-z)\,\theta_3^2(0)}{\theta_1^2(zi)\,\theta_3^2(z)}. \tag{83}$$

To show that indeed $S=S'$ we use (B6) and (B7), and apply to the first term of the right-hand side of each equation Jacobi's imaginary transformations (75)–(77) and

$$\theta_2(z,\tau)=\alpha\,\theta_4(z\tau',\tau'). \tag{84}$$

We get (with $u=z$ and $v=zi$, and recalling that, in our problem, $\tau=i$, and, consequently, $\tau'=i$)

$$\theta_3^2(0)\,\theta_3(z+zi)\,\theta_3(z-zi)=2\,\theta_4^2(z)\,\theta_4^2(zi), \tag{85}$$

$$\theta_3^2(0)\,\theta_1(z+zi)\,\theta_1(z-zi)=-2\,\theta_3^2(z)\,\theta_1^2(zi) \tag{86}$$

or

$$\frac{\theta_3(z+zi)\,\theta_3(z-zi)}{\theta_1(z+zi)\,\theta_1(zi-z)}=\frac{\theta_4^2(z)\,\theta_4^2(zi)}{\theta_3^2(z)\,\theta_1^2(zi)}. \tag{87}$$

Then, substituting (87) in (83) we obtain that $S'=S$. By a similar procedure we can prove that $(\pi/2)\,i$ is also a period of S. Thus, S is an elliptic function of periods $\pi/2$ and $(\pi/2)\,i$.

We now prove that S is an elliptic function of order less than two, and, by Liouville theorem,[9,10] a constant.

Since, in the problem we are dealing with, z is real, S has only one zero which occurs when $z=\pi/2$, i.e., $\theta_3[(\pi/2)+(\pi/2)\,i]=0$. Then, since the number of zero's of an elliptic function is equal to the number of poles in the fundamental parallelogram we conclude that S is an elliptic function of order one, and, by Liouville theorem, a constant.[11] Another way to analyze this is the following. Since when $z=\pi/2$ the function $\theta_4^2(zi)$ in the denominator of S has a double zero and the function $\theta_3(z+zi)$ has a single zero, this single zero will knock a zero of $\theta_4^2(zi)$ and, consequently, S will have only one pole and will be an elliptic function of order one and, by Liouville theorem, a constant.

The constant value of S in the fundamental parallelogram is found by selecting an appropriate value of z, which in our case is, naturally, 0 (corresponding to $a=0$). Thus, putting $z=0$ in Eq. (61) we get

$$S=\ln\left(\frac{\theta_3(0)}{\theta_4(0)}\right)^4$$

$$=\ln 2.$$

Further, it can be shown by the same methodology that when $a\neq b$, S_g is an elliptic function of periods 0 in $\pi(a-b)/4$ and π in $\pi(a+b)/4$ (i.e., periods 2 in a and b), and periods 0 in $\pi(a-b)/4$ and πi in $\pi(a+b)/4$ (i.e., periods $2i$ in a and b). Also, it can be shown that when $a\neq b$ S_g is an elliptic function of order two and, by Liouville theorem, is not a constant.

V. CONCLUSIONS

A recent mathematical result,[1] Eq. (1), derived as a consequence of the application of the Thompson–Lampard theorem of electrostatics,[2–4] has been given an entirely mathematical proof. Our approach has been, first, to generalize the left-hand side of Eq. (1) in terms of two parameters and to express it in terms of the logarithm of a ratio of products of Jacobi's theta functions of the types $\theta_3(x)$ and $\theta_4(x)$. Second, we have proved that the constancy of the sum indicated corresponds to the particular case when both parameters are equal to each other. We have done this by either of two procedures. The first one was based on the manipulation of some relations among Jacobi's theta functions, and the second one made use of Liouville theorem of the theory of doubly periodic functions.[9,10]

APPENDIX A: A FORMULA INVOLVING A SUM OF PRODUCTS OF COSINES AND EXPONENTIALS

Here we will derive a formula involving a sum of a product of cosines and exponentials.

Using the following relations[5]

$$\cos(x-y)=\cos x\cos y+\sin x\sin y, \tag{A1}$$

$$\sum_{k=1}^{\infty}\frac{p^k\cos kx}{k}=\ln\frac{1}{\sqrt{1-2p\cos x+p^2}}, \tag{A2}$$

with $p=e^{-2|t|}$, and Eq. (7) we obtain

$$\begin{aligned}
&\sum_{k=1}^{\infty}\frac{\cos kx\cos ky}{k}e^{-2k|t|}\\
&\quad=\sum_{k=1}^{\infty}\frac{\cos k(x-y)}{k}e^{-2k|t|}-\sum_{k=1}^{\infty}\frac{\sin kx\sin ky}{k}e^{-2k|t|}\\
&\quad=-\tfrac{1}{2}\ln(1-e^{-2|t|+i(x-y)})-\tfrac{1}{2}\ln(1-e^{-2|t|-i(x-y)})\\
&\qquad-\frac{1}{4}\ln\left[\frac{\sin^2\dfrac{x+y}{2}+\sinh^2|t|}{\sin^2\dfrac{x-y}{2}+\sinh^2|t|}\right].
\end{aligned}\tag{A3}$$

On the other hand,

$$\sum_{n=1}^{\infty}\frac{\cos nx\cos ny}{n}e^{-2n|t|}=\sum_{n\ \text{even}}\frac{\cos nx\cos ny}{n}e^{-2n|t|}+\sum_{n\ \text{odd}}\frac{\cos nx\cos ny}{n}e^{-2n|t|}.\tag{A4}$$

The sum over n even in the preceding equation can be evaluated easily using (A3),

$$\begin{aligned}
\sum_{n\ \text{even}}\frac{\cos nx\cos ny}{n}e^{-2n|t|}&=\sum_{j=1}^{\infty}\frac{\cos 2jx\cos 2jy}{2j}e^{-2j(2|t|)}\\
&=-\tfrac{1}{4}\ln(1-e^{-4|t|+2i(x-y)})-\tfrac{1}{4}\ln(1-e^{-4|t|-2i(x-y)})\\
&\quad-\frac{1}{8}\ln\left[\frac{\sin^2(x+y)+\sinh^2 2|t|}{\sin^2(x-y)+\sinh^2 2|t|}\right].
\end{aligned}\tag{A5}$$

We now substitute (A3) and (A5) in (A4) and solve the sum over n odd obtaining

$$\begin{aligned}
&\sum_{n\ \text{odd}}\frac{\cos nx\cos ny}{n}e^{-2n|t|}\\
&\quad=-\tfrac{1}{2}\ln(1-e^{-2|t|+i(x-y)})-\tfrac{1}{2}\ln(1-e^{-2|t|-i(x-y)})\\
&\qquad-\frac{1}{4}\ln\left[\frac{\sin^2\dfrac{x+y}{2}+\sinh^2|t|}{\sin^2\dfrac{x-y}{2}+\sinh^2|t|}\right]+\frac{1}{4}\ln(1-e^{-4|t|+2i(x-y)})+\frac{1}{4}\ln(1-e^{-4|t|-2i(x-y)})\\
&\qquad+\frac{1}{8}\ln\left[\frac{\sin^2(x+y)+\sinh^2 2|t|}{\sin^2(x-y)+\sinh^2 2|t|}\right].
\end{aligned}\tag{A6}$$

APPENDIX B: RELATIONS AMONG JACOBI'S THETA FUNCTIONS RELEVANT TO THE PRESENT WORK

In this appendix we list the relevant theta function relations[6] that will be needed in the proof presented in Sec. IV:

$$\theta_4^2(0)\,\theta_4(u+v)\,\theta_4(u-v)=\theta_4^2(u)\,\theta_4^2(v)-\theta_1^2(u)\,\theta_1^2(v),\tag{B1}$$

$$\theta_3^2(0)\,\theta_4(u+v)\,\theta_4(u-v)=\theta_1^2(u)\,\theta_2^2(v)+\theta_3^2(u)\,\theta_4^2(v), \tag{B2}$$

$$\theta_4^2(u)=k\,\theta_1^2(u)+k'\,\theta_3^2(u), \tag{B3}$$

$$\theta_2^2(u)=-k'\,\theta_1^2(u)+k\,\theta_3^2(u), \tag{B4}$$

$$\theta_3^2(0)\,\theta_3(u+v)\,\theta_3(u-v)=\theta_1^2(u)\,\theta_1^2(v)+\theta_3^2(u)\,\theta_3^2(v), \tag{B5}$$

$$\theta_3^2(0)\,\theta_3(u+v)\,\theta_3(u-v)=\theta_2^2(u)\,\theta_2^2(v)+\theta_4^2(u)\,\theta_4^2(v), \tag{B6}$$

$$\theta_3^2(0)\,\theta_1(u+v)\,\theta_1(u-v)=\theta_1^2(u)\,\theta_3^2(v)-\theta_3^2(u)\,\theta_1^2(v). \tag{B7}$$

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Generalization of the Darboux transform

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This article presents a generalization of the standard Darboux transform applied to Sturm–Liouville differential equations. This is achieved with the aid of an ansatz as a particular solution for the Riccati relationship involved, which in turn led us to obtain its generalized Darboux solution that contains, as a particular case, the standard Darboux transform. The proposed generalized Darboux transform (GDT), applied to the quantum mechanical field, gives the opportunity to prove the existence of standard and generalized Darboux potentials that match with the so-called isospectral potentials. This is exemplified by obtaining, through the GDT, a set of standard and generalized Darboux potentials that form the partner of the one-dimensional harmonic oscillator model for any quantum principal number. The worked example indicates how the GDT can be used to obtain the isospectral potentials associated to any known specific potential. We consider also the application of our method as proposed to the theory of solitons in order to show why the GDT will be important in other fields of application where the standard Darboux transform is usually concerned.
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I. INTRODUCTION

Although the Darboux transform was given a long time ago,[1] such an exceptional procedure is actually of great interest as has been demonstrated by several applications in the theory of solitons.[2–4] Essentially, the Darboux proposition is based on the covariance properties of ordinary and partial differential equations with respect to a gauge transformation in the special case of the Sturm–Liouville relationship. Moreover, the N-times repeated Darboux transform has been given by Crum[5] and applied for radial Schrödinger equations.[6] Furthermore, in the field of quantum mechanics, several studies have turned to the Gelfand–Levitan procedure[7] for the inverse scattering method to generate anharmonic potentials.[8] Other research has been directed to standard and modified factorizations and SUSY[9] in relation to the so-called isospectral potentials.[10] In this regard, Korolev[11] has disclosed the interplay between Liouville equations and Darboux transform in relation to the isospectral problem. Besides, Morales and Peña[12] have recently proposed a procedure to obtain all the related isospectral potentials, standard, modified and generalized, proving also[13] that their modified potentials match those obtained by means of the standard Darboux transform. Taking into consideration the aforesaid aspects, in this work we extend the procedure that we have already proposed, aiming to find the matching that corresponds to generalized potentials. Then we proceeded to follow the spirit of the method used to obtain generalized potentials, in order to generalize the Darboux transform with the purpose to transcend the scope of the standard Darboux transform field. Thus, in the next section the standard Darboux transform is reviewed within the frame of the Sturm–Liouville equations in such a way that in Sec. III we give

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the corresponding generalization. Specifically, the generalized Darboux transform applied to quantum mechanical problems is given in Sec. IV where we analyze the problem of isospectrality. Finally, just as an example, the usefulness of the proposed generalized Darboux transform, on quantum mechanical situations, is shown by obtaining the corresponding standard and generalized Darboux potentials that are partner to the one-dimensional harmonic oscillator potential model. In order to compare our findings with results already published we give explicitly the set of isospectral potentials that corresponds to each eigenvalue of the former Hamiltonian as well as the general formula for the generalized and standard Darboux potentials for any arbitrary n quantum principal number. This example shows straightforwardly by how to generalize any known potential model exactly solved, for which it will be possible, in the same manner, to improve any application where the standard Darboux transform is involved as shown in Sec. V with an application to the theory of solitons.

II. THE STANDARD DARBOUX TRANSFORM

According to the Darboux statement of the Sturm–Liouville equation

$$-\psi''+u(x)\psi=\lambda\psi, \tag{1}$$

if ψ_1 and λ_1 exist and are such that

$$-\psi_1''+u(x)\psi_1=\lambda_1\psi_1, \tag{2}$$

then the Darboux transform

$$\varphi=\psi'-\sigma_1(x)\psi \tag{3}$$

is a solution of

$$-\varphi''+U(x)\varphi=\lambda\varphi, \tag{4}$$

where

$$\sigma_1(x)=\psi_1'/\psi_1 \tag{5}$$

which is equivalent to

$$\psi_1=e^{\int\sigma_1(x)dx}. \tag{6}$$

Clearly, the Sturm–Liouville relationship given in Eq. (1) is covariant with respect to the Darboux transform on condition that

$$U(x)=U_{\mathrm{D}}(x)=u(x)-2\sigma_1'(x), \tag{7}$$

where the subscript D is used to denote $U_{\mathrm{D}}(x)$ as the ''standard Darboux potential'' when concerned with quantum mechanical applications.

III. THE GENERALIZED DARBOUX TRANSFORM

In order to differentiate the purpose of this work regarding the so-called generalized Darboux transform,[2] or Crum generalization,[5] it is important to point out that we are not involved with the N-times repeated Darboux transform. We are interested in the use of the Darboux transformation method in order to obtain the *generalized Darboux solution* which includes the *standard Darboux solution* as particular case, i.e., to find our generalized Darboux transform (GDT).

According to this, it should be noticed that the Darboux transform given in Eq. (3) fulfills the covariance of Eq. (4) on condition that

$$(\lambda - u(x) + 2\sigma_1'(x))\sigma_1(x)\psi - u'(x)\psi + \sigma_1(x)\psi'' + \sigma_1''(x)\psi = 0, \tag{8}$$

which is equivalent to showing that

$$(\sigma_1''(x) + 2\sigma_1(x)\sigma_1'(x) - u'(x))\psi = 0. \tag{9}$$

That is, the relationship

$$\sigma_1''(x) + 2\sigma_1(x)\sigma_1'(x) - u'(x) = 0 \tag{10}$$

can be written as

$$\frac{d}{dx}(\sigma_1'(x) + \sigma_1^2(x) - u(x)) = 0, \tag{11}$$

which leads to

$$\sigma_1'(x) + \sigma_1^2(x) - u(x) = B \tag{12}$$

where B is a constant.

Regarding this point, it can be shown that the Riccati equation

$$y' = Q(x)y^2 + P(x)y + R(x) \tag{13}$$

has the general solution[14]

$$y = y_p + \frac{b}{\mu}, \tag{14}$$

where y_p is a particular solution and

$$\mu = e^{-\int^x [2Q(x)y_p + P(x)]dx}\left(\gamma - b\int^x e^{\int^x [2Q(x)y_p + P(x)]dx} Q(x)dx\right), \tag{15}$$

γ and b being constants. This means that we can consider $\sigma_1(x) = \sigma_{p_1}(x)$ as a particular solution of the specific Riccati relationship

$$\sigma_{p_1}'(x) + \sigma_{p_1}^2(x) - u(x) = C, \tag{16}$$

where C is any constant, in such a way that the corresponding generalized solution of Eq. (12) is

$$\sigma_{g_1}(x) = \sigma_{p_1}(x) + \frac{b}{\rho_1(x)}, \tag{17}$$

where the subindex g is used to denote the general solution and

$$\rho_1(x) = e^{2\int \sigma_{p_1}(x)dx}\left(\gamma + b\int e^{-2\int \sigma_{p_1}(x)dx}dx\right). \tag{18}$$

At this point, just before considering the generalized Darboux transform, it is very important to notice that we can use Eq. (15) to identify the particular potential $u(x)$ from an appropriate ansatz $\sigma_{p_1}(x)$ in order to find the Darboux potential. Such a procedure is by far simpler than the usual procedure requiring the knowledge of both the particular solution ψ_1 and the eigenvalue λ_1 associated to $u(x)$. Instead, with the identification of the former potential from Eq. (16) it is possible to perform the direct calculation of the $U_D(x)$ Darboux potential by means of

$$U_{\mathrm{D}}(x)=u(x)-2\sigma'_{p_1}(x). \tag{19}$$

Finally, for the full eigenfunction spectra, the generalized Darboux transform is given by

$$\varphi_g=\left(\frac{d}{dx}-\sigma_{g_1}(x)\right)\psi, \tag{20}$$

where $\sigma_{g_1}(x)=\varphi'_{g_1}/\varphi_{g_1}$ is such that

$$\varphi_{g_1}=e^{\int(\sigma_{p_1}(x)+\,b/\rho_1(x))dx}=\psi_1\left(\gamma+\int\frac{b\,dx}{\psi_1^2}\right). \tag{21}$$

This transformed function, φ_g, is a solution of

$$-\varphi''_g+U_{\mathrm{GD}}(x)\varphi_g=\lambda\varphi_g, \tag{22}$$

where

$$U_{\mathrm{GD}}(x)=U_{\mathrm{D}}(x)-2b\frac{d}{dx}\left(\frac{1}{\rho_1(x)}\right) \tag{23}$$

is the ''generalized Darboux potential'' appropriate for situations in quantum mechanics.

IV. THE GENERALIZED DARBOUX TRANSFORM IN QUANTUM MECHANICS

In order to show the usefulness of the generalized Darboux transform in quantum mechanics, this section is devoted to analyzing the isospectrality of the $U_{\mathrm{GD}}(x)$ associated Hamiltonian as well as to find the Darboux potentials, standard and generalized, for the specific case of the one-dimensional harmonic oscillator (HO) model.

A. Isospectrality of the $U_{\mathrm{GD}}(x)$ associated Hamiltonian

In order to prove the isospectrality of the generalized Hamiltonian that involves the potential $U_{\mathrm{GD}}(x)$, it is important to remember that the generalized Darboux transform applied to quantum mechanics can be seen by means of the Schrödinger relationship

$$H_g\varphi_g=E_g\varphi_g, \tag{24}$$

where H_g is given by

$$H_g=-\frac{d^2}{dx^2}+U_{\mathrm{GD}}(x) \tag{25}$$

assuming natural units $\hbar^2/2m=1$. In such a case, according to the generalized Darboux transform given in Eq. (20), it follows that

$$H_g\varphi_g=\left(-\frac{d^2}{dx^2}+u(x)-2\sigma'_{g_1}\right)\left(\frac{d}{dx}-\sigma_{g_1}\right)\psi, \tag{26}$$

which is equivalent to

$$H_g\varphi_g=-\psi'''+\sigma_{g_1}\psi''+\sigma''_{g_1}\psi+u(x)\psi'-u(x)\sigma_{g_1}\psi+2\sigma_{g_1}\sigma'_{g_1}\psi. \tag{27}$$

On the other hand, the use of the Sturm–Liouville relationship given by Eq. (1) leads to

$$\psi'''=(u(x)-\lambda)\psi'+u'(x)\psi. \tag{28}$$

With this identity and with the corresponding second derivative ψ'', Eq. (27) is rewritten as

$$H_g\varphi_g=\lambda(\psi'-\sigma_{g_1}\psi)+(\sigma''_{g_1}-u'(x)+2\sigma_{g_1}\sigma'_{g_1})\psi. \tag{29}$$

Finally, due to the fact that σ_{g_1} is a solution of Eq. (12), we use in Eq. (28) the Darboux transform given in Eq. (19) in order to obtain

$$H_g\varphi_g=\lambda\varphi_g, \tag{30}$$

which means that the relation $\lambda=E_g$ proves the isospectrality of the Darboux generalized Hamiltonian. In a similar way one can prove the isospectrality of the Hamiltonian associated to the standard Darboux potential.

B. The Darboux potentials of the HO model for specific principal quantum numbers

In order to find the corresponding standard and generalized Darboux potentials that are associated to the one-dimensional harmonic oscillator model, the algorithm to be used is straightforward: from the Schrödinger relationship we choose a particular eigenfunction ψ_1 in order to find λ_1 (or vice versa) to determine the function $\sigma_p(x)$ that will be necessary for obtaining the standard Darboux potential $U_{\mathrm{D}}(x)$ as well as the generalized wavefunction ψ_g. This last wavefunction is used to find the corresponding $\sigma_g(x)$ that will permit us to obtain the generalized Darboux potential.

In the present case, the Schrödinger relationship is given by

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V_{\mathrm{HO}}(x)\right)\psi_n=\lambda_n\psi_n, \tag{31}$$

where $V_{\mathrm{HO}}(x)=\frac{1}{2}m\omega^2x^2$ is the one-dimensional harmonic oscillator potential and where $n=0, 1, 2, 3,\ldots$. Next, it will be shown that for each n there exists a standard and a generalized Darboux potential that are partners to the former potential.

When $n=0$ we have

$$\psi_0=\left(\frac{1}{\pi}\right)^{1/4}e^{-(m\omega/2\hbar)x^2}\quad\text{and}\quad\lambda_0=\frac{\hbar\omega}{2} \tag{32}$$

for which, according to Eq. (5), it follows that

$$\sigma_{p_0}(x)=-\frac{m\omega}{\hbar}x \tag{33}$$

and, consequently, from Eq. (7), the standard Darboux potential becomes

$$V_{\mathrm{D}_0}(x)=\tfrac{1}{2}m\omega^2x^2+\hbar\omega, \tag{34}$$

where the subscript $_0$ in $V_{\mathrm{D}}(x)$ is used to emphasize that this potential comes from the choice of $n=0$. Also, it should be remembered that we have used $\hbar^2/m=2$.

Similarly, for the generalized Darboux potential the wavefunction

$$\psi_{g_0}=e^{-(m\omega/2\hbar)x^2}\left(\gamma+b\int e^{(m\omega/\hbar)x^2}dx\right) \tag{35}$$

is used in Eq. (17) in order to find

$$\sigma_{g_0}(x) = -\frac{m\omega}{\hbar}x + \frac{be^{(m\omega/\hbar)x^2}}{\gamma + b\int^x e^{(m\omega/\hbar)x^2}dx} \tag{36}$$

which, after using Eq. (23), leads to

$$V_{\mathrm{DG}_0}(x) = \frac{1}{2}m\omega^2x^2 + \hbar\omega - \frac{\hbar^2}{m}\frac{d}{dx}\left(\frac{be^{(m\omega/\hbar)x^2}}{\gamma + b\int^x e^{(m\omega/\hbar)x^2}dx}\right). \tag{37}$$

This potential has been identified by Mielnik[8] as a new isospectral potential that matches the spectra obtained for the harmonic oscillator Hamiltonian.

When $n=1$, following the procedure already displayed, we have

$$\psi_1 = \sqrt{\frac{2m\omega}{\hbar\sqrt{\pi}}}xe^{-(m\omega/2\hbar)x^2} \quad \text{and} \quad \lambda_1 = \frac{3\hbar\omega}{2} \tag{38}$$

for which

$$\sigma_{p_1}(x) = \frac{1}{x} - \frac{m\omega}{\hbar}x \tag{39}$$

and, consequently,

$$V_{\mathrm{D}_1}(x) = \frac{1}{2}m\omega^2x^2 + \hbar\omega\left(1 + \frac{\hbar}{m\omega x^2}\right) \tag{40}$$

is the standard Darboux potential associated to $n=1$.

Consequently, for the generalized Darboux potential we use Eq. (17) in order to find

$$\sigma_{g_1}(x) = \frac{1}{x} - \frac{m\omega}{\hbar}x + \frac{be^{(m\omega/\hbar)x^2}/x^2}{\gamma + b\int^x (e^{(m\omega/\hbar)x^2}/x^2)\,dx} \tag{41}$$

and Eq. (23) to obtain

$$V_{\mathrm{DG}_1}(x) = \frac{1}{2}m\omega^2x^2 + \hbar\omega + \frac{\hbar^2}{m}\left\{\frac{1}{x^2} - \frac{d}{dx}\left(\frac{be^{(m\omega/\hbar)x^2}/x^2}{\gamma + b\int^x (e^{(m\omega/\hbar)x^2}/x^2)\,dx}\right)\right\}, \tag{42}$$

which is an isospectral potential set that comes from the second eigenfunction of the harmonic oscillator potential.

In the case of $n=2$, we have

$$\psi_2 = \left(\frac{1}{8\sqrt{\pi}}\right)^{1/2}\left(\frac{4m\omega}{\hbar}x^2 - 2\right)e^{-(m\omega/2\hbar)x^2} \quad \text{and} \quad \lambda_2 = \frac{5\hbar\omega}{2} \tag{43}$$

for which

$$\sigma_{p_2}(x) = \frac{4(m\omega/\hbar))x}{2(m\omega/\hbar)x^2 - 1} - \frac{m\omega}{\hbar}x \tag{44}$$

and

$$V_{D_2}(x) = \frac{1}{2}m\omega^2x^2 + \hbar\omega\left\{1 - \frac{4}{2(m\omega/\hbar)x^2 - 1} + \left(\frac{4\sqrt{m\omega/\hbar}x}{2(m\omega/\hbar)x^2 - 1}\right)^2\right\} \tag{45}$$

is the standard Darboux potential associated to $n=2$.

Similarly, the generalized Darboux potential that corresponds to this case is obtained from

$$\sigma_{g_2}(x)=\frac{4(m\omega/\hbar)x}{2(m\omega/\hbar)x^2-1}-\frac{m\omega}{\hbar}x+\frac{be^{(m\omega/\hbar)x^2}/(2(m\omega/\hbar)x^2-1)^2}{\gamma+b\int^x[e^{(m\omega/\hbar)x^2}/(2(m\omega/\hbar)x^2-1)^2]\,dx} \tag{46}$$

and Eq. (23) in order to have

$$V_{\mathrm{DG}_2}(x)=\frac{1}{2}m\omega^2x^2+\hbar\omega\left\{1-\frac{4}{2(m\omega/\hbar)x^2-1}+\left(\frac{4\sqrt{m\omega/\hbar}x}{2(m\omega/\hbar)x^2-1}\right)^2 - \frac{\hbar}{m\omega}\frac{d}{dx}\left(\frac{b\,e^{(m\omega/\hbar)x^2}/(2(m\omega/\hbar)x^2-1)^2}{\gamma+b\int^x[e^{(m\omega/\hbar)x^2}/(2(m\omega/\hbar)x^2-1)^2]\,dx}\right)\right\} \tag{47}$$

from the eigenvalue $n=2$ of the harmonic oscillator potential.

C. The Darboux potentials of the HO model for any *n* eigenfunction

As can be appreciated in the preceding paragraph, the choice of each quantum number leads to specific eigenvalues for which one can find each time the corresponding standard and generalized Darboux potentials. In this section we give the general formulas that allow us to obtain the Darboux potentials in the most general case, any n quantum principal number. That is, by using the wavefunction

$$\psi_n=C_ne^{-(m\omega/2\hbar)x^2}H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\quad\text{and}\quad\lambda_n=\hbar\omega\left(n+\frac{1}{2}\right), \tag{48}$$

where $C_n=(\sqrt{\pi}n!2^n)^{-1/2}$, it follows that

$$\sigma_{p_n}(x)=\frac{d}{dx}\ln H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)-\left(\frac{m\omega}{\hbar}\right)x \tag{49}$$

in order to get

$$\sigma'_{g_n}(x)=\sigma'_{p_n}(x)+\frac{b}{\rho_n(x)} \tag{50}$$

where

$$\frac{1}{\rho_n(x)}=\frac{d}{bdx}\ln\left(\gamma+\int\frac{be^{(m\omega/\hbar)x^2}dx}{H_n^2(\sqrt{m\omega/\hbar}x)}\right). \tag{51}$$

Hence, the n-generalized Darboux potential becomes

$$V_{\mathrm{DG}_n}(x)=\frac{1}{2}m\omega^2x^2+\hbar\omega-\frac{\hbar^2}{m}\frac{d^2}{dx^2}\ln\left(H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\left(\gamma+\int\frac{be^{(m\omega/\hbar)x^2}dx}{H_n^2(\sqrt{m\omega/\hbar}x)}\right)\right), \tag{52}$$

which reduces, for $b=0$ and $\gamma=1$, to the n-standard Darboux potential

$$V_{\mathrm{D}_n}(x)=\frac{1}{2}m\omega^2x^2+\hbar\omega\left(1-\frac{\hbar}{m\omega}\frac{d^2}{dx^2}\ln H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\right). \tag{53}$$

These Darboux potentials are isospectral with respect to the original Hamiltonian of the standard HO with the corresponding wavefunctions

$$\varphi_{Dg_n}=\left(\frac{d}{dx}-\sigma_{g_n}(x)\right)\psi_n \tag{54}$$

and

$$\varphi_{D_n}=\psi_n'-\sigma_{p_n}(x)\psi_n \tag{55}$$

as mentioned before.

With this example, we have shown the usefulness of the proposed generalized Darboux transform in quantum mechanical problems dedicated to obtain new sets of isospectral potentials which, as shown above, are the standard and generalized Darboux potentials. That is, the application to other specific potential models different from the case here exemplified is straightforward. For these, it can be easily proved that the generalized Darboux transform leads to various new isospectral potentials recently published, such as the free particle,[12] Hulthen,[13] hydrogenic and isotonic,[15] Morse,[16] Coulomb,[17] anharmonic oscillators[18] and other potential models.

In any case, the use of different eigenfunctions leads to different varieties of potential that can give more possibilities to understand exactly solved problems. That is, it is interesting to know whether there are some physical quantities which can be used to characterize different potentials, in the same class, with the same energy spectrum, as solution of relevant physical problems. So, the importance of the isospectral potentials is equivalent to the importance of supersymmetry in quantum mechanics due to the fact that the Darboux transform provides a basis for the supersymmetry theory.[11] In a similar way, the generalized Darboux transform applied to other fields, such as solitons, should improve the findings already published elsewhere as will be shown in the next section with the linear Bargmann potential[19] as a worked example.

V. THE GENERALIZED DARBOUX TRANSFORM AND SOLITONS

The connection between a nonlinear partial differential equation that exhibits soliton behavior, the Korteweg–deVries (KdV) relationship, and a linear eigenvalue problem such as the Schrödinger equation is well known. In fact, although the partial differential equations that govern the motion of solitons are nonlinear, they are closely related to the Sturm–Liouville equations for which the analytical expressions that describe multisoliton interactions are merely Bargmann potentials. Thus, as another example of the usefulness of the proposed generalized Darboux transform, in this section we consider its application in solitons by assuming that the Sturm–Liouville equation

$$y''+(k^2-u(x))y=0 \tag{56}$$

has as solution

$$y=e^{ikx}F(k,x). \tag{57}$$

According to our method, applying Eq. (5) to the linear k form

$$F(k,x)=2k+ia(x) \tag{58}$$

leads to

$$\sigma_{p_1}(x)=\frac{2ik^2+ia'(x)-ka(x)}{2k+ia(x)} \tag{59}$$

for which Eq. (16), with $C=-k^2$, is written as

$$ia''(x)-2ka'(x)=u(x)(2k+ia(x)). \tag{60}$$

The above relationship for $k\neq 0$ gives place to the conditions

$$u(x)=-a'(x) \quad \text{and} \quad a''(x)=a(x)u(x) \tag{61}$$

that are put together in order to find the equivalent of Eq. (11),

$$\frac{d}{dx}\left(a'(x)+\frac{1}{2}a^2(x)\right)=0. \tag{62}$$

Thus, integration of the latter equation yields the Riccati relationship

$$a'(x)+\tfrac{1}{2}a^2(x)=2\mu^2, \tag{63}$$

which, with $a(x)=2g'(x)/g(x)$, leads to the second order differential equation

$$g''(x)-\mu^2 g(x)=0 \tag{64}$$

which has as solution

$$g(x)=\alpha e^{\mu x}+\beta e^{-\mu x}. \tag{65}$$

That is,

$$\frac{1}{2\mu}a(x)=\frac{\alpha e^{\mu x}-\beta e^{-\mu x}}{\alpha e^{\mu x}+\beta e^{-\mu x}}=\tanh(\mu x-\phi), \tag{66}$$

where $\phi=\frac{1}{2}\ln\beta/\alpha$, permits us to obtain the linear Bargmann potential[19]

$$u(x)=-2\mu^2\,\mathrm{sech}^2(\mu x-\phi) \tag{67}$$

that is the single soliton solution of the Korteweg–deVries relationship[20]

$$u(x)_t-6u(x)u(x)_x+u(x)_{xxx}=0 \tag{68}$$

on condition that $\phi_t=4\mu^3$. As usual, the subscripts in KdV mean total derivative with respect to the index variable.

On the other hand, due to the fact that Eq. (16) indicates that $u(x)$ is given in terms of $\sigma_{p_1}(x)$, it becomes that $\sigma_{p_1}(x)=\sigma(x)$ is at the time a solution of

$$\sigma(x)_t=(-\sigma(x)_{xx}+2\sigma(x)^3+6k^2\sigma(x))_x \tag{69}$$

which has been identified as the modified KdV relationship.

Thus, in a similar way it can be shown that the associated Darboux potential given in Eq. (19) is a solution of

$$U_{\mathrm{D}}(x)_t=-U_{\mathrm{D}}(x)_{xxx}+6U_{\mathrm{D}}(x)U_{\mathrm{D}}(x)_x \tag{70}$$

as well as the generalized Darboux potential that corresponds to the Bargmann model. The details of these calculations and a more complete analysis on this application will be given in a forthcoming publication. However, we hope that with these examples we have shown the usefulness of the GDT and that the method proposed has significance and interest beyond that of a purely mathematical device.

VI. CONCLUDING REMARKS

In the present work the standard Darboux transform applied to Sturm–Liouville problems has been generalized. This generalization has been possible due to the fact that the standard Darboux transform is related to Riccati-type equations whose general solutions can be obtained straightforwardly. As a useful application of the generalized Darboux transform we consider explicitly the quantum mechanical problem associated to the one-dimensional harmonic oscillator potential. As expected, we obtain the generalized and standard Darboux potentials associated to the harmonic oscillator model, one for each quantum principal number. Besides, a general formula for the corresponding Darboux potential for any n is given. In all cases considered, the standard and generalized Darboux potentials correspond to a new set of isospectral potentials whose energy is that of the former potential, indicating a direct procedure for generalizing any known potential model. Similarly, in other fields where the standard Darboux transform is involved, our proposition of generalized Darboux transform will be an important improvement *vis a vis* to other alternative procedures usually used with similar purposes such as that exemplified with the treatment of the linear Bargmann potential in the theory of solitons.

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Erratum: ''Structure and properties of Hughston's stochastic extension of the Schrödinger equation'' [J. Math. Phys. 41, 2485 (2000)]

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In the line immediately following Eq. (20b), the text Eq. (18a) should read Eq. (16a). In other words, the density matrix evolution of Eq. (21a) follows directly from Hughston's equation [Eq. (16a)], and does not use the state vector evolution assumed in Eq. (17a) through Eq. (19), as the misprint would suggest.

Erratum: "On characteristic equations, trace identities and Casimir operators of simple Lie algebras" [J. Math. Phys. 41, 3192–3225 (2000)]

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First, there is a typographical error in Eq. (4.50a). This equation, cf. (A37a), should read

$$\mathrm{tr}(x_{(i_1}\cdots x_{i_4)}) = \tfrac{1}{12} d^{(2)}_{(i_1 i_2} d^{(2)}_{i_3 i_4)}\,. \tag{4.50a}$$

Second, Eqs. (4.41a) and (4.41b) as well as (4.43a) and (4.43b) are inconsistent with (A40b) and (A42c) and (A42d) due to the normalization of $A = a_j x_j$ in Appendix A7(i). We wish to retain the definition $A = a_j x_j$, and so the former set of equations have to be corrected:

$$\mathrm{tr}(x_{(i_1}\cdots x_{i_8)}) = -\tfrac{5}{12}\delta_{(i_1 i_2}\delta_{i_3 i_4}\delta_{i_5 i_6}\delta_{i_7 i_8)} + \tfrac{4}{3}\delta_{(i_1 i_2} d^{(6)}_{i_3\cdots i_8)}\,, \tag{4.41a}$$

$$\mathrm{tr}(x_{(i_1}\cdots x_{i_{10})}) = -\tfrac{1}{2}\delta_{(i_1 i_2}\delta_{i_3 i_4}\delta_{i_5 i_6}\delta_{i_7 i_8}\delta_{i_9 i_{10})} + \tfrac{5}{4}\delta_{(i_1 i_2}\delta_{i_3 i_4} d^{(6)}_{i_5\cdots i_{10})}\,, \tag{4.41b}$$

and

$$\mathrm{tr}(F_{(i_1}\cdots F_{i_6)}) = 30\,\delta_{(i_1 i_2}\delta_{i_3 i_4}\delta_{i_5 i_6)} - 26\, d^{(6)}_{(i_1\cdots i_6)}\,, \tag{4.43a}$$

$$\mathrm{tr}(F_{(i_1}\cdots F_{i_8)}) = \tfrac{515}{6}\,\delta_{(i_1 i_2}\delta_{i_3 i_4}\delta_{i_5 i_6}\delta_{i_7 i_8)} - \tfrac{320}{3}\,\delta_{(i_1 i_2} d^{(6)}_{i_3\cdots i_8)}\,. \tag{4.43b}$$

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Erratum: "A note on families of spin observables and a generalization of Wigner's theorem in $\mathbb{C}^2$" [J. Math. Phys. 41, 7832 (2000)]

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Due to a production error, a box symbol (□) was placed incorrectly on p. 7837. It should have been placed at the end of the proof of Lemma IV.5, but was placed incorrectly at the end of the previous paragraph. AIP apologizes for this error.

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Uncertainty for spin systems

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A modified definition of quantum mechanical uncertainty Δ for spin systems, which is invariant under the action of SU(2), is suggested. Its range is shown to be $\hbar^2 j \leqslant \Delta \leqslant \hbar^2 j(j+1)$ within any irreducible representation j of SU(2) and its mean value in Hilbert space computed using the Fubini–Study metric is determined to be $\text{mean}(\Delta) = \hbar^2 j(j+1/2)$. The most used sets of coherent states in spin systems coincide with the set of minimum Δ uncertainty states. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1336515]

I. INTRODUCTION

Coherent states are an important tool in the study of wave phenomena finding many relevant applications in quantum physics.[1,2] The familiar Glauber states[3,4] can be equivalently defined as the elements of the orbit of the Heisenberg–Weyl group which contains the ground state, as the eigenstates of the annihilation operator or as the minimum uncertainty wave packets. Following these different definitions there are different approaches to the generalization of the concept of coherent states, the one based on the first definition[5] being the most popular. The generalization procedure has been extended to include spin systems[6,7] and others.[8–11] A full account of applications of coherent states in different areas of physics can be found in Ref. 12. In the group theoretical approach to coherent states Hilbert space is decomposed into the union of disjoint sets of coherent states, the group orbits. For spin systems the orbit space (the set of orbits) is composed almost entirely of three-dimensional orbits with the exception of a finite number of two-dimensional orbits which consist of the eigenvectors of $\mathbf{r}\cdot\mathbf{J}$, with $\mathbf{J}$ the generators of the Lie algebra of SU(2) and $\mathbf{r}$ any numeric vector.[13,14] In each irreducible representation of SU(2) there is one particular orbit which admits an analytic representation in the complex plane,

$$|z\rangle = \frac{1}{(1+|z|^2)^j} e^{zJ_-}|j\rangle.$$

It turns out that this orbit is singled out by the structure of orbit space; it is the two-dimensional orbit composed of the eigenvectors of $\mathbf{r}\cdot\mathbf{J}$ with the highest absolute value of its eigenvalue.[14] However the states belonging to this orbit are not all minimum uncertainty states; they do not even have constant uncertainty.

Uncertainty is an important property of a physical state, and it would be desirable to keep it playing a major role in the definition of coherent states. Minimum uncertainty states have been studied in Ref. 15 and, in the context of spin systems, states saturating the equality in the Heisenberg relation have been studied in Ref. 16 and called intelligent states. States saturating the equality in the Robertson relation have also been studied.[17,18] One unsatisfactory feature of intelligent states and of the commonly used definition of uncertainty for spin systems is that they are not invariants under the action of SU(2). As a consequence sets of coherent states based on these definitions cannot be represented as orbits of SU(2). This is in contrast with the situation in

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particle mechanics where the Heisenberg inequality and the uncertainty function used are invariants under the action of the Heisenberg–Weyl group. Here we propose a new definition of uncertainty for spin systems,

$$\Delta = \Delta J_x^2 + \Delta J_y^2 + \Delta J_z^2,$$

which is a positive increasing function of the variances and which is invariant under the action of SU(2). It obeys the following invariant inequalities,

$$\hbar^2 j \leqslant \Delta \leqslant \hbar^2 j(j+1),$$

which play the role of uncertainty relations. As an immediate application we show that the particular set of coherent states which admits an analytic representation in the complex plane coincides with the set of minimum uncertainty states for this inequality. We use the Fubini–Study metric to compute the mean value of the uncertainty Δ in Hilbert space with the result,

$$\text{mean}(\Delta) = \hbar^2 j(j+\tfrac{1}{2}),$$

for any irreducible representation j. This shows that in higher dimensional representation spaces of SU(2) most of the states have high values of uncertainty. In particular one has

$$\lim_{j\to\infty} \frac{\text{mean}(\Delta)}{\max(\Delta)} = 1. \tag{1}$$

The paper is organized as follows: In Sec. II we review some mathematical definitions concerning group orbits and invariants, the Glauber coherent states and their generalization, and the construction of spin coherent states. In Sec. III we discuss the issue of Heisenberg-type inequalities and uncertainty relations. We propose the new definition of uncertainty Δ for spin systems and we state and prove the statements about Δ made above. We include an appendix on how to average quantities in CP^N using the Fubini–Study metric.

II. REVIEW OF GROUP ORBITS AND COHERENT STATES

A. Group orbits and invariants

Let $U(g)$ be a representation of the Lie group G on the Hilbert space $\mathcal{H}$. The G-orbit through $|\phi\rangle \in \mathcal{H}$ is the subset of $\mathcal{H}$ given by

$$\mathcal{C}_\phi = \{|\psi\rangle \in \mathcal{H} : |\psi\rangle = U(g)|\phi\rangle,\ g \in G\}. \tag{2}$$

It follows that

$$\dim \mathcal{C}_\phi \leqslant \dim G \quad \text{and} \quad \dim \mathcal{C}_\phi \leqslant \dim \mathcal{H}. \tag{3}$$

The relation "$|\phi'\rangle$ lies on the same orbit as $|\phi\rangle$" is clearly an equivalence relation: reflexive, symmetric and transitive. As a consequence $\mathcal{H}$ can be partitioned into disjoint orbits

$$\mathcal{H} = \bigcup_\phi \mathcal{C}_\phi, \tag{4}$$

where the label ϕ runs over orbits (equivalence classes) and not over vectors. The quotient space $\mathcal{H}/G$ is called the orbit space. A function $f(|\psi\rangle)$ in Hilbert space $\mathcal{H}$ is said to be G-invariant if

$$f(U(g)|\psi\rangle) = f(|\psi\rangle), \quad \forall g \in G, \quad \forall |\psi\rangle \in \mathcal{H}. \tag{5}$$

It follows that G-invariant functions are also functions on orbit space $\mathcal{H}/G$.

For more information on these issues see, for instance, Refs. 19 and 20,

B. Glauber states

The familiar Glauber states $|q,p\rangle$ in particle mechanics can be seen as the G-orbit of the Heisenberg–Weyl group through the vacuum state $|0\rangle$,

$$|q,p\rangle = U(q,p)|0\rangle, \tag{6}$$

where $U(p,q)$ is the Weyl operator,

$$U(q,p) = e^{i(pQ-qP)/\hbar}. \tag{7}$$

They are eigenstates of the annihilation operator and they admit the useful analytic representation in the complex plane,

$$|p,q\rangle = e^{(za^+ - z^* a)}|0\rangle = e^{-|z|^2/2}\sum_n \frac{z^n}{\sqrt{n!}}|n\rangle, \tag{8}$$

with $z=(q+ip)/\sqrt{2\hbar}$. It can be shown that the Glauber states are minimum uncertainty states since

$$\Delta Q^2 = \Delta P^2 = \hbar/2, \tag{9}$$

and the equality sign is satisfied in the Heisenberg uncertainty relation (sometimes the square root of this relation is used; here we prefer this form)

$$\Delta Q^2 \Delta P^2 \geqslant \hbar^2/4. \tag{10}$$

The remaining G-orbits of the Heisenberg–Weyl group can be seen as generalized coherent states[5,12] but they are not eigenstates of any particularly simple operator, they do not admit an analytic representation in the complex plane, and they are not minimum uncertainty states. Nevertheless they have constant values of uncertainty since both factors ΔQ^2 and ΔP^2 are G-invariant functions.[14]

C. Spin coherent states

The group SU(2) admits representations classified according to integer and semi-integer values j with the Casimir operator $J^2 = j(j+1)\hbar^2$. Let $\mathcal{H}$ be a Hilbert space carrying one such representation. Sets of generalized coherent states can be generated as the orbits of SU(2) in $\mathcal{H}$,

$$\mathcal{C}_\phi = \{|\mathbf{r}\rangle \in \mathcal{H} : |\mathbf{r}\rangle = U(\mathbf{r})|\phi\rangle, \mathbf{r} \in (4\pi)^3\} \tag{11}$$

$$U(\mathbf{r}) = e^{i\mathbf{r}\cdot\mathbf{J}/\hbar}, \tag{12}$$

where we used the so-called canonical group coordinates for generality.

Using the group parameterization

$$U(z,\theta) = N e^{zJ_-/\hbar} e^{-z^* J_+/\hbar} e^{-i\theta J_z/\hbar}, \tag{13}$$

where $J_\pm$ are the ladder operators $J_\pm = J_x \pm iJ_y$, and choosing the fiducial state $|\phi\rangle$ to be an eigenstate of J_z, $|m\rangle$ with $m=-j,\ldots,j$, one has[7]

$$|z;m\rangle = U(z)|m\rangle = N e^{zJ_-/\hbar} e^{-z^* J_+/\hbar}|m\rangle, \tag{14}$$

where the phase factor resulting from $e^{-i\theta J_z/\hbar}$ has been ignored and N stands for a normalization factor. Further choosing $|j\rangle$ as the fiducial state one has $e^{-z^* J_+/\hbar}|j\rangle = |j\rangle$ and

$$|z\rangle = \frac{1}{(1+|z|^2)^j} e^{zJ_-}|j\rangle, \tag{15}$$

after determination of the normalization factor. This analytic representation is not available in general for the sets (12) generated from arbitrary fiducial vectors. The analogous relation for spin systems to the Heisenberg inequality for canonically conjugate operators (10) is

$$\Delta J_x^2 \Delta J_y^2 \geqslant \frac{\hbar^2}{4} \overline{J_z}^2. \tag{16}$$

Notice the important difference with (10) that now the right-hand side of the inequality is not a constant. Following Ref. 16 we shall call the left-hand side of (16) the uncertainty $\Delta J_x^2 \Delta J_y^2$. Then it is clear that the set of states for which the equality in (16) is saturated and the set of states of minimum uncertainty are not the same. Moreover none of them coincide with any set of coherent states (11). On the other hand in particle mechanics the Glauber states satisfy the Heisenberg inequality and they are states of minimum uncertainty. In Ref. 16 the spin states satisfying the equality sign in (16) have been called intelligent states. They are given by

$$|\tau,N\rangle = \frac{A_N}{(1+|\tau|^2)^j} \sum_{l=0}^{N} \binom{N}{l} (2j-l)! \left(-\frac{2}{\hbar}\tau J_+\right)^l e^{\tau J_+/\hbar}|-j\rangle, \tag{17}$$

where N is a discrete label satisfying $0 \leqslant N \leqslant 2j$ and τ is a continuous label which can be either real or purely imaginary. A_N is a normalization factor.

Finally we comment that the space of physical states for the irreducible representation j of SU(2) is CP^N with $N=2j$ (see the Appendix),

$$j \to \dim \mathcal{H} = 2j+1 \to \text{projective space} : CP^{2j}. \tag{18}$$

Its real dimension is $4j$.

III. UNCERTAINTY

A. Uncertainty relations

We recall the inequality valid for Hermitian operators A and B,[21]

$$\Delta A^2 \Delta B^2 \geqslant \tfrac{1}{4}(\sigma_{AB}^2 - \overline{[A,B]}^2), \tag{19}$$

where ΔA and ΔB are the standard deviations of the operators A and B

$$\Delta A^2 = \overline{A^2} - \overline{A}^2 = \langle\psi|A^2|\psi\rangle - \langle\psi|A|\psi\rangle^2. \tag{20}$$

and where

$$\sigma_{AB} = \overline{\{A,B\}} - 2\overline{A}\,\overline{B} \geqslant 0 \tag{21}$$

is the covariance of A and B. Since for Hermitian operators σ_{AB} is real and $\overline{[A,B]}$ is purely imaginary, both parcels on the right-hand side of (19) are positive and one can state that

$$\Delta A^2 \Delta B^2 \geqslant -\tfrac{1}{4}\overline{[A,B]}^2. \tag{22}$$

This is called the Heisenberg relation while (19) is often called the Robertson relation. For canonically conjugate operators Q and P one has $[Q,P]=i\hbar$ and the Heisenberg uncertainty relation (10) follows immediately from (22). For spin systems (16) follows from $[J_x,J_y] = i\hbar J_z$. Notice that the equality can hold only if $\sigma_{AB}=0$. The left-hand side of the Heisenberg

inequality (22) is sometimes called the uncertainty. It is invariant under the action of the Heisenberg–Weyl group. And the right-hand side of (22) is a constant. It is therefore natural to assign a particular physical significance to $\Delta Q^2 \Delta P^2$ and to the states satisfying the equality sign in this inequality. But the left hand side of the analogous spin inequality (16) is not invariant under the action of SU(2) neither is its right hand side a constant. Therefore there seems to be no reason why $\Delta J_x^2 \Delta J_y^2$ should play a role for spin systems similar to the one played by $\Delta Q^2 \Delta P^2$ in particle mechanics, nor why states saturating the equality in (22) or in (19) should be particularly distinguished. Such states (intelligent states) have been studied in Ref. 16 and in Refs. 17 and 18, respectively, and may certainly be important for the study of spin systems with Hamiltonians that break the SU(2) symmetry such as systems under the action of one particular magnetic field pointing in the *z*-direction, but in what concerns the study of CP^N as the representation space for spin systems prior to the definition of the Hamiltonian one should look for a *G*-invariant definition of uncertainty. We look for an uncertainty function which is positive and which increases with increasing values of the variances of the elements of the Lie algebra. The following additive rather than multiplicative combination of variances does the job,

$$\Delta = \Delta J_x^2 + \Delta J_y^2 + \Delta J_z^2. \tag{23}$$

The following results hold:

(I) The uncertainty Δ is *G*-invariant and therefore it is constant within sets of coherent states generated as orbits of SU(2) in CP^N;

(II) The uncertainty Δ is bounded from below and from above

$$\hbar^2 j \leqslant \Delta \leqslant \hbar^2 j(j+1). \tag{24}$$

All values within this range are present in Hilbert space except for the representation $j = 1/2$ where all states have the same uncertainty $\Delta = \hbar^2 j$;

(III) The set

$$\{|\psi\rangle \in \mathcal{H}: \Delta(|\psi\rangle) = \hbar^2 j\} \tag{25}$$

of minimum uncertainty vectors in the irreducible representation j of SU(2) coincides with the set of coherent states

$$|z\rangle = (1+|z|^2)^{-j} e^{zJ_-}|j\rangle \tag{26}$$

generated as an orbit of SU(2) in $\mathcal{H}$ and admitting an analytic representation in the complex plane;

(IV) The mean value evaluated with the volume element naturally associated to the Fubini–Study metric of uncertainty on the whole of Hilbert space is given by

$$\text{mean}(\Delta) = \hbar^2 j(j+1/2) \tag{27}$$

for any irreducible representation j of SU(2). Notice that the last statement is consistent with the second one for the $j = 1/2$ representation.

B. Proof

(I) We have

$$U^+(\mathbf{r}) J_i U(\mathbf{r}) = \Lambda_i^j(\mathbf{r}) J_j, \tag{28}$$

where Λ_i^j are the matrices of the adjoint representation of SU(2), satisfying

$$\Lambda_i^j(\mathbf{r}) \Lambda_i^k(\mathbf{r}) = \delta^{jk}, \forall \mathbf{r}. \tag{29}$$

The mean values of J_i transforms, within an orbit, according to the adjoint representation too,

$$\overline{J_i} = \langle \mathbf{r}|J_i|\mathbf{r}\rangle = \langle \phi|U^+(\mathbf{r}) J_i U(\mathbf{r})|\phi\rangle = \Lambda_i^j(\mathbf{r}) \langle \phi|J_j|\phi\rangle. \tag{30}$$

Then $\overline{J_i J_i}$ is a G-invariant function

$$\overline{J_i J_i} = \Lambda_i^j(\mathbf{r})\langle\phi|J_j|\phi\rangle\Lambda_i^k(\mathbf{r})\langle\phi|J_k|\phi\rangle = \langle\phi|J_i|\phi\rangle\langle\phi|J_i|\phi\rangle. \tag{31}$$

This is one example of a wider set of invariants defined in Ref. 14. The Casimir operator $J_i J_i$ is invariant within the whole representation and consequently $\overline{J_i J_i}$ is G-invariant. Then,

$$\Delta = \sum_{i=x,y,z} \Delta J_i^2 = \sum_{i=x,y,z} \overline{J_i J_i} - \overline{J_i J_i} \tag{32}$$

is the difference between two G-invariant functions and is therefore G-invariant too.

(II) It is always possible to choose a representative $|\psi\rangle = \Sigma_{m=-j}^{m} c_m|m\rangle$ within each orbit such that $\langle\psi|\mathbf{J}|\psi\rangle = \overline{J_z}\mathbf{e}_z$. Then $\overline{J_i J_i} = \overline{J_z}^2$. But

$$\overline{J_z} = \sum_{m=-j}^{j} m\hbar|c_m|^2 \Rightarrow |\overline{J_z}| \leqslant \hbar j. \tag{33}$$

Therefore $\overline{J_i J_i} \leqslant \hbar^2 j^2$, and this inequality is valid all over Hilbert space since it concerns a G-invariant function. On the other hand it is obvious that $\overline{J_i J_i} \geqslant 0$. Since $J_i J_i = \hbar^2 j(j+1)$ it follows that

$$0 \leqslant \overline{J_i J_i} \leqslant \hbar^2 j^2 \Leftrightarrow \hbar^2 j \leqslant \Delta \leqslant \hbar^2 j(j+1). \tag{34}$$

Now we consider the one-parameter set of vectors

$$|\alpha\rangle = \cos\alpha|j\rangle + \sin\alpha|-j\rangle \quad \text{with} \quad \alpha \in [0, \pi/2]. \tag{35}$$

We have

$$\begin{aligned} &\overline{J_x} = \hbar\sqrt{j/2}\sin(2\alpha)\,\delta_j^{1-j},\ \overline{J_y} = 0,\ \overline{J_z} = \hbar j\cos(2\alpha) \\ &\Rightarrow \overline{J_i J_i} = \begin{cases} \hbar^2 j^2 & \text{for } j = 1/2 \\ \hbar^2 j^2\cos^2(2\alpha) & \text{for } j \neq 1/2. \end{cases} \end{aligned} \tag{36}$$

There is only one orbit in the $j = 1/2$ representation;[14] since Δ is G-invariant it can only assume the value $\hbar^2 j^2$. On the other hand, for $j \neq 1/2$ it is clear that $\overline{J_i J_i}$ maps α onto $[0, \hbar^2 j^2]$, and the statements about the range of $\overline{J_i J_i}$ in Hilbert space are proven.

(III) We notice from (33) that the maximum value of $\overline{J_i J_i}$ is attained only at the vectors $|j\rangle$ and $|-j\rangle$ which we know to belong to the same orbit.[14] This single orbit coincides with the set (15) of coherent states $|z\rangle$ since for $z = 0$ we have $|z\rangle = |j\rangle$.

(IV) We use the coordinates (A16) defined in the Appendix to label physical states

$$|\psi\rangle = \sum_{m=-j}^{j} c_m|m\rangle = \sum_{n=0}^{N} Z_n(\theta_i, \beta_j)|n - N/2\rangle = |\{\theta_i\}, \{\beta_j\}\rangle. \tag{37}$$

Using the standard representation of the generator J_z of the SU(2) Lie algebra[22] its mean value on a state $|\{\theta_i\}, \{\beta_j\}\rangle$ is

$$\overline{J_z} = \sum_{m=-j}^{j} |c_m|^2 \hbar m = \hbar \sum_{n=0}^{N} x_n^2 \left(n - \frac{N}{2}\right). \tag{38}$$

The mean value of $\overline{J_z}^2$ in the whole of Hilbert space is thus [see (A24) in the appendix],

$$\text{mean}(\overline{J_z}^2)=\frac{\hbar^2}{V_N}\int_{CP^N}dv\,\overline{J_z}^2=\frac{\hbar^2}{V_N}\sum_{m,n=0}^{N}\left[\left(m-\frac{N}{2}\right)\left(n-\frac{N}{2}\right)\int_{CP^N}dv\,(x_m x_n)^2\right]. \tag{39}$$

Now we compute

$$\int_{CP^N}dv\,(x_m x_n)^2=\frac{\pi^N}{(N+2)!}(1+\delta_{mn}) \tag{40}$$

and

$$\sum_{m,n=0}^{N}\left(m-\frac{N}{2}\right)\left(n-\frac{N}{2}\right)(1+\delta_{mn})=\sum_{n=0}^{N}\left(n-\frac{N}{2}\right)^2=\frac{N(N+1)(N+2)}{12} \tag{41}$$

to arrive at

$$\text{mean}(\overline{J_z}^2)=\frac{\hbar^2}{V_N}\frac{\pi^N}{(N+2)!}\frac{N(N+1)(N+2)}{12}=\frac{\hbar^2 N}{12}. \tag{42}$$

By symmetry one has

$$\text{mean}(\overline{J_x}^2)=\text{mean}(\overline{J_y}^2)=\text{mean}(\overline{J_z}^2), \tag{43}$$

and consequently

$$\text{mean}(\overline{J_i J_i})=3\,\text{mean}(\overline{J_z}^2)=\frac{\hbar^2 N}{4}=\frac{\hbar^2 j}{2}. \tag{44}$$

The mean value of uncertainty (32) in Hilbert space is therefore

$$\text{mean}(\Delta)=\text{mean}(\overline{J_i J_i})-\text{mean}(\overline{J_i J_i})=\hbar^2 j(j+1)-\frac{\hbar^2 j}{2}=\hbar^2 j\left(j+\frac{1}{2}\right). \tag{45}$$

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APPENDIX: THE FUBINI–STUDY METRIC AND THE VOLUME ELEMENT IN CP^N

Two vectors in Hilbert space $\mathcal{H}$ differing by a multiplicative non-zero complex constant α represent the same physical state,

$$|z'\rangle\sim|z\rangle \quad \text{if} \quad |z'\rangle=\alpha|z\rangle. \tag{A1}$$

Therefore the space of physical states is the space of rays in Hilbert space or projective space, that is the space of equivalence classes defined by (A1) and excluding the vector $|\psi\rangle=0$. The projective spaces constructed from finite-dimensional Hilbert spaces are called CP^N and are well studied spaces.[23,24] The superscript N stands for their complex dimension which is one unit lower then the complex dimension of the Hilbert space from which they are constructed. If $|n\rangle$ is a basis for $(N+1)$-dimensional Hilbert space any vector $|\psi\rangle$ can be written as

$$|\psi\rangle=\sum_{n=0}^{N}Z_n|n\rangle. \tag{A2}$$

The complex numbers Z_n are homogeneous coordinates in $\mathcal{H}$ and they can also be used as coordinates in CP^N provided one makes the identifications

$$Z'_n \sim Z_n \text{ if } \exists \alpha : \forall n, Z'_n = \alpha Z_n . \tag{A3}$$

We start by reminding the reader that the unit N-sphere can be defined as the hyper-surface in $(N+1)$-dimensional Euclidean space with coordinates $x_i, i=0,..,N$ that satisfies

$$\sum_{i=0}^{N} x_i^2 = 1. \tag{A4}$$

Intrinsic coordinates θ_i can be defined by

$$x_i = \cos\theta_i \prod_{j=i+1}^{N} \sin\theta_j . \tag{A5}$$

Their range is $(0,\pi)$ except for θ_1 with range $(0,2\pi)$. $\theta_0 = 0$ is not a coordinate. The metric induced on the N-sphere by its embedding in $(N+1)$-dimensional Euclidean space in this coordinates is diagonal with components

$$g_{ii} = \left(\prod_{j=i+1}^{N} \sin\theta_j \right)^2 , \tag{A6}$$

and the volume element is

$$dv = \prod_{i=1}^{N} \sin^{(n-1)}\theta_i d\theta_i . \tag{A7}$$

Real projective space RP^N follows the same construction with the range of θ_1 being $(0,\pi)$ too, plus the identifications

$$(0,\theta_2,\ldots,\theta_N) \equiv (\pi, \pi-\theta_2,\ldots,\pi-\theta_N). \tag{A8}$$

For quantum mechanical purposes the metric of interest in CP^N is the Fubini–Study metric.[24] Its line element in the homogeneous coordinates Z_i is

$$ds^2 = \frac{1}{X^2}\sum_{i=0}^{N} dZ_i d\overline{Z_i} - \frac{1}{X^4}\sum_{i=0}^{N} dZ_i \overline{Z_i} \sum_{j=0}^{N} Z_j d\overline{Z_j} , \tag{A9}$$

where we have defined

$$X^2 = \sum_{i=0}^{N} Z_i \overline{Z_i} . \tag{A10}$$

Splitting the complex homogeneous coordinates into their absolute values and phases

$$Z_i = X_i e^{i\alpha_i}, \tag{A11}$$

the Fubini–Study metric splits into two blocks relative to the X_i and to the α_i,

$$ds^2 = ds_X^2 + ds_\alpha^2, \tag{A12}$$

with

$$ds_X^2=\frac{1}{X^2}\left(\sum_{i=0}^{N} dX_i^2-dX^2\right), \tag{A13}$$

$$ds_\alpha^2=\frac{1}{X^2}\sum_{i=0}^{N} X_i^2 d\alpha_i^2-\frac{1}{X^4}\left(\sum_{i=0}^{N} x_i^2 d\alpha_i\right)^2. \tag{A14}$$

The intrinsic coordinates on the sphere (A5) and the phases relative to α_0

$$\beta_i=\alpha_i-\alpha_0, \quad i=1,...,N \tag{A15}$$

can be used as intrinsic coordinates on CP^N. However we should remark that the ranges of all the coordinates θ_i are $(0,\pi/2)$ since the X_i are absolute values and cannot therefore be negative. Moreover these coordinates are clearly singular whenever $\theta_i=\{0,\pi/2\}$. The relation of this coordinates with the homogeneous ones is

$$Z_i=Xe^{i\alpha_0}x_i(\theta_j)e^{i\beta_i}. \tag{A16}$$

Plugging this expression into the previous formulas for the line elements (A13)–(A14) one gets

$$ds_X^2=\sum_{i=0}^{N} dx_i^2=\sum_{i=1}^{N} g_{ii}d\theta_i^2, \tag{A17}$$

$$ds_\alpha^2=\sum_{i=1}^{N} x_i^2 d\beta_i^2-\left(\sum_{i=1}^{N} x_i^2 d\beta_i\right)^2=\sum_{i,j=1}^{N} h_{ij}d\beta_i d\beta_j. \tag{A18}$$

The first is the line element in the unit sphere (A6) and in the phase line element ds_α^2 we have defined the metric

$$h_{ij}=x_i^2(\delta_{ij}-x_j^2) \tag{A19}$$

with inverse

$$h^{ij}=\frac{1}{x_0^2}+\frac{\delta_{ij}}{x_i^2}. \tag{A20}$$

The volume element for the phase coordinates is

$$\begin{aligned} dv_\alpha&=\sqrt{\det(h_{ij})}\prod_{k=1}^{N} d\beta_k \\ &=\sqrt{\det(\delta_{ij}-x_j^2)}\prod_{k=1}^{N} x_k d\beta_k \\ &=\sqrt{1-\sum_{i=1}^{N} x_i^2}\prod_{k=1}^{N} x_k d\beta_k \\ &=\prod_{i=0}^{N} x_i\prod_{j=1}^{N} d\beta_j=\prod_{i=1}^{N} \cos\,\theta_i \sin^i\,\theta_i d\beta_i, \end{aligned} \tag{A21}$$

where we used (A5) for x_i in the last equality. Using (A7) for dv_X the combined volume element is

$$dv = dv_X dv_\alpha = \prod_{i=1}^{N} \cos\theta_i \, \sin^{2i-1}\theta_i d\theta_i d\beta_i \, . \tag{A22}$$

The total volume of CP^N becomes easy to compute

$$V_N = \prod_{i=1}^{N} \int_0^{\pi/2} d\theta_i \cos\theta_i \sin^{2i-1}\theta_i \int_0^{2\pi} d\beta_i = \prod_{i=1}^{N} \frac{1}{2i} 2\pi = \frac{\pi^N}{N!} . \tag{A23}$$

Now we are able to compute mean values of functions in Hilbert space as their integral in CP^N weighted with the Fubini–Study volume element (A22) and divided by the volume V_N of CP^N (A23). Since the functions we are interested in are of the type $<\psi|A|\psi> = \overline{A}$ we shall write explicitly mean$(\overline{A})$ to emphasize that the mean value is not taken on quantum states but rather on the whole of CP^N,

$$\text{mean}(\overline{A}) = \frac{1}{V_N} \int_{CP^N} dv \overline{A} . \tag{A24}$$

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Three-quark exchange operators, crossing matrices and Fierz transformations in SU(2) and SU(3)

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We give explicit expressions for the three-quark exchange operators, crossing matrices and Fierz transforms for the SU(2) and SU(3) groups. We identify the invariant terms in these operators and express them in terms of Casimir operators.
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I. INTRODUCTION

Dirac[1] was the first to express the two-particle spin-exchange operator,

$$\mathrm{P}_{12}=\tfrac{1}{2}+\tfrac{1}{2}\,\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\,, \tag{1}$$

in terms of Pauli matrices $\boldsymbol{\tau}_{1,2}$ of the two particles, where $\boldsymbol{\tau}\cdot\boldsymbol{\tau}=\Sigma_{a=1}^{3}\tau^a\tau^a$. This, and the following result:

$$\mathrm{P}_{12}\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2=\tfrac{3}{2}-\tfrac{1}{2}\,\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\,, \tag{2}$$

are equivalent to a ''Fierz reordering formula'' for the quartic field interaction, or to the SU(2) crossing matrix,

$$\mathbf{C}=\frac{1}{2}\begin{pmatrix}1 & 1\\ 3 & -1\end{pmatrix}, \tag{3}$$

for two-body processes. The same trick has been extended to the SU(3) Lie algebra,

$$\mathrm{P}_{12}=\tfrac{1}{3}+\tfrac{1}{2}\boldsymbol{\lambda}_1\cdot\boldsymbol{\lambda}_2\,, \tag{4a}$$

$$\mathrm{P}_{12}\boldsymbol{\lambda}_1\cdot\boldsymbol{\lambda}_2=\tfrac{16}{9}-\tfrac{1}{3}\boldsymbol{\lambda}_1\cdot\boldsymbol{\lambda}_2\,, \tag{4b}$$

again only for two particles,[2] with the resulting crossing matrix (or the equivalent Fierz reordering formulas for bilinear products of Gell–Mann matrices) being

$$\mathbf{C}=\begin{pmatrix}\frac{1}{3} & \frac{1}{2}\\ \frac{16}{9} & -\frac{1}{3}\end{pmatrix}. \tag{5}$$

Here the lower index indicates the number of the quark, λ^a are the Gell–Mann matrices, and f^{abc}, d^{abc} are the usual SU(3) structure constants.

In the meantime a need has arisen for tri-linear Fierz formulas/crossing relations in connection with applications of the three-flavor 't Hooft interaction.[3] Such relations do not seem to exist in the literature.[4–6] In this paper we present the corresponding three-body exchange operators for quarks

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[particles in the fundamental representation of SU(2) and/or SU(3)], as well as the equivalent Fierz reordering formulas for the sextic field interaction.

II. THREE-QUARK EXCHANGE OPERATORS

A. The SU(2) algebra

1. Three-body exchange operators

Using the symmetric group $\mathcal{S}_3$ it is straightforward, if tedious, to derive the SU(2) version of the three-quark/spin exchange operator,

$$\mathrm{P}_{123}=\mathrm{P}_{23}\mathrm{P}_{12}=\frac{1}{4}+\frac{1}{4}\sum_{i<j}^{3}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j+\frac{i}{4}\varepsilon^{abc}\boldsymbol{\tau}_1^a\boldsymbol{\tau}_2^b\boldsymbol{\tau}_3^c, \tag{6a}$$

$$\mathrm{P}_{132}=\mathrm{P}_{123}^2=\frac{1}{4}+\frac{1}{4}\sum_{i<j}^{3}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j-\frac{i}{4}\varepsilon^{abc}\boldsymbol{\tau}_1^a\boldsymbol{\tau}_2^b\boldsymbol{\tau}_3^c. \tag{6b}$$

Similar results are

$$\mathrm{P}_{123}\sum_{i<j}^{3}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j=\frac{1}{2}\left(9+\sum_{i<j}^{3}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j-3i\varepsilon^{abc}\boldsymbol{\tau}_1^a\boldsymbol{\tau}_2^b\boldsymbol{\tau}_3^c\right), \tag{7a}$$

$$\mathrm{P}_{132}\sum_{i<j}^{3}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j=\frac{1}{4}\left(9+\sum_{i<j}^{3}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j+3i\varepsilon^{abc}\boldsymbol{\tau}_1^a\boldsymbol{\tau}_2^b\boldsymbol{\tau}_3^c\right), \tag{7b}$$

as well as

$$i\mathrm{P}_{123}\varepsilon^{abc}\boldsymbol{\tau}_1^a\boldsymbol{\tau}_2^b\boldsymbol{\tau}_3^c=\frac{1}{2}\left(-3+\sum_{i<j}^{3}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j-i\varepsilon^{abc}\boldsymbol{\tau}_1^a\boldsymbol{\tau}_2^b\boldsymbol{\tau}_3^c\right), \tag{8a}$$

$$i\mathrm{P}_{132}\varepsilon^{abc}\boldsymbol{\tau}_1^a\boldsymbol{\tau}_2^b\boldsymbol{\tau}_3^c=\frac{1}{2}\left(3-\sum_{i<j}^{3}\boldsymbol{\tau}_i\cdot\boldsymbol{\tau}_j-i\varepsilon^{abc}\boldsymbol{\tau}_1^a\boldsymbol{\tau}_2^b\boldsymbol{\tau}_3^c\right). \tag{8b}$$

2. Crossing matrix

These results are summarized by the crossing matrices:

$$\mathbf{C}=\frac{1}{4}\begin{pmatrix}1&1&1\\9&1&-3\\-6&2&-2\end{pmatrix}, \tag{9}$$

for P_{123}, and

$$\mathbf{C}^2=\frac{1}{4}\begin{pmatrix}1&1&-1\\9&1&3\\6&-2&-2\end{pmatrix}, \tag{10}$$

for P_{132}. A valuable check is the constraint $\mathbf{C}^3=1$.

3. Three-body Fierz identities

$$\delta_{\alpha\delta}\delta_{\gamma\rho}\delta_{\sigma\beta}=\tfrac{1}{4}(\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho}+\delta_{\alpha\beta}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\gamma\delta}\boldsymbol{\tau}_{\alpha\beta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\sigma\rho}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\alpha\beta}+i\varepsilon^{abc}\boldsymbol{\tau}^a_{\alpha\beta}\boldsymbol{\tau}^b_{\gamma\delta}\boldsymbol{\tau}^c_{\sigma\rho}), \tag{11a}$$

$$\delta_{\alpha\rho}\delta_{\gamma\beta}\delta_{\sigma\delta}=\tfrac{1}{4}(\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho}+\delta_{\alpha\beta}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\gamma\delta}\boldsymbol{\tau}_{\alpha\beta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\sigma\rho}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\alpha\beta}-i\varepsilon^{abc}\boldsymbol{\tau}^a_{\alpha\beta}\boldsymbol{\tau}^b_{\gamma\delta}\boldsymbol{\tau}^c_{\sigma\rho}), \tag{11b}$$

$$\delta_{\alpha\delta}\boldsymbol{\tau}_{\gamma\rho}\cdot\boldsymbol{\tau}_{\sigma\beta}+\delta_{\gamma\rho}\boldsymbol{\tau}_{\alpha\delta}\cdot\boldsymbol{\tau}_{\sigma\beta}+\delta_{\sigma\beta}\boldsymbol{\tau}_{\gamma\rho}\cdot\boldsymbol{\tau}_{\alpha\delta}=\tfrac{1}{4}(9\,\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho}+\delta_{\alpha\beta}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\gamma\delta}\boldsymbol{\tau}_{\alpha\beta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\sigma\rho}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\alpha\beta}-3i\varepsilon^{abc}\boldsymbol{\tau}^a_{\alpha\beta}\boldsymbol{\tau}^b_{\gamma\delta}\boldsymbol{\tau}^c_{\sigma\rho}), \tag{12a}$$

$$\delta_{\alpha\rho}\boldsymbol{\tau}_{\gamma\beta}\cdot\boldsymbol{\tau}_{\sigma\delta}+\delta_{\gamma\beta}\boldsymbol{\tau}_{\alpha\rho}\cdot\boldsymbol{\tau}_{\sigma\delta}+\delta_{\sigma\beta}\boldsymbol{\tau}_{\gamma\rho}\cdot\boldsymbol{\tau}_{\alpha\delta}=\tfrac{1}{4}(9\,\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho}+\delta_{\alpha\beta}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\gamma\delta}\boldsymbol{\tau}_{\alpha\beta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\sigma\rho}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\alpha\beta}+3i\varepsilon^{abc}\boldsymbol{\tau}^a_{\alpha\beta}\boldsymbol{\tau}^b_{\gamma\delta}\boldsymbol{\tau}^c_{\sigma\rho}), \tag{12b}$$

$$i\varepsilon^{abc}\boldsymbol{\tau}^a_{\alpha\delta}\boldsymbol{\tau}^b_{\gamma\rho}\boldsymbol{\tau}^c_{\sigma\beta}=\tfrac{1}{2}(-3\,\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho}+\delta_{\alpha\beta}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\gamma\delta}\boldsymbol{\tau}_{\alpha\beta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\sigma\rho}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\alpha\beta}-i\varepsilon^{abc}\boldsymbol{\tau}^a_{\alpha\beta}\boldsymbol{\tau}^b_{\gamma\delta}\boldsymbol{\tau}^c_{\sigma\rho}), \tag{13a}$$

$$i\varepsilon^{abc}\boldsymbol{\tau}^a_{\alpha\rho}\boldsymbol{\tau}^b_{\gamma\beta}\boldsymbol{\tau}^c_{\sigma\delta}=\tfrac{1}{2}(3\,\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho}-(\delta_{\alpha\beta}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\gamma\delta}\boldsymbol{\tau}_{\alpha\beta}\cdot\boldsymbol{\tau}_{\sigma\rho}+\delta_{\sigma\rho}\boldsymbol{\tau}_{\gamma\delta}\cdot\boldsymbol{\tau}_{\alpha\beta})-i\varepsilon^{abc}\boldsymbol{\tau}^a_{\alpha\beta}\boldsymbol{\tau}^b_{\gamma\delta}\boldsymbol{\tau}^c_{\sigma\rho}). \tag{13b}$$

B. The SU(3) algebra

1. Three-body exchange operators

Similarly, we have

$$\mathrm{P}_{123}=\frac{1}{9}+\frac{1}{6}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j+\frac{1}{4}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c+\frac{i}{4}f^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c, \tag{14a}$$

$$\mathrm{P}_{132}=\frac{1}{9}+\frac{1}{6}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j+\frac{1}{4}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c-\frac{1}{4}if^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c, \tag{14b}$$

as well as similar relations for the operators,

$$\mathrm{P}_{123}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j=\frac{1}{9}+\frac{1}{6}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j+\frac{1}{4}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c+\frac{i}{4}f^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c, \tag{15a}$$

$$\mathrm{P}_{132}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j=\frac{1}{9}+\frac{1}{6}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j+\frac{1}{4}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c-\frac{1}{4}if^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c, \tag{15b}$$

and

$$\mathrm{P}_{123}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c=\frac{80}{81}-\frac{5}{27}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j+\frac{13}{18}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c-\frac{5}{18}if^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c, \tag{16a}$$

$$\mathrm{P}_{132}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c=\frac{80}{81}-\frac{5}{27}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j+\frac{13}{18}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c+\frac{5}{18}if^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c, \tag{16b}$$

$$\mathrm{P}_{123}if^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c=-\frac{16}{9}+\frac{1}{3}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j+\frac{1}{2}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c-\frac{1}{2}if^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c, \tag{16c}$$

$$\mathrm{P}_{132} if^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c = \frac{16}{9} - \frac{1}{3}\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j - \frac{1}{2}d^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c - \frac{1}{2}if^{abc}\boldsymbol{\lambda}_1^a\boldsymbol{\lambda}_2^b\boldsymbol{\lambda}_3^c . \tag{16d}$$

2. Crossing matrix

This leads to the following first cyclic permutation three-quark crossing matrix:

$$\mathbf{C} = \begin{pmatrix} \frac{1}{9} & \frac{1}{6} & \frac{1}{4} & \frac{1}{4} \\ \frac{16}{9} & \frac{2}{3} & -\frac{1}{2} & \frac{1}{2} \\ \frac{80}{81} & -\frac{5}{27} & \frac{13}{18} & -\frac{5}{18} \\ -\frac{16}{9} & \frac{1}{3} & \frac{1}{2} & -\frac{1}{2} \end{pmatrix}. \tag{17}$$

Similarly, for the second cyclic permutation we find

$$\mathbf{C}^2 = \begin{pmatrix} \frac{1}{9} & \frac{1}{6} & \frac{1}{4} & -\frac{1}{4} \\ \frac{16}{9} & \frac{2}{3} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{80}{81} & -\frac{5}{27} & \frac{13}{18} & \frac{5}{18} \\ \frac{16}{9} & -\frac{1}{3} & -\frac{1}{2} & -\frac{1}{2} \end{pmatrix}, \tag{18}$$

and, of course satisfying $\mathbf{C}^3 = 1$.

3. Three-body Fierz identities

$$\begin{aligned}\delta_{\alpha\delta}\delta_{\gamma\rho}\delta_{\sigma\beta} = {}& \tfrac{1}{9}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho} + \tfrac{1}{6}(\delta_{\alpha\beta}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\gamma\delta}\boldsymbol{\lambda}_{\alpha\beta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\sigma\rho}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\alpha\beta}) \\ & + \tfrac{1}{4}d^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho} + \tfrac{1}{4}if^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho},\end{aligned} \tag{19a}$$

$$\begin{aligned}\delta_{\alpha\rho}\delta_{\gamma\beta}\delta_{\sigma\delta} = {}& \tfrac{1}{9}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho} + \tfrac{1}{6}(\delta_{\alpha\beta}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\gamma\delta}\boldsymbol{\lambda}_{\alpha\beta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\sigma\rho}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\alpha\beta}) \\ & + \tfrac{1}{4}d^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho} - \tfrac{1}{4}if^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho},\end{aligned} \tag{19b}$$

$$\begin{aligned}\delta_{\alpha\delta}\boldsymbol{\lambda}_{\gamma\rho}\cdot\boldsymbol{\lambda}_{\sigma\beta} + \delta_{\gamma\rho}\boldsymbol{\lambda}_{\alpha\delta}\cdot\boldsymbol{\lambda}_{\sigma\beta} + \delta_{\sigma\beta}\boldsymbol{\lambda}_{\gamma\rho}\cdot\boldsymbol{\lambda}_{\alpha\delta} = {}& \tfrac{2}{3}(\delta_{\alpha\beta}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\gamma\delta}\boldsymbol{\lambda}_{\alpha\beta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\sigma\rho}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\alpha\beta}) \\ & + \tfrac{16}{9}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho} - \tfrac{1}{2}d^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho} \\ & + \tfrac{1}{2}if^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho},\end{aligned} \tag{20a}$$

$$\begin{aligned}\delta_{\alpha\rho}\boldsymbol{\lambda}_{\gamma\beta}\cdot\boldsymbol{\lambda}_{\sigma\delta} + \delta_{\gamma\beta}\boldsymbol{\lambda}_{\alpha\rho}\cdot\boldsymbol{\lambda}_{\sigma\delta} + \delta_{\sigma\beta}\boldsymbol{\lambda}_{\gamma\rho}\cdot\boldsymbol{\lambda}_{\alpha\delta} = {}& \tfrac{2}{3}(\delta_{\alpha\beta}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\gamma\delta}\boldsymbol{\lambda}_{\alpha\beta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\sigma\rho}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\alpha\beta}) \\ & + \tfrac{16}{9}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho} - \tfrac{1}{2}d^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho} \\ & - \tfrac{1}{2}if^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho},\end{aligned} \tag{20b}$$

$$\begin{aligned}d^{abc}\boldsymbol{\lambda}^a_{\alpha\delta}\boldsymbol{\lambda}^b_{\gamma\rho}\boldsymbol{\lambda}^c_{\sigma\beta} = {}& -\tfrac{5}{27}(\delta_{\alpha\beta}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\gamma\delta}\boldsymbol{\lambda}_{\alpha\beta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\sigma\rho}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\alpha\beta}) + \tfrac{80}{81}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho} \\ & + \tfrac{13}{18}d^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho} - \tfrac{5}{18}if^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho},\end{aligned} \tag{21a}$$

$$\begin{aligned}d^{abc}\boldsymbol{\lambda}^a_{\alpha\rho}\boldsymbol{\lambda}^b_{\gamma\beta}\boldsymbol{\lambda}^c_{\sigma\delta} = {}& -\tfrac{5}{27}(\delta_{\alpha\beta}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\gamma\delta}\boldsymbol{\lambda}_{\alpha\beta}\cdot\boldsymbol{\lambda}_{\sigma\rho} + \delta_{\sigma\rho}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\alpha\beta}) + \tfrac{80}{81}\,\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho} \\ & + \tfrac{13}{18}d^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho} + \tfrac{5}{18}if^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho},\end{aligned} \tag{21b}$$

$$if^{abc}\boldsymbol{\lambda}^a_{\alpha\delta}\boldsymbol{\lambda}^b_{\gamma\rho}\boldsymbol{\lambda}^c_{\sigma\beta}=\tfrac{1}{3}(\delta_{\alpha\beta}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\sigma\rho}+\delta_{\gamma\delta}\boldsymbol{\lambda}_{\alpha\beta}\cdot\boldsymbol{\lambda}_{\sigma\rho}+\delta_{\sigma\rho}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\alpha\beta})-\tfrac{16}{9}\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho}$$
$$+\tfrac{1}{2}d^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho}-\tfrac{1}{2}if^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho}, \tag{22a}$$

$$if^{abc}\boldsymbol{\lambda}^a_{\alpha\rho}\boldsymbol{\lambda}^b_{\gamma\beta}\boldsymbol{\lambda}^c_{\sigma\delta}=-\tfrac{1}{3}(\delta_{\alpha\beta}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\sigma\rho}+\delta_{\gamma\delta}\boldsymbol{\lambda}_{\alpha\beta}\cdot\boldsymbol{\lambda}_{\sigma\rho}+\delta_{\sigma\rho}\boldsymbol{\lambda}_{\gamma\delta}\cdot\boldsymbol{\lambda}_{\alpha\beta})+\tfrac{16}{9}\delta_{\alpha\beta}\delta_{\gamma\delta}\delta_{\sigma\rho}$$
$$-\tfrac{1}{2}d^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho}-\tfrac{1}{2}if^{abc}\boldsymbol{\lambda}^a_{\alpha\beta}\boldsymbol{\lambda}^b_{\gamma\delta}\boldsymbol{\lambda}^c_{\sigma\rho}. \tag{22b}$$

III. COMMENTS

Two of the three operators $\Sigma^3_{i<j}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j, d^{abc}\boldsymbol{\lambda}^a_1\boldsymbol{\lambda}^b_2\boldsymbol{\lambda}^c_3, if^{abc}\boldsymbol{\lambda}^a_1\boldsymbol{\lambda}^b_2\boldsymbol{\lambda}^c_3$ are SU(3) invariants, i.e., they can be expressed in terms of the two Casimir operators of SU(3) as follows:

$$\sum_{i<j}^{3}\boldsymbol{\lambda}_i\cdot\boldsymbol{\lambda}_j=2C^{(1)}-4, \tag{23a}$$

$$d^{abc}\boldsymbol{\lambda}^a_1\boldsymbol{\lambda}^b_2\boldsymbol{\lambda}^c_3=\tfrac{4}{3}[C^{(2)}-\tfrac{5}{2}C^{(1)}+\tfrac{20}{3}]; \tag{23b}$$

where the two Casimir operators of SU(3) are defined as $C^{(1)}=\mathbf{F}^2, C^{(2)}=d^{abc}\mathbf{F}^a\mathbf{F}^b\mathbf{F}^c$ and $\mathbf{F}^a$ are the SU(3) algebra generators. The third operator, $if^{abc}\boldsymbol{\lambda}^a_1\boldsymbol{\lambda}^b_2\boldsymbol{\lambda}^c_3$, is a peculiar object: it is an SU(3) invariant, because it commutes with the SU(3) generators $\mathbf{F}^a=1/2(\boldsymbol{\lambda}^a_1+\boldsymbol{\lambda}^a_2+\boldsymbol{\lambda}^a_3)$ in the special case when these generators are formed from three Gell–Mann matrices, but it is also an off-diagonal operator [it annihilates the two three-quark SU(3) eigenstates with definite exchange symmetry properties, i.e., the **1** and **10**, and turns one **8** state into another] that cannot be expressed in terms of Casimir operators. This result does not violate the Casimir–v.d. Waerden theorem relating the rank of the group to the number of independent invariant operators, as it is representation dependent. This example, however, points out the existence of such invariants which is not widely known.

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Towards an analytical formula for the eigenvalues of the Aharonov–Bohm annular billiard

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We derive an asymptotic formula for the eigenvalues of the Aharonov–Bohm annular billiard (ABAB) that improves and corrects previous estimates. Employing semiclassical arguments we relate the limitations of the procedure to the topology of the classical phase space of the system. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1341235]

I. INTRODUCTION

In recent years, the interest in quantum billiards has increased considerably. Owing to advances in nanotechnology, it has been possible to fabricate small devices in which the carriers are mainly scattered by the boundaries of the sample.[1] The high resemblance between these systems, commonly referred to as quantum dots, and the quantum billiards, it is very appealing to study the transport properties of ballistic samples employing quantum billiards as models.

Quantum billiards threaded by a magnetic flux ϕ are suitable configurations to model problems related to persistent currents.[2,3] These equilibrium currents are a consequence of the nature of the eigenfunctions' flux sensitivity, which is strictly of the Aharonov–Bohm type.[4,5] The current, at zero temperature, carried by the level E_n is $I \propto \partial E_n / \partial \phi$. The first theoretical works on persistent currents have been in one-dimensional (1D) ring geometries,[6] in two-dimensional (2D) the computations have been performed employing discrete models or cylindrical geometries.[7,8] In the last case, the mathematical description of the problem is essentially the same as for the ring geometries because the eigenenergies are pure quadratic forms of the two quantum numbers with a functional dependence on the flux that is identical to 1D systems.

To describe the real ''rings'' employed in the experiments on persistent currents,[9] it seems to be more suitable to consider the 2D Aharonov–Bohm annular billiard (ABAB) depicted in Fig. 1. The eigenenergies for this system can be numerically determined from the zeros of the cross products of Bessel functions, but a closed analytical formula for the eigenvalues does not exist.

In a recent paper Samandra and Healy introduced an asymptotic formula for the eigenvalues of a charged particle confined in an annular shell in which there was a cylindrically symmetric static magnetic field inside the inner cylinder.[10] This configuration is equivalent to thread the annular shell by an static magnetic flux ϕ and, therefore, equivalent to the ABAB. In this article we present an asymptotic analytical formula for the eigenenergies of the ABAB that corrects and improves the previous one.[10] Moreover, we will show that the eigenenergies obtained in Ref. 10 fail to describe quantum states that are present at all the energy scales, even in the semiclassical limit. These states are associated with classical orbits that do not hit the inner radius of the ABAB and cannot be described by the asymptotic expansion presented in Ref. 10. We find that the eigenenergies for these states can be obtained, under certain conditions, through the Debye's expansion for the zeros of the Bessel functions of first kind.

The paper is organized as follows. In Sec. II we introduce the system and summarize the results concerning the solutions of the Schrödinger equation. In Sec. III we obtain the asymptotic expansion for the eigenenergies and compare it to the one obtained in Ref. 10. Part of this section

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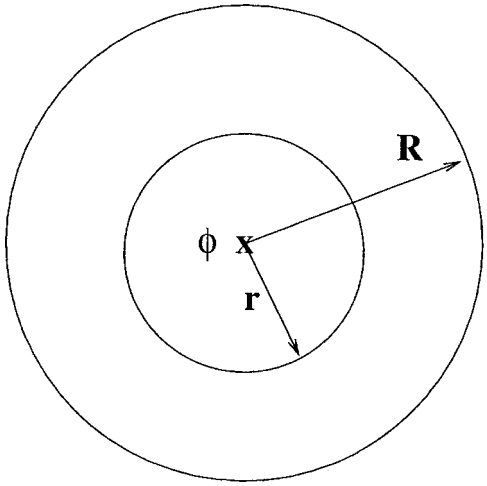

FIG. 1. Aharonov–Bohm annular billiard (ABAB) threaded by a magnetic flux ϕ. The inner and outer radii are denoted r and R, respectively.

is devoted to a detailed discussion about the limitations of the analytical results. We present in Sec. IV the numerical results and in Sec. V the concluding remarks.

II. THE AHARONOV–BOHM ANNULAR CAVITY

In this section we introduce the ABAB and the relevant equations involved in the problem. The annular shell is defined in terms of the polar coordinates (ρ, θ). The radial coordinate ρ varies between r and R and the azimutal angle $0 \leqslant \theta \leqslant 2\pi$ (see Fig. 1). We take the area equal to π and we define the parameter $\lambda = R/r$, such that $R = \lambda/\sqrt{\lambda^2 - 1}$ and $r = 1/\sqrt{\lambda^2 - 1}$. When $\lambda \to 1$ the system resembles a 1D ring, while for $\lambda > 1$ it is an annular cavity.

We fix the gauge $\mathbf{A} = \phi/(2\pi\rho)\hat{\theta}$, where $\hat{\theta}$ is the azimutal unit vector, and there is no magnetic field piercing the body of the annulus.

The single particle spectrum results from the eigenvalue equation

$$\Delta\Psi + \frac{2i\alpha}{\rho^2}\frac{\partial\Psi}{\partial\theta} - \frac{\alpha^2}{\rho^2}\Psi + k^2\Psi = 0, \tag{2.1}$$

where Δ is the Laplacian in polar coordinates. We define the scaled flux $\alpha = \phi/\phi_0$ with $\phi_0 = hc/e$ the flux quantum. We use units such $\hbar^2/2m = 1$, so the energy is $E = k^2$.

We apply Dirichlet boundary conditions at $\rho = r$ and $\rho = R$ and periodic boundary condition in the azimutal direction. The Eq. (2.1) is separable in polar coordinates and we factorize $\Psi(\rho, \theta) = \mathcal{F}(\rho)\exp(im\theta)$ with $m = 0, \pm 1, \pm 2, \ldots$ the orbital quantum number. The wave numbers $k_{\nu,n}$ result from the solution of the equation

$$J_\nu(z\lambda)N_\nu(z) - J_\nu(z)N_\nu(z\lambda) = 0, \quad \nu \equiv m - \alpha, \tag{2.2}$$

where we have defined $z \equiv kr$ and $n = 1,2\ldots$, is the radial quantum number. J_ν and N_ν are the Bessel functions of the first and second kind, respectively. The corresponding eigenfunctions $\Psi(\rho, \theta)$ are

$$\Psi_{\nu,n}(\rho, \theta) = A_{\nu,n}\exp(im\theta)[J_\nu(k_{\nu,n}\rho)N_\nu(k_{\nu,n}r) - J_\nu(k_{\nu,n}r)N_\nu(k_{\nu,n}\rho)], \tag{2.3}$$

where $A_{\nu,n}$ is the normalization constant.

All the eigenstates and all the equilibrium physical properties of the system are periodic functions of the flux with period ϕ_0. Moreover, as the energy spectrum is symmetric with respect to $\phi=\phi_0/2$, in the following the parameter α will take values between 0 and 1/2. For $\alpha\neq 0$, the states with m and $-m$ are, in general, not degenerate.

We remark that the eigenenergies $E_{\nu,n}$ cannot be written down as simple functions of the numbers ν and n as it happens, for example, in the case of the cylindrical geometries where the eigenenergies are pure quadratic functions of both quantum numbers. Moreover, there is not a closed analytical expression for the eigenenergies of the Aharonov–Bohm annular cavity.

III. THE ASYMPTOTIC EXPANSION FOR THE EIGENENERGIES

To derive an estimate for the eigenenergies $E_{\nu,n}$, we begin rewriting the asymptotic expansion of the nth zero of Eq. (2.2) that appears in Ref. 11, in such a way that the dependence on n, that is hidden in the expression given in Ref. 11 becomes explicit:

$$k_{\nu,n}\approx n\pi\frac{\sqrt{\lambda^2-1}}{\lambda-1}+\frac{(\lambda-1)\sqrt{\lambda^2-1}}{2n\pi\lambda}\nu^2-\frac{(\lambda-1)\sqrt{\lambda^2-1}}{8n\pi\lambda}+\frac{(\lambda-1)^3\sqrt{\lambda^2-1}}{n^3\pi^3}Q+\frac{(\lambda-1)^5\sqrt{\lambda^2-1}}{n^5\pi^5}P, \tag{3.1}$$

with

$$Q\equiv\nu^4\left(16f(\lambda)-\frac{1}{4\lambda^2}\right)+\nu^2\left(\frac{1}{8\lambda^2}-104f(\lambda)\right)-25f(\lambda)-\frac{1}{64\lambda^2},$$

$$P\equiv-\frac{f(\lambda)(-25+4\nu^2)(-1+4\nu^2)^2}{2\lambda}+\frac{(-1+4\nu^2)^3}{256\lambda^3}+\frac{(-1+\lambda^5)(-1+4\nu^2)}{5120(\lambda-1)\lambda^5}(1073-456\nu^2+16\nu^4). \tag{3.2}$$

As Eq. (3.1) is asymptotic in $1/n$, the symbol $\approx$ comes from neglecting all the terms of $\mathcal{O}(1/n^7)$ and higher. We have defined for convenience

$$f(\lambda)\equiv(\lambda^3-1)/(384\lambda^3(\lambda-1)).$$

Equation (3.1) contains terms in orders $\mathcal{O}(1/n)$, $\mathcal{O}(1/n^3)$, and $\mathcal{O}(1/n^5)$ that must be taken into account for small n and values of $\lambda\gtrsim 1$. One can solve by numerical methods Eq. (2.2) to obtain the (exact) eigenvalues of the ABAB. This will be done in the next section. Nevertheless, we now want to stress that for fixed values of λ and $n>1$, the accuracy of the expansion Eq. (3.1) to the exact eigenvalues depends, not only on n, but also on the other quantum number m through ν.

We expand Eq. (3.1) explicitly as a function of both quantum numbers m and n. Keeping the terms up to order α^2 (this is not a crude approximation taking into account that α varies between 0 and 1/2) we obtain the corresponding eigenenergies

$$E_{\nu,n}\equiv E_{m,n}(\alpha)\approx A\alpha^2+B\alpha+C+\mathcal{O}(\alpha^3), \tag{3.3}$$

with A, B, and C polynomials in the quantum number m

$$A\equiv a_0+a_2m^2+a_4m^4+a_6m^6+a_8m^8+a_{10}m^{10}, \tag{3.4}$$

$$B\equiv b_1m+b_3m^3+b_5m^5+b_7m^7+b_9m^9, \tag{3.5}$$

$$C\equiv c_0+c_2m^2+c_4m^4. \tag{3.6}$$

In the Appendix we write down the explicit formulae for the coefficients a_i which although rather cumbersome, will be useful in the following. They are analytic functions of the parameter λ and the radial quantum number n.

The second-order approximation Eq. (3.3) is not the Taylor expansion in α of the eigenenergies. The coefficients in Eqs. (3.4)–(3.6) have been obtained from the asymptotic expansion Eq. (3.1) that, when the radial quantum number $n \lesssim m$, does not work. This important fact has not been taken into account in Ref. 10. Moreover, even in the limit $n \gg m$ the results of Ref. 10 are, in general, very poor estimates of the eigenenergies. To clarify this point we compare Eq. (3.3) to the equation obtained in Ref. 10 for the eigenenergies, that we have rewritten in the form of Eq. (3.3)

$$\tilde{E}_{m,n}(\alpha) = \tilde{A}\alpha^2 + \tilde{B}\alpha + \tilde{C}, \tag{3.7}$$

with

$$\tilde{A} \equiv \frac{\lambda^2 - 1}{\lambda},$$

$$\tilde{B} \equiv -\left(\frac{\lambda^2 - 1}{\lambda}\right) 2m, \tag{3.8}$$

$$\tilde{C} \equiv n^2\pi^2 \left(\frac{\lambda + 1}{\lambda - 1}\right) + \frac{(\lambda^2 - 1)}{\lambda}(m^2 - 1/4).$$

Comparing Eqs. (3.4)–(3.6) [and the Eq. (A1) for a_i] to Eq. (3.8) we conclude that, even in the limit $n \gg m$, it is only for $\lambda = 1 + \epsilon (\epsilon \ll 1)$ that the Eqs. (3.7) and (3.8) give satisfactory values for the eigenenergies of the ABAB. In this case the annulus resembles a thin cylindrical surface of height $(\lambda - 1)/\sqrt{\lambda^2 - 1} = R - r$. Let us remark that for a cylindrical surface of area $L \times L_y$, the exact eigenenergies are parabolas as a function of α. The corresponding coefficients are: $A = (2\pi/L)^2$ (without any dependence on the quantum numbers) for the quadratic term, $B = 2m(2\pi/L)^2$ (depending only on the orbital quantum number m) for the linear term, and the constant term $C = (n\pi/L_y)^2$ which is a function only of the transverse quantum number n.

On the contrary, Eqs. (3.4)–(3.6) are valid for larger values of λ. As an example, Fig. 2 shows a plot of the coefficients A [Eq. (3.4)] and $\tilde{A}$ as a function of the quantum number m for $\lambda = 10$ and $n = 30$. In the same figure the empty circles are the exact numerical values for this coefficient (obtained following the prescription that will be describe in the next section). Whereas the coefficient $\tilde{A}$ only gives the constant value for $m = 0$, the behavior of A is quite satisfactory for values of $m \lesssim 10$. Nevertheless, for $m \lesssim n$ the coefficients given in Eqs. (3.4)–(3.6) do not reproduce the actual values obtained in the numerical computations. The inclusion of additional terms in these equations does not give a better approximation to the eigenenergies. Under the present condition, Eqs. (3.4)–(3.6) are not perturbative because $|m/n| \gtrsim 1$, and any truncation of the expansion is misleading.

The difficulty to obtain a uniform perturbative expansion for the eigenenergies of the ABAB is related to the very different characteristics of the eigenstates as a function of the quantum numbers. This fact can be understood through semiclassical arguments. Since the problem is integrable, the classical phase space is foliated by tori that are labeled by the values of the actions $I_i(l,E), i = 1,2$, with l and E the angular momentum and the energy, respectively.[12] Moreover, this kind of system can be quantized through the E.B.K rule that establishes a correspondence between each eigenstate and a classical torus labeled by $I_i = (k_i + \alpha_i/4)\hbar$, where k_i is an integer and α_i is the Maslov index that depends on the topology of the classical orbits of the system.[13]

Given the values of l and E, and according to the ratio $\eta \equiv l\sqrt{(\lambda^2 - 1)/E}$, we can distinguish two type of classical orbits: Those that do not hit the inner circle ($\eta > 1$), and orbits that hit the inner circle ($\eta < 1$). The special value of $\eta_c = 1$ corresponds to orbits that are tangent to the inner

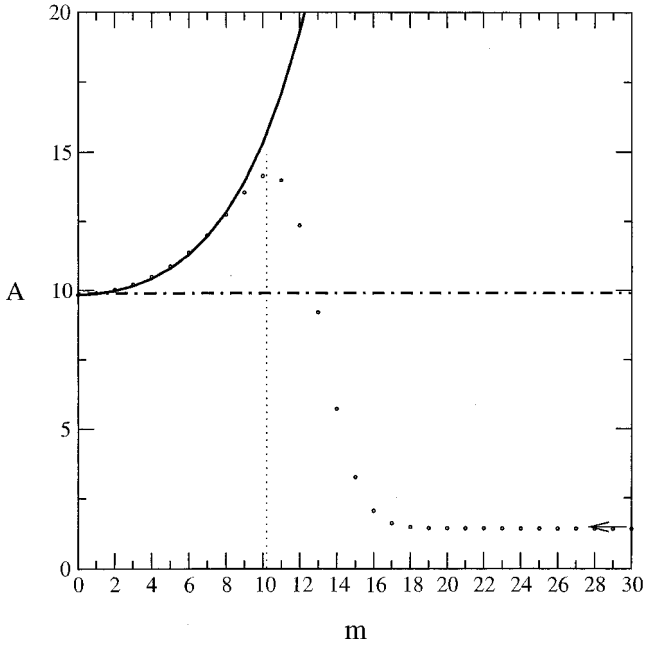

FIG. 2. Coefficient A obtained from Eq. (3.4) (solid lined) and $\tilde{A}$ obtained from Eq. (3.8) (dotted-dashed line) as a function of the quantum number m, for $n=30$ and $\lambda=10$. The empty circles correspond to the numerical values A_{mn} for $n=30$ obtained in Sec. IV. The vertical dotted line is the value m_c defined in Eq. (4.3). The left down arrow indicates the analytical estimate A_e [Eq. (4.4)] for values of $m>m_c$.

circle. The parameter η is the ratio between the radius of the caustic of the classical orbit for a disk of radius $R=\lambda/\sqrt{(\lambda^2-1)}$ and the inner radius of the ABAB, $r=1/\sqrt{(\lambda^2-1)}$.

According to the preceding remarks, given two values of the quantum numbers m and n the classical motion associated to the quantized torus will correspond either to $\eta>1$ or to $\eta<1$. Therefore, two kind of eigenstates are expected according to the value of η. Equation (3.3) is valid for quantum states such that $\eta<1$ and becomes a better approximation as η decreases.

For $\eta>1$, the classical motion on the ABAB is indistinguishable from that on a disk of radius R. Therefore, one would expect that analytical expressions for the eigenvalues corresponding to such a quantum states could be obtained from the Debye's asymptotic expansions for the Bessel functions of the first kind.[11]

However, it is well-known that the Debye's expansions fail to describe states localized on the whispering gallery modes.[14] In terms on the parameter $\epsilon\equiv\sqrt{E/(\lambda^2-1)}\lambda/l$ the whispering gallery modes correspond to $\epsilon\to 1$. As ϵ increases from 1 the Debye's expansion improves. Therefore, the Debye's expansion will be useful to describe states in the ABAB if the conditions $\eta>1$ and $\epsilon>1$ are simultaneously satisfied. As $\eta\cdot\epsilon=\lambda$, the fraction of such states increases with λ.

Figure 3 shows in the k-l plane the two critical lines labeled L_1 and L_2 defined, respectively by the equations $\eta_c=1$ and $\epsilon_c=1$ for $\lambda=10$. The states lying on the shadowed region in between L_1 and L_2 can be approximated by the Debye expansion. As a consequence, while for $\eta<1$ the eigenenergies for the ABAB are given by Eq. (3.1), for $\eta>1$ they could be obtained through the Debye's approximation. In the next section we will explore this approach.

It is important to emphasize that the nature of the failure of the Debye's expansion is quite different from that of the expansion Eq. (3.1). While the former is originated by the pathological behavior of the semiclassical approximation when the classical motion exhibits caustics,[14] the second one is due to the impossibility of the perturbative expansion Eq. (3.1) to cross the separatrix defined by $\eta=\eta_c$. In the next section we will show how this separatrix affects the actual eigenenergies.

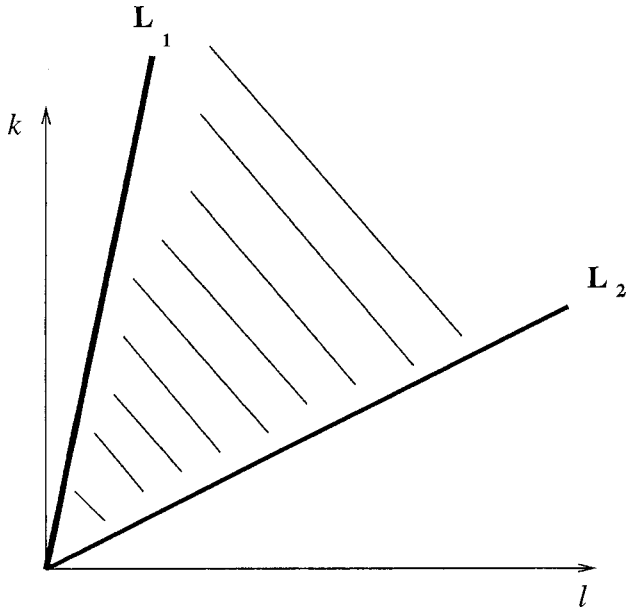

FIG. 3. Critical lines labeled L_1 and L_2 defined, respectively, by the equations $\eta_c=1$ and $\epsilon_c=1$ for $\lambda=10$. The states lying on the shadowed region in between L_1 and L_2 can be approximated by the Debye's expansion.

IV. NUMERICAL RESULTS AND ANALYTICAL ESTIMATES

To obtain each eigenenergy $E_{m,n}$ as a function of the flux α, we have numerically solved Eq. (2.2) employing the Newton–Raphson method. For a given value of λ, we have repeated this procedure for six equally spaced values of α between 0 and 1/2. Then we have fitted the numerical values with a quadratic function that minimizes the sum of the squares of the deviations from the numerical values. Figure 4 shows a region of the energy spectrum as a function of α for $\lambda=10$, obtained by the described procedure. The dotted lines are the quadratic fits, superimposed on the numerical values (circles). In the following we will consider

$$E_{m,n}=A_{mn}(\lambda)\alpha^2+B_{mn}(\lambda)\alpha+C_{mn}(\lambda), \tag{4.1}$$

where A_{mn}, B_{mn}, and C_{mn} have been obtained from the quadratic fit mentioned above.

To illustrate the statements of the preceding section, we will analize the coefficient A_{mn} as a function of both quantum numbers for two values of the parameter λ. Figure 5 shows a surface plot of the coefficient A_{mn} as a function of m and n for $\lambda=10$. We can see a pronounced crest separating two plateaux. One of them (labeled as *I*) corresponds to values of the quantum numbers m and n such that $\eta<1$. The other plateau (labeled as *II*) corresponds to $\eta>1$. The values of the coefficient A_{mn} that correspond to eigenstates such that $\eta\approx1$ are launched on the crest of the surface plot. The crest is a quantum signature of the classical separatrix previously mentioned. For this value of λ the fraction of states on the plateau *II* is much greater than the fraction of those on the plateau *I*.

Figure 6 shows a surface plot of the coefficient A_{mn} as a function of m and n for $\lambda=2$. The exhibited behavior is qualitatively the same as in Fig. 5. Nevertheless, opposite to the previous case, the fraction of states on the plateau *II* is smaller than the fraction of those on the plateau *I*.

As we have mentioned in Sec. III, Fig. 2 shows a transverse section of the surface plot Fig. 5 for $n=30$, together with the coefficient A evaluated for $n=30$ [Eq. (3.4)] and the coefficient $\tilde{A}$ given in Eq. (3.8) that only reproduces the plateau *I* ($A=9.9$ for the present value of $\lambda=10$). On the other hand, the coefficient A follows quite satisfactory the numerical values up to the crest of the plot, but it fails to reproduce the behavior of A_{mn} in the complete range of values of m.

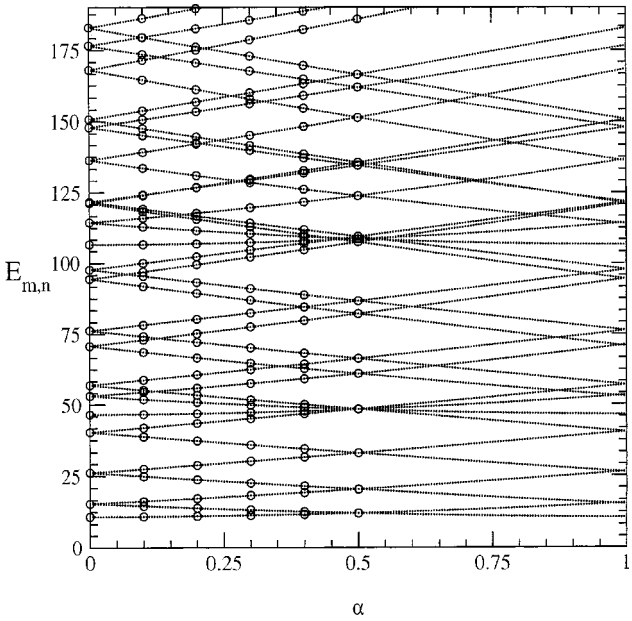

FIG. 4. Single particle energy levels as a function of the adimensional flux α, corresponding to the lowest region of the spectrum for the ABAB with $\lambda = 10$. The circles correspond to exact values obtained from the zeros of the cross products of Bessel functions. The small dotted lines are the quadratic fits obtained in Eq. (4.1). See the text for details.

To reproduce the numerical values A_{mn} in the region of the second plateau *II* we employ the Debye's approximation[11] that gives the asymptotic expansion for the zeros of the Bessel functions of the first kind $J_\nu(kR)$. If $j_{\nu,n}$ is a zero, $E_{\nu,n}=(j_{\nu,n}/R)^2$ will be the eigenenergy. Expanding $E_{\nu,n}$ as a function of the flux $\alpha(\nu=m-\alpha)$ and keeping the terms up to second order in α, we finally obtain

$$E_{m,n}\sim\frac{1}{R^2}\left[\left(\frac{\pi^2}{4}-1\right)\alpha^2+2m\left(\frac{\pi^2}{4}-1\right)\alpha+\pi^2\left(n^2+\left(\frac{\pi^2}{4}-1\right)m^2+\frac{1}{16}\right)\right]. \tag{4.2}$$

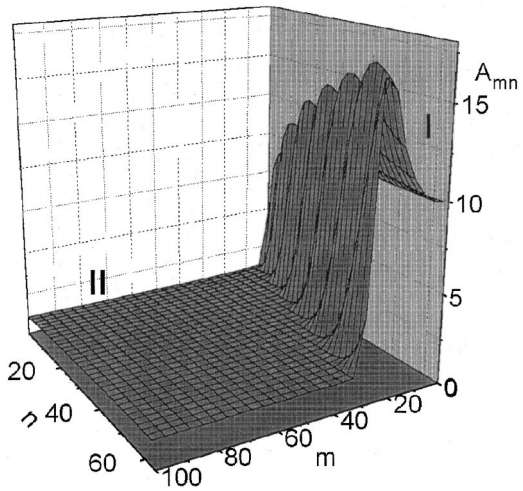

FIG. 5. Surface plot of the coefficient A_{mn} as a function of the quantum numbers m and n for $\lambda = 10$. The plateau labeled with I corresponds to values $\eta<1$, whereas the plateau labeled with II to $\eta>1$.

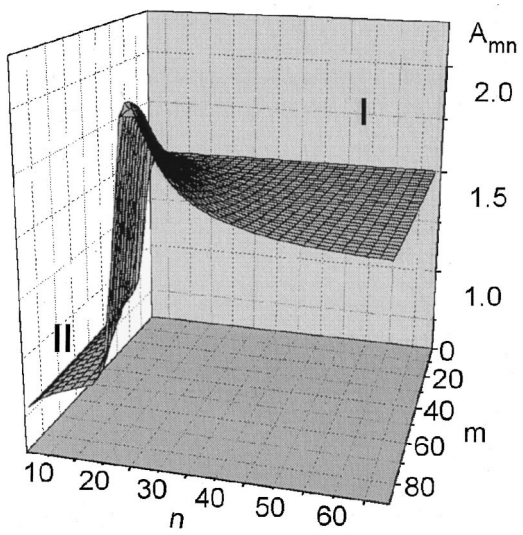

FIG. 6. Surface plot of the coefficient A_{mn} as a function of the quantum numbers m and n for $\lambda=2$. The plateau labeled with I corresponds to values $\eta<1$, whereas the plateau labeled with II to $\eta>1$.

The prefactor in the quadratic term of Eq. (4.2) gives the estimate of A_{mn} in the region of the second plateau *II* ($\eta>1$). For $\lambda=10$ is $R=1.005$ and the value of the coefficient is 1.452. This value is indicated in the right down part of Fig. 2 by an arrow and it agrees with the numerical values of A_{mn} on the plateau *II*.

Equation (4.2) can be used to obtain the critical condition $\eta_c=1$, in the *n*-*m* plane ($\eta_c=1$ defines the line L_1 in *k*-*l* plane). For a given value of the radial quantum number n, $\eta_c=1$ determines a critical value for the orbital quantum number m_c given by

$$m_c\sqrt{\frac{\lambda^2}{\pi^2}+1-\frac{\pi^2}{4}}\simeq n, \tag{4.3}$$

where the fact that $m\equiv l$ was used. Figure 7 shows in the *n*-*m* plane the critical line defined by the

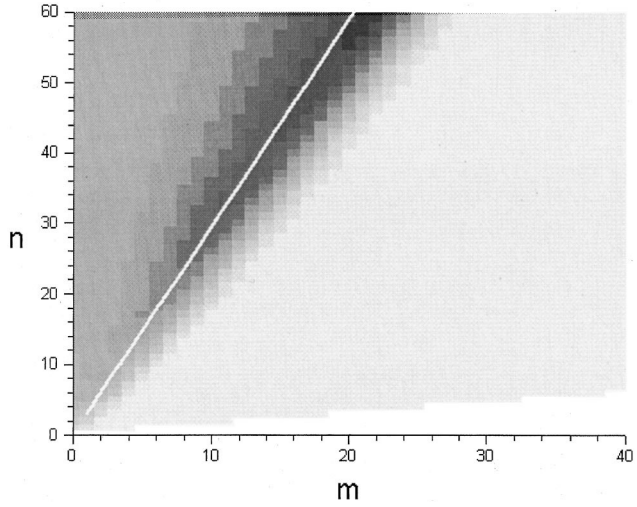

FIG. 7. Gray level density plot in the *m*-*n* plane corresponding to the surface plot Fig. 5. The solid white line is the critical line defined in Eq. (4.3) for $\lambda=10$.

Eq. (4.3) for $\lambda=10$ together with the gray scale density plot of the numerical values of A_{mn} taken from Fig. 5. In the present figure the crest of the surface plot Fig. 5 corresponds to the highest gray level intensity region in where, as expected, the critical line Eq. (4.3) is launched. As a consequence of the preceding analysis, we establish the following functional form to evaluate the coefficients $A_{mn}(\lambda)$

$$A_e=\begin{cases} \text{A given by Eq. (3.4),} & \text{for } m\leqslant m_c \\ \left(\dfrac{\pi^2}{4}-1\right)\dfrac{(\lambda^2-1)}{\lambda}, & \text{for } m>m_c \end{cases}, \tag{4.4}$$

where m_c is given in Eq. (4.3).

V. CONCLUDING REMARKS

In the present article we have explored the possibility to obtain an analytical expansion for the eigenenergies of the Aharonov–Bohm annular billiard valid for the whole range of values of the two relevant quantum numbers. We have shown that the well-known expansion for the zeros of the cross products of Bessel functions fail to reproduce the actual behavior of the eigenenergies for some kind of states that are present in all regions of the spectrum (namely for quantum states such that the parameter $\eta>1$). Based on semiclassical arguments we have demonstrated that these quantum states are associated with classical orbits that do not hit the inner circle of the annulus. These orbits, when the system is a genuine annulus ($\lambda>1$), are relevant in all the energy scales. For $\eta>1$ and $\lambda>1$, we have shown that the eigenenergies of the ABAB can be obtained through the Debye's expansions for the zeros of the Bessel functions of first kind, if the condition $\epsilon>1$ is also acomplished. As $\eta\cdot\epsilon=\lambda$, the fraction of states whose eigenenergies can be approximated by the Debye's expansion increases with λ. We have illustrated our results proposing an analytical estimate A_e, that reproduces quite satisfactory the exact numerical values $A_{mn}(\lambda)$ at both sides of the critical line defined in m-n plane by the Eq. (4.3), irrespective of the value of the parameter ϵ. That is, although the Debye's expansions fail for $\epsilon\to1$, the numerical values A_{mn} are not sensitive to that limit. Therefore, the value predicted by A_e for $m>m_c$ is valid even in the limit $\epsilon\to1$. We should remark that doing analogous calculations to those performed in Sec. IV, it is possible to derive the analytical estimates for the numerical coefficients B_{mn} and C_{mn}. This should be equivalent, in view of Eq. (4.1), to find an analytical expansion for the eigenenergies of the ABAB valid at both sides of the critical line $\eta_c=1$.

Last but not least, we would like to remark that the present study is far from being purely academic. The analytical expression of the eigenenergies as a function of the normalized flux α can be employed to determine the actual prefactors in the magnitude of the typical persistent current for a ballistic ABAB with N carriers, $I_{\text{typ}}\equiv\sqrt{\int_0^1 I^2 d\alpha}$.

In a recent paper it was found that $I_{\text{typ}}\propto A_T/N^{1/4}$, being $A_T\equiv\Sigma_{m,n}A_{mn}(\lambda)$.[3] Taking into account the analytical expression given in Eq. (4.4) we have obtained, to leading order in N

$$A_T=N\frac{(\lambda^2-1)}{\lambda}\left(\frac{\pi^2}{4}-1+\frac{(8-\pi^2)(\lambda-1)}{\pi(\lambda+1)\sqrt{4(\lambda^2+\pi^2)-\pi^4}}\right)+\mathcal{O}(N^{1/2}),$$

which gives a value of I_{typ} 1.4–1.5 times larger than the obtained in case of employing Eq. (3.8). This result could help to understand the existent discrepancy between the large experimental values of the persistent current measured in all the experiments performed up to date, and previous theoretical estimates that did not consider the corrections introduced in the present work.

ACKNOWLEDGMENTS

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APPENDIX

In this Appendix we write down the explicit expressions for the coefficients a_m of the different powers of m in the formula Eq. (3.4)

$$a_0=\frac{\lambda^2-1}{\lambda}-\frac{(\lambda-1)^2(\lambda^2-1)}{8\lambda^2\pi^2n^2},$$

$$a_2=\frac{3(\lambda-1)^2(\lambda^2-1)}{2\lambda^2\pi^2n^2}-\frac{69(\lambda-1)^3(1+\lambda)}{16\lambda^5\pi^4n^4},$$

$$a_4=(\lambda-1)^3\left(\frac{3(1+\lambda)}{8\lambda^5\pi^4n^4}\,\frac{-1109+4253\lambda+3812\lambda^2+450\lambda^3+775\lambda^4-935\lambda^5+290\lambda^6}{192\lambda^6\pi^6n^6}\right),$$

$$a_6=\frac{-7(\lambda-1)^3}{720\lambda^6\pi^6n^6}(-41+377\lambda+188\lambda^2+90\lambda^3+115\lambda^4-155\lambda^5+50\lambda^6)$$
$$+\frac{7(\lambda-1)^9}{2880\lambda^8\pi^8n^8}(-423+1897\lambda+2320\lambda^2),$$

$$a_8=\frac{(\lambda-1)^{10}(\lambda^2-1)}{512\lambda^{10}\pi^{10}n^{10}}[-207+1290\lambda-364\lambda^2+2916\lambda^3-1611\lambda^4$$
$$+2916\lambda^5-3621\lambda^6+1290\lambda^7-207\lambda^8]$$
$$+\frac{(\lambda-1)^8(\lambda^2-1)}{64\lambda^8\pi^8n^8}(3-32\lambda-131\lambda^2-249\lambda^3+131\lambda^4-32\lambda^5+3\lambda^6),$$

$$a_{10}=\frac{(\lambda-1)^{10}(\lambda^2-1)}{9600\lambda^{10}\pi^{10}n^{10}}[99-1122\lambda+6017\lambda^2-17204\lambda^3$$
$$+26895\lambda^4-17204\lambda^5+6017\lambda^6+1122\lambda^7+99\lambda^8].$$

(A1)

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Classical analogs of quasifree quantum stochastic processes given by stochastic states of the quantized electromagnetic field

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The mathematical model describing a light beam prepared in an arbitrary quantum optical state is a quasifree quantum stochastic process on the C^* algebra of the canonical commutatation relations. For such quantum stochastic processes the concept of stochastic states is introduced. Stochastic quantum states have a classical analog in the following sense: If the light beam is prepared in a stochastic state, one can construct a generalized classical stochastic process, such that the distributions of the quantum observables and the classical random variables coincide. A sufficient algebraic condition for the stochasticity of a quantum state is formulated. The introduced formalism generalizes the Wigner representation from a single field mode to a continuum of modes. For the special case of a single field mode the stochasticity condition provides a new criterion for the positivity of the Wigner function related to the given state. As an example the quantized eletromagnetic field in empty space at temperature $T=0$ is discussed. It turns out that the corresponding classical stochastic process is not a white noise but a colored noise with a linearly increasing spectrum. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The physical system considered throughout this paper is a light beam propagating in free space into the x direction of a fixed coordinate system. The beam is assumed to be prepared in an arbitrary quantum optical state. This situation can be described mathematically by a quasifree quantum stochastic process on the C^* algebra of the canonical commutation relations (CCR algebra).[1] Investigating this quantum stochastic process, the main question is the following: For which quantum optical states is it possible to construct a corresponding classical stochastic process, such that the classical random variables have the same distributions as the quantum observables in the given state?

The paper is organized as follows: in Sec. II we summarize some facts about the quantization of infinite dimensional linear Hamiltonian systems, i.e., of systems with the following properties: The state space is a linear space on which the Hamilton function is a strictly positive quadratic form determining the so called energy scalar product. The dynamics of the system defines a strongly continuous group of unitary transformations on state space. The described quantization procedure generalizes the quantization approach of Mackey[2] to the infinite dimensional case. It is closely related to some work of Lewis and Maassen,[3] Hinz[4] and to the Segal–Weinless-approach to quantization.[5,6]

In order to connect this quantization procedure to the Fock space formalism generally used in quantum optics,[7] it is necessary to identify the up to unitary equivalence uniquely determined Fock representation of the resulting CCR algebra. However, it is well known that there is an infinity of

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inequivalent Fock states on the CCR algebra over an infinite dimensional real symplectic space.[8] As a main result of Sec. II it is shown that among these Fock states there is exactly one, which is left invariant by the dynamics of the system. The Fock representation corresponding to this state connects the described quantization procedure to the Fock space formalism used in quantum optics. Generalizing a uniqueness result of Kay[9] an explicit construction of the invariant Fock state is given.

In Sec. III the quantization procedure is applied to the electromagnetic field. A one dimensional light beam is described as a linear Hamiltonian system, its time invariant Fock state is determined and the quasifree quantum stochasic process describing the quantized field in a given state is defined.

In Sec. IV a class of quantum optical states having a classical analog in the following sense is introduced: There exists a generalized classical stochastic process in the sense of Hida,[10] whose generalized random variables have the same distributions as the quantized observables in the given quantum state. Such states are called stochastic states. The generalized classical stochastic process corresponding to an arbitrary stochastic state of the quantized electromagnetic field is constructed.

In Sec. V we provide some deeper insight into the mathematical structure of stochastic states. On the basis of the Kolmogorov decomposition of positive definite kernels a sufficient algebraic condition for the stochasticity of a quantum state is formulated. The approach generalizes the well known Wigner representation[11] to a continuum of field modes. For a single mode the stochastic states correspond to the states whose Wigner spectrum[12] contains the points 0 and 1. In Ref. 12 these states are identified as mixed states with a positive Wigner function. Restricted to the one dimensional case, the stochasticity condition leads to a new criterion for the positivity of the Wigner function.

In Sec. VI the invariant Fock state describing the free electromagnetic field at temperature $T=0$ is discussed as an example for a stochastic quantum state. As it turns out, the corresponding generalized classical stochastic process is not a white noise, but a colored noise with a linearly increasing spectrum. This provides a new argument for an experimantally motivated assumption of Gardiner,[13] that the spectrum of the quantized electromagnetic field at $T=0$, which cannot be directly observed by photon counting, might be linearly increasing.

II. QUANTIZATION OF LINEAR HAMILTONIAN SYSTEMS

A triple $[\mathcal{H},\langle\cdot,\cdot\rangle,(U_t=e^{At})_t]$ consisting of a real Hilbert space $\mathcal{H}$ with scalar product $\langle\cdot,\cdot\rangle$ and a strongly continuous one parameter group of unitary transformations $(U_t)_{t\in\mathbb{R}}$ with a densely defined, skew adjoint, injective generator $A:\mathcal{D}(A)\to\mathcal{H}$ is called a *linear Hamiltonian system*, if the following conditions hold: The energy of the system prepared in an arbitrary state $f\in\mathcal{H}$ is given by the expression $\frac{1}{2}\langle f,f\rangle$. The unitary group $(U_t)_{t\in\mathbb{R}}$ describes the dynamics of the system, i.e., starting in the state $f_0\in\mathcal{H}$ at time $t=0$, the state at time $t>0$ will be $f_t=U_tf_0$. Since we consider only systems in continuous time, we write $(U_t)_t$ in the following. We call the scalar product $\langle\cdot,\cdot\rangle$ the *energy scalar product* and $\mathcal{H}$ the *state space* of the system.

Given a linear Hamiltonian system $[\mathcal{H},\langle\cdot,\cdot\rangle,(U_t=e^{At})_t]$, the starting point for its quantization is the corresponding *symplectic system* $[D,\sigma,(\tilde{U}_t)_t]$. It consists by definition of the real linear space $D:=\mathcal{D}(A)\subseteq\mathcal{H}$, the nondegenerate symplectic form $\sigma:D\times D\to\mathbb{R}:(f,g)\mapsto\langle Af,g\rangle$ and the symplectic dynamics $(\tilde{U}_t)_t:=(U_{-t})_t$, which leaves the symplectic form σ invariant. The pair (D,σ) is called a *symplectic space*.

For any $f\in D$ the corresponding *classical linear observable* $\varphi(f)$ is defined as the linear functional,

$$\varphi(f):\mathcal{H}\to\mathbb{R}:g\mapsto\langle g,f\rangle.$$

Parallel to the Heisenberg picture, we will use on the level of quantum mechanics, we fix the states $f\in\mathcal{H}$ and let the observables $\varphi(f)$ evolve in time. Their time evolution is given by $\varphi_t(f)=\phi(\tilde{U}_tf)$, $\forall f\in D$, $t\in\mathbb{R}$.

In this setting the problem of quantizing a linear Hamiltonian system can be formulated as follows: For any classical linear observable $\varphi(f)$ find a corresponding *quantum observable* $\Phi(f)$, i.e., a densely defined, self-adjoint operator $\Phi(f)$ acting on a complex Hilbert space $\mathcal{F}$, such that the *canonical commutation relations*,

$$[\Phi(f),\Phi(g)]=-i\sigma(f,g)\mathbf{1}_{\mathcal{F}},\quad \forall f,g\in D,$$

are fullfilled on a properly chosen dense subspace of $\mathcal{F}$. $\mathbf{1}_{\mathcal{F}}$ denotes the identity on $\mathcal{F}$. Note that we have set $\hbar=1$.

It is well known that this problem can be solved in the following way: Let $\mathrm{CCR}(D,\sigma)$ the CCR algebra over the symplectic space (D,σ),[14] which is by definition the up to C^* isomorphism uniquely determined C^* algebra generated by unitary elements $\{W(f):f\in D\}$, which fullfill the *canonical commutation relations* in their *Weyl form*,

$$W(f)W(g)=e^{i\sigma(f,g)}W(f+g),\quad \forall f,g\in D. \tag{1}$$

Take a regular state ψ on $\mathrm{CCR}(D,\sigma)$ and denote the corresponding Gelfand Naimark Segal (GNS) representation[15] by $(\mathcal{F}_\psi,\Pi_\psi,\xi_\psi)$. $\mathcal{F}_\psi$ is a complex Hilbert space, $\Pi_\psi:\mathrm{CCR}(D,\sigma)\to\mathcal{B}(\mathcal{F}_\psi)$ denotes the representation itself, which is a $*$ homomorphism from the C^* algebra $\mathrm{CCR}(D,\sigma)$ into the bounded linear operators $\mathcal{B}(\mathcal{F}_\psi)$ on $\mathcal{F}_\psi$, and $\xi_\psi\in\mathcal{F}_\psi$ is a cyclic vector, i.e., the vectors $\{\Pi_\psi(W(f)):f\in D\}$ span a dense subspace of $\mathcal{F}_\psi$. The GNS representation of $\mathrm{CCR}(D,\sigma)$ corresponding to a given state is unique up to unitary equivalence. The unitary operators $\{W_\psi(f):=\Pi_\psi(W(f)):f\in D\}$ are called *Weyl operators*. Since ψ is regular, by definition the map $\mathbb{R}\ni t\mapsto W_\psi(tf)$ defines for every $f\in D$ a strongly continuous group of unitary operators acting on $\mathcal{F}_\psi$. Starting from the relations (1), it follows that the unbounded, self-adjoint generators $\{B_\psi(f):=(d/dt)\,W_\psi(tf)|_{t=0}:f\in D\}$, the so called *field operators*, fullfill the commutation relations

$$[B_\psi(f),B_\psi(g)]=-2i\sigma(f,g)\mathbf{1}_{\mathcal{F}_\psi},\quad \forall f,g\in D,$$

on a properly chosen dense subspace of $\mathcal{F}_\psi$. Therefore the *quantized observables*,

$$\Phi_\psi(f):=\frac{1}{\sqrt{2}}B_\psi(f),\quad \forall f\in D,$$

solve the quantization problem formulated above.

The symplectic dynamics $(\tilde{U}_t)_t$ induces on the C^* algebra $\mathrm{CCR}(D,\sigma)$ the quasifree automorphism group $(\beta_t)_t$ determined by

$$\beta_t(W(f))=W(\tilde{U}_tf),\quad \forall f\in D,t\in\mathbb{R}. \tag{2}$$

The resulting time evolution of the quantized observables is

$$B_\psi(f)_t=B_\psi(\tilde{U}_tf),\quad \forall f\in D,t\in\mathbb{R}.$$

The GNS Hilbert space $\mathcal{F}_\psi$ and the quantized observables $\Phi_\psi(f)$ depend on the chosen state ψ. The representation generally used in quantum optics is the so called *Fock representation*: the GNS Hilbert space $\mathcal{F}_\psi$ is the symmetric Fock space $\mathcal{F}^+(\mathcal{K})$ over the so called *one particle space* $\mathcal{K}$, which is a properly chosen complex Hilbert space. (The examples considered in this paper are $\mathcal{K}=\mathbb{C}$ for a single field mode and $\mathcal{K}=L^2(\mathbb{R}_+)$ for the light beam propagating in one dimension of space.) The cyclic vector ξ_ψ is the *vacuum vector* $\Omega=1\oplus0\oplus0\cdots\in\mathcal{F}^+(\mathcal{K})$. The Fock representation is unitary equivalent to the GNS representation of the C^* algebra $\mathrm{CCR}(\mathcal{K})$ over the complex Hilbert space $\mathcal{K}$ induced by the state ψ_F with the generating functional

$$\psi_F(W(\tilde{f}))=e^{-(1/2)\|\tilde{f}\|^2_{\mathcal{K}}},\quad \forall \tilde{f}\in\mathcal{K}.$$

By definition the CCR algebra CCR($\mathcal{K}$) over a **complex** Hilbert space $\mathcal{K}$ is generated by the unitary elements $\{W(\tilde{f}):\tilde{f}\in\mathcal{K}\}$ fullfilling the relations

$$W(\tilde{f})W(\tilde{g})=e^{i\mathrm{Im}\langle\tilde{f},\tilde{g}\rangle}W(\tilde{f}+\tilde{g}),\quad \forall \tilde{f},\tilde{g}\in\mathcal{K}.$$

However starting from a given linear Hamiltonian system, the solution of the quantization problem leads to the CCR algebra CCR(D,σ) over the **real** symplectic space (D,σ). In the rest of this section we will be concerned with connecting the real quantization procedure described above to the complex picture generally used in quantum optics. The bridge will be a construction called *unitary embedding*.

Let (D,σ) a symplectic space and $\alpha:D\times D\to\mathbb{R}$ a positive bilinear form, such that

$$\sigma(f,g)^2\leqslant\alpha(f,f)\alpha(g,g),\quad \forall f,g\in D.$$

Then there is exactly one so called *quasifree state* ψ_α on CCR(D,σ), such that

$$\psi_\alpha(W(f))=e^{-(1/2)\alpha(f,f)},\quad \forall f\in D.$$

A *Fock state* is a quasifree state ψ_α on CCR(D,σ) with the additional property that D carries the structure of a complex linear space with complex scalar product $\langle\cdot,\cdot\rangle_c$, such that

$$\langle f,g\rangle_c=\alpha(f,g)+i\sigma(f,g),\quad \forall f,g\in D.$$

There is a common way to supply a real symplectic space (D,σ) with the structure of a complex scalar product space: Let $J:D\to D$ a linear map, such that $J^2=-\mathbf{1}$, $\sigma(Jf,f)\geqslant 0$, $\forall f\in D$, $\sigma(Jf,f)=0$ iff $f=0$ and $\sigma(Jf,Jg)=\sigma(f,g)$, $\forall f,g\in D$. Then J is called a *complex structure* on the symplectic space (D,σ). With the definitions

$$(x+iy)f:=xf+yJf,\quad \forall x,\ y\in\mathbb{R},f\in D,$$

and

$$\langle f,g\rangle_c:=\sigma(Jf,g)+i\sigma(f,g),\quad \forall f,g\in D,$$

D becomes a complex scalar product space, which will be denoted in the following by D_J. Note that for any complex structure J on (D,σ) the real scalar product,

$$\alpha_J:D\times D\to\mathbb{R}:(f,g)\mapsto\sigma(Jf,g),$$

uniquely determines a Fock state on CCR(D,σ). This state will be denoted in the following by ψ_J.

Theorem 1: *Let* $[\mathcal{H},\langle\cdot,\cdot\rangle,(U_t=e^{At})_t]$ *be a linear Hamiltonian system and* $[D,\sigma,(\tilde{U}_t)_t]$ *the corresponding symplectic system. Let* $A=-J|A|$ *the unique polar decomposition of the infinitesimal generator* A *into the positive operator* $|A|=\sqrt{A^*A}$ *and the partial isometry* $-J$. *Then* J *is a complex structure on* (D,σ) *and the Fock state* ψ_J *on* CCR(D,σ) *is the only Fock state on* (D,σ) *which is left invariant by the automorphism group* $(\beta_t)_t$ *defined in Eq. (2).*

Proof: From the fact that A is injective and skew adjoint one deduces that the partial isometry J is unitary with $J^*=J^{-1}=-J$ and that J is a complex structure. Because $A=-J|A|=-A^*=-|A|J$ it holds $JA=AJ$ or equivalently $\tilde{U}_tJ=J\tilde{U}_t$, $\forall t\in R$. From here it follows directly that

$$\alpha(\tilde{U}_t f,\tilde{U}_t g)=\sigma(J\tilde{U}_t f,\tilde{U}_t g)$$
$$=\sigma(\tilde{U}_t J f,\tilde{U}_t g)$$
$$=\sigma(Jf,g)=\alpha(f,g),\quad \forall f,g\in D,t\in\mathbb{R},$$

which proves the asserted time invariance of ψ_J.

For the proof of uniqueness assume the existence of another time invariant Fock state $\psi_{\tilde{J}}$ on CCR(D,σ) or equivalently of another complex structure $\tilde{J}$ on (D,σ) with $\tilde{J}A=A\tilde{J}$. Since A is injective and skew adjoint, ran$A$ is a dense subspace of $\mathcal{H}$. Consequently from

$$\langle\tilde{J}Af,\tilde{J}g\rangle=\langle A\tilde{J}f,\tilde{J}g\rangle=\sigma(\tilde{J}g,\tilde{J}g)=\sigma(f,g)$$
$$=\langle Af,g\rangle=\forall f,g\in\mathcal{H},$$

it follows that $\tilde{J}$ is isometric and therefore unitary, since $\tilde{J}^2=-\mathbf{1}$. Now it is obvious that $\tilde{J}^*=\tilde{J}^{-1}=-\tilde{J}$. Since $\tilde{J}A$ is easily shown to be a positive operator, since $\tilde{J}(-J)$ is unitary and since the polar decomposition is unique, from $\mathbf{1}(\tilde{J}A)=\tilde{J}(-J)|A|$ it follows $\mathbf{1}=\tilde{J}(-J)$ or $\tilde{J}=J$. ■

Definition 1: Let $[D,\sigma,(\tilde{U}_t)_t]$ *be the symplectic system corresponding to a given linear Hamiltonian system* $[\mathcal{H},\langle\cdot,\cdot\rangle,(U_t=e^{At})_t]$, *and let J be the unique complex structure defined in Theorem 1. A real linear map* $\mathcal{I}:D\to\mathcal{K}_0\subseteq\mathcal{K}$, *where* $\mathcal{K}_0$ *is a dense subspace of a complex Hilbert space* $\mathcal{K}$, *is called a* unitary embedding *of the given linear Hamiltonian system, if* $\mathcal{I}$ *is unitary as a map from the complex scalar product space* D_J to $\mathcal{K}_0$.

Given a unitary embedding $\mathcal{I}:D\to\mathcal{K}_0\subseteq\mathcal{K}$, the map $I_0:\mathrm{CCR}(D,\sigma)\ni W(f)\mapsto W(\mathcal{I}f)\in\mathrm{CCR}(\mathcal{K})$ extends to a C^* isomorphism $I:\mathrm{CCR}(D,\sigma)\to\mathrm{CCR}(\mathcal{K}_0)$. The Fock state ψ_J is mapped onto the state $\psi_J\circ I^{-1}$ with the generating functional,

$$\psi_J\circ I^{-1}(W(\tilde{f}))=\psi_J(W(\mathcal{I}^{-1}\tilde{f}))$$
$$=e^{-(1/2)\,\alpha_J(\mathcal{I}^{-1}\tilde{f},\mathcal{I}^{-1}\tilde{g})}$$
$$=e^{-(1/2)\,\|\tilde{f}\|^2_{\mathcal{K}}},\quad \forall\tilde{f}\in\mathcal{K}_0.$$

Therefore the GNS representation of CCR(σ,D) corresponding to the Fock state ψ_J and the GNS representation of CCR$(\mathcal{K}_0)$ corresponding to the state $\psi_J\circ I^{-1}$ are unitary equivalent. Since the latter can be realized in the usual manner on the symmetric Fock space $\mathcal{F}^+(\mathcal{K})$, the connection between the real quantization procedure and the complex picture used in quantum optics, we were looking for, is given by the unitary embedding $\mathcal{I}:D_J\to\mathcal{K}_0\subseteq\mathcal{K}$ under the condition that $\mathcal{I}$ is chosen such that $\mathcal{K}$ coincides with the complex one particle space of the considered system.

III. QUANTIZATION OF THE FREE ELECTROMAGNETIC FIELD

Specializing the Maxwell equations,

$$\mathrm{div}\,\vec{E}=0,\quad \mathrm{div}\,\vec{B}=0,$$

$$\mathrm{rot}\,\vec{E}=-\frac{\partial\vec{B}}{\partial t},\quad \mathrm{rot}\,\vec{B}=\frac{1}{c^2}\frac{\partial\vec{E}}{\partial t},$$

to the case of a linear in the y direction polarized light beam propagating into the x direction of a fixed coordinate system, leads to the *linear Hamiltonian system*,

$$[\mathcal{H}=L^2_r(\mathbb{R}),\langle\cdot,\cdot\rangle,(U_t)_t=(S_{-ct})_t]. \tag{3}$$

The *state space* $\mathcal{H}=L^2(\mathbb{R})$ is the Hilbert space of real valued quadratic integrable functions on the real axis with the energy scalar product $\langle f,g\rangle=\int_{-\infty}^{\infty}f(x)g(x)dx$. In the following we will often consider functions in the Schwartz space $\mathcal{S}_r:=\mathcal{S}_r(\mathbb{R})\subseteq\mathcal{H}$ of real valued rapidly decreasing functions. Since the magnetic induction vector $(0,0,B)^T$ is always orthogonal to the electric field vector $(0,E,0)^T$ and $cB(x,t)=E(x,t)$, $\forall x,t\in\mathbb{R}$, the state of the light beam is completely determined by the scalar electric field amplitude $E\in\mathcal{H}$.

We consider a cylindric volume of space with cross section F in the yz plane and infinite extension in the x direction. Given a function $E_0\in\mathcal{S}_r$ describing the electric field at time $t=0$, we define the corresponding *state* of the light beam as

$$f_0(x):=\sqrt{2\epsilon_0 F}E_0(x),\quad \forall x\in\mathbb{R}.$$

Then the electromagnetic energy contained in the considered volume can be written as

$$W_F(E_0)=\epsilon_0 F\int_{-\infty}^{\infty}E_0(x)^2dx=\frac{1}{2}\langle f_0,f_0\rangle.$$

The *dynamics* $(S_{-ct})_t$ is the right shift with the velocity of light c,

$$S_{-ct}(f)(x)=f(x-ct),\quad \forall x,\ t\in\mathbb{R},\ f\in\mathcal{S}_r.$$

The skew adjoint infinitesimal generator of the dynamics $A:\mathcal{D}(A)=H_r^1(\mathbb{R})\to\mathcal{H}:f\mapsto -cf'$, which is defined on the Sobolev space $H_r^1(\mathbb{R})$ of real valued absolutely continuous functions with a quadratic integrable derivative, is obviously injective, since constant functions are not in $L_r^2(\mathbb{R})$. In the following we use the notation $A=-c\,(d/dx)$.

The *symplectic system* corresponding to the linear Hamiltonian system (3) is

$$[D=\mathcal{D}(A)=H_r^1(\mathbb{R}),\sigma,(S_{ct})_t],\tag{4}$$

with the symplectic form

$$\sigma(f,g)=\int_{-\infty}^{\infty}(-cf'(x))g(x)dx,\quad \forall f,g\in D,$$

and the left shift $(S_{ct})_t$.

Since the polar decomposition of the generator $A=-c\,(d/dx)$ is obvious in the Fourier transformed picture, we will construct the complex structure J determining the time invariant Fock state of the light beam with the help of Fourier transformation,

$$\hat{f}(k):=FT(f)(k):=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}f(x)e^{-ikx}dx,\quad \forall f\in\mathcal{S}_r.$$

Proposition 1: The unique complex structure J determining the time invariant Fock state ψ_J of the linear Hamiltonian system (3) according to Theorem 1 is

$$J=FT^{-1}\circ M_{i\,\mathrm{sign}(k)}\circ FT,$$

where $M_{i\mathrm{sign}(k)}$ denotes pointwise multiplication with

$$i\mathrm{sign}(k)=\begin{cases}+i, & \text{for } k>=0,\\ -i, & \text{for } k<0.\end{cases}$$

Proof: Since the multiplication operator $M_{c|k|}$ is obviously positive and the polar decomposition is unique, the statement follows immediately from

$$\widehat{Af}(k)=(-\widehat{cf'})(k)=-ick\hat{f}(k)=-(i\mathrm{sign}(k))(c|k|)\hat{f}(k),\quad \forall k\in\mathbb{R},$$

or in formal notation,

$$FT\circ A=FT\circ(-J|A|)=(-M_{i\mathrm{sign}(k)}M_{c|k|})\circ FT. \qquad \blacksquare$$

Note that the Fourier transformation maps real valued elements $f\in\mathcal{H}$ onto symmetric complex elements $\hat{f}\in L^2_{\mathrm{sym}}(\mathbb{R}):=\{h\in L^2(\mathbb{R}):h(-k)=\overline{h(k)}a.e.\}$ and that the multiplication operator $M_{i\mathrm{sign}(k)}$ leaves the subspace $L^2_{\mathrm{sym}}(\mathbb{R})\subseteq L^2(\mathbb{R})$ invariant.

Next we will construct the unitary embedding $\mathcal{I}$ that connects the formalism described above to the Fock space formalism. The complex one particle space used in quantum optics for the description of a one dimensional quantized light beam is the complex Hilbert space $\mathcal{K}:=L^2(\mathbb{R}_+)$ of quadratic integrable functions on the positive real axis $\mathbb{R}_+=[0,\infty[$, referring to the continuum of positive frequencies contained in the light beam.

Proposition 2: Let $\mathcal{K}_0:=\{h\in\mathcal{K}:\int_0^\infty k|h(k)|^2dk<\infty\}\subseteq\mathcal{K}$ *and define the orthogonal projection* $P_{[0,\infty[}:L^2(\mathbb{R})\to\mathcal{K}:f\mapsto\chi_{[0,\infty[}f$, *where* $\chi_{[0,\infty[}$ *denotes the characteristic function of the interval* $[0,\infty[$. *Then the real linear map,*

$$\mathcal{I}:D\to\mathcal{K}_0:f\mapsto -i\sqrt{2}(M_{\sqrt{ck}}\circ P_{[0,\infty[}(\hat{f})), \tag{5}$$

is a unitary embedding of the linear Hamiltonian system (3).

Proof: A direct computation shows that $\mathcal{I}$ is a complex linear map from the complex scalar product space D_J into the complex Hilbert space $\mathcal{K}$. It is isometric, because

$$\begin{aligned}\langle\mathcal{I}f,\mathcal{I}f\rangle_{\mathcal{K}}&=2\int_0^\infty ck|\hat{f}(k)|^2dk\\&=\int_{-\infty}^\infty c|k||\hat{f}(k)|^2dk\\&=\langle|A|f,f\rangle=\alpha_J(f,f),\quad\forall f\in D_J.\end{aligned}$$

Furthermore $\mathcal{I}$ is a surjective map from D_J onto $\mathcal{K}_0$, since

$$\begin{aligned}&f\in D_J\subseteq\mathcal{H}\Leftrightarrow f\in\mathcal{H}\text{ and }f\in H^1(\mathbb{R})\\&\Leftrightarrow\hat{f}\in L^2_{\mathrm{sym}}(\mathbb{R})\text{ and}\int_{-\infty}^\infty k^2|\hat{f}(k)|^2dk=2\int_0^\infty k|\sqrt{k}\hat{f}(k)|^2dk<\infty\\&\Leftrightarrow\mathcal{I}f\in\mathcal{K}_0\subseteq\mathcal{K}.\end{aligned}\qquad\blacksquare$$

With the help of this unitary embedding the quantized electric field operator as it is found in quantum optics literature,[16]

$$\mathbf{E}(x,t)=\frac{i\sqrt{c}}{\sqrt{4\pi\epsilon_0 F}}\int_0^\infty(e^{ikx}e^{-i\omega t}a_k-e^{-ikx}e^{i\omega t}a_k^+)\sqrt{k}dk,$$

can be connected to the mathematical quantization approach described above as follows: The measurement of the classical electric field amplitude $E(x,t)$ at the point $x\in\mathbb{R}$ at time $t\in\mathbb{R}$ is described in a distributional sense by the linear observable $\varphi((1/\sqrt{2\epsilon_0 F})\,\delta_{x-ct})$, where δ_{x-ct} denotes the delta distribution at the point $x-ct\in\mathbb{R}$. The corresponding quantized observable represented on the Fock space $\mathcal{F}_+(L^2(\mathbb{R}_+))$ is formally given by

$$\Phi_{\mathcal{F}}\left(\mathcal{I}\left(\frac{1}{\sqrt{2\epsilon_0 F}}\delta_{x-ct}\right)\right) = -\frac{\sqrt{c}}{\sqrt{2\pi\epsilon_0 F}}\Phi_{\mathcal{F}}(i\sqrt{k}e^{-ik(x-ct)})$$

$$= -\frac{i\sqrt{c}}{\sqrt{4\pi\epsilon_0 F}}\int_0^\infty (e^{ikx}e^{-i\omega t}a_k - e^{-ikx}e^{i\omega t}a_k^+)\sqrt{k}dk$$

$$= \mathbf{E}(x,t),$$

with $w=ck$, $\Phi_{\mathcal{F}}(\tilde{f}) = (1/\sqrt{2})(a(\tilde{f}) + a^+(\tilde{f}))$, $\forall \tilde{f} \in \mathcal{K}$ and $a_k := a(\delta_k)$, $a_k^+ := a^+(\delta_k)$, where a_k and a_k^+ denote the annihilation and creation operator of a photon in the field mode k. Note that this observable does not exist in a strict sense, because classical linear observables $\varphi(f)$ and their quantized couterparts $\Phi_{\mathcal{F}}(\mathcal{I}f)$ are only defined for test functions $f \in D$. But it can be approximated by properly defined quantized observables.

IV. STOCHASTIC STATES OF THE QUANTIZED ELECTROMAGNETIC FIELD

Definition 2: Let ψ be a regular state on the CCR algebra $\mathrm{CCR}(\mathcal{K}=L^2(\mathbb{R}_+))$ *of the quantized electromagnetic field. The familiy of quantized observables* $\Lambda_\psi := \{\Phi_\psi(\tilde{f}) : \tilde{f} \in \mathcal{I}\mathcal{S}_r \subseteq \mathcal{K}\}$ *is called the* quasifree quantum stochastic process given by the state ψ.

Λ_ψ is a family of self-adjoint operators acting on the GNS Hilbert space $\mathcal{F}_\psi$. As usual the *distribution* μ_ψ of the quantized observable $\Phi_\psi(\tilde{f})$, which is now interpreted as a quantum random variable, is defined as the spectral measure of the self-adjoint operator $\Phi_\psi(\tilde{f})$ in the state ψ.

Next we will introduce a class of quantum states for which Λ_ψ has a classical analog.

Definition 3: A state ψ on $CCR(\mathcal{K})$ is called a stochastic state *if its generating functional,*

$$G_\psi : \mathcal{K} \to \mathbb{C} : \tilde{f} \mapsto G_\psi(\tilde{f}) := \psi(W(\tilde{f})),$$

is continuous and the kernel,

$$k : \mathcal{K} \times \mathcal{K} \to \mathbb{C} : (\tilde{g}, \tilde{f}) \mapsto G_\psi(\tilde{f} - \tilde{g}),$$

is positive definite, i.e., $\Sigma_{i,j=1}^n \overline{\lambda_i}\lambda_j k(\tilde{f}_i, \tilde{f}_j) \geqslant 0$, $\forall n \in \mathbb{N}$ *and for arbitrary elements* $\lambda_1, \ldots, \lambda_n \in \mathbb{C}$, $\tilde{f}_1, \ldots, \tilde{f}_n \in \mathcal{K}$.

For the special case $\mathcal{K}=\mathbb{C}$ of a single field mode the definition of stochastic states reduces to the definition of so called η-positive states with $\eta=0$ and $\eta=1$ given in Ref. 12. As it is shown there, these states are one to one with the states having a positive Wigner function.

Starting from a stochastic state ψ of the electromagnetic field we will associate in the following a classical analog to the quantum stochastic process Λ_ψ. Let $\mathcal{S}_r \subseteq \mathcal{H} \subseteq \mathcal{S}_r'$ be the real countable nuclear Hilbert space introduced in Ref. 10, where $\mathcal{S}_r$ denotes the space of real valued Schwartz functions, $\mathcal{H}=L_r^2(\mathbb{R})$ denotes the real state space of the linear Hamiltonian system describing the considered light beam and $\mathcal{S}_r'$ denotes the tempered distributions.

Proposition 3: Let G_ψ be the generating functional of a stochastic state ψ of the quantized electromagnetic field on $CCR(\mathcal{K}=L^2(\mathbb{R}_+))$ and let $\mathcal{I}: D \to \mathcal{K}_0$ the unitary embedding defined in Eq. (5). Then the functional,

$$C_\psi : \mathcal{S}_r \to \mathbb{R} : f \mapsto G_\psi\left(\frac{1}{\sqrt{2}}\mathcal{I}f\right), \tag{6}$$

is a characteristic functional, i.e., it is continuous and positive definite with $C_\psi(0)=1$.

Proof: Since $\mathcal{S}_r \subseteq D$ and $\mathcal{I}: D \to \mathcal{K}_0$ is isometric and therefore continuous with respect to the scalar product $\alpha_J(\cdot,\cdot) = \langle |A| \cdot, \cdot \rangle$ on $D \subseteq \mathcal{H}$ and since G_ψ is continuous as a map from $\mathcal{K}_0$ to $\mathbb{C}$, C_ψ is continuous with respect to the scalar product α_J. With $|A| = |c\,(d/dx)|$ it follows from the

definition of the topology on $\mathcal{S}_r$ that C_ψ is continuous with respect to this topology as well (see Ref. 10). The positive definiteness of C_ψ is shown by a direct computation starting from the positive definiteness of G_ψ. $C_\psi(0)=G_\psi(0)=1$ is obvious. ■

According to the theorem of Bochner and Minlos (see Ref. 10) for any characteristic functional C on $\mathcal{S}_r$ there exists exactly one probability measure ν on $(\mathcal{S}_r',\Sigma)$, where Σ denotes a suitable constructed σ algebra over $\mathcal{S}_r'$, such that

$$C(f)=\int_{\mathcal{S}_r'} e^{i\langle f,x\rangle} d\nu(x), \quad \forall f\in\mathcal{S}_r.$$

The random variables,

$$X_f:(\mathcal{S}_r',\Sigma,d\nu)\to\mathbb{R}:x\mapsto\langle f,x\rangle,$$

where $\langle\cdot,\cdot\rangle$ denotes the canonical bilinear form connecting $\mathcal{S}_r$ with its dual $\mathcal{S}_r'$, build the *generalized classical stochastic process* $\{X_f:f\in\mathcal{S}_r\}$ induced by the characteristic functional C.

Starting from a stochastic state ψ of the quantized electromagnetic field the characteristic functional defined in Eq. (6) induces a corresponding generalized classical stochastic process $Y_\psi:=\{X_f:f\in\mathcal{S}_r\}$. The following proposition shows that Y_ψ can be seen as a classical analog of the quasifree quantum stochastic process Λ_ψ.

Proposition 4: Let Λ_ψ the quasifree quantum stochastic process of the quantized electromagnetic field given by a stochastic state ψ and let Y_ψ be the corresponding generalized classical stochastic process. Then for any $f\in\mathcal{S}_r$ the distribution ν_f of the generalized classical random variable $X_f\in Y_\psi$ and the distribution μ_f of the quantized random variable $\Phi_\psi(\mathcal{I}f)\in\Lambda_\psi$ coincide.

Proof: For any $t\in\mathbb{R}$, $f\in\mathcal{S}_r$ it holds on one hand side,

$$C(tf)=\int_{\mathcal{S}_r'} e^{it<f,x>} d\nu(x)=\int_{\mathcal{S}_r'} e^{itX_f(x)} d\nu(x)$$

$$=\int_{\mathbb{R}} e^{ity} d\nu_f(y),$$

and on the other hand side,

$$C(tf)=G_\psi\left(\frac{1}{\sqrt{2}}\mathcal{I}tf\right)=\psi\left(W\left(\frac{1}{\sqrt{2}}\mathcal{I}tf\right)\right)$$

$$=\psi(e^{itB_\psi((1/\sqrt{2})\mathcal{I}f)})$$

$$=\psi(e^{it\Phi_\psi(\mathcal{I}f)})$$

$$=\int_{\mathbb{R}} e^{ity}\, d\mu_f(y).$$

The assertion follows from the uniqueness of Fourier transformation. ■

V. A STOCHASITICITY CRITERION

Since it can be difficult to prove the positive definiteness of the characteristic functional directly, there is a need for a stochasiticity criterion which is easier to check. Such a criterion will be provideed in the following.

Lemma 1: Let $\mathcal{K}$ be a complex Hilbert space. Then there exist real orthogonal projections p_1, $p_2:\mathcal{K}\to\mathcal{K}$ onto closed real subspaces $\mathcal{K}_1:=p_1\mathcal{K},\mathcal{K}_2:=p_2\mathcal{K}$ such that $p_1+p_2=\mathbf{1}\mathcal{K}$, $\mathcal{K}_2=i\mathcal{K}_1$,

$\mathrm{Re}\langle p_1\tilde{f},p_2\tilde{f}\rangle_{\mathcal{K}}=0$ *and* $\mathrm{Im}\langle p_1\tilde{f},p_1\tilde{g}\rangle_{\mathcal{K}}=\mathrm{Im}\langle p_2\tilde{f},p_2\tilde{g}\rangle_{\mathcal{K}}=0,\forall\tilde{f},\tilde{g}\in\mathcal{K}$. ($p_1,p_2$ *being real projections means that they are real linear, idempotent and self-adjoint with respect to the real scalar product* $\mathrm{Re}\langle\cdot,\cdot\rangle_{\mathcal{K}}$.)

Proof: Take an arbitrary orthogonal basis $\{\tilde{h}_k:k\in\mathbb{N}\}\subseteq\mathcal{K}$ and define for every $\tilde{f}=\Sigma_k\alpha_k\tilde{h}_k\in\mathcal{K}$,

$$p_1\tilde{f}:=\sum_k \mathrm{Re}(\alpha_k)\tilde{h}_k,\quad p_2\tilde{f}:=\sum_k \mathrm{Im}(\alpha_k)\tilde{h}_k. \qquad \blacksquare$$

Definition 4: Under the conditions described above, the decomposition,

$$\tilde{f}=p_1\tilde{f}+p_2\tilde{f}:=\tilde{f}_1+\tilde{f}_2,\quad \forall\tilde{f}\in\mathcal{K},$$

is called a generalized decomposition into real and imaginary parts.

Theorem 2: *A state ψ on $CCR(\mathcal{K})$ is a stochastic state, if its generating functional G_ψ is continuous and if there is at least one generalized decomposition $\tilde{f}=\tilde{f}_1+\tilde{f}_2$, $\forall\tilde{f}\in\mathcal{K}$ into real and imaginary parts, such that G_ψ fullfills the factorization condition*

$$G_\psi(\tilde{f})=G_\psi(\tilde{f}_1)G_\psi(\tilde{f}_2),\quad \forall\tilde{f}\in\mathcal{K}.$$

Proof: In the GNS representation $(\Pi_\psi,\mathcal{F}_\psi,\xi_\psi)$ the vectors,

$$\{\gamma_{\tilde{f}}:=W_\psi(\tilde{f})\xi_\psi:\tilde{f}\in\mathcal{K}\}\subseteq\mathcal{F}_\psi,$$

span a dense subspace of $\mathcal{F}_\psi$ and fullfill the condition

$$\langle\gamma_{\tilde{f}},\gamma_{\tilde{g}}\rangle=G_\psi(\tilde{f}-\tilde{g})e^{i\,\mathrm{Im}\langle\tilde{f},\tilde{g}\rangle},\quad \forall\tilde{f},\tilde{g}\in\mathcal{K}.$$

(See Ref. 14.) In other words $(\mathcal{F}_\psi,\gamma_{\tilde{f}})$ provides a Kolmogorov decomposition[17] of the positive definite kernel,

$$k:\mathcal{K}\times\mathcal{K}\to\mathbb{C}:(\tilde{g},\tilde{f})\mapsto G_\psi(\tilde{f}-\tilde{g})e^{i\,\mathrm{Im}\langle\tilde{f},\tilde{g}\rangle}.$$

For every $\tilde{f}=\tilde{f}_1+\tilde{f}_2\in\mathcal{K}$ define the vector

$$\eta_{\tilde{f}}:=\gamma_{\tilde{f}_1}\otimes\gamma_{\tilde{f}_2}\in\mathcal{F}_\psi\otimes\mathcal{F}_\psi,$$

in the Hilbert space tensor product $\mathcal{F}_\psi\otimes\mathcal{F}_\psi$ and let $\mathcal{G}$ be the complex Hilbert space spanned by the vectors $\{\eta_{\tilde{f}}:\tilde{f}\in\mathcal{K}\}$. Then $(\mathcal{G},\eta_{\tilde{f}})$ provides a Kolmogorov decomposition for the kernel,

$$k_0:\mathcal{K}\times\mathcal{K}\to\mathbb{C}:(\tilde{g},\tilde{f})\mapsto G_\psi(\tilde{f}-\tilde{g}),$$

since it holds

$$\begin{aligned}
\langle\eta_{\tilde{f}},\eta_{\tilde{g}}\rangle&=\langle\gamma_{\tilde{f}_1}\otimes\gamma_{\tilde{f}_2},\gamma_{\tilde{g}_1}\otimes\gamma_{\tilde{g}_2}\rangle\\
&=\langle\gamma_{\tilde{f}_1},\gamma_{\tilde{g}_1}\rangle\langle\gamma_{\tilde{f}_2},\gamma_{\tilde{g}_2}\rangle\\
&=G_\psi(\tilde{f}_1-\tilde{g}_1)e^{i\,\mathrm{Im}\langle\tilde{f}_1,\tilde{g}_1\rangle}G_\psi(\tilde{f}_2-\tilde{g}_2)e^{i\,\mathrm{Im}\langle\tilde{f}_2,\tilde{g}_2\rangle}\\
&=G_\psi(\tilde{f}_1-\tilde{g}_1)G_\psi(\tilde{f}_2-\tilde{g}_2)\\
&=G_\psi(p_1(\tilde{f}-\tilde{g}))G_\psi(p_2(\tilde{f}-\tilde{g}))\\
&=G_\psi(\tilde{f}-\tilde{g}),\quad \forall\tilde{f},\tilde{g}\in\mathcal{K}.
\end{aligned}$$

Because a kernel has a Kolmogorov decomposition if and only if it is positive definite, the proof is complete. ■

VI. THE ELECTROMAGNETIC FIELD AT $T=0$

At $T=0$ the quantized electromagnetic field is described by the Fock state ψ_F on CCR($\mathcal{K}=L^2(\mathbb{R})$) with the generating functional

$$G_{\mathrm{F}}(\tilde{f})=e^{-(1/2)\|\tilde{f}\|_{\mathcal{K}}^2}, \quad \forall \tilde{f}\in\mathcal{K}.$$

Since for any generalized decomposition into real and imaginary part it holds that

$$\begin{aligned} G_{\mathrm{F}}(\tilde{f}_1+\tilde{f}_2)&=e^{-(1/2)\|\tilde{f}_1+\tilde{f}_2\|_{\mathcal{K}}^2}\\ &=e^{-(1/2)\mathrm{Re}\langle \tilde{f}_1+\tilde{f}_2,\tilde{f}_1+\tilde{f}_2\rangle_{\mathcal{K}}}\\ &=e^{-(1/2)(\langle \tilde{f}_1,\tilde{f}_1\rangle_{\mathcal{K}}+\langle \tilde{f}_2,\tilde{f}_2\rangle_{\mathcal{K}})}=G_{\mathrm{F}}(\tilde{f}_1)G_F(\tilde{f}_2), \quad \forall \tilde{f}\in\mathcal{K}, \end{aligned}$$

ψ_{F} is a stochastic state. Consequently the quasifree quantum stochastic process $\Lambda_{\mathrm{F}}=\{\Phi_{\mathrm{F}}(\tilde{f}):\tilde{f}\in\mathcal{I}\mathcal{S}_r\}$ given by ψ_{F} has a classical analog $Y_f=\{X_f:f\in\mathcal{S}_r\}$. This analog will be constructed in the following.

The quantum observables $\Phi_{\mathrm{F}}(\tilde{f})$ act on the symmetric Fock space $\mathcal{F}_+(\mathcal{K})$. Y_{F} is uniquely determined by its characteristic functional,

$$C_{\mathrm{F}}(f)=G_{\mathrm{F}}\left(\frac{1}{\sqrt{2}}\mathcal{I}f\right)=e^{-(1/4)\|\mathcal{I}f\|_{\mathcal{K}}^2}, \quad \forall f\in\mathcal{S}_r.$$

Since the unitary embedding $\mathcal{I}$ is isometric with respect to the scalar product $\langle |A|\cdot,\cdot\rangle$ on $\mathcal{S}_r\subseteq\mathcal{H}$, it follows that

$$C_{\mathrm{F}}(f)=e^{-(1/4)\langle |A|f,f\rangle}, \quad \text{with } A=-c\frac{d}{dx}, \ \forall f\in\mathcal{S}_r.$$

The characteristic functional C_{F} determines a zero mean Gaussian generalized stochastic process with covariance,

$$\mathrm{cov}(X_f,X_g)=\int_{\mathcal{S}_r'}X_f(x)X_g(x)d\mu_{\mathrm{F}}(x)=\langle |A|f,g\rangle, \quad \forall f,g\in\mathcal{S}_r$$

(see Ref. 10).

Obviously Y_{F} is not a white but a colored noise. Its spectrum is given by the linearly increasing spectrum of the positive operator $|A|=FT^{-1}\circ M_{|ck|}\circ FT$. This result provides a new argument for an assumption of Gardiner, that the spectrum of the electromagnetic field at $T=0$, which cannot be observed by photon counting, might be linearly increasing. (See Ref. 13.)

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Integrable Yang–Mills–Higgs equations in three-dimensional de Sitter space–time

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This paper describes an integrable Yang–Mills–Higgs system on (2+1)-dimensional de Sitter space–time. It is the curved-space–time analog of the Bogomolnyi equations for monopoles on $\mathbf{R}^3$. A number of solutions, of various types, are constructed. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The background to this paper is the question of the existence of integrable nonlinear partial differential equations (and more specifically of soliton equations) in curved space–times. For a given (fixed) space–time M, are there integrable systems which live on M (i.e., are covariantly coupled to its geometry)? In general, this places severe restrictions both on M and on the equations that are coupled to it. In this paper, we concentrate on one example, namely an integrable Yang–Mills–Higgs system on (2+1)-dimensional de Sitter space–time.

In effect, this generalizes examples which have long been known. Consider the chiral equation $g^{\mu\nu}\partial_\mu(U^{-1}\partial_\nu U)=0$, where $U(x^\mu)$ takes values in a Lie group, and where $g_{\mu\nu}$ is the metric of M. This system is integrable if M is (1+1)-dimensional (this being related to conformal invariance). In higher-dimensional flat space–times, the chiral equation is not integrable;[1] and this is probably also the case for curved space-times of dimension greater than two. But if one modifies the equation by adding a torsion term, then integrability is possible;[1,2] in particular, there is an integrable (modified) chiral equation in flat three-dimensional space–time $\mathbf{R}^{2+1}$. The system is equivalent to one involving a gauge field (Yang–Mills field) coupled to a Higgs field, and may be seen to arise from the self-dual Yang–Mills equations in $\mathbf{R}^{2+2}$, by dimensional reduction. The soliton solutions can be understood in terms of algebraic geometry, and the soliton dynamics is (in general) nontrivial.[3–10]

Other ways of reducing the self-dual Yang–Mills equations in $\mathbf{R}^{2+2}$ can lead to integrable Yang–Mills–Higgs systems in curved (2+1)-dimensional space–times. These are the Lorentzian analog of hyperbolic monopoles, which live on (positive-definite) hyperbolic 3-space. The space–time has to have constant curvature; and so there are two Lorentzian possibilities, namely anti-de Sitter and de Sitter space–time. Some preliminary results on the anti-de Sitter case have appeared previously;[11] the present paper deals with the de Sitter case. In particular, we construct various explicit solutions. One new feature that appears here is associated with the nontrivial topology of de Sitter space.

II. (2+1)-DIMENSIONAL DE SITTER SPACE–TIME

(2+1)-dimensional de Sitter space–time M is the manifold $\mathbf{R}\times S^2$ equipped with the metric

$$ds^2=g_{\mu\nu}\,dx^\mu\,dx^\nu=\cosh^2 T(d\theta^2+\sin^2\theta\,d\varphi^2)-dT^2. \tag{1}$$

Here $T\in\mathbf{R}$ is a time coordinate, and (θ,φ) are polar coordinates on the spatial sphere. It is a space of constant curvature, with scalar curvature $R=6$ (conventions are those of Ref. 12).

There is a relation between this space–time M and flat (2+2)-dimensional space $\mathbf{R}^{2+2}$, and we shall use this to obtain equations on M from equations on $\mathbf{R}^{2+2}$. The relation is as follows. Let u and w be complex coordinates on $\mathbf{R}^{2+2}$, so that its metric is $du\,d\overline{u}-dw\,d\overline{w}$. First, define new coordinates $(\theta,\varphi,\tilde{\theta},\tilde{\varphi})$ by

$$u=\frac{(\sin\theta)\mathrm{e}^{-i\varphi}}{(\cos\theta+\cos\tilde{\theta})},\quad w=\frac{(\sin\tilde{\theta})\mathrm{e}^{i\tilde{\varphi}}}{(\cos\theta+\cos\tilde{\theta})}. \tag{2}$$

Then

$$du\,d\overline{u}-dw\,d\overline{w}=2(\cos\theta+\cos\tilde{\theta})^{-1}\,ds^2_{\tilde{M}}, \tag{3}$$

where

$$ds^2_{\tilde{M}}=(d\theta^2+\sin^2\theta\,d\varphi^2)-(d\tilde{\theta}^2+\sin^2\tilde{\theta}\,d\tilde{\varphi}^2). \tag{4}$$

In other words, R^{2+2} is conformal to part of the product $\tilde{M}=S^2\times S^2$; we interpret (θ,φ) as polar coordinates on the first sphere of $\tilde{M}$, and $(\tilde{\theta},\tilde{\varphi})$ on the second. The 4-space $\tilde{M}$ is conformally flat and has vanishing scalar curvature; it is a double cover of a conformal compactification[13,14] of $\mathbf{R}^{2+2}$.

The next step is to reduce to 2+1 dimensions: this is done by factoring out by the Killing vector $\partial/\partial\tilde{\varphi}$, i.e., by a rotation of the second sphere. First we remove $\tilde{\theta}=0$ and $\tilde{\theta}=\pi$, which are fixed points of the rotation. On the complement of these fixed points, we can write

$$ds^2_{\tilde{M}}=\sin^2\tilde{\theta}\ [\mathrm{cosec}^2\tilde{\theta}(d\theta^2+\sin^2\theta\,d\varphi^2-d\tilde{\theta}^2)-d\tilde{\varphi}^2]. \tag{5}$$

So $\tilde{M}$ (minus the fixed points) is conformal to the product of S^1 and a space with topology $\mathbf{R}\times S^2$ and metric

$$ds^2=\mathrm{cosec}^2\tilde{\theta}(d\theta^2+\sin^2\theta\,d\varphi^2-d\tilde{\theta}^2). \tag{6}$$

This is exactly (2+1)-dimensional de Sitter space–time (1), where the coordinates T and $\tilde{\theta}$ are related by $\tanh T=-\cos\tilde{\theta}$.

III. INTEGRABLE EQUATIONS ON *M*

In view of the conformal relation between $\tilde{M}$ and M, we may obtain integrable equations on M by reducing conformally-invariant integrable equations on $\tilde{M}$ (or $\mathbf{R}^{2+2}$). The simplest conformally-invariant equation on $\tilde{M}$ is the conformally-invariant wave equation. Bearing in mind the absence of scalar curvature, this has the form

$$\Delta\chi-\tilde{\Delta}\chi=0, \tag{7}$$

where Δ and $\tilde{\Delta}$ are the Laplacians on the two spheres. The $\tilde{\varphi}$-independent solutions of (7) correspond to solutions of the conformally-invariant wave equation on M, namely,

$$g^{\mu\nu}\nabla_\mu\nabla_\nu\Psi-\Psi=0, \tag{8}$$

where χ and Ψ are related by the relevant conformal factor, $\Psi=(\mathrm{sech}\,T)\chi$. Solutions can be obtained (in terms of Legendre polynomials and spherical harmonics) by separating variables or

by twistor methods.[13] For example, the simplest case $\chi=1$ (constant) gives $\Psi=\operatorname{sech} T$, i.e., a solution of (8) which is spatially constant. Using $l=1$ spherical harmonics yields the examples $\Psi=\operatorname{sech} T\tanh T\cos\theta$, $\Psi=\operatorname{sech} T\tanh T\sin\theta\cos\varphi$, etc.

Another example, and the one which we concentrate on in this article, is that of the self-dual Yang–Mills equations (these are integrable on any conformally-flat 4-space, and so in particular on $\tilde{M}$). When we reduce to the (2+1)-dimensional space–time M, the self-dual Yang–Mills field becomes a Yang–Mills–Higgs system (Φ,A_μ) satisfying the Bogomolny-type equations,

$$D_\alpha\Phi=\tfrac{1}{2}\eta_{\alpha\beta\gamma}F^{\beta\gamma}. \tag{9}$$

The Higgs field Φ (taking values in the Lie algebra G of the gauge group) is identified with the $\tilde{\varphi}$-component $A_{\tilde{\varphi}}$ of the gauge potential, with the remaining three components A_μ becoming a gauge potential on M. As usual, D_α denotes the covariant derivative $D_\alpha\Phi=\partial_\alpha\Phi+[A_\alpha,\Phi]$, $F_{\mu\nu}$ is the gauge field $[D_\mu,D_\nu]$, and $\eta_{\alpha\beta\gamma}=[-\det(g_{\mu\nu})]^{1/2}\varepsilon_{\alpha\beta\gamma}$ is the volume 3-form on M. In terms of the polar coordinates $(\theta,\tilde{\theta},\varphi)$, Eq. (9) is

$$\begin{aligned} D_{\tilde{\theta}}\Phi&=(\sin\tilde{\theta}\ /\sin\theta)F_{\theta\varphi},\\ D_\theta\Phi&=(\sin\tilde{\theta}\ /\sin\theta)F_{\tilde{\theta}\varphi},\\ D_\varphi\Phi&=(\sin\tilde{\theta}\sin\theta)F_{\theta\tilde{\theta}}. \end{aligned} \tag{10}$$

So (9), or equivalently (10), form a set of covariant integrable partial differential equations on M. They are linear if the gauge algebra G is abelian, but otherwise are nonlinear. In the remaining sections, we shall construct and examine some solutions of (10), for gauge algebras u(1) and su(2).

IV. A U(1) EXAMPLE

For gauge algebra $G=u(1)$, Eqs. (10) reduce to

$$\partial_\alpha\Phi=\tfrac{1}{2}\eta_{\alpha\beta\gamma}F^{\beta\gamma}, \tag{11}$$

where $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$. Note that from (11) it follows immediately that $g^{\mu\nu}\nabla_\mu\nabla_\nu\Phi=0$; so this case is related to, but different from, that of the wave equation (8) discussed previously. Since space is a sphere S^2, there can be nontrivial topology: U(1) gauge fields over S^2 are classified topologically by the integer

$$k=\frac{-\mathrm{i}}{2\pi}\int_\Sigma F_{\mu\nu}dx^\mu\wedge dx^\nu, \tag{12}$$

where Σ is a space section (spacelike surface with topology S^2).

An example of a topologically nontrivial solution of (11) is

$$\Phi=\tfrac{1}{2}\mathrm{i}k(\cos\tilde{\theta}-1),\quad A_\varphi=\tfrac{1}{2}\mathrm{i}k(\cos\theta-1),\quad A_\theta=0=A_{\tilde{\theta}}.$$

For smoothness, we need $A_\varphi=0$ at $\theta=0,\pi$; so the above gauge potential has a singularity at $\theta=\pi$. This is the familiar ''Dirac-string'' singularity, and is removable: the gauge-transformed potential

$$A_\varphi+\exp(-\mathrm{i}k\varphi)\partial_\varphi\exp(\mathrm{i}k\varphi)=\tfrac{1}{2}\mathrm{i}k(\cos\theta+1)$$

is smooth near $\theta=\pi$. In other words, this Maxwell–Higgs system is smooth throughout M. The apparent singularities are a consequence of the fact that the gauge field is topologically nontrivial:

its magnetic charge equals k. Furthermore, it is spatially-homogeneous: note in particular that Φ depends only on the time coordinate $\tilde{\theta}$, and that the gauge 2-form [the integrand of (12)] is a (time-dependent) multiple of the spatial area element $\sin\theta\, d\theta\wedge d\varphi$.

V. SPATIALLY-HOMOGENEOUS SU(2) SOLUTIONS

Spatially-homogeneous SU(2) fields may be characterized as follows. Temporarily, think of the spatial 2-sphere as the unit sphere in $\mathbf{R}^3$, with coordinates $x^j=(x^1,x^2,x^3)$. Take the Higgs field and gauge potential to have the form

$$\Phi = \mathrm{i}g(\tilde{\theta})x^j\sigma_j\,,$$

$$A_j = \mathrm{i}f(\tilde{\theta})\varepsilon_{jkl}x^l\sigma^k, \tag{13}$$

$$A_{\tilde{\theta}}=0, \quad \text{(a gauge choice)},$$

where σ_j are the the Pauli matrices, and f and g are two scalar functions of $\tilde{\theta}$ only. This implements SO(3) symmetry: recall, for example, that the spherically-symmetric 1-monopole in $\mathbf{R}^3$ has the ''hedgehog'' form (13). The components A_θ and A_φ are obtained from A_j in the obvious way, by transforming to polar coordinates. Although Φ and A_μ depend on the spatial variables (θ,φ), the effect of a spatial rotation is to make a gauge transformation; and gauge-invariant quantities such as $-\mathrm{tr}\,\Phi^2=2g^2$ depend only on $\tilde{\theta}$.

Substituting (13) into (10) gives the pair of ordinary differential equations

$$g'=2f(1-f)\sin\tilde{\theta}, \quad f'=g(2f-1)/\sin\tilde{\theta}. \tag{14}$$

Eliminating g from these leaves an equation for f which, after the transformation

$$f(\tilde{\theta})=\tfrac{1}{2}(\mathrm{e}^{2T}+1)P(T)+\tfrac{1}{2}, \quad \tanh T=-\cos\tilde{\theta},$$

is

$$P''=(P')^2/P-4\mathrm{e}^{2T}P^3, \tag{15}$$

where $P'=dP/dT$. This is the third Painlevé equation P_{III}. In terms of the variable $t=\mathrm{e}^T=\tan(\tilde{\theta}/2)\in(0,\infty)$, it takes the more usual form

$$\ddot{P}=(\dot{P})^2/P-\dot{P}/t-4P^3, \tag{16}$$

where $\dot{P}=dP/dt$. Solutions of (15) or (16) therefore determine spatially-homogeneous SU(2) solutions of the Yang–Mills–Higgs–Bogomolny equations (10).

VI. THE TWISTOR CORRESPONDENCE

One can in principle construct all solutions of the self-dual Yang–Mills equations, and hence of (10), by using the twistor correspondence.[15,14] The details of the construction are well-known, and here we simply give some brief details in order to establish notation and conventions.

Twistor space is the complex projective space $\mathbf{CP}^3$, with homogeneous coordinates $Z^\alpha=(Z^0,Z^1,Z^2,Z^3)$. (Strictly speaking, the twistor space of $\tilde{M}$ is a non-Hausdorff space[14] obtained by glueing together two copies of $\mathbf{CP}^3$; but for simplicity we shall avoid going into the details of this.) The correspondence between $\mathbf{CP}^3$ and $\tilde{M}$ is expressed by the relations

$$Z^0=uZ^2+wZ^3, \quad Z^1=\overline{w}Z^2+\overline{u}Z^3. \tag{17}$$

Here u and w are the complex coordinates defined by (2) (recall that they only cover ''half'' of $\tilde{M}$—it is for this reason that the true twistor space is a non-Hausdorff ''doubling'' of $\mathbf{CP}^3$).

A matrix-valued twistor function $F(Z^\alpha)$ is said to be *real* if $F^\dagger = F$, where $F^\dagger(Z^\alpha) = F(\overline{Z^1}, \overline{Z^0}, \overline{Z^3}, \overline{Z^2})^*$, and $*$ denotes complex conjugate transpose. There is a correspondence between certain holomorphic vector bundles over twistor space, and solutions of the self-dual Yang–Mills equations on $\tilde{M}$; in particular, if $F(Z^\alpha)$ is a real ''patching matrix'' for a vector bundle of rank n, then ''splitting'' F yields a self-dual U(n) gauge field. In addition to being real, the matrix function $F(Z^\alpha)$ has to be homogeneous of degree zero in Z^α; and in order to have $\tilde{\varphi}$-invariance, we require F to be annihilated by the vector field

$$V = Z^3 \frac{\partial}{\partial Z^3} - Z^2 \frac{\partial}{\partial Z^2} + Z^1 \frac{\partial}{\partial Z^1} - Z^0 \frac{\partial}{\partial Z^0}. \tag{18}$$

For example, all three requirements (reality, homogeneity and V-invariance) are met by the (scalar) function $Q = (Z^0 Z^1 + Z^2 Z^3)/(Z^2 Z^3)$. Indeed, the line bundle defined by the patching matrix $F = Q^k$, where k is an integer, yields the U(1) solution of Sec. IV.

VII. AN SU(2) EXAMPLE

In order to obtain SU(2) solutions by this construction, we look for examples of 2×2 twistor matrices $F(Z^\alpha)$ which are upper-triangular, and which are equivalent to ''real'' matrices. Given an upper-triangular F, one can obtain explicit expressions for Φ and A_μ (see, for example, Sec. 8.2 of Ref. 15). The analog of the 'tHooft ansatz, and its generalizations (corresponding to example 8.2.3 of Ref. 15) does not work—it produces only SU(1,1) fields. But the analog (changed-signature version) of example 8.2.4 of Ref. 15 does work, and produces SU(2) solutions in our case. Some brief details are as follows.

Write $\zeta = Z^3/Z^2$, and think of $F(Z^\alpha)$ as defining a vector bundle by the patching relation $\hat{\psi} = F\psi$, where ψ and $\hat{\psi}$ are (2-vector) fiber-coordinates over $U = \{|\zeta| \leqslant 1\}$ and $\hat{U} = \{|\zeta| \geqslant 1\}$, respectively. Take $F(Z^\alpha)$ to have the form

$$F(Z^\alpha) = \begin{pmatrix} \zeta^k \mathrm{e}^f & 2Q^{-1} \cosh f \\ 0 & \zeta^{-k} \mathrm{e}^{-f} \end{pmatrix}, \tag{19}$$

where k is a positive integer, $f(Z^\alpha)$ is real, and $Q = P/(Z^2 Z^3)^k$ with $P(Z^\alpha)$ being a real polynomial (homogeneous of degree $2k$). Then, because

$$R(Z^\alpha) = \begin{pmatrix} 0 & -1 \\ 1 & \zeta^k Q \end{pmatrix}$$

is holomorphic on U and FR is real, it follows that the construction will yield a real [i.e., SU(2)-valued] solution.

As an example of this construction, take $P = (Z^0 Z^1 + Z^2 Z^3)$ and $k = 1$ (or $k = -1$, which leads to the same solution). The simplest choice for f, namely, $f = 0$, gives nothing new: the field is then effectively abelian, and is an embedding into SU(2) of the U(1) solution described in Sec. IV. To get something genuinely non-abelian, we may take $f = \log Q$, where $Q = (Z^0 Z^1 + Z^2 Z^3)/(Z^2 Z^3)$, so that

$$F(Z^\alpha) = \begin{pmatrix} \zeta Q & 1 + Q^{-2} \\ 0 & (\zeta Q)^{-1} \end{pmatrix}. \tag{20}$$

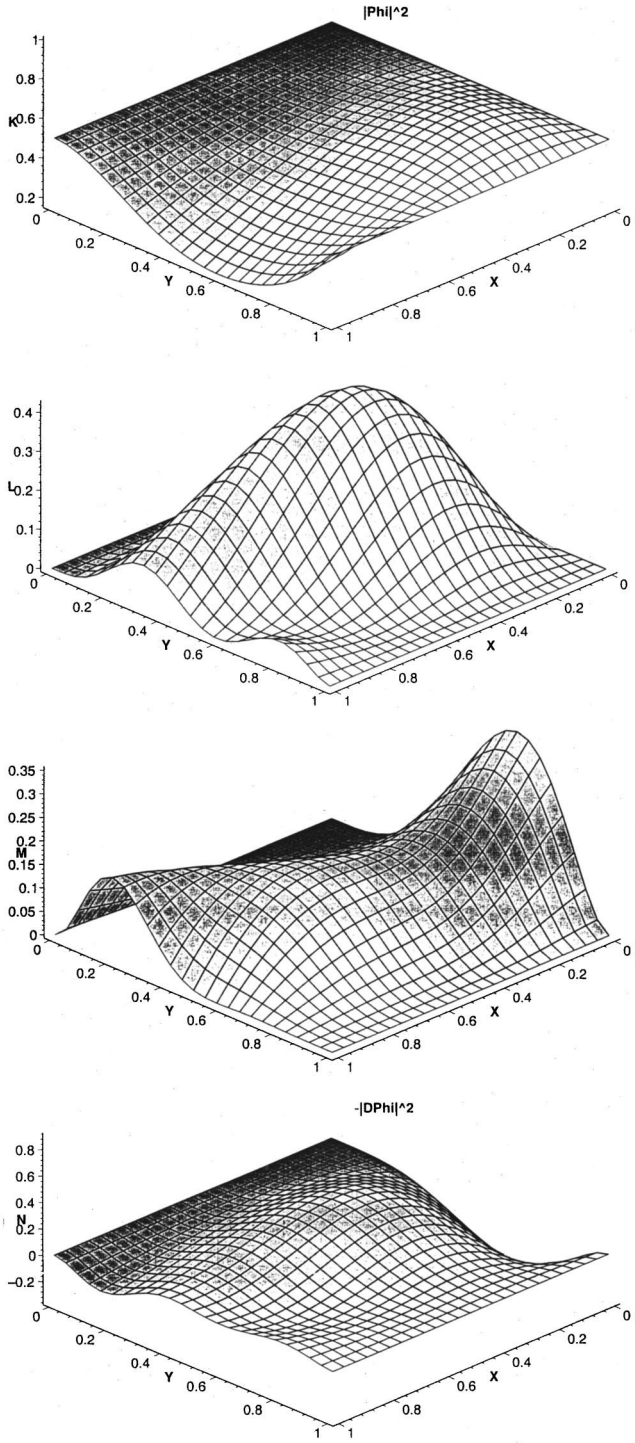

FIG. 1. The quantities $K=-\operatorname{tr}\Phi^2$, $L=-\sin^2\tilde{\theta}\operatorname{tr}(D_{\tilde{\theta}}\Phi)^2$, $M=-\sin^2\tilde{\theta}\operatorname{tr}[(D_\theta\Phi)^2+(D_\varphi\Phi)^2/\sin^2\theta]$ and $N=g^{\mu\nu}\operatorname{tr}[(D_\mu\Phi)(D_\nu\Phi)]$ as functions of $X=\cos^2(\theta/2)$ and $Y=\cos^2(\tilde{\theta}/2)$.

The procedure[15] referred to above then yields explicit (although rather complicated) expressions for Φ and A_μ, as rational functions of $\cos\theta$, $\cos\tilde{\theta}$, and $\exp(i\varphi)$. The dependence on φ can be compensated by a gauge transformation, so in effect the solution depends only on θ and $\tilde{\theta}$: it is an SO(2)-invariant solution of the Yang–Mills–Higgs equations (9) on M.

The functions are somewhat simpler when expressed in terms of the variables $X=\cos^2(\theta/2)$ and $Y=\cos^2(\tilde{\theta}/2)$; for example, $-\operatorname{tr}\Phi^2=\frac{1}{2}H(X,Y)/(1+X^2Y^2)^2$, where

$$H(X,Y)=1+16X^4Y^6-24X^4Y^5+9X^4Y^4+16X^2Y^4-8X^2Y^3-6X^2Y^2-16XY^4+16XY^3.$$

Figure 1 contains plots of four gauge-invariant quantities, namely,

$$K:=-\operatorname{tr}\Phi^2,$$

$$L:=-\sin^2\tilde{\theta}\,\operatorname{tr}(D_{\tilde{\theta}}\Phi)^2,$$

$$M:=-\sin^2\tilde{\theta}\,\operatorname{tr}[(D_\theta\Phi)^2+(D_\varphi\Phi)^2/\sin^2\theta],$$

$$N:=L-M=g^{\mu\nu}\operatorname{tr}[(D_\mu\Phi)(D_\nu\Phi)],$$

as functions of ''spatial latitude'' X and ''time'' Y. A couple of features that may be noted are:

(1) In the distant future or past (i.e., as $Y\to 1$ or $Y\to 0$), the field approaches a ''vacuum value,'' where $-\operatorname{tr}\Phi^2=\frac{1}{2}$ and $-\operatorname{tr}(D_\mu\Phi)^2=0$;
(2) At the point $X=0$ on the spatial sphere, we have $-\operatorname{tr}\Phi^2=\frac{1}{2}$, $-\operatorname{tr}(D_{\text{time}}\Phi)^2=0$ and $-\operatorname{tr}(D_{\text{space}}\Phi)^2=16Y^4(Y-1)^2$.

VIII. CONCLUDING REMARKS

For the corresponding systems in (2+1)-dimensional flat[2] and anti-de Sitter[11] space–time, there are localized soliton solutions; and a single soliton travels (as one would expect) along a timelike geodesic. More investigation is needed to determine whether the same is true in the de Sitter case. The method used to construct solutions in the former cases does not work so well here; the construction of Sec. VII is, by contrast, the analog of one which yields the one-monopole solution[15] of the Yang–Mills–Higgs–Bogomolnyi equations on $\mathbf{R}^3$. One question, therefore, is whether there is a meaningful correspondence between between these two systems, i.e., between the Yang–Mills–Higgs systems on $\mathbf{R}^3$ and on (2+1)-dimensional de Sitter space.

In addition to exact solution methods, one may wish to investigate the equations numerically, as was done in the flat case.[5] For this, an alternative sigma-model or chiral-model formulation is useful; and this may be of interest in any event. For example, there exists a gauge in which $A_{\bar{u}}=H^{-1}\partial_{\bar{u}}H$ and $A_w=H^{-1}\partial_w H$, where H takes values in the complexified gauge group [i.e., SL(2,C) if $G=\mathrm{su}(2)$]. Then the Hermitian matrix $K=HH^*$ satisfies

$$\partial_u(K^{-1}\partial_{\bar{u}}K)-\partial_{\bar{w}}(K^{-1}\partial_w K)=0. \tag{21}$$

And this single matrix equation (21) is equivalent, after transforming coordinates as in (2) and imposing a suitable dependence on $\tilde{\varphi}$, to the Yang–Mills–Higgs equations (10).

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States of quantum systems and their liftings

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Let H_1, H_2 be complex Hilbert spaces, H be their Hilbert tensor product and let tr_2 be the operator of taking partial trace, with respect to the space H_2, of trace class operators in H. The operation tr_2 maps states in H (=positive trace class operators in H with trace equal to 1) into states in H_1. In this paper we give the full description of mappings that are linear right inverse to tr_2. More precisely, we prove that any affine mapping $F(W)$ of the convex set of states in H_1 into the states in H that is right inverse to tr_2 is given by $W \mapsto W \otimes D$ for some state D in H_2. In addition we investigate a representation of the quantum mechanical state space by probability measures on the set of pure states and a representation—used in the theory of stochastic Schrödinger equations—by probability measures on the Hilbert space. We prove that there are no affine mappings from the state space of quantum mechanics into these spaces of probability measures. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1343882]

I. INTRODUCTION

In quantum mechanics the states of a physical system are given by the statistical operators or density matrices in the Hilbert space associated to this system. The state of a subsystem is uniquely calculated as the reduced statistical operator by the partial trace. But it seems that the inverse problem, to define a linear mapping from the set of states of a subsystem to the set of states of an enlarged system such that the reduced state coincides with the original state, has not been studied systematically in the literature. In this article we want to investigate this lifting problem of states and the adjoint problem of reducing observables in some detail.

In the sequel all Hilbert spaces are assumed to be complex (and separable). For any Hilbert space we denote by $\mathcal{L}(H)$ the (complex) vector space of all linear bounded operators in H; by $\mathcal{L}^a(H)$ we denote the real vector subspace of $\mathcal{L}(H)$ consisting of all self-adjoint operators from $\mathcal{L}(H)$, by $\mathcal{L}^+(H)$ we denote the cone of positive operators within $\mathcal{L}(H)$ [and hence within $\mathcal{L}^a(H)$]. The (complex) vector space of all trace class operators in H is denoted by $\mathcal{L}_1(H)$. In addition we use the following notations: $\mathcal{L}_1^+(H) = \mathcal{L}^+(H) \cap \mathcal{L}_1(H)$, $\mathcal{L}_1^a(H) = \mathcal{L}_1^+(H) \cap \mathcal{L}^a(H)$, and $\mathcal{D}(H)$ is the convex set of all operators from $\mathcal{L}_1^+(H)$ having trace equal to one. If H is the Hilbert space associated to a physical system, then the elements of $\mathcal{L}^a(H)$ represent the (bounded) observables of the system, the elements of $\mathcal{D}(H)$ represent (mixed and pure) states, and the closed subset $\mathcal{P}(H) \subset \mathcal{D}(H)$ of rank one projection operators represents the pure states.

If $\mathcal{S}$ and $\mathcal{E}$ are physical systems with Hilbert spaces H_S and H_E, then the Hilbert space of the composite system—denoted by $\mathcal{S} \times \mathcal{E}$—of these systems is the Hilbert tensor product of Hilbert spaces H_S and H_E, i.e., $H = H_S \otimes H_E$. The scalar product in H is written as $\langle , \rangle_H$; the corresponding notations are used for scalar products in H_S and H_E. Hence $\mathcal{S}$ is a subsystem of the quantum system $\mathcal{S} \times \mathcal{E}$, and the system $\mathcal{E}$ can be interpreted as an environment of H_S. For any state W

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$\in \mathcal{D}(H)$ of the total system $\mathcal{S}\times\mathcal{E}$ the state of the system $\mathcal{S}$—called the reduced state—is given by the partial trace $\mathrm{tr}_{H_E} W \in \mathcal{D}(H_S)$. This partial trace is uniquely defined for all $W \in \mathcal{L}_1(H)$ as the operator $\mathrm{tr}_{H_E} W \in \mathcal{L}_1(H_S)$ which satisfies the identity $\langle \mathrm{tr}_{H_E} W x_1, x_2\rangle_{H_S} = \Sigma_j \langle W(x_1 \otimes e_j^E), (x_2 \otimes e_j^E)\rangle_H$ for an orthonormal basis $\{e_j^E\}$ of H_E and all $x_1, x_2 \in H_S$. The mapping $W \to \mathrm{tr}_{H_E} W$, $\mathcal{L}_1(H) \to \mathcal{L}_1(H_S)$, is obviously linear and continuous.

By the partial trace we can calculate the Schrödinger dynamics of the subsystem $\mathcal{S}$—the so called reduced dynamics—from the Schrödinger dynamics of the whole system $\mathcal{S}\times\mathcal{E}$. But in general, this dynamics does not depend linearly on the initial state of the subsystem; see Remark 2. In order to obtain the linear dependence one has to find a linear solution for the lifting problem, which can be formulated as follows. For any state $W_S \in \mathcal{L}_1(H_S)$ to find a state $F(W_S) \in \mathcal{L}_1(H)$ such that $\mathrm{tr}_{H_E} F(W_S) = W_S$; such a mapping F_S is called the lifting.

The simplest solution of this problem is given by the mapping $F_D : \mathcal{L}_1(H_S) \to \mathcal{L}_1(H)$, $W \mapsto W \otimes D$, where D is an element of $\mathcal{L}_1(H_E)$, which is usually called a reference state. This choice is well known from the theory of open systems, see, e.g., Refs. 1–3.

The main theorem of the paper—Theorem 1 of the next section—implies that actually any linear lifting coincides with F_D, for some D.

Remark 1: The vector space $\mathcal{L}^a(H)$ of bounded observables can be identified with the space of continuous affine linear functionals on the state space $\mathcal{D}(H)$ equipped with the topology induced by the trace norm $\|.\|_1$ of $\mathcal{L}_1(H) \supset \mathcal{D}(H)$; see, e.g., Ref. 4. Affine linearity means that such a functional $f : \mathcal{D}(H) \to \mathbb{R}$ respects the mixing property: $f(\alpha W_1 + \beta W_2) = \alpha f(W_1) + \beta f(W_2)$ for $0 \leqslant \alpha, \beta \leqslant 1$ with $\alpha + \beta = 1$, and $W_1, W_2 \in \mathcal{D}(H)$. In fact, any such a functional can be uniquely extended to a continuous $\mathbb{C}$-linear functional $\overline{f} : \mathcal{L}_1(H) \to \mathbb{C}$, see, e.g., Ref. 5. Since $\mathcal{L}(H)$ is dual to $\mathcal{L}_1(H)$, with the duality pairing

$$\mathcal{L}(H) \times \mathcal{L}_1(H) \to \mathbb{C} : (A, W) \mapsto \langle A, W\rangle \equiv \mathrm{tr}_H AW, \tag{1}$$

there exists $A_f \in \mathcal{L}(H)$ such that for any $W \in \mathcal{L}_1(H)$ the identity $\overline{f}(W) = \mathrm{tr}_H WA_f$ is true.

On the other side, according to Gleason's theorem,[6] the state space $\mathcal{D}(H)$ can be identified with the set of linear functionals $\omega : \mathcal{L}(H) \to \mathbb{C}$ having the following properties:

(1) *if $A \in \mathcal{L}^+(H)$ then $\omega(A) \geqslant 0$;*
(2) *$\omega(Id) = 1$;*
(3) *$\omega(\Sigma_j P_j) = \Sigma_j \omega(P_j)$ for any finite or countable family of mutually orthogonal projectors.*

For any ω which satisfies these constraints there exists an element $W_\omega \in \mathcal{D}(H)$ such that $\omega(A) = \mathrm{tr}_H W_\omega A$ is true for all $A \in \mathcal{L}(H)$. The natural norm of the state space is $\sup_{\|A\|=1} |\omega(A)|$ which coincides with the trace norm of W_ω.

Remark 2: The time evolution of a composite system with Hilbert space $H = H_S \otimes H_E$ in the Schrödinger picture is given by a family Φ_t, $t \in \mathbb{R}$ or $t \in \mathbb{R}_+$, of continuous affine linear mappings $\Phi_t : \mathcal{D}(H) \to \mathcal{D}(H)$. We normalize these evolutions by $\Phi_0(W) = W$. The affine linear mappings Φ_t can be extended to $\mathbb{C}$-linear mappings on $\mathcal{L}_1(H)$, again denoted by Φ_t. In the usual case of a Hamiltonian (unitary) dynamics we have $\Phi_t(W) = U(t) W U^+(t)$ with the unitary group $U(t)$ on H generated by the Hamiltonian. But more general evolutions like semigroups are admitted in the sequel. The mappings Φ_t have unique extensions to continuous $\mathbb{C}$-linear mappings $\overline{\Phi}_t$ of $\mathcal{L}_1(H)$ into $\mathcal{L}_1(H)$. The duality (1) then allows us to determine the Heisenberg evolution, a family Ψ_t of continuous linear operators on $\mathcal{L}(H)$. Any Schrödinger evolution Φ_t on $\mathcal{D}(H_S \otimes H_E)$ induces a unique time evolution $\rho_t = tr_{H_E} \Phi_t(W)$ of the system H_S. In order to obtain a linear dependence on the initial state $\rho = \rho_{t=0}$ we need an affine linear mapping F of $\mathcal{D}(H_S)$ into $\mathcal{D}(H_S \otimes H_E)$. Then the mapping $\rho \mapsto W = F(\rho) \mapsto \rho_t = \mathrm{tr}_{H_E} \Phi_t(W)$ is a linear time evolution on $\mathcal{D}(H_S)$. This time evolution has the correct initial condition $\rho_{t=0} = \rho$ if F satisfies the constraint $\mathrm{tr}_{H_E} F(\rho) = \rho$. The Heisenberg dynamics of the system then follows from the duality (1) applied to $\mathcal{L}(H_S)$ and $\mathcal{L}_1(H_S)$.

The paper is organized a follows. In Sec. II we prove the main result of the paper—Theorem 1—describing all linear liftings. In Sec. III we consider a theorem—Theorem 2—that is in a sense dual to Theorem 1 and describes a reduction of observables of the system H to observables of the system H_S.

In the final section (Sec. IV) we consider the case of a classical state space, i.e., a space of probability measures, and the representation of the quantum mechanical state space $\mathcal{D}(H)$ by probability measures either on the set of pure states—the Choquet representation—or on the Hilbert space—a representation used in the theory of stochastic Schrödinger equations. The space $\mathcal{D}(H)$ is a convex set with the closed set $\mathcal{P}(H)$ of pure states as extremal points. Any $W \in \mathcal{D}(H)$ can be represented by an integral over the pure states $W=\int_{\mathcal{P}(H)}\mu(dP)\,P$, where $\mu(dP)$ is a probability measure on $\mathcal{P}(H)$. Since this representation has been derived by Choquet for general convex sets, see, e.g., Ref. 7, we denote the (nonunique) measure $\mu(dP)$ as Choquet measure of W. In Theorem 3 we prove that there does not exist a linear mapping γ from the space $\mathcal{D}(H)$ into the set of probability measures on the set $\mathcal{P}(H)$ such that the measure $\gamma(W)$ is the Choquet measure of the state $W \in \mathcal{D}(H)$. This theorem is in fact a consequence of Theorem 1. In Sec. IV we deduce Theorem 3 from the structural difference between the classical and the quantum mechanical state spaces. Both these spaces are convex sets. But the classical state space is a simplex whereas $\mathcal{D}(H)$ not; see, e.g., Ref. 8. Finally we investigate the representation of the state space by probability measures on the Hilbert space. Also in this case the structural difference between the quantum mechanical state space and the space of probability measures does not allow an affine linear mapping from $\mathcal{D}(H)$ into the measure space.

II. LINEAR LIFTINGS

The main result of the paper is the following theorem.

Theorem 1: *Let* $F:\mathcal{D}(H_S)\to\mathcal{D}(H_S\otimes H_E)$ *be an affine linear mapping such that* $\mathrm{tr}_{H_E}F(\rho)=\rho$ *for all* $\rho\in\mathcal{D}(H_S)$. *Then there exists an element* $\rho_E\in\mathcal{D}(H_E)$ *such that* $F(\rho)=\rho\otimes\rho_E$.

Proof: The mapping F can be extended (uniquely) to the $\mathbb{C}$-linear mapping of $\mathcal{L}_1(H_S)$ into $\mathcal{L}_1(H_S\otimes H_E)$ that we shall denote by the same symbol. This extension has the following properties:

$$F(\mathcal{L}_1^{+}(H_S))\subset\mathcal{L}_1^{+}(H_S\otimes H_E), \tag{2}$$

$$F(\mathcal{L}_1^{a}(H_S))\subset\mathcal{L}_1^{a}(H_S\otimes H_E); \tag{3}$$

we shall use these properties later.

Let $\{e_i, i\in\mathbb{N}\}$ (respectively, $\{f_j, j\in\mathbb{N}\}$) be an orthonormal basis in H_S (respectively, in H_E). Without loss of generality we assume H_S and H_E to be infinite-dimensional. Then $H=\mathrm{span}\{e_i\otimes f_j,\ i\in\mathbb{N}, j\in\mathbb{N}\}$. We realize $\mathcal{L}_1(H_S)$ as a vector space of complex valued functions on $\mathbb{N}^2$: $g_{ij}\in\mathbb{C}: i\in\mathbb{N}, j\in\mathbb{N}$. Analogously, we realize $\mathcal{L}_1(H)=\mathcal{L}_1(H_S\otimes H_E)$ as a vector space of complex valued functions on $\mathbb{N}^4$: $F(g)_{ij}^{kl}, i,j,k,l\in\mathbb{N}$. We say that $b_{ij}, i,j\in\mathbb{N}$ is a (k,l)-component of $F\in\mathcal{L}_1(H)$ and denote it by $(F)^{kl}$ if $F_{ij}^{kl}=b_{ij}$ for all $i,j\in\mathbb{N}$. We say that F has only the components of some type if all components of other types are equal to zero. Let us note that

$$\mathrm{tr}_{H_E}F(g)=g\Leftrightarrow\sum_{i=1}^{\infty}F(g)_{ii}^{kl}=g_{kl},\quad\forall k,l\in\mathbb{N}. \tag{4}$$

Consider the following basis $\{g^{kl}, k\leqslant l, g^{kl*}, k<l\}$ in $\mathcal{L}_1(H_S)$:

$$g_{ij}^{kl}=\begin{cases}1, & \text{if } (i,j)\in\{(k,k),(k,l),(l,k),(l,l)\},\\ 0, & \text{otherwise,}\end{cases} \qquad g_{ij}^{kl*}=\begin{cases}1, & \text{if } (i,j)=(k,k),\\ i, & \text{if } (i,j)=(k,l),\\ -i, & \text{if } (i,j)=(l,k),\\ 1, & \text{if } (i,j)=(l,l),\\ 0, & \text{otherwise.}\end{cases}$$

First, all g^{kl} and g^{kl*} are positive operators, therefore $F(g^{kl})$ and $F(g^{kl*})$ are also positive and hence $F(g^{kl})_{ii}^{mm}\geqslant 0$ and $F(g^{kl*})_{ii}^{mm}\geqslant 0$ for all $i,m\in\mathbb{N}$. Due to (4) $\Sigma_{i=1}^{\infty}F(g^{kl})_{ii}^{mm}=g_{mm}^{kl}=0$ for $m\neq k, m\neq l$ and $\Sigma_{i=1}^{\infty}F(g^{kl*})_{ii}^{mm}=g_{mm}^{kl*}=0$ for $m\neq k, m\neq l$. From this follows that

$$F(g^{kl})_{ii}^{mm}=0,\ m\neq k,\ m\neq l,\ i\in\mathbb{N};\quad F(g^{kl*})_{ii}^{mm}=0,\ m\neq k,\ m\neq l,\ i\in\mathbb{N}. \tag{5}$$

Second, all g^{kl} and g^{kl*} are self-adjoint, therefore $F(g^{kl})$ and $F(g^{kl*})$ are also self-adjoint and hence

$$F(g^{kl})_{ji}^{nm}=\overline{F(g^{kl})_{ij}^{mn}} \text{ and } F(g^{kl*})_{ji}^{nm}=\overline{F(g^{kl*})_{ij}^{mn}}, \quad \text{for all } i,j,k,l,m,n\in\mathbb{N}. \tag{6}$$

□

The further proof is organized as follows. First, we show that $F(g^{kk})$ has only a (k,k)-component (Step 1), $F(g^{kl}),k<l$ [resp., $F(g^{kl*}),k<l$] has only (k,k)-, (k,l)-, (l,k)-, (l,l)-components (Step 2). Furthermore, we prove that nonzero components of $F(g^{kl})$ are equal (Step 3) and that nonzero components of $F(g^{kl*})$ satisfy $(F)^{kk}=-i(F)^{kl}=i(F)^{lk}=(F)^{ll}$ (Step 4). Finally, we denote elements of the only nonzero component of $F(g^{11})$ by a_{ij} and show that any nonzero component of $F(g^{kl})$ is equal to a_{ij} (Step 5) and that the nonzero components of $F(g^{kl*})$ satisfy $(F)^{kk}=-i(F)^{kl}=i(F)^{lk}=(F)^{ll}=a_{ij}$ (Step 6), which completes the proof.

In the proof we shall also use the following (obvious) lemma.

Lemma 1: Let $a\geqslant 0, b\geqslant 0, c\geqslant 0$ be real numbers; then

$$\begin{aligned}&\{(t,p)\in\mathbb{R}^2:(1+t)(1+p)\geqslant 1, t+1\geqslant 0\}\\ &\quad\subset\{(t,p)\in\mathbb{R}^2:(b+at)(b+cp)\geqslant b^2, b+at\geqslant 0\}\\ &\quad\Leftrightarrow a=c\leqslant b.\end{aligned}$$

Proof of Theorem 1 (continued):

Step 1. Consider $g^{kk}\in\mathcal{L}_1(H_S),k\in\mathbb{N}$ and restrict $F(g^{kk})$ to the space $\langle e_m\otimes f_i, e_n\otimes f_j\rangle$, where $(m,n)\neq(k,k)$. In this basis $F(g^{kk})$ has the form

$$\begin{pmatrix} F(g^{kk})_{ii}^{mm} & F(g^{kk})_{ji}^{nm}\\ F(g^{kk})_{ij}^{mn} & F(g^{kk})_{jj}^{nn}\end{pmatrix}.$$

Because either $m\neq k$ or $n\neq k$ we have due to (5) that either $F(g^{kk})_{ii}^{mm}=0$ or $F(g^{kk})_{jj}^{nn}=0$. $F(g^{kk})$ is positive, hence $F(g^{kk})_{ii}^{mm}F(g^{kk})_{jj}^{nn}-F(g^{kk})_{ji}^{nm}F(g^{kk})_{ij}^{mn}\geqslant 0$. Combining these conditions together with (6) we get

$$F(g^{kk})_{ij}^{mn}=0,\ \forall i,\ j,m,n\in\mathbb{N},\ (m,n)\neq(k,k),$$

i.e., $F(g^{kk})$ has only a (k,k)-component.

Step 2. Consider $g^{kl}\in\mathcal{L}_1(H_S),k,l\in\mathbb{N},k<l$ and restrict $F(g^{kl})$ to the subspace $\langle e_m\otimes f_i, e_n\otimes f_j\rangle$, where (m,n) does not take values (k,k), (k,l), (l,k), (l,l). In this basis $F(g^{kl})$ has the form

$$\begin{pmatrix} F(g^{kl})_{ii}^{mm} & F(g^{kl})_{ji}^{nm} \\ F(g^{kl})_{ij}^{mn} & F(g^{kl})_{jj}^{nn} \end{pmatrix}.$$

Due to the conditions on (m,n) it follows from (5) that either $F(g^{kl})_{ii}^{mm}=0$ or $F(g^{kl})_{jj}^{nn}=0$. $F(g^{kl})$ is positive, hence $F(g^{kl})_{ii}^{mm}F(g^{kl})_{jj}^{nn}-F(g^{kl})_{ji}^{nm}F(g^{kl})_{ij}^{mn}\geqslant 0$. Combining this condition together with (6) we get

$$F(g^{kl})_{ij}^{mn}=0, \quad \forall i,\ j,m,n\in\mathbb{N}, \quad \text{with } (m,n)\notin\{(k,k),(k,l),(l,k),(l,l)\},$$

i.e., $F(g^{kl})$ has only (k,k)-, (k,l)-, (l,k)-, (l,l)-components.

Analogously (substituting $g^{kl}*$ for g^{kl}) we prove that $F(g^{kl}*)$ has only (k,k)-, (k,l)-, (l,k)-, (l,l)-components.

Step 3. First, let us show that the main diagonals of the nonzero components of $F(g^{kl})$ are equal, i.e., $F(g^{kl})_{ii}^{kk}=F(g^{kl})_{ii}^{kl}=F(g^{kl})_{ii}^{lk}=F(g^{kl})_{ii}^{ll}$. Restrict $F(g^{kl})$ to the subspace $\langle e_k\otimes f_i, e_l\otimes f_i\rangle$. In this basis $F(g^{kl})$ has the form

$$\begin{pmatrix} F(g^{kl})_{ii}^{kk} & F(g^{kl})_{ii}^{lk} \\ F(g^{kl})_{ii}^{kl} & F(g^{kl})_{ii}^{ll} \end{pmatrix}.$$

This matrix is positive, hence $F(g^{kl})_{ii}^{kk}F(g^{kl})_{ii}^{ll}-F(g^{kl})_{ii}^{lk}F(g^{kl})_{ii}^{kl}\geqslant 0$, i.e., $|F(g^{kl})_{ii}^{kl}|\leqslant\sqrt{F(g^{kl})_{ii}^{kk}F(g^{kl})_{ii}^{ll}}$ [note that $F(g^{kl})_{ii}^{kk}$ and $F(g^{kl})_{ii}^{ll}$ are real and non-negative]. Due to (4) $\Sigma_{i=1}^{\infty}F(g^{kl})_{ii}^{kk}=\Sigma_{i=1}^{\infty}F(g^{kl})_{ii}^{kl}=\Sigma_{i=1}^{\infty}F(g^{kl})_{ii}^{lk}=\Sigma_{i=1}^{\infty}F(g^{kl})_{ii}^{ll}=1$ and hence

$$\begin{aligned} 1=\sum_{i=1}^{\infty}\operatorname{Re}F(g^{kl})_{ii}^{kl}\leqslant\sum_{i=1}^{\infty}|F(g^{kl})_{ii}^{kl}|&\leqslant\sum_{i=1}^{\infty}\sqrt{F(g^{kl})_{ii}^{kk}F(g^{kl})_{ii}^{ll}} \\ &\leqslant\sum_{i=1}^{\infty}\frac{F(g^{kl})_{ii}^{kk}+F(g^{kl})_{ii}^{ll}}{2}=1, \end{aligned}$$

and therefore all parts of the inequality must be equal. We have

$$\sqrt{F(g^{kl})_{ii}^{kk}F(g^{kl})_{ii}^{ll}}=\frac{F(g^{kl})_{ii}^{kk}+F(g^{kl})_{ii}^{ll}}{2}\Rightarrow F(g^{kl})_{ii}^{kk}=F(g^{kl})_{ii}^{ll}$$

and

$$\operatorname{Re}F(g^{kl})_{ii}^{kl}=|F(g^{kl})_{ii}^{kl}|=F(g^{kl})_{ii}^{kk}\Rightarrow F(g^{kl})_{ii}^{kl}=F(g^{kl})_{ii}^{lk}=F(g^{kl})_{ii}^{kk}.$$

Hence the diagonal elements $F(g^{kl})_{ii}^{kk}=F(g^{kl})_{ii}^{kl}=F(g^{kl})_{ii}^{lk}=F(g^{kl})_{ii}^{ll}$ are equal.

Second, let us show that the corresponding nondiagonal elements of the nonzero components of $F(g^{kl})$ are equal, i.e., $F(g^{kl})_{ij}^{kk}=F(g^{kl})_{ij}^{kl}=F(g^{kl})_{ij}^{lk}=F(g^{kl})_{ij}^{ll}$, where $i\neq j$. Denote $a_i=F(g^{kl})_{ii}^{kk}$. Restrict $F(g^{kl})$ to the subspace $\langle e_k\otimes f_i, e_k\otimes f_j, e_l\otimes f_j\rangle$. In this basis $F(g^{kl})$ has the form

$$\begin{pmatrix} F(g^{kl})_{ii}^{kk} & F(g^{kl})_{ji}^{kk} & F(g^{kl})_{ji}^{lk} \\ F(g^{kl})_{ij}^{kk} & F(g^{kl})_{jj}^{kk} & F(g^{kl})_{jj}^{lk} \\ F(g^{kl})_{ij}^{kl} & F(g^{kl})_{jj}^{kl} & F(g^{kl})_{jj}^{ll} \end{pmatrix}=\begin{pmatrix} a_i & \overline{y} & \overline{x} \\ y & a_j & a_j \\ x & a_j & a_j \end{pmatrix}=A.$$

If $a_j=0$ then obviously $x=y=0$ as A is positive. If $a_j\neq 0$ then

$$\det A=-y(\overline{y}a_j-\overline{x}a_j)+x(\overline{y}a_j-\overline{x}a_j)=-a_j|y-x|^2\geqslant 0\Rightarrow x=y,$$

and we have derived $F(g^{kl})_{ij}^{kk}=F(g^{kl})_{ij}^{kl}=F(g^{kl})_{ij}^{lk}=F(g^{kl})_{ij}^{ll}$, for all i,j.

Step 4. First, let us prove $F(g^{kl*})^{kk}_{ii}=-iF(g^{kl*})^{kl}_{ii}=iF(g^{kl*})^{lk}_{ii}=F(g^{kl*})^{ll}_{ii}$, i.e., that this condition holds on the main diagonals of nonzero components of $F(g^{kl*})$. Analogously to the previous step, we get $|F(g^{kl*})^{kl}_{ii}|\leqslant\sqrt{F(g^{kl*})^{kk}_{ii}F(g^{kl*})^{ll}_{ii}}$ [note that $F(g^{kl*})^{kk}_{ii}$ and $F(g^{kl*})^{ll}_{ii}$ are real and non-negative]. Due to (4) $\Sigma_{i=1}^{\infty}F(g^{kl*})^{kk}_{ii}=\Sigma_{i=1}^{\infty}F(g^{kl*})^{ll}_{ii}=1$, $\Sigma_{i=1}^{\infty}F(g^{kl*})^{kl}_{ii}=i$, $\Sigma_{i=1}^{\infty}F(g^{kl*})^{lk}_{ii}=-i$ and hence

$$1=\sum_{i=1}^{\infty}\operatorname{Im}F(g^{kl*})^{kl}_{ii}\leqslant\sum_{i=1}^{\infty}|F(g^{kl*})^{kl}_{ii}|\leqslant\sum_{i=1}^{\infty}\sqrt{F(g^{kl*})^{kk}_{ii}F(g^{kl})^{ll}_{ii}}$$

$$\leqslant\sum_{i=1}^{\infty}\frac{F(g^{kl*})^{kk}_{ii}+F(g^{kl*})^{ll}_{ii}}{2}=1,$$

and therefore all parts of inequality must be equal. Analogously to the previous step we have

$$F(g^{kl*})^{kk}_{ii}=F(g^{kl*})^{ll}_{ii}$$

and

$$\operatorname{Im}F(g^{kl*})^{kl}_{ii}=|F(g^{kl*})^{kl}_{ii}|=F(g^{kl*})^{kk}_{ii}\Rightarrow F(g^{kl*})^{kl}_{ii}=F(g^{kl*})^{lk}_{ii}=F(g^{kl*})^{kk}_{ii},$$

and hence $F(g^{kl*})^{kk}_{ii}=-iF(g^{kl*})^{kl}_{ii}=iF(g^{kl*})^{lk}_{ii}=F(g^{kl*})^{ll}_{ii}$.

Second, let us show that this property holds also for corresponding nondiagonal elements of the nonzero components of $F(g^{kl*})$, i.e., $F(g^{kl*})^{kk}_{ij}=-iF(g^{kl*})^{kl}_{ij}=iF(g^{kl*})^{lk}_{ij}=F(g^{kl*})^{ll}_{ij}$ if $i\neq j$.

Denote $a_i=F(g^{kl*})^{kk}_{ii}$. Restrict $F(g^{kl*})$ to the subspace $\langle e_k\otimes f_i,e_k\otimes f_j,e_l\otimes f_j\rangle$. In this basis $F(g^{kl*})$ has the form

$$\begin{pmatrix}F(g^{kl*})^{kk}_{ii} & F(g^{kl*})^{kk}_{ji} & F(g^{kl*})^{lk}_{ji}\\ F(g^{kl*})^{kk}_{ij} & F(g^{kl*})^{kk}_{jj} & F(g^{kl*})^{lk}_{jj}\\ F(g^{kl*})^{kl}_{ij} & F(g^{kl*})^{kl}_{jj} & F(g^{kl*})^{ll}_{jj}\end{pmatrix}=\begin{pmatrix}a_i & \overline{y} & \overline{x}\\ y & a_j & ia_j\\ x & -ia_j & a_j\end{pmatrix}=A.$$

If $a_j=0$ then obviously $x=iy=0$ as A is positive. If $a_j\neq 0$ then

$$\det A=-y(\overline{y}a_j-i\overline{x}a_j)+x(-i\overline{y}a_j-\overline{x}a_j)=-a_j|iy-x|^2\geqslant 0\Rightarrow x=iy,$$

and hence $F(g^{kl*})^{kk}_{ij}=-iF(g^{kl*})^{kl}_{ij}=iF(g^{kl*})^{lk}_{ij}=F(g^{kl*})^{ll}_{ij}$ holds for all i,j.

Step 5. First, let us show that the main diagonals of nonzero components of all $F(g^{kl})$, $k\leqslant l$, are equal, i.e., we have to prove

$$F(g^{kk})^{kk}_{ii}=F(g^{ll})^{ll}_{ii}=F(g^{kl})^{kl}_{ii},\quad\text{for all}\quad k<l.$$

Consider $g(t)=g^{kl}+tg^{kk}+pg^{ll}$, where $t+p+tp\geqslant 0$, $p+1\geqslant 0$ and $k<l$. The operator $g(t)$ is positive hence $F(g(t))$ is also positive. Restrict $F(g(t))$ to the subspace $\langle e_k\otimes f_i,e_l\otimes f_i\rangle$. In this basis $F(g(t))$ has the form

$$\begin{pmatrix}F(g(t))^{kk}_{ii} & F(g(t))^{lk}_{ii}\\ F(g(t))^{kl}_{ii} & F(g(t))^{ll}_{ii}\end{pmatrix}=\begin{pmatrix}F(g^{kl})^{kk}_{ii}+tF(g^{kk})^{kk}_{ii} & F(g^{kl})^{lk}_{ii}\\ F(g^{kl})^{kl}_{ii} & F(g^{kl})^{ll}_{ii}+pF(g^{ll})^{ll}_{ii}\end{pmatrix}.$$

This matrix is positive, hence

$$(F(g^{kl})^{kk}_{ii}+tF(g^{kk})^{kk}_{ii})(F(g^{kl})^{ll}_{ii}+pF(g^{ll})^{ll}_{ii})\geqslant(F(g^{kl})^{kl}_{ii})^2$$

[note that $F(g^{kl})^{kl}_{ii}$, $F(g^{kl})^{kk}_{ii}+tF(g^{kk})^{kk}_{ii}$, and $F(g^{kl})^{ll}_{ii}+pF(g^{ll})^{ll}_{ii}$ are real and non-negative]. We apply Lemma 1 with $a=F(g^{kk})^{kk}_{ii}$, $b=F(g^{kl})^{kl}_{ii}$, $c=F(g^{ll})^{ll}_{ii}$, which gives us

$$F(g^{kk})^{kk}_{ii}=F(g^{ll})^{ll}_{ii}\leqslant F(g^{kl})^{kl}_{ii}.$$

Taking into account the fact that $\Sigma_{i=1}^{\infty}F(g^{kk})^{kk}_{ii}=\Sigma_{i=1}^{\infty}F(g^{ll})^{ll}_{ii}=\Sigma_{i=1}^{\infty}F(g^{kl})^{kl}_{ii}=1$ we get

$$F(g^{kk})^{kk}_{ii}=F(g^{ll})^{ll}_{ii}=F(g^{kl})^{kl}_{ii}.$$

Second, let us show that the remaining elements of the nonzero components of $F(g^{kl}),k\leqslant l$ are equal. For that purpose we prove

$$F(g^{kk})^{kk}_{ij}=F(g^{ll})^{ll}_{ij}=F(g^{kl})^{kl}_{ij},\ \text{for all}\ i\neq j\ \text{and all}\ k<l$$

using again the operator $g(t)$. Denote $a_i=F(g^{kl})^{kk}_{ii}$. Restrict $F(g(t))$ to the subspace $\langle e_k\otimes f_i,e_k\otimes f_j,e_l\otimes f_j\rangle$. In this basis $F(g(t))$ has the form

$$\begin{aligned}
&\begin{pmatrix} F(g(t))^{kk}_{ii} & F(g(t))^{kk}_{ji} & F(g(t))^{lk}_{ji}\\ F(g(t))^{kk}_{ij} & F(g(t))^{kk}_{jj} & F(g(t))^{lk}_{jj}\\ F(g(t))^{kl}_{ij} & F(g(t))^{kl}_{jj} & F(g(t))^{ll}_{jj}\end{pmatrix}\\
&=\begin{pmatrix} F(g^{kl})^{kk}_{ii}+tF(g^{kk})^{kk}_{ii} & F(g^{kl})^{kk}_{ji}+tF(g^{kk})^{kk}_{ji} & F(g^{kl})^{lk}_{ji}\\ F(g^{kl})^{kk}_{ij}+tF(g^{kk})^{kk}_{ij} & F(g^{kl})^{kk}_{jj}+tF(g^{kk})^{kk}_{jj} & F(g^{kl})^{lk}_{jj}\\ F(g^{kl})^{kl}_{ij} & F(g^{kl})^{kl}_{jj} & F(g^{kl})^{ll}_{jj}+pF(g^{ll})^{ll}_{jj}\end{pmatrix}\\
&=\begin{pmatrix} a_i+ta_i & x+ty & x\\ \overline{x}+t\overline{y} & a_j+ta_j & a_j\\ \overline{x} & a_j & a_j+pa_j\end{pmatrix}\\
&=A.
\end{aligned}$$

If $a_j=0$ then obviously $x=y=0$ as A is positive. If $a_j\neq 0$ then

$$\begin{aligned}
\det A=&\,a_ia_j^2(1+t)^2(1+p)+(x+ty)a_j\overline{x}+x(\overline{x}+t\overline{y})a_j-xa_j(1+t)\overline{x}\\
&-(x+ty)(\overline{x}+t\overline{y})a_j(1+p)-a_ia_j^2(1+t)\\
=&-\frac{a_j}{1+t}|x(1+t)-(x+ty)|^2\geqslant 0\Rightarrow x=y.
\end{aligned}$$

This means that

$$F(g^{kl})^{kk}_{ij}=F(g^{kk})^{kk}_{ij}.$$

Step 6. First, let us show that the main diagonals of nonzero components of all $F(g^{kl*})$, $k<l$ satisfy the equality

$$F(g^{kk})^{kk}_{ii}=-iF(g^{kl*})^{kl}_{ii}=iF(g^{kl*})^{lk}_{ii}=F(g^{ll})^{ll}_{ii}.$$

Thereby we use the same arguments as in the previous step considering the operator $g^*(t)=g^{kl*}+tg^{kk}+pg^{ll}$, where $t+p+tp\geqslant 0$, $p+1\geqslant 0$ and $k<l$. The operator $g^*(t)$ is positive, hence $F(g^*(t))$ is also positive. Restrict $F(g^*(t))$ to the subspace $\langle e_k\otimes f_i,e_l\otimes f_i\rangle$. In this basis $F(g^*(t))$ has the form

$$\begin{pmatrix} F(g^*(t))^{kk}_{ii} & F(g^*(t))^{lk}_{ii}\\ F(g^*(t))^{kl}_{ii} & F(g^*(t))^{ll}_{ii}\end{pmatrix}=\begin{pmatrix} F(g^{kl*})^{kk}_{ii}+tF(g^{kk})^{kk}_{ii} & -F(g^{kl*})^{kl}_{ii}\\ F(g^{kl*})^{kl}_{ii} & F(g^{kl*})^{ll}_{ii}+pF(g^{ll})^{ll}_{ii}\end{pmatrix}. \tag{7}$$

Note that $-iF(g^{kl*})^{kl}_{ii}$, $F(g^{kl*})^{kk}_{ii}+tF(g^{kk})^{kk}_{ii}$, and $F(g^{kl*})^{ll}_{ii}+pF(g^{ll})^{ll}_{ii}$ are real and nonnegative. The matrix (7) is positive, hence

$$(F(g^{kl*})^{kk}_{ii}+tF(g^{kk})^{kk}_{ii})(F(g^{kl*})^{kk}_{ii}+pF(g^{ll})^{ll}_{ii})\geqslant -|F(g^{kl*})^{kl}_{ii}|^2=|-iF(g^{kl*})^{kl}_{ii}|^2.$$

We apply Lemma 1 with $a=F(g^{kk})^{kk}_{ii}$, $b=-iF(g^{kl*})^{kl}_{ii}$, $c=F(g^{ll})^{ll}_{ii}$, which gives us

$$F(g^{kk})^{kk}_{ii}=F(g^{ll})^{ll}_{ii}\leqslant -iF(g^{kl*})^{kl}_{ii}.$$

Taking into account the fact that $\Sigma_{i=1}^{\infty}F(g^{kk})^{kk}_{ii})=\Sigma_{i=1}^{\infty}F(g^{ll})^{ll}_{ii}=-\Sigma_{i=1}^{\infty}iF(g^{kl*})^{kl}_{ii}=1$ we get

$$F(g^{kk})^{kk}_{ii}=-iF(g^{kl*})^{kl}_{ii}=iF(g^{kl*})^{lk}_{ii}=F(g^{ll})^{ll}_{ii},\ \text{for all}\ k<l.$$

Second, let us show that the remaining elements of the nonzero components of $F(g^{kl*})$, $k<l$, satisfy

$$F(g^{kk})^{kk}_{ij}=F(g^{kl*})^{kk}_{ij},\ \text{if}\ i\neq j,$$

using again the operator $g^*(t)$. Denote $a_i=F(g^{kl*})^{kk}_{ii}$. Restrict $F(g^*(t))$ to the subspace $\langle e_k\otimes f_i, e_k\otimes f_j, e_l\otimes f_j\rangle$. In this basis $F(g^*(t))$ has the form

$$\begin{pmatrix} F(g^*(t))^{kk}_{ii} & F(g^*(t))^{kk}_{ji} & F(g^*(t))^{lk}_{ji} \\ F(g^*(t))^{kk}_{ij} & F(g^*(t))^{kk}_{jj} & F(g^*(t))^{lk}_{jj} \\ F(g^*(t))^{kl}_{ij} & F(g^*(t))^{kl}_{jj} & F(g^*(t))^{ll}_{jj} \end{pmatrix}$$

$$=\begin{pmatrix} F(g^{kl*})^{kk}_{ii}+tF(g^{kk})^{kk}_{ii} & F(g^{kl*})^{kk}_{ji}+tF(g^{kk})^{kk}_{ji} & F(g^{kl*})^{lk}_{ji} \\ F(g^{kl*})^{kk}_{ij}+tF(g^{kk})^{kk}_{ij} & F(g^{kl*})^{kk}_{jj}+tF(g^{kk})^{kk}_{jj} & F(g^{kl*})^{lk}_{jj} \\ F(g^{kl*})^{kl}_{ij} & F(g^{kl*})^{kl}_{jj} & F(g^{kl*})^{ll}_{jj}+pF(g^{ll})^{ll}_{jj} \end{pmatrix}$$

$$=\begin{pmatrix} a_i+ta_i & x+ty & -ix \\ \overline{x}+t\overline{y} & a_j+ta_j & -ia_j \\ i\overline{x} & ia_j & a_j+pa_j \end{pmatrix}=A.$$

If $a_j=0$ then obviously $x=y=0$ as A is positive. If $a_j\neq 0$ then, analogously to the previous step,

$$\det A=-\frac{a_j}{1+t}|x(1+t)-(x+ty)|^2\geqslant 0\Rightarrow x=y.$$

This means that

$$F(g^{kl*})^{kk}_{ij}=F(g^{kk})^{kk}_{ij}.$$

Denote $a_{ij}=F(g^{11})^{11}_{ij}$ and consider $\rho_E\in\mathcal{L}_1^+(H_S)$ that has the form a_{ij} in the basis $\{e_i, i\in\mathbb{N}\}$. It is easy to see now that $F(\rho)=\rho\otimes\rho_E$ for each $\rho\in\mathcal{L}_1(H)$. The theorem is proved. □

Remark 3: The theorem implies that the linear lifting F is continuous.

Remark 4: If we skip the constraint $\mathrm{tr}_{H_E}F(\rho)=\rho$, *more general liftings are possible. Let* $\rho_E\in\mathcal{D}(H_E)$ *be a reference state, and* K_n *a family of bounded operators in* H *which satisfy* $\Sigma_n K_n^+K_n=Id$; *then*

$$\rho\mapsto F(\rho)=\sum_n K_n(\rho\otimes\rho_E)K_n^+ \tag{8}$$

is a linear and continuous mapping $\mathcal{D}(H_S)\to\mathcal{D}(H)$. Such liftings are used in general investigations of the process of measurement[9] *and in information theory; see, e.g., Ref. 10.*

Remark 5: It is well known that any mixed state ρ of a system $\mathcal{S}$ can be obtained as the reduced state of a pure state in an extended system $\mathcal{S}\times\mathcal{E}$, if only $\dim H_E \geqslant \dim H_S$; *see, e.g., Ref. 11. But due to Theorem 1 the pure state cannot depend linearly on the state ρ. The representation by a pure state is actually a generalization of the classical Gram's theorem from linear algebra. To see this let H_S be realized as $\mathcal{L}_2(\Omega,\mathcal{B}_\Omega,\mu_\Omega)$ where Ω is a set, $\mathcal{B}_\Omega$ is a σ-algebra of its subsets, μ_Ω a non-negative σ-additive measure on $\mathcal{B}_\Omega$. Then the space $H=H_S\otimes H_E$ is isomorphic to the space $\mathcal{L}_2(\Omega,\mathcal{B}_\Omega,\mu_\Omega,H_E)$ of H_E-valued Bochner square μ_Ω-integrable functions on Ω. The corresponding isomorphic map $H_S\otimes H_E\to\mathcal{L}_2(\Omega,\mathcal{B}_\Omega,\mu_\Omega,H_E)$ is denoted by φ. On the other hand, the space $H_S\otimes H_S$ can be realized as $\mathcal{L}_2(\Omega\times\Omega,\mathcal{B}_\Omega\otimes\mathcal{B}_\Omega,\mu_\Omega\otimes\mu_\Omega)$, and hence the space $\mathcal{L}_1(H_S)$ can be considered as a vector subspace of the latter space which includes all Hilbert–Schmidt operators in H_S. Any normalized vector $a\in H_S\otimes H_E$, $\|a\|=1$, spans a one-dimensional subspace of $H_S\otimes H_E$ and defines a unique projection operator $P_a\in\mathcal{D}(H_S\otimes H_E)$. If $f_a\in\mathcal{L}_2(\Omega,\mathcal{B}_\Omega,\mu_\Omega,H_E)$ is defined by $f_a=\varphi(a)$ then the reduced state of the pure state P_a is given by*

$$S(\omega_1,\omega_2)=\langle f_a(\omega_1),f_a(\omega_2)\rangle_{H_E}. \tag{9}$$

Now the generalization of Gram's theorem can be formulated as follows: For any $S\in\mathcal{L}_1^+(H_S)$ there exists a vector $a\in H_S\otimes H_E$, $\|a\|=1$, for which (9) holds. If Ω is a finite set and μ_Ω is the counting measure, we obtain the classical Gram's theorem.

III. REDUCING OBSERVABLES

The problem of linear liftings of states is closely related to the problem of reducing observables of the total system H to observables of the subsystem H_S.

Lemma 2: Let $F:\mathcal{L}_1(H_S)\to\mathcal{L}_1(H_S\otimes H_E)$ be a continuous mapping and let $F^*:\mathcal{L}(H_S\otimes H_E)\to\mathcal{L}(H_S)$ be its adjoint mapping; then $F^*(B\otimes\mathrm{Id}_E)=B$ for all $B\in\mathcal{L}(H_S)$ iff $\mathrm{tr}_{H_E}F(\rho)=\rho$ for all $\rho\in\mathcal{L}_1(H_S)$.

Proof: If $B\in\mathcal{L}(H_S)$ then, according to the definition of the duality between $\mathcal{L}(H)$ and $\mathcal{L}_1(H)$, $\langle B\otimes\mathrm{Id}_E,F(\rho)\rangle=\mathrm{tr}_H(B\otimes\mathrm{Id}_E)F(\rho)=\mathrm{tr}_{H_S}B\rho=\langle B,\rho\rangle$. This identity together with the definition of the duality between $\mathcal{L}(H_S)$ and $\mathcal{L}_1(H_S)$ implies that

$$F^*(B\otimes\mathrm{Id})=B. \tag{10}$$

On the other hand, if F^* satisfies (10) then, for $B\in\mathcal{L}(H_S)$ and $\rho\in\mathcal{L}_1(H_S)$,

$$\langle B\otimes\mathrm{Id}_E,F(\rho)\rangle=\langle F^*(B\otimes\mathrm{Id}_E),\rho\rangle=\langle B,\rho\rangle=\mathrm{tr}_{H_S}B\rho. \tag{11}$$

But $\langle B\otimes\mathrm{Id}_E,F(\rho)\rangle=\mathrm{tr}_{H_S}B(\mathrm{tr}_{H_E}F(\rho))$. Hence $\langle B,\rho\rangle=\mathrm{tr}_{H_S}B\rho=\langle B,\mathrm{tr}_{H_E}F(\rho)\rangle$, and as the latter identity holds for any B, we finally obtain $\rho=\mathrm{tr}_{H_E}F(\rho)$. The lemma is proved. □

Theorem 1 and Lemma 2 imply the following theorem.

Theorem 2: *If $R:\mathcal{L}(H_S\otimes H_E)\to\mathcal{L}(H_S)$ is a linear mapping, continuous in the ultraweak or $(\sigma(\mathcal{L}(H),\mathcal{L}_1(H)),\sigma(\mathcal{L}(H_S),\mathcal{L}_1(H_S)))$ topology; see, e.g., Sec. VI.6 of Ref. 4, and if $R(B\otimes\mathrm{Id}_E)=B$ is true for all $B\in\mathcal{L}(H_S)$ then there exists an element $\rho_E\in\mathcal{D}(H_S)$ such that $R(A)=\mathrm{tr}_{H_E}A(\mathrm{Id}_S\otimes\rho_E)$ for all $A\in\mathcal{L}(H)$.*

IV. PROBABILITY MEASURES

The classical analog of the case considered in Theorem 1 is much simpler and admits nonfactorizing answers. Let T be a topological space; then $\mathcal{C}_b(T)$ is the vector space of all bounded continuous functions on T, $\mathcal{M}(T)$ is the vector space of all Borel (signed) measures on T equipped with the topology $\sigma(\mathcal{M}(T),\mathcal{C}_b(T))$, and $\mathcal{M}_p(T)$ is the closed convex set of probability measures on T. The Dirac measure at point $t\in T$ will be denoted by δ_t. Let Q and P be

topological spaces, $E=Q\times P$ the product space, and $\mathcal{G}:\mathcal{M}_p(E)\to\mathcal{M}_p(Q)$ be the mapping induced by the projection $\mathrm{pr}_Q:E\to Q$. The mapping $\mathcal{G}$ can be (uniquely) extended by linearity to an $\mathbb{R}$-linear mapping $\mathcal{M}(E)\to\mathcal{M}(Q)$. For any measure $\mu\in\mathcal{M}(E)$ the measure $\mathcal{G}\mu\in\mathcal{M}(Q)$ is called the marginal of μ. The right inverse of $\mathcal{G}$ will be called a lifting.

Lemma 3: Let $f:Q\to\mathcal{M}_p(E)$ be a continuous function such that $\mathcal{G}f(q)=\delta_q$; then the mapping $\mathcal{F}:\mathcal{M}(Q)\to\mathcal{M}(E)$, defined by

$$\mathcal{F}\nu:=\int_Q f(q)\,\nu(dq), \tag{12}$$

is a linear lifting. Any linear lifting has this representation.

Proof: Take the Dirac measure δ_q; then the integral is $\mathcal{F}\delta_q=f(q)\in\mathcal{M}_p(E)$ and we have $\mathcal{G}F\,\delta_q=\mathcal{G}f(q)=\delta_q$. The general case follows by linearity and continuity. On the other hand, if G is a linear lifting, then (12) follows with the function $f(q)=\mathcal{F}\delta_q$. □

If $f(q)$ factorizes into $f(q)=\delta_q\times\chi$ with $\chi\in\mathcal{M}(P)$, the lifting (12) factorizes into $\mathcal{F}(\nu)=\nu\times\chi$. But one can obviously choose nonfactorizing functions $f(q)$ such that $\mathcal{F}(\nu)$ is not a product measure. To give an explicit example we split Q into two disjoint measurable sets $Q=Q_1\cup Q_2$ and denote by $\chi_1(q)$ and $\chi_2(q)$ the characteristic functions of the sets Q_1 and Q_2. Then

$$f(q)=\chi_1(q)\,\delta_q\times\delta_{p_1}+\chi_2(q)\,\delta_q\times\delta_{p_2}, \tag{13}$$

with two points $p_j\in P$, $j=1,2$, $p_1\neq p_2$, yields an example of a nonfactorizing lifting.

The state space $\mathcal{D}(H)$ of a quantum mechanical system is a closed convex set with the pure states $\mathcal{P}(H)$ as extremal points. Any $W\in\mathcal{D}(H)$ can be represented by the Choquet integral,[7]

$$W=\int_{\mathcal{P}(H)} P\;\mu(dP), \tag{14}$$

where $\mu(dP)$ is a—in general nonunique—measure in the convex set $\mathcal{M}_p(\mathcal{P}(H))$ of probability measures on $\mathcal{P}(H)$; see, e.g., Ref. 12. This representation relates the quantum mechanical state space with the space of probability measures, and one might ask whether it is possible to find an affine linear mapping $\gamma:\mathcal{D}(H)\to\mathcal{M}(\mathcal{P}(H))$ such that (12) is valid for all $W\in\mathcal{D}(H)$ with the measure $\mu(dP)=\gamma_W(dP)$.

Theorem 3: *There does not exist an affine linear mapping $\gamma:\mathcal{D}(H)\to\mathcal{M}_p(\mathcal{P}(H))$ such that the representation* (12) *holds for all $W\in\mathcal{D}(H)$ with $\mu(dP)=(\gamma W)(dP)$.*

Proof: If such a mapping γ exists then any pure state has to be represented by an atomic measure on the one-point set containing just this pure state. Moreover this mapping can be extended to an $\mathbb{R}$-linear mapping $\gamma:\mathcal{L}_1^a(H)\to\mathcal{M}(\mathcal{P}(H))$. Since there are finite sets of pure states which are linearly dependent in $\mathcal{L}_1^a(H)$—e.g., any four projection operators on the Hilbert subspace $\mathbb{C}^2$ of $\mathcal{H}$—whereas the set of atomic measures is linear independent in $\mathcal{M}(\mathcal{P}(H))$ we obtain a contradiction to the linearity of γ. □

The proof given here exploits the different structures of the convex sets $\mathcal{D}(H)$ and $\mathcal{M}_p(\mathcal{P}(H))$: the space of measures is a simplex whereas $\mathcal{D}(H)$ not. Theorem 3 is also closely related to Theorem 1; it is actually a consequence of it. To see that implication assume such an affine linear mapping γ exists. Then the lifting problem of Sec. II has the following solution in contradiction to Theorem 1.

In the first step the statistical operator $\rho\in\mathcal{D}(H_S)$ is mapped onto the measure $\gamma\rho\in\mathcal{M}_p(\mathcal{P}(H_S))$. Following Lemma 3 we can lift this measure to a measure $\sigma\in\mathcal{M}_p(\mathcal{P}(H_S)\times\mathcal{P}(H_E))$. Thereby we can choose a lifting such that σ is not a product measure; take, e.g., (13). The operator

$$W=\int_{\mathcal{P}(H_S)\times\mathcal{P}(H_E)} P_S\otimes P_E\sigma(dP_S\times dP_E) \tag{15}$$

has the partial trace $\mathrm{tr}_{H_E}W=\int_{\mathcal{P}(H_S)}P_S(\gamma\rho)(dP_S)=\rho$. All steps of the mapping $\rho\to W$ are affine linear. Since the measure σ does not factorize, the statistical operator W has not the product form $\rho\otimes\rho_E$, and we have obtained a contradiction to Theorem 1.

In addition to the representation of states by a probability distribution on the set of pure states there exists a representation of any state by a random vector distributed by a probability measure on the Hilbert space. Such a representation is used in the theory of Schrödinger (–Belavkin) stochastic equations (see Refs. 13, 14 and references therein), which gives both a phenomenological description of continuous measurements and a Markovian approximations for the reduced dynamics.

By $\mathcal{M}(H)$ we denote the space of all σ-additive signed measures on the σ-algebra of Borel subsets of H. The space of probability measures on H is denoted by $\mathcal{M}_p(H)$, the set of all measures concentrated on $H\backslash\{0\}$ by $\mathcal{M}^0(H)$, and the set of all probability measures concentrated on $H\backslash\{0\}$ by $\mathcal{M}_p^0(H)=\mathcal{M}^0(H)\cap\mathcal{M}_p(H)$.

In the theory of stochastic Schrödinger equations a probability measure $\nu\in\mathcal{M}_p^0(H)$ represents the state $B\in\mathcal{D}(H)$ if

$$\int_H\langle z,Az\rangle\|z\|^{-2}\nu(dz)=\omega_B(A)\equiv\mathrm{tr}_H AB \tag{16}$$

is valid for all observables $A\in\mathcal{L}(H)$. Thereby any measure $\nu\in\mathcal{M}_p^0(H)$ represents a state, and any state $W\in\mathcal{D}(H)$ can be represented by such a measure.

For the proof of the first statement take $A\in\mathcal{L}(H)$. Then the function $|\langle z,Az\rangle|\|z\|^{-2}$ is bounded by $\|A\|$ for all $z\neq 0$, and the integral $\omega_\nu(A):=\int_H\|z\|^{-2}\langle z,Az\rangle\nu(dz)$ is defined. Moreover, it is easy to see that all the demands of Gleason's theorem, see Remark 1, are fulfilled. Hence there exists a state $W\in\mathcal{D}(H)$ such that $\omega_\nu(A)=\mathrm{tr}_H AW$.

On the other hand, given a statistical operator a probability measure for the representation (16) can be constructed as follows. For any $B\in\mathcal{D}(H)$, let $\nu_B^0\in\mathcal{M}_p^0(H)$ be a probability measure with the correlation operator B, i.e., for all $z_1,z_1\in H$ the identity $\langle z_1,Bz_2\rangle=\int\langle z_1,z\rangle\langle z,z_2\rangle\nu_B^0(dz)$ is true. It is worth noticing that among the measures ν_B^0 there exist precisely one Gaussian measure with zero mean value. The positive measure $\nu_B\in\mathcal{M}^0(H)$ is then defined by $\nu_B=\langle z,z\rangle\nu_B^0=\|z\|^2\nu_B^0$; i.e., for any Borel subset $\mathcal{A}$ of $H^{\mathbb{R}}$ we have $\nu_B(\mathcal{A})=\int_{\mathcal{A}}\langle z,z\rangle\nu_B^0(dz)$. The identity $\mathrm{tr}_H B=1$ implies that ν_B is a probability measure on H; in fact $\nu_B(H)=\int\langle z,z\rangle\nu_B^0(dz)=\mathrm{tr}_H B=1$. For any observable $A\in\mathcal{L}(H)$ the function $H\mapsto\mathbb{R}^1: z\mapsto(1/\|z\|^2)\langle z,Az\rangle$ is a random variable on the probability space (H,ν_B). The mean value $\overline{A}$ of this random variable,

$$\overline{A}=\int_H\langle z,Az\rangle\|z\|^{-2}\nu_B(dz)=\int_H\langle z,Az\rangle\nu_B^0(dz)=\mathrm{tr}_H AB,$$

is exactly the expectation of the observable A in the state $B\in\mathcal{D}(H)$. Hence the measure $\nu_B\in\mathcal{M}_p^0(H)$ represents the state B.

There exists an affine linear mapping from the measures $\nu\in\mathcal{M}_p^0(H)$ into the set of measures of the Choquet representation. Let $\varphi: H\backslash\{0\}\to\mathcal{P}(H)$ be the mapping $a\mapsto P_a$, where P_a is the projection operator onto the subspace $\{\lambda a|\lambda\in\mathbb{C}\}$, i.e., $P_a b=\langle b|a\rangle\|a\|^{-2}a$ for all $b\in H$. Then the measure $\nu\varphi^{-1}\in\mathcal{M}_p(\mathcal{P}(H))$ is defined by $\nu\varphi^{-1}(\mathcal{R})=\nu(\varphi^{-1}(\mathcal{R}))$ for any measurable set $\mathcal{R}\subset\mathcal{P}(H)$ of projection operators. This mapping $\nu\mapsto\nu\varphi^{-1}$ is affine linear. If $\nu\in\mathcal{M}_p^0$ represents a state $W\in\mathcal{D}(H)$, then (16) and the definition of $\nu\varphi^{-1}$ yield

$$\langle z_1|Wz_2\rangle \overset{(16)}{=} \int_H \langle z_1|z\rangle\langle z|z_2\rangle \|z\|^{-2}\nu(dz) = \int_{\mathcal{P}(H)} \langle z_1|Pz_2\rangle(\nu\varphi^{-1})(dP).$$

But that means $W=\int_{\mathcal{P}(H)}P(\nu\varphi^{-1})(dP)$, and $\nu\varphi^{-1}$ is the Choquet measure of the state W.

The measures in the representation (16) are highly nonunique; the arbitrariness is even larger than in the case of the Choquet representation, and one might ask again for an affine linear lifting $\mathcal{D}(H)\to\mathcal{M}_p^0(H)$. But assume such an affine linear lifting $\gamma:\mathcal{D}(H)\to\mathcal{M}_p^0(H)$ exists, then it induces an affine linear lifting $\mathcal{D}(H)\to\mathcal{M}_p(\mathcal{P}(H))$ by $W\mapsto\gamma(W)\mapsto(\gamma(W))\varphi^{-1}$ and we have obtained a contradiction to Theorem 3.

Corollary 1: There does not exist an affine linear mapping $\gamma:\mathcal{D}(H)\to\mathcal{M}_p^0(H)$ *such that for any* $W\in\mathcal{D}(H)$ *the measure* $\gamma(W)$ *represents the state* W.

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A generalized Weyl relation approach to the time operator and its connection to the survival probability

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The time operator, an operator which satisfies the canonical commutation relation with the Hamiltonian, is investigated, on the basis of a certain algebraic relation for a pair of operators T and H, where T is symmetric and H self-adjoint. This relation is equivalent to the Weyl relation, in the case of self-adjoint T, and is satisfied by the Aharonov–Bohm time operator T_0 and the free Hamiltonian H_0 for the one-dimensional free-particle system. In order to see the qualitative properties of T_0, the operators T and H satisfying this algebraic relation are examined. In particular, it is shown that the standard deviation of T is directly connected to the survival probability, and H is absolutely continuous. Hence, it is concluded that the existence of the operator T implies the existence of scattering states. It is also shown that the minimum uncertainty states do not exist. Other examples of these operators T and H, than the one-dimensional free-particle system, are demonstrated. [DOI: 10.1063/1.1346598]

I. INTRODUCTION

The concept of the time operator is strongly connected with the time–energy uncertainty relation. The time operator, denoted by T, is usually defined to satisfy the canonical commutation relation (CCR) with the Hamiltonian H: $[T,H]=i$ (see Ref. 1 and the references therein). If such an operator were defined consistently on the Hilbert space corresponding to a certain quantum system, then the time–energy uncertainty relation could be automatically reduced from the Cauchy–Schwarz inequality, as in the case between the position and momentum operators on $L^2(\mathbf{R}^1)$. For instance, if we take the operator T_0 suggested by Aharonov and Bohm,[2] as a time operator for the one-dimensional free-particle system (1DFPS), we formally have $[T_0,H_0]=i$ and derive the uncertainty relation between T_0 and H_0. Here $H_0:=P^2/2$ is the free Hamiltonian for the 1DFPS, and T_0 is defined as

$$T_0:=\tfrac{1}{2}(QP^{-1}+P^{-1}Q), \tag{1}$$

where Q and P are the position and momentum operators on $L^2(\mathbf{R}^1)$ (a more precise definition is given in Sec. III). T_0 is often called the Aharonov–Bohm time operator. It is, however, not clear whether the inverse P^{-1} could be well-defined. We should also remember the criticism posed by Pauli,[3] although it is not rigorous, that the time operator cannot necessarily be defined for all quantum systems without contradiction. Furthermore the physical meaning of the time operator, if any, still remains unclear.

We shall base our discussion on the axiomatic quantum mechanics. Then it is possible to comment on the above difficulties from the axiomatic points of view. We first see that the inverse P^{-1} is a well-defined self-adjoint operator on $L^2(\mathbf{R}^1)$ (more details are given in Sec. III). Recently, the operator T_0 was shown to be well-defined, and its mathematical character was clarified, through the study of the time-of-arrival problem.[4] Observe that in Pauli's criticism, it is implicitly

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assumed that if there exists a self-adjoint operator T which satisfies the CCR with the Hamiltonian H for some system,

$$TH\psi - HT\psi = i\psi, \quad \forall \psi \in \mathrm{Dom}(TH) \cap \mathrm{Dom}(HT), \tag{2}$$

one would be able to derive the following relation:

$$He^{i\epsilon T}\psi = e^{i\epsilon T}(H+\epsilon)\psi, \quad \forall \psi \in \mathrm{Dom}(H), \quad \forall \epsilon \in \mathbf{R}^1. \tag{3}$$

We have to be careful, however, about this kind of logic, since it is not generally true whereas its converse is true. For example, consider a pair of operators, the position and momentum operators on $L^2([0,1])$, Q and P, for the above T and H, respectively.[5] They satisfy Eq. (2) but Eq. (3) is satisfied only for the particular values $\epsilon = 2\pi n, n \in \mathbf{Z}$, since, in order that P be self-adjoint, the domain $\mathrm{Dom}(P)$ has to be supplemented with a boundary condition $\psi(0) = \theta\psi(1)$ with a fixed $\theta \in \mathbf{C}$, $|\theta| = 1$, $\forall \psi \in \mathrm{Dom}(P)$.[6] Furthermore, there is no *a priori* reason why we have to consider the time operator an observable, that is, a self-adjoint operator: we do not have any interpretation of the time operator as an observable. In this paper, we shall require the time operator to be symmetric, satisfying Eq. (2) with the Hamiltonian, but not necessarily to be self-adjoint.

The investigation of the time operator is important to understanding the time–energy uncertainty relation, and may have a significance for the analysis of the dynamics of quantum systems. A reason for the latter is that the time operator is directly connected to the Hamiltonian through the CCR, and this is algebraically so strong a relation between operators as to prescribe qualitative aspects of their spectra, we can expect that the time operator brings us information about qualitative aspects of the time evolution of quantum systems. Hence, our purposes here are to examine for which quantum systems such a symmetric time operator is allowed to exist consistently, and to disclose its relevance to the dynamics of the quantum system under consideration.

From what is mentioned above, the investigation of the time operator is involved in that of the commutator (not necessarily canonical). The connection between the commutator of the form $[H, iA] = C$ $(C \geqslant 0)$ and the spectra of self-adjoint operators, H, A, and C, has been widely studied by Putnam,[7] Kato,[8] Lavine,[9,10] and others (see also Ref. 11). We here, however, restrict our consideration to the more strong form, which will be called the ''T-weak'' Weyl relation.

Definition 1.1: Let $\mathcal{H}$ be a Hilbert space, T be a symmetric operator on $\mathcal{H}$, and H be a self-adjoint operator on $\mathcal{H}$. If, for any $\psi \in \mathrm{Dom}(T)$ and for any $t \in \mathbf{R}^1$, the relations $e^{-itH}\psi \in \mathrm{Dom}(T)$ and

$$Te^{-itH}\psi = e^{-itH}(T+t)\psi \tag{4}$$

hold, then a pair of operators T and H is said to satisfy the T-weak Weyl relation (T-weak WR), or T (H) is said to satisfy the T-weak WR with H (T).

One can find, from the above definition, that $\mathrm{Dom}(Te^{-itH}) = \mathrm{Dom}(T)$, $\forall t \in \mathbf{R}^1$. Thus the T-weak WR are represented merely by

$$Te^{-itH} = e^{-itH}(T+t), \quad \forall t \in \mathbf{R}^1. \tag{5}$$

Here it should be notified that there is the excellent work about the T-weak WR, done by Schmüdgen[12] (also see the references therein). In his work, he found, under a mild regularity condition, that T and H is unitary equivalent to the momentum operator, satisfying some boundary condition, and the position operator on a certain Hilbert space.

It will follow that the time operator T_0, in Eq. (1), is a symmetric operator on $L^2(\mathbf{R}^1)$ and one of its symmetric extensions, denoted by $\tilde{T}_0$, satisfies the $\tilde{T}_0$-weak WR with H_0 (see Sec. III). Thus as long as it is to see the qualitative properties of T_0 (or $\tilde{T}_0$), it may suffice to examine the T-weak WR and the operators T and H satisfying this relation, by paying a particular attention to their spectra and to the uncertainty relation between them. From another viewpoint to the T-weak WR

than that of Schmüdgen, we have obtained the fact that the time operator is deeply connected to the survival probablility. Indeed, if a pair of operators T and H satisfies the T-weak WR, the following inequality:

$$\frac{4(\Delta T)_\psi^2 \|\psi\|^2}{t^2} \geqslant |\langle \psi, e^{-itH}\psi\rangle|^2 \tag{6}$$

holds for every $\psi \in \mathrm{Dom}(T)$ and for every $t \in \mathbf{R}^1\setminus\{0\}$, where $(\Delta T)_\psi$ is the standard deviation of T with respect to ψ, and $|\langle \psi, e^{-itH}\psi\rangle|^2$ is the survival probability of ψ at time t. This is shown in Theorem 4.1. As an application of this inequality, we have Corollary 4.3 which states that H has no point spectrum. Furthermore, it is shown that H is absolutely continuous,[13] as in Theorem 4.4. This means that the existence of the time operator, which satisfies the T-weak WR with the Hamiltonian for some system, infers that the system consists of only scattering states. Also, in Theorem 5.1, the absence of minimum-uncertainty states, for the uncertainty relation between T and H, is proved, under some condition satisfied by the operators $\tilde{T}_0$ and H_0.

In Sec. II, the connection among the CCR, Weyl relation, and T-weak WR is mentioned. Section III is devoted to the brief study of the Aharonov–Bohm time operator in Eq. (1), to see a sign of the deep connection between the operator T and the survival probability, followed by several statements in Sec. IV. They include the inequality (6) and the spectral properties of both T and H, e.g., Theorem 4.4. Theorem 5.1 is proved in Sec. V. Further discussion about the time operator is developed in Sec. VI, on the basis of the results of the preceding sections and of the theory of Schrödinger operators. We mention other quantum systems than the 1DFPS for which an operator T exists, to satisfy the T-weak WR with the Hamiltonian. In fact, for a certain class of quantum systems, time operators are easily constructed by unitary transformations of $\tilde{T}_0$. Concluding remarks are given in Sec. VII.

II. THE CANONICAL COMMUTATION RELATION, WEYL RELATION, AND *T*-WEAK WEYL RELATION

The T-weak WR in Eq. (4) or (5) is characterized more clearly, in the Heisenberg picture. The T-weak WR is represented, in an alternative form, as

$$T_t = T + tI, \quad \forall t \in \mathbf{R}^1, \tag{7}$$

where $T_t := e^{itH}Te^{-itH}$. It is now clear that T, which satisfies the T-weak WR with H, is shifted proportionally to the time parameter t in the Heisenberg picture. This fact bring us an image of time for T. We also see, from this form, that T is necessarily unbounded. It is, however, noted that in our investigation the T-weak WR in Eq. (5) is more convenient than in Eq. (7). The connection among the Weyl relation (WR),[14] the CCR and the T-weak WR is very important, when one considers whether a symmetric operator T, satisfying the T-weak WR with the Hamiltonian for some system, is the time operator. Recall that the latter is defined as a symmetric operator satisfying the CCR with the same Hamiltonian as in Eq. (2). In this respect, we put forward the next proposition.

Proposition 2.1: Let $\mathcal{H}$ be a Hilbert space, T be a closed symmetric operator on $\mathcal{H}$, and H be a self-adjoint operator on $\mathcal{H}$. If a pair of operators T and H satisfies the T-weak WR, then there is a dense subspace $\mathcal{D}\subset\mathcal{H}$ such that

(i) $\mathcal{D}\subset \mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$,
(ii) $H:\mathcal{D}\to\mathcal{D}$,
(iii) *The CCR holds in the meaning of that $TH-HT=i$ on $\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$. Moreover, if T is self-adjoint, then the operators T and H satisfy the WR,*

$$e^{-isT}e^{-itH} = e^{-ist}e^{-itH}e^{-isT}, \quad \forall s, \ \forall t \in \mathbf{R}^1. \tag{8}$$

The above (i), (ii), and (iii) are proved in the same manner as in the proof,[15] by noting the strong continuity of $Te^{-itH}\psi$, $\forall\psi\in\mathrm{Dom}(T)$, by virtue of the T-weak WR, and the closedness of T, and also by considering the subspace spaned by the following subset of $\mathcal{H}$, as a subspace $\mathcal{D}$ in this proposition:

$$\left\{\psi_f\in\mathcal{H}\,\middle|\,\psi_f:=\int_{-\infty}^{\infty}f(s)e^{-isH}\psi\,ds,\forall f\in C_0^{\infty}(\mathbf{R}^1)\ \text{ and }\ \forall\psi\in\mathrm{Dom}(T)\right\},$$

where the integral is defined by Riemann's sense and thus a strong limit. The last part of the proposition is proved as follows. In the case of T being self-adjoint, we see, from the T-weak WR (5), that $\forall\phi\in\mathcal{H}$ and $\forall\psi\in\mathrm{Dom}(T)$,

$$\begin{aligned}\int_{\mathbf{R}^1}\lambda\,d\langle\phi,e^{itH}F(\lambda)e^{-itH}\psi\rangle&=\langle\phi,e^{itH}Te^{-itH}\psi\rangle\\&=\langle\phi,(T+t)\psi\rangle\\&=\int_{\mathbf{R}^1}(\lambda+t)d\langle\phi,F(\lambda)\psi\rangle=\int_{\mathbf{R}^1}\lambda\,d\langle\phi,F_t(\lambda)\psi\rangle,\end{aligned}$$

where $\{F(B)|B\in\mathbf{B}^1\}$ is the spectral measure of T, $\mathbf{B}^1$ is the σ-field which is generated by all open sets of $\mathbf{R}^1$, and $F_t(B):=F(\{\lambda-t|\lambda\in B\})$. From the uniqueness of the spectral resolution, this means that $e^{itH}F(B)e^{-itH}=F_t(B)$, for all $t\in\mathbf{R}^1$. Then it follows that $\forall\psi\in\mathcal{H}$ and $\forall s\in\mathbf{R}^1$,

$$\begin{aligned}\langle\psi,e^{itH}e^{-isT}e^{-itH}\psi\rangle&=\int_{\mathbf{R}^1}e^{-is\lambda}d\langle\psi,e^{itH}F(\lambda)e^{-itH}\psi\rangle\\&=\int_{\mathbf{R}^1}e^{-is\lambda}d\langle\psi,F_t(\lambda)\psi\rangle=\int_{\mathbf{R}^1}e^{-is(\lambda+t)}d\langle\psi,F(\lambda)\psi\rangle=\langle\psi,e^{-ist}e^{-isT}\psi\rangle.\end{aligned}$$

By using the polarization identity, we can obtain the WR (8). According to von Neumann's uniqueness theorem, with respect to the solution of the WR,[14] we had better to define T, which appears in the T-weak WR, as a symmetric operator, to allow the operator H (corresponding to the Hamiltonian) to be bounded from below. We note here that if a symmetric operator T satisfies the T-weak WR with some self-adjoint operator H, then the closure of T, denoted by $\overline{T}$, also satisfies the $\overline{T}$-weak WR with the same H. This is easily verified by the usual calculation. It is guaranteed, from this proposition, that a symmetric operator T, satisfying the T-weak WR with the Hamiltonian for some system, is the time operator, and thus it is significant to examine the T-weak WR in the general analysis of the time operator. As a summary, we remark again that the following relations:

$$\mathrm{WR}\Rightarrow T-\text{weak WR}\Rightarrow\mathrm{CCR}$$

hold, in the sense of Proposition 2.1, even though, in general the converses do not hold, as is already mentioned in Sec. I.

III. THE AHARONOV–BOHM TIME OPERATOR

Let us consider the Hilbert space $L^2(\mathbf{R}^1)$. The operator T_0 on $L^2(\mathbf{R}^1)$ in Eq. (1),

$$T_0:=\tfrac{1}{2}(QP^{-1}+P^{-1}Q),$$

is defined in its domain $\mathrm{Dom}(T_0):=\mathrm{Dom}(QP^{-1})\cap\mathrm{Dom}(P^{-1}Q)$, where P is the momentum operator on $L^2(\mathbf{R}^1)$ for the 1DFPS, and P^{-1} its inverse. In the axiomatic quantum mechanics, P is defined as $P:=-iD_x$, where D_x is a differential operator on $L^2(\mathbf{R}^1)$, and its domain consists of the L^2-functions which belong to $AC(\mathbf{R}^1)$, and satisfy that their derivatives are also included in

$L^2(\mathbf{R}^1)$.[5] $AC(\Omega)$ (Ω is an open set of $\mathbf{R}^1$) is the set of functions on Ω, which are absolutely continuous on all bounded closed intervals of Ω. The free Hamiltonian H_0 for this system is $H_0 := P^2/2$. The position operator Q on $L^2(\mathbf{R}^1)$ is defined as an operator of multiplication by x on $L^2(\mathbf{R}^1)$, denoted by M_x, and its domain consists of L^2-functions, defined by ψ, such that $\int_{\mathbf{R}^1}|x\psi(x)|^2dx$ is finite. It is noted that in the definition of T_0, P^{-1} is well-defined and becomes a self-adjoint operator on $L^2(\mathbf{R}^1)$. This is because, for any self-adjoint operator A, if its inverse A^{-1} exists, A^{-1} should be self-adjoint.[16] In our case, P^{-1} exists since P is an injection, i.e., $\mathrm{Ker}(P^{-1})=\{0\}$, where $\mathrm{Ker}(A) := \{\psi \in \mathrm{Dom}(A) \mid A\psi = 0\}$.

In the momentum representation of T_0, we have

$$FT_0F^{-1} = \tfrac{1}{2}(iD_kM_{1/k} + M_{1/k}iD_k),$$

and its domain

$$\begin{aligned}\mathrm{Dom}(FT_0F^{-1}) &= \mathrm{Dom}(D_kM_{1/k}) \cap \mathrm{Dom}(M_{1/k}D_k)\\ &= \{\psi \in \mathrm{Dom}(M_{1/k}) \mid M_{1/k}\psi \in \mathrm{Dom}(D_k)\}\\ &\quad \cap \{\psi \in \mathrm{Dom}(D_k) \mid D_k\psi \in \mathrm{Dom}(M_{1/k})\},\end{aligned} \tag{9}$$

where F is the Fourier transformation from $L^2(\mathbf{R}^1)$ onto $L^2(\mathbf{R}^1_k)$, and use has been made of the relations $FQF^{-1} = iD_k$, $FPF^{-1} = M_k$, and $FP^{-1}F^{-1} = M_{1/k}$. At first sight, $\mathrm{Dom}(T_0)$ seems to be rather restricted, because of the existence of P^{-1} in the definition of T_0. The following simple example by Kobe[1] may be considered to support this anticipation.

Example 1: Let us consider the functions $\phi_n(k) := k^n N_n e^{-a_0k^2} \in L^2(\mathbf{R}^1_k)$, where $n \in \mathbf{Z}$, $n \geqslant 0$, $a_0 > 0$, and N_n is a normalization factor. We see that for any integer $n \geqslant 2$, $\phi_n \in \mathrm{Dom}(FT_0F^{-1})$. The action of FT_0F^{-1} on each $\phi_n (n \geqslant 2)$ is, by direct calculation,

$$FT_0F^{-1}\phi_n(k) = \frac{i}{2}[(2n-1)k^{n-2} - 2a_0k^{n-1} - 2a_0k^n]N_ne^{-a_0k^2}.$$

In the case of $n = 0, 1$, however, the right-hand side of the above equation is formally not square integrable, and thus $\phi_0, \phi_1 \notin \mathrm{Dom}(FT_0F^{-1})$.

Notice that in spite of this example, $\mathrm{Dom}(T_0)$ is dense in $L^2(\mathbf{R}^1)$. This can be seen from the fact that the subspace $\mathcal{C}_\mathrm{i}$ is included in $\mathrm{Dom}(FT_0F^{-1})$ and is dense in $L^2(\mathbf{R}^1_k)$. $\mathcal{C}_\mathrm{i}$ is defined as

$$\mathcal{C}_\mathrm{i} := \{\psi \in C_0^\infty(\mathbf{R}^1_k) \mid \mathrm{supp}\,\psi \subset \mathbf{R}^1_k \backslash \{0\}\}, \tag{10}$$

where supp ψ denotes the support of ψ, i.e., the closure of $\{k \in \mathbf{R}^1_k \mid \psi(k) \neq 0\}$. Therefore the adjoint operator of T_0, denoted by T_0^*, can be defined. Then, T_0 is symmetric, because

$$T_0^* \supset \tfrac{1}{2}((QP^{-1})^* + (P^{-1}Q)^*) \supset \tfrac{1}{2}((P^{-1})^*Q^* + Q^*(P^{-1})^*) = T_0,$$

where we have used the fact that $Q^* = Q$ and $(P^{-1})^* = P^{-1}$. It is noted that T_0 and H_0 do not satisfy the T_0-weak WR, $T_0e^{-itH_0} = e^{-itH_0}(T_0 + t)$, $\forall t \in \mathbf{R}^1$. Because $\mathrm{Dom}(FT_0F^{-1})$ in Eq. (9) is not invariant under the action of $e^{-itM_{k^2/2}}$ for all $t \neq 0$, that is for any $t \neq 0$, there is some vector $\psi \in \mathrm{Dom}(FT_0F^{-1})$ satisfying $e^{-itM_{k^2/2}}\psi \notin \mathrm{Dom}(FT_0F^{-1})$. For instance, consider the following L^2-function g of $k \in \mathbf{R}^1_k$:

$$g(k) := \begin{cases} e^{-1/k^2}\dfrac{1}{1+|k|^s} & (k \neq 0),\\ 0 \quad (k = 0), \end{cases}$$

where $1/2 < s \leqslant 3/2$. Then g is C^∞-function. One can see that $g \in \mathrm{Dom}(FT_0F^{-1})$, however, $e^{-itM_{k^2/2}}g \notin \mathrm{Dom}(FT_0F^{-1})$, $\forall t \neq 0$. This follows from the fact that $e^{-itM_{k^2/2}}g \notin \mathrm{Dom}(D_k)$, $\forall t$

$\neq 0$. Here we introduce a symmetric extension of T_0 on $L^2(\mathbf{R}^1)$, denoted by $\tilde{T}_0$, which will satisfy the $\tilde{T}_0$-weak WR with H_0, and is defined, in the momentum representation, as follows:

$$\mathrm{Dom}(F\tilde{T}_0F^{-1}) := \left\{ \psi \in L^2(\mathbf{R}^1_k) \;\middle|\; \begin{array}{c} \psi \in AC(\mathbf{R}^1_k\backslash\{0\}), \lim_{k\to 0}\dfrac{\psi(k)}{|k|^{1/2}} = 0, \\ \text{and} \\ \displaystyle\int_{\mathbf{R}^1_k\backslash\{0\}} \left| \frac{d\psi(k)/k}{dk} + \frac{1}{k}\frac{d\psi(k)}{dk} \right|^2 dk < \infty \end{array} \right\},$$

and its action,

$$F\tilde{T}_0F^{-1}\psi(k) = \frac{i}{2}\left(\frac{d\psi(k)/k}{dk} + \frac{1}{k}\frac{d\psi(k)}{dk} \right), \quad \text{a.e. } k \in \mathbf{R}^1_k\backslash\{0\}, \quad \forall \psi \in \mathrm{Dom}(F\tilde{T}_0F^{-1}). \tag{11}$$

It is seen that $\mathrm{Dom}(F\tilde{T}_0F^{-1})$ is a subspace of $L^2(\mathbf{R}^1_k)$, and $F\tilde{T}_0F^{-1}$ is a linear operator on $L^2(\mathbf{R}^1_k)$.

Proposition 3.1: $\tilde{T}_0$ is a symmetric extension of T_0.

Proof: $F\tilde{T}_0F^{-1}$ being symmetric follows from that $\forall \psi, \forall \phi \in \mathrm{Dom}(F\tilde{T}_0F^{-1})$,

$$\begin{aligned} &\int_{(0,\infty)} \overline{\phi}(k)\frac{i}{2}\left(\frac{d\psi(k)/k}{dk} + \frac{1}{k}\frac{d\psi(k)}{dk} \right) dk - \int_{(0,\infty)} \frac{-i}{2}\left(\frac{d\overline{\phi}(k)/k}{dk} + \frac{1}{k}\frac{d\overline{\phi}(k)}{dk} \right)\psi(k)\,dk \\ &\quad = i\left(\lim_{b\to\infty}\frac{\overline{\phi}(b)\psi(b)}{b} - \lim_{a\downarrow 0}\frac{\overline{\phi}(a)\psi(a)}{a} \right) = 0, \end{aligned}$$

where $\lim_{b\to\infty}\overline{\phi}(b)\psi(b)/b = 0$ and $\lim_{a\downarrow 0}\overline{\phi}(a)\psi(a)/a = 0$ are used. The former is brought from the integrability of $\overline{\phi}(k)\psi(k)$, and the latter from the boundary conditions of $\overline{\phi}(k)$ and $\psi(k)$ at the origin. By considering the left half-line in the same manner, we can obtain that $\forall \psi, \forall \phi \in \mathrm{Dom}(F\tilde{T}_0F^{-1})$, $\langle \phi, F\tilde{T}_0F^{-1}\psi\rangle = \langle F\tilde{T}_0F^{-1}\phi, \psi\rangle$, that is, $F\tilde{T}_0F^{-1}$ is symmetric. To see that $\tilde{T}_0$ is an extension of T_0, i.e., $\tilde{T}_0 \supset T_0$, it is sufficient that every $\psi \in \mathrm{Dom}(FT_0F^{-1})$ satisfies the boundary condition at the origin, which appears in the definition of $\mathrm{Dom}(F\tilde{T}_0F^{-1})$. This is easily verified as follows. Consider a $\psi \in \mathrm{Dom}(FT_0F^{-1})$ in Eq. (9); then $\psi(k)/k$ belongs to $AC(\mathbf{R}^1_k)$, and thus, $\lim_{k\to 0}\psi(k)/k$ exists. Thus $\lim_{k\to 0}|\psi(k)/|k|^{1/2}| = \lim_{k\to 0}|k|^{1/2}|\psi(k)/k| = 0$. □

This operator may be more understood, from the view of the energy representation which was emphasized by Egusquiza and Muga, and many other authors (see Ref. 4 and the references therein).

It is, now, noted that $\mathrm{Dom}(\tilde{T}_0)$ is an invariant subspace of e^{-itH_0}. Because, for every $\psi \in \mathrm{Dom}(F\tilde{T}_0F^{-1})$ and $t \in \mathbf{C}$ $(\mathrm{Im}t \leqslant 0)$, $\lim_{k\to 0}e^{-itk^2/2}\psi(k)/|k|^{1/2} = 0$, and for almost everywhere $k \in \mathbf{R}^1_k\backslash\{0\}$,

$$\frac{i}{2}\left(\frac{de^{-itk^2/2}\psi(k)/k}{dk} + \frac{1}{k}\frac{de^{-itk^2/2}\psi(k)}{dk} \right) = te^{-itk^2/2}\psi(k) + e^{-itk^2/2}\frac{i}{2}\left(\frac{d\psi(k)/k}{dk} + \frac{1}{k}\frac{d\psi(k)}{dk} \right),$$

where the right-hand side is square-integrable. Therefore $e^{-itM_{k^2/2}}\psi$ is included in $\mathrm{Dom}(F\tilde{T}_0F^{-1})$, and, as a result, $\tilde{T}_0$ can satisfy the $\tilde{T}_0$-weak WR with H_0,

$$\tilde{T}_0e^{-itH_0} = e^{-itH_0}(\tilde{T}_0 + t), \quad \forall t \in \mathbf{C}(\mathrm{Im}t \leqslant 0), \tag{12}$$

whereas T_0 does not satisfy the T_0-weak WR with H_0. It is seen that $\tilde{T}_0$ is not self-adjoint. Because, if it was so, $\tilde{T}_0$ and H_0 would have to satisfy the WR from Proposition 2.1. The latter is, however, in contradiction to the non-negativity $H_0 \geqslant 0$.

Consider the subspace $\mathcal{C}_{\rm i}$ in Eq. (10). It is easily seen that $\mathcal{C}_{\rm i}$ is an invariant subspace of $F\tilde{T}_0F^{-1}$, that is, $F\tilde{T}_0F^{-1}:\mathcal{C}_{\rm i}\to\mathcal{C}_{\rm i}$. Thus $F\tilde{T}_0F^{-1}$ can act any times on $\mathcal{C}_{\rm i}$. In the position representation, this property is described as $\tilde{T}_0: F^{-1}\mathcal{C}_{\rm i}\to F^{-1}\mathcal{C}_{\rm i}$ where $F^{-1}\mathcal{C}_{\rm i}:=\{\psi\in L^2(\mathbf{R}^1)|\,\psi = F^{-1}\eta, \eta\in\mathcal{C}_{\rm i}\}$. $\mathcal{C}_{\rm i}$ may be regarded as an important subspace which determines the property of $\tilde{T}_0$. Indeed, using the $\tilde{T}_0$-weak WR in Eq. (12), we can obtain the following statement:

Proposition 3.2: For any non-negative integer n, m and for any $\psi,\phi\in F^{-1}\mathcal{C}_{\rm i}$,

$$\lim_{t\to\pm\infty}|t|^n\left|\frac{d^m\langle\phi,e^{-itH_0}\psi\rangle}{dt^m}\right|=0.$$

That is, the probability amplitude, $\langle\phi,e^{-itH_0}\psi\rangle$, is a rapidly decreasing function of $t\in\mathbf{R}^1$.

Proof: Let $\psi,\phi\in F^{-1}\mathcal{C}_{\rm i}$. Since $F^{-1}\mathcal{C}_{\rm i}$ is an invariant subspace of $\tilde{T}_0$, thus $\tilde{T}_0\phi,\tilde{T}_0\psi\in F^{-1}\mathcal{C}_{\rm i}$. By using Eq. (12), we have

$$\langle\phi,e^{-itH_0}\tilde{T}_0\psi\rangle=\langle\phi,(\tilde{T}_0-t)e^{-itH_0}\psi\rangle=\langle\tilde{T}_0\phi,e^{-itH_0}\psi\rangle-t\langle\phi,e^{-itH_0}\psi\rangle, \tag{13}$$

where $\langle\cdot,\cdot\rangle$ denotes the inner product in $L^2(\mathbf{R}^1)$. Note that $\forall\psi\in L^2(\mathbf{R}^1)$, $\mathrm{w}-\lim_{t\to\pm\infty}e^{-itH_0}\psi=0$,[17] because H_0 is (spectrally) absolutely continuous.[13] This means that $\lim_{t\to\pm\infty}\langle\phi,e^{-itH_0}\tilde{T}_0\psi\rangle=\lim_{t\to\pm\infty}\langle\tilde{T}_0\phi,e^{-itH_0}\psi\rangle=0$, which leads to the relation $\lim_{t\to\pm\infty}t\langle\phi,e^{-itH_0}\psi\rangle=0$. In order to show that for any integer $n\geqslant 2$ and for any $\psi,\phi\in\mathcal{C}_{\rm i}$, $\lim_{t\to\pm\infty}t^n\langle\phi,e^{-itH_0}\psi\rangle=0$, we observe that $\tilde{T}_0{}^k:F^{-1}\mathcal{C}_{\rm i}\to F^{-1}\mathcal{C}_{\rm i}$, and that the following relations similar to Eq. (13) hold for every $n\in\mathbf{N}$:

$$\begin{aligned}\langle\phi,e^{-itH_0}\tilde{T}_0{}^{n+1}\psi\rangle&=\langle\phi,(\tilde{T}_0-t)^{n+1}e^{-itH_0}\psi\rangle\\&=\sum_{k=0}^{n}(-t)^k\binom{n+1}{k}\langle\tilde{T}_0{}^{n+1-k}\phi,e^{-itH_0}\psi\rangle+(-t)^{n+1}\langle\phi,e^{-itH_0}\psi\rangle.\end{aligned}$$

Then $\lim_{t\to\pm\infty}t^n\langle\phi,e^{-itH_0}\psi\rangle=0$ is proved recursively for any integer $n\geqslant 2$. In order to show that $\langle\phi,e^{-itH_0}\psi\rangle$ is infinitely differentiable on $\mathbf{R}^1$, it is sufficient to use the fact that $\forall\psi\in F^{-1}\mathcal{C}_{\rm i}$, $e^{-itH_0}\psi$ is infinitely and strongly differentiable on $\mathbf{R}^1$, and $F^{-1}\mathcal{C}_{\rm i}$ is also an invariant subspace of H_0, that is, $H_0:F^{-1}\mathcal{C}_{\rm i}\to F^{-1}\mathcal{C}_{\rm i}$. □

We note that $\forall\psi,\phi\in F^{-1}\mathcal{C}_{\rm i}$, $\langle\phi,e^{-itH_0}\psi\rangle$ converges to 0 as $t\to\pm\infty$, more rapidly than any inverse-power of t. This fact is not trivial and is seen from the next example.

Example 2: Define the survival probability of ψ as a function of $t\in\mathbf{R}^1$, i.e., $P_\psi(t):=|\langle\psi,e^{-itH_0}\psi\rangle|^2$, where ψ is an arbitrary element in $L^2(\mathbf{R}^1_k)$. Then, for a particular ϕ_n, $n\geqslant 2$ in Example 1, $P_{\phi_n}(t)=(1+t^2/16a_0^2)^{-n-1/2}$ and this converges to 0 as $t\to\pm\infty$ as, at most, a power function of t.

From the above statement and example, we may expect that there is a connection between T_0 (or $\tilde{T}_0$) and the survival probability. This expectation is also inspired from the works done by Bhattacharyya.[18]

IV. CONNECTION BETWEEN THE TIME OPERATOR AND THE SURVIVAL PROBABILITY

If we assume the existence of a symmetric operator T which satisfies the T-weak WR with the Hamiltonian for some system, i.e., the time operator, several statements are derived, in a rigorous form, which concern to the connection between the time operator and the survival probability. Before deriving these statements, we introduce a few definitions. Let T be a symmetric operator on the Hilbert space $\mathcal{H}$ and define

$$\langle T\rangle_\psi := \langle \psi, T\psi\rangle, \quad (\Delta T)_\psi := \|(T-\langle T\rangle_\psi)\psi\|, \quad \forall \psi \in \mathrm{Dom}(T), \tag{14}$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product in $\mathcal{H}$, and $\|\cdot\|$ the norm in $\mathcal{H}$, defined by this inner product. $\langle T\rangle_\psi$ and $(\Delta T)_\psi$ are, respectively, called the expectation and standard deviation of T with respect to the state ψ.

Theorem 4.1: *Let T be a symmetric operator on $\mathcal{H}$, and H be a self-adjoint operator on $\mathcal{H}$. Then if a pair of operators T and H satisfies the T-weak WR, the inequality (6) holds.*

Proof: Let us define self-adjoint operators $\cos(tH) := (e^{itH}+e^{-itH})/2$ and $\sin(tH) := (e^{itH} - e^{-itH})/2i$. Then, from the T-wea WR in Eq. (5), we can obtain two commutation relations,

$$[T, \cos(tH)] = -it\sin(tH), \quad [T, \sin(tH)] = it\cos(tH). \tag{15}$$

From the above commutation relations, we can derive the uncertainty relations. From the first relation in Eq. (15), we have that

$$(\Delta T)_\psi^2 \|\cos(tH)\psi\|^2 \geqslant \frac{t^2}{4}|\langle \psi, [T, \cos(tH)]\psi\rangle|^2 = \frac{t^2}{4}|\mathrm{Im}\langle \psi, e^{-itH}\psi\rangle|^2,$$

$\forall \psi \in \mathrm{Dom}(T)$, $\forall t \in \mathbf{R}^1$. Similarly, the second relation in Eq. (15) gives us an inequality,

$$(\Delta T)_\psi^2 \|\sin(tH)\psi\|^2 \geqslant \frac{t^2}{4}|\mathrm{Re}\langle \psi, e^{-itH}\psi\rangle|^2, \quad \forall \psi \in \mathrm{Dom}(T), \ \forall t \in \mathbf{R}^1.$$

Adding these inequalities together, and taking into account the relation $\|\cos(tH)\psi\|^2 + \|\sin(tH)\psi\|^2 = \|\psi\|^2$, the inequality (6) can be obtained. □

Two corollarys follow from the inequality (6).

Corollary 4.2: Let T be a symmetric operator on $\mathcal{H}$, and H be a self-adjoint operator on $\mathcal{H}$. Then if a pair of operators T and H satisfies the T-weak WR, T has no point spectrum.

Proof: Suppose that there existed an eigenvector $\psi_0 \in \mathrm{Dom}(T)$ belonging to an eigenvalue $\lambda \in \mathbf{R}^1$ of T, that is, $T\psi_0 = \lambda\psi_0$ and $\|\psi_0\| = 1$. Then we see that $(\Delta T)_{\psi_0} = 0$, from the definition in Eq. (14). It follows, from Theorem 4.1, that $\langle \psi_0, e^{-itH}\psi_0\rangle = 0$, $\forall t \in \mathbf{R}^1\backslash\{0\}$. Since e^{-itH} is strongly continuous at any $t \in \mathbf{R}^1$, we have that $\|\psi_0\|^2 = \lim_{t\to 0}\langle \psi_0, e^{-itH}\psi_0\rangle = 0$, and this is in contradiction to the premise. Thus T has no point spectrum. □

Corollary 4.3: Let T be a symmetric operator on $\mathcal{H}$, and H be a self-adjoint operator on $\mathcal{H}$. If a pair of operators T and H satisfies the T-weak WR, then H has no point spectrum.

Proof: Since $\mathrm{Dom}(T)$ is dense in $\mathcal{H}$, for each $\psi \in \mathcal{H}$ there is a sequence $\{\psi_n\}_{n=1}^\infty \subset \mathrm{Dom}(T)$, satisfying $\psi_n \to \psi$, $n \to \infty$. It follows that

$$\begin{aligned}|\langle \psi, e^{-itH}\psi\rangle - \langle \psi_n, e^{-itH}\psi_n\rangle| &= |\langle \psi, e^{-itH}\psi\rangle - \langle \psi, e^{-itH}\psi_n\rangle + \langle \psi, e^{-itH}\psi_n\rangle - \langle \psi_n, e^{-itH}\psi_n\rangle| \\ &\leqslant \|e^{itH}\psi\|\|\psi - \psi_n\| + \|\psi - \psi_n\|\|e^{-itH}\psi_n\| \leqslant (\|\psi\| + \|\psi_n\|)\|\psi - \psi_n\|,\end{aligned}$$

and thus,

$$\begin{aligned}\lim\ \sup_{t\to\pm\infty}|\langle \psi, e^{-itH}\psi\rangle| &\leqslant \lim\ \sup_{t\to\pm\infty}|\langle \psi_n, e^{-itH}\psi_n\rangle| + (\|\psi\| + \|\psi_n\|)\|\psi - \psi_n\| \\ &= (\|\psi\| + \|\psi_n\|)\|\psi - \psi_n\|,\end{aligned}$$

where we use the inequality (6) and $\psi_n \in \mathrm{Dom}(T)$, in the last equality. Note that the above inequality holds for any $n \in \mathbf{N}$. Thus, in the limit $n \to \infty$, we obtain that

$$\forall \psi \in \mathcal{H}, \quad \lim_{t\to\pm\infty}\langle \psi, e^{-itH}\psi\rangle = 0. \tag{16}$$

This means that H has no point spectrum. Because if H has a nonempty point spectrum, say $\lambda \in \mathbf{R}^1$, then there is a corresponding eigenvector ψ_λ, which satisfies $H\psi_\lambda = \lambda\psi_\lambda$. Obviously ψ_λ does not satisfy the above condition (16). □

Moreover, it is seen that H is absolutely continuous, under the same assumption as in Corollary 4.3. Its proof is, essentially, based on the theorem in Ref. 19. For later convenience, here we introduce the closed subspace of $\mathcal{H}$, with respect to a self-adjoint operator H on $\mathcal{H}$, that is, $\mathcal{H}_{\mathrm{ac}}(H) := \{\psi \in \mathcal{H} | \|E(\cdot)\psi\|^2 \text{is absolutely continuous}\}$, where $\{E(B) \mid B \in \mathbf{B}^1\}$ is the spectral measure of H.[20]

Theorem 4.4: *Let T be a symmetric operator on $\mathcal{H}$, and H be a self-adjoint operator on $\mathcal{H}$. If a pair of operators T and H satisfies the T-weak WR, then*

$$\|E(B)\psi\|^2 \leqslant \|T\psi\|\|\psi\||B|, \tag{17}$$

for all $\psi \in \mathrm{Dom}(T)$ and all $B \in \mathbf{B}^1$, where $|B|$ is the Lebesgue measure of B. In particular, H is absolutely continuous.

Proof: Let us, first, derive the inequality that, $\forall \epsilon > 0$, $\forall \lambda \in \mathbf{R}^1$, and $\forall \psi \in \mathrm{Dom}(T)$,

$$|\mathrm{Im}\langle \psi, R(\lambda + i\epsilon)\psi\rangle| \leqslant \pi \|T\psi\|\|\psi\|, \tag{18}$$

where $R(\lambda \pm i\epsilon) := (H - (\lambda \pm i\epsilon))^{-1}$. It is seen that

$$\begin{aligned} i\,\mathrm{Im}\langle \psi, R(\lambda + i\epsilon)\psi\rangle &= \frac{1}{2}\int_{\mathbf{R}^1}\left(\frac{1}{\lambda' - \lambda - i\epsilon} - \frac{1}{\lambda' - \lambda + i\epsilon}\right) d\langle \psi, E(\lambda')\psi\rangle \\ &= \frac{i}{2}\int_{\mathbf{R}^1}\left[\int_0^\infty (e^{-it(\lambda' - \lambda - i\epsilon)} + e^{it(\lambda' - \lambda + i\epsilon)})dt\right] d\langle \psi, E(\lambda')\psi\rangle \\ &= i\int_0^\infty e^{-\epsilon t}\langle \psi, \cos t(H - \lambda)\psi\rangle dt \\ &= \lim_{\delta \downarrow 0}\int_\delta^\infty \frac{e^{-\epsilon t}}{t}\langle \psi, [T, \sin t(H - \lambda)]\psi\rangle dt, \end{aligned} \tag{19}$$

where Fubini's theorem has been used in the third equality, and Eq. (15) in the last. To evaluate Eq. (19), it is sufficient to see that

$$\lim_{\delta \downarrow 0}\int_\delta^\infty \frac{e^{-\epsilon t}}{t}\langle T\psi, \sin t(H - \lambda)\psi\rangle dt. \tag{20}$$

We define, here, a function $f(\epsilon, \lambda): (0, \infty) \times \mathbf{R}^1 \to \mathbf{R}^1$, as follows:

$$f(\epsilon, \lambda) := \int_0^\infty e^{-\epsilon t}\frac{\sin t\lambda}{t} dt.$$

$f(\epsilon, \lambda)$ is continuous on $(0, \infty) \times \mathbf{R}^1$, because of the fact that $|e^{-\epsilon t}\sin t\lambda/t| \leqslant e^{-\epsilon t}|\lambda|$ for any $t > 0$, and of the use of the dominated convergence theorem. Furthermore, since $\forall \epsilon > 0$, $\forall \lambda \in \mathbf{R}^1$ $e^{-\epsilon t}\sin t\lambda$ is integrable on $[0, \infty)$, $f(\epsilon, \lambda)$ is differentiable with respect to any $\epsilon > 0$, for each fixed λ. Thus, it is obtained, through the partial integrations, that $\forall \lambda \neq 0$,

$$\partial_\epsilon f(\epsilon, \lambda) = -\frac{1}{\lambda}\frac{1}{1 + \epsilon^2/\lambda^2}.$$

Note that $\forall \lambda \in \mathbf{R}^1$, $\lim_{\epsilon \to \infty} f(\epsilon, \lambda) = 0$, we obtain

$$f(\epsilon,\lambda)=\pm\frac{\pi}{2}-\frac{1}{\lambda}\int_0^{\epsilon}\frac{1}{1+\tau^2/\lambda^2}d\tau, \tag{21}$$

where each $\pm$ corresponds to the sign of λ. From this expression, $f(\epsilon,\lambda)$ is bounded, i.e. $|f(\epsilon,\lambda)|\leqslant\pi/2$. Equation (20) is expressed by $f(\epsilon,\lambda)$,

$$\begin{aligned}\lim_{\delta\downarrow 0}\int_{\delta}^{\infty}\frac{e^{-\epsilon t}}{t}\langle T\psi,\sin t(H-\lambda)\psi\rangle dt&=\lim_{\delta\downarrow 0}\int_{\delta}^{\infty}\frac{e^{-\epsilon t}}{t}\left[\int_{\mathbf{R}^1}\sin t(\lambda'-\lambda)d\langle T\psi,E(\lambda')\psi\rangle\right]dt\\&=\lim_{\delta\downarrow 0}\int_{\mathbf{R}^1}\left[\int_{\delta}^{\infty}e^{-\epsilon t}\frac{\sin t(\lambda'-\lambda)}{t}dt\right]d\langle T\psi,E(\lambda')\psi\rangle\\&=\int_{\mathbf{R}^1}f(\epsilon,\lambda'-\lambda)d\langle T\psi,E(\lambda')\psi\rangle=\langle T\psi,f(\epsilon,H-\lambda)\psi\rangle,\end{aligned}$$

where Fubini's theorem is used in the second equality, and the dominated convergence theorem is in the third. Substituting above relation into Eq. (19),

$$i\,\mathrm{Im}\langle\psi,R(\lambda+i\epsilon)\psi\rangle=\langle T\psi,f(\epsilon,H-\lambda)\psi\rangle-\langle f(\epsilon,H-\lambda)\psi,T\psi\rangle.$$

Note that $\|f(\epsilon,H-\lambda)\|\leqslant\pi/2$, then Equation (18) is obtained. Equation (17) follows from Eq. (18) through Stone's formula. By virtues of Eq. (17) and the denseness of $\mathrm{Dom}(T)$ in $\mathcal{H}$, it is seen that H is absolutely continuous. □

V. ABSENCE OF MINIMUM-UNCERTAINTY STATES

When a pair of operators T and H satisfies the T-weak WR, the following uncertainty relation between them:

$$(\Delta T)_{\psi}(\Delta H)_{\psi}\geqslant\tfrac{1}{2},\quad\forall\psi\in\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)\ \ (\|\psi\|=1), \tag{22}$$

is automatically derived, from the CCR between T and H, the validity of which follows from Proposition 2.1 (a more detailed explanation will be given in the proof of Theorem 5.1). For operators Q and P in Sec. III, it is well known that there is a state $\psi\in\mathrm{Dom}(QP)\cap\mathrm{Dom}(PQ)$ $(\|\psi\|=1)$, which minimizes the uncertainty, that is, a Gaussian packet. The following statement, on the contrary, shows that, under some additional conditions, there is no state $\psi\in\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$ $(\|\psi\|=1)$ which satisfies the equality in Eq. (22).

Theorem 5.1: *Let T be a symmetric operator on $\mathcal{H}$, H be a self-adjoint operator on $\mathcal{H}$, and these operators satisfy the T-weak WR. Then if H is non-negative and if the T-weak WR is analytically continued for all $t\in\mathbf{C}$ $(\mathrm{Im}\,t\leqslant 0)$, the equality in Eq. (22) can never be satisfied by any $\psi\in\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$ $(\|\psi\|=1)$.*

In order to prove this theorem, let us first consider two lemmas.

Lemma 5.2: Let T and H be symmetric operators on $\mathcal{H}$, and they satisfy the CCR $TH-HT=i$, on a subspace of $\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$, denoted by $\mathcal{D}$. Then neither eigenvector of T nor that of H belongs to $\mathcal{D}$.

Proof: Assume that an eigenvector of T, $\psi_\lambda\neq 0$, belonging to an eigenvalue λ exists in $\mathcal{D}$. Then $T\psi_\lambda=\lambda\psi_\lambda$, and thus we have $\langle\psi_\lambda,(TH-HT)\psi_\lambda\rangle=0$. On the other hand, the condition in this lemma requires that $\langle\psi_\lambda,(TH-HT)\psi_\lambda\rangle=i\|\psi_\lambda\|^2\neq 0$. Thus the subspace $\mathcal{D}$ contains no eigenvector of T. The rest of the proof for H can be done, as in the same way for T. □

Lemma 5.3: Let T and H be symmetric operators on $\mathcal{H}$, and let them satisfy the CCR $TH-HT=i$, on a subspace of $\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$, denoted by $\mathcal{D}$. If a state $\eta\in\mathcal{D}$ $(\|\eta\|=1)$ and a pair of complex numbers $a,b\in\mathbf{C}$, satisfying the following two equalities:

$$(T+aH+b)\eta=0, \tag{23}$$

$$\langle T\eta,H\eta\rangle+\langle H\eta,T\eta\rangle-2\langle T\rangle_\eta\langle H\rangle_\eta=0, \tag{24}$$

exist, then $\mathrm{Re}\,a=0$ *and* $\mathrm{Im}\,a>0$.

Proof: Let η be a state which satisfies the conditions in this lemma. Then we have that

$$\langle T\eta,H\eta\rangle+\langle H\eta,T\eta\rangle=\langle\eta,(HT+i)\eta\rangle+\langle H\eta,T\eta\rangle=i-2a\|H\eta\|^2-2b\langle\eta,H\eta\rangle.$$

From Eq. (23), we also have that

$$2\langle T\rangle_\eta\langle H\rangle_\eta=-2\langle\eta,(aH+b)\eta\rangle\langle\eta,H\eta\rangle=-2a\langle\eta,H\eta\rangle^2-2b\langle\eta,H\eta\rangle.$$

Therefore the condition Eq. (24) leads us to the relation

$$i-2a\|H\eta\|^2=-2a\langle\eta,H\eta\rangle^2. \tag{25}$$

Let us consider the real and imaginary parts of the above equality, separately. It follows, from the real part $(\mathrm{Re}\,a)\|H\eta\|^2=(\mathrm{Re}\,a)\langle\eta,H\eta\rangle^2$, that $\mathrm{Re}\,a=0$. This is because if $\mathrm{Re}\,a\neq0$, then $\|H\eta\|^2-\langle\eta,H\eta\rangle^2=0$ and this means that η is an eigenvector of H, belonging to the eigenvalue $\langle\eta,H\eta\rangle$, in spite of the premise $\eta\in\mathcal{D}$ $(\|\eta\|=1)$. This is in contradiction to Lemma 5.2. It is also seen, from the imaginary part, $1-2(\mathrm{Im}\,a)\|H\eta\|^2=-2(\mathrm{Im}\,a)\langle\eta,H\eta\rangle^2$, that $\mathrm{Im}\,a>0$. □

Proof of Theorem 5.1: Let $\psi\in\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$ and $\|\psi\|=1$. Since the T-weak WR holds for T and H, the CCR in Eq. (2) follows. Then the uncertainty relation between T and H, in Eq. (22), is derived as

$$\begin{aligned}(\Delta T)_\psi(\Delta H)_\psi&=\|(T-\langle T\rangle_\psi)\psi\|\|(H-\langle H\rangle_\psi)\psi\|\\&\geqslant|\langle(T-\langle T\rangle_\psi)\psi,(H-\langle H\rangle_\psi)\psi\rangle|\\&\geqslant|\mathrm{Im}\langle(T-\langle T\rangle_\psi)\psi,(H-\langle H\rangle_\psi)\psi\rangle|\\&=\tfrac{1}{2}|\langle T\psi,H\psi\rangle-\langle H\psi,T\psi\rangle|=\tfrac{1}{2}.\end{aligned}$$

In the second line, which is nothing but the Cauchy–Schwarz inequality, the equality holds if and only if there exists a complex number $\alpha\in\mathbf{C}$, satisfying

$$(T-\langle T\rangle_\psi)\psi+\alpha(H-\langle H\rangle_\psi)\psi=0.$$

In the third line, the equality holds if and only if

$$\mathrm{Re}\langle(T-\langle T\rangle_\psi)\psi,(H-\langle H\rangle_\psi)\psi\rangle=\langle T\psi,H\psi\rangle+\langle H\psi,T\psi\rangle-2\langle T\rangle_\psi\langle H\rangle_\psi=0.$$

In order to show that no $\psi\in\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$ $(\|\psi\|=1)$ can satisfy the equality in the uncertainty relation between T and H, in Eq. (22), it is sufficient to see that the above two conditions cannot be satisfied simultaneously, for any $\psi\in\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$ $(\|\psi\|=1)$ and for any $\alpha\in\mathbf{C}$. Observe that these conditions take just the same form as the two equalities (23) and (24) in Lemma 5.3.

Let us now assume that there exist such a state $\eta\in\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$ $(\|\eta\|=1)$, and a pair of complex numbers $a,b\in\mathbf{C}$, that satisfy both of Eqs. (23) and (24), and derive a contradiction. Lemma 5.3 implies that the parameter a is pure imaginary and is expressed as $a=iq$, $q>0$, to lead to $T\eta+iqH\eta+b\eta=0$. Then we must have that $-q\langle\eta,H\eta\rangle=\mathrm{Im}\,b\leqslant0$, because $\langle\eta,T\eta\rangle\in\mathbf{R}^1$ and $H\geqslant0$ (see the conditions of Theorem 5.1). It is also noted that e^{-itH} is bounded and $e^{-itH}H\subset He^{-itH}$, for all $t\in\mathbf{C}$ $(\mathrm{Im}\,t\leqslant0)$. Then it follows that $Te^{-itH}\eta=e^{-itH}(T\eta+t\eta)=(-iqH-b+t)e^{-itH}\eta$. Since $\mathrm{Im}\,b\leqslant0$ and $\mathrm{Im}\,t\leqslant0$, we can put $t=b$ and obtain $Te^{-ibH}\eta=-iqHe^{-ibH}\eta$. It is here noted that $e^{-ibH}\eta\neq0$, because e^{-ibH} is an injection and $\eta\neq0$. This is seen from the following relations:

$$\|e^{-ibH}\eta\|^2=\int_{[0,\infty)}|e^{-ib\lambda}|^2 d\|E(\lambda)\eta\|^2\geqslant\int_{[0,N]}|e^{-ib\lambda}|^2 d\|E(\lambda)\eta\|^2$$

$$\geqslant \inf_{\lambda\in[0,N]}|e^{-ib\lambda}|^2\int_{[0,N]} d\|E(\lambda)\eta\|^2$$

$$=e^{-2|\mathrm{Im}\, b|N}\int_{[0,N]} d\|E(\lambda)\eta\|^2,$$

where $\{E(B)|B\in\mathbf{B}^1\}$ is the spectral measure of H, N is an arbitrary natural number, and we have used the fact that the spectrum of H should be included in $[0,\infty)$, because $H\geqslant 0$. Providing that $e^{-ibH}\eta=0$, one would obtain that $0=\lim_{N\to\infty}\int_{[0,N]}d\|E(\lambda)\eta\|^2=\|\eta\|^2$, which contradicts $\|\eta\|=1$. By taking the inner products between $e^{-ibH}\eta$ and each side of $Te^{-ibH}\eta=-iqHe^{-ibH}\eta$, we have

$$\langle e^{-ibH}\eta, Te^{-ibH}\eta\rangle=-iq\langle e^{-ibH}\eta, He^{-ibH}\eta\rangle.$$

Notice that the both sides of this equality have to vanish. Since $q>0$ and $e^{-ibH}\eta\neq 0$, we have that $0=\langle e^{-ibH}\eta, He^{-ibH}\eta\rangle=\langle H^{1/2}e^{-ibH}\eta, H^{1/2}e^{-ibH}\eta\rangle=\|H^{1/2}e^{-ibH}\eta\|^2$, where $H^{1/2}$ is a self-adjoint operator, satisfying $H=H^{1/2}H^{1/2}$ and $H^{1/2}\geqslant 0$. Thus $He^{-ibH}\eta=0$. It is also seen that $e^{-ibH}\eta\in\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$, because $\eta\in\mathrm{Dom}(TH)\cap\mathrm{Dom}(HT)$. These facts are in contradiction to Lemma 5.2. Therefore, Eqs. (23) and (24) in Lemma 5.3 cannot be satisfied simultaneously. This means that the equality, in the uncertainty relation between T and H in Eq. (22), never holds under the condition of Theorem 5.1. □

The question about minimum-uncertainty states is motivated by the following result by Kobe:[1]

$$\lim_{n\to\infty}(\Delta\tilde{T}_0)_{F^{-1}\phi_n}(\Delta H_0)_{F^{-1}\phi_n}=\tfrac{1}{2},$$

where ϕ_n $(n\geqslant 2)$ is defined as in Example 1. Note, however, that ϕ_n does not converge in the L^2-norm, as $n\to\infty$. This Kobe's result implies the absence of minimum-uncertainty states. This result was also derived by Wigner[21] and Baute *et al.*,[22] in different ways from ours. It should be notified that the absence of minimum-uncertainty states expresses a crucial difference between the Weyl relation and the T-weak WR.

VI. CONSTRUCTION OF THE TIME OPERATORS FOR GENERAL QUANTUM SYSTEMS

We first summarize the several results so far obtained about the time operator T_0 in Eq. (1), or its extension $\tilde{T}_0$ in Eq. (11), for the 1DFPS.

Example 3: $\tilde{T}_0$ satisfies the $\tilde{T}_0$-weak WR with H_0, as is seen in Eq. (12). Then we have the following properties about $\tilde{T}_0$.

(i) The inequality (6) between $(\Delta\tilde{T}_0)_\psi$ and the survival probability of ψ holds for all $\psi\in\mathrm{Dom}(\tilde{T}_0)$ (Theorem 4.1).
(ii) $\tilde{T}_0$ has no point spectrum (Corollary 4.2).
(iii) The inequality (17) holds for all $\psi\in\mathrm{Dom}(\tilde{T}_0)$ and all $B\in\mathbf{B}^1$ (Theorem 4.4).
(iv) The uncertainty relation (22) between $\tilde{T}_0$ and H_0 holds on $\mathrm{Dom}(\tilde{T}_0H_0)\cap\mathrm{Dom}(H_0\tilde{T}_0)$ (Proposition 2.1), although there exists no state in $\mathrm{Dom}(\tilde{T}_0H_0)\cap\mathrm{Dom}(H_0\tilde{T}_0)$, which satisfies equality in the uncertainty relation between $\tilde{T}_0$ and H_0 (Theorem 5.1).

It is seen, from the above (i), that the Gaussian packet $F\phi_0$ in Example 1 is not included in $\mathrm{Dom}(\tilde{T}_0)$. Because, for large $|t|$, the survival probability of the Gaussian packet for the 1DFPS decays with an inverse-power law $|t|^{-1}$, and this is in contradiction to the behavior of the survival

probability predicted by the inequality (6). It is, however, noticed that this kind of estimation about the domain $\mathrm{Dom}(\tilde{T}_0)$ is valid for the one-dimensional case. Because, as the dimension becomes higher, the survival probability decays faster, in general than $|t|^{-2}$. We also obtain, from the inequality (6) for $\tilde{T}_0$ and H_0, that

$$2\sqrt{2}(\Delta\tilde{T}_0)_\psi \geqslant \tau_h(\psi), \tag{26}$$

where $\tau_h(\psi)$ is defined as $\tau_h(\psi) := \sup\{t \geqslant 0 \,|\, |\langle \psi, e^{-itH_0}\psi\rangle|^2 = 1/2\}$, $\forall \psi \in \mathrm{Dom}(\tilde{T}_0)$ $(\|\psi\| = 1)$. This relation is important, to give the direct connection between $(\Delta\tilde{T}_0)_\psi$ and the measurable quantity $\tau_h(\psi)$, although we do not know whether $\tilde{T}_0$ itself is an observable. Let us also consider the physical meaning of the above (iii). The following inequality is derived from Eq. (17):

$$\|E_{H_0}(B)\psi\|^2 \leqslant (\Delta\tilde{T}_0)_\psi |B|,$$

for all $\psi \in \mathrm{Dom}(\tilde{T}_0)$ $(\|\psi\| = 1)$ and $B \in \mathbf{B}^1$, because of the fact that the $\tilde{T}_0$-weak WR is not changed, with replacing $\tilde{T}_0$ by $\tilde{T}_0 - \langle \tilde{T}_0 \rangle_\psi$. Note that $\|E_{H_0}(B)\psi\|^2$ is the probability which one finds a measured energy-value in the range B for the fixed ψ. Suppose that $(\Delta\tilde{T}_0)_\psi$ is small; then the probability $\|E_{H_0}(B)\psi\|^2$ should be uniformly small for all $B \in \mathbf{B}^1$. This concludes that the probability distribution $\|E_{H_0}(\cdot)\psi\|^2$ has a broad deviation, for $\|E_{H_0}(\mathbf{R}^1)\psi\|^2 = 1$. Hence $(\Delta\widetilde{H_0})_\psi$ must be large and this result is consistent with the uncertainty relation.

In order to find other quantum systems than the 1DFPS, for which a time operator exists, let us recall the results obtained by Putnam, in the theory of Schrödinger operators.[23] According to this theorem, if a potential $V(x)$ is a real-valued measurable function on $\mathbf{R}^1$ satisfying $0 \leqslant V(x) \leqslant \mathrm{const}$, *a.e.* and $V(x) \in L^1(\mathbf{R}^1)$; then H_0 and $H_1 := H_0 + V(x)$ defined on $L^2(\mathbf{R}^1)$ are absolutely continuous, and furthermore the wave operators $U_\pm := \mathrm{s}-\lim_{t \to \pm\infty} e^{itH_1}e^{-itH_0}$ exist and are unitary operators satisfying $H_1 = U_\pm H_0 U_\pm^*$. For our purpose, we first define the operators $T_{1,\pm} := U_\pm \tilde{T}_0 U_\pm^*$ on $L^2(\mathbf{R}^1)$, where $U_\pm$ are the wave operators defined in this Putnam's theorem. Then $T_{1,\pm}$ are symmetric and satisfy the $T_{1,\pm}$-weak WR with H_1, i.e.,

$$T_{1,\pm}e^{-itH_1} = e^{-itH_1}(T_{1,\pm} + t),$$

which are nothing but the unitary transformations of Eq. (12). These operators $T_{1,\pm}$ are the time operators we have sought for other quantum systems than the 1DFPS, and they satisfy all the properties, described in Example 3, with this H_1.

For a quantum system which allows bound states, we can also construct a time operator satisfying the T-weak WR with the Hamiltonian H, by restricting it to act on the set of scattering states. The latters are usually identified with the subspace $\mathcal{H}_{\mathrm{ac}}(H)$ of the Hilbert space $\mathcal{H}$ under consideration. Because, in this case, the wave operator (if exits) is not a unitary operator on $\mathcal{H}$ in general, that is, the range $\mathrm{Ran}(U_\pm)$ becomes a proper subspace of $\mathcal{H}$. In fact, according to Kuroda,[24] if the potential $V(x)$ is a real-valued measurable function on $\mathbf{R}^1$ satisfying $V(x) \in L^1(\mathbf{R}^n) \cap L^2(\mathbf{R}^n)$, $n \leqslant 3$, and the Hamiltonian H_1 on $L^2(\mathbf{R}^1)$ is defined as $H_1 := H_0 + V(x)$, then the wave operators $U_\pm$ exist and are complete, i.e., $\mathrm{Ran}(U_\pm) = L^2_{\mathrm{ac}}(H_1)$, where $L^2_{\mathrm{ac}}(H_1)$ is a subspace in $L^2(\mathbf{R}^1)$, similarly defined as $\mathcal{H}_{\mathrm{ac}}(H)$ just before Theorem 4.4. As in the same way for Putnam's theorem, by the use of the wave operators $U_\pm$ defined for H_0 and H_1 in this Kuroda's theorem, we can define the operators $T_{1,\pm} := U_\pm \tilde{T}_0 U_\pm^*$ on $L^2_{\mathrm{ac}}(H_1)$ and their domains, $\mathrm{Dom}(T_{1,\pm}) := U_\pm \mathrm{Dom}(\tilde{T}_0)$. Then they are symmetric operators on $L^2_{\mathrm{ac}}(H_1)$, and satisfy

$$T_{1,\pm}e^{-itH_{1,ac}} = e^{-itH_{1,ac}}(T_{1,\pm} + t).$$

$H_{1,\mathrm{ac}}$ is defined as $H_{1,\mathrm{ac}} := H_1|_{L^2_{\mathrm{ac}}(H_1)} = U_\pm H_0 U_\pm^*$, and is called the (spectrally) absolutely continuous part of H_1.[13] By the unitary equivalence, Example 3 is also valid for the pair $T_{1,\pm}$ and $H_{1,\mathrm{ac}}$.

We cannot, however, extend these $T_{1,\pm}$ to the densely defined symmetric operators on $L^2(\mathbf{R}^1)$, so that they satisfy the $T_{1,\pm}$-weak WR with H_1, when H_1 has a point spectrum, i.e., $L^2_{\rm pp}(H_1) \neq \{0\}$. This is because such an extension contradicts Corollary 4.3 and Theorem 4.4.

VII. CONCLUDING REMARKS

Analyzing the T-weak Weyl relation (T-weak WR) in Eq. (4), and obtaining several statements about the time operator, we have seen that the Aharonov–Bohm time operator T_0 in Eq. (1) [or its symmetric extension $\tilde{T}_0$ in Eq. (11)] is characterized by the $\tilde{T}_0$-weak WR in Eq. (12). We have, in particular, recognized the fact that the time operator is deeply connected to the survival probability. In relation to this considerable connection, we would like, first, to revisit the inequality (6) in Theorem 4.1, Theorem 4.4, and their implications.

The inequality (6) is important to bring us a possibility of understanding the time operator from the two different points. The first point is related to the measurement of the survival probability. Since the inequality (26) derived from the inequality (6) gives the quantitative relation between the standard deviation of the time operator $\tilde{T}_0$ and the maximum half-time of the survival probability in the 1DFPS, we may associate the time operator in quantum systems, with both the real and theoretical measurements of the survival probability. Another point is related to the connection with the dynamics of quantum systems. In order to see this possibility, we may refer to Proposition 3.2, and Corollary 4.3 which is one of the applications of the inequality (6). These facts imply a possibility of associating the time operator (or its domain), with the scattering state and its dynamics, through the survival probability.

As a remark on Theorem 4.4, the following suggestion by Putnam should be recalled, that is, the existence of the absolutely continuous part of the Hamiltonian can be inferred from the behavior of specific observables.[25] He considered the following system, in which there is a self-adjoint operator A_0 satisfying $A_t = A_0 + tI$, $\forall t \in \mathbf{R}^1$, where $A_t := e^{itH} A_0 e^{-itH}$ and H is the Hamiltonian for this system. He showed that H must be absolutely continuous (note that this is the case to which the last statement in Proposition 2.1 is applicable). The essence of its proof, that is, the uniqueness of the spectral resolution of A_0, also implies that if A_0 is maximally symmetric (not necessarily self-adjoint), H must be absolutely continuous. Because A_0 is uniquely represented by the generalized resolution of identity.[26] In this context, Theorem 4.4 is a generalization of the above statement by Putnam, to nonmaximally symmetric operators. However the absolute continuity of H seems to be obvious in the light of the works by Schmüdgen.[12] Because, under some condition, H is unitary equivalent to the position operator. Here we would like to emphasize the inequality (17), rather than the absolute continuity of H, which is explained as follows.

The proof of the absolute continuity of H, which satisfies the T-weak Weyl relation with T, depends on Eq. (17). It is similar to the following inequality which was derived by Putnam[27] and Kato,[8] on the study of the commutator of the form, $[H, iA] = C$, where H, A and C are bounded self-adjoint operators, and $C \geqslant 0$,

$$\|C^{1/2} E_H(B)\psi\|^2 \leqslant \|A\| \|\psi\|^2 |B|, \quad \forall \psi \in \mathcal{H}, \ \forall B \in \mathbf{B}^1. \tag{27}$$

It is seen that Eq. (17) is an unbounded case of theirs, and is not trivial. Because one cannot replace directly C with the identity, for both bounded H and A. They showed, through Eq. (27), that H is absolutely continuous, provided that $\mathrm{Ker}(C) = \{0\}$, i.e., $\overline{\mathrm{Ran}(C)} = \mathcal{H}$. This statement is sometimes valid when the above H and A are unbounded, however, its proof originates in the more fundamental notion, T-smoothness,[8] rather than the inequality like the above one, and the appropriate technique. Lavine applied it to Schrödinger operators in an especially good manner.[9–11] It should be noted that his work is closely related to the our problem. He found self-adjoint operators A which satisfy $[H, iA] = C$, with a certain class of Schrödinger operators H and positive bounded C. In the case of the absolute continuity of the free Hamiltonian H_0, we can choose the self-adjoint operator $A := (f(P)Q + Qf(P))/2$, where $f(P) := P(P^2 + \delta^2)^{-1}$ and $C := Pf(P)$. When $\delta > 0$, A is self-adjoint, because $\mathrm{Ker}(A^* \mp i) = \{0\}$. And also C is bounded and

$C>0$. They satisfy $[H_0, iA]=C$ and one can consider the case that a parameter δ approaches to 0, which is just $A=T_0$. Hence this scheme has the advance in the approach to the absolute continuity of H_0 and its connection with the Aharonov–Bohm time operator T_0.

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Path integral for relativistic Aharonov–Bohm–Coulomb system on the pseudo-sphere

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The Green's function for relativistic spinless Aharonov–Bohm–Coulomb (ABC) system on the pseudo-sphere $\Lambda^{(2)}$ is calculated using Kleinert's path integral representation for relativistic spinless particles. The energy spectrum and the corresponding wave functions are extracted for bound and scattering states. The results in the nonrelativistic and flat space limits are considered. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1329660]

I. INTRODUCTION

Quantum motion on spaces with constant curvature, positive as well negative, is of great interest for various fields of theoretical physics.[1] Examples are provided by the structure of the pseudo-sphere $\Lambda^{(2)}$, which makes it very interesting in Polyakov path integral approach to string theory and in $(1+1)$-dimensional quantum gravity.[2] We can also cite the path integral treatment of the nonrelativistic Kepler problem in space of constant curvature.[3] On the other hand, the path integral formalism is the most suitable tool to treat topological defects such as the Aharonov–Bohm (AB) effect. The path integral treatment of a nonrelativistic particle on the hyperbolic plane under the action of the AB field has been done recently.[4]

In this paper we would like to add, to the short list of solvable path integrals for relativistic systems,[5,6] another application, namely the relativistic spinless Aharonov–Bohm–Coulomb (ABC) system on the pseudo-sphere $\Lambda^{(2)}$.

In Sec. II, we present a brief review of the path integral formulation on spaces with constant curvature. In Sec. III, using the Duru–Kleinert's technique of space–time transformations, we obtain in a closed form the Green's function for the relativistic ABC system. In Sec. IV the energy spectrum and the wave functions for bound states are explicitly evaluated and the special cases of the flat space limit and the nonrelativistic limit are considered. In Sec. V, using the integral representation of the Green's function, we deduce the scattering states. Our concluding remarks are given in Sec. VI.

II. PATH INTEGRAL REPRESENTATION ON $\Lambda^{(2)}$

The spherical coordinates in the pseudo-Euclidean space $E_{2,1}$ are given by

$$x^1 = r\sinh\tau\sin\varphi, \quad x^2 = r\sinh\tau\cos\varphi, \quad x^3 = r\cosh\tau, \tag{1}$$

where $r>0, \tau>0$ and $\varphi\in[0,2\pi)$.

The discretized propagator of a free particle moving in such a space is given by[7]

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$$K(\mathbf{x}_b,\mathbf{x}_a;T)=\lim_{N\to\infty}\int\prod_{n=1}^{N}\left(\frac{m}{2\pi i\varepsilon}\right)\left(\frac{mi}{2\pi\varepsilon}\right)^{1/2N-1}\prod_{n=1}^{N-1}dx_n^1dx_n^2dx_n^3$$
$$\times\prod_{n=1}^{N}\exp\left\{\frac{im}{2\varepsilon}[(\Delta x_n^1)^2+(\Delta x_n^2)^2-(\Delta x_n^3)^2]\right\}$$
$$=\lim_{N\to\infty}\int\prod_{n=1}^{N}\left(\frac{m}{2\pi i\varepsilon}\right)\left(\frac{mi}{2\pi\varepsilon}\right)^{1/2N-1}\prod_{n=1}^{N-1}r_n^2dr_n\sinh\tau_nd\tau_nd\varphi_n$$
$$\times\prod_{n=1}^{N}\exp\left\{-\frac{im}{2\varepsilon}\Delta r_n^2-\frac{im}{\varepsilon}r_nr_{n-1}[1+(\mathbf{e}_n,\mathbf{e}_{n-1})]\right\}. \tag{2}$$

A regularizating scheme for this path integral consists in adding, to the mass, a small positive imaginary term for the compact variables (x^1 and x^2) and a small negative imaginary term for the noncompact variable (x^3). The particular form of the measure, which is a consequence of the indefinite metric, is necessary to obtain the correct normalization contition, $\lim_{T\to0}K(\mathbf{x}_{b,},\mathbf{x}_a;T)=\delta(\mathbf{x}_b-\mathbf{x}_a)$.

The scalar product between the unit vectors $\mathbf{e}_n$ and $\mathbf{e}_{n-1}$ is given by

$$(\mathbf{e}_n,\mathbf{e}_{n-1})=-[\sinh\tau_n\sinh\tau_{n-1}(1-\cos\Delta\varphi_n)+\cosh\Delta\tau_n]. \tag{3}$$

The propagator on the pseudo-sphere $\Lambda^{(2)}$ is easily obtained by fixing r_n to a constant R via the relation

$$\lim_{\epsilon\to0}\left(\frac{mi}{2\pi\varepsilon}\right)^{1/2}\exp\left(-\frac{im}{2\varepsilon}(r_n-r_{n-1})^2\right)=\delta(r_n-r_{n-1}). \tag{4}$$

Then performing the integrations over r_j in (2), we obtain

$$K(\mathbf{x}_b,\mathbf{x}_a;T)=\frac{1}{R^2}\lim_{N\to\infty}\int\prod_{n=1}^{N}\left(\frac{mR^2}{2\pi i\varepsilon}\right)\prod_{n=1}^{N-1}\sinh\tau_nd\tau_nd\varphi_n$$
$$\times\prod_{n=1}^{N}\exp\left\{-\frac{im}{\varepsilon}R^2[1+(\mathbf{e}_n,\mathbf{e}_{n-1})]\right\}. \tag{5}$$

Let us set $v_n=-mR^2\sinh\tau_n\sinh\tau_{n-1}$. Using the decomposition

$$e^{i/\varepsilon\,v_n\cos\Delta\varphi_n}=\sum_{l_n=-\infty}^{\infty}I_{l_n}\left(\frac{iv_n}{\varepsilon}\right)e^{il_n\Delta\varphi_n}, \tag{6}$$

and the following relation valid for $\varepsilon\to0$:

$$I_{l_n}\left(\frac{iv_n}{\varepsilon}\right)\approx\sqrt{\frac{\varepsilon}{2\pi iv_n}}\exp\left(\frac{iv_n}{\varepsilon}-\frac{\varepsilon}{2iv_n}\left(l_n^2-\frac{1}{4}\right)\right), \tag{7}$$

we obtain

$$K(\mathbf{x}_b,\mathbf{x}_a;T)=[R^4\sinh\tau_b\sinh\tau_a]^{-1/2}\lim_{N\to\infty}\int\prod_{n=1}^{N}\frac{1}{2\pi}\left(\frac{mR^2}{2\pi i\varepsilon}\right)$$
$$\times\prod_{n=1}^{N-1}d\tau_n d\varphi_n\prod_{n=1}^{N}\exp\left\{-\frac{im}{\varepsilon}R^2[1-\cosh\Delta\varphi_n]\right\}$$
$$\times\sum_{l_n=-\infty}^{\infty}\exp\left(-\frac{i\varepsilon}{2mR^2}\frac{l_n^2-\frac{1}{4}}{\sinh\tau_n\sinh\tau_{n-1}}\right)e^{il_n\Delta\varphi_n}. \tag{8}$$

The $N-1$ successive integrations over the variables φ_n produce the factor $\Pi_{n=1}^{N-1}2\pi\delta_{l_n,l_{n-1}}$, such that the propagator becomes

$$K(\mathbf{x}_b,\mathbf{x}_a;T)=[R^4\sinh\tau_b\sinh\tau_a]^{-1/2}\lim_{N\to\infty}\int\prod_{n=1}^{N}\left(\frac{mR^2}{2\pi i\varepsilon}\right)^{1/2N-1}\prod_{n=1}d\tau_n\sum_{l=-\infty}^{\infty}\frac{e^{il(\varphi_b-\varphi_a)}}{2\pi}$$
$$\times\prod_{n=1}^{N}\exp\left\{-\frac{im}{\varepsilon}R^2[1-\cosh\Delta\tau_n]-\frac{i\varepsilon}{2mR^2}\frac{l^2-\frac{1}{4}}{\sinh\tau_n\sinh\tau_{n-1}}\right\}. \tag{9}$$

Now we use the approximation valid for $\varepsilon\to 0$

$$1-\cosh\Delta\tau_n\approx-\tfrac{1}{2}(\Delta\tau_n)^2-\tfrac{1}{24}(\Delta\tau_n)^4. \tag{10}$$

We note that $(\Delta\tau_n)^4/\varepsilon=O(\varepsilon)$ and hence contributes to the path integral. Its contribution can be evaluated via the procedure of McLaughlin–Schulman[8] based on the formula

$$\int_{-\infty}^{+\infty}\exp(-ax^2+bx^4)dx=\int_{-\infty}^{+\infty}\exp\left(-ax^2+\frac{3b}{4a^2}\right)dx, \tag{11}$$

valid for large a and $\mathrm{Re}a>0$ and for b purely imaginary or even with a negative imaginary part. The condition on a can be satisfied by adding a small imaginary part to the mass in the kinetic term.

Finally the path integral representation of the propagator on the pseudo-sphere $\Lambda^{(2)}$ is given by

$$K(\mathbf{x}_b,\mathbf{x}_a;T)=[R^4\sinh\tau_b\sinh\tau_a]^{-1/2}\sum_{l=-\infty}^{\infty}\frac{e^{il(\varphi_b-\varphi_a)}}{2\pi}\lim_{N\to\infty}\int\prod_{n=1}^{N}\left(\frac{mR^2}{2\pi i\varepsilon}\right)^{1/2N-1}\prod_{n=1}d\tau_n$$
$$\times\exp\left\{i\sum_{n=1}^{N}\left[\frac{mR^2}{2\varepsilon}(\Delta\tau_n)^2-\varepsilon\left(\frac{1}{2mR^2}\frac{l^2-1/4}{\sinh\tau_n\sinh\tau_{n-1}}+\frac{1}{8mR^2}\right)\right]\right\}. \tag{12}$$

III. RELATIVISTIC ABC ON $\Lambda^{(2)}$

The Green's function of a relativistic particle in a $(D+1)$-dimensional Minkowski space is given by Kleinert's path integral representation[9]

$$G(\mathbf{x}_b,\mathbf{x}_a;E)=\frac{1}{2mc}\int_0^\infty dL\int\mathcal{D}\rho(t)\Phi[\rho(t)]\int\mathcal{D}\mathbf{x}(t)\exp(i\mathcal{A}), \tag{13}$$

with the action

$$\mathcal{A}=\int_0^T dt\left[\frac{m}{2\rho(t)}\dot{\mathbf{x}}^2(t)+\frac{e}{c}\mathbf{A}\dot{\mathbf{x}}(t)+\rho(t)\frac{(E-V(\mathbf{x}))^2}{2mc^2}-\rho(t)\frac{mc^2}{2}\right]. \tag{14}$$

Here $\mathbf{A}$ and $V(\mathbf{x})$ are, respectively, the vector and scalar potentials, L is a length defined by

$$L=\int_0^T dt\rho(t), \tag{15}$$

and $\Phi[\rho(t)]$ is a gauge-fixing functional of the dimensionless fluctuating scale variable $\rho(t)$ which obeys the condition

$$\int D\rho(t)\Phi[\rho(t)]=1. \tag{16}$$

In the following we fix the value of $\rho(t)$ to unity by simply choosing $\Phi[\rho(t)]=\delta[\rho(t)-1]$ and we consider the case of rotationally invariant scalar potential.

We begin our investigation of the relativistic spinless ABC system by considering the Coulomb potential on $\Lambda^{(2)}$ defined by[3,4]

$$V(\tau)=-\frac{\alpha}{R}(\coth\tau-1), \tag{17}$$

where the coupling constant α is the analogue of e^2 on a flat space.

Using the path integral representation (12), the Green's function for the relativistic Coulomb field on $\Lambda^{(2)}$ is given by

$$\begin{aligned}
&G(\mathbf{x}_b,\mathbf{x}_a;E)\\
&\quad=[R^4\sinh\tau_b\sinh\tau_a]^{-1/2}\left(\frac{1}{2mc}\right)\int_0^\infty dT\lim_{N\to\infty}\int\prod_{n=1}^{N}\left(\frac{mR^2}{2\pi i\varepsilon}\right)^{1/2}\prod_{n=1}^{N-1}d\tau_n\\
&\qquad\times\sum_{l=-\infty}^{\infty}\frac{e^{il(\varphi_b-\varphi_a)}}{2\pi}\exp\left\{i\epsilon\sum_{n=1}^{N}\left[\frac{mR^2}{2\varepsilon^2}(\Delta\tau_n)^2\right.\right.\\
&\qquad\left.\left.+\left(A\coth\tau_n-\frac{B_l}{\sinh\tau_n\sinh\tau_{n-1}}+C\right)\right]\right\}.
\end{aligned} \tag{18}$$

In the limit $N\to\infty$ we have

$$\begin{aligned}
G(\mathbf{x}_b,\mathbf{x}_a;E)&=[R^4\sinh\tau_b\sinh\tau_a]^{-1/2}\left(\frac{1}{2mc}\right)\int_0^\infty dT\sum_{l=-\infty}^{\infty}\frac{e^{il(\varphi_b-\varphi_a)}}{2\pi}\\
&\quad\times\int_{\tau_a}^{\tau_b}\mathcal{D}\tau(t)\exp\left\{i\int_0^T dt\left[\frac{mR^2}{2}\dot{\tau}^2+A\coth\tau-\frac{B_l}{\sinh^2\tau}+C\right]\right\},
\end{aligned} \tag{19}$$

where we have set $\mathcal{D}\tau(t)=\lim_{N\to\infty}\Pi_{n=1}^{N}(mR^2/2\pi i\varepsilon)^{1/2}\Pi_{n=1}^{N-1}d\tau_n$ and

$$A=\frac{\alpha}{mc^2R}\left(E-\frac{\alpha}{R}\right), \tag{20}$$

$$B_l=\frac{1}{2mR^2}\left(l^2-\frac{1}{4}\right)-\frac{\alpha^2}{2mc^2R^2}, \tag{21}$$

$$C=\frac{1}{2mc^2}\left[\left(\frac{\alpha}{R}\right)^2+\left(E-\frac{\alpha}{R}\right)^2\right]-\frac{1}{8mR^2}-\frac{mc^2}{2}. \tag{22}$$

According to an ansatz by Kuperin *et al.*[10] for the AB field we write the magnetic interaction in (14) as

$$A_{\mathrm{mag}} = -2\pi n \nu, \tag{23}$$

where we have set

$$n = \frac{1}{2\pi}\int_0^T \dot{\varphi}(t)dt, \quad \nu = -\frac{e}{2\pi c}\int d^2x B_3. \tag{24}$$

Here n is a topological invariant, $\varphi(t) = \arctan(x^2/x^1)$ is the azimuthal angle around the AB tube, B_3 represents the magnetic field confined to an infinitely thin tube along the third axis and $\int d^2x B_3$ is the flux through the tube.

Adding (23) to the action in (19) and converting the sum over the azimuthal quantum number l to an integral via the Poisson's summation formula

$$\sum_{l=-\infty}^{\infty} f(l) = \int_{-\infty}^{+\infty} d\mu \sum_{p=-\infty}^{\infty} e^{2i\pi p\mu} f(\mu), \tag{25}$$

we write the Green's function for the ABC system in the following form:

$$G(\mathbf{x}_b, \mathbf{x}_a; E) = \sum_{l=-\infty}^{\infty} \frac{e^{il(\varphi_b - \varphi_a)}}{2\pi} G_{l+\nu}(\tau_b, \tau_a; E), \tag{26}$$

where the radial part is given by

$$G_{l+\nu}(\tau_b, \tau_a; E) = [R^4 \sinh\tau_b \sinh\tau_a]^{-1/2}\left(\frac{1}{2mc}\right)\int_0^\infty dT \times \int_{\tau_a}^{\tau_b} \mathcal{D}\tau(t) \exp\left\{ i\int_0^T dt\left[\frac{mR^2}{2}\dot{\tau}^2 + A\coth\tau - \frac{B_{l+\nu}}{\sinh^2\tau} + C\right]\right\}, \tag{27}$$

with $B_{l+\nu}$ defined by Eq. (21).

This is exactly the path integral representation of the Manning–Rosen potential[11] analyzed by several authors.[12]

In order to link Eq. (27) with the Green's function for the motion of a mass point near the surface of a sphere in four dimensions projected in a state of fixed angular momentum, we use Duru–Kleinert's technique of space–time transformations.[13,14]

Indeed we introduce the following space transformation $\tau \in [0,\infty) \to \theta \in [0,\pi)$

$$\tanh\frac{\tau}{2} = \frac{1-\cos(\theta/2)}{1+\cos(\theta/2)}, \tag{28}$$

combined to the path-dependent time transformation $t \to s$

$$dt = ds \tan^2\frac{\theta}{2}. \tag{29}$$

Taking into account all the contributions arising from the slicing of the path-dependent time, the Green's function (27) becomes

$$G_{l+\nu}(\tau_b,\tau_a;E)=\frac{2}{R^2}\left[\sin\frac{\theta_b}{2}\sin\frac{\theta_a}{2}\right]^{-1/2}\left(\frac{1}{2mc}\right)\int_0^S dS\int \mathcal{D}\theta(s)$$
$$\times\exp\left\{i\int_0^S ds\left[\frac{mR^2}{8}\dot{\theta}^2+\frac{A+C+1/8mR^2}{\cos^2(\theta/2)}-\frac{4B_{l+\nu}+3/8mR^2}{\sin^2(\theta/2)}+A-C\right]\right\}. \tag{30}$$

Following Ref. 14, let us introduce the following parameters:

$$m_1=\tfrac{1}{2}(\sqrt{-2mR^2(A+C)})+\sqrt{1+8mR^2B_{l+\nu}}), \tag{31}$$

$$m_2=\tfrac{1}{2}(\sqrt{-2mR^2(A+C)})-\sqrt{1+8mR^2B_{l+\nu}}), \tag{32}$$

$$E_{PT'}=A-C-\tfrac{1}{8}mR^2. \tag{33}$$

Then (30) is given by

$$G_{l+\nu}(\tau_b,\tau_a;E)=\frac{4}{R^2}\sqrt{\cos(\theta_b/2)\cos(\theta_a/2)}\left(\frac{1}{2mc}\right)$$
$$\times\sum_{L=\max(m_1,m_2)}\frac{i}{E_{PT'}-((L+1)^2-1/4)/2mR^2}$$
$$\times\frac{L+1}{2}d^{L/2}_{m_1,m_2}(\theta_b)d^{L/2}_{m_1,m_2}(\theta_a), \tag{34}$$

where $d^L_{m,n}(\theta)$ is the analytical continuation of the Wigner function.

The summation over L in (34) is performed with the help of Sommerfeld–Watson's transformation,[15,16] which is essentially based on the following substitution:

$$\sum_L \rightarrow\frac{1}{2i}\int_C d\sigma\frac{e^{-2i\pi\sigma}}{\sin\pi\sigma}, \tag{35}$$

where the contour of integration C is the entire real axis in a counterclockwise direction.

Then following Ref. 17, we put the Green's function in the following compact form:

$$G_{l+\nu}(\tau_b,\tau_a;E)=-im\sqrt{\cos(\theta_b/2)\cos(\theta_a/2)}\left(\frac{1}{2mc}\right)\Gamma(m_1-L_E)\Gamma(L_E-m_1+1)$$
$$\times d^{L_E}_{m_1,-m_2}(\theta_b-\pi)d^{L_{E^*}}_{m_1,m_2}(\theta_a), \tag{36}$$

where $\theta_b<\theta_a$ and L_E is given by

$$L_E=-\frac{1}{2}+\sqrt{\frac{1}{16}+\frac{mR^2}{2}E_{PT'}}=-\frac{1}{2}[1-\sqrt{2mR^2(A-C)}]. \tag{37}$$

Using the old variables we obtain the radial part of the Green's function in the following closed form:

$$G_{l+\nu}(\tau_b,\tau_a;E)=-im\left(\frac{1}{2mc}\right)\left(\frac{1-\tanh(\tau_b/2)}{1+\tanh(\tau_b/2)}\right)^{1/2}\left(\frac{1-\tanh(\tau_a/2)}{1+\tanh(\tau_a/2)}\right)^{1/2}$$
$$\times\Gamma(m_1-L_E)\Gamma(L_E-m_1+1)d^{L_E}_{m_1,-m_2}(\theta(\tau_b)-\pi)d^{L_{E^*}}_{m_1,m_2}(\theta(\tau_a)), \tag{38}$$

with $\theta(\tau)$ defined by (28).

IV. BOUND STATES

The allowed energy levels are extracted from the poles of $\Gamma(m_1-L_E)$ in (38) which occur when the argument is a negative integer $-n_r$

$$m_1-L_E=-n_r, \quad n_r=0,1,2,3,\ldots. \tag{39}$$

Using the expressions (31) and (37), it is easy to show that

$$C+\frac{2mR^2A^2}{N^2}+\frac{N^2}{8mR^2}=0, \tag{40}$$

where

$$N=2n_r+s+1, s=\sqrt{1+8mR^2B_{l+\nu}}. \tag{41}$$

The solutions of (40) give the energy spectrum for the relativistic ABC system on $\Lambda^{(2)}$

$$E_{n_r}-\frac{\alpha}{R}=\pm mc^2\left[\frac{1+(1-(2\alpha/c)^2-N^2)/(2mcR)^2}{1+(2\alpha/Nc)^2}\right]^{1/2}. \tag{42}$$

The maximum number of bound states is given by

$$N_{\max}=\{\sqrt{(2mcR)^2-(2\alpha/c)^2+1}\}. \tag{43}$$

Here the symbol $\{k\}$ means the largest integer smaller than k.

The corresponding energy eigenfunctions for the bound states are now derived from the residues of the Green's function at the poles

$$\Gamma(m_1-L_E)\approx\frac{(-1)^{n_r}}{n_r!}\frac{1}{m_1-L_E+n_r}. \tag{44}$$

After some mathematical manipulations we find

$$\begin{aligned}\Gamma(m_1-L_E)\approx&\frac{(-1)^{n_r+1}}{n_r!}\left(\frac{E-\alpha/R}{mc^2}\right)^2\frac{2mc^2}{(E-\alpha/R)^2-(E_{n_r}-\alpha/R)^2}\\&\times\frac{16m^2R^4A^2/N^2-N^2}{2mR^2N}\left[1+\frac{1-(2\alpha/c)^2-N^2}{(2mcR)^2}\right]^{-1}.\end{aligned} \tag{45}$$

Now using the following symmetry relation:[18]

$$d^{L_E}_{m_1,-m_2}(\theta-\pi)=(-1)^{m_1-L_E}d^{L_E}_{m_1,m_2}(\theta), \tag{46}$$

and the relation connecting the Wigner function and the hypergeometric function

$$\begin{aligned}d^{L_E}_{m_1,m_2}(\theta)=&\left[\frac{\Gamma(L_E+m_1+1)\Gamma(L_E-m_2+1)}{\Gamma(L_E-m_1+1)\Gamma(L_E+m_2+1)}\right]^{1/2}\frac{1}{\Gamma(m_1-m_2+1)}\\&\times\left(\frac{1-\cos(\theta)}{2}\right)^{(m_1-m_2)/2}\left(\frac{1+\cos(\theta)}{2}\right)^{(m_1+m_2)/2}\\&\times{}_2F_1\left(-L_E+m_1,L_E+m_1+1,m_1-m_2+1;\frac{1-\cos(\theta)}{2}\right),\end{aligned} \tag{47}$$

we obtain the following decomposition of the radial Green's function:

$$G_{l+\nu}(\tau_b,\tau_a;E)=\frac{1}{2mc}\sum_{N=s+1}^{N_{\max}}\left(\frac{E-\alpha/R}{mc^2}\right)^2\frac{2imc^2}{(E-\alpha/R)^2-(E_{n_r}-\alpha/R)^2}\Psi_{n_r}(\tau_b)\Psi^*_{n_r}(\tau_a), \tag{48}$$

where the radial wave functions are

$$\begin{aligned}\Psi_{n_r}(\tau)=&\left[\frac{16m^2R^4A^2/N^2-N^2}{2R^2N}\right]^{1/2}\left[1+\frac{1-(2\alpha/c)^2-N^2}{(2mcR)^2}\right]^{-1/2}\\&\times\frac{2^{m_1-m_2}}{\Gamma(m_1-m_2+1)}\left[\frac{\Gamma(L_E+m_1+1)\Gamma(L_E-m_2+1)}{\Gamma(L_E-m_1+1)\Gamma(L_E+m_2+1)}\right]^{1/2}\\&\times(1-\tanh\tau/2)^{m_1+m_2+1/2}(1+\tanh\tau/2)^{-2m_1-1/2}(\tanh\tau/2)^{(m_1-m_2)/2}\\&\times{}_2F_1\left(-L_E+m_1,L_E+m_1+1,m_1-m_2+1;\frac{4\tanh\tau/2}{(1+\tanh\tau/2)^2}\right),\end{aligned} \tag{49}$$

with

$$m_{1,2}=mR^2\left(\frac{A_{n_r}}{N}-\frac{N}{4mR^2}\right)\pm\frac{s}{2},\quad L_E=-\frac{1}{2}+mR^2\left(\frac{A_{n_r}}{N}+\frac{N}{4mR^2}\right), \tag{50}$$

and A_{n_r} is the expression of A given by (18) with E replaced by E_{n_r}.

In the following we treat two important cases namely, the relativistic ABC in a flat space and the nonrelativistic ABC on the pseudo-sphere. To this aim we first expand s in terms of (α/c) which is the analog of the fine structure constant in the flat space

$$s=2|l+\nu|\left[1-\frac{(\alpha/c)^2}{2|l+\nu|^2}-\frac{(\alpha/c)^4}{8|l+\nu|^4}-\cdots\right]. \tag{51}$$

Then the energy levels are rewritten as

$$\begin{aligned}E_{n_r}-\frac{\alpha}{R}=\pm mc^2\Bigg\{&1-\frac{1}{2}\left(\frac{\alpha}{c}\right)^2\left[\frac{\tilde{N}^2-1/4}{m^2\alpha^2R^2}+\frac{1}{\tilde{N}^2}\right]-\frac{1}{2}\left(\frac{\alpha}{c}\right)^4\Bigg[\left(\frac{\tilde{N}^2-1/4}{2m^2\alpha^2R^2}\right)^2\\&+\frac{\tilde{N}^2-1/4}{2m^2\alpha^2R^2\tilde{N}^2}+\frac{3}{4\tilde{N}^4}+\frac{1}{\tilde{N}^3|l+\nu|}+\frac{1}{m^2\alpha^2R^2}\frac{n_r+1/2}{|l+\nu|}\Bigg]-\cdots\Bigg\},\end{aligned} \tag{52}$$

where

$$\tilde{N}=|l+\nu|+n_r+\tfrac{1}{2}. \tag{53}$$

A. Nonrelativistic limit

In the nonrelativistic limit $c\to\infty$, expression (52) reduces to the energy spectrum for the nonrelativistic ABC system on $\Lambda^{(2)4}$

$$E_{n_r}=\frac{\alpha}{R}-\frac{\tilde{N}^2-1/4}{2mR^2}-\frac{m\alpha^2}{2\tilde{N}^2}. \tag{54}$$

The corresponding wave function is easily obtained from (49) by making use of the following relations:

$$m_{1,2}=-\frac{m\alpha R^2}{2\tilde{N}}\left(\frac{\tilde{N}^2-1/4}{2mR^2}-\frac{m\alpha^2}{2\tilde{N}^2}\right)-\frac{\tilde{N}}{2}\pm 2|l+\nu|, \tag{55}$$

$$L_E=-\frac{1}{2}-\frac{m\alpha R^2}{2\tilde{N}}\left(\frac{\tilde{N}^2-1/4}{2mR^2}-\frac{m\alpha^2}{2\tilde{N}^2}\right)+\frac{\tilde{N}}{2}. \tag{56}$$

B. Flat space limit

In the flat space limit $R\to\infty$, the energy levels reduce to

$$E_{n_r}=\pm mc^2\left\{1-\frac{1}{2}\frac{(\alpha/c)^2}{\tilde{N}^2}-\frac{1}{2}\frac{(\alpha/c)^4}{\tilde{N}^3}\left[\frac{1}{\tilde{N}-n_r-1/2}-\frac{3}{4\tilde{N}}\right]+\cdots\right\}. \tag{57}$$

For the wave function, it is easy to show that

$$\lim_{R\to\infty}\frac{16m^2R^4A^2/N^2-N^2}{2mR^2N}=\left(\frac{8\alpha^2E^2}{N^3c^4}\right). \tag{58}$$

Using the radial variable $r=R\tau$ in Euclidean spaces, we obtain for $R\to\infty$

$$(1-\tanh\tau/2)^{m_1+m_2+1/2}(1+\tanh\tau/2)^{-2m_1-1/2}(\tanh\tau/2)^{(m_1-m_2)/2}\to\left(\frac{r}{2R}\right)^{s/2}e^{-2\alpha E/Nc^2 r}. \tag{59}$$

Now using the following relation[19] valid for $|z|\to\infty$:

$$\frac{\Gamma(z+a)}{\Gamma(z)}\to z^a, \tag{60}$$

we show that

$$\frac{\Gamma(L_E+m_1+1)\Gamma(L_E-m_2+1)}{\Gamma(L_E-m_1+1)\Gamma(L_E+m_2+1)}\to\frac{\Gamma(n_r+s+1)}{\Gamma(n_r+1)}\left(\frac{2\alpha Er}{(2n_r+s+1)c^2}\right)^s. \tag{61}$$

On the other hand we have

$$\lim_{R\to\infty}{}_2F_1\left(-L_E+m_1,L_E+m_1+1,m_1-m_2+1;\frac{4\tanh\tau/2}{(1+\tanh\tau/2)^2}\right)={}_1F_1\left(-n_r,s+1;\frac{4\alpha E}{Nc^2}r\right). \tag{62}$$

Collecting all the terms leads to

$$\Psi_{n_r}(r)=\frac{1}{\sqrt{r}}\frac{1}{\Gamma(1+s)}\sqrt{\frac{\Gamma(n_r+s+1)}{\Gamma(n_r+1)}}\frac{2}{2n_r+s+1}\frac{1}{\tilde{a}_H^{1/2}}\left(\frac{4r}{(2n_r+s+1)\tilde{a}_H}\right)^{(s+1)/2}$$
$$\times e^{-2r/(2n_r+s+1)\tilde{a}_H}{}_1F_1\left(-n_r,s+1;\frac{4\alpha E}{(2n_r+s+1)c^2}r\right), \tag{63}$$

where $\tilde{a}_H=a_H(mc^2/E)$ and a_H is Bohr radius. Expressions (57) and (63) are exactly the ones obtained recently in Ref. 5.

V. SCATTERING STATES

We begin by considering the reduced Green's function defined in Eq. (38)

$$g_{l+\nu}(\tau_b,\tau_a;E)=-im\Gamma(m_1-L_E)\Gamma(L_E-m_1+1)d^{L_E}_{m_1,-m_2}(\theta_b-\pi)d^{L_E*}_{m_1,m_2}(\theta_a). \tag{64}$$

This can be rewritten in the following integral form:[20]

$$g_{l+\nu}(\tau_b,\tau_a;E)=\frac{m}{2\pi}\oint_C\frac{dE}{E^2-E_k^2}(2E)\Gamma(m_1-L_E)\Gamma(L_E-m_1+1)\times d^{L_E}_{m_1,-m_2}(\theta_b-\pi)d^{L_E*}_{m_1,m_2}(\theta_a), \tag{65}$$

where the contour C is a semicircle in the upper half plane.

Using the spectral decomposition of the Manning–Rosen propagator,[12] we easily get the continuous spectrum for a relativistic particle moving on the pseudo-sphere $\Lambda^{(2)}$

$$E_k^2=m^2c^4+\frac{c^2}{R^2}\left(k^2+\frac{1}{4}\right). \tag{66}$$

In comparison with the flat space continuous spectrum we have the correspondence

$$k_f^2\rightarrow(k^2+\tfrac{1}{4})/R^2. \tag{67}$$

In the following we restrict ourself to positives energies and write (65) as

$$g_{l+\nu}(\tau_b,\tau_a;E)=\frac{1}{2\pi R^2}\oint_C kdk\left(\frac{E}{mc^2}\right)^2\frac{2mc^2}{E^2-E_k^2}\times\frac{\Gamma(m_1-L_E)\Gamma(L_E-m_1+1)}{[1+(1/mcR)^2(k^2+1/4)]}d^{L_E}_{m_1,-m_2}(\theta_b-\pi)d^{L_E*}_{m_1,m_2}(\theta_a). \tag{68}$$

It is easy to show that

$$m_1=\frac{s}{2}+\frac{ik}{2},\quad m_2=-\frac{s}{2}+\frac{ik}{2},\quad L_E=\frac{\gamma-1}{2}, \tag{69}$$

where we have set $\gamma=\sqrt{2mR^2(A-C)}$. Taking into account the asymptotic behavior of the Wigner's functions, we write (68) in the form

$$g_{l+\nu}(\tau_b,\tau_a;E)=-\frac{1}{2\pi R^2}\int_{-\infty}^{\infty}kdk\left(\frac{E}{mc^2}\right)^2\frac{2mc^2}{E^2-E_k^2}\times\frac{\Gamma((1+s-\gamma+ik)/2)\Gamma((1-s+\gamma-ik)/2)}{[1+(1/mcR)^2(k^2+1/4)]}\times d^{(\gamma-1)/2}_{m_1,-m_2}(\theta_b-\pi)d^{(\gamma-1)/2*}_{m_1,m_2}(\theta_a). \tag{70}$$

Thanks to the following properties:[18]

$$d^{-L-1}_{m_1,m_2}(\theta)=d^{L}_{m_1,m_2}(\theta),\quad d^{L}_{-m_2,-m_1}(\theta)=(-1)^{2(m_2-m_1)}d^{L}_{m_1,m_2}(\theta), \tag{71}$$

we show that (71) becomes

$$g_{l+\nu}(\tau_b,\tau_a;E)=\frac{(-1)^{(s-1)/2}}{2\pi R^2}\int_0^\infty kdk\left(\frac{E}{mc^2}\right)^2\frac{2mc^2}{E^2-E_k^2}\frac{e^{i\pi\gamma/2}}{[1+(1/mcR)^2(k^2+1/4)]}$$
$$\times\{e^{\pi k/2}\Gamma((1+s-\gamma+ik)/2)\Gamma((1-s+\gamma-ik)/2)$$
$$-e^{-\pi k/2}\Gamma((1+s-\gamma-ik)/2)\Gamma((1-s+\gamma+ik)/2)\}$$
$$\times d^{(\gamma-1)/2}_{m_1,m_2}(\theta_b)d^{(\gamma-1)/2*}_{m_1,m_2}(\theta_a). \tag{72}$$

Now using the following identity which is a consequence of Gauss's transformation formula:[19]

$$e^{i\pi a/2}\frac{\Gamma(b-a)\Gamma(a-b+1)}{\Gamma(b)\Gamma(1-b)}+e^{i\pi b/2}\frac{\Gamma(a-b)\Gamma(b-a+1)}{\Gamma(a)\Gamma(1-a)}=1, \tag{73}$$

we get

$$g_{l+\nu}(\tau_b,\tau_a;E)=\frac{i}{2\pi R^2}\int_0^\infty kdk\frac{2mc^2}{E^2-E_k^2}\left(\frac{E}{mc^2}\right)^2\frac{1}{[1+(1/mcR)^2(k^2+1/4)]}$$
$$\times\frac{\Gamma((1+s-\gamma+ik)/2)\Gamma((1-s+\gamma-ik)/2)(k\to-k)}{|\Gamma(ik)|^2}$$
$$\times d^{(\gamma-1)/2}_{m_1,m_2}(\theta_b)d^{(\gamma-1)/2*}_{m_1,m_2}(\theta_a). \tag{74}$$

Finally the continuous part of the radial Green's function is given by

$$G_{l+\nu}(\tau_b,\tau_a;E)=\frac{1}{2mc}\int_0^\infty\frac{dk}{R}\frac{2imc^2}{E^2-E_k^2}\left(\frac{E}{mc^2}\right)^2\Psi_k(\tau_b)\Psi_k^*(\tau_a), \tag{75}$$

where the normalized continuous wave functions are

$$\Psi_k(\tau)=\sqrt{\frac{1}{\pi R}}\frac{2^s}{\sqrt{1+(k^2+1/4)/(mcR)^2}}$$
$$\times\frac{[\Gamma((1+s-\gamma+ik)/2)\Gamma((1+s+\gamma+ik)/2)(k\to-k)]^{1/2}}{|\Gamma(ik)|\Gamma(1+s)}$$
$$\times(1-\tanh\tau/2)^{ik+1/2}(1+\tanh\tau/2)^{-ik-s-1/2}(\tanh\tau/2)^{s/2}$$
$$\times{}_2F_1\left((1+s-\gamma+ik)/2,(1+s+\gamma+ik)/2,1+s;4\frac{\tanh\frac{\tau}{2}}{\left(1+\tanh\frac{\tau}{2}\right)^2}\right). \tag{76}$$

We go now to the flat space limit $R\to\infty$. To this aim we use the correspondence (67) between k on the pseudo-sphere and k_f on the flat space.

Owing to the following relations valid for $R\to\infty$

$$\gamma\to-\frac{2i\alpha}{c^2k_f}E_{k_f}, \tag{77}$$

$$\frac{[\Gamma((1+s-\gamma+ik)/2)\Gamma((1+s+\gamma+ik)/2)(k\to-k)]^{1/2}}{|\Gamma(ik)|\Gamma(1+s)}$$
$$\to|\Gamma((s+1)/2+i\alpha E_{k_f}/c^2k_f)|(Rk_f)^{(s+1)/2}, \tag{78}$$

$$(1-\tanh\tau/2)^{ik+1/2}(1+\tanh\tau/2)^{-ik-s-1/2}(\tanh\tau/2)^{s/2}\rightarrow\left(\frac{r}{2R}\right)^{s/2}e^{-ik_f r}, \tag{79}$$

and

$$ {}_2F_1\left((1+s-\gamma+ik)/2,(1+s+\gamma+ik)/2,1+s;4\,\frac{\tanh\frac{\tau}{2}}{\left(1+\tanh\frac{\tau}{2}\right)^2}\right)$$
$$\rightarrow {}_1F_1((1+s)/2+i\alpha E_{k_f}/c^2k_f,1+s;2ik_f r), \tag{80}$$

we obtain the following representation of the Green's function for the relativistic spinless ABC system in a flat space:

$$G_{l+\nu}(r_b,r_a;E)=\frac{1}{2mc}\int_0^\infty dk_f\,\frac{2imc^2}{E^2-E_{k_f}^2}\left(\frac{E}{mc^2}\right)^2\Psi_{k_f}(r_b)\Psi_{k_f}^*(r_a), \tag{81}$$

where the continuous wave function $\Psi_{k_f}(r)$ is given by[21]

$$\Psi_{k_f}(r)=\frac{1}{\sqrt{2\pi r}}\,\frac{1}{\sqrt{1+(k_f/mc)^2}}\,\frac{|\Gamma((s+1)/2+i\alpha E_{k_f}/c^2k_f)|}{\Gamma(1+s)}$$
$$\times e^{\pi\alpha E_{k_f}/2c^2k_f}(2k_f r)^{(1+s)/2}e^{-ik_f r}\,{}_1F_1((1+s)/2+i\alpha E_{k_f}/c^2k_f,1+s;2ik_f r). \tag{82}$$

The correctness of this expression is assured by the presence of the factor $e^{-\pi\alpha E_{k_f}/2c^2k_f}$, which is essential for the particle density at $r=0$. However this factor has been missing in path integral treatments based on the SU(1, 1) group manifold.[3,22]

VI. CONCLUSION

In this paper we have explicitly evaluated the Green's function for the relativistic spinless Aharonov–Bohm–Coulomb system on the pseudo-sphere $\Lambda^{(2)}$ using Kleinert's path integral representation for the motion of relativistic spinless particles in $(D+1)$-dimensional Minkowski space. We have obtained the energy spectrum and the corresponding wave-functions for bound states. The scattering states are deduced from the integral representation of the Green's function. In the nonrelativistic limit and the flat space limit our results are in agreement with those of the literature. We hope that the results presented in this paper may be useful to investigate other features, like the interference pattern, of the Aharonov–Bohm–Coulomb system on the pseudo-sphere $\Lambda^{(2)}$.

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Alternative $SU(N)$ Skyrme models and their solutions

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We consider alternative $SU(N)$ Skyrme models in 3 spatial dimensions. We show that when $N=2$ they reduce to the usual $SU(2)$ Skyrme model but for $N\geqslant 3$ they are different. We show that the harmonic map ansatz previously applied to the usual Skyrme models can also be applied to these models giving spherically symmetric solutions (when the number of projectors is $N-1$) and low energy field approximants when the number of projectors is lower. We compare our results with the results for the usual Skyrme models. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1346596]

I. INTRODUCTION

The usual Skyrme model was originally proposed by Skyrme,[1] and recently, since Witten's demonstration that it arises in the large N_c limit[2] of QCD, it has been used to study various properties of low energy mesons and baryons.[3]

While the basic fields of the model describe mesons the topologically nontrivial solutions of the model, known as skyrmions, are identified with classical ground states of light nuclei. Although the preliminary results of the investigations of the implications of this idea are very encouraging[4] a thorough understanding of the structure and dynamics of multi-skyrmion configurations is required before a more qualitative assessment of the validity of this application can be made.

The $SU(N)$ Skyrme models, usual or alternative, involves fields which take value in $SU(N)$; i.e., are described by $SU(N)$ valued functions of $\vec{x}$ and t. The two classes of models differ only in the form of their Lagrangians and so in their equations of motion.

Multi-skyrmions are stationary points (either minima or saddle points) of the static energy functional, which, for the usual Skyrme models, is given by

$$E=\frac{1}{12\pi^2}\int_{R^3}\left\{-\frac{1}{2}\mathrm{Tr}(\partial_i U\,U^{-1})^2-\frac{1}{16}\mathrm{Tr}[\partial_i U\,U^{-1},\ \partial_j U\,U^{-1}]^2\right\}d^3\vec{x}, \tag{1}$$

where $U(\vec{x})\in SU(N)$.

The equations for multi-skyrmions, in the usual Skyrme model, are therefore

$$\partial_i(\partial_i U\,U^{-1}-\tfrac{1}{4}[\partial_j U\,U^{-1},[\partial_j U\,U^{-1},\partial_i U\,U^{-1}]])=0. \tag{2}$$

In these expressions we have, for simplicity, set the mass terms to zero. This has been done for convenience, as the conventional mass terms introduce only small changes.

Finiteness of the energy functional, for the usual Skyrme models and for the, soon to be introduced, alternative Skyrme models, requires that $U(\vec{x})$ approaches a constant matrix at spatial infinity, which can be reduced to the identity matrix by a global chiral transformation. So, without any loss of generality, one normally imposes the following boundary conditions on U: $U\to I$ as $|\vec{x}|\to\infty$.

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Since $U \to I$ as $|\vec{x}| \to \infty$ is a mapping from $S^3 \to SU(N)$, it can be classified by the third homotopy group $\pi_3(SU(N)) \equiv Z$ or, equivalently, by the integer valued winding number

$$B = \frac{1}{24\pi^2} \int_{R^3} \varepsilon_{ijk} \, \mathrm{Tr}(\partial_i U \, U^{-1} \partial_j U \, U^{-1} \partial_k U \, U^{-1}) d^3\vec{x}, \tag{3}$$

which is a topological invariant which classifies the solitonic sectors in the model. And following the idea of Skyrme[1] and Witten,[2] B is to be identified with the baryon number of the field configuration.

Until very recently most of the studies involving the Skyrme model have concentrated on the $SU(2)$ version of the model and its embeddings into $SU(N)$. However, when one considers $SU(N)$, for $N \geqslant 3$, one has to bear in mind that the Skyrme model is not unique. In fact, there are two possible versions of the fourth-order Skyrme term[5] and so in this paper we initiate the study of the model based on the alternative form of the fourth-order Skyrme term.

Thus instead of looking at

$$-\tfrac{1}{16} \mathrm{Tr}[\partial_i U \, U^{-1}, \ \partial_j U \, U^{-1}]^2 \tag{4}$$

in (1) we consider

$$\tfrac{1}{8} (\mathrm{Tr}(\partial_i U \, U^{-1} \, \partial_i U \, U^{-1}))^2 - \tfrac{1}{8} (\mathrm{Tr}(\partial_i U \, U^{-1} \, \partial_j U \, U^{-1}))^2. \tag{5}$$

Note that when $N=2$ the two expressions are the same. To see this we introduce

$$R_i = U^{-1} \, \partial_i U = i R_i^k \sigma^k, \tag{6}$$

where σ^k, $k=1,2,3$, are Pauli matrices. Then, using the properties of Pauli matrices, we find that

$$\mathrm{Tr}(\partial_i U \, U^{-1} \, \partial_j U \, U^{-1}) = -2(R_i^k R_j^k), \tag{7}$$

and so

$$\begin{aligned} -\tfrac{1}{16} \mathrm{Tr}[\partial_i U \, U^{-1}, \ \partial_j U \, U^{-1}]^2 &= \tfrac{1}{2}[(R_i^k R_i^k)^2 - R_i^k R_j^k R_i^l R_j^l] \\ &= \tfrac{1}{8} (\mathrm{Tr}(\partial_i U \, U^{-1} \, \partial_i U \, U^{-1}))^2 \\ &\quad - \tfrac{1}{8} (\mathrm{Tr}(\partial_i U \, U^{-1} \, \partial_j U \, U^{-1}))^2. \end{aligned} \tag{8}$$

However, for $N>2$ the two expressions are different.

Until very recently very little attention has been paid to field configurations describing many skyrmions in $SU(N)$ models which were not embeddings of $SU(2)$ skyrmions. Although some work has been done earlier[6,7] the real progress has only been made since Houghton, Manton and Sutcliffe had produced their harmonic map ansatz.[8]

This ansatz, when generalized to $SU(N)$ models,[9] has lead to the construction of whole families of solutions of $SU(N)$ Skyrme models—with spherically symmetric energy densities.[10] Moreover, it also presents field configurations, which though not solutions of the equations, are close to them—thus providing us with good approximants to other solutions.[9]

In this paper we apply the same ideas to the alternative Skyrme models. We find that, although the actual values of energies etc., and the properties of the field configurations, are different, the situation is qualitatively the same as in the usual Skyrme models; the harmonic map ansatz produces good approximants and the appropriate multiprojector fields provide solutions of the full equations (the only difference lies in the profile functions).

In the next section, for completeness, we discuss the harmonic maps ansatz and its generalization to $SU(N)$ fields. In the following section we present the discussion of the one projector

approximants. In it we study the $SU(N)$ fields with $N=3,4$ and 5, and compare the values of energies of such fields in the usual and the alternative Skyrme models. This is followed by sections on the spherically symmetric solutions of the alternative Skyrme models and a discussion of some of their properties.

II. HARMONIC MAPS

In Ref. 9 the $SU(2)$ ansatz of Houghton *et al.*[8] was generalized to the usual $SU(N)$ Skyrme models. This generalization involved rewriting the expression of Houghton *et al.* as a projector from S^2 to CP^{N-1}. It not only gave a new way of interpreting old results but also a new way of deriving expressions for low energy $SU(N)$ field configurations which are **not** simple embeddings of $SU(2)$ fields. In particular, the energy distributions of the field configurations given in Ref. 9 exhibited symmetries very different from those of the embeddings.

The method of Ref. 9 was then generalized further in Ref. 10, to involve more projectors. This generalization exploited some ideas from the theory of harmonic maps of $S^2\to CP^{N-1}$ and $S^2\to U(N)$.[11] Here, for completeness, we follow Ref. 10 and recall some properties of harmonic maps $S^2\to CP^{N-1}$.

We recall[12] that an N dimensional space possesses a ''natural'' set of mutually orthogonal projectors constructed from $S^2\to CP^{N-1}$ maps. To construct them we proceed as follows.

First we write each projector P as

$$P(V)=\frac{V\otimes V^\dagger}{|V|^2}, \tag{9}$$

where V is an N-component complex vector dependent on ξ and its complex conjugate $\bar{\xi}$. These are related to the more familiar θ and φ, which locally parametrize S^2, via $\xi=\tan(\theta/2)\,e^{i\varphi}$.

Then for the first projector we take $V=f(\xi)$, i.e., an analytic vector of ξ. Its components are chosen to be polynomials in ξ. Next we construct further vectors V^α, $\alpha=1,2,\ldots,$ by

$$V^\alpha=\frac{\partial^\alpha}{\partial\xi^\alpha}V, \tag{10}$$

and Gram Schmidt orthogonalize the whole sequence.

It is then easy to check[12] that the kth vector, $k=0,1,\ldots,$ in the resultant sequence of vectors, can be written as $P_+^k f$ and considered as having come from a sequence of k successive application to f of the operator P_+ defined by its action on any vector $v\in \mathrm{C}^N$ as

$$P_+ v=\partial_\xi v-\frac{v\,(v^\dagger\,\partial_\xi v)}{|v|^2}, \tag{11}$$

i.e., $P_+^k v=P_+(P_+^{k-1}v)$.

Then as further projectors we take projectors given by (9) with V given by $P_+^k f$. This way we end up with

$$P_0=P(f),\quad P_1=P(P_+f),\quad P_2=P(P_+^2 f),\quad \ldots,\quad P_k=P(P_+^k f), \tag{12}$$

and note, that due to the orthogonality of P_i, $\Sigma_{k=0}^{N-1}P_k=1$.

The orthogonality properties of our projectors follow from their construction and translate into the following properties of $P_+^k f$ when f is holomorphic:

$$(P_+^k f)^\dagger\,P_+^l f=0,\quad k\neq l, \tag{13}$$

$$\partial_{\bar{\xi}}(P_+^k f)=-P_+^{k-1}f\frac{|P_+^k f|^2}{|P_+^{k-1}f|^2},\quad \partial_\xi\left(\frac{P_+^{k-1}f}{|P_+^{k-1}f|^2}\right)=\frac{P_+^k f}{|P_+^{k-1}f|^2}. \tag{14}$$

It is easy to check that for $SU(N)$ the last projector P_{N-1} in this sequence corresponds to an anti-analytic vector; [i.e., up to an overall factor, which cancels in (9), the components of $V=P_+^{N-1}f$ are functions of only $\bar{\xi}$].

As $\Sigma_{k=0}^{N-1}P_k=1$ we see that for $SU(N)$ only $N-1$ projectors are independent.

The properties (13)–(14) are independent of the choice of the starting vector f. However, there are further properties of vectors $P_+^k f$ which depend on f. Namely, in Ref. 10 it was shown that if, for a given N, we choose the vector f to be given by

$$N=2, \quad f=(1,\xi)^t, \tag{15}$$

$$N=3, \quad f=(1,\sqrt{2}\,\xi,\xi^2)^t, \tag{16}$$

$$N=4, \quad f=(1,\sqrt{3}\xi,\sqrt{3}\,\xi^2,\xi^3)^t, \tag{17}$$

$$N=n, \quad f=(f_0,f_1,\ldots,f_{n-1})^t: \quad f_k=\xi^k\sqrt{C_k^{n-1}}, \tag{18}$$

where C_k^{n-1} denotes the binomial coefficients, then not only $|f|^2$ is a power of $(1+|\xi|^2)$ but so are also all $|P_+^k f|^2$, for $k=1,2,\ldots,N-1$. In fact, in Ref. 10 it was shown that

$$|P_+^k f|^2=k!(N-1)(N-2)\cdots(N-k)(1+|\xi|^2)^{N-2k-1}.$$

The reason for choosing vectors of the form (18) is that they correspond to spherically symmetric configurations.

Let us note that in the mathematical literature our sequence of vectors $P_+^k f$, $k=0,1,\ldots,$ is called the Veronese sequence.[13] In Refs. 9 and 10 it was then shown that for the usual $SU(N)$ Skyrme models it is convenient to take our sequence of projectors (12) and so to consider U of the form

$$\begin{aligned} U&=\exp\left[-ig_0\left(\frac{I}{N}-P_0\right)-ig_1\left(\frac{I}{N}-P_1\right)-\ldots-ig_{N-2}\left(\frac{I}{N}-P_{N-2}\right)\right] \\ &=e^{-ig_0/N}(I+A_0P_0)\,e^{-ig_1/N}(I+A_1P_1)\ldots e^{-ig_{N-2}/N}(I+A_{N-1}P_{N-2}), \end{aligned} \tag{19}$$

where $g_k=g_k(r)$, for $k=0,\ldots,N-2$, are the profile functions and $A_k=e^{ig_k}-1$. The profile functions $g_k(r)$ are required to satisfy the boundary conditions $g_k(\infty)=0$ and $g_k(0)=2\alpha\pi$, where $\alpha=0$ or ±1. The vector V in the projector P_i is given by $V=P_+^i f$, and so depends only on θ,φ, and r is the usual radial variable. Then, as shown in Ref. 10, the full equations for the field U are automatically satisfied if the appropriate equations (just ordinary differential equations) for the profile functions $g_k(r)$ are satified.

If we take a smaller number of projectors (i.e., fewer than $N-1$) and/or take different initial vectors f, the resultant field does not solve the full equations but may provide a good approximation to such a solution. Good, in the sense that the energy (and even the energy density) of the configuration (for a ''good'' choice of the vector f) is very close to an exact solution (which had to be found numerically); this was checked for different vectors f for the $SU(2)$ model where the numerical solutions are known. The same is expected to be the case for other $SU(N)$ models.

In the next sections we show that the same is true for the alternative Skyrme models.

III. SOME APPROXIMATE SOLUTIONS OF THE ALTERNATIVE $SU(N)$ SKYRME MODELS

In this section we look at the 1 projector approximants to the minimal field configuration of the alternative Skyrme models and compare them with the similar approximations to the solutions of the usual Skyrme models.

To do this we note, using the definition

$$R_i = U^{-1}\,\partial_i U, \tag{20}$$

where $i=x,y,z$, that the alternative Skyrme term is proportional to

$$K(x,y) = \mathrm{Tr}\,R_x^2\,\mathrm{Tr}\,R_y^2 - (\mathrm{Tr}\,R_x R_y)^2, \tag{21}$$

plus $K(x,z)+K(z,y)$—i.e., the corresponding (xz) and (zy) contributions. The usual related Skyrme term is

$$M(x,y) = \mathrm{Tr}\,(R_x R_x R_y R_y - R_x R_y R_x R_y), \tag{22}$$

plus the corresponding $M(y,z)$ and $M(z,x)$ contributions.

Next we change variables $(x,y,z)\to(r,\xi,\bar{\xi})$, as discussed in the previous section; i.e., r is the radial variable ($r=\sqrt{x^2+y^2+z^2}$) and ξ and $\bar{\xi}$ are related to the spherical angles (θ,φ).

If we now use our harmonic map ansatz [taking only the first projector in (19) and putting $g_0=2g$],

$$U = e^{-2ig/N}\,(1+(e^{2ig}-1)P), \tag{23}$$

we find that

$$R_x = -\frac{2ig_x}{N}1 + 2ig_x P + HP_\xi\frac{1-\xi^2}{2r} - \bar{H}P_{\bar{\xi}}\frac{1-\bar{\xi}^2}{2r}, \tag{24}$$

$$R_y = -\frac{2ig_y}{N}1 + 2ig_y P + HP_\xi\frac{i(1+\xi^2)}{2r} + \bar{H}P_{\bar{\xi}}\frac{i(1+\bar{\xi}^2)}{2r}, \tag{25}$$

and

$$R_z = -\frac{2ig_z}{N}1 + 2ig_z P - HP_\xi\frac{\xi}{r} + \bar{H}P_{\bar{\xi}}\frac{\bar{\xi}}{r}, \tag{26}$$

where $H=e^{2ig}-1$.

Moreover, as $V=f$ is a function of only ξ,

$$P = \frac{ff^\dagger}{|f|^2}, \quad P_\xi = \frac{P_+ ff^\dagger}{|f|^2}, \quad P_{\bar{\xi}} = \frac{f(P_+ f)^\dagger}{|f|^2}. \tag{27}$$

Next we calculate various terms in the energy. We look at various products of R_i and take appropriate traces. Then using the orthogonality properties of vectors f and $P_+ f$ and

$$\mathrm{Tr}\,P = 1, \quad \mathrm{Tr}\,1 = N, \quad \mathrm{Tr}P_\xi P_{\bar{\xi}} = \frac{|P_+ f|^2}{|f|^2} = \mathcal{B}, \tag{28}$$

$$\mathrm{Tr}\,P_\xi P_{\bar{\xi}} P_\xi P_{\bar{\xi}} = \frac{|P_+ f|^4}{|f|^4} = \mathcal{B}^2, \tag{29}$$

we find, for the usual Skyrme model [for the (x,y) contribution],

$$M(x,y) = \mathcal{B}^2(\gamma_x\delta_y - \delta_x\gamma_y) - \mathcal{B}(\gamma_x\beta_y - \beta_x\gamma_y)(\delta_x\beta_y - \beta_x\delta_y), \tag{30}$$

while for the alternative Skyrme term the $\mathcal{B}^2$ term is the same and the $\mathcal{B}$ term is altered to

$$\mathcal{B}\to\mathcal{B}^{\frac{2(N-1)}{N}}=\mathcal{B}A_N, \tag{31}$$

where

$$A_N=\frac{2(N-1)}{N}. \tag{32}$$

In the expression above β_i, γ_i and δ_i are the coefficients of P, $P_{\bar{\xi}}$ and P_ξ, respectively, in the expansion of R_i (24)–(26).

Adding all the contributions, and the contribution of the usual (σ model) terms we find that while the energy of the usual Skyrme model is given by

$$E_u=\frac{1}{3\pi}\int dr\left(A_N g_r^2 r^2+2\mathcal{N}\sin^2 g\,(1+g_r^2)+\mathcal{I}\frac{\sin^4 g}{r^2}\right), \tag{33}$$

its value in the alternative model is given by

$$E_a=\frac{1}{3\pi}\int dr\left(A_N g_r^2 r^2+2\mathcal{N}\sin^2 g\,(1+A_N g_r^2)+\mathcal{I}\frac{\sin^4 g}{r^2}\right), \tag{34}$$

where

$$\mathcal{N}=\frac{i}{2\pi}\int d\xi\, d\bar{\xi}\,\mathrm{tr}(|\partial_\xi P|^2), \tag{35}$$

$$\mathcal{I}=\frac{i}{4\pi}\int d\xi\, d\bar{\xi}\,(1+|\xi|^2)^2\,\mathrm{tr}([\partial_\xi P,\partial_{\bar{\xi}}P])^2. \tag{36}$$

Note that $\mathcal{N}$ is the expression for the energy of the 2-dimensional $CP^{(N-1)}$ sigma model, so $\mathcal{N}$ is given by the degree of f. It should be noted that Eq. (34) implies that the same projector minimizes the energy in both the usual and alternative Skyrme models within this ansatz.

Note also that for $N=2$ both expressions agree, as they should.

Which energy E_u or E_a is larger for the same projector? Clearly, as all the terms in E_u and E_a are positive, $E_a>E_u$. This is true even though both expressions (33) and (34) have to be extremized first for the shape of the profile function $g(r)$ [subject to the conditions: $g(0)=\pi$, $g(\infty)=0$]; i.e., we have to solve the resultant equation for g and then calculate the value of E_u or E_a.

However, note that the profile function $g(r)$, corresponding to E_a, when put into the expression for E_u will give a lower value; taking $g(r)$ which extremizes E_u can only lower this value further.

So we conclude that the energies of the harmonic field approximants are higher in the alternative models than in the usual Skyrme models. How much higher? To assess this we took maps of the form (18) (with n replaced by $n+1$) for which $N=n+1$ and one can compute that $\mathcal{N}=n$ and $\mathcal{I}=n^2$. We have calculated the corresponding energies for a few special cases with $n=2$, 3 and 4, and we have found that for $n=2$ $E_u=2.44404$, $E_a=2.70614$ while for $n=3$ and $n=4$ the corresponding numbers are $E_u=3.64410$, $E_a=4.18918$ and $E_u=4.83792$, $E_a=5.66929$, respectively. We see that the difference (and even the relative difference) grows with n. These numerical values were obtained both by the shooting method and by the finite difference scheme with 48,000 grid points and lattice spacing $\delta r=10^{-3}$.

IV. SPHERICALLY SYMMETRIC SOLUTIONS—GENERAL DISCUSSION

Next we show that, like for the usual Skyrme models, our ansatz (19) gives us also many exact solutions of the alternative Skyrme models. In fact, we will show that for each $SU(N)$ model our ansatz involving $N-1$ projectors leads to exact solutions involving $N-1$ profile functions.

To show this, like for the usual Skyrme models,[10] we first rewrite our equations for U, which for the alternative models are given by

$$\partial_i[\partial_i U\, U^{-1} - \tfrac{1}{2}(\mathrm{Tr}(\partial_j U\, U^{-1})^2)\partial_i U\, U^{-1} + \tfrac{1}{2}(\mathrm{Tr}(\partial_i U\, U^{-1}\, \partial_j U\, U^{-1}))\partial_j U U^{-1}] = 0, \quad (37)$$

in spherical polar coordinates (r,θ,φ).

We then use R_i given by the definition (20) and find that these equations take the form

$$\partial_r\left[r^2\left(R_r - \frac{1}{2}(A_r - B_r)\right)\right] + \frac{1}{\sin\theta}\partial_\theta\left[\sin\theta\left(R_\theta - \frac{1}{2}(A_\theta - B_\theta)\right)\right] + \frac{1}{\sin^2\theta}\partial_\varphi\left[R_\varphi - \frac{1}{2}(A_\varphi - B_\varphi)\right] = 0, \quad (38)$$

where

$$A_d = \left[\mathrm{Tr}\, R_r^2 + \frac{1}{r^2}\left(\mathrm{Tr}\, R_\theta^2 + \frac{1}{\sin^2\theta}\mathrm{Tr}\, R_\varphi^2\right)\right]R_d, \quad (39)$$

$$B_d = \mathrm{Tr}(R_d R_r)R_r + \frac{1}{r^2}\left[\mathrm{Tr}(R_d R_\theta)R_\theta + \frac{1}{\sin^2\theta}\mathrm{Tr}(R_d R_\varphi)R_\varphi\right], \quad (40)$$

and $d = r,\theta,\varphi$. Next we note that with U given by the ansatz (19),

$$R_r = -i\sum_{k=0}^{N-2}\dot{g}_k\left(\frac{1}{N} - P_k\right), \quad (41)$$

where $\dot{g}_k = dg_k/dr$. To proceed further we introduce the holomorphic variables ξ and $\bar{\xi}$ and find that

$$R_\xi = \exp\left(-i\sum_{k=0}^{N-2} g_k P_k\right)\left[\exp\left(i\sum_{l=0}^{N-2} g_l P_l\right)\right]_\xi .$$

Using the orthogonality properties of the projectors we rewrite this as

$$R_\xi = \left[1 + \sum_{k=0}^{N-2}(e^{-ig_k} - 1)P_k\right]\left[\sum_{l=0}^{N-2}(e^{ig_l} - 1)P_{l\xi}\right] = \sum_{k=1}^{N-1}[e^{-i(g_k - g_{k-1})} - 1]\frac{V_k V_{k-1}^\dagger}{|V_{k-1}|^2}, \quad (42)$$

where $V_k = P_+^k f$ and where $g_{N-1} = 0$. Moreover, $R_{\bar{\xi}} = -(R_\xi)^\dagger$. Next we note that

$$\partial_\theta = \frac{(1+|\xi|^2)}{2|\xi|}(\xi\partial_\xi + \bar{\xi}\partial_{\bar{\xi}}), \quad (43)$$

$$\partial_\varphi = i(\xi\partial_\xi - \bar{\xi}\partial_{\bar{\xi}}), \quad (44)$$

which allows us to rewrite all the terms in (39) and (40) in terms of R_ξ, $R_{\bar{\xi}}$ and R_r giving

$$r^2(A_r-B_r)=\frac{(1+|\xi|^2)^2}{2}[2\,\mathrm{Tr}(R_\xi R_{\bar\xi})R_r-\mathrm{Tr}(R_rR_\xi)R_{\bar\xi}-\mathrm{Tr}(R_rR_{\bar\xi})R_\xi], \tag{45}$$

and

$$\begin{aligned}&\sin\theta(A_\theta-B_\theta)+i(A_\varphi-B_\varphi)\\&\quad=2\bar\xi\left[(\mathrm{Tr}\,R_r^2)R_{\bar\xi}-\mathrm{Tr}(R_{\bar\xi}R_r)R_r-\frac{(1+|\xi|^2)^2}{2r^2}\{\mathrm{Tr}(R_\xi^2)R_\xi-\mathrm{Tr}(R_\xi R_{\bar\xi})R_{\bar\xi}\}\right].\end{aligned} \tag{46}$$

Reexpressing all the derivatives involving ∂_θ and ∂_φ in terms of ∂_ξ and $\partial_{\bar\xi}$ using (43) and (44) we find that the equations (38) become

$$\begin{aligned}&\partial_r(r^2R_r)+\frac{(1+|\xi|^2)^2}{2}(\partial_\xi R_{\bar\xi}+\partial_{\bar\xi}R_\xi)-\frac{(1+|\xi|^2)^2}{4}\partial_r[\{\mathrm{Tr}(R_\xi R_{\bar\xi})R_r-\mathrm{Tr}(R_rR_\xi)R_{\bar\xi}\}+(\xi\leftrightarrow\bar\xi)]\\&\quad-\frac{(1+|\xi|^2)^2}{4}[\partial_\xi\{\mathrm{Tr}(R_r^2)R_{\bar\xi}-\mathrm{Tr}(R_{\bar\xi}R_r)R_r\}+(\xi\leftrightarrow\bar\xi)]+\frac{(1+|\xi|^2)^2}{4r^2}\\&\quad\times\left[\partial_\xi\left\{\frac{(1+|\xi|^2)^2}{2}(\mathrm{Tr}(R_\xi^2)R_\xi-\mathrm{Tr}(R_\xi R_{\bar\xi})R_\xi\right\}+(\xi\leftrightarrow\bar\xi)\right]=0.\end{aligned} \tag{47}$$

Next we calculate the traces. From the expressions for R_r as given by (41) we find that

$$\mathrm{Tr}(R_r^2)=\frac{1}{N}\left(\sum_{i=0}^{N-2}\dot g_i\right)^2-\sum_{i=0}^{N-2}\dot g_i^2\,. \tag{48}$$

On the other hand, from (42) we find that

$$\mathrm{Tr}(R_\xi R_{\bar\xi})=-2\sum_{i=1}^{N-1}(1-\cos(g_{i-1}-g_i))\frac{|V_i|^2}{|V_{i-1}|^2}. \tag{49}$$

For the other traces the orthogonality of the vectors V makes them vanish, i.e.,

$$\mathrm{Tr}(R_rR_\xi)=\mathrm{Tr}(R_\xi^2)=\mathrm{Tr}(R_{\bar\xi}^2)=0. \tag{50}$$

Using these results and the fact that $\mathrm{Tr}(R_r^2)$ is independent of $(\xi,\bar\xi)$ we see that (47) reduces to

$$\begin{aligned}&\partial_r\left[\left(r^2-\frac{1}{2}Q\right)R_r\right]+\frac{(1+|\xi|^2)^2}{2}\left[(\partial_\xi R_{\bar\xi}+\partial_{\bar\xi}R_\xi)\left\{1-\frac{1}{2}\mathrm{Tr}(R_r^2)\right\}\right.\\&\qquad\left.-\frac{1}{4r^2}\{\partial_\xi(QR_{\bar\xi})+\partial_{\bar\xi}(QR_\xi)\}\right]=0,\end{aligned} \tag{51}$$

where

$$Q=Q(r,\xi,\bar\xi)=(1+|\xi|^2)^2\,\mathrm{Tr}(R_\xi R_{\bar\xi}). \tag{52}$$

Next we note that

$$\partial_r(r^2R_r)=2rR_r+r^2R_{rr}=-i\sum_{k=0}^{N-2}\left(\frac{1}{N}-P_k\right)(2r\dot g_k+r^2\ddot g_k), \tag{53}$$

and that

$$\partial_{\xi} R_{\bar{\xi}} + \partial_{\bar{\xi}} R_{\xi} = \sum_{k=1}^{N-1} h_k \frac{|V_k|^2}{|V_{k-1}|^2} (P_k - P_{k-1}), \tag{54}$$

where h_k are only functions of g_l.

For our choice of vectors V corresponding to the map (18), we find that $|V_k|^2/|V_{k-1}|^2$ is proportional to $1/(1+|\xi|^2)^2$ and so all the dependence on ξ and $\bar{\xi}$ in (51) resides only in the projectors. The terms involving $\partial_r(r^2 R_r)$ give us expressions involving $1/N - P_k$ while all other terms give us expressions involving $P_k - P_{k-1}$. It is easy to check that all N projectors arise in our expressions but we can always reexpress P_{N-1} in terms of the previous ones so we end up with $N-1$ factors involving $P_k - 1/N$ (for $k=0,\ldots,N-2$). To satisfy our equations (51) the coefficients of such factors have to vanish. This requirement gives us $N-1$ equations for $N-1$ functions g_i. Hence, if these equations have solutions, we have solutions of the equations of the alternative $SU(N)$ Skyrme models.

To find the $N-1$ equations for g_i we can either look in detail at all our terms in (51) or put our expression into (1) with (4)→(5), integrate out ξ and $\bar{\xi}$ variables and derive the equations for the profile functions $g_i(r)$. The two methods give the same equations. In the next section we use the second one as we want to determine the energies of our solutions. The first method is described in the Appendix.

Note that, like for the usual Skyrme models, the whole procedure hinges on having $N-1$ profile functions and on the very special form of our vectors V. Had we taken other vectors f, and so V, we would have not gotten all the ξ and $\bar{\xi}$ dependence residing only in the projectors and had we taken less than $N-1$ profile functions and projectors we would have gotten too many equations for our functions. It is only in the case of $N-1$ projectors that we get the right number of equations and our equations of motion (PDE's) reduce to a system of ODE's.

V. EQUATIONS FOR THE PROFILE FUNCTIONS

To derive the equation for our profile functions g_i we rewrite our energy function [(1) with (4)→(5)] in terms of r, ξ and $\bar{\xi}$. We find

$$E = -\frac{i}{12\pi^2} \int \frac{d\xi\, d\bar{\xi}}{(1+|\xi|^2)^2} r^2\, dr \left[\mathrm{Tr}(R_r^2) + \frac{1}{r^2} Q \left(1 - \frac{1}{2} \mathrm{Tr}(R_r^2) - \frac{1}{8r^2} Q \right) \right], \tag{55}$$

where Q is given by (52).

Next, we use the fact that

$$\frac{|V_k|^2}{|V_{k-1}|^2} = \frac{k(N-k)}{(1+|\xi|^2)^2}, \tag{56}$$

and find that $\mathrm{Tr}|R_{\xi}|^2$ has a factor $1/(1+|\xi|^2)^2$ showing us that the function Q is independent of ξ and $\bar{\xi}$. Thus as

$$i \int d\xi\, d\bar{\xi} \frac{1}{(1+|\xi|^2)^2} = 2\pi, \tag{57}$$

we find that the ξ and $\bar{\xi}$ integration gives us

$$E=\frac{1}{6\pi}\int r^2 dr\left[\left(-\frac{1}{N}\left(\sum_{i=0}^{N-2}\dot{g}_i\right)^2+\sum_{i=0}^{N-2}\dot{g}_i^2\right)\left(1+\frac{1}{r^2}\sum_{k=1}^{N-1}D_k\right)\right.$$
$$\left.+\frac{2}{r^2}\sum_{i=1}^{N-1}D_i\left(1+\frac{1}{4r^2}\sum_{k=1}^{N-1}D_k\right)\right], \tag{58}$$

where $D_k=k(N-k)(1-\cos(g_{k-1}-g_k))$.

Next we observe that, apart from the first two terms above, all the dependence on the profile functions g_k comes via their combinations g_k-g_{k-1}. To exploit this observation we change variables and introduce F_k defined by

$$F_k=g_k-g_{k+1}\quad (k=0,\ldots,N-2), \tag{59}$$

where, of course, $F_{N-2}=g_{N-2}$. Next we note that

$$\frac{\partial\mathcal{E}}{\partial\dot{F}_l}=\left[-\frac{2(l+1)}{N}\sum_{i=0}^{N-2}(i+1)\dot{F}_i+2\sum_{i=0}^{l}\left(\sum_{j=i}^{N-2}\dot{F}_j\right)\right]\left[r^2+\sum_{k=1}^{N-1}D_k\right], \tag{60}$$

where $\mathcal{E}$ denotes the integrand of E and $D_k=k(N-k)(1-\cos F_{k-1})$.

We can now determine our equations for the functions F_i and so also for g_i. They are

$$\left[-\frac{l+1}{N}\sum_{i=0}^{N-2}(i+1)\ddot{F}_i+\sum_{i=0}^{l}\sum_{j=i}^{N-2}\ddot{F}_j\right]A_{N2}+\frac{2}{r}\left[-\frac{l+1}{N}\sum_{i=0}^{N-2}(i+1)\dot{F}_i+\sum_{i=0}^{l}\sum_{j=i}^{N-2}\dot{F}_j\right]A_{N1}$$
$$-\frac{1}{r^2}[(l+1)(N-l-1)\sin F_l]A_{N0}=0, \tag{61}$$

where

$$A_{N2}=1+\frac{1}{r^2}\sum_{k=1}^{N-1}D_k,$$
$$A_{N1}=1+\frac{1}{2r}\sum_{k=1}^{N-1}\dot{D}_k, \tag{62}$$
$$A_{N0}=-\frac{1}{2N}\left(\sum_{i=0}^{N-2}(i+1)\dot{F}_i\right)^2+\frac{1}{2}\sum_{i=0}^{N-2}\left(\sum_{j=i}^{N-2}\dot{F}_j\right)^2+1+\frac{1}{2r^2}\sum_{k=1}^{N-1}D_k,$$

and where $\dot{D}_k=k(N-k)\dot{F}_{k-1}\sin(F_{k-1})$.

Note that the equations (61) have to be solved numerically. To do this we have to consider each N and diagonalize the terms involving second derivatives. In the next two sections, to compare the obtained results with the results discussed in Ref. 10, we look in detail at the simplest cases of $N=3$, 4 and 5, which involve 2, 3 or 4 functions.

VI. GENERAL TOPOLOGICAL PROPERTIES AND SYMMETRIES

Let us first note that the topological properties of our solutions are controlled by the values of F_i at 0.

To see this we rewrite the topological charge B, (3) in our variables. We get

$$B=\frac{1}{8\pi^2}\int dr\,d\xi\,d\bar{\xi}\,\mathrm{Tr}(R_r[R_\xi,R_{\bar{\xi}}]). \tag{63}$$

Using the expression for R_ξ in (42), we find that the commutator $[R_\xi, R_{\bar{\xi}}]$ is given by

$$[R_\xi,\ R_{\bar{\xi}}]=2\sum_{k=1}^{N-1}(P_{k-1}-P_k)C_k, \tag{64}$$

where $C_k=(1-\cos F_{k-1})(|V_k|^2/|V_{k-1}|^2)$.

Then, using this result and R_r as given in (41) we find that, when we take the trace, the terms involving $\dot{g}_k/N$ in R_r cancel and we are left with

$$\begin{aligned} B&=-\frac{i}{4\pi^2}\int dr\,d\xi\,d\bar{\xi}\sum_{k=0}^{N-2}\dot{F}_k(1-\cos F_k)\frac{|V_{k+1}|^2}{|V_k|^2}\\ &=\frac{1}{2\pi}\int dr\sum_{k=0}^{N-2}\dot{F}_k(1-\cos F_k)(k+1)(k+1-N)\\ &=\frac{1}{2\pi}\sum_{k=0}^{N-2}(k+1)(k+1-N)[F_k-\sin F_k]_{r=0}^{r=\infty}. \end{aligned} \tag{65}$$

As $g_k(\infty)=0$ we see that the only contributions to the topological charge come from $F_k(0)$.

Our $N-1$ equations (61) for functions F_k, $k=0,\ldots,N-2$ and so g_i have many symmetries. These symmetries allow us to find special solutions which involve only a smaller number of functions. So, before looking at special cases, let us mention some of these symmetries.

The main symmetry, which is relatively easy to spot is the symmetry under the independent interchanges,

$$F_0\leftrightarrow F_{N-2},\quad F_1\leftrightarrow F_{N-3},\quad F_k\leftrightarrow F_{N-k-2},\quad \ldots. \tag{66}$$

To see this symmetry we look at the expression for the energy and note that as

$$D_k=k(N-k)(1-\cos F_{k-1}),$$

D_k have this symmetry; i.e., $D_k\leftrightarrow D_{N-k}$, when $F_{k-1}\leftrightarrow F_{N-k-1}$.

This symmetry is evident in all terms involving D_k's and so we are left with having to look at the terms involving $\dot{F}_k$'s.

However, clearly the terms involving $\dot{F}_k^2 D_{k+1}$ have this symmetry as they come in the combination

$$\sum_{k=0}^{N-2}\dot{F}_k^2 D_{k+1}=\sum_{k=0}^{N-2}\dot{F}_k^2(k+1)(N-k-1)(1-\cos F_k). \tag{67}$$

Next we rewrite the remaining terms as

$$-\frac{1}{N}\left(\sum_{i=0}^{N-2}\dot{g}_i\right)^2+\sum_{i=0}^{N-2}\dot{g}_i^2=-\frac{1}{N}\left(\sum_{i=0}^{N-2}(i+1)\dot{F}_i\right)^2+\sum_{i=0}^{N-2}\left(\sum_{j=i}^{N-2}\dot{F}_j\right)^2 \tag{68}$$

and note that the coefficient of $\dot{F}_i^2$ is given by

$$-\frac{1}{N}(i+1)^2+(i+1)=(i+1)\frac{(N-i-1)}{N}, \tag{69}$$

which is also the coefficient of $\dot{F}_{N-i-2}^2$. Moreover, as the coefficient of $\dot{F}_i\dot{F}_j$ (when $i>j$) is

$$2i-\frac{2}{N}(i+1)(j+1), \tag{70}$$

which is also the coefficient of $\dot{F}_{N-i-2}\dot{F}_{N-j-2}$ we see that we have demonstrated the validity of our symmetry.

VII. SPECIAL CASES

Now we look at the cases of low N.

A. *SU*(3)

In the $SU(3)$ case we have two functions: F_0 and F_1. The radial energy density $\mathcal{E}$ is given by

$$\mathcal{E}=\frac{2}{3}(\dot{F}_0^2+\dot{F}_1^2+\dot{F}_0\dot{F}_1)[r^2+2(1-\cos F_0)+2(1-\cos F_1)]+4[(1-\cos F_0)+(1-\cos F_1)]$$
$$\times\left[1+\frac{1}{2r^2}(1-\cos F_0)+\frac{1}{2r^2}(1-\cos F_1)\right]. \tag{71}$$

The equations for F_0 and F_1 are

$$\begin{aligned}(2\ddot{F}_0+\ddot{F}_1)A_{32}+\frac{2}{r}(2\dot{F}_0+\dot{F}_1)A_{31}-\frac{6}{r^2}(\sin F_0)A_{30}=0,\\ (\ddot{F}_0+2\ddot{F}_1)A_{32}+\frac{2}{r}(\dot{F}_0+2\dot{F}_1)A_{31}-\frac{6}{r^2}(\sin F_1)A_{30}=0,\end{aligned} \tag{72}$$

where

$$\begin{aligned}A_{32}&=1+\frac{2}{r^2}(1-\cos F_0)+\frac{2}{r^2}(1-\cos F_1),\\ A_{31}&=1+\frac{1}{r}\dot{F}_0\sin F_0+\frac{1}{r}\dot{F}_1\sin F_1,\\ A_{30}&=\frac{1}{3}(\dot{F}_0^2+\dot{F}_1^2+\dot{F}_0\dot{F}_1)+1+\frac{1}{r^2}(1-\cos F_0)+\frac{1}{r^2}(1-\cos F_1).\end{aligned} \tag{73}$$

The equations (72) can be solved for the two functions F_0 and F_1. Clearly, we cannot put either of them to zero but, due to the symmetry, we can take $F_0=F_1=F$ in which case both equations reduce to

$$\ddot{F}\left[1+\frac{4}{r^2}(1-\cos F)\right]+\frac{2}{r}\dot{F}+\frac{2}{r^2}\sin F\left[\dot{F}^2-1-\frac{2}{r^2}(1-\cos F)\right]=0. \tag{74}$$

This equation coincides with the equation of the usual $SU(2)$ Skyrme model after rescaling the coordinate $r=2\tilde{r}$. Performing this coordinate rescaling in the corresponding energy integral, we find that its energy is $E=8\times 1.232$, i.e., is exactly 8 times the energy of one $SU(2)$ skyrmion [taking $F(0)=2\pi$]. This agrees with our numerical result 9.85242 obtained from (74) [within our numerical accuracy the energy of one $SU(2)$ skyrmion is 1.23146]. The topological charge of this configuration is clearly $B=4$, so energy per baryon is 2 times the energy of one $SU(2)$ skyrmion.

In addition, there is a further symmetry; we can put $F_0=-F_1=G$. In this case both equations reduce to

$$\ddot{G}\left[1+\frac{4}{r^2}(1-\cos G)\right]+\frac{2}{r}\dot{G}+\frac{2}{r^2}\sin G\left[\dot{G}^2-3-\frac{6}{r^2}(1-\cos G)\right]=0. \tag{75}$$

This case, as $F_0=g_0-g_1$ and $F_1=g_1$, corresponds to the case of $g_0=0$ and so our solution involves only one projector, namely P_1. Its topological charge is $B=2-2=0$ and its energy is 5.11338. A similar solution was discussed, in the usual Skyrme model case, in Ref. 9 (there its energy is 3.861).

In general, however, our solutions depend on two functions F_0 and F_1. For example, by imposing the boundary conditions: $F_0(0)=2\pi, F_0(\infty)=0$ and $F_1(0)=0, F_1(\infty)=0$ in (72) we found that the energy of this solution is $E=2.61503$ and its baryon number is $B=2$. (In the usual Skyrme model, a similar solution has energy 2.3764.)

B. *SU*(4)

In this case we have three functions F_0, F_1 and F_2. The energy density becomes

$$\begin{aligned}\mathcal{E}=&\tfrac{1}{4}[3\dot{F}_0^2+4\dot{F}_1^2+3\dot{F}_2^2+4\dot{F}_0\dot{F}_1+2\dot{F}_0\dot{F}_2+4\dot{F}_1\dot{F}_2][r^2+3(1-\cos F_0)+4(1-\cos F_1)\\&+3(1-\cos F_2)]+2[3(1-\cos F_0)+4(1-\cos F_1)+3(1-\cos F_2)]\\&\times\left[1+\frac{3}{4r^2}(1-\cos F_0)+\frac{1}{r^2}(1-\cos F_1)+\frac{3}{4r^2}(1-\cos F_2)\right].\end{aligned} \tag{76}$$

The equations for F_0, F_1 and F_2 are very complicated. They read as

$$\begin{aligned}&(3\ddot{F}_0+2\ddot{F}_1+\ddot{F}_2)A_{42}+\frac{2}{r}(3\dot{F}_0+2\dot{F}_1+\dot{F}_2)A_{41}-\frac{12}{r^2}(\sin F_0)A_{40}=0,\\&(\ddot{F}_0+2\ddot{F}_1+\ddot{F}_2)A_{42}+\frac{2}{r}(\dot{F}_0+2\dot{F}_1+\dot{F}_2)A_{41}-\frac{8}{r^2}(\sin F_1)A_{40}=0,\\&(\ddot{F}_0+2\ddot{F}_1+3\ddot{F}_2)A_{42}+\frac{2}{r}(\dot{F}_0+2\dot{F}_1+3\dot{F}_2)A_{41}-\frac{12}{r^2}(\sin F_2)A_{40}=0,\end{aligned} \tag{77}$$

where

$$\begin{aligned}A_{42}=&1+\frac{3}{r^2}(1-\cos F_0)+\frac{4}{r^2}(1-\cos F_1)+\frac{3}{r^2}(1-\cos F_2),\\A_{41}=&1+\frac{3}{2r}\dot{F}_0\sin F_0+\frac{2}{r}\dot{F}_1\sin F_1+\frac{3}{2r}\dot{F}_2\sin F_2,\\A_{40}=&\frac{3}{8}\left(\dot{F}_0^2+\frac{4}{3}\dot{F}_1^2+\dot{F}_2^2+\frac{4}{3}\dot{F}_0\dot{F}_1+\frac{2}{3}\dot{F}_0\dot{F}_2+\frac{4}{3}\dot{F}_1\dot{F}_2\right)\\&+1+\frac{3}{2r^2}(1-\cos F_0)+\frac{2}{r^2}(1-\cos F_1)+\frac{3}{2r^2}(1-\cos F_2).\end{aligned} \tag{78}$$

These equations have the previously mentioned symmetry $F_0\leftrightarrow F_2$ which allows us to set $F_0=F_2=F$ while keeping F_1 arbitrary. In this case the above equations reduce to the following two coupled equations:

$$(2\ddot{F}+\ddot{F}_1)\tilde{A}_{42}+\frac{2}{r}(2\dot{F}+\dot{F}_1)\tilde{A}_{41}-\frac{6}{r^2}(\sin F)\tilde{A}_{40}=0,$$
$$(\ddot{F}+\ddot{F}_1)\tilde{A}_{42}+\frac{2}{r}(\dot{F}+\dot{F}_1)\tilde{A}_{41}-\frac{4}{r^2}(\sin F_1)\tilde{A}_{40}=0, \tag{79}$$

where

$$\tilde{A}_{42}=1+\frac{6}{r^2}(1-\cos F)+\frac{4}{r^2}(1-\cos F_1),$$
$$\tilde{A}_{41}=1+\frac{3}{r}\dot{F}\sin F+\frac{2}{r}\dot{F}_1\sin F_1, \tag{80}$$
$$\tilde{A}_{40}=\left(\dot{F}^2+\frac{1}{2}\dot{F}_1^2+\dot{F}\dot{F}_1\right)+1+\frac{3}{r^2}(1-\cos F)+\frac{2}{r^2}(1-\cos F_1).$$

By imposing $F(0)=2\pi, F(\infty)=0$ and $F_1(0)=0, F_1(\infty)=0$ the corresponding solution is found to have energy 13.2006 and its baryon number is 6.

If we further set $F_1=F=G$ then the above coupled equations reduce to

$$\ddot{G}\left[1+\frac{10}{r^2}(1-\cos G)\right]+\frac{2}{r}\dot{G}+\frac{1}{r^2}\sin G\left[5\dot{G}^2-2-\frac{10}{r^2}(1-\cos G)\right]=0. \tag{81}$$

This equation coincides with the usual $SU(2)$ Skyrme model equation, after rescaling the coordinate $r=\sqrt{10}\tilde{r}$. Performing this coordinate rescaling in the corresponding energy integral we find that this configuration has energy $E=10\sqrt{10}\times 1.232$. Our numerical result for the energy obtained from (81) is 38.9551 which is in good agreement with the above exact result. Note that the topological charge of this solution is 10, so energy per baryon is $\sqrt{10}$ times the energy of one $SU(2)$ skyrmion.

Another solution can be found by setting $F_0=-F_2=Z$. Then the equations have a solution if $F_1=0$. This case corresponds to $g_0=0$ and $g_1=g_2$ and so, effectively, the field configuration is described by a one projector of rank two; namely, P_1+P_2. The corresponding equation for Z is

$$\ddot{Z}\left[1+\frac{6}{r^2}(1-\cos Z)\right]+\frac{2}{r}\dot{Z}+\frac{3}{r^2}\sin Z\left[\dot{Z}^2-2-\frac{6}{r^2}(1-\cos Z)\right]=0. \tag{82}$$

This solution has energy 9.39388 and its charge is $B=3-3=0$.

When we use all 3 functions we get results which depend on $F_i(0)$. In the following table we present our results for E_a and compare them with the similar results for E_u derived in the usual Skyrme models.[10]

$F_0(0)$	$F_1(0)$	$F_2(0)$	B	E_a	E_u
2π	0	0	3	3.96601	3.518
0	2π	0	4	5.87187	4.788
2π	0	2π	6	13.2006	7.22553
2π	2π	0	7	18.9833	8.45219
2π	2π	2π	10	38.9551	12.32
2π	-2π	2π	6–4	14.3419	8.852
2π	2π	-2π	7–3	20.5668	9.896
2π	0	-2π	3–3	9.39388	6.63422
-2π	2π	0	4–3	9.07753	6.61478

We see that our energies are higher (especially for larger values of B).

C. *SU*(5)

This time we have four functions F_0, F_1, F_2 and F_3. The energy density becomes

$$\begin{aligned}\mathcal{E}=&\tfrac{2}{5}[2\dot{F}_0^2+3\dot{F}_1^2+3\dot{F}_2^2+2\dot{F}_3^2+3\dot{F}_0\dot{F}_1+2\dot{F}_0\dot{F}_2+\dot{F}_0\dot{F}_3+4\dot{F}_1\dot{F}_2+2\dot{F}_1\dot{F}_3+3\dot{F}_2\dot{F}_3]\\&\times[r^2+2\{2(1-\cos F_0)+3(1-\cos F_1)+3(1-\cos F_2)+2(1-\cos F_3)\}]\\&+4[2(1-\cos F_0)+3(1-\cos F_1)+3(1-\cos F_2)+2(1-\cos F_3)]\\&\times\left[1+\frac{1}{2r^2}\{2(1-\cos F_0)+3(1-\cos F_1)+3(1-\cos F_2)+2(1-\cos F_3)\}\right].\end{aligned}\tag{83}$$

The equations for F_0, F_1, F_2 and F_3 are now given by

$$\begin{aligned}&(4\ddot{F}_0+3\ddot{F}_1+2\ddot{F}_2+\ddot{F}_3)A_{52}+\frac{2}{r}(4\dot{F}_0+3\dot{F}_1+2\dot{F}_2+\dot{F}_3)A_{51}-\frac{20}{r^2}(\sin F_0)A_{50}=0,\\&(3\ddot{F}_0+6\ddot{F}_1+4\ddot{F}_2+2\ddot{F}_3)A_{52}+\frac{2}{r}(3\dot{F}_0+6\dot{F}_1+4\dot{F}_2+2\dot{F}_3)A_{51}-\frac{30}{r^2}(\sin F_1)A_{50}=0,\\&(2\ddot{F}_0+4\ddot{F}_1+6\ddot{F}_2+3\ddot{F}_3)A_{52}+\frac{2}{r}(2\dot{F}_0+4\dot{F}_1+6\dot{F}_2+3\dot{F}_3)A_{51}-\frac{30}{r^2}(\sin F_2)A_{50}=0,\\&(\ddot{F}_0+2\ddot{F}_1+3\ddot{F}_2+4\ddot{F}_3)A_{52}+\frac{2}{r}(\dot{F}_0+2\dot{F}_1+3\dot{F}_2+4\dot{F}_3)A_{51}-\frac{20}{r^2}(\sin F_3)A_{50}=0,\end{aligned}\tag{84}$$

where

$$\begin{aligned}A_{52}=&1+\frac{2}{r^2}[2(1-\cos F_0)+3(1-\cos F_1)+3(1-\cos F_2)+2(1-\cos F_3)],\\A_{51}=&1+\frac{1}{r}[2\dot{F}_0\sin F_0+3\dot{F}_1\sin F_1+3\dot{F}_2\sin F_2+2\dot{F}_3\sin F_3],\\A_{50}=&\frac{1}{5}[2\dot{F}_0^2+3\dot{F}_1^2+3\dot{F}_2^2+2\dot{F}_3^2+3\dot{F}_0\dot{F}_1+2\dot{F}_0\dot{F}_2+\dot{F}_0\dot{F}_3+4\dot{F}_1\dot{F}_2+2\dot{F}_1\dot{F}_3+3\dot{F}_2\dot{F}_3]\\&+1+\frac{1}{r^2}[2(1-\cos F_0)+3(1-\cos F_1)+3(1-\cos F_2)+2(1-\cos F_3)].\end{aligned}\tag{85}$$

It is easy to spot, as we have mentioned before, that these expressions have symmetries $F_0\leftrightarrow F_3$ and, independently, $F_1\leftrightarrow F_2$.

So we can seek solutions involving only two functions $F_0=F_3=F$ and $F_1=F_2=G$. If we impose this condition our equations reduce to the following two coupled equations:

$$\begin{aligned}&(\ddot{F}+\ddot{G})\tilde{A}_{52}+\frac{2}{r}(\dot{F}+\dot{G})\tilde{A}_{51}-\frac{4}{r^2}(\sin F)\tilde{A}_{50}=0,\\&(\ddot{F}+2\ddot{G})\tilde{A}_{52}+\frac{2}{r}(\dot{F}+2\dot{G})\tilde{A}_{51}-\frac{6}{r^2}(\sin G)\tilde{A}_{50}=0,\end{aligned}\tag{86}$$

where

$$\tilde{A}_{52}=1+\frac{4}{r^2}[2(1-\cos F)+3(1-\cos G)],$$

$$\tilde{A}_{51}=1+\frac{2}{r}[2\dot{F}\sin F+3\dot{G}\sin G], \tag{87}$$

$$\tilde{A}_{50}=[\dot{F}^2+2\dot{G}^2+2\dot{F}\dot{G}]+1+\frac{2}{r^2}[2(1-\cos F)+3(1-\cos G)].$$

By imposing $F(0)=0,F(\infty)=0$ and $G(0)=2\pi,G(\infty)=0$, the corresponding solution is found to have energy 37.3436 and its baryon number is 12. We observe that the equations (86) coincide with the equations (79) in the $SU(4)$ case, after rescaling the coordinate $r=\sqrt{2}\tilde{r}$. Performing this coordinate rescaling in the corresponding energy integral of (86), we find that its energy is $2\sqrt{2}$ times the energy of (79) which agrees with our numerical results above.

Note that if in addition, we further let $G=F$ then the above coupled equations reduce to

$$\ddot{F}\left[1+\frac{20}{r^2}(1-\cos F)\right]+\frac{2}{r}\dot{F}+\frac{2}{r^2}\sin F\left[5\dot{F}^2-1-\frac{10}{r^2}(1-\cos F)\right]=0. \tag{88}$$

This equation, again, coincides with the usual $SU(2)$ Skyrme model equation after rescaling the coordinate $r=\sqrt{20}\tilde{r}$ and from the corresponding energy integral we find that its energy is $E=20\sqrt{20}\times 1.232$. Our numerical result for the energy obtained from (88) is 110.251 which is also in good agreement with the above exact result. As its topological charge is 20 we see that the energy per baryon of this solution is $\sqrt{20}$ times the energy of one $SU(2)$ skyrmion.

There is still a further symmetry, which we could exploit, and which allows us to put $F_0=-F_3=Y$ and $F_1=-F_2=Z$. The corresponding equations for Y and Z are

$$\begin{aligned}(3\ddot{Y}+\ddot{Z})\tilde{A}_{52}+\frac{2}{r}(3\dot{Y}+\dot{Z})\tilde{A}_{51}-\frac{20}{r^2}(\sin Y)\tilde{A}_{50}=0,\\ (\ddot{Y}+2\ddot{Z})\tilde{A}_{52}+\frac{2}{r}(\dot{Y}+2\dot{Z})\tilde{A}_{51}-\frac{30}{r^2}(\sin Z)\tilde{A}_{50}=0,\end{aligned} \tag{89}$$

where

$$\tilde{A}_{52}=1+\frac{4}{r^2}[2(1-\cos Y)+3(1-\cos Z)],$$

$$\tilde{A}_{51}=1+\frac{2}{r}[2\dot{Y}\sin Y+3\dot{Z}\sin Z], \tag{90}$$

$$\tilde{A}_{50}=\frac{1}{5}[3\dot{Y}^2+2\dot{Z}^2+2\dot{Y}\dot{Z}]+1+\frac{2}{r^2}[2(1-\cos Y)+3(1-\cos Z)].$$

This case corresponds to $g_0=0$ and $g_1=g_3$ and so the corresponding field configurations are described by two projectors—namely P_2 and P_1+P_3. By imposing $Y(0)=2\pi,Y(\infty)=0$ and $Z(0)=0,Z(\infty)=0$, we found that this configuration has energy 13.4618. Its charge is $B=4-4=0$.

More general solutions, however, depend on all four functions.

Finally, let us note that for $SU(N)$ with $N>2$, when all profile functions F_i are the same, i.e., $F_0=F_1=\cdots=F_{N-2}=F$ the equations (61) reduce to the single equation

$$\ddot{F}\left[1+\frac{\tilde{B}}{r^2}(1-\cos F)\right]+\frac{2}{r}\dot{F}+\frac{2}{r^2}\sin F\left[\frac{\tilde{B}}{4}\dot{F}^2-1-\frac{\tilde{B}}{2r^2}(1-\cos F)\right]=0, \tag{91}$$

and the corresponding energy integral (58) reduces to

$$E=\frac{1}{6\pi}\int r^2\,dr\left[\frac{\tilde{B}}{2}\dot{F}^2\left(1+\frac{\tilde{B}}{r^2}(1-\cos F)\right)+2\frac{\tilde{B}}{r^2}(1-\cos F)+\frac{\tilde{B}^2}{2r^4}(1-\cos F)^2\right], \tag{92}$$

where

$$\tilde{B}=\frac{(N-1)N(N+1)}{6}, \tag{93}$$

and $\tilde{B}$ is the baryon number of our configuration.

We observe that by rescaling the radial coordinate r to

$$r=\tilde{r}\sqrt{\tilde{B}}, \tag{94}$$

the equation (91) reduces to the usual $SU(2)$ Skyrme model equation (in the coordinate $\tilde{r}$) and the energy integral (92) becomes

$$E=\tilde{B}\sqrt{\tilde{B}}\,E_{SU(2)}, \tag{95}$$

where $E_{SU(2)}$ is the energy integral of the usual $SU(2)$ Skyrme model (in the coordinate $\tilde{r}$). Thus this configuration has energy $E=\tilde{B}\sqrt{\tilde{B}}\times 1.232$ [taking $F(0)=2\pi$], which agrees with our results for the cases: $N=3$, 4 and 5 above. As the baryon number of this configuration is $\tilde{B}$, the energy per baryon is $\sqrt{\tilde{B}}$ times the energy of one $SU(2)$ skyrmion.

VIII. CONCLUSIONS

In this paper we have discussed the alternative $SU(N)$ Skyrme models. We have shown that for $N=2$ they reduce to the usual Skyrme models but for $N\neq 2$ they are different.

We have also shown that to study these models we can use the rational map ansatz[8] in the form of its generalization to the usual Skyrme models.[9]

Like for the usual Skyrme models when we use only one projector we find field configurations which have low energies and which we hope are close to the true solutions of this model. We have also found that, as in the case of usual Skyrme models, the use of $N-1$ projectors constructed from the Veronese sequence of vectors gives us radially symmetric solutions of the alternative models. These solutions are characterized by the appropriate profile functions, which have to be determined numerically. In some cases we can exploit symmetries of the energy densities and reduce the number of functions.

Thus, almost everything works exactly like for the usual Skyrme models; only the equations for the profile functions are a little modified. When we have solved the equations for the profile functions we have found that the solutions of the alternative models have energies higher than the corresponding solutions of the usual models. This can be traced to the extra terms in the expression for the energy density after the integration over the angular variables has been performed which give an additional positive contribution to the total energy.

It is not clear, both for the usual and alternative models, how to generalize the harmonic map ansatz to derive an analytical or quasi-analytical form of the nonradially symmetric solutions.

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APPENDIX: DERIVATION OF EQUATIONS (61)

In this appendix, we derive the equations for the profile functions g_k directly from the equations (51). To do this we look in detail at all the terms in these equations.

Using the very special form of our vectors V, we find that

$$\partial_\xi R_{\bar{\xi}} + \partial_{\bar{\xi}} R_\xi = \frac{2i}{(1+|\xi|^2)^2} \sum_{k=1}^{N-1} k(N-k)\sin(g_{k-1}-g_k)(P_k - P_{k-1}), \tag{A1}$$

and

$$Q = (1+|\xi|^2)^2 \,\mathrm{Tr}(R_\xi R_{\bar{\xi}}) = -2\sum_{k=1}^{N-1} D_k, \tag{A2}$$

where $D_k = k(N-k)(1-\cos(g_{k-1}-g_k))$. The term R_r is given in (41), while $\mathrm{Tr}(R_r^2)$ is given in (48).

Using these results we find that (51) reduce to the the following factorized form:

$$\sum_{k=0}^{N-2} \left[\left(P_k - \frac{1}{N} \right) \alpha_k + (P_{k+1} - P_k)\beta_{k+1} \right] = 0, \tag{A3}$$

where

$$\alpha_k = \partial_r [(r^2 - \tfrac{1}{2}Q)\dot{g}_k], \tag{A4}$$

and

$$\beta_k = k(N-k)\sin(g_{k-1}-g_k)\left[1 - \frac{1}{2}\mathrm{Tr}(R_r^2) - \frac{1}{4r^2}Q \right]. \tag{A5}$$

Next we take the inner product of (A3) with the vectors V_m $(m=0,1,\ldots,N-2)$ from the right. Using

$$P_k V_m = \left(\frac{V_k V_k^\dagger}{|V_k|^2} \right) V_m = V_k \delta_{km},$$

where δ_{km} is the Kronecker's delta, and the fact that the vectors V_k are independent, we see that the requirement of the vanishing of the corresponding coefficients leaves us with

$$\left(\alpha_k - \frac{1}{N} \sum_{n=0}^{N-2} \alpha_n \right) + (\beta_k - \beta_{k+1}) = 0. \tag{A6}$$

Finally, using the relation

$$\sum_{k=0}^{l} (\beta_k - \beta_{k+1}) = -\beta_{l+1}, \tag{A7}$$

for $(l=0,1,\ldots,N-2)$, as $\beta_0 = 0$ $(g_{-1}=0)$, and summing (A6) from $k=0$ to l yields

$$\sum_{k=0}^{l} \alpha_k - \frac{(l+1)}{N} \sum_{n=0}^{N-2} \alpha_n - \beta_{l+1} = 0. \tag{A8}$$

Introducing $F_k = g_k - g_{k+1}$ we find that the equations (A8) coincide with the equations for the profile functions that we have derived from the energy integral in Sec. V, i.e., Eqs. (61).

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Solutions of the Yang–Mills–Higgs equations in 2+1-dimensional anti-de Sitter space–time

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The solutions of the Bogomolny equation in $2+1$-dimensional anti-de Sitter space–time are obtained by using Darboux transformations with both constant spectral parameters and variable ''spectral parameters.'' These solutions give the Yang–Mills–Higgs fields in $2+1$-dimensional anti-de Sitter space–time. Some examples in the SU(2) case are considered and qualitative asymptotic behaviors of the solutions as $t\to\infty$ are discussed in detail. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1337799]

I. INTRODUCTION

The Yang–Mills–Higgs fields satisfying the Bogomolny equations in $\mathbf{R}^3$ and $\mathbf{R}^{2,1}$ were widely investigated and the equations are known to be integrable. On the other hand, the Yang–Mills–Higgs fields satisfying the Bogomolny equations in some curved spaces such as the hyperbolic space H^3, the $2+1$-dimensional anti-de Sitter space–time are also integrable.[1–3] In the present paper, we consider the solutions of the Bogomolny equation in the $2+1$-dimensional anti-de Sitter space–time, the Lax pair of which has been known and the soliton solutions (with constant spectral parameters) were also obtained.[3]

With the Darboux transformation method, we obtain exact multisoliton solutions. Moreover, the ''spectral parameters'' in the construction of Darboux transformation can depend on the space–time variables as in some other problems with dimensions $\geqslant 3$, like the self-dual Yang–Mills equation, modified principal chiral field, the Bolgomolny equation in $\mathbf{R}^3$, etc.[4–8] These kinds of equations are also called breaking soliton equations, since the spectral parameter may not be constant and satisfies an equation whose solution can blow up at finite time.[9,10]

In Secs. II and III the Darboux transformations for $\mathrm{GL}(N,\mathbf{C})$ and $\mathrm{U}(N)$ cases are discussed. As a special case, the general construction of soliton solutions is given in Sec. IV. Then, in Sec. V, some examples of single solitons and multisolitons are considered, with both constant spectral parameters and variable ''spectral parameters.'' Their qualitative asymptotic behavior as $t\to\infty$ is discussed in detail. When the spectral parameters are constants, we find solutions globally defined on the whole $2+1$-dimensional anti-de Sitter space–time. When the ''spectral parameters'' are not constants, the solutions derived here are only locally defined in $2+1$-dimensional anti-de Sitter space–time.

Our problem is as follows.

Let M be a three-dimensional Lorentz manifold with metric g. A_μ is a gauge potential and Φ is a (scalar) Higgs field, both of which are valued in the Lie algebra of a Lie group G. Hereafter, we always suppose G is a matrix Lie group and the matrices in G are of order N.

The $2+1$-dimensional anti-de Sitter space–time is the universal covering space of the hyperboloid

$$U^2+V^2-X^2-Y^2=1 \tag{1.1}$$

in $\mathbf{R}^{2,2}$ with the metric

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$$ds^2 = -dU^2 - dV^2 + dX^2 + dY^2. \tag{1.2}$$

Define

$$r = \frac{1}{U+X}, \quad x = \frac{Y}{U+X}, \quad t = -\frac{V}{U+X}, \tag{1.3}$$

then a part of the $2+1$-dimensional anti-de Sitter space–time with $U+X>0$ is represented by the Poincaré coordinates (r,x,t) with $r>0$ and the metric is

$$ds^2 = r^{-2}(-dt^2 + dr^2 + dx^2) = r^{-2}(dr^2 + du\, dv), \tag{1.4}$$

where $u=x+t$, $v=x-t$.

The Yang–Mills–Higgs field in $2+1$-dimensional anti-de Sitter space–time satisfies the Bogomolny equation[1,11]

$$D\Phi = *F, \tag{1.5}$$

or, written in terms of the components,

$$D_\mu \Phi = \frac{1}{2\sqrt{|g|}} g_{\mu\nu} \epsilon^{\nu\alpha\beta} F_{\alpha\beta}, \tag{1.6}$$

where the action of the covariant derivative $D_\mu = \partial_\mu + A_\mu$ on Φ is $D_\mu \Phi = \partial_\mu \Phi + [A_\mu, \Phi]$, $\partial_\mu = \partial/\partial x^\mu$. $\{F_{\mu\nu}\}$ is the curvature corresponding to $\{A_\mu\}$, $F_{\mu\nu} = [D_\mu, D_\nu]$.

With the Poincaré coordinates (1.3), (1.6) becomes

$$D_u \Phi = rF_{ur}, \quad D_v \Phi = -rF_{vr}, \quad D_r \Phi = -2rF_{uv}. \tag{1.7}$$

It was proposed in Ref. 3 that this system of nonlinear partial differential equations had a Lax pair

$$\begin{aligned} &(rD_r + \Phi - 2(\zeta - u)D_u)\psi = 0, \\ &\left(2D_v + \frac{\zeta - u}{r} D_r - \frac{\zeta - u}{r^2}\Phi\right)\psi = 0, \end{aligned} \tag{1.8}$$

where $D_\mu \psi = \partial_\mu \psi + A_\mu \psi$ and ζ is a complex spectral parameter. That is, (1.7) is the integrability condition of the overdetermined system (1.8).

II. DARBOUX TRANSFORMATION IN GL(N,C) CASE

In this section, we consider the case $G = \mathrm{GL}(N, \mathbf{C})$. This is the simplest case because no reduction should be considered. Let

$$\tilde{\psi} = (\zeta - u)R\psi - T\psi, \tag{2.1}$$

where $R(u,v,r)$ and $T(u,v,r)$ are $N \times N$ matrices and R is invertible, then the transformation $\psi \to \tilde{\psi}$ is called a Darboux transformation (of degree one) if there are $(\tilde{A}_\mu, \tilde{\Phi})$ such that

$$\begin{aligned} &(r\tilde{D}_r + \tilde{\Phi} - 2(\zeta - u)\tilde{D}_u)\tilde{\psi} = 0, \\ &\left(2\tilde{D}_v + \frac{\zeta - u}{r}\tilde{D}_r - \frac{\zeta - u}{r^2}\tilde{\Phi}\right)\tilde{\psi} = 0 \end{aligned} \tag{2.2}$$

hold. Here $\tilde{D}_\mu=\partial_\mu+\tilde{A}_\mu$.

We should first determine R and T so that (2.1) is a Darboux transformation. For given (A,Φ), $(\tilde{A},\tilde{\Phi})$ and arbitrary matrix function Q, let

$$\Delta_\mu Q=\partial_\mu Q+\tilde{A}_\mu Q-QA_\mu,$$
$$\delta Q=\tilde{\Phi}Q-Q\Phi. \tag{2.3}$$

Expressed in ψ, both equations of (2.2) are polynomials of ζ of degree two. The coefficients of the second, first, and zeroth order of ζ in the two equations of (2.2) lead to

$$\Delta_u R=0,\quad r\Delta_r R+2\Delta_u T+\delta R+2R=0,$$
$$r\Delta_r T+\delta T=0, \tag{2.4}$$

and

$$\Delta_r R-\frac{1}{r}\delta R=0,\quad 2\Delta_v R-\frac{1}{r}\Delta_r T+\frac{1}{r^2}\delta T=0,$$
$$\Delta_v T=0. \tag{2.5}$$

These two systems are equivalent to

$$\Delta_u R=0, \tag{2.6}$$

$$\Delta_v T=0, \tag{2.7}$$

$$\Delta_v R=\frac{1}{r}\Delta_r T, \tag{2.8}$$

$$\Delta_r R+\frac{1}{r}\Delta_u T+\frac{1}{r}R=0, \tag{2.9}$$

$$\Delta_r R-\frac{1}{r}\delta R=0, \tag{2.10}$$

$$\Delta_r T+\frac{1}{r}\delta T=0. \tag{2.11}$$

$\tilde{A}_u$ and $\tilde{A}_v$ are solved from (2.6) and (2.7) as

$$\tilde{A}_u=RA_uR^{-1}-(\partial_u R)R^{-1}, \tag{2.12}$$

$$\tilde{A}_v=TA_vT^{-1}-(\partial_v T)T^{-1}, \tag{2.13}$$

while (2.10) and (2.11) lead to

$$\tilde{A}_r=\frac{1}{2}(TA_r-\partial_r T)T^{-1}+\frac{1}{2}(RA_r-\partial_r R)R^{-1}+\frac{1}{2r}(T\Phi T^{-1}-R\Phi R^{-1}), \tag{2.14}$$

$$\tilde{\Phi}=\frac{r}{2}(TA_r-\partial_r T)T^{-1}-\frac{r}{2}(RA_r-\partial_r R)R^{-1}+\frac{1}{2}(T\Phi T^{-1}+R\Phi R^{-1}). \tag{2.15}$$

Now let Z be an $N\times N$ matrix function of (u,v,r), H be a solution of

$$\begin{aligned} &r((\partial_r H)H^{-1}+A_r)+\Phi-2((\partial_u H)H^{-1}+A_u)S=0,\\ &2((\partial_v H)H^{-1}+A_v)+\frac{1}{r}((\partial_r H)H^{-1}+A_r)S-\frac{1}{r^2}\Phi S=0, \end{aligned} \tag{2.16}$$

where $S=HZH^{-1}-u$, then S satisfies

$$\begin{aligned} \partial_r S&=H\left(\partial_r Z-\frac{2}{r}(\partial_u Z)(Z-u)\right)H^{-1}+\frac{2}{r}S+\frac{2}{r}(\partial_u S)S-[A_r,S]+\frac{2}{r}[A_u,S]S-\frac{1}{r}[\Phi,S],\\ \partial_v S&=H\left(\partial_v Z+\frac{1}{2r}(\partial_r Z)(Z-u)\right)H^{-1}-\frac{1}{2r}(\partial_r S)S-[A_v,S]-\frac{1}{2r}[A_r,S]S+\frac{1}{2r^2}[\Phi,S]S. \end{aligned} \tag{2.17}$$

Remark 1: If Z is diagonal and $Z=\mathrm{diag}(\zeta_1,...,\zeta_N)$, then $H=(h_1,\ldots,h_N)$ where h_i is a column solution of the Lax pair (1.8) with $\zeta=\zeta_i(u,v,r)$.

If $T=RS$, then (2.8) and (2.9) hold if and only if

$$\begin{aligned} &\partial_r Z-\frac{2}{r}(\partial_u Z)(Z-u)=0,\\ &\partial_v Z+\frac{1}{2r}(\partial_r Z)(Z-u)=0. \end{aligned} \tag{2.18}$$

Therefore, we have

Theorem 1: *Suppose $R(u,v,r)$ is an arbitrary invertible matrix function. If $Z(u,v,r)$ is an $N\times N$ matrix solution of (2.18) and H is a solution of (2.16) with $S=HZH^{-1}-u$, then $\psi\mapsto\tilde{\psi}=(\zeta-u)R\psi-RS\psi$ is a Darboux transformation for (1.8).*

If $Z=\mathrm{diag}(\zeta_1,...,\zeta_N)$, then each ζ_i is a solution of

$$\begin{aligned} &\partial_r\zeta-\frac{2}{r}(\zeta-u)\partial_u\zeta=0,\\ &\partial_v\zeta+\frac{1}{2r}(\zeta-u)\partial_r\zeta=0. \end{aligned} \tag{2.19}$$

Apart from the constant solution, the general nonconstant solution of (2.19) is given implicitly by

$$v-\frac{r^2}{\zeta-u}=C(\zeta), \tag{2.20}$$

where C is an arbitrary holomorphic function. We still call ζ_i as a ''spectral parameter.'' However, here the ''spectral parameters'' ζ_i's in Z can be either constant or variable. In the latter case, they are given by (2.20).

Remark 2: Note that the spectral parameter ζ in the Lax pair is still a complex constant. Only ζ_i's in Z can depend on (u,v,r).

According to Theorem 1, we can get the exact solution of (1.7) from a known solution of (1.7) and the corresponding solution of the linear system (2.16). When Z is diagonal, solving (2.16) is equivalent to solving (1.8).

Theorem 1 gives the construction of Darboux transformations of degree one. The Darboux transformations of higher degrees can be obtained by the composition of several Darboux transformations of degree one.

III. DARBOUX TRANSFORMATION IN THE U(N) CASE

When $G=\mathrm{U}(N)$, the Lie algebra consists of all anti-Hermitian matrices. Hence $A_\mu^*=-A_\mu$, $\Phi^*=-\Phi$.

In order to construct Darboux transformation which keeps this reduction, some constraints on ζ_j's and h_j's should be added.

Suppose ψ is a solution of (1.8), ϕ is a solution of (1.8) with $\zeta\to\overline{\zeta}$. Then

$$\begin{aligned} &r\partial_r(\phi^*\psi)-2(\zeta-u)\partial_u(\phi^*\psi)=0,\\ &2\partial_v(\phi^*\psi)+\frac{\zeta-u}{r}\partial_r(\phi^*\psi)=0. \end{aligned} \tag{3.1}$$

It is uniquely solvable for a given initial value of $\phi^*\psi$ at $r=r_0>0$ and $v=v_0$. Hence if $\phi^*\psi|_{r=r_0,v=v_0}=0$, then $\phi^*\psi=0$ identically for $r>0$.

Let ζ_0 be a constant number or a nonconstant solution of (2.19). Take $Z=\mathrm{diag}(\zeta_1,...,\zeta_N)$ with $\zeta_j=\zeta_0$ or $\overline{\zeta_0}$, $H=(h_1,\ldots,h_N)$ where h_j is a column solution of (1.8) with $\zeta=\zeta_j$ such that $\det H\neq 0$ and $h_i^*h_j=0$ for $\zeta_i=\overline{\zeta_j}$. Then, the Darboux transformation given by Theorem 1 keeps the U(N) reduction. That is, $\tilde{A}_\mu^*=-\tilde{A}_\mu$, $\tilde{\Phi}^*=-\tilde{\Phi}$. This is proved similarly to the U(N) reduction for other systems like the AKNS system.

Darboux transformation of higher degree can be obtained by composition of Darboux transformations of degree one. However, when $G=\mathrm{U}(N)$, there is the following special and more explicit construction.

Let $\zeta^{(i)}$ $(i=1,\ldots,r)$ be constant numbers or nonconstant solutions of (2.19), $h^{(i)}$ be a column solution of (1.8) with $\zeta=\zeta^{(i)}$. Consider the composition of r Darboux transformations of degree one. In the ith Darboux transformation, let

$$Z=Z^{(j)}\equiv\mathrm{diag}(\zeta^{(j)},\overline{\zeta}^{(j)},\ldots,\overline{\zeta}^{(j)}),\quad H=H^{(j)}\equiv(h_1^{(j)},\ldots,h_N^{(j)}), \tag{3.2}$$

where $h_1^j=h^{(j)}$ and $h_k^{(j)}$ $(k=2,3,\ldots,n)$ are solutions of (1.8) with $\zeta=\overline{\zeta}^{(j)}$ and satisfy $h_k^{(j)*}h^{(j)}=0$. In this case, the Darboux transformation of degree r can be constructed in the following way, which does not depend on $h_k^{(j)}$ $(j=1,2,\ldots,r;\ k=2,3,\ldots,n)$.

Let

$$\Gamma_{ij}=\frac{h^{(i)*}h^{(j)}}{\overline{\zeta}^{(i)}-\zeta^{(j)}}, \tag{3.3}$$

then $G=(G_{ij})$ with

$$G_{ij}=\prod_{j=1}^{r}(\zeta-\overline{\zeta}^{(j)})\left(1+\sum_{i,j=1}^{r}\frac{h^{(i)}(\Gamma^{-1})_{ij}h^{(j)*}}{\zeta-\overline{\zeta}^{(j)}}\right) \tag{3.4}$$

is a Darboux matrix for (1.8).[6,7]

IV. SOLITON SOLUTIONS

Soliton solutions are obtained in the following way.

Take seed solution $A_\mu=0$ $(\mu=u,v,r)$, $\Phi=0$. Considering the gauge equivalence in (2.12), we can always choose $R=1$ and $T=S$. From (2.12)–(2.15), (2.17), and (2.18), we have

$$\tilde{A}_u=0,\quad \tilde{A}_v=-(\partial_vS)S^{-1}=\frac{1}{2r}\partial_rS, \tag{4.1}$$

$$\tilde{A}_r=-\frac{1}{2}(\partial_r S)S^{-1}=-\frac{1}{r}(\partial_u S+1),\quad \tilde{\Phi}=-\frac{r}{2}(\partial_r S)S^{-1}=-\partial_u S-1,$$

and

$$\tilde{F}_{uv}=[\tilde{D}_u,\tilde{D}_v]=\frac{1}{2r}\partial_u\partial_r S,$$

$$\tilde{F}_{ur}=[\tilde{D}_u,\tilde{D}_r]=-\frac{1}{r}\partial_u\partial_u S, \tag{4.2}$$

$$\tilde{F}_{vr}=[\tilde{D}_v,\tilde{D}_r]=-\frac{1}{2r}(\partial_r\partial_r+2\partial_u\partial_v)S+\frac{1}{2r^2}\partial_r S-\frac{1}{2r^2}[\partial_r S,\partial_u S].$$

Here we always suppose Z is diagonal with $Z=\mathrm{diag}(\zeta_1,\ldots,\zeta_N)$. Then the corresponding h_i's are solved from (1.8) explicitly.

Case 1: ζ_i is a constant.

Then h_i satisfies

$$\begin{aligned} r\partial_r h_i-2(\zeta_i-u)\partial_u h_i=0,\\ 2\partial_v h_i+\frac{\zeta_i-u}{r}\partial_r h_i=0. \end{aligned} \tag{4.3}$$

Hence

$$h_i=f_i(\omega(\zeta_i)), \tag{4.4}$$

where f_i is an arbitrary holomorphic vector function of $\omega(\zeta_i)$ and

$$\omega(\zeta)=v-\frac{r^2}{\zeta-u}. \tag{4.5}$$

Case 2: ζ_i is not a constant.

According to (2.20), ζ_i satisfies

$$v-\frac{r^2}{\zeta_i-u}=C_i(\zeta_i), \tag{4.6}$$

where C_i is an arbitrary holomorphic function. h_i should be a solution of (4.3) with this ζ_i, which is

$$h_i=f_i(\zeta_i), \tag{4.7}$$

where f_i is an arbitrary holomorphic vector function. The Darboux transformation is also given by $S=HZH^{-1}-u$ with $H=(h_1,\ldots,h_N)$ when $\det H\neq 0$.

Multisolitons can be obtained by the composition of Darboux transformations of degree one or by (3.3) and (3.4) directly in U(N) case.

V. EXAMPLES FOR SU(2) CASE

Now we consider the soliton solutions for the simplest non-Abelian group $G=\mathrm{SU}(2)$.

A. Single soliton solutions with constant spectral parameter

Take ζ_0 to be a complex constant which is not real, $Z=\mathrm{diag}(\zeta_0,\overline{\zeta_0})$. Let $\tau=\omega(\zeta_0)$, then

$$H=\begin{pmatrix}\alpha(\tau) & -\overline{\beta(\tau)}\\ \beta(\tau) & \overline{\alpha(\tau)}\end{pmatrix}, \tag{5.1}$$

where α, β are two holomorphic functions. Let $\sigma(\tau)=\beta(\tau)/\alpha(\tau)$, then

$$S=\frac{\zeta_0-\overline{\zeta_0}}{1+|\sigma|^2}\begin{pmatrix}1 & \overline{\sigma}\\ \sigma & |\sigma|^2\end{pmatrix}+\overline{\zeta_0}-u, \tag{5.2}$$

$$\tilde{\Phi}=-\partial_u S-1=\frac{\zeta_0-\overline{\zeta_0}}{(1+|\sigma|^2)^2}\begin{pmatrix}(|\sigma|^2)_u & \overline{\sigma}^2\sigma_u-\overline{\sigma}_u\\ \sigma^2\overline{\sigma}_u-\sigma_u & -(|\sigma|^2)_u\end{pmatrix}, \tag{5.3}$$

and

$$-\mathrm{tr}\,\tilde{\Phi}^2=\frac{8(\mathrm{Im}\,\zeta_0)^2}{(1+|\sigma|^2)^2}|\partial_u\sigma|^2. \tag{5.4}$$

According to (1.1) and (4.5),

$$\tau=\frac{\zeta_0(Y+V)(U+X)-1-Y^2+V^2}{(\zeta_0(U+X)-Y+V)(U+X)}=\frac{\zeta_0(Y+V)+X-U}{\zeta_0(U+X)-Y+V}. \tag{5.5}$$

Denote

$$\xi=\zeta_0(Y+V)+X-U,\quad \eta=\zeta_0(X+U)-Y+V, \tag{5.6}$$

then both ξ and η cannot be zero anywhere on (1.1) when ζ_0 is not real. Hence τ is a smooth function of U,V,X,Y on (1.1). Moreover,

$$\partial_u\tau=-\frac{r^2}{(\zeta_0-u)^2}=-\frac{1}{\eta^2}. \tag{5.7}$$

Since $\sigma(\tau)$ is a meromorphic function of τ, suppose $\sigma(\tau)=\sigma_1(\tau)/\sigma_2(\tau)$ where $\sigma_1(\tau)$ and σ_2 are two holomorphic functions of τ without common zero. According to (5.4),

$$-\mathrm{tr}\,\tilde{\Phi}^2=\frac{8(\mathrm{Im}\,\zeta_0)^2|\sigma_2(\tau)\partial_\tau\sigma_1(\tau)-\sigma_1(\tau)\partial_\tau\sigma_2(\tau)|^2}{(|\sigma_1(\tau)|^2+|\sigma_2(\tau)|^2)^2}|\eta|^{-4}. \tag{5.8}$$

Hence, $\tilde{\Phi}$ can be extended smoothly to (1.1). Likewise, according to (4.1),

$$\begin{aligned}-\mathrm{tr}\,\tilde{A}_u^2=0,\quad -\mathrm{tr}\,\tilde{A}_v^2&=\frac{8(\mathrm{Im}\,\zeta_0)^2(|\sigma_2(\tau)\partial_\tau\sigma_1(\tau)-\sigma_1(\tau)\partial_\tau\sigma_2(\tau)|^2}{(|\sigma_1(\tau)|^2+|\sigma_2(\tau)|^2)^2}(U+X)^2|\eta|^{-2},\\ -\mathrm{tr}\,\tilde{A}_r^2&=\frac{8(\mathrm{Im}\,\zeta_0)^2(|\sigma_2(\tau)\partial_\tau\sigma_1(\tau)-\sigma_1(\tau)\partial_\tau\sigma_2(\tau)|^2}{(|\sigma_1(\tau)|^2+|\sigma_2(\tau)|^2)^2}(U+X)^2|\eta|^{-4}.\end{aligned} \tag{5.9}$$

Therefore, the solution $(\tilde{\Phi},\tilde{A}_u,\tilde{A}_v,\tilde{A}_r)$ is smooth on (1.1), hence is smooth on the whole $2+1$-dimensional anti-de Sitter space–time.

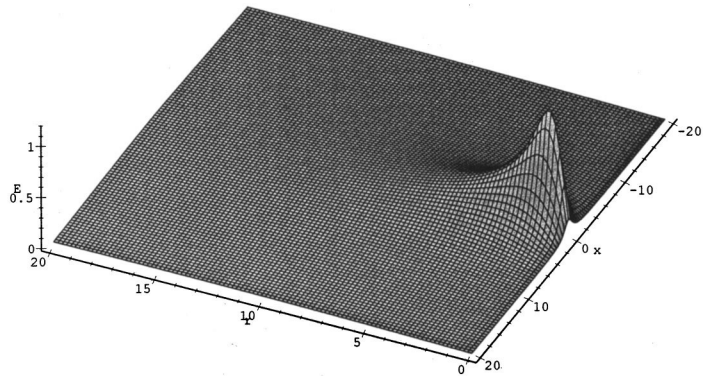

FIG. 1.

The infinity of the $2+1$-dimensional anti-de Sitter space–time includes only $r\to 0$. However, for the parameter space (t,r,x) $(r>0)$ with fixed t, the infinity of the derived half plane contains $r\to 0$ and $r^2+x^2\to\infty$. Here we call a solution localized if $-\operatorname{tr}\tilde{\Phi}^2\to 0$ when $r\to 0$ or $r^2+x^2\to\infty$ for fixed t.

Example 1: If $\zeta_0=\mathrm{i}$, $\tau=\omega(\zeta_0)$, $\sigma(\tau)=\tau$, this is just the localized solution (25) of Ref. 3, and

$$-\operatorname{tr}\tilde{\Phi}^2=\frac{8r^4}{((r^2+x^2-t^2)^2+2x^2+2t^2+1)^2}.$$

Let

$$x=tR\cos\theta,\quad r=tR\sin\theta. \tag{5.10}$$

When t and θ are fixed, $-\operatorname{tr}\tilde{\Phi}^2$ is a function of R only. Its maximum appears at $R=\pm\sqrt{t^2+1}/t$. Hence as $t\to\infty$, the ridge of the solution locates on the circle $x^2+r^2=t^2+1$.

Figures 1 and 2 describe this soliton at $t=0$ and $t=10$, respectively. In Figs. 1 and 2, the vertical axis is $(-\operatorname{tr}\tilde{\Phi}^2)^{1/4}$.

Example 2: $\tau=\omega(\zeta_0)$, $\sigma(\tau)$ is a polynomial of τ of degree k $(k\geqslant 1)$.

If $r\to 0$, then $\tau\to v$, $\partial_v\tau\to 1$ and all the other derivatives of τ (including derivatives of higher orders) tend to zero. According to (5.4), $-\operatorname{tr}\tilde{\Phi}^2\to 0$.

If $r^2+x^2\to\infty$, then (for fixed t)

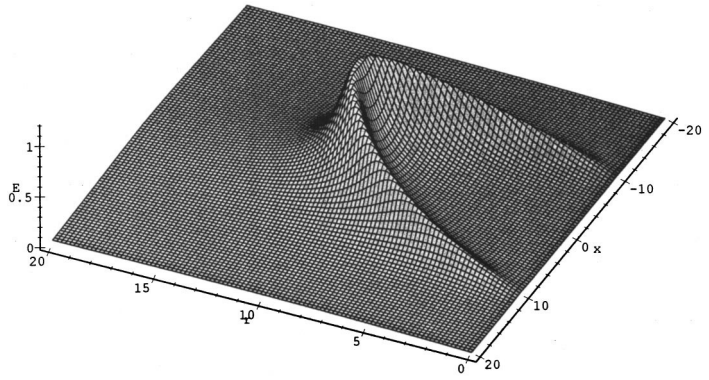

FIG. 2.

$$\tau=\frac{\zeta_0(x-t)-(r^2+x^2-t^2)}{\zeta_0-x-t}\to\infty. \tag{5.11}$$

Moreover, when t fixed, r^2+x^2 and $|\tau|$ are large enough, we have the estimates

$$\begin{aligned}&\frac{|\tau|^{k+1}|\partial_\tau\sigma|}{1+|\sigma|^2}\leqslant C_1\frac{|\tau|^{k+1}|\tau|^{k-1}}{1+|\tau|^{2k}}\leqslant C_1,\\ &\left|\frac{\partial_u\tau}{\tau^2}\right|(r^2+x^2)=\frac{r^2}{|\zeta_0(x-t)-(r^2+x^2-t^2)|^2}(r^2+x^2)\leqslant C_2,\end{aligned} \tag{5.12}$$

where C_1 and C_2 are independent of x and r, but may depend on ζ_0 and t. According to (5.4),

$$-\operatorname{tr}\tilde{\Phi}^2\leqslant\frac{8(\operatorname{Im}\zeta_0)^2C_1^2C_2^2}{|\tau|^{2k-2}}\frac{1}{(x^2+r^2)^2}\to 0. \tag{5.13}$$

Hence the solution is also localized whenever $\sigma(\tau)$ is a nonconstant polynomial of τ.

Now we consider the asymptotic behavior of the solution as $t\to\infty$ for $\zeta_0=i$. The following discussion in this example is qualitative and not rigorous.

Suppose all the roots of $\sigma(\tau)$ are simple roots. Denote $E=-\operatorname{tr}\tilde{\Phi}^2$. By (5.4), when τ is near a root of $\sigma(\tau)$, E may be large. Hence when τ is near a root of $\sigma(\tau)$, perhaps there will be a ridge in the graph of E.

From (4.5), the real and imaginary parts of $\tau=\omega(i)$ are

$$\begin{aligned}\operatorname{Re}\tau&=\frac{x-t+(x+t)(r^2+x^2-t^2)}{1+(x+t)^2},\\ \operatorname{Im}\tau&=\frac{r^2}{1+(x+t)^2}.\end{aligned} \tag{5.14}$$

When t is large and $x+t$ is not very small,

$$\operatorname{Re}\tau\approx\frac{r^2+x^2-t^2}{x+t}. \tag{5.15}$$

For a root ρ of $\sigma(\cdot)$, the points with

$$\frac{r^2+x^2-t^2}{x+t}=\operatorname{Re}\rho \tag{5.16}$$

are on the circle

$$C:\quad r^2+(x-\tfrac{1}{2}\operatorname{Re}\rho)^2=(t+\tfrac{1}{2}\operatorname{Re}\rho)^2. \tag{5.17}$$

On this circle C, for fixed t and $\operatorname{Re}\rho$, $\operatorname{Im}\tau$ can be expressed by x as

$$\operatorname{Im}\tau=\frac{t^2-x^2+\operatorname{Re}\rho(x+t)}{1+(x+t)^2}. \tag{5.18}$$

By computing $(\mathrm{d}/\mathrm{d}x)\operatorname{Im}\tau$, we know that $\operatorname{Im}\tau$ decreases when x increases if $x\geqslant -t+1$ and $t\geqslant -\operatorname{Re}\rho/2$. Hence it is easy to derive that $|\operatorname{Im}\tau|\leqslant 2$ when $t>|\operatorname{Re}\rho|$ and $x\geqslant 0$. Therefore, when $|\operatorname{Im}\rho|$ is not large, there will be a ridge of E on C.

When $|\operatorname{Im}\rho|\geqslant 1$, E is large on C only when $\operatorname{Im}\tau\approx\operatorname{Im}\rho$. If t is large and $x+t$ is not very small,

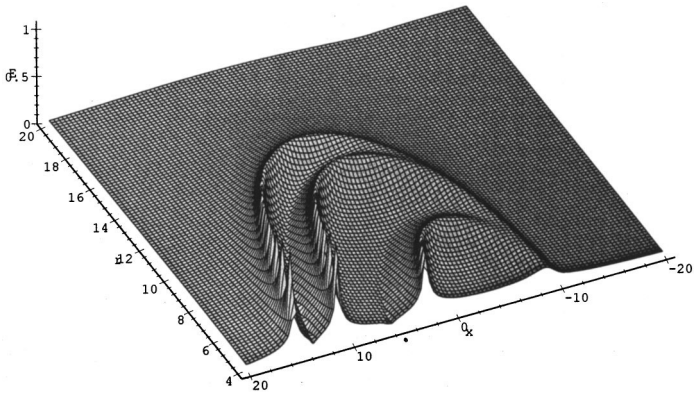

FIG. 3.

$$\operatorname{Im}\tau \approx \frac{t-x+\operatorname{Re}\rho}{x+t}. \tag{5.19}$$

The equation

$$\frac{t-x+\operatorname{Re}\rho}{x+t}=\operatorname{Im}\rho \tag{5.20}$$

has a unique solution

$$x=\frac{-(\operatorname{Im}\rho-1)t+\operatorname{Re}\rho}{\operatorname{Im}\rho+1}. \tag{5.21}$$

If $\operatorname{Im}\rho \gg 1$, then when t is large enough, x satisfies $-t \leqslant x \leqslant t+\operatorname{Re}\rho$. Hence there exists unique $r>0$ such that $(x,r)\in C$. This means that when $\operatorname{Im}\rho \gg 1$, there will be a peak rather than a ridge. If $\operatorname{Im}\rho \ll -1$, then when t is large enough, $x<-t$. Hence there does not exist $r>0$ such that $(x,r)\in C$, that is, there is neither ridge nor peak in the graph of E.

The above-presented discussion on the graph of E is summarized as follows. As $t\to\infty$, a root ρ with $|\operatorname{Im}\rho| \ll 1$ corresponds to a ridge, a root ρ with $\operatorname{Im}\rho \gg 1$ corresponds to a peak, and a root ρ with $\operatorname{Im}\rho \ll -1$ corresponds to nothing.

Figure 3 ($t=10$) shows the solution for

$$\sigma(\tau)=(\tau-2)(\tau-6)(\tau+6), \tag{5.22}$$

which has three real roots. It is plotted for $r \geqslant 4$ because the ridge is perpendicular to $r=0$ and the figures cannot be plotted well near $r=0$. Figure 4 shows its local behavior for a part of the region with $0 \leqslant r \leqslant 4$.

Figure 5 ($t=10$) shows the solution for

$$\sigma(\tau)=(\tau-2)(\tau-6)(\tau+6)(\tau-2i)(\tau-6i)(\tau+6i), \tag{5.23}$$

which has three real roots and three purely imaginary roots, but one imaginary root has the negative imaginary part. The solution has three ridges and two peaks.

Figure 6 ($t=10$) shows the solution for

$$\sigma(\tau)=(\tau-2-2i)(\tau-6-6i)(\tau+6-4i), \tag{5.24}$$

which has no real roots. In Fig. 6, there are three peaks.

Figure 7 ($t=10$) shows the solution for

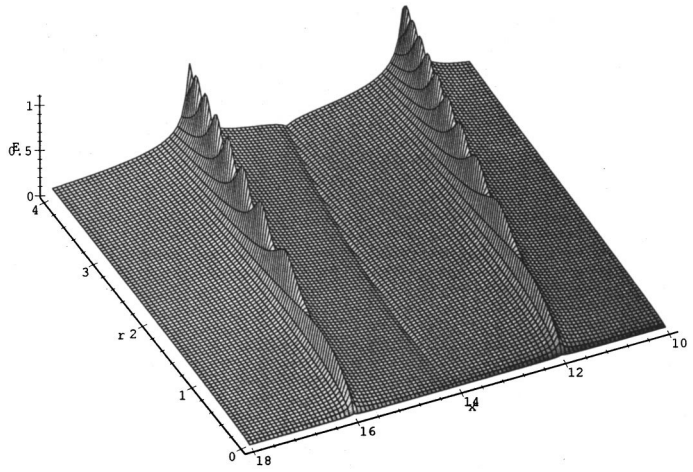

FIG. 4.

$$\sigma(\tau)=(\tau-2-2i)(\tau-6-6i)(\tau+6+6i), \tag{5.25}$$

which has no real roots, and only two roots have positive imaginary parts. In Fig. 7, there are only two peaks.

In all these figures (Figs. 3–7), the vertical axis is $(-\operatorname{tr}\tilde{\Phi}^2)^{1/8}$.

Example 3: $\zeta_0=i$, $\tau=\omega(i)$, $\sigma(\tau)=\sin(\mu\tau)$ where μ is a real constant.

If $r\to 0$, then $\tau\to v$, hence $E\to 0$. When the point $(x,r)\to\infty$ along the straight line $r=kx+b$ (k,b are real constants), (5.14) gives

$$\begin{aligned}\operatorname{Im}\tau&=\frac{(kx+b)^2}{1+(x+t)^2}\to k^2,\\ \operatorname{Re}\tau&=\frac{x-t+(x+t)((kx+b)^2+x^2-t^2)}{1+(x+t)^2}\sim(k^2+1)x.\end{aligned} \tag{5.26}$$

Denote $\mu\tau=p+qi$ where p and q are real, then

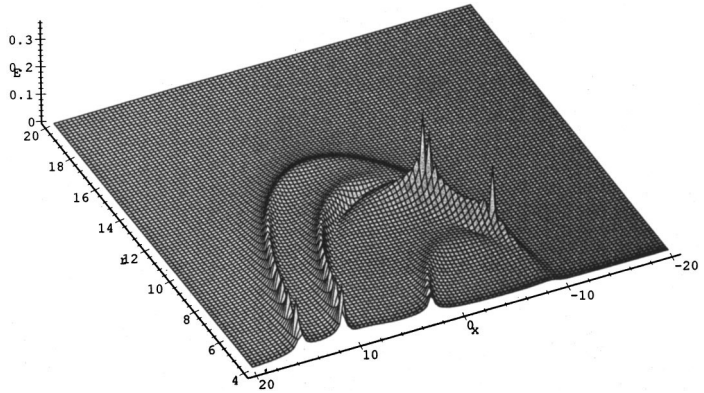

FIG. 5.

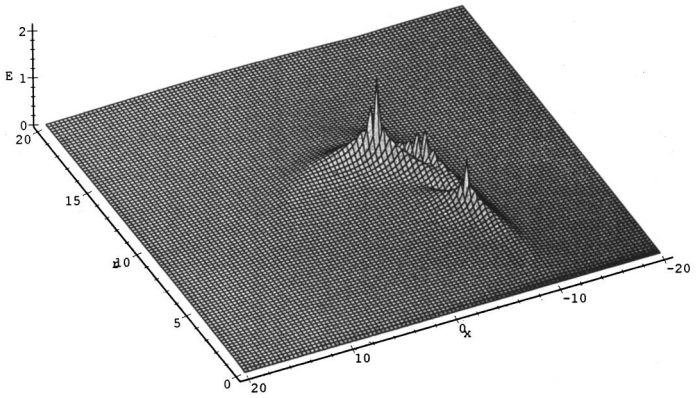

FIG. 6.

$$E=\frac{16\mu^2(\cosh(2q)+\cos(2p))}{(\cosh(2q)-\cos(2p)+2)^2}\frac{r^4}{(1+(x+t)^2)^2}\sim\frac{16\mu^2k^4(\cosh(2\mu k^2)+\cos(2\mu(k^2+1)x)}{(\cosh(2\mu k^2)-\cos(2\mu(k^2+1)x)+2)^2} \tag{5.27}$$

as $x^2+r^2\to\infty$. Hence the solution is bounded, but not localized in our definition [on the half (r,x,t) space]. However, as is shown, E tends to zero at the infinity of the $2+1$-dimensional anti-de Sitter space–time ($r=0$).

This solution is shown in Fig. 8 ($t=10$).

B. Single soliton solutions with nonconstant "spectral parameter"

In this case, ζ_0 should satisfy

$$v-\frac{r^2}{\zeta_0-u}=C(\zeta_0). \tag{5.28}$$

S, $\tilde{\Phi}$ are given by (5.2) and (5.3), and $-\operatorname{tr}\tilde{\Phi}^2$ is given by (5.4). However, in these expressions, ζ_0 is no longer a constant.

Contrary to the case where ζ_0 is a constant, here the solutions are defined only on the half (r,x,t) space. In general, they cannot be extended to the whole $2+1$-dimensional anti-de Sitter space–time.

Example 4: $C(\zeta_0)=C_0$ (constant), then

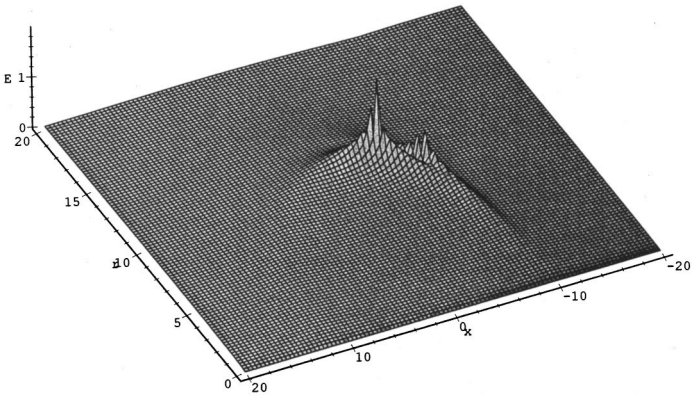

FIG. 7.

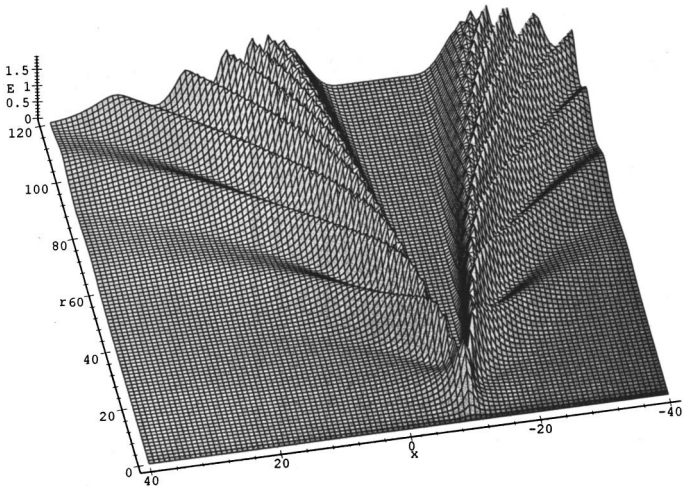

FIG. 8.

$$\zeta_0 = u - \frac{r^2}{C_0 - v}. \tag{5.29}$$

Let

$$H = \begin{pmatrix} \alpha(\zeta_0) & -\overline{\beta(\zeta_0)} \\ \beta(\zeta_0) & \overline{\alpha(\zeta_0)} \end{pmatrix},$$

where α and β are holomorphic functions of ζ_0 and $\sigma = \beta(\zeta_0)/\alpha(\zeta_0)$, then the Darboux matrix S is also given by (5.2). For example, if $\sigma(\zeta) = \zeta$ and $C_0 = i$, then $-\operatorname{tr}\tilde{\Phi}^2$ is completely the same as that in Example 1.

Example 5: $C(\zeta_0) = \zeta_0 + C_0$ where $C_0 = \alpha + \beta i$, α and β are real constants with $\beta \neq 0$, $\sigma(\zeta_0) = \zeta_0$.

Then

$$\zeta_0^2 - (u + v - C_0)\zeta_0 + uv + r^2 - C_0 u = 0. \tag{5.30}$$

The criteria of this quadratic equation is

$$\begin{aligned} \Delta &= (u + v - C_0)^2 - 4(uv + r^2 - C_0 u) \\ &= (u - v + C_0)^2 - 4r^2 \\ &= (2t + \alpha)^2 - 4r^2 - \beta^2 + 2\beta(2t + \alpha)i. \end{aligned} \tag{5.31}$$

When $t > -\alpha/2$, the imaginary part of Δ is never zero. Hence we can choose

$$\zeta_0 = \frac{u + v - C_0 + \sqrt{(u - v + C_0)^2 - 4r^2}}{2}, \tag{5.32}$$

where the square root takes the specific branch in the upper half-plane.

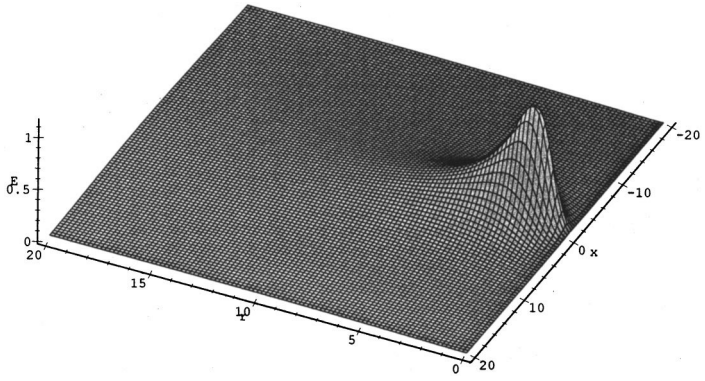

FIG. 9.

If $r\to 0$, then $\zeta_0\to u$, $\partial_u\zeta_0\to 1$ and all the other derivatives of ζ_0 tend to zero. Hence by (5.4), $-\mathrm{tr}\tilde{\Phi}^2\to 0$.

If $x^2+r^2\to\infty$ (t fixed),

$$\frac{|\zeta_0|}{\sqrt{x^2+r^2}}=\frac{1}{\sqrt{x^2+r^2}}\left|\frac{2x-C_0+\sqrt{(2t+C_0)^2-4r^2}}{2}\right|\to 1,$$

$$|\partial_u\zeta_0|=\frac{1}{2}\left|1+\frac{2t+C_0}{\sqrt{(2t+C_0)^2-4r^2}}\right|\leqslant C_3,\quad \frac{|\mathrm{Im}\,\zeta_0|}{r}\leqslant 2, \tag{5.33}$$

where C_3 is independent of x and r, but may depend on t, α, and β. According to (5.4) for $\sigma(\zeta_0)=\zeta_0$, $-\mathrm{tr}\,\tilde{\Phi}^2\to 0$ as $x^2+r^2\to\infty$. Hence the solution is also localized. However, it cannot be extended to the whole $2+1$-dimensional anti-de Sitter space–time smoothly because of the condition $t>-\alpha/2$.

This soliton is shown in Fig. 9 ($t=1$) and Fig. 10 ($t=10$) for $\alpha=0$ and $\beta=2$.

Example 6: $C(\zeta_0)=\zeta_0+C_0$, $C_0=\alpha+\beta i$ ($\beta\neq 0$) as previously, $\sigma(\zeta_0)$ is a polynomial of ζ_0 of degree k.

Then similar to (5.12), we have the estimates

$$\frac{|\zeta_0|^{k+1}|\partial_{\zeta_0}\sigma|}{1+|\sigma|^2}\leqslant C_1\frac{|\zeta_0|^{k+1}|\zeta_0|^{k-1}}{1+|\zeta_0|^{2k}}\leqslant C_1, \tag{5.34}$$

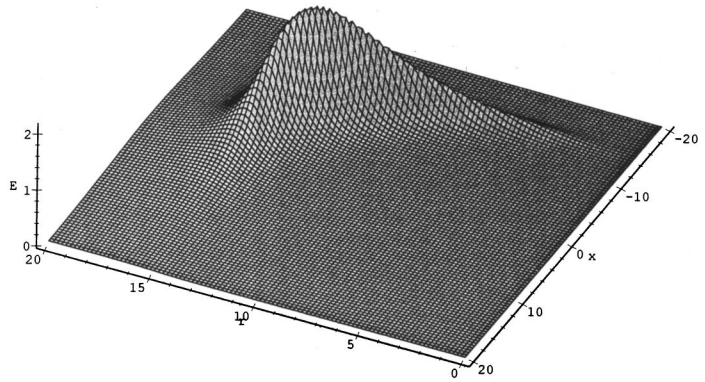

FIG. 10.

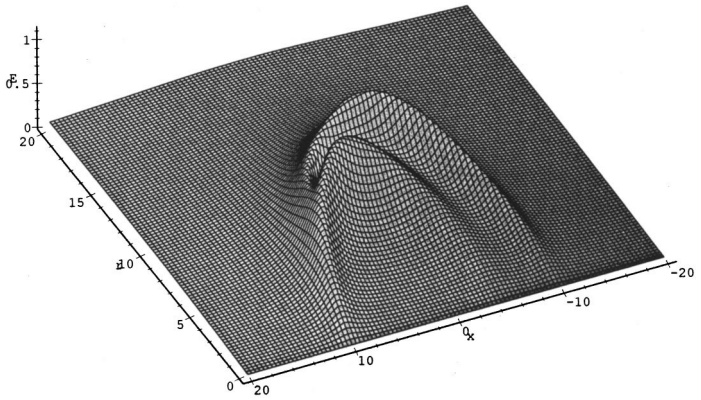

FIG. 11.

$$\left|\frac{\partial_u \zeta_0}{\zeta_0^2}\right|(r^2+x^2)\leqslant 2C_3$$

as $x^2+r^2\to\infty$ by (5.33). From (5.4), when $x^2+r^2\to\infty$,

$$-\operatorname{tr}\tilde{\Phi}^2\leqslant \frac{128C_1^2C_3^2}{|\zeta_0|^{2k-2}}\frac{r^2}{(r^2+x^2)^2}\to 0. \tag{5.35}$$

The solution is localized. As in the last example, this solution cannot be extended to the whole $2+1$-dimensional anti-de Sitter space–time.

C. Double soliton solutions

Double soliton solutions are obtained by Darboux transformations of degree two. Here we only show the following simple case for constant spectral parameters. In more complicated cases the double soliton solutions can also be derived similarly.

Example 7: Let $\zeta_1=i$, $\zeta_2=5+2i$, $\tau_j=\omega(\zeta_j)$, $\sigma_j(\tau_j)=\tau_j$ $(j=1,2)$. The double soliton is shown in Fig. 11 $(t=10)$.

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Quadratic Poisson algebras of two-dimensional classical superintegrable systems and quadratic associative algebras of quantum superintegrable systems

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The integrals of motion of the classical two-dimensional superintegrable systems with quadratic integrals of motion close in a restrained quadratic Poisson algebra, whose the general form is investigated. Each classical superintegrable problem has a quantum counterpart, a quantum superintegrable system. The quadratic Poisson algebra is deformed into a quantum associative algebra, the finite-dimensional representations of this algebra are calculated by using a deformed parafermion oscillator technique. It is shown that the finite dimensional representations of the quadratic algebra are determined by the energy eigenvalues of the superintegrable system. The calculation of energy eigenvalues is reduced to the solution of algebraic equations, which are universal, that is for all two-dimensional superintegrable systems with quadratic integrals of motion. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In classical mechanics, an integrable system is a system possessing more constants of motion than just the energy one. A comprehensive review of the two-dimensional integrable classical systems is given by Hietarinta,[1] where the space was assumed to be a flat real one. The case of nonflat space is under current investigation.[2,3] An interesting subset of the totality of integrable systems is the set of systems, which possess a maximum number of integrals, these systems are termed as superintegrable ones. The Coulomb and the harmonic oscillator potentials are the most familiar classical superintegrable systems, whose their quantum counterpart has nice symmetry properties, which are described by the $so(2N)$ and $su(N)$ Lie algebras, respectively.

The Hamiltonian of a classical system is generally a quadratic function of the momenta. All the ''nondegenerate'' superintegrable systems with quadratic integrals of motion in a complex flat space have been classified recently by Kalnins, Miller and Pogosyan.[4] In that paper the term ''nondegenerate'' means that the potential depends on four independent parameters. These potentials are indeed separable in more than one orthogonal system of coordinates. This classification enlarges the class of the known two-dimensional superintegrable systems with quadratic integrals of motion in the real flat space. These potentials are simultaneously separable in more than two orthogonal coordinate systems.[5] The notions of the multiseparability and superintegrability do not coincide. There are several known examples, the most illustrative one is the anisotropic harmonic oscillator with a rational ratio of frequencies. These potentials do not possess quadratic integrals of motion. An example, where the integrals of motion are quadratic ones but nonseparable in more than one system of coordinates, is given in Ref. 6.

The integrals of motion of a two-dimensional superintegrable system in flat space close in a restrained classical Poisson algebra.[4,7–9] The general form of the Poisson algebra has been studied in Ref. 4. In the case of the potentials with two quadratic integrals of motion the Poisson algebra is a quadratic Poisson algebra. In Ref. 4 these quadratic Poisson algebras are listed for all super-

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integrable systems in the complex flat space. In Ref. 10 the quadratic algebras for the superintegrable on the sphere are given for all classified cases.

The study of the quadratic Poisson algebras is a matter under investigation, related to several branches of physics as the solution of the classical Yang–Baxter equation,[11] the two-dimensional superintegrable systems in flat space or on the sphere,[9] the statistics[12] or the case of ''exactly solvable'' classical problems.[13]

The quantization of a classical integrable system corresponds generally to a quantum integrable system. The mechanism of quantum deformation of a classical system to a quantum one is not fully understood. Initially the problem of quantization of classical superintegrable system was viewed as a relatively simple and somehow trivial problem,[14] but several authors have proved that this quantization procedure has to add correction terms to the integrals of motion or to the Hamiltonian, these correction terms are of order $\mathcal{O}(\hbar^2)$.[15,16] The result of the quantum deformation of a superintegrable system is realized by the shift of the classical Poisson algebra to some quantum polynomial associative algebra. The same fact is true in the case of quadratic Poisson algebra corresponding to the Yang–Baxter equation,[11] which is turned into a quantum quadratic associative algebra[17] with four generators. The same idea was discussed in reference Ref. 13, where the classical problems, which are expressed by a quadratic Poisson algebra, are mapped to quantum ones described by the corresponding quantum operator quadratic algebra. The same shift is indeed true for the superintegrable systems, where the classical ones correspond to the quantum ones and the classical quadratic Poisson algebra is mapped to a quadratic associative algebra.[18–22]

The deformation of the classical Poisson algebra to a quadratic associative algebra implies a deformation of the parameters of the quadratic algebra.[4] The general form of the quadratic algebras, which are encountered in the case of the two-dimensional quantum superintegrable systems, is investigated in this paper. In Refs. 7, 8, 18–20,23–26 there was conjectured that the energy eigenvalues correspond to finite-dimensional representations of the latent quadratic algebras. Granovskii *et al.* in Ref. 13 studied the representations of the quadratic Askey–Wilson algebras $QAW(3)$. In their work using there the proposed ladder representation, the finite dimensional representations are calculated and this method was applied to several superintegrable systems.[18–20,24,26] Another method[7,8] for calculating the finite dimensional representations is the use of the deformed oscillator algebra[27] and their finite-dimensional version which are termed as ''generalized deformed parafermionic algebras.''[28] Our main task in this paper is to reduce the calculations of eigenvalues to a system of two algebraic equations with two parameters to be determined. These equations are universal equations, which are valid of all superintegrable systems, with quadratic integrals of motion.

This paper is organized as follows: In Sec. II the general form of the quadratic Poisson algebra for a two-dimensional system with quadratic integrals of motion is derived. In Sec. III the special form of the Poisson algebra of the known two-dimensional superintegrable systems in flat space is written. In Sec. IV the quantum version of the Poisson quadratic algebra is studied. The deformed parafermionic oscillator algebra is reviewed and the oscillator realization of the quadratic algebras is realized. The finite-dimensional representations of the quadratic algebras are generated by using the technique of deformed parafermionic algebras. The problem is reduced to the solution of a system of two algebraic equations in Sec. VI. In Sec. VII the energy eigenvalues of all the known superintegrable systems in the flat two-dimensional space are determined by solving the appropriate algebraic equations. Finally, in Sec. VIII there is a discussion of the results of this paper.

II. QUADRATIC POISSON ALGEBRAS

Let us consider a two-dimensional superintegrable system. The general form of the Hamiltonian is

$$H=a(q_1,q_2)p_1^2+2b(q_1,q_2)p_1p_2+c(q_1,q_2)p_2^2+V(q_1,q_2); \tag{1}$$

this Hamiltonian is a quadratic form of the momenta. The system is superintegrable, therefore

there are two additional integrals of motion A and B. In that section, we assume that these integrals of motion are quadratic functions of the momenta, i.e., they are given by the general forms:

$$A=A(q_1,q_2,p_1,p_2)=c(q_1,q_2)p_1^2+2d(q_1,q_2)p_1p_2+e(q_1,q_2)p_2^2 + f(q_1,q_2)p_1+g(q_1,q_2)p_2+Q(q_1,q_2).$$

The integral of motion B is assumed to be indeed a quadratic form, which is analogous to above one:

$$B=B(q_1,q_2,p_1,p_2)=h(q_1,1_2)p_1^2+2k(q_1,q_2)p_1p_2+l(q_1,q_2)p_2^2 + m(q_1,q_2)p_1+n(q_1,q_2)p_2+S(q_1,q_2).$$

By definition the following relations are satisfied:

$$\{H,A\}_P=\{H,B\}_P=0, \tag{2}$$

where $\{\,.\,,.\,\}_P$ is the usual Poisson bracket.

From the integrals of motion A, B, we can construct the integral of motion:

$$C=\{A,B\}_P\,. \tag{3}$$

The integral of motion C is not a new independent integral of motion, which is a cubic function of the momenta. The integral C is not independent from the integrals H, A and B as it will be shown later. The fact that the integral C is a cubic function of momenta implies the impossibility of expressing C as a polynomial function of the other integrals, which are quadratic functions of momenta. Starting from the integral of motion C, we can construct the (nonindependent) integrals $\{A,C\}_P$ and $\{B,C\}_P$. These integrals are quartic functions of the momenta, i.e., functions of fourth order. Therefore these integrals could be expressed as quadratic combinations of the integrals H, A and B. Therefore the following relations are assumed to be valid:

$$\{A,C\}_P=\alpha A^2+\beta B^2+2\gamma AB+\delta A+\epsilon B+\zeta \tag{4}$$

and

$$\{B,C\}_P=aA^2+bB^2+2cAB+dA+eB+z. \tag{5}$$

By taking an appropriate linear combination of the integrals A and B, we can always consider the case $\beta=0$.

The Jacobi equality for the Poisson brackets induces the relation

$$\{A,\{B,C\}_P\}_P=\{B,\{A,C\}_P\}_P\,.$$

The following relations:

$$b=-\gamma,\quad c=-\alpha \text{ and } e=-\delta$$

must be satisfied.

The integrals A, B and C satisfy the quadratic Poisson algebra:

$$\{A,B\}_P=C,$$

$$\{A,C\}_P=\alpha A^2+2\gamma AB+\delta A+\epsilon B+\zeta, \tag{6}$$

$$\{B,C\}_P=aA^2-\gamma B^2-2\alpha AB+dA-\delta B+z,$$

where α, γ, a are constants and

$$\delta=\delta(H)=\delta_0+\delta_1 H,$$

$$\epsilon=\epsilon(H)=\epsilon_0+\epsilon_1 H,$$

$$\zeta=\zeta(H)=\zeta_0+\zeta_1 H+\zeta_2 H^2,$$

$$d=d(H)=d_0+d_1 H,$$

$$z=z(H)=z_0+z_1 H+z_2 H^2,$$

where δ_i, ϵ_i, ζ_i, d_i and z_i are constants. The associative algebra, whose the generators satisfy equations (6), is the general form of the closed Poisson algebra of the integrals of superintegrable systems with integrals quadratic in momenta.

The quadratic Poisson algebra (6) possess a Casimir which is a function of momenta of degree 6 and it is given by

$$\begin{aligned}K=&C^2-2\alpha A^2B-2\gamma AB^2-2\delta AB-\epsilon B^2-2\zeta B\\&+\frac{2}{3}aA^3+dA^2+2zA\\=&k_0+k_1H+k_2H^2+k_3H^3.\end{aligned}\tag{7}$$

Obviously

$$\{K,A\}_P=\{K,B\}_P=\{K,C\}_P=0.$$

Therefore the integrals of motion of a superintegrable two-dimensional system with quadratic integrals of motion close a constrained classical quadratic Poisson algebra (6), corresponding to a Casimir equal at most to a cubic function of the Hamiltonian (7).

In the general case of a superintegrable system the integrals are not necessarily quadratic functions of the momenta, but rather polynomial functions of the momenta. The case of the systems with a quadratic and a cubic integral of motion are recently studied by Tsiganov.[29] The general form of the Poisson algebra of generators A, B and C is characterized by a polynomial function $h(A,B)$, which satisfy the following equations:

$$\begin{aligned}\{A,B\}_P&=C,\\\{A,C\}_P&=\partial h/\partial B,\\\{B,C\}_P&=-\partial h/\partial A.\end{aligned}\tag{8}$$

The above general forms of the Poisson algebra were introduced by Kalnins, Miller and Pogosyan.[4] The Casimir of the algebra is given by

$$K=K(H)=C^2-2h(A,B),\quad \{K,A\}_P=\{K,B\}_P=0,\tag{9}$$

where $h(A,B)$ is a polynomial function of the integrals of motion A and B. These relations are also discussed in Ref. 4 in a slightly different context.

In the case of the quadratic Poisson algebra (6) the form of the function $h(A,B)$ is given by the equation

$$\begin{aligned}h(A,B)=&-\frac{a}{3}A^3+\alpha A^2B+\gamma AB^2\\&-\frac{d}{2}A^2+\delta AB+\frac{\epsilon}{2}B^2-zA+\zeta B.\end{aligned}$$

In the general case of a two-dimensional superintegrable system, with quadratic Hamiltonian, one integral A of order m in momenta and one integral B of order n $(n \geqslant m)$, the form of the function $h(A,B)$, in most cases, can be given by the general form

$$h(A,B)=h_0(A)+h_1(A)B+h_2(A)B^2,$$

where $h_i(A)$ are polynomials of the integrals A and H. The proof of this assumption is based on the dependence of the integrals of motion on the momenta. This is true almost for the potentials with a cubic integral of motion.

III. POISSON ALGEBRAS FOR SUPERINTEGRABLE SYSTEMS

Let us consider the superintegrable systems with quadratic integrals of motion, these potentials are given by several authors starting from different but comparable points of view. In Refs. 1, 2 the integrals of motion are generated by solving the Darboux conditions for the integrability of quadratic integrals. In Ref. 5 the Hamilton–Jacobi equation is solved by the separation of variables and the two-dimensional Hamiltonians which are separable in more than one coordinate system are obtained. The separation of variables is essential for solving the quantum counterpart of the superintegrable system and the solution of the associate Schrödinger equations is given in Ref. 9. Using this method the quantum superintegrable systems have been solved on the sphere[9] and the hyperboloid.[9,22] From a classical point of view the super integrable systems are given in Ref. 3, while the case of a pseudo Euclidean kinetic term has been studied in Ref. 2. The extension on the systems with a quadratic and a cubic integral of motion is sytematized in Ref. 29.

In this section we consider the case of superintegrable systems given in Ref. 9, because in the next sections we study the quantum counterparts of these potentials. The study of these cases has been extended in the complex flat space in Ref. 4.

In this paper the following superintegrable systems are considered.

Potential (i):

$$H=\frac{1}{2}\left(p_x^2+p_y^2+\omega^2 r^2+\frac{\mu_1}{x^2}+\frac{\mu_2}{y^2}\right).$$

This potential has the following independent integrals of motion:

$$A=p_x^2+\omega^2 x^2+\frac{\mu_1}{x^2}$$

and

$$B=(xp_y-yp_x)^2+r^2\left(\frac{\mu_1}{x^2}+\frac{\mu_2}{y^2}\right).$$

The constants, which characterize the corresponding quadratic algebra (6), are given by

$$\begin{array}{lll} \alpha=-8, & \gamma=0, & \delta=16H, \\ \epsilon=-16\omega^2, & \zeta=16(\mu_1+\mu_2)\omega^2, & \\ a=0, & d=0, & z=16(\mu_2-\mu_1)\omega^2, \end{array}$$

the value of the Casimir (7) is

$$K=-16((\mu_2-\mu_1)^2\omega^2+4\mu_1 H^2).$$

Potential (ii):

$$H=\frac{1}{2}\left(p_x^2+p_y^2+\omega^2(4x^2+y^2)+\frac{\mu}{y^2}\right).$$

This potential has the following independent integrals of motion:

$$A=p_x^2+4\omega^2x^2$$

and

$$B=(xp_y-yp_x)p_y+\frac{\mu x}{y^2}-\omega^2xy^2.$$

The constants, which characterize the corresponding quadratic algebra (6), are given by

$$\begin{aligned}&\alpha=0, \quad \gamma=0, \quad \delta=0,\\ &\epsilon=-16\omega^2, \quad \zeta=0,\\ &a=-6, \quad d=16H, \quad z=8\mu\omega^2-8H^2,\end{aligned}$$

the value of the Casimir (7) is

$$K=0.$$

Potential (iii):

$$H=\frac{1}{2}\left(p_x^2+p_y^2+\frac{k}{r}+\frac{1}{r}\left(\frac{\mu_1}{r+x}+\frac{\mu_2}{r-x}\right)\right).$$

This potential has the following independent integrals of motion:

$$A=(xp_y-yp_x)^2+r\left(\frac{\mu_1}{r+x}+\frac{\mu_2}{r-x}\right)$$

and

$$B=(xp_y-yp_x)p_y-\frac{\mu_1}{2r}\frac{r-x}{r+x}+\frac{\mu_2}{2r}\frac{r+x}{r-x}+\frac{kx}{2r}.$$

The constants, which characterize the corresponding quadratic algebra (6), are given by

$$\begin{aligned}&\alpha=0, \quad \gamma=0, \quad \delta=0,\\ &\epsilon=0, \quad \zeta=-\mu_1\mu_2/2,\\ &a=0, \quad d=-2H, \quad z=4\frac{\mu_1^2-\mu_2^2}{4},\end{aligned}$$

the value of the Casimir (7) is

$$K=2(\mu_1-\mu_2)^2H-k^2(\mu_1+\mu_2).$$

Potential (iv):

$$H=\frac{1}{2}\left(p_x^2+p_y^2+\frac{k}{r}+\mu_1\frac{\sqrt{r+x}}{r}+\mu_2\frac{\sqrt{r-x}}{r}\right).$$

This potential has the following independent integrals of motion:

$$A=(yp_x-xp_y)p_y+\frac{\mu_1(r-x)\sqrt{r+x}}{2r}-\frac{\mu_2(r+x)\sqrt{r-x}}{2r}-\frac{kx}{2r}$$

and

$$B=(xp_y-yp_x)p_x-\frac{\mu_1 x\sqrt{r-x}}{2r}+\frac{\mu_2 x\sqrt{r+x}}{2r}-\frac{ky}{2r}.$$

The constants, which characterize the corresponding quadratic algebra (6), are given by

$$\alpha=0,\qquad \gamma=0,\qquad \delta=0,$$
$$\epsilon=2H,\quad \zeta=-\mu_1\mu_2/2,$$
$$a=0,\qquad d=-2H,\qquad z=\frac{\mu_1^2-\mu_2^2}{4},$$

the value of the Casimir (7) is

$$K=-k^2H/2-k(\mu_1^2+\mu_2^2)/4.$$

IV. THE QUADRATIC ASSOCIATIVE ALGEBRA

The quantum counterparts of the classical systems, which have been studied in Sec. II, are quantum superintegrable systems. The quadratic classical Poisson algebra (6) possesses a quantum counterpart, which is a quadratic associative algebra of operators. The form of the quadratic algebra is similar to the classical Poisson algebra, the involved constants are generally functions of $\hbar$ and they should coincide with the classical constants in the case $\hbar\to 0$. Let us consider the quadratic associative algebra generated by the generators $\{A, B, C\}$, which satisfy the commutation relations,

$$[A,B]=C,$$
$$[A,C]=\alpha A^2+\beta B^2+\gamma\{A,B\}+\delta A+\epsilon B+\zeta, \tag{10}$$
$$[B,C]=aA^2+bB^2+c\{A,B\}+dA+eB+z.$$

After rotating the generators A and B, we can always consider the case $\beta=0$.

The Jacobi equality for the commutator induces the relation

$$[A,[B,C]]=[B,[A,C]],$$

the following relations:

$$b=-\gamma,\quad c=-\alpha\quad\text{and}\quad e=-\delta,$$

must be satisfied, and consequently the general form of the quadratic algebra (10) can be explicitly written as follows:

$$[A,B]=C, \tag{11}$$
$$[A,C]=\alpha A^2+\gamma\{A,B\}+\delta A+\epsilon B+\zeta, \tag{12}$$
$$[B,C]=aA^2-\gamma B^2-\alpha\{A,B\}+dA-\delta B+z. \tag{13}$$

The Casimir of this algebra is given by

$$K=C^2-\alpha\{A^2,B\}-\gamma\{A,B^2\}+(\alpha\gamma-\delta)\{A,B\}+(\gamma^2-\epsilon)B^2+(\gamma\delta-2\zeta)B+\frac{2a}{3}A^3+\left(d+\frac{a\gamma}{3}+\alpha^2\right)A^2+\left(\frac{a\epsilon}{3}+\alpha\delta+2z\right)A, \tag{14}$$

another useful form of the Casimir of the algebra is given by

$$K=C^2+\frac{2a}{3}A^3-\frac{\alpha}{3}\{A,A,B\}-\frac{\gamma}{3}\{A,B,B\}+\left(\frac{2\alpha^2}{3}+d+\frac{2a\gamma}{3}\right)A^2+\left(-\epsilon+\frac{2\gamma^2}{3}\right)B^2+\left(-\delta+\frac{a\gamma}{3}\right)\{A,B\}+\left(\frac{2\alpha\delta}{3}+\frac{a\epsilon}{3}+\frac{d\gamma}{3}+2z\right)A+\left(-\frac{\alpha\epsilon}{3}+\frac{2\delta\gamma}{3}-2\zeta\right)B+\frac{\gamma z}{3}-\frac{\alpha\zeta}{3}, \tag{15}$$

where

$$\{A,B,C\}=ABC+ACB+BAC+BCA+CAB+CBA.$$

This quadratic algebra has many similarities to the Racah algebra $QR(3)$, which is a special case of the Askey–Wilson algebra $QAW(3)$. The algebra (11)–(13) does not coincide with the Racah algebra $QR(3)$, if $a\neq 0$ in the relation (13). A representation theory can be constructed by following the same procedures as they were described by Granovskii, Lutzenko and Zhedanov in Refs. 13, 18, 19. In this paper we shall give another realization of this algebra using the deformed oscillator techniques.[27] The finite-dimensional representations of the algebra (10) will be constructed by constructing a realization of the algebra with the generalized parafermionic algebra introduced by Quesne.[28]

V. DEFORMED PARAFERMIONIC ALGEBRA

Let us now consider a realization of the algebra (11)–(13), by using the deformed oscillator technique, i.e., by using a deformed oscillator algebra[27] $\{b^\dagger,b,\mathcal{N}\}$, which satisfies the

$$[\mathcal{N},b^\dagger]=b^\dagger,\quad [\mathcal{N},b]=-b,\quad b^\dagger b=\Phi(\mathcal{N}),\quad bb^\dagger=\Phi(\mathcal{N}+1), \tag{16}$$

where the function $\Phi(x)$ is a ''well behaved'' real function which satisfies the boundary condition

$$\Phi(0)=0,\ \text{and}\ \Phi(x)>0,\quad \text{for}\ x>0. \tag{17}$$

As it is well known[27] this constraint imposes the existence a Fock type representation of the deformed oscillator algebra, i.e., there is a Fock basis $|n>$, $n=0,1,\ldots$, such that

$$\mathcal{N}|n\rangle=n|n\rangle,$$

$$b^\dagger|n\rangle=\sqrt{\Phi(n+1)}|n+1\rangle,\quad n=0,1,\ldots,$$

$$b|0\rangle=0,$$

$$b|n\rangle=\sqrt{\Phi(n)}|n-1\rangle,\quad n=1,2,\ldots.$$

The generalized deformed algebra given in Ref. 27 is equivalent to several deformed oscillator schemes as the Odaka–Kishi–Kamefuchi unification scheme,[30] the Beckers–Debergh unification scheme,[31] The Fibonacci oscillator,[32] for a discussion of deformation schemes see Ref. 33.

In the case of nilpotent deformed oscillator algebras, there is a positive integer p, such that

$$b^{p+1}=0,\ (b^{\dagger})^{p+1}=0;$$

the above equations imply that

$$\Phi(p+1)=0. \tag{19}$$

In that case the deformed oscillator (16) has a finite-dimensional representation, with dimension equal to $p+1$, these kinds of oscillators are called deformed parafermion oscillators of order p.

An interesting property of the deformed parafermionic algebra is that the existence of a faithful finite-dimensional representation of the algebra implies that

$$\mathcal{N}(\mathcal{N}-1)(\mathcal{N}-2)\cdots(\mathcal{N}-p)=0. \tag{20}$$

The above restriction and the constraints (17) and (19) imply that the general form of the structure function $\Phi(\mathcal{N})$ has the general form[28]

$$\Phi(\mathcal{N})=\mathcal{N}(p+1-\mathcal{N})(a_0+a_1\mathcal{N}+a_2\mathcal{N}^2+\cdots a_{p-1}\mathcal{N}^{p-1}).$$

A systematic study and applications of the parafermionic oscillator is given in references Refs. 28, 34–36.

We shall show that there is a realization of the quadratic algebra, such that

$$A=A(\mathcal{N}), \tag{21}$$

$$B=b(\mathcal{N})+b^{\dagger}\rho(\mathcal{N})+\rho(\mathcal{N})b, \tag{22}$$

where the $A(x)$, $b(x)$ and $\rho(x)$ are functions, which will be determined. In that case (11) implies

$$C=[A,B]\Rightarrow C=b^{\dagger}\Delta A(\mathcal{N})\rho(\mathcal{N})-\rho(\mathcal{N})\Delta A(\mathcal{N})b, \tag{23}$$

where

$$\Delta A(\mathcal{N})=A(\mathcal{N}+1)-A(\mathcal{N}).$$

Using Eqs. (21), (22) and (12) we find

$$\begin{aligned}
[A,C]&=[A(\mathcal{N}),b^{\dagger}\Delta A(\mathcal{N})\rho(\mathcal{N})-\rho(\mathcal{N})\Delta A(\mathcal{N})b]\\
&=b^{\dagger}(\Delta A(\mathcal{N}))^2\rho(\mathcal{N})+\rho(\mathcal{N})(\Delta A(\mathcal{N}))^2b\\
&=\alpha A^2+\gamma\{A,B\}+\delta A+\epsilon B+\zeta\\
&=b^{\dagger}(\gamma(A(\mathcal{N}+1)+A(\mathcal{N}))+\epsilon)\rho(\mathcal{N})\\
&\quad+\rho(\mathcal{N})(\gamma(A(\mathcal{N}+1)+A(\mathcal{N}))+\epsilon)b\\
&\quad+\alpha A(\mathcal{N})^2+2\gamma A(\mathcal{N})b(\mathcal{N})+\delta A(\mathcal{N})+\epsilon B(\mathcal{N})+\zeta;
\end{aligned} \tag{24}$$

therefore we have the following relations:

$$(\Delta A(\mathcal{N}))^2=\gamma(A(\mathcal{N}+1)+A(\mathcal{N}))+\epsilon, \tag{25}$$

$$\alpha A(\mathcal{N})^2+2\gamma A(\mathcal{N})b(\mathcal{N})+\delta A(\mathcal{N})+\epsilon b(\mathcal{N})+\zeta=0, \tag{26}$$

while the function $\rho(\mathcal{N})$ can be arbitrarily determined. In fact this function can be fixed, in order to have a polynomial structure function $\Phi(x)$ for the deformed oscillator algebra (16).

The solutions of equation (25) depend on the value of the parameter γ, while the function $b(\mathcal{N})$ is uniquely determined by Eq. (26) (provided that almost one of the parameters γ or ϵ is not zero). At this stage, the cases $\gamma\neq 0$ or $\gamma=0$ should be treated separately. We can see the following.

Case 1: $\gamma\neq 0$

In that case the solutions of Eqs. (25) and (26) are given by

$$A(\mathcal{N})=\frac{\gamma}{2}\left((\mathcal{N}+u)^2-1/4-\frac{\epsilon}{\gamma^2}\right), \tag{27}$$

$$b(\mathcal{N})=-\frac{\alpha((\mathcal{N}+u)^2-1/4)}{4}+\frac{\alpha\epsilon-\delta\gamma}{2\gamma^2} -\frac{\alpha\epsilon^2-2\delta\epsilon\gamma+4\gamma^2\zeta}{4\gamma^4}\frac{1}{((\mathcal{N}+u)^2-1/4)}. \tag{28}$$

Case 2: $\gamma=0$, $\epsilon\neq 0$

The solutions of Eqs. (25) and (26) are given by

$$A(\mathcal{N})=\sqrt{\epsilon}(\mathcal{N}+u), \tag{29}$$

$$b(\mathcal{N})=-\alpha(\mathcal{N}+u)^2-\frac{\delta}{\sqrt{\epsilon}}(\mathcal{N}+u)-\frac{\zeta}{\epsilon}. \tag{30}$$

The constant u will be determined later.

Using the above definitions of equations $A(\mathcal{N})$ and $b(\mathcal{N})$, the left hand side and right hand side of Eq. (13) give the following equation:

$$\begin{aligned}&2\Phi(\mathcal{N}+1)\left(\Delta A(\mathcal{N})+\frac{\gamma}{2}\right)\rho(\mathcal{N})-2\Phi(\mathcal{N})\left(\Delta A(\mathcal{N}-1)-\frac{\gamma}{2}\right)\rho(\mathcal{N}-1)\\ &\quad=aA^2(\mathcal{N})-\gamma b^2(\mathcal{N})-2\alpha A(\mathcal{N})b(\mathcal{N})+dA(\mathcal{N})-\delta b(\mathcal{N})+z.\end{aligned} \tag{31}$$

Equation (14) gives the following relation:

$$\begin{aligned}K=&\Phi(\mathcal{N}+1)(\gamma^2-\epsilon-2\gamma A(\mathcal{N})-\Delta A^2(\mathcal{N}))\rho(\mathcal{N})\\ &+\Phi(\mathcal{N})(\gamma^2-\epsilon-2\gamma A(\mathcal{N})-\Delta A^2(\mathcal{N}-1))\rho(\mathcal{N}-1)-2\alpha A^2(\mathcal{N})b(\mathcal{N})\\ &+(\gamma^2-\epsilon-2\gamma A(\mathcal{N}))b^2(\mathcal{N})+2(\alpha\gamma-\delta)A(\mathcal{N})b(\mathcal{N})+(\gamma\delta-2\zeta)b(\mathcal{N})\\ &+\tfrac{2}{3}aA^3(\mathcal{N})+(d+\tfrac{1}{3}a\gamma+\alpha^2)A^2(\mathcal{N})+(\tfrac{1}{3}a\epsilon+\alpha\delta+2z)A(\mathcal{N}).\end{aligned} \tag{32}$$

Equations (31) and (32) are linear functions of the expressions $\Phi(\mathcal{N})$ and $\Phi(\mathcal{N}+1)$; then the function $\Phi(\mathcal{N})$ can be determined, if the function $\rho(\mathcal{N})$ is given. The solution of this system, i.e., the function $\Phi(\mathcal{N})$ depends on two parameters u and K and it is given by the following formulas.

Case 1: $\gamma\neq 0$

$$\rho(\mathcal{N})=\frac{1}{3\cdot 2^{12}\cdot\gamma^8(\mathcal{N}+u)(1+\mathcal{N}+u)(1+2(\mathcal{N}+u))^2}$$

and

$$\Phi(\mathcal{N}) = -3072\gamma^6 K(-1+2(\mathcal{N}+u))^2$$
$$-48\gamma^6(\alpha^2\epsilon-\alpha\delta\gamma+a\epsilon\gamma-d\gamma^2)\cdot(-3+2(\mathcal{N}+u))(-1+2(\mathcal{N}+u))^4(1+2(\mathcal{N}+u))$$
$$+\gamma^8(3\alpha^2+4a\gamma)(-3+2(\mathcal{N}+u))^2(-1+2(\mathcal{N}+u))^4(1+2(\mathcal{N}+u))^2$$
$$+768(\alpha\epsilon^2-2\delta\epsilon\gamma+4\gamma^2\zeta)^2+32\gamma^4(-1+2(\mathcal{N}+u))^2(-1-12(\mathcal{N}+u)$$
$$+12(\mathcal{N}+u)^2)\cdot(3\alpha^2\epsilon^2-6\alpha\delta\epsilon\gamma+2a\epsilon^2\gamma+2\delta^2\gamma^2-4d\epsilon\gamma^2+8\gamma^3 z+4\alpha\gamma^2\zeta)$$
$$-256\gamma^2(-1+2(\mathcal{N}+u))^2\cdot(3\alpha^2\epsilon^3-9\alpha\delta\epsilon^2\gamma+a\epsilon^3\gamma+6\delta^2\epsilon\gamma^2-3d\epsilon^2\gamma^2$$
$$+2\delta^2\gamma^4+2d\epsilon\gamma^4+12\epsilon\gamma^3 z-4\gamma^5 z+12\alpha\epsilon\gamma^2\zeta-12\delta\gamma^3\zeta+4\alpha\gamma^4\zeta). \tag{33}$$

Case 2: $\gamma=0$, $\epsilon\neq 0$

$$\rho(\mathcal{N})=1,$$

$$\Phi(\mathcal{N}) = \frac{1}{4}\left(-\frac{K}{\epsilon}-\frac{z}{\sqrt{\epsilon}}-\frac{\delta}{\sqrt{\epsilon}}\frac{\zeta}{\epsilon}+\frac{\zeta^2}{\epsilon^2}\right)$$
$$-\frac{1}{12}\left(3d-a\sqrt{\epsilon}-3\alpha\frac{\delta}{\sqrt{\epsilon}}+3\left(\frac{\delta}{\sqrt{\epsilon}}\right)^2-6\frac{z}{\sqrt{\epsilon}}+6\alpha\frac{\zeta}{\epsilon}-6\frac{\delta}{\sqrt{\epsilon}}\frac{\zeta}{\epsilon}\right)(\mathcal{N}+u)$$
$$+\frac{1}{4}\left(\alpha^2+d-a\sqrt{\epsilon}-3\alpha\frac{\delta}{\sqrt{\epsilon}}+\left(\frac{\delta}{\sqrt{\epsilon}}\right)^2+2\alpha\frac{\zeta}{\epsilon}\right)(\mathcal{N}+u)^2$$
$$-\frac{1}{6}\left(3\alpha^2-a\sqrt{\epsilon}-3\alpha\frac{\delta}{\sqrt{\epsilon}}\right)(\mathcal{N}+u)^3+\frac{1}{4}\alpha^2(\mathcal{N}+u)^4. \tag{34}$$

The above formula is valid for $\epsilon>0$.

VI. FINITE-DIMENSIONAL REPRESENTATIONS OF QUADRATIC ALGEBRAS

Let us consider a representation of the quadratic algebra, which is diagonal to the generator A and the Casimir K. Using the parafermionic realization defined by Eqs. (21) and (22), we see that is this a representation diagonal to the parafermionic number operator $\mathcal{N}$ and the Casimir K. The basis of a such representation corresponds to the Fock basis of the parafermionic oscillator, i.e., the vectors $|k, n>$, $n=0,1,\ldots$, of the carrier Fock space satisfy the equations

$$\mathcal{N}|k,n\rangle = n|k,n\rangle, \quad K|k,n\rangle = k|k,n\rangle .$$

The structure function (33) [or, respectively, (33)] depend on the eigenvalues of the of the parafermionic number operator $\mathcal{N}$ and the Casimir K. The vectors $|k,n\rangle$ are also eigenvectors of the generator A, i.e.,

$$A|k,n\rangle = A(k,n)|k,n\rangle.$$

In the case $\gamma\neq 0$ we find from Eq. (27),

$$A(k,n)=\frac{\gamma}{2}\left((n+u)^2-1/4-\frac{\epsilon}{\gamma^2}\right).$$

In the case $\gamma=0$, $\epsilon\neq 0$ we find from Eq. (29),

$$A(k,n)=\sqrt{\epsilon}(n+u).$$

If the deformed oscillator corresponds to a deformed parafermionic oscillator of order p then the two parameters of the calculation k and u should satisfy the constraints (17) and (19) of the system:

$$\Phi(0,u,k)=0,$$
$$\Phi(p+1,u,k)=0; \tag{35}$$

then the parameter $u=u(k,p)$ is a solution of the system of Eqs. (35).

Generally there are many solutions of the above system, but a unitary representation of the deformed parafermionic oscillator is restrained by the additional restriction

$$\Phi(x)>0, \text{ for } x=1,2,\ldots,p\ .$$

We must point out that the system (35) corresponds to a representation with dimension equal to $p+1$.

The proposed method of calculation of the representation of the quadratic algebra is an alternative to the method given by Granovskii *et al.*[13,18–20] and reduces the search of the representations to the solution of a system of polynomial equations (35). Also it is applied to an algebra not included in the cases of the algebras, which are treated in the above references. We must point out, that there are several papers on the representations of quadratic (or generally polynomial algebras),[37–43] these algebras are deformations of the su(2) or osp(1/2) algebras. The general form of the quadratic algebra, which is studied in this paper, is different by definition from the deformed versions of su(2) or osp(1/2).

VII. QUADRATIC ALGEBRAS FOR THE QUANTUM SUPERINTEGRABLE SYSTEMS

In this section, we shall give an example of the calculation of eigenvalues of a superintegrable two-dimensional system, by using the methods of the previous section. The calculation by an empirical method was performed in Ref. 8 and the solution of the same problem by using the separation of variables was studied in Ref. 9. Here in order to show the effects of the quantization procedure we do not use $\hbar=1$ as considered in Refs. 8 and 9. That means that the following commutation relations are taken into consideration:

$$[x,p_x]=i\hbar, \quad [y,p_y]=i\hbar.$$

A. Potential (i)

$$H=\frac{1}{2}\left(p_x^2+p_y^2+\omega^2r^2+\frac{\mu_1}{x^2}+\frac{\mu_2}{y^2}\right).$$

This potential has the following independent integrals of motion:

$$A=p_x^2+\omega^2x^2+\frac{\mu_1}{x^2}$$

and

$$B=(xp_y-yp_x)^2+r^2\left(\frac{\mu_1}{x^2}+\frac{\mu_2}{y^2}\right).$$

The constants, which characterize the corresponding quadratic algebra (10), are given by

$$\alpha=8\hbar^2, \qquad \gamma=0, \qquad \delta=-16h^2H,$$
$$\epsilon=16\hbar^2\omega^2, \quad \zeta=-16\hbar^2(\mu_1+\mu_2)\omega^2+8\hbar^4\omega^2,$$
$$a=0, \qquad d=16\hbar^4, \qquad z=-16\hbar^2(\mu_2-\mu_1)\omega^2-16\hbar^4H;$$

the value of the Casimir (14) is

$$K=16\hbar^2((\mu_2-\mu_1)^2\omega^2+4\mu_1H^2)-16\hbar^4(3H^2+2\hbar^2\omega^2-2(\mu_1+\mu_2)).$$

For simplicity reasons we introduce the positive parameters k_1 and k_1, which are related to the potential parameters μ_1 and μ_2 by the relations

$$\mu_1=(k_1^2-\tfrac{1}{4})\hbar^2, \quad \mu_2=(k_2^2-\tfrac{1}{4})\hbar^2.$$

This quadratic algebra corresponds to the case $\gamma=0$ and $\epsilon>0$ of the algebra given by Eqs. (11)–(13). In that case, the structure function (34) of the deformed parafermionic algebra of Sec. V can be given by the simple form

$$\Phi(x)=16\hbar^4\left(x+u-\frac{1}{2}-\frac{k_1}{2}\right)\left(x+u-\frac{1}{2}+\frac{k_1}{2}\right)$$
$$\times\left(x+u-\frac{1}{2}-\frac{k_2}{2}-\frac{E}{2\hbar\omega}\right)\left(x+u-\frac{1}{2}+\frac{k_2}{2}-\frac{E}{2\hbar\omega}\right).$$

In the above formula E is the eigenvalue of the energy. The values of the parameters u and E corresponding to the representation of the parafermionic algebra of dimension $p+1$ are determined by the restrictions (35), which are transcribed as

$$\Phi(0)=0, \quad \Phi(p+1)=0.$$

One should notice that only the solutions which correspond to positive eigenvalues of the integral A must be retained. The acceptable solutions are four and correspond to the following values of the parameters u and E:

$$u=\frac{1}{2}+\frac{\epsilon_1k_1}{2}, \quad E=2\hbar\omega\left(p+1+\frac{\epsilon_1k_1+\epsilon_2k_2}{2}\right),$$

where $\epsilon_i=\pm1$. The corresponding structure function is

$$\Phi(x)=16\hbar^4x(p+1-x)(x+\epsilon_1k_1)(p+1-x+\epsilon_2k_2).$$

The corresponding eigenvalues of the operator A are given by

$$A(m)=4\hbar\omega\left(m+\frac{1+\epsilon_1k_1}{2}\right), \quad m=0,1,\ldots,p.$$

The structure function $\Phi(x)$ should be a positive function, for $x=1,2,\ldots,p$ therefore the constants k_i are restricted by the relations

$$\epsilon_1k_1>-1, \quad \epsilon_2k_2>-1.$$

B. Potential (ii)

$$H=\frac{1}{2}\left(p_x^2+p_y^2+\omega^2(4x^2+y^2)+\frac{\mu}{y^2}\right).$$

This potential has the following independent integrals of motion:

$$A=p_x^2+4\omega^2x^2$$

and

$$B=\frac{1}{2}\{xp_y-yp_x,p_y\}+\frac{\mu x}{y^2}-\omega^2xy^2.$$

The constants, which characterize the corresponding quadratic algebra (10), are given by

$$\begin{aligned}&\alpha=0, && \gamma=0, && \delta=0,\\ &\epsilon=16\hbar^2\omega^2, && \zeta=0, &&\\ &a=6\hbar^2, && d=-16\hbar^2H, && z=-8\hbar^2(\mu\omega^2-H^2)+6\hbar^4\omega^2;\end{aligned}$$

the value of the Casimir (14) is

$$K=64\hbar^4\omega^2H.$$

For simplicity reasons we introduce the positive parameter k, which is related to the potential parameter μ by the relation

$$\mu=(k^2-\tfrac{1}{4})\hbar^2.$$

This quadratic algebra corresponds to the case $\gamma=0$ and $\epsilon>0$ of the algebra given by Eqs. (11)–(13). In that case, the structure function (34) of the deformed parafermionic algebra of Sec. V can be given by the simple form

$$\Phi(x)=8\hbar^3\omega\left(x+u-\frac{1}{2}\right)\left(x+u-\frac{1}{2}-\frac{k}{2}-\frac{E}{2\hbar\omega}\right)\left(x+u-\frac{1}{2}+\frac{k}{2}-\frac{E}{2\hbar\omega}\right).$$

In the above formula E is the eigenvalue of the energy. The values of the parameters u and E corresponding to the representation of the parafermionic algebra of dimension $p+1$ are determined by the restrictions (35), which are transcribed as

$$\Phi(0)=0, \quad \Phi(p+1)=0.$$

One should notice that only the solutions which correspond to positive eigenvalues of the integral A must be retained. The acceptable solutions are four and correspond to the following values of the parameters u and E:

$$u=\frac{1}{2}, \quad E=2\hbar\omega\left(p+1+\frac{\epsilon k}{2}\hbar\right),$$

where $\epsilon=\pm1$. The corresponding structure function is

$$\Phi(x)=4\hbar^3x(p+1-x)(p+1-x+\epsilon k).$$

The structure function should be a positive function; therefore the values of the parameter k are restrained by

$$\epsilon k > -1.$$

The eigenvalues of the operator A are given by

$$A(m) = 4\hbar\omega(m + \tfrac{1}{2}), \quad m = 0,1,\ldots,p.$$

C. Potential (iii)

$$H = \frac{1}{2}\left(p_x^2 + p_y^2 + \frac{k}{r} + \frac{1}{r}\left(\frac{\mu_1}{r+x} + \frac{\mu_2}{r-x} \right) \right).$$

In Ref. 9 the parabolic coordinates have been used:

$$\begin{aligned} x &= \frac{1}{2}(\xi^2 - \eta^2), \quad & p_x &= \frac{\xi}{\xi^2+\eta^2} p_\xi - \frac{\eta}{\xi^2+\eta^2} p_\eta, \\ y &= \xi\eta, & p_y &= \frac{\eta}{\xi^2+\eta^2} p_\xi + \frac{\xi}{\xi^2+\eta^2} p_\eta, \\ [\xi, p_\xi] &= i\hbar, & [\eta, p_\eta] &= i\hbar. \end{aligned}$$

For comparison reasons we quote all the relations in both cartesian and parabolic systems, so

$$H = \frac{1}{\xi^2+\eta^2}\left(\frac{1}{2}(p_\xi^2 + p_\eta^2) + k + \frac{\mu_1}{\xi^2} + \frac{\mu_2}{\eta^2} \right).$$

This potential has the following independent integrals of motion:

$$\begin{aligned} A &= (xp_y - yp_x)^2 + r\left(\frac{\mu_1}{r+x} + \frac{\mu_1}{r-x} \right) \\ &= \frac{1}{2}\left(\frac{1}{2}(\eta p_\xi - \xi p_\eta)^2 + (\xi^2+\eta^2)\left(\frac{\mu_1}{\xi^2} + \frac{\mu_2}{\eta^2} \right) \right). \end{aligned}$$

and

$$\begin{aligned} B &= \frac{1}{2}\left(\{xp_y - yp_x, p_y\} - \frac{\mu_1}{r}\frac{r-x}{r+x} + \frac{\mu_2}{r}\frac{r+x}{r-x} + \frac{kx}{r} \right) \\ &= \frac{1}{\xi^2+\eta^2}\left(\frac{1}{2}(\xi^2 p_\eta^2 - \eta^2 p_\xi^2) + \mu_2\frac{\xi^2}{\eta^2} - \mu_1\frac{\eta^2}{\xi^2} + \frac{k}{2}\frac{\xi^2-\eta^2}{\xi^2+\eta^2} \right). \end{aligned}$$

The constants, which characterize the corresponding quadratic algebra (10), are given by

$$\begin{aligned} &\alpha = 0, && \gamma = 2\hbar^2, && \delta = 0, \\ &\epsilon = -\hbar^4, && \zeta = -\hbar^2 k(\mu_1 - \mu_2), && \\ &a = 0, && d = 8\hbar^2 H, && z = -\hbar^2(4(\mu_1+\mu_2)H - k^2/2) + \hbar^4 H; \end{aligned}$$

the value of the Casimir (14) is

$$K = -\hbar^2(2(\mu_1-\mu_2)^2 H - k^2(\mu_1+\mu_2)) - 2\hbar^4\left((\mu_1+\mu_2)H - \frac{k^2}{4} \right) + \hbar^6 H.$$

For simplicity reasons we introduce the positive parameters k_1 and k_1, which are related to the potential parameters μ_1 and μ_2 by the relations

$$\mu_1=\frac{\hbar^2}{2}\left(k_1^2-\frac{1}{4}\right),\quad \mu_2=\frac{\hbar^2}{2}\left(k_2^2-\frac{1}{4}\right).$$

This quadratic algebra corresponds to the case $\gamma\neq 0$ of the algebra given by Eqs. (11)–(13). In that case, the structure function (33) of the deformed parafermionic algebra of Sec. V can be given by the simple form

$$\Phi(x)=3\cdot 2^{14}\hbar^{16}(2x-1+k_1+k_2)(2x-1+k_1-k_2)(2x-1-k_1+k_2)$$
$$\cdot(2x-1-k_1-k_2)(8\hbar^2Hx^2-8\hbar^2Hx+2\hbar^2H+k^2)$$

In the above formula E is the eigenvalue of the energy. The values of the parameters u and E corresponding to the representation of the parafermionic algebra of dimension $p+1$ are determined by the restrictions (35), which are transcribed as

$$\Phi(0)=0,\quad \Phi(p+1)=0.$$

One should notice, that only the solutions which correspond to positive eigenvalues of the integral A must be retained. The acceptable solutions are four and correspond to the following values of the parameters u and E:

$$u=\frac{1}{2}(2+\epsilon_1k_1+\epsilon_2k_2),\quad E=-\frac{k^2}{2\hbar^2(2(p+1)+\epsilon_1k_1+\epsilon_2k_2)^2},$$

where $\epsilon_i=\pm 1$. The corresponding structure function is

$$\Phi(x)=3\cdot 2^{20}\cdot k^2\hbar^{16}\cdot x(p+1-x)(x+\epsilon_1k_1)(x+\epsilon_2k_2)\cdot(x+\epsilon_1k_1+\epsilon_2k_2)$$
$$\times\frac{(x+p+1+\epsilon_1k_1+\epsilon_2k_2)}{(2(p+1)+\epsilon_1k_1+\epsilon_2k_2)^2}.$$

The eigenvalues of the operator A are given by the formula

$$A(m)=\hbar^2\left(m+\epsilon_1k_1+\epsilon_2k_2+\frac{3}{2}\right)^2,\quad m=0,1,\ldots,p.$$

The positive sign of the structure function for $x=1,2,\ldots,p$ is obtained when

$$\epsilon_1k_1>-1,\quad \epsilon_2k_2>-1\quad\text{and}\quad \epsilon_1k_1+\epsilon_2k_2>-1.$$

D. Potential (iv)

$$H=\frac{1}{2}\left(p_x^2+p_y^2+\frac{k}{r}+\mu_1\frac{\sqrt{r+x}}{r}+\mu_2\frac{\sqrt{r-x}}{r}\right)$$

$$=\frac{1}{\xi^2+\eta^2}\left(\frac{1}{2}(p_\xi^2+p_\eta^2)+k+\mu_1\xi+\mu_2\eta\right).$$

This potential has the following independent integrals of motion:

$$A=\frac{1}{2}\left(\{(yp_x-xp_y),p_y\}+\frac{\mu_1(r-x)\sqrt{r+x}}{r}-\frac{\mu_2(r+x)\sqrt{r-x}}{r}-\frac{kx}{r}\right)$$

$$=\frac{1}{2(\xi^2+\eta^2)}(\eta^2p_\xi^2-\xi^2p_\eta^2+k(\eta^2-\xi^2)+2\xi\eta(\mu_1\eta-\mu_2\xi))$$

and

$$B=\frac{1}{2}\left(\{xp_y-yp_x,p_x\}-\frac{\mu_1 x\sqrt{r-x}}{r}+\frac{\mu_2 x\sqrt{r+x}}{r}-\frac{ky}{r}\right)$$

$$=-\frac{1}{2(\xi^2+\eta^2)}(\xi\eta(p_\xi^2+p_\eta^2)-(\xi^2+\eta^2)p_\xi p_\eta+2k\xi\eta$$
$$+(\mu_2\xi-\mu_1\eta)(\eta^2-\xi^2)).$$

The constants, which characterize the corresponding quadratic algebra (10), are given by

$$\alpha=0,\quad \gamma=0,\quad \delta=0,$$
$$\epsilon=-2\hbar^2H,\quad \zeta=\hbar^2\mu_1\mu_2/2,$$
$$a=0,\quad d=2\hbar^2H,\quad z=-\hbar^2(\mu_1^2-\mu_2^2)/4,$$

the value of the Casimir (14) is

$$K=\hbar^2k^2H/2+\hbar^2k(\mu_1^2+\mu_2^2)/4+\hbar^4H^2.$$

This quadratic algebra corresponds to the case $\gamma=0$ and $\epsilon>0$ of the algebra given by Eqs. (11)–(13). It is worth noticing that algebra is extremely simple, which can be reduced to the usual $su(2)$. We prefer to treat this algebra with the proposed methods in this paper for pedagogical reasons. The existence of the finite-dimensional representations of this algebra implies that the coefficient ϵ in Eq. (12) should be positive, therefore the energy operator H must have energy eigenvalues $E<0$. For simplicity reasons we introduce the new parameters:

$$\varepsilon=\sqrt{-2E}/\hbar,\quad \lambda=k/\hbar^2,$$

$$\nu_1=\mu_1/\hbar^2,\quad \nu_2=\mu_2/\hbar^2,\quad \nu^2=\nu_1^2+\nu_2^2.$$

The structure function (34) of the deformed parafermionic algebra of Sec. V can be given by the form

$$\Phi(x)=\frac{\hbar^4}{16\varepsilon^4}\left(\nu_1^2-\lambda\varepsilon^2+2\left(x+u-\frac{1}{2}\right)\varepsilon^3\right)\left(\nu_2^2-\lambda\varepsilon^2-2\left(x+u-\frac{1}{2}\right)\varepsilon^3\right).$$

In the above formula the parameter ε is related to the the eigenvalue E of the energy. The values of the parameters u and ε, corresponding to the representation of the parafermionic algebra of dimension $p+1$, are determined by the restrictions (35), which are transcribed as

$$\Phi(0)=0,\quad \Phi(p+1)=0.$$

The first condition can be used for determining the acceptable values of the parameter u. Two possible solutions are found:

$$u=u_1=\frac{\nu_2^2-\lambda\varepsilon^2+\varepsilon^3}{2\varepsilon^3},\tag{36}$$

$$u=u_2=-\frac{\nu_1^2-\lambda\varepsilon^2-\varepsilon^3}{2\varepsilon^3}.\tag{37}$$

Using these solutions and the condition $\Phi(p+1)=0$, we find that ε must satisfy two possible cubic equations:

$$u_1 \to 2(p+1)\varepsilon^3 - 2\lambda\varepsilon^2 + \nu^2 = 0, \tag{38}$$

$$u_2 \to 2(p+1)\varepsilon^3 + 2\lambda\varepsilon^2 - \nu^2 = 0. \tag{39}$$

If ε is a solution of Eq. (38) then $-\varepsilon$ is the solution of the other equation (39); therefore there is at least one solution which is positive. This solution leads to the structure function

$$\Phi(x) = \frac{\varepsilon^2}{4} x(p+1-x),$$

which is positive for $x = 1,2,\ldots,p$.

VIII. DISCUSSION

If we compare the quadratic associative algebra, introduced in Sec. IV with the corresponding Poisson algebra given in Sec. II, we see that in general, the quantum constants are similar to the classical ones up to a factor equal to $-h^2$, but there are quantum corrections of order h^4 and h^6. The knowledge of the classical constants of the Poisson algebra is not sufficient to reproduce the rules of quantum associative operator algebra. Therefore, the passage from the classic Poisson algebra to the noncommutative quantum algebra cannot be realized by simple replacements of the Poisson brackets by commutators and by a symmetrization procedure.

The energy eigenvalues of Sec. VII corroborate the results of Ref. 9 [the differences in the case of the potential (iv) are due to some misprints in that reference]. The calculation of the energy eigenvalues in Ref. 9 was achieved by solving the corresponding Schrödinger differential equations, while in this paper the energy eigenvalues are obtained by algebraic methods. The advantage of the proposed method is that the energy eigenvalues are reduced to simple algebraic calculations of the roots of polynomial equations, whose form is universally determined by the structure functions (33), (33) and the system (35). These equations are valid for any two-dimensional superintegrable system with integrals of motion, which are quadratic functions of the momenta. The same equations should be valid in the case of two-dimensional superintegrable systems in curved space.[44] The superintegrable systems bring up the open problem of the quantization of a Poisson algebra in a well determined context, because these systems and their quantum counterparts are explicitly known.

From the above discussion several open problems are risen.

- The calculation of the classical Poisson algebras and their quantum counterparts for the totality of the two-dimensional problems in curved space. This study will lead to the calculation of the energy eigenvalues by algebraic methods. In Ref. 10 the case of the complex sphere has been investigated.
- The two-dimensional ''nondegenerate'' [4] superintegrable systems are classified by the values of the constants of the Darboux equations[3,4] and the constants of the system. The relation of these constants with the constants of the quadratic Poisson algebra is not yet known.
- The Poisson algebras for the Drach superintegrable systems with a cubic integral of motion were written by using a classical analog of the deformed parafermionic algebra.[29] Their quantum counterparts and the calculation of their energy eigenvalues are topics under investigation.
- The Poisson algebras and the associated quantum counterparts for the three-dimensional superintegrable systems are not yet fully studied. Recently[45] the quantum quadratic algebras have been written down, but a systematic calculation of energy eigenvalues has not been performed yet.

The above points show that, the study of nonlinear Poisson algebras and their quantum counterparts are topics of interest.

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Asymptotics of electromagnetic radiation off a spherical superconductor

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Asymptotics of electromagnetic radiation off a spherical superconductor is analyzed in terms of creeping waves. Temporal damping behavior of the charge distribution on the surface when the sphere is rendered superconducting is studied and is compared with that on a superconductor with an infinite plane surface. Finally, the coherent states of light waves outside a spherical superconductor and a superconductor with an infinite plane surface are constructed. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1331100]

I. INTRODUCTION

Arnold Sommerfeld, student of Boltzmann and teacher of Debye, Bethe, Heisenberg, Herzfeld, and many another distinguished physicists, established not once, but twice a standard of thoroughness for the analysis of a field of mathematical physics. First, he treated the propagation of the electromagnetic field à la Maxwell in geometry after geometry of this, that, or the other interesting symmetry, and, second, he analyzed the atomic structure à la Bohr, Heisenberg, Jordan, Schrödinger, and Pauli and its correlation with the observed pattern configurations can be attributed to Sommerfield, who put out Volume VI (partial differential equations in physics) while slashing his way into the heartland of atomic physics. But had there stood at his side an Arnold Sommerfeld clone who could have continued with the analysis of electromagnetic field configurations of interesting symmetry, there surely would have appeared at least one more volume on the subject.

We do not have to look far to find the obvious candidate for the first chapter in that Volume IV. Kamerlingh Onnes, working in his Leiden low-temperature laboratory, had in 1911 just discovered superconductivity. At last one could visualize an interesting configuration of spherical symmetry. Here, we spell out the simple model and analyze the associated field configuration. As is well known, the spherical superconductor has two modes, TE and TM. Neither mode of oscillation is stationary. Both damp. Characteristic features of these modes are the appearance of new integers in addition to familiar spherical harmonic indices l and m. These integers also appear in the homogeneous integral equation for light waves hitting the sphere and undergoing diffraction behind the sphere. Analytic approximate expressions for these eigenvalues were already obtained by Debye, Sommerfeld, and others. We try to give the physical meanings to this new characteristic integer in this paper.

Normal modes of oscillation for infinite plane superconductors are stationary. But, we shall show that physics on the plane looks similar to the physics on the sphere, by looking at the time dependence of the decaying charge distribution, when a sphere with axially symmetric charge distribution on one hand, and a plane with sinusoidal charge distribution on the other hand, are suddenly rendered superconducting.

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Finally, we construct the coherent state (''coherent'' means here that the superposed solitary waves progress keeping their forms unaltered) for electromagnetic waves outside a spherical superconductor and an infinite plane superconductor. For a spherical superconductor we have a reasonable result, and for a plane superconductor we have a perfectly satisfactory result.

II. SIMPLE MODEL

A. The Hamilton–Jacobi theory of a pseudophoton

Before we discuss in detail the asymptotics of electromagnetic radiation off a spherical superconductor, we recall how light waves diffract behind a spherical superconductor when they hit it, simply by using classically the concept of a pseudophoton.[1]

We start with the basic equation of a pseudophoton,

$$k_r^2+\frac{(l+\frac{1}{2})^2}{r^2}=\frac{\omega^2}{c^2}. \tag{2.1}$$

We rewrite this equation as follows:

$$\frac{c^2}{\alpha_1}\left\{p_r^2+\frac{\alpha_\theta^2}{r^2}\right\}=\alpha_1, \tag{2.2}$$

where we have

$$\alpha_\theta=(l+\tfrac{1}{2})\hbar, \tag{2.3}$$

and

$$\alpha_1=\hbar\omega. \tag{2.4}$$

Using Hamilton's characteristic function, $W=W_1(r)+\alpha_\theta\theta$, we have

$$\frac{c^2}{\alpha_1}\left\{\left(\frac{\partial W_1}{\partial r}\right)^2+\frac{\alpha_\theta^2}{r^2}\right\}=\alpha_1. \tag{2.5}$$

Therefore we have

$$W=\int dr\left(\frac{\alpha_1^2}{c^2}-\frac{\alpha_\theta^2}{r^2}\right)^{1/2}+\alpha_\theta\theta. \tag{2.6}$$

Then, the Hamilton–Jacobi theory gives us

$$t+\beta_1=\frac{\partial W}{\partial\alpha_1} \tag{2.7}$$

and

$$\beta_2=\frac{\partial W}{\partial\alpha_\theta}. \tag{2.8}$$

We solve these equations and we obtain

$$r=\left\{c^2t^2+\left(l+\frac{1}{2}\right)^2\frac{c^2}{\omega^2}\right\}^{1/2} \tag{2.9}$$

and

$$r=\frac{\left(l+\frac{1}{2}\right)\frac{c}{\omega}}{\cos\theta}, \tag{2.10}$$

where we have put $\beta_1=\beta_2=0$.

These expressions give a simple picture of a pseudophoton that creeps around and peels off the surface of a spherical superconductor, and underlies a full analysis in the following chapters.

B. Quantum theory of a pseudophoton

In this section, we discuss the field configurations outside a spherical superconductor, when the charge distribution over a spherical superconductor and therefore the electromagnetic field outside it oscillates, simply by using quantum mechanically the concept of a pseudophoton.

Here we, again, begin with the basic formula for the motion of a pseudophoton,

$$k_r^2+\frac{(l+\frac{1}{2})^2}{r^2}=\frac{\omega^2}{c^2}. \tag{2.1}$$

Transforming this equation into the quantum mechanical form, we have

$$-\frac{d^2S}{dr^2}+\frac{(l+\frac{1}{2})^2}{r^2}S=\frac{\omega^2}{c^2}S. \tag{2.11}$$

For large r, we have

$$-\frac{d^2S}{dr^2}=\frac{\omega^2}{c^2}S. \tag{2.12}$$

The solution of this equation is certainly

$$S(r)=e^{-i(\omega/c)r}. \tag{2.13}$$

Thus we put

$$S(r)=H(r)e^{-i(\omega/c)r}. \tag{2.14}$$

Then, the differential equation that $H(r)$ satisfies, is

$$\frac{d^2H}{dr^2}-i\frac{2\omega}{c}\frac{dH}{dr}-\frac{(l+\frac{1}{2})^2}{r^2}H=0. \tag{2.15}$$

We put

$$r=i\frac{c}{2\omega}z. \tag{2.16}$$

Then, we have

$$\frac{d^2H}{dz^2}+\frac{dH}{dz}-\frac{(l+\frac{1}{2})^2}{z^2}H=0. \tag{2.17}$$

The solution of this equation is given by

$$H(z)=z^{1/2}e^{-z/2}Z_{[l(l+1)+1/2]^{1/2}}\left(i\frac{z}{2}\right). \tag{2.18}$$

Or, we have

$$H(r)=e^{-i(\pi/4)}\left(\frac{2\omega}{c}r\right)^{1/2}e^{i(\omega/c)r}Z_{[l(l+1)+1/2]^{1/2}}\left(\frac{\omega}{c}r\right). \tag{2.19}$$

Here Z_ν is a cylindrical function. Since we are dealing with a pseudophoton, we have, putting $\omega/c=k$, the following results:

$$S(r)=(2kr)^{1/2}e^{-i(\pi/4)}J_{[l(l+1)+1/2]^{1/2}}(kr). \tag{2.20}$$

Or

$$S(r)=(2kr)^{1/2}e^{-i(\pi/4)}N_{[l(l+1)+1/2]^{1/2}}(kr). \tag{2.21}$$

Finally, we have, for $r\to\infty$,

$$S(r)\sim\frac{2}{\pi^{1/2}}e^{-i(\pi/4)}\cos\left\{kr-\frac{(2[l(l+1)+\frac{1}{2}]^{1/2}+1)\pi}{4}\right\}. \tag{2.22}$$

Or

$$S(r)\sim\frac{2}{\pi^{1/2}}e^{-i(\pi/4)}\sin\left\{kr-\frac{(2[l(l+1)+\frac{1}{2}]^{1/2}+1)\pi}{4}\right\}. \tag{2.23}$$

We rewrite the expression for $S(r)$ in the following way:

$$S(r)=\frac{2}{\pi^{1/2}}e^{-i(\pi/4)}krj_{[l(l+1)+1/2]^{1/2}-1/2}(kr). \tag{2.24}$$

Or

$$S(r)=\frac{2}{\pi^{1/2}}e^{-i(\pi/4)}krn_{[l(l+1)+1/2]^{1/2}-1/2}(kr). \tag{2.25}$$

Also, we have

$$S(r)=\frac{2}{\pi^{1/2}}e^{-i(\pi/4)}krh^{(1)}_{[l(l+1)+1/2]^{1/2}-1/2}(kr). \tag{2.26}$$

Further, we have, by adding the angular dependence and the time-dependent factor,

$$S(r,\theta,t)=\frac{2}{\pi^{1/2}}e^{-i(\pi/4)}krh^{(1)}_{[l(l+1)+1/2]^{1/2}-1/2}(kr)P_l(\cos\theta)e^{-i\omega t}. \tag{2.27}$$

Now we ask the boundary condition for the wave function of a pseudophoton, on the surface of a spherical superconductor with radius a:

$$S(r,\theta,t)_{r=a}=0. \tag{2.28}$$

This condition leads to the same condition as that in the TE mode (see Chap. III) for large l in which we are interested, such that

$$\{h^{(1)}_{[l(l+1)+1/2]^{1/2}-1/2}(kr)\}_{r=a}=0. \tag{2.29}$$

Also, we can ask the regularity condition for the wave function of a pseudophoton, on the surface of a spherical superconductor:

$$\left\{\frac{\partial}{\partial r}S(r,\theta,t)\right\}_{r=a}=0. \tag{2.30}$$

This condition leads to the same condition as that in the TM mode (see Chap. III) for large l, such that

$$\left\{\frac{d}{dr}[rh^{(1)}_{[l(l+1)+1/2]^{1/2}-1/2}(kr)]\right\}_{r=a}=0. \tag{2.31}$$

Either one of the above boundary conditions is equally definite to fix the eigenvalues.

Finally, we give the asymptotic formula of $S(r,\theta,t)$ for $r\to\infty$,

$$S(r\to\infty,\theta,t)\sim\frac{2}{\pi^{1/2}}\exp\left\{i\left(kr-\frac{(2[l(l+1)+\frac{1}{2}]^{1/2}+2)\pi}{4}\right)\right\}P_l(\cos\theta)e^{-i\omega t}. \tag{2.32}$$

Since the eigenvalues for both conditions have the negative imaginary parts, this expression shows the characteristic, spatially increasing, and temporally decreasing behavior.

Now we go over to the detailed analysis of TE and TM modes and their related subjects of the charge distribution over a spherical superconductor and the electromagnetic field outside it.

III. TRANSVERSE ELECTRIC MODES AND TRANSVERSE MAGNETIC MODES OF A SPHERICAL SUPERCONDUCTOR

As the student of wave mechanics works out the solution of the Schrödinger equation for the $1s$, $2p$, $3d$, $4f$, and further states of the electron moving around the hydrogen nucleus, he sees the first maximum of the wave function becomes more and more sharply defined and moving outward in clearer and clearer correspondence to the radius of the corresponding classical circular Bohr orbit. Does any similar asymptotology hold for the modes of oscillation of electromagnetic field around a spherical superconductor (and the accompanying vibrations of the electric charge on the surface of the superconductor)?

This question arose in a junior level course that one of us taught at the University of Texas at Austin in 1975 when, among the homework, the student encountered the following question from the familiar text of Jackson:[2]

> 16.10 Discuss the normal modes of oscillation of a perfectly conducting solid sphere of radius a in free space. (This problem was solved by J.J. Thomson in the 1880(s.)
> (a) Determine the characteristic equations for the eigenfrequencies for TE and TM modes of oscillation. Show that the roots for ω always have a negative imaginary part, assuming a time dependence of $e^{-i\omega t}$.
> (b) Calculate the eigenfrequencies for the $l=1$ and $l=2$ TE and TM modes. Tabulate the wavelength (defined in terms of the real part of the frequency) in units of the radius a and the decay time (defined as the time taken for the energy to fall to e^{-1} of its initial value) in units of the transit time (a/c) for each of the modes.

In this problem there are two conditions at one boundary, the surface of the superconducting sphere $(r=a)$, rather than one condition, $\psi=0$ (3.1), at two locations ($r=0$ and $r=$infinity), but their power to fix the eigenvalues is equally definite.

For concreteness we picture a sphere of radius a on the surface of which we spray an axially symmetric distribution of electric charge $\sigma(\theta)=\sigma_0 P_l(\cos\theta)$. At time $t=0$ we render the sphere superconducting. The charge thereupon goes into a superposition of damped oscillations. But with what frequencies and what damping constants, we ask, knowing that the electromagnetic field for some modes is transverse electric (TE) and for the others is transverse magnetic (TM).

For transverse electric (TE) modes of oscillation of the electromagnetic field one may write[3]

$$\mathbf{E}=\mathbf{r}\times\text{grad}\,\psi, \tag{3.2}$$

(guaranteeing that **E** stands perpendicular to **r**) and

$$\mathbf{B}=\left(\frac{1}{i\omega}\right)\mathbf{del}\times\mathbf{E}, \tag{3.3}$$

where

$$\psi(r,\theta,\varphi,t)=h_l^{(1)}(kr)Y_l^m(\theta,\varphi)e^{-ikct}, \tag{3.4}$$

with $h_l^{(1)}$ the spherical Hankel function of the first kind.[3] It satisfies the differential equation

$$\frac{d^2h_l^{(1)}}{dz^2}+\frac{2}{z}\frac{dh_l^{(1)}}{dz}+\left[1-\frac{l(l+1)}{z^2}\right]h_l^{(1)}=0, \tag{3.5}$$

and admits an expression in the form

$$h_l^{(1)}(z)=z^{-(l+1)}[\text{polynomial in } z \text{ of order } l]e^{iz}. \tag{3.6}$$

For transverse magnetic (TM) modes of oscillation of the electromagnetic field one may write[3]

$$\mathbf{H}=\mathbf{r}\times\text{grad}\,\psi, \tag{3.7}$$

(guaranteeing that **H** stands perpendicular to **r**) and

$$\mathbf{E}=\left(\frac{i}{\omega\varepsilon_0}\right)\mathbf{del}\times\mathbf{H}. \tag{3.8}$$

On the surface, the tangential component of the electric field for each mode of oscillation must vanish at all times, whence every spherical Hankel function that is relevant must satisfy the eigenvalue condition

$$h_l^{(1)}(ka)=0, \tag{3.9}$$

for TE modes, and

$$\left\{\frac{d}{dr}[rh_l^{(1)}(kr)]\right\}_{r=a}=0, \tag{3.10}$$

for TM modes. One of the students, Iraj Emami, went beyond the Jackson problem in its stated form and sought the 41 roots (3.10) for $l=40$. For this purpose Emami programmed a computer to get the real part of each root, to about 8 decimals, and likewise the imaginary part. His results appear in Fig. 1(a). Figure 1(a): complex roots of Eq. (3.10) for TM modes with a spherical Hankel function of the first kind of order $l=40$ as determined to perhaps around eight places of decimals by Iraj Emami in the spring of 1983, about the time when he was called back to Iran for military service. In this figure, a parameter, $K=[ka-(l+\frac{1}{2})]/(l+\frac{1}{2})^{1/3}$ is plotted. Contrary to the

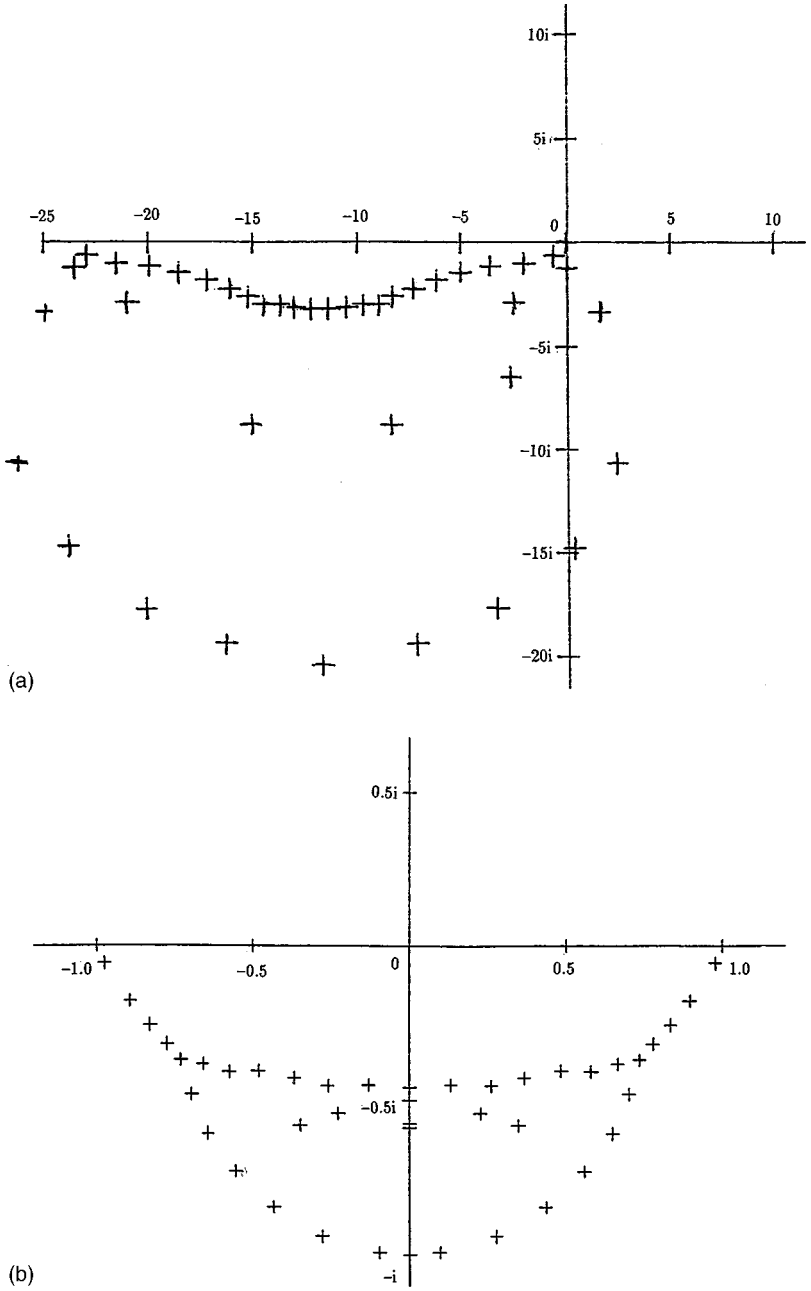


FIG. 1. (a) The complex roots of Eq. (3.10) for TM modes with a spherical Hankel function of the first kind, of order $l=40$, as determined to around eight places of decimals by Iraj Emami. (b) The 41 complex roots of Eq. (3.10) normalized by $l(=40)$, obtained to eight places of decimals by one of us (M.W.).

note that Emami left, and also to other calculations of him for several l values smaller than 40, in Fig. 1(a), only 40 roots are shown instead of 41 roots. All attempts have failed to contact him to get his participation in this report. On leaving Austin he had said, ''Don't worry about me. The Iraqis can't shoot straight.'' Maybe he was wrong. To examine the reproducibility of his result, we show, in Fig. 1(b), 41 complex roots of Eq. (3.10) normalized by $l(=40)$, obtained to eight places of decimals by one of us (M.W.). We could say that the diagrams have some features in common.

The pattern of complex frequencies in Fig. 1(a) fall into oval, below, and above a bow. Supply some simple physical interpretation of these two features, we asked ourselves and a succession of

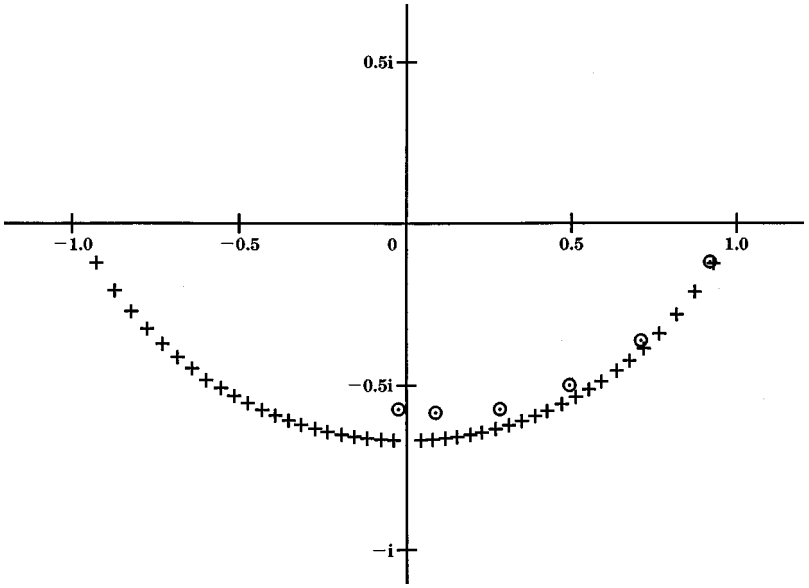


FIG. 2. Complex eigenvalues for the 45 characteristic modes of decay of the transverse electric field around a charged superconductor. All expressed in units of the basic frequency, cl/a. Crosses: our calculations; circles: the prediction of the asymptotic formula of Debye (Ref. 9) and Sommerfeld (Ref. 10).

distinguished visitors. ''Crazy'' replied one after several hours of study, and rightly so, we now realize, because Fig. 1(a) is mistaken, through not having been calculated to enough decimal places. That perceptive visitor was later honored with a knighthood, but not for this. Clarity first came when one of us (M.W.) repeated the calculations to a higher number of decimal places, 16 for the real part and 16 for the imaginary part, by finding 45 roots of a polynomial of 45th order with real coefficients in (3.9) for TE modes, yielding the pattern of complex eigenvalues of Fig. 2.

Both modes of oscillation appear as poles in the S matrix for the scattering of a plane electromagnetic wave by a spherical superconductor.[3] The TM modes of oscillation describe the temporal behavior of the charge distribution on a sphere, which is rendered superconducting at $t=0$, while for $t<0$, the charge is distributed axially symmetrically and given by $\sigma(\theta) = \sigma_0 P_l(\cos\theta)$. We start with the following integral expression:

$$E_r(r,\theta,t) = \frac{\sigma_0}{\varepsilon_0}\left(\frac{a}{r}\right) P_l(\cos\theta)\,\frac{1}{2\pi i}\int \frac{dk}{k}\left\{\frac{-l}{\left\{\frac{d}{dz}[zh_l^{(1)}(z)]\right\}_{z=ka}}\right\}$$

$$\times[A(k,a)h_l^{(2)}(kr)+h_l^{(1)}(kr)]e^{-ikct}, \tag{3.11}$$

$$A(k,a) = -\frac{\left\{\frac{d}{dr}[rh_l^{(1)}(kr)]\right\}_{r=a}}{\left\{\frac{d}{dr}[rh_l^{(2)}(kr)]\right\}_{r=a}}, \tag{3.12}$$

$$\left\{\frac{d}{dr}[rh_l^{(1)}(k_l^n r)]\right\}_{r=a} = 0. \tag{3.13}$$

The integration should be performed along the real axis except for going below zero, in the complex k plane. Equation (3.12) for factor $A(k,a)$ arises from the boundary condition that the tangential component of the electric field must vanish on the surface of the spherical superconductor, as guaranteed by

$$E_\theta(r,\theta,t)=\frac{\sigma_0}{\varepsilon_0}\left(\frac{a}{r}\right)\frac{P_l^1(\cos\theta)}{l(l+1)}\frac{1}{2\pi i}\int\frac{dk}{k}\left\{\frac{-l}{\left\{\frac{d}{dz}[zh_l^{(1)}(z)]\right\}_{z=ka}}\right\}$$
$$\times\left\{\frac{d}{dr}[A(k,a)rh_l^{(2)}(kr)+rh_l^{(1)}(kr)]\right\}e^{-ikct} \tag{3.14}$$

and

$$E_\varphi=0. \tag{3.15}$$

For the space–time points, $(r-a-ct)>0$, we have

$$E_r(r,\theta)=\frac{\sigma_0}{\varepsilon_0}\left(\frac{a}{r}\right)^{(l+2)}P_l(\cos\theta) \tag{3.16}$$

and

$$E_\theta(r,\theta)=-\frac{\sigma_0}{\varepsilon_0}\left(\frac{a}{r}\right)^{(l+2)}\frac{P_l^1(\cos\theta)}{(l+1)}, \tag{3.17}$$

where we have $P_l^1(\cos\theta)=(d/d\theta)P_l(\cos\theta)$.

For the space–time points, $(r-a-ct)<0$, we have

$$E_r(r,\theta,t)=\frac{\sigma_0}{\varepsilon_0}\left(\frac{a}{r}\right)P_l(\cos\theta)\sum_n\frac{l}{[l(l+1)-(k_l^na)^2]}\frac{h_l^{(1)}(k_l^nr)}{h_l^{(1)}(k_1^na)}e^{-ik_l^nct} \tag{3.18}$$

and

$$E_\theta(r,\theta,t)=\frac{\sigma_0}{\varepsilon_0}\left(\frac{a}{r}\right)\frac{P_l^1(\cos\theta)}{(l+1)}\sum_n\frac{1}{[l(l+1)-(k_l^na)^2]}\frac{\frac{d}{dr}[rh_l^{(1)}(k_l^nr)]}{h_l^{(1)}(k_l^na)}e^{-ik_l^nct}. \tag{3.19}$$

For $r=a$ and $t=0$, Eq. (3.18) reduces to $E_r(\theta)=(\sigma_0/\epsilon_0)P_l(\cos\theta)$. Here we have used the relation[4]

$$\frac{h_l^{(1)}(z)}{\frac{d}{dz}[zh_l^{(1)}(z)]}=\sum_n\frac{z_l^n}{[l(l+1)-(z_l^n)^2](z-z_l^n)}. \tag{3.20}$$

The charge distribution on the surface of a sphere for $t>0$, is given by

$$\sigma(\theta,t)=\sigma_0P_l(\cos\theta)\sum_n\frac{l}{[l(l+1)-(k_l^na)^2]}e^{-ik_l^nct}. \tag{3.21}$$

A very naive insight [5] to understanding the pattern of eigenfrequencies in Fig. 2 can be gained from the studies done for the creeping waves going into the shadow region around the surface (1) of the cylindrical perfect conductor,[6] when the light wave hits the cylinder perpendicularily to its

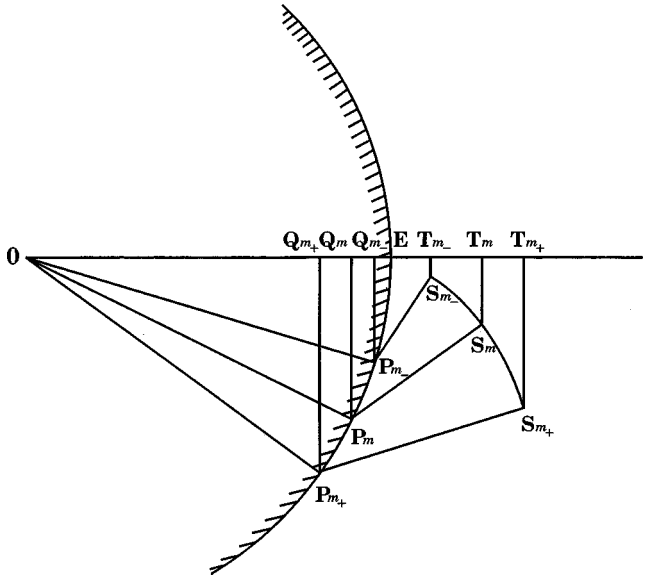


FIG. 3. Two light rays meet at a point S_m. The length, S_mT_m is the path difference between the light ray coming from a point P_m and the light ray coming from a point lying, on the straight line, T_mS_m, and far from a point T_m by the length, Q_mP_m, and is equal to $m\times$(the wavelength of the light). Here the length, P_mS_m is equal to the length, P_mQ_m. Angle, $\angle Q_mP_mS_m$ is nearly twice angle, $\angle EOP_m$. The figure is just schematic alone. These situations are same for other light rays drawn here. Thus the length, $S_{m+}T_{m+}$ is equal to $(m+1/4)\times$(the wavelength of the light), and the length, $S_{m-}T_{m-}$, is equal to $(m-1/4)\times$(the wavelength of the light).

axis, and (2) of the spherical perfect conductor,[7] when the light wave hits the sphere from its north pole, along the z axis. The damping factors of the wave amplitude in both cases are shown, by Franz,[8] to have the content equivalent to the Debye[9] and Sommerfeld[10] formula for eigenvalues of TM modes,

$$l=ka+\frac{1}{2}(ka)^{1/3}\left(\frac{3\pi}{4}\right)^{2/3}(4m+1)^{2/3}e^{i\pi/3},$$
$$m=0,1,2,3,\cdots, \tag{3.22}$$

and for TE modes,

$$l=ka+\frac{1}{2}(ka)^{1/3}\left(\frac{3\pi}{4}\right)^{2/3}(4m-1)^{2/3}e^{i\pi/3}$$
$$m=1,2,3,\cdots\ . \tag{3.23}$$

As m increases, the corresponding creeping wave is localized farther and farther from the surface.[11] The pattern of this localization can be inferred from the following simple consideration. Let us think of a plane electromagnetic wave hitting a sphere. The interference phenomena of the light going straightforwardly and the light reflected on the surface of a sphere are shown in Fig. 3. (Here we do not take into account the polarization effect of the light.)

In Fig. 3, the width $T_{m_-}T_{m_+}$ is the mth trapped or localized region of energy produced by the constructive interference of two light rays, one coming straightforwardly and the other reflected on the surface of a sphere. Following the concept of a creeping wave, we assume that the light rays within this width go around the circular small zone apart from the surface by the distance, ET_m. One can easily calculate the time ΔT_m needed for the pseudophoton[1] coming grazingly at point E

in Fig. 3 to clear the mth trapped region. The inverse of the angle $\Delta\varphi_m$ spanned by the light ray circulating within the mth trapped region for the time ΔT_m gives the angularwise decay rate of a creeping wave in our picture. We have

$$0.63(ka)^{1/3}, \quad 2.31(ka)^{1/3}, \ 3.68(ka)^{1/3}, \cdots, \tag{3.24}$$

while the Debye and Sommerfeld formula gives, for TM modes,

$$0.77(ka)^{1/3}, \quad 2.24(ka)^{1/3}, \quad 3.32(ka)^{1/3}, \cdots \tag{3.25}$$

The largest decay rate is simply given by the WKB approximation method as follows:[12]

$$\omega_{\text{imaginary}} = -0.6627\left(l+\frac{1}{2}\right)\frac{c}{a}. \tag{3.26}$$

The corresponding decay factor of the electromagnetic field around an oscillating charged spherical superconductor, is $\exp[-ct/a/0.6627(l+\frac{1}{2})]$. Therefore the effective reduced wavelength, $\lambda/2\pi$ is $a/0.6627(l+\frac{1}{2}) = (1+0.5090)a/(l+\frac{1}{2})$. This means that in terms of a creeping wave, the effective radius is elongated by $0.5a$ from the surface of a sphere, and the pseudophoton departs this outermost trapped region when it moves over one reduced wavelength.

In the trapped regions near the surface of a cylindrical or spherical superconductor, the property of light waves as an aggregate of photons is evident, but in those far from the surface, the property as an individual photon is evident. Further, in the latter case, the following quite an elementary argument suggests, implicitly, the appearance of quantum h.

The angular momentum A of a circulating pseudophoton over a circle with radius $1.5a$ is given as follows:

$$A = 1.5ap, \tag{3.27}$$

where the momentum p of a pseudophoton is equal to $\hbar k$, by de Broglie's relation. Thus we have

$$A = 1.5a\hbar k. \tag{3.28}$$

Further, we have, for the quantized angular momentum of a circulating pseudophoton,

$$A = l\hbar. \tag{3.29}$$

Therefore, we have the final equation,

$$l = 1.5ak. \tag{3.30}$$

That is, quantum h is implicitly included in this equation. These considerations correspond to the situation in the hydrogen atom stated in the beginning.

At this point, we consider the resonance curve of normal oscillations for TE modes. The cross section[3] for scattering of plane light waves by a spherical superconductor of radius a is given by

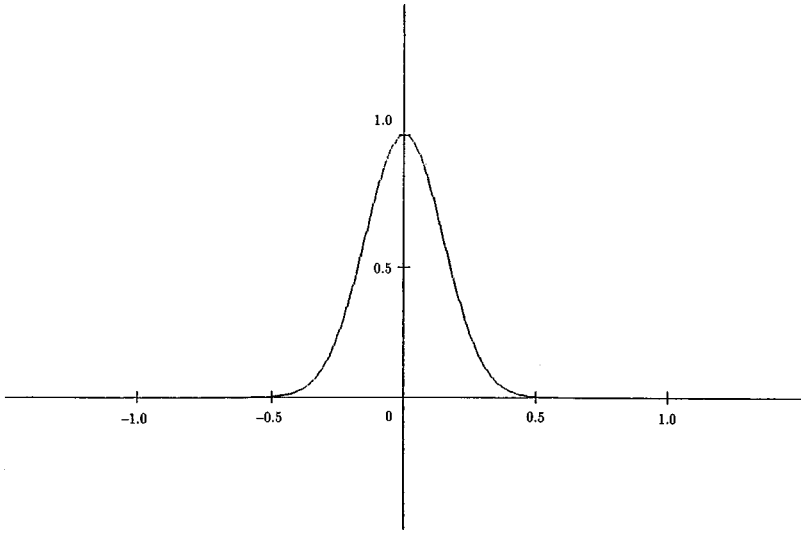


FIG. 4. Diagram for the resonance factor, Eq. (3.33) for $l=45$ of the TE mode appearing in the total scattering cross section of the light by a spherical superconductor is drawn. The curve is plotted as a function of $z=ka$. All quantities, $z, z_{\text{real}}^{(k)}$ and $z_{\text{imag}}^{(k)}$ are normalized by $l(=45)$. The horizontal axis stands for z, and the vertical axis stands for the resonance factor, Eq. (3.33). The diagram does not show the slightest indication of the resonance feature of the individual mode.

$$\sigma=\frac{2\pi}{k^2}\sum_l (2l+1)(|a_l|^2+|b_l|^2),$$

$$a_l=-\frac{j_l(ka)}{h_l^{(1)}(ka)}, \tag{3.31}$$

$$b_l=-\left\{\frac{\dfrac{d}{dr}[rj_l(kr)]}{\dfrac{d}{dr}[rh_l^{(1)}(kr)]}\right\}_{r=a}.$$

Let us consider the resonance factor produced by the zeros of $h_l^{(1)}(z)$ in the complex z plane. We use the following representation for $h_l^{(1)}(z)$:

$$h_l^{(1)}(z)=\frac{e^{iz}}{z^{(l+1)}}(\text{polynomial in } z \text{ of order } l)$$

$$=\frac{e^{iz}}{z^{(l+1)}}f(0)\left(1-\frac{z}{z^{(1)}}\right)\left(1-\frac{z}{z^{(2)}}\right)\cdots\left(1-\frac{z}{z^{(l)}}\right). \tag{3.32}$$

Here $f(0)$ is the value of the polynomial at $z=0$, and $z^{(k)}$ is the kth complex root of $h_l^{(1)}(z)=0$. Then the resonance curve is given by the following expression:

$$\Pi_{k=1}^{l}\frac{[(z_{\text{real}}^{(k)})^2+(z_{\text{imag}}^{(k)})^2]}{[(z-z_{\text{real}}^{(k)})^2+(z_{\text{imag}}^{(k)})^2]}. \tag{3.33}$$

We present this resonance curve for $l=45$ in Fig. 4. Here we do not have the slightest indication of a resonance feature in the individual mode.

IV. NORMAL MODES IN A SUPERCONDUCTOR WITH AN INFINITE PLANE SURFACE

The superconductor with an infinite plane surface is an insulator for $t<0$. We take the charge to be distributed according to the surface density, $\sigma(x)=\sigma_0\cos(kx)$. The corresponding electromagnetic fields in space are

$$E_x(x,z)=\frac{\sigma_0}{\epsilon_0}\sin(kx)e^{-kz},$$

$$E_y=0,$$

$$E_z(x,z)=\frac{\sigma}{\epsilon_0}\cos(kx)e^{-kz},$$

$$\mathbf{H}=0. \tag{4.1}$$

The electric energy associated with the charge distribution on the surface is

$$U_{\text{charge}}=\frac{1}{2}\int\int dx\,dy\,\sigma(x)\phi(x)$$

$$=\frac{\sigma_0^2}{2\epsilon_0 k}\int\int dx\,dy\cos^2(kx)$$

$$=\frac{\sigma_0^2}{4\epsilon_0 k}\int\int dx\,dy. \tag{4.2}$$

Here $\phi(x)=(\sigma_0/\epsilon_0 k)\cos(kx)$ is the electric potential on the surface. The transition from the second to the last equation in (4.2) is performed by taking the average over x dependence, as done in the following discussion as well.

On the other hand, the electric energy stored in space is

$$U_{\text{field}}=\int\int\int dx\,dy\,dz\,\frac{\epsilon_0}{2}(E_x^2+E_z^2)$$

$$=\frac{\sigma_0^2}{4\epsilon_0 k}\int\int dx\,dy. \tag{4.3}$$

We see that the electric energy, U_{charge} associated with the charge distribution on the surface is equal to the electric energy, U_{field} stored in space as it should be in static electricity.

At time $t=0$ we render the substance superconducting. General solutions are stationary and given by

$$
\begin{aligned}
E_x(x,z,t) &= k_z \sin(kx)\sin(k_z z)\cos(\omega t),\\
E_y &= 0,\\
E_z(x,z,t) &= k \cos(kx)\cos(k_z z)\cos(\omega t),\\
H_x &= 0,\\
H_y(x,z,t) &= -\frac{\omega}{\mu_0 c^2}\sin(kx)\cos(k_z z)\sin(\omega t),\\
H_z &= 0,
\end{aligned}
\tag{4.4}
$$

where we have $\omega = c(k^2+k_z^2)^{1/2}$.

Then we superpose the individual electromagnetic field components with a weight factor, $(2\sigma_0/\pi\epsilon_0)/(k^2+k_z^2)$. We write down the resulting electromagnetic field components below. For $z>ct$ we have

$$
\begin{aligned}
E_x(x,z) &= \frac{\sigma_0}{\epsilon_0}\sin(kx)e^{-kz},\\
E_y &= 0,\\
E_z(x,z) &= \frac{\sigma_0}{\epsilon_0}\cos(kx)e^{-kz},\\
\mathbf{H} &= 0.
\end{aligned}
\tag{4.5}
$$

For $z<ct$ we have

$$
\begin{aligned}
E_x(x,z,t) &= -\left(\frac{2}{\pi}\right)^{1/2}\frac{\sigma_0}{\epsilon_0}\sin(kx)\,\frac{z}{k^{1/2}ct(c^2t^2-z^2)^{1/4}}\sin\left[k(c^2t^2-z^2)^{1/2}+\frac{\pi}{4}\right],\\
E_y &= 0,\\
E_z(x,z,t) &= \left(\frac{2}{\pi}\right)^{1/2}\frac{\sigma_0}{\epsilon_0}\cos(kx)\,\frac{(c^2t^2-z^2)^{1/4}}{k^{1/2}ct}\cos\left[k(c^2t^2-z^2)^{1/2}+\frac{\pi}{4}\right],\\
H_x &= 0,\\
H_y(x,z,t) &= -\left(\frac{2}{\pi}\right)^{1/2}\frac{\sigma_0}{\epsilon_0\mu_0 c}\sin(kx)\,\frac{1}{k^{1/2}(c^2t^2-z^2)^{1/4}}\sin\left[k(c^2t^2-z^2)^{1/2}+\frac{\pi}{4}\right],\\
H_z &= 0.
\end{aligned}
\tag{4.6}
$$

Now we define the total electromagnetic field energy stored in the whole space surrounding the infinite superconducting plane surface,

$$
U_{\text{field}}(t) = \int\int dx\,dy\int_{ct}^{\infty} dz\,\frac{\epsilon_0}{2}(E_x^2+E_z^2) + \int\int dx\,dy\int_0^{ct} dz\left[\frac{\epsilon_0}{2}(E_x^2+E_z^2)+\frac{\mu_0}{2}H_y^2\right]. \tag{4.7}
$$

Inserting Eqs. (4.5) and (4.6) into Eq. (4.7), we have the final result,

$$U_{\text{field}}(t)=\frac{\sigma_0^2}{4\epsilon_0 k}\left[e^{-2kct}+1+\frac{1}{2kct}\mathbf{H}_1(2kct)\right]\int\int dx\,dy. \tag{4.8}$$

Here the function $\mathbf{H}_1(2kct)$ is the Struve function, which is defined by[13]

$$\mathbf{H}_\nu(z)=\sum_{m=0}^{\infty}\frac{(-1)^m\left(\frac{z}{2}\right)^{\nu+2m+1}}{\Gamma\left(m+\frac{3}{2}\right)\Gamma\left(\nu+m+\frac{3}{2}\right)}. \tag{4.9}$$

When z is large, we can better use the following expression:[13]

$$\mathbf{H}_\nu(z)=Y_\nu(z)+\frac{1}{\pi}\sum_{m=0}^{\infty}\frac{\Gamma(m+\frac{1}{2})}{\Gamma\left(\nu+\frac{1}{2}-m\right)\left(\frac{z}{2}\right)^{2m-\nu+1}}. \tag{4.10}$$

Thus we have

$$U_{\text{field}}(t=\infty)=\frac{\sigma_0^2}{4\epsilon_0 k}\int\int dx\,dy. \tag{4.11}$$

Now we calculate the charge distribution on the surface for $t>0$. We start with the correct expression,

$$\sigma(x,t)=\sigma_0\cos(kx)\left(\frac{2}{\pi}\right)\int_0^{\pi/2}d\phi\cos\left(\frac{kct}{\cos\phi}\right). \tag{4.12}$$

For large times, we can make an approximation, $\cos\phi=1-\phi^2/2$, which is equivalent to that in the case where smaller values of ϕ are important. We have

$$\sigma(x,t)=\sigma_0\cos(kx)\left(\frac{2}{\pi kct}\right)^{1/2}\cos\left(kct+\frac{\pi}{4}\right). \tag{4.13}$$

This is equivalent to that derived from Eq. (4.6). For small times, we can make an approximation, $1/\cos\phi=\tan\phi$, which is equivalent to that in the case where values of ϕ near $\pi/2$ are important. We have

$$\begin{aligned}\sigma(x,t)&=\sigma_0\cos(kx)\left(\frac{2}{\pi}\right)\int_0^{\pi/2}d\phi\cos(kct\tan\phi)\\&=\sigma_0\cos(kx)e^{-kct}.\end{aligned} \tag{4.14}$$

This result can be derived exactly in the following way:

$$\begin{aligned}\int_0^{\pi/2}d\phi\cos\left(\frac{kct}{\cos\phi}\right)&=\int_1^{\infty}d\tau\frac{\cos(kct\tau)}{\tau(\tau^2-1)^{1/2}}\\&=\frac{\pi}{2}-\pi\sum_{n=0}^{\infty}J_{2n+1}(z).\end{aligned} \tag{4.15}$$

The transition to the last expression is performed by using the formulas on pp. 546–547 of Ref. 13. Further we have the relation

$$\int dz\, J_0(z) = 2\sum_{n=0}^{\infty} J_{2n+1}(z). \tag{4.16}$$

For small values of z we have the following expansion formula:

$$J_0(z) = 1 - \frac{z^2}{4} + \frac{z^4}{64} - \cdots. \tag{4.17}$$

Thus we have the expression of the charge distribution for small values of t given by

$$\sigma(x,t) = \sigma_0 \cos(kx)\left[1 - kct + \frac{(kct)^3}{12} - \frac{(kct)^5}{320} + \cdots\right]. \tag{4.18}$$

This equation verifies Eq. (4.14).

Thus, we see that the temporal damping pattern of the charge distribution on the infinite superconducting plane surface contains a continuous form from e^{-kct} to $1/(kct)^{1/2}$. From this situation, the infinite plane superconductor could be regarded as an approximation of a spherical superconductor in the sense that large decay factors make the oscillation of the charge distribution to decrease faster at smaller times, and at larger times the charge distribution oscillates with smaller decay factors.

The similarity of the infinite plane superconductor to the spherical superconductor can be seen in the surface diffraction wave (for a cylinder or a sphere, this is called ''creeping wave''). In fact, when the plane incident wave hits the infinite very thin plane superconductor, the surface diffraction wave on the surface in the shadow region, decreases proportionally to $\exp(ikr)/(kr)^{1/2}$ as r goes to infinity.[14] This implies no radiation loss during the wave propagation, because this expression expresses just the propagation of the cylindrical wave starting at the infinite edge of the infinite plane superconductor. On the other hand, for the radius of a sphere going to infinity, the creeping wave becomes an undamped plane Maxwell wave of infinite extent in the radial direction.

V. COHERENT STATES

A. A spherical superconductor

As stated in the Introduction, ''coherent'' means here that the superposed solitary waves progress keeping their forms unaltered for electromagnetic waves both outside a spherical superconductor and outside an infinite plane superconductor.

Now we pursue another analogy for the connection of two pictures of the hydrogen atom electron, (1) as a point going around and around in a circular orbit and (2) as a Schrödinger wave function spreading out all over the space. This connection is done by superposing waves within a certain effective range of n values to build a wave packet. It goes around and around like a point. We stated that the Debye and Sommerfeld formula has the content equivalent to the damping factor in the amplitude of the waves creeping into the shadow region around the surface of a spherical superconductor. This content is exemplified in the φ dependence of the light wave amplitude near the equator, when the wave hits the sphere along the x axis. As a preliminary work to study this characteristic, we superpose electromagnetic waves with spherical harmonic indices, l and m, such that $(l,m) = \cdots,(42,42),(43,43),(44,44),(45,45),\cdots$.

For this purpose we write down the electromagnetic field components for TM modes:

$$
\begin{aligned}
E_r &= \frac{-i}{\omega\epsilon_0}\frac{l(l+1)}{r}\psi, \\
E_\theta &= \frac{-i}{\omega\epsilon_0}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial\theta}\right), \\
E_\varphi &= \frac{m}{\omega\epsilon_0}\frac{1}{r\sin\theta}\frac{\partial}{\partial r}(r\psi), \\
H_r &= 0, \\
H_\theta &= \frac{-im}{\sin\theta}\psi, \\
H_\varphi &= \frac{\partial}{\partial\theta}\psi,
\end{aligned}
\tag{5.1}
$$

where ψ is given by Eq. (3.4). According to the prescription stated above we superpose the electromagnetic field components such that

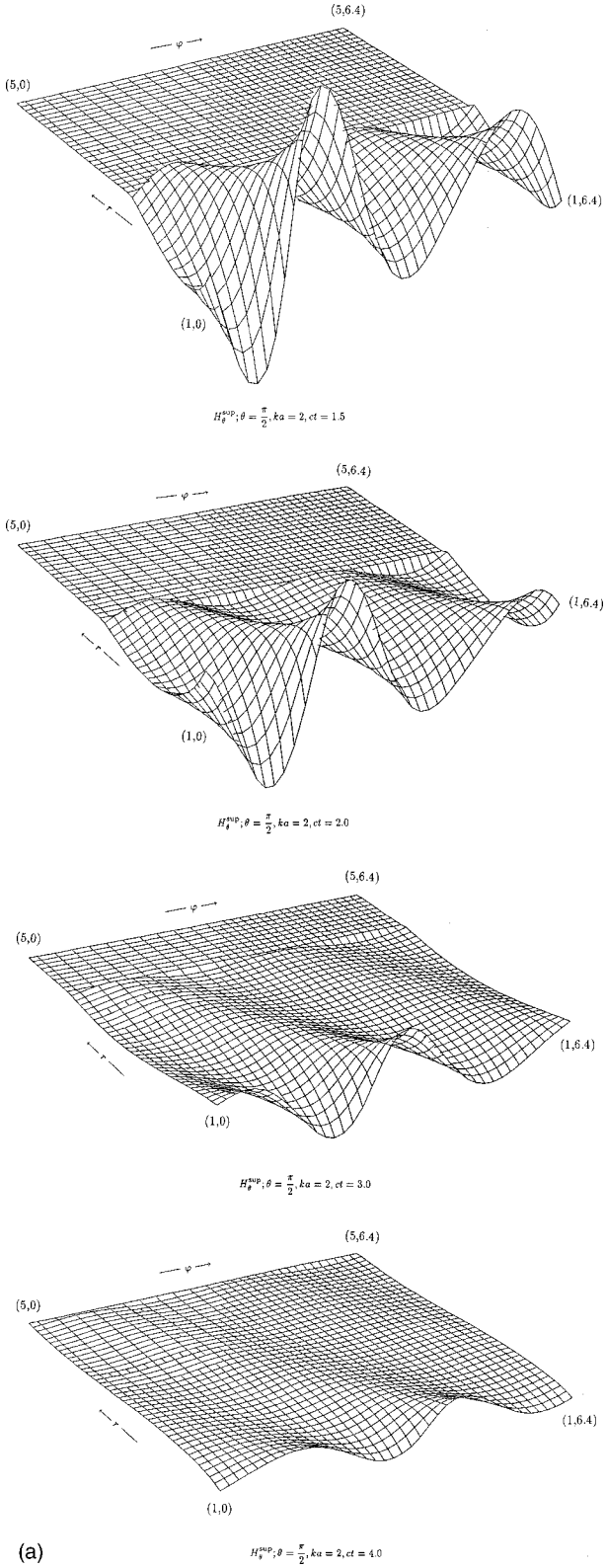
$$
\begin{aligned}
H_\theta^{\mathrm{sup}} &= \sum_l \frac{\frac{l_{\mathrm{imag}}}{\pi}}{(l-l_{\mathrm{real}})^2+l_{\mathrm{imag}}^2}\left(\frac{-il}{\sin\theta}\right)\frac{h_l^{(1)}(k_l^{\mathrm{lowest}}r)}{h_l^{(1)}(k_l^{\mathrm{lowest}}a)}(\sin\theta)^l e^{il\varphi}e^{-ik_l^{\mathrm{lowest}}ct}, \\
l_{\mathrm{real}} &= ka+\frac{1}{2}(ka)^{1/3}\left(\frac{3\pi}{4}\right)^{2/3}\cos\frac{\pi}{3}, \\
l_{\mathrm{imag}} &= \frac{1}{2}(ka)^{1/3}\left(\frac{3\pi}{4}\right)^{2/3}\sin\frac{\pi}{3}.
\end{aligned}
\tag{5.2}
$$

Here the superscript, ''*lowest*'' in k_l^{lowest} stands for the eigenvalue with the lowest decay rate in magnitude and the largest real part for given l, that is, the trajectory, $m=0$ in the Debye and Sommerfeld formula for TM modes. Calculations are shown in Figs. 5(a)–5(d).

From Figs. 5(a)–5(d), we could well infer that the electromagnetic fields of the creeping wave are not restricted on the surface of the sphere, but spread out in the space, apart from the surface, even at very small times. More interesting results concerning this important point might be obtained when we choose next to the *lowest* mode, in l_{real} and l_{imag} in the weight factor of Eq. (5.2). The fact that so much difference between Fig. 5(a) and Fig. 5(b) is not seen, might be due to the fact that high l's values do not make significant contributions to H_θ^{sup}. From Figs. 5(c) and 5(d), we see that the wave amplitude gets concentrated more and more near the surface of the sphere, as ka increases. Energy conservation cannot be discussed from these figures, because now we are limiting ourselves to the essential features of the creeping wave, the r dependence and φ dependence that it takes near the equator as time goes on, which is realized in the formation of H_θ^{sup} in Eq. (5.2).

B. A superconductor with an infinite plane surface

For the present purpose, we had better take the following general solutions for electromagnetic fields in the free space:



(a)

FIG. 5. The superposed magnetic field component, $H_\theta^{\mathrm{sup}}(r,\theta,\varphi,t)$ outside a spherical superconductor is shown for $ka=2$ and $\theta=\pi/2$, $\pi/4$ [(a) and (b)] and $ka=5$, 10, and $\theta=\pi/2$ [(c) and (d)]. We made the calculations of wave amplitudes until the distance where $(r-a-ct)\leqslant 0$, and beyond that distance, we made them equal to zero. All lengths, r and ct, are measured in unit a. Coordinates, (r,φ) stand for r values and φ values, which they take when the amplitudes of electromagnetic fields are zero, and in figures, they are drawn on the positions that the amplitudes actually take at corresponding cases and corresponding times.

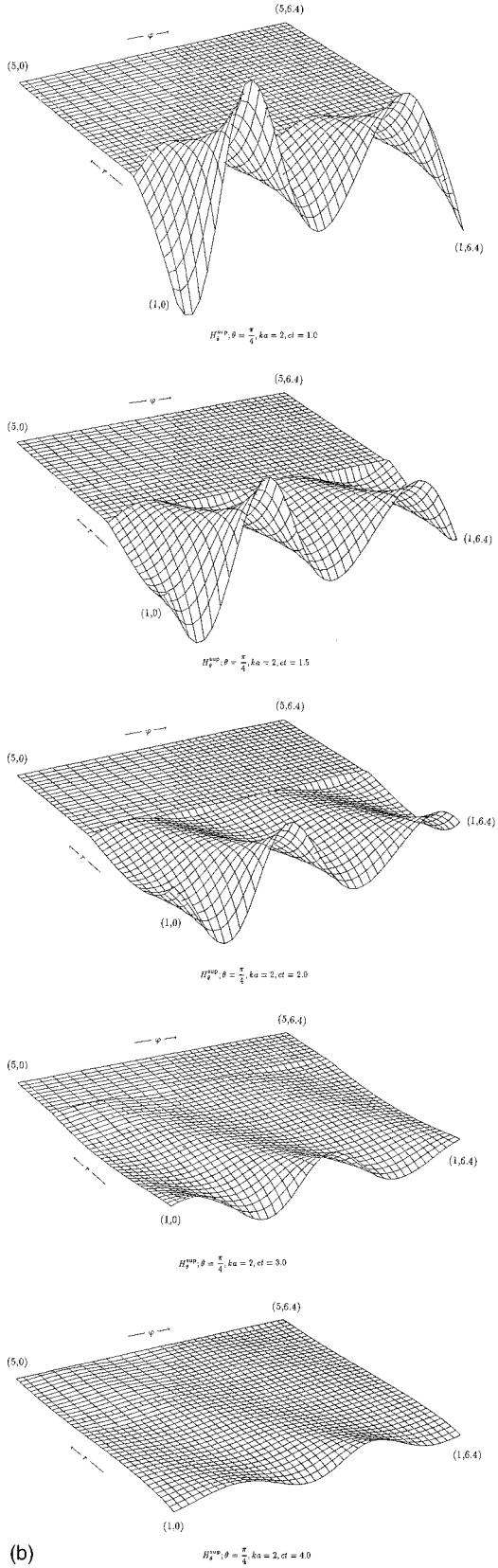
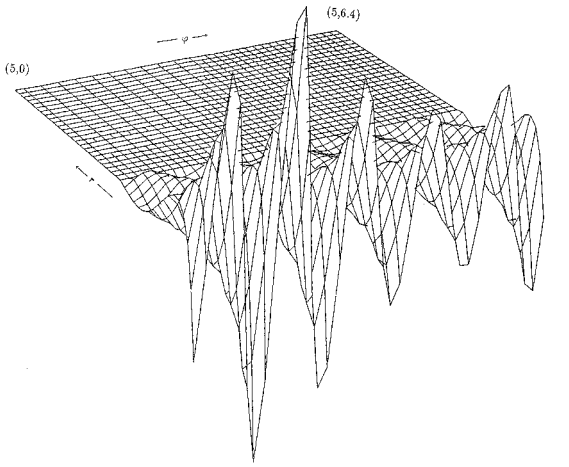
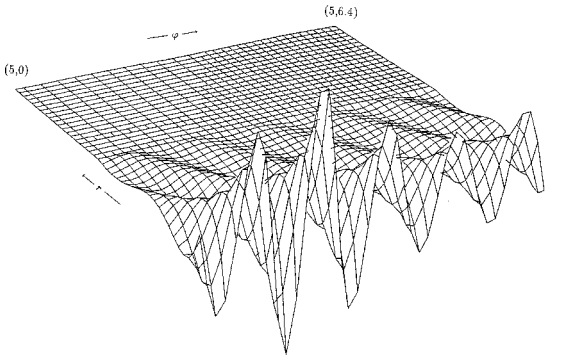


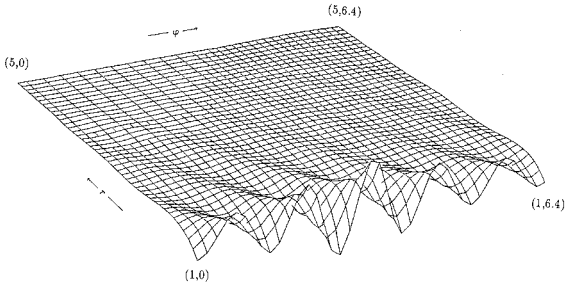
FIG. 5 (*Continued.*)



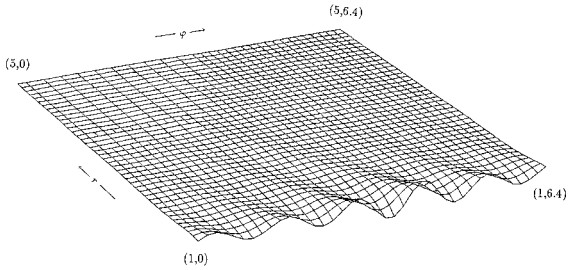
$H_\theta^{\text{sup}}; \theta = \frac{\pi}{2}, ka = 5, ct = 1.5$



$H_\theta^{\text{sup}}; \theta = \frac{\pi}{2}, ka = 5, ct = 2.0$



$H_\theta^{\text{sup}}; \theta = \frac{\pi}{2}, ka = 5, ct = 3.0$



(c) $H_\theta^{\text{sup}}; \theta = \frac{\pi}{2}, ka = 5, ct = 4.0$

FIG. 5 (*Continued.*)

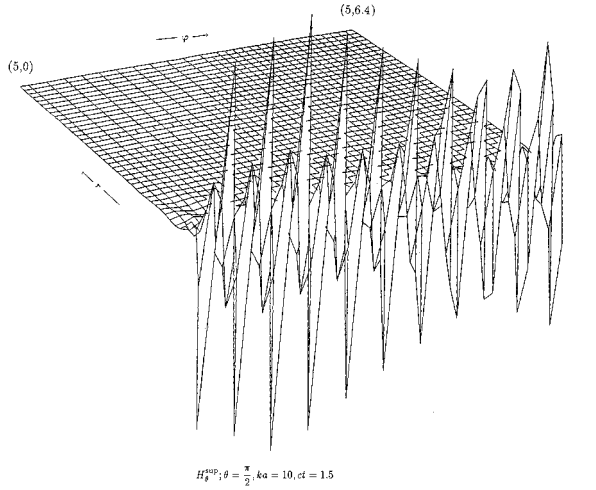


FIG. 5 (*Continued.*)

$$
\begin{aligned}
E_x(x,z,t) &= k_z \sin(k_z z) e^{i(kx-\omega t)},\\
E_y &= 0,\\
E_z(x,z,t) &= ik \cos(k_z z) e^{i(kx-\omega t)},\\
H_x &= 0,\\
H_y(x,z,t) &= -i \frac{\omega}{\mu_0 c^2} \cos(k_z z) e^{i(kx-\omega t)},\\
H_z &= 0,
\end{aligned}
\tag{5.3}
$$

where we have $\omega = c(k^2 + k_z^2)^{1/2}$.

We superpose these expressions by multiplying with a Gaussian weight factor, $a^2 e^{-(k_z a)^2}$ and integrating in k_z from 0 to ∞. Here a is an arbitrary length.
For $ct = 0$ we have

$$
\begin{aligned}
E_x^{\sup}(x,z) &= \frac{\pi^{1/2} z}{4a} e^{-z^2/4a^2} e^{ikx},\\
E_y^{\sup} &= 0,\\
E_z^{\sup}(x,z) &= i \frac{\pi^{1/2} ka}{2} e^{-z^2/4a^2} e^{ikx},\\
H_x^{\sup} &= 0,\\
H_y^{\sup}(x,z) &= -i \frac{\pi^{1/2}}{2\mu_0 c} \left(k^2 a^2 - \frac{z^2}{4a^2} \right)^{1/2} e^{-z^2/4a^2} e^{ikx},\\
H_z^{\sup} &= 0.
\end{aligned}
\tag{5.4}
$$

For $ct > z$ we have

$$
\begin{aligned}
E_x^{\sup}(x,z,t) &= \frac{(2\pi)^{1/2} e^{-i(3\pi/4)}}{2} \frac{(ka)^{3/2} z c t a^{1/2}}{(c^2 t^2 - z^2)^{5/4}} e^{-(ka)^2 z^2/(c^2 t^2 - z^2)} e^{ik[x-(c^2 t^2 - z^2)^{1/2}]},\\
E_y^{\sup} &= 0,\\
E_z^{\sup}(x,z,t) &= \frac{(2\pi)^{1/2} e^{i(\pi/4)}}{2} \frac{(ka)^{3/2} c t a^{1/2}}{(c^2 t^2 - z^2)^{3/4}} e^{-(ka)^2 z^2/(c^2 t^2 - z^2)} e^{ik[x-(c^2 t^2 - z^2)^{1/2}]},\\
H_x^{\sup} &= 0,\\
H_y^{\sup}(x,z,t) &= -\frac{(2\pi)^{1/2} e^{i(\pi/4)}}{2\mu_0 c} \frac{(ka)^{3/2} (ct)^2 a^{1/2}}{(c^2 t^2 - z^2)^{5/4}} e^{-(ka)^2 z^2/(c^2 t^2 - z^2)} e^{ik[x-(c^2 t^2 - z^2)^{1/2}]},\\
H_z^{\sup} &= 0.
\end{aligned}
\tag{5.5}
$$

Next, we superpose electromagnetic field components given by Eqs. (5.4) and (5.5) by multiplying with a Gaussian weight factor, $a e^{-(ka)^2}$, and integrating in k from 0 to ∞. For $ct = 0$ we have

$$E_x^{\sup}(x,z)=\frac{\pi^{1/2}}{4}\frac{z}{a}e^{-z^2/4a^2}\left[\frac{\pi^{1/2}}{2}e^{-x^2/4a^2}+i\frac{x}{2a}e^{-x^2/4a^2}\,{}_1F_1\left(\frac{1}{2};\frac{3}{2};\frac{x^2}{4a^2}\right)\right],$$

$$E_y^{\sup}=0,$$

$$E_z^{\sup}(x,z)=i\frac{\pi^{1/2}}{4}e^{-z^2/4a^2}\left[{}_1F_1\left(1;\frac{1}{2};-\frac{x^2}{4a^2}\right)+i\frac{\pi^{1/2}}{2}\frac{x}{a}e^{-x^2/4a^2}\right],$$

$$H_x^{\sup}=0,$$

$$H_y^{\sup}(x,z)=-i\frac{\pi^{1/2}}{4\mu_0 c}e^{-z^2/4a^2}\left[{}_1F_1\left(1;\frac{1}{2};-\frac{x^2}{4a^2}\right)+i\frac{\pi^{1/2}}{2}\frac{x}{a}e^{-x^2/4a^2}\right],$$

$$H_z^{\sup}=0. \tag{5.6}$$

For $ct>z$ we have

$$E_x^{\sup}(x,z,t)=\frac{(2\pi)^{1/2}e^{-i(3\pi/4)}}{4}\frac{za^{1/2}}{(ct)^{3/2}}F(x,z,t),$$

$$E_y^{\sup}=0,$$

$$E_z^{\sup}(x,z,t)=\frac{(2\pi)^{1/2}e^{i(\pi/4)}}{4}\frac{(c^2t^2-z^2)^{1/2}a^{1/2}}{(ct)^{3/2}}F(x,z,t),$$

$$H_x^{\sup}=0,$$

$$H_y^{\sup}(x,z,t)=-\frac{(2\pi)^{1/2}e^{i(\pi/4)}}{4\mu_0 c}\frac{a^{1/2}}{(ct)^{1/2}}F(x,z,t),$$

$$H_z^{\sup}=0. \tag{5.7}$$

Here we have

$$\begin{aligned}F(x,z,t)=&\Gamma\left(\frac{5}{4}\right)\,{}_1F_1\left(\frac{5}{4};\frac{1}{2};-\frac{(c^2t^2-z^2)[x-(c^2t^2-z^2)^{1/2}]^2}{4c^2t^2a^2}\right)\\&+i\frac{(c^2t^2-z^2)^{1/2}}{ct}\frac{[x-(c^2t^2-z^2)^{1/2}]}{a}e^{-(c^2t^2-z^2)[x-(c^2t^2-z^2)^{1/2}]^2/4c^2t^2a^2}\\&\times{}_1F_1\left(-\frac{3}{2};\frac{3}{2};\frac{(c^2t^2-z^2)[x-(c^2t^2-z^2)^{1/2}]^2}{4c^2t^2a^2}\right).\end{aligned} \tag{5.8}$$

We show $E_z^{\sup}(x,z,t)$ and $H_y^{\sup}(x,z,t)$ in Fig. 6, by taking their real parts. We made the calculations of wave amplitude until the distance, $(z-ct)\leqslant 0$, and beyond that distance we made them equal to zero. Therefore, the wave amplitude at $ct=0$ and those for $ct>0$ are not directly connected. The value at $z=0$ of the wave amplitude at $ct=0$ should be smoothly connected to the limiting value at $ct=0$ continued from $ct>0$, of the wave amplitude for $ct>0$. The fact that it does not look so in figures is due to the stationary phase approximations used in obtaining Eq. (5.5). Waves propagate in the x direction and simultaneously in the z direction as time goes on, without loss of the energy, and as a bulk.

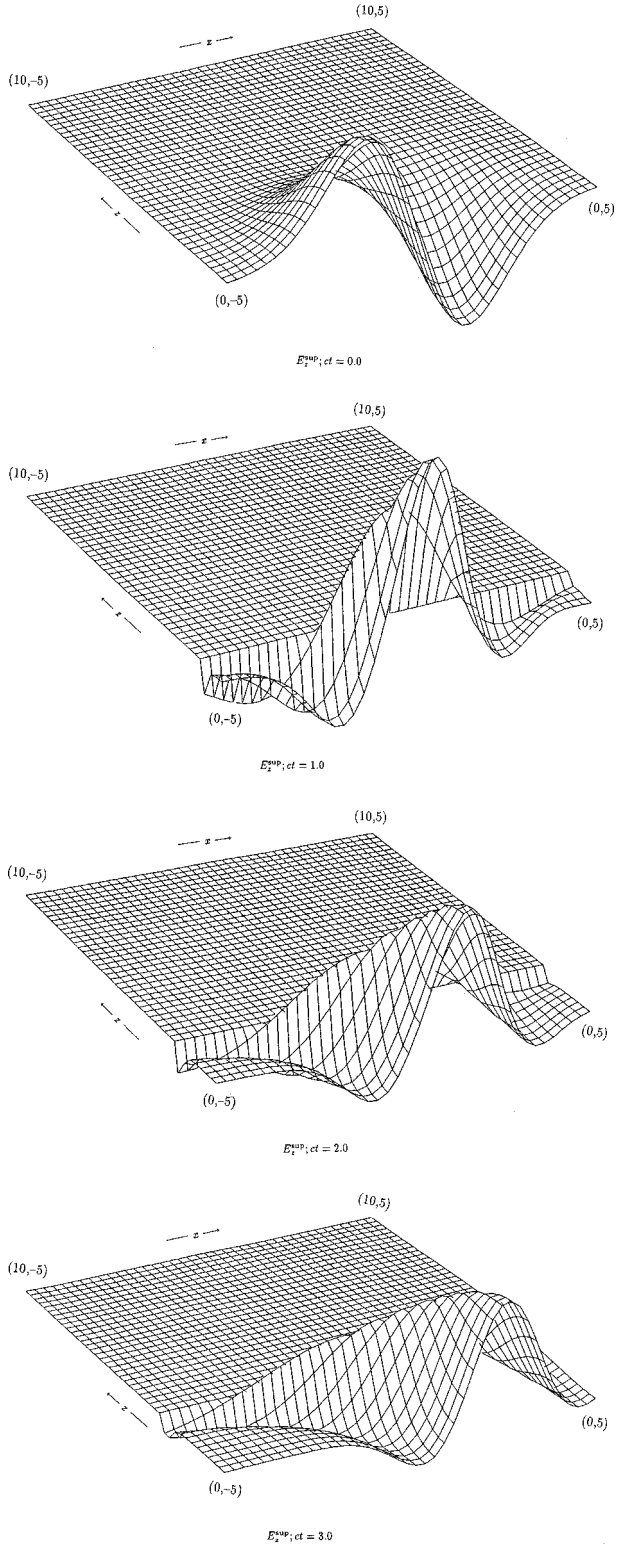


FIG. 6. Temporal behaviors of electromagnetic components, $E_x^{\mathrm{sup}}(x,z,t)$ and $H_y^{\mathrm{sup}}(x,z,t)$ in x and z space are drawn. Coordinates (z,x) stand for z values and x values, which they take when the amplitudes of electromagnetic fields are equal to zero, and in figures, they are drawn at the positions that the amplitudes actually take for corresponding cases and corresponding times. Electromagnetic waves move simultaneously to the z direction and x direction, as time goes on, without loss of the energy, and as a bulk.

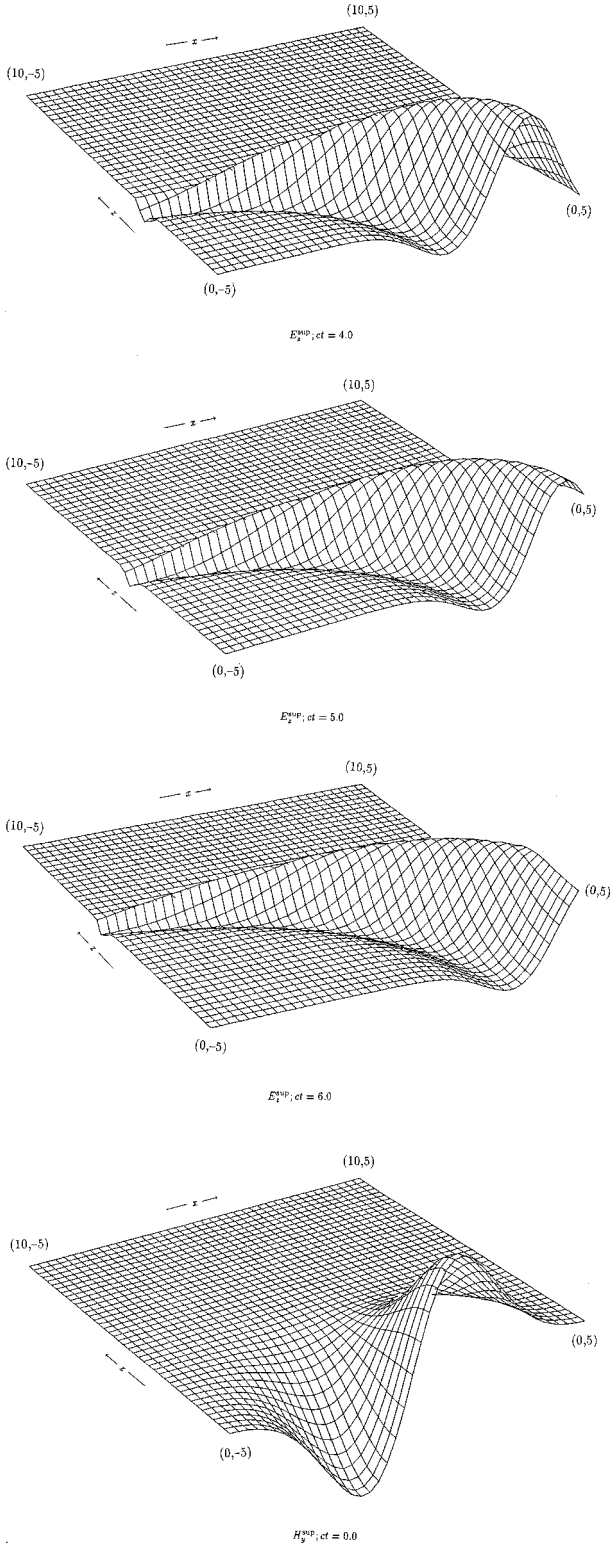
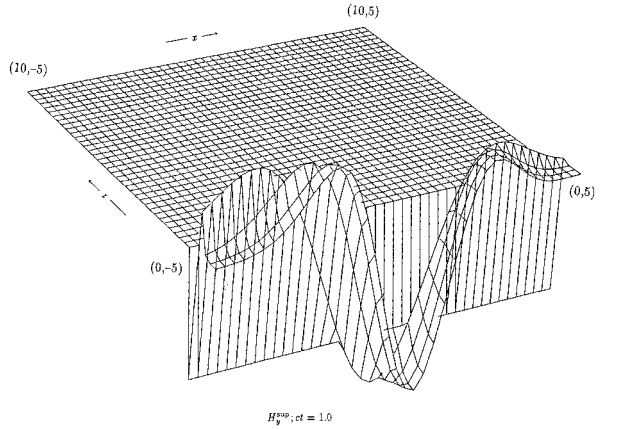
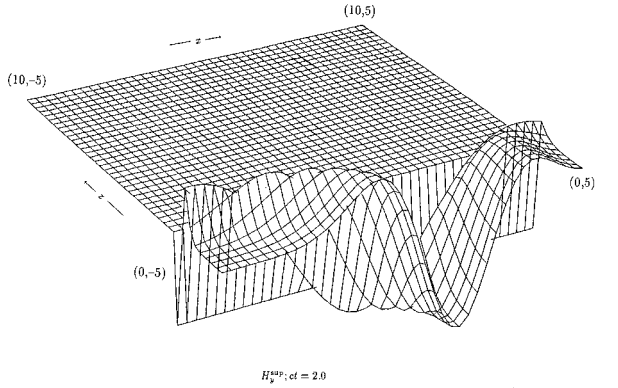


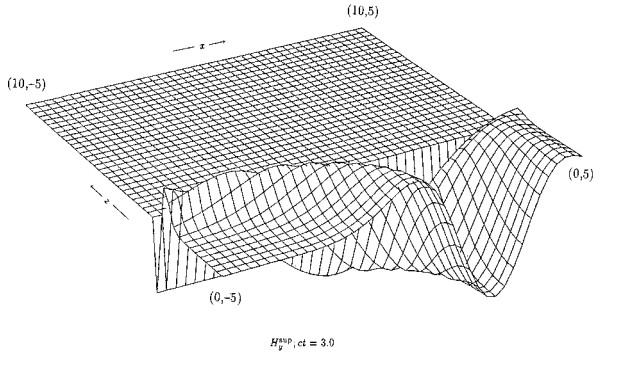
FIG. 6 (*Continued.*)



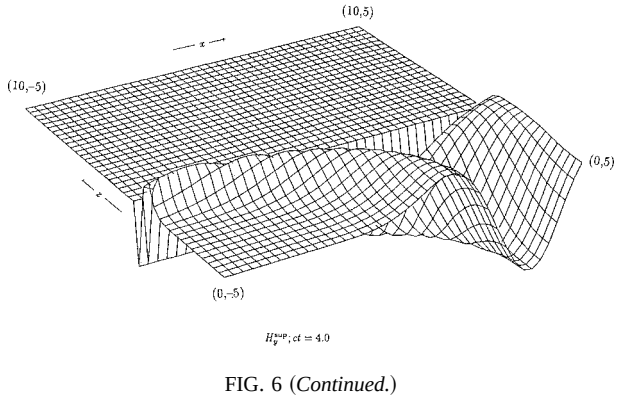
$H_y^{sup}; ct = 1.0$



$H_y^{sup}; ct = 2.0$



$H_y^{sup}, ct = 3.0$



$H_y^{sup}; ct = 4.0$

FIG. 6 (*Continued.*)

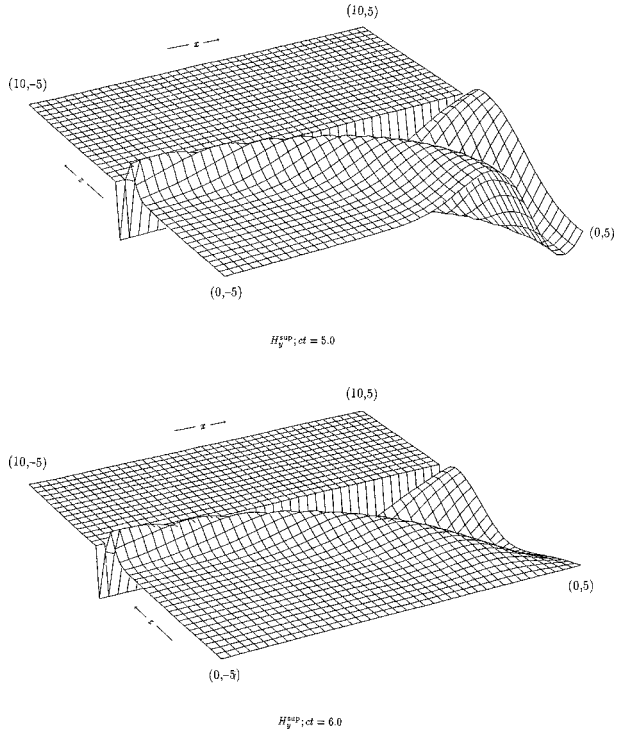


FIG. 6 (*Continued.*)

VI. SUMMARY

With a classical model of pseudophotons we obtained the qualitative picture of light waves diffracting a spherical superconductor. A quantum mechanical treatment of the same model gave the well-known TE and TM modes of an oscillating charged spherical superconductor with oscillating electromagnetic fields surrounding it.

Then we studied the temporal behavior of the charge distribution of the sphere and the electromagnetic field outside it, when the sphere with the axially symmetric charge distribution is suddenly rendered superconducting. A similar analysis was also made for an infinite plane superconductor. All complex eigenvalues for TM modes appear for given spherical harmonic index l in the first case, while continuous eigenvalues for given wave number k appear in the latter case. Nevertheless, physics looks similar in two cases.

The eigenvalues of TE and TM modes for a spherical superconductor are well approximated by the Debye and Sommerfeld formula. In this formula, a new characteristic integer appears in addition to spherical harmonic indices, l and m. Guided by the simple model stated above, and following the physical picture suggested by the works[6,7] by Franz and Deppermann (see Chap. III), we give a heuristic interpretation to the damping factor of the diffracting light waves in the shadow region of a spherical superconductor. This explanation automatically gives the physical meaning to the characteristic integer stated above.

We have made the computation of eigenvalues of Eq. (3.9) for TE modes, and Eq. (3.10) for TM modes, until spherical harmonic index $l=45$. With these values of TM modes we constructed the temporally changing states of coherent electromagnetic waves surrounding a spherical superconductor. The same analysis has been done for electromagnetic waves outside an infinite plane superconductor, and we obtained reasonable results in both cases.

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Exact equation of state for 2-dimensional gravitating system within Tsallis statistical mechanics

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We obtain an exact expression for the equation of state for a classical 2-dimensional gravitating system, using Tsallis's statistical mechanics. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1335553]

I. INTRODUCTION

The statistical mechanical description of gravitating systems, regarding the granularity of matter, is very important to the study of astrophysical systems. Unfortunately, there are only a few toy models that can be analytically worked. However, due to the long-range nature of gravity, some additional problems arise when standard statistical mechanics is applied to these systems—the divergences of phase volume $g(E)$ in the microcanonical description and partition function in the canonical description, in the short and long distances of gravitational potential. Depending on the system, divergence in a short distance may occur in one or both descriptions.[1]

An other approach which is usually employed to describe the gravitating systems is based on the distribution function $f(\mathbf{x},\mathbf{v},\mathbf{t})$ in phase space, by considering the smooth gravitational potential and ignoring the granularity of the system. However, this approach applied to the equilibrium configuration due to some mechanisms like violent relaxation, also leads to a problem of infinite total mass.[2]

Recently, an alternative entropy function called Tsallis's entropy[3] has been used by Plastino to study the problem above. The author has shown that Tsallis's entropy can determine the meaningful distribution function as described by polytropic models,[4] and it may represent an important starting point for investigating the subject by using Tsallis's description.

In this paper, for simplicity, we study the two-dimensional gravitating system by using Tsallis's description and we obtain the corresponding exact equation of state, regarding the granularity of the system.

II. TSALLIS FORMALISM

In this section, we introduce some quantities of Tsallis's formalism, for simplicity, based on unnormalized constraints (second version).[3] We also present the relations between the second and the third (normalized constraints[5]) versions for the q-averages. Tsallis's entropy with probability p_i is given by

$$S_q = k\frac{1-\Sigma_{i=1}^{W} p_i^q}{q-1}, \tag{1}$$

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where k is a positive constant, W is total number of microscopic configurations of the system and q is a real parameter. It should be noted that the standard entropy is recovered from (1) by taking it to the limit $q\to 1$. For simplicity, $k=1$, hereafter.

The connection with thermodynamics is obtained by extremizing S_q with the constraints

$$E_q=\langle H\rangle_q=\sum_{i=1}^{W} p_i^q \varepsilon_i \tag{2}$$

and

$$\sum_{i=1}^{W} p_i=1, \tag{3}$$

where E_q is the generalized internal energy. Hence, the probability of the canonical ensemble is given by

$$p_i=\frac{[1-\beta(1-q)\varepsilon_i]^{1/(1-q)}}{Z_q}, \tag{4}$$

where

$$Z_q=\sum_{i=1}^{W} [1-\beta(1-q)\varepsilon_i]^{1/(1-q)} \tag{5}$$

is the partition function of a canonical ensemble and β is a Lagrange multiplier. In order to retain a consistent probabilistic interpretation (eigenvalues of p_i must be nonnegative real numbers monotonically decreasing with the energy), the cut-off condition imposes $p_i(\varepsilon_i)=0$ whenever $[1-(1-q)\beta H]\leqslant 0$ ($\{\varepsilon_i\}$ is the set of eigenvalues of the Hamiltonian H).[3,5,6] From Eqs. (4) and (5) we can easily verify that

$$-\frac{\partial}{\partial\beta}\frac{Z_q^{1-q}-1}{1-q}=E_q. \tag{6}$$

Other useful relations:

$$\frac{Z_q^{1-q}-1}{1-q}+\beta E_q=S_q \tag{7}$$

and

$$\frac{\partial S_q}{\partial E_q}=\frac{1}{T}, \tag{8}$$

with $T\equiv 1/\beta$. From the definition of generalized free energy,

$$F_q=E_q-TS_q, \tag{9}$$

we obtain that

$$F_q=-\frac{1}{\beta}\frac{Z_q^{1-q}-1}{1-q}. \tag{10}$$

Notice that the constraint (2) is unnormalized, i.e., $\langle 1\rangle_q \neq 1$. A formulation based on the normalized constraint, has been worked in Ref. 5. The relation between the averages obtained within these formulations, based on the unnormalized and normalized constraints, can be established as follows:

$$\langle\langle \mathcal{O}\rangle\rangle_q(\beta)=\frac{\langle \mathcal{O}\rangle_q(\beta')}{\langle 1\rangle_q(\beta')}, \tag{11}$$

where $\langle\langle \mathcal{O}\rangle\rangle_q$ is the normalized constraint and β' is given by

$$\beta'=\frac{\beta}{\mathrm{Tr}\,\rho_q^q+(1-q)\beta\langle\langle H\rangle\rangle_q}. \tag{12}$$

III. 2-DIMENSIONAL GRAVITATING SYSTEM

The Hamiltonian of a two-dimensional gravitating system of N particles is given by

$$H=\sum_{i=1}^{N}\frac{P_i^2}{2m}+\frac{1}{2}\sum_{i\neq j}2Gm^2\ln|\mathbf{x}_i-\mathbf{x}_j|. \tag{13}$$

It should be noted that this system is analogous to that of 2-dimensional plasma when the constant (Gm^2) is replaced by $(-e_ie_j)$, where e_ie_j are the charges of particles.[7] Although the functional forms of these systems are similar, their physical properties are different because the charge particles may create screening.[8]

It is easy to show that the phase volume $g(E)$ of the system above, in the microcanonical ensemble, does not diverge since the particles are confined inside a large square box with length $2L$ $(-L,+L)$.[1] However, $g(E)$ cannot be analytically calculated.

In a canonical description, the central quantity is the partition function. From it one can calculate any thermodynamical quantity. It is given by

$$Z(\beta)=\int_{-L}^{+L}\prod_{i=1}^{N}\mathrm{d}^2P_i\,\mathrm{d}^2x_i\exp(-\beta H), \tag{14}$$

in classical statistical mechanics. Integrating out the momenta we obtain

$$Z(\beta)=\left(\frac{2\pi m}{\beta}\right)^N\int_{-L}^{+L}\prod_{i=1}^{N}\mathrm{d}^2x_i\exp\left(-\beta\sum_{i\neq j}Gm^2\ln|\mathbf{x}_i-\mathbf{x}_j|\right). \tag{15}$$

We observe that this last integral does not exist near the origin, except for

$$\beta<\beta_c=2[Gm^2(N-1)]^{-1}. \tag{16}$$

This means that below T_c the partition function diverges.

We now calculate the equation of state of the system above by using Tsallis's description. As in standard statistical mechanics, we replace the sum of Eq. (5) by the following integral:

$$Z_q(\beta)=\int_{-L}^{+L}\prod_{i=1}^{N}\mathrm{d}^2P_i\,\mathrm{d}^2x_i[1-\beta(1-q)H]^{1/(1-q)}. \tag{17}$$

We should note that Z_q does not exist near the origin for $q>1$. For this reason, we restrict our analysis for $q<1$. Moreover, we also assume that the particles are confined inside a large box which each x_i given by $(-L,+L)$, in order to maintain the integral (17) finite for large x_i. It

should be also noticed that the integration of Z_q over the momenta has a cutoff and should be adequately treated. To do so, we use the following integral representation of the gamma function:[9]

$$\frac{e^{ab}b^{z-1}}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}t\,\frac{e^{ibt}}{(a+\mathrm{i}t)^z}=\begin{cases}\dfrac{1}{\Gamma(z)} & \text{for} \quad b>0,\\ 0 & \text{for} \quad b<0,\end{cases} \tag{18}$$

by setting $b=[1-(1-q)\beta\Sigma_{i=1}^{N}(P_i^2/2m)/(1+\beta(q-1)\Sigma_{i\neq j}Gm^2\ln|\mathbf{x}_i-\mathbf{x}_j|)]^{1/(1-q)}$, $a=1$ and $z-1=1/(1-q)$. The representation (18) was also used in Ref. 10. An other integral representation valid for $q<1$ was established by Prato,[11] while the integral representation for $q>1$ was established by Hilhorst and was applied to study noninteracting particles.[12] Using Eq. (18) to take into account the cutoff of Eq. (17), we obtain

$$Z_q(\beta)=A\int_{-L}^{+L}\mathrm{d}^2x_1\ldots.\mathrm{d}^2x_N\left(1+\beta(q-1)\sum_{i\neq j}Gm^2\ln|\mathbf{x_i}-\mathbf{x_j}|\right)^{N+1/(1-q)}, \tag{19}$$

where

$$A=\left(\frac{2\pi m}{\beta(1-q)}\right)^N\frac{\Gamma\left(1+\dfrac{1}{1-q}\right)}{\Gamma\left(1+N+\dfrac{1}{1-q}\right)}. \tag{20}$$

We note that the integral (19) is similar of that of phase volume [see Eq. (3.40) of Ref. 1]. It has the form $\int\mathrm{d}x\,x[\ln(x^{\beta(1-q)Gm^2})^{-1}]^{N+1/(1-q)}$ in polar coordinates and it transforms into $\int\mathrm{d}z\,z^{N+1/(1-q)}\exp[-2z/(\beta(1-q)Gm^2)]$ with the variable $z=-\ln x^{(\beta(1-q)Gm^2)}$. Near the origin ($x\to 0$ and $z\to\infty$), the exponential function suppresses the power function, therefore, the integral does not diverge. This means that the partition function (19) is finite. We now redefine the variables $y_i=x_i/L$ in Eq. (19); then we get

$$Z_q(\beta,L)=A\int_{-1}^{1}\mathrm{d}^2y_1\ldots\mathrm{d}^2y_N\times\left[1+(q-1)\beta Gm^2\left(N(N-1)\ln L+\sum_{i\neq j}\ln|\mathbf{y_i}-\mathbf{y_j}|\right)\right]^{N+1/1(-q)}. \tag{21}$$

Differentiating $Z_q(\beta,L)$ with respect to L and using the following expression for the pressure:

$$P=-\frac{\partial F_q}{\partial V}=\frac{1}{\beta Z_q^q}\frac{\partial Z_q}{\partial V}, \tag{22}$$

where V is the two-dimensional volume (L^2), we obtain

$$P=\frac{N}{V\beta}\left\{Z_q^{1-q}-[1+N(1-q)]\frac{N-1}{2}\beta Gm^2H(\beta,L)\right\} \tag{23}$$

and

$$H(\beta,L)=A\int_{-L}^{+L}\mathrm{d}^2x_1\ldots\mathrm{d}^2x_N\left(1+\beta(q-1)\sum_{i\neq j}Gm^2\ln|\mathbf{x_i}-\mathbf{x_j}|\right)^{-1+N+1/(1-q)}. \tag{24}$$

Although the partition function Z_q is finite, the pressure P becomes negative for all V if $[1+N(1-q)](N-1)\beta Gm^2H(\beta,L)/(2Z_q^{1-q})>1$. Using now the expressions (9) and (10), we can write the expression (23) as follows:

$$P=\frac{N}{V\beta}\left\{1-\frac{N-1}{2}\beta Gm^2-(1-q)\beta\left[F_q+\frac{N-1}{2}Gm^2S_q\right]\right\}. \tag{25}$$

For $q\to 1$, we recover the standard result[1]

$$P=\frac{N}{V\beta}\left\{1-\frac{N-1}{2}\beta Gm^2\right\}. \tag{26}$$

For completeness, we now discuss about the three-dimensional gravitating system. In this case, the Hamiltonian is given by

$$H=\sum_{i=1}^{N}\frac{P_i^2}{2m}-\frac{1}{2}\sum_{i\neq j}\frac{Gm^2}{|\mathbf{x_i}-\mathbf{x_j}|}. \tag{27}$$

The phase volume $g(E)$ of this system diverges for $N\geqslant 3$.[1] In the standard canonical ensemble, the partition function diverges near the origin because the integrand has the form $r^2\exp(1/r)$. In the case of Tsallis's description, for $q<1$, we have

$$Z_q(\beta)=B\int_{-L}^{+L}\prod_{i=1}^{N}\mathrm{d}^3x_i\left[1+\beta(1-q)\frac{1}{2}\sum_{i\neq j}\frac{Gm^2}{|\mathbf{x_i}-\mathbf{x_j}|}\right]^{3N/2+1/(1-q)}, \tag{28}$$

where

$$B=\left(\frac{2\pi m}{\beta(1-q)}\right)^{3N/2}\frac{\Gamma\left(1+\dfrac{1}{1-q}\right)}{\Gamma\left(1+\dfrac{3N}{2}+\dfrac{1}{1-q}\right)}. \tag{29}$$

The integral to be calculated in (28) is of the form

$$\int_0^{\varepsilon}\mathrm{d}x\,x^2\left[1+\beta(1-q)\frac{1}{2}\frac{Gm^2}{x}\right]^{3N/2+1/(1-q)}=\lim_{\varepsilon\to 0}x^{3-1/(1-q)-3N/2}, \tag{30}$$

which diverges for $N\geqslant 2-2/[3(1-q)]$. This condition is more restrictive than that given in the calculation of phase volume.

Let us now consider the third version of Tsallis's statistics,[5] with the use of normalized constraint $E_q^{(3)}=\Sigma_{i=1}^{W}p_i^q\varepsilon_i/\Sigma_{j=1}^{W}p_j^q$. The partition function of the system (13), for $q<1$, is given by

$$(Z_q^{(3)}(\beta))^2=A\int_{-L}^{+L}\prod_{i=1}^{N}\mathrm{d}^2x_i\left\{(Z_q^{(3)})^{1-q}+\beta(1-q)\left[E_q^{(3)}-\sum_{i\neq j}Gm^2\ln|\mathbf{x_i}-\mathbf{x_j}|\right]\right\}^{N+1/(1-q)}, \tag{31}$$

in which we have integrated out all the momenta. We now change the variables $y_i=x_i/L$, then

$$(Z_q^{(3)}(\beta,L))^2=A\int_{-1}^{+1}\Pi_{i=1}^{N}\mathrm{d}^2y_i\times L^{2N}\left\{(Z_q^{(3)})^{1-q}+\beta(1-q)\left[E_q^{(3)}-\sum_{i\neq j}Gm^2\ln(L|\mathbf{y_i}-\mathbf{y_j}|)\right]\right\}^{N+1/(1-q)}. \tag{32}$$

We observe that this last equation depends implicitly on $Z_q^{(3)}$ and L. Thus, it turns out to be very difficult (according to our analysis) to obtain an exact expression for the equation of state.

IV. CONCLUSION

Contrary to standard statistical mechanics, we have shown that Tsallis's statistical mechanics[3] can describe the toy model of the two-dimensional gravitating system, in a canonical ensemble, without divergence near the origin of gravitational potential, even for $N \gg 1$. Moreover, for the limit $q \to 1$, we have recovered the standard result. Since the partition function Z_q is finite for $q < 1$, the system is thermodynamically acceptable, in principle. In the three-dimensional gravitating system, the phase volume diverges for $N \geqslant 3$. In Tsallis's description, the condition of divergence for Z_q is more restrictive than that given by phase volume, i.e., it diverges for $N > 2 - 2/[3(1-q)]$. This last condition is not thermodynamically acceptable because none of the thermodynamic quantities is well-defined for $N > 1$.

Despite the success of Tsallis's statistics applied to several systems,[13] a deeper investigation into the subject is needed to understand this interesting generalization of standard statistical mechanics.

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How does a shock in supersonic flow grow out of smooth data?

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This paper is devoted to the precise description of the process of formation and construction of shock waves. If a steady supersonic flow moves above a concavely curved wall, then the flow is compressed by the bending wall, and a suspended shock will be formed in the flow field. This fact with the existence of solution having an assigned singularity structure is rigorously proved. It is indicated that the suspended shock will start from the cusp of the envelope of λ_+ characteristics. Moreover, some estimates describing the behavior of the solution near the cusp are also obtained. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1343094]

I. INTRODUCTION

In the study of the quasilinear hyperbolic system of conservation laws a most important phenomena is that smooth initial data may develop discontinuities. The fact corresponding to such phenomena in fluid dynamics is that supersonic flow often contains shocks and other singularities in the flow field, even though all data to determine the flow are smooth. Besides some of the simplest examples for the Cauchy problem of the scalar equation (see Refs. 1 and 2), Sideris proved in Refs. 3 and 4 that under rather general assumptions the smooth solution of the Euler system, describing compressible flow, must blow up in finite time. In the case of steady flow, when a supersonic flow passes around a smooth concave wall, the flow is compressive due to the bending of the wall. Then, a suspended shock will be formed in a bounded domain (see Refs. 5 and 6).

In this paper we will give a detailed analysis of the problem arising in supersonic flow past a bended rigid wall. Though people have known the fact from physical experience that a shock will be formed somewhere above the bended wall, more accurate information is obviously important. The information includes the location of blowup points and the precise structure and estimate of the solution near the place of blowup. It will not only offer us the knowledge of how the discontinuity comes from smooth data, but also gives us a preparation to construct a global solution. In this aspect we mention Alinhac's work on the mechanism of blowup. In Refs. 7 and 8, Alinhac introduces two kinds of mechanism of blowup, namely, ordinary differential equation blowup and geometric blowup. According to this classification the blowup caused by the curved rigid wall in steady supersonic flow belongs to geometric blowup. As we will show, the derivatives of solution become infinity at the point of blowup, while the solution itself remains bounded. Besides, the strength of the shock is zero at the blowup point and then gradually increases.

The process of shock formation for scalar quasilinear hyperbolic equations has been well known for a long time. In this case, the shock appears, starting from the cusp of the envelope of characteristics of the equation. Meanwhile the shock can be determined by solving an ordinary differential equation (see Refs. 1 and 2). In the case of the p system, Lebaud discussed the problem of shock formation under the assumption that one Riemann invariant remains constant in Ref. 9. For steady potential flow, which is an approximation of the Euler system under the assumption of ''isentropic'' and ''irrotational,'' such a discussion is also presented (see Ref. 6).

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Certainly, people are more interested in the case without such assumptions, because in fact the flow will be neither isentropic nor irrotational once the shock appears. In this paper we will use the original Euler system to describe steady flow, and give a complete construction of the shock in the neighborhood of the starting point of the shock. In the whole paper we only consider the flow with two space variables.

The Euler system describing the two-dimensional steady flow is

$$\frac{\partial}{\partial x}\begin{pmatrix} \rho u \\ p+\rho u^2 \\ \rho uv \\ \rho uE+pu \end{pmatrix}+\frac{\partial}{\partial y}\begin{pmatrix} \rho v \\ \rho uv \\ p+\rho v^2 \\ \rho vE+pv \end{pmatrix}=0, \tag{1.1}$$

where (u,v), p, ρ, E represent components of velocity, pressure, density, and energy, respectively. For polytropic gas $E=\frac{1}{2}(q^2)+e, p=A(S)\rho^{\gamma}$, where S is entropy, γ is the adiabatic exponent, $q^2=u^2+v^2$, $e=p/(\gamma-1)\rho$, $A(S)=(\gamma-1)e^{c_v(S-S_0)}$ with c_v being a constant.

From (1.1) we know that along every streamline Bernoulli's relation holds

$$\frac{1}{2}(u^2+v^2)+\frac{a^2}{\gamma-1}=\text{const}, \tag{1.2}$$

where a is sonic speed, which is

$$a=\left(\frac{\mathrm{d}p}{\mathrm{d}\rho}\right)_S^{1/2}=A(S)\gamma\rho^{\gamma-1}=A(S)^{1/\gamma}\gamma p^{(\gamma-1)/\gamma}. \tag{1.3}$$

We also remark here that the constant in (1.2) may be different along different streamlines.

Assume that there is a curved wall with equation $y=f(x)$, $f(x)\in C^{p+1}$, $p\geqslant 4$, which satisfies

$$\begin{cases} f(x)\equiv 0, & x\leqslant 0, \\ f(x)>0, f'(x)>0, f''(x)>0, & x>0. \end{cases} \tag{1.4}$$

According to (1.4) the wall is curved up starting from the right side of the origin. Therefore, when a supersonic flow comes from the left side with velocity $(q_\infty,0)$, it is compressed in $x\geqslant 0$ by the wall. The compression will cause formation of a shock.

On the shock the solution of (1.1) is discontinuous, and the parameters of the flow on the both sides satisfy the Rankine–Hugoniot condition

$$\begin{gathered} \rho_0 u_{0n}=\rho_1 u_{1n}, \\ p_0+\rho_0 u_{0n}^2=p_1+\rho_1 u_{1n}^2, \\ u_{0t}=u_{1t}, \\ \frac{1}{2}q_0^2+\frac{\gamma p_0}{(\gamma-1)\rho_0}=\frac{1}{2}q_1^2+\frac{\gamma p_1}{(\gamma-1)\rho_1}, \end{gathered} \tag{1.5}$$

where u_n, u_t represent the normal and tangential components of velocity, the subscript ''0'' or ''1'' represents the value of corresponding quantities ahead or behind the shock. Besides, on the shock the entropy condition

$$S_1>S_0 \tag{1.6}$$

should also be satisfied. To simplify notations we often omit the subscript ''1,'' if no confusion is caused.

Ahead of the shock the flow is assumed to be uniform. So the constant in (1.3) equals $\frac{1}{2}u_0^2 + [1/(\gamma-1)]a_0^2$. Corespondingly, the system (1.12) can be reduced to a system with three equations

$$\begin{cases} K(p,\theta,S)\dfrac{\mathrm{d}p}{\mathrm{d}\ell_+} + \dfrac{\mathrm{d}\theta}{\mathrm{d}\ell_+} = 0, \\ \dfrac{\mathrm{d}S}{\mathrm{d}\ell_0} = 0, \\ K(p,\theta,S)\dfrac{\mathrm{d}p}{\mathrm{d}\ell_-} - \dfrac{\mathrm{d}\theta}{\mathrm{d}\ell_-} = 0, \end{cases} , \tag{1.7}$$

where

$$\frac{\mathrm{d}}{\mathrm{d}\ell_{\pm,0}} = \frac{\partial}{\partial x} + \lambda_{\pm,0}\frac{\partial}{\partial y}$$

is the directional derivative along the characteristics

$$\ell_{\pm,0}, \theta = \arctan\frac{v}{u}, K(p,\theta,S) = \frac{1}{\rho q^2 \tan A},$$

A is the Mach angle. Besides,

$$\lambda_\pm = \frac{uv \pm \sqrt{q^2-a^2}}{u^2-a^2}, \quad \lambda_0 = \frac{v}{u}. \tag{1.8}$$

It is convenient to introduce new unknown functions z, w, which amount to Riemannian invariants in the irrotational case. Let $z = \theta - F(q)$, $w = \theta + F(q)$ with

$$F(q) = \int \frac{\sqrt{q^2-a^2}}{aq}\mathrm{d}q,$$

(1.7) can be rewritten as

$$\begin{cases} \dfrac{\mathrm{d}z}{\mathrm{d}\ell_+} - \mathrm{d}\dfrac{\mathrm{d}S}{\mathrm{d}\ell_+} = 0, \\ \dfrac{\mathrm{d}S}{\mathrm{d}\ell_0} = 0, \\ \dfrac{\mathrm{d}w}{\mathrm{d}\ell_-} + \mathrm{d}\dfrac{\mathrm{d}S}{\mathrm{d}\ell_-} = 0, \end{cases} \tag{1.9}$$

where

$$d = \frac{1}{\gamma(\gamma-1)A(s)}\frac{a\sqrt{q^2-a^2}}{q^2}.$$

According to the shock theory of compressible flow (see Ref. 10), across λ_+ shock the jump of z is the main part of the jump of parameters of the flow, while the jump of w and S is only a quantity of third order, comparing the strength of shock.

Before the formation of shock the uniform upstream flow has become a nonuniform flow by the influence of the curved wall. If the wall is not greatly bended, the flow near the wall can be obtained by a characteristic method. The flow in this region is called the Prandtl–Meyer flow,

where all parameters keep constant on each λ_+ characteristic line. In this case, by viewing $u(x,y)$, $v(x,y)$ as a map from the plane (x,y) to the plane (u,v), the whole region of the Prandtl–Meyer flow is mapped to an epicycloidal (see Ref. 5)

$$\begin{cases} u = a_*(\cos\mu(\omega-\omega_*)\cos\omega + \mu^{-1}\sin\mu(\omega-\omega_*)\sin\omega), \\ v = a_*(\cos\mu(\omega-\omega_*)\sin\omega - \mu^{-1}\sin\mu(\omega-\omega_*)\cos\omega), \end{cases} \tag{1.10}$$

where

$$\mu = \left(\frac{\gamma-1}{\gamma+1}\right)^{1/2},$$

a_* is the critical sound speed, $\omega_* = \mu^{-1}\arccos(a_0/a_*)$, and a_0 is the sound speed of the upstream flow.

Since the direction of the velocity on the wall must be tangential to the surface of the body, we have at the point $(\overline{x}, f(\overline{x}))$

$$f'(\overline{x}) = \frac{\cos\mu(\omega-\omega_*)\sin\omega - \mu^{-1}\sin\mu(\omega-\omega_*)\cos\omega}{\cos\mu(\omega-\omega_*)\cos\omega + \mu^{-1}\sin\mu(\omega-\omega_*)\sin\omega}. \tag{1.11}$$

Correspondingly, we must require that the angle γ of the tangential line with the x axis is always less than ω_*, i.e.,

$$\arctan f'(\overline{x}) < \omega_* \quad \text{for any } \overline{x}. \tag{1.12}$$

The derivative of the right-hand side of (1.11) with respect to ω is

$$(\cos\mu(\omega-\omega_*)\cos\omega + \mu^{-1}\sin\mu(\omega-\omega_*)\sin\omega)^{-2}\mu^{-1}(\mu^{-1}-\mu)\sin^2\mu(\omega-\omega_*),$$

which is positive identically. Therefore, from the assumption $f''>0$ we know that (1.11) determines a one-to-one map between $\overline{x}$ and ω. Moreover, $\omega(\overline{x})$ is a C^p increasing function.

Notice that the geometric meaning of the parameter ω is the angle of y axis with the normal to λ_+ characteristics (see Ref. 5). Then the equation of the characteristics issuing from $(\overline{x}, f(\overline{x}))$ is

$$\begin{cases} x = \overline{x} + t\cos\left(\omega - \dfrac{\pi}{2}\right) = \overline{x} + t\sin\omega, \\ y = f(\overline{x}) + t\sin\left(\omega - \dfrac{\pi}{2}\right) = f(\overline{x}) - t\cos\omega, \end{cases} \tag{1.13}$$

where $\omega = \omega(\overline{x})$ is determined by (1.11).

The family of characteristics of (1.13) is compressed and then forms an envelope, because the wall is curved up. The envelope is determined by

$$\Delta \equiv \frac{\partial(x,y)}{\partial(t,\overline{x})} = 0. \tag{1.14}$$

Equation (1.14) implies

$$t = -\frac{1}{\omega'}(f'\sin\omega + \cos\omega).$$

Substituting it into (1.13) we obtain

$$\begin{cases} x=\overline{x}-\dfrac{1}{\omega'}(f'\sin\omega(\overline{x})+\cos\omega(\overline{x}))\sin\omega(\overline{x}), \\ y=f(\overline{x})+\dfrac{1}{\omega'}(f'\sin\omega(\overline{x})+\cos\omega(\overline{x}))\cos\omega(\overline{x}). \end{cases} \tag{1.15}$$

Simply denote (1.15) as $x=k(\overline{x})$, $y=h(\overline{x})$. If $k(\overline{x})$ takes its minimum at $\overline{x}=\overline{x_0}$:

$$k'(\overline{x_0})=0, \quad (\overline{x}-\overline{x_0})k'(\overline{x})>0, \tag{1.16}$$

then the envelope has a cusp at $(x_0,y_0)=(k(\overline{x_0}),h(\overline{x_0}))$, which will be the starting point of shock.

The main result of this paper is:

Theorem 1.1: Assume that a uniform upstream flow with velocity $(u_0,0)$ moves above the wall $y=f(x)$ from left to right, $u_0>a_0$, $f(x)$ satisfies (1.4), (1.11), and (1.16), then system (1.1) admits a solution, which is continuously differentiable in $x<x_0$ and has a shock $\Gamma: y=\phi(x)$ starting from the point (x_0,y_0). In the neighborhood Ω of (x_0,y_0), the solution is also continuously differentiable in $\Omega\backslash\Gamma$. Besides, the solution satisfies the Rankine–Hugoniot condition and entropy condition on Γ, and their estimates in Ω can be expressed through z,w,S as follows:

$$\begin{cases} \phi(x)=y_0+\alpha(x-x_0)+O((x-x_0)^2), \\ w=w_0+O((x-x_0)^{3/2}), \\ z=z_0+O((x-x_0)^3+(y-y_0-\alpha(x-x_0))^2)^{1/6}, \\ S=S_0+O((x-x_0)^{3/2}), \end{cases} \tag{1.17}$$

where w_0,z_0,S_0 are the values of the corresponding functions at the point (x_0,y_0), and α is the slope of the λ_+ characteristics at this point.

We remark here that some weaker singularities of the solution of (1.1) may propagate into the domain $x>x_0$ along the characteristics through (x_0,y_0), though the solution is continuous there.

The solution (z,w,S) in $x\geqslant x_0$ will be constructed by an iterative procedure. To this end we are going to construct a sequence of solutions $\{z^{(\nu)}(x,y)\}$, $\{w^{(\nu)}(x,y)\}$, $\{S^{(\nu)}(x,y)\}$ and a corresponding sequence $\phi^{(\nu)}(x)$ standing for the location of the approximate shock, and then prove the convergence of these sequences. Here we take $w^{(0)}(x,y)=w_0, S^{(0)}(x,y)=S_0$ as the first approximation of w and S, while $z^{(0)}(x,y)$ as well as the position of the approximate shock $y=\phi_0(x)$ are determined by a conservation law corresponding to the first equation of (1.9). Then the whole sequence $\{z^{(\nu)}\}$, $\{w^{(\nu)}\}\{S^{(\nu)}\}$ can be successively determined by the characteristic method, while $\{\phi^{(\nu)}(x)\}$ can be determined by the Rankine–Hugoniot condition correspondingly.

The remainder of this paper is arranged as follows: In Sec. II we give a first approximation of system (1.9), which defines $z^{(0)}(x,y)$, $\phi^{(0)}(x)$, and give some description of the approximation as a preparation for further discussion. In Sec. III we give an iterative scheme to construct the sequence of approximate solutions, and set up a proposition $F^{(\nu)}$, which indicates the estimates satisfied by the approximate solutions and which should be verified inductively later. According to this scheme, Sec. IV is devoted to the estimates of $\{z^{(\nu+1)}\}$, $\{w^{(\nu+1)}\}$, $\{S^{(\nu+1)}\}$, and $\{\phi^{(\nu)}\}$ under the assumption $F^{(\nu)}$. Section V is devoted to the estimates of derivatives of all these functions. Finally, in Sec. VI we establish the convergence of all these sequences, and then prove the main conclusion in this paper.

II. FIRST APPROXIMATION

As mentioned previously, we take $w^{(0)}(x,y)=w_0$, $S^{(0)}(x,y)=S_0$ as the first approximation of w,S in $x>x_0$. Since both $w^{(0)}$ and $S^{(0)}$ can be added by an arbitrary constant, so we simply take $w_0=S_0=0$. Take δ as a suitable small number, then $\Gamma:\{x=x_0-\delta, y>f(x_0-\delta)\}$ locates in the domain of Prandtl–Meyer flow. All parameters of the flow on Γ are known. So the flow near

(x_0,y_0) can also be determined by the data on Γ. It means that the problem to determine the solution near (x_0,y_0) can be reduced to a Cauchy problem of system (1.1) [or (1.9)] with data $w=S=0, z=z_0(y)\in C^p$ on Γ.

To seek the first approximation of $z(x,y)$ we substitute $w=S=0$ into (1.9). The first equation (1.9) is then reduced to

$$\partial_x z(x,y)+\lambda_+\partial_y z(x,y)=0, \tag{2.1}$$

where

$$\lambda_+=\frac{uv+a\sqrt{q^2-a^2}}{u^2-a^2}.$$

In the domain $x<x_0$, $w=S=0$ combined with the solution of the first equation (2.1) coincides with the solution of the whole system (1.9). Since the solution of (2.1) may have discontinuity in the domain $x\geqslant x_0$, to describe the discontinuity condition on shock we need to reduce (2.1) to a suitable form of conservation law and let the discontinuity condition for (2.1) coinside with the Rinkine–Hugoniot condition of (1.1).

Recall the definitions of z and w, we have $\theta=\frac{1}{2}(z+w), F(q)=\frac{1}{2}(w-z)$. Denote G as the inverse function of $F(q)$, then

$$q=G\left(\frac{w-z}{2}\right),$$

and

$$\lambda_+=\frac{G^2\cos\frac{z}{2}\sin\frac{z}{2}+\sqrt{G^2-(\gamma-1)\left(c_0-\frac{1}{2}G^2\right)}}{G^2\cos^2\frac{z}{2}-(\gamma-1)\left(c_0-\frac{1}{2}G^2\right)}, \tag{2.2}$$

where $G=G(-z/2)$.

Compare Eq. (2.1) with the conservation law of mass in (1.1). The first equation in (1.1) for $w=S=0$ can be written as

$$(\rho_z u+\rho u_z)z_x+(\rho_z v+\rho v_z)z_y=0. \tag{2.3}$$

On the other hand, under the assumption $S=\text{const}$ we have

$$qq_z+\frac{a^2}{\rho}\rho\rho_z=0.$$

Direct calculation implies

$$\rho_z u+\rho u_z=\frac{1}{2}\frac{\rho q^2 u}{a\sqrt{q^2-a^2}}-\frac{1}{2}\frac{\rho a u}{\sqrt{q^2-a^2}}-\frac{1}{2}\rho v, \tag{2.4}$$

$$\rho_z v+\rho v_z=\frac{1}{2}\frac{\rho q^2 v}{a\sqrt{q^2-a^2}}-\frac{1}{2}\frac{\rho a v}{\sqrt{q^2-a^2}}+\frac{1}{2}\rho u. \tag{2.5}$$

Moreover,

$$\lambda_+\left(\frac{\rho q^2 u}{a\sqrt{q^2-a^2}}-\frac{\rho a u}{\sqrt{q^2-a^2}}-\rho v\right)=\frac{\rho q^2 v}{a\sqrt{q^2-a^2}}-\frac{\rho a v}{\sqrt{q^2-a^2}}+\rho u.$$

Therefore, multiplying (2.1) by $(\rho_z u+\rho u_z)_{w=S=0}$ we obtain

$$((\rho u)_z)_{w=S=0}\partial_x z+((\rho v)_z)_{w=S=0}\partial_y z=0, \tag{2.6}$$

which coincides with (2.3).

To analyze the weak solution of (2.6), we view ρu as a new unknown function m. Notice that

$$(\rho u)_z>0$$

for $u>a$, then $m(z)$ is an increasing function, and (2.6) can be written as

$$m_x+f(m)_y=0. \tag{2.7}$$

Viewing the coordinate $\overline{y}$ on Γ as a parameter, the family of λ_+ characteristics can be denoted as

$$y=\overline{y}+xg(\overline{y}). \tag{2.8}$$

The envelope of the family (2.8) is

$$x=-\frac{1}{g'(\overline{y})},\quad y=\overline{y}-\frac{g(\overline{y})}{g'(\overline{y})}, \tag{2.9}$$

which is another form of (1.14). Correspondingly, we have

$$k(\overline{x})=-\frac{1}{g'(\overline{y})},\quad k'(\overline{x})=\frac{g''(\overline{y})}{g'(\overline{y})^2}\frac{d\overline{y}}{d\overline{x}}, \tag{2.10}$$

Let us choose $\overline{y_0}$, so that the straight line $y=\overline{y_0}+xg(\overline{y_0})$ is just the λ_+ characteristics through $(k(\overline{x_0}),h(\overline{x_0}))$. In view of the fact that the slope of λ_+ characteristics is positive and bounded away from zero, there is a constant c, such that $c^{-1}(x-x_0)\leqslant y-y_0\leqslant c(x-x_0)$. Hence

$$\begin{gathered}k'(\overline{x_0})=0\leftrightarrow g''(\overline{y_0})=0,\\ (\overline{x}-\overline{x_0})k'(\overline{x_0})\geqslant 0,\leftrightarrow(\overline{y}-\overline{y_0})g''(\overline{y})\geqslant 0.\end{gathered} \tag{2.11}$$

Generally, for the initial problem of quasilinear equation (2.7), when the family of characteristics forms an envelope with a cusp, the solution with a shock starting from the cusp has been constructed (see Refs. 1 and 2). Moreover, denote $x-x_0$ by $\tilde{x}$, $y-y_0-\alpha(x-x_0)$ with $\alpha=g(y_0)$ by $\tilde{y}$, and recalling the result in Ref. 9 we have the following propositions:

Lemma 2.1: If $f(m)\in C^\infty$, $m_0(y)=m(x_0-\delta,y)\in C^p$, then there is a weak solution $m(x,y)$ of (2.7) and a $C^{p/2}$ function $y=\phi(x)$ defined on $x\geqslant 0$, such that $m(x,y)$ is of C^p away from $y=\phi(x)$, and satisfies estimates

$$\begin{gathered}|m(x,y)-m(0,0)|\leqslant C(\tilde{x}^3+\tilde{y}^2)^{1/6},\\ |\partial_{\not}m(x,y)|\leqslant C(\tilde{x}^3+\tilde{y}^2)^{-1/6},\\ |\partial_y m(x,y)|\leqslant C(\tilde{x}^3+\tilde{y}^2)^{-1/3},\\ |\partial_{yy}m(x,y)|\leqslant C(\tilde{x}^3+\tilde{y}^2)^{-5/6},\end{gathered} \tag{2.12}$$

where $\partial_{\not}=\partial_x+\alpha\partial_y$. Besides, $z(x,y)$ satisfies the same estimates.

Lemma 2.2: The leftward characteristics $y=\eta_{\pm}(x,a,b)$ through point (a,b) with $a>0$ in the neighborhood of the origin (above or below x axis, respectively) does not intersect with the shock $y=\phi(x)$, and satisfies the estimates

$$\pm\eta_{\pm}(0,a,b)=\sqrt{a}+O(a)+|O(b^{1/3})|, \tag{2.13}$$

$$\pm(\eta_{\pm}(x,a,b)-b)=\sqrt{a}(a-x)+|O(b^{1/3}(a-x))|+O(a(a-x)). \tag{2.14}$$

Lemma 2.3: For any point (a,b) in the neighborhood of the origin, $\eta_{\pm}(x,a,b)$ satisfies

$$x^3+\eta_{\pm}(x,a,b)^2\geqslant\tfrac{5}{16}(a^3+b^2). \tag{2.15}$$

Lemma 2.4: Suppose that $\zeta(x,a,b)$ is a function satisfying

$$|\zeta(x,a,b)-\eta(x,a,b)|\leqslant Ca(a-x), \tag{2.16}$$

then for small a

$$0<-\int_0^a(\lambda_u\cdot u_y)(x,\zeta(x,a,b))\mathrm{d}x<\log\tfrac{3}{2}+C\sqrt{a}. \tag{2.17}$$

III. ITERATION SCHEME

Next we are going to improve the approximation of the sequence successively. To avoid the difficulty caused by the change of the location of the shock we perform a coordinate transformation to fix the location of the shock. Suppose that the location of the shock at νth step is $y=\phi^{(\nu)}(x)$, then the transformation is

$$T^{(\nu)}:\tilde{x}=x-x_0,\tilde{y}=\begin{cases}y-\phi^{(\nu)}(x), & \text{if } \geqslant x_0\\ y_0+\alpha(x-x_0), & \text{if } {}_0-\delta\leqslant x\leqslant x_0,\end{cases} \tag{3.1}$$

where α is the slope of λ^+ characteristics through (x_0,y_0). Obviously, the location of shock is fixed on $\tilde{x}=x_0$ by the transformation (3.1).

To simplify the notation we will denote $\tilde{x}$, $\tilde{y}$ by x,y again, move (x_0,y_0) to (0,0), and restrict our discussion on $\Omega=\Omega_0\cup\Omega_+\cup\Omega_-$, where

$$\Omega_0=\{(x,y),-\delta\leqslant x\leqslant 0,-\epsilon\leqslant y\leqslant\epsilon\},$$

$$\Omega_+=\left\{(x,y);0\leqslant x\leqslant\frac{\epsilon}{K},0\leqslant y\leqslant\epsilon-Kx\right\}, \tag{3.2}$$

$$\Omega_-=\left\{(x,y);0\leqslant x\leqslant\frac{\epsilon}{K},-\epsilon-Kx\leqslant y\leqslant 0\right\}.$$

Obviously, when ϵ is small, and K is large, the domain Ω locates above the rigid wall. Besides, $\Omega_{\pm}$ locates in the determinate region of Ω_0.

The approximate solutions $\{z^{(\nu)}\}$, $\{w^{(\nu)}\}$, $\{S^{(\nu)}\}$ and the approximate slope of shock $\{\sigma^{(\nu)}(x)\}$ are costructed as follows.

First, $w^{(0)}(x,y)=S^{(0)}(x,y)=0$, $z^{(0)}(x,y)$ is determined as the solution of (2.1), and $\sigma^{(0)}(x)$ is obtained in the process of determining $z^{(0}(x,y)$.

Now assume that $z^{(\nu)}$, $w^{(\nu)}$, $S^{(\nu)}$ are given, then $\rho^{(\nu)}$, $u^{(\nu)}$, $v^{(\nu)}$ are known correspondingly. Take

$$\sigma^{(\nu)}=\begin{cases} -\dfrac{[\rho^{(\nu)}v^{(\nu)}]}{[\rho^{(\nu)}u^{(\nu)}]}, & \geqslant 0 \\ \alpha, & <0, \end{cases} \tag{3.3}$$

where $[\cdot]$ means the difference of the lower limit from the upper limit of the quantity inside the brackets. Then, as indicated in Sec. II, $\sigma^{(\nu)}$ with $\nu=0$ in (3.3) coincides with the slope of the shock in the solution of Eq. (2.1).

In the sequel we define $z^{(\nu+1)}$, $w^{(\nu+1)}$, $S^{(\nu+1)}$ as the solution of the following linear system:

$$\left.\begin{array}{c} \partial_x z^{(\nu+1)}+(\lambda_+^{(\nu)}-\sigma^{(\nu)})\partial_y z^{(\nu+1)}-d^{(\nu)}(\partial_x S^{(\nu)}+(\lambda_+^{(\nu)}-\sigma^{(\nu)})\partial_y S^{(\nu)})=0, \\ \partial_x S^{(\nu+1)}+(\lambda_0^{(\nu)}-\sigma^{(\nu)})\partial_y S^{(\nu+1)}=0, \\ \partial_x w^{(\nu+1)}+(\lambda_-^{(\nu)}-\sigma^{(\nu)})\partial_y w^{(\nu+1)}+d^{(\nu)}(\partial_x S^{(\nu)}+(\lambda_-^{(\nu)}-\sigma^{(\nu)})\partial_y S^{(\nu)})=0 \end{array}\right), \tag{3.4}$$

satisfying initial conditions

$$w^{(\nu+1)}(-\delta,y)=0, S^{(\nu+1)}(-\delta,y)=0, z^{(\nu+1)}(-\delta,y)=z_0(y). \tag{3.5}$$

Problem (3.4),(3.5) can be solved by a characteristic method. Since λ_-, λ_0 characteristics may intersect with $y=0$, we have also to estimate $w^{(\nu+1)}$ and $S^{(\nu+1)}$ on $y=0$ in order to obtain estimates of $w^{(\nu+1)}$ and $S^{(\nu+1)}$ in Ω_-. This is given in the following lemma:

Lemma 3.1: On λ_+ shock

$$[\theta]=k[F(q)], \tag{3.6}$$

where k is a smooth function of $(\theta_u,\ \theta_\swarrow,\ q_u,\ q_\swarrow,\ \rho_u,\ \rho_\swarrow)$, and it tends to -1 as $[q]\to 0$. Here θ_u means the value of θ on the upper side of the shock, while $\theta_\swarrow$ means the value of θ on the lower side of the shock. The meaning q_u, $q_\swarrow$, ρ_u, $r_\swarrow$ are similar.

Proof: From the shock relation one has

$$\sigma=-\frac{[u]}{[v]}=\frac{[\rho v]}{[\rho u]}.$$

Write $u=q\cos\theta$, $v=q\cos\theta$, we obtain

$$\cos[\theta]=\frac{\rho_\swarrow q_\swarrow^2-\rho_u q_u^2}{(\rho_\swarrow+\rho_u)q_\swarrow q_u}, \tag{3.7}$$

then

$$\sin^2[\theta]=-\frac{(q_\swarrow+q_u)^2\left(\rho_+^2+q_u^2\dfrac{\rho_\swarrow^2-\rho_u^2}{q_\swarrow^2-q_u^2}\right)}{(\rho_\swarrow+\rho_u)^2 q_\swarrow^2 q_u^2}[q]^2. \tag{3.8}$$

When $[q]\to 0$, the limit of the coefficient of $[q]^2$ on the right-hand side equals

$$-\frac{4q^2}{4\rho^2 q^4}\left(\rho^2+q^2\frac{\rho}{q}\frac{\mathrm{d}\rho}{\mathrm{d}q}\right)=-\frac{1}{\rho q^2}\left(\rho+q\frac{\mathrm{d}\rho}{\mathrm{d}q}\right).$$

Since the difference of entropy across shock is a small quantity of third order of the strength of the shock, again using Bernoulli's relation (1.3) we have $\mathrm{d}S/\mathrm{d}q=0$, $q\,dq+(a^2/\rho)\,d\rho=0$. In view of $\sin[\theta]\sim[\theta]$ for $[\theta]\sim 0$, we have from (3.8)

$$[\theta]^2=E(\rho_\swarrow,\rho_u,q_\swarrow,q_u,\theta_\swarrow,\theta_u)[F(q)]^2,$$

where

$$\lim_{[q]\to 0} E=-\frac{1}{\rho q^2}\left(\rho+q\frac{d\rho}{dq}\right)\frac{1}{F'(q)^2}=-\frac{1}{\rho q^2}\frac{\rho(a^2-q^2)}{a^2}\frac{a^2q^2}{q^2-a^2}=1.$$

Furthermore, notice that $[\theta]$ and $[q]$ take different signs, then $[\theta]$ and $[F(q)]$ take different signs. Hence the coefficient k in (3.6) tends to -1 as $[q]\to 0$.

Lemma 3.2: If $w=S=0$ on the upper side of λ_+ shock, then

$$S_{\swarrow}=O([z]^3),\quad w_{\swarrow}=O([z]^3). \tag{3.9}$$

Proof: The first equality is well known, because the change of entropy across a shock is a small quanity of third order of the strength of the shock. To prove the second equality in (3.9), we apply Lemma 3.1, which implies

$$[\theta]=(-1+h(\theta_{\swarrow},\theta_u,q_{\swarrow},q_u,\rho_{\swarrow},\rho_u)[F(q)])[F(q)]. \tag{3.10}$$

Exchanging the subscript u and subscript $\swarrow$ in (3.10) causes the function h to change its sign. Therefore, (3.10) can be rewritten as

$$[\theta]=(-1+h_1[F(q)]^2)[F(q)].$$

Substituting $z=\theta-F(q), w=\theta+F(q)$ leads to

$$[z+w]^2=\left(1+\frac{h_2}{4}[z-w]^2\right)[z-w]^2,$$

$$[z+w]^2-[z-w]^2=\frac{h_2}{4}[z-w]^2.$$

The above-mentioned equality is equivalent to

$$w_{\swarrow}([z-w]+w_{\swarrow})=\tfrac{1}{16}h_2[z-w]^4$$

due to $w_r=0$. Denote

$$r=\frac{w_{\swarrow}}{[z-w]},$$

then r satisfies

$$r(1+r)=\tfrac{1}{16}h_2[z-w]^2. \tag{3.11}$$

By using the fact $[z-w]\to 0$ for $[z]\to 0$, we obtain $r=O([z-w]^2)$ from (3.11), and then $w_{\swarrow}=O([z-w]^3)$. Writing $[z-w]$ as $[z]+w_{\swarrow}$, the second equality of (3.10) is obtained immediately.

Next we will indicate that the sequence $\{z^{(\nu)}\}$, $\{w^{(\nu)}\}$, $\{S^{(\nu)}\}$, $\{\sigma^{(\nu)}\}$ is well defined, and the sequence is convergent. To do that, let us first set up a proposition $F^{(\nu)}$ as follows:

(1) $z^{(\nu)}(x,y), w^{(\nu)}(x,y), S^{(\nu)}(x,y)\in C^1(\overline{\Omega}_-\backslash(0,0))$,

(2) $|z^{(\nu)}(x,y)-z^{(0)}(x,y)|\leqslant Cx$,

(3) $|S^{(\nu)}(x,y), w^{(\nu)}(x,y)|\leqslant Cx^{3/2}$,

$$(4)\quad |\nabla_{x,y}(z^{(\nu)}-z^{(0)})|\leqslant C(x^3+y^2)^{-1/6},$$

$$(5)\quad |\nabla_{x,y}S^{(\nu)},\nabla_{x,y}w^{(\nu)}|\leqslant Cx^{1/2}.$$

Then we will prove these facts by induction with respect to ν.

IV. ESTIMATES OF $z^{(\nu+1)}$, $w^{(\nu+1)}$, $S^{(\nu+1)}$

In this section we are going to give estimates of $z^{(\nu+1)}$, $w^{(\nu+1)}$, $S^{(\nu+1)}$ from the validity of $F^{(\nu)}$. In the following discussion, ''C'' represents a constant independent of ν, which may take different values in different inequality.

Lemma 4.1: Under the assumption $F^{(\nu)}$,

$$|\sigma^{(\nu)}-\sigma^{(0)}|\leqslant Cx. \tag{4.1}$$

Proof: $\sigma^{(\nu)}$ is determined by (3.3). On the other hand, by using (2.6) $\sigma^{(0)}$ can also be written as

$$\sigma^{(0)}=\left(\frac{[f(m)]}{[m]}\right)_{z=z^{(0)}},$$

where $m=(\rho u)_{w=S=0}$, $f(m)=(\rho v)_{w=S=0}$. Notice that $z^{(\nu)}$, $S^{(\nu)}$, $w^{(\nu)}$ in Ω_+ is independent of ν, then

$$|\sigma^{(\nu)}-\sigma^{(0)}|=\left|\frac{[\rho v]}{[\rho u]}-\left(\frac{[\rho v]}{[\rho u]}\right)_{w=S=0,z=z^{(0)}}\right|\leqslant C(|z^{(\nu)}-z^{(0)}|+|S^{(\nu)}|+|w^{(\nu)}|). \tag{4.2}$$

Here all functions on the right-hand side of the inequality take value in domain Ω_-. Thus (4.1) is obtained from $F^{(\nu)}$.

Lemma 4.2: Under the assumption $F^{(\nu)}$,

$$|\eta^{(\nu)}(x,a,b)-\eta^{(0)}(x,a,b)|\leqslant Ca(a-x), \tag{4.3}$$

where $\eta^{(\nu)}(x,a,b)$ is a characteristic through (a,b) corresponding to the eigenvalue $\lambda_+^{(\nu)}-\sigma^{(\nu)}$.

Proof: From the definition of $\eta^{(\nu)}$,

$$\eta^{(\nu)}(x,a,b)=b+\int_a^x(\lambda_+^{(\nu)}(\alpha,\eta^{(\nu)}(\alpha,a,b))-\sigma^{(\nu)}(\alpha))\mathrm{d}\alpha. \tag{4.4}$$

To estimate $\eta^{(\nu)}(x,a,b)$ we introduce another iterative process. Temporarily fix ν, and determine a sequence $\{\zeta_n\}$ according to

$$\begin{aligned}\zeta_0(x,a,b)&=\eta^{(0)}(x,a,b),\\ \zeta_{n+1}(x,a,b)&=b+\int_a^x(\lambda_+^{(\nu)}(\alpha,\zeta_n(\alpha,a,b))-\sigma^{(\nu)}(\alpha))\mathrm{d}\alpha.\end{aligned} \tag{4.5}$$

Obviously, since $\eta^{(0)}$ satisfies the integral equation

$$\eta^{(0)}(x,a,b)=b+\int_a^x(\lambda_+^{(0)}(\alpha,\eta^{(0)}(\alpha,a,b))-\sigma^{(0)}(\alpha))\mathrm{d}\alpha$$

we have

$$\zeta_{n+1}(x,a,b)-\zeta_0(x,a,b)=\int_a^x \lambda_+^{(\nu)}(\alpha,\zeta_n(\alpha,a,b))-\lambda_+^{(0)}(\alpha,\zeta_0(\alpha,a,b))\mathrm{d}\alpha + \int_a^x (\sigma^{(0)}(\alpha)-\sigma^{(\nu)}(\alpha))\mathrm{d}\alpha.$$

Now we confirm that the sequence $\{\zeta_i(x,a,b)\}$ satisfies the estimate

$$|\zeta_i(x,a,b)-\zeta_0(x,a,b)|\leqslant Ca(a-x), \tag{4.6}$$

and the sequence $\{\zeta_i\}$ is convergent. Obviously, if these two facts are true, then the limit of $\{\zeta_i\}$ is just $\eta^{(\nu)}$, and (4.3) is valid.

The inequality (4.6) can be proved inductively. Evidently, it holds for $i=0$. Now if it holds for $i=n$, then

$$\begin{aligned}\zeta_{n+1}(x,a,b)-\zeta_0(x,a,b)&=\int_a^x\Big(\lambda_+^{(0)}(\alpha,\zeta_n(\alpha,a,b))-\lambda_+^{(0)}(\alpha,\zeta_0(\alpha,a,b))\mathrm{d}\alpha\\&\quad+\int_a^x \lambda_+^{(\nu)}(\alpha,\zeta_n(\alpha,a,b))-\lambda^{(0)}(\alpha,\zeta_n(\alpha,a,b))\mathrm{d}\alpha\\&\quad+\int_a^x(\sigma^{(0)}(\alpha)-\sigma^{(\nu)}(\alpha))\mathrm{d}\alpha.\end{aligned} \tag{4.7}$$

Notice that

$$\begin{aligned}&\left|\int_a^x \lambda_+^{(0)}(\alpha,\zeta_n(\alpha,a,b))-\lambda_+^{(0)}(\alpha,\zeta_0(\alpha,a,b))\mathrm{d}\alpha\right|\\&\quad\leqslant\left|\int_a^x\left(\frac{\partial\lambda_+^{(0)}}{\partial z}z_y^{(0)}(\alpha,\zeta_0+\theta(\zeta_n-\zeta_0))(\alpha,a,b)\right.\right.\\&\qquad\left.\left.\cdot(\zeta_n(\alpha,a,b)-\zeta_0(\alpha,a,b))\mathrm{d}\alpha\right|,\end{aligned}$$

where $0<\theta<1$. Because ζ_n is assumed to satisfy (4.6), then $\zeta_0+\theta(\zeta_n-\zeta_0)$ also satisfies (4.6). Therefore, Lemma 2.4 yields

$$\left|\int_a^x \lambda_+^{(0)}(\alpha,\zeta_n(\alpha,a,b))-\lambda_+^{(0)}(\alpha,\zeta_0(\alpha,a,b))\mathrm{d}\alpha\right|\leqslant\left(\log\frac{3}{2}+C\sqrt{a}\right)a(a-x). \tag{4.8}$$

Then, taking account of (4.1) and the estimate

$$|\lambda_+^{(\nu)}-\lambda_+^{(0)}|\leqslant\|\nabla\lambda_+\|_{L^\infty}(|z^{(\nu)}-z^{(0)}|+|w^{(\nu)}|+|S^{(\nu)}|)\leqslant C\alpha \tag{4.9}$$

derived from $F^{(\nu)}$, we obtain the validity of (4.6) for $i=n+1$. To obtain the convergence of $\{\zeta_n\}$, we estimate the difference $\zeta_{n+1}-\zeta_n$,

$$
\begin{aligned}
&|\zeta_{n+1}(x,a,b)-\zeta_n(x,a,b)| \\
&\quad\leqslant\left|\int_0^x(\partial_y\lambda_+^{(\nu)})(\alpha,((1-\theta)\zeta_{n-1}+\theta\zeta_n)(\alpha,a,b))\right. \\
&\qquad\left.\cdot(\zeta_n(\alpha,a,b)-\zeta_{n-1}(\alpha,a,b))d\alpha\right| \\
&\quad\leqslant\int_0^a|(\partial_y\lambda_+^{(\nu)})(\alpha,((1-\theta)\zeta_{n-1}+\theta\zeta_n)(\alpha,a,b)|\mathrm{d}\alpha\cdot\|\zeta_n-\zeta_{n-1}\|_{L^\infty}. \qquad (4.10)
\end{aligned}
$$

Since $\zeta_{n-1}+\theta(\zeta_n-\zeta_{n-1})$ satisfies the condition (4.6), then Lemma 2.4 implies

$$
\int_0^a|\partial_y\lambda_+^{(\nu)}(\alpha,\zeta_{n-1}+\theta(\zeta_n-\zeta_{n-1})(\alpha,a,b)|\mathrm{d}\alpha\leqslant\log\frac{3}{2}+C\sqrt{a}<\frac{1}{2}, \qquad (4.11)
$$

Therefore,

$$
\|\zeta_{n+1}-\zeta_n\|_{L^\infty}\leqslant\tfrac{1}{2}\|\zeta_n-\zeta_{n-1}\|_{L^\infty}, \qquad (4.12)
$$

which leads to the convergence of $\{\zeta_n\}$. By taking the limit in (4.5) and (4.6), we know the limit of ζ_n satisfies (4.4), and the limit is nothing but $\eta^{(\nu)}(\alpha,a,b)$. Hence (4.3) is also obtained.

Lemma 4.3: Under the assumption $F^{(\nu)}$,

$$
|(z^{\nu+1)}-z^{(0)})(x,y)|\leqslant Cx. \qquad (4.13)
$$

Proof: Denote $v(x,y)=(z^{(\nu+1)}-z^{(0)})(x,y)$, then $v(x,y)$ satisfies

$$
\partial_x v+(\lambda_+^{(\nu)}-\sigma^{(\nu)})\partial_y v=(-\lambda_+^{(\nu)}+\lambda_+^{(0)}+\sigma^{(\nu)}-\sigma^{(0)})\partial_y z^{(0)}+d^{(\nu)}(\partial_x S^{(\nu)}+(\lambda_+^{(\nu)}-\sigma^{(\nu)})\partial_y S^{(\nu)}). \qquad (4.14)
$$

The fact $S^{(\nu)}$, $w^{(\nu)}=0$ in $\Omega_0\cup\Omega_+$ is known. Then intergrating (4.14) along the characteristics $y=\eta_+(x,a,b)$ corresponding to the eigenvalue $\lambda_+^{(\nu)}-\sigma^{(\nu)}$, and taking the assumption $F^{(\nu)}$ into account, we have

$$
|v(x,y)|\leqslant\int_0^x|(-\lambda_+^{(\nu)}+\lambda_+^{(0)}+\sigma^{(\nu)}-\sigma^{(0)})\cdot(\partial_y z^{(0)})(\alpha,\eta_+(\alpha,x,y))|\mathrm{d}\alpha+\int_0^x C\alpha^{1/2}\mathrm{d}\alpha. \qquad (4.15)
$$

Lemma 2.1 indicates

$$
|\partial_y z^{(0)}(\alpha,\eta_+(\alpha,x,y))|\leqslant C(\alpha^3+\eta_+^2)^{-1/3}\leqslant C\alpha^{-1}.
$$

Again by using assumption $F^{(\nu)}$, we obtain from (4.15)

$$
|v(x,y)|\leqslant C\int_0^x\alpha\cdot\alpha^{-1}\,\mathrm{d}\alpha\leqslant Cx. \qquad (4.16)
$$

Lemma 4.4: Under the assumption $F^{(\nu)}$,

$$
|S^{(\nu+1)}(x,y),w^{(\nu+1)}(x,y)|\leqslant Cx^{1/2}. \qquad (4.17)
$$

Proof: $S^{(\nu+1)}(x,y)$ and $w^{(\nu+1)}(x,y)$ are identically zero in $\Omega_+\cup\Omega_0$. In the domain Ω_- the value of $S^{(\nu+1)},w^{(\nu+1)}$ in Ω_- can be obtained by integrating along $\not{\ell}_0$ or $\not{\ell}_-$ characteristics with their data on $x=0$ or $y=0$, respectively. On $x=0$ the data of $S^{(\nu+1)}$, $w^{(\nu+1)}$ are zero, while on $y=0$

$$|S^{(\nu+1)}(x,0_{\swarrow})|+|w^{(\nu+1)}(x,0_{\swarrow})|\leqslant C|[z^{(\nu+1)}(x,0)]^3|$$

due to (3.9), where $0_{\swarrow}$ means the limit from below. Notice that

$$[z^{(\nu+1)}(x,0)]=[z^{(\nu+1)}(x,0)-z^{(0)}(x,0)]+[z^{(0)}(x,0)]\leqslant Cx^{1/2}$$

by means of Lemma 2.1 and (4.16), then

$$|S^{(\nu+1)}(x,0_{\swarrow})|+|w^{(\nu+1)}(x,0_{\swarrow})|\leqslant Cx^{3/2}. \tag{4.18}$$

Denote $y'=\eta_0(x',x,y)$ the equation of characteristics $\swarrow_0$ from (x,y) corresponding to the eigenvalue $\lambda_0^{(\nu)}-\sigma^{(\nu)}$, namely

$$\begin{cases} \dfrac{\mathrm{d}\eta_0(x',x,y)}{dx'}=(\lambda_0^{(\nu)}-\sigma^{(\nu)})(x',\eta_0(x',x,y)), \\ \eta_0(x,x,y)=y, \end{cases} \tag{4.19}$$

then $S^{(\nu+1)}$ takes constant on $\swarrow_0$ by using (3.4), that is $S^{(\nu+1)}(x',\eta_0(x',x,y))$ is independent of x'. If $\swarrow_0$ intersects with the y axis before it meets the x axis, then $S^{(\nu+1)}(x,y)=0$. Otherwise,

$$S^{(\nu+1)}(x,y)=S^{(\nu+1)}(\xi^{(\nu)}(x,y),0_{\swarrow}), \tag{4.20}$$

where $\xi^{(\nu)}(x,y)$ is the coordinate of the intersection of $\swarrow_0$ with the x axis, and then satisfies $\eta_0(\xi^{(\nu)}(x,y),x,y))=0$. Hence

$$S^{(\nu+1)}(x,y)=O\big(\xi^{(\nu)}(x,y)^{3/2}\big)=O\big(x^{3/2}\big) \tag{4.21}$$

by virtue of $0\leqslant\xi^{(\nu)}(x,y)\leqslant x$.

Turn to the estimate of $w^{(\nu+1)}$. The estimate of $w^{(\nu+1)}(x,0_{\swarrow})$ on $y=0$ has been obtained by (4.18). Now if the characteristics $\swarrow_-$ corresponding to the eigenvalue $\lambda_-^{(\nu)}-\sigma^{(\nu)}$ intersects with $y=0$ at $\tilde{\xi}^{(\nu)}(x,y)$, then

$$w^{(\nu+1)}(x,y)=w^{(\nu+1)}(\tilde{\xi}^{(\nu)},0)+\int_{\tilde{\xi}^{(\nu)}}^{x}-d^{(\nu)}(\partial_x S^{(\nu)}+(\lambda_-^{(\nu)}-\sigma^{(\nu)})\partial_y S^{(\nu)})\mathrm{d}\alpha. \tag{4.22}$$

Then by using the estimate of $w^{(\nu+1)}(x,0_{\swarrow})$ and the assumption $F^{(\nu)}$ on $\nabla S^{(\nu)}$ we obtain

$$|w^{(\nu+1)}(x,y)|\leqslant C(\tilde{\xi}^{(\nu)})^{3/2}+C\int_{\tilde{\xi}^{(\nu)}}^{x}\alpha^{1/2}\,\mathrm{d}\alpha\leqslant Cx^{3/2}. \tag{4.23}$$

In the case when $\swarrow_-$ intersects with $x=0$ before it meets $y=0$, the initial value of $w^{(\nu+1)}$ is 0. And the required estimate can be derived in the same way.

V. ESTIMATES OF DERIVATIVES

Lemma 5.1: Under the assumption $F^{(\nu)}$,

$$|\nabla(z^{(\nu+1)}-z^{(0)})|\leqslant C(x^3+y^2)^{-1/6}. \tag{5.1}$$

Proof: Setting $v=\partial_y(z^{(\nu+1)}-z^{(0)})$, and differentiating the equation satisfied by v with respect to y we obtain

$$\partial_{\swarrow_+}(v-d^{(\nu)}S_y^{(\nu)})=r_1, \tag{5.2}$$

where

$$r_1=(-\lambda_+^{(\nu)}+\lambda_+^{(0)}+\sigma^{(\nu)}-\sigma^{(0)})\partial_{yy}z^{(0)}-\lambda_{+y}^{(\nu)}v$$
$$-(\lambda_{+y}^{(\nu)}-\lambda_{+y}^{(0)})\partial_y z^{(0)}+d_y^{(\nu)}S_x^{(\nu)}-d_x^{(\nu)}S_y^{(\nu)}+d^{(\nu)}\lambda_{+y}^{(\nu)}S_y^{(\nu)}.$$

Integrating along the characteristics $\not{\ell}_+$ yields

$$v(a,b)-d^{(\nu)}S_y^{(\nu)}(a,b)=\int_0^a r_1\,\mathrm{d}\alpha. \tag{5.3}$$

Applying Lemmas 2.1 and 2.3 and the assumption $F^{(\nu)}$, we have

$$\left|\int_0^a[(-\lambda_+^{(\nu)}+\lambda_+^{(0)}+\sigma^{(\nu)}-\sigma^{(0)})\partial_{yy}z^{(0)}]\mathrm{d}\alpha\right|$$
$$\leqslant\int_0^a C\alpha(\alpha^3+\eta^2)^{-5/6}\mathrm{d}\alpha$$
$$\leqslant\int_0^a C\alpha\mathrm{d}\alpha\cdot(a^3+b^2)^{-5/6}$$
$$\leqslant Ca^2(a^3+b^2)^{-5/6}$$
$$\leqslant C(a^3+b^2)^{-1/6},$$

$$\left|\int_0^a\partial_y(\lambda_+^{(\nu)}-\lambda_+^{(0)})\partial_y z^{(0)}\mathrm{d}\alpha\right|$$
$$\leqslant\int_0^a|\lambda_{+w}^{(\nu)}w_y^{(\nu)}+\lambda_{+z}^{(\nu)}(z_y^{(\nu)}-z_y^{(0)})+(\lambda_{+z}^{(\nu)}-\lambda_z^{(0)})z_y^{(0)}|\cdot|\partial_y z^{(0)}|\mathrm{d}\alpha$$
$$\leqslant C\int_0^a\left|(\alpha^3+\eta^2)^{-1/6}+\alpha^{-1/2}+\alpha(\alpha^3+\eta^2)^{-1/3}\right|\cdot(\alpha^3+\eta^2)^{-1/3}\mathrm{d}\alpha$$
$$\leqslant C\int_0^a\alpha^{-1/2}\mathrm{d}\alpha(a^3+b^2)^{-1/3}$$
$$\leqslant C(a^3+b^2)^{-1/6},$$

$$\left|\int_0^a(d_y^{(\nu)}S_x^{(\nu)}-d_x^{(\nu)}S_y^{(\nu)}+d^{(\nu)}\lambda_{+y}^{(\nu)}S_y^{(\nu)})\mathrm{d}\alpha\right|\leqslant C\int_0^a\alpha^{-1/2}\cdot\alpha^{1/2}\mathrm{d}\alpha\leqslant Ca.$$

Therefore,

$$|v-d^{(\nu)}S_y^{(\nu)}|\leqslant\int_0^a g(\alpha)|v|d\alpha+h(a,b), \tag{5.4}$$

where $|h(a,b)|\leqslant C(a^3+b^2)^{-1/6}$, $|g(\alpha)|\leqslant C\alpha^{-1/2}$. Namely, $v_1=v-d^{(\nu)}S_y^{(\nu)}$ satisfies

$$|v_1|\leqslant\int_0^a g(\alpha)|v_1|d\alpha+h_1(a,b),$$

where h_1 still satisfies $|h_1(a,b)|\leqslant C(a^3+b^2)^{-1/6}$.

Recall that Lemma 2.4 implies $\int_0^a g(\alpha)d\alpha\leqslant\log\frac{3}{2}+C\sqrt{a}$. Then by using Gronwall inequality v_1 is dominated by $C(a^3+b^2)^{-1/6}$, and so does v. Again using the system (3.4) we obtain the estimate of $\partial_x(z^{(\nu+1)}-z^{(0)})$. Hence (5.1) holds.

Lemma 5.2: Under the assumption $F^{(\nu)}$,

$$|\nabla S^{(\nu+1)}, \nabla w^{(\nu+1)}| \leqslant C x^{1/2}. \tag{5.5}$$

Proof: To obtain the estimate of $\nabla w^{(\nu+1)}$, we define $v_2(x,y) = w_y^{(\nu+1)} + d^{(\nu)} S_y^{(\nu)}(x,y)$. By differentiating the third equation of (3.4) we have

$$\partial_x v_2 + (\lambda_-^{(\nu)} - \sigma^{(\nu)}) \partial_y v_2 + \lambda_{-y}^{(\nu)} v_2 = -\lambda_{-y}^{(\nu)} d^{(\nu)} S_y^{(\nu)} - d_y^{(\nu)} S_x^{(\nu)} + d_x^{(\nu)} S_y^{(\nu)}. \tag{5.6}$$

Denoting the right-hand side by r_2, (5.6) can be rewritten as

$$\partial_{\swarrow_-} v_2 = r_2.$$

Then integrating (4.5) along $\swarrow_-$, we obtain

$$v_2(a,b) = v(\tilde{\xi}, 0_{\swarrow}) + \int_{\tilde{\xi}}^{a} \lambda_{-y}^{(\nu)} v_2 \, \mathrm{d}\alpha + \int_{\tilde{\xi}}^{a} r_2(\alpha) \mathrm{d}\alpha, \tag{5.7}$$

provided $\swarrow_-$ intersects with $y=0$ before it meets $x=0$. Otherwise, two integrals in (5.7) should be replaced by the corresponding integrals from 0 to a, while the term $v(\xi,0)$ should be replaced by 0.

Let us analyze three terms an the right-hand side of (5.7). The estimate (4.18) indicates

$$|w_x^{(\nu+1)}(\xi, 0_{\swarrow})| \leqslant C|\xi|^{1/2},$$

and the same estimate for $|w_y^{(\nu+1)}(\xi,0)|$ also holds, because $|\lambda_0|$ and $|\lambda_-|$ are bounded away from zero. The fact means $|v_2(\xi,0_{\swarrow})| \leqslant C|\xi|^{1/2}$. Moreover, according to the assumption $F^{(\nu)}$, r_2 satisfies

$$|r_2| \leqslant C(x^3 + y^2)^{-1/6} x^{1/2} \leqslant C,$$

then $\int_0^a r_2(\alpha)\mathrm{d}\alpha \leqslant Ca$, and (5.7) can be written as

$$v(a,b) = \int_{\xi}^{a} \lambda_{-y}^{(\nu)} v \, \mathrm{d}\alpha + O(a^{1/2}),$$

where $\lambda_{-y}^{(\nu)}$ is also dominated by $Cx^{-1/2}$. Therefore, we can use the same method in Lemma 4.1 to obtain

$$|v(a,b)| \leqslant Ca^{1/2}, \tag{5.8}$$

which implies $|w_y^{(\nu+1)}(a,b)| \leqslant Ca^{1/2}$, and again applying the system (3.4) itself yields $|w_x^{(\nu+1)}(a,b)| \leqslant Ca^{1/2}$.

The same method is available to estimate $\nabla S^{(\nu+1)}$. In the above-mentioned process replacing $w^{(\nu+1)}$ by $S^{(\nu+1)}$, $\lambda_-^{(\nu)}$ by $\lambda_0^{(\nu)}$, and $d^{(\nu)}$ by 0, we obtain $|\nabla S^{(\nu+1)}| \leqslant Cx^{1/2}$ immediately.

According to Lemma 4.2 and Lemmas 5.1 and 5.2 we know that the assumption $F^{(\nu)}$ implies the validity of $F^{(\nu+1)}$. Then $F^{(\nu)}$ holds for any ν by induction.

VI. CONVERGENCE

To obtain the convergence of $\{z^{(\nu)}\}$, $\{w^{(\nu)}\}$, $\{S^{(\nu)}\}$, we are going to prove the contractivity of these sequences. In the sequel we denote $e_z^{(\nu)} = z^{(\nu+1)} - z^{(\nu)}$, $e_w^{(\nu)} = w^{(\nu+1)} - w^{(\nu)}$, $e_s^{(\nu)} = S^{(\nu+1)} - S^{(\nu)}$ for notational simplicity, and will estimate these differences.

First, (3.3) implies that $|\sigma^{(\nu)} - \sigma^{(\nu-1)}|$ can be dominated by

$$C(\|e_z^{(\nu-1)}\|_{L^\infty} + \|e_w^{(\nu-1)}\|_{L^\infty} + \|e_s^{(\nu-1)}\|_{L^\infty}).$$

Since the formation of shock is caused by compression of λ^+ characteristics, the difference $e_z^{(\nu-1)}$ plays the principal role among these three terms.

Lemma 6.1: If ϵ is small and K is large in (3.2), then

$$|\sigma^{(\nu)}-\sigma^{(\nu-1)}|\leqslant C(\|e_s^{(\nu-1)}\|_{L^\infty}+\|e_w^{(\nu-1)}\|_{L^\infty})+\frac{1}{2}|\lambda_+'|\cdot\|e_z^{(\nu-1)}\|_{L^\infty}(1+O(x)). \tag{6.1}$$

Proof: Denote

$$H(z^{(\nu)},w^{(\nu)},S^{(\nu)})=\frac{[\rho^{(\nu)}v^{(\nu)}]}{[\rho^{(\nu)}u^{(\nu)}]}$$

then

$$\begin{aligned}|\sigma^{(\nu)}-\sigma^{(\nu-1)}|&=|H(z^{(\nu)},w^{(\nu)},S^{(\nu)})-H(z^{(\nu-1)},w^{(\nu-1)},S^{(\nu-1)})|\\&\leqslant C(\|e_w^{(\nu-1)}\|_{L^\infty}+\|e_s^{(\nu-1)}\|_{L^\infty})+|H(z^{(\nu)},w^{(\nu)},S^{(\nu)})-H(z^{(\nu-1)},w^{(\nu)},S^{(\nu)})|\\&\leqslant C(\|e_w^{(\nu-1)}\|_{L^\infty}+\|e_s^{(\nu-1)}\|_{L^\infty})+|H(z^{(\nu)},0,0)-H(z^{(\nu-1)},0,0)|\\&\quad+|(H(z^{(\nu)},w^{(\nu)},S^{(\nu)})-H(z^{(\nu)},0,0))\\&\quad-(H(z^{(\nu-1)},w^{(\nu)},S^{(\nu)})-H(z^{(\nu-1)},0,0))|.\end{aligned} \tag{6.2}$$

Here $H(z,0,0)$ is just the expression $[f(m)]/[m]$ in the Rankine–Hugoniot condition for (2.7), so

$$\begin{aligned}|H(z^{(\nu)},0,0)-H(z^{(\nu-1)},0,0)|&=\left(\frac{d}{dz}\frac{[f(m(z))]}{[m(z)]}\right)_{z=z^*}e_z^{(\nu-1)}\\&=\left(\frac{[m]f'(m)-[f(m)]}{[m]^2}\frac{dm}{dz}\right)_{z=z^*}e_z^{(\nu-1)}.\end{aligned}$$

Since

$$f''(m)\frac{dm}{dz}=\partial_z\lambda_+^{(0)},\quad \frac{[m]f'(m)-[f(m)]}{[m]^2}=-\frac{1}{2}f''(m^*),$$

we have

$$|H(z^{(\nu)},0,0)-H(z^{(\nu-1)},0,0)|=\left|\tfrac{1}{2}\partial_z\lambda_+^{(0)}+O(z^{(\nu)}-z^{(0)})\right|\cdot\left|e_z^{(\nu-1)}\right|.$$

Moreover, notice that the last term in (6.2) is dominated by $C(|w^{(\nu)}|+|S^{(\nu)}|)\|e_z^{(\nu-1)}\|_{L^\infty}$ we obtain (6.1).

Lemma 6.2: Under the assumption of Lemma 6.1

$$\|e_z^{(\nu)}\|_{L^\infty}\leqslant\tfrac{4}{5}\|e_z^{(\nu-1)}\|_{L^\infty}+C(\|e_s^{(\nu-1)}\|_{L^\infty}+\|e_w^{(\nu-1)}\|_{L^\infty}). \tag{6.3}$$

Proof: (3.4) implies

$$\begin{aligned}&(\partial_x+(\lambda_+^{(\nu)}-\sigma^{(\nu)}\partial_y)e_z^{(\nu)}\\&\quad=-(\lambda_+^{(\nu)}-\sigma^{(\nu)}-\lambda_+^{(\nu-1)}+\sigma^{(\nu-1)})\partial_y z^{(0)}\\&\qquad-(\lambda_+^{(\nu)}-\sigma^{(\nu)}-\lambda_+^{(\nu-1)}+\sigma^{(\nu-1)})\partial_y(z^{(\nu)}-z^{(0)})\\&\qquad+(d^{(\nu)}S_x^{(\nu)}-d^{(\nu-1)}S_x^{(\nu-1)})+d^{(\nu)}(\lambda_+^{(\nu)}-\sigma^{(\nu)})S_y^{(\nu)}-d^{(\nu-1)}\end{aligned}$$

$$\times(\lambda_+^{(\nu-1)}-\sigma^{(\nu-1)})S_y^{(\nu-1)}. \tag{6.4}$$

Integrating (6.4) along $\not{C}_+^{(\nu)}$ characteristics we have

$$e_z^{(\nu)}(x,y)=\int_0^x r_3(\alpha,\eta_+(\alpha,x,y))\mathrm{d}\alpha, \tag{6.5}$$

where r_3 represents the right-hand side of (6.4). Notice that

$$|\lambda_+^{(\nu)}-\lambda_+^{(\nu-1)}|\leqslant|e_z^{(\nu-1)}|\cdot|\partial_z\lambda_+^{(0)}+O(x)|+C(|e_s^{(\nu-1)}+e_w^{(\nu-1)}|),$$

$$|\sigma^{(\nu)}-e^{(\nu-1)}|\leqslant|\tfrac{1}{2}e_z^{(\nu-1)}|\cdot|\partial_z\lambda_+^{(0)}+O(x)|+C(|e_s^{(\nu-1)}|+e_w^{(\nu-1)}|),$$

and

$$\begin{aligned}|\partial_y z^{(0)}(\alpha,\eta^{(\nu)}(\alpha,x,y))|&\leqslant C(\alpha^3+|\eta^{(\nu)}(\alpha,x,y)|^2)^{-1/3}\\&\leqslant C_1(\alpha^3+|\eta(\alpha,x,y)|^2)^{-1/3}\\&\leqslant C_2(x^3+y^2)^{-1/3}\end{aligned}$$

by virture of Lemmas 2.3 and 4.2. Then by using Lemma 2.4

$$\begin{aligned}&\int_0^x|(\lambda_+^{(\nu)}-\sigma^{(\nu)}-\lambda_+^{(\nu-1)}+\sigma^{(\nu-1)})\partial_y z^{(0)}(\alpha,\eta^{(\nu)}(\alpha,x,y))|\mathrm{d}\alpha\\&\quad\leqslant\left(\frac{3}{2}\log\frac{3}{2}+C\sqrt{a}\right)(\|e_z^{(\nu-1)}\|_{L^\infty}+C(\|e_s^{(\nu-1)}\|_{L^\infty}+\|e_w^{(\nu-1)}\|_{L^\infty}).\end{aligned}$$

Besides, by using the assumption $F^{(\nu)}$, the integral of all other terms on the right-hand side of (6.4) are dominated by

$$C\sqrt{a}(\|e_z^{(\nu-1)}\|_{L^\infty}+\|e_s^{(\nu-1)}\|_{L^\infty}+\|e_w^{(\nu-1)}\|_{L^\infty}).$$

Therefore, for small a we have

$$\|e_z^{(\nu)}\|_{L^\infty}\leqslant\tfrac{4}{5}\|e_z^{(\nu-1)}\|_{L^\infty}+C(\|e_s^{(\nu-1)}\|_{L^\infty}+\|e_w^{(\nu-1)}\|_{L^\infty}).$$

Lemma 6.3: Under the assumption of Lemma 6.1 we can find a constant C_0 such that

$$\|e_z^{(\nu)}\|_{L^\infty}+C_0\|e_s^{(\nu)}\|_{L^\infty}+C_0\|e_w^{(\nu)}\|_{L^\infty}\leqslant\tfrac{9}{10}(\|e_z^{(\nu-1)}\|_{L^\infty}+C_0\|e_s^{(\nu-1)}\|_{L^\infty}+C_0\|e_w^{(\nu-1)}\|_{L^\infty}). \tag{6.6}$$

Proof: Lemma 3.2 indicates

$$\|e_s^{(\nu)}(x,0_{\not{C}})\|_{L^\infty}\leqslant Cx\|e_z^{(\nu)}\|_{L^\infty},\quad \|e_w^{(\nu)}(x,0_{\not{C}})\|_{L^\infty}\leqslant Cx\|e_z^{(\nu)}\|_{L^\infty}.$$

Substracting the second equation in (3.4) with index $\nu+1$ by the corresponding equation with index ν we obtain

$$\partial_x e_s^{(\nu)}+(\lambda_0^{(\nu)}-\sigma^{(\nu)})\partial_y e_s^{(\nu)}+(\lambda_0^{(\nu)}-\sigma^{(\nu)}-\lambda_0^{(\nu-1)}+\sigma^{(\nu-1)})\partial_y S^{(\nu)}=0. \tag{6.7}$$

Integrating (6.7) along $\not{C}_0$ characteristics yields (in the case when leftward characteristic $\not{C}_0$ intersects with $y=0$ before it meets $x=0$)

$$e_s^{(\nu)}(a,b)=e_s^{(\nu)}(x,0_{\not{C}})-\int_x^a(\lambda_0^{(\nu)}-\sigma^{(\nu)}-\lambda_0^{(\nu-1)}+\sigma^{(\nu-1)})\partial_y S^{(\nu)}\mathrm{d}\alpha. \tag{6.8}$$

Applying the proposition $F^{(\nu)}$ we have

$$\begin{aligned}\|e_s^{(\nu)}\|_{L^\infty} &\leqslant Cx\|e_z^{(\nu)}\|_{L^\infty}+C\sqrt{a}(\|e_z^{(\nu-1)}\|_{L^\infty}+\|e_s^{(\nu-1)}\|_{L^\infty}+\|e_w^{(\nu-1)}\|_{L^\infty})\\ &\leqslant C\sqrt{a}(\|e_z^{(\nu)}\|_{L^\infty}+\|e_z^{(\nu-1)}\|_{L^\infty}+\|e_s^{(\nu-1)}\|_{L^\infty}+\|e_w^{(\nu-1)}\|_{L^\infty}).\end{aligned} \tag{6.9}$$

When ℓ_0 intersect with $x=0$ before it meets $y=0$, the computation is similar.

By using the same method we have

$$\|e_w^{(\nu)}\|_{L^\infty}\leqslant C\sqrt{a}(\|e_z^{(\nu)}\|_{L^\infty}+\|e_z^{(\nu-1)}\|_{L^\infty}+\|e_s^{(\nu-1)}\|_{L^\infty}+\|e_w^{(\nu-1)}\|_{L^\infty}). \tag{6.10}$$

Then from (6.3), (6.9), and (6.11) we obtain

$$\begin{aligned}&\|e_z^{(\nu)}\|_{L^\infty}+2C\|e_s^{(\nu)}\|_{L^\infty}+2C\|e_w^{(\nu)}\|_{L^\infty}\\ &\quad\leqslant\left(\frac{4}{5}+4C^2\sqrt{a}\right)\|e_z^{(\nu-1)}\|_{L^\infty}+(C+4C^2\sqrt{a})\|e_s^{(\nu-1)}\|_{L^\infty}\\ &\qquad+(C+4C^2\sqrt{a})\|e_w^{(\nu-1)}\|_{L^\infty}+4C^2\sqrt{a}\|e_z^{(\nu)}\|_{L^\infty}.\end{aligned} \tag{6.11}$$

Let a satisfy $4C^2\sqrt{a}<\frac{1}{20}$ we obtain (6.6).

Proof of Theorem 1.1: From Lemma 6.3 we know the sequences $\{z^{(\nu)}(x,y)\}$, $\{w^{(\nu)}(x,y)\}$, $\{S^{(\nu)}(x,y)\}$ are uniformly convergent. Then from expression (3.3) of $\sigma^{(\nu)}(x)$ we also have the convergence of $\{\sigma^{(\nu)}(x)\}$. As the integral of $\sigma^{(\nu)}$, the location of approximate shock is also convergent.

The limit of the above-mentioned sequences satisfies the system (1.9). In fact, the proposition $F^{(\nu)}$ implies that the sequences $\{\nabla z^{(\nu)}\}$, $\{\nabla w^{(\nu)}\}$, $\{\nabla S^{(\nu)}\}$ are uniformly bounded in any domain $\omega\subset\Omega$ away from the point (x_0,y_0). Then using the standard argument on compact sequences we know $\{z^{(\nu)}\}$, $\{w^{(\nu)}\}$, $\{S^{(\nu)}\}$ and their derivatives are pointwise convergent. By taking limit we confirm that z,w,S satisfy (1.9).

Returning to original coordinates we have locally constructed a piecewise continuous solution with shock starting from the point (x_0,y_0). The strength of the shock is zero at the point and then graduately increases along with $x-x_0$. Meanwhile, the solution has bounded derivatives away from (x_0,y_0), and the estimates (1.16) hold near (x_0,y_0).

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Nöther charges, Brown–York quasilocal energy, and related topics

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The Lagrangian proposed by York *et al.* and the covariant first-order Lagrangian for general relativity are reviewed. They both deal with the (vacuum) gravitational field on a reference background and were conjectured to be equivalent. The two corresponding actions are compared and we show that the first one can in fact be obtained from the latter under suitable hypotheses. A conditioned correspondence among Nöther conserved quantities of covariant first-order Lagrangian, Brown–York quasilocal energy and the standard ADM Hamiltonian is also established. [DOI: 10.1063/1.1336514]

I. INTRODUCTION

Many approaches to variational principles, conserved quantities, and related topics can be found in the current literature about general relativity (see, e.g., Refs. 1–13, and references quoted therein). We shall hereafter compare two of them, both dealing with a dynamical metric g and a reference background metric $\overline{g}$ over a space–time manifold M of arbitrary dimension n, with $n \geqslant 3$. A large part of the paper will deal with the explicit case $n=4$, in view of applications to standard general relativity. We shall deal with the vacuum case; the generalization to the matter case is straightforward.

The first action we shall deal with is based on the covariant first-order action functional for general relativity (see Refs. 12, 14–16). The second one[3,7] is based on the action functional due to York *et al.*, which is defined with the aim of dealing with the fixing of the $(n-1)$ metric induced on the boundary ∂D of any region D of space–time M.

In the present situation it seems to us that there are two (quite separated) groups of researchers on the subjects, each one using a single one of these variational principles and both claiming that the two approaches should be *basically* equivalent. Even though there is quite a widespread feeling that the two approaches in fact have to be (at least in most cases) equivalent, we are not aware of a rigorous theoretical comparison between these two variational principles in the current literature which clarifies the matter once and for all by proving if, how, and when they are really equivalent.

Furthermore, this situation is even worse when one considers conserved quantities. In the context of a covariant first-order Lagrangian, *energy* is in fact defined by the Nöther theorem in a covariant and geometrical framework (see Refs. 14 and 15). Brown and York gave an interesting alternative definition, the so-called *quasilocal energy*, oriented to statistical considerations. Both these *energies* are often quoted in the literature since they reproduce the ADM mass in the asymptotically flat case, though they have been recognized as also suitable for more general boundary conditions [e.g., in asymptotically anti-de Sitter (see Ref. 17) or asymptotically locally flat cases; see Refs. 18–21]. *Both* methods allow one to define the *energy within a finite region* as

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well as the total one. In this way, the advantages of the Brown–York framework can also be obtained by covariant first-order formalism and Nöther theorem.

We also remark that in both cases it has been recognized that *absolute conserved quantities* have a meaning just in particular cases, while for general boundary conditions just *conserved quantities relative to something* (e.g., *a reference background*) are meaningful. Furthermore, even ''*absolute*'' *conserved quantities* should be interpreted as *conserved quantities relative to some canonical background* (e.g., flat Minkowski space in asymptotically flat spaces). We also stress that reference backgrounds are particularly relevant in general relativity, as well as in other nonlinear field theories, since whenever fields are endowed with a vector space structure a canonical choice for the reference exists, namely the *zero* section. If the configuration bundle is not a vector bundle, as happens in general relativity (as well as, e.g., in Yang–Mills theories) there is instead no canonical choice for the vacuum state. The vacuum state thence has to be ''*arbitrarily*'' fixed. When doing that it sounds physically reasonable to also require the background to be a solution of field equations, so that the relative energy can be interpreted as the energy ''*spent to go*'' from the background solution to the dynamical one (and analogously for other physically relevant conserved quantities). Furthermore, it is essential that the choice of the reference background does not effect the evolution of the dynamical fields, i.e., these solutions have to be decoupled. In view of these considerations both the covariant first-order and the York action functionals incorporate the background from the very beginning.

Again these very evident similarities are not supported by a rigorous equivalence proof. Moreover, we are not aware of any detailed analysis which clarifies whether these analogies are unconditioned or are subjected to some restrictive hypotheses. We thence believe that the matter still deserves a detailed and rigorous investigation aimed to cover both the variational aspects as well as those related to conserved quantities.

Accordingly, in this paper we shall compare the covariant first-order Lagrangian and York action functionals. Since both these *labels* hide in themselves a number of slightly different variational principles, each one adapted to a particular situation, we shall briefly review the literature on the subject to fix notation.

In Sec. II we shall review some material about covariant first-order Lagrangian and its Nöther conserved quantities, while Sec. III is devoted to introducing the Brown–York approach and the notion of quasilocal energy. Sections II and III could be considered trivial by the appropriate research group, but (in view of the existing separation we mentioned before) we hope it will serve as a short review for the complementary group. They are therefore included to make the paper self-contained as well as for uniformity of notation. The most standard and technical aspects are omitted or reported in the Appendix.

In Sec. IV we shall compare the action functionals introduced in Secs. II and III. There we shall establish a conditioned equivalence which holds under suitable boundary prescriptions required on the metric g and the background $\overline{g}$. The fact that the claimed equivalence is not completely unconditioned is in our opinion particularly important, since it sets a basis to choose between the two methods. However, the requirements on boundary conditions needed to provide equivalence are sufficiently general to support the general belief that the two methods are *basically equivalent*.

In Sec. V we shall compare the conserved quantities reviewed in Secs. II and III. We shall obtain the standard ADM Hamiltonian as well as the quasilocal energy (under the aforementioned boundary conditions) as Nöther quantities associated with the covariant first-order Lagrangian. While the first comparison with the ADM Hamiltonian already appeared in literature (although in a simplified version; see Ref. 22 and references quoted therein) the second, i.e., the comparison between quasilocal energy and Nöther charges, is, as far as we know, new.

In Sec. VI we shall also discuss the very notion of *conserved quantity*. On the one hand, in fact, the Nöther theorem provides currents $\mathcal{E}$ which are *covariantly conserved*, i.e., $d\mathcal{E}=0$ identically or on shell (i.e., along solutions), meaning that their integral on the boundary ∂D of any n-region D in space–time M vanishes or, equivalently, that the conserved quantity obeys a continuity equation. On the other hand, physicists are often interested in quantities Q which are

conserved in time, meaning that, once an ADM foliation of a region of space–time has been chosen, such a quantity Q may be computed by integration on each leaf and it turns out to be independent of the particular leaf labeled by *time* t. Clearly, ADM foliations are far from unique and different foliations of the same region D correspond to different ways of defining *time*. Furthermore, such a quantity Q may be conserved in the time defined by an ADM foliation without being conserved with respect to other foliations (i.e., with respect to different time parameters). From a theoretical general relativity viewpoint, quantities conserved in time are not (manifestly) covariant in nature. They are, in fact, conserved with respect to a special parameter, while, at a fundamental level, the principle of general covariance forbids, at least in principle, the selection of a preferred time. Different sets of conditions under which conservation ''*in time*'' follows from covariant conservation will be discussed.

In Sec. VII we shall present two simple examples illustrating the difference between time-conserved and covariantly conserved quantities. The first one is the computation of various Nöther charges of the Schwarzschild solution relative to a Minkowski background matched on a *finite sphere*. Conservation in time of various foliations is analyzed and quasilocal energy is obtained via the Nöther theorem, in full agreement with previously known results (see Ref. 3). The second example is a Kerr solution matched at spatial infinity with the Minkowski metric. The Nöther conserved quantities are obtained. Such an example is interesting because it does not obey the same matching conditions required throughout the rest of the paper. Nevertheless it produces a current which is time conserved, showing that all the conditions discussed along the paper are sufficient but not necessary. We believe that these examples are important also from a pedagogical viewpoint.

In the Appendix we collect formulas which are used throughout the paper to translate covariant objects into objects adapted to the ADM foliation and vice versa. We omit the details about the geometric framework for variational calculus and refer the reader to Refs. 23 and 24, and references therein, for specifics.

II. THE COVARIANT FIRST-ORDER LAGRANGIAN

The covariant first-order action was introduced to set general relativity in a standard *covariant first-order* variational framework. As is well known, in fact, the Hilbert Lagrangian $L=(1/2\kappa)\sqrt{g}R\,\mathbf{ds}$ is second order in the metric field, so that field equations are expected to be of fourth order. Einstein field equations are second-order equations instead, as if the action were first order only. This is due to the well-known fact that *locally* second derivatives of the metric field appearing in the scalar curvature may be hidden under a divergence, thus not appearing in field equations (a fact which was clear to Einstein from the very beginning; see, e.g., Ref. 25). Of course, however, this cannot be done in general in a global and covariant way; that is why general relativity is usually considered as a second-order field theory or, whenever it is treated on a first-order basis, something is lost (e.g., covariance or boundary terms; see Refs. 4 and 5). The problem of a covariant splitting of the Hilbert Lagrangian can be globally solved by introducing a background connection $\overline{\Gamma}^{\alpha}_{\beta\nu}$. Hereafter, for reasons which will be clear later, we shall further restrict ourselves to introducing a background metric $\overline{g}_{\mu\nu}$ so that $\overline{\Gamma}^{\alpha}_{\beta\nu}$ is its Levi-Civita connection.

The *covariant first-order action functional in a region* $D\subset M$ is the following:

$$A_D[g,\overline{g}]=\frac{1}{2\kappa}\int_D\sqrt{g}R\,\mathbf{ds}-\frac{1}{2\kappa}\int_{\partial D}\sqrt{g}g^{\mu\nu}w^{\alpha}_{\mu\nu}\,\mathbf{ds}_{\alpha}-\frac{1}{2\kappa}\int_D\sqrt{\overline{g}}\overline{R}\,\mathbf{ds}, \tag{2.1}$$

where κ is a constant [$\kappa=8\pi G/c^4$ in general relativity with $\dim(M)=4$], $\sqrt{g}$ is the square root of the absolute value of the determinant of the dynamical metric g, $\sqrt{\overline{g}}=\sqrt{|\det\overline{g}|}$ is the analogous quantity for the background metric $\overline{g}$, and $\mathbf{ds}$ and $\mathbf{ds}_{\alpha}=\partial_{\alpha}\lrcorner\mathbf{ds}$ are the standard local bases for n forms and $(n-1)$ forms over M, respectively. We systematically denote by a bar the quantities referred to the background, i.e., we shall use the following notation:

$g_{\mu\nu}$	$\overline{g}_{\mu\nu}$	Covariant metric
$g^{\mu\nu}$	$\overline{g}^{\mu\nu}$	Contravariant metric
$\Gamma^{\alpha}_{\beta\nu}$	$\overline{\Gamma}^{\alpha}_{\beta\nu}$	Levi-Civita connection
$R^{\alpha}_{\beta\mu\nu}$	$\overline{R}^{\alpha}_{\beta\mu\nu}$	Riemann tensor
$R_{\mu\nu}=R^{\alpha}_{\mu\alpha\nu}$	$\overline{R}_{\mu\nu}=\overline{R}^{\alpha}_{\mu\alpha\nu}$	Ricci tensor
$R=g^{\mu\nu}R_{\mu\nu}$	$\overline{R}=\overline{g}^{\mu\nu}\overline{R}_{\mu\nu}$	Scalar curvature
$u^{\mu}_{\alpha\beta}=\Gamma^{\mu}_{\alpha\beta}-\delta^{\mu}_{(\alpha}\Gamma^{\epsilon}_{\beta)\epsilon}$	$\overline{u}^{\mu}_{\alpha\beta}=\overline{\Gamma}^{\mu}_{\alpha\beta}-\delta^{\mu}_{(\alpha}\overline{\Gamma}^{\epsilon}_{\beta)\epsilon}$	

We also introduced the following *relative quantities*:

$$q^{\mu}_{\alpha\beta}=\Gamma^{\mu}_{\alpha\beta}-\overline{\Gamma}^{\mu}_{\alpha\beta}, \quad w^{\mu}_{\alpha\beta}=u^{\mu}_{\alpha\beta}-\overline{u}^{\mu}_{\alpha\beta}.$$

The action functional (2.1) is associated with the so-called *covariant first-order Lagrangian*

$$L=\frac{1}{2\kappa}\left(\sqrt{g}R-d_{\alpha}(\sqrt{g}g^{\mu\nu}w^{\alpha}_{\mu\nu})-\sqrt{\overline{g}}\overline{R}\right)\mathbf{ds} \tag{2.2a}$$

or equivalently

$$L=\frac{1}{2\kappa}((\sqrt{g}g^{k\nu}-\sqrt{\overline{g}}\overline{g}^{\mu\nu})\overline{R}_{\mu\nu}+\sqrt{g}g^{\alpha\beta}(q^{\rho}_{\alpha\sigma}q^{\sigma}_{\rho\beta}-q^{\sigma}_{\sigma\rho}q^{\rho}_{\alpha\beta}))\mathbf{ds}. \tag{2.2b}$$

From (2.2a), it can easily be seen that the fields g and $\overline{g}$ do not interact and they both obey vacuum Einstein field equations (provided that variations are performed with suitable boundary conditions). From (2.2b), the Lagrangian is, however, recognized to be first order in g and second order in $\overline{g}$. Being both $q^{\mu}_{\alpha\beta}$ and $w^{\mu}_{\alpha\beta}$ tensors, L is a covariant Lagrangian. It is, of course, the truly covariant counterpart of the so-called Hilbert–Palatini first-order Lagrangian (see Ref. 26), to which it reduces by suitable noncovariant cancellations and background fixings. We stress that in the variational principle induced by (2.1) the dynamical metric g is endowed with a direct physical meaning, while the reference background metric $\overline{g}$ is, at least for the moment, introduced to provide covariance and as a reference value for conserved quantities, as discussed in the following. Notice that if the action (2.1) is computed for $g=\overline{g}$, then it identically vanishes.

The Nöther theorem (see, e.g., Refs. 14–16, 23, and references quoted therein) is related to the general covariance of the theory. It *algorithmically* defines a *Nöther conserved current*, i.e., a map $\mathcal{E}[\xi,\sigma]$ which associates with any space–time vector field ξ and any field configuration $\sigma=(g,\overline{g})$ an $(n-1)$-form $\mathcal{E}[\xi,\sigma]$ on space–time M of dimension n which is closed on-shell, i.e., when the configuration σ is a solution of field equations. For the action functional (2.1) we obtain

$$\begin{aligned}\mathcal{E}[\xi,\sigma]=\frac{1}{2\kappa}[&\sqrt{g}((g^{\lambda\alpha}g_{\mu\nu}-\delta^{(\lambda}_{\mu}\delta^{\alpha)}_{\nu})\nabla_{\alpha}\pounds_{\xi}g^{\mu\nu}-\xi^{\lambda}R)\\&-(\pounds_{\xi}(\sqrt{g}g^{\mu\nu}w^{\lambda}_{\mu\nu})-\xi^{\lambda}d_{\alpha}(\sqrt{g}g^{\mu\nu}w^{\alpha}_{\mu\nu}))\\&-\sqrt{\overline{g}}((\overline{g}^{\lambda\alpha}\overline{g}_{\mu\nu}-\delta^{(\lambda}_{\mu}\delta^{\alpha)}_{\nu}))\overline{\nabla}_{\alpha}\pounds_{\xi}\overline{g}^{\mu\nu}-\xi^{\lambda}\overline{R}]\mathbf{ds}_{\lambda}.\end{aligned} \tag{2.3}$$

The differential of the $(n-1)$-form $\mathcal{E}[\xi,\sigma]$ satisfies the following property:

$$d\mathcal{E}[\xi,\sigma]=\mathcal{W}[\xi,\sigma], \tag{2.4}$$

where $\mathcal{W}[\xi,\sigma]=-(1/2\kappa)(G_{\mu\nu}\pounds_{\xi}g^{\mu\nu}-\overline{G}_{\mu\nu}\pounds_{\xi}\overline{g}^{\mu\nu})$ **ds** is proportional to field equations. Consequently, the Nöther current $\mathcal{E}[\xi,\sigma]$ is closed along solutions.

Of course, the Nöther currents, as well as the conserved quantities associated with them, explicitly depend on boundary terms in the Lagrangian. This is a very well known feature in Physics, as it can be simply seen, e.g., in thermodynamics. It is in fact well known that boundary

terms are related to boundary conditions. Different boundary terms need different boundary conditions to keep field equations satisfied by action extremals (see Refs. 7, 27, and 28). And it is well known that, e.g., for a correct definition of energy in thermodynamics, different boundary conditions correspond to different definitions of energy, such as *internal energy*, *free energy*, etc. We stress that all these energies are *true* physical energies of thermodynamical systems. Which one has to be used in practice is determined by the particular system under consideration and the boundary conditions *we* decided to impose. As it is physically relevant to notice, we may decide to keep temperature fixed on the boundary of a gas box or we may impose adiabatic conditions; this different choice corresponds to a different apparatus which selects a different energy flow through the boundary so that the boundary conditions are satisfied. We stress that this corresponds to an external action on the system which turns out to change the physical energy of the system itself. In the covariant first-order approach to general relativity something fully analogous holds: The background $\overline{g}$ canonically selects both the boundary conditions and the corresponding energy to be used and different choices of the background correspond to different physically meaningful definitions of energy.

As shown in Refs. 23 and 24, one can also define the *superpotential* $\mathcal{U}[\xi,\sigma]$ and the *reduced current* $\tilde{\mathcal{E}}[\xi,\sigma]$ as those currents such that

$$\mathcal{E}[\xi,\sigma]=\tilde{\mathcal{E}}[\xi,\sigma]+d\mathcal{U}[\xi,\sigma], \tag{2.5}$$

where the reduced current is required to vanish on shell.

The *conserved quantity in a* $(n-1)$*-region* Ω is defined as

$$Q_\Omega[\xi,\sigma]=\int_\Omega \mathcal{E}[\xi,\sigma]=\int_\Omega \tilde{\mathcal{E}}[\xi,\sigma]+\int_{\partial\Omega}\mathcal{U}[\xi,\sigma]=\int_{\partial\Omega}\mathcal{U}[\xi,\sigma], \tag{2.6}$$

where, in the last equality, σ is assumed to be a solution so that $\tilde{\mathcal{E}}[\xi,\sigma]=0$.

In the case of the first-order covariant action functional (2.1) we obtain in particular:

$$\begin{aligned}\mathcal{U}[\xi,\sigma]&=\frac{1}{2\kappa}[\sqrt{g}\nabla^\beta.\xi^\alpha+\sqrt{g}g^{\mu\nu}w^\beta_{\mu\nu}\xi^\alpha-\sqrt{\overline{g}}\overline{\nabla}^\beta.\xi^\alpha]\mathbf{ds}_{\alpha\beta},\\ \tilde{\mathcal{E}}[\xi,\sigma]&=\frac{1}{\kappa}[\sqrt{g}g^{\mu\lambda}G_{\mu\nu}\xi^\nu-\sqrt{\overline{g}}\overline{g}^{\mu\lambda}\overline{G}_{\mu\nu}\xi^\nu]\mathbf{ds}_\lambda .\end{aligned} \tag{2.7}$$

The conserved quantity $Q_\Omega[\xi,\sigma]$ depends on the dynamical metric g and on the reference background metric $\overline{g}$. It has to be interpreted as the *relative conserved quantity of g with respect to* $\overline{g}$. If one chooses g to be a solution asymptotically flat according to one of the current definitions (e.g., the Kerr–Newman solution), assuming $\overline{g}$ to be the flat reference background (which matches the dynamical metric at infinity where ''infinity'' is prescribed by the definition of asymptotic flatness) and Ω to be a spacelike hypersurface in M, then $Q_\Omega[\xi,\sigma]$ reproduces the expected value for mass (by choosing $\xi=\partial_t$, i.e., the vector field which corresponds to asymptotic time translation) and angular momentum (by choosing $\xi=-\partial_\phi$, i.e., the vector field which corresponds to asymptotic rotation; see, e.g., Refs. 11, 15, and 23). Furthermore, the same results are achieved for nonasymptotically flat solutions by choosing suitable reference backgrounds. Examples are the $(2+1)$ BTZ solution (which is asymptotically anti-de Sitter; see Ref. 16), the Euclidean Taub–Bolt solution (which is asymptotically locally flat; see Ref. 29). In addition, the same techniques are successfully used in *gauge-natural theories*, i.e., when the field theory owns both covariance and gauge invariance (e.g., BCEA theory, Einstein–Maxwell theory; see Refs. 23 and 30).

We stress that the conserved quantities $Q_\Omega[\xi,\sigma]$ associated with the covariant first-order action principle (2.1) *are not* affected by the anomalous factor problems as are the ones associated with the standard Hilbert–Einstein Lagrangian (see Refs. 14 and 16).

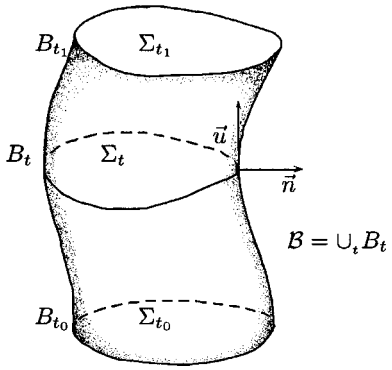

FIG. 1.

III. YORK'S VARIATIONAL PRINCIPLE

York's action was originally introduced (see Refs. 3, 7, and 31) to provide a variational principle suited to deal with the boundary conditions which are specified by keeping the induced metric on ∂D fixed. Boundary terms are added to the standard Hilbert–Einstein action $(1/2\kappa)\int_D R\sqrt{g}\,\mathbf{ds}$. They are exactly needed so that the boundary contribution to the variation of the action vanishes when the induced $(n-1)$ metric is kept fixed on ∂D.

York's action functional is adapted to an ADM foliation induced by dragging a spacelike hypersurface Σ along a timelike vector field ζ.

An ADM foliation of a space–time region D is obtained and it is parametrized by the affine parameter t of ζ (see Fig. 1). The region D is thence topologically the product of Σ times a real line interval $[t_0,t_1]$. Let the generic leaf be Σ_t and B_t its boundary, which is obviously $(n-2)$ dimensional. Let us then denote by $\vec{u}$ the future directed timelike unit normal to the leaf Σ_t.

The boundary ∂D is formed by the union of all $(n-2)$-boundaries B_t, which will be denoted by $\mathcal{B}$, together with the initial and final leaves Σ_{t_0} and Σ_{t_1} of the sandwich, which will be called *lids*. Let us denote by $\vec{n}$ the outward spacelike unit normal to $\mathcal{B}$, by γ_{ij} the metric induced by g on $\mathcal{B}$, by h_{ab} the metric induced on Σ_t, and by σ_{AB} the metric induced on the $(n-2)$-boundary B_t. Here and in the sequel indices run in the following ranges: Greek indices from 0 to $n-1$, lower case Roman letters $a,b,\ldots$ from 1 to $n-1$, lower case middle Roman letters $i,j,\ldots$ take the values 0,2,...,$n-1$, and upper case Roman letters $A,B,\ldots$ range from 2 to $n-1$ (see also the Appendix for the notation).

We shall finally denote by Θ_{ij} the extrinsic curvature of $\mathcal{B}$ in the space–time M, by K_{ab} the extrinsic curvature of Σ_t in M, and by $\mathcal{K}_{AB}$ the extrinsic curvature of B_t in Σ_t (see the Appendix). We shall denote by $\Theta=\gamma^{ij}\Theta_{ij}$, $K=h^{ab}K_{ab}$, and $\mathcal{K}=\sigma^{AB}\mathcal{K}_{AB}$ the traces of the extrinsic curvatures of $\mathcal{B}$, Σ_t, and B_t, respectively. It is assumed that the dynamical metric g and the reference background $\overline{g}$ induce the same metric γ_{ij} on $\mathcal{B}$. Furthermore, let us also assume that the hypersurfaces $\mathcal{B}$ and Σ_t *intersect orthogonally* (or equivalently that $\vec{n}$ and $\vec{u}$ are orthogonal on any B_t, i.e., $u^\mu n_{\mu|\mathcal{B}}=0$). We stress that here we are considering a region D in which the timelike vector field ζ has no fixed points, so that the hypersurfaces Σ_t do not intersect each other and span the whole region D. Let us also denote by Π^{ij} and P^{ab} the *gravitational momenta* conjugated to the metrics γ_{ij} and h_{ab}, respectively; they are given by

$$\Pi^{ij}=-\frac{1}{2\kappa}\sqrt{\gamma}(\Theta\gamma^{ij}-\Theta^{ij}),$$
$$P^{ab}=\frac{1}{2\kappa}\sqrt{h}(Kh^{ab}-K^{ab}). \tag{3.1}$$

According to this notation, York's action in the presence of a background $\overline{g}$ may be written as

$$I_D[g,\overline{g}]=I_D[g]-I_D[\overline{g}], \tag{3.2}$$

where the functional $I_D[g]$ is defined by

$$I_D[g]=\frac{1}{2\kappa}\int_D \sqrt{g}R\,\mathbf{ds}+\frac{1}{\kappa}\int_{\Sigma_{t_0}}^{\Sigma_{t_1}} Ku^\alpha\sqrt{g}\,\mathbf{ds}_\alpha-\frac{1}{\kappa}\int_{\mathcal{B}}\Theta n^\alpha\sqrt{g}\,\mathbf{ds}_\alpha \tag{3.3}$$

and $I_D[\overline{g}]$ is the same functional calculated for the background $\overline{g}$. Notice that $\sqrt{g}u^\alpha\,\mathbf{ds}_\alpha=\sqrt{h}\,\mathrm{d}^3x$ and $\sqrt{g}n^\alpha\,\mathbf{ds}_\alpha=\sqrt{\gamma}\,d^3x$ are the volume elements on Σ_t and $\mathcal{B}$, respectively. In the functional (3.3) we also set the convenient notation

$$\int_{\Sigma_{t_0}}^{\Sigma_{t_1}}\equiv\int_{\Sigma_{t_1}}-\int_{\Sigma_{t_0}}.$$

In the current literature, there exists a whole family of action functionals similar to (3.2) each adapted to the particular problem under consideration. In general, one can add to the functional (3.3) an arbitrary functional depending on the data fixed on the boundary, i.e., depending on the boundary metric (see Ref. 3). This arbitrariness does not affect the equations of motion since the boundary metric is kept fixed in the variational principle. The choice (3.2) is motivated by the requirement $I_D[\overline{g},\overline{g}]=0$, i.e., the requirement that the action functional vanishes when computed with $g=\overline{g}$. The same property is satisfied by (2.1).

Moreover, under additional hypotheses, the integral on the lids Σ_{t_0} and Σ_{t_1} in (3.3) is usually discarded since the lids are either ignored or identified. This is usually done by restricting to situations in which the lids are not present (e.g., by considering a noncompact region D in which t_0 and t_1 are let to tend to $-\infty$ and ∞, respectively) or are identified. [Identification is obtained, e.g., when the solution is time periodic, as may happen in the Euclidean sector (see Refs. 32, 27, and 19) and in approaches based on path integrals for evaluating the grand-canonical partition function or the density of states for general relativity, where the sum over periodic histories has to be considered (see Ref. 27). In all those cases the boundary ∂D is *required* to have the topology $\partial\Sigma\times S^1$, i.e., it is assumed to be a single boundary component $\partial D=\mathcal{B}$.]

Accordingly, let us assume from now on that lids are not present unless otherwise stated. The quasilocal energy $E[g]$ (for motivations and details see Ref. 3), i.e., the energy of a region of finite spatial extent, is obtained by considering the change of the action in time, where changes in time are governed by the lapse N on the boundary $\mathcal{B}$. We stress that the interpretation of this quantity as the energy of a gravitating system was suggested in Ref. 3 through a Hamilton–Jacobi analysis of the action functional. It is given by

$$E_t[g]=\frac{1}{\kappa}\int_{B_t}\mathcal{K}\sqrt{\sigma}\,\mathrm{d}^2x, \tag{3.4}$$

where $\sqrt{\sigma}\,\mathrm{d}^2x$, is the volume element on B_t. A contribution analogous to (3.4) comes from the background action $I_D[\overline{g}]$ in (3.2). Assuming that the induced three metric γ and $\overline{\gamma}$ are matched on the surface $\mathcal{B}$ we finally have

$$E_t[g,\overline{g}]=\frac{1}{\kappa}\int_{B_t}(\mathcal{K}-\overline{\mathcal{K}})\sqrt{\sigma}\,\mathrm{d}^2x. \tag{3.5}$$

This is the explicit expression of Brown and York quasilocal energy computed for the action functional (3.2).

Another standard quantity which can be defined by the (3.2) action functional is the ADM Hamiltonian. It is obtained by a $(3+1)$ decomposition of the action which leads by standard techniques to

$$I_D[g]=\int \mathrm{d}t \int_{\Sigma_t}(P^{ab}\partial_t h_{ab}-N\mathcal{H}-N_a\mathcal{H}^a)\mathrm{d}^3x$$
$$-\int \mathrm{d}t\int_{B_t}\left(\frac{N}{\kappa}\mathcal{K}+N^a 2\frac{P^{bc}}{\sqrt{h}}n_b\sigma_{ac}\right)\sqrt{\sigma}\,\mathrm{d}^2x, \tag{3.6}$$

where

$$\mathcal{H}=-\frac{1}{2\kappa}\sqrt{h}\mathcal{R}+\frac{\kappa}{\sqrt{h}}(2P_{ab}P^{ab}-P^a_aP^b_b),$$
$$\mathcal{H}^a=-2D_bP^{ab} \tag{3.7}$$

are the Hamiltonian and the momentum constraint, respectively. The Hamiltonian for vacuum general relativity is thus identified with the term

$$H(g)=\int_{\Sigma_t}(N\mathcal{H}+N_a\mathcal{H}^a)\mathrm{d}^3x+\frac{1}{\kappa}\int_{B_t}(N\mathcal{K}-N^aK^{bc}n_b\sigma_{ac})\sqrt{\sigma}\,\mathrm{d}^2x. \tag{3.8}$$

In the latter term we have taken into account that $h^{bc}n_b\sigma_{ac}=0$ (see the Appendix for details).

The Hamiltonian $H(g)$ is the sum of a *constrained volume* term, which is vanishing when computed on a solution, and a *boundary* term.

We may repeat the above-mentioned analysis also for the background action functional $I_D[\overline{g}]$ obtaining an Hamiltonian $H(\overline{g})$ which agrees with (3.8) provided that we replace the terms there involved with the corresponding barred ones. The total Hamiltonian $H(g,\overline{g})$ is then given by the following difference:

$$H(g,\overline{g})=H(g)-H(\overline{g}). \tag{3.9}$$

When it is evaluated on solutions of field equations, the constrained volume terms vanish and (3.9) reduces to the boundary terms:

$$H(g,\overline{g})\simeq\frac{1}{\kappa}\int_{B_t}(N\mathcal{K}-N^aK^{bc}n_b\sigma_{ac})\sqrt{\sigma}\,\mathrm{d}^2x$$
$$-\frac{1}{\kappa}\int_{B_t}(\overline{N\mathcal{K}}-\overline{N}^a\overline{K}^{bc}\overline{n}_b\overline{\sigma}_{ac})\sqrt{\overline{\sigma}}\,\mathrm{d}^2x, \tag{3.10}$$

where the symbol $\simeq$ denotes equality on shell.

Moreover, if the metric g and its relative background $\overline{g}$ agree on the boundary the Hamiltonian simplifies as follows:

$$H(g,\overline{g})\simeq\frac{1}{\kappa}\int_{B_t}\{N(\mathcal{K}-\overline{\mathcal{K}})-N^a(K^{bc}-\overline{K}^{bc})n_b\sigma_{ac}\}\sqrt{\sigma}\,\mathrm{d}^2x. \tag{3.11}$$

The *mass* associated with the time translation $t^\mu=Nu^\mu+N^\mu$, relative to two solutions g and $\overline{g}$, is simply defined to be the value of the Hamiltonian (3.10). Clearly the mass $H(\overline{g},\overline{g})$ of the background is equal to zero.

Notice that, whenever it is possible to choose a Gaussian gauge, i.e., setting $N=1$ and $N^a=0$ in (3.11), we obtain the quasilocal energy (3.5) (see Ref. 3).

In Ref. 33 it was shown that the definition (3.10) agrees with the expressions of energy already defined in the literature for space–times with different asymptotic behavior.

IV. COMPARISON OF THE ACTION FUNCTIONALS

We shall here decompose the first-order covariant action functional (2.1) along an ADM foliation of D in order to prove that the action functional (3.2) and (2.1) are equal if the four-metrics g and $\overline{g}$ are required to coincide on ∂D.

Of course, the ADM splitting breaks down the explicit covariance in the action allowing a comparison with respect to the same ADM foliation. In particular, the boundary term in the covariant action (2.1) splits into a contribution on $\mathcal{B}$ and a contribution on the *lids* Σ_{t_0} and Σ_{t_1}.

Let us consider local coordinates (t,r,x^A) adapted both to $\mathcal{B}$ and the ADM splitting on D. In this coordinate system $\mathcal{B}$ has the expression $r=$constant while the leaves Σ_t are the hypersurfaces of equation $t=$constant. The metric tensor g can be split with respect to the ADM foliation obtaining

$$\begin{aligned} g=g_{\mu\nu}\,\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu&=(h_{\mu\nu}-u_\mu u_\nu)\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu\\ &=-N^2\,\mathrm{d}t^2+h_{ab}(\mathrm{d}x^a+N^a\,\mathrm{d}t)\otimes(\mathrm{d}x^b+N^b\,\mathrm{d}t). \end{aligned} \tag{4.1}$$

Similarly, one can consider the foliation of space–time in the hypersurfaces $r=$constant and obtain

$$\begin{aligned} g=g_{\mu\nu}\,\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu&=(\gamma_{\mu\nu}+n_\mu n_\nu)\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu\\ &=V^2\,\mathrm{d}r^2+\gamma_{ij}(\mathrm{d}x^i+V^i\,\mathrm{d}r)\otimes(\mathrm{d}x^j+V^j\,\mathrm{d}r). \end{aligned} \tag{4.2}$$

Analogous expressions can be obtained for the reference background metric $\overline{g}$. Let us evaluate the boundary term of the covariant first-order action functional (2.1) on $\mathcal{B}$ and on the lids Σ_{t_0} and Σ_{t_1}, i.e.,

$$A_{\mathcal{B}}=-\frac{1}{2\kappa}\int_{\mathcal{B}}\sqrt{g}g^{\mu\nu}w^\alpha_{\mu\nu}\,\mathbf{ds}_\alpha,\quad A^{\Sigma_{t_1}}_{\Sigma_{t_0}}=-\frac{1}{2\kappa}\int^{\Sigma_{t_1}}_{\Sigma_{t_0}}\sqrt{g}g^{\mu\nu}w^\alpha_{\mu\nu}\,\mathbf{ds}_\alpha. \tag{4.3}$$

By using results which are summarized in the Appendix [see Eqs. (A18) and (A23)] one obtains

$$\begin{aligned} A_{\mathcal{B}}=-\frac{1}{2\kappa}\int_{\mathcal{B}}g^{\mu\nu}w^\alpha_{\mu\nu}n_\alpha\sqrt{\gamma}\,\mathrm{d}^3x=-\frac{1}{2\kappa}\int_{\mathcal{B}}\Bigg\{&2\Theta-\overline{\Theta}_{ij}\left(\frac{\overline{V}}{V}\overline{\gamma}^{ij}+\frac{V}{\overline{V}}\gamma^{ij}\right)\\ &-\frac{\overline{\Theta}_{ij}}{V\overline{V}}(V^i-\overline{V}^i)(V^j-\overline{V}^j)+\frac{1}{V\overline{V}}\partial_i\overline{V}(V^i-\overline{V}^i)-\frac{1}{V}\overline{\mathcal{D}}_i(V^i-\overline{V}^i)\Bigg\}\sqrt{\gamma}\,\mathrm{d}^3x, \end{aligned} \tag{4.4}$$

where $\overline{\mathcal{D}}_i$ is the covariant derivative with respect to the three-metric $\overline{\gamma}_{ij}$ induced on $\mathcal{B}$ by the background metric $\overline{g}$, while V and V^i are the *radial lapse* and the *radial shift* [see (4.2)].

Analogously, on the lids the ADM splitting of the boundary term (4.3) gives an extra contribution of the following form:

$$\begin{aligned} A^{\Sigma_{t_1}}_{\Sigma_{t_0}}&=+\frac{1}{2\kappa}\int^{\Sigma_{t_1}}_{\Sigma_{t_0}}g^{\mu\nu}w^\alpha_{\mu\nu}u_\alpha\sqrt{h}\,\mathrm{d}^3x\\ &=-\frac{1}{2\kappa}\int^{\Sigma_{t_1}}_{\Sigma_{t_0}}\Bigg\{-2K+\overline{K}_{ab}\left(\frac{\overline{N}}{N}\overline{h}^{ab}+\frac{N}{\overline{N}}h^{ab}\right)-\frac{\overline{K}_{ab}}{N\overline{N}}(N^a-\overline{N}^a)(N^b-\overline{N}^b)\\ &\quad-\frac{1}{N\overline{N}}\partial_a\overline{N}(N^a-\overline{N}^a)+\frac{1}{N}\overline{D}_a(N^a-\overline{N}^a)\Bigg\}\sqrt{h}\,\mathrm{d}^3x, \end{aligned} \tag{4.5}$$

where $\overline{D}_a$ is the covariant derivative with respect to the three-metric $\overline{h}_{ab}$ induced on Σ by the background metric $\overline{g}$, while N and N^a are the lapse and the shift of the metric [see (4.1)]. We stress that no matching condition is required to obtain the above-mentioned results. The behaviors of the metrics g and $\overline{g}$ are completely unrelated until now. In general the two action functionals (2.1) and (3.2) are fairly different.

However, let us assume that the dynamical metric g and the background $\overline{g}$ coincide on the hypersurface $\mathcal{B}$ so that, in particular, they induce the same three-metric on $\mathcal{B}$ (i.e., $\gamma_{ij}|_{\mathcal{B}}=\overline{\gamma}_{ij}|_{\mathcal{B}}$) and they have the same *radial* lapse function (i.e. $V|_{\mathcal{B}}=\overline{V}|_{\mathcal{B}}$) and *radial* shift vector (i.e. $V^i|_{\mathcal{B}}=\overline{V}^i|_{\mathcal{B}}$). Then, under these additional hypotheses, the contribution $A_{\mathcal{B}}$ reduces to

$$A_{\mathcal{B}}=-\frac{1}{\kappa}\int_{\mathcal{B}}(\sqrt{\gamma}\Theta-\sqrt{\overline{\gamma}}\overline{\Theta})\mathrm{d}^3x=-\frac{1}{\kappa}\int_{\mathcal{B}}(\sqrt{g}\Theta-\sqrt{\overline{g}}\overline{\Theta})n^\alpha\,\mathbf{ds}_\alpha. \tag{4.6}$$

Analogously, if the metric g and $\overline{g}$ are required to agree on the lids (i.e., if $h_{ij}=\overline{h}_{ij}$, $N=\overline{N}$, and $N^i=\overline{N}^i$ on Σ_{t_0} and Σ_{t_1}), then the contribution (4.5) on the lids reduces to

$$A^{\Sigma_{t_1}}_{\Sigma_{t_0}}=\frac{1}{\kappa}\int_{\Sigma_{t_0}}^{\Sigma_{t_1}}(\sqrt{h}K-\sqrt{\overline{h}}\overline{K})\mathrm{d}^3x=\frac{1}{\kappa}\int_{\Sigma_{t_0}}^{\Sigma_{t_1}}(\sqrt{g}K-\sqrt{\overline{g}}\overline{K})u^\alpha\,\mathbf{ds}_\alpha. \tag{4.7}$$

Then the boundary term in the covariant first-order action (2.1) can be written as

$$A_{\mathcal{B}}+A^{\Sigma_{t_1}}_{\Sigma_{t_0}}=-\frac{1}{\kappa}\int_{\mathcal{B}}(\sqrt{g}\Theta-\sqrt{\overline{g}}\overline{\Theta})n^\alpha\mathbf{ds}_\alpha+\frac{1}{\kappa}\int_{\Sigma_{t_0}}^{\Sigma_{t_1}}(\sqrt{g}K-\sqrt{\overline{g}}\overline{K})u^\alpha\,\mathbf{ds}_\alpha \tag{4.8}$$

and the action functionals (2.1) and (3.2) clearly coincide.

We stress that this result has been obtained by requiring the aforementioned matching conditions between g and $\overline{g}$ on the complete boundary $\partial D=\mathcal{B}+\Sigma_{t_1}-\Sigma_{t_0}$ of the region D.

We should also remark that for time-independent solutions the matching on the lids cannot be required, because if the two metrics g and $\overline{g}$ agree on a spacelike hypersurface Σ_t, they necessarily agree on the whole region D. Also for this reason, the contributions on the lids are never considered in applications.

The matching condition of the four-metrics g and $\overline{g}$ is a stronger requirement than the one introduced in Ref. 10. There, only the induced three-metrics γ_{ij} and $\overline{\gamma}_{ij}$ are required to agree on $\mathcal{B}$, where $\mathcal{B}$ is let to tend to *infinity*. Although the matching of the four-metrics at infinity is not too hard to be implemented in applications (see Refs. 15, 16, and 19), we are aware that this matching, when possible, may become hard to implement in a *finite region*. Here the matching is required to have a direct theoretical comparison between the action functionals (2.1) and (3.2) (and between their Hamiltonians and conserved charges).

V. QUASILOCAL ENERGY AS A NÖTHER CURRENT

Nöther theorem provides a map Q which associates to each space–time vector field ξ a covariantly conserved quantity $Q[\xi]$ [see Eqs. (2.6) and (2.7)]. The quantity Q will be compared with the standard ADM Hamiltonian and with the quasilocal energy defined in Sec. III.

Let us consider the covariant conserved quantity $Q_{\Sigma_t}[\xi,\sigma]$ for the first-order action functional (2.1) in the domain Σ_t and relative to a vector field ξ and a section $\sigma=(g,\overline{g})$. As we have already outlined in Sec. II, the quantity $Q_{\Sigma_t}[\xi,\sigma]$ is defined to be the integral of the superpotential (2.7) on the two-dimensional surfaces B_t (see Fig. 1 for the notation). Since the Lagrangian (2.1) decomposes in three terms [see Eq. (2.2a)], we can also decompose each derived quantity (in particular the superpotential, the Nöther currents, and the conserved quantities) in three terms. In particular,

$$Q^{\mathrm{tot}}_{\Sigma_t}[\xi,\sigma]=Q_{\Sigma_t}[\xi,g]+Q_{\Sigma_t}[\xi,g,\overline{g}]+Q_{\Sigma_t}[\xi,\overline{g}], \tag{5.1}$$

where

$$Q_{\Sigma_t}[\xi,g]=\frac{1}{2\kappa}\int_{B_t}\sqrt{g}\nabla^{\beta}\xi^{\alpha}\,\mathbf{ds}_{\alpha\beta},$$

$$Q_{\Sigma_t}[\xi,g,\overline{g}]=\frac{1}{2\kappa}\int_{B_t}\sqrt{g}g^{\mu\nu}w^{\beta}_{\mu\nu}\xi^{\alpha}\,\mathbf{ds}_{\alpha\beta}, \tag{5.2}$$

$$Q_{\Sigma_t}[\xi,\overline{g}]=-\frac{1}{2\kappa}\int_{B_t}\sqrt{\overline{g}}\overline{\nabla}^{\beta}\xi^{\alpha}\,\mathbf{ds}_{\alpha\beta}.$$

In order to simplify the ADM decomposition of the expression (5.1) so to be able to compare the results obtained with the standard ones of Sec. III and Ref. 3 let us assume, as usual, that the metrics g and $\overline{g}$ are matched on the hypersurface $\mathcal{B}$ and that the boundaries are orthogonal (i.e., $u^{\mu}n_{\mu}|_{\mathcal{B}}=0$).

[We stress that under our viewpoint the matching condition between g and $\overline{g}$ is unessential, since Nöther currents are always covariantly conserved. One may consider the second example analyzed in Sec. VII, where the Kerr solution is studied and its *mass* inside the finite R sphere is obtained with respect to a flat background matched at spatial infinity. In this section we require the matching on $\mathcal{B}$ in order to compare the Nöther charges' expression with the aforementioned standard $(3+1)$ Hamiltonian and quasilocal energy.]

Let us also assume that the vector field ξ is tangent to the hypersurface $\mathcal{B}$ (i.e., $\xi^{\mu}n_{\mu}|_{\mathcal{B}}=0$). First of all let us consider the first contribution $Q_{\Sigma_t}[\xi,g]$ into (5.1), i.e., the integral of the Komar superpotential. It may be rewritten as

$$Q_{\Sigma_t}[\xi,g]=\frac{1}{2\kappa}\int_{B_t}(u_{\beta}n_{\alpha}-u_{\alpha}n_{\beta})g^{\beta\mu}\nabla_{\mu}\xi^{\alpha}\sqrt{\sigma}\,\mathrm{d}^2x. \tag{5.3}$$

Taking formula (A9) repeatedly into account together with the condition of orthogonal boundaries $u^{\mu}n_{\mu}|_{\mathcal{B}}=0$ and the condition $\xi^{\mu}n_{\mu}|_{\mathcal{B}}=0$ we finally obtain

$$Q_{\Sigma_t}[\xi,g]=\frac{1}{\kappa}\int_{B_t}\{\Theta_{\mu\alpha}u^{\mu}\xi^{\alpha}\}\sqrt{\sigma}\,\mathrm{d}^2x+\frac{1}{2\kappa}\int_{B_t}u_{\alpha}\pounds_{\xi}n^{\alpha}\sqrt{\sigma}\,\mathrm{d}^2x. \tag{5.4}$$

A similar expression may be found for the third contribution $Q_{\Sigma_t}[\xi,\overline{g}]$ into formula (5.2), i.e., the Komar contribution of the matched bakground $\overline{g}$:

$$Q_{\Sigma_t}[\xi,\overline{g}]=-\frac{1}{\kappa}\int_{B_t}\{\overline{\Theta}_{\mu\alpha}u^{\mu}\xi^{\alpha}\}\sqrt{\sigma}\,\mathrm{d}^2x-\frac{1}{2\kappa}\int_{B_t}u_{\alpha}\pounds_{\xi}\overline{n}^{\alpha}\sqrt{\sigma}\,\mathrm{d}^2x. \tag{5.5}$$

It now remains to calculate the second contribution $Q_{\Sigma_t}[\xi,g,\overline{g}]$ into formula (5.2). We stress that this is the contribution arising from the boundary term into the action functional (2.1). By standard techniques it can be recasted as

$$Q_{\Sigma_t}[\xi,g,\overline{g}]=-\frac{1}{\kappa}\int_{B_t}u_{\alpha}\xi^{\alpha}(\Theta-\overline{\Theta})\sqrt{\sigma}\,\mathrm{d}^2x. \tag{5.6}$$

[Notice that only the projection $u_{\alpha}\xi^{\alpha}$ of the vector field ξ^{α} along the timelike normal u^{α} gives a contribution to the term $Q_{\Sigma_t}[\xi,g,\overline{g}]$. This is the reason why the boundary term into the action

(2.1) allows one to correct the anomalous factor of the Komar superpotential which, as we said previously, appears in the computation of mass while it does not enter in the computation of angular momentum.]

The *conserved quantity* in the region Σ_t relative to the infinitesimal generator of space–time symmetries ξ is then given by the sum of (5.4), (5.5), and (5.6). Using (A11) and since in this case $K_{\mu\nu}u^\nu=0$ and $\sigma^\mu_\nu u^\nu=0$ it can be recasted as

$$Q^{\mathrm{tot}}_{\Sigma_t}[\xi,\sigma]=-\frac{1}{\kappa}\int_{B_t}\{u_\alpha\xi^\alpha(\mathcal{K}-\overline{\mathcal{K}})+\sigma^\rho_\alpha\xi^\alpha n^\beta(K_{\rho\beta}-\overline{K}_{\rho\beta})\}\sqrt{\sigma}\,\mathrm{d}^2x$$
$$+\frac{1}{2\kappa}\int_{B_t}u_\alpha(\pounds_\xi n^\alpha-\pounds_\xi\overline{n^\alpha})\sqrt{\sigma}\,\mathrm{d}^2x. \tag{5.7}$$

Let us stress that, until now, no assumption has been made on the vector field ξ, apart from the requirement $\xi^\mu n_\mu|_{\mathcal{B}}=0$.

An easy computation shows that *the difference* $u_\alpha(\pounds_\xi n^\alpha-\pounds_\xi\overline{n^\alpha})$ is always zero if the metrics g and $\overline{g}$ are matched on $\mathcal{B}$. Furthermore, the terms $u_\alpha\pounds_\xi n^\alpha$ and $u_\alpha\overline{\pounds_\xi n^\alpha}$ appearing in the last contribution to (5.7) *separately* disappear if we choose ξ to be tangent to the two-surfaces B_t, that is $\xi^\mu u_\mu|_{B_t}=0$, or also if we choose ξ to be the timelike vector field ∂_t, i.e., $\xi^\alpha=Nu^\alpha+N^\alpha$. In both cases the flow of the vector field ξ maps each hypersurface Σ_t into itself or, respectively, into another surface $\Sigma_{t'}$. Since the vector field n^α is tangent to each Σ_t it also turns out that $\pounds_\xi n^\alpha$ is tangent to Σ_t and then $u_\alpha\pounds_\xi n^\alpha=0$ in these cases.

Hence if we specialize formula (5.7) for the vector field $\xi=\partial_t$ we obtain the covariant conserved quantity which we call the *Hamiltonian* of the system. It is given by

$$Q^{\mathrm{tot}}_{\Sigma_t}[\partial_t,\sigma]=\frac{1}{\kappa}\int_{B_t}\{N(\mathcal{K}-\overline{\mathcal{K}})-N^a(K^{bc}-\overline{K}^{bc})n_b\sigma_{ac}\}\sqrt{\sigma}\,\mathrm{d}^2x \tag{5.8}$$

and it coincides exactly with the expression of the $(3+1)$ Hamiltonian (3.11).

Let us notice that this definition of the Hamiltonian can be correctly considered as the definition of a *covariant* ADM formulation (see Refs. 22, 34, and 35). In fact it does not require, *a priori*, a $(3+1)$ decomposition of space–time. We stress that in the covariant ADM approach, the Hamiltonian, or energy, contained in a three-dimensional region Ω and relative to a solution σ, is defined by (2.6) as a Nöther conserved quantity:

$$Q^{\mathrm{tot}}_{\Omega}[\xi,\sigma]=\int_{\partial\Omega}\mathcal{U}[\xi,\sigma]. \tag{5.9}$$

This is a well-posed definition of the Hamiltonian provided only that the nonvanishing vector field ξ be transverse to the hypersurface Ω. Hence, by considering the parameter of the flow of ξ as the ''time'' parameter and transporting Ω along the flow of ξ we obtain a world tube foliated by hypersurfaces diffeomorphic to Ω. In this covariant context, rather than starting from a preferred local foliation into hypersurfaces, the starting point is a nonvanishing vector field the flow of which defines the local time, i.e., the flow of evolution. Then, by specializing the definition (5.9) to the ADM foliation depicted in Fig. 1, under the additional assumptions of orthogonal boundaries and of the matching between the metric and its background, the *covariant* Hamiltonian $Q^{\mathrm{tot}}_{\Sigma_t}[\partial_t,\sigma]$ exactly coincides with the standard Hamiltonian $H(g,\overline{g})$ derived from a $(3+1)$ splitting of the York action functional [see Eq. (3.11)].

Another relevant Nöther conserved quantity is obtained by specializing formula (5.7) to a vector field $\xi^\alpha=N^\alpha$ tangent to the two-surfaces B_t, i.e., $N^\alpha u_\alpha|_{B_t}=0$ and $\sigma^\rho_\alpha N^\alpha=N^\rho$. Because of the vanishing of the first and third terms on the right-hand side of (5.7) we obtain

$$Q^{\mathrm{tot}}_{\Sigma_t}[N^\alpha,\sigma]=-\frac{1}{\kappa}\int_{B_t}N^\alpha n^\beta(K_{\alpha\beta}-\overline{K}_{\alpha\beta})\sqrt{\sigma}\,\mathrm{d}^2x. \tag{5.10}$$

In asymptotically flat space–times when ξ corresponds to a rotation at spatial infinity, the Nöther charge (5.10) may be taken as the definition of *angular momentum*.

The last Nöther charge we consider is the one relative to the unit vector field $\xi=u$ normal to the leaves of the ADM foliation. From (5.7) we obtain

$$Q^{\mathrm{tot}}_{\Sigma_t}[u,\sigma]=\frac{1}{\kappa}\int_{B_t}(\mathcal{K}-\overline{\mathcal{K}})\sqrt{\sigma}\,\mathrm{d}^2x. \tag{5.11}$$

We observe that it agrees with the definition (3.5) of quasilocal energy. In the aforementioned hypotheses, *quasilocal energy may then be considered as a Nöther charge associated with the normal generator of the ADM foliation.*

VI. TIME CONSERVATION

Despite the fact that quantities conserved along the *time* of a fixed ADM foliation are not manifestly covariant in nature they may be interesting to investigate. In our perspective, in fact, they can be obtained from covariantly conserved quantities. To be more precise, we can consider a variational principle, a space–time vector field ξ which is an infinitesimal generator of Lagrangian symmetries and a solution of field equations. Then we can compute covariantly conserved currents $\mathcal{E}[\xi]$ by Nöther theorem. Let us then fix a spacelike $(n-1)$-region Σ and integrate the Nöther current on it to define a conserved quantity $Q_\Sigma[\xi,\sigma]$ [see (2.6)]. Any timelike vector field ζ then allows one to evolve the region Σ along its flow, parameterized by its affine parameter t. Under this viewpoint, the question arises whether there exists a vector field ζ (possibly depending on the region Σ) such that the covariantly conserved quantity generated by ξ is also conserved in the ''time'' induced by ζ. At a first glance, if we have $\partial D=\Sigma_{t_1}-\Sigma_{t_0}+\mathcal{B}$ (see Fig. 1), conservation in time is equivalent to requiring that the integral of the Nöther current $\mathcal{E}[\xi]$ on $\mathcal{B}$ vanishes (for any time interval $[t_0,t_1]$). In fact, we have the covariant conservation law $\mathrm{d}\mathcal{E}[\xi]=0$, so that

$$0=\int_D\mathrm{d}\mathcal{E}[\xi]=\int_{\partial D}\mathcal{E}[\xi]=\int_{\Sigma_{t_1}}\mathcal{E}[\xi]-\int_{\Sigma_{t_0}}\mathcal{E}[\xi]+\int_{\mathcal{B}}\mathcal{E}[\xi]\Rightarrow\int_{\Sigma_{t_1}}\mathcal{E}[\xi]-\int_{\Sigma_{t_0}}\mathcal{E}[\xi]=-\int_{\mathcal{B}}\mathcal{E}[\xi]. \tag{6.1}$$

Thence the conserved quantity $\int_{\Sigma_t}\mathcal{E}[\xi]$ computed on a leaf does not depend on the particular leaf if and only if $\int_{\mathcal{B}}\mathcal{E}[\xi]=0$ (for any time interval $[t_0,t_1]$). Physically speaking, this amount to require that the flow of the current $\mathcal{E}[\xi]$ through $\mathcal{B}$ is vanishing. Clearly, different ADM foliations may evolve Σ in different ways. In general, just a few of them will lead to time-conserved quantities. The vanishing of $\int_{\mathcal{B}}\mathcal{E}[\xi]$ then has to be guaranteed by additional hypotheses, possibly in many different ways. Under stronger hypotheses on ξ (or on ζ, or on the boundary conditions which g and $\overline{g}$ have to satisfy) the set of ADM foliations leading to time-conserved quantities with respect to different times may be possibly enlarged. Different sets of conditions which guarantee time conservation will be discussed in the following and we shall compare them to those found in the current literature; see also Sec. VII for some examples.

Here we shall discuss two different sets of sufficient conditions for time conservation. The quantities (5.8), (5.10), and (5.11) are all covariantly conserved quantities independent of the hypothesis that ξ is or is not a Killing vector field. In fact they have been defined by means of Nöther theorem through a construction which relies only on the covariant nature of the Lagrangian. Hence, on a solution of field equations, the covariant conservation law $d_\mu\mathcal{E}^\mu[\xi,\sigma]=0$ always holds for the Nöther current $\mathcal{E}[\xi,\sigma]$ and for all vector fields ξ. This property, together with the property of existence of superpotentials for any natural theory, has allowed us to define the covariantly conserved Nöther charges $Q^{\mathrm{tot}}_\Omega[\xi,\sigma]$ [see (2.6)]. On the contrary the charges $Q^{\mathrm{tot}}_{\Sigma_t}[\xi,\sigma]$

are *conserved in ''time''* if they do not depend on the chosen hypersurface Σ_t, i.e., if $Q^{\mathrm{tot}}_{\Sigma_t}[\xi,\sigma] = Q^{\mathrm{tot}}_{\Sigma_{t'}}[\xi,\sigma]$. This is a stronger condition that has to be supported by additional requirements. If $\mathcal{B}$ is the three-dimensional region such that $\Sigma_{t'} - \Sigma_t + \mathcal{B}$ is the boundary of a region D, from the conservation law $d_\mu \mathcal{E}^\mu[\xi,\sigma] = 0$ we obtain, as we already claimed, a time-conserved quantity if $\int_{\mathcal{B}} \mathcal{E}^\mu \, \mathrm{d}s_\mu = 0$. A stronger condition amounts to requiring that the integrand be equal to zero on $\mathcal{B}$, i.e., $\mathcal{E}^\mu n_\mu|_{\mathcal{B}} = 0$. In this case $Q^{\mathrm{tot}}[\xi,\sigma]$ is conserved not only with respect to the given foliation in hypersurfaces Σ_t but it is time conserved with respect to the time of *any* foliation of the same region D.

For the action functional (2.1) the Nöther current (2.3) may be rewritten as

$$\mathcal{E}^\alpha[\xi,\sigma] = \frac{1}{2\kappa}\{(\sqrt{g}g^{\mu\nu} - \sqrt{\overline{g}}\overline{g}^{\mu\nu})\pounds_\xi \overline{u}^\alpha_{\mu\nu} - \pounds_\xi(\sqrt{g}g^{\mu\nu})w^\alpha_{\mu\nu} - \xi^\alpha \mathcal{L}\}. \tag{6.2}$$

The corresponding quantity $\mathcal{E}^\mu n_\mu|_{\mathcal{B}}$ will be equal to zero if some condition is verified. We do not explicitly know a set of necessary requirements for the occurrence of this situation; we can only provide two examples of sufficient conditions.
We may require, as a first example, that the following properties hold true:

(A) the vector field ξ is a Killing vector field for the metric, i.e., $\pounds_\xi g_{\mu\nu} = 0$;
(B) the vector field ξ is a symmetry for the background in the sense that $\pounds_\xi \overline{u}^\alpha_{\mu\nu} = 0$;
(C) ξ is tangent to the boundary $\mathcal{B}$, i.e., $\xi^\mu n_\mu|_{\mathcal{B}} = 0$.

These three requirements together ensure that $\mathcal{E}^\mu n_\mu|_{\mathcal{B}} = 0$. These properties are clearly satisfied if we are dealing with the Killing vector fields of an asymptotically flat stationary solution and we choose the flat metric as a background. Nevertheless, we stress that the time-conserved quantities $Q^{\mathrm{tot}}_{\Sigma_t}[\xi,\sigma] = \int_{B_t} \mathcal{U}[\xi,\sigma]$ can be computed on a finite region, i.e., it is not necessary that B_t is identified with spatial infinity. Moreover, we have not explicitly required the matching between the metrics on $\mathcal{B}$ (see the example of the Kerr metric in Sec. VII).

Another set of sufficient conditions may be imposed to fulfill the condition $\mathcal{E}^\mu n_\mu|_{\mathcal{B}} = 0$. They closely resemble the ones of Ref. 3. We may require the matching of the metrics on the boundary $\mathcal{B}$ [so that the first term in (6.2) vanishes] and we again require ξ to be tangent to the boundary $\mathcal{B}$: $\xi^\mu n_\mu|_{\mathcal{B}} = 0$ [in order to make the third term in (6.2) vanishing when contracted with the normal n_α]. We are left with the following term:

$$\int_{\mathcal{B}} \mathcal{E}^\alpha \, \mathrm{d}s_\alpha = -\frac{1}{2\kappa}\int_{\mathcal{B}} \pounds_\xi(\sqrt{g}g^{\mu\nu})w^\alpha_{\mu\nu}\mathbf{ds}_\alpha .$$

Owing to the matching requirement $g_{\mu\nu}|_{\mathcal{B}} = \overline{g}_{\mu\nu}|_{\mathcal{B}}$ the latter expression may be recasted into the equivalent form:

$$\int_{\mathcal{B}} \mathcal{E}^\alpha \, \mathrm{d}s_\alpha = \int_{\mathcal{B}} (\Pi^{ij} - \overline{\Pi}^{ij})\pounds_\xi \gamma_{ij} \, \mathrm{d}^3x.$$

It vanishes if we require ξ to be a Killing vector of the boundary three-metric: $\pounds_\xi \gamma_{ij} = \mathcal{D}_i\xi_j + \mathcal{D}_i\xi_j = 0$. Hence, also in this latter situation, we obtain time-conserved quantities $Q^{\mathrm{tot}}_{\Sigma_t}[\xi,\sigma]$ for the time t of *any foliation* of D in hypersurfaces Σ_t.

VII. EXAMPLES

Here we shall discuss some simple examples to illustrate and clarify some of the topics introduced previously in the paper.

Let us first consider the conserved quantities of the Schwarzschild solution given in its standard form:

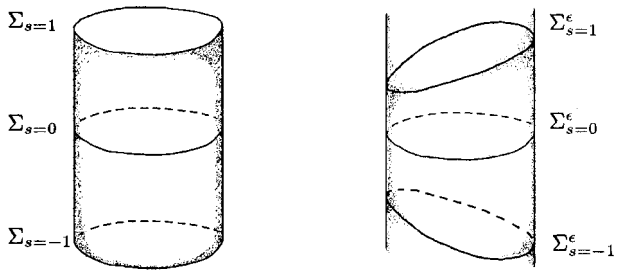

FIG. 2.

$$g = -\left(1 - \frac{2M}{\rho}\right) dt^2 + \frac{1}{\left(1 - \frac{2M}{\rho}\right)} d\rho^2 + \rho^2 (d\theta^2 + \sin^2\theta\, d\phi^2). \tag{7.1}$$

For computational convenience we rewrite it in isotropic coordinates (t, r, θ, ϕ):

$$g = -\frac{(2r-M)^2}{(2r+M)^2} dt^2 + \left(1 + \frac{M}{2r}\right)^4 (dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\phi^2)), \tag{7.2}$$

where, see Ref. 6,

$$2r = -M + \rho + \sqrt{\rho(\rho - 2M)} \Leftrightarrow \rho = \frac{(M+2r)^2}{4r}. \tag{7.3}$$

Let us choose as a background the Minkowski space–time in isotropic coordinates

$$\overline{g} = -\frac{(2R-M)^2}{(2R+M)^2} dt^2 + \left(1 + \frac{M}{2R}\right)^4 (dr^2 + r^2(d\theta^2 + \sin^2\theta\, d\phi^2)). \tag{7.4}$$

The background $\overline{g}$ is in fact a flat metric as one can easily check by direct computation of the Riemann tensor. Furthermore, the two metrics g and $\overline{g}$ are matched on the hypersurface $\mathcal{B}$ defined by the equation $r = R$.

Let us then consider a family of foliations of the region $r \leqslant R$ generated by the infinitesimal generator

$$\zeta = (1 + \epsilon(\sin(\phi) + 1))\partial_t, \tag{7.5}$$

where ϵ is a (small) parameter. The flow parameter is denoted by s so that, if Σ is a spacelike hypersurface, it can be dragged along the flow Φ_s of ζ to obtain the foliation:

$$\Sigma^{\epsilon}_s = \{s \ \text{constant}\}, \quad s = t/(1 + \epsilon(\sin(\phi) + 1)).$$

Since s denotes the affine parameter along the flow of ζ, it can be interpreted as the *time* associated with the ADM foliation. We remark that we are in the hypothesis of orthogonal boundaries as required throughout the paper. Notice also that for $\epsilon = 0$ we recover the ordinary asymptotic time translation $\zeta = \partial_t$ and the ordinary ADM foliation by the hypersurfaces $t = \text{constant}$ (see Fig. 2).

Let us then choose the (three-parameter) vector field

$$\xi = \alpha\partial_t + (\beta + \gamma \sin(\theta)\cos\phi)\partial_\phi \tag{7.6}$$

(where α, β, and γ are three real constants), which is a generator of symmetries for the first-order Lagrangian (2.1). We remark that ξ is a well-defined vector field on $\mathcal{B}$; in particular it extends to $\theta=0$ and $\theta=\pi$. For $\alpha=1$ and $\beta=\gamma=0$, ξ reduces to the ordinary time translation $\xi=\partial_t$ so that we expect the corresponding conserved quantity $Q^{\mathrm{tot}}_{\Sigma^\epsilon_s}[\xi]$ to be interpreted as the *mass* of g *relative* to $\overline{g}$ on the leaf Σ^ϵ_s in the region $r\leqslant R$. We also stress that for $\gamma=0$ the vector field ξ is a Killing vector both for g and $\overline{g}$. On the contrary, for $\gamma\neq 0$, ξ is not Killing both for g and $\overline{g}$. In the case $\gamma\neq 0$, ξ does not have a direct physical interpretation, though it is a symmetry generator for the Lagrangian (2.1) and it algorithmically generates the covariant Nöther conserved quantity $Q^{\mathrm{tot}}_{\Sigma^\epsilon_s}[\xi]$. We shall use it to illustrate how time conservation may be related to covariant conservation along different foliations.

If we calculate the Nöther conserved quantity [according to Eq. (5.1) with $2k=16\pi$, i.e., in geometric units $G=c=1$] we get the following result:

$$
\begin{aligned}
Q_{\Sigma^\epsilon_s}[\xi,g] &= \alpha\frac{M}{2}-\gamma\frac{\pi}{16}R\left(1-\frac{M}{2R}\right)^2 s\epsilon,\\
Q_{\Sigma^\epsilon_s}[\xi,g,\overline{g}] &= \left(\alpha\frac{M}{2}-\gamma\frac{\pi M}{16}s\epsilon\right)\left(1-\frac{M}{R}\right),\\
Q_{\Sigma^\epsilon_s}[\xi,g] &= \gamma\frac{\pi R}{16}\left(1-\frac{M^2}{4R^2}\right)s\epsilon,\\
Q^{\mathrm{tot}}_{\Sigma^\epsilon_s}[\xi] &= \alpha\left(M-\frac{M^2}{2R}\right)+\gamma\left(\frac{\pi M^2}{32R}s\epsilon\right).
\end{aligned}
\tag{7.7}
$$

Thus, when ξ is the Killing vector ∂_t ($\alpha=1$, $\beta=\gamma=0$) the *relative mass*

$$
Q^{\mathrm{tot}}_{\Sigma^\epsilon_s}[\partial_t]=M-\frac{M^2}{2R} \tag{7.8}
$$

is time conserved along any foliation of the family generated by ζ, since it does not depend on the affine parameter s. We also stress that the *conserved quantity* (i.e., letting R tend to infinity) is always $Q^{\mathrm{tot}}_{\infty}[\partial_t]=M$, i.e., it reduces to the expected value for total mass.

If $\gamma\neq 0$ the vector ξ is not Killing. Despite the fact that the conserved quantity is not time conserved in general, it is still time conserved along a particular foliation [namely, the one corresponding to $\epsilon=0$, i.e., $\zeta=\partial_t$; see Fig. 2(a)]. We remark that in this case the flow of the Nöther current $\mathcal{E}[\xi]=\mathcal{E}^\mu\mathbf{ds}_\mu$ through $\partial\Sigma_s$ vanishes even if $\mathcal{E}^\mu n_\mu|_{\mathcal{B}}\neq 0$.

On the contrary, when $\epsilon\neq 0$ [see Fig. 2(b)] the Nöther charge $Q^{\mathrm{tot}}_{\Sigma^\epsilon_s}$ explicitly depends on the time s, i.e., on the particular leaf on which it is computed.

We finally remark that in any case the quantity $Q^{\mathrm{tot}}_{\Sigma^\epsilon_s}[\xi]$ given by Eq. (7.7) is covariantly conserved (as any Nöther conserved quantity is) and it consequently obeys a continuity equation.

To wrap up this first example let us now compute the quasilocal energy (5.11). We consider the case depicted in Fig. 2(a), i.e., the foliation induced by $\zeta=\partial_t$. We choose, as infinitesimal symmetry ξ, the unit timelike normal u:

$$
\xi=u=\frac{2r+M}{2r-M}\,\partial_t\,. \tag{7.9}
$$

If we calculate the Nöther conserved quantity (5.1) we now obtain the following result:

$$
\begin{aligned}
Q_{\Sigma_t}[u,g] &= \frac{1}{4}\frac{M(2R+M)}{2R-M},\\
Q_{\Sigma_t}[u,g,\bar{g}] &= \frac{1}{2}\frac{(2R^2-MR-M^2)M}{R(2R-M)},\\
Q_{\Sigma_t}[u,\bar{g}] &= \frac{1}{4}\frac{M(4R^2-M^2)}{(2R-M)^2},\\
Q^{\mathrm{tot}}_{\Sigma_t}[u] &= M+\frac{M^2}{2R}.
\end{aligned}
\tag{7.10}
$$

In spherical coordinates (t,ρ,θ,ϕ) the fourth expression of (7.10) may be rewritten as

$$
Q^{\mathrm{tot}}_{\Sigma_t}[u]=\rho_0\left[1-\sqrt{1-\frac{2M}{\rho_0}}\right], \tag{7.11}
$$

where $2R=-M+\rho_0+\sqrt{\rho_0(\rho_0-2M)}$; see (7.3). As expected, expression (7.11) perfectly agrees with the value of the energy computed in Ref. 3, formula (6.14).

Let us now consider another example of a conserved quantity in a finite region D. It is a completely different example since it does not require the matching of the solutions on the boundary $\mathcal{B}$ of the finite region under consideration. Neither is the condition of orthogonal boundaries required here.

Let us consider the Kerr space–time in ingoing Kerr–Schild coordinates (t,r,θ,ϕ), given by

$$
g=\bar{g}+2Mr\rho^{-2}[dt+dr-a\sin^2\theta\, d\phi]^2, \tag{7.12}
$$

where $\rho^2=r^2+a^2\cos^2\theta$, $M^2\geqslant a^2$. Let us choose the flat background $\bar{g}$ as

$$
\bar{g}=-dt^2+[dr-a\sin^2\theta\, d\phi]^2+\rho^2[d\theta^2+\sin^2\theta\, d\phi^2]. \tag{7.13}
$$

The metrics g and $\bar{g}$ are matched at infinity. Let us consider the regions D *inside* the hypersurface $\mathcal{B}$ defined by $r=R$ and the ADM foliation $\Sigma_t=\{t=\text{constant}\}$ generated by the vector field ∂_t. We stress that g and $\bar{g}$ do not match on $\mathcal{B}$ unless R is let to tend to infinity.

Let us finally choose as the symmetry generator the (two-parameter) vector

$$
\xi=\alpha\partial_t+\beta\partial_\phi, \tag{7.14}
$$

which is a Killing vector for both g and $\bar{g}$ (α and β are two real constants).

The Nöther conserved quantities one obtains are

$$
\begin{aligned}
Q_\Sigma[\xi,g] &= \left(\alpha\frac{M}{2}-\beta Ma\right),\\
Q_\Sigma[\xi,g,\bar{g}] &= \alpha\frac{M}{2},\\
Q_\Sigma[\xi,\bar{g}] &= 0,\\
Q^{\mathrm{tot}}_\Sigma[\xi] &= \alpha M-\beta Ma,
\end{aligned}
\tag{7.15}
$$

which reproduce the expected values of the *relative mass* and of the *angular momentum* in the region $t=$ constant and $r\leqslant R$. Notice that the result is independent of R meaning that all the energy and angular momentum is ''buried in the singularity.'' We remark that setting anywhere $a=0$ the

Schwarzschild solution is recovered. The relative mass M we obtain in this case [see Eq. (7.15) with $\alpha=1$, $\beta=0$] does not agree with the value found previously [see Eq. (7.8)] because of the two different matches selected.

We remark that the quantities (7.15) are also time conserved (even if the metrics are not matched at $\mathcal{B}$). In fact the flow integral $\int_{\mathcal{B}}\mathcal{E}$ vanishes since ξ is tangent to $\mathcal{B}$ and it is a Killing vector of both g and $\overline{g}$ (see Sec. VI). Notice also that $\mathcal{E}^{\alpha}n_{\alpha}=0$, i.e., the Nöther current has no flow through any part of $\mathcal{B}$. Consequently, the associated conserved quantity is time conserved along *any* ADM foliation of the region D.

[The calculations in this section have been carried out by using tensor package of MAPLEV, see Ref. 36. They are the very direct application of formula (5.1), just computed on the configuration $(g,\overline{g})$.]

VIII. CONCLUSION AND PERSPECTIVES

We proved that once suitable matching conditions are required (i.e., the four-metrics g and $\overline{g}$ are required to agree on the boundary of the region under consideration) the two action functionals (2.1) and (3.2) agree. Consequently the action functional (3.2) may be considered as the ADM counterpart of the covariant action functional (2.1).

The second important result achieved here is the use of the Nöther theorem to define conserved quantities in a finite region and the characterization of the quasilocal energy as the Nöther charge associated with the (timelike) unit vector normal to the leaves of the ADM foliation [see (5.11)].

These seem to be new results which should enable us to extend the analysis further ahead to the prescription for the entropy in general relativity. In fact, the quasilocal energy as well as the action functional (3.2) also appeared as the starting point of a statistically oriented approach to black hole entropy (see Refs. 17, 27, 19, 33, 20, 21, and references therein). A different approach to black hole entropy based on the Nöther approach (see Refs. 16, 23, 29, 37 and references therein) may be found in the literature. In view of the present comparison between the covariant first-order approach (which the Nöther approach is based on) and the York's action functional (which quasilocal energy is based on) as well as between the Nöther charges and the quasilocal energy themselves, we believe that the two different approaches to entropy can be now successfully compared (see also Refs. 38 and 39).

Another interesting perspective is to extend the present comparison to the more general situation of nonorthogonal boundaries which sometimes appeared in the literature (see Refs. 8–10). It would be of some interest to know whether nonorthogonality of the boundaries in the ADM decomposition of the covariant action functional (2.1) exactly produces the additional boundary terms which are derived for the (modified) York's action (see Ref. 9), as we guess to be true.

ACKNOWLEDGMENTS

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APPENDIX: NOTATION

In order to make this paper self-contained here we briefly summarize some of the formulas and expressions which are used throughout the paper. We follow the convention and notation adopted in Ref. 3 and we also refer the reader to Fig. 1 for notation.

We assume the hypersurfaces Σ_t to be spacelike and we assume the hypersurface $\mathcal{B}$ to be timelike. The metric $h_{\mu\nu}$ induced on the hypersurfaces Σ_t may be written as

$$h_{\mu\nu}=g_{\mu\nu}+u_{\mu}u_{\nu}, \tag{A1}$$

while for the metric $\gamma_{\mu\nu}$ on the hypersurface $\mathcal{B}$ we have

$$\gamma_{\mu\nu}=g_{\mu\nu}-n_\mu n_\nu \tag{A2}$$

(in the sequel Greek indices are always raised and lowered with the four-dimensional metric). The two vectors $\vec{u}$ and $\vec{n}$ denote the future directed unit normal to Σ_t and the outward pointing unit normal to the hypersurfaces $\mathcal{B}$, respectively. They satisfy the normalization relations $u^\mu u_\mu=-1$ and $n^\mu n_\mu=1$, respectively. Any space–time tensor may be projected onto the hypersurfaces Σ_t by means of the projection tensor:

$$h^\mu_\nu=\delta^\mu_\nu+u^\mu u_\nu. \tag{A3}$$

Any tensorial object may be also projected onto $\mathcal{B}$ with the projection tensor

$$\gamma^\mu_\nu=\delta^\mu_\nu-n^\mu n_\nu. \tag{A4}$$

The two-metric $\sigma_{\mu\nu}$ on the boundaries B_t is given by

$$\sigma_{\mu\nu}=\gamma_{\mu\nu}+u_\mu u_\nu=h_{\mu\nu}-n_\mu n_\nu \tag{A5}$$

and the respective projection tensor is $\sigma^\mu_\nu=g^{\mu\rho}\sigma_{\rho\nu}$.

The extrinsic curvatures $K_{\mu\nu}$ of Σ_t in M, $\Theta_{\mu\nu}$ of $\mathcal{B}$ in M and $\mathcal{K}_{\mu\nu}$ of B_t embedded in Σ_t are defined, respectively, as follows:

$$\begin{aligned} K_{\mu\nu}&=-h^\alpha_\mu\nabla_\alpha u_\nu,\\ \Theta_{\mu\nu}&=-\gamma^\alpha_\mu\nabla_\alpha n_\nu,\\ \mathcal{K}_{\mu\nu}&=-\sigma^\alpha_\mu D_\alpha n_\nu, \end{aligned} \tag{A6}$$

where D_α denotes the covariant derivative on Σ_t compatible with the metric h.

The extrinsic curvature $K_{\mu\nu}$ is a *symmetric tensor on* Σ_t, i.e., it satisfies the conditions $K_{\mu\nu}u^\mu=0$, $K_{\mu\nu}h^\mu_\rho=K_{\rho\nu}$. Instead the extrinsic curvature $\Theta_{\mu\nu}$ is a symmetric tensor on $\mathcal{B}$: $\Theta_{\mu\nu}n^\mu=0$, $\Theta_{\mu\nu}\gamma^\mu_\rho=\Theta_{\rho\nu}$, while the extrinsic curvature $\mathcal{K}_{\mu\nu}$ is a symmetric tensor on B_t, i.e., $\mathcal{K}_{\mu\nu}u^\mu=\mathcal{K}_{\mu\nu}n^\mu=0$.

We also denote by

$$\begin{aligned} a^\nu&=u^\mu\nabla_\mu u^\nu,\\ b^\nu&=n^\mu\nabla_\mu n^\nu \end{aligned} \tag{A7}$$

the (covariant) *accelerations* of the two normals u^μ and n^μ, respectively. They satisfy the orthogonality properties: $u^\mu a_\mu=0$ and $n^\mu b_\mu=0$.

By making use of the property (A4), we obtain

$$\nabla_\nu n^\mu=\delta^\alpha_\nu\nabla_\alpha n^\mu=\gamma^\alpha_\nu\nabla_\alpha n^\mu+n^\alpha n_\nu\nabla_\alpha n^\mu. \tag{A8}$$

Taking into account definitions (A6) and (A7) we have

$$\nabla_\nu n^\mu=-\Theta^\mu_\nu+n_\nu b^\mu. \tag{A9}$$

Performing calculations in the same manner for the vector u^μ, it is easy to check the analogous relation:

$$\nabla_\nu u^\mu=-K^\mu_\nu-u_\nu a^\mu. \tag{A10}$$

Moreover, projecting the indices of the extrinsic curvature $\Theta_{\mu\nu}$ normally and tangentially to the hypersurfaces Σ_t we obtain the useful formula (see Ref. 3 for detailed computations):

$$\Theta_{\mu\nu}=\mathcal{K}_{\mu\nu}+u_\mu u_\nu n_\alpha a^\alpha+2\sigma^\alpha_{(\mu}u_{\nu)}n^\beta K_{\alpha\beta}. \tag{A11}$$

[We recall that this relation is true only under the assumption of orthogonal boundaries, i.e., $u^\mu n_\mu|_{\mathcal{B}}=0$.] Contracting the latter expression with $g^{\mu\nu}$ we also easily obtain

$$\Theta=\mathcal{K}-n_\alpha a^\alpha. \tag{A12}$$

Let us now consider the ADM decomposition of the metric:

$$\begin{aligned} g=g_{\mu\nu}\,\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu&=(h_{\mu\nu}-u_\mu u_\nu)\,\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu\\ &=-N^2\,\mathrm{d}t^2+h_{ab}(\mathrm{d}x^a+N^a\,\mathrm{d}t)\otimes(\mathrm{d}x^b+N^b\,\mathrm{d}t). \end{aligned} \tag{A13}$$

The coordinate system $(x^\mu)=(t,x^a)=(t,r,x^A)$ is adapted both to $\mathcal{B}$ and to the ADM foliation on D. The surfaces Σ_t are surfaces of constant t while $\mathcal{B}$ is the hypersurface of constant r. In other words, indices $a,b,c,\ldots$ run from 1 to 3 and denote indices on the spacelike hypersurfaces Σ_t, while indices $A,B,C,\ldots$ run from 2 to 3 and they instead denote indices on the boundary B_t of Σ_t. Hence, tensors on Σ_t are labeled by early Roman letters $a,b,\ldots$. When they are considered as tensors on space–time M the same tensors are instead denoted by Greek letters. For example, the extrinsic curvature K in (A6) can be denoted as $K_{\mu\nu}$ or K_{ab}, according to notational convenience.

The unit normal is given by $(u_\mu)=(-N,0,0,0)$ while the timelike coordinate vector field $\vec{\partial}_0=\partial/\partial t$ reads as $\vec{\partial}_0=N\vec{u}+\vec{N}$, N being the lapse function and $\vec{N}=(N^\mu)=(0,N^a)$ the spatial shift vector: $\vec{N}\cdot\vec{u}=N^\mu u_\mu=0$ (we remind the reader that if we also assume the vector field $\vec{\partial}_0$ be tangent to the three-dimensional hypersurface $\mathcal{B}$, the orthogonal boundary conditions reads as $\vec{N}\cdot\vec{n}|_{\mathcal{B}}=N^\mu n_\mu|_{\mathcal{B}}=0$. Nevertheless this latter hypothesis will be not relevant for the computations in the rest of this Appendix). The extrinsic curvature $K_{\mu\nu}$ and the acceleration a^μ defined in (A6) and (A7), respectively, read as

$$\begin{aligned} K_{ab}&=-N\Gamma^0_{ab}=\frac{1}{2N}[-\partial_0 h_{ab}+D_aN_b+D_bN_a],\\ (a^\mu)&=(0,a^b)=\left(0,\frac{\partial^b N}{N}\right). \end{aligned} \tag{A14}$$

(Roman indices are here raised and lowered with the three-metric h_{ab}.)

The Levi-Civita connection coefficients are given by

$$\begin{aligned} \Gamma^0_{0a}&=\frac{1}{N}(\partial_a N-N^bK_{ba}),\\ \Gamma^0_{ab}&=-\frac{K_{ab}}{N},\\ \Gamma^0_{00}&=\frac{\partial_0 N}{N}+\frac{N^b}{N}\partial_b N-\frac{N^aN^b}{N}K_{ab},\\ \Gamma^a_{b0}&=-NK^a_b+\frac{N^aN^c}{N}K_{cb}+D_bN^a-\frac{N^a}{N}\partial_b N,\\ \Gamma^a_{bc}&={}^3\Gamma^a_{bc}+\frac{N^a}{N}K_{bc} \end{aligned} \tag{A15}$$

(where ${}^3\Gamma^a_{bc}$ denotes the Levi-Civita connection of the three-metric h_{ab}). A similar splitting may be performed with the background metric $\overline{g}$; we obviously obtain the same relations by replacing the objects involved with the corresponding barred ones. By means of formula (A15) one may easily compute the quantities $u^\mu_{\alpha\beta}=\Gamma^\mu_{\alpha\beta}-\delta^\mu_{(\alpha}\Gamma^\epsilon_{\beta)\epsilon}$. For example, one can verify the following:

$$g^{\mu\nu}u^0_{\mu\nu}=-\frac{2}{N}K^a_a+\frac{1}{N^2}\partial_a N^a \tag{A16}$$

and

$$g^{\mu\nu}\overline{u}^0_{\mu\nu}=\overline{K}_{ab}\left[\frac{1}{N^2\overline{N}}(\overline{N}^a-N^a)(\overline{N}^b-N^b)-\frac{1}{N}\left(\frac{\overline{N}}{N}\overline{h}^{ab}+\frac{N}{\overline{N}}h^{ab}\right)\right]$$
$$-\frac{1}{\overline{N}N^2}(\overline{N}^a-N^a)\partial_a\overline{N}+\frac{1}{N^2}\partial_a\overline{N}^a+\frac{\overline{N}^b}{N^2}{}^3\overline{\Gamma}^a_{ab}-\frac{N^b}{N^2}{}^3\overline{\Gamma}^a_{ab}, \tag{A17}$$

which together give

$$g^{\mu\nu}w^\alpha_{\mu\nu}u_\alpha=g^{\mu\nu}(u^\alpha_{\mu\nu}-\overline{u}^\alpha_{\mu\nu})u_\alpha=-Ng^{\mu\nu}(u^0_{\mu\nu}-\overline{u}^0_{\mu\nu}). \tag{A18}$$

The latter term is involved in the contribution on the lids of the boundary term in the action functional (2.1). To evaluate instead the action functional contribution on the hypersurface $\mathcal{B}$ we have to make use of the adapted splitting of the metric:

$$g=g_{\mu\nu}\,\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu=(\gamma_{\mu\nu}+n_\mu n_\nu)\mathrm{d}x^\mu\otimes\mathrm{d}x^\nu$$
$$=V^2\,\mathrm{d}r^2+\gamma_{ij}(\mathrm{d}x^i+V^i\,\mathrm{d}r)\otimes(\mathrm{d}x^j+V^j\,\mathrm{d}r), \tag{A19}$$

where $(x^i)=(t,x^A)$. Middle Roman letters $i,j,k,\ldots$ denote indices on the timelike hypersurface $\mathcal{B}$ while x^A $(A=2,3)$ again denote the coordinates over the two-dimensional surfaces B_t. The function V is the *radial lapse* while V^i is the *radial shift*. Hence the unit, outward pointing, radial normal $\vec{n}$ reads as $\vec{n}=(1/V)[\vec{\partial}_r-V^i\vec{\partial}_i]$. The extrinsic curvature Θ_{ij} of the ''cylinder'' $\mathcal{B}=\{r\ \text{constant}\}$ is given by

$$\Theta_{ij}=V\Gamma^r_{ij}=\frac{1}{2V}[-\partial_r\gamma_{ij}+\mathcal{D}_iV_j+\mathcal{D}_jV_i], \tag{A20}$$

where $\mathcal{D}_i$ denotes the covariant derivative on $\mathcal{B}$ induced by the Levi-Civita connection ${}^3\Gamma^i_{jk}$ of the three-metric γ_{ij}. The coefficients of the four-dimensional Levi-Civita connection can now be decomposed as

$$\Gamma^r_{ri}=\frac{1}{V}(\partial_iV+V^j\Theta_{ji}),$$

$$\Gamma^r_{ij}=\frac{\Theta_{ij}}{V},$$

$$\Gamma^r_{rr}=\frac{1}{V}\partial_rV+\frac{V^i}{V}\partial_iV+\frac{V^iV^j}{V}\Theta_{ij}, \tag{A21}$$

$$\Gamma^i_{jr}=-V\Theta^i_j-\frac{V^iV^k}{V}\Theta_{kj}+\mathcal{D}_jV^i-\frac{V^i}{V}\partial_jV,$$

$$\Gamma^i_{jk} = {}^3\Gamma^i_{jk} - \frac{V^i}{V}\Theta_{jk}.$$

The latter expressions are not simply obtained from (A15) by exchanging tensors on Σ_t with the corresponding tensors on $\mathcal{B}$. Because the metrics h_{ab} and γ_{ij} have different signatures, a change of sign may appear in some terms of (A21) if compared with the decomposition (A15).

By means of (A21), the following expressions are then easily computed:

$$\begin{aligned} g^{\mu\nu}u^r_{\mu\nu} &= \frac{2}{V}\Theta^i_i - \frac{1}{V^2}\partial_i V^i, \\ g^{\mu\nu}\overline{u}^r_{\mu\nu} &= \overline{\Theta}_{ij}\left[\frac{1}{V^2\overline{V}}(\overline{V^i}-V^i)(\overline{V^j}-V^j) + \frac{1}{V}\left(\frac{\overline{V}}{V}\overline{\gamma}^{ij} + \frac{V}{\overline{V}}\gamma^{ij}\right)\right] \\ &\quad + \frac{1}{\overline{V}V^2}(\overline{V^i}-V^i)\partial_i\overline{V} - \frac{1}{V^2}\partial_i\overline{V^i} - \frac{\overline{V^j}}{V^2}{}^3\overline{\Gamma}^i_{ij} + \frac{V^j}{V^2}{}^3\overline{\Gamma}^i_{ij}. \end{aligned} \tag{A22}$$

Expressions (A22) gives

$$g^{\mu\nu}w^\alpha_{\mu\nu}n_\alpha = g^{\mu\nu}(u^\alpha_{\mu\nu} - \overline{u}^\alpha_{\mu\nu})n_\alpha = Vg^{\mu\nu}(u^r_{\mu\nu} - \overline{u}^r_{\mu\nu}), \tag{A23}$$

which is the contribution on $\mathcal{B}$ of the boundary term in the action functional (2.1).

We stress that in (A18) and (A23) computations are performed without any hypothesis of orthogonal boundaries and without requiring any matching conditions between the metric g and its background $\overline{g}$.

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Far field behavior of noncompact static spherically symmetric solutions of Einstein SU(2) Yang Mills equations

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There exist static spherically symmetric solutions of the Einstein equations with cosmological constant Λ coupled to the SU(2) Yang Mills equations that are smooth at the origin $r=0$ and with a horizon which can be transformed away with a change of coordinates in which the radius increases across the singularity. We establish the global behavior of these solutions. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1287918]

I. INTRODUCTION

Reference 1 analyzes spherically symmetric static solutions of the Einstein SU(2) Yang Mills equations with small positive cosmological constant that are smooth at the origin of spherical symmetry. In particular, it is proven that the presence of a positive cosmological constant Λ causes each such solution to give rise to a horizon at some $r_c \leqslant \sqrt{3/\Lambda}$. For small Λ a class of solutions was found in which this singularity is only due to choice of Schwarzschild coordinates and can be transformed away with a Kruskal-type change of coordinates in such a way that r increases in the extended solution. Furthermore, the Yang Mills curvature is well behaved under the change of coordinates. In this paper we prove that such solutions are defined globally in Schwarzschild coordinates and that the solutions (except for the one coordinate singularity) are everywhere smooth. We also determine their asymptotic behavior.

With a spherical symmetric metric

$$ds^2 = C^2 A\, dt^2 - \frac{1}{A} dr^2 - r^2\, d\Omega^2 \tag{1-1}$$

($d\Omega^2 = d\phi^2 + \sin^2\phi\, d\theta^2$, the standard metric on the unit 2-sphere) and spherically symmetric connection on an SU(2) bundle,

$$\omega = a(r,t)\tau_3\, dt + b(r,t)\tau_3\, dr + w(r,t)\tau_2\, d\phi + (\cos\phi\tau_3 - w(r,t)\sin\phi\tau_1)\, d\theta, \tag{1-2}$$

the Einstein–Yang Mills equations take the form of three ordinary differential equations for the coefficients A, C, and w,

$$rA' + 2Aw'^2 = 1 - A - \frac{(1-w^2)^2}{r^2} - \Lambda r^2, \tag{1-3}$$

$$r^2 A w'' + r\left(1 - A - \frac{(1-w^2)^2}{r^2} - \Lambda r^2\right) w' + w(1-w^2) = 0, \tag{1-4}$$

and

$$rC' = 2w'^2 C. \tag{1-5}$$

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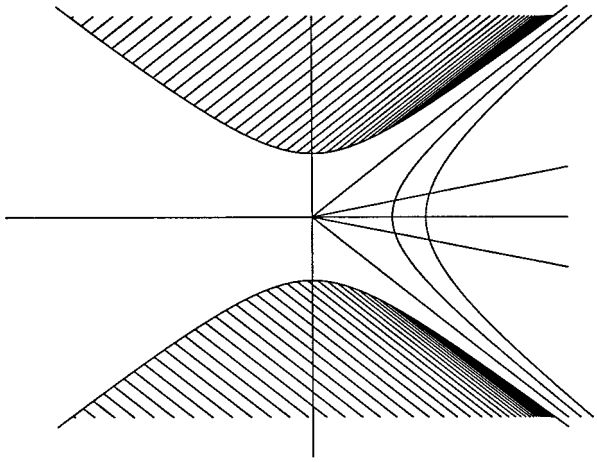

FIG. 1. Space–time geometry near $r=r_h$. The space–time manifold M is the unshaded region. The hyperbolas are curves of constant r and the rays through the origin are curves of constant t. The rays at angles $\pm 45°$ represent $t=\pm\infty$, respectively. The hyperbola for $r=r_h$ degenerates to the point at the origin.

The τ_i in Eq. (1-2) are the following matrices which form a basis of SU(2):

$$\tau_1=i/2\begin{bmatrix}0 & -1\\ -1 & 0\end{bmatrix},\quad \tau_2=i/2\begin{bmatrix}0 & i\\ -i & 0\end{bmatrix},\quad \tau_3=i/2\begin{bmatrix}-1 & 0\\ 0 & 1\end{bmatrix}.$$

By appropriate change of gauge, one of a and b can be made to vanish. We assume that in this gauge, the other vanishes too.

There are known explicit solutions to Eqs. (1-3)–(1-5). Among these is the Schwarzchild–deSitter metric with constant Yang Mills connection

$$ds^2=\left(1-\frac{\Lambda r^2}{3}\right)dt^2-\left(1-\frac{\Lambda r^2}{3}\right)^{-1}dr^2-r^2\,d\Omega^2,\quad w\equiv 1. \tag{1-6}$$

This solution is defined for all r and is smooth except at the horizon which occurs on the sphere $r=r_h=\sqrt{3/\Lambda}$, and serves as a prototype of solutions which have the following characteristic:

$$\lim_{r\nearrow r_h} w^2(r)<\infty \quad\text{and}\quad \lim_{r\nearrow r_h} A'(r)<0. \tag{1-7}$$

We call solutions that satisfy Eq. (1-7) *noncompact*. For such solutions, a change in coordinates (t,r) to new coordinates (u,v) can be found that transforms the metric (1-1) to

$$ds^2=g(u,v)(du^2-dv^2)-r^2(u,v)\,d\Omega^2, \tag{1-8}$$

such that $g\neq 0$ in a neighborhood of the singularity at r_h.[2,3] Constant r and t curves are shown in Fig. 1.

II. GLOBAL BEHAVIOR

We now prove that any solution of Eqs. (1-3)–(1-5) that satisfies Eq. (1-7) behaves qualitatively like the solution (1-6); namely, the solution is defined and smooth for all $r\neq r_h$, the metric approaches the metric (1-6) as $r\nearrow\infty$, and the Yang Mills connection approaches a finite w_∞ asymptotically as $r\nearrow\infty$.

Because the singularity at r_h of such a solution is only a coordinate singularity and because of condition (1-7), the solution $(A(r),w(r),C(r))$ can be extended to some $\rho>r_h$. We define ρ to be the largest value for which the solution is valid and such that $A(r)<0$ for all $r\in(r_h,\rho)$.

We now define the function

$$h(r)=(1-w^2)^2-2r^2Aw'^2. \tag{2-1}$$

The global smoothness and asymptotic behavior of w, A and C will follow from the following:

Lemma 2.1: $\lim_{r\nearrow\rho}h(r)$ *exists and is finite.*

Proof: A simple calculation yields

$$h'(r)=2rw'^2(\Phi+2Aw'^2-2A), \tag{2-2}$$

where

$$\Phi(r)=1-A-\frac{(1-w^2)^2}{r^2}-\Lambda r^2. \tag{2-3}$$

To simplify notation, we define

$$k(r)=\frac{\Phi+2Aw'^2-2A}{r}, \tag{2-4}$$

and rewrite Eq. (2-2) as

$$h'=2r^2w'^2k. \tag{2-5}$$

Another routine calculation yields

$$r^2k'+2r(w'^2+1)k+2p=0, \tag{2-6}$$

where

$$p=1-\frac{2(1-w^2)^2}{r^2}-2Aw'^2. \tag{2-7}$$

Clearly, since $r_h>1/\sqrt{\Lambda}$ and $A(r_h)=0$,

$$k(r_h)=\frac{\Phi(r_h)}{r_h}<0. \tag{2-8}$$

We claim, furthermore, that $k<0$ for all $r\in(r_h,\rho)$. For otherwise, let $\tilde{r}$ be the smallest $r\in(r_h,\rho)$ that satisfies

$$k(\tilde{r})=0. \tag{2-9}$$

Equations (2-5) and (2-1) imply

$$h(r)<h(r_h)<1 \text{ for all } r\in[r_h,\tilde{r}]; \tag{2-10}$$

in particular, $(1-w^2(\tilde{r}))^2<1$ and since $\tilde{r}>\sqrt{2}$,

$$\left[\frac{2(1-w^2)^2}{r^2}\right]_{r=\tilde{r}}<1. \tag{2-11}$$

Therefore,

$$p(\tilde{r})>0. \tag{2-12}$$

Now, on the one hand, from Eqs. (2-6), (2-9), and (2-12) it follows that

$$k'(\tilde{r})<0. \tag{2-13}$$

On the other hand, because of Eq. (2-8) and the definition of $\tilde{r}$, we must have

$$k'(\tilde{r})\geqslant 0. \tag{2-14}$$

Since both Eqs. (2-13) and (2-14) cannot hold, there can be no $\tilde{r}$ that satisfies Eq. (2-9). This establishes the claim. Since $h>0$ for all $r\in(r_h,\rho)$, the Lemma follows. ■

We shall prove that $\rho=\infty$. Assuming this, we have the following:

Corollary 2.1: $A\sim-\Lambda r^2/3$.

Proof: Lemma 2.1 implies that $\lim_{r\nearrow\infty}[(1-w^2)^2/r+2rAw'^2](r)=0$. Equation (1-3) then gives, for any $\epsilon>0$, an $\bar{r}$ such that

$$|1-\Lambda r^2-(rA)'|<\frac{\epsilon}{r} \tag{2-15}$$

whenever $r>\bar{r}$. Integrating Eq. (2-15) from $\bar{r}$ to any $r>\bar{r}$ implies

$$\left|1-\frac{\Lambda r^2}{3}+\frac{c}{r}-A\right|<\frac{\epsilon\ln r}{r} \tag{2-16}$$

(c is a constant of integration). The result follows upon taking the limit as $r\nearrow\infty$. ■

Corollary 2.2: $\lim_{r\nearrow r_h}w'(r)=0$ *and* $\lim_{r\nearrow r_h}w(r)$ *exists and is finite.*

Corollary 2.3: $\lim_{r\nearrow\infty}C(r)$ *exists and is finite.*

Proof: Choosing $C(0)=1$ and integrating Eq. (1-5) gives

$$C(r)=e^{\int_0^r 2w'^2(s)/s\,ds}. \tag{2-17}$$

From Eq. (2-17) it is clear that $\lim_{r\nearrow\infty}C(r)$ exists although, *a priori*, it might be infinite. Lemma 2.1 and Corollary 2.1 imply $w'^2\sim r^{-4}$. Consequently,

$$\int_0^\infty\frac{2w'^2}{r}<\infty.$$

■

Substituting corollaries (2.1) and (2.2) into Eq. (1-1) and scaling t by a factor of $[\lim_{r\nearrow\infty}C(r)]^{-1}$ yields a metric that is asymptotic to Eq. (1-6). It is also clear that the Yang Mills field vanishes as $r\nearrow\infty$.

It remains to prove the following:

Theorem I: $\rho=\infty$.

Proof: From Lemma 2.1 it follows that $\overline{\lim}_{r\nearrow\rho}w^2(r)<\infty$. Substituting this into Eq. (1-3) gives $\lim_{r\nearrow\rho}A'(r)>-\infty$. Thus, $\lim_{r\nearrow\rho}A(r)$ exists. Standard results now imply $\rho<\infty$ only if one of the following holds:

(1) $A(\rho)=0$,
(2) $\underline{A(\rho)}<0$ and $\overline{\lim}_{r\nearrow\rho}w'^2(r)=\infty$, or
(3) $\overline{\lim}_{r\nearrow\rho}w'^2(r)<\infty$ and $\underline{\lim}_{r\nearrow\rho}A'^2(r)=\infty$.

We now eliminate all three possibilities.

Case 1. We first claim that

$$\lim_{r\nearrow\rho}Aw'^2(r)\ \text{ exists and is finite.} \tag{2-18}$$

Clearly, $Aw'^2 \leqslant 0$ in the interval $[r_h, \rho]$; i.e., Aw'^2 is bounded from above. It suffices to prove that near ρ, $(Aw'^2)'$ is bounded also from below.

Now, because $\lim_{r \nearrow \rho} A(r) = 0$ and $r_h > 1/\sqrt{\Lambda}$, there exist $\epsilon > 0$ and $\delta > 0$ such that $\Phi < -\epsilon$, and consequently,

$$\Phi + 2Aw'^2 < -\epsilon, \quad \text{whenever} \quad r \in (\rho - \delta, \rho). \tag{2-19}$$

Also, Lemma 2.1 implies the existence of $M > 0$ such that $w < M$. For arbitrary constant β, we obtain easily from Eqs. (1-3) and (1-4) the following equation:

$$r^2(Aw'^\beta)' + rw'^\beta[(\beta - 1)\Phi + 2Aw'^2] + \beta w w'^{\beta - 1}(1 - w^2) = 0. \tag{2-20}$$

With $\beta = 2$, this becomes Eq. (2-21):

$$r^2(Aw'^2)' + rw'^2[\Phi + 2Aw'^2] + 2ww'(1 - w^2) = 0. \tag{2-21}$$

From Eq. (2-21) and inequality (2-19) it follows that

$$(Aw'^2)' \geqslant \frac{3M(1 - M^2)}{\rho^2} \tag{2-22}$$

whenever $w'^2 \leqslant 1$ and $r \in (\rho - \delta, \rho)$. Also, whenever $w'^2 > 1$ and $r \in (\rho - \delta, \rho)$,

$$(Aw'^2)' > \frac{w'}{r^2}[r\epsilon w' - 2M(1 - M^2)]. \tag{2-23}$$

It is clear from inequalities (2-22) and (2-23) that $(Aw'^2)'$ is bounded from below. This establishes (2-18).

To eliminate this case, we note that on the one hand, $\lim_{r \nearrow \rho} Aw'^2(r) < 0$. Indeed, if $\lim_{r \nearrow \rho} Aw'^2(r) = 0$, then Eq. (1-3) would give

$$\overline{\lim}_{r \nearrow \rho}(rA)' = \overline{\lim}_{r \nearrow \rho} \Phi(r) \leqslant \lim_{r \nearrow \rho}(1 - \Lambda r^2) < 0.$$

However, because $rA < 0$ throughout the interval (r_h, ρ) and $A(\rho) = 0$, we must have $\overline{\lim}_{r \nearrow \rho}(rA)'(r) \geqslant 0$.

On the other hand, the assumption $\lim_{r \nearrow \rho} Aw'^2(r) < 0$ leads to a contradiction. Indeed, since $\lim_{r \nearrow \rho} A(r) = 0$, we must have

$$\lim_{r \nearrow \rho} w'^2(r) = \infty.$$

The invariance of Eqs. (1-3) and (1-4) under the transformation $w \mapsto -w$ allows us to assume, without any loss of generality, that $\lim_{r \nearrow \rho} w'(r) = +\infty$. We next consider Eq. (2-20) with $\beta = 3$ to obtain

$$r^2(Aw'^3)' + rw'^3(2\Phi + 2Aw'^2) + 3ww'^2(1 - w^2) = 0. \tag{2-24}$$

Near ρ, $\Phi < 0$ and thus

$$2\Phi + 2Aw'^2 < \lim_{r \nearrow \rho} Aw'^2(r) < -c < 0$$

for some $c > 0$. Also, Lemma 2.1 implies w is bounded. These facts imply that in Eq. (2-24) the second term on the left dominates the third term on the same side. It follows that

$$\lim_{r\nearrow\rho}(Aw'^3)'=+\infty. \tag{2-25}$$

However, $\lim_{r\nearrow\rho}Aw'^2(r)<0$ implies that $\lim_{r\nearrow\rho}Aw'^3=-\infty$. Therefore

$$\underline{\lim}_{r\nearrow\rho}(Aw'^3)'(r)=-\infty.$$

But this contradicts Eq. (2-25). This eliminates Case 1.

Case 2. Without any loss of generality, we assume that

$$\overline{\lim}_{r\nearrow\rho}w'(r)=+\infty \quad \text{and} \quad \lim_{r\nearrow\rho}A(r)<0.$$

Thus, there exists a sequence $\{r_n\}\nearrow\rho$ such that $\lim_{n\to\infty}(Aw')(r_n)=-\infty$ and $\lim_{n\to\infty}(Aw')'=-\infty$. Equation (2-20) with $\beta=1$ gives

$$r^2(Aw')'+2rw'^2(Aw')+w(1-w^2)=0. \tag{2-26}$$

Evaluating Eq. (2-26) at r_n implies $\lim_{n\to\infty}w(r_n)=-\infty$. We claim that

$$\lim_{r\nearrow\rho}w(r)=-\infty. \tag{2-27}$$

For if not, then there exist $c>0$ and a sequence $\{s_n\}\nearrow\rho$ such that $w(s_n)>-c$, $2s_nAw'^3(s_n)\nearrow+\infty$, and $(Aw')'(s_n)>0$. This in turn implies that, for sufficiently large n,

$$[r^2(Aw')'+2rAw'^3+w(1-w^2)]_{r=s_n}>0,$$

contradicting Eq. (2-26). This establishes Eq. (2-27).

Similarly, we assert that

$$\underline{\lim}_{r\nearrow\rho}w'(r)\geqslant 0.$$

For otherwise, there exists a sequence $\{t_n\}\nearrow\rho$ such that $Aw'(t_n)>0$ and $(Aw')'(t_n)>0$. Now,

$$[r^2(Aw')'+2rAw'^3+w(1-w^2)]_{r=t_n}>0$$

which also contradicts Eq. (2-26).

Since $\lim_{r\nearrow\rho}w(r)=-\infty$ implies $\lim_{r\nearrow\rho}w'(r)<0$, Case 2 is impossible.

Case 3. Equation (1-3) gives $M>\overline{0}$ such that

$$(rA)'=1-\frac{(1-w^2)^2}{r^2}-\Lambda r^2-2Aw'^2>-M$$

throughout the interval (r_h,ρ). It follows that $\lim_{r\nearrow\rho}(rA)$, and thus, also $\lim_{r\nearrow\rho}A(r)$ exist and are finite provided $\rho<\infty$. Now, Eq. (1-3), written as

$$A'=\frac{1}{r}\left[1-\frac{(1-w^2)^2}{r^2}-\Lambda r^2-2Aw'^2\right],$$

shows that in the finite interval $[r_h,\rho)$ A' is bounded on both sides. ■

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Scattering on graphs and one-dimensional approximations to *N*-dimensional Schrödinger operators

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In the present article we develop the spectral analysis of Schrödinger operators on lattice-type graphs. For the basic example of a cubic periodic graph the problem is reduced to the spectral analysis of certain regular differential operators on a fundamental star-like subgraph with a selfadjoint condition at the central node and quasiperiodic conditions at the boundary vertices. Using an explicit expression for the resolvent of lattice-type operator we develop in the second section appropriate Lippmann–Schwinger techniques for the perturbed periodic operator and construct the corresponding scattering matrix. It serves as a base for the approximation of the multi-dimensional Schrödinger operator by a one-dimensional operator on the graph: in the third section of the paper for given N-dimensional Schrödinger operators with rapidly decreasing potential we construct a lattice-type operator on a cubic graph embedded into $\mathbf{R}^N$ and show that the original N-dimensional scattering problem can be approximated in a proper sense by the corresponding scattering problem for the perturbed lattice operator.
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I. INTRODUCTION

Modern interest in spectral properties of Schrödinger operators on graphs and corresponding scattering problems arises from the natural expectation that a dense lattice may serve as a natural approximation for the corresponding solid body. This basic idea is intensely exploited when constructing approximate solutions of partial differential equations on *zero-dimensional* meshes.[1]

From a geometrical point of view, graphs are *one-dimensional* objects, but they have new interesting properties, which distinguish one-dimensional Schrödinger operators on graphs from one-dimensional Schrödinger operators on finite and infinite intervals. One property is the absence of a ''global'' solution of the Cauchy problem. Still we may describe the whole set of solutions of the corresponding homogeneous differential equation on a graph as a *spline* of solutions of local Cauchy problems for ordinary differential equations on edges. But now the whole structure of the finite-dimensional subspace of solutions of the homogeneous equation depends on the *topology* of the graph. Hence we see that Schrödinger operators on graphs have interesting mathematical structures which take an intermediate position between ordinary and partial differential equations. On the other hand, this makes them a useful tool for mathematical modeling and for a study of real physical systems, like nanowires, thin waveguides and networks. This is the reason of recent

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interest in differential operators on graphs, both for pure mathematics[2–12] and applications.[13–18]

In the present article we study cubic lattice type graphs in $\mathbf{R}^N$. Lattice type graphs are periodic infinite graphs with no infinite edges. Our main objective is to study the possibility of an approximation of high-dimensional Schrödinger dynamics by corresponding dynamics on lattice-type graphs. One-dimensional geometry of graphs makes the spectral analysis and solution of scattering problems essentially less difficult than in high-dimensional systems. On the other hand, the *partial discretization* of the problem obtained by replacing the differential equation on the multi-dimensional space by the corresponding problem for an ordinary differential operator on the lattice-type graph, may serve not only for the aims of computing with use of the corresponding *one-dimensional* (or, generally, *multi-dimensional*) *meshes* viewed as approximations of domains of the original space, but also for qualitative modeling of spectral properties of the original multi-dimensional Schrödinger operator. This modeling is more natural, due to the continuous nature of graphs, compared with discrete zero-dimension lattice approximations of high-dimensional domains[19,20] normally used for the construction of approximate solutions of partial differential equations.

The article is organized as follows. In Sec. II we consider the Schrödinger operator on a periodic cubic lattice graph in $\mathbf{R}^N$. We would like to notice that we generalize results of Exner, who studied[9] the Schrödinger operator on a cubic lattice type graph in $\mathbf{R}^2$. We derive the dispersion equation and explicit expressions for Bloch waves, for the resolvent kernel and obtain the Krein's formula for the finitely perturbed periodic lattice. In Sec. III we consider the Schrödinger operator $H=-\Delta+V(\mathbf{X})$ in Euclidean space $\mathbf{R}^N$ supplied with the cubic lattice-type graph Γ with edges of the length $2a$. For given H we construct a family of Schrödinger operators $L^{(a)}$ on Γ which have the following property: the restrictions of the solutions of the equation $H\mathcal{U}=\lambda\mathcal{U}+F$ onto the lattice Γ are asymptotically close to the solutions of the equation $L^{(a)}u=\lambda u+F|_\Gamma$ when $a\to 0$. We construct an effective equation for the resolvent of the operator $L^{(a)}$ and prove that it is of the Hilbert–Schmidt type, thus allowing for a straightforward numerical solution by iterative methods. Finally we compare the scattering matrix for the operators $L^{(a)}$ on the graph Γ with the scattering matrix of the original N-dimensional operator H.

II. ONE-BODY PROBLEM ON CUBIC LATTICE-TYPE GRAPHS

A. Periodic cubic graph in $\mathbf{R}^N$

In this section we consider a periodic cubic graph Γ in Euclidean space $\mathbf{R}^N$. We assume that the edges of the graph are parallel to the vectors of a fixed orthogonal and normalized basis $\{e_i\}$, $i=1,2,\ldots,N$. If each edge of the graph has length $2a$, then the whole graph may be produced by shifts of a fragment Ω_a of the graph Γ (see Fig. 1) which is called a fundamental subgraph (the fundamental domain of the subgroup of all translations in the basic directions by distances multiple of $2a$):

$$\Omega_a := \{-a<x_s<a,\ \ s=1,2,\ldots,N\}.$$

Denoting by μ the Lebesgue measure on Γ we may consider the Hilbert Space $\mathcal{H}=L_2(\Gamma)$ of all square-integrable functions on Γ. It is clear that $\mathcal{H}$ may be interpreted as an orthogonal sum of a countable number of copies of $L_2(\Omega_a)$:

$$\mathcal{H}=L_2(\Gamma)=l_2(\mathbf{Z}^2,L_2(\Omega_a)).$$

In accordance with the last decomposition any function $u(X)\in\mathcal{H}$ may be represented as a function of two variables: the discrete variable $\mathbf{m}$ which numerates the tiles $\Omega_{a,\mathbf{m}}$ of all discrete translations (multiple to $2a$) of the fundamental subgraph Ω_a, and the inner coordinate x which defines the position of the point inside the given tile:

$$u(X)=u(x,\mathbf{m}),\quad \text{if}\quad X=2a\sum_{i=1}^{N} m_i e_i+x,$$

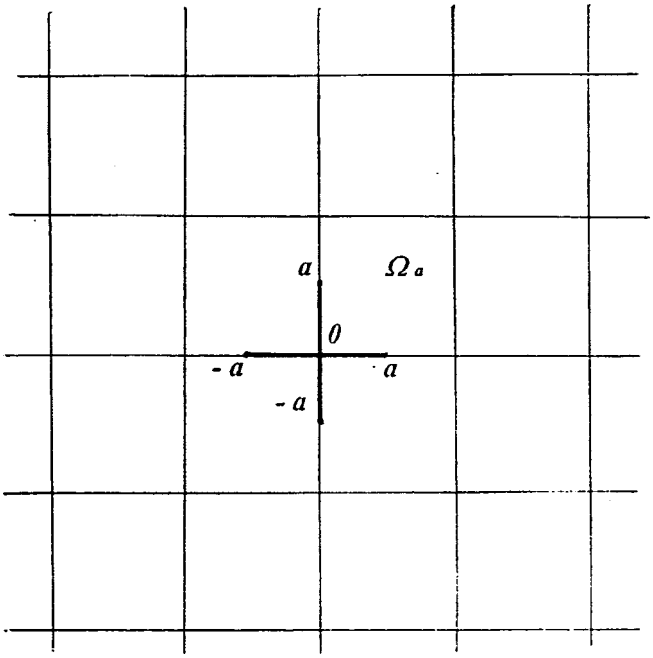

FIG. 1. Cubic lattice type graph Γ_a and its fundamental subgraph Ω_a in $\mathbf{R}^2$.

$$x=\{x_i\}_{i=1}^N, \quad -a<x_i<a; \quad \mathbf{m}=\{m_i\}_{i=1}^N \in \mathbf{Z}^N.$$

We introduce the differential operator L_γ acting in the Hilbert space $\mathcal{H}$ on smooth functions as a second order differentiation in basic direction e_i on each edge parallel to e_i.

$$L_\gamma u=-\frac{d^2u}{dx^2}.$$

One may easily check that this operator is symmetric on the domain of all smooth functions with compact support submitted to the following boundary condition at each node $\mathbf{m}$ $:=(2am_1,2am_2,2am_3,\ldots 2am_n)$:

$$\begin{gathered} u(\mathbf{m}\pm 0e_i)=u(\mathbf{m}\pm 0e_k):=u(\mathbf{m}), \quad 1\leqslant i,k\leqslant N, \\ \sum_{i=1}^N \left[\frac{du}{dx_i}(\mathbf{m}+0e_i)-\frac{du}{dx_i}(\mathbf{m}-0e_i)\right]:=[u'](\mathbf{m})=\gamma(\mathbf{m})u(\mathbf{m}), \end{gathered} \tag{1}$$

where $\gamma(\mathbf{m})=\overline{\gamma}(\mathbf{m})$. One may also easily check, using the strong subordination condition and embedding theorems, that for each *bounded sequence* $\gamma(\mathbf{m})$ the closure of the operator L_γ is a self-adjoint operator in $\mathcal{H}$ defined on the orthogonal sum of the Sobolev spaces W_2^2 on the edges submitted to the above boundary condition (1) at the nodes of the lattice. Our next aim is to explore the spectral structure of L_γ in the simplest case when the function γ is constant: $\gamma(\mathbf{m})=\gamma$. We do it for general N, but for the convenience of the reader we supply some figures for the simplest nontrivial case $N=2$. In this case the infinite graph Γ is represented by a square lattice of nodes each one connected with four neighbors (see Fig. 1). The internode distance is $2a$. This graph can be represented in the form (1) where the fundamental subgraph Ω_a shown in Fig. 1 is a union of four branches $(0,\pm ae_i):=\Omega_a^{i,\pm}$ with a common origin. In this case the total number of edges attached to each node is equal to $2N=4$.

The periodic self-adjoint operator L_γ is singular. Following Gelfand's approach[21] we reduce the construction of the spectral decomposition for it to an analysis of the regular Sturm–Liouvilles problem for the operator L_γ^P on the fundamental subgraph Ω_a:

$$L_\gamma^P u := -\frac{d^2}{dx^2}\Xi_\lambda^P = \lambda \Xi_\lambda^P,$$

with the boundary condition (1) at the node and special quasiperiodic conditions at the ends of branches of Ω_a^s fixed by the vector parameter $P=(p_1,p_2,\ldots,p_s,\ldots,p_N)$. We call this vector parameter varying on N-dimensional torus $\mathbf{T}^N$ a *quasimomentum* and write down the boundary conditions as

$$\Xi_\lambda^P(\mathbf{m}+ae_s)=e^{ip_s}\Xi_\lambda^P(\mathbf{m}-ae_s), \quad -\pi<p_s<\pi, \quad s=1,2,3,\ldots,N. \tag{2}$$

The operator L_γ may be represented as

$$L_\gamma = \int_{\mathbf{T}^N} \oplus L_\gamma^P d^N P,$$

which reduces the spectral analysis of operator L_γ to the spectral analysis of the operators L_γ^P.

Lemma 1: For any quasimomentum P the spectrum σ_γ^P of the operator L_γ^P is real, discrete and bounded from below. It has multiplicity one for almost all P. The eigenvalues $\lambda=k^2$ may be calculated as the roots of the transcendental equation,

$$\sum_{s=1}^{N} \cos p_s + \frac{\gamma \sin 2ka}{2k} = N\cos 2ka. \tag{3}$$

The components of the eigenfunctions on the branches of the fundamental subgraph may be constructed in the form

$$\Xi_\lambda^P := \sum_{s=1}^{N} \oplus \Xi_\lambda^{p_s}, \quad \Xi_\lambda^{p_s}(x_s)=\frac{G_\lambda^{p_s}(x_s,0)}{G_\lambda^{p_s}(0,0)}, \quad s=1,2,3,\ldots,N, \tag{4}$$

where $G_\lambda^{p_s}(x,y)$ is the Green's function of the one-dimensional quasiperiodic problem [integral kernel of the resolvent $(L_\gamma^P-\lambda)^{-1}$] on the s-branch Ω_s of the fundamental subgraph $-a<x_s<a$. Then

$$G_\lambda^p(0,0)=\frac{\sin ka}{2k(\cos p-\cos 2ka)},$$

$$\Xi_\lambda^{p_s}(x_s)=\frac{e^{-ip/2}}{2\sin ka}\left[e^{-ik(x+a/2)}\sin\left(\frac{ka-p}{2}\right)+e^{ik(x+a/2)}\sin\left(\frac{ka+p}{2}\right)\right], \quad -a<x_s<0,$$

$$\Xi_\lambda^{p_s}(x_s)=\frac{e^{ip/2}}{2\sin ka}\left[e^{-ik(x-a/2)}\sin\left(\frac{ka+p}{2}\right)+e^{ik(x-a/2)}\sin\left(\frac{ka-p}{2}\right)\right], \quad 0<x_s<a.$$

The normalizing coefficients $\rho_\lambda^P=\int_\Omega|\Xi_\lambda^P(x)|^2\,d\mu$ of the eigenfunctions $\Xi_\lambda^P(x)=\{\Xi_\lambda^{p_s}(x_s),\ s=1,2,\ldots N\}$ are calculated as

$$\rho_\lambda^P = 2Na+\gamma\frac{ka\cos 2ka-\sin 2ka}{2ak^2\sin 2ka},$$

and are positive on the spectrum σ_γ^P of the regular periodic problem. The spectral resolution and the Green's function of the regular quasiperiodic problem are represented by the spectral series converging in L_2 for $x \neq y$:

$$\sum_\lambda \Xi_\lambda^P(x)\langle \Xi^P, f\rangle \frac{1}{\rho_\lambda^P} = f(x),$$

$$G_\lambda^P(x,y) = \sum_\lambda \frac{\Xi_\lambda^P(x)\overline{\Xi_\lambda^P}(y)}{\lambda(P)-\lambda}\frac{1}{\rho_\lambda^P}.$$

Proof: Consider the following ratio of Green's functions of the quasiperiodic problem on the s-branch of the fundamental subgraph:

$$\Xi_\lambda^{p_s}(x_s) = \frac{G_\lambda^{p_s}(x,0)}{G_\lambda^{p_s}(0,0)}, \quad s = 1,2,3,\ldots,N. \tag{5}$$

Then the quasiperiodicity condition is automatically fulfilled, and the boundary condition at the node is fulfilled for values of the spectral parameter λ which satisfy the dispersion equation we derive now. Note that $\Xi_\lambda^{p_s}(0) = 1$ and the jump-condition $G_\lambda'(+0,0) - G_\lambda'(-0,0) = -1$ is fulfilled at the pole 0. Then the dispersion equation for $\Xi_\lambda^P := \Sigma_s \oplus \Xi_\lambda^{p_s}$ has the form

$$\sum_{s=1}^N \frac{1}{G_\lambda^{p_s}(0,0)} + \gamma = 0. \tag{6}$$

At the value $\mathbf{m} = 0$ we calculate the expression for the Green's function G_λ^p in explicit form:

$$G_\lambda^p(x,y) = \sum_{l=-\infty}^{\infty} e^{-ipl}\frac{e^{ik|x-y+2al|}}{2ik} = \frac{e^{ik|x-y|}}{2ik} + \frac{1}{2ik}\frac{e^{i(2ka-p)}}{1-e^{i(2ka-p)}}e^{ik(x-y)} + \frac{1}{2ik}\frac{e^{i(ka+p)}}{1-e^{i(ka+p)}}e^{ik(y-x)}, \quad k^2 = \lambda,$$

which implies $G_\lambda^p(0,0) = \sin 2ka/2k(\cos p - \cos 2ka)$. Then the dispersion equation acquires the form

$$\sum_{s=1}^N \cos p_s + \frac{\gamma \sin 2ka}{2k} = N\cos 2ka, \quad k^2 = \lambda. \tag{7}$$

The solutions λ of this equation give the spectrum σ_γ^P of the regular spectral problem on the fundamental subgraph with the quasiperiodic boundary condition (2). The spectrum σ_γ^P depends on the quasimomentum $P = (p_1, p_2, \ldots, p_N)$. Hence due to the general spectral properties of the periodic problems[21] the spectrum σ_γ of the periodic operator on the whole space is calculated as a union of all σ_γ^P,

$$\sigma_\gamma = \bigcup_{P \in \mathbf{T}^N} \sigma_\gamma^P.$$

The restrictions of the eigenfunctions of the periodic problem from the whole lattice (Bloch-functions) onto the fundamental subgraph are calculated as eigenfunctions of the regular quasiperiodic spectral problem with all possible quasimomenta. It is easy to check that each s-component of it on the s-branch $-a < x_s < a$ of the fundamental subgraph may be calculated as

$$\Xi_\lambda^P(x_s)=\frac{\cos p_s-\cos(2ka)}{\sin 2ka}\,2kG_{k^2}(x_s,0),\quad s=1,2,3,\ldots,N,\quad \lambda=k^2, \tag{8}$$

and then may be continued on the whole graph via the quasiperiodicity condition (2).

To calculate the spectral density of the periodic problem we need the normalizing coefficients of the Bloch waves for the regular problem with fixed $P=(p_1,p_2,\ldots,p_N)$ on the fundamental subgraph centered at $\mathbf{m}=\mathbf{0}$. According to the previous analysis, the s-component of the Bloch wave $\Xi_\lambda^{p_s}(x)$ is presented for $x=x_s$ as the ratio

$$\Xi_P(x_s)=\frac{G_\lambda^{p_s}(x,0)}{G_\lambda^{p^s}(0,0)}=\frac{\dfrac{e^{ik|x|}}{2ik}+\dfrac{1}{4k}\dfrac{e^{i(2ka-p)/2}}{\sin\left(\dfrac{2ka-p}{2}\right)}e^{ikx}+\dfrac{1}{4k}\dfrac{e^{i(2ka+p)/2}}{\sin\left(\dfrac{2ka+p}{2}\right)}e^{-ikx}}{G_\lambda^p(0,0)},\quad p:=p_s. \tag{9}$$

For $x<0$, that is on the branch $\Omega_a^{s,-}$ of the fundamental subgraph, the numerator of the Bloch wave (9) may be represented as

$$\begin{aligned}G_\lambda^p(x,0)&=\frac{1}{2ik}\left[e^{-ikx}\frac{i}{2}\frac{e^{-i(2ka+p)/2}}{\sin\left(\dfrac{2ka+p}{2}\right)}+e^{ikx}\frac{i}{2}\frac{e^{i2ka-p/2}}{\sin\left(\dfrac{2ka-p}{2}\right)}\right]\\&=\frac{e^{-ip/2}}{4k}\left[\frac{e^{-ik(x+a)}\sin\left(\dfrac{2ka-p}{2}\right)+e^{ik(x+a)}\sin\left(\dfrac{2ka+p}{2}\right)}{\cos p-\cos 2ka}\right],\\&\qquad x<0.\end{aligned}$$

The same numerator on the complementary branch Ω_a^{s+} (for $x>0$) is given by the formula

$$G_\lambda^p(x,0)=\frac{e^{ip/2}}{4k}\left[\frac{e^{-ik(x-a)}\sin\left(\dfrac{2ka+p}{2}\right)+e^{ik(x-a)}\sin\left(\dfrac{2ka-p}{2}\right)}{\cos p-\cos 2ka}\right],\quad x>0.$$

The normalizing coefficient $\int_\Omega|\Xi^P|^2dx$ of the Bloch-wave is calculated as a sum of integrals of the squares of all components of the Bloch-wave over all branches $\Omega_a^{s\pm}$ of the fundamental subgraph Ω_a:

$$\sum_{s=1}^N\frac{[\mathcal{J}_-^s+\mathcal{J}_+^s]}{|G_\lambda^{p_s}(0,0)|^2},$$

where $\mathcal{J}_\pm^s=\int_{\Omega_a^{s\pm}}|G_\lambda^{p_s}(x,0)|^2\,dx$. These integrals are positive and they are represented by the formula

$$\begin{aligned}\mathcal{J}_\pm^s=\frac{a}{4k^2|\cos p-\cos 2ka|^2}&\left[\sin^2\left(\frac{2ka-p}{2}\right)+\sin^2\left(\frac{2ka+p}{2}\right)\right.\\&\left.+2\sin\left(\frac{2ka+p}{2}\right)\sin\left(\frac{2ka-p}{2}\right)\frac{\sin 2ka}{2ka}\right],\quad p:=p_s.\end{aligned}$$

Summing the result over all branches and using the dispersion equation (3) we obtain for the integral over the fundamental subgraph:

$$\int_{\Omega_a} |\Xi_\lambda^P|^2\, dx = 2Na + \gamma \frac{2ka\cos 2ka - \sin 2ka}{2ak^2 \sin 2ka} \equiv \rho_\lambda^P. \tag{10}$$

Hence the spectral expansion for the regular spectral problem on the fundamental subgraph with the quasiperiodic boundary conditions (2) has the form

$$\sum_\lambda \Xi_\lambda^P(x)\Xi_\lambda^P(y)\frac{1}{\rho_\lambda^P} = \delta(x-y), \tag{11}$$

where the summation is over the spectrum $\lambda \in \sigma_P^\gamma$ of the regular quasiperiodic problem. The expression for the square norm ρ_λ^P remains positive on the spectrum σ where the dispersion equation (3) is valid for $-\pi < p_s < \pi$. In particular we see that the norm of the Bloch-functions (4) for Kirchhoff's (''zero-current'') boundary conditions $\gamma = 0$ is trivial, $\rho_\lambda^P = 2aN$.

□

The spectral properties of the periodic operator L_γ on the whole graph Γ may be easily derived from the spectral properties of the regular operator L_γ^P on the fundamental subgraph. We already mentioned that $\sigma_\gamma = \cup_P \sigma_\gamma^P$, and the eigenfunctions of the periodic problem (Bloch functions) may be obtained as the quasiperiodic continuation of the eigenfunctions Ξ_λ^P of the regular quasiperiodic problem. The spectral resolution for the periodic problem and the resolvent kernel may be obtained by averaging the corresponding expressions for the regular problem over the elementary cube of the dual lattice of quasimomenta $-\pi < p_s < \pi$, $s = 1,2,\ldots,N$:

$$\frac{1}{(2\pi)^N}\int_{\mathbf{T}^N} \sum_{\lambda \in \sigma_\gamma^P} \Xi_\lambda^P(x)\overline{\Xi_\lambda^P}(y)\frac{1}{\rho_\lambda^P} d^N P = \delta(x-y). \tag{12}$$

Each term of the series (12) above represents a spectral band of the periodic problem defined by corresponding branch $\lambda(P)$ of the solution of the dispersion equation (3), $P \in \mathbf{T}^N$. The resolvent kernel $G_z^\gamma(x,y)$ of the periodic problem [the integral kernel of the operator $R_\gamma(z) = (L_\gamma - z)^{-1}$] may be represented now as a spectral integral:

$$G_z^\gamma(x,y) = \frac{1}{(2\pi)^N}\int_{\mathbf{T}^N} \sum_{\lambda \in \sigma_\gamma^P} \frac{\Xi_\lambda^P(x)\overline{\Xi_\lambda^P}(y)}{\lambda(P) - z}\frac{d^N P}{\rho_\lambda^P}. \tag{13}$$

B. Perturbation in a finite number of nodes

Consider now a perturbed periodic lattice with only finite number $M < \infty$ of nodes $(\mathbf{m}_1, \mathbf{m}_2, \ldots \mathbf{m}_M)$ affected. Actually we replace[22–24] the standard boundary condition with $\gamma(\mathbf{m}) = \gamma$ [see the second condition in Eq. (1)] at the nodes $\mathbf{m}_1, \mathbf{m}_2, \ldots, \mathbf{m}_M$ by the local boundary condition

$$[u'](\mathbf{m}_r) = (\gamma + \beta_r)u(\mathbf{m}_r), \quad r = 1,2,\ldots,M, \tag{14}$$

with real β_r. Our next aim is to construct the resolvent and scattered waves of the corresponding self-adjoint operator $L_{\gamma\beta}$. We shall obtain both applying the Krein formula for generalized resolvents to our case. In fact we will rederive this remarkable formula in the present context; see also Refs. 24–26.

For given nodes $\mathbf{m}_1, \mathbf{m}_2, \mathbf{m}_3, \ldots, \mathbf{m}_M$ consider the finite-dimensional Hilbert space $\mathcal{E}$ of complex M-vectors $U = (u_1, u_2, u_3, \ldots, u_M)$. Each continuous function u on the cubic lattice may generate a corresponding vector $\vec{u}$ by the rule $(\vec{u})_s = u(\mathbf{m}_s)$, $s = 1,2,\ldots,M$. The scalar product in $\mathcal{E}$ we denote as $<\vec{u},\vec{v}>_\mathcal{E} = \Sigma_{s=1}^M u_s\overline{v_s}$. We need also a *real* scalar product in $\mathcal{E}$ with complex conjugation absent on the second term. We denote it just by the angular brackets $\langle \vec{u},\vec{v}\rangle = \Sigma_{s=1}^M u_s v_s$. We also consider a finite-dimensional operator $\mathcal{G}_\lambda^\gamma$ in $\mathcal{E}$ defined by the matrix

$$(\mathcal{G}_\lambda^\gamma)_{st} = G_\lambda^\gamma(\mathbf{m}_s, \mathbf{m}_t).$$

The operator defined in $\mathcal{E}$ by the diagonal matrix $\mathrm{diag}\{\beta_s\}$ will be denoted by

$$\mathcal{B} := \mathrm{diag}\{\beta_s\}.$$

Theorem 1: *The resolvent kernel $G_\lambda^\beta(x,y), x,y \in \Gamma$, of the operator $L_{\gamma\beta}$ is represented by the following Krein formula:*

$$G_\lambda^{\gamma\beta}(x,y) = G_\lambda^\gamma(x,y) - \left\langle \vec{G}_\lambda^\gamma(x), \frac{I}{I+\mathcal{B}\mathcal{G}_\lambda^\gamma} \vec{G}_\lambda^\gamma(x) \right\rangle, \tag{15}$$

where $\vec{G}_\lambda^\gamma(x)$ is an M-dimensional vector-function with the components $G_\lambda^\gamma(x,\mathbf{m}_s)$, $s = 1,2,\ldots,M$. The spectrum of the operator $L_{\gamma\beta}$ consists of an absolutely-continuous branch(es) which coincides with the (absolutely-continuous) spectrum σ_γ of L_γ and a finite number of eigenvalues in each spectral gap, which may be found from the dispersion equation $\det[I+\mathcal{B}\mathcal{G}_\lambda^\gamma] = 0$. *The scattered waves Φ_λ^P which serve as eigenfunctions of the absolutely-continuous spectrum of the operator $L_{\gamma\beta}$ are parameterized by the quasimomenta P of the initial Bloch-waves and may be constructed in analogy to the resolvent kernel*:

$$\Phi_\lambda^P = \Xi_\lambda^P(x) - \left\langle \vec{G}_\lambda^\gamma(x), \frac{I}{I+\mathcal{B}\mathcal{G}_\lambda^\gamma} \vec{\Xi}_\lambda^P \right\rangle. \tag{16}$$

Proof: We begin with an auxiliary statement concerning the resolvent of the periodic problem. Let us denote by $[']_\mathbf{m} - \gamma I_\mathbf{m}$ the following boundary value at the node $\mathbf{m}$ for the function u defined on the cubic graph:

$$([']_\mathbf{m} - \gamma I_\mathbf{m})u := \sum_{i=1}^N \left[\frac{du}{dx_i}(\mathbf{m}+0e_i) - \frac{du}{dx_i}(\mathbf{m}-0e_i) \right] - \gamma u(\mathbf{m}).$$

Then for the resolvent kernel $G_\lambda^\gamma(x,s)$ the following statement is true:

$$([']_\mathbf{m} - \gamma I_\mathbf{m}) G_\lambda^\gamma(x,\mathbf{s}) = -\delta_{\mathbf{ms}}. \tag{17}$$

Indeed, let us introduce the delta-function $\delta(x-\mathbf{m})$ attached to the node $\mathbf{m}$ of the cubic graph. It may be represented as a sum of delta-functions constructed on the one-dimensional branches of the fundamental subgraph as

$$\delta(x-\mathbf{m}) = \frac{1}{N} \sum_{i=1}^N \delta(x_i - m_i), \tag{18}$$

since both left and right parts define the same functional on the class of all continuous functions on the graph. This means that the periodic operator L_γ may be represented as

$$L_\gamma = -\frac{d^2}{dx^2} + \gamma \sum_\mathbf{m} \delta(x-\mathbf{m}),$$

and the Green's function $G_\lambda^\gamma(x,\mathbf{s})$ which satisfies the equation

$$-\frac{d^2}{dx^2} G_\lambda^\gamma(x,\mathbf{n}) + \gamma \sum_\mathbf{m} \delta(x-\mathbf{m}) G_\lambda^\gamma(x,\mathbf{n}) = \lambda G_\lambda^\gamma(x,\mathbf{n}) + \delta(x-\mathbf{n}),$$

may be integrated on a small subgraph $\Omega_{\epsilon,\mathbf{m}} = (-\epsilon < x_i - 2am_i < \epsilon,\ \epsilon \ll 1)$ which gives the following result due to (27):

$$\lim_{\epsilon\to 0}\int_{\Omega_\epsilon}(L^\gamma-\lambda I)G_\lambda^\gamma(x,\mathbf{n})d\mu=\delta_{\mathbf{mn}}.$$

The left side of the last formula coincides with $([']_{\mathbf{m}}-\gamma I_{\mathbf{m}})G_\lambda^\gamma(x,\mathbf{n})$, as announced. It is clear that the statement is true for any bounded sequence $\gamma(\mathbf{m})$ depending on $\mathbf{m}$ as well.

To prove the first relation (15) we consider the Ansatz for the resolvent kernel of the perturbed periodic operator in the form

$$G_\lambda^{\gamma\beta}(x,y)=G_\lambda^\gamma(x,y)+\sum_{t=1}^{M}A_tG_\lambda^\gamma(x,\mathbf{m}_t). \tag{19}$$

Then applying the operation $[']_{\mathbf{m}_r}-\gamma I_{\mathbf{m}_r}$ to the ansatz $G_\lambda^{\gamma\beta}(x,\mathbf{m}_s)$ we obtain the vector $-\delta_{sr}-\Sigma_{t=1}^{M}A_t\delta_{st}$ in $\mathcal{E}$. On the other hand if the boundary condition (14) for $G_\lambda^{\gamma\beta}(x,\mathbf{m}_s)$ is fulfilled, then this vector must coincide with the vector $\beta_rG_\lambda^\gamma(\mathbf{m}_r,\mathbf{m}_s)+\Sigma_{t=1}^{M}G_\lambda^\gamma(\mathbf{m}_r,\mathbf{m}_t)A_t$. This gives a *finite-dimensional* equation for A_t, $t=1,2,...,N$.

$$-(I+\mathcal{B}\mathcal{G})\vec{A}=\vec{G}_\lambda.$$

If the operator $I+\mathcal{B}\mathcal{G}_\lambda$ is invertible, then the vector $\vec{A}$ of coefficients A_t may be obtained as

$$\vec{A}=-\frac{I}{I+\mathcal{B}\mathcal{G}_\lambda}\vec{G}_\lambda,$$

which gives the first relation (15). The second relation (16) may be obtained in a similar way by using the ansatz

$$\Phi_\lambda^P(x)=\Xi_\lambda^P(x)+\sum_{t=1}^{M}A_tG_\lambda^\gamma(x,\mathbf{m}_t).$$

□

III. APPROXIMATION OF *N*-DIMENSIONAL SCHRÖDINGER DYNAMICS BY DYNAMICS ON CUBIC GRAPH

A. Approximation theorems

We have seen above that quantum systems on the corresponding embedded graphs inherit some basic spectral features from relevant systems on bulk space. On the other hand, the less the dimension of mesh we are using for approximation of the multi-dimensional problem, the easier the corresponding computing; see the article[20] by McCormic. At the same time the analysis for *one-dimensional* graphs may be developed in terms of solutions of corresponding Cauchy problems for *ordinary* differential equations on the edges of the graph, which is almost as simple to solve with the use of modern computers as discrete equations. But the continuous nature of ordinary differential equations allows us to observe high-energy phenomena in a most natural form. In particular one may derive the realistic asymptotic formulas, e.g., for a description of the scattering processes. This is our motivation for analyzing Schrödinger dynamics in N-dimensional space in terms of the corresponding dynamics on one-dimensional cubic graphs filling the whole space $\mathbf{R}^N$.

Let us consider a Schrödinger operator in $\mathbf{R}^N$,

$$H=-\Delta+V(\mathbf{X}),\quad \mathbf{X}\in\mathbf{R}^N, \tag{20}$$

with a continuous, rapidly decreasing potential $V(\mathbf{X})\in L_2(\mathbf{R}^N)\cap C(\mathbf{R}^N)$. For any $a>0$ we can discretize the space $\mathbf{R}^N$ representing it as a tiling

$$\mathbf{R}^N = K_a \times \mathbf{Z}^N := \bigcup_{\mathbf{m}\in\mathbf{Z}^N} K_{a\mathbf{m}},$$

where the tile $K_{a\mathbf{m}}$ is produced by the shift of the basic tile K_a,

$$K_a = \{\mathbf{x}: |\mathbf{x}_j| \leqslant a;\ \ j = 1,2,\ldots,N\}.$$

Here and in what follows we use the following notations:

$\mathbf{x} = \{\mathbf{x}_j\}_{j=1}^N$ is a point of N-dimensional cube K_a with the edges of the length $2a$ parallel to the vectors of a standard orthogonal and normalized basis $\{e_i\}_{i=1}^N$;

$\mathbf{X} = \{\mathbf{X}_j\}_{j=1}^N = 2a\mathbf{m} + \mathbf{x}$, $\mathbf{m}\in\mathbf{Z}^N$, is a point of $\mathbf{R}^N$ with coordinates;

$\mathbf{X}_j = 2a\mathbf{m}_j + \mathbf{x}_j$ with respect to the basis $\{e_i\}_{i=1}^N$;

$\mathbf{X}_\mathbf{m} = 2a\mathbf{m}$ is the $\mathbf{m}$-th node of the cubic lattice with the edge $2a$.

Together with the space $\mathbf{R}^N$ we consider a graph Γ_a which has the structure of a cubic lattice:

$$\Gamma_a = \Omega_a \times \mathbf{Z}^N,$$

where Ω_a is a union of N pairwise orthogonal edges $[-ae_i, ae_i]$ directed along the basic vector of the same orthogonal and normalized basis $\{e_i\}_{i=1}^N$ and having only one common point at the origin. The structure of this lattice is obviously compatible with the tiling introduced above in the sense that the graph Γ_a can be naturally embedded in the space $\mathbf{R}^N$ as a cubic lattice with the step $2a$ so that the fundamental subgraph of it forms the boundary of the fundamental domain K_a of the subgroup of the shift group forming the tiling above. Indeed, when using the following notations:

x is a point of the fundamental subgraph $\Omega_a = \cup_{j=1}^N [-ae_j, ae_j] := \cup_{j=1}^N \Omega_a^j$;

X is a point of the graph Γ_a; $X = 2a\mathbf{m} + x$, $\mathbf{m}\in\mathbf{Z}^N$;

$X_\mathbf{m} = 2a\mathbf{m}$ is the $\mathbf{m}$-th node of the graph Γ_a;

x_j is a point of the interval $\Omega_a^j = [-ae_j, ae_j]$ (the j-edge of the fundamental subgraph $\Omega_a \subset \Gamma_a$),

we describe the *natural embedding* of the graph Γ_a into $\mathbf{R}^N$ as an identification of points $\mathbf{X}_\mathbf{m}$ and X_m and a realization of the edges of the graph as intervals parallel to coordinate axes in $\mathbf{R}^N$ connected to the orthogonal basis $\{e_i\}_{i=1}^N$. In particular the fundamental subgraph Ω_a is then embedded into the cube K_a such that each j-axis of this cube $\{\mathbf{X}: \mathbf{X}_l = 0, l \neq j\}$ corresponds to the component Ω_a^j of the fundamental subgraph and $x_j = \mathbf{x}_j$.

One can consider the Hilbert space $\mathcal{H}_a$ of functions on the graph Γ_a:

$$\mathcal{H}_a = L_2(\Gamma_a, \nu\, dX) = l_2(\mathbf{Z}^N, L_2(\Omega_a, \nu\, dx)) = l_2\left(\mathbf{Z}^N, \sum_{j=1}^N \oplus L_2([-a,a], \nu\, dx_j)\right),$$

where the coefficient in the measure

$$\nu = (2a)^{N-1}/N \tag{21}$$

is chosen in order to preserve the measure under the embedding described above:

$$\int_{K_a} d^N\mathbf{x} = \nu \int_{\Omega_a} dx. \tag{22}$$

The Laplace operator on the graph is given as

$$L_0^{(a)} = -N \sum_{\mathbf{m}\in\mathbf{Z}^N} \sum_{j=1}^N \oplus \partial_{x_j}^2 := -N\frac{d^2}{dx^2}, \tag{23}$$

in the Hilbert space $\mathcal{H}_a$ with the domain $D^{(a)}$ described as a linear variety,

$$l_2\left(\mathbf{Z}^N, \sum_{j=1}^{N} \oplus W_2^2([-a,a]\setminus\{0\}, \nu\, dx_j)\right),$$

of all W_2^2-smooth elements in $\mathcal{H}_2$ which satisfy the boundary condition (1) with $\gamma=0$ (Kirchhoff's ''zero-current'' condition).

We shall approximate the initial Schrödinger operator (20) in $\mathbf{R}_N$ by the following Schrödinger operator on the graph:

$$L^{(a)} = L_0^{(a)} + q_a(X), \tag{24}$$

with the (generalized) potential $q_a(X)=q_a(x,\mathbf{m})$ which will be specified later.

It is obvious that general elements of the basic Hilbert space $L_2(\mathbf{R}^N)$ of all square-integrable functions on $\mathbf{R}^N$ cannot be restricted onto the embedded one-dimensional graph as square-integrable functions. In fact we need even more. The restrictions of functions on $\mathbf{R}^N$ to the lattice Γ_a should be in a proper sense twice differentiable. Exact additional conditions of the smoothness of elements of the original Hilbert space $L_2(\mathbf{R}_N)$ may be easily derived from Sobolev's embedding theorems,[27] but for the moment we just consider the trivial class $W_2^l(\mathbf{R}^N)$, $2l>N$ which consists of continuous ($\mathrm{Lip}_{1/l+1}$) Lipshitz-functions in $\mathbf{R}^N$ and the class

$$\mathcal{F} := W_2^l(\mathbf{R}^N), \quad 2l-N>4,$$

which gives after restriction onto the one-dimensional lattice Γ_a functions in $C^{2+(1/l+1)}(\Gamma_a)$. Below we prove two preparatory statements which will be summarized later in form of the theorem on approximations announced above.

Lemma 2: For any function $u\in W_2^l(\mathbf{R}^N)$, $2l>N$ its restriction u_a onto the graph Γ_a belongs to $L_2(\Gamma_a)\cap \mathrm{Lip}_{2l-N/2(2l-N+2)}$, and the modulo of continuity,

$$\omega_{\mathbf{X}}^u(\delta) := \sup_{|\mathbf{K}|\leqslant\delta} |u(\mathbf{X}+\mathbf{K})-u(\mathbf{X})|,$$

of the function u at the point $\mathbf{X}\in\mathbf{R}^N$ is a square-integrable function of $\mathbf{X}$ in $\mathbf{R_N}$ for any $\delta\ll 1$:

$$\int_{\mathbf{R}^N} |\omega_{\mathbf{X}}^u(\delta)|^2\, d\mathbf{X}^N \leqslant C\delta^{2/(l+1)} \|u\|_{W_2^1}^2.$$

The restriction operator $u\mapsto u_a$ is asymptotically isometric for $a\to 0$:

$$\left|\int_{\mathbf{R}^N} |u|^2\, d\mathbf{X}^N - \int_{\Gamma_a} |u_a|^2(X)\,\nu\, dX\right| \leqslant aC_0\left[\int_{\mathbf{R}_N} |u|^2\, d\mathbf{X}^N + \int_{\mathbf{R}^N} |\nabla u|^2 d\mathbf{X}^N\right] + a^{2l}\left(a+\frac{1}{a}\right) C_l \int_{\mathbf{R}^N} |\nabla^l u|^2\, d\mathbf{X}^N.$$

Similarly, there is a constant $C<\infty$, such that for any functions $u,v\in W_2^l(\mathbf{R}^N)$, $2l>N$, and its restrictions u_a, v_a onto the graph Γ_a,

$$\left|\int_{\mathbf{R}^N} u\overline{v}\, d\mathbf{X}^N - \int_{\Gamma_a} u_a\overline{v}_a \nu\, dX\right| \leqslant aC[\|u\|_{W_2^l}^2 + \|v\|_{W_2^l}^2].$$

Proof: We begin with the proof of the second statement. Note first of all that in the case $2l>N$ the function $u\in W_2^l$ in the unit cube K_1 may be estimated as

$$\sup_{K_1} |u|^2 \leqslant C_0 \int_{K_1} |u|^2\, d\mathbf{x}^N + C_l \int_{K_1} |\nabla^l u|^2\, d\mathbf{x}^N,$$

and the increment of u on any direct path $(\mathbf{x},\mathbf{x}')$ in the unit cube the following estimate holds with some absolute constants C_1, C_l:

$$|u(\mathbf{x})-u(\mathbf{x}')|^2 \leqslant \left[\int_{(\mathbf{x},\mathbf{x}')} |\nabla u|(s)\,ds\right]^2 \leqslant C_0 \int_{K_1} |\nabla u|^2\, d\mathbf{x}^N + C_l \int_{K_1} |\nabla^l u|^2 d\mathbf{x}^N.$$

By scaling this gives

$$\sup_{\mathbf{x}\in K_a} |u|^2 \leqslant C_0 (2a)^{-N} \int_{K_a} |u|^2\, d\mathbf{x}^N + (2a)^{2l-N} C_l \int_{K_a} |\nabla^l u|^2\, d\mathbf{x}^N,$$

$$\sup_{\mathbf{x},\mathbf{x}'\in K_a} |u(\mathbf{x})-u(\mathbf{x}')|^2 \leqslant C_0 (2a)^{2-N} \int_{K_a} |\nabla u|^2\, d\mathbf{x}^N + (2a)^{2l-N} C_l \int_{K_1} |\nabla^l u|^2\, d\mathbf{x}^N.$$

Hence for the real function u the estimate for the increment of u^2 for $u \in W_2^l(K_a)$ along any direct path $(\mathbf{x}, \mathbf{x}')$, in K_a may be reduced to an estimation of the product

$$|u^2(\mathbf{x})-u^2(\mathbf{x}')| = |u(\mathbf{x})+u(\mathbf{x}')\|u(\mathbf{x})-u(\mathbf{x}')|,$$

which may be transformed with use of Cauchy's inequality to the form

$$|u^2(\mathbf{x})-u^2(\mathbf{x}')| \leqslant \left[(2a)^{1-N} C_0 \int_{K_a} (|u|^2+|\nabla u|^2) d\mathbf{x}^N + (2a)^{2l-N}\left(2a+\frac{1}{2a}\right) C_l \int_{K_a} |\nabla^l u|^2\, d\mathbf{x}^N\right].$$

Having j fixed somehow we choose the point $\mathbf{x}' = X'$ on Ω_a^j and then integrate over K_a and sum over all j and over the tiling $K_{\mathbf{m}}$. Then redefining we obtain the estimate for the integral over Lebesgue measure μ on the lattice Γ:

$$\left|\int_{\mathbf{R}^N} |u|^2\, d\mathbf{X}^N - \frac{(2a)^{N-1}}{N} \int_{\Gamma_a} |u_a|^2\, dX\right| \leqslant \left[\frac{(2a)}{N} C_0 \int_{\mathbf{R}^N} (|u|^2+|\nabla u|^2) d\mathbf{X}^N + (2a)^{2l-N} \times \left(2a+\frac{1}{2a}\right)\frac{C_l}{N} \int_{K_a} |\nabla^l u|^2\, d\mathbf{x}^N\right].$$

To obtain a similar estimate for complex-valued functions one may derive it separately for real and imaginary parts of them, and then add both parts. The final result for the estimation of the scalar product $\langle u,v\rangle$ is obtained with use of the polarization identity.

Using the assertion proved above we may reduce the verification of the first statement of the lemma to the proof of the corresponding fact in $\mathbf{R}^N$. This may be easily derived for rapidly decreasing smooth functions. The increment of the function $u(\mathbf{X})$ may be estimated in the usual way:

$$u(\mathbf{X}+\mathbf{K})-u(\mathbf{X}) = \frac{1}{(2\pi)^{N/2}} \int_{\mathbf{R}_N} e^{i\mathbf{P}\mathbf{X}} \frac{(-1+e^{\mathbf{P}\mathbf{K}})}{(1+\mathbf{P}^2)^{l/2}} u(\mathbf{P})(1+\mathbf{P}^2)^{l/2}\, d\mathbf{P}^N.$$

Denoting the Fourier transform by $\mathbf{F}$ we may rewrite the last expression in the form

$$u(\mathbf{X}+\mathbf{K})-u(\mathbf{X}) = \mathbf{F}^{-1} A(\mathbf{K},*)\mathbf{F}(1+D^2)^{l/2} u(\mathbf{X}),$$

where A is the pseudo-differential operator with the symbol

$$A(\mathbf{K},\mathbf{P}) = \frac{e^{i\mathbf{P}\mathbf{K}}}{(1+\mathbf{P}^2)^{l/2}},$$

and D^2 is the Laplace operator in $L_a(\mathbf{R}^N)$. Using the uniform estimate $|A(\mathbf{K},\mathbf{P})| \leqslant C\delta^{1/(1+l)}$ for the symbol in the ball $|K| \leqslant \delta$ and the unitarity of the Fourier-transform in $L_2(\mathbf{R}^N)$ we see that for any continuous function $K(\mathbf{X})$, $|K(\mathbf{X})| \leqslant \delta$ we may estimate $\int_{\mathbf{R}^N} |u(\mathbf{X}+\mathbf{K}(\mathbf{X}))-u(\mathbf{X})|^2\, d\mathbf{X}^N$ by the product $C\delta^{2/(1+l)}\|u\|^2_{W_2^l(\mathbf{R}^N)}$. The function $K(\mathbf{X})$ may be chosen such that

$$|u(\mathbf{X}+\mathbf{K}(\mathbf{X}))-u(\mathbf{X})| = \sup_{|\mathbf{X}|\leqslant\delta} |u(\mathbf{X}+\mathbf{K}(\mathbf{X}))-u(\mathbf{X})| = \omega^u_{\mathbf{X}}(\delta).$$

This gives the first statement of the lemma.

□

Lemma 2 permits us to substitute the pre-Hilbert space of all W_2^l-smooth, $2l>N$, square-integrable functions in $\mathbf{R}^N$ by the pre-Hilbert space of Lipshits–continuous functions on the cubic graph. We need one more step to substitute the Laplace operator on $\mathbf{R}^N$ by the Laplace on the cubic lattice, $-\Delta \to L_0^a$.

Define the classes

$$\mathcal{F}_0 := W_2^l(\mathbf{R}^N); \quad \mathcal{F}_2 := W_2^{l+2}(\mathbf{R}^N).$$

Then the following statement may be considered as a motivation for the substitution of the Laplace operator $-\Delta$ by the operator L_0^a on the graph.

Lemma 3: The restriction u_a of any function $u \in \mathcal{F}_2$ onto the graph Γ_a,

$$u_a(x) := u(\mathbf{X}), \quad if \quad \mathbf{X} = X \in \Gamma_a,$$

in $C^{2+(2l-N)/2(2l-N+2)}(\Gamma_a) \cap L_2(\Gamma_a)$ exists and the diagram

$$\begin{array}{ccc} u & \xrightarrow{\text{differentiation}} & -\Delta u \\ \downarrow \text{restriction} & & \text{restriction} \downarrow \\ u_a & \xrightarrow{\text{differentiation}} & L_0^a u_a \leftrightarrow -\Delta u|_a \end{array} \tag{25}$$

is ''almost commutative'' in the following weak sense: for any test-function $\varphi \in W_2^l(\Gamma_a)$ the weak deviation of $L_0^a u_a$ **from** $-\Delta u|_a$ for small a may be estimated as

$$\left| \int_{\Gamma_a} (L_0^a u_a + \Delta u|_a)\, \overline{\varphi}\, \nu\, dx \right| \leqslant \mathbf{C} a^{1/(l+1)},$$

where $\mathbf{C}$ is a constant depending on $\|u\|^2_{W_2^{l+2}(\mathbf{R}^N)}$, $\|\varphi\|^2_{W_2^l(\Gamma_a)}$.

Proof: Due to Lemma 2 it is sufficient to derive the required estimate on the fundamental subgraph and then sum it over the whole tiling. If we denote by $u_0(\mathbf{m})$, $\mathbf{u_s}(\mathbf{m})$, $\mathbf{u_{st}}(\mathbf{m})$, respectively, the values of the function u and the values of its first derivatives with respect to x_s and second derivatives with respect to x_s, x_t at the node $\mathbf{m}$, we may write down the Taylor formula on the tile $\Omega_{a,\mathbf{m}}$ for the function u,

$$u(2a\mathbf{m}+\mathbf{x}) = u_0(\mathbf{m}) + \sum_s u_s(\mathbf{m})\mathbf{x}_s + \tfrac{1}{2}\sum_{s,t} u_{st}(\mathbf{m})\mathbf{x}_s\mathbf{x}_t + O(\omega^u_{\mathbf{m}}(|\mathbf{x}|)),$$

and for the restriction u_a of u onto the lattice Γ_a, $x \in \Omega_a^s$:

$$u_a(2a\mathbf{m}+x_s) = u_0(\mathbf{m}) + u_s(\mathbf{m})x_s + \tfrac{1}{2}u_{ss}(\mathbf{m})x_s^2 + O(\omega^u_{\mathbf{m}}(|\mathbf{x}|)).$$

A straightforward calculation of the multi-dimensional Laplace on u gives on the tile $\Omega_{\mathbf{m}}$:

$$\Delta u = \sum u_{ss}(\mathbf{m}) + O(\omega_{\mathbf{m}}^{\Delta u}(|x_s|)), \tag{26}$$

where $\omega_{\mathbf{m}}^{f}(\delta)$ stands for the modulo of continuity of the function f on the tile $\Omega_{\mathbf{m}}$. The application of the lattice Laplace L_0^a to the branch $\Omega_{a,\mathbf{m}}^s$ of the tile $\Omega_{a,\mathbf{m}}$ gives

$$L_0^a u_a = N u_{ss} + O(\omega_{\mathbf{m}}^{u}(|x_s|)). \tag{27}$$

It is clear that the last two expressions (26), (27) have a lot in common: the restriction of the first of them onto the branch $\Omega_{a,\mathbf{m}}^s$ gives $\Sigma u_{ss}(\mathbf{m}) + O(\omega_{\mathbf{m}}^{u}(a))$, hence integrating over $\Omega_{a,\mathbf{m}}$ with the test-function φ we obtain

$$\varphi(2a\mathbf{m} + x_s) = \varphi(2a\mathbf{m}) + O(\omega_{\mathbf{m}}^{\varphi}(|x_s|)).$$

Summing over s, $s = 1,2,\ldots,N$ and $\mathbf{m}$ results in

$$\begin{aligned}\left| \int_{\Gamma_a} [(-\Delta u)|_{\Gamma_a} - L_0^a u_a] \varphi \nu \, dX \right| \leqslant \mathbf{C} \sum_{\mathbf{m}} \Bigg\{ & \left(\int_{\Omega_{a,\mathbf{m}}} |\varphi|^2 \nu \, dx \right)^{1/2} \left(\int_{\Omega_{a,\mathbf{m}}} |\omega_{\mathbf{m}}^{D^2 u}(x)|^2 \, dx \right)^{1/2} \\ & + \left(\int_{\Omega_{a,\mathbf{m}}} |\omega_{\mathbf{m}}^{\varphi}(x)|^2 \nu \, dx \right)^{1/2} \left(\int_{\Omega_{a,\mathbf{m}}} |D^2 u|^2 \nu \, dx \right)^{1/2} \\ & + \left(\int_{\Omega_{a,\mathbf{m}}} |\omega_{\mathbf{m}}^{D^2 u}(x)|^2 \, dx \right)^{1/2} \left(\int_{\Omega_{a,\mathbf{m}}} |\omega_{\mathbf{m}}^{\varphi}(x)|^2 \nu \, dx \right)^{1/2} \Bigg\},\end{aligned}$$

where $\mathbf{C}$ is an absolute constant and $|D^2 u|^2$, $|\omega_{\mathbf{m}}^{D^2 u}|^2$ stay for sums of squares of second derivatives and of the moduli of continuity of them, respectively. The integrals of the squares of the moduli of continuity may be estimated via the mean-value theorem as

$$\int_{\Omega_{a,\mathbf{m}}} |\omega_{\mathbf{m}}^{f}(x)|^2 \nu \, dx \leqslant (2a)^N |\omega_{\mathbf{m}}^{f}(2a)|^2,$$

and hence

$$\sum_{\mathbf{m}} \int_{\Omega_{a,\mathbf{m}}} |\omega_{\mathbf{m}}^{f}(x)|^2 \nu \, dx \leqslant \sum_{\mathbf{m}} (2a)^N |\omega_{\mathbf{m}}^{f}(2a)|^2,$$

which coincides with an integral sum for the integral $\int_{\Gamma_a} |\omega_X^f(2a)|^2 \nu \, dx$. Using the local estimate for $X \in \Omega_{a,\mathbf{m}}$,

$$\omega_{\mathbf{m}}^{f}(2a) \leqslant \omega_X^f(4a),$$

we may substitute the integral sum by the integral $\int_{\Gamma_a} |\omega_X^f(4a)|^2 \nu \, dx$ and estimate it using Lemma 2. These steps give the announced estimate with some constant $\mathbf{C}$ depending on $\|u\|_{W_2^{l+2}(\mathbf{R}^N)}, \|\varphi\|_{W_2^l(\Gamma_a)}$.

□

Consider a pair of differential equations,

$$-\Delta \mathcal{U} + V(\mathbf{X})\mathcal{U} = \lambda \mathcal{U} + F,$$

$$L_0^{(a)} u + q(x) u = \lambda u + F_a,$$

with nonhomogeneous terms $F \in W_2^l(\mathbf{R}^N)$ and with $F_a = F|_{\Gamma_a}$. To approximate the multi-dimensional dynamics in $\mathbf{R}^N$ by the corresponding one-dimensional dynamics on the graph Γ_a we have to compare the resolvents of corresponding Schrödinger operators. For given continuous potential $V(\mathbf{X})$ in $\mathbf{R}^N$ [see Eq. (20)], we have to construct a potential $q_a(X)$ (continuous, singular or generalized) on the graph Γ_a [see Eq. (24)] so that following diagram:

$$\begin{array}{ccc} -\Delta\mathcal{U} + V(X)\mathcal{U} = \lambda\mathcal{U} + F & \overset{\text{solution}}{\rightarrow} & \mathcal{U}(\mathbf{X}) \\ \downarrow \text{approximation} & & \text{restriction} \downarrow \\ L_0^{(a)} u + q(x)u := L^{(a)} u = \lambda u + F|_{\Gamma_a} & \overset{\text{solution}}{\rightarrow} & u(X) \rightarrow_{a\to 0} \mathcal{U}|_{\Gamma_a} \end{array} \tag{28}$$

is ''approximately commutative'' in a sense similar to one of the diagrams discussed in Lemma 3. Now the exact meaning of the diagram (28) is clarified by the following.

Theorem 2: *Let $H = -\Delta + V(\mathbf{X})$ be a Schrödinger operator in $L_2(\mathbf{R}^N)$ with a real uniformly bounded square-integrable and continuous potential $V(\mathbf{X})$. Consider the family of lattice-type graphs Γ_a naturally embedded into $\mathbf{R}^N$ as described above and the family $\{L^{(a)}\}$ of operators (each acting in its own space $\mathcal{H}_a$) given by Eq. (24) with the generalized delta-functional potentials,*

$$q_a(X) = (2N\nu)^{-1} \sum_{\mathbf{m}\in\mathbf{Z}^N} \delta(X - X_{\mathbf{m}}) \int_{K_a} V(\mathbf{x} + 2a\mathbf{m}) d^N\mathbf{x}. \tag{29}$$

Then for any pair of test functions $\Upsilon(\mathbf{X}) \in \mathcal{F}_2$, $\Psi(\mathbf{X}) \in \mathcal{F}_0$ and the restrictions $\upsilon^{(a)}(X), \psi^{(a)}$ onto the graph Γ_a the following weak approximation property is valid when $a \to 0$:

$$|\langle H\Upsilon, \Psi\rangle_{L_2(\mathbf{R}^N)} - \langle L^a \upsilon^{(a)}, \psi^{(a)}\rangle_{\mathcal{H}^{(a)}}| \leqslant \mathbf{C} a^{1(l+1)} \|\Upsilon\|_{W_2^{l+2}(\mathbf{R}^N)} \|\Psi\|_{W_2^l(\mathbf{R}^N)}. \tag{30}$$

Proof: First let us notice that the choice of the (generalized) potential $q_a(x)$ is not unique; however, the one given leads to an essential simplification.

The comparison of the bilinear forms of the differential operator parts Δ and $L^{(a)}$ was done in Lemma 3. It remains to compare the parts which contain the potentials. Using Taylor expansions for the test functions Υ and Ψ, we have for instance,

$$\Upsilon(\mathbf{x}, \mathbf{m}) = \upsilon^{(a)}(2a\mathbf{m}) + \sum_{l=1}^{2} \sum_{n\geqslant 1} \frac{\partial^n \Upsilon}{\partial \mathbf{x}_l^n}(2a\mathbf{m}) \frac{\mathbf{x}^n}{n!} + O(\omega_{\mathbf{m}}^{D^2\Upsilon}(2a)),$$

where the symbolic notations for a high-order differential are used. Therefore we may obtain the approximate formula for the bilinear term with the potential

$$\begin{aligned} \langle V\Upsilon, \Psi\rangle_{L_2(\mathbf{R}^N)} &= \sum_{\mathbf{m}\in\mathbf{Z}^N} \int_{K_a} V(\mathbf{x} + 2a\mathbf{m}) \Upsilon(\mathbf{x} + 2a\mathbf{m}) \overline{\Psi}(\mathbf{x} + \mathbf{m}) d\mathbf{x}^N \\ &= \sum_{\mathbf{m}\in\mathbf{Z}^N} \upsilon^{(a)}(2a\mathbf{m}) \overline{\psi^{(a)}}(2a\mathbf{m}) \int_{K_a} V(\mathbf{x} + \mathbf{m}) d\mathbf{x} + a^{1/(1+l)} [\|\Upsilon\|_{W_2^l(\mathbf{R}^N)} \|\Psi\|_{W_2^l(\mathbf{R}^N)}]. \end{aligned}$$

Due to the continuity of the restrictions υ, ψ we may approximate the potential $V(\mathbf{X})$ by the combination $q_a(X)$ of delta functions on the lattice Γ_a attached to the points $2a\mathbf{m}$ [see Eq. (29)]. Using the bracket notations for functionals on continuous functions we have

$$\upsilon^{(a)}(2a\mathbf{m})\overline{\psi^{(a)}}(2a\mathbf{m})=\int_{\Gamma_a}\delta(X-2a\mathbf{m})\upsilon^{(a)}(X)\overline{\psi^{(a)}}(X)dX=\nu^{-1}\langle\delta(X-X_M)\upsilon^{(a)}(X),\psi^{(a)}(X)\rangle_{\mathcal{H}_a},$$

hence

$$\begin{aligned}\langle V(\mathbf{X})\Upsilon,\Psi\rangle_{L_2(\mathbf{R}^N)}&=\nu^{-1}\sum_{\mathbf{m}\in\mathbf{Z}^N}\langle\delta(X-X_\mathbf{m})\upsilon^{(a)},\psi^{(a)}\rangle_{\mathcal{H}_a}\int_{K_a}V(\mathbf{x}+\mathbf{m})d\mathbf{x}^N\\&\quad+O(a^{1/(1+l)}[\|\Upsilon\|_{W_2^l(\mathbf{R}^N)}\|\Psi\|_{W_2^l(\mathbf{R}^N)}])\\&=\langle q_a(X)\upsilon^{(a)},\psi^{(a)}\rangle_{\mathcal{H}_a}+O(a^{1/(1+l)}[\|\Upsilon\|_{W_2^l(\mathbf{R}^N)}\|\Psi\|_{W_2^l(\mathbf{R}NN)}]).\end{aligned}\tag{31}$$

Using Lemma 3 and Eq. (30) concludes the proof of the theorem.

□

We see now that the family of the operators $L^{(a)}$ on the graphs Γ_a approximates in the weak sense the N-dimensional Schrödinger operator H when $a\to 0$. This result will now lead to the desired interpretation of the ''weak commutativity'' of the diagram (28).

Definition 1: The function $\mathcal{U}\in\mathcal{F}_2$ is called a weak solution of the equation

$$-\Delta\mathcal{U}+V\mathcal{U}=\lambda\mathcal{U}+F,\quad F\in\mathcal{F},\tag{32}$$

if for all test-functions $\Psi\in\mathcal{F}_0$ the following equation holds:

$$\langle(-\Delta+V-\lambda)\mathcal{U},\Psi\rangle_{L_2(\mathbf{R}^N)}=\langle F,\Psi\rangle_{L_2(\mathbf{R}^N)}.$$

Definition 2: The function $u\in W_2^l(\Gamma_a)$ is called a weak solution of the equation solution,

$$L_0^{(a)}u+q_au=\lambda u+f,\tag{33}$$

if for all restrictions ψ of the test-functions $\Psi\in\mathcal{F}_0$ onto the lattice Γ_a the following equation holds:

$$\langle(H_0^{(a)}+q-\lambda)u,\psi\rangle_{\mathcal{H}_a}=\langle f,\psi\rangle_{\mathcal{H}_a},$$

for all functions $\psi\in\mathcal{H}_a$.

The following theorem is valid.

Theorem 3: *If $\mathcal{U}$ is a weak solution of Eq. (32), then its restriction $\mathcal{U}|_{\Gamma_a}$ to the graph Γ_a is approximated by a weak solution of Eq. (33) with $f=F|_{\Gamma_a}$ in the following sense:*

$$\langle(L_0^{(a)}+q-\lambda)\mathcal{U}|_{\Gamma_a},\psi\rangle_{\mathcal{H}_a}-\langle F|_{\Gamma_a},\psi\rangle_{\mathcal{H}_a}\to 0,\ \text{if}\ a\to 0,\tag{34}$$

for any $\psi\in\mathcal{H}_a$, where $q_a(x)$ is given by Eq. (29).

Proof: The class $\mathcal{F}_2$ of test functions is dense in the space $L_2(\mathbf{R}^N)$, therefore we can restrict our consideration to the case $\mathcal{U}\in\mathcal{F}_2$. Applying Theorem 2 we have

$$\langle(-\Delta+V)\mathcal{U},\Psi\rangle_{L_2(\mathbf{R}^N)}=\langle(L_0^{(a)}+q_a)\mathcal{U}|_{\Gamma_a},\Psi|_{\Gamma_a}\rangle_{\mathcal{H}_a}+O(a^{1/(1+l)}[|U|_{W_2^{l+2}(\mathbf{R}^N)}|\Psi|_{W_2^l(\mathbf{R}^N)}]).$$

Following the pattern of the proof of Theorem 2 one can see that

$$\langle\mathcal{U},\Psi\rangle_{L_2(\mathbf{R}^N)}=\langle\mathcal{U}|_{\Gamma_a},\Psi|_{\Gamma_a}\rangle_{\mathcal{H}_a}+O(a^{1/(1+l)}[|U|_{W_2^l(\mathbf{R}^N)}|\Psi|_{W_2^l(\mathbf{R}^N)}]);$$

$$\langle F,\Psi\rangle_{L_2(\mathbf{R}^N)}=\langle F|_{\Gamma_a},\Psi|_{\Gamma_a}\rangle_{\mathcal{H}_a}+O(a^{1/(1+l)}[|F|_{W_2^l(\mathbf{R}^N)}|\Psi|_{W_2^l(\mathbf{R}^N)}]);$$

for any $\mathcal{U}\in\mathcal{F}_2,\Psi,F\in\mathcal{F}_0$. The function $\mathcal{U}\in\mathcal{F}_2\subset\mathcal{F}_0$ is a weak solution of Eq. (32), and the restriction $\mathcal{F}_0|_{\Gamma_a}$ of the class $\mathcal{F}_0$ to the graph Γ_a is dense in the space $\mathcal{H}_a$; therefore formula (34) is true.

□

The last statement confirms the ''approximate commutativity'' of diagram (28) in the weak sense when $a\to 0$, thus motivating the study of the operators $L^{(a)}$.

B. Analysis of operators $L^{(a)}$

Due to the specific (delta-functional) perturbation, the easiest way to investigate the operators $H^{(a)}$ is to use the Lippmann–Schwinger equation for the resolvents,

$$R(z)=R_0(z)-R_0(z)q_aR(z), \tag{35}$$

where we omit index a and use the notations

$$R_0(z)=(L_0^{(a)}-z)^{-1};$$

$$R(z)=(L^{(a)}-z)^{-1}=(L_0^{(a)}+q_a(X)-z)^{-1}. \tag{36}$$

The unperturbed resolvent $R_0(z)$ was constructed in Sec. II A through its kernel (the Green's function) $G_z^\gamma(x,y)$ [see Eq. (13)]. The case under consideration is given by $\gamma=0$ (Kirchhoff's condition). In this case we see from Eq. (3) that the spectrum of the unperturbed operator $L_0^{(a)}$ being the union of spectra of fiber the operators $L_0^{(a)P}$, $P\in\mathbf{T}^N$, is absolutely continuous and fills the positive semiaxis. Indeed, $-1\leqslant(1/N)\sum_{s=1}^N\cos p_s\leqslant 1$ for all $P=\{p_s\}_{s=1}^N\in\mathbf{T}^N$, and $(1/N)\sum_{s=1}^N\cos p_s$ takes all values in the interval $[-1,1]$ when P varies on $\mathbf{T}^N$. Therefore, solutions k of Eq. (3) in case $\gamma=0$ fill the whole real axis after integration over $\mathbf{T}^N$, and the spectrum $\sigma_0\ni\lambda=k^2$ of the operator $L_0^{(a)}$ fills the positive semiaxis.

The kernel of the unperturbed resolvent (the Green's function) constructed in Sec.II A has a tensor structure. We denote its tensor elements as $R_{\mathbf{mm}'}^{(0)jj'}(x,x',z)$, $1\leqslant j,j'\leqslant N$, $\mathbf{m},\mathbf{m}'\in\mathbf{Z}^N$. Tensor elements of the local perturbation $q_a(X)$ given by Eq. (29) are

$$q_{\mathbf{mm}'}^{jj'}(x,x')=\nu^{-2}V_{\mathbf{m}}\delta_{\mathbf{mm}'}\delta_{jj'}\delta(x')\delta(x), \tag{37}$$

where

$$V_{\mathbf{m}}\overset{\text{def}}{=}\int_{K_a}V(\hat{X},\mathbf{m})d^N\hat{X}. \tag{38}$$

Therefore the Lippmann–Schwinger equation (35) for the tensor elements of the perturbed resolvent takes the form

$$R_{\mathbf{mm}'}^{jj'}(x,x',z)=R_{\mathbf{mm}'}^{(0)jj'}(x,x',z)-\sum_{\mathbf{n}\in\mathbf{Z}^N}V_{\mathbf{n}}\sum_{l=1}^N R_{\mathbf{mn}}^{(0)jl}(x,0,z)R_{\mathbf{nm}'}^{lj'}(0,x',z), \tag{39}$$

which for $x=0$ implies

$$R_{\mathbf{mm}'}^{jj'}(0,x',z)=R_{\mathbf{mm}'}^{(0)jj'}(0,x',z)-\sum_{\mathbf{n}\in\mathbf{Z}^N}V_P\sum_{l=1}^N R_{\mathbf{mn}}^{(0)jl}(0,0,z)R_{\mathbf{nm}'}^{lj'}(0,x',z). \tag{40}$$

Let us show that the elements $R_{\mathbf{mn}}^{(0)jl}(0,0,z)$ do not depend on j,l. Indeed, let $r_0^P(z)=(L_0^{(a)P}-z)^{-1}$ be the resolvent of the fiber operator $L_0^{(a)P}$. Using the spectral decomposition a tensor element of its kernel can be constructed in terms of the eigenfunctions [see Eq. (13)]:

$$r^P_{(0)jl}(x,x',z)=\sum_{n=-\infty}^{\infty}\frac{\Xi^{p_j}_{Nk_n^2(P)}(x)\overline{\Xi}^{p_l}_{Nk_n^2(P)}(x')}{Nk_n^2(P)-z},$$

where $Nk_n^2(P)$ are the eigenvalues of the operator $L_0^{(a)P}$. One can check by straightforward calculations that in our case ($\gamma=0$) the eigenfunctions have the form

$$\Xi^{p_l}_{Nk_n^2}(x)=\begin{cases}(Na\nu)^{-1/2}[\cos k_n x+\alpha_l^-\sin k_n x], & -a\leqslant x<0,\\ (Na\nu)^{-1/2}[\cos k_n x-\alpha_l^+\sin k_n x], & 0<x\leqslant a,\end{cases}\tag{41}$$

where

$$\alpha_l^{\pm}=\frac{e^{\pm ip_l}-\cos 2k_n a}{\cos 2k_n a}.$$

Using Eq. (41), we have

$$r^P_{(0)jl}(0,0,z)=\frac{1}{2\nu Na}\sum_{n=-\infty}^{\infty}\frac{1}{Nk_n^2(P)-z},$$

where $k_n(P)$ are the solutions of Eq. (3) with $\gamma=0$. Therefore we can see for any j, $l=1,2,\ldots,N$

$$\begin{aligned}\mathcal{A}_{\mathbf{mn}}(z)&\overset{\text{def}}{=}R^{(0)jl}_{\mathbf{mn}}(0,0,z)\\&=\frac{1}{(2\pi)^N}\int_{\mathbf{T}^N}r^P_{(0)jl}(0,0,z)e^{i(\mathbf{m}-\mathbf{n},P)}\,d^NP\\&=\frac{1}{2\nu Na(2\pi)^N}\int_{\mathbf{T}^N}e^{i(\mathbf{m}-\mathbf{n},P)}\sum_{n=-\infty}^{\infty}\frac{d^N\Theta}{Nk_n^2(\Theta)-z}.\end{aligned}\tag{42}$$

From Eqs. (39), (40), (42) we have

$$R^{jj'}_{\mathbf{mm}'}(0,x',z)=R^{(0)jj'}_{\mathbf{mm}'}(0,x',z)-\sum_{\mathbf{n}\in\mathbf{Z}^N}\mathcal{A}_{\mathbf{mn}}(z)V_{\mathbf{n}}\sum_{l=1}^{N}R^{jj'}_{\mathbf{nm}'}(0,x',z).\tag{43}$$

Summation over $j=1,2,\ldots,N$ gives

$$\sum_{j=1}^{N}R^{jj'}_{\mathbf{mm}'}(0,x',z)=\sum_{j=1}^{N}R^{(0)jj'}_{\mathbf{mm}'}(0,x',z)-N\sum_{\mathbf{n}\in\mathbf{Z}^N}\mathcal{A}_{\mathbf{mn}}(z)V_P\sum_{l=1}^{N}R^{jj'}_{\mathbf{nm}'}(0,x',z).\tag{44}$$

One can also check that $\Sigma_{j=1}^N R^{(0)jl}_{\mathbf{mm}'}(0,x,z)$ does not depend on index l. Indeed, using Eq. (13) we have

$$\sum_{j=1}^{N}R^{(0)jl}_{\mathbf{mm}'}(0,x,z)=\sum_{j=1}^{N}\int_{\mathbf{T}^N}d^NPe^{i(\mathbf{m}-\mathbf{m}',P)}\sum_{n=-\infty}^{\infty}\frac{\Xi^{p_j}_{Nk_n^2(P)}(0)\overline{\Xi}^{p_l}_{Nk_n^2(P)}(x)}{Nk_n^2(P)-z}.$$

Therefore, using Eq. (41) we get

$$\sum_{j=1}^{N}R^{(0)jl}_{\mathbf{mm}'}(0,x,z)=\frac{1}{\nu a}\int_{\mathbf{T}^N}d^NPe^{i(\mathbf{m}-\mathbf{m}',P)}\sum_{n=-\infty}^{\infty}\frac{1}{Nk_n^2(P)-z}(\cos k_n(P)x+\alpha_l(P)\sin k_n(P)x).$$

The only possible dependence on l is given through the coefficients $\alpha_l^{\pm}$ defined in Eq. (41). Therefore, the only l-dependent contribution to the latter expression is given by

$$\frac{1}{\nu a}\int_{\mathbf{T}^N} d^N P e^{\pm i p_l} e^{i(\mathbf{m}-\mathbf{m}',P)} \sum_{n=-\infty}^{\infty} \frac{\sin k_n(P)x}{Nk_n^2(P)-z}.$$

From Eq. (3) at $\gamma=0$ we see that $k_n^2(P)$ is invariant with respect to every permutation of indices $P=(p_1,p_2,\ldots,p_N)\to P'=(p_{l_1},p_{l_2},\ldots,p_{l_N})$. Therefore the same is true for the function $\Sigma_{n=-\infty}^{\infty}\sin k_n(P)x/Nk_n^2(P)-z$. Hence, the latter integral actually does not depend on l, and the same is true for $\Sigma_{j=1}^{N} R_{\mathbf{mm}'}^{(0)jj'}(0,x,z)$. Therefore we can introduce the notation

$$G_{\mathbf{mm}'}^{(0)}(x,z)\overset{\text{def}}{=}\sum_{j=1}^{N} R_{\mathbf{mm}'}^{(0)jl}(0,x,z),$$

and from Eq. (44) see that

$$G_{\mathbf{mm}'}(x,z)\overset{\text{def}}{=}\sum_{j=1}^{N} R_{\mathbf{mm}'}^{jl}(0,x,z)$$

does not depend on l as well. Eq. (40) implies

$$G_{\mathbf{mm}'}(x,z)=G_{\mathbf{mm}'}^{(0)}(x,z)-N\sum_{\mathbf{n}\in\mathbf{Z}^N}\mathcal{A}_{\mathbf{mn}}(z)V_P G_{\mathbf{nm}'}(x,z). \tag{45}$$

Combining Eqs. (39), (40), (43), (44) we can express the tensor elements of the perturbed resolvent in terms of solutions of Eq. (45):

$$R_{\mathbf{mm}'}^{jj'}(x,x',z)=R_{\mathbf{mm}'}^{(0)jj'}(x,x',z)-\sum_{\mathbf{n}\in\mathbf{Z}^N}V_{\mathbf{n}}\sum_{l=1}^{N}R_{\mathbf{mn}}^{(0)jl}(x,0,z)$$
$$\times\left(R_{\mathbf{nm}'}^{(0)lj'}(0,x',z)-\sum_{\mathbf{n}'\in\mathbf{Z}^N}\mathcal{A}_{\mathbf{nn}'}(z)V_{\mathbf{n}'}G_{\mathbf{n}'\mathbf{m}'}(x',z)\right). \tag{46}$$

Therefore, the construction of the resolvent of the operator $L^{(a)}$ is reduced to the solution of the effective tensor equation (45). Let us notice that x and z play the role of parameters in this effective equation. We omit the parameter x in the further notations and rewrite the effective equation (45) in the tensor form

$$G(z)=G^{(0)}(z)-N\mathcal{A}(z)\hat{V}G, \tag{47}$$

where tensor elements of the tensors $G(z)$, $G^0(z)$ and $\mathcal{A}(z)$ are $G_{\mathbf{mm}'}(x,z)$, $G_{\mathbf{mm}'}^{(0)}(x,z)$ and $\mathcal{A}_{\mathbf{mm}'}(z)$, respectively; $\hat{V}$ stands for a diagonal tensor with the elements $V_{\mathbf{m}}$.

We can formulate the above result in the form of the following.

Lemma 4: The tensor elements of the resolvent $R(Z)=(L_0^{(a)}+q(X)-z)^{-1}$ are given by Eq. (46), where the tensor $G(z)$ is the solution of the equation (47).

In order to study properties of the equation (47) we need the following technical result.

Lemma 5: The function

$$\tau_z(P)\overset{\text{def}}{=}\sum_{n=-\infty}^{\infty}\frac{1}{Nk_n^2(P)-z} \tag{48}$$

has bounded derivatives $\partial_{p_1p_2\ldots p_N}^N\tau_z(P)$ *on* $\mathbf{T}^N$ *for all* $z\in\mathbf{C}\setminus\mathbf{R}_+$.

Proof: Introducing the notation

$$\mu(P)\overset{\text{def}}{=}\frac{1}{N}\sum_{j=1}^{N}\cos p_j\,.$$

Due to Eq. (3) at $\gamma=0$ we have

$$k_n(P)=\frac{1}{2a}\left((-1)^n\,\mathrm{Arccos}\{\mu(P)\}+2\pi\left[\frac{n+1}{2}\right]\right),\quad n\in\mathbf{Z},\tag{49}$$

where the square bracket $[z]$ stand for the integer part of z and the inverse cosine function is assumed to take values in the interval $0\leqslant \mathrm{Arccos}\ \mu<\pi$. Hence the function $\tau_z(P)$ depends on the single variable $\mu(P)$ only,

$$\tau_z(\mu)=\sum_{n=-\infty}^{\infty}\chi_z^n(\mu),$$

where

$$\chi_z^n(\mu)\overset{\text{def}}{=}\frac{1}{N\left\{(-1)^n\mathrm{Arccos}\,\mu+2\pi\left[\frac{n+1}{2}\right]\right\}^2-z},\tag{50}$$

and one can calculate

$$\partial^2_{p_jp_l}\mu(P)=\delta_{jl}N^{-1}\sin p_j\,,$$

$$\begin{aligned}\partial^N_{p_1p_2\ldots p_N}\tau_z(\mu(P))&=\left(\prod_{j=1}^{N}\frac{\partial\mu(P)}{\partial p_j}\frac{\partial}{\partial\mu}\right)\tau_z(\mu)\\&=(-N)^N\frac{\partial^N\tau_z(\mu)}{\partial\mu^N}\prod_{j=1}^{N}\sin p_j\\&=(-N)^N\sum_{n=-\infty}^{\infty}\frac{\partial^N\chi_z^n(\mu)}{\partial\mu^N}\prod_{j=1}^{N}\sin p_j\,.\end{aligned}\tag{51}$$

The function $\mathrm{Arccos}(\mu)$ is an infinitely differentiable function everywhere in the open interval $(-1,1)\ni\mu$. Since $d/d\mu\,\mathrm{Arccos}(\mu)=-(1-\mu^2)^{-1/2}$, the derivatives $(d^s/d\mu^s)\,\mathrm{Arccos}(\mu)$ in the points $\mu=\pm1$ have has only singularities defined by the factor $(1-\mu^2)^{-s+1/2}$. The derivative $(d^N/d\mu^N)\,\chi_z^n(\mu)$ has no other singularities for any $z\in\mathbf{C}\backslash\mathbf{R}_+$ and contains the derivatives $(d^s/d\mu^s)\mathrm{Arccos}(\mu)$ with $s=0,1,2,\ldots,N$. Hence it is finite everywhere in the open interval $(-1,1)\ni\mu$ and can have poles of the order not higher than $(1-\mu^2)^{-N+1/2}$ in the points $\mu=\pm1$. However, due to the definition of function $\mu(P)$ if $\mu=\pm1$ then $\cos p_j=\pm1$ for all $j=1,1,\ldots,d$, thus $\sin p_j=0$ for all $j=1,2,\ldots,N$. Therefore the function $\Pi_{j=1}^N\sin p_j$ has zeros of the order $(1-\mu^2)^N$ in these points. Consequently, the functions $[\partial^N\chi_z^n(\mu(P))/\partial\mu^N]\,\Pi_{j=1}^N\sin\theta_j$ are bounded in the closed interval $[-1,1]\ni\mu$ (i.e., in the whole torus $\mathbf{T}^N\ni P$) for any $n\in\mathbf{Z}$ and any $z\in\mathbf{C}\backslash\mathbf{R}_+$.

One can also check that

$$\chi_z^n(\mu(P))=O(n^2)(1+o(1));$$

$$\left|\frac{\partial^N\chi_z^n(\mu(P))}{\partial\mu^N}\right|\leqslant O(n^2)(1+o(1)),$$

when $n\to\pm\infty$ for all $P\in\mathbf{T}^N$, $z\in\mathbf{C}\setminus\mathbf{R}_+$. Hence the series (49) converges.

□

The following statement is true.

Theorem 4: *For any potential $V(\mathbf{X})\in L_2(\mathbf{R}^N)\cap C(\mathbf{R}^N)$ the operator $\mathcal{A}(z)\hat{V}$ is a Hilbert–Schmidt operator in the space $l_2(\mathbf{Z}^N)$ for all $z\in\mathbf{C}\setminus\mathbf{R}_+$ if the tensor elements $\mathcal{A}_{\mathbf{mm}'}(z)$ are given by Eq. (42) and $\hat{V}$ is the diagonal tensor with elements $V_{\mathbf{m}}=\int_{K_a}V(\hat{X},\mathbf{m})d^N\hat{X}$, $\mathbf{m}\in\mathbf{Z}^N$.*

Proof: It suffices to prove that

$$\sum_{\mathbf{m},\mathbf{n}\in\mathbf{Z}^N}|(\mathcal{A}(z)\hat{V})_{\mathbf{mn}}|^2<\infty. \tag{52}$$

We have

$$\sum_{\mathbf{m},\mathbf{n}}|(\mathcal{A}(z)\hat{V})_{\mathbf{mn}}|^2=(Na(2\pi)^N)^{-2}\sum_{\mathbf{m},\mathbf{n}}\left|\int_{\mathbf{T}^N}e^{i(\mathbf{m}-\mathbf{n},P)}\tau_z(P)d^NP\int_{K_a}V(\hat{X},P)d^N\hat{X}\right|^2$$

$$=(Na(2\pi)^N)^{-2}\sum_{\mathbf{q}}\left|\int_{\mathbf{T}^N}e^{i(\mathbf{q},P)}\tau_z(P)d^NP\right|^2\sum_{\mathbf{n}}\left|\int_{K_a}V(\hat{X},\mathbf{n})d^N\hat{X}\right|^2. \tag{53}$$

First, using the Hölder inequality we estimate

$$\sum_{\mathbf{n}}\left|\int_{K_a}V(\hat{X},\mathbf{n})d^N\hat{X}\right|^2\leqslant(2a)^N\sum_{\mathbf{n}}\int_{K_a}|V(\hat{X},\mathbf{n})|^2\,d^N\hat{X}$$

$$=(2a)^N\int_{\mathbf{R}^N}|V(\mathbf{X})|^2\,d^N\mathbf{X}$$

$$=(2a)^N||V(\mathbf{X})||^2_{L_2(\mathbf{R}^N)}<\infty. \tag{54}$$

Next, using Lemma 5 we can integrate by parts and get the estimation

$$\sum_{\mathbf{n}\in\mathbf{Z}^N}\left|\int_{\mathbf{T}^N}e^{i(\mathbf{n},P)}\tau_z(P)d^NP\right|^2$$

$$=\left|\int_{\mathbf{T}^N}\tau_z(P)d^NP\right|^2+\sum_{n_1n_2\dots n_N\neq0}\left|\frac{1}{\Pi_{j=1}^Nn_j}\int_0^{2\pi}dp_1\dots\int_0^{2\pi}dp_N\,\partial^N_{p_1p_2\dots p_N}\tau_z(P)\prod_{j=1}^N e^{in_jp_j}\right|^2$$

$$\leqslant\left|\int_{\mathbf{T}^N}\tau_z(P)d^NP\right|^2+\left(\int_{\mathbf{T}^N}|\partial^N_{p_1p_2\dots p_N}\tau_z(P)|d^NP\right)^2\sum_{n_1n_2\dots n_N\neq0}\frac{1}{\Pi_{j=1}^Nn_j^2}$$

$$=\left|\int_{\mathbf{T}^N}\tau_z(P)d^NP\right|^2+\left(\frac{\pi}{3}\right)^N\left(\int_{\mathbf{T}^N}|\partial^N_{p_1p_2\dots p_N}\tau_z(P)|d^NP\right)^2<\infty. \tag{55}$$

Combining Eqs. (53)–(55) and Lemma 5 we get the proof.

□

This theorem allows us to use iteration methods in order to find the solutions of Eq. (48) and construct the resolvent of the operator $L^{(a)}$.

C. Scattering matrix

In order to discuss scattering for the pair of operators $L_0^{(a)}$ and $L^{(a)}$ it is enough to impose the condition[28]

$$\left|\int_{\Omega_a}q(x+2a\mathbf{m})dx\right|\leqslant\frac{C}{1+|\mathbf{m}|^{2+\varepsilon}},\quad\varepsilon>0.$$

By construction it is equivalent to the following condition on the potential $V(\mathbf{X})$:

$$\left| \int_{K_a} V(\mathbf{x}+2a\mathbf{m})d^N\mathbf{x} \right| \leqslant \frac{C}{1+|\mathbf{m}|^{2+\varepsilon}}.$$

Under this condition we will calculate the scattering matrix for the pair of operators $L_0^{(a)}$, $L^{(a)}$. We start with the equation for the T-matrix:[28]

$$T(z)=q_a-q_aR_0(z)T(z), \tag{56}$$

which can be solved in the same manner as the Lippmann–Schwinger equation (35) for the resolvent. Indeed, substituting Eq. (29) into Eq. (56) we have for the tensor elements of the kernel of the T-matrix,

$$T^{jj'}_{\mathbf{mm}'}(x,x',z)=\nu^{-2}V_{\mathbf{m}}\delta(x)C^{jj'}_{\mathbf{mm}'}(x',z), \tag{57}$$

where

$$C^{jj'}_{\mathbf{mm}'}(x,z)\overset{\text{def}}{=}\nu^{-2}\delta(x-x')\,\delta_{\mathbf{mm}'}\delta_{jj'}-\sum_{\mathbf{n}}\sum_{l}\int_0^a dy R^{(0)jl}_{\mathbf{mn}}(0,y,z)T^{lj'}_{\mathbf{nm}'}(y,x,z).$$

Hence $C^{jj'}_{\mathbf{mm}'}(x,z)$ obeys the following equation:

$$C^{jj'}_{\mathbf{mm}'}(x,z)=\nu^{-2}\delta(x)\,\delta_{\mathbf{mm}'}\delta_{jj'}-\sum_{\mathbf{n}}\sum_{l}V_{\mathbf{n}}R^{(0)jl}_{\mathbf{mn}}(0,0,z)C^{lj'}_{\mathbf{mn}'}(x,z). \tag{58}$$

Using the fact that the coefficients $R^{(0)jl}_{\mathbf{mn}}(0,0,z)$ do not depend on indices j,l, we denote

$$J^l_{\mathbf{mn}}(x,z)\overset{\text{def}}{=}\sum_{j=1}^{2N}C^{(0)jl}_{\mathbf{mn}}(x,z) \tag{59}$$

and get

$$Q^l_{\mathbf{mm}'}(x,z)=\delta(x)\,\delta_{\mathbf{mm}'}-N\sum_{\mathbf{n}}\mathcal{A}_{\mathbf{mn}}V_PQ^l_{\mathbf{nm}'}(x,z). \tag{60}$$

This equation shows that $J^l_{\mathbf{mm}'}(x,z)$ does not depend on the index l. Therefore it can be omitted and we get the equation

$$\sum_{\mathbf{n}}(\delta_{\mathbf{mn}}+N\mathcal{A}_{\mathbf{mn}}V_P)J_{\mathbf{nm}'}(x,z)=\nu^{-2}\delta(x)\,\delta_{\mathbf{mm}'}, \tag{61}$$

or in tensor form,

$$(I+N\mathcal{A}(z)\hat{V})J(x,z)=\nu^{-2}\delta(x)I. \tag{62}$$

By Eqs. (56)–(60) tensor elements of the T-matrix can be expressed in terms of the solution of Eq. (62) as

$$T^{jj'}_{\mathbf{mm}'}(x,x',z)=\nu^{-2}\delta(x)\,\delta(x')V_{\mathbf{m}}\left(\delta_{\mathbf{mm}'}\delta_{jj'}-\sum_{\mathbf{n}}\mathcal{A}_{\mathbf{mn}}(z)V_{\mathbf{n}}(I+N\mathcal{A}(z)\hat{V})^{-1}_{\mathbf{nm}'}\right)$$

$$=\nu^{-2}\delta(x)\,\delta(x')V_{\mathbf{m}}(\delta_{mm'}\delta_{jj'}-(\mathcal{A}(z)\hat{V}(I+N\mathcal{A}(z)\hat{V})^{-1})_{\mathbf{mm}'}).$$

Introducing the notation

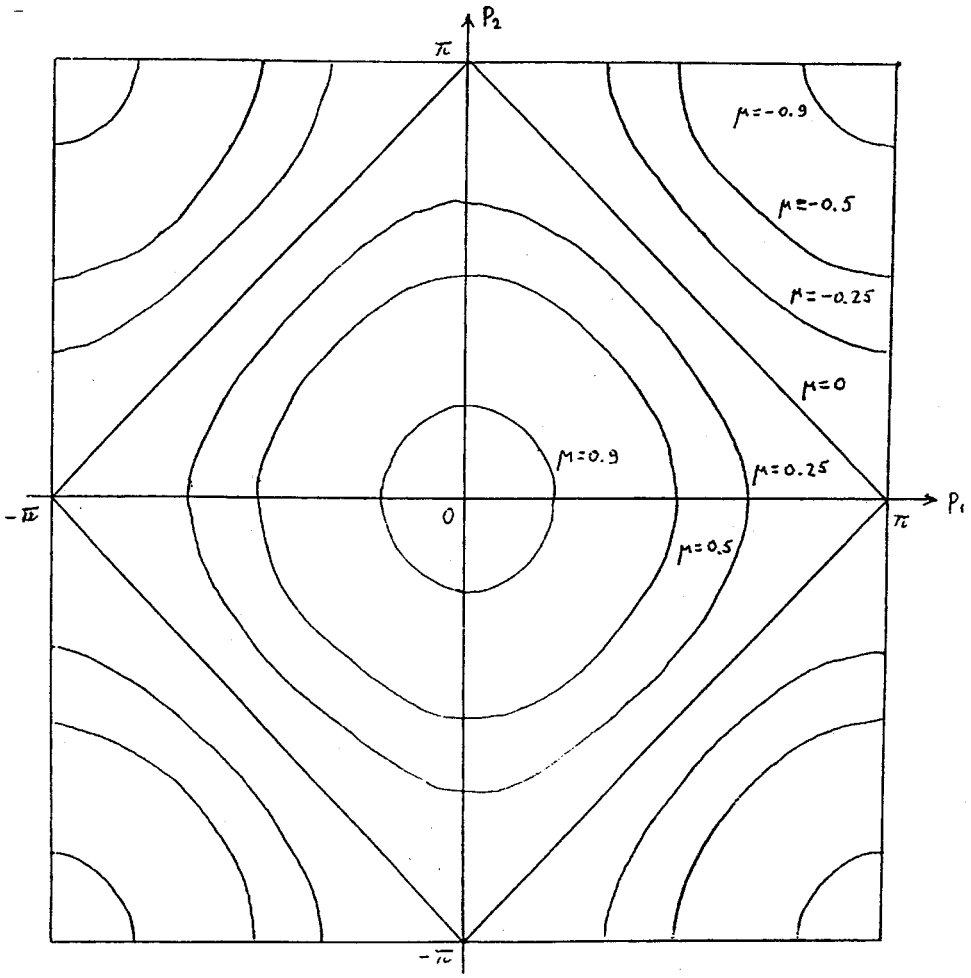

FIG. 2. Isoenergetic surfaces $\mu(P)=\text{const}$ of the Hamiltonian $L^{(a)}$ in the quasimomentum torus $\mathbf{T}^N$ in case $N=2$.

$$\mathcal{D}(z)\overset{\text{def}}{=}\mathcal{A}(z)\hat{V}(I+N\mathcal{A}(z)\hat{V})^{-1}, \tag{63}$$

we can write down the latter formula as

$$T^{jj'}_{\mathbf{mm}'}(x,x',z)=\nu^{-2}\delta(x)\,\delta(x')V_{\mathbf{m}}(\delta_{\mathbf{mm}'}\delta_{jj'}-\mathcal{D}_{\mathbf{mm}'}(z)). \tag{64}$$

Knowing the kernel of the T-matrix we can construct the scattering matrix in the standard way.[28] In order to construct the scattering matrix for a fixed energy, let us define the isoenergetic surface $\mathcal{T}_\lambda\subset\mathbf{T}^N$ for any fixed energy $\lambda>0$ as follows. The set of all possible quasimomenta P for the fixed energy λ:

$$\mathcal{T}_\lambda\overset{\text{def}}{=}\{P\in\mathbf{T}^N:\mu(P)=\cos 2a\sqrt{\lambda/N}\},$$

where $\mu(P)=(1/N)\,\Sigma_{j=1}^{N}\cos p_j$. Isoenergetic surfaces in case $N=2$ are shown in Fig. 2. Due to Eq. (3) with $\gamma=0$ for a fixed energy $\lambda=Nk_n^2(P)$ we have $\cos 2ak_n(P)=\mu(P)$. Let us fix some energy $\lambda>0$ and suppose that $P,P'\in\mathcal{T}_\lambda$. The corresponding unit vectors are denoted by $\hat{P},\hat{P}'$.

The corresponding wave functions of the unperturbed Hamiltonian $L_0^{(a)}$ given by Eq. (23) we denote by Ξ_λ^P, $\Xi_\lambda^{P'}$. We can calculate the kernel of the scattering operator in the unperturbed representation as[28]

$$S_\lambda(P,P') = \delta(\hat{P}-\hat{P}') - 2\pi i \langle T(\lambda+i0)\Xi_\lambda^{P'}, \Xi_\lambda^P \rangle_{\mathcal{H}_a}.$$

For fixed energy $\lambda = Nk_n^2(P)$ we can write

$$S_{nn'}(P,P') = \delta_{nn'}[\,\delta(\hat{P}-\hat{P}') - 2i\pi\delta(\mu(P)-\mu(P'))\langle T(Nk_n^2(P)+i0)\Xi_{Nk_n^2}^{P'}, \Xi_{Nk_n^2}^P\rangle_{\mathcal{H}_a}]. \tag{65}$$

This leads to the following statement.

Theorem 5: *Under the condition of the existence of the scattering matrix for the pair of operators* $L_0^{(a)}$, $L_0^{(a)}+q_a$, *its matrix elements* $S_{nn'}(P,P')$ *for fixed energy* $\lambda = Nk_n^2(P)$ *are given by the following formula*:

$$S_{nn'}(P,P') = \delta_{nn'}\Bigg[\,\delta(\hat{P}-\hat{P}') - \delta(\mu(P)-\mu(P'))\Bigg(\frac{2\pi i}{a\nu}\sum_{\mathbf{m}} V_{\mathbf{m}} e^{-i(P-P',\mathbf{m})} + \frac{2\pi i N}{a\nu}\sum_{\mathbf{m}} V_{\mathbf{m}} e^{-i(P,\mathbf{m})}\sum_{\mathbf{m}'} \mathcal{D}_{\mathbf{m}\mathbf{m}'}(Nk_n^2(P)+i0)e^{i(P',\mathbf{m}')}\Bigg)\Bigg], \tag{66}$$

where $\mathcal{D}_{\mathbf{m}\mathbf{m}'}(z)$ *are the tensor elements of the tensor* $\mathcal{D}(z)$ *given by Eq. (64).*

The proof is obvious by substituting Eqs. (41), (64) into Eq. (65).

□

A natural question appears. Is the above constructed scattering matrix for the system on the graph Γ_a related to the scattering matrix associated with the original N-dimensional Schrödinger dynamics? In order to clarify this question one has to construct the ''representative'' of the plane wave $e^{i(Q,X)}$; $Q,X \in \mathbf{R}^N$, on the graph Γ_a, observe its scattering under the evolution on Γ_a, and, finally, associate the resulting scattered waves in Γ_a with scattered waves in $\mathbf{R}^N$.

We propose the following procedure. As the main aim in the description of scattering processes is to obtain the angular distribution of the scattered wave given the incoming plane wave, we have to establish a correspondence between the direction of the propagation of the plane wave $e^{i(Q,\mathbf{X})}$ and of its Γ_a-''representative.'' In this context, the correspondence between the angle $\hat{Q} = Q/|Q|$ and the direction of the wave propagation in Γ_a should be kept intact. The following steps meet this requirement.

(1) Given the $\mathbf{R}^N$-plane wave $e^{i(Q,\mathbf{X})}$ we calculate the quasimomentum $P_Q = 2aQ(\mathrm{mod}\,2\pi)$.
(2) We calculate the function $\mu(P_Q) = (1/N)\sum_{j=1}^N \cos(P_Q)_j = (1/N)\sum_{j=1}^N \cos 2aq_j$. In case $\mu(P_Q)<0$ or $\mu(P_Q)>0$ (as illustrated in Fig. 3 for $N=2$) we fix the direction of the quasimomentum P_Q, i.e., the ray Λ_Q with the origin in the point $P_+ = \{p_j = 0\}_{j=1}^N$ [for $\mu(P_Q)>0$] or in the point $P_- = \{p_j = \pi\}_{j=1}^N$ [for $\mu(P_Q)>0$] and containing the point P_Q.
(3) Given the $\mathbf{R}^N$-dynamics energy $E = |Q|^2$, we introduce the value $\tilde{\mu}_Q \overset{\text{def}}{=} \cos 2a|Q|$. Then, for any quasimomentum $P \in \tilde{\mathcal{T}}_Q$ on the isoenergetic surface $\tilde{\mathcal{T}}_Q = \{P:\mu(P) = \tilde{\mu}_Q\}$ (see Fig. 3) we have the correspondence between the $\mathbf{R}^N$-energy and the Γ_a-energy.
(4) We find the intersection point $\tilde{P}_Q = \tilde{\mathcal{T}}_Q \cap \Lambda_Q$. The quasimomentum $\tilde{P}_Q$ corresponds to the Γ_a-energy equal to $|Q|^2$ (because $\tilde{P}_Q \in \tilde{\mathcal{T}}_Q$), if the number of the mode n: $E = |Q|^2 = Nk_n^2(\tilde{P}_Q)$ is chosen properly (see step 5). On the other hand, it corresponds to the same direction of the wave propagation as the $\mathbf{R}^N$-plane wave $e^{i(Q,\mathbf{X})}$ (because $\tilde{\Theta}_Q \in \Lambda_Q$).

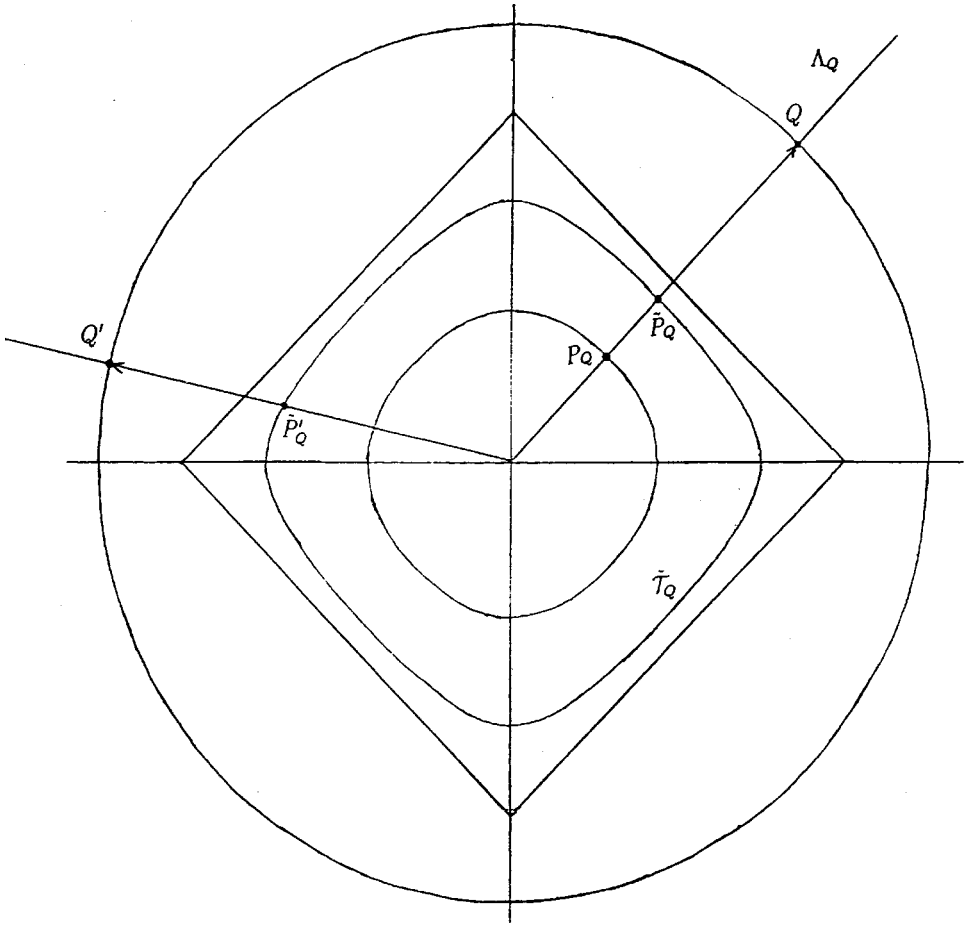

FIG. 3. Procedure for the approximation of the scattering of N-dimensional plane wave $e^{i(Q,\mathbf{X})}$ through the scattering process on the graph Γ_a.

(5) Given the $\mathbf{R}^N$-dynamics energy $E=|Q|^2$, we calculate the number of the mode of the corresponding wave function in Γ_a:

$$n_Q=\left[\frac{2a}{\pi}|Q|\right].$$

(6) ' We take the corresponding eigenfunction $\Xi^{\tilde{P}_Q}_{Nk^2_{n_Q}}(x)$ of the fiber Hamiltonian $L_0^{(a)\tilde{P}_Q}$ and consider the function

$$\Xi^{\tilde{P}_Q}_{Nk^2_{n_Q}}(x)e^{i(\mathbf{m},\tilde{P}_Q)}, \tag{67}$$

as the ''representative'' of the $\mathbf{R}^N$-plane wave $e^{i(Q,\mathbf{X})}$ on the graph Γ_a. By construction, this wave propagates in the same direction as $e^{i(Q,\mathbf{X})}$ and has the same Γ_a-energy $Nk^2_{n_Q}(\tilde{P}_Q)=|Q|^2$ as the $\mathbf{R}^N$-energy of the plane wave $e^{i(Q,\mathbf{X})}$.

(7) We consider the scattering of the wave (67) in the graph Γ_a:

$$S:\Xi^{\tilde{P}_Q}_{Nk^2_{n_Q}}(x)e^{i(\mathbf{m},\tilde{P}_Q)}\mapsto\int_{\tilde{\mathcal{T}}_Q}S_{n_Qn_Q}(\tilde{P}'_Q,\tilde{P}_Q)\Xi^{\tilde{P}'_Q}_{Nk^2_{n_Q}}(x)e^{i(\mathbf{m},\tilde{P}'_Q)}d\tilde{P}'_Q.$$

The scattered wave thus obtained is a composition of the waves $\Xi^{\tilde{P}'_Q}_{Nk^2_{n_Q}}(x)e^{i(\mathbf{m},\tilde{P}'_Q)}$, $\tilde{P}'_Q\in\tilde{\mathcal{T}}_Q$ (see Fig. 3).

(8) For every $\tilde{P}'_Q \in \tilde{\mathcal{T}}_Q$ we calculate the momentum $Q' = \tilde{P}'_Q(|Q|/|\tilde{P}'_Q|)$ (see Fig. 3) and construct the $\mathbf{R}^N$-plane wave $e^{i(Q',\mathbf{X})}$. It propagates in the same direction as the Γ_a-wave $\Xi^{\tilde{P}'_Q}_{Nk^2_{n_Q}}(x)e^{i(\mathbf{m},\tilde{P}'_Q)}$ and has the energy $|Q'|^2 = |Q|^2$.

(9) We define the action of the approximate scattering matrix for the $\mathbf{R}^N$-dynamics as

$$\mathbf{S}_a^{approx}: e^{i(Q,\mathbf{X})} \mapsto \int_{\tilde{\mathcal{T}}_Q} S_{n_Q n_Q}(\tilde{P}'_Q, \tilde{P}_Q) e^{i|Q|(\tilde{P}'_{Q'}|\tilde{P}'_Q|,\mathbf{X})}\, d\tilde{P}'_Q. \tag{68}$$

This 9-step procedure is necessary. Indeed a simple restriction of the plane wave $e^{(Q,\mathbf{X})}$ to the graph Γ_a,

$$e^{i(Q,X)}|_{\Gamma_a} = v_Q(x)e^{i2a(\mathbf{m},P_Q)}, \tag{69}$$

where $P_Q = 2aQ(\mathrm{mod}\, 2\pi)$, i.e., $(P_Q)_l = 2aq_l(\mathrm{mod}\, 2\pi)$, $l = 1,2,\ldots,N$, and $v^j_Q(x_j) = e^{iq_j x_j}$, brings the following difficulty. Function (69) is associated with the quasimomentum $P_Q = 2aQ(\mathrm{mod}2\pi)$, but it corresponds to a wave packet containing components with different energies. Indeed, one can decompose the function $v_Q(x)$ defined on the fundamental subgraph Ω_a in terms of the eigenfunctions of the fiber Hamiltonian $L_0^{(a)P_Q}$:

$$v_Q(x) = \sum_{n\geqslant 0} c^n_Q \Xi^{P_Q}_{Nk^2_n}(x),$$

where

$$c^n_Q = \langle v_Q(x), \Xi^{P_Q}_{Nk^2_n}\rangle_{L_2(\Omega_a)},$$

and Eq. (69) can be rewritten as

$$e^{i(Q,X)}|_{\Gamma_a} = \sum_{n\geqslant 0} c^n_Q \Xi^{P_Q}_{Nk^2_n}(x)e^{i2a(\mathbf{m},P_Q)}. \tag{70}$$

This is a wave packet with the components all having the same quasimomentum $P_Q = 2aQ(\mathrm{mod}\, 2\pi)$ but different energies $Nk^2_n(P_Q)$. However, all these energies may be different from the energy $|Q|^2$ of the plane wave $e^{i(Q,\mathbf{X})}$ if the latter is considered in the frame of the original N-dimensional Schrödinger dynamics. Indeed, this energy equals

$$|Q|^2 = \sum_{l=1}^{N} q_l^2, \tag{71}$$

while the energies $Nk^2_n(\Theta_P)$ are determined by the equation

$$\cos 2ak_n(P_Q) = \mu(P_Q) = \frac{1}{N}\sum_{l=1}^{N} \cos(P_Q)_l = \frac{1}{N}\sum_{l=1}^{N} \cos 2aq_l,$$

i.e.,

$$Nk^2_n(P_Q) = \frac{N}{4a^2}\left((-1)^n \mathrm{Arccos}\left(\frac{1}{N}\sum_{l=1}^{N} \cos 2aq_l\right) + 2\pi\left[\frac{n+1}{2}\right]\right)^2. \tag{72}$$

Obviously, the right hand sides of Eqs. (71) and (72) are different for almost all sets $\{q_l\}$. Therefore, if we have the same direction of the wave propagation in $\mathbf{R}^N$ and in Γ_a [i.e., the quasimomentum $P = P_Q = 2aQ(\mathrm{mod}\, 2\pi)$], we cannot, in the general case, have the correspon-

dence of the energies. This is a manifestation of the fact that the relations between energy and momentum (quasimomentum) are not the same for the dynamics in $\mathbf{R}^N$ and in Γ_a. Therefore, if one takes the function (69) as the ''representative'' of the plane wave $e^{i(Q,\mathbf{X})}$, the scattering process in Γ_a will not preserve the energy of the $\mathbf{R}^N$-dynamics. It makes it difficult to approximate in this way the $\mathbf{R}^N$-scattering process by the Γ_a-scattering process. This problem does not appear if one uses the 9-step procedure described above.

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Families of exact solutions of a two-dimensional gravity model minimally coupled to electrodynamics

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Three families of exact solutions for two-dimensional gravity minimally coupled to electrodynamics are obtained in the context of $\mathcal{R}=T$ theory. It is shown, by supersymmetric formalism of quantum mechanics, that the quantum dynamics of a neutral bosonic particle on static backgrounds with both varying curvature and electric field is exactly solvable. © *2001 American Institute of Physics.*
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I. INTRODUCTION

It is well-known that Einstein's gravitational theory in two-dimensions is trivial. This is because the Einstein tensor is identically zero for all two-dimensional metrics. Consequently, the Einstein equations require the energy-momentum tensor to be vanished and this result is inconsistent with some nontrivial matter configurations.[1] Also, in the mathematical language the Euler class χ of a compact and two-dimensional manifold M with boundary ∂M is defined by[2]

$$2\pi\chi=\frac{1}{2}\int_M d^2x\sqrt{-g}\mathcal{R}-\int_{\partial M}\sqrt{-g}K,$$

where $\mathcal{R}$ is the Ricci scalar and K is the trace of the extrinsic curvature K_{ij}. Therefore, if we demand more useful information on a two-dimensional space–time a different gravitational action is required. An interesting action for two-dimensional gravity has been derived in the context of string theory.[3] However, despite the string theory approach it has been recently shown that gravity in two-dimensions is not necessarily trivial.[1,4] Of particular interest among these new approaches is the $\mathcal{R}=T$ theory of two-dimensional gravity in which the scalar curvature $\mathcal{R}$ is equal to the trace of the energy-momentum tensor T.[1,4] This theory has provided some remarkable classical and semiclassical results such as: Well defined Newtonian limit,[5] black hole solutions,[4,6] gravitational radiation, Friedmann–Robertson–Walker (FRW) cosmology, gravitational collapse,[7] black hole radiation,[8] and their thermodynamical properties.[4] On the other hand, there are some similarities between four-dimensional and two-dimensional gravity. Therefore, the study of classical and quantum behavior of $\mathcal{R}=T$ theory of two-dimensional gravity may help us to get a deeper insight into the problems involved in four-dimensional gravity.

In this paper (We use the units in which $\hbar=c=8\pi G=1$.), we find families of exact solutions of two-dimensional $\mathcal{R}=T$ type gravity minimally coupled to electrodynamics. Then, we investigate the quantum dynamics of a neutral bosonic particle on the obtained class of static solutions by using the supersymmetric quantum mechanics and obtain the energy spectrum and eigenfunctions exactly. In Secs. II and III, we introduce the model and obtain three families of exact solutions for: (a) two-dimensional manifolds with constant curvature and varying electric field, (b) two-

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dimensional manifolds with varying curvature and constant electric field, and (c) two-dimensional manifolds with both varying curvature and electric field. Then, in Sec. IV the quantum dynamics of a neutral bosonic particle on the obtained static backgrounds with both varying curvature and electric field is investigated in the context of supersymmetric quantum mechanics. The paper ends with a brief conclusion.

II. THE MODEL

It is well-known that in two dimensions one can write locally the metric in the form[9]

$$g(X)=e^{\phi(X)}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \tag{1}$$

where $X:=(t,x)$ and $\phi(X)$ is a scalar field. The Ricci scalar for the metric (1) is given by

$$\mathcal{R}(X)=e^{-\phi(X)}(\partial_x^2-\partial_t^2)\phi(X). \tag{2}$$

Now, we put the matter as a Maxwell field with strength tensor $F_{\mu\nu}(\mu,\nu=0,1)$ on the above two dimensional Lorentzian geometry. We are interested in $\mathcal{R}=T$ theory of two-dimensional gravity in which ''T'' is the trace of electromagnetic energy-momentum tensor given by

$$T_{\alpha\beta}=-\epsilon(F_{\alpha\mu}F^{\mu}_{\beta}-\tfrac{1}{4}g_{\alpha\beta}F_{\lambda\sigma}F^{\lambda\sigma}), \tag{3}$$

where $|\epsilon|=1$ and its sign is arbitrary. The $T_{\alpha\beta}$ in Eq. (3) is the special case of one which was already considered by Mann *et al.*[6] for charged point particles.

The coupled Einstein–Maxwell field equations are as follows:[6]

$$\mathcal{R}=T, \tag{4}$$

$$\frac{1}{\sqrt{-g}}\partial_\nu(\sqrt{-g}F^{\mu\nu})=J^\mu, \tag{5}$$

where the first is the Einstein gravity in two-dimensions and the second is the Maxwell equation in two-dimensional curved space–time from which the current conservation is easily derived. We note that the electromagnetic field $F_{\mu\nu}$ in two-dimensions has only one independent nonzero component as electric field namely

$$F_{tx}=E(X). \tag{6}$$

Therefore, considering the form of strength tensor $F_{\mu\nu}$ in Eq. (6) the trace of energy-momentum tensor (3) is obtained as

$$T=\epsilon e^{-2\phi}E^2. \tag{7}$$

Substituting the scalar curvature (2) and the trace (7) into Eq. (4) we have

$$(\partial_t^2-\partial_x^2)\phi(X)+\epsilon e^{-\phi(X)}E^2(X)=0. \tag{8}$$

III. THREE FAMILIES OF EXACT SOLUTIONS

Now, we classify the solutions of Einstein–Maxwell field equations in three categories.

A. 2D manifolds with constant scalar curvature and varying electric field

Assuming the constant scalar curvature $\mathcal{R}(X)=\mathcal{R}_0$ and considering Eq. (4) we find the varying electric field as

$$E(X)=\pm\sqrt{\frac{\mathcal{R}_0}{\epsilon}}e^{\phi(X)}. \tag{9}$$

In Eq. (9) the parameter ϵ is suitably chosen so that for negative or positive scalar curvature $\mathcal{R}_0$ the electric field is always a real quantity. In this way, for $\mathcal{R}_0<0$ (one-sheet hyperboloid or a half plane) and for $\mathcal{R}_0>0$ (a strip or a half plane) we should correspond $T<0$ and $T>0$, respectively. Using (9), Eq. (8) becomes

$$(\partial_t^2-\partial_x^2)\phi(X)+\mathcal{R}_0 e^{\phi(X)}=0, \tag{10}$$

which is known as Liouville equation.[10] It is worth noting that Eq. (10) was considered, at first, in the study of *pure mathematical theory* of two-dimensional surfaces with constant curvature and is derived here through the *physical* $\mathcal{R}=T$ theory of gravity in two-dimensions with constant curvature. Of course, it is not so surprising because in the matter coupled gravity theory here, with dynamical variables $g_{\mu\nu},F_{\mu\nu}$, and ϕ, the condition $\mathcal{R}=T$ may give rise to a dynamical equation in gravity (geometry) sector with variables $\mathcal{R},\phi$, and by taking a constant value for $\mathcal{R}$ it falls into the Liouville's mathematical context. In other words, Eq. (10) is the Liouville equation in which the constancy of curvature is introduced through the physical theory as $\mathcal{R}=T=\text{Const}$.
General solutions of Eq. (10) is given by[11]

$$\phi(x^+,x^-)=\log\frac{8A'_+(x^+)A'_-(x^-)}{|\mathcal{R}_0|\left[A_+(x^+)-\dfrac{|\mathcal{R}_0|}{\mathcal{R}_0}A_-(x^-)\right]^2}, \tag{11}$$

where

$$A'_\pm:=\frac{dA_\pm}{dx^\pm},\quad x^\pm=t\pm x.$$

Substituting the solutions for ϕ, Eq. (11), into Eqs. (1) and (9) the metric solution and electric field are explicitly obtained with respect to arbitrary functions $A_\pm(x^\pm)$ as

$$ds^2=\frac{8A'_+(x^+)A'_-(x^-)}{|\mathcal{R}_0|\left[A_+(x^+)-\dfrac{|\mathcal{R}_0|}{\mathcal{R}_0}A_-(x^-)\right]^2}dx^+dx^-, \tag{12}$$

$$E(x^+,x^-)=\pm\sqrt{\frac{\mathcal{R}_0}{\epsilon}}\frac{8A'_+(x^+)A'_-(x^-)}{|\mathcal{R}_0|\left[A_+(x^+)-\dfrac{|\mathcal{R}_0|}{\mathcal{R}_0}A_-(x^-)\right]^2}. \tag{13}$$

Using Eq. (5) one can easily show that the covariant current J^μ corresponding to the solutions (12), (13) vanishes. The metric (12) describes a family of two-dimensional Lorentzian manifolds with the same constant curvature $\mathcal{R}_0$. In Ref. 11 it was shown that all two-dimensional Lorentzian manifolds with the same constant curvature are locally isometric. Therefore, as a result, it may be said that all metrics defined by (12) are locally isometric.

B. 2D manifolds with varying scalar curvature and constant electric field

In this case, by assumption of a constant electric field as $E(X)=E_0$ Eq. (8) is written as

$$(\partial_t^2-\partial_x^2)\phi(X)+\epsilon E_0^2 e^{-\phi(X)}=0. \tag{14}$$

As before, one can show that general solution to Eq. (14) is given by

$$\phi(x^+,x^-)=-\log\frac{8B'_+(x^+)B'_-(x^-)}{E_0^2\left[B_+(x^+)+\frac{1}{\epsilon}B_-(x^-)\right]^2}, \tag{15}$$

where $B_\pm(x^\pm)$ are arbitrary functions of their arguments. Considering the solution (15) the metric solution and the scalar curvature are given as

$$ds^2=\frac{E_0^2\left[B_+(x^+)+\frac{1}{\epsilon}B_-(x^-)\right]^2}{8B'_+(x^+)B'_-(x^-)}dx^+dx^-, \tag{16}$$

$$\mathcal{R}(x^+,x^-)=\frac{64\epsilon}{E_0^2}\left[\frac{B'_+(x^+)B'_-(x^-)}{\left[B_+(x^+)+\frac{1}{\epsilon}B_-(x^-)\right]^2}\right]^2. \tag{17}$$

The current **J** corresponding to the solutions (16) and (17) has the components

$$J^\pm=\mp 2E_0e^{-2\phi}\partial_\mp\phi, \tag{18}$$

where the functions ϕ are given by Eq. (15).

C. 2D manifolds with varying scalar curvature and varying electric field

In this case considering Eqs. (2) and (8) the following relation between the scalar curvature and the electric field is obtained

$$E(X)=e^{\phi(X)}\sqrt{\frac{\mathcal{R}(X)}{\epsilon}}. \tag{19}$$

For each given function $\phi(X)$ one can find, using Eqs. (1), (2), and (19), the corresponding metric solution and electric field. Moreover, the current which produces the electric field (19) is obtainable by Eq. (5). For example, for ϕ as merely a function of spatial coordinate x, namely for a static space–time, we find $J^x=0$ and that the static electric field is produced by J^t component. The importance of two-dimensional manifolds with both varying scalar curvature and electric field in the static case, as will be shown in the next section, is that the quantum dynamics of a neutral bosonic particle on these manifolds is solvable exactly by using the *Supersymmetric quantum mechanics* and *Shape invariance*.

IV. QUANTUM DYNAMICS OF A NEUTRAL BOSONIC PARTICLE ON STATIC 2D MANIFOLDS WITH VARYING SCALAR CURVATURE AND VARYING ELECTRIC FIELD

Quantization of particle dynamics in two-dimensions with constant curvature for both massive and massless particles was investigated in Ref. 11. Here, our aim is to quantize the particle dynamics on the manifold discussed in Sec. III C of the previous section in the static case. Quantum dynamics of a massive neutral bosonic particle is described by two-dimensional Klein–Gordon equation

$$\frac{1}{\sqrt{-g}}\partial_\alpha(\sqrt{-g}g^{\alpha\beta}\partial_\beta)\Psi(X)+m^2\Psi(X)=0,$$

where m is the mass of the particle. Assuming the scalar wave function $\Psi(X)$ as

$$\Psi(x,t)=e^{-i\mathcal{E}t}\psi(x),$$

the Klein–Gordon equation on the two-dimensional (2D) manifold obtained by the metric (1) in the static case $[\phi=\phi(x)]$ becomes

$$\left[-\frac{d^2}{dx^2}+m^2(e^{\phi(x)}-1)\right]\psi(x)=(\mathcal{E}^2-m^2)\psi(x). \tag{20}$$

Equation (20) is mathematically equivalent to one-dimensional time-independent Schrödinger equation. We use the supersymmetric quantum mechanics to solve this equation. In supersymmetric quantum mechanics the *creation* and *annihilation* operators are defined, respectively, as[12,13]

$$\mathcal{A}^{\dagger}:=-\frac{d}{dx}+W(x),$$

$$\mathcal{A}:=\frac{d}{dx}+W(x),$$

where $W(x)$ is called the *Superpotential*. The supersymmetric *Partner* Hamiltonians namely $H_+=\mathcal{A}\mathcal{A}^{\dagger}, H_-=\mathcal{A}^{\dagger}\mathcal{A}$ have the following form:

$$H_{\pm}=-\frac{d^2}{dx^2}+V_{\pm}(x) \tag{21}$$

where the partner potentials $V_{\pm}(x)$ are given with respect to the superpotential $W(x)$ as

$$V_{\pm}(x)=W^2(x)\pm\frac{dW(x)}{dx}. \tag{22}$$

If the partner potentials $V_{\pm}(a_0,x)$ (with a_0 as a constant parameter) are related according to the relation

$$V_+(a_0,x)=V_-(a_1,x)+R(a_1), \tag{23}$$

then they are called *Shape-invariant* potentials.[14] In Eq. (23), $a_1=F(a_0)$ is a new set of parameters and the term $R(a_1)$ is x independent. For shape-invariant potentials given by Eq. (23) the spectrum and eigenfunctions are obtained by algebraic approach.[12] Comparing the left-hand side of Eq. (20) with Eq. (21) we deduce

$$m^2(e^{\phi_{\pm}(x)}-1)=V_{\pm}(x), \tag{24}$$

which relates the conformal factors $e^{\phi_{\pm}(x)}$ to the partner potentials $V_{\pm}(x)$. In fact, the supersymmetry and conformal degree of freedom let us to have two sets of two-dimensional static manifolds with varying curvature

$$ds_{\pm}^2=e^{\phi_{\pm}(x)}(dt^2-dx^2),$$

together with static electric fields $E_{\pm}(x)$. For example, by a suitable choice for the conformal factor as

$$e^{\phi_-(x)}=\frac{\omega}{2m^2}\left(\frac{\omega}{2}x^2-1\right)+1, \tag{25}$$

we may consider the following superpotential

$$W(x)=\tfrac{1}{2}\omega x, \quad \omega>0, \tag{26}$$

where ω is a quantity with the dimension of $(mass)^2$ or $(length)^{-2}$ in the units $\hbar=c=1$. Now, in order to study the one set of solutions we calculate the partner potential $V_-(x)$, by using Eq. (24), as

$$V_-(x)=\frac{\omega}{2}\left(\frac{\omega}{2}x^2-1\right). \tag{27}$$

Using Eq. (24) we can obtain the energy and wave function[12,13]

$$\mathcal{E}_n^2=m^2+n\omega, \quad n=0,1,2,\ldots,$$

$$\psi_n(x)=C_n\exp\left(-\frac{\omega}{4}x^2\right)H_n\left(\sqrt{\frac{\omega}{2}}x\right), \tag{28}$$

where C_n is the normalization constant. The static metric solution and electric field corresponding to the conformal factor given by (25) are as follows:

$$ds_-^2=\left[1+\frac{\omega}{2m^2}\left(\frac{\omega}{2}x^2-1\right)\right](dt^2-dx^2), \tag{29}$$

$$E_-(x)=\sqrt{\frac{\omega^2}{2m^2\epsilon}\frac{1-\frac{\omega}{2m^2}\left(\frac{\omega}{2}x^2+1\right)}{1+\frac{\omega}{2m^2}\left(\frac{\omega}{2}x^2-1\right)}}. \tag{30}$$

The current corresponding to the electric field (30) has the nonvanishing component

$$J^t(x)=-e^{-\phi_-(x)}\partial_x[e^{-\phi_-(x)}E_-(x)]. \tag{31}$$

It is easy to show that for $1-2m^2/\omega\geqslant 0$ the metric (29) is degenerate at

$$x=\pm\sqrt{\frac{2}{\omega}\left(1-\frac{2m^2}{\omega}\right)}. \tag{32}$$

On the other hand, by calculating the Ricci scalar corresponding to the metric (29) as

$$\mathcal{R}=\frac{\omega^2}{2m^2}\frac{1-\frac{\omega}{2m^2}-\frac{\omega^2x^2}{4m^2}}{\left[1+\frac{\omega}{2m^2}\left(\frac{\omega}{2}x^2-1\right)\right]^3}, \tag{33}$$

we find that the geometry defined by (29) has also essential singularities at the points (32). The general existence of these *naked* singular points indicates that the particle dynamics is exactly solvable in the part of the manifold not including these singular points. Alternatively, it seems possible to avoid the singular behavior only in a sub-class of manifold by appropriate choices of the values on ω and m. To this end, we may restrict ourselves to the values of m and ω satisfying the relation $1-2m^2/\omega<0$, which makes the metric (29) free of singularity. Then, we have

$$\begin{cases} \mathcal{R}=0 & \text{at the points} \quad x_0^{\pm}=\pm\sqrt{-\frac{2}{\omega}\left(1-\frac{2m^2}{\omega}\right)} \\ \mathcal{R}>0 & \text{for the range} \quad x_0^-<x<x_0^+ \\ \mathcal{R}<0 & \text{for } x>x_0^+ \quad \text{and } x<x_0^- \end{cases}.$$

Finally, we point out that for each partner potential $V_+(x)$ corresponding to the conformal factor $e^{\phi_+(x)}$ we may obtain a set of static two-dimensional manifolds with varying curvature together with nonvanishing electric field with nontrivial current distribution. Obviously, the same procedure may be exactly applied for other shape-invariant potentials given by Refs. 12 and 13.

V. CONCLUDING REMARKS

In this paper we have found three families of exact solutions for two-dimensional $\mathcal{R}=T$ theory of gravity minimally coupled to electrodynamics. By the study of quantum dynamics of a neutral bosonic particle on a static two-dimensional space–time background we have shown that: *Supersymmetric formalism of quantum mechanics leads to two disjoint sets of static two-dimensional manifolds with both varying curvature and electric field*. It is possible to solve exactly the quantum dynamics of a neutral bosonic particle on these manifolds. It seems that the study of quantum dynamics of a fermionic particle in two-dimensional space–time may lead to two-dimensional Lorentzian manifolds as the solutions of 2D gravity coupled to electrodynamics and also to the quantum solvability of particle dynamics on these manifolds.[15]

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On combined standard–nonstandard or hybrid (q,h)-deformations

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Combined (q,h)-deformations proposed by Kupershmidt and Ballesteros–Herranz–Parashar are studied. In each case a transformation is shown to lead to an equivalent, standard q-deformation. We briefly indicate that appropriate singular limits of the same type of transformations can however lead from standard biparametric (p,q)-deformations to nonhybrid but biparametric nonstandard (g,h) ones. Finally a case of hybrid (q,h)-deformation is recalled, related to the superalgebra $GL(1|1)$. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1343881]

I. INTRODUCTION

Not only the standard q-deformation but also the nonstandard (Jordanian) h-deformation of $GL(2)$ can be considered to be well-known. In each of these domains biparametric generalizations, (p,q) and (g,h), respectively, have been studied by a number of authors. A large number of previous sources are cited in Refs. 1 and 2. The dual quantum algebras of GL_{pq} and GL_{gh} were found in Refs. 3 and 4, respectively. Here we are concerned with certain proposals for combining these two distinct types into (q,h)-deformations. They will often be denoted as hybrid ones. In particular, we analyze the results of Kupershmidt[1] and of Ballesteros–Herranz–Parashar.[2] In each case, we show that a well-defined transformation eliminates h leaving a standard q-deformation. This transformation is not an arbitrary twist, but a straightforward similarity relation performed by a tensor square of an operator. This will be demonstrated explicitly in Secs. II and III.

In Sec. II we start, in fact, with the 3-parameter (q,h,h') deformation of Ref. 1. Already at this level we are able to construct a similarity transformation reducing the formalism to a 1-parameter deformation. The surviving single parameter q' is expressed explicitly as a function

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of (q,h,h'). For the case particularly advocated in Ref. 1, namely $h'=0$, one has simply $q'=q$.

In Sec. III we start by transforming the $R_{q,h}$ matrix of Ref. 2 to R_q. Then we show how their relevant results can be much better understood in the context of an explicitly presented, ''coalgebra conserving'' map. This illuminates several aspects and goes beyond the case of 4×4 matrices.

In Sec. IV we add some comments on maps and singular limits of transformations. Their nontrivial consequences[5–8] are indicated by citing appropriate references. The passage from a standard biparametric (p,q)-deformation to a nonstandard (g,h) one is presented in this context.

In Sec. V we arrive (at last) to a hybrid (q,h)-deformation where h cannot be transformed away. This turns out to be a hybrid deformation of the superalgebra $GL(1|1)$, already studied in Ref. 9. It is located as the case $R_{H1.2}$ in the classification of 4×4 R-matrices in Ref. 10, which we briefly recall.

Finally we would like to come back to Secs. II and III. Instead of briefly stating the equivalence $(q,h)\rightarrow(q)$, we have chosen to present our elementary analysis explicitly and in some detail. We consider this worthwhile for dissipating some confusions. Several authors have presented attractive looking hybrid deformations without noticing disguised equivalences. We ourselves devoted time and effort to their study before reducing them to usual deformations. We hope that our analysis will create a more acute awareness of traps in this domain.

II. KUPERSHMIDT'S (q,h,h') AND (q,h) DEFORMATIONS

We start by noting that the group relations given by the set of equations (5) of Ref. 1 can be written as

$$\begin{aligned} ca&=ac, \quad bd=db,\\ cb&=qbc-hac-h'db,\\ ad&=da+(q-1)bc-hac-h'db,\\ qba&=ab+ha^2+h'b^2-h(da-bc),\\ cd&=q\,dc-hc^2-h'd^2+h'(da-bc). \end{aligned} \tag{II.1}$$

From the second and the third equations of (II.1) one obtains

$$ad-qbc+hac+h'bd=da-bc=ad-cb. \tag{II.2}$$

Substituting from (II.2) the l.h.s. for $(da-bc)$ in the fourth and fifth equations of (II.1) one gets back exactly (5) of Ref. 1. Compared to his original version ours has the following advantages.

- Adopting the ordering,
$$d>a>b>c; \tag{II.3}$$
all the terms in increasing order $(ca,\ bd,\ldots)$ are on the l.h.s. of (II.1), whereas the square terms and terms in decreasing order are on the r.h.s. This solves the ordering problem encountered in Ref. 1 when h' was taken different from 0.
- The roles of the parameters h,h' are now more simple and symmetrical. The terms bilinear in them (like $hh'bd$ and h'^2bd) do not appear in (II.1). The corresponding complementary (upper and lower triangular) linear contributions of h and h' in the R-matrix to be presented below correspond directly to this feature [the possibility of linearizing the contributions in (II.1)].
- The simpler form of (II.1) facilitates the construction of the R-matrix form of the RTT relations. This, in turn, facilitates the construction of the explicit similarity transformation leading to a 1-parametric equivalent deformation,

$$(q,h,h') \leftrightarrow q', \tag{II.4}$$

where q' is a specific function of (q,h,h') to be presented below. We could have derived the same final results using the more complicated version of (II.1) in Ref. 1. But (II.1) is preferable.

A. Solution of the RTT constraints

Let

$$T=\begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad T_1 = T\otimes 1, \quad T_2 = 1\otimes T, \tag{II.5}$$

where a,b,c,d satisfy (II.1) and let R satisfy

$$RT_1T_2 = T_2T_1R. \tag{II.6}$$

Using (II.1) systematically, one obtains a solution involving an arbitrary parameter κ. It is

$$R=\begin{pmatrix} 1 & -h\kappa & h\kappa & 0 \\ 0 & q\kappa & (1-q\kappa) & 0 \\ 0 & (1-\kappa) & \kappa & 0 \\ 0 & -h'\kappa & h'\kappa & 1 \end{pmatrix}. \tag{II.7}$$

This does *not* satisfy the Yang–Baxter (YB) relations for all values of κ. In fact, in order that R satisfies YB the parameter κ must satisfy the following quadratic equation:

$$\kappa^2(q+hh') - \kappa(q+1) + 1 = 0. \tag{II.8}$$

(Thus, for example, the particularly simple form for $\kappa = 1$ does not satisfy YB unless $hh' = 0$.) The presence of κ at this stage permits the existence of two solutions satisfying YB constraints and related through $R \leftrightarrow R_{21}^{-1}$.

We find it convenient for the similarity transformation to be introduced below to write down the two solutions of (II.8) in the following manner:

$$\kappa = \kappa_1 = (1+\eta^{-1}h)^{-1}, \quad \kappa = \kappa_2 = (1+\eta h')^{-1}, \tag{II.9}$$

where the parameter η satisfies the quadratic

$$\eta^{-1}h + \eta h' = q - 1. \tag{II.10}$$

Our equation (II.10) is the same as the one used in Ref. 1 Eq. (15), to eliminate h' at the level of the vector basis of the Poisson bracket algebra. But the rôle of our η (corresponding to t in Ref. 1) is different. We continue to allow h' to be arbitrary and finally use a similarity transformation to arrive at an equivalent 1-parameter deformation.

B. Similarity transformation to a 1-parameter deformation

Define

$$G=\begin{pmatrix} 1 & \eta \\ \zeta & (1+\eta\zeta) \end{pmatrix}, \quad G^{-1}=\begin{pmatrix} (1+\eta\zeta) & -\eta \\ -\zeta & 1 \end{pmatrix}, \tag{II.11}$$

where the parameters η,ζ are given by

$$h=(q-1)\frac{\eta(1+\eta\zeta)}{1+2\eta\zeta},\quad h'=(q-1)\frac{\eta}{1+2\eta\zeta},\tag{II.12}$$

or

$$\eta=(2h')^{-1}((q-1)\pm\lambda),\quad \eta^{-1}=(2h)^{-1}((q-1)\mp\lambda),$$
$$\zeta=\mp h'\lambda^{-1},\quad \lambda=\sqrt{(q-1)^2-4hh'}.\tag{II.13}$$

(For $\lambda=0$, ζ diverges. This point should be approached as a limit after transforming.)

One obtains, after subtle simplifications,

$$R'=(G\otimes G)R(G^{-1}\otimes G^{-1})=\begin{pmatrix}1&0&0&0\\0&\kappa/\kappa_1&(1-\kappa/\kappa_1)&0\\0&(1-\kappa/\kappa_2)&\kappa/\kappa_2&0\\0&0&0&1\end{pmatrix},\tag{II.14}$$

where κ_1,κ_2 are given by (II.9). [In light of the remarks following (II.13), note that ζ does not appear in R', only η through κ_1 and κ_2. Reality restrictions are discussed at the end of this section.]

Now the statement leading to (II.9) is evident: for $\kappa=\kappa_1$ one gets

$$R'=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&(1-\kappa_1/\kappa_2)&\kappa_1/\kappa_2&0\\0&0&0&1\end{pmatrix},\tag{II.15}$$

the standard lower triangular form of the YB solution for the single parameter κ_1/κ_2. Similarly, for $\kappa=\kappa_2$, one gets

$$R'=\begin{pmatrix}1&0&0&0\\0&\kappa_2/\kappa_1&(1-\kappa_2/\kappa_1)&0\\0&0&1&0\\0&0&0&1\end{pmatrix},\tag{II.16}$$

the standard upper-triangular YB solution for the single parameter κ_2/κ_1. In fact (II.15) and (II.16) are related as the pair R', $(R'_{21})^{-1}$.

Let us now define

$$T'=\begin{pmatrix}a'&b'\\c'&d'\end{pmatrix},\tag{II.17}$$

such that it satisfies

$$R'T'_1T'_2=T'_2T'_1R'.\tag{II.18}$$

The group relations turn out to be independent of the parameter κ of (II.14) [just as (II.1) are independent of κ in (II.7)]. One obtains

$$c'a'=a'c',\quad b'd'=d'b',\quad c'b'=q'b'c',$$
$$a'd'=d'a'+(q'-1)b'c',\quad q'b'a'=a'b',\quad c'd'=q'd'c',\tag{II.19}$$

where we have set

$$q' = \frac{\kappa_2}{\kappa_1} = \frac{1+\eta^{-1}h}{1+\eta h'}, \tag{II.20}$$

with $\eta^{-1}h+\eta h' = q-1$. Note that

$$\begin{aligned} &\text{for } h'=0, \quad q'=q; \\ &\text{for } h=0, \quad q'=q^{-1}. \end{aligned} \tag{II.21}$$

A more complete discussion of the domains of q' follows below.

Setting $h=h'=0$ in (II.1) and adding primes one obtains (II.19).

The relations (II.19) can also be obtained from (II.1) by transforming with G. We have preferred to construct the corresponding R-matrices first from their intrinsic interest and also for elucidating the significance of the free parameter κ arising at the RTT level before imposing the YB constraints.

In Ref. 1, after setting $h'=0$ the (q,h) deformed system is reformulated using a certain ordering. Our preceding study contains the R-matrix for this case as the particular one obtained by setting in (II.7),

$$\begin{aligned} &\kappa=\kappa_2=(1+\eta h')^{-1}=1 \quad (\text{for } h'=0), \\ &\kappa_1=(1+\eta^{-1}h)^{-1}=q^{-1} \end{aligned} \tag{II.22}$$

giving

$$R' = \begin{pmatrix} 1 & -h & h & 0 \\ 0 & q & (1-q) & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{II.23}$$

The transformation to 1-parameter form is now by

$$G = \begin{pmatrix} 1 & \eta \\ 0 & 1 \end{pmatrix}, \quad \text{with } \zeta=0, \ \eta=\frac{h}{q-1}, \tag{II.24}$$

in (II.11). The upper triangular form (II.16) now becomes

$$R' = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & q & (1-q) & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{II.25}$$

The transformed (a,b,c,d), namely (a',b',c',d'), now satisfies (II.19) with $q'=q$.

The results for $h'=0$ can be obtained directly by starting with a (q,h) system given by (16) of Ref. 1 with one necessary correction. The group relations should be written as

$$ba = q^{-1}a(b+ha) - q^{-1}hda + q^{-2}hc(b+ha),$$

$$bd = db,$$

$$bc=q^{-1}c(b+ha),$$

$$ad=da+(1-q^{-1})cb-q^{-1}hca, \tag{II.26}$$

$$ac=ca,$$

$$dc=q^{-1}c(d+hc).$$

[The last two terms of the first equation has each an extra factor q^{-1} as compared to (16) of Ref. 1. Setting $h'=0$ in (5) of Ref. 1 and reordering one indeed gets our version. Starting directly with (II.26), the RTT relations and the YB constraints can indeed be shown to lead to (II.23). Then (II.24) eliminates h leading to (II.25) and to (II.19) with $q'=q$. The case $h=0$ can be treated quite analogously setting (taking the lower sign in (II.13) for η,ζ.]

$$\eta=0, \quad G=\begin{pmatrix} 1 & 0 \\ \zeta & 1 \end{pmatrix}, \quad \zeta=\frac{h'}{q-1}. \tag{II.27}$$

In Ref. 1 h' was eliminated at the stage of Poisson brackets and h was retained. It was assumed that one thus obtains an authentic 2-parameter (q,h)-deformation. We have shown that this is not the case. Our transformation for the original (q,h,h') case shows that, from the start, one has always been dealing with a heavily disguised q-deformation. This statement should however be qualified by taking a closer look at different domains of the parameter space of (q,h,h'). We consider below real values of (q,h,h').

For both $(h,h')\neq 0$ (the cases $h'=0$ and $h=0$, with $q'=q$ and $q'=q^{-1}$, respectively, can be considered simply and analogously), from (II.20),

$$q'=\frac{q+1\pm\sqrt{(q-1)^2-4hh'}}{q+1\mp\sqrt{(q-1)^2-4hh'}}. \tag{II.28}$$

Apart from the very special case

$$q=-1, \quad q'=-1, \tag{II.29}$$

we note that more generally (i) for any q and $hh'<0$ and (ii) for $(q-1)^2>4hh'>0$, q' is always real. We consider this as the generic case.

Another very special case is (for $hh'>0$) $|q-1|=2\sqrt{hh'}$ when $q'=1$. See the remark following (II.13) concerning this singular point. Here one has a classical solution with commuting a',b',c',d' !

For $hh'>0$ and $|q-1|<2\sqrt{hh'}$, $q'=e^{\pm i\delta}$, a complex phase. Here q' can even be a root of unity. Thus starting from a complex deformation, one can obtain by the transformation with G an equivalent deformation with 3 real parameters related through (II.28).

III. THE BALLESTEROS–HERRANZ–PARASHAR CASE

A. Transformation to R_q

The Ballesteros–Herranz–Parashar (BHP) two-parametric deformation (Sec. 4 of Ref. 2) leads to the R-matrix

$$R_{q,h}=\begin{pmatrix} 1 & h & -qh & h^2 \\ 0 & q & 1-q^2 & qh \\ 0 & 0 & q & -h \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{III.1}$$

The authors present it as a superposition of standard (q) and nonstandard (h) deformations. It has indeed the attractive property that for $h=0$ and $q=1$, respectively, one obtains the standard R_q and the nonstandard R_h matrices.

Now consider a similarity transformation of $R_{q,h}$ by $M\otimes M$ where

$$M=\begin{pmatrix} x & y \\ 0 & 1 \end{pmatrix}, \quad M^{-1}=x^{-1}\begin{pmatrix} 1 & -y \\ 0 & x \end{pmatrix}, \tag{III.2}$$

with $y=h/(q-1)$ $(h\neq 0,\ q\neq 1)$ and x is an arbitrary nonzero parameter. In the notation of Ref. 2,

$$y=\frac{a_+}{2a} \quad (q=e^a). \tag{III.3}$$

One obtains, independently of the choice of x,

$$(M^{-1}\otimes M^{-1})R_{q,h}(M\otimes M)=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & q & 1-q^2 & 0 \\ 0 & 0 & q & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}=R_q\,. \tag{III.4}$$

Thus it is seen that h can be transformed away.

B. A coalgebra preserving map

The significance of this equivalence (and that of the related Hopf algebraic results of Ref. 2) are better understood in the context of a simple class of coalgebra preserving maps, presented below. (The content of the mapping can be considered, in a certain sense, to be trivial. Elucidating this aspect is precisely our purpose.) These maps can be generalized to higher dimensional algebras. But we here consider only $\mathcal{U}_q(gl(2))$.

One starts with the standard $\mathcal{U}_q(sl(2))$ algebra,

$$\begin{aligned} &[J_0,J_\pm]=\pm 2J_\pm\,, \quad (q^{J_0}J_\pm=q^{\pm 2}J_\pm q^{J_0}), \\ &[J_+,J_-]=\frac{q^{J_0}-q^{-J_0}}{q-q^{-1}}\equiv[J_0], \end{aligned} \tag{III.5}$$

with the coalgebra structure

$$\begin{aligned} \Delta(J_0)&=J_0\otimes 1+1\otimes J_0 \quad (\Delta(q^{J_0})=q^{J_0}\otimes q^{J_0}), \\ \Delta(J_\pm)&=q^{J_0/2}\otimes J_\pm+J_\pm\otimes q^{-J_0/2}, \\ S(q^{J_0/2})&=q^{-J_0/2}, \\ S(J_\pm)&=-q^{-J_0/2}J_\pm q^{J_0/2}, \\ \epsilon(q^{J_0/2})&=1, \quad \epsilon(J_\pm)=0. \end{aligned} \tag{III.6}$$

[Note that for the antipode S, we have not replaced $q^{-J_0/2}J_\pm q^{J_0/2}$ by $q^{\mp 1}J_\pm$. This last form uses (III.5) which will be modified by the map, keeping the structure (III.6) intact in terms of the new generators.]

Next one sets

$$J_0' = J_0,$$

$$J_+' = J_+,$$

$$J_-' = b_1 J_- + b_2 (q^{J_0/2} - q^{-J_0/2}) + b_3 J_+ . \tag{III.7}$$

Choosing (with $q = e^a$)

$$b_1 = \frac{\sinh(a)}{a}, \quad b_2 = -\frac{a_+}{2a^2}, \quad b_3 = -\frac{a_+^2}{4a^2}, \tag{III.8}$$

one obtains the case (4.6) of Ref. 2 [our (J_0', J_+', J_-') corresponding to their (J_3', J_+, J_-)]. Indeed

$$[J_0', J_+'] = 2J_+',$$

$$[J_0', J_-'] = -2J_-' - \frac{a_+}{a} \frac{\sinh(aJ_0'/2)}{a/2} - \frac{a_+^2}{a^2} J_+', \tag{III.9}$$

$$[J_+', J_-'] = \frac{\sinh(aJ_0')}{a} + \frac{a_+}{a} \frac{e^a - 1}{2a} (e^{-aJ_0'/2} J_+' + J_+' e^{aJ_0'/2}).$$

Moreover, the coalgebra structure induced by this map has the same expression in terms of the new generators, i.e.,

$$\Delta(J_0') = J_0' \otimes 1 + 1 \otimes J_0',$$

$$\Delta(J_\pm') = q^{J_0'/2} \otimes J_\pm' + J_\pm' \otimes q^{-J_0'/2}, \tag{III.10}$$

and so on. This is achieved under the single condition that the coefficients of $q^{\pm J_0}$ in (III.7) are opposite. [Note that the latter statement would be true also if, in addition, we write $J_+' = a_1 J_+ + a_2 (q^{J_0/2} - q^{-J_0/2}) + a_3 J_-$.] The whole Hopf algebra described by (J_0', J_+', J_-') then reproduces that of BHP. This means that the BHP Hopf algebra is equivalent to $\mathcal{U}_q(gl(2))$.

IV. COMMENTS ON SINGULAR LIMITS OF TRANSFORMATIONS

Up to now we have been considering regular, invertible transformations making evident the trivial nature of the passage

$$R_q \leftrightarrow R_{q,h}. \tag{IV.1}$$

The map (III.7) is consistent with this due to the conservation of the structure of the coalgebra. When a map has to be followed by a twist[11,12] to arrive at a sought for coalgebra, the situation can be of interest. It has been shown elsewhere[5] how the universal $\mathcal{R}_h$ matrix (introduced first in Ref. 13) can be obtained, through a twist, starting from the trivial classical one [$\mathcal{U}_h(sl(2))$ is a triangular Hopf algebra]. Another interesting possibility is the use of a transformation singular in the limit $q \to 1$ but in such a specific fashion that [$G(q,h)$ being singular at $q=1$],

$$(G(q,h)^{-1} \otimes G(q,h)^{-1} R_q G(q,h) \otimes G(q,h))|_{q=1} = R_h. \tag{IV.2}$$

In contrast to (IV.1) this passage is noninvertible and the end-product is not a hybrid $R_{q,h}$ but a nonstandard R_h. This can be considered as an operator equation between universal R-matrices and G given by (as shown in Ref. 6):

$$G(q,h)=E_q(\eta J_+), \quad \text{with} \quad \eta=\frac{h}{q-1} \tag{IV.3}$$

and

$$E_q(x)=\sum_{n=0}^{\infty}\frac{x^n}{[n]!}, \quad [n]\equiv\frac{q^n-q^{-n}}{q-q^{-1}}. \tag{IV.4}$$

Alternatively (IV.2) can be regarded as a matrix equation implementing $j_1\otimes j_2$ representations. This technique can be generalized to $GL(N)_q$[6] and also to obtain nonstandard quasi-Hopf algebras.[7]

Note that in (IV.2) η has the same form as in (II.11) or (III.2). But the crucial difference is that one takes the limit $q\to 1$.

In the above-mentioned references universal $\mathcal{R}$-matrices have been studied but only for R_q and R_h. Here, in conclusion, we indicate how one can treat the biparametric case involving $R_{p,q}$ and $R_{g,h}$. (Note that no hybrid deformation is involved here.) We restrict the study to the fundamental case of 4×4 matrices.

We start with

$$R_{pq}=\begin{pmatrix} p & 0 & 0 & 0 \\ 0 & pq & p-q & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & p \end{pmatrix}, \tag{IV.5}$$

and define [with $j_1\otimes j_2=\frac{1}{2}\otimes\frac{1}{2}$ in (IV.3)]

$$G=\begin{pmatrix} 1 & \eta \\ 0 & 1 \end{pmatrix}, \tag{IV.6}$$

but now η will be chosen differently. One obtains

$$(G^{-1}\otimes G^{-1})R_{p,q}(G\otimes G)=\begin{pmatrix} p & p(1-q)\eta & (q-1)\eta & (1-p)(q-1)\eta^2 \\ 0 & pq & p-q & q(p-1)\eta \\ 0 & 0 & 1 & (1-p)\eta \\ 0 & 0 & 0 & p \end{pmatrix}. \tag{IV.7}$$

Now let $q\to 1$ and $p\to 1$ in such a fashion that

$$\left(\frac{q-1}{p-1}\right)^{1/2}=\lambda=\text{const.} \tag{IV.8}$$

Set

$$\eta=\frac{\eta_0}{((p-1)(q-1))^{1/2}}, \quad \lambda\eta_0=h, \quad \lambda^{-1}\eta_0=-g. \tag{IV.9}$$

Then

$$((G^{-1}\otimes G^{-1})R_{p,q}(G\otimes G))\big|_{(p\to 1,q\to 1)}=\begin{pmatrix} 1 & -h & h & gh \\ 0 & 1 & 0 & -g \\ 0 & 0 & 1 & g \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{IV.10}$$

Thus we obtained the 2-parametric nonstandard R-matrix. For $g=h$ and $g=0$, we obtain the two known forms of R_h. The 2-parametric universal colored, nonstandard R-matrix for deformed $gl(2)$ is obtained in Sec. 3 of Ref. 8 implementing a twist. Here we presented the 4×4 case to show how η is quite simply modified from (IV.3) to (IV.9) as one passes from the 1- to the 2-parametric case.

V. AN AUTHENTIC HYBRID (q,h) DEFORMATION: $GL_{q,h}(1|1)$

In Sec. II and Sec. III we have shown that the hybrid (q,h) deformations in Refs. 1 and 2 are in fact disguised q-ones. In the search of hybrid deformation we also check with the classification of 4×4 R-matrices in Ref. 10. There we find seven triangular cases:

$$R_{S2,1}=\begin{pmatrix} 1 & 0 & 0 & 0 \\ & p & 1-pq & 0 \\ & & q & 0 \\ & & & 1 \end{pmatrix}, \tag{V.1}$$

$$R_{S2,2}=\begin{pmatrix} 1 & 0 & 0 & 0 \\ & p & 1-pq & 0 \\ & & q & 0 \\ & & & -pq \end{pmatrix}, \tag{V.2}$$

$$(R_{H1,3})_{|_{k=1,p=-h,q=-g}}=\begin{pmatrix} 1 & -h & h & gh \\ & 1 & 0 & -g \\ & & 1 & g \\ & & & 1 \end{pmatrix}, \tag{V.3}$$

$$(R_{H2,3})_{|_{k=1},p=x_1,q=x_2,s=x_3}=\begin{pmatrix} 1 & x_1 & x_2 & x_3 \\ & 1 & 0 & x_2 \\ & & 1 & x_1 \\ & & & 1 \end{pmatrix}, \tag{V.4}$$

$$R_{S0,1}=\begin{pmatrix} 1 & 0 & 0 & 1 \\ & 1 & 0 & 0 \\ & & 1 & 0 \\ & & & 1 \end{pmatrix}, \tag{V.5}$$

$$R_{S0,2}=\begin{pmatrix} 1 & 0 & 0 & 1 \\ & -1 & 0 & 0 \\ & & -1 & 0 \\ & & & 1 \end{pmatrix}, \tag{V.6}$$

$$R_{q,h}=(R_{H1,2})_{|_{p=1,k=h}}=\begin{pmatrix} 1 & 0 & 0 & h \\ & 1 & 1-q & 0 \\ & & q & 0 \\ & & & -q \end{pmatrix}. \tag{V.7}$$

Note that in Ref. 10 the R-matrices are given in two versions: homogeneous $R_{H\ldots}$ and scaled $R_{S\ldots}$. The scaled versions are simpler but in some cases, in order not to lose some symmetry among the parameters we use the homogeneous versions with only an overall rescaling.

The case $R_{S2,1}$ is the 2-parameter p,q deformation, $GL_{pq}(2)$, the dual of which is given in Ref. 3. The case $R_{S2,2}$ is a superalgebra—the known p,q deformation of $GL_{pq}(1|1)$, the dual of which is given in Refs. 14–16.

Remark: Note that here (and below for $R_{q,h}$) we consider ordinary, not graded, R-matrices. The results can be translated to the graded formalism. There is a one-to-one correspondence between the results obtained through the two approaches (which was noticed first for solutions of YBE and graded YBE in Ref. 17). This correspondence may be given also through ''transmutation'' in the sense of Ref. 18. This aspect is considered in the context of $sl(1|2)$ in Ref. 19. In our paper the superalgebraic aspect becomes evident after implementation of the RTT formalism.

In the third case we have written the homogeneous version $R_{H1,3}$ of Ref. 10 with $k=1$ and renamed parameters. This seems the natural scaling (and not the $R_{S1,3}$). The result is indeed with 2 parameters, i.e., this is the 2-parameter Jordanian $GL_{gh}(2)$. The dual was found in Ref. 4.

In the fourth case we have written the homogeneous version $R_{H2,3}$ of Ref. 10 with $k=1$ and renamed parameters. From the RTT relations we obtain the following:

$$
\begin{gathered}
acx_1+cax_2+c^2x_3=0,\\
ac-ca+c^2x_2=0,\\
-ac+ca+c^2x_1=0,\\
-c^2x_1+cd-dc=0,\\
-c^2x_2-cd+dc=0,\\
c^2x_3+c\,dx_1+dc\,x_2=0,\\
ad-cax_1+c\,dx_2-da=0,\\
-acx_2-ad+da+dc\,x_1=0,\\
bc-cax_2-cb+dc\,x_2=0,\\
-acx_1-bc+cb+c\,dx_1=0,\\
-a^2x_1+ab+a\,dx_1-ba+cbx_2+c\,dx_3=0,\\
-a^2x_2-ab+ba+bcx_1+da\,x_2+dc\,x_3=0,\\
bd-cax_3-cbx_1-da\,x_2-db+d^2x_2=0,\\
-acx_3-a\,dx_1-bcx_2-bd+db+d^2x_1=0,\\
-a^2x_3-abx_1-bax_2+b\,dx_1+db\,x_2+d^2x_3=0.
\end{gathered}
\tag{V.8}
$$

It is necessary to consider several cases.

(1) In the case $x_1+x_2\neq 0$ (and arbitrary x_3) from the above follow:

$$
\begin{gathered}
c^2=0,\quad ca=ac=0,\quad dc=cd=0,\\
da=ad,\quad cb=bc,\\
a^2=d^2=ad+bc
\end{gathered}
\tag{V.9}
$$

$$ab=bd=ba+(x_1-x_2)bc, \quad db=bd+(x_2-x_1)bc.$$

These relations make the resulting algebra rather degenerate. Moreover, in order to build a PBW basis we have to look also for higher order relations. For instance, using these relations we obtain

$$a^3=a^2d+abc=a^2d.$$

Furthermore one can eliminate $bc=a^2-ad$, and $bd=ba+(x_1-x_2)(a^2-ad)$. From all these it follows that the PBW basis may have only the following monomials:

$$b^n a^k, \quad a^{\ell} d, \quad c, \quad n,k\in\mathbb{Z}_+, \quad \ell=0,1. \tag{V.10}$$

(2) Next we consider the case $x_1=-x_2=h$, $x_3\neq -h^2$; then from (V.8) follows that

$$\begin{gathered} c^2=0, \quad ca=ac=0, \quad dc=cd=0, \\ da=ad, \quad cb=bc, \quad a^2=d^2, \\ ab=ba+h(a^2+bc-ad), \quad db=bd-h(a^2+bc-ad). \end{gathered} \tag{V.11}$$

The resulting algebra is also degenerate, though the above relations are less restrictive than the previous case and the possible PBW basis is richer:

$$b^n a^k d^{\ell}, \quad b^n c^{\ell}, \quad n,k\in\mathbb{Z}_+, \quad \ell=0,1. \tag{V.12}$$

(3) Finally in the case $x_1=-x_2=h$, $x_3=-h^2$ this coincides with the case $R_{H1,3}$ when $g=-h$.

The fifth case $R_{S0,1}$ is a special case of $R_{H2,3}$ when $x_1=x_2=0$, $x_3=1$. Thus, the resulting algebra relations are obtained from (V.11) setting $h=0$.

In the sixth case $R_{S0,2}$ the RTT relations give

$$\begin{gathered} c^2=0, \quad ca=ac=0, \quad dc=cd=0, \\ da=ad, \quad cb=bc, \quad a^2=d^2, \\ ab+ba=0, \quad db+bd=0. \end{gathered} \tag{V.13}$$

This is a superalgebra, also degenerate like the previous two cases. The PBW basis would be as in (V.12).

Finally, we are left with the seventh case, which we have anticipated to be a hybrid one by the notation $R_{q,h}$. Note that setting $q=1$,

$$R_h=R_{1,h}=\begin{pmatrix} 1 & 0 & 0 & h \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{V.14}$$

still depends on h and is triangular (in the sense $R_{21}=R^{-1}$).

Now we obtain the RTT relations by implementing (V.7) in (II.6) with (II.5):

$$\begin{gathered} ba=ab+hcd, \quad ca=q^{-1}ac, \\ da=ad-(1-q^{-1})bc, \quad cb=q^{-1}bc, \\ db=-bd+hq^{-1}ac, \quad dc=-qcd, \\ c^2=0, \quad ha^2=(q+1)b^2+hd^2. \end{gathered} \tag{V.15}$$

This is a superalgebra which we shall denote by $GL_{q,h}(1|1)$. It was first written in Ref. 9, where also the dual quantum algebra was given. This is indeed a hybrid deformation of $GL(1|1)$ since it is known from Ref. 10 that no transformation of the form

$$R_{qh} \rightarrow (M \otimes M) R_{qh} (M^{-1} \otimes M^{-1}) \tag{V.16}$$

can lead to R_q.

Using the transformation (V.16) with

$$M = \begin{pmatrix} x & y \\ 0 & x^{-1} \end{pmatrix}, \tag{V.17}$$

one gets

$$R_{q,h} = \begin{pmatrix} 1 & 0 & 0 & hx^4 - (1+q)(xy)^2 \\ 0 & 1 & 1-q & -2xy \\ 0 & 0 & q & -2qxy \\ 0 & 0 & 0 & -q \end{pmatrix}, \tag{V.18}$$

For no choice of x,y one obtains for the transformed R the form $R_{q;h=0}$, in contrast with the results of Secs. II and III.

For $1+q \neq 0$ one may choose to eliminate the top right hand element by setting $y = \pm x(h/(1+q))^{1/2}$. Denoting $h' = -2xy$,

$$R_{q,h} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1-q & h' \\ 0 & 0 & q & qh' \\ 0 & 0 & 0 & -q \end{pmatrix}. \tag{V.19}$$

In conclusion we repeat that in order to display the sharp contrast between the mixed deformations of Secs. II and III and the present case we have restricted our considerations in both cases to similarity transformations, i.e., coboundary twists $\mathcal{F} \equiv (g^{-1} \otimes g^{-1}) \Delta(g)$, which transform $\mathcal{R}$-matrices as $\mathcal{R}^{\mathcal{F}} \equiv \mathcal{F}_{21} \mathcal{R} \mathcal{F}^{-1} = (g^{-1} \otimes g^{-1}) \mathcal{R} (g \otimes g)$. Other interesting aspects can be explored by implementing more general twists. We refer to the discussion in Ref. 20 concerning the three deformed versions of $gl(1|1)$.

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Symmetry properties and explicit solutions of the generalized Weierstrass system

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The method of symmetry reduction is systematically applied to derive several classes of invariant solutions for the generalized Weierstrass system inducing constant mean curvature surfaces and to the associated two-dimensional nonlinear sigma model. A classification of subgroups with generic orbits of codimension one of the Lie point symmetry group for these systems provides a tool for introducing symmetry variables and reduces the initial systems to different nonequivalent systems of ordinary differential equations. We perform a singularity analysis for them in order to establish whether these ordinary differential equations have the Painlevé property. These ordinary differential equations can then be transformed to standard forms and next solved in terms of elementary and Jacobi elliptic functions. This results in a large number of new solutions and in some cases new interesting constant mean curvature surfaces are found. Furthermore, this symmetry analysis is extended to include conditional symmetries by subjecting the original system to certain differential constraints. In this case, several new types of nonsplitting algebraic, trigonometric, and hyperbolic multisoliton solutions have been obtained in explicit form. Some physical interpretation of these results in the areas of fluid membranes, string theory, two-dimensionl gravity, and cosmology are given. [DOI: 10.1063/1.1337796]

I. INTRODUCTION

The expressions describing minimal surfaces imbedded in three-dimensional Euclidean space were first formulated by Enneper and Weierstrass[1,2] one and a half centuries ago. They start by introducing two holomorphic functions $\psi(z)$, $\phi(z)$ and three complex valued functions ω_1, ω_2, and ω_3 which satisfy the following system of equations

$$\partial\omega_1 = i(\psi^2+\phi^2), \quad \partial\omega_2 = \psi^2-\phi^2, \quad \partial\omega_3 = -2\psi\phi, \quad \bar{\partial}\psi = 0, \quad \bar{\partial}\phi = 0, \tag{1.1}$$

where the derivatives are abbreviated $\partial = \partial/\partial z$ and $\bar{\partial} = \partial/\partial\bar{z}$. The bar denotes the complex conjugate. They show that if the system of three real-valued functions $X_i(z,\bar{z}), i = 1,2,3$ are considered as a coordinate system for a surface immersed in $\mathbb{R}^3$, defined as

$$X_1 = \mathrm{Re}\,\omega_1 = \mathrm{Re}\int_C i(\psi^2+\phi^2)\,\mathrm{d}z,$$

$$X_2 = \mathrm{Re}\,\omega_2 = \mathrm{Re}\int_C (\psi^2-\phi^2)\,\mathrm{d}z, \tag{1.2}$$

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$$X_3 = \mathrm{Re}\,\omega_3 = -\mathrm{Re}\int_C 2\psi\phi\,\mathrm{d}z$$

(where C is any contour in the domain of common holomorphicity of both functions ψ and ϕ), then the functions $X_i(z,\overline{z})$ determine a minimal surface. The minimal lines on this surface are given by the parametric lines $z=$ constant and $\overline{z}=$ constant, respectively.

More recently, this idea was substantially generalized by Konopelchenko,[3] who established the connection between certain classes of constant mean curvature surfaces and the trajectories of an infinite-dimensional Hamiltonian system. Namely, he considered the nonlinear Dirac-type system of equations for two complex valued functions ψ_1 and ψ_2 given by

$$\begin{aligned} &\partial\psi_1 = p\psi_2, \quad \overline{\partial}\psi_2 = -p\psi_1, \\ &\overline{\partial}\overline{\psi}_1 = p\overline{\psi}_2, \quad \partial\overline{\psi}_2 = -p\overline{\psi}_1, \\ &p = |\psi_1|^2 + |\psi_2|^2. \end{aligned} \tag{1.3}$$

The system (1.3) possesses several conserved quantities,[4] including the following.

(1) The conservation of current

$$J = \overline{\psi}_1\partial\psi_2 - \psi_2\partial\overline{\psi}_1, \tag{1.4}$$

which satisfies

$$\overline{\partial}J = \overline{\partial}(\overline{\psi}_1\partial\psi_2 - \psi_2\partial\overline{\psi}_1) = -p(\partial p) + p(\partial p) \equiv 0, \tag{1.5}$$

whenever (1.3) holds.

(2) The conservation of a potential function

$$\partial(\psi_1^2) + \overline{\partial}(\psi_2^2) = 0, \quad \overline{\partial}(\psi_1^2) + \partial(\overline{\psi}_2^2) = 0. \tag{1.6}$$

(3) Another conserved quantity,

$$\partial(\psi_1\overline{\psi}_2) + \overline{\partial}(\overline{\psi}_1\psi_2) = 0.$$

Making use of these conserved quantities, there exists three real valued functions $X_i(z,\overline{z})$, $i=1,2,3$, such that

$$\begin{aligned} X_1 + iX_2 &= 2i\int_\gamma (\overline{\psi}_1^2\,\mathrm{d}z' - \overline{\psi}_2^2\,\mathrm{d}\overline{z}'), \\ X_1 - iX_2 &= 2i\int_\gamma (\psi_2^2\,\mathrm{d}z' - \psi_1^2\,\mathrm{d}\overline{z}'), \\ X_3 &= -2\int_\gamma (\overline{\psi}_1\psi_2\,\mathrm{d}z' + \psi_1\overline{\psi}_2\,\mathrm{d}\overline{z}'). \end{aligned} \tag{1.7}$$

On account of system (1.3), the right-hand side of (1.7) does not depend on the choice of contour γ in $\mathbb{C}$. We treat the functions $X^i(z,\overline{z})$ as the coordinates of a surface immersed into $\mathbb{R}^3$. The Gaussian curvature, the constant mean curvature, and first fundamental form of the surface are given by[3]

$$K=-\frac{\partial\overline{\partial}(\ln p)}{p^2},\quad H=1,\quad \Omega=4p^2\,\mathrm{d}z\mathrm{d}\overline{z}, \tag{1.8}$$

in isothermic coordinates, respectively. Konopelchenko called the modified version (1.3) of the Weierstrass–Enneper system (1.1) the generalized Weierstrass (GW) system. These formulas are the starting point for the symmetry analysis in this paper, and we will refer to it as such. The theory of constant mean curvature surfaces has had a great impact on many problems with physical applications. In particular, the model has found many applications to such diverse areas as in the fields of two-dimensional gravity,[5,6] quantum field theory,[5,7] statistical physics,[8,9] and fluid dynamics.[10,11] It is worth mentioning an application of recent interest, namely, the propagation of a string through space–time.[12] It describes a surface called its world sheet. When one quantizes a string, the result is an ordinary two-dimensional point particle quantum field theory on a given surface. Thus, one can say that first quantized string theory is the study of conformal field theories on Riemann surfaces. Another relevant application of recent interest is in the area of statistical mechanics. Any two-dimensional statistical system near a second-order phase transition can be described by a conformally invariant theory.[8] Near a phase transition, fluctuations of the fields are correlated over very long length scales and appear on all scales essentially equally. Since no scale is preferred, it becomes scale or conformally invariant. Thus, the specific lattice becomes relatively unimportant, and so a type of universal behavior is displayed. A recent interesting application is to the theory of fluid membranes,[8] in which one introduces the free energy per molecule f_e. Then two invariants of the surface which appear directly in the theory are the mean curvature H and Gaussian curvature K. Since the free energy of a fluid membrane must be invariant under rotations of the coordinate system, f_e must be a function of H, H^2, and K to the order we consider

$$f_e(\Sigma,H,K)=f_0(\Sigma)+f_1(\Sigma)H+f_2(\Sigma)H^2+f_3(\Sigma)K,$$

where Σ is the equilibrium area per molecule and the coefficients $f_i, i=0,1,2,3$ are typically functions of Σ, which itself may depend on the curvature. The free energy of the flat film is f_0 and f_1, f_2, and f_3 are the derivatives of the free energy with respect to H, H^2, and K, respectively. One then minimizes f_e to find the equilibrium area per molecule of the curved interface. This defines the curvature free energy. Physically speaking, it is found that if the chains are allowed to adjust their area per molecule depending on the curvature, the monolayer will be less rigid upon bending than with a fixed area per molecule. We would like to stress that results for these curvatures can be obtained from the solutions of the GW system (1.3), which is the object of our study here.

It has been demonstrated[13] that GW system (1.3) can be decoupled into a direct sum of elliptic Sh–Gordon and Laplace equations. If we change the dependent variables ψ_1 and ψ_2 in (1.3) to the new dependent variables p and J, then the GW system (1.3) can be written in the equivalent form

$$\partial\overline{\partial}\ln p=\frac{|J|^2}{p^2}-p^2,\quad \overline{\partial}J=0. \tag{1.9}$$

It was shown using the conditional symmetry method,[14] that the GW system admits an auto-Bäcklund transformation for any holomorphic function J,

$$\partial p=-\lambda q p^2+\frac{\partial q}{q}p-\frac{\lambda J}{q},\quad \overline{\partial}p=-\frac{\overline{J}}{\lambda q}p^2-\frac{\overline{\partial}q}{q}p-\frac{q}{\lambda},\quad \overline{\partial}J=0,\quad \lambda\in\mathbb{C}, \tag{1.10}$$

where the function q satisfies the elliptic Sh–Gordon equation (1.9). The arbitrary complex constant λ is the Bäcklund parameter. The compatibility condition for (1.10) reproduces the system (1.9) in the variable q. It has also been shown,[14] that for a chosen solution q of (1.9), the symmetry group G of the overdetermined system (1.9) and (1.10) with two-dimensional orbits has

a complete set of two functionally independent invariants. Thus, the solution p of the initial equations (1.9) and (1.10) can be expressed in terms of these invariants. In other words, they are invariant under the finite Abelian Lie algebra given by

$$Z_1=\partial-\left(\frac{\lambda J}{q}-\frac{\partial q}{q}p+\lambda q p^2\right)\partial_p,\quad Z_2=\overline{\partial}-\left(\frac{q}{\lambda}+\frac{\overline{\partial}q}{q}p+\frac{\overline{J}}{\lambda q}p^2\right)\partial_p,\quad \overline{\partial}J=0, \tag{1.11}$$

where these vector fields are parametrized by the function q which satisfies (1.9), and constant $\lambda\in\mathbb{C}$. The difference between the classical symmetry reduction and the conditional one[15] is that the group associated with a classical approach to system (1.9) maps all solutions into other solutions of the same system, whereas for a conditional symmetry method, the associated group G maps only a subset of solutions of system (1.9) into solutions of the overdetermined system, that is, the original system (1.9) subjected to given differential constraints (1.10).

Furthermore, by linearizing the Riccati system (1.10), that is, by taking the homogeneous coordinates ϕ_1 and ϕ_2 in (1.10) such that $p=\phi_1/\phi_2$, we obtain, for any holomorphic function J, the associated linear spectral problem for (1.9),

$$\partial\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}=\begin{pmatrix}\dfrac{\partial q}{2q} & -\dfrac{\mu J}{q}\\ \mu q & -\dfrac{\partial q}{2q}\end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix},\quad \overline{\partial}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}=\begin{pmatrix}-\dfrac{\overline{\partial}q}{2q} & -\dfrac{q}{\mu}\\ \dfrac{\overline{J}}{\mu q} & \dfrac{\overline{\partial}q}{2q}\end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix},\quad \overline{\partial}J=0. \tag{1.12}$$

The permutability theorem for the auto-Bäcklund transformation for system (1.3) has recently been formulated by the authors[14] and new classes of nonsplitting multisoliton solutions of system (1.3) have been obtained.

The objective of this paper is a systematic analysis of GW system (1.3) from the symmetry group point of view. We focus on constructing several classes of solutions obtained from the symmetry reduction method.[16,17] It will be demonstrated that the symmetry reduction method applied directly to GW system (1.3) provides limited classes of solutions. However, large classes of solutions of GW system (1.3) can be obtained from a systematic use of the subgroup structure of the invariance group of the sigma model associated with the GW system. Among analytic solutions of (1.3) which are particularly important are those which can be expressed in terms of Jacobi elliptic functions, since they lead to solutions which are not necessarily local.[2] In view of the integrals (1.7), the presented method can provide new, interesting surfaces with constant mean curvature. Our motivation in the present paper is to report on a systematic way of constructing these types of solutions of (1.3), and discuss solitonlike applications. Among these solutions which are particularly significant are those whose total energy

$$E=\int_D\left(p^2+\frac{|J|^2}{p^2}\right)\mathrm{d}x\,\mathrm{d}y,\quad D\in\mathbb{R}^2, \tag{1.13}$$

is finite over all space.

This paper is organized as follows. Section II is devoted to the construction of Lie point symmetries and their subalgebras for GW system (1.3). The reductions of (1.3) to ordinary differential equations (ODEs) requires consideration of three-dimensional subalgebras. The general integrals of these ODEs are presented. In Sec. III, we investigate the connection between GW system (1.3) and a two-dimensional nonlinear sigma model. This link together with conservation laws for (1.3) allows us to establish several useful transformations which simplify the structure of GW system (1.3). Section IV deals with the associated sigma model. The symmetry algebra, list of representatives of conjugacy classes of subalgebras, the corresponding invariants, and reduced differential equations are given. Solutions of GW system (1.3) are provided by means of a number of reduced equations of the associated sigma model. In some cases, solitary and doubly periodic

solutions of the GW system in terms of Jacobi elliptic functions are obtained. Section V contains the extension of the classical Lie approach to group invariant solutions of (1.3) admitting differential constraints (DCs). Each of the solutions presented provides us with different classes of constant mean curvature surface imbedded in three-dimensional Euclidean space. Section VI discusses in detail a set of DCs which allow GW system (1.3) to become a decoupled linear system of equations, and we solve these in terms of Bessel functions of zero order. Section VII contains a future outlook concerning surfaces immersed in multidimensional spaces.

II. THE SYMMETRY GROUP, ITS SUBALGEBRAS, AND THEIR REDUCTIONS TO ODEs

The symmetry group of GW system (1.3) can be computed using the appropriate MACSYMA program.[18] This provides us with a set of determining equations from which we can find the symmetry algebra L of infinitesimal symmetries of system (1.3). It is spanned by the vector fields

$$
\begin{aligned}
&T_1=\partial, \quad T_2=\overline{\partial},\\
&D_1=z\partial-\tfrac{1}{2}(\overline{\psi}_1\partial_{\overline{\psi}_1}+\psi_2\partial_{\psi_2}), \quad D_2=\overline{z}\overline{\partial}-\tfrac{1}{2}(\psi_1\partial_{\psi_1}+\overline{\psi}_2\partial_{\overline{\psi}_2}),\\
&K_1=z^2\partial-z(\overline{\psi}_1\partial_{\overline{\psi}_1}+\psi_2\partial_{\psi_2}), \quad K_2=\overline{z}^2\overline{\partial}-\overline{z}(\psi_1\partial_{\psi_1}+\overline{\psi}_2\partial_{\overline{\psi}_2}),\\
&H=\psi_1\partial_{\psi_1}-\overline{\psi}_1\partial_{\overline{\psi}_1}+\psi_2\partial_{\psi_2}-\overline{\psi}_2\partial_{\overline{\psi}_2}.
\end{aligned}
\tag{2.1}
$$

The physical interpretation of the Lie algebra L is as follows. Here, T_1 and T_2 generate translations in the z and $\overline{z}$ directions, respectively. The generators D_1 and D_2 correspond to two different types of dilations and the generators K_1 and K_2 represent two types of conformal transformations. The generator H reflects the fact that the GW system is invariant under phase transformations. To show this, it is convenient to use polar coordinates for the functions ψ_j, that is to put

$$
\psi_j=R_j e^{i\alpha_j}, \quad j=1,2, \tag{2.2}
$$

and then write the generator H in terms of R_j and α_j. In this case, the field H takes the simple form

$$
H=-i(\partial_{\alpha_1}+\partial_{\alpha_2}).
$$

The nonzero commutation relations for the algebra (2.1) are given by

$$
[D_i,K_i]=K_i, \quad [T_i,K_i]=2D_i, \quad [T_i,D_i]=T_i, \quad i=1,2.
$$

We see that the Lie algebra can be decomposed into a direct sum of two sl(2,$\mathbb{C}$) subalgebras in addition with generator H. The vector field H represents the center of the Lie algebra L. Thus we find that

$$
L=\{\mathrm{sl}(2,\mathbb{C})\}_1\oplus\{sl(2,\mathbb{C})\}_2\oplus H, \tag{2.3}
$$

where the subalgebras $\{\mathrm{sl}(2,\mathbb{C})\}_i$ are spanned by $\{T_i,D_i,K_i\}$, $i=1,2$, respectively. Subalgebras of the direct sum $\{\mathrm{sl}(2,\mathbb{C})\}_1\oplus\{\mathrm{sl}(2,\mathbb{C})\}_2$ can be classified by using an adaptation of the Goursat twist method to Lie algebras.[19,20] Note that the vector fields K_i can be rectified by a point transformation involving independent and dependent variables in such a way that K_i is equivalent to T_i. This fact simplifies considerably the classification of subalgebras of L.

The results for representatives of the conjugacy classes of one-dimensional subalgebras of the symmetry algebra L are listed in Table I using a standard method.[21] The discrete transformations of GW system (1.3) were used in order to restrict the range of parameters appearing in the classification. The proposition is that any one-dimensional subalgebra of L is conjugate under the

TABLE I. The one-dimensional subalgebras of (2.1) leading to a system of first order ODEs where α, $\beta \in \mathbb{C}$. Similar results to those of L_4 are obtained for $L_6 = D_2 + \beta H$ when z is replaced by $\overline{z}$, $(\psi_1, \overline{\psi}_1, \psi_2, \overline{\psi}_2)$ is replaced by $(\psi_2, \overline{\psi}_2, \psi_1, \overline{\psi}_1)$ and for $L_7 = T_2 + \epsilon H$ to those of L_5 when $\overline{z}$ is replaced by z and $(\psi_1, \overline{\psi}_1, \psi_2, \overline{\psi}_2)$ is replaced by $(\overline{\psi}_1, \psi_1, \overline{\psi}_2, \psi_2)$, respectively.

No.	Subalgebras	Symmetry variable ξ	Reduction to ODEs	A solution of (1.3)	CMC surfaces are cylinders
L_1	$D_1 - D_2 + \beta H$	$\overline{z}^{-1} z^{-1}$	$\alpha \xi \dot{A} + \left(\beta - \frac{\alpha}{2}\right) A$	$\psi_1 = \lambda \overline{a}^{1/2} (z\overline{z})^{a/2}$	$X_1^2 + X_2^2 = 1$
			$= (AD + BC) B$	$\psi_2 = \lambda a^{1/2} (z\overline{z})^{(a-1)/2} \overline{z}$	$z^a \overline{z^a} = e^{-2X_3}$
	$\alpha \neq 0$		$\xi^2 \dot{B} = (AD + BC) A$	$a + \overline{a} = 1, \lvert\lambda\rvert^4 = 1/16$	
L_2	$T_2 + D_1 + \beta H$	$z^{-1} e^{\overline{z}}$	$-\xi \dot{A} + \beta A = (AB + CD) C$	Trivial constant	$\cdots$
			$\xi \dot{C} = -(AB + CD) A$		
L_3	$T_1 + T_2 + \epsilon H$	$z - \overline{z}$	$\dot{A} + \epsilon A = C(AB + CD) e^{\epsilon \xi}$	$\psi_1 = \lambda (a - i\epsilon)^{1/2} \exp(F)$	$X_1^2 + X_2^2 = 1$
	$\epsilon = \pm 1$		$\dot{C}(\xi) = A(AB + CD) e^{\epsilon \xi}$	$\psi_2 = \lambda (a + i\epsilon)^{1/2} \exp(F)$	$X_3 = -\mathrm{Re}((a + i\epsilon) z)$
				$F = a(z - \overline{z})/2 + i\epsilon(z + \overline{z})/2$	
				$\epsilon = \pm 1, a \in \mathbb{R}, \lvert\lambda\rvert^4 = 1/16$	
L_4	$D_1 + \beta H$	$\overline{z}$	$\beta A = D(AC + BD)$	$\psi_1 = \sqrt{\beta/2} e^{i\theta} z^{\beta} \overline{z}^{-\beta - 1/2}$	$X_1^2 + X_2^2 = \frac{1}{4}$
			$\dot{D} = -A(AC + BD)$	$\psi_2 = \sqrt{\beta/2} e^{i\theta} z^{\beta - 1/2} \overline{z}^{-\beta}$	$X_3 = -2\beta \ln(\lvert z\rvert)$
				$\beta, \theta \in \mathbb{R}$	
L_5	$T_1 + \epsilon H$	$\overline{z}$	$\epsilon A_0 = C_0 (A_0 B_0 + C_0 D_0)$	$\psi_1 = \frac{e^{i\theta}}{\sqrt{2}} e^{\epsilon(z - \overline{z})}$	$X_1^2 + X_2^2 = 1$
	$\epsilon = \pm 1$		$C_0 = A_0 (A_0 B_0 + C_0 D_0)$	$\psi_2 = \frac{e^{i\theta}}{\sqrt{2}} e^{\epsilon(z - \overline{z})} \epsilon = \pm 1$	

action of the group G to precisely one algebra L_j, $1 \leqslant j \leqslant 7$ in the list. No two members occurring in the list are mutually conjugate. The list of invariants of the corresponding Lie subalgebras and also the corresponding reduced ODEs are given in Table I. The functions A, B, C, D, and ξ denote the five invariants for the given subalgebras L_j, where ξ is the symmetry variable. The main feature of the symmetry reduction method is that the set of symmetry variables enables us to reduce, after some transformations, the original system of PDEs to sets of four coupled ODEs. These ODEs can very often be explicitly integrated in terms of known functions or at least their singularity structure can be investigated using the Painlevé test.[22] It is shown in many cases that the result of the test is positive for the reduced systems of ODEs. After some change of variables, these ODEs can be written in closed analytic form which can be decoupled and solved in many cases. The Lie algebra obtained from the infinitesimal symmetries of the GW system (1.3), listed in Table I, have to obey the restriction coming from the requirement that the quantities z and $\overline{z}$ as well as the values of ψ_i and $\overline{\psi}_i$ cannot be viewed as independent variables in $\mathbb{C}$, respectively, as demanded by symmetry criterion. This fact is a strong limitation on the admitted class of invariant solutions of (1.3). Thus if we interpret z and $\overline{z}$ as coordinates in the complex plane $\mathbb{C}$, and ψ_i and $\overline{\psi}_i$ as complex conjugate valued functions on $\mathbb{C}$, then the following is a list of representatives of conjugacy classes of one-dimensional subalgebras, the corresponding invariants, and their associated reductions and solutions of (1.3). The four invariants A, B, C, D depend on the argument ξ. Here, we only summarize the results in Table I.

We classify two-dimensional subalgebras of the symmetry algebra (2.1) into conjugacy classes under the action of the symmetry group G including discrete transformations of (1.3). It turns out that only two classes of two-dimensional subalgebras exist for GW system (1.3). They can be represented by

$$L_{2,1} = \{D_1, T_1 + aH\}, \quad L_{2,2} = \{D_2, T_2 + aH\}, \quad a \in \mathbb{C}.$$

The corresponding invariant solutions of the reduced equations of GW system (1.3) lead to trivial constant solutions.

Let us now sum up the results. We remark that solutions of the GW system obtained from one- and two-dimensional reductions are elementary solutions, that is, constant, algebraic polynomial and exponential solutions. Thus the classical symmetry reduction method in the version presented here does not prove to be a very useful tool, since it leads to rather limited classes of solutions. In the framework of group theoretical methods applied to PDEs, there exists in the recent liturature several approaches such as nonclassical and conditional symmetry methods[23,24] which evolved in the process of extending Lie's classical theory of symmetry for PDEs. This approach consists basically in modifying the original system by adding to it certain differential constraints for which a symmetry criterion is identically satisfied. The overdetermined system of equations obtained in this way admits, in some cases, a larger class of Lie point symmetry groups and consequently, can provide other classes of solutions of the original system than the ones obtained by the classic approach. Thus, one of our objectives is to study the conditional symmetries of the GW system and look for new classes of solutions, which is presented in Sec. IV.

III. THE ASSOCIATED SIGMA MODEL EQUATIONS

In our investigation it is more convenient to introduce a new dependent variable which links the GW system with the Euclidean sigma model. Such a link has been discovered first by Kenmotsu[25] for the linear Weierstrass equations inducing mean curvature surfaces. This will be extended to the case of the GW system, and it will allow us to establish several useful transformations in order to simplify the structure of system (1.3).

Let us define a new complex variable

$$\rho=\frac{\psi_1}{\overline{\psi}_2}, \tag{3.1}$$

and its complex conjugate. Differentiating (3.1) with respect to ∂ and using the relation

$$p=|\psi_2|^2(1+|\rho|^2),$$

we obtain

$$\partial\rho=(1+|\rho|^2)^2\psi_2^2. \tag{3.2}$$

Note that $\partial\rho$ and ψ_2^2 have the same polar angle in the complex plane, since they are related by a real quantity $(1+|\rho|^2)^2$. Taking into account (3.1) we get the following transformation from the variable ρ into the variables ψ_1 and ψ_2:

$$\psi_1=\epsilon\rho\frac{(\overline{\partial\rho})^{1/2}}{1+|\rho|^2},\quad \psi_2=\epsilon\frac{(\partial\rho)^{1/2}}{1+|\rho|^2},\quad \epsilon=\pm 1. \tag{3.3}$$

According to Ref. 26, if ψ_1 and ψ_2 are solutions of GW system (1.3), then the function ρ defined by (3.1) is a solution to the two-dimensional Euclidean sigma-model equations

$$\text{(i)}\quad \partial\overline{\partial}\rho-\frac{2\overline{\rho}}{1+|\rho|^2}\partial\rho\,\overline{\partial}\rho=0,\quad \text{(ii)}\quad \partial\overline{\partial}\overline{\rho}-\frac{2\rho}{1+|\rho|^2}\partial\overline{\rho}\,\overline{\partial}\overline{\rho}=0. \tag{3.4}$$

Conversely, according to Ref. 26, if ρ is a solution of the sigma model (3.4), then the solutions ψ_1 and ψ_2 of GW system (1.3) have the form (3.3). Hence, some classes of solutions to GW system (1.3) can be obtained directly by applying the transformation (3.3) to the solutions of the sigma-

model (3.4). For example, a very large class of solutions can be found simply by requiring the holomorphicity or antiholomorphicity of the function ρ. This choice for the function ρ leads to so-called splitting solutions (1.3), which satisfy the Laplace equation

$$\partial\bar{\partial}\rho=0,$$

and have been extensively investigated in Ref. 14 and 26. We discuss in detail a technique for constructing nonsplitting solutions of (1.3) for which $\partial\bar{\partial}\rho\neq 0$ holds in Secs. V and VI. Note that the only trivial solution of GW system (1.3) is the null solution $\psi_i\equiv 0$, which corresponds to ρ equal to any constant.

The conservation of current (1.5) and conservation of a potential function imply that there exists a complex function $g:\mathbb{C}\to\mathbb{C}$ such that

$$\psi_1=\epsilon(\bar{\partial}g)^{1/2},\quad \psi_2=\epsilon(\partial g)^{1/2},\quad \epsilon=\pm 1. \tag{3.5}$$

Substituting these into the GW system (1.3), we obtain the following second order system of PDEs:

$$\begin{aligned}\partial\bar{\partial}g&=2i\epsilon[(\bar{\partial}g)(\partial\bar{g})^{1/2}(\partial g)^{1/2}+(\bar{\partial}g)^{1/2}(\partial g)(\bar{\partial}\bar{g})^{1/2}],\\ \bar{\partial}\partial\bar{g}&=-2i\epsilon[(\partial\bar{g})(\bar{\partial}g)^{1/2}(\bar{\partial}\bar{g})^{1/2}+(\partial\bar{g})^{1/2}(\bar{\partial}\bar{g})(\partial g)^{1/2}].\end{aligned} \tag{3.6}$$

Hence,[27] if g is a solution of the system (3.6), then the functions ψ_1 and ψ_2 defined by (3.5) satisfy the GW system (1.3). Under the above-mentioned conservation law, we can formulate the following.

Proposition 1: If ψ_1 and ψ_2 are solutions of GW system (1.3), then the current J in terms of the function ρ defined by (3.1) takes the form

$$J(z,\bar{z})=-\frac{\partial\rho\,\partial\bar{\rho}}{(1+|\rho|^2)^2}, \tag{3.7}$$

and is a holomorphic function, $\bar{\partial}J=0$.

Proof: Indeed, differentiation of Eq. (3.1) with respect to z gives transformation (3.3). Substituting Eq (3.3) into expression (1.7), we get

$$\begin{aligned}J&=\frac{\bar{\rho}\,\partial^2\rho}{2(1+|\rho|^2)^2}-\frac{\bar{\rho}\partial\rho}{(1+|\rho|^2)^3}(\rho\partial\bar{\rho}+\bar{\rho}\partial\rho)-\frac{\partial\rho\,\partial\bar{\rho}}{(1+|\rho|^2)^3}-\frac{\bar{\rho}\,\partial^2\rho}{2(1+|\rho|^2)^2}+\bar{\rho}^2\frac{(\partial\rho)^2}{(1+|\rho|^2)^3}\\ &=-\frac{\partial\rho\,\partial\bar{\rho}}{(1+|\rho|^2)^2}.\end{aligned} \tag{3.8}$$

Differentiation of (3.8) yields

$$\bar{\partial}J=\frac{(\bar{\partial}\partial\rho)(\partial\bar{\rho})+(\partial\rho)(\bar{\partial}\partial\bar{\rho})}{(1+|\rho|^2)^2}-2\frac{(\partial\rho)(\partial\bar{\rho})(\rho\bar{\partial}\bar{\rho}+\bar{\rho}\bar{\partial}\rho)}{(1+|\rho|^2)^3}. \tag{3.9}$$

Substituting sigma model equation (3.4) into (3.9), we obtain that (3.9) is identically satisfied

$$2\bar{\rho}(\partial\rho)(\bar{\partial}\rho)(\partial\bar{\rho})+2\rho(\partial\bar{\rho})(\bar{\partial}\bar{\rho})(\partial\rho)-2\rho(\partial\rho)(\partial\bar{\rho})(\bar{\partial}\bar{\rho})-2\bar{\rho}(\partial\rho)(\partial\bar{\rho})(\bar{\partial}\rho)\equiv 0,$$

which completes the proof. Q.E.D.

Proposition 2: If ρ is a solution of sigma model system (3.4), then the functions ψ_1 and ψ_2 defined by (3.3) in terms of ρ satisfy the conservation of potential (1.6) identically.

Proof: Indeed, substituting (3.3) into expression (1.6), we obtain

$$2\rho\,\partial\rho\frac{\overline{\partial\rho}}{(1+|\rho|^2)^2}+\rho^2\frac{\partial\overline{\partial\rho}}{(1+|\rho|^2)^2}-2\rho^2\frac{\overline{\partial\rho}}{(1+|\rho|^2)^3}(\overline{\rho}\partial\rho+\rho\partial\overline{\rho})$$
$$+\frac{\overline{\partial}\partial\rho}{(1+|\rho|^2)^2}-2\frac{\partial\rho}{(1+|\rho|^2)^3}(\overline{\rho}\overline{\partial}\rho+\rho\overline{\partial\rho})=0.$$

By virtue of sigma model equations (3.4), the above-mentioned equation is an identity,

$$\rho\,\partial\rho\,\overline{\partial\rho}-\frac{\rho}{1+|\rho|^2}(1+|\rho|^2)\,\partial\rho\,\overline{\partial\rho}\equiv 0.$$

An analogous result holds for the conjugate equation. Q.E.D.

IV. GROUP INVARIANT SOLUTIONS OF THE SIGMA MODEL

This section is devoted to finding explicit solutions of GW system (1.3) based on transformation (3.3) and uses a variety of classes of invariant solutions of the sigma model (3.4). In order to construct and investigate solutions of sigma model (3.4) obtained by means of the symmetry reduction method[16,17] to ODEs, we need to find its symmetry group G, and then classify all subgroups G_i of G having generic orbits of codimension one in the space of independent variables. We then find the associated invariants of each of its subgroups G_i, and perform for each of these invariants the symmetry reduction of (3.4) to a system of ODEs and then solve these ODEs. The last step requires that a singularity analysis be carried out to determine whether they are of the Painlevé type, and thus whether all their critical points are fixed, or independent of the initial data.

The reductions of sigma model (3.4) to systems of ODEs require consideration of one-dimensional subalgebras of the symmetry algebra of (3.4). Using the MACSYMA program,[18] we find that the classical symmetry groups G of the sigma model equations (3.4) are the conformal and scaling transformations. The corresponding symmetry algebra L is spanned by the vector fields

$$X^1=\xi(z)\partial,\quad X^2=\eta(\overline{z})\overline{\partial},\quad D=\rho\partial_\rho-\overline{\rho}\partial_{\overline{\rho}}. \tag{4.1}$$

Here, ξ and η are arbitrary functions of z and $\overline{z}$, respectively. Now, since the distribution of the vector fields (4.1) is Abelian, it determines that the algebra $\mathcal{L}$ can be decomposed as a direct sum of two infinite-dimensional simple Lie subalgebras with direct sum given by a one-dimensional algebra generated by D,

$$\mathcal{L}=\{X^1\}\oplus\{X^2\}\oplus D. \tag{4.2}$$

If we assume that the functions ξ and η are analytic in a proper open subset Ω of $\mathbb{C}$, then they can be developed in a Laurent series. In this case, we can provide a basis for two centerless Virasoro algebras. Finite-dimensional subalgebras of $\{X^1\}$ and $\{X^2\}$ are spanned only by

$$\{\partial\},\{\partial,z\partial\},\{\partial,z\partial,z^2\partial\},\cdots,\quad \{\overline{\partial}\},\{\overline{z}\overline{\partial}\},\{\overline{\partial},\overline{z}\overline{\partial},\overline{z}^2\partial\},\cdots, \tag{4.3}$$

respectively. The invariant solutions of the one-dimensional subalgebras (4.3) are only holomorphic or antiholomorphic functions and lead to splitting solutions of (3.4), which have been discussed in detail in Ref. 26. According to Refs. 21 and 28, we can apply the method of classifying finite subalgebras of direct-sum algebras (4.2). Here, we state only the result of this classification. We give in the following a list of representatives of conjugacy classes of one-dimensional subalgebras of symmetry algebra $\mathcal{L}$. The statement is that any one-dimensional subalgebra of $\mathcal{L}$ is conjugate under G to give precisely one algebra $L_{1,j}(j=1,\ldots,5)$ in the list and no two members of this list are mutually conjugate. The results are summarized by the following cases:

$$L_{1,1}=\partial, \quad L_{1,2}=D,$$
$$L_{1,3}=\partial+\overline{\partial}, \quad L_{1,4}=D+\partial, \quad L_{1,5}=D+\partial+\overline{\partial}. \tag{4.4}$$

Note that complex conjugate subalgebras to those given in (4.4) were excluded in our classification list. The discrete subgroups of system (3.4) presented in the Appendix were used to restrict the range of parameters appearing in this classification.

For computational purposes, it is useful to examine the real system of PDEs equivalent to the two-dimensional Euclidean sigma model equations (3.4). If we introduce the polar coordinates

$$\rho=\mathrm{R}e^{i\phi} \tag{4.5}$$

into system (3.4), then the real and imaginary parts of the so obtained equations have the following form for the unknown functions R and ϕ:

$$\phi_{xx}+\phi_{yy}+\frac{2(1-R^2)}{R(1+R^2)}(R_x\phi_x+R_y\phi_y)=0, \tag{4.6i}$$

$$R_{xx}+R_{yy}-\frac{R(1-R^2)}{1+R^2}(\phi_x^2+\phi_y^2)-\frac{2R}{1+R^2}(R_x^2+R_y^2)=0. \tag{4.6ii}$$

Note that if we put $R=1$, then (4.6ii) is identically satisfied and the first one reduces to the Laplace equation for the phase ϕ. This implies that ϕ has to be a periodic, harmonic function with a period equal to 2π. Otherwise, if the period of ϕ is not 2π, then the solution (4.6) may become a multivalued function. In our analysis, if we construct solutions that disobey the above-mentioned restriction, then these solutions have to be excluded from our consideration in general.

Equation (4.6) is invariant under the discrete transformations generated by the reflections

$$x\to\epsilon_1 x, \quad y\to\epsilon_2 y, \quad R\to\epsilon_3 R, \quad \phi\to\epsilon_4\phi, \quad \epsilon_i=\pm 1, \quad i=1,\ldots,4, \tag{4.7i}$$

and also the inversion given by

$$R\to\frac{1}{\eta}, \quad \phi\to\phi. \tag{4.7ii}$$

Making use of the MACSYMA program[18] for determining the symmetry algebra of a differential equation, we find that the symmetry algebra $\mathcal{L}$ of Eq. (4.6) is spanned by the following vector fields:

$$X^1=\tfrac{1}{2}\xi(z)(\partial_x-i\partial_y), \quad X^2=\tfrac{1}{2}\overline{\xi}(\overline{z})(\partial_x+i\partial_y), \quad \Phi=\partial_\phi, \tag{4.8}$$

where ξ is an arbitrary function of $z=x+iy$ and $\overline{\xi}$ denotes its complex conjugate. Note the vector fields X^1 and X^2 can be rectified by any conformal transformation $z=z(u)$ and $\overline{z}=\overline{z}(\overline{u})$,

$$X^1=\xi(z)\partial\to\partial_u, \quad X^2=\overline{\xi}(\overline{z})\overline{\partial}\to\partial_{\overline{u}}.$$

It is easy to check that this transformation preserves the form of the sigma model equation (3.4).

For computational purposes, it is useful to change the base of vector fields (4.8). The corresponding symmetry algebra $\mathcal{L}$ is spanned by

$$\alpha^{\pm}=X^1\pm\overline{X^1}=\tfrac{1}{2}\{(\xi\pm\overline{\xi})\partial_x-i(\xi\mp\overline{\xi})\partial_y\}, \quad \Phi=\partial_\phi,$$

since we have

$$\alpha^{+}=X^1+\overline{X^1}=X^2+\overline{X^2}, \quad \alpha^{-}=-i(X^1-\overline{X^1})=-i(X^2-\overline{X^2}).$$

The algebra $\mathcal{L}$ can be decomposed as a direct sum of two infinite-dimensional simple Lie subalgebras with direct sum composed of a one-dimensional algebra generated by Φ,

$$\mathcal{L}=\{\alpha^+\}\oplus\{\alpha^-\}\oplus\{\Phi\}. \tag{4.9}$$

Note that the vector field Φ commutes with the vector fields α^+ and α^-, so it represents the center of the algebra $\mathcal{L}$. Assuming that the function ξ is analytic in a proper open subset of $\mathcal{D}\subset\mathbb{C}$, we can develope ξ as a power series and can provide the following basis:

$$\begin{aligned}\alpha_n^+&=X^1+\overline{X^1}=\frac{1}{2}\{(x+iy)^n+(x-iy)^n\}\partial_x-\frac{i}{2}\{(x+iy)^n-(x-iy)^n\}\partial_y,\\ \alpha_n^-&=-i(X^1-\overline{X^1})=-\frac{i}{2}\{(x+iy)^n-(x-iy)^n\}\partial_x-\frac{1}{2}\{(x+iy)^n+(x-iy)^n\}\partial_y,\end{aligned} \tag{4.10}$$

where $n\in\mathbb{Z}^+$. The vector fields (4.10) generate an infinite-dimensional simple algebra that contains only one finite-dimensional subalgebra spanned by

$$\begin{aligned}&P_1=\partial_x,\quad P_2=\partial_y,\\ &D=x\partial_x+y\partial_y,\quad L_3=y\partial_x-x\partial_y,\\ &C_1=(x^2-y^2)\partial_x+2xy\,\partial_y,\quad C_2=2xy\,\partial_x-(x^2-y^2)\,\partial_y,\end{aligned} \tag{4.11}$$

which corresponds to the case in which the index $n=0,1,2$ in Eq. (4.10). The physical interpretation of this Lie algebra is the following. The operators P_1 and P_2 generate translations in the x and y directions, respectively. The vector fields D and L_3 correspond to dilation and rotation, respectively. The operators C_1 and C_2 generate two different types of conformal transformations. The nonvanishing commutation relations for the algebra (4.11) are given by

$$\begin{aligned}&[C_1,L_3]=C_1,\quad [C_1,D]=-C_2,\quad [C_1,P_1]=-2D,\quad [C_1,P_2]=2L_3,\\ &[C_2,L_3]=-C_2,\quad [C_2,D]=C_1,\quad [C_2,P_1]=-2L_3,\quad [C_2,P_2]=-2D,\\ &[L_3,P_1]=P_2,\quad [L_3,P_2]=-P_1,\quad [D,P_1]=-P_1,\quad [D,P_2]=-P_2.\end{aligned} \tag{4.12}$$

These relations show that this algebra is isomorphic to the $O(3,1)$ algebra. We refer the reader to Ref. 17 and 29 for details of the classification of subalgebras of the symmetry algebra $O(3,1)$ into conjugacy classes under the action of the symmetry group G. In our case, among all nonconjugate subalgebras, the ones that have generic orbits of codimension one in the space of independent variables and three in the space of independent and dependent variables $\{x,y,R,\phi\}$ reduce the original system (4.6) to a system of ODEs via the symmetry reduction method. The one-dimensional subalgebras are given by

$$P_1+b\Phi,\quad L_3+b\Phi,\quad D+b\Phi,\quad D+aL_3+b\Phi, \tag{4.13}$$

where a and b are real parameters. The discrete subgroups (4.7) admitted by (4.6) were used to restrict the range of parameters occurring in this classification. In order to find the reduction associated with subalgebras (4.13), we compute for each of them the corresponding invariants by solving the PDE

$$XH(x,y,R,\phi)=0, \tag{4.14}$$

where H is an auxilliary function of four variables (x,y,R,ϕ), and X is one of the generators listed in (4.13). The solution of (4.14) is found by integrating the associated characteristic system.

TABLE II. The symmetry reduction for Eq. (4.6).

No	Algebra	Symmetry variable ξ	One-dimensional orbits of subgroups	Coefficients of the reduction to ODEs (3.16)	Reduction to second order ODE
1.	$P_1+b\Phi$	y	$R=R(\xi)$	$g=g_0, h=0, s=0$	$\ddot{R}-\frac{2R}{1+R^2}\dot{R}^2-A^2g_0^2\frac{(1-R^2)(1+R^2)^3}{R^3}$
			$\phi=bx+F(\xi)$	$l=1, m=0$	$-\frac{R(1-R^2)}{1+R^2}=0$
2.	$L_3+b\Phi$	$\sqrt{x^2+y^2}$	$R=R(\xi)$	$\frac{\dot{g}}{g}=-\frac{1}{\xi}, h=0, s=0$	$\ddot{R}-\frac{2R}{1+R^2}\dot{R}^2+\frac{1}{\xi}\dot{R}$
			$\phi=b\sin^{-1}\frac{x}{\sqrt{x^2+y^2}}$	$l=\frac{b^2}{\xi^2}, m=0$	$-\frac{A^2C^2}{\xi^2}\frac{(1-R^2)(1+R^2)^3}{R^3}$
			$+F(\xi)$		$-\frac{b^2}{\xi^2}\frac{R(1-R^2)}{1+R^2}=0$
3.	$D+b\Phi$	$\frac{x}{y}$	$R=R(\xi)$	$\frac{\dot{g}}{g}=-\frac{2\xi}{1+\xi^2}, h=\frac{b}{\xi(1+\xi^2)}$	$\ddot{R}-\frac{2R}{1+R^2}\dot{R}^2+\frac{2\xi}{1+\xi^2}\dot{R}$
			$\phi=b\ln x+F(\xi)$	$s=-\frac{b}{\xi^2(1+\xi^2)}, l=\frac{b^2}{\xi^2(1+\xi^2)}$	$-\frac{A(\xi)^2C^2}{(1+\xi^2)^2}\frac{(1-R^2)(1+R^2)^3}{R^3}$
				$m=-\frac{4b}{(1+\xi^2)^2}$	$-\frac{R(1-R^2)}{(1+\xi^2)^2(1+R^2)}=0$
4.	$D+aL_3+b\Phi$	$\ln\sqrt{x^2+y^2}$	$R=R(\xi)$	$g=g_0, h=-\frac{2b}{1+a^2}, l=\frac{b^2}{1+a^2}$	$\ddot{R}-\frac{2R}{1+R^2}\dot{R}^2-A^2g_0^2\frac{(-R^2)(1+R^2)^3}{R^3}$
	$a>0$	$+\frac{1}{a}\tan^{-1}\frac{x}{y}$	$\phi=-\frac{b}{a}\tan^{-1}\frac{x}{y}$	$s=0, m=0$	$+\frac{R(1-R^2)}{1+R^2}b^2\left(\frac{3-a^2}{(1+a^2)^2}\right)=0$
			$+F(\xi)$		

The result of it is that we find three invariants ξ, R, and F which are listed for all cases in Table II. The orbits of the subgroups of G for all considered cases (4.13) can be expressed in terms of two functions R and ϕ in the following form:

$$R=R(\xi), \quad \phi=\alpha(x,y)+F(\xi), \quad \xi=\xi(x,y), \tag{4.15}$$

where α and ξ are given functions of x and y for each subalgebra. Here, the function ξ is the symmetry variable of the invariance subgroup having generic orbits of codimension one. Substituting each specific form (4.15) into system (4.6) leads to the coupled system of ODEs in terms of the symmetry variable ξ only

$$\begin{aligned} &\text{(i)} \quad \ddot{R}-\frac{2R}{1+R^2}\dot{R}^2-\frac{R(1-R^2)}{1+R^2}\dot{\phi}^2-\frac{\dot{g}}{g}\dot{R}-2h\frac{R(1-R^2)}{1+R^2}\dot{\phi}-l\frac{R(1-R^2)}{1+R^2}=0,\\ &\text{(ii)} \quad \ddot{\phi}+2\dot{R}\dot{\phi}\frac{(1-R^2)}{R(1+R^2)}-\frac{\dot{g}}{g}\dot{\phi}+2h\frac{(1-R^2)}{R(1+R^2)}\dot{R}+s=0, \end{aligned} \tag{4.16}$$

where functions g, h, l, and s are given for each of the subalgebras in Table II. The dot means differentiation with respect to ξ. The results of these calculations are summarized in Table II for each of the subalgebras.

The obtained reduced system of ODEs (4.16) has a form similar to the one obtained from the symmetry reduction method for the CP^1 sigma model in $(2+1)$ dimensions as given in Ref. 30. So, following the procedure presented in Ref. 30, Eq. (4.16) can be solved in an analogous way. The results of the Painlevé analysis for system (4.16) and the integration of these reduced ODEs

in terms of elementary functions, Jacobi elliptic functions, or Painlevé transcendents are summarized in Table II. The system of ODEs (4.16) for R and ϕ can be decoupled. If we perform the transformation,

$$\dot{\phi}=V-h, \tag{4.17}$$

on equation (4.16ii), then the function V has to satisfy the nonhomogeneous ODE

$$\dot{V}+2\dot{R}\frac{1-R^2}{R(1+R^2)}V-\frac{\dot{g}}{g}V-m=0, \tag{4.18}$$

where

$$m=\dot{h}-\frac{\dot{g}}{g}h-s_0. \tag{4.19}$$

Let us consider two cases separately.

(1) When $m=0$ Eq. (4.18) is an homogeneous ODE for the function V. This case corresponds to subalgebras $\{P_1+b\Phi\}$, $\{L_3+b\Phi\}$ and $\{D+aL_3+b\Phi\}$ (see Table II). The general integral of the homogeneous ODE (4.18) has the form

$$V=Ag\frac{(1+R^2)^2}{R^2}, \quad A\in\mathbb{R}. \tag{4.20}$$

Hence, transformation (4.17) becomes

$$\dot{\phi}=Ag\frac{(1+R^2)^2}{R^2}-h. \tag{4.21}$$

Elimination of $\dot{\phi}$ from (4.21) and (4.16i) gives

$$\ddot{R}-\frac{2R}{1+R^2}\dot{R}^2-\frac{\dot{g}}{g}\dot{R}-A^2g^2\frac{(1-R^2)(1+R^2)^3}{R^3}+(h^2-l)\frac{R(1-R^2)}{1+R^2}=0. \tag{4.22}$$

(2) When $m\neq 0$ Eq. (4.18) is a nonhomogeneous ODE for the function V. This case is related to subalgebra $D+b\Phi$, as in Table II. The general solution of ODE (4.18) is obtained by the method of variation of parameters and has the following form:

$$V=A(\xi)g\frac{(1+R^2)^2}{R^2}, \tag{4.23}$$

with

$$A(\xi)=\int\frac{mR^2}{g(1+R^2)^2}d\xi'. \tag{4.24}$$

Substituting (4.23) and (4.24) into (4.17), we can eliminate $\dot{\phi}$ from (4.16i), and we get (4.22). In order to construct solutions of (4.22), we have to analyze the singularity structure in the sense of Painlevé and Gambier[31,32] and transform these equations to one of the standard forms listed in Ref. 33. If we perform the transformation of the dependent variable in (4.22) given by

$$R(\xi)=(-U(\xi))^{1/2}, \tag{4.25}$$

then the function U has to satisfy the second-order ODE

$$\ddot{U}=\left(\frac{1}{2U}-\frac{1}{1-U}\right)\dot{U}^2-\frac{\dot{g}}{g}\dot{U}+\frac{2C^2}{g^2}\frac{(1+U)(1-U)^3}{U}. \tag{4.26}$$

Changing the independent variable

$$\eta=\int_{\xi_0}^{\xi}\frac{dt}{g(t)}, \quad g(t)\neq 0, \tag{4.27}$$

in (4.26), we obtain the following ODE in the η variable:

$$\ddot{U}=\left(\frac{1}{2U}-\frac{1}{1-U}\right)\dot{U}^2+\frac{2C^2}{U}(1+U)(1-U)^3. \tag{4.28}$$

If $C=0$, then from (4.17), $\phi=\phi_0$, and Eq. (4.28) becomes Eq. (PXXXVII) listed by Ince[33] with the solution given by

$$U=\tanh^2(K_1\eta+K_2), \quad K_1,K_2\in\mathbb{R}. \tag{4.29}$$

If $C\neq 0$, then Eq. (4.28) is Eq. (PXXXVIII) listed in Ince,[33] where in Ince's notation, $\beta=-\alpha=2C^2$ and $\gamma=\delta=0$. This equation admits a first integral and can be reduced to a first-order ODE for U,

$$U'=-4C^2U^4+4C_1U^3+8(C^2-C_1)U^2+4C_1U-4C^2, \quad C_1\in\mathbb{C}, \tag{4.30}$$

where differentiation is with respect to η. Equation (4.30) can be written in equivalent form for $C\neq 0$,

$$U'^2=-4C^2(U-U_1)(U-U_2)(U-U_3)(U-U_4), \tag{4.31}$$

where U_i, $i=1,\cdots,4$ denote the constant roots of the right-hand side of (4.31). These roots can be expressed in terms of the constants C and C_1. It is well known[30] that the behavior of the solutions of (4.31) depends upon the relationships between the roots of the quartic polynomial on the right-hand side of (4.31). This equation is a known equation which can be solved in terms of elliptic Jacobi functions (see Byrd and Friedman[34]) or in the degenerate cases, as when the roots have multiplicity greater than one, in terms of elementary algebraic functions with one or two simple poles, trigonometric and hyperbolic solitons.

Localized solutions can also be obtained. Suppose that $C=0$, then (4.30) takes the form

$$\dot{U}^2=(4C_1U^2-2(B+4C_1)U+4C_1)U.$$

When $C_1=0$, this can be integrated easily to give

$$U=D\exp(\pm\sqrt{-2B}\,\eta). \tag{4.32}$$

When $C_1\neq 0$, one can write the quadratic in factorized form

$$\dot{U}^2=4C_1(U-U_1)(U-U_2)U,$$

where the roots are given as follows:

$$U_{1,2}=(n+1)\pm\sqrt{n(n+2)}, \tag{4.33}$$

with $n=B/4C_1$. We have summarized all individual possibilities in Tables III–V. It is worth noting, in the case of elliptic doubly periodic solutions of (4.31), we can construct global solutions of GW system through the use of transformation (3.3). Note that nonsingular periodic solutions

TABLE III. The elliptic solutions of the sigma model (4.6), $\rho = R\exp(i\phi)$ with $R = \sqrt{-U(\eta)}$.

No.	Order of roots	Function $U(\eta)$	Function β modulus k
1.	$U_1 > U_2 \geqslant U > 0$	$U_2 sn^2\left(\frac{\sqrt{4K}}{\beta}(\eta-\eta_0),k\right)$	$\beta = \frac{2}{\sqrt{U_1}}$, $k^2 = \frac{U_2}{U_1}$
2.	$U_1 > U_2 > U \geqslant 0$	$\frac{U_1U_2\left(1-sn^2\left(\frac{\sqrt{4K}}{\beta}(\eta-\eta_0),k\right)\right)}{U_1-U_2sn^2\left(\frac{\sqrt{4K}}{\beta}(\eta-\eta_0),k\right)}$	$\beta = \frac{2}{\sqrt{U_1}}, k^2 = \frac{U_2}{U_1}$
3.	$U_1 \geqslant U > U_2 > 0$	$\frac{U_1U_2}{U_1-(U_1-U_2)sn^2\left(\frac{\sqrt{4K}}{\beta}(\eta-\eta_0),k\right)}$	$\beta = \frac{2}{\sqrt{U_1}}, k^2 = \frac{U_1-U_2}{U_1}$
4.	$U_1 > U \geqslant U_2 > 0$	$U_1-(U_1-U_2)sn^2\left(\frac{\sqrt{4K}}{\beta}(\eta-\eta_0),k\right)$	$\beta = \frac{2}{\sqrt{U_1}}, k^2 = \frac{U_1-U_2}{U_1}$
5.	$U > U_1 > U_2 > 0$	$-\frac{U_1-U_2sn^2\left(\frac{\sqrt{4K}}{\beta}(\eta-\eta_0),k\right)}{sn^2\left(\frac{\sqrt{4K}}{\beta}(\eta-\eta_0),k\right)-1}$	$\beta = \frac{2}{\sqrt{U_1}}, k^2 = \frac{U_2}{U_1}$
6.	$\infty > U \geqslant U_1 > U_2 > 0$	$\frac{U_1}{sn^2\left(\frac{\sqrt{4K}}{\beta}(\eta-\eta_0),k\right)}$	$\beta = \frac{2}{\sqrt{U_1}}, k^2 = \frac{U_2}{U_1}$

can be physically interpreted as elementary excitations, kinks as domain walls, and bumps as nucleation centers. Singular solutions represent static defect structures—''charges'' with the quantity which defines order. Some of them develop from a point or a line into a growing sphere or a cylinder g.[35]

As an example to illustrate how this method works, let us write the functions ψ_i for a particular case of the roots of (4.31) and two cases 1 and 4 listed in Table II. Suppose that three of the roots are the same, so that $U_4 = U_3 = U_2 < U \leqslant U_1 < 0$. Equation (4.31) can be integrated and we can solve to obtain U as given in Table V as follows:

$$U = \frac{U_2C^2(U_1-U_2)^2(\eta-\eta_0)^2+U_1}{C^2(U_1-U_2)^2(\eta-\eta_0)^2+1}.$$

For the symmetry algebras $\{P_1+b\Phi\}$ and $\{D+aL_3+b\Phi\}$ in Table II, $g = g_0$ is constant, so from (4.27), we obtain

$$\eta-\eta_0 = \frac{1}{g_0}(\xi-\xi_0),$$

and putting (4.25) into (4.21), we get

$$\phi = -g_0A\int \frac{(1-U)^2}{U}d\xi - h\xi.$$

In the case of subalgebra $\{P_1+b\Phi\}$, for which the symmetry variable is given by $\xi = y$, and $h = 0$, we can determine the function ρ given by (4.5) in the following form:

TABLE IV. The elliptic solutions of the sigma model (4.6), $R=\sqrt{-U(\eta)}$ with $(\dot{U})^2=-4C^2(U-U_1)(U-U_2)(U-U_3)(U-U_4)$ $C\neq 0$ and phase ϕ specified in this table, and $A^2=(U_1-b_1)^2+a_1^2$, $B^2=(U_2-b_1)^2+a_1^2$ $a_1=-(c-\overline{c})^2/4$, and $b_1=(c+\overline{c})/2$.

No.	Order of roots	Function $U(\eta)$	Function β	Modulus k
1.	$U_1>U_2>U_3>U_4>U$	$\dfrac{U_4(U_1-U_3)-U_3(U_1-U_4)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}{U_1-U_3-(U_1-U_4)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}$	$\dfrac{2}{\sqrt{(U_1-U_3)(U_2-U_4)}}$	$\dfrac{(U_2-U_3)(U_1-U_4)}{(U_1-U_3)(U_2-U_4)}$
2.	$U_1>U_2>U_3\geqslant U>U_4$	$\dfrac{U_3(U_2-U_4)-U_2(U_3-U_4)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}{U_2-U_4-(U_3-U_4)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}$	$\dfrac{2}{\sqrt{(U_1-U_3)(U_2-U_4)}}$	$\dfrac{(U_1-U_2)(U_3-U_4)}{(U_1-U_3)(U_2-U_4)}$
3.	$U_1>U_2>U_3>U\geqslant U_4$	$\dfrac{U_3(U_2-U_4)-U_2(U_3-U_4)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}{U_2-U_4-(U_3-U_4)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}$	$\dfrac{2}{\sqrt{(U_1-U_3)(U_2-U_4)}}$	$\dfrac{(U_1-U_2)(U_3-U_4)}{(U_1-U_3)(U_2-U_4)}$
4.	$U_1>U_2\geqslant U>U_3>U_4$	$\dfrac{U_3(U_4-U_2)+U_4(U_2-U_3)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}{U_4-U_2-(U_2-U_3)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}$	$\dfrac{2}{\sqrt{(U_1-U_3)(U_2-U_4)}}$	$\dfrac{(U_2-U_3)(U_1-U_4)}{(U_1-U_3)(U_2-U_4)}$
5.	$U_1\geqslant U>U_2>U_3>U_4$	$\dfrac{U_2(U_3-U_2)+U_3(U_1-U_4)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}{U_3-U_1+(U_1-U_4)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}$	$\dfrac{2}{\sqrt{(U_1-U_3)(U_2-U_4)}}$	$\dfrac{(U_2-U_3)(U_1-U_4)}{(U_1-U_3)(U_2-U_4)}$
6.	$U_1\geqslant U>U_2>U_3>U_4$	$\dfrac{U_2(U_3-U_2)+U_3(U_1-U_2)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}{U_3-U_1+(U_1-U_2)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}$	$\dfrac{2}{\sqrt{(U_1-U_3)(U_2-U_4)}}$	$\dfrac{(U_1-U_2)(U_3-U_4)}{(U_1-U_3)(U_2-U_4)}$
7.	$U_1>U\geqslant U_2>U_3>U_4$	$\dfrac{U_4(U_3-U_1)+U_3(U_1-U_4)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}{U_3-U_1+(U_1-U_4)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}$	$\dfrac{2}{\sqrt{(U_1-U_3)(U_2-U_4)}}$	$\dfrac{(U_1-U_2)(U_3-U_4)}{(U_1-U_3)(U_2-U_4)}$
8.	$U>U_1>U_2>U_3>U_4$	$\dfrac{U_1(U_2-U_4)+U_2(U_4-U_1)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}{U_2-U_4+(U_4-U_1)sn^2\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}$	$\dfrac{2}{\sqrt{(U_1-U_3)(U_2-U_4)}}$	$\dfrac{(U_2-U_3)(U_1-U_4)}{(U_1-U_3)(U_2-U_4)}$
9.	$U_1\geqslant U>U_2, c,\overline{c}\in\mathbb{C}$	$\dfrac{-U_2A-U_1B+(U_1B-U_2A)cn\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}{-A-B+(B-A)cn\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}$	$\dfrac{1}{\sqrt{AB}}$	$\dfrac{(U_1-U_2)^2-(A-B)^2}{4AB}$
10.	$U_2<U_1<U<\infty, c,\overline{c}\in\mathbb{C}$	$\dfrac{-U_2A-U_1B+(U_2A+U_1B)cn\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}{-A+B+cn\left(\dfrac{\sqrt{-4C^2}}{\beta}(\eta-\eta_0),k\right)}$	$\dfrac{1}{\sqrt{AB}}$	$\dfrac{(A+B)^2-(U_1-U_2)^2}{4AB}$

TABLE V. The solitary wave or bump type elliptic solutions of the sigma model (4.6), $R=\sqrt{-U(\eta)}$, $C\neq 0$, $B>4(C^2-K)>0$, $K<0$, and phase ϕ specified in Table IV.

No.	Order of roots	Function $U(\eta)$	Modulus k and parameters
1.	$U_4=U_3=U_2<U\leqslant U_1<0$	$U_2+\dfrac{U_1-U_2}{1+(U_1-U_4)^2C^2(\eta-\eta_0)^2}$	
2.	$U_4\leqslant U<U_3=U_2=U_1<0$	$U_1-\dfrac{U_1-U_4}{1+(U_1-U_4)^2C^2(\eta-\eta_0)^2}$	
3.	$U_4<U_3=U_2<U\leqslant U_1<0$	$U_2+\dfrac{(U_1-U_2)(U_2-U_4)}{(U_1-U_4)\cosh^2 C\sqrt{(U_1-U_2)(U_2-U_4)}(\eta-\eta_0)-(U_1-U_2)}$	
4.	$U_4\leqslant U\leqslant=U_2<U_1<0$	$U_2-\dfrac{(U_1-U_2)(U_2-U_4)}{(U_1-U_4)\cosh^2 C\sqrt{(U_1-U_2)(U_2-U_4)}(\eta-\eta_0)-(U_2-U_4)}$	
5.	$U_4=U_3<U_2\leqslant U\leqslant U_1<0$	$U_3+\dfrac{(U_1-U_3)(U_2-U_3)}{U_2-U_3+(U_1-U_2)\cos^2 C\sqrt{(U_1-U_3)(U_2-U_3)}(\eta-\eta_0)}$	$K<0$ $B>4(C^2-K)>0$
6.	$U_4\leqslant U\leqslant U_3<U_2=U_1$	$U_1-\dfrac{(U_1-U_4)(U_1-U_3)}{U_1-U_3+(U_3-U_4)\cos^2 C\sqrt{(U_1-U_4)(U_1-U_3)}(\eta-\eta_0)}$	
7.	$U_2\leqslant U\leqslant U_1<0$	$\dfrac{U_1U_2}{U_2+(U_1-U_2)sn^2(\sqrt{-U_2K/2}(\eta-\eta_0),k)}$	$k^2=\dfrac{U_1-U_2}{-U_2}$ $C=0,B<-8K<0$
8.	$U_2<U_1\leqslant U\leqslant 0$	$U_1sn^2\sqrt{\dfrac{U_2K}{2}}(\eta-\eta_0,k)$	$k^2=\dfrac{U_1}{U_2},C=0$ $K<0,B>-8K>0$
9.	$U_4\leqslant U\leqslant U_3<U_2<U_1$	$\dfrac{U_1(U_3-U_4)sn^2[\beta(\eta-\eta_0),k]+U_4(U_1-U_3)}{(U_3-U_4)sn^2[\beta(\eta-\eta_0),k]+U_1-U_3}$	$k^2=\dfrac{(U_1-U_2)(U_3-U_4)}{(U_1-U_3)(U_2-U_3)}$ $\beta=C\sqrt{(U_1-U_3)(U_2-U_4)}$ $C\neq 0$
10.	$U_4<U_3<U_2\leqslant U\leqslant U_1<0$	$\dfrac{U_4(U_1-U_2)sn^2[\beta(\eta-\eta_0),k]+U_1(U_2-U_4)}{(U_1-U_2)sn^2[\beta(\eta-\eta_0),k]+U_2-U_4}$	$k^2=\dfrac{(U_1-U_2)(U_3-U_4)}{(U_1-U_3)(U_2-U_3)}$ $\beta=C\sqrt{(U_1-U_3)(U_2-U_4)}$ $C\neq 0,B>4(C^2+(-K))>0$

$$\rho=\mathrm{Re}^{i\phi}=\sqrt{-\frac{U_2C^2g_0^{-2}(U_1-U_2)^2(y-y_0)^2+U_1}{C^2g_0^{-2}(U_1-U_2)^2(y-y_0)^2+1}}\exp\Bigg[i\Bigg(bx+\frac{g_0^2A}{C}\tan^{-1}((y-y_0)\times(U_2-U_1)g_0^{-1}C)-\frac{g_0^2A(U_2-U_1)}{CU_2(U_1U_2)^{1/2}(U_1-U_2)}\tan^{-1}\Bigg(\frac{U_2C(U_2-U_1)^2(y-y_0)}{g_0(U_1U_2)^{1/2}(U_1-U_2)}\Bigg)-g_0A\frac{(U_2-1)^2}{U_2}y\Bigg)\Bigg].$$

To evaluate the ψ_i, one next calculates the derivatives $\partial\rho$ and $\overline{\partial\rho}$, and then substitutes these into transformation (3.3). To abbreviate the notation, let us define the quantities

$$k=C^2g_0^{-2}(U_1-U_2)^2,\quad f=g_0(U_1U_2(U_1-U_2)^2)^{1/2},\quad Q=g_0^2(A(U_2-U_1)/CU_2). \tag{4.34}$$

Then for the case of the subalgebra $\{P_1+b\Phi\}$, the ψ_i are as follows:

$$\psi_1=\epsilon\frac{\rho}{1-U}\Bigg[-\frac{iU_2k(\xi-\xi_0)}{2Rk(\xi-\xi_0)^2+1}-\frac{1}{2}iRk(\xi-\xi_0)-iR\Bigg(\frac{1}{2}b+\frac{ig_0A(U_2-U_1)}{2(1+(U_2-U_1)^2g_0^{-2}C^2(\xi-\xi_0)^2)}$$
$$-\frac{ig_0QU_2C(U_2-U_1)^2}{2(f^2+U_2^2C^2(U_2-U_1)^4(\xi-\xi_0)^2)}-\frac{ig_0A(U_2-1)^2}{2U_2}\Bigg)\Bigg]^{1/2}\exp(-i\phi/2),$$

$$\psi_2=\frac{\epsilon}{1-U}\Bigg[\frac{iU_2k(\xi-\xi_0)}{2Rk(\xi-\xi_0)^2+1}+\frac{1}{2}iRk(\xi-\xi_0)+iR\Bigg(\frac{1}{2}b-\frac{ig_0A(U_2-U_1)}{2(1+(U_2-U_1)^2g_0^{-2}C^2(\xi-\xi_0)^2)}$$
$$+\frac{ig_0QCU_2(U_2-U_1)^2}{2(f^2+U_2^2C^2(U_2-U_1)^4(\xi-\xi_0)^2)}+\frac{ig_0A(U_2-1)^2}{2U_2}\Bigg)\Bigg]^{1/2}\exp(i\phi/2). \tag{4.35}$$

For the subalgebra $\{D+aL_3+b\Phi\}$, the function ρ given by (4.5) can be written down in terms of the symmetry variable abbreviated as $\xi=\ln\sqrt{x^2+y^2}+(1/a)\tan^{-1}x/y$ and $h=2b/(1+a^2)$,

$$\rho=\sqrt{-\frac{U_2C^2g_0^{-2}(U_1-U_2)^2(\xi-\xi_0)^2+U_1}{C^2g_0^{-2}(U_1-U_2)^2(\xi-\xi_0)^2+1}}\exp\Bigg[i\Bigg(-\frac{b}{a}\tan^{-1}\frac{x}{y}+\frac{g_0^2A}{C}\Bigg)\tan^{-1}((\xi-\xi_0)(U_2$$
$$-U_1)g_0^{-1}C)-\frac{g_0^2A(U_2-U_1)}{CU_2(U_1U_2)^{1/2}(U_1-U_2)}\tan^{-1}\Bigg(\frac{U_2C(U_2-U_1)^2(\xi-\xi_0)}{g_0(U_1U_2)^{1/2}(U_1-U_2)}-g_0A\frac{(U_2-1)^2}{U_2}\xi$$
$$+\frac{2b}{1+a^2}\xi\Bigg)\Bigg].$$

Defining the additional variables

$$s_1=1+\frac{x^2}{y^2},\quad s_2=\frac{1}{2iy}+\frac{x}{2y^2},\quad \tilde{s}_2=\frac{1}{2iy}-\frac{x}{2y^2},\quad w_1=\frac{1}{2z}+\frac{is_2}{as_1},\quad w_2=\frac{1}{2\bar{z}}+\frac{i\tilde{s}_2}{as_1},$$

and with k, f, and Q defined by (4.34), the functions ψ_i are calculated by differentiating ρ and using transformation (3.3)

$$\psi_1=\epsilon\frac{\rho}{1-U}\Bigg[-\frac{U_2k(\xi-\xi_0)w_2}{(k(\xi-\xi_0)^2+1)R}+\frac{(U_2k(\xi-\xi_0)^2+U_1)k(\xi-\xi_0)w_2}{R(k(\xi-\xi_0)^2+1)^2}-iR\Bigg(-\frac{ib\tilde{s}_2}{as_1}$$
$$+\frac{g_0A(U_2-U_1)w_2}{1+(U_2-U_1)^2g_0^{-2}C^2(\xi-\xi_0)^2}-\frac{g_0QCU_2(U_2-U_1)^2w_2}{f^2+U_2^2C^2(U_2-U_1)^4(\xi-\xi_0)^2}-\frac{g_0A(U_2-1)^2}{U_2}w_2$$
$$+\frac{2b}{1+a^2}w_2\Bigg)\Bigg]^{1/2}\exp(-i\phi/2),$$

$$\psi_2=\frac{\epsilon}{1-U}\Bigg[-\frac{U_2k(\xi-\xi_0)w_1}{(k(\xi-\xi_0)^2+1)R}+\frac{(U_2k(\xi-\xi_0)^2+U_1)k(\xi-\xi_0)w_1}{R(k(\xi-\xi_0)^2+1)^2}+iR\Bigg(-\frac{ibs_2}{as_1}$$
$$+\frac{g_0A(U_2-U_1)w_1}{1+(U_2-U_1)^2g_0^{-2}C^2(\xi-\xi_0)^2}-\frac{g_0QCU_2(U_2-U_1)^2w_1}{f^2+U_2^2C^2(U_2-U_1)^4(\xi-\xi_0)^2}-\frac{g_0A(U_2-1)^2}{U_2}w_1$$
$$+\frac{2b}{1+a^2}w_1\Bigg)\Bigg]^{1/2}\exp(i\phi/2). \tag{4.36}$$

A class of solutions of (4.26), which are different from those obtained above, can be constructed by introducing the change of independent variables

$$\eta = \int g(\xi)\, \mathrm{d}\xi, \tag{4.37}$$

into (4.26). We obtain

$$U'' = \left(\frac{1}{2U} + \frac{1}{U-1}\right) U'^2 + 2\frac{g'}{g} U' - \frac{2C^2}{g^4}(1-U)^2\left(\frac{1}{U} - U\right), \tag{4.38}$$

where differentiation is with respect to η. Note that if $g = g_0$, then we obtain the previously discussed case (PXXXVIII). The symmetry reduction to ODE (4.38) with $g = A\xi$ is related to the symmerty algebra L_3. In this case, Eq. (4.38) is the standard form for the fifth Painlevé transcendent,[33] where in Ince's notation, $\beta = -\alpha = 2C^2/A^4$ and $\gamma = \delta = 0$. However, if we make the transformation

$$g = \exp\left(\int_{\xi_0}^{\xi} r(\eta)\, \mathrm{d}\eta \right),$$

for which the function r is given by one of the following two cases

$$r = \frac{1}{A\xi^2}, \quad r = \frac{2\xi}{A(1+\xi^2)^2},$$

which are related to the algebra L_3 or D, respectively, then Eq. (4.38) is Eq. (PXXXX) listed in Ref. 33. According to Ref. 33, Eq. (4.38) can be reduced to the first-order ODE after the transformation

$$\frac{1}{u-1} u' - B e^{-2\int r\, \mathrm{d}\eta} u = -2w, \quad B \in \mathbb{R},$$

to a Riccati equation of the form

$$w' + w^2 + 2rw - \tfrac{1}{2} B^2 e^{-4\int r\, \mathrm{d}\eta} = E e^{-2\int r\, \mathrm{d}\eta}. \tag{4.39}$$

If g in Eq. (4.38) is a constant, then we can perform a new transformation on the independent variable

$$\eta = e^{i g_0 (\xi - \xi_0)},$$

into (4.38) and obtain

$$U'' = \left(\frac{1}{2U} + \frac{1}{U-1}\right) U'^2 - \frac{1}{\eta} U' + \frac{2C^2}{g^4}(1-U)^2\left(\frac{1}{U} - U\right). \tag{4.40}$$

This is the equation for the fifth Painlevé transcendent, where in Ince's notation, $\beta = -\alpha = 2C^2/g_0^4$ and $\gamma = \delta = 0$, which is related to the reduction obtained from the symmetry algebras P_1 and $\{D + aL_3\}$, respectively.

In many solitonlike problems in field theory, the field configuration of finite energy (1.13) is relevant to many applications.[5,8,9] Such a situation takes place for the following reductions: In the case of Eq. (4.29), we obtain a kink soliton solution. Bump-type solutions appear in 3 and 4 of Table V. Localized solitonlike solutions are listed in Tables III and IV, cases 1–8, and Table V, cases 7–10.

V. THE NONSPLITTING SOLUTIONS OF THE GENERALIZED WEIERSTRASS SYSTEM

Now we discuss the case when some classes of solutions of GW system (1.3) can be obtained from transformation (3.3) for which the solutions of the sigma model (3.4) are invariant under the scaling transformation D as given in (4.1). This means that we subject system (1.3) to the algebraic constraint

$$|\rho|^2=1. \tag{5.1}$$

It follows from (5.1) that sigma model (3.4) can be written

$$\partial\overline{\partial}\rho-\overline{\rho}\partial\rho\overline{\partial}\rho=0, \quad \overline{\partial}\partial\overline{\rho}-\rho\partial\overline{\rho}\overline{\partial}\overline{\rho}=0, \tag{5.2}$$

and has a solution of the exponential form

$$\rho=e^{i\varphi}, \tag{5.3}$$

where φ is any real harmonic function of z and $\overline{z}$, since from (3.4), we get the following identity:

$$\partial\overline{\partial}\rho-\overline{\rho}\partial\rho\overline{\partial}\rho=e^{i\varphi}(i\partial\overline{\partial}\varphi-\partial\varphi\overline{\partial}\varphi)+e^{i\varphi}(e^{-i\overline{\varphi}}e^{i\varphi}\partial\varphi\overline{\partial}\varphi)\equiv 0.$$

The transformation (3.3) becomes

$$\psi_1=\frac{\epsilon}{2}e^{i\varphi/2}(\overline{\partial}\varphi)^{1/2}, \quad \psi_2=\frac{\epsilon}{2}e^{i\varphi/2}(\partial\varphi)^{1/2}, \quad \epsilon=\pm 1,$$

and satisfies GW system (1.3).

In this section, we shall study nonsplitting solutions of overdetermined system (3.4) and (5.1) depending on one arbitrary complex valued function of one complex variable z and its complex conjugate

$$\rho=\frac{f(z)}{\overline{f(z)}}.$$

In this case, transformation (3.3) defined in terms of a function f takes the form

$$\psi_1=\frac{\epsilon}{2\overline{f}}(f\,\overline{\partial f})^{1/2}, \quad \psi_2=\frac{\epsilon}{2\overline{f}}(\overline{f}\partial f)^{1/2}, \quad p=\frac{1}{2}\left|\frac{\partial f}{f}\right|.$$

The associated surface determined from Eq. (1.7) becomes

$$\begin{aligned}
X_1+iX_2&=\frac{i}{2}\int_\gamma\left(\frac{\overline{f}\partial f}{f^2}\mathrm{d}z'-\frac{\overline{\partial f}}{\overline{f}}\mathrm{d}\overline{z}'\right),\\
X_1-iX_2&=\frac{i}{2}\int_\gamma\left(\frac{\partial f}{f}\mathrm{d}z'-\frac{f\overline{\partial f}}{\overline{f}^2}\mathrm{d}\overline{z}'\right),\\
X_3&=-\frac{1}{2}\int_\gamma\left(\frac{\partial f}{f}\mathrm{d}z'+\frac{\overline{\partial f}}{\overline{f}}\mathrm{d}\overline{z}'\right).
\end{aligned} \tag{5.4}$$

The constant mean curvature surfaces corresponding to (5.4) for $f(z)=z^n$, $n=6,8,9$ are shown in Figs. 1–3. The induced metric on the surface and its Gaussian curvature (1.8) are given by

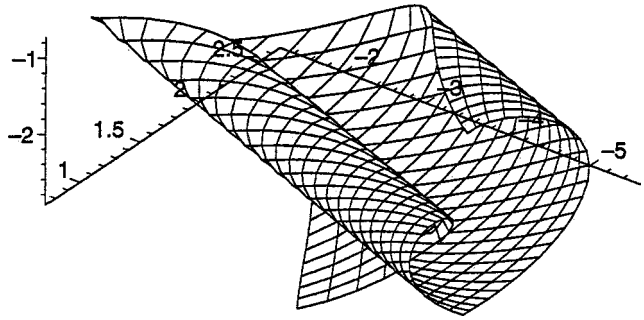

FIG. 1. The constant mean curvature surface for the case (5.4) with $f(z)=z^6$.

$$ds^2=\left|\frac{\partial f}{f}\right|^2 dz\, d\bar{z}, \quad K=-\left(\frac{1}{2}\left|\frac{\partial f}{f}\right|\right)^{-2}\partial\bar{\partial}\left(\ln\left|\frac{\partial f}{f}\right|\right)=0,$$

respectively.

Note that if function ρ is a solution of (3.4), and ρ satisfies algebraic condition (5.1), then both of the functions ρ^{-1} and $\bar{\rho}$ are also solutions of Eq. (3.4). In fact, the derivatives of ρ are

$$\partial\bar{\rho}=-\frac{1}{\rho^2}\partial\rho, \quad \bar{\partial}\bar{\rho}=-\frac{1}{\rho^2}\bar{\partial}\rho, \quad \partial\bar{\partial}\bar{\rho}=\frac{2}{\rho^3}(\partial\rho\,\bar{\partial}\rho)-\frac{1}{\rho^2}\partial\bar{\partial}\rho. \tag{5.5}$$

Substituting (5.5) into Eq. (3.4), we obtain

$$2\frac{\partial\rho\,\bar{\partial}\rho}{\rho^3}-\frac{1}{\rho^2}\partial\bar{\partial}\rho-\frac{1}{\rho^3}\partial\rho\bar{\partial}\rho=0,$$

which is just the identity

$$\partial\bar{\partial}\rho-\frac{1}{\rho}\partial\rho\,\bar{\partial}\rho\equiv 0,$$

since $\bar{\rho}=1/\rho$, and whenever (3.4) holds. Then we have the following Propositions.

Proposition 3: Suppose that for any complex-valued function F of class C^1, the function ρ satisfies the algebraic condition (5.1) and the differential constraints

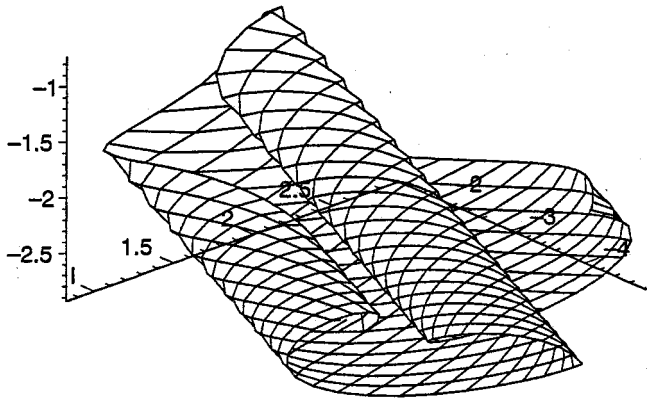

FIG. 2. The constant mean curvature surface for the case (5.4) with $f(z)=z^8$.

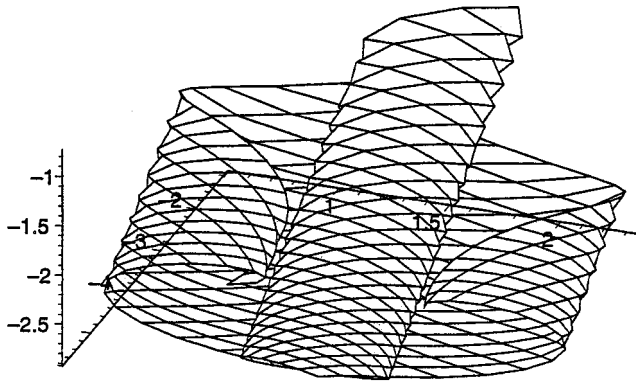

FIG. 3. The constant mean curvature surface for the case (5.4) with $f(z)=z^9$.

$$\partial\rho = F(z)\rho, \quad \overline{\partial}\rho = -\overline{F}(\overline{z})\rho. \tag{5.6}$$

Then the complex valued function ρ is a nonsplitting solution of the system (3.4). The associated surface has zero Gaussian curvature (1.8).

Proof: Note that from Eq. (5.6), we have

$$\overline{\partial}\partial\rho = F(z)\overline{\partial}\rho.$$

Thus, system (3.4) is identically satisfied, since

$$F(\overline{\partial}\rho) - \overline{\rho}(F\rho)(-F\rho) = F(-\overline{F}\rho) - F\overline{F}\rho \equiv 0$$

holds. Moreover, from (3.3), we get

$$\partial\psi_1 = \frac{\epsilon}{4}(\overline{F}\rho)^{1/2}F, \quad \overline{\partial}\psi_2 = -\frac{\epsilon}{4}(F\rho)^{1/2}\overline{F}, \quad p = \frac{1}{2}(F\overline{F})^{1/2}, \quad \epsilon = \pm 1.$$

So in view of (4.7), the GW system is also identically satisfied. Moreover, we have

$$\partial \ln p = \frac{\partial p}{p} = \frac{\partial F}{2F},$$

which implies that $\overline{\partial}(\partial p) = 0$, since F is a function of only z. Thus from formula (1.8), the Gaussian curvature K is zero. Q.E.D.

We now discuss the possibility of constructing more general classes of solutions of GW system (1.3) which are based on nonlinear superpositions of N elementary solutions of sigma model (3.4).

Proposition 4: (Factorization) Suppose that for each $i=1,\ldots,N$ the complex valued functions ρ_i satisfy the sigma model system (3.4) and the conditions $|\rho_i|^2 = 1$. Then the product function

$$\rho = \prod_{i=1}^{N} \rho_i \tag{5.7}$$

is also a solution of system (3.4). The corresponding solution of the GW system (1.3) takes the following factorized form:

$$\psi_1 = \frac{1}{2}\epsilon \prod_{i=1}^{N} \rho_i \left(\overline{\partial} \prod_{j=1}^{N} \overline{\rho_j} \right)^{1/2}, \quad \psi_2 = \frac{1}{2}\epsilon \left(\partial \prod_{j=1}^{N} \rho_j \right)^{1/2}.$$

Proof: It suffices to prove this for $N=2$, and then to invoke induction to extend this to any N. Suppose that ρ_1,ρ_2 are solutions to (3.4). Substituting the function $\rho=\rho_1\rho_2$ into (3.4), we obtain

$$(\overline{\partial}\partial\rho_1)\rho_2+\partial\rho_1\overline{\partial}\rho_2+\overline{\partial}\rho_1\partial\rho_2+\rho_1\overline{\partial}\partial\rho_2-\overline{\rho}_1\rho_2\partial\rho_1\overline{\partial}\rho_1-\overline{\partial}\rho_1\partial\rho_2-\partial\rho_1\overline{\partial}\rho_2-\rho_1\overline{\rho}_2\partial\rho_2\overline{\partial}\rho_2$$
$$=\rho_2(\overline{\partial}\partial\rho_1-\overline{\rho}_1\partial\rho_1\overline{\partial}\rho_1)+\rho_1(\overline{\partial}\partial\rho_2-\overline{\rho}_2\partial\rho_2\overline{\partial}\rho_2)=0,$$

whenever the functions ρ_i satisfy sigma model equations (3.4). Thus, the product of two solutions is a solution. Consequently, proceeding inductively from the product form of ρ given in (5.7), if the equation is satisfied for a solution with k factors, it is satisfied for a solution with $k+1$ factors. Substituting (5.7) into (3.3), we obtain ψ_1 and ψ_2 which satisfy system (1.3). Q.E.D.

Propositions 3 and 4 provide us with the possibility of constructing a class of nonsplitting solutions of Eq. (1.3). We now present several examples of such solutions.

(1) Let us discuss now the construction of an algebraic multisoliton solution of the GW system (1.3). First, we look for a particular class of rational solutions of (3.4) admitting simple poles at the points $\overline{z}=\overline{a_j}$,

$$\rho_j=\frac{z-a_j}{\overline{z}-\overline{a}_j},\quad a_j\in\mathbb{C},\quad j=1,\ldots,N. \tag{5.8}$$

By virtue of Propositions 3 and 4, a more general case than (5.8) can be constructed by taking products over j in (5.8), when the solution ρ_j of (3.4) admits an arbitrary number of simple poles,

$$\rho=\prod_{k=1}^{N}\frac{z-a_k}{\overline{z}-\overline{a}_k},\quad a_k\in\mathbb{C}, \tag{5.9}$$

where we assume that all a_k are distinct. Note that the complex function ρ admits a removable singularity since

$$\lim_{z\to a_k}(\overline{z}-\overline{a}_k)\left(\frac{z-a_k}{\overline{z}-\overline{a}_k}\right)=0,$$

and thus

$$\lim_{z\to a_k}(\overline{z}-\overline{a}_k)\prod_{j=1}^{N}\left(\frac{z-a_j}{\overline{z}-\overline{a}_j}\right)=0.$$

In that case the function ρ satisfies both conditions $\partial\overline{\partial}\rho\neq 0$ and $|\rho|^2=1$. Substituting (5.9) into (3.4), we obtain that Eq. (3.4) is satisfied identically, where the required first derivatives of ρ are given by

$$\partial\rho=\sum_{j=1}^{N}\frac{1}{(z-a_j)}\rho\equiv F(z)\rho,\quad \overline{\partial}\rho=-\sum_{j=1}^{N}\frac{1}{(\overline{z}-\overline{a}_j)}\rho\equiv-\overline{F}(\overline{z})\rho. \tag{5.10}$$

Substituting (5.9) and (5.10) into (3.3), we determine the explicit form of an algebraic multisoliton solution of the GW system

$$\psi_1=\frac{\epsilon}{2}\left(\sum_{j=1}^{N}\frac{1}{(\overline{z}-\overline{a}_j)}\overline{\rho}\right)^{1/2},\quad \psi_2=\frac{\epsilon}{2}\left(\sum_{j=1}^{N}\frac{1}{(z-a_j)}\rho\right)^{1/2},\quad \epsilon=\pm 1. \tag{5.11}$$

For the case $N=1$, substituting (5.11) into relation (1.4), we obtain that the corresponding constant mean curvature surface is determined by

$$(X_1^2+X_2^2)^2-\left(2+\frac{a^2}{4}e^{2X_3}\right)(X_1^2+X_2^2)+\frac{a^2}{2}e^{2X_3}X_2+1-\frac{a^2}{4}e^{2X_3}=0.$$

(2) Another class of rational solutions can be written down by noting that, by Proposition 4, a new solution can be found by taking products of ρ_k with itself k times and so

$$\rho_k=\left(\frac{z-a_k}{\overline{z}-\overline{a}_k}\right)^k$$

satisfies identically Eq. (3.4) for any integer k and complex a_k. Consequently, we can generalize the form of this solution to another type of nonsplitting multisoliton solution of (3.4) by applying Proposition 4 again and forming products over k. This solution is generated by a ρ of the form

$$\rho=\prod_{k=1}^{N}\left(\frac{z-a_k}{\overline{z}-\overline{a}_k}\right)^k. \tag{5.12}$$

Note that for each a_k, the function ρ has a removable singularity. So in this case, the function ρ satisfies $|\rho|^2=1$, and the derivatives of ρ are given by

$$\partial\rho=\sum_{k=1}^{N}\frac{k}{z-a_k}\rho\equiv H\rho,\quad \overline{\partial}\rho=-\sum_{k=1}^{N}\frac{k}{\overline{z}-\overline{a}_k}\rho\equiv\overline{H}\rho. \tag{5.13}$$

Substituting (5.12) and (5.13) into Eq. (3.4), we find that

$$\overline{\partial}\partial\rho-\overline{\rho}\partial\rho\overline{\partial}\rho=-\sum_{k=1}^{N}\frac{k}{z-a_k}\sum_{j=1}^{N}\frac{j}{\overline{z}-\overline{a}_j}\rho+\overline{\rho}\sum_{k=1}^{N}\frac{k}{z-a_k}\rho\sum_{j=1}^{N}\frac{j}{\overline{z}-\overline{a}_j}\rho=0.$$

From (5.12) and (5.13), we can determine through the transformation (3.3) the explicit form of an algebraic multisoliton solution of the GW system

$$\psi_1=\frac{\epsilon}{2}\left(\sum_{k=1}^{N}\frac{k}{(\overline{z}-\overline{a}_k)}\overline{\rho}\right)^{1/2},\quad \psi_2=\frac{\epsilon}{2}\left(\sum_{k=1}^{N}\frac{k}{(z-a_k)}\rho\right)^{1/2}. \tag{5.14}$$

Similarly, these solutions as in the previous case (5.11) also admit simple poles at $z=a_k$

(3) An interesting class of nonsplitting solution can be found by applying Proposition 4 to ρ_k a total of n times for a fixed number n, to obtain a new solution, and then applying Proposition 4 again by taking products over k,

$$\rho=\prod_{k=1}^{N}\left(\frac{z-a_k}{\overline{z}-\overline{a}_k}\right)^n. \tag{5.15}$$

The function ρ satisfies (5.1), and the derivatives of ρ are given by

$$\partial\rho=n\sum_{j=1}^{N}\frac{1}{(z-a_j)}\rho,\quad \overline{\partial}\rho=-n\sum_{j=1}^{N}\frac{1}{(\overline{z}-\overline{a}_j)}\rho. \tag{5.16}$$

From (3.3), the solution of GW system (1.3) in this case takes the form

$$\psi_1=\frac{\epsilon}{2}\left(n\sum_{j=1}^{N}\frac{1}{(\overline{z}-\overline{a}_j)}\overline{\rho}\right)^{1/2},\quad \psi_2=\frac{\epsilon}{2}\left(n\sum_{j=1}^{N}\frac{1}{(z-a_j)}\rho\right)^{1/2}. \tag{5.17}$$

Note that the function ψ_i admits only simple poles.

(4) There exists an exponential class of nonsplitting solution of GW system (1.3) which is generated by the products of functions of the form $\rho_j = e^{\overline{\alpha_i} z - \alpha_i \overline{z}}$ as follows:

$$\rho = \prod_{j=1}^{N} \rho_j = e^{\overline{A} z - A \overline{z}}. \tag{5.18}$$

This satisfies condition (5.1), and generates, using Proposition 4, the following class of solutions of GW system (1.3):

$$\psi_1 = \frac{\epsilon}{2} A^{1/2} e^{(\overline{A} z - A \overline{z})/2}, \quad \psi_2 = \frac{\epsilon}{2} \overline{A}^{1/2} e^{(\overline{A} z - A \overline{z})/2}. \tag{5.19}$$

(5) An explicit class of solutions to GW system (1.3) admitting two arbitrary real-valued functions of one real variable can be constructed based on the idea of Proposition 4. Suppose that h and χ are real-valued functions of one variable $s = z + \overline{z}$, then the following function

$$\rho = e^{-i\chi(s)} \frac{c_1 e^{h(s)} + c_2 e^{-h(s)}}{\overline{c_1} e^{h(s)} + \overline{c_2} e^{-h(s)}}, \quad c_1, c_2 \in \mathbb{C}, \tag{5.20}$$

satisfies the constraint (5.1) and system (3.4), provided that the condition $c_1 \overline{c_2} - c_2 \overline{c_1} = 0$ on the complex constants c_1 and c_2 holds. Defining the quantities

$$f^{(\pm)}(s) = c_1 e^{h(s)} \pm c_2 e^{-h(s)},$$

and using Proposition 2, we can write a general solution of the sigma model (3.4) as follows:

$$\rho = \exp\left[-i \sum_{j=1}^{N} \chi_j(s) \right] \prod_{i=1}^{N} \frac{f_i^{(+)}(s)}{\overline{f_i^{(+)}}(s)}. \tag{5.21}$$

So, we have

$$\partial\rho = \left[-i \sum_{j=1}^{N} \chi_j' + \sum_{k=1}^{N} \frac{f_k^{(-)} h_k'}{f_k^{(+)}} - \sum_{k=1}^{N} \frac{\overline{f_k^{(-)}} h_k'}{\overline{f_k^{(+)}}} \right] \rho, \tag{5.22}$$

where the prime represents differentiation of χ and h with respect to s. Substituting (5.21) and (5.22) into transformation (3.3), we determine explicitly the corresponding form of multisoliton solution of GW system (1.3),

$$\begin{aligned} \psi_1 &= \frac{\epsilon}{2} \left(\rho \left[i \sum_{j=1}^{N} \chi_j' + \sum_{k=1}^{N} \frac{\overline{f_k^{(-)}} h_k'}{\overline{f_k^{(+)}}} - \sum_{k=1}^{N} \frac{\overline{f_k^{(-)}} h_k'}{\overline{f_k^{(+)}}} \right] \right)^{1/2}, \\ \psi_2 &= \frac{\epsilon}{2} \left(\rho \left[-i \sum_{j=1}^{N} \chi_j' + \sum_{k=1}^{N} \frac{f_k^{(-)} h_k'}{f_k^{(+)}} - \sum_{k=1}^{N} \frac{\overline{f_k^{(-)}} h_k'}{\overline{f_k^{(+)}}} \right] \right)^{1/2}. \end{aligned} \tag{5.23}$$

Note that solutions (5.23) do not admit any singularities when $c_1 \neq c_2$.

(6) Using Proposition 4, an interesting class of periodic nonsplitting solutions of (3.4) satisfying the algebraic constraint (5.1) has the form

$$\rho = \exp\left(\sum_{j=1}^{N} (\cos(z - a_j) - \cos(\overline{z} - \overline{a_j})) \right). \tag{5.24}$$

The derivatives of ρ are given by

$$\partial\rho=-\sum_{j=1}^{N}\sin(z-a_j)\rho,\quad \overline{\partial}\rho=\sum_{j=1}^{N}\sin(\overline{z}-\overline{a}_j)\rho.$$

Then using (3.3), we can find that the solutions of GW system (1.3) are

$$\psi_1=\frac{\epsilon}{2}\left(-\sum_{j=1}^{N}\sin(\overline{z}-\overline{a}_j)\overline{\rho}\right)^{1/2},\quad \psi_2=\frac{\epsilon}{2}\left(-\sum_{j=1}^{N}\sin(z-a_j)\rho\right)^{1/2},\quad p=\frac{1}{2}\left|\sum_{j=1}^{N}\sin(z-a_j)\right|. \tag{5.25}$$

Note that solutions (5.19) and (5.25) do not admit any singularities. When $N=1$, the associated constant mean curvature surface can be computed from relation (1.7),

$$u(X_1+iX_2)=-iv,\quad v(X_1-iX_2)=iu,\quad uv=e^{2X_3},$$

where $u=\exp(\cos(z-a))$ and $v=\exp(\cos(\overline{z}-\overline{a}))$. The corresponding surface is a cylinder having X_3 as a symmetry axis since X_1 and X_2 satisfy $X_1^2+X_2^2=1$. Similar calculations to the one given by (5.24) can be performed when cos in (5.24) is replaced by trigonometric and hyperbolic functions sin and cosh or sinh, respectively. This procedure provides us with several classes of periodic solutions of GW system (1.3).

Finally, one can apply Proposition 4 again to solutions of the form (5.24) of sigma model (3.4) by replacing the cos function by sin and taking products of these resulting solutions, namely (5.24) and the modified one,

$$\begin{aligned}\rho&=\exp\left(\sum_{j=1}^{N}(\cos(z-a_j)-\cos(\overline{z}-\overline{a}_j)+\sin(z-a_j)-\sin(\overline{z}-\overline{a}_j))\right)\\&=\exp\left(\sum_{j=1}^{N}\left(-2\sin\left(\frac{z+\overline{z}-a_j-\overline{a}_j}{2}\right)\sin\left(\frac{z-\overline{z}-a_j+\overline{a}_j}{2}\right)\right.\right.\\&\quad\left.\left.+2\cos\left(\frac{z+\overline{z}-a_j-\overline{a}_j}{2}\right)\sin\left(\frac{z-\overline{z}-a_j+\overline{a}_j}{2}\right)\right)\right).\end{aligned} \tag{5.26}$$

The corresponding solution of GW system (1.3) has the form

$$\begin{aligned}\psi_1&=\frac{1}{2}\epsilon\left(\overline{\rho}\sum_{j=1}^{N}(-\sin(\overline{z}-\overline{a}_j)+\cos(\overline{z}-\overline{a}_j))\right)^{1/2},\\\psi_2&=\frac{1}{2}\epsilon\left(\rho\sum_{j=1}^{N}(-\sin(z-a_j)+\cos(z-a_j))\right)^{1/2}.\end{aligned} \tag{5.27}$$

Note that there exists a resemblance of function ρ given by (5.26) to a Calogero–Sutherland type potential.[36] A large class of hyperbolic nonsplitting solution can be obtained by replacing the trigonometric functions appearing in (5.26) by hyperbolic functions, and these solutions lead to spherical surfaces, namely, $X_1^2+X_2^2+X_3^2=1$. Solutions which yield cylinders and spheres can have applications to certain types of cosmological models.[5]

Recently, a new approach to classical configurations of strings in three-dimensional Euclidean space has been proposed.[6,12] It is basically done by representing the Euler–Lagrange equation for the Nambu–Goto–Polyakov action in a simple form. One then looks for common solutions of this equation and the GW system. From a physical point of view, it has been proposed to describe QCD flux tubes in this way. Conformal invariance is important here because one is involved in the

construction of a Lorentz invariant extended object. The world sheet of the string will obey a two-dimensional wave equation, and using the conformal invariance of this equation, by a suitable choice of conformal frame, one may get rid of the vibrations in, for example, the timelike direction.

In the case in which the mean curvature is constant, the Euler–Lagrange equation reduces to the Liouville equation in the variable $\theta=\ln p^2$ as follows, $\partial\bar{\partial}\theta+\beta e^{\theta}=0$. All of the new solutions here can be made to satify this if β is taken to be zero. Konopelchenko[6] has pointed out that the Liouville equation is of importance since it can be thought of as describing a theory of metrics. In fact, the idea that a geometric realization of gravity as extended two-dimensional gravity involves $\mathbb{R}^3$ surfaces of constant mean curvature.[6] Generalized exponential solutions generated by (1.3) in the case $\partial p=\bar{\partial}\bar{p}$ have applications to gravity. In a certain limit of Laplace–Beltrami gravity, the action of the theory corresponds to the action of the sigma model and the equation of motion then corresponds to (3.4). It turns out[6] that multi-instanton or anti-instanton solutions of the form (5.9) are the only solutions of (3.4) with finite action.

VI. DIFFERENTIAL CONSTRAINTS AND SOLUTIONS OF THE GW SYSTEM

We now discuss the existence of certain classes of solutions to the GW system (1.3) which can be obtained by subjecting (1.3) to specific differential constraints which allows us to reduce the overdetermined system to a system admitting a first integral. This fact simplifies considerably the process of solving the initial system (1.3) and consequently, certain classes of nonsplitting solutions can be constructed.

First let us discuss the case when we append two differential constraints to GW system (1.3) of the form

$$\psi_1\partial\bar{\psi}_1+\bar{\psi}_2\partial\psi_2=0,\quad \bar{\psi}_1\bar{\partial}\psi_1+\psi_2\bar{\partial}\bar{\psi}_2=0. \tag{6.1}$$

In terms of the complex functions ψ_i, it has been shown[26] that the reduction of the overdetermined system composed of (1.3) and (6.1) is equivalent to a linear decoupled system

$$\bar{\partial}\partial\psi_i+p_0^2\psi_i=0,\quad i=1,2, \tag{6.2}$$

with the first integral of the motion

$$|\psi_1|^2+|\psi_2|^2=p_0\in\mathbb{R}. \tag{6.3}$$

Indeed, making use of GW system (1.3) and condition (6.1), we have

$$\partial p=\psi_1(\partial\bar{\psi}_1)+\bar{\psi}_2(\partial\psi_2)=0,\quad \bar{\partial}\bar{p}=\bar{\psi}_1(\bar{\partial}\psi_1)+\psi_2(\bar{\partial}\bar{\psi}_2)=0. \tag{6.4}$$

This means that p is a real constant. The overdetermined system (1.3) and (6.1) admits a three-dimensional symmetry group, namely, the similitude group Sim(2,$\mathbb{C}$). Its Lie subalgebra of algebra (2.1) is spanned by $\{T_1,T_2,H\}$ and the corresponding invariant is given by (6.3).

Now let us express the constraints in (6.4) in terms of the function ρ. Taking into account (3.4), the differential constraints in (6.4) become

$$\frac{\partial p}{\bar{\psi}_2}=\rho\partial\bar{\psi}_1+\partial\psi_2=\frac{\epsilon}{2}(\partial\rho)^{-1/2}\partial^2\rho-\epsilon\frac{(\partial\rho)^{1/2}}{1+|\rho|^2}(\rho\partial\bar{\rho}+\bar{\rho}\partial\rho)+\epsilon\rho\frac{(\partial\rho)^{1/2}(\partial\bar{\rho})}{1+|\rho|^2}=0,\quad \epsilon=\pm1, \tag{6.5}$$

and its respective complex conjugate. As a result, the overdetermined system composed of Eqs. (3.4) and (6.5) for the function ρ take the form

$$\begin{aligned}&\bar\partial\partial\rho-\frac{2\bar\rho}{1+|\rho|^2}\partial\rho\bar\partial\rho=0,\quad \partial\bar\partial\bar\rho-\frac{2\rho}{1+|\rho|^2}\partial\bar\rho\bar\partial\bar\rho=0,\\&\partial^2\rho-\frac{2\bar\rho}{1+|\rho|^2}(\partial\rho)^2=0,\quad \bar\partial^2\bar\rho-\frac{2\rho}{1+|\rho|^2}(\bar\partial\bar\rho)^2=0.\end{aligned}\tag{6.6}$$

We show now that if the current J given by (3.7) is constant, then all second derivatives of ρ are determined in terms of ρ and their first derivatives. In fact, differentiating the current J with respect to ∂ we get

$$(1+|\rho|^2)(\partial\bar\rho\partial^2\rho+\partial\rho\partial^2\bar\rho)-2\,\partial\rho\partial\bar\rho(\bar\rho\partial\rho+\rho\partial\bar\rho)=0.$$

Taking into account the system (6.6), we obtain

$$\partial^2\bar\rho-\frac{2\rho}{1+|\rho|^2}(\partial\bar\rho)^2=0,\quad \bar\partial^2\rho-\frac{2\bar\rho}{1+|\rho|^2}(\bar\partial\rho)^2=0.\tag{6.7}$$

Hence, all second-order derivatives of ρ are known in terms of ρ and its derivatives. Note that all compatibility conditions are identically satisfied whenever Eq. (3.4) holds. Moreover, the nonsplitting exponential class of solution (5.18) is a solution of the system (6.6) and (6.7). Thus, we can formulate the following:

Proposition 5: The overdetermined system (6.6) and (6.7) for the function ρ admits a first integral of the form

$$\frac{(\partial\rho\,\bar\partial\bar\rho)^{1/2}}{1+|\rho|^2}=p_0,\quad p_0\in\mathbb{R}.\tag{6.8}$$

Proof: Differentiating the left-hand side of (6.8) with respect to ∂, we obtain

$$\partial\left(\frac{(\partial\rho\bar\partial\bar\rho)^{1/2}}{1+|\rho|^2}\right)=\frac{(\partial\rho)^{-1/2}(\bar\partial\bar\rho)^{1/2}}{2(1+|\rho|^2)}\left[(\bar\partial\bar\rho)\partial^2\rho+\partial\rho(\partial\bar\partial\bar\rho)-2\frac{(\partial\rho)(\bar\partial\bar\rho)}{1+|\rho|^2}(\partial\rho\,\bar\rho+\rho\partial\bar\rho)\right].\tag{6.9}$$

Substituting (6.6) and (6.7) into system (6.9), this is identically zero, since

$$\frac{2\bar\rho}{1+|\rho|^2}(\bar\partial\bar\rho)(\partial\rho)^2+\frac{2\rho}{1+|\rho|^2}\partial\rho\partial\bar\rho\bar\partial\bar\rho-\frac{2\bar\rho}{1+|\rho|^2}\bar\partial\bar\rho(\partial\rho)^2-\frac{2\rho}{1+|\rho|^2}\partial\rho\partial\bar\rho\bar\partial\bar\rho\equiv0.$$

Similarly, differentiating the left-hand side of (6.8) with respect to $\bar\partial$ and making use of (6.6) and (6.7), we obtain that the resulting equation is identically satisfied. Q.E.D.

Proposition 6: If the functions ψ_1 and ψ_2 satisfy the overdetermined system composed of the initial value problem for GW system (1.3) with $\psi_i(0)=0$ and differential constraints (6.1),

$$\begin{aligned}&\partial\psi_1=p\psi_2,\quad \bar\partial\psi_2=-p\psi_1,\quad \psi_i(0)=0,\\&\psi_1\partial\bar\psi_1+\bar\psi_2\partial\psi_2=0,\quad \bar\psi_1\bar\partial\psi_1+\psi_2\bar\partial\bar\psi_2=0,\end{aligned}\tag{6.10}$$

then the general solution has the form

$$\psi_i=J_0(p_0\sqrt{(z-z_i^1)(\bar z-\bar z_i^2)}),\quad p_0\in\mathbb{R},\quad z_i^1,z_i^2\in\mathbb{C},\quad i=1,2,\tag{6.11}$$

where J_0 is a Bessel function of order zero. The general solution of (6.6) and (6.7) has the form

$$\rho=\frac{J_0(p_0\sqrt{(z-z_1^1)(\overline{z}-\overline{z}_1^2)})}{J_0(p_0\sqrt{(z-z_2^1)(\overline{z}-\overline{z}_2^2)})}. \tag{6.12}$$

Proof: If the function W is a solution of the second-order differential equation

$$s_iW^{(2)}(s_i)+W^{(1)}(s_i)+p_0^2W(s_i)=0, \tag{6.13}$$

where the differentiation of W is with respect to s_i, then the general solution of the system (6.2) has the form

$$\psi_i=W(s_i),$$

where

$$s_i=\frac{1}{4p_0^2}(z-z_i^1)(\overline{z}-\overline{z}_i^2), \quad p_0\in\mathbb{R}, \quad z_i^1,z_i^2\in\mathbb{C}.$$

After a change of variable $s_i=r_i^2$, the differential equation (6.13) is reduced to the Bessel equation

$$r_i^2J''(r_i)+r_iJ'(r_i)+4p_0^2r_i^2J(r_i)=0,$$

and the general solution is given by

$$\psi_i=J_0(p_0\sqrt{s_i})=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!^2}(p_0^{2k}(z-z_i^1)^k(\overline{z}-\overline{z}_i^2)^k),$$

and hence (6.10) holds. Then using the definition (3.1) for the function ρ, we find that the general solution of the overdetermined system (6.6) and (6.7) is given by (6.12). Q.E.D.

Finally, let us discuss the case when the GW system (1.3) is subjected to a single constraint

$$\psi_1\partial\overline{\psi}_1+\overline{\psi}_2\partial\psi_2-\epsilon(\overline{\psi}_1\overline{\partial}\psi_1+\psi_2\overline{\partial\psi}_2)=0, \quad \epsilon=\pm1. \tag{6.14}$$

This is a weaker condition than (6.1), since two constraints have been combined. In terms of the complex function ρ, Eq. (6.14) becomes

$$\left(\partial^2\rho-\frac{2\overline{\rho}}{1+|\rho|^2}(\partial\rho)^2\right)\overline{\partial\rho}-\epsilon\left(\overline{\partial}^2\overline{\rho}-\frac{2\rho}{1+|\rho|^2}(\overline{\partial\rho})^2\right)\partial\rho=0. \tag{6.15}$$

Note that if the function ρ satisfies the overdetermined system composed of Eqs. (3.4) and (6.15), then there exists a conserved quantity

$$\frac{(\partial\rho)^{1/2}(\overline{\partial\rho})^{1/2}}{1+|\rho|^2}=p(z+\epsilon\overline{z}). \tag{6.16}$$

In fact, from Eq. (6.16) and taking into account Eqs. (3.4) and (6.15), we obtain

$$(\partial-\epsilon\overline{\partial})\left(\frac{(\partial\rho)^{1/2}(\overline{\partial\rho})^{1/2}}{1+|\rho|^2}\right)=p\left\{\frac{\partial^2\rho}{2\partial\rho}-\frac{\overline{\rho}\partial\rho}{1+|\rho|^2}-\epsilon\left(\frac{\overline{\partial}^2\overline{\rho}}{2\overline{\partial\rho}}-\frac{\rho\overline{\partial\rho}}{1+|\rho|^2}\right)\right\}\equiv0. \tag{6.17}$$

Hence, the quantity p is a real valued function of the argument $s=z+\epsilon\overline{z}$. This means that the solution of the system (1.3) and (6.14) is invariant under a two-dimensional symmetry algebra $\{T_1+\epsilon T_2,H\}$. This class of solutions has been discussed in detail in Ref. 27.

VII. SUMMARY AND CONCLUDING REMARKS

The main aim of the paper has been to provide a great variety of exact analytic solutions through the systematic use of the subgroup structure of the invariance group of the generalized Weierstrass system. We concentrated mainly on classical symmetries as well on conditional symmetries for the GW system. The latter case refers to the symmetry of the overdetermined system obtained by supplementing the original system (1.3) with the differential constraints (6.1), and the original system (3.4) subjected to constraints (5.1). Thus, the solutions obtained for this overdetermined system are invariant under the action of the conditional symmetry algebras. They were investigated and a procedure for constructing them was proposed. We can summarize the results which were obtained using both symmetry methods in our work in the following cases:

(1) Elementary solutions, that is, constant, algebraic with one or two simple poles, trigonometric and hyperbolic solutions.
(2) Doubly periodic solutions which can be expressed in terms of Jacobi elliptic functions sn, cn, and dn.
(3) Some of the reduced equations can be written in terms of Painlevé transcendents.

It is worth noting that the symmetry analysis of the sigma model (3.4) provides much larger classes of solutions to the original system (1.3) by means of transformation (3.3), than the symmetry analysis of GW system applied directly. This is due to the fact that there exists a gauge freedom in the definition of the function ρ, since the numerator and denominator of (3.1) can be multiplied by any complex function. Note also that the inverse mapping of (3.1) is a double valued function, and is provided by (3.3). We found that when, at least locally, the solutions of GW system (1.3) are single valued as a function of its complex independent variables, the system is a completely integrable one. Such a phenomena has been known since the the time of Kovalevsky[37] in connection with the equations of the spinning top. In this case, the single-valued solutions of these equations are integrable, and wide classes of solutions have been constructed.

The construction of constant mean curvature surfaces which are embedded in three-dimensional Euclidean space, by means of expression (1.7), is more difficult to integrate explicitly in the case when solutions of (1.3) are expressed in terms of Jacobi elliptic functions. In many of these cases, we deal with hyperelliptic integrals and the formulas obtained are quite complex expressions, and we skip them. However, the qualitative features, such as asymptotic behavior, geometrical description, of these integrals can be investigated numerically (i.e., their singularity structure such as the existence of different types of poles, etc.).

The question arises whether our approach can be extended to GW systems describing surfaces immersed in multidimensional Euclidean and pseudo-Riemannian spaces and if this may provide new classes of solutions. Recently, such generalization of the GW system has been achieved by Konopelchenko *et al.*[12,38,39] where, in particular, the explicit representations for generic surfaces conformally immersed into multidimensional Euclidean and pseudo-Euclidean spaces with different signatures have been derived.

In particular, the Dirac-type system for the four complex-valued functions ψ_α and φ_α describing constant mean curvature surfaces immersed in four-dimensional Euclidean space is given by[37]

$$\partial\psi_\alpha = p\varphi_\alpha, \quad \bar{\partial}\varphi_\alpha = -p\psi_\alpha, \quad \bar{\partial}\bar{\psi}_\alpha = p\bar{\varphi}_\alpha, \quad \partial\bar{\varphi}_\alpha = -p\bar{\psi}_\alpha, \quad \alpha = 1,2, \tag{7.1}$$

where the following notation has been introduced:

$$p = (u_1 u_2)^{1/2}, \quad u_\alpha = |\psi_\alpha|^2 + |\varphi_\alpha|^2, \quad \alpha = 1,2. \tag{7.2}$$

The GW system (7.1) possesses several conserved quantities and admits compatible differential constraints, among them the following:

$$\text{(i)} \quad \partial(\psi_\alpha\psi_\beta) + \bar{\partial}(\varphi_\alpha\varphi_\beta) = 0, \quad \bar{\partial}(\bar{\psi}_\alpha\bar{\psi}_\beta) + \partial(\bar{\varphi}_\alpha\bar{\varphi}_\beta) = 0, \quad \alpha \neq \beta = 1,2,$$

$$\begin{aligned}
&\text{(ii)} \quad \partial(\psi_\alpha\overline{\varphi}_\beta)-\overline{\partial}(\varphi_\alpha\overline{\psi}_\beta)=0, \quad \overline{\partial}(\overline{\psi}_\alpha\varphi_\beta)-\partial(\overline{\varphi}_\alpha\psi_\beta)=0 \quad \alpha\neq\beta=1,2,\\
&\text{(iii)} \quad \varphi_\alpha\partial\overline{\varphi}_\alpha+\overline{\psi}_\alpha\partial\psi_\alpha=0, \quad \overline{\varphi}_\alpha\overline{\partial}\varphi_\alpha+\psi_\alpha\overline{\partial\psi}_\alpha=0, \quad \alpha=1,2,\\
&\text{(iv)} \quad \partial(\ln\psi_\alpha)\overline{\partial}(\ln\varphi_\alpha)=-p^2, \quad \overline{\partial}(\ln\overline{\psi}_\alpha)\partial(\ln\overline{\varphi}_\alpha)=-p^2, \quad \alpha=1,2..
\end{aligned} \tag{7.3}$$

It has been shown,[38] that for each pair of complex fields $(\psi_\alpha,\varphi_\alpha)$ resulting from system (7.1), a set of constant mean curvature surfaces is obtained by means of the following parametrization:

$$(z,\overline{z})\to\mathbf{r}=(X_1(z,\overline{z}),\ldots,X_4(z,\overline{z})),$$

such that

$$\begin{aligned}
X_1+iX_2&=\int_\Gamma(i\overline{\psi_1\psi_2}\,\mathrm{d}z'-i\overline{\varphi_1\varphi_2}\,\mathrm{d}\overline{z}'),\\
X_1-iX_2&=\int_\Gamma(i\varphi_1\varphi_2\,\mathrm{d}z-i\psi_1\psi_2\,\mathrm{d}\overline{z}),\\
X_4+iX_3&=\int_\Gamma(-i\overline{\psi}_2\varphi_1\,\mathrm{d}z'-i\psi_1\overline{\varphi}_2\,\mathrm{d}\overline{z}'),\\
X_4-iX_3&=\int_\Gamma(i\overline{\psi}_1\varphi_2\,\mathrm{d}z'+i\psi_2\overline{\varphi}_1\,\mathrm{d}\overline{z}'),
\end{aligned} \tag{7.4}$$

where Γ is any contour in $\mathbb{C}$. Note the functions $X_i(z,\overline{z})$ are real valued functions since Eq. (7.3) holds. These functions can be identified with the components of a position vector $\mathbf{r}$ of a surface imbedded in $\mathbb{R}^4$.

Making use of (7.2), one can differentiate p to obtain

$$\begin{aligned}
p\partial\overline{\partial}p-\partial p\overline{\partial}p=&-\frac{1}{2p^2}(\partial u_1u_2+u_1\partial u_2)(\overline{\partial}u_1u_2+u_1\overline{\partial}u_2)+\frac{1}{2}(\partial\overline{\partial}u_1u_2+\overline{\partial}u_1\partial u_2+\partial u_1\overline{\partial}u_2\\
&+u_1\partial\overline{\partial}u_2).
\end{aligned} \tag{7.5}$$

Substituting the derivatives of u_α, namely,

$$\partial u_1=\psi_1\partial\overline{\psi}_1+\overline{\varphi}_1\partial\varphi_1, \quad \partial u_2=\psi_2\partial\overline{\psi}_2+\overline{\varphi}_2\partial\varphi_2,$$

and their conjugates, as well as their second derivatives,

$$\partial\overline{\partial}u_1=\partial\overline{\psi}_1\overline{\partial}\overline{\psi}_1+\partial\varphi_1\overline{\partial}\overline{\varphi}_1-p^2u_1, \quad \partial\overline{\partial}u_2=\partial\overline{\psi}_2\overline{\partial}\overline{\psi}_2+\partial\varphi_2\overline{\partial}\overline{\varphi}_2-p^2u_2,$$

into Eq. (7.5), we get the following expression:

$$\begin{aligned}
p\partial\overline{\partial}p-\partial p\overline{\partial}p=&\frac{1}{2p^2}[u_2^2(|\varphi_1|^2\overline{\partial}\psi_1\partial\overline{\psi}_1-\overline{\varphi}_1\overline{\psi}_1\partial\varphi_1\overline{\partial}\psi_1-\psi_1\varphi_1\partial\overline{\psi}_1\overline{\partial}\overline{\varphi}_1+|\psi_1|^2\partial\varphi_1\overline{\partial}\overline{\varphi}_1)\\
&+u_1^2(|\varphi_2|^2\partial\overline{\psi}_2\overline{\partial}\psi_2-\overline{\varphi}_2\overline{\psi}_2\partial\varphi_2\overline{\partial}\psi_2-\varphi_2\psi_2\partial\overline{\psi}_2\overline{\partial}\overline{\varphi}_2+|\psi_2|^2\partial\varphi_2\overline{\partial}\overline{\varphi}_2)-2p^6].
\end{aligned} \tag{7.6}$$

Defining the quantities $J_1=\varphi_1\partial\overline{\psi}_1-\overline{\psi}_1\partial\varphi_1$ and $J_2=\varphi_2\partial\overline{\psi}_2-\overline{\psi}_2\partial\varphi_2$, and dividing both sides by p^2, it is straightforward to show that Eq. (7.6) can be written in the form

$$\partial\overline{\partial}(\ln p)=\frac{1}{2p^4}[u_2^2|J_1|^2+u_1^2|J_2|^2-2p^6]. \tag{7.7}$$

In the next stage of this research, using group theoretical techniques, the authors plan to generate in a systematic way large classes of solutions of GW system (7.1), which can be expressed as elementary and doubly periodic functions which are written in terms of the Jacobi elliptic functions. These solutions will lead to the construction of several classes of constant mean curvature surfaces embedded in four-dimensional Euclidean space by making use of Eq. (7.4), which can describe more diverse types of surfaces than the ones discussed in three-dimensional space.

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APPENDIX

It is worth noting that the sigma model equations (3.4) are invariant under discrete transformations generated by

(i) the reflections

$$\begin{aligned} &Z_1: z\to z, \quad \overline{z}\to -\overline{z}, \quad \rho\to\rho, \quad \overline{\rho}\to\overline{\rho},\\ &Z_2: z\to z, \quad \overline{z}\to\overline{z}, \quad \rho\to -\rho, \quad \overline{\rho}\to -\overline{\rho},\\ &Z_3: z\to -z, \quad \overline{z}\to\overline{z}, \quad \rho\to -\rho, \quad \overline{\rho}\to\overline{\rho}, \end{aligned} \tag{A1}$$

and their complex conjugates;

(ii) the inversion

$$I: z\to z, \quad \overline{z}\to\overline{z}, \quad \rho\to\frac{1}{\overline{\rho}}, \quad \overline{\rho}\to\frac{1}{\rho}; \tag{A2}$$

(iii) the Caley transformation which maps the circle into the upper half plane

$$C: z\to z, \quad \overline{z}\to\overline{z}, \quad \rho\to\frac{1+i\eta}{1-i\eta}, \quad \overline{\rho}\to\frac{1-i\overline{\eta}}{1+i\overline{\eta}}; \tag{A3}$$

(iv) the generalized $U(2)$ transformation for any $a,b\in\mathbb{C}$,

$$U: z\to z, \quad \overline{z}\to\overline{z}, \quad \rho\to\frac{a\eta+b}{-\overline{b}\eta+\overline{a}}, \quad \overline{\rho}\to\frac{\overline{a\eta}+\overline{b}}{-b\overline{\eta}+a}, \quad a,b\in\mathbb{C}. \tag{A4}$$

Note that the inversion transformation (iii) preserves the form of the sigma model equations (3.4), since substituting (A2) into (3.4i), we get (3.4ii). Clearly, applying this mapping a second time, we obtain (3.4i) again. This means that the square of the mapping has the same effect as the identity transformation. Note also that transformations (iii) and (iv) preserve the form of Eq. (3.4). Substituting (A3) or (A4) into the sigma model equations (3.4), we get

$$\partial\overline{\partial}\rho-\frac{2\overline{\rho}}{1+|\rho|^2}\partial\rho\overline{\partial}\rho=\frac{\eta+i}{(1+i\eta)^3(1+|\eta|^2)}\left(\partial\overline{\partial}\eta-\frac{2\overline{\eta}}{1+|\eta|^2}\partial\eta\overline{\partial}\eta\right)=0,$$

and

$$\partial\overline{\partial}\rho-\frac{2\overline{\rho}}{1+|\rho|^2}\partial\rho\overline{\partial}\rho=\frac{(|a|^2+|b|^2)}{(\overline{b}\eta-\overline{a})^2}\left(\partial\overline{\partial}\eta-\frac{2\overline{\eta}}{1+|\eta|^2}\partial\eta\overline{\partial}\eta\right)=0,$$

respectively. The discrete subgroups were used to limit the range of parameters occurring in the classification list of one-dimensional subalgebras of the symmetry algebra of sigma model (3.4).

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Differential geometry of $GL_h(1|1)$

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We construct a differential calculus on the quantum supergroup $GL_h(1|1)$ and obtain the h-deformed superalgebra of $GL_h(1|1)$. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1319856]

I. INTRODUCTION

In the last few years, the theory of quantum (super) groups like GL(2), GL(1|1), etc. were generalized in two ways. Both of the generalizations are based on the deformation of the algebra of functions on the matrix (super) groups generated by coordinate functions T^i_j which normally commute. These deformations of Lie (super) groups are algebraic structures depending on one (or more) continuous parameter. We have a standard Lie (super) group for particular values of the deformation parameters. Quantum (super) groups[1,2] present the examples of (graded) Hopf algebras. They have found application in diverse areas of physics and mathematics.[3]

The q-deformation of Lie (super) groups can be realized on a quantum (super) space in which coordinates are noncommuting.[2] Recently the differential calculus on noncommutative (super) space has been intensively studied both by mathematicians and mathematical physicists. There is much activity in differential geometry[4] on quantum groups. Throughout the recent development of differential calculus on the quantum groups two principal concepts are readily seen. The first of them, formulated by Woronowicz,[5] is known as bicovariant differential calculus on the quantum groups. Another concept, introduced by Woronowicz[6] and Schirmacher *et al.*[7] proceeds from the requirement of a calculus only. There are many papers in this field.[8] We shall consider the second concept.

Another type of deformation, the so-called h-deformation, which is a new class of quantum deformations of Lie groups and Lie algebras, has recently been intensively studied.[9] This deformation may be obtained as a contraction of the q-deformation.[10] There is much interest in studies relating to various aspects of the h-deformed algebra. The differential geometry of $SL_h(2)$ was given in Ref. 11. In this work, we introduce a differential calculus on the quantum supergroup $GL_h(1|1)$. This quantum supergroup was obtained in Ref. 12 using a contraction procedure given in Ref. 10.

Let us briefly discuss the content of the article. In the second section, the basic notations of the Hopf algebra structure on the quantum supergroup $GL_h(1|1)$ are introduced. In the third section we shall obtain the commutation relations for the matrix elements and their differentials so we have a differential algebra. This differential algebra (extended algebra) has a Hopf algebra structure. Later, we shall construct the Cartan–Maurer one-forms and obtain the needed commutation relations. Using these commutation relations, we shall describe the quantum algebra for the vector fields (superalgebra generators) for $GL_h(1|1)$ and derive the commutation relations between the matrix elements and the algebra generators. We shall also show that the obtained quantum algebra can be rederived using the partial derivatives and their relations.

II. THE ALGEBRA OF FUNCTIONS ON $GL_h(1|1)$

Elementary properties of quantum supergroup $GL_h(1|1)$ are described in Ref. 12. We state briefly the properties we are going to need in this work. Here we denote q-deformed objects by

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primed quantities. Unprimed quantities will represent transformed coordinates. As usual, it is known that even (bosonic) objects commute with everything and odd (Grassmann) objects anticommute among themselves. In this work, to obtain the quantum supergroup $\mathrm{GL}_h(1|1)$, we shall only assume that odd elements β and γ anticommute with the ''new'' deformation parameter h.

Let us begin with the q-deformed counterparts of $\mathrm{GL}(1|1)$. The quantum supergroup $\mathrm{GL}_q(1|1)$ is defined by the matrices of the form

$$T'=\begin{pmatrix} a' & \beta' \\ \gamma' & d' \end{pmatrix},$$

where the matrix entries satisfy the following commutation relations:[2]

$$\begin{gathered} a'\beta'=q\beta' a', \quad d'\beta'=q\beta' d', \\ a'\gamma'=q\gamma' a', \quad d'\gamma'=q\gamma' d', \\ \beta'\gamma'+\gamma'\beta'=0, \quad \beta'^2=0=\gamma'^2, \\ a'd'=d'a'+(q-q^{-1})\gamma'\beta'. \end{gathered} \tag{1}$$

We now consider the following similarity transformation:[10]

$$T=\begin{pmatrix} a & \beta \\ \gamma & d \end{pmatrix}=g^{-1}T'g, \tag{2}$$

where

$$g=\begin{pmatrix} 1 & 0 \\ h/(q-1) & 1 \end{pmatrix}, \quad h^2=0. \tag{3}$$

Assuming that β and γ anticommute with the Grassmann number h and substituting (2) into (1), we arrive at the following relations:[12]

$$\begin{gathered} a\beta=\beta a, \quad a\gamma=\gamma a+ha^2(1-\mathcal{D}_h^{-1}), \\ d\beta=\beta d, \quad d\gamma=\gamma d+hd^2(\mathcal{D}_h-1), \\ \beta^2=0, \quad \gamma^2=h\gamma d(1-\mathcal{D}_h), \\ \beta\gamma=-\gamma\beta+h\beta d(1-\mathcal{D}_h), \\ ad=da+h\beta d(\mathcal{D}_h-1), \end{gathered} \tag{4}$$

where

$$\mathcal{D}_h=ad^{-1}-\beta d^{-1}\gamma d^{-1} \tag{5}$$

is the quantum superdeterminant of T. It can be checked that $\mathcal{D}_h$ commutes with all matrix elements of T. Note that, by imposing the relation

$$\mathcal{D}_h=1$$

as an interesting case, we obtain the classical special supergroup $SL(1|1)$, instead of $SL_h(1|1)$. In other words, the restriction of the superdeterminant to unity does not give the quantum supergroup $SL_h(1|1)$. It is known that, in the q-deformed case, the restriction to unity ($\mathcal{D}_q = ad^{-1} - \beta d^{-1}\gamma d^{-1} = 1$) gives the quantum supergroup $SL_q(1|1)$.

Let us denote the algebra generated by the elements a, β, γ, d with the relations (4) by $\mathcal{A}$. We know that the algebra $\mathcal{A}$ is a graded Hopf algebra with the following co-structures: the usual coproduct

$$\Delta: \mathcal{A} \to \mathcal{A} \otimes \mathcal{A}, \quad \Delta(T^i_j) = T^i_k \otimes T^k_j, \tag{6}$$

the counit

$$\varepsilon: \mathcal{A} \to \mathcal{C}, \quad \varepsilon(T^i_j) = \delta^i_j, \tag{7}$$

and the coinverse $S: \mathcal{A} \to \mathcal{A}$,

$$S(T) = T^{-1} = \begin{pmatrix} a^{-1} + a^{-1}\beta d^{-1}\gamma a^{-1} & -a^{-1}\beta d^{-1} \\ -d^{-1}\gamma a^{-1} & d^{-1} + d^{-1}\gamma a^{-1}\beta d^{-1} \end{pmatrix}. \tag{8}$$

It is not difficult to verify the following properties of the co-structures:

$$(\Delta \otimes \mathrm{id}) \circ \Delta = (\mathrm{id} \otimes \Delta) \circ \Delta, \tag{9a}$$

$$\mu \circ (\varepsilon \otimes \mathrm{id}) \circ \Delta = \mu' \circ (\mathrm{id} \otimes \varepsilon) \circ \Delta, \tag{9b}$$

$$m \circ (S \otimes \mathrm{id}) \circ \Delta = \varepsilon = m \circ (\mathrm{id} \otimes S) \circ \Delta, \tag{9c}$$

where id denotes the identity mapping, $\mu: \mathcal{C} \otimes \mathcal{A} \to \mathcal{A}$, and $\mu': \mathcal{A} \otimes \mathcal{C} \to \mathcal{A}$ are the canonical isomorphisms, defined by $\mu(k \otimes a) = ka = \mu'(a \otimes k)$, $\forall a \in \mathcal{A}$, $\forall k \in \mathcal{C}$, and m is the multiplication map $m: \mathcal{A} \otimes \mathcal{A} \to \mathcal{A}$, $m(a \otimes b) = ab$.

The multiplication in $\mathcal{A} \otimes \mathcal{A}$ follows the rule

$$(A \otimes B)(C \otimes D) = (-1)^{p(B)p(C)} AC \otimes BD, \tag{10}$$

where $p(X)$ is the z_2-grade of X.

III. DIFFERENTIAL CALCULUS ON $GL_h(1|1)$

In this section, we shall build up the differential calculus on the quantum supergroup $GL_h(1|1)$. The differential calculus on the quantum supergroups involves functions on the supergroup, differentials and differential forms.

A. Differential algebra

We first note the properties of the exterior differential. We can introduce the exterior differential d to be an operator that is nilpotent and obeys the graded Leibniz rule:

$$\mathrm{d}^2 = 0, \tag{11a}$$

and

$$\mathrm{d}(fg) = (\mathrm{d}f)g + (-1)^{p(f)} f(\mathrm{d}g), \tag{11b}$$

where f and g are functions of the matrix elements. Note that, since the deformation parameter h is an odd (Grassmann) number, it must anticommute with the exterior differential d. In fact,

$$\mathrm{d}(hf) = (-1)^{p(h)} h(\mathrm{d}f) = -h(\mathrm{d}f) \Rightarrow \mathrm{d}h = -h\mathrm{d}. \tag{11c}$$

We have seen, in the previous section, that $\mathcal{A}$ is an associative algebra generated by the matrix elements of T with the relations (4). A differential algebra on $\mathcal{A}$ is a z_2-graded associative algebra Γ equipped with an operator d given in (11). Also the algebra Γ has to be generated by $\mathcal{A}\cup\mathrm{d}\mathcal{A}$.

First, we wish to obtain the relations between the matrix elements of T and their differentials. To do this, we shall use the method of Ref. 13. For this reason, we decompose the algebra $\mathcal{A}$ into subalgebras. We denote by $\mathcal{A}_{a'\beta'}$ the algebra generated by the elements a' and β' with the relations

$$a'\beta'=q\beta'a', \quad \beta'^2=0. \tag{12}$$

Then, a possible set of commutation relations between generators of $\mathcal{A}_{a'\beta'}$ and $\mathrm{d}\mathcal{A}_{\mathrm{d}a'\mathrm{d}\beta'}$ is of the form

$$\begin{aligned} a'\mathrm{d}a'&=A_1\mathrm{d}a'a',\\ a'\mathrm{d}\beta'&=F_{11}\mathrm{d}\beta'a'+F_{12}\mathrm{d}a'\beta',\\ \beta'\mathrm{d}a'&=F_{21}\mathrm{d}a'\beta'+F_{22}\mathrm{d}\beta'a',\\ \beta'\mathrm{d}\beta'&=A_2\mathrm{d}\beta'\beta', \end{aligned} \tag{13}$$

where the coefficients A_i and F_{ij} are related to the complex deformation parameter q. To determine them we use the consistency of calculus (see, for details, Ref. 13). Continuing in this way, we can obtain the other relations.

Let us now substitute the matrix elements of $\mathrm{d}T'$,

$$\mathrm{d}T'=\begin{pmatrix}\alpha' & b'\\ c' & \delta'\end{pmatrix}=\begin{pmatrix}\alpha-\dfrac{h}{q-1}b & b\\ c+\dfrac{h}{q-1}(\delta-\alpha) & \delta-\dfrac{h}{q-1}b\end{pmatrix}, \tag{14}$$

and T' into (13). After rather complicated and tedious calculations by using the consistency of calculus, as the final result one has the following commutation relations:

$$\begin{aligned} &a\alpha=\alpha a+h(\alpha\beta-ba), \quad ab=ba-hb\beta,\\ &ac=ca+h(\alpha a-c\beta+\delta a),\\ &a\delta=\delta a+h(ba+\delta\beta),\\ &\beta\alpha=-\alpha\beta+hb\beta, \quad \beta b=b\beta,\\ &\beta c=c\beta+h(\alpha+\delta)\beta, \quad \beta\delta=-\delta\beta-hb\beta,\\ &\gamma\alpha=-\alpha\gamma+h(\alpha a+\alpha d+b\gamma),\\ &\gamma b=b\gamma+hb(a+d),\\ &\gamma c=c\gamma+h(\alpha\gamma+ca+cd+\delta\gamma),\\ &\gamma\delta=-\delta\gamma+h(\delta a+\delta d-b\gamma),\\ &d\alpha=\alpha d-h(\alpha\beta+bd), \quad db=bd+hb\beta,\\ &dc=cd+h(\alpha d+c\beta+\delta d), \end{aligned} \tag{15}$$

$$d\delta = \delta d + h(bd - \delta\beta).$$

It is easy to verify that the deformation parameter h anticommutes with α and δ. In fact, since $ah = ha$ we have

$$0 = \mathrm{d}(ah - ha) = \alpha h + h\alpha.$$

To find the commutation relations between differentials, we apply the exterior differential d on the relations (15) and use the nilpotency of d with (11c). Then it is easy to see that

$$\begin{gathered}
\alpha b = b\alpha + hb^2, \quad \alpha c = c\alpha + h(cb + \delta\alpha), \\
\delta b = b\delta - hb^2, \quad \delta c = c\delta - h(cb - \alpha\delta), \\
\alpha^2 = h\alpha b, \quad \alpha\delta = -\delta\alpha + h(\delta - \alpha)b, \\
\delta^2 = -h\delta b, \quad bc = cb + h(\delta + \alpha)b.
\end{gathered} \tag{16}$$

These relations are the relations of $\mathrm{Gr}_h(1|1)$ in Ref. 14. Note that the central element of $\mathrm{d}\mathcal{A}$, which is generated by the elements α, b, c, δ with the relations (16), is

$$\hat{\mathcal{D}} = bc^{-1} - \alpha c^{-1}\delta c^{-1}. \tag{17}$$

However, the element $\hat{\mathcal{D}}$ also commutes with the generators of $\mathcal{A}$. So, the element $\hat{\mathcal{D}}$ is the central element of the algebra $\mathcal{A}$, too. Thus $\hat{\mathcal{D}}$ is the central element of the differential algebra Γ.

An interesting note is also the following. The central element of the q-deformed differential algebra[13] is only the element $\hat{\mathcal{D}}$. However, the superdeterminant of $T \in \mathrm{GL}_h(1|1)$ commutes with the generators of $\mathrm{d}\mathcal{A}$, too. So the superdeterminant $\mathcal{D}_h$ is also a central element for the h-deformed differential algebra Γ.

B. Hopf algebra structure on Γ

We first note that consistency of a differential calculus with commutation relations (4) means that the algebra Γ is a graded associative algebra generated by the elements of the set $\{a, \beta, \gamma, d, \alpha, b, c, \delta\}$. So, it is sufficient to only describe the actions of co-maps on the subset $\{\alpha, b, c, \delta\}$.

We consider a map $\phi_R : \Gamma \to \Gamma \otimes \mathcal{A}$ such that

$$\phi_R \circ \mathrm{d} = (\mathrm{d} \otimes \mathrm{id}) \circ \Delta. \tag{18}$$

and define a map Δ_R as follows:

$$\Delta_R(u_1 \mathrm{d}v_1 + \mathrm{d}v_2 u_2) = \Delta(u_1)\phi_R(\mathrm{d}v_1) + \phi_R(\mathrm{d}v_2)\Delta(u_2). \tag{19}$$

Then it can be checked that the map Δ_R leaves invariant the relations (15) and (16). One can also check that the following identities are satisfied:

$$(\Delta_R \otimes \mathrm{id}) \circ \Delta_R = (\mathrm{id} \otimes \Delta) \circ \Delta_R, \quad (\mathrm{id} \otimes \epsilon) \circ \Delta_R = \mathrm{id}. \tag{20}$$

However, we do not have a coproduct for the differential algebra because the map ϕ_R does not give an analog for the derivation property (11), yet. So we consider another map $\phi_L : \Gamma \to \mathcal{A} \otimes \Gamma$ such that

$$\phi_L \circ \mathrm{d} = (\tau \otimes \mathrm{d}) \circ \Delta \tag{21}$$

and a map Δ_L with again (19) by replacing L with R. Here $\tau:\Gamma\to\Gamma$ is the linear map of degree zero which gives $\tau(u)=(-1)^{p(u)}u$. The map Δ_L also leaves invariant the relations (15) and (16), and the following identities are satisfied:

$$(\mathrm{id}\otimes\Delta_L)\circ\Delta_L=(\Delta\otimes\mathrm{id})\circ\Delta_L, \quad (\epsilon\otimes\mathrm{id})\circ\Delta_L=\mathrm{id}. \tag{22}$$

To denote the coproduct, counit and coinverse which will be defined on the algebra Γ with those of $\mathcal{A}$ may be inadvisable. For this reason, we shall denote them with a different notation. Let us define the map $\hat{\Delta}$ as

$$\hat{\Delta}=\Delta_R+\Delta_L, \tag{23}$$

which will allow us to define the coproduct of the differential algebra. We denote the restriction of $\hat{\Delta}$ to the algebra $\mathcal{A}$ by Δ and the extension of Δ to the differential algebra Γ by $\hat{\Delta}$. It is possible to interpret the relation

$$\hat{\Delta}|_{\mathcal{A}}=\Delta \tag{24}$$

as the definition of $\hat{\Delta}$ on the generators of $\mathcal{A}$ and (23) as the definition of $\hat{\Delta}$ on differentials. One can see that $\hat{\Delta}$ is a coproduct for the differential algebra Γ where

$$\hat{\Delta}(\mathrm{d}T^i_j)=\mathrm{d}T^i_k\otimes T^k_j+(-1)^{p(T^i_k)}T^i_k\otimes\mathrm{d}T^k_j. \tag{25}$$

It is not difficult to verify the following conditions:

(a) Γ is an $\mathcal{A}$-bimodule.

(b) Γ is an $\mathcal{A}$-bicomodule with left and right coactions Δ_L and Δ_R, respectively, making Γ a left and right $\mathcal{A}$-comodule with (20) and (22), and

$$(\Delta_L\otimes\mathrm{id})\circ\Delta_R=(\mathrm{id}\otimes\Delta_R)\circ\Delta_L, \tag{26}$$

which is the $\mathcal{A}$-bimodule property. So, the triple $(\Gamma,\Delta_L,\Delta_R)$ is a bicovariant bimodule over Hopf algebra $\mathcal{A}$. In additional, since

(c) (Γ,d) is a first order differential calculus over $\mathcal{A}$, and

(d) d is both a left and a right comodule map, i.e., for all $u\in\mathcal{A}$,

$$(\tau\otimes\mathrm{d})\Delta(u)=\Delta_L(\mathrm{d}u), \quad (\mathrm{d}\otimes\mathrm{id})\Delta(u)=\Delta_R(\mathrm{d}u), \tag{27}$$

the quadruple $(\Gamma,\mathrm{d},\Delta_L,\Delta_R)$ is a first order bicovariant differential calculus over Hopf algebra $\mathcal{A}$.

Now let us return to the Hopf algebra structure of Γ. If we define a counit $\hat{\epsilon}$ for the differential algebra as

$$\hat{\epsilon}\circ\mathrm{d}=\mathrm{d}\circ\epsilon=0 \tag{28}$$

and

$$\hat{\epsilon}|_{\mathcal{A}}=\epsilon, \quad \epsilon|_{\Gamma}=\hat{\epsilon}, \tag{29}$$

we have

$$\hat{\epsilon}(\mathrm{d}T^i_j)=0, \tag{30}$$

where

$$\hat{\epsilon}(u_1\mathrm{d}v_1+\mathrm{d}v_2u_2)=\epsilon(u_1)\hat{\epsilon}(\mathrm{d}v_1)+\hat{\epsilon}(\mathrm{d}v_2)\epsilon(u_2). \tag{31}$$

Here we used the fact that $\mathsf{d}(1)=0$.

As the next step we obtain a coinverse $\hat{S}$. For this, it suffices to define $\hat{S}$ such that

$$\hat{S}\circ\mathsf{d}=\mathsf{d}\circ S \tag{32}$$

and

$$\hat{S}|_{\mathcal{A}}=S, \quad S|_{\Gamma}=\hat{S}, \tag{33}$$

where

$$\hat{S}(u_1\mathsf{d}v_1+\mathsf{d}v_2u_2)=\hat{S}(\mathsf{d}v_1)S(u_1)+S(u_2)\hat{S}(\mathsf{d}v_2). \tag{34}$$

Thus the action of $\hat{S}$ on the generators α, b, c and γ is as follows:

$$\hat{S}(\mathsf{d}T^i_j)=-(-1)^{p[(T^{-1})^i_k]}(T^{-1})^i_k\mathsf{d}T^k_l(T^{-1})^l_j. \tag{35}$$

Note that it is easy to check that $\hat{\epsilon}$ and $\hat{S}$ leave invariant the relations (15) and (16). Consequently, we can say that the structure $(\Gamma,\hat{\Delta},\hat{\epsilon},\hat{S})$ is a graded Hopf algebra.

C. Cartan–Maurer one-forms and their relations

To complete the differential geometric scheme we need the Cartan–Maurer one-forms. As in analogy with the one-forms on a Lie group in classical differential geometry, one can construct the matrix valued one-form Ω where

$$\Omega=\mathsf{d}T\ \ T^{-1}. \tag{36}$$

So, we can write the matrix elements (one-forms) of Ω as follows:

$$\begin{aligned} w_1&=\alpha A+bC, \quad u=\alpha B+bD,\\ w_2&=\delta D+cB, \quad v=cA+\delta C, \end{aligned} \tag{37}$$

where $T^{-1}=\left(\begin{smallmatrix}A & B\\ C & D\end{smallmatrix}\right)$. We now wish to find the commutation relations of the matrix entries of T with those of Ω. So we need the commutation relations between the matrix elements of T and T^{-1}, which may be computed directly, as follows:

$$\begin{gathered} aA=Aa+h(A-D)\beta, \quad aB=Ba,\\ aC=Ca+h(1-\mathcal{D}_h), \quad aD=Da,\\ \beta A=A\beta, \quad \beta B=-B\beta,\\ \beta C=-C\beta+h(D-A)\beta, \quad \beta D=D\beta,\\ \gamma A=A\gamma+h(1-\mathcal{D}_h^{-1}),\\ \gamma B=-B\gamma+h(A-D)\beta,\\ \gamma C=-C\gamma, \quad \gamma D=D\gamma+h(\mathcal{D}_h-1),\\ dA=Ad, \quad dC=Cd+h(\mathcal{D}_h^{-1}-1),\\ dB=Bd, \quad dD=Dd+h(D-A)\beta. \end{gathered} \tag{38}$$

Using these relations, we now find the commutation relations of the matrix entries of T with those of Ω :

$$
\begin{gathered}
aw_1 = w_1 a - hua, \quad au = ua, \\
av = va + h(w_1 + w_2)a, \quad aw_2 = w_2 a + hua, \\
\beta w_1 = -w_1 \beta + hu\beta, \quad \beta u = u\beta, \\
\beta v = v\beta + h(w_1 + w_2)\beta, \quad \beta w_2 = -w_2 \beta - hu\beta, \\
\gamma w_1 = -w_1 \gamma + h(2w_1 a + u\gamma), \quad \gamma u = u\gamma + 2hua, \\
\gamma v = v\gamma + h(w_1 \gamma + 2va + w_2 \gamma), \quad \gamma w_2 = -w_2 \gamma + h(2w_2 a - u\gamma), \\
dw_1 = w_1 d - h(2w_1 \beta + ud), \quad du = ud + 2hu\beta, \\
dv = vd + h(w_1 d + 2v\beta + w_2 d), \quad dw_2 = w_2 d + h(ud - 2w_2 \beta).
\end{gathered}
\tag{39}
$$

To obtain the commutation relations among the Cartan—Maurer one-forms, we use the commutation relations of the matrix elements of T^{-1} with the differentials of the group parameters which are given in the following:

$$
\begin{gathered}
A\alpha = \alpha A + h(bA - \alpha B), \quad Ab = bA + hbB, \\
Ac = cA - h(\alpha A + \delta A - cB), \quad A\delta = \delta A - h(bA + \delta B), \\
B\alpha = -\alpha B - hbB, \quad Bb = bB, \\
Bc = cB - h(\alpha + \delta)B, \quad B\delta = -\delta B + hbB, \\
C\alpha = -\alpha C - h(\alpha A + \alpha D + bC), \quad Cb = bC - hb(A + D), \\
Cc = cC - h(\alpha C + cA + cD + \delta C), \\
C\delta = -\delta C + h(bC - \delta A - \delta D), \\
D\alpha = \alpha D + h(\alpha B + bD), \quad Db = bD - hbB, \\
Dc = cD - h(\alpha D + cB + \delta D), \quad D\delta = \delta D + h(\delta B - bD).
\end{gathered}
\tag{40}
$$

Using these relations, we obtain the commutation relations of the Cartan–Maurer forms with the differentials of the matrix elements of T as follows:

$$
\begin{gathered}
w_1 \alpha = -\alpha w_1 - h\alpha u, \quad w_1 b = bw_1 - hbu, \\
w_1 c = cw_1 - hcu, \quad w_1 \delta = -\delta w_1 - h\delta u, \\
u\alpha = \alpha u, \quad ub = bu, \\
uc = cu, \quad u\delta = \delta u, \\
v\alpha = \alpha v + h\alpha(w_1 - w_2), \quad vb = bv - hb(w_1 - w_2), \\
vc = cv - hc(w_1 - w_2), \quad v\delta = \delta v + h\delta(w_1 - w_2),
\end{gathered}
\tag{41}
$$

$$w_2\alpha=-\alpha w_2-h\alpha u,\quad w_2b=bw_2-hbu,$$

$$w_2c=cw_2-hcu,\quad w_2\delta=-\delta w_2-h\delta u.$$

We now obtain the commutation relations of the Cartan–Maurer forms,

$$w_1u=uw_1-2hu^2,\quad w_2u=uw_2,$$

$$w_1v=vw_1+2h(w_1w_2-uv),\quad w_2v=vw_2,$$

$$w_1w_2=-w_2w_1-2huw_2, \tag{42}$$

$$w_1^2=-2huw_1,\quad w_2^2=0,$$

$$uv=vu-2huw_2.$$

It can be checked that the elements $\mathcal{D}_h$ and $\hat{\mathcal{D}}$ commute with the Cartan–Maurer one-forms, i.e, both of the $\mathcal{D}_h$ and $\hat{\mathcal{D}}$ are still central elements. In the q-deformation, $\mathcal{D}_q$ does not commute with the Cartan–Maurer forms.

Of course, the relations (4), (15), (16), and (38)–(42) can be obtained with the help of a matrix R that acts on the square tensor space of the supergroup. The matrix R is a solution of the quantum supergroup equation. The quantum supergroup relations (4) follows from the equation

$$RT_1T_2=T_2T_1R,$$

where, in usual grading tensor notation, $T_1=T\otimes I$ and $T_2=I\otimes T$ and

$$R=\begin{pmatrix}1&0&0&0\\-h&1&0&0\\h&0&1&0\\0&h&h&1\end{pmatrix}.$$

The relations (15) are equivalent to the equation

$$T_1'\hat{T}_2=R^{-1}\hat{T}_2T_1R,$$

where

$$T_1'=(-1)^{p(T_1)}T_1,\quad \hat{T}_2=\mathrm{d}T_2.$$

Applying the exterior differential d on both sides of the above equation, one has

$$(\hat{T}_1)'\hat{T}_2=R\hat{T}_2'\hat{T}_1R,\quad (\hat{T}_1)'=d(T_1'),$$

which is equivalent to the relations (16). Similarly, the relations (39), (41) and (42) can be written, in a compact form, as follows, respectively:

$$T_1'\Omega_2=R^{-1}\Omega_2RT_1,$$

$$\hat{T}_1'\Omega_2=R\Omega_2'R\hat{T}_1,$$

$$\Omega_1'R^{-1}\Omega_2R=-R\Omega_2'R\Omega_1.$$

Note that one can check that the action of d on (39), (41) and also (42) is consistent. These relations allow us to evaluate the quantum superalgebra of $\mathrm{GL}_h(1|1)$ by relating the generators of the superalgebra to the one-forms.

IV. QUANTUM SUPERALGEBRA

The commutation relations of Cartan–Maurer forms allow us to construct the algebra of the generators. To obtain the quantum superalgebra of the algebra generators we first write the Cartan–Maurer forms as

$$\begin{aligned} \alpha &= w_1 a + u\gamma, \quad b = w_1\beta + ud, \\ \delta &= w_2 d + v\beta, \quad c = w_2\gamma + va. \end{aligned} \tag{43}$$

The differential d can then be expressed in the form

$$\mathsf{d} = w_1 T_1 + w_2 T_2 + u\nabla_+ + v\nabla_- . \tag{44}$$

Here T_1, T_2 and $\nabla_\pm$ are the quantum superalgebra generators. We now shall obtain the commutation relations of these generators. Considering an arbitrary function f of the matrix elements of T and using the nilpotency of the exterior differential d one has

$$(\mathsf{d}w_i)T_i f + (\mathsf{d}u_i)\nabla_i f = w_i \mathsf{d}T_i f - u_i \mathsf{d}\nabla_i f, \tag{45}$$

where

$$w_i \in \{w_1, w_2\}, \quad u_i \in \{u, v\}, \quad \nabla_i \in \{\nabla_+, \nabla_-\}.$$

So we need the four two-forms. To obtain these, using the nilpotency of the differential d, we can write $\mathsf{d}\Omega$ of the form

$$\mathsf{d}\Omega = \sigma_3 \Omega \sigma_3 \Omega, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{46}$$

In terms of the two-forms, these become

$$\begin{aligned} \mathsf{d}w_1 &= w_1^2 - uv, \quad \mathsf{d}u = w_1 u - u w_2, \\ \mathsf{d}w_2 &= w_2^2 - vu, \quad \mathsf{d}v = w_2 v - v w_1 . \end{aligned} \tag{47}$$

Using the Cartan–Maurer equations we find the following commutation relations for the quantum superalgebra:

$$\begin{gathered} T_1 T_2 - T_2 T_1 = 2h\nabla_- T_1, \\ T_1\nabla_+ - \nabla_+ T_1 = -\nabla_+ + 2h(T_1^2 - T_1), \\ T_2\nabla_+ - \nabla_+ T_2 = \nabla_+ - 2h(T_2 T_1 + T_2 - \nabla_+\nabla_-), \\ T_1\nabla_- - \nabla_- T_1 = \nabla_- , \\ T_2\nabla_- - \nabla_- T_2 = -\nabla_- , \\ \nabla_+^2 = -2hT_1\nabla_+ , \quad \nabla_-^2 = 0, \\ \nabla_-\nabla_+ + \nabla_+\nabla_- = T_1 + T_2 - 2h\nabla_- T_1 . \end{gathered} \tag{48}$$

The commutation relations (48) of the algebra generators should be consistent with monomials of the matrix elements of T. To do this, we evaluate the commutation relations between the generators of algebra and the matrix elements of T. The commutation relations of the generators with the matrix elements can be extracted from the Leibniz rule:

$$\mathrm{d}(af)=(\mathrm{d}a)f+a(\mathrm{d}f)\Rightarrow(w_iT_i+u_i\nabla_i)a=\mathrm{d}a+a(w_iT_i+u_i\nabla_i), \tag{49}$$

etc. This yields

$$\begin{gathered}
T_1a=a+aT_1-ha\nabla_-,\\
T_1\beta=\beta+\beta T_1+h\beta\nabla_-,\\
T_1\gamma=\gamma T_1+h(2aT_1+\gamma\nabla_-),\\
T_1d=dT_1+h(2\beta T_1-d\nabla_-),\\
T_2a=aT_2-ha\nabla_-,\\
T_2\beta=\beta T_2+h\beta\nabla_-,\\
T_2\gamma=\gamma+\gamma T_2+h(2aT_2+\gamma\nabla_-),\\
T_2d=d+dT_2+h(2\beta T_2-d\nabla_-),\\
\nabla_+a=\gamma+a\nabla_+-ha(T_1-T_2),\\
\nabla_+\beta=d-\beta\nabla_+-h\beta(T_1-T_2),\\
\nabla_+\gamma=-\gamma\nabla_+-h(2a\nabla_-+\gamma T_1-\gamma T_2),\\
\nabla_+d=d\nabla_++h(2\beta\nabla_+-dT_1+dT_2),\\
\nabla_-a=a\nabla_-,\quad \nabla_-\beta=-\beta\nabla_-,\\
\nabla_-\gamma=a-\gamma\nabla_--2ha\nabla_-,\\
\nabla_-d=\beta+d\nabla_-+2h\beta\nabla_-.
\end{gathered} \tag{50}$$

V. CONCLUSION

To conclude, we introduce here commutation relations between the matrix elements and their partial derivatives and thus illustrate the connection between the relations in Sec. IV and the relations which will be now obtained.

To proceed, let us first obtain the relations of the matrix elements with their partial derivatives. We know that the exterior differential d can be expressed in the form

$$\mathrm{d}f=(\alpha\partial_a+b\partial_\beta+c\partial_\gamma+\delta\partial_d)f. \tag{51}$$

Then, replacing f with af, etc., we obtain the following commutation relations:

$$\begin{gathered}
\partial_aa=1+a\partial_a-h(\beta\partial_a+a\partial_\gamma),\\
\partial_a\beta=\beta\partial_a+h\beta\partial_\gamma,\\
\partial_a\gamma=\gamma\partial_a+h(a\partial_a+d\partial_a+\gamma\partial_\gamma),
\end{gathered}$$

$$
\begin{aligned}
&\partial_a d = d\partial_a + h(\beta\partial_a - d\partial_\gamma),\\
&\partial_\beta a = a\partial_\beta - h(a\partial_a - a\partial_d + \beta\partial_\beta),\\
&\partial_\beta \beta = 1 - \beta\partial_\beta - h\beta(\partial_a - \partial_d),\\
&\partial_\beta \gamma = -\gamma\partial_\beta - h(a\partial_\beta + \gamma\partial_a - \gamma\partial_d + d\partial_\beta),\\
&\partial_\beta d = d\partial_\beta + h(\beta\partial_\beta - d\partial_a + d\partial_d),\\
&\partial_\gamma a = a\partial_\gamma - h\beta\partial_\gamma, \quad \partial_\gamma \beta = -\beta\partial_\gamma,\\
&\partial_\gamma \gamma = 1 - \gamma\partial_\gamma - h(a\partial_\gamma + d\partial_\gamma),\\
&\partial_\gamma d = d\partial_\gamma + h\beta\partial_\gamma,\\
&\partial_d a = a\partial_d - h(a\partial_\gamma + \beta\partial_d),\\
&\partial_d \beta = \beta\partial_d + h\beta\partial_\gamma,\\
&\partial_d \gamma = \gamma\partial_d + h(a\partial_d + \gamma\partial_\gamma + d\partial_d),\\
&\partial_d d = 1 + d\partial_d + h(\beta\partial_d - d\partial_\gamma).
\end{aligned}
\tag{52}
$$

We thus find the commutation relations between the derivatives. These relations can be obtained by using the nilpotency of the exterior differential d and they have the form

$$
\begin{aligned}
&\partial_a\partial_\beta = \partial_\beta\partial_a + h(\partial_d\partial_a - \partial_\beta\partial_\gamma - \partial_a^2),\\
&\partial_d\partial_\beta = \partial_\beta\partial_d - h(\partial_a\partial_d + \partial_\beta\partial_\gamma - \partial_d^2),\\
&\partial_a\partial_\gamma = \partial_\gamma\partial_a, \quad \partial_d\partial_\gamma = \partial_\gamma\partial_d,\\
&\partial_\beta\partial_\gamma = -\partial_\gamma\partial_\beta + h\partial_\gamma(\partial_a - \partial_d),\\
&\partial_\beta^2 = h\partial_\beta(\partial_a - \partial_d), \quad \partial_\gamma^2 = 0,\\
&\partial_a\partial_d = \partial_d\partial_a + h\partial_\gamma(\partial_d - \partial_a).
\end{aligned}
\tag{53}
$$

The (graded) Hopf algebra structure for ∂ is given by

$$
\begin{aligned}
&\Delta(\partial_a) = \partial_a\otimes\partial_a + \partial_\beta\otimes\partial_\gamma, \quad \Delta(\partial_\beta) = \partial_a\otimes\partial_\beta + \partial_\beta\otimes\partial_d,\\
&\Delta(\partial_d) = \partial_d\otimes\partial_d + \partial_\gamma\otimes\partial_\beta, \quad \Delta(\partial_\gamma) = \partial_\gamma\otimes\partial_a + \partial_d\otimes\partial_\gamma,\\
&\varepsilon(\partial_a) = 1 = \varepsilon(\partial_d), \quad \varepsilon(\partial_\beta) = 0 = \varepsilon(\partial_\gamma),\\
&S(\partial_a) = \partial_a^{-1} + \partial_a^{-1}\partial_\beta\partial_d^{-1}\partial_\gamma\partial_a^{-1}, \quad S(\partial_\beta) = -\partial_a^{-1}\partial_\beta\partial_d^{-1},\\
&S(\partial_d) = \partial_d^{-1} + \partial_d^{-1}\partial_\gamma\partial_a^{-1}\partial_\beta\partial_d^{-1}, \quad S(\partial_\gamma) = -\partial_d^{-1}\partial_\gamma\partial_a^{-1},
\end{aligned}
\tag{54}
$$

provided that the formal inverses ∂_a^{-1} and ∂_d^{-1} exist. However, these co-maps do not leave invariant the relations (52).

We know, from Sec. IV, that the exterior differential d can be expressed in the form (31), which we repeat here:

$$\mathrm{d}f=(w_1T_1+u\nabla_+ +v\nabla_- +w_2T_2)f. \tag{55}$$

Considering (51) together (55) and using (43) one has

$$\begin{aligned} T_1&=a\partial_a+\beta\partial_\beta, \quad \nabla_+=\gamma\partial_a+d\partial_\beta,\\ T_2&=d\partial_d+\gamma\partial_\gamma, \quad \nabla_-=a\partial_\gamma+\beta\partial_d. \end{aligned} \tag{56}$$

Using the relations (52) and (53), one can check that the relations of the generators in (56) coincide with (48). It can also be verified that the action of the generators in (56) on the group parameters coincide with (50).

The classical limit $h\to 0$ of the differential calculus is the undeformed (ordinary) differential calculus.

Note that if we make the identification

$$u\to\frac{x}{2}, \quad w_1\to\theta,$$

where x and θ are the coordinates of superplane, we have

$$x\theta=\theta x+hx^2, \quad \theta^2=-hx\theta.$$

One of the interesting problems may be to construct linear connections[15] on the h-superplane.

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On the existence of stationary states for quantum dynamical semigroups

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We provide two criteria on the existence of stationary states for quantum dynamical semigroups. The first one is based on the semigroup itself, while the second criterion is based on the generator which is in general unbounded and interpreted as a sesquilinear form. These results are illustrated by physical examples drawn from quantum optics. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Quantum dynamical semigroups (QDS) appeared for the first time in the physical literature during the 1970s motivated by studies on the evolution of open systems.

This class of semigroups is indeed an appropriate noncommutative counterpart of the classical Markov theory. On the other hand, numerous important properties of open systems, like the approach to equilibrium, represented by a normal stationary state, can be properly analyzed within the mathematical framework of QDS.

In 1978, the seminal paper of Frigerio[1] showed the importance of assuming the existence of a normal faithful stationary state to study ergodic properties of QDS. Indeed, under that hypothesis, the family of fixed points of the semigroup becomes a von Neumann algebra and a unique conditional expectation onto that algebra does exist. This allows to prove the Ergodic theorem for QDS. As for the stronger result on the weak convergence of the so-called predual semigroup of the given QDS, the crucial hypothesis is the existence of a normal stationary state (see Refs. 2 and 3). This is often taken for granted as a ''physical reasonable'' hypothesis.

In spite of their importance, truly applicable methods to prove the existence of normal stationary states, for an infinite dimensional system, are lacking in the extensive literature on QDS.

This paper is aimed at providing powerful, although simple, criteria for the existence of stationary states for QDS. Assume a quantum dynamical semigroup $(\mathcal{T}_t)_{t\geqslant 0}$, with generator $\mathcal{L}$, be given over the von Neumann algebra $\mathcal{B}(h)$ of all bounded linear operators on a complex separable Hilbert space h. Loosely speaking, a normal stationary state exists, whenever one can find two self-adjoint operators X, Y where, in addition, X is positive and Y is bounded from below, with finite dimensional spectral projections associated with bounded intervals such that either

$$\int_0^\infty \mathcal{T}_s(Y)\,ds \leqslant X \tag{1}$$

or

$$\mathcal{L}(X) \leqslant -Y. \tag{2}$$

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The first inequality clearly reads as a property of the potential associated with the semigroup $(\mathcal{T}_t)_{t\geqslant 0}$. The inequality (2) allows us, under favorable circumstances, to deduce (1). Moreover it is easier to check in the physical applications where the generator usually is given instead of the semigroup. For this reason we think that it is the main result of this paper.

The plan of the paper is as follows. Section II contains some general results on QDS on $\mathcal{B}(h)$ and on tightness (relative compactness) of sets of normal states. This allows us to prove our first criterion for the existence of stationary states based on the inequality (1). The main result, based on the inequality (2), is proved in Sec. IV. Finally, Sec. V contains applications to physical models arising in quantum optics (Alli–Sewell and Jaynes–Cummings).

II. PRELIMINARIES

Let h be a complex separable Hilbert space and let $\mathcal{B}(h)$ be the von Neumann algebra of all bounded linear operators on h. The identity operator on h will be denoted by $\mathbb{1}$.

A quantum dynamical semigroup (QDS) on $\mathcal{B}(h)$ is a w^* continuous semigroup $\mathcal{T}=(\mathcal{T}_t;t\geqslant 0)$ of normal completely positive maps on $\mathcal{B}(h)$. It is conservative or Markov if $\mathcal{T}_t(\mathbb{1})=\mathbb{1}$ for all $t\geqslant 0$. In this case we shall call $\mathcal{T}$ a quantum Markov semigroup (QMS).

The infinitesimal generator, denoted by $\mathcal{L}$, is the operator in $\mathcal{B}(h)$ whose domain is given by the set $D(\mathcal{L})$ of all $x\in\mathcal{B}(h)$ for which the w^* limit of $t^{-1}(\mathcal{T}_t(x)-x)$ exists when $t\to 0$; such a limit defines $\mathcal{L}(x)$.

The predual space of $\mathcal{B}(h)$ is the Banach space $\mathcal{I}_1(h)$, the space of trace-class operators on h. The subspace of $\mathcal{I}_1(h)$ of all positive trace-class operators with unit trace is the set of normal states, which we denote by $\mathcal{S}$. Throughout this paper we will limit ourselves to consider nothing but normal states. Note that $\mathcal{T}_t$ is the dual of an operator $\mathcal{T}_{*t}$ defined on $\mathcal{I}_1(h)$, which is called the predual of $\mathcal{T}_t$.

Definition II.1: A normal state ρ is stationary (or invariant) for a QDS $\mathcal{T}$ if $\mathrm{tr}(\rho\mathcal{T}_t(x))=\mathrm{tr}(\rho x)$ for all $t\geqslant 0$ and all $x\in\mathcal{B}(h)$.

A sequence of states $(\rho_n)_n$ is said to converge *weakly* to $\rho\in\mathcal{S}$ if it converges in the weak topology of the Banach space $\mathcal{I}_1(h)$, i.e.,

$$\lim_{n\to\infty}\mathrm{tr}(\rho_n x)=\mathrm{tr}(\rho x)$$

for all $x\in\mathcal{B}(h)$.

We recall here a useful result on weak convergence of states.

Definition II.2: A sequence of normal states $(\rho_n)_n$ is tight if for any $\epsilon>0$ there exists a finite rank projection p and $n_0\in\mathbb{N}$ such that

$$\mathrm{tr}(\rho_n p)\geqslant 1-\epsilon,$$

for all $n\geqslant n_0$.

Theorem II.1: Any tight sequence of normal states admits a weakly convergent subsequence.

The reader is referred to Ref. 4 Lemma 4.3, p. 291 or Ref. 5 Theorem 2, p. 27 (see also Ref. 6, Appendix 1.4) for the proof. A detailed exposition of this kind of result is contained in Ref. 7.

We recall also the following well-known fact.

Proposition II.1: For each normal state ρ all the weak limits of the family

$$\frac{1}{t}\int_0^t \mathcal{T}_{*s}(\rho)\,ds,\quad t>0$$

on sequences $(t_n)_{n\geqslant 1}$ diverging to infinity are normal stationary states for $\mathcal{T}$.

For each self-adjoint operator Y, bounded from below, we denote by $Y\wedge r$ the truncated operator

$$Y\wedge r=YE_r+rE_r^{\perp},\tag{3}$$

where E_r denotes the spectral projection of Y associated with the interval $[-\infty, r]$.

We are now in a position to prove our first result on the existence of normal stationary states.

Theorem II.2: Let $\mathcal{T}$ be a QMS. Suppose that there exist two self-adjoint operators X and Y with X positive and Y bounded from below and with finite dimensional spectral projections associated with bounded intervals such that

$$\int_0^t \langle u, \mathcal{T}_s(Y \wedge r)u\rangle ds \leqslant \langle u, Xu\rangle \tag{4}$$

for all $t, r \geqslant 0$ and all $u \in D(X)$. Then the QMS $\mathcal{T}$ has a normal stationary state.

Proof: Let $-b$ (with $b>0$) be a lower bound for Y. Note that, for each $r \geqslant 0$ we have

$$Y \wedge r \geqslant -bE_r + rE_r^{\perp} = -(b+r)E_r + r\mathbb{1},$$

so that (4) yields

$$-(b+r)\int_0^t \langle u, \mathcal{T}_s(E_r)u\rangle ds + rt\|u\|^2 \leqslant \langle u, Xu\rangle$$

for all $u \in D(X)$. Normalize u and denote by $|u\rangle\langle u|$ the pure state with unit vector u. Dividing by $t(b+r)$, for all $t, r>0$ we have then

$$\frac{1}{t}\int_0^t \mathrm{tr}(\mathcal{T}_{*s}(|u\rangle\langle u|)E_r)ds \geqslant \frac{r}{b+r} - \frac{\langle u, Xu\rangle}{t(b+r)}.$$

It follows that, for all $\varepsilon>0$, there exists $t(\varepsilon)>0$, $r(\varepsilon)>0$ such that

$$\frac{1}{t}\int_0^t \mathrm{tr}(\mathcal{T}_{*s}(|u\rangle\langle u|)E_{r(\varepsilon)})ds \geqslant 1-\varepsilon$$

for all $t>t(\varepsilon)$. Therefore the family of normal states

$$\frac{1}{t}\int_0^t \mathcal{T}_{*s}(|u\rangle\langle u|)ds, \quad t>t(\varepsilon)$$

is tight. The conclusion follows then from Theorem II.1 and Proposition II.1. □

Remark: It is worth noticing that we wrote the inequality (4) with truncations (integral on $[0,t]$, and $Y \wedge r$) in order to cope with divergence of the integral and unboundedness of Y. Defining appropriately the supremum of a family of self-adjoint operators and then the potential $\mathcal{U}$ for positive self-adjoint operators, formula (4) can be written as

$$\mathcal{U}(Y) \leqslant X.$$

In the applications, however, the QMS usually is not explicitly given. Therefore we shall look for conditions involving the infinitesimal generator. To this end we introduce now the class of QMS with possibly unbounded generators that concerns our research. This is sufficiently general to cover a wide class of applications.

III. THE MINIMAL QUANTUM DYNAMICAL SEMIGROUP

The characterization of a QMS from its generator has been obtained for the first time by Gorini, Kossakowsky, and Sudharshan in Ref. 8 in the finite dimensional case. This result was extended later by Lindblad to the case of an infinite dimensional Hilbert space in the celebrated paper.[9] However, Lindblad restricted himself to consider *bounded generators*, or equivalently, uniformly continuous semigroups. This hypothesis is hardly satisfied in physical models, for

instance in those commonly arising in quantum optics. For that reason several authors, starting from Davies,[10] have been looking for a characterization of nonuniformly continuous QDS for which the generator is usually given as a sesquilinear form, appearing in the so-called *master equations*. At present there is not a definite answer to this question because, even ''good forms'' could have an infinite family of associated QDS which renders the characterization ambiguous. As a way to solve this ambiguity, the notion of *minimal quantum dynamical semigroup* has been proposed by Davies and used by different authors to enlarge the class of semigroups which can be used in applications to Physics. This notion is recalled here for easier reference in the sequel.

Let G and L_ℓ, ($\ell \geqslant 1$) be operators in h which satisfy the following hypothesis:

(**H**) G is the infinitesimal generator of a strongly continuous contraction semigroup in h, $D(G)$ is contained in $D(L_\ell)$, for all $\ell \geqslant 1$, and, for all $u,v \in D(G)$, we have

$$\langle Gv,u\rangle + \sum_{\ell=1}^{\infty} \langle L_\ell v, L_\ell u\rangle + \langle v, Gu\rangle = 0.$$

Under the above assumption (**H**), for each $x \in \mathcal{B}(h)$ let $\mathfrak{L}(x)$ be the sesquilinear form on h with domain $D(G)\times D(G)$ defined by

$$\mathfrak{L}(x)(v,u) = \langle Gv, xu\rangle + \sum_{\ell=1}^{\infty} \langle L_\ell v, xL_\ell u\rangle + \langle v, xGu\rangle. \tag{5}$$

It is well known (see, e.g., Ref. 10, Sec. 3, and Ref. 11, Sec. 3.3) that, given a domain $D \subseteq D(G)$, which is a core for G, it is possible to build up a QDS, called the *minimal* QDS, satisfying the equation

$$\langle v, \mathcal{T}_t(x)u\rangle = \langle v, xu\rangle + \int_0^t \mathfrak{L}(\mathcal{T}_s(x))(v,u)ds, \tag{6}$$

for $u,v \in D$.

This equation, however, in spite of the hypothesis (**H**) and the fact that D is a core for G, does not necessarily determine a unique semigroup. The minimal QDS is characterized by the following property: for any w^* continuous family $(\mathcal{T}_t)_{t\geqslant 0}$ of positive maps on $\mathcal{B}(h)$ satisfying (6) we have $\mathcal{T}_t^{(\min)}(x) \leqslant \mathcal{T}_t(x)$ for all positive $x \in \mathcal{B}(h)$ and all $t \geqslant 0$ (see, e.g., Ref. 11, Theorem 3.21).

Let $\mathcal{T}_*^{(\min)}$ denote the predual semigroup on $\mathcal{I}_1(h)$ with infinitesimal generator $\mathcal{L}^{(\min)}$. It is worth noticing here that $\mathcal{T}_*^{(\min)}$ is a *weakly* continuous semigroup on the Banach space $\mathcal{I}_1(h)$, hence it is *strongly* continuous. The linear span $\mathcal{V}$ of elements of $\mathcal{I}_1(h)$ of the form $|u\rangle\langle v|$ is contained in the domain of $\mathcal{L}^{(\min)}$. Thus we can write the equation (6) as follows:

$$\mathrm{tr}(|u\rangle\langle v|\mathcal{T}_t(x)) = \mathrm{tr}(|u\rangle\langle v|x) + \int_0^t \mathrm{tr}(\mathcal{L}_*^{(\min)}(|u\rangle\langle v|)\mathcal{T}_s(x))ds.$$

This equation reveals that the solution to (6) is unique whenever the linear manifold $\mathcal{L}_*^{(\min)}(\mathcal{V})$ is big enough. Indeed, the following characterization holds.

Proposition III.1: Under the assumption (**H**) the following conditions are equivalent:

(i) the minimal QDS is Markov [i.e., $\mathcal{T}_t^{(\min)}(\mathbb{1}) = \mathbb{1}$],
(ii) $(\mathcal{T}_t^{(\min)})_{t\geqslant 0}$ is the unique w^*-continuous family of positive contractive maps on $\mathcal{B}(h)$ satisfying (6) for all positive $x \in \mathcal{B}(h)$ and all $t \geqslant 0$,
(iii) the domain $\mathcal{V}$ is a core for $\mathcal{L}_*^{(\min)}$.

We refer to Ref. 10 Theorem 3.2 or Ref. 11, Prop. 3.31 (respectively, Ref. 11 Theorem 3.21) for the proof of the equivalence of (i) and (iii) [respectively, (i) and (ii)].

The above discussion has shown the importance of getting a minimal quantum dynamical semigroup which preserves the identity, that is, a quantum Markov semigroup. Chebotarev and Fagnola have obtained an easier criterion to verify the Markov property (see Ref. 12, Theorem 4.4, p. 394). We will recall later this result in one of our applications.

IV. MAIN RESULT

Definition IV.1: Given two self-adjoint operators X, Y, with X positive and Y bounded form below, we write $\mathfrak{L}(X)\leqslant -Y$ on D, whenever the inequality

$$\langle Gu, Xu\rangle + \sum_{\ell=1}^{\infty} \langle X^{1/2}L_\ell u, X^{1/2}L_\ell u\rangle + \langle Xu, Gu\rangle \leqslant -\langle u, Yu\rangle, \tag{7}$$

holds for all u in a linear manifold D dense in h, contained in the domains of G, X, and Y, which is a core for X and G, such that $L_\ell(D)\subseteq D(X^{1/2})$, $(\ell\geqslant 1)$.

Theorem IV.1: Assume that the hypothesis (**H**) holds and that the minimal QDS associated with G, $(L_\ell)_{\ell\geqslant 1}$ is Markov. Suppose that there exist two self-adjoint operators X and Y, with X positive and Y bounded from below and with finite dimensional spectral projections associated with bounded intervals, such that

(i) $\mathfrak{L}(X)\leqslant -Y$ on D,
(ii) G is relatively bounded with respect to X,
(iii) $L_\ell(n+X)^{-1}(D)\subseteq D(X^{1/2})$ $(n,\ell\geqslant 1)$.

Then the minimal QDS associated with G, $(L_\ell)_{\ell\geqslant 1}$ has a normal stationary state.

It is worth noticing that the above sufficient conditions always hold for a finite dimensional space h. Indeed, by the hypothesis (**H**), it suffices to take $X=\mathbb{1}$, $Y=0$, and $D=h$.

We begin the proof by building up approximations $\mathcal{T}^{(n)}$ of $\mathcal{T}^{(\min)}$.

Lemma IV.1: Under the hypotheses of Theorem IV.1, for all integer $n\geqslant 1$ the operators $G^{(n)}$ and $L_\ell^{(n)}$ with domain D defined by

$$G^{(n)}=nG(n+X)^{-1}, \quad L_\ell^{(n)}=nL_\ell(n+X)^{-1},$$

admit a unique bounded extension. The operator on $\mathcal{B}(h)$ defined by

$$\mathcal{L}^{(n)}(x)=G^{(n)*}x+\sum_{\ell} L_\ell^{(n)*}xL_\ell^{(n)}+xG^{(n)} \tag{8}$$

$(n\geqslant 1)$ generates a uniformly continuous QDS $\mathcal{T}^{(n)}$.

Proof: First notice that $G^{(n)}$ and the $L_\ell^{(n)}$'s are bounded. Indeed, by the hypothesis (ii), the resolvent $(n+X)^{-1}$ maps h into the domain of the operators G and L_ℓ, therefore, $G^{(n)}$ and $L_\ell^{(n)}$ are everywhere defined. Moreover, since G is relatively bounded with respect to X, there exist two constants c_1, $c_2>0$ such that, for each $u\in h$ we have

$$\|nG(n+X)^{-1}u\|\leqslant c_1\|nX(n+X)^{-1}u\|+c_2\|n(n+X)^{-1}u\|.$$

By well-known properties of the Yosida approximation the right-hand side is bounded by $(nc_1+c_2)\|u\|$.

On the other hand, by (**H**), for each $u\in h$ we also have

$$\sum_{\ell=1}^{\infty}\|nL_\ell(n+X)^{-1}u\|^2=-2\Re\langle n(n+X)^{-1}u, G^{(n)}u\rangle\leqslant 2(nc_1+c_2)\|u\|^2.$$

Thus the $L_\ell^{(n)}$'s are bounded. Moreover, replacing u,v in condition (**H**) by $n(n+X)^{-1}u$, $u\in h$, leads to

$$\langle u,\mathcal{L}^{(n)}(\mathbb{1})u\rangle = 2\Re\langle u,G^{(n)}u\rangle + \sum_{\ell=1}^{\infty}\|L_\ell^{(n)}u\|^2$$

$$= 2\Re\langle X(n+X)^{-1}u,G^{(n)}u\rangle$$

$$\leqslant 2(nc_1+c_2)\|u\|^2.$$

It follows that the sum $\Sigma_{\ell=1}^{\infty}L_\ell^{(n)*}L_\ell^{(n)}$ converges strongly. Therefore by Lindblad's theorem (see Refs. 9 and 13), the equation (8) defines the generator of a uniformly continuous QDS. □

We recall the following well-known result on semigroup convergence.

Proposition IV.1: Let A, $A^{(n)}$ $(n\geqslant 1)$ be infinitesimal generators of strongly continuous contraction semigroups $(T_t)_{t\geqslant 0}$, $(T_t^{(n)})_{t\geqslant 0}$ on a Banach space and let D_0 be a core for A. Suppose that each element x of D_0 belongs to the domain of $A^{(n)}$ for n big enough and the sequence $(A^{(n)}x)_{n\geqslant 1}$ converges strongly to Ax. Then the operators $T_t^{(n)}$ converge strongly to T_t uniformly for t in bounded intervals.

We refer to Ref. 14, Theorem 1.5, p. 429, Theorem 2.16, p. 504 for the proof.

We shall need also the following elementary lemma.

Lemma IV.2: Let $(r_\ell)_{\ell\geqslant 1}$, $(s_\ell^{(n)})_{\ell\geqslant 1}$ $(n\geqslant 1)$ be square-summable sequences of positive real numbers such that, for every $\ell\geqslant 1$, $s_\ell^{(n)}\to 0$ as n tends to infinity and there exists a positive constant c such that

$$\sum_{\ell\geqslant 1}(s_\ell^{(n)})^2\leqslant c$$

for every $n\geqslant 1$. Then

$$\lim_{n\to\infty}\sum_{\ell\geqslant 1} r_\ell s_\ell^{(n)} = 0.$$

Proof: Suppose that our conclusion is false. Then, by extracting a subsequence (in n) if necessary, we can choose $\varepsilon>0$ such that, for every n,

$$\sum_{\ell\geqslant 1} r_\ell s_\ell^{(n)} > \varepsilon. \tag{9}$$

The sequences $s^{(n)}$ can be viewed as vectors in $l^2(\mathbb{N}^*)$ uniformly bounded in norm by c. Therefore we can extract a subsequence $(n_m)_{m\geqslant 1}$ such that $(s^{(n_m)})_{m\geqslant 1}$ converges weakly as m tends to infinity. Since $s_\ell^{(n)}\to 0$ as n tends to infinity for each $\ell\geqslant 1$, it follows that the weak limit must be the vector 0. This contradicts (9). □

Lemma IV.3: Let $G^{(n)}$, $L_\ell^{(n)}$ the operators on h defined in Lemma IV.1. Then, under the hypotheses of Theorem IV.1, for all $u\in D(X)$, we have

$$\lim_{n\to\infty} G^{(n)}u = Gu, \quad \lim_{n\to\infty} L_\ell^{(n)}u = L_\ell u.$$

Moreover the operators $\mathcal{T}_{*t}^{(n)}$ on $\mathcal{I}_1(h)$ converge strongly, as n tends to infinity, to $\mathcal{T}_{*t}$, uniform for t in bounded intervals.

Proof: For all $u\in D(X)$, we have

$$\|G^{(n)}u-Gu\| = \|G(n(n+X)^{-1}-\mathbb{1})u\|$$

$$\leqslant c_1\|(n(n+X)^{-1}-\mathbb{1})Xu\| + c_2\|(n(n+X)^{-1}-\mathbb{1})u\|.$$

Therefore the sequence $(G^{(n)}u)_{n\geqslant 1}$ converges strongly to Gu as n tends to infinity by well-known properties of Yosida approximations. Moreover, by (**H**), for $u\in D(X)$, we have also

$$\sum_{\ell=1}^{\infty} \|L_\ell^{(n)}u - L_\ell u\|^2 = -2\Re\langle (n(n+X)^{-1}-\mathbb{1})u, G(n(n+X)^{-1}-\mathbb{1})u\rangle. \tag{10}$$

This shows the convergence of sequences $(L_\ell^{(n)}u)_{n\geqslant 1}$ to $L_\ell u$ for all $\ell \geqslant 1$.

For all $u,v \in D(X)$ we have

$$\mathcal{L}_*^{(n)}(|u\rangle\langle v|) - \mathcal{L}_*^{(\min)}(|u\rangle\langle v|) = |(G^{(n)}-G)u\rangle\langle v| + |u\rangle\langle (G^{(n)}-G)v| + \sum_{\ell=1}^{\infty} |(L_\ell^{(n)}-L_\ell)u\rangle\langle v| + \sum_{\ell=1}^{\infty} |u\rangle\langle (L_\ell^{(n)}-L_\ell)v|.$$

Therefore the trace norm of $\mathcal{L}_*^{(n)}(|u\rangle\langle v|) - \mathcal{L}_*^{(\min)}(|u\rangle\langle v|)$ can be estimated by

$$\|v\|\cdot\|(G^{(n)}-G)u\| + \|u\|\cdot\|(G^{(n)}-G)v\| + \sum_{\ell=1}^{\infty} \|L_\ell u\|\cdot\|(L_\ell^{(n)}-L_\ell)v\| + \sum_{\ell=1}^{\infty} \|L_\ell v\|\cdot\|(L_\ell^{(n)}-L_\ell)u\|.$$

Clearly the first two terms vanish as n tends to infinity. Moreover, by the inequality (10), since the operators $X(n+X)^{-1}$ are contractive, we have

$$\begin{aligned}\sum_{\ell=1}^{\infty} \|L_\ell^{(n)}u - L_\ell u\|^2 &\leqslant 2\|(n+X)^{-1}Xu\|\cdot\|(G^{(n)}-G)u\| \\ &\leqslant 2\|u\|(c_1\|(n(n+X)^{-1}-\mathbb{1})Xu\| + c_2\|(n(n+X)^{-1}-\mathbb{1})u\|) \\ &= 2\|u\|(c_1\|(X(n+X)^{-1})Xu\| + c_2\|(X(n+X)^{-1})u\|) \\ &\leqslant 2\|u\|(c_1\|Xu\| + c_2\|u\|).\end{aligned}$$

An application of Lemma IV.2 shows then that the trace norm of $\mathcal{L}_*^{(n)}(|u\rangle\langle v|) - \mathcal{L}_*^{(\min)}(|u\rangle\langle v|)$ converges to 0 as n tends to infinity.

Since the minimal QDS associated with G, $(L_\ell)_{\ell\geqslant 1}$ is Markov and $D(X)$ is a core for G (it contains D), the linear manifold generated by $|u\rangle\langle v|$ with $u \in D(X)$ is a core for $\mathcal{L}_*^{(\min)}$. The conclusion follows then from Proposition IV.1. □

Lemma IV.4: Let $Y \wedge r$ the operator defined by (3) and let $X^{(n)} = nX(n+X)^{-1}$ $(n \geqslant 1)$. Define $Y_r^{(n)} = n^2(n+X)^{-1}(Y\wedge r)(n+X)^{-1}$. Then, under the hypotheses of Theorem IV.1, the operator

$$X^{(n)} - \int_0^t \mathcal{T}_s^{(n)}(Y_r^{(n)})\,ds$$

is positive for each $t \geqslant 0$.

Proof: Notice that $Y_r \leqslant Y$. Therefore, by the hypothesis (i) of Theorem IV.1, we have the inequality

$$\langle Gu, Xu\rangle + \sum_{\ell=1}^{\infty} \langle X^{1/2}L_\ell u, X^{1/2}L_\ell u\rangle + \langle Xu, Gu\rangle \leqslant -\langle u, (Y\wedge r)u\rangle, \tag{11}$$

for all $u \in D$.

The domain D being a core for X and G being relatively bounded with respect to X, for every $u \in D(X)$ we can find a sequence $(u_n)_{n\geqslant 1}$ in D such that $(Xu_n)_{n\geqslant 1}$ converges to Xu and

$(Gu_n)_{n\geqslant 1}$ converges to Gu. Then the convergence of $(L_\ell u_n)_{n\geqslant 1}$ to $L_\ell u$ (for all $\ell\geqslant 1$) follows readily form the hypothesis (**H**). Moreover, for every $n,m\geqslant 1$, the inequality (11) yields

$$\sum_{\ell=1}^{\infty} \|X^{1/2}L_\ell(u_n-u_m)\|^2 \leqslant -2\Re\langle G(u_n-u_m),X(u_n-u_m)\rangle - \langle (u_n-u_m),(Y\wedge r)(u_n-u_m)\rangle.$$

Therefore, replacing u by u_n, and letting n tend to infinity we show that (11) holds for all $u \in D(X)$.

Since $n(n+X)^{-1}$ is a contraction and $Y_r \leqslant Y$, under the hypotheses of Theorem IV.1, for all $u \in h$, we have

$$\begin{aligned}\langle u,\mathcal{L}^{(n)}(X^{(n)})u\rangle &\leqslant 2\Re\langle G^{(n)}u,X^{(n)}u\rangle + \sum_{\ell=1}^{\infty}\langle X^{1/2}L_\ell^{(n)}u,X^{1/2}L_\ell^{(n)}u\rangle \\ &\leqslant -\langle n(n+X)^{-1}u,Y_r n(n+X)^{-1}u\rangle \\ &= -\langle u,Y_r^{(n)}u\rangle.\end{aligned}$$

It follows then $\mathcal{L}^{(n)}(X^{(n)}) \leqslant -Y_r^{(n)}$.

Now, notice that

$$\frac{d}{dt}\left(X^{(n)} - \mathcal{T}_t^{(n,\eta)}(X^{(n)}) - \int_0^t \mathcal{T}_s^{(n)}(Y_r^{(n)})ds\right) = -\mathcal{T}_t^{(n)}(\mathcal{L}^{(n)}(X^{(n)}) + Y_r^{(n)}) \geqslant 0.$$

Therefore,

$$X^{(n)} - \int_0^t \mathcal{T}_s^{(n)}(Y_r^{(n)})ds \geqslant \mathcal{T}_t^{(n)}(X^{(n)}) \geqslant 0$$

for all $t\geqslant 0$. □

Proof (of Theorem IV.1): By Lemma IV.4 for each $u \in D(X)$, $t,r\geqslant 0$, and $n\geqslant 1$, we have

$$\int_0^t \mathrm{tr}(\mathcal{T}_{*s}^{(n)}(|u\rangle\langle u|)Y_r^{(n)})ds \leqslant \langle u,X^{(n)}u\rangle.$$

The sequence $(Y_r^{(n)})_{n\geqslant 1}$ converges strongly to $Y\wedge r$. Thus, by Lemma IV.3, we can let n tend to infinity to obtain

$$\int_0^t \mathrm{tr}(\mathcal{T}_{*s}(|u\rangle\langle u|)(Y\wedge r))ds \leqslant \langle u,Xu\rangle.$$

This inequality coincides with (4). Therefore Theorem IV.1 follows from Theorem II.2. □

V. APPLICATIONS

V.1. A multimode Dicke laser model. We follow Alli and Sewell[15] where a model is proposed for a Dicke laser or maser. We begin by establishing the corresponding notations.

The system consists of N identical two-level atoms coupled with the radiation corresponding to n modes. Therefore, one can choose the Hilbert space h which consists of the tensor product of N copies of $\mathbb{C}^2$ and n copies of $l^2(\mathbb{N})$. To simplify notations we simply identify any operator acting on a factor of the above tensor product with its canonical extension to h.

Let σ_1, σ_2, σ_3 be the Pauli matrices and define the spin raising and lowering operators $\sigma_\pm = (\sigma_x \pm \sigma_y)/2$. The atoms are located on the sites $r=1,\ldots,N$ of a one-dimensional lattice, so

that we denote by $\sigma_{\epsilon,r}(\epsilon=1,2,3,+,-)$ the spin component of the atom at the site r. The free evolution of the atoms is described by a generator $\mathcal{L}_{\mathrm{mat}}$ which is bounded and given in Lindblad form as

$$\mathcal{L}_{\mathrm{mat}}(x)=i[H,x]-\frac{1}{2}\sum_j\ (V_j^*V_jx-2V_j^*xV_j+xV_j^*V_j), \tag{12}$$

where the sum contains a finite number of elements, H is self-adjoint and the V_j's are bounded operators.

Moreover, we denote by a_j^*, a_j, the creation and annihilation operators corresponding to the jth mode of the radiation $(j=1,\ldots,n)$. These operators satisfy the canonical commutation relations:

$$[a_j,a_k^*]=\delta_{jk}I,\quad [a_j,a_k]=0.$$

The free evolution of the radiation is given by the formal generator

$$\mathcal{L}_{\mathrm{rad}}(x)=\sum_{\ell=1}^{n}\ (\kappa_\ell(-a_\ell^*a_\ell x+2a_\ell^*xa_\ell-xa_\ell^*a_\ell)+i\omega_\ell[a_\ell^*a_\ell,x]), \tag{13}$$

where κ_ℓ are the damping and ω_ℓ are the frequencies corresponding to the ℓth mode of the radiation.

The coupling between the matter and the radiation corresponds to a Hamiltonian interaction of the form

$$H_{\mathrm{int}}=\frac{i}{N^{1/2}}\sum_{r=1}^{N}\sum_{\ell=1}^{n}\lambda_\ell(\sigma_{-,r}a_\ell^*\mathrm{e}^{-2\pi ik_\ell r}-\sigma_{+,r}a_\ell\mathrm{e}^{2\pi ik_\ell r}), \tag{14}$$

where k_ℓ is the wave number of the ℓth mode and the λ's are real valued, N independent coupling constants.

With the above notations, the formal generator of the whole dynamics is given by

$$\mathcal{L}(x)=\mathcal{L}_{\mathrm{mat}}(x)+\mathcal{L}_{\mathrm{rad}}(x)+i[H_{\mathrm{int}},x]. \tag{15}$$

To identify L_ℓ and G in our notations, we use in force the convention on the abridged version of tensor products with the identity. That is, here we find

$$L_\ell=\sqrt{\kappa_l}a_\ell,\quad (\ell=1,\ldots,n) \tag{16}$$

All the remaining L_ℓ's are bounded operators. Among them a finite number (indeed $3N$) coincides with some of the V_j's appearing in (12) and the others vanish.

So that the operator G becomes formally

$$G=-\frac{1}{2}\sum_\ell\ (\kappa_\ell-2i\omega_\ell)a_\ell^*a_\ell-iH-iH_{\mathrm{int}}, \tag{17}$$

where the sum contains only a finite number of nonzero terms.

To make the above expression rigorous some preliminary work is needed. Call $(f_m)_{m\geqslant 0}$ the canonical orthonormal basis on the space $l^2(\mathbb{N})$. In the radiation space, which consists of the tensor product of n copies of $l^2(\mathbb{N})$, we denote

$$f_\alpha=f_{\alpha_1}^{(1)}\otimes\cdots\otimes f_{\alpha_n}^{(n)},$$

where $\alpha=(\alpha_1,\ldots,\alpha_n)$ and $f_{\alpha_\ell}^{(\ell)}$ is an element of the canonical basis of the ℓ copy of $l^2(\mathbb{N})$. Thus, $(f_\alpha)_{\alpha\in\mathbb{N}^n}$ is the canonical orthonormal basis of the radiation space.

With these notations we have

$$a_\ell^* f_\alpha=\sqrt{\alpha_\ell+1}\,f_{\alpha+1_\ell},\quad a_\ell f_\alpha=\begin{cases}\sqrt{\alpha_\ell}\,f_{\alpha-1_\ell}, & \text{if } \alpha_\ell>0,\\ 0, & \text{if } \alpha_\ell=0,\end{cases} \tag{18}$$

where 1_ℓ is the vector with a 1 at the ℓth coordinate and zero elsewhere.

Thus, the operator G is well defined over vectors of the form uf_α where $u\in\mathbb{C}^{2N}$ and the symbol of tensor product is dropped.

It can be shown (e.g., as in Ref. 11, Prop. 4.9) that the closure of G generates a strongly continuous contraction semigroups and the hypothesis (**H**) is easily checked. Therefore, we choose X formally given by $X=\Sigma_{\ell=1}^n a_\ell^* a_\ell$. That is, $Xuf_\alpha=|\alpha|uf_\alpha$, where $|\alpha|=\alpha_1+\cdots+\alpha_n$.

Since $X^k uf_\alpha=|\alpha|^k uf_\alpha$ it follows that the linear span of vectors of the form uf_α is a dense subset of the analytic vectors for X. Therefore, by a theorem of Nelson (see, e.g., Ref. 16), X is essentially self-adjoint on the referred domain. From now on we identify X with its closure which is self-adjoint.

We show now that H_{int} is relatively bounded with respect to X. Let ξ be a finite linear combination of elements of the form $u_\alpha f_\alpha$. By Schwarz' inequality, and elementary inequalities like $\sqrt{t+s}\leqslant\sqrt{t}+\sqrt{s}\leqslant\sqrt{2(t+s)}$, $2\sqrt{ts}\leqslant\epsilon t+\epsilon^{-1}s$, we obtain

$$\begin{aligned}\|H_{\text{int}}\xi\|&\leqslant\frac{1}{N^{1/2}}\sum_{r=1}^N\sum_{\ell=1}^n|\lambda_\ell|(\|a_\ell^*\xi\|+\|a_\ell\xi\|)\\&\leqslant\frac{1}{N^{1/2}}\sum_{r=1}^N\sum_{\ell=1}^n|\lambda_\ell|(4\langle\xi,a_\ell^*a_\ell\xi\rangle+2\|\xi\|^2)^{1/2}\\&\leqslant\frac{1}{N^{1/2}}\left[\sum_{r=1}^N\sum_{\ell=1}^n 2(|\lambda_\ell|^2\langle\xi,a_\ell^*a_\ell\xi\rangle)^{1/2}+\sqrt{2}\sum_{r=1}^N\sum_{\ell=1}^n|\lambda_\ell|\|\xi\|\right]\\&\leqslant\frac{1}{N^{1/2}}\left[\sum_{r=1}^N\sum_{\ell=1}^n(\epsilon\|a_\ell^*a_\ell\xi\|+\epsilon^{-1}|\lambda_\ell|^2\|\xi\|)+\sqrt{2}\sum_{r=1}^N\sum_{\ell=1}^n|\lambda_\ell|\|\xi\|\right].\end{aligned}$$

Finally, by the elementary inequality $\Sigma_{\ell=1}^n\|s_\ell\|\leqslant\sqrt{n}\|\Sigma_{\ell=1}^n s_\ell\|$, it follows

$$\|H_{\text{int}}\xi\|\leqslant\frac{n^{1/2}\epsilon}{N^{1/2}}\sum_{r=1}^N\left\|\sum_{\ell=1}^n a_\ell^*a_\ell\xi\right\|+\frac{1}{N^{1/2}}\sum_{r=1}^N\sum_{\ell=1}^n(\sqrt{2}+\epsilon^{-1}|\lambda_\ell|)|\lambda_\ell|\|\xi\|$$

$$\leqslant\epsilon N^{1/2}n^{1/2}\|X\xi\|+\frac{1}{N^{1/2}}\sum_{r=1}^N\sum_{\ell=1}^n(\sqrt{2}+\epsilon^{-1}|\lambda_\ell|)|\lambda_\ell|\|\xi\|,$$

thus, choosing $2\epsilon<(Nn)^{-1/2}$, the above inequality yields the required relative boundedness of H_{int} with respect to X. Note that the domain of G coincides with the domain of X.

To apply our main result, we fix the domain D as the space of vectors ξ which are finite linear combinations of the form $u_\alpha f_\alpha$. Notice that this is an invariant for X, G, and all the L_ℓ's. To identify an appropriate operator Y to have $\mathcal{L}(X)\leqslant -Y$, we first perform the computation of $\mathcal{L}(X)$.

For the sake of clarity, we avoid handling forms in the computations below. However, the reader may easily notice that all the expressions are well defined since the domain D is invariant under the action of the operators X, G, and L_ℓ.

First, it holds $\mathcal{L}_{\mathrm{mat}}(X)=0$. Second, a straightforward computation using the canonical commutation relations, yields

$$\mathcal{L}_{\mathrm{rad}}(X)=-2\sum_{\ell=1}^{n}\kappa_\ell a_\ell^* a_\ell.$$

Another easy computation leads us to

$$i[H_{\mathrm{int}},X]=-iN^{-1/2}\sum_{r=1}^{N}\sum_{\ell=1}^{n}\lambda_\ell(\sigma_{-,r}a_\ell e^{-2\pi ik_\ell r}+\sigma_{+,r}a_\ell^* e^{2\pi ik_\ell r}).$$

Summing up,

$$\mathfrak{L}(X)=-2\sum_{\ell=1}^{n}\kappa_\ell a_\ell^* a_\ell-\frac{i}{N^{1/2}}\sum_{r=1}^{N}\sum_{\ell=1}^{n}\lambda_\ell(\sigma_{-,r}a_\ell e^{-2\pi ik_\ell r}+\sigma_{+,r}a_\ell^* e^{2\pi ik_\ell r}).$$

To identify Y it suffices to control the term $i[H_{\mathrm{int}},X]$. For each $\xi\in D$, it follows

$$\begin{aligned}
|\langle\xi,i[H_{\mathrm{int}},X]\xi\rangle| &= \frac{1}{N^{1/2}}\left|\sum_{r=1}^{N}\sum_{\ell=1}^{n}\lambda_\ell\langle\xi,(\sigma_{-,r}a_\ell e^{-2\pi ik_\ell r}+\sigma_{+,r}a_\ell^* e^{2\pi ik_\ell r}\xi\rangle\right| \\
&\leqslant \frac{1}{2N^{1/2}}\sum_{r=1}^{N}\sum_{\ell=1}^{n}2|\lambda_\ell|\|\xi\|(\|a_\ell\xi\|+\|a_\ell^*\xi\|) \\
&\leqslant \frac{\epsilon}{2N^{1/2}}\sum_{r=1}^{N}\sum_{\ell=1}^{n}(\langle\xi,a_\ell^* a_\ell\xi\rangle+\langle\xi,a_\ell a_\ell^*\xi\rangle)+\frac{1}{2\epsilon N^{1/2}}\sum_{r=1}^{N}\sum_{\ell=1}^{n}|\lambda_\ell|^2\|\xi\|^2 \\
&\leqslant \epsilon N^{1/2}\langle\xi,X\xi\rangle+\frac{\epsilon N^{1/2}n}{2}\|\xi\|^2+\frac{1}{2\epsilon N^{1/2}}\sum_{r=1}^{N}\sum_{\ell=1}^{n}|\lambda_\ell|^2\|\xi\|^2.
\end{aligned}$$

So that choosing $0<\epsilon<(2/N^{1/2})\min_{1\leqslant\ell\leqslant n}\kappa_\ell$ the required operator Y may be taken as

$$Y=\left(2\min_{1\leqslant\ell\leqslant n}\kappa_\ell-\epsilon N^{1/2}\right)(X+c),$$

where $c>0$ is a suitable constant.

The spectrum of X coincides with $\mathbb{N}$. For each $m\in\mathbb{N}$, the corresponding eigenspace is generated by the f_α with $|\alpha|=m$. Therefore, it follows that all spectral projections of X and Y associated with bounded intervals are finite dimensional.

In Ref. 15 it is proven that the minimal QDS with G, L_ℓ is Markov.

To summarize, our main theorem combined with the Markov property of the semigroup imply the following corollary.

Corollary V.1: There exists a normal stationary state for the multimode Dicke model.

To finish with this example we want to comment that one can prove the Markov property alternatively, following similar arguments to those used to check the hypotheses of our main theorem. Indeed, it suffices to apply the Proposition below from Ref. 12 with $C=X$ to show that the minimal QDS is conservative.

Proposition V.1: Under the hypothesis (**H**) suppose that there exists a self-adjoint operator C in h with the following properties:

(a) the domain of G is contained in the domain of $C^{1/2}$ and is a core for $C^{1/2}$,
(b) the linear manifold $L_\ell(D(G^2))$ is contained in the domain of $C^{1/2}$,
(c) there exists a self-adjoint operator Φ, with $D(G)\subseteq D(\Phi^{1/2})$ and $D(C)\subseteq D(\Phi)$, such that, for all $u\in D(G)$, we have

$$-2\Re\langle u,Gu\rangle=\sum_\ell \|L_\ell u\|^2=\|\Phi^{1/2}u\|^2,$$

(a) for all $u\in D(C^{1/2})$ we have $\|\Phi^{1/2}u\|\leqslant\|C^{1/2}u\|$,
(b) for all $u\in D(G^2)$ the following inequality holds

$$2\Re\langle C^{1/2}u,C^{1/2}Gu\rangle+\sum_{\ell=1}^{\infty}\|C^{1/2}L_\ell u\|^2\leqslant b\|C^{1/2}u\|^2, \tag{19}$$

where b is a positive constant depending only on G, L_ℓ, C.

Then the minimal QDS is Markov.

V.2 The Jaynes–Cummings model. We follow our paper[17] to introduce the Jaynes–Cummings model in quantum optics. To this aim we use the same space $h=l^2(\mathbb{N})$, since here $n=1$, we drop the index ℓ from the notations of creation and annihilation operators and S denotes the right-shift operator.

In this framework the formal generator is given by

$$\mathcal{L}(x)=-\frac{\mu^2}{2}(a^*ax-2a^*xa+xa^*a)-\frac{\lambda^2}{2}(aa^*x-2axa^*+xaa^*)$$
$$+R^2(\cos(\phi\sqrt{aa^*})x\cos(\phi\sqrt{aa^*})-x)+R^2\sin(\phi\sqrt{aa^*})S^*xS\sin(\phi\sqrt{aa^*}),$$

where λ, μ, R, and ϕ are positive constants. In Ref. 17 the rigorous construction of the minimal QDS was done showing also that it is identity preserving.

The above Jaynes–Cummings generator has a faithful normal stationary state if and only if $\mu^2>\lambda^2$. This state can be computed explicitly. The interested reader is referred to Ref. 17.

To check conditions of Theorem IV.1, one can take $X=a^*a$, the value of $\mathcal{L}(X)$ becoming

$$\mathcal{L}(X)=-(\mu^2-\lambda^2)a^*a+R^2\sin^2(\phi\sqrt{aa^*}).$$

Thus, it suffices to take $Y=(\mu^2-\lambda^2)a^*a-R^2$ to prove the existence of a stationary state via our main result.

To prove the necessity, one can follow the argument explained in Ref. 17 inspired from classical probability.

Thus, in this case, our result IV.1 turns out to be sharp.

VI. FINAL COMMENTS

Theorems II.2 and IV.1 provide a useful method for deciding whether a normal stationary state exists for a given physical model, when this is not given at the outset. Some other concrete examples of application will be considered by the authors in a forthcoming paper.

On the other hand, the natural question which arises is whether there exists a *faithful* normal stationary state for a given quantum dynamical semigroup. An answer to this supplementary question will be provided in Ref. 18.

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Recursion operators of some equations of hydrodynamic type

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We give a general method for constructing recursion operators for some equations of hydrodynamic type, admitting a nonstandard Lax representation. We give several examples for $N=2$ and $N=3$ containing the equations of shallow water waves and its generalizations with their first two general symmetries and their recursion operators. We also discuss a reduction of $N+1$ systems to N systems of some new equations of hydrodynamic type. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Most of the integrable nonlinear partial differential equations admit Lax representations,

$$L_t=[A,L], \tag{1}$$

where L is a pseudo-differential operator of order m and A is a pseudo-differential operator. Recently[1] we established a new method for such integrable equations to construct their recursion operators. This method uses the hierarchy of equations,

$$L_{t_n}=[A_n,L], \tag{2}$$

and the Gel'fand–Dikkii[2] construction of the A_n-operators. Defining an operator R_n in the form

$$A_n=LA_{n-m}+R_n, \tag{3}$$

one then obtains relations among the hierarchies,

$$L_{t_n}=LL_{t_{n-m}}+[R_n;L]. \tag{4}$$

This equation allows to find L_{t_n} in terms of $L_{t_{n-m}}$. It is important to note that one does not need to know the exact form of A_n. For further details of the method see Ref. 1.

In Ref. 1 we introduced a direct method to determine a recursion operator of a system of evolution equations when its Lax representation is known. It has no direct reference to the Hamiltonian operators. Hence one may be able to determine the recursion operators when any one of the Hamiltonian operators are degenerate. In the same paper we gave several applications of the method. In all these examples we have considered the Lax representation is given either in a pseudo-differential operator or in matrix form (taking values in some lower dimensional Lie algebras). We call such Lax representations as standard Lax representation. On the other hand there are some systems of evolution equations, such as the equations of hydrodynamic type, which are obtained by nonstandard Lax represenations used in the present paper. We first show that the method introduced in Ref. 1 is also applicable here in the case of systems of equations of hydrodynamic types and we give several examples for illustration. These equations and their Hamil-

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tonian formulation (sometimes called the dispersion-less KdV system) were studied by Dubrovin and Novikov.[3] See Ref. 4 for more details on this subject (see also Ref. 5). It is known that these equations admit a nonstandard Lax representation,

$$\frac{\partial L}{\partial t}=\{A,L\}_k, \tag{5}$$

where A,L are differentiable functions of t,x,p on a Poisson manifold M with local coordinates (x,p) and $\{,\}_k$ is the Poisson bracket. On M we take this Poisson bracket $\{,\}_k=p^k\{,\}$, where $\{,\}$ is the canonical Poisson bracket and k is an integer. For more information on Poisson manifolds see Refs. 6 and 7. Equations of hydrodynamic type with the above Lax representations were studied in Refs. 8–11. Having such a Lax representation, we can consider a whole hierarchy of equations,

$$\frac{\partial L}{\partial t_n}=\{A_n,L\}_k. \tag{6}$$

We can also represent function A_n in the form given in (3) and apply our method[1] for the construction of a recursion operator for the equation (6). There are some other works[12–14] which also give recursion operators of some equations of hydrodynamic type. The form of these operators are different than the recursion operators presented in this work. Our method[1] produces recursion operators for hydrodynamic type of equations in the form $\mathcal{R}=A+B\,D^{-1}$ where A and B are functions of dynamical variables and their derivatives. All higher symmetries obtained by the repeated application of this recursion operator to translational symmetries also belong to the hydrodynamic type of equations. The recursion operators obtained in Refs. 12–14 are of the form $\mathcal{R}=C\,D+A+B\,D^{-1}E$, where A,B,C, and E are functions of dynamical variables and their derivatives.

In the next section we discuss the Lax representation with Poisson brackets for polynomial Lax functions. In Sec. III we give the method of construction of the recursion operators following Ref. 1. In Sec. IV we give several examples for $k=0$ and $k=1$. In Sec. V we consider the Poisson bracket for general k and let

$$L=p+S+Pp^{-1}, \tag{7}$$

and find the Lax equations and the corresponding recursion operator for $N=2$. In Sec. VI we consider the Lax function

$$L=p^{\gamma-1}+u+\frac{v^{\gamma-1}}{(\gamma-1)^2}p^{-\gamma+1}, \tag{8}$$

and take $k=0$. We obtain the equations corresponding to the polytropic gas dynamics and its recursion operators.[6,10] It is interesting to note that the systems of equations and their recursion operators obtained in Secs. V and VI are transformable into each other. In Sec. VII we give a method reduction from an $N+1$ system to an N system and from an $N+1$ system to an $N-1$ system by letting one of the symmetrical variables (defined in the text) either to zero or equating to another variable. The systems obtained by the reduction are equivalent to the systems obtained by the Lax function (in symmetrical variables) having zeros with multiplicities greater than one. Reduced systems are shown to be also integrable, i.e., they admit recursion operators.

II. LAX FORMULATION WITH POISSON BRACKET

We start with the definition of the standard Poisson bracket. Let $f(x,p)$ and $g(x,p)$ be differentiable functions of their arguments. Then the standard Poisson bracket is defined by (see Refs. 6 and 9 for more details)

$$\{f,g\}=\frac{\partial f}{\partial p}\frac{\partial g}{\partial x}-\frac{\partial f}{\partial x}\frac{\partial g}{\partial p}. \tag{9}$$

We give a slight modification of this bracket as[9]

$$\{f,g\}_k=p^k\{f,g\}, \tag{10}$$

where k is an integer. It is easy to prove that $\{,\}_k$ also defines a Poisson bracket for all $k\in\mathbb{Z}$. Although this bracket is equivalent to $\{,\}$, under $p^k(d/dp)=d/dq$ where q is the new variable, we shall keep using it. The main reason is technical. There is a nice duality between the systems obtained by polynomial Lax representation, $L=p^N+\cdots$, with Poisson bracket $\{,\}_k$ and by Lax represention $L=p^\gamma[p^N+\cdots]$ with Poisson bracket $\{,\}$. For illustration we have examples, equations governing the polytropic gas dynamics, given in Propositions 6 and 7.

For each $k\in\mathbf{Z}$ we can consider hierarchies of equations of hydrodynamic type, defined in terms of the Lax function,

$$L=p^{N-1}+\sum_{i=-1}^{N-2}p^iS_i(x,t), \tag{11}$$

by the Lax equation

$$\frac{\partial L}{\partial t_n}=\{(L^{n/(N-1)})_{\geqslant -k+1};L\}_k, \tag{12}$$

where $n=j+l(N-1)$ and $j=1,2,\ldots,(N-1), l\in\mathbf{N}$. So we have a hierarchy for each k and $j=1,\ldots,(N-1)$. Also, we require $n\geqslant -k+1$ to ensure that $(L^{n/(N-1)})_{\geqslant -k+1}$ is not zero. With the choice of Poisson brackets $\{,\}_k$, we must take a certain part of the series expansion of $L^{n/(N-1)}$ to get the consistent equation (12). This part is $(L^{n/(N-1)})_{\geqslant -k+1}$.

The Lax function (11) can also be written in terms of symmetric variables $u_1,\ldots,u_N$,

$$L=\frac{1}{p}\prod_{j=1}^{N}(p-u_j), \tag{13}$$

that is $u_1,\ldots,u_N$ are roots of the polynomial

$$p^{N-1}+S_{N-2}p^{N-2}+\ldots+S_{-1}p^{-1}.$$

In new variables the equation (12) is invariant under transposition of variables.

III. RECURSION OPERATORS

For each hierarchy of the equations (12), depending on the pair (N,k), we can find a recursion operator.

Lemma 1: For any n,

$$L_n=LL_{n-(N-1)}+\{R_n;L\}_k, \tag{14}$$

where function R_n has a form

$$R_n=\sum_{i=0}^{N-2}p^{i-k}A_i(S_{-1}\ldots S_{N-2},\partial S_{-1}/\partial t_{n-(N-1)}\ldots\partial S_{N-2}/\partial t_{n-(N-1)}). \tag{15}$$

Proof:

$$(L^{n/(N-1)})_{\geqslant -k+1}=[L(L^{n/(N-1)-1})_{\geqslant -k+1}+L(L^{n/(N-1)-1})_{<-k+1}]_{\geqslant -k+1}.$$

So,

$$(L^{n/(N-1)})_{\geqslant -k+1}=L(L^{n/(N-1)-1})_{\geqslant -k+1}+(L(L^{n/(N-1)-1})_{<-k+1})_{\geqslant -k+1}$$
$$-(L(L^{n/(N-1)-1})_{\geqslant -k+1})_{<-k+1}. \tag{16}$$

If we put

$$R_n=(L(L^{n/(N-1)-1})_{<-k+1})_{\geqslant -k+1}-(L(L^{n/(N-1)-1})_{\geqslant -k+1})_{<-k+1},$$

then

$$(L^{n/(N-1)})_{\geqslant -k+1}=L(L^{n/(N-1)-1})_{\geqslant -k+1}+R_n.$$

Hence,

$$L_n=\{(L^{n/(N-1)})_{\geqslant -k+1};L\}_k=\{L(L^{n/(N-1)-1})_{\geqslant -k+1}+R_n;L\}_k=LL_{n-(N-1)}+\{R_n;L\}_k, \tag{17}$$

and (14) is satisfied. Evaluating powers of $(L(L^{n/(N-1)-1})_{<-k+1})_{\geqslant -k+1}$ and $-(L(L^{n/(N-1)-1})_{\geqslant -k+1})_{<-k+1}$ we get that R_n has form (15). □

Lemma 2: A recursion operator for the hierarchy (12) is given by equalities, for $m=N-2,N-3,\ldots,-1$,

$$\frac{\partial S_m}{\partial t_n}=\sum_{j=-1}^{m+1} S_j \frac{\partial S_{m-j}}{\partial t_{n-(N-1)}}+\sum_{j=-1}^{m+1}(j+1-k)A_{j+1}S_{m-j,x}-\sum_{j=-1}^{m+1}(m-j)A_{j+1,x}S_{m-j}, \tag{18}$$

where to simplify the above formula we have defined that $S_{N-1}=1$ and $S_{N-1,x}=0$, $(\partial S_{N-1}/\partial t_n)=0$. *Coefficients* $A_{N-2},A_{N-3},\ldots,A_0$ *can be found from the recursion relations, for* $m=N-2,\ldots,-1$,

$$(N-1)A_{m,x}=\sum_{j=m}^{N-1} S_j \frac{\partial S_{(N-2)+m-j}}{\partial t_{n-(N-1)}}+\sum_{j=m}^{N-2}(j+1-k)A_{j+1}S_{N-2+m-j,x}$$
$$-\sum_{j=m}^{N-2}(N-2+m-j)A_{j+1,x}S_{N-2+m-j}. \tag{19}$$

Proof: Let us write the equality (14), using (15) for R_n,

$$\sum_{i=-1}^{N-2} p^i \frac{\partial S_i}{\partial t_n}=\left(p^{N-1}+\sum_{i=-1}^{N-2}p^i S_i\right)\left(\sum_{i=-1}^{N-2}p^i \frac{\partial S_{(N-2)+m-j}}{\partial t_{n-(N-1)}}\right)+p^k\left(\sum_{j=0}^{N-1}(j-k)p^{j-k-1}A_j\right)$$
$$\times\left(\sum_{j=-1}^{N-2}p^j S_{j,x}\right)-p^k\left(\sum_{j=0}^{N-1}p^{j-k}A_{j,x}\right)\left((N-1)p^{N-2}+\sum_{j=-1}^{N-2}jp^{j-1}S_j\right).$$

To have the equality, the coefficients of $p^{2N-3},\ldots,p^{N-1}$ and p^{-2} must be zero; it gives recursion relations to find $A_{N-2},\ldots,A_0$. The coefficients of $p^{N-2},\ldots,p^{-1}$ give the expressions for $\partial S_{N-2}/\partial t_{n,}\ldots,\partial S_{-1}/\partial t_n$. □

Although the recursion operator $\mathcal{R}$, given by (18), is a pseudo-differential operator, but it gives a hierarchy of local symmetries starting from the equation itself. Indeed, equalities (18), (19)

give expressions $\partial S_{N-2}/\partial t_{n,\ldots,}\partial S_{-1}/\partial t_n$ in terms of $S_{N-2},\ldots,S_{-1}$ and $\partial S_{N-2}/\partial t_{n-(N-1),\ldots,}$ $\partial S_{-1}/\partial t_{n-(N-1)}$. Hence, the recursion operator $\mathcal{R}$ is constructed in such a way that

$$\{(L^{n/(N-1)+1})_{\geqslant -k+1};L\}_k=\mathcal{R}(\{(L^{n/(N-1)})_{\geqslant -k+1};L\}_k). \tag{20}$$

IV. SOME INTEGRABLE SYSTEMS

We shall consider first some examples for $k=0$, $k=1$ and the general case in the next section.

A. Multicomponent hierarchy containing also the shallow water wave equations, $k=0$

This hierarchy corresponds to the case $k=0$. Let us give the first equation of hierarchy and a recursion operator for $N=2,3$.

Proposition 1: In the case $N=2$ one has the Lax function,

$$L=p+S+P\,p^{-1},$$

and the Lax equation for $n=2$, given by (47), when $k=0$,

$$\begin{aligned}\tfrac{1}{2}S_t&=SS_x+P_x,\\ \tfrac{1}{2}P_t&=SP_x+PS_x,\end{aligned} \tag{21}$$

and the recursion operator, given by (48),

$$\mathcal{R}=\begin{pmatrix} S+S_xD_x^{-1} & 2\\ 2P+P_xD_x^{-1} & S\end{pmatrix}. \tag{22}$$

These equations are known as the shallow water wave equations or as the equations of polytropic gas dynamics for $\gamma=2$ (See Sec. VI).

The first two symmetries of the system (21) are given by

$$S_{t_1}=(S^3+6SP)_x,$$

$$P_{t_1}=(3S^2P+3P^2)_x, \tag{23}$$

$$S_{t_2}=(S^4+12S^2P+6P^2)_x,$$

$$P_{t_2}=(4S^3P+12SP^2)_x. \tag{24}$$

These are all commuting symmetries.

Remark 1: In symmetric variables the system (21) is written as

$$\begin{aligned}\tfrac{1}{2}u_t&=(u+v)u_x+uv_x,\\ \tfrac{1}{2}v_t&=vu_x+(u+v)v_x,\end{aligned} \tag{25}$$

and the recursion operator (22) takes the form

$$\mathcal{R}=\begin{pmatrix} u+v+u_xD_x^{-1} & 2u+u_xD_x^{-1}\\ 2v+v_xD_x^{-1} & u+v+v_xD_x^{-1}\end{pmatrix}. \tag{26}$$

Proposition 2: In the case $N=3$ one has the Lax function

$$L=p^2+pS+P+p^{-1}Q,$$

and the Lax equation with $n=3$ is

$$\begin{aligned}
\tfrac{1}{3}S_t&=(\tfrac{1}{2}P-\tfrac{1}{8}S^2)S_x+\tfrac{1}{2}SP_x+Q_x,\\
\tfrac{1}{3}P_t&=\tfrac{1}{2}QS_x+(\tfrac{1}{8}S^2+\tfrac{1}{2}P)P_x+SQ_x,\\
\tfrac{1}{3}Q_t&=\tfrac{1}{4}SQS_x+\tfrac{1}{2}QP_x+(\tfrac{1}{8}S^2+\tfrac{1}{2}P)Q_x.
\end{aligned}\tag{27}$$

The recursion operator, corresponding to this equation, is

$$\mathcal{R}=\begin{pmatrix}
-\dfrac{S^2}{4}+P+P_xD_x^{-1}-\dfrac{S_x}{4}D_x^{-1}\cdot S & \dfrac{S}{2}+\dfrac{S_x}{2}D_x^{-1} & 3\\
\dfrac{3Q}{2}+\left(Q_x+\dfrac{P_xS}{2}\right)D_x^{-1}-\dfrac{P_x}{4}D_x^{-1}\cdot S & P+\dfrac{P_x}{2}D_x^{-1} & 2S\\
\dfrac{SQ}{4}+\left(\dfrac{SQ_x}{2}+\dfrac{S_xQ}{2}\right)D_x^{-1}-\dfrac{Q_x}{4}D_x^{-1}\cdot S & \dfrac{3Q}{2}+\dfrac{Q_x}{2}D_x^{-1} & P
\end{pmatrix}.\tag{28}$$

Proof: Using (19) we find the function R_n and using (18) we find the recursion operator (28). □

Remark 2: In symmetric variables the equation (27) is written as

$$\begin{aligned}
\tfrac{1}{3}u_t&=(-\tfrac{1}{8}u^2+\tfrac{1}{2}(uv+uw+vw)+\tfrac{1}{8}(v+w)^2)u_x+(\tfrac{1}{4}u^2+\tfrac{1}{4}uv+\tfrac{3}{4}uw)v_x+(\tfrac{1}{4}u^2+\tfrac{1}{4}uw+\tfrac{3}{4}uv)w_x,\\
\tfrac{1}{3}v_t&=(\tfrac{1}{4}v^2+\tfrac{1}{4}uv+\tfrac{3}{4}vw)u_x+(\tfrac{1}{4}v^2+\tfrac{1}{4}vw+\tfrac{3}{4}uv)w_x+(-\tfrac{1}{8}v^2+\tfrac{1}{2}(uv+uw+vw)+\tfrac{1}{8}(u+w)^2)v_x,\\
\tfrac{1}{3}w_t&=(\tfrac{1}{4}w^2+\tfrac{1}{4}uw+\tfrac{3}{4}wv)u_x+(\tfrac{1}{4}w^2+\tfrac{1}{4}wv+\tfrac{3}{4}uw)v_x+(-\tfrac{1}{8}w^2+\tfrac{1}{2}(uv+uw+vw)+\tfrac{1}{8}(v+u)^2)w_x,
\end{aligned}\tag{29}$$

and the recursion operator takes the form (A1) given in the Appendix.

B. Toda hierarchy ($k=1$)

Toda hierarchy corresponds to the case $k=1$.[9] Let us give the first equation of hierarchy and a recursion operator for $N=2$ and $N=3$.

Proposition 3: In the case $N=2$ and $n=1$ one has the Lax function

$$L=p+S+P\,p^{-1},$$

and the Lax equation for $n=1$, given by (41),

$$\begin{aligned}
S_t&=P_x,\\
P_t&=PS_x,
\end{aligned}\tag{30}$$

and the recursion operator, given by (42),

$$\mathcal{R}=\begin{pmatrix} S & 2+P_xD_x^{-1}\cdot P^{-1}\\ 2P & S+S_xPD_x^{-1}\cdot P^{-1}\end{pmatrix}.\tag{31}$$

The first two symmetries of the equation (30) are given by

$$S_{t_1}=(2SP)_x,$$
$$P_{t_1}=P(2P+S^2)_x, \tag{32}$$

$$S_{t_2}=(3S^2P+3P^2)_x,$$
$$P_{t_2}=P(6PS+S^3)_x. \tag{33}$$

Remark 3: In symmetric variables the equation (30) is written as

$$u_t=uv_x,$$
$$v_t=vu_x, \tag{34}$$

and the recursion operator (31) takes the form

$$\mathcal{R}=\begin{pmatrix} u+v+uv_xD_x^{-1}\cdot u^{-1} & 2u+uv_xD_x^{-1}\cdot v^{-1} \\ 2v+vu_xD_x^{-1}\cdot u^{-1} & u+v+vu_xD_x^{-1}\cdot v^{-1} \end{pmatrix}. \tag{35}$$

Proposition 4: In the case $N=3$ and $n=1$ one has the Lax function

$$L=p^2+pS_1+P+p^{-1}Q,$$

and the Lax equation with $n=1$ is

$$S_t=P_x-\tfrac{1}{2}SS_x,$$
$$P_t=Q_x, \tag{36}$$
$$Q_t=\tfrac{1}{2}QS_x.$$

The recursion operator, corresponding to this equation, is

$$\mathcal{R}=\begin{pmatrix} P-\frac{1}{4}S^2+(\frac{1}{2}P_x-\frac{1}{4}SS_x)D_x^{-1} & \frac{1}{2}S & 3+2Q_xD_x^{-1}\cdot Q^{-1} \\ \frac{3}{2}Q+\frac{1}{2}Q_xD_x^{-1} & P & 2S+(SQ)_xD_x^{-1}\cdot Q^{-1} \\ \frac{1}{4}SQ+\frac{1}{4}S_xQD_x^{-1} & \frac{3}{2}Q & P+P_xQD_x^{-1}\cdot Q^{-1} \end{pmatrix}. \tag{37}$$

Proof: Using equalities (19) we find the function R_n and using (18) we find the recursion operator (37). □

Remark 4: In symmetric variables the equation (36) is written as

$$u_t=\tfrac{1}{2}u(-u_x+v_x+w_x),$$
$$v_t=\tfrac{1}{2}v(+u_x-v_x+w_x), \tag{38}$$
$$w_t=\tfrac{1}{2}w(+u_x+v_x-w_x),$$

and the recursion operator takes the form (A2) given in the Appendix.

V. LAX EQUATION FOR GENERAL *k*

We shall only consider the case where $N=2$. We have the Lax function

$$L=p+S+Pp^{-1}, \tag{39}$$

and the Lax equation

$$\frac{\partial L}{\partial t_n}=\{(L^n)_{\geqslant -k+1};L\}_k. \tag{40}$$

We consider two cases $k\geqslant 1$ and $k\leqslant 0$.

A. The first case $k\geqslant 1$

Proposition 5: In the case $N=2$ and $k\geqslant 1$ one has the Lax equation

$$\begin{aligned} S_t&=kP^{k-1}P_x,\\ P_t&=kP^kS_x, \end{aligned} \tag{41}$$

and the recursion operator for this equation is

$$\mathcal{R}=\begin{pmatrix} S+(1-k)S_xD_x^{-1} & 2+kP^{k-1}P_xD_x^{-1}\cdot P^{-k}\\ 2P+(1-k)P_xD_x^{-1} & S+kS_xP^kD_x^{-1}\cdot P^{-k}\end{pmatrix}. \tag{42}$$

Proof: The smallest power of p in L^n is $-n$. To have powers less than $-k+1$ we must put $n=k$. If there are no such powers then Poisson brackets are $\{(L^n);L\}_k=0$.

Let us calculate the Lax equation,

$$L_t=\{(L^k)_{\geqslant -k+1};L\}_k=-\{(L^k)_{\leqslant -k};L\}_k.$$

We have $(L^k)_{\leqslant -k}=[(p+S+Pp^{-1})^k]_{\leqslant -k}=P^kp^{-k}$, thus

$$L_t=-\{P^kp^{-k};p+S+Pp^{-1}\}_k.$$

And we get the equation (41). Using (18), (19) we find the recursion operator (42). □

First two symmetries are given as follows:

$$\begin{aligned} S_{t_1}&=(k+1)(P^kS)_x,\\ P_{t_1}&=(k+1)P^k\left(P+\frac{k}{2}S^2\right)_x. \end{aligned} \tag{43}$$

$$\begin{aligned} S_{t_2}&=(k+1)(k+2)\left(\frac{1}{2}P^kS^2+\frac{1}{k+1}P^{k+1}\right)_x,\\ P_{t_2}&=(k+1)(k+2)P^k\left(PS+\frac{k}{6}S^3\right)_x. \end{aligned} \tag{44}$$

Remark 5: In symmetric variables the equation (41) is written as

$$\begin{aligned} u_t&=ku^kv^{k-1}v_x,\\ v_t&=ku^{k-1}v^ku_x, \end{aligned} \tag{45}$$

and the recursion operator (42) takes the form

$$\mathcal{R}=\begin{pmatrix} u+v+(1-k)u_xD_x^{-1}+ & 2u+(1-k)u_xD_x^{-1}+ \\ ku^kv^{k-1}v_xD_x^{-1}\cdot u^{-k}v^{-k+1} & ku^kv^{k-1}v_xD_x^{-1}\cdot u^{-k+1}v^{-k} \\ 2v+(1-k)v_xD_x^{-1}+ & u+v+(1-k)v_xD_x^{-1}+ \\ ku^{k-1}v^ku_xD_x^{-1}\cdot u^{-k}v^{-k+1} & ku^{k-1}v^ku_xD_x^{-1}\cdot u^{-k+1}v^{-k} \end{pmatrix}. \tag{46}$$

B. The second case $k\leqslant 0$

Proposition 6: In the case $N=2$ and $k\leqslant 0$ one has the Lax equation

$$\begin{aligned} S_t&=(-k+2)(-k+1)SS_x+(-k+2)P_x, \\ P_t&=(-k+2)(-k+1)SP_x+(-k+2)S_xP, \end{aligned} \tag{47}$$

and the recursion operator for this equation is

$$\mathcal{R}=\begin{pmatrix} S+(1-k)S_xD_x^{-1} & 2+kP^{k-1}P_xD_x^{-1}\cdot P^{-k} \\ 2P+(1-k)P_xD_x^{-1} & S+kS_xP^kD_x^{-1}\cdot P^{-k} \end{pmatrix}. \tag{48}$$

Proof: The largest power of p in L^n is p^n. To have powers larger than $-k+1$ we must put $n=-k+1$. Then we have

$$(L^{-k+1})_{\geqslant -k+1}=[(p+S+Pp^{-1})^{-k+1}]_{\geqslant -k+1}=p^{-k+1};$$

thus

$$L_t=\{p^{-k+1};p+S+Pp^{-1}\}_k.$$

Then the Lax equation becomes

$$\begin{aligned} S_t&=S_x, \\ P_t&=P_x. \end{aligned}$$

This is a trivial equation; let us calculate the second symmetry. We have $(L^{-k+2})_{\geqslant -k+1}=[(p+S+Pp^{-1})^{-k+1}]_{\geqslant -k+1}=p^{-k+2}+(-k+2)Sp^{-k+1}$, thus

$$L_t=\{p^{-k+2}+(-k+2)Sp^{-k+1};p+S+Pp^{-1}\}_k.$$

We get the equation (47). Using (18), (19) we find the recursion operator (48). □

First two symmetries are given as follows:

$$\begin{aligned} S_{t_1}&=(k-2)(k-3)(PS+\tfrac{1}{6}(1-k)S^3)_x, \\ P_{t_1}&=(k-2)(k-3)(SS_xP+\tfrac{1}{2}(1-k)S^2P_x+PP_x), \end{aligned} \tag{49}$$

$$\begin{aligned} S_{t_2}&=(2-k)(3-k)(4-k)\left(\frac{1}{2}S^2P+\frac{1}{6}S^4+\frac{1}{2(2-k)}P^2\right)_x, \\ P_{t_2}&=(2-k)(3-k)(4-k)\left(\frac{1}{2}S^2S_xP+\frac{1}{6}(1-k)S^3P_x+SPP_x+\frac{1}{(2-k)}P^2S_x\right). \end{aligned} \tag{50}$$

Remark 6: In symmetric variables the equation (47) is written as

$$u_t=(-k+2)(1-k)(u+v)u_x+(-k+2)uv_x,$$

$$v_t=(-k+2)vu_x+(-k+2)(1-k)(u+v)v_x, \tag{51}$$

and the recursion operator (48) takes the form

$$\mathcal{R}=\begin{pmatrix} u+v+(1-k)u_xD_x^{-1}+ & 2u+(1-k)u_xD_x^{-1}+ \\ ku^kv^{k-1}v_xD_x^{-1}\cdot u^{-k}v^{-k+1} & ku^kv^{k-1}v_xD_x^{-1}\cdot u^{-k+1}v^{-k} \\ 2v+(1-k)v_xD_x^{-1}+ & u+v+(1-k)v_xD_x^{-1}+ \\ ku^{k-1}v^ku_xD_x^{-1}\cdot u^{-k}v^{-k+1} & ku^{k-1}v^ku_xD_x^{-1}\cdot u^{-k+1}v^{-k} \end{pmatrix}. \tag{52}$$

In this section, to obtain the recursion operators we have considered two different cases $k\leqslant 0$ and $k\geqslant 1$ to simplify some technical problems in the method. At the end we obtained recursion operators having the same forms (42) and (48). Hence any one of these represent the recursion operator for $k\in\mathbb{Z}$. It seems, comparing the results, that the systems of equations in one case are symmetries of the other case. For instance, the system (47) is a symmetry of system (41). Hence we may consider only one case with recursion operator (42) for all integer values of k.

VI. LAX FUNCTION FOR POLYTROPIC GAS DYNAMICS

In this section we consider another Lax function, introduced in Ref. 10,

$$L=p^{\gamma-1}+u+\frac{v^{\gamma-1}}{(\gamma-1)^2}p^{-\gamma+1}, \tag{53}$$

and the Lax equation

$$\frac{\partial L}{\partial t}=\frac{\gamma-1}{\gamma}\{(L^{\gamma/(\gamma-1)})_{\geqslant 1},L\}_0, \tag{54}$$

gives the equations of the polytropic gas dynamics.

Proposition 7: The Lax equation corresponding to (54) is

$$u_t+uu_x+v^{\gamma-2}v_x=0,$$

$$v_t+(uv)_x=0. \tag{55}$$

Proof: Expanding the function (53) around the point $p=\infty$, we have

$$\left(p^{\gamma-1}+u+\frac{v^{\gamma-1}}{(\gamma-1)^2}p^{-\gamma+1}\right)^{\gamma/(\gamma-1)}=p^{\gamma}+\frac{\gamma}{\gamma-1}pu+\ldots;$$

all other terms have negative powers of p. Therefore

$$(L^{\gamma/(\gamma-1)})_{\geqslant 1}=p^{\gamma}+\frac{\gamma}{\gamma-1}pu,$$

and the Lax equation (54) corresponds to (55). □

Proposition 8: The recursion operator for the equation (55) is

$$\mathcal{R}=\begin{pmatrix} u+\dfrac{u_x}{\gamma-1}D_x^{-1} & \dfrac{2v^{\gamma-2}}{\gamma-1}+\dfrac{(v^{\gamma-2})_x}{\gamma-1}D_x^{-1} \\ \dfrac{2v}{\gamma-1}+\dfrac{v_x}{\gamma-1}D_x^{-1} & u+\dfrac{\gamma-2}{\gamma-1}u_xD_x^{-1} \end{pmatrix}. \tag{56}$$

Proof: Using the equation

$$\frac{\partial L}{\partial t_{n+1}} = L\frac{\partial L}{\partial t_n} + \{R_n, L\},$$

in the same way as for the polynomial Lax function one can find the recursion operator (56). □

It is interesting to note that the equation (47) and equations of polytropic gas dynamics (55) are related by the following change of variables:

$$S = \frac{u}{(-k+2)(-k+1)}, \qquad P = \frac{v^{1/(-k+1)}}{(-k+2)^2}, \tag{57}$$

where $\gamma = (-k+2)/(-k+1)$. We note that under this change of variables recursion operator (48) is mapped to the recursion operator (56).

VII. REDUCTION

In this section we consider reductions of the equation (12), written in symmetric variables, by setting $u_1 = 0$, or $u_1 = u_N, \ldots$, or $u_1 = u_2 = \cdots, = u_N$. These reductions correspond to the Lax equations with different Lax functions. For reduction $u_1 = 0$ we have a polynomial Lax function with simple roots $L = (p-u_N)\cdots(p-u_2)$ and for reduction $u_N = u_1$ we have a polynomial Lax function with a root of multiplicity two $L = (1/p)(p-u_N)^2(p-u_{N-1})\ldots(p-u_2)$, etc. We note that instead of working on the Lax functions with higher multiplicities like the last example one can take a polynomial Lax function without any multiplicities and perform the reductions we propose in this section.

A. Reduction $u_1 = 0$

Let us write the equation (12) as

$$\Delta(u_N, \ldots, u_1) = 0, \tag{58}$$

where Δ is a differential operator. Then

$$\Delta(u_N, \ldots, u_1)|_{u_1=0} = \begin{pmatrix} \tilde{\Delta}(u_N, \ldots, u_2), \\ 0 \end{pmatrix}, \tag{59}$$

where $\tilde{\Delta}$ is another differential operator. Indeed, following Ref. 8 for the Lax function $L = (1/p)\,\Pi_{j=1}^{N}(p-u_j)$ we have

$$\frac{\partial L}{\partial t} = L\sum_{j=1}^{N}\frac{u_{j,t}}{p+u_j},$$

$$\frac{\partial L}{\partial x} = L\sum_{j=1}^{N}\frac{u_{j,x}}{p+u_j},$$

and

$$\frac{\partial L}{\partial p} = L\left(-\frac{1}{p} + \sum_{j=1}^{N}\frac{1}{p+u_j}\right).$$

Thus $u_{j,t} = \mathrm{Res}_{p=-u_j}\{M, L\}_k$, where $M = (L^{n/(N-1)})_{\geqslant -k+1}$. The Lax equation (12) can be written as

$$\sum_{j=1}^{N}\frac{u_{j,t}}{p+u_j}=p^kM_p\sum_{j=1}^{N}\frac{u_{j,x}}{p+u_j}-p^kM_x\left(-\frac{1}{p}+\sum_{j=1}^{N}\frac{1}{p+u_j}\right). \tag{60}$$

Note that p^kM_x and p^kM_p are polynomials. So, if we put $u_1=0$ and calculate the residue of the right hand side at $p=0$ we get (59). A new equation,

$$\tilde{\Delta}(u_N,\ldots,u_2)=0, \tag{61}$$

is also integrable and a recursion operator of this equation can be obtained as a reduction of the recursion operator of the equation (58). Let $\mathcal{R}$ be the recursion operator of (58) given by Lemma 2, then

$$\mathcal{R}|_{u_1=0}=\left(\begin{array}{c|c}\tilde{R} & *\\ \hline 0\cdots 0 & 0\end{array}\right). \tag{62}$$

Indeed, we found the recursion operator using formula (14). This formula can be written as

$$\sum_{j=1}^{N}\frac{u_{j,t_n}}{p+u_j}=LL_{n-(N-1)}+p^kR_{n,p}\sum_{j=1}^{N}\frac{u_{j,x}}{p+u_j}-p^kR_{n,x}\left(-\frac{1}{p}+\sum_{j=1}^{N}\frac{1}{p+u_j}\right) \tag{63}$$

and in the same way as for the reduction of (58) we have (62); note, that $p^kR_{n,x}$ and $p^kR_{n,p}$ are also polynomials.

Lemma 3: The operator $\tilde{R}$ is a recursion operator of the equation (61).

Proof: Equation (61) is an evolution equation, so, to prove that $\tilde{R}$ is a recursion operator we must prove that for any solution $(u_N,\ldots,u_2)$ of (61) the following equality holds (see Ref. 6):

$$D_{\tilde{\Delta}}\tilde{R}=\tilde{R}D_{\tilde{\Delta}},$$

where $D_{\tilde{\Delta}}$ is a Frechet derivative of $\tilde{\Delta}$.

If $(u_N,\ldots,u_2)$ is a solution of (61) then $(u_N,\ldots,u_2,u_1=0)$ is a solution of (58) and for the solution $(u_N,\ldots,u_2,u_1=0)$ we have

$$D_\Delta\mathcal{R}=\mathcal{R}D_\Delta. \tag{64}$$

Next

$$D_\Delta|_{u_1=0}=\left(\begin{array}{c|c}\tilde{D} & *\\ \hline 0\cdots 0 & *\end{array}\right)$$

and

$$\mathcal{R}|_{u_1=0}=\left(\begin{array}{c|c}\tilde{R} & *\\ \hline 0\cdots 0 & 0\end{array}\right).$$

Hence by (64) we have $\tilde{D}\tilde{R}=\tilde{R}\tilde{D}$. Calculating the Frechet derivative, we take derivatives with respect to one variable, considering other variables as constants. Thus, to calculate $\tilde{D}$ we can put $u_1=0$ and differentiate with respect to other variables or we can first differentiate and then put $u_1=0$. It means that $\tilde{D}=D_{\tilde{\Delta}}$ and

$$D_{\tilde{\Delta}}\tilde{R}=\tilde{R}D_{\tilde{\Delta}}.$$

□

Let us consider the reduction of systems, given by Remark 2 and Remark 4 and their recursion operators.

Proposition 9: Putting $w=0$ in (38) and (A2) we obtain a new system,

$$u_t=\tfrac{1}{2}u(-u_x+v_x),$$
$$v_t=\tfrac{1}{2}v(+u_x-v_x), \tag{65}$$

and its recursion operator,

$$\mathcal{R}=\begin{pmatrix} -uv+\frac{u}{4}(u+v) & -\frac{u}{4}(u+v) \\ +\frac{u}{4}(u_x-v_x)D_x^{-1} & +\frac{u}{4}(u_x-v_x)D_x^{-1} \\ -\frac{v}{4}(u+v) & -uv+\frac{v}{4}(u+v) \\ +\frac{v}{4}(-u_x+v_x)D_x^{-1} & +\frac{v}{4}(-u_x+v_x)D_x^{-1} \end{pmatrix}, \tag{66}$$

respectively. □

Proposition 10: Putting $w=0$ in (29) and (A1) we obtain a new system,

$$\tfrac{1}{3}u_t=(-\tfrac{1}{8}u^2+\tfrac{1}{2}uv+\tfrac{1}{8}v^2)u_x+(\tfrac{1}{4}u^2+\tfrac{1}{4}uv)v_x,$$
$$\tfrac{1}{3}v_t=(\tfrac{1}{4}v^2+\tfrac{1}{4}uv)u_x+(-\tfrac{1}{8}v^2+\tfrac{1}{2}uv+\tfrac{1}{8}u^2)v_x, \tag{67}$$

and its recursion operator,

$$\mathcal{R}=\begin{pmatrix} -\frac{u^2}{4}+\frac{3uv}{4}+\left(\frac{u_xv}{2}+\frac{uv_x}{2}\right)D_x^{-1} & \frac{u}{4}(u+v)+\left(\frac{u_xv}{2}+\frac{uv_x}{2}\right)D_x^{-1} \\ -\frac{u_x}{4}D_x^{-1}\cdot u+\frac{u_x}{4}D_x^{-1}\cdot v & +\frac{u_x}{4}D_x^{-1}\cdot u-\frac{u_x}{4}D_x^{-1}\cdot v \\ \frac{v}{4}(u+v)+\left(\frac{uv_x}{2}+\frac{u_xv}{2}\right)D_x^{-1} & -\frac{v^2}{4}+\frac{3uv}{4}+\left(\frac{uv_x}{2}+\frac{u_xv}{2}\right)D_x^{-1} \\ -\frac{v_x}{4}D_x^{-1}\cdot u+\frac{v_x}{4}D_x^{-1}\cdot v & +\frac{v_x}{4}D_x^{-1}\cdot u-\frac{v_x}{4}D_x^{-1}\cdot v \end{pmatrix}, \tag{68}$$

respectively. □

It is worth mentioning that by reduction we obtain a new equation. For example, consider the case $k=0$. The equation (25), corresponding to $N=2$, and reduction of the equation (29), corresponding to $N=3$, are not related by a linear transformation of variables. Indeed, in the equation (25) coefficients of u_x,v_x are linear in u,v but in the equation (67) coefficients of u_x,v_x contain quadratic terms. Hence they cannot be related by a linear transformation.

B. Reduction $u_N=u_1$

It follows from (60) that the Lax equation (12) can be written as

$$u_{i,t}=\sum_{j=1}^{N} h_i^j(u_N,\ldots,u_1)u_{j,x}, \tag{69}$$

where $i,j=1,\ldots,N$ and $h_i^j=h_1(u_i,u_N,\ldots,\hat{u}_i,\ldots,u_1)$ when $i\neq j$ and $h_i^i=h_2(u_i,u_N,\ldots,\hat{u}_i,\ldots,u_1)$, the overcaret denotes the absence of the corresponding variable. It also follows from (60) that the functions $h_1(x_N,\ldots,x_1)$ and $h_2(x_N,\ldots,x_1)$ are symmetric under permutations of variables $x_{N-1},\ldots,x_1$.

Reduction $u_N=u_1$ gives us a new integrable equation,

$$
\begin{aligned}
u_{N,t} &= (h_N^N(u_N,u_{N-1},\ldots,u_2,u_N)+h_N^1(u_N,u_{N-1},\ldots,u_2,u_N))u_{N,x} \\
&\quad + \sum_{j=2}^{N-1} h_N^j(u_N,u_{N-1},\ldots,u_2,u_N)u_{j,x}, \\
u_{i,t} &= 2h_i^N(u_N,u_{N-1},\ldots,u_2,u_N)u_{N,x}+\sum_{j=2}^{N-1} h_i^j(u_N,u_{N-1},\ldots,u_2,u_N)u_{j,x},
\end{aligned}
\tag{70}
$$

where $i=(N-1),\ldots,2$.

The Frechet derivative of (69), under condition $u_N=u_1$, has the form

$$
D_\Delta|_{u_N=u_1}=\begin{pmatrix}
a_{11} & a_{12} & \cdots & a_{1(N-1)} & a_{1N} \\
a_{21} & a_{22} & \cdots & a_{2(N-1)} & a_{21} \\
\vdots & \vdots & \cdots & \vdots & \vdots \\
a_{(N-1)1} & a_{(N-1)2} & \cdots & a_{(N-1)(N-1)} & a_{(N-1)1} \\
a_{1N} & a_{12} & \cdots & a_{1(N-1)} & a_{11}
\end{pmatrix}, \tag{71}
$$

where a_{ij}, $i,j=1,\ldots,N$ are differential operatos. So, the Frechet derivative of (70) can be writen as

$$
\bar{D_\Delta}=\begin{pmatrix}
a_{11}+a_{1N} & a_{12} & \cdots & a_{1(N-1)} \\
2a_{21} & a_{22} & \cdots & a_{2(N-1)} \\
\vdots & \vdots & \cdots & \vdots \\
2a_{(N-1)1} & a_{(N-1)2} & \cdots & a_{(N-1)(N-1)}
\end{pmatrix}. \tag{72}
$$

Now let us write the recurcion operator of (69), given by Lemma 2. From (63) it follows that, under condition $u_N=u_1$, it has the form

$$
\mathcal{R}|_{u_N=u_1}=\begin{pmatrix}
b_{11} & b_{12} & \cdots & b_{1(N-1)} & b_{1N} \\
b_{21} & b_{22} & \cdots & b_{2(N-1)} & b_{21} \\
\vdots & \vdots & \cdots & \vdots & \vdots \\
b_{(N-1)1} & b_{(N-1)2} & \cdots & b_{(N-1)(N-1)} & b_{(N-1)1} \\
b_{1N} & b_{12} & \cdots & b_{1(N-1)} & b_{11}
\end{pmatrix}, \tag{73}
$$

where b_{ij}, $i,j=N,\ldots,1$ are differential operators.

Now we can write a recursion operator for Eq. (70),

$$
\bar{\mathcal{R}}=\begin{pmatrix}
b_{11}+b_{1N} & b_{12} & \cdots & b_{1(N-1)} \\
2b_{21} & b_{22} & \cdots & b_{2(N-1)} \\
\vdots & \vdots & \cdots & \vdots \\
2b_{(N-1)1} & b_{(N-1)2} & \cdots & b_{(N-1)(N-1)}
\end{pmatrix}. \tag{74}
$$

The form of (74) can be deduced by applaing operator $\mathcal{R}|_{u_N=u_1}$ to a symmetry $(\partial u_N/\partial t_n,\partial u_{N-1}/\partial t_{n,\ldots,}\partial u_2/\partial t_n,\partial u_n/\partial t_n)$.

Lemma 4: The operator $\bar{R}$ in (74) is a recursion operator of the equation (70).

Proof: Equation (70) is an evolution equation, so, to prove that $\bar{R}$ is a recursion operator we must prove that for any solution $(u_N,\ldots,u_2)$ of (70) the following equality holds (see Ref. 6):

$$
D_{\bar{\Delta}}\bar{R}=\bar{R}D_{\bar{\Delta}}.
$$

If $(u_N,\ldots,u_2)$ is a solution of (70) then $(u_N,\ldots,u_2,u_1=u_N)$ is a solution of (69) and for the solution $(u_N,\ldots,u_2,u_1=u_N)$ we have

$$D_\Delta \mathcal{R}=\mathcal{R} D_\Delta . \tag{75}$$

One can show that from commutation of (71) and (73) follows the commutation of (72) and (74) that is equality (75). □

Let us consider reduction of systems, given by Remark 2 and Remark 4 and their recursion operators.

Proposition 11: Putting $w=u$ in (38) and (A2) we obtain a new system,

$$\begin{aligned} u_t&=\tfrac{1}{2}uv_x,\\ v_t&=\tfrac{1}{2}v(2u_x-v_x), \end{aligned} \tag{76}$$

and its recursion operator

$$\mathcal{R}=\begin{pmatrix} -(2uv+u^2)-\frac{3}{2}uv & -\frac{1}{4}u(2u+v)-\frac{3}{2}u^2\\ +\frac{1}{2}uv_xD_x^{-1} & +\frac{1}{4}u(2u_x-v_x)D_x^{-1}\\ -2u(uv)_xD_x^{-1}\cdot u^{-1} & -u(uv)_xD_x^{-1}\cdot v^{-1}\\ -\frac{1}{2}v(2u+v)-3uv & -(2uv+u^2)+\frac{1}{4}v(2u+v)\\ +\frac{1}{2}v(-2u_x+v_x)D_x^{-1} & +\frac{1}{4}v(2-u_x+v_x)D_x^{-1}\\ -2v(uv)_xD_x^{-1}\cdot u^{-1} & -v(u^2)_xD_x^{-1}\cdot v^{-1} \end{pmatrix}. \tag{77}$$

□

Proposition 12: Putting $w=u$ in (29) and (A1) we obtain a new system,

$$\begin{aligned} \tfrac{1}{3}u_t&=(u^2+2uv+\tfrac{1}{8}v^2)u_x+(u^2+\tfrac{1}{4}uv)v_x,\\ \tfrac{1}{3}v_t&=(\tfrac{1}{2}v^2+2uv)u_x+(-\tfrac{1}{8}v^2+uv+u^2)v_x, \end{aligned} \tag{78}$$

and its recursion operator,

$$\mathcal{R}=\begin{pmatrix} u^2+\frac{7}{2}uv+(u^2+uv)_xD_x^{-1} & 2u^2+\frac{1}{4}uv+\frac{1}{2}(u^2+uv)D_x^{-1}\\ +\frac{1}{2}u_xD_x^{-1}\cdot v & +\frac{1}{2}u_xD_x^{-1}\cdot u-\frac{1}{4}u_xD_x^{-1}\cdot v\\ 4uv+\frac{1}{2}v^2+2(uv)_xD_x^{-1} & -\frac{1}{4}v^2+\frac{3}{2}uv+u^2+(uv)_xD_x^{-1}\\ +\frac{1}{2}v_xD_x^{-1}\cdot v & +\frac{1}{2}v_xD_x^{-1}\cdot u-\frac{1}{4}v_xD_x^{-1}\cdot v \end{pmatrix}. \tag{79}$$

□

We may go on introducing new reductions. For instance a reduction of the type $u_1=u_2=u_N$, $(N>3)$, reduces an N-system to an $(N-2)$-system. One may obtain this $(N-2)$-system also from the polynomial Lax function having the form $L=p^{-1}(p-u_1)^3(p-u_3)\cdots(p-u_{N-1})$ (a zero of L with multiplicity three). In this way one obtains an infinite number of different classes of $N=2$, $N=3$ systems.

VIII. CONCLUSION

We have constructed the recursion operators of some equations of hydrodynamic type. The form of the these operators fall into the class of pseudo-differential operators $A+BD^{-1}$ where A and B are functions of dynamical variables and their derivatives. The generalized symmetries of these equations are local and all belong to the same class (i.e., they are also equations of hydro-

dynamic type). We have introduced a method of reduction which leads also to integrable classes. Depending upon the type of reductions we may obtain infinitely many different classes of $N=k$ systems. These properties, the bi-Hamiltonian structure of the equations we obtained and equations with rational Lax functions, will be communicated elsewhere.

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APPENDIX: RECURSION OPERATORS FOR *N*=3 SYSTEMS (29) AND (38)

Recursion operators of the systems (29) and (38) are, respectively, given by

$$\mathcal{R}=\begin{pmatrix}
-\frac{u^2}{4}+\frac{3}{4}(uv+uw)+wv & \frac{u}{4}(u+v+w)+\frac{3uw}{2} & \frac{u}{4}(u+v+w)+\frac{3uv}{2}\\
+\frac{u_x}{2}(v+w)D_x^{-1} & +\frac{u_x}{2}(v+w)D_x^{-1} & +\frac{u_x}{2}(v+w)D_x^{-1}\\
+\frac{u}{2}(v_x+w_x)D_x^{-1} & +\frac{u}{2}(v_x+w_x)D_x^{-1} & +\frac{u}{2}(v_x+w_x)D_x^{-1}\\
-\frac{u_x}{4}D_x^{-1}\cdot u+\frac{u_x}{4}D_x^{-1}\cdot v & +\frac{u_x}{4}D_x^{-1}\cdot u-\frac{u_x}{4}D_x^{-1}\cdot v & +\frac{u_x}{4}D_x^{-1}\cdot u+\frac{u_x}{4}D_x^{-1}\cdot v\\
+\frac{u_x}{4}D_x^{-1}\cdot w & +\frac{u_x}{4}D_x^{-1}\cdot w & -\frac{u_x}{4}D_x^{-1}\cdot w\\
\frac{v}{4}(u+v+w)+\frac{3vw}{2} & -\frac{v^2}{4}+\frac{3}{4}(uv+vw)+uw & \frac{v}{4}(u+v+w)+\frac{3uv}{2}\\
+\frac{v_x}{2}(u+w)D_x^{-1} & +\frac{v_x}{2}(u+w)D_x^{-1} & +\frac{v_x}{2}(u+w)D_x^{-1}\\
+\frac{v}{2}(u_x+w_x)D_x^{-1} & +\frac{v}{2}(u_x+w_x)D_x^{-1} & +\frac{v}{2}(u_x+w_x)D_x^{-1}\\
-\frac{v_x}{4}D_x^{-1}\cdot u+\frac{v_x}{4}D_x^{-1}\cdot v & +\frac{v_x}{4}D_x^{-1}\cdot u-\frac{v_x}{4}D_x^{-1}\cdot v & +\frac{v_x}{4}D_x^{-1}\cdot u+\frac{v_x}{4}D_x^{-1}\cdot v\\
+\frac{v_x}{4}D_x^{-1}\cdot w & +\frac{v_x}{4}D_x^{-1}\cdot w & -\frac{v_x}{4}D_x^{-1}\cdot w\\
\frac{w}{4}(u+v+w)+\frac{3vw}{2} & \frac{w}{4}(u+v+w)+\frac{3uw}{2} & -\frac{w^2}{4}+\frac{3}{4}(uw+vw)+uv\\
+\frac{w_x}{2}(u+v)D_x^{-1} & +\frac{w_x}{2}(u+v)D_x^{-1} & +\frac{w_x}{2}(u+v)D_x^{-1}\\
+\frac{w}{2}(u_x+v_x)D_x^{-1} & +\frac{w}{2}(u_x+v_x)D_x^{-1} & +\frac{w}{2}(u_x+v_x)D_x^{-1}\\
-\frac{w_x}{4}D_x^{-1}\cdot u+\frac{w_x}{4}D_x^{-1}\cdot v & +\frac{w_x}{4}D_x^{-1}\cdot u-\frac{w_x}{4}D_x^{-1}\cdot v & +\frac{w_x}{4}D_x^{-1}\cdot u+\frac{w_x}{4}D_x^{-1}\cdot v\\
+\frac{w_x}{4}D_x^{-1}\cdot w & +\frac{w_x}{4}D_x^{-1}\cdot w & -\frac{w_x}{4}D_x^{-1}\cdot w
\end{pmatrix}, \tag{A1}$$

$$\mathcal{R}=\begin{pmatrix}
-(uv+uw+vw) & -\frac{u}{4}(u+v+w) & -\frac{u}{4}(u+v+w) \\
+\frac{u}{4}(u+v+w) & -\frac{3uw}{2} & -\frac{3uv}{2} \\
+\frac{u}{4}(u_x-v_x-w_x)D_x^{-1} & +\frac{u}{4}(u_x-v_x-w_x)D_x^{-1} & +\frac{u}{4}(u_x-v_x-w_x)D_x^{-1} \\
-u(wv_x+vw_x)D_x^{-1}\cdot u^{-1} & -u(wv_x+vw_x)D_x^{-1}\cdot v^{-1} & -u(wv_x+vw_x)D_x^{-1}\cdot w^{-1} \\
-\frac{v}{4}(u+v+w) & -(uv+uw+vw) & -\frac{v}{4}(u+v+w) \\
-\frac{3vw}{2} & +\frac{v}{4}(u+v+w) & -\frac{3uv}{2} \\
+\frac{v}{4}(-u_x+v_x-w_x)D_x^{-1} & +\frac{v}{4}(-u_x+v_x-w_x)D_x^{-1} & +\frac{v}{4}(-u_x+v_x-w_x)D_x^{-1} \\
-v(wu_x+uw_x)D_x^{-1}\cdot u^{-1} & -v(wu_x+uw_x)D_x^{-1}\cdot v^{-1} & -v(wu_x+uw_x)D_x^{-1}\cdot w^{-1} \\
-\frac{w}{4}(u+v+w) & -\frac{w}{4}(u+v+w) & -(uv+uw+vw) \\
-\frac{3uw}{2} & -\frac{3vw}{2} & +\frac{w}{4}(u+v+w) \\
+\frac{w}{4}(-u_x-v_x+w_x)D_x^{-1} & +\frac{w}{4}(-u_x-v_x+w_x)D_x^{-1} & +\frac{w}{4}(-u_x-v_x+w_x)D_x^{-1} \\
-w(uv_x+vu_x)D_x^{-1}\cdot u^{-1} & -w(uv_x+vu_x)D_x^{-1}\cdot v^{-1} & -w(uv_x+vu_x)D_x^{-1}\cdot w^{-1}
\end{pmatrix}. \tag{A2}$$

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The q-Laplace operator and q-harmonic polynomials on the quantum vector space

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The aim of this paper is to study q-harmonic polynomials on the quantum vector space generated by q-commuting elements $x_1, x_2, \ldots, x_n$. They are defined as solutions of the equation $\Delta_q p = 0$, where p is a polynomial in $x_1, x_2, \ldots, x_n$ and the q-Laplace operator Δ_q is determined in terms of q-derivatives. The projector $H_m : \mathcal{A}_m \to \mathcal{H}_m$ is constructed, where $\mathcal{A}_m$ and $\mathcal{H}_m$ are the spaces of homogeneous (of degree m) polynomials and q-harmonic polynomials, respectively. By using these projectors, a q-analog of classical associated spherical harmonics is constructed. They constitute an orthonormal basis of $\mathcal{H}_m$. A q-analog of separation of variables is given. Representations of the nonstandard q-deformed algebra $U_q'(\mathrm{so}_n)$ [which plays the role of the rotation group $\mathrm{SO}(n)$ in the case of classical harmonic polynomials] on the spaces $\mathcal{H}_m$ are explicitly constructed. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1343092]

I. INTRODUCTION

The Laplace operator, harmonic polynomials, and related separations of variables are of a great importance for physics and mathematics. They are closely related to the rotation groups $\mathrm{SO}(n)$ and to its subgroups (see, e.g., Ref. 1, Chap. 10).

Harmonic polynomials are defined by the equation $\Delta p = 0$, where Δ is the Laplace operator and p belongs to the space $\mathcal{R}$ of polynomials on the Euclidean space $E_n \sim \mathbb{R}^n$. The space $\mathcal{H}$ of all harmonic polynomials on E_n decomposes as a direct sum of the subspaces $\mathcal{H}_m$ of homogeneous harmonic polynomials of degree m: $\mathcal{H} = \oplus_{m=0}^{\infty} \mathcal{H}_m$. The Laplace operator Δ on the n-dimensional Euclidean (vector) space E_n commutes with the natural action of the rotation group $\mathrm{SO}(n)$ on this space. This means that the subspaces $\mathcal{H}_m$ are invariant with respect to $\mathrm{SO}(n)$. The irreducible representation T_m of the group $\mathrm{SO}(n)$ with highest weight $(m,0,\ldots,0)$ is realized on $\mathcal{H}_m$.

The Laplace operator Δ permits separation of variables on the space $\mathcal{H}_m$. In other words, there exist different coordinate systems (spherical, polyspherical, etc.) on $E_n \sim \mathbb{R}^n$ and for each of them it is possible to find the corresponding basis of the space of solutions of the equation $\Delta p = 0$ consisting of products of functions depending on separated variables. To different coordinate systems there correspond different separations of variables. From the other side, to different coordinate systems there correspond different chains of subgroups of the group $\mathrm{SO}(n)$ (see Ref. 1, Chap. 10, for details of this correspondence). The basis of the space $\mathcal{H}_m$ in separated variables, e.g., in spherical coordinates, consists of products of certain Gegenbauer polynomials multiplied by r^m, where r is the radius. These polynomials (considered only on the sphere S^{n-1}) are matrix elements of the class 1 [with respect to the subgroup $\mathrm{SO}(n-1)$] irreducible representations T_m of $\mathrm{SO}(n)$ belonging to the zero column. The basis of $\mathcal{H}_m$ in polyspherical separated variables consists of products of Jacobi polynomials multiplied by r^m. Considered on S^{n-1}, these polynomials are zero column matrix elements of the representation T_m with respect to the subgroup $\mathrm{SO}(p) \times \mathrm{SO}(n-p)$ for a certain value of p (see Ref. 1, Sec. 10.2).

Many new directions of mathematical physics are related to quantum groups and noncommutative geometry. It is natural to generalize the above-described theory to noncommutative spaces.

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Such generalizations can be of a great importance for further development of some branches of mathematical and theoretical physics related to noncommutative geometry.

The aim of this paper is to construct a q-deformation of the above-described classical theory. In the q-case, instead of the Euclidean space we take the quantum vector space. It is defined in terms of the associative algebra $\mathcal{A}$ generated by the elements $x_1, x_2, \ldots, x_n$, satisfying the defining relations $x_i x_j = q x_j x_i$ for $i < j$. These elements play the role of Cartesian coordinates of E_n.

The q-Laplace operator Δ_q on $\mathcal{A}$ is defined in terms of q-derivatives [see formula (12)]. There exists no quantum group G_q which would relate to Δ_q as the rotation group $\mathrm{SO}(n)$ relates to the classical Laplace operator. For this reason, we involve into the theory a nonstandard q-deformation of the universal enveloping algebra $U(\mathrm{so}_n)$ of the Lie algebra so_n. This q-deformed associative algebra [we denote it by $U'_q(\mathrm{so}_n)$] is obtained by deformation of the defining relations for the elements $I'_{i,i-1} = E_{i,i-1} - E_{i-1,i}$, $i = 2,3,\ldots,n$, of $U(\mathrm{so}_n)$, where E_{ks} are the $n \times n$ matrices with entries $(E_{ks})_{ij} = \delta_{ki}\delta_{sj}$. The algebra $U'_q(\mathrm{so}_n)$ was constructed in Ref. 2. (It was shown in Ref. 3 that this algebra is related to the algebra of observables for quantum gravity constructed in Ref. 4.) The algebra $U'_q(\mathrm{so}_n)$ replaces the group $\mathrm{SO}(n)$ for the q-Laplace operator.

q-harmonic polynomials on the quantum vector space are defined as elements p of $\mathcal{A}$ (that is, polynomials in $x_1, x_2, \ldots, x_n$) for which $\Delta_q p = 0$. By using the algebra $U'_q(\mathrm{so}_n)$ (instead of the rotation group $\mathrm{SO}(n)$ in the classical case) we construct for q-harmonic polynomials a theory similar to the theory for classical harmonic polynomials described previously. Namely, we construct projectors $H_m : \mathcal{A}_m \to \mathcal{H}_m$, where $\mathcal{A}_m$ and $\mathcal{H}_m$ are the subspaces of homogeneous (of degree m) polynomials in $\mathcal{A}$ and in the space $\mathcal{H}$ of all q-harmonic polynomials from $\mathcal{A}$, respectively. Using these projectors we construct in $\mathcal{H}_m$ a q-analog of associated spherical harmonics with respect to the subalgebra $U'_q(\mathrm{so}_{n-1})$. They constitute an orthonormal basis of the space $\mathcal{H}_m$ corresponding to the chain of the subalgebras $U'_q(\mathrm{so}_n) \supset U'_q(\mathrm{so}_{n-1}) \supset U'_q(\mathrm{so}_{n-2}) \supset \cdots \supset U'_q(\mathrm{so}_2)$. Here we obtain a q-analog of the spherical separated coordinates. We construct explicitly the representation T_m of the algebra $U'_q(\mathrm{so}_n)$ on the space $\mathcal{H}_m$ and identify it with one of the representations of $U'_q(\mathrm{so}_n)$ known from literature. It is a class 1 [with respect to the subalgebra $U'_q(\mathrm{so}_{n-1})$] irreducible representation. Then we construct a q-analog of associated spherical harmonics with respect to the subalgebra $U'_q(\mathrm{so}_p) \times U'_q(\mathrm{so}_{n-p})$, where $1 < p < n-1$. Again, these harmonics constitute a basis of $\mathcal{H}_m$ corresponding to the separation of variables related to this subalgebra. We explicitly construct the representation T_m of $U'_q(\mathrm{so}_n)$ in this basis.

Our constructions use essentially the results of Ref. 5, where the operator Δ_q and the spaces $\mathcal{H}_m$ were defined.

Everywhere in the following we suppose that q is not a root of unity.

II. THE q-DEFORMED ALGEBRA $U'_q(\mathrm{so}_n)$

There exist the well known Drinfeld–Jimbo quantum algebras $U_q(\mathrm{so}_n)$ corresponding to the Lie algebras of the types B_l and D_l. However, they are not satisfactory from the point of view of some problems in quantum physics and representation theory. In particular, the reductions $U_q(\mathrm{so}_n) \supset U_q(\mathrm{so}_{n-1})$ and the embedding $U_q(\mathrm{so}_n) \subset U_q(\mathrm{sl}_n)$ are not allowed. For this reason, an analog of the Gel'fand–Tsetlin bases for finite-dimensional irreducible representations of $U_q(\mathrm{so}_n)$ does not exists. To be able to exploit reductions of such types, we have to consider q-deformations of the universal enveloping algebra $U(\mathrm{so}_n)$ of the Lie algebra so_n defined in terms of the generators $I_{k,k-1} = E_{k,k-1} - E_{k-1,k}$ [where E_{is} is the matrix with entries $(E_{is})_{rt} = \delta_{ir}\delta_{st}$] rather than by means of Cartan subalgebras and root elements. To construct such deformations we have to deform trilinear relations for elements $I_{k,k-1}$ instead of Serre's relations (as in the case of Drinfeld–Jimbo quantum algebras). As a result, we obtain the associative algebra which is denoted as $U'_q(\mathrm{so}_n)$.

This q-deformation was first constructed in Ref. 2. It permits the reduction $U'_q(\mathrm{so}_{n-1}) \subset U'_q(\mathrm{so}_n)$. Moreover, this q-deformed algebra $U'_q(\mathrm{so}_n)$ can be embedded into the Drinfeld–Jimbo algebra $U_q(\mathrm{sl}_n)$ (see Ref. 6). As a disadvantage of the algebra $U'_q(\mathrm{so}_n)$ we have

to mention difficulties with a Hopf algebra structure. Nevertheless, $U_q'(\mathrm{so}_n)$ turns out to be a coideal in $U_q(\mathrm{sl}_n)$.

The q-deformed algebra $U_q'(\mathrm{so}_n)$ is defined as the associative algebra (with a unity) generated by the elements $I_{i,i-1}$, $i=2,3,\ldots,n$, satisfying the defining relations

$$I_{i,i-1}I_{i-1,i-2}^2-(q+q^{-1})I_{i-1,i-2}I_{i,i-1}I_{i-1,i-2}+I_{i-1,i-2}^2I_{i,i-1}=-I_{i,i-1}, \tag{1}$$

$$I_{i,i-1}^2I_{i-1,i-2}-(q+q^{-1})I_{i,i-1}I_{i-1,i-2}I_{i,i-1}+I_{i-1,i-2}I_{i,i-1}^2=-I_{i-1,i-2}, \tag{2}$$

$$[I_{i,i-1},I_{j,j-1}]=0, \quad |i-j|>1, \tag{3}$$

where $[\cdot,\cdot]$ denotes the usual commutator. In the limit $q\to 1$, formulas (1)–(3) give the relations defining the universal enveloping algebra $U(\mathrm{so}_n)$ (see Ref. 7). Note also that relations (1) and (2) principally differ from the q-deformed Serre relations in the approach of Drinfeld in Ref. 8 and Jimbo in Ref. 9 (see also Ref. 10) to quantum algebras $U_q(\mathrm{so}_n)$ by the presence of a nonzero right-hand side. It is evident from (1) to (3) that we can construct for $U_q'(\mathrm{so}_n)$ the chain of subalgebras

$$U_q'(\mathrm{so}_n)\supset U_q'(\mathrm{so}_{n-1})\supset\cdots\supset U_q'(\mathrm{so}_3)\supset U_q'(\mathrm{so}_2),$$

where the subalgebras $U_q'(\mathrm{so}_k)$ are generated by the elements $I_{i,i-1}$, $i=2,3,\ldots,k$, respectively. Recall that in the standard Drinfeld–Jimbo approach to the definition of quantum algebras, the algebras $U_q(\mathrm{so}_{2m})$ and the algebras $U_q(\mathrm{so}_{2m+1})$ are distinct series of quantum algebras which are constructed independently of each other.

The algebra $U_q'(\mathrm{so}_n)$ can be embedded into the Drinfeld–Jimbo quantum algebra $U_q(\mathrm{sl}_n)$. The last algebra is generated by the elements $k_i\equiv q^{h_i}$, $k_i^{-1}\equiv q^{-h_i}$, e_i, f_i, $i=1,2,\ldots,n-1$, satisfying the relations $k_ik_i^{-1}=k_i^{-1}k_i=1$, $k_ik_j=k_jk_i$ and

$$k_ie_jk_i^{-1}=q^{a_{ij}}e_j, \quad k_if_jk_i^{-1}=q^{-a_{ij}}f_j,$$

$$[e_i,f_j]\equiv e_if_j-f_je_i=\delta_{ij}\frac{k_i-k_i^{-1}}{q-q^{-1}},$$

$$e_i^2e_{i\pm1}-(q+q^{-1})e_ie_{i\pm1}e_i+e_{i\pm1}e_i^2=0,$$

$$f_i^2f_{i\pm1}-(q+q^{-1})f_if_{i\pm1}f_i+f_{i\pm1}f_i^2=0,$$

$$[e_i,e_j]=[f_i,f_j]=0, \quad |i-j|>1,$$

where $a_{ii}=2$, $a_{i,i\pm1}=-1$ and $a_{ij}=0$ for $|i-j|>1$. Then there exists a unique homomorphism

$$\varphi: U_q'(\mathrm{so}_n)\to U_q(\mathrm{sl}_n) \tag{4}$$

such that $\varphi(I_{i+1,i})=f_i-qq^{-h_i}e_i$ (see Ref. 6). Moreover, this homomorphism is an embedding, that is, a one-to-one mapping (see Refs. 5 and 11).

III. CLASS 1 REPRESENTATIONS OF $U_q'(\mathrm{so}_n)$

We shall use the term ''a class 1 representation'' for those finite-dimensional irreducible representations of $U_q'(\mathrm{so}_n)$ which contain the trivial representation of the subalgebra $U_q'(\mathrm{so}_{n-1})$. In the case of the algebra $U_q'(\mathrm{so}_3)$, class 1 representations are defined with respect to the commutative subalgebra $U_q'(\mathrm{so}_2)$, generated by one element I_{21}.

The algebra $U_q'(\mathrm{so}_n)$ has two types of finite-dimensional irreducible representations (see Ref. 12): representations of the classical type (at $q\to 1$ they turn into corresponding irreducible repre-

sentations of the Lie algebra so_n) and representations of the nonclassical type (they have no classical analog). It is seen from the formulas for representations of the nonclassical type that none of these representations can be of class 1.

Analyzing the representations of the classical type (formulas for these representations see, e.g., those in Ref. 12) we see that like the classical case, class 1 representations are characterized by ''a highest weight'' $(m_n,0,\ldots,0)$, where m_n is a non-negative integer. These representations are denoted R_{m_n}. Under restriction onto the subalgebra $U_q'(\mathrm{so}_{n-1})$ the representation R_{m_n} decomposes into those and only those class 1 representations $R_{m_{n-1}}$ of this subalgebra for which

$$m_n \geqslant m_{n-1} \geqslant 0 \quad \text{if} \quad n>3, \quad -m_3 \leqslant m_2 \leqslant m_3 \quad \text{if} \quad n=3.$$

The orthonormal basis obtained by restriction of class 1 representations T_{m_n} onto the subalgebras $U_q'(\mathrm{so}_k)$, $k=n-1,n-2,\ldots,2$, is nothing but a q-analog of the Gel'fand–Tsetlin basis. We denote the Gel'fand–Tsetlin basis elements of the representation space of R_{m_n} by

$$|m_n,m_{n-1},m_{n-2},\ldots,m_3,m_2\rangle,$$

where m_k characterizes the set $(m_k,0,\ldots,0)$ of integers giving the class 1 representation R_{m_k} of $U_q'(\mathrm{so}_k)$. With respect to this basis the operators $R_{m_n}(I_{k,k-1})$ of the representation R_{m_n} of $U_q'(\mathrm{so}_n)$ are given by

$$R_{m_n}(I_{21})|m_n,m_{n-1},\ldots,m_2\rangle = i[m_2]|m_n,m_{n-1},\ldots,m_2\rangle, \tag{5}$$

$$\begin{aligned} R_{m_n}(I_{k,k-1})|m_n,m_{n-1},\ldots,m_2\rangle = {} & ([m_k+m_{k-1}+k-2][m_k-m_{k-1}])^{1/2} \\ & \times A(m_{k-1})|m_n,\ldots,m_k,m_{k-1}+1,m_{k-2},\ldots m_2\rangle \\ & -([m_k+m_{k-1}+k-3][m_k-m_{k-1}+1])^{1/2} \\ & \times A(m_{k-1}-1)|m_n,\ldots,m_k,m_{k-1}-1,m_{k-2},\ldots,m_2\rangle, \end{aligned} \tag{6}$$

where $n \geqslant k \geqslant 3$, the symbol $[m] \equiv [m]_q$ denotes a q-number defined as

$$[m]=\frac{q^m-q^{-m}}{q-q^{-1}},$$

and

$$A(m_{k-1})=\left(\frac{[m_{k-1}+m_{k-2}+k-3][m_{k-1}-m_{k-2}+1]}{[2m_{k-1}+k-3][2m_{k-1}+k-1]}\right)^{1/2}.$$

Note that in the case $k=3$ we have to put $m_1=0$ in formula (6); then for $A(m_2)$ we have the expression $([m_2][m_2+1]/[2m_2][2m_2+2])^{1/2}$.

IV. REPRESENTATIONS ON THE QUANTUM VECTOR SPACE

Let $\mathcal{A} \equiv \mathbb{C}[x_1,x_2,\ldots,x_n]$ be the associative algebra (with unity) generated by elements $x_1,x_2,\ldots,x_n$ satisfying the defining relations $x_ix_j=qx_jx_i$, $i<j$. This algebra is called the algebra of functions on the n-dimensional quantum vector space. Elements of $\mathcal{A}$ are called polynomials on this quantum vector space and are denoted by $p \equiv p(x_1,x_2,\ldots,x_n) \equiv p(\mathbf{x})$.

We define on $\mathcal{A}$ the q-differentiations ∂_i and ∂_i' which are linear operators acting as $\partial_i p = \partial_i' p = 0$ on monomials p not containing x_i and as

$$\partial_i = \check{x}_i^{-1}\frac{\gamma_i-\gamma_i^{-1}}{q-q^{-1}}, \quad \partial_i' = \hat{x}_i^{-1}\frac{\gamma_i-\gamma_i^{-1}}{q-q^{-1}} \tag{7}$$

on monomials containing x_i, where $\hat{x}_i$ and $\check{x}_i$ are the operators of left and right multiplication by x_i, respectively, and

$$\gamma_i p(x_1,\dots,x_n)=p(x_1,\dots,x_{i-1},qx_i,x_{i+1},\dots,x_n).$$

$$\gamma_i^{-1} p(x_1,\dots,x_n)=p(x_1,\dots,x_{i-1},q^{-1}x_i,x_{i+1},\dots,x_n).$$

We have $\partial_i\hat{x}_j=\hat{x}_j\partial_i$, $i\neq j$, and

$$\partial_i\partial_j=q^{-1}\partial_j\partial_i, \quad \partial_i\check{x}_j=q\check{x}_j\partial_i, \quad i<j,$$

$$\gamma_i\hat{x}_j=q^{\delta_{ij}}\hat{x}_j\gamma_i, \quad \gamma_i\partial_j=q^{-\delta_{ij}}\partial_j\gamma_i.$$

It is possible to introduce a q-analog of the Fischer scalar product on $\mathcal{A}$ (see Ref. 5). It is defined by

$$\langle p_1,p_2\rangle=p_1(\partial_1',\dots,\partial_n')p_2^*|_{x=0}, \tag{8}$$

where p_2^* is the polynomial p_2 in which numerical coefficients are replaced by complex conjugate ones, $p_1(\partial_1',\dots,\partial_n')$ means the q-differential operator obtained from a polynomial p by replacement of x_i by ∂_i', $i=1,2,\dots,n$, and the symbol $p|_{x=0}$ means a constant term of the polynomial p.

We can define an action of the quantum algebra $U_q(\mathrm{sl}_n)$ on the space $\mathcal{A}$ determining its representation on $\mathcal{A}$. This action is given by

$$\rho(k_i)=\gamma_i\gamma_{i+1}^{-1}, \quad \rho(e_i)=\check{x}_i\gamma_i\partial_{i+1}, \quad \rho(f_i)=\check{x}_{i+1}\gamma_i^{-1}\partial_i. \tag{9}$$

The action ρ and formulas (4) lead to the representation $T=\rho\circ\varphi$ of $U_q'(\mathrm{so}_n)$ on $\mathcal{A}$. We introduce the notation $\theta_j=T(I_{j+1,j})$, $i=1,2,\dots,n-1$. Then it is easy to calculate that

$$\theta_j=\check{x}_{j+1}\gamma_j^{-1}\partial_j-\check{x}_j\gamma_{j+1}\partial_{j+1} \tag{10}$$

(see also Ref. 5).

The representation T of $U_q'(\mathrm{so}_n)$ is reducible. It is easy to check by using the explicit form (10) of the operators θ_j that the subspaces $\mathcal{A}_m\in\mathcal{A}$ of homogeneous polynomials of degrees m are invariant with respect to this representation. Clearly,

$$\mathcal{A}=\bigoplus_{m=0}^{\infty}\mathcal{A}_m.$$

We denote the restriction of the representation T to the subspace $\mathcal{A}_m$ by $T^{(m)}$.

The representation ρ of $U_q(\mathrm{sl}_n)$ on the space $\mathcal{A}$ is also reducible, and the subspaces $\mathcal{A}_m$ are invariant for this representation. We denote the restriction of the representation ρ of $U_q(\mathrm{sl}_n)$ to the space $\mathcal{A}_m$ by ρ_m. A direct calculation shows that the representation ρ_m is irreducible and has the highest weight $(m,0,\dots,0)$. The monomials $x_1^{m_1}x_2^{m_2}\cdots x_n^{m_n}$, $m_1+m_2+\cdots+m_n=m$, are weight vectors of this representation. The highest weight vector coincides with x_1^m.

In general, the representations $T^{(m)}$ of $U_q'(\mathrm{so}_n)$ on the spaces $\mathcal{A}_m$ are reducible. It is checked by a direct computation that the element

$$Q=x_1^2+q^{-1}x_2^2+\cdots+q^{-n+1}x_n^2\in\mathcal{A}_2 \tag{11}$$

is invariant with respect to the representation $T^{(2)}$ (and hence with respect to the representation T), that is, $T^{(2)}(I_{k,k-1})Q=0$ for $k=2,3,\dots,n$. Similarly, the element $Q^k\in\mathcal{A}_{2k}$ is invariant with respect to the representation $T^{(2k)}$.

To the element (11) there corresponds the operator

$$\hat{Q}=\hat{x}_1^2+q^{-1}\hat{x}_2^2+\cdots+q^{-n+1}\hat{x}_n^2$$

on $\mathcal{A}$ which commutes with operators of the representation T. We also consider on $\mathcal{A}$ the operator

$$\Delta_q\equiv\Delta=q^{n-1}\partial_1^2+q^{n-2}\partial_2^2+\cdots+\partial_n^2. \tag{12}$$

It is called the *q-Laplace operator* on the quantum vector space. It is clear that $\Delta:\mathcal{A}_m\to\mathcal{A}_{m-2}$.

The following relations are proved by direct calculations (see Ref. 5):

$$\Delta\hat{Q}^k-\hat{Q}^k\Delta=\hat{Q}^{k-1}[2k]\{q^{2k+n-2}\gamma^2\}, \tag{13}$$

$$\Delta(Q^k)=Q^{k-1}[2k][2k+n-2], \tag{14}$$

where $[r]$ are q-numbers and

$$\{a\}=\frac{a-a^{-1}}{q-q^{-1}}.$$

We also have

$$\hat{Q}^*=q^{-n+1}\Delta,\quad \Delta^*=q^{n-1}\hat{Q},\quad \theta_j^*=-\theta_j,$$

where an asterisk means Hermitian conjugation with respect to the scalar product (8) (see Ref. 5).

A polynomial $p\in\mathcal{A}$ is called *q-harmonic* if $\Delta p=0$. The linear subspace of $\mathcal{A}$ consisting of all q-harmonic polynomials is denoted by $\mathcal{H}$. Let $\mathcal{H}_m=\mathcal{A}_m\cap\mathcal{H}$. Then

$$\mathcal{H}=\bigoplus_{m=0}^{\infty}\mathcal{H}_m.$$

Similar to the classical case, the space $\mathcal{A}_m$ can be represented in the form of the direct sum (see Ref. 5)

$$\mathcal{A}_m=\mathcal{H}_m\oplus Q\mathcal{A}_{m-2}. \tag{15}$$

This decomposition has the following consequence:

$$\mathcal{A}_m=\bigoplus_{0\leqslant 2j\leqslant m}Q^j\mathcal{H}_{m-2j} \tag{16}$$

(the summation here is over $j=0,1,2,\ldots,\lfloor m/2\rfloor$, where $\lfloor m/2\rfloor$ is the integral part of $m/2$). The following proposition is proved in Ref. 5:

Proposition 1: The q-Laplace operator Δ commutes with all operators of the representation T of $U_q'(\mathrm{so_n})$.

It follows from Proposition 1 that the subspace $\mathcal{H}_m$ is invariant with respect to the representation $T^{(m)}$. We denote the restriction of this representation to $\mathcal{H}_m$ by T_m. Since Q is invariant with respect to $U_q'(\mathrm{so}_n)$, it follows from (16) that

$$T^{(m)}=\bigoplus_{0\leqslant 2j\leqslant m}T_{m-2j}. \tag{17}$$

In the following we identify the representations T_{m-2j} with the corresponding representations of Sec. III.

Proposition 2: If $h_m(\mathbf{x})\in\mathcal{H}_m$, then $\tilde{h}_{m-1}(\mathbf{x}):=\gamma_n^{-1}\partial_n h_m(\mathbf{x})\in\mathcal{H}_{m-1}$ and

$$\hat{h}_{m+1}(\mathbf{x}) := h_m(\mathbf{x})x_n - \frac{Q\gamma_n^{-1}\partial_n h_m(\mathbf{x})}{[n+2m-2]} \in \mathcal{H}_{m+1}. \tag{18}$$

Proof: Since $\tilde{h}_{m-1} \in \mathcal{A}_{m-1}$ and $\hat{h}_{m+1} \in \mathcal{A}_{m+1}$, it is enough to prove that $\Delta\tilde{h}_{m-1}=0$ and $\Delta\hat{h}_{m+1}=0$. The first relation follows from the equalities

$$\Delta(\gamma_n^{-1}\partial_n) = (\partial_n^2 + q\Delta_{(n-1)})\gamma_n^{-1}\partial_n = q^{-2}\gamma_n^{-1}\partial_n(\partial_n^2 + q\Delta_{(n-1)}) = q^{-2}(\gamma_n^{-1}\partial_n)\Delta,$$

where $\Delta_{(n-1)}) = q^{n-2}\partial_1^2 + q^{n-3}\partial_2^2 + \cdots + \partial_{n-1}^2$ is the q-Laplace operator for the elements $x_1, x_2, \ldots, x_{n-1}$. In order to prove the relation $\Delta\hat{h}_{m+1}=0$ we first note that for $p \in \mathcal{A}$ one has

$$\begin{aligned}
\partial_n^2(p(\mathbf{x})x_n) &= \partial_n\left(\left(\frac{\gamma_n - \gamma_n^{-1}}{q-q^{-1}}p(\mathbf{x})x_n\right)x_n^{-1}\right) = \partial_n\left(\frac{q\gamma_n - q^{-1}\gamma_n^{-1}}{q-q^{-1}}p(\mathbf{x})x_n x_n^{-1}\right) \\
&= \frac{q^2\gamma_n - q^{-2}\gamma_n^{-1}}{q-q^{-1}}\partial_n p(\mathbf{x}) = \left(q^2\frac{\gamma_n - \gamma_n^{-1}}{q-q^{-1}} + \frac{q^2-q^{-2}}{q-q^{-1}}\gamma_n^{-1}\right)\partial_n p(\mathbf{x}) \\
&= q^2(\partial_n^2 p(\mathbf{x}))x_n + [2]\gamma_n^{-1}\partial_n p(\mathbf{x}).
\end{aligned}$$

Hence,

$$\begin{aligned}
\Delta(h_m(\mathbf{x})x_n) &= (\partial_n^2 + q\Delta_{(n-1)})(h_m(\mathbf{x})x_n) = \partial_n^2(h_m(\mathbf{x})x_n) + q^3(\Delta_{(n-1)}h_m(\mathbf{x}))x_n \\
&= q^2(\Delta h_m(\mathbf{x}))x_n + [2]\gamma_n^{-1}\partial_n h_m(\mathbf{x}) = [2]\tilde{h}_{m-1}(\mathbf{x}).
\end{aligned} \tag{19}$$

Using relation (13) at $k=1$ we also have

$$\Delta(Q\gamma_n^{-1}\partial_n h_m(\mathbf{x})) = Q\Delta\tilde{h}_{m-1}(\mathbf{x}) + [2][n+2m-2]\tilde{h}_{m-1}(\mathbf{x}). \tag{20}$$

Now the relation $\Delta\hat{h}_{m+1}=0$ follows from (19) and (20). Proposition is proved.

It is shown in Ref. 5 that $\mathcal{A} \simeq \mathbb{C}[Q]\otimes\mathcal{H}$. This decomposition is a q-analog of the theorem on separation of variables for Lie groups in an abstract form (see, e.g., Ref. 13). We have

$$\mathcal{A} \simeq \mathbb{C}[Q]\otimes\mathcal{H} \simeq \mathbb{C}[Q]\otimes\bigoplus_{m\geqslant 0}\mathcal{H}_m = \bigoplus_{m\geqslant 0}(\mathbb{C}[Q]\otimes\mathcal{H}_m). \tag{21}$$

If $h_m(\mathbf{x}) \in \mathcal{H}_m$ and $h_s'(\mathbf{x}) \in \mathcal{H}_s$, then [since $\hat{Q}^* = q^{-n+1}\Delta$ with respect to the scalar product (8)] we have

$$\langle Q^k h_m, Q^l h_s'\rangle = q^{k(-n+1)}\langle h_m, \Delta^k Q^l h_s'\rangle.$$

Using (13) we derive that $\Delta(Q^l h_s') = Q^{l-1}[2l][2l+n+2s-2]h_s'$. Applying repeatedly this formula we obtain from the previous formula that

$$\langle Q^k h_m, Q^l h_s'\rangle = \delta_{kl}q^{k(-n+1)}[2l]!!\frac{[2k+n+2s-2]!!}{[n+2s-2]!!}\langle h_m, h_s'\rangle. \tag{22}$$

Remark: In an analogy with the classical case, we may consider the scalar product (8) as an integral of the function $p_1 p_2^*$. Then the formula (22) means a fulfillment of ''integration'' with respect to the q-radial part. Like in the classical case, the scalar product $\langle h_m, h_s'\rangle$ can be treated as ''integration'' over q-spherical coordinates for q-harmonic polynomials.

A direct calculation shows that

$$\langle Q^l, Q^s\rangle = q^{l(1-n)}\langle 1, \Delta^l Q^s\rangle = \delta_{ls}q^{l(-n+1)}\frac{[2l]!![2l+n-2]!!}{[n-2]!!}. \tag{23}$$

V. THE PROJECTION $\mathcal{A}_m \to \mathcal{H}_m$

The decomposition (15) is orthogonal with respect to the scalar product (8). Let us construct the projector $H_m : \mathcal{A}_m = \mathcal{H}_m \oplus Q\mathcal{A}_{m-2} \to \mathcal{H}_m$. We present this projector in the form

$$H_m p = \sum_{k=0}^{\lfloor m/2 \rfloor} \alpha_k \hat{Q}^k \Delta^k p, \quad \alpha_k \in \mathbb{C}, \quad p \in \mathcal{A}_m, \tag{24}$$

where $\lfloor m/2 \rfloor$ means the integral part of $m/2$. We have to calculate values of the coefficients α_k. In order to do this, we act by the q-Laplace operator Δ upon both parts of (24) and use the relation (13). Under this action, the left-hand side vanishes. Equating the right-hand side to 0, we derive a recurrence relation for α_k which gives

$$\begin{aligned} \alpha_k &= \frac{(-1)^k}{[2k]!![n+2m-4][n+2m-6]\cdots[n+2m-2k-2]} \\ &= \frac{(-1)^k [n+2m-2k-4]!!}{[2k]!![n+2m-4]!!}, \end{aligned} \tag{25}$$

where $[s]!! = [s][s-2][s-4]\cdots[2]$ (or $[1]$) and $[0]!! = 1$.

Note that the coefficients α_k are determined by the recurrence relation uniquely up to a constant. In (25) we chose this constant in such a way that $H_m p = p$ for $p \in \mathcal{H}_m$. This means that $H_m^2 = H_m$.

Proposition 3: (a) The operator H_m commutes with the operators θ_j of the representation $T^{(m)}$ of $U_q'(\mathrm{so_n})$. (b) Considering the scalar product (8) on the space $\mathcal{A}_m$ we have $H^* = H$.

Proof: The assertion (a) follows from the fact that θ_j commutes with $\hat{Q}$ and Δ. The assertion (b) is a consequence of the equalities $\hat{Q}^* = q^{-n+1}\Delta$ and $\Delta^* = q^{n-1}\hat{Q}$.

Let us show how to construct by using the operator H_m a zonal polynomial [that is an invariant element with respect to the subalgebra $U_q'(\mathrm{so}_{n-1})$] in the space $\mathcal{H}_m$. In order to do this, we have to take a polynomial $p \in \mathcal{A}_m$ invariant with respect to $U_q'(\mathrm{so}_{n-1})$ and to act upon it by the operator H_m. Since the projector H_m commutes with the action of $U_q'(\mathrm{so}_{n-1})$, a polynomial obtained in this way is a zonal polynomial. Clearly, the polynomial $p(x) = x_n^m$ belongs to $\mathcal{A}_m$ and is invariant under the action of $U_q'(\mathrm{so}_{n-1})$. We have

$$\begin{aligned} \varphi_m' &:= H_m x_n^m = \sum_{k=0}^{\lfloor m/2 \rfloor} \alpha_k \hat{Q}^k \Delta^k x_n^m = \sum_{k=0}^{\lfloor m/2 \rfloor} \alpha_k \hat{Q}^k \partial_n^{2k} x_n^m \\ &= \sum_{k=0}^{\lfloor m/2 \rfloor} (-1)^k \frac{[m]![n+2m-2k-4]!!}{[m-2k]![2k]!![n-2m-4]!!} Q^k x_n^{m-2k}. \end{aligned} \tag{26}$$

Using the notation

$$(a;q)_s = (1-a)(1-qa)(1-q^2a)\cdots(1-q^{s-1}a),$$

we reduce the zonal polynomial (26) to the form

$$\varphi_m' = \sum_{k=0}^{\lfloor m/2 \rfloor} \frac{(q^{-2m};q^4)_k (q^{-2m+2};q^4)_k}{(q^4;q^4)_k (q^{-2n-4m+8};q^4)_k} q^{-k(n-5)} Q^k x_n^{m-2k}. \tag{27}$$

It concides with the formula for a zonal polynomial found by another method in Ref. 5.

VI. q-ANALOG OF ASSOCIATED SPHERICAL HARMONICS WITH RESPECT TO $U_q'(\mathrm{so}_{n-1})$

It is known (see Ref. 1, Chaps. 9 and 10) that in the space of classical homogeneous harmonic polynomials there exist different orthonormal bases. They correspond to different separations of variables. Each separation of variables corresponds to a certain chain of subgroups of the rotation group $\mathrm{SO}(n)$. We show in the following that a similar picture has place for spaces $\mathcal{H}_m$ of homogeneous q-harmonic polynomials.

In the classical case, the tree method distinguishes different separations of variables or, equivalently, different chains of subgroups of $\mathrm{SO}(n)$. The same tree method can be used for q-harmonic polynomials, but instead of chains of subgroups of $\mathrm{SO}(n)$ we have to take the corresponding chains of subalgebras of the algebra $U_q'(\mathrm{so}_n)$.

The aim of this section is to construct an orthonormal basis of the space $\mathcal{H}_m$ of homogeneous q-harmonic polynomials which corresponds to the chain

$$U_q'(\mathrm{so}_n)\supset U_q'(\mathrm{so}_{n-1})\supset\cdots\supset U_q'(\mathrm{so}_3)\supset U_q'(\mathrm{so}_2), \tag{28}$$

where $U_q'(\mathrm{so}_2)$ is the commutative subalgebra generated by the element I_{21}. This basis is a q-analog of the well-known set of associated spherical harmonics which are products of certain Gegenbauer polynomials (see, Ref. 1, Chap. 9).

Proposition 4: Let $h_s(\mathbf{x}')$ be a homogeneous harmonic polynomial of degree s in $\mathbf{x}'=(x_1,x_2,\ldots,x_{n-1})$. Then for $x_n^{m-s}h_s(\mathbf{x}')\in\mathcal{A}_m$ we have

$$H_m(x_n^{m-s}h_s(\mathbf{x}'))=\left(\sum_{k=0}^{\lfloor (m-s)/2\rfloor}\frac{(-1)^k q^{-2sk}[m-s]![2m+n-2k-4]!!}{[m-s-2k]![2k]!![2m+n-4]!!}Q^k x_n^{m-s-2k}\right)h_s(\mathbf{x}'). \tag{29}$$

Proof: Since

$$\Delta_{(n-1)}(x_n^{m-s}h_s(\mathbf{x}'))=x_n^{m-s}(\Delta_{(n-1)}h_s(\mathbf{x}'))=0,$$

where $\Delta_{(n-1)}$ is the q-Laplace operator for the elements $x_1,x_2,\ldots,x_{n-1}$, we have

$$\Delta(x_n^{m-s}h_s(\mathbf{x}'))=(q\Delta_{(n-1)}+\partial_n^2)(x_n^{m-s}h_s(\mathbf{x}'))=q^{-2s}[m-s][m-s-1]x_n^{m-s}h_s(\mathbf{x}').$$

Applying repeatedly the last relation to the right-hand side of the equality

$$H_m(x_n^{m-s}h_s(\mathbf{x}'))=\sum_{k=0}^{\lfloor m/2\rfloor}\alpha_k\hat{Q}^k\Delta_{(n)}^k(x_n^{m-s}h_s(\mathbf{x}'))$$

we derive the relation (29). The proposition is proved.

We denote by $\hat{t}_s^{n,m}(Q,x_n)$ the expression at $h_s(\mathbf{x}')$ on the right-hand side of (29):

$$\hat{t}_s^{n,m}(Q,x_n)=\sum_{k=0}^{\lfloor (m-s)/2\rfloor}\frac{(-1)^k q^{-2sk}[m-s]![2m+n-2k-4]!!}{[m-s-2k]![2k]!![2m+n-4]!!}Q^k x_n^{m-s-2k}. \tag{30}$$

In particular, we have $\hat{t}_0^{n,m}(Q,x_n)=\varphi_m'=H_m x_n^m$.

In order to construct an orthonormal basis of $\mathcal{H}_m$, we have to normalize expression (29). Let us first consider a normalization of φ_m'. We have

$$\langle\varphi_m',\varphi_m'\rangle=\langle H_m x_n^m,H_m x_n^m\rangle=\langle x_n^m,H_m^*H_m x_n^m\rangle=\langle x_n^m,H_m x_n^m\rangle=\langle x_n^m,\varphi_m'\rangle=c_m^{(0)}\langle x_n^m,x_n^m\rangle,$$

where $c_m^{(0)}$ is the coefficient at x_n^m in expression (27) for φ_m' [the last equality is due to the definition (8) of the scalar product]. We have

$$c_m^{(0)}=\sum_{k=0}^{\lfloor m/2\rfloor}\frac{(q^{-2m};q^4)_k(q^{-2m+2};q^4)_k}{(q^{-2n-4m+8};q^4)_k}\frac{q^{k(-2n+6)}}{(q^4;q^4)_k}$$
$$={}_2\varphi_1(q^{-2m},q^{-2m+2};q^{8-2n-4m};q^4,q^{-2n+6}).$$

This q-hypergeometric series can be summed by means of the formula

$${}_2\varphi_1(a,q^{-n};c;q,cq^n/a)=\frac{(c/a;q)_n}{(c;q)_n} \tag{31}$$

(see Ref. 14, Sec. 1.5). As a result, we derive that

$$c_m^{(0)}=\frac{(q^{-2(n+m-3)};q^4)_{m/2}}{(q^{-2(n+2m-4)};q^4)_{m/2}} \quad \text{if} \quad m-s \quad \text{is} \quad \text{even},$$

$$c_m^{(0)}=\frac{(q^{-2(n+m-4)};q^4)_{(m-1)/2}}{(q^{-2(n+2m-4)};q^4)_{(m-1)/2}} \quad \text{if} \quad m-s \quad \text{is} \quad \text{odd}.$$

Since $\langle x_n^m,x_n^m\rangle=(\partial_n')^n x_n^m=[n]!$, then the normalized zonal polynomial from $\mathcal{H}_m$ has a form

$$\varphi_m=(c_m^{(0)}[m]!)^{-1/2}\varphi_m'.$$

Now let τ_s^m denote expression (29). We similarly have

$$\langle\tau_s^m,\tau_s^m\rangle=\langle H_m(x_n^{m-s}h_s(\mathbf{x}')),H_m(x_n^{m-s}h_s(\mathbf{x}'))\rangle=\langle x_n^{m-s}h_s(\mathbf{x}'),\tau_s^m\rangle$$
$$=c_m^{(s)}\langle x_n^{m-s}h_s(\mathbf{x}'),x_n^{m-s}h_s(\mathbf{x}')\rangle=c_m^{(s)}q^{-s(m-s)}\langle h_s(\mathbf{x}')x_n^{m-s},x_n^{m-s}h_s(\mathbf{x}')\rangle$$
$$=c_m^{(s)}q^{-s(m-s)}[m-s]!\langle h_s(\mathbf{x}'),h_s(\mathbf{x}')\rangle,$$

where $c_m^{(s)}$ is the coefficient at x_n^{m-s} in expression (30) for $\hat{t}_s^{n,m}(Q,x_n)$. We obtain from (30) that

$$c_m^{(s)}=\sum_{k=0}^{\lfloor (m-s)/2\rfloor}\frac{(q^{-2(m-s)};q^4)_k(q^{-2(m-s)+2};q^4)_k}{(q^{-2n-4m+8};q^4)_k}\frac{q^{k(-2n-4s+6)}}{(q^4;q^4)_k}$$
$$={}_2\varphi_1(q^{2(s-m)},q^{2(s-m)+2};q^{8-2n-4m};q^4,q^{6-2n-4s}).$$

This q-hypergeometric series can be summed by means of formula (31) and we receive

$$c_m^{(s)}=\frac{(q^{2(-n-m-s+3)};q^4)_{(m-s)/2}}{(q^{2(-n-2m+4)};q^4)_{(m-s)/2}} \quad \text{if} \quad m-s \quad \text{is} \quad \text{even}, \tag{32}$$

$$c_m^{(s)}=\frac{(q^{2(-n-m-s+4)};q^4)_{(m-s-1)/2}}{(q^{2(-n-2m+4)};q^4)_{(m-s-1)/2}} \quad \text{if} \quad m-s \quad \text{is} \quad \text{odd}. \tag{33}$$

Instead of $\hat{t}_s^{n,m}(Q,x_n)$ we shall use the normalized expression

$$t_s^{n,m}(Q,x_n)=\frac{q^{s(m-s)/2}}{\sqrt{c_m^{(s)}[m-s]!}}\hat{t}_s^{n,m}(Q,x_n). \tag{34}$$

In order to construct an orthonormal basis of the space $\mathcal{H}_m$ in an explicit form, we take into account that

$$\langle t_s^{n,m}(Q,x_n)h_s(\mathbf{x}'),t_s^{n,m}(Q,x_n)h_s(\mathbf{x}')\rangle=\langle h_s(\mathbf{x}'),h_s(\mathbf{x}')\rangle.$$

We apply the previous reasoning of this section to homogeneous q-harmonic polynomials of $x_1,x_2,\ldots,x_{n-1}$. As a result, we obtain q-harmonic polynomials of the form

$$t_s^{n,m}(Q,x_n)t_r^{n-1,s}(Q_{n-1},x_{n-1})h_r(\mathbf{x}''), \quad s=0,1,2,\ldots,m, \quad r=0,1,2,\ldots,s,$$

where

$$Q_{n-1}=x_1^2+q^{-1}x_2^2+\cdots+q^{-n+2}x_{n-1}^2, \quad \mathbf{x}''=(x_1,x_2,\ldots,x_{n-2}),$$

$h_r(\mathbf{x}'')$ are elements of the space of homogeneous q-harmonic polynomials of degree r in $x_1,x_2,\ldots,x_{n-2}$, and $t_r^{n-1,s}(Q_{n-1},x_{n-1})$ is defined by (30) and (34).

Continuing this procedure, we obtain the normalized polynomials of $\mathcal{H}_m$ of the form

$$\begin{aligned}\Xi_{\mathbf{m}}(\mathbf{x})&\equiv\Xi_{m,m_{n-1},m_{n-2},\ldots,m_2}(\mathbf{x})\\&=t_{m_{n-1}}^{n,m}(Q,x_n)t_{m_{n-2}}^{n-1,m_{n-1}}(Q_{n-1},x_{n-1})\cdots t_{m_2}^{3,m_3}(Q_3,x_3)t^{2,m_2}(x_1,x_2),\end{aligned} \tag{35}$$

$$m\geqslant m_{n-1}\geqslant m_{n-2}\geqslant\cdots\geqslant m_3\geqslant|m_2|, \tag{36}$$

where the polynomials $t^{2,m_2}(x_1,x_2)$ are determined in the following way. A complete set of linearly independent harmonic polynomials in x_1 and x_2 coincides with

$$z^{(0)}\equiv 1, \quad z^{(s)}=(ix_1+x_2)(ix_1+qx_2)\cdots(ix_1+q^{s-1}x_2), \quad s>0,$$

$$z^{(s)}=(ix_1-x_2)(ix_1-qx_2)\cdots(ix_1-q^{-s+1}x_2), \quad s<0$$

(see Ref. 5). A direct computation shows that $c^{(0)}\equiv\langle z^{(0)},z^{(0)}\rangle=1$ and

$$c^{(s)}\equiv\langle x^{(s)},x^{(s)}\rangle=c^{(-s)}\equiv\langle x^{(-s)},x^{(-s)}\rangle=2q^{s(s-1)/2}[s][2s-2]!!, \quad s>0.$$

We set

$$t^{2,m_2}(x_1,x_2)=(c^{(m_2)})^{-1/2}z^{(m_2)}.$$

To every set of integers $m_{n-1},m_{n-2},\ldots,m_3,m_2$ satisfying the condition (36) corresponds a polynomial (35). (For fixed m_3 the number m_2 takes the values $-m_3,-m_3-1,\ldots,m_3$.) A direct calculation shows that the number of these polynomials is equal to the dimension of the space $\mathcal{H}_m$ given in Corollary 3.1.4 of Ref. 5. From the other side, the polynomials (35) are pairwise orthogonal [a proof of this fact is fulfilled by taking into account the definition (8) of the scalar product and repeating the above-mentioned reasoning of this section]. This means that *the set of all polynomials (35) constitute an orthonormal basis of the space $\mathcal{H}_m$. This basis corresponds to the chain of subalgebras (28).*

Representation of the basis of the space $\mathcal{H}_m$ of solutions of the equation $\Delta p_m=0$ in the form (35) gives us a q-analog of separation of variables of the classical analysis. This q-separation of variables corresponds to the chain of subalgebras (28). q-analogs of other types of separations of variables will be given in the following.

VII. REPRESENTATION OF $U_q'(\mathrm{so}_n)$ ON $\mathcal{H}_m$

In this section we derive how the operators θ_j act upon the basis elements (35).

Lemma 1: Let $h_m(\mathbf{x})=\hat{t}_s^{n,m}(Q,x_n)h_s(\mathbf{x}')$, where $\hat{t}_s^{n,m}$ is given by (30) and $h_s(\mathbf{x}')$ is a homogeneous q-harmonic polynomial of degree s in $\mathbf{x}'=(x_1,x_2,\ldots,x_{n-1})$. Then for the corresponding q-harmonic polynomials $\tilde{h}_{m-1}(\mathbf{x})$ and $\hat{h}_{m+1}(\mathbf{x})$, given by Proposition 2, we have

$$\tilde{h}_{m-1}(\mathbf{x})=q^{-s}[m-s]\frac{[n+m+s-3]}{[n+2m-4]}\hat{t}_s^{n,m-1}(Q,x_n)h_s(\mathbf{x}'), \tag{37}$$

$$\hat{h}_{m+1}(\mathbf{x})=q^s\hat{t}_s^{n,m+1}(Q,x_n)h_s(\mathbf{x}'). \tag{38}$$

Proof: It was proved in Sec. VI that

$$h_m(\mathbf{x})=c_m^{(s)}x_n^{m-s}h_s(\mathbf{x}')+\alpha Q_{n-1}x_n^{m-s-2}h_s(\mathbf{x}')+\beta Q_{n-1}x_n^{m-s-4}h_s(\mathbf{x})+\cdots,$$

where α and β are certain coefficients (we do not need their explicit form) and $c_m^{(s)}$ is given by (32) and (33). Therefore, for $\tilde{h}_{m-1}(\mathbf{x})=\gamma_n^{-1}\partial_n h_m(\mathbf{x})$ we have

$$\tilde{h}_{m-1}(\mathbf{x})=q^{-s}q^{-(m-s-1)}[m-s]c_m^{(s)}x_n^{m-s-1}h_s(\mathbf{x}')+\alpha' Q_{n-1}x_n^{m-s-3}h_s(\mathbf{x}')+\cdots. \tag{39}$$

This polynomial is of the form $\tilde{h}_{m-1}(\mathbf{x})=\sigma\hat{t}_s^{n,m-1}(Q,x_n)h_s(\mathbf{x}')$, where σ is a constant and $h_s(\mathbf{x}')$ is as noted earlier. To show this we note that by Proposition 2 we have $\tilde{h}_{m-1}(\mathbf{x})\in\mathcal{H}_{m-1}$. Therefore, $\tilde{h}_{m-1}(\mathbf{x})$ is a linear combination of the basis polynomials (35) taken for $\mathcal{H}_{m-1}$. In the set of these basis polynomials there is a single polynomial of the form $p(Q,x_n)h_s(\mathbf{x}')$. Up to a constant it coincides with $\hat{t}_s^{n,m-1}(Q,x_n)h_s(\mathbf{x}')$. This proves the desired form of $\tilde{h}_{m-1}(\mathbf{x})$.

In order to compute the constant σ in $\tilde{h}_{m-1}(\mathbf{x})=\sigma\hat{t}_s^{n,m-1}(Q,x_n)h_s(\mathbf{x}')$ we represent $\tilde{h}_{m-1}(\mathbf{x})$ in the form

$$\tilde{h}_{m-1}(\mathbf{x})=\sigma(c_{m-1}^{(s)}x_n^{m-s-1}h_s(\mathbf{x}')+\alpha'' Q_{n-1}x_n^{m-s-3}h_s(\mathbf{x}')+\cdots). \tag{40}$$

Comparing the coefficients at $x_n^{m-s-1}h_s(\mathbf{x}')$ in (39) and (40) we derive that

$$\sigma=q^{-m+1}[m-s]\frac{c_m^{(s)}}{c_{m-1}^{(s)}}=q^{-s}[m-s]\frac{[n+m+s-3]}{[n+2m-4]}.$$

This proves relation (37).

Now for our $h_m(\mathbf{x})$ we consider the expression $\hat{h}_{m+1}(\mathbf{x})$ given by (18). We have

$$h_m(\mathbf{x})x_n=q^s c_m^{(s)}x_n^{m-s+1}h_s(\mathbf{x}')+\cdots,$$

$$\frac{Q\gamma_n^{-1}\partial_n h_m(\mathbf{x})}{[n+2m-2]}=\frac{q^{1-n}q^{-m+1}[m-s]}{[n+2m-2]}c_m^{(s)}x_n^{m-s+1}h_s(\mathbf{x}')+\cdots,$$

where the dots mean summands with lower degrees of x_n. Making some calculations with q-numbers we derive from these equalities that

$$\hat{h}_{m+1}(\mathbf{x})=\frac{q^m[n+m+s-2]}{[n+2m-2]}x_n^{m-s+1}h_s(\mathbf{x}')+\cdots. \tag{41}$$

Taking into account that $\hat{h}_{m+1}\in\mathcal{H}_{m+1}$ and using the above-mentioned reasoning of this proof, one easily proves that $\hat{h}_{m+1}(\mathbf{x})=\tau\hat{t}_s^{n,m+1}(Q,x_n)h_s(\mathbf{x}')$, where τ is a constant. In order to calculate this constant, we represent $\hat{h}_{m+1}$ in the form

$$\hat{h}_{m+1}(\mathbf{x})=\tau(c_{m+1}^{(s)}x_n^{m-s+1}h_s(\mathbf{x}')+\cdots). \tag{42}$$

Comparing the coefficients at $x^{m-s+1}h_s(\mathbf{x}')$ in (41) and (42), we derive that

$$\tau=\frac{q^m[n+m+s-2]}{[n+2m-2]}\frac{c_m^{(s)}}{c_{m+1}^{(s)}}=q^s.$$

This proves relation (38). The lemma is proved.

Theorem 1: *The operators* $T_m(I_{k,k-1})=\theta_{k-1}$, $k=2,3,\ldots,n$, *act upon the basis elements* $\Xi_{\mathbf{m}}\equiv|\mathbf{m}\rangle$, *given by (35), as*

$$T_m(I_{k,k-1})|\mathbf{m}\rangle=-([m_k+m_{k-1}+k-2][m_k-m_{k-1}])^{1/2}A(m_{k-1})|\mathbf{m}_{k-1}^{+}\rangle+([m_k+m_{k-1}+k-3]\times[m_k-m_{k-1}+1])^{1/2}A(m_{k-1}-1)|\mathbf{m}_{k-1}^{-}\rangle,\quad k\neq 2,$$

$$T_m(I_{21})|\mathbf{m}\rangle=i[m_2]|\mathbf{m}\rangle,$$

where $m_n\equiv m$, $\mathbf{m}_{k-1}^{\pm}$ *denote the set of the numbers* $\mathbf{m}$ *with* m_{k-1} *replaced by* $m_{k-1}\pm 1$, *respectively, and*

$$A(m_{k-1})=\left(\frac{[m_{k-1}+m_{k-2}+k-3][m_{k-1}-m_{k-2}+1]}{[2m_{k-1}+k-3][2m_{k-1}+k-1]}\right)^{1/2}.$$

Proof: Let us find how the operator

$$T_m(I_{n,n-1})\equiv\theta_{n-1}=\check{x}_n\gamma_{n-1}^{-1}\partial_{n-1}-\check{x}_{n-1}\gamma_n\partial_n$$

acts upon the polynomial $x_n^{m-s}\hat{t}_r^{n-1,s}(Q_{n-1},x_{n-1})h_r(\mathbf{x}'')$, where $h_r(\mathbf{x}'')$ is a homogeneous q-harmonic polynomial in $x_1,x_2,\ldots,x_{n-2}$. We have

$$\check{x}_n\gamma_{n-1}^{-1}\partial_{n-1}(x_n^{m-s}\hat{t}_r^{n-1,s}(Q_{n-1},x_{n-1})h_r(\mathbf{x}''))=\check{x}_n(x_n^{m-s}\gamma_{n-1}^{-1}\partial_{n-1}\hat{t}_r^{n-1,s}(Q_{n-1},x_{n-1})h_r(\mathbf{x}''))=q^{s-1}x_n^{m-s+1}\gamma_{n-1}^{-1}\partial_{n-1}\hat{t}_r^{n-1,s}h_r(\mathbf{x}'').$$

Using Lemma 1 we derive that

$$\check{x}_{n-1}\gamma_n\partial_n(x_n^{m-s}\hat{t}_r^{n-1,s}h_r(\mathbf{x}''))=q^{m-2s-1}[m-s]\check{x}_{n-1}(x_n^{m-s-1}\hat{t}_r^{n-1,s}h_r(\mathbf{x}''))=q^{m-2s-1}[m-s]x_n^{m-s-1}\left(q^r\hat{t}_r^{n-1,s+1}h_r(\mathbf{x}'')+\frac{Q_{n-1}\gamma_{n-1}^{-1}\partial_{n-1}\hat{t}_r^{n-1,s}h_r(\mathbf{x}'')}{[n+2s-3]}\right),$$

where $\hat{t}_r^{n-1,s}\equiv\hat{t}_r^{n-1,s}(Q_{n-1},x_{n-1})$. Using the above-given equalities and the relation

$$x_n^{m-s-1}Q_{n-1}=q^{-2(m-s-1)}(Q-q^{-n+1}x_n^2)x_n^{m-s-1}=q^{-2(m-s-1)}Qx_n^{m-s-1}-q^{-2(m-s-1)-n+1}x_n^{m-s+1}$$

we obtain that

$$\theta_{n-1}(x_n^{m-s}\hat{t}_r^{n-1,s}h_r(\mathbf{x}''))=\left(q^{s-1}+q^{-2(m-s)-n+3}\frac{q^{m-2s-1}[m-s]}{[n+2s-3]}\right)x_n^{m-s+1}\gamma_{n-1}^{-1}\partial_{n-1}\hat{t}_r^{n-1,s}h_r(\mathbf{x}'')-q^{m-2s+r-1}[m-s]x_n^{m-s-1}\hat{t}_r^{n-1,s+1}h_r(\mathbf{x}'')-\frac{q^{-m+1}}{[n+2s-3]}Qx_n^{m-s-1}\partial_n\hat{t}_r^{n-1,s}h_r(\mathbf{x}'').$$

Now we act by the projection operator H_m upon both sides of this relation, taking into account that the last summand on the right-hand side belongs to $\mathrm{Ker}\, H_m$. Since θ_{n-1} commutes with H_m (see Proposition 3), we derive

$$\theta_{n-1}(\hat{t}_s^{n,m}\hat{t}_r^{n-1,s}h_r(\mathbf{x}''))=-q^{m-2s+r-1}[m-s]\hat{t}_{s+1}^{n,m}\hat{t}_r^{n-1,s+1}h_r(\mathbf{x}'')$$
$$+q^{-m+2s-r-1}[s-r]\frac{[n+m+s-3][n+s+r-4]}{[n+2s-3][n+2s-5]}\hat{t}_{s-1}^{n,m}\hat{t}_r^{n-1,s-1}h_r(\mathbf{x}'').$$

If we rewrite this formula for the normalized polynomials $\Xi_{\mathbf{m}}$, then we obtain the action formula for the operator $T_m(I_{n,n-1})=\theta_{n-1}$, given by the formulation of the theorem.

The above-given proof is valid for the action of any operator $T_m(I_{j,j-1})=\theta_{j-1}$, $j\geqslant 3$, since θ_{j-1} act upon basis polynomials (35) on the right. The formula for $T_m(I_{21})$ is derived in Ref. 5. The theorem is proved.

Comparing the operators $T_m(I_{k,k-1})$ of Theorem 1 with the operators of the irreducible representation R_m of $U_q'(\mathrm{so}_n)$ from Sec. III we obtain

Corollary: The representation T_m realized on the space $\mathcal{H}_m$ of homogeneous q-harmonic polynomials is equivalent to the class 1 irreducible representation R_m of $U_q'(\mathrm{so_n})$.

VIII. q-ANALOG OF ASSOCIATED SPHERICAL HARMONICS WITH RESPECT TO $U_q'(\mathrm{so}_p)\times U_q'(\mathrm{so}_{n-p})$

In Sec. VI we found an orthonormal basis of the space $\mathcal{H}_m$ of homogeneous harmonic polynomials corresponding to the chain of subalgebras (28). In this section we shall find orthonormal bases of the same space corresponding to the reductions

$$U_q'(\mathrm{so}_n)\supset U_q'(\mathrm{so}_p)\times U_q'(\mathrm{so}_{n-p}). \tag{43}$$

As in the classical case (see Ref. 1, Chap. 10), further reductions can be made as in (28) or as (43). In particular, the usual tree method (see Ref. 1, Sec. 10.2) can be used to describe different chains of subalgebras corresponding to different orthonormal bases of $\mathcal{H}_m$.

We represent the set $\mathbf{x}=(x_1,x_2,\ldots,x_n)$ as $\mathbf{x}=(\mathbf{y},\mathbf{t})$, where $\mathbf{y}=(x_1,x_2,\ldots,x_p)$ and $\mathbf{t}=(x_{p+1},x_{p+2},\ldots,x_n)$. Then the q-Laplace operator Δ can be written as

$$\Delta=q^{n-p}\Delta_{(\mathbf{y})}+\Delta_{(\mathbf{t})},$$

where $\Delta_{(\mathbf{y})}$ and $\Delta_{(\mathbf{t})}$ are the q-Laplace operators for $\mathbf{y}$ and $\mathbf{t}$, respectively.

In order to find bases of $\mathcal{H}_m$ corresponding to the reduction (43) we take non-negative numbers s_1 and s_2 such that m and s_1+s_2 are of the same evenness and $m-s_1-s_2\geqslant 0$. Let us find a harmonic projection of the function

$$Q_{\mathbf{t}}^{(m-s_1-s_2)/2}h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y})\in\mathcal{A}_m,$$

where $Q_{\mathbf{t}}:=x_{p+1}+q^{-1}x_{p+2}+\cdots+q^{-(n-p)+1}x_n$ and $h_{s_1}(\mathbf{t})$ [respectively $h_{s_2}(\mathbf{y})$] is a homogeneous of degree s_1 (respectively, of degree s_2) harmonic polynomial in $\mathbf{t}$ (respectively, in $\mathbf{y}$). By definition (7) of the derivatives ∂_i from (12), we have

$$\Delta(Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y}))=\Delta_{(\mathbf{t})}(Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y}))+q^{n-p}Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t})\Delta_{(\mathbf{y})}h_{s_2}(\mathbf{y})$$
$$=q^{-2s_2}\Delta_{(\mathbf{t})}(Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t}))h_{s_2}(\mathbf{y}),$$

where $r=(m-s_1-s_2)/2$. Taking into account relation (13) we obtain

$$\Delta(Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y}))=q^{-2s_2}Q_{\mathbf{t}}^{r-1}[2r][2r+n-p+2s_1-2]h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y}).$$

Repeatedly applying this formula we derive

$$
\begin{aligned}
&H_m(Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y}))\\
&\quad=\sum_{k=0}^{\lfloor m/2\rfloor}\alpha_k\hat{Q}^k\Delta^k(Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y}))\\
&\quad=\left(\sum_{k=0}^{r}\frac{(-1)^k q^{-2s_2k}[2r]!!}{[n+2m-4]!!}\,\frac{[2r+n-p+2s_1-2]!![n+2m-2k-4]!!}{[2r-2k]!![2r+n-p+2s_1-2k-2]!![2k]!!}Q^kQ_{\mathbf{t}}^{r-k}\right)\\
&\qquad\times h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y}),
\end{aligned}
\tag{44}
$$

where, as before, $r=(m-s_1-s_2)/2$.

We denote by $\hat{t}_{s_1,s_2}^{n,p;\,m}(Q_{\mathbf{t}},Q_{\mathbf{y}})$ the expression at $h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y})$ on the right-hand side of (44):

$$
\begin{aligned}
\hat{t}_{s_1,s_2}^{n,p;\,m}(Q_{\mathbf{t}},Q_{\mathbf{y}})&=\sum_{k=0}^{r}\frac{(-1)^k q^{-2s_2k}[2r]!!}{[n+2m-4]!!}\\
&\quad\times\frac{[2r+n-p+2s_1-2]!![n+2m-2k-4]!!}{[2r-2k]!![2r+n-p+2s_1-2k-2]!![2k]!!}Q^kQ_{\mathbf{t}}^{r-k}.
\end{aligned}
\tag{45}
$$

In particular,

$$
\hat{t}_{0,0}^{n,p;\,m}(Q_{\mathbf{t}},Q_{\mathbf{y}})=\frac{[2r]!![2r+n-p-2]!!}{[n+2m-4]!!}\sum_{k=0}^{r}\frac{(-1)^k[n+2m-2k-4]!!Q^kQ_{\mathbf{t}}^{r-k}}{[2r-2k]!![2r+n-p-2k-2]!![2k]!!},
\tag{46}
$$

where m is even, is a zonal polynomial of the space $\mathcal{H}_m$ with respect to the subalgebra $U_q'(\mathrm{so}_p)\times U_q'(\mathrm{so}_{n-p})$. When m is not even, then the space $\mathcal{H}_m$ does not have a zonal polynomial.

In order to normalize expression (45) we have to calculate the coefficient $c_m^{(s_1,s_2)}$ at $Q_{\mathbf{t}}^r$ in $\hat{t}_{s_1,s_2}^{n,p;\,m}(Q_{\mathbf{t}},Q_{\mathbf{t}})$. It follows from (45) and from $Q=Q_{\mathbf{y}}+q^{-p}Q_{\mathbf{t}}$ that

$$
\begin{aligned}
c_m^{(s_1,s_2)}&=\sum_{k=0}^{r}\frac{(-1)^k q^{-2s_2k-pk}[2r]!!}{[n+2m-4]!!}\,\frac{[2r+n-p+2s_1-2]!![n+2m-2k-4]!!}{[2r-2k]!![2r+n-p+2s_1-2k-2]!![2k]!!}\\
&={}_2\varphi_1(q^{-2(2r+n-p+2s_1-2)},q^{-4r};\quad q^{-2n-4m+8};\quad q^4,q^{4-4s_2-2p}).
\end{aligned}
$$

By formula (31) we have

$$
c_m^{(s_1,s_2)}=\frac{(q^{4-4s_2-2p-4r};q^4)_r}{(q^{-2n-4m+8};q^4)_r}.
$$

Repeating the reasoning of Sec. VI for derivation of formula (34), we fulfill a normalization of expression (45). The normalized expression has the form

$$
t_{s_1,s_2}^{n,p;\,m}(Q_{\mathbf{t}},Q_{\mathbf{y}})=\left(\frac{[n+2s_1-p-2]!!q^{(n-p-1)r+2s_2r+s_1s_2}}{[2r]!![2s_1+n+2r-p-2]!!c_m^{(s_1,s_2)}}\right)^{1/2}\hat{t}_{s_1,s_2}^{n,p;\,m}(Q_{\mathbf{t}},Q_{\mathbf{y}}).
$$

In order to construct an orthonormal basis of the space $\mathcal{H}_m$ corresponding to the reduction $U_q'(\mathrm{so}_n)\supset U_q'(\mathrm{so}_p)\times U_q'(\mathrm{so}_{n-p})$ in an explicit form, we note that

$$
\langle t_{s_1,s_2}^{n,p;\,m}(Q_{\mathbf{t}},Q_{\mathbf{y}})h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y}),t_{s_1,s_2}^{n,p;\,m}(Q_{\mathbf{t}},Q_{\mathbf{y}})h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y})\rangle=\langle h_{s_1}(\mathbf{t}),h_{s_1}(\mathbf{t})\rangle\langle h_{s_2}(\mathbf{y}),h_{s_2}(\mathbf{y})\rangle.
$$

Therefore, for construction of such a basis we have to take orthonormal bases $h^{(i)}_{s_1}(\mathbf{t})$ and $h^{(j)}_{s_2}(\mathbf{y})$ of the spaces $\mathcal{H}^{(\mathbf{t})}_{s_1}$ and $\mathcal{H}^{(\mathbf{y})}_{s_2}$ of homogeneous q-harmonic polynomials in $\mathbf{t}$ and $\mathbf{y}$, respectively, and to construct the products

$$t^{n,p;\,m}_{s_1,s_2}(Q_{\mathbf{t}},Q_{\mathbf{y}})h^{(i)}_{s_1}(\mathbf{t})h^{(j)}_{s_2}(\mathbf{y}), \tag{47}$$

$$s_1+s_2\equiv m(\mathrm{mod}\,2),\quad s_1+s_2\leqslant m,\quad i=1,2,\ldots,\dim\mathcal{H}^{(\mathbf{t})}_{s_1},\quad j=1,2,\ldots,\dim\mathcal{H}^{(\mathbf{y})}_{s_2}.$$

It is easy to calculate that the number of elements (47) is equal to $\dim\mathcal{H}_m$. From the other side, it is proved as in the case of the basis elements (35) that the elements (47) are orthogonal to each other. Therefore, the polynomials (47) constitute an orthonormal basis of the space $\mathcal{H}_m$. In particular, we can take the elements $\Xi_{\mathbf{s}_1}(\mathbf{t})$, $\mathbf{s}_1=(s_1,s_1',\ldots)$, and $\Xi_{\mathbf{s}_2}(\mathbf{y})$, $\mathbf{s}_2=(s_2,s_2',\ldots)$, of the type (35) as orthonormal bases of the spaces $\mathcal{H}^{(\mathbf{t})}_{s_1}$ and $\mathcal{H}^{(\mathbf{y})}_{s_2}$, respectively. Then the elements

$$t^{n,p;\,m}_{s_1,s_2}(Q_{\mathbf{t}},Q_{\mathbf{y}})\Xi_{\mathbf{s}_1}(\mathbf{t})\Xi_{\mathbf{s}_2}(\mathbf{y}) \tag{48}$$

form an orthonormal basis of $\mathcal{H}_m$ corresponding to the chain

$$U'_q(\mathrm{so}_n)\supset U'_q(\mathrm{so}_p)\times U'_q(\mathrm{so}_{n-p})\supset U'_q(\mathrm{so}_{p-1})\times U'_q(\mathrm{so}_{n-p-1})\supset\cdots. \tag{49}$$

As was mentioned previously, in order to construct different orthonormal bases of $\mathcal{H}_m$ the tree method from Sec. 10.2 in Ref. 1 can be used. To different trees there correspond different chains of subalgebras of $U'_q(\mathrm{so}_n)$ and orthonormal bases corresponding to them. As in Sec. VI, in this way we obtain q-analogs of different separation of variables.

In the following, for derivation of formulas of action of the operators θ_j upon basis elements corresponding to the reduction (49), we need another basis of $\mathcal{H}_m$. It is obtained from the basis (48) if the elements $\Xi_{\mathbf{s}_1}(\mathbf{t})$ of $\mathcal{H}^{(\mathbf{t})}_{s_1}$ are replaced by the polynomials $\tilde{\Xi}_{\mathbf{s}_1}(\mathbf{t})$, where $\tilde{\Xi}_{\mathbf{s}_1}(\mathbf{t})$ is obtained from $\Xi_{\mathbf{s}_1}(\mathbf{t})$ by replacement of $x_{p+1},x_{p+2},\ldots,x_n$ by $x_n,x_{n-1},\ldots,x_{p+1}$, respectively, and q by q^{-1}. It is proved by a direct calculation that $\Delta_{\mathbf{t}}\tilde{\Xi}_{\mathbf{s}_1}(\mathbf{t})=0$. Thus, we have the orthonormal basis

$$\Xi^{n,p}_{\mathbf{s}_1,\mathbf{s}_2}(\mathbf{x})=t^{n,p;\,m}_{s_1,s_2}(Q_{\mathbf{t}},Q_{\mathbf{y}})\tilde{\Xi}_{\mathbf{s}_1}(\mathbf{t})\tilde{\Xi}_{\mathbf{s}_2}(\mathbf{y}) \tag{50}$$

of $\mathcal{H}_m$.

For calculation in the following we shall use the polynomials

$$\tilde{h}^{n-p}_{s_1,s_2}(\mathbf{t}):=\tilde{t}^{\,p,s_1}_{s_1'}(Q_{\mathbf{t}},x_{p+1})\tilde{h}_{s_1'}(\mathbf{t}') \tag{51}$$

multiple to $\tilde{\Xi}_{s_1}(\mathbf{t})$, where $\mathbf{t}'=(x_{p+2},x_{p+3},\ldots,x_n)$ and $\tilde{t}^{\,p,s_1}_{s_1'}(Q_{\mathbf{t}},x_{p+1})$ and $\tilde{h}_{s_1'}(\mathbf{t}')$ are obtained from $\hat{t}^{\,p,s_1}_{s_1'}(Q_{\mathbf{t}},x_n)$ and $h_{s_1'}(x_{p+1},\ldots,x_{n-1})$ by the replacement mentioned previously. For the polynomials (51) the following lemma is proved in the same way as Lemma 1.

Lemma 2: The following relations are true in the space of q-harmonic polynomials in $x_{p+1},x_{p+2},\ldots,x_n$:

$$\gamma_{p+1}\partial_{p+1}\tilde{h}^{n-p}_{s_1,s_1'}(\mathbf{t})=q^{s_1'}[s_1-s_1']\frac{[n-p+s_1+s_1'-3]}{[n-p+2s_1-4]}\tilde{h}^{n-p}_{s_1-1,s_1'}(\mathbf{t}),$$

$$\tilde{h}^{n-p}_{s_1,s_1'}(\mathbf{t})x_{p+1}-\frac{q^{n-p-1}Q_{\mathbf{t}}\gamma_{p+1}\partial_{p+1}\tilde{h}^{n-p}_{s_1,s_1'}(\mathbf{t})}{[n-p+2s_1-2]}=q^{-s_1'}\tilde{h}^{n-p}_{s_1+1,s_1'}(\mathbf{t}).$$

IX. REPRESENTATIONS T_m IN $U'_q(\mathrm{so}_p)\times U'_q(\mathrm{so}_{n-p})$ BASIS

The aim of this section is to derive formulas giving the action of the operators θ_j upon the basis (50) corresponding to the reduction (49).

First, we obtain the action of the operator $T_m(I_{p+1,p})=\theta_p$ upon non-normalized basis vectors. For this, we calculate

$$\theta_p(Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y}))=Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t})x_{p+1}q^{s_2-1}(\gamma_p^{-1}\partial_p h_{s_2}(\mathbf{y}))-q^{-s_2}(\gamma_{p+1}\partial_{p+1}(Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t}))h_{s_2}(\mathbf{y})x_p,$$

where $h_{s_1}\in\mathcal{H}_{s_1}^{(\mathbf{t})}$ and $h_{s_2}\in\mathcal{H}_{s_2}^{(\mathbf{y})}$. Using the Leibnitz rule

$$\partial_{p+1}(f_1(x_{p+1},\ldots,x_n)f_2(x_{p+1},\ldots,x_n))=(\gamma_{p+1}^{-1}f_1)(\partial_{p+1}f_2)+(\partial_{p+1}f_1)(\gamma_{p+1}\gamma_{p+2}\cdots\gamma_n f_2)$$

we obtain

$$\begin{aligned}\gamma_{p+1}\partial_{p+1}(Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t}))&=\gamma_{p+1}((\gamma_{p+1}^{-1}Q_{\mathbf{t}}^r)\partial_{p+1}h_{s_1}(\mathbf{t})+(\partial_{p+1}Q_{\mathbf{t}}^r)(\gamma_{p+1}\gamma_{p+2}\ldots\gamma_n h_{s_1}(\mathbf{t})))\\&=Q_{\mathbf{t}}^r(\gamma_{p+1}\partial_{p+1}h_{s_1}(\mathbf{t}))+(\gamma_{p+1}\partial_{p+1}Q_{\mathbf{t}}^r)q^{s_1}\gamma_{p+1}h_{s_1}(\mathbf{t})\\&=Q_{\mathbf{t}}^r(\gamma_{p+1}\partial_{p+1}h_{s_1}(\mathbf{t}))+[2r]q^{2r+2s_1-1}Q_{\mathbf{t}}^{r-1}h_{s_1}(\mathbf{t})x_{p+1},\end{aligned}$$

where

$$\gamma_{p+1}\partial_{p+1}Q_{\mathbf{t}}^r=Q_{\mathbf{t}}^{r-1}x_{p+1}q^{2r-1}[2r].$$

By means of this relation and Lemmas 1 and 2 we get

$$\begin{aligned}\theta_p(Q_{\mathbf{t}}^r h_{s_1}(\mathbf{t})h_{s_2}(\mathbf{y}))=&\frac{q^{s_2-2s_1-2r}[n-4+2s_1+2s_2+2r]}{[n-p+2s_1-2][p+2s_2-2]}Q_{\mathbf{t}}^{r+1}(\gamma_{p+1}\partial_{p+1}\tilde{h}_{s_1,s_1'}^{n-p}(\mathbf{t}))\\&\times(\gamma_p^{-1}\partial_p h_{s_2,s_2'}^p(\mathbf{y}))+q^{s_2-s_1'-2r-1}\frac{[p+2s_2+2r-2]}{[p+2s_2-2]}Q_{\mathbf{t}}^r\tilde{h}_{s_1+1,s_1'}^{n-p}(\mathbf{t})\\&\times(\gamma_p^{-1}\partial_p h_{s_2,s_2'}^p(\mathbf{y}))-q^{-s_2+s_2'+2r}\frac{[n-p+2s_1+2r-2]}{[n-p+2s_1-2]}Q_{\mathbf{t}}^r\\&\times(\gamma_{p+1}\partial_{p+1}\tilde{h}_{s_1,s_1'}^{n-p}(\mathbf{t}))h_{s_2+1,s_2'}^p(\mathbf{y})\\&-q^{2s_1-s_2-s_1'+s_2'+2r-1}[2r]Q_{\mathbf{t}}^{r-1}\tilde{h}_{s_1+1,s_1'}^{n-p}(\mathbf{t})h_{s_2+1,s_2'}^p(\mathbf{y}),\end{aligned}\tag{52}$$

where the expressions $\gamma_{p+1}\partial_{p+1}\tilde{h}_{s_1,s_1'}^{n-p}(\mathbf{t})$ and $\gamma_p^{-1}\partial_p h_{s_2,s_2'}^p(\mathbf{y})$ are equal to

$$\gamma_{p+1}\partial_{p+1}\tilde{h}_{s_1,s_1'}^{n-p}(\mathbf{t})=q^{s_1'}[s_1-s_1']\frac{[n-p+s_1+s_1'-3]}{[n-p+2s_1-4]}\tilde{h}_{s_1-1,s_1'}^{n-p}(\mathbf{t}),$$

$$\gamma_p^{-1}\partial_p h_{s_2,s_2'}^p(\mathbf{y})=q^{-s_2'}[s_2-s_2']\frac{[p+s_2+s_2'-3]}{[p+2s_2-4]}h_{s_2-1,s_2'}^p(\mathbf{y}).$$

Acting by H_m upon both sides of (52) and taking into account that H_m commutes with θ_p, we obtain the action formula for the non-normalized vectors. It follows from this formula how θ_p acts upon normalized polynomials $\Xi_{\mathbf{s}_1,\mathbf{s}_2}^{n,p}(\mathbf{x})\equiv|m;\mathbf{s}_1,\mathbf{s}_2\rangle$, where, as before, $\mathbf{s}_1=(s_1,s_1',s_1'',\ldots)$, $\mathbf{s}_2=(s_2,s_2',s_2'',\ldots)$. This action is given by

$$\theta_p|m;\mathbf{s}_1,\mathbf{s}_2\rangle=-K_{s_1}L_{s_2}([m-s_1-s_2][m+s_1+s_2+n-2])^{1/2}|m;\mathbf{s}_1^{+1},\mathbf{s}_2^{+1}\rangle$$
$$+K_{s_1}L_{s_2-1}([m-s_1+s_2+p-2][m+s_1-s_2+n-p])^{1/2}|m;\mathbf{s}_1^{+1},\mathbf{s}_2^{-1}\rangle$$
$$-K_{s_1-1}L_{s_2}([m+s_1-s_2+n-p-2][m-s_1+s_2+p])^{1/2}|m;\mathbf{s}_1^{-1},\mathbf{s}_2^{+1}\rangle$$
$$+K_{s_1-1}L_{s_2-1}([m-s_1-s_2+2][m+s_1+s_2+n-4])^{1/2}|m;\mathbf{s}_1^{-1},\mathbf{s}_2^{-1}\rangle,$$

where $\mathbf{s}_i^{\pm 1}$ is the set $\mathbf{s}_i$ with s_i replaced by $s_i\pm 1$, respectively, and

$$K_{s_1}=\left(\frac{[s_1-s_1'+1][s_1+s_1'+n-p-2]}{[2s_1+n-p][2s_1+n-p-2]}\right)^{1/2},$$

$$L_{s_2}=\left(\frac{[s_2-s_2'+1][s_2+s_2'+p-2]}{[2s_2+p][2s_2+p-2]}\right)^{1/2}.$$

This formula coincides with one given for this type of irreducible representation of $U_q'(\mathrm{so}_n)$ in Ref. 15.

The action of operators θ_k, $1\leqslant k<p$, upon the basis (50) is given by the formulas of Theorem 1 written for the algebra $U_q'(\mathrm{so}_p)$ with $m_p=s_2$, $m_{p-1}=s_2',\ldots$. The action of operators θ_k, $p<k<n$, is given by the formulas of Theorem 1 for the operators $-\theta_{n-k}$ of the algebra $U_q'(\mathrm{so}_{n-p})$, respectively, with $m_{n-p}=s_1$, $m_{n-p-1}=s_1',\ldots$.

X. SPECTRAL DECOMPOSITIONS OF SOME REPRESENTATIONS

The above-obtained results allow us to decompose the reducible representations constructed in the previous sections into irreducible constituents. In Sec. IV we gave the representation ρ_m of $U_q(\mathrm{sl}_n)$ on the space $\mathcal{A}_m$ of homogeneous polynomials. It is an irreducible representation with highest weight $(m,0,\ldots,0)$. The restriction of this representation to the subalgebra $U_q'(\mathrm{so}_n)$ was denoted by $T^{(m)}$. Since for $T^{(m)}$ we have the decomposition (17) and $T_{m-2j}\sim R_{m-2j}$, where R_k are the irreducible class 1 representations of $U_q'(\mathrm{so}_n)$, then

$$\rho_m\downarrow_{U_q'(\mathrm{so}_n)}=\bigoplus_{0\leqslant 2j\leqslant m}R_{m-2j},\quad T^{(m)}=\bigoplus_{0\leqslant 2j\leqslant m}R_{m-2j},$$

where summations are such as in (17).

The results of Sec. IX show how the restriction of the representation $T_m\sim R_m$ of $U_q'(\mathrm{so}_n)$ onto the subalgebra $U_q'(\mathrm{so}_p)\times U_q'(\mathrm{so}_{n-p})$ decomposes into irreducible representations:

$$R_m\downarrow_{U_q'(\mathrm{so}_p)\times U_q'(\mathrm{so}_{n-p})}=\bigoplus_{s_1,s_2}(R_{s_1}\times R_{s_2}),$$

where summation is over non-negative integers s_1 and s_2 such that $s_1+s_2\equiv 0(\mathrm{mod}\,m)$ and $s_1+s_2\leqslant m$.

The formulas

$$ke=q^4ek,\quad kf=q^{-4}fk,\quad ef-fe=\frac{k-k^{-1}}{q^2-q^{-2}}$$

determine the quantum algebra $U_{q^2}(\mathrm{sl}_2)$. The algebra homomorphism $\omega: U_{q^2}(\mathrm{sl}_2)\to\mathcal{A}$ uniquely determined by

$$w(e)=\frac{\hat{Q}}{q+q^{-1}},\quad w(f)=-\frac{\Delta}{q+q^{-1}},\quad \omega(k)=q^n\gamma_1^2\cdots\gamma_n^2\equiv q^n\gamma^2$$

is a representation of $U_{q^2}(\mathrm{sl}_2)$ (see Ref. 5). Since the operators $\omega(e)$, $\omega(f)$, and $\omega(k)$ commute with the operators θ_j (see Ref. 5), the representation $\omega \times T$ of the algebra $U_{q^2}(\mathrm{sl}_2) \times U'(\mathrm{so}_n)$ acts on $\mathcal{A}$, where T is determined by formula (10). This representation is reducible. Let us decompose it into irreducible components.

By (21), we have $\mathcal{A} = \oplus_{m \geqslant 0}(\mathbb{C}[Q] \otimes \mathcal{H}_m)$. The subspaces $\mathbb{C}[Q] \otimes \mathcal{H}_m$ are irreducible under $U_{q^2}(\mathrm{sl}_2) \times U'(\mathrm{so}_n)$, since the space $\mathbb{C}[Q]$ is pointwise invariant under $U'(\mathrm{so}_n)$ and for $f \in \mathbb{C}[Q]$ and $h_m \in \mathcal{H}_m$ we have

$$\hat{Q}(f(Q) \otimes h_m) = Qf(Q) \otimes h_m, \tag{53}$$

$$\Delta(Q^r \otimes h_m) = [2r][2r+2m+n-2]Q^{r-1} \otimes h_m, \tag{54}$$

$$k(Q^r \otimes h_m) = q^n \gamma^2 (Q^r \otimes h_m) = q^{4r+2m+n}(Q^r \otimes h_m). \tag{55}$$

These formulas show that $U_{q^2}(\mathrm{sl}_2)$ acts on $\mathbb{C}[Q]$ and $U'(\mathrm{so}_n)$ acts on $\mathcal{H}_m$. However, this action of $U_{q^2}(\mathrm{sl}_2)$ depends on the component $\mathcal{H}_m$. Taking the basis

$$|r\rangle := [2r]!\, Q^r, \quad r = 0,1,2,\ldots,$$

in the space $\mathbb{C}[Q]$, we find from (53) to (55) that

$$\omega(f)|r\rangle = -[r+m-1+n/2]_{q^2}|r-1\rangle,$$

$$\omega(e)|r\rangle = [r+1]_{q^2}|r+1\rangle, \quad \omega(k)|r\rangle = (q^2)^{m+2r+n/2}|r\rangle.$$

Comparing this representation with the known irreducible representations of $U_{q^2}(\mathrm{sl}_2)$ (see, e.g., Ref. 16) we derive that the irreducible representation of $U_{q^2}(\mathrm{sl}_2)$ of the discrete series with lowest weight $m+n/2$ is realized on the component $\mathbb{C}[Q]$ of the space $\mathbb{C}[Q] \otimes \mathcal{H}_m$. We denote this representation of $U_{q^2}(\mathrm{sl}_2)$ by $D_{m+n/2}$.

Thus, we derived that on the subspace $\mathbb{C}[Q] \otimes \mathcal{H}_m$ of the space $\mathcal{A}$ acts the irreducible representation $D_{m+n/2} \times T_m$ of the algebra $U_{q^2}(\mathrm{sl}_2) \times U'(\mathrm{so}_n)$. This means that for the reducible representation $\omega \otimes T$ we have the following decomposition into irreducible components:

$$\omega \otimes T = \bigoplus_{m=0}^{\infty} D_{m+n/2} \times T_m.$$

It is a q-analog of the corresponding decomposition of the classical case (see Ref. 1, Sec. 12.3).

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Diagram projection rules for recoupling diagrams in the Racah–Wigner category

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This paper gives three important techniques for recoupling coefficients of an arbitrary number or irreducible representations: factorization as a product of smaller degree recoupling coefficients, diagram projection projecting a recoupling diagram to obtain constraints on recoupling coefficients, and primitive expansion expressing a recoupling coefficient in terms of primitive recoupling coefficients. The first technique reduces a recoupling coefficient to its essential and simplest form. The second is many faceted allowing one to work at the recoupling level. Importantly, recoupling diagrams can be used to construct a complete set of constraints on the recoupling coefficients. The third allows large degree recoupling coefficients to be expressed in terms of primitive recoupling coefficients. An example of this is the fact that the $9j$ symbol is defined by the $3j$ and $6j$ symbols. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1339830]

I. INTRODUCTION

The central goals of group representation theory[1] are to determine the representations of a group, determine which of these are irreducible, and decompose any representation into a direct sum of irreducible representations. The converse, namely given the irreducible representations and rules concerning direct sum decomposition determine the original group, is given by Tannaka–Krein duality.[2] The Racah–Wigner calculus[3,4] assumes this knowledge and proceeds to unravel the properties of the mappings between representations. This falls squarely into the realm of category theory[5] and homological algebra. The important properties are Schur's lemma, naturality, coherence,[6] and universal property.

Furthermore, given the number of labels often needed to index a recoupling coefficient, it is important to choose appropriate notation. This notation has to be precise to account for the complex relationships between labels yet still represent the underlying structure of recoupling. This we achieve through a suitable bra ket format together with the pictorial power of binary trees. Also the often complex relationships between mappings requires a mathematical formalism to cope with the ideas involved; such a formalism is best given using category theory which provides a concrete link between binary trees and the bra ket notation. In recent years category theory is finding relevance to knot theory and quantum groups.[7]

The formulation of the Racah–Wigner calculus as a ring category is given in Joyce and Butler,[8] Joyce.[9] The original sources on ring categories are Kelly[10] and Laplaza.[11] The reader should consult these sources for a complete understanding of the category theoretic issues. This paper gives concise definitions for statement, coupling, recoupling, and recoupling coefficient. The notion of coupling relies on the concept of universal property and the notion of recoupling on naturality and coherence; all ideas only found in category theory. The recoupling coefficient is generated through the notion of a projection scheme. This paper utilizes these notions to give three important techniques for effectively handling recoupling coefficients: factorization of recoupling coefficients as a product of lower degree recoupling coefficients (without summation), expansion in terms of primitive recoupling coefficients, and a set of rules for obtaining recoupling coefficient

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constraints corresponding to a given recoupling diagram. These three techniques provide us with the basic tools to handle recoupling coefficient equations at the formal recoupling level.

An important application of these techniques is to obtain recoupling coefficient constraints underlying any recoupling diagram. It is a mechanical application of the rules, regardless of the number of irreducible representations coupled together, to obtain the equations of constraint. The constraint equations can be reduced further using primitive expansions. The primitive expansion technique allows one to write a general recoupling coefficient in terms of primitive associativity and commutativity recoupling coefficients. These ideas underlie a paper in preparation devoted to the algorithmic calculation of general recoupling coefficients from an initial set. The method is by direct calculation and unlike present methods; for example, see Butler *et al.*,[12] Searle,[13] and Searle and Butler.[14] All of these methods are based on solving linear recursion equations.

Finally, we use the method of diagram projection to determine complete sets of constraints on the recoupling coefficients. For the diagrams of a symmetric tensor category we deduce the symmetry, pentagon, and hexagon equations. For the j symbols of Wigner we deduce the symmetry, Biedenharn–Elliott and Racah backcoupling equations.

In what follows the following conventions are assumed. The group G underlying all representations is assumed to be reductive. The set Irr_G is a family of irreducible representations of G containing exactly one representation for each isomorphism class. The elements of Irr_G serve to label the isomorphism classes of irreducible representations. We call the elements of Irr_G irreps for short. The Racah–Wigner category $\mathbf{RW}_G$ is generated from Irr_G as a full ring subcategory of $\mathbf{URep}_G$. $\mathbf{URep}_G$ is the category of unitary representations whose objects are unitary representations of G and morphisms are G-equivariant linear maps (intertwining operators). Moreover, $\mathbf{URep}_G$ is a ring category with bifunctors direct sum $\oplus:\mathbf{URep}_G\times\mathbf{URep}_G\rightarrow\mathbf{URep}_G$ and tensor product $\otimes:\mathbf{URep}_G\times\mathbf{URep}_G\rightarrow\mathbf{URep}_G$. The objects of $\mathbf{RW}_G$ are all finite words of irreps generated by direct sum and tensor product. The important point is that we have made a choice of irreducible representation for each isomorphism class and restricted our attention to that set. The morphisms of $\mathbf{RW}_G$ are those inherited from $\mathbf{URep}_G$.

II. COUPLING

The notion of coupling is essential to the construction of recoupling coefficients. In this section we give a precise definition and the properties of couplings required by latter sections. Coupling provides the link between the notion of recoupling and recoupling coefficient. A coupling is a prescription for decomposing the tensor product of two irreps μ and ν into a direct sum

$$\mu\otimes\nu\cong\bigoplus_{\lambda\in\mathrm{Irr}_G} m_\lambda^{\mu,\nu}\lambda, \tag{1}$$

where $m_\lambda^{\mu,\nu}$ is the multiplicity of λ in $\mu\otimes\nu$. We assume the convention that if $m_\lambda^{\mu,\nu}=0$ then λ is not part of the direct sum.

Definition 1: A coupling between two irreps μ and ν is a family of bra kets $\{\langle k\lambda|\mu.\nu\rangle:\mu\otimes\nu\rightarrow\lambda\}_{k\lambda}$ where $k=1,2,\ldots,m_\lambda^{\mu,\nu}$ for each λ, satisfying the universal property of a category product: Let a be a representation. Given a family $\{\langle k\lambda|f|a\rangle:a\rightarrow\lambda\}_{k\lambda}$ of bra kets there exists a unique map $\langle\mu.\nu|f|a\rangle:a\rightarrow\mu.\nu$ such that the diagram of Fig. 1 commutes, or equivalently $\langle k\lambda|f|a\rangle=\langle k\lambda|\mu.\nu\rangle\langle\mu.\nu|f|a\rangle$.

A coupling projects out the components of the direct sum decomposition from a tensor product of two irreps. This is equivalent to choosing a basis for the vector space of intertwining operators from $\mu\otimes\nu$ to λ. Dual to the notion of coupling is that of a co-coupling, embedding the components of the direct sum decomposition into the tensor product of two irreps. This is equivalent to choosing a basis for the vector space of intertwining operators from λ to $\mu\otimes\nu$. The unique existence for expressions of vectors as linear combinations of basis vectors is expressed in lemma 1.

Lemma 1: For every coupling $\{\langle k\lambda|\mu.\nu\rangle\}_{k\lambda}$ there exists a unique family of bra kets $\{\langle\mu.\nu|k\lambda\rangle:\lambda\rightarrow\mu\otimes\nu\}_{k\lambda}$ with the following properties:

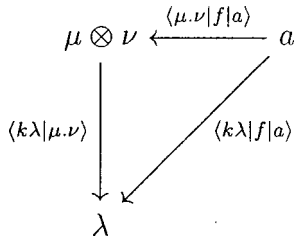

FIG. 1. The universal property of a category product.

(i) The bra kets $\{\langle \mu.\nu|k\lambda\rangle\}_{k\lambda}$ *have the universal property of a category coproduct: Let a be a representation. Given a family* $\{\langle a|f|k\lambda\rangle:\lambda\to a\}_{k\lambda}$ *of bra kets there exists a unique* $\langle a|f|\mu.\nu\rangle:\mu\otimes\nu\to a$ *such that the diagram of Fig. 2 commutes, or equivalently* $\langle a|f|k\lambda\rangle = \langle a|f|\mu.\nu\rangle\langle\mu.\nu|k\lambda\rangle$.

(ii) Every coupling bra ket has a co-coupling bra ket left inverse

$$\langle k\lambda|\mu\nu\rangle\langle\mu.\nu|k\lambda\rangle = 1_\lambda\,, \tag{2}$$

(*iii*)

$$\sum_{k\lambda} \langle\mu.\nu|k\lambda\rangle\langle k\lambda|\mu.\nu\rangle = 1_{\mu.\nu}\,. \tag{3}$$

The family of bra kets $\{\langle \mu.\nu|k\lambda\rangle\}_{k\lambda}$ is called a co-coupling and said to be the dual of the coupling $\{\langle k\lambda|\mu.\mu\rangle\}_{k\lambda}$. The dual co-coupling brackets are often denoted $\{\overline{\langle k\lambda|\mu.\nu\rangle}\}_{k\lambda}$.

An orthogonal choice of coupling can always be made as attested by lemma 2.

Lemma 2: Given irreps μ *and* ν *there exists an orthogonal coupling. That is,*

$$\langle k\lambda|\mu.\nu\rangle\langle\mu.\nu|k'\lambda'\rangle = \delta_{kk'}\delta_{\lambda\lambda'}\,. \tag{4}$$

A collection of couplings is called a family if for every ordered pair of irreps (μ,ν) there exists a unique coupling in the collection with domain $\mu\otimes\nu$.

III. RECOUPLING

In order to give a precise definition of recoupling we need to introduce the notion of a statement. Loosely a statement of irreps is any binary bracketed *n*-fold tensor product of irreps. We make this precise using the connection between binary trees and binary bracketings. Let *B* be a binary tree. We define the map

$$B\mapsto [\_]^B:\bigoplus_{n=1}^{\infty}\left(\prod_{i=1}^{n}\mathrm{Irr}_G\right)\to \mathbf{RW}_G \tag{5}$$

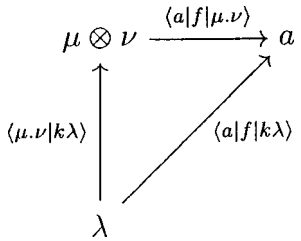

FIG. 2. The universal property of a category coproduct.

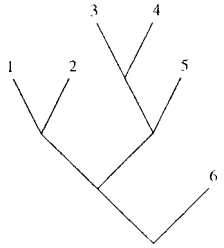

FIG. 3. Binary tree representation of the statement $((\lambda_1\otimes\lambda_2)\otimes((\lambda_3\otimes\lambda_4)\otimes\lambda_5))\otimes\lambda_6$.

by $(\lambda_1,\ldots,\lambda_n)\mapsto[\otimes_i]^B\lambda_i$ where the square brackets around the direct sum means that the irreps have been bracketed according to the binary tree B in the standard way. A full description of this association is given in Joyce[9] and Biedenharn and Louck.[3] A brief outline will now be given. The irreps of an ordered pair $(\lambda_1,\ldots,\lambda_n)$ are bijectively mapped onto the terminal vertices of the binary tree B starting with the left hand side terminal vertex and then working ones way around the terminal vertices of the binary tree in order. Each internal vertex represents a bracketed product of the left hand side branch with the right hand side branch. Inductively this generates a binary bracketed tensored product of the irreps $\lambda_1,\ldots,\lambda_n$. Each object $[\otimes_i]^B\lambda_i$ is called a statement of irreps. The number of irreps defines the length of the statement. For example, the statement $((\lambda_1\otimes\lambda_2)\otimes((\lambda_3\otimes\lambda_4)\otimes\lambda_5))\otimes\lambda_6$ of length six is represented by the binary tree of Fig. 3.

The permutation groups have an obvious action on an n-fold Cartesian product of irreps: Let $\pi\in S_n$ then

$$\pi:\prod_{i=1}^{n}\ \mathrm{Irr}_G\to\prod_{i=1}^{n}\ \mathrm{Irr}_G,(\lambda_1,\ldots,\lambda_n)\mapsto(\lambda_{\pi(1)},\ldots,\lambda_{\pi(n)}). \tag{6}$$

Hence we can define the obvious extension; the map $(\pi,B)\mapsto[\pi\_]^B$. Moreover, each map $[\pi\_]^B$ extends to a functor from the n-fold Cartesian product $\Pi_{i=1}^n\mathbf{RW}_G$ to $\mathbf{RW}_G$, again in an obvious way.

Intuitively a recoupling is an isomorphism between the two statements which at a formal level reorders and rebrackets the irreps. There is a potential problem of consistency where two alternative chains of composed isomorphisms representing recouplings achieving the same formal recoupling may differ. This is avoided by using the natural isomorphisms of associativity and commutativity provided by $\mathbf{RW}_G$ to generate the recoupling isomorphisms. The consistency issue is resolved in the affirmative by the coherence property of $\mathbf{RW}_G$. See Joyce[9] and Mac Lane[5] for the details. We make the following formal definition of a recoupling.

Definition 2: A recoupling rebracketing B as B' and reordering according to the permutation π is the natural isomorphism $\imath_\pi^{B'B}:[\_]^B\to[\pi\_]^{B'}$ generated by the multiplicative associativity and commutativity natural isomorphisms in $\mathbf{RW}_G$.

The degree of a recoupling is defined to be the length of the statement it acts upon.

IV. RECOUPLING COEFFICIENTS

In this section we set up a procedure for obtaining the recoupling coefficients corresponding to a recoupling using a family of couplings. Consider a statement $S=[\lambda_1,\ldots,\lambda_n]^B=[\otimes_{i=1}^n]^B\lambda_i$. We make the following useful definitions. A consecutive pair $\lambda_i\otimes\lambda_{i+1}$ of irreps bracketed together within the statement S is called a couple. The degree of a couple is the number of brackets it is embedded within. The degree of the statement S is defined to be the maximum degree of all its couples. We denote the degree of S by $\deg(S)$. As an example consider the statement $((\lambda_1\otimes\lambda_2)\otimes((\lambda_3\otimes\lambda_4)\otimes\lambda_5))\otimes\lambda_6$ of length six. The couples are $\lambda_1\otimes\lambda_2$ and $\lambda_3\otimes\lambda_4$ with degrees 1 and 2, respectively. Hence the degree of this statement is $\deg(S)=2$.

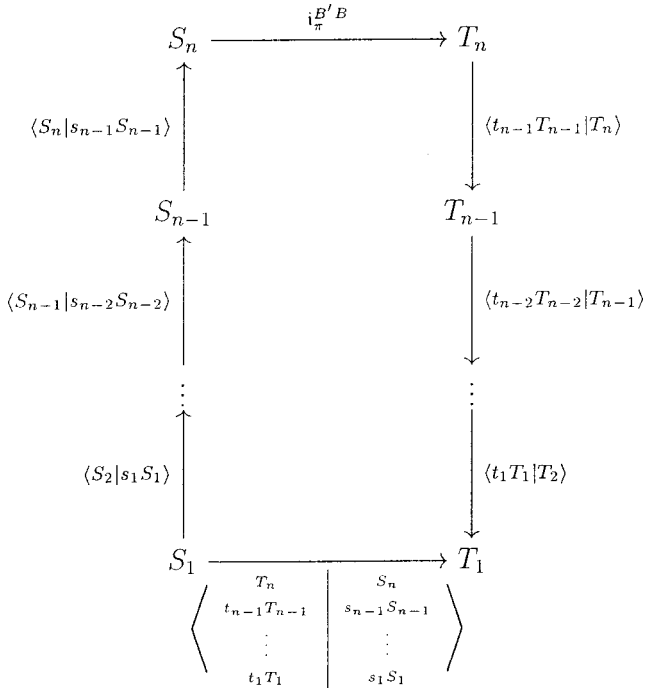

FIG. 4. Construction of recoupling coefficients.

To mechanize the projection of a statement S_n, where the subscript n is the length of the statement, we introduce the notion of a projection scheme which is a finite sequence $S_n,\ldots,S_1$ of statements, of decreasing degree constructed as follows. Let S_n be the given statement of length n. Define the statement S_{n-1} to be the statement of length $n-1$ derived from S_n as follows: Reading from left to right locate the first couple of degree $\deg(S_n)$. We call this the principal couple of S_n. We replace this couple with a dummy irrep label. This label stands in for the irreps in the decomposition of the principal couple and is said to be an internal irrep label. Note that we will also associate a dummy multiplicity label of which more will be said later. Continuing this process inductively we obtain a finite sequence $S_n,\ldots,S_1$ of statements. The last statement has length one and is a single irrep. The sequence obtained in this way we call the projection scheme of S_n. The number of (dummy) internal irreps is one less than the length of the statement and largely independent of the degree of the statement.

Let $\mathfrak{i}_\pi^{B'B}: S_n \to T_n$ be a recoupling of degree n between the statements S_n and T_n. The recoupling component bra kets for the recoupling are obtained as suggested by the diagram of Fig. 4. The vertical arms of the diagram represent the projection schemes for S_n and T_n. The vertical arrow at the ith level and on the left (resp. right) hand side of the diagram represents a co-coupling bra ket $\langle s_i \lambda | \mu.\nu \rangle$ (resp. coupling bra ket $\langle t_i \lambda | \mu.\nu \rangle$) taking the principal couple, $\mu \otimes \nu$ of S_{i+1} (resp. T_{i+1}) to the corresponding internal irrep λ of S_i (resp. T_i). Note that s_i (resp. t_i) is the multiplicity label appearing in the recoupling bra ket. In future the vertical arrows will only be labeled with the multiplicity instead of the entire bra ket. By Schur's lemma the recoupling bra kets are nonzero only if $S_1 = T_1$ and, moreover, are multiples of the identity. These multiples are called recoupling coefficients. We denote a recoupling coefficient with the same symbol as its recoupling bra ket. The order of a recoupling coefficient is defined to be the length n of the statement recoupled.

As an example of the procedure consider the recoupling depicted by the diagram in Fig. 5. In this example the vertical arrows are labeled by the multiplicity labels of the (co-)coupling brackets. The bottom horizontal arrow is the recoupling coefficient, denoted by

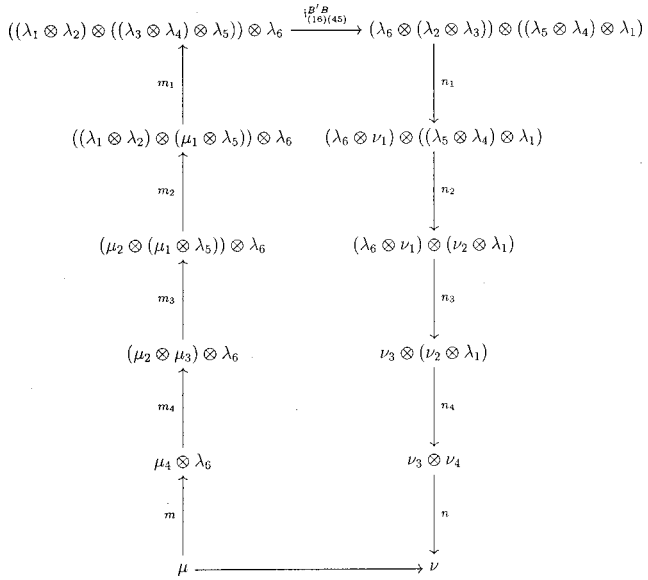

FIG. 5. Construction of the recoupling coefficients corresponding to the recoupling $i^{B'B}_{(16)(45)}:((\lambda_1\otimes\lambda_2)\otimes((\lambda_3\otimes\lambda_4)\otimes\lambda_5))\otimes\lambda_6\rightarrow(\lambda_6\otimes(\lambda_2\otimes\lambda_3))\otimes((\lambda_5\otimes\lambda_4)\otimes\lambda_1)$.

$$
\left\langle \begin{array}{ccccccccc}
(\lambda_6 & & (\lambda_2 & & \lambda_3)) & & ((\lambda_5 & & \lambda_4) & & \lambda_1) \\
& (\lambda_6 & & n_1\nu_1) & & ((\lambda_5 & & \lambda_4) & & \lambda_1) & \\
& & (\lambda_6 & & \nu_1) & & (n_2\nu_2 & & \lambda_1) & & \\
& & & n_3\nu_3 & & (\nu_2 & & \lambda_1) & & & \\
& & & & \nu_3 & & n_4\nu_4 & & & & \\
& & & & & n\nu & & & & &
\end{array} \right|
\left| \begin{array}{ccccccccc}
((\lambda_1 & & \lambda_2) & & ((\lambda_3 & & \lambda_4) & & \lambda_5)) & & \lambda_6 \\
& ((\lambda_1 & & \lambda_2) & & (m_1\mu_1 & & \lambda_5)) & & \lambda_6 & \\
& & (m_2\mu_2 & & (\mu_1 & & \lambda_5)) & & \lambda_6 & & \\
& & & (\mu_2 & & m_3\mu_3) & & \lambda_6 & & & \\
& & & & m_4\mu_4 & & \lambda_6 & & & & \\
& & & & & m\mu & & & & &
\end{array} \right\rangle . \tag{7}
$$

Note that for simplicity the tensor product symbols are not written in the recoupling coefficient at all and each multiplicity label appears below the couple it originates from and in front of the internal irrep to which it corresponds.

V. RECOUPLING COEFFICIENT FACTORIZATION

Often a recoupling coefficient can be factored as a product of smaller degree recoupling coefficients. This is always the case if the recoupling only modifies isolated subsections of the statement. A procedure will be developed here to reduce a recoupling coefficient to a product of essential (sub)recoupling coefficients. First we develop further the connection between binary trees and statements.

As we have seen, a statement S_n of length n is represented by a binary tree B_n with n terminal vertices. This binary tree can also represent the projection scheme for S_n. By removing the principal couple from B_n and labeling the new terminal vertex with the internal irrep label, one

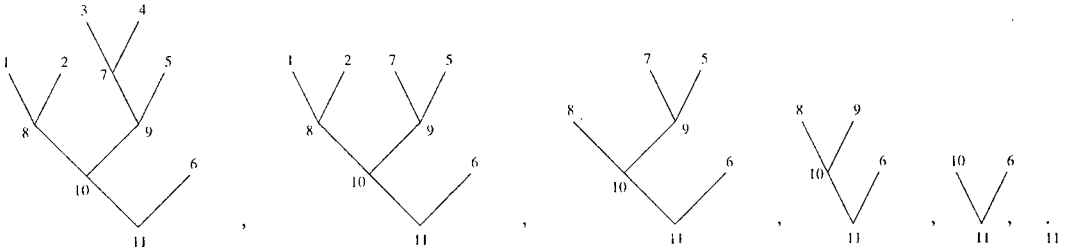

FIG. 6. Projection scheme of the statement $((\lambda_1\otimes\lambda_2)\otimes((\lambda_3\otimes\lambda_4)\otimes\lambda_5))\otimes\lambda_6$.

obtains the binary tree B_{n-1} representing the statement S_{n-1}. This process inductively generates the sequence $B_n,\ldots,B_1$ of binary trees corresponding to the projection scheme $S_n,\ldots,S_1$. Moreover, we can label the internal vertices of the binary trees with the dummy variables introduced by the projection scheme. Since such a close connection exists between binary trees and statements then we often denote the binary trees $B_n,\ldots,B_1$ by their corresponding statements $S_n,\ldots,S_1$. For example, consider the statement $((\lambda_1\otimes\lambda_2)\otimes((\lambda_3\otimes\lambda_4)\otimes\lambda_5))\otimes\lambda_6$ of Fig. 3. The binary tree sequence representing the projection scheme of this statement is given in Fig. 6.

Finally we introduce the following definition. Given an internal vertex μ for a binary tree B, define $B(\mu)$ to be the maximal binary subtree embedded in B with principal vertex μ. This $B(\mu)$ is obtained by removing the portion of the binary tree below the vertex μ.

The factorization of recoupling coefficients is in two steps. The first is more of a cosmetic simplification. Let $\mathrm{i}_\pi^{T_nS_n}:S_n\to T_n$ be the recoupling we wish to reduce. Given internal vertices μ of S_n and ν of T_n such that the binary subtrees $S_n(\mu)$ and $T_n(\nu)$ have the same set of terminal vertices then we identify the internal irrep labels ($\mu=\nu$). This makes sense because of the following.

Proposition 1: Let $\mathrm{i}_\pi^{T_nS_n}:S_n\to T_n$ *be a recoupling. If there exist internal vertices* μ, ν *such that the binary subtrees* $S_n(\mu)$ *and* $T_n(\nu)$ *have the same set of terminal vertex labels then*

$$\left\langle \begin{array}{c|c} T_n & S_n \\ t_{n-1}T_{n-1} & t_{n-1}S_{n-1} \\ \vdots & \vdots \\ t_1T_1 & s_1S_1 \end{array} \right\rangle \neq 0 \tag{8}$$

only if $\mu=\nu$.

This is a result of Schur's lemma and the linearity of couplings and recouplings.

The second step of the factorization is as follows. We divide each of the binary trees S_n and T_n into a finite sequence of nontrivial binary subtrees. We begin by taking S_n and T_n to be the initial sequences. Suppose there exist nontrivial binary trees B_S and B_T such that B_S is a subtree of S_n and B_T is a subtree of T_n. Furthermore, suppose B_S and B_T have the same set of vertex labels. (Note that the order of labeling may differ.) We divide the binary tree S_n at the vertex labeled by the principal vertex of B_S and replace S_n in the sequence with these two binary trees retaining the left/right hand distinction. Similarly divide T_n at the vertex labeled by the principal vertex of B_T and replace T_n in the sequence. Inductively we repeat this process on each member of the two growing sequences of binary trees until all pairs of nontrivial such binary trees have been exhausted. Thus S_n and T_n have each been divided into a finite sequence of binary trees. Denote these sequences by $(S_{n_1,1},\ldots,S_{n_m,m})$ and $(T_{n_1,1},\ldots,T_{n_m,m})$, respectively, where m is the number of binary trees and n_k is the number of terminal vertices of the kth binary tree. For each $k=1,2,...,m$ there is a recoupling $\mathrm{i}_k:S_{n_k,k}\to T_{n_k,k}$. Moreover, the original recoupling is given by composing the i_k's. This composition is independent of order.

Theorem 1: *The factorization procedure outlined above gives rise to the following factorization:*

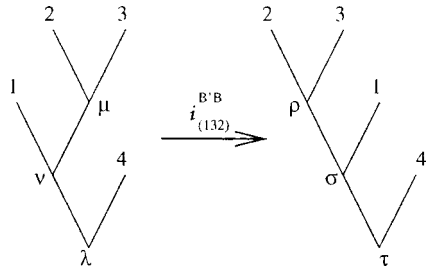

FIG. 7. Binary tree representation of the recoupling $i^{B'B}_{(132)}:(\lambda_1\otimes(\lambda_2\otimes\lambda_3))\otimes\lambda_4\rightarrow((\lambda_2\otimes\lambda_3)\otimes\lambda_1)\otimes\lambda_4$.

$$\left\langle \begin{array}{c|c} S_n & T_n \\ s_{n-1}S_{n-1} & t_{n-1}T_{n-1} \\ \vdots & \vdots \\ s_1S_1 & t_1T_1 \end{array} \right\rangle = \prod_{k=1}^{m} \left\langle \begin{array}{c|c} S_{n_k,k} & T_{n_k,k} \\ s_{n_k-1,k}S_{n_k-1,k} & t_{n_k-1,k}T_{n_k-1,k} \\ \vdots & \vdots \\ s_{1,k}S_{1,k} & t_{1,k}T_{1,k} \end{array} \right\rangle , \tag{9}$$

where $T_1=S_1=T_{1,k}=S_{1,k}$.

To illustrate the above factorization process consider the following recoupling $i^{B'B}_{(132)}:(\lambda_1\otimes(\lambda_2\otimes\lambda_3))\otimes\lambda_4\rightarrow((\lambda_2\otimes\lambda_3)\otimes\lambda_1)\otimes\lambda_4$. This recoupling is depicted by Fig. 7. The first step of the factorization procedure relabels ρ with μ, σ with ν, and τ with λ. The second step results in the sequences of binary trees given by Fig. 8 and the recouplings indicated between corresponding members. Finally by Theorem 1 we obtain the recoupling factorization

$$\left\langle \begin{array}{ccccc|ccccc} ((\lambda_2 & & \lambda_3) & & \lambda_1) & \lambda_4 & (\lambda_1 & & (\lambda_2 & & \lambda_3)) & \lambda_4 \\ & (m'\mu & & \lambda_1) & & \lambda_4 & & (\lambda_1 & & m\mu) & & \lambda_4 \\ & & n'\nu & & \lambda_4 & & & & n\nu & & \lambda_4 & \\ & & & k'\lambda & & & & & & k\lambda & & \end{array} \right\rangle$$

$$= \left\langle \begin{array}{ccc|ccc} \nu & & \lambda_4 & \nu & & \lambda_4 \\ & k'\lambda & & & k\lambda & \end{array} \right\rangle \left\langle \begin{array}{ccc|ccc} \mu & & \lambda_1 & \lambda_1 & & \mu \\ & n'\nu & & & n\nu & \end{array} \right\rangle$$

$$\cdot \left\langle \begin{array}{ccc|ccc} \lambda_2 & & \lambda_3 & \lambda_2 & & \lambda_3 \\ & m'\mu & & & m\mu & \end{array} \right\rangle . \tag{10}$$

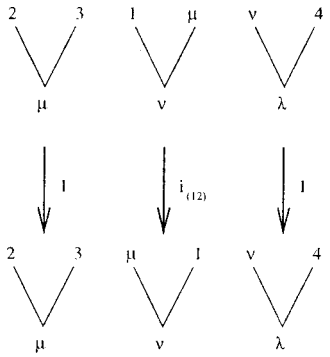

FIG. 8. Binary tree factorization of the recoupling $i^{B'B}_{(132)}:(\lambda_1\otimes(\lambda_2\otimes\lambda_3))\otimes\lambda_4\rightarrow((\lambda_2\otimes\lambda_3)\otimes\lambda_1)\otimes\lambda_4$.

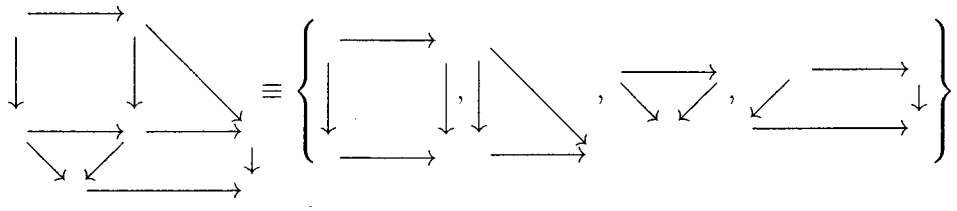

FIG. 9. An example of fragmentation.

Two of these are recoupling coefficients arising from identity recouplings. If the couplings are orthogonal then the identity recoupling coefficients are Kronecker deltas. Hence the recoupling coefficient would further reduce to

$$\delta_{kk'}\delta_{mm'}\left\langle \begin{matrix} \mu & & \lambda_1 \\ & n'\nu & \end{matrix} \middle| \begin{matrix} \lambda_1 & & \mu \\ & n\nu & \end{matrix} \right\rangle. \tag{11}$$

In this case an imposing recoupling coefficient was reduced to a product of small recoupling coefficients.

VI. RECOUPLING DIAGRAM PROJECTION RULES

Recouplings are isomorphisms that formally reorganize statements of irreps. Hence recouplings give rise to the notion of a recoupling diagram such as those in Figs. 11–17. These diagrams represent differing sequences of formal rearrangements resulting in the same recoupling. Because recouplings are isomorphisms there is no guarantee that differing sequences achieving the same recoupling compose to give the same isomorphism. Any diagram for which they are the same is said to commute. Recall that each recoupling corresponds to a recoupling coefficient. Hence the commutativity of a recoupling diagram is equivalent to a collection of constraint equations on the recoupling coefficients. In principle the manipulation of recoupling coefficient equations can be replaced by the formal manipulation of recoupling diagrams (or equivalently binary trees). To perform this replacement one requires a procedure for obtaining equations of constraint from recoupling diagrams. We call this process diagram projection. This section develops a set of simple rules which perform the task of diagram projection.

A recoupling diagram is any two dimensional connected directed graph such that each vertex has at least two arrows and no edges cross. The edges are labeled by statements and each arrow corresponds to the obvious recoupling. For examples see the various recoupling diagrams given in Figs. 11–17. Every recoupling diagram is equivalent to a collection of polygonal diagrams. Moreover, a minimal collection is given by the polygons bounding each interior region of the diagram. We call this process fragmentation and each polygon a fragment. For an example of fragmentation see Fig. 9.

Recall that each vertex of a diagram generates a projection scheme. Hence every arrow (or recoupling) can be projected onto its corresponding recoupling coefficient. The projection of a polygonal recoupling diagram results in a polygonal diagram whose arrows are recoupling bra kets and vertices are single irrep statements. Such a diagram is equivalent to an equation of constraint. Projecting the collection of fragments for a diagram gives the collection of constraints equivalent to the commutativity of the original recoupling diagram. The process may be visualized by the scheme given in Fig. 10.

The procedure for obtaining the constraint equation from a given recoupling polygon is given by the following set of rules.

Theorem 2: (*Polygonal Diagram Projection Rules*) *A given polygonal recoupling diagram commutes if and only if the recoupling coefficient constraint constructed by the following rules holds:*

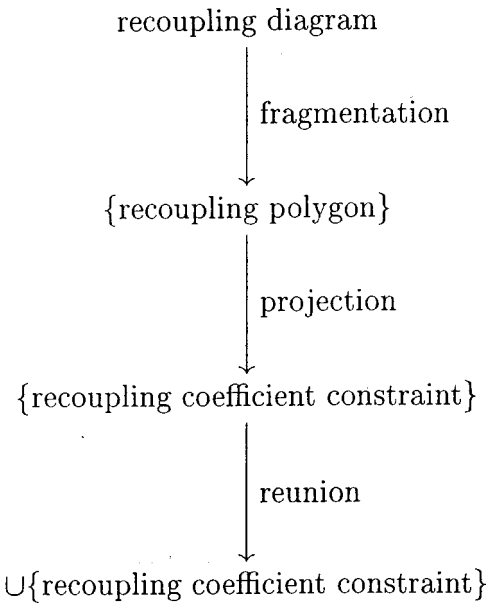

FIG. 10. Schematic depicting the extraction of the recoupling coefficient constraints corresponding to a recoupling diagram.

(i) Choose two vertices (possibly the same vertex) as a start and end vertex to split the polygonal diagram into two (resp. one) directed chains;
(ii) represent each arrow by the factorization of its corresponding recoupling coefficient;
(iii) compose the recoupling coefficients from right to left along each directed chain;
(iv) sum over all internal irrep labels and multiplicity labels that appear first in a ket and last in a bra (reading from left to right) for each recoupling expression;
(v) equate the recoupling coefficient expressions obtained. (Equate to the identity recoupling coefficient if there is only one expression.);
(vi) contract all identity recoupling coefficients with other recoupling coefficients where possible.

Two illustrations of the diagram projection rules are given in the proof of Theorem 3. We further illustrate these rules by deriving the generalized orthogonality condition satisfied by every recoupling coefficient. Let $\mathfrak{i}:S_n\rightarrow T_n$ be a recoupling. Consider the diagram projection of the trivial recoupling diagram given in Fig. 11. Diagram projection of this diagram, using the rules for polygonal diagram projection, gives the generalized recoupling coefficient orthogonality constraint

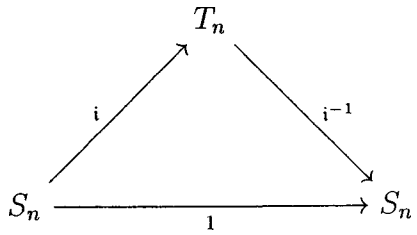

FIG. 11. The recoupling diagram $i^{-1}i=1$.

$$\sum_{i=1}^{n-1}\sum_{t_iT_i}\left\langle\begin{array}{c|c}S_n & T_n\\ s'_{n-1}S'_{n-1} & t_{n-1}T_{n-1}\\ \vdots & \vdots\\ s'_1S'_1 & t_1T_1\end{array}\right\rangle\left\langle\begin{array}{c|c}T_n & S_n\\ t_{n-1}T_{n-1} & s_{n-1}S_{n-1}\\ \vdots & \vdots\\ t_1T_1 & s_1S_1\end{array}\right\rangle=\left\langle\begin{array}{c|c}S_n & S_n\\ s'_{n-1}S'_{n-1} & s_{n-1}S_{n-1}\\ \vdots & \vdots\\ s'_1S'_1 & s_1S_1\end{array}\right\rangle. \tag{12}$$

If the couplings are orthogonal then the identity bra ket is a product of Kronecker deltas giving the standard orthogonality of recoupling coefficients. In particular the generalized orthogonality conditions for associative, commutative, and identity recoupling coefficients are given by taking $\mathfrak{i}$ to be $\mathfrak{a}$, $\mathfrak{c}$ and 1, respectively.

Note that not all recoupling diagrams give constraints on the recoupling coefficients as the following demonstrates.

Proposition 2: Given a recoupling polygon, then it is a natural diagram if and only if its diagram projection gives rise to no recoupling constraint.

This follows by noting that a polygon is a natural diagram if and only if the projection schema are not entangled. Hence the constraint obtained after diagram projection has recoupling coefficients with either an exact match on the other side of the expression or their inverse on the same side. Either way the sum over labels are not entangled and allow one to simply cancel coefficients on opposite sides or contract on the same side of the equation. Ultimately the constraint collapses completely to the equality of identity recoupling coefficients.

VII. RECOUPLING COEFFICIENT EXPANSION

Every recoupling can be built from a composed sequence of primitive recouplings. We call this a primitive expansion for the recoupling. In a symmetric tensor category the building block recouplings are the natural isomorphisms

$$\begin{gathered}1:1\to 1,\quad \alpha\mapsto 1_\alpha:\alpha\to\alpha,\\ \mathfrak{c}:\otimes\to\otimes\tau,\quad (\alpha,\beta)\mapsto\mathfrak{c}_{\alpha,\beta}:\alpha\otimes\beta\to\beta\otimes\alpha,\\ \mathfrak{a}:\otimes(\otimes\times 1)\to\otimes(1\times\otimes),\quad (\alpha,\beta,\gamma)\mapsto\mathfrak{a}_{\alpha,\beta,\gamma}:(\alpha\otimes\beta)\otimes\gamma\to\alpha\otimes(\beta\otimes\gamma),\end{gathered} \tag{13}$$

where τ is the flip map taking $(\alpha,\beta)\mapsto(\beta,\alpha)$. The primitive recouplings are those natural isomorphisms constructed from exactly one $\mathfrak{a}$ or $\mathfrak{c}$, as many 1s as required concatenated through $\otimes$ and finally binary bracketed. An example is $\mathfrak{i}:(((\lambda_1\otimes\lambda_2)\otimes\lambda_3)\otimes\lambda_4)\otimes\lambda_5\to\lambda_5\otimes((\lambda_2\otimes\lambda_3)\otimes(\lambda_1\otimes\lambda_4))$ given by the primitive expansion $\mathfrak{i}=(1.\mathfrak{a})[1.((1.\mathfrak{c}).1)][1.(\mathfrak{a}.1)]\mathfrak{c}$ where the recouplings $1.\mathfrak{a}$, $1.((1.\mathfrak{c}).1)$, $1.(\mathfrak{a}.1)$, and $\mathfrak{c}$ are primitive. Note that this is far from the only choice of primitive expansion for $\mathfrak{i}$.

A recoupling $\mathfrak{i}$ with a primitive expansion $\mathfrak{p}_1\ldots\mathfrak{p}_m$ forms the obvious polygonal recoupling diagram. Diagram projection of this diagram gives a primitive expansion of the recoupling coefficient for $\mathfrak{i}$ thus

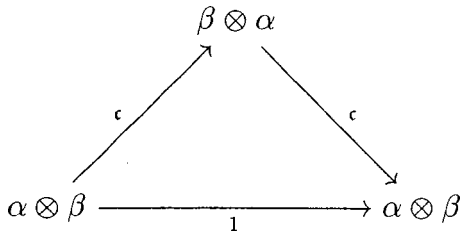

FIG. 12. The symmetry diagram.

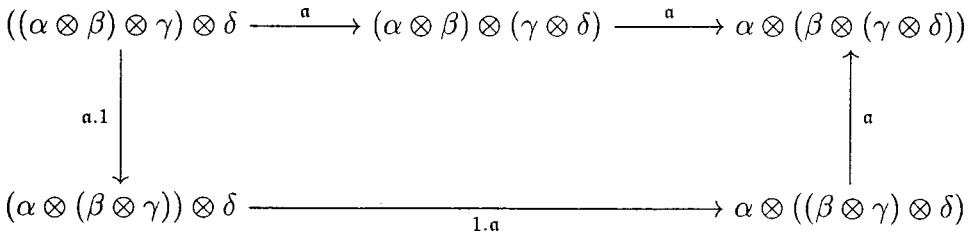

FIG. 13. The pentagon diagram.

$$\langle \vdots | \mathfrak{i} | \vdots \rangle = \sum_{\cdots} \langle \vdots | \mathfrak{p}_1 | \vdots \rangle \cdots \langle \vdots | \mathfrak{p}_m | \vdots \rangle, \tag{14}$$

where each $\langle \vdots | \mathfrak{p}_i | \vdots \rangle$ represents the recoupling coefficient factorization of the recoupling coefficient corresponding to $\mathfrak{p}_i$ and summation is over all labels appearing only on the left hand side of the expression.

VIII. COMPLETE SETS OF RECOUPLING COEFFICIENT CONSTRAINTS

There are many ways to recouple two statements that are obtained from differing sequences of formal rearrangements on statements of irreps. For example, the pentagon diagram given in Fig. 13 shows two different paths recoupling $((\alpha\otimes\beta)\otimes\gamma)\otimes\delta$ to $\alpha\otimes(\beta\otimes(\gamma\otimes\delta))$. The property of oherence demands that these two paths compose to give the same isomorphism. More generally coherence demands that all formally constructed recoupling diagrams commute. The standard coherence result of Mac Lane[5] in symmetric tensor categories guarantees that all (formal) recoupling diagrams commute if and only if the symmetry, pentagon, and hexagon diagrams given in Figs. 12, 13, and 14 commute.

A (minimal) generating set of recoupling coefficient constraints is obtained by diagram projecting the symmetry, pentagon, and hexagon diagrams.

Theorem 3: *All recoupling diagrams commute if and only if the following list of recoupling coefficient constraints hold:*

(i) The symmetry equation

$$\sum_l \left\langle \begin{matrix} \alpha & & \beta \\ & k'\lambda & \end{matrix} \middle| \begin{matrix} \beta & & \alpha \\ & l\lambda & \end{matrix} \right\rangle \left\langle \begin{matrix} \beta & & \alpha \\ & l\lambda & \end{matrix} \middle| \begin{matrix} \alpha & & \beta \\ & k\lambda & \end{matrix} \right\rangle = \left\langle \begin{matrix} \alpha & & \beta \\ & k'\lambda & \end{matrix} \middle| \begin{matrix} \alpha & & \beta \\ & k\lambda & \end{matrix} \right\rangle, \tag{15}$$

(ii) The pentagon equation

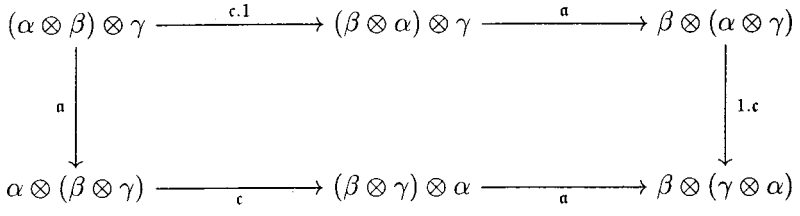

FIG. 14. The hexagon diagram.

$$\sum_{k'} \left\langle \begin{matrix} \alpha & & (\beta & & \rho) \\ & \alpha & & s\sigma & \\ & & l\lambda & & \end{matrix} \middle| \begin{matrix} (\alpha & & \beta) & & \rho \\ & m\mu & & & \\ & & k'\lambda & & \end{matrix} \right\rangle$$
$$\cdot \left\langle \begin{matrix} \mu & & (\gamma & & \delta) \\ & \mu & & r\rho & \\ & & k'\lambda & & \end{matrix} \middle| \begin{matrix} (\mu & & \gamma) & & \delta \\ & n\nu & & & \\ & & k\lambda & & \end{matrix} \right\rangle$$
$$= \sum_{\eta s' n'} \left\langle \begin{matrix} \beta & & (\gamma & & \delta) \\ & \beta & & r\rho & \\ & & s\sigma & & \end{matrix} \middle| \begin{matrix} (\beta & & \gamma) & & \delta \\ & h\eta & & & \\ & & s'\sigma & & \end{matrix} \right\rangle$$
$$\cdot \left\langle \begin{matrix} \alpha & & (\eta & & \delta) \\ & \alpha & & s'\sigma & \\ & & l\lambda & & \end{matrix} \middle| \begin{matrix} (\alpha & & \eta) & & \delta \\ & n'\nu & & & \\ & & k\lambda & & \end{matrix} \right\rangle$$
$$\cdot \left\langle \begin{matrix} \alpha & & (\beta & & \gamma) \\ & \alpha & & h\eta & \\ & & \eta'\nu & & \end{matrix} \middle| \begin{matrix} (\alpha & & \beta) & & \gamma \\ & m\mu & & & \gamma \\ & & n\nu & & \end{matrix} \right\rangle, \tag{16}$$

(iii) The hexagon equation

$$\sum_{m'n'} \left\langle \begin{matrix} \gamma & & \alpha \\ & n\nu & \end{matrix} \middle| \begin{matrix} \alpha & & \gamma \\ n'\nu & & \end{matrix} \right\rangle \left\langle \begin{matrix} \beta & & (\alpha & & \gamma) \\ & \beta & & n'\nu & \\ & & l\lambda & & \end{matrix} \middle| \begin{matrix} (\beta & & \alpha) & & \gamma \\ & m'\mu & & & \\ & & k\lambda & & \end{matrix} \right\rangle$$
$$\cdot \left\langle \begin{matrix} \beta & & \alpha \\ & m'\mu & \end{matrix} \middle| \begin{matrix} \alpha & & \beta \\ & m\mu & \end{matrix} \right\rangle$$
$$= \sum_{\eta k' l'} \left\langle \begin{matrix} \beta & & (\gamma & & \alpha) \\ & \beta & & n\nu & \\ & & l\lambda & & \end{matrix} \middle| \begin{matrix} (\beta & & \gamma) & & \alpha \\ & h\eta & & & \\ & & l'\lambda & & \end{matrix} \right\rangle \left\langle \begin{matrix} \eta & & \alpha \\ & l'\lambda & \end{matrix} \middle| \begin{matrix} \alpha & & \alpha \\ & & k'\lambda \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} \alpha & & (\beta & & \gamma) \\ & \alpha & & h\eta & \\ & & k'\lambda & & \end{matrix} \middle| \begin{matrix} (\alpha & & \beta) & & \gamma \\ & m\mu & & & \\ & & k\lambda & & \end{matrix} \right\rangle. \tag{17}$$

Proof: The proof is by diagram projection of the symmetry, pentagon, and hexagon diagrams. The symmetry equation follows immediately. Cutting the pentagon diagram at the top left hand side and top right hand side vertices [rule (i)], diagram projection gives [rules (ii) to (v)]

$$\sum_{m'k'r'} \left\langle \begin{matrix} \alpha & & (\beta & & \rho) \\ & \alpha & & s\sigma & \\ & & l\lambda & & \end{matrix} \middle| \begin{matrix} (\alpha & & \beta) & & \rho \\ & m'\mu & & & \\ & & k'\lambda & & \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} \gamma & & \delta \\ & r\rho & \end{matrix} \middle| \begin{matrix} \gamma & & \delta \\ & r'\rho & \end{matrix} \right\rangle \cdot \left\langle \begin{matrix} \mu & & (\gamma & & \delta) \\ & \mu & & r'\rho & \\ & & k'\lambda & & \end{matrix} \middle| \begin{matrix} (\mu & & \gamma) & & \delta \\ & n\nu & & & \\ & & k\lambda & & \end{matrix} \right\rangle$$
$$\times \left\langle \begin{matrix} \alpha & & \beta \\ & m'\mu & \end{matrix} \middle| \begin{matrix} \alpha & & \beta \\ & m\mu & \end{matrix} \right\rangle$$

$$= \sum_{\eta h' s' n' p q} \left\langle \begin{matrix} \beta & & (\gamma & & \delta) \\ & \beta & & r\rho & \\ & & s\sigma & & \end{matrix} \middle| \begin{matrix} (\beta & & \gamma) & & \delta \\ & h'\eta & & & \\ & & & s'\sigma & \end{matrix} \right\rangle$$

$$\times \left\langle \begin{matrix} \alpha & & \sigma \\ & l\lambda & \end{matrix} \middle| \begin{matrix} \alpha & & \sigma \\ & q\lambda & \end{matrix} \right\rangle \cdot \left\langle \begin{matrix} \alpha & & (\eta & & \delta) \\ & \alpha & & s'\sigma & \\ & & q\lambda & & \end{matrix} \middle| \begin{matrix} (\alpha & & \eta) & & \delta \\ & n'\nu & & & \\ & & & p\lambda & \end{matrix} \right\rangle$$

$$\times \left\langle \begin{matrix} \beta & & \gamma \\ & h'\eta & \end{matrix} \middle| \begin{matrix} \beta & & \gamma \\ & h\eta & \end{matrix} \right\rangle \cdot \left\langle \begin{matrix} \alpha & & (\beta & & \gamma) \\ & \alpha & & h\eta & \\ & & n'\nu & & \end{matrix} \middle| \begin{matrix} (\alpha & & \beta) & & \gamma \\ & m\mu & & & \\ & & & n\nu & \end{matrix} \right\rangle$$

$$\times \left\langle \begin{matrix} \nu & & \delta \\ & p\lambda & \end{matrix} \middle| \begin{matrix} \nu & & \delta \\ & k\lambda & \end{matrix} \right\rangle. \tag{18}$$

Similarly cutting the hexagon diagram at the top left hand and bottom right hand vertices [rule (i)], diagram projection gives [rules (i) to (v)]

$$\sum_{k' l' m' n'} \left\langle \begin{matrix} \gamma & & \alpha \\ & n\nu & \end{matrix} \middle| \begin{matrix} \alpha & & \gamma \\ & n'\nu & \end{matrix} \right\rangle \left\langle \begin{matrix} \beta & & \nu \\ & l\lambda & \end{matrix} \middle| \begin{matrix} \beta & & \nu \\ & l'\lambda & \end{matrix} \right\rangle$$

$$\times \left\langle \begin{matrix} \beta & & (\alpha & & \gamma) \\ & \beta & & n'\nu & \\ & & l'\lambda & & \end{matrix} \middle| \begin{matrix} (\beta & & \alpha) & & \gamma \\ & m'\mu & & & \\ & & & k'\lambda & \end{matrix} \right\rangle$$

$$\times \left\langle \begin{matrix} \beta & & \alpha \\ & m'\mu & \end{matrix} \middle| \begin{matrix} \alpha & & \beta \\ & m\mu & \end{matrix} \right\rangle \cdot \left\langle \begin{matrix} \mu & & \gamma \\ & k'\lambda & \end{matrix} \middle| \begin{matrix} \mu & & \gamma \\ & k\lambda & \end{matrix} \right\rangle$$

$$= \sum_{\eta h' k' l'} \left\langle \begin{matrix} \beta & & (\gamma & & \alpha) \\ & \beta & & n\nu & \\ & & l\lambda & & \end{matrix} \middle| \begin{matrix} (\beta & & \gamma) & & \alpha \\ & h'\eta & & & \\ & & & l'\lambda & \end{matrix} \right\rangle$$

$$\times \left\langle \begin{matrix} \eta & & \alpha \\ & l'\lambda & \end{matrix} \middle| \begin{matrix} \alpha & & \eta \\ & k'\lambda & \end{matrix} \right\rangle \cdot \left\langle \begin{matrix} \beta & & \gamma \\ & h'\eta & \end{matrix} \middle| \begin{matrix} \beta & & \gamma \\ & h\eta & \end{matrix} \right\rangle$$

$$\times \left\langle \begin{matrix} \alpha & & (\beta & & \gamma) \\ & \alpha & & h\eta & \\ & & k'\lambda & & \end{matrix} \middle| \begin{matrix} (\alpha & & \beta) & & \gamma \\ & m\mu & & & \\ & & & k\lambda & \end{matrix} \right\rangle. \tag{19}$$

Finally, the pentagon and hexagon equations follow by contracting the identities with the non-identity recoupling coefficients in the above two equations [rule (vi)]. The validity of this rule is seen by projecting the trivial diagrams $1^2=1$, $\mathfrak{i}1=\mathfrak{i}$ and $1\mathfrak{i}=1$.

IX. THE WIGNER *j* SYMBOLS

In this section we derive a set of constraints for the Wigner 3j and 6j symbols that turn out to give the symmetry equation, the Biedenharn–Elliott equation, and the Racah backcoupling equation. These equations arise from an alternative choice of primitive recouplings and consequently an alternative collection of recoupling diagrams guaranteeing coherence.[9] Define the primitive recouplings

$$3\mathrm{j}: \otimes \to \otimes\tau, \quad (\alpha,\beta) \mapsto \mathfrak{c}_{\alpha,\beta}: \alpha\otimes\beta \to \beta\otimes\alpha \tag{20}$$

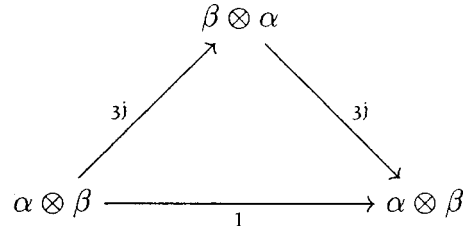

FIG. 15. The symmetry diagram.

$$6\mathrm{j}:\otimes(\otimes\times 1)\to\otimes(\otimes\times 1)\tau_{(13)},\quad(\alpha,\beta,\gamma)\mapsto[(\mathfrak{c}.1)\mathfrak{ca}]_{\alpha,\beta,\gamma}:(\alpha\otimes\beta)\otimes\gamma\to(\gamma\otimes\beta)\otimes\alpha. \quad (21)$$

These primitive recouplings are formally transpositions. The 3j recoupling flips two irrep statements. The 6j recoupling interchanges the first and third irrep (sub)statements in a binary bracketed triplet. Loosely speaking the first generates the $3j$ symbol and the second the $6j$ symbol. Specifically from Joyce[9] the 3j symbol is given by

$$\{(12),\alpha\beta\lambda\}^{k}_{l}=\left\langle \begin{matrix}\beta & & \alpha\\ & l\lambda^{*} & \end{matrix}\middle|\begin{matrix}\alpha & & \beta\\ & k\lambda^{*} & \end{matrix}\right\rangle \quad (22)$$

and the $6j$ symbol by

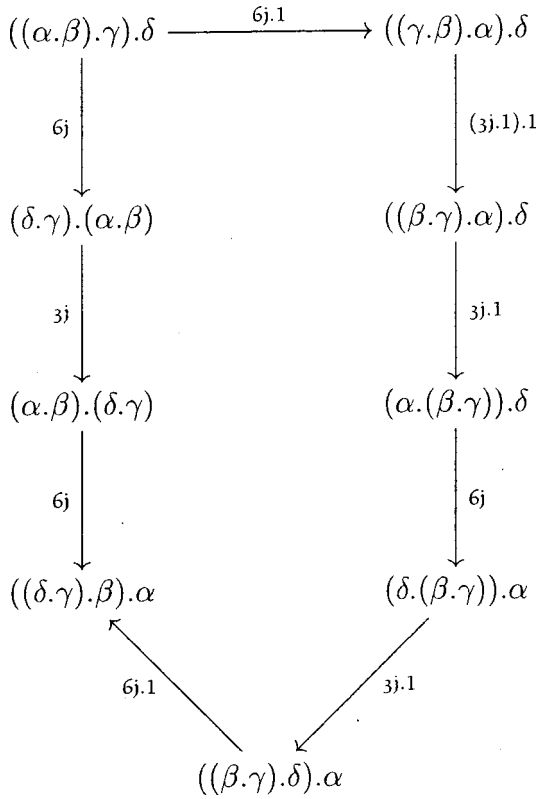

FIG. 16. A nonagonal diagram.

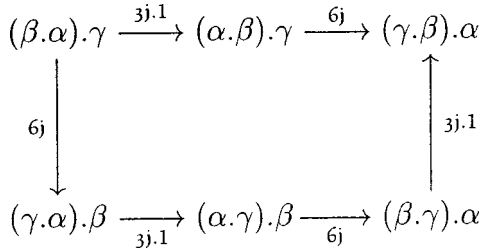

FIG. 17. A hexagonal diagram.

$$\begin{Bmatrix} \alpha & \beta & \mu \\ \gamma & \lambda & \nu \end{Bmatrix}_{lnkm} = \sum_{rs} \{\lambda\}\{*,\alpha\beta\mu\}^{m}_{r}\{*,\mu^{*}\gamma\lambda^{*}\}^{k}_{s} \cdot \left\langle \begin{matrix} (\gamma & & \beta) & & \alpha \\ & n\nu & & \alpha & \\ & & l\lambda & & \end{matrix} \middle| \begin{matrix} (\alpha & & \beta) & & \gamma \\ & r\mu^{*} & & \gamma & \\ & & s\lambda & & \end{matrix} \right\rangle . \tag{23}$$

These symbols differ from the usual definitions (see Butler[15]) by dimension factors and historical phase choices both of which are unnecessary complications.[9] Note that the 6j symbol is defined without using 3j symbols and consequently should not be viewed as being generated by the $\mathfrak{a}$ recoupling. The 3j symbol is equivalent to the M matrices of Derome and Sharp[16] and the $\{*,\mu^{*}\gamma\lambda^{*}\}^{k}_{s}$ symbols to the A matrices of Derome and Sharp.[16]

Direct substitution of $\mathfrak{c}$=3j and $\mathfrak{a}$=3j(3j.1)6j into the symmetry, pentagon, and hexagon diagrams gives an equivalent set of recoupling coherence conditions given by Figs. 15, 16, and 17. Diagram projection of the recoupling diagrams in Figs. 15, 16, and 17 gives the following result by the previous theorem.

Theorem 4: *All recoupling diagrams commute if and only if the following list of recoupling coefficient constraints hold.*

(i) The symmetry equation

$$\sum_{l} \{(12),\beta\alpha\lambda\}^{l}_{k'}\{(12),\alpha\beta\lambda\}^{k}_{l} = \left\langle \begin{matrix} \alpha & & \beta \\ & k'\lambda & \end{matrix} \middle| \begin{matrix} \alpha & & \beta \\ & k\lambda & \end{matrix} \right\rangle , \tag{24}$$

(ii) The Biedenharn–Elliott equation

$$\begin{aligned} &\sum_{ra} \{\lambda\}(\{*,\alpha\beta\mu\}^{-1})^{r}_{a}\{(12),\beta\alpha\mu\}^{m}_{r}\begin{Bmatrix} \alpha & \beta & \mu \\ \gamma & \lambda & \nu \end{Bmatrix}_{lnka} \\ &\quad = \sum_{\sigma stuvpqw} (\{*,\alpha\gamma\sigma^{*}\}^{-1})^{t}_{p}(\{*,\sigma\beta\lambda^{*}\}^{-1})^{v}_{q}(\{*,\beta\alpha\mu\})^{-1^{m}}_{w} \\ &\qquad \cdot \{(12),\beta\gamma\nu^{*}\}^{s}_{n}\{(12),\gamma\alpha\sigma^{*}\}^{u}_{t}\begin{Bmatrix} \alpha & \gamma & \sigma^{*} \\ \beta & \lambda & \nu \end{Bmatrix}_{lsqp} \cdot \begin{Bmatrix} \beta & \alpha & \mu \\ \gamma & \lambda & \sigma \end{Bmatrix}_{vukw} , \end{aligned} \tag{25}$$

(iii) The Racah backcoupling equation

$$\sum_{abf} \{\sigma\}\{\eta\}(\{*,\mu^*\rho\lambda^*\}^{-1})^b_f\{(12),\rho\mu^*\lambda^*\}^a_b \cdot \begin{Bmatrix} \alpha & \beta & \mu \\ \rho & \lambda & \eta \end{Bmatrix}_{lnfm} \begin{Bmatrix} \mu^* & \gamma & \sigma^* \\ \delta & \lambda & \rho \end{Bmatrix}_{arks}$$

$$= \sum_{\nu cdpntqjvu} (\{*,\beta\gamma\nu^*\})^{-1^n}_j(\{*,\nu\delta\eta^*\}^{-1})^c_u(\{*,\alpha\nu\sigma^*\}^{-1})^p_v$$

$$\cdot\{(12),\delta\nu\eta^*\}^d_c\{(12),\nu\alpha\sigma^*\}^q_p\{(12),\gamma\beta\nu^*\}^t_n$$

$$\cdot \begin{Bmatrix} \beta & \gamma & \nu^* \\ \delta & \eta & \rho \end{Bmatrix}_{hruj} \begin{Bmatrix} \alpha & \nu & \sigma^* \\ \delta & \lambda & \eta \end{Bmatrix}_{ldkv} \begin{Bmatrix} \alpha & \beta & \mu \\ \gamma & \sigma & \nu \end{Bmatrix}_{qtsm}. \tag{26}$$

Diagram projection of the symmetry, nonagonal, and hexagonal diagrams given in Figs. 15, 16, and 17, followed by substitution of each j symbol for its corresponding recoupling coefficient and finally rearrangement and contraction of terms gives the three, j symbol constraints in the hypothesis. The explicit details are to be found in Joyce.[9]

X. CONCLUSION

We have given a concise definition to the concept of coupling and its important properties. Note that we did not require the couplings to be orthogonal. The notion of a projection scheme was defined giving a canonical mechanism for obtaining recoupling coefficients from a recoupling. The language of category theory was found to be the best framework for these ideas. These definitions were a necessary prerequisite to what followed.

Next we gave three important and useful techniques for recoupling coefficients. The first, recoupling coefficient factorization allows one to write a recoupling as a product (without summation) of smaller degree coefficients. The second, primitive expansion, allows a recoupling coefficient to be expressed in terms of primitive recoupling coefficients. The third and most useful, diagram projection, allows one to obtain the underlying recoupling coefficient constraints associated with a recoupling diagram. This affords one the convenience of working at the combinatorial recoupling level. The recoupling coefficient constraints may be obtained at any stage using the rules of diagram projection. A forthcoming paper will use this idea to give an algorithm for the direct calculation of recoupling coefficients that is not based on solving linear recursion equations.

The diagram projection rules allow one to obtain a complete set of constraints for the recoupling coefficients. We diagram projected the recoupling diagrams defining a symmetric tensor category to obtain the symmetry, pentagon, and hexagon equations. These form a complete set of constraints having less recoupling coefficient factors than the classical Biedenharn–Elliott and Racah backcoupling equations and are a viable alternative for any computation scheme. Finally, we gave the recouplings corresponding to the j symbols of Wigner, derived a collection of recoupling diagrams guaranteeing coherence, and recovered from these using diagram projection the Biedenharn–Elliott and Racah backcoupling equations.

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Quotient of a loop group and Witten genus

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We define a Dirac–Ramond operator over the quotient $(LG)/H$ of a loop group by a subgroup H of the compact Lie group G. We state the conjecture that its equivariant Index with respect of the natural circle action over the quotient of the loop group is equal to the Witten genus of the homogeneous manifold G/H. We motivate the conjecture by a short time argument which allows to come back to a Dirac–Ramond operator at the manner of Taubes on a limit model where all the computations can be done by hand. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Let us consider the free loop space $L(M)$ of a compact manifold; it is endowed with a natural circle action. The fixed point set of this circle action is the manifold itself.

In finite dimension, when there is a circle action over a manifold, there are two types of relations between the fixed point set and the total space. It is the purpose of the Berline–Vergne localization formulas[1] and of the Lefschetz formulas.[2,3] In the first case, we localize the integrals over the fixed point set; in the second case, using the method of Taubes,[3] we localize the operators over the fixed point set.

Over the loop space, the Berline–Vergne localization formulas give the index theorem for the Dirac operator over a manifold.[4,5] If we localize an operator, this gives the Index theorem over the loop space, which gives quantities which are very important for algebraic topology as it was noticed by Witten.[6–8]

The problem for Lefschetz formula over the loop space is that it is purely hypothetical. Taubes[3] gives a rigorous construction for a limit model. He considers as model of the free loop space the family of flat loops on the tangent space. He considers a measure over the flat loop space, which lives over random distributions, and whose choice comes from quantum field theory. So we cannot curve its model.

There is another way to attack the problem of defining the Dirac–Ramond operator over the loop space and others geometrical operators: it is the way followed by Léandre-Roan,[9] Jones-Léandre,[10] and Léandre[11] (see in Ref. 12 the survey of Léandre). We consider the Brownian bridge measure. There is a tangent Hilbert space, which allows us to state integration by parts formulas over the free loop space. Reference 9 meets the problem that the tangent Hilbert space is not stable by Lie brackets; a connection allows us to compute a regularized stochastic exterior derivative and to compute its adjoint. This gives a rigorous approach to the Euler–Poincaré characteristic of Dixon–Harvey–Vafa–Witten of an orbifold.[13] Reference 11 meets the same problem for the Dolbeault operator over the loop space of a Kaehler manifold, with the natural polarization over the loop space which results from the polarization of the Kaehler manifold. This gives a rigorous approach to Hirzebruch's genus of level N.[14]

The problem is to construct the Dirac–Ramond operator over the loop space. Reference 10 present only a beginning of construction of it. Namely, if we follow Taubes approach to construct the Dirac–Ramond operator over the free loop space, we have to extend over the free loop space the natural polarization which arises from Fourier series. This leads to complicated considerations.

We remark that over a loop group, if we consider the tangent space of a loop group, we do not meet the previous difficulties. For instance, the tangent space of a loop group is stable by Lie

bracket. This allows us to compute a true exterior derivative and its adjoint (and not a regularized one as in Refs. 10 and 9) in Ref. 15. The polarization by Fourier series is well defined over the loop group. But the Witten genus of a group is trivial, because the tangent bundle of a Lie group G is trivial.

The idea is to consider $(LG)/H$ where H is a maximal torus of G, where G is a noncommutative Lie group. It inherits clearly a circle action over it, and its fixed point set coincides with a countable disjoint unions of the homogeneous space G/H.

So the natural conjecture is the following:

Conjecture (Bismut): Over $(LG)/H$, there is a Dirac–Ramond–Taubes operator which is invariant under the natural circle action over $(LG)/H$ and it is possible to define its ''renormalized'' equivariant Index which is equal to the Witten genus of G/H.

The purpose of this work is to give a stochastic approach to this conjecture.

We construct in the first part an H-equivariant operator over LG, which generalizes the construction of Taubes. For that, we suppose that the homogeneous space G/H is Kaehlerian and spin. This operator is invariant under the natural circle action over LG. The space of functionals over $(LG)/H$ can be seen as a functional over LG which is invariant under the H action, which induces an action by isometries over it. Since H is finite dimensional, the analysis over $(LG)/H$ comes ultimately to the analysis over LG for H invariant functionals. This allows us to define a Dirac–Ramond operator over $(LG)/H$, which follows precisely the prescriptions of Taubes.

In a second time, we consider the loop group in small time, and we repeat the considerations in this loop group context of Refs. 9, 10, and 11 to motivate the conjecture. We deform the Hilbert space of the theory and we arrive at the limit to a limit operator at the manner of Taubes, whose equivariant index is the Witten genus G/H. The price to pay in order to be able to do the asymptotic expansion of the Dirac–Ramond–Taubes operator near the constant loops is that we have to change completely the structure of the considered Dirac operator. In particular we suppose G/H spin and Kaehlerian, and we work in order to perform Bismut's dilatation over the small elements of $(LG)/H$. The reader interested by short time asymptotic expansion can see the surveys of Kusuoka,[16] Watanabe,[17] and Léandre.[18]

The question which is put by this work is the following: Taubes construction of the Dirac–Ramond operator over the loop space is a construction by hand, which avoids the theory of spin representation of loop group. On the other hand, there is a theory of spinor fields over the loop space,[19–21] and in particular, by using the fact that there is a measure over the loop space, the definition of Hilbert spaces of sections of the spin bundle over the loop space,[22–24] where the Dirac–Ramond operator should act. What is the relation between the two point of view?

We refer to the two surveys of Léandre[12,25] for the interaction between analysis over loop space and topology.

II. CONSTRUCTION OF THE DIRAC–RAMOND–TAUBES OPERATOR

Let G be a compact simply connected Lie group. We consider the Killing metric over its Lie algebra Lie G. We consider the Brownian motion over G staring from g. It is the solution of the following stochastic differential equation starting from g:

$$dg_s = g_s dB_s, \tag{2.1}$$

where B_s is a Brownian motion over Lie G and where d denotes the Stratonovitch differential. It has an heat kernel $p_t(g,g')$ with respect to the Haar measure $d\pi(g)$ over G. Over the free loop group of G called $L(G)$ of continuous loops, we consider the following measure:

$$d\mu_{G,1} = \frac{p_1(g,g)d\pi(g)\otimes dP_{1,g}}{\int p_1(g,g)dg}, \tag{2.2}$$

where $P_{1,g}$ is the law of the Brownian bridge starting from g and arriving in g in time 1. For a cylindrical functional $F(g_{s_1},\ldots,g_{s_r})$, $s_1<s_2<\cdots<s_r$, we have a more explicit description of $\mu_{G,1}$ in terms of the heat kernel,

$$E[F(g_{s_1},\ldots,g_{s_r})]=\frac{1}{\int p_1(g,g)d\pi(g)}\int\ldots\int p_{s_2-s_1}(g_1,g_2)$$

$$p_{s_3-s_2}(g_2,g_3)\ldots p_{s_r-s_1}(g_r,g_1)F(g_1,\cdots,g_r)d\pi(g_1)\cdots d\pi(g_r). \tag{2.3}$$

Let us remark that by the symmetry of Eq. (2.1), $p_1(g,g)=p_1(e,e)$ such that $\int p_1(g,g)d\pi(g)=p_1(e,e)$.

We consider as tangent space of an element $g_.$ of the loop group the set of $X_.$ where $X_s=g_sK_s$ such that $K_0=K_1$ and where the path $K_.$ in the Lie algebra of G is of finite energy. We introduce the following Hilbert structure:

$$\|X_.\|_{g_.}=\int_0^1|K_s|^2ds+\int_0^1|K_s'|^2ds. \tag{2.4}$$

There is a natural circle action over $L(G)$; if $q=\exp[2i\pi t]$ belongs to the circle, $q(g_.)_s=g_{s-t}$.

This natural circle action preserves the measure as well the tangent bundle of the loop group: it preserves therefore the metric, since g induce a rotation from Lie(G) into the tangent space of G at g. If we complify the tangent space of $g_.$ $T_{g_.}$ into $T_{g_.}\otimes C$ and if the real complex structure (2.4) is transformed into the natural complex Hilbert structure over the complexified tangent space, there is a natural orthonormal basis of $T_{g_.}\otimes C$ starting from a real orthonormal basis e_i of Lie(G). It is given by

$$X_n(e_i)_s=g_s\frac{\exp[2\pi ins]e_i}{\sqrt{Cn^2+1}}. \tag{2.5}$$

This splits $T_{g_.}\otimes C$ into H_-+E+H_+. H_+ corresponds to a strictly positive n, H_- corresponds to $n<0$, and E to $n=0$. We have therefore a polarization over the loop group which comes from the Fourier expansion.

We remark that the tangent bundle is stable by Lie bracket. If $X_s=g_sK_s(X)$ and $Y_s=g_sK_s(Y)$, where $K_s(X)$ and $K_s(Y)$ are deterministic, we have

$$[X,Y]_s=g_s[K_s(X),K_s(Y)]. \tag{2.6}$$

Moreover, H_+ and H_- are stable by the Lie bracket. Under the natural circle action by q in the circle, $X_n(e_i)_.$ behaves as q^{-n} if e_i is deterministic.

There is a Levi-Civita connection over $L(G)$ which is given for real vector fieds $X_.$, $Y_.$, and $Z_.$ by a formula of [K.N] p. 160. We have

$$2\langle\nabla_{X_.}Y_.,Z_.\rangle=X_..\langle Y_.,Z_.\rangle+Y_..\langle X_.,Z_.\rangle-Z_..\langle X_.,Y_.\rangle+\langle[X_.,Y_.],Z_.\rangle$$
$$+\langle[Z_.,X_.],Y_.\rangle+\langle X_.,[Z_.,Y_.]\rangle. \tag{2.7}$$

If we consider the vector fields $X_n(e_i)_.$ for e_i deterministic, $\langle X_n(e_i)_.,X_m(e_j)\rangle=\delta_{n,m}\delta_{i,j}$ and

$$\langle\nabla_{X_{p(e)_.}}X_n(f)_.,X_m(f')_.\rangle=C(p,n,m,e,f,f') \tag{2.8}$$

is deterministic. Moreover, (2.7) show, if n and m are positive, that $\nabla_{X_n(e_i)_.}X_m(e_j)_.$ is a linear combination of $X_{n+m}(e_k)_.$

The problem is to understand E now. For that we introduce a compact Lie group H which is a maximal torus of G. We suppose that G/H is spin and Kaehlerian. We suppose that the Kaehler structure is compatible with the action of G over G/H. We can decompose the complexified Lie algebra of G into $n_+ + \mathrm{Lie}(H) + n_-$. Let us detail how we proceed. Let us introduce the canonical projection $p: G \to G/H$. G becomes a fibration over G/H with fiber H. Let us consider $g \in p^{-1}(x)$, where x denoted the typical element of G/H. At g, the complexified tangent space of G, $T_g \otimes C$, has the direct orthogonal decomposition $n_+(g) + T_{p^{-1}(x)} \otimes C + n_-(g)$. The fact that we have a Kaehler structure over G/H implies that $[h, f_+]$ belongs still in n_+ if h belongs to the Lie algebra of H and if f_+ belongs to n_+. The analogous statement remains true for n_-. By the action of G, $n_+(g)$ can be identified with the set of $T^{1,0}$ vectors $\partial/\partial z$ over G/H and $n_-(g)$ can be identified with the sets of $T^{0,1}$ vectors $\partial/\partial\overline{z}$ over G/H. (Let us recall that $T^{1,0}$ is the set of eigenvectors $\partial/\partial z$ associated with the eigenvalue i for the complex structure J over G/H and that $T^{0,1}$ is the set of eigenvectors $\partial/\partial\overline{z}$ associated with the eigenvalue $-i$ for the complex structure J.)

We deduce a decomposition of E into $N_+ + O + N_-$ which is orthogonal. Moreover, this decomposition is invariant by rotation, because the action of $g \in G$ preserves the Kaehler structure of G/H.

Let us recall that over G/H, there is a $\overline{\partial}$ operator: $T^{1,0}$ forms are called dz and $T^{0,1}$ forms are called $d\overline{z}$. We introduce the Levi-Civita connection over G/H: it preserves, since G/H is supposed Kaehlerian, the decomposition of the complexified tangent space in $T^{1,0}$ and in $T^{0,1}$. The same is true for the forms. We consider the bundle $\Lambda(T^{0,1})$ and we consider the $\overline{\partial}$ operator,

$$\overline{\partial}_f = \sum d\overline{z}_i \wedge \nabla_{\partial/\partial\overline{z}_i} \tag{2.9}$$

for the Levi-Civita connection (see Ref. 26) where we take the sum over a local orthonormal basis of $T^{0,1}$. We can tensorize this operator by an auxiliary complex hermitian bundle ξ endowed with an Hermitian connection.

This allows us to construct the Dirac operator over G/H in terms of a twisted Dolbeault operator, if we suppose G/H spin (see Ref. 26, p. 186). We consider a square root of the canonical bundle $\Lambda^{n,0}$, whose curvature is given by $2R$, which is a closed $4\pi i Z$ valued form over G/H. We consider its dual ξ', which can be endowed with a Hermitian structure and a connection whose curvature is $-R$. We consider the $\overline{\partial}$ operator twisted by ξ'. This gives a realization of the Dirac operator over G/H.

Let $-R$ be the curvature of ξ'. We construct a complex line bundle over $L(G)$ by proceeding as follows; we consider the form $-p^*R$ over G: it is $2\pi i Z$ valued. We construct the form $\sigma = -\int_0^1 p^*(R)(g_s)(.)ds$ over $L(G)$. It is still closed $2i\pi Z$ valued. This form determines, since G is supposed simply connected and therefore $L(G)$ is simply connected, a complex line bundle ξ_∞ over $L(G)$. Let us recall[20,27,24,28] how to do it, in order to construct it. In order to simplify the exposure, we will work over the Hoelder loop space $L_{1/2-\epsilon}(G)$: it is possible to assume this because the Brownian loop is almost surely Hoelder,

$$\sup \frac{d(g_s, g_t)}{d(s,t)^{1/2-\epsilon}} < \infty, \tag{2.10}$$

where $d(g_s, g_t)$ denoted the Riemannian distance over the group between g_s and g_t and $d(s,t)$ denoted the Riemannian distance over the circle between s and t. This will allow us to produce smooth sections of the line bundle ξ_∞, whose existence is strongly based upon the existence of partition of unity over the loop space, which does not exist if the loops $g_.$ are only continuous.

We consider the system of balls $B(g_{\alpha.}; \delta)$ for the uniform distance of radius δ and of center the smooth loop $g_{\alpha.}$. We construct over this ball the curve

$$l_\alpha(g_.)(t)_s = \exp[t(g_s - g_{\alpha,s})], \tag{2.11}$$

where we consider the exponential of the Lie group. Let us explain what we mean by this notation: there is a unique geodesic joining $g_{\alpha,s}$ to g_s whose driving vector is denoted by $g_s - g_{\alpha,s}$ and belongs to the tangent space of G in $g_{\alpha,s}$. We consider the geodesic joining $g_{\alpha,s}$ to g_s, which coincide since we consider over G the binvariant metric with the traditional exponential over a Lie group, since g_s and $g_{\alpha,s}$ are closed. If $g_.$ belongs to the intersection of $B(g_{\alpha.};\delta)$ and of $B(g_{\beta.};\delta)$, we can construct a system of transition functionals as follows: we join the two loops $l_\alpha(g_.)(t)_.$ and $l_\beta(g_.)(t)_.$ by using the Lie group exponential. This constitutes a small triangle. We use the fact that $\Pi_2(G)=0$ in order to find a big triangle whose boundary is any path joining $e_.$ to $g_{\alpha.}$, the exponential curve joining $g_{\alpha.}$ to $g_{\beta.}$ and any curve joinning $g_{\beta.}$ to $e_.$. We produced a distinguished surface $S_{\alpha,\beta}(g_.)$ in $L_{1/2-\epsilon}(G)$ whose boundary is the distinguished path $l_\alpha(g_.)$ joining $e_.$ to $g_.$ and the path $l_\beta(g_.)$ circled in the opposite sense.

We put

$$\rho_{\alpha,\beta}(g_.)=\exp\left[-2i\pi\int_{S_{\alpha,\beta}(g_.)}\sigma\right]. \tag{2.12}$$

It is a smooth functional in the traditional sense over the intersection of the two ball $B(g_{\alpha.};\delta)$ and $B(g_{\beta.};\delta)$ (and not in the generalized sense of the infinite dimensional analysis). We get clearly, since σ is Z-valued, over $B(g_{\alpha_1.};\delta)\cap B(g_{\alpha_2.};\delta)\cap B(g_{\alpha_3.};\delta)$,

$$\rho_{\alpha_1,\alpha_2}(g_.)\rho_{\alpha_2,\alpha_3}(g_.)\rho_{\alpha_3,\alpha_1}(g_.)=1. \tag{2.13}$$

This determines a complex line bundle endowed with a natural Hermitian structure over it.

We define a Hermitian connection form over the small ball $B(g_{\alpha.};\delta)$,

$$A_\alpha(g_.)(X_.)=\int_0^1\sigma(d/dt\, l_\alpha(g_.)(t),D_{X_.}l_\alpha(g_.)(t)). \tag{2.14}$$

Let us remark that this Calculus does not need all the schochastic apparatus of Refs. 22–24 and 28, because the quantities are here surely defined. The next lemma uses deeply that there exist a partition of unity over $L_{1/2-\epsilon}(G)$ associated with the cover $B(g_{\alpha.};\delta)$ (see Ref. 28):

Lemma II.1: There exists a smooth section τ_{ξ_∞} of ξ_∞ such that for all $m>1$,

$$\sum_{n,i}E[|\nabla_{X_n(e_i)_.}\tau_{\xi_\infty}|^{2m}]<\infty. \tag{2.15}$$

Proof: We choose the section over $B(g_{\alpha.};\delta)$ which corresponds to any cylindrical functional in the trivialization given for $A_\alpha(g_.)$. It is not smooth. We multiply it by a mollifer; it is possible, because we consider the Hoelder loop space. We follow Ref. 28. Let us introduce a smooth function f from $[0,\infty]$ into $[1,\infty]$ which is exactly exactly on $[0,\delta']$ for $\delta'<\delta$. We suppose that f behaves as $|\delta''-r|^{-n}$ for a big integer n when $r\to\delta''_-$ for some $\delta''<\delta$ and is infinite for $r>\delta''$. We introduce a smooth function h from $[1,\infty]$ into $[0,1]$ with compact suppost which is equal to 1 only at 1. We consider the functional,

$$F_\alpha(g_.)=h\left(\int_0^1 f(d(g_s,g_{\alpha,s}))ds\right). \tag{2.16}$$

F_α is smooth with support included in $B(g_{\alpha.};\delta)$, because we work over the Hoelder loop space (This property is wrong over the continuous loop space). Moreover,

$$X_n(e_i)_\cdot . F_\alpha(g_\cdot) = h'\left(\int_0^1 f(d(g_s, g_{\alpha,s}))ds \right) \times \int_0^1 f'(d(g_s, g_{\alpha,s}) \langle d'(g_s, g_{\alpha,s}), X_n(e_i)_s \rangle ds. \tag{2.17}$$

We get

$$|X_n(e_i)_\cdot . F_\alpha(g_\cdot)|^2 \leqslant C\left(h'\left(\int_0^1 f(d(g_s, g_{\alpha,s}))ds \right)^2 \int_0^1 |f'(d(g_s, g_{\alpha,s}))|^2 ds \times \int_0^1 |\langle d'(g_s, g_{\alpha,s}), X_n(e_i)_s \rangle|^2 1_{B(g_{\alpha,s};\delta)}(g_s) ds. \tag{2.18}$$

The product of the two first term in the right-hand side of (2.18) is bounded in all the L^p by the exponential inequality. The last term has a bound in n and i in $1/(cn^2+1)$. ◇

Over $L_{1/2-\epsilon}(G)$, we can consider the following natural action of H: $g_\cdot \to g_\cdot h$. This preserves the measure, the tangent space as well as the Hilbert space structure over the Hilbert space. It commutes with the natural circle action over the loop group. Since σ is invariant under the action of H over the loop group, the action of H over the loop group lifts to an action of H over ξ_∞, which preserves the Hermitian structure and the connection. It transforms clearly a smooth section of ξ_∞ into a smooth section (in the traditional sense). Moreover, if τ_{ξ_∞} satifies to (2.15), $\tau_{\xi_\infty}.h$ satisfies still to (2.15). We can produce an H-invariant section by using $\int_H \tau_{\xi_\infty}.h d\pi(h)$. The space of H-invariant sections and of finite linear combinations of H-invariant sections produced by Lemma II.1 is dense in the space of L^2 H-invariant section of ξ_∞.

This allows us to construct the Hilbert space of the theory; we consider $\Lambda(H_-)$ the Fermionic Fock bundle of the bundle H_- and $\Lambda(N_-)$ the space of forms associated with the bundle spanned by $X_0(f_i)_\cdot, f_i$. being a orthonormal basis of n_-. We consider the bundle $\Xi = \Lambda(H_-) \otimes \Lambda(N_-) \otimes \xi_\infty$. It is a Hermitian bundle over the Holderian loop group, endowed with a product connection. Over $\Lambda(H_-)$, we consider the lift to the Levi-Civita connection defined by (2.7). Over $\Lambda(N_-)$, we consider the connection given by $\nabla_\cdot X_0(f_j)_\cdot = 0$ if f_j is a deterministic orthonormal basis of n_-. This connection is clearly invariant by rotation. Over ξ_∞, we consider the connection which is invariant under the H-action. The H-action over the Hoelder loop group lift to Ξ. More precisely a vector $X_n(e_i)_\cdot$ is transformed under the H-action into a vector $X_n(h^{-1}e_i h)$. This lift keeps the metric and is compatible with the connection which are considered.

Moreover the natural circle action over the loop groups lifts to $\Lambda(H_-)$, and the connection and the Hermitian metric are compatible with this lift, because the Levi-Civita connection is invariant under the circle action, because the circle acts by isometries. The same considerations work for $\Lambda(N_-)$ and for ξ_∞, because the form σ which determines ξ_∞ is invariant under the circle action.

The Hilbert space $E_H[\Xi]$ of the theory is the space of sections τ_Ξ of Ξ which are invariant under the H-action and which are in L^2: this means that $E[|\tau_\Xi|^2] < \infty$.

We will define a dense core $\Lambda_H[\Xi]$, where we can define a regularized Dirac–Ramond–Taubes operator, which is symmetric, therefore closable.

Let us introduce $I = ((n_1, i_1), \ldots, (n_r, i_r))$ for $n_i < 0$ and let us consider $X_{I_\cdot} = X_{n_1}(e_{i_1})_\cdot \wedge \ldots X_{n_r}(e_{i_r})_\cdot$. Let f_j a given deterministic orthonormal basis of n_-. Let J be equal to $(j_1, \ldots, j_r)$ and let $Y_{J_\cdot}$ be equal to $X_0(f_{j_1})_\cdot \wedge \ldots \wedge X_{j_0}(f_{j_r})_\cdot \ldots$. Let $F_{I,J,K}(g_\cdot)$ be a cylindrical function and let $\tau_{\xi_\infty,K}$ a finite family of sections of τ_{ξ_∞} satisfying (2.15).

A typical section τ_{Ξ} of the core $\Lambda_H[\Xi]$ is a section which is a finite sum of the type,

$$\tau_{\Xi}=\sum F_{I,J,K}(g_.)X_{I.}\wedge Y_{J.}\otimes \tau_{\xi_\infty,K}, \tag{2.19}$$

where we afterwards average under the H-action in order to get H-invariant sections of Ξ. Moreover, it is a dense subspace of the Hilbert space $E_H[\Xi]$. We remark that $\Lambda_H[\Xi]$ is invariant under the natural circle action over the loop group. It is clearly true for $X_{I.}$ and $Y_{J.}$, and for the cylindrical functioanls $F_{I,J,K}(g_.)$ whose set is invariant under the circle action. This result arises for $\tau_{\xi_\infty,K}$ because the space of sections τ_{ξ_∞} satisfying (2.15) is invariant under the circle action.

We consider as an operator,

$$\overline{\partial}_{r,\infty}=\sum_{n>0,i} X_n(e_i)_.\wedge\nabla_{X_n(e_i)_.}+\sum_{f_j} X_0(f_j)_.\wedge\nabla_{X_0(f_j)_.}. \tag{2.20}$$

$X_n(e_i)_.$ corresponds to the form $Y_.\to<Y_.,X_n(e_i)_.>$ in the wedge product. By antilinearity of the Hermitian product, it behaves as q^n under the action of $q\in S_1$, if it is considered as a form. Unfortunately, $\overline{\partial}_{r,\infty}$ is not well defined over $\Lambda_H[\Xi]$. In order to see that, we have to estimate $\nabla_{X_{m(e_i)_.}}X_k(e_j)_.$ when $m\to\infty$. Let us denote by $\overline{X_.}$ the natural conjugation of a vector field $X_.$ which arises from Fourier series. Let us suppose that $X_.$, $Y_.$, and $Z_.$ are 3 vector fields of the type $X_n(e_k)_.$ with e_k deterministic. By (2.7), we have

$$2\langle\nabla_{X_.}Y_.,Z_.\rangle=\langle[X_.,Y_.],Z_.\rangle+\langle Y_.,[Z_.,\overline{X_.}]\rangle+\langle X_.,[Z_.,\overline{Y_.}]\rangle. \tag{2.21}$$

We deduce that

$$\nabla_{X_{m(e_i)_.}}X_l(e_j)_.=\sum_k \alpha_k(i,j)X_{m+l}(e_k)_.\frac{\sqrt{C(m+l)^2+1}}{\sqrt{C(m^2)+1}\sqrt{Cl^2+1}} \tag{2.22}$$

for $m>0$ and $l>0$. Therefore $\overline{\partial}_{r,\infty}\tau_{\Xi}$ has absolutely no reason to belong to $E_H[\Xi]$, if τ_{Ξ} belongs to $\Lambda_H[\Xi]$.

In order to overcome this difficulty, we will change of connection. We choose

$$\nabla_.X_m(e_i)_.=0. \tag{2.23}$$

This connection is clearly invariant by rotation because the vector field $X_n(e_i)_.$ considered as a vector field behaves as q^{-n} under the natural action of the element q of the circle. Moreover this connection is clearly invariant under the H-action, because a vector $X_n(e_i)_.$ is transformed under the H-action in a vector $X_n(h^{-1}e_ih)_.$. Therefore, if we change in the definition (2.19) of $\overline{\partial}_{r,\infty}$ of connection following the last prescriptions, $\overline{\partial}_{r,\infty}(\tau_{\Xi})$ belongs to $E_H[\Xi]$ as soon as τ_{Ξ} belongs to $E_H[\Xi]$ because $X_m(e_i)_..F_{I,J,K}(g_.)$ as a behavior in $C/\sqrt{Cm^2+1}$ when $m\to\infty$ and because (2.15).

Let us recall that over the Loop group, we have some integration by parts formulas called the Albévério–Hoegh–Krohn integration by parts formulas (Refs. 29 and 30). There exists a functional $\mathrm{div}(X_n(e_i)_.)$ which belongs to all the L^p over the loop group such that for all cylindrical functional F,

$$E[X_n(e_i)_..F]=E[F\,\mathrm{div}(X_n(e_i)_.)]. \tag{2.24}$$

We deduce, since the connection is ∇ is Hermitian over Ξ, that we can compute the formal adjoint of $\overline{\partial}_{r,\infty}$ called $\overline{\partial}^*_{r,\infty}$,

$$\overline{\partial}^{*}_{r,\infty}=\sum_{n<0,i}\left(-\nabla_{X_n(e_i)_\cdot}i_{X_{-n}(e_i)_\cdot}+\operatorname{div}X_n(e_i)_\cdot i_{X_{-n}(e_i)_\cdot}\right)$$

$$+\sum_{j}\left(-\nabla_{X_0(f'_j)_\cdot}i_{X_0(f_j)}+\operatorname{div}X_0(f'_j)_\cdot i_{X_0(f_j)_\cdot}\right), \tag{2.25}$$

where f'_j is the orthonormal basis of n_+ corresponding to the orthonormal basis f_j of n_-. $i_{X_\cdot}$ denotes the interior product by a vector field $X_\cdot$. The sum is in fact finite if τ_Ξ belongs to $\Lambda_H[\Xi]$. We take $\operatorname{div}X_n(e_i)_\cdot$ for $n<0$ in (2.25), because we consider complexified L^2 Hilbert space.

This motivates the following definition:

Definition II.2: We call regularized Dirac–Ramond–Taubes operator over the quotient of the loop group the operator,

$$D_{r,\infty}=\overline{\partial}_{r,\infty}+\overline{\partial}^{*}_{r,\infty}. \tag{2.26}$$

It is defined over $\Lambda_H[\Xi]$, symmetric and therefore closable over $E_H[\Xi]$.

Let us compute the fixed point set under the circle action of $(LG)/H$. It is the only place in this work where it is important to suppose that H is a torus.

Let $g_\cdot$ be a representative of an element of the fixed point set. We have, for all s,

$$g_{s+t}=g_s k_t \tag{2.27}$$

for k_t in H and

$$g_{s+t+t'}=g_{s+t}k_{t'}=g_s k_t k_{t'}=g_s k_{t+t'}. \tag{2.28}$$

It follows that $k_t=\exp[et]$ for e belonging to the Lie algebra of H. We identify $g\exp[e.]$ and $g'\exp[e'.]$ we get for a given element h' of H,

$$g\exp[et]=g'\exp[e't]k. \tag{2.29}$$

Therefore, $g=g'k$, and since H is commutative, $e=e'$. Moreover, since we consider loops, e must belong to the canonical lattice L of Lie H of e such that $\exp[e]=1$

We have proved:

Theorem II.3: The fixed point set of $(LG)/H$ under the natural circle action is $G/H\times L$.

III. LIMIT THEOREMS

We consider over the group the equation

$$dg_{\epsilon,s}=g_{\epsilon,s}(\epsilon dB_s) \tag{3.1}$$

starting from g, where B_s is a Brownian motion over the the Lie algebra of G.

It has an heat kernel $p_{s,\epsilon}(g,g')$. Moreover, $p_{1,\epsilon}(g,g)=p_{1,\epsilon}(e,e)$ clearly. Over the loop group, we consider the probability measure $d\mu_{G,\epsilon}=d\pi g\otimes dP_\epsilon(g)$. $P_\epsilon(g)$ is the law of the diffusion $g_{\epsilon,\cdot}$ starting from g constrained to come back at g. We consider a new Hilbert structure for vector fields of the type $X_s=g_s K_s$. It is given by

$$\|X_\cdot\|^2_{g_\cdot,\epsilon}=\int_0^1(|K_s|^2+\epsilon^{-2}|d/dsK_s|^2)ds, \tag{3.2}$$

where $K_\cdot$ is a finite energy application from the circle into the Lie algebra of H. This Hilbert structure is invariant under rotation.

An orthogonal basis of the tangent space is given by

$$X_{n,\epsilon}(e_i)_s = g_{\epsilon,s}\frac{\exp[2i\pi ns]e_i}{\sqrt{Cn^2\epsilon^{-2}+1}}, \tag{3.3}$$

where e_i is an orthonormal basis of the orthogonal of the Lie algebra of G.

Let us compute the divergence of a vector field $X^1_{n,\epsilon}(e_i)_.$ for $\mu_{G,\epsilon}$. For that, we consider $g^\lambda_{\epsilon,s} = \exp[\lambda(\cos[2\pi ns]e_i/\sqrt{cn^2\epsilon^{-2}+1})]$. We consider Eq. (3.1) starting from e. $g_{\epsilon,.}g^\lambda_{\epsilon,.}$ is the solution of a differential equation starting from $g^\lambda_{\epsilon,0}$,

$$d(g_{\epsilon,s}g^\lambda_{\epsilon,s}) = (g_\epsilon dg^\lambda_{\epsilon,s}) + g_{\epsilon,s}(\epsilon dB_s)g^\lambda_{s,\epsilon}. \tag{3.4}$$

It follows that the law of $g_{\epsilon,s}g^\lambda_{\epsilon,.}$ is equivalent to the original law, if we do not fix the starting point and the end point, that is if we consider the free path group, because the Haar measure is invariant under rotation and because $(g^\lambda_{\epsilon,s})^{-1}(dB_s)g^\lambda_{\epsilon,s}$ is still the differential of a Brownian motion on the Lie algebra of G. By differentiating in $\lambda = 0$, we get infinitisimal integration by parts formulas. By using, the quasisure analysis,[31] this integration by parts formulas can be desintegrated over the loop group. For cylindrical functionals F, we get

$$E[X^1_{n,\epsilon}(e_i)_..F] = E[F\ \mathrm{div}\, X^1_{n,\epsilon}(e_i)_.], \tag{3.5}$$

where $\mathrm{div}\, X^1_{n,\epsilon}(e_i)_.$ behaves in small time in $C\int_0^1\langle\exp[2i\pi ns]e_i, dB_s\rangle$ because the law of $g_{\epsilon,.}$ has an equivalent in $g\exp[\epsilon B_. + O(\epsilon^2)]$, where $B_.$ is a flat Brownian bridges over the Lie algebra of G. We have supposed that $g_{\epsilon,.}$ starts from g.

So we have the lemma:

Lemma III.1: In law, when $\epsilon \to 0$, we have over the loop group,

$$\mathrm{div}\, X_{n,\epsilon}(e_i)_. \to \int_0^1 C\langle\exp[2i\pi ns]e_i, dB_s\rangle, \tag{3.6}$$

where B_s is a flat Brownian bridge over the Lie algebra of G.

Let us remark that if we consider the vector field $X_{0,\epsilon}(e_i)_. = g_{\epsilon,.}e_i$, its divergence is equal to 0, because the probability law $P_\epsilon(g)$ is equal to the probability law of $P_\epsilon(gg')$ by the transformation $g_. \to g_.g'$.

This leads to the introduction of a limit limit model, according Taubes.

Let us recall that G is endowed with the Haar measure $d\pi(.)$. G/H is equipped of a Kaehler structure and over G/H, there is the complex line bundle ξ', which allows to define the spin structure. We consider the projection p: $G \to G/H$, and the line bundle $p^*\xi'$, and the bundle $p^*(T(G/H))$. We consider the bundle V_g of ge, e belonging to the orthogonal of the Lie algebra of Lie H. It is isomorphic to the bundle $p^*(T(G/H))$. It is constituted of vector ge orthogonal to vectors ge_i where e_i belongs to the Lie algebra of H. It can be assimilitated to vectors of the shape e where e belongs to the orthogonal of the Lie algebra of H. Let us recall that the complexification of the orthogonal of the Lie algebra of H in the Lie algebra of G can be splitt in $n_+(g) + n_-(g)$ Moreover, this decomposition is invariant under the action of H by inner product. We consider the family of flat Brownian bridges $g_{\mathrm{flat}_.}$ in $V_.$ starting from 0 in V_g endowed with the measure $d\pi(g)\otimes dP_{1,g,\mathrm{flat}}$. It is the same as $gB^1_s(g)$, where $B^1_s(g)$ is a Brownian bridge in the orthogonal of Lie H. The tangent space is the space $X_{l,t}$ of path in V_g with finite energy. As the Hilbert norm, we take

$$\|X_{l,0}\|^2 + \int_0^1 \|d/ds X_{l,t}\|^2 dt = \|X_{l,.}\|^2_1. \tag{3.7}$$

For forms, we take the Hilbert structure,

$$\int_0^1 |X_{l,t}|^2 dt + \int_0^1 |d/dt X_{l,t}|^2 dt = \|X_l\|_2^2. \tag{3.8}$$

It has the orthogonal basis $g\int_0^{\cdot} \exp[2i\pi ns]e_i = X_{n,l}(e_i)$ if $n \neq 0$ and $ge_i = X_{0,l}(e_i)_{\cdot}$ if $n=0$. The complexified tangent space, considered as forms, for the Hilbert structure $\|.\|_2^2$ has an orthonormal basis $\overline{X}_{n,l}(e_i)_s = g\,(\exp[2i\pi ns]/\sqrt{Cn^2+1})\,e_i$ for $n \neq 0$. This splits the space of finite energy paths with values in V_g in $H_{\text{flat},+} + H_{\text{flat},-}$, where $H_{\text{flat},+}$ corresponds to positive n and $H_{\text{flat}-}$ to negative n in the choice of $\overline{X}_{n,l}(e_i)$. We consider the bundle $n_-(g)$ over G and we introduce the following limit bundle:

$$\Xi_l = \Lambda(H_{\text{flat},-}) \otimes \Lambda(n_-(g)) \otimes p^*\xi'. \tag{3.9}$$

The two last parts in Ξ_l are pullback bundles by the evaluation map $g_{\text{flat},\cdot} \to g$ of bundles over G. This bundle inherites a natural H-action, by transforming $\overline{X}_{n,l}(e_i)$ into $\overline{X}_{n,l}(h^{-1}e_i h)$, where h is an element of h and by transforming $X_0(f)$ into $X_0(h^{-1}fh)$, and by an immediate action over $p^*\xi$.

We consider the Bosonic Fock space $B(V_g)$ over $g_{\text{flat},\cdot}$ in V_g and we consider the bundle over G,

$$B(V_g) \otimes \Xi_l. \tag{3.10}$$

Over this limit supersymmetric Fock bundle, we have a connection, which acts as follow: we take the derivative of e_i in $\overline{X}_{n,l}(e_i)_{\cdot}$ for the trivial connection of G. [let us recall that V_g is isomorphic to $p^*T(G/H)$], which is equal to the pullback of the canonical connection over ξ', and which acts over the Wick polynomial $:\langle e_i \alpha_i g, g_{\text{flat},\cdot}\rangle:$ by taking the derivative of e_i and of g in the following formula, but not of $dB^1_{\cdot}(g)$. Namely for α_s a smooth path, we have

$$\begin{aligned}
\langle ge_i\alpha_{\cdot}, g_{\text{flat},\cdot}\rangle &= \int_0^1 \langle ge_i\alpha_s, dg_{\text{flat},s}\rangle \\
&= \int_0^1 \langle ge_i\alpha_s, gdB^1_s(g)\rangle \\
&= \int_0^1 \langle e_i, dB_s(g)\rangle.
\end{aligned} \tag{3.11}$$

This induces a connection over the bundle over G $B(V_g) \otimes \Xi_l$. This bundle inherites clearly an H-action, which is compatible with the connection.

We will construct a core where a ''limit'' Dirac–Ramond operator will act. Let us denote this core $\Lambda_H(\Xi_l)$. We consider the set of finite combination of $:\langle ge_i'\alpha_i, g_{\text{flat},\cdot}\rangle: \otimes \overline{X}_{-n,l}(e_i)_{\cdot} \wedge \overline{X}_{0,l}(f_j')_{\cdot} \otimes \psi$, where e_i depends only on g ($e_i g$ belongs in fact to V_g), f_j' depends only on g, the section ψ on $p^*\xi'$ depends only on g. We consider a finite wedge product of forms $\overline{X}_{-n,l}(e_i)_{\cdot}$, with a different convention of sign from (2.21), because these expressions are considered as forms and not as vectors. The same remarks works for $\overline{X}_{0,l}(f_j')_{\cdot}$. We remark that each of the elements of $\Lambda_H(\Xi_l)$ is not invariant under the H-action, in order to get a section of Ξ_l which is invariant under the H-action, we average it under the H-action.

We consider as orthogonal basis of the path with values in V_g of finite energy the set constituted of paths $g\int_0^t \exp[2i\pi ns]e_i\,ds = X_{n,l}(e_i)_t$ and $X_{0,l}(f_j) = gf_j$ and $X_0(f_j') = gf_j'$.

The infinite dimensional part of the limit Dirac–Ramond–Taubes operator is built of the following operator and its adjoint. If we consider a local orthonormal basis e_i of V_g which depends only on g, we have

$$\overline{\partial}_{\infty,l}=\sum_{i,n>0} c(n)\nabla_{X_{n,l}(e_i)_.}\wedge\overline{X}_{-n,l}(e_i) \tag{3.12}$$

for a family of deterministics constants $c(n)$ for a family of deterministic constant satisfying $\Sigma c(n)^2<\infty$ and we take the sum over an orthogonal basis of the orthogonal of the Lie algebra of H. This operator is clearly invariant under the H-action, because the set of he_ih^{-1} is still an orthogonal basis of the orthogonal of the Lie algebra of H. It acts over $\Lambda_H(\Xi_l)$. Namely, if $n\neq 0$, $X_{n,l}(e_i)_.\langle ge_j\alpha,g_{\text{flat},.}\rangle=\int_0^1\langle ge_j\alpha_s,g\exp[2i\pi ns]e_ids\rangle$, if e_i belongs to the orthogonal of Lie H, which is quickly decreasing because α_s is chosen smooth. This means that the infinitesimal variation of dB_s under $X_{n,l}(e_i)_.$ is $\exp[2i\pi ns]e_ids$ if e_i belongs to the orthogonal of the Lie algebra of H.

The adjoint of $\overline{\partial}_{\infty,l}$, denoted by $\overline{\partial}^*_{\infty,l}$ is defined by the following formula:

$$\overline{\partial}^*_{\infty,l}=\sum_{i,n<0} i_{X_{-n,l}(e_i)}c(n)(-\nabla_{X_{n,l}(e_i)_.}+\operatorname{div}X_{n,l}(e_i)_.). \tag{3.13}$$

We put

$$D_{\infty,l}=\overline{\partial}_{\infty,l}+\overline{\partial}^*_{\infty,l}. \tag{3.14}$$

This operator is clearly invariant under the H-action and defined over $\Lambda_H(\Xi_l)$. Namely, a vector field $X_{n,l}(e_i)_.$ is transformed under the H-action into $X_{n,l}(he_ih^{-1})$.

The finite dimensional part of the limit Dirac–Ramond–Taubes operator is constructed as follow. We add a finite dimensional $\overline{\partial}_{f,l}$ operator,

$$\overline{\partial}_{f,l}=\sum_{f_j} X_{0,l}(f_j)_.\wedge\nabla_{X_0(f_j)_.} \tag{3.15}$$

with the notations of (2.20), which operates over the bundle $B(V_g)\otimes\Xi_l$.

We compute its adjoint: with the notations of Eq. (2.26), we have

$$\overline{\partial}^*_{f,l}=\sum_j -\nabla_{X_0(f_j')_.}i_{X_0(f_j)_.}+\operatorname{div}X_0(f_j')_.i_{X_0(f_j)_.}. \tag{3.16}$$

In order to summarize, there are two parts in the limit Dirac–Ramond–Taubes operator,

$$D_l=\overline{\partial}_{f,l}+\overline{\partial}_{f,l}+\overline{\partial}_{\infty,l}+\overline{\partial}^*_{\infty,l}. \tag{3.17}$$

There is a finite dimensional part which acts over the bundle $B(V_g)\otimes\Xi_l$ and and infinite dimensional part which acts over the Brownian bridge paths in the fiber of the linear bundle V_g.

The limit model inherites a natural limit circle action. The form $\overline{X}_{n,l}(e_i)_.$ behaves as q^n as we have seen after (2.20).

Let us compute the behavior under the limit action of the circle of the considered limit functional $\int_0^1\langle ge_i\exp[2i\pi ns],dg_{\text{flat},s}\rangle$ for e_i a section of V_g which depends only on g. For that, let us study the action of the circle of the functional $\int_0^1\langle g_{\epsilon,s}e_i\exp[2i\pi ns]ds,dg_{\epsilon,s}\rangle/\epsilon$ which tends in law to $\int_0^1\langle ge_i\exp[2i\pi ns],dg_{\text{flat},s}\rangle$. But

$$\int_0^1\langle g_{\epsilon,s-t}e_i\exp[2i\pi n(s-t)],dg_{s-t,\epsilon}\rangle=\int_0^1\langle g_{\epsilon,s}e_i\exp[2i\pi ns],dg_{\epsilon,s}\rangle. \tag{3.18}$$

If we put $F(g_{\epsilon,.})=\int_0^1\langle g_{\epsilon,s}e_i\exp[2i\pi ns],dg_{\epsilon,s}\rangle$, we have then

$$F(qg_{\epsilon,.})=q^nF(g_{\epsilon,.}) \tag{3.19}$$

for an element q of the circle. This means that F behaves as q^n by himself under the natural action of the circle over the loop group. Therefore, $\int_0^1 \langle g e_i \exp[2i\pi ns], dg_{\text{flat},s}\rangle$ behaves as q^n by himself under the limit circle action which arises by limit of the circle action over the loop group.

Let us compute the behavior of this functional under the H-action: $g_{\epsilon,s}\exp[2i\pi ns]e_i$ is transformed in $g_{\epsilon,s}\exp[2i\pi ns]e_i h$ and $g_{\epsilon,s}$ is transformed into $g_{\epsilon,s}h$. This shows that the functional F is invariant under the H action, and therefore that the limit functional is invariant under the H-action. The core $\Lambda_H(\Xi_l)$ is invariant under the limit circle action.

Let us recall what is the Witten genus of G/H: we consider the Atiyah–Singer genus of G/H which gives the Index of the Dirac operator over G/H, because G/H is supposed spin. It is too equal to $\text{Todd}(G/H)\wedge\text{ch}(\xi')$, where $\text{Todd}(G/H)$ is the Todd genus of the Kaehlerian manifold G/H. We consider the symmetric tensor algebra of $T(G/H)\otimes C$, where a tensor product of length j is counted with the power q^{nj}, where q is the generic element of S^1. The Witten genus is given by the following formula:

$$Wi(G/H)=\int_{G/H}\hat{A}(G/H)\wedge\text{ch}\otimes_{n>0}S_{q^n}(T(G/H)\otimes C) \tag{3.20}$$

(see Refs. 6, 3, 7, 8). It is given by the characterisic series (see Ref. 8, p. 83 modulo some normalizing factors)

$$Q(x)=\frac{x/2}{\sinh(x/2)}\prod_{n>0}\frac{1}{(1-q^n\exp[x])(1-q^n\exp[-x])}. \tag{3.21}$$

It is a formal series in q. So the Witten genus has to be seen as a formal series in q.

In the sequel, we will suppose that $c(n)\neq 0$ for $n>0$.

The operator D_l commutes with the limit circle action over $\Lambda_H(\Xi_l)$. We can define its ''formal'' equivariant index,

$$\text{Ind}_q D_l=\text{Tr}_{\text{Ker}\,D_l^+}q-\text{Tr}_{\text{Ker}\,D_l^-}q. \tag{3.22}$$

D_l^+ is the restriction of D_l to $\Lambda_H^+(\Xi_l)$, where $\Lambda_H^+(\Xi_l)$ is the subset of elements of $\Lambda_H(\Xi_l)$, where we choose an even power of $\overline{X}_{-n,l}(e_i)_.$, and $\Lambda_H^-(\Xi_l)$ is the subset of $\Lambda_H(\Xi_l)_.$, where we have an odd power of $\overline{X}_{-n,l}(e_i)_.$.

Theorem III.2: The equivariant Index of the limit Dirac–Ramond–Taubes operator over $\Lambda_H(\Xi_l)$ is equal to the Witten genus of G/H.

Proof: Let us compute $\Delta_l=D_l^2$. The infinite dimensional part and the finite dimensional part of the limit Dirac operator anticommute. Therefore, we have

$$\Delta_l=(\overline{\partial}_{f,l}+\overline{\partial}^*_{f,l})^2+(\overline{\partial}_{\infty,l}+\overline{\partial}^*_{\infty,l})^2=\Delta_{f,l}+\Delta_{\infty,l}. \tag{3.23}$$

To the polarization given, is associated a class of holomorphic bosons; they are combinations in the Wick products, $:\int_0^1\langle g e_j\exp[2i\pi n_j s], dg_{\text{flat},s}\rangle:$ where $n_j>0$. Let $N_{B,c}(\text{anti})$ be the second quantized operator of $c(n)^2$ which counts the number of antiholomorphic bosons and let $N_{F,c}$ be the second quantized operator of $c(n)^2$ which counts the number of fermions of the type $\overline{X}_{-n,l}(e_i)$ with $n>0$. We have[32]

$$\Delta_{\infty,l}=N_{B,c}(\text{anti})+N_{F,c}. \tag{3.24}$$

Namely, in the Gaussian space $B_.$, we do the infinitesimal transformation by $\exp[2i\pi ns]e_i$, where e_i belongs to the orthogonal of $\text{Lie}\,H$. Therefore $\Delta_{\infty,l}$ has a set of eigenvectors, which can be seen following Taubes as a countable set of finite dimensional bundles over G. Moreover, $\overline{\partial}_{f,l}+\overline{\partial}^*_{f,l}$ transforms a section of each bundle into a section of the same finite dimensional bundle. D_l has,

therefore, a self-adjoint extension which is compatible with the self-adjoint extension of Δ_l. Moreover, these constructions are compatible with the natural H-action over the limit model.

This implies that we can compute the elements which are H-invariants of the kernel of Δ_l as follows: we take first the kernel of $\Delta_{\infty,l}$, and the elements which are H-invariant under the natural H-action over it. This gives a countable set of finite dimensional bundles over G/H.

$\overline{\partial}_{f,l}+\overline{\partial}^{*}_{f,l}$ acting over H-invariant elements of the kernel of $\Delta_{\infty,l}$ tensorized by H-invariant sections of $\Lambda(n_{-}(g))\otimes p^{*}\xi'$ can be seen as homotopic to the Dirac operator over G/H tensorized by the previous countable sets of these finite dimensional bundles over G/H. The kernel of the Bosonic number operator is constitute of the holomorphic bosons since $c(n)\neq 0$, or in others words of linear combinations of Wick products, $\int_0^1 \langle g e_j \exp[2i\pi n_j s], dg_{\text{flat},s}\rangle$, with $n_j>0$. This last quantity behaves under the natural circle action as $q^{\sum n_j}$. This explains that only positive n appear in the expression of the equivariant index of D_l acting over $\Lambda_H(\Xi_l)$. The index formula (see Ref. 26) gives

$$\mathrm{Ind}_q(D_l)=\int_{G/H}\hat{A}(G/H)\wedge ch\otimes_{n>0}S_{q^n}(T(G/H)\otimes C). \tag{3.25}$$

◇

Remark: If we do not suppose that G/H is spin, we get for any complex auxiliary line bundle ξ, the equivariant index formula,

$$\mathrm{Ind}_q D_l=\int_{G/H}\mathrm{Todd}(G/H)\wedge \mathrm{ch}\,\xi'\wedge \mathrm{ch}\otimes_{n>0}S_{q^n}(T(G/H)\otimes C). \tag{3.26}$$

Let $B(x_i;\delta_i)$ be a finite cover of G/H, such that for all i, there exists a small ball B_i included in $B(x_i;\delta_i)$ such that the intersection of B_i with $B(x_j;\delta_j)$ is empty for $j\neq i$. We consider the open subset $p^{-1}B(x_i;\delta_i)$ of G. It constitutes a finite open cover of G.

Let $g_.$ be a loop. We consider a smooth function f_i from $R^{+}\to[0,\infty]$ which behaves has $1/(-\delta_i''+r)^{+n}$ for a big integer n when $r\to\delta_{i,+}''$, and which is infinite if $r<\delta_i''$ for a convenient δ_i'', and which is equal to zero outside a bounded set. We consider the functional,

$$G_i'(g_.)=\int_H d\pi(h)\int_0^1 f_i(d(g_s,hg_i)ds \tag{3.27}$$

for some $g_i\in p^{-1}(x_i)$. We multiply this by a functional of the type (2.16) such that it is equal to infinite over a small neighborhood for the uniform norm of $p^{-1}B(x_i;\delta_i)$ and it is equal to 0 outside a small neighborhood of the same set for the uniform distance in the Holderian loop space. Let us call the functional which is got by this procedure $G_i(g_.)$. Let us introduce a function h from $[0,\infty]\to[0,1]$ which is equal to 1 if $r>C$ and which is equal to zero in a neighborhood of 0.

We introduce the functional

$$F(g_.)=h\left(\sum G_i(g_.)\right). \tag{3.28}$$

This functional is clearly invariant by rotation, invariant under the H-action. It checks clearly the hypothesis (2.15) and is equal to outside a neighborhood of the constants loops in G, and is equal to 1 in a neighborhood of the constant loops in G.

Moreover,

$$P[F(g_{\epsilon,.})\neq 1]\leqslant C\exp\left[-\frac{C}{\epsilon^2}\right] \tag{3.29}$$

by the exponential inequality.

We put

$$F_i(g_.)=h(G_i(g_.)). \tag{3.30}$$

Let us suppose that $F_i(g_.)\neq 0$. $g_.$ lies in a small neighborhood for the uniform topology over the Hoelderian loop space of $p^{-1}B(x_i;\delta_i)$, if δ_i'' is chosen enough well. This neighborhood is invariant under the H-action and under the natural circle action over the loop group. Let $\tau_{i,\xi_\infty}(g_.)$ be the section of the bundle ξ_∞ given by the trivialization which is given after (2.12) by 1. Since the connection form is invariant by rotation, $\tau_{i,\xi_\infty}(g_.)$ is invariant under rotation. It is too invariant under the H-action. Namely the connection form (2.14) is invariant under the H-action. Let us precise a bit this statement: we consider the set $B(g;\delta'')$ where $g\in p^{-1}(x_i)$ for the uniform distance over the Hoelder loop space. We introduce following (2.12) the path in the loop space:

$$l_g(g_.)(t)_s=\exp[t(g_s-g)] \tag{3.31}$$

joining the loop $g_.$ to the constant loop g, and after we go to g to any fixed given element g' of $p^{-1}(x_i)$. [Recall the notation of (2.11).] If we multiply $g_.$ by h, we consider the ball $B(gh;\delta'')$ for the uniform distance over the Hoelder loop space, and the path $l_{hg}(hg_.)(t)_s=\exp[t(hg_s-hg)]$ with the notations of (2.11) and any given curve in $p^{-1}(x_i)$ joining gh to the given element g' of $p^{-1}(x_i)$. Since $-p^*R$ is in fact a basical form over G/H, the extra integral from curves in $p^{-1}x_i$ which appears in the transition functional gives a contribution which is equal to 0. This explains why the section $\tau_{i,\xi_\infty}(g_.)$ is invariant under the H-action.

We consider a section τ_{ξ_∞} of ξ_∞ such that

$$\sup_{\epsilon\leqslant 1}\sum_{n,i} E[|\nabla_{X_n(e_i)_.}\tau_{\xi_\infty}(g_{\epsilon,.})|^{2m}]<\infty. \tag{3.32}$$

It is possible by a small refinement of lemma II.1 to find such a section. By using an argument similar to Ref. 12, the second remark after Theorem II.10, it is possible to show that these sections are dense in the space of the L^2 section of ξ_∞ if ϵ is small enough.

Let us introduce a set of expressions. We consider as functionals

$$\xi(A)=\prod \int_0^1 \langle g_{\epsilon,s}e_i\exp[2i\pi ns],\delta g_{\epsilon,s}\rangle, \tag{3.33}$$

where e_i is a fixed element of Lie(G) and i and n describes the finite set A and δ denotes the Itô integral. We consider as form $X_{-n}(e_i)_.$ for the e_i element of an orthogonal basis of the orthogonal of the Lie algebra of H, i and the negative integers $-n$ describing the finite set B. We consider $X_n(e_i)_.$ for e_i belonging to the Lie algebra of G and the negative integers describing a finite set C. We consider the wedge product of all and we get an expression called $X_-(B,C)_.$. The different conventions of signs with (2.20) result that here we consider forms.

At a last step, we consider forms $X_0(f_i')$ for f_i' describing a finite set C of f_i'. [Let us recall that in (2.20), $X_0(f_j)$ considered as a vector corresponds to $X_0(f_j')$ considered as a form.] We choose a wedge product of these forms and we call it $X_0(D_.)$.

We consider as core $\Lambda_{H,\epsilon}(\Xi)$ the space of section of Ξ defined by

$$\tau_\Xi(g_{\epsilon,.})=\sum \lambda(A,B,C,D,i)F_i(g_{\epsilon,.})\xi(A,i)X_-(B,C,i)_.\wedge X_0(D,i)_.\otimes\tau_{i,\xi_\infty}(g_{\epsilon,.})$$

$$+(1-F(g_{\epsilon,.}))\sum F_{I,J,K}(g_{\epsilon,.})(X_I)_.\wedge Y_{J,.}\otimes\tau_{\xi_\infty,K}. \tag{3.34}$$

$\lambda(A,B,C,D,i)$ are constants, where the second sum in (3.34) is defined as in (2.20) and $\tau_{\xi_\infty}(g_{\epsilon,.})$ satisfies (3.33). $F_{I,J,K}(g_{\epsilon,.})$ is a cylindrical functional.

This core is invariant under the H-action and not under the natural circle action over the loop group. Namely, it is not clear that $X_{n,\epsilon}(e_i)_.$ is invariant under rotation. For that, we average under the circle the vector $X_{n,\epsilon}(e_i)_.$. It is not clear that it remains an independent family. But if $g_{\epsilon,.}$ is a small loop, it remains an independent family. For that, we introduce some cuttofs as it was done in Ref. 10, p. 270. If $\sup_{s,t}|g_{\epsilon,s}g_{\epsilon,t}^{-1}-e|$ remains small, the averaged vector fields are still an independent family of vectors. We introduce the mollifer of Ref. 10, p. 270, which is invariant by rotation and invariant under the H action because $\sup_{s,t}|g_{\epsilon,s}g_{\epsilon,t}^{-1}-e|$ is invariant under the H-action in order to conclude. We localize the core $\Lambda_{H,\epsilon}(\Xi)$ by using this others restrictions, and by using the average vector fields which are invariant by rotations, and which are independent, and which are supposed orthogonal by modifying a bit the metric.

We define Bismut's dilatation B_ϵ which acts over $\xi(A)$ by

$$B_\epsilon \xi(A)=\prod_{(i,n)\in A}\int_0^1 \frac{\langle g_{\epsilon,s}e_i \exp[2i\pi ns], dg_{\epsilon,s}\rangle}{\epsilon^{\alpha_i}}, \tag{3.35}$$

where $\alpha_i=1$ if e_i belongs to the orthogonal of the Lie algebra as H and $\alpha_i=1/2$ if e_i belongs to the Lie algebra of H. Bismut's dilatation acts over wedge products $X_-(C,D)$ by multiplying each elements of the wedge product of the type $X_n(e_i)$ with e_i belonging to the Lie algebra of H by ϵ.

Definition III.3: Bismut's dilatation over $\Lambda_{H,\epsilon}(\Xi)$ is defined by

$$B_\epsilon \tau_\Xi(g_{\epsilon,.})=\sum F_i(g_{\epsilon,.})\lambda(A,B,C,D,i)B_\epsilon\xi(A,i)B_\epsilon(X_-(B,C,i))\wedge X_0(D,i)\otimes\tau_{i,\xi_\infty}(g_{\epsilon,.})$$
$$+\left(1-F(g_.\epsilon,.)\right)\sum F_{I,J,K}(X_{I.})\wedge Y_{J_.}\otimes\tau_{\xi_\infty,K}. \tag{3.36}$$

Lemma III.4: Bismut's dilatation are well defined over $\Lambda_{H,\epsilon}(\Xi)$.

Proof: We suppose in order to simplify that $\epsilon=1$.

Since there is a small neighborhood O_i of $p^{-1}x_i$ for the uniform distance for the Hoelder loop space such that the intersection of O_i with the set $\{F_j(g_{\epsilon,.})\neq 0\}$ is empty, the result will follow the following property: if

$$i_{O_i}\sum_{A,B,C,D}\lambda(A,B,C,D,i)\xi(A,i)X_-(B,C,i)\wedge X_0(D,i)\otimes\tau_{i,\xi_\infty}(g_{\epsilon,.})=0, \tag{3.37}$$

then $\lambda(A,B,C,D,i)=0$.

We can find a mollifer functional $\tilde{F}_i$ which belongs to all the Sobolev spaces and of the type studied before such that $\tilde{F}_i(g)\neq 0$ for some $g\in p^{-1}x_i$ and such that the set $\{\tilde{F}_i(g_.)\neq 0\}$ is included in O_i.

Let us introduce the random variables $\zeta(i,n)=\int_0^1\langle e_i\cos[2\pi ns], dB_s\rangle$ for $n\geqslant 0$ and $\zeta(i,n)=\int_0^1\langle e_i\sin[2\pi ns], dB_s\rangle$ for $n<0$.

We suppose in order to simplify the exposure that the diffusion $g_.$ starts from e. We consider the measure over $G\times R^N$ μ,

$$F\to E[\tilde{F}_i(g_.)f(g_1,\zeta(.,.)], \tag{3.38}$$

where we consider $|n|\leqslant n_0$. We can suppose that $\tilde{F}_i(e)\neq 0$. Let us show that μ has an absolutely continuous part which has a strictly positive density in (e,ζ) for some convenient ζ. This will show the result. It is enough to show the following property: let us replace formally dB_s by $h_s\,ds$ with the L^2 topology over $h_.$. g_1 is replaced by $g_1(h_.)$ and $\zeta(.,.)$ by $\zeta(.,.)(h_.)$. The property says that the application Ψ: $h_.\to(g_1(h_.),\zeta(.,.)(h_.))$ is a submersion for a small $h_.$ such that $g_1(h_.)=e$. By the positivity theorem of Ref. 33 (see Ref. 34 for an abstract version), the density part of μ in $(e,\zeta(.,.)(h_.))$ is strictly positive.

If we do not suppose that n can be equal to zero, it is clearly a submersion in $h_\cdot=0$. The only problem in order that Ψ is a submersion in $h=0$ is $n=0$. But, we can perturb a little bit $h_\cdot$ in order to get a submersion, because there are multiple iterated integrals which appear in the expression of $g_1(h_\cdot)$. Let us precise a little bit this statement, after plunging the Lie group in an orthogonal matrix group. Let us denote by $Dg_s(h_\cdot)(h'_\cdot)$ the expression of the derivative of $g_s(h_\cdot)$ in the direction $h'_\cdot$. It is the solution of the differential equation,

$$dDg_s(h_\cdot)(h'_\cdot)=Dg_s(h_\cdot)(h'_\cdot)h_s ds+g_s(h_\cdot)h'_s ds. \tag{3.39}$$

We can solve this equation by the method of variation of constants. We get

$$Dg_1(h_\cdot)(h'_\cdot)=\int_0^1 g_s(h_\cdot)h'_s g_s^{-1}(h_\cdot)ds g_1(h_\cdot). \tag{3.40}$$

It is enough to choose a small h such that $s\to g_s(h_\cdot).g_s^{-1}(h_\cdot)$ is not proportional to $s\to\cos[2\pi ns]$ and to $s\to\sin[2\pi ns]$ for $|n|\leqslant n_0$ such that $g_1(h)=e$. ◇

We would like to compute the limit of $B_\epsilon\tau_\Xi(g_{\epsilon,\cdot})$ when $\epsilon\to 0$ in order to justify the appellation ''limit model'' which was used previously.

Definition III.5: We say that a sequence of sections $\tau_\xi(g_{\epsilon,\cdot},\epsilon)$ of the type

$$\tau_\Xi(g_{\epsilon,\cdot},\epsilon)=\sum_{B,C,D,i} F_{I,J,K}(g_{\epsilon,\cdot},\epsilon)X_-(B,C,i)_\cdot\wedge X_0(D,i)_\cdot\otimes\tau_{\xi_\infty,K}(g_{\epsilon,0}) \tag{3.41}$$

tends in law to the section $\tau_{\Xi_l}(g_{\text{flat},\cdot})$ of the limit model defined by

$$\tau_{\xi_l}(g_{\text{flat},\cdot})=\sum_{B,C,D,i}\xi_{(B,C,D,i)}g_{\text{flat},\cdot}\overline{X}_{-,l}(B,C,i)_\cdot\wedge\overline{Y}_{0,l}(D,i)_\cdot\otimes\tau_{\xi'}(g) \tag{3.42}$$

if the family of random variables $F_{B,C,D,i}(g_{\epsilon,\cdot},\epsilon)$ in $L^2(N)$ tends in law to the family of random variable $\xi_{B,C,D,i}(g_{\text{flat},\cdot})$ and if $E[\Sigma|F_{I,J,K}(g_{\epsilon,\cdot},\epsilon)|^2]$ remains bounded.

In this definition, it is supposed that the random variables $F_{A,B,C,i}(g_{\epsilon,\cdot},\epsilon)$ tends in law to zero if there is in $X_-(B,C,i)_\cdot$ a $X_n(e_i)_\cdot$ considered as vector or a $\overline{X}_{-n,l}(e_i)_\cdot$ considered as a form at the limit (with $n>0$) associated to an element e_i of the Lie algebra of H.

Proposition III.6: If $\tau_\Xi(g_{\epsilon,\cdot})$ is a section of Ξ of the type (3.34), $B_\epsilon\tau_\Xi(g_{\epsilon,\cdot})$ tends in law to a section of the limit model τ_{Ξ_l}.

Proof: It will result from the following observation. The contribution which is normalized at which comes from the loop close of the constant loops can be handled by the following remark: in law, when $\epsilon\to 0$,

$$g_{\epsilon,\cdot}=g\exp[\epsilon B_s+O(\epsilon^2)] \tag{3.43}$$

for a Brownian bridge $B_\cdot$ over the Lie algebra of G (see Refs. 35 and 36).

This shows that, in law,

$$B_\epsilon\xi(A)\to\prod_{i,n\in A}\int_0^1\langle ge_i\exp[2i\pi ns],dg_{\text{flat},s}\rangle \tag{3.44}$$

if all the e_i belong to the orthogonal of the Lie algebra of H and tends to 0 in law in the others cases. ◇

We consider the core $\Lambda_{H,\epsilon}(\Xi)$ as the set of sections in (3.34), where the contributions which are far from the constant loops are equal to 0. So this core is a space of sections over a small neighborhood of the constant loops in the loop group which is invariant under the circle action and

invariant under the H-action. Since the contribution outside the constant loops vanishes, it is natural to introduce a deformation of the infinite dimensional Dirac–Ramond–Taubes operator near the constant loops.

We define the regularized Dirac–Ramond–Taubes operator over the core $\Lambda_{H,\epsilon}(\Xi)$ by

$$D_\epsilon = \overline{\partial}_{\epsilon,\infty} + \overline{\partial}^*_{\epsilon,\infty}, \tag{3.45}$$

where

$$\overline{\partial}_{\epsilon,\infty} = \sum_{n>0,i} X_{-n}(e_i)_\cdot \wedge \nabla_{X_{n,\epsilon}(e_i)_\cdot} + \sum_{f_j} X_0(f'_j)_\cdot \wedge \nabla_{X_0(f_j)_\cdot}, \tag{3.46}$$

and where

$$\begin{aligned}\overline{\partial}^*_{\epsilon,\infty} = &\sum_{n<0,i} -\nabla_{X_{n,\epsilon}(e_i)_\cdot} i_{X_n(e_i)_\cdot} + \operatorname{div} X_{n,\epsilon}(e_i)_\cdot i_{X_n(e_i)_\cdot} \\ &+ \sum_j -\nabla_{X_0(f'_j)_\cdot} i_{X_0(f_j)_\cdot} + \operatorname{div} X_0(f'_j)_\cdot i_{X_0(f_j)_\cdot}.\end{aligned} \tag{3.47}$$

Let us remark that D_ϵ operates over the core $\Lambda_{H,\epsilon}(\Xi)$. Namely,

$$\begin{aligned}&X_{m,\epsilon}(e_j)_\cdot \cdot \int_0^1 \langle g_{\epsilon,s} \exp[2i\pi ns] e_i, dg_{\epsilon,s}\rangle \\ &= O(1/n) + C(\epsilon,m) \\ &\quad \times \int_0^1 \langle g_{\epsilon,s} \exp[2i\pi ns] e_i, g_{\epsilon,s} \exp[2i\pi ms] e_j\rangle \\ &= O(1/n) + C(\epsilon,m,n)\,\delta_{m,n}.\end{aligned} \tag{3.48}$$

The problem is that this operator is not invariant under rotation. For that, we average the vector fields $X_{n,\epsilon}(e_i)_\cdot$ under the natural circle action. The problem is that the averaged vector fields do not constitute an independent family in general. But it remains an independent family, because we work over a small neighborhood of the constant loops. We have the following theorem:

Theorem III. 7: When $\epsilon \to 0$, we have in law if $\tau_\Xi(g_{\epsilon,\cdot})$ is a section belonging to $\Lambda'_{H,\epsilon}(\Xi)$,

$$D_\epsilon B_\epsilon \tau_\Xi(g_{\epsilon,\cdot}) \to D_l \tau_{\Xi_l} \tag{3.49}$$

for some $c(n) \neq 0$, $\tau_\Xi(g_{\epsilon,\cdot})$ and τ_{Ξ_l} being given as in Proposition III.6.

Proof: We remark first that the contribution of the derivatives of $F_i(g_{\epsilon,\cdot})$ vanishes as it was seen previously.

There is the contribution of the covariant $\tau_{i,\xi_\infty}(g_{\epsilon,\cdot})$. If $n \neq 0$, $\nabla_{X_{n,e_i(e_i)_\cdot}} \tau_{i,\xi_\infty}(g_{\epsilon,\cdot})$ tends clearly to 0 because $X_{n,\epsilon}(e_i) \to 0$. If $n=0$, we remark that ξ_∞ restricts over G to $p^*\xi'$, and the connection forms over the first bundle over the loop group restricts over the connection form over G. Let us look at formula (2.15). The distinguished path $l_{g'}(\epsilon,\cdot)(t)$ tends to the distinguished path joining g to the given element g' of $p^{-1}(x_i)$. Therefore,

$$A_{g'}(g_{\epsilon,\cdot})(X_0(e_i)_\cdot) \to A_{g'}(e_i g), \tag{3.50}$$

where A_i is the connection form associated to $p^*\xi'$ over $p^{-1}B(x_i;\delta)$. Therefore the expression which comes to the covariant derivative of $\tau_{i,\xi_\infty}(g_{\epsilon,\cdot})$ pass to the limit.

The treatment of the covariant derivative of $B_\epsilon(X_-(B,C,i)_\cdot)$ and $X_0(D,i)_\cdot$ is trivial, with the chosen connections.

The treatment of $\operatorname{div} X_{n,\epsilon}(e_i)_.$ is given at Lemma III.1. It remains to remark that $\operatorname{div} X_{n,\epsilon}(e_i)_.$ if e_i belongs to Lie H at the limit does not appear, because there is an interior product in D_ϵ, $i_{X_n(e_i)_.}$, and that the corresponding forms are multiplied by ϵ and disappear at the limit.

It remains to consider

$$X_{n,\epsilon}(e_i)_.\,.B_\epsilon\xi(A) \tag{3.51}$$

or equivalently,

$$X_{n,\epsilon}(e_i)_.\,.\int_0^1\langle g_{\epsilon,s}\exp[2i\pi ms]e_j,\delta g_{\epsilon,s}\rangle/\epsilon. \tag{3.52}$$

Let us consider first $n\neq 0$ and e_j belonging to the orthogonal of Lie H. It tends in law, too,

$$\int_0^1\langle g\exp[2i\pi ns]e_j,g\exp[2i\pi ms]e_i\rangle \tag{3.53}$$

which is the derivative of $\int_0^1\langle g\exp[2i\pi ms]e_j,dg_{\mathrm{flat},s}\rangle$ along $X_{n,l}(e_i)_.$.

If $n\neq 0$ and e_j belongs to Lie H, $X_{n,\epsilon}(e_i)_.=O(\epsilon)$ and

$$X_{n,\epsilon}(e_i)_.\,.\int_0^1\langle g_{\epsilon,s}\exp[2i\pi ms]e_j,\delta g_{\epsilon,s}\rangle/\sqrt{\epsilon}=O(\epsilon^{1/2})) \tag{3.54}$$

and tends to zero, which is the derivative of the limit of this expression, which is 0.

If $n=0$ and if e_j belongs to the orthogonal of the Lie algebra of H,

$$\begin{aligned}X_0(e_i)_.\,.\int_0^1\langle g_{\epsilon,s}\exp[2i\pi ms]e_j,\delta g_{\epsilon,s}\rangle/\epsilon&\\ =\int_0^1\langle g_{\epsilon,s}e_i\exp[2i\pi ms]e_j,\delta g_{\epsilon,s}\rangle/\epsilon&\\ +\int_0^1\langle g_{\epsilon,s}\exp[2i\pi ms]e_j,\delta g_{\epsilon,s}(e_i)\rangle/\epsilon,&\end{aligned} \tag{3.55}$$

which tends in law to

$$\begin{aligned}\int_0^1\langle ge_i\exp[2i\pi msd]e_j,gdB_s\rangle&\\ +\int_0^1\langle g\exp[2i\pi ms]e_j,ge_idB_s\rangle=0&\end{aligned} \tag{3.56}$$

which is the derivative of

$$\int_0^1\langle g\exp[2i\pi ms]e_j,dg_{\mathrm{flat},s}\rangle=\int_0^1\langle\exp[2i\pi ms]e_j,dB_.\rangle$$

in the direction ge_i.

We have considered the limit in law of each component of the section $\tau_\Xi(g_{\epsilon,.})$, but the collections of each components converges in law.

The last property of Proposition III.5. is clearly checked. ◇

Remark: It is enough to suppose the G/H spin, by extending the Clifford multiplication over small loops as it was done in Ref. 10, (2.10), because we work over a small neighborhood of the constant loops.

Remark: The previous argument should justify, but not prove the following assertion: over $(LG)/H$, there is a Dirac–Ramond–Taubes operator, and its ''renormalized'' equivariant index is equal to the Witten genus of G/H. The contribution of the others fixed points should be treated by looking at the ''homeomorphism'' $g_\cdot \to \exp[e_\cdot] g_\cdot$.

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To the Gel'fand–Tsetlin realization of irreducible representations of classical semisimple algebras

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It is shown that the Gel'fand–Tsetlin realization of irreducible representations of the A_n algebra is directly connected with a linear exactly integrable system in the n-dimensional space. General solutions for this system is explicitly given.
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I. INTRODUCTION

Almost 50 years ago Gel'fand and Tsetlin (GZ) discovered the explicit form of irreducible representations of the classical semisimple Lie algebras such as A_n, B_n, and D_n.[1] Their purely algebraic arguments were based on the possibility of the consequent embedding of one algebra into another. Under such kind of embedding the number of necessary additional ''quantum numbers'' is equal to the number of arising Cazimir operators.

In the present paper we consider GZ results from another point of view in order to connect them with some exactly integrable system of finite difference equations or with its continuous limit which has a form of partial differential equations in the n-dimensional space. The key point is that we propose the operator realization of the generators of the simple roots $X_i^{\pm}$ and Cartan elements h_i of the A_n algebra. The selection rules used by us (the assumed form of operators) are of course initiated by GZ results.

As a consequence of the commutation relations between $3n$ elements of the A_n algebra ($2n$ generators of its simple roots $X_i^{\pm}$ and n elements h_i of its Cartan subalgebra)

$$[X_i^+, X_j^-] = \delta_{i,j} h_i, \quad [h_i, X_j^{\pm}] = \pm k_{j,i} X_j^{\pm}, \tag{1}$$

in some specific form of their realization arises a discrete system of equations for n unknown functions depending on n arguments. This system allows the exact integration. Finally, the particular solution of this system under some additional requirements of irreducibility overgoes to the matrix elements the famous GZ paper.

It is more suitable to perform continuous limit not from the limiting procedure from discrete variables but by independently considering (1) on the level of Poisson brackets. Then we can use the Darboux theorem for resolving the arising functional group. (We use the old sense of this term, see, e.g., the book of Eisenhart.[2]) In this way it is possible to obtain the GZ expressions in the classical region. This method is much simpler technically and may be used as an additional hint for introducing and understanding the algebraic GZ formulas:

Such a general approach to the problem of constructing the irreducible representations of the Lie algebras was proposed many years ago in Ref. 3 but up to now has not been used (to the best of our knowledge).

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We begin our discussion in Secs. II and III with the simplest cases of A_1 and A_2 algebras, discribing in detail all necessary steps of calculations. In Sec. IV we consider the general case of A_n algebra. In Sec. V we summarize the results of the paper and discuss the perspectives of the further investigations.

II. THE CASE OF $A_1 \simeq$ SU(2) AND U(2)

Every section will be divided into two parts; the classical case (the functional group level) and proper algebraic construction (''quantum case''). As it was remarked in the Introduction, the classical results may be used as good hint in further algebraic (quantum) calculations.

A. The functional algebra case

The functional U(2) algebra contains four elements $X^{\pm},H,I$ connected among themselves by Poisson brackets,

$$\{I,X^{\pm}\}=\{I,H\}=0, \quad \{X^{+},X^{-}\}=H, \quad \{H,X^{\pm}\}=\pm 2X^{\pm}. \tag{2}$$

In correspondence with the Darboux theorem[2] out of the elements of the U(2) functional group (2) it is possible to construct a pair of canonically conjugated variables M,m, $\{M,m\}=1$ and two cyclic variables $I,L\equiv X^{+}X^{-}+\frac{1}{4}H^{2}$ which have zero Poisson brackets among themselves and with all the other elements of the U(2) functional group (clearly, up to an arbitrary canonical transformation). Let us choose $M=H$ and $m=\frac{1}{4}\ln(X^{+}/X^{-})+f(H)$. With the help of the Poisson brackets (2) it is not difficult to see that thus constructed M,m are really canonically conjugate variables. Resolving these relations with respect to the functional group elements leads to following realization of the functional group elements in terms of the canonical conjugated coordinate m and momenta M and the two cyclic momenta L_1,L_2,

$$\begin{gathered} X^{+}=\tfrac{1}{2}e^{2m}(L_1-M), \quad X^{-}=\tfrac{1}{2}e^{-2m}(M-L_2), \quad H=M, \\ K^{1}\equiv I=L_1+L_2, \quad K^{2}=\frac{1}{4}\left(\frac{L_1-L_2}{2}\right)^{2}. \end{gathered} \tag{3}$$

By direct calculations it is not difficult to verify that (3) is indeed a realization of the functional group (2). If we want to restrict ourselves with the case of A_1 algebra it is necessary to put $I=0$.

B. Algebraic case

As always, to pass from the classical expressions to the quantum ones it is necessary to order in some way the operators involved and replace the Poisson brackets by commutators. Equations (3) give us a hint about the very tempting possibility to rewrite them as

$$\begin{gathered} X^{+}=\tfrac{1}{2}e^{m}(L_1-M)e^{m}, \quad X^{-}=\tfrac{1}{2}e^{-m}(M-L_2)e^{-m}, \\ H=M-\frac{L_1+L_2}{2}, \quad Q=L_1+L_2, \quad L=\frac{1}{2}\left(\frac{(L_1-L_2)^{2}}{2}-1\right) \end{gathered} \tag{4}$$

and consider now M,m as generators of the Heisenberg algebra ($[M,m]=1$, $[M,1]=0$, $[m,1]=0$, and L_1,L_2 commute with all of the generators involved in (4)). Keeping in mind the following operator relation for the Heisenberg algebra, $e^{\pm x}pe^{\mp x}=p\mp 1$, we conclude that the generators, defined in (4) satisfy the commutation relations (2) of U(2) algebra (of course with square brackets instead of the curly ones).

Two Cazimir operators under realization (4) take on the constant values

$$K^{(1}=L_1+L_2, \quad K^{(2}=X^+X^-+X^-X^+ +\frac{1}{2}H^2=\left(\frac{(L_1-L_2)^2}{2}-1\right), \tag{5}$$

which proves the irreducibility of the constructed representation.

III. $A_2 \simeq$ SU(3) AND U(3) CASES

In this case the problem consists in resolving the system of commutation relations

$$[X_1^+,X_1^-]=h_1, \quad [X_1^+,X_2^-]=0, \quad [h_1,X_1^\pm]=\pm 2X_1^\pm, \quad [h_1,X_2^\pm]=\mp X^\pm,$$

$$[X_1^+,X_2^-]=0, \quad [X_2^+,X_2^-]=h_2, \quad [h_2,X_2^\pm]=\pm 2X_2^\pm, \quad [h_2,X_1^\pm]=\mp X_1^\pm. \tag{6}$$

Algebra representation theory insures us that this is equivalent to the construction of some representation (possibly a reducible one) of the A_2 algebra.

The ''selection rules'' of the GZ paper allow us to try to find a solution of this problem in the following form:

$$\begin{gathered} X_1^+=\tfrac{1}{2}e^m(L_1-M)e^m, \quad X_2^+=e^{l_1}f^1e^{l_1}+e^{l_2}f^2e^{l_2}, \\ h_1=M-\frac{L_1+L_2}{2}, \\ X_1^-=\tfrac{1}{2}e^{-m}(M-L_2)e^{-m}, \quad X_2^-=e^{-l_1}\overline{f^1}e^{-l_1}+e^{-l_2}\overline{f^2}e^{-l_2}, \\ h_2=-\frac{M}{2}+L_1+L_2-\frac{N_1+N_2+N_3}{2}, \end{gathered} \tag{7}$$

where all ''structural'' functions $f^{1,2},\overline{f^{1,2}}$ depend only on momentum (capital letters) variables. We intentionally preserve the order of operators to avoid rewriting the same formulas for several times.

A. Classical case

In this case it is necessary to understand all of the above relations at the functional group level. The commutators have to be replaced by the Poisson brackets understood as usually,

$$\{A,B\}=\sum_1^3\left(\frac{\partial A}{\partial p_i}\frac{\partial B}{\partial x_i}-\frac{\partial A}{\partial x_i}\frac{\partial B}{\partial p_i}\right), \quad x_i=(m,l_1,l_2), \quad p_i=(M,L_1,L_2).$$

Now all of the objects are commutative and the order of the factors in (7) is unimportant. As a consequence of the vanishing Poisson brackets $\{X_1^+,X_2^-\}=\{X_2^+,X_1^-\}=0$, we obtain the explicit dependence of structural functions on momentum M. Namely,

$$\begin{gathered} X_1^+=\tfrac{1}{2}e^m(L_1-M)e^m, \quad X_2^+=e^{l_1}f^1e^{l_1}+e^{l_2}(M-L_2)f^2e^{l_2}, \\ X_{12}^+\equiv[X_1^+,X_2^+]=e^m\{e^{l_1}f^1e^{l_1}-e^{l_2}(L_1-M)f^2e^{l_2}\}e^m, \\ h_1=M-\frac{L_1+L_2}{2}, \quad h_2=-\frac{M}{2}+L_1+L_2-\frac{N_1+N_2+N_3}{2}, \end{gathered} \tag{8}$$

$$X_{12}^-\equiv[X_2^-,X_1^-]=e^{-m}\{e^{-l_1}(L_1-M)\overline{f^1}e^{-l_1}-e^{l_2}\overline{f^2}e^{-l_2}\}e^{-m},$$

$$X_1^-=\tfrac{1}{2}e^{-m}(M-L_2)e^{-m}, \quad X_2^-=e^{-l_1}(L_1-M)\overline{f^1}e^{-l_1}+e^{-l_2}\overline{f^2}e^{-l_2}. \tag{9}$$

Keeping in mind the above arguments, we have preserved the order of factors essential for the consideration in the next subsection. Moreover, we have presented also the explicit form of the generators of the composed roots $X_{12}^{\pm}$, which will be necessary below for constructing of the Cazimir operators. The additional constant in h_2 will be explained a little bit later. In the case of the A_2 algebra this constant is equal to zero.

The remaining Poisson bracket $\{X_2^+, X_2^-\}=h_2$, unused up to now, has as its consequence the system of equations for structural functions. Technically, all these operations are simple and we represent only the result,

$$(f^1\overline{f^1})_{L_1}-(f^2\overline{f^2})_{L_2}=-\tfrac{1}{4},\quad -(L_1 f^1\overline{f^1})_{L_1}+(L_2 f^2\overline{f^2})_{L_2}=\frac{L_1+L_2}{2}-\frac{N_1+N_2+N_3}{4}, \tag{10}$$

$$f^2_{L_1}\overline{f^1}+f^2\overline{f^1}_{L_2}=0,\quad f^1_{L_2}\overline{f^2}+f^1\overline{f^2}_{L_1}=0. \tag{11}$$

By shifts of independent variables $L_1\to L_1+(N_1+N_2+N_3)/3$ and $L_2\to L_2+(N_1+N_2+N_3)/3$ the constant term from the second Eq. (10) may be taken away. This corresponds to the transition from the algebra U(3) to SU(3).

From now on we can divide our problem into two parts and formulate it more precisely. First of all, we want to prove that the linear system of Eqs. (10) is exactly integrable and to give its general solution. In the case of arbitrary A_n algebra it will be the linear system of equations in partial derivatives for n unknown functions in the n-dimensional space. Secondly, we can solve this system under additional restrictions, which follow from (11), and in this way to obtain once again the GZ formulas for matrix elements of irreducible representations of the A_n algebra.

In this section we present the solution of the second part of the problem. The functional group possesses two cyclic variables (Cazimir operators on the algebra representation level), which may be constructed as the traces of the second and third degree of the following matrix:

$$K=\begin{pmatrix} h^1 & X_1^- & X_{12}^- \\ X_1^+ & h^2-h^1 & X_2^- \\ X_{12}^+ & X_2^+ & -h^2 \end{pmatrix},$$

where $h^1=(2h_1+h_2)/3=(M/2)$, and $h^2=(h_1+2h_2)/3=(L_1+L_2)/2$. Explicit forms of Cazimir operators of the second- and the third-order are as follows:

$$\begin{aligned} K^{(2}&=X_{12}^+X_{12}^-+X_1^+X_1^-+X_2^+X_2^-+(h^1)^2-h^1h^2+(h^2)^2\\ &=(L_1-L_2)(f^1\overline{f^1}+f^2\overline{f^2})+\tfrac{1}{4}(L_1^2+L_1L_2+L_2^2),\end{aligned}$$

$$\begin{aligned} K^{(3}&=X_{12}^+X_1^-X_2^-+X_{12}^-X_1^+X_2^+-h^1X_2^+X_2^-+h^2X_1^+X_1^-+(h^1-h^2)X_{12}^+X_{12}^-+h^1h^2(h^1+h^2)\\ &=\tfrac{1}{2}\{(L_1-L_2)(L_1f^1\overline{f^1}+L_2f^2\overline{f^2})+\tfrac{1}{4}L_1L_2(L_1+L_2).\end{aligned}$$

Equating the Cazimir operators to constant values, we obtain additional system of linear algebraic equations for the functions $x\equiv f^1\overline{f^1}$, $y\equiv f^2\overline{f^2}$, which is consistent with (10), (11),

$$x+y=\frac{\sigma_2-(L_1^2+L_1L_2+L_2^2)}{4(L_1-L_2)^2},\quad L_2x+L_1y=\frac{\sigma_3-L_1L_2(L_1+L_2)}{4(L_1-L_2)^2}.$$

The solution of the last system is given as follows:

$$f^1\overline{f^1}=\frac{P_3(L_1)}{4(L_1-L_2)^2},\quad f^2\overline{f^2}=\frac{-P_3(L_2)}{4(L_1-L_2)^2}, \tag{12}$$

where $P_3(z)=(z-N_1)(z-N_2)(z-N_3)$ and $N_1+N_2+N_3=0$ in the case of A_2 algebra. We emphasize that solution (12) is only a particular solution of system (10), but not of the general one.

B. General solution of the linear system

To stress the symmetry properties of (10), we rewrite it in the variables $X^1\equiv f^1\overline{f^1}, X^2\equiv -f^2\overline{f^2}, x_1\equiv L_1, x_2\equiv L_2$, keeping only the homogeneous part of it,

$$X^1_{x_1}+X^2_{x_2}=0, \quad (x_1X^1)_{x_1}+(x_2X^2)_{x_2}=0. \tag{13}$$

The system (13) is a particular case of the following system for n unknown functions X^i in n-dimensional coordinate space x_i,

$$\sum_{i=1}^{n}(x_i^kX^i)_{x_i}=0, \ \ k=0,1,2,...,n-1 \tag{14}$$

the particular case (13) corresponds to the choice $n=2$ in (14).

Now we would like to demonstrate the direct way for obtaining the general solution of (13). Multiplying the first equation of the system (13) correspondingly by x_1, x_2 and subtracting it from the second equation we obtain

$$((x_2-x_1)X^2)_{x_2}+X^1=0, \quad ((x_1-x_2)X^1)_{x_1}+X^2=0.$$

Introducing new unknown functions $Y^{1,2}\equiv(x_1-x_2)^2X^{1,2}$, we transform the system (13) to the form

$$(x_2-x_1)(Y^2)_{x_2}+Y^1-Y^2=0, \quad (x_1-x_2)(Y^1)_{x_1}+Y^2-Y^1=0,$$

from which we conclude that $(Y^1)_{x_1}=(Y^2)_{x_2}$. At last, differentiating the first equation with respect to x_1 and the second one with respect to x_2, we present each of them in the integrable form,

$$\frac{\partial \ln Y^2_{x_1}}{\partial x_2}=\frac{1}{x_2-x_1}, \quad \frac{\partial \ln Y^1_{x_2}}{\partial x_1}=\frac{1}{x_1-x_2}. \tag{15}$$

Finally, the general solution of the system (13) takes the form,

$$\begin{aligned}(x_1-x_2)^2X^1&=\Phi(x_2)_{x_2}(x_1-x_2)+\Theta(x_1)+\Phi(x_2),\\ (x_1-x_2)^2X^2&=\Theta(x_1)_{x_1}(x_2-x_1)+\Phi(x_2)+\Theta(x_1),\end{aligned} \tag{16}$$

where $\Theta(x_1),\Phi(x_2)$ are arbitrary functions of a single argument.

C. Algebraic cases $A_2\simeq$ SU(3) and U(3)

In this section we will consider a realization of (8), where the pairs M,m,L_1,l_1,L_2,l_2 are the elements of the three independent mutually commutative Heisenberg algebras $[M,m]=1$, $[L_1,l_1]=1$, $[L_2,l_2]=1$. The involved structural functions are supposed to depend only on the momentum operators M,L_1,L_2,N_1,N_2,N_3.

Explicit dependence of the structural functions upon the momentum M arises immediately, if we take into account commutation relations $[X_1^+,X_2^-]=[X_2^+,X_1^-]=0$.

Commutation relation $[X_2^+,X_2^-]=h_2$, after using the well-known from the theory of the Heisenberg algebra relations $\exp(\pm x)p\exp(\mp x)=p\mp 1$ is equivalent to the system of equations in finite differences, which will be convenient to write in the following notation:

$$F^{(1}_{\pm}=f^{(1}(L_1\pm 1,L_2)\overline{f}^{(1}(L_1\pm 1,L_2),$$

$$F^{(2}_{\pm}=f^{(2}(L_1,L_2\pm 1)\overline{f}^{(2}(L_1,L_2\pm 1),$$

$$F^{(1}_{+}-F^{(1}_{-}+F^{(2}_{+}-F^{(2}_{-}=-\tfrac{1}{2},$$

$$-(L_1+1)F^{(1}_{+}+(L_1-1)F^{(1}_{-}-(L_2-1)F^{(2}_{-}+(L_2+1)F^{(2}_{+}=L_1+L_2-\frac{N_1+N_2+N_3}{2}, \tag{17}$$

$$\begin{aligned} &f^{(2}(L_1-1,L_2)\overline{f}^{(1}(L_1,L_2-1)=f^{(2}(L_1+1,L_2)\overline{f}^{(1}(L_1,L_2+1),\\ &f^{(1}(L_1,L_2-1)\overline{f}^{(2}(L_1-1,L_2)=f^{(1}(L_1,L_2+1)\overline{f}^{(2}(L_1+1,L_2). \end{aligned} \tag{18}$$

In the continuous limit (17) coincides with (10), and (18) coincides with (11).

The Cazimir operators may be constructed as traces of the first, second, and third degrees of the K matrix as in the previous subsection. But in this case it is necessary to take into account noncommutativity of operators involved. In this way we obtain their explicit expressions,

$$K^{(1}=\frac{N_1+N_2+N_3}{2},$$

$$\begin{aligned} K^{(2}&=X^+_{12}X^-_{12}+X^-_{12}X^+_{12}+X^+_1X^-_1+X^-_1X^+_1+X^+_2X^-_2+X^-_2X^+_2+2((h^1)^2-h^1h^2+(h^2)^2),\\ K^{(3}&=X^-_2X^+_{12}X^-_1+X^+_1X^-_{12}X^+_2-\tfrac{1}{2}h^1\{X^+_2X^-_2\}+\tfrac{1}{2}h^2\{X^+_1X^-_1\}\\ &\quad+\tfrac{1}{2}(h^1-h^2-2)\{X^+_{12}X^-_{12}\}+h^1h^2(h^1+h^2)+(h^1+h^2)-((h^1)^2-h^2h^1+(h^2)^2). \end{aligned} \tag{19}$$

Equating Cazimir's operators to constant values, we obtain the additional and consistent with (17), (18) equations,

$$\begin{aligned} F^{(1}_{+}+F^{(1}_{+}+F^{(2}_{+}+F^{(2}_{-}=&\frac{\sigma_2-(L_1^2+L_1L_2+L_2^2)}{2(L_1-L_2)}\left[\frac{(L_2-1)(L_1+L_2+4)}{4}-(L_1+1)(L_2+1)\right]F^{(1}_{+}\\ &+\frac{(L_2+1)(L_1+L_2+4)}{4}F^{(1}_{-}-\frac{(L_1+1)(L_1+L_2+4)}{4}F^{(2}_{-}\\ &+\left[(L_2+1)(L_1+1)-\frac{(L_1-1)(L_1+L_2+4)}{4}\right]F^{(2}_{+}\\ =&\sigma_3+\frac{1}{8}L_1L_2(L_1+L_2)+\frac{5}{8}(L_1+L_2)+\frac{1}{4}(L_1+L_2)^2. \end{aligned} \tag{20}$$

In connection with the last system the following comments will be appropriate. (17) is the system of the two equations for two unknown functions $F^{(1,2}$ with shifted ± 1 arguments. In this sense it is a closed one. (18) and (20) may be considered as additional to (17) conditions, by which are necessary to choose from the general solution only those that correspond to the realization of the irreducible (Cazimir operators are fixed) representations of the A_2 algebra.

As in the previous section, here two problems arises; to find a general solution of the system (17) and, as the second step, to satisfy additional conditions which follow from (18) and (20).

Here we present a solution of the second part of the above formulated problem. Combining the first equation of (17) with the first equation from (20), we immediately obtain

$$F_+^{(1}+F_-^{(2}=-\frac{1}{4}+\frac{\sigma_2-(L_1^2+L_1L_2+L_2^2)}{4(L_1-L_2)},\quad F_+^{(1}+F_+^{(2}=\frac{1}{4}+\frac{\sigma_2-(L_1^2+L_1L_2+L_2^2)}{4(L_1-L_2)}.$$

For unknown functions, $v\equiv(L_1-L_2-2)(F_-^{(1}-F_+^{(2})$, $u\equiv(L_1-L_2+2)(F_+^{(1}-F_-^{(2})$, we obtain the linear system from the remaining equations,

$$v-u=\tfrac{3}{2}(L_1+L_2),$$

$$(L_1-L_2+2)v+(L_1-L_2-2)u=\frac{(L_1+L_2+4)(\sigma_2-(L_1^2+L_1L_2+L_2^2))}{4}+L_1L_2(L_1+L_2)$$
$$+2(L_1^2+L_1L_2+L_2^2)+2(L_1+L_2)+\sigma_3,$$

with the explicit solution,

$$4(L_1-L_2-1)(L_1-L_2+1)F^{(1}=P_3(L_1),\quad 4(L_1-L_2-1)(L_1-L_2+1)F^{(2}=P_3(L_2),\quad (21)$$

where $P_3(z)=(z-N_1)(z-N_2)(z-N_3)$.

The square roots of $F^{(1},F^{(2}$ are exactly the matrix elements of Gel'fand–Tsetlin realization of U(3) algebra.

IV. GENERAL CASE OF ARBITRARY *n*

A. The algebra representation level

Let us assume that the generators of the simple roots and Cartan elements of elements of $U(n+1)$ algebra may be represented in the form

$$X_s^+=\sum_{k=1}^{s} e^{l_k^s}g_k^s e l_k^s,\quad X_s^-=\sum_{k=1}^{s} e^{-l_k^s}\overline{g}_k^s e^{-l_k^s},\qquad (22)$$

$$h_s=-\frac{1}{2}\sum_{r=1}^{s-1}L_r^{s-1}+\sum_{k=1}^{s}L_k^s-\frac{1}{2}\sum_{l=1}^{s+1}L_l^{s+1},\quad 1\leqslant s\leqslant n,$$

where nonzero commutators of operators involved are only those

$$[L_k^s,l_l^t]=\delta_{st}\delta_{kl}I$$

and structural functions are the functions only of the following arguments: $g_k^s\equiv g_k^s(L^{s+1},L^s,L^{s-1})$, $\overline{g}_k^s\equiv\overline{g}_k^s(L^{s+1},L^s,L^{s-1})$. The reader may identify without any difficulties L^1 with M,L^2 with L_1,L_2 and at last L^3 with N_1,N_2,N_3. We will assume also that structural functions may be represented in factorizable form

$$g_k^s\equiv F_k^s(L^{s+1};L^s)f_k^s(L^s;L^{s-1}),\quad \overline{g}_k^s\equiv\overline{F}_k^s(L^{s+1};L^s)\overline{f}_k^s(L^s;L^{s-1}),$$

and

$$(F_k^{s-1})^2=(\overline{F}_k^{s-1})^2=\frac{\Pi_{r=1}^s(L_k^{s-1}-L_r^s)}{\Phi(L^{s-1})},$$

where function Φ is translation invariant with respect to the shift of all of its arguments L_k^{s-1}.

The last proposition we will prove by induction.

It is obvious that under such kinds of restrictions commutation relation between generators of Cartan subalgebra h_l and generators of the simple roots $X_k^{\pm}$ are correctly satisfied. It is also clear that the generators $X_s^{\pm}$ commute with all generators $X_k^{\mp}$ with $k \leqslant (s-2)$ because they act on essentially different arguments. And finally, commutation relations

$$[X_s^{\pm}, X_{s-1}^{\mp}] = 0$$

allow us to reconstruct in explicit form the dependence of structural functions $f_k^s, \overline{f_k^s}$ on arguments L_k^{s-1}.

As a direct consequence of the last commutation relations we obtain

$$f_k^s(L^s;\ldots,L_r^{s-1}-1,\ldots)\overline{F_r^s}^{s-1}(\ldots,L_k^s-1,\ldots;L^{s-1}) = f_k^s(L^s;\ldots,L_r^{s-1}+1,\ldots)\overline{F_r^s}^{s-1}(\ldots,L_k^s+1,\ldots;L^{s-1}),$$

$$\overline{f_k^s}(L^s;\ldots,L_r^{s-1}-1,\ldots)F_r^{s-1}(\ldots,L_k^s-1,\ldots;L^{s-1}) = \overline{f_k^s}(L^s;\ldots,L_r^{s-1}+1,\ldots)F_r^{s-1}(\ldots,L_k^s+1,\ldots;L^{s-1}).$$

The last relations must be satisfied for all possible values of the indices k and r. Keeping in mind the explicit form of the structural functions $F_k^{s-1} = \overline{F_k^s}^{s-1}$, proposed above, we can resolve the last equations in the form,

$$g_k^s = F_k^s(L^{s+1};L^s)\sqrt{\prod_{r=1}^{s-1}(L_k^s - L_r^{s-1})},\quad \overline{g_k^s} = \overline{F_k^s}(L^{s+1};L^s)\sqrt{\prod_{r=1}^{s-1}(L_k^s - L_r^{s-1})}. \tag{23}$$

Up to now we have not satisfied the only commutation relation

$$[X_s^+, X_s^-] = h_s. \tag{24}$$

This equation contains a ''diagonal'' part (which does not contain the coordinates of Heisenberg subalgebras l_i) and a nondiagonal one (in above sense). It is suitable to write the emerged equation for the diagonal part in the following notations:

$$X_k^{\pm s} = F_k^s(L^{s+1};\ldots,L_k^s \pm 1,\ldots)\overline{F_k^s}(L^{s+1};\ldots,L_k^s \pm 1\ldots),$$

$$\sum_{k=1}^{s}\prod_{r=1}^{s-1}(L_k^s + 1 - L_r^{s-1})X_k^{+s} - \sum_{k=1}^{s}\prod_{r=1}^{s-1}(L_k^s - 1 - L_r^{s-1})X_k^{(-s}$$

$$= -\frac{1}{2}\sum_{r=1}^{s-1}L_r^{s-1} + \sum_{k=1}^{s}L_k^s - \frac{1}{2}\sum_{j=1}^{s+1}L_j^{s+1}. \tag{25}$$

The left-hand side of this equation may be represented as linear combination of $s-1$ symmetrical functions, constructed out of $(s-1)$ momentum variables L_r^{s-1}. The right-hand side of (25) contains only terms of the first and zero degree with respect to such functions. Thus, as a corollary of (25), we obtain the system of s equations in finite differences for determining s unknown functions X_k^s,

$$\sum_{k=1}^{s}[(L_k^s+1)^{s-1}X_k^{+s} - (L_k^s-1)^{s-1}X_k^{-s}] = \sum_{k=1}^{s}L_k^s - \frac{1}{2}\sum_{j=1}^{s+1}L_j^{s+1},$$

$$\sum_{k=1}^{s}[(L_k^s+1)^{s-2}X_k^{+s} - (L_k^s-1)^{s-2}X_k^{-s}] = \frac{1}{2}, \tag{26}$$

$$\sum_{k=1}^{s}\left[(L_k^s+1)^i X_k^{+s}-(L_k^s-1)^i X_k^{-s}\right]=0 \quad 0\leqslant i\leqslant(s-3).$$

The zero value of ''nondiagonal'' part of (24) is equivalent to additional conditions which structural functions must satisfy

$$\begin{aligned}&F_k^s(L^{s+1};\ldots,L_j^s-1,\ldots)\overline{F_j^s}(L^{s+1};\ldots,L_k^s-1,\ldots)=F_k^s(L^{s+1};\ldots,L_j^s+1,\ldots)\overline{F_j^s}(L^{s+1};\ldots,L_k^s+1,\ldots),\\&\overline{F_k^s}(L^{s+1};\ldots,L_j^s-1,\ldots)F_j^s(L^{s+1};\ldots,L_k^s-1,\ldots)=\overline{F_k^s}(L^{s+1};\ldots,L_j^s+1,\ldots)F_j^s(L^{s+1};\ldots,L_k^s+1,\ldots).\end{aligned}\tag{27}$$

From (27) we see that the solution $F_j^s=\overline{F_j^s}$ is possible and the functions X_k^s (as the solutions of (25)) must satisfy the additional conditions,

$$X_k^s(L^{s+1};\ldots,L_j^s-1,\ldots)X_j^s(L^{s+1};\ldots,L_k^s-1,\ldots)=X_k^s(L^{s+1};\ldots,L_j^s+1,\ldots)X_j^s(L^{s+1};\ldots,L_k^s+1,\ldots).\tag{28}$$

Putting $s=2$, the reader can easily obtain from general equations of the present subsection all results of the previous section, in particular, Eqs. (17). At this point we interrupt our consideration for a moment in order to represent a general solution of the continuous version of Eq. (26).

B. General solution of the linear system in the continuous limit

The continuous limit of the homogeneous part of the system (26) in variables $X^i\equiv F_i^n$, $x_i\equiv L_i^n$ has the form

$$\sum_{i=1}^{n}(x_i^k X^i)_{x_i}=0, \quad k=0,1,\ldots, \ n-1.\tag{29}$$

We do not know the simple regular methods of the direct resolution of (29). The way of solving of this problem known to us for the particular case $n=3$ is given in the Appendix. Here we represent the final result and the proof of its validity.

General solution of the system (29) is given by the formula

$$X^s=\left(\frac{\Theta}{\Pi'^n_{k=1}(x_i-x_k)}\right)_{x_1\ldots x_{s-1}x_{s+1}\ldots x_n},\tag{30}$$

where the function Θ satisfies the equation $\Theta_{x_1\ldots x_n}=0$ (here the differentiation is performed with respect to all independent coordinates of the problem!).

The following result from the theory of symmetrical functions will be necessary for us to prove that (30) is indeed a solution of (29),

$$\sum_{i=1}^{n}\frac{x_i^r}{\Pi'^n_{k=1}(x_i-x_k)}=(0,1,S^{r-n+1}).$$

In the parentheses in the right-hand side different possibilities are given. The first one (0) takes place if r is strictly less then $n-1$; the second one occurs if $r=n-1$ and the third possibility corresponds to the case when r is strictly more the $n-1$ and S^k is some symmetrical function of the kth degree.

It is possible to understand the above proposition without any calculations. Indeed, the written sum is a symmetrical function. After reducing it to the common denominator we obtain the ratio of two n-dimensional polynomial functions, one of which (the denominator) is exactly the Wandermond determinant (an only function which is antisymmetrical with respect to permutation of

each pair of coordinates). Hence the numerator must also be antisymmetrical polynomial (since the ratio is symmetric!). This is impossible if r is less then $n-1$ (the degree of the numerator in this case is less than the degree of the Wandermond determinant).

After these comments let us consider an arbitrary equation from the system (30). We have consequently

$$\sum_{s=1}^{n}\left(x_s^r\left(\frac{\Theta}{\Pi'^{n}_{k=1}(x_s-x_k)}\right)_{x_1\cdots x_{s-1}x_{s+l}\cdots x_n}\right)_{x_s}=\left(\sum_{s=1}^{n}\frac{x_s^r}{\Pi'^{n}_{k=1}(x_s-x_k)}\Theta\right)_{x_1\cdots x_n}=0.$$

In the case when r is strictly less than $n-1$ the sum by itself equals zero; in the case when $r=(n-1)$ the sum is equal to unity but the condition for the function Θ equates to zero the corresponding equation of the system.

Thus, our proposition is proven and (30) is indeed a general solution of the linear system (29).

C. Continuation of the discussion

Now we can present the solution of inhomogeneous system (27) together with the additional conditions (28). We begin with the continuous case, using the notations of the previous subsection. In this case system (27) takes the form,

$$2\sum_{i=1}^{n}(x_i^{n-1}X^i)_{x_i}=-\frac{1}{2}\sum_{j=1}^{n+1}y_j+\sum_{i=1}^{n}x_i 2\sum_{i=1}^{n}(x_i^{n-2}X^i)_{x_i}=\frac{1}{2},$$
$$\sum_{i=1}^{n}(x_i^rX^i)_{x_i}=0,\quad 0\leqslant r\leqslant n-3. \tag{31}$$

Keeping in mind the solution for the particular case $n=2$ (21) we will try to find a solution of the last system in the form,

$$X^i=\frac{1}{4}\left(\frac{P_{n+1}(x_i)}{\Pi'^{n}_{k=1}(x_i-x_k)}\right)_{x_1\cdots x_{i-1}x_{i+1},\cdots x_n}\equiv\frac{1}{4}\frac{P_{n+1}(x_i)}{\Pi'^{n}_{k=1}(x_i-x_k)^2}, \tag{32}$$

where $P_{n+1}(x_i)=\Pi_{j=1}^{n+1}(x_i-y_j)$. Substituting (32) into each Eq. (31) we consequently check all equations,

$$\sum_{i=1}^{n}(x_i^rX^i)_{x_i}=\frac{1}{4}\left(\frac{x^rP_{n+1}(x_i)}{\Pi'^{n}_{k=1}(x_i-x_k)}\right)_{x_1,\cdots x_n},$$

where in the last expression it is necessary to perform the differentiation on all coordinates.

In connection with the facts from the theory of the symmetrical functions, mentioned in the previous subsection, the sum under the symbol of differentiation in the case $(0\leqslant r\leqslant(n-3))$ is nothing else but the linear combination of the symmetrical functions with the degree not greater than $n-1$. After differentiating with respect to all coordinates such functions vanish. By the same reason only the term with the highest power of polynomial gives contribution different from zero in the case when $(r=n-2)$ and the terms $x_i^{n+1}-(\Sigma_{j=1}^{n+1}y_j)x_i^n$ in the case when $r=n-1$. Numerical values for corresponding sums, which can be calculated without big difficulties, shows that the first pair of Eqs. (31) is also satisfied. It is not difficult to check that the solution (32) satisfies additional conditions (28).

In the algebraic case situation is very similar. To show this let us introduce the operation of the discrete differentiation, defined as

$$\Delta_i f(x_1,\ldots,x_n)=\frac{f(\ldots x_i+1,\ldots)-f(\ldots,x_i-1,\ldots)}{2}.$$

Operations Δ_i and Δ_j are obviously mutually commutative and satisfy the linear condition in the following sense:

$$\Delta_i(f^1+f^2)=\Delta_i f^1+\Delta_i f^2,\ \ \Delta_i c f=c\Delta_i f,$$

if c is some function independent of the x_i coordinate.

In this notations general solution of homogeneous system (26) has the form

$$X^i=(\Delta_1\cdots\Delta_{i-1}\Delta_{i+1}\cdots\Delta_n)\frac{\Theta}{\Pi'^n_{k=1}(L^n_i-L^n_k)},\tag{33}$$

where the function Θ is an arbitrary solution of the equation in finite differences

$$(\Delta_1\cdots\Delta_n)\Theta=0.$$

Solution of the inhomogeneous system (26) satisfying additional conditions (28) is given by

$$F^i=(\Delta_1\cdots\Delta_{i-1}\Delta_{i+1}\cdots\Delta_n)\frac{P_{n+1}(L^n_i)}{\Pi'^n_{k=1}(L^n_i-L^n_k)},\ \ P_{n+1}(x)=\prod_{j=1}^{n+1}(x-L^{n+1}_j).\tag{34}$$

We omit the proofs of the last propositions because it does not change in essential points in comparison with the continuous case. This fact is extremely interesting and remarkable and it will take some time to comprehend it.

V. OUTLOOK AND POSSIBLE PERSPECTIVES

In the present paper we have presented some new (unknown before or may be forgotten at the present moment) linear integrable systems in the space of arbitrary n dimensions. This system is invariant with respect to transformations from the whole group of permutations of n symbols. Particular solutions of this system are in the deep connection with the algebra A_n and matrix elements of its irreducible representations, discovered many years ago by Gel'fand and Tsetlin.[1] This fact allows us to reproduce the GZ result by a new method and moreover, to make them more understandable. Remarkably, under our formulation of the problem it was sufficient to perform calculations only on the functional group level. But to give any explanation or comment of this fact we are now not ready.

By some reasons (which are not clear for us at this moment) the quasiclassical approach gives a functionally correct quantum result. We hope that the method proposed in this paper can be generalized to the case of arbitrary semisimple algebra, relating the used parameterization with the properties of the Weyl discrete group of corresponding semisimple algebra.

We hope also that by a method of the present paper it will be possible to find new realizations of quantum and deformed algebras.

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APPENDIX

The initial system in the case $n=3$ has the form

$$X^1_{x_1}+X^2_{x_2}+X^3_{x_3}=0,$$

$$(x_1X^1)_{x_1}+(x^k_iX^i)_{x_i}+(x_3X^3)_{x_3}=0, \tag{35}$$

$$(x^2_1X^1)_{x_1}+(x^2_2X^2)_{x_2}+(x^2_3X^3)_{x_3}=0.$$

Multiplying the first equation by x_2x_3, the second one by $-(x_2+x_3$ and summing them with the third one we obtain

$$((x_3-x_2)(x_3-x_1)X^3)_{x_3}+\frac{(x_1-x_2)(x_1-x_3)X^1}{(x_1-x_3)}+\frac{(x_2-x_1)(x_2-x_3)X^2}{(x_2-x_3)}=0.$$

Let us introduce the new unknown functions $\overline{X^i}\equiv\Pi'^n_{k=1}(x_i-x_k)X^i$ and rewrite the last equation (together with those which arise from it after obvious permutations of the indexes), we come to a system

$$\overline{X^1}_{x_1}+\frac{\overline{X^2}}{(x_2-x_1)}+\frac{\overline{X^3}}{(x_3-x_1)}=0,$$

$$\overline{X^2}_{x_2}+\frac{\overline{X^1}}{(x_1-x_2)}+\frac{\overline{X^3}}{(x_3-x_2)}=0, \tag{36}$$

$$\overline{X^3}_{x_3}+\frac{\overline{X^1}}{(x_1-x_3)}+\frac{\overline{X^2}}{(x_2-x_3)}=0.$$

The next transformation $\tilde{X}^i=\equiv\Pi'^n_{k=1}(x_i-x_k)\tilde{X}^i$ would be possible to realize independently on the first step, but the form of the system (36) will be necessary for further consideration and for this reason we represent it above. In the new variables we obtain

$$(x_1-x_2)(\tilde{X}^2_{x_2}+\tilde{X}^1_{x_1})+2(\tilde{X}^2-\tilde{X}^1)=0,$$

$$(x_2-x_3)(\tilde{X}^3_{x_3}+\tilde{X}^2_{x_2})+2(\tilde{X}^3-\tilde{X}^2)=0, \tag{37}$$

$$(x_1-x_2)(\tilde{X}^1_{x_1}+\tilde{X}^3_{x_3})+2(\tilde{X}^1-\tilde{X}^3)=0.$$

After excluding unknown $\tilde{X}^3$ from the two last equations and introducing $v\equiv\tilde{X}^2_{x_3}$ and $u\equiv\tilde{X}^1_{x_3}$ we obtain the system of two equations,

$$v_{x_2}-u_{x_1}-\frac{2v}{x_2-x_3}-\frac{2u}{x_3-x_1}=0,\quad v_{x_2}+u_{x_1}+\frac{2v}{x_1-x_2}-\frac{2u}{x_1-x_2}=0.$$

Finally excluding the unknown u we obtain an equation for v in the integrable form,

$$v_{x_1x_2}=v_{x_1}\left(\frac{1}{x_2-x_1}+\frac{1}{x_2-x_3}\right).$$

Returning back, after some algebraic manipulations we obtain the general solution of the initial system in the form

$$\overline{X^1}=\Theta_{x_2x_3}+\frac{\Theta_{x_3}}{x_1-x_2}+\frac{\Theta_{x_2}}{x_1-x_3}+\frac{\Theta}{(x_1-x_2)(x_1-x_3)},$$

$$\overline{X^2}=\Theta_{x_1x_3}+\frac{\Theta_{x_3}}{x_1-x_2}+\frac{\Theta_{x_1}}{x_2-x_3}+\frac{\Theta}{(x_2-x_1)(x_2-x_3)},$$

$$\overline{X^3}=\Theta_{x_2x_1}+\frac{\Theta_{x_2}}{x_3-x_1}+\frac{\Theta_{x_1}}{x_3-x_2}+\frac{\Theta}{(x_3-x_2)(x_3-x_1)}, \tag{38}$$

where $\Theta=\Theta^1(x_2x_3)+\Theta^2(x_1x_3)+\Theta^3(x_1x_2)$ and Θ^i are arbitrary functions of two independent arguments. So it is possible to state that Θ is an arbitrary solution of the equation

$$\Theta_{x_1x_2x_3}=0.$$

Of course, (38) is equivalent to one represented in the main text and used as an initial guess to find the general solution in the form (30).

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Deformation of surfaces, integrable systems, and Chern–Simons theory

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A few years ago, some of us devised a method to obtain integrable systems in $(2+1)$-dimensions from the classical non-Abelian pure Chern–Simons action via the reduction of the gauge connection in Hermitian symmetric spaces. In this article we show that the methods developed in studying classical non-Abelian pure Chern–Simons actions can be naturally implemented by means of a geometrical interpretation of such systems. The Chern–Simons equation of motion turns out to be related to time evolving two-dimensional surfaces in such a way that these deformations are both locally compatible with the Gauss–Mainardi–Codazzi equations and completely integrable. The properties of these relationships are investigated together with the most relevant consequences. Explicit examples of integrable surface deformations are displayed and discussed. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1339831]

I. INTRODUCTION

Many authors have extensively studied the deep relations among completely integrable systems and the basic equations of the differential geometry, like the Frenet formulas defining curves embedded in $\mathbf{R}^3$, or their analogous formulas for the surfaces, the Gauss–Weingarten (GW) equations, and the corresponding integrability conditions, i.e., the Gauss–Mainardi–Codazzi (GMC) equations (see for instance Refs. 1–3). In these approaches the main idea is to add to a generic differential geometry setting certain auxiliary conditions, containing from the beginning the properties of the completely integrable systems.

A slightly different situation occurs in the study of the so-called Darboux system,[4,5] which naturally arises in looking for classes of orthogonal curvilinear coordinates in Euclidean spaces and whose integrability has been detected in Ref. 6. Such a system has been investigated mainly in connection with the topological field theory.[7] On the other hand, some years ago some of us proposed a simple method to obtain completely integrable systems in $(2+1)$-dimensions, from classes of non-Abelian Chern–Simons (CS) field theories, taking values in Hermitian symmetric spaces.[8] In this context completely integrable systems are seen as particular gauge choices in which the theory is formulated. Moreover, linear spectral problems are naturally related to the geometrical constraints imposed on the target space. From this point of view, integrable systems arise as special reductions, which break the general covariance and the gauge invariance of the original field theory, but preserve a residual symmetry in order to allow the Lax representation and the complete integrability, although the solvability is lost.

In the present work we show that this approach can be naturally implemented by resorting to a geometrical interpretation of the completely integrable systems mentioned above. Precisely, we

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show, as the CS equation of motion can describe, time evolving two-dimensional surfaces in such a way that the deformation is not only locally compatible with the GMC equation, but completely integrable as well. The nature and the properties of such relationships are investigated together with the most important consequences. Furthermore, explicit examples of integrable deformations of surfaces are displayed.

The article is organized as follows. Section II contains some results on the CS theory. In Sec. III the fundamental terminology and notations related to the theory of two-dimensional surfaces are reviewed. In Sec. IV the general formulation of deformation of two-dimensional surfaces is presented. Section V is devoted to the analysis of certain spin models in $(2+1)$-dimensions. Section VI is addressed the bilinear representations of the spin systems fields and the trihedral moving frame. Sections VII and VIII are concerned with the deformations of surfaces from integrable $(2+1)$-dimensional spin systems and equations of the nonlinear Schrödinger type, respectively. In Secs. IX and X some solutions and special surfaces associated with spin system vortices are considered. Finally, in Sec. XI some concluding remarks are reported.

II. CHERN–SIMONS THEORY AND COMPLETELY INTEGRABLE SYSTEMS

Here we shall review some preliminaries concerning the CS theory and we show how one can connect them to the completely integrable systems in $(2+1)$ dimensions. We are dealing with the field theory defined by the action

$$S[J]=\frac{k}{4\pi}\int_M \mathrm{Tr}\left(J\wedge dJ+\frac{2}{3}J\wedge J\wedge J\right), \tag{1}$$

where J is a one-form gauge connection taking values in a simple Lie algebra $\hat{g}$ on an oriented closed three-manifold M, and k is a coupling constant which should be quantized in a quantum theory.[9] The related classical equation of motion is the zero-curvature condition,

$$F\equiv dJ+J\wedge J=0. \tag{2}$$

The action (1) is manifestly invariant under general coordinate transformations (preserving orientation and volumes). Moreover, under a generic gauge map $G:M\to\hat{G}$ the gauge connection transforms as $J\to G^{-1}JG+G^{-1}\,dG$. Correspondingly, the action (1) changes as $S[J]\to S[J]+2\pi k\,W(G)$, where

$$W(J)=\frac{1}{24\pi^2}\int_M \mathrm{Tr}(G^{-1}\,dG\wedge G^{-1}\,dG\wedge G^{-1}\,dG) \tag{3}$$

is the winding number of the map G and takes integer values, because of the result $\pi_3(\hat{G})=\mathbf{Z}$ from the homotopy theory.[10] This is a topological field theory in the sense that it possesses quantum observables, which are independent of the metric and are related to the Jones polynomials of the knot theory.[11] From other points of view, the action (1) has been used as an effective interaction for quasiparticles and vortices in two space-dimensional systems, of interest in the physics of high temperature superconductivity,[12] and in the context of the low-dimensional gravity models (see Ref. 13 and references therein). In the static self-dual reductions the system of equations (2) becomes the two-dimensional Toda field theory,[14] the static reductions of the Ishimori model, or of the Davey–Stewartson equation.[15]

In Ref. 8 the general action (1) was reduced assuming that the Lie algebra $\hat{g}$ admits a $\mathbf{Z}_2$ graduation, in such a way the form J splits in two parts, taking values on an isotropy subalgebra and a complement linear space, respectively. The former component will play the role of a gauge field with the isotropy group as a gauge group; the latter could be considered as a sort of coupled ''matter'' field. At any point of the corresponding coset space we can introduce in a natural way a Riemannian torsion-free connection.[10] Furthermore, the three-manifold M is trivialized into $\Sigma\times\mathbf{R}$, where Σ is a Riemann surface endowed with a set of local complex coordinates $z=x^1$

$+ix^2$, and $\mathbf{R}$ is interpreted as the time axis. Thus the connection J can be further decomposed into time- and space-like components. In the simplest SU(2)/U(1)$\sim CP^1\sim S^2$ case the connection takes the form

$$J=\begin{pmatrix} iv_\mu & -q_\mu^* \\ q_\mu & -iv_\mu \end{pmatrix} dx^\mu,$$

which can be rewritten in terms of complex forms

$$v\,dz=\tfrac{1}{2}(v_1-iv_2)dz, \quad \psi_- dz=\tfrac{1}{2}(q_1-iq_2)dz, \quad \psi_+ d\bar{z}=\tfrac{1}{2}(q_1+iq_2)d\bar{z}.$$

This allows us to write the action (1) as follows:

$$S=-\frac{k}{\pi}\int_{\Sigma\times\mathbf{R}}\left\{\frac{1}{2}\varepsilon^{\lambda\mu\nu}v_\lambda\partial_\mu v_\nu+\frac{i}{2}(\psi_+^* D_0\psi_+-\psi_+(D_0\psi_+)^*-\psi_-^* D_0\psi_-+\psi_-(D_0\psi_-)^*)\right.$$
$$\left.-iq_0^*(D\psi_+-\bar{D}\psi_-)+iq_0(D\psi_+-\bar{D}\psi_-)^*\right\}dx^0\,dx^1\,dx^2, \tag{4}$$

where $D_0=\partial_0-2iv_0$, $D=\partial_z-2iv$, $\bar{D}=\partial_{\bar{z}}-2iv^*$ (* denotes the complex conjugation). The first-order Lagrangian involved in (4) is constrained by the torsion-free condition

$$D\psi_+-\bar{D}\psi_-=0, \tag{5}$$

and by what we call the Gauss–Chern–Simons (GCS) law

$$\partial_z v^*-\partial_{\bar{z}}v=-i(|\psi_+|^2-|\psi_-|^2), \tag{6}$$

enforced by the Lagrangian multipliers q_0 and v_0, respectively. Of course, here we are looking in a different way to a subset of the equations of motion (2), in which the general covariance is broken. Indeed, only the isotropic U(1) invariance is left. Furthermore, by exploiting the local isomorphism between so(3) and su(2) realized by the adjoint representation of the connection

$$J^{(\mathrm{ad})}=\begin{pmatrix} 0 & -v_0 & -\mathrm{Re}(q_0) \\ v_0 & 0 & -\mathrm{Im}(q_0) \\ \mathrm{Re}(q_0) & \mathrm{Im}(q_0) & 0 \end{pmatrix} dx^0$$
$$+\begin{pmatrix} 0 & -2\,\mathrm{Re}(v) & -\mathrm{Re}(\psi_++\psi_-) \\ 2\,\mathrm{Re}(v) & 0 & -\mathrm{Im}(\psi_++\psi_-) \\ \mathrm{Re}(\psi_++\psi_-) & \mathrm{Im}(\psi_++\psi_-) & 0 \end{pmatrix} dx^1$$
$$+\begin{pmatrix} 0 & 2\,\mathrm{Im}(v) & -\mathrm{Im}(\psi_+-\psi_-) \\ -2\,\mathrm{Im}(v) & 0 & -\mathrm{Re}(\psi_+-\psi_-) \\ \mathrm{Im}(\psi_+-\psi_-) & \mathrm{Re}(\psi_+-\psi_-) & 0 \end{pmatrix} dx^2,$$

we are able to introduce the so-called moving trihedral frame $\{\mathbf{e}_i\}$ in $\mathbf{R}^3$,[10] which satisfies the orthonormal conditions

$$\mathbf{e}_i\cdot\mathbf{e}_j=\delta_{ij}, \quad \mathbf{e}_i\wedge\mathbf{e}_j=\varepsilon_{ijk}\mathbf{e}_k, \tag{7}$$

and changes accordingly to

$$\partial_\mu\mathbf{e}_i=(J_\mu)_{ik}^{(\mathrm{ad})}\mathbf{e}_k, \quad \mu=0,1,2, \quad i=1,2,3. \tag{8}$$

Its integrability is assured by the zero-curvature condition, namely by Eq. (2). For instance, assigning to $\mathbf{e}_3$ the special role of unimodular normal vector to a given surface $\mathcal{S}$, whose tangent plane is defined by the vectors $(\mathbf{e}_1,\mathbf{e}_2)$, the equations (8) for $\mu=1,2$ and $i=1,2,3$ can be seen as the Gauss–Weingarten equations of such a surface. Moreover, the mapping $\mathbf{e}_3:\mathcal{S}\to S^2$ is the well-known Gauss map. Furthermore, the corresponding integrability equations, rewritten as

$$\partial_1 J_2^{(\mathrm{ad})}-\partial_2 J_1^{(\mathrm{ad})}+[J_1^{(\mathrm{ad})},J_2^{(\mathrm{ad})}]=0,$$

are the Gauss–Codazzi–Mainardi equations for a surface S immersed in $\mathbf{R}^3$. They are the real form of Eqs. (5) and (6). The U(1) invariance of such equations is readily interpreted as the invariance under local rotations of the tangent plane at the surface $\mathcal{S}$. This identification is one of the motivations of the present article and it will be fully developed from the geometrical point of view in the next sections. Here we would like to show how to use effectively the remaining equations in (8) for $\mu=0$ and $i=1,2,3$ and the corresponding integrability conditions. In particular, we ask if structures related to the integrable systems can be detected in the above general picture. Then, since we show that it is the case, we are allowed to introduce a completely integrable dynamics for the trihedral frame and, by consequence, we can infer an integrable dynamics for the corresponding surfaces.

First, we can rewrite Eqs. (5) and (6) by introducing the quantities

$$V=\begin{pmatrix} v^* & \\ & v \end{pmatrix},\quad \Psi_\pm=\begin{pmatrix} & \psi_\pm \\ -\psi_\pm^* & \end{pmatrix},\quad B=\frac{i}{2}\sigma_3(\Psi_- -\Psi_+).$$

Indeed, the torsionless condition (5) and its complex conjugate can be written as

$$\begin{pmatrix} \partial_z & \\ & \partial_{\bar z} \end{pmatrix} B+\frac{i}{2}(\partial_{\bar z}-\partial_z)\Psi_- +V\Psi_- -\Psi_+ V=0,$$

while combining the GCS law (6) and its complex conjugate yields

$$\mathrm{Tr}\left\{\sigma_3\left[\begin{pmatrix} \partial_z & \\ & \partial_{\bar z} \end{pmatrix} V+B\Psi_- -\Psi_+ B\right]\right\}=0.$$

These equations involve independent components in the basis of the complex 2×2 matrices, and we have no information about the identity component σ_0. So the last two equations provide

$$L_+\left[\frac{i}{2}(\partial_{\bar z}-\partial_z)+V+B\right]-\left[\frac{i}{2}(\partial_{\bar z}-\partial_z)+V+B\right]L_-=f\sigma_0, \tag{9}$$

$$L_\pm=\begin{pmatrix} \partial_z & \\ & \partial_{\bar z} \end{pmatrix}-\Psi_\pm, \tag{10}$$

where f is an arbitrary function. Equation (10) has the form of the two-dimensional principal Zakharov–Shabat spectral operator[16] of elliptic type. Moreover, putting $f\equiv 0$ in Eq. (9), we obtain the so-called space part of the Bäcklund transformations associated with $L_\pm$, defining the first-order Bäcklund-gauge operator

$$\hat B=\frac{i}{2}(\partial_{\bar z}-\partial_z)+V+B.$$

This means that $\hat B$ maps solutions between the two linear problems

$$L_-\phi_-=0\Rightarrow L_+B\phi_-=L_+\phi_+=0. \tag{11}$$

The previous considerations tell us that in the above formalism the Gauss–Codazzi–Mainardi equations are expressed in terms of products of first-order differential operators, which have a precise meaning in the theory of the completely integrable systems. Of course, in this context an essential role is played by the second (evolution) linear operator of the Lax pair, in order to introduce a compatible time evolution. The latter, generally speaking, is nonlinear, while the corresponding equations from the CS theory still contains the arbitrary functions interpreted as Lagrangian multipliers in the action (4). Indeed, the corresponding equations read

$$D_0\psi_+ = \bar{D}q_0, \quad D_0\psi_- = Dq_0, \tag{12}$$

$$\partial_0 v - \partial_z v_0 = i(q_0\psi_+^* - q_0^*\psi_-), \tag{13}$$

and their complex conjugated. However, we can exploit the freedom in the choice of q_0 and v_0 in order to fix the evolution of $\psi_\pm$ and v in the x^0 variable. In fact, let us take

$$q_0 = 2i\left[\left(\bar{D} - \frac{i}{2}(\partial_{\bar{z}}\omega - i\partial_{\bar{z}}\chi)\right)\psi_+ + \left(D - \frac{i}{2}(\partial_z\omega + i\partial_z\chi)\right)\psi_-\right], \tag{14}$$

where we require that the real functions χ and ω satisfy the supplementary conditions

$$\partial_z\partial_{\bar{z}}\chi = -4(|\psi_+|^2 - |\psi_-|^2), \quad \partial_z\partial_{\bar{z}}\omega = 0. \tag{15}$$

Furthermore, by introducing an irrotational field $\mathbf{A} = (\partial_z\Lambda, \partial_{\bar{z}}\Lambda, \partial_0\Lambda)$ (Λ is an arbitrary real function) in such a way that

$$v = \frac{1}{4}\partial_z\Lambda - \frac{i}{8}\partial_z\chi, \quad v_0 = \frac{1}{4}(\partial_0\Lambda + u_0), \quad \psi_\pm = \Psi_\pm \exp\left(\frac{i}{2}\Lambda\right),$$

the ''time evolutions'' (12) become

$$i\partial_0\Psi_\pm + 2(\partial_z^2 + \partial_{\bar{z}}^2)\Psi_\pm + \tfrac{1}{2}u_0^\pm\Psi_\pm - i(\partial_{\bar{z}}\omega\partial_{\bar{z}} + \partial_z\omega\partial_z)\Psi_\pm = 0, \tag{16}$$

where we have suitably defined in terms of u_0, χ, and ω the scalar fields $u_0^\pm$, which obey the consistency conditions arising from (13),

$$\partial_z\partial_{\bar{z}}u_0^\pm = 8(\partial_z^2 + \partial_{\bar{z}}^2)|\Psi_\pm|^2. \tag{17}$$

Thus, to summarize, the gauge fixing conditions (14) and (15) destroy the arbitraryness contained in the equations (12) in favor of a formally decoupled pair of Davey–Stewartson equations (16) and (17). Actually, between the two pairs of fields $(\Psi_\pm, u_0^\pm)$ there still exists the coupling provided by the torsionless condition (5), which in the new variables takes the form

$$(\partial_{\bar{z}} + \tfrac{1}{4}\partial_{\bar{z}}\chi)\Psi_- = (\partial_z + \tfrac{1}{4}\partial_z\chi)\Psi_+. \tag{18}$$

As we discussed above, Eq. (18) is in essence the space part of the Bäcklund transformations. Starting from a known solution, say (Ψ_-, u_0^-), and fixing ω, one can reconstruct the function χ, and solving (18) for Ψ_+, finally we find u_0^+ from (17). Furthermore, we observe that the gauge choice (14)–(15) is equivalent to fix the second operator of the Lax pair, denoted here by $M_\pm = \partial_{x^0} + \Sigma_{k=0}^2 M_\pm^{(k)}[i/2(\partial_{\bar{z}} - \partial_z)]^{2-k}$, where $M_\pm^{(k)}$ are specific matrices. $M_\pm$ provide the system (16)–(17) and (18) by the compatibility relations

$$[L_\pm, M_\pm] = 0, \quad M_+\hat{B} - \hat{B}M_- = 0.$$

Moreover, by using a suitable particular eigenfunction ϕ_-^0 of Eq. (11), it is well-known (see Refs. 17, 18) that one can construct a new spectral problem of the form

$$L_-^I=(\phi_-^0)^{-1}L_-\phi_-^0=\partial_{x^1}+iS\partial_{x^2},\quad M_-^I=(\phi_-^0)^{-1}M_-\phi_-^0,$$

where

$$S=i(\phi_-^0)^{-1}\sigma_3\phi_-^0$$

is an element of SU(2)/U(1) coset space and the corresponding eigenfunction is $\phi_-^I=(\phi_-^0)^{-1}\phi_-$. The resulting integrable system is known as Ishimori model and it describes the evolution of a classical spin in a background generated by the density of the topological charge. Since this equation will be discussed in the next sections, we do not give other details about it. But here we want to stress that such a system is an alternative integrable restriction of the possible configurations of the CS field, exactly as the Davey–Stewartson equation does. Furthermore, one can purpose the question does the spin field S have something to do with the trihedral frame introduced above. The consequences arising from the identification of S with one of the unimodular vector fields $\mathbf{e}_i$ is the main subject of the next sections.

III. SURFACES IN R^3

To introduce our terminology and notations and to make the exposition self-contained, we recall some basic facts from the theory of two-dimensional surfaces. So, we consider a smooth surface in a three-dimensional Euclidean space $\mathbf{R}^3$. Let x,y be the local coordinates on the surface. At the same time, the surface can be described by the position vector $(x_1,x_2,x_3)=\mathbf{r}(x,y)$, where the x_i are coordinates of $\mathbf{R}^3$. The surface is uniquely defined within rigid motions by the two fundamental forms

$$I=E\,dx^2+2F\,dx\,dy+G\,dy^2 \tag{19}$$

and

$$II=L\,dx^2+2M\,dx\,dy+N\,dy^2, \tag{20}$$

where E,F,G,L,M,N can be defined by

$$E=\mathbf{r}_x\cdot\mathbf{r}_x=g_{11},\quad F=\mathbf{r}_x\cdot\mathbf{r}_y=g_{12}=g_{21},\quad G=\mathbf{r}_y\cdot\mathbf{r}_y=g_{22}, \tag{21}$$

$$L=\mathbf{n}\cdot\mathbf{r}_{xx}=b_{11},\quad M=\mathbf{n}\cdot\mathbf{r}_{xy}=b_{12}=b_{21},\quad N=\mathbf{n}\cdot\mathbf{r}_{yy}=b_{22}. \tag{22}$$

In Eqs. (21) and (22),

$$\mathbf{n}(x,y)=\frac{\mathbf{r}_x\wedge\mathbf{r}_y}{|\mathbf{r}_x\wedge\mathbf{r}_y|}=\frac{\mathbf{r}_x\wedge\mathbf{r}_y}{\sqrt{g}} \tag{23}$$

is introduced, where $g=\det(g_{ij})=EG-F^2=|\mathbf{r}_x\wedge\mathbf{r}_y|^2$, is the normal vector field at each point of the surface. Then the triple $(\mathbf{r}_x,\mathbf{r}_y,\mathbf{n})$ represents a local frame of $\mathbf{R}^3$, the changes of which are characterized by the GW equations

$$\mathbf{r}_{xx}=\Gamma_{11}^1\mathbf{r}_x+\Gamma_{11}^2\mathbf{r}_y+L\mathbf{n}, \tag{24}$$

$$\mathbf{r}_{xy}=\Gamma_{12}^1\mathbf{r}_x+\Gamma_{12}^2\mathbf{r}_y+M\mathbf{n}, \tag{25}$$

$$\mathbf{r}_{yy}=\Gamma_{22}^1\mathbf{r}_x+\Gamma_{22}^2\mathbf{r}_y+N\mathbf{n}, \tag{26}$$

$$\mathbf{n}_x=p_{11}\mathbf{r}_x+p_{12}\mathbf{r}_y, \tag{27}$$

$$\mathbf{n}_y=p_{21}\mathbf{r}_x+p_{22}\mathbf{r}_y, \tag{28}$$

where the Christoffel symbols of the second kind are defined by g_{ij} ($g^{ij}=(g_{ij})^{-1}$) as

$$\Gamma^i_{jk}=\frac{1}{2}g^{il}\left(\frac{\partial g_{lk}}{\partial x^j}+\frac{\partial g_{jl}}{\partial x^k}-\frac{\partial g_{jk}}{\partial x^l}\right), \tag{29}$$

with $i,j,k=1,2$ and

$$p_{ij}=-b_{ik}g^{kj}. \tag{30}$$

The principal curvatures k_1,k_2 are the eigenvalues of the Weingarten operator

$$\Lambda=\begin{pmatrix}E & F\\ F & G\end{pmatrix}^{-1}\begin{pmatrix}L & M\\ M & N\end{pmatrix}, \tag{31}$$

which for the mean and the Guassian curvature implies

$$H=\frac{k_1+k_2}{2}=\mathrm{Tr}(\Lambda)=\frac{EN+LG-2MF}{2(EG-F^2)}, \tag{32}$$

$$K=k_1k_2=\det(\Lambda)=\frac{LN-M^2}{EG-F^2}. \tag{33}$$

One of the global characteristics of surfaces is the integral curvature

$$\chi=\frac{1}{2\pi}\int K\sqrt{g}\,dx\,dy, \tag{34}$$

which for compact oriented surfaces is the integer

$$\chi=2(1-\Delta), \tag{35}$$

where Δ is the genus of the surface. The compatibility conditions of the GW Eqs. (24)–(28) furnish the GMC equations, which in two dimensions read

$$R_{1,2,1,2}=K,\quad \frac{\partial b^{ij}}{\partial x^k}-\frac{\partial b_{ik}}{\partial x^j}=\Gamma^s_{ik}b_{js}-\Gamma^s_{ij}b_{ks}, \tag{36}$$

where $i,j=1,2$, $b^j_i=g^{jl}b_{il}$, and the curvature tensor, defined in the standard way,

$$R^l_{ijk}=\frac{\partial\Gamma^l_{ij}}{\partial x^k}-\frac{\partial\Gamma^l_{ik}}{\partial x^j}+\Gamma^s_{ij}\Gamma^l_{ks}-\Gamma^s_{ik}\Gamma^l_{js}, \tag{37}$$

has only one (i.e., $R^1_{2,1,2}$) independent component. For our purposes it is convenient to employ the triad of orthonormal vectors,

$$\mathbf{e}_1=\frac{\mathbf{r}_x}{\sqrt{E}},\quad \mathbf{e}_2=\mathbf{n},\quad \mathbf{e}_3=\mathbf{e}_1\wedge\mathbf{e}_2. \tag{38}$$

In terms of these vectors the GW Eqs. (24)–(28) take the form

$$\mathbf{e}_{jx}=\mathbf{X}\wedge\mathbf{e}_j,\quad \mathbf{e}_{jy}=\mathbf{Y}\wedge\mathbf{e}_j, \tag{39}$$

where

$$\mathbf{X}=\tau\mathbf{e}_1+\sigma\mathbf{e}_2+k\mathbf{e}_3,\quad \mathbf{Y}=m_1\mathbf{e}_1+m_2\mathbf{e}_2+m_3\mathbf{e}_3, \tag{40}$$

and

$$k=\frac{L}{\sqrt{E}},\quad \sigma=\frac{2EF_x-EE_y-FE_x}{2E\sqrt{g}},\quad \tau=\frac{ME-LF}{\sqrt{gE}}, \tag{41}$$

$$m_1=\frac{NE-MF}{\sqrt{gE}},\quad m_2=\frac{FE_y-EG_x}{2E\sqrt{g}},\quad m_3=\frac{M}{\sqrt{E}}. \tag{42}$$

Similarly, we can rewrite the GMC Eqs. (36) in the following form:

$$A_y-B_x+[A,B]=0, \tag{43}$$

with

$$A=\begin{pmatrix} 0 & k & -\sigma \\ -k & 0 & \tau \\ \sigma & -\tau & 0 \end{pmatrix},\quad B=\begin{pmatrix} 0 & m_3 & -m_2 \\ -m_3 & 0 & m_1 \\ m_2 & -m_1 & 0 \end{pmatrix}. \tag{44}$$

Then, the GMC equation turns out to be equivalent to the set of equations for the coefficients of the first and second fundamental forms. This system, which is in general nonintegrable, reduces to integrable partial differential equations for certain particular surfaces.[10]

IV. DEFORMATIONS OF SURFACES IN (2+1)-DIMENSIONS: THE GENERAL FORMULATION

It is well-known that in some cases deformations of surfaces can be associated with integrable equations.[1–3] Here we are interested in the deformation of the two-dimensional surfaces discussed in Sec. III. In other words, we have to deal with the motion of such surfaces. To this aim, let us introduce the vector field

$$\mathbf{r}_t=a_1\mathbf{r}_x+a_2\mathbf{r}_y+a_3\mathbf{n}, \tag{45}$$

where the a_i are some real functions. It is easy to show that the evolution of the local trihedral frame is given by

$$\mathbf{e}_{jt}=\mathbf{T}\wedge\mathbf{e}_j, \tag{46}$$

$$\mathbf{T}=\omega_1\mathbf{e}_1+\omega_2\mathbf{e}_2+\omega_3\mathbf{e}_3, \tag{47}$$

ω_j being real functions. Summarizing, the changes of the local frame are provided by

$$\mathbf{e}_{jx}=\mathbf{X}\wedge\mathbf{e}_j,\quad \mathbf{e}_{jy}=\mathbf{Y}\wedge\mathbf{e}_j,\quad \mathbf{e}_{jt}=\mathbf{T}\wedge\mathbf{e}_j, \tag{48}$$

where the vectors **X** and **Y** are defined by (40). This system is analogous to the system (8) in Sec. II.

The system (48) represents the simplest form of the (2+1)-dimensional GW equations.

By introducing the matrix

$$C=\begin{pmatrix} 0 & \omega_3 & -\omega_2 \\ -\omega_3 & 0 & \omega_1 \\ \omega_2 & -\omega_1 & 0 \end{pmatrix}, \tag{49}$$

and using the matrices A and B [see (44)], the compatibility conditions of Eqs. (48) entail

$$A_y - B_x + [A,B] = 0, \tag{50}$$

$$A_t - C_x + [A,C] = 0, \tag{51}$$

$$B_t - C_y + [B,C] = 0. \tag{52}$$

Of the nine funcions $k, \sigma, \tau, m_i, \omega_i$ involved in A, B, and C, only three are independent. In fact, we can express the functions m_i, ω_i in terms of k, σ, τ, and their derivatives. This point will be discussed later.

A. Some geometrical invariants and integrals of motion as a consequence of the geometrical formalism

The formalism developed above yields some important invariants having a pure geometrical nature. Indeed, in terms of the triad vectors these geometrical invariants take the form

$$K_1^{(t)} = \int \mathbf{e}_1 \cdot (\mathbf{e}_{1x} \wedge \mathbf{e}_{1y}) dx\, dy, \quad K_2^{(t)} = \int \mathbf{e}_2 \cdot (\mathbf{e}_{2x} \wedge \mathbf{e}_{2y}) dx\, dy,$$

$$K_3^{(t)} = \int \mathbf{e}_3 \cdot (\mathbf{e}_{3x} \wedge \mathbf{e}_{3y}) dx\, dy. \tag{53}$$

In a similar way we can write down the other two classes of invariants with respect to x and y directions, respectively. These geometrical invariants can be interpreted as ''topological charges.'' However, three of them, namely $K_i^{(t)}$ $(i = 1,2,3)$ behave as integrals of motion of the $(2+1)$-dimensional geometrical models under consideration. This will be elucidated in the next sections. These invariants can be related to the topological Chern index of a curvature two-form on a two-dimensional space.[19]

V. INTEGRABLE SPIN MODELS IN (2+1)-DIMENSIONS

Now let us dwell upon the problem of finding or building up integrable deformations of $(2+1)$-dimensional surfaces. Among several possibilities, within the geometrical formalism previously presented, we shall consider multidimensional integrable spin (field) systems (MISS) to recognize integrable deformations of surfaces.

A. The spin model

A few words on MISS. At present there exist many integrable spin systems in $(2+1)$-dimensions (see, for example, Refs. 20–25). A well-known prototype of these systems is the Ishimori model (IM).[20] A more general $(2+1)$-dimensional integrable spin model is described by the pair of equations

$$\mathbf{S}_t + \mathbf{S} \wedge \{(b+1)\mathbf{S}_{\xi\xi} - b\mathbf{S}_{\eta\eta}\} + b u_\eta \mathbf{S}_\eta + (b+1) u_\xi \mathbf{S}_\xi = 0, \tag{54}$$

$$u_{\xi\eta} = \mathbf{S} \cdot (\mathbf{S}_\xi \wedge \mathbf{S}_\eta), \tag{55}$$

where ξ, η are real or complex variables, b is a real constant, $\mathbf{S} = (S_1, S_2, S_3)$ is the spin (field) vector, $\mathbf{S}^2 = 1$, and u is a scalar function. These equations, which are called M-XX equations (about our conditional notations, see e.g., Refs. 21–25), are one of the $(2+1)$-dimensional integrable generalizations of the isotropic Landau–Lifshitz (LL) equation

$$\mathbf{S}_t = \mathbf{S} \wedge \mathbf{S}_{xx}. \tag{56}$$

In $(1+1)$-dimensions, Eqs. (54) and (55) reduce to the LL equation. In fact, assuming that the variables $\mathbf{S}, u$ are, for example, independent of η, then Eqs. (54) and (55) reproduce Eq. (56) within a simple scale transformation.

We notice that Eqs. (54) and (55) are not the only integrable generalization of the LL equation in $(2+1)$-dimensions. Actually, other integrable generalizations exist, such as the IM or the model defined by

$$\mathbf{S}_t=(\mathbf{S}\wedge\mathbf{S}_y+u\mathbf{S})_x, \tag{57}$$

$$u_x=-\mathbf{S}\cdot(\mathbf{S}_x\wedge\mathbf{S}_y). \tag{58}$$

These equations, which are called M-I equations (see Ref. 21) are again completely integrable. Some properties of these equations are studied in Refs. 21–23.

1. The Lax representation

Equations (54) and (55) can be solved by the inverse spectral transform (IST) method. The applicability of the IST method to Eqs. (54) and (55) is based on the equivalence of these equations to the compatibility condition of the following linear equations [the Lax representation (LR)]

$$\Phi_{Z^+}=S\Phi_{Z^-}, \tag{59}$$

$$\Phi_t=2i[S+(2b+1)I]\Phi_{Z^-Z^-}+W\Phi_{Z^-}, \tag{60}$$

where $Z^{\pm}=\xi\pm\eta$ and

$$W=2i\left\{(2b+1)(F^++F^-S)+(F^+S+F^-)+(2b+1)SS_{Z^-}+\frac{1}{2}S_{Z^-}+\frac{1}{2}SS_{Z^+}\right\},$$

$$S=\begin{pmatrix} S_3 & rS^- \\ rS^+ & -S_3 \end{pmatrix}, \quad S^{\pm}=S_1\pm iS_2, \quad S^2=EI, \quad E=\pm 1, \quad r^2=\pm 1,$$

$$F^+=2iu_{Z^-}, \quad F^-=2iu_{Z^+}.$$

In fact, from the condition $\Phi_{Z^+t}=\Phi_{tZ^+}$ we deduce

$$iS_t+\tfrac{1}{2}[S,(b+1)S_{\xi\xi}-bS_{\eta\eta}]+ibu_{\eta}S_{\eta}+i(b+1)u_{\xi}S_{\xi}=0, \tag{61}$$

$$u_{\xi\eta}=\frac{1}{4i}\,\mathrm{Tr}(S[S_{\xi},S_{\eta}]), \tag{62}$$

which is the matrix form of Eqs. (54) and (55).

2. Special cases

Equations (54) and (55) contain both well-known and less-known integrable cases in $(2+1)$- and $(1+1)$-dimensions. Below we shall report some of them.

(i) If $b=0$, Eqs. (54) and (55) yield

$$\mathbf{S}_t+\mathbf{S}\wedge\mathbf{S}_{\xi\xi}+w\mathbf{S}_{\xi}=0, \tag{63}$$

$$w_{\eta}-\mathbf{S}\cdot(\mathbf{S}_{\xi}\wedge\mathbf{S}_{\eta})=0, \tag{64}$$

where $w=u_{\xi}$. This system, which is known as the M-VIII model,[24] is one of the simplest spin systems in $(2+1)$-dimensions integrable by IST. It affords a different type of solutions (solitons, vortices, etc.). In particular, vortex solutions of Eqs. (63)–(64) can be derived from vortex solutions of the spin system (54)–(55) discussed in Sec. IX (for $b=0$).

(ii) Let us introduce the coordinates $x=\xi-\eta$, $y=\alpha(\xi+\eta)$, and put $b=-\frac{1}{2}$. Then, the spin system (54)–(55) reduces to the IM

$$\mathbf{S}_t+\mathbf{S}\wedge(\mathbf{S}_{xx}+\alpha^2\mathbf{S}_{yy})+u_x\mathbf{S}_y+u_y\mathbf{S}_x=0, \tag{65}$$

$$u_{xx}-\alpha^2u_{yy}=-2\alpha^2\mathbf{S}\cdot(\mathbf{S}_x\wedge\mathbf{S}_y). \tag{66}$$

The IM is the first integrable spin (field) system in the plane which can be solved by the IST method. The IM was studied by many authors from different points of view (e.g., Refs. 16, 17, 20, 23, 26).

(iii) By setting $b=0$, $\eta=t$, Eqs. (54) and (55) reduce to the following $(1+1)$-dimensional spin system:

$$\mathbf{S}_t+\mathbf{S}\wedge\mathbf{S}_{\xi\xi}+w\mathbf{S}_\xi=0, \tag{67}$$

$$w_t+\tfrac{1}{2}(\mathbf{S}_\xi^2)_\xi=0. \tag{68}$$

This integrable model describes the nonlinear dynamics of compressible magnets.[27] It is the first (and, to the best of our knowledge, at present the unique) example of an integrable spin system governing the nonlinear interactions of spin $(\mathbf{S})$ and lattice (u) subsystems in $(1+1)$-dimensions.

VI. BILINEAR REPRESENTATIONS

One of the powerful tools in the soliton theory is the Hirota method. Now we show how to construct the bilinear representations of the fields of the spin system by using geometry. First, let e_{ji} be the components of the unit vector $\mathbf{e}_j$, i.e., $\mathbf{e}_j=(e_{j1},e_{j2},e_{j3})$. We can take the following representation for the components of the vector $\mathbf{e}_1$:

$$e_1^+=e_{11}+ie_{12}=\frac{2\bar{f}g}{\bar{f}f+\bar{g}g},\quad e_{13}=\frac{\bar{f}f-\bar{g}g}{\bar{f}f+\bar{g}g}, \tag{69}$$

where f and g are complex functions of (x,y,t). Then, the consistency of the system (48) implies

$$e_2^+=e_{21}+ie_{22}=\frac{\bar{f}^2+g^2}{\bar{f}f+\bar{g}g},\quad e_{23}=i\frac{fg-\bar{f}\bar{g}}{\bar{f}f+\bar{g}g}, \tag{70}$$

$$e_3^+=e_{31}+ie_{32}=\frac{\bar{f}^2-g^2}{\bar{f}f+\bar{g}g},\quad e_{33}=-\frac{fg+\bar{f}\bar{g}}{\bar{f}f+\bar{g}g}, \tag{71}$$

with

$$k=-i\frac{D_x(g\circ f-\bar{g}\circ\bar{f})}{\bar{f}f+\bar{g}g},\quad m_3=-i\frac{D_y(g\circ f-\bar{g}\circ\bar{f})}{\bar{f}f+\bar{g}g}, \tag{72}$$

$$\sigma=-\frac{D_x(g\circ f+\bar{g}\circ\bar{f})}{\bar{f}f+\bar{g}g},\quad m_2=-\frac{D_y(g\circ f+\bar{g}\circ\bar{f})}{\bar{f}f+\bar{g}g}, \tag{73}$$

$$\tau=i\frac{D_x(\bar{f}\circ f+\bar{g}\circ g)}{\bar{f}f+\bar{g}g},\quad m_1=i\frac{D_y(\bar{f}\circ f+\bar{g}\circ g)}{\bar{f}f+\bar{g}g}, \tag{74}$$

$$\omega_3=-i\frac{D_t(g\circ f-\bar{g}\circ\bar{f})}{\bar{f}f+\bar{g}g},\quad \omega_2=-\frac{D_t(g\circ f+\bar{g}\circ\bar{f})}{\bar{f}f+\bar{g}g}, \tag{75}$$

$$\omega_1 = i\frac{D_t(\overline{f}\circ f + \overline{g}\circ g)}{\overline{f}f + \overline{g}g}. \tag{76}$$

The Hirota operators D_x, D_y, and D_t are defined by

$$D_x^l D_y^m D_t^n f(x,y,t)\circ g(x,y,t) = (\partial_x - \partial_{x'})^l (\partial_y - \partial_{y'})^m (\partial_t - \partial_{t'})^n f(x,y,t)\circ g(x',y',t')\big|_{x=x',y=y',t=t'}.$$

Now we write the bilinear representation for the spin vector and for the derivatives of the potential u, identifying $\mathbf{S}$ and $\mathbf{e_1}$. Taking into account (69), we find

$$S^+ = S_1 + iS_2 = \frac{2\overline{f}g}{\overline{f}f + \overline{g}g}, \quad S_3 = \frac{\overline{f}f - \overline{g}g}{\overline{f}f + \overline{g}g}. \tag{77}$$

This is the general representation for the components of the spin vector for all the spin systems. However, for the potential, the bilinear forms for every spin system should be different. In the following we shall consider some examples.

A. The Ishimori model

In this case we have

$$\tau = \frac{1}{2}u_y, \quad m_1 = \frac{1}{2\alpha^2}u_x. \tag{78}$$

Hence, from (74) we get

$$u_y = -2i\frac{D_x(\overline{f}\circ f + \overline{g}\circ g)}{\overline{f}f + \overline{g}g}, \quad u_x = -2i\alpha^2\frac{D_y(\overline{f}\circ f + \overline{g}\circ g)}{\overline{f}f + \overline{g}g}. \tag{79}$$

On the other hand, from (74) it also follows that

$$\tau_x = \alpha^2 m_{1y}, \tag{80}$$

so that

$$m_1 = \alpha^{-2}\partial_y^{-1}\tau_x. \tag{81}$$

B. The isotropic M-I equation

Let us take

$$\tau = 0, \quad m_1 = u. \tag{82}$$

Then, from (74) and (82) we obtain

$$D_x(\overline{f}\circ f + \overline{g}\circ g) = 0, \quad u = -i\frac{D_y(\overline{f}\circ f + \overline{g}\circ g)}{\overline{f}f + \overline{g}g}. \tag{83}$$

C. The spin system (54)–(55)

Let us start from

$$\tau=\frac{1}{2}u_{\xi},\quad m_1=-\frac{1}{2}u_{\eta}. \tag{84}$$

Then we have

$$u_{\xi}=-2i\frac{D_{\xi}(\bar{f}\circ f+\bar{g}\circ g)}{\bar{f}f+\bar{g}g},\quad u_{\eta}=2i\frac{D_{\eta}(\bar{f}\circ f+\bar{g}\circ g)}{\bar{f}f+\bar{g}g},$$

and

$$\tau_{\eta}=-m_{1\xi}, \tag{85}$$

$$m_1=-\partial_{\xi}^{-1}\tau_{\eta}. \tag{86}$$

An important consequence of these results is the possibility to determine the time evolution of the potential (and/or its derivatives). For instance, for the IM the time evolution of the derivatives of the potential are given by

$$\frac{1}{2}(u_y)_t-\omega_{3x}+\sigma\omega_1-\tau\omega_2=0, \tag{87}$$

$$\frac{1}{2\alpha^2}(u_x)_t-\omega_{1y}+m_3\omega_3-m_2\omega_3=0. \tag{88}$$

VII. DEFORMATIONS OF SURFACES BY INTEGRABLE SPIN SYSTEMS IN (2+1) DIMENSIONS

As we said above, examples of surface integrable deformations can be found out by identifying the tangent unit vector $\mathbf{e}_1$ with the spin vector, i.e.,

$$\mathbf{e}_1\equiv\mathbf{S}. \tag{89}$$

In such a way, the spin model (54)–(55) takes the form

$$\mathbf{e}_{1t}+\mathbf{e}_1\wedge\{(b+1)\mathbf{e}_{1\xi\xi}-b\mathbf{e}_{1\eta\eta}\}+bu_{\eta}\mathbf{e}_{1\eta}+(b+1)u_{\xi}\mathbf{e}_{1\xi}=0, \tag{90}$$

$$u_{\xi\eta}=\mathbf{e}_1\cdot(\mathbf{e}_{1\xi}\wedge\mathbf{e}_{1\eta}). \tag{91}$$

The functions m_i,ω_i can be expressed in terms of the three independent functions k,τ,σ. Using the GW Eq. (48), Eqs. (90)–(91) can be written as

$$\mathbf{e}_{1t}=\omega_3\mathbf{e}_2-\omega_2\mathbf{e}_3, \tag{92}$$

$$u_{\xi\eta}=\sigma m_3-km_2, \tag{93}$$

where

$$\omega_2=b[m_{3\eta}-m_2^2-u_{\eta}m_2]-(b+1)[k_{\xi}+\sigma\tau+u_{\xi}\sigma], \tag{94}$$

$$\omega_3=(b+1)[\sigma_{\xi}-k\tau-ku_{\xi}]-b[m_{2\eta}-m_1m_3+u_{\eta}m_3]. \tag{95}$$

Now by choosing m_1 according to the special reduction (84), the remaining functions m_2 and m_3 are given by

$$m_2=\frac{\sigma m_3-u_{\xi\eta}}{k}, \quad m_3=\frac{\sigma\tau u_{\xi\eta}+(a_2/2)u_\xi-a_3}{a_1+\sigma^2\tau}, \tag{96}$$

where

$$a_1=k^2\tau-k\sigma_\xi+\sigma k_\xi, \quad a_2=-k^3-\sigma^2 k,$$
$$a_3=k^2\sigma_\eta-\sigma k k_\eta+k u_{\xi\xi\eta}-k_\xi u_{\xi\eta}. \tag{97}$$

By virtue of these formulas we derive the function ω_1 from (50)–(52).

Thus, all the unknown functions m_i,ω_i are defined via the three functions k,τ,σ only and their derivatives. This is the consequence of the identification of the motion of surface with the spin system (90)–(91). This means that the motion of surface is fully determined by these three functions. Since the spin model (90)–(91) is integrable, we can conclude that the deformation of the surface characterized by Eqs. (50)–(52) is integrable.

VIII. DEFORMATIONS OF SURFACES RELATED TO THE (2+1)-DIMENSIONAL NLS-TYPE EQUATION

One of the most remarkable consequences of the geometrical formalism previously outlined is that it allows to find the equivalent counterpart of the spin system (54)–(55). To show this property, let us introduce two complex functions q,p according to the following expressions:

$$q=a_1e^{ib_1}, \quad p=a_2e^{ib_2}, \tag{98}$$

where a_j,b_j are real functions. Now let us choose the functions a_j,b_j in such a way that

$$a_1^2=\frac{1}{4}k^2+\frac{|\alpha|^2}{4}(m_3^2+m_2^2)-\frac{1}{2}\alpha_R k m_3-\frac{1}{2}\alpha_I k m_2, \tag{99}$$

$$b_1=\partial_x^{-1}\left\{-\frac{\gamma_1}{2ia_1'^2}-(\bar{A}-A+D-\bar{D})\right\}, \tag{100}$$

$$a_2^2=\frac{1}{4}k^2+\frac{|\alpha|^2}{4}(m_3^2+m_2^2)+\frac{1}{2}\alpha_R k m_3-\frac{1}{2}\alpha_I k m_2, \tag{101}$$

$$b_2=\partial_x^{-1}\left\{-\frac{\gamma_2}{2ia_2'^2}-(A-\bar{A}+\bar{D}-D)\right\}, \tag{102}$$

where

$$\gamma_1=i\left\{\frac{1}{2}k^2\tau+\frac{|\alpha|^2}{2}(m_3 k m_1+m_2k_y)-\frac{1}{2}\alpha_R(k^2m_1+m_3k\tau+m_2k_x)\right.$$
$$\left.+\frac{1}{2}\alpha_I[k(2k_y-m_{3x})-k_x m_3]\right\}, \tag{103}$$

$$\gamma_2=-i\left\{\frac{1}{2}k^2\tau+\frac{|\alpha|^2}{2}(m_3 k m_1+m_2k_y)+\frac{1}{2}\alpha_R(k^2m_1+m_3k\tau+m_2k_x)\right.$$
$$\left.+\frac{1}{2}\alpha_I[k(2k_y-m_{3x})-k_x m_3]\right\}. \tag{104}$$

In this case, q,p satisfy the $(2+1)$-dimensional equations of the nonlinear Schrödinger (NLS) type[27]

$$iq_t+(1+b)q_{\xi\xi}-bq_{\eta\eta}+vq=0, \tag{105}$$

$$ip_t-(1+b)p_{\xi\xi}+bp_{\eta\eta}-vp=0, \tag{106}$$

$$v_{\xi\eta}=-2\{(1+b)(pq)_{\xi\xi}-b(pq)_{\eta\eta}\}. \tag{107}$$

These equations are the geometrical equivalent counterpart of the spin system (54)–(55). Therefore, the spin system and the $(2+1)$-dimensional NLS equations (105)–(107) turn out to be mutually geometrical equivalent.

A. Gauge equivalence

Now we prove that the spin system (54)–(55) and Eqs. (105)–(107) are not only equivalent in the geometrical sense, but are also gauge equivalent. To this purpose, let us perform the gauge transformation $\Psi=g\Phi$, where the function Φ is the solution of Eqs. (59)–(60) and g is a 2×2 matrix such that

$$S=g^{-1}\sigma_3 g, \tag{108}$$

and

$$g_{Z^+}g^{-1}-\sigma_3 g_{Z^-}g^{-1}=\begin{pmatrix}0 & q\\ p & 0\end{pmatrix}. \tag{109}$$

Under this transformation the function Ψ obeys the following set of linear equations

$$\Psi_{Z^+}=\sigma_3\Psi_{Z^-}+B_0\Psi, \tag{110}$$

$$\Psi_t=4iC_2\Psi_{Z^-Z^-}+2C_1\Psi_{Z^-}+C_0\Psi, \tag{111}$$

where B_0,C_j are given by

$$B_0=\begin{pmatrix}0 & q\\ p & 0\end{pmatrix},\quad C_2=\begin{pmatrix}b+1 & 0\\ 0 & b\end{pmatrix},$$

$$C_1=\begin{pmatrix}0 & iq\\ ip & 0\end{pmatrix},\quad C_0=\begin{pmatrix}c_{11} & c_{12}\\ c_{21} & c_{22}\end{pmatrix}, \tag{112}$$

and the functions c_{ij} $(i,j=1,2)$ fulfill the equations

$$c_{12}=i[(4b+3)q_{Z^-}+q_{Z^+}],\quad c_{21}=-i[(4b+1)p_{Z^-}+p_{Z^+}], \tag{113}$$

$$c_{11Z^-}-c_{11Z^+}=i[(4b+3)(pq)_{Z^-}+(pq)_{Z^+}], \tag{114}$$

$$c_{22Z^-}+c_{22Z^+}=i[(4b+1)(pq)_{Z^-}+(pq)_{Z^+}], \tag{115}$$

with $v=i(c_{22}-c_{11})$ [see (105)–(107)].

The compatibility condition of Eqs. (110)–(111) gives the equations (105)–(107). This means that the spin model (54)–(55) and the NLS—type equations (105)–(107) are gauge equivalent. Moreover, it is easy to check that if g satisfies Eq. (109), then S given by (108) satisfies Eqs. (54)–(55) with

$$u=-2\ln\det g. \tag{116}$$

B. Reductions

Equations (105)–(107), as its and equivalent spin system (54)–(55), contain several integrable cases, namely

(i) $b=0$. Equations (105)–(107) yield the equations[27]

$$iq_t+q_{\xi\xi}+vq=0, \tag{117}$$

$$ip_t-p_{\xi\xi}-vp=0, \tag{118}$$

$$v_\eta=-2(pq)_\xi. \tag{119}$$

(ii) $a=b=-\frac{1}{2}$. Then, we give the Davey–Stewartson (DS) equations[27]

$$iq_t+q_{xx}+\alpha^2q_{yy}+vq=0, \tag{120}$$

$$ip_t-p_{xx}-\alpha^2p_{yy}-vq=0, \tag{121}$$

$$v_{xx}-\alpha^2v_{yy}=2\{(pq)_{xx}+\alpha^2(pq)_{yy}\}, \tag{122}$$

where $x=\xi-\eta, y=\alpha(\xi+\eta)$.

(iii) Putting $b=0, \eta=t$, Eqs. (105)–(107) reduce to the $(1+1)$-dimensional Ma[28]–Yajima–Oikawa[29] equations,

$$iq_t+q_{\xi\xi}+vq=0, \tag{123}$$

$$ip_t-p_{\xi\xi}-vp=0, \tag{124}$$

$$v_t+2(pq)_\xi=0, \tag{125}$$

which are known to be integrable.

IX. SOLUTIONS OF THE SPIN SYSTEM

It could be of interest to study Eqs. (54)–(55) by the IST method. However, to look for some special solutions, it is convenient to exploit the Hirota bilinear method. To this aim, let us build up the bilinear form of (54)–(55) for the compact case.

We obtain

$$S^+=S_1+iS_2=\frac{2\overline{f}g}{\overline{f}f+\overline{g}g}, \quad S_3=\frac{\overline{f}f-\overline{g}g}{\overline{f}f+\overline{g}g}, \tag{126}$$

$$u_\xi=-2i\frac{D_\xi(\overline{f}\circ f+\overline{g}\circ g)}{\overline{f}f+\overline{g}g}, \quad u_\eta=2i\frac{D_\eta(\overline{f}\circ f+\overline{g}\circ g)}{\overline{f}f+\overline{g}g}, \tag{127}$$

where S_j $(j=1,2,3)$ are the components of spin vector $\mathbf{S}$, $S^\pm=S_1\pm iS_2$, and u is the scalar potential.

Hence, from (116) we get

$$u(\xi,\eta,t)=-2\ln(|f|^2+|g|^2). \tag{128}$$

Substituting formulas (126) and (127) into the spin system (54)–(55), we obtain the bilinear equations

$$[iD_t-(b+1)D_\xi^2+bD_\eta^2](\overline{f}\circ g)=0, \tag{129}$$

$$[iD_t-(b+1)D_\xi^2+bD_\eta^2](\overline{f}\circ f-\overline{g}\circ g)=0, \tag{130}$$

$$\{D_\xi D_\eta+D_\eta D_\xi\}(\overline{f}f+\overline{g}g)\circ(\overline{f}f+\overline{g}g)=0. \tag{131}$$

Equation (131) coincides with the compatibility condition $u_{\xi\eta}=u_{\eta\xi}$.

Now we can construct some special solutions of Eqs. (54)–(55). In particular, to construct vortex solutions, we start from Eqs. (129)–(130) and assume that

$$f=f(\xi,t), \quad g=g(\xi,t). \tag{132}$$

Then Eq. (131) is satisfied automatically. At the same time, Eqs. (129)–(130) are fulfilled if

$$if_t+(b+1)f_{\xi\xi}=0, \quad ig_t+(b+1)g_{\xi\xi}=0. \tag{133}$$

Consequently, we are led to the following multivortex solutions:

$$g_N=\sum_{j=0}^{N}\sum_{m+2n=j}\frac{a_j}{m!n!}\left(\frac{2}{b+1}\right)^{m/2}\xi^m(2it)^n, \tag{134}$$

$$f_N=\sum_{j=0}^{N-1}\sum_{m+2n=j}\frac{b_j}{m!n!}\left(\frac{2}{b+1}\right)^{m/2}\xi^m(2it)^n, \tag{135}$$

where a_j and b_j are arbitrary complex constants, and m,n are nonnegative integer numbers. In particular, the one-vortex solution can be derived by choosing

$$f=b_0, \quad g=a_1'\xi+a_0, \tag{136}$$

where $a_1'=a_1(2/(b+1))^{1/2}$.

So, the one-vortex solution is static. To find a dynamic solution, we have to consider the N-vortex solution using the forms

$$f(\xi,t)=b_0\prod_{j=1}^{N}[\xi-p_j(t)], \tag{137}$$

$$g(\xi,t)=a_0\prod_{j=1}^{N}[\xi-q_j(t)], \tag{138}$$

where p_j and q_j denote the positions of the zeros of f and g, and a_0,b_0 are constants. The evolution of p_j and q_j is

$$p_{jt}=-i(b+1)\sum_{k[n0]=j}^{N}\frac{1}{p_j-p_k}, \tag{139}$$

$$q_{jt}=-i(b+1)\sum_{k\neq j}^{N}\frac{1}{q_j-q_k}, \tag{140}$$

where $j,k=1,2,\ldots,N$. These equations are related to the Calogero–Moser system.

X. SPECIAL SURFACES CORRESPONDING TO VORTEX SOLUTIONS OF THE SPIN SYSTEM

This section is devoted to the construction of explicit surfaces. To this aim, let us start from the one-vortex solution of the spin system (54)–(55). By choosing for simplicity $E=1$, Eqs. (41)–(42) become

$$k=L, \quad \sigma=\frac{F_x}{\sqrt{g}}, \quad \tau=\frac{M-LF}{\sqrt{g}}, \tag{141}$$

$$m_1=\frac{N-MF}{\sqrt{g}}, \quad m_2=-\frac{G_x}{2\sqrt{g}}, \quad m_3=M. \tag{142}$$

On the other hand, from (38) and (89) we get

$$\mathbf{r}_x(\xi,\eta,t)=\mathbf{S}(\xi,\eta,t). \tag{143}$$

Now let us consider by way of example the surface associated with the one-vortex solution of the Ishimori system, whose components are

$$S_3=\frac{1-b^2|\Xi|^2}{1+b^2|\Xi|^2}, \quad S^+=2be^{i\delta}\frac{\Xi}{1+b^2|\Xi|^2},$$

$$u=2(\ln(b)+\ln[1+b^2|\Xi|^2]),$$

where Ξ denotes the complex variable $\Xi=2a\exp(i\gamma)(x+iy)+1$, a,b, γ, and δ being real constants.

Then, by resorting to the formula $e_1=r_x/\sqrt{E}$ (with $E\equiv 1$), we can integrate to yield the following components for the position vector:

$$r_1=\frac{\hat{c}\ln(1+b^2|\Xi|^2)}{a\,b}-\frac{\sqrt{2}\arctan\left[b\sqrt{\frac{2}{\Omega}}(a\,x+c)\right](\tilde{c}-2\,a\,\hat{s}y)}{a\sqrt{\Omega}},$$

$$r_2=\frac{\hat{s}\ln(1+b^2|\Xi|^2)}{a\,b}-\frac{\sqrt{2}\arctan\left[b\sqrt{\frac{2}{\Omega}}(a\,x+c)\right](2\,a\,\hat{c}y+\tilde{s})}{a\sqrt{\Omega}}, \tag{144}$$

$$r_3=-x+\frac{2\sqrt{2}\arctan\left[b\sqrt{\frac{2}{\Omega}}(a\,x+c)\right]}{a\,b\sqrt{\Omega}},$$

where for the sake of clarity we have introduced the second degree polynomial $\Omega=2+b^2[1+2a^2y^2-\cos(2\gamma)+4a\sin(\gamma)y]$ and the constants $c=\cos(\gamma)$, $s=\sin(\gamma)$, $\hat{c}=\cos(\gamma+\delta)$, $\hat{s}=\sin(\gamma+\delta)$, $\tilde{c}=-\cos(\delta)+\cos(2\gamma+\delta)$, and $\tilde{s}=-\sin(\delta)+\sin(2\gamma+\delta)$. Furthermore, we have put identically equal to zero any arbitrary function of integration in y only.

From them, with the help of the various formulas given in Sec. III, we obtain the coefficients of the I-fundamental form,

$$E=1, \quad F=\frac{4\,b\,(s+a\,y)\,(b\,(c+a\,x)\sqrt{\Omega}+\sqrt{2}\,(1+b^2|\Xi|^2)\,At[x,y])}{(1+b^2|\Xi|^2)\,\Omega^{3/2}},$$

$$G=\frac{2\,(4\,b^2\,(s+a\,y)^2\,\Omega+8\,(1+b^2\,|\Xi|^2)\,At[x,y]^2)}{(1+b^2\,|\Xi|^2)\,\Omega^2},$$

where $At[x,y]=\arctan[\,b\,\sqrt{2/\Omega}\,(a\,x+c)]$, and analogously for the II-fundamental form,

$$\sqrt{g}L=\frac{8\,a\,b\,[-(b^3\,(c+a\,x)\,(s+a\,y)^2\,\sqrt{\Omega})+\sqrt{2}\,(1+b^2\,|\Xi|^2)\,At[x,y]]}{(1+b^2\,|\Xi|^2)^2\,\Omega^{3/2}},$$

$$\sqrt{g}M=\frac{-4\,a\,b^2\,(s+a\,y)}{(1+b^2\,|\Xi|^2)^2},$$

$$\sqrt{g}N=\frac{8\,a\,b(2\sqrt{2}(1+b^2|\Xi|^2)\,\sqrt{\Omega}\;At[x,y]+8\,b\,(c+a\,x)\,(1+b^2\,|\Xi|^2)\;At[x,y]^2+b^3\,(c+a\,x)\,(s+a\,y)^2\,\Omega\,(2+\Omega))}{(1+b^2|\,\Xi|^2)^2\,\Omega^3},$$

where g in the metric factor $\sqrt{g}$ is expressed by

$$g=\frac{8}{(1+b^2\,|\Xi|^2)^2\,\Omega^3}\{\,b^2\,(s+a\,y)^2\,\Omega-2\,b^2\,(c+a\,x)^2+(1+b^2\,|\Xi|^2)\,\Omega)$$
$$-4\sqrt{2}\,b^3\,(c+a\,x)\,(s+a\,y)^2\,(1+b^2\,|\Xi|^2)\,\sqrt{\Omega}\,At[x,y]+4\,(1+b^2\,|\Xi|^2)^2\,At[x,y]^2\}.$$

The Gauss curvature K and the mean curvature H are given by [see (32) and (33)] are given by

$$K=\frac{8\,a^2\,b^2}{(1+b^2\,\Xi^2)^4\,\Omega^{9/2}}\{-b^2\,(s+a\,y)^2\,\Omega^{3/2}\,(\Omega^3+4\,b^4\,(c+a\,x)^2\,(s+a\,y)^2\,(2+\Omega))$$
$$+4\sqrt{2}b^3(c+ax)(s+ay)^2(1+b^2|\Xi|^2)\Omega^2At[x,y]-16(1+b^2|\Xi|^2)$$
$$\times[2\,b^4\,(c+a\,x)^2\,(s+a\,y)^2-(1+b^2|\Xi|^2)]\sqrt{\Omega}\,At[x,y]^2$$
$$+32\sqrt{2}b(c+ax)(1+b^2|\Xi|^2)^2At[x,y]^3\},$$

$$H=\frac{4ab}{(1+b^2\,|\Xi|^2)^3\Omega^{7/2}\sqrt{g}}\{b^3\,(c+a\,x)\,(s+a\,y)^2\,\Omega^{3/2}[(1+b^2\,|\Xi|^2)\,(2+\Omega)$$
$$+4\,(2\,b^2\,(s+a\,y)^2+\Omega)]+2\,\sqrt{2}\,(1+b^2\,|\Xi|^2)\,\Omega\,(1-4\,b^2\,(s+a\,y)^2+b^2\,|\Xi|^2$$
$$+2\,b^2\,(s+a\,y)^2\,\Omega)\,At[x,y]+8\,b\,(c+a\,x)\,(1+b^2\,|\Xi|^2)$$
$$\times(1+2\,b^2\,(s+a\,y)^2+b^2\,|\Xi|^2)\,\sqrt{\Omega}\,At[x,y]^2-16\sqrt{2}\,(1+b^2\,|\Xi|^2)^2\,At[x,y]^3\},$$

respectively.

An example of a surface associated with the one-vortex solution of the Ishimori system is drawn in Fig 1.

XI. CONCLUSIONS

In this article we have established some notable connections among the purely topological CS theory, deformations of surfaces, and integrable equations in $(2+1)$-dimensions. However, many questions remain open and deserve further investigation, such as, for example, the search for other integrable classes of deformations of surfaces, the determination of the Hamiltonian structure, and the possible interpretation of the solutions from a physical point of view. To this regard, in particular we have found the surface associated with the exact vortex solutions of the $(2+1)$-dimensional spin system. We notice that another approach exists to study integrable $(2+1)$-dimensional deformations of surfaces, i.e., the method developed mainly by Konopelchenko, Taimanov, and co-workers.[3,30] The essential tool of their procedure is the use of a generalized

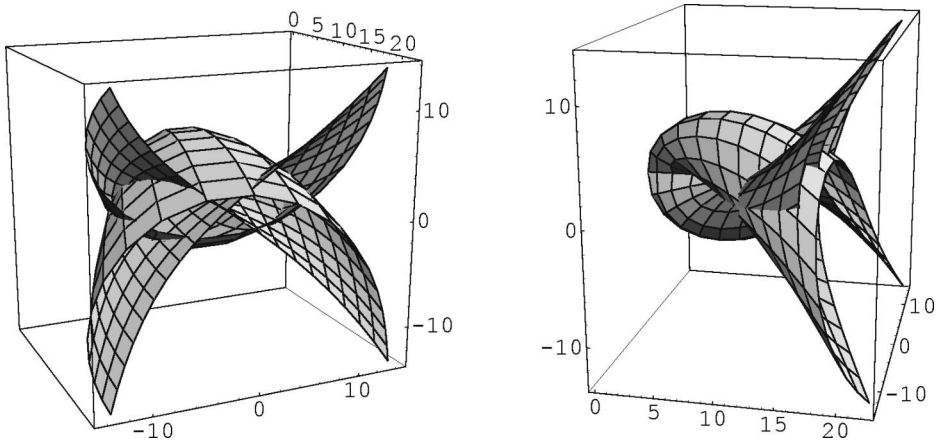

FIG. 1. We drew the same surface from two different points of view. The parameters used in Eq. (144) are $a=1$, $b=0.1$, $\gamma=\delta=0$.

Weierstrass representation for a conformal immersion of surfaces into R^3 or R^4, together with a linear problem related to this representation. The method devised in Refs. 3, 30 allows one to express integrable deformations of surfaces via hierarchies of integrable equations, such as the Nizhnik–Veselov–Novikov, the DS equations, and so on. We think that our approach and that described in Ref. 3 should be pursued in parallel, with the purpose to achieve possible complementary results on the link between integrable deformations of surfaces and completely integrable partial differential equations. Finally, we have shown that the non-Abelian Chern–Simons field theory can be interpreted in a more classical geometrical setting. From this aspect, by a suitable choice of the configuration space of the fields and under certain assumptions on the gauge conditions, notable equations of the mathematical physics arise. In this case, since large classes of solutions are known, our results could be useful in the studies of related problems in the low-dimensional classical and quantum physics, where the peculiar properties of the Chern–Simons interaction are involved.[14,15,31–33]

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Harmonic functions and angular momentum for anyon systems

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A method of construction of harmonic functions for the system of anyons on a plane is given. Spectra of angular momentum are derived. Anyonic statistics implies a restriction of the range of angular momentum which is stronger in comparison to the bosonic and fermion case. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1339220]

I. INTRODUCTION

We consider the system of N anyons on a plane, with the statistical parameter $\nu \in [0,2)$. The configuration space of the system is $Q_N = C^N \backslash D_N / \Sigma_N$ (we identify the plane with the complex plane C, D_N denotes the fat diagonal, and Σ_N is the symmetric group). The fundamental group of this space is the so called braid group $B_N = \pi_1(Q_N)$.[1–4] Wave functions describing this system will be referred to as the ν-equivariant functions, that is functions which transform according to one-dimensional unitary irreducible representations of the corresponding braid group B_N, labeled uniquely by ν.

In the theory of anyons on a (complex) plane it is convenient to separate the motion of the system into the mass center and the relative part. Because the mass center part corresponds to a simply connected space we will deal only with the relative one. The relative part of the motion is orthogonal to the mass center part because the former is generated by differences of positions of particles. It is obvious that the space of the relative part has complex dimension $M := N-1$.

Anyonic harmonic functions (it means those satisfying the Laplace equation and being ν-equivariant) are very important in the anyon theory. For example, solutions of the stationary Schrödinger equation for free anyons or anyons in a homogeneous harmonic oscillator potential can be written by means of products of homogeneous anyonic harmonic functions and suitable special functions depending only on the length of the relative radius. So the relative angular momentum depends only on the harmonic factor, the other factor does not affect the value of angular momentum. Solutions for the system was given in the papers of Refs. 5, 6 by means of homogeneous holomorphic functions, but more general formulas we obtain replacing them by homogeneous harmonic functions.

It is well known [3,4] that the relative part of ν-equivariant functions can be presented as

$$V^{\nu}(u) F_{\mathrm{sym}}(u,u^*) \tag{1}$$

or

$$V^{2-\nu}(u^*) F_{\mathrm{sym}}(u,u^*), \tag{2}$$

where

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$$u=(u_1,\ldots,u_M), \quad u^*=(u_1^*,\ldots,u_M^*) \tag{3}$$

are orthonormal system of holomorphic (resp., antiholomorphic) coordinates of the relative motion space,

$$V(u)=\prod_{k<l}(z_l-z_k) \tag{4}$$

is the Vandermonde determinant of positions of particles $(z_k, k=1,2,\ldots,N)$, expressed by the relative coordinates, and $F_{\mathrm{sym}}(u,u^*)$ is a power series of variables u,u^*, symmetric with respect to transpositions of particles.

Our aim in the present paper is the construction of anyonic harmonic functions, that is such ν-equivariant functions $H(u,u^*)$ of the form of Eqs. [(1)–(2)], which satisfy the Laplace equation:

$$\sum_{k=1}^{M}\frac{\partial}{\partial u_k}\frac{\partial}{\partial u_k^*}H=0. \tag{5}$$

In Sec. II we propose the construction of such functions, in Sec. III we deal with the angular momentum, in Sec. IV we give an example, and in Sec. V, some general remarks and conclusions.

II. CONSTRUCTION OF ANYONIC HARMONIC FUNCTIONS

We start with the following evident commutation relations:

$$\left[\frac{\partial}{\partial u_k},\frac{\partial}{\partial u_l}\right]=0, \tag{6}$$

$$\left[\frac{\partial}{\partial u_k},u_l^*\right]=0, \tag{7}$$

$$\left[\frac{\partial}{\partial u_k},\frac{\partial}{\partial u_l^*}\right]=0. \tag{8}$$

They imply that despite the fact that the Laplace Equation (5) is of the second order, we can treat it as a first order partial differential equation with respect to the antiholomorphic variables. This equation is linear, and its coefficients are operators $\partial/\partial u_k$, which are constant with respect to antiholomorphic variables. Thus the solutions are given in a full analogy with the case of equations with constant number coefficients,

$$\sum_{k=1}^{M}a_k\frac{\partial}{\partial x_k}p(x)=0. \tag{9}$$

The solution can be written in the form

$$p(x)=P(x_1a_2-x_2a_1,x_1a_3-x_3a_1,\ldots,x_{M-1}a_M-x_Ma_{M-1}), \tag{10}$$

with P being an arbitrary function of the class C_1. It suggests we look for the solutions of Eq. (5) in the form

$$H(u,u^*)=P\left(u_1^*\frac{\partial}{\partial u_2}-u_2^*\frac{\partial}{\partial u_1},u_1^*\frac{\partial}{\partial u_3}-u_3^*\frac{\partial}{\partial u_3{}_1},\ldots,u_{M-1}^*\frac{\partial}{\partial u_M}-u_M^*\frac{\partial}{\partial u_{M-1}}\right)\tilde{f}(u), \tag{11}$$

where $\tilde{f}$ depends only upon holomorphic variables u. Moreover, we admit in our consideration only a polynomial form of the functions P, to avoid detailed discussion of domains, etc.

The right-hand side of Eq. (11) is the result of acting of the differential operator $P(u_1^*(\partial/\partial u_2) - u_2^*(\partial/\partial u_1),\ldots]$ on holomorphic function $\tilde{f}(u)$.

To impose the fractional statistics ν, we take the function $\tilde{f}(u)$ in the form

$$\tilde{f}(u) = f(u)V^{\nu}(u), \tag{12}$$

where $f(u)$ is a polynomial. The condition of hard core for anyons implies that H should vanish at the fat diagonal.[3] Thus, it cannot exhibit any pole there. It follows that the polynom f should be divisible by V^n, where n is the total degree of the polynom P. Moreover, (Eq. (1) implies that either both $P[u_1^*(\partial/\partial u_2) - u_2^*(\partial/\partial u_1),\ldots]$ and $f(u)$ are symmetric with respect to transpositions of particles, or both are antisymmetric.

For homogeneous polynomials P and f the function H is a bihomogeneous one, which means that H is an eigenfunction of holomorphic and antiholomorphic homogeneity degree operators:

$$\hat{n}_h = \sum_k u_k \frac{\partial}{\partial u_k}, \quad \hat{n}_a = \sum_k u_k^* \frac{\partial}{\partial u_k^*}, \tag{13}$$

i.e.,

$$\hat{n}_h H = n_h H, \quad \hat{n}_a H = n_a H. \tag{14}$$

We have therefore the following formulas:

$$H(u,u^*) = P_{\mathrm{sym}}\left(u_1^* \frac{\partial}{\partial u_2} - u_2^* \frac{\partial}{\partial u_1},\ldots\right)(f_{\mathrm{sym}}(u)V^{\nu+2k}(u)), \tag{15}$$

$$H(u,u^*) = P_{\mathrm{antisym}}\left(u_1^* \frac{\partial}{\partial u_2} - u_2^* \frac{\partial}{\partial u_1},\ldots\right)(f_{\mathrm{sym}}(u)V^{\nu+2k-1}(u)), \tag{16}$$

or

$$H(u,u^*) = P_{\mathrm{sym}}\left(u_1 \frac{\partial}{\partial u_2^*} - u_2 \frac{\partial}{\partial u_1^*},\ldots\right)(f_{\mathrm{sym}}(u^*)V^{2-\nu+2k}(u^*)), \tag{17}$$

$$H(u,u^*) = P_{\mathrm{antisym}}\left(u_1 \frac{\partial}{\partial u_2^*} - u_2 \frac{\partial}{\partial u_1^*},\ldots\right)(f_{\mathrm{sym}}(u^*)V^{1-\nu+2k}(u^*)), \tag{18}$$

where f_{sym} is a symmetric bihomogeneous polynomial indivisible by V. In all of Eqs. (15)–(18), the degree of polynomial P_{sym} (P_{antisym}) is less than the exponent of Vandermonde determined (the hardcore condition). Equations (15)–(18) provide general formulas for anyonic harmonic functions for arbitrary N, and constitute the basis for the following considerations. We proceed to demonstrate some special cases in more detail.

III. ANGULAR MOMENTUM OF ANYON SYSTEM

Let us consider the operators

$$\hat{l} = \hat{n}_h + \hat{n}_a \tag{19}$$

and

$$\hat{m} = \hat{n}_h - \hat{n}_a. \tag{20}$$

Clearly, $\hat{m}$ is the operator of the two-dimensional angular momentum, and a bihomogeneous function $H(u,u^*)$ is its eigenfunction, with eigenvalue $m=n_h-n_a$.

The operator $\hat{l}$ has the meaning of the total degree of homogeneity $l=n_h+n_a$ and bears some resemblance to the quantum number of the square of angular momentum in the three-dimensional theory. Namely, we are going to demonstrate that it provides some bounds to the range of m.

We start with the observation that in the three-dimensional case the (z-projection of) the angular momentum m varies with the step 1, whereas in our case m varies with the step 2, for fixed value of the total homogeneity degree l. It is an immediate consquence of Eqs. (19), (20), which follow from the fact that our system is two-dimensional.

Let us consider in particular harmonic functions of the form

$$H_I=P\left(u_k^*\frac{\partial}{\partial u_l}-u_l^*\frac{\partial}{\partial u_k}\right)(V^{n+\nu}(u)f(u)), \tag{21}$$

where P is a polynomial of degree n, which is symmetric (antisymmetric) for n even (odd), and f is a holomorphic homogeneous symmetric polynomial. The total homogeneity degree and the angular momentum of the function are given by

$$l_I=(n+\nu)\binom{N}{2}+d(f), \quad m_I=l_I-2n, \tag{22}$$

where $d(f)$ is the homogeneity degree of the polynomial f. Note that $\binom{N}{2}$ is equal to the homogeneity degree of the Vandermonde determinant $V(u)$. For given l_I we obtain the minimal value of m_I for $n=(n_I)_{\max}$,

$$(n_I)_{\max}=\left[\frac{l_I-\binom{N}{2}\nu}{\binom{N}{2}}\right], \tag{23}$$

where the square bracket denotes the integer part,

$$(m_I)_{\min}=l_I-2(n_I)_{\max}>0. \tag{24}$$

Bounds (23) and (24) follow from the fact that ν is genuinely nonintegral. Namely, it is easy to observe that $P[u_k^*(\partial/\partial u_l)-u_l^*\partial/\partial u_k)$ in Eq. (21) generates poles when the degree of P is bigger than $(n_I)_{\max}$. In other words, the spectrum of the angular momentum m_I is

$$l_I-2(n_I)_{\max}, \quad l_I-2(n_I)_{\max}+2, \ldots l_I-2, \quad l_I. \tag{25}$$

For harmonic functions of the form

$$H_{II}=P\left(u_k\frac{\partial}{\partial u_l^*}-u_l\frac{\partial}{\partial u_k^*}\right)(V^{n+2-\nu}(u^*)f(u^*)), \tag{26}$$

we obtain in a similar way the spectrum of the angular momentum m_{II}:

$$-(l_{II}-2(n_{II})_{\max}), -(l_I-2(n_{II})_{\max}+2), \ldots -(l_{II}-2), -l_{II}, \tag{27}$$

where l_{II} is the total homogeneity degree of the function (26), and

$$(n_{II})_{\max}=\left[\frac{l_{II}-\binom{N}{2}(2-\nu)}{\binom{N}{2}}\right], \tag{28}$$

$$(m_{II})_{\max}=-(l_{II}-2(n_{II})_{\max})<0. \tag{29}$$

Thus in the case of boson ($\nu=0$) or fermion ($\nu=1$) statistics, the angular momentum m varies in the range from $-l$ to l with the step 2 (for the two-dimensional system). For fractional statistics we obtain some bounds the range of m under fixed l, given by Eqs. (23), (24) and Eqs. (28), (29).

When considering purely fractional statistics ($\nu\neq 0$ and $\nu\neq 1$), we should distinguish between two cases: the generic $N(N-1)\nu\notin Z$, and the special one $N(N-1)\nu\in Z$.

The consideration given above imply that for the generic case the spectra of the total homogeneity degree l_I and l_{II} are mutually different. In this case the equality $l_I=l_{II}$ cannot be satisfied because the difference l_I-l_{II} is not an integer. In special cases a series of positive values [Eq. (25)] of angular momentum m_I joins with suitable series of negative values m_{II} [Eq. (27)] such that $l_I=l_{II}$.

We conclude that in the generic case the spectrum of the angular momentum m for fixed l is either positive or negative, whereas in special cases it encompasses both positive and negative values.

IV. THE CASE OF THREE ANYONS. EXAMPLES

Now we discuss the case of three anyons. The complex dimension of the relative space is $M=2$, so that P depends only upon a single argument, e.g., $u_1^*(\partial/\partial u_2)-u_2^*(\partial/\partial u_1)$ (cf. Eq. (11)]. Thus we take

$$P(x)=x^n. \tag{30}$$

For the sake of definiteness, we restrict our further discussion to Eq. (15). Other cases follow correspondingly.

The Vandermonde determinant for three anyons in Fourier coordinates:[7]

$$u_k=\frac{1}{\sqrt{3}}\sum_{l=1}^{3} e^{2\pi ikl/3}z_l, \quad k=0,1,2, \tag{31}$$

is given, up to a multiplicative constant, by the formula

$$V(u)=u_2^3-u_1^3. \tag{32}$$

So Eq. (15) yields $H(u,u^*)=[u_1^*(\partial/\partial u_2)-u_2^*(\partial/\partial u_1)]^n[f(u)(u_2^3-u_1^3)^r]$, where $r\geqslant n$; $[r]=[\nu]$ with $[x]$ denoting the integer part of x. For simplicity we put $f(u)=u_1^k u_2^l$, which is not symmetric generally, and then we get a formula for symmetric polynomials.

The case $n=0$ in Eq. (30) corresponds to the constant function $P=1$, so the multivalued function H is locally holomorphic.

In the case $n=1$ (the antiholomorphic homogenity rank is equal to 1, we have

$$\left(u_1^*\frac{\partial}{\partial u_2}-u_2^*\frac{\partial}{\partial u_1}\right)[(u_1^k u_2^l(u_2^3-u_1^3)^r)]=(lu_1u_1^*-ku_2u_2^*)u_1^{k-1}u_2^{l-1}(u_2^3-u_1^3)^r + 3r(u_2^2u_1^*+u_1^2u_2^*)u_1^k u_2^l(u_2^3-u_1^3)^{r-1}. \tag{33}$$

In particular, we have a very simple form of harmonics for $k,l=0$, which reads as

$$(u_2^2u_1^*+u_1^2u_2^*)(u_2^3-u_1^3)^{r-1}. \tag{34}$$

The case $n=2$ yields

$$\begin{aligned}
&\left(u_1^*\frac{\partial}{\partial u_2}-u_2^*\frac{\partial}{\partial u_1}\right)^2[(u_1^ku_2^l(u_2^3-u_1^3)^r)]\\
&\quad=-(k+l)u_1^*u_2^*u_1^{k-1}u_2^{l-1}(u_2^3-u_1^3)^r\\
&\qquad+(lu_1u_1^*-ku_2u_2^*)[(l-1)u_1u_1^*-(k-1)u_2u_2^*]u_1^{k-2}u_2^{l-2}(u_2^3-u_1^3)^r\\
&\qquad+6r(u_2^2u_1^*+u_1^2u_2^*)(lu_1u_1^*-ku_2u_2^*)u_1^{k-1}u_2^{l-1}(u_2^3-u_1^3)^{r-1}\\
&\qquad+6r(u_2u_1^{*2}+u_1u_2^{*2})u_1^ku_2^l(u_2^3-u_1^3)^{r-1}\\
&\qquad+9r(r-1)(u_2^2u_1^*+u_1^2u_2^*)^2u_1^ku_2^l(u_2^3-u_1^3)^{r-2}.
\end{aligned}$$

It shows that the number of terms increases rapidly with n.

Now let us consider the spectrum of the angular momentum operator for the relative part of anyonic harmonic functions of the three anyon system. The total homogeneity rank of the function of the form (42) is

$$l_I=3(n+\nu)+k, \tag{35}$$

and of the form (43),

$$l_{II}=3(n+2-\nu)+k, \tag{36}$$

where k is the homogeneity rank of $f(u)$, $(f(u^*))$.

The permutation group S_3 acts on variables u_0,u_1,u_2 in the standard way as on functions of z_1,z_2,z_3:

$$(\sigma f)(z_1,z_2,z_3)=f(z_{\sigma(1)},z_{\sigma(2)},z_{\sigma(3)}). \tag{37}$$

This action is trivial on u_0, and

$$\sigma_1u_1=u_2,\quad \sigma_1u_2=u_1,\quad \sigma_2u_1=\epsilon^2u_2,\quad \sigma_2u_2=\epsilon u_1, \tag{38}$$

where $\epsilon=e^{2\pi i/3}$. The relative space is a carrying space of the irreducible representation $\Gamma_{\{1,2\}}$ of the group S_3. In the coordinate (u_1,u_2) the matrix elements are

$$\Gamma_{\{1,2\}}(\sigma_1)=\begin{bmatrix}0&1\\1&0\end{bmatrix},\quad \Gamma_{\{1,2\}}(\sigma_2)=\begin{bmatrix}0&\epsilon^2\\\epsilon&0\end{bmatrix}. \tag{39}$$

The symmetrization $S=\frac{1}{6}\Sigma\sigma$ of the monomial $u_1^{n_1}u_2^{n_2}$ is equal 0 for n_1-n_2 indivisible by 3:

$$S(u_1^{n_1}u_2^{n_2})=\tfrac{1}{6}(1+\epsilon^{n_1-n_2}+\epsilon^{n_2-n_1})u_1^{n_1}u_2^{n_2}+(1+\epsilon^{n_1-n_2}+\epsilon^{n_2-n_1})u_2^{n_1}u_1^{n_2}. \tag{40}$$

So the basis of the holomorphic relative symmetric polynomials is formed by such functions:

$$u_1^{n_1}u_2^{n_2}+u_1^{n_2}u_2^{n_1},\quad n_1\geqslant n_2, \tag{41}$$

where the difference n_1-n_2 is divisible by three. In a similar way one can show that $u_1^*(\partial/\partial u_2-u_2^*(\partial/\partial u_1)$ is an antisymmetric operator. So general formulas for the relative part of harmonic functions for a three anyon system of the type (15.) can be written in the form

$$H_I(u,u^*)=\left(u_1^*\frac{\partial}{\partial u_2}-u_2^*\frac{\partial}{\partial u_1}\right)^n(u_2^3-u_1^3)^{n+\nu}f(u), \tag{42}$$

where $f(u)$ is a relative holomorphic symmetric polynomial.

The other formula of the type (18) is given in such a way,

$$H_{II}(u,u^*)=\left(u_1\frac{\partial}{\partial u_2^*}-u_2\frac{\partial}{\partial u_1^*}\right)^n(u_2^{*3}-u_1^{*3})^{n+2-\nu}f(u^*), \tag{43}$$

where $f(u^*)$ is a relative antiholomorphic symmetric polynomial.

The dimension of the space X_k (X_k^*) of homogeneous relative holomorphic (antiholomorphic) symmetric polynomials of degree k is equal to $d(k)$, where

$$d(6n+a)=n+1 \quad \text{for } a=0,2,3,4,5 \text{ and } d(6n+1)=n. \tag{44}$$

The pairs (l_I,m_I) and (l_{II},m_{II}) in general are degenerate. The degree of the degeneration of the pair (l_I,m_I) or (l_{II},m_{II}) is equal to the dimension $d(k)$ of the space X_k.

Now let us consider two examples—one for the generic case: $\nu=\frac{1}{7}$, $l_I=8\frac{3}{7}$, the nearest value of l_{II} to $8\frac{3}{7}$ is $l_{II}=8\frac{4}{7}$, and one for the special case $\nu=\frac{1}{6}$, $l_I=l_{II}=l=8\frac{1}{2}$.

The spectrum of the angular momentum for $\nu=\frac{1}{7}$ and for $8\frac{3}{7}$ the spectrum of the angular momentum is

$$m_I=4\,\tfrac{3}{7},\quad 6\,\tfrac{3}{7},\quad 8\,\tfrac{3}{7}, \tag{45}$$

and for $\nu=\frac{1}{7}$, $l_{II}=8\frac{4}{7}$ the spectrum of the angular momentum is

$$m_{II}=-8\,\tfrac{4}{7},\quad -6\,\tfrac{4}{7}. \tag{46}$$

For the special case $\nu=\frac{1}{6}$, $l_I=l_{II}=l=8\frac{1}{2}$ the spectrum of angular momentum is given as

$$m_{II}=-8\,\tfrac{1}{2},\quad -6\,\tfrac{1}{2},4\,\tfrac{1}{2},\ 6\,\tfrac{1}{2},\quad 8\,\tfrac{1}{2}. \tag{47}$$

V. CONCLUSIONS

The construction of anyonic harmonic functions for the system of N anyons on the plane has been given. The separation of holomorphic and antiholomorphic variables allows us to reduce the Laplace equation to a homogeneous linear first order partial differential equation with constant operatorial coefficients. The solution of the problem is given by Eqs. (15)–(18).

We have already reported another approach to the construction presented above.[8,9] The anyonic harmonic functions are presented there in terms of covariant derivatives. It is related to the fact that the differential operators in these papers are acting upon polynomials $f(u)$ instead of multivalued functions $\tilde{f}(u)$:

$$\frac{\partial\tilde{f}}{\partial u_k}=V^\nu\left(\nu\frac{\partial \ln V}{\partial u_k}+\frac{\partial}{\partial u_k}\right)f. \tag{48}$$

As the result the derivation presented here is formally equivalent to that given before, but is remarkably simpler, since it avoids a double change of gauge transformation.

The angular momentum of an anyonic harmonic function H is quantized with step 2 for fixed total homogeneity degree $l=d(H)$. This observation follows from the fact that the system is two-dimensional. The angular momentum for boson or fermion statistics is constrained to the range $-l,-l+2,\ldots,l$. The case of intrinsically fractional statistics imposes a further restriction of this range specified by the formulas in Eqs. (25), (27). This effect follows from the fact that

bosonic or fermionic harmonic functions are polynoms and thus any differentiation cannot lead to poles on the fat diagonal. Contrary for an intrinsically fractional statistic, an appropriately large number of differentiations yields unavoidably poles on the fat diagonal which is inconsistent with the hard-core requirement.

This formalism can be adapted for more general systems. For example, for a system of many kinds of anyons on a plane with different statistical parameters or for a system of distinguishable particles with hard cores on a plane.

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Stability of nonconservative hyperbolic systems and relativistic dissipative fluids

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A stability theorem for general quasi-linear symmetric hyperbolic systems (not necessarily conservation laws) is proved in this work. The key assumption is the ''stability eigenvalue condition,'' which requires all the eigenvalues of the constant coefficient system symbol to have negative real part for nonzero Fourier frequency, decaying no faster than $|\omega|^2$ when $|\omega|\to 0$. The decay of the solution to zero, as time grows to infinity, is proved when the space dimension is bigger than or equal to 3. As an application of the general theorem, stability is proved for the equations describing relativistic dissipative fluids. © *2001 American Institute of Physics.*
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I. INTRODUCTION

It is the purpose of this work to prove the linear and nonlinear stability of stationary constant solutions to the Cauchy problem in the whole space of a general quasi-linear symmetric hyperbolic system of equations. It is also the purpose of this work to present a concrete, physically relevant application of the stability result, namely to the systems of equations describing dissipative relativistic fluids.

The Cauchy problems considered are those of the form

$$\partial_t u=\sum_{j=1}^{d}\,[A_{0j}+\varepsilon A_{1j}(x,t,u,\varepsilon)]\partial_j u+[B_0+\varepsilon B_1(x,t,u,\varepsilon)]u+F(x,t),$$
$$u(x,0)=f(x). \tag{1}$$

Here $x\in\mathbf{R}^d$, $t\geqslant 0$, and $u(x,t)$ and $f(x)$ take values in $\mathbf{R}^n$. Partial differentiation with respect to t and x_j are denoted by ∂_t and ∂_j, respectively. The assumptions on the coefficients, source, and initial data to be used in the theorems throughout the article are given below after introducing some notation.

As usual, for $u,v\in\mathbf{C}^n$, and $A\in\mathbf{C}^{n\times n}$,

$$\langle u,v\rangle=\sum_{j=1}^{n}\,u_j^*\,v_j,\quad |u|=\langle u,u\rangle^{1/2}\quad\text{and}\quad |A|=\max_u\{|Au|:|u|=1\}$$

denote the inner product, Euclidean norm, and corresponding matrix norm. For vector functions u,v of the space variables, $\|u\|_1$, (u,v), $\|u\|=(u,u)^{1/2}$, and $\|u\|_{H^p}$ denote the L_1-norm, L_2-inner product, L_2-norm, and the H^p-Sobolev norm, respectively.

For the squared L_1-norm in space and time the following notation will be used

$$K_F(T):=\left[\int_0^T\int_{\mathbf{R}^d}|F(x,t)|\,dx\,dt\right]^2.$$

Given multi-indices $\alpha=(\alpha_1,\alpha_2,\ldots,\alpha_d)$ and $\beta=(\beta_1,\beta_2,\ldots,\beta_n)$ the following notation will be used for partial derivatives

$$\partial_x^\alpha=\partial_1^{\alpha_1}\cdots\ \partial_d^{\alpha_d},\quad \text{and}\quad |\alpha|=\alpha_1+\cdots+\alpha_d,$$

and

$$\partial_u^\beta=\left(\frac{\partial}{\partial u_1}\right)^{\beta_1}\cdots\left(\frac{\partial}{\partial u_n}\right)^{\beta_n}\quad \text{and}\quad |\beta|=\beta_1+\cdots+\beta_n.$$

Assumption 1: The constant matrices A_{0j} and B_0 are real and symmetric. The matrices A_{1j} are also real and symmetric.

The following is an assumption on the regularity of the coefficients, source, and initial data.

Assumption 2: (a) Given $C>0$, there are constants $k_{A,C}$ and $k_{B,C}$ such that, for $j=1,2,\ldots,d$,

$$|A_{1j}(x,t,u,\varepsilon)|\leqslant k_{A,C}|u(x,t)|$$

and

$$|B(x,t,u,\varepsilon)|\leqslant k_{B,C}|u(x,t)|,$$

provided that $|u|\leqslant C$.

(b) Given $C>0$, for every $p=0,1,2,\ldots$ there is a constant $K(C,p)$ such that

$$|\partial_x^\alpha\partial_u^\beta A_{1j}(x,t,u,\varepsilon)|+|\partial_x^\alpha\partial_u^\beta\partial_t A_{1j}(x,t,u,\varepsilon)|\leqslant K(C,p)$$

and

$$|\partial_x^\alpha\partial_u^\beta B_1(x,t,u,\varepsilon)|+|\partial_x^\alpha\partial_u^\beta\partial_t B_1(x,t,u,\varepsilon)|\leqslant K(C,p),$$

provided that $|u|\leqslant C$, and for all multi-indices α and β with $|\alpha|+|\beta|=p$.

(c) The source F is such that

$$K_F(\infty)<\infty\quad \textit{and}\quad \int_0^\infty \|F(\cdot,t)\|_{H^p}^2\,dt<\infty,\ \ p=0,1,2,\ldots.$$

(d) The initial data function f satisfies

$$f\in L_1(\mathbf{R}^d,\mathbf{R}^n)\cap H^p(\mathbf{R}^d,\mathbf{R}^n),\ \ for\ \ p=0,1,2,\ldots.$$

The first two assumptions are just the usual assumptions for short time existence theorems plus adequate decay rates in time. The third assumption, given later, is the one that implies global in time existence and stability, and is not necessary for local existence. We introduce notation for the first-order partial differential operators and associated symbol first:

$$P_0=\sum_{j=1}^d A_{0j}\partial_j\quad \text{and}\quad P_1=\sum_{j=1}^d A_{1j}(x,t,u,\varepsilon)\partial_j.$$

The symbol of the constant coefficient system, (1) with $\varepsilon=0$, is given by

$$\hat{P}_0(i\omega)+B_0=\sum_{j=1}^d i\omega_j A_{0j}+B_0,\quad \text{for}\ \ \omega\in\mathbf{R}^d. \tag{2}$$

Assumption 3: The symbol of the constant coefficient system satisfies the ''stability eigenvalue condition,'' i.e., there are positive constants ω_0, μ, *and* δ *such that all eigenvalues* $\lambda(\omega)$ *of (2) satisfy*

(a) $\mathrm{Re}\,\lambda(\omega)\leqslant -\mu|\omega|^2$, *for* $|\omega|\leqslant\omega_0$;
(b) $\mathrm{Re}\,\lambda(\omega)\leqslant -\delta$, *for* $|\omega|>\omega_0$.

Let $\hat{u}(\omega,t)$ denote the Fourier transform of $u(x,t)$. The following splitting in high and low frequencies of u will be useful:

$$u(x,t)=u^I(x,t)+u^{II}(x,t),\quad \text{where}\quad \hat{u}^I(\omega,t)=\begin{cases}\hat{u}(\omega,t) & \text{if } |\omega|\leqslant\omega_0,\\ 0 & \text{if } |\omega|>\omega_0.\end{cases} \tag{3}$$

This article presents a generalization of the work by Kreiss *et al.*,[1] where stability is proved for a wide class of systems of conservation laws. The symmetric hyperbolic systems studied in the present work are more general since they are not required to be systems of conservation laws. This generalization requires the dimension of space to be bigger than or equal to 3. In this article the initial data function is explicitly included in the estimates, as opposed to absorbing it in the source by means of a transformation as done by Kreiss *et al.*

This work also extends previous stability results[2] by including noncompact domains. This extension is necessary for some physical applications such as the theories of relativistic dissipative fluids.[3] Stability of the Cauchy problem of these fluid theories, under periodic boundary conditions, was shown in a previous work.[4]

Sections II and III of this work follow the paper by Kreiss *et al.*[1] In Sec. II the estimates for the solution of the linear equation [Eq. (1) with coefficients independent of u] are found and linear stability is proved. In Sec. III the linear estimates together with Sobolev's inequalities are used to prove global existence and stability in the nonlinear case. A proof of the following theorem is given.

Theorem 1: *Consider the Cauchy problem for the nonlinear equation (1), let Assumptions 1–3 hold, and let the dimension of space be* $d\geqslant 3$. *Then there exists* $\varepsilon_0>0$ *such that for* $|\varepsilon|\leqslant\varepsilon_0$ *the solution* u *is* C^∞ *and exists globally in time. Furthermore, the Cauchy problem is stable in the sense that*

$$\lim_{t\to\infty}|u(\cdot,t)|_\infty=0.$$

In Sec. IV the stability theorem is applied to an example of physical relevance, namely that of the general theories of relativistic dissipative fluids. Most of the effort done in Sec. IV is devoted to proving that these fluid theories comply with the stability eigenvalue condition required by Assumption 3.

Along this work C_l and $C_l(p)$, $l=1,2,\ldots$, will denote positive constants that may depend on P_0, B_0, and p when indicated, but are independent of P_1, B_1, ε, F, and f.

II. ESTIMATES AND LINEAR STABILITY

Consider the Cauchy problem for the linear, symmetric hyperbolic system of equations

$$\begin{aligned}\partial_t u&=\sum_{j=1}^{d}[A_{0j}+\varepsilon A_{1j}(x,t,\varepsilon)]\partial_j u+[B_0+\varepsilon B_1(x,t,\varepsilon)]u+F(x,t),\\ u(x,0)&=f(x).\end{aligned} \tag{4}$$

The first step to prove global existence and stability is to obtain estimates for the constant coefficient problem. Application of the Fourier–Laplace transformation to the constant coefficient system, (4) with $\varepsilon=0$, gives

$$[sI-\hat{P}_0(i\omega)-B_0]\tilde{u}(\omega,s)=\hat{f}(\omega)+\tilde{F}(\omega,s), \quad s=\eta+i\xi, \quad \eta>0. \tag{5}$$

Here $\tilde{u}(\omega,s)=\mathcal{L}_{t\to s}[\mathcal{F}_{x\to\omega}u(x,t)]$ and $\hat{f}(\omega)=\mathcal{F}_{x\to\omega}f(x)$.

Recall the decomposition (3) of u in low and high frequencies.

A. Estimates for u^I (low frequencies)

Assumption 3(a) implies $B_0\leqslant 0$, Then

$$[\hat{P}_0(i\omega)+B_0]+[\hat{P}_0(i\omega)+B_0]^{\dagger}=2B_0\leqslant 0,$$

where the symmetry was used. Consequently $|e^{(\hat{P}_0+B_0)t}|\leqslant 1$ and Kreiss' matrix theorem[5] can be applied. There are two constants C_1 and C_2 such that for each ω there is a transformation $S(\omega)$ such that

$$S^{-1}(\hat{P}_0+B_0)S=\begin{pmatrix}\lambda_1 & b_{12} & \cdots & b_{1n}\\ & \lambda_2 & \cdots & b_{2n}\\ & & \ddots & \vdots\\ 0 & & & \lambda_n\end{pmatrix}$$

with $|S^{-1}|+|S|\leqslant C_1$ and $|b_{ij}|\leqslant C_2|\mathrm{Re}\,\lambda_i|$, $1\leqslant i<j\leqslant n$. Therefore, it can be proved that

$$|[(\eta+i\xi)I-(\hat{P}_0+B_0)]^{-1}|^2\leqslant C_3\sum_j \frac{1}{(\eta-\mathrm{Re}\,\lambda_j)^2+(\xi-\mathrm{Im}\,\lambda_j)^2}.$$

By Assumption 3(a), $\eta-\mathrm{Re}\,\lambda_j\geqslant-\mu|\omega|^2$ when $|\omega|\leqslant\omega_0$. Then integration of the previous inequality gives

$$\int_{-\infty}^{\infty}|[(\eta+i\xi)I-(\hat{P}_0+B_0)]^{-1}|^2d\xi\leqslant\frac{C_4}{|\omega|^2}. \tag{6}$$

Lemma 1: Let u solve the constant coefficient Cauchy problem (4) with $\varepsilon=0$. If Assumptions 1, 2(c), 2(d), and 3(a) hold, and the dimension of space is $d\geqslant 3$, then for every $p=0,1,2,\ldots$ there exists a constant $C_0(p)$, which is independent of T, F, and f such that

$$\int_0^T\|u^I(\cdot,t)\|_{H^p}^2dt\leqslant C_0(p)[\|f\|_1^2+K_F(T)].$$

Proof: Equation (5) implies

$$|\tilde{u}|^2\leqslant 2|(sI-\hat{P}_0-B_0)^{-1}|^2|\hat{f}|^2+2|(sI-\hat{P}_0-B_0)^{-1}|^2|\tilde{F}|^2. \tag{7}$$

Notice that $|\hat{f}|^2\leqslant\|f\|_1^2$ and

$$|\tilde{F}|^2\leqslant\left|\int_0^{\infty}\int_{\mathbf{R}^d}e^{-i\langle\omega,x\rangle}e^{-\eta t}F(x,t)dxdt\right|^2\leqslant\left(\int_0^{\infty}\int_{\mathbf{R}^d}e^{-\eta t}|F(x,t)|dxdt\right)^2\leqslant K_F(\infty),$$

so that Parseval's relation,

$$\int_0^{\infty}e^{-2\eta t}\|u^I\|^2dt=\frac{1}{(2\pi)^{d+1}}\int_{|\omega|\leqslant\omega_0}\int_{-\infty}^{\infty}|\tilde{u}(\omega,\eta+i\xi)|^2d\xi\,d\omega,$$

together with estimates (6) and (7) imply

$$\int_0^\infty e^{-2\eta t}\|u^I\|^2 dt \leq C_4[\|f\|_1^2 + K_F(\infty)] \int_{|\omega|\leq\omega_0} \frac{d\omega}{|\omega|^2}.$$

As the dimension of space is $d \geq 3$, the integral of $|\omega|^{-2}$ is finite, and as the right-hand side is independent of η, the inequality also holds in the limit $\eta \to 0^+$. Thus,

$$\int_0^\infty \|u^I\|^2 dt \leq C_5[\|f\|_1^2 + K_F(\infty)]. \tag{8}$$

The space derivatives $\partial_x^\alpha u$ satisfy the same constant coefficient partial differential equation (PDE) as u. Therefore

$$|\widetilde{\partial_x^\alpha u}(\omega,s)| \leq |\omega|^{|\alpha|} |\tilde{u}(\omega,s)| \leq \omega_0^{|\alpha|} |\tilde{u}(\omega,s)|$$

and Eq. (8) imply

$$\int_0^\infty \|u^I\|_{H^p}^2 dt \leq \frac{1}{(2\pi)^{d+1}} \sum_{|\alpha|\leq p} \int_0^\infty \int_{|\omega|\leq\omega_0} |\widetilde{\partial_x^\alpha u}(\omega, \eta + i\xi)|^2 d\omega d\xi \leq C_0(p)[\|f\|_1^2 + K_F(\infty)]. \tag{9}$$

Finally, as the values of $u^I(x,t)$ for $t \leq T$ do not depend on the values of $F(x,t)$ for $t > T$, ∞ can be replaced by a finite time T in the previous estimate. This concludes the proof.

Consider now the Cauchy problem for the variable coefficient system (4). In this case the following assumption is needed.

Assumption 2(a′):

$$\sum_j \int_0^\infty \|A_{1j}(\cdot,t,\varepsilon)\|^2 \, dt + \int_0^\infty \|B_1(\cdot,t,\varepsilon)\|^2 \, dt \leq K_1 < \infty.$$

An estimate for the solution u in the variable coefficient case can be obtained, for $p \geq 1$, from the estimate (9) by redefining the source term to include the variable coefficients

$$G(x,t) = F(x,t) + \varepsilon \sum_j A_{1j}(x,t,\varepsilon)\partial_j u(x,t) + \varepsilon B_1(x,t,\varepsilon)u(x,t). \tag{10}$$

Notice that

$$\begin{aligned} K_G(\infty) &\leq 3K_F(\infty) + 3\varepsilon^2 \left(\int_0^\infty \int_{\mathbf{R}^d} \sum_j |A_{1j}||\partial_j u| dx \, dt \right)^2 \\ &\quad + 3\varepsilon^2 \left(\int_0^\infty \int_{\mathbf{R}^d} |B_1||u| dx \, dt \right)^2 \\ &\leq 3K_F(\infty) + 3\varepsilon^2 K_1 \int_0^\infty \|u\|_{H^1}^2 dt. \end{aligned}$$

Thus, application of (9) with F replaced by G gives

$$\begin{aligned} \int_0^\infty \|u^I\|_{H^p}^2 dt &\leq C_0(p)\|f\|_1^2 + 3C_0(p)K_F(\infty) + 6\varepsilon^2 C_0(p)K_1 \int_0^\infty \|u^I\|_{H^1}^2 dt \\ &\quad + 6\varepsilon^2 C_0(p)K_1 \int_0^\infty \|u^{II}\|_{H^1}^2 dt, \end{aligned}$$

where $u=u^I+u^{II}$ was used. Then, choosing ε small enough and repeating the argument for replacing ∞ by a finite time T, we have proved the following.

Lemma 2: Let u solve (4). If Assumptions 1, 2(a′), 2(c), 2(d), and 3(a) hold, and the dimension of space is $d\geqslant 3$, *then for* $p=1,2,\ldots,$

$$\int_0^T \|u^I\|_{H^p}^2 dt \leqslant 2C_0(p)\left[\|f\|_1^2+3K_F(T)+6\varepsilon^2 K_1\int_0^T \|u^{II}\|_{H^1}^2 dt\right], \tag{11}$$

where $C_0(p)$ *is the same constant of Lemma 1 and* ε *is assumed to be small enough so that* $6\varepsilon^2 C_0(p)K_1\leqslant \frac{1}{2}$.

B. Estimates for u^{II} (high frequencies)

Given $u\in L_2(\mathbf{R}^d,\mathbf{R}^n)$ [respectively $u\in H^p(\mathbf{R}^d,\mathbf{R}^n)$] and using the decomposition in low and high frequencies for u given by (3), the decomposition $L_2=L_2^I\oplus L_2^{II}$ (respectively $H^p=H^{pI}\oplus H^{pII}$) is defined so that $u^I\in L_2^I$ and $u^{II}\in L_2^{II}$.

It was shown in a previous work[2] that if the system (4) satisfies Assumption 3(b), then there exists a constant C_6 and a time independent pseudo-differential operator S, acting on $L_2^{II}(\mathbf{R}^d,\mathbf{R}^n)$ and depending on P_0+B_0 only, with the following properties.

(a) S is self-adjoint and bounded, i.e., $\|S\|_{L_2^{II}}\leqslant C_6$.

(b) $I+S$ is positive definite with $\|I+S\|_{L_2^{II}}+\|(I+S)^{-1}\|_{L_2^{II}}\leqslant C_6$.

(c) $2\,\mathrm{Re}(I+S)(P_0+B_0)\leqslant -\delta(I+S)$.

(d) S is a smoothing operator, i.e., its symbol satisfies $|\hat{S}(\omega)|=C_6/|\omega|$, for $|\omega|\geqslant\omega_0$.

The action of S is extended to L_2 by defining $S=I$ on L_2^I. It is clear from the properties above that there exists a constant C_7 such that the operator $H=I+S$ has the following properties.

(*i*) H is self-adjoint and bounded, i.e., $\|H\|\leqslant C_7$.
(*ii*) H is positive definite with $\|H\|+\|H^{-1}\|\leqslant C_7$.
(*iii*) $2\,\mathrm{Re}\,H(P_0+B_0)\leqslant -\delta H$ when restricted to L_2^{II}.
(*iv*) $|(u,H\partial_j v)-(u,\partial_j v)|\leqslant C_7\|u\|\,\|v\|$, for all $u\in L_2$, $v\in H^1$, and $j=1,2,\ldots,d$.

The last property follows from Parseval's relation and property (d) of S.

New inner products and norms in L_2 and H^p are defined using H:

$$(u,v)_H=(u,Hv),\quad (u,v)_{p,H}=\sum_{|\alpha|\leqslant p}(\partial_x^\alpha u,H\partial_x^\alpha v),$$

and

$$\|u\|_H=(u,u)_H^{1/2},\quad \|u\|_{p,H}=(u,u)_{p,H}^{1/2}.$$

Properties (*i*) and (*ii*) of H imply the equivalence

$$\frac{1}{C_7}\|u\|_{H^p}\leqslant\|u\|_{p,H}\leqslant C_7\|u\|_{H^p},\quad \text{for } p=0,1,2,\ldots. \tag{12}$$

The estimate for u^{II} will be obtained in the H-norm:

$$\begin{aligned}\frac{d}{dt}\|u^{II}\|_H^2 &= 2\,\mathrm{Re}(u^{II},u_t^{II})_H\\ &= 2\,\mathrm{Re}(u^{II},u_t)_H\\ &= 2\,\mathrm{Re}(u^{II},[P_0+B_0]u)_H+2\varepsilon\,\mathrm{Re}(u^{II},P_1u)_H\\ &\quad +2\varepsilon\,\mathrm{Re}(u^{II},B_1u)_H+2\,\mathrm{Re}(u^{II},F)_H.\end{aligned} \tag{13}$$

Let us estimate the four terms above separately. Using the property (iii) of H we obtain

$$\begin{aligned} 2\,\mathrm{Re}(u^{II},[P_0+B_0]u)_H &= 2\,\mathrm{Re}(u^{II},[P_0+B_0]u^{II})_H \\ &\leqslant (u^{II},2\,\mathrm{Re}H[P_0+B_0]u^{II}) \\ &\leqslant -\delta\|u^{II}\|_H^2. \end{aligned}$$

The second term in (13) can be separated as

$$2\varepsilon\,\mathrm{Re}(u^{II},P_1u)_H = 2\varepsilon\,\mathrm{Re}(u^{II},P_1u^I)_H + 2\varepsilon\,\mathrm{Re}(u^{II},P_1u^{II})_H.$$

However,

$$\begin{aligned} |2\,\mathrm{Re}(u^{II},P_1u^I)_H| &\leqslant 2\|u^{II}\|\,\|HP_1u^I\| \\ &\leqslant 2\,C_7\|u^{II}\|\left\|\sum_j A_{1j}\partial_j u^I\right\| \\ &\leqslant 2\,C_7\,|A_1|_\infty\omega_0\|u^I\|\,\|u^{II}\|, \end{aligned}$$

where $|A_1|_\infty=\Sigma_j|A_{1j}|_\infty$ and $\|\partial_j u^I\|\leqslant\omega_0\|u^I\|$. Also,

$$P_1u^{II}=\sum_j \partial_j(A_{1j}u^{II})-\left(\sum_j \partial_jA_{1j}\right)u^{II}.$$

Symmetry of A_{1j} and properties (i) and (iv) of H imply

$$\begin{aligned} |2\,\mathrm{Re}(u^{II},P_1u^{II})_H| &\leqslant |2\,\mathrm{Re}\sum_j (u^{II},\partial_j[A_{1j}u^{II}])_H| + \left|2\left(u^{II},\left[\sum_j \partial_jA_{1j}\right]u^{II}\right)_H\right| \\ &\leqslant \sum_j |2\,\mathrm{Re}(u^{II},\partial_j[A_{1j}u^{II}])| + 2\sum_j C_7\|u^{II}\|\|A_{1j}u^{II}\| \\ &\quad + 2\|u^{II}\|\left\|H\left(\sum_j \partial_jA_{1j}\right)u^{II}\right\| \\ &\leqslant \sum_j |(u^{II},[\partial_jA_{1j}]u^{II})| + 2C_7|A_1|_\infty\|u^{II}\|^2 \\ &\quad + 2C_7|DA_1|_\infty\|u^{II}\|^2 \\ &\leqslant 2[C_7|A_1|_\infty+(1+C_7)|DA_1|_\infty]\|u^{II}\|^2, \end{aligned}$$

where $|DA_1|_\infty=\Sigma_j|\partial_jA_{1j}|_\infty$. Therefore the estimate

$$\begin{aligned} |2\varepsilon\,\mathrm{Re}(u^{II},P_1u)_H| &\leqslant \{\rho+2|\varepsilon|[C_7|A_1|_\infty+(1+C_7)|DA_1|_\infty]\}\|u^{II}\|^2 \\ &\quad +(\varepsilon^2/\rho)C_7{}^2|A_1|_\infty^2\omega_0^2\|u^I\|^2 \end{aligned}$$

holds for any $\rho>0$. By property (i) of H

$$\begin{aligned} |2\varepsilon\,\mathrm{Re}(u^{II},B_1u)_H| &\leqslant 2|\varepsilon|C_7|B_1|_\infty\|u^{II}\|\,\|u^I\| \\ &\leqslant \rho\|u^{II}\|^2+(\varepsilon^2/\rho)C_7{}^2|B_1|_\infty^2\,\|u^I\|^2. \end{aligned}$$

Also,

$$|2\,\mathrm{Re}(u^{II},F)_H| \leqslant \rho\|u^{II}\|^2 + (C_7{}^2/\rho)\|F\|^2.$$

The last four estimates and the equivalence (12) for $p=0$ imply

$$\frac{d}{dt}\|u^{II}\|_H^2 = \{-\delta + 3\rho C_7{}^2 + 2|\varepsilon| C_7{}^2[C_7|A_1|_\infty + (1+C_7)|DA_1|_\infty]\}\,\|u^{II}\|_H^2$$

$$+\varepsilon^2\frac{C_7}{\rho}(\omega_0^2|A_1|_\infty^2 + |B_1|_\infty^2)\,\|u^I\|^2 + \frac{C_7{}^2}{\rho}\|F\|^2.$$

Thus, choosing $\rho = \delta(18C_7{}^2)^{-1}$ and calling

$$\varepsilon_1 = \delta\{12C_7{}^2[C_7|A_1|_\infty + (1+C_7)|DA_1|_\infty]\}^{-1}$$

we have proved the following.

Lemma 3: Let u be a solution of (4), and let Assumptions 1, 2(b), 2(c), and 3(b) hold. Then there exists ε_1 such that

$$\frac{d}{dt}\|u^{II}\|_H^2 = -\frac{2}{3}\,\delta\,\|u^{II}\|_H^2 + \varepsilon^2 C_{A,B}\|u^I\|^2 + C_0\|F\|^2, \quad \text{if } |\varepsilon| \leqslant \varepsilon_1. \tag{14}$$

Here $C_{A,B}$ depends on P_0+B_0, $|A_1|_\infty$ and $|B_1|_\infty$, and C_0 depends on P_0+B_0 only.

This result can be generalized to include derivatives. Applying ∂_x^α to (4), it becomes

$$\partial_t(\partial_x^\alpha u) = \sum_j\,(A_{0j}+\varepsilon A_{1j})\partial_j\partial_x^\alpha u + (B_0+\varepsilon B_1)\partial_x^\alpha u + \varepsilon R^\alpha + \partial_x^\alpha F,$$

$$\partial_x^\alpha u(x,0) = \partial_x^\alpha f, \tag{15}$$

where $R^\alpha = \Sigma_j[\partial_x^\alpha(A_{1j}\partial_j u) - A_{1j}\partial_j\partial_x^\alpha u] + \partial_x^\alpha(B_1 u) - B_1\partial_x^\alpha u$ is made of lower order terms only, i.e., derivatives of A_{1j}, B_1 and u up to order $|\alpha|$.

Lemma 4: Let u be a solution of (4), and let Assumptions 1, 2(a′), 2(b), 2(c), and 3(b) hold. Then, if $|\varepsilon| \leqslant \varepsilon_1(A,B,p)$, we get for $p=1,2,\ldots$

$$\frac{d}{dt}\|u^{II}\|_{p,H}^2 = -\frac{2}{3}\,\delta\,\|u^{II}\|_{p,H}^2 + \varepsilon^2 C_{A,B,p}\|u^I\|_{H^p}^2 + C_0\|F\|_{H^p}^2. \tag{16}$$

Here, $\varepsilon_1(A,B,p)$ and $C_{A,B,p}$ are constants that depend P_0+B_0 and the L_∞-norms of A_{1j} and B_1 and their derivatives up to order p, but are independent of F. C_0 depends on P_0+B_0 only.

Proof: For $|\alpha| \leqslant p$, Lemma 3 can be applied to the system (15), thinking of $\partial_x^\alpha F + \varepsilon R^\alpha$ as the source term. This gives

$$\frac{d}{dt}\|\partial_x^\alpha u^{II}\|_H^2 = -\frac{2}{3}\,\delta\|\partial_x^\alpha u^{II}\|_H^2 + \varepsilon^2 C_{A,B}\|\partial_x^\alpha u^I\|^2 + 2\varepsilon^2 C_0\|R^\alpha\|^2 + 2C_0\|\partial_x^\alpha F\|^2.$$

All terms in R^α are proportional to a derivative of u of order less than or equal to $|\alpha|$. Addition of all the inequalities with $|\alpha| \leqslant p$ gives

$$\frac{d}{dt}\|u^{II}\|_{p,H}^2 = -\frac{2}{3}\,\delta\|u^{II}\|_{p,H}^2 + \varepsilon^2 C_{A,B}\|u^I\|^2 + 2\varepsilon^2 C_0\tilde{C}_{A,B,p}\|u^I + u^{II}\|_{H^p}^2 + 2C_0\|F\|_{H^p}^2.$$

Here $\tilde{C}_{A,B,p}$ depends on the L_∞-norms of A_{1j} and B_1 and their derivatives up to order p. Using the equivalence (12) and defining an appropriate $\varepsilon_1=\varepsilon_1(\tilde{C}_{A,B,p})$ the lemma follows.

C. Linear stability

Global existence for the linear problem shown in this section is well known. As a simple application of the estimates for the low and high frequency parts of the solution obtained earlier, linear stability is shown here. The fundamental estimates, Lemmas 1 and 3, will be the base for the nonlinear stability, too.

Theorem 2: *Assume that u solves the linear system (4), Assumptions 1, 2(a′), 2(b), 2(c), 2(d), and 3 hold, and the dimension of space is* $d\geqslant 3$. *Then, for any* $p=1,2,3,\ldots$ *there are positive constants* $C_0(p)$ *and* $\varepsilon_0(A,B,p)$ *such that*

$$\int_0^\infty (\|u\|^2_{H^{p+1}}+\|\partial_t u\|^2_{H^p})dt\leqslant C_0(p)\left[\|f\|_1^2+\|f\|^2_{H^{p+1}}+K_F(\infty)+\int_0^\infty \|F\|^2_{H^{p+1}}dt\right], \tag{17}$$

provided that $|\varepsilon|\leqslant\varepsilon_0(A,B,p)$. $C_0(p)$ *depends only on* P_0+B_0 *and* p, *while* $\varepsilon_0(A,B,p)$ *depends also on the constants* K_1 *of Assumption 2(a′) and* $K(0,0)$, $K(0,1),\ldots,K(0,p+1)$ *of Assumption 2(b). Furthermore,*

$$\lim_{t\to\infty}|u(\cdot,t)|_\infty=0.$$

Proof: Denote

$$y_1(t)=\|u^I(\cdot,t)\|^2_{H^p},\quad y_2(t)=\|u^{II}(\cdot,t)\|^2_{p,H}.$$

The results of Lemmas 2 and 4 can be written as

$$\int_0^\infty y_1 dt\leqslant C_8(p)\left[\|f\|_1^2+K_F(\infty)+\varepsilon^2 C_0(p)K_1\int_0^\infty \|u^{II}\|^2_{H^1}dt\right] \tag{18}$$

and

$$\frac{dy_2}{dt}\leqslant -\frac{2}{3}\delta y_2+\varepsilon^2\tilde{C}_{A,B,p}y_1+C_0\|F\|^2_{H^p}.$$

This last estimate is equivalent to

$$y_2(t)\leqslant y_2(0)e^{-(2/3)\,\delta t}+C_0\int_0^t e^{-(2/3)\,\delta(t-\tau)}\|F(\cdot,\tau)\|^2_{H^p}d\tau$$

$$+\varepsilon^2\tilde{C}_{A,B,p}\int_0^t e^{-(2/3)\,\delta(t-\tau)}y_1(\tau)d\tau. \tag{19}$$

Notice that

$$\int_0^\infty\int_0^t e^{-a(t-\tau)}f(\tau)d\tau dt=\int_0^\infty\int_\tau^\infty e^{-a(t-\tau)}f(\tau)dtd\tau=\frac{1}{a}\int_0^\infty f(\tau)d\tau.$$

Using this identity, the estimate (19) implies

$$\int_0^\infty y_2(t)dt\leqslant\frac{3}{2\delta}y_2(0)+\frac{3C_0}{2\delta}\int_0^\infty\|F(\cdot,\tau)\|^2_{H^p}dt+\varepsilon^2\frac{3\tilde{C}_{A,B,p}}{2\delta}\int_0^\infty y_1(\tau)d\tau. \tag{20}$$

The equivalence of norms, Eq. (12), implies

$$\int_0^\infty \|u\|_{H^p}^2 dt \leqslant 2\int_0^\infty y_1 dt + 2C_7 \int_0^\infty y_2 dt.$$

Thus (18) and (20) imply, for $|\varepsilon| \leqslant \tilde{\varepsilon}_0$,

$$\int_0^\infty \|u\|_{H^p}^2 dt \leqslant C_9(p)\left[\|f\|_1^2 + \|f\|_{H^p}^2 + K_F(\infty) + \int_0^\infty \|F\|_{H^p}^2 dt\right]. \tag{21}$$

Here $\tilde{\varepsilon}_0 = \tilde{\varepsilon}_0(\tilde{C}_{A,B,p}, K_1)$. To estimate $\partial_t u$ and its space derivatives we apply ∂_x^α to Eq. (4) and take the norm. Adding all the estimates for $|\alpha| \leqslant p$ we obtain

$$\|\partial_t u\|_{H^p}^2 \leqslant C_{10}(p)\|u\|_{H^{p+1}}^2 + \varepsilon^2 \tilde{C}_{A,B,p}\|u\|_{H^{p+1}}^2 + C(p)\|F\|_{H^p}^2.$$

Finally, integrating this last estimate and using (21) for $p+1$ we get the desired estimate (17), with ε_0 conveniently defined. The stability follows from the convergence of the integral in (17). More precisely,

$$|u(\cdot,T)|_\infty^2 \leqslant C\int_T^\infty (\|u\|_{H^{p+1}}^2 + \|\partial_t u\|_{H^p}^2) dt \to 0, \text{ when } T \to \infty,$$

for $p > d/2$.

III. NONLINEAR STABILITY

A proof of Theorem 1 is given in this section. The construction of the estimates for the nonlinear solution is based on the estimates of Lemmas 1 and 3 and Sobolev's inequalities.

Proof of Theorem 1: Local (in time) existence is well known for quasi-linear symmetric hyperbolic systems; let u denote such a solution to the problem (1) for a given initial data function f and source F. It will be shown that, for ε small enough, the ''energy''

$$\|f\|_{H^{p+1}}^2 + \int_0^{t_1} (\|u\|_{H^{p+1}}^2 + \|\partial_t u\|_{H^p}^2) dt, \quad p = d+3,$$

remains bounded by a constant M sufficiently large, even when $t_1 \to \infty$; thus the solution exists globally. Suppose this is not the case. Then there exists a time $T(M,\varepsilon)$ such that

$$\|f\|_{H^{p+1}}^2 + \int_0^T (\|u\|_{H^{p+1}}^2 + \|\partial_t u\|_{H^p}^2) dt = M. \tag{22}$$

In what follows C_M^l, $l = 1,2,\ldots$, will denote constants that may depend on M, $P_0 + B_0$, and the constants in Assumption 2, but not on ε or T.

Recall that, for all $f(t) \in H^1([0,T], \mathbf{R})$,

$$\max_{0 \leqslant t \leqslant T} |f(t)|^2 \leqslant \min_{0 \leqslant t \leqslant T} |f(t)|^2 + \int_0^T [|f(t)|^2 + |f'(t)|^2] dt.$$

Sobolev's Lemma and (22) imply, for $|\alpha| + (d/2) < p$,

$$|\partial_x^\alpha u|_{\infty,T}^2 = \sup_{0 \leqslant t \leqslant T} |\partial_x^\alpha u(\cdot,t)|_\infty^2 \leqslant C\left[\|f\|_{H^p}^2 + \int_0^T (\|u\|_{H^p}^2 + \|\partial_t u\|_{H^p}^2) dt\right] \leqslant CM, \tag{23}$$

where C is a constant independent of ε, T, and M.

To apply the estimates obtained for the linear case we rewrite (1) as

$$\begin{aligned} \partial_t u &= (P_0+B_0)u+\varepsilon\sum_{j=1}^{d} A'_{1j}(x,t,\varepsilon)\partial_j u+B'_1(x,t,\varepsilon)u+F(x,t), \\ u(x,0) &= f(x), \end{aligned} \tag{24}$$

with

$$A'_{1j}(x,t,\varepsilon)=A_{1j}(x,t,u(x,t),\varepsilon)$$

and

$$B'_1(x,t,\varepsilon)=B_1(x,t,u(x,t),\varepsilon).$$

Application of Lemma 1, with F replaced by $G=F+\varepsilon\Sigma_{j=1}^{d}A'_{1j}\partial_j u+\varepsilon B'_1 u$, gives

$$\int_0^T \|u^I(\cdot,t)\|^2_{H^{p+1}}dt\leqslant C_{11}(p)[\|f\|_1^2+K_G(T)].$$

Notice that, using (23) and Assumption 2(a),

$$\begin{aligned} K_G(T) &= 3\Bigg\{K_F(T)+\varepsilon^2 k^2_{A,CM}\Bigg(\sum_{j=1}^{d}\int_0^T\int_{\mathbf{R}^d}|u|\,|\partial_j u|dxdt\Bigg)^2 \\ &\quad +\varepsilon^2 k^2_{B,CM}\Bigg(\sum_{j=1}^{d}\int_0^T\int_{\mathbf{R}^d}|u|^2dxdt\Bigg)^2\Bigg\} \\ &\leqslant 3K_F(T)+\varepsilon^2 C_M^1. \end{aligned}$$

Thus,

$$\int_0^T \|u^I(\cdot,t)\|^2_{H^{p+1}}dt\leqslant C_{11}(p)[\|f\|_1^2+3K_F(T)+\varepsilon^2 C_M^1]. \tag{25}$$

The estimate of u^{II} is constructed in the H-norm. Lemma 3 applied to (24) gives

$$\frac{d}{dt}\|u^{II}\|_H^2\leqslant -\frac{2}{3}\,\delta\|u^{II}\|_H^2+\varepsilon^2 C_M^3\|u^I\|^2+C_{12}\|F\|^2. \tag{26}$$

To estimate the derivatives of u^{II} we first apply ∂_x^α, $1\leqslant|\alpha|\leqslant p+1$, to (24),

$$\partial_t\partial_x^\alpha u=(P_0+B_0)\partial_x^\alpha u+\varepsilon\sum_{j=1}^{d}A'_{1j}\partial_j\partial_x^\alpha u+\varepsilon\,\partial_x^\alpha(B'_1u)+\partial_x^\alpha F+\varepsilon R^\alpha, \tag{27}$$

with

$$R^\alpha=\sum_{j=1}^{d}R_j^\alpha=\sum_{j=1}^{d}[\partial_x^\alpha(A'_{1j}\partial_j u)-A'_{1j}\partial_j\partial_x^\alpha u].$$

The chain rule implies that each R_j^α is a sum of terms of the form

$$r_j(x,t,\alpha,\sigma)\partial_x^{\sigma_1}u\cdots\partial_x^{\sigma_r}u, \tag{28}$$

where, for all $|\alpha|\leqslant p+1$,

$$|\sigma_1|+\cdots+|\sigma_r|\leqslant p+2,\ |\sigma_l|\leqslant p+1,\ l=1,\ldots,r,$$

and $r_j(x,t,\alpha,\sigma)$ are partial derivatives $\partial_x^\beta\partial_u^\gamma A_{1j}$, $|\beta|+|\gamma|\leqslant p+1$. On the one hand, all factors $\partial_x^{\sigma_l}u$ in (28), with the exception of at most one of them, can be bounded in the infinite norm, otherwise there would be two factors with

$$|\sigma_l|+\frac{d}{2}\geqslant p,\ |\sigma_m|+\frac{d}{2}\geqslant p,$$

and, consequently,

$$p+2+d\geqslant|\sigma_l|+|\sigma_m|+d\geqslant 2p,$$

which would contradict the choice $p=d+3$. On the other hand, the factors $r_j(x,t,\alpha,\sigma)$ can be bounded in terms of the constants $K(CM,0),K(CM,1),\ldots,K(CM,p+1)$ of Assumption 2(b). Therefore,

$$\|R^\alpha\|^2\leqslant C_M^4\|u\|^2_{H^{|\alpha|}}.$$

Similarly,

$$\|\partial_x^\alpha(B_1'u)\|\leqslant C_M^5\|u\|^2_{H^{|\alpha|}}.$$

Lemma 3 applied to (27), with F replaced by $\partial_x^\alpha F+\varepsilon R^\alpha+\partial_x^\alpha(B_1'u)$, gives

$$\frac{d}{dt}\|\partial_x^\alpha u^{II}\|_H^2\leqslant-\frac{2}{3}\,\delta\|\partial_x^\alpha u^{II}\|_H^2+\varepsilon^2C_M^6\|\partial_x^\alpha u^I\|^2+C_{13}\|\partial_x^\alpha F+\varepsilon R^\alpha+\varepsilon\partial_x^\alpha(B_1'u)\|^2.$$

So, adding these estimates for $1\leqslant|\alpha|\leqslant p+1$ to (26), and using the bounds for R^α and $\partial_x^\alpha(B_1'u)$ and the equivalence (12) we obtain

$$\frac{d}{dt}\|u^{II}\|^2_{p+1,H}\leqslant-\frac{1}{3}\,\delta\|\partial_x^\alpha u^{II}\|_H^2+\varepsilon^2C_M^7\|u^I\|^2_{H^{p+1}}+C_{14}\|F\|^2_{H^{p+1}}.$$

Integration like in the proof of Theorem 2, plus the equivalence (12), gives

$$\int_0^T\|u^{II}\|^2_{p+1,H}dt\leqslant C_{15}\left(\|f\|_1^2+\|f\|^2_{H^{p+1}}+\int_0^T\|F\|^2_{H^{p+1}}dt\right)+\varepsilon^2C_M^8.$$

Equivalence (12) together with (25) give

$$\int_0^T\|u\|^2_{H^{p+1}}dt\leqslant C_{16}(p)\left[\|f\|_1^2+\|f\|^2_{H^{p+1}}+K_F(T)+\int_0^T\|F\|^2_{H^{p+1}}dt\right]+\varepsilon^2C_M^9 \tag{29}$$

if $|\varepsilon|\leqslant\varepsilon_2(M)$.

The differential equation (1) will be used now to estimate $\partial_t u$ in the H^p-norm. Notice that

$$\|\partial_x^\alpha\partial_t u\|^2\leqslant 3\|(P_0+B_0)\partial_x^\alpha u\|^2+3\varepsilon^2\|\partial_x^\alpha[(P_1+B_1)u]\|^2+3\|\partial_x^\alpha F\|^2.$$

The highest derivative of u in each of the first two terms is of order $|\alpha|+1$. The second term can be treated as we did before with R^α. The addition of the resulting estimates for $0\leqslant|\alpha|\leqslant p$ gives

$$\|\partial_t u\|^2_{H^p}\leqslant C_{17}(p)\|u\|^2_{H^{p+1}}+3\|F\|^2_{H^p}+\varepsilon^2C_M^{10}\|u\|^2_{H^{p+1}},$$

and, using (29),

$$\|f\|^2_{H^{p+1}}+\int_0^T(\|u\|^2_{H^{p+1}}+\|\partial_t u\|^2_{H^p})dt\leqslant C_{18}(p)\left[\|f\|^2_1+\|f\|^2_{H^{p+1}}+K_F(\infty)+\int_0^\infty\|F\|^2_{H^{p+1}}dt\right]+\varepsilon^2 C_M^{11}.$$

Therefore, choosing

$$M=1+C_{18}(p)\left[\|f\|^2_1+\|f\|^2_{H^{p+1}}+K_F(\infty)+\int_0^\infty\|F\|^2_{H^{p+1}}\,dt\right],$$

and if $|\varepsilon|\leqslant\varepsilon_0(M)$ with $\varepsilon_0(M)$ conveniently defined, we arrive at a contradiction and the time T cannot exist. Then the solution exists globally in time and standard arguments show that it is C^∞. Stability is shown as in the proof of Theorem 2.

IV. STABILITY OF RELATIVISTIC DISSIPATIVE FLUIDS

As an application of the stability theorem given in the Introduction, stability of the standard theories of dissipative relativistic fluids[3,6,7] is shown in this section. Stability for these theories has already been shown,[4] but only on compact domains with periodic boundary conditions.

The dynamical equations in these theories constitute a symmetric hyperbolic system of equations with zeroth-order dissipation. The Cauchy problem will be considered on the Minkowski space–time—$\mathbf{R}^4$ with a flat Lorentzian metric, and the stability shown for constant equilibrium solutions.

Calling $v(x,t)$ the vector of dynamical fields in the theory ($v:\mathbf{R}^3\times\mathbf{R}\to\mathbf{R}^n$) the system of equations, when written on Cartesian coordinates $\{x_i,t\}$, $i=1,2,3$, takes the form[4]

$$\begin{aligned}N(v)\partial_t v&=\sum_{j=1}^3 A_j(v)\partial_j v+B(v)v,\\ v(x,0)&=g(x).\end{aligned}\tag{30}$$

Here N is a symmetric, positive definite matrix, the matrices A_j are symmetric, and B is symmetric and negative semi-definite (at least when evaluated at constant equilibrium).

If v_0 is a constant solution of (30), the smallness parameter ε is introduced so that

$$g(x)=v_0+\varepsilon f(x)\quad\text{and}\qquad v(x,t)=v_0+\varepsilon\,u(x,t).$$

Thus, the coefficient matrices in (30) can be written as

$$A_j(v)=A_{0j}+\varepsilon A_{1j}(u,\varepsilon),\quad A_{0j}=A_j(v_0),$$

$$B(v)=B_0+\varepsilon B_1(u,\varepsilon),\quad B_0=B(v_0).$$

All the coefficients are assumed to be C^∞ functions of v, therefore it is clear that all the matrices A_{1j} and B_1 vanish at least linearly with u. The matrix B_0 is the one introducing dissipation into the system, and it is a physical requirement that this matrix is negative semi-definite. The Cauchy problem for the variable u is like the problem (1) with vanishing source function. The presence of the matrix $N(u)$ in front of the time derivative does not change the character of the problem, and though, for simplicity, the stability was proved for the case $N=I$, the estimates can be built also with a general N and the stability result holds.

The regularity assumptions on the coefficients and initial data, Assumptions 1 and 2, are physically reasonable and will be assumed to be satisfied. The requirement that the initial data are

functions on L_2 implies that the only equilibrium solution to be considered is $v_0=0$. This is, in turn, the only physically relevant equilibrium solution when the Cauchy problem is considered in the whole space, in the sense that it is the only constant solution with finite total energy.

The only critical condition that needs verification so that the stability theorem can be applied is Assumption 3. This is an assumption on the eigenvalues λ of the symbol of the constant coefficient system. This system can be written as

$$N_0\partial_t u=\sum_{j=0}^{3} A_{0j}\partial_j u+B_0 u.$$

The Fourier transformed system is

$$N_0\partial_t \hat{u}(\omega,t)=[\hat{P}_0(i\omega)+B_0]\hat{u}(\omega,t).$$

The eigenvalue problem for the symbol, in the presence of N_0, is

$$[\hat{P}_0(i\omega)+B_0]a(\omega)=\lambda(\omega)N_0 a(\omega). \tag{31}$$

Here $a(\omega)$ is an eigenvector, normalized so that $\langle a(\omega),N_0 a(\omega)\rangle=1$, with eigenvalue $\lambda(\omega)$.

In the previous work,[4] the first part of Assumption 3 was proved to follow from a condition previously required in the literature to characterize equilibrium states. This condition can be written as the injectivity of a linear map, and the result in Ref. 4 can be written as follows.[8]

Lemma 5: If for all complex numbers z and unit frequency vectors $\hat{\omega}$, the linear map

$$zN_0+\hat{P}(i\hat{\omega}):\ker(B_0)\to\mathbf{C}^n \tag{32}$$

is injective, then for all $\omega_0>0$ there exists $\delta>0$ such that $\mathrm{Re}\{\lambda(\omega)\}\leqslant-\delta$, *for all* $|\omega|\geqslant\omega_0$.

It will be shown in this section that the second part of Assumption 3 also follows from the injectivity condition of Lemma 5.

To simplify notation the work will be carried out in a basis of $\mathbf{C}^n$ where N_0 becomes the identity and B_0 becomes block diagonal. To see that such a basis exists notice that, as N_0 is symmetric and positive definite, there exists a constant, nonsingular matrix R_0 such that $N_0=R_0^{\dagger}R_0$. On the one hand, the eigenvalue problem (31) is equivalent to

$$(R_0^{-1})^{\dagger}[\hat{P}_0(i\omega)+B_0]R_0^{-1}b(\omega)=\lambda(\omega)b(\omega),$$

with $b(\omega)=R_0 a(\omega)$ denoting the eigenvector, which satisfies $\langle b(\omega),b(\omega)\rangle=1$. On the other hand, the injectivity condition of Lemma 5 is equivalent to the following: The map

$$zI+\tilde{P}_0(i\hat{\omega}):\ker(\tilde{B}_0)\to\mathbf{C}^n$$

is injective for all $z\in\mathbf{C}$ and unit $\hat{\omega}$; where $\tilde{P}_0(i\hat{\omega})=(R_0^{-1})^{\dagger}\hat{P}_0(i\hat{\omega})R_0^{-1}$, and $\tilde{B}_0=(R_0^{-1})^{\dagger}B_0R_0^{-1}$. One further change of basis, with a unitary matrix U_0, takes $\tilde{B}_0$ to block diagonal form

$$B=U_0^{\dagger}\tilde{B}_0U_0=\begin{pmatrix}B_{11} & 0\\ 0 & 0\end{pmatrix}, \tag{33}$$

where B_{11} is symmetric and negative definite. The eigenvalue problem becomes

$$[iA(\hat{\omega})+B]c(\omega)=\lambda(\omega)c(\omega), \tag{34}$$

where $A(\hat{\omega})$ is a self-adjoint matrix given by

$$A(\hat{\omega}) = -iU_0^{\dagger}(R_0^{-1})^{\dagger}\hat{P}_0(i\hat{\omega})R_0^{-1}U_0 = U_0^{\dagger}(R_0^{-1})^{\dagger}\left(\sum_{j=1}^{d}\hat{\omega}_j A_{0j}\right)R_0^{-1}U_0,$$

$c(\omega) = U_0 R_0 a(\omega)$, and B is given by (33). The injectivity condition now reads as follows.

Assumption 4: For all complex numbers z and unit frequency vectors $\hat{\omega}$, the linear map

$$zI + iA(\hat{\omega}):\ker(B) \to \mathbf{C}^n$$

is injective.

Using the block structure of B to block also $A(\hat{\omega})$ and the eigenvector, the eigenvalue problem can be written as

$$\begin{pmatrix} i|\omega|A_{11}(\hat{\omega}) + B_{11} & i|\omega|A_{12}(\hat{\omega}) \\ i|\omega|A_{12}^{\dagger}(\hat{\omega}) & i|\omega|A_{22}(\hat{\omega}) \end{pmatrix}\begin{pmatrix} u(\omega) \\ v(\omega) \end{pmatrix} = \lambda(\omega)\begin{pmatrix} u(\omega) \\ v(\omega) \end{pmatrix}. \tag{35}$$

The eigenvalues $\lambda(\omega)$ are continuous functions of ω and therefore they separate into two disjoint sets when $|\omega|$ is small; the set of eigenvalues that approach the eigenvalues of B_{11}, and the set of those that approach zero. Moreover, there exists $\omega_1 > 0$ such that, for $|\omega| \leqslant \omega_1$, the whole symbol can be transformed to block diagonal form by a smooth transformation (to simplify notation the dependence on $\hat{\omega}$ will be omitted in what follows):

$$S^{-1}\begin{pmatrix} i|\omega|A_{11} + B_{11} & i|\omega|A_{12} \\ i|\omega|A_{12}^{\dagger} & i|\omega|A_{22} \end{pmatrix}S = \begin{pmatrix} P_{11} & 0 \\ 0 & P_{22} \end{pmatrix}, \tag{36}$$

where

$$P_{11} = B_{11} + i|\omega|A_{11} - |\omega|^2 A_{12}A_{12}^{\dagger}B_{11}^{-1} + \mathcal{O}(|\omega|^3),$$

$$P_{22} = i|\omega|A_{22} + |\omega|^2 A_{12}^{\dagger}B_{11}^{-1}A_{12} + \mathcal{O}(|\omega|^3),$$

and where the transformation

$$S = \begin{pmatrix} I & S_{12} \\ S_{21} & S_{22} \end{pmatrix},$$

with

$$S_{12} = -i|\omega|B_{11}^{-1}A_{12} + \mathcal{O}(|\omega|^2),$$

$$S_{21} = i|\omega|A_{12}^{\dagger}B_{11}^{-1} + \mathcal{O}(|\omega|^2),$$

$$S_{22} = I + \mathcal{O}(|\omega|^2),$$

is a smooth function of ω for $|\omega| \leqslant \omega_1$.

The eigenvalues of (36) are the same ones of (35). The eigenvalues of P_{11} are the ones close to those of B_{11}. For these eigenvalues there exist $\delta > 0$ and $\omega_2 > 0$ ($\omega_2 \leqslant \omega_1$) such that $\mathrm{Re}\,\lambda \leqslant -\delta < 0$ for $|\omega| \leqslant \omega_2$. Assumption 3 is certainly true for these eigenvalues.

In what follows the eigenvalues $\lambda(\omega)$ of P_{22}, which are the ones approaching zero, and their eigenvectors will be studied.

Lemma 6: There exists $\omega_3 > 0$ such that the functions $\lambda(\omega)/|\omega|$ are continuous functions of $(|\omega|, \hat{\omega})$ for $|\omega| \leqslant \omega_3$.

Proof: Consider the matrix $P_{22}(\omega)/|\omega|$:

$$\frac{P_{22}(\omega)}{|\omega|} = iA_{22}(\hat{\omega}) + |\omega| M_{22}(|\omega|, \hat{\omega}). \tag{37}$$

Here A_{22} is a smooth function of $\hat{\omega}$, and M_{22} is a smooth function of $(|\omega|, \hat{\omega})$ for $|\omega| > 0$ that stays bounded when $|\omega| \to 0$. As

$$\| |\omega| M_{22}(|\omega|, \hat{\omega}) | \to 0 \quad \text{when} \quad |\omega| \to 0,$$

perturbation theory says that each eigenvalue of (37) is of the form

$$\frac{\lambda(\omega)}{|\omega|} = i\alpha(\hat{\omega}) + \gamma(|\omega|, \hat{\omega}). \tag{38}$$

Here $\alpha(\hat{\omega})$, an eigenvalue of $A_{22}(\hat{\omega})$, is a continuous function of $\hat{\omega}$, and γ is a continuous function of its arguments that vanishes at least as a rational power of $|\omega|$ when $|\omega| \to 0$. This proves the lemma.

An important property of the eigenvectors in (35) is proved next.

Lemma 7: Assumption 4 implies that there exist $c > 0$ *and* $\omega_0 > 0$ *such that, for all* $|\omega| \leqslant \omega_0$, $|u(\omega)| \geqslant c|\omega|$.

Proof: If $|\lambda|$ does not vanish when $|\omega| \to 0$, the lemma is clearly true since $\mathrm{Re}\,\lambda = \langle u, B_{11} u \rangle$. Consider the case $|\lambda| \to 0$ when $|\omega| \to 0$ (eigenvalues of P_{22}).

The equation (35) can be written as

$$\left(\frac{\lambda}{|\omega|} I - iA - \frac{1}{|\omega|} B \right) \begin{pmatrix} u \\ 0 \end{pmatrix} = \left(-\frac{\lambda}{|\omega|} I + i\hat{A} \right) \begin{pmatrix} 0 \\ v \end{pmatrix}. \tag{39}$$

Let us define

$$F(|\omega|, \hat{\omega}, y) = (zI + iA) \begin{pmatrix} 0 \\ y \end{pmatrix}, \quad \text{with} \quad z = -\frac{\lambda(\omega)}{|\omega|}, \quad \text{and} \quad |y| = 1.$$

The injectivity assumption (Assumption 4) implies that $|F|$ is a strictly positive function, and Lemma 6 implies that, for $|\omega| \leqslant \omega_3$, the function $|F|$ is continuous on all its arguments. Therefore, as $(|\omega|, \hat{\omega}, y)$ moves on a compact set, there exist $\tilde{c} > 0$ such that $|F(|\omega|, \hat{\omega}, y)| \geqslant \tilde{c}$. As $|u|$ goes to zero when $|\omega|$ goes to zero (otherwise $|\mathrm{Re}\,\lambda|$ would not go zero), $|v|$ stays close to one and we can divide (39) by $|v|$ to obtain

$$\left| \left(\frac{\lambda}{|\omega|} I - iA - \frac{1}{|\omega|} B \right) \frac{1}{|v|} \begin{pmatrix} u \\ 0 \end{pmatrix} \right| = |F(|\omega|, \hat{\omega}, v/|v|)| \geqslant \tilde{c},$$

and consequently

$$\left| (\lambda I - i|\omega| A - B) \begin{pmatrix} u \\ 0 \end{pmatrix} \right| \geqslant \tilde{c} |\omega| |v|. \tag{40}$$

Now assume the lemma is false. Thus for all $c > 0$ and $\omega_0 > 0$, there exists ω, with $|\omega| < \omega_0$, such that $|u(\omega)| < c|\omega|$. Then, it follows from (40) that

$$|B_{11}||u(\omega)| \geqslant \tilde{c}|\omega| \sqrt{1 - |u(\omega)|^2} - |\lambda(\omega)||u(\omega)| - |\omega||A||u(\omega)|,$$

$$> (\tilde{c}\sqrt{1 - c^2|\omega|^2} - c|\lambda(\omega)| - c|A||\omega|)|\omega|,$$

which, as $|\lambda(\omega)| \to 0$ when $|\omega| \to 0$, gives a contradiction for $c = \tilde{c}/2|B_{11}|$ and $\omega_0 \leqslant \omega_3$ small enough so that

$$\tilde{c}\sqrt{1-c^2|\omega|^2}-c|\lambda(\omega)|-c|A||\omega|>\frac{\tilde{c}}{2}.$$

This concludes the proof.

Corollary 1: For $|\omega|\leqslant\omega_0$, *the eigenvalues of* P_{22} *satisfy* $\mathrm{Re}\,\lambda\leqslant-\mu|\omega|^2$ *with* $\mu>0$.

Proof: Left multiply (35) by the eigenvector and take the real part to obtain

$$\mathrm{Re}\,\lambda(\omega)=\langle u,B_{11}u\rangle\leqslant-\beta|u(\omega)|^2\leqslant-\beta c^2|\omega|^2,$$

where $\beta>0$ exists because B_{11} is negative definite and Lemma 7 was used. Corollary 1 holds with $\mu=\beta c^2$.

We can summarize the results of Lemma 5 and Corollary 1 in the following.

Theorem 3: *If Assumption 4 holds, there are positive constants* ω_0, δ, *and* μ *such that all eigenvalues* $\lambda(\omega)$ *of the symbol satisfy*

$$\mathrm{Re}\,\lambda(\omega)\leqslant\begin{cases}-\mu|\omega|^2, & \text{or } -\delta, \quad \text{if } |\omega|\leqslant\omega_0,\\ -\delta, & \text{if } |\omega|\geqslant\omega_0.\end{cases}$$

This says that the physically based Assumption 4 implies that Assumption 3 holds for the general dissipative relativistic fluids. Therefore Theorem 1 applies and the constant solutions of these theories are stable.

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Painlevé–Calogero correspondence revisited

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We extend the work of Fuchs, Painlevé and Manin on a Calogero-like expression of the sixth Painlevé equation (the ''Painlevé–Calogero correspondence'') to the other five Painlevé equations. The Calogero side of the sixth Painlevé equation is known to be a nonautonomous version of the (rank one) elliptic model of Inozemtsev's extended Calogero systems. The fifth and fourth Painlevé equations correspond to the hyperbolic and rational models in Inozemtsev's classification. Those corresponding to the third, second and first are not included therein. We further extend the correspondence to the higher rank models, and obtain a ''multi-component'' version of the Painlevé equations. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The so called Painlevé equations are the following six equations discovered by Painlevé[1] and Gambier:[2]

$$(\mathrm{P_{VI}}) \quad \frac{d^2\lambda}{dt^2} = \frac{1}{2}\left(\frac{1}{\lambda}+\frac{1}{\lambda-1}+\frac{1}{\lambda-t}\right)\left(\frac{d\lambda}{dt}\right)^2 - \left(\frac{1}{t}+\frac{1}{t-1}+\frac{1}{\lambda-t}\right)\frac{d\lambda}{dt} + \frac{\lambda(\lambda-1)(\lambda-t)}{t^2(t-1)^2}\left(\alpha+\frac{\beta t}{\lambda^2}+\frac{\gamma(t-1)}{(\lambda-1)^2}+\frac{\delta t(t-1)}{(\lambda-t)^2}\right),$$

$$(\mathrm{P_V}) \quad \frac{d^2\lambda}{dt^2} = \left(\frac{1}{2\lambda}+\frac{1}{\lambda-1}\right)\left(\frac{d\lambda}{dt}\right)^2 - \frac{1}{t}\frac{d\lambda}{dt} + \frac{\lambda(\lambda-1)^2}{t^2}\left(\alpha+\frac{\beta}{\lambda^2}+\frac{\gamma t}{(\lambda-1)^2}+\frac{\delta t^2(\lambda+1)}{(\lambda-1)^3}\right),$$

$$(\mathrm{P_{IV}}) \quad \frac{d^2\lambda}{dt^2} = \frac{1}{2\lambda}\left(\frac{d\lambda}{dt}\right)^2 + \frac{3}{2}\lambda^3 + 4t\lambda^2 + 2(t^2-\alpha)\lambda + \frac{\beta}{\lambda},$$

$$(\mathrm{P_{III}}) \quad \frac{d^2\lambda}{dt^2} = \frac{1}{\lambda}\left(\frac{d\lambda}{dt}\right)^2 - \frac{1}{t}\frac{d\lambda}{dt} + \frac{\lambda^2}{4t^2}\left(\alpha+\frac{\beta t}{\lambda^2}+\gamma\lambda+\frac{\delta t^2}{4\lambda^3}\right),$$

$$(\mathrm{P_{II}}) \quad \frac{d^2\lambda}{dt^2} = 2\lambda^3 + t\lambda + \alpha,$$

$$(\mathrm{P_I}) \quad \frac{d^2\lambda}{dt^2} = 6\lambda^2 + t.$$

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The third equation P_{III} is slightly modified; the original equation can be reproduced by the simple change of variables $(t,\lambda)\to(t^2,t\lambda)$. It is well known that these equations are characterized by the absence of ''movable singularities'' other than poles.

Fuchs[3] proposed two more approaches to the sixth equation P_{VI}. One approach is the concept of isomonodromic deformations. In this approach, P_{VI} is interpreted as a differential equation describing isomonodromic deformations of a linear ordinary differential equation on the Riemann sphere. This is the origin of many subsequent researches. Another approach relates P_{VI} to an incomplete elliptic integral. Painlevé[4] took the second approach, and derived a new expression of P_{VI} in term of the Weierstrass $\wp$-function. This work of Painlevé is briefly reviewed in Okamoto's work on affine Weyl group symmetries of P_{VI}.[5]

Manin[6] revived the almost forgotten work of Fuchs and Painlevé after nearly ninety years. Manin's remarkable idea is to use the elliptic modulus τ, rather than t, as an independent variable. The outcome is a Hamiltonian system with a Hamiltonian of the normal form $\mathcal{H}=p^2/2+V(q)$, where the potential is a linear combination of the Weierstrass $\wp$-function and its shift by three half periods. This is a nonautonomous system, because the Hamiltonian depends on the ''time'' τ through the τ-dependence of the $\wp$-function.

Levin and Olshanetsky[7] pointed out that Manin's equation resembles the so called Calogero–Moser systems, i.e., the various extensions[8] of the integrable many-body systems first discovered by Calogero.[9] More precisely, the Hamiltonian $\mathcal{H}$ is identical to a special case (the rank-one elliptic model) of Inozemtsev's extensions[10,11] of the Calogero–Moser systems. Levin and Olshanetsky called this relation the ''Painlevé–Calogero correspondence.''

One will naturally ask if this correspondence can be extended to the other Painlevé equations. Manin himself raised this problem in his paper. Olshanetsky[12] conjectured that a degenerate version of Inozemtsev's elliptic model will emerge therein.

In this paper we aim to answer this question affirmatively. A guiding principle is the degeneration relation of the six Painlevé equations.[13] This relation can be schematically expressed as follows:

$$\begin{array}{ccccccc} P_{VI} & \to & P_V & \to & P_{IV} & & \\ & & \downarrow & & \downarrow & & \\ & & P_{III} & \to & P_{II} & \to & P_I \end{array}$$

This diagram means, for instance, that P_V can be derived from P_{VI} by a degeneration process, which amounts to confluence of singular points of the aforementioned linear ordinary differential equation in the isomonodromic approach. We shall trace this process carefully on the ''Calogero side,'' and find a P_V-version of Manin's equation. In principle, one can thus find an analog of Manin's equation for all the six Painlevé equations (though, actually, one can resort to a more direct approach that bypasses the complicated degeneration process).

Remarkably (or rather naturally?), all the six equations on the Calogero side turn out to become a (nonautonomous) Hamiltonian system with a Hamiltonian of the normal form $\mathcal{H}=p^2/2+V(q)$. Furthermore, the Hamiltonians on the Calogero side of P_V and P_{IV} coincide with the Hamiltonians of the (rank one) hyperbolic and rational models in Inozemtsev's classification[10] (which were discovered by Levi and Wojciechowski[14] before Inozemtsev's work). Those corresponding to the other three Painlevé equations are not included therein, but may be thought of as a further degeneration of the hyperbolic and rational models.

One can further proceed to the higher rank models, and ask if there is still a Painlevé–Calogero correspondence. We shall show that this is also the case. The Painlevé side of the correspondence is a kind of multi-dimensional extension of the Painlevé equations. They are obviously different from another multi-dimensional extension called the ''Garnier systems.''[13] For this reason, we call our multi-dimensional extension a *multi-component* version of the Painlevé equations.

This paper is organized as follows. Section II is a brief review of the work of Fuchs, Painlevé and Manin. In Sec. III we deal with P_V, P_{IV} and P_{III}. The degeneration process is discussed in

detail for the case of P_V. The direct approach is illustrated for the case of P_{IV} and P_{III}. In Sec. IV we show a reformulation of the foregoing calculations in the Hamiltonian formalism. The status of P_{II} and P_I is also clarified therein. Section V is devoted to the higher rank Inozemtsev Hamiltonians and the multi-component Painlevé equations. Section VI is for concluding remarks. Part of the technical details are gathered in the Appendices.

II. PAINLEVÉ–CALOGERO CORRESPONDENCE FOR P_{VI}

We here briefly review the work of Fuchs, Painlevé and Manin.

Fuchs rewrites P_{VI} into the following form:

$$t(1-t)\mathcal{L}_t\int_\infty^\lambda \frac{dz}{\sqrt{z(z-1)(z-t)}} = \sqrt{\lambda(\lambda-1)(\lambda-t)}\left[\alpha+\frac{\beta t}{\lambda^2}+\frac{\gamma(t-1)}{(\lambda-1)^2}+\left(\delta-\frac{1}{2}\right)\frac{t(t-1)}{(\lambda-t)^2}\right]. \tag{1}$$

Here $\mathcal{L}_t$ is the linear differential operator (Picard–Fuchs operator)

$$\mathcal{L}_t = t(1-t)\frac{d^2}{dt^2}+(1-2t)\frac{d}{dt}-\frac{1}{4}, \tag{2}$$

which also appears in the Picard–Fuchs equation of complete elliptic integrals. In this respect, P_{VI} may be thought of as an inhomogeneous (and nonlinear) analog of the Picard–Fuchs equation.

Painlevé and Manin make use of a parametrization of the elliptic curve,

$$y^2 = z(z-1)(z-t), \tag{3}$$

by the Weierstrass $\wp$-function. Let $\wp(u)$ be the $\wp$-function with primitive periods 1 and τ:

$$\wp(u)=\wp(u|1,\tau)=\frac{1}{u^2}+\sum_{(m,n)\neq(0,0)}\left(\frac{1}{(u+m+n\tau)^2}-\frac{1}{(m+n\tau)^2}\right). \tag{4}$$

The parametrization is now given by

$$z=\frac{\wp(u)-e_1}{e_2-e_1},\quad y=\frac{\wp'(u)}{2(e_2-e_1)^{3/2}}, \tag{5}$$

where $e_n=\wp(\omega_n)$, $n=1,2,3$ are the values of $\wp(u)$ at the three half period points $\omega_1=1/2$, $\omega_2=-(1+\tau)/2$, $\omega_3=\tau/2$.

Manin's excellent idea is to do a simultaneous change of the dependent variable $\lambda\to q$ by

$$\lambda=\frac{\wp(q)-e_1}{e_2-e_1}, \tag{6}$$

and the independent variable $t\to\tau$ by

$$t=\frac{e_3-e_1}{e_2-e_1}. \tag{7}$$

Manin presents the beautiful formula

$$\frac{d\tau}{dt}=\frac{\pi i}{t(t-1)(e_2-e_1)}, \tag{8}$$

for the Jacobian of the latter, which plays a key role in his calculations. P_{VI} is thereby mapped to the equation

$$(2\pi i)^2 \frac{d^2 q}{d\tau^2} = \sum_{n=0}^{3} \alpha_n \wp'(q+\omega_n), \tag{9}$$

where the parameters on the right hand side are connected with the parameters of P_{VI} as $\alpha_0 = \alpha$, $\alpha_1 = -\beta$, $\alpha_2 = \gamma$, $\alpha_3 = -\delta + 1/2$. This equation is equivalent to the Hamiltonian system,

$$2\pi i \frac{dq}{d\tau} = \frac{\partial \mathcal{H}}{\partial p}, \quad 2\pi i \frac{dp}{d\tau} = -\frac{\partial \mathcal{H}}{\partial q}, \tag{10}$$

with the Hamiltonian

$$\mathcal{H} = \frac{p^2}{2} - \sum_{n=0}^{3} \alpha_n \wp(q+\omega_n). \tag{11}$$

III. CORRESPONDENCE FOR P_V, P_{IV} AND P_{III}

A. Degeneration of P_{VI} to P_V

The degeneration of P_{VI} to P_V is achieved by rescaling the time variable and the parameters as

$$t = 1 + \epsilon \tilde{t}, \quad \alpha = \tilde{\alpha}, \quad \beta = \tilde{\beta}, \quad \gamma = \frac{\tilde{\gamma}}{\epsilon} - \frac{\tilde{\delta}}{\epsilon^2}, \quad \delta = \frac{\tilde{\delta}}{\epsilon^2}, \tag{12}$$

and letting $\epsilon \to 0$ while leaving $\tilde{\alpha}, \ldots, \tilde{\gamma}$ and $\tilde{t}$ finite.[13]

The building blocks of Fuchs' equation (1) turn out to survive this scaling limit as follows.

(1) The Picard–Fuchs operator:

$$t(1-t)\mathcal{L}_t \to \tilde{t}^2 \frac{d^2}{d\tilde{t}^2} + \tilde{t}\frac{d}{d\tilde{t}} = \left(\tilde{t}\frac{d}{d\tilde{t}}\right)^2.$$

(2) The sum $\alpha + \cdots$ of four terms on the right hand side:

$$\alpha + \frac{\beta t}{\lambda^2} + \frac{\gamma(t-1)}{(\lambda-1)^2} + \left(\delta - \frac{1}{2}\right)\frac{t(t-1)}{(\lambda-t)^2} \to \tilde{\alpha} + \frac{\tilde{\beta}}{\lambda^2} + \frac{\tilde{\gamma}\tilde{t}}{(\lambda-1)^2} + \frac{\tilde{\delta}\tilde{t}^2(\lambda+1)}{(\lambda-1)^3}.$$

(3) The square root on the right hand side:

$$\sqrt{\lambda(\lambda-1)(\lambda-t)} \to \sqrt{\lambda}(\lambda-1).$$

(4) The incomplete elliptic integral:

$$\int_\infty^\lambda \frac{dz}{\sqrt{z(z-1)(z-t)}} \to \int_\infty^\lambda \frac{dz}{\sqrt{z}(z-1)}.$$

In particular, the degeneration of P_{VI} to P_V is associated with the degeneration of the elliptic curve to a rational curve,

$$y^2 = z(z-1)(z-t) \to y^2 = z(z-1)^2, \tag{13}$$

or, equivalently, the degeneration of the torus $\mathbb{C}/(\mathbb{Z} + \tau\mathbb{Z})$ to the cylinder $\mathbb{C}/\mathbb{Z}$.

Thus, rewriting $\tilde{\alpha}$, $\tilde{\beta}$, $\tilde{\gamma}$, $\tilde{\delta}$ and $\tilde{t}$ to α, β, γ, δ and t, we obtain the following equation as a P_V-version of Fuchs' equation:

$$\left(t\frac{d}{dt}\right)^2\int_\infty^\lambda \frac{dz}{\sqrt{z}(z-1)}=\sqrt{\lambda}(\lambda-1)\left(\alpha+\frac{\beta}{\lambda^2}+\frac{\gamma t}{(\lambda-1)^2}+\frac{\delta t^2(\lambda+1)}{(\lambda-1)^3}\right). \tag{14}$$

B. Analog of Manin's equation for P_V

As a counterpart of the q-variable for P_{VI}, we now consider

$$q=\int_\infty^\lambda \frac{dz}{\sqrt{z}(z-1)}. \tag{15}$$

If one prefers to be more faithful to Manin's parametrization, one should rather define q as

$$q=\frac{1}{2\pi i}\int_\infty^\lambda \frac{dz}{\sqrt{z}(z-1)},$$

because $2(e_2-e_1)^{1/2}\to 2\pi i$ as $\mathrm{Im}\,\tau\to+\infty$ (see Appendix B). Since there is no substantial difference, let us take the first definition that is slightly simpler for calculations.

Let us rewrite (14) in terms of q. The integral can be readily calculated as

$$q=\log\left(\frac{\sqrt{\lambda}-1}{\sqrt{\lambda}+1}\right), \tag{16}$$

so that the inverse relation can be written as

$$\sqrt{\lambda}=-\coth(q/2). \tag{17}$$

Terms on the right hand side of (14) can be calculated as follows:

$$\sqrt{\lambda}(\lambda-1)=-\frac{\cosh(q/2)}{\sinh^3(q/2)},$$

$$\sqrt{\lambda}(\lambda-1)\frac{1}{\lambda^2}=-\frac{\sinh(q/2)}{\cosh^3(q/2)},$$

$$\sqrt{\lambda}(\lambda-1)\frac{1}{(\lambda-1)^2}=-\frac{1}{2}\sinh(q),$$

$$\sqrt{\lambda}(\lambda-1)\frac{(\lambda+1)}{(\lambda-1)^3}=-\frac{\lambda^{3/2}+\lambda^{1/2}}{(\lambda-1)^2}=-\frac{1}{4}\sinh(2q).$$

The differential equation for q eventually takes the form

$$\left(t\frac{d}{dt}\right)^2 q=-\frac{\partial V(q)}{\partial q}, \tag{18}$$

where

$$V(q)=-\frac{\alpha}{\sinh^2(q/2)}-\frac{\beta}{\cosh^2(q/2)}+\frac{\gamma t}{2}\cosh(q)+\frac{\delta t^2}{8}\cosh(2q). \tag{19}$$

This gives a P_V-version of Manin's equation. Note that this equation can be readily converted to a Hamiltonian system with the Hamiltonian $\mathcal{H}=p^2/2+V(q)$.

Remark: A very similar change of dependent variable for P_V is discussed in the book of Iwasaki *et al.*[15]

C. Idea of direct approach

Although the degeneration process can be continued to the other Painlevé equations, we now present a more direct approach. Note that the integrand is connected with the coefficient of $(d\lambda/dt)^2$ in the original Painlevé equation by the following very simple relation:

$$\frac{1}{\sqrt{z(z-1)(z-t)}} = \exp\left[-\int \frac{1}{2}\left(\frac{1}{z} + \frac{1}{z-1} + \frac{1}{z-t}\right) dz \right],$$

$$\frac{1}{\sqrt{z}(z-1)} = \exp\left[-\int \left(\frac{1}{2z} + \frac{1}{z-1}\right) dz \right].$$

If this is a correct prescription, one will be able to define the q-variable for P_{III} and P_{II} directly without the cumbersome degeneration process. This is indeed the case, as we shall show below.

D. q-variable for P_{IV}

Since the expected integrand is given by

$$\exp\left(-\int \frac{dz}{2z} \right) = \frac{1}{\sqrt{z}}, \tag{20}$$

we define

$$q = \int^{\lambda} \frac{dz}{\sqrt{z}} = 2\sqrt{\lambda}. \tag{21}$$

This can be solved for λ as

$$\lambda = \left(\frac{q}{2}\right)^2. \tag{22}$$

Honest calculations show that all derivative terms of P_{IV} can be absorbed by the second derivative of q:

$$\frac{d^2q}{dt^2} = \frac{1}{\sqrt{\lambda}} \frac{d^2\lambda}{dt^2} - \frac{1}{2\lambda\sqrt{\lambda}} \left(\frac{d\lambda}{dt}\right)^2$$

$$= \frac{1}{\sqrt{\lambda}} \left(\frac{3}{2}\lambda^3 + 4t\lambda^2 + 2(t^2 - \alpha)\lambda + \frac{\beta}{\lambda} \right). \tag{23}$$

Substituting $\lambda = (q/2)^2$ gives the second order differential equation,

$$\frac{d^2q}{dt^2} = -\frac{\partial V(q)}{\partial q}, \tag{24}$$

with the potential

$$V(q) = -\frac{1}{2}\left(\frac{q}{2}\right)^6 - 2t\left(\frac{q}{2}\right)^4 - 2(t^2 - \alpha)\left(\frac{q}{2}\right)^2 + \beta\left(\frac{q}{2}\right)^{-2}. \tag{25}$$

E. q-variable for P_{III}

The integrand is expected to be given by

$$\exp\left(-\int \frac{dz}{z}\right)=\frac{1}{z}. \tag{26}$$

We consider

$$q=\int^{\lambda}\frac{dz}{z}=\log\lambda, \tag{27}$$

and its inversion

$$\lambda=e^{q}. \tag{28}$$

All derivatives terms of P_{III} are now absorbed by the second derivative of q with respect to $\log t$:

$$\left(t\frac{d}{dt}\right)^2 q=\frac{t^2}{\lambda}\frac{d^2\lambda}{dt^2}+\frac{t}{\lambda}\frac{d\lambda}{dt}-\frac{t^2}{\lambda^2}\left(\frac{d\lambda}{dt}\right)^2$$

$$=\frac{\alpha\lambda}{4}+\frac{\beta t}{4\lambda}+\frac{\gamma\lambda^2}{4}+\frac{\delta t^2}{4\lambda^2}. \tag{29}$$

Substituting $\lambda=e^{q}$ gives the second order equation,

$$\left(t\frac{d}{dt}\right)^2 q=-\frac{\partial V(q)}{\partial q}, \tag{30}$$

with the potential

$$V(q)=-\frac{\alpha}{4}e^{q}+\frac{\beta t}{4}e^{-q}-\frac{\gamma}{8}e^{2q}+\frac{\delta t^2}{8}e^{-2q}. \tag{31}$$

F. Summary

Let us summarize the results of this section.

Theorem 1: *The foregoing change of variable $\lambda\to q$ maps P_V, P_{IV} and P_{III} to a second order differential equation for the new dependent variable q. These equations are equivalent to a non-autonomous Hamiltonian system with a Hamiltonian of the normal form $\mathcal{H}=p^2/2+V(q)$.*
(P_V) *The Hamiltonian system takes the form*

$$t\frac{dq}{dt}=\frac{\partial\mathcal{H}}{\partial p},\quad t\frac{dp}{dt}=-\frac{\partial\mathcal{H}}{\partial q}, \tag{32}$$

with the Hamiltonian

$$\mathcal{H}=\frac{p^2}{2}-\frac{\alpha}{\sinh^2(q/2)}-\frac{\beta}{\cosh^2(q/2)}+\frac{\gamma t}{2}\cosh(q)+\frac{\delta t^2}{8}\cosh(2q). \tag{33}$$

(P_{IV}) *The Hamiltonian system takes the form*

$$\frac{dq}{dt}=\frac{\partial\mathcal{H}}{\partial p},\quad \frac{dp}{dt}=-\frac{\partial\mathcal{H}}{\partial q}, \tag{34}$$

with the Hamiltonian

$$\mathcal{H}=\frac{p^2}{2}-\frac{1}{2}\left(\frac{q}{2}\right)^6-2t\left(\frac{q}{2}\right)^4-2(t^2-\alpha)\left(\frac{q}{2}\right)^2+\beta\left(\frac{q}{2}\right)^{-2}. \tag{35}$$

(P_{III}) *The Hamiltonian system takes the form*

$$t\frac{dq}{dt}=\frac{\partial\mathcal{H}}{\partial p},\quad t\frac{dp}{dt}=-\frac{\partial\mathcal{H}}{\partial q}, \tag{36}$$

with the Hamiltonian

$$\mathcal{H}=\frac{p^2}{2}-\frac{\alpha}{4}e^q+\frac{\beta t}{4}e^{-q}-\frac{\gamma}{8}e^{2q}+\frac{\delta t^2}{8}e^{-2q}. \tag{37}$$

Remark:

(1) The Hamiltonians for P_V and P_{IV} coincide with those of the hyperbolic and rational models of Inozemtsev,[10] Levi and Wojciechowski.[14] The Hamiltonian for P_{III} has no counterpart in their work, but nowadays can be found in the literature.[16]
(2) The foregoing construction of the q-variable does not literally work for P_{II} and P_I, because there is no $(d\lambda/dt)^2$ term. The status of these equations will be clarified in the next section from a different point of view.

IV. HAMILTONIAN FORMALISM OF CORRESPONDENCE

A. Hamiltonians of Painlevé equations

All the six Painlevé equations are known to be expressed in the Hamiltonian form

$$\frac{d\lambda}{dt}=\frac{\partial H}{\partial\mu},\quad \frac{d\lambda}{dt}=-\frac{\partial H}{\partial\lambda},$$

with a suitable choice of the canonical conjugate variable μ and the Hamiltonian H.[17] This expression is by no means unique; we here consider the following Hamiltonians.[13] These Hamiltonians are referred to as the ''polynomial Hamiltonians'' because they are polynomials in λ and μ:

$$(P_{VI})\quad H=\frac{\lambda(\lambda-1)(\lambda-t)}{t(t-1)}\left[\mu^2-\left(\frac{\kappa_0}{\lambda}+\frac{\kappa_1}{\lambda-1}+\frac{\theta-1}{\lambda-t}\right)\mu+\frac{\kappa}{\lambda(\lambda-1)}\right],$$

$$(P_V)\quad H=\frac{\lambda(\lambda-1)^2}{t}\left[\mu^2-\left(\frac{\kappa_0}{\lambda}+\frac{\theta_1}{\lambda-1}-\frac{\eta_1 t}{(\lambda-1)^2}\right)\mu+\frac{\kappa}{\lambda(\lambda-1)}\right],$$

$$(P_{IV})\quad H=2\lambda\left[\mu^2-\left(\frac{\lambda}{2}+t+\frac{\kappa_0}{\lambda}\right)\mu+\frac{\theta_\infty}{2}\right],$$

$$(P_{III})\quad H=\frac{\lambda^2}{t}\left[\mu^2-\left(\eta_\infty+\frac{\theta_0}{\lambda}-\frac{\eta_0 t}{\lambda^2}\right)\mu+\frac{\eta_\infty(\theta_0+\theta_\infty)}{2\lambda}\right],$$

$$(P_{II})\quad H=\frac{\mu^2}{2}-\left(\lambda^2+\frac{t}{2}\right)\mu-\left(\alpha+\frac{1}{2}\right)\lambda,$$

$$(P_I)\quad H=\frac{\mu^2}{2}-2\lambda^3-t\lambda.$$

Here $\kappa_0, \kappa_1, \theta$, etc. are constants that are connected with the parameters $\alpha, \beta, \gamma, \delta$ of the Painlevé equations by simple algebraic relations:

$$(\mathrm{P_{VI}}) \quad \alpha = \frac{(\kappa_0+\kappa_1+\theta-1)^2}{2} - 2\kappa, \quad \beta = -\frac{\kappa_0^2}{2}, \quad \gamma = \frac{\kappa_1^2}{2}, \quad \delta = \frac{1-\theta^2}{2};$$

$$(\mathrm{P_V}) \quad \alpha = \frac{(\kappa_0+\theta_1)^2}{2} - 2\kappa, \quad \beta = -\frac{\kappa_0^2}{2}, \quad \gamma = \eta_1(\theta_1+1), \quad \delta = -\frac{\eta_1^2}{2};$$

$$(\mathrm{P_{IV}}) \quad \alpha = 2\theta_\infty - \kappa_0 + 1, \quad \beta = -2\kappa_0^2;$$

$$(\mathrm{P_{III}}) \quad \alpha = -4\eta_\infty\theta_\infty, \quad \beta = 4\eta_0(\theta_0+1), \quad \gamma = 4\eta_\infty^2, \quad \delta = -4\eta_0^2.$$

B. How to find canonical transformations

The goal of this section is to show that the Painlevé–Calogero correspondence is, in fact, a (time-dependent) canonical transformation of two Hamiltonian systems. By this, we mean that the functional relation between λ and q can be extended to (λ,μ) and (q,p) so as to satisfy the equation

$$\mu\, d\lambda - H dt = \text{constant} \cdot (p\, dq - \mathcal{H}\, dT) + \text{exact form}, \tag{38}$$

with a suitably redefined time variable T (such as the logarithmic time $\log t$ in $\mathrm{P_V}$ and $\mathrm{P_{III}}$). The constant factor on the right hand side is inserted simply for convenience; if necessary, one can normalize the constant to 1 by suitably rescaling p, q, $\mathcal{H}$ and T. For this reason, we call this type of coordinate transformation a ''canonical'' transformation even if the constant factor is not equal to 1.

Let us illustrate, in the case of $\mathrm{P_{VI}}$, how to find such a canonical transformation. Suppose that λ and μ be a solution of $\mathrm{P_{VI}}$ in the aforementioned Hamiltonian formalism, and that q be a corresponding solution of Manin's equation. The canonical equation for λ takes the form

$$\frac{d\lambda}{dt} = \frac{\lambda(\lambda-1)(\lambda-t)}{t(t-1)}\left(2\mu - \frac{\kappa_0}{\lambda} - \frac{\kappa_1}{\lambda-1} - \frac{\theta-1}{\lambda-t}\right).$$

This equation can be solved for μ:

$$\mu = \frac{t(t-1)}{2\lambda(\lambda-1)(\lambda-t)}\frac{d\lambda}{dt} + \frac{1}{2}\left(\frac{\kappa_0}{\lambda} + \frac{\kappa_1}{\lambda-1} + \frac{\theta-1}{\lambda-t}\right).$$

Our task is to rewrite the right hand side in terms of p and q. We first consider $d\lambda/dt$. Differentiating (6) against t gives

$$\frac{d\lambda}{dt} = \left(\frac{\wp'(q)}{e_2-e_1}\frac{dq}{d\tau} + f_\tau(q)\right)\frac{d\tau}{dt},$$

where we have introduced the functions

$$f(u) = \frac{\wp(u)-e_1}{e_2-e_1}, \quad f_\tau(u) = \frac{\partial f(u)}{\partial \tau}. \tag{39}$$

The derivative $dq/d\tau$ can be read off from the canonical equation for q:

$$\frac{dq}{d\tau} = \frac{1}{2\pi i}\frac{\partial \mathcal{H}}{\partial p} = \frac{p}{2\pi i}.$$

As for the Jacobian $d\tau/dt$, Manin's formula (8) is available. One can thus express $d\lambda/dt$ as a function of p, q and τ. The other part of the foregoing expression of μ contains λ only, which can be readily converted to a function of q and τ by (6). We thus obtain the following expression of μ:

$$\mu = \frac{e_2-e_1}{\wp'(q)}p + \frac{2\pi i(e_2-e_1)^2}{\wp'(q)^2}f_\tau(q) + \frac{e_2-e_1}{2}\left(\frac{\kappa_0}{\wp(q)-e_1} + \frac{\kappa_1}{\wp(q)-e_2} + \frac{\theta-1}{\wp(q)-e_3}\right). \tag{40}$$

We now move the point of view, and think of (6) and (40) as defining a coordinate transformation $(\lambda,\mu)\to(q,p)$. This gives a canonical transformation that we have sought for the following.

Theorem 2: *(6) and (40) define a canonical transformation that connects the Hamiltonian form of* P_{VI} *and Manin's Hamiltonian system. The canonical coordinates and the Hamiltonians of the two systems obey the equation*

$$\mu\, d\lambda - H dt = p\, dq - \mathcal{H}\frac{d\tau}{2\pi i} + \text{exact form}. \tag{41}$$

C. Proof of Theorem 2

The total differential of (6) gives

$$d\lambda = \frac{\wp'(q)}{e_2-e_1}dq + f_\tau(q)d\tau,$$

so that $\mu\, d\lambda$ can be expressed as

$$\begin{aligned}\mu\, d\lambda &= \left(\frac{e_2-e_1}{\wp'(q)}p + \frac{2\pi i(e_2-e_1)^2}{\wp'(q)^2}f_\tau(q)\right)\left(\frac{\wp'(q)}{e_2-e_1}dq + f_\tau(q)d\tau\right) \\ &\quad + \frac{1}{2}\left(\frac{\kappa_0}{\lambda} + \frac{\kappa_1}{\lambda-1} + \frac{\theta-1}{\lambda-t}\right)d\lambda \\ &= p\, dq + (\mathrm{A}) + (\mathrm{B}) + (\mathrm{C}),\end{aligned}$$

where

$$(\mathrm{A}) = \frac{2\pi i(e_2-e_1)}{\wp'(q)}f_\tau(q)dq,$$

$$(\mathrm{B}) = \left(\frac{e_2-e_1}{\wp'(q)}p + \frac{2\pi i(e_2-e_1)^2}{\wp'(q)^2}f_\tau(q)\right)f_\tau(q)d\tau,$$

$$(\mathrm{C}) = \frac{1}{2}\left(\frac{\kappa_0}{\lambda} + \frac{\kappa_1}{\lambda-1} + \frac{\theta-1}{\lambda-t}\right)d\lambda.$$

As we shall prove in Appendix A, (A) can be further rewritten as

$$(\mathrm{A}) = \left[\frac{\wp(q+\omega_3)}{4\pi i} - \pi\left(\frac{f_\tau(q)}{f'(q)}\right)^2\right]d\tau + \text{exact form}, \tag{42}$$

where $f'(u)$ denotes the u-derivative of $f(u)$:

$$f'(u)=\frac{\partial f(u)}{\partial u}=\frac{\wp'(u)}{e_2-e_1}. \tag{43}$$

For (B) and (C), we have

$$(\mathrm{B})=\left[\frac{f_\tau(q)}{f'(q)}p+2\pi i\left(\frac{f_\tau(q)}{f'(q)}\right)^2\right]d\tau,$$

$$(\mathrm{C})=\frac{\theta-1}{2(\lambda-t)}dt+\frac{1}{2}(\kappa_0\log\lambda+\kappa_1\log(\lambda-1)+(\theta-1)\log(\lambda-t))$$

$$=\frac{\theta-1}{2(\lambda-t)}dt+\text{exact form}.$$

Thus we find that

$$\mu\,d\lambda-H dt=p\,dq-\tilde{\mathcal{H}}\frac{d\tau}{2\pi i}+\text{exact form}, \tag{44}$$

where

$$\tilde{\mathcal{H}}=2\pi i\frac{dt}{d\tau}\left(H-\frac{\theta-1}{2(\lambda-t)}\right)-2\pi i\left[\frac{\wp(q+\omega_3)}{4\pi i}+\frac{f_\tau(q)}{f'(q)}p+\pi i\left(\frac{f_\tau(q)}{f'(q)}\right)^2\right]. \tag{45}$$

Our task is to prove that the transformed Hamiltonian $\tilde{\mathcal{H}}$ coincides, modulo irrelevant terms, with the Hamiltonian of Manin's equation. Here ''irrelevant'' means that the term is a function of t only. Such a ''nondynamical'' term can be absorbed by the ''exact form'' part of the foregoing relation of 1-forms, thereby being negligible.

Let us evaluate the contribution of $2\pi i(dt/d\tau)H$. By Manin's formula (8) of $d\tau/dt$, and also by the identity

$$\lambda(\lambda-1)(\lambda-t)=\frac{\wp'(q)^2}{4(e_2-e_1)^3},$$

we can rewrite $2\pi i(dt/d\tau)H$ as follows:

$$2\pi i\frac{dt}{d\tau}H=\frac{\wp'(q)^2}{2(e_2-e_1)^2}\left[\mu^2-\left(\frac{\kappa_0}{\lambda}+\frac{\kappa_1}{\lambda-1}+\frac{\theta-1}{\lambda-t}\right)\mu+\frac{\kappa}{\lambda(\lambda-1)}\right]$$

$$=\frac{\wp'(q)^2}{2(e_2-e_1)^2}\left[\mu-\frac{1}{2}\left(\frac{\kappa_0}{\lambda}+\frac{\kappa_1}{\lambda-1}+\frac{\theta-1}{\lambda-t}\right)\right]^2$$

$$+\frac{\wp'(q)^2}{2(e_2-e_1)^2}\left[-\frac{1}{4}\left(\frac{\kappa_0}{\lambda}+\frac{\kappa_1}{\lambda-1}+\frac{\theta-1}{\lambda-t}\right)^2+\frac{\kappa}{\lambda(\lambda-1)}\right].$$

The first term on the right hand side is equal to

$$\frac{1}{2}\left(p+2\pi i\frac{f_\tau(q)}{f'(q)}\right)^2=\frac{p^2}{2}+2\pi i\frac{f_\tau(q)}{f'(q)}p+\left(2\pi i\frac{f_\tau(q)}{f'(q)}\right)^2,$$

by which the terms proportional to $f_\tau(q)/f'(q)$ and its square in the definition of $\tilde{\mathcal{H}}$ are cancelled out. The transformed Hamiltonian $\tilde{\mathcal{H}}$ can now be expressed as

$$\widetilde{\mathcal{H}}=\frac{p^2}{2}-\frac{\wp'(q)^2}{2(e_2-e_1)^2}-\frac{(\theta-1)t(t-1)(e_2-e_1)}{\lambda-t}+\frac{\wp'(q)}{2(e_2-e_1)^2}\left[-\frac{1}{4}\left(\frac{\kappa_0}{\lambda}+\frac{\kappa_1}{\lambda-1}+\frac{\theta-1}{\lambda-t}\right)^2+\frac{\kappa}{\lambda(\lambda-1)}\right]. \tag{46}$$

Note that this is already of the normal form $p^2/2+\widetilde{V}(q)$ with the potential

$$\widetilde{V}(q)=-\frac{\wp'(q)^2}{2(e_2-e_1)^2}-\frac{(\theta-1)t(t-1)(e_2-e_1)}{\lambda-t}+\frac{\wp'(q)}{2(e_2-e_1)^2}\left[-\frac{1}{4}\left(\frac{\kappa_0}{\lambda}+\frac{\kappa_1}{\lambda-1}+\frac{\theta-1}{\lambda-t}\right)^2+\frac{\kappa}{\lambda(\lambda-1)}\right]. \tag{47}$$

What remains is to express $\widetilde{V}(q)$ as an explicit function of q. To this end, we substitute the factor $\wp'(q)^2/2(e_2-e_1)^2$ by $2(e_2-e_1)\lambda(\lambda-1)(\lambda-t)$, and rewrite the main part of $\widetilde{V}(q)$ as a linear combination of λ, $1/\lambda$, $1/(\lambda-1)$ and $1/(\lambda-t)$. This leads to the following expression of $\widetilde{V}(q)$:

$$\widetilde{V}(q)=-\frac{(\kappa_0+\kappa_1+\theta-1)^2-4\kappa}{2}(e_2-e_1)\lambda-\frac{\kappa_0^2}{2}\cdot\frac{(e_2-e_1)t}{\lambda}-\frac{\kappa_1^2}{2}\cdot\frac{(e_2-e_1)(1-t)}{\lambda-1}-\frac{(\theta-1)^2+1}{2}\cdot\frac{(e_2-e_1)t(t-1)}{\lambda-t}-\frac{1}{2}\wp(q+\omega_3)+\text{function of } t \text{ only}.$$

The final piece of the ring is the general formula

$$\wp(u+\omega_j)=e_j+\frac{(e_j-e_k)(e_j-e_l)}{\wp(u)-e_j}, \tag{48}$$

where (j,k,l) is a cyclic permutation of (1,2,3). This implies that

$$\frac{(e_2-e_1)t}{\lambda}=\wp(q+\omega_1)-e_1,$$

$$\frac{(e_2-e_1)(1-t)}{\lambda-1}=\wp(q+\omega_2)-e_2,$$

$$\frac{(e_2-e_1)t(t-1)}{\lambda-t}=\wp(q+\omega_3)-e_3,$$

so that

$$\widetilde{V}(q)=-\frac{(\kappa_0+\kappa_1+\theta-1)^2-4\kappa}{2}\wp(q)-\frac{\kappa_0^2}{2}\wp(q+\omega_1)-\frac{\kappa_1^2}{2}\wp(q+\omega_2)-\frac{\theta^2}{2}\wp(q+\omega_3)+\text{function of } \tau \text{ only}. \tag{49}$$

Apart from the last term which is negligible, this potential is indeed the same as Manin's potential $V(q)$ (recall the algebraic relations connecting the constants κ_0, etc. and the parameters of P_{VI}). This completes the proof of the theorem. Q.E.D.

D. Canonical transformation for P_V

This heuristic method for constructing a canonical transformation can be applied to the other Painlevé equations. Here we consider the case of P_V.

Let λ be a solution of P_V, μ the canonical conjugate variable, and q the corresponding solution of (18). The canonical equation for λ can be written as

$$\frac{d\lambda}{dt}=\frac{\lambda(\lambda-1)^2}{t}\left(2\mu-\frac{\kappa_0}{\lambda}-\frac{\theta_1}{\lambda-1}+\frac{\eta_1 t}{(\lambda-1)^2}\right).$$

This equation can be solved for μ as

$$\mu=\frac{1}{2\lambda(\lambda-1)^2}t\frac{d\lambda}{dt}+\frac{1}{2}\left(\frac{\kappa_0}{\lambda}+\frac{\theta_1}{\lambda-1}-\frac{\eta_1 t}{(\lambda-1)^2}\right).$$

By differentiating (17) against t and using the canonical equation $t\,dq/dt=\partial\mathcal{H}/\partial p=p$, we obtain the identity

$$t\frac{d\lambda}{dt}=\sqrt{\lambda}(\lambda-1)p,$$

which can be used to rewrite the expression of μ as

$$\mu=\frac{p}{2\sqrt{\lambda}(\lambda-1)}+\frac{1}{2}\left(\frac{\kappa_0}{\lambda}+\frac{\theta_1}{\lambda-1}-\frac{\eta_1 t}{(\lambda-1)^2}\right). \tag{50}$$

We now reinterpret (17) and (50) as defining a coordinate transformation $(\lambda,\mu)\to(q,p)$. This indeed turns out to give a canonical transformation that we have sought for the following.

Theorem 3: *(17) and (50) define a canonical transformation that connects* P_V *and the* P_V*-version of Manin's Hamiltonian system. The canonical coordinates and the Hamiltonians of the two systems obey the equation*

$$\mu\,d\lambda-H\,dt=\frac{1}{2}\left(p\,dq-\mathcal{H}\frac{dt}{t}\right)+\text{exact form}. \tag{51}$$

Proof: Since $d\lambda$ and dq are connected by the relation

$$d\lambda=\sqrt{\lambda}(\lambda-1)dq,$$

$\mu\,d\lambda$ can be expressed as

$$\begin{aligned}\mu\,d\lambda&=\frac{1}{2}pdq+\frac{1}{2}\left(\frac{\kappa_0}{\lambda}+\frac{\theta_1}{\lambda-1}-\frac{\eta_1 t}{(\lambda-1)^2}\right)d\lambda\\&=\frac{1}{2}p\,dq-\frac{\eta_1}{2(\lambda-1)}dt+\frac{1}{2}d\left(\kappa_0\log\lambda+\theta_1\log(\lambda-1)+\frac{\eta_1 t}{\lambda-1}\right),\end{aligned}$$

so that

$$\mu\, d\lambda - H\, dt = \frac{1}{2}\left(p\, dq - \widetilde{\mathcal{H}}\frac{dt}{t}\right) + \text{exact form}, \tag{52}$$

where

$$\widetilde{\mathcal{H}} = 2Ht + \frac{\eta_1 t}{\lambda - 1}. \tag{53}$$

We can rewrite $\widetilde{\mathcal{H}}$ to a normal form as

$$\begin{aligned}\widetilde{\mathcal{H}} &= 2\lambda(\lambda-1)^2\left[\mu - \frac{1}{2}\left(\frac{\kappa_0}{\lambda} + \frac{\theta_1}{\lambda-1} - \frac{\theta_1 t}{(\lambda-1)^2}\right)\right]^2 \\ &\quad + 2\lambda(\lambda-1)^2\left[-\frac{1}{4}\left(\frac{\kappa_0}{\lambda} + \frac{\theta_1}{\lambda-1} - \frac{\eta_1 t}{(\lambda-1)^2}\right)^2 + \frac{\kappa}{\lambda(\lambda-1)}\right] + \frac{\eta_1 t}{\lambda-1} \\ &= \frac{p^2}{2} + \widetilde{V}(q),\end{aligned} \tag{54}$$

where

$$\begin{aligned}\widetilde{V}(q) &= -\frac{\lambda(\lambda-1)^2}{2}\left(\frac{\kappa_0}{\lambda} + \frac{\theta_1}{\lambda-1} - \frac{\eta_1 t}{(\lambda-1)^2}\right)^2 + 2\kappa(\lambda-1) + \frac{\eta_1 t}{\lambda-1}. \\ &= -\left(\frac{\kappa_0}{2} + \frac{\theta_1^2}{2} + \kappa_1\theta_1 - 2\kappa\right)\frac{1}{\sinh^2(q/2)} + \frac{\kappa_0^2}{2}\,\frac{1}{\cosh^2(q/2)} \\ &\quad + \frac{\eta_1(\theta_1+1)t}{2}\cosh(q) - \frac{\eta_1^2 t^2}{2}\cosh(2q) + \text{function of } t \text{ only}.\end{aligned} \tag{55}$$

Apart from the last negligible term, this coincides with the potential $V(q)$ in the statement of the theorem. Q.E.D.

E. Canonical transformation for P_{IV}

We now consider the case of P_{IV}.

Let λ be a solution of P_{IV}, μ the canonical conjugate variable, and q the corresponding solution of (24). The canonical equation for λ can be written as

$$\frac{d\lambda}{dt} = 4\lambda\mu - (\lambda^2 + 2t\lambda + 2\kappa_0),$$

which can be solved for μ as

$$\mu = \frac{1}{4\lambda}\frac{d\lambda}{dt} + \frac{1}{4}\left(\lambda + 2t + \frac{2\kappa_0}{\lambda}\right).$$

By (22) and the canonical equation $dq/dt = \partial\mathcal{H}/\partial p = p$, we have the identity

$$\frac{d\lambda}{dt} = \sqrt{\lambda}\frac{dq}{dt} = \sqrt{\lambda}p,$$

so that

$$\mu = \frac{p}{4\sqrt{\lambda}} + \frac{1}{4}\left(\lambda + 2t + \frac{2\kappa_0}{\lambda}\right). \tag{56}$$

Theorem 4: *(22) and (55) define a canonical transformation that connects* P_{IV} *and the* P_{IV}*-version of Manin's Hamiltonian system. The canonical coordinates and Hamiltonians of the two systems obey the equation*

$$\mu\, d\lambda - H\, dt = \tfrac{1}{4}(p\, dq - \mathcal{H}\, dt) + \text{exact form}. \tag{57}$$

Proof: Since $d\lambda$ and dq are connected by the relation

$$d\lambda = \sqrt{\lambda}\, dq,$$

$\mu\, d\lambda$ can be expressed as

$$\begin{aligned}\mu\, d\lambda &= \frac{1}{4}p\, dq + \frac{1}{4}\left(\lambda + 2t + \frac{2\kappa_0}{\lambda}\right)d\lambda \\ &= \frac{1}{4}p\, dq - \frac{1}{2}\lambda\, dt + \frac{1}{4}d\left(\frac{\lambda^2}{2} + 2t\lambda + 2\kappa_0 \log\lambda\right),\end{aligned}$$

so that

$$\mu\, d\lambda - H\, dt = \tfrac{1}{4}(p\, dq - \tilde{\mathcal{H}}\, dt) + \text{exact form}, \tag{58}$$

where

$$\tilde{\mathcal{H}} = 4H + 2\lambda. \tag{59}$$

We can rewrite the transformed Hamiltonian $\tilde{\mathcal{H}}$ to a normal form as

$$\begin{aligned}\tilde{\mathcal{H}} &= 8\lambda\left[\mu - \frac{1}{2}\left(\frac{\lambda}{2} + t + \frac{\kappa_0}{\lambda}\right)\right]^2 + 8\lambda\left[-\frac{1}{4}\left(\frac{\lambda}{2} + t + \frac{\kappa_0}{\lambda}\right)^2 + \frac{\theta_\infty}{2}\right] + 2\lambda \\ &= \frac{p^2}{2} + \tilde{V}(q),\end{aligned} \tag{60}$$

where

$$\begin{aligned}\tilde{V}(q) &= -2\lambda\left(\frac{\lambda}{2} + t + \frac{\kappa_0}{\lambda}\right)^2 + 4\theta_\infty\lambda + 2\lambda \\ &= -\frac{1}{2}\lambda^3 - 2t\lambda^2 - 2(t^2 + \kappa_0 - 2\theta_\infty - 1)\lambda - 2\kappa_0^2\lambda^{-1} \\ &\quad + \text{function of } t \text{ only}.\end{aligned} \tag{61}$$

Substituting $\lambda = (q/2)^2$ gives the potential $V(q)$ modulo an irrelevant term. Q.E.D.

F. Canonical transformations for P_{III}

The situation of P_{III} is somewhat similar to P_V.

Let λ, again, be a solution of $\mathrm{P}_{\mathrm{III}}$, λ the canonical conjuage variable, and q be the corresponding solution of (30). The canonical equation for λ takes the form

$$\frac{d\lambda}{dt} = \frac{\lambda^2}{t}\left(2\mu - \eta_\infty - \frac{\theta_0}{\lambda} + \frac{\eta_0 t}{\lambda^2}\right),$$

which can be solved for μ as

$$\mu = \frac{t}{2\lambda^2}\frac{d\lambda}{dt} + \frac{1}{2}\left(\eta_\infty + \frac{\theta_0}{\lambda} - \frac{\eta_0 t}{\lambda^2}\right).$$

By differentiating (28) and using the canonical equation $t\,dq/dt = \partial\mathcal{H}/\partial p = p$, the t-derivative of λ can be written as

$$t\frac{d\lambda}{dt} = \lambda p,$$

so that we obtain

$$\mu = \frac{p}{2\lambda} + \frac{1}{2}\left(\eta_\infty + \frac{\theta_0}{\lambda} - \frac{\eta_0 t}{\lambda^2}\right). \tag{62}$$

This relation, again, can be used to define a canonical transformation.

Theorem 5: *(28) and (62) define a canonical transformation that connects* $\mathrm{P}_{\mathrm{III}}$ *and the* $\mathrm{P}_{\mathrm{III}}$*-version of Manin's Hamiltonian system. The canonical coordinates and the Hamiltonians of the two systems obey the equation*

$$\mu\,d\lambda - H dt = \frac{1}{2}\left(p\,dq - \mathcal{H}\frac{dt}{t}\right) + \text{exact form}. \tag{63}$$

Proof: Since $d\lambda$ and dq are connected by the relation

$$d\lambda = \lambda\,dq,$$

$\mu\,d\lambda$ can be written as

$$\begin{aligned}\mu\,d\lambda &= \frac{1}{2}p\,dq + \frac{1}{2}\left(\eta_\infty + \frac{\theta_0}{\lambda} - \frac{\eta_0 t}{\lambda^2}\right)d\lambda \\ &= \frac{1}{2}p\,dq - \frac{\eta_0}{2\lambda}dt + \frac{1}{2}d\left(\eta_\infty\lambda + \theta_0\log\lambda + \frac{\eta_0 t}{\lambda}\right),\end{aligned}$$

so that

$$\mu\,d\lambda - H\,dt = \frac{1}{2}\left(p\,dq - \tilde{\mathcal{H}}\frac{dt}{t}\right) + \text{exact form}, \tag{64}$$

where

$$\tilde{\mathcal{H}} = 2Ht + \frac{\eta_0 t}{\lambda}. \tag{65}$$

We can convert the transformed Hamiltonian $\tilde{\mathcal{H}}$ to a normal form as

$$\tilde{\mathcal{H}}=2\lambda^2\left[\mu-\frac{1}{2}\left(\eta_\infty+\frac{\eta_0}{\lambda}-\frac{\eta_0 t}{\lambda^2}\right)\right]^2$$
$$+2\lambda^2\left[-\frac{1}{2}\left(\eta_\infty+\frac{\eta_0}{\lambda}-\frac{\eta_0 t}{\lambda^2}\right)^2+\frac{\eta_\infty(\theta_0+\theta_\infty)}{2\lambda}\right]+\frac{\eta_0 t}{\lambda}$$
$$=\frac{p^2}{2}+\tilde{V}(q), \tag{66}$$

where

$$\tilde{V}(q)=-\frac{\lambda^2}{2}\left(\eta_\infty+\frac{\theta_0}{\lambda}-\frac{\eta_0 t}{\lambda^2}\right)^2+\eta_\infty(\theta_0+\theta_\infty)\lambda+\frac{\eta_0 t}{\lambda}$$
$$=\eta_\infty\theta_\infty e^q+\eta_0(\theta_0+1)te^{-q}-\frac{\eta_\infty^2}{2}e^{2q}-\frac{\eta_0^2 t^2}{2}e^{-2q}$$
$$+\text{function of } t \text{ only}. \tag{67}$$

Thus, apart from the last irrelevant term, $\tilde{V}(q)$ coincides with the potential $V(q)$ in the statement of the theorem. Q.E.D.

G. Status of P_{II} and P_I

Let us turn to P_{II} and P_I. The Hamiltonian of P_I is already of the normal form $\mathcal{H}=p^2/2+V(q)$ with $\lambda=q$, $\mu=p$ and $H=\mathcal{H}$. Although this is not the case for P_{II}, one can directly find a canonical transformation that converts the Hamiltonian H to a normal form.

Theorem 6: *A* P_{II}*-version of Manin's Hamiltonian system is defined by the Hamiltonian*

$$\mathcal{H}=\frac{p^2}{2}-\frac{1}{2}\left(q^2+\frac{t}{2}\right)^2-\alpha q. \tag{68}$$

This system is connected with P_{II} *by the canonical transformation,*

$$\lambda=q, \quad \mu=p+\lambda^2+\frac{t}{2}. \tag{69}$$

The canonical coordinates and the Hamiltonians of the two systems obey the equation

$$\mu\, d\lambda-H\, dt=p\, dq-\mathcal{H}\, dt+\text{exact form}. \tag{70}$$

Proof: The foregoing relation between (λ,μ) and (q,p) implies that

$$\mu\, d\lambda=p\, dq+\left(\lambda^2+\frac{t}{2}\right)d\lambda=p\, dq-\frac{\lambda}{2}dt+d\left(\frac{\lambda^3}{3}+\frac{t\lambda}{2}\right),$$

so that

$$\mu\, d\lambda-H\, dt=p\, dq-\tilde{\mathcal{H}}\, dt+\text{exact form}, \tag{71}$$

where

$$\begin{aligned}\widetilde{\mathcal{H}} &= H + \frac{\lambda}{2} \\ &= \frac{1}{2}\left[\mu - \left(\lambda^2 + \frac{t}{2}\right)\right]^2 - \frac{1}{2}\left(\lambda^2 + \frac{t}{2}\right)^2 - \left(\alpha + \frac{1}{2}\right)\lambda + \frac{\lambda}{2} \\ &= \frac{p^2}{2} - \frac{1}{2}\left(q^2 + \frac{t}{2}\right)^2 - \alpha q. \end{aligned} \tag{72}$$

This is nothing but the Hamiltonian in the statement of the theorem. Q.E.D.

V. MULTI-COMPONENT PAINLEVÉ EQUATIONS

A. Inozemtsev Hamiltonians of higher rank

The rank l version of Inozemtsev's Hamiltonians have l coordinates $q_1,\dots,q_l$ and canonical conjugate momenta $p_1,\dots,p_l$. The Hamiltonians of the elliptic, hyperbolic and rational models take the following form:[10,11,14]

- Elliptic model:

$$\mathcal{H} = \sum_{j=1}^{l}\left(\frac{p_j^2}{2} + \sum_{n=0}^{3} g_n^2 \wp(q_j + \omega_n)\right) + g_4^2 \sum_{j\neq k} (\wp(q_j - q_k) + \wp(q_j + q_k)).$$

- Hyperbolic model:

$$\begin{aligned}\mathcal{H} = \sum_{j=1}^{l}&\left(\frac{p_j^2}{2} + \frac{g_0^2}{\sinh^2(q_j/2)} + \frac{g_1^2}{\cosh^2(q_j/2)} + g_2^2\cosh(q_j) + g_3^2\cosh(2q_j)\right) \\ &+ g_4^2 \sum_{j\neq k}\left(\frac{1}{\sinh^2((q_j - q_k)/2)} + \frac{1}{\sinh^2((q_j + q_k)/2)}\right).\end{aligned}$$

- Rational model:

$$\mathcal{H} = \sum_{j=1}^{l}\left(\frac{p_j^2}{2} + g_0^2 q_j^6 + g_1^2 q_j^4 + g_2^2 q_j^2 + g_3^2 q_j^{-2}\right) + g_4^2 \sum_{j\neq k}\left(\frac{1}{(q_j - q_k)^2} + \frac{1}{(q_j + q_k)^2}\right).$$

Here g_0, g_1, g_2, g_3 and g_4 are coupling constants. The Painlevé–Calogero correspondence for P_{III}, P_{II} and P_I suggests the existence of further degeneration of these models.

Our goal in this section is to extend the Painlevé–Calogero correspondence to these higher rank models. Since a complete exposition will become inevitably lengthy, we shall illustrate the elliptic and hyperbolic models in detail, leaving the other cases rather sketchy. The strategy is as follows: The point of departure is the Hamiltonian of Inozemtsev's rank l elliptic model. This gives rise to a rank l version of Manin's equation. Starting with this nonautonomous Hamiltonian system, we seek an analog of the degeneration process for the Painlevé equations. We can thus obtain six types of nonautonomous Hamiltonian systems. At each stage of the degeneration process, we confirm that the nonautonomous Hamiltonian system on the Calogero side can be mapped, by a canonical transformation, to a multicomponent analog of the Painlevé equation of the corresponding type.

B. Elliptic model and multi-component P_{VI}

We now consider the nonautonomous Hamiltonian system,

$$2\pi i \frac{dq_j}{d\tau} = \frac{\partial \mathcal{H}}{\partial p_j}, \quad 2\pi i \frac{dp_j}{d\tau} = -\frac{\partial \mathcal{H}}{\partial q_j}, \tag{73}$$

defined by the Hamiltonian of Inozemtsev's elliptic model. This is a rank l version of Manin's equation. This nonautonomous system is known to describe a family of isomonodromic deformations on the torus.[18]

An honest generalization of the canonical transformation for the case of $l=1$ leads to a multi-component version of P_{VI} as follows.

Theorem 7: *The time-dependent canonical transformation defined by*

$$\lambda_j=\frac{\wp(q_j)-e_1}{e_2-e_1},$$

$$\mu_j=\frac{e_2-e_1}{\wp'(q)}p_j+\frac{2\pi i(e_2-e_1)^2}{\wp'(q_j)^2}f_\tau(q_j)+\frac{e_2-e_1}{2}\left(\frac{\kappa_0}{\wp(q_j)-e_1}+\frac{\kappa_1}{\wp(q_j)-e_2}+\frac{\theta-1}{\wp(q_j)-e_3}\right), \tag{74}$$

and

$$t=\frac{e_3-e_1}{e_2-e_1}. \tag{75}$$

maps (73) to the Hamiltonian system,

$$\frac{d\lambda_j}{dt}=\frac{\partial H}{\partial\mu_j},\quad \frac{d\mu_j}{dt}=-\frac{\partial H}{\partial\lambda_j}, \tag{76}$$

with the Hamiltonian

$$H=\sum_{j=1}^{l}\frac{\lambda_j(\lambda_j-1)(\lambda_j-t)}{t(t-1)}\left[\mu_j^2-\left(\frac{\kappa_0}{\lambda_j}+\frac{\kappa_1}{\lambda_j-1}+\frac{\theta-1}{\lambda_j-t}\right)\mu_j+\frac{\kappa}{\lambda_j(\lambda_j-1)}\right]+\frac{g_4^2}{2t(t-1)}\sum_{j\neq k}\left[\frac{\lambda_j(\lambda_j-1)(\lambda_j-t)+\lambda_k(\lambda_k-1)(\lambda_k-t)}{8(\lambda_j-\lambda_k)^2}-2(\lambda_j+\lambda_k)\right]. \tag{77}$$

Proof: The method of proof for the case of $l=1$ can be applied to the present case as well, yielding the equality

$$\sum_{j=1}^{l}p_j\,dq_j-\mathcal{H}\frac{d\tau}{2\pi i}=\sum_{j=1}^{l}\mu_j\,d\lambda_j-\tilde{H}\,dt+\text{exact form}, \tag{78}$$

where

$$\tilde{H}=\sum_{j=1}^{l}\frac{\lambda_j(\lambda_j-1)(\lambda_j-t)}{t(t-1)}\left[\mu_j^2-\left(\frac{\kappa_0}{\lambda_j}+\frac{\kappa_1}{\lambda_j-1}+\frac{\theta-1}{\lambda_j-t}\right)\mu_j+\frac{\kappa}{\lambda_j(\lambda_j-1)}\right]+\frac{g_4^2}{2t(t-1)(e_2-e_1)}\sum_{j\neq k}(\wp(q_j-q_k)+\wp(q_j+q_k)). \tag{79}$$

What remains is to express the ''two-body potential'' part in terms of λ_j. To this end, let us recall the addition formula,

$$\wp(u-v)+\wp(u+v)=-2\wp(u)-2\wp(v)+\frac{\wp'(u)^2+\wp'(v)^2}{2(\wp(u)-\wp(v))^2}, \tag{80}$$

of the $\wp$-function. Applying it to the case where $(u,v)=(\lambda_j,\lambda_k)$, and substituting

$$\wp(q_j)=e_1+(e_2-e_1)\lambda_j,$$

$$\wp(q_k)=e_1+(e_2-e_1)\lambda_k,$$

$$\wp'(q_j)^2=\frac{(e_2-e_1)^3}{4}\lambda_j(\lambda_j-1)(\lambda_j-t),$$

$$\wp'(q_k)^2=\frac{(e_2-e_1)^3}{4}\lambda_k(\lambda_k-1)(\lambda_k-t),$$

we can rewrite the two-body potential terms as

$$\begin{aligned}\wp(q_j-q_k)+\wp(q_j+q_k)&=-2(e_1+(e_2-e_1)\lambda_j)-2(e_1+(e_2-e_1)\lambda_k)\\&\quad+\frac{(e_2-e_1)^3}{8}\cdot\frac{\lambda_j(\lambda_j-1)(\lambda_j-t)+\lambda_k(\lambda_k-1)(\lambda_k-t)}{(e_1+(e_2-e_1)\lambda_j-e_1-(e_2-e_1)\lambda_k)^2}\\&=-4e_1-2(e_2-e_1)(\lambda_j+\lambda_k)\\&\quad+\frac{e_2-e_1}{8}\cdot\frac{\lambda_j(\lambda_j-1)(\lambda_j-t)+\lambda_k(\lambda_k-1)(\lambda_k-t)}{(\lambda_j-\lambda_k)^2}.\end{aligned}\tag{81}$$

The first term $-4e_1$ is nondynamical, thereby negligible (i.e., can be absorbed by the ''exact form'' part). Removing these terms from $\tilde{H}$, we obtain the Hamiltonian H. Q.E.D.

C. Degeneration of elliptic model to hyperbolic model

The degeneration of the elliptic model is achieved by letting Im $\tau\to+\infty$. Like the degeneration process from P_{VI} to P_V, this is a kind of scaling limit, namely, the coupling constants g_n and the elliptic modulus τ have to be suitably rescaled. To this end, we have to understand the asymptotic behavior of the constants e_1, e_2, e_3 and the $\wp$-function in the limit as Im $\tau\to+\infty$. All necessary data are collected in Appendix B. For instance, the asymptotic expression of e_1, e_2 and e_3 imply that

$$t=1+\frac{e_3-e_2}{e_2-e_1}=1+16\pi^2e^{\pi i\tau}+O(e^{2\pi i\tau}).\tag{82}$$

This is indeed consistent with the scaling rule $t=1+\epsilon\tilde{t}$ in the degeneration process of P_{VI} to P_V.

Having these data, we now rescale the coupling constants and the elliptic modulus as

$$g_0^2=\tilde{g}_0^2,\quad g_1^2=\tilde{g}_1^2,\quad g_2^2=\frac{\tilde{g}_2^2}{\epsilon}+\frac{\tilde{g}_3^2}{\epsilon^2},\quad g_3^3=\frac{\tilde{g}_3^2}{\epsilon^2},\quad g_4^2=\tilde{g}_4^2,\tag{83}$$

and

$$16e^{\pi i\tau}=\epsilon\tilde{t},\tag{84}$$

and consider the limit as $\epsilon\to0$ while leaving $\tilde{g}_n$ and $\tilde{t}$ finite. Note that letting $\epsilon\to0$ amounts to letting Im $\tau\to+\infty$.

The asymptotic expression of $\wp(u)$ and $\wp(u+\omega_n)$ in Appendix B shows that the potential $V(q)$ of the elliptic model behaves as

$$V(q)=\sum_{j=1}^{l}\left(\frac{\tilde{g}_0^2\pi^2}{\sin^2(\pi q_j)}+\frac{\tilde{g}_1^2\pi^2}{\cos^2(\pi q_j)}+\frac{\tilde{g}_2^2\pi^2\tilde{t}}{2}\cos(2\pi q_j)-\frac{\tilde{g}_3^2\pi^2\tilde{t}^2}{8}\cos(4\pi q_j)\right)$$
$$+\tilde{g}_4^2\sum_{j\neq k}\left(\frac{1}{\sin^2(\pi(q_j-q_k))}+\frac{1}{\sin^2(\pi(q_j+q_k))}\right)$$
$$+\text{function of }\epsilon\text{ and }\tilde{t}\text{ only}+O(\epsilon).$$

Thus, removing negligible terms, we obtain the following Hamiltonian in the limit

$$\tilde{\mathcal{H}}=\sum_{j=1}^{l}\left(\frac{p_j^2}{2}+\frac{\tilde{g}_0^2\pi^2}{\sin^2(\pi q_j)}+\frac{\tilde{g}_1^2\pi^2}{\cos^2(\pi q_j)}+\frac{\tilde{g}_2^2\pi^2\tilde{t}}{2}\cos(2\pi q_j)-\frac{\tilde{g}_3^2\pi^2\tilde{t}^2}{8}\cos(4\pi q_j)\right)$$
$$+\tilde{g}_4^2\sum_{j\neq k}\left(\frac{1}{\sin^2(\pi(q_j-q_k))}+\frac{1}{\sin^2(\pi(q_j+q_k))}\right).\tag{85}$$

The asymptotic expression of t determines the equation of motion in the limit. In fact, since

$$\frac{d\tau}{dt}=\frac{\pi}{t(t-1)(e_2-e_1)}=\frac{\pi i}{(1+\epsilon\tilde{t})(-\epsilon\tilde{t})(-\pi^2+O(\epsilon))}$$

and

$$2\pi i\frac{d}{d\tau}=2\pi i\frac{dt}{d\tau}\frac{d\tilde{t}}{dt}\frac{d}{dt}=(2\pi^2\tilde{t}+O(\epsilon^2))\frac{d}{dt},$$

we find that the equations of motion take the following form:

$$2\pi^2\tilde{t}\frac{dq_j}{d\tilde{t}}=\frac{\partial\tilde{\mathcal{H}}}{\partial p_j},\quad 2\pi^2\tilde{t}\frac{dp_j}{d\tilde{t}}=-\frac{\partial\tilde{\mathcal{H}}}{\partial q_j}.\tag{86}$$

The final step is to rescale the variables and the Hamiltonian as

$$q_j\to\frac{q_j}{2\pi i},\quad p_j\to\pi i q_j,\quad \tilde{\mathcal{H}}\to-\pi^2\tilde{\mathcal{H}},\tag{87}$$

and to rename $\tilde{t}$ and $\tilde{\mathcal{H}}$ to t and $\mathcal{H}$. Let us also define the new constants

$$\alpha=-\frac{\tilde{g}_0^2}{2},\quad \beta=\frac{\tilde{g}_1^2}{2},\quad \gamma=-\frac{\tilde{g}_2^2}{2},\quad \delta=\frac{\tilde{g}_3^2}{2},\tag{88}$$

which are to be identified with the four parameters of P_V. The outcome is the nonautonomous Hamiltonian system

$$t\frac{dq_j}{dt}=\frac{\partial\mathcal{H}}{\partial p_j},\quad t\frac{dp_j}{dt}=-\frac{\partial\mathcal{H}}{\partial q_j},\tag{89}$$

with the Hamiltonian

$$\mathcal{H}=\sum_{j=1}^{l}\left(\frac{p_j^2}{2}-\frac{\alpha}{\sinh^2(q_j/2)}-\frac{\beta}{\cosh^2(q_j/2)}+\frac{\gamma t}{2}\cosh(q_j)+\frac{\delta t^2}{8}\cosh(2q_j)\right)$$
$$+g_4^2\sum_{j\neq k}\left(\frac{1}{\sinh^2((q_j-q_k)/2)}+\frac{1}{\sinh^2((q_j+q_k)/2)}\right). \tag{90}$$

This gives a rank l version of the nonautonomous Hamiltonian system on the Calogero side of P_V. Note that the Hamiltonian is essentially the same as the Hamiltonian of Inozemtsev's hyperbolic model, except that the effective coupling constants are now time-dependent.

Remark: The foregoing prescription of scaling limit of the coupling constants and the elliptic modulus is reminiscent of ''renormalization'' in quantum field theories. In this analogy, one can interpret the equations of motion of the Hamiltonian system as ''renormalization group equations,'' in which $\tilde{t}$ plays the role of a ''mass scale'' parameter.

D. Canonical transformation to multi-component P_V

Again, an honest generalization of the canonical transformation for the case of $l=1$ leads to a multi-component version of P_V.

Theorem 8: *The time-dependent canonical transformation defined by*

$$\sqrt{\lambda_j}=-\coth(q_j/2),$$
$$\mu_j=\frac{p_j}{2\sqrt{\lambda_j}(\lambda_j-1)}+\frac{1}{2}\left(\frac{\kappa_0}{\lambda_j}+\frac{\theta_1}{\lambda_j-1}-\frac{\eta_1 t}{(\lambda_j-1)^2}\right), \tag{91}$$

maps (89) to the Hamiltonian system,

$$\frac{d\lambda_j}{dt}=\frac{\partial H}{\partial\mu_j},\quad \frac{d\mu_j}{dt}=-\frac{\partial H}{\partial\lambda_j}, \tag{92}$$

with the Hamiltonian

$$H=\sum_{j=1}^{l}\frac{\lambda_j(\lambda_j-1)^2}{t}\left[\mu_j^2-\left(\frac{\kappa_0}{\lambda_j}+\frac{\theta_1}{\lambda_j-1}-\frac{\eta_1 t}{(\lambda_j-1)^2}\right)\mu_j+\frac{\kappa}{\lambda_j(\lambda_j-1)}\right]$$
$$+\frac{g_4^2}{2t}\sum_{j\neq k}\frac{2(\lambda_j-1)(\lambda_k-1)(\lambda_j+\lambda_k)}{(\lambda_j-\lambda_k)^2}. \tag{93}$$

Proof: The method of proof for the case of $l=1$ can be used as it is. The outcome is the equality

$$\sum_{j=1}^{l}p_j\,dq_j-\mathcal{H}\frac{dt}{t}=2\left(\sum_{j=1}^{l}\mu_j\,d\lambda_j-H\,dt\right)+\text{exact form}, \tag{94}$$

where

$$H=\sum_{j=1}^{l}\frac{\lambda_j(\lambda_j-1)^2}{t}\left[\mu_j^2-\left(\frac{\kappa_0}{\lambda_j}+\frac{\theta_1}{\lambda_j-1}-\frac{\eta_1 t}{(\lambda_j-1)^2}\right)\mu_j+\frac{\kappa}{\lambda_j(\lambda_j-1)}\right]$$
$$+\frac{g_4^2}{2t}\sum_{j\neq k}\left(\frac{1}{\sinh^2((q_j-q_k)/2)}+\frac{1}{\sinh^2((q_j+q_k)/2)}\right). \tag{95}$$

The two-body potential part can be rewritten by use of the identity

$$\frac{1}{\sinh^2(u-v)}+\frac{1}{\sinh^2(u+v)}=4\frac{\cosh(2u)\cosh(2v)-1}{(\cosh(2u)-\cosh(2v))^2}. \tag{96}$$

Substituting $u=q_j/2$, $v=q_k/2$, and also using the equality $\cosh(q_j)=(\lambda_j+1)/(\lambda_j-1)$, we find that

$$\frac{1}{\sinh^2((q_j-q_k)/2)}+\frac{1}{\sinh^2((q_j+q_k)/2)}=\frac{2(\lambda_j-1)(\lambda_k-1)(\lambda_j+\lambda_k)}{(\lambda_j-\lambda_k)^2}, \tag{97}$$

which gives the two-body potential term in H. Q.E.D.

E. Other models

The degeneration process can be further continued, and leads to four more models that correspond to a multi-component version of P_{IV}, P_{III}, P_{II} and P_I. Since the details of derivation are more or less parallel, we show the final results only. The Hamiltonian of each model, like those in the foregoing cases, becomes a sum of l copies of the one-component Hamiltonian and Calogero-like two-body potential terms.

1. Rational model and multi-component P_{IV}

This model can be derived from the hyperbolic model by degeneration. The degeneration process consists of putting the variables and the parameters as

$$t=1+2\epsilon\tilde{t}, \quad q_j=\pi i+\epsilon^{1/2}\tilde{q_j}, \quad p_j=\frac{\tilde{p_j}}{2\epsilon^{1/2}}, \tag{98}$$

and

$$\alpha=\frac{1}{8\epsilon^4}, \quad \beta=\frac{\tilde{\beta}}{4}, \quad \gamma=\frac{1}{4\epsilon^4}, \quad \delta=-\frac{1}{8\epsilon^4}+\frac{\tilde{\alpha}}{2\epsilon^2}, \tag{99}$$

and letting $\epsilon\to 0$ while leaving the ''renormalized'' quantities $\tilde{t}$, etc. finite.

The equations of motion of this model takes the canonical form

$$\frac{dq_j}{dt}=\frac{\partial\mathcal{H}}{\partial p_j}, \quad \frac{dp_j}{dt}=-\frac{\partial\mathcal{H}}{\partial q_j}, \tag{100}$$

with the Hamiltonian

$$\mathcal{H}=\sum_{j=1}^{l}\left[\frac{p_j^2}{2}-\frac{1}{2}\left(\frac{q_j}{2}\right)^6-2t\left(\frac{q_j}{2}\right)^4-2(t^2-\alpha)\left(\frac{q_j}{2}\right)^2+\beta\left(\frac{q_j}{2}\right)^{-2}\right]$$
$$+g_4^2\sum_{j\neq k}\left(\frac{1}{(q_j-q_k)^2}+\frac{1}{(q_j+q_k)^2}\right). \tag{101}$$

The canonical transformation defined by

$$\lambda_j=\left(\frac{q_j}{2}\right)^2, \quad \mu_j=\frac{p_j}{4\sqrt{\lambda_j}}+\frac{1}{4}\left(\lambda_j+2t+\frac{2\kappa_0}{\lambda_j}\right), \tag{102}$$

maps the foregoing nonautonomous system to the Hamiltonian system,

$$\frac{d\lambda_j}{dt}=\frac{\partial H}{\partial\mu_j}, \quad \frac{d\mu_j}{dt}=-\frac{\partial H}{\partial\lambda_j}, \tag{103}$$

with the Hamiltonian

$$H=\sum_{j=1}^{l} 2\lambda_j^2\left[\mu_j^2-\left(\frac{\lambda_j}{2}+t+\frac{\kappa_0}{\lambda}\right)\mu_j+\frac{\theta_0}{2}\right]+\frac{g_4^2}{4}\sum_{j\neq k}\frac{2(\lambda_j+\lambda_k)}{(\lambda_j-\lambda_k)^2}. \tag{104}$$

2. Exponential-hyperbolic model and multi-component $\mathrm{P_{III}}$

This model, too, can be derived from the hyperbolic model by degeneration. This degeneration is achieved by the putting the variables and the parameters as

$$q_j=-\tilde{q}_j-\log\frac{\epsilon}{4},\quad p_j=-\tilde{p}_j, \tag{105}$$

and

$$\alpha=\frac{\tilde{\alpha}}{4\epsilon}+\frac{\tilde{\gamma}}{8\epsilon^2},\quad \beta=-\frac{\tilde{\gamma}}{8\epsilon^2},\quad \gamma=\frac{\tilde{\beta}\epsilon}{4},\quad \delta=\frac{\tilde{\delta}\epsilon^2}{8}, \tag{106}$$

and letting $\epsilon\to 0$.

The equations of motion of this model takes the canonical form

$$t\frac{dq_j}{dt}=\frac{\partial\mathcal{H}}{\partial p_j},\quad t\frac{dp_j}{dt}=-\frac{\partial\mathcal{H}}{\partial q_j}, \tag{107}$$

with the Hamiltonian

$$\mathcal{H}=\sum_{j=1}^{l}\left(\frac{p_j^2}{2}-\frac{\alpha}{4}e^{q_j}+\frac{\beta t}{4}e^{-q_j}-\frac{\gamma}{8}e^{2q_j}+\frac{\delta t^2}{8}e^{-2q_j}\right)$$
$$+g_4^2\sum_{j\neq k}\frac{1}{\sinh^2((q_j-q_k)/2)}. \tag{108}$$

The canonical transformation defined by

$$\lambda_j=e^{q_j},\quad \mu_j=\frac{p_j}{2\lambda_j}+\frac{1}{2}\left(\eta_\infty+\frac{\theta_0}{\lambda_j}-\frac{\eta_0 t}{\lambda_j^2}\right), \tag{109}$$

maps the foregoing nonautonomous system to the Hamiltonian system,

$$\frac{d\lambda_j}{dt}=\frac{\partial H}{\partial\mu_j},\quad \frac{d\mu_j}{dt}=-\frac{\partial H}{\partial\lambda_j}, \tag{110}$$

with the Hamiltonian

$$H=\sum_{j=1}^{l}\frac{\lambda_j^2}{t}\left[\mu_j^2-\left(\eta_\infty+\frac{\theta_0}{\lambda_j}-\frac{\eta_0 t}{\lambda_j^2}\right)\mu_j+\frac{\eta_\infty(\theta_0+\theta_\infty)}{2\lambda_j}\right]+\frac{g_4^2}{2t}\sum_{j\neq k}\frac{4\lambda_j\lambda_k}{(\lambda_j-\lambda_k)^2}. \tag{111}$$

3. Second rational model and multi-component $\mathrm{P_{II}}$

This model can be derived from *both* the rational model and the exponential-hyperbolic model by degeneration. For the degeneration from the rational model, we write the variables and the parameters as

$$t=\frac{-1+4^{-1/3}\epsilon^4\tilde{t}}{\epsilon},\quad \frac{q_j}{2}=\frac{1+2^{-1/3}\epsilon^2\tilde{q}_j}{\epsilon^{3/2}},\quad p_j=\frac{4^{2/3}\tilde{p}_j}{\epsilon^{1/2}},\tag{112}$$

and

$$\alpha=-2\tilde{\alpha}-\frac{1}{2\epsilon^6},\quad \beta=-\frac{1}{2\epsilon^{12}},\tag{113}$$

and let $\epsilon\to 0$. The degeneration from the exponential-hyperbolic model is similarly achieved by putting

$$t=1+2\epsilon^2\tilde{t},\quad q_j=2\epsilon\tilde{q}_j,\quad p_j=\frac{\tilde{p}_j}{\epsilon},\tag{114}$$

and

$$\alpha=-\frac{1}{2\epsilon^6},\quad \beta=\frac{1+4\epsilon^3\tilde{\alpha}}{2\epsilon^6},\quad \gamma=\frac{1}{4\epsilon^6},\quad \delta=-\frac{1}{4\epsilon^6},\tag{115}$$

and again letting $\epsilon\to 0$.

The equations of motion of this model takes the canonical form

$$\frac{dq_j}{dt}=\frac{\partial\mathcal{H}}{\partial p_j},\quad \frac{dp_j}{dt}=-\frac{\partial\mathcal{H}}{\partial q_j},\tag{116}$$

with the Hamiltonian

$$\mathcal{H}=\sum_{j=1}^{l}\left[\frac{p_j^2}{2}-\frac{1}{2}\left(q_j^2+\frac{t}{2}\right)^2-\alpha q_j\right]+g_4^2\sum_{j\neq k}\frac{1}{(q_j-q_k)^2}.\tag{117}$$

The canonical transformation defined by

$$\lambda_j=q_j,\quad \mu_j=p_j+\lambda_j^2+\frac{t}{2},\tag{118}$$

maps the foregoing nonautonomous system to the Hamiltonian system,

$$\frac{d\lambda_j}{dt}=\frac{\partial H}{\partial\mu_j},\quad \frac{d\mu_j}{dt}=-\frac{\partial H}{\partial\lambda_j},\tag{119}$$

with the Hamiltonian

$$H=\sum_{j=1}^{l}\left[\frac{\mu_j^2}{2}-\left(\lambda_j^2+\frac{t}{2}\right)\mu_j-\left(\alpha+\frac{1}{2}\right)\lambda_j\right]+g_4^2\sum_{j\neq k}\frac{1}{(\lambda_j-\lambda_k)^2}.\tag{120}$$

4. Multi-component $\mathrm{P_I}$

This model can be derived from the second rational model, and takes the *same* form on both the Painlevé and Calogero sides. The degeneration process is achieved by putting

$$t=\frac{-6+\epsilon^{12}\tilde{t}}{\epsilon^{10}},\quad q_j=\frac{1+\epsilon^6\tilde{q}_j}{\epsilon^5},\quad p_j=\frac{\tilde{p}_j}{\epsilon},\quad \alpha=4\epsilon^{15},\tag{121}$$

and letting $\epsilon\to 0$. The equations of motion takes the canonical form

$$\frac{dq_j}{dt}=\frac{\partial H}{\partial p_j},\quad \frac{dp_j}{dt}=-\frac{\partial H}{\partial q_j}, \tag{122}$$

with the Hamiltonian

$$H=\sum_{j=1}^{l}\left(\frac{p_j^2}{2}-2q_j^3-tq_j\right)+g_4^2\sum_{j\neq k}\frac{1}{(q_j-q_k)^2}. \tag{123}$$

VI. CONCLUDING REMARKS

We have shown that the Painlevé–Calogero correspondence persists for all the six Painlevé equations and their multi-component generalizations. The Calogero side of this correspondence is a nonautonomous version of Inozemtsev's elliptic model and its various degenerations. Those for P_V and P_{IV} are a nonautonomous version of Inozemtsev's hyperbolic and rational models. The others corresponding to P_{III}, P_{II} and P_I are further degenerations of the hyperbolic and rational models. The pattern of degeneration on the Calogero side repeats the degeneration diagram,

$$\begin{array}{ccccc} P_{VI} & \rightarrow & P_V & \rightarrow & P_{IV} \\ & & \downarrow & & \downarrow \\ & & P_{III} & \rightarrow & P_{II} \quad \rightarrow \quad P_I \end{array}$$

of the Painlevé equations.

This picture applies to the autonomous systems as well. Actually, such degeneration relations in the autonomous case have been more or less well known to experts of Calogero–Moser systems (see the Introduction of van Diejen's paper[16]). The autonomous systems are defined by a Hamiltonian of the same form with the time-dependent coupling constants being replaced by absolute constants (except for the elliptic model, in which case an independent time variable is introduced). Those in the position of the first row of the degeneration diagram are, of course, Inozemtsev's elliptic, hyperbolic and rational models (see Sec. V). Those in the position of P_{III} and P_{II} are defined by the following Hamiltonians:

- Exponential-hyperbolic model:
$$\mathcal{H}=\sum_{j=1}^{l}\left(\frac{p_j^2}{2}+g_0^2e^{q_j}+g_1^2e^{2q_j}+g_2^2e^{-q_j}+g_3^2e^{-2q_j}\right)+g_4^2\sum_{j\neq k}\frac{1}{\sinh^2((q_j-q_k)/2)}.$$
- Second rational model:
$$\mathcal{H}=\sum_{j=1}^{l}\left(\frac{p_j^2}{2}+g_0^2q_j^4+g_1^2q_j^3+g_2^2q_j^2+g_3^2q_j\right)+g_4^2\sum_{j\neq k}\frac{1}{(q_j-q_k)^2}.$$

The Hamiltonian in the position of P_I is redundant in the automonous case, because it is a specialization, rather than a degeneration, of the last Hamiltonian.

Note that the Hamiltonian of the second rational model is a *quartic* perturbation of the usual (A_l type) rational Calogero Hamiltonian. According to the recent work of Caseiro, Françoise and Sasaki,[19] such a quartic (integrable) perturbation always exists for any rational Calogero–Moser system. Inozemtsev's rational model, which is a *sextic* perturbation of the D_l type rational Calogero–Moser system, might admit a similar interpretation.

Back to the Painlevé equations, the extended Painlevé–Calogero correspondence raises many interesting problems. A central issue will be to find an isomonodromic description of the multi-component Painlevé equations. If such an isomonodromic description does exist, it should be related to a new geometric structure.

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APPENDIX A: PROOF OF (42)

Let us introduce the two auxiliary functions:

$$g(u)=\frac{f_\tau(u)}{f'(u)},\quad h(u)=\frac{\vartheta'(u+\omega_1)}{\vartheta(u+\omega_1)}, \tag{A1}$$

associated with the function

$$f(u)=\frac{\wp(u)-e_1}{e_2-e_1} \tag{A2}$$

and the standard elliptic theta function,

$$\vartheta(u)=\sum_{n=-\infty}^{\infty}\exp(\pi i\tau n^2+2\pi i n u). \tag{A3}$$

Lemma 1: $g(u)$ *is a meromorphic function on the* u*-plane with additive quasi-periodicity,*

$$g(u+1)=g(u),\quad g(u+\tau)=g(u)-1. \tag{A4}$$

All poles are of the first order and contained in the lattice $\omega_3+\mathbb{Z}+\tau\mathbb{Z}$*. Furthermore,* $g(u)$ *has zeros at* $u=0$ *and* $u=\omega_1$.

Proof: Since $f(u)$ is a doubly periodic function with primitive periods 1 and τ, $f'(u)$ and $f_\tau(u)$ transform as

$$f'(u+1)=f'(u),\quad f'(u+\tau)=f'(u),$$

$$f_\tau(u+1)=f_\tau(u),\quad f_\tau(u+\tau)=f_\tau(u)-f'(u),$$

under the shift by 1 and τ. This implies the additive quasi-periodicity of $g(u)$. Furthermore, by the construction, $g(u)$ is a meromorphic function on the u-plane, and all possible poles are of the first order and located at the points of $\omega_k+\mathbb{Z}+\tau\mathbb{Z}$. Let us examine the behavior of $g(u)$ at the representative points $u=\omega_0,\omega_1,-\omega_2,\omega_3$:

- As $u\to\omega_0=0$,

$$f(u)=\frac{1}{(e_2-e_1)u^2}+O(1),$$

thereby

$$f'(u)=-\frac{2}{(e_2-e_1)u^3}+O(1),\quad f_\tau(u)=-\frac{e_{2,\tau}-e_{1,\tau}}{(e_2-e_1)^2u^2}+O(1),$$

so that $g(u)$ has rather a zero at $u=0$:

$$g(u)=O(u). \tag{A5}$$

- As $u\to\omega_1=\frac{1}{2}$,

$$f(u)=\frac{1}{e_2-e_1}(\wp(\omega_1)-e_1+\wp'(\omega_1)(u-\omega_1)+O((u-\omega_1)^2))$$

$$= O((u-\omega_1)^2),$$

thereby

$$f'(u) = O(u-\omega_1), \quad f_\tau(u) = O((u-\omega_1)^2),$$

so that $g(u)$ has another zero at $u=\omega_1$:

$$g(u) = O(u-\omega_1). \tag{A6}$$

- As $u \to -\omega_2 = \frac{1}{2} + \tau/2$,

$$f(u) = \frac{1}{e_2-e_1}(\wp(-\omega_2) - e_1 + \wp'(-\omega_2)(u+\omega_2) + O((u+\omega_2)^2))$$
$$= O((u+\omega_2)^2),$$

thereby

$$f'(u) = O(u+\omega_2), \quad f_\tau(u) = O(u+\omega_2),$$

so that $g(u)$ behaves as

$$g(u) = O(1). \tag{A7}$$

- As $u \to \omega_3 = \tau/2$,

$$f(u) = \frac{1}{e_2-e_1}(\wp(\omega_3) - e_1 + \wp'(\omega_3)(u-\omega_3) + O((u-\omega_3)^2))$$
$$= t + O((u-\omega_3)^2),$$

thereby

$$f'(u) = O(u-\omega_3), \quad f_\tau(u) = O(1),$$

so that $g(u)$ turns out to have a pole of the first order at $u=\omega_3$:

$$g(u) = 0((u-\omega_3)^{-1}). \tag{A8}$$

The behavior of $g(u)$ at the other points of $\omega_n + \mathbb{Z} + \tau\mathbb{Z}$ can be deduced from these results by the additive quasi-periodicity of $g(u)$. Q.E.D.

Lemma 2: $h(u)$ is a meromorphic function on the u-plane with additive quasi-periodicity,

$$h(u+1) = h(u), \quad h(u+\tau) = h(u) - 2\pi i. \tag{A9}$$

All poles are of the first order and contained in the lattice $\omega_3 + \mathbb{Z} + \tau\mathbb{Z}$. Furthermore, $h(u)$ has zeros at $u=0$ and $u=\omega_1$.

Proof: Let us recall the fundamental properties of $\vartheta(u)$:

- $\vartheta(u)$ is an entire function on the u-plane with zeros of the first order at the lattice points $\omega_2 + m + n\tau$ $(m,n \in \mathbb{Z})$.
- $\vartheta(u)$ is quasi-periodic,

$$\vartheta(u+1) = \vartheta(u), \quad \vartheta(u+\tau) = e^{-\pi i\tau - 2\pi i u}\vartheta(u).$$

- $\theta(u)$ and $\vartheta(u+1/2)$ are even under the reflection $u \to -u$.

All the properties of $h(u)$ in the statement of the lemma are an immediate consequence of these properties of $\vartheta(u)$. Q.E.D.

Lemma 3: The function $f(u)$ satisfies the equation

$$2\pi i \frac{f_\tau(u)}{f'(u)} = \frac{\vartheta'(u+\omega_1)}{\vartheta(u+\omega_1)}, \tag{A10}$$

where the prime stands for $\partial/\partial u$.

Proof: The foregoing properties of $g(u)$ and $h(u)$ imply the following:

- $2\pi i g(u)-h(u)$ is a doubly periodic meromorphic function with primitive period 1 and τ.
- All poles of $2\pi i g(u)-h(u)$ are of the first order and contained in the lattice $\omega_3+\mathbb{Z}+\tau\mathbb{Z}$.
- $2\pi i g(u)-h(u)$ has zeros at $u=0$ and $u=\omega_1$.

The first two properties imply that $2\pi i g(u)-h(u)$ is a constant. By the last one, this constant has to be zero. We thus find that $2\pi i g(u)-h(u)=0$. Q.E.D.

Lemma 4: $\vartheta(u)$ satisfies the equation

$$(\log \vartheta(u+\omega_1))''=-\wp(u+\omega_3)+\text{function of } \tau \text{ only.} \tag{A11}$$

Proof: The aforementioned complex analytic properties of $\vartheta(u)$ imply the following:

- $(\log \vartheta(u+\omega_1))''$ is a doubly periodic meromorphic function with primitive period 1 and τ.
- All poles of this meromorphic function are contained in the lattice $\omega_3+\mathbb{Z}+\tau\mathbb{Z}$.
- As $u\to-\omega_3$, this function behaves as

$$(\log \vartheta(u+\omega_1))''=-\frac{1}{(u+\omega_3)^2}+O(1).$$

The function $-\wp(u+\omega_3)$, too, has these properties. Accordingly, their difference is a constant function on the u-plane, namely, a function of τ only. Q.E.D.

We now return to the proof of (42). By the third lemma, we have the identity

$$2\pi i\frac{f_\tau(u)}{f'(u)}du=\frac{\vartheta'(u+\omega_1)}{\vartheta(u+\omega_1)}du=\frac{d\vartheta(u+\omega_1)}{\vartheta(u+\omega_1)}-\frac{\partial\vartheta(u+\omega_1)/\partial\tau}{\vartheta(u+\omega_1)}d\tau. \tag{A12}$$

On the other hand, the well known ''heat equation,''

$$4\pi i\frac{\partial\vartheta(u)}{\partial\tau}=\vartheta(u)'', \tag{A13}$$

implies that

$$\frac{\partial\vartheta(u+\omega_1)/\partial\tau}{\vartheta(u+\omega_1)}=\frac{1}{4\pi}\frac{\vartheta(u+\omega_1)''}{\vartheta(u+\omega_2)}=\frac{1}{4\pi i}\left[(\log\vartheta(u+\omega_1))''+\left(\frac{\vartheta'(u+\omega_1)}{\vartheta(u+\omega_1)}\right)^2\right].$$

By the third and fourth lemmas, the last line can be rewritten as

$$\frac{1}{4\pi i}\left[-\wp(u+\omega_3)+\left(2\pi i\frac{f_\tau(u)}{f'(u)}\right)^2\right]+\text{function of } \tau \text{ only,}$$

so that

$$2\pi i\frac{f_\tau(u)}{f'(u)}du=\frac{1}{4\pi i}\left[\wp(u+\omega_3)-\left(2\pi i\frac{f_\tau(u)}{f'(u)}\right)^2\right]d\tau+\text{exact form.} \tag{A14}$$

Substituting $u=q$ gives (42).

APPENDIX B: ASYMPTOTICS OF ELLIPTIC FUNCTIONS

The asymptotic behavior of the $\wp$-function $\wp(u)$, the shifted $\wp$-functions $\wp(u+\omega_k)$ and the constants $e_k=\wp(\omega_k)$, in the limit as $\mathrm{Im}\,\tau\to+\infty$, can be deduced from the well known formula

$$\wp(u)=\sum_{n=-\infty}^{\infty}\frac{\pi^2}{\sin^2(\pi(u+n\tau))}-\frac{\pi^2}{3}-\sum_{n=1}^{\infty}\frac{2\pi^2}{\sin^2(\pi n\tau)}. \tag{B1}$$

Let us first consider the asymptotic behavior of $\wp(u)$ itself. The constant $(n=0)$ term in the first sum is of order 1 and the n-th term is of order $e^{2n\pi i\tau}$. Similarly, the n-th term in the second sum is of order $e^{2n\pi i\tau}$. Therefore

$$\wp(u)=\frac{\pi^2}{\sin^2(\pi u)}-\frac{\pi^2}{3}+O(e^{2\pi i\tau}). \tag{B2}$$

A similar estimate leads to the following asymptotic expression for the shifted $\wp$-functions:

$$\begin{aligned}\wp(u+\omega_1)&=\frac{\pi^2}{\cos^2(\pi u)}-\frac{\pi^2}{3}+O(e^{2\pi i\tau}),\\ \wp(u+\omega_2)&=-\frac{\pi^2}{3}+8\pi^2\cos(2\pi u)e^{\pi i\tau}+O(e^{2\pi i\tau}),\\ \wp(u+\omega_3)&=-\frac{\pi^2}{3}-8\pi^2\cos(2\pi u)e^{2\pi i\tau}+O(e^{2\pi i\tau}).\end{aligned} \tag{B3}$$

In fact, the degeneration process of the elliptic model requires us to know the asymptotic expression of $\wp(u+\omega_2)+\wp(u+\omega_3)$ to the order $e^{2\pi i\tau}$. This can be achieved by the following calculations:

$$\begin{aligned}\wp(u+\omega_2)+\wp(u+\omega_3)&=\sum_{n=-\infty}^{\infty}\frac{\pi^2}{\cos^2\left(u+\frac{\tau}{2}+n\tau\right)\sin^2\left(u+\frac{\tau}{2}+n\tau\right)}-\frac{2\pi^2}{3}-\sum_{n=1}^{\infty}\frac{4\pi^2}{\sin^2(\pi n\tau)}\\ &=-\frac{2\pi^2}{3}-32\pi^2\cos(2\pi u)e^{2\pi i\tau}+16\pi^2e^{2\pi i\tau}+O(e^{3\pi i\tau}).\end{aligned} \tag{B4}$$

We now consider the constants e_k. For instance, e_1 can be written as

$$\begin{aligned}e_1&=\sum_{n=-\infty}^{\infty}\frac{\pi^2}{\cos^2(\pi n\tau)}-\frac{\pi^2}{3}-\sum_{n=1}^{\infty}\frac{2\pi^2}{\sin^2(\pi n\tau)}\\ &=\frac{2}{3}\pi^2+\sum_{n=1}^{\infty}\frac{2\pi^2}{\cos^2(\pi n\tau)}-\sum_{n=1}^{\infty}\frac{2\pi^2}{\sin^2(\pi n\tau)}.\end{aligned} \tag{B5}$$

The constant $2\pi^2/3$ becomes the leading term; the leading $(n=1)$ terms of the last two series give the next-leading term of the order $e^{2\pi i\tau}$. e_2 and e_3 can be similarly analyzed. Thus the following asymptotic formulas are obtained:

$$\begin{aligned}e_1&=\frac{2\pi^2}{3}+16\pi^2e^{2\pi i\tau}+O(e^{4\pi i\tau}),\\ e_2&=-\frac{\pi^2}{3}+8\pi^2e^{\pi i\tau}+O(e^{2\pi i\tau}),\\ e_3&=-\frac{\pi^2}{3}-8\pi^2e^{\pi i\tau}+O(e^{2\pi i\tau}).\end{aligned} \tag{B6}$$

In particular, $e_2-e_1\to-\pi^2$, as expected.

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On the problem of algebraic completeness for the invariants of the Riemann tensor: I

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We present a new determining set, CZ, of Riemann invariants which possesses the minimum degree property. From an analysis on the possible independence of CZ, we are led to the division of all space–times into two distinct, invariantly characterized, classes: a general class $\mathcal{M}_{G^+}$, and a special, singular class $\mathcal{M}_S$. For each class, we provide an independent set of invariants ($\mathcal{I}_{G^+} \subset \mathrm{CZ}$ and $\mathcal{I}_S \subset \mathrm{CZ}$, respectively) which, with the results of a sequel paper, will be shown to be algebraically complete. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In the literature, there are many papers devoted to the study of the scalar invariants of the Riemann tensor. The motivation behind this study has been, primarily, the coordinate invariant characterization of certain geometrical properties of space–times. For example, it has been shown that these invariants play an important role in the study of curvature singularities, classification of the Weyl and Ricci tensors and more fundamentally in the problem of the equivalence of two space–time metrics.

It is well known that, in general, there are 14 (algebraically) independent, second-order, invariants formed from the Riemann tensor R_{abcd}. This is simply a consequence of the fact that the 20 independent components of R_{abcd} can be reduced to 14 using the 6-parameter group freedom of the Lorentz transformations. Alternatively, the 14 independent algebraic invariants can be considered to be made up of the 4 independent eigenvalues of each of the Weyl and Ricci tensors together with the 6 parameters specifying the Lorentz transformation between the Weyl and Ricci canonical tetrads.[1,2] However, there is no guidance as to how these invariants may be constructed.

In the literature, there are different definitions of ''complete.'' Our definition of an ''algebraically complete'' set is motivated by the folllowing questions: How much algebraically independent information that is in the Riemann tensor is present in its polynomial invariants, and what is the minimum number of invariants of lowest possible degree, needed so that this maximum amount of information is contained? Accordingly, we define an ''algebraically complete'' set of Riemann invariants $\mathcal{I}=\{I_1, I_2, \ldots, I_n\}$ as one having the following properties: (i) any other invariant can be expressed in an algebraic relation (not necessarily equal to a polynomial) which determines that invariant for all Petrov or Segre types, with some or all of $I_1, I_2, \ldots, I_n$ and their complex conjugates, and (ii) no invariant $I_i \in \mathcal{I}$ can <u>always</u> (i.e., for all Petrov or Segre types) be expressed in an algebraic relation, which determines I_i, with the remaining invariants in $\mathcal{I}$. Note that this definition would essentially lead to that given by Zakhary and McIntosh.[3] Any set of invariants which satisfies property (i) will be called ''determining'' and any set which satisfies property (ii) is said to be ''not always dependent.'' Hence, a set $\mathcal{I}$ is said to be ''always dependent'' if there exists an invariant $I_i \in \mathcal{I}$ such that I_i can always be expressed in an algebraic relation which determines (for all Petrov or Segre types) I_i, with the remaining invariants in $\mathcal{I}$.

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TABLE I. Equivalent invariants in Sneddon's set.

CZ	$\mathcal{K}$
R	R
w_1	$[A^2]=[\Psi^2]$
w_2	$\det A=\det \Psi$
r_1	$[B]=[K]$
r_2	$\Delta=\det \Gamma$
r_3	$[B^2]=[K^2]$
m_1	$[AB]=[\Psi K]=\overline{[C]}$
m_2	$[A^2B]=[\Psi^2K]=\overline{[D]}$
m_3	$[AB^2]=[\Psi K^2]=\overline{[BC]}$
m_4	$[AC]=[\Psi\Gamma\overline{\Psi\Gamma}]$
m_5	$[AD]=[\Psi\Gamma\overline{\Psi^2\Gamma}]=\overline{[A^2C]}$
m_6	$[A^2D]=[\Psi^2\Gamma\overline{\Psi^2\Gamma}]$

For simplicity, in the remainder of this article, we will use the term ''dependent'' to mean ''always dependent'' and use the term ''independent'' to mean ''not always dependent,'' when referring to a set of invariants.

Recently, Bonanos[4] and Sneddon[5–7] have studied the problem of completeness for a set of Riemann tensor invariants. Bonanos studied invariants formed from contractions with only Ψ_{ABCD} and the Plebanski spinor $\chi_{ABCD}=\Phi_{(AB}{}^{\dot{C}\dot{D}}\Phi_{CD)\dot{C}\dot{D}}$ but not with $\overline{\Psi}_{\dot{A}\dot{B}\dot{C}\dot{D}}$, while Sneddon examined the problem, in general, in a comprehensive study using rotor calculus. It is interesting to compare our work with theirs.

First, we note that *algebraically complete* is different from *complete* in the usual classical sense which is the one that both Bonanos and Sneddon use (it is more restrictive than ours in that in the construction of a complete set, they include an invariant in a set if it is not equal to some *polynomial* of the already existing elements in the set. On the other hand, in terms of our definition, an invariant is independent of a ''base'' set if it cannot be expressed for all Segre and Petrov types in an *algebraic* relation with the elements of that set). On this matter, we believe that our definition is more appropriate for relativity. Second, our primary concern is always with how much algebraic information that is in the Riemann tensor is present in its polynomial invariants. As will be shown below, no set of curvature invariants formed from contractions with only Ψ_{ABCD} and $\Phi_{AB}{}^{\dot{C}\dot{D}}$ can contain all of the possible algebraic information that is in R_{abcd}. It is essential that contraction ''mixing'' between Ψ_{ABCD} and $\overline{\Psi}_{\dot{A}\dot{B}\dot{C}\dot{D}}$ be included. This is also evident from Sneddon's work. We conclude that Bonanos' set cannot be algebraically complete. On the other hand, Sneddon's set $\mathcal{K}$ is complete in the usual classical sense. However, within the context of this work, his set is unnecessarily large (consisting of the equivalent of 38 real invariants) and of too high degree (going up to overall degree 11). This could make his set unwieldy to work with in many practical applications (the general expansion of some of the high-degree invariants would lead to extremely large expressions). What we will show in this and a sequel paper is that for a determining set, we need at most the equivalent of 18 real invariants with a maximum overall degree of 6. Also, our proposed set of invariants is essentially contained in $\mathcal{K}$, and in Table I we list the equivalence.

As an additional point, it is important to note that there are space–times where the set of all polynomial invariants does not contain all of the information that is in R_{abcd}. An illustrative example will be given below.

Prior to 1991, there were a number of sets of 14 invariants in the literature claiming to be independent.[8–16] However, none of these sets can be algebraically complete.[14,17] This suggests that such a set should contain more than 14 invariants and hence, in general, be redundant. Some of the members of this set would then be connected by a number of algebraic relations for different Petrov or Segre types, with no one relation holding for all types. Also, Carminati and

McLenaghan,[17] for the first time, pointed out two highly desirable properties of an algebraically complete set, namely (a) it must consist of invariants of the lowest possible degree, and (b) it must be the smallest set which contains the maximum number (less than or equal to 14) of independent invariants for any Petrov or Segre type. In this article, we intend to construct a determining set of invariants subject to property (a) while attempting to satisfy properties (ii) and (b). However, we note that our construction process would generally lead to a set having a reduced number of elements but not necessarily the minimum number, since we are satisfying property (a) as well. Theoretically, it could be possible to have a determining or algebraically complete set with a smaller number of invariants if higher degree scalars were to be introduced. This issue still remains unresolved. Priority will be given to property (a).

As will be evident from the backsolving method presented in this and a sequel paper, given particular values for our invariants, multiple solutions will result (as a consequence of taking roots of algebraic equations) for the curvature components. This is not an issue in the process of establishing the determining nature of the proposed set of invariants since we are trying to establish sufficiency. In practical terms, one is not concerned with explicitly applying this process but rather to invariantly express (if possible) certain geometrical properties [like alignment between principal null directions (PND's) of the Weyl and Ricci tensor, or electric and magnetic characteristics of the Weyl tensor, etc.] with the use of just the polynomial invariants of the Riemann tensor for a given particular space–time.

This is the first of two papers dedicated to eventually establishing an algebraically complete set of second-order Riemann invariants for each canonically different space–time. In this paper, we will show that the set CM, as proposed by Carminati and McLenaghan, is not algebraically complete. Further, although the set of invariants as proposed by Zakhary and McIntosh (ZM)[3] is algebraically complete (as shown later) for the general class, $\mathcal{M}_{G^+}$, we will also show that it fails for the special singular class, $\mathcal{M}_S$ (as described below), since it is missing an essential invariant. Our main purpose in this paper is to propose a new determining set of invariants CZ that contains that missing invariant, possesses the minimum degree property (a), and simultaneously attempts to satisfy properties (ii) and (b). The possible independence of the invariants of this set is analyzed[18,19] and as a consequence we are led to the division of all space–times into two distinct, invariantly characterized, classes: a general class $\mathcal{M}_{G^+}$, and a singular class $\mathcal{M}_S$. For each class, we provide an independent set of invariants ($\mathcal{I}_{G^+} \subset \mathrm{CZ}$ and $\mathcal{I}_S \subset \mathrm{CZ}$, respectively) which, with the results of a sequel paper, will be shown to be algebraically complete.

The CZ set consists of the following invariants, using the notation (but different definitions of the invariants) of Carminati and McLenaghan:

$$R := g^{ab} g^{cd} R_{acdb},$$

$$w_1 := \frac{1}{6} \Psi_{ABCD} \Psi^{ABCD},$$

$$w_2 := \frac{1}{6} \Psi_{ABCD} \Psi^{CD}{}_{EF} \Psi^{EFAB},$$

$$r_1 := \frac{1}{3} \Phi_{AB\dot{A}\dot{B}} \Phi^{AB\dot{A}\dot{B}},$$

$$r_2 := \frac{1}{6} \Phi_{AB\dot{A}\dot{B}} E^{AB\dot{A}\dot{B}},$$

$$r_3 := \frac{1}{12} E_{AB\dot{A}\dot{B}} E^{AB\dot{A}\dot{B}},$$

TABLE II. Relations between sets.

CZ	ZM	CM
R	R	R
w_1	I	$\frac{1}{6}w_1$
w_2	J	$\frac{1}{6}w_2$
r_1	I_6	$\frac{1}{3}r_1$
r_2	I_7	$\frac{1}{3}r_2$
r_3	I_8	$\frac{1}{3}r_3-\frac{1}{12}r_1^2$
m_1	K	m_1
m_2	L	$m_2-\frac{1}{3}w_1r_1$
m_3	$-M$	—
m_4	M_1	m_3
m_5	M_2	$m_5-\frac{1}{3}w_1\overline{m_1}$
m_6	—	—

$$m_1 := \Psi_{ABCD}\Phi^{CD}{}_{\dot{C}\dot{D}}\Phi^{AB\dot{C}\dot{D}},$$

$$m_2 := \Psi^{EF}{}_{(AB}\Psi_{CD)EF}\Phi^{AB}{}_{\dot{C}\dot{D}}\Phi^{CD\dot{C}\dot{D}},$$

$$m_3 := \Psi_{ABCD}\Phi^{AE\dot{A}\dot{B}}\Phi^{B}{}_{E\dot{A}\dot{C}}\Phi^{CF\dot{C}\dot{D}}\Phi^{D}{}_{F\dot{D}\dot{B}},$$

$$m_4 := \Psi^{AB}{}_{CD}\Phi^{CD}{}_{\dot{A}\dot{B}}\overline{\Psi}^{\dot{A}\dot{B}}{}_{\dot{C}\dot{D}}\Phi_{AB}{}^{\dot{C}\dot{D}},$$

$$m_5 := \Psi_{(AB}{}^{CD}\Psi_{EF)CD}\overline{\Psi}_{\dot{A}\dot{B}\dot{C}\dot{D}}\Phi^{AB\dot{C}\dot{D}}\Phi^{EF\dot{A}\dot{B}},$$

$$m_6 := \Psi^{AB}{}_{CD}\Psi^{CD}{}_{EF}\Phi^{EF}{}_{\dot{A}\dot{B}}\overline{\Psi}^{\dot{A}\dot{B}}{}_{\dot{C}\dot{D}}\overline{\Psi}^{\dot{C}\dot{D}}{}_{\dot{E}\dot{F}}\Phi_{AB}{}^{\dot{E}\dot{F}},$$

where $E^{AB}{}_{\dot{C}\dot{D}} := 2\Phi^{A}{}_{E\dot{F}(\dot{C}}\Phi^{BE\dot{F}}{}_{\dot{D})}$.

For future reference, we give, in Table II, the relations between the various sets. In Tables III and IV below,[20,3] we summarize the syzygies for the different Petrov and Segre types of the Weyl and Ricci tensors, respectively.

TABLE III. The Weyl Syzygies.

Petrov Types	Syzygies
I	—
II, D	$w_1^3=w_2^2$
III, N, O	$w_1=w_2=0$

TABLE IV. The Ricci Syzygies.

Ricci Degeneracy	Segre Types	Syzygies
{1111}	[1,111], $[Z\bar{Z}11]$	—
{112}	[1,1(11)], [(1,1)11], $[Z\bar{Z}(11)]$, [211]	$r_2^2(4r_1^3-6r_1r_3+r_2^2)=r_3^2(3r_1^2-4r_3)$
{22}	[(1,1)(11)], [2(11)]	$r_2=r_3=0$
{13}	[1,(111)], [(1,11)1], [(21)1], [31]	$r_2^2=r_1^3$, $r_3=r_1^2$
{4}	[(31)], [(211)], [(1,111)]	$r_1=r_2=r_3=0$

II. AN INDEX THEOREM

Before proceeding with the analysis of our invariants, we shall need to establish a result on the general structure of any invariant formed from the Weyl and Ricci spinors:

$$\Psi_{ABCD}=\Psi_0\iota_A\iota_B\iota_C\iota_D-4\Psi_1o_{(A}\iota_B\iota_C\iota_{D)}+6\Psi_2o_{(A}o_B\iota_C\iota_{D)}-4\Psi_3o_{(A}o_Bo_C\iota_{D)}+\Psi_4o_Ao_Bo_Co_D,$$

$$\Phi_{AB\dot{A}\dot{B}}=\Phi_{00}\iota_A\iota_B\bar{\iota}_{\dot{A}}\bar{\iota}_{\dot{B}}-2\Phi_{01}\iota_A\iota_B\bar{\iota}_{(\dot{A}}\bar{o}_{\dot{B})}+\Phi_{02}\iota_A\iota_B\bar{o}_{\dot{A}}\bar{o}_{\dot{B}}-2\Phi_{10}o_{(A}\iota_{B)}\bar{\iota}_{\dot{A}}\bar{\iota}_{\dot{B}}+4\Phi_{11}\iota_{(A}o_{B)}\bar{\iota}_{(\dot{A}}\bar{o}_{\dot{B})}$$
$$-2\Phi_{12}\iota_{(A}o_{B)}\bar{o}_{\dot{A}}\bar{o}_{\dot{B}}+\Phi_{20}o_Ao_B\bar{\iota}_{\dot{A}}\bar{\iota}_{\dot{B}}-2\Phi_{21}o_Ao_B\bar{\iota}_{(\dot{A}}\bar{\iota}_{\dot{B})}+\Phi_{22}o_Ao_B\bar{o}_{\dot{A}}\bar{o}_{\dot{B}}.$$

Index Theorem: Let a, b, c be non-negative integers and let $\boldsymbol{\Psi}^a\bar{\boldsymbol{\Psi}}^b\boldsymbol{\Phi}^c$ represent any of the complete contractions (invariant) of a copies of the Weyl spinor, b copies of its complex conjugate and c copies of the Ricci spinor. Then any term in the expansion of this invariant has the form

$$\Psi_0^{a_0}\Psi_1^{a_1}\Psi_2^{a_2}\Psi_3^{a_3}\Psi_4^{a_4}\bar{\Psi}_0^{b_0}\bar{\Psi}_1^{b_1}\bar{\Psi}_2^{b_2}\bar{\Psi}_3^{b_3}\bar{\Psi}_4^{b_4}\Phi_{00}^{c_{00}}\Phi_{01}^{c_{01}}\Phi_{02}^{c_{02}}\Phi_{10}^{c_{10}}\Phi_{11}^{c_{11}}\Phi_{12}^{c_{12}}\Phi_{20}^{c_{20}}\Phi_{21}^{c_{21}}\Phi_{22}^{c_{22}}$$

where $a_0,\ldots,a_4,b_0,\ldots,b_4,c_{00},\ldots,c_{22}$ are non-negative integers which must satisfy the following conditions:

$$a_0+a_1+a_2+a_3+a_4=a,$$

$$b_0+b_1+b_2+b_3+b_4=b,$$

$$c_{00}+c_{01}+c_{02}+c_{10}+c_{11}+c_{12}+c_{20}+c_{21}+c_{22}=c,$$

$$a_1+2a_2+3a_3+4a_4+c_{10}+c_{11}+c_{12}+2c_{20}+2c_{21}+2c_{22}=2a+c,$$

$$b_1+2b_2+3b_3+4b_4+c_{01}+2c_{02}+c_{11}+2c_{12}+c_{21}+2c_{22}=2b+c.$$

The proof of this result is readily established by counting the number of contracting pairs of dotted and undotted indices.

When applying the index theorem, note the following:

(1) If $\Phi_{ij}=0$ (or $\Psi_i=0$), we set $c_{ij}=0$ (or $a_i=b_i=0$).
(2) If an invariant does not include Ψ_i's, we set all $b_i=0$ and $b=0$.
(3) If $\Phi_{ij}=1$ (or $\Psi_i=1$), we do not set $c_{ij}=0$ (or $a_i=b_i=0$).
(4) If $\Phi_{ij}=\Phi_{kl}$, we do not set $c_{ij}=c_{kl}$.

To illustrate this theorem's use, consider the Segre type [(3,1)] in the canonical frame where the only nonzero Ricci components are $\Phi_{12}=\Phi_{21}=1$. In this case, we set $c_{ij}=0$, except c_{12} and c_{21}. For an invariant of the form $\mathbf{\Psi}\overline{\mathbf{\Psi}}\mathbf{\Phi}^2$, $a=b=1$ and $c=2$. Hence, the index theorem implies the following:

$$a_0+a_1+a_2+a_3+a_4=1,$$

$$b_0+b_1+b_2+b_3+b_4=1,$$

$$c_{12}+c_{21}=2,$$

$$a_1+2a_2+3a_3+4a_4+c_{12}+2c_{21}=4,$$

$$b_1+2b_2+3b_3+4b_4+2c_{12}+c_{21}=4.$$

These equations allow only three solutions:

$$\{c_{12}=0,c_{21}=2,a_2=1,a_0=a_1=a_3=a_4=0,b_0=1,b_1=b_2=b_3=b_4=0\},$$

$$\{c_{12}=1,c_{21}=1,a_1=1,a_0=a_2=a_3=a_4=0,b_1=1,b_0=b_2=b_3=b_4=0\},$$

$$\{c_{12}=2,c_{21}=0,a_0=1,a_1=a_2=a_3=a_4=0,b_2=1,b_0=b_1=b_3=b_4=0\}.$$

This agrees with the expression of m_4 which contains exactly the correct three terms. In fact, $m_4=4(\Psi_0\overline{\Psi}_2\Phi_{21}^2+2\Psi_1\overline{\Psi}_1\Phi_{12}\Phi_{21}+\Psi_2\overline{\Psi}_0\Phi_{12}^2)$.

III. PROPERTIES OF THE CZ SET

We have carried out a detailed study[21] of the possible canonical frames for the different Segre types using Hall's approach.[22] Our analysis is somewhat more detailed than Hall's in that we give more explicit descriptions of the canonical forms together with the remaining tetrad freedom for each case. The details of this work will be published in a sequel paper. For our current purposes, we will only need canonical frames for the Segre types [1,111], [1,1(11)], [(2,11)] and [2,11].

In this section, we shall construct the CZ set so that it possesses the minimum degree property (a) and attempts to satisfy properties (i), (ii) and (b). To begin with, we will look at Ricci tensors that are of Segre Type [1,111]. The canonical frame is completely fixed by the Ricci tensor and described by $\Phi_{00}=\Phi_{22}\neq 0$, Φ_{11}, $\Phi_{02}=\Phi_{20}\neq 0$, $\Phi_{01}=\Phi_{12}=0$, with $4\Phi_{11}^2\neq(\Phi_{00}\pm\Phi_{02})^2$.

We will now show that the set of invariants $\mathcal{I}_G=\{R,w_1,w_2,r_1,r_2,r_3,m_1,m_2,m_3\}$ is algebraically complete, for this Segre type, by completely backsolving for the curvature components in terms of the invariants where, in terms of equivalent real invariants, the number of nonzero curvature components equals the number of invariants. We begin with the backsolving for the Ricci components Φ_{ab}. In our canonical frame, the Ricci invariants are

$$r_1=\tfrac{2}{3}(\Phi_{00}^2+\Phi_{02}^2+2\Phi_{11}^2),$$

$$r_2=2\Phi_{11}(\Phi_{00}^2-\Phi_{02}^2),$$

$$r_3=\tfrac{1}{3}(\Phi_{00}^4-2\Phi_{00}^2\Phi_{02}^2+8\Phi_{00}^2\Phi_{11}^2+8\Phi_{02}^2\Phi_{11}^2+\Phi_{02}^4).$$

The Jacobian of this system is $\frac{64}{9}J$, where

$$J=\Phi_{00}\Phi_{02}(\Phi_{00}+\Phi_{02}+2\Phi_{11})(\Phi_{00}+\Phi_{02}-2\Phi_{11})(\Phi_{00}-\Phi_{02}+2\Phi_{11})(\Phi_{00}-\Phi_{02}-2\Phi_{11}),$$

and consequently is always nonzero. Thus it follows that the Ricci invariants r_1,r_2,r_3 are always backsolvable for Φ_{ab}. We note that

FIG. 1. Quadratic-degree invariants.

$$J^2=\tfrac{27}{16}(r_3^2(3r_1^2-4r_3)-r_2^2(4r_1^3-6r_1r_3+r_2^2)),$$

and that $J=0$, which can be alternatively written as $4(r_1^2-r_3)^3=(2r_1^3-3r_1r_3+r_2^2)^2$ (similar to the condition $w_1^3=w_2^2$), is the condition for the Ricci spinor to be algebraically special.

To facilitate the backsolving of the Weyl components Ψ_i, we make the following substitutions:

$$\Psi_0=x+y,\quad \Psi_1=u+v,\quad \Psi_3=u-v,\quad \Psi_4=x-y.$$

The Weyl and mixed invariants then take the form

$$w_1=\tfrac{1}{3}(x^2-y^2-4u^2+4v^2+3\Psi_2^2),$$

$$w_2=2\Psi_2u^2-2\Psi_2v^2-\Psi_2^3-2u^2x+4yuv-2v^2x+\Psi_2x^2-\Psi_2y^2,$$

$$m_1=2\Psi_2\Phi_{00}^2-8\Psi_2\Phi_{11}^2+4\Phi_{00}\Phi_{02}x+2\Psi_2\Phi_{02}^2,$$

$$\begin{aligned}m_2=&-2\Psi_2^2\Phi_{02}^2+8\Psi_2^2\Phi_{11}^2-2\Psi_2^2\Phi_{00}^2+\tfrac{16}{3}\Phi_{11}^2v^2-\tfrac{4}{3}\Phi_{02}^2v^2-\tfrac{4}{3}\Phi_{00}^2v^2-\tfrac{16}{3}\Phi_{11}^2u^2+\tfrac{4}{3}\Phi_{02}^2u^2\\&+\tfrac{4}{3}\Phi_{00}^2u^2-8\Phi_{00}v^2\Phi_{02}-8\Phi_{00}u^2\Phi_{02}-\tfrac{8}{3}\Phi_{11}^2x^2+\tfrac{8}{3}\Phi_{11}^2y^2+\tfrac{2}{3}\Phi_{02}^2x^2-\tfrac{2}{3}\Phi_{02}^2y^2+\tfrac{2}{3}\Phi_{00}^2x^2\\&-\tfrac{2}{3}\Phi_{00}^2y^2+8\Psi_2\Phi_{00}\Phi_{02}x,\end{aligned}$$

$$m_3=8\Psi_2\Phi_{11}^2\Phi_{00}^2-16\Phi_{02}\Phi_{00}\Phi_{11}^2x+4\Psi_2\Phi_{00}^2\Phi_{02}^2+8\Psi_2\Phi_{02}^2\Phi_{11}^2-2\Psi_2\Phi_{00}^4-2\Psi_2\Phi_{02}^4.$$

We begin by noting that the system $\{m_1,m_3\}$ which contains only the Weyl variables x and Ψ_2 has Jacobian equal to $-8J$ which is nonzero. Hence, we may regard x and Ψ_2 as (locally) implicit functions of m_1 and m_3 and Φ_{ab} (which in turn are determined by the Ricci invariants). Next, we solve w_1 for u^2 and use this equation to eliminate u from m_2. We can always solve this resulting equation for v^2, since its coefficient is nonzero. Finally, after solving w_2 for $4yuv$ and squaring, we substitute the solutions for u^2 and v^2 into this expression to obtain a polynomial equation of degree 6 in y with the coefficients being polynomials in x, Ψ_2, Φ_{ab}, and invariants. This polynomial can always be solved for y, since the coefficient of y^6 is $J/\Phi_{00}\Phi_{02}\neq 0$. Thus complete backsolving has been achieved.

Next, we will show that the set $\mathcal{I}_G$ is of the lowest possible degree. We begin by listing all (inequivalent and excluding complex conjugates and trivially dependent invariants which have separable product contractions) invariants at the various degree levels. This is done diagramatically as follows. A straight line between quantities indicates a contraction between undotted spinor indices and a dashed line indicates a contraction between dotted indices (see Fig. 1–4).

By direct calculation, it can be readily shown that all of the quadratic, cubic and quartic scalars represented in Fig. 1-3, constitute an equivalent set to $\mathcal{I}_4$

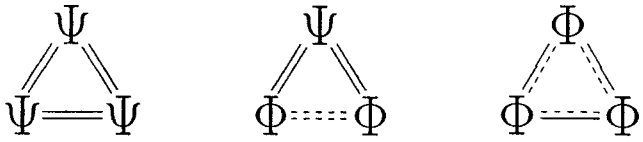

FIG. 2. Cubic-degree invariants.

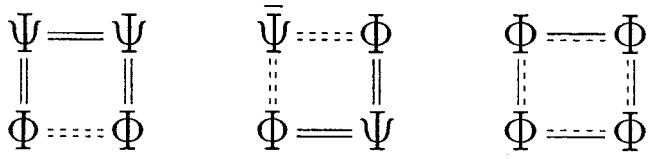

FIG. 3. Independent quartic-degree invariants.

$=\{R,w_1,w_2,r_1,r_2,r_3,m_1,m_2,m_4\}$. It is also easy to show that all the remaining quartic scalars represented in Fig. 4 are either identically zero or dependent on the remaining ones. Now we observe that this set $\mathcal{I}_4$, differs from $\mathcal{I}_G$ in that it contains m_4 but does not contain m_3 and therefore $\mathcal{I}_4$ contains the equivalent of 13 independent real invariants (less information than $\mathcal{I}_G$ since m_4 is real whereas m_3 is complex, in general). Thus, we conclude that the set $\mathcal{I}_4$, which is constructed using the minimum degree property, and contains all of the information in all scalars up to and including quartic degree, cannot contain all possible information for this Segre type, whereas $\mathcal{I}_G$ does. Next, we note that adding one more real invariant of degree five to $\mathcal{I}_4$ will not make it algebraically complete (in general). This can be shown as follows. First, all real, nontrivial invariants of degree five must be of the form $\Psi\bar{\Psi}\Phi^3$ and they are equivalent[7] (if independent of $\mathcal{I}_4$). Consider one such invariant to be $m:=\Psi_A{}^B{}_{DE}\Phi^{DE}{}_{\dot{A}}{}^{\dot{B}}\bar{\Psi}_{\dot{B}}{}^{\dot{C}}{}_{\dot{D}\dot{E}}\Phi_B{}^{C\dot{D}\dot{E}}\Phi_C{}^{A}{}_{\dot{C}}{}^{\dot{A}}$. For Segre type [1,111] and Petrov type **N**, we have, by direct calculation, $m^2=Em_4$, where E is a polynomial in Weyl and Ricci components. Hence, in the special case that $m_4=0$ (which is possible), we have $m=0$ but $m_3\neq 0$. This means that with one real condition, two real invariants vanish. Thus we conclude that m_4 and m cannot replace m_3 in general.

Since $\mathcal{I}_G$ is obtained from $\mathcal{I}_4$ by removing m_4 and adding m_3 and the addition of a real invariant of degree five to $\mathcal{I}_4$ is not sufficient, it follows that the set $\mathcal{I}_G$ must satisfy the minimum degree property (a).

We have thus far established the fact that an algebraically complete set satisfying property (a) must contain all of the invariants (or their equivalent at each corresponding degree level) in $\mathcal{I}_G$. Now, let us address the following key question: ''*Is* $\mathcal{I}_G$ *algebraically complete for all Segre Types*?'' To answer this question, we need to consider the Segre Type [(2,11)].

For Segre Type [(2,11)], the canonical frame is fixed (up to a 2-p null rotation plus a spatial rotation) by the Ricci tensor and described by $\Phi_{00}=\Phi_{01}=\Phi_{02}=\Phi_{11}=\Phi_{12}=0,\Phi_{22}=1$.

Case 1: $\Psi_0\neq 0$: In this case, we can make Ψ_0 real and $\Psi_1=0$. Hence, the elements of $\mathcal{I}_G$ (except R) are given by

$$w_1=\tfrac{1}{3}(\Psi_0\Psi_4+3\Psi_2^2),$$

$$w_2=\Psi_0\Psi_2\Psi_4-\Psi_0\Psi_3^2+3\Psi_2^3,$$

$$r_1=0,$$

$$r_2=0,$$

$$r_3=0,$$

$$m_1=0,$$

$$m_2=0,$$

$$m_3=0.$$

It is clear that we do not have sufficient curvature information in the invariants of $\mathcal{I}_G$ (there are the equivalent of seven real unknowns, Ψ_0, Ψ_2, Ψ_3, Ψ_4, to be solved for, whereas $\mathcal{I}_G$

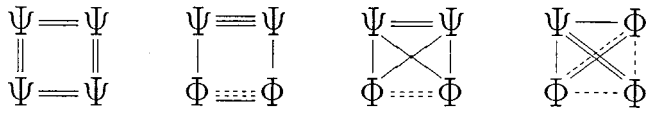

FIG. 4. Dependent quartic-degree invariants.

contains only the nontrivial invariants w_1, w_2, excluding R). We conclude that we need the equivalent of three more real invariants. Using the index theorem, it follows that any further curvature information must come from an invariant which contains contractions with $\bar{\mathbf{\Psi}}$ as well as $\mathbf{\Psi}$ and $\mathbf{\Phi}$ (i.e. a, b and c must be nonzero in the contraction $\mathbf{\Psi}^a\bar{\mathbf{\Psi}}^b\mathbf{\Phi}^c$).

Guided by criteria (a), (b) and (ii), it follows that we must include the two invariants m_4 and m_5 to obtain the new set $\mathcal{I}_{G^+}=\mathcal{I}_G\cup\{m_4,m_5\}$ so that complete backsolving is possible in this case. This is established as follows. The necessary inclusion of m_4 follows immediately from the application of the Index theorem and properties (a), (b) and (ii). Hence, all of the information in the scalars up to and including quartic degree has now been included. Thus we must next consider degree five. In this case, the inclusion of m_5 is justified as follows. First, by appealing to the Index theorem, the required invariant must be of the form $\mathbf{\Psi}^2\bar{\mathbf{\Psi}}\mathbf{\Phi}^2$.

In Fig. 5, we list all (inequivalent and excluding complex conjugates and trivially dependent invariants which have separable product contractions) degree five invariants of this form. By direct calculation, it follows that the second invariant, in the list below, is equivalent to the product of lower degree invariants. Also, we find that the first and third invariants are both equivalent to m_5. Note that we are still maintaining the minimum degree requirement. In this case, we have $m_4=\Psi_0^2$ and $m_5=2\Psi_0^2\Psi_2$. Now, complete backsolving is possible since m_4 determines Ψ_0, m_5 determines Ψ_2, w_1 determines Ψ_4, and w_2 determines Ψ_3. There remains to consider whether it is possible to remove the invariant m_3 retaining only the invariant m_5. In fact, this is impossible since by a direct calculation it follows that the invariant m_5 always vanishes for Petrov type **N** while m_3 does not, and m_3 is generally needed in the backsolving for these cases. It now follows that the CM set cannot be algebraically complete.

Case 2: $\Psi_0=0$, & $\Psi_1\neq 0$: In this case, we can make Ψ_1 real and $\Psi_2=0$. Hence, the elements of $\mathcal{I}_{G^+}$ (except R) are given by

$$w_1=-\tfrac{4}{3}\Psi_1\Psi_3,$$

$$w_2=-\Psi_1^2\Psi_4,$$

$$r_1=0,$$

$$r_2=0,$$

$$r_3=0,$$

$$m_1=0,$$

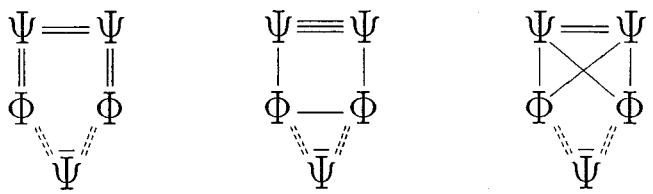

FIG. 5. Fifth-degree invariants of the form $\Psi^2\bar{\Psi}\Phi^2$.

TABLE V. Invariant conditions for the class $\mathcal{M}_S$.

Group A: $r_1 \neq 0$	Group B: $r_1 = 0$
Characterization	Characterization
$r_2 = 0$	$r_2 = 0$
$r_3 = \frac{3}{4} r_1^2$	$r_3 = 0$
$m_1^3 - 27 r_1^2 w_1 m_1 - 54 r_1^3 w_2 = 0$	$m_1 = 0$
$6 r_1 m_2 + m_1^2 + 9 r_1^2 w_1 = 0$	
$2 m_3 + 3 r_1 m_1 = 0$	
$3 r_1 m_4 - m_1 \overline{m}_1 = 0$	$m_4 = 0$
$m_6 - 3 r_1 w_1 \overline{w}_1 \neq 0$	$m_6 \neq 0$
Consequence:	Consequence:
$18 r_1^2 m_5 + m_1^2 \overline{m}_1 + 9 r_1^2 w_1 \overline{m}_1 = 0$	$m_2 = m_3 = m_5 = 0$

$$m_2 = 0,$$

$$m_3 = 0,$$

$$m_4 = 0,$$

$$m_5 = 0.$$

In this case, we do not have sufficient curvature information in the invariants of $\mathcal{I}_{G^+}$ (there are the equivalent of five real unknowns, Ψ_1, Ψ_3, Ψ_4, to be solved for, whereas $\mathcal{I}_{G^+}$ contains only the nontrivial invariants w_1, w_2, excluding R). We conclude that we need the equivalent of one more real invariant, since we can view the above system as determining Ψ_3 and Ψ_4 in terms of Ψ_1 and invariants. Using the Index theorem, it follows that any further curvature information must come from an invariant which must be of sixth degree or higher and of the form $\mathbf{\Psi}^2 \overline{\mathbf{\Psi}}^2 \mathbf{\Phi}^2$ for sixth degree. We choose to include the new real invariant m_6. Since in this case $m_6 = 4\Psi_1^4$, complete backsolving is possible because m_6 determines Ψ_1. Also, the inclusion of m_6 maintains the minimum degree property since $\mathcal{I}_{G^+}$ has the minimum degree property. We now have arrived at the proposed determining set $\mathrm{CZ} = \mathcal{I}_{G^+} \cup \{m_6\}$. It follows from this that the set $\mathrm{ZM} = \mathcal{I}_{G^+}$ is not determining and hence is not algebraically complete. We note that m_6 cannot replace m_4 since the invariant m_6 always vanishes for Petrov type **N** while m_4 does not, and m_4 is generally needed in the backsolving for these cases.

Again, we stress that the set CZ is of the lowest possible degree. This does not mean that CZ is unique, since other invariants, at the same degree level, may be substituted for some of the invariants in our set.

As a consequence of our analysis in this and a sequel paper, on the possible independence of CZ, we are led to the partitioning of all space–times into two disjoint classes: a special class $\mathcal{M}_S$ and a general class $\mathcal{M}_{G^+}$ containing the remaining space–times. The space–times in $\mathcal{M}_S$ are invariantly characterized by the conditions given in Table V. Thus, all the mixed invariants of $\mathcal{I}_{G^+}$ are dependent, hence the need for m_6. Specifically, $\mathcal{M}_S$ consists of special cases within some Segre types (see Table VI) and splits into two groups **A** and **B**.[23]

For $\mathcal{M}_S$, $\mathcal{I}_S = \{R, w_1, w_2, r_1, m_6\}$ is an independent set of invariants. It will be shown in a sequel paper that $\mathcal{I}_S$ is also determining, and hence it follows that $\mathcal{I}_S$ is algebraically complete for $\mathcal{M}_S$.

Next, we will now show that the set $\mathcal{I}_{G^+}$ is independent for $\mathcal{M}_{G^+}$. First, it is clear that any mixed invariant m_i cannot replace any of the Ricci invariants r_i or Weyl invariants w_i. This follows from consideration of conformally flat spaces and Einstein spaces. Second, the invariants in $\mathcal{I}_G$ are independent since they are all needed for the Segre type [1,111] as shown before. Hence, it remains to show that m_4 or m_5 or any ''parts'' of these invariants cannot replace any (''parts'')

TABLE VI. Space–times for the class $\mathcal{M}_S$.

Group	Subclasses of Segre types	
	Segre type	Restrictions in the Ricci canonical frame
Group A: $r_1 \neq 0$	[1,1(11)]	$\Psi_0=\Phi_{11}=\Psi_4=0$ with $\Psi_1\overline{\Psi}_1+\Psi_3\overline{\Psi}_3\neq 0$
	$[Z\overline{Z}(11)]$	$\Psi_0=\Phi_{11}=\Psi_4=0$ with $\Psi_1\overline{\Psi}_1+\Psi_3\overline{\Psi}_3\neq 0$
	[(1,1)11]	$\Psi_0=\Phi_{11}=\Psi_4=0$ with $\Psi_1\Psi_3\neq 0$
Group B: $r_1=0$	[(2,11)]	$\Psi_0=0$ with $\Psi_1\neq 0$

of the invariants in $\mathcal{I}_G$. The invariant m_4 cannot replace any parts of m_1 or m_2 because these three invariants are all needed (essential)[3] for the Segre type [(1,1)11] as will be shown in the sequel paper. Since, for the Segre type [31], $m_4=0$ for some special cases, while $m_3\neq 0$, then m_4 cannot replace m_3. For the invariant m_5, it cannot replace m_1 or m_3 or parts of these invariants, since m_5 vanishes identically for Petrov type N while m_1 and m_3 do not, in general (and they are both needed in general for backsolving). For Segre type [(1,1)(11)], $3r_1m_5=\overline{m}_1m_2$,[3] and therefore $m_5=0$ if $m_1=0$. Hence, m_5 cannot replace m_2, for this Segre type, since $m_1=0$ does not imply $m_2=0$, in general, and m_2 is generally needed in the backsolving. Details will be given in the sequel paper. Finally, no part of m_5 can replace m_4 since they are both (entirely) needed for Segre type [(211)], as shown above. This completes the proof that $\mathcal{I}_{G^+}$ is independent for $\mathcal{M}_{G^+}$

In a sequel paper, we will show that the set $\mathcal{I}_{G^+}$ is determining (and hence algebraically complete) for the class $\mathcal{M}_{G^+}$. As regards the set CZ, it is possible that m_6 could replace $m_2\overline{m}_2$ or $m_5\overline{m}_5$, or both (this is the only possible redundancy that could exist) but as yet we have been unable to resolve this issue. Hence, we cannot claim, at this stage, that CZ is independent, but it will be shown, at least, that it is determining for the set of all space–times.

As previously mentioned, there are some space–times where the information in R_{abcd} is not contained in the set CZ. In these cases, it follows that the missing information cannot be contained in any other invariants. An example of such space–times is Segre type [2,11] with $\Psi_0=\Psi_1=0$ in the canonical frame where the only nonzero Φ_{ab} are $\Phi_{02}=\Phi_{20}$, Φ_{11}, $\Phi_{22}=\pm 1$. In this case, there is no remaining tetrad freedom as the Ricci tensor determines the frame completely. Applying the Index theorem, for any invariant, we obtain $a_2+a_3+a_4=a$, $b_2+b_3+b_4=b$, $c_{02}+c_{11}+c_{20}+c_{22}=c$, $2a_2+3a_3+4a_4+c_{11}+2c_{20}+2c_{22}=2a+c$, $2b_2+3b_3+4b_4+2c_{02}+c_{11}+2c_{22}=2b+c$. This gives $a_3+2a_4+b_3+2b_4+2c_{22}=0$ and hence, $a_3=a_4=b_3=b_4=c_{22}=0$. This means that no invariant will ever contain Ψ_3, Ψ_4, $\overline{\Psi}_3$ or $\overline{\Psi}_4$ and hence there will always be missing information in the Riemann invariants of any degree.

IV. CONCLUSION

A set, CZ, of second-order Riemann invariants has been presented. This set has been constructed so that it is determining, possessing the minimum degree property while attempting to include a minimum number of independent invariants. An analysis on the possible independence of CZ leads to the division of all space–times into two distinct, invariantly characterized, classes: a general class $\mathcal{M}_{G^+}$, and a very special, singular class $\mathcal{M}_S$. Explicitly, in this paper, we have shown that CZ is the union of two sets $\mathcal{I}_S$ and $\mathcal{I}_{G^+}$. The set $\mathcal{I}_S$ has been shown to be independent for the class $\mathcal{M}_S$ while $\mathcal{I}_{G^+}$ has been shown to be independent for the class $\mathcal{M}_{G^+}$. In a sequel paper, we will show that $\mathcal{I}_S$ and $\mathcal{I}_{G^+}$ are also determining and hence algebraically complete for their respective classes $\mathcal{M}_S$ and $\mathcal{M}_{G^+}$. An Index theorem has also been introduced to assist in establishing our results. Finally, an illustrative example has been given to show that in some space–times, no set of second-order invariants can contain all of the information in the Riemann tensor. In such cases, ''complete backsolving'' is not possible. Interestingly, this can only occur for those Segre types in which the Ricci tensor possesses a null eigenvector. In our sequel paper, we will explicitly list all such space–times and show that in these cases there is a geometric

common theme, that being, of alignment between the repeated PND of the Weyl tensor with the null eigenvector of the Ricci tensor. We suspect that some space–times within such classes will, in general, prove to be more difficult to distinguish as inequivalent.

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Clifford algebra as quantum language

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We suggest Clifford algebra as a useful simplifying language for present quantum dynamics. Clifford algebras arise from representations of the permutation groups as they arise from representations of the rotation groups. Aggregates using such representations for their permutations obey *Clifford statistics*. The vectors supporting the Clifford algebras of permutations and rotations are plexors and spinors, respectively. Physical spinors may actually be plexors describing quantum ensembles, not simple individuals. We use Clifford statistics to define quantum fields on a quantum space–time, and to formulate a quantum dynamics-field-space–time unity that evades the compactification problem. The quantum bits of history regarded as a quantum computation seem to obey a Clifford statistics. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1353183]

I. SPINORS AND PLEXORS

Pauli represented electron rotations in SO(3) with elements of the Clifford algebra of a **3**, and Dirac represented Lorentz transformation in SO(1, 3) with elements of the Clifford algebra of a **4**. (In what follows, all representations and their homomorphisms are projective, and may be double valued, unless they are stated to be linear or vector representations, which are single valued. **1**, **2**, **3**,... represent real quadratic spaces of dimension 1, 2, 3,... and of signature specified in context.)

It is unlikely that they knew that Wiman[1] and Schur[2] had represented permutations in the permutation group S_N (also called ''the symmetric group,'' no doubt because its elements are not symmetric) with elements of the Clifford algebra of $(N-1)\mathbf{1}$. A vector space (or module) on which these Clifford algebras are faithfully represented as endomorphism algebra (or ring) are called spinors for the orthogonal groups and *plexors* for the permutation groups. Plexors and spinors are isomorphic mathematical objects of different physical meaning. Spinors arise in one-body quantum physics, plexors in N-body quantum physics with $N>3$.

In the first years of quantum theory, physicists overlooked spinors because they do not occur in the tensor product of vectors. We then proceeded to overlook plexors until Nayak and Wilczek[3] for much the same reason.

Clifford representation of the permutation groups. We write the free Clifford algebra over a quadratic space V as

$$\mathrm{Cliff}(V)=\mathbf{2}^V \tag{1}$$

and the spinor space S of V defined by the isomorphism $\mathbf{2}^V\cong S\otimes S^\dagger$, as

$$S=\sqrt{\mathbf{2}^V}=\sqrt{2}^V. \tag{2}$$

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We construct a reducible Clifford representation R of the permutation group S_N by associating the ath individual of the N-ad being permuted with a first-degree Clifford unit $i_a \in \mathbf{2}^{N1}$, for $a = 1,...,N$, obeying Clifford relations

$$i_a i_b + i_b i_a = 2\delta_{ab}. \tag{3}$$

For quantum applications we define an adjoint † on $\mathbf{2}^V$ by

$$i_a^\dagger = i_a. \tag{4}$$

Then R represents each swap $(ab) \in S_N$ (for $a<b$) by the Clifford difference $R(ab) = i_b - i_a$:

$$R: S_N \to \mathbf{2}^{N1}, \quad (ab) \mapsto i_a - i_b. \tag{5}$$

It is straightforward to see that R is a (projective!) representation of S_N. The i_a make up an orthonormal basis for the first-degree subspace $\mathcal{V} = \mathrm{Cliff}_1(N,0) \subset \mathrm{Cliff}(N,0)$. Let us call R the *orthonormal* Clifford representation of S_N.

R', a useful variant of R, replaces Eq. (3) by

$$i_a i_b + i_b i_a = 2t_{ab}, \tag{6}$$

where

$$t_{ab} = \frac{N+1}{N-1}\delta_{ab} - \frac{2}{N-1}. \tag{7}$$

The form t_{ab} is the inner product between two unit vectors i_a, i_b from the center of a regular $N-1$-simplex $\sigma^{N-1} \subset (N-1)\mathbf{1}$ to its N vertices $i_1,\ldots,i_N$. The i_a of Eq. (6) can be identified with the N simplex vertices permuted. We therefore call R' the *simplicial* representation of S_N. It is isomorphic to a representation given less symmetrically by Schur (1911). The R' image of S_N is an irreducible group of Clifford-algebra elements $\tilde{S}(N)$ that is a (universal) covering group $\tilde{S}_N$ of the discrete group S_N. [Schur (1911) would call $\tilde{S}(N)$ a ''representation group'' of S_N, but today this seems apt to be confused with a group representation.]

The concept of rotation presupposes physical concepts of angle and length. The concept of permutation does not. It presupposes the more primal concept of identity. Therefore permutation groups can enter theoretical physics at finer levels of resolution and higher energies than rotation groups. Plexors may be more basic than spinors.

Representations of permutation groups, and hence plexors, enter quantum physics by two specially deep routes, statistics and dynamics.

II. CLIFFORD STATISTICS

A *statistics* describes how we compose individual quantum elements into an aggregate quantum system. Such a transition from the individual to the collective is sometimes called ''second quantization,'' merely because it introduces new operators, but is better called quantification. Quantification has little to do with quantization and is thousands of years older.

A quantification or statistics is often defined by giving a representation of each permutation group S_N. A *Clifford statistics* represents permutations doubly by Clifford algebra elements of degree 1.[4–8] A *cliffordon* is a quantum whose aggregates have Clifford statistics. A *squadron* is a quantum assembly of cliffordons.

The operators representing operations on a squadron of cliffordons, including the observables of the squadron, form the Clifford algebra of the one-cliffordon mode space. Modes of the squadron are plexors of its Clifford algebra, representable by elements of a minimal left ideal of the algebra.

A statistics is *Abelian* (or central, or scalar, respectively) as its representation of the permutation group is. The Bose and Fermi statistics are Abelian, and the Maxwell, Clifford, and braid statistics are non-Abelian. Read and Moore[9] suggested non-Abelian statistics for quasiparticles of the fractional quantum Hall effect. Nayak and Wilczek[3] recognized this as a Clifford statistics in the first application of the Schur[2] theory to physics. While anyonic and braid statistics are confined to two dimensions, Clifford statistics works in any dimensionality.

A. Spinors describe aggregates

When a spinor of SO_N describes one quantum individual with N possible modes, a plexor of S_N describes a complex of at least N isomorphic individuals. Thus our belated encounter with Schur[2] disabuses us of a long-held notion that spinors represent simpler entities than vectors, a notion that has blocked important research directions. Spinors represent aggregates.[10]

This deserves to be said three times, differently.

B. Spinors describe aggregates

That spinors describe aggregates in quantum theory was already implicit in Cartan's theory of spinors. Cartan starts from a complex vector space $\mathcal{V}$ with a symmetric quadratic form g. The complex space $\mathcal{V}$ can be decomposed (in many ways) into two maximal null subspaces $\mathcal{V}_\pm$ as $\mathcal{V}=\mathcal{V}_+\otimes\mathcal{V}_-$. (A *null space* is one composed entirely of null vectors.) A Cartan spinor—relative to such a decomposition!—is an element of the Grassmann algebra $\bigvee\mathcal{V}_+$. The spinor space $\mathcal{S}$ then has dimension

$$\mathrm{Dim}\,\mathcal{S}=2^{\lceil (D-1)/2\rceil}, \tag{8}$$

where $\mathrm{Dim}\,\mathcal{V}=D=2\,\mathrm{Dim}\,\mathcal{V}_+$ and $\lceil N\rceil$ is the greatest integer $n\leqslant N$. Quantum theory interprets $\mathcal{V}_\pm$ as mode spaces for a fermion and the Grassmann algebra $\bigvee\mathcal{V}_+$ as the algebra of an aggregate of such fermions. Thus Cartan spinors describe fermionic quantum aggregates, not elementary individuals.

C. Spinors describe aggregates

The fact that a vector v can be expressed through a spinor ψ bilinearly as $v^\mu=\psi^\dagger\sigma^\mu\psi$ is sometimes cited to indicate that the vector is less elementary. This is a categorical error. The relation $v^\mu=\psi^\dagger\sigma^\mu\psi$ indicates that a spinor, like an aggregate of vectors, carries enough information to define a vector. But a vector cannot define a spinor. Therefore the vectorial object is a subobject of the spinorial object, not conversely.

Some have called Dirac's spinor space a ''square root of space–time,'' because v^μ is quadratic in ψ^α. More accurately, a spinor space $\mathcal{S}$ is the square root of the Clifford algebra $\mathcal{C}=2^{\mathcal{X}}\cong\mathcal{S}\otimes\mathcal{S}^\dagger$ over space–time; or half thereof, after reduction:

$$\mathcal{S}=\sqrt{2}^{\mathcal{X}}. \tag{9}$$

$\mathrm{Dim}\,\mathcal{S}$ is never less than $\mathrm{Dim}\,\mathcal{X}$, and is exponentially greater for high dimension.

Since plexors describe aggregates, plexor theory can be a quantum substitute for set theory. We apply it to quantum dynamics next.

III. CLIFFORD DYNAMICS

A *dynamics*, too, can be defined by a permutation. First we give a fixed set $\mathcal{V}$ of elementary processes that the system under study can undergo. Then we give a permutation

$$D:\mathcal{V}\to\mathcal{V}. \tag{10}$$

For any elementary process $s \in \mathcal{V}$, we interpret Ds as the immediate successor of s in the dynamical development defined by D. We write the group of such permutations of $\mathcal{V}$ as $S(\mathcal{V})$.

It is customary to avoid messy boundary questions by imagining experiments that have gone on forever and will continue forever. We shall use periodic boundary conditions. Now the experimental space–time region ultimately closes on itself, outside the interesting part of the experiment. This is no more fantastic than the infinite domain and it permits us to work in a finite-dimensional algebra.

A permutation D partitions its domain $\mathcal{V}$ into a congruence of orbits. These are the threads that tie the dynamical elements together. They do not intersect. The intersecting geodesics and the light cones of space–time must arise when we project orbits from eight dimensions down to the four dimensions of space-time. They arise from and describe a quantum entanglement that occurs in the dynamical development.

Then a possible quantum concept of a dynamics mode D is an operator D in the algebra of a representation of $S(\mathcal{V})$, e.g., in the algebra of the covering group $\tilde{S}(\mathcal{V})$. Since S_N is not simple in general, and distinguishes a basis in SO_N, we do not found our theory on this concept. Instead we imbed S_N in the simple group SO_N as the axis-permuting elements, and represent SO_N. We still interpret the operator D as defining a dynamical succession.

Everything we know about a system is in the record of our dynamical operations on the system. A good language for quantum dynamics is then a language of great expressive power.

As syntax for the dynamics language, abstract † algebra is not sufficient. It deals only with how to combine actions in series and parallel, by multiplication and addition, and how to reverse their internal chronological order, by forming the adjoint. It omits space–time fine structure, which is supplied in standard quantum theory by classical constructions prior to the definition of the algebra. How to express space–time concepts within the algebra is part of the problem of marrying quantum theory with gravity theory. We use a high-dimensional Clifford algebra to express quantum space–time.

The statistics and the dynamics roads to the permutation group join when we postulate that ordinary dynamical processes are aggregates too, namely of elementary dynamical processes. In the standard field theory the general process is composed of operations that go on everywhere in the system all the time, described by the Hamiltonian or Lagrangian density. Space–time is how the parts of the dynamics are interconnected.

Any quantum-dynamical theory must give the statistics of its elementary quantum-dynamical processes. In standard physics they are tagged with space–time coordinates, so they are distinguishable and implicity obey Maxwell–Boltzmann statistics.

A. Plexic dynamics

To learn the structure of the dynamical process, we dissect it into its atomic constituents and reassemble it out of them. Evidently these elements of dynamics must still have the nature of dynamical processes themselves. The dynamics is built out of elementary dynamical actions χ, represented by arrows joining states. The simplest classical concept of dynamics is a topological dynamics D.[11] This is usually presented as a map $D:S \to S$ of a set of states S into itself. Instead we deal only with dynamical actions and not with states. We define the dynamics as a mapping D sending each arrow χ to its dynamical successor D_χ.

A theory that puts states of being prior to modes of action is called ontic, the reverse *praxic*. Praxism is an acute case of the pragmatism of Charles Peirce and William James and the operationalism of Einstein and Heisenberg. Here we dissect dynamical operations into micro-operations as James proposed to analyze experience into microexperiences.

This praxic concept of classical dynamics introduces our two principals: a set X of atomic actions $\chi \in X$, and a semigroup $S(X)$ of possible dynamical developments

$$D:X \to X. \tag{11}$$

Dynamical developments are 1-1 mappings or permutations of $X \to X$.

To formulate a quantum dynamics we ''quantize'' the structure (11). That is, we replace classical variables described by sample spaces with corresponding quantum variables described by full matrix algebras. Our prime variable is not space–time, as Einstein proposed, but the dynamical law. Anandan[12] has proposed (like Newton) that dynamical law is variable and Smolin[13,14] that it evolves. We sharpen this assumption and take the dynamical law as the only independent variable, on which all others depend.

The individual elementary quantum process making up the dynamics we call the chronon χ. Its mode space $\mathcal{X}$ and algebra Endo($\mathcal{X}$) replace the set X of atomic actions. Its operator algebra $\mathcal{A}(\mathcal{X}) := \mathrm{Endo}\,\mathcal{X}$ replaces and synthesizes the commutative Boolean algebra of X and the arrow semigroup of ordered pairs $X \times X$. The nearest classical analog of a chronon is not a space–time point, which has no natural dynamical successor, but a tangent or cotangent vector (x, v) or (x,p), which does. These form an eight-dimensional manifold, not a four-dimensional one.

To describe an aggregate of chronons we need a statistics for the chronon.

Neither Fermi, Bose, nor Maxwell statistics will do. A dynamics is a permutation. A Fermi aggregate, like a classical set, is invariant under any permutation of its elements. It cannot represent its dynamics by its permutations. Nor can a Bose aggregate.

And Maxwell statistics are reducible.

Evidently chronons, to be permuted effectively, must be distinguishable, like classical space–time points, which are implicitly supposed to have Maxwell statistics.

In nature the ambient dynamics has modes with spin 1/2.

The simplest statistics that supports two-valued representations of S_N is the *Clifford statistics*. The operator algebra of this aggregate is a Clifford algebra $\mathcal{C} = \mathrm{Cliff}(\mathcal{V}I)$ generated by individual unit modes i_a obeying Eq. (3). The difference of two units $C(ab) = i_a - i_b$ represents their swap (ab). We identify the individual mode space $\mathcal{V}I$ with the first-degree subspace $\mathcal{C}_1 \subset \mathcal{C}$. Here there is no doubt that the spinor represents an aggregate, namely the aggregate that the permutations permute.

Schur[2] and Nayak and Wilczek[3] use complex coefficients throughout. They represent some swaps by sums $i_a + i_b$ and others by differences $i_a - i_b$, depending on an arbitrary choice of $N-1$ generating swaps. It is not possible to represent all swaps (ab) by sums $i_a + i_b$. But their representation is isomorphic to the simplex representation (7), of all swaps by differences.

Choosing Clifford statistics for chronons expresses the distinguishability of events and the existence of spin 1/2. The grade of a Clifford element gives the minimal number of swaps or chronons in its factorization, corresponding roughly to classical phase-space volume.

In the quantum theory of a variable dynamics D, we distinguish between the dynamics D and some dynamics operator D that describes D maximally, just as we distinguish between a hydrogen atom H and a mode vector ψ maximally describing H. A Hamiltonian is a kind of dynamics operator of the continuum limit.

Standard quantum theory uses modes in a complex † space $\mathcal{V}$ whose † defines a nonsingular sesquilinear form $\psi\dagger\phi$. Gauge invariance requires that the gauge generators be anti-Hermitian, and the gauge group structure requires that some of them be nilpotent. Only in an indefinite sesquilinear space can a nilpotent other than the trivial 0 be anti-Hermitian. Therefore † is usually indefinite, and the quantum theories that work in Hilbert spaces, with their definite *, are not sufficiently relativistic for physics.

B. Field theory under the microscope

Clifford statistics also resolves a question that has beset quantum space–time physics from its inception. What is the algebra of quantum fields on a quantum space–time? When we first asked this question[15] we imagined that the q bits of the space–time quantum computer all commuted, and had serious difficulties with this question. Now that they all anticommute it answers itself.

First the problem. In classical physics, the field fiber $\mathcal{F}$ of field values and the Minkowski manifold $\mathcal{M}$ of space–time points are combined (at least locally) by exponentiation into a space

$$\Phi = \mathcal{F}^{\mathcal{M}} \tag{12}$$

of fields, each field $f \in \mathcal{F}^{\mathcal{M}}$ being a function $f:\mathcal{M}\to\mathcal{F}$.

Question: How do we define the exponential F^M when the classical spaces $\mathcal{F}$ and $\mathcal{M}$ have been replaced by operator algebras describing quantum field and space–time entities?

Answer: Take the logarithms of the algebras. This reduces the computation of the exponential to the computation of products, an already solved problem.

We expand on this answer a bit.

One's first guess for the algebra F^M is apt to be the algebra of linear morphisms $M\to F$, but this reduces merely to the tensor product $M^\dagger\otimes F$ when M and F are algebras, and represents merely a pair of one M quantum and one F quantum. This is to be expected, since M and F describe individuals, not aggregates, and a mapping from one individual to another is merely one ordered pair.

For a better answer, one must express algebraically the fact that $\mathcal{M}$ is a plenum, not a point. All the points of $\mathcal{M}$ are actual, not mutually exclusive possibilities.

This is just the case for the Clifford statistics, which permutes entities that are all present at once. We designate a real free Clifford algebra $\mathcal{C}$ over a quadratic space $\mathcal{X}$ with endomorphisms algebra $\mathcal{A}=\mathrm{Endo}(\mathcal{X})$ by

$$\mathcal{C}=\mathbf{2}^{\mathcal{X}}=\sqrt{\mathbf{2}}^{\mathcal{A}}=\mathrm{Cliff}\,\mathcal{X}. \tag{13}$$

This makes $\mathcal{A}$ a logarithm of $\mathcal{C}$ and tells us how to define any quantum exponential of $\mathcal{C}$:

$$\mathcal{C}^{\mathcal{M}}:=(\sqrt{\mathbf{2}}^{\mathcal{A}})^{\mathcal{M}}:=(\sqrt{\mathbf{2}})^{\mathcal{A}\otimes\mathcal{M}}=\mathrm{Cliff}(\mathcal{X}\otimes\mathcal{Y}), \tag{14}$$

where $\mathcal{M}=\mathrm{Endo}(\mathcal{Y})$.

It is not hard to see that the observed field algebras do have logarithm algebras, using the Chevalley[16] representation of spinors within their Clifford algebra.

Definitions: An *octad* is a squadron of eight cliffordons with neutral quadratic form. An octad space is a real neutral quadratic space

$$\mathbf{8}=\mathbf{4}\oplus\overline{\mathbf{4}} \tag{15}$$

of eight dimensions, where the bar indicates a reversal of metric, $\dagger\to-\dagger$. An *octon* is a hypothetical quantum whose mode space is **8**. An *octadic space* is a real neutral quadratic space whose dimension is a multiple of 8: The general octadic space is

$$\mathcal{O}=\mathbf{8}\oplus\ldots\oplus\mathbf{8}=N\mathbf{8} \tag{16}$$

with $N>0$ terms.

C. Examples

The tangent–cotangent space to Minkowskian space–time $\mathcal{M}$ is the octad space $\mathbf{8}=\mathbb{M}\oplus\overline{\mathbb{M}^\dagger}$, where $\mathbb{M}:=\mathbf{1}\oplus\overline{\mathbf{3}}$ is the Minkowski tangent space. The irreducible spinor spaces of **8** are again octad spaces (Chevalley triality).

The Clifford algebra of an octadic space, with its neutral quadratic form, is algebra-isomorphic to the Clifford algebra of a space of the same dimension with a definite quadratic form.

Octad lemma: An octadic chronon algebra $\mathbf{2}^{N\mathbf{S}}$ factors as a Maxwell–Boltzmann ensemble of N octads each with algebra $\mathbf{2}^{\mathbf{S}}$.

$$\mathbf{2}^{N\mathbf{S}}=\mathbf{2}^{\mathbf{S}}\otimes\ldots\otimes\mathbf{2}^{\mathbf{S}}\quad(N\ \text{terms}) \tag{17}$$

In the limit $N\to\infty$, this Maxwell–Boltzmann ensemble includes a Bose–Einstein aggregate of octads.

It is easy to see that this Bose–Einstein aggregate admits condensation into an eight-dimensional symplectic manifold isomorphic to the tangent bundle to space–time. A field of operators on space–time is a similar condensation of a squadron of octads as $N\to\infty$, $\hbar\to 0$.

This is a great simplification. The group of a bundle is never simple; the base couples to the fiber without reverse coupling. In Galilean relativity the base was time, while in field theory the base is space–time, but the illness is the same, and the cure too: relativization. In Eq. (14) the field and the space–time are unified in the simple space–time-field entity $\mathcal{S}$. When we first attempted to express field theory in terms of q bits or chronons[15] we imagined an absolute split between field fiber and space–time base. Now the field/space–time split appears to be a factorization of a field-space–time unity $\mathcal{S}$. It is as relative as the factorization of space–time into space/time.

IV. QUANTIFICATION OPERATORS

Each of the usual statistics, Fermi, Bose, and Maxwell, has an operator-valued form $Q^\dagger$ and dual form Q that defines how infinitesimal actions on the individual can act on the aggregate.

In each statistics the individual I has a mode vector space $\mathcal{V}(I)$ and operator algebra $\mathcal{A}(I)$. The aggregate has a mode vector space $\mathcal{V}(S)$ and operator algebra $\mathcal{A}(S)$. Let $d\mathcal{A}$ be the infinitesimal Lie algebra of $\mathcal{A}$ with Lie product $[\alpha,\beta]:=\alpha\beta-\beta\alpha$. The quantification operator $Q^\dagger$ is a linear morphism

$$Q^\dagger:\mathcal{V}(I)\to\mathcal{A}(S),\qquad \psi\mapsto Q^\dagger\psi, \tag{18}$$

transforming a mode vector (or a ket) $\psi\in\mathcal{V}(I)$ for the individual to an operator $Q^\dagger\psi\in\mathcal{A}(S)$ for the aggregate. The operators $\psi^\dagger Q$ generate $\mathcal{A}(S)$ † algebraically. The mapping

$$\langle\ldots\rangle:d\mathcal{A}(I)\to d\mathcal{A}(S),\qquad w\mapsto\hat{w}=Q^\dagger wQ \tag{19}$$

is a Lie-algebra homomorphism.

We call the Q with these properties, when it exists, the *quantification operator* of the statistics. If w represents an additive quantity or infinitesimal transformation of the individual, we call $Q^\dagger wQ$ the *quantified w* for the quantified system. The quantification operators of Fermi, Bose, and Maxwell statistics map individual mode vectors ψ into annihilation operators $Q^\dagger\psi$, and individual quantities q into additive total quantities $Q^\dagger qQ$. Clifford statistics also has a quantification operator $Q^\dagger$, which maps mode vectors into swaps instead of creation operators.

The Clifford quantification operator Q_0 obeys the Clifford law

$$(\forall v\in\mathcal{V})(Q_0^\dagger v)^2=\|v\|. \tag{20}$$

We chose the sign in Eq. (3) so that the mapping (19) is a Lie algebra homomorphism, preserving the commutation relations of the individual within those of the aggregate, as for Fermi and Bose statistics. This is just the familiar fact that the commutators $L_{ab}=i_{[ab]}$ generate a representation of the orthogonal group.

We write the quantification operators for Clifford, Fermi, and Bose statistics as Q_0, Q_1, and Q_2. The numerical subscripts count the independent imaginaries in the coefficient field $\mathbb{R}$, $\mathbb{C}$, and $\mathbb{H}$ of the classical group of the statistics. We write Q_M for the Maxwell–Boltzmann quantifiation operator. We call the most important aggregates (Maxwell) *sequences*, (Bose) *sibs*, (Fermi) *sets* and (Clifford) *squadrons* for brevity. We call the Clifford composite a *squadron* to remind us that it is an essentially *quantum* structure. There are classical sets and classical sibs, but no classical squadrons. Clifford statistics, like anyonic and other multivalued statistics, involves quantum superposition more deeply than the single-valued composites such as the sequence, sib, or set.

For example if L is a component of individual angular momentum, then for Fermi quantification $Q=Q_1$ and Bose quantification $Q=Q_2$, $Q^\dagger LQ$ is the total angular momentum of the aggregate. These quantifications *totalize* the operator on which they act.

The Maxwell quantification operator Q_M does not totalize. The quantified operator $Q_M^\dagger L Q_M$ represents the L of only the last individual in the sequence, not the total ω. Totals have somewhat more complicated expressions in Maxwell statistics.

Clifford quantification, like Fermi and Bose, totalizes.

Clifford statistics relates a quadratic space $\mathcal{V}$, its endomorphism algebra $\mathcal{A}$, its Clifford algebra $\mathcal{C}$, and its spinor space $\mathcal{S}$, by the commutative diagram

$$\begin{array}{ccc} & \overset{\text{Endo}}{} & \\ \mathcal{V} & \rightarrow & \mathcal{A} \\ Sq\downarrow & \searrow \text{Cliff} & Sq\downarrow \\ & \overset{\text{Endo}}{} & \\ \mathcal{S} & \rightarrow & \mathcal{C} \end{array} \tag{21}$$

When we apply Clifford statistics to dynamics, $\mathcal{V}$ is the mode space $\mathcal{X}$ for a chronon. The composite system described by a spinor of $\mathcal{S}$ consists of all the chronons transpiring in the experimental space–time region. The algebra $\mathcal{A}$ consists of endomorphisms of $\mathcal{V}$. The Clifford algebra $\mathcal{C}$ consists of descriptions D of the global dynamics of the squadron.

The real Clifford algebra $\mathcal{C}=\text{Cliff}(\mathcal{V},\mathbb{R})$ of Clifford statistics is the endomorphism algebra of an underlying spinor module $\mathcal{S}$ over one of the five rings $\mathbb{R}$, $\mathbb{C}$, $\mathbb{H}$, $2\mathbb{R}$, $2\mathbb{H}$, depending on the dimension and signature of ν according to the spinorial chessboard.[17]

Clifford statistics can readily simulate Bose and Fermi statistics with pseudobosons and pseudofermions. In Eq. (17), Clifford statistics exactly simulates an aggregate of octads obeying mutual Maxwell–Boltzmann statistics and internal Clifford statistics at the same time.

The most striking difference between the Clifford statistics and Fermi statistics cannot be read from their algebras. Orthogonal ψ's anticommute in both statistics, and every fermionic algebra is algebra isomorphic to a neutral Clifford algebra, but fermions are identical and cliffordons are not. An algebra does not define its interpretation. The exchange of two fermions is represented by factor exchange, one stipulates, and hence by -1, which is projectively equivalent to the identity. The exchange of cliffordons 1 and 2, however, is represented by i_1-i_2. Cliffordon swaps, far from being trivial, scalar, or central, may generate the entire aggregate action algebra.

V. CHRONON DYNAMICS

We hypothesize that the dynamics of a suitably isolated physical system is a squadron of elementary dynamical processes or chronons, and that the ambient vacuum breaks its Clifford algebra $\mathcal{C}$ down into many mutually commuting local octadic Clifford algebras as in Eq. (17).

We construct a simple finite-dimensional Clifford algebra $\mathcal{C}=\check{\mathcal{A}}$ that approaches (or ''contracts to'' (cf. Ref. 18) the Minkowski manifold algebra, the associative algebra $\mathcal{A}=\mathcal{A}(x^\mu,\partial_\mu)$ of coordinates x and derivations ∂ of space–time differential geometry. $\mathcal{A}$ may be regarded as a generalization of the Heisenberg algebra of x and p and a variant of the Bose–Einstein algebra. Expanding it into a Clifford algebra is mathematically akin to approximating bosonic fields with fermionic ones, the process of bosonization.

Since $\mathcal{A}$ is infinite dimensional, the dimensions of $\mathcal{C}$ and its orthogonal group are huge, like the number of phase-space cells in the experiment, which is likely $\gg 10^{20}$ for atomic experiments, and approach infinity in the contraction to the continuum.

Chronons and the basic Clifford variables i_a that represent them are prelocal in the extreme, since they all anticommute. Nevertheless they are the raw material of our universe, we propose.

This only apparently clashes with quasilocality, due to Eq. (17).

A. Localization

We begin construction with an octadic chronon space $\mathbf{8}N$ and its Clifford algebra $\mathcal{C}$.

We decompose $\mathcal{C}$ into N mutually commuting octad algebras of independent local variables $\gamma_\mu(n)$ obeying local commutation relations

$$\{\gamma_\nu(n),\gamma_\mu(m)\}=t_{\nu\mu}\delta_{nm}. \tag{22}$$

We define the Lorentz algebra and group of such a Clifford algebra by the usual expression for the angular momentum of a spin aggregate,

$$\check{L}_{\nu\mu}:=\frac{1}{2}\sum_{n=1}^{N}\sum_{\beta=0}^{1}\gamma_{\mu\nu}(n,\beta). \tag{23}$$

We assume that p_μ and x^μ for the N squadrons are, like $L_{\mu\nu}$, additively composed of terms from each squadron, corresponding to how the displacement $\Delta x=\int_C \mathrm{d}x(\tau)$ along a curve $C{:}x=x(\tau)$ is an integral over C of a contribution from each differential element $\mathrm{d}x(\tau)$:

$$\Delta x^\mu=\sum_{n,\beta}\delta x^\mu(n,\beta),\quad \Delta p_\mu=\frac{1}{2N}\sum_{n,\beta}\delta p_\mu(n,\beta). \tag{24}$$

Here we use $\hbar=c=л=1$.

Suppose each tetrad has contributions

$$\delta x^\mu=2^{-1/2}\gamma^\mu,\quad \delta p_\mu=2^{-1/2}\gamma^\uparrow\gamma_\mu,\quad \delta i=\gamma^\uparrow. \tag{25}$$

The unit of x is $л$ and the unit of p is $\hbar/л$, while i is dimensionless.

Then for each tetrad

$$\begin{aligned}[\delta x^\nu,\delta p_\mu]&=\delta i\,\delta_{\nu\mu},\\ [\delta i,\delta x^\mu]&=+2\,\delta p^\mu,\\ [\delta i,\delta p_\mu]&=-2\,\delta x_\mu.\end{aligned} \tag{26}$$

The first equation of (26) makes $\gamma^\uparrow$ the expansion of Heisenberg's i, much as Hestenes[19] proposed. Presumably this builds in a violation of parity.

The second and third equations tell us that the expanded i generates the symplectic symmetry between x and p, as Segal[20] proposed. On the chronon scale, this violates Heisenberg's commutation relations seriously. In the standard quantum theory i is central.

We recover the Heisenberg commutation relations as a contraction of the Clifford relations by summation and a subsequent correlation:

$$\begin{aligned}\check{x}^\mu&=\sum_{n,\beta}\delta x^\mu(n,\beta),\\ \check{p}_\mu&=\frac{1}{2N}\sum_{n,\beta}\delta p_\mu(n,\beta),\\ \check{i}&=\sum_{n,\beta}\delta i(n,\beta).\end{aligned} \tag{27}$$

Here and in what follows, the breve on a variable, like $\check{i}$ Eq. (27) is a semantic annotation rather than a syntactic one. It declares that the accented variable is an expansion of the standard unaccented one, and reduces to it upon contraction. It thus tells us how to measure the variable in the contracted domain of experience. If one set of physical concepts successfully covers both domains, as in quantum theory and relativity, for example, we drop such labels.

Feynman[21] proposed that the space–time coordinate-difference operator is the sum of many mutually commuting tetrads of Dirac vectors:

$$\Delta x^{\mu} = \text{const} \sum \gamma^{\mu}(n) \tag{28}$$

as a quantum form of the proper-time Heisenberg–Dirac equation $\mathrm{d}x^{\mu}/\mathrm{d}r = \gamma^{\mu}(\tau)$. Feynman's proposal returns in Eq. (27) as a result of the octad lemma. Each of his γ's represents one chronon i^{a} in a large octadic squadron.

B. Correlation

We now have far too many *i*'s: one for every tetrad. In the standard physics there is only one imaginary *i* and one Clifford vector γ^{μ} for the whole system. We correlate all the δi so that they are effectively one *i*, and all the tetrads $\gamma^{\mu}(n)$ so that they are effectively one tetrad γ^{μ}. We suppose that the vacuum Bose–Einstein condensation establishes this correlation. The local departure of $\breve{i}$ from its global mean *i* is presumably a Higgs operator.

To be sure, the tetrads of the tetrad lemma obey Maxwell statistics, not Bose. But the mode space of Maxwell statistics is the direct sum of the spaces of all the tensorial statistics, including Fermi and Bose and parastatistics. Any Bose projection is *a fortiori* a Maxwell projection.

We require a projection operator $P \in \mathcal{C}$ expressing this alleged Bose–Einstein correlation, projecting onto the symmetric subspace.

We have constructed this symmetrizer elsewhere. The symmetric subspace of $\mathcal{S}$ is $P\mathcal{S}$, the *P* image of $\mathcal{S}$. The restrictions of the $\breve{i}(n)$ to $P\mathcal{S}$ are all equal to $P\breve{i}P$, the restriction of $\breve{i}$ to $\mathcal{S}$, with $\breve{i}$ given by Eq. (27).

It is then straightforward to see that this restriction of $\breve{i}$ is a square root of the restriction of -1 to *P*:

$$(P\breve{i}P)^{2} = -P. \tag{29}$$

It remains to be seen whether the variable $P\breve{i}P$ is sufficiently close to being central in processes close to the vacuum. If so then it can pass for the physical *i* of quantum mechanics in such processes.

The Clifford elements

$$L_{\mu\nu} = \sum_{\beta,\tau} [i_{\mu,\beta,\tau}, i_{\nu,\beta,\tau}] \tag{30}$$

are infinitesimal generators of the connected Lorentz group $\mathcal{L}$ of this model. The operators *x* and *p* constructed by Eq. (27) are covariant under the connected Lorentz group $\mathcal{L}$.

VI. RELATIVISTIC DYNAMICS OPERATOR

To recover Maxwell statistics in the classical space–time limit we were forced to order the octads with a ''proper time'' index τ. This permits us to formulate an ''octad-cycling'' dynamics operator D_o that advances τ by unity and so is a scalar invariant, unlike the Hamiltonian, which increases *t* and is one component of a vector.

A covariant development in proper time is generated by *a rest mass operator* just as a coordinate-time development is generated by a Hamiltonian energy operator. A covariant proper-time dynamics with a second-order mass operator is used by Schwinger among others. The present theory is a kind of ''quantum square-root'' of such theories.

D_o is then an ordered product of eight disjoint cycles of length *N* according to Clifford statistics. Defining $\Delta i_{\mu,\beta,\tau} := (i_{\mu,\beta,\tau+1} - i_{\mu,\beta,\tau})$, we write this basic dynamics operator as

$$D_o = \overleftarrow{\prod_{\beta}} \; \overleftarrow{\prod_{\mu}} \; \overleftarrow{\prod_{\tau}} \; \Delta i_{\mu,\beta,\tau}. \tag{31}$$

In the τ ordering, $\Delta i_{\mu,\beta,\tau}$ is to be treated as a whole with one index τ, not divided between τ and $\tau+1$. Each cycle of Eq. (31) swaps the μ, β chronon of octad τ with the μ, β chronon of octad $\tau+1$ according to the orthonormal statistics (5).

Now two apparently separate conceptual streams, special relativity and combinatorics, merge almost unexpectedly.

The octadic chronon dynamics D_o is Lorentz invariant. The proof is straightforward. It rests on the familiar fact that the Dirac top gamma $\gamma^{\uparrow}=``\gamma^5"$ is invariant under the connected Lorentz group. This confluence gives us renewed hope for a chronon dynamics.

D_o has several easily constructed brothers that are also Lorentz invariant and also shift tetrads or octads forward in τ by small steps.

D_o is still unsatisfactory for many reasons. Above all, it does not define the Minkowskian metrical structure of space–time. In a simple theory, Poincaré invariance of the ambient dynamics operator D is not enough. D must also define the space–time metric.

Physically, we must know the momentum of a moving particle to predict its next position sharply. This means a coupling among the eight components of space–time–energy–momentum. The dynamics D_0 is an uncoupled development. Lorentz-invariant couplings are now under study.

VII. SIMPLIFYING THE STANDARD MODEL

The simplification of the space–time structure of the standard model that we have performed so far suggests that we can simplify its internal structure as well by dissolving the separation between field variables and space–time variables. This was the goal of our earlier Fermi quantizations of space–time, and it comes closer in the present Clifford quantization.

The standard theory needs internal variables to describe hypercharge, isospin, color, and family because it assumes that the immediate neighborhood of any event is exactly Minkowskian. *At any one point all gauge vectors can be transformed to zero by a gauge transformation.*

In the case of gravity this assumption of the standard model specializes to Einstein's equivalence principle. We call this italicized proposition the *generalized equivalence principle* when we intend to include gravity among the gauge fields.

We have supposed that the field variables actually describe finite quasilocal defects of size $л$ in the vacuum condensate. In the continuum limit $л\to 0$, these vanish, and surrogate variables have to be invented. Variables that describe the condensate in maximal quantum detail, with $л\neq 0$, should suffice to describe its defects.

This approach to simplification avoids the compactification problem that plagues theories of the Kaluza kind. It replaces mysteriously small extra dimensions by physically small neighborhoods. The same chronon variables i^a that combine to form the external x's and ∂'s, also combine into the internal γ's and τ's, the fields, and the Lagrangian, a contraction of the dynamics operator. In the condensate many of these degrees of freedom are frozen. A high-energy interaction thaws and excites some of them. We require that the same i's give us the external modes when they sing in unison and the internal modes when they sing polyphonically.

VIII. DISCUSSION

The revolutions of the past hundred years of physics have simplified certain algebras. Several nonsimple algebras still wait to be simplified, notably the Heisenberg algebra of quantum theory, the algebra of the field bundle, and the algebra of dynamics. These couple to each other so that the next revolution must likely simplify them all at once. The result will be a nonlocal quantum theory.

We have given one obvious simplification of these algebras, postulating a dynamics operator D that contracts to the standard Hamiltonian and Lagrangian in a suitable limit but consists of many elementary quantum actions, chronons. The key unifying element is the Clifford statistics for the chronon.

This leads us to a quantum correspondent for the standard gauge principle: Remote comparisons are effected by a succession of quantum swaps. It also suggests a host of relativistic candidates for the dynamics operator D.

Some of these results were presented at the American Physical Society Centennial Meeting, Atlanta, 25 March 1999.[22]

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Magnetic fields and factored two-spheres

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A magnetic monopole is placed at the center of a ball whose surface S^2 is tiled by the symmetry group, Γ, of a regular solid. The quantum mechanics on the two-dimensional quotient S^2/Γ is developed and the monopole charge is found to be quantized in an expected manner. The heat-kernel and ζ-functions are evaluated and the Casimir energy is computed. Numerical approaches to the calculation of the derivative of the Barnes ζ-function are presented. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1345501]

I. INTRODUCTION

In previous work,[1] we have discussed quantum field theory on orbifold factors of spheres S^n/Γ, where Γ is a discrete subgroup of the orthogonal group, $O(n+1)$. In this paper we wish to present an extension in the two-dimensional case $(n=2)$ to the situation where there is a uniform radial magnetic field passing through the surface of the sphere. This can be thought of as due to a magnetic monopole at the center of a ball in an embedding R^3. The motivation is partly to investigate the interplay between a magnetic field and a nontrivial topology/geometry induced by identification. Specifically we would be interested in what happens to the Dirac quantization in topologically interesting or singular manifolds (orbifolds). There is also continuing statistical mechanical interest in magnetic fields and two-dimensional domains.

The quotient group is the complete symmetry group of a regular solid and can be generated by reflections in the three (concurrent) planes of symmetry of the solid. The elements fall into two sets depending on whether they contain an even or an odd number of reflections. The even subset forms the rotational subgroup denoted now by $\Gamma \in \mathrm{SO}(3)$. The odd subset is denoted by Γ_1'. If γ' is any fixed element of Γ' then as γ runs over Γ, $\gamma\gamma'$ exhausts Γ_1'. In particular we can choose $\gamma'=\sigma$ where σ is a reflection in a symmetry plane and so the complete group is

$$\Gamma' = \Gamma \cup \Gamma_1' = \Gamma \cup \Gamma\sigma. \tag{1}$$

The standard classification of finite subgroups (reflection groups) is given by Meyer,[2] and we use his notation. The general construction of the quotients, S^2/Γ', which in this case are certain geodesic triangles on S^2 is sketched later. The vertices of these triangles are singular points. Joining them to the origin of the ambient $\mathbb{R}^3$ produces singular strings and our analysis can be extended to this three-dimensional setting.[3] The two-dimensional models that we study can be thought of as toy models for more general ''textures'' in higher dimensions as laid down by Kibble [see, e.g., Ref. 4].

Our main interest is in setting up the general framework and then applying it to some specific calculations such as the evaluation of vacuum energies. This will involve a certain amount of technical manipulation, especially with the properties of the Barnes ζ-function. This function appears quite commonly, particularly in spherically symmetric situations and in the presence of magnetic fields or harmonic oscillators and we expect that our methods will have an applicability beyond the immediate one here.

A very brief summary of our findings is given in Sec. XIII.

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II. MODES AND GROUP ACTIONS ON THE FULL SPHERE

As modes on the full sphere, we can take the angular part of the Schrödinger equation solutions derived long ago by Tamm[5] and Fierz.[6] It would be more rigorous to use a fibre bundle formulation (Greub and Petry,[7] Wu and Yang[8]) or geometric quantization[9,10] but this is unnecessary for our purposes. For definiteness, we employ the modes denoted by $(Y_{qm})_a$ in Wu and Yang, corresponding to the string running down the negative z-axis. The modes are, up to normalization, the SU(2) representation matrices $\mathcal{D}^{(l)*}_{m,-q}(\phi,\theta,-\phi)$ with $l=|q|,|q+1|\ldots,-l\leqslant m\leqslant l$.[11] $2q$ is the monopole number with $q\equiv eg/\hbar$, and $2q\in\mathbb{Z}$. If the string runs up the positive z-axis, the modes are $\mathcal{D}^{(l)*}_{m,-q}(\phi,\theta,\phi)$.

The corresponding eigenvalues of H_{S^2}, the angular part of $-(\nabla-ie\mathbf{A})^2$, are

$$\lambda_l=l(l+1)-q^2=(l+\tfrac{1}{2})^2-\tfrac{1}{4}-q^2 \tag{2}$$

with degeneracy $2l+1$.

It is helpful to give the explicit form of the angular eigenfunctions in spherical polar coordinates,

$$Y^{(l)}_{qm}(\theta,\phi)=N_{qlm}\sin^{|q+m|}(\theta/2)\cos^{|q-m|}(\theta/2)P^{|q+m|,|q-m|}_{l-(q|q+m|+|q-m|)/2}(\cos\theta)e^{i(q+m)\phi}, \tag{3}$$

where N_{qlm} is a normalization constant and the $P^{\alpha,\beta}_n(x)$ are Jacobi polynomials. In the Wu–Yang formalism these are the solutions (sections) in the upper hemisphere. In the lower hemisphere the potential is taken to have a string along the positive z-axis. The two sets of solutions are related on the equator by the factor $\exp(i2q\phi)$. Making this single valued gives the quantization condition on q, in this approach.

The basic means of finding the modes is to write $H_{S^2}\psi=\lambda\psi$ explicitly as a differential equation in spherical polar coordinates,

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial\psi}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+i\frac{2q}{1+\cos\theta}\frac{\partial\psi}{\partial\phi}-q^2\frac{1-\cos\theta}{1+\cos\theta}\psi=\lambda\psi, \tag{4}$$

and solve it assuming the separation $\psi(\theta,\phi)=\exp(iu\phi)P(\cos\theta)$. Using this method we can suppose initially that q is arbitrary which leads to the same solutions as in (3) but which are characterized by two integers $u\in\mathbb{Z}^+$ and $v\in\mathbb{Z}$.[5] The relationship to the SU(2) labels l and m is given by

$$l=u+\tfrac{1}{2}(|q+m|+|q-m|),\quad v=m-q \tag{5}$$

and thus it would appear that we could have any value of q as long as u and v are integers (with suitable $l,m\in\mathbb{R}$). However, in this case the solutions would not be single-valued and all the solutions would vanish on the string axis. Setting $2q\in\mathbb{Z}$ gives the same values of l and m as before.

As usual, when one tries to adapt wave functions to some symmetry (here Γ') there is the problem that the magnetic potential, $\mathbf{A}$, might not possess the same symmetry so that compensating gauge transformations are necessary. Peierls[12] calls this process ''umeichen.'' It is a well known situation, with extensive discussion,[13] which we have encountered in an earlier calculation on the tetrahedron,[14] an orbifold factor of the plane. A similar procedure has also been applied to factors of the Poincaré half-plane.

In the present case, under the action of Γ', the string is rotated and reflected and has to be brought back to its original position if we are to implement the identification in S^2/Γ' consistently. The equation that contains the relevant information is the behavior of the modes under arbitrary rotations-reflections. For the moment we deal with the easier, pure rotational case, $g\in\mathrm{SO}(3)$. Then the behavior is an elementary consequence of the SU(2) group combination law and one has explicitly (Wu and Yang,[8] Frenkel and Hraskó[15]),

$$Y^{(l)}_{qm'}(g^{-1}\hat{\mathbf{r}}) = e^{iq\Lambda_g(\hat{\mathbf{r}})} Y^{(l)}_{qm}(\hat{\mathbf{r}}) \mathcal{D}^{(l)}_{mm'}(g), \quad g \in \mathrm{SO}(3). \tag{6}$$

The exponential factor is the compensating gauge rotation with

$$\Lambda_g(\hat{\mathbf{r}}) = \alpha(g) + \gamma(g) - \Omega_g, \tag{7}$$

where α, β, and γ are the Euler angles of the rotation g and Ω_g is the solid angle subtended by the geodesic triangle on the (unit) sphere cut out by $-\mathbf{r}$, the string axis, $\mathbf{n}$ (here the negative z-axis) and the rotated string axis, $g\mathbf{n}$,

$$\Omega_g(\hat{\mathbf{r}}) = \Omega(g\mathbf{n}, \mathbf{n}; \mathbf{r}), \quad \mathbf{r} = (\hat{\mathbf{r}}, r).$$

(Our conventions regarding rotations and actions are generally those of Brink and Satchler.[16]) The gradient of Ω gives the gauge transformation between the potentials of the two strings.

An alternative expression for Λ is (Wu and Yang[8])

$$\Lambda_g(\hat{\mathbf{r}}) = \phi_g - \phi - A_g, \tag{8}$$

where A_g is the angle at $-\hat{\mathbf{r}}$ in the above mentioned triangle on S^2 and $g^{-1}\hat{\mathbf{r}} = (\theta_g, \phi_g)$

In order that (6) be consistently iterated, it is necessary that the group combination (cocycle) condition,

$$\Lambda_{gh}(\hat{\mathbf{r}}) = \Lambda_g(\hat{\mathbf{r}}) + \Lambda_h(g^{-1}\hat{\mathbf{r}}), \tag{9}$$

should hold, and this can be checked directly from (7). The geometrical details are to be found in the useful article by Frenkel and Hraskó.[15]

The magnetic rotation operator, T_g, is defined, on scalars, by the action

$$(T_g\psi)(\mathbf{r}) = e^{-iq\Lambda_g(\hat{\mathbf{r}})} \psi(g^{-1}\mathbf{r}), \tag{10}$$

or, equivalently,

$$\langle \mathbf{r} | T_g = e^{-iq\Lambda_g(\hat{\mathbf{r}})} \langle g^{-1}\mathbf{r} |. \tag{11}$$

In the present spherical case, because of (9), the magnetic rotations provide a true, as opposed to a ray, representation of the *double* of SO(3) [denoted $\mathrm{SO}^{\bullet}(3)$] in the sense that

$$T_{gh} = T_g T_h$$

and

$$T_E = (-1)^{2q}\mathbf{1}, \tag{12}$$

where E is a 2π rotation. This is not unexpected considering that for q a half odd-integer all the monopole harmonics have half odd-integer angular momentum. $\mathrm{SO}^{\bullet}(3)$ is isomorphic to SU(2).

Magnetic rotations on the plane[17] also provide true representations but not so *translations*, unless the flux through a fundamental domain is quantized.[18]

We record the action of T_g on the modes which is easily obtained from (10) and (6),

$$T_g Y^{(l)}_{qm'}(\hat{\mathbf{r}}) = Y^{(l)}_{qm}(\hat{\mathbf{r}}) \mathcal{D}^{(l)}_{mm'}(g). \tag{13}$$

III. PARITY AND REFLECTIONS

The singularity (string) preserving magnetic parity operator on monopole wave functions is defined by the action,[15]

$$(\Pi\psi)(\mathbf{r}) = e^{-iq\Omega(-\mathbf{n},\mathbf{n};\mathbf{r})} \psi(-\mathbf{r}) \tag{14}$$

under the inversion $\iota:\mathbf{r}\to-\mathbf{r}$.

On the modes we have, as an easy calculation shows

$$\Pi Y^{(l)}_{qm}=(-1)^l Y^{(l)}_{-qm}. \tag{15}$$

The parity operator can be used to extend the magnetic rotation operator T to include reflections. The reflection, σ, in the plane with normal $\mathbf{t}$ can be written as a rotation through π about the axis $\mathbf{t}$ combined with the parity inversion ι. This can be written as $\sigma=g_\pi\iota=\iota g_\pi$. The extension of T to reflections is thus defined by

$$T_\sigma\psi=T_{ig_\pi}\psi=T_\iota T_{g_\pi}\psi=\Pi T_{g_\pi}\psi.$$

From (10) and (14),

$$(T_\sigma\psi)(\mathbf{r})=e^{-iq\Omega_\sigma(\hat{\mathbf{r}})+iq\pi}(R_{g_\pi}\psi)(-\mathbf{r}), \tag{16}$$

and on the modes,

$$(T_\sigma Y^{(l)}_{qm'})(\hat{\mathbf{r}})=(-1)^l Y^{(l)}_{-qm}(\hat{\mathbf{r}})\mathcal{D}^{(l)}_{mm'}(g_\pi). \tag{17}$$

IV. CONSTRUCTION OF THE DOMAINS S^2/Γ'

It is convenient now to formalize briefly what we mean by the space S^2/Γ' where Γ' is a finite subgroup of O(3). A region of the sphere $\mathcal{F}\in S^2$ is called a fundamental domain for Γ if it satisfies the following criteria:

(i) $\mathcal{F}$ is open in S^2,
(ii) $\mathcal{F}\cap\gamma\mathcal{F}=\varnothing$, $\forall\,\gamma\in\Gamma'-\{id\}$,
(iii) $S^2=\cup_{\gamma\in\Gamma'}\overline{\gamma\mathcal{F}}$.

We also assume that $\mathcal{F}$ is connected.

Physically, $\mathcal{F}\cup\partial\mathcal{F}$ represents the space on which our theory is defined, and all the copies of $\mathcal{F}$ on S^2 must be physically equivalent.

The space S^2/Γ' is the the sphere S^2 with the points $\mathbf{r}$ and $\gamma\mathbf{r}$ identified for all $\gamma\in\Gamma'$. If Γ' acts freely on S^2, i.e., there are no fixed points, then S^2/Γ' is closed and can be taken to be $\mathcal{F}$ with identified boundary. If there are fixed points, these will be contained in $\partial\mathcal{F}$ and can be considered as boundary singular points of S^2/Γ'.

When Γ is purely rotational the fixed points form a discrete set of which there are two, or three, in $\partial\mathcal{F}$. For the extended, reflection groups, as already indicated, the boundary $\partial\mathcal{F}$ is constructed from the intersections of two or three reflection planes with the sphere. Thus there are transformations that map $\mathcal{F}$ into adjacent domains and which leave part of the boundary of $\mathcal{F}$ fixed. The conclusion here is that, unlike the rotational case, the boundary $\partial\mathcal{F}$ is a real boundary and the physical manifold is termed a Möbius triangle.

V. PROJECTION TO S^2/Γ

Still restricting to purely rotational Γ, we will now formally project everything down to S^2/Γ in a more or less standard fashion.

In order that a function $\tilde{\psi}(\mathbf{r})$ on S^2 project down consistently to S^2/Γ, it is necessary that it satisfy the magnetic periodicity condition,

$$T_g\cdot\tilde{\psi}(\mathbf{r})=a(g^\bullet)\tilde{\psi}(\mathbf{r}),\quad g\in\Gamma^\bullet, \tag{18}$$

where $a(g^\bullet)$ forms a one-dimensional representation of $\Gamma^\bullet$, the double of Γ, and labels the projection. For ease we have put $\mathbf{r}$ in place of $\hat{\mathbf{r}}$. We show later that there is a minimal choice for $a(g^\bullet)$.

If q is integral, there is no need to introduce the group doubles. However, if one does, there is a simple duplication, which is easily dealt with in practice as we can show with the following, somewhat superfluous, constructions.

Since the action of $\Gamma^\bullet$ covers the sphere S^2 twice, we introduce the trivial double covering, $S^{2^\bullet}$, of two identical copies of S^2, with $S^{2^\bullet}/\Gamma^\bullet = S^2/\Gamma$.

The modes themselves do not change sign on a 2π rotation, even when l is half odd-integral, and neither does the wave function. So $\psi^\bullet(\mathbf{r}) = \psi^\bullet(E\mathbf{r})$, where E is a 2π rotation, and therefore, $\tilde{\psi}(\mathbf{r}) = \psi^\bullet(\mathbf{r})$.

We then have, somewhat non-rigorously, for the function, $\psi(\mathbf{r})$, on $S^{2^\bullet}/\Gamma^\bullet$ the numerical equality

$$\psi(\mathbf{r}) = \psi^\bullet(\mathbf{r}), \tag{19}$$

where we do not distinguish between the projected and original coordinates, both being denoted by $\mathbf{r}$. The $\mathbf{r}$ on the right belongs to the fundamental domain of $\Gamma^\bullet$ on $S^{2^\bullet}$, which is, of course, isomorphic to that of Γ on S^2. Then,

$$T_{g^\bullet}\psi(\mathbf{r}) = a(g^\bullet)\psi(\mathbf{r}). \tag{20}$$

The heat-kernel on S^2, written in mode form,

$$K_{S^2}(\mathbf{r},\mathbf{r}';\tau) = \sum_{l=|q|}^{\infty} e^{-\lambda_l \tau}\,\mathrm{Tr}[\mathbf{Y}_q^{(l)}(\mathbf{r})\mathbf{Y}_q^{(l)\dagger}(\mathbf{r}')], \tag{21}$$

propagates arbitrary wave functions on S^2 and satisfies the important switching relation

$$K_S(\mathbf{r},g^{-1}\mathbf{r}';\tau) = e^{-iq\Lambda_g(\mathbf{r}')-iq\Lambda_{g^{-1}}(\mathbf{r})}K_S(g\mathbf{r};\mathbf{r}';\tau),$$

which realizes in coordinate representation the operator rotational symmetry,

$$T_g K_{S^2} = K_{S^2} T_g$$

[see (11)].

The heat-kernel that propagates wave functions on $S^{2^\bullet}/\Gamma^\bullet$ obeying (20) is, by general theory,

$$K_{S^{2^\bullet}/\Gamma^\bullet}(\mathbf{r},\mathbf{r}') = \sum_{g^\bullet \in \Gamma^\bullet} a(g^\bullet) T_{g^{\bullet -1}} K_{S^2}(\mathbf{r},\mathbf{r}'), \tag{22}$$

which is referred to as the preimage form of this propagator in terms of that on $S^{2^\bullet}$.

The double group $\Gamma^\bullet$ can be decomposed,

$$\Gamma^\bullet = \Gamma \cup E\Gamma,$$

and the sum over $\Gamma^\bullet$ reduced to a sum over the subset Γ,

$$K_{S^{2\bullet}/\Gamma^\bullet}(\mathbf{r},\mathbf{r}') = \sum_{g\in\Gamma} (a(g)T_{g^{-1}} + a(Eg)T_{(Eg)^{-1}})K_{S^{2\bullet}}(\mathbf{r},\mathbf{r}'). \tag{23}$$

We know, (12), that $T_E = (-1)^{2q}\mathbf{1}$ and so from (20), $a(E) = (-1)^{2q}$. Hence $a(E)T_E = \mathbf{1}$ and so

$$K_{S^{2\cdot}/\Gamma\cdot}(\mathbf{r},\mathbf{r}')=2\sum_{g\in\Gamma}a(g)T_{g^{-1}}K_{S^{2}\cdot}(\mathbf{r},\mathbf{r}'), \tag{24}$$

which means we can finally write what was almost obvious from the start, the preimage sum,

$$K_{S^2/\Gamma}(\mathbf{r},\mathbf{r}')=\sum_{g\in\Gamma}a(g)T_{g^{-1}}K_{S^2}(\mathbf{r},\mathbf{r}'). \tag{25}$$

The factor of 2 is a normalization (volume) factor between $S^{2\cdot}$ and S^2, $K_{S^{2\cdot}}=2K_{S^2}$.

This result shows that we can effectively ignore the complication of the double group and just proceed with Γ as usual.

Given an arbitrary field $\tilde{\phi}(\mathbf{r})$ on S^2, a quasiperiodic field on S^2 and hence, via (19), a field on S^2/Γ is constructed by the projection

$$\psi(\mathbf{r})=\frac{1}{|\Gamma|}\sum_{g\in\Gamma}a(g)T_{g^{-1}}\tilde{\phi}(\mathbf{r}). \tag{26}$$

In particular the projected (i.e., adapted) modes are

$$Y^{\Gamma(l)}_{qm}(\mathbf{r})=\frac{1}{\sqrt{|\Gamma|}}\sum_{g\in\Gamma}a(g)(T_{g^{-1}}Y^{(l)}_{qm})(\mathbf{r})=\sqrt{|\Gamma|}Y^{(l)}_{qm'}(\mathbf{r})P_{m'm}, \tag{27}$$

where, using (13),

$$P_{m'm}=\frac{1}{|\Gamma|}\sum_{g\in\Gamma}a(g)\mathcal{D}^{(l)}_{m'm}(g^{-1}) \tag{28}$$

is a Hermitian projection matrix, $P^2=P$. Since the eigenvalues of P are 0 and 1, this shows that in a suitable, i.e., diagonal, basis the projected eigenfunctions are a subset of the unprojected ones, a general result and independent of the magnetic field.

Depending on whether q and l are integral or half odd-integral together, the representations a and $\mathcal{D}$ of the doubled elements, $E\gamma$, have the same or opposite sign as those of γ and we can see explicitly that it is adequate to restrict the sum in (28) to Γ, as we have done.

Let us pursue this a little further to make sure everything is satisfactory. It is much more elegant to express everything in abstract form but we will retain the coordinate representation. The discussion is a textbook one in applied group theory.

From (27), using periodicity, one easily derives the integral

$$\int_{S^2/\Gamma}Y^{\Gamma(l)}_{qm}{}^{*}(\mathbf{r})Y^{\Gamma(l)}_{qm'}(\mathbf{r})d\mathbf{r}=P_{mm'}.$$

Diagonalizing A, $A=UDU^{-1}$, introduces the linear combinations $Y^{(\Gamma)}U$, which, from (27) equals $\sqrt{|\Gamma|}YUD$ showing that certain linear combinations of the modes on S^2 vanish and others do not, after adaptation which takes on the nature of a filtering process. We write for the nonzero combinations,

$$\mathcal{Y}^{(l)}_{q\alpha}=\sqrt{|\Gamma|}Y^{(l)}_{qm}U_{m\alpha}, \tag{29}$$

which form a complete, orthogonal set on S^2/Γ.

The factors of $\sqrt{|\Gamma|}$ have been chosen to give suitably normalized eigenfunctions on S^2/Γ so that

$$K_{S^2/\Gamma}(\mathbf{r},\mathbf{r}';\tau)=\sum_{l=|q|}^{\infty} e^{-\lambda_l \tau}\,\mathrm{Tr}[\mathcal{Y}_q^{(l)}(\mathbf{r})\mathcal{Y}_q^{(l)\dagger}(\mathbf{r}')]. \tag{30}$$

The matrix U reduces the l-representation of $\Gamma^\bullet$ into irreducible ones and, from (28), the range of α, i.e., the degeneracy, is the number of times the irreducible a-representation occurs in this decomposition.

VI. EFFECT OF FIXED POINTS

The standard theory of coverings applies when the covering group acts freely. This is not so in the present case and the result is a singular space—an orbifold. We can still maintain the standard covering terminology, as we already have done when referring to fundamental domains, in an obvious way by firstly removing the fixed points, so that the standard theory applies, and then extending the action of the covering group, Γ, to these points.

We now investigate the implications of the periodicity condition (18) when extended to the fixed point set of Γ. For any $\gamma\in\Gamma$ there are two fixed points on the sphere, $\pm\mathbf{r}_\gamma$. Going back to the mathematical result (6), we see that the monopole modes on the full sphere satisfy the *identity*,

$$Y_{qm'}^{(l)}(\pm\mathbf{r}_\gamma)=e^{iq\Lambda_\gamma(\pm\mathbf{r}_\gamma)}Y_{qm}^{(l)}(\pm\mathbf{r}_\gamma)\mathcal{D}_{mm'}^{(l)}(\gamma), \tag{31}$$

where γ is the rotation about $\pm\mathbf{r}_\gamma$, obviously.

Using the relation (29) we can determine the action of the magnetic rotation operator T_γ on the $\mathcal{Y}$,

$$T_\gamma\mathcal{Y}(\mathbf{r})=\sqrt{|\Gamma|}(T_\gamma Y)(\mathbf{r})U=e^{-iq\Lambda_\gamma(\mathbf{r})}\sqrt{|\Gamma|}Y(\gamma^{-1}\mathbf{r})U=e^{iq\Lambda_\gamma(\mathbf{r})}\mathcal{Y}(\gamma^{-1}\mathbf{r})$$

as expected. However we also have, from (27),

$$T_\gamma\mathcal{Y}(\mathbf{r})=a(\gamma)\mathcal{Y}(\mathbf{r})$$

and therefore

$$e^{-iq\Lambda_\gamma(\mathbf{r})}\mathcal{Y}(\gamma^{-1}\mathbf{r})=a(\gamma)\mathcal{Y}(\mathbf{r})$$

and of course

$$e^{-iq\Lambda_\gamma(\mathbf{r})}\psi(\gamma^{-1}\mathbf{r})=a(\gamma)\psi(\mathbf{r}).$$

If there were no fixed points there would be no problem to discuss. However if $\mathbf{r}=\mathbf{r}_\gamma$ is fixed by γ we have the consistency condition,

$$e^{iq\Lambda_\gamma(\mathbf{r}_\gamma)}\psi(\mathbf{r}_\gamma)=a(\gamma)\psi(\mathbf{r}_\gamma),$$

$$e^{-iq\Lambda_\gamma(\mathbf{r}_\gamma)}\mathcal{Y}(\mathbf{r}_\gamma)=a(\gamma)\mathcal{Y}(\mathbf{r}_\gamma). \tag{32}$$

This says that the phase is undetermined at the fixed points. If the fixed point is removed there is no problem. We are then effectively working arbitrarily close to the fixed point and all the points $\gamma\mathbf{r}$, $\gamma\in\Gamma$, belong to different images of the fundamental domain. When the fixed point is put back and the limit $\mathbf{r}\to\mathbf{r}_\gamma$ taken, all these images coalesce and the phase becomes indeterminate, unless something special happens such as $e^{-iq\Lambda_\gamma(\mathbf{r}_\gamma)}$ equaling $a(\gamma)$ or if the wave function has a node at $\mathbf{r}_\gamma$. We analyze this situation further.

Since Γ can be generated by a set of cyclic rotations, it is helpful first to take the case when Γ is cyclic, C_k, about the z-axis. Everything in (28) is then explicit. Let the generator of C_k be $\hat{\gamma}$, ($\hat{\gamma}^k=\mathbf{1}$). Also let the generator of the double group $\mathbb{Z}^\bullet$ be $\gamma^\bullet$ with $(\gamma^\bullet)^k=E$ and $(\gamma^\bullet)^{2k}=\mathbf{1}$. E is the 2π doubling rotation.

The representations $a(g^{\bullet})$ are

$$a((\gamma^{\bullet})^{p})=e^{2\pi ipr/k}, \quad p=0,1,...,2k-1, \tag{33}$$

where, for integral q, the label r, is in the range 0 to $k-1$, while for half-odd integral q, $r=(2s+1)/2$ with $0\leqslant s\leqslant k-1$.

$\mathcal{D}^{(l)}_{mm'}(g^{\bullet})$ is diagonal

$$\mathcal{D}^{(l)}_{mm'}((\gamma^{\bullet})^{p})=e^{-2\pi ipm/k}\delta_{mm'}, \quad -l\leqslant m, \ \ m'\leqslant l, \tag{34}$$

and $P_{mm'}$ is easily found,

$$P_{mm'}=\frac{1}{k}\,\frac{1-e^{2\pi i(m+r)}}{1-e^{2\pi i(m+r)/k}}\,\delta_{mm'}. \tag{35}$$

This expression vanishes unless $m+r$ is 0 mod k, in which case it equals unity making the filtering obvious.

It is comforting to check things by looking at the explicit forms of some modes. For $q=0$, the modes $Y^{(l)}_{m}$ are ordinary spherical harmonics. At the north pole only the $m=0$ component survives which then forces r to be zero and (32) is trivially satisfied since $a(\gamma)=1$.

One can proceed generally but let us use the modes exhibited in Wu and Yang, Sec. VII. For $q=1/2$ we see that only the $m=-1/2$ survives at the north pole making $r=1/2$ and now to check (32) we need the expression for Λ. For a rotation through ω about the z-axis, from (7) or (8), $\Lambda=-\omega$, and again the check works. For $q=1$, the nonzero mode corresponds to $r=1$.

In general one finds that $r=q$ and looking at the ϕ dependence of the modes, $Y^{(l)}_{mq}$, (3), i.e., $\exp(i(m+q)\phi)$, we see that the modes $Y^{\Gamma(l)}$ are periodic as ϕ increases by $2\pi/k$ and so, therefore, is the wave function.

It should be noted that if (8) is used, the azimuthal angle of the north pole changes by ω even though it is a fixed point. The string's location may be unchanged, but a nonzero compensating gauge transformation is still required.

It is clear geometrically that the same results will hold if C_k is cyclic about any axis so that it is consistent to set

$$a(\gamma)=e^{-iq\Lambda_{\gamma}(\mathbf{r}_{\gamma})}, \tag{36}$$

for any Γ. The consequence of replacing $\mathbf{r}_{\gamma}$ by $-\mathbf{r}_{\gamma}$ is discussed in the next section.

The minimal choice (36) clearly corresponds to untwisted fields in the sense that the more general form,

$$a(\gamma)=e^{-iq\Lambda_{\gamma}(\mathbf{r}_{\gamma})}b(\gamma), \tag{37}$$

where $b(\gamma)$ is some nontrivial representation of $\Gamma^{\bullet}$, encodes physics over and above the magnetic monopole, such as Aharonov–Bohm fluxes through the fixed points. In this latter case, (18) implies that the wave function vanishes at the fixed points.

VII. CHARGE QUANTIZATION ON ROTATIONAL DOMAINS

We now have expressions for the modes and heat-kernel on S^2/Γ in the rotational case and have tacitly assumed that all integer values of $2q$ are allowed. However $2q$ need only form a subset of the integers. A geometric, Dirac-type argument will first be used to calculate this subset.

Choose a fundamental domain $\mathcal{F}$ which does not contain the string. Let $L\subset\mathcal{F}$ be a piecewise continuous loop in $\mathcal{F}$ and construct the parallel propagator,

$$\mathcal{I}[L]=e^{ie\int_L A}=e^{-iq\Omega}, \tag{38}$$

where A is the potential one-form, Ω is the area within L. This follows from the explicit form of the monopole potential. As L shrinks to a point in $\mathcal{F}$, $\mathcal{I}[L]$ clearly tends to unity as the area vanishes. Now L also describes a loop with (oriented) area $-(|\mathcal{F}|-\Omega)$ in S^2/Γ, since S^2/Γ is closed for rotational Γ (except for the fixed points which we can ignore for these purposes as a set of measure zero). Thus if we let L expand to fill the boundary $\partial\mathcal{F}\subset S^2$, the propagator will also take the value 1. This requires that $q|\mathcal{F}|$ be a multiple of 2π which gives the possible values of the magnetic charge as

$$q=|\Gamma|\frac{n}{2}, \quad n\in\mathbb{Z}, \tag{39}$$

the expected value since the magnetic charge per closed domain, $\overline{q}\equiv q/|\Gamma|$, equals the Dirac value, $n/2$.

If the string passes through $\mathcal{F}$ there is an extra phase $-4\pi q$ in (38) which makes no difference to the final result.

For the cyclic group, C_k, according to (33), and (36),

$$a(\gamma^{\bullet p})=e^{2\pi ipq/\nu}=(-1)^{np} \tag{40}$$

so all the $a(\gamma)$ are ± 1.

A further restriction occurs if C_k is a subgroup of a point group Γ, for then

$$a(\gamma^{\bullet})=e^{i\pi|\Gamma|n/k},$$

but, by observation, for a noncyclic point group, all $|\Gamma|/k$ are even and the $a(\gamma)$ are unity. Furthermore the monopole charge q is integral and there are no spinor modes.

The quantization (39) or (36), will now be derived in another way. The consistency condition (32) must hold for both fixed points of γ. Geometry shows, if orientation effects are taken correctly into account, that $\Lambda_\gamma(-\mathbf{r}_\gamma)=-\Lambda_\gamma(\mathbf{r}_\gamma)$. This also follows from the mode transformation (31) and the behavior under parity (14), which involves $q\to -q$.

The two definitions of $a(\gamma)$ require

$$q=\frac{k_\gamma}{2}n_\gamma \tag{41}$$

for some integer n_γ, where k_γ is the order of the cyclic subgroup generated by γ. Since $\Lambda_\gamma(\mathbf{r}_\gamma)=2\pi/n_\gamma$, all the $a(\gamma)$ are ± 1.

If Γ is not cyclic, the minimum requirement of (41) is $q=(K/2)p$, where $p\in\mathbb{Z}$ and K is the LCM of all the n_γ. Looking at the character tables of the double point groups it is easily checked that it is not possible to reconcile the tabulated ± 1 representations $a(\gamma^{\bullet})$ with (41) unless all the $a(\gamma^{\bullet})$ are unity, implying that p is even or $q=(2K/2)p'$ for $p'\in\mathbb{Z}$. But $2K$ is nothing but the group order Γ leading to (39) for all n. Q.E.D.

VIII. INTEGRATED KERNELS AND ZETA FUNCTIONS

Special interest attaches itself to the integrated kernel,

$$\begin{aligned} K_\Gamma(\tau)&\equiv\int_{S^2/\Gamma}K_{S^2/\Gamma}(\mathbf{r},\mathbf{r};\tau)d\mathbf{r}\\ &=\sum_{g\in\Gamma}a(g)\int_{S^2/\Gamma}(T_{g^{-1}}K_{S^2})(\mathbf{r},\mathbf{r};\tau)d\mathbf{r}\\ &=\frac{1}{|\Gamma|}\sum_{g\in\Gamma}a(g)\int_{S^2}(T_{g^{-1}}K_{S^2})(\mathbf{r},\mathbf{r};\tau)d\mathbf{r}. \end{aligned} \tag{42}$$

It is convenient to write everything in terms of the covering S^2 quantities because we can use the mode form (21) in (42) to obtain

$$K_\Gamma(\tau)=\sum_{l=|q|}^{\infty} d_\Gamma(l)e^{-\lambda_l\tau} \tag{43}$$

with

$$d_\Gamma(l)=\frac{1}{|\Gamma|}\sum_g a(g)\chi^{(l)}(g^{-1}), \tag{44}$$

where we have used the orthogonality of the S^2 monopole modes and $\chi^{(l)}(g)$ is the usual $\mathrm{SO}^\bullet(3)\sim\mathrm{SU}(2)$ character of g. In particular,

$$\int_{S^2}\mathrm{Tr}[(T_g\mathbf{Y}_{ql})(\mathbf{r})\mathbf{Y}^\dagger_{ql}(\mathbf{r})]d\mathbf{r}=\chi_l(g). \tag{45}$$

Algebraically we can see that the degeneracy, $d_\Gamma(l)$, is the number of times the irreducible representation ''a'' occurs in the l-representation. Since degeneracies are real $a(g)$ in (44) and in the following equations, can be replaced by its real part, $\mathrm{Re}\,a(g)$, although in the present case the minimal $a(g)=\pm1$.

(44) shows that the summand in $d_\Gamma(l)$, is a class function so that we can make a convenient geometrical decomposition of the traced kernel, as in our earlier work.[1] The preimage sum, i.e., the sum over Γ, is firstly replaced by a sum over conjugacy classes, $\{g\}$,

$$d_\Gamma(l)=\frac{2l+1}{|\Gamma|}+\frac{1}{|\Gamma|}\sum_{\{g\}} a(g)|\{g\}|\chi^{(l)}(g)$$

with g being a typical element in $\{g\}$.

We now recall that the elements of a class correspond to rotations through one fixed angle about a set of conjugate axes. For a given set of such axes, one corresponding class can be considered to be the primitive class, all others associated with these axes then being generated by this one. Thus the sum over all classes can be rewritten as a sum over primitive classes and powers of these. Let k be the generic order of the rotation associated with the generic primitive class $\{\hat g\}$ so that $\hat g^k=id$. Then $|\{\hat g\}|$ is just the number, n_k, of conjugate k-fold axes and we can write

$$d_\Gamma(l)=\frac{2l+1}{|\Gamma|}+\frac{1}{|\Gamma|}\sum_{\hat g} n_k\sum_{p=1}^{k-1} a^p(\hat g)\chi^{(l)}(\hat g^p) \tag{46}$$

which is the same as when there is no magnetic field, apart from the restriction $l\geqslant|q|$ and one sees again that the cyclic groups, C_k, form the basic building blocks. This can be made explicit as follows. In the case that Γ is just C_k, one has from (46)

$$d_k(l)=\frac{1}{k}\sum_{p=0}^{k-1} a^p(\hat g)\chi^{(l)}(\hat g^p)=\frac{2l+1}{k}+\frac{1}{k}\sum_{p=1}^{k-1} a^p(\hat g)\chi^{(l)}(\hat g^p) \tag{47}$$

so that, substituting back,

$$d_\Gamma(l)=\frac{d_1(l)}{|\Gamma|}\left(1-\sum_{\hat g} n_k\right)+\frac{1}{|\Gamma|}\sum_{\hat g} kn_kd_k(l), \tag{48}$$

where $d_1(l)=2l+1$ is the full sphere degeneracy.

Having now the degeneracies and the eigenvalues, we can turn to the explicit construction of the integrated heat-kernel (43) and its Mellin transform, the ζ-function,

$$\zeta_\Gamma(s)=\sum_l \frac{d_\Gamma(l)}{\lambda_l^s}. \tag{49}$$

The eigenvalues are given by (2) and we face the old problem of computing spherical spectral quantities. We will approach this by firstly looking at a ''linearized'' system, one whose eigenvalues are $l+1/2$. The corresponding heat-kernel, denoted $\tilde{K}_\Gamma(\tau)$, can be considered as that for the pseudo-operator $(H_{S^2}+1/4+q^2)^{1/2}$ and will allow us to find the ζ-function for the eigenvalues $(l+1/2)^2$ quickly and that for the λ_l of (2), more elaborately. The expressions are also of some statistical mechanical interest if τ is interpreted as an inverse temperature.

From (43), we have the linearized, or square root, kernel

$$\tilde{K}_\Gamma(\tau)=\sum_{l=|q|}^{\infty} d_\Gamma(l)e^{-(l+1/2)r} \tag{50}$$

with degeneracies given by (44).

In accordance with (48), it is sufficient to consider the cyclic group case, $K_k(\tau)$ and $\zeta_k(s)$.

Since the cyclic axis is immaterial, we choose it to lie along the z-axis and could use the expressions in the previous section since $d_k(l)$ is $\mathrm{Tr}\,\mathbf{P}$, where $\mathbf{P}$ is given by (35) with $r=q$. Therefore,

$$\tilde{K}_k(\tau)=\frac{1}{k}\sum_{l=|q|}^{\infty}\sum_{m=-l}^{l} e^{-(l+1/2)r}\frac{1-e^{2\pi i(m+q)}}{1-e^{2\pi i(m+q)/k}}. \tag{51}$$

The summations can be relabeled using (5) and performed, but it is perhaps more elegant to substitute (44) into (43) and do the l-summation first, as in Ref. 1.

Remembering the charge quantization condition, (40), the degeneracies are

$$d_k(l,q)=\frac{1}{k}\sum_{p=0}^{k-1}\cos(\pi np)\frac{\sin((2l+1)\pi p/k)}{\sin(\pi p/k)},\quad q=nk/2, \tag{52}$$

where n is even or odd. If n is even, the degeneracies are identical to the case when $q=0$, $d_k(l,q)=d_k(l,0)$.

We now introduce the generating function

$$h_k(\sigma,q)=\sum_{l=|q|}^{\infty} d_k(l,q)\sigma^l \tag{53}$$

closely connected with the traced heat-kernel, (43), if $\sigma=e^{-\tau}$. For n even the only effect of the monopole is to make the series start at $l=|q|$. However it is better to continue with the summations. We have, for both integral and half odd-integral q,

$$
\begin{aligned}
h_k(\sigma,q)&=\frac{1}{k}\sum_{l=|q|}^{\infty}\sum_{p=0}^{k-1}\cos(\pi np)\,\frac{\sin(2l+1)\pi p/k)}{\sin(\pi p/k)}\,\sigma^l\\
&=\frac{1}{k}\sum_{p=0}^{k-1}\cos(\pi np)\sum_{l=|q|}^{\infty}\frac{\sin(2l+1)\pi p/k}{\sin(\pi p/k)}\,\sigma^l\\
&=\sigma^q\frac{(q+\sigma+2q(1-\sigma))}{k(1-\sigma)^2}+\frac{1}{k}\sum_{p=1}^{k-1}\cos(\pi np)\sum_{l=|q|}^{\infty}\frac{\sin(2l+1)\pi p/k)}{\sin(\pi/k)}\,\sigma^l\\
&=\sigma^q\left(\frac{1}{1-\sigma}\,\frac{1+\sigma^k}{1-\sigma^k}+\frac{2q}{k(1-\sigma)}\right)
\end{aligned}
\tag{54}
$$

and so the corresponding heat-kernel is related in the simple way,

$$
\tilde{K}^q_k(\tau)=e^{-q\tau}\left(\tilde{K}_k(\tau)+\frac{2q}{k}\tilde{K}_\infty(\tau)\right) \tag{55}
$$

to the monopole-less ($q=0$) expression,[1]

$$
\tilde{K}_k(\tau)=\frac{\coth(k\tau/2)}{2\sinh(\tau/2)}.
$$

The decomposition into conjugacy classes, (48), shows that this relation will follow through for all groups Γ,

$$
\tilde{K}^q_\Gamma(\tau)=e^{-q\tau}(\tilde{K}_\Gamma(\tau)+2\overline{q}\tilde{K}_\infty(\tau)), \tag{56}
$$

where $\overline{q}$ is the charge per domain and $\tilde{K}_\Gamma(\tau)$ has been determined in Ref. 1,

$$
\tilde{K}_\Gamma(\tau)=\frac{\cosh(d_0\tau/2)}{2\sinh(d_1\tau/2)\sinh(d_2\tau/2)}. \tag{57}
$$

Here d_0, d_1, and d_2 are integer invariants associated with the reflection group having Γ as its rotation subgroup.

The zeta function corresponding to the linear heat kernel is easily determined as the Mellin transform of (57). In fact we shall find it more useful to consider the slightly more general zeta function defined by

$$
\begin{aligned}
\zeta^q_\Gamma(s,a)&=\frac{1}{\Gamma(s)}\int_0^\infty\tau^{s-1}e^{\tau/2-a\tau}\tilde{K}^q_\Gamma(\tau)d\tau\\
&=\zeta_2(s,a+q|d_1,d_2)+\zeta_2(s,a+q+d_0|d_1,d_2)+\overline{q}\zeta_H(s,a+q),
\end{aligned}
\tag{58}
$$

where ζ_H is the Hurwitz zeta function, and ζ_2 is the two-dimensional Barnes zeta function defined for $s>2$ by,[19]

$$
\zeta_2(s,a|d_1,d_2)=\sum_{n_1,n_2=0}^{\infty}\frac{1}{(a+n_1d_1+n_2d_2)^s}. \tag{59}
$$

ζ_H is actually a one-dimensional Barnes ζ-function.

To conclude this section we shall present some properties of the Barnes zeta function needed later.

The function $\zeta_2(s,a|d_1,d_2)$ has simple poles at $s=1,2$ whose residues can be written in terms of generalized Bernoulli polynomials,

$$\mathrm{Res}_{s\to r}\zeta_2(s,a|d_1,d_2)=\frac{(-1)^r}{d_1d_2}B^{(2)}_{2-r}(a|d_1,d_2) \tag{60}$$

for $r=1,2$. Here we have used the more standard notation as in Erdelyi.[20] The values of the Barnes ζ-function at negative integers are also given in terms of generalized Bernoulli polynomials. For $n\in\mathbb{Z}^+$ we have,

$$\zeta_2(-n,a|d_1,d_2)=\frac{1}{(n+1)(n+2)d_1d_2}B^{(2)}_{2+n}(a|d_1,d_2) \tag{61}$$

The explicit generalized Bernoulli polynomials required in this paper are

$$\begin{aligned}
B^{(2)}_0(a|d_1,d_2)&=1,\\
B^{(2)}_1(a|d_1,d_2)&=a-\tfrac{1}{2}(d_1+d_2),\\
B^{(2)}_2(a|d_1,d_2)&=a^2-(d_1+d_2)a+\tfrac{1}{6}(d_1^2+3d_1d_2+d_2^2),\\
B^{(2)}_3(a|d_1,d_2)&=a^3-\tfrac{3}{2}(d_1+d_2)a^2+\tfrac{1}{2}(d_1^2+3d_1d_2+d_2^2)a-\tfrac{1}{4}(d_1^2d_2+d_1d_2^2).
\end{aligned} \tag{62}$$

Finally we present a useful Bernoulli identity which will be used to simplify some expressions later on,

$$B^{(2)}_n(d_1+d_2-a|d_1,d_2)=(-1)^nB^{(2)}_n(a|d_1,d_2). \tag{63}$$

IX. EXTENSION TO REFLECTION GROUPS

Before showing how to deal with the eigenvalues (2), we extend the analysis to orbifolds S^2/Γ' where Γ' is a finite reflection group—the complete symmetry group of a regular solid as outlined in Sec. I. The domain of interest is a Möbius triangle on S^2.

As shown in Sec. III, under reflection, the magnetic charge, q, changes sign and the projection has to take this into account. The rotational projection is given by (22) and (27) and all that is necessary is to combine this with the group decomposition (1). We start by writing down the projected modes

$$W^{(l)}_{qm}(\mathbf{r})=Y^{\Gamma(l)}_{qm}(\mathbf{r})+a(\sigma)T_\sigma Y^{\Gamma(l)}_{-qm}(\mathbf{r}), \tag{64}$$

where σ is a reflection, say in one of the symmetry planes, so that $a(\sigma)=\pm1$. We can choose either sign.

Note the extended periodicity condition

$$T_{\gamma'}W^{(l)}_{qm}(\mathbf{r})=a(\gamma)a(\sigma)W^{(l)}_{-qm}(\mathbf{r}),\quad \gamma'=\gamma\sigma,$$

which shows that the wave function on the domain $\gamma'\mathcal{F}$ has monopole charge $-q$ if that on $\mathcal{F}$ has charge q.

The group decomposition of Γ' gives

$$S^2=\Big(\bigcup_{\gamma\in\Gamma}\overline{\gamma\mathcal{F}}\Big)\cup\Big(\bigcup_{\gamma\in\Gamma'_1}\overline{\gamma'\mathcal{F}}\Big)=\bigcup_{\gamma\in\Gamma}\overline{\gamma(\mathbf{1}+\sigma)\mathcal{F}},$$

and we see that the only possible theory using images requires that adjacent domains on the sphere have opposite numerical monopole charge.[23] The charge is q on $\gamma\mathcal{F}$ and $-q$ on $\gamma'\mathcal{F}$ for all $\gamma\in\Gamma,\gamma'\in\Gamma'_1$.

For the theory to be consistent, we must at least show that the fundamental domains with charge q and $-q$ define equivalent physical theories. There are two points. The first is that the

sign of the charge is arbitrary, being essentially a matter of definition for the observer. The second point is that any physically significant quantities will depend only on $F_{\mu\nu}F^{\mu\nu}\sim q^2$. Our theory therefore has the possibility of being consistent and we now derive the values of q for which it is consistent.

Across the boundaries of the fundamental domains we have $\mathbf{B}\to-\mathbf{B}$ and $\mathbf{A}\to-\mathbf{A}$. For consistency we should define these vector quantities to vanish on the reflecting boundaries. Consider now the parallel propagator, (38), where the loop $L\in\mathcal{F}$. Since we have defined $\mathbf{A}$ to vanish on $\partial\mathcal{F}$ we have $\mathcal{I}[\partial\mathcal{F}]=1$. Thus for an arbitrary loop approaching the boundary we require trivial parallel transport just as in the pure rotational case. This gives the *possible* values of q as

$$q=|\Gamma'|\frac{n'}{2}=|\Gamma|n', \quad n'\in\mathbb{Z}, \tag{65}$$

so q is integral and there are no spinor modes.

The existence of fixed points imposes certain conditions. The situation is more restricting than in the pure rotational case because the fixed points form a continuous set, the boundary of our domain, $\mathcal{F}$. Let σ be a reflection ($\sigma^2=\mathbf{1}$). The fixed point set, $\mathcal{P}$, is the intersection of the reflecting plane with the S^2, i.e., a great circle. Extending the periodicity condition (18) to Γ' we see that ψ would have to satisfy

$$e^{-iq\Omega_\sigma(\mathbf{r})+iq\pi}\psi(\mathbf{r})=a(\sigma)\psi(\mathbf{r}), \quad \forall\,\mathbf{r}\in\mathcal{P}. \tag{66}$$

Since $\Omega_\sigma(\mathbf{r})$ is not constant on $\mathcal{P}$, this equation cannot be satisfied on all of $\mathcal{P}$ unless one of $q=0$, $\psi|_{\mathcal{P}}=0$, $\mathbf{n}\perp\mathcal{P}$ or $\mathbf{n}\in\mathcal{P}$ is true. Applying this argument to the two, or three, reflection generators removes the last two possibilities and we are left with either $q=0$ or $\psi|_{\mathcal{P}}=0$ (or both).

The fact that the magnetic charge, q, has to be of opposite sign on adjacent domains under the action of Γ' for the image method to work indicates, crudely, that q is zero on the boundary and suggests that our construction satisfies the restrictions following from (66).

Developing this nonrigorous analysis, since the magnetic field $\mathbf{B}$ vanishes on the reflecting boundaries we must insist that the monopole modes take the value $W^{(l)}_{0m}$ on the boundaries. Thus the consistency Eq. (66) is satisfied. Let γ be an arbitrary rotation in Γ. The rotational consistency (32) is satisfied for all γ since q is an integer multiple of $|\Gamma|$ and, as already stated, $a(\gamma)=1$, $\forall\gamma$. It would thus appear that all the values of q in (65) produce a consistent theory.

For clarity we restate that the mode labeled by qlm takes the values

$$\begin{gathered} W^{(l)}_{qm} \ \text{ on } \ \Gamma\mathcal{F}, \\ W^{(l)}_{-qm} \ \text{ on } \ \Gamma'_1\mathcal{F}, \\ W^{(l)}_{0m} \ \text{ on } \ \partial(\Gamma\mathcal{F})\sim-\partial(\Gamma'_1\mathcal{F}). \end{gathered} \tag{67}$$

The modes (64) can be used to define a heat-kernel analogous to the rotational case. We skip straight to the linear heat-kernel which may be written

$$\tilde{K}^q_{\Gamma'}(\tau)=\int_{S^2/\Gamma'}\sum_{l=q}^{\infty}e^{-(l+1/2)\tau}\mathrm{Tr}[\mathbf{W}^{(l)}_q(\mathbf{r})\mathbf{W}^{(l)\dagger}_q(\mathbf{r})]d\mathbf{r}.$$

Here $\mathbf{W}^{(l)}_q$ is the vector of solutions $W^{(l)}_{qm}$. We can extend this integral to all S^2 just as we did in Eq. (42), in the rotational case (this is not entirely trivial but it is possible using the invariance of the theory under $q\to-q$),

$$\tilde{K}^q_{\Gamma'}(\tau)=\frac{1}{|\Gamma'|}\int_{S^2}\sum_{l=q}^{\infty}e^{-(l+1/2)\tau}\mathrm{Tr}[\mathbf{W}^{(l)}_q(\mathbf{r})\mathbf{W}^{(l)\dagger}_q(\mathbf{r})]d\mathbf{r}.$$

The next step is to the use the explicit rotational modes (27) or (29) [with $a(g)=1$], Eqs. (13) and (17), and the invariance of the heat kernel under charge reversal. The result is

$$\tilde{K}^q_{\gamma'}(\tau)=\tfrac{1}{2}\tilde{K}^q_\Gamma(\tau)+\frac{a(\sigma)}{|\Gamma'|}\sum_{\gamma'\in\Gamma_1}\int_{S^2}\sum_{l=q}^{\infty}e^{-(l+1/2)}\,\mathrm{Tr}[(T_{\gamma'}\mathbf{Y}^{(l)}_{-q})(\mathbf{r})\mathbf{Y}^{(l)\dagger}_q(\mathbf{r})]d\mathbf{r}. \tag{68}$$

This equation actually represents two heat kernels for the cases $a(\sigma)=\pm 1$. For $a(\sigma)=-1$ we shall use the term ''Dirichlet'' and write $K^q_D(\tau)$. For $a(\sigma)=+1$ we use the term ''Neumann'' and write $K^q_N(\tau)$. These names are used in analogy to the case with no monopole field, $q=0$. In this case $W^{(l)}_{0m}$ is, by construction, a solution on the whole sphere [see (67)] and must satisfy $T_{\gamma'}W^{(l)}_{0m}=a(\sigma)W^{(l)}_{0m}$ everywhere. On the reflecting boundaries, $a(\sigma)=-1$ requires $W^{(l)}_{0m}$ to vanish, i.e., Dirichlet boundary conditions, and $a(\sigma)=+1$ requires the normal derivative of $W^{(l)}_{0m}$ to vanish, i.e., Neumann boundary conditions.

We now turn to some specific calculations of the heat kernels. Using (45) we can write the second term in (68) as,

$$\frac{a(\sigma)}{|\Gamma'|}\int_{S^2}\sum_{l=q}^{\infty}\sum_{\gamma'\in\Gamma_1}\chi_l(\gamma')e^{-(l+1/2)r}. \tag{69}$$

Our first calculation is for the reflection group Γ' with rotational subgroup C_k. In this case Γ'_1 consists of k reflection planes with a common invariant axis, and with angle $2\pi/k$ between adjacent planes. If we take one plane to be the $z-x$ plane then we can write $\Gamma'_1=\{\Pi g_\pi\hat{\gamma}^p|p=0,1,2,\ldots,k-1\}$ where Π is parity, g_π is a rotation by angle π about the y axis, and $\hat{\gamma}$ is a rotation by angle $2\pi/k$ about the z-axis. Using the explicit result

$$\mathcal{D}^{(l)}_{mm'}(g_\pi)=(-1)^{l-m}\delta^m_{-m'} \tag{70}$$

and Eqs. (15), (34) we find $\chi_l(\gamma')=1$ for all $\gamma'\in\Gamma'_1$ and all l. Thus (69) is trivial to calculate in this case, and from (68), (55) we find[23]

$$\tilde{K}^q_D(\tau)=e^{-q\tau}\frac{e^{-k\tau/2}}{4\sinh(\tau/2)\sinh(k\tau/2)}+\frac{q}{2k}\frac{e^{-q\tau}}{\sinh(\tau/2)}, \tag{71}$$

$$\tilde{K}^q_N(\tau)=e^{-q\tau}\frac{e^{k\tau/2}}{4\sinh(\tau/2)\sinh(k\tau/2)}+\frac{q}{2k}\frac{e^{-q\tau}}{\sinh(\tau/2)}. \tag{72}$$

The first term in each of these expressions is simply $\exp(-q\tau)$ times the monopoleless heat kernel.[1] Notice that the extra monopole contribution is the same in both heat kernels.

We can also calculate the heat kernels for the group Γ' with dihedral rotational subgroup D_k. We take Γ'_1 as σD_k where σ is a reflection in the $x-y$ plane, and D_k is the dihedral group with the k-fold cyclic group about the z axis, and a rotation by π about the y axis. Using (34) and (70), we find $\chi_l(\gamma')=1$ for elements $\gamma'\in\Gamma'_1$ involving the rotation by angle π about y. These elements are $|\Gamma|$ in number and contribute to (69) the expression

$$\frac{a(\sigma)}{8}\frac{e^{-q\tau}}{\sinh(\tau/2)}. \tag{73}$$

The remaining elements can be written $\Pi g_\pi\hat{\gamma}^p$, where g_π is a rotation by π about the z axis, and Π, $\hat{\gamma}$ are as defined above. Using (15) and (34) we find the transformation matrix $(-1)^{l+m}\delta^m_{m'}\exp(-i2\pi mp/k)$. This transformation is nontrivial and we have to construct a sum similar to (51).

For technical variety we use the relations (5) so that the sum can be written,

$$\frac{a(\sigma)}{4}e^{-\tau/2}\sum_{u=0}^{\infty}\sum_{t=-\infty}^{\infty}(-1)^{kt}(-e)^{-\tau(u+(|tk+q|+|tk-q|)/2)}=a(\sigma)e^{-q\tau}\frac{\cosh(k\tau/2)}{8\cosh(\tau/2)\sinh(k\tau/2)}. \tag{74}$$

Adding together (73) and (74), and using (55) gives the results from (68),

$$\tilde{K}_D^q(\tau)=e^{-q\tau}\frac{e^{-(k+1)\tau/2}}{4\sinh(2\tau/2)\sinh(k\tau/2)}+\frac{q}{4k}\frac{e^{-q\tau}}{\sinh(\tau/2)}, \tag{75}$$

$$\tilde{K}_N^q(\tau)=e^{-q\tau}\frac{e^{(k+1)\tau/2}}{4\sinh(2\tau/2)\sinh(k\tau/2)}+\frac{q}{4k}\frac{e^{-q\tau}}{\sinh(\tau/2)}. \tag{76}$$

Again the first terms are simply $\exp(-q\tau)$ times the $q=0$ case.

For all the heat kernels derived above the extra monopole contribution is simply given by

$$\frac{q}{|\Gamma'|}\frac{e^{-q\tau}}{\sinh(\tau/2)}. \tag{77}$$

Since we may construct the heat kernel for an arbitrary reflection group from the heat kernels calculated above,[2] the simplicity of (77) leads us to conclude that in the general case,[23]

$$\tilde{K}_D^q(\tau)=e^{-q\tau}\frac{e^{-d_0\tau/2}}{4\sinh(d_1\tau/2)\sinh(d_2\tau/2)}+\overline{q}'\frac{e^{-q\tau}}{\sinh(\tau/2)}, \tag{78}$$

$$\tilde{K}_N^q(\tau)=e^{-q\tau}\frac{e^{-d_0\tau/2}}{4\sinh(d_1\tau/2)\sinh(d_2\tau/2)}+\overline{q}'\frac{e^{-q\tau}}{\sinh(\tau/2)}. \tag{79}$$

These two equations are the culmination of this section.

The first terms in these heat kernels are just $\exp(-q\tau)$ times the $q=0$ expressions,[1] and we have defined the monopole charge per reflection domain

$$\overline{q}'=\frac{q}{|\Gamma'|}.$$

Equation (68) predicts that the linear Dirichlet and Neumann heat kernels should add up to give the rotational linear heat kernel (56), and this is seen to be true (in performing this sum we must use the relation $\overline{q}=2\overline{q}'$ for the same value of q).

The linear zeta functions for $\tilde{K}_D^q$ and $\tilde{K}_N^q$ are calculated using Eq. (58) with $\tilde{K}_\Gamma^q(\tau)$ suitably replaced. In terms of the Barnes zeta function we find,

$$\zeta_D^q(s,a)=\zeta_2(s,a+q+d_0|d_1,d_2)+\overline{q}'\zeta_H(s,a+q), \tag{80}$$

$$\zeta_N^q(s,a)=\zeta_2(s,a+q|d_1,d_2)+\overline{q}'\zeta_H(s,a+q). \tag{81}$$

It should be remembered that although we may add these two zeta functions to produce the rotational zeta function, the physical theories are completely different due to the changing sign of the magnetic field. Thus the procedure can only be regarded as a formal trick.

X. GENERAL ZETA FUNCTION AND ITS DERIVATIVE

Equations (58), (80), and (81) give zeta functions for the eigenvalues $(l+a)^2$ if s is replaced with $2s$. In general we need the zeta functions for the more general eigenvalues $\lambda_l=(l+a)^2-\alpha^2$, with suitable constants a and α. For example we may add curvature coupling and mass terms to the Hamiltonian H_{S^2}. In this case the eigenvalue equation is,

$$(H_{S^2}+\xi R+m^2)Y_{qm}^{(l)}=\lambda_l Y_{qm}^{(l)}$$

and we find $a=1/2$, $\alpha^2=q^2+(1/4-2\xi)-m^2$ ($R=2$ on the unit two-sphere). It is assumed that α^2 is positive. To analyze these general zeta functions we use similar methods to those found in Ref. 21; For brevity we shall just write $\zeta(s)$ to represent a general zeta function. For $s>1$, we have the explicit mode sum

$$\zeta(s)=\sum_{l=|q|}^{\infty}\frac{d(l)}{[(l+a)^2-\alpha^2]^s}. \tag{82}$$

The function $d(l)$ is the degeneracy of the eigenvalue λ_l for some linear zeta function (i.e., rotational, Dirichlet or Neumann). If we assume that $|\alpha|<|q|+a$ we can perform a binomial expansion on the summand which leads to a continuation of $\zeta(s)$ given by

$$\zeta(s)=\sum_{r=0}^{\infty}\alpha^{2r}\frac{\Gamma(s+r)}{r!\Gamma(s)}\zeta^q(2s+2r,a). \tag{83}$$

In the the above equation $\zeta^q(s,a)$ is intended to be any one of the rotational, Dirichlet, or Neumann zeta functions defined by Eqs. (58), (80), and (81), respectively.

In order to tie in with Ref. 21 we generalize to the case where $\zeta^q(s)$ represents an arbitrary zeta function on a d-dimensional space with simple poles (only) at $s=1,2,...,d$. This is the situation encountered in Ref. 21, where $\zeta^q(s)$ would just be a d-dimensional Barnes function $\zeta_d(s,a|\mathbf{d})$ (of course the label q is defunct in the general case). Near the poles we define,

$$\zeta^q(s+r,a)=\frac{N_r}{s}+R_r+O(s),\quad s\to 0,$$

for $r=1,2,...,d$. For our three cases (with $d=2$) the residues N_r for $r=1,2$ can be calculated from the specific forms of the zeta functions and (60).

The important fact is that the series (83) reduces to a finite sum when s is a negative integer. Thus we concentrate on these values of s and find for $n\in\mathbb{Z}^+$,

$$(-\alpha^2)^{-n}\zeta(-n)=\sum_{r=0}^{n}(-\alpha^2)^{-r}\binom{n}{r}\zeta^q(-2r,a)+\frac{1}{2}\sum_{r=1}^{u}\alpha^{2r}\frac{n!(r-1)!}{(r+n)!}N_{2r}. \tag{84}$$

The number u in the above is defined as $[d/2]$ where d is the dimension of the space under consideration. The derivative of the zeta function at $s=-n$ can also be calculated from (83),

$$\begin{aligned}(-\alpha^2)^{-n}\zeta'(-n)=&2\sum_{r=0}^{n}\binom{n}{r}(-\alpha^2)^{-r}\zeta^{q\prime}(-2r,a)-\sum_{r=0}^{n}\binom{n}{r}(-\alpha^2)^{-r}(\psi(n+1)-\psi(r+1))\zeta^q\\&\times(-2r,a)-\sum_{r=1}^{u}\alpha^{2r}\frac{n!(r-1)!}{(r+n)!}\left\{R_{2r}+\frac{1}{2}N_{2r}(\psi(r)-\psi(n+1))\right\}\\&+\sum_{r=u+1}^{\infty}\alpha^{2r}\frac{n!(r-1)!}{(r+n)!}\zeta^q(2r,a),\end{aligned} \tag{85}$$

where $\psi(z)=\Gamma'(z)/\Gamma(z)$ is the logarithmic derivative of the gamma function.

The problem now rests on the evaluation of the infinite sum on the last line of this expression. We show that this sum can be written in finite terms. It is expected that the sum will be finite since we expect $\zeta'(-n)$ to be finite, and all other terms on the right-hand side are finite. A word of caution is that in singular situations, there is the possibility that logarithmic terms, $\log\tau$, may

appear in the asymptotic expansion of the heat-kernel. If this were so, more care would have to be taken over the evaluation of the determinants. However no such terms occur here.

Using the integral representation (58) extended to the arbitrary zeta function $\zeta^q(s,a)$, we may write the last line in (85) as,

$$2n!\sum_{n=u+1}^{\infty}\alpha^{2r}\frac{r!}{(r+n)!(2r)!}\int_0^\infty \tau^{2r-1}e^{\tau/2-a\tau}\widetilde{K}^q(\tau)d\tau, \tag{86}$$

where $\widetilde{K}^q(\tau)$ is the linear heat kernel associated with $\zeta^q(s,a)$. Since (86) is assumed finite we may take the sum inside the integral. Thus our problem can be reduced to evaluating the sequence of sums,

$$T_n(\tau)=n!\sum_{r=1}^{\infty}\frac{r!\,\tau^{2r}}{(2r)!(r+n)!}.$$

Using the simple result $\sqrt{\pi}(2r)!=2^{2r}r!\Gamma(r+1/2)$ and changing the summation variable to $r'=r+n$ gives the result

$$T_n(\tau)=n!\sqrt{\pi}\left(\frac{1}{2}\tau\right)^{1/2-n}I_{-n-1/2}(\tau)-\sum_{r=0}^{n}\binom{n}{r}(2r)!(-\tau^2)^{-r},$$

where $I_\nu(x)$ is the modified Bessel function.

To find a closed form for $T_n(\tau)$ we employ a useful integral representation given in Ref. 22; For $\nu>0$,

$$\Gamma\left(\frac{1}{2}+\nu\right)I_{-\nu}(x)=\frac{2}{\sqrt{\pi}}\left(\frac{1}{2}x\right)^{\nu}\left[\int_{-1}^{1}e^{-xt}(1-t^2)^{\nu-1/2}dt+\sin(\pi\nu)\int_1^\infty e^{-xt}(t^2-1)^{\nu-1/2}dt\right].$$

Setting $\nu=n+1/2$ in this expression we may expand the integrand factors $(1-t^2)^n$ using the binomial theorem leaving simple exponential integrals. After a little work we find,

$$T_n(\tau)=\sum_{r=0}^{n}\binom{n}{r}(-1)^r\left\{(-\tau^2)^{-n}(2\tau)^r(2n-r)!\frac{1}{2}(e^\tau+(-1)^\tau e^{-\tau})-(2r)!\,\gamma t^{-2r}\right\}. \tag{87}$$

Having found a suitable expression for T_n we can now go back to (86) and write it in the new form,

$$\int_0^\infty\left\{2T_n(\alpha\tau)-\sum_{r=1}^{u}(\alpha\tau)^{2r}\frac{n!(r-1)!}{(r+n)!(2r-1)!}\right\}\tau^{s-1}e^{\tau/2-a\tau}\widetilde{K}^q(\tau)d\tau. \tag{88}$$

We have introduced into the integral a regulator τ^s (the expression that we want is given for the value $s=0$). The continuation variable s has been introduced so that we may evaluate the integrals of the individual terms in the sum definition (87) of T_n, and of the sum subtracted from it, *before* we perform the sums. We assume that s is large enough so that all the individual integrals are well defined. In fact this requires $s>2n$. Performing the integrations leaves

$$(-\alpha^2)^{-n}\sum_{r=0}^{n}\binom{n}{r}(2\alpha)^{\tau}(2n-r)!\Gamma(s+r-2n)\{\zeta^q(s+r-2n,a+\alpha)$$

$$+(-1)^r\zeta^q(s+r-2n,a-\alpha)\}-2\sum_{r=0}^{n}(-\alpha^2)^{-r}\binom{n}{r}(2r)!$$

$$\times\Gamma(s-2r)\zeta^q(s-2r,a)-\sum_{r=1}^{u}\alpha^{2r}\frac{n!(r-1)!\Gamma(s+2r)}{(r+n)!(2r-1)!}\zeta^q(s+2r,a). \tag{89}$$

As $s\to 0$ all of these terms diverge, although taking all terms together we must get a finite result, i.e., all poles must cancel as $s\to 0$. This cancellation of the poles leads to the equation,

$$(-\alpha^2)^{-n}\sum_{r=0}^{n}\binom{n}{r}(2\alpha)^r\{\zeta^q(r-2n,a-\alpha)+(-1)^r\zeta^q(r-2n,a+\alpha)\}$$

$$-2\sum_{r=0}^{n}(-\alpha^2)^{-r}\binom{n}{r}\zeta^q(-2r,a)-\sum_{r=1}^{u}\alpha^{2r}\frac{n!(r-1)!}{(r+n)!}N_{2r}=0. \tag{90}$$

Comparing Eqs. (90) and (84) we see that the pole cancellation is precisely the statement,

$$\zeta(-n)=\frac{1}{2}\sum_{r=0}^{n}\binom{n}{r}(2\alpha)^r\{\zeta^q(r-2n,a-\alpha)+(-1)^r\zeta^q(r-2n,a+\alpha)\}. \tag{91}$$

This expression contains equally terms with arguments $a+\alpha$ and $a-\alpha$. We shall say that $\zeta(-n)$ is ''symmetric.'' It is a generalization to general n of the symmetric expression for $n=0$ found in Ref. 21. The methods used in this reference do not produce a suitable pole cancellation to give a symmetric result for $\zeta(-n)$.

The finite remainder part of (89) as $s\to 0$ is given by the expression,

$$(-\alpha^2)^{-n}\sum_{r=0}^{n}\binom{n}{r}(2\alpha)^r\{\zeta^{q\prime}(r-2n,a-\alpha)+(-1)^r\zeta^{q\prime}(r-2n,a+\alpha)\}-2\sum_{r=0}^{n}(-\alpha^2)^{-r}\binom{n}{r}\zeta^{q\prime}$$

$$\times(-2r,a)-\sum_{r=1}^{u}\alpha^{2r}\frac{n!(r-1)!}{(r+n)!}R_{2r}+(-\alpha^2)^{-n}\sum_{r=0}^{n}\binom{n}{r}(2\alpha)^r\psi(2n-r+1)$$

$$\times\{\zeta^q(r-2n,a-\alpha)+(-1)^r\zeta^q(r-2n,a+\alpha)\}-2\sum_{r=0}^{n}(-\alpha^2)^{-r}\binom{n}{r}\psi(2r+1)\zeta^q(-2r,a)$$

$$-\sum_{r=1}^{u}\alpha^{2r}\frac{n!(r-1)!}{(r+n)!}\psi(2r)N_{2r}.$$

Inserting this expression into (85), and adding zero in the form of $\psi(2n+1)$ times (90) gives

$$\zeta'(-n)=\sum_{r=0}^{n}\binom{n}{r}(2\alpha)^r\{\zeta^{q\prime}(r-2n,a-\alpha)+(-1)^r\zeta^{q\prime}(r-2n,a+\alpha)\}-\sum_{r=1}^{n}\binom{n}{r}(2\alpha)^r\sigma_r$$
$$\times\{\zeta^q(r-2n,a-\alpha)+(-1)^r\zeta^q(r-2n,a+\alpha)\}-\sum_{r=0}^{n-1}(-\alpha^2)^{n-r}\binom{n}{r}(2\psi(2r+1)$$
$$-\psi(r+1)+\psi(n+1)-2\psi(2n+1))\zeta^q(-2r,a)-(-1)^n$$
$$\times\sum_{r=1}^{u}\alpha^{2(r+n)}\frac{n!(r-1)!}{2(r+n)!}(2\psi(2r)-\psi(r)+\psi(n+1)-2\psi(2n+1))N_{2r}. \tag{92}$$

The quantities σ_r in the above equation are defined as the sums,

$$\sigma_r=\sum_{k=0}^{r-1}\frac{1}{2n-k}.$$

Equation (92) is not symmetric in the sense that, unlike (91), it does not depend only on the quantities $a\pm\alpha$. If we assume that the sum over the residues is a true feature of $\zeta'(-n)$, as it is for $\zeta'(0)$ in Ref. 21, then we are still left with a sum over $\zeta^q(-2r,a)$. We will now rewrite this sum in a more natural, i.e., symmetric, form.

To this end we introduce the intermediate zeta function, $\overline{\zeta}(s)$, on the space $\overline{\mathcal{M}}=\mathbb{R}^{2n}\times S^2/\Gamma$, which is given by

$$\overline{\zeta}(s)=\frac{\Gamma(s-n)}{(4\pi)^n\Gamma(s)}\zeta(s-n). \tag{93}$$

Combining this with (83) gives an expansion for $\overline{\zeta}(s)$,

$$\overline{\zeta}(s)=\sum_{r=0}^{\infty}\alpha^{2r}\frac{\Gamma(s+r)}{r!\Gamma(s)}\overline{\zeta^q}(2s+2r,a), \tag{94}$$

where we have defined the new linear zeta function via

$$\overline{\zeta^q}(s,a)=\frac{\Gamma\left(\frac{1}{2}s-n\right)}{(4\pi)^n\Gamma\left(\frac{1}{2}s\right)}\zeta^q(s-2n,a). \tag{95}$$

The dimension of $\overline{\mathcal{M}}$ is $\overline{d}=2n+d$ (remember, for our monopole case $d=2$). We see from (95) that $\overline{\zeta^q}(s)$ has poles at $s=2,4,...,2n$ and $s=2n+1,2n+2,...,\overline{d}$. The residues are given by the formulas,

$$\overline{N}_{2r}=\frac{2(-1)^r}{(4\pi)^n(r-1)!(n-r)!}\zeta^q(2r-2n,a),\quad r=1,2,...,n, \tag{96}$$

$$\overline{N}_{2n+r}=\frac{\Gamma\left(\frac{1}{2}r\right)}{(4\pi)^n\Gamma\left(\frac{1}{2}r+n\right)}N_r,\quad r=1,2,...,d. \tag{97}$$

The purpose of making these new definitions is the functional similarity between (83) and (94). This implies that results like (91) and (92) should exist for $\overline{\zeta}(s)$ in terms of $\overline{\zeta^q}(s)$. The

important point is that we know that $\zeta'(0)$ can be written as a symmetric part and a sum over the residues of $\zeta^q(s,a)$, either from Ref. 21, or setting $n=0$ in (92). Thus we might expect $\overline{\zeta'}(0)$ to consist of a symmetric part and a sum over the residues of $\overline{\zeta^q}(s,a)$. Differentiating (93) and setting $s=0$ gives,

$$\overline{\zeta'}(0)=\frac{(-1)^n}{(4\pi)^n n!}(\zeta'(-n)+(\psi(n+1)-\psi(1))\zeta(-n)). \tag{98}$$

Now $\zeta(-n)$ is symmetric in terms of $\zeta^q(s,a\pm\alpha)$ and extends easily to a symmetric form for $\overline{\zeta^q}(s,a)$ using (95). Thus by our reasoning we expect $\zeta'(-n)$ to contain a sum over the residues $\overline{N}_r$. This is exactly what we find, and the final result, in this section, is the *symmetrical* expression,[23]

$$\begin{aligned}\zeta'(-n)=&\sum_{r=0}^{n}\binom{n}{r}(2\alpha)^r\{\zeta^{q\prime}(r-2n,a-\alpha)+(-1)^r\zeta^{q\prime}(r-2n,a+\alpha)\}\\&-\sum_{r=1}^{n}\binom{n}{r}(2\alpha)^r\sigma_r\{\zeta^q(r-2n,a-\alpha)+(-1)^r\zeta^q(r-2n,a+\alpha)\}\\&-(-1)^n(4\pi)^n n!\sum_{r=1}^{\overline{u}}\frac{\alpha^{2r}}{\tau}\rho_r\overline{N}_{2r},\end{aligned} \tag{99}$$

with the definitions $\overline{u}=[\overline{d}/2]$ and

$$\rho_r=\psi(2r-2n+1)-\frac{1}{2}\psi(r-n+1)-\left(\psi(2n+1)-\frac{1}{2}\psi(n+1)\right)=\sum_{k=0}^{r-1}\frac{2}{2k+1}-\sum_{k=0}^{n-1}\frac{1}{2k+1}.$$

The conclusion of these manipulations is that, despite the apparent awkwardness of the binomial expansion, (83), to obtain the required ζ-function, the quantities that we want are given in finite terms, (91), (92), (99), and involve only relatively standard functions such as generalized Bernoulli polynomials introduced via the Barnes ζ-function.

XI. VACUUM ENERGY CALCULATIONS

Simply as an example of the use of the preceding expressions, we evaluate some vacuum (Casimir) energies on S^2/Γ'.

Let $\zeta^q(s,a)$ represent one of the rotational, Dirichlet or Neumann linear zeta functions as in the previous section. Then $\zeta^q(s,a)$ can be extended to the odd-dimensional space–time $\mathbb{R}\times S^2/\Gamma$ (or $\mathbb{R}\times S^2/\Gamma'$) by defining a new zeta function $\zeta(s)$ given by (with $a=1/2$),

$$\zeta(s)=\frac{\Gamma(s-1/2)}{(4\pi)^{1/2}\Gamma(s)}\zeta^q(2s,1/2). \tag{100}$$

This zeta function corresponds to the rather artificial case of a conformally coupled field in three dimensions with mass q^2. [For a scalar field conformally coupled in N dimensions we have $4\xi=(N-2)/(N-1)$. In fact we only require that $\alpha^2=0$ or equivalently $m^2=q^2+(1/4-2\xi)$.] The vacuum energy associated with this physical situation is defined by the simple formula[24]

$$E=-\frac{1}{2}\mu_r\frac{d}{ds}\left(\frac{\mu}{\mu_r}\right)^{2s}\zeta(s)\bigg|_{s=0}. \tag{101}$$

In this equation μ is an arbitrary mass scale and $\mu_r=1/r$ is the mass scale associated with the sphere radius r (which has the value $r=1$). Equation (101) is in fact just half the logarithmic determinant. Inserting Eq. (100) into (101) gives the simpler expression

$$E=\tfrac{1}{2}\zeta^q(-1,1/2), \tag{102}$$

which is finite and independent of μ (we have set $r=1$ again).

The vacuum energy on the space $\mathbb{R}\times\mathbb{R}^{2n}\times S^2/\Gamma(')$ can also be found and gives E proportional to $\zeta^q(-1-2n,\frac{1}{2})$. The calculation for general n is entirely equivalent to the $n=0$ case, which we now calculate.

Using the definitions (80), (80) and Eq. (61), we find from (102) the Dirichlet and Neumann vacuum energies,

$$E_{\{{}^D_N\}}=\pm\frac{d_0}{48|\Gamma'|}(d_0^2-d_1^2-d_2^2)+\frac{\overline{q}'}{24}\left(3d_0^2-d_1^2+\frac{1}{2}\pm 6d_0q-2q^2\right).$$

The constant (q independent) terms are exactly the same as those calculated in Ref. 1 for $q=0$, as required. Adding together the Dirichlet and Neumann vacuum energies gives the rotational vacuum energy

$$E_\Gamma=\frac{\overline{q}}{24}(3d_0^2-d_1^2-d_2^2-2q^2),$$

where we have used the relation $\overline{q}=2\overline{q}'$ for fixed q. This vacuum energy necessarily vanishes for $q=0$, as proven in Ref. 1. We now list the vacuum energies $E_{\{{}^D_N\}}$ for all possible reflection groups Γ',

$$O^*:\quad \pm\frac{29}{256}+\frac{\overline{q}'}{48}(383\pm 108q-4q^2),$$

$$Y^*:\quad \pm\frac{89}{384}+\frac{\overline{q}'}{48}(1079\pm 90q-4q^2),$$

$$O]T:\quad \pm\frac{11}{192}+\frac{\overline{q}'}{48}(167\pm 36q-4q^2),$$

$$D_n]C_n:\quad \mp\frac{1}{96}+\frac{\overline{q}'}{48}(4n^2-1\pm 6nq-4q^2),$$

$$D_n^*(n\ \text{even}),\ D_{2n}]D_n(n\ \text{ odd}):\quad \pm\frac{(n+1)(2n-3)}{192n}\frac{\overline{q}'}{48}(4(n+1)(n+2)-9\pm 6(n+1)q-4q^2).$$

Those for the corresponding rotational subgroups are obtained by adding the D and N values.

We now go on to calculate the vacuum energy on the even-dimensional space $\mathbb{R}^{2n}\times S^2/\Gamma(')$. Using Eqs. (93), (98), and (101) we find the expression,

$$E=\frac{(-1)^{n+1}\mu_r}{2(4\pi)^n n!}\left(\zeta'(-n)+\left[\ln\left(\frac{\mu}{\mu_r}\right)^2+\psi(n+1)-\psi(1)\right]\zeta(-n)\right). \tag{103}$$

Here $\zeta(s)$ is the general zeta function defined via Eqs. (82) and (83).

An infinite contribution has been (arbitrarily) dropped to arrive at (103), the logarithmic term being a relic of this divergence. Since $\zeta(0)$ is not zero for any of the three monopole theories, we

conclude from (103) that the vacuum energy is explicitly dependent on the arbitrary scale μ. However for simplicity we shall assume $\mu=\mu_r=1$ for the rest of this section. Our concern in this paper is not with realistic quantum field theory considerations.

Equations (91) and (92) imply that the calculation for increasing n merely requires the evaluation of more and more zeta functions and their derivatives. Thus we shall concentrate on the simplest case $n=0$ corresponding to $S^2/\Gamma(')$ itself. This will also allow us to compare with the results for $q=0$ studied in Ref. 21.

We consider the case of a massless field with minimal coupling, that is $m^2=0$ and $\xi=0$. Thus we have $a=1/2$ and $2\alpha=\sqrt{4q^2+1}$ (we shall still write α when convenient). From the definitions (80), (81), and Eqs. (91), (61), we find for Dirichlet and Neumann boundary conditions,

$$\zeta_{\{N\}}^{D}(0)=\frac{1}{12}+\frac{1}{6|\Gamma'|}(d_0(d_0-1)+1\pm 6d_0q+18q^2).$$

These expressions reduce to those found earlier for $q=0$.[21] For the rotational case we simply add the Dirichlet and Neumann results to give

$$\zeta_{\Gamma}(0)=\frac{1}{6}+\frac{1}{6|\Gamma|}(d_0(d_0-1)+1+18q^2).$$

To calculate the vacuum energy we have still to calculate $\zeta'(0)$. Considering Eq. (92) with $n=0$ requires the evaluation of the residue N_2. For both Dirichlet and Neumann zeta functions we find from (60) and (62) the value $N_2=2/|\Gamma'|$. Using the derivative of the Hurwitz zeta function in Ref. 20 then gives the zeta function derivatives

$$\begin{aligned}\zeta_D'(0)=&\zeta_2'\left(0,\frac{1}{2}+q-\alpha+d_0\right)+\zeta_2'\left(0,\frac{1}{2}+q+\alpha+d_0\right)\\&+\overline{q}'\ln\left\{\Gamma\left(\frac{1}{2}+q-\alpha\right)\Gamma\left(\frac{1}{2}+q+\alpha\right)\right\}-\overline{q}'\ln(2\pi)-\frac{1+4q^2}{2|\Gamma'|},\end{aligned}\tag{104}$$

$$\begin{aligned}\zeta_N'(0)=&\zeta_2'\left(0,\frac{1}{2}+q-\alpha\right)+\zeta_2'\left(0,\frac{1}{2}+q+\alpha\right)\\&+\overline{q}'\ln\left\{\Gamma\left(\frac{1}{2}+q-\alpha\right)\Gamma\left(\frac{1}{2}+q+\alpha\right)\right\}-\overline{q}'\ln(2\pi)-\frac{1+4q^2}{2|\Gamma'|}.\end{aligned}\tag{105}$$

(The rotational zeta function derivative is just the sum of these two.) The triangle inequality $|x|+|y|\geqslant\sqrt{x^2+y^2}(x,y\in\mathbb{R})$ implies that $1/2+q\geqslant\alpha$. The equality is only met for $q=0$, and in this case we have to remove the singularity in the first term $\zeta_2'(0,1/2+q-\alpha|d_1,d_2)$ of the Dirichlet zeta function as in (21) (we shall do this later). For $q>0$ all terms in (105) and (104) are well defined.

There is no known analytic form for the derivatives of the Barnes zeta functions appearing in (105) and (104), and so we have to calculate them numerically. To do this we obviously need a continuation of the Barnes zeta function which is open to easy numerical computation. In Ref. 21 several efficient continuations are presented which are valid for positive integer values of d_1 and d_2. However as we shall show in the next section, it is useful to have an expression which is valid for all d_1, $d_2\in\mathbb{R}^+$. We shall now derive such an expression.

Our starting point is the Plana sum formula which we display here,[25]

$$\sum_{n=a}^{b}f(n)=\frac{1}{2}(f(a)+f(b))+\int_a^b f(t)dt+i\int_0^\infty\frac{f(a+it)-f(a-it)-f(b+it)+f(b-it)}{e^{2\pi t}-1}dt.\tag{106}$$

To be valid $f(t)$ must be an analytic function in the region of the complex t plane $a \leqslant \mathrm{Re}(t) \leqslant b$, and the integrals must exist. Applying (106) twice to the sum definition (59) of the Barnes zeta function gives immediately, for $s>2$,

$$\zeta_2(s,a|d_1,d_2)=\frac{1}{2}d_1^{-s}\zeta_H\left(s,\frac{a}{d_1}\right)+\frac{1}{d_2(s-1)}d_1^{-s}\zeta_H\left(s-1,\frac{a}{d_1}\right)$$
$$+i\int_0^\infty\frac{dt}{e^{2\pi t}-1}\left\{\frac{1}{2}((a+id_2t)^{-s}-(a-id_2t)^{-s})+\frac{1}{d_1(s-1)}((a+id_2t)^{1-s}\right.$$
$$\left.-(a-id_2t)^{1-s})\right\}+\int_0^\infty\frac{du}{e^{2\pi u}-1}\int_0^\infty\frac{dt}{e^{2\pi t}-1}\{(a+id_1u-id_2t)^{-s}$$
$$+(a-id_1u+id_2t)^{-s}-(a+id_{21}u+id_2t)^{-s}-(a-id_1u-id_2t)^{-s}\}. \qquad (107)$$

It is simple to verify that we are meeting the conditions required for the validity of the sum formula. In order to get rid of the single integrals in (107) we use the Plana sum definition of the Hurwitz zeta function which is, from (106),

$$\zeta_H(s,a)=\frac{1}{2}a^{-s}+\frac{a^{1-s}}{s-1}+i\int_0^\infty\frac{dt}{e^{2\pi t}-1}\{(a+it)^{-s}-(a-it)^{-s}\}. \qquad (108)$$

The integral part of this expression is equivalent to the integrals appearing in (107).

To simplify the double integral in (107) we first perform a change of variables from t, u to $d_1u\pm d_2t$. Following this, we use the easily proven formula,

$$(x+iy)^s+(x-iy)^s=2\cos(s\tan^{-1}y/x),$$

which is valid for $\mathrm{Re}(x)\geqslant 0$. After a little work we find the more convenient form for the double integral,

$$\frac{2}{d_1d_2}\int_0^\infty dw\,\frac{G(w)}{e^{2\pi w}-1}\,\frac{\cos(s\tan^{-1}(w/a))}{(a^2+w^2)^{s/2}}. \qquad (109)$$

All the nontrivial d_1, d_2 dependence has been absorbed into the function $G(w)$ which is independent of s and has the explicit form,

$$G(w)=(e^{2\pi w}-1)\left\{\int_0^w\frac{dy}{(e^{\delta_1 y}-1)(e^{\delta_2(w-y)}-1)}-\int_0^\infty\frac{dy}{(e^{\delta_1 y}-1)(e^{\delta_2(w+y)}-1)}\right.$$
$$\left.-\int_0^\infty\frac{dy}{(e^{\delta_1(w+y)}-1)(e^{\delta_2 y}-1)}\right\}, \qquad (110)$$

where we have defined $\delta_i=2\pi/d_i$, $i=1,2$. This function is symmetric under the interchange of d_1, d_2 as one would expect. The factor $(e^{2\pi w}-1)$ has been included into the definition to ensure that $G(w)$ is finite as $w\to 0$.

All the integrals in the definition of $G(w)$ are divergent at their lower limits, and the first integral is also divergent at its upper limit. However one can check that the combination is well defined. In fact by expanding the integrands at their limits of integration we find that for small $\epsilon>0$,

$$G(w)=(e^{2\pi w}-1)\left\{\int_{\epsilon}^{w-\omega}\frac{dy}{(e^{\delta_1 y}-1)(e^{\delta_2(w-y)}-1)}-\int_{\epsilon}^{\infty}\frac{dy}{(e^{\delta_1 y}-1)(e^{\delta_2(w+y)}-1)}\right.$$
$$\left.-\int_{\epsilon}^{\infty}\frac{dy}{(e^{\delta_1(w+y)}-1)(e^{\delta_2 y}-1)}\right\}+O(\epsilon).$$

Thus $G(w)$ is easy to calculate numerically, with the error being of order ϵ. We may also make ϵ the lower limit of the integration over w in (109). Since the integrand with respect to w is finite at the lower limit, the error incurred will still be $O(\epsilon)$.

The full expression for our continuation of the Barnes zeta function, after dealing with both the single and double integrals in (107), is

$$\zeta_2(s,a|d_1,d_2)=-\frac{1}{4}a^{-s}-\frac{a^{2-s}}{d_1d_2(s-1)(s-2)}-\frac{(d_1+d_2)a^{1-s}}{2d_1d_2(s-1)}+\frac{1}{2}d_1^{-s}\zeta_H\left(s,\frac{a}{d_1}\right)$$
$$+\frac{1}{2}d_2^{-s}\zeta_H\left(s,\frac{a}{d_2}\right)+\frac{1}{d_1d_2(s-1)}\left\{d_1^{2-s}\zeta_H\left(s-1,\frac{a}{d_1}\right)+d_2^{2-s}\zeta_H\left(s-1,\frac{a}{d_2}\right)\right\}$$
$$+\frac{2}{d_1d_2}\int_0^{\infty}\frac{G(w)dw}{e^{2\pi w}-1}\frac{\cos(s\tan^{-1}(w/a))}{(a^2+w^2)^{s/2}}. \tag{111}$$

Although this formula was derived for $s>2$, it is actually a continuation to all values of (complex) s except at the points $s=1,2$ where there are simple poles. It is easy to check that these poles are correct in that their residues match those given in (60). From (111) we can calculate the derivative of the Barnes zeta function at $s=0$,[23]

$$\zeta_2'(0,a|d_1,d_2)=-\frac{1}{4}\ln a-\frac{1}{2}\left(1-\frac{a}{d_1}-\frac{a}{d_2}\right)\ln(2\pi)+\frac{1}{2}a\ln a\left(\frac{1}{d_1}+\frac{1}{d_2}\right)-\frac{a^2}{2d_1d_2}\left(\frac{5}{2}+\ln a\right)$$
$$+\left(\frac{1}{2}-\frac{a}{d_1}\right)\left(\frac{1}{2}-\frac{a}{d_2}\right)\ln\frac{a^2}{d_1d_2}+\left(\frac{1}{2}-\frac{a}{d_1}\right)\ln\Gamma\left(\frac{a}{d_2}\right)+\left(\frac{1}{2}-\frac{a}{d_2}\right)\ln\Gamma\left(\frac{a}{d_1}\right)+\frac{d_1^2+d_2^2}{12d_1d_2}$$
$$+\frac{1}{d_1d_2}\int_0^{\infty}\frac{dw}{e^{2\pi w}-1}(2G(w)-d_1^2w\ln(a^2+d_1^2w^2)-d_2^2w\ln(a^2+d_2^2w^2)). \tag{112}$$

Here we have used (108) again to convert derivatives of the Hurwitz zeta function $\zeta_H(s,a)$ at $s=-1$ into integrals suitable for numerical evaluation.

The expression (112) can be used directly in equation (105) and (104). Figures 1–4 show plots of $E=-\zeta'(0)/2$ for small values of $\overline{q}$. The lines on the graphs for T, O, and Y are for labeling only. The graphs for C_k and D_k are plotted for all k, although at the moment we are only concerned with the integral values $k=1,2,...$ marked with crosses. On each graph the value $\overline{q}$ of the charge per rotational domain is always twice the reflection value $\overline{q}'$ so as to give the same value of q.

The graphs with $\overline{q}=q=0$ are exactly the same as those calculated in Ref. 21. To plot the graphs in this case we have had to remove the divergence in the first Barnes zeta function derivative in (105). This is due to a zero mode appearing in the spectrum of the operator H_{S^2}. The divergence is logarithmic and can be removed by defining the so called Γ-modular form ρ_2 defined by[19,21]

$$\lim_{a\to 0}\zeta_2'(0,a|d_1,d_2)=-\ln a-\ln\rho_2.$$

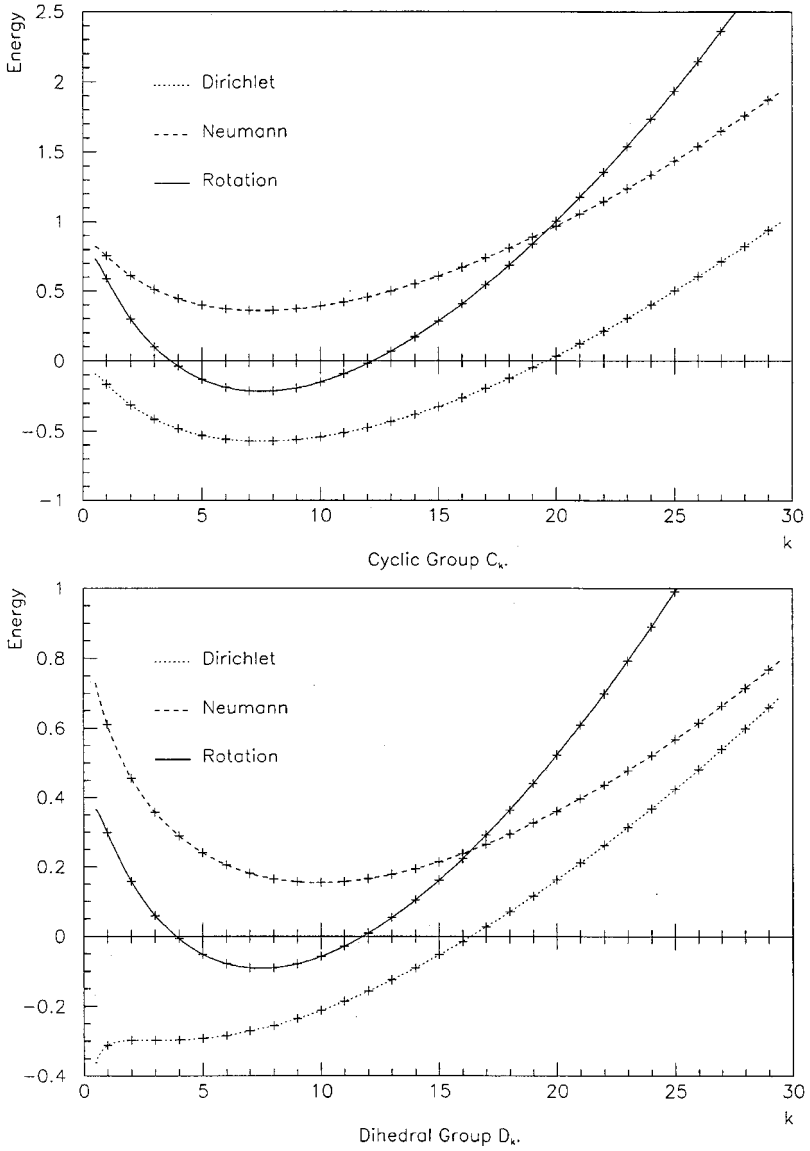

FIG. 1. Vacuum energies for C_k and D_k with $\overline{q}'=0$.

The leading term $-\ln a$ on the right-hand side is the divergent zero mode contribution which must be removed. The form ρ_2 has been calculated in terms of the multiple gamma function by Barnes.[19,26] The Γ-modular form can be more easily calculated by using the simply proved relation,

$$\zeta_2(s,a|d_1,d_2)=a^{-s}+d_1^{-s}\zeta_H\left(s,1+\frac{a}{d_1}\right)+d_2^{-s}\zeta_H\left(s,1+\frac{a}{d_2}\right)+\zeta_2(s,a+d_1+d_2|d_1,d_2).$$

Differentiating this with respect to s at $s=0$, and taking the limit $a\to 0$ leaves the expression

$$-\ln\rho_2=\tfrac{1}{2}\ln(d_1d_2)-\ln(2\pi)+\zeta_2'(0,d_0+1|d_1,d_2).$$

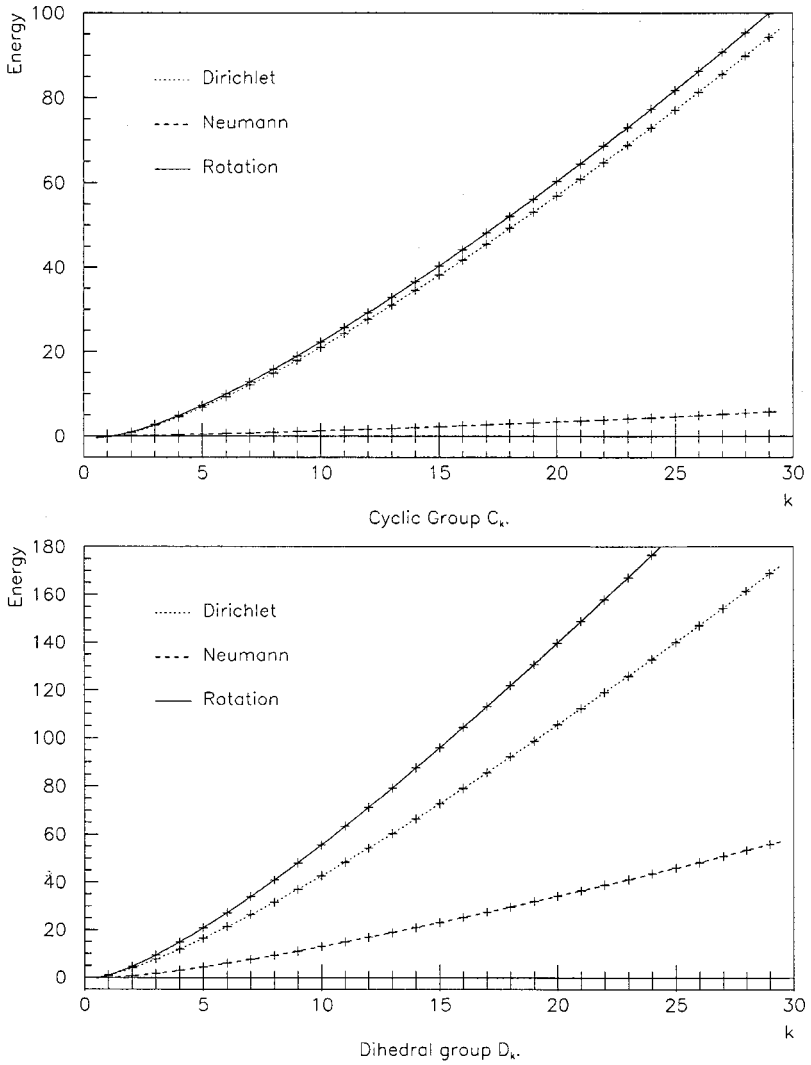

FIG. 2. Vacuum energies for C_k and D_k with $\overline{q}=1/2$.

For $q>0$, the zero mode that we have just removed for $q=0$ is still almost zero. This is the reason why the vacuum energy for the Dirichlet zeta function increases more rapidly with $\overline{q}$ than in the Neumann case.

XII. THEORY FOR A SPHERICAL SLICE

By a spherical slice of width β we mean the space $S_\beta=\{(\theta,\phi)\,|\,\theta\in[0,\pi],\ \phi\in[0,\beta]\}$ with the points $(\theta, 0)$ and (θ, β) identified [here (θ, ϕ) are the spherical polar coordinates on the sphere which shall be used throughout this section]. One might also term this space a ''periodic lune.''

The starting point for the monopole theory on S_β is the solution to the explicit differential Eq. (4) with arbitrary q. As mentioned in the discussion surrounding the differential equation the solutions are characterized by integers u, v, and are given by Eqs. (3) and (5). We shall now show that it is possible to define consistent monopole theories on S_β corresponding to the rotational, Dirichlet and Neumann cases already given. The rotational case is considered first.

Define k by $k=2\pi/\beta$ and let $\hat{\gamma}$ denote a rotation by angle β about the z axis. Due to the identification of points in S_β at $\phi=0,\beta$, we will proceed conventionally and take the wave

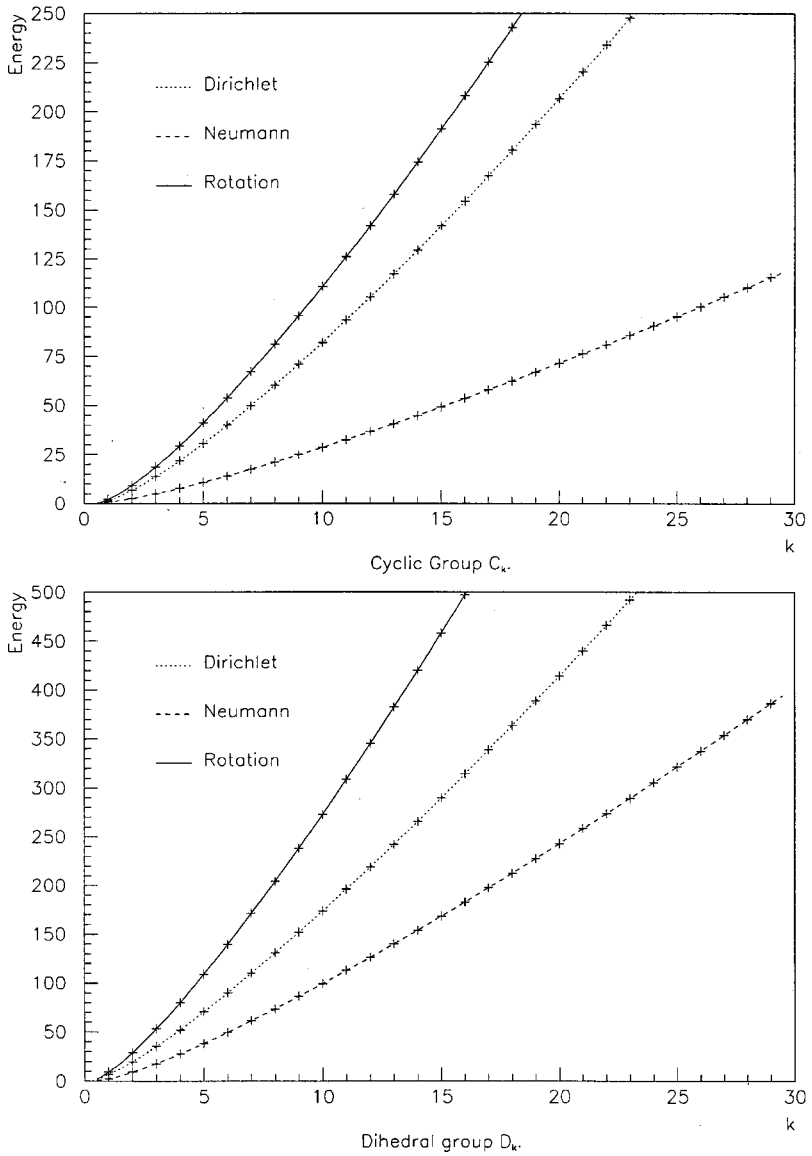

FIG. 3. Vacuum energies for C_k and D_k with $\overline{q}'=1$.

function to be single valued, i.e., to have period β. Also, for rapidity, the monopole charge quantization will be obtained by requiring the connecting function $\exp(i2q\phi)$ to have period β. This yields

$$q=\frac{k}{2}n, \quad n\in\mathbb{Z}. \tag{113}$$

Corresponding to these values of q we find $a(\hat{\gamma})=(-1)^n$. If k is an integer then S_β is a fundamental domain for the group C_k (generated by $\hat{\gamma}$), and the relation $|C_k|=k$ gives an equivalence between the quantization conditions (39) and (113). Thus we see that the quantization condition for arbitrary k is a generalization of the previous theory for C_k (with integer k). From single valuedness, $\varphi(\theta,\beta)=\varphi(\theta,0)$, for the monopole harmonics (5), we see from the explicit ϕ dependence that,

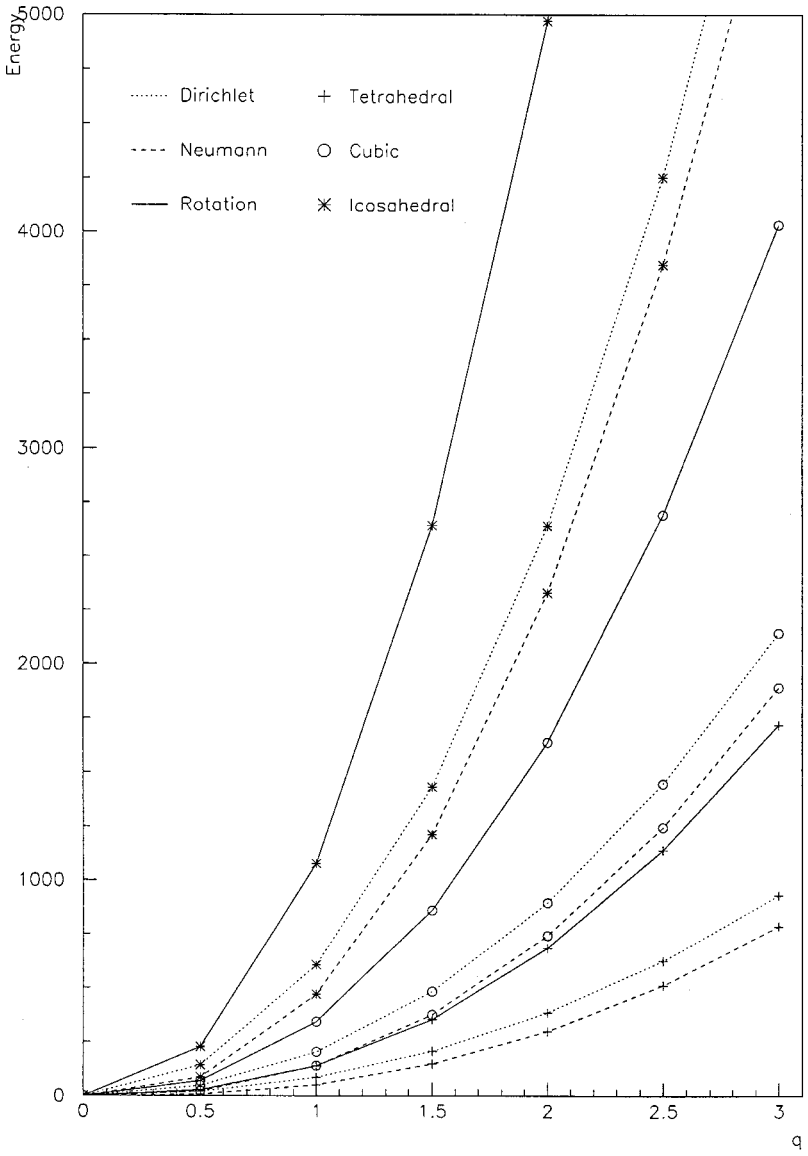

FIG. 4. Vacuum energies for groups T, O, and Y as functions of $\overline{q}'$.

$$m = jk - q, \quad j \in \mathbb{Z}. \tag{114}$$

In this more general setting it would appear that we can always choose n to be odd, whereas before this was only possible for k odd also. From (5) we find the possible values of l,

$$l = u + \frac{k}{2}(|j| + |n-j|), \quad u \in \mathbb{Z}^+, j \in \mathbb{Z}.$$

The eigenvalues λ appearing in the mode Eq. (4) are still given by $l(l+1) - q^2$. As in Sec. VII we shall calculate the linear heat kernel for the eigenvalues $(l+1/2)$.

Using the values of q, l, and m above gives the sum form for the linear heat kernel analogous to (51), with (5),

$$\tilde{K}_k^q(\tau)=e^{-\tau/2}\sum_{u=0}^{\infty}\sum_{j=-\infty}^{\infty}e^{-r(u+k(|j|+|j+n|)/2)}. \tag{115}$$

Evaluating this sum gives exactly the result found before, Eq. (56), except that now k is not an integer, and q need not be an integer multiple of k. A corollary of this result is that (56) is also valid for the case when $\Gamma=C_k$ with k and $2q$ odd integers. The zeta function defined by Eq. (58) is also correct for $d_1=1$, $d_2=k$ and hence we conclude that the vacuum energies calculated in the previous section are valid for *arbitrary* k.

For the Dirichlet and Neumann theories defined in section 8 we consider the slice $S_{\beta/2}$ and two reflection planes P_0 and P_1 which leave $\phi=0$ and $\phi=\beta/2$ invariant respectively. Following the same arguments as in section 8 gives the values of the monopole charge

$$q=kn', \tag{116}$$

which is equivalent to Eq. (65). Taking γ' in (64) to be a reflection in P_0 and using (17) gives the modes $W_{qm}^{(l)}$ as the combinations,

$$W_{qm}^{(l)}(\theta,\phi)=Y_{qm}^{(l)}(\theta,\phi)+a(\sigma)Y_{q-m}^{(l)}(\theta,\phi).$$

Here $Y_{qm}^{(l)}$ are those defined in (3) with the string along the negative z axis, and $a(\sigma)=\pm1$ as before (the reflection in P_0 is expressed simply as $\phi\to-\phi$).

The ϕ dependent part of the modes $W_{qm}^{(l)}$ is given by

$$W_{qm}^{(l)}\sim e^{iq\phi}\times\begin{cases}\cos(m\phi), & a(\sigma)=+1\\ \sin(m\phi), & a(\sigma)=-1\end{cases}.$$

Reflection in P_0 is equivalent to $\phi\to-\phi$ and we see explicitly that this transforms $W_{qm}^{(l)}(\theta,0)$ into $a(\sigma)W_{-qm}^{(l)}(\theta,0)$ as required. Reflection in P_1 is equivalent to $\phi\to\beta-\phi$ and results in the condition on m,

$$m=kj, \quad j\in\mathbb{Z}^+. \tag{117}$$

For the Dirichlet case $a(\sigma)=-1$ the $m=0$ mode is in fact zero and has to be removed. Comparing (117) with (114) (with $n=2n'$ even) we see that the only difference between the rotation and reflection cases is that in the reflection case the values of m are restricted to positive integers.

The linear heat kernel for the Neumann case $a(\sigma)=+1$ is given by

$$\tilde{K}_N^q(\tau)=e^{-\tau/2}\sum_{u=0}^{\infty}\sum_{j=0}^{\infty}e^{-r(u+k(|j+n'|+|j-n'|)/2)}. \tag{118}$$

Explicit evaluation of the sum gives exactly the heat kernel as before, Eq. (55). The Dirichlet case involves subtracting the $j=0$ term from (71) and yields the previous expression (75). Thus the zeta functions are given exactly as before and we conclude that the vacuum energy calculated for C_k is in fact valid for all k.

To extend the results of D_k to arbitrary k we consider the slice of the upper hemisphere $S'_\beta=\{(\theta,\phi)\,|\,\theta\in[0,\pi/2],\ \phi\in[0,\beta]\}$ with again $k=2\pi/\beta$. This is a fundamental domain for D_k when k is an integer. The theory then follows as for the C_k extension above, but we must include in this case a rotation about the x axis by angle π. This rotation can be thought of as a reflection in the plane P_0 followed by a reflection in the x–y plane, which we call P_2. The theory for S_β above is adapted to the reflection P_0 and thus we see that P_2 is the essential extra detail here.

The reflection P_2 is equivalent to the transformation $\theta\to\pi-\theta$ which does not affect the ϕ dependence of the modes $Y_{qm}^{(l)}(\theta,\phi)$. Since the extension to arbitrary k is entirely linked with the

ϕ dependence, we conclude that all the heat kernels, zeta functions and vacuum energies for D_k can be extended to arbitrary k. The values of the monopole charge in the reflection case are calculated using the theory of Sec. IX as

$$q = 2kn', \quad n' \in \mathbb{Z},$$

which is the generalization of (65) with $|\Gamma'| = 4k$.

XIII. SUMMARY AND DISCUSSION

We have thoroughly adapted Dirac's monopole theory to the orbifold, S^2/Γ, for the cases that Γ contains only rotations and when Γ is generated by reflections. In the former case we imposed rotational (periodic) boundary conditions on the monopole solutions. In the latter we had a choice of boundary conditions defined so as to reproduce Dirichlet and Neumann conditions for no monopole charge, $q=0$. We found that it was the monopole charge $\overline{q} = q/|\Gamma|$ through S^2/Γ that was Dirac quantized with $2\overline{q} \in \mathbb{Z}$.

After all the formalities of the theory had been tidied we explicitly calculated the vacuum energies on the orbifolds S^2/Γ and $\mathbb{R}\times S^2/\Gamma$. Formal expressions are given for the generalization to the spaces $\mathbb{R}^{2n}\times S^2/\Gamma$ and $\mathbb{R}\times\mathbb{R}^{2n}\times S^2/\Gamma$. Finally we provided an extension of the monopole theory to arbitrary slices of the sphere and hemisphere. In this case the flux through the spherical region is still quantized, although now the overall monopole charge q is not, in general, an integer or half odd-integer.

We feel that the scalar theory has been developed essentially to its analytical limit on the factored sphere. The next step would be the extension to $\mathbb{R}^3/\Gamma$ for Γ a reflection or rotation group. This requires modes of the full Hamiltonian which are given by

$$Y^{(l)}_{qm}(\theta,\phi) J_\nu(kr)\sqrt{k/r}, \quad \nu = \sqrt{(l+1/2)^2 - q^2}$$

with eigenvalues k^2. Since the radial dependence does not involve m, the underlying facts of the theory (modes on factored space, charge quantization, etc.) are the same as in the spherical case. However the heat-kernel calculation, and hence the ζ-function, is completely different. Due to the complicated index, $\sqrt{(l+1/2)^2-q^2}$, closed forms do not seem possible and asymptotic methods are needed. One could always arbitrarily add a term q^2/r to the (total) Hamiltonian and then a closed form would exist. This fact suggests that there is some significance to this modification.

The spinor theory on the factored sphere S^2/Γ has been considered by Chang.[27] He found a consistent theory only for $\Gamma = C_k$ with k odd. For $q \neq 0$ we claim that the same restriction still holds. This follows from the lack of half odd-integral solutions to the scalar monopole problem for $\Gamma \neq C_k$.

A possible extension of the scalar calculation would be to consider if (high temperature) Bose–Einstein condensation occurs. The general theory has been laid down by Toms[28] See also Kirsten and Toms.[29] Basically, all that is required is to ensure that the ζ-function for the theory, and its derivative, are finite at zero as the chemical potential approaches a critical value. On the two-sphere we can use the calculations of $\zeta(-n)$ and $\zeta'(-n)$ given in Sec. X to study the theory on $\mathbb{R}^{2n}\times S^2$. In fact we could also discuss $\mathbb{R}^{2n}\times S^d$.

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Geometric invariant theory approach to the determination of ground states of *D*-wave condensates in isotropic space

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A complete and rigorous determination of the possible ground states for *D*-wave pairing Bose condensates is presented, using a geometrical invariant theory approach to the problem. The order parameter is argued to be a vector, transforming according to a ten-dimensional real representation of the group $G=\mathbf{O}_3\otimes\mathbf{U}_1\times\langle\mathcal{T}\rangle$. We determine the equalities and inequalities defining the orbit space of this linear group and its symmetry strata, which are in a one-to-one correspondence with the possible distinct phases of the system. We find 15 allowed phases (besides the unbroken one), with different symmetries, that we thoroughly determine. The group–subgroup relations between bordering phases are pointed out. The perturbative sixth degree corrections to the minimum of a fourth degree polynomial *G*-invariant free energy, calculated by Mermin, are also determined. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1345871]

I. INTRODUCTION

Superfluidity and superconductivity are justified on the basis of the macroscopic condensation of Bose quasiparticles. The classical Bardeen, Cooper, and Schrieffer (BCS) theory for superconductivity dates to 1957. Soon after, a BCS-type transition was proposed for the Fermi system ^{3}He by Anderson and Morel.[1] Cooper pair formation was thought to occur in an $L\neq 0$ state, to take into account the hard core nature of ^{3}He atom interaction. The superfluid phases were actually observed,[2] and the nature of *p*-wave pairing is now well established for ^{3}He. The theory of $L\neq 0$ superfluids is relevant for ''unconventional'' superconductivity too. The high temperature superconducting (HTS) oxides are anomalous in their non-Fermi liquid normal state properties and in many cases share with heavy fermion superconductors unconventional *d*-wave pairing behavior.[3,4] In fact, experiments probing the phase and the nodes of the gap show a sign reversal of the order parameter, compatible with the *d*-wave scenario. Nevertheless, other experiments on the same HTS compounds point in the direction of a significant *s*-wave component. In the presence of external magnetic fields, defects, and interface phenomena there is also evidence of a mixed pairing symmetry (see, e.g., the Introduction of Ref. 5, and references therein). Such a

controversial experimental situation is reflected in the fact that the underlying microscopic mechanism inducing superconductivity in HTS materials is still unclear and is one of today's major challenges.[6,7]

Such a situation has motivated the efforts at studying the macroscopic properties of unconventional superconductors through the Landau theory of phase transitions[8] and the identification of the order parameter symmetry has become a preliminary task in the construction of viable models describing the attractive nature of the pairing interaction.

Direct experimental evidence of an order parameter unconventional structure lies on multiple phase transitions. The heavy fermion compounds $U_{1-x}Th_xBe_{13}$ display four different superconducting phases in the $T-x$ phase diagram and UPt_3 displays three superconducting phases in a $T-H$ phase diagram.[3] Furthermore, from power-law temperature behavior of thermodynamic and transport properties (e.g., specific heat, magnetic penetration depth), a nontrivial node structure for the gap function may be inferred, compatible with high L-pairing. That is the case also for HTS oxides, for which, at present, clear proofs are lacking of the existence of more than one superconducting state.

Actually, it must be pointed out that, unlike superfluid ^{3}He, which is an isotropic fermion system, Bloch electrons in a superconductor crystal lattice exhibit, in general, a reduced finite symmetry; in addition, the existence of imperfections, even in the cleanest samples, can partly destroy the gap node structure at low energy. So, the very fact that the experimental observation cannot at present completely unravel the node structure of the gap function, reinforces the necessity of classifying all the possible symmetry breaking schemes.

Moreover, the role of Fermi isotropic space beyond a zeroth-order approximation in phenomenological theories is still supported by some recent studies: In HTS oxides, low symmetrical crystal fields (tetragonal and orthorombic), as well as spontaneous strain, have weak influence on the temperature of the superconducting phase transition[9] or on the penetration depth.[10] So, even if the spectrum of the interactions which are responsible for the pairing (whatever there origins may be) must be anisotropic in the crystal, it is worth analyzing the possibility that they act in a way not directly dependent on the crystal structure (like in isotropic space).

The possible ground states of a high L superfluid was the object of intense investigations during the 1960s and the 1970s. From the solution of the state equations, Anderson and Morel[1] and Mermin[11] identified five different phases, through the minimization of a fourth degree Landau potential. Schakel and Bias[12] analyzed the problem using only group theoretical arguments. Capel and Schakel,[13] taking advantage of the results in Ref. 12, computed the possible ground states of condensates driven by p-waves. They also investigated the consequences of lowering the residual symmetry by means of strong spin–orbit interactions. Since, in this case, the Cooper pair is in a $J=2$ state $(S=1, L=1)$, the order parameter is represented by a traceless symmetric tensor. The same holds true for an $(S=0, L=2)$ state order parameter, so their results may be directly applied to D-wave pairing. According to the authors of Ref. 13, eleven different phases are allowed. Their analysis, however, is questionable, since time reversal symmetry cannot be neglected in the theory of condensate states and the use of a fourth degree polynomial Landau free energy strongly limits the number of phases that would be allowed by the symmetry of the system.

Our aim is to give a definitive answer to the classification of possible symmetry breaking patterns in D-wave pairing Bose condensate, in the framework of the Landau theory of phase transitions. In this paper, we shall mainly be concerned with the mathematical aspects of the problem, which will be solved making use of the geometrical invariant theory approach, proposed in Ref. 14. The strategy is to exploit a set of basic invariant polynomials of the symmetry group of the system, as fundamental variables in the description of the phase space of the system and in the minimization procedure of the free energy.[15] In the realization of this program, we shall meet some substantial computational difficulties, which will be overcome by means of innovative procedures.

II. THE GEOMETRICAL INVARIANT THEORY APPROACH TO SPONTANEOUS SYMMETRY BREAKING

Let us briefly recall some basic elements of the geometrical invariant theory approach, or orbit space approach (see Ref. 16, and references therein) to the determination of possible patterns of spontaneous symmetry breaking.

Let $x \in \mathbf{R}^n$ be a vector order parameter, transforming linearly and orthogonally under the compact real symmetry group G, and let $\Phi(\alpha;x)$ be the G-invariant free energy, expressed in terms, also, of state variables α. The points $x_0(\alpha)$, where the function $\phi_\alpha(x)=\Phi(\alpha;x)$ takes on its absolute minimum, determine the stable phase of the system, whose residual symmetry is defined by the isotropy subgroup of G at x_0, G_{x_0}. Owing to its G-invariance, the free energy is a constant along each G-orbit, so each of its stationary points is degenerate along the G-orbit through it. Since the isotropy subgroups of G at points of the same orbit are conjugate in G, only the conjugate class, $[G_{x_0}]$, of G_{x_0} in G, i.e., the *orbit type* (or *symmetry*) of the orbit through x_0, is physically relevant.

The set of all G-orbits, endowed with the quotient topology and differentiable structure, forms the *orbit space*, $\mathbf{R}^n/G$, of G and the subset of all the G-orbits with the same orbit type forms a *stratum* of $\mathbf{R}^n/G$. Phase transitions take place when, by varying the values of the α's, the point $x_0(\alpha)$ is shifted to an orbit lying on a different stratum.

If $\Phi(\alpha;x)$ is a sufficiently general function of the α's, by varying these parameters, the point $x_0(\alpha)$ can be shifted to any stratum of $\mathbf{R}^n/G$. So, *the strata are in a one-to-one correspondence with the symmetry phases allowed by the G-invariance of the free energy*. On the contrary, extra restrictions on the form of the free energy function, not coming from G-symmetry requirements (e.g., the assumption that the free energy is a polynomial of low degree), can limit the number of allowed phases for the system in its ground state.

Being constant along each G-orbit, the free energy may be conveniently thought of as a function defined in the orbit space of G. This fact can be formalized using some basic results of invariant theory. In fact, the G-invariant polynomial functions separate the G-orbits, meaning that, for any two distinct orbits, there is at least a polynomial G-invariant function assuming different values on them. Moreover, every G-invariant polynomial can be built as a real polynomial function of a *finite* set, $\{p_1(x),\ldots,p_q(x)\}$, of basic polynomial invariants (*integrity basis of the ring of G-invariant polynomials*). Thus, the elements of an integrity basis can be conveniently used as coordinates of the orbit space points. They need not, for general compact groups, be algebraically independent, but can, and will, be chosen to be homogeneous polynomials in x. The number of algebraically independent elements in a *minimal* set of basic polynomial invariants is $n-\nu$, where ν is the dimension of a generic (principal) orbit of G. Information on the number and degrees of a minimal set of basic invariants, and the degrees of the algebraic relations (*syzygies*) among them, can be inferred from the Mölien function of G.

Let us call q_0 the number of independent elements of the set $\{p\}$. The range of the *orbit map*, $x \mapsto p(x)=(p_1(x),\ldots,p_q(x)) \in \mathbf{R}^q$, yields a realization of the orbit space of the linear group G, as a connected semialgebraic surface, i.e., a subset of $\mathbf{R}^q$, determined by algebraic equations and inequalities. The orbit space of G will, therefore, be identified with a closed and connected region, $\hat{S}$, of a q_0-dimensional algebraic surface, delimited by lower dimensional semialgebraic surfaces.

If an integrity basis has been determined, the equations and inequalities defining the orbit space of a compact group can be obtained from a simple recipe. It has been shown, in fact, that the orbit space of a reductive linear group can be identified with the semialgebraic variety formed by the points $p \in \mathbf{R}^q$, satisfying the following conditions:[14,17]

(i) p lies on the surface, Z, defined by the syzygies.

(ii) The $q \times q$ matrix $\hat{P}(p)$, defined by the relations

$$\hat{P}_{ab}(p(x))=\sum_{j=1}^{n} \partial_j p_a(x)\partial_j p_b(x), \quad \forall x \in \mathbf{R}^n \tag{1}$$

is positive semidefinite and has rank $\leqslant q_0$ at p.

The minimum of $\Phi(\alpha;x)$ can be computed as a *constrained* minimum of the function, $\hat{\Phi}(\alpha;p)$, $p\in\hat{S}$, defined by

$$\hat{\Phi}(\alpha;p(x))=\Phi(\alpha;x), \quad \forall x\in\mathbf{R}^n. \tag{2}$$

It has also been shown[14] that the state equation

$$\partial\Phi(\alpha;x)/\partial x_j=0, \quad j=1,...,n,$$

determining the extremal points of $\Phi(\alpha;x)$, is equivalent to the following equation in orbit space:

$$\sum_{b=1}^{q}\hat{P}_{ab}(p)\partial_b\hat{\Phi}(\alpha;p)=0, \quad a=1,...,q, \quad p\in\hat{S}. \tag{3}$$

Like all semialgebraic sets, the orbit space of G presents a natural *stratification*. It can, in fact, be considered as the disjoint union of a *finite number* of semialgebraic subsets of decreasing dimensions (*geometrical strata*), each geometrical stratum being in the border of a higher dimensional one, but for the highest dimensional stratum, which is unique (*principal stratum*). The *geometrical strata* are the connected components of the *symmetry strata*. The symmetries of two bordering strata are related by a group–subgroup relation and the orbit type of the lower dimensional stratum is larger.

In order to determine the minimum of $\hat{\Phi}(\alpha;p)$, $p\in\hat{S}$, as a constrained minimum, one needs the relations defining the geometrical strata of $\mathbf{R}^n/G$. These can be obtained from positivity and rank conditions on the matrix $\hat{P}(p)$ and from the syzygies, as already stated.

The geometrical and symmetry strata are determined in the following way. Let $\hat{W}^{(d)}$ denote the (generally nonconnected) d dimensional algebraic subset of Z, defined by the relation

$$\hat{W}^{(d)}=\{p\in Z|\operatorname{rank}(\hat{P}(p))=d, \ \hat{P}(p)\geqslant 0\}, \tag{4}$$

then, the geometrical d dimensional strata are the connected components of $\hat{W}^{(d)}$ and each d dimensional symmetry stratum, $\hat{S}^{(d,\alpha)}$, $\alpha=1,...$, is the union of all the geometrical d dimensional strata, $\hat{W}^{(d,\alpha,r)}$, $r=1,...k_\alpha$, with the same orbit type, $[G^{(d,r)}]$. A representative in $[G^{(d,r)}]$ can be obtained as the isotropy subgroup at an arbitrarily chosen point $x^{(d,r)}$ of the image in $\mathbf{R}^n$, $W^{(d,r)}$, of the geometric stratum $\hat{W}^{(d,r)}$. The point $x^{(d,r)}$ can be obtained as a solution of the equation $p(x)=p^{(d,r)}$, where $p^{(d,r)}$ is an arbitrarily chosen point in $\hat{W}^{(d,r)}$. Note that for $p^{(0)}\in\hat{S}$, all the solutions, x, of the equation $\tilde{p}(x)=\tilde{p}^{(0)}$ form a unique G-orbit. The equation has no solutions for $p^{(0)}\notin\hat{S}$.

In the following, we shall classify and characterize all the allowed symmetry phases and possible phase transitions between contiguous phases, for D-wave phase condensates in isotropic space. In particular, in Sec. III we shall identify the linear symmetry group, G, of these systems and a minimal set of basic polynomial invariants of G. In Sec. IV, we shall determine the geometrical features of the orbit space of G, i.e., its stratification (including connection properties and bordering relations of the strata) and the orbit types of its strata. In Sec. V, using an innovative method, we shall provide relatively simple expressions for the equalities and inequalities determining each stratum. These are essential for establishing the connection properties of the strata and make much easier the determination of the minima of a specific free energy function. A simple example of the determination of the minima of a general fourth degree G-invariant polynomial and their stability against sixth-order perturbations will be given in Sec. V.

III. SYMMETRY OF THE ALLOWED *D*-WAVE CONDENSATE STATES IN ISOTROPIC SPACE

The formation of *D*-wave condensate ground states breaks the symmetry of the isotropic three-dimensional space, which corresponds to the group $\mathbf{O}_3 \otimes \mathbf{U}_1 \times \langle \mathcal{T} \rangle$, where $\mathbf{O}_3$ is the complete rotation group, $\mathbf{U}_1$ is the gauge group, and $\langle \mathcal{T} \rangle$ is the group generated by the time reversal operator $\mathcal{T}$. Also, here and in the following, we shall denote by $\langle g_1,\ldots,g_n \rangle$ the group generated by the set $\{g_1,\ldots,g_n\}$.

The symmetry of the allowed *D*-wave condensate ground states is defined by the relative values of the complex coefficients in the decomposition of the gap function, Δ, in terms of spherical harmonics with $L=2$:

$$\Delta(\theta,\phi)=\sum_{m=-2}^{2} D_m Y_2^m(\theta,\phi).$$

The set of functions $\{Y_2^m, Y_2^{m*}\}$ yields a basis of a ten-dimensional (10 D) space, hosting a real representation of the symmetry group $\mathbf{O}_3 \otimes \mathbf{U}_1 \times \langle \mathcal{T} \rangle$. A general element, γ, of the group will be denoted by a triple

$$\gamma=(\rho, e^{i\phi}, \epsilon),$$

where, $\rho \in \mathbf{O}_3$, $0 \leqslant \phi < 2\pi$ and $\epsilon = -1$, or $+1$ according to whether a time reflection is involved in the transformation, or not. In the following, we shall also use the shortened notations ρ for $(\rho,1,1)$, $U_1(\phi)$ for $(\mathbf{1}_3, U_1(\phi),1)$, and $\mathcal{T}$ for $(\mathbf{1}_3,1,-1)$.

The action of G can be transferred to a real irreducible action on the 10 D vector formed by the coefficients $\{D_2,\ldots,D_{-2},D_{-2}^*,\ldots,D_2^*\}$. The representation of G thus obtained can be realized in the 10 D real vector space generated by a couple of two independent, real, second rank, symmetric, traceless tensors, $X_{ij}^{(1)}$ and $X_{ij}^{(2)}$, $i, j=1, 2, 3$, which can be considered as the real and imaginary parts of a complex 3×3 matrix ψ, whose elements will be written in terms of five complex coordinates, z_j:

$$z_j = x_j + i x_{5+j}, \quad j=1,\ldots,5, \quad x_i \in \mathbf{R}, \tag{5}$$

$$\psi = \frac{1}{\sqrt{2}} \begin{pmatrix} z_2 + \dfrac{z_5}{\sqrt{3}} & z_1 & z_4 \\ z_1 & -z_2 + \dfrac{z_5}{\sqrt{3}} & z_3 \\ z_4 & z_3 & -\dfrac{2z_5}{\sqrt{3}} \end{pmatrix}. \tag{6}$$

The coordinates D_α are connected to the z_j by the following relations:

$$D_2 = -\frac{iz_1+z_2}{\sqrt{2}}, \quad D_1 = \frac{iz_3+z_4}{\sqrt{2}}, \quad D_0 = z_5, \quad D_{-1} = \frac{iz_3-z_4}{\sqrt{2}}, \quad D_{-2} = \frac{iz_1-z_2}{\sqrt{2}}. \tag{7}$$

The matrix ψ transforms in the following way under a general transformation, $\gamma=(\rho,\phi,\epsilon) \in G$:

$$\gamma \cdot \psi = e^{i\phi} \rho \psi' \rho^T, \tag{8}$$

where $\psi' = \psi$ or ψ^*, according to whether $\epsilon = +1$ or -1 and the apex T denotes transposition. As a consequence, the group G acts as a group of linear, real, *orthogonal* transformations on the vector order parameter $x = (x_1, \ldots, x_{10}) \in \mathbf{R}^{10}$.

The kernel of the representation of G just defined is the group generated by the space reflection, so it will not be restrictive to assume that the symmetry group is

$$G = \mathbf{SO}_3 \otimes \mathbf{U}_1 \times \langle \mathcal{T} \rangle$$

and, when referring to G, in the following, we shall always mean this linear group acting in the vector space $\mathbf{R}^{10}$.

The group G has a trivial principal isotropy subgroup (the isotropy subgroup of generic points of $\mathbf{R}^{10}$), thus the principal G-orbits have the same dimensions, four, as G and its *orbit space*, $\mathbf{R}^{10}/G$, has dimensions $q_0 = 10 - 4 = 6$.

The Mölien function of $G, M_G(\eta)$, can be calculated in the form of an invariant Haar integral over G (see, for instance, Refs. 18 and 19):

$$M_G(\eta) = \int_G \frac{\mathrm{d}\mu(g)}{\det(\mathbf{1} - \eta g)}, \quad |\eta| < 1,$$

where $\mu(g)$ is a normalized invariant measure on the group G, the integration is over the whole group G, and $g \in G$. In terms of the Euler angles ϕ_1, θ, ϕ_2 and of the gauge angle α, the integral can be written in the form of a sum over the two connected components of G,

$$M_G(\eta) = \frac{1}{16\pi^2} \int_0^{2\pi} \mathrm{d}\phi_1 \int_0^{2\pi} \mathrm{d}\phi_2 \int_0^{\pi} \sin\theta \, \mathrm{d}\theta \times \left\{ \int_0^{2\pi} \frac{\mathrm{d}\alpha}{2\pi} \prod_{k=-2}^{2} [(1 - \eta e^{i(k\chi + \alpha)}) \times (1 - \eta e^{i(k\chi - \alpha)})]^{-1} + \prod_{k=-2}^{2} [(1 - \eta e^{ik\chi})(1 + \eta e^{ik\chi})]^{-1} \right\}, \tag{9}$$

where $\{e^{ik\chi}\}_{-2 \leqslant k \leqslant 2}$ are the distinct eigenvalues of the 10 D rotation matrix and $\cos\chi$ is a function of the Euler angles:

$$\cos\chi = \tfrac{1}{2}[\cos\theta + \cos(\phi_1 + \phi_2) + \cos\theta \cos(\phi_1 + \phi_2) - 1]. \tag{10}$$

It has to be noted that, in principle, the denominators in (9) are polynomials in $\sin\chi$ and $\cos\chi$; but, by definition, they are also even functions of χ, so they can be expressed as polynomials only in $\cos\chi$.

An explicit calculation of the integrals (see Appendix A) leads to

$$M_G(\eta) = \frac{1 + \eta^8 + \eta^{10} + \eta^{12} + \eta^{20}}{(1 - \eta^2)(1 - \eta^4)^2 (1 - \eta^6)^2 (1 - \eta^8)}, \tag{11}$$

a relation that can also be written in the following equivalent suggestive form:

$$M_G(\eta) = \frac{1 - \eta^{16} - \eta^{18} - \eta^{20} - \eta^{22} - \eta^{24} + \eta^{26} + \eta^{28} + \eta^{30} + \eta^{32} + \eta^{34} - \eta^{50}}{(1 - \eta^2)(1 - \eta^4)^2 (1 - \eta^6)^2 (1 - \eta^8)^2 (1 - \eta^{10})(1 - \eta^{12})}. \tag{12}$$

Any G-invariant homogeneous polynomial of degree 20 in $x \in \mathbf{R}^{10}$ can be written as a polynomial in $p_1(x), \ldots, p_9(x)$; Eqs. (11) and (12) yield the following indications, whose validity has been checked through direct calculations.

(1) A minimal integrity basis (IB) for the linear group G contains nine elements, $\{p_1, \ldots, p_9\}$ with degrees $(d_1, \ldots, d_9) = (2, 4, 4, 6, 6, 8, 8, 10, 12)$.

(2) The invariants p_i are connected by five independent syzygies of degrees 16, 18, 20, 22, and 24. The group is, therefore, *noncoregular*.

(3) It is possible to find a *nonminimal homogeneous* IB, $\{\xi_1,\ldots,\xi_6,\theta_1,\ldots,\theta_4\}$, with degrees (2, 4, 4, 6, 6, 8, 8, 10, 12, 20), such that any invariant polynomial, F, can be written in the form[20]

$$F=Q_0(\xi)+\sum_{i=1}^{4} Q_i(\xi)\,\theta_i, \tag{13}$$

where the Q's, are polynomials in the *algebraically independent* polynomial invariants $(\xi_1,\ldots,\xi_6)$.

A possible choice for the IBs $\{p\}$ and $\{\xi,\ \theta\}$ is the following:

$$\begin{gathered}
p_1=\mathrm{Tr}(\psi\psi^*)=\Sigma_{i=1}^{10}x_i^2,\\
p_2=\mathrm{Tr}[(\psi\psi^*)^2],\quad p_6=\Re[\mathrm{Tr}(\psi^2)\mathrm{Tr}(\psi^2\psi^*)\mathrm{Tr}(\psi^{*3})],\\
p_3=|\mathrm{Tr}(\psi^2)|^2,\quad p_7=\Re[\mathrm{Tr}(\psi^{*2})(\mathrm{Tr}(\psi^2\psi^*))^2],\\
p_4=|\mathrm{Tr}(\psi^3)|^2,\quad p_8=\Re[\mathrm{Tr}(\psi^2\psi^*)\mathrm{Tr}(\psi^3)(\mathrm{Tr}(\psi^{*2}))^2],\\
p_5=|\mathrm{Tr}(\psi^2\psi^*)|^2,\quad p_9=\Re[(\mathrm{Tr}(\psi^2))^3(\mathrm{Tr}(\psi^{*3}))^2].
\end{gathered} \tag{14}$$

and

$$\begin{gathered}
\xi_i=p_i,\quad i=1,\ldots,5,\quad \xi_6=p_6+p_7,\\
\theta_1=p_6-p_7,\quad \theta_2=p_8,\quad \theta_3=p_9,\quad \theta_4=(p_6-p_7)p_9.
\end{gathered} \tag{15}$$

Thus, the most general nonequilibrium polynomial Landau potential, $\hat{\Phi}(\alpha;p)$, can be written in the form

$$\hat{\Phi}=Q_0+Q_1p_7+Q_2p_8+Q_3p_9+Q_4p_7p_9. \tag{16}$$

Using the above-mentioned definitions, the explicit form of the syzygies and of the $\hat{P}$-matrix elements can be obtained through the following simple procedure.

After defining the *weight* of an element, p_i, of the IB to be equal to the degree, d_i, of the homogeneous polynomial $p_i(x)$, and the degree of $\Pi_i p_i^{n_i}$ as $\Sigma_i n_i d_i$, one writes down the most general homogeneous polynomial, $\hat{\Theta}^{(d)}(\xi,\theta)$, of the relevant weight, d, in the weighted variables ξ_i, $i=1,\ldots,6$ and θ_i, $i=1,\ldots,4$. With the definitions $\theta_0=1$, $d_0=0$, the polynomial $\hat{\Theta}^{(d)}(\xi,\theta)$ can be written in the compact form

$$\hat{\Theta}^{(d)}(\xi,\theta)=\sum_{j=0}^{3}\delta_{N_j,d}A^{(j,d)}_{n_i,\ldots,n_6}\theta_j\prod_{k=1}^{6}\xi^{n_k},$$

where $N_j=\Sigma_{i=1}^{6}n_id_i-d_j$, $\delta_{N_{j,d}}$ is a Kronecker symbol and the A's are real coefficients to be determined through the following conditions:

(i) In the case of the syzygies $\hat{s}_d(\xi,\theta)$, $d=16,\ 18,\ 20,\ 22,\ 24$: The expression $\hat{s}_d(\xi(x),\theta(x))$ has to vanish identically in x.

(ii) In the case of the matrix elements $\hat{P}_{a,b}(\xi,\theta)$, $a,b=1,\ldots,9$, $d=d_a+d_b-2$: The expression $\hat{P}_{ab}(\xi(x),\theta(x))=\Sigma_{i=1}^{10}\partial_i p_a(x)\partial_i p_b(x)$ has to be an identity in x.

The explicit expressions of the syzygies are reported in Appendix B and the elements of the matrix $\hat{P}(p)$ in Appendix C. In the following we shall always use the minimal IB $\{p\}$.

On the algebraic surface, Z, defined by the syzygies in the nine-dimensional space of the p's, the 9×9 symmetric matrix $\hat{P}(p)$ has rank $\leqslant 6$, as it has to be, since the orbit space is six dimensional.

IV. THE ORBIT SPACE OF THE LINEAR GROUP *G*

As recalled in Sec. I, the orbit space of G can be identified with the range of the orbit map $x\mapsto p(x)$, which is the same as the set of values of $p\in Z$, that render the matrix $\hat{P}(p)$ positive semidefinite.

The analytic conditions determining the geometrical strata, $\hat{W}^{(d,\alpha,r)}$, are not difficult to specify, in principle, but, in the case of the higher dimensional strata, their explicit expressions (as sets of equalities and inequalities in the p's) become difficult to obtain, too large to be written down extensively and uneasy to handle, if they are derived only from rank and positivity conditions of the matrix $\hat{P}(p)$. An elegant way to bypass this difficulty is the following.

One starts with the relatively easy determination of the *geometrical* strata of dimensions $\leqslant 2$ [i.e., the connected components of the sets $\hat{W}^{(d)}$, $d=1$, 2, defined in (4)], starting from the positivity and rank properties of the matrix $\hat{P}(p)$ and from the syzygies. The subsequent step consists in the identification of the orbit type of each geometrical stratum. This allows one to identify the connected components, $\hat{W}^{(d,\alpha,r)}$, $r=1,...$, with the same orbit type, $[G^{d,\alpha}]$, and belonging, therefore, to the same *symmetry* stratum, $\hat{S}^{(d,\alpha)}$. There is a unique zero-dimensional stratum, corresponding to the point $p=p(0)=0$, whose symmetry is $[G]$. It will be ignored in the following. All the groups $G^{(2,\alpha)}$ turn out to be finite groups of low order ($\leqslant 8$).

The determination of the higher dimensional strata bordered by a given two-dimensional stratum, $\hat{S}^{(2,\alpha)}$, can be obtained starting from the identification of their orbit types, which are necessarily contained in the orbit type of $\hat{S}^{(2,\alpha)}$. The task is easily accomplished by selecting, out of the set of maximal subgroups of $G^{(2,\alpha)}$, those which are isotropy subgroups of G. To this end, the following criterion can be used. Let H be one of the maximal subgroups of a $G^{(d,\alpha)}$ and denote by V_H the linear subspace formed by all the points $x\in\mathbf{R}^{10}$, which are stable under H. Then, H is an isotropy subgroup of G, if and only if the following condition is satisfied:

$$\operatorname*{Max}_{x\in V_H}\operatorname{rank}(P(x))<d.$$

If this condition is satisfied, when x spans V_H, the point $p(x)\in\mathbf{R}^9$ spans the topological closure of a stratum $\hat{S}^{(d',\alpha')}$ and

$$\dim(\hat{S}^{(d',\alpha')})=\operatorname*{Max}_{x\in V_H}\operatorname{rank}(P(x)).$$

To get the full set of higher dimensional strata, the last part of the procedure just described has to be repeated for each newly determined stratum.

The derivation of the equalities and inequalities determining each of the higher dimensional strata requires a more sophisticated method,[21] which we shall explain and exploit in Sec. V.

Before resuming the results obtained with the realization of the program just presented, let us note that, owing to the linearity of G, its isotropy subgroups coincide at the points $x\in\mathbf{R}^{10}$ and κx, $0\neq\kappa\in\mathbf{R}$. Thus, also taking into account the homogeneity of the polynomials $p_i(x)$, the points $(p_1,...,p_9)$ and $(1,p_2/p_1^{d_2/2},...,p_9/p_1^{d_9/2})$ lie on the same stratum and the equalities and inequalities defining the strata can be written as homogeneous relations in the weighted variables p_i. It will be useful, therefore, to introduce the definitions

$$\tilde{p}_i=p_i/p_1^{d_i/2},\quad \tilde{p}=(\tilde{p}_2,...,\tilde{p}_9). \tag{17}$$

TABLE I. Relations defining 1 D geometrical strata, $\hat{S}^{(1,A)}=\hat{W}^{(1,A)}$ in orbit space. For $2\leqslant i\leqslant 9$, $\tilde{p}_i=p_i/(p_1^{d_i/2})$, d_i denotes the degree of the polynomial $p_i(x)$ in the order parameter x and the values, $p^{(1,A)}$, taken on by $\tilde{p}$ on $\hat{W}^{(1,A)}$ are listed in the columns from 2 to 9.

A	$\tilde{p}_2$	$\tilde{p}_3$	$\tilde{p}_4$	$\tilde{p}_5$	$\tilde{p}_6$	$\tilde{p}_7$	$\tilde{p}_8$	$\tilde{p}_9$
1	1	0	0	0	0	0	0	0
2	1/2	1	1/6	1/6	1/6	1/6	1/6	1/6
3	1/2	1	0	0	0	0	0	0
4	1/3	0	1/3	0	0	0	0	0
5	1/2	0	0	0	0	0	0	0

The relations determining the one- and two-dimensional strata can be easily obtained by selecting those solutions, $\overline{p}$, of the condition rank $(\hat{P}(p))=1$ and, respectively, rank $(\hat{P}(p))=2$, at which the matrix $\hat{P}(\overline{p})$ is positive semidefinite. In this way, one obtains five connected components, $\hat{W}^{(1,A)}$,$A=1,...,5$, of $\hat{W}^{(1)}$ and seven connected components, $\hat{W}^{(2,A)}$, $A=1_+, 1_-, 2, 3_+, 3_-, 4, 5$, of $\hat{W}^{(2)}$. The parametric equations defining these semialgebraic sets are listed in Tables I and II.

In order to identify the distinct 1 D and 2 D symmetry strata, for each connected component $\hat{W}^{(d,A)}$, $d=1,2$, we have picked up a point $p^{(d,A)}$ and, for each $p^{(d,A)}$, a ''simple'' solution, $x^{(d,A)}$, of the equation $\tilde{p}(x)=\tilde{p}^{d,A}$. Then, at each point $x^{(d,A)}$ we have determined, and compared for conjugation, the isotropy subgroup of G,$G^{(d,A)}$. These subgroups turn out to be nonconjugate in G, but for $G^{(2,1_+)}$, which is conjugate to $G^{(2,1_-)}$, and $G^{(2,3_+)}$, which is conjugate to $G^{(2,3_-)}$. Thus, there are five distinct 1 D and five 2 D symmetry strata, $\hat{S}^{(d,\alpha)}$, with orbit-types $[G^{(d,\alpha)}]$, $d=1,2$, $\alpha=1,...,5$.

After choosing an element, H, in each class $[G^{(d,\alpha)}]$, it is easy to determine the subspace $V_H\subset\mathbf{R}^{10}$, formed by the vectors which are H-invariant.

The results we have obtained are listed in Tables III and IV and the bordering relations among the strata are illustrated in Fig. 1. The definitions of the rotation matrices appearing in the tables and in the following text are recalled in Appendix D. We have used standard notations for the corresponding geometrical transformations (see, e.g, Ref. 22).

V. RELATIONS DEFINING THE STRATA WITH DIMENSIONS ⩾3

In order to derive the relations defining the higher dimensional strata we shall exploit the following results,[21] which we shall briefly recall, without proof. Let H be an isotropy subgroup of G, $S_{[H]}$ and $\hat{S}_{[H]}$ the associated strata in $\mathbf{R}^{10}$ and $\mathbf{R}^{10}/G$ respectively, and let $\mathrm{Stab}(H,G)$ be the stabilizer of H in G:

TABLE II. Parametric equations defining the geometrical strata, $\hat{W}^{(2,A)}$ (A is listed in the head row) in orbit space. For $2\leqslant i\leqslant 9$, $\tilde{p}_i=p_i/(p_1^{d_i/2})$ and d_i denotes the degree of the polynomial $p_i(x)$, in the order parameter x, and $\epsilon=\pm 1$.

$\tilde{p}\backslash A$	1_ϵ	2	3_ϵ	4	5
$\tilde{p}_2$	$(2+\xi^2)/6$	1/2	$(2+\xi^2)/6$	1/2	ξ
$\tilde{p}_3$	0	ξ	ξ^2	1	$2-2\xi$
$\tilde{p}_4$	$(2-\xi)^2(1+\xi)/12$	0	$(2-\xi)^2(1+\xi)/12$	ξ	0
$\tilde{p}_5$	0	0	$\xi^2(1+\xi)/12$	ξ	0
$\tilde{p}_6$	0	0	$(2-\xi)(1+\xi)\xi^2/12$	ξ	0
$\tilde{p}_7$	0	0	$(1+\xi)\xi^3/12$	ξ	0
$\tilde{p}_8$	0	0	$(2-\xi)(1+\xi)\xi^3/12$	ξ	0
$\tilde{p}_9$	0	0	$(2-\xi)^2(1+\xi)\xi^3/12$	ξ	0
ξ range	$]0,\frac{1+3\epsilon}{2}[$	$]0,1[$	$]0,\epsilon[$	$]0,\frac{1}{6}[$	$]\frac{1}{2},1[$

TABLE III. Possible symmetry strata, $S^{(d,r)}$ for D-wave driven pairing in isotroic space (d denotes the dimension of the stratum and r is an enumeration index). From left to right, the columns refer to the phase reference numbers according to our $((d,r))$ and Ref. 12 ($\mathcal{N}$) classification, the order ($|H|$) and the residual symmetry group, H, the complex coordinates ($z_j=x_j+ix_{5+j}$, $j=1,...,5$) of the H-invariant superconducting vector order parameter and corresponding values of the partial wave amplitudes $(D_2,\ldots,D_{-2})$. In columns five and six, the t's are real parameters, while the v's are complex ones. The definitions of the group elements are recalled in Appendix D.

(d,r)	$\mathcal{N}$	$\lvert H\rvert$	H	$(z_1,\ldots,z_5)$	$\sqrt{2}(D_2,D_1,D_0,D_{-1},D_{-2})$
(1,1)	II	∞	$\langle C_{2x}\mathcal{T}\rangle\times\{R_z(\phi)U_1(2\phi)\}_\phi$	$(it,-t,0,0,0)$	$(2t,0,0,0,0)$
(1,2)	VIII	∞	$\mathbf{O}_2^z\otimes\langle\mathcal{T}\rangle$	$(0,0,0,0,t)$	$(0,0,t\sqrt{2},0,0)$
(1,3)	IX,X	16	$\langle C_{2x},\mathcal{T},C_{4z}U_1(\pi)\rangle$	$(0,t,0,0,0)$	$(-t,0,0,0,-t)$
(1,4)	XI	24	$\langle C_{2x},C_{2a}\mathcal{T},C_{3\delta}U_1(4\pi/3)\rangle$	$(0,-it,0,0,t)$	$(it,0,t\sqrt{2},0,it)$
(1,5)	I	∞	$\langle C_{2x}\mathcal{T}\rangle\times\{R_z(\phi)U_1(-\phi)\}_\phi$	$(0,0,t,-it,0)$	$(0,0,0,2it,0)$
(2,1)	V	6	$\langle C_{2x}\mathcal{T},C_{3z}U_1(4\pi/3)\rangle$	$(it_1,-t_1,t_2,-it_2,0)$	$(2t_1,0,0,2it_2,0)$
(2,2)	IV	4	$\langle C_{2x}\mathcal{T},C_{2z}U_1(\pi)\rangle$	$(0,0,t_1,it_2,0)$	$(0,it_1+it_2,0,it_1-it_2,0)$
(2,3)	$\cdots$	8	$\langle C_{2x},C_{4z}\mathcal{T}\rangle$	$(0,it_1,0,0,t_2)$	$(-it_1,0,t_2\sqrt{2},0,-it_1)$
(2,4)	VII	8	$\langle C_{2x},C_{2z},\mathcal{T}\rangle$	$(0,t_1,0,0,t_2)$	$(-t_1,0,t_2\sqrt{2},0,-t_1)$
(2,5)	VI	8	$\langle C_{2x}\mathcal{T},C_{4z}U_1(\pi)\rangle$	$(it_1,t_2,0,0,0)$	$(t_1-t_2,0,0,0,-t_1-t_2)$
(3,1)	III	4	$\langle C_{2x},C_{2x}\mathcal{T}\rangle$	$(it_1,t_2,0,0,t_3)$	$(t_1-t_2,0,t_3\sqrt{2},0,-t_1-t_2)$
(3,2)	$\cdots$	4	$\langle C_{2x},C_{2z}\rangle$	$(0,v_1,0,0,v_2)$	$(-v_1,0,v_2\sqrt{2},0,-v_1)$
(4,1)	$\cdots$	2	$\langle C_{2x}\mathcal{T}\rangle$	(it_1,t_2,t_3,it_4,t_5)	$(t_1-t_2,it_3+it_4,t_5\sqrt{2},it_3-it_4,-t_1-t_2)$
(4,2)	$\cdots$	2	$\langle C_{2z}\rangle$	$(v_1,v_2,0,0,v_3)$	$(-iv_1-v_2,0,v_3\sqrt{2},0,iv_1-v_2)$
(6,1)	$\cdots$	1	$\{1\}$	(v_1,v_2,v_3,v_4,v_5)	$(-iv_1-v_2,iv_3+v_4,v_5\sqrt{2},iv_3-v_4,iv_1-v_2)$

$$\mathrm{Stab}(H,G)=\{g\in G\,|\,gHg^{-1}=H\}.$$

We have denoted by V_H the linear subspace formed by the H-invariant vectors of $\mathbf{R}^{10}$:

$$V_H=\{x\in\mathbf{R}^{10}\,|\,hx=x,\forall h\in H\},\tag{18}$$

and we shall denote by $V_H^{(H)}$ the subset of V_H formed by the points at which the isotropy subgroup of G is H:

$$V_H^{(H)}=\{x\in\mathbf{R}^{10}\,|\,G_x=H\}.\tag{19}$$

TABLE IV. Strata of dimensions $\geqslant 3$, bordering each stratum $\hat{S}^{(d,r)}$ (d denotes the dimension of the stratum and r is an enumeration index). From left to right, the columns refer to the enumeration numbers, (d,r), of the lower bordering stratum, $\hat{S}^{(d,r)}$, its orbit type, $[G^{(d,r)}]$, the maximal conjugacy classes of subgroups of $[G^{(d,r)}]$, $[H]_M$, the order, $|H_M|$, of H_M and the indices, (d',r'), of the corresponding strata, if any. The definitions of the group elements are recalled in Appendix D.

(d,r)	$[G^{(d,r)}]$	$[H]_M$	$\lvert H_M\rvert$	(d',r')
(2,1)	$[\langle C_{2x}\mathcal{T},C_{3z}U_1(4\pi/3)\rangle]$	$[\langle C_{3z}U_1(4\pi/3)\rangle]$	3	$\cdots$
		$[\langle C_{2x}\mathcal{T}\rangle]$	2	(4,1)
(2,2)	$[\langle C_{2x}\mathcal{T},C_{2z}U_1(\pi)\rangle]$	$[\langle C_{2x}\mathcal{T}\rangle]$	2	(4,1)
		$[\langle C_{2z}U_1(\pi)\rangle]$	2	$\cdots$
(2,3)	$[\langle C_{2z},C_{4x}\mathcal{T}\rangle]$	$[\langle C_{2z},C_{2x}\mathcal{T}\rangle]$	4	(3,1)
		$[\langle C_{2x},C_{2z}\rangle]$	4	(3,2)
		$[\langle C_{4z}\mathcal{T}\rangle]$	4	$\cdots$
(2,4)	$[\langle C_{2x},C_{2z},\mathcal{T}\rangle]$	$[\langle C_{2x},C_{2z}\rangle]$	4	(3,2)
		$[\langle C_{2z},C_{2x}\mathcal{T}\rangle]$	4	(3,1)
(2,5)	$[\langle C_{2x}\mathcal{T},C_{4z}U_1(\pi)\rangle]$	$[\langle C_{2z},C_{2x}\mathcal{T}\rangle]$	4	(3,1)
		$[\langle C_{4z}U_1(\pi)\rangle]$	4	$\cdots$
(3,1)	$[\langle C_{2z},C_{2x}\mathcal{T}\rangle]$	$[\langle C_{2x}\mathcal{T}\rangle]$	2	(4,1)
		$[\langle C_{2z}\rangle]$	2	(4,2)
(3,2)	$[\langle C_{2x},C_{2z}\rangle]$	$[\langle C_{2z}\rangle]$	2	(4,2)
(4,1)	$[\langle C_{2x}\mathcal{T}\rangle]$	$[\mathbf{1}]$	1	(6,1)
(4,2)	$[\langle C_{2z}\rangle]$	$[\mathbf{1}]$	1	(6,1)

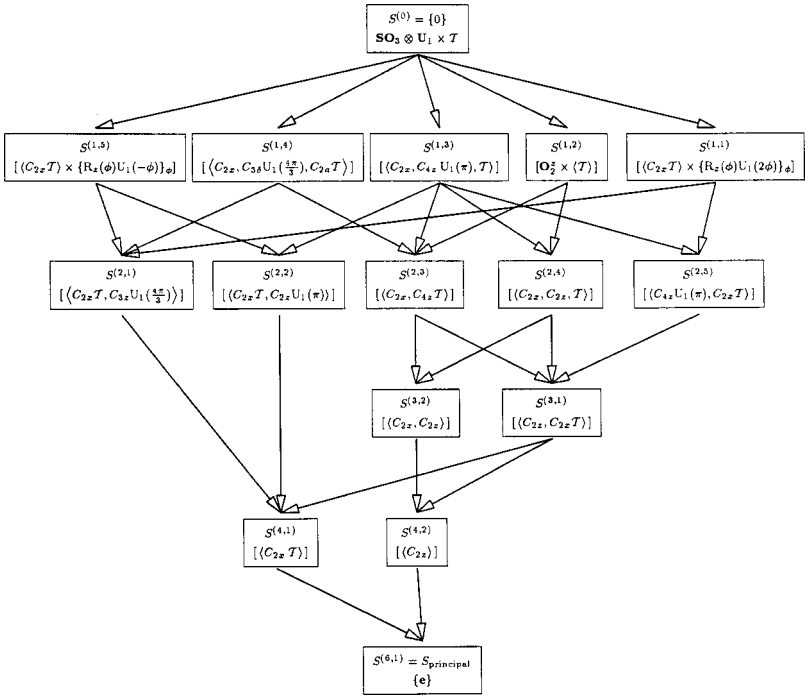

FIG. 1. Possible phase transitions between bordering strata, connected by continuous sequences of one or more arrows. The group elements are defined in Appendix D.

The set $V_H^{(H)}$ is the intersection of V_H with the stratum of orbit-type $[H]$.

The group $\mathrm{Stab}(H,G)$ acts linearly on V_H; let us call $\tilde{H}$ the linear group defined by this action. The $\tilde{H}$-orbit through $x \in V_H$ is the intersection of the G-orbit through x with V_H. There is, therefore, a one-to-one correspondence between the G-orbits lying in the closure of $\hat{S}_{[H]}$ and the $\tilde{H}$ orbits. This correspondence can be restricted to a one-to-one correspondence between the interior points of the closure of $\hat{S}_{[H]}$ and the points of the principal stratum of $V_H/\tilde{H}$. If $\hat{S}_{[H]}$ is connected, the one-to-one correspondence is between the principal stratum of $V_H/\tilde{H}$ and $\hat{S}_{[H]}$, otherwise the inverse image of $\hat{S}_{[H]}$ in the correspondence reduces to the points of the principal stratum of $V_H/\tilde{H}$, corresponding to $\tilde{H}$-orbits through points of $V_H^{(H)}$. Thus an IB, $\{\lambda\}$, of $\tilde{H}$ can be used to parametrize the points of $\hat{S}_{[H]}$:

$$p = p(\lambda).$$

The range of the parameters λ will be determined by the positivity conditions of the $\hat{P}$ matrix associated to the IB $\{\lambda\}$, $\hat{P}^{(H)}(\lambda)$, and convenient additional conditions obtained from positivity and rank conditions of $\hat{P}(p)$, if $\hat{S}_{[H]}$ is not connected. To this end it will be worth noting that, for $p \in \hat{S}_{[H]}$, the matrix $\hat{P}(p)$ can be written in the following form:

$$\hat{P}(p(\lambda)) = J^T(\lambda)\hat{P}^{(H)}(\lambda)J(\lambda), \tag{20}$$

where, $J(\lambda)$ is the Jacobian matrix

$$J_{ai}(\lambda) = \frac{\partial p_a(\lambda)}{\partial \lambda_i}. \tag{21}$$

Owing to a well-known theorem in matrix theory, from (20) one obtains the following upper limit:

$$\mathrm{rank}(\hat{P}(p(\lambda))) \leqslant \mathrm{rank}(J(\lambda)). \tag{22}$$

In the following, we shall use this approach to derive rational parametric equations for all the strata of $\hat{S}$ with dimensions three and four. The results obtained in this way, starting from each of the strata of dimensions $\geqslant 2$, are summarized in Table IV and in the lower part of Table III.

A. Stratum $\hat{S}^{(3,1)}$

The stabilizer in G of the group $H=G^{(3,1)}=\langle C_{2z}, C_{2x}\mathcal{T}\rangle$, is the group $\mathrm{Stab}(H)=\langle C_{2x}, C_{2a}, U_1(\pi), \mathcal{T}\rangle$.

An easy calculation shows that the space V_H is defined by the equations $x_i=0$, $i=1, 3, 4, 7, 8, 9, 10$. The elements of $\tilde{H}$ act on the x_i, $i=2, 5, 6,$ by changing the signs of one or two or all of these coordinates, so, an IB of $\tilde{H}$ can be chosen to be

$$\lambda_1=x_5^2, \quad \lambda_2=x_2^2, \quad \lambda_3=x_6^2 \tag{23}$$

and the expression of the p's in terms of the λ's turns out to be the following:

$$\begin{aligned}
p_1&=\lambda_1+\lambda_2+\lambda_3,\\
p_2&=(3\lambda_1^2+6\lambda_1\lambda_2+3\lambda_2^2+2\lambda_1\lambda_3+18\lambda_2\lambda_3+3\lambda_3^2)/6,\\
p_3&=(\lambda_1+\lambda_2-\lambda_3)^2,\\
p_4&=\lambda_1(\lambda_1-3\lambda_2+3\lambda_3)^2/6,\\
p_5&=\lambda_1(\lambda_1-3\lambda_2-\lambda_3)^2/6,\\
p_6&=\lambda_1(\lambda_1-3\lambda_2-\lambda_3)(\lambda_1+\lambda_2-\lambda_3)(\lambda_1-3\lambda_2+3\lambda_3)/6,\\
p_7&=\lambda_1(\lambda_1-3\lambda_2-\lambda_3)^2(\lambda_1+\lambda_2-\lambda_3)/6,\\
p_8&=\lambda_1(\lambda_1-3\lambda_2-\lambda_3)(\lambda_1+\lambda_2-\lambda_3)^2(\lambda_1-3\lambda_2+3\lambda_3)/6,\\
p_9&=\lambda_1(\lambda_1+\lambda_2-\lambda_3)^3(\lambda_1-3\lambda_2+3\lambda_3)^2/6,
\end{aligned} \tag{24}$$

with

$$\lambda_1, \lambda_2, \lambda_3 > 0. \tag{25}$$

For values of the λ's satisfying (25), the values of the p's defined in (24) render $\hat{P}(p)$ everywhere positive semidefinite and of rank three. We can conclude, therefore, that they yield parametric equations for the three-dimensional (3D) stratum $\hat{S}^{(3,1)}$. Being the continuous image of a connected set, the stratum is *connected*.

By eliminating the parameters λ's from (24) and (25), one obtains the following relations:

$$\begin{aligned}
p_4&=9(2p_1{}^2-2p_2-p_3)(2p_1{}^2-2p_2+2p_1\sqrt{p_3}+p_3)^2\tau,\\
p_5&=(2p_1{}^2-2p_2-p_3)(2p_1{}^2-6p_2-2p_1\sqrt{p_3}-p_3)^2\tau,\\
p_6&=-3\sqrt{p_3}(2p_1{}^2-2p_2-p_3)(2p_1{}^2-6p_2-2p_1\sqrt{p_3}-p_3)(2p_1{}^2-2p_2+2p_1\sqrt{p_3}+p_3)\tau,
\end{aligned}$$

$$p_7 = -\sqrt{p_3}(2{p_1}^2 - 2p_2 - p_3)(2{p_1}^2 - 6p_2 - 2p_1\sqrt{p_3} - p_3)^2\tau,$$

$$p_8 = 3p_3(2{p_1}^2 - 2p_2 - p_3)(2{p_1}^2 - 6p_2 - 2p_1\sqrt{p_3} - p_3)(2{p_1}^2 - 2p_2 + 2p_1\sqrt{p_3} + p_3)\tau,$$

$$p_9 = -9\sqrt{p_3^3}(2{p_1}^2 - 2p_2 - p_3)(2{p_1}^2 - 2p_2 + 2p_1\sqrt{p_3} + p_3)^2\tau, \tag{26}$$

$$\begin{cases} 0 < p_3 < p_1^2, \\ 2p_1^2 + p_3 < 6p_2 < 3(2p_1^2 - p_3), \end{cases} \tag{27}$$

where

$$\tau^{-1} = 64(p_1 + \sqrt{p_3})^3, \tag{28}$$

and the square root of p_3 has to be intended in an algebraic sense.

B. Stratum $\hat{S}^{(3,2)}$

The stabilizer in G of the group $H = G^{(3,2)} = \langle C_{2x}, C_{2x} \rangle$, is a group of ∞ order: Stab(H) $= \langle C_{4x}, C_{4z}, \mathcal{T} \rangle \times \mathbf{U}_1$.

The space V_H is defined by the equations $x_i = 0$, $i = 1, 3, 4, 6, 8, 9$. The transformation properties of the coordinates x_i, $i = 2, 5, 7, 10$, under the transformations of $\tilde{H}$ can be conveniently described in the following way. Let us define:

$$\eta_1 = x_2 + ix_5 + i(x_7 + ix_{10}), \quad \eta_2 = x_2 - ix_5 + i(x_7 - ix_{10}), \tag{29}$$

then

(i) under a gauge transformation, $U_1(\phi)$:$(\eta_1, \eta_2) \to (e^{i\phi}\eta_1, e^{i\phi}\eta_2)$;
(ii) under time reversal $\mathcal{T}$:$(\eta_1, \eta_2) \to (\eta_2^*, \eta_1^*)$;
(iii) under a transformation C_{4x}:$(\eta_1, \eta_2) \to (e^{i\pi/3}\eta_2, e^{-i\pi/3}\eta_1)$;
(iv) under a transformation C_{4z}:$(\eta_1, \eta_2) \to (-\eta_2, -\eta_1)$.

The group $\tilde{H}$ is coregular and admits the following minimal IB:

$$\lambda_1 = (|\eta_1|^2 + |\eta_2|^2)/2 = {x_2}^2 + {x_5}^2 + {x_7}^2 + {x_{10}}^2,$$

$$\lambda_2 = (|\eta_1|^2 - |\eta_2|^2)^2/16 = (x_5x_7 - x_2x_{10})^2, \tag{30}$$

$$\lambda_3 = \Re[(\eta_1\eta_2^*)^3] = ({x_2}^2 - {x_5}^2 + {x_7}^2 - {x_{10}}^2)({x_2}^4 - 14{x_2}^2{x_5}^2 + {x_5}^4 + 2{x_2}^2{x_7}^2 - 2{x_5}^2{x_7}^2 + {x_7}^4$$
$$- 24x_2x_5x_7x_{10} - 2{x_2}^2{x_{10}}^2 + 2{x_5}^2{x_{10}}^2 - 14{x_7}^2{x_{10}}^2 + {x_{10}}^4).$$

It has to be noted that the invariant $(\Im[(\eta_1\eta_2^*)^3])^2$ can be expressed as a polynomial in $\lambda_1, \lambda_2, \lambda_3$.

The corresponding $\hat{P}$-matrix turns out to be

$$\begin{pmatrix} 4\lambda_1 & 8\lambda_2 & 12\lambda_3 \\ 8\lambda_2 & 4\lambda_1\lambda_2 & 0 \\ 12\lambda_3 & 0 & 36\lambda_1(\lambda_1^2 - 4\lambda_2)^2 \end{pmatrix} \tag{31}$$

and the p's can be expressed in terms of the λ's in the following form:

$$p_1 = \lambda_1,$$

$$p_2 = (3\lambda_1^2 - 4\lambda_2)/6,$$

$$
\begin{aligned}
p_3&=\lambda_1^2-4\lambda_2,\\
p_4&=(\lambda_1^3+12\lambda_1\lambda_2-\lambda_3)/12,\\
p_5&=(\lambda_1^3-4\lambda_1\lambda_2-\lambda_3)/12,\\
p_6&=(\lambda_1^4-16\lambda_2^2-\lambda_1\lambda_3)/12,\\
p_7&=(\lambda_1^4-8\lambda_1^2\lambda_2+16\lambda_2^2-\lambda_1\lambda_3)/12,\\
p_8&=(\lambda_1^5-8\lambda_1^3\lambda_2+16\lambda_1\lambda_2^2-\lambda_1^2\lambda_3-4\lambda_2\lambda_3)/12,\\
p_9&=(\lambda_1^6-12\lambda_1^4\lambda_2+48\lambda_1^2\lambda_2^2-64\lambda_2^3-\lambda_1^3\lambda_3-12\lambda_1\lambda_2\lambda_3)/12,
\end{aligned}
\tag{32}
$$

where the parameters λ have to satisfy the conditions:

$$
\begin{cases}
\lambda_1>0,\\
0<4\lambda_2<\lambda_1^2,\\
\lambda_3^2<(\lambda_1^2-4\lambda_2)^3.
\end{cases}
\tag{33}
$$

For values of the λ's satisfying (33), the values of the p's defined in (32) render $\hat{P}(p)$ everywhere positive semidefinite and of rank three. We can conclude, therefore, that they yield parametric equations for the 3D stratum $\hat{S}^{(3,1)}$. Being the continuous image of a connected set, the stratum is *connected*.

By eliminating the parameters λ from (32) and (33) one obtains the following relations:

$$
\begin{aligned}
p_2&=(2p_1^2+p_3)/6,\\
p_5&=(-p_1^3+p_1p_3+3p_4)/3,\\
p_6&=(-4p_1^4+5p_1^2p_3-p_3^2+12p_1p_4)/12,\\
p_7&=(-4p_1^4+3p_1^2p_3+p_3^2+12p_1p_4)/12,\\
p_8&=(-4p_1^5+5p_1^3p_3-p_1p_3^2+12p_1^2p_4-6p_3p_4)/6,\\
p_9&=(-16p_1^6+24p_1^4p_3-9p_1^2p_3^2+p_3^3+48p_1^3p_4-36p_1p_3p_4)/12
\end{aligned}
\tag{34}
$$

and

$$
\begin{cases}
p_1>0,\\
0<p_3<p_1^2,\\
p_3^3<[12p_4-(4p_1^2-3p_3)p_1]^2
\end{cases}
.
\tag{35}
$$

C. Stratum $\hat{S}^{(4,1)}$

The stabilizer in G of the group $H=G^{(4,1)}=\langle C_{2x},\mathcal{T}\rangle$, is the group $\mathrm{Stab}(H,G)=\mathbf{O}_2^x\times\langle U_1(\pi),\mathcal{T}\rangle$.

The space V_H is defined by the equations $x_i=0$, $i=1, 4, 7, 8, 10$. The transformation properties of the coordinates, x_i, $i=2, 3, 5, 6, 9$ of V_H are easily derived from (8) and can be put in the following advantageous form. Let us define

$$\eta_1=\frac{\sqrt{3}x_2+x_5}{2},\quad \eta_2=x_3+i\frac{x_2-\sqrt{3}x_5}{2},\quad \eta_3=x_6-ix_9, \tag{36}$$

then,

(i) under a proper rotation, $O_2^x(\phi):(\eta_1,\eta_2,\eta_3)\to(\eta_1,e^{-2i\phi}\eta_2,e^{i\phi}\eta_3)$;
(ii) under a gauge transformation, $U_1(\pi):(\eta_1,\eta_2,\eta_3)\to(-\eta_1,-\eta_2,-\eta_3)$;
(iii) under a transformation $C_{2z}:(\eta_1,\eta_2,\eta_3)\to(\eta_1,-\eta_2^*,\eta_3^*)$;
(iv) under time reversal $\mathcal{T}:(\eta_1,\eta_2,\eta_3)\to(\eta_1,\eta_2,-\eta_3)$.

The group $\tilde{H}$ is not coregular and admits the following minimal IB:

$$\lambda_1=3|\eta_1|^2=\tfrac{3}{4}(\sqrt{3}x_2+x_5)^2,$$

$$\lambda_2=|\eta_2|^2=\tfrac{1}{4}(x_2^2+4x_3^2-2\sqrt{3}x_2x_5+3x_5^2),$$

$$\lambda_3=|\eta_3|^2=x_6^2+x_9^2, \tag{37}$$

$$\lambda_4=\sqrt{3}\,\eta_1\mathfrak{I}(\eta_2\eta_3^2)=\frac{\sqrt{3}}{4}(\sqrt{3}x_2+x_5)(x_2x_6^2-\sqrt{3}x_5x_6^2-4x_3x_6x_9-x_2x_9^2+\sqrt{3}x_5x_9^2),$$

$$\lambda_5=[\mathfrak{I}(\eta_2\eta_3^2)]^2=\tfrac{1}{4}(x_2x_6^2-\sqrt{3}x_5x_6^2-4x_3x_6x_9-x_2x_9^2+\sqrt{3}x_5x_9^2)^2$$

with the syzygy

$$\lambda_4^2-\lambda_1\lambda_5=0 \tag{38}$$

and the $\hat{P}$ matrix

$$\begin{pmatrix} 12\lambda_1 & 0 & 0 & 6\lambda_4 & 0 \\ 0 & 4\lambda_2 & 0 & 2\lambda_4 & 4\lambda_5 \\ 0 & 0 & 4\lambda_3 & 4\lambda_4 & 8\lambda_5 \\ 6\lambda_4 & 2\lambda_4 & 4\lambda_4 & 4\lambda_1\lambda_2\lambda_3+\lambda_1\lambda_3^2+2\lambda_3(4\lambda_2+\lambda_3)\lambda_4 & 2\lambda_3(4\lambda_2+\lambda_3)\lambda_4 \\ 0 & 4\lambda_5 & 8\lambda_5 & 2\lambda_3(4\lambda_2+\lambda_3)\lambda_4 & 4\lambda_3(4\lambda_2+\lambda_3)\lambda_5 \end{pmatrix}. \tag{39}$$

The conditions $\hat{P}(\lambda)\geqslant 0$ and rank $(\hat{P}(\lambda))=4$, added to (38), yield the following restrictions on the acceptable range for the λ's:

$$\begin{cases} \lambda_1,\lambda_2,\lambda_3\geqslant 0, \\ 0\leqslant\lambda_5<\lambda_2\lambda_3^2, \\ \lambda_1+\lambda_5>0. \end{cases} \tag{40}$$

The p's can be expressed in terms of the λ's in the following form:

$$p_1=(\lambda_1+3\lambda_2+3\lambda_3)/3,$$

$$p_2=(\lambda_1^2+6\lambda_1\lambda_2+9\lambda_2^2+14\lambda_1\lambda_3+18\lambda_2\lambda_3+9\lambda_3^2+24\lambda_4)/18,$$

$$p_3=(\lambda_1+3\lambda_2-3\lambda_3)^2/9,$$

$$p_4=(4\lambda_1^3-72\lambda_1^2\lambda_2+324\lambda_1\lambda_2^2-36\lambda_1^2\lambda_3+324\lambda_1\lambda_2\lambda_3+81\lambda_1\lambda_3^2$$
$$+108\lambda_1\lambda_4-972\lambda_2\lambda_4-486\lambda_3\lambda_4+729\lambda_5)/648,$$

$$p_5=(4\lambda_1^3-72\lambda_1^2\lambda_2+324\lambda_1\lambda_2^2+12\lambda_1^2\lambda_3-108\lambda_1\lambda_2\lambda_3+9\lambda_1\lambda_3^2 -36\lambda_1\lambda_4+324\lambda_2\lambda_4-54\lambda_3\lambda_4+81\lambda_5)/648, \tag{41}$$

$$p_6=(\lambda_1+3\lambda_2-3\lambda_3)(4\lambda_1^3-72\lambda_1^2\lambda_2+324\lambda_1\lambda_2^2-12\lambda_1^2\lambda_3+108\lambda_1\lambda_2\lambda_3 -27\lambda_1\lambda_3^2+36\lambda_1\lambda_4-324\lambda_2\lambda_4+162\lambda_3\lambda_4-243\lambda_5)/1944,$$

$$p_7=(\lambda_1+3\lambda_2-3\lambda_3)(4\lambda_1^3-72\lambda_1^2\lambda_2+324\lambda_1\lambda_2^2+12\lambda_1^2\lambda_3-108\lambda_1\lambda_2\lambda_3 +9\lambda_1\lambda_3^2-36\lambda_1\lambda_4+324\lambda_2\lambda_4-54\lambda_3\lambda_4+81\lambda_5)/1944,$$

$$p_8=(\lambda_1+3\lambda_2-3\lambda_3)^2(4\lambda_1^3-72\lambda_1^2\lambda_2+324\lambda_1\lambda_2^2-12\lambda_1^2\lambda_3+108\lambda_1\lambda_2\lambda_3 -27\lambda_1\lambda_3^2+36\lambda_1\lambda_4-324\lambda_2\lambda_4+162\lambda_3\lambda_4-243\lambda_5)/5832,$$

$$p_9=(\lambda_1+3\lambda_2-3\lambda_3)^3(4\lambda_1^3-72\lambda_1^2\lambda_2+324\lambda_1\lambda_2^2-36\lambda_1^2\lambda_3+324\lambda_1\lambda_2\lambda_3 +81\lambda_1\lambda_3^2+108\lambda_1\lambda_4-972\lambda_2\lambda_4-486\lambda_3\lambda_4+729\lambda_5)/17\,496.$$

For values of the λ's satisfying (38) and (40), the values of the p's defined in (41) render $\hat{P}(p)$ everywhere positive semidefinite and of rank four. We can conclude, therefore, that they yield parametric equations for the four-dimensional (4D) stratum $\hat{S}^{(4,1)}$. Being the continuous image of a connected set, the stratum is *connected*.

For $\lambda_1\neq 0$ $[\lambda_5\neq 0]$, the syzygy can be solved with respect to $\lambda_5[\lambda_1]$ and the expression one obtains can be substituted into (41), so, in this region, $(\lambda_1,\ldots,\lambda_4)[(\lambda_2,\ldots,\lambda_5)]$ play the role of local coordinates for the manifold underlying the stratum. Since, owing to (40), λ_1 and λ_5 cannot vanish simultaneously, the whole stratum is covered by two rational charts of local coordinates.

The elimination of the parameters λ from (41) and (40) leads to cumbersome relations, which are not worth writing down.

D. Stratum $\hat{S}^{(4,2)}$

The stabilizer in G of the isotropy subgroup $H=G^{(4,2)}=\langle C_{2z}\rangle$, is the group $\mathrm{Stab}(H)=\mathbf{O}_2^z\times\mathbf{U}_1$.

The space V_H is defined by the equations $x_i=0$, $i=3,4,8,9$. The transformation properties of the coordinates, x_i, $i=1, 2, 5, 6, 7, 10$ of V_H can be put in the following advantageous form. Let us define

$$\eta_1=x_5+ix_{10},\quad \eta_2=\frac{x_7+ix_6+i(x_2+ix_1)}{\sqrt{2}},\quad \eta_3=\frac{x_7+ix_6-i(x_2+ix_1)}{\sqrt{2}}, \tag{42}$$

then,

(i) under a proper rotation, $O_2^z(\phi)$: $(\eta_1,\eta_2,\eta_3)\to(\eta_1,e^{-2i\phi},e^{-2i\phi}\eta_3)$;
(ii) under a gauge transformation, $U_1(\phi)$: $(\eta_1,\eta_2,\eta_3)\to(e^{i\phi}\eta_1,e^{-i\phi}\eta_2,e^{i\phi}\eta_3)$;
(iii) under a transformation C_{2x}: $(\eta_1,\eta_2,\eta_3)\to(\eta_1,\eta_3^*,\eta_2^*)$;
(iv) under time reversal $\mathcal{T}$: $(\eta_1,\eta_2,\eta_3)\to(\eta_1^*,-\eta_3,-\eta_2)$.

A minimal IB of $\tilde{H}$, which is coregular, can be chosen to be

$$\lambda_1=\Sigma_{j=1}^3|\eta_j|^2=x_1^2+x_2^2+x_5^2+x_6^2+x_7^2+x_{10}^2,$$

$$\lambda_2=|\eta_1|^2=x_5^2+x_{10}^2, \tag{43}$$

$$\lambda_3=(|\eta_2|^2-|\eta_3|^2)^2/4=(x_2x_6-x_1x_7)^2,$$

$$\lambda_4=2\Re(\eta_1^2\eta_2\eta_3^*)=-x_1^2x_5^2-x_2^2x_5^2+x_5^2x_6^2+x_5^2x_7^2-4x_1x_5x_6x_{10}-4x_2x_5x_7x_{10}+x_1^2x_{10}^2+x_2^2x_{10}^2-x_6^2x_{10}^2-x_7^2x_{10}^2.$$

The $\hat{P}$ matrix relative to the IB $\{\lambda\}$ has the following form:

$$\hat{P}(\lambda)=4\begin{pmatrix}\lambda_1 & \lambda_2 & 2\lambda_3 & 2\lambda_4\\ \lambda_2 & \lambda_2 & 0 & \lambda_4\\ 2\lambda_3 & 0 & (\lambda_1-\lambda_2)\lambda_3 & 0\\ 2\lambda_4 & \lambda_4 & 0 & \lambda_2(\lambda_1^2-\lambda_1\lambda_2-4\lambda_3)\end{pmatrix}. \tag{44}$$

The conditions $\hat{P}(\lambda)>0$ and rank $(\hat{P}(p))=4$ yield the following restrictions on the acceptable values of the λ's:

$$\begin{cases}0<\lambda_2<\lambda_1\\ 0<4\lambda_3<(\lambda_1-\lambda_2)^2\\ \lambda_4^2<\lambda_2^2[(\lambda_1-\lambda_2)^2-4\lambda_3]\end{cases}. \tag{45}$$

The expressions of the p's in terms of the λ's turn out to be the following:

$$p_1=\lambda_1,$$

$$p_2=(3\lambda_1^2-2\lambda_1\lambda_2+2\lambda_2^2+12\lambda_3-2\lambda_4)/6,$$

$$p_3=\lambda_1^2-2\lambda_1\lambda_2+2\lambda_2^2-4\lambda_3-2\lambda_4,$$

$$p_4=\lambda_2(9\lambda_1^2-18\lambda_1\lambda_2+10\lambda_2^2-36\lambda_3+6\lambda_4)/6,$$

$$p_5=(5\lambda_1^2\lambda_2-14\lambda_1\lambda_2^2+10\lambda_2^3-4\lambda_2\lambda_3-4\lambda_1\lambda_4+6\lambda_2\lambda_4)/6, \tag{46}$$

$$p_6=(6\lambda_1^3\lambda_2-17\lambda_1^2\lambda_2^2+14\lambda_1\lambda_2^3-2\lambda_2^4-24\lambda_1\lambda_2\lambda_3+20\lambda_2^2\lambda_3-3\lambda_1^2\lambda_4+2\lambda_1\lambda_2\lambda_4+4\lambda_2^2\lambda_4+12\lambda_3\lambda_4-2\lambda_4^2)/6,$$

$$p_7=(4\lambda_1^3\lambda_2-11\lambda_1^2\lambda_2^2+6\lambda_1\lambda_2^3+2\lambda_2^4-16\lambda_1\lambda_2\lambda_3+28\lambda_2^2\lambda_3-5\lambda_1^2\lambda_4+10\lambda_1\lambda_2\lambda_4-4\lambda_2^2\lambda_4+4\lambda_3\lambda_4+2\lambda_4^2)/6,$$

$$p_8=(3\lambda_1^4\lambda_2+2\lambda_1^3\lambda_2^2-36\lambda_1^2\lambda_2^3+52\lambda_1\lambda_2^4-20\lambda_2^5-24\lambda_1^2\lambda_2\lambda_3-8\lambda_1\lambda_2^2\lambda_3+80\lambda_2^3\lambda_3+48\lambda_2\lambda_3^2-6\lambda_1^3\lambda_4+16\lambda_1^2\lambda_2\lambda_4-16\lambda_1\lambda_2^2\lambda_4+8\lambda_2^3\lambda_4+24\lambda_1\lambda_3\lambda_4-16\lambda_2\lambda_3\lambda_4-4\lambda_1\lambda_4^2+12\lambda_2\lambda_4^2)/6,$$

$$p_9=(33\lambda_1^4\lambda_2^2-132\lambda_1^3\lambda_2^3+168\lambda_1^2\lambda_2^4-72\lambda_1\lambda_2^5+4\lambda_2^6-264\lambda_1^2\lambda_2^2\lambda_3+528\lambda_1\lambda_2^3\lambda_3-144\lambda_2^4\lambda_3+528\lambda_2^2\lambda_3^2-9\lambda_1^4\lambda_4+36\lambda_1^3\lambda_2\lambda_4-60\lambda_1^2\lambda_2^2\lambda_4+48\lambda_1\lambda_2^3\lambda_4-12\lambda_2^4\lambda_4+72\lambda_1^2\lambda_3\lambda_4-144\lambda_1\lambda_2\lambda_3\lambda_4+96\lambda_2^2\lambda_3\lambda_4-144\lambda_3^2\lambda_4-12\lambda_1^2\lambda_4^2+24\lambda_1\lambda_2\lambda_4^2+12\lambda_2^2\lambda_4^2+48\lambda_3\lambda_4^2-4\lambda_4^3)/6.$$

In the range of values for the λ's defined in (45), the values of the p's defined in (46) render $\hat{P}(p)$ everywhere positive semidefinite and of rank four. We can conclude, therefore, that they yield parametric equations for the four dimensional stratum $\hat{S}^{(4,2)}$. Being the continuous image of a connected set, the stratum is *connected*.

The elimination of the parameters λ from (46) and (45) leads to cumbersome relations, which are not worthwhile writing down.

E. Principal stratum $\hat{S}^{(6,1)}$

Implicit equations for the principal stratum are yielded in $\mathbf{R}^9$ by the syzygies relating the invariants p_i, $i=1,...,9$, which can be easily obtained from the syzygies (B1)–(B5), using (15). At the points of $\hat{S}_p=\hat{S}^{(6,1)}$ the matrix $\hat{P}(p)$ has to be positive semidefinite and its rank has to be 6.

The method used for the singular strata does not help to obtain parametric equations for $\hat{S}_p$ and to attain the goal one has to resort to less elegant and more pedantic procedures. A possibility is to use the invariants of an IB of the subgroup $\mathbf{SO}_3$ of G as parameters in terms of which to express the p's, but in this case, great care has to be paid to the determination of the range of the parameters that render one-to-one correspondence with the points $p\in\hat{S}_p$.

The Mölien function for the subgroup $\mathbf{SO}_3$ of G can be obtained as a byproduct of the calculation of the Mölien function for G (see Appendix A):

$$M_{\mathbf{SO}_3}(\eta)=\frac{1+\eta^4+\eta^8}{(1-\eta^2)^3(1-\eta^3)^4}, \tag{47}$$

which, after multiplying numerator and denominator by $(1-\eta^4)$, becomes

$$M_{\mathbf{SO}_3}(\eta)=\frac{1-\eta^{12}}{(1-\eta^2)^3(1-\eta^3)^4(1-\eta^4)}. \tag{48}$$

Equations (47) and (48) indicate that a minimal IB for the subgroup $\mathbf{SO}_3$ of G is formed by eight invariants, with degrees (2, 2, 2, 3, 3, 3, 3, 4) related by only one syzygy of degree 12. A possible choice is the following:

$$\begin{aligned}
&\lambda_1=\mathrm{Tr}(\psi\psi^*), \quad \lambda_5=\Im[\mathrm{Tr}(\psi^3)],\\
&\lambda_2=\Re[\mathrm{Tr}(\psi^2)], \quad \lambda_6=\Re[\mathrm{Tr}(\psi^2\psi^*)],\\
&\lambda_3=\Im[\mathrm{Tr}(\psi^2)], \quad \lambda_7=\Im[\mathrm{Tr}(\psi^2\psi^*)],\\
&\lambda_4=\Re[\mathrm{Tr}(\psi^3)]), \quad \lambda_8=\mathrm{Tr}(\psi\psi^*\psi\psi^*).
\end{aligned} \tag{49}$$

Only the first seven elements of the basis are algebraically independent. The explicit expression of the syzygy relating the λ's is reported in Appendix B [see (B7)].

The $\hat{P}$ matrix relative to the IB $\{\lambda_1,\ldots,\lambda_8\}$ is the following and for values of the λ's satisfying the syzygy (B7), it has rank seven:

$$\hat{P}_{1i}=2d_i^{(\lambda)}\lambda_i, \quad d^{(\lambda)}=(2,2,2,3,3,3,3,4), \quad i=1,...,8,$$

$$\hat{P}_{22}=4\lambda_1, \quad \hat{P}_{45}=0,$$

$$\hat{P}_{23}=0, \quad \hat{P}_{46}=\tfrac{1}{2}(2\lambda_1\lambda_2+\lambda_2^2-\lambda_3^2),$$

$$\hat{P}_{24}=6\lambda_6, \quad \hat{P}_{47}=-(\lambda_1-\lambda_2)\lambda_3,$$

$$\hat{P}_{25}=6\lambda_7, \quad \hat{P}_{48}=2(2\lambda_1\lambda_4+\lambda_2\lambda_6-\lambda_3\lambda_7),$$

$$\hat{P}_{26}=2(\lambda_4+2\lambda_6), \quad \hat{P}_{55}=\tfrac{3}{4}(6\lambda_1^2-\lambda_2^2-\lambda_3^2-6\lambda_8),$$

$$\hat{P}_{27}=2(\lambda_5-2\lambda_7),\quad \hat{P}_{56}=(\lambda_1+\lambda_2)\lambda_3,$$

$$\hat{P}_{28}=4\lambda_1\lambda_2,\quad \hat{P}_{57}=\tfrac{1}{2}(2\lambda_1\lambda_2-\lambda_2^2+\lambda_3^2),$$

$$\hat{P}_{33}=4\lambda_1,\quad \hat{P}_{58}=2(2\lambda_1\lambda_5+\lambda_3\lambda_6+\lambda_2\lambda_7),$$

$$\hat{P}_{34}=-6\lambda_7,\quad \hat{P}_{66}=\tfrac{1}{12}(2\lambda_1^2+8\lambda_1\lambda_2+5\lambda_2^2+5\lambda_3^2+6\lambda_8),$$

$$\hat{P}_{35}=6\lambda_6,\quad \hat{P}_{67}=\tfrac{2}{3}\lambda_1\lambda_3,$$

$$\hat{P}_{36}=2(\lambda_5+2\lambda_7),\quad \hat{P}_{68}=-\tfrac{2}{3}(3\lambda_2\lambda_4+3\lambda_3\lambda_5-14\lambda_1\lambda_6+2\lambda_2\lambda_6+2\lambda_3\lambda_7),$$

$$\hat{P}_{37}=-2(\lambda_4-2\lambda_6),\quad \hat{P}_{77}=\tfrac{1}{12}(2\lambda_1^2-8\lambda_1\lambda_2+5\lambda_2^2+5\lambda_3^2+6\lambda_8),$$

$$\hat{P}_{38}=4\lambda_1\lambda_3,\quad \hat{P}_{78}=\tfrac{2}{3}(3\lambda_3\lambda_4-3\lambda_2\lambda_5-2\lambda_3\lambda_6+14\lambda_1\lambda_7+2\lambda_2\lambda_7),$$

$$\hat{P}_{44}=\tfrac{3}{4}(6\lambda_1^2-\lambda_2^2-\lambda_3^2-6\lambda_8),\quad \hat{P}_{88}=-\tfrac{8}{3}(3\lambda_1^3-2\lambda_4^2-2\lambda_5^2+2\lambda_6^2+2\lambda_7^2-9\lambda_1\lambda_8).\tag{50}$$

The connection between the p's and the λ's can be immediately obtained from their very definitions:

$$p_1=\lambda_1,$$

$$p_2=\lambda_8,$$

$$p_3=\lambda_2^2+\lambda_3^2,$$

$$p_4=\lambda_4^2+\lambda_5^2,$$

$$p_5=\lambda_6^2+\lambda_7^2,\tag{51}$$

$$p_6=\lambda_2\lambda_4\lambda_6+\lambda_3\lambda_5\lambda_6-\lambda_3\lambda_4\lambda_7+\lambda_2\lambda_5\lambda_7,$$

$$p_7=\lambda_2\lambda_6^2+2\lambda_3\lambda_6\lambda_7-\lambda_2\lambda_7^2,$$

$$p_8=\lambda_2^2\lambda_4\lambda_6-\lambda_3^2\lambda_4\lambda_6+2\lambda_2\lambda_3\lambda_5\lambda_6+2\lambda_2\lambda_3\lambda_4\lambda_7-\lambda_2^2\lambda_5\lambda_7+\lambda_3^2\lambda_5\lambda_7,$$

$$p_9=\lambda_2^3\lambda_4^2-3\lambda_2\lambda_3^2\lambda_4^2+6\lambda_2^2\lambda_3\lambda_4\lambda_5-2\lambda_3^3\lambda_4\lambda_5-\lambda_2^3\lambda_5^2+3\lambda_2\lambda_3^2\lambda_5^2.$$

As already noted, there is not one-to-one correspondence between the points $\lambda=(\lambda_1,\ldots,\lambda_8)$, lying on the surface determined by the syzygy (B7) and rendering positive semidefinite and of rank seven the $\hat{P}$ matrix associated with the integrity basis $\{\lambda\}$, and the points p of the principal stratum of $\mathbf{R}^{10}/G$. In fact, the action of the group G in $\mathbf{R}^{10}$ induces a linear action of G on the variables λ_i. With the definitions

$$\eta_1=\lambda_2+i\lambda_3,\quad \eta_2=\lambda_4+i\lambda_5,\quad \eta_3=\lambda_6+i\lambda_7,\tag{52}$$

the variables λ and η have the following transformation properties:

(i) λ_1 and λ_8 are invariant under the whole group;
(ii) under gauge transformations, $U_1(\phi)$: $(\eta_1,\eta_2,\eta_3)\rightarrow(e^{2i\phi}\eta_1,e^{3i\phi}\eta_2,e^{i\phi}\eta_3)$;
(iii) under time reversal $\mathcal{T}$: $(\eta_1,\eta_2,\eta_3)\rightarrow(\eta_1^*,\eta_2^*,\eta_3^*)$.

The one-to-one correspondence problem can be solved by finding a criterion enabling one to select a unique point in each orbit of the action of G in the λ space. To this end, let us make some preliminary remarks:

(i) A direct check shows that for $\eta_1=0$ and general values of η_2 and η_3 the rank of $\hat{P}(p(\lambda))$ is six.

(ii) Using (22) one easily realizes that $\mathrm{rank}(\hat{P}(p(\lambda)))<\mathrm{rank}(J(\lambda))<6$, for $\lambda_3=\lambda_5=\lambda_7=0$.

Now, let us choose any orbit, $\overline{\Omega}$, in the principal stratum of $\mathbf{R}^{10}/G$, i.e., a $\overline{p}\in\hat{S}_p$, and let $\overline{\lambda}$ be such that $p(\overline{\lambda})=\overline{p}$. At least one of the parameters $\overline{\eta}_i$, $i=1, 2, 3$, has to be different from zero. Let us say that $\overline{\eta}_i$, is the first one, in lexicographic order (in a lexicographic ordering, $(v_1,\ldots,v_k)>(v_1',\ldots,v_k')$ means that the first nonvanishing component v_i-v_i', $i=1,\ldots,k$, is positive). Then, on $\overline{\Omega}$ there will be a point $\overline{\lambda}'$, such that $\overline{\eta}_i'$ is real and positive; this point can be attained from $\overline{\lambda}$ by means of a convenient gauge transformation. Since at least a $\overline{\eta}_j$, $j=1, 2, 3$, has to be $\neq 0$, this means $\overline{\imath}<3$. At this point we still have at our disposal time reversal transformations to fix the sign of the imaginary part of one of the $\overline{\eta}_i, i>\overline{\imath}$ [recall that at least one of the $\Im(\overline{\eta}_j)$ has to be $\neq 0$]. So, if $\overline{J}$ is such that $\Im(\overline{\eta}_{\overline{J}})$ is the first (in lexicographic order) nonvanishing imaginary part of the $\overline{\eta}$'s, we can choose $\Im(\overline{\eta}_{\overline{J}})>0$.

After introducing a lexicographic order in the real vector spaces generated by the vectors formed, respectively, with the real and imaginary parts of the η's, the criterion that we have devised can be resumed in the following simple additional conditions on these vectors:

$$\lambda_3=0,\quad (\lambda_2,\lambda_4,\lambda_6)>0,\quad (\lambda_3,\lambda_5,\lambda_7)>0,\quad \lambda_5=0 \ \text{ for } \ \lambda_2=0. \tag{53}$$

Using these conditions, the expressions (51) of the p's can be simplified as follows:

$$\begin{gathered} p_1=\lambda_1,\quad p_6=\lambda_2(\lambda_4\lambda_6+\lambda_5\lambda_7),\\ p_2=\lambda_8,\quad p_7=\lambda_2(\lambda_6^2-\lambda_7^2),\\ p_3=\lambda_2^2,\quad p_8=\lambda_2^2(\lambda_4\lambda_6-\lambda_5\lambda_7),\\ p_4=\lambda_4^2+\lambda_5^2,\quad p_9=\lambda_3(\lambda_4^2-\lambda_5^2),\\ p_5=\lambda_6^2+\lambda_7^2, \end{gathered} \tag{54}$$

where the λ's are required to satisfy the syzygy (B7), the conditions rendering the matrix $\hat{P}(p)$ positive semidefinite and of rank six and $(\lambda_5,\lambda_7)>0$.

VI. AN EXAMPLE: MINIMA OF A GENERAL FOURTH DEGREE LANDAU POLYNOMIAL

As a simple example, we have also calculated the minimum of a general fourth degree polynomial free energy

$$\hat{\Phi}^{(4)}(p)=\frac{\alpha_0}{2}p_1^2+\sum_{j=1}^{3}\alpha_j p_j,\quad \alpha_i\in\mathbf{R},\quad i=0,\ldots,3, \tag{55}$$

with the additional assumptions that it is bounded below and has a local maximum at the origin $(\alpha_1<0)$. In (55) the α's are phenomenological parameters.

Recalling the definition $\tilde{p}_i=p_i/p_1^{d_i/2}$, the polynomial $\hat{\Phi}^{(4)}(p)$ can be put in the following form:

TABLE V. Absolute minimum, $\hat{\Phi}^{(4)}_{\min}=-\alpha_1^2/(2\delta)$, of a general, bounded below, *G*-invariant fourth degree polynomial, $\hat{\Phi}^{(4)}(\alpha,p)=\alpha_0 p_1^2/2+\Sigma_{j=1}^3\,\alpha_j p_j$, $\alpha_1<0$, and hosting strata, $S^{(d,r)}$, as functions of the coefficients α. The denomination of the strata is the same as in Table III.

α range	δ	(d,r)
$\mathcal{R}_1$: Max$(0-3\alpha_0/2,-6\alpha_3)<\alpha_2$	$\alpha_0+2\alpha_2/3$	(1,4)
$\mathcal{R}_2$: $-6\alpha_3>\alpha_2>$Max$(-\alpha_0-2\alpha_3,2\alpha_3)$	$\alpha_0+\alpha_2+2\alpha_3$	(1,2), (1,3), (2,4)
$\mathcal{R}_3$: $-\alpha_0/2<\alpha_2<$Min$(0,2\alpha_3)$	$\alpha_0+2\alpha_2$	(1,1)
$\mathcal{R}_{13}$: $0=\alpha_2<$Min(α_0,α_3)	α_0	(1,1), (1,4), (1,5), (2,1), (3,1), (4,1)
$\mathcal{R}_{12}$: Max$(-3\alpha_0/2,0)<\alpha_2=-6\alpha_3$	$\alpha_0-4\alpha_3$	(1,2), (1,3), (1,4), (2,3), (2,4), (3,2)
$\mathcal{R}_{23}$: $-\alpha_0/2<\alpha_2=2\alpha_3<0$	$\alpha_0+4\alpha_3$	(1,1), (1,2), (1,3), (2,4), (2,5)
$\mathcal{R}_{123}$: $\alpha_2=\alpha_3=0<\alpha_0$	α_0	All, except (0,1)

$$\hat{\Phi}^{(4)}(p)=\frac{p_1^2}{2}\Delta+\alpha_1 p_1, \tag{56}$$

where we have defined

$$\Delta=\alpha_0+2\alpha_2\tilde{p}_2+2\alpha_3\tilde{p}_3. \tag{57}$$

Since, owing to its definition (14), p_1 ranges over the whole non-negative real numbers, in the orbit space, the polynomial $\hat{\Phi}^{(4)}(p)$ is bounded below (in the assumption $\alpha_1<0$) if and only if the minimum of Δ, δ, evaluated in the section $p_1=1$ of the orbit space, is positive. Being the minimum of the right-hand side of (56), thought of as a function only of $p_1\geqslant 0$, equal to $-\alpha_1/(2\Delta)$, the absolute minimum of $\hat{\Phi}^{(4)}(p)|_{p\in S}$ is $-\alpha_1^2/(2\delta)$. In this way, the determination of the minimum of $\hat{\Phi}^{(4)}(p)$ is reduced to the calculation of δ.

The absolute minimum of δ in each singular stratum can be easily computed using the equations of the strata. For the principal stratum the determination of the minimum of the restriction of $\hat{\Phi}^{(4)}$ to the surface $p_1=1$ as a constrained minimum is difficult and it is easier to solve Eq. (2) and to check subsequently if the solutions lie in the principal stratum. A comparison of the values of the minima in the different strata, in order to determine the absolute minimum, leads to the results summarized in Table V and illustrated in Fig. 2, where the denomination of the strata introduced in the text has been used. Owing to the low degree of the polynomial defining $\hat{\Phi}^{(4)}\times(p)$ in (55), and the consequent low number of free parameters α, the absolute minimum exhibits strong degeneracy, particularly for special values of the α's. If these special values are excluded, spontaneous breaking of the symmetry can generate only five distinct phases out of fifteen permitted in the *G*-symmetry; some of them are unstable. For no nontrivial values of (α_2,α_3) does the absolute minimum lie on the stratum $S^{(2,2)}$.

For general values of the α's, our results are in agreement with Mermin's ones.[11] Let us add a few words about the perturbative stability of the three degenerate phases in the region $\mathcal{R}_2$ (see Table V). For $(\alpha_0,\alpha_2,\alpha_3)\in\mathcal{R}_2$, the addition to the free energy, $\Phi^{(4)}$, of a ''small'' perturbation, consisting in an invariant polynomial of degree six:

$$\Theta^{(6)}=\alpha_4 p_4+\alpha_5 p_5, \tag{58}$$

splits the three degenerate minima determined by the fourth degree term.[23] This is easy to check, at least in the additional assumption that the perturbation leaves the absolute minimum in one of the strata corresponding to the degenerate phases. In fact, at the first perturbative order, one obtains from Tables I and II the following shifts, $\Theta^{(6)}_{(d,r)}$, in the values of the sixth-order free energy at the points where $\Phi^{(4)}(p)$ takes on its degenerate absolute minimum under consideration:

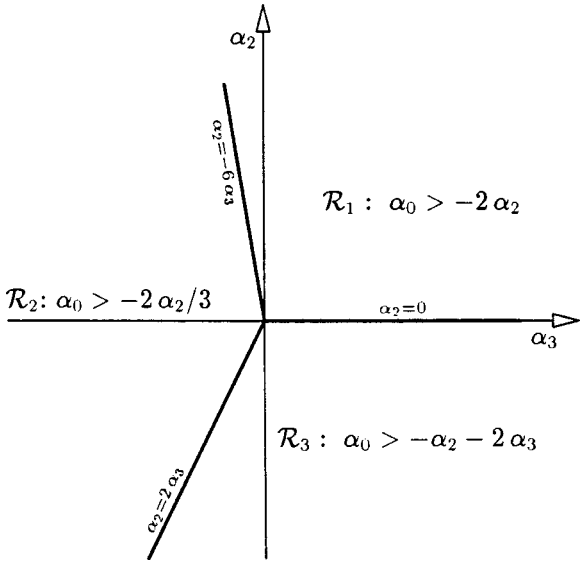

FIG. 2. Localization of the absolute minimum of a fourth degree G-invariant polynomial, $\hat{\Phi}^{(4)}(\alpha,p)=\alpha_0 p_1^2/2+\Sigma_{j=1}^{3}\alpha_j p_j$, $\alpha_1<0$, as a function of its coefficients. For values of $(\alpha_0,\alpha_2,\alpha_3)$ in $\mathcal{R}_1$ or in $\mathcal{R}_2$ or in $\mathcal{R}_3$, the absolute minimum lies, respectively, in the strata $S^{(1,4)}$ or $\{S^{(1,2)},S^{(1,3)},S^{(2,4)}\}$ (degenerate minimum) or $S^{(1,1)}$. For particular values of the α's, see Table IV.

$$\Theta^{(6)}_{(1,2)}=\frac{\alpha_1^3}{\delta^3}\,\frac{\alpha_4+\alpha_5}{6},\quad \Theta^{(6)}_{(1,3)}=0,\quad \Theta^{(6)}_{(2,4)}=\frac{\alpha_1^3}{\delta^3}(\alpha_4+\alpha_5)\xi, \tag{59}$$

where $0<\xi<1/6$.

Since $-\alpha_1/\delta>0$, the absolute minimum will be perturbatively stable on $\hat{S}^{(1,2)}$ or, respectively, $\hat{S}^{(1,3)}$, depending on whether $\alpha_4+\alpha_5$ is negative or positive.

As stressed in Sec. I, the above-mentioned difficulties can be overcome if one puts less restrictive upper limits to the degree of the polynomial describing the free energy. It is trivial, for instance, to realize that the following class of bounded below polynomial functions[16] have a vanishing maximum at the origin of $\mathbf{R}^{10}$ and display an absolute minimum at the arbitrarily chosen point $\overline{p}\in\hat{S}$:

$$\sum_{i=1}^{9}\alpha_i[(p_i-\overline{p}_i)^{2n_i}-\overline{p}_i^{2n_i}], \tag{60}$$

where the α's are positive constants and the n's are positive integers.

The physical implications of our results and the derivation of a more realistic form of the free energy will be discussed in forthcoming papers. We shall limit ourselves, here, to note that, the D-wave content in terms, e.g., of d- or extended s-waves (mentioned in Sec. I) can be directly read off the fourth column of Table III for each of the possible symmetry phases of the system under consideration.

VII. CONCLUSIONS

Through a detailed and rigorous analysis, we have determined and characterized the possible ground states of D-wave condensates in isotropic space, which are relevant both in high T_c superconductivity and in ^{3}He phase transitions. The problem has been formulated and solved in the framework of geometric invariant theory, which, as noted long ago,[14] is the natural mathemati-

cal setting in which to deal with minimization of invariant potentials, which are plagued by degeneracy problems. This enabled us to complete and/or correct results previously obtained by other authors, using different methods.

Until now, the kind of approach we have used had only been applied to relatively simple models, with coregular symmetry groups, in condensed matter[24] and in elementary particle physics.[25] In this paper, we have fully characterized the geometry of the orbit space of the linear group $\mathbf{SO}_3 \otimes \mathbf{U}_1 \times \langle \mathcal{T} \rangle$, acting in the space $\mathbf{R}^{10}$, a highly nontrivial group, with a noncoregular minimal integrity basis, formed by nine elements with degrees up to 12. For this group we have determined the explicit form of the elements of an integrity basis and of the syzygies relating these elements, the equations and inequalities determining the orbit space and its stratification and the corresponding isotropy subgroups chains. The minima of a general fourth degree polynomial invariant free energy have been recalculated and the sixth degree polynomial perturbative corrections to its absolute minimum have been determined. Some of our conclusions have been compared with previous results obtained by other authors.

To overcome some computational difficulties in the full characterization of the stratification of the orbit space, difficulties originating from the high dimensionality of the problem, we had to devise a sophisticated procedure, allowing us to obtain *rational* parametric equations also for the higher dimensional singular strata. The procedure is absolutely general and is reminiscent, but in a different context and in higher dimensions, of classical techniques for parametrizing plane algebraic curves.[26]

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APPENDIX A: CALCULATION OF MÖLIEN FUNCTIONS

In this Appendix, we shall explicitly calculate the two integrals, I_1 and I_2, appearing in the expression of $M_G(\eta)$ [see (9)]:

$$I_1 = \frac{1}{32\pi^3} \int_0^{2\pi} \mathrm{d}\phi_1 \int_0^{2\pi} \mathrm{d}\phi_2 \int_0^{\pi} \sin\theta \, \mathrm{d}\theta \int_0^{2\pi} \frac{\mathrm{d}\alpha}{f_1(\cos\chi, \alpha)},$$

$$I_2 = \frac{1}{16\pi^2} \int_0^{2\pi} \mathrm{d}\phi_1 \int_0^{2\pi} \mathrm{d}\phi_2 \int_0^{\pi} \frac{\sin\theta \, \mathrm{d}\theta}{f_2(\cos\chi)}, \tag{A1}$$

where

$$f_1(\cos\chi, \alpha) = \prod_{k=-2}^{2} [(1 - \eta e^{i(k\chi + \alpha)})(1 - \eta e^{i(k\chi - \alpha)})],$$

$$f_2(\cos\chi) = \prod_{k=-2}^{2} [(1 - \eta e^{ik\chi})(1 + \eta e^{ik\chi})] \tag{A2}$$

and $\cos\chi$ is defined in (10).

Using as new integration variables ϕ_2, $u = \cos(\phi_1 + \phi_2)$, and $v = \cos\chi$, the integral over ϕ_2 can be immediately performed and one remains with

$$
\begin{aligned}
I_1 &= \frac{1}{2\pi^2}\int_0^{2\pi} d\alpha \int_{-1}^{1} \frac{dv}{f_1(v,\alpha)} \int_v^1 \frac{du}{(1+u)\sqrt{1-u^2}} \\
&= \frac{1}{2\pi^2}\int_0^{2\pi} d\alpha \int_{-1}^{1} \frac{dv}{f_1(v,\alpha)} \frac{\sqrt{1-v^2}}{1+v} \\
&= \frac{1}{2\pi^2}\int_0^{2\pi} d\alpha \int_0^{2\pi} d\chi \frac{\sin^2(\chi/2)}{f_1(\cos\chi,\alpha)}
\end{aligned} \tag{A3}
$$

and, analogously,

$$
I_2 = \frac{1}{\pi}\int_0^{2\pi} d\chi \frac{\sin^2(\chi/2)}{f_2(\cos\chi)}. \tag{A4}
$$

After defining

$$
\zeta_1 = e^{i\chi}, \quad \zeta_2 = e^{i\alpha}, \tag{A5}
$$

the remaining integrals can be conveniently thought of as integrals on unit circles of complex planes of the variables ζ_1 and ζ_2,

$$
\begin{aligned}
I_1 &= -\frac{1}{8\pi^2\eta^4} \oint \frac{d\zeta_2}{(\zeta_2-\eta)(\zeta_2\eta-1)} \oint d\zeta_1 F_1(\zeta_1,\zeta_2,\eta), \\
I_2 &= \frac{1}{4\pi i\eta^4(\eta^2-1)} \oint d\zeta_1 F_2(\zeta_1,\eta),
\end{aligned} \tag{A6}
$$

where

$$
\begin{aligned}
&F_1(\zeta_1,\zeta_2,\eta) \\
&= \frac{\zeta_1^4(\zeta_1-1)^2}{\left(\zeta_1^2-\frac{\eta}{\zeta_2}\right)(\zeta_1^2-\zeta_2\eta)\left(\zeta_1-\frac{\eta}{\zeta_2}\right)(\zeta_1-\zeta_2\eta)\left(\zeta_1-\frac{\zeta_2}{\eta}\right)\left(\zeta_1-\frac{1}{\zeta_2\eta}\right)\left(\zeta_1^2-\frac{\zeta_2}{\eta}\right)\left(\zeta_1^2-\frac{1}{\zeta_2\eta}\right)},
\end{aligned} \tag{A7}
$$

$$
F_2(\zeta_1,\eta) = \frac{\zeta_1^4(\zeta_1-1)^2}{(\zeta_1^2-\eta^2)(\zeta_1^4-\eta^2)\left(\zeta_1^2-\frac{1}{\eta^2}\right)\left(\zeta_1^4-\frac{1}{\eta^2}\right)}.
$$

Using the Cauchy theorem and recalling that $|\eta|<1$, the calculation reduces to a computation of residues at the internal poles to the unit circles. So, one ends up with the following expressions for I_1 and I_2:

$$
\begin{aligned}
I_1 &= \frac{1+3\eta^8+2\eta^{10}+3\eta^{12}+\eta^{20}}{2(1-\eta^2)^3(1-\eta^4)^2(1-\eta^8)(1-\eta+\eta^2)^2(1+\eta+\eta^2)^2}, \\
I_2 &= \frac{1-\eta^2+\eta^4}{2(1-\eta^2)^3(1-\eta^4)(1-\eta+\eta^2)(1+\eta+\eta^2)}.
\end{aligned} \tag{A8}
$$

The sum of I_1 and I_2 gives to the expression of $M_G(\eta)$ reported in (11).

As a by-product of the calculation, one finds also the following expression for the Mölien function of the subgroup $\mathbf{SO}_3$ of G:

$$M_{\mathbf{SO}_3}(\eta)=\frac{1}{8\pi^2}\int_0^{2\pi}\mathrm{d}\phi_1\int_0^{2\pi}\mathrm{d}\phi_2\int_0^{\pi}\mathrm{d}\theta\sin\theta f_1(\cos\chi,0)$$
$$=-\frac{1}{4\pi i\,\eta^4(1-\eta^2)}\oint\mathrm{d}\zeta_1 F_1(\zeta_1,1,\eta)$$
$$=\frac{1+\eta^4+\eta^8}{(1-\eta^2)^3(1-\eta^3)^4}. \tag{A9}$$

APPENDIX B: SYZYGIES

1. Explicit form of the syzygies for the group *G*

The ten elements of the nonminimal IB $\{\xi,\theta\}$ defined in (14) and (15) are related by the following syzygies:

$$\theta_1^2=\tfrac{1}{192}[36\xi_1^6\xi_3-144\xi_1^4\xi_2\xi_3+180\xi_1^2\xi_2^2\xi_3-72\xi_2^3\xi_3-36\xi_1^4\xi_3^2+108\xi_1^2\xi_2\xi_3^2-72\xi_2^2\xi_3^2+9\xi_1^2\xi_3^3$$
$$-18\xi_2\xi_3^3-80\xi_1^3\xi_3\xi_4+144\xi_1\xi_2\xi_3\xi_4+24\xi_1\xi_3^2\xi_4+48\xi_3\xi_4^2+144\xi_1^3\xi_3\xi_5-144\xi_1\xi_2\xi_3\xi_5$$
$$+72\xi_1\xi_3^2\xi_5-288\xi_3\xi_4\xi_5-144\xi_3\xi_5^2-96\xi_1^2\xi_3\xi_6-24\xi_3^2\xi_6+192\xi_6^2$$
$$+24\theta_1(8\xi_1^2-12\xi_2-\xi_3)\xi_3+96\theta_2(\xi_1\xi_3-4\xi_5)-16\theta_3\xi_3], \tag{B1}$$

$$\theta_1\theta_2=-\tfrac{1}{2}(\xi_3\xi_4\xi_6+\theta_1\xi_3\xi_4-2\theta_2\xi_6+2\theta_3\xi_5), \tag{B2}$$

$$\theta_2^2=\tfrac{1}{768}[-36\xi_1^6\xi_3^2+144\xi_1^4\xi_2\xi_3^2-180\xi_1^2\xi_2^2\xi_3^2+72\xi_2^3\xi_3^2+36\xi_1^4\xi_3^3-108\xi_1^2\xi_2\xi_3^3+72\xi_2^2\xi_3^3-9\xi_1^2\xi_3^4$$
$$+18\xi_2\xi_3^4+80\xi_1^3\xi_3^2\xi_4-144\xi_1\xi_2\xi_3^2\xi_4-24\xi_1\xi_3^3\xi_4-48\xi_3^2\xi_4^2-44\xi_1^3\xi_3^2\xi_5+144\xi_1\xi_2\xi_3^2\xi_5$$
$$-72\xi_1\xi_3^3\xi_5+1056\xi_3^2\xi_4\xi_5+144\xi_3^2\xi_5^2+96\xi_1^2\xi_3^2\xi_6+24\xi_3^3\xi_6-384\xi_3\xi_6^2+24\theta_1\xi_3$$
$$\times(-8\xi_1^2\xi_3+12\xi_2\xi_3+\xi_3^2-16\xi_6)-96\theta_2\xi_3(\xi_1\xi_3-4\xi_5)+16\theta_3(\xi_3^2+24\xi_6)-384\theta_4], \tag{B3}$$

$$\theta_2\theta_3=\tfrac{1}{128}[-36\xi_1^7\xi_3^2+144\xi_1^5\xi_2\xi_3^2-180\xi_1^3\xi_2^2\xi_3^2+72\xi_1\xi_2^3\xi_3^2+36\xi_1^5\xi_3^3-108\xi_1^3\xi_2\xi_3^3+72\xi_1\xi_2^2\xi_3^3$$
$$-9\xi_1^3\xi_3^4+18\xi_1\xi_2\xi_3^4+144\xi_1^6\xi_3\xi_4-576\xi_1^4\xi_2\xi_3\xi_4+720\xi_1^2\xi_2^2\xi_3\xi_4-288\xi_2^3\xi_3\xi_4-64\xi_1^4\xi_3^2\xi_4$$
$$+288\xi_1^2\xi_2\xi_3^2\xi_4-288\xi_2^2\xi_3^2\xi_4+12\xi_1^2\xi_3^3\xi_4-72\xi_2\xi_3^3\xi_4-320\xi_1^3\xi_3\xi_4^2+576\xi_1\xi_2\xi_3\xi_4^2$$
$$+48\xi_1\xi_3^2\xi_4^2+192\xi_3\xi_4^3+144\xi_1^6\xi_3\xi_5-576\xi_1^4\xi_2\xi_3\xi_5+720\xi_1^2\xi_2^2\xi_3\xi_5-288\xi_2^3\xi_3\xi_5$$
$$-288\xi_1^4\xi_3^2\xi_5+576\xi_1^2\xi_2\xi_3^2\xi_5-288\xi_2^2\xi_3^2\xi_5-36\xi_1^2\xi_3^3\xi_5-72\xi_2\xi_3^3\xi_5+256\xi_1^3\xi_3\xi_4\xi_5$$
$$+1440\xi_1\xi_3^2\xi_4\xi_5-960\xi_3\xi_4^2\xi_5+576\xi_1^3\xi_3\xi_5^2-576\xi_1\xi_2\xi_3\xi_5^2+432\xi_1\xi_3^2\xi_5^2-4800\xi_3\xi_4\xi_5^2$$
$$-576\xi_3\xi_5^3+96\xi_1^3\xi_3^2\xi_6+24\xi_1\xi_3^3\xi_6+384\xi_1^2\xi_3\xi_4\xi_6-1152\xi_2\xi_3\xi_4\xi_6-192\xi_3^2\xi_4\xi_6$$
$$-384\xi_1^2\xi_3\xi_5\xi_6-96\xi_3^2\xi_5\xi_6-384\xi_1\xi_3\xi_6^2+1536\xi_4\xi_6^2+1536\xi_5\xi_6^2-24\theta_1$$
$$\times(8\xi_1^3\xi_3^2-12\xi_1\xi_2\xi_3^2-\xi_1\xi_3^3-32\xi_1^2\xi_3\xi_5+48\xi_2\xi_3\xi_5+4\xi_3^2\xi_5+16\xi_1\xi_3\xi_6+64\xi_4\xi_6$$
$$-64\xi_5\xi_6)+8\theta_2(36\xi_1^6-144\xi_1^4\xi_2+180\xi_1^2\xi_2^2-72\xi_2^3-36\xi_1^4\xi_3+108\xi_1^2\xi_2\xi_3-72\xi_2^2\xi_3$$
$$-3\xi_1^2\xi_3^2-18\xi_2\xi_3^2-80\xi_1^3\xi_4+144\xi_1\xi_2\xi_4+72\xi_1\xi_3\xi_4+48\xi_4^2+144\xi_1^3\xi_5-144\xi_1\xi_2\xi_5$$

$$+168\xi_1\xi_3\xi_5-480\xi_4\xi_5-336\xi_5^2-288\xi_1^2\xi_6+288\xi_2\xi_6)+16\theta_3(\xi_1\xi_3^2-4\xi_3\xi_4+96\xi_1^2\xi_5$$
$$-144\xi_2\xi_5-16\xi_3\xi_5+24\xi_1\xi_6)-384\theta_4\xi_1], \tag{B4}$$

$$\theta_3{}^2=\tfrac{1}{256}[-144\xi_1{}^8\xi_3{}^2+144\xi_1{}^6\xi_2\xi_3{}^2+1008\xi_1{}^4\xi_2{}^2\xi_3{}^2-1872\xi_1{}^2\xi_2{}^3\xi_3{}^2+864\xi_2{}^4\xi_3{}^2+108\xi_1{}^6\xi_3{}^3$$
$$+144\xi_1{}^4\xi_2\xi_3{}^3-1188\xi_1{}^2\xi_2{}^2\xi_3{}^3+936\xi_2{}^3\xi_3{}^3-144\xi_1{}^2\xi_2\xi_3{}^4+288\xi_2{}^2\xi_3{}^4-9\xi_1{}^2\xi_3\xi^5$$
$$+18\xi_2\xi_3{}^5+1728\xi_1{}^7\xi_3\xi_4-6912\xi_1{}^5\xi_2\xi_3\xi_4+8640\xi_1{}^3\xi_2{}^2\xi_3\xi_4-3456\xi_1\xi_2{}^3\xi_3\xi_4$$
$$-1408\xi_1{}^5\xi_3{}^2\xi_4+5568\xi_1{}^3\xi_2\xi_3{}^2\xi_4-5184\xi_1\xi_2{}^2\xi_3{}^2\xi_4+416\xi_1{}^3\xi_3{}^3\xi_4-1296\xi_1\xi_2\xi_3{}^3\xi_4$$
$$-24\xi_1\xi_3{}^4\xi_4-3840\xi_1{}^4\xi_3\xi_4{}^2+6912\xi_1{}^2\xi_2\xi_3\xi_4{}^2+960\xi_1{}^2\xi_3{}^2\xi_4{}^2-576\xi_2\xi_3{}^2\xi_4{}^2-48\xi_3{}^3\xi_4{}^2$$
$$+2304\xi_1\xi_3\xi_4{}^3+1728\xi_1{}^7\xi_3\xi_5-6912\xi_1{}^5\xi_2\xi_3\xi_5+8640\xi_1{}^3\xi_2{}^2\xi_3\xi_5-3456\xi_1\xi_2{}^3\xi_3\xi_5$$
$$-2304\xi_1{}^5\xi_3{}^2\xi_5+4032\xi_1{}^3\xi_2\xi_3{}^2\xi_5-1728\xi_1\xi_2{}^2\xi_3{}^2\xi_5-1584\xi_1\xi_2\xi_3{}^3\xi_5-72\xi_1\xi_3{}^4\xi_5$$
$$+3072\xi_1{}^4\xi_3\xi_4\xi_5+14\,976\xi_1{}^2\xi_3{}^2\xi_4\xi_5+3456\xi_2\xi_3{}^2\xi_4\xi_5+288\xi_3{}^3\xi_4\xi_5-11\,520\xi_1\xi_3\xi_4{}^2\xi_5$$
$$+6912\xi_1{}^4\xi_3\xi_5{}^2-6912\xi_1{}^2\xi_2\xi_3\xi_5{}^2+4032\xi_1{}^2\xi_3{}^2\xi_5{}^2+1728\xi_2\xi_3{}^2\xi_5{}^2+144\xi_3{}^3\xi_5{}^2$$
$$-57\,600\xi_1\xi_3\xi_4\xi_5{}^2-6912\xi_1\xi_3\xi_5{}^3+864\xi_1{}^6\xi_3\xi_6-3456\xi_1{}^4\xi_2\xi_3\xi_6+4320\xi_1{}^2\xi_2{}^2\xi_3\xi_6$$
$$-1728\xi_2{}^3\xi_3\xi_6-480\xi_1{}^4\xi_3{}^2\xi_6+3744\xi_1{}^2\xi_2\xi_3{}^2\xi_6-1728\xi_2{}^2\xi_3{}^2\xi_6+408\xi_1{}^2\xi_3{}^3\xi_6$$
$$-144\xi_2\xi_3{}^3\xi_6+24\xi_3{}^4\xi_6+2688\xi_1{}^3\xi_3\xi_4\xi_6-10\,368\xi_1\xi_2\xi_3\xi_4\xi_6-1344\xi_1\xi_3{}^2\xi_4\xi_6$$
$$-384\xi_3\xi_4{}^2\xi_6-1152\xi_1{}^3\xi_3\xi_5\xi_6-3456\xi_1\xi_2\xi_3\xi_5\xi_6+576\xi_1\xi_3{}^2\xi_5\xi_6-14\,592\xi_3\xi_4\xi_5\xi_6$$
$$-3456\xi_3\xi_5{}^2\xi_6-5376\xi_1{}^2\xi_3\xi_6{}^2-2304\xi_2\xi_3\xi_6{}^2-768\xi_3{}^2\xi_6{}^2+18\,432\xi_1\xi_4\xi_6{}^2$$
$$+18\,432\xi_1\xi_5\xi_6{}^2+6144\xi_6{}^3+8\theta_1(36\xi_1{}^6\xi_3-144\xi_1{}^4\xi_2\xi_3+180\xi_1{}^2\xi_2{}^2\xi_3-72\xi_2{}^3\xi_3$$
$$-132\xi_1{}^4\xi_3{}^2-36\xi_1{}^2\xi_2\xi_3{}^2+360\xi_2{}^2\xi_3{}^2-3\xi_1{}^2\xi_3{}^3+54\xi_2\xi_3{}^3+3\xi_3{}^4-80\xi_1{}^3\xi_3\xi_4$$
$$+144\xi_1\xi_2\xi_3\xi_4-24\xi_1\xi_3{}^2\xi_4+240\xi_3\xi_4{}^2+1296\xi_1{}^3\xi_3\xi_5-1872\xi_1\xi_2\xi_3\xi_5-72\xi_1\xi_3{}^2\xi_5$$
$$-864\xi_3\xi_4\xi_5-144\xi_3\xi_5{}^2-96\xi_1{}^2\xi_3\xi_6-864\xi_2\xi_3\xi_6-96\xi_3{}^2\xi_6-2304\xi_1\xi_4\xi_6+2304\xi_1\xi_5\xi_6$$
$$+768\xi_6{}^2)+96\theta_2(36\xi_1{}^7-144\xi_1{}^5\xi_2+180\xi_1{}^3\xi_2{}^2-72\xi_1\xi_2{}^3-36\xi_1{}^5\xi_3+108\xi_1{}^3\xi_2\xi_3$$
$$-72\xi_1\xi_2{}^2\xi_3+5\xi_1{}^3\xi_3{}^2-30\xi_1\xi_2\xi_3{}^2-\xi_1\xi_3{}^3-80\xi_1{}^4\xi_4+144\xi_1{}^2\xi_2\xi_4+72\xi_1{}^2\xi_3\xi_4+48\xi_1\xi_4{}^2$$
$$+144\xi_1{}^4\xi_5-144\xi_1{}^2\xi_2\xi_5+136\xi_1{}^2\xi_3\xi_5+48\xi_2\xi_3\xi_5+4\xi_3{}^2\xi_5-480\xi_1\xi_4\xi_5-336\xi_1\xi_5{}^2$$
$$-288\xi_1{}^3\xi_6+288\xi_1\xi_2\xi_6+16\xi_1\xi_3\xi_6+64\xi_4\xi_6-64\xi_5\xi_6)+16\theta_3(36\xi_1{}^6-144\xi_1{}^4\xi_2$$
$$+180\xi_1{}^2\xi_2{}^2-72\xi_2{}^3-36\xi_1{}^4\xi_3+108\xi_1{}^2\xi_2\xi_3-72\xi_2{}^2\xi_3+13\xi_1{}^2\xi_3{}^2-6\xi_2\xi_3{}^2+\xi_3{}^3$$
$$-80\xi_1{}^3\xi_4+144\xi_1\xi_2\xi_4-24\xi_1\xi_3\xi_4+48\xi_4{}^2+1296\xi_1{}^3\xi_5-1872\xi_1\xi_2\xi_5-72\xi_1\xi_3\xi_5$$
$$-480\xi_4\xi_5-336\xi_5{}^2+192\xi_1{}^2\xi_6-48\xi_3\xi_6)-512\theta_4(3\xi_1{}^2+9\xi_2+\xi_3)], \tag{B5}$$

$$\theta_4=\theta_1\theta_3. \tag{B6}$$

2. Explicit form of the syzygy for the rotation subgroup of *G*

The invariants $\lambda_1,\ldots,\lambda_8$ of the subgroup $\mathbf{SO}_3$ of G, defined in (49), satisfy the following syzygy:

$$
\begin{aligned}
\lambda_8^3=\tfrac{1}{72}(&36\lambda_1{}^6-36\lambda_1{}^4\lambda_2{}^2+9\lambda_1{}^2\lambda_2{}^4-36\lambda_1{}^4\lambda_3{}^2+18\lambda_1{}^2\lambda_2{}^2\lambda_3{}^2+9\lambda_1{}^2\lambda_3{}^4-80\lambda_1{}^3\lambda_4{}^2\\
&+24\lambda_1\lambda_2{}^2\lambda_4{}^2-16\lambda_2{}^3\lambda_4{}^2+24\lambda_1\lambda_3{}^2\lambda_4{}^2+48\lambda_2\lambda_3{}^2\lambda_4{}^2+48\lambda_4{}^4-96\lambda_2{}^2\lambda_3\lambda_4\lambda_5\\
&+32\lambda_3{}^3\lambda_4\lambda_5-80\lambda_1{}^3\lambda_5{}^2+24\lambda_1\lambda_2{}^2\lambda_5{}^2+16\lambda_2{}^3\lambda_5{}^2+24\lambda_1\lambda_3{}^2\lambda_5{}^2-48\lambda_2\lambda_3{}^2\lambda_5{}^2\\
&+96\lambda_4{}^2\lambda_5{}^2+48\lambda_5{}^4+96\lambda_1{}^2\lambda_2\lambda_4\lambda_6+96\lambda_1\lambda_2{}^2\lambda_4\lambda_6-48\lambda_2{}^3\lambda_4\lambda_6-96\lambda_1\lambda_3{}^2\lambda_4\lambda_6\\
&-48\lambda_2\lambda_3{}^2\lambda_4\lambda_6+96\lambda_1{}^2\lambda_3\lambda_5\lambda_6+192\lambda_1\lambda_2\lambda_3\lambda_5\lambda_6-48\lambda_2{}^2\lambda_3\lambda_5\lambda_6-48\lambda_3{}^2\lambda_5\lambda_6\\
&+144\lambda_1{}^3\lambda_6{}^2-288\lambda_1{}^2\lambda_2\lambda_6{}^2+72\lambda_1\lambda_2{}^2\lambda_6{}^2+72\lambda_1\lambda_3{}^2\lambda_6{}^2-288\lambda_4{}^2\lambda_6{}^2-288\lambda_5{}^2\lambda_6{}^2\\
&+384\lambda_4\lambda_6{}^3-144\lambda_6{}^4-96\lambda_1{}^2\lambda_3\lambda_4\lambda_7+192\lambda_1\lambda_2\lambda_3\lambda_4\lambda_7+48\lambda_2{}^2\lambda_3\lambda_4\lambda_7+48\lambda_3{}^3\lambda_4\lambda_7\\
&+96\lambda_1{}^2\lambda_2\lambda_5\lambda_7-96\lambda_1\lambda_2{}^2\lambda_5\lambda_7-48\lambda_2{}^3\lambda_5\lambda_7+96\lambda_1\lambda_3{}^2\lambda_5\lambda_7-48\lambda_2\lambda_3{}^2\lambda_5\lambda_7\\
&-576\lambda_1{}^2\lambda_3\lambda_6\lambda_7+1152\lambda_5\lambda_6{}^2\lambda_7+144\lambda_1{}^3\lambda_7{}^2+288\lambda_1{}^2\lambda_2\lambda_7{}^2+72\lambda_1\lambda_2{}^2\lambda_7{}^2+72\lambda_1\lambda_3{}^2\lambda_7{}^2\\
&-288\lambda_4{}^2\lambda_7{}^2-288\lambda_5{}^2\lambda_7{}^2-1152\lambda_4\lambda_6\lambda_7{}^2-288\lambda_6{}^2\lambda_7{}^2-384\lambda_5\lambda_7{}^3-144\lambda_7{}^4-144\lambda_1{}^4\lambda_8\\
&+108\lambda_1{}^2\lambda_2{}^2\lambda_8-18\lambda_2{}^4\lambda_8+108\lambda_1{}^2\lambda_3{}^2\lambda_8-36\lambda_2{}^2\lambda_3{}^2\lambda_8-18\lambda_3{}^4\lambda_8+144\lambda_1\lambda_4{}^2\lambda_8\\
&+144\lambda_1\lambda_5{}^2\lambda_8-288\lambda_2\lambda_4\lambda_6\lambda_8-288\lambda_3\lambda_5\lambda_6\lambda_8-144\lambda_1\lambda_6{}^2\lambda_8+288\lambda_2\lambda_6{}^2\lambda_8\\
&+288\lambda_3\lambda_4\lambda_7\lambda_8-288\lambda_2\lambda_5\lambda_7\lambda_8+576\lambda_3\lambda_6\lambda_7\lambda_8-144\lambda_1\lambda_7{}^2\lambda_8-288\lambda_2\lambda_7{}^2\lambda_8+180\lambda_1{}^2\lambda_8{}^2\\
&-72\lambda_2{}^2\lambda_8{}^2-72\lambda_3{}^2\lambda_8{}^2). \qquad \text{(B7)}
\end{aligned}
$$

APPENDIX C: EXPLICIT FORM OF THE $\hat{P}$ MATRIX FOR THE GROUP G

For

$$(d_1,\ldots,d_9)=(2,4,4,6,6,8,8,10,12), \qquad \text{(C1)}$$

the explicit form of the $\hat{P}$ matrix related to the integrity basis $\{p\}$ of the group G is the following:

$$P_{1,i}=2d_ip_i, \quad i=1,...,9,$$

$$P_{2,2}=-\tfrac{8}{3}(3p_1{}^3-9p_1p_2-2p_4+2p_5),$$

$$P_{2,3}=8p_1p_3,$$

$$P_{2,4}=4(2p_1p_4+p_6),$$

$$P_{2,5}=\tfrac{4}{3}(14p_1p_5-3p_6-2p_7),$$

$$P_{2,6}=-\tfrac{2}{3}(3p_3p_4-3p_3p_5-26p_1p_6+2p_8),$$

$$P_{2,7}=-\tfrac{4}{3}(2p_3p_5-17p_1p_7+3p_8),$$

$$P_{2,8}=-\tfrac{2}{3}(2p_3p_6-3p_3p_7-32p_1p_8+3p_9),$$

$$P_{2,9}=4(p_3p_8+5p_1p_9),$$

$$P_{3,3}=16p_1p_3,$$

$$P_{3,4}=24p_6,$$

$$P_{3,5}=8(p_6+2p_7),$$

$$P_{3,6}=4(p_3p_4+3p_3p_5+2p_1p_6+2p_8),$$

$$P_{3,7}=8(2p_3p_5+p_1p_7+p_8),$$

$$P_{3,8}=4(2p_3p_6+3p_3p_7+4p_1p_8+p_9),$$

$$P_{3,9}=24(p_3p_8+p_1p_9),$$

$$P_{4,4}=3(6p_1^2-6p_2-p_3)p_4,$$

$$P_{4,5}=2(2p_1p_6+p_8),$$

$$P_{4,6}=\tfrac{1}{2}(4p_1p_3p_4+24p_4p_5+18p_1^2p_6-18p_2p_6-3p_3p_6+2p_9),$$

$$\begin{aligned}P_{4,7}=\tfrac{1}{32}(&-36p_1^6+144p_1^4p_2-180p_1^2p_2^2+72p_2^3+36p_1^4p_3-108p_1^2p_2p_3+72p_2^2p_3-9p_1^2p_3^2\\&+18p_2p_3^2+80p_1^3p_4-144p_1p_2p_4-24p_1p_3p_4-48p_4^2-144p_1^3p_5+144p_1p_2p_5\\&-72p_1p_3p_5+288p_4p_5+144p_5^2-96p_1^2p_6+288p_2p_6+112p_3p_6+288p_1^2p_7-288p_2p_7\\&+32p_1p_8+16p_9),\end{aligned}$$

$$P_{4,8}=\tfrac{1}{2}(2p_3^2p_4+48p_4p_7+18p_1^2p_8-18p_2p_8-3p_3p_8+4p_1p_9),$$

$$P_{4,9}=3(12p_4p_8+6p_1^2p_9-6p_2p_9-p_3p_9),$$

$$P_{5,5}=\tfrac{1}{3}(2p_1^2p_5+6p_2p_5+5p_3p_5+8p_1p_7),$$

$$\begin{aligned}P_{5,6}=\tfrac{1}{48}(&-36p_1^6+144p_1^4p_2-180p_1^2p_2^2+72p_2^3+36p_1^4p_3-108p_1^2p_2p_3+72p_2^2p_3-9p_1^2p_3^2\\&+18p_2p_3^2+80p_1^3p_4-144p_1p_2p_4-24p_1p_3p_4-48p_4^2-144p_1^3p_5+144p_1p_2p_5\\&+24p_1p_3p_5+480p_4p_5+144p_5^2-80p_1^2p_6+336p_2p_6+88p_3p_6+288p_1^2p_7-288p_2p_7\\&+48p_3p_7-32p_1p_8+16p_9),\end{aligned}$$

$$\begin{aligned}P_{5,7}=\tfrac{1}{96}(&-36p_1^6+144p_1^4p_2-180p_1^2p_2^2+72p_2^3+36p_1^4p_3-108p_1^2p_2p_3+72p_2^2p_3-9p_1^2p_3^2\\&+18p_2p_3^2+80p_1^3p_4-144p_1p_2p_4-24p_1p_3p_4-48p_4^2-144p_1^3p_5+144p_1p_2p_5\\&+184p_1p_3p_5+288p_4p_5+912p_5^2-96p_1^2p_6+288p_2p_6+48p_3p_6+352p_1^2p_7-96p_2p_7\\&+160p_3p_7-96p_1p_8+16p_9),\end{aligned}$$

$$P_{5,8}=\tfrac{1}{6}(6p_3^2p_5+8p_1p_3p_6+96p_5p_6+12p_1p_3p_7+48p_4p_7+2p_1^2p_8+6p_2p_8+5p_3p_8),$$

$$P_{5,9}=2(-12p_3p_4p_5+p_3^2p_6+24p_6^2+2p_1p_3p_8+6p_4p_8),$$

$$\begin{aligned}P_{6,6}=\tfrac{1}{12}(&2p_1^2p_3p_4+6p_2p_3p_4+5p_3^2p_4+54p_1^2p_3p_5-54p_2p_3p_5-9p_3^2p_5+48p_1p_4p_5\\&+24p_1p_3p_6+48p_4p_6+144p_5p_6+96p_4p_7+12p_3p_8+8p_1p_9),\end{aligned}$$

$$\begin{aligned}P_{6,7}=\tfrac{1}{96}(&-36p_1^7+144p_1^5p_2-180p_1^3p_2^2+72p_1p_2^3+36p_1^5p_3-108p_1^3p_2p_3+72p_1p_2^2p_3\\&-9p_1^3p_3^2+18p_1p_2p_3^2+80p_1^4p_4-144p_1^2p_2p_4-24p_1^2p_3p_4-48p_1p_4^2-144p_1^4p_5\\&+144p_1^2p_2p_5-72p_1^2p_3p_5+96p_3^2p_5+288p_1p_4p_5+144p_1p_5^2-96p_1^3p_6+288p_1p_2p_6\\&+176p_1p_3p_6+1152p_5p_6+288p_1^3p_7-288p_1p_2p_7+192p_1p_3p_7+576p_4p_7+576p_5p_7\end{aligned}$$

$$-64p_1{}^2p_8+96p_2p_8+80p_3p_8+16p_1p_9),$$

$$P_{6,8}=\tfrac{1}{12}(8p_1p_3{}^2p_4+48p_3p_4p_5+12p_3{}^2p_6+96p_6{}^2+54p_1{}^2p_3p_7-54p_2p_3p_7-9p_3{}^2p_7+96p_1p_4p_7$$
$$+24p_1p_3p_8+72p_4p_8+216p_5p_8+2p_1{}^2p_9+6p_2p_9+5p_3p_9),$$

$$P_{6,9}=\tfrac{1}{2}(2p_3{}^3p_4+24p_3p_4p_6+18p_1{}^2p_3p_8-18p_2p_3p_8-3p_3{}^2p_8$$
$$+24p_1p_4p_8+4p_1p_3p_9+12p_4p_9+60p_5p_9),$$

$$P_{7,7}=\tfrac{1}{3}(2p_1{}^2p_3p_5+6p_2p_3p_5+5p_3{}^2p_5+12p_1p_5^2+24p_4p_6+8p_1p_3p_7+48p_5p_7),$$

$$P_{7,8}=\tfrac{1}{6}(12p_1p_3{}^2p_5+36p_3p_4p_5-36p_3p_5{}^2+2p_1{}^2p_3p_6+6p_2p_3p_6+5p_3{}^2p_6$$
$$+48p_1p_5p_6+24p_6{}^2+6p_3{}^2p_7+72p_7{}^2+8p_1p_3p_8+120p_5p_8),$$

$$P_{7,9}=-12p_1p_3p_4p_5+4p_1p_3{}^2p_6+12p_3p_4p_6-12p_3p_5p_6$$
$$+24p_1p_6{}^2+2p_3{}^2p_8+24p_7p_8+24p_5p_9,$$

$$P_{8,8}=\tfrac{1}{12}(2p_1{}^2p_3{}^2p_4+6p_2p_3{}^2p_4+5p_3{}^3p_4+54p_1{}^2p_3{}^2p_5-54p_2p_3{}^2p_5-9p_3{}^3p_5+192p_1p_3p_4p_5$$
$$+24p_1p_3{}^2p_6+96p_3p_4p_6-288p_3p_5p_6+12p_3{}^2p_8+576p_7p_8+8p_1p_3p_9+192p_5p_9),$$

$$P_{8,9}=\tfrac{1}{2}(4p_1p_3{}^3p_4+12p_3{}^2p_4{}^2+18p_1{}^2p_3{}^2p_6-18p_2p_3{}^2p_6-3p_3{}^3p_6+48p_1p_3p_4p_6-84p_3p_6{}^2$$
$$-24p_3p_4p_8+84p_8{}^2+2p_3{}^2p_9+48p_6p_9+84p_7p_9),$$

$$P_{9,9}=3(6p_1{}^2p_3{}^3p_4-6p_2p_3{}^3p_4-p_3{}^4p_4+12p_1p_3{}^2p_4{}^2+288p_1p_3{}^2p_4p_5-1152p_3p_4p_5{}^2$$
$$-24p_3{}^2p_4p_6-288p_1p_3p_6{}^2+1152p_5p_6{}^2+144p_1{}^2p_3p_4p_7-432p_2p_3p_4p_7-72p_3{}^2p_4p_7$$
$$+1152p_4p_7{}^2+108p_1{}^6p_8-432p_1{}^4p_2p_8+540p_1{}^2p_2{}^2p_8-216p_2{}^3p_8-108p_1{}^4p_3p_8$$
$$+324p_1{}^2p_2p_3p_8-216p_2{}^2p_3p_8+27p_1{}^2p_3{}^2p_8-54p_2p_3{}^2p_8-240p_1{}^3p_4p_8+432p_1p_2p_4p_8$$
$$+72p_1p_3p_4p_8+144p_4{}^2p_8+432p_1{}^3p_5p_8-432p_1p_2p_5p_8+216p_1p_3p_5p_8-864p_4p_5p_8$$
$$-432p_5{}^2p_8-864p_1{}^2p_7p_8+864p_2p_7p_8+144p_1{}^2p_5p_9-432p_2p_5p_9-72p_3p_5p_9$$
$$+288p_1p_7p_9).$$

APPENDIX D: EXPLICIT FORM OF THE GENERATORS OF THE ISOTROPY SUBGROUPS OF SO_3

In this Appendix are collected the definitions of the groups and of the elements and the generators of the subgroups of $\mathbf{SO}_3$, involved in the body of the paper, in the tables and in the figures.

1. Generators or group elements

$$C_{2x}=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix},\quad C_{2z}=\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix},\quad C_{3z}=\begin{pmatrix}-\frac{1}{2}&\frac{\sqrt{3}}{2}&0\\-\frac{\sqrt{3}}{2}&-\frac{1}{2}&0\\0&0&1\end{pmatrix},$$

$$C_{4z}=\begin{pmatrix}0&1&0\\-1&0&0\\0&0&1\end{pmatrix},\quad C_{4x}=\begin{pmatrix}1&0&0\\0&0&1\\0&-1&0\end{pmatrix},\quad C_{2a}=\begin{pmatrix}0&1&0\\1&0&0\\0&0&-1\end{pmatrix},\tag{D1}$$

$$C_{3\delta}=\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix},\quad R_z(\phi)=\begin{pmatrix}\cos(\phi)&\sin(\phi)&0\\-\sin(\phi)&\cos(\phi)&0\\0&0&1\end{pmatrix},$$

$$R_x(\phi)=\begin{pmatrix}1&0&0\\0&\cos(\phi)&\sin(\phi)\\0&-\sin(\phi)&\cos(\phi)\end{pmatrix}.$$

2. Groups

By $\mathbf{SO}_3$ and $\mathbf{O}_3$ we denote the proper and, respectively, the complete 3D rotation group and, by $\mathbf{O}_2^{\alpha}$, $\alpha=x,z$ the following $\mathbf{O}_2$ subgroups of $\mathbf{SO}_3$: $\mathbf{O}_2^x=\{\mathrm{R}_x(\phi)\}_{0\leqslant\phi<2\pi}\cup\{C_{2z}\mathrm{R}_x(\phi)\}_{0\leqslant\phi<2\pi}$ and $\mathbf{O}_2^z=\{\mathrm{R}_z(\phi)\}_{0\leqslant\phi<2\pi}\cup\{C_{2x}\mathrm{R}_z(\phi)\}_{0\leqslant\phi<2\pi}$.

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The generalized star product and the factorization of scattering matrices on graphs

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In this article we continue our analysis of Schrödinger operators on arbitrary graphs given as certain Laplace operators. In the present article we give the proof of the composition rule for the scattering matrices. This composition rule gives the scattering matrix of a graph as a generalized star product of the scattering matrices corresponding to its subgraphs. We perform a detailed analysis of the generalized star product for arbitrary unitary matrices. The relation to the theory of transfer matrices is also discussed. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Potential scattering for one-particle Schrödinger operators on the line possesses a remarkable property concerning its (on-shell) scattering matrix given as a 2×2 matrix-valued function of the energy. Let the potential V be given as the sum of two potentials V_1 and V_2 with disjoint support. Then the scattering matrix for V at a given energy is obtained from the two scattering matrices for V_1 and V_2 at the same energy by a certain nonlinear, noncommutative but associative composition rule. This fact has been discovered independently by several authors (see, e.g., Refs. 1–7) and is an easy consequence of the multiplicative property of the transfer matrix of the Schrödinger equation (see e.g., Ref. 8). It has also been well known in the theory of mesoscopic systems and multichannel conductors (see, e.g., Refs. 9–18). In higher space dimensions a similar rule is not known. However, for large separation between the supports of the potentials the scattering matrix at a given energy is asymptotically related to the scattering matrices for V_1 and V_2 at the same energy.[19,20]

To the best of our knowledge the composition rule for 2×2 scattering matrices was first observed in network theory by Redheffer,[2,3] who called it the star product. In an earlier article[21] we extended this result to quasi-one-dimensional quantum systems—Schrödinger operators on graphs. Such systems are nowadays a subject of intensive study (see, e.g., Refs. 22–27). Some other related works are quoted in Ref. 21. In Refs. 28–31 differential operators with Neuman boundary conditions on ''fat graphs'' were considered, i.e., on thin domains in $\mathbb{R}^d$ which asymptotically shrink to a graph.

There is also a large amount of literature on linear difference operators on graphs. The motivation for the study of such operators comes from the graph theory, where the spectra of these operators are known to be related to topological properties of the graph.[32–34] Scattering theory for such operators was developed in Refs. 35 and 36.

In Ref. 21 we considered the (continuous) Laplace operator on graphs with an arbitrary number n of open ends (i.e., channels) and with arbitrary boundary conditions at the edges resulting in a self-adjoint operator. We formulated and proved necessary and sufficient conditions

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for such operators to be self-adjoint. We provided an explicit expression for the resulting unitary $n\times n$ scattering matrix in terms of the boundary conditions, the lengths of the internal lines, and the given energy. Furthermore, we generalized Redheffer's star product to what we called the generalized star product. This is a nonlinear, noncommutative but associative composition rule for unitary matrices not necessarily of equal rank and resulting in a unitary matrix.

Under special circumstances there is an alternative way to describe the generalized star product. Fix $p\geqslant 1$ and consider the group $\mathsf{U}(p,p)$ with its natural multiplication. As a set this group is isomorphic to some subgroup of $\mathsf{U}(2p)$. This nonlinear set isomorphism is well known in the case $p=1$ (see, e.g., Ref. 37) and can be easily generalized to the case of arbitrary $p>1$. Under this isomorphism the multiplication in $\mathsf{U}(p,p)$ induces new nonlinear multiplication $*_p$ in this subgroup of $\mathsf{U}(2p)$, which is our generalized star product. The operation $*_p$ can be extended by continuity to the whole $\mathsf{U}(2p)$. The set $\mathsf{U}(2p)$ with $*_p$ as multiplication is no longer a group, but only a semigroup.

Employing this generalized star product in Ref. 21 we provided a formal proof based on the quantum mechanical superposition principle to show how the scattering matrix at the same energy for the whole graph can be obtained from the scattering matrices of two subgraphs obtained by cutting the graph in any way in two. Again for the special case of two-channel scattering matrices, like potential scattering on the line, this formal argument is well known (see, e.g., Ref. 17). In this article we will provide a rigorous proof of this composition rule. It is interesting to note that in this general case the composition rule cannot be reduced to the multiplicative property of the transfer matrix of the Schrödinger equation on the graph.

Such composition rules are important in the study of the electric conduction in multi-terminal mesoscopic systems. By the Landauer–Büttiker theory the electric conduction in mesoscopic systems is directly related to the transmission probability and thus to the scattering matrix.[38–41] A good introduction into the theory of electronic transport in such systems is given in the book[17] by S. Datta. The formal arguments leading to the composition rule for the scattering matrices are presented on pp. 125–126 of Ref. 17.

The composition rules are also very useful in the study of statistical properties of large random or periodic systems. Examples of such systems can be found, e.g., in Refs. 42, 24, and 25. In Refs. 8 and 43–45 we proved that in arbitrary dimensions the scattering phase (or more generally of the spectral shift function) per interaction volume equals (up to a factor π) the difference of the integrated densities of states for the free and interaction theories, respectively. In the strictly one-dimensional situation (Schrödinger operators on the line) the Lyapunov exponent is known to be related to the logarithmic density of transmission probability.[46–48,8] Due to the Ishii-Pastur-Kotani theorem (see, e.g., Ref. 49) the vanishing of the transmission amplitude for almost all values of energy implies localization (i.e., the spectrum must be purely point) (see also the related works Refs. 9–16):

Certain Laplace operators on (infinite) periodic graphs were previously considered in Refs. 24 and 25. There are also some attempts to consider differential operators on regular graphs with random boundary conditions or on random graphs with deterministic boundary conditions (see, e.g., Ref. 42). Some other examples can be found also in Ref. 50, Chap. 3. A difference Laplace operator on the edges of aperiodic tilings was considered in Ref. 51. Such systems provide a main field of application for our composition rule which will be discussed in a forthcoming publication.

The article is organized as follows. In Sec. II we recall the general quantum scattering theory on graphs as given in Ref. 21. In Sec. III we recall the definition of the generalized star product and study some its properties. In particular we show that this product applies to arbitrary unitary matrices. In Sec. IV we give a rigorous proof of the composition rule for scattering matrices on arbitrary finite graphs. Section V is devoted to the special case of graphs having an even number $2p$ of external lines. If the new graph is obtained by gluing of exactly p lines, then it has again $2p$ external lines. We consider the question whether in this case the composition rule for the scattering matrices can be reduced to the multiplication rule of the corresponding transfer matrices. In general for $p>1$ the answer is negative. We formulate a necessary and sufficient condition, which

guarantees that the composition rule for the scattering matrices is equivalent to the standard multiplication of transfer matrices.

After completing the work we received the preprint[52] by M. Harmer where, among other questions, the composition rule for the scattering matrices is also considered. The results there partially recover our Theorem IV.1 below.

We are indebted to P. Kuchment for sending us the preliminary version of the preprint[29] and also for pointing out the works of R. Carlson.[26,27,53]

II. THE LAPLACIAN ON A GRAPH AND ITS SCATTERING MATRIX

In this section we will recall the definition of Schrödinger operators on an arbitrary but finite graph and the construction of their scattering matrices.[21]

We consider an arbitrary graph Γ with a finite number $n \geqslant 1$ of external and a finite number $m \geqslant 0$ of internal lines (edges). More precisely this means that outside of a finite domain the graph is isomorphic to the union of n positive half-lines. Any internal line ends at two, not necessary different, vertices and has a finite length. We assume that any vertex of Γ has nonzero degree, i.e., for any vertex there is at least one edge (internal or external) with which it is incident.

Let the set $\mathcal{E}$ label the external and the set $\mathcal{I}$ the internal lines of the graph. We assume that the sets $\mathcal{E}$ and $\mathcal{I}$ are ordered in an arbitrary but fixed way. To each $e \in \mathcal{E}$ we associate the infinite interval $[0,\infty)$ and to each $i \in \mathcal{I}$ the finite directed interval $[0,a_i]$, where $a_i > 0$ is the length of this line. With this association the graph becomes directed, such that the initial vertex of an edge of length a corresponds to $x=0$ and the terminal vertex corresponds to $x=a$. The external lines are assumed to be directed in the positive direction of half-lines.

We define the Hilbert space $\mathcal{H}=L^2(\Gamma)$ as

$$\mathcal{H}=\mathcal{H}_{\mathcal{E}} \oplus \mathcal{H}_{\mathcal{I}}, \quad \mathcal{H}_{\mathcal{E}}=\bigoplus_{e \in \mathcal{E}} \mathcal{H}_e, \quad \mathcal{H}_{\mathcal{I}}=\bigoplus_{i \in \mathcal{I}} \mathcal{H}_i,$$

where $\mathcal{H}_e=L^2(0,\infty)$ and $\mathcal{H}_i=L^2(0,a_i)$. Elements of $\mathcal{H}$ are written as column vectors

$$\psi=(\{\psi_e\}_{e \in \mathcal{E}},\{\psi_i\}_{i \in \mathcal{I}})^T=(\psi_{\mathcal{E}},\psi_{\mathcal{I}})^T, \quad \psi_e \in M\mathcal{H}_e, \quad \psi_i \in \mathcal{H}_i. \tag{2.1}$$

Similarly we define the Sobolev space $W^{2,2}(\Gamma)$ as

$$W^{2,2}(\Gamma)=\bigoplus_{e \in \mathcal{E}} W^{2,2}(0,\infty) \oplus \bigoplus_{i \in \mathcal{I}} W^{2,2}(0,a_i),$$

where $W^{2,2}(0,\infty)$ and $W^{2,2}(0,a_i)$ are the usual Sobolev spaces of square integrable functions whose distributional second derivatives are also square integrable (see, e.g., Ref. 54). Let $[\,]: W^{2,2}(\Gamma) \to \mathbb{C}^{2(n+2m)}$ be the surjective linear map which associates to each ψ the element $[\psi]$ given as

$$[\psi]=\begin{pmatrix} (\{\psi_e(0)\}_{e \in \mathcal{E}},\ \{\psi_i(0)\}_{i \in \mathcal{I}},\ \{\psi_i(a_i)\}_{i \in \mathcal{I}})^T \\ (\{\psi_e'(0)\}_{e \in \mathcal{E}},\ \{\psi_i'(0)\}_{i \in \mathcal{I}},\ \{-\psi_i'(a_i)\}_{i \in \mathcal{I}})^T \end{pmatrix}=\begin{pmatrix} \underline{\psi} \\ \underline{\psi}' \end{pmatrix}$$

again viewed as a column vector with the same ordering as in ψ, i.e., with the ordering given by the ordering of $\mathcal{E}$ and $\mathcal{I}$.

In Ref. 21 we showed that for any two $(n+2m)\times(n+2m)$ complex matrices A and B with AB^* being Hermitian and the $(n+2m)\times 2(n+2m)$ matrix (A,B) having maximal rank equal to $n+2m$, one can define the self-adjoint Laplace operator $\Delta(A,B,\underline{a})$ in $\mathcal{H}$ corresponding to the boundary condition

$$A\underline{\psi}+B\underline{\psi}'=0. \tag{2.2}$$

Here $\underline{a}=(a_1,\ldots,a_m)^T\in\mathbb{R}_+^m$, $m=\#(\mathcal{I})$. Furthermore, any self-adjoint extension of the Laplacian on the given graph is given by $\Delta(A,B,\underline{a})$ with some matrices A and B satisfying the properties stated above. If $\mathcal{I}=\varnothing$, we simply write $(\Delta(A,B)$ instead of $\Delta(A,B,\cdot)$.

Before we turn to the scattering theory for $\Delta(A,B,\underline{a})$ we recall some well-known facts from scattering theory in two Hilbert spaces $\mathfrak{h}_1$ and $\mathfrak{h}_2$ (see, e.g., Ref. 55). Let H_1 and H_2 be self-adjoint operators in the Hilbert spaces $\mathfrak{h}_1$ and $\mathfrak{h}_2$, respectively. Let $\mathcal{J}$ be a bounded operator from $\mathfrak{h}_1$ into $\mathfrak{h}_2$. The two-space wave operators are defined as the strong limits

$$\Omega^{\pm}(H_2,H_1;\mathcal{J})=\operatorname*{s-lim}_{t\to\mp\infty} e^{iH_2t}\mathcal{J}e^{-iH_1t}P_{\mathrm{ac}}(H_1),$$

where $P_{\mathrm{ac}}(H)$ denotes the projection onto the absolute continuous subspace of H. We consider the sets $\mathfrak{N}_{\pm}$ of elements $g\in\mathfrak{h}_2$ for which $\lim_{t\to\mp\infty}\|\mathcal{J}^*e^{iH_2t}P_{\mathrm{ac}}(H_2)g\|=0$. The wave operators $\Omega^{\pm}$ are called $\mathcal{J}$-complete if $\mathfrak{h}_2=\overline{\mathrm{Ran}(\Omega^{\pm})}\oplus\mathfrak{N}_{\pm}$. For details we refer to, e.g., to Chap. 3 of Ref. 56.

Now we consider a graph $\Gamma_{\mathcal{E}}$ consisting of the external lines of the original graph Γ. On the graph $\Gamma_{\mathcal{E}}$ we consider the operator $-\Delta(A_{\mathcal{E}}=0,B_{\mathcal{E}}=\mathbb{I})$ corresponding to Neumann boundary conditions. Let $\mathcal{J}:\mathcal{H}\to\mathcal{H}_{\mathcal{E}}$ be given as $\mathcal{J}\psi=\psi_{\mathcal{E}}$ according to the notation (2.1). In particular $\mathcal{J}$ is identity if $m=0$. Since we actually deal with finite-dimensional perturbations by the Kato-Rosenblum theorem (see, e.g., Ref. 56, Theorem 6.2.3 and Corollary 6.2.4) the wave operators $\Omega^{\pm}(-\Delta(A,B,\underline{a}),-\Delta(A_{\mathcal{E}}=0,B_{\mathcal{E}}=\mathbb{I});\mathcal{J})$ exist and are $\mathcal{J}$-complete. Thus the scattering operator

$$S(-\Delta(A,B,\underline{a}),-\Delta(A_{\mathcal{E}}=0,B_{\mathcal{E}}=\mathbb{I};\mathcal{J})=(\Omega^-)^*\Omega^+:\mathcal{H}_{\mathcal{E}}\to\mathcal{H}_{\mathcal{E}} \tag{2.3}$$

is unitary and its layers $S_{A,B,\underline{a}}(\lambda):\mathbb{C}^n\to\mathbb{C}^n$ [in the direct integral representation with respect to $-\Delta(A_{\mathcal{E}}=0,B_{\mathcal{E}}=\mathbb{I})$] are also unitary for almost all energies $\lambda\in\mathbb{R}_+$.

The resulting scattering matrix is related to the scattering wave function for the operator $-\Delta(A,B,\underline{a})$ at energy $\lambda>0$ as follows. The function $\psi^k(\cdot,\lambda)$ indexed by $k\in\mathcal{E}$ and with components

$$\psi_j^k(x,\lambda)=\begin{cases} S_{jk}(\lambda)e^{i\sqrt{\lambda}x} & \text{for } j\in\mathcal{E}, j\neq k,\\ e^{-i\sqrt{\lambda}x}+S_{kk}(\lambda)e^{i\sqrt{\lambda}x} & \text{for } j\in\mathcal{E}, j=k,\\ \alpha_{jk}(\lambda)e^{i\sqrt{\lambda}x}+\beta_{jk}(\lambda)e^{-i\sqrt{\lambda}x} & \text{for } j\in\mathcal{J},\end{cases} \tag{2.4}$$

solves the Schrödinger equation with the operator $-\Delta(A,B,\underline{a})$ for energy $\lambda>0$.

Recall that in potential scattering for one-particle Schrödinger operators the wave operators give precise meaning to the scattering wave functions, i.e., solutions of the Schrödinger equation at positive energy $\lambda>0$. Similarly the wave operators $\Omega^{\pm}(-\Delta(A,B,\underline{a}),-\Delta(A_{\mathcal{E}}=0,B_{\mathcal{E}}=\mathbb{I});\mathcal{J})$ determine the ''external part'' of the scattering wave function, i.e., $\psi_j^k(x,\lambda)$ for $j\in\mathcal{E}$. The completeness of usual wave operators means that any solution of the Schrödinger equation at energy $\lambda>0$ can be uniquely represented as a superposition of the scattering wave functions. Similarly, in the present context the $\mathcal{J}$-completeness of the wave operators $\Omega^{\pm}(-\Delta(A,B,\underline{a}),-\Delta(A_{\mathcal{E}}=0,B_{\mathcal{E}}=\mathbb{I});\mathcal{J})$ means that the external part of any solution for the Schrödinger equation with the operator $-\Delta(A,B,\underline{a})$ at energy $\lambda>0$ can uniquely be represented as a linear combination of the external parts of the scattering wave functions (2.4).

The scattering matrix $S_{A,B,\underline{a}}(\lambda)$ as well as the $m\times n$ matrix amplitudes $\alpha_{A,B,\underline{a}}(\lambda)$ and $\beta_{A,B,\underline{a}}(\lambda)$ are determined as solutions to the equation

$$Z_{A,B,\underline{a}}(\lambda)\begin{pmatrix} S(\lambda)\\ \alpha(\lambda)\\ \beta(\lambda)\end{pmatrix}=-A(-i\sqrt{\lambda}B)\begin{pmatrix}\mathbb{I}\\0\\0\end{pmatrix}, \tag{2.5}$$

where

$$Z_{A,B,\underline{a}}(\lambda)=AX_{\underline{a}}(\lambda)+i\sqrt{\lambda}BY_{\underline{a}}(\lambda) \tag{2.6}$$

is the $(n+2m)\times(n+2m)$ matrix with

$$X_{\underline{a}}(\lambda)=\begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & \mathbb{I} \\ 0 & e^{i\sqrt{\lambda}\underline{a}} & e^{-i\sqrt{\lambda}\underline{a}} \end{pmatrix}$$

and

$$Y_{\underline{a}}(\lambda)=\begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & -\mathbb{I} \\ 0 & -e^{i\sqrt{\lambda}\underline{a}} & e^{-i\sqrt{\lambda}\underline{a}} \end{pmatrix}.$$

Here $e^{\pm i\sqrt{\lambda}\underline{a}}$ stands for the $m\times m$ diagonal matrix with elements

$$(e^{\pm i\sqrt{\lambda}\underline{a}})_{jk}=e^{\pm i\sqrt{\lambda}\underline{a}_j}\delta_{jk}, \quad j,k\in\mathcal{J}.$$

If $\det Z_{A,B,\underline{a}}(\lambda)\neq 0$, the scattering matrix $S(\lambda)=S_{A,B,\underline{a}}(\lambda)$ as well as the $m\times n$ matrices $\alpha(\lambda)=\alpha_{A,B,\underline{a}}(\lambda)$ and $\beta(\lambda)=\beta_{A,B,\underline{a}}(\lambda)$ can be uniquely determined by solving the equation (2.5) in the form

$$\begin{pmatrix} S(\lambda) \\ \alpha(\lambda) \\ \beta(\lambda) \end{pmatrix} = -Z_{A,B,\underline{a}}(\lambda)^{-1}(A-i\sqrt{\lambda}B)\begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix}. \tag{2.7}$$

We denote by $\Sigma_{A,B,\underline{a}}=\{\lambda>0|\det Z_{A,B,\underline{a}}(\lambda)=0\}$ the set of exceptional points for which $Z_{A,B,\underline{a}}(\lambda)$ is not invertible.

Let ϕ be an arbitrary measurable function on the graph Γ. The subset supp ϕ of all edges of the graph Γ will be called the *support* of the function ϕ if $\phi\neq 0$ a.e. on supp ϕ.

In Ref. 21 we proved the following.

Theorem II.1: *For any boundary condition* (A, B) *and arbitrary* $\underline{a}\in\mathbb{R}_+^m$ *the set* $\Sigma_{A,B,\underline{a}}$ *equals the set* $\sigma_{A,B,\underline{a}}$ *of all positive eigenvalues of* $-\Delta(A,B,\underline{a})$. *This set is discrete and has no finite accumulation points in* $\mathbb{R}_+$. *The eigenfunctions of* $-\Delta(A,B,\underline{a})$ *have support on the internal lines of the graph. For all* $\lambda\in\Sigma_{A,B,\underline{a}}$ *the equation (2.5) is still solvable and determines* $S_{A,B,\underline{a}}(\lambda)$ *uniquely*.

Given an arbitrary $n\times n$ unitary matrix U and an energy $\lambda_0>0$ we can find boundary conditions A,B defining a self-adjoint operator $-\Delta(A,B)$ on a single-vertex graph (i.e., with $m=0$) with n external lines such that the corresponding scattering matrix is given as $S_{A,B}(\lambda_0)=U$. The proof of this fact can be found in Ref. 57. For other inverse problems on graphs we refer to Refs. 58 and 53.

Recall that by definition the operator $\Delta(A,B,\underline{a})$ is real if it commutes with complex conjugation, i.e., for any $\psi\in\mathcal{D}(\Delta(A,B,\underline{a}))$ the function $\overline{\psi}$ also belongs to $\mathcal{D}(\Delta(A,B,\underline{a}))$ and $\Delta(A,B,\underline{a})\psi=\overline{\Delta(A,B)\overline{\psi}}$. Equivalently, this means that any $\psi\in\mathcal{D}(\Delta(A,B,\underline{a}))$ [i.e., $\psi\in W^{2,2}(\Gamma)$ satisfying $A\psi+B\psi'=0$] also satisfies the equation $\overline{A}\overline{\psi}+\overline{B}\overline{\psi}'=0$. Thus, $\Delta(A,B,\underline{a})$ is real iff $\mathrm{Ker}(A,B)=\mathrm{Ker}(\overline{A},\overline{B})$. The last condition is satisfied iff there is an invertible matrix C_1 such that $A=C_1\overline{A}$, $B=C_1\overline{B}$ or alternatively there is an invertible matrix C_2 such that both C_2A and C_2B are real. We recall that $\Delta(A,B,\underline{a})=\Delta(CA,CB,\underline{a})$ for any invertible C (see Ref. 21).

In Ref. 21, Corollary 3.2, we have proved the following.

Theorem II.2: *For arbitrary* $\underline{a}\in\mathbb{R}_+^m$, $\lambda>0$, *and all boundary conditions A, B defining the self-adjoint operator* $\Delta(A,B,\underline{a})$

$$S_{\overline{A},\overline{B},\underline{a}}(\lambda)^T=S_{A,B,\underline{a}}(\lambda). \tag{2.8}$$

In particular, if the operator $\Delta(A,B,\underline{a})$ *is real, then* $S_{A,B,\underline{a}}(\lambda)=S_{A,B,\underline{a}}(\lambda)^T$ *for all* $\lambda>0$.

Here we give an alternative proof.

Proof: From the self-adjointness of the operator $\Delta(A,B,\underline{a})$ it follows that the matrix $A+i\sqrt{\lambda}B$ is invertible for all $\lambda>0$ (see Ref. 21). The relation (2.5) implies that

$$\begin{pmatrix} S_{A,B,\underline{a}}(\lambda) \\ \alpha_{A,B,\underline{a}}(\lambda) \\ e^{-i\sqrt{\lambda}\underline{a}}\beta_{A,B,\underline{a}}(\lambda) \end{pmatrix} = -(A+i\sqrt{\lambda}B)^{-1}(A-i\sqrt{\lambda}B)\begin{pmatrix} \mathbb{I} \\ \beta_{A,B,\underline{a}}(\lambda) \\ e^{i\sqrt{\lambda}\underline{a}}\alpha_{A,B,\underline{a}}(\lambda) \end{pmatrix}.$$

Similarly, for the operator $\Delta(\overline{A},\overline{B},\underline{a})$ we have

$$\begin{pmatrix} S_{\overline{A},\overline{B},\underline{a}}(\lambda) \\ \alpha_{\overline{A},\overline{B},\underline{a}}(\lambda) \\ e^{-i\sqrt{\lambda}\underline{a}}\beta_{\overline{A},\overline{B},\underline{a}}(\lambda) \end{pmatrix} = -(\overline{A}+i\sqrt{\lambda}\overline{B})^{-1}(\overline{A}-i\sqrt{\lambda}\overline{B})\begin{pmatrix} \mathbb{I} \\ \beta_{\overline{A},\overline{B},\underline{a}}(\lambda) \\ e^{i\sqrt{\lambda}\underline{a}}\alpha_{\overline{A},\overline{B},\underline{a}}(\lambda) \end{pmatrix}.$$

Taking the complex conjugate and multiplying by $(A+i\sqrt{\lambda}B)^{-1}(A-i\sqrt{\lambda}B)$ from the left we obtain

$$\begin{pmatrix} \mathbb{I} \\ \overline{\beta_{\overline{A},\overline{B},\underline{a}}(\lambda)} \\ e^{-i\sqrt{\lambda}\underline{a}}\overline{\alpha_{\overline{A},\overline{B},\underline{a}}(\lambda)} \end{pmatrix} = -(A+i\sqrt{\lambda}B)^{-1}(A-i\sqrt{\lambda}B)\begin{pmatrix} \overline{S_{\overline{A},\overline{B},\underline{a}}(\lambda)} \\ \overline{\alpha_{\overline{A},\overline{B},\underline{a}}(\lambda)} \\ e^{i\sqrt{\lambda}\underline{a}}\overline{\beta_{\overline{A},\overline{B},\underline{a}}(\lambda)} \end{pmatrix}.$$

We multiply this relation by $S_{\overline{A},\overline{B}}(\lambda)^T$ from the right and make use of the unitarity of the scattering matrix in the form $\overline{S_{\overline{A},\overline{B}}(\lambda)}S_{\overline{A},\overline{B}}(\lambda)^T=\mathbb{I}$, thus obtaining

$$\begin{pmatrix} S_{\overline{A},\overline{B},\underline{a}}(\lambda)^T \\ \overline{\beta_{\overline{A},\overline{B},\underline{a}}(\lambda)}S_{\overline{A},\overline{B},\underline{a}}(\lambda)^T \\ e^{-i\sqrt{\lambda}\underline{a}}\overline{\alpha_{\overline{A},\overline{B},\underline{a}}(\lambda)}S_{\overline{A},\overline{B},\underline{a}}(\lambda)^T \end{pmatrix} = -(A+i\sqrt{\lambda}B)^{-1}(A-i\sqrt{\lambda}B)\begin{pmatrix} \mathbb{I} \\ \overline{\alpha_{\overline{A},\overline{B},\underline{a}}(\lambda)}S_{\overline{A},\overline{B},\underline{a}}(\lambda)^T \\ e^{i\sqrt{\lambda}\underline{a}}\beta_{\overline{A},\overline{B},\underline{a}}(\lambda)S_{\overline{A},\overline{B},\underline{a}}(\lambda)^T \end{pmatrix}.$$

Equivalently, this relation can be written in a form analogous to (2.5),

$$Z_{A,B,\underline{a}}(\lambda)\begin{pmatrix} S_{\overline{A},\overline{B},\underline{a}}(\lambda)^T \\ \overline{\beta_{\overline{A},\overline{B},\underline{a}}(\lambda)}S_{\overline{A},\overline{B},\underline{a}}(\lambda)^T \\ \overline{\alpha_{\overline{A},\overline{B},\underline{a}}(\lambda)}S_{\overline{A},\overline{B},\underline{a}}(\lambda)^T \end{pmatrix} = -(A-i\sqrt{\lambda}B)\begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix}. \tag{2.9}$$

In Ref. 21 we proved that equation (2.5) has a solution for all $\lambda>0$. If $\lambda>0$ is not an eigenvalue of the operator $\Delta(A,B,\underline{a})$, then it has a unique solution. If $\lambda>0$ is an eigenvalue of $\Delta(A,B,\underline{a})$, this solution is nonunique, but still determines the scattering matrix uniquely. Therefore, from comparison of (2.5) and (2.9) the relation (2.8) follows. If $\Delta(A,B,\underline{a})$ is real, by the remark preceding the theorem we can choose the matrices A and B to be real. From this and from (2.8) the second claim of the theorem follows. □

We note that the comparison of (2.5) with (2.9) also gives the relations

$$\alpha_{A,B,\underline{a}}(\lambda)=\overline{\beta_{\overline{A},\overline{B},\underline{a}}(\lambda)}S_{A,B,\underline{a}}(\lambda)^T,$$

$$\beta_{A,B,\underline{a}}(\lambda)=\overline{\alpha_{\overline{A},\overline{B},\underline{a}}(\lambda)}S_{A,B,\underline{a}}(\lambda)^T,$$

III. THE GENERALIZED STAR PRODUCT

Let $U^{(1)}$ and $U^{(2)}$ be arbitrary $n_1\times n_1$ and $n_2\times n_2$ unitary matrices, respectively. Let p be some integer satisfying $1\leqslant p<(n_1+n_2)/2$, $p\leqslant n_j$, $j=1$, 2, and V be an arbitrary $p\times p$ unitary matrix. We write $U^{(1)}$ and $U^{(2)}$ in a 2×2-block form

$$U^{(1)}=\begin{pmatrix} U_{11}^{(1)} & U_{12}^{(1)} \\ U_{21}^{(1)} & U_{22}^{(1)} \end{pmatrix}, \quad U^{(2)}=\begin{pmatrix} U_{11}^{(2)} & U_{12}^{(2)} \\ U_{21}^{(2)} & U_{22}^{(2)} \end{pmatrix}, \tag{3.1}$$

where $U_{22}^{(1)}$ and $U_{11}^{(2)}$ are $p\times p$ matrices, $U_{11}^{(1)}$ is an $(n_1-p)\times(n_1-p)$ matrix, $U_{22}^{(2)}$ is an $(n_2-p)\times(n_2-p)$ matrix, etc. The unitarity condition for $U^{(1)}$ then reads

$$U_{11}^{(1)*}U_{11}^{(1)}+U_{21}^{(1)*}U_{21}^{(1)}=\mathbb{I},$$

$$U_{12}^{(1)*}U_{12}^{(1)}+U_{22}^{(1)*}U_{22}^{(1)}=\mathbb{I},$$

$$U_{11}^{(1)*}U_{12}^{(1)}+U_{21}^{(1)*}U_{22}^{(1)}=0,$$

$$U_{12}^{(1)*}U_{11}^{(1)}+U_{22}^{(1)*}U_{21}^{(1)}=0,$$

and similarly for $U^{(2)}$.

*Definition III.1: The unitary matrix $U^{(1)}$ is called V-***compatible** *with the unitary matrix $U^{(2)}$ if the $p\times p$ matrix $VU_{22}^{(1)}V^*U_{11}^{(2)}$ does not have* 1 *as an eigenvalue. For the case $V=\mathbb{I}$ the matrix $U^{(1)}$ is simply called* **compatible** *with $U^{(2)}$ (for given $p\geqslant 1$).*

Note that the compatibility of the matrices is not a symmetric relation, i.e., if $U^{(1)}$ is V-compatible with $U^{(2)}$, then $U^{(2)}$ need not be V-compatible with $U^{(1)}$.

Obviously, if $U^{(1)}$ is V-compatible with $U^{(2)}$, then also the matrix $V^*U_{11}^{(2)}VU_{22}^{(1)}$ does not have 1 as an eigenvalue. Indeed, let us assume the converse, i.e., let there be nonzero $c\in\mathbb{C}^p$ such that $V^*U_{11}^{(2)}VU_{22}^{(1)}c=c$ and thus

$$VU_{22}^{(1)}V^*U_{11}^{(2)}VU_{22}^{(1)}c=VU_{22}^{(1)}c.$$

Since $VU_{22}^{(1)}c\neq 0$ the matrix $VU_{22}^{(1)}V^*U_{11}^{(2)}$ has 1 as an eigenvalue, which is a contradiction. From this it also follows that if $U^{(1)}$ is not V-compatible with $U^{(2)}$, then the matrix $V^*U_{11}^{(2)}VU_{22}^{(1)}$ has 1 as an eigenvalue.

From the unitarity conditions it follows that

$$0\leqslant U_{11}^{(1)*}U_{11}^{(1)}=\mathbb{I}-U_{21}^{(1)*}U_{21}^{(1)}\leqslant\mathbb{I},$$

$$0\leqslant U_{22}^{(1)*}U_{22}^{(1)}=\mathbb{I}-U_{12}^{(1)*}U_{12}^{(1)}\leqslant\mathbb{I},$$

and thus $\|U_{11}^{(1)}\|\leqslant 1, \|U_{22}^{(1)}\|\leqslant 1$. Similar inequalities hold for $U_{11}^{(2)}$ and $U_{22}^{(2)}$. Therefore $\|VU_{22}^{(1)}V^*U_{11}^{(2)}\|\leqslant 1$. Strict inequality holds whenever $\|U_{22}^{(1)}\|<1$ or $\|U_{11}^{(2)}\|<1$ and then $U^{(1)}$ is V-compatible with $U^{(2)}$ and $U^{(2)}$ is V-compatible with $U^{(1)}$ for all unitary $p\times p$ matrices V.

In general, if $U^{(1)}$ is V-compatible with $U^{(2)}$, then it is easy to see that the following $p\times p$ matrices exist:

$$\begin{aligned} K_1&=(\mathbb{I}-VU_{22}^{(1)}V^*U_{11}^{(2)})^{-1}V=V(\mathbb{I}-U_{22}^{(1)}V^*U_{11}^{(2)}V)^{-1}, \\ K_2&=(\mathbb{I}-V^*U_{11}^{(2)}VU_{22}^{(1)})^{-1}V^*=V^*(\mathbb{I}-U_{11}^{(2)}VU_{22}^{(1)}V^*)^{-1}. \end{aligned} \tag{3.2}$$

An easy calculation establishes the following relations

$$\begin{aligned} K_1&=V+VU_{22}^{(1)}V^*U_{11}^{(2)}K_1=V+VU_{22}^{(1)}K_2U_{11}^{(2)}V=V+K_1U_{22}^{(1)}V^*U_{11}^{(2)}V, \\ K_2&=V^*+V^*U_{11}^{(2)}VU_{22}^{(1)}K_2=V^*+V^*U_{11}^{(2)}K_1U_{22}^{(1)}V^*=V^*+K_2U_{11}^{(2)}VU_{22}^{(1)}V^*. \end{aligned} \tag{3.3}$$

Note that formally one has the power series expansion

$$K_1=\sum_{m=0}^{\infty}(VU_{22}^{(1)}V^*U_{11}^{(2)})^mV,$$

$$K_2=\sum_{m=0}^{\infty}(V^*U_{11}^{(2)}VU_{22}^{(1)})^mV^*,$$

which is rigorous if $\|U_{22}^{(1)}\|<1$ or $\|U_{11}^{(2)}\|<1$. These power series expansions combined with the superposition principle were used in Ref. 21 to give a formal proof that the composition rule for scattering matrices was given by the generalized star product.

With these preparations the generalized star product $U=U^{(1)}*_VU^{(2)}$ of the unitary matrices $U^{(1)}$ and $U^{(2)}$ is defined as follows. Write the $(n_1+n_2-2p)\times(n_1+n_2-2p)$ matrix U in a 2×2 block form as

$$U=\begin{pmatrix}U_{11} & U_{12}\\ U_{21} & U_{22}\end{pmatrix},$$

where U_{11} is an $(n_1-p)\times(n_1-p)$ matrix, U_{22} is an $(n_2-p)\times(n_2-p)$ matrix, etc. These matrices are now defined as

$$\begin{aligned}U_{11}&=U_{11}^{(1)}+U_{12}^{(1)}K_2U_{11}^{(2)}VU_{21}^{(1)},\\ U_{22}&=U_{22}^{(2)}+U_{21}^{(2)}K_1U_{22}^{(1)}V^*U_{12}^{(2)},\\ U_{12}&=U_{12}^{(1)}K_2U_{12}^{(2)},\\ U_{21}&=U_{21}^{(2)}K_1U_{21}^{(1)}.\end{aligned}\tag{3.4}$$

In particular for an arbitrary $n\times n$ unitary matrix U and all p such that $1\leqslant p<n$ the $2p\times2p$ matrices $\mathbb{E}=\left(\begin{smallmatrix}0 & \mathbb{I}\\ \mathbb{I} & 0\end{smallmatrix}\right)$ serve as units for the $*_V$-product when $V=\mathbb{I}$,

$$\begin{pmatrix}0 & \mathbb{I}\\ \mathbb{I} & 0\end{pmatrix}*_VU=U_{*V}\begin{pmatrix}0 & \mathbb{I}\\ \mathbb{I} & 0\end{pmatrix}=U.$$

Further, we will need the following Perron–Frobenius-type result which, for the sake of generality, will be formulated to cover also the infinite-dimensional case:

Lemma III.2: Let a compact operator A on a separable Hilbert space $\mathfrak{h}$ be a contraction, i.e. $\|A\|\leqslant1$. Suppose that $\lambda=l$ is an eigenvalue of A. Then

(i) *every $c\in\mathfrak{h}$ such that $Ac=c$ also satisfies $A^*c=c$ and hence also $A^*Ac=AA^*c=c$,* and
(ii) *the geometric and algebraic multiplicities of the eigenvalue $\lambda=1$ are equal.*

Proof: The claim (*i*) is an easy consequence of the singular values decomposition (see, e.g., Ref. 59, p. 155). Thus we have $\mathrm{Ker}(A-1)=\mathrm{Ker}(A^*-1)=(\mathrm{Ran}(A-1))^{\perp}$. The claim (*ii*) now follows from the fact that the geometric and algebraic multiplicities of an eigenvalue λ are unequal iff $\mathrm{Ran}(A-\lambda)\cap\mathrm{Ker}(A-\lambda)$ is nontrivial. □

Also, we will make use of the following.

Lemma III.3: Let A and B be linear compact operators on a separable Hilbert space $\mathfrak{h}$ such that $\|A\|\leqslant1$, $\|B\|\leqslant1$, and $ABb=b$ for some $b\in\mathfrak{h}$. Then $B^*Bb=b$.

Proof: Without loss of generality we may assume that $\|b\|_{\mathfrak{h}}=1$. By Lemma III.2

$$B^*A^*ABb=b.\tag{3.5}$$

Therefore, by well-known inequalities for the singular values of compact operators (see, e.g., Ref. 60) we have

$$1 \leqslant s(AB) \leqslant s(A)s(B) \leqslant \|A\|\|B\| \leqslant 1,$$

where $s(K)$ denotes the maximal singular value of a compact operator K, i.e., the maximal eigenvalue of the self-adjoint non-negative operator K^*K. This gives $s(AB)=s(A)=s(B)=1$. From $s(A)=s(B)=1$ it follows that $\lambda=1$ is a maximal eigenvalue of A^*A and B^*B. By the min-max principle (see, e.g., Ref. 61, Theorem XIII.2) any $c \in \mathfrak{h}$, $\|c\|_{\mathfrak{h}}=1$ maximizing $(c,K^*Kc) \leqslant 1$, satisfies $K^*Kc=c$. Moreover, if $(c,K^*Kc)=1$ with some $\|c\|_{\mathfrak{h}} \leqslant 1$, then $K^*Kc=c$ and $\|c\|_{\mathfrak{h}}=1$. Therefore, since

$$(Bb,A^*ABb)=(b,B^*A^*ABb)=1,$$

we obtain

$$A^*ABb=Bb \tag{3.6}$$

and $\|Bb\|=1$. The relations (3.5) and (3.6) imply that $B^*Bb=B^*A^*ABb=b$. □

Suppose now that the unitary matrix $U^{(1)}$ is not V-compatible with $U^{(2)}$. In this case the linear subspaces of $\mathbb{C}^p$

$$\mathcal{C}=\mathrm{Ker}(\mathbb{I}-VU_{22}^{(1)}V^*U_{11}^{(2)}, \quad \tilde{\mathcal{C}}=\mathrm{Ker}(\mathbb{I}-U_{22}^{(1)}V^*U_{11}^{(2)}V),$$

$$\mathcal{B}=\mathrm{Ker}(\mathbb{I}-V^*U_{11}^{(2)}VU_{22}^{(1)}), \quad \tilde{\mathcal{B}}=\mathrm{Ker}(\mathbb{I}-U_{11}^{(2)}VU_{22}^{(1)}V^*)$$

are nontrivial. By Lemma III.2 we also have

$$\mathcal{C}=\mathrm{Ker}(\mathbb{I}-U_{11}^{(2)*}VU_{22}^{(1)*}V^*), \quad \tilde{\mathcal{C}}=\mathrm{Ker}(\mathbb{I}-V^*U_{11}^{(2)*}VU_{22}^{(1)*}),$$

$$\mathcal{B}=\mathrm{Ker}(\mathbb{I}-U_{22}^{(1)*}V^*U_{11}^{(2)*}V), \quad \tilde{\mathcal{B}}=\mathrm{Ker}(\mathbb{I}-VU_{22}^{(1)*}V^*U_{11}^{(2)*}).$$

Obviously $\tilde{\mathcal{C}}=V^*\mathcal{C}$ and $\tilde{\mathcal{B}}=V\mathcal{B}$. Since V is unitary this implies $\dim\tilde{\mathcal{C}}=\dim\mathcal{C}$ and $\dim\tilde{\mathcal{B}}=\dim\mathcal{B}$. Furthermore, we have the following.

Lemma III.4: The subspaces $\mathcal{B}$ and $\mathcal{C}$ have equal dimensions, $\dim\mathcal{B}=\dim\mathcal{C}$. *Moreover,*

(i) $\mathcal{B}=\mathrm{lin\ span}\{V^*U_{11}^{(2)}c, c\in\mathcal{C}\}=\mathrm{lin\ span}\{U_{22}^{(1)*}V^*c, c\in\mathcal{C}\}$,

$\mathcal{C}=\mathrm{lin\ span}\{VU_{22}^{(1)}b, b\in\mathcal{B}\}=\mathrm{lin\ span}\{U_{11}^{(2)*}Vb, b\in\mathcal{B}\}$,

and

$\tilde{\mathcal{B}}=\mathrm{lin\ span}\{U_{11}^{(2)}V\tilde{c}, \tilde{c}\in\tilde{\mathcal{C}}\}=\mathrm{lin\ span}\{VU_{22}^{(1)*}\tilde{c}, \tilde{c}\in\tilde{\mathcal{C}}\}$,

$\tilde{\mathcal{C}}=\mathrm{lin\ span}\{U_{22}^{(1)}V^*\tilde{b}, \tilde{b}\in\tilde{\mathcal{B}}\}=\mathrm{lin\ span}\{V^*U_{11}^{(2)*}\tilde{b}, \tilde{b}\in\tilde{\mathcal{B}}\}$,

(ii) $U_{21}^{(2)}c=0$ *for all* $c\in\mathcal{C}$,

(iii) $U_{12}^{(1)}b=0$ *for all* $b\in\mathcal{B}$,

(iv) $U_{21}^{(1)*}\tilde{c}=0$ *for all* $\tilde{c}\in\tilde{\mathcal{C}}$,

(v) $U_{12}^{(2)*}\tilde{b}=0$ *for all* $\tilde{b}\in\tilde{\mathcal{B}}$.

Proof: Let $c_i\in\mathbb{C}^p$, $i=1,...,k\leqslant p(k\geqslant 1)$, be a (not necessarily orthogonal) basis in $\mathcal{C}$. For all $i=1,...,k$ we have

$$(\mathbb{I}-VU_{22}^{(1)}V^*U_{11}^{(2)})c_i=0. \tag{3.7}$$

Multiplying these equations by $V^*U_{11}^{(2)}$ from the left we obtain

$$(\mathbb{I}-V^*U_{11}^{(2)}VU_{22}^{(1)}V^*U_{11}^{(2)}c_i=0.$$

Thus

$$\text{lin span}\{V^*U_{11}^{(2)}c, \quad c\in\mathcal{C}\}\subseteq\mathcal{B}. \tag{3.8}$$

By Lemma III.3 it follows from (3.7) that

$$U_{11}^{(2)*}U_{11}^{(2)}c_i=c_i, \quad i=1,...,k. \tag{3.9}$$

Hence,

$$\dim \text{ lin span}\{V^*U_{11}^{(2)}c, \quad c\in\mathcal{C}\}=\dim\ \mathcal{C} \tag{3.10}$$

and therefore by (3.8) $\dim\mathcal{C}\leqslant\dim\mathcal{B}$.

Let $b_i\in\mathbb{C}^p$, $i=1,...,k'\leqslant p$ be some basis in $\mathcal{B}$. We have

$$(\mathbb{I}-V^*U_{11}^{(2)}VU_{22}^{(1)})b_i=0 \tag{3.11}$$

for all $i=1,...,k'$. Multiplying these equations by $VU_{22}^{(1)}$ we obtain

$$(\mathbb{I}-VU_{22}^{(1)}V^*U_{11}^{(2)})VU_{22}^{(1)}b_i=0,$$

and thus

$$\text{lin span}\{VU_{22}^{(1)}b, \quad b\in\mathcal{B}\}\subseteq\mathcal{C}. \tag{3.12}$$

Again by Lemma III.3 it follows from (3.11) that

$$U_{22}^{(1)*}U_{22}^{(1)}b_i, \quad i=1,...,k'. \tag{3.13}$$

Thus

$$\dim \text{ lin span}\{VU_{22}^{(1)}b, \quad b\in\mathcal{B}\}=\dim\mathcal{B} \tag{3.14}$$

and therefore by (3.12) $\dim\mathcal{B}\leqslant\dim\mathcal{C}$. So we have proved that $\dim\mathcal{B}=\dim\mathcal{C}$. The inclusion (3.8) and the equality (3.10) imply that

$$\text{lin span}\{V^*U_{11}^{(2)}c, \quad c\in\mathcal{C}\}=\mathcal{B}.$$

The inclusion (3.12) and the equality (3.14) imply that

$$\text{lin span}\{VU_{22}^{(1)}b, b\in\mathcal{B}\}=\mathcal{C}.$$

The proof of the relations

$$\mathcal{B}=\text{lin span}\{U_{22}^{(1)*}V^*c, \quad c\in\mathcal{C}\},$$

$$\mathcal{C}=\text{lin span}\{U_{11}^{(2)*}Vb, \quad b\in\mathcal{B}\}$$

is similar and will therefore be omitted.

We turn to the proof of (ii)–(v). By the unitarity of $U^{(2)}$ from (3.9) it follows that $U_{21}^{(2)*}U_{21}^{(2)}c_i=0$. Since $\text{Ker}\,A^*A=\text{Ker}\,A$ for any linear operator A we obtain the claim (*ii*). By the unitarity of $U^{(1)}$ from (3.13) it follows that $U_{12}^{(1)*}U_{12}^{(1)}b_i=0$, which proves the claim (*iii*).

As already noted the vectors c_i and b_i also satisfy

$$(\mathbb{I}-U_{11}^{(2)*}VU_{22}^{(1)*}V^*)c_i=0, \quad (\mathbb{I}-U_{22}^{(1)*}V^*U_{11}^{(2)*}V)b_i=0.$$

A final application of Lemma III.3 yields

$$VU_{22}^{(1)}U_{22}^{(1)*}V^*c_i=c_i, \quad V^*U_{11}^{(2)}U_{11}^{(2)*}Vb_i=b_i,$$

which by the unitarity of $U^{(1)}$, $U^{(2)}$ and V implies (*iv*) and (v), which completes the proof of the lemma. □

Lemma III.5:

(i) *The matrices* $\mathbb{I}-VU_{22}^{(1)}V^*U_{11}^{(2)}$ *and* $\mathbb{I}-U_{11}^{(2)*}VU_{22}^{(1)*}V^*$ *map* $\mathcal{C}^\perp$ *bijectively onto itself.*

(ii) *The matrices* $\mathbb{I}-V^*U_{11}^{(2)}VU_{22}^{(1)}$ *and* $\mathbb{I}-U_{22}^{(1)*}V^*U_{11}^{(2)*}V$ *map* $\mathcal{B}^\perp$ *bijectively onto itself.*

(iii) *The matrices* $\mathbb{I}-U_{22}^{(1)}V^*U_{11}^{(2)}V$ *and* $\mathbb{I}-V^*U_{11}^{(2)*}VU_{22}^{(1)*}$ *map* $\tilde{\mathcal{C}}^\perp$ *bijectively onto itself.*

(iv) *The matrices* $\mathbb{I}-U_{11}^{(2)}VU_{22}^{(1)}V^*$ *and* $\mathbb{I}-VU_{22}^{(1)*}V^*U_{11}^{(2)*}$ *map* $\tilde{\mathcal{B}}^\perp$ *bijectively onto itself.*

Proof: Since V is unitary by the definitions of $\tilde{\mathcal{B}}$ and $\tilde{\mathcal{C}}$ it suffices to prove (*i*) and (*ii*). By the definition of $\mathcal{C}$ we have that

$$(c,VU_{22}^{(1)}V^*U_{11}^{(2)}c_\perp)=(U_{11}^{(2)*}VU_{22}^{(1)*}V^*c,c_\perp)=(c,c_\perp)=0$$

for any $c\in\mathcal{C}$ and any $c_\perp\in\mathcal{C}^\perp$. Thus $(\mathbb{I}-VU_{22}^{(1)}V^*U_{11}^{(2)})c_\perp\in\mathcal{C}^\perp$ for all $c_\perp\in\mathcal{C}^\perp$. Conversely, by Lemma III.2 for any $c_\perp\in\mathcal{C}^\perp$ there is a unique $d\in\mathcal{C}^\perp$ which satisfies the equation $(\mathbb{I}-VU_{22}^{(1)}V^*U_{11}^{(2)})d=c_\perp$. This proves the claim (*i*). The claim (*ii*) is proved similarly. □

Theorem III.6: *If at least one of the off-diagonal blocks of the matrices* $U^{(1)}$ *and* $U^{(2)}$ (*i.e.*, $U_{12}^{(1)}$, $U_{21}^{(1)}$, $U_{12}^{(2)}$, *or* $U_{21}^{(2)}$ *is of maximal rank, then the matrix* $U^{(1)}$ *is* V*-compatible with* $U^{(2)}$ *for all unitary* $p\times p$ *matrices* V.

Proof: We recall that for $p\leqslant n_1/2$ the $(n_1-p)\times p$ matrix $U_{12}^{(1)}$ is not of maximal rank ($=\min\{n_1-p,p\}$) iff there is a vector $b\in\mathbb{C}^p$ such that $U_{12}^{(1)}b=0$. For $p\geqslant n_1/2$ the matrix $U_{12}^{(1)}$ is not of maximal rank iff there is a vector $c\in\mathbb{C}^p$ such that $U_{12}^{(1)*}c=0$.

Let us suppose that the matrix $U^{(1)}$ is not V-compatible with $U^{(2)}$. Then by Lemma III.4 it follows that all off-diagonal blocks of $U^{(1)}$ and $U^{(2)}$ are not of maximal rank. □

Actually we have also the following result. Let a unitary $n\times n$ matrix U be written in the block form

$$U=\begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix},$$

where U_{11} is an $(n-p)\times(n-p)$ matrix, U_{22} is a $p\times p$ matrix, etc. with p being an arbitrary integer such that $1\leqslant p<n$.

Lemma III.7: The matrices U_{12} *and* U_{21} *are simultaneously either of maximal rank or not of maximal rank.*

Proof: Let us suppose that $p\leqslant n/2$. Then the $(n-p)\times p$ matrix U_{12} is not of maximal rank iff there is a nonzero vector $b\in\mathbb{C}^p$ such that $U_{12}b=0$. From the unitarity of U it follows that

$$U_{11}^*U_{12}+U_{21}^*U_{22}=0, \quad U_{22}^*U_{22}+U_{12}^*U_{12}=\mathbb{I},$$

and therefore

$$U_{21}^*U_{22}b=0, \quad U_{22}^*U_{22}b=b.$$

Thus $U_{22}b\neq 0$ and $U_{22}b\in\operatorname{Ker}U_{21}^*$. From this it follows that the $(n-p)\times p$ matrix U_{21}^* is not of maximal rank, and thus the $p\times(n-p)$ matrix U_{21} is also not of maximal rank.

Now let us suppose that $n>p\geqslant n/2$. Then the matrix U_{12} is not of maximal rank iff there is a nontrivial vector $b\in\mathbb{C}^{n-p}$ such that $U_{12}^*b=0$. Again from the unitarity we have

$$U_{21}U_{11}^*+U_{22}U_{12}^*=0, \quad U_{11}U_{11}^*+U_{12}U_{12}^*=\mathbb{I},$$

and therefore

$$U_{21}U_{11}^{*}b=0, \quad U_{11}U_{11}^{*}b=b.$$

Thus, the $p\times(n-p)$ matrix U_{21} is not of maximal rank. □

We will show now that the *-product can be extended to arbitrary, not necessarily V-compatible, unitary matrices. We will prove that the operators

$$U_{21}^{(2)}K_1=U_{21}^{(2)}(\mathbb{I}-VU_{22}^{(1)}V^{*}U_{11}^{(2)})^{-1}V$$

and

$$U_{12}^{(1)}K_2=U_{12}^{(1)}(\mathbb{I}-V^{*}U_{11}^{(2)}VU_{22}^{(1)})^{-1}V^{*}$$

are actually well defined. From Lemma III.5 it follows (see Ref. 62, Section 1.5.3) that

$$P_{\mathcal{C}^{\perp}}(\mathbb{I}-VU_{22}^{(1)}V^{*}U_{11}^{(2)})^{-1} \quad \text{and} \quad P_{\mathcal{B}^{\perp}}(\mathbb{I}-V^{*}U_{11}^{(2)}VU_{22}^{(1)})^{-1}$$

are well defined. From (*ii*) and (*iii*) of Lemma III.4 it follows that $\mathcal{C}\subseteq\operatorname{Ker}U_{21}^{(2)}$ and $\mathcal{B}\subseteq\operatorname{Ker}U_{12}^{(1)}$ and thus

$$U_{21}^{(2)}(\mathbb{I}-VU_{22}^{(1)}V^{*}U_{11}^{(2)})^{-1}=U_{21}^{(2)}P_{\mathcal{C}^{\perp}}(\mathbb{I}-VU_{22}^{(1)}V^{*}U_{11}^{(2)})^{-1}$$

and

$$U_{12}^{(1)}(\mathbb{I}-V^{*}U_{11}^{(2)}VU_{22}^{(1)})^{-1}=U_{12}^{(1)}P_{\mathcal{B}^{\perp}}(\mathbb{I}-V^{*}U_{11}^{(2)}VU_{22}^{(1)})^{-1}$$

are well defined. Similarly one can show that the operators

$$U_{21}^{(2)}V(\mathbb{I}-U_{22}^{(1)}V^{*}U_{11}^{(2)}V)^{-1} \quad \text{and} \quad U_{12}^{(1)}V^{*}(\mathbb{I}-U_{11}^{(2)}VU_{22}^{(1)}V^{*})^{-1}$$

are also well defined. With this we obtain that the relations (3.4) indeed also define the generalized star product of two noncompatible unitary matrices. Moreover, we have

$$\begin{gathered}U_{21}^{(2)}(\mathbb{I}-VU_{22}^{(1)}V^{*}U_{11}^{(2)})^{-1}c=0, \quad U_{12}^{(1)}(\mathbb{I}-V^{*}U_{11}^{(2)}VU_{22}^{(1)})^{-1}b=0,\\ U_{21}^{(2)}V(\mathbb{I}-U_{22}^{(1)}V^{*}U_{11}^{(2)}V)^{-1}\tilde{c}=0, \quad U_{12}^{(1)}V^{*}(\mathbb{I}-U_{11}^{(2)}VU_{22}^{(1)}V^{*})^{-1}\tilde{b}=0\end{gathered} \tag{3.15}$$

for all $c\in\mathcal{C}$, $b\in\mathcal{B}$, $\tilde{c}\in\tilde{\mathcal{C}}$, and $\tilde{b}\in\tilde{\mathcal{B}}$.

Theorem III.8: *For arbitrary unitary matrices $U^{(1)}$, $U^{(2)}$, and V the matrix $U=U^{(1)}*_{V}U^{(2)}$ is unitary.*

This theorem was proved in Appendix C of Ref. 21 in the case when $U^{(1)}$ is V-compatible with $U^{(2)}$. For the general case the proof is given in the Appendix.

Analogously one can prove associativity of the generalized star product. More precisely, let $U^{(3)}$ be a unitary $n_3\times n_3$ and V' a unitary $p'\times p'$ matrix with $p'\leqslant n_2$, $p'\leqslant n_3$. If $p+p'\leqslant n_1$, then

$$U^{(1)}*_{V}(U^{(2)}*_{V'}U^{(3)})=(U^{(1)}*_{V}U^{(2)})*_{V'}U^{(3)}$$

holds.

Theorem III.9: *The generalized star product is a continuous operation in each of its two arguments, i.e., for any unitary matrices $U^{(1)}$, $U^{(2)}$, $U^{(3)}$, and V such that $U^{(2)}$ and $U^{(3)}$ have equal size there is a constant $C>0$ depending on $U^{(1)}$ and V only such that*

$$\|U^{(1)}*_{V}U^{(2)}-U^{(1)}*_{V}U^{(3)}\|\leqslant C\|U^{(2)}-U^{(3)}\|,$$

where the norm $\|\cdot\|$ is an arbitrary matrix norm. A similar estimate holds with respect to the first argument.

In Ref. 21 we proved that the scattering matrix of a self-adjoint Laplacian on an arbitrary graph is a continuous function of $\lambda>0$. Theorem III.9 together with the composition rule given in Sec. IV below allows us to give an alternative proof of this fact. We will not dwell on the details here.

In the sequel we will use the notion of the Moore–Penrose pseudoinverse (see, e.g., Ref. 63). Recall that for any (not necessarily square) matrix M its pseudoinverse $M^\star$ is uniquely defined by the Penrose equations

$$MM^\star M=M, M^\star MM^\star=M^\star,$$

$$(M^\star M)^*=M^\star M, (MM^\star)^*=MM^\star.$$

One also has

$$M^{\star *}=M^{**},$$

$$\text{Ran}\ \ M^\star=\text{Ran}\ \ M^*,$$

$$\text{Ker}\ \ M^\star=\text{Ker}\ \ M^*,$$

and $MM^\star=P_{\text{Ran}M}$, $M^\star M=P_{\text{Ran}M^*}$, where $P_{\mathcal{H}}$ denotes the orthogonal projection onto the linear subspace $\mathcal{H}$. Moreover $0^\star=0$. If M is a square matrix of maximal rank, then $M^\star=M^{-1}$.

Let U again be an arbitrary unitary $n\times n$ matrix written in the block form with some $1\leqslant p<n$.

Lemma III.10: If $\text{Ker}\,U_{12}=\{0\}$, *then* $\text{Ker}\,(U_{21}-U_{22}U_{12}^\star U_{11})^*=\{0\}$.

Proof: Assume the converse, i.e., let there be $c\in\mathbb{C}^p$, $c\neq 0$, such that

$$(U_{21}-U_{22}U_{12}^\star U_{11})^*c=0,$$

or, equivalently,

$$U_{21}^*c-U_{11}^*U_{12}^{\star *}U_{22}^*c=0.$$

We multiply this equation by U_{21} from the left and use the unitarity of U which in particular implies

$$U_{21}U_{21}^*+U_{22}U_{22}^*=\mathbb{I}.$$

This yields

$$c-U_{22}U_{22}^*c-U_{21}U_{11}^*U_{12}^{\star *}U_{22}^*c=0. \tag{3.16}$$

Again by unitarity we have $U_{21}U_{11}^*=-U_{22}U_{12}^*$. Recall that

$$U_{12}^*U_{12}^{\star *}=(U_{12}^\star U_{12})^*=(\mathbb{I}-P_{\text{Ker}\,U_{12}})^*=\mathbb{I}$$

by the hypothesis of the lemma. Thus, from (3.16) it follows that $c=0$. □

Now we turn to a discussion of the inverse of a unitary $2p\times 2p$ matrix U with respect to the generalized star product $*_p$, i.e., the existence of the unitary matrices U^L and U^R such that

$$U^L*_pU=U*_pU^R=\mathbb{E},$$

where $\mathbb{E}$ is the $2p\times 2p$ matrix $\left(\begin{smallmatrix}0 & \mathbb{I}\\ \mathbb{I} & 0\end{smallmatrix}\right)$ (in the $p\times p$ block notation). We will not discuss general necessary and sufficient conditions for the existence of U^L and U^R, but simply restrict ourselves to a special case. We will prove the following.

Theorem III.11: *Let U be an arbitrary $2p\times 2p (p\geqslant 1)$ unitary matrix. Let at least one of the $p\times p$ matrices U_{12} and U_{21} be of maximal rank $(=p)$. Then there exists a unique unitary $2p\times 2p$ matrix U' such that*

$$U'*_p U = U*_p U' = \mathbb{E}. \tag{3.17}$$

Proof: By Lemma III.7 both matrices U_{12} and U_{21} have maximal rank. We will discuss only the second of the relations (3.17). In block notation this relation has the form

$$\begin{aligned} &U_{11}+U_{12}(\mathbb{I}-U'_{11}U_{22})^{-1}U'_{11}U_{21}=0,\\ &U'_{22}+U'_{21}(\mathbb{I}-U_{22}U'_{11})^{-1}U_{22}U'_{12}=0,\\ &U_{12}(\mathbb{I}-U'_{11}U_{22})^{-1}U'_{12}=\mathbb{I},\\ &U'_{21}(\mathbb{I}-U_{22}U'_{11})^{-1}U_{21}=\mathbb{I}. \end{aligned} \tag{3.18}$$

By Theorem III.6 the matrix U must be compatible with U' such that $(\mathbb{I}-U'_{11}U_{22})^{-1}$ and $(\mathbb{I}-U_{22}U'_{11})^{-1}$ are both well defined. We multiply the first of the relations (3.18) by U_{12}^{-1} from the left. Next we multiply the resulting expression by $\mathbb{I}-U'_{11}U_{22}$, thus obtaining

$$U'_{11}(U_{21}-U_{22}U_{12}^{-1}U_{11}) = -U_{12}^{-1}U_{11}.$$

By Lemma III.10 we have that $U_{21}-U_{22}U_{12}^{-1}U_{11}$ is invertible and thus

$$U'_{11} = -U_{12}^{-1}U_{11}(U_{21}-U_{22}U_{12}^{-1}U_{11})^{-1}. \tag{3.19}$$

From the third relation in (3.18) we obtain

$$U'_{12}=(\mathbb{I}-U'_{11}U_{22})U_{12}^{-1}=U_{12}^{-1}+U_{12}^{-1}U_{11}(U_{21}-U_{22}U_{12}^{-1}U_{11})^{-1}U_{22}U_{12}^{-1}.$$

The fourth relation in (3.18) gives

$$U'_{21}=U_{21}^{-1}(\mathbb{I}-U_{22}U'_{11})=(U_{21}-U_{22}U_{12}^{-1}U_{11})^{-1}. \tag{3.20}$$

The second relation in (3.18) determines U'_{22}.

It remains to prove that U' is unitary. By the unitarity of the matrix U we have

$$(U_{21}^*-U_{11}^*U_{12}^{*-1}U_{22}^*)(U_{21}-U_{22}U_{12}^{-1}U_{11})=\mathbb{I}+U_{11}^*U_{12}^{*-1}U_{12}^{-1}U_{11}.$$

Therefore

$$(U_{21}^*-U_{11}^*U_{12}^{*-1}U_{22}^*)^{-1}[\mathbb{I}+U_{11}^*U_{12}^{*-1}U_{12}^{-1}U_{11}](U_{21}-U_{22}U_{12}^{-1}U_{11})^{-1}=\mathbb{I},$$

and thus by (3.19) and (3.20) we obtain

$$U_{11}'^*U'_{11}+U_{21}'^*U'_{21}=\mathbb{I}.$$

The relations $U_{12}'^*U'_{12}+U_{22}'^*U'_{22}=\mathbb{I}$, $U_{11}'^*U'_{12}+U_{21}'^*U'_{22}=0$, and $U_{12}'^*U'_{11}+U_{22}'^*U'_{21}=0$ can be proved similarly.

The left inverse is constructed similarly and by means of the obvious relation

$$(U_{21}-U_{22}U_{12}^{-1}U_{11})^{-1}U_{22}U_{12}^{-1}=U_{21}^{-1}U_{22}(U_{21}-U_{22}U_{12}^{-1}U_{11})^{-1}U_{22}U_{12}^{-1}$$

is easily shown to be equal to the right inverse. □

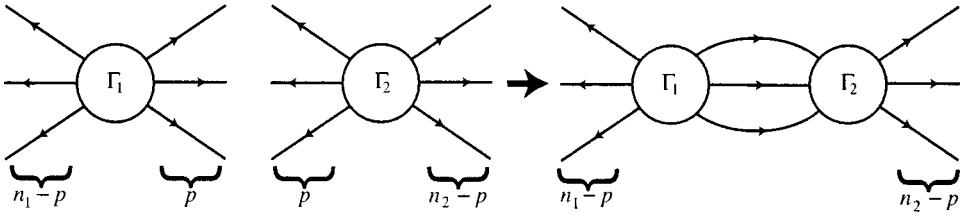

FIG. 1. Gluing of two graphs.

Corollary III.12: *Let* G *be the set of all* $2p\times 2p$ *unitary matrices with* $p\times p$ *blocks* U_{12} *and* U_{21} *both being of maximal rank, endowed with the generalized star product* $*_p$ *as a multiplication and* $\mathbb{E}$ *as a unit. Then* G *is a group isomorphic to* $\mathsf{U}(p,p)$.

The proof will follow from the arguments given in Sec. V. In particular, the group isomorphism between G and $\mathsf{U}(p,p)$ is given by the formulas (5.9) and (5.13). We note that this isomorphism generalizes the well-known *set* isomorphism between the group $\mathsf{SU}(1,1)$ and a subgroup of $\mathsf{SU}(2)$.

The set of *all* $2p\times 2p$ unitary matrices endowed with the generalized star product $*_p$ as a multiplication and $\mathbb{E}$ as a unit is no longer a group but only a semigroup.

IV. COMPOSITION RULE FOR THE SCATTERING MATRICES

Now we apply the generalized star product to prove the composition rule for the scattering matrices on graphs. For this we only need the special case $V=\mathbb{I}_p$, the $p\times p$ unit matrix, and so we introduce the notation $*_p := *_{V=\mathbb{I}_p}$. Let Γ_1 and Γ_2 be two graphs with $n_1\geqslant 1$ and $n_2\geqslant 1$ external lines, respectively, labeled by $\mathcal{E}_1$ and $\mathcal{E}_2$, i.e., $\#(\mathcal{E}_1)=n_1$, $\#(\mathcal{E}_2)=n_2$ and an arbitrary number of internal lines with given fixed lengths (see Fig. 1). Furthermore, at all vertices we have local boundary conditions giving Laplace operators $\Delta(\Gamma_1)$ on Γ_1 and $\Delta(\Gamma_2)$ on Γ_2 and the scattering matrices $S_1(\lambda)$ and $S_2(\lambda)$. Let now $\mathcal{E}_1^0$ and $\mathcal{E}_2^0$ be subsets of $\mathcal{E}_1$ and $\mathcal{E}_2$ respectively having an equal number $1\leqslant p\leqslant \min\{n_1,n_2\}$ of elements. Also let $\varphi_0:\mathcal{E}_1^0\to\mathcal{E}_2^0$ be a one-to-one map. Finally, to each $k\in\mathcal{E}_1^0$ we associate a number $a_k>0$. With these data we can now form a graph Γ by connecting the external line $k\in\mathcal{E}_1^0$ with the line $\varphi_0(k)\in\mathcal{E}_2^0$ to form a line of length a_k. In other words any interval $[0_k,\infty_k)$, $k\in\mathcal{E}_1^0$ belonging to Γ_1 and the interval $[0_{\varphi_0(k)},\infty_{\varphi_0(k)}]$ belonging to Γ_2 is replaced by the finite interval $[0_k,a_k]$ with 0_k being associated to the same vertex in Γ_1 as previously and a_k being associated to the same vertex in Γ_2 as $0_{\varphi_0(k)}$ before in the sense of the discussion at the end of the previous section. Recall that the graphs need not be planar. Thus Γ has $n=n_1+n_2-2p$ external lines indexed by elements in $(\mathcal{E}_1\backslash\mathcal{E}_1^0)\cup(\mathcal{E}_2\backslash\mathcal{E}_2^0)$ and p internal lines indexed by elements in $\mathcal{E}_1^0$ in addition to those of Γ_1 and of Γ_2. We denote this set by $\mathcal{I}_{12}$ such that the set of all internal lines of the graph Γ is given by $\mathcal{I}=\mathcal{I}_1\cup\mathcal{I}_2\cup\mathcal{I}_{12}$. There are no new vertices in addition to those of Γ_1 and Γ_2 so the boundary conditions on Γ_1 and Γ_2 define boundary conditions on Γ resulting in a Laplace operator $\Delta(\Gamma)$. Suppose that the indices of $\mathcal{E}_1^0$ in $\mathcal{E}_1$ come after the indices in $\mathcal{E}_1\backslash\mathcal{E}_1^0$ (in an arbitrary but fixed order) [see (3.1)]. Via the map φ_0 we may identify $\mathcal{E}_2^0$ with $\mathcal{E}_1^0$ so let these indices now come first in $\mathcal{E}_2$, but again in the same order. Finally, let the diagonal $n_2\times n_2$ matrix $V(\underline{a})$ be given as

$$V(\underline{a})=\begin{pmatrix}\exp i\sqrt{\lambda}\underline{a} & 0\\ 0 & \mathbb{I}\end{pmatrix},$$

where $\exp(i\sqrt{\lambda}\underline{a})$ again is the diagonal $p\times p$ matrix given by the p new lengths a_k, $k\in\mathcal{E}_2^0$.

Recall that by Theorem II.1 all eigenfunctions of the operator $-\Delta(\Gamma)$ have the form

$$\psi=\begin{cases}0, & j\in\mathcal{E},\\ \alpha_j e^{i\sqrt{\lambda}x}+\beta_j e^{-i\sqrt{\lambda}x}, & j\in\mathcal{I},\end{cases}$$

where the coefficients α_j and β_j satisfy the homogeneous equation

$$Z_{A,B,\underline{a}}(\lambda)\begin{pmatrix}0\\ \alpha\\ \beta\end{pmatrix}=0, \quad \alpha=\{\alpha_j\}_{j=1}^m, \quad \beta=\{\beta_j\}_{j=1}^m$$

with the matrix $Z_{A,B,\underline{a}}(\lambda)$ defined by (2.6). We define the linear subspace $\mathcal{L}_{12}(\lambda)$ of $\mathbb{C}^{n+2m}$ as a set of all vectors $(0,\alpha,\beta)^T$ for which $\alpha_j=\beta_j=0$ for all $j\in\mathcal{I}_{12}$,

$$\mathcal{L}_{12}(\lambda)=\{l=(0,\alpha,\beta)^T\in \operatorname{Ker} Z_{A,B,\underline{a}}(\lambda)\subset\mathbb{C}^{n+2m}\,|\,\alpha_j=\beta_j \forall j\in\mathcal{I}_{12}\}. \tag{4.1}$$

Obviously for $\lambda\notin\sigma_{A,B,\underline{a}}$ this subspace is trivial, i.e., $\mathcal{L}_{12}(\lambda)=\{0\}$. Let $\Upsilon(\Gamma,\mathcal{I}_{12})\subset\mathbb{R}$ be the set of those eigenvalues of $-\Delta(\Gamma)$ for which $\operatorname{Ker} Z_{A,B,\underline{a}}(\lambda)\ominus\mathcal{L}_{12}(\lambda)$ is nontrivial. Obviously the eigenfunctions corresponding to the eigenvalues from $\Upsilon(\Gamma,\mathcal{I}_{12})$ have nontrivial overlap with $\mathcal{I}_{12}$, i.e., $\operatorname{supp}\phi\cap\mathcal{I}_{12}$ has nonzero measure.

Let $\Xi(\Gamma_1,\Gamma_2)\subset\mathbb{R}_+$ be the set of those $\lambda>0$ for which $\operatorname{Ker}(V(\underline{a})S_{22}^{(1)}(\lambda)V(\underline{a})S_{11}^{(2)}(\lambda)-1)$ is nontrivial.

Theorem IV.1: *With the above notations* $\Xi(\Gamma_1,\Gamma_2)=\Upsilon(\Gamma,\mathcal{I}_{12})\cap\mathbb{R}_+$. *The composition rule*

$$S(\lambda)=S_1(\lambda)*_pV(\underline{a})S_2(\lambda)V(\underline{a}) \tag{4.2}$$

holds for all $\lambda\in\mathbb{R}_+$. *If* $\lambda\in\Upsilon(\Gamma,\mathcal{I}_{12})$ *and* $\lambda>0$, *then its multiplicity equals*

$$\dim\operatorname{Ker}(-\Delta(\Gamma_1)-\lambda)+\dim\operatorname{Ker}(-\Delta(\Gamma_2-\lambda)+\dim\operatorname{Ker}(V(\underline{a})S_{22}^{(1)}(\lambda)V(\underline{a})S_{11}^{(2)}(\lambda)-).$$

In particular, if the eigenvalue $\lambda>0$ *is such that* $\lambda\notin\Upsilon(\Gamma,\mathcal{I}_{12})$, *then its multiplicity equals*

$$\dim\operatorname{Ker}(-\Delta(\Gamma_1)-\lambda)+\dim\operatorname{Ker}(-\Delta(\Gamma_2)-\lambda).$$

Here $\dim\operatorname{Ker}(-\Delta(\Gamma_1)-\lambda)$ denotes the multiplicity of the eigenvalue λ regardless whether it is embedded into the absolutely continuous spectrum or not.

Note that by Lemma III.2 $\dim\operatorname{Ker}(V(\underline{a})S_{22}^{(1)}(\lambda)V(\underline{a})S_{11}^{(2)}(\lambda)-1)$ equals the algebraic multiplicity of the eigenvalue $\mu=1$ of $V(\underline{a})S_{22}^{(1)}(\lambda)V(\underline{a})S_{11}^{(2)}(\lambda)$.

If by cutting p internal lines of an arbitrary graph Γ with local boundary conditions, the graph will be decomposed into two disjoint subgraphs Γ_1 and Γ_2, by Theorem IV.1 the scattering matrix S_Γ can be obtained from the scattering matrices S_{Γ_1} and S_{Γ_2} at the same energy. Thus, using (4.2) iteratively the scattering matrix associated to any graph can be obtained from the scattering matrices associated to its subgraphs each having one vertex only. In fact, pick one vertex and choose all the internal lines connecting to all other vertices. This leads to two graphs and the rule (4.2) may be applied. Iterating this procedure L times, where L is the number of vertices, gives the desired result.

Proof of Theorem IV.1: We split the proof into several steps.

(1) First we suppose that $S_1(\lambda)$ is compatible with $V(\underline{a})S_2(\lambda)V(\underline{a})$ and prove that the composition rule (4.2) holds. Let $\psi_j^k(x,\lambda;\Gamma_l)$, $j\in\mathcal{E}_l\cup\mathcal{I}_l$ for any $k\in\mathcal{E}_l$ be the solution of the Schrödinger equation with the operator $-\Delta(\Gamma_l)$, $l=1,2$ [see (2.4)] at energy λ. Let $\Psi_l(x,\lambda)$ be $n_l\times n_l$ matrices

$$[\Psi_l(x,\lambda)]_{jk}=\psi_j^k(x,\lambda;\Gamma_l), \quad j,k\in\mathcal{E}_l, \quad l=1,2, \tag{4.3}$$

such that

$$\Psi_l(x,\lambda)=e^{-i\sqrt{\lambda}x}\mathbb{I}+e^{i\sqrt{\lambda}x}S_l(\lambda), \quad l=1,2. \tag{4.4}$$

Observe that $e^{-i\sqrt{\lambda}x}$ and $e^{i\sqrt{\lambda}x}$ are linearly independent functions and therefore the scattering matrices may uniquely be recovered from $\Psi_l(x,\lambda)$. The columns of $\Psi_l(x,\lambda)$ define the external part of solutions of the Schrödinger equation for $-\Delta(\Gamma_l)$ at energy λ. We are looking for a square matrix

$$\Psi(x,\lambda)=e^{-i\sqrt{\lambda}x}\mathbb{I}+e^{i\sqrt{\lambda}x}S(\lambda)$$

such that its $(n_1-p)+(n_2-p)=n_1+n_2-2p$ columns defines the external parts of a solution to the Schrödinger equation for $-\Delta(\Gamma)$. Here the indices are assumed to be arranged such that the first indices are those of $\mathcal{E}_1\backslash\mathcal{E}_1^0$ followed by the indices of $\mathcal{E}_2\backslash\mathcal{E}_2^0$. The aim is to obtain $\Psi(x,\lambda)$ from $\Psi_1(x,\lambda)$, $\Psi_2(x,\lambda)$, and the lengths $\underline{a}=\{a_s\}_{s\in\mathcal{I}_{12}}$ of the new internal lines $\mathcal{I}_{12}$. By the above observation this will determine the scattering matrix $S(\lambda)$. The strategy will be to find new solutions of the Schrödinger equations for $-\Delta(\Gamma_l)$ with incoming plane waves $(e^{-i\sqrt{\lambda}x})$ in the channels $k\in\mathcal{E}_l\backslash\mathcal{E}_l^0$ which agree suitably in the channels $k\in\mathcal{E}_1^0$ and $\varphi_0(k)\in\mathcal{E}_2^0$.

With the conventions made above we write

$$\begin{aligned}S_1(\lambda)&=\begin{pmatrix}S_1^{(n_1-p)\times(n_1-p)}(\lambda) & S_1^{(n_1-p)\times p}(\lambda)\\ S_1^{p\times(n_1-p)}(\lambda) & S_1^{p\times p}(\lambda)\end{pmatrix},\\ S_2(\lambda)&=\begin{pmatrix}S_2^{p\times p}(\lambda) & S_2^{p\times(n_2-p)}(\lambda)\\ S_2^{(n_2-p)\times p}(\lambda) & S_2^{(n_2-p)\times(n_2-p)}(\lambda)\end{pmatrix},\end{aligned}\tag{4.5}$$

where the superscripts denote the sizes of the blocks. For arbitrary $p\times(n_1-p)$ matrices C_1 and C_2, respectively, consider the $n_1\times(n_1-p)$ and $n_2\times(n_1-p)$ matrices

$$\begin{aligned}\Phi_1(x,\lambda;C_1)&=e^{-i\sqrt{\lambda}x}\begin{pmatrix}\mathbb{I}\\ C_1\end{pmatrix}+e^{i\sqrt{\lambda}x}S_1(\lambda)\begin{pmatrix}\mathbb{I}\\ C_1\end{pmatrix},\\ \Phi_2(x,\lambda;C_2)&=e^{-i\sqrt{\lambda}x}\begin{pmatrix}C_2\\ 0\end{pmatrix}+e^{i\sqrt{\lambda}x}S_2(\lambda)\begin{pmatrix}C_2\\ 0\end{pmatrix}.\end{aligned}\tag{4.6}$$

Here $\mathbb{I}$ stands for the $(n_1-p)\times(n_1-p)$ unit matrix and 0 stands for the $(n_2-p)\times(n_1-p)$ zero matrix. Obviously, the columns of $\Phi_l(x,\lambda;C_l)$ are the external parts of linear combinations of the columns of $\Psi_l(x,\lambda;\Gamma_l)$, and thus define the external parts of solutions of the Schrödinger equations for the operators $-\Delta(\Gamma_l)$, $l=1,2$. Note that $\Phi_1(x,\lambda;C_1)$ has an incoming plane wave in any of the channels $k\in\mathcal{E}_1\backslash\mathcal{E}_1^0$ and $\Phi_2(x,\lambda;C_2)$ has no incoming plane wave in all channels $k\in\mathcal{E}_2\backslash\mathcal{E}_2^0$.

Now we make the coordinate transformations $x\to a_k-x$ on the lines $\varphi_0(k)\in\mathcal{E}_2^0(k\in\mathcal{E}_1^0)$. The reason for this is as follows. Under the gluing process $\Gamma_1,\Gamma_2\to\Gamma$ (see Fig. 1) the two half-lines corresponding to $k\in\mathcal{E}_1^0$ and $\varphi_0(k)\in\mathcal{E}_2^0$ are replaced by the interval $[0,a_k]$, giving the new lines in $\mathcal{I}_{12}$. This may be realized by identifying a point P on the half-line corresponding to $k\in\mathcal{E}_1^0$ and with coordinate $x(0\leqslant x\leqslant a_k)$ with the point Q on the half-line corresponding to $\varphi_0(k)\in\mathcal{E}_2^0$ with coordinate a_k-x. In particular, $x=a_k$ on the k-line corresponds to $x=0$ on the $\varphi_0(k)$-line and vice versa. Applying this transformation to $\Phi_2(x,\lambda;C_2)$ we obtain in this new coordinate system

$$\Phi_2^{(a)}(x,\lambda;C_2)=\begin{pmatrix}e^{-i\sqrt{\lambda}(\underline{a}-x)} & 0\\ 0 & e^{-i\sqrt{\lambda}x}\end{pmatrix}+\begin{pmatrix}C_2\\ 0\end{pmatrix}+\begin{pmatrix}e^{-i\sqrt{\lambda}(\underline{a}-x)} & 0\\ 0 & e^{-i\sqrt{\lambda}x}\end{pmatrix}S_2(\lambda)\begin{pmatrix}C_2\\ 0\end{pmatrix}.$$

We now require that $\Phi_1(x,\lambda;C_1)$ and $\Phi_2^{(a)}(x,\lambda;C_2)$ agree on the lines labeled by $\mathcal{I}_{12}$. This will fix C_1 and C_2. Indeed, we then obtain

$$e^{-i\sqrt{\lambda}x}C_1+e^{i\sqrt{\lambda}x}S_1^{p\times(n_1-p)}(\lambda)+e^{i\sqrt{\lambda}x}S_1^{p\times p}(\lambda)C_1=e^{-i\sqrt{\lambda}(\underline{a}-x)}C_2+e^{i\sqrt{\lambda}(\underline{a}-x)}S_2^{p\times p}(\lambda)C_2.$$

By the linear independence of the functions $e^{i\sqrt{\lambda}x}$ and $e^{-i\sqrt{\lambda}x}$ it follows that

$$\begin{aligned} C_1 &= e^{i\sqrt{\lambda}\underline{a}} S_2^{p\times p}(\lambda) C_2, \\ S_1^{p\times p}(\lambda) C_1 + S_1^{p\times(n_1-p)}(\lambda) &= e^{-i\sqrt{\lambda}\underline{a}} C_2, \end{aligned} \tag{4.7}$$

and thus

$$\begin{aligned} C_2 &= [\mathbb{I} - e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}} S_2^{p\times p}(\lambda)]^{-1} e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times(n_1-p)}(\lambda), \\ C_1 &= e^{i\sqrt{\lambda}\underline{a}} S_2^{p\times p}(\lambda) [\mathbb{I} - e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}} S_2^{p\times p}(\lambda)]^{-1} e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times(n_i-p)}(\lambda). \end{aligned} \tag{4.8}$$

Since for any invertible A and U the identities $UA^{-1} = (AU^{-1})^{-1}$ and $A^{-1}U = (U^{-1}A)^{-1}$ hold, we have

$$\begin{aligned} [\mathbb{I} - e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}} S_2^{p\times p}(\lambda)]^{-1} e^{i\sqrt{\lambda}\underline{a}} &= [e^{-i\sqrt{\lambda}\underline{a}} - S_1^{p\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}} S_2^{p\times p}(\lambda)]^{-1} \\ &= e^{i\sqrt{\lambda}\underline{a}} [\mathbb{I} - S_1^{p\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}} S_2^{p\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}}]^{-1}. \end{aligned}$$

Since $S_1(\lambda)$ is assumed to be compatible with $V(\underline{a}) S_2(\lambda) V(\underline{a})$ the inverses in (4.8) are well defined.

Similar to (4.5) and according to the ordering convention made previously we write the scattering matrix $S(\lambda)$ for the graph Γ in the block form

$$S(\lambda) = \begin{pmatrix} S^{(n_1-p)\times(n_1-p)}(\lambda) & S^{(n_1-p)\times(n_2-p)}(\lambda) \\ S^{(n_2-p)\times(n_1-p)}(\lambda) & S^{(n_2-p)\times(n_2-p)}(\lambda) \end{pmatrix},$$

where the superscripts denote again the sizes of the blocks. Since $\Phi_1(x,\lambda;C_1)$ has an incoming plane wave in any of the first n_1-p channels $k \in \mathcal{E}_1 \backslash \mathcal{E}_1^0$, Eqs. (4.8) allow one to determine $S^{(n_1-p)\times(n_1-p)}(\lambda)$ and $S^{(n_1-p)\times(n_2-p)}(\lambda)$:

$$\begin{aligned} S^{(n_1-p)\times(n_1-p)}(\lambda) &= S_1^{(n_1-p)\times(n_1-p)}(\lambda) + S_1^{(n_1-p)\times p}(\lambda) C_1 \\ &= S_1^{(n_1-p)\times(n_1-p)}(\lambda) + S_1^{(n_1-p)\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}} S_2^{p\times p}(\lambda) \\ &\quad \times e^{i\sqrt{\lambda}\underline{a}} \cdot [\mathbb{I} - S_1^{p\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}} S_2^{p\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}}]^{-1} S_1^{p\times(n_1-p)}(\lambda), \end{aligned}$$

$$\begin{aligned} S^{(n_2-p)\times(n_1-p)}(\lambda) &= S_2^{(n_2-p)\times p}(\lambda) C_2 \\ &= S_2^{(n_2-p)\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}} \cdot [\mathbb{I} - S_1^{p\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}} S_2^{p\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}}]^{-1} S_1^{p\times(n_1-p)}(\lambda). \end{aligned}$$

To determine the remaining blocks of the scattering matrix $S(\lambda)$ instead of (4.6) we consider the $n_1\times(n_2-p)$ and $n_2\times(n_2-p)$ matrices

$$\begin{aligned} \tilde{\Phi}_1(x,\lambda;\tilde{C}_1) &= e^{-i\sqrt{\lambda}x} \begin{pmatrix} 0 \\ \tilde{C}_1 \end{pmatrix} + e^{i\sqrt{\lambda}x} S_1(\lambda) \begin{pmatrix} 0 \\ \tilde{C}_1 \end{pmatrix}, \\ \tilde{\Phi}_2(x,\lambda;\tilde{C}_2) &= e^{-i\sqrt{\lambda}x} \begin{pmatrix} \tilde{C}_2 \\ \mathbb{I} \end{pmatrix} + e^{i\sqrt{\lambda}x} S_2(\lambda) \begin{pmatrix} \tilde{C}_2 \\ \mathbb{I} \end{pmatrix}, \end{aligned} \tag{4.9}$$

with arbitrary $p\times(n_2-p)$ matrices $\tilde{C}_1$ and $\tilde{C}_2$. Again $\tilde{\Phi}_l(x,\lambda;\tilde{C}_l)$ are the external parts of some solutions of the Schrödinger equations with the operators $-\Delta(\Gamma_l)$, $l=1,2$. Now $\tilde{\Phi}_1(x,\lambda;\tilde{C}_1)$ has no incoming plane waves in the channels $k\in\mathcal{E}_1\setminus\mathcal{E}_1^0$, but $\tilde{\Phi}_2(x,\lambda;\tilde{C}_2)$ has an incoming plane wave in any of the channels $k\in\mathcal{E}_2\setminus\mathcal{E}_2^0$.

Repeating the arguments used above we obtain the following matching conditions for $\tilde{C}_1$ and $\tilde{C}_2$:

$$\begin{aligned}\tilde{C}_2&=e^{i\sqrt{\lambda}\underline{a}}S_1^{p\times p}\tilde{C}_1,\\ S_2^{p\times p}(\lambda)\tilde{C}_2+S_2^{p\times(n_2-p)}(\lambda)&=e^{-i\sqrt{\lambda}\underline{a}}\tilde{C}_1,\end{aligned}\tag{4.10}$$

and thus

$$\tilde{C}_1=[\mathbb{I}-e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times p}(\lambda)e^{i\sqrt{\lambda}\underline{a}}S_1^{p\times p}(\lambda)]^{-1}e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times(n_2-p)}(\lambda),$$

$$\tilde{C}_2=e^{i\sqrt{\lambda}\underline{a}}S_1^{p\times p}(\lambda)[\mathbb{I}-e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times p}(\lambda)e^{i\sqrt{\lambda}\underline{a}}S_1^{p\times p}(\lambda)]^{-1}e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times(n_2-p)}(\lambda).$$

Since $S_1(\lambda)$ is compatible with $V(\underline{a})S_2(\lambda)V(\underline{a})$ the inverses are again well defined. From this and from (4.9) it follows that

$$\begin{aligned}S^{(n_2-p)\times(n_2-p)}(\lambda)&=S_2^{(n_2-p)\times(n_2-p)}(\lambda)+S_2^{(n_2-p)\times p}(\lambda)\tilde{C}_2\\&=S_2^{(n_2-p)\times(n_2-p)}(\lambda)+S_2^{(n_2-p)\times p}(\lambda)e^{i\sqrt{\lambda}\underline{a}}S_1^{p\times p}(\lambda)\\&\quad\cdot[\mathbb{I}-e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times p}(\lambda)e^{i\sqrt{\lambda}\underline{a}}S_1^{p\times p}(\lambda)]^{-1}e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times(n_2-p)}(\lambda),\end{aligned}$$

$$\begin{aligned}S^{(n_1-p)\times(n_2-p)}(\lambda)&=S_1^{(n_1-p)\times p}(\lambda)\tilde{C}_1\\&=S_1^{(n_1-p)\times p}(\lambda)\cdot[\mathbb{I}-e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times p}(\lambda)e^{i\sqrt{\lambda}\underline{a}}S_1^{p\times p}(\lambda)]^{-1}e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times(n_2-p)}(\lambda).\end{aligned}$$

By the definition of the generalized star product (3.4) we obtain (4.2).

(2) Now suppose that $\lambda\in\Xi(\Gamma_1,\Gamma_2)$. We prove that the composition rule (4.2) remains valid. Also $\lambda\in\Upsilon(\Gamma,\mathcal{I}_{12})$ and the multiplicity of λ equals

$$\dim\mathrm{Ker}(-\Delta(\Gamma_1)-\lambda)+\dim\ker(-\Delta(\Gamma_2)-\lambda)+\dim\mathrm{Ker}(V(\underline{a})S_{22}^{(1)}(\lambda)V(\underline{a})S_{11}^{(2)}(\lambda)-1).\tag{4.11}$$

The assumption $\lambda\in\Xi(\Gamma_1,\Gamma_2)$ implies that

$$\mathbb{I}-S_1^{p\times p}(\lambda)e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times p}(\lambda)e^{i\sqrt{\lambda}\underline{a}}$$

and

$$\mathbb{I}-e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times p}(\lambda)e^{i\sqrt{\lambda}\underline{a}}S_1^{p\times p}(\lambda)$$

have nontrivial kernels. This implies that the homogeneous form of the equations (4.7) and (4.10),

$$\begin{aligned}C_1&=e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times p}(\lambda)C_2,\\S_1^{p\times p}(\lambda)C_1&=e^{-i\sqrt{\lambda}\underline{a}}C_2,\end{aligned}\tag{4.12}$$

and

$$\begin{aligned}\widetilde{C}_2 &= e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times p}(\lambda)\widetilde{C}_1,\\ S_2^{p\times p}(\lambda)\widetilde{C}_2 &= e^{-i\sqrt{\lambda}\underline{a}}\widetilde{C}_1,\end{aligned} \tag{4.13}$$

respectively, have nontrivial solutions. It is easy to prove that the inhomogeneous equations (4.7) and (4.10) still have solutions in this case. Consider, for instance, the equation (4.7), which is equivalent to

$$C_2 = e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times(n_1-p)}(\lambda) + e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times p}(\lambda) e^{i\sqrt{\lambda}\underline{a}} S_2^{p\times p}(\lambda) C_2.$$

By the Fredholm alternative this equation has a nontrivial solution iff

$$S_1^{p\times(n_1-p)}(\lambda)^* e^{-i\sqrt{\lambda}\underline{a}} b = 0 \tag{4.14}$$

for any $0 \neq b \in \mathbb{C}^p$ satisfying

$$S_2^{p\times p}(\lambda)^* e^{-i\sqrt{\lambda}\underline{a}} S_1^{p\times p}(\lambda)^* e^{-i\sqrt{\lambda}\underline{a}} b = b.$$

By Lemma III.3 with $A = S_2^{p\times p}(\lambda)^*$ and $B = e^{-i\sqrt{\lambda}\underline{a}} S_1^{p\times p}(\lambda)^* e^{-i\sqrt{\lambda}\underline{a}}$ we have

$$e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times p}(\lambda) S_1^{p\times p}(\lambda)^* e^{-i\sqrt{\lambda}\underline{a}} b = b. \tag{4.15}$$

From the unitarity of $V(\underline{a})S_1(\lambda)V(\underline{a})$, which states in particular that

$$e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times p}(\lambda) S_1^{p\times p}(\lambda)^* e^{-i\sqrt{\lambda}\underline{a}} + e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times(n_1-p)}(\lambda) S_1^{p\times(n_1-p)}(\lambda)^* e^{-i\sqrt{\lambda}\underline{a}} = \mathbb{I},$$

and from (4.15) it follows that

$$e^{i\sqrt{\lambda}\underline{a}} S_1^{p\times(n_1-p)}(\lambda) S_1^{p\times(n_1-p)}(\lambda)^* e^{-i\sqrt{\lambda}\underline{a}} b = 0.$$

Since $\operatorname{Ker} C^*C = \operatorname{Ker} C$ for any operator C we obtain (4.14). Equation (4.10) is discussed similarly.

From (4.6) and (4.9) it follows that the Schrödinger equation with the operator $-\Delta(\Gamma)$ for given value of the spectral parameter $\lambda > 0$ has (nonunique) solutions which have the form

$$\begin{aligned}\Phi_1(x,\lambda;C_1) &= e^{-i\sqrt{\lambda}x}\begin{pmatrix}0\\ C_1\end{pmatrix} + e^{i\sqrt{\lambda}x} S_1(\lambda)\begin{pmatrix}0\\ C_1\end{pmatrix},\\ \Phi_2(x,\lambda;C_2) &= e^{-i\sqrt{\lambda}x}\begin{pmatrix}C_2\\ 0\end{pmatrix} + e^{i\sqrt{\lambda}x} S_2(\lambda)\begin{pmatrix}C_2\\ 0\end{pmatrix},\end{aligned} \tag{4.16}$$

and

$$\begin{aligned}\widetilde{\Phi}_1(x,\lambda;\widetilde{C}_1) &= e^{-i\sqrt{\lambda}x}\begin{pmatrix}0\\ \widetilde{C}_1\end{pmatrix} + e^{i\sqrt{\lambda}x} S_1(\lambda)\begin{pmatrix}0\\ \widetilde{C}_1\end{pmatrix},\\ \widetilde{\Phi}_2(x,\lambda;\widetilde{C}_2) &= e^{-i\sqrt{\lambda}x}\begin{pmatrix}\widetilde{C}_2\\ 0\end{pmatrix} + e^{i\sqrt{\lambda}x} S_2(\lambda)\begin{pmatrix}\widetilde{C}_2\\ 0\end{pmatrix},\end{aligned} \tag{4.17}$$

where C_1 and C_2 ($\widetilde{C}_1$ and $\widetilde{C}_2$) solve (4.12) [(4.13), respectively]. Note that $C_1 = \widetilde{C}_1$ and $C_2 = \widetilde{C}_2$. On the lines in the set $\mathcal{I}_{12}$ the quantity Φ_1 coincides with Φ_2 and $\widetilde{\Phi}_1$ and $\widetilde{\Phi}_2$. We will now prove that

$$S_1^{(n_1-p)\times p}(\lambda)C_1=0, \quad S_2^{(n_2-p)\times p}(\lambda)C_2=0. \tag{4.18}$$

Thus, the functions (4.16) and (4.17) are zero on all external lines of the graph Γ and their support has nontrivial overlap with the interval lines $\mathcal{I}_{12}$.

From (4.12) it follows that $C_1=e^{i\sqrt{\lambda}a}S_2^{p\times p}(\lambda)e^{i\sqrt{\lambda}a}S_1^{p\times p}(\lambda)C_1$. By Lemma III.3 we have

$$S_1^{p\times p}(\lambda)*S_1^{p\times p}(\lambda)C_1=C_1.$$

By unitarity it follows that

$$S_1^{(n_1-p)\times p}(\lambda)*S_1^{(n_1-p)\times p}(\lambda)C_1=0$$

and thus $S_1^{(n_1-p)\times p}(\lambda)C_1=0$. The second relation in (4.18) is proved similarly.

Now we note that from (4.12) and (4.13) it follows that

$$\text{Rank } C_1=\text{Rank } C_2= \dim \text{Ker}(e^{i\sqrt{\lambda}a}S_2^{p\times p}(\lambda)e^{i\sqrt{\lambda}a}S_1^{p\times p}(\lambda)-1).$$

The columns of (4.16) correspond to linear-independent eigenfunctions of $-\Delta(\Gamma)$ for the eigenvalue λ. There are precisely $\dim \text{Ker}(e^{i\sqrt{\lambda}a}S_2^{p\times p}(\lambda)e^{i\sqrt{\lambda}a}S_1^{p\times p}(\lambda)-1)$ such eigenfunctions and the supports of all of them have nontrivial overlap with the internal lines $\mathcal{I}_{12}$.

(3) Let $\lambda\in\Upsilon(\Gamma,\mathcal{I}_{12})\cap\mathbb{R}_+$ and let

$$\dim(\text{Ker } Z_{A,B,a}(\lambda)\ominus\mathcal{L}_{12}(\lambda))=k, \tag{4.19}$$

where the linear subspace $\mathcal{L}_{12}(\lambda)$ is defined by (4.1). This means that there are precisely k eigenfunctions of $-\Delta(\Gamma)$ which disappear if we cut the internal lines $\mathcal{I}_{12}$. We will prove that $\lambda\in\Xi(\Gamma_1,\Gamma_2)$ and that

$$\dim \text{Ker}(V(a)S_{22}^{(1)}(\lambda)V(a)S_{11}^{(2)}(\lambda)-1)=k, \tag{4.20}$$

which in turn implies that

$$\begin{aligned}\dim \text{Ker}(-\Delta(\Gamma)-\lambda)&=\dim \text{Ker}(-\Delta(\Gamma_1)-\lambda)+\dim \text{Ker}(-\Delta(\Gamma_2)-\lambda)\\&\quad+\dim \text{Ker}(V(a)S_{22}^{(1)}(\lambda)V(a)S_{11}^{(2)}(\lambda)-1).\end{aligned}$$

From the existence of the above-mentioned eigenfunctions it follows that these eigenfunctions can be constructed by means of superposition and matching of the solutions (4.4) of the Schrödinger equation for the operators $-\Delta(\Gamma_1)$ and $-\Delta(\Gamma_2)$ at energy $\lambda>0$. For any vectors $C_1,C_2\in\mathbb{C}^p$ the functions

$$\phi_1(x,\lambda,C_1)=e^{-i\sqrt{\lambda}x}\begin{pmatrix}0\\C_1\end{pmatrix}+e^{i\sqrt{\lambda}x}S_1(\lambda)\begin{pmatrix}0\\C_1\end{pmatrix},$$

$$\phi_2(x,\lambda,C_2)=e^{-i\sqrt{\lambda}x}\begin{pmatrix}C_2\\0\end{pmatrix}+e^{i\sqrt{\lambda}x}S_2(\lambda)\begin{pmatrix}C_2\\0\end{pmatrix},$$

define the external parts of solutions of the Schrödinger equations for the operators $-\Delta(\Gamma_l)$, $l=1,2$. Since the eigenfunctions are supported on internal lines of the graph Γ (Theorem II.1) the vectors C_1 and C_2 must satisfy

$$S_1^{(n_1-p)\times p}(\lambda)C_1=0, \quad S_2^{p\times(n_2-p)}(\lambda)C_2=0$$

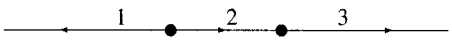

FIG. 2. The graph from Example IV.2.

such that $\phi_1(x,\lambda,C_1)$ vanishes in any of the channels $k\in\mathcal{E}_1\backslash\mathcal{E}_1^0$ and $\phi_2(x,\lambda,C_2)$ vanishes in all channels $k\in\mathcal{E}_2\backslash\mathcal{E}_2^0$. Making the coordinate transformation $x\to\underline{a}-x$ on the lines $\varphi_0(k)\in\mathcal{E}_2^0(k\in\mathcal{E}_1^0)$ and requiring that $\phi_1(x,\lambda,C_1)$ and $\phi_2(\underline{a}-x,\lambda,C_2)$ agree on the lines labeled by $\mathcal{I}_{12}$, we obtain

$$C_1=e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times p}(\lambda)C_2,$$

$$S_1^{p\times p}(\lambda)C_1=e^{-i\sqrt{\lambda}\underline{a}}C_2,$$

or equivalently

$$\begin{aligned} e^{i\sqrt{\lambda}\underline{a}}S_2^{p\times p}(\lambda)e^{i\sqrt{\lambda}\underline{a}}S_1^{p\times p}(\lambda)C_1&=C_1,\\ C_2&=e^{i\sqrt{\lambda}\underline{a}}S_1^{p\times p}(\lambda)C_1. \end{aligned} \tag{4.21}$$

Linear-independent solutions of (4.21) correspond to linear-independent eigenfunctions of $-\Delta(\Gamma)$ and vise versa. Thus the condition (4.19) implies (4.20). This completes the proof of the theorem. □

Note that if Γ is simply the disjoint union of Γ_1 and Γ_2, i.e., if no connections are made (corresponding to $p=0$ and $n=n_1+n_2$), then $S(\lambda)$ is just the direct sum of $S_1(\lambda)$ and $S_2(\lambda)$. Also $V^*S(\lambda)V=S_{2n}^{\text{free}}(\lambda)*_V S(\lambda)$ for any scattering matrix with n open ends and any unitary $n\times n$ matrix V, where

$$S_{2n}^{\text{free}}(\lambda)=\begin{pmatrix}0 & \mathbb{I}\\ \mathbb{I} & 0\end{pmatrix}.$$

Similarly $S(\lambda)*_V S_{2n}^{\text{free}}(\lambda)=VS(\lambda)V^*$.

Example IV.2: Consider an arbitrary self-adjoint Laplacian $\Delta(A,B)$ with local boundary conditions on the graph depicted in Fig. 2, where the distance between the two vertices is a. The composition rule (4.2) with

$$V(a)=\begin{pmatrix}e^{i\sqrt{\lambda}a} & 0\\ 0 & 1\end{pmatrix}.$$

easily gives

$$\begin{aligned} S_{11}&=S_{11}^{(1)}+S_{12}^{(1)}S_{11}^{(2)}S_{21}^{(1)}(1-S_{22}^{(1)}S_{11}^{(2)}e^{2ia\sqrt{\lambda}})^{-1},\\ S_{22}&=S_{22}^{(2)}+S_{22}^{(1)}S_{21}^{(2)}S_{12}^{(2)}(1-S_{22}^{(1)}S_{11}^{(2)}e^{2ia\sqrt{\lambda}})^{-1},\\ S_{12}&=S_{12}^{(1)}S_{12}^{(2)}(1-S_{22}^{(1)}S_{11}^{(2)}e^{2ia\sqrt{\lambda}})^{-1},\\ S_{21}&=S_{21}^{(2)}S_{21}^{(1)}(1-S_{22}^{(1)}S_{11}^{(2)}e^{2ia\sqrt{\lambda}})^{-1}, \end{aligned} \tag{4.22}$$

where the S-matrices are written in the form analogous to (3.1)

$$S^{(1)}=\begin{pmatrix}S_{11}^{(2)} & S_{12}^{(1)}\\ S_{21}^{(1)} & S_{22}^{(1)}\end{pmatrix},\quad S^{(2)}=\begin{pmatrix}S_{11}^{(2)} & S_{12}^{(2)}\\ S_{21}^{(2)} & S_{22}^{(2)}\end{pmatrix},$$

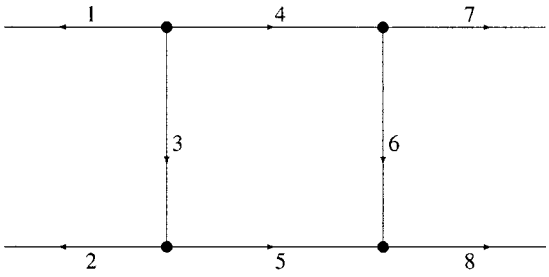

FIG. 3. The graph from Example IV.3. The arrows show the positive direction for every edge. The edges 3 and 6 have the length *a* and the edges 4 and 5 the length *b*.

leaving out the λ *dependence. These relations are equivalent to the well-known factorization formula*[2–4,1,5–7] *applied to the Laplacian on a line with boundary conditions posed at* $x=0$ *and* $x=a$.

Example IV.3: Consider the graph depicted in Fig. 3 where the length of the edges 3 and 6 equals a and the length of the edges 4 and 5 equals b. Let the boundary conditions be given as

$$\begin{aligned}
&\psi_1(0)=\psi_3(0)=\psi_4(0),\\
&\psi_2(0)=\psi_3(a)=\psi_5(0),\\
&\psi_1'(0)+\psi_3'(0)+\psi_4'(0)=0,\\
&\psi_2'(0)+\psi_5'(0)-\psi_3'(a)=0,\\
&\psi_4(b)=\psi_6(0)=\psi_7(0),\\
&\psi_5(b)=\psi_6(a)=\psi_8(0),\\
&-\psi_4'(b)+\psi_6'(0)+\psi_7'(0)=0,\\
&-\psi_5'(b)-\psi_6'(a)+\psi_8'(0)=0.
\end{aligned} \tag{4.23}$$

Obviously they define a self-adjoint operator which we denote by $\Delta(a,b)$. *The scattering matrix corresponding to this operator [as defined by (2.3) and (2.4)] will be denoted by* $S_{a,b}(\lambda)$. *To determine this* 4×4 *matrix we first consider the graph depicted in Fig. 4 where the length of the edge 3 is supposed to be equal a. The boundary conditions (4.23) determine the self-adjoint operator. The corresponding scattering matrix we denote by* $S_a(\lambda)$. *From (2.7) it follows that*

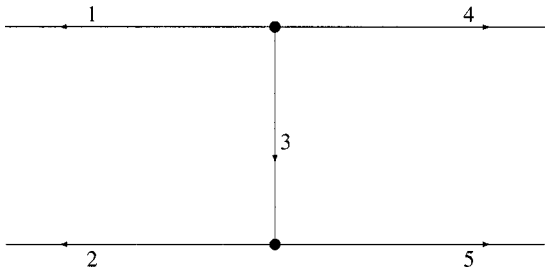

FIG. 4. The graph from Example IV.3. The arrows show the positive direction for every edge.

$$S_a(\lambda)=(e^{i\sqrt{\lambda}a}-9e^{-i\sqrt{\lambda}a})^{-1}$$
$$\times\begin{pmatrix} e^{i\sqrt{\lambda}a}+3e^{-i\sqrt{\lambda}a} & -4 & 2(e^{i\sqrt{\lambda}a}-3e^{-i\sqrt{\lambda}a}) & -4 \\ -4 & e^{i\sqrt{\lambda}a}+3e^{-i\sqrt{\lambda}a} & -4 & 2(e^{i\sqrt{\lambda}a}-3e^{-i\sqrt{\lambda}a}) \\ 2(e^{i\sqrt{\lambda}a}-3e^{-i\sqrt{\lambda}a}) & -4 & e^{i\sqrt{\lambda}a}+3e^{-i\sqrt{\lambda}a} & -4 \\ -4 & 2(e^{i\sqrt{\lambda}a}-3e^{-i\sqrt{\lambda}a}) & -4 & e^{i\sqrt{\lambda}a}+3e^{-i\sqrt{\lambda}a} \end{pmatrix}. \tag{4.24}$$

By Theorem IV.1 the scattering matrix $S_{a,b}(\lambda)$ is given by

$$S_{a,b}(\lambda)=S_a(\lambda)*_2V(\underline{b})S_a(\lambda)V(\underline{b}), \tag{4.25}$$

where

$$V(\underline{b})=\mathrm{diag}(e^{i\sqrt{\lambda}b},e^{i\sqrt{\lambda}b},1,1),\quad \underline{b}=(b,b)\in\mathbb{R}^2.$$

We now compute the 2×2 matrices K_1 and K_2 entering the definition (3.4) *of the generalized star product, thus obtaining*

$$K_1^{-1}=K_2^{-1}=(e^{i\sqrt{\lambda}a}-9e^{-i\sqrt{\lambda}a})^{-2}L,$$

$$(L)_{11}=(L)_{22}=e^{2i\sqrt{\lambda}a}(1-e^{2i\sqrt{\lambda}b})+9e^{-2i\sqrt{\lambda}a}(9-e^{2i\sqrt{\lambda}b})-2(9+11e^{2i\sqrt{\lambda}b}),$$

$$(L)_{12}=(L)_{21}=8e^{2i\sqrt{\lambda}b}(e^{i\sqrt{\lambda}a}+3e^{-i\sqrt{\lambda}a}).$$

From this it follows that

$$\det K_1^{-1}=\det K_2^{-1}=(e^{i\sqrt{\lambda}a}-9e^{-i\sqrt{\lambda}a})^{-4}\cdot e^{-4i\sqrt{\lambda}a}[\xi(\xi\eta^2-64)(\xi-8)^2$$
$$+16\eta(-256-128\xi+44\xi^2-3\xi^3)],$$

where $\xi=\exp\{2i\sqrt{\lambda}a\}-1$ and $\eta=\exp\{2i\sqrt{\lambda}b\}-1$. Obviously these determinants vanish if $e^{2i\sqrt{\lambda}a}=e^{2i\sqrt{\lambda}b}=1$. One can show that there are no other zeros. Note that the embedded eigenvalues of the operator $-\Delta(a,b)$ are determined by the equation $e^{2i\sqrt{\lambda}a}=e^{2i\sqrt{\lambda}b}=1$ such that for incommensurable a and b there are no embedded eigenvalues.

For $e^{2i\sqrt{\lambda}a}=e^{2i\sqrt{\lambda}b}=1$ the matrix $S_a(\lambda)$ is not compatible with $V(\underline{b})S_a(\lambda)V(\underline{b})$ and

$$K_1^{-1}=K_2^{-1}=\frac{1}{2}\begin{pmatrix} 1 & \pm1 \\ \pm1 & 1 \end{pmatrix},$$

where ±1 corresponds to $\exp\{i\sqrt{\lambda}a\}=\pm1$. Obviously $\mathrm{Ker}\,K_1^{-1}=\mathrm{Ker}\,K_2^{-1}$ is the subspace spanned by the vector $(1,\mp1)^T$. Further,

$$(S_a(\lambda))_{12}\begin{pmatrix} 1 \\ \mp1 \end{pmatrix}=\frac{1}{2}\begin{pmatrix} 1 & \pm1 \\ \pm1 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ \mp1 \end{pmatrix}=0$$

and

$$V(\underline{b})S_a(\lambda)V(\underline{b}))_{12}\begin{pmatrix} 1 \\ \mp1 \end{pmatrix}=\frac{1}{2}e^{i\sqrt{\lambda}b}\begin{pmatrix} 1 & \pm1 \\ \pm1 & 1 \end{pmatrix}\begin{pmatrix} 1 \\ \mp1 \end{pmatrix}=0.$$

Thus, as proved in Sec. III, the generalized star product is well defined also in the case when the matrix $S_a(\lambda)$ is not compatible with $V(\underline{b})S_a(\lambda)V(\underline{b})$.

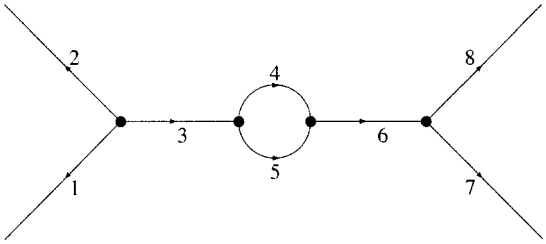

FIG. 5. The graph from Example IV.3. The arrows show the positive direction for every edge. The edges 3 and 6 have the length a and the edges 4 and 5 the length b.

Example IV.4: Consider the graph depicted in Fig. 5 where the length of the edges 3 and 6 equals a and the length of the edges 4 and 5 equals b. Let the boundary conditions be given by

$$\psi_1(0)=\psi_2(0)=\psi_3(0),$$

$$\psi_4(0)=\psi_5(0)=\psi_3(a),$$

$$\psi_1'(0)+\psi_2'(0)+\psi_3'(0)=0,$$

$$\psi_4'(0)+\psi_5'(0)-\psi_3'(a)=0,$$

$$\psi_4(b)=\psi_5(b)=\psi_6(0),$$

$$\psi_6(a)=\psi_7(0)=\psi_8(0),$$

$$-\psi_4'(b)-\psi_5'(b)+\psi_6'(0)=0,$$

$$-\psi_6'(a)+\psi_7'(0)+\psi_8'(0)=0.$$

Obviously they define a self-adjoint operator which we denote by $\Delta(a,b)$. The scattering matrix corresponding to this operator [as defined by (2.3) and (2.4)] will be denoted by $S_{a,b}(\lambda)$. To determine this 4×4 matrix we first consider the graph depicted in Fig. 4 where the length of the edge 3 is supposed to be equal a. The boundary conditions (4.23) determine the self-adjoint operator. The corresponding scattering matrix $S_a(\lambda)$ can be obtained from (4.24) by means of the permutation of its lines and columns thus giving

$$S_a(\lambda)=(e^{i\sqrt{\lambda}a}-9e^{-i\sqrt{\lambda}a})^{-1}$$
$$\times\begin{pmatrix} e^{i\sqrt{\lambda}a}+3e^{-i\sqrt{\lambda}a} & 2(e^{i\sqrt{\lambda}a}-3e^{-i\sqrt{\lambda}a}) & -4 & -4 \\ 2(e^{i\sqrt{\lambda}a}-3e^{-i\sqrt{\lambda}a}) & e^{i\sqrt{\lambda}a}+3e^{-i\sqrt{\lambda}a} & -4 & -4 \\ -4 & -4 & e^{i\sqrt{\lambda}a}+3e^{-i\sqrt{\lambda}a} & 2(e^{i\sqrt{\lambda}a}-3e^{-i\sqrt{\lambda}a}) \\ -4 & -4 & 2(e^{i\sqrt{\lambda}a}-3e^{-i\sqrt{\lambda}a}) & e^{i\sqrt{\lambda}a}+3e^{-i\sqrt{\lambda}a} \end{pmatrix}.$$

By Theorem IV.1 the scattering matrix $S_{a,b}(\lambda)$ is given by

$$S_{a,b}(\lambda)=S_a(\lambda)*_2V(\underline{b})S_a(\lambda)V(\underline{b}), \tag{4.26}$$

where

$$V(\underline{b})=\mathrm{diag}(e^{i\sqrt{\lambda}b},e^{i\sqrt{\lambda}b},1,1), \quad \underline{b}=(b,b).$$

We now compute the 2×2 *matrices* K_1 and K_2 *entering the definition* (3.4) *of the generalized star product, thus obtaining*

$$K_1^{-1}=K_2^{-1}=(e^{i\sqrt{\lambda}a}-9e^{-i\sqrt{\lambda}a})^2L,$$

$$(L)_{11}=(L)_{22}=e^{2i\sqrt{\lambda}a}(1-5e^{2i\sqrt{\lambda}b})+9e^{-2i\sqrt{\lambda}a}(9-5e^{2i\sqrt{\lambda}b})-18(1-e^{2i\sqrt{\lambda}}),$$

$$(L)_{12}=(L)_{21}=-4e^{2i\sqrt{\lambda}b}(e^{2i\sqrt{\lambda}a}-9e^{-2i\sqrt{\lambda}a}).$$

From this it follows that

$$\begin{aligned}\det K_1^{-1}=\det K_2^{-1}=(e^{i\sqrt{\lambda}a}-9e^{-i\sqrt{\lambda}a})^{-4}[&e^{4i\sqrt{\lambda}a}(1-10e^{2i\sqrt{\lambda}b}+9e^{4i\sqrt{\lambda}b})\\&+9^3e^{-4i\sqrt{\lambda}a}(9-10e^{2i\sqrt{\lambda}b}+e^{4i\sqrt{\lambda}b})-36e^{2i\sqrt{\lambda}a}(1-6e^{2i\sqrt{\lambda}b}+5e^{4i\sqrt{\lambda}b})\\&-18^2e^{-2i\sqrt{\lambda}a}(9-14e^{2i\sqrt{\lambda}b}+5e^{4i\sqrt{\lambda}b})+18(27-86e^{2i\sqrt{\lambda}b}+59e^{4i\sqrt{\lambda}b})].\end{aligned}$$

Obviously these determinants vanish if $e^{2i\sqrt{\lambda}b}=1$. *One can show that there are no other zeros. Note that the embedded eigenvalues of the operator* $-\Delta(a,b)$ *are determined by the equation* $e^{2i\sqrt{\lambda}b}=1$.

For $e^{2i\sqrt{\lambda}b}=1$ *the matrices* $S_a(\lambda)$ *and* $V(\underline{b})S_a(\lambda)V(\underline{b})$ *are not compatible and*

$$K_1^{-1}=K_2^{-1}=-4\,\frac{e^{2i\sqrt{\lambda}a}-9e^{-2i\sqrt{\lambda}a}}{(e^{i\sqrt{\lambda}a}-9e^{-i\sqrt{\lambda}a})^2}\begin{pmatrix}1&1\\1&1\end{pmatrix}.$$

Obviously $\operatorname{Ker}K_1^{-1}=\operatorname{Ker}K_2^{-1}$ *is the subspace spanned by the vector* $(1,-1)^T$. *Further,*

$$(S_a(\lambda))_{12}\begin{pmatrix}1\\-1\end{pmatrix}=-4\begin{pmatrix}1&1\\1&1\end{pmatrix}\begin{pmatrix}1\\-1\end{pmatrix}=0$$

and

$$(V(\underline{b})S_a(\lambda)V(\underline{b}))_{12}\begin{pmatrix}1\\-1\end{pmatrix}=-4e^{i\sqrt{\lambda}b}\begin{pmatrix}1&1\\1&1\end{pmatrix}\begin{pmatrix}1\\-1\end{pmatrix}=0.$$

Thus, as proved in Sec. III, the generalized star product is well defined also in the case when the matrices $S_a(\lambda)$ *and* $V(\underline{b})S_a(\lambda)V(\underline{b})$ *are not compatible.*

As already discussed in Ref. 21, multiple application of (4.2) to an arbitrary graph allows one by complete induction on the number of vertices to calculate its scattering matrix from the scattering matrices corresponding to single-vertex graphs. If these single-vertex graphs contain no tadpoles, i.e., internal lines starting and ending at the same vertex, then (4.2) give a complete explicit construction of the scattering matrix in terms of the scattering matrices for single vertex graphs. In the case when a resulting single-vertex graph contains tadpoles we proceed as follows. Let the graph Γ have one vertex, n external lines, and m tadpoles of lengths a_i. To calculate the scattering matrix of Γ we insert an extra vertex on each of the internal lines (for definiteness, say, at $x=a_i/2$). At these new vertices we impose trivial boundary conditions corresponding to continuous differentiability at this point. With these new vertices we may now repeat our previous procedure. Thus in the end we arrive at graphs with one vertex only and no tadpoles.

V. SPECIAL CASE $n_1=n_2=2p$: TRANSFER MATRICES

This section is devoted to the construction of the transfer matrix for Schrödinger operators on graphs with an even number of external lines. The transfer matrix formalism for general Schrödinger operators on the line is well known (see, e.g., Ref. 49). Its relation to the scattering matrix is discussed in, e.g., Refs. 9 and 8.

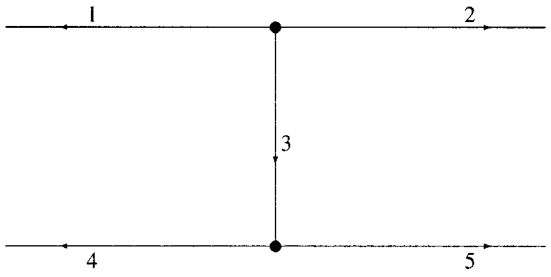

FIG. 6. The same graph as in Fig. 4 but with different ordering of the external lines.

We start with the simplest example of a Laplace operator on the graph with $n=2$ and $m=0$ (see Fig. 6) which is equivalent to a Schrödinger operator on the line with point interaction. The boundary conditions given by the relation

$$\begin{pmatrix} \psi_2(0) \\ \psi_2'(0) \end{pmatrix} = e^{i\mu} \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \psi_1(0) \\ -\psi_1'(0) \end{pmatrix}, \tag{5.1}$$

where the matrix

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \in \mathsf{SL}(2,\mathbb{R}),$$

and μ is real, lead to self-adjoint Laplacians (see Refs. 21 and 64–67). Conversely, from the viewpoint of the von Neumann extension theory (see, e.g., Ref. 54) relation (5.1) describes almost all [with respect to the Haar measure on $\mathsf{U}(2)$] self-adjoint Laplacians $\Delta(A,B)$. If $\exp\{2i\mu\}=1$, the operator $\Delta(A,B)$ is real, i.e., commutes with complex conjugation. In particular, the choice $a-1=d-1=b=0$, $\exp\{2i\mu\}=1$ corresponds to the δ-potential of strength c (see, e.g., Ref. 68).

By definition the transfer matrix is a 2×2 matrix $M(\lambda)\in \mathsf{U}(1)\times\mathsf{SL}(2,\mathbb{R})$ satisfying

$$M(\lambda)\begin{pmatrix} \psi_1(0) \\ \psi_1'(0) \end{pmatrix} = \begin{pmatrix} \psi_2(0) \\ -\psi_2'(0) \end{pmatrix}. \tag{5.2}$$

In fact, in the case at hand it is given explicitly as follows:

$$M(\lambda) = e^{i\mu} \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

If $\exp\{2i\mu\}=1$, the matrix $M(\lambda)$ is unimodular, i.e., $M(\lambda)\in\mathsf{SL}(2;\mathbb{R})$.

The transfer matrix possesses the following equivalent description. Any solution of the Schrödinger equation with the operator $-\Delta(A,B)$ for the energy $\lambda>0$ has the form

$$u_1(x) = a_1 e^{i\sqrt{\lambda}x} + b_1 e^{-i\sqrt{\lambda}x},$$

$$u_2(x) = a_2 e^{i\sqrt{\lambda}x} + b_2 e^{-i\sqrt{\lambda}x}.$$

From this and (5.2) it follows that there is a matrix $\Lambda(\lambda)\in\mathsf{U}(1)\times\mathsf{SU}(1,1)\subset\mathsf{U}(1)\times\mathsf{SL}(2;\mathbb{C})$ (with the inclusion in the group-theoretical sense) such that

$$\Lambda(\lambda)\begin{pmatrix} a_1 \\ b_1 \end{pmatrix} = \begin{pmatrix} b_2 \\ a_2 \end{pmatrix} \tag{5.3}$$

and

$$M(\lambda)=\begin{pmatrix} 1 & 1 \\ i\sqrt{\lambda} & -i\sqrt{\lambda} \end{pmatrix}\Lambda(\lambda)\begin{pmatrix} 1 & 1 \\ i\sqrt{\lambda} & -i\sqrt{\lambda} \end{pmatrix}^{-1}.$$

For $\lambda>0$ the matrix $\Lambda(\lambda)$ is related to the scattering matrix

$$S_{A,B}(\lambda)=\begin{pmatrix} R(\lambda) & T_1(\lambda) \\ T_2(\lambda) & L(\lambda) \end{pmatrix}$$

by the relation

$$\Lambda(\lambda)=\begin{pmatrix} \dfrac{1}{T_2(\lambda)} & -\dfrac{R(\lambda)}{T_2(\lambda)} \\ \dfrac{L(\lambda)}{T_2(\lambda)} & \dfrac{T_1(\lambda)}{|T_2(\lambda)|^2} \end{pmatrix},$$

where

$$T_1(\lambda)=2e^{i\mu}(a-ib\sqrt{\lambda}+ic/\sqrt{\lambda}+d)^{-1},$$

$$T_2(\lambda)=2e^{-i\mu}(a-ib\sqrt{\lambda}+ic/\sqrt{\lambda}+d)^{-1},$$

$$R(\lambda)=(a-ib\sqrt{\lambda}+ic/\sqrt{\lambda}+d)^{-1}(a-ib\sqrt{\lambda}-ic/\sqrt{\lambda}-d),$$

$$L(\lambda)=(a-ib\sqrt{\lambda}+ic/\sqrt{\lambda}+d)^{-1}(-a-ib\sqrt{\lambda}-ic/\sqrt{\lambda}+d),$$

Note that $T_1(\lambda)=T_2(\lambda)$ for all $\lambda>0$ if the operator $\Delta(A,B)$ is real, i.e., $\exp\{2i\mu\}=1$. This is in analogy with Schrödinger operators on the line with potentials which are necessarily real (see, e.g., Refs. 69 and 70).

The factorization rule from Example IV.2 can now be written in the form

$$\Lambda(\lambda)=\Lambda^{(1)}(\lambda)U(a)\Lambda^{(2)}(\lambda)U(a)^{-1}, \tag{5.4}$$

where

$$U(a)=\begin{pmatrix} e^{-i\sqrt{\lambda}a} & 0 \\ 0 & e^{i\sqrt{\lambda}a} \end{pmatrix}.$$

The relation (5.4) is the special case of the well-known factorization formula[1–7] applied to the Laplacian on a line with point interaction.

It is easy to realize that the transfer matrix cannot be defined for *arbitrary* boundary conditions. For instance, the Dirichlet $[\psi_2(0+)=\psi_1(0+)=0]$ or Neuman $[\psi_2'(0+)=\psi_1'(0+)=0]$ or mixed $[\psi_2(0+)+k_2\psi_2'(0+)=\psi_1(0+)+k_1\psi_1'(0+)=0]$ boundary conditions introduce the decoupling $\Delta(A,B)=\Delta_1\oplus\Delta_2$, where Δ_j, $j=1,2$, are the Laplacians on $L^2(0,\infty)$ with corresponding boundary conditions. Recall, however, that the scattering matrix is well defined even in these cases. The composition rule (4.22) (see Example IV.2) remains valid.

Now we consider an arbitrary graph Γ with an even number of external lines $n=2p$. We enumerate the external lines in an arbitrary but fixed order. The external part of an arbitrary solution of the Schrödinger equation with $-\Delta(A,B)$ at the energy $\lambda>0$ has the form

$$u_j(x)=a_je^{i\sqrt{\lambda}x}+b_je^{-i\sqrt{\lambda}x}, \quad j=1,...,n. \tag{5.5}$$

We define the transfer matrix

$$\Lambda(\lambda)\begin{pmatrix} a_1 \\ \vdots \\ a_p \\ b_1 \\ \vdots \\ b_p \end{pmatrix} = \begin{pmatrix} b_{p+1} \\ \vdots \\ b_n \\ a_{p+1} \\ \vdots \\ a_n \end{pmatrix}. \tag{5.6}$$

To prove that $\Lambda(\lambda)$ is correctly defined it suffices to show that for arbitrary constants (a_j, b_j), $j = 1,\ldots,p$, there is a solution to the Schrödinger equation with the operator $-\Delta(A,B)$ whose external part has the form (5.5) and this solution is unique up to its internal part. The external part of any solution to the Schrödinger equation with the operator $-\Delta(A,B)$ is a linear combination of the columns of the matrix-valued function

$$\Psi(x,\lambda) = e^{-i\sqrt{\lambda}x}\mathbb{I} + e^{i\sqrt{\lambda}x}S(\lambda). \tag{5.7}$$

Thus, the columns of (5.7) have to satisfy (5.6), i.e.,

$$\Lambda(\lambda)\begin{pmatrix} S_{11}(\lambda) & S_{12}(\lambda) \\ \mathbb{I} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \mathbb{I} \\ S_{21}(\lambda) & S_{22}(\lambda) \end{pmatrix},$$

where the $p \times p$ block notation is adopted. Writing $\Lambda(\lambda)$ as

$$\Lambda(\lambda) = \begin{pmatrix} \Lambda_{11}(\lambda) & \Lambda_{12}(\lambda) \\ \Lambda_{21}(\lambda) & \Lambda_{22}(\lambda) \end{pmatrix}$$

we obtain

$$\begin{gathered} \Lambda_{11}(\lambda)S_{11}(\lambda) + \Lambda_{12}(\lambda) = 0, \\ \Lambda_{11}(\lambda)S_{12}(\lambda) = \mathbb{I}, \\ \Lambda_{21}(\lambda)S_{11}(\lambda) + \Lambda_{22}(\lambda) = S_{21}(\lambda), \\ \Lambda_{21}(\lambda)S_{12}(\lambda) = S_{22}(\lambda). \end{gathered} \tag{5.8}$$

Let us suppose that $\det S_{12}(\lambda) \neq 0$. Then

$$\Lambda_{11}(\lambda) = S_{12}(\lambda)^{-1}, \Lambda_{12}(\lambda) = -S_{12}(\lambda)^{-1}S_{11}(\lambda),$$

$$\Lambda_{21}(\lambda) = S_{22}(\lambda)S_{12}(\lambda)^{-1}, \Lambda_{22}(\lambda) = S_{21}(\lambda) - S_{22}(\lambda)S_{12}(\lambda)^{-1}S_{11}(\lambda).$$

Thus, we proved that for $\det S_{12}(\lambda) \neq 0$ the transfer matrix exists and has the form

$$\Lambda(\lambda) = \begin{pmatrix} S_{12}(\lambda)^{-1} & -S_{12}(\lambda)^{-1}S_{11}(\lambda) \\ S_{22}(\lambda)S_{12}(\lambda)^{-1} & S_{21}(\lambda) - S_{22}(\lambda)S_{12}(\lambda)^{-1}S_{11}(\lambda) \end{pmatrix}. \tag{5.9}$$

Also, its definition (5.6) immediately leads to the following factorization formula,

$$\Lambda(\lambda) = \Lambda^{(1)}(\lambda)U(\underline{a})\Lambda^{(2)}(\lambda)U(\underline{a})^{-1}, \tag{5.10}$$

where the diagonal unitary matrix $U(\underline{a})$ is given by

$$U(\underline{a})=\begin{pmatrix} e^{-i\sqrt{\lambda}\underline{a}} & 0 \\ 0 & e^{i\sqrt{\lambda}\underline{a}} \end{pmatrix}.$$

Note that formal arguments based on the superposition principle leading to (5.10) have appeared earlier in Ref. 17. As for related results we mention that in Ref. 71 it was shown that the transfer matrix of a Schrödinger operator on the line with a matrix-valued potential can be written in the form (5.9).

Lemma V.1: If $\det S_{12}(\lambda)\neq 0$, *then* $\Lambda(\lambda)\in \mathsf{U}(p,p)$.

Proof: Obviously the coefficients $a_1,\ldots,a_n,b_1,\ldots,b_n$ in (5.5) satisfy the relation

$$\begin{pmatrix} a_1 \\ \vdots \\ a_n \end{pmatrix}=S(\lambda)\begin{pmatrix} b_1 \\ \vdots \\ b_n \end{pmatrix}.$$

From the unitarity of the scattering matrix it follows that

$$|a_1|^2+\cdots+|a_n|^2=|b_1|^2+\cdots+|b_n|^2,$$

or, equivalently,

$$|a_1|^2+\cdots+|a_p|^2-|b_1|^2-|b_p|^2=|b_{p+1}|^2+\cdots+|b_n|^2-|a_{p+1}|^2-\cdots-|a_n|^2.$$

This relation and (5.6) complete the proof of the lemma. □

Let us summarize the above results of the present section:

Theorem V.2: *If* $\det S_{12}(\lambda)\neq 0$, *then the transfer matrix* $\Lambda(\lambda)\in \mathsf{U}(p,p)$ *as given by* (5.9) *exists such that for an arbitrary* $(a_1,\ldots,a_p,b_1,\ldots,b_p)\in\mathbb{C}^n$ *there is a solution of the Schrödinger equation with* $-\Delta(A,B)$ *at the energy* $\lambda>0$ *whose external part has the form* (5.5) *and the coefficients* $(b_{p+1},\ldots,b_n,a_{p+1},\ldots,a_n)\in\mathbb{C}^n$ *are given by* (5.6). *The composition rule for the scattering matrices* (4.2) *is equivalent to the multiplication formula* (5.10) *for the transfer matrices.*

In addition for real operators we have the following.

Theorem V.3: *If the operator* $\Delta(A,B,\underline{a})$ *is real and if in addition* $\det S_{12}(\lambda)\neq 0$, *then* $\Lambda(\lambda)\in \mathsf{SU}(p,p)\subset \mathsf{SL}(2p;\mathbb{C})$.

Proof: From the well-known determinant formula for block matrices (see, e.g., Ref. 72, Section II.5)

$$\det\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}=\det A_{11}\det(A_{22}-A_{21}A_{11}^{-1}A_{12}), \tag{5.11}$$

which follows from the decomposition

$$\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}=\begin{pmatrix} A_{11} & 0 \\ A_{21} & \mathbb{I} \end{pmatrix}\begin{pmatrix} \mathbb{I} & A_{11}^{-1}A_{12} \\ 0 & A_{22}-A_{21}A_{11}^{-1}A_{12} \end{pmatrix},$$

it follows that

$$\det\Lambda(\lambda)=\frac{\det S_{21}(\lambda)}{\det S_{12}(\lambda)}.$$

By Theorem II.2 we have $S_{12}(\lambda)^T=S_{21}(\lambda)$ and thus $\det\Lambda(\lambda)=1$. □

We turn now to a discussion of the assumption $\det S_{12}(\lambda)\neq 0$. For the scattering matrix of the graph depicted in Fig. 4 with the boundary conditions (4.23) (see Example IV.3) $\det(S_a(\lambda))_{12}=0$ for all $\lambda>0$.

Theorem V.4: *Suppose that* $\det S_{12}(\lambda)=0$. *Then the transfer matrix* $\Lambda(\lambda)$ *exists such that for arbitrary*

$$(a_1,\ldots,a_p,b_1,\ldots,b_p)\in \mathrm{Ran}\begin{pmatrix}\mathbb{I} & 0\\ 0 & P_{(\mathrm{Ker}\, S_{12}(\lambda))^\perp}\end{pmatrix}\subset\mathbb{C}^n$$

there is a solution of the Schrödinger equation with $-\Delta(A,B,\underline{a})$ *at energy* $\lambda>0$ *whose external part has the form (5.5) and the coefficients* $(b_{p+1},\ldots,b_n,a_{p+1},\ldots,a_n)\in\mathbb{C}^n$ *are given by* (5.6).

Proof: The external part of any solution to the Schrödinger equation with the operator $-\Delta(A,B,\underline{a})$ satisfying the conditions of the theorem is a linear combination of the columns of the matrix-valued function

$$\Psi(x,\lambda)\begin{pmatrix}\mathbb{I} & 0\\ 0 & P_{(\mathrm{Ker}\, S_{12}(\lambda))^\perp}\end{pmatrix}, \tag{5.12}$$

where $\Psi(x,\lambda)$ is given by (5.7). Thus, the columns of (5.12) have to satisfy (5.6), i.e.,

$$\begin{pmatrix}\Lambda_{11}(\lambda) & \Lambda_{12}(\lambda)\\ \Lambda_{21}(\lambda) & \Lambda_{22}(\lambda)\end{pmatrix}\begin{pmatrix}S_{11}(\lambda) & S_{12}(\lambda)P_{(\mathrm{Ker}\, S_{12}(\lambda))^\perp}\\ \mathbb{I} & 0\end{pmatrix}=\begin{pmatrix}0 & P_{(\mathrm{Ker}\, S_{12}(\lambda))^\perp}\\ S_{21}(\lambda) & S_{22}(\lambda)P_{(\mathrm{Ker}\, S_{12}(\lambda))^\perp}\end{pmatrix}.$$

The solution of this equation can be wiritten in the form

$$\Lambda_{11}(\lambda)=S_{12}(\lambda)^\star,\Lambda_{12}(\lambda)=-S_{12}(\lambda)^\star S_{11}(\lambda),$$

$$\Lambda_{21}(\lambda)=S_{22}(\lambda)S_{12}(\lambda)^\star,\Lambda_{22}=S_{21}(\lambda)-S_{22}(\lambda)S_{12}(\lambda)^\star S_{11}(\lambda),$$

where $\star$ stands for the Penrose–Moore pseudoinverse. □

Note that any vector of the form $(c,0)^T$ with $c\in\mathrm{Ker}\, S_{12}(\lambda)$ satisfies $\Lambda(\lambda)\binom{c}{0}=0$. Thus $\det\Lambda(\lambda)=0$.

Inspection of the proof of Theorem V.4 shows that the transfer matrix cannot be extended to a subspace larger than

$$\mathrm{Ran}\begin{pmatrix}\mathbb{I} & 0\\ 0 & P_{(\mathrm{Ker}\, S_{12}(\lambda))^\perp}\end{pmatrix}.$$

If $\det\Lambda^{(1)}(\lambda)=\det\Lambda^{(2)}(\lambda)=0$, then $\mathrm{Ran}\, U(\underline{a})\Lambda^{(2)}(\lambda)U(\underline{a})$ and $\mathrm{Ker}\,\Lambda^{(1)}(\lambda)$ may have a nontrivial overlap and therefore the multiplication formula (5.10) does not hold in this case.

Example V.5: Consider the graph depicted in Fig. 4 with the boundary conditions from Example IV.3. For all $\lambda\in\mathbb{R}_+$ *such that* $e^{2i\sqrt{\lambda}a}=1$ *we have that* $\mathrm{Ker}\, S_{12}(\lambda)$ *is nontrivial and*

$$P_{\mathrm{Ker}\, S_{12}(\lambda)}=\frac{1}{2}\begin{pmatrix}1 & \mp 1\\ \mp 1 & 1\end{pmatrix},$$

$$P_{(\mathrm{Ker}\, S_{12}(\lambda))^\perp}=\frac{1}{2}\begin{pmatrix}1 & \pm 1\\ \pm 1 & 1\end{pmatrix},$$

where ± 1 *corresponds to* $\exp\{i\sqrt{\lambda}a\}=\pm 1$. *Suppose that*

$$(a_1,a_2,b_1,b_2)^T\notin\mathrm{Ran}\begin{pmatrix}\mathbb{I} & 0\\ 0 & P_{(\mathrm{Ker}\, S_{12}(\lambda))^\perp}\end{pmatrix},$$

or, equivalently,

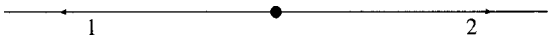

FIG. 7. The graph with $n=2$ and $m=0$.

$$(a_1,a_2,b_1,b_2)^T \in \mathrm{Ran}\begin{pmatrix} 0 & 0 \\ 0 & P_{\mathrm{Ker}\, S_{12}(\lambda)} \end{pmatrix}.$$

In particular, we can choose

$$a_1=a_2=0, \quad b_1=1, \quad b_2=\mp 1.$$

It is easy to check that there is no solution to the Schrödinger equation with these boundary conditions.

Example V.6: Consider the graph depicted in Fig. 7 with the boundary conditions as in Example IV.4. $\mathrm{Ker}\, S_{12}(\lambda)$ *is nontrivial for all* $\lambda \in \mathbb{R}_+$ *and*

$$P_{\mathrm{Ker}\, S_{12}(\lambda)}=\frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad P_{(\mathrm{Ker}\, S_{12}(\lambda))^\perp}=\frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

Suppose again that

$$(a_1,a_2,b_1,b_2)^T \notin \mathrm{Ran}\begin{pmatrix} \mathbb{I} & 0 \\ 0 & P_{(\mathrm{Ker}\, S_{12}(\lambda))^\perp} \end{pmatrix}$$

and choose

$$a_1=a_2=0, \quad b_1=1, \quad b_2=1.$$

Again it is easy to check that there is no solution to the Schrödinger equation with these boundary conditions.

The statement converse to Theorem V.2 immediately follows from Theorem V.4.

Theorem V.7: *If the transfer matrix* $\Lambda(\lambda)$ *exists in the sense of Theorem V.2, then* $\det S_{12}(\lambda)\neq 0$ *and the corresponding scattering matrix is given by*

$$S(\lambda)=\begin{pmatrix} -\Lambda_{11}(\lambda)^{-1}\Lambda_{12}(\lambda) & \Lambda_{11}(\lambda)^{-1} \\ \Lambda_{22}(\lambda)-\Lambda_{21}(\lambda)\Lambda_{11}(\lambda)^{-1}\Lambda_{12}(\lambda) & \Lambda_{21}(\lambda)\Lambda_{11}(\lambda)^{-1} \end{pmatrix}. \tag{5.13}$$

Proof: Suppose that $\det S_{12}(\lambda)=0$. Then by Theorem V.4 we get $\det \Lambda(\lambda)=0$, which is a contradiction. Thus, $\det S_{12}(\lambda)\neq 0$ and therefore by Theorem V.2 $\det \Lambda(\lambda)\neq 0$. The representation (5.13) follows from (5.8). □

ACKNOWLEDGMENT

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APPENDIX: PROOF OF THEOREM III.8

Here we give the proof of Theorem III.8 which claims that for arbitrary unitary matrices $U^{(1)}$, $U^{(2)}$, and V the matrix $U=U^{(1)}*_V U^{(2)}$ defined by (3.4) is unitary. As already noted in Ref. 21 it suffices to prove only the relations

$$U_{11}^* U_{11}+U_{21}^* U_{21}=\mathbb{I},$$

$$U_{11}^* U_{12}+U_{21}^* U_{22}=0. \tag{A1}$$

The remaining relations,

$$U_{12}^{*}U_{12}+U_{22}^{*}U_{22}=\mathbb{I},$$

$$U_{12}^{*}U_{11}+U_{22}^{*}U_{21}=0, \tag{A2}$$

follow immediately from (A1). To see this for an arbitrary unitary matrix U we define an involutive map $U\mapsto U^{\tau}$ given as

$$U=\begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}\mapsto U^{\tau}=\begin{pmatrix} U_{22} & U_{21} \\ U_{12} & U_{11} \end{pmatrix}.$$

Direct calculations show that the following ''transposition law,''

$$U^{\tau}=U^{(2)^{\tau}}*_{V^{*}}U^{(1)^{\tau}} \tag{A3}$$

holds whenever $U=U^{(1)}*_{V}U^{(2)}$. Assume that (A1) holds for arbitrary unitary U. Replacing the matrix U by U^{τ} given by (A3) transforms the relations (A1) into (A2).

By the definition of the generalized star product (3.4) and by the unitarity of $U^{(1)}$ the first of the relations (A1) is equivalent to

$$\begin{aligned} &-U_{21}^{(1)*}U_{21}^{(1)}+U_{21}^{(1)*}V^{*}U_{11}^{(2)*}K_{2}^{*}U_{12}^{(1)*}U_{11}^{(1)}+U_{11}^{(1)*}U_{12}^{(1)}K_{2}U_{11}^{(2)}VU_{21}^{(1)} \\ &\quad+U_{21}^{(1)*}V^{*}U_{11}^{(2)*}K_{2}^{*}U_{12}^{(1)*}U_{12}^{(1)}K_{2}U_{11}^{(2)}VU_{21}^{(1)}+U_{21}^{(1)*}K_{1}^{*}U_{21}^{(2)*}U_{21}^{(2)}K_{1}U_{21}^{(1)}=0. \end{aligned} \tag{A4}$$

Since the opposite case was already considered in Ref. 21, we further assume that the matrix $U^{(1)}$ is not V-compatible with $U^{(2)}$. From Theorem III.6 it follows that all off-diagonal blocks $U_{12}^{(1)}$, $U_{21}^{(1)}$, $U_{12}^{(2)}$, and $U_{21}^{(2)}$ are not of maximal rank and thus $\operatorname{Ker}U_{21}^{(1)}$ is nontrivial. Let d_i, $1\leqslant i\leqslant k=\dim\ \operatorname{Ker}U_{21}^{(1)}$, be an arbitrary basis in $\operatorname{Ker}U_{21}^{(1)}$. From the unitary of the matrix $U^{(1)}$ we get $U_{12}^{(1)*}U_{11}^{(1)}d_i=0$ for all $1\leqslant i\leqslant k$. Thus

$$\begin{aligned} &[-U_{21}^{(1)*}U_{21}^{(1)}+U_{21}^{(1)*}V^{*}U_{11}^{(2)*}K_{2}^{*}U_{12}^{(1)*}U_{11}^{(1)}+U_{11}^{(1)*}U_{12}^{(1)}K_{2}U_{11}^{(2)}VU_{21}^{(1)} \\ &\quad+U_{21}^{(1)*}V^{*}U_{11}^{(2)*}K_{2}^{*}U_{12}^{(1)*}U_{12}^{(1)}K_{2}U_{11}^{(2)}VU_{21}^{(1)}+U_{21}^{(1)*}K_{1}^{*}U_{21}^{(2)*}U_{21}^{(2)}K_{1}U_{21}^{(1)}]d_i=0 \end{aligned}$$

for all $1\leqslant i\leqslant k$. Hence to prove (A4) it remains to show that

$$\begin{aligned} &[-U_{21}^{(1)*}U_{21}^{(1)}+U_{21}^{(1)*}V^{*}U_{11}^{(2)*}K_{2}^{*}U_{12}^{(1)*}U_{11}^{(1)}+U_{11}^{(1)*}U_{12}^{(1)}K_{2}U_{11}^{(2)}VU_{21}^{(1)} \\ &\quad+U_{21}^{(1)*}V^{*}U_{11}^{(2)*}K_{2}^{*}U_{12}^{(1)*}U_{12}^{(1)}K_{2}U_{11}^{(2)}VU_{21}^{(1)}+U_{21}^{(1)*}K_{1}^{*}U_{21}^{(2)*}U_{21}^{(2)}K_{1}U_{21}^{(1)}]d=0. \end{aligned} \tag{A5}$$

for any $d\in(\operatorname{Ker}U_{21}^{(1)})^{\perp}=\operatorname{Ran}U_{21}^{(1)*}$. Therefore we set $d=U_{21}^{(1)*}\tilde{d}$, where $\tilde{d}\in\mathbb{C}^{p}$ is an arbitrary vector. Thus, the relation (A5) holds whenever

$$\begin{aligned} &[-U_{21}^{(1)*}U_{21}^{(1)}U_{21}^{(1)*}+U_{21}^{(1)*}V^{*}U_{11}^{(2)*}K_{2}^{*}U_{12}^{(1)*}U_{11}^{(1)}U_{21}^{(1)*}+U_{11}^{(1)*}U_{12}^{(1)}K_{2}U_{11}^{(2)}VU_{21}^{(1)}U_{21}^{(1)*} \\ &\quad+U_{21}^{(1)*}V^{*}U_{11}^{(2)*}K_{2}^{*}U_{12}^{(1)*}U_{12}^{(1)}K_{2}U_{11}^{(2)}VU_{21}^{(1)}U_{21}^{(1)*}+U_{21}^{(1)*}K_{1}^{*}U_{21}^{(2)*}U_{21}^{(2)}K_{1}U_{21}^{(1)}U_{21}^{(1)*}]\tilde{d}=0 \end{aligned} \tag{A6}$$

for all $\tilde{d}\in\mathbb{C}^{p}$.

First we note that by Lemma III.4 (*iv*) the relation (A6) holds for all $\tilde{d}\in\tilde{\mathcal{C}}$. Therefore it suffices to prove that (A6) holds for all $\tilde{d}\in\tilde{\mathcal{C}}^{\perp}$. Observe that in this case by Lemma III.4 (*i*) and by the unitarity of the matrices $U^{(1)}$ and $U^{(2)}$ we have

$$U_{12}^{(1)*}U_{11}^{(1)}U_{21}^{(1)*}\tilde{d}=-U_{12}^{(1)*}U_{12}^{(1)}U_{22}^{(1)*}\tilde{d}=-U_{22}^{(1)*}\tilde{d}+U_{22}^{(1)*}U_{22}^{(1)}U_{22}^{(1)*}\tilde{d}\in\mathcal{B}^{\perp},$$

$$U_{11}^{(2)}VU_{21}^{(1)}U_{21}^{(1)*}\tilde{d}=U_{11}^{(2)}V\tilde{d}-U_{11}^{(2)}VU_{22}^{(1)}U_{22}^{(1)*}\tilde{d}\in\tilde{B}^{\perp}, \tag{A7}$$

$$U_{21}^{(1)}U_{21}^{(1)*}\tilde{d}=\tilde{d}-U_{22}^{(1)}U_{22}^{(1)*}\tilde{d}\in\tilde{\mathcal{C}}^{\perp}.$$

To prove the first relation in (A7) it suffices to show that for any $\tilde{d}\in\tilde{\mathcal{C}}^{\perp}$ and any $b\in\mathcal{B}$

$$-(b,U_{22}^{(1)*}\tilde{d})+(b,U_{22}^{(1)*}U_{22}^{(1)}U_{22}^{(1)*}\tilde{d})=-(U_{22}^{(1)}b,\tilde{d})+(U_{22}^{(1)}U_{22}^{(1)*}U_{22}^{(1)}b,\tilde{d})=0. \tag{A.8}$$

By the definition of $\mathcal{B}$ and by Lemma III.3 $U_{22}^{(1)*}U_{22}^{(1)}b=b$ for any $b\in\mathcal{B}$ which proves (A8). To prove the second relation in (A7) it suffices to show for any $\tilde{d}\in\tilde{\mathcal{C}}^{\perp}$ and any $\tilde{b}\in\tilde{\mathcal{B}}$

$$(\tilde{b},U_{11}^{(2)}V\tilde{d})-(\tilde{b},U_{11}^{(2)}VU_{22}^{(1)}U_{22}^{(1)*}\tilde{d})=(V^{*}U_{11}^{(2)}\tilde{b},\tilde{d})-(U_{22}^{(1)}U_{22}^{(1)*}V^{*}U_{11}^{(2)*}\tilde{b},\tilde{d})=0. \tag{A9}$$

By Lemma III.4 (*i*) $V^{*}U_{11}^{(2)}\tilde{b}\in\tilde{\mathcal{C}}$. By the definition of $\tilde{\mathcal{C}}$ and by Lemma III.3 $U_{22}^{(1)}U_{22}^{(1)*}\tilde{c}=\tilde{c}$ for any $\tilde{c}\in\tilde{\mathcal{C}}$ which proves (A9). This also proves that

$$(\tilde{c},\tilde{d})-(\tilde{c},U_{22}^{(1)}U_{22}^{(1)*}\tilde{d})=(\tilde{c},\tilde{d})-(U_{22}^{(1)}U_{22}^{(1)*}\tilde{c},\tilde{d})=0$$

for all $\tilde{d}\in\tilde{\mathcal{C}}^{\perp}$ and all $\tilde{c}\in\tilde{\mathcal{C}}$ from which the third relation in (A7) follows.

From Lemma III.5 and the definition (3.2) of the matrices K_1 and K_2 it follows that

$$\begin{aligned}
&(i)\quad K_1 \text{ maps } \tilde{\mathcal{C}}^{\perp} \text{ onto } \mathcal{C}^{\perp} \text{ bijectively},\\
&(ii)\quad K_1^{*} \text{ maps } \mathcal{C}^{\perp} \text{ onto } \tilde{\mathcal{C}}^{\perp} \text{ bijectively},\\
&(iii)\quad K_2 \text{ maps } \tilde{\mathcal{B}}^{\perp} \text{ onto } \mathcal{B}^{\perp} \text{ bijectively},\\
&(iv)\quad K_2^{*} \text{ maps } \mathcal{B}^{\perp} \text{ onto } \tilde{\mathcal{B}}^{\perp} \text{ bijectively},
\end{aligned} \tag{A10}$$

Noting that $U_{12}^{(1)*}U_{12}^{(1)}b_{\perp}=b_{\perp}-U_{22}^{(1)*}U_{22}^{(1)}b_{\perp}\in\mathcal{B}^{\perp}$ and $U_{21}^{(2)*}U_{21}^{(2)}c_{\perp}=c_{\perp}-U_{11}^{(2)*}U_{11}^{(2)}c_{\perp}\in\tilde{\mathcal{C}}^{\perp}$ due to (A7) and (A10) we can write the lhs of (A6) in the form

$$\begin{aligned}
U_{21}^{(1)*}[&-\mathbb{I}-V^{*}U_{11}^{(2)*}K_2U_{22}^{(1)*}-U_{22}^{(1)}K_2U_{11}^{(2)}V+V^{*}U_{11}^{(2)*}K_2^{*}K_2U_{11}^{(2)}V\\
&-V^{*}U_{11}^{(2)*}K_2^{*}U_{22}^{(1)*}U_{22}^{(1)}K_2U_{11}^{(2)}V+K_1^{*}K_1-K_1^{*}U_{11}^{(2)*}U_{11}^{(2)}K_1]U_{21}^{(2)*}U_{21}^{(2)}\tilde{d}.
\end{aligned} \tag{A11}$$

Similar to Ref. 21 one can easily prove that for any $\tilde{b}_{\perp}\in\tilde{\mathcal{B}}^{\perp}$ and $\tilde{c}_{\perp}\in\tilde{\mathcal{C}}^{\perp}$ the following relations hold:

$$K_1^{*}K_1\tilde{c}_{\perp}=\tilde{c}_{\perp}+U_{22}^{(1)}K_2U_{11}^{(2)}V\tilde{c}_{\perp}+V^{*}U_{11}^{(2)*}K_2^{*}U_{22}^{(1)*}\tilde{c}_{\perp}+V^{*}U_{11}^{(2)*}K_2^{*}U_{22}^{(1)*}U_{22}^{(1)}K_2U_{11}^{(2)}V\tilde{c}_{\perp}.$$

$$K_1^{*}U_{11}^{(2)*}U_{11}^{(2)}K_1\tilde{c}_{\perp}=V^{*}(\mathbb{I}+U_{11}^{(2)*}K_2^{*}U_{22}^{(1)*}V^{*})U_{11}^{(2)*}U_{11}^{(2)}(\mathbb{I}+VU_{22}^{(1)}K_2U_{11}^{(2)})V\tilde{c}_{\perp},$$

$$K_2^{*}K_2\tilde{b}_{\perp}=\tilde{b}_{\perp}+K_2^{*}U_{22}^{(1)*}V^{*}U_{11}^{(2)*}+U_{11}^{(2)}VU_{22}^{(1)}K_2\tilde{b}_{\perp}+K_2^{*}U_{22}^{(1)*}V^{*}U_{11}^{(2)*}U_{11}^{(2)}VU_{22}^{(1)}K_2\tilde{b}_{\perp}.$$

Inserting these relations in (A11) with the choice $\tilde{c}_\perp = U_{21}^{(2)*} U_{21}^{(2)} \tilde{d}$ and $\tilde{b}_\perp = U_{11}^{(2)} V \tilde{c}_\perp$ we obtain that it vanishes, thus completing the proof of the first relation in (A1). The proof of the second relation in (A1) is similar and will therefore be omitted.

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Chirality in the context of spin $\frac{3}{2}$ particles

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In this paper we apply the chiral spinorial approach to the description of spin $\frac{3}{2}$ particles. Chiral components of rank 3 spinor fields are considered to be the dynamical variables of the theory. The free Lagrangian is built from the same principles as in the case of spin 1 and spin 2 particles: chiral symmetry at the free field level and chiral symmetry breakdown at the interaction level. We show how the chiral spinorial approach provides an unambiguous Lagrangian approach for massless spin $\frac{3}{2}$ particles. This approach provides a fairly rich set of effective Lagrangians for the interaction of spin $\frac{3}{2}$ particles. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1316061]

I. INTRODUCTION

The usual way to describe a massive (or massless) spin $\frac{3}{2}$ field is to use the Rarita–Schwinger[1] (RS) spinor-vector $\Phi^{\mu}_{,a}$ field (four vector indices $\mu=0,1,2,3$ and four spinor indices $a=1,2,3,4$) which satisfies the equations

$$(i\partial\!\!\!/-m)_{ab}\Phi_{\mu,b}=0, \tag{1.1}$$

$$\gamma^{\mu}_{ab}\Phi_{\mu,b}=0, \tag{1.2}$$

$$\partial^{\mu}\Phi_{\mu,a}=0. \tag{1.3}$$

The RS theory can be obtained as a consequence of the more general Bargmann–Wigners[2] (BW) approach, which assigns to a massive particle of spin s, a spinorial symmetric field of rank $2s$, obeying a Dirac equation in each index.

This paper deals with the extension to particles of spin $\frac{3}{2}$, of our chiral spinorial approach.[3,4] We show in this paper that our method provides an ambiguity free approach to the description of spin $\frac{3}{2}$ particles.

In our approach we use a set of 8 chiral fields which are built from the rank 3 spinor field. These chiral fields are treated as independent field variables. We have in this way, a set of eight Dirac-type equations. The fact that we have a larger number of equations than the BW method, means that we are able to describe particles with more degrees of freedom than Bargmann and Wigner did. We shall come back to this point in a future paper.

Besides the enlargement of the number of degrees of freedom our method relies upon a Lagrangian from which we can derive all equations of motion. These equations can be written either in terms of the chiral fields or alternatively, in terms of tensor fields. Within this Lagrangian approach one can easily discuss internal and discrete symmetries such as C, P, and T.

In this paper we shall see that RS equations follow from chiral invariance at the free field level and chiral asymmetry at the interaction level. In this way we have extended to spin $\frac{3}{2}$ the description used by us to particles of spin 1 (Ref. 3) and spin 2.[4]

The chiral spinorial method is also useful in the construction of effective interactions.[5] In this approach the interactions are represented as effective Lagrangians involving the coupling of the eight chiral components, with matter fields and the other fields.

The plan of this paper is the following: in Sec. II we review the BW method and discuss some aspects of this theory. We have pointed out in this section some ambiguities of this approach for spin $\frac{3}{2}$ particles.

In Sec. III we define the chiral components and show how they can be written in terms of vector–spinor and tensor–spinor fields.

Chiral invariance is defined in Sec. IV. The free field Lagrangian is required to be chiral invariant. This is enough to fix the first order derivative Lagrangian for spin $\frac{3}{2}$ particles. The chiral invariant Lagrangian is shown to lead to the right equations for massless $\frac{3}{2}$ particles in Sec. V. This is done through the use of the set of equations for the chiral components.

In Sec. VI we show that in the massive case our Lagrangian leads to a Lagrangian approach for the Rarita–Schwinger equation. The Lagrangian is written in terms of the vector–spinor and tensor–spinor fields which are now treated as independent field variables.

The approach developed here is particularly useful in phenomenological applications. In Sec. VII we show how this method will lead to a large number of Lagrangians for the interaction of spin $\frac{3}{2}$ particles to other particles.

We end this paper by drawing some conclusions in Sec. VIII.

II. SPINORS AND THE BARGMANN–WIGNER APPROACH

We take the generally accepted view that particles of spin s can be described by a rank $2s$ spinor field $\psi_{a_1 a_2 \cdots a_{2s}}(x)$. In the case of spin 1 and 2 particles this is a departure of the usual approach that relies upon the use of vector and tensor fields. For particles of spin $\frac{3}{2}$ the basic field is a rank 3 spinor field $\psi_{a_1 a_2 a_3}(x)$.

The problem with this approach is that we deal with a field having too many degrees of freedom. In fact, in the case of the spin $\frac{3}{2}$ particles we are dealing with a field with 64 components, and so we have 64 degrees of freedom.

How to we deal with so many degrees of freedom? Some of these degrees of freedom are fields which can be expressed in terms of more fundamental fields. One expects some relations among them. There might also be constraints upon these fields.

These relations, or constraints, can be obtained from three equations proposed by Bargmann and Wigner:[2]

$$i\partial\!\!\!/ \otimes 1 \otimes 1\,\psi = m\psi, \tag{2.1a}$$

$$1 \otimes i\partial\!\!\!/ \otimes 1\,\psi = m\psi, \tag{2.1b}$$

$$1 \otimes 1 \otimes i\partial\!\!\!/\,\psi = m\psi. \tag{2.1c}$$

where m is the mass of the Bargmann–Wigner field, which is associated to the mass of the spin $\frac{3}{2}$ particles.

The first problem with the Bargmann–Wigner equations is that they cannot be obtained from a Lagrangian density. BW method is not based on a Lagrangian approach.

The second problem with the BW method is that for a general 64 component spinor field three equations are not enough to impose all restrictions and relations among the components. It is enough however for symmetric spinors. We shall come to this point later.

Finally, we would like to stress the fact that the Bargmann–Wigner method fails in the case of zero mass particles.

We shall see that the chiral spinorial method proposed by us provides a better description for particles of spin $\frac{3}{2}$, since we are able to cure all these three problems associated with the BW method.

In order to understand the problems discussed before let us reduce the number of degrees of freedom to 40 by imposing the symmetry of ψ into two indices. This can be achieved by means of a decomposition of the field ψ in terms of the symmetric matrices $(\gamma^\mu C)$ and $(\sigma^{\mu\nu}C)$. We write

$$\psi_{a_1a_2a_3}(x)=\psi_{a_1a_3a_2}(x)=D_1\mathbf{\Phi}_{\mu,a_1}(x)(\gamma^\mu C)_{a_2a_3}+D_2\mathcal{G}_{\mu\nu,a_1}(x)(\sigma^{\mu\nu}C)_{a_2a_3} \tag{2.2a}$$

or

$$\psi_{a_2a_3a_1}(x)=\psi_{a_2a_1a_3}(x)=D_1\mathbf{\Phi}_{\mu,a_2}(x)(\gamma^\mu C)_{a_3a_1}+D_2\mathcal{G}_{\mu\nu,a_2}(x)(\sigma^{\mu\nu}C)_{a_3a_1} \tag{2.2b}$$

or

$$\psi_{a_3a_1a_2}(x)=\psi_{a_3a_2a_1}(x)=D_1\mathbf{\Phi}_{\mu,a_3}(x)(\gamma^\mu C)_{a_1a_2}+D_2\mathcal{G}_{\mu\nu,a_3}(x)(\sigma^{\mu\nu}C)_{a_1a_2}. \tag{2.2c}$$

where $\mathcal{G}_{\mu\nu,a}$ is a tensor-spinor field and $\mathbf{\Phi}_{\mu,a}$ is the RS vector–spinor field. Clearly each of the above decompositions takes into account the symmetry in only two indices.

A decomposition that takes into account the symmetry in all indices is

$$\begin{aligned}\psi_{a_1a_2a_3}(x)=\psi_{a_2a_3a_1}(x)=\psi_{a_3a_1a_2}(x)=\cdots=d_1\{&\varphi_{\mu,a_1}(x)(\gamma^\mu C)_{a_2a_3}+\varphi_{\mu,a_2}(x)(\gamma^\mu C)_{a_3a_1}\\&+\varphi_{\mu,a_3}(x)(\gamma^\mu C)_{a_1a_2}\}+d_2\{G_{\mu\nu,a_1}(x)(\sigma^{\mu\nu}C)_{a_2a_3}\\&+G_{\mu\nu,a_2}(x)(\sigma^{\mu\nu}C)_{a_3a_1}+G_{\mu\nu,a_3}(x)(\sigma^{\mu\nu}C)_{a_1a_2}\}.\end{aligned} \tag{2.3}$$

For a totally symmetric tensor the BW equations reduces to just one equation since for a symmetric ψ we have the identity

$$(i\partial\!\!\!/\otimes 1\otimes 1)\psi=(1\otimes i\partial\!\!\!/\otimes 1)\psi=(1\otimes 1\otimes i\partial\!\!\!/)\psi. \tag{2.4}$$

For a symmetric spinor we are left with just one equation. One equation is not enough to impose all relations and constraints expected for the $\mathbf{\Phi}_{\mu,a}$ and $\mathcal{G}_{\mu\nu,a}$ fields. There is, however, a way of getting around this problem. It amounts, in fact, to the use of a simple trick. We use the partially symmetric decomposition in the BW equations and then assume that ψ is totally symmetric.

Let us consider the simple example of $\psi_{a_1a_2a_3}$ as given by decomposition (2.2a). Since C^{-1}, $C^{-1}\gamma^5$, and $C^{-1}\gamma^5\gamma^\mu$ are antisymmetric matrices, the following projections are obviously zero:

$$\mathrm{Tr}(C^{-1}_{a_1a_2}\cdot\psi_{a_1a_2a_3})=0,$$

$$\mathrm{Tr}((C^{-1}\gamma^5)_{a_1a_2}\cdot\psi_{a_1a_2a_3})=0,$$

$$\mathrm{Tr}((C^{-1}\gamma^5\gamma^\mu)_{a_1a_2}\cdot\psi_{a_1a_2a_3})=0.$$

Let us use in the above equations the nonsymmetrical decomposition (2.2a). We will be led to the following independent conditions:

$$\gamma^\mu_{a_1a_2}\mathbf{\Phi}_{\mu,a_2}=0, \tag{2.5}$$

$$\mathbf{\Phi}^\mu_{a_1}=2i\frac{D_2}{D_1}(\gamma_\nu)_{a_1a_2}\mathcal{G}^{\mu\nu}_{a_2}. \tag{2.6}$$

The first constraint, (2.5), is just one of the Rarita–Schwinger (RS) equations for the spinor–vector $\mathbf{\Phi}^\mu_{,a}$. The use of the second constraint (2.6), and of the BW equations (2.1b) gives rise, after further extra manipulations, to the other two RS equations:

$$(i\partial\!\!\!/ - m)_{ab}\mathbf{\Phi}_{\mu,b} = 0 \tag{2.7}$$

and

$$\partial^{\mu}\mathbf{\Phi}_{\mu,a} = 0. \tag{2.8}$$

Clearly we will obtain the same results if we use expressions (2.2b) or (2.2c) for ψ and take the appropriate projections.

The conclusion is that the way of getting the RS equations from the BW method, works but is a tricky method. We use an asymmetric decomposition but assume that the field is a symmetric one.

Finally let us relate the superposition coefficients φ_{μ} and $G_{\mu\nu}$ of the totally symmetric decomposition (2.3) of ψ, to the coefficients $\mathbf{\Phi}^{\mu}$ and $\mathcal{G}^{\mu\nu}$. We get

$$2D_1\mathbf{\Phi}^{\mu}_{,a_1} = d_1\{2\varphi^{\mu}_{,a_1} + (\gamma^{\alpha}\gamma^{\mu})_{a_1a_2}\varphi_{\alpha,a_2}\} + d_2(\sigma^{\alpha\beta}\gamma^{\mu})_{a_1a_2}G_{\alpha\beta,a_2}, \tag{2.9}$$

$$2D_2\mathcal{G}^{\mu\nu}_{,a_1} = d_1(\gamma^{\alpha}\sigma^{\mu\nu})_{a_1a_2}\varphi_{\alpha,a_2} + 4d_2G_{\mu\nu,a_1} + d_2(\sigma^{\alpha\beta}\sigma^{\mu\nu})_{a_1a_2}G_{\alpha\beta,a_2}. \tag{2.10}$$

III. CHIRAL COMPONENTS

Let us analyze the relativistic equations for spin $\frac{3}{2}$ particles by using the spinorial approach. Within the spinorial approach we treat chiral components as independent field variables. For spin $\frac{1}{2}$ particles we define two chiral components as

$$\psi_R = \tfrac{1}{2}(1+\gamma^5)\psi$$

$$\psi_L = \tfrac{1}{2}(1-\gamma^5)\psi.$$

For the rank 3 spinor field ψ, one can introduce, in close analogy with the spin $\frac{1}{2}$ case, the chiral components:

$$\begin{aligned}
\psi^{RRR}_{a_1a_2a_3} &= \tfrac{1}{2}(1+\gamma^5)\otimes\tfrac{1}{2}(1+\gamma^5)\otimes\tfrac{1}{2}(1+\gamma^5)\psi,\\
\psi_{RRL} &= \tfrac{1}{2}(1+\gamma^5)\otimes\tfrac{1}{2}(1+\gamma^5)\otimes\tfrac{1}{2}(1-\gamma^5)\psi,\\
\psi_{RLR} &= \tfrac{1}{2}(1+\gamma^5)\otimes\tfrac{1}{2}(1-\gamma^5)\otimes\tfrac{1}{2}(1+\gamma^5)\psi,\\
\psi_{LRR} &= \tfrac{1}{2}(1-\gamma^5)\otimes\tfrac{1}{2}(1+\gamma^5)\otimes\tfrac{1}{2}(1+\gamma^5)\psi,\\
\psi_{LLR} &= \tfrac{1}{2}(1-\gamma^5)\otimes\tfrac{1}{2}(1-\gamma^5)\otimes\tfrac{1}{2}(1+\gamma^5)\psi,\\
\psi_{LRL} &= \tfrac{1}{2}(1-\gamma^5)\otimes\tfrac{1}{2}(1+\gamma^5)\otimes\tfrac{1}{2}(1-\gamma^5)\psi,\\
\psi_{RLL} &= \tfrac{1}{2}(1+\gamma^5)\otimes\tfrac{1}{2}(1-\gamma^5)\otimes\tfrac{1}{2}(1-\gamma^5)\psi,\\
\psi_{LLL} &= \tfrac{1}{2}(1-\gamma^5)\otimes\tfrac{1}{2}(1-\gamma^5)\otimes\tfrac{1}{2}(1-\gamma^5)\psi,
\end{aligned} \tag{3.1}$$

where by definition

$$\psi = \psi_{RRR} + \psi_{RRL} + \psi_{RLR} + \psi_{LRR} + \psi_{LLR} + \psi_{LRL} + \psi_{RLL} + \psi_{LLL}\,. \tag{3.2}$$

To each possible expansions of the spinor ψ, there corresponds a set of chiral components: there is a set of equations obtained from a nonsymmetric decomposition and another set obtained from the symmetrized decomposition. We shall analyze both sets of equations. We shall see that the method works in both cases.

The chiral components defined in (3.1) assumes, after inserting the nonsymmetrized expression in (3.1), the following form:

$$
\begin{aligned}
\psi^{RRR}_{a_1a_2a_3} &= D_2(\mathcal{G}_{\mu\nu R})_{a_2}(\sigma^{\mu\nu}C)_{Ra_3a_1},\\
\psi_{RRL} &= D_1(\mathbf{\Phi}_{\mu R})(\gamma^{\mu}C)_L,\\
\psi_{RLR} &= D_2(\mathcal{G}_{\mu\nu L})(\sigma^{\mu\nu}C)_R,\\
\psi_{LRR} &= D_1(\mathbf{\Phi}_{\mu R})(\gamma^{\mu}C)_R,\\
\psi_{LLR} &= D_1(\mathbf{\Phi}_{\mu L})(\gamma^{\mu}C)_R,\\
\psi_{LRL} &= D_2(\mathcal{G}_{\mu\nu R})(\sigma^{\mu\nu}C)_L,\\
\psi_{RLL} &= D_1(\mathbf{\Phi}_{\mu L})(\gamma^{\mu}C)_L,\\
\psi_{LLL} &= D_2(\mathcal{G}_{\mu\nu L})(\sigma^{\mu\nu}C)_L,
\end{aligned}
\tag{3.3}
$$

where in (3.3), we have introduced the more compact following notation:

$$
\begin{aligned}
&\tfrac{1}{2}(1\pm\gamma^5)_{a_1a_2}\mathbf{\Phi}_{\mu a_2} = (\mathbf{\Phi}_{\mu})^{Ra_1}_{L},\\
&\tfrac{1}{2}(1\pm\gamma^5)\mathcal{G}_{\mu\nu} = (\mathcal{G}_{\mu\nu})^{R}_{L},\\
&(\tfrac{1}{2}(1\pm\gamma^5)\gamma^{\mu}C)_{a_1a_2} = (\gamma^{\mu}C)^{R}_{L},\\
&(\tfrac{1}{2}(1\pm\gamma^5)\sigma^{\mu\nu}C) = (\sigma^{\mu\nu}C)^{R}_{L}.
\end{aligned}
\tag{3.4}
$$

We will refer to the chiral components (3.3) as to the nonsymmetrized chiral components. One can see that the chiral components provides a way of separating the vector–spinor from the tensor–spinor contributions.

The chiral components defined in (3.1) assumes after inserting the symmetrized expansion of ψ into (3.1) and having in mind the notation (3.4), the following form:

$$
\begin{aligned}
\psi^{RRR}_{a_1a_2a_3} &= d_2\{(G_{\mu\nu R})_{a_1}(\sigma^{\mu\nu}C)_{Ra_2a_3}+(G_{\mu\nu R})_{a_2}(\sigma^{\mu\nu}C)_{Ra_3a_1}+(G_{\mu\nu R})_{a_3}(\sigma^{\mu\nu}C)_{Ra_1a_2}\},\\
\psi^{RRL}_{a_1a_2a_3} &= d_1\{(\varphi_{\mu R})_{a_1}(\gamma^{\mu}C)_{Ra_2a_3}+(\varphi_{\mu R})_{a_2}(\gamma^{\mu}C)_{La_3a_1}\}+d_2(G_{\mu\nu L})_{a_3}(\sigma^{\mu\nu}C)_{Ra_1a_2},\\
\psi^{RLR}_{a_1a_2a_3} &= d_1\{(\varphi_{\mu R})_{a_1}(\gamma^{\mu}C)_{La_2a_3}+(\varphi_{\mu R})_{a_3}(\gamma^{\mu}C)_{Ra_1a_2}\}+d_2(G_{\mu\nu L})_{a_2}(\sigma^{\mu\nu}C)_{Ra_3a_1},\\
\psi^{LRR}_{a_1a_2a_3} &= d_1\{(\varphi_{\mu R})_{a_2}(\gamma^{\mu}C)_{Ra_3a_1}+(\varphi_{\mu R})_{a_3}(\gamma^{\mu}C)_{La_1a_2}\}+d_2(G_{\mu\nu L})_{a_1}(\sigma^{\mu\nu}C)_{Ra_2a_3},\\
\psi^{LLR}_{a_1a_2a_3} &= d_1\{(\varphi_{\mu L})_{a_1}(\gamma^{\mu}C)_{La_2a_3}+(\varphi_{\mu L})_{a_2}(\gamma^{\mu}C)_{Ra_3a_1}\}+d_2(G_{\mu\nu R})_{a_3}(\sigma^{\mu\nu}C)_{La_1a_2},\\
\psi^{LRL}_{a_1a_2a_3} &= d_1\{(\varphi_{\mu L})_{a_1}(\gamma^{\mu}C)_{Ra_2a_3}+(\varphi_{\mu L})_{a_3}(\gamma^{\mu}C)_{La_1a_2}\}+d_2(G_{\mu\nu R})_{a_2}(\sigma^{\mu\nu}C)_{La_3a_1},
\end{aligned}
\tag{3.5}
$$

$$\psi^{RLL}_{a_1a_2a_3} = d_1\{(\varphi_{\mu L})_{a_2}(\gamma^\mu C)_{La_3a_1} + (\varphi_{\mu L})_{a_3}(\gamma^\mu C)_{Ra_1a_2}\} + d_2(G_{\mu\nu R})_{a_1}(\sigma^{\mu\nu}C)_{La_2a_3},$$

$$\psi^{LLL}_{a_1a_2a_3} = d_2\{(G_{\mu\nu L})_{a_1}(\sigma^{\mu\nu}C)_{La_2a_3} + (G_{\mu\nu L})_{a_2}(\sigma^{\mu\nu}C)_{La_3a_1} + (G_{\mu\nu L})_{a_3}(\sigma^{\mu\nu}C)_{La_1a_2}\}.$$

Chiral components (3.5) will be named symmetrized chiral components.

Our next step will be to write the free Lagrangian for the chiral components.

IV. CHIRAL TRANSFORMATION AND CHIRAL INVARIANCE

Let us turn now to the construction of the free field Lagrangian. If one imposes the requirement of Lorentz invariance and requires further that the Lagrangian be first order, the Lagrangian density will be written under the general form

$$\mathcal{L}_0 = a_1\overline{\psi}(i\partial\!\!\!/\otimes 1\otimes 1)\psi + a_2\overline{\psi}(1\otimes i\partial\!\!\!/\otimes 1)\psi + a_3\overline{\psi}(1\otimes 1\otimes i\partial\!\!\!/)\psi. \tag{4.1}$$

For spin $\frac{1}{2}$ particles, chiral transformation is defined as the following transformation of the field:

$$\psi \to \psi^{\text{chi}} = e^{i\theta\gamma^5}\psi = (\cos\theta + i\gamma^5\sin\theta)\psi. \tag{4.2}$$

The natural extension of (4.2) will be the following general chiral transformation:

$$\psi \to \psi^{\text{chi}} = e^{i\theta_1\gamma^5}\otimes e^{i\theta_2\gamma^5}\otimes e^{i\theta_3\gamma^5}\psi. \tag{4.3}$$

Under this general chiral transformation, the chiral components will be transformed as

$$\begin{aligned}
\psi_{RRR} &\to \psi^{\text{chi}}_{RRR} = e^{i(\theta_1+\theta_2+\theta_3)}\psi_{RRR},\\
\psi_{RRL} &\to \psi^{\text{chi}}_{RRL} = e^{i(\theta_1+\theta_2-\theta_3)}\psi_{RRL},\\
\psi_{RLR} &\to \psi^{\text{chi}}_{RLR} = e^{i(\theta_1-\theta_2+\theta_3)}\psi_{RLR},\\
\psi_{LRR} &\to \psi^{\text{chi}}_{LRR} = e^{i(-\theta_1+\theta_2+\theta_3)}\psi_{LRR},\\
\psi_{LLR} &\to \psi^{\text{chi}}_{LLR} = e^{i(-\theta_1-\theta_2+\theta_3)}\psi_{LLR},\\
\psi_{LRL} &\to \psi^{\text{chi}}_{LRL} = e^{i(-\theta_1+\theta_2-\theta_3)}\psi_{LRL},\\
\psi_{RLL} &\to \psi^{\text{chi}}_{RLL} = e^{i(\theta_1-\theta_2-\theta_3)}\psi_{RLL},\\
\psi_{LLL} &\to \psi^{\text{chi}}_{LLL} = e^{i(-\theta_1-\theta_2-\theta_3)}\psi_{LLL}.
\end{aligned} \tag{4.4}$$

As far as the chiral components are concerned, chiral transformation stands for phase transformations. Each chiral component transforms under a different phase.

In order to get a chiral invariant Lagrangian, we are left with just one among the following three options:

$$a_1 = a_2 = 0 \Rightarrow \theta_1 = \theta_2 = 0$$

or

$$a_1 = a_3 = 0 \Rightarrow \theta_1 = \theta_3 = 0$$

or

$$a_2 = a_3 = 0 \Rightarrow \theta_2 = \theta_3 = 0.$$

In the third case, that will be considered, from now on, the chiral invariant Lagrangian is

$$\mathcal{L}_0 = \overline{\psi}(i\not{\partial} \otimes 1 \otimes 1)\psi, \tag{4.5}$$

which is invariant under the chiral transformation

$$\psi \rightarrow \psi^{\text{chi}} = e^{i\theta_1 \gamma^5} \otimes 1 \otimes 1 \psi. \tag{4.6}$$

Our proposal for treating massless spin $\frac{3}{2}$ particles is, in close analogy with spin $\frac{1}{2}$ particles,[3,4] to treat all chiral components as independent field variables. In this way we consider all chiral components as dynamical variables. It is simple to check that the substitution of (3.2) into (4.5) leads to the following Lagrangian density:

$$\begin{aligned}\mathcal{L} = {} & \overline{\psi}_{RRR}(\ )\psi_{RLL} + \overline{\psi}_{RRL}(\ )\psi_{RLR} + \overline{\psi}_{RLR}(\ )\psi_{RRL} + \overline{\psi}_{LRR}(\ )\psi_{LLL} \\ & + \overline{\psi}_{LLR}(\ )\psi_{LRL} + \overline{\psi}_{LRL}(\ )\psi_{LLR} + \overline{\psi}_{RLL}(\ )\psi_{RRR} + \overline{\psi}_{LLL}(\ )\psi_{LRR},\end{aligned} \tag{4.7}$$

where ( ) stands for the operator $i\not{\partial} \otimes 1 \otimes 1$.

Treating all chiral components as independent field variables, one gets from (4.7) the following equations of motion:

$$\begin{aligned}
&(i\not{\partial} \otimes 1 \otimes 1)\psi_{RLL} = 0, \\
&(i\not{\partial} \otimes 1 \otimes 1)\psi_{RLR} = 0, \\
&(i\not{\partial} \otimes 1 \otimes 1)\psi_{RRL} = 0, \\
&(i\not{\partial} \otimes 1 \otimes 1)\psi_{LLL} = 0, \\
&(i\not{\partial} \otimes 1 \otimes 1)\psi_{LRL} = 0, \\
&(i\not{\partial} \otimes 1 \otimes 1)\psi_{LLR} = 0, \\
&(i\not{\partial} \otimes 1 \otimes 1)\psi_{RRR} = 0, \\
&(i\not{\partial} \otimes 1 \otimes 1)\psi_{LRR} = 0.
\end{aligned} \tag{4.8}$$

We write the equations of motion (4.8) for the symmetric and nonsymmetric decompositions of the chiral components. The nonsymmetrized chiral components leads to the following set of equations:

$$\begin{aligned}
&(\tfrac{1}{2}(1-\gamma^5)\gamma^\mu \not{\partial} C)_{a_3 a_1}(\mathbf{\Phi}_{\mu_L^R})_{a_2} = 0, \\
&(\tfrac{1}{2}(1+\gamma^5)\gamma^\mu \not{\partial} C)(\mathbf{\Phi}_{\mu_L^R}) = 0, \\
&(\tfrac{1}{2}(1-\gamma^5)\sigma^{\mu\nu} \not{\partial} C)(\mathcal{G}_{\mu\nu_L^R}) = 0, \\
&(\tfrac{1}{2}(1+\gamma^5)\sigma^{\mu\nu} \not{\partial} C)(\mathcal{G}_{\mu\nu_L^R}) = 0.
\end{aligned} \tag{4.9}$$

From the above equations it follows that

$$(\gamma^{\mu}\partial\!\!\!/ C)_{a_3a_1}\mathbf{\Phi}_{\mu,a_2}=0, \tag{4.10}$$

$$(\sigma^{\mu\nu}\partial\!\!\!/ C)_{a_3a_1}\mathcal{G}_{\mu\nu,a_2}=0. \tag{4.11}$$

Multiplying (4.10) successively by $(C^{-1})_{a_1a_3}$ and $(C^{-1}\gamma^{\alpha}\gamma^{\beta})_{a_1a_3}$, we obtain after some additional trivial manipulations, the massless Rarita–Schwinger equations for the vector spinor $\mathbf{\Phi}^{\mu}_{,a}$.

The symmetrized decomposition of the spinor field will result in the following set of equations:

$$\begin{aligned}
&(\partial\!\!\!/ G_{\mu\nu}{}^{R}_{L})_{a_1}(\sigma^{\mu\nu}C^{R}_{L})_{a_2a_3}-(G_{\mu\nu}{}^{R}_{L})_{a_2}(\sigma^{\mu\nu}{}^{R}_{L}\partial\!\!\!/ C)_{a_3a_1}+(G_{\mu\nu}{}^{R}_{L})_{a_3}(\partial\!\!\!/(\sigma^{\mu\nu}C)^{R}_{L})_{a_1a_2}=0,\\
&d_1\{(\partial\!\!\!/\varphi_{\mu}{}^{R}_{L})_{a_1}(\gamma^{\mu}C^{R}_{L})_{a_2a_3}-(\varphi_{\mu}{}^{R}_{L})_{a_2}[(\gamma^{\mu})^{R}_{L}\partial\!\!\!/ C]_{a_3a_1}\}+d_2(G_{\mu\nu}{}^{R}_{L})_{a_3}(\partial\!\!\!/(\sigma^{\mu\nu}C)^{R}_{L})_{a_1a_2}=0,\\
&d_1\{(\partial\!\!\!/\varphi_{\mu}{}^{R}_{L})_{a_1}(\gamma^{\mu}C^{R}_{L})_{a_2a_3}+(\varphi_{\mu}{}^{R}_{L})_{a_3}[\partial\!\!\!/(\gamma^{\mu}C)^{R}_{L}]_{a_1a_2}\}-d_2(G_{\mu\nu}{}^{L}_{R})_{a_2}[(\sigma^{\mu\nu})^{R}_{L}\partial\!\!\!/ C]_{a_3a_1}=0,\\
&d_1\{-(\varphi_{\mu}{}^{R}_{L})_{a_2}[(\gamma^{\mu})^{R}_{L}\partial\!\!\!/ C]_{a_3a_1}+(\varphi_{\mu}{}^{R}_{L})_{a_3}[\partial(\gamma^{\mu}C)^{R}_{L}{}_{a_1a_2}+d_2(\partial\!\!\!/ G_{\mu\nu}{}^{L}_{R})_{a_1}(\sigma^{\mu\nu}C)^{R}_{L}{}_{a_2a_3}=0.
\end{aligned} \tag{4.12}$$

From (4.12) it follows that

$$\begin{aligned}
&d_1\{(\partial\!\!\!/)_{a_1a'_1}\varphi_{\mu a'_1}(\gamma^{\mu}C)_{a_2a_3}-\varphi_{\mu a_2}(\gamma^{\mu}\partial\!\!\!/ C)_{a_3a_1}+\varphi_{\mu a_3}(\partial\!\!\!/\gamma^{\mu}C)_{a_1a_2}\}\\
&\quad+d_2\{(\partial\!\!\!/)_{a_1a'_1}G_{\mu\nu a'_1}(\sigma^{\mu\nu}C)_{a_2a_3}+G_{\mu\nu a_3}(\partial\!\!\!/\sigma^{\mu\nu}C)_{a_1a_2}-G_{\mu\nu a_2}(\sigma^{\mu\nu}\partial\!\!\!/ C)_{a_3a_1}\}=0.
\end{aligned} \tag{4.13}$$

Now, the multiplication of (4.13) by C^{-1}, $C^{-1}\gamma^{\eta}$, and $C^{-1}\gamma^{\eta}\gamma^{\lambda}$ gives rise to three equations in φ^{μ}, $G^{\mu\nu}$ and derivatives of these fields. We get

$$\partial^{\mu}\mathbf{\Phi}_{\mu}=0, \tag{4.14a}$$

$$\partial^{\mu}\mathcal{G}_{\mu\nu}=0, \tag{4.14b}$$

$$g^{\alpha\beta}\partial^{\mu}\mathbf{\Phi}_{\mu}-\partial^{\alpha}\mathbf{\Phi}^{\beta}-\partial^{\beta}\mathbf{\Phi}^{\alpha}=0. \tag{4.14c}$$

It is easy to check that the equations (4.14a), (4.14b), (4.14c) will lead us, remembering also condition (2.5) for $\mathbf{\Phi}^{\mu}$ (trivially satisfied in the symmetrized version), to the RS massless equations.

Chiral components remove the ambiguity in the Lagrangian approach to spin $\frac{3}{2}$ massless particles. We have a well-defined Lagrangian, built from first principles, and it does not matter which decomposition one uses.

As we shall see in the next section the chiral spinorial approach is the only anomaly free framework for massless particles.

V. MASSIVE SPIN $\frac{3}{2}$ PARTICLES

We know that at some level chiral invariance is broken. For example, a mass term breaks chiral invariance. We propose then that the Lagrangian in the massive case, be of the form

$$\mathcal{L}=\overline{\psi}(i\partial\!\!\!/\otimes 1\otimes 1)\psi-m\overline{\psi}\psi. \tag{5.1}$$

By making the variation over the field $\overline{\psi}$ we will get just one equation for the field ψ, that is,

$$i\partial\!\!\!/\otimes 1\otimes 1\psi=m\psi. \tag{5.2}$$

Let us consider first the explicitly symmetric expansion of ψ. The advantage of this symmetric expression is that we can deduce all properties and equations for φ_μ and $G_{\mu\nu}$ from just one Dirac-type equation. In this case it does not matter which of the three equations (2.1) one uses. We take equation (2.1a).

From (5.2) it follows the following equations for φ_μ and $G_{\mu\nu}$:

$$\partial_\mu\{d_1(2\varphi^{\mu}_{,a_1}+(\gamma^\alpha\gamma^\mu)_{a_1a_2}\varphi_{\alpha,a_2})+d_2(\sigma^{\alpha\beta}\gamma^\mu)_{a_1a_2}G_{\alpha\beta,a_2}\}=0, \tag{5.3}$$

$$\begin{aligned} &i\{d_1(\gamma^\mu\partial^\nu\varphi_\mu-\gamma^\mu\gamma^\rho\gamma^\nu\partial_\rho\varphi_\mu)+d_2(\sigma^{\alpha\beta}\partial^\nu G_{\alpha\beta}-\sigma^{\alpha\beta}\gamma^\rho\gamma^\nu)\partial_\rho G_{\alpha\beta}\}+4d_2\partial_\rho G^{\nu\rho}\\ &\quad=md_1\{2\varphi^\nu+(\gamma^\alpha\gamma^\nu)\varphi_\alpha\}+md_2(\sigma^{\alpha\beta}\gamma^\nu)G_{\alpha\beta}, \end{aligned} \tag{5.4}$$

$$\begin{aligned} &i\{d_1[\partial^\lambda(2\varphi^\eta+\gamma^\mu\gamma^\eta\varphi_\mu)+\partial^\eta(2\varphi^\lambda+\gamma^\mu\gamma^\lambda\varphi_\mu)-\partial_\alpha g^{\lambda\eta}(2\varphi^\alpha+\gamma^\mu\gamma^\alpha\varphi_\mu)]\\ &\quad+d_2[\partial^\lambda(\sigma^{\mu\nu}\gamma^\eta)-\partial^\eta(\sigma^{\mu\nu}\gamma^\lambda)-\partial_\alpha g^{\lambda\eta}(\sigma^{\mu\nu}\gamma^\alpha)]G_{\mu\nu}\}\\ &\quad=md_1\gamma^\mu(g^{\lambda\eta}-\gamma^\lambda\gamma^\eta)\varphi_\mu+md_2\{-4iG^{\eta\lambda}-(\sigma^{\mu\nu}\gamma^\lambda\gamma^\eta)G_{\mu\nu}+g^{\lambda\eta}\sigma^{\mu\nu}G_{\mu\nu}\} \end{aligned} \tag{5.5}$$

[spinor indices omitted in (5.3), (5.4), and (5.5)].

The equations (5.3), (5.4), and (5.5) can be rewritten in a simpler form if one uses properties (2.9) and (2.10). These alternative expressions are

$$\partial^\mu\mathbf{\Phi}_\mu=0, \tag{5.6}$$

$$-2D_2\partial_\alpha\mathcal{G}^{\alpha\nu}=mD_1\mathbf{\Phi}^\nu, \tag{5.7}$$

$$D_1(\partial^\lambda\mathbf{\Phi}^\eta-\partial^\eta\mathbf{\Phi}^\lambda-g^{\lambda\eta}\partial_\alpha\mathbf{\Phi}^\alpha)=2mD_2\mathcal{G}^{\lambda\eta}. \tag{5.8}$$

As a consequence of the above equations we establish that the spinor vector $\mathbf{\Phi}^\mu_{,a}$, obeys a Dirac-type equation

$$(i\partial\!\!\!/-m)_{a_1a_2}\mathbf{\Phi}^\mu_{,a_2}=0. \tag{5.9}$$

So that, the symmetric expansion (2.3) gives rise to a vector spinor $\mathbf{\Phi}^\mu_{,a}$ which satisfies the RS equations.

Let us turn now to the nonsymmetric decomposition of the ψ field. At first sight it might appear that we cannot get Rarita–Schwinger equation from just one Dirac-type equation [like Eq. (5.2)]. We can get RS equations if one uses decomposition (2.2b). Decompositions (2.2a) and (2.2c) will lead to RS equations by using (2.1b) and (2.1c). That is, for each decomposition we need to use a different equation.

As a final remark we would like to comment on the massless case. We can show explicitly that the $m=0$ limit of (5.3)–(5.5) do not lead to the Rarita–Schwinger equations. In this case the only alternative is to use our previous equations for the chiral components.

VI. SIMPLER LAGRANGIANS IN THE MASSIVE CASE

The usual RS Lagrangian involving the spinor–vector $\mathbf{\Phi}^\mu$, is built in a somehow artificial manner.[6] That is, it is constructed in such a way as to give rise to the equations and constraints satisfied by the vector-spinor field.

We should see that the chiral approach lead naturally to an unambiguous Lagrangian formulation. The difference from the usual approaches is that our Lagrangians are written in terms of $\mathcal{G}^{\mu\nu}_a$ and $\mathbf{\Phi}^\mu_a$ which are then treated as dynamical variables.

If one wants to write simpler Lagrangians in terms of the fields $\mathbf{\Phi}^\mu_{,a}$ and $\mathcal{G}^{\mu\nu}_{,a}$, all we have to do is to substitute ψ given in (2.2b) into Lagrangian (5.1). Doing so we get

$$\mathcal{L}=4D_1^*D_2\overline{\mathbf{\Phi}}_{\mu,a}(\partial_\alpha\mathcal{G}^{\alpha\mu}_{,a}-\partial_\alpha\mathcal{G}^{\mu\alpha}_{,a})+4D_2^*D_1\overline{\mathcal{G}}_{\mu\nu,a}(\partial^\nu\mathbf{\Phi}^\mu_{\ a}-\partial^\mu\mathbf{\Phi}^\nu_{\ a})$$
$$+4D_1^*D_1m\overline{\mathbf{\Phi}}^\mu_{,a}\mathbf{\Phi}_{\mu,a}+8D_2^*D_2m\overline{\mathcal{G}}^{\mu\nu}_{,a}\mathcal{G}_{\mu\nu,a}. \tag{6.1}$$

Considering $\mathbf{\Phi}^\mu_{,a}$ and $\mathcal{G}^{\mu\nu}_{,a}$ as independent field variables, we get the following Euler-Lagrange equations:

$$2D_2\partial_\mu\mathcal{G}^{\mu\nu}_{,a}=-mD_1\mathbf{\Phi}^\nu_{,a}, \tag{6.2}$$

$$2mD_2\mathcal{G}^{\mu\nu}_{,a}=D_1(\partial^\mu\mathbf{\Phi}^\nu_{\ a}-\partial^\nu\mathbf{\Phi}^\mu_{\ a}). \tag{6.3}$$

Now, by construction, $\mathcal{G}^{\mu\nu}_{\ a}$ is antisymmetric in its vector indices, from this fact and Eq. (6.2) it follows that

$$\partial^\mu\mathbf{\Phi}_{\mu,a}=0. \tag{6.4}$$

Now, if one considers Eqs. (6.2)–(6.4) together with the conditions (2.5) and (2.6) satisfied by $\mathbf{\Phi}^\mu_{,a}$ and $\mathcal{G}^{\mu\nu}_{,a}$, we can see that $\mathbf{\Phi}^\mu_{,a}$ obeys Dirac equation

$$(i\not\partial-m)_{a_1a_2}\mathbf{\Phi}^\mu_{a_2}=0. \tag{6.5}$$

Equations (2.5), (6.4), and (6.5) for the vector–spinor $\mathbf{\Phi}^\mu_{,a}$, are exactly the RS equations.

Now let us use the symmetrized expansion (2.3) of ψ. The results are a little bit different. To illustrate this point, we consider just the massless case, and use the expression (4.5).

Substituting ψ by the decomposition (2.3) in (4.5), we obtain the following expression for the massless Lagrangian:

$$\mathcal{L}=i\{-2d_1^*d_1(2\overline{\varphi}_\mu\not\partial\varphi^\mu+\overline{\varphi}^\mu\not\partial\gamma^\alpha\gamma^\mu\varphi_\alpha+\overline{\varphi}_\mu\gamma^\alpha\gamma^\mu\not\partial\varphi_\alpha-\overline{\varphi}_\mu\gamma^\alpha\not\partial\gamma^\mu\varphi_\alpha)$$
$$-2d_1^*d_2(\overline{\varphi}_\mu\not\partial\sigma^{\alpha\beta}\gamma^\mu G_{\alpha\beta}+\overline{\varphi}_\mu\sigma^{\alpha\beta}\gamma^\mu\not\partial G_{\alpha\beta}-\overline{\varphi}_\mu\sigma^{\alpha\beta}\not\partial\gamma^\mu G_{\alpha\beta}+8i\overline{\varphi}_\mu\partial^\alpha G_\alpha{}^\mu)$$
$$-2d_2^*d_1(\overline{G}_{\mu\nu}\not\partial\gamma^\alpha\sigma^{\mu\nu}\varphi_\alpha+\overline{G}_{\mu\nu}\gamma^\alpha\sigma^{\mu\nu}\not\partial\varphi_\alpha-\overline{G}_{\mu\nu}\gamma^\alpha\not\partial\sigma^{\mu\nu}\varphi_\alpha+4i\overline{G}_{\mu\nu}(\partial^\nu\varphi^\mu-\partial^\mu\varphi^\nu))$$
$$-2d_2^*d_2(4\overline{G}_{\mu\nu}\not\partial G^{\mu\nu}+\overline{G}_{\mu\nu}\not\partial\sigma^{\alpha\beta}\sigma^{\mu\nu}G_{\alpha\beta}+\overline{G}_{\mu\nu}\sigma^{\alpha\beta}\sigma^{\mu\nu}\not\partial G_{\alpha\beta}-\overline{G}_{\mu\nu}\sigma^{\alpha\beta}\not\partial\sigma^{\mu\nu}G_{\alpha\beta})\}, \tag{6.6}$$

where φ^μ stands for $\varphi^\mu_{,a}$ (for example), and the obvious summed spinor indices were omitted.

Considering $\varphi^\mu_{,a}$ and $G^{\mu\nu}_{,a}$ as independent field variables, we write the Euler–Lagrange equations and obtain two equations. We give here the ''translated'' expression of this two equations, obtained using ''the dictionary'' equations (2.9) and (2.10), in order to have simpler, but equivalent, equations than the original ones. We have

$$D_1\not\partial_{a_1a_2}\mathbf{\Phi}^\mu_{a_2}-4iD_2\partial_\alpha\mathcal{G}^{\mu\alpha}_{,a_1}=0, \tag{6.7}$$

$$D_2\not\partial_{a_1a_2}\mathcal{G}^{\mu\nu}_{a_2}+iD_1(\partial^\nu\mathbf{\Phi}^\mu_{a_1}-\partial^\mu\mathbf{\Phi}^\nu_{a_1})=0. \tag{6.8}$$

Clearly the conditions (2.5) and (2.6) with respect to $\mathbf{\Phi}^\mu$ and $\mathcal{G}^{\mu\nu}$ are understood. Having this last point in mind, it is easy to show that in fact (6.7) is a consequence of (6.8), and therefore we have only one independent equation relating $\mathbf{\Phi}^\mu$ and $\mathcal{G}^{\mu\nu}$ in this case. This symmetric approach gives rise to too few equations for too many fields. We need to fix or to impose extra conditions in order to reduce this number of degrees of freedom. Having in mind the results obtained using a nonsymmetric expansion for ψ, we propose to separate equations (6.7) and (6.8) into two vanishing parts:

$$D_1 \not\partial_{a_1 a_2} \mathbf{\Phi}^{\mu}_{a_2} = 4iD_2 \partial_\alpha \mathcal{G}^{\mu\alpha}_{a_1} = 0, \tag{6.9}$$

$$D_2 \not\partial_{a_1 a_2} \mathcal{G}^{\mu\nu}_{a_2} = iD_1 (\partial^\mu \mathbf{\Phi}^{\nu}_{a_1} - \partial^\nu \mathbf{\Phi}^{\mu}_{a_1}). \tag{6.10}$$

Now, as a consequence of the two last equations and the condition (2.5) we have

$$\partial^\mu \mathbf{\Phi}_{\mu,a} = 0.$$

We get in this way the RS equations, for the spinor vector $\mathbf{\Phi}^{\mu}_{,a}$. We can justify the method used here only when one looks back to Sec. IV. There we have made use of the chiral components.

VII. EFFECTIVE INTERACTIONS

In previous papers[5,7] we have constructed effective interactions for particles of arbitrary spin. In Ref. 5 we have made the description of a particle of spin s by using a symmetric rank $2s$ spinor (BW method) and by using this field we obtain interactions making contractions of the spinor indices. For example, an interaction involving one spin $\frac{3}{2}$ particle and three spin $\frac{1}{2}$ particles, can be written as

$$\overline{\psi}_{a_1 a_2 a_3} (\eta^C)_{a_1} \eta_{a_2} \eta_{a_3}, \tag{7.1}$$

η^C is a charge conjugated spin $\frac{1}{2}$ spinor.

An interaction term involving spin $\frac{3}{2}$ with spin 1 and spin $\frac{1}{2}$ particles can be written in this approach as

$$\overline{\psi}_{a_1 a_2 a_3} \psi_{a_1 a_2} \eta_{a_3} \tag{7.2}$$

or

$$\overline{\psi}_{a_1 a_2 a_3} \psi_{a_1 a_3} \eta_{a_2}. \tag{7.3}$$

If we rememember[3] the decomposition (7.4) for a spin 1 field:

$$\psi_{a_1 a_2} = C_1 A_\alpha (\gamma^\alpha C)_{a_1 a_2} + C_2 F_{\alpha\beta} (\sigma^{\alpha\beta} C)_{a_1 a_2} \tag{7.4}$$

the interaction term (7.2) involving particles of spin $\frac{3}{2}$, 1 and $\frac{1}{2}$ may be written as

$$-D_1^* C_1 A_\alpha \overline{\mathbf{\Phi}}_{\mu,a_2} (\gamma^\alpha \gamma^\mu)_{a_2 a_3} \eta_{a_3} - D_2^* C_1 A_\alpha \overline{\mathcal{G}}_{\mu\nu,a_2} (\gamma^\alpha \sigma^{\mu\nu})_{a_2 a_3} \eta_{a_3},$$

$$-D_1^* C_2 F_{\alpha\beta} \overline{\mathbf{\Phi}}_{\mu,a_2} (\sigma^{\alpha\beta} \gamma^\mu)_{a_2 a_3} \eta_{a_3} - D_2^* C_2 F_{\alpha\beta} \overline{\mathcal{G}}_{\mu\nu,a_2} (\sigma^{\alpha\beta} \sigma^{\mu\nu})_{a_2 a_3} \eta_{a_3}. \tag{7.5}$$

The chiral method introduces some improvements for the construction of effective interactions. We have now a richer set of alternative Lagrangians. Furthermore, we are now able to separate vector–spinor and tensor–spinor parts. For example, in the case of the nonsymmetric decomposition of the rank 3 spinor $\psi_{a_1 a_2 a_3}$, we have

$$(\overline{\psi}_{RRL} + \overline{\psi}_{LRR} + \overline{\psi}_{LLR} + \overline{\psi}_{RLL})_{a_1 a_2 a_3} = -D_1^* \overline{\Phi}_{\mu,a_2} (C^{-1} \gamma^\mu)_{a_3 a_1}, \tag{7.6}$$

whereas the combination associated to $\overline{\mathcal{G}}_{\mu\nu}$ is

$$(\overline{\psi}_{RRR} + \overline{\psi}_{LRL} + \overline{\psi}_{RLR} + \overline{\psi}_{LLL})_{a_1 a_2 a_3} = -D_2^* \overline{\mathcal{G}}_{\mu\nu,a_2} (C^{-1} \sigma^{\mu\nu})_{a_3 a_1}. \tag{7.7}$$

In expression (7.6) we have just the vector spinor $\mathbf{\Phi}^{\mu}_{a}$ whereas in (7.7) we have just the tensor spinor $\mathcal{G}^{\mu\nu}_{a}$.

The interaction resulting from (7.6) for spin $\frac{1}{2}$ particles is, from (7.1):

$$D_1^*(\overline{\eta}_{a_2}\gamma^{\mu}_{a_2a_3}\eta_{a_3})(\overline{\Phi}_{\mu,a_2}\eta_{a_2}). \tag{7.8}$$

We are also able to separe the purely vector, vector–tensor and purely tensor parts of the expansion of the field ψ by using the chiral components.

The purely vector part is given by the interaction Lagrangian

$$\begin{aligned}&(\overline{\psi}_{RRL}+\overline{\psi}_{LRR}+\overline{\psi}_{LLR}+\overline{\psi}_{RLL})_{a_1a_2a_3}(\psi_{RL}+\psi_{LR})_{a_1a_2}\eta_{a_3}\\&\quad=-D_1^*C_1A_{\alpha}\overline{\mathbf{\Phi}}_{\mu,a_2}(\gamma^{\alpha}\gamma^{\mu})_{a_2a_3}\eta_{a_3}.\end{aligned} \tag{7.9}$$

The interaction between vector field A_{μ} and tensor components ($\mathcal{G}_{\mu\nu,a}$) is given by the following interaction terms:

$$\begin{aligned}&(\overline{\psi}_{RRR}+\overline{\psi}_{LRL}+\overline{\psi}_{RLR}+\overline{\psi}_{LLL})_{a_1a_2a_3}(\psi_{RL}+\psi_{LR})_{a_1a_2}\eta_{a_3}\\&\quad=-D_2^*C_1A_{\alpha}\overline{\mathcal{G}}_{\mu\nu,a_2}(\gamma^{\alpha}\sigma^{\mu\nu})_{a_2a_3}\eta_{a_3}\end{aligned} \tag{7.10}$$

and between the tensor field $F_{\mu\nu}$ and the vector spinor $\mathbf{\Phi}_{\mu}$ by the Lagrangian

$$\begin{aligned}&(\overline{\psi}_{RRL}+\overline{\psi}_{LRR}+\overline{\psi}_{LLR}+\overline{\psi}_{RLL})_{a_1a_2a_3}(\psi_{RR}+\psi_{LL})_{a_1a_2}\eta_{a_3}\\&\quad=-D_1^*C_2F_{\alpha\beta}\overline{\mathbf{\Phi}}_{\mu,a_2}(\sigma^{\alpha\beta}\gamma^{\mu})_{a_2a_3}\eta_{a_3},\end{aligned} \tag{7.11}$$

whereas the purely tensor interaction is associated to the following chiral components interaction:

$$(\overline{\psi}_{RRR}+\overline{\psi}_{LRL}+\overline{\psi}_{RLR}+\overline{\psi}_{LLL})_{a_1a_2a_3}(\psi_{RR}+\psi_{LL})_{a_1a_2}\eta_{a_3}=-D_2^*C_2F_{\alpha\beta}\overline{\mathcal{G}}_{\mu\nu,a_2}(\sigma^{\alpha\beta}\sigma^{\mu\nu})_{a_2a_3}\eta_{a_3}. \tag{7.12}$$

We can also introduce effective interactions involving just one, or more chiral components. That is, at the interaction level the different chiral components might interact with different strengths. This means that at the interaction level we might have left–right asymmetry. For example, if one couples just the ψ_{RRL} spin $\frac{3}{2}$ component with three spin $\frac{1}{2}$ particles we get the only nonzero term:

$$\begin{aligned}&(\overline{\psi}_{RRL})_{a_1a_2a_3}(\eta_R^C)_{a_1}(\eta_L)_{a_2}(\eta_R)_{a_3}\\&\quad=-D_1^*\overline{\Phi}_{\mu,a}\tfrac{1}{2}(1-\gamma^5)_{aa_1}\eta_{a_1}\overline{\eta}_{a_2}(\tfrac{1}{2}(1-\gamma^5)\gamma^{\mu})_{a_2a_3}\eta_{a_3}.\end{aligned} \tag{7.13}$$

Clearly the consequence of such an interaction term is that there will be parity violation.

VIII. CONCLUSIONS

In this paper we have expanded even further the idea that chirality is a basic notion in the description of particles of arbitrary spin. We have shown that a consistent description of spin $\frac{3}{2}$ particles can be achieved by using our chiral spinorial method.

Our approach is different from others in the sense that we take the interaction of spin $\frac{1}{2}$ particles as a guide to other interactions. That is, at the free field level one imposes chiral invariance as a guide to establish the Lagrangian.

Another important distinction from other approaches is that we treat all eight chiral components as independent field variables. This allows us to get a consistent Lagrangian method for massless spin $\frac{3}{2}$ particles.

The extension of this Lagrangian to the massive case is straightforward. In the massive case, we have shown how the description here proposed (using the prescription that the chiral components be treated as independent field variables) lead to the same results as in the case of RS theory. It is important to stress here the main distinction between our approach and RS theory. In our case there is a Lagrangian, the equations of motion for all chiral components are very similar to each other, the discrete symmetries can be analyzed and the zero mass limit can be properly treated.

For the massive case we have shown that our Lagrangian provides a way of getting Rarita–Schwinger equations by using three different methods.

At the free field level we show that the chiral approach lead to an unambiguous Lagrangian for the description of spin $\frac{3}{2}$ particles. This is the only consistent Lagrangian method for massless particles.

As far as interactions of spin $\frac{3}{2}$ particles are concerned, our approach provides a very simple method for the construction of effective interactions. We get, by treating the chiral components as independent variables, a large number of effective Lagrangians. Some of them might be useful in phenomenological applications.

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High-frequency asymptotics for Maxwell's equations in anisotropic media Part I: Linear geometric and diffractive optics

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This paper is devoted to the derivation of the equations that govern the propagation of pulses in noncentrosymmetric crystals. The method is based upon high-frequency expansions techniques for Maxwell's equations. By suitable choices of the scalings we are able to derive two classical models: Geometric optics and diffractive optics (Schrödinger-type equations). In the so-called geometric regime we recover the standard results on the propagation of pulses in crystals (dispersion equation, polarization states, group velocity). In the diffractive regime we exhibit original results and give a closed-form expression for the diffraction operator which reads as an anisotropic operator. Given this expression we identify a critical configuration where the diffraction reduces to a one-dimensional second-order operator instead of the standard transverse Laplacian. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1354639]

I. INTRODUCTION

Many crystals and liquid crystals have optical properties which depend on the direction of propagation and the polarization of light. A precise understanding of light propagation in such anisotropic media is important for both theoretical and practical applications. Indeed this problem is theoretically interesting in that it exhibits many optical phenomena such as polarizations effects, optical rotation, and conical refraction.[1] It is also practically relevant since anisotropic media are essential components for many optical devices such as prism polarizers, birefringent filters, and Pockels cells.[2] Anisotropic media are also used for phase-matched frequency conversion.[3] The aim of this paper is to describe the effects of the anisotropy of the medium so as to derive evolution equations for the slowly varying envelopes of fields. Such results have been already obtained using more or less ad hoc methods (see Ref. 4 and references therein). In particular a modern method of solving optical problems is based on the integral formulation of the field equation and the determination of the Green function.[5] The method requires an explicit representation of the Green function which is obtained by the use of a Fourier transform. Then applying stationary phase method one gets the asymptotic form of the Green function. This method is efficient for linear media, but it is not well-adapted for addressing nonlinear problems since the use of Fourier transforms, and thus the derivation of an explicit form of the solution, are then prohibited.

We shall use a technique based on high-frequency expansions of the fields which has already been successfully applied to systems of linear, semilinear and quasilinear hyperbolic partial differential equations (see Ref. 6 and references therein). This technique is more robust than the Green function approach in the sense that the approximate solutions are not derived by an asymptotic analysis of an explicit solution, but through a direct asymptotic analysis of Maxwell's equations. This high-frequency asymptotics method can deal with boundary conditions and—more important—it can handle nonlinearities. Applying this technique to Maxwell's equations in anisotropic media allows us to get evolution equations for the field envelopes in both the scales

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corresponding to geometric optics and diffractive optics. We are then able to write equations which recover the classical results and also exhibit original results such as the explicit form of the anisotropic second-order operator which plays the role of the transverse Laplace operator in the standard Schrödinger equation.

The theoretical derivations of the equations and the physically relevant applications are quite long, but they can be divided into two parts. In this paper we restrict ourselves to linear propagation. Nonlinear propagation is addressed in the companion paper[7] that requires the results derived here below. The framework for high-frequency expansions of the solutions of Maxwell's equations follows from the appearance of the small parameter δ which has the order of magnitude of the carrier wavelength of light divided by the next smallest characteristic length present in the problem. If we consider the propagation along the z axis of a broadband and divergent pulse with carrier frequency ω, then there exists a wave number $k=k(\omega)$ such that the electric field $\mathcal{E}$ can be expanded as a series of slowly varying functions modulated by a rapid phase $\phi=kz-\omega t$

$$\mathcal{E}(t,x,y,z)=\frac{1}{2}\left(\sum_{j=0}^{\infty}\delta^j\mathbf{E}_j(\delta t,\delta x,\delta y,\delta z)e^{i(kz-\omega t)}+cc\right), \tag{1}$$

where *cc* is a shorthand for ''complex conjugate.'' We are particularly interested in determining the leading profile $\mathbf{E}_0$, the so-called slowly varying envelope of the field. We shall derive the evolution equation for $\mathbf{E}_0$ by using the fact that it reads as the compatibility condition for the existence of the expansion (1). We shall see that for propagation length (z) of order δ^{-1} times the wavelength, which corresponds to the scales of the so-called geometric optics, evolution equations read as transport equations with constant velocity. Further, in the moving pulse-time frame (moving according to the velocity exhibited by the geometric transport equations), we can study the evolution of the field for propagation lengths of order δ^{-2} times the wavelength, which corresponds to the scales of the so-called diffractive optics. The evolution of the slowly varying envelope of the field is then governed by a Schrödinger-type equation.

The paper is organized as follows. First we describe the general configuration at hand in Sec. II. Sections III–V are devoted to an extensive study of the linear propagation of pulses in biaxial crystals. We finally apply these results to specific configurations and discuss some applications in the last sections of this paper.

II. FORMULATION AND SCALING

We aim at focusing on the derivation of the propagation equation, so we consider simple boundary conditions. We refer to Refs. 8 and 9 for extensive treatments of very general boundary conditions. In this paper the plane $\Sigma:=\{(x',y,z)\in\mathbb{R}^3,z=0\}$ is the boundary surface that separates the semi-infinite vacuum $\mathbb{R}^3_-:=\{(x,y,z)\in\mathbb{R}^3,z<0\}$ on the left and a biaxial crystal on the right $\mathbb{R}^3_+:=\{(x,y,z)\in\mathbb{R}^3,z>0\}$. We consider an incident beam incoming from the left whose propagation axis is perpendicular to the boundary surface Σ and is collinear to the z axis.

We assume absence of free charges or currents ($\mathbf{j}=0$, $\rho=0$), and that the crystal is nonmagnetic so that its magnetic permeability $\mu\equiv\mu_0$. Inside the domain $\mathbb{R}^3_+$, the electric field $\mathcal{E}$ and magnetic induction $\mathcal{B}$ obey the Maxwell equations

$$\partial_t\mathcal{B}+\mathbf{rot}\,\mathcal{E}=0,$$

$$\mu_0\partial_t\mathcal{D}-\mathbf{rot}\,\mathcal{B}=0,$$

where $\mathcal{D}$ is the electric induction which contains the physic interaction between light and matter and can be expressed in terms of $\mathcal{E}$. The magnetic field $\mathcal{H}$ is simply given by $\mathcal{B}=\mu_0\mathcal{H}$. By differentiating the second equation with respect to time t and substituting into the first one, the magnetic induction is eliminated so that we get the equation which governs the evolution of the electric field

$$\mathbf{rot}\,\mathbf{rot}\,\mathcal{E}=-\mu_0\partial_t^2\mathcal{D}. \tag{2}$$

Equation (2) is insufficient to determine the electric field and has to be supplemented by a constitutive equation showing how the field is related to the properties of the medium. Assuming that the wave intensity is small enough so that the response of the medium is linear, the electric induction reads

$$\mathcal{D}=\varepsilon_0\mathcal{E}+\mathcal{P} \tag{3}$$

$$\mathcal{P}=\varepsilon_0\chi^{(1)}*\mathcal{E}=\varepsilon_0\int_{-\infty}^{t}dt_1\chi^{(1)}(t-t_1)\mathcal{E}(t_1), \tag{4}$$

where $\mathcal{P}$ is the polarization of the medium. We assume that the electromagnetic wave is far enough from all absorption lines of the medium so that we can neglect absorption and the tensor $\chi^{(1)}$ is real and symmetric. ε_0 and μ_0 are, respectively, the dielectric constant and magnetic permeability of vacuum. These constant quantities are related to the light velocity c by the identity $\varepsilon_0\mu_0c^2=1$.

In order to deal with a well-posed problem we must state boundary conditions in time and space domains. The boundary condition at the boundary surface Σ is imposed by the continuity of the tangential components of the magnetic and electric fields. If we know the total field $\mathcal{S}_{\text{tot}}$ in vacuum just in the limit slab $z=0^-$, then the electric field $\mathcal{E}$ within the crystal in $z=0^+$ should satisfy $\mathcal{E}\times\mathbf{n}=\mathcal{S}_{\text{tot}}\times\mathbf{n}$, where $\mathbf{n}$ is the outgoing normal direction $(0, 0, -1)$. Unfortunately we do not know *a priori* the total source, which divides into the sum of the incoming wave and the reflected wave. It is much more appropriate to consider as a boundary condition the incoming wave condition which is a well-adapted condition for almost normally incident pulses. The boundary conditions then read as the following equation over the interface Σ:

$$(\mathcal{E}-c\mathcal{B}\times\mathbf{n})\times\mathbf{n}=2\mathcal{S}\times\mathbf{n}, \tag{5}$$

where $\mathcal{S}$ is the source corresponding to the field of the incoming pulse given at the interface Σ by

$$\mathcal{S}(x,y,t)=\begin{pmatrix}\mathcal{S}_x(x,y,t)\\ \mathcal{S}_y(x,y,t)\\ 0\end{pmatrix}.$$

Last we assume that all unknown quantities are vanishing at time $t\leqslant 0$

$$\mathcal{E},\mathcal{B},\mathcal{D}(t=0)=0 \quad \text{in } \mathbb{R}^3_+.$$

The source is assumed to be a modulation of a high-frequency signal whose carrier wavelength is λ_0, or the superposition of a finite number of such modes. From the characteristic spatial (resp. temporal) variations of the envelope of the source we can also define a length scale R_0 (resp. a time scale T_0). In order to make comparison we associate to the time scale T_0 the corresponding length scale $L_0:=cT_0$. Our study will take place in the framework where the dimensionless parameter $\delta=\min\{\lambda_0/R_0,\lambda_0/L_0\}$ is small. Note that this assumption prevents from addressing the cases of ultrashort pulses (whose duration is of the order of a few femtoseconds) and of ultrafocused beams (whose radius is of the order of a few micrometers). The most interesting case is then the configuration where R_0 and L_0 are of the same order: $\lambda_0\ll R_0\sim L_0$, since it is the case that contains all physical phenomena and the other configurations $\lambda_0\ll R_0\ll L_0$ and $\lambda_0\ll L_0\ll R_0$ can be deduced from the first one by straightforward approximations. Setting $\delta=\lambda_0/R_0$, $\tilde{x}=x/\lambda_0$, $\tilde{y}=y/\lambda_0$, $\tilde{z}=z/\lambda_0$, and $\tilde{t}=ct/\lambda_0$, the dimensionless Maxwell equation reads as:

$$\tilde{\mathbf{rot}}\,\tilde{\mathbf{rot}}\,\mathcal{E}=-\tilde{\mu}_0\partial_t^2\mathcal{D},$$

where $\tilde{\mu}_0=\mu_0 c^2$. If we denote $\tilde{\varepsilon}_0=\varepsilon_0$ and $\tilde{c}=1$, then we still have the conservation relation $\tilde{\mu}_0\tilde{\varepsilon}_0\tilde{c}^2=1$. The source $\mathcal{S}$ has a high-frequency expansion of the form

$$\mathcal{S}(\tilde{x},\tilde{y},\tilde{t})=\frac{1}{2}\sum_{\omega_f\in\Omega_{\mathcal{S}}}\begin{pmatrix} v_x^f(\delta\tilde{t},\delta\tilde{x},\delta\tilde{y}) \\ v_y^f(\delta\tilde{t},\delta\tilde{x},\delta\tilde{y}) \\ 0 \end{pmatrix} e^{-i\omega_f\tilde{t}}+cc. \tag{6}$$

$\Omega_{\mathcal{S}}$ is the collection (with finite cardinality) of the high carrier frequencies ω_f of the modes that the source contains. These carrier frequencies are now of order 1. $\mathbf{v}^f$ is the slowly varying envelope of the mode with carrier frequency ω_f, and the typical scale of the variations of the smooth function $(T,X,Y)\mapsto\mathbf{v}^f(T,X,Y)$ is of order 1. Note that a dimensionless propagation distance $\tilde{z}$ of the order of δ^{-1} corresponds to a physical distance of the order of R_0. Further a dimensionless propagation distance $\tilde{z}$ of the order of δ^{-2} corresponds to a physical distance of the order of R_0^2/λ_0 which is the well-known Rayleigh distance.

From now on we drop the tildes. We assume *a priori* that the electric field, the electric induction and the polarization can be expanded in a power series of the small parameter δ and in a series with respect to a set of rapid phases $k^f z-\omega_f t$:

$$\mathcal{E}=\frac{1}{2}\sum_{(\omega_f,k^f)\in H}(\mathbf{E}^f(\delta t,\delta x,\delta y,\delta z)e^{i(k^f z-\omega_f t)}+cc), \tag{7a}$$

$$\mathbf{E}^f(T,X,Y,Z)=\sum_{j=0}^{\infty}\delta^j\mathbf{E}_j^f(T,X,Y,Z), \tag{7b}$$

where $\mathbf{E}^f$ is the slowly varying envelope of the mode whose rapid phase is (ω_f,k^f). The functions $\mathbf{E}_j^f$ are smooth in all their arguments. H denotes the set of the rapid phases (ω_f,k^f) which are contained in the field $\mathcal{E}$. Finally note that the slow variables will be denoted throughout the paper by capital letters (say T), while the fast variables, or microscopic, will be represented by lower case letters (say t).

III. LINEAR POLARIZATION

A. Geometry

We introduce the geometric framework. We first define a reference frame (x, y, z) associated with the pulse where the carrier wave vector of the incoming pulse is collinear to the z axis. We then introduce a reference frame (1, 2, 3) associated with the optic axis of the crystal, where $\mathbf{e}_3$ is the main optic axis. The description of the carrier wave vector in the crystal reference frame is given in Fig. 1. θ stands for the angle between the wave vector $\mathbf{k}_0$ and the main optic axis. ϕ is the angle between the projection of the wave vector onto the plane $(\mathbf{e}_1,\mathbf{e}_2)$ and the axis collinear to $\mathbf{e}_1$. In such a configuration the transition matrix between the reference frames (x, y, z) and (1, 2, 3) is

$$U:=\begin{pmatrix} \cos\theta\cos\phi & -\sin\phi & \sin\theta\cos\phi \\ \cos\theta\sin\phi & \cos\phi & \sin\theta\sin\phi \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}.$$

The matrix U is unitary and satisfies $U^{-1}=U^T$. Throughout the paper we use the notation M^T for the transpose of a matrix M. If $\mathbf{v}$ is a row vector (resp. line vector), $\mathbf{v}^T$ stands for the line vector (resp. row vector) whose coefficients are v_j.

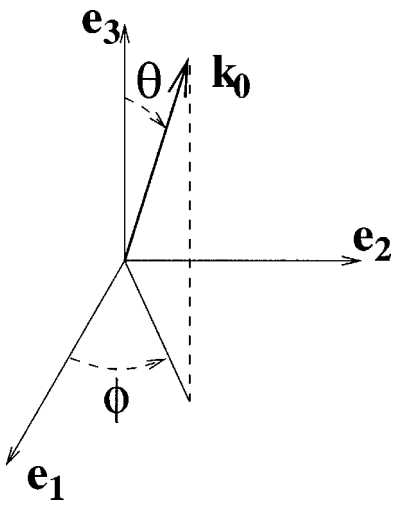

FIG. 1. Description of the wave vector in the crystallographic reference frame.

B. Linear susceptibility

The linear susceptibility is defined as the Fourier transform of the $\chi^{(1)}$ tensor[10]

$$\hat{\chi}^{(1)}(\omega) := \int_0^\infty dt_1 \chi^{(1)}(t_1) e^{i\omega t_1}.$$

Time integration starts from 0 to satisfy the causality property. In the crystallographic reference frame (1, 2, 3) the linear susceptibility is diagonal and reads:

$$\hat{\chi}^{(1)}_{123} = \begin{pmatrix} \chi_1 & 0 & 0 \\ 0 & \chi_2 & 0 \\ 0 & 0 & \chi_3 \end{pmatrix},$$

so that in the reference frame (x, y, z) the tensor $\hat{\chi}^{(1)}_{xyz}$ is $U^{-1}\hat{\chi}^{(1)}_{123}U$

$$\hat{\chi}^{(1)}_{xyz} = \begin{pmatrix} \chi_4 \cos^2\theta + \chi_3 \sin^2\theta & \frac{\sin(2\phi)}{2}(\chi_2 - \chi_1)\cos\theta & \frac{\sin(2\theta)}{2}(\chi_4 - \chi_3) \\ \frac{\sin(2\phi)}{2}(\chi_2 - \chi_1)\cos\theta & \chi_1 \sin^2\phi + \chi_2 \cos^2\phi & \frac{\sin(2\phi)}{2}(\chi_2 - \chi_1)\sin\theta \\ \frac{\sin(2\theta)}{2}(\chi_4 - \chi_3) & \frac{\sin(2\phi)}{2}(\chi_2 - \chi_1)\sin\theta & \chi_4 \sin^2\theta + \chi_3 \cos^2\theta \end{pmatrix}, \quad (8)$$

where $\chi_4 = \chi_1 \cos^2\phi + \chi_2 \sin^2\phi$. In the following χ is a shorthand for the matrix $\hat{\chi}^{(1)}_{xyz} + I_d$.

C. Expansion of the linear polarization

The linear induction is $\mathcal{D} = \varepsilon_0 \mathcal{E} + \mathcal{P}$. If $\mathcal{E} = \frac{1}{2}(\mathbf{E}(\delta t, \delta \mathbf{x}) e^{i(kz - \omega t)} + cc)$ and if we denote by $T = \delta t$ the slowly varying time variable, then the contribution of the linear induction to the Maxwell equation (2) can be expanded as

$$-\mu_0 \partial_t^2 \mathcal{D} = \tfrac{1}{2}(\mathbf{D}_0(\mathbf{E}) + \delta \mathbf{D}_1(\mathbf{E}) + \delta^2 \mathbf{D}_2(\mathbf{E}) + O(\delta^3)) e^{i(kz - \omega t)} + cc, \quad (9)$$

where the $\mathbf{D}_j(\mathbf{E})$ are linear functions of $\mathbf{E}$ given by

$$\mathbf{D}_0(\mathbf{E})=\frac{\omega^2}{c^2}\chi\mathbf{E},\quad \mathbf{D}_1(\mathbf{E})=\frac{i}{c^2}(\omega^2\chi)'\,\partial_T\mathbf{E},\quad \mathbf{D}^2(\mathbf{E})=-\frac{1}{2c^2}(\omega^2\chi)''\,\partial_T^2\mathbf{E}, \tag{10}$$

and the primes indicate partial derivatives with respect to ω.

Proof: If $\mathcal{E}=\frac{1}{2}(\mathbf{E}(\delta t,\delta\mathbf{x})e^{i(kz-\omega t)}+cc)$, then by expanding the linear induction as powers of δ we get

$$\mathcal{D}=\tfrac{1}{2}(\mathbf{D}(\delta t,\delta\mathbf{x})e^{i(kz-\omega t)}+cc),$$

$$\mathbf{D}=\varepsilon_0\mathbf{E}+\varepsilon_0\sum_{j=0}^{\infty}\frac{\delta^j(-1)^j}{j!}\left(\int_0^{\infty}dt'\,t'^j\,\chi^{(1)}(t')e^{i\omega t'}\right)\partial_T^j\mathbf{E}.$$

We introduce the derivatives of the linear susceptibility:

$$\hat{\chi}^{(1,j)}(\omega)=\frac{\partial^j\hat{\chi}^{(1)}}{\partial\omega^j}(\omega)=\int_0^{\infty}dt_1(it_1)^j\chi^{(1)}(t_1)e^{i\omega t_1},$$

so that the above expression reduces

$$\mathbf{D}=\varepsilon_0\mathbf{E}+\varepsilon_0\sum_{j=0}^{\infty}\frac{\delta^j i^j}{j!}\hat{\chi}^{(1,j)}(\omega)\partial_T^j\mathbf{E}.$$

If only the coefficients of order smaller than δ^2 are retained, then the contribution of the linear polarization to the Maxwell equation reads

$$-\mu_0\partial_t^2\mathcal{D}=\frac{1}{2}\left\{\frac{\omega^2}{c^2}(I_d+\hat{\chi}^{(1)})\mathbf{E}+i\delta\frac{\omega}{c^2}(\omega\hat{\chi}^{(1,1)}+2\hat{\chi}^{(1)})\partial_T\mathbf{E}\right.$$
$$\left.-\delta^2\frac{1}{c^2}\left(\frac{1}{2}\omega^2\hat{\chi}^{(1,2)}+2\omega\hat{\chi}^{(1,1)}+\hat{\chi}^{(1)}\right)\partial_T^2\mathbf{E}+O(\delta^3)\right\}e^{i(kz-\omega t)}+cc,$$

which establishes the desired result since $\chi=I_d+\hat{\chi}^{(1)}$. □

Notice that an expansion of the field of the form $\mathcal{E}=\frac{1}{2}\mathbf{E}(\delta t,\delta\mathbf{x})e^{i(kz-\omega t)}+cc$ provides an expansion of the contribution of the linear induction of the form $\frac{1}{2}(\mathbf{D}_0(\mathbf{E})+\delta\mathbf{D}_1(\mathbf{E})+\delta^2\mathbf{D}_2(\mathbf{E})+\cdots)e^{i(kz-\omega t)}+cc$. If one desires similar forms in both expansions, then it is sufficient to consider an expansion of the field of the form $\mathcal{E}=\frac{1}{2}(\mathbf{E}_0+\delta\mathbf{E}_1+\delta^2\mathbf{E}_2+\cdots)(\delta t,\delta\mathbf{x})e^{i(kz-\omega t)}+cc$. This remark will appear determining in the establishing of a suitable ansatz for the solution of the Maxwell equation which is discussed in the next section.

IV. ELECTROMAGNETIC PROPAGATION IN ANISOTROPIC MEDIA

A. Principle of the high-frequency expansion

We aim at outlining the principle of the high-frequency expansion method. It can be applied if the source can be expanded as (6). Then we proceed to *a priori* expansions of the field inside the crystal of the form (7). In linear media the set of the frequencies ω which are contained in H is imposed by the source and is equal to $\Omega_{\mathcal{S}}$. In nonlinear media the generation of harmonics should be taken into account so that the set H could be much larger than in the linear case.

The establishing of the propagation equations for the slowly varying envelopes obeys the following scheme. The form (7) is substituted into Eq. (2): **rot rot** $\mathcal{E}=-\mu_0\partial_t^2\mathcal{D}$. We get the expansion with respect to δ by applying formulas (9) and (11) for the right-hand side of Eq. (2) (contribution of the linear induction) and the left-hand side of Eq. (2) (**rot rot** $\mathcal{E}$), respectively. Collecting the terms with similar orders in δ and the same rapid phases (ω_f,k^f), we get a family

of equations. These equations can be decomposed into independent systems of equations parametrized by the rapid phases. The system corresponding to a rapid phase (ω_f, k^f) reads as a closed form system for the coefficients $\mathbf{E}_j^f$ of the series expansion of the envelope $\mathbf{E}^f$. This means that the envelopes of the different modes propagate independently. Note that in nonlinear media there may be coupling between the propagation equations of the modes. Considering the system for the mode with rapid phase (ω_f, k^f), we shall show on the one hand that a dispersion equation on (ω_f, k^f) appears as a compatibility condition for the existence of the high-frequency expansion (7a), and on the other hand that the form of the leading order term $\mathbf{E}_0^f$ is imposed by a compatibility condition for the existence of the series expansion (7b).

The form (7) is an ansatz, that is to say an *a priori* form of the solution which is valid in a given domain, here for $z \lesssim \delta^{-1}$. As an ansatz it satisfies basic properties. First it is compatible with the boundary conditions and the source. Second it is self-similar with respect to the operators that are encountered in the Maxwell equation. Indeed we have already established in Sec. III C that applying the operator corresponding to the right-hand side of the Maxwell equation to a an expansion of the kind (7) provides the same form. We are going to see in the next section devoted to the action of the **rot rot** operation that the expansion (7) is also self-similar with respect to this operator.

B. Expansion of the rot rot $\mathcal{E}$ term

If $\mathcal{E}$ is of the form $\mathcal{E}=\frac{1}{2}(\mathbf{E}(\delta t, \delta x, \delta y, \delta z)e^{i(kz-\omega t)}+cc)$, then **rot rot** $\mathcal{E}$ can be expanded as powers of δ. Denoting by $T=\delta t$, $X=\delta x$, $Y=\delta y$, and $Z=\delta z$ the slowly varying variables we find that

$$\mathbf{rot\,rot}\,\mathcal{E}=\tfrac{1}{2}(\mathbf{R}_0(\mathbf{E})+\delta\mathbf{R}_1(\mathbf{E})+\delta^2\mathbf{R}_2(\mathbf{E}))e^{i(kz-\omega t)}+cc, \tag{11}$$

where the mappings $\mathbf{R}_j(\mathbf{E})$ are given by

$$\mathbf{R}_0(\mathbf{E})=\begin{pmatrix} k^2E_x \\ k^2E_y \\ 0 \end{pmatrix}, \tag{12a}$$

$$\mathbf{R}_1(\mathbf{E})=\begin{pmatrix} ik\partial_X E_z-2ik\partial_Z E_x \\ ik\partial_Y E_z-2ik\partial_Z E_y \\ ik\partial_X E_x+ik\partial_Y E_y \end{pmatrix}, \tag{12b}$$

$$\mathbf{R}_2(\mathbf{E})=\begin{pmatrix} -\partial_Y^2E_x-\partial_Z^2E_x+\partial_X\partial_Y E_y+\partial_X\partial_Z E_z \\ -\partial_X^2E_y-\partial_Z^2E_y+\partial_X\partial_Y E_x+\partial_Y\partial_Z E_z \\ -\partial_X^2E_z-\partial_Y^2E_z+\partial_X\partial_Z E_x+\partial_Y\partial_Z E_y \end{pmatrix}. \tag{12c}$$

Note that (11) actually holds true as an identity, and not only as an expansion. Furthermore $\mathbf{R}_2(\mathbf{E})$ is simply the standard ''**Rot Rot E**'' when the spatial derivatives are taken with respect to the slow variables (X, Y, Z).

C. Dispersion equation

Let us first assume that the input pulse has a single carrier frequency ω. By substituting the ansatz (7) into Eq. (2) and collecting the coefficients with power δ^0, we get by applying the identities (9) and (11) that $\mathbf{R}_0(\mathbf{E}_0)=\mathbf{D}_0(\mathbf{E}_0)$

$$k^2J\mathbf{E}_0=\omega^2c^{-2}\chi\mathbf{E}_0, \tag{13}$$

where J is the matrix

$$J=\begin{pmatrix}1&0&0\\0&1&0\\0&0&0\end{pmatrix}. \tag{14}$$

The projection of Eq. (13) onto the z axis implies

$$E_{0z}=-\chi_{zz}^{-1}(\chi_{zx}E_{0x}+\chi_{zy}E_{0y}),$$

and substituting this identity into Eq. (13) we get that (E_{0x},E_{0y}) should fulfill

$$k^2\begin{pmatrix}E_{0x}\\E_{0y}\end{pmatrix}=\frac{\omega^2}{c^2}M\begin{pmatrix}E_{0x}\\E_{0y}\end{pmatrix},$$

where M is the 2×2 matrix

$$M=\begin{pmatrix}\chi_{xx}-\dfrac{\chi_{xz}\chi_{zx}}{\chi_{zz}} & \chi_{xy}-\dfrac{\chi_{xz}\chi_{zy}}{\chi_{zz}}\\ \chi_{yx}-\dfrac{\chi_{yz}\chi_{zx}}{\chi_{zz}} & \chi_{yy}-\dfrac{\chi_{yz}\chi_{zy}}{\chi_{zz}}\end{pmatrix}.$$

Note that, since χ is symmetric, M is also symmetric. The existence of a nonzero field $\mathbf{E}_0$ with carrier wave number k is equivalent to the Fresnel equation expressing the determinant of the system (13) equaling 0

$$\det(M-n^2I_d)=0. \tag{15}$$

The relationship $k=n\omega c^{-1}$ describes the normal waves that can propagate in the media with dielectric tensor χ. Eq. (15) also reads in terms of χ_1, χ_2, and χ_3 as

$$n^4-Sn^2+P=0,$$

$$S=\frac{(\chi_1\chi_2+\chi_3\chi_4)\sin^2\theta+\chi_3(\chi_1+\chi_2)\cos^2\theta}{\chi_3\cos^2\theta+\chi_4\sin^2\theta},$$

$$P=\frac{\chi_1\chi_2\chi_3}{\chi_3\cos^2\theta+\chi_4\sin^2\theta}.$$

The sum $n_a^2+n_b^2$ is equal to S and the product $n_a^2n_b^2$ is equal to P. Since S and P are positive it is easy to check that the Fresnel equation (15) has two positive solutions n_a and n_b. Consequently there exist two possible polarizations $\mathbf{s}_a$ and $\mathbf{s}_b$ so that $\mathbf{s}_a$ and $\mathbf{s}_b$ are unit vectors and $(n_a\omega c^{-1},\mathbf{s}_a)$ and $(n_b\omega c^{-1},\mathbf{s}_b)$ are solutions of Eq. (13). Furthermore the vectors (s_{ax},s_{ay}) and (s_{bx},s_{by}) are orthogonal. We define the dispersion relationship, the group velocity and the dispersion coefficient of the waves as follows:

$$k_m(\omega):=\frac{\omega n_m(\omega)}{c},\quad v_m(\omega):=\left(\frac{\partial k_m}{\partial\omega}\right)^{-1},\quad \sigma_m(\omega):=k_m\frac{\partial^2k_m}{\partial\omega^2},\quad m=a,b. \tag{16}$$

Accordingly, if the polarization of the incoming pulse has components on both the x and y axis, then it should be decomposed into the sum of a type a and type b waves. We shall discuss this decomposition precisely in the next section. Further, if the incoming pulse is a superposition of

several modes with different carrier frequencies, then for each carrier frequency ω_f the above results can be applied, so that each mode should be decomposed into the sum of a type a and type b waves.

Note that the occurrence of the case $n_a=n_b$ corresponds to very particular configurations. If the three indices χ_1, χ_2, and χ_3 are distinct (biaxial crystals), then the only cases for which $n_a=n_b$ are (assuming for instance $\chi_1>\chi_2>\chi_3$): $\phi=0$ or π and $\theta=\pm\theta_c(\omega)$, where

$$\sin^2\theta_c=\frac{\chi_1/\chi_2-1}{\chi_1/\chi_3-1}, \tag{17}$$

which defines the two optic axes of the biaxial crystal. If χ_3 is different from $\chi_1=\chi_2$ (uniaxial crystals), then the only cases for which $n_a=n_b$ are $\theta=0$ or π, and any ϕ. This defines the optic axis of the uniaxial crystal. Of course in isotropic medium $\chi_1=\chi_2=\chi_3$ one has $n_a=n_b$, but this trivial case will not be addressed in this paper.

Section V is devoted to an extensive study of the propagation of the pulse in anisotropic media in the general case when $n_a\neq n_b$. These results are then applied to the case of uniaxial crystals in Sec. VI. In Secs. VII–VIII we study the critical cases when $n_a=n_b$. Finally in Sec. IX we give some more results about the case when the crystal is biaxial but two of the crystal indices χ_j are close to each other.

D. Boundary condition

This condition reads as (5). We first eliminate the magnetic induction by differentiating with respect to time

$$(\partial_t\mathcal{E}+c\,\mathbf{rot}\,\mathcal{E}\times\mathbf{n})\times\mathbf{n}=2\partial_t\mathcal{S}\times\mathbf{n}.$$

If we assume that the source $\mathcal{S}$ can be expanded as (6), and accordingly that the field $\mathcal{E}$ inside the crystal is of the form (7), then collecting the coefficients with power δ^0 and high carrier frequency ω_f establishes the continuity conditions which impose that the components parallel to the boundary surface of the input field $\mathcal{S}$ and of the field $\mathcal{E}$ should be equal, while there are no condition for the normal components. Consequently, the type m mode ($m=a,b$) with carrier frequency ω_f should be at $z=0^+$

$$\mathbf{E}^f_{0,m}(\delta t,\delta x,\delta y,z=0^+)=c_{tr,m}(\omega_f)\mathbf{v}^f(\delta t,\delta x,\delta y),$$

where the transmission matrices $c_{tr,m}$ are

$$c_{tr,m}(\omega)=\frac{2}{1+n_m(\omega)}\frac{1}{s_{mx}^2+s_{my}^2}\begin{pmatrix} s_{mx}^2 & s_{mx}s_{my} & 0\\ s_{mx}s_{my} & s_{my}^2 & 0\\ s_{mx}s_{mz} & s_{my}s_{mz} & 0\end{pmatrix}.$$

Note that, if the input field at frequency ω_f is linearly polarized along the $(s_{ax},s_{ay},0)$-axis, then the field inside the crystal is purely type a. Moreover $c_{tr,m}(s_{mx},s_{my},0)^T=(2/[1+n_m(\omega)])\mathbf{s}_m$.

V. THE GEOMETRIC AND DIFFRACTIVE REGIMES IN THE GENERAL CASE

In this section we assume that the input pulse has only one carrier frequency ω and that the dispersion equation has two distinct solutions $n_a\neq n_b$. In such a configuration, the input pulse can be decomposed into a type a wave and a type b wave which propagate independently. We shall express our results in the case when the input pulse is linearly polarized according to the $(s_{ax},s_{ay},0)$. The generalization to any polarization is then straightforward by application of the superposition principle. The case when $n_a=n_b$ require a specific study since the rapid phases of the type a and type b waves are equal, so their propagations may be coupled. This study will be carried out in Secs. VII and VIII.

A. Geometric optics

We assume in this section that the input pulse with carrier frequency ω is linearly polarized according to the $(s_{ax}(\omega),s_{ay}(\omega),0)$-axis

$$\mathcal{S}=\tfrac{1}{2}v(\delta x,\delta y,\delta t)(s_{ax},s_{ay},0)^T e^{-i\omega t}+cc. \tag{18}$$

Consequently we adopt the ansatz (7) with $H=\{(\omega,k_a(\omega))\}$

$$\mathcal{E}=\frac{1}{2}\left(\sum_{j=0}^{\infty}\delta^j\mathbf{E}_j(\delta t,\delta x,\delta y,\delta z)\right)e^{i(k_a(\omega)z-\omega t)}+cc. \tag{19}$$

We denote $T=\delta t,\ X=\delta x,\ Y=\delta y,\ Z=\delta z,$ and k_a is a shorthand for $k_a(\omega)$.

Proposition 1. If the source $\mathcal{S}$ can be expanded as (18), then the leading order term $\mathbf{E}_0$ of the slowly varying envelope is linearly polarized along the $\mathbf{s}_a$-axis and satisfies the transport equation:

$$u_{ax}\partial_X E_0+u_{ay}\partial_Y E_o-\partial_Z E_0-v_a(\omega)^{-1}\partial_T E_0=0, \tag{20}$$

starting from $\mathbf{E}_0(T,X,Y,Z=0)=2/[1+n_a(\omega)]v(T,X,Y)$, *where* $\mathbf{u}_a=(s_{ax}s_{az}/(s_{ax}^2+s_{ay}^2),s_{ay}s_{az}/(s_{ax}^2+s_{ay}^2),-1)^T$. The solution of the above transport equation reads

$$E_0(T,X,Y,Z)=\frac{2}{1+n_a(\omega)}v(T-Z/v_a(\omega),X+u_{ax}Z,Y+u_{ay}Z).$$

It corresponds to the framework of the geometric optics, where the slowly varying envelope propagates without deformation with the group velocity. Note that the group velocity $v_a(\omega)$ and $v_b(\omega)$ are different. This phenomenon is called walk-off in the classical literature. It means that an input pulse will break into the sum of a type a and type b waves which propagate without interaction at different velocities. Furthermore the rays along which the waves propagate are not parallel. The Poynting vector of a type a wave is collinear to the vector $\mathbf{u}_a$ which means that the energy flow does not propagate along the direction of the carrier wave vector $\mathbf{k}_a$ which is collinear to the z axis. This is the so-called angular walk-off phenomenon. Finally note that $\mathbf{u}_a$ is orthogonal to the polarization vector $\mathbf{s}_a$: $\mathbf{u}_a.\mathbf{s}_a=0$, and that the three vectors $\mathbf{s}_a$, $\mathbf{u}_a$, and $\mathbf{k}_a$ lie in the same plane.

Proof: Let us substitute the ansatz (19) into Eq. (2) and collect the coefficients of each power of δ.

Order δ^0. The equations obtained at order δ^0 give the dispersion relationship and the fact that $\mathbf{E}_0=E_0\mathbf{s}_a$ (see Sec. IV C).

Order δ^1. The identity $\mathbf{R}_0(\mathbf{E}_1)+\mathbf{R}_1(\mathbf{E}_0)=\mathbf{D}_0(\mathbf{E}_1)+\mathbf{D}_1(\mathbf{E}_0)$ reads

$$\frac{\omega^2}{c^2}\chi\mathbf{E}_1+\frac{i}{c^2}(\omega^2\chi)'\partial_T\mathbf{E}_0=k_a^2J\mathbf{E}_1+ik_a\begin{pmatrix}\partial_X E_{0z}-2\partial_Z E_{0x}\\ \partial_Y E_{0z}-2\partial_Z E_{0y}\\ \partial_X E_{0x}+\partial_Y E_{0y}\end{pmatrix}, \tag{21}$$

where J is the matrix (14). We project this equation onto the vector $\mathbf{s}_a$. Since the matrix χ is symmetric, Eq. (13) implies

$$(\mathbf{s}_a^T)\chi-k_a^2(\mathbf{s}_a^T)J\equiv 0, \tag{22}$$

so that the terms in $\mathbf{E}_1$ cancel. Furthermore $\mathbf{E}_0=E_0\mathbf{s}_a$, so that it remains

$$\frac{i}{c^2}((\mathbf{s}_a^T)(\omega^2\chi)'\mathbf{s}_a)\partial_T E_0=2ik_a(s_{ax}s_{az}\partial_X E_0+s_{ay}s_{az}\partial_Y E_0-(s_{ax}^2+s_{ay}^2)\partial_Z E_0). \tag{23}$$

Besides, differentiating with respect to ω the equation $(\omega^2/c^2)\chi\mathbf{s}_a=k_a^2J\mathbf{s}_a$ yields

$$\frac{1}{c^2}(\omega^2\chi)\mathbf{s}_a+\frac{\omega^2}{c^2}\chi\mathbf{s}_a=k_a^2J\mathbf{s}_a+2k_ak_a'J\mathbf{s}_a\,. \tag{24}$$

Left-multiplying this equation by $\mathbf{s}_a$, the terms in $\mathbf{s}_a'$ cancel by (22), so it comes

$$c^{-2}((\mathbf{s}_a^T)(\omega^2\chi)'\mathbf{s}_a)=2k_ak_a'(s_{ax}^2+s_{ay}^2).$$

Substituting into (23) finally establishes Eq. (20). □

B. Diffractive optics

Eq. (20) describes the propagation of the envelope of the pulse for distances z of the order of δ^{-1}. The propagation is a pure transport without deformation. Consequently no evolution is noticeable in the moving reference frame $(\delta(t-z/v_a),\delta(x+u_{ax}z),\delta(y+u_{ay}z))$ when one looks at z of the order of δ^{-1}. We are now considering longer propagation distances z of the order of the Rayleigh distance δ^{-2} and we adopt the following ansatz:

$$\mathcal{E}=\frac{1}{2}\left(\sum_{j=0}^{\infty}\delta^j\mathbf{E}_j(\delta(t-z/v_a),\delta(x+u_{ax}z),\delta(y+u_{ay}z),\delta^2z)\right)e^{i(k_az-\omega t)}+cc. \tag{25}$$

We denote $T=\delta(t-z/v_a)$, $X=\delta(x+u_{ax}z)$, $Y=\delta(y+u_{ay}z)$ and the long scale variation of the envelope will be characterized by the variable $\zeta=\delta^2z$.

Proposition 2. If the source $\mathcal{S}$ can be expanded as (18), then the leading order term of the slowly varying envelope is linearly polarized along the $\mathbf{s}_a$-axis and satisfies in the moving frame the Schrödinger equation

$$\begin{aligned}&2ik_a\partial_\zeta E_0+c_{a,xx}\partial_X^2E_0+c_{a,yy}\partial_Y^2E_0+2c_{a,xy}\partial_X\partial_YE_0-\sigma_a\partial_T^2E_0\\&\quad+2k_a(u_{ax}'\partial_T\partial_XE_0+u_{ay}'\partial_T\partial_YE_0)=0,\end{aligned} \tag{26}$$

starting from $E_0(T,X,Y,\zeta=0)=(2/[1+n_a(\omega)])v(T,X,Y)$, where the prime stands for the partial derivative with respect to ω. The diffraction coefficients are given by

$$c_{a,xx}(\omega)=\frac{n_a^2}{n_b^2-n_a^2}\left(\frac{\chi_{zy}}{\chi_{zz}}+2u_{ay}\right)^2+\frac{n_a^2s_{ax}^2}{\chi_{zz}(s_{ax}^2+s_{ay}^2)}+\frac{s_{ay}^2}{(s_{ax}^2+s_{ay}^2)^2},$$

$$c_{a,xy}(\omega)=-\frac{n_a^2}{n_b^2-n_a^2}\left(\frac{\chi_{zy}}{\chi_{zz}}+2u_{ay}\right)\left(\frac{\chi_{zx}}{\chi_{zz}+2u_{ax}}\right)+\frac{n_a^2s_{ax}s_{ay}}{\chi_{zz}(s_{ax}^2+s_{ay}^2)}-\frac{s_{ax}s_{ay}}{(s_{ax}^2+s_{ay}^2)^2},$$

$$c_{a,yy}(\omega)=\frac{n_a^2}{n_b^2-n_a^2}\left(\frac{\chi_{zx}}{\chi_{zz}}+2u_{ax}\right)^2+\frac{n_a^2s_{ay}^2}{\chi_{zz}(s_{ax}^2+s_{ay}^2)}+\frac{s_{ax}^2}{(s_{ax}^2+s_{ay}^2)^2}.$$

This proposition gives the equation which governs the propagation of the envelope of the field in the framework of the slowly varying envelope. We get here the result that the envelope in the moving framework satisfies a Schrödinger-type equation with an anisotropic diffraction operator, and that coupled time–space derivatives of the envelope are coming into the equation.

It thus appears that there exists a disagreement between the propagation equations which are proposed in standard references,[4] where the diffraction effect is represented as an isotropic Laplace operator with respect to the transverse coordinates, and our Eq. (26) where the diffraction effect reads as an anisotropic second order operator. We aim here at underlying the point where we feel the departure comes from. The direction of the polarization vector is assumed to be constant during propagation in previous derivations of the evolution equations. We have shown in this paper that this hypothesis holds true for the leading term $\mathbf{E}_0$, but it is wrong when considering

the corrective term $\mathbf{E}_1$. We feel that the departure between the results essentially originates from the improper assumption about the constancy of the direction of the polarization vector.

The crossed space–time derivatives essentially originate from the fact that the Poynting vector of a monochromatic pulse is collinear to $\mathbf{u}_a(\omega)$ whose direction depends on the frequency ω. Accordingly the different frequencies of a broadband pulse (or equivalently a short pulse) do not propagate exactly in the same direction which involves this additive ''dispersion.''

PROOF: We substitute the ansatz (25) into Eq. (2) and we collect the coefficients with the same power of δ. In the expressions (12b) and (12c) of $\mathbf{R}_1$ and $\mathbf{R}_2$ we must take care to replace $\partial_Z(.)$ by $-v_a^{-1}\partial_T(.)+u_{ax}\partial_X(.)+u_{ay}\partial_Y(.)$ and to take into account the new slow variable ζ.

Order δ^1. Once rewritten in terms of the new variables, the transport equation (20) becomes trivial. Furthermore, since

$$((\omega^2\chi)'\mathbf{s}_a)_z=(\omega^2\chi\mathbf{s}_a)_z'-(\omega^2\chi\mathbf{s}_a')_z=0-\omega^2(\chi_{zx}s_{ax}'+\chi_{zy}s_{ay}'+\chi_{zz}s_{az}'),$$

the projection of Eq. (21) onto the z axis establishes that

$$E_{1z}=-\chi_{zz}^{-1}(\chi_{zx}E_{1x}+\chi_{zy}E_{1y})+\frac{ik_ac^2}{\omega^2\chi_{zz}}(\partial_XE_{0x}+\partial_YE_{0y})+i\left(\frac{\chi_{zx}}{\chi_{zz}}s_{ax}'+\frac{\chi_{zy}}{\chi_{zz}}s_{ay}'+s_{az}'\right)\partial_TE_0. \tag{27}$$

Substituting into the projections of Eq. (21) onto the axes x and y

$$\left(\frac{\omega^2}{c^2}M-k_a^2I_d\right)\begin{pmatrix}E_{1x}\\E_{1y}\end{pmatrix}=ik_a\begin{pmatrix}-s_{ay}\\s_{ax}\end{pmatrix}\left(\left(-\frac{\chi_{yz}}{\chi_{zz}}-2u_{ay}\right)\partial_XE_0+\left(\frac{\chi_{xz}}{\chi_{zz}}+2u_{ax}\right)\partial_YE_0\right)$$
$$+i\left(\left(\frac{\omega^2}{c^2}M-k_a^2I_d\right)\begin{pmatrix}s_{ax}'\\s_{ay}'\end{pmatrix}-2k_ak_a'\begin{pmatrix}s_{ax}\\s_{ay}\end{pmatrix}\right)\partial_TE_0. \tag{28}$$

Since the vectors (s_{ax},s_{ay}) and $(-s_{ay},s_{ax})$ are orthogonal, there exist two scalars A_a and B_a such that

$$\begin{pmatrix}E_{1x}\\E_{1y}\end{pmatrix}=A_a\begin{pmatrix}s_{ax}\\s_{ay}\end{pmatrix}+B_a\begin{pmatrix}-s_{ay}\\s_{ax}\end{pmatrix}, \tag{29}$$

and two scalars C_a and D_a such that

$$\left(\frac{\omega^2}{c^2}M-k_a^2I_d\right)\begin{pmatrix}-s_{ay}\\s_{ax}\end{pmatrix}=C_a\begin{pmatrix}s_{ax}\\s_{ay}\end{pmatrix}+D_a\begin{pmatrix}-s_{ay}\\s_{ax}\end{pmatrix}.$$

Since $\binom{s_{ax}}{s_{ay}}$ is an eigenvector of $\omega^2c^{-2}M$ with eigenvalue k_a^2, left-multiplying this equation by $\binom{s_{ax}}{s_{ay}}$ yields: $0=C_a(s_{ax}^2+s_{ay}^2)$ so $C_a=0$. Thus $\binom{-s_{ay}}{s_{ax}}$ is an eigenvector of $\omega^2c^{-2}M$ with eigenvalue $D_a+k_a^2$, and by definition of the eigenvalues this proves that $D_a=k_b^2-k_a^2$. Eq. (28) now reads

$$B_a=i\frac{s_{ax}s_{ay}'-s_{ay}s_{ax}'}{s_{ax}^2+s_{ay}^2}\partial_TE_0+\frac{ik_a}{k_b^2-k_a^2}\left(\left(-\frac{\chi_{yz}}{\chi_{zz}}-2u_{ay}\right)\partial_XE_0+\left(\frac{\chi_{xz}}{\chi_{zz}}+2u_{ax}\right)\partial_YE_0\right). \tag{30}$$

Order δ^2. Collecting the coefficients of order δ^2 we get:

$$\mathbf{R}_0(\mathbf{E}_2)+\mathbf{R}_1(\mathbf{E}_1)+\mathbf{R}_2(\mathbf{E}_0)=\mathbf{D}_0(\mathbf{E}_2)+\mathbf{D}_1(\mathbf{E}_1)+\mathbf{D}_2(\mathbf{E}_0).$$

Projecting onto the vector $\mathbf{s}_a$ the terms in $\mathbf{E}_2$ cancel and it remains

$$\mathbf{s}_a.\mathbf{R}_1(\mathbf{E}_1)+\mathbf{s}_a.\mathbf{R}_2(\mathbf{E}_0)=\mathbf{s}_a.\mathbf{D}_1(\mathbf{E}_1)+\mathbf{s}_a.\mathbf{D}_2(\mathbf{E}_0). \tag{31}$$

We now compute the four terms of this identity.

(i) Computation of $\mathbf{S}_a.\mathbf{D}_1(\mathbf{E}_1)$.
By definition:

$$\mathbf{S}_a.\mathbf{D}_1(\mathbf{E}_1)=ic^{-2}(\mathbf{s}_a^T)(\omega^2\chi)'\partial_T\mathbf{E}_1.$$

From (22) this expression simplifies

$$\mathbf{s}_a.\mathbf{D}_1(\mathbf{E}_1)=2ik_ak_a'\partial_T(s_{ax}E_{1x}+s_{ay}E_{1y})-i(\mathbf{s}_a'^T)(\omega^2c^{-2}\chi-k_a^2J)\partial_T\mathbf{E}_1. \tag{32}$$

Differentiating Eq. (21) with respect to time and multiplying by $\mathbf{s}_a'^T$ establishes

$$\begin{aligned}&(\mathbf{s}_a'^T)(\omega^2c^{-2}\chi-k_a^2J)\partial_T\mathbf{E}_1\\&\quad=i(\mathbf{s}_a'^T)(\omega^2c^{-2}\chi-k_a^2J)\mathbf{s}_a'\partial_T^2E_0+ik_a(s_{ax}^2+s_{ay}^2)(u_{ax}'\partial_T\partial_XE_0+u_{ay}'\partial_T\partial_YE_0).\end{aligned}$$

On the one hand, differentiating Eq. (24) with respect to ω and multiplying by $\mathbf{s}_a^T$

$$\begin{aligned}&c^{-2}(\mathbf{s}_a^T)(\omega^2\chi)''\mathbf{s}_a+2c^{-2}(\mathbf{s}_a^T)(\omega^2\chi)'\mathbf{s}_a'\\&\quad=4k_ak_a'(s_{ax}s_{ax}'+s_{ay}s_{ay}')+2((k_a')^2+k_ak_a'')(s_{ax}^2+s_{ay}^2).\end{aligned}$$

On the other hand, multiplying Eq. (24) by $\mathbf{s}_a'^T$

$$c^{-2}(\mathbf{s}_a'^T)(\omega^2\chi)'\mathbf{s}_a+\omega^2c^{-2}(\mathbf{s}_a'^T)\chi\mathbf{s}_a'=k_a^2((s_{ax}')^2+(s_{ay}')^2)+2k_ak_a'(s_{ax}'s_{ax}+s_{ay}'s_{ay}).$$

Multiplying by 2 the last identity and subtracting the last two identities establish:

$$c^{-2}(\mathbf{s}_a^T)(\omega^2\chi)''\mathbf{s}_a=2(\mathbf{s}_a'^T)(\omega^2c^{-2}\chi-k_a^2J)\mathbf{s}_a'+2((k_a')^2+k_ak_a'')(s_{ax}^2+s_{ay}^2).$$

Finally, substituting into (32)

$$\begin{aligned}\mathbf{s}_a.\mathbf{D}_1(\mathbf{E}_1)=&2ik_ak_a'\partial_T(s_{ax}E_{1x}+s_{ay}E_{1y})+k_a(s_{ax}^2+s_{ay}^2)(u_{ax}'\partial_T\partial_XE_0+u_{ay}'\partial_T\partial_YE_0)\\&+(-((k_a')^2+k_ak_a'')(s_{ax}^2+s_{ay}^2)+2^{-1}c^{-2}(\mathbf{s}_a^T)(\omega^2\chi)''\mathbf{s}_a)\partial_T^2E_0.\end{aligned} \tag{33}$$

(ii) Computation of $\mathbf{s}_a.\mathbf{D}_2(\mathbf{E}_0)$.
By definition and using the fact that $\mathbf{E}_0$ reads $\mathbf{s}_aE_0$

$$\mathbf{s}_a.\mathbf{D}_2(\mathbf{E}_0)=-2^{-1}c^{-2}(\mathbf{s}_a^T)(\omega^2\chi)''\mathbf{s}_a\partial_T^2E_0. \tag{34}$$

(iii) Computation of $\mathbf{s}_a.\mathbf{R}_2(\mathbf{E}_0)$.
Computing $\mathbf{s}_a.\mathbf{R}_2(\mathbf{E}_0)$ is easy

$$\begin{aligned}\mathbf{s}_a.\mathbf{R}_2(\mathbf{E}_0)=&\frac{-s_{ay}^2}{s_{ax}^2+s_{ay}^2}\partial_X^2E_0+\frac{2s_{ax}s_{ay}}{s_{ax}^2+s_{ay}^2}\partial_X\partial_YE_0+\frac{-s_{ax}^2}{s_{ax}^2+s_{ay}^2}\partial_Y^2E_0\\&-2ik_a(s_{ax}^2+s_{ay}^2)\partial_\xi E_0-\frac{s_{ax}^2+s_{ay}^2}{v_a^2}\partial_T^2E_0.\end{aligned} \tag{35}$$

(iv) Computation of $\mathbf{s}_a.\mathbf{R}_1(\mathbf{E}_1)$.
We first compute $\mathbf{s}_a.\mathbf{R}_1(\mathbf{E}_1)$ by taking into account (27)

$$\mathbf{s}_a.\mathbf{R}_1(\mathbf{E}_1)=ik_a\left[\left(-\frac{\chi_{zy}}{\chi_{zz}}-2u_{ay}\right)\partial_X+\left(\frac{\chi_{zx}}{\chi_{zz}}+2u_{ax}\right)\partial_Y\right](s_{ax}E_{1y}-s_{ay}E_{1x})$$
$$-\frac{k_a^2c^2}{\omega^2\chi_{zz}}(s_{ax}^2\partial_X^2E_0+2s_{ax}s_{ay}\partial_X\partial_YE_0+s_{ay}^2\partial_Y^2E_0)+2i\frac{k_a}{v_a}\partial_T(s_{ax}E_{1x}+s_{ay}E_{1y})$$
$$-k_a\left(\frac{\chi_{zx}}{\chi_{zz}}s'_{ax}+\frac{\chi_{zy}}{\chi_{zz}}s'_{ay}+s'_{az}\right)(s_{ax}\partial_T\partial_XE_0+s_{ay}\partial_T\partial_YE_0).$$

Using the representation (29) and the identity (30)

$$\mathbf{s}_a.\mathbf{R}_1(\mathbf{E}_1)=-\left[\frac{n_a^2(s_{ax}^2+s_{ay}^2)}{n_b^2-n_a^2}\left(\frac{\chi_{zy}}{\chi_{zz}}+2u_{ay}\right)^2+\frac{n_a^2s_{ax}^2}{\chi_{zz}}\right]\partial_X^2E_0-\left[\frac{n_a^2(s_{ax}^2+s_{ay}^2)}{n_b^2-n_a^2}\left(\frac{\chi_{zx}}{\chi_{zz}}+2u_{ax}\right)^2\right.$$
$$\left.+\frac{n_a^2s_{ay}^2}{\chi_{zz}}\right]\partial_Y^2E_0+2\left[\frac{n_a^2(s_{ax}^2+s_{ay}^2)}{n_b^2-n_a^2}\left(\frac{\chi_{zx}}{\chi_{zz}}+2u_{ax}\right)\left(\frac{\chi_{zy}}{\chi_{zz}}+u_{ay}\right)\right.$$
$$\left.-\frac{n_a^2s_{ax}s_{ay}}{\chi_{zz}}\right]\partial_X\partial_YE_0+2i\frac{k_a}{v_a}\partial_T(s_{ax}E_{1x}+s_{ay}E_{1y})-k_a\left(\frac{\chi_{zx}}{\chi_{zz}}s'_{ax}+\frac{\chi_{zy}}{\chi_{zz}}s'_{ay}+s'_{az}\right)$$
$$\times(s_{ax}\partial_T\partial_XE_0+s_{ay}\partial_T\partial_YE_0). \tag{36}$$

By collecting the expressions (33)–(36) of the four terms which are coming into the identity (31), we conclude that Eq. (26) holds true. □

C. Anomalous diffraction for biradial waves in biaxial crystals

We examine in this section the propagation in biaxial crystals in the particular configuration $\theta=\theta_r(\omega)$ and $\phi=0$ or π where

$$\sin^2\theta_r=\frac{1-\chi_2/\chi_1}{1-\chi_3/\chi_1},$$

where we have assumed that $\chi_1>\chi_2>\chi_3$. Computing all relevant quantities we have found that the eigenindices are $n_a^2=\chi_2$ and $n_b^2=\chi_1\chi_3/(\chi_1+\chi_3-\chi_2)$. The corresponding unit polarization vectors are

$$\mathbf{s}_a=(\cos\beta_r,0,\sin\beta_r)^T,$$

where the angle β_r is given by

$$\tan\beta_r=-\frac{\sqrt{(\chi_2-\chi_3)(\chi_1-\chi_2)}}{\chi_1+\chi_3-\chi_2}.$$

The diffraction coefficients are:

$$c_{a,xx}=1,\quad c_{a,xy}=0,\quad c_{a,yy}=0,$$

$$c_{b,xx}=\frac{\chi_1\chi_3}{(\chi_1+\chi_3-\chi_2)^2},\quad c_{b,xy}=0,\quad c_{b,yy}=\frac{\chi_1+\chi_3}{\chi_1+\chi_3-\chi_2}.$$

The striking point is that the diffraction operator for the type a wave is degenerate, in the sense that there is no diffraction in the y direction. The a wave is polarized along the y axis and satisfies the Schrödinger equation

$$2ik_a\partial_\zeta E_{0y}+\partial_X^2 E_{0y}-\sigma_a\partial_T^2 E_{0y}=0.$$

Such an anomalous behavior is consistent with the results derived in Ref. 11 where the authors show that the asymptotic form of the Green function is proportional to $z^{-1/2}$ instead of the standard z^{-1}-decay. This phenomenon is made transparent from our results, since the solution of a Schrödinger equation with a d-dimensional second-order operator spreads out as $z^{-d/2}$. This configuration could involve an interesting application in nonlinear optics. Consider high-intensity pulses so that the nonlinearity of the medium should be taken into account. Choose a carrier frequency such that the phase matching condition for the second-harmonic generation is not fulfilled. We may then expect that the main nonlinear term reads as a cubic Kerr effect, so that the field should satisfy (neglecting group velocity dispersion):

$$2ik_a\partial_\zeta E_{0y}+\partial_X^2 E_{0y}+\gamma|E_{0y}|^2E_{0y}=0.$$

This one-dimensional nonlinear Schrödinger equation possesses the complete integrability property, which implies that stable solitons should be generated and propagate over large distances. This configuration will be studied in the companion paper.[7]

VI. UNIAXIAL CRYSTALS

We assume in this section that the dielectric tensor $\chi^{(1)}$ corresponds to the uniaxial case, that is to say $\chi_1=\chi_2:=\chi_o$ and $\chi_3=\chi_e$, with $\chi_e\neq\chi_o$. The results derived in the above sections can then be rewritten in simpler terms. In the general framework $\theta\neq 0$ there are two distinct eigenindices, the so-called ordinary and extraordinary refractive indices

$$n_o(\omega)=\chi_o(\omega)^{1/2},\quad n_e(\omega)=\left(\frac{\chi_o(\omega)\chi_e(\omega)}{\cos^2\theta\chi_e(\omega)+\sin^2\theta\chi_o(\omega)}\right)^{1/2}. \tag{37}$$

These configurations correspond to an ordinary wave and an extraordinary wave, respectively. The unit polarization vector of an ordinary wave is simply $\mathbf{s}_o=(0,1,0)^T$, while the polarization vector of an extraordinary wave lies in the plane (xz) and is given by $\mathbf{s}_e(\omega)=(\cos\beta,0,\sin\beta)^T$, where the angle $\beta(\omega)$ is

$$\tan\beta(\omega)=\frac{\cos\theta\sin\theta(\chi_e(\omega)-\chi_o(\omega))}{\cos^2\theta\chi_e(\omega)+\sin^2\theta\chi_o(\omega)}.$$

A. Ordinary wave

The vector $\mathbf{u}_o$ which gives the direction of the rays along which the wave propagates in the geometric framework is simply $\mathbf{u}_o=(0,0,-1)^T$. The diffraction coefficients are $c_{o,xy}=0$, $c_{o,xx}=c_{o,yy}=1$, and $\mathbf{u}_o'=\mathbf{0}$, so that the propagation equation in the moving frame $(\delta(t-z/v_o),\delta x,\delta y,\delta^2 z))$ reads as the standard Schrödinger equation:

$$2ik_o\partial_\zeta E_{0y}+\partial_X^2 E_{0y}+\partial_Y^2 E_{0y}-\sigma_o\partial_T^2 E_{0y}=0.$$

An ordinary wave propagates according to the usual rules which govern the propagation of waves in linear isotropic media.

B. Extraordinary wave

The Poynting vector is $\mathbf{u}_e=(\tan\beta,0,-1)^T$. Thus β is the walk-off angle, that is to say the angle between the carrier wave vector $\mathbf{k}$ and the Poynting vector. The transverse diffraction coefficient $c_{e,xy}$ is zero while

$$c_{e,xx}(\omega)=\frac{\chi_o\chi_e}{(\cos^2\theta\chi_e+\sin^2\theta\chi_o)^2},\quad c_{e,yy}(\omega)=\frac{\chi_o}{\cos^2\theta\chi_e+\sin^2\theta\chi_o}.$$

Furthermore $u'_{e,x}=(\tan\beta)'$ and $u'_{e,y}=0$. The extraordinary wave $E_0=\mathbf{s}_e.\mathbf{E}_0$ in the moving frame $(\delta(t-z/v_e),\delta(x+\tan\beta z),\delta y,\delta^2 z)$ thus satisfies the equation

$$2ik_e\partial_\zeta E_0+c_{e,xx}\partial_X^2E_0+c_{e,yy}\partial_Y^2E_0+2k_e(\tan\beta)'\partial_T\partial_XE_0-\sigma_e\partial_T^2E_0=0.$$

In a negative crystal $\chi_o>\chi_e$ we have $c_{e,xx}<c_{e,yy}$, which proves that diffraction effects are more important along the y axis than along the x axis. Note that, as $\theta\to0$, we have $n_e\to n_o$ while the coefficients $c_{e,xx}$ and $c_{e,yy}$ converge to χ_o/χ_e. But as pointed out in Sec. V B, this extrapolation is not correct since terms of order δ are inversely proportional to n_o-n_e and consequently tend to infinity. At the limit $\theta\to0$ new terms of order 1 must be introduced. This will be done in the next section. Finally note that the expressions of the diffraction coefficients $c_{m,\dots}$, $m=o,e$, are compatible with the asymptotic form of the Green function in the case of a uniaxial medium given by Lax and Nelson.[12]

VII. CRITICAL CONFIGURATION IN UNIAXIAL CRYSTALS

As demonstrated in Sec. IV C, if $\chi_1=\chi_2:=\chi_o$ and $\chi_3:=\chi_e$ there exists a family of critical configurations characterized by $\theta=0$ and any ϕ for which the indices n_a and n_b are both equal to $\sqrt{\chi_o}$. We assume in this section that the crystal is uniaxial and tailored so that its principal axis and the propagation axis z of the input pulse are collinear. In such a configuration there is no distinction between ordinary and extraordinary waves, and the field is transverse (there is no component E_{0z}). Further the propagations of the components E_{0x} and E_{0y} which used to be independent in the configuration $\theta\neq0$ are now coupled since they have the same rapid phase $(\omega,n_o\omega/c)$. To deal with this coupling we consider a general form for the source

$$\mathcal{S}=\tfrac{1}{2}(v_x(\delta x,\delta y,\delta t),v_y(\delta x,\delta y,\delta t),0)^Te^{-i\omega t}+cc. \tag{38}$$

The dispersion relationship, group velocity coefficient and dispersion are similar to those of a standard ordinary wave and given by (37).

A. Geometric optics

We adopt the ansatz (7) with $H=\{(\omega,k_o(\omega))\}$

$$\mathcal{E}=\frac{1}{2}\left(\sum_{j=0}^{\infty}\delta^j\mathbf{E}_j(\delta t,\delta x,\delta y,\delta z)\right)e^{i(k_o(\omega)z-\omega t)}+cc.$$

We denote $T=\delta t$, $X=\delta x$, $Y=\delta y$, $Z=\delta z$, and $k_o=k_o(\omega)$.

Proposition 3: If the source $\mathcal{S}$ can be expanded as (38), then the leading order term $\mathbf{E}_0$ of the slowly varying envelope is transverse. It has the same polarization as the incoming pulse, and it satisfies the transport equation

$$\partial_Z\mathbf{E}_0+v_o^{-1}\partial_T\mathbf{E}_0=0, \tag{39}$$

starting from $\mathbf{E}_0(T,X,Y,Z=0)=(2/[1+n_o(\omega)])\mathbf{v}(T,X,Y)$.

In the geometric optics framework, this proposition demonstrates that the leading order terms of the components of the wave with perpendicular polarizations propagate without interaction according to the standard law of ordinary waves.

B. Diffractive optics

Equation (39) describe the propagation of the slowly varying envelope of the wave over propagation distance z of the order of δ^{-1}. It appears that the envelope is transported without deformation. Accordingly, if one considers the envelope in the moving reference frame $(\delta(t-z/v_o),\delta x,\delta y)$, then no evolution is noticeable as far as $z\sim\delta^{-1}$. It is therefore, necessary to address the problem of long-range propagation, over distances z of the order of δ^{-2}. The corresponding ansatz is the following:

$$\mathcal{E}=\frac{1}{2}\left(\sum_{j=0}^{\infty}\delta^j\mathbf{E}_j(\delta(t-z/v_o),\delta x,\delta y,\delta^2 z)\right)e^{i(k_o(\omega)z-\omega t)}+cc. \tag{40}$$

We denote $T=\delta(t-z/v_o)$, $X=\delta x$, $Y=\delta y$ and the long-range scale is represented by the slow variable $\zeta=\delta^2 z$.

Proposition 4: If the source $\mathcal{S}$ can be expanded as (38), then the leading order term $\mathbf{E}_0$ of the slowly varying envelope is elliptically polarized in the plane (x, y) and it obeys the coupled system of Schrödinger equations in the moving frame:

$$2ik_o\partial_\zeta E_{0x}+\rho\partial_X^2E_{0x}+\partial_Y^2E_{0x}+(\rho-1)\partial_X\partial_YE_{0y}-\sigma_o\partial_T^2E_{0x}=0, \tag{41a}$$

$$2ik_o\partial_\zeta E_{0y}+\partial_X^2E_{0y}+\rho\partial_Y^2E_{0y}+(\rho-1)\partial_X\partial_YE_{0x}-\sigma_o\partial_T^2E_{0y}=0, \tag{41b}$$

starting from $\mathbf{E}_0(T,X,Y,Z=0)=(2/[1+n_o(\omega)])\mathbf{v}(T,X,Y)$, *where* $\rho(\omega):=\chi_o(\omega)/\chi_e(\omega)$.

Note that the result of this proposition was reported in Ref. 13, which is as far as we know the only paper which provides an explicit form for the diffraction operator in an anisotropic medium. Nevertheless Ref. 13 only addressed the propagation of pulses along the principal axis of a uniaxial crystal, while our formulas are valid for more general configurations and systems (41a) and (41b) is just a particular application. As in the diffractive regime of the propagation of an extraordinary wave in the framework $\theta\neq0$, we find an anisotropic diffraction operator. Further systems (41a) and (41b) puts into evidence a coupling between the linear Schrödinger type equations satisfied by the components of the field which are polarized along the x and y axes, respectively. This coupling shows itself in crossed second-order spatial derivatives which act onto the orthogonally polarized components. Accordingly, if the input wave is linearly polarized, then the spatial spectrum of the orthogonally polarized output field will present a dark cross which is known as the Maltese cross.

C. Almost-critical configuration $\theta=\delta\eta$

The condition $\theta=0$ is very stringent. It seems hardly possible to reach such a perfect level in realistic experimental configurations. It is consequently relevant to address the problem of the influence of a small perturbation of the ideal case $\theta=0$ by considering that the main optic axis of the crystal is collinear to the propagation axis up to a term of order δ. The second motivation of this section is to make smooth the transition between the results of the cases $\theta\neq0$ and $\theta=0$, since it appears at first glance that there is discontinuity. As we shall see in this section, this apparent disagreement is involved by the fact that the transition is continuous at $\theta=0$ when considering a change of θ at rate δ. Accordingly we set $\theta=\delta\eta$. In the geometric optics framework, one finds the very same equations as in the case $\eta=0$. In the diffractive optics framework, one finds the following perturbed Schrödinger equations:

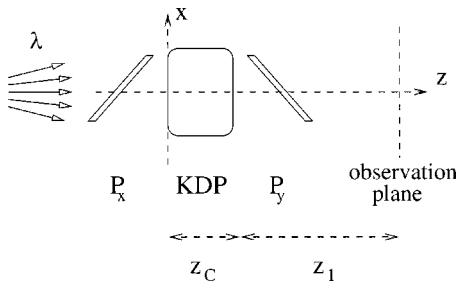

FIG. 2. Experimental setup of a Pockels cell.

$$2ik_o\partial_\zeta E_{0x}+\rho\partial_X^2E_{0x}+\partial_Y^2E_{0x}+(\rho-1)\partial_X\partial_YE_{0y}-\sigma_o\partial_T^2E_{0x}$$
$$=\eta^2k_o^2(\rho-1)E_{0x}-i\eta k_o(\rho-1)(2\partial_XE_{0x}+\partial_YE_{0y}), \tag{42a}$$

$$2ik_o\partial_\zeta E_{0y}+\partial_X^2E_{0y}+\rho\partial_Y^2E_{0y}+(\rho-1)\partial_X\partial_YE_{0x}-\sigma_o\partial_T^2E_{0y}=-i\eta k_o(\rho-1)\partial_YE_{0x}. \tag{42b}$$

These equations involve an interesting application that we discuss in the next section.

D. Application: Detection of the optic axis of a crystalline medium

This section is devoted to a useful and straightforward application of the propagation equations derived here above. We aim at determining the optic axis of a uniaxial crystal by a simple and efficient method. The technique which is described here below is widely used to bring into alignment Pockels cells in experimental setups. We consider the experimental configuration presented in Fig. 2. A linearly polarized divergent light beam emerging from a polarizer P_x is normally incident onto a plane parallel crystal plate of thickness z_c. The optic axis of the crystal is assumed to be almost collinear to the propagation axis z, and we are looking for the angle mismatch η between these axes.

We consider in this section long pulses with carrier wavelength λ so that the time-dependence of the envelope is much slower than its transverse spatial dependence and can be neglected. We take the Fourier transform with respect to the transverse spatial coordinates

$$\hat{\mathbf{E}}_0=\int\mathbf{E}_0e^{-i(k_xx+k_yy)}dxdy.$$

Inside the crystal plate the field evolution is ruled by the systems (42a) and (42b) which reduces to a system of ordinary differential equations (we drop the 0-index)

$$2ik_o\partial_z\hat{E}_x=\rho k_x^2\hat{E}_x+k_y^2\hat{E}_x+(\rho-1)k_xk_y\hat{E}_y+(\rho-1)\eta k_o((\eta k_o-2k_x)\hat{E}_x-k_y\hat{E}_y),$$

$$2ik_o\partial_z\hat{E}_y=k_x^2\hat{E}_y+\rho k_y^2\hat{E}_y+(\rho-1)k_xk_y\hat{E}_x-(\rho-1)\eta k_ok_y\hat{E}_x,$$

that can be solved exactly by a straightforward exponentiation. The input field is linearly polarized along the x axis by the P_x polarizer, and the P_y polarizer eliminates the x component of the output field. Consequently the spectral intensity of the output field is

$$|\hat{E}_y|^2(z_c,k_x,k_y)=F\left((k_x-\eta k_o)\sqrt{\frac{(\rho-1)z_c}{4k_o}},\quad k_y\sqrt{\frac{(\rho-1)z_c}{4k_o}}\right)|\hat{E}_x|^2(0,k_x,k_y), \tag{43a}$$

$$F(u,v)=4u^2v^2\,\mathrm{sinc}^2(u^2+v^2), \tag{43b}$$

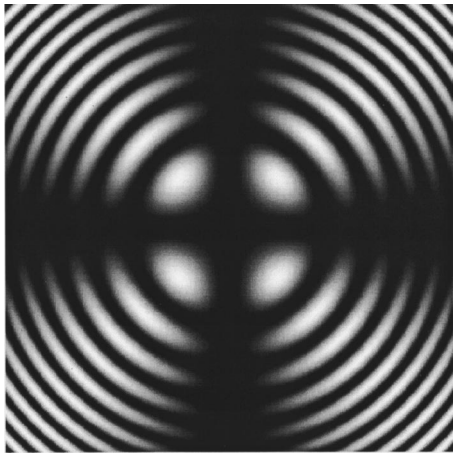

FIG. 3. Interference pattern from uniaxial crystal plate cut perpendicular to the optic axis, between two crossed polarizers. Function $(u,v)\mapsto F(u,v)$ over the domain $(-4,4)\times(-4,4)$.

where $\mathrm{sinc}(s)=\sin(s)/s$. The function F is plotted in Fig. 3. From z_c to $z_{\mathrm{obs}}:=z_c+z_1$ the pulse propagates in vacuum, so in the far field configuration $(z_1\gg\lambda)$ the intensity distribution $|E_y|^2(z_{\mathrm{obs}},x,y)$ is proportional to the power spectral density of the near field:

$$|E_y|^2(z_{\mathrm{obs}},x_o,y_o)=\frac{1}{\lambda^2 z_1^2}|\hat{E}_y|^2\left(z_c,\frac{2\pi x_o}{\lambda z_1},\frac{2\pi y_o}{\lambda z_1}\right).$$

Substituting Eq. (43a) into this identity yields

$$|E_y|^2(z_{\mathrm{obs}}x_o,y_o)=\frac{1}{\lambda^2 z_1^2}F\left(\left(\frac{x_o}{z_1}+\eta n_o\right)\sqrt{\frac{(\rho-1)\pi z_c}{2n_o\lambda}},\quad\frac{y_o}{z_1}\sqrt{\frac{(\rho-1)\pi z_c}{2n_o\lambda}}\right)|\hat{E}_x|^2(0,k_x,k_y).$$

Conclusion. If the optic axis of the crystal is perfectly collinear to the propagation axis of the beam, then the far field intensity presents a centered dark cross. If there exists an angle mismatch η between the optic axis and the propagation axis, then the cross is shifted by the quantity $\Delta x_o=\eta n_o z_1$.

VIII. CONICAL REFRACTION IN BIAXIAL CRYSTAL

As pointed out in Sec. IV C, if $\chi_1>\chi_2>\chi_3$ are distinct, then a simple study of the matrix χ shows that there exists only one case when $n_a=n_b$, which corresponds to the configuration when $\phi=0$ and $\theta=\pm\theta_c(\omega)$ where $\theta_c(\omega)$ is defined by (17). In such a configuration $n_a=n_b=\chi_2^{1/2}$, and the two mutually orthogonal polarization vectors are:

$$\mathbf{s}_a=(\cos\beta_c,0,\sin\beta_c)^T,\quad \mathbf{s}_b=(0,1,0)^T,$$

where the angle $\beta_c(\omega)$ between the polarization vector $\mathbf{s}_a$ and the propagation axis z is given by

$$\tan\beta_c=-\sqrt{\left(1-\frac{\chi_2}{\chi_1}\right)\left(\frac{\chi_2}{\chi_3}-1\right)}.$$

Substituting the ansatz (19) into Eq. (2) and collecting the coefficients of each power of δ, we get the following result.

Proposition 5: If we denote the projections of the field $\mathbf{E}_0$ *onto the vectors* $\mathbf{s}_a$ *and* $\mathbf{s}_b$ *by* $E_{0a}=\mathbf{s}_a\cdot\mathbf{E}_0$ *and* $E_{0b}=\mathbf{s}_b\cdot\mathbf{E}_0$, *then the scalar fields* E_{0a} *and* E_{0b} *satisfy the coupled equations*

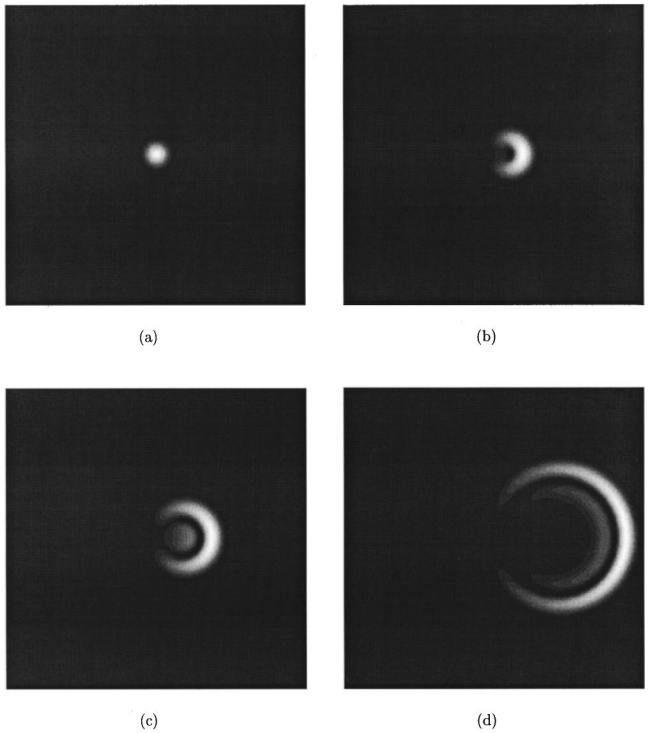

FIG. 4. Conical refraction of a Gaussian pulse polarized along the x axis for different values of Z. $Z=0$ (a), $Z=4.13$ (b), $Z=8.26$ (c), and $Z=20.65$ (d). Here $\cos\beta_c=0.9$ or equivalently $(\tan\beta_c)/2=0.24$.

$$v_a^{-1}\partial_T E_{0_a}+\partial_Z E_{0a}-\tan\beta_c\partial_X E_{0a}=\frac{\tan\beta_c}{2\cos\beta_c}\partial_Y E_{ob}, \tag{44a}$$

$$v_a^{-1}\partial_T E_{0b}+\partial_Z E_{0b}=\frac{\sin\beta_c}{2}\partial_Y E_{0a}, \tag{44b}$$

starting from $E_{0a}(T,X,Y,Z=0)=(2/[1+n_a(\omega)])v_x(T,X,Y)$ *and* $E_{0b}(T,X,Y,Z=0)=(2/[1+n_a(\omega)])v_y(T,X,Y)$.

Taking the spatial Fourier transform with respect to the transverse coordinates (X,Y), the solution field reads

$$\begin{pmatrix}\hat{E}_{0a}\\ \hat{E}_{0b}\end{pmatrix}(Z,T,k_x,k_y)=\frac{2e^{ik_xZ'}}{1+n_a}\left[\cos(k_rZ')\begin{pmatrix}1&0\\0&1\end{pmatrix}\right.$$
$$\left.+i\sin(k_rZ')\frac{1}{k_r}\begin{pmatrix}k_x & \dfrac{k_y}{\cos\beta_c}\\ k_y\cos\beta_c & -k_x\end{pmatrix}\right]\hat{\mathbf{v}}(T-Z/v_a,k_x,k_y),$$

where $k_r=\sqrt{k_x^2+k_y^2}$ and $Z'=Z(\tan\beta_c)/2$. The evolution of an input Gaussian field is plotted in Fig. 4. Let us study the field in the framework $|Z'|>1$ but not so large so as to be allowed to neglect the diffractive terms (i.e., $\delta^{-1}\leqslant z\ll\delta^{-2}$). In the physical space, using the stationary phase method, we get that the field is concentrated on the circle with center Z' and radius Z' if the input field is localized around 0. In other words the wave surface has the shape of a cone. This conical refraction is a well-known phenomena which was predicted in 1832 by Hamilton and observed thereafter by Lloyd. Historical references and an elementary study of conical refraction can be found in Ref. 1. More advanced treatments are devoted to the subject.[14,15] In particular Warnick and Arnold[16] predicts additional fringes by computing the asymptotic form of the Green func-

tion. These results can be exhibited in our framework quite easily. Let us denote by $(\cos\gamma,\sin\gamma,0)$ the unit polarization vector of the source $\mathbf{v}$, and by R_0 the radius of the input beam. If (X,Y) is farther than R_0 from the cone $(X-Z')^2+Y^2=Z'^2$, then we have $|E_0|^2(Z,X,Y)=o(Z^{-1})$. If (X,Y) is close to the cone $(X-Z')^2+Y^2=Z'^2$ by less than R_0, then denoting $X=Z'+Z'\cos\alpha$ and $Y=Z'\sin\alpha$

$$|E_0|^2(Z,X,Y)\simeq\frac{Z_0}{Z}\left(\cos\left(\frac{\alpha}{2}\right)\cos(\gamma)\cos(\beta_c)+\sin\left(\frac{\alpha}{2}\right)\sin(\gamma)\right)^2\left(1+\cos^2\left(\frac{\alpha}{2}\right)\tan^2(\beta_c)\right),$$

where Z_0 is a characteristic distance proportional to $R_0/\tan\beta_c$. If Z is so large that it reaches values of order δ^{-1} (i.e., z reaches values of order δ^{-2}), then one should take into account the second-order derivatives, which makes the evolution of the field more complicated. The strategy is still the same as in the other configurations. It consists in looking at the evolution of the field at the long scale $\delta^2 z$ around the points defined by the transport equation, that is to say the cone defined by $(x-z(\tan\beta_c)/2)^2+y^2=(z(\tan\beta_c)/2)^2$. This specific study will be carried out elsewhere. Nevertheless, we would like to add the following comment that gives a new insight into the phenomena that govern conical refraction. In the moving reference frame $(\delta(t-z/v_a),\delta(x+z(\tan\beta_c)/2),\delta y,\delta z)$ Eqs. (44a) and (44b) read as

$$\partial_Z E_{0a}=\frac{\tan\beta_c}{2}\partial_X E_{0a}+\frac{\tan\beta_c}{2\cos\beta_c}\partial_Y E_{0b}, \tag{45a}$$

$$\partial_Z E_{0b}=\frac{\sin\beta_c}{2}\partial_Y E_{0a}-\frac{\tan\beta_c}{2}\partial_X E_{0b}. \tag{45b}$$

Composing these equations establishes that the modes E_{0m} for $m=a$ and b obey the standard wave equations with uniform ''velocity'' $(\tan\beta_c)/2$

$$\partial_Z^2 E_{0a}=\frac{\tan^2\beta_c}{4}(\partial_X^2+\partial_Y^2)E_{0_a}, \tag{46a}$$

$$\partial_Z^2 E_{0b}=\frac{\tan^2\beta_c}{4}(\partial_X^2+\partial_Y^2)E_{0b}, \tag{46b}$$

where Z plays the role of the usual time. The initial conditions are imposed by $E_{0m}(Z=0)$ and $\partial_Z E_{0m}(Z=0)$. As is well-known the solution of the wave equation $u_{tt}=c^2\Delta u$ satisfies the Huygens principle which states that, if the Laplacian acts on a space with odd dimension d, then the solution $u(x,t)$ depends only on the initial data at $t=0$ for $x_0\in\{x_0\in\mathbb{R}^d,|x_0-x|=ct\}$. Thus an initial delta-like pulse at $t=0$, $x=0$ will give rise at time t to a pulse concentrated on the circle with center 0 and radius ct. This property does not hold true for even dimension, since the solution $u(x,t)$ then depends on the initial data at $t=0$ in the cone $x_0\in\{x_0\in\mathbb{R}^d,|x_0-x|\leqslant t\}$. In the standard wave equation, the space has dimension $d=3$ and the Huygens principle is satisfied. In our case, Z plays the role of t and $d=2$, which proves that complex structure inside the main cone can be generated during the propagation. We refer to the standard literature on the wave equation for a description of the different phenomena that can arise.[17,18]

IX. TRANSITION BETWEEN UNIAXIAL AND BIAXIAL CONFIGURATIONS

We assume in this section that the crystal is tailored so that its principal axis and the propagation axis z of the input pulse are collinear. Furthermore the susceptibilities χ_1 and χ_2 are close to each other so that they can be written as: $\chi_1=\chi_o$ and $\chi_2=\chi_o-\delta^2\eta_\chi$, where η_χ is of order 1. Accordingly the tensor χ in the (x,y,z)-frame reads as

$$\chi=\chi^0-\delta^2\eta_x M_\phi, \quad \chi^0:=\begin{pmatrix}\chi_o & 0 & 0\\ 0 & \chi_o & 0\\ 0 & 0 & \chi_e\end{pmatrix}, \quad M_\phi=N_\phi\oplus 0, \quad N_\phi:=\begin{pmatrix}\sin^2\phi & \cos\phi\sin\phi\\ \cos\phi\sin\phi & \cos^2\phi\end{pmatrix}.$$

In such a configuration the dispersion equation is the same as in the uniaxial case considered in Sec. VII since the mismatch only appears at order δ^2. Thus the two eigenindices are equal to $\chi_o^{1/2}$, the group velocity coefficient and dispersion are similar to those of a standard ordinary wave and given by (37), and the leading order term $\mathbf{E}_0$ of the field is transverse. Further the propagations of the components E_{0x} and E_{0y} are coupled. To deal with this coupling we consider the general form (38) for the source. The weak biaxial property (of order δ^2) does not involve any modification of the transport equations which govern the propagation of the wave in the geometric scales with respect to the uniaxial case. We thus consider the scales of diffractive optics and we adopt the ansatz (40).

Proposition 6: If the source $\mathcal{S}$ can be expanded as (38), then the leading order term $\mathbf{E}_0$ of the slowly varying envelope is transverse and it satisfies the coupled Schrödinger equations:

$$2ik_o\partial_\zeta E_{0x}+\rho\partial_X^2 E_{0x}+\partial_Y^2 E_{0x}+(\rho-1)\partial_X\partial_Y E_{0y}-\sigma_o\partial_T^2 E_{0x}=k_o^2\eta_\chi(M_\phi\mathbf{E}_0)_x, \tag{47a}$$

$$2ik_o\partial_\zeta E_{0y}+\partial_X^2 E_{0y}+\rho\partial_Y^2 E_{0y}+(\rho-1)\partial_X\partial_Y E_{0x}-\sigma_o\partial_T^2 E_{0y}=k_o^2\eta_\chi(M_\phi\mathbf{E}_0)_y, \tag{47b}$$

starting from $\mathbf{E}_0(T,X,Y,\zeta=0)=(2/[1+n_o(\omega)])\mathbf{v}(T,X,Y)$, *where* $\rho=\chi_o/\chi_e$.

Taking the spatial Fourier transform with respect to the transverse coordinates (X, Y), the systems (47a) and (47b) reduces to a system of ordinary differential equations. If the initial pulse is polarized along the x axis, and if we retain only the component of the output pulse which is y polarized, then we have

$$|\hat{E}_y(z_c,k_x,k_y)|^2=F_\phi\left(k_x\sqrt{\frac{(\rho-1)z_c}{4k_o}},k_y\sqrt{\frac{(\rho-1)z_c}{4k_o}},\frac{\eta_\chi k_o z_c}{4}\right)|\hat{E}_x(0,k_x,k_y)|^2,$$

$$F_\phi(u,v,\eta)=(2uv+\eta\sin(2\phi))^2 \times\operatorname{sinc}^2\left(\sqrt{(u^2+v^2)^2+\eta^2+2\eta((v^2-u^2)\cos(2\phi)+2uv\sin(2\phi))}\right),$$

where $\operatorname{sinc}(s)=\sin(s)/s$. Figure 5 plots the function $(u,v)\mapsto F_\phi(u,v,\eta)$ for different values of the parameters ϕ and η. Comparisons with experimental observations show excellent agreement. See Figure 14.26 in Ref. 1 for an observation of Fig. 5(f), Figures 465 to 466 in Ref. 19 for observations of Figs. 5(d) and Fig. 5(e), and Fig. 5.30 in Ref. 20 for another observation of Fig. 5(e). In particular Fig. 5(f) is the theoretical counterpart of the cover of the sixth edition of the book ''Principles of Optics'' by Born and Wolf![1] Let us briefly discuss the main properties of the functions F_ϕ. If the initial polarization vector is collinear to one of the axis of the crystal ($\phi=0$ or π), then F_0 has a factor u^2v^2, which shows that there is a centered dark cross, whatever η. If the initial polarization vector is collinear to the bisecting line of the axes of the crystal ($\phi=\pi/4$), then we have

$$F_{\pi/4}(u,v,\eta)=(2uv+\eta)^2\operatorname{sinc}^2\left(\sqrt{(u^2+v^2)^2+\eta^2+4\eta uv}\right), \tag{48}$$

which shows that the transmission at the center gets nonzero when η increases and may even be 1 at some particular values (see Fig. 5). Indeed, whatever ϕ, the transmission at $u=v=0$ is $F_\phi(0,0,\eta)=\sin(\eta)^2\sin(2\phi)^2$. If $\phi=0$, it is always 0, but if $\phi=\pi/4$, it is equal to $\sin(\eta)^2$ which is maximal and equal to 1 when $\eta=\pi/2 \bmod \pi$. This implies that a plane wave is fully transmitted in this configuration.

The results derived in this section provide the principle and the precise characterization of electro-optic switching devices of the family of Pockels cells.[2] Indeed, the experimental setup

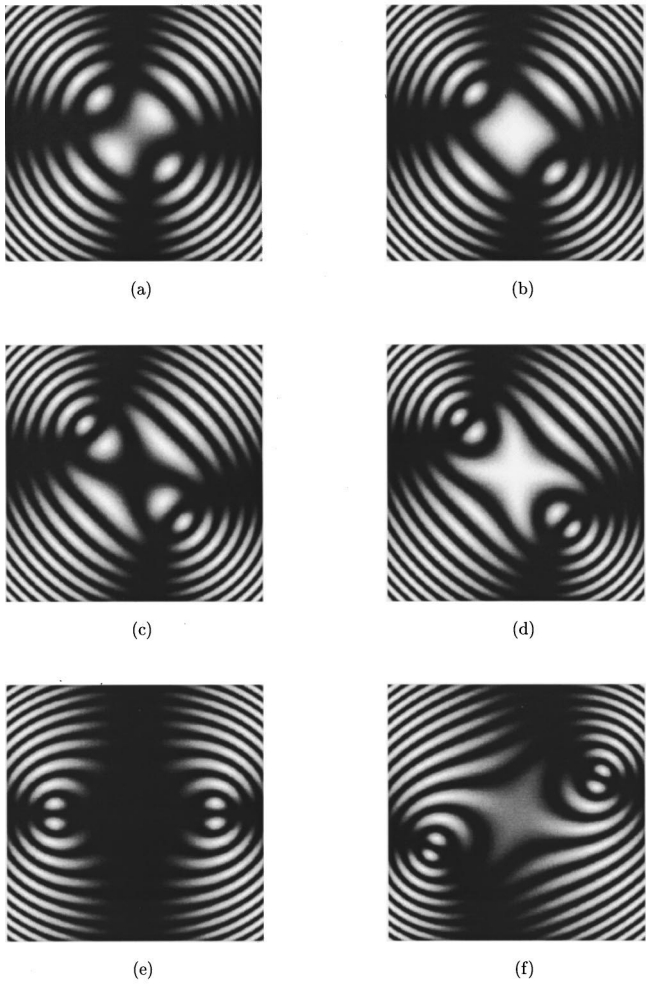

FIG. 5. Interference patterns from biaxial crystal plates between two crossed polarizers. Functions $(u,v)\mapsto F_\phi(\eta,u,v)$ over the domain $(-4,4)\times(-4,4)$ for different values of η and ϕ. $\eta=\pi/4$ and $\phi=\pi/4$ (a), $\eta=\pi/2$ and $\phi=\pi/4$ (b), $\eta=\pi$ and $\phi=\pi/4$ (c), $\eta=3\pi/2$ and $\phi=\pi/4$ (d), $\eta=2\pi$ and $\phi=\pi$ (e), and $\eta=5\pi/2$ and $\phi=7\pi/8$ (f). The case $\eta=0$ (and any ϕ) is plotted in Fig. 3.

depicted in Fig. 2 corresponds to the case $\eta_\chi=0$. Applying an electric field between two faces of the potassium dihydrogen phosphate (KDP) crystal plate involves an alteration of the distribution of the electric charges of the atoms and molecules which constitute the crystal, which affect the optical properties of the medium. The theory of electro-optics is well-known, and we refer for instance to Ref. 21, Section 87, for a survey. In the case of point group $\bar{4}2m$ to which KDP crystal belongs, it is known that the crystals become biaxial while they are uniaxial in the absence of external electric field, that is to say η_χ takes nonzero values which are imposed by the applied electric field. By applying the tension from 0 to the value corresponding to $\eta_\chi=2\pi/(k_o(\omega)z_c)$, the transmittivity goes from 0 to 1 for an input plane wave with carrier frequency ω. Finally note also that the transfer function $(u,v)\mapsto F_{\pi/4}(u,v,\pi/2)$ possesses a flat top hat. This configuration could then be used as a spatial filter as well.

X. CONCLUSION

In this paper we have derived the equations which govern the linear propagation of the slowly varying envelopes of pulses in a bulk medium presenting anisotropic properties. The strategy mainly consists in two steps. We first consider the Maxwell equations in the scales of optic

geometric, that is to say for propagation distance of the same order as the radius of the beam or the duration of the pulse times the light velocity. In this framework the propagation equations read as transport equations, which actually give the propagation of the rays according to the law of geometric optics. Second we revisit the Maxwell equations in the moving frame indicated by the above-derived transport equations. In the scales of the geometric optics, the propagation equations are then trivial, which allows to consider larger propagation distances, of the order of the Rayleigh distance or the dispersion distance. In this framework the propagation equations read as Schrödinger-type equations, which actually give the propagations of the slowly varying envelope according to the law of diffractive optics.

By applying this methodology we have put into evidence that we can deal with many situations. We have recovered well-known results, but we have also exhibited closed form expressions for the diffraction operator which has led to original results regarding an anomalous diffraction in a very particular configuration. Another advantage of this method is that it can still be applied when we take into account the nonlinear susceptibility of the medium. This generalization is addressed in the companion paper.[7]

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High-frequency asymptotics for Maxwell's equations in anisotropic media Part II: Nonlinear propagation and frequency conversion

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This paper is devoted to the derivation of the equations that govern the propagation and frequency conversion of pulses in noncentrosymmetric crystals. The method is based upon high-frequency expansions techniques for hyperbolic quasi-linear and semilinear equations. In the so-called geometric regime we recover the standard results on the frequency conversion of pulses in nonlinear crystals. In the diffractive regime we show that the anisotropy of the diffraction operator involves remarkable phenomena. In particular the phase matching angle of a divergent pulse depends on the distance between the waist and the crystal plate. Finally we detect a configuration where the beam propagation in a biaxial crystal involves the generation of spatial solitons thanks to an anomalous one-dimensional diffraction. [DOI: 10.1063/1.1354640]

I. INTRODUCTION

In 1961 Franken *et al.*[1] observed radiation at a double frequency when a ruby laser beam was directed into a quartz crystal. Unfortunately, because of phase mismatch of the fundamental and converted waves, the efficiency of conversion proved to be very low (about $10^{-10}\%$). The so-called phase matching condition which should be fulfilled for the second harmonic generation $\omega+\omega \mapsto 2\omega$ reads as $2\mathbf{k}(\omega)=\mathbf{k}(2\omega)$, or equivalently $n(2\omega)=n(\omega)$, where n is the refractive index. In the optical transparency region of isotropic crystals, and in anisotropic crystals for waves of identical polarizations, this condition is never fulfilled because of normal dispersion ($n(\omega) < n(2\omega)$). The use of anomalous dispersion is prohibited because the energy absorption is then very high. In 1962 Giordmaine[2] and Maker[3] simultaneously and independently proposed an ingenious method of matching the phase velocities of the fundamental and converted waves. The technique is based on the difference between the refractive indices of the waves with different polarizations in an anisotropic crystal. It is now current to reach efficiency of conversion of several ten percents.[4]

Anisotropy is a necessary condition for a medium to have a nonzero second order nonlinearity.[5] The χ^2-tensor is zero for any centrosymmetric crystal. The study of sum-frequency generation thus takes place in anisotropic media. The aim of this paper is to describe the effects of the anisotropy of the medium and to take a rigorous account of it in the study of the nonlinear regime and especially the frequency conversion phenomenon. The case of plane waves has been carefully studied in Ref. 6. We aim at deriving evolution equations for the slowly varying envelopes of broadband and divergent pulses by using a technique based on high-frequency expansions of the fields.[7]

The derived equations find practical applications in the framework of frequency conversion of high-power laser beams. Indeed the phase matching condition for efficient frequency doubling and tripling of laser beams is very drastic,[4] and it is therefore, necessary to detect the principal axis of the crystal with great precision. The standard process consists in observing the main output

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direction of the frequency converted pulse of a divergent pulse. This work was originally triggered by the experimental observation that the direction of the frequency converted pulse of a fundamental Gaussian pulse depends on the distance between the waist of the fundamental pulse and the crystal, even with a perfectly normal incidence. The departures for different distances exceed the high-precision level required for reaching the expected conversion performance. The results derived in this paper predict the phenomenon and allow to compute the direction of the phase matching angle as a function of the direction of the frequency converted pulse and the distance between the waist of the fundamental pulse and the crystal.

The results of this paper are also necessary for a careful treatment of the propagation and frequency conversion of partially coherent pulses. Indeed incoherent light with short coherence time is of interest for smoothing techniques for uniform irradiation in plasma physics.[8] If propagation of incoherent light in isotropic linear media is now rather well understood, the evolution of the statistical properties of incoherent pulses in anisotropic and/or nonlinear media has been insufficiently examined.[9] A high level of irradiation uniformity is required for both direct and indirect drive for Inertial Confinement Fusion.[8] This criterion can be reached by implementing active smoothing methods, such as Induced Spatial Incoherence with echelons,[10] Smoothing by Spectral Dispersion (SSD),[11] Smoothing by multimode Optical Fiber (SOF).[12] All these methods involve the illumination on the target with an intensity which is a time varying speckle pattern, so that the time integrated intensity averages towards a flat profile. As an unavoidable drawback the optical smoothing techniques also involve phase modulations in the amplifiers and frequency converters (SSD), or even intensity modulations (SOF).

The framework for high-frequency expansions of the solutions of Maxwell's equations follows from the appearance of the small parameter δ which has the order of magnitude of the carrier wavelength of light divided by the next smallest characteristic length present in the problem. If we assume that the carrier wavelength is 1, then we have seen in Ref. 13 that for propagation length of order δ^{-1}, which corresponds to the scales of the so-called geometric optics, evolution equations read as transport equations with constant velocity. Further, in the moving pulse-time frame (moving according to the velocity exhibited by the geometric transport equations), for propagation length of order δ^{-2}, which corresponds to the scales of diffractive optics, the evolution of the field is governed by a Schrödinger equation.

The first nonlinear effect we discuss in this paper is the sum frequency generation. A nonlinear χ^2-type function applied to expressions of the form $\Sigma_f \mathbf{E}_f^{\delta}(\delta t, \delta \mathbf{x}) \exp i(k^f z - \omega_f t)$ will produce harmonics, that is to say expression with phase $(k^{f_1} + k^{f_2})z - (\omega_{f_1} + \omega_{f_2})t$. If the couples (ω_f, k^f) satisfy the dispersion relation, then the natural harmonic phases generally do not, due to the dispersive property of the material. The set of harmonics which satisfy the dispersion relation is generally very small (sometimes empty), because they need to fulfill a very drastic phase matching condition.

We must also take care that the strength of interaction and, therefore, the scale for interaction depends on the amplitude of the wave. If the amplitude of the wave is δ^{α}, then a p-wave interaction process will be noticeable for propagation length of order $\delta^{-(p-1)\alpha}$. Since we are mainly concerned in this paper with second-order nonlinearity, it means that the nonlinear effect will appear for propagation length of the order of $\delta^{-\alpha}$. Accordingly $\alpha = 1$ will correspond to nonlinear geometric optics and $\alpha = 2$ to nonlinear diffractive optics.

The paper is organized as follows. First we describe the general configuration at hand in Sec. II. Section III is devoted to the derivations of the dispersion relation, the phase matching and the suitable expanded form of the solution of the Maxwell equations. We address in Secs. IV and V the frequency conversion in birefringent crystals. In Sec. VI we derive the propagation equation of the slowly varying envelope of the field when the phase-matching conditions for frequency generation are not fulfilled. In Sec. VII we study a particular configuration which should allow the generation and propagation of spatial solitons.

II. FORMULATION AND SCALING

We consider an incident beam incoming from the left onto a nonmagnetic nonlinear crystal that occupies the domain $\mathbb{R}^3_+ := \{(x,y,z) \in \mathbb{R}^3, z>0\}$. The propagation axis is perpendicular to the boundary surface $\Sigma := \{(x,y,z) \in \mathbb{R}^3, z=0\}$ and is collinear to the z axis. The evolution of the electric field $\mathcal{E}$ is governed by the Maxwell equation

$$\mathbf{rot}\ \mathbf{rot}\ \mathcal{E} = -\mu_0 \partial_t^2 \mathcal{D}, \tag{1}$$

where the electric induction divides into the sum $\mathcal{D} = \mathcal{D}_l + \mathcal{P}_{nl}$ of a linear and a nonlinear part

$$\mathcal{D}_l = \varepsilon_0 \mathcal{E} + \varepsilon_0 \chi^{(1)} * \mathcal{E}, \tag{2}$$

$$\mathcal{P}_{nl} = \varepsilon_0 \chi^{(2)} * (\mathcal{E},\mathcal{E}) + \varepsilon_0 \chi^{(3)} * (\mathcal{E},\mathcal{E},\mathcal{E}) + \cdots, \tag{3}$$

$$\chi^{(j)} * (\mathcal{E},\ldots,\mathcal{E}) = \int_{-\infty}^{t} dt_1 \cdots \int_{-\infty}^{t} dt_j \chi^{(j)}(t-t_1,\ldots,t-t_j) : \mathcal{E}(t_1)\cdots\mathcal{E}(t_j). \tag{4}$$

ε_0 and μ_0 are, respectively, the dielectric constant and magnetic permeability of vacuum. The electromagnetic wave is assumed to be far enough from all absorption lines of the medium so that we can neglect absorption and the tensors $\chi^{(j)}$ are real.

The boundary condition at the surface Σ is imposed by the continuity of the tangential components of the magnetic and electric fields. The source $\mathcal{S}$ corresponding to the electric field of the incoming pulse at the interface Σ is assumed to be a modulation of a high-frequency signal whose carrier wavelength is λ_0, or the superposition of a finite number of such modes. From the characteristic spatial (resp. temporal) variations of the source we can also define a length scale R_0 (resp. a time scale T_0, associated with the length $L_0 := cT_0$). Our study will take place in the framework where the dimensionless parameter $\delta := \min\{\lambda_0/R_0, \lambda_0/L_0\}$ is small. As pointed out in the introduction, the order of magnitude $\overline{\mathcal{S}}$ of the source also plays a crucial role in that it determines the strength of the nonlinear interaction. Let us denote by $\overline{\chi_1}$ (resp. $\overline{\chi_2}$) the typical value taken by the Fourier transforms of the components of the $\chi^{(1)}$-tensor (resp. $\chi^{(2)}$-tensor) evaluated at frequency $2\pi c/\lambda_0$. The characteristic nonlinear amplitude is defined by $\overline{E_{nl}} := \overline{\chi_1}/\overline{\chi_2}$. Our study takes place in the framework of weakly nonlinear waves, which reads as $\overline{\mathcal{S}}/\overline{E_{nl}} \ll 1$. This ratio may be related to the small parameter δ through a new parameter $\alpha > 0$ such that $\overline{\mathcal{S}}/\overline{E_{nl}} = \delta^\alpha$. Setting $\tilde{x} = x/\lambda_0$, $\tilde{y} = y/\lambda_0$, $\tilde{z} = z/\lambda_0$, $\tilde{t} = ct/\lambda_0$, $\tilde{\mathcal{D}} = \mathcal{D}/(\varepsilon_0 \overline{E_{nl}})$, and $\tilde{\mathcal{E}} = \mathcal{E}/\overline{E_{nl}}$ the dimensionless Maxwell equation reads as

$$\tilde{\mathbf{rot}}\ \tilde{\mathbf{rot}}\ \tilde{\mathcal{E}} = -\tilde{\mu}_0 \partial_{\tilde{t}}^2 \tilde{\mathcal{D}},$$

where $\tilde{\mu}_0 = \varepsilon_0 \mu_0 c^2 = 1$. The source $\tilde{\mathcal{S}}$ has a high-frequency expansion of the form

$$\tilde{\mathcal{S}}(\tilde{x},\tilde{y},\tilde{t}) = \frac{1}{2}\delta^\alpha \sum_{\omega_f \in \Omega_s} \begin{pmatrix} v_x^f(\delta\tilde{t},\delta\tilde{x},\delta\tilde{y}) \\ v_y^f(\delta\tilde{t},\delta\tilde{x},\delta\tilde{y}) \\ 0 \end{pmatrix} e^{-i\omega_f \tilde{t}} + cc, \tag{5}$$

where *cc* is a shorthand for ''complex conjugate.'' $\Omega_{\mathcal{S}}$ is the collection of the high-carrier frequencies ω_f. $\mathbf{v}^f$ is the slowly varying envelope of the mode with carrier frequency ω_f. Note that a dimensionless propagation distance $\tilde{z}$ of the order of δ^{-1} corresponds to a physical distance of the order of R_0, while a dimensionless distance $\tilde{z}$ of the order of δ^{-2} corresponds to a physical distance of the order of R_0^2/λ_0 which is the well-known Rayleigh distance.

From now on we drop the tildes. We assume *a priori* that the electric field can be expanded in a power series of the small parameter δ and in a series with respect to a set of rapid phases $k^f z - \omega_f t$

$$\mathcal{E}=\tfrac{1}{2}\delta^{\alpha}\sum_{(\omega_f,k^f)\in H}(\mathbf{E}^f(\delta t,\delta x,\delta y,\delta z)e^{i(k^f z-\omega_f t)}+cc), \tag{6a}$$

$$\mathbf{E}^f(T,X,Y,Z)=\sum_{j=0}^{\infty}\delta^j\mathbf{E}_j^f(T,X,Y,Z), \tag{6b}$$

where $\mathbf{E}^f$ is the slowly varying envelope of the mode whose rapid phase is (ω_f,k^f). The functions $\mathbf{E}_j^f$ are smooth in all their arguments. H denotes the set of the rapid phases (ω_f,k^f) which are contained in the field $\mathcal{E}$. In case of linear medium[13] the modes propagate without interaction and the set of high frequencies $\{\omega_f,\exists k^f$ such that $(\omega_f,k^f)\in H\}$ is equal to Ω_S. In case of nonlinear medium, the generation of new phases (the so-called harmonics) is expected so that the series (6) may contain much more terms than in the source (5).

III. PROPAGATION IN A BIREFRINGENT CRYSTAL

We introduce the geometric framework. We first define a reference frame (x,y,z) associated with the pulse whose carrier wave vector $\mathbf{k}_0$ is collinear to the z axis. We then introduce a reference frame (1, 2, 3) associated with the optic axis of the crystal, where $\mathbf{e}_3$ is the main optic axis. We denote by θ the angle between the wave vector and the main optic axis. ϕ is the angle between the projection of the carrier wave vector onto the plane $(\mathbf{e}_1,\mathbf{e}_2)$ and the axis collinear to $\mathbf{e}_1$. The transition matrix between the reference frames (x,y,z) and (1, 2, 3) is denoted by U.

A. Principle of the high-frequency expansion

We present the principle of the high-frequency expansion method. It can be applied if the source can be expanded as (5). We proceed to *a priori* expansions of the field inside the crystal of the kind (6) with $\alpha>0$ (weak nonlinearity). In linear media (or equivalently for evanescent sources $\alpha\gg 1$) all nonlinear phenomena can be neglected, and the set of the frequencies ω which are contained in H is imposed by the source and is equal to Ω_S. Otherwise the generation of harmonics should be taken into account so that the set H could be much larger than in the linear case.

The establishing of the propagation equations for the slowly varying envelopes obeys the following scheme. The form (6) is substituted into Eq. (1). Collecting the terms with similar orders in δ and the same rapid phases (ω_f,k^f), we get a family of equations. These equations can be decomposed into coupled systems of equations parametrized by the rapid phases. In linear media these systems are independent so that the envelopes of the different modes propagate independently,[13] but in nonlinear media there are coupling between the propagation equations of the envelopes. If the form (6) is suitable, then the derived systems should have unique solutions. Actually we shall show the two following statements. First, the rapid phases must satisfy dispersion relations which read as compatibility conditions for the existence of the high-frequency expansion (6a). Second, the leading order terms $\mathbf{E}_0^f$ are determined by compatibility conditions for the existence of the series expansion (6b).

The form (6) is an ansatz, that is to say an *a priori* form of the solution which is valid in a given domain, here for $z\lesssim\delta^{-1}$. It is compatible with the boundary conditions and the source. It is self-similar with respect to the operators that are encountered in the Maxwell equation. This fact was established in Ref. 13 for the linear operators, and we shall see in the following that the expansion (6) is also self-similar with respect to the nonlinear operators.

B. Expansions of the linear terms

The linear susceptibility is defined as the Fourier transform of the tensor $\chi^{(1)}$ defined by (2). It is a diagonal matrix $\hat{\chi}^{(1)}_{123}$ in the frame (1, 2, 3), while in the reference frame (x,y,z) the tensor $\hat{\chi}^{(1)}_{xyz}$ is $U^{-1}\hat{\chi}^{(1)}_{123}U$. In the following χ is a shorthand for the matrix $\hat{\chi}^{(1)}_{xyz}+I_d$. If $\mathcal{E}$ is of the form $\mathcal{E}=\frac{1}{2}\delta^{\alpha}(\mathbf{E}(\delta t,\delta x,\delta y,\delta z)e^{i(kz-\omega t)}+cc)$, then the contribution of the linear induction to the Max-

well equation (1) and the **rot rot** $\mathcal{E}$ term can be expanded as powers of δ. Denoting by $T=\delta t$, $X=\delta x$, $Y=\delta y$, and $Z=\delta z$ the slowly varying variables, we have on the one hand

$$-\mu_0\partial_t^2\mathcal{D}_l=\tfrac{1}{2}\delta^\alpha(\mathbf{D}_0(\mathbf{E})+\delta\mathbf{D}_1(\mathbf{E})+\delta^2\mathbf{D}_2(\mathbf{E})+O(\delta^3))e^{i(kz-\omega t)}+cc, \tag{7}$$

where the $\mathbf{D}_j(\mathbf{E})$ are linear functions of $\mathbf{E}$ given by

$$\mathbf{D}_0(\mathbf{E})=\frac{\omega^2}{c^2}\chi\mathbf{E},\quad \mathbf{D}_1(\mathbf{E})=\frac{i}{c^2}(\omega^2\chi)'\partial_T\mathbf{E},\quad \mathbf{D}_2(\mathbf{E})=-\frac{1}{2c^2}(\omega^2\chi)''\partial_T^2\mathbf{E}, \tag{8}$$

and the primes stand for partial derivatives with respect to ω. On the other hand the **rot rot** $\mathcal{E}$ term writes

$$\textbf{rot rot}\ \mathcal{E}=\tfrac{1}{2}\delta^\alpha(\mathbf{R}_0(\mathbf{E})+\delta\mathbf{R}_1(\mathbf{E})+\delta^2\mathbf{R}_2(\mathbf{E}))e^{i(kz-\omega t)}+cc, \tag{9}$$

where the mappings $\mathbf{R}_j(\mathbf{E})$ are sums of partial derivatives of E with respect to space coordinates of order j that are given in Ref. 13.

C. Dispersion relations for the rapid phases

We aim at showing here that the rapid phases (ω_f,k^f) of the set H should fulfill the so-called dispersion equation. By substituting the ansatz (6) into Eq. (1) and collecting the coefficients with power δ^α and phases (ω_f,k^f), we get by applying the identities (7) and (9) that the leading order term $\mathbf{E}_0^f$ should satisfy

$$\mathbf{R}_0(\mathbf{E}_0^f)=\mathbf{D}_0(\mathbf{E}_0^f), \tag{10}$$

similarly as in the linear case. This is of course expected, since the weakness of the amplitude of the pulse (of order δ^α with $\alpha>0$) prevents nonlinear terms from coming into the leading part of the expansion with respect to δ.

As established in Ref. 13 there exist two positive solutions n_a and n_b and two polarizations $\mathbf{s}_a$ and $\mathbf{s}_b$ so that $\mathbf{s}_a$ and $\mathbf{s}_b$ are unit vectors and $(n_a\omega c^{-1},\mathbf{s}_a)$ and $(n_b\omega c^{-1},\mathbf{s}_b)$ are solutions of Eq. (10). We define the dispersion relationship, the group velocity and the dispersion coefficient of the waves as follows:

$$k_m(\omega):=\frac{\omega n_m(\omega)}{c},\quad v_m(\omega):=\left(\frac{\partial k_m}{\partial\omega}\right)^{-1},\quad \sigma_m(\omega):=k_m\frac{\partial^2 k_m}{\partial\omega^2},\quad m=a,b, \tag{11}$$

and we denote by β_m the angle between the polarization vector $\mathbf{s}_m$ and the z axis

$$\cos^2(\beta_m(\omega))=s_{mx}^2(\omega)+s_{my}^2(\omega).$$

In order to fulfill condition (10), the set $(\omega_f,k^f,\mathbf{E}_0^f)$ must satisfy one of the three following alternatives:

(i) Either $k^f=k_a(\omega_f)$ and the components of $\mathbf{E}_0^f$ parallel to $\mathbf{s}_a(\omega_f)$ may be nonvanishing;
(ii) either $k^f=k_b(\omega_f)$ and the components of $\mathbf{E}_0^f$ parallel to $\mathbf{s}_b(\omega_f)$ may be nonvanishing;
(iii) or $k^f\notin\{k_a(\omega_f),k_b(\omega_f)\}$, and then necessarily $\mathbf{E}_0^f\equiv 0$.

Note that the third option simply means that modes which are not phase-matched cannot have an envelope of order δ^α.

We can now give a suitable description of the set H of the rapid phases. The set H in the general nonlinear framework should at least contain the rapid phases that were exhibited in the linear framework for a given source $\mathcal{S}$ that is to say

$$H_{\mathcal{S}}=H_{a,\mathcal{S}}\cup H_{b,\mathcal{S}},$$

where $H_{a,\mathcal{S}}$ and $H_{b,\mathcal{S}}$ are the subsets of the rapid phases which satisfy either the a dispersion relation or the b relation

$$H_{m,\mathcal{S}}=\{(\omega,k) \text{ such that } \omega\in\Omega_{\mathcal{S}} \text{ and } k=k_m(\omega)\}.$$

In a nonlinear medium the generation of new frequencies is expected. The choice of the ansatz should take into account this phenomenon and that is why the set H of all possible rapid phases reads as the extended formulation

$$H=\left\{(\omega,k) \text{ such that } \exists j_1,\ldots,j_n\in\mathbb{Z},(\omega_i,k^i)\in H_{\mathcal{S}},\omega=\sum_{j=1}^{n} j_i\omega_i, \text{ and } k=\sum_{j=1}^{n} j_i k_i\right\}.$$

The rapid phases $(\omega,k)\in H$ for which $\omega\notin\Omega_{\mathcal{S}}$ correspond to the so-called harmonic modes. Since the pairs (ω_f,k^f) are algebraic sums of adapted rapid phases which originate from $H_{\mathcal{S}}$, and since the media we usually consider have a normal dispersion, there is only two types of phase matching (assuming that $n_a<n_b$):

(i) Type I: Both fundamental modes are of type a and the harmonic mode is of type b with $\omega_h=\omega_p+\omega_q$ and $k_a(\omega_q)+k_a(\omega_p)=k_b(\omega_h)$;
(ii) Type II: One of the fundamental modes is of type a and the other one of type b, while the harmonic mode is also of type b with $\omega_h=\omega_p+\omega_q$ and $k_a(\omega_p)+k_b(\omega_q)=k_b(\omega_h)$.

Only the rapid phases of H which satisfy one of the two phase matching conditions may possess a nonvanishing zeroth-order component $\mathbf{E}_0^f$. That is why the physically relevant modes are those for which the rapid phases belong to H_{ac}

$$H_{ac}=\{(\omega,k)\in H \text{ such that } k=k_a(\omega) \text{ or } k=k_b(\omega)\}.$$

The leading order terms for the other harmonic phases $(\omega_f,k^f)\in H\backslash H_{ac}$ are at most of order $\delta^{2\alpha}$, that is to say $\mathbf{E}^f\sim\delta^\alpha\mathbf{E}_\alpha^f+O(\delta^{\alpha+1})$. Nevertheless it is necessary to take into account the harmonic modes that are not phase-matched so as to close the propagation equations. To complete this section we would like to add that the phase matching condition is only required to be fulfilled at order 1. A phase matching condition satisfied up to a term of order δ: $k_b(\omega_h)-k^p-k^q\sim O(\delta)$ or $k_b(\omega_h)-k^p-k^q\sim O(\delta)$, is a sufficient condition for an harmonic phase to possess an envelope with a nonvanishing leading order term $\mathbf{E}_0^h$. We shall encounter such situations in the forthcoming sections.

D. Boundary condition

If we assume that the source $\mathcal{S}$ can be expanded as (5), and accordingly that the field $\mathcal{E}$ inside the crystal is of the form (6), then collecting the coefficients with power δ^α and high carrier frequency ω_f establishes the continuity conditions which impose that the components parallel to the boundary surface of the input field $\mathcal{S}$ and of the field $\mathcal{E}$ should be equal, while there are no condition for the normal components. Since $\alpha>0$ these conditions are the same as in the linear configuration, so the type m mode $(m=a,b)$ with carrier frequency ω_f should be at $z=0^+$

$$\mathbf{E}_{0,m}^f(\delta t,\delta x,\delta y,z=0^+)=\frac{2}{1+n_m(\omega)}\frac{1}{s_{mx}^2+s_{my}^2}\begin{pmatrix} s_{mx}^2 & s_{mx}s_{my} & 0\\ s_{mx}s_{my} & s_{my}^2 & 0\\ s_{mx}s_{mz} & s_{my}s_{mz} & 0\end{pmatrix}\mathbf{v}^f(\delta t,\delta x,\delta y).$$

E. Poynting vector and diffraction operator in the linear framework

In this section we remember the reader with the main results of Ref. 13 in the case when the nonlinear polarization is neglected. The following results hold true when the two eigenindices (n_a,n_b) are different from each other. Note that the occurrence of the case $n_a=n_b$ corresponds to

very particular configurations which were thoroughly studied in Ref. 13. In the framework of frequency conversion, these configurations are not interesting since we aim at using the existence of two different dispersion relations for the modes to fulfill the phase matching conditions. The input wave break into the sum of modulations of high-frequency signals, which also divide into two modes which all propagate independently. For each high frequency ω and mode $m=a,b$, the Poynting vector of the mode is collinear to

$$\mathbf{u}_m(\omega)=\left(\frac{s_{mx}s_{mz}}{s_{mx}^2+s_{my}^2},\frac{s_{my}s_{mz}}{s_{mx}^2s_{my}^2},-1\right)^T. \tag{12}$$

In the reference frame $(\delta t,\delta x,\delta y,\delta z)$ the slowly varying envelope E_m^ω of the mode satisfies the transport equation $\partial_Z E_m^\omega+\mathcal{T}_m(\omega)E_m^\omega=0$ where

$$\mathcal{T}_m(\omega)=-u_{mx}(\omega)\partial_X-u_{my}(\omega)\partial_Y+v_m(\omega)^{-1}\partial_T. \tag{13}$$

In the moving reference frame $(\delta(t-z/v_m),\delta(x+u_{mx}z),\delta(y+u_{my}z),\delta^2 z)$ the slowly varying envelope E_m^ω of the mode satisfies a Schrödinger-type equation with respect to the long scale variable $\zeta=\delta^2 z$

$$2ik_m(\omega)\partial_\zeta E_m^\omega+\mathcal{L}_m(\omega)E_m^\omega+\mathcal{K}_m(\omega)E_m^\omega=0, \tag{14}$$

where the diffraction operator $\mathcal{L}_m(\omega)$ is anisotropic (see Ref. 13 for the complete expressions of the $c_{m,\ldots}$)

$$\mathcal{L}_m(\omega)=c_{m,xx}(\omega)\partial_X^2+2c_{m,xy}(\omega)\partial_X\partial_Y+c_{m,yy}(\omega)\partial_Y^2, \tag{15}$$

and the dispersion operator $\mathcal{K}_m(\omega)$ contains crossed space–time derivatives

$$\mathcal{K}_m(\omega)=-\sigma_m(\omega)\partial_T^2+2k_m(\omega)(\partial_\omega u_{mx})(\omega)\partial_T\partial_X+2k_m(\omega)(\partial_\omega u_{my})(\omega)\partial_T\partial_Y. \tag{16}$$

F. Second-order nonlinear polarization

The nonlinear susceptibility is the Fourier transform of the tensor $\chi^{(2)}$ defined by (3)

$$\hat{\chi}^{(2)}(\omega_1,\omega_2):=\int_0^\infty dt_1\int_0^\infty dt_2\chi^{(2)}(t_1,t_2)e^{i\omega_1 t_1+i\omega_2 t_2}.$$

Time integration starts from 0 to satisfy the causality property. We introduce the projector Θ_{ω_c,k^c} acting on fields of the form $\mathcal{A}=\frac{1}{2}\Sigma_{(\omega_f,k^f)\in H}\mathbf{A}_\delta^f e^{i(k^f z-\omega_f t)}+cc$ by

$$\Theta_{\omega_c,k^c}(\mathcal{A})=\mathbf{A}_\delta^c \text{ if } (\omega_c,k^c)\in H, \text{ and } 0 \text{ otherwise.}$$

The (ω_h,k^h) component of the nonlinear polarization in the crystallographic frame then reads as

$$\Theta_{\omega_h,k^h}(\mathcal{P}_{nl})=\frac{\epsilon_0}{2}\sum_{p,q,\omega_p+\omega_q=\omega_h,k^p+k^q=k^h}\hat{\chi}^{(2)}(\omega_p,\omega_q):(\mathbf{E}^p,\mathbf{E}^q).$$

For frequencies ω_p and ω_q and for types m_1 and m_2 in $\{a,b\}$ we denote by $\mathbf{s}_{m_1,m_2}(\omega_p,\omega_q)$ the vector

$$\mathbf{s}_{m_1,m_2}(\omega_p,\omega_q):=\hat{\chi}^{(2)}(\omega_p,\omega_q):(\mathbf{s}_{m_1}(\omega_p),\mathbf{s}_{m_2}(\omega_q)). \tag{17}$$

We list in the following the processes which can give rise to the generation of new frequencies:

(i) Type I conversion.
Let us denote $\omega_h=\omega_p+\omega_q$, $k^p=k_a(\omega_p)$, $k^q=k_a(\omega_q)$, and $k^h=k^p+k^q$. Then $\mathcal{E}^p+\mathcal{E}^q$ is of the form $\frac{1}{2}E^p\mathbf{s}_a(\omega_p)e^{i(k^pz-\omega_pt)}+\frac{1}{2}E^q\mathbf{s}_a(\omega_q)e^{i(k^qz-\omega_qt)}+cc$. In the (xyz)-reference frame the nonlinear polarization reads $\mathcal{P}_{nl,xyz}=U^{-1}\mathcal{P}_{nl,123}U$ and the (ω_h,k^h) component is

$$\Theta_{\omega_h,k^h}(\mathcal{P}_{nl,xyz})=\epsilon_0\mathbf{s}_{a,a}(\omega_p,\omega_q)E^pE^q. \tag{18}$$

(i) Type II conversion.
Let us denote $\omega_h=\omega_p+\omega_q$, $k^p=k_a(\omega_p)$, $k^q=k_b(\omega_q)$, and $k^h=k^p+k^q$. Then $\mathcal{E}^p+\mathcal{E}^q$ is of the form $\frac{1}{2}E^p\mathbf{s}_a(\omega_p)e^{i(k^pz-\omega_pt)}+\frac{1}{2}E^q\mathbf{s}_b(\omega_q)e^{i(k^qz-\omega_qt)}$. In the (xyz)-reference frame the nonlinear polarization reads $\mathcal{P}_{nl,xyz}=U^{-1}\mathcal{P}_{nl,123}U$ and the (ω_h,k^h) component is

$$\Theta_{\omega_h,k^h}(\mathcal{P}_{nl,xyz})=\epsilon_0\mathbf{s}_{a,b}(\omega_p,\omega_q)E^pE^q. \tag{19}$$

In the case of the class $\overline{4}2m$ which contains in particular potassium dihydrogen phosphate (KDP) crystal, the $\chi^{(2)}$-tensor has only six nonvanishing components which are equal to the coefficient $2d$: $\hat{\chi}^{(2)}_{123}=\hat{\chi}^{(2)}_{132}=\hat{\chi}^{(2)}_{213}=\hat{\chi}^{(2)}_{231}=\hat{\chi}^{(2)}_{312}=\hat{\chi}^{(2)}_{321}=2d$. The vectors $\mathbf{s}_{o,o}$ and $\mathbf{s}_{o,e}$ then read as

$$\mathbf{s}_{o,o}=2d\begin{pmatrix}\sin\theta\sin(2\phi)\\0\\-\cos\theta\sin(2\phi)\end{pmatrix},\quad \mathbf{s}_{o,e}=2d\begin{pmatrix}\cos(2\phi)\sin(\beta-2\theta)\\-\sin(2\phi)\sin(\beta-\theta)\\\cos(2\phi)\cos(\beta-2\theta)\end{pmatrix}.$$

IV. TYPE I PHASE-MATCHING

We assume that the incoming pulse consists of two modes with carrier frequencies ω_p and ω_q which are linearly polarized along the $\mathbf{s}_a(\omega_p)$-axis and $\mathbf{s}_a(\omega_q)$-axis, respectively

$$\mathcal{S}=\tfrac{1}{2}\delta^\alpha(v^p(\delta x,\delta y,\delta t)\mathbf{s}_a(\omega_p)e^{-i\omega_pt}+v^q(\delta x,\delta y,\delta t)\mathbf{s}_a(\omega_q)e^{-i\omega_qt})+cc. \tag{20}$$

The type I phase matching conditions are assumed to be satisfied for the sum $\omega_p+\omega_q=\omega_h$

$$k_a(\omega_p)+k_a(\omega_q)=k_b(\omega_h). \tag{21}$$

We also assume that the pair $(\omega_h,k_b(\omega_h))$ is the only adapted harmonic phase, that is to say the phase matching condition is not fulfilled for a subtraction or a sum between ω_p, ω_q, and ω_h different from $\omega_h=\omega_p+\omega_q$. As a consequence $H_{ac}=\{(\omega_p,k^p),(\omega_q,k^q),(\omega_h,k^h)\}$ where $k^p=k_a(\omega_p)$, $k^q=k_a(\omega_q)$, and $k^h=k_b(\omega_h)$. The adapted ansatz is accordingly

$$\mathcal{E}=\mathcal{E}^p+\mathcal{E}^q+\mathcal{E}^h+\mathcal{R}, \tag{22a}$$

$$\mathcal{E}^f=\frac{1}{2}\,\delta^\alpha\left(\sum_{j=0}^{\infty}\delta^j\mathbf{E}^f_j(\delta t,\delta x,\delta y,\delta z)\right)e^{i(k^fz-\omega_ft)}+cc, \tag{22b}$$

where $\mathcal{R}$ indicates a series of harmonic modes whose leading order coefficients $\mathbf{E}^f_0$ are vanishing. The parameter α will then play a crucial part since the order of magnitude of the input pulse imposes the distance scale at which the nonlinear effects become noticeable.

A. Geometric optics $\alpha=1$

We denote $T=\delta t$, $X=\delta x$, $Y=\delta y$, $Z=\delta z$.

Proposition 1: If the source can be expanded as (20), then the fundamental modes are of type a for the carrier frequencies ω_p and ω_q while the harmonic mode at frequency ω_h is of type b. By denoting $E^p_0=\mathbf{s}_a(\omega_p).\mathbf{E}^p_0$, $E^q_0=\mathbf{s}_a(\omega_q).\mathbf{E}^q_0$, and $E^h_0=\mathbf{s}_b(\omega_h).\mathbf{E}^h_0$ the projections of the modes onto their respective unit polarization vectors, the slowly varying envelopes E^f_0 satisfy the following coupled equations:

$$\partial_Z E_0^p + \mathcal{T}_a(\omega_p)(E_0^p) = \frac{i\omega_p d^{(I)}}{n_a(\omega_p)\cos^2(\beta_a(\omega_p))} E_0^q * E_0^h, \tag{23a}$$

$$\partial_Z E_0^q + \mathcal{T}_a(\omega_q)(E_0^q) = \frac{i\omega_q d^{(I)}}{n_a(\omega_q)\cos^2(\beta_a(\omega_q))} E_0^p * E_0^h, \tag{23b}$$

$$\partial_Z E_0^h + \mathcal{T}_b(\omega_h)(E_0^h) = \frac{i\omega_h d^{(I)}}{n_b(\omega_h)\cos^2(\beta_b(\omega_h))} E_0^p E_0^q, \tag{23c}$$

starting from $E_0^p(T,X,Y,Z=0) = (2/[1+n_a(\omega_p)])v^p(T,X,Y)$, $E_0^q(T,X,Y,Z=0) = (2/[1+n_a(\omega_q)])v^q(T,X,Y)$ *and* $E_0^h(T,X,Y,Z=0) = 0$, *where the transport operator* $\mathcal{T}_m(\omega)$ *is given by* (13) *and*

$$d^{(I)} = \frac{\mathbf{s}_a(\omega_p).\mathbf{s}_{a,b}(\omega_q,\omega_h)}{2c}.$$

Proof: The strategy is formally the same as in linear configurations. We substitute the ansatz (22a) and (22b) with $\alpha = 1$ into Eq. (1) and we collect the coefficients with the same power of δ and the same carrier frequency. At order δ we find the dispersion relation and phase matching conditions discussed in Sec. III C. At order δ^2, we project the equation onto the three axes.
For the frequency ω_p (resp. $-\omega_p$), denoting $k^p = k_a(\omega_p)$

$$\mathbf{R}_0(\mathbf{E}_1^p) + \mathbf{R}_1(\mathbf{E}_0^p) = \mathbf{D}_0(\mathbf{E}_1^p) + \mathbf{D}_1(\mathbf{E}_0^p) + \mu_0\omega_p^2\Theta_{\omega_p,k^p}(\mathcal{P}_{nl}(\mathcal{E}_0,\mathcal{E}_0)), \tag{24}$$

where we retain only the terms of order δ in $\mathcal{P}_{nl}$, which are the ones that give a contribution of the nonlinear polarization of order δ^2. Further in the nonlinear term $\mathcal{P}_{nl}(\mathcal{E}_0,\mathcal{E}_0)$ we only retain the coefficients with rapid phase $+(k^p z - \omega_p t)$. Only the frequencies ω_h and $-\omega_q$ can generate ω_p (resp. $-\omega_h$ and ω_q for $-\omega_p$). We, therefore, compute the sum of a type a wave at frequency $-\omega_q$ with a type b wave at frequency ω_h. By applying (19) we get in the reference frame (x,y,z):

$$\Theta_{\omega_p,k^p}(\mathcal{P}_{nl}(\mathcal{E}_0,\mathcal{E}_0)) = \epsilon_0\mathbf{s}_{a,b}(\omega_q,\omega_h)E_0^q * E_0^h.$$

The projection of Eq. (24) onto $\mathbf{s}_a(\omega_p)$ then provides the compatibility condition which reads as Eq. (23a).

For the frequency ω_q, the situation is similar. We get Eq. (23b) with an expression of $d^{(I)}$ which is $d^{(I)'} = (\mathbf{s}_a(\omega_q).\mathbf{s}_{a,b}(\omega_p,\omega_h))/(2c)$, and using the symmetry properties of $\hat{\chi}^{(2)}$[14] it is easy to prove that $d^{(I)'} = d^{(I)}$.

For the frequency ω_h, denoting $k^h = k_b(\omega_h)$:

$$\mathbf{R}_0(\mathbf{E}_1^h) + \mathbf{R}_1(\mathbf{E}_0^h) = \mathbf{D}_0(\mathbf{E}_1^h) + \mathbf{D}_1(E_0^h) + \mu_0\omega_h^2\Theta_{\omega_h,k^h}(\mathcal{P}_{nl}(\mathcal{E}_0,\mathcal{E}_0)), \tag{25}$$

where we retain only the terms of order δ in $\mathcal{P}_{nl}$, which are the ones that give a contribution of the nonlinear polarization of order δ^2. Further in the nonlinear term $\mathcal{P}_{nl}(\mathcal{E}_0,\mathcal{E}_0)$ we only retain the coefficients with rapid phase $+(k^h z - \omega_h t)$. Only the frequencies ω_p and ω_q can generate ω_h (resp. $-\omega_p$ and $-\omega_q$ for $-\omega_h$). We therefore compute the sum of a type a wave at frequency ω_p with a type a wave at frequency ω_q. By applying (18), we get in the reference frame (x,y,z)

$$\Theta_{\omega_h,k^h}(\mathcal{P}_{nl,xyz}) = \epsilon_0\mathbf{s}_{a,a}(\omega_p,\omega_q)E_0^p E_0^q.$$

The projection of Eq. (25) onto $\mathbf{s}_b(\omega_h)$ then provides the compatibility condition which reads as Eq. (23c) with $d^{(I)''} = (\mathbf{s}_b(\omega_h).\mathbf{s}_{a,a}(\omega_p,\omega_q))/(2c)$, and using the symmetry properties of $\hat{\chi}^{(2)}$ it is easy to prove that $d^{(I)''} = d^{(I)}$. □

B. Approximate phase matching

In the above section we have considered a perfect phase matching condition. This condition is indeed very stringent and should be fulfilled at the leading order. Nevertheless it is barely possible in realistic experimental configurations to reach such a level of perfection. It is therefore relevant to address the case of a slight perturbation of the ideal case $\theta=\theta_{pm}$ where θ_{pm} is the angle which satisfies (21). We consider in this section that the phase matching condition is fulfilled up to a term of order δ and we set $\theta=\theta_{pm}+\delta\eta$. The corresponding propagation equations read

$$\partial_Z E_0^p+\mathcal{T}_a(\omega_p)E_0^p=\frac{i\omega_p d^{(I)}}{n_a(\omega_p)\cos^2(\beta_a(\omega_p))}E^{q*}\tilde{E}_0^h,$$

$$\partial_Z E_0^q+\mathcal{T}_a(\omega_q)E_0^q=\frac{i\omega_q d^{(I)}}{n_a(\omega_q)\cos^2(\beta_a(\omega_q))}E_0^{p*}E_0^h,$$

$$\partial_Z E_0^h+\mathcal{T}_b(\omega_h)E_0^h=\frac{i\omega_h d^{(I)}}{n_b(\omega_h)\cos^2(\beta_b(\omega_h))}E_0^pE_0^q+i\eta_k E_0^h,$$

where $\eta_k=\eta[\partial k_b(\omega_h)/\partial\theta]|_{\theta=\theta_{pm}}$. By setting $\tilde{E}_0^h=E_0^h e^{-i\eta_k Z}$, this system reduces:

$$\partial_Z E_0^p+\mathcal{T}_a(\omega_p)E_0^p=\frac{i\omega_p d^{(I)}}{n_a(\omega_p)\cos^2(\beta_a(\omega_p))}E_0^{q*}\tilde{E}_0^h e^{i\eta_k Z},$$

$$\partial_Z E_0^q+\mathcal{T}_a(\omega_q)E_0^q=\frac{i\omega_q d^{(I)}}{n_a(\omega_q)\cos^2(\beta_a(\omega_q))}E_0^{p*}\tilde{E}_0^h e^{i\eta_k Z},$$

$$\partial_Z \tilde{E}_0^h+\mathcal{T}_b(\omega_h)\tilde{E}_0^h=\frac{i\omega_h d^{(I)}}{n_b(\omega_h)\cos^2(\beta_b(\omega_h))}E_0^pE_0^q e^{-i\eta_k Z}.$$

It appears that it is necessary to add a phase $-\eta_k Z$ to the harmonic field so as to make the frequency conversion equations into a standard form. It shows that the rapid phase of the harmonic is imposed by the product of the phases of the fundamental modes: $\exp i((k^p+k^q)z-(\omega_p+\omega_q)t)$, which is different from the ''natural'' type b phase $\exp i(k_b(\omega_h)z-\omega_h t)$, with $\omega_h=\omega_p+\omega_q$.

C. Diffractive optics $\alpha=2$

In this configuration the nonlinear effects are weaker, of the order of $\delta^{2\alpha}=\delta^4$, so that they can show themselves only after a longer propagation distance z of the order of δ^{-2}. The technique is the same as for the derivations of the propagation equations in the linear framework. The final result is expressed in terms of the original variables x,y,z,t:

Proposition 2: Let us assume that the input field $\mathcal{S}$ consists of two modes with carrier frequencies ω_p and ω_q which are linearly polarized along the $\mathbf{s}_a(\omega_p)$-axis and $\mathbf{s}_a(\omega_q)$-axis, respectively. Then the fundamental modes are of type a and the harmonic mode is of type b ($\omega_h=\omega_p+\omega_q$). We denote $k^p=k_a(\omega_p)$, $k^q=k_a(\omega_q)$, $k^h=k_b(\omega_h)$, $\eta_k=k^h-k^p-k^q$, and $\tilde{\mathbf{E}}^h=\mathbf{E}^h e^{-i\eta_k z}$. We introduce the projections of the envelopes of the modes onto their respective unit polarization vectors: $E^p=\mathbf{s}_a(\omega_p).\mathbf{E}^p$, $E^q=\mathbf{s}_a(\omega_q).\mathbf{E}^q$, and $\tilde{E}^h=\mathbf{s}_b(\omega_h).\tilde{\mathbf{E}}^h$. The system which governs the propagation and conversion is:

$$\partial_z E^p+\mathcal{T}_a(\omega_p)E^p-\frac{i}{2k^p}\mathcal{L}_a(\omega_p)E^p-\frac{i}{2k^p}\mathcal{K}_a(\omega_p)E^p=\frac{i\omega_p d^{(I)}}{n_a(\omega_p)\cos^2(\beta_a(\omega_p))}E^{q*}\tilde{E}^h e^{i\eta_k z},$$

$$\partial_z E^q+\mathcal{T}_a(\omega_q)E^q-\frac{i}{2k^q}\mathcal{L}_a(\omega_q)E^q-\frac{i}{2k^q}\mathcal{K}_a(\omega_q)E^q=\frac{i\omega_q d^{(I)}}{n_a(\omega_q)\cos^2(\beta_a(\omega_q))}E^{p*}\tilde{E}^h e^{i\eta_k z},$$

$$\partial_z \tilde{E}^h + \mathcal{T}_b(\omega_h)\tilde{E}^h - \frac{i}{2k^h}\mathcal{L}_b(\omega_h)\tilde{E}^h - \frac{i}{2k^h}\mathcal{K}_b(\omega_h)\tilde{E}^h = \frac{i\omega_h d^{(I)}}{n_b(\omega_h)\cos^2(\beta_b(\omega_h))}E^p E^q e^{-i\eta_k z},$$

where the transport operator $\mathcal{T}_m$ and the diffraction-dispersion operators $\mathcal{L}_m$ and $\mathcal{K}_m$ are given by (13), (15), and (16), respectively (where small letters should be substituted for capital letters).

V. TYPE II PHASE-MATCHING

We assume that the source can be expanded as

$$\mathcal{S} = \frac{1}{2}\delta^2 \begin{pmatrix} v_x(\delta x, \delta y, \delta t)e^{-i\omega_q t} \\ v_y(\delta x, \delta y, \delta t)e^{-i\omega_p t} \\ 0 \end{pmatrix} + cc, \tag{26}$$

and that the type II phase matching condition is almost satisfied by the sum $\omega_p + \omega_q = \omega_h$:

$$k_b(\omega_h) - k_a(\omega_p) - k_b(\omega_q) = O(\delta).$$

We also assume that the pair $(\omega_h, k_b(\omega_h))$ is the only adapted harmonic phase, that is to say the phase matching condition is not fulfilled for a subtraction or a sum between ω_p, ω_q, and ω_h different from $\omega_h = \omega_p + \omega_q$, so that the suitable ansatz is (22a) and (22b) with $H_{ac} = \{(\omega_p, k^p), (\omega_q, k^q), (\omega_h, k^h)\}$ where $k^p = k_a(\omega_p)$, $k^q = k_b(\omega_q)$, and $k^h = k_b(\omega_h)$. The main result is obtained by using the very same techniques as in the previous sections so that we only state it in the original variables *x,y,z,t*. We denote the phase mismatch by $\eta_k := k^h - k^p - k^q$.

Proposition 3. Let us assume that the input field $\mathcal{S}$ consists of two modes with carrier frequencies ω_p and ω_q which are linearly polarized along the y axis and x axis, respectively. Then the modes of the field $\mathcal{E}$ are ordinary for the fundamental ω_p and extraordinary for the fundamental ω_q and harmonic $\omega_h = \omega_p + \omega_q$. By introducing $\tilde{\mathbf{E}}^h = \mathbf{E}^h e^{-i\eta_k z}$ and denoting $E^p = \mathbf{s}_a(\omega_p).\mathbf{E}^p$, $E^q = \mathbf{s}_b(\omega_q \mathbf{E}^q)$. and $\tilde{E}^h = \mathbf{s}_b(\omega_h).\tilde{\mathbf{E}}^h$ the projections of the envelopes of the modes onto their respective unit polarization vectors, the system which governs the propagation and conversion is:

$$\partial_z E^p + \mathcal{T}_a(\omega_p)E^p - \frac{i}{2k^p}\mathcal{L}_a(\omega_p)E^p - \frac{i}{2k^p}\mathcal{K}_a(\omega_p)E^p = \frac{i\omega_p d^{(II)}}{n_a(\omega_p)\cos^2(\beta_a(\omega_p))}E^{q*}\tilde{E}^h e^{i\eta_k z},$$

$$\partial_z E^q + \mathcal{T}_b(\omega_q)E^q - \frac{i}{2k^q}\mathcal{L}_b(\omega_q)E^q - \frac{i}{2k^q}\mathcal{K}_b(\omega_q)E^q = \frac{i\omega_q d^{(II)}}{n_b(\omega_q)\cos^2(\beta_b(\omega_q))}E^{p*}\tilde{E}^h e^{i\eta_k z},$$

$$\partial_z \tilde{E}^h + \mathcal{T}_b(\omega_h)\tilde{E}^h - \frac{i}{2k^h}\mathcal{L}_b(\omega_h)\tilde{E}^h - \frac{i}{2k^h}\mathcal{K}_b(\omega_h)\tilde{E}^h = \frac{i\omega_h d^{(II)}}{n_b(\omega_h)\cos^2(\beta_b(\omega_h))}E^p E^q e^{-i\eta_k z},$$

where

$$d^{(II)} = \frac{\mathbf{s}_a(\omega_p).\mathbf{s}_{b,b}(\omega_q, \omega_h)}{2c}.$$

VI. PROPAGATION FAR FROM PHASE-MATCHING

In the two previous sections we have examined the two cases corresponding to phase-matching for sum-frequency generation. In this section we consider the general situation where the phase-matching condition is not fulfilled so as to derive the propagation equation of the fundamental wave, and also some information for the different harmonic waves. Such a work has been performed by Leblond[15] who considered the propagation of a pulse along the principal axis of a uniaxial crystal. In this section we consider the general case of biaxial crystals in the configuration when the two eigenindices are different from each other. We assume a source of the form

$$\mathcal{S}=\tfrac{1}{2}\delta v(\delta x,\delta y,\delta t)(s_{ax}(\omega),s_{ay}(\omega),0)^T e^{-i\omega t}+cc, \tag{27}$$

and we shall see that the suitable ansatz for the scales corresponding to diffractive optics is:

$$\mathcal{E}=\mathcal{E}^{0\omega}+\mathcal{E}^{1\omega}+\mathcal{E}^{2\omega}+\mathcal{R}, \tag{28a}$$

$$\mathcal{E}^{l\omega}=\frac{1}{2}\delta\sum_{j=0}^{\infty}\delta^j\mathbf{E}_j^{l\omega}(\delta(t-z/v_a),\delta(x+u_{ax}z),\delta(y+u_{ay}z),\delta^2 z)e^{il(k_a(\omega)z-\omega t)}+cc, \tag{28b}$$

where $\mathcal{R}$ is a sum of harmonic waves whose leading order term is of order δ^3 or smaller, and v_a, $\mathbf{u}_a$ are shorthands for $v_a(\omega)$, $\mathbf{u}_a(\omega)$, respectively.

Proposition 4: If we assume that the input field $\mathcal{S}$ consists of one mode with carrier frequency ω which is linearly polarized along the $\mathbf{s}_a(\omega)$-axis, then the slowly varying envelope of the field $\mathcal{E}$ is of type a and $E_0=\mathbf{s}_a(\omega).\mathbf{E}_0^{1\omega}$ satisfies the nonlinear Schrödinger equation

$$2ik_a\partial_\zeta E_0+\mathcal{L}_a(\omega)E_0+\mathcal{K}_a(\omega)E_0+P_3(E_0)=0, \tag{29}$$

starting from $E_0(T,X,Y,\zeta=0)=(2/[1+n_a(\omega)])v(T,X,Y)$, *where* $P_3(E_0)=(\gamma_1+\gamma_2)|E_0|^2E_0+\mathbf{s}_a.\hat{\chi}^{(2)}(0,\omega)(\mathbf{E}_1^{0\omega^*},\mathbf{E}_0^{1\omega})$,

$$\gamma_1=\tfrac{3}{4}\mathbf{s}_a(\omega).\hat{\chi}^{(3)}(\omega,\omega,-\omega):(\mathbf{s}_a(\omega),\mathbf{s}_a(\omega),\mathbf{s}_a(\omega)),$$

$$\gamma_2=\tfrac{1}{2}\mathbf{s}_a(\omega).\hat{\chi}^{(2)}(2\omega,-\omega):((n_a^2(\omega)J-\chi(2\omega))^{-1}\mathbf{s}_{a,a}(\omega,\omega),\mathbf{s}_a(\omega)),$$

where J is the 3×3 matrix whose entries are vanishing but $J_{11}=J_{22}=1$. The second harmonic is of order δ^2 and its leading order term $\mathbf{E}_1^{2\omega}$ is given by (30). The zero harmonic is of order δ^2 and its leading order term $\mathbf{E}_1^{0\omega}$ is given by (32). All other harmonic are of order smaller than δ^3.

Note that far from phase matching, the second harmonic does not propagate with its natural phase velocity and group velocity, but with those of the fundamental. But it is smaller by an order of magnitude. The same holds true for the zero-harmonic term. By ''zero-harmonic'' we mean an electromagnetic wave whose wavelength is of the order of δ^{-1}.

Proof:

(i) Computation of the leading order term at 2ω.
Collecting the terms of order δ^2 at frequency 2ω provides an explicit representation for $\mathbf{E}_1^{2\omega}$:

$$\mathbf{E}_1^{2\omega}=\tfrac{1}{2}(n_a^2(\omega)J-\chi(2\omega))^{-1}\hat{\chi}^{(2)}(\omega,\omega):(\mathbf{E}_0^{1\omega},\mathbf{E}_0^{1\omega}). \tag{30}$$

Note that the matrix $n_a^2(\omega)J-\chi(2\omega)$ is invertible since we assume that there is no phase-matching for second harmonic generation.

(ii) Computation of the leading order term at 0ω.
Collecting the terms of order δ^4 at frequency 0ω yields:

$$\mathbf{R}_2(\mathbf{E}_1^{0\omega})=\mathbf{D}_2(\mathbf{E}_1^{0\omega})-c^{-2}\partial_T^2\mathbf{P}_2,$$

where $\mathbf{P}_2$ is given by

$$\mathbf{P}_2=\hat{\chi}^{(2)}(\omega,-\omega)(\mathbf{E}_0^{1\omega},\mathbf{E}_0^{1\omega^*}).$$

Note that $\mathbf{D}_2(\mathbf{E}_1^{0\omega})=-c^{-2}\chi(0\omega)\partial_T^2\mathbf{E}_1^{0\omega}$. The computation of $\mathbf{E}_1^{0\omega}$ is formally identical as for the second-harmonic wave, that is to say the zero-harmonic wave is obtained by applying an inversion operator [here $(\mathbf{R}_2-\mathbf{D}_2)^{-1}$] to a functional of the leading-order term of the fundamental wave (here $-c^{-2}\partial_T^2\mathbf{P}_2$). But the inversion is a little more elaborate, since it requires to apply the Green function of a linear nondispersive Maxwell equation. We give in what follows an explicit formulation of this inversion. First denote by **Rot** the standard ''**rot**'' operator operating on the macroscopic variables (X,Y,Z). Consider the

problem of finding the solution $\mathbf{E}$ of the following Maxwell equation with a source:

$$\mathbf{Rot}\ \mathbf{Rot}\ \mathbf{E}=-c^{-2}\chi(0\omega)\partial_T^2\mathbf{E}-c^{-2}\partial_T^2\mathbf{P},$$

where $\mathbf{P}(T,X,Y,Z)$ is the polarization induced by the source. Taking the Fourier transform with respect to time and space

$$(|\mathbf{K}|^2 I_d-\mathbf{K}\otimes\mathbf{K}-\nu^2c^{-2}\chi(0\omega))\hat{\mathbf{E}}(\nu,\mathbf{K})=\nu^2c^{-2}\hat{\mathbf{P}}(\nu,\mathbf{K}), \tag{31}$$

where ν is the frequency, $\mathbf{K}$ the wave number, and $\mathbf{S}\otimes\mathbf{U}$ is the matrix whose entries are S_iU_j. We denote by N_a and N_b the two solutions of the Fresnel equation associated with the tensor $\chi(0\omega)$:

$$\det(N^2I_d-N^2|\mathbf{K}|^2\mathbf{K}\otimes\mathbf{K}-\chi(0\omega))=0,$$

and by $\mathbf{S}_a$ and $\mathbf{S}_b$ the corresponding unit eigenvectors. The Green function $\hat{g}(\nu,\mathbf{K})$ corresponding to Eq. (31) is defined by the equation

$$\hat{\mathbf{E}}(\nu,\mathbf{K})=\hat{g}(\nu,\mathbf{K})\hat{\mathbf{P}}(\nu,\mathbf{K}).$$

It was shown by Lax and Nelson that the Green function can be written in the form[16]

$$\hat{g}(\nu,\mathbf{K})=\frac{\nu^2}{c^2}\left(\frac{e_a}{|\mathbf{K}|^2/N_a^2-\nu^2/c^2-io}+\frac{e_b}{|\mathbf{K}|^2/N_b^2-\nu^2/c^2-io}\right)-\frac{\mathbf{K}\otimes\mathbf{K}}{\mathbf{K}^T\chi(0\omega)\mathbf{K}},$$

$$e_m=\frac{\mathbf{S}_m\otimes\mathbf{S}_m}{\mathbf{S}_m^T\chi(0\omega)\mathbf{S}_m}.$$

If $\nu<0$, then the term $-io$ should be replaced by $+io$. We then introduce the auxiliary function $\hat{G}$ which is the projection of $\hat{g}$ onto the characteristic equation satisfied by $\mathbf{P}_2$

$$\hat{G}(\nu,K_x,K_y)=\hat{g}(\nu,K_x,K_y,K_xu_{ax}(\omega)+K_yu_{ay}(\omega)-\nu/v_a(\omega)),$$

$$G(T,X,Y)=\frac{1}{(2\pi)^3}\int\hat{G}(\nu,K_x,K_y)e^{i(K_xX+K_yY-\nu T)}dXdYdT.$$

We finally define the convolution operator Ψ which associates to any pair of vector-valued functions $\mathbf{A}_1(T,X,Y)$ and $\mathbf{A}_2(T,X,Y)$ the vector-valued function

$$\Psi*(\mathbf{A}_1,\mathbf{A}_2)(T,X,Y):=\int G(T-s,X-u,Y-v)[\hat{\chi}^{(2)}(\omega,-\omega):(\mathbf{A}_1,\mathbf{A}_2)(s,u,v)]dsdudv.$$

The leading order term $\mathbf{E}_1^{0\omega}(T,X,Y,\zeta)$ of the zero-harmonic wave can then be expressed for every ζ as the application of the Ψ-operator to the pair $(\mathbf{E}_0^{1\omega}(.,.,.,\zeta),\mathbf{E}_0^{1\omega^*}(.,.,.,\zeta))$:

$$\mathbf{E}_1^{0\omega}(T,X,Y,\zeta)=\Psi*(\mathbf{E}_0^{1\omega}(.,.,.,\zeta),\mathbf{E}_0^{1\omega^*}(.,.,.,\zeta))(T,X,Y). \tag{32}$$

(iii) Equation for the corrective term at ω.
Collecting the terms of order δ^2 at frequency ω we get an explicit form for the first corrective term $\mathbf{E}_1^{1\omega}$ of the fundamental wave. No nonlinear term is coming to at this order, so the expression is identical to the linear framework (see Ref. 13).

(iv) Equation for the leading order term at ω.
Collecting the terms of order δ^3 at frequency ω we get

$$\mathbf{R}_2(\mathbf{E}_0^{1\omega})+\mathbf{R}_1(\mathbf{E}_1^{1\omega})+\mathbf{R}_0(\mathbf{E}_2^{1\omega})=\mathbf{D}_2(\mathbf{E}_0^{1\omega})+\mathbf{D}_1(\mathbf{E}_1^{1\omega})+\mathbf{D}_0(\mathbf{E}_2^{1\omega})-c^{-2}\mathbf{P}_3,$$

where the contribution of the nonlinear polarization is:

$$\mathbf{P}_3=(\tfrac{3}{4})\hat{\chi}^{(3)}(\omega,\omega,-\omega):(\mathbf{E}_0^{1\omega},\mathbf{E}_0^{1\omega},\mathbf{E}_0^{1\omega^*})+\hat{\chi}^{(2)}(2\omega,-\omega):(\mathbf{E}_1^{2\omega},\mathbf{E}_0^{1\omega^*})$$
$$+\hat{\chi}^{(2)}(0\omega,\omega):(\mathbf{E}_1^{0\omega},\mathbf{E}_0^{1\omega}).$$

Projecting onto $\mathbf{s}_a(\omega)$ we get

$$\mathbf{s}_a(\omega).\mathbf{R}_2(\mathbf{E}_0^{1\omega})+\mathbf{s}_a(\omega).\mathbf{R}_1(\mathbf{E}_1^{1\omega})=\mathbf{s}_a(\omega).\mathbf{D}_2(\mathbf{E}_0^{1\omega})+\mathbf{s}_a(\omega).\mathbf{D}_1(\mathbf{E}_1^{1\omega})-c^{-2}\mathbf{s}_a(\omega).\mathbf{P}_3.$$

Substituting the expression of $\mathbf{E}_1^{1\omega}$ establishes the result.

Note that the long-scale variable ζ plays the role of a parameter in the expression (32) of $\mathbf{E}_1^{0\omega}$. Consequently Eq. (29) reads as a simple first-order evolution equation with respect to the ζ-variable for the envelope E_0. This provides a simple numerical scheme to compute $E_0(.,.,.,\zeta+\Delta\zeta)$ from $E_0(.,.,.,\zeta)$.

VII. SPATIAL SOLITON PROPAGATION IN BIAXIAL CRYSTALS

We examine in this section the propagation in biaxial crystals of the modulation of a high-frequency signal with frequency ω in the particular configuration $\theta=\theta_r(\omega)$ and $\phi=0$ or π where

$$\sin^2\theta_r(\omega)=\frac{1-\chi_2(\omega)/\chi_1(\omega)}{1-\chi_3(\omega)/\chi_1(\omega)}.$$

Computing all relevant quantities according to the general formulas we have found in particular that the type a eigenindex and unit polarization eigenvector are $n_a^2(\omega)=\chi_2(\omega)$ and $\mathbf{s}_a(\omega)=(0,1,0)^T$, respectively (for the type b we refer to Ref. 13). The diffraction coefficients for the a-mode are $c_{a,xx}(\omega)=1$, $c_{a,xy}(\omega)=0$, and $c_{a,yy}(\omega)=0$, while the dispersion operator reads $\mathcal{K}_a(\omega)=-\sigma_a(\omega)\partial_T^2$. The striking point is that the diffraction operator for the type a wave is degenerate, in the sense that there is no diffraction in the y-direction. Let us assume that the carrier frequency ω of the input pulse is such that the phase matching condition for the second-harmonic generation is not fulfilled. For the sake of simplicity we first restrict ourselves to one of the three following classes:[17]

(1) triclinic class with point group $\overline{1}$, such as Mica or Al_2SiO_5;
(2) monoclinic class with point group $2/m$, such as $AgAuTe_4$ or $PbSiO_3$;
(3) orthorhombic class with point group mmm, such as $CaCl_2$, or Al_2BeO_4 (also called alexandrite).

The crystals of these classes are biaxial and have a vanishing $\chi^{(2)}$-tensor. This simplification allows us to get rid of the $\chi^{(2)}$-cascaded terms and to deal with a simple $\chi^{(3)}$-component which then reads as a simple Kerr effect. The result is the following:

Proposition 5. In cases 1, 2, 3, if we assume that the input field $\mathcal{S}$ consists of one mode with carrier frequency ω which is linearly polarized along the y axis, then the slowly varying envelope of the field $\mathcal{E}$ is polarized along the y axis and $E_0=(0,1,0).\mathbf{E}_0^{1\omega}$ satisfies the nonlinear Schrödinger equation

$$2ik_a\partial_\zeta E_0+\partial_X^2E_0-\sigma_a\partial_T^2E_0+\gamma|E_0|^2E_0=0, \tag{33}$$

starting from $E_0(T,X,Y,\zeta=0)=(2/[1+n_a(\omega)])v(T,X,Y)$, where $\gamma=(\frac{3}{4})\hat{\chi}^{(3)}_{2222}(-\omega,\omega,\omega)$.

The removal of the time variable is involved by the assumption that there is no modulation of the input pulse at the time scale δ^{-1}, which is typically of the order of the picosecond, but only at scale δ^{-2}, which is typically of the order of the nanosecond. Then the slowly varying envelope of the field satisfies the standard one-dimensional Schrödinger equation

$$2ik_a\partial_\zeta E_0+\partial_X^2E_0+\gamma|E_0|^2E_0=0. \tag{34}$$

The one-dimensional nonlinear Schrödinger equation possesses the complete integrability property, which implies that stable solitons should be generated and propagate over large distances. If a pulse is focused onto a crystal plate according to the incident angle and polarization described here above, then in the x-transverse direction the profile of the pulse will not diffract and keep its original form while in the transverse y-direction the pulse will break into a soliton (or eventually

several solitons) and radiation whose amplitude will decay as standard one-dimensional waves do in linear media, that is to say at rate $z^{-1/2}$. The incident pulse must at least fulfill a well-known power criterion so that a soliton can be generated[18]

$$\int_{-\infty}^{\infty} |E_0| dx \geqslant 1.279 \gamma^{-1/2},$$

which simply means that the incident pulse should be sufficient focused so that its power $\int |E_0|^2 dx$ be concentrated on a small segment. Nevertheless one should still remain in the domain where Eq. (33) holds true, which is basically the paraxial approximation.

In case of biaxial crystals with nonvanishing $\chi^{(2)}$-tensor the result is qualitatively the same, in the sense that the diffraction operator still reads as a one-dimensional second-order derivative, but $\chi^{(2)}$-cascaded terms make the nonlinear term more complicated. We aim in the following proposition at generalizing Proposition 5 to any biaxial crystal.

Proposition 6. For any biaxial crystal in the configuration $\theta=\theta_r$ and $\phi=0$, if we assume that the input field $\mathcal{S}$ consists of one mode with carrier frequencies ω which is linearly polarized along the y axis, then the slowly varying envelope of the field $\mathcal{E}$ is polarized along the y axis and $E_0=(0,1,0).\mathbf{E}_0$ satisfies the nonlinear Schrödinger equation

$$2ik_a \partial_\zeta E_0 + \partial_X^2 E_0 - \sigma_a \partial_T^2 E_0 + P_3(E_0) = 0, \tag{35}$$

where $P_3(E_0)=(\gamma_1+\gamma_2)|E_0|^2E_0+\Sigma_{j,l=1}^3 \gamma_{3_{jl}} \Phi_{jl}(|E_0|^2(.,.,.,\zeta))E_0$, *with*

$$\gamma_1 = \tfrac{3}{4}\hat{\chi}^{(3)}_{2222}(\omega,\omega,-\omega),$$

$$\gamma_2 = \frac{1}{2}\sum_{j=1}^{3} \hat{\chi}^{(2)}_{2j2}(2\omega,-\omega)[(n_a^2(\omega)J-\chi(2\omega))^{-1}\chi^{(2)}_{.22}(\omega,\omega)]_j,$$

$$\gamma_{3_{jl}} = \hat{\chi}^{(2)}_{2j2}(0,\omega)\hat{\chi}^{(2)}_{l22}(\omega,-\omega),$$

$$\Phi_{jl}(I(.,.,.))(T,X,Y) = \sum_{j',l'=1}^{3} U_{jj'}U_{ll'} \int G_{j'l'}(T-s,X-u,Y-v) I(s,u,v) ds du dv.$$

G is the Green function whose Fourier transform is $\hat{G}(\nu,K_x,K_y)=\hat{g}(\nu,K_x,K_y,-\nu/v_a(\omega))$ *with*:

$$\hat{g}(\nu,\mathbf{K}) = \frac{\nu^2}{c^2}\left(\frac{e_a}{|\mathbf{K}|^2/n_a(0\omega)^2-\nu^2/c^2-io} + \frac{e_b}{|\mathbf{K}|^2/n_b^2(0\omega)-\nu^2/c^2-io}\right) - \frac{\mathbf{K}\otimes\mathbf{K}}{\mathbf{K}^T\chi(0\omega)\mathbf{K}},$$

$$e_m = \frac{\mathbf{s}_m(0\omega)\otimes\mathbf{s}_m(0\omega)}{(\mathbf{s}_m(0\omega)^T)\chi(0\omega)\mathbf{s}_m(0\omega)},$$

where $n_m(0\omega)$ *and* $\mathbf{s}_m(0\omega)$ *are the eigenindices and unit eigenvectors of the Fresnel equation corresponding to the tensor* $\chi(0\omega)$ *at angles* $\theta_r(\omega)$, $\phi=0$

$$(n^2 I_d - n^2|\mathbf{K}|^{-2}\mathbf{K}\otimes\mathbf{K} - \chi(0\omega,\theta_r(\omega),0))\mathbf{s}=0.$$

All terms in P_3 are proportional to $|E_0|^2E_0$ or a product of three terms proportional to E_0. Note that the only coefficient of the $\chi^{(3)}$-tensor which plays a role is $\hat{\chi}^{(3)}_{2222}(\omega,\omega,-\omega)$. The coefficients of the $\chi^{(2)}$-tensor which play a role are the ones with at least two indices equal to 2. In case of orthorhombic class with point group 222, the only non-vanishing coefficients of the $\chi^{(2)}$-tensor are the ones with three different indices. Consequently all components of P_3 vanish but $\gamma_1|E_0|^2E_0$ so that we get back the result of Proposition 5.

VIII. SPATIAL SPECTRUM OF THE SECOND HARMONIC PULSE

In this section we aim at giving the explanation of a recent experimental observation. The framework is the following. In the context of Inertial Confinement Fusion, many high-power laser beams are focused onto a spherical target composed of a mixture of deuterium–tritium so as to compress it and to obtain density and pressure conditions which involve thermonuclear burning. The laser energy production is based on the amplification of an infrared pulse in glass amplifiers, which are the only ones capable to deliver an energy of the order of 1 to 2 megajoules. Nevertheless it is necessary to frequency convert the pulse in the ultraviolet (UV) domain so as to optimize the plasma-laser interaction between the laser beams and the inertial confinement-fusion (ICF) target. Thus the frequency tripling performance conditions the feasibility of the project. Two successive KDP crystals, which can be produced in large dimensions, are used for the frequency doubling and summing operations. In order to get a high tripling rate, it is necessary to adjust the positions of the KDP crystals in the laser chain with very high accuracy, since a precision of the order of 15 μrad is required. The method consists in focusing a fundamental beam and to detect the main output angle of the second harmonic pulse (''test'' configuration), which should correspond to the optimal frequency conversion angle. However it appears that the direction of the frequency converted pulse of a fundamental Gaussian pulse depends on the distance between the waist of the fundamental pulse and the crystal. The departures for different distances far exceed the high precision level required for reaching the expected conversion performance for applications to ICF. It is, therefore, necessary to give a precise account of this unexpected phenomenon.

We assume that the fundamental pulse has Gaussian shape in the waist plane $z=0$. We denote by z_0 the distance from the waist plane to the crystal plate, and by z_c the thickness of the plate. If w_0 is the beam radius in the waist plane, A_0 is its maximal amplitude, and **e** is its unit polarization vector, then in the plane just before the plate the input field writes

$$\hat{\mathbf{E}}(z=z_0^-,k_x,k_y)=A_0\pi w_0^2\exp\left(-\frac{(k_x^2+k_y^2)w_0^2}{4}-i\frac{(k_x^2+k_y^2)z_0}{2k}\right)\mathbf{e},$$

where k is the free wave number and we have performed a Fourier transform with respect to the transverse coordinates $(x,y)\mapsto(k_x,k_y)$. By continuity of the tangential components of the electric field, the field just inside the plate is the sum of an ordinary wave and an extraordinary wave

$$\hat{E}_{o,\omega}(z=z_0^+,k_x,k_y)=A_0\pi w_0^2 e_y\exp\left(-\frac{(k_x^2+k_y^2)w_0^2}{4}-i\frac{(k_x^2+k_y^2)n_o(\omega)z_0}{2k_o(\omega)}\right),$$

$$\hat{E}_{e,\omega}(z=z_0^+,k_x,k_y)=\frac{A_0\pi w_0^2 e_x}{\cos(\beta(\omega))}\exp\left(-\frac{(k_x^2+k_y^2)w_0^2}{4}-i\frac{(k_x^2+k_y^2)n_e(\omega)z_0}{2k_e(\omega)}\right).$$

For the type I configuration we consider the case $e_x=0$, $e_y=1$. For the type II configuration we choose an equiphotonic repartition $e_x=1/\sqrt{2}$, $e_y=1/\sqrt{2}$.

A. Type I conversion

Applying Proposition 2 the system which governs the second harmonic generation in the type I configuration is:

$$\partial_z E_{o,\omega}-\frac{i}{2k_o(\omega)}\partial_x^2 E_{o,\omega}-\frac{i}{2k_o(\omega)}\partial_y^2 E_{o,\omega}=\frac{i2\omega d^{(I)}}{n_o(\omega)}E_{o,\omega}^* E_{e,2\omega}e^{i\eta_k z},$$

$$\partial_z E_{e,2\omega}-\eta\partial_x E_{e,2\omega}-\frac{ic_x(2\omega)}{2k_e(2\omega)}\partial_x^2 E_{e,2\omega}-\frac{ic_y(2\omega)}{2k_e(2\omega)}\partial_y^2 E_{e,2\omega}=\frac{i2\omega d^{(I)}}{n_e(2\omega)\cos^2\beta(2\omega)}E_{o,\omega}^2 e^{-i\eta_k z},$$

where $\eta_k=k_e(2\omega)-2k_o(\omega)$, $\eta=\tan\beta(2\omega)$, and

$$c_x(2\omega)=\frac{\chi_o(2\omega)\chi_e(2\omega)}{(\cos^2(\theta)\chi_e(2\omega)+\sin^2(\theta)\chi_o(2\omega))^2},\quad c_y(2\omega)=\frac{\chi_o(2\omega)}{\cos^2(\theta)\chi_e(2\omega)+\sin^2(\theta)\chi_o(2\omega)}.$$

We assume that the frequency conversion rate is low. Taking the Fourier transform with respect to the spatial transverse coordinates $(x,y)\mapsto(k_x,k_y)$:

$$\partial_z\hat{E}_{o,\omega}+\frac{ik_x^2}{2k_o(\omega)}\hat{E}_{o,\omega}+\frac{ik_y^2}{2k_o(\omega)}\hat{E}_{o,\omega}=0, \tag{36a}$$

$$\partial_z\hat{E}_{e,2\omega}+ik_x\eta\hat{E}_{e,2\omega}+\frac{ik_x^2c_x(2\omega)}{2k_e(2\omega)}\hat{E}_{e,2\omega}+\frac{ik_y^2c_y(2\omega)}{2k_e(2\omega)}\hat{E}_{e,2\omega}=id^I_{e,2\omega}\hat{E}_{o,\omega}*\hat{E}_{o,\omega}e^{i(2k_o-k_e)z}, \tag{36b}$$

where $*$ stands for the convolution operation. It is easy to find the explicit form of $\hat{E}_{o,\omega}$ from Eq. (36a) by a simple exponentiation, and convoluting this expression with itself

$$\hat{E}_{o,\omega}*\hat{E}_{o,\omega}(z_0+z,k_x,k_y)=\frac{A_0\pi w_0^2}{\frac{w_0^2}{2}+i\frac{n_o(\omega)z_0+z}{k_o(\omega)}}\exp-\frac{k_x^2+k_y^2}{2}\left(\frac{w_0^2}{4}+i\frac{n_o(\omega)z_0+z}{2k_o(\omega)}\right).$$

In order to compute $|\hat{E}_{e,2\omega}|$ we set:

$$\hat{E}_{e,2\omega}=\hat{E}_{e,2\omega}\exp iz\left(k_x\eta+\frac{k_x^2c_x(2\omega)}{2k_e(2\omega)}+\frac{k_y^2c_y(2\omega)}{2k_e(2\omega)}\right),$$

whose modulus is equal to the modulus of $\hat{E}_{e,2\omega}$ and which satisfies

$$\partial_z\overline{E}_{e,2\omega}=id^{II}_{e,2\omega}\hat{E}_{o,\omega}*\hat{E}_{o,\omega}\exp iz\left(k_x\eta+\frac{k_x^2c_x(2\omega)}{2k_e(2\omega)}+\frac{k_y^2c_y(2\omega)}{2k_e(2\omega)}+2k_o(\omega)-k_e(2\omega)\right).$$

The right-hand side is known, so by a simple exponentiation we get that, up to a multiplicative constant

$$|\hat{E}_{e,2\omega}|^2(z_0+z_c,k_x,k_y)=e^{-\gamma(k_x,k_y)k_ow_0^2}|E_i(-\gamma(k_x,k_y)(z_1+iz_c))-E_i(-\gamma(k_x,k_y)z_1)|^2, \tag{37}$$

where E_i is the integral exponential function: $E_i(x):=\int_1^\infty[\exp(-xt)/t]dt$ and

$$z_1=\frac{k_o(\omega)w_0^2}{2}+iz_0n_0(\omega),$$

$$\gamma(k_x,k_y)=k_x\eta+k_x^2\left(\frac{c_x(2\omega)}{2k_e(2\omega)}-\frac{1}{4k_o(\omega)}\right)+k_y^2\left(\frac{c_y(2\omega)}{2k_e(2\omega)}-\frac{1}{4k_o(\omega)}\right)+2k_o(\omega)-k_e(2\omega).$$

A study of the function (37) proves that the locations of the minima of the spectral intensity (which are experimentally detectable with high precision) do not depend on the waist distance z_0.

B. Type II conversion

We still assume that the frequency conversion rate is low. Taking the Fourier transform for the spatial transverse coordinates and applying Proposition 3, the system which governs the second harmonic generation in the type II configuration is:

$$\partial_z \hat{E}_{o,\omega} + \frac{ik_x^2}{2k_o(\omega)}\hat{E}_{o,\omega} + \frac{ik_y^2}{2k_o(\omega)}\hat{E}_{o,\omega} = 0, \tag{38a}$$

$$\partial_z \hat{E}_{e,\omega} + ik_x\eta_1\hat{E}_{e,\omega} + \frac{ik_x^2 c_x(\omega)}{2k_e(\omega)}\hat{E}_{e,\omega} + \frac{ik_y^2 c_y(\omega)}{2k_e(\omega)}\hat{E}_{e,\omega} = 0, \tag{38b}$$

$$\partial_z \hat{E}_{e,2\omega} + ik_x\eta_2\hat{E}_{e,2\omega} + \frac{ik_x^2 c_x(2\omega)}{2k_e(2\omega)}\hat{E}_{e,2\omega} + \frac{ik_y^2 c_y(2\omega)}{2k_e(2\omega)}\hat{E}_{e,2\omega} = \frac{2i\omega d^{(II)}}{n_e(2\omega)\cos^2\beta(2\omega)}\hat{E}_{o,\omega} * \hat{E}_{e,\omega}e^{-i\eta_k z}, \tag{38c}$$

where $\eta_k = k_e(2\omega) - k_e(\omega) - k_o(\omega)$, $\eta_1 = \tan\beta(\omega)$, and $\eta_2 = \tan\beta(2\omega)$. The calculations are identical to the ones performed in the type I configuration. One first compute the closed-form expressions of the fields $\hat{E}_{o,\omega}$ and $\hat{E}_{e,\omega}$ from Eqs. (38a) and (38b). These expressions are then substituted into the right-hand side of Eq. (38c) which can then be solved. We have found that, up to a multiplicative constant

$$|\hat{E}_{e,2\omega}|(2k\theta_x, 2k\theta_y) = \left| \int_0^{z_c} \frac{1}{(\bar{\alpha} + iC_x z)^{1/2}} \exp k \frac{A_x(\theta_x)z^2 + i\bar{\alpha}B_x(\theta_x)z - \bar{\alpha}^2\theta_x^2}{\bar{\alpha} + iC_x z} \times \frac{1}{(\bar{\alpha} + iC_y z)^{1/2}} \exp k \frac{A_y(\theta_y)z^2 + i\bar{\alpha}B_y(\theta_y)z - \bar{\alpha}^2\theta_y^2}{\bar{\alpha} + iC_y z} \times \exp(-i\eta_k z)\, dz \right|, \tag{39}$$

where $\bar{\alpha} = z_r + iz_0$, $z_r = kw_0^2/2$, $k = 2\pi/\lambda = \omega/c$, and

$$A_x(\theta_x) = \theta_x^2\left(\frac{c_x(\omega)}{n_o(\omega)n_e(\omega)} - \frac{c_x(2\omega)}{n_e(2\omega)}C_x\right) + \theta_x\left(\frac{\eta_1}{n_o(\omega)} - 2\eta_2 C_x\right) - \frac{\eta_1^2}{4},$$

$$B_x(\theta_x) = \theta_x^2\left(\frac{c_x(2\omega)}{n_e(2\omega)} - 2C_x\right) + \theta_x(2\eta_2 - \eta_1),$$

$$C_x = \frac{1}{2}\left(\frac{1}{n_o(\omega)} + \frac{c_x(\omega)}{n_e(\omega)}\right),$$

$$A_y(\theta_y) = \theta_y^2\left(\frac{c_y(\omega)}{n_o(\omega)n_e(\omega)} - \frac{c_y(2\omega)}{n_e(2\omega)}C_y\right),$$

$$B_y(\theta_x) = \theta_y^2\left(\frac{c_y(2\omega)}{n_e(2\omega)} - 2C_y\right),$$

$$C_y = \frac{1}{2}\left(\frac{1}{n_o(\omega)} + \frac{c_y(\omega)}{n_e(\omega)}\right).$$

In the type II configuration the positions of the minima of the spectral intensity depend on the waist distance z_0.

IX. CONCLUSION

In this paper we have derived the equations which govern the evolutions of the slowly varying envelopes of pulses in a bulk medium presenting anisotropic properties and nonlinear suscepti-

bilities. In case of phase-matching we have derived the equations that govern the frequency conversion of the source. In case of no phase matching we have derived the nonlinear Schrödinger-type equation that governs the evolution of the pulse. We have shown that the diffraction operator is anisotropic, and that the nonlinear term may be more complicated than the standard Kerr effect due to $\chi^{(2)}$-cascaded effects. We have in particular detected a configuration where stable solitons should be naturally generated since the equation then reads as the standard one-dimensional Schrödinger equation with Kerr nonlinearity. As a natural extension of this work we may also think at the propagation of partially coherent light in a linear or nonlinear anisotropic medium. Indeed the intensity profiles of the speckle spots along the propagation axis are imposed by the diffraction. So an anisotropic diffraction should involve interesting and original characteristics of the speckle spots.

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Computing the inertia operator of a rigid body

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We prove that the inertia operator A of a rigid body is generically determined, up to a scalar multiple, by the curve Ω in $\mathbf{R}^3$ that describes its angular velocity in the body. The precise condition is that Ω not be contained in a two-dimensional subspace of $\mathbf{R}^3$. We derive two indirect methods to compute A from the values of Ω over an arbitrary interval, and a direct method to compute A from the second- and fourth-order moments of Ω. The direct method utilizes moment identities derived from symmetries in Euler's equation. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In this section we review some of the kinematics and dynamics of rigid bodies as presented in Ref. 1. Consider a rigid body whose center of mass is fixed at $\mathbf{0}\in\mathbf{R}^3$, and let F be an orthonormal frame at $\mathbf{0}$ fixed relative to the body. At time t during the motion, F is an orthonormal frame $B(t)=(b_1(t),b_2(t),b_3(t))$ relative to ambient space $\mathbf{R}^3$. Suppose that $B(0)$ is the standard basis of $\mathbf{R}^3$. Identifying triples of column vectors with 3×3 matrices, $B(t)$ lies in the rotation group $SO(3)$, and $B(0)$ is the identity I. Relative to the standard basis, the position at time t of a point fixed relative to the body is then $q(t)=B(t)q(0)$, where $q(0)\in\mathbf{R}^3$ is the position at time 0. For $u\in\mathbf{R}^3$ define the skew-symmetric operator $\alpha(u):\mathbf{R}^3\to\mathbf{R}^3$ by $\alpha(u)v=u\times v$, $v\in\mathbf{R}^3$ where $\times$ is the cross product. The *angular velocity in the body* is the function $\Omega:\mathbf{R}\to\mathbf{R}^3$ defined by

$$\dot{B}=B\alpha(\Omega). \tag{1}$$

The *angular velocity in space* is $\omega=B\Omega$ and Eq. (1) implies that

$$\dot{\omega}=B\dot{\Omega}. \tag{2}$$

Inertial motion of the body is described by *Euler's equation*[2]

$$A\dot{\Omega}=(A\Omega)\times\Omega, \tag{3}$$

where A is the symmetric positive-definite 3×3 matrix that represents the inertia operator with respect to the standard basis (the inertia operator is defined from the mass distribution of the body). It follows from Eq. (1) and (3) that the *kinetic energy* $E=\frac{1}{2}\Omega^T A\Omega$ and the *angular momentum in space* $\mathbf{m}=BA\Omega$ are constant. Write $m=\|\mathbf{m}\|$. Evidently $\Omega^T A^2\Omega=m^2$, and $\omega^T\mathbf{m}=2E$. Notice that Ω is analytic, since it is bounded and its derivative is an analytic function of Ω. Suppose from now on that the rigid body is not fixed, namely q is a nonconstant function of t. Then $E,m>0$.

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There is an extensive classical literature including Refs. 2–4 that addresses the problem of computing the solution Ω of Euler's equation from A and the initial value of Ω. For the remainder of this paper we consider the inverse problem of computing A from a solution Ω. For future investigations we record the fact that Euler's equation describes uniform speed parametrized geodesics on the rotation group with a left-invariant Riemmanian metric induced by the inertia operator, and that it can be generalized to describe geodesics on Lie groups[1] and Riemannian manifolds.[5] An important objective of this paper, and one motivation for our detailed derivations of three distinct methods to compute the inertia operator, is to develop techniques for investigating more inverse problems in these more general contexts.

II. DEGENERACY

Let $\Omega : \mathbf{R} \to \mathbf{R}^3$ be a solution of Euler's equation (3). Call Ω *degenerate* when its range is contained in a two-dimensional subspace of $\mathbf{R}^3$. Otherwise Ω is *nondegenerate*. The distinction turns out to be useful in determining A from Ω in Sec. III. Euler's equation is invariant with respect to SO(3) in the sense that for any $O \in \mathrm{SO}(3)$, $\tilde{\Omega} = O\Omega$ satisfies Euler's equation where A is replaced by $\tilde{A} = OAO^T$. Evidently $\tilde{\Omega}$ is degenerate if and only if Ω is degenerate. Choose $O \in \mathrm{SO}(3)$ such that

$$OAO^T = \mathrm{diag}(I_1, I_2, I_3), \tag{4}$$

where $0 < I_1 \leqslant I_2 \leqslant I_3$ are the eigenvalues of A (Arnold lists the eigenvalues in the opposite order).

Proposition 1: The function Ω is degenerate if and only if $m^2/2E \in \{I_1, I_2, I_3\}$. If Ω is nondegenerate then $\|\dot{\Omega}\|$ is bounded below by a positive number and Ω is periodic.

Proof: It suffices to prove these assertions for $\tilde{\Omega}$. Define $\alpha_j \equiv I_j - m^2/(2E)$, $j = 1,2,3$. Since the range of $\tilde{\Omega}$ is contained in both the energy ellipsoid $\epsilon_E \equiv \{ x \in \mathbf{R}^3 : I_1 x_1^2 + I_2 x_2^2 + I_3 x_3^2 = 2E \}$ and the momentum (or co-adjoint) ellipsoid $\epsilon_m \equiv \{ x \in \mathbf{R}^3 : I_1^2 x_1^2 + I_2^2 x_2^2 + I_3^2 x_3^2 = m^2 \}$, it is contained in $\epsilon_h \equiv \{ x \in \mathbf{R}^3 : \alpha_1 I_1 x_1^2 + \alpha_2 I_2 x_2^2 + \alpha_3 I_3 x_3^2 = 0 \}$ and $I_1 \leqslant m^2/2E \leqslant I_3$. If $m^2/2E \in \{I_1, I_3\}$ then $\tilde{\Omega}$ is degenerate since it is constant. If $I_1 < m^2/2E = I_2 < I_3$ then the range of $\tilde{\Omega}$ is contained in the union $\{ x \in \mathbf{R}^3 : \sqrt{-\alpha_1 I_1}\, x_1 = \sqrt{\alpha_3 I_3}\, x_3 = 0 \} \cup \{ x \in \mathbf{R}^3 : \sqrt{-\alpha_1 I_1}\, x_1 = \sqrt{\alpha_3 I_3}\, x_3 = 0 \}$ of two two-dimensional subspaces of $\mathbf{R}^3$. Therefore, since $\tilde{\Omega}$ is analytic, its range is entirely contained in one of these two subspaces and it is degenerate (the orbits consist of two fixed points and four heteroclinic connections between them). To complete the proof, observe that if $m^2/2E \notin \{I_1, I_2, I_3\}$ then the ellipsoids ϵ_E and ϵ_m intersect transversally. Hence their intersection is diffeomorphic to the disjoint union of two circles and Euler's equation implies that $\|\dot{\Omega}\|$ is bounded below by a positive number. Furthermore, the range of $\tilde{\Omega}$ is contained in a half-space $H \subset \mathbf{R}^3$. Therefore, $\tilde{\Omega}$ is nondegenerate and periodic.

III. *A* FROM Ω: METHODS 1 AND 2

Consider the problem of determining the inertia matrix A from the solution Ω of Euler's equation (3). Clearly A is at most determined up to a positive scalar multiple. When this happens we say A is *almost-determined* by Ω.

Theorem 2: *A is almost-determined by Ω if and only if Ω is nondegenerate.*

Proof: Assume Ω is degenerate. Then there is a nonzero $v \in \mathbf{R}^3$ such that $v^T \Omega = v^T \dot{\Omega} = 0$. Define a symmetric positive definite matrix $A_v = A + vv^T$. Then Ω satisfies Eq. (3) with A replaced by A_v, and A_v is not a scalar multiple of A. This proves the only if part. To prove the if part choose any $s_2 > s_1$ and define three matrices and one vector

$$M_\Omega = \int_{s_1}^{s_2} \Omega(t)\, \Omega(t)^T\, dt, \quad M_\omega = \int_{s_1}^{s_2} \omega(t)\, \omega(t)^T\, dt,$$

$$M_{\mathbf{m}}=\int_{s_1}^{s_2}\Omega(t)\,\mathbf{m}^T B(t)\,dt, \quad u_\omega=\int_{s_1}^{s_2}\omega(t)dt.$$

Then $M_{\mathbf{m}}$ is linear in $\mathbf{m}$, and A and $\mathbf{m}$ satisfy

$$M_\Omega A=M_{\mathbf{m}}, \tag{5}$$

$$M_\omega \mathbf{m}=2E\,u_\omega. \tag{6}$$

Proposition 3: If Ω is nondegenerate then the matrices M_Ω and M_ω are nonsingular.

Proof: Suppose that M_Ω is singular and choose a nonzero vector $w\in\mathbf{R}^3$ such that $w^T M_\Omega w=0$. Then $w^T\Omega(t)\,\Omega(t)^T w=0$ for all $t\in[s_1,s_2]$, namely $\|\Omega(t)^T w\|=0$. Then $\Omega(t)$ lies in the plane V orthogonal to w for all $t\in[s_1,s_2]$ and hence for all $t\in\mathbf{R}$ since Ω is analytic, therefore Ω is degenerate. To show that M_ω is nonsingular it suffices to show that the range of ω is not contained in any two-dimensional subspace of $\mathbf{R}^3$. Assume to the contrary that the range of $\omega([s_1,s_2])$ is contained in a two-dimensional subspace V of $\mathbf{R}^3$ and hence in the line $V\cap\{x: x^T\mathbf{m}=2E\}$. By Proposition 1 $\|\dot\Omega\|=\|\dot\omega\|$ is bounded below by a positive number, thus the range of ω is unbounded. This is impossible since $\|\omega\|=\|\Omega\|$ and $\|\Omega\|$ is bounded above and the proposition is proved.

Define $C(t), t\in[s_1,s_2]$ by the nonautonomous linear differential equation $\dot C=C\alpha(\Omega)$ and initial value $C(s_1)=I$. Then $B(t)=B(s_1)C(t)$, $\omega(t)=B(s_1)C(t)\Omega(t)$, $u_\omega=B(s_1)\int_{s_1}^{s_2}C(t)\Omega(t)dt$, and Eq. (6) implies that

$$\left(\int_{s_1}^{s_2}C(t)\Omega(t)\Omega(t)^T C(t)^T dt\right)B(s_1)^T\mathbf{m}=2E\int_{s_1}^{s_2}C(t)\Omega(t)dt.$$

Proposition 3 implies that $B(s_1)^T\mathbf{m}$ is determined up to a positive scalar multiple by Ω, hence $\mathbf{m}^T B(t)$ and $M_{\mathbf{m}}$ are also determined up to a positive scalar multiple. Finally, Eq. (5) and Proposition 3 show that A is determined up to a positive scalar multiple from Ω. This proves Theorem 2 and provides a constructive method (Method 1) for almost-determining A from Ω.

Method 1 requires Ω to be observed on a continuous interval $[s_1,s_2]$, and may be difficult to apply in cases where Ω is known only on finite subsets of $[s_1,s_2]$. When sampling is coarse or noise contaminated, solving the ordinary differential equation for C is especially problematic. Notice also that Method 1 uses the associations between t and $\Omega(t)$: It is not enough to observe the image of Ω over $[s_1,s_2]$. Alternatively, we can apply Theorem 2 in a less direct way to almost-determine A as follows. Let Ω be a nondegenerate solution of Eq. (3), and let $s_2>s_1$. Denote the space of symmetric 3×3 matrices by S, and define a quadratic form $Q: S\to\mathbf{R}$ by

$$Q(D)=\int_{s_1}^{s_2}\|D\dot\Omega(t)-(D\Omega(t))\times\Omega(t)\|^2 dt, \quad D\in S.$$

Corollary 4: Q has co-rank 1 and A is a null-eigenvector of Q. So Q defines A up to a positive scalar multiple.

Proof: Clearly $A\in S$ and $Q(A)=0$. Let $D\in S$ with $Q(D)=0$. It suffices to show that there exists $\mu\in\mathbf{R}$ such that $D=\mu A$. Choose $\epsilon>0$ such that $A_\epsilon=A+\epsilon D$ is positive definite. Clearly $Q(A_\epsilon)=0$, hence Ω satisfies Eq. (3) with inertia matrix A_ϵ over the interval $[s_1,s_2]$ and thus over $\mathbf{R}$ since Ω is analytic. Theorem 2 implies that there exists $\lambda>0$ such that $A_\epsilon=\lambda A$. Therefore $D=\mu A$ where $\mu=(\lambda-1)/\epsilon$ and the corollary is proved.

The quadratic form Q is determined by values of Ω and $\dot\Omega$ over $[s_1,s_2]$, thus Corollary 4 gives another method (Method 2) to almost-determine A from Ω. We observe that (i) Q can be approximated by sampling $(\Omega,\dot\Omega)$ uniformly over $[s_1,s_2]$, (ii) the associations between t and $(\Omega(t),\dot\Omega(t))$ are not needed, (iii) when observations of $(\Omega,\dot\Omega)$ are contaminated by noise, the

effects in the formula for Q are approximately additive, and (iv) Method 2 does not require the intermediate step of solving an ODE for $C(t)$. These observations suggest that Method 2 may be more robust and practical than Method 1. However, Method 2 requires us to know $\dot{\Omega}$. It may be difficult to accurately estimate $\dot{\Omega}$ from values of Ω that are coarsely sampled or noise contaminated. These difficulties are overcome (to some degree) by using a method, based on moments of Ω (Method 3 in Sec. VIII), to almost-determine A. It turns out that moments of orders 0, 2, and 4 give most of the needed information, and it seems these quantities can be reliably estimated from uniform samples of Ω over $[s_1,s_2]$ (without regard to their time association). To simplify the discussion we assume that the moments of Ω are calculated over an entire orbit of the motion: The more general case of sampling over $[s_1,s_2]$ is a straightforward extension. Even so, the analysis is lengthy and not as clean as for Methods 1 and 2. We also note that genericity assumptions are required for Sec. VIII.

IV. MOMENTS

Let Ω be a periodic solution of Euler's equation (3), of period $T>0$.

Definition 5: Given a monomial $\mu:\mathbf{R}^3\to\mathbf{R}$ the associated moment Ω^μ is defined to be

$$\int_0^T \mu\circ\Omega(t)dt.$$

The moment Ω^μ associated with the monomial $\mu=x_{i_1}x_{i_2}\ldots x_{i_d}$ is denoted by $\Omega^{i_1i_2\cdots i_d}$. The degree d of the monomial μ is said to be the order of the moment Ω^μ.

We shall see that the moments satisfy many interesting identities involving the inertia matrix A. As before, we frequently use conservation of energy

$$E=\tfrac{1}{2}\Omega^T A\Omega \tag{7}$$

and conservation of squared length of angular momentum

$$m^2=\|A\Omega\|^2. \tag{8}$$

Assume that the eigenspaces of A are one-dimensional, namely that the I_j are distinct where $j=1,2,3$. Then any orthogonal matrix O satisfying (4) maps eigenvectors of A to nonzero multiples of standard basis elements of $\mathbf{R}^3$. Furthermore, O is *almost-unique* in the sense that, if $O'\in O(3)$ diagonalizes A then $O'=DO$, where D is a diagonal matrix whose diagonal entries are ± 1.

Let Ω be nondegenerate. Write $\alpha_j\equiv I_j-m^2/2E$. Theorem 1 says $\alpha_j\neq 0$ for $j=1,2,3$ and, because the I_j are distinct, $\alpha_1<0,\alpha_2<\alpha_3$. Moments of Ω may be called *empirical*: They can be inferred from observations of the trajectory of the rigid body. Moments of $\tilde{\Omega}\equiv O\Omega$, where $O\in \mathrm{SO}(3)$ satisfies (4), are said to be *almost-canonical* (they are not quite canonical because O is not quite unique). Empirical moments are linear combinations of almost-canonical moments (and vice versa) with coefficients polynomial in entries of O. In order to obtain identities there are some simple things we can try with almost-canonical moments. First, integration of Eqs. (7) and (8) gives

$$I_1\tilde{\Omega}^{11}+I_2\tilde{\Omega}^{22}+I_3\tilde{\Omega}^{33}=2TE, \tag{9}$$

$$I_1^2\tilde{\Omega}^{11}+I_2^2\tilde{\Omega}^{22}+I_3^2\tilde{\Omega}^{33}=Tm^2. \tag{10}$$

Solving Eqs. (9) and (10) gives

$$\tilde{\Omega}^{22}=\frac{2\alpha_3 TE-I_1(I_3-I_1)\tilde{\Omega}^{11}}{I_2(I_3-I_2)}, \tag{11}$$

$$\tilde{\Omega}^{33}=\frac{-2\alpha_2 TE+I_1(I_2-I_1)\tilde{\Omega}^{11}}{I_3(I_3-I_2)}. \tag{12}$$

From Eqs. (11) and (12) we obtain the following bounds on $\tilde{\Omega}^{11}$ in terms of E, m^2, T and the I_j:

$$\frac{2\alpha_2 TE}{I_1(I_2-I_1)}<\tilde{\Omega}^{11}<\frac{2\alpha_3 TE}{I_1(I_3-I_1)}. \tag{13}$$

This begs the question of how to calculate $\tilde{\Omega}^{11}$. This can be done by quadrature, as in Secs. V and VI, where we also consider third-order moments. Before doing that, we say some things about fourth-order moments. Multiplying Eqs. (7) and (8) by $\tilde{\Omega}_i^2$ and integrating gives

$$I_1\tilde{\Omega}^{1111}+I_2\tilde{\Omega}^{1122}+I_3\tilde{\Omega}^{1133}=2E\tilde{\Omega}^{11}, \tag{14}$$

$$I_1\tilde{\Omega}^{1122}+I_2\tilde{\Omega}^{2222}+I_3\tilde{\Omega}^{2233}=2E\tilde{\Omega}^{22}, \tag{15}$$

$$I_1\tilde{\Omega}^{1133}+I_2\tilde{\Omega}^{2233}+I_3\tilde{\Omega}^{3333}=2E\tilde{\Omega}^{33}, \tag{16}$$

$$I_1^2\tilde{\Omega}^{1111}+I_2^2\tilde{\Omega}^{1122}+I_3^2\tilde{\Omega}^{1133}=m^2\tilde{\Omega}^{11}, \tag{17}$$

$$I_1^2\tilde{\Omega}^{1122}+I_2^2\tilde{\Omega}^{2222}+I_3^2\tilde{\Omega}^{2233}=m^2\tilde{\Omega}^{22}, \tag{18}$$

$$I_1^2\tilde{\Omega}^{1133}+I_2^2\tilde{\Omega}^{2233}+I_3^2\tilde{\Omega}^{3333}=m^2\tilde{\Omega}^{33}. \tag{19}$$

The system of equations (14)–(18) has rank 5. We now need to consider the cases $\alpha_2<0$ and $\alpha_2>0$ separately.

V. THE CASE $\alpha_2<0$

Suppose $\alpha_2<0$. Then $x_3\neq 0$ for $x\in\epsilon_E\cap\epsilon_m$. Solving Eqs. (7) and (8), x lies on at least one of eight arcs $x_{\sigma_1,\sigma_2,\sigma_3}$ given parametrically by

$$x_{\sigma_1,\sigma_2,\sigma_3}(v)=\begin{bmatrix}\sigma_1\sqrt{\dfrac{I_3v^2(I_3-I_2)+2\alpha_2E}{I_1(I_2-I_1)}}\\ \sigma_2\sqrt{\dfrac{-2\alpha_1E-I_3v^2(I_3-I_1)}{I_2(I_2-I_1)}}\\ \sigma_3 v\end{bmatrix}, \quad v\in[\beta_L,\beta_U], \tag{20}$$

where $\sigma_j=\pm$, $j=1,2,3$, $\beta_L=\sqrt{-2\alpha_2E/(I_3(I_3-I_2))}$, and $\beta_U=\sqrt{-2\alpha_1E/(I_3(I_3-I_1))}$. Then $0<\beta_L<\beta_U$, and

$$x_{\sigma_1,\sigma_2,\sigma_3 1}(v)\neq 0 \quad \text{for} \quad v\in(\beta_L,\beta_U], \quad x_{\sigma_1,\sigma_2,\sigma_3 1}(\beta_L)=0, \tag{21}$$

$$x_{\sigma_1,\sigma_2,\sigma_3 2}(v)\neq 0 \quad \text{for} \quad v\in[\beta_L,\beta_U), \quad x_{\sigma_1,\sigma_2,\sigma_3 2}(\beta_U)=0, \tag{22}$$

$$x_{\sigma_1,\sigma_2,\sigma_3 3}(v)\neq 0 \quad \text{for} \quad v\in[\beta_L,\beta_U]. \tag{23}$$

Since the image C of $\tilde{\Omega}$ is diffeomorphic to a circle, C is a union of arcs. By Eq. (23) and because C is connected, σ_3 is fixed. Given σ_3, there are at most four such arcs in C, corresponding to choices of σ_1,σ_2. Inspection of Eqs. (21) and (22) show that, in order for C to be connected, all four arcs are needed: C is the track sum of

$$x_{+,+,\sigma_3}(v),\quad x_{+,-,\sigma_3}(\beta_U-\beta_L-v),\quad x_{-,-,\sigma_3}(v),\quad x_{-,+,\sigma_3}(\beta_U-\beta_L-v),$$

where $v\in[\beta_L,\beta_U]$. By Eq. (3) $I_3\dot{\tilde{\Omega}}_3(v)=-(I_2-I_1)\tilde{\Omega}_1(v)\tilde{\Omega}_2(v)\neq 0$ for $v\in(\beta_L,\beta_U)$, and so $\tilde{\Omega}^\mu=[I_3/(I_2-I_1)]\int_{\beta_L}^{\beta_U}P(v)dv$, where

$$P=\frac{\mu(x_1,x_2,x_3)+\mu(x_1,-x_2,x_3)+\mu(-x_1,-x_2,x_3)+\mu(-x_1,x_2,x_3)}{x_1x_2}$$

and $x\equiv x_{+,+,\sigma_3}(v)$. From this formula the moments $\tilde{\Omega}^\mu$ can be evaluated by quadrature. The following result follows directly from the form of P.

Proposition 6: Write $\mu=x_1^{a_1}x_2^{a_2}x_3^{a_3}$. *If* a_1 *or* a_2 *is odd then* $\tilde{\Omega}^\mu=0$. *Otherwise*

$$\tilde{\Omega}^\mu=\frac{4I_3}{I_2-I_1}\int_{\beta_L}^{\beta_U}x_1(v)^{a_1-1}x_2(v)^{a_2-1}x_3(v)^{a_3}\,dv\neq 0.$$

This result provides the following examples of zeroth-, first-, and second-order almost-canonical moment identities.

Example 7: If μ *is the monomial of degree* 0 *whose value is* 1 *everywhere then the corresponding moment is the period*

$$T=4I_3\sqrt{I_1I_2}\int_{\sqrt{-2\alpha_2E/I_3(I_3-I_2)}}^{\sqrt{-2\alpha_1E/I_3(I_3-I_1)}}\times\frac{1}{\sqrt{(2\alpha_2E+I_3v^2(I_3-I_2))(-2\alpha_1E-I_3v^2(I_3-I_1))}}\,dv.$$

Example 8: $\tilde{\Omega}^1=\tilde{\Omega}^2=0$, *and*

$$\tilde{\Omega}^3=4I_3\sqrt{I_1I_2}\,\mathrm{sign}(\tilde{\Omega}_3)\int_{\sqrt{-2\alpha_2E/I_3(I_3-I_2)}}^{\sqrt{-2\alpha_1E/I_3(I_3-I_1)}}\times\frac{v}{\sqrt{(2\alpha_2E+I_3v^2(I_3-I_2))(-2\alpha_1E-I_3v^2(I_3-I_1))}}\,dv\neq 0.$$

Example 9: $\tilde{\Omega}^{12}=\tilde{\Omega}^{23}=\tilde{\Omega}^{31}=0$, *and the* $\tilde{\Omega}^{ii}$ *are nonzero. In particular*

$$\tilde{\Omega}^{11}=\frac{4I_3}{I_2-I_1}\sqrt{\frac{I_2}{I_1}}\int_{\sqrt{-2\alpha_2E/I_3(I_3-I_2)}}^{\sqrt{-2\alpha_1E/I_3(I_3-I_1)}}\sqrt{\frac{2\alpha_2E+I_3v^2(I_3-I_2)}{-2\alpha_1E-I_3v^2(I_3-I_1)}}dv>0,$$

and the two remaining nonzero second-order almost-canonical moments can be calculated algebraically in terms of $\tilde{\Omega}^{11}$ *as in Sec. IV. Alternatively, we can calculate either* $\tilde{\Omega}^{22}$ *or* $\tilde{\Omega}^{33}$ *by quadrature and solve algebraically for the other nonzero second-order moments.*

Theorem 10: *There are ten third-order almost-canonical moments, all except three are zero, and these are given by* $(\tilde{\Omega}^{113},\tilde{\Omega}^{223},\tilde{\Omega}^{333})=\tilde{\Omega}^3Q/((I_3-I_1)(I_3-I_2))$ *where* $Q=((I_3-I_2)\alpha_3/I_1,(I_3-I_1)\alpha_3/I_2,(-I_3(\alpha_1+\alpha_2)+I_1\alpha_2+I_2\alpha_1)/I_3)$.

Proof: We multiply both sides of Eq. (7) and (8) by $\tilde{\Omega}_3$ and integrate to obtain

$$I_1\tilde{\Omega}^{113}+I_2\tilde{\Omega}^{223}+I_3\tilde{\Omega}^{333}=2E\tilde{\Omega}^3, \tag{24}$$

$$I_1^2\tilde{\Omega}^{113}+I_2^2\tilde{\Omega}^{223}+I_3^2\tilde{\Omega}^{333}=m^2\tilde{\Omega}^3. \tag{25}$$

We integrate

$$\tilde{\Omega}_1\dot{\tilde{\Omega}}_2+\dot{\tilde{\Omega}}_1\Omega_2=\frac{I_2-I_3}{I_1}\tilde{\Omega}_2^2\tilde{\Omega}_3+\frac{I_3-I_1}{I_2}\tilde{\Omega}_1^2\tilde{\Omega}_3$$

(from Euler's Equation) and use $\tilde{\Omega}(0)=\tilde{\Omega}(T)$ to obtain

$$\frac{I_2-I_3}{I_1}\tilde{\Omega}^{223}+\frac{I_3-I_1}{I_2}\tilde{\Omega}^{113}=0, \tag{26}$$

and then solve the system (24), (25), (26) to complete the proof.

Theorem 11: *There are fifteen almost-canonical fourth-order moments. All of these are zero except for* $\tilde{\Omega}^{1111},\tilde{\Omega}^{1122},\tilde{\Omega}^{1133},\tilde{\Omega}^{2222},\tilde{\Omega}^{2233},\tilde{\Omega}^{3333}$. *These are positive and they satisfy a nondegenerate system of six linear equations whose matrix coefficients are rational functions of the* I_j *and whose right-hand sides are linear separately in* E,m^2, *and the second-order almost-canonical moments* $\tilde{\Omega}^{jj}, j=1,2,3$.

Proof: We integrate

$$\tilde{\Omega}_2\tilde{\Omega}_3\dot{\tilde{\Omega}}_1+\tilde{\Omega}_3\tilde{\Omega}_1\dot{\tilde{\Omega}}_2+\tilde{\Omega}_1\tilde{\Omega}_2\dot{\tilde{\Omega}}_3=-\frac{I_3-I_2}{I_1}\tilde{\Omega}_2^2\tilde{\Omega}_3^2+\frac{I_3-I_1}{I_2}\tilde{\Omega}_1^2\tilde{\Omega}_3^2-\frac{I_2-I_1}{I_3}\tilde{\Omega}_1^2\tilde{\Omega}_2^2,$$

[from Eq. (3)] to obtain

$$-\frac{I_3-I_2}{I_1}\tilde{\Omega}^{2233}+\frac{I_3-I_1}{I_2}\tilde{\Omega}^{1133}-\frac{I_2-I_1}{I_3}\tilde{\Omega}^{1122}=0. \tag{27}$$

The proof is complete since the determinant of the coefficient matrix of the system (14), (15), (16), (17), (18), (27) equals $3I_1I_2I_3(I_2-I_1)(I_3-I_1)(I_3-I_2)$, which is positive.

Comparing Theorem 11 with Example 9 we obtain

Corollary 12: The second- and fourth-order almost-canonical moments are independent of the choice of O. *They are determined algebraically by* E,m^2,T, *the* I_j, $j=1,2,3$, *and any one of* $\tilde{\Omega}^{ii}$, $j=1,2,3$.

VI. THE CASE $\alpha_2>0$

When $\alpha_2>0$, $x_1\neq 0$ for $x\in\epsilon_E\cap\epsilon_m$, and x lies on at least one of eight arcs $x_{\sigma_1,\sigma_2,\sigma_3}$ given by

$$x_{\sigma_1,\sigma_2,\sigma_3}(v)=\begin{bmatrix}\sigma_1 v\\ \sigma_2\sqrt{\dfrac{2\alpha_3E-I_1v^2(I_3-I_1)}{I_2(I_3-I_2)}}\\ \sigma_3\sqrt{\dfrac{I_1v^2(I_2-I_1)-2\alpha_2E}{I_3(I_3-I_2)}}\end{bmatrix}, \tag{28}$$

where the $\sigma_j=\pm$. The arguments of Sec. V then adapt as follows: $v\in[\beta_L,\beta_U]$ where

$$\beta_L = \sqrt{\frac{2\alpha_2 E}{I_1(I_2 - I_1)}}, \quad \beta_U = \sqrt{\frac{2\alpha_3 E}{I_1(I_3 - I_1)}}.$$

In this case

$$x_{\sigma_1,\sigma_2,\sigma_3 1}(v) \neq 0 \quad \text{for} \quad v \in [\beta_L, \beta_U], \tag{29}$$

$$x_{\sigma_1,\sigma_2,\sigma_3 2}(v) \neq 0 \quad \text{for} \quad v \in [\beta_L, \beta_U), \quad x_{\sigma_1,\sigma_2,\sigma_3 2}(\beta_U) = 0, \tag{30}$$

$$x_{\sigma_1,\sigma_2,\sigma_3 3}(v) \neq 0 \quad \text{for} \quad v \in (\beta_L, \beta_U], \quad \text{and} \quad x_{\sigma_1,\sigma_2,\sigma_3 3}(\beta_L) = 0. \tag{31}$$

As before, the image C of $\tilde{\Omega}$ is a union of arcs, but this time σ_1 is fixed. Given σ_1, we argue as before, but using Eqs. (30) and (31), that C is parametrized by four arcs, namely the track sum of

$$x_{\sigma_1,+,+}(v), \quad x_{\sigma_1,-,+}(\beta_U - \beta_L - v), \quad x_{\sigma_1,-,-}(v), \quad x_{\sigma_1,-,+}(\beta_U - \beta_L - v),$$

where $v \in [\beta_L, \beta_U]$. By Eq. (3) $I_1 \tilde{\Omega}_1(v) = (I_3 - I_2)\tilde{\Omega}_2(v)\tilde{\Omega}_3(v) \neq 0$ for $v \in (\beta_L, \beta_L)$, and so

$$\tilde{\Omega}^\mu = \frac{I_1}{I_3 - I_2} \int_{\beta_L}^{\beta_U} P(v)\, dv,$$

where

$$P = \frac{\mu(x_1, x_2, x_3) + \mu(x_1, -x_2, x_3) + \mu(-x_1, -x_2, x_3) + \mu(-x_1, x_2, x_3)}{x_1 x_2}$$

and $x \equiv x_{\sigma_1,+,+}(v)$. The following result is analogous to Proposition (6).

Proposition 13: Write $\mu = x_1^{a_1} x_2^{a_2} x_3^{a_3}$. *If* a_2 or a_3 *is odd then* $\tilde{\Omega}^\mu = 0$. *Otherwise*

$$\tilde{\Omega}^\mu = \frac{4I_1}{I_3 - I_2} \int_{\beta_L}^{\beta_U} x_1(v)^{a_1} x_2(v)^{a_2 - 1} x_3(v)^{a_3 - 1} dv \neq 0.$$

Example 14: The moment that corresponds to the monomial of degree 0 ($which = 1$) *is the period*

$$T = 4I_1 \sqrt{I_2 I_3} \int_{\sqrt{2\alpha_2 E / I_1(I_2 - I_1)}}^{\sqrt{2\alpha_3 E / I_1(I_3 - I_1)}} \times \frac{1}{\sqrt{(-2\alpha_2 E + I_1 v^2(I_2 - I_1))(2\alpha_3 E - I_1 v^2(I_3 - I_1))}} dv.$$

Example 15: Let $\tilde{\Omega}^j$ *be the first-order moments corresponding to* x_j *where* $j = 1,2,3$. *Then* $\tilde{\Omega}^2 = \tilde{\Omega}^3 = 0$, *and* $\tilde{\Omega}^1 \neq 0$.

Example 16: Let $\tilde{\Omega}^{ij}$ *be the second-order moments corresponding to* $x_1^i x_2^j$. *Then* $\tilde{\Omega}^{12} = \tilde{\Omega}^{23} = \tilde{\Omega}^{31} = 0$, *and the* $\tilde{\Omega}^{ii}$ *are nonzero. As in Example 9, it suffices to calculate a single* $\tilde{\Omega}^{ii}$ *by quadrature. The other nonzero second-order moments are then determined algebraically.*

Example 17: Of the ten almost-canonical third-order moments, the nonzero ones are $\tilde{\Omega}^{111}, \tilde{\Omega}^{122}, \tilde{\Omega}^{133}$, *which can be calculated algebraically from* $\tilde{\Omega}^1$, E, m^2, *and the* I_j, *by imitating the proof of Theorem 10.*

Example 18: Of the fifteen almost-canonical moments of order 4, the nonvanishing ones are the same as in Theorem 11. The proofs of Theorem 11 and Corollary 12 are valid in the present case where $\alpha_2 > 0$.

VII. *G* AND NULL VECTORS: THE GENERIC CASE

Given $\overline{O} \in O(3)$ write $\overline{A} = \overline{O} A \overline{O}^T$, and $\overline{\Omega}(t) = \overline{O}\Omega(t)$. The transformations $A \mapsto \overline{A}$, $\Omega \mapsto \overline{\Omega}$ leave Eq. (3) invariant and, using $\overline{O}$, moments $\overline{\Omega}^\mu$ of $\overline{\Omega}$ can be calculated from empirical moments. Suppose $\overline{O} \in O(3)$ diagonalizes the symmetric matrix

$$E^{[2]} \equiv \begin{bmatrix} \Omega^{11} & \Omega^{12} & \Omega^{13} \\ \Omega^{12} & \Omega^{22} & \Omega^{23} \\ \Omega^{13} & \Omega^{23} & \Omega^{33} \end{bmatrix}$$

of empirical second-order moments, namely $\overline{O} E^{[2]} \overline{O}^T$ is diagonal. Suppose that the eigenvalues of $E^{[2]}$ are distinct, and let $\mathbf{e}_j$ denote the jth standard basis vector of $\mathbf{R}^3$. Examples 9 and 16 imply that $\overline{O} = \Pi O$ where $\Pi(\mathbf{e}_j) = \pm \mathbf{e}_{\pi(j)}$, $j = 1,2,3$, and π is a permutation of $\{1,2,3\}$. The eigenvalues of $E^{[2]}$ are the nonvanishing second-order almost-canonical moments $\tilde{\Omega}^{jj}$, and $\overline{A} = \mathrm{diag}(\overline{I}_1, \overline{I}_2, \overline{I}_3)$. where $\overline{I}_{\pi(j)} \equiv I_j$. Write $\overline{I} \equiv [\overline{I}_1\, \overline{I}_2\, \overline{I}_3]^T$. Equations (9), (14), (15), (16) are invariant with respect to permutations of coordinates in monomials. Substitution of Eq. (9) in the right-hand sides of (14), (15), (16) shows that $\overline{I}$ is a null-vector of $G \equiv TF^{[4]} - F^{[2]} F^{[2]T}$, where

$$F^{[4]} \equiv \begin{bmatrix} \overline{\Omega}^{1111} & \overline{\Omega}^{1122} & \overline{\Omega}^{1133} \\ \overline{\Omega}^{1122} & \overline{\Omega}^{2222} & \overline{\Omega}^{2233} \\ \overline{\Omega}^{1133} & \overline{\Omega}^{2233} & \overline{\Omega}^{3333} \end{bmatrix}, \quad F^{[2]} \equiv \begin{bmatrix} \overline{\Omega}^{11} \\ \overline{\Omega}^{22} \\ \overline{\Omega}^{33} \end{bmatrix}.$$

In the same way, with (10), (17), (18), (19) in place of (9), (14), (15), (16), $\overline{I}^{(2)} \equiv [\overline{I}_1^2\, \overline{I}_2^2\, \overline{I}_3^2]^T$ is also a null-vector of the symmetric matrix G. Because $\{\overline{I}, \overline{I}^{(2)}\}$ is linearly independent, G is either trivial or rank 1.

Theorem 19: *G has rank 1, with non-null eigenvector*

$$w \equiv \left[\frac{\overline{I}_2 - \overline{I}_3}{\overline{I}_1} \quad \frac{\overline{I}_3 - \overline{I}_1}{\overline{I}_2} \quad \frac{\overline{I}_1 - \overline{I}_2}{\overline{I}_3} \right]^T.$$

Proof: Given $v \in \mathbf{R}^3$ define $f(t) = v_1 \overline{\Omega}_1(t)^2 + v_2 \overline{\Omega}_2(t)^2 + v_3 \overline{\Omega}_3(t)^2$, where $t \in [0,T]$. Let $g: [0,T] \to \mathbf{R}$ be identically 1. Cauchy–Schwarz for $f, g \in L^2[0,T]$ says

$$(F^{[2]T} v)^2 < T v^T F^{[4]} v \tag{32}$$

unless f is a scalar multiple of g. Let v be a nonzero null-vector of G. By Eq. (32) f is constant, and by Eq. (3)

$$0 = v^T \begin{bmatrix} \overline{\Omega}_1(t) \dot{\overline{\Omega}}_1(t) \\ \overline{\Omega}_2(t) \dot{\overline{\Omega}}_2(t) \\ \overline{\Omega}_3(t) \dot{\overline{\Omega}}_3(t) \end{bmatrix} = 2 \overline{\Omega}_1(t) \overline{\Omega}_2(t) \overline{\Omega}_3(t) v^T w$$

for $t\in[0,T]$. By Eq. (20), and the corresponding equation (28) for the other case, $\overline{\Omega}_1\overline{\Omega}_2\overline{\Omega}_3 = \tilde{\Omega}_1\tilde{\Omega}_2\tilde{\Omega}_3$ vanishes for only finitely many parameter values. Therefore v is orthogonal to w. Because w is nonzero it is not a null-vector of G. However it is an eigenvector, because it is orthogonal to the null-vectors $\overline{I}, \overline{I^{(2)}}$, and G is symmetric.

Remark 20: The eigenvalue of w is

$$-R\frac{\overline{I}_3^2\overline{I}_1^2(\overline{I}_3-\overline{I}_1)^2+\overline{I}_2^2\overline{I}_3^2(\overline{I}_2-\overline{I}_3)^2+\overline{I}_1^2\overline{I}_2^2(\overline{I}_1-\overline{I}_2)^2}{3\overline{I}_1^2\overline{I}_2^2\overline{I}_3^2(\overline{I}_1-\overline{I}_2)(\overline{I}_2-\overline{I}_3)(\overline{I}_3-\overline{I}_1)}$$

where $R\equiv\overline{I}_2\overline{I}_3(\overline{I}_2-\overline{I}_3)\overline{\Omega}^{22}\overline{\Omega}^{33}+\overline{I}_3\overline{I}_1(\overline{I}_3-\overline{I}_1)\overline{\Omega}^{33}\overline{\Omega}^{11}+\overline{I}_1\overline{I}_2(\overline{I}_1-\overline{I}_2)\overline{\Omega}^{11}\overline{\Omega}^{22}$.

VIII. METHOD 3: *A* FROM MOMENTS

Let Ω be a nondegenerate solution of Eq. (3) of period $T>0$. In Sec. III A is almost-determined by the restriction of Ω to an interval $[s_1,s_2]$ of positive length. It turns out that in generic cases we can obtain a similar result using moments of Ω of order $\leqslant 4$, together with a small amount of auxiliary information. First we explain what is meant by *generic*.

Definition 21: The symmetric positive-definite matrix A is generic *when its eigenvalues* I_j *are distinct for* $j=1,2,3$. *When A is generic a solution* Ω *of Eq. (3) is* generic *provided the matrix* $E^{[2]}$ *of Sec. VII has distinct eigenvalues.*

Let Ω be generic. In Secs. VI and V we see that either Ω_3 or Ω_1 has constant sign on $[0,T]$, but not both: The *index* of Ω is defined to be 3 or 1 accordingly.

Theorem 22: *For* Ω *generic, A is almost-determined by the index of* Ω *and the moments of* Ω *of orders* 0,1,2,4.

Proof: As in Sec. VII, the matrix $E^{[2]}$ of second-order moments determines O up to conjugation with a permutation matrix Π. As in Sec. VII, the corresponding permutation of $\{1,2,3\}$ is denoted by π. Examining first-order moments with Examples 15, 8, choose π so that $\pi(\iota)=\iota$ where ι is the index of Ω. Second- and fourth-order moments determine a rank 1 symmetric matrix G. By Theorem 19 any non-null eigenvector $\hat{w}$ of G has all coordinates nonzero. Choose $\hat{w}$ so that $\hat{w}_\iota<0$. Furthermore, the permutation π of $\{1,2,3\}\backslash\{\iota\}$ is uniquely determined by the condition

$$\hat{w}_{\pi(2)}>0. \tag{33}$$

Knowing π, return to Sec. VII and rechoose $\overline{O}$ so that Π becomes a diagonal matrix with entries ± 1. Define w and choose $\hat{w}$ as before, but with the new $\overline{O}$. Then $\overline{I}_j=I_j$ for $j=1,2,3$, and w becomes

$$\left[\frac{I_2-I_3}{I_1}\ \frac{I_3-I_1}{I_2}\ \frac{I_1-I_2}{I_3}\right]^T=\sigma\hat{w}, \tag{34}$$

where $\sigma>0$. For $j=1,2$, set $v_j=\hat{w}_j/\hat{w}_3$. The v_j are determined by the index and the moments. Since $I_1<I_2<I_3$,

$$v_1>0,\ v_2<0. \tag{35}$$

Proposition 23: Suppose that $J\in\mathbf{R}^3$ *satisfies*

$$\left[\frac{J_2-J_3}{J_1}\ \frac{J_3-J_1}{J_2}\ \frac{J_1-J_2}{J_3}\right]^T=\sigma\hat{w}, \tag{36}$$

where $\sigma>0$ *is unknown, and* $J_j>0$ *for* $j=1,2,3$. *Then J is a positive scalar multiple of I.*

Proof: Since $\hat{w}_1<0,\hat{w}_2>0,\hat{w}_3<0$, we have

$$0<J_1<J_2<J_3.$$

Define $\Delta_1,\Delta_2>0$ by $J_2=(1-\Delta_2)J_3$ and $J_1=(1-\Delta_1-\Delta_2)J_3$. Then $\Delta_1+\Delta_2<1$. Substituting for the J_j in Eq. (36), and eliminating σ,

$$\frac{\Delta_2}{\Delta_1(1-\Delta_1-\Delta_2)}=v_1, \tag{37}$$

$$-\frac{\Delta_1+\Delta_2}{\Delta_1(1-\Delta_2)}=v_2. \tag{38}$$

Consider the possible solutions for $\Delta\equiv(\Delta_1,\Delta_2)$ of the simultaneous equations (37) and (38). We consider two cases.

Case 1: When $v_1+v_2\neq 0$ there are at most two possible solutions, namely

$$\Delta=\left(\frac{\sqrt{-v_1v_2(1+v_1+v_2)}}{v_1v_2},\frac{(1+v_1+v_2)v_2-\sqrt{-v_1v_2(1+v_1+v_2)}}{(v_1+v_2)v_2}\right), \tag{39}$$

and

$$\Delta=\left(-\frac{\sqrt{-v_1v_2(1+v_1+v_2)}}{v_1v_2},\frac{(1+v_1+v_2)v_2+\sqrt{-v_1v_2(1+v_1+v_2)}}{(v_1+v_2)v_2}\right). \tag{40}$$

Since Eqs. (35) and (39) imply that $\Delta_1<0$, hence Eq. (40) is the only possible solution.

Case 2: When $v_1+v_2=0$ there is at most one solution, namely

$$\Delta=\left(\frac{1}{v_1},\frac{v_1-1}{2v_1}\right).$$

In both cases there is at most one solution Δ (corresponding to $J=I$). This proves the proposition.

Proposition 23 implies that Eq. (34) determines $[I_1\,I_2\,I_3]$ up to positive scalar multiple. Since O is determined up to multiplication by a scalar matrix with entries ± 1, A is almost-determined. This completes the proof of Theorem 22 and provides Method 3, for almost-determining A from qualitative information about Ω (the index) and moments of Ω of orders 0,1,2,4.

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Systems of reaction diffusion equations and their symmetry properties

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A constructive algorithm is proposed for the investigation of symmetries of partial differential equations. The algorithm is used to present classical Lie symmetries of systems of two nonlinear reaction diffusion equations. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1331318]

I. INTRODUCTION

Mathematical models which ultimately involve the analysis of coupled systems of nonlinear diffusion equations are often discussed in the literature. The Schrödinger equation in m-dimensional space is an obvious example from mathematical physics while activator-inhibitor reactions,[1] predator-prey systems, and $\lambda-\omega$ reaction systems[2] are common examples from mathematical biology. These systems are very complex in nature and admit fundamental particular solutions (for example, traveling waves and spiral waves) which have a clear group-theoretical interpretation and which can be obtained using the classical Lie approach. The existence of such solutions suggests an important role for both the classical and nonclassical symmetry analysis of systems of reaction diffusion equations. However, to the best of our knowledge, a comprehensive group analysis has not been undertaken previously although analyses of some special cases do exist.

In this article we discuss symmetries of equations in the general form

$$\frac{\partial u}{\partial t}-A\sum_i \frac{\partial^2 u}{\partial x_i^2}-f(u)=0, \tag{1}$$

where $u\in\mathbb{R}^n$, $f\in\mathbb{R}^n$, $(x,t)\in\mathbb{R}^m\times\mathbb{R}$ and A is a $n\times n$ constant non singular matrix. Actually we restrict ourselves to the case $n=2$ but all results present in Sec. II and the main part of results of Sec. III are valid for arbitrary n.

We note that Eq. (1) with $m=n=1$, $f\equiv 0$ was the subject of a group analysis by Sophus Lie.[3] In addition, classical Lie symmetries of Eq. (1), with $n=m=1$, were investigated by Ovsiannikov[4] whose results were completed by Dorodnitsyn[5] and then generalized to the case $m=2,3$ by Dorodnitsyn, Kniazeva and Svirishchevski.[6] The related conditional (nonclassical) symmetries were described by Fushchych and Serov[7] and Clarkson and Mansfield.[8] The classical symmetries are summarized in Table I.

Here Greek letters denote arbitrary parameters and are the translation, X_0; Galilei, G_α $(\alpha=0,1)$; scale, $\hat{D}_\mu$ $(\mu=0,1,\ldots,4)$ and conformal, $\hat{A}_s$ $(\sigma=0,1,2)$ generators respectively, where

$$X_0=\alpha\frac{\partial}{\partial t}+\beta\frac{\partial}{\partial x},\quad G_\alpha=t\frac{\partial}{\partial x}-\frac{1}{2}xu\frac{\partial}{\partial u}+\frac{1}{2}\delta_{\alpha 1}tx\frac{\partial}{\partial u},\quad \hat{D}_0=2t\frac{\partial}{\partial t}+x\frac{\partial}{\partial x},$$

TABLE I. Symmetries of the scalar diffusion equation with source

$f(u)$	Infinitesimals generator, X
arbitrary	X_0
0	$X_0+\nu G_0+\mu\hat{D}_0+\lambda\hat{A}_0+\sigma u\frac{\partial}{\partial u}+\psi_0\frac{\partial}{\partial u}$
1	$X_0+\nu G_1+\mu\hat{D}_1+\lambda\hat{A}_1+\sigma(u-t)\frac{\partial}{\partial u}+\psi_0\frac{\partial}{\partial u}$
u	$X_0+\nu G_0+\mu\hat{D}_2+\alpha\hat{A}_2+\sigma u\frac{\partial}{\partial u}+\psi_1\frac{\partial}{\partial u}$
$u^n,\ n\neq 1$	$X_0+\mu\hat{D}_3$
e^u	$X_0+\mu\hat{D}_4$
$f=u\ln u$	$X_0+\nu e^t\left(\frac{\partial}{\partial x}-\frac{1}{2}xu\frac{\partial}{\partial u}\right)+\mu e^t u\frac{\partial}{\partial u}$

$$\hat{D}_1=\hat{D}_0+2t\frac{\partial}{\partial u},\quad \hat{D}_2=\hat{D}_0+2tu\frac{\partial}{\partial u},\quad \hat{D}_3=\hat{D}_0-\frac{2}{n-1}u\frac{\partial}{\partial u},\tag{2}$$

$$\hat{D}_4=D_0-2\frac{\partial}{\partial u},\quad \hat{A}_\mu=\frac{1}{2}t\hat{D}_\mu-\frac{1}{4}(x^2+2t)(1-\delta_{\mu 1}t)u\frac{\partial}{\partial u}.$$

In addition, $\delta_{\mu\nu}$ is the Kronecker symbol and $\psi_n(n=0,1)$ is an arbitrary solution of the linear diffusion equation $(\partial/\partial t-\partial^2/\partial x^2)\psi_n=n\psi_n$.

A systematic investigation of the symmetries of the general Eq. (1) with $m>1$ and $n>1$ has so far not been considered in detail, although partial results are available in Refs. 2 and 9–11. In a recent paper[12] Lie symmetries of a subclass of systems (1) for $n=2$ and arbitrary m were investigated. In this subclass the matrix A was diagonal but not a multiple of the unit matrix. We shall demonstrate that the results[12] are incomplete.

It is the aim here to undertake such an investigation for the most general case of an *arbitrary* 2×2 matrix A. In this way we present a complete description of Lie symmetries of all possible systems (1) including the cases of the unit matrix A. This latter case corresponds to the most rich of symmetries with many interesting applications. In particular, we find all nonlinear Schrödinger equations admitting nontrivial Lie symmetries since these equations can also be represented in the form (1) with an *antidiagonal* matrix A, as is demonstrated in Sec. VII. Moreover, we find new symmetries of (1) also in the subclass studied in Ref. 12.

The additional main aim of this article is to present the novel use of a rather conventional algorithm for investigation of symmetries of a special class of partial differential equations which includes (1) as a particular case. More precisely we will show that the classical Lie approach (refer to, for example, Refs. 13 and 11) when applied to systems (1) admits a rather simple formulation in terms of commutator algebra which may also be applied to extended classes of partial differential equations. Furthermore, the algorithm may be used to determine nonclassical (or conditional) symmetries of (1). It will be shown that for $n>1$ there is a proliferation of symmetries, including for the case when $f(u)$ is linear, which do not have origins in symmetries of Table I for the one dimensional scalar diffusion equation with source.

II. AN ALGORITHM FOR THE DETERMINING EQUATIONS OF SYMMETRY FOR THE SYSTEM (1)

We require form invariance of the system of reaction diffusion equations (1) with respect to the one-parameter group of transformations:

$$t\to t'(t,x,\varepsilon),\quad x\to x'(t,x,\varepsilon),\quad u\to u'(t',x',\varepsilon),\tag{3}$$

where ε is a group parameter. In other words, we require that $u'(t',x',\varepsilon)$ satisfies the same equation as $u(t,x)$:

$$L'u'=f(u'), \quad L'=\frac{\partial}{\partial t'}-A\sum_i \frac{\partial_i^2}{\partial x_i'^2}. \tag{4}$$

From the infinitesimal transformations,

$$\begin{gathered} t\to t'=t+\Delta t=t+\varepsilon\eta, \quad x_a\to x_a'=x_a+\Delta x_a=x_a+\varepsilon\xi^a, \\ u_a\to u_a'=u_a+\Delta u_a=u_a+\varepsilon\pi_a, \end{gathered} \tag{5}$$

we obtain the following representation for the operator L':

$$L'=\left[1+\varepsilon\left(\eta\frac{\partial}{\partial t}+\xi^a\frac{\partial}{\partial x_a}\right)\right]L\left[1-\varepsilon\left(\eta\frac{\partial}{\partial t}+\xi^a\frac{\partial}{\partial x_a}\right)\right]+O(\varepsilon^2). \tag{6}$$

Using the classical Lie algorithm it is possible to find the determining equations for the functions η,ξ_a and π_a which specify the generator X of the symmetry group:

$$X=\eta\frac{\partial}{\partial t}+\xi^a\frac{\partial}{\partial x_a}-\pi^b\frac{\partial}{\partial u_b}, \tag{7}$$

where a summation from 1 to m and from 1 to n is assumed over repeated indices a and b, respectively. This system will not be reproduced here, but we note that three of the equations are

$$\frac{\partial\eta}{\partial u_a}=0, \quad \frac{\partial\xi^a}{\partial u_b}=0, \quad \frac{\partial^2\pi^a}{\partial u_c\partial u_b}=0. \tag{8}$$

So from (8) η and ξ^a are functions of t and x_a and π^a is linear in u_a. Thus,

$$\pi^a=-\pi^{ab}u_b-\omega^a, \tag{9}$$

where π^{ab} and ω^a are functions of t and $x=(x_1,x_2,\ldots,x_m)$.

From (4) it is possible to deduce all the remaining determining equations. Indeed, substituting (5), and (9) into (6), using (1), and neglecting the terms of order ε^2 we find that

$$[Q,L]u-L\omega=\pi f+\frac{\partial f}{\partial u_a}(-\pi^{ab}u_b-\omega^a), \quad Q=\eta\frac{\partial}{\partial t}+\xi^a\frac{\partial}{\partial x_a}+\pi \tag{10}$$

and π is a matrix whose elements π^{ab} are defined by the relation (9).

To guarantee that Eq. (10) is compatible with (1) and does not impose new nontrivial conditions for u in addition to (1) it is necessary to suppose that the commutator $[Q,L]$ admits the representation

$$[Q,L]=\Lambda L+\varphi(t,x), \tag{11}$$

where Λ and φ are $n\times n$ matrices dependent on (t,x_a).

Substituting (11) into (10) the following determining equations for f are obtained:

$$(\Lambda^{kb}-\pi^{kb})f^b+\varphi^{kb}u^b-(L\omega)^k=-(\omega^a+\pi^{ab}u_b)\frac{\partial f^k}{\partial u^a}. \tag{12}$$

Thus, to find all nonlinearities f^k generating Lie symmetries for Eq. (1) it is necessary to solve the operator equation (11) for L, Q given in (4) and (10) and to determine the corresponding

matrices Λ, π, φ and functions η and ξ. In the second step the nonlinearities f^a may be found by solving the system of first-order equations (12) with their known coefficients.

Equation (11) is a straightforward generalization of the invariance condition for the *linear* system of diffusion equations (1) with $f(u)=0$, so that $[Q,L]=\Lambda L$, which may readily be solved. By means of this ''linearization'' the problem of investigating symmetries of systems of nonlinear diffusion equations is reduced to the rather simple application of elements of matrix calculus in order to classify nonequivalent solutions of the determining equations.

We notice that this approach is valid for the extended class of equations $Lu=f(u)$ where L is a linear differential operator with constant coefficients and where $u\in\mathbb{R}^n$. We note also that calculations of the nonclassical (conditional) symmetries for the system (1) may be reduced to the solution of the determining equations (12) where now Λ, π, φ, η and ξ are defined as solutions of the following relationship,

$$[Q,L]=\Lambda L+\varphi(t,x)+\mu(t,x)Q, \tag{13}$$

and where $\mu(t,x)$ is an unknown function of the independent variables.

III. THE SYMMETRY OPERATORS AND THEIR SIMPLIFICATION

We now determine the general solutions for matrices Λ, φ, π and also the functions ξ, η, π which satisfy (12) and (11).

Evaluating the commutator in (11) and equating the coefficients for linearly independent differential operators we obtain the five determining equations:

$$2A\xi^a_b=-\delta_{ab}(\Lambda A+[A,\pi]),\quad \dot\eta_a=0,\quad \dot\eta=\Lambda, \tag{14}$$

$$\dot\xi^a-2A\pi_a-A\xi^a_{nn}=0,\quad \varphi=A\pi_{nn}-\dot\pi. \tag{15}$$

Here the dots denote derivatives with respect to t and subscripts denote derivatives with respect to the spatial variables, so, for example, $\eta_a=\partial\eta/\partial x_a$.

From (14) Λ is proportional to the unit matrix, $\Lambda=\lambda I$ and from (14) $[A,\pi]=0$. Indeed, choosing $a=b$ we obtain

$$\pi-A^{-1}\pi A=(2\xi^a_a-\lambda)I. \tag{16}$$

The trace of the left hand side of (16) is equal to zero, and so $2\xi^a_a-\lambda\equiv 0$ and $A\pi-\pi A=0$.

Equations (14) and (15) contain matrices which commute, and so they may easily be integrated using, for example, the method of characteristics. The general solution of (14) and (15) is

$$\xi^a=C^{[ab]}x_b+\dot d x^a+g^a,\quad \eta=-2d,$$

$$\pi=\frac{1}{2}A^{-1}\left(\frac{\ddot d}{2}x^2+\dot g^a x^a\right)+C,\quad \Lambda=-2\dot d I, \tag{17}$$

$$\varphi=\frac{m}{2}\ddot d-\dot C-\frac{1}{2}A^{-1}\left(\frac{\dddot d}{2}x^2+\ddot g^a x^a\right),$$

where d and g^a are arbitrary functions of t and C is a t-dependent matrix commuting with A.

By considering the x dependence of functions (17) it is convenient to represent still unknown functions ω_a, occurring in (12), as

$$\omega_a=\omega^a_2x^2+\omega^{ab}_1x_b+\omega^a_0+\mu^a, \tag{18}$$

where $\omega_2^a, \omega_1^{ab}, \omega_0^a$ are functions of t, and μ^a is a function of t and x. Without loss of generality we suppose that all terms on the right hand side of (18) are linearly independent. Then comparing with (12) and (17) the functions μ^k have to satisfy

$$(L\mu)^k = \lambda^{kb}\mu^b + \xi_0^k + \xi_1^{kb}x_b + \xi_2^k x^2, \tag{19}$$

where λ^{kb} are constants and $\xi_0^k, \xi_1^{kb}, \xi_2^k$ are functions of t.

The final step is to substitute (17) and (19) into (12) and equate coefficients for all different powers of x_a. As a result we obtain the system of equations

$$\ddot{d}(A^{-1})^{kb}f^b + \dddot{d}(A^{-1})^{kb}u^b - \ddot{d}(A^{-1})^{ab}u^b\frac{\partial f^k}{\partial u^a} = 4\left(\dot{\omega}_2^k + \xi_2^k - \omega_2^b\frac{\partial f^k}{\partial u_b}\right), \tag{20}$$

$$\dot{g}^a(A^{-1})^{kb}f^b + \ddot{g}^a(A^{-1})^{kb}u^b - \dot{g}^a(A^{-1})^{kb}u^b\frac{\partial f^k}{\partial u^a} = 2\left(\dot{\omega}_1^{ka} + \xi_1^{ka} - \omega_1^{ba}\frac{\partial f^k}{\partial u_a}\right), \tag{21}$$

$$2\dot{d}f^k - C^{kb}f^b - \left(\dot{C}^{kb} + \frac{m}{2}\ddot{d}\,\delta^{kb}\right)u^b + (\omega_0^a + C^{ab}u^b)\frac{\partial f^k}{\partial u_a} = \dot{\omega}_0^k - 2mA^{kb}\omega_2^b + \xi_0^k, \tag{22}$$

$$\frac{\partial f^k}{\partial u_b}\mu^b = \lambda^{kb}\mu^b. \tag{23}$$

Thus, the general form of symmetry group generators for Eq. (1) is given by relations (7), (17), and (18) where $d, g^a, C^{ab}, \omega_0^k, \omega_1^{kb}, \omega_2^a, \mu^a$ are functions of t to be specified using Eqs. (20)–(23). These results are valid for Eq. (1) with arbitrary $n\times n$ constant nonsingular matrix A.

In the following we restrict ourselves to the case of 2×2 matrix A. The related Eq. (1) is reduced to the form

$$\begin{aligned}
&\frac{\partial}{\partial t}u_1 - \sum_i \frac{\partial^2}{\partial x_i^2}(A^{11}u_1 + A^{12}u_2) = f^1,\\
&\frac{\partial}{\partial t}u_2 - \sum_i \frac{\partial^2}{\partial x_i^2}(A^{21}u_1 + A^{22}u_2) = f^2,
\end{aligned} \tag{24}$$

where A^{11}, A^{12}, A^{21} and A^{22} are elements of matrix A, and f^1 and f^2 are functions of u_1, u_2 to be specified.

First we present all nonequivalent matrices A which have to be considered in the analysis. The *ad hoc* nonequivalent versions of Eq. (24) correspond to the following matrices A:

$$\text{(Ia) } A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \text{(Ib) } A = \begin{pmatrix} 1 & 0 \\ 0 & a \end{pmatrix}; \quad \text{(II) } A = \begin{pmatrix} b & -c \\ c & b \end{pmatrix}; \quad \text{(III) } A = \begin{pmatrix} 1 & 0 \\ e & 1 \end{pmatrix}, \tag{25}$$

where a, b, c and e are arbitrary parameters, $a \neq 0,1$. All 2×2 matrices can be reduced to one of the forms (25) using linear and scale transformations of the dependent variables. Moreover, without loss of generality it is possible to set $c=1$ and $e=1$.

The analysis of symmetries of systems of nonlinear diffusion equations present in Ref. 12 was restricted to the case when matrix A had the form Ib. We consider here the most general case, that is, all possible forms of the matrix A given by relations (25). We present now an outline of the approach used to solve the system (20)–(23)and begin by noticing the following.

(i) Except for the functions μ_a depending on t, x and the constant matrix A^{-1}, all quantities in the determining equations belong to one of two classes. Either the quantities depend on u

but are independent of t, or, alternatively, the quantities depend on t but are independent of u. This enables us to separate variables and so decouple the equations.

(ii) To simplify calculations it is convenient to use the equivalence transformations

$$u^a \to (u')^a = \lambda^{ab} u^b + \sigma^a, \quad f^a \to (f')^a = \lambda^{ab} f^b, \tag{26}$$

where λ^{ab} is an invertable constant matrix and σ^a are constants. Such transformations leave Eq. (1) form invariant and so make it possible to reduce A^{-1} (and other matrices used in the analysis) to canonical forms (25).

(iii) Many solutions of (20)–(23) are such that f is linear in u. Such possibilities are considered separately.

An important *a priori* simplification of the determining equations can be obtained by considering the compatibility of (20)–(23).

Lemma 1: Let Eqs. (20) and (22) be compatible and f^k be nonlinear in u. Then, up to equivalence transformations (26), the functions d and ω_2^k have to satisfy one of the following relations:

$$\dddot{d} = 0, \quad \omega_2^1 = 0, \quad \dot{\omega}_2^k = \mu \omega_2^k - \xi_2^k + \mu \ddot{d}, \quad \text{or} \quad \dddot{d} = \mu \ddot{d}, \quad \omega_2^1 = \omega_2^2 = 0, \tag{27}$$

where $\mu \neq 0$, ν_1 and ν_2 are constants, at least one of constants ν_α is nonzero, and nontrivial ω_2^k are linearly independent of $\ddot{d}$.

The proof of Lemma 1 depends on the analysis of the consequences of differentiating Eq. (20) first, with respect to u_c, and then with respect to u_a, and further considering the conditions for consistency of the resulting system. Details of this analysis are straightforward and are omitted here.

An analogous result with a similar proof is valid for Eq. (21) which generates the following restrictions:

$$\ddot{g}_a = 0, \quad \omega_1^{1b} = 0, \quad \dot{\omega}_1^{2b} = \nu \omega_1^{2b} - \xi_1^{2b}, \quad \text{or} \quad \ddot{g}_a = \nu \dot{g}_a, \quad \omega_1^{1b} = \omega_1^{2b} = 0. \tag{28}$$

These conditions are compatible with (20) and (21) only when

$$\dot{d} = d_3 t + d_4, \quad g^a = g_3^a t + g_4^a, \quad \omega_1^{2b} = \nu^b \omega_2^2, \tag{29}$$

$$\dot{d} = d_1 \exp(\nu t) + d_2, \quad g^a = g_1^a \exp(\nu t) + g_2^a, \quad \omega_1^{2b} = \nu^b \omega_2^2, \tag{30}$$

where ν, ν^a, g_k^a, d_k, $k = 1,...,4$, are constant.

Let μ^α be trivial. Then substituting these into (20)–(22) we find that

$$(A^{-1})^{kb} f_b = (A^{-1})^{ab} u_b \frac{\partial f^k}{\partial u^a}, \quad d_3 \neq 0 \quad \text{or/and} \quad g_3^a \neq 0, \tag{31}$$

$$[-2(d_3 t + d_4)\delta^{kb} + C^{kb}] f^b + \left(\frac{m}{2} d_3 \delta_{kb} + \dot{C}^{kb} \right) u^b = \dot{\omega}_0^k - 2mA^{k2} \omega_2^2 - (\omega_0^a - C^{ab} u^b) \frac{\partial f^k}{\partial u^a}, \tag{32}$$

$$\omega_2^2 \left(\mu \delta_{k2} - \frac{\partial f^k}{\partial u_2} \right) = 0, \tag{33}$$

or alternatively, the system which includes (33) and the two following equations,

$$(A^{-1})^{kb} (f^b + \mu u^b) = (A^{-1})^{ab} u_b \frac{\partial f^k}{\partial u^a}, \quad \mu \neq 0, \quad d_1 \neq 0 \quad \text{or} \quad g_1 \neq 0, \tag{34}$$

$$[(2d_1\exp(\mu t)+d_2)\,\delta^{kb}+C^{kb}]f^b+\left(\frac{1}{2}\mu d_1\exp(\nu t)\,\delta^{kb}+\dot{C}^{kb}\right)u^b$$

$$=\dot{\omega}_0^k-2A^{k2}\omega_2^2-(\omega_0^a-C^{ab}u_b)\frac{\partial f^k}{\partial u^a}. \tag{35}$$

Thus, the investigation of symmetries for systems of diffusion equations depends on solving the determining equations (31)–(33) and (34), (35), (33). These include arbitrary parameters d_k, and μ, arbitrary functions of t, i.e., ω_0^a,ω_2^a, and an arbitrary matrix C^{ab} which commutes with A and also depends on t. The form of C is given as follows.

Lemma 2: A necessary condition of compatibility of system (31)–(33) is that the matrix function C^{ab} has the form

$$C^{ab}=\phi_0F^{ab}+\phi_1B^{ab}+\nu(\delta^{ab}-F^{ab}) \tag{36}$$

where F^{ab}, B^{ab} are constants and ϕ_0, ϕ_1 are functions of t satisfying the conditions

$$F^{ak}B^{kb}-B^{ak}F^{kb}=\alpha B^{ab}+\beta F^{ab},$$
$$\dot{\phi}_0=k_0\phi_0+k_1\phi_1+k_2,\quad \dot{\phi}_1=n_0\phi_0+n_1\phi_1+n_2. \tag{37}$$

Here α, β, ν, k_0, k_1, k_2, n_0, n_1 and n_2 are arbitrary constants.

Proof is straightforward but rather cumbersome, so we present its sketch only.

An arbitrary 2×2 matrix C whose elements are C^{ab} can be expanded as

$$C=C_0I+C_1\sigma_1+C_2\sigma_2+C_3\sigma_3, \tag{38}$$

where

$$I=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0&-1\\1&0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}, \tag{39}$$

and C_0, C_1, C_2 and C_3 are functions of t. Let k $(1\leqslant k\leqslant 4)$ of these functions be linearly independent. Then equating in (32) the coefficients for these functions we obtain k systems of equations for f^a.

Considering the case $k=4$ it is possible to convince ourselves that the related overdetermined systems are incompatible. For $k=3$ the compatibility condition for (32) reduces to the form (36). Then equating coefficients for independent functions ϕ_0 and ϕ_1 in (32) we come to systems of equations for f^a, which are compatible provided relations (36) and (37) are satisfied.

Substituting (27) and (28) into (32) we obtain

$$\phi_0\left[F^{kb}(f^b+k_0u^b)-F^{ab}u_b\frac{\partial f^k}{\partial u_a}+n_0B^{kb}u^b\right]+\phi_1\left[B^{kb}(f^b+n_1u^b)-B^{ab}u_b\frac{\partial f^k}{\partial u^a}+k_1F^{kb}u^b\right]$$
$$+\nu\left[(\delta^{kb}-F^{kb})F^b-(\delta^{ab}-F^{ab})u_b\frac{\partial f^k}{\partial u_a}\right]+(n_2F^{kb}+k_2B^{ab})u_b-2(d_3t+d_4)f^k+\frac{1}{2}d_3u^k$$
$$=-\dot{\omega}_0^k+2m\,\delta_{k2}A^{k2}\omega_2^2+2\omega_0^a\frac{\partial f^k}{\partial u^a}. \tag{40}$$

This equation has to be imposed together with (31) provided $g_3^a\neq0$ or $d_3\neq0$. Moreover, different combinations of values of these parameters correspond to different systems of determining equations. We specify the following five cases:

$$d_3=0,\quad g_3^a=0,\quad \phi_0\not\equiv0,\quad \omega_2^2=\omega_1^{2b}=0,\quad \omega_0^a=\text{const},\quad n_2=k_2=0,$$

$$d_3=0,\quad g_3^a=0,\quad \phi_0\equiv 0,\quad \omega_2^2=\omega_1^{2b}=0,\quad \omega_0^a=\text{const},\quad n_2=k_2=0,$$

$$d_3=0,\quad g_3^a\neq 0,\quad \omega_2^2=\omega_1^{2b}=0,\quad \omega_0^a=\text{const},$$

$$d_3\neq 0,\quad \omega_2^2=\omega_1^{2b}=0,\quad \omega_0^a=\text{const},$$

$$\omega_2^2\neq 0,\quad \omega_1^{2b}\neq 0.$$

In this way the system of equations (31)–(33) may be solved explicitly using the method of characteristics to determine f^k and their corresponding symmetries. A similar approach can be used for the alternative system (34) and (35) and for the case when μ^α are not trivial. In the last case very strong restrictions are imposed on f^k by relation (23) which has only few solutions.

IV. NON-LINEARITIES AND SYMMETRIES

We will not give the detailed calculations but present the general solution of relations (20)–(23). In the following tables we present the results of the symmetry analysis for the case where f^k is nonlinear in u.

First we present the list of nonlinearities of the most general form which are defined up to arbitrary functions (Table II). To make this we specify matrices B which commute with A (25) according to the following categories:

$$\begin{aligned}
&\text{(I) } B=\begin{pmatrix}1&0\\0&d\end{pmatrix},\quad A^{-1}=\begin{pmatrix}1&0\\0&a^{-1}\end{pmatrix}\ \text{if}\ a\neq 1;A^{-1}\ \text{is arbitrary if}\ a=1;\\
&\text{(II) } B=\begin{pmatrix}d&-1\\1&d\end{pmatrix},\quad A^{-1}=\frac{1}{b^2+c^2}\begin{pmatrix}b&c\\-c&b\end{pmatrix},\\
&\text{(IIIa) } B=\begin{pmatrix}0&0\\1&0\end{pmatrix},\quad A^{-1}=\begin{pmatrix}1&0\\-c&1\end{pmatrix},\\
&\text{(IIIb) } B=\begin{pmatrix}1&0\\1&1\end{pmatrix},\quad A^{-1}=\begin{pmatrix}1&0\\-e&1\end{pmatrix}.
\end{aligned}\tag{41}$$

Here $R=\sqrt{u_1^2+u_2^2},\theta=\arctan(u_2/u_1)$, the Greek letters in the right column of Table II denote arbitrary coefficients while D_μ, G_a^i and $\overline{G_a^i}, X_A, Y_a, \hat{B}$ are various types of dilatation, Galilei and special transformation generators as follows:

$$\begin{aligned}
&D_0=2t\frac{\partial}{\partial t}+x_a\frac{\partial}{\partial x_a},\quad D_1=D_0-\frac{2}{k}\hat{B},\quad D_2=D_0+\frac{2}{k}\left(\frac{\partial}{\partial u_2}+nu_1\frac{\partial}{\partial u_1}\right),\\
&D_3=D_0-\frac{2}{k}\left(\frac{\partial}{\partial u_1}-nu_1\frac{\partial}{\partial u_2}\right),\quad D_4=D_0-\frac{2}{k}\omega_a\frac{\partial}{\partial u_a},\\
&G_a=t\frac{\partial}{\partial x_a}-\frac{1}{2}x_a(A^{-1})^{nb}u_b\frac{\partial}{\partial u_n},\quad \hat{G}_a=e^{nt}\left(\frac{\partial}{\partial x_a}-\frac{1}{2}nx_a(A^{-1})^{nb}u_b\frac{\partial}{\partial u_n}\right),\\
&X_0=\alpha\frac{\partial}{\partial t}+\beta_a\frac{\partial}{\partial x_a}+\nu^{[a,b]}x_a\frac{\partial}{\partial x_b},\quad \nu^{[a,b]}=-\nu^{[b,a]},\\
&Y_1=ntu_1\frac{\partial}{\partial u_2}+u_2\frac{\partial}{\partial u_2},\quad Y_2=u_1\frac{\partial}{\partial u_1}+n\frac{\partial}{\partial u_2},\quad Y_3=e^{st}\left(u_1\frac{\partial}{\partial u_1}+n\frac{\partial}{\partial u_2}\right),
\end{aligned}\tag{42}$$

TABLE II. Nonlinearities with arbitrary functions.

No.	Nonlinear terms	Type of matrix B (41)	Arguments of φ_1, φ_2	Conditions for parameters	Symmetries, Z_N for $A^{-1}\neq\kappa B$ and Z_E for $A^{-1}=\kappa B$
1	$f^1=u_1^{k+1}\varphi_1$, $f^2=u_1^{k+d}\varphi_2$	I	u_2/u_1^d	$k\neq 0$	$Z_N=Z_E$ $=X_0+\nu D_1$
				$k=0$, $d\neq 0$	$Z_N=X_0+\lambda\hat{B}$, $Z_E=Z_N+\sigma_a G_a$
				$k=d=0$, $\varphi_1\neq$ const	$Z_N=X_0+\alpha u_1\dfrac{\partial}{\partial u_1}$
				$k=d=0$, $\varphi_1=n=$ const	$Z_N=X_0$ $+\alpha u_1\dfrac{\partial}{\partial u_1}+\tilde{\psi}_n\dfrac{\partial}{\partial u_1}$
2	$f^1=e^{k\theta}(\varphi_1 u_2+\varphi_2 u_1)$, $f^2=e^{k\theta}(\varphi_2 u_{2-}\varphi_1 u_1)$	II	$Re^{-d\theta}$	$k\neq 0$	$Z_N=Z_E$ $=X_0+\nu D_1$
3	$f^1=\varphi_1 u_1^{k+1}$, $f^2=(\varphi_1\ln u_1+\varphi_2)u_1^{k+1}$	IIIb	$u_1 e^{-u_2/u_1}$	$k\neq 0$	$Z_N=Z_E$ $=X_0+\nu D_1$
4	$f^1=e^{k(u_2/u_1)}\varphi_1 u_1$, $f^2=e^{k(u_2/u_1)}(\varphi_1 u_2+\varphi_2)$	IIIa	u_1	$k\neq 0$	$Z_N=X_0+\nu D_1$
5	$f^1=u_1(n\ln u_1+\varphi_1)$, $f^2=u_2(n\ln u_2+\varphi_2)$	I	u_2/u_1^d	$n\neq 0$	$Z_N=X_0+\mu e^{nt}\hat{B}$, $Z_E=Z_N+\nu_a\hat{G}_a$
6	$f^1=\varphi_1 u_2+\varphi_2 u_1$ $+\dfrac{n}{2}\left(\dfrac{1}{d}\ln R+\theta\right)(du_1-u_2)$, $f^2=\varphi_2 u_{2-}\varphi_1 u_1$ $+\dfrac{n}{2}\left(\dfrac{1}{d}\ln R+\theta\right)(du_2+u_1)$	II, $d\neq 0$	$Re^{-d\theta}$	$n\neq 0$	$Z_N=X_0+\mu e^{nt}\hat{B}$, $Z_E=Z_N+\nu_a\hat{G}_a$
				$n=0$	$Z_N=X_0+\mu\hat{B}$, $Z_E=Z_N+\lambda_a G_a$
7	$f^1=(\varphi_1-n\theta)u_2+\varphi_2 u_1$, $f^2=\varphi_2 u_2-\varphi_1 u_1$	II, $d=0$	R	$n\neq 0$	$Z_N=X_0+\mu e^{nt}\hat{B}$, $Z_E=Z_N+\nu_a\hat{G}_a$
				$n=0$	$Z_N=X_0+\mu\hat{B}$, $Z_E=Z_N+\lambda_a G_a$
8	$f^1=\varphi_1 u_1+nu_2$, $f^2=(\varphi_1 u_2+u_1\varphi_2)$ $+nu_2\left(1+\dfrac{u_2}{u_1}\right)$	IIIb	$u_2/u_1-\ln u_1$	$n\neq 0$ $n=0$	$Z_N=X_0+\mu e^{nt}\hat{B}$, $Z_E=Z_N+\nu_a\hat{G}_a$ $Z_N=X_0+\mu\hat{B}$, $Z_E=Z_N+\lambda_a G_a$
9	$f^1=\varphi u_1-su_1$,	IIIa	u_1	$s=0,n\neq 0$	$Z_N=X_0+\mu u_1\dfrac{\partial}{\partial u_2}$ $+\nu Y_1$
	$f^2=\varphi u_2-nu_1$			$s\neq 0,n=0$	$Z_N=X_0+\nu u_2\dfrac{\partial}{\partial u_2}$ $+\mu e^{st}u_1\dfrac{\partial}{\partial u_2}$
				$n=s=0$	$Z_N=X_0+\nu u_2\dfrac{\partial}{\partial u_2}$ $+\mu u_1\dfrac{\partial}{\partial u_2}$

TABLE II. (*Continued.*)

No.	Nonlinear terms	Type of matrix B (41)	Arguments of φ_1, φ_2	Conditions for parameters	Symmetries, Z_N for $A^{-1}\neq\kappa B$ and Z_E for $A^{-1}=\kappa B$
10	$f^1=\varphi_1 u_1$,	IIIa	u_1	$\varphi_1\neq 0$	$Z_N=X_0+\mu e^{nt}\hat{B}$,
	$f^2=\varphi_1 u_2+\varphi_2 u_1+nu_2$			$\varphi_1=0$	$Z_N=X_0+\mu\hat{B}+\psi_n\frac{\partial}{\partial u_2}$
11	$f^1=\varphi_1\exp(-ku_2)u_1$, $f^2=\varphi_2\exp(-ku_2)$	I, $d=0$	$\ln u_1+nu_2$	$k\neq 0$	$Z_N=X_0+\nu D_2$
12	$f^1=\varphi_1 u_1+\frac{s}{n}u_1u_2$,	I,	$u_2-n\ln u_1$	$n\neq 0, s=0$	$Z_N=X_0+\lambda Y_2$
	$f^2=\varphi_2+su_2$	$d=0$		$s\neq 0, n\neq 0$	$Z_N=X_0+\lambda Y_3$
13	$f^1=e^{ku_1}\varphi_1$,	IIIa	$nu_1^2+2u_2$	$k\neq 0$	$Z_N=X_0+\lambda D_3$
	$f^2=e^{ku_1}(\varphi_2-n\varphi_1u_1)$			$k=0, n\neq 0$	$Z_N=X_0+\lambda Y_4$
14	$f^1=n$,	IIIa	u_1	$\varphi\neq$ const	$Z_N=X_0+\lambda Y_5$
	$f^2=ku_2+\varphi$				$+\psi_k\frac{\partial}{\partial u_2}$
15	$f^1=u_1\varphi_1+nu_1\ln u_1$,	I,	u_2	$n\neq 0$	$Z_N=X_0+\lambda Y_6$
	$f^2=\varphi_2$	$d=0$			
16	$f^\alpha=e^{k/\omega(\omega_1u_1+\omega_2u_2)}\varphi^\alpha$, $\alpha=1,2$, $\omega^2=\omega_1^2+\omega_2^2$	any	ω_1u_2- $-\omega_2u_1$	$k\neq 0$	$Z_N=Z_E$ $=X_0+\nu D_4$
17	$f^1=\varphi_1+ku_1+u_2$,	any	u_2-ku_1	$k\neq 0$,	$Z_N=Z_E=X_0$
	$f^2=\varphi_2+k(ku_1+u_2)$			$A\neq\varkappa I$	$+e^{2kt}\psi(x)\left(\frac{\partial}{\partial u_1}+k\frac{\partial}{\partial u_2}\right)$
		$A=\varkappa I$	u_1	$k=0, A=\varkappa I$	$Z_N=X_0+\tilde{\psi}_0\frac{\partial}{\partial u_2}$
18	$f^1=\varphi_1, f^2=\varphi_2$	any	u_1, u_2		$Z_N=Z_E=X_0$

$$Y_4=nu_1\frac{\partial}{\partial u_2}-\frac{\partial}{\partial u_1},\quad Y_5=e^{kt}\left(u_1\frac{\partial}{\partial u_2}+\frac{nx^2}{2m}\frac{\partial}{\partial u_2}\right),\quad Y_6=e^{nt}u_1\frac{\partial}{\partial u_1},$$

$$\hat{B}=B^{ab}u_b\frac{\partial}{\partial u_a},$$

where B^{ab} are elements of the corresponding matrices (41).

In Tables III and IV we use triplets of matrices (F, B, A^{-1}) with F and B forming a two-dimensional Lie algebra and commuting with A (25). We classify such triplets according to the categories

$$\text{(I) } F=\begin{pmatrix}1&0\\0&d\end{pmatrix},\quad B=\begin{pmatrix}0&0\\0&1\end{pmatrix},\quad A^{-1}=\begin{pmatrix}1&0\\0&a^{-1}\end{pmatrix};$$

$$\text{(IIa) } F=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad B=\begin{pmatrix}0&-1\\1&0\end{pmatrix},\quad A^{-1}=\frac{1}{b^2+c^2}\begin{pmatrix}b&c\\-c&b\end{pmatrix}; \tag{43}$$

$$\text{(IIb) } F=\begin{pmatrix}d&-1\\1&d\end{pmatrix},\quad B=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad A^{-1}=\frac{1}{b^2+c^2}\begin{pmatrix}b&c\\-c&b\end{pmatrix};$$

TABLE III. Nonlinearities which generate dilatation symmetry.

No.	Nonlinear terms	Conditions for parameters	Symmetries, Z_N for $A^{-1}\neq\kappa F$ and Z_E for $A^{-1}=\kappa F$	Matrices (43) and generator parameters
1	$f^1=(gu_1^q u_2^r+n)u_1$,	$q\neq 0,-1$, $p\neq 0, n=0$	$Z_N=X_0+\mu\hat{F}+\nu D_5$,	I, $k=\frac{4}{m}$,
		$q+r=\frac{4}{m}$		$d=-\frac{q}{r}$
		$q=-1$, $p=n=0$,	$Z_E=Z_N+\sigma_a G_a+\lambda\hat{A}$	$I, k=\frac{4}{m}$
		$r=\frac{4+m}{m}$		$d=-\frac{q}{r}$
		$q\neq 0,-1, r\neq 0$	$Z_N=X_0+\mu\hat{F}+\mu D_5$ $+\tilde{\psi}_0\frac{\partial}{\partial u_1}$	I, $k=r+q$,
	$f^2=\left(pu_1^q u_2^r-\frac{qn}{r}\right)u_2$	$q+r\neq 0,\frac{4}{m}$;	$Z_E=Z_N+\sigma_a G_a+\lambda\hat{A}$	$d=-\frac{q}{r}$
		$p=n=0, g\neq 0$	$Z_N=X_0+\nu\hat{F}+\mu D_5$,	I, $d=\frac{1}{r}$,
		$q=-1, r\neq 0,1$	$Z_E=Z_N+\sigma_a G_a$	$k=r$
		$q=g=0$,	$Z_N=X_0+\nu\hat{F}$ $+\mu D_6+\tilde{\psi}_0\frac{\partial}{\partial u_1}$	I, $d=0$,
		$r\neq 0,1; p\neq 0$	$Z_E=Z_N+\sigma_a G_a$	$k=r$
2	$f^1=e^{q\theta}R^r(gu_1-pu_2)+su_2-lu_1$,	$s=l=0$,	$Z_N=X_0+\nu\hat{F}+\mu D_6$ $+\tilde{\psi}_n\frac{\partial}{\partial u_1}$,	IIb, $k=\frac{4}{m}$,
		$r=\frac{4}{m}$		$d=-\frac{q}{r}, n=0$
		$r\neq\frac{4}{m}, r\neq 0$,	$Z_N=X_0+\nu\hat{F}+\mu D_5$,	IIb, $k=r$,
	$f^2=e^{q\theta}R^r(gu_2+pu_1)-su_1-lu_2$,	$s=l=0$	$Z_E=Z_N+\sigma_a G_a+\lambda\hat{A}$	$d=-\frac{q}{r}, n=0$
		$l=(sq/r)$,	$Z_N=X_0+\nu\hat{F}+\mu D_5$,	IIb, $k=r$, $n=-s$,
	$R^2=u_1^2+u_2^2$	$s\neq 0, r\neq 0$	$Z_E=Z_N+\sigma_a G_a$	$d=-\frac{q}{r}$
	$\theta=\arctan\left(\frac{u_2}{u_1}\right)$	$s=0, l\neq 0$, $q\neq 0, r=0$	$Z_N=X_0+\nu\hat{F}+\mu D_6$, $Z_E=Z_N+\sigma_a G_a$	IIa, $k=q$, $n=-l$
3	$f^1=pu_1^{r+1}e^{q(u_2/u_1)}-su^1$,	$r=-q=\frac{4}{m}$,	$Z_N=X_0+\nu\hat{F}+\mu D_6$,	IIIb, $d=1$,
		$s=0$	$Z_E=Z_N+\alpha_a G_a$	$k=\frac{4}{m}$
	$f^2=e^{q(u_2/u_1)}(pu_2+gu_1)u_1^r$	$-q=r\neq\frac{4}{m}$,	$Z_N=X_0+\nu\hat{F}+\mu D_5$,	IIIb, $d=1$,
		$s=0, r\neq 0$	$Z_E=Z_N+\alpha_a G_a+\lambda\hat{A}$	$k=r$
	$-s\left(u_2-\frac{r}{q}u_1\right)$	2	$Z_N=X_0+\nu\hat{F}+\mu D_5$,	IIIb, $k=q$,
		$q\neq 0, s\neq 0$	$Z_E=Z_N+\alpha_a G_a$	$n=-sq$,
			$Z_N=X_0+\nu\hat{F}+\mu D_6$, $Z_E=Z_N+\alpha_a G_a$	$d=-\frac{r}{q}$

TABLE III. (*Continued*.)

No.	Nonlinear terms	Conditions for parameters	Symmetries, Z_N for, $A^{-1}\neq\kappa F$ and Z_E for $A^{-1}=\kappa F$	Matrices (43) and generator parameters
4	$f^1=pu_1^{k+1}$,	$d+k\neq 1$, $k\neq 0, q\neq 0$, $s=n\neq 0, p\neq 0$	$Z_N=X_0+\nu\hat{F}+\mu D_6$	IIIa
	$f^2=u_1^k(pu_2+qu_1^d)+\dfrac{s}{d+k-1}u_1$	$k\neq 0, s=0$, $q=0, p\neq 0$	$Z_N=X_0+\nu\hat{F}+\mu D_5+\lambda u_2\dfrac{\partial}{\partial u_2}$	IIIa, $d=0$
		$pk\neq 0, q=0$, $s=n(k-1)\neq 0$	$Z_N=X_0+\nu\hat{F}+\mu D_5+\lambda Y_1$	IIIa, $d=0$
		$d+k\neq 0,1$, $k\neq 0, q\neq 0$, $s=n\neq 0, p=0$	$Z_N=X_0+\nu\hat{F}+\mu D_6+\psi_0\dfrac{\partial}{\partial u_a}$	IIIa
5	$f^1=pu_1^{k+1}$, $f^2=pu_1^k u_2+qu_1-knu_1\ln u_1$	$k\neq 0, n\neq 0$, $p\neq 0$	$Z_N=X_0+\nu\hat{F}+\mu D_6$	IIIa, $d=1-k$
		$k\neq 0, n\neq 0$, $p=0$	$Z_N=X_0+\nu\hat{F}+\mu D_6+\psi_0\dfrac{\partial}{\partial u_2}$	IIIa, $d=1-k$
6	$f^1=qu_1^{r+1}e^{ku_2}+su_1$, $f^2=pu_1^r e^{ku_2}-\dfrac{sr}{k}$	$r\neq 0,-1; k\neq 0$, $p\neq 0, q\neq 0$	$Z_n=X_0+\nu D_7+\mu Y_2$	I, $d=0$, $n=-\dfrac{r}{k}$
		$p=0, r=-1$, $q\neq 0, s=0$,	$Z_N=X_0+\nu D_7$	I, $d=0$, $r=-1$,
		$k\neq 0$	$+\mu Y_2+\tilde{\psi}_0\dfrac{\partial}{\partial u_1}$	$n=\dfrac{1}{k}$
7	$f^1=pe^{(n-k)u_2}+hu_2$, $f^2=ge^{-ku_2}+q$	$q=h=0$, $k\neq 0, n\neq 0$	$Z_N=X_0+\nu D_2+\tilde{\psi}_0\dfrac{\partial}{\partial u_1}$	I, $d=0$
		$p=q=0$, $k\neq 0, h\neq 0$	$Z_N=X_0+\nu D_8+\tilde{\psi}_0\dfrac{\partial}{\partial u_1}$	I, $d=0$
		$p=q=0$, $h=0, k\neq 0$	$Z_N=X_0+\nu D_2+\sigma u_1\dfrac{\partial}{\partial u_1}+\tilde{\psi}_0\dfrac{\partial}{\partial u_1}$	I, $d=0$, $n=0$
		$n=q=g=0$, $p\neq 0$	$Z_N=X_0+\nu D_9+\mu u_2\dfrac{\partial}{\partial u_1}+\tilde{\psi}_0\dfrac{\partial}{\partial u_1}$	IIIa
8	$f^1=ge^{u_2+ku_1}$, $f^1=qe^{u_2+ku_1}+p$	$k\neq 0$	$Z_N=Z_E=X_0+\nu D_{10}+\psi(x)\left(\dfrac{\partial}{\partial u_1}-k\dfrac{\partial}{\partial u_2}\right)$	I, $a\neq 1$
			$Z_N=Z_E=X_0+\nu D_{11}+\psi(x)\left(\dfrac{\partial}{\partial u_1}-k\dfrac{\partial}{\partial u_2}\right)$	IIa, IIb, $c\neq 0$
		$k=0$	$Z_N=Z_E=X_0+\nu D_{12}+\psi(x)\dfrac{\partial}{\partial u_1}$	IIIb, $e\neq 0$

TABLE III. (*Continued.*)

No.	Nonlinear terms	Conditions for parameters	Symmetries, Z_N for, $A^{-1}\neq\kappa F$ and Z_E for $A^{-1}=\kappa F$	Matrices (43) and generator parameters
	$f^1=p(u_2+nu_1^2)^{s+1/2}+\dfrac{1}{2n(2s+1)}$,	$s\neq 0,-\frac{1}{2}$,		
9	$f^2=-\dfrac{1}{2s+1}u_1+(q-2npu_1)$	$p\neq 0, n\neq 0$	$Z_N=X_0+\nu D_{13}$	IIIa
	$\times(u_2+nu_1^2)^{s+1/2}$			I $k=-1$ I $k=-1$
10	$f_1=gu_1^{k+1}$,	$k=-1, q=0,$ $p\neq 0, g\neq 0$	$Z_N=Z_E=X_0$	IIIb, $d=1$
		$k=-1, p\neq 0$ $q=g=0$		
	$f_2=(p\ln u_1+q)u_1^{k+1}$	$k\neq 0,-1$ $g=p$	$+\nu D_1+\psi_0\dfrac{\partial}{\partial u_2}$	
		$k\neq 0,-1;$ $s\neq 0$		
	$f^1=g(u_2+su_1)^{k+1}$,	$k\neq 0,-1;$	$Z_N=Z_E$	
11		$s=0,$	$=X_0+\nu D_{14}$	I, $a\neq 1$
	$f^2=q(u_2+su_1)^{k+1}+p$	$s\neq 0$	$+\psi(x)\left(\dfrac{\partial}{\partial u_1}-s\dfrac{\partial}{\partial u_2}\right)$	
12	$f^1=p\ln(u_2+su_1)$, $f^2=q\ln(u_2+su_1)$		$Z_N=Z_E$ $=X_0+\nu D_{15}$ $+\psi(x)\left(\dfrac{\partial}{\partial u_1}-s\dfrac{\partial}{\partial u_2}\right)$	IIa, IIb, $c\neq 0$
		$s=0$	$Z_N=Z_E=X_0$ $+\nu D_{16}+\psi(x)\dfrac{\partial}{\partial u_1}$	IIIb, $b=1$ $c\neq 0$
13	$f^1=gu_1^{k+1}$,	$g\neq 0, k\neq 0$	$Z_N=Z_E=X_0$	I $a\neq 1$ IIa, IIb $k=-1,$ $c\neq 0;$
	$f^2=qu_1^{k+d}$		$+\nu D_1+\psi_0\dfrac{\partial}{\partial u_2}$	IIIb, $k=-1,$ $b=1,$ $c\neq 0$ I

$$\text{(IIIa)}\ F=\begin{pmatrix}0&0\\1&0\end{pmatrix},\quad B=\begin{pmatrix}1&0\\0&d\end{pmatrix},\quad A^{-1}=\begin{pmatrix}1&0\\0&1\end{pmatrix};$$

$$\text{(IIIb)}\ F=\begin{pmatrix}1&0\\d&1\end{pmatrix},\quad B=\begin{pmatrix}0&0\\1&0\end{pmatrix},\quad A^{-1}=\begin{pmatrix}1&0\\-e&1\end{pmatrix};$$

where a,b,c,e and d are real parameters $(a\neq 0, b^2+c^2\neq 0)$.

In Table IV, columns 4 and 5 refer to both the nonlinearities specified as cases 9 and 10. However, the conditions marked by * are related to case 9 only and the symmetries marked by ** correspond only to case 10.

Here $\kappa=$constant, $\Delta=k_0n_1-n_0k_1$, $\delta=\frac{1}{4}(k_0-n_1)^2+k_1n_0$, $\hat{\mathcal{F}}_\alpha=\mathcal{F}_\alpha^{ab}u_b\,\partial/\partial u_a$, $\hat{F}=F^{ab}u_b\,\partial/\partial u_a$ and:

TABLE IV. Further non-linearities with arbitrary parameters.

No.	Nonlinear terms	Matrix Class (43)	Conditions for parameters and matrices $\mathcal{F}_\alpha$	Symmetries, Z_N for $A^{-1}\neq\kappa\mathcal{F}_a$, Z_E for $A^{-1}=\kappa\mathcal{F}_1$, and $\tilde{Z}_E$ for $A^{-1}=\kappa\mathcal{F}_2$
1	$f^1=(k_0\ln u_1+k_1\ln u_2+q)u_1$,	I, $d=0$	$\delta>0,\Delta\neq 0,k_1\neq 0$, $\mathcal{F}_1=k_1F+(n_+-k_0)B$, $\mathcal{F}_2=k_1F+(n_--k_0)B$, $n_\pm=\frac{k_0+n_1}{2}\pm\delta$	$Z_N=X_0+\lambda e^{n_+t}\hat{\mathcal{F}}_1+\nu e^{n_-t}\hat{\mathcal{F}}_2$, $Z_E=Z_N+\sigma_a\hat{G}_a(n=n_+)$, $\tilde{Z}_E=Z_N+\sigma_a\hat{G}_a(n=n_-)$
	$f^2=(n_0\ln u_1+n_1\ln u_2+p)u_2$		$k_1=n_0=0,k_0n_1\neq 0$	$Z_N=X_0+\nu e^{k_0t}u_1\frac{\partial}{\partial u_1}+\nu e^{n_1t}u_2\frac{\partial}{\partial u_2}$
			$k_1=n_0=n_1=0$	$Z_N=X_0+\psi_p\frac{\partial}{\partial u_2}+\nu e^{k_0t}u_1\frac{\partial}{\partial u_1}$
			$\Delta=0,k_0\neq 0$, $\mathcal{F}_1=k_1F+n_1B$, $\mathcal{F}_2=k_0B-k_1F$;	$Z_N=X_0+\lambda e^{(n_1+k_0)t}\hat{\mathcal{F}}_1+\nu\hat{\mathcal{F}}_2$, $Z_E=Z_N+\sigma_a\hat{G}_a(n_1\neq 0)$, $\hat{Z}_E=Z_N+\sigma_aG_a(k_0\neq 0)$
			$k_0=n_1=n$,	$Z_N=X_0+\alpha e^{nt}u_1\frac{\partial}{\partial u_1}+\lambda e^{nt}u_2\frac{\partial}{\partial u_2}$,
			$k_1=n_0=0$, $\mathcal{F}_1=\mu F+\nu B,\mu\nu\neq 0$	$\tilde{Z}_E=Z_N+\sigma_a\hat{G}_a$
			$k_0=n_1=n$, $n_0=0,k_1\neq 0$	$Z_N=X_0+\lambda e^{nt}u_1\frac{\partial}{\partial u_1}+\nu e^{nt}\left(k_1tu_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right)$
			$\delta=0,\Delta\neq 0,k_0+n_1=2n$ $\mathcal{F}_1=2k_1F+(n_1-k_0)B$, $\mathcal{F}_2=t\mathcal{F}_1+2B$	$Z_N=X_0+\nu X_1+\mu X_2$, $Z_E=Z_N+\sigma_a\hat{G}_a$
			$\delta=\Delta=0$, $n_0k_1\neq 0$, $\mathcal{F}_1=k_1F-k_0B$	$Z_N=X_0+\nu\left[k_1tu_1\frac{\partial}{\partial u_1}+(1-k_0t)u_2\frac{\partial}{\partial u_2}\right]+\mu\left(k_1u_1\frac{\partial}{\partial u_1}-k_0u_2\frac{\partial}{\partial u_2}\right)$, $Z_E=Z_N+\sigma_aG_a$
			$k_1=n_1=0,q=p$,	$Z_N=X_0+\nu u_2\frac{\partial}{\partial u_2}+\mu u_1\frac{\partial}{\partial u_2}+\lambda e^{nt}\left(u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right)$,
			$k_0=n_0=n$, $a=1$ $\mathcal{F}_1=F+B$	$Z_E=Z_N+\sigma_a\tilde{G}_a$
			$k_1=n_1=0,p=0$,	$Z_N=X_0+\nu u_2\frac{\partial}{\partial u_2}+\mu e^{pt}u_1\frac{\partial}{\partial u_2}+\lambda e^{nt}\left(u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right)$,
			$k_0=n_0=n,q\neq 0$,	

TABLE IV. (*Continued*.)

No.	Nonlinear terms	Matrix Class (43)	Conditions for parameters and matrices $\mathcal{F}_\alpha$	Symmetries, Z_N for $A^{-1}\neq\kappa\mathcal{F}_a$, Z_E for $A^{-1}=\kappa\mathcal{F}_1$, and $\tilde{Z}_E$ for $A^{-1}=\kappa\mathcal{F}_2$
	$f^1=qu_1$,		$d\neq 0,1,2;k=0$,	$Z_N=X_0+\nu\hat{B}+\psi_n\dfrac{\partial}{\partial u_2}$,
2	$f^2=nu_2+pu_1^d+su_1+k$	IIIa	$s=0,n\neq q,\mathcal{F}_1=B$	$Z_E=Z_N+\sigma_a G_a$
			$d\neq 0,2;n=0$,	$Z_N=X_0+\psi_0\dfrac{\partial}{\partial u_2}$
			$s=0$,	$+\nu\left(\hat{B}-dkt\dfrac{\partial}{\partial u_2}\right)$,
			$\mathcal{F}_1=B$	$Z_E=Z_N+\sigma_a G_a$
			$d\neq 0,1,2;k=0$,	$Z_N=X_0+\nu\hat{F}$
			$s=\dfrac{1}{1-d},\mathcal{F}_1=B$	$+\mu\hat{B}+\psi_q\dfrac{\partial}{\partial u_2}$,
				$Z_E=Z_N+\sigma_a G_a$
			$d=2,k=0,s\neq 0$	$Z_N=X_0+\mu Y_7+\psi_q\dfrac{\partial}{\partial u_2}$
			$k=s=0$,	$Z_N=X_0+\nu\hat{B}+\psi_0\dfrac{\partial}{\partial u_2}$,
			$d=2,\mathcal{F}_1=B$	$Z_E=Z_N+\sigma_a G_a+e^{qt}\hat{F}$
			$n=2(q+p)$	$Z_N=X_0+\nu Y_8$
			$d=2,k=s=0$,	$+\mu\hat{B}+\psi_0\dfrac{\partial}{\partial u_2}$,
			$\mathcal{F}_1=B$	$Z_E=Z_N+\sigma_a G_a$
			$d=2,p=-q$,	$Z_N=X_0+\nu Y_8+\psi_0\dfrac{\partial}{\partial u_2}$
			$n=s=0$	$+\mu\left(\hat{B}-2kt\dfrac{\partial}{\partial u_2}\right)$
3	$f^1=ku_1\ln u_1+pu_1$,	I	$b=k=q=0$,	$Z_N=X_0+\nu Y_9$
	$f^2=bu_2+n\ln u_1+q$		$p\neq 0$	$+\psi_0\dfrac{\partial}{\partial u_2}$
			$q=p=0,b=k$	$Z_N=X_0+\nu Y_{10}+\psi_b\dfrac{\partial}{\partial u_2}$
			$q=p=0$,	$Z_N=X_0+\nu Y_{11}$
			$b\neq k,b\neq 0$	$+\psi_b\dfrac{\partial}{\partial u_2}$
4	$f^1=k_0u_1\ln u_1+k_1u_1u_2$,	I	$k_1\neq 0,\delta=0$	$Z_N=X_0+\nu Y_{12}$
	$f^2=n_0\ln u_1+n_1u_2$	$d=0$	$k_1\neq 0,\delta>0$	$+\mu\left(tY_{12}+e^{(k_0+n_1/2)t}\dfrac{\partial}{\partial u_2}\right)$
			$k_1\neq 0,\delta=-\omega^2<0$	$Z_N=X_0+\nu Y_{13}^+ +\mu Y_{13}^-$
				$Z_N=X_0+\nu Y_{14}+\mu Y_{15}$
5	$f^1=pu_2^k+qu_1$,	I,	$p\neq 0,kg\neq q$,	$Z_N=X_0+\nu\hat{F}+\tilde{\psi}_q\dfrac{\partial}{\partial u_1}$,
	$f^2=gu_2$	$d=\dfrac{1}{k}$	$k\neq 0,1;\mathcal{F}_1=F$	$Z_E=Z_N+\sigma_a G_a$

TABLE IV. (*Continued*.)

No.	Nonlinear terms	Matrix Class (43)	Conditions for parameters and matrices $\mathcal{F}_\alpha$	Symmetries, Z_N for $A^{-1}\neq\kappa\mathcal{F}_a$, Z_E for $A^{-1}=\kappa\mathcal{F}_1$, and $\tilde{Z}_E$ for $A^{-1}=\kappa\mathcal{F}_2$
6	$f^1=nu_1\ln u_1$,	I,	$n\neq 0, p\neq 0$,	$Z_N=X_0+\mu u_1\frac{\partial}{\partial u_2}$
	$f^2=nu_2\ln u_1+pu_1$	$d=0$	$\mathcal{F}_1=B+F$	$+\nu\left(\hat{B}-ptu_1\frac{\partial}{\partial u_2}\right)$
				$+\lambda e^{nt}\left(u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right)$
				$Z_E=Z_N+\sigma_a\tilde{G}_a$
7	$f^1=pu_1^{k+1}$, $f^2=pu_1^k u_2+su_2$	IIIa, $d=0$	$k\neq 0, s\neq 0$	$Z_N=X_0+\nu u_2\frac{\partial}{\partial u_2}$ $+\mu e^{st}u_1\frac{\partial}{\partial u_2}+\lambda D_6$
8	$f^1=(k_0u_1-n_0u_2)\ln R$ $+\theta(k_1u_1-n_1u_2)+pu_1-qu_2$,	IIa	$\delta>0,\Delta\neq 0,n_0^2+k_1^2\neq 0$ $\mathcal{F}_1=\frac{1}{2}(k_0-n_1)+\sqrt{\delta}]F$ $+n_0B,\mathcal{F}_2$ $=-[\frac{1}{2}(k_0-n_1)$ $+\sqrt{\delta}]B+k_1F$	$Z_N=X_0$ $+\lambda e^{n_+t}\hat{\mathcal{F}}_1+\nu e^{n_-t}\hat{\mathcal{F}}_2$, $n_\pm=\frac{1}{2}(k_0+n_1)\pm\sqrt{\delta}$, $Z_E=Z_N+\sigma_a\hat{G}_a$, $\tilde{Z}_E=Z_E(k_1\neq 0^*)$
	$f^2=(k_0u_2+n_0u_1)\ln R$ $+\theta(n_1u_1+k_1u_2)+qu_1+pu_2$		$\delta>0,\Delta=0,n=n_1+k_0$. $(n_1=0,k_0\neq 0)$: $\mathcal{F}_1=k_0F+n_0B$, $\mathcal{F}_2=k_0B-k_1F$; $(k_0=0$ or $n_1\neq 0)$: $\mathcal{F}_1=k_1F+n_1B(k_1\neq 0^*)$, $\mathcal{F}_2=n_1F-n_0B(n_1\neq 0^*)$	$Z_N=X_0+\mu e^{nt}\hat{\mathcal{F}}_1$ $+\nu\hat{\mathcal{F}}_2$, $Z_E=Z_N+\sigma_a\hat{G}_a$, $\tilde{Z}_E=Z_N+\sigma_aG_a$,
9	$f^1=(k_0u_1-n_0u_2)\ln R$ $+\theta(k_1u_1-n_1u_2)+pu_1-qu_2$,	IIa	$\delta>0,\Delta\neq 0,k_1\neq 0$, $\mathcal{F}_1=k_1F+(n_+-k_0)B$, $\mathcal{F}_2=k_1F+(n_--k_0)B$, $n_\pm=\frac{k_0+n_1}{2}\pm\delta$	$Z_N=X_0+\lambda e^{n_+t}\hat{\mathcal{F}}_1+\nu e^{n_-t}\hat{\mathcal{F}}_2$, $Z_E=Z_N+\sigma_a\hat{G}_a$, $\tilde{Z}_E=Z_E\ (k_1\neq 0^*)$
	$f^2=(k_0u_2+n_0u_1)\ln R$ $+\theta(n_1u_1+k_1u_2)+qu_1+pu_2$		$\Delta=0,k_0+n_1=n\neq 0$, $k_1\neq 0$: $\mathcal{F}_1=k_1F+n_1B$, $\mathcal{F}_2=k_0B-k_1F$; $k_1=0,n_0\neq 0$: $\mathcal{F}_1=n_0B+k_0F$, $(k_0\neq 0^*)$ $\mathcal{F}_2=n_1F-n_0B$; $(n_1\neq 0^*)$	$Z_N=X_0+\mu e^{nt}\hat{\mathcal{F}}_1+\nu\hat{\mathcal{F}}_2$, $Z_E=Z_N+\sigma_a\hat{G}_a$, $\hat{Z}_E=Z_N+\sigma_aG_a$,

TABLE IV. (*Continued.*)

10	$f^1=(k_0\ln u_1+q)u_1+k_1u_2,$ $f^2=(n_0u_1+k_0u_2)\ln u_1$ $k_1\frac{u_2^2}{u_1}+pu_1$ $+(n_1+q)u_2$	IIIb, $d=0$	$k_1=n_0=0,\ k_0=n_1=n,$ $\mathcal{F}_1=\nu F\mu B\ (\nu\neq 0^*)$ $\delta=n_0=0,\ \Delta\neq 0,$ $k_1\neq 0,\ \mathcal{F}_1=F,$ $n=\frac{1}{2}(k_0+n_1)$ $\delta=k_1=0,$ $k_0=n_1,$ $n_0\neq 0,\ \mathcal{F}_1=B$ $\delta=0,\ \Delta\neq 0,\ k_0+n_1=2n$ $\mathcal{F}_1=2k_1F+(n_1-k_0)B,$ $F_2=t\mathcal{F}_1+2B$ $k_0=k_1=n_1=0,$ $n_0\neq 0,\ \mathcal{F}_1=B$ $k_0=n_0=n_1=0,$ $k_1\neq 0,\ \mathcal{F}_1=F$ $\delta=\Delta=0,$ 12 $n_0k_1<0,$ $\mathcal{F}_1=k_1F-k_0B$	$Z_N=X_0+\alpha e^{nt}\hat{\mathcal{F}}_1,$ $Z_E=Z_N+\sigma_a\hat{G}_a$ $Z_N=X_0+\mu e^{nt}(k_1t\hat{F}+B)$ $+\nu e^{nt}\hat{F},$ $Z_E=Z_N+\sigma_a\hat{G}_a$ $Z_N=X_0+\mu e^{n_1t}(\hat{F}+n_0t\hat{B})$ $\nu e^{n_1t}\hat{B},$ $Z_E^{**}=Z_N+\sigma_a\hat{G}_a$ $Z_N=X_0+\nu X_1+\mu X_2,$ $Z_E=Z_N+\sigma_a\hat{G}_a$ $Z_N=X_0+\nu\hat{B}$ $+\mu(\hat{F}+n_0t\hat{B}),$ $Z_E^{**}=Z_N+\sigma_aG_a$ $Z_N=X_0+\nu\hat{F}$ $+\mu(\hat{B}+k_1t\hat{F})$ $Z_E=Z_N+\sigma_aG_a$ $Z_N=X_0+\mu(k_1\hat{F}-k_0\hat{B})$ $\nu[k_1t\hat{F}+(1-k_0t)\hat{B}],$ $Z_E=Z_N+\sigma_aG_a$

$$\left(\frac{\partial}{\partial t}-A\sum_{i=1}^{m}\frac{\partial^2}{\partial x_i^2}\right)\begin{pmatrix}0\\ \psi_n\end{pmatrix}=n\begin{pmatrix}0\\ \psi_n\end{pmatrix},\quad \left(\frac{\partial}{\partial t}-A\sum_{i=1}^{m}\frac{\partial^2}{\partial x_i^2}\right)\begin{pmatrix}\tilde{\psi}_n\\ 0\end{pmatrix}=n\begin{pmatrix}\tilde{\psi}_n\\ 0\end{pmatrix},$$

$$\sum_{i=1}^{m}\frac{\partial^2}{\partial x_i^2}\psi(x)=0,$$

and n is an arbitrary parameter (including the case $n=0$). The generators $D_\mu,\hat{A},G_a,\hat{G}_a,X_\nu,Y_s$, when not specified in (42), are given by

$$\hat{A}=t^2\frac{\partial}{\partial t}+tx_a\frac{\partial}{\partial x_a}-\frac{1}{4}x^2(A^{-1})^{ab}u_b\frac{\partial}{\partial u_a}-\frac{m}{2}t\left(u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right)+nt^2\hat{F},$$

$$D_5=D_0-\frac{2}{k}\left(u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right),\quad D_6=D_0+2tn\hat{F}-\frac{2}{k}\hat{B},$$

$$D_7=D_0+2\left(st-\frac{1}{r}\right)u_1\frac{\partial}{\partial u_1}-\frac{2srt}{k}\frac{\partial}{\partial u_2},\quad D_8=D_0+2u_1\frac{\partial}{\partial u_1}+\frac{2ht}{k}\frac{\partial}{\partial u_1}+\frac{2}{k}\frac{\partial}{\partial u_2},$$

$$D_9=D_0-2ht(u_2-1)\frac{\partial}{\partial u_1}-\frac{2}{k}\frac{\partial}{\partial u_2},$$

$$D_{10}=D_0-2\frac{\partial}{\partial u_2}-\frac{p}{k(1-a)}\left(\frac{x^2}{m}+2t\right)\left(\frac{\partial}{\partial u_1}-k\frac{\partial}{\partial u_2}\right),$$

$$D_{11}=D_0-2\frac{\partial}{\partial u_2}-\frac{p}{c(1+k^2)}\left(\frac{x^2}{m}+2t(ck+b)\right)\left(\frac{\partial}{\partial u_1}-k\frac{\partial}{\partial u_2}\right),$$

TABLE V. Symmetries for linear systems.

No.	Form of f^1 and f^2	Type of A (25)	Conditions	Symmetries
1	$f^1=f^2=0$	Ia		$X_5+\lambda u_1\frac{\partial}{\partial u_2}$ $+\nu u_2\frac{\partial}{\partial u_2}+\mu u_2\frac{\partial}{\partial u_1}$
		Ib		$X_5+\mu u_2\frac{\partial}{\partial u_2}$
		II		$X_5+\lambda\left(u_1\frac{\partial}{\partial u_2}-u_2\frac{\partial}{\partial u_1}\right)$
		III		$X_5+\lambda u_1\frac{\partial}{\partial u_2}$
2	$f^1=u_2$,	Ib		$X_0+\psi^\beta_\Lambda\frac{\partial}{\partial u_a}$
	$f^2=0$	Ib		$+\alpha\left(D_0+2u_1\frac{\partial}{\partial u_1}\right)$ $+\lambda\left(u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right)$
3	$f^1=au_1+bu_2$,	Ib	$\delta>0$	$X_0+\psi^\beta_\Lambda\frac{\partial}{\partial u_a}$
	$f^2=cu_1+du_2$			$+\nu\left(u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right)$
4	$f^1=au_1+bu_2$,	II	$(a-d)^2+(b+c)^2\neq 0$	$X_0+\psi^\beta_\Lambda\frac{\partial}{\partial u_a}$
	$f^2=cu_1+du_2$			$+\nu\left(u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right)$
5	$f^1=au_1+bu_2$,	III	$b^2+(a-d)^2\neq 0$	$X_0+\psi^\beta_\Lambda\frac{\partial}{\partial u_a}$
	$f^2=cu_1+du_2$			$+\nu\left(u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right)$

$$
\begin{aligned}
D_{12}&=D_0-2\frac{\partial}{\partial u_2}-\frac{p}{e}\left(\frac{x^2}{m}+2t\right)\frac{\partial}{\partial u_1},\\
D_{13}&=D_0-\frac{1}{s}\left(u_1\frac{\partial}{\partial u_1}+2u_2\frac{\partial}{\partial u_2}\right)+\frac{t}{2sn}\frac{\partial}{\partial u_1}-\frac{t}{s}u_1\frac{\partial}{\partial u_2},\\
D_{14}&=D_5+\frac{p(k+1)}{ks(a-1)}\left(2t+\frac{x^2}{m}\right)\left(\frac{\partial}{\partial u_1}-s\frac{\partial}{\partial u_2}\right),\\
D_{15}&=D_5-\frac{p(k+1)}{ksc(1+s^2)}\left(2t(cs+b)+\frac{x^2}{m}\right)\frac{\partial}{\partial u_1}-s\frac{\partial}{\partial u_2},\\
D_{16}&=D_5-\frac{p(k+1)}{kc}\left(2t+\frac{x^2}{m}\right)\frac{\partial}{\partial u_1}
\end{aligned}
\tag{44}
$$

$$X_1=\exp(nt)[(\sqrt{-n_0k_1}t+1)\hat{F}+n_0t\hat{B}],\quad X_2=[(k_1\hat{F}-\sqrt{-n_0k_1}\hat{B})t+\hat{B}],$$

$$X_3=\exp(nt)[\tfrac{1}{2}(n_1-k_0)\cos(\omega t)+\omega\ \sin\ (\omega t)]\hat{F}-n_0\ \cos(\omega t)\hat{B},$$

$$X_4=\exp(nt)[\omega\ \sin(\omega t)+\tfrac{1}{2}(k_0-n_1)\cos(\omega t)]\hat{B}-k_1\cos(\omega t)\hat{F},$$

$$Y_7=\exp(nt)\left(u_1\frac{\partial}{\partial u_2}-\frac{q}{2p}\left(\frac{sx^2}{2m}\frac{\partial}{\partial u_2}-\frac{\partial}{\partial u_1}\right)\right),\quad Y_8=\exp(nt)\left(u_1\frac{\partial}{\partial u_2}-\frac{\partial}{\partial u_1}\right),$$

$$Y_9=u_1\frac{\partial}{\partial u_1}+nt\frac{\partial}{\partial u_2},\quad Y_{10}=\exp(kt)\left(u_1\frac{\partial}{\partial u_1}+nt\frac{\partial}{\partial u_2}\right),$$

$$Y_{11}=\exp(kt)\left(u_1\frac{\partial}{\partial u_1}+\frac{n}{k-b}\frac{\partial}{\partial u_2}\right),\quad Y_{12}=\exp(nt)\left(\sin(pt)u_1\frac{\partial}{\partial u_1}+\cos(pt)\frac{\partial}{\partial u_2}\right),$$

$$Y_{13}=\exp(nt)\left(\cos(pt)u_1\frac{\partial}{\partial u_1}-\sin(pt)\frac{\partial}{\partial u_2}\right),\quad Y_{14}=\exp(nt)\left(ptu_1\frac{\partial}{\partial u_1}+\frac{\partial}{\partial u_2}\right).$$

V. LINEAR SYSTEMS

Consider now the linear case when f^1 and f^2 have the form $f^a=\Lambda^{ab}u_b+\lambda_a$. In contrast to the one-dimensional cases we find nontrivial possibilities corresponding to the noncommutation of the matrices A and Λ where we specify A in formulas (25).

In Table V the following notation has been employed:

$$\delta=bc-\tfrac{1}{4}(a-d)^2,$$

$$X_5=X_0+\nu\left(u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right)+\lambda D_0+\psi^a_\Lambda\frac{\partial}{\partial u_a}+\mu\left(t^2\frac{\partial}{\partial t}+tx_a\frac{\partial}{\partial x_a}-\frac{1}{4}x^2(A^{-1})^{ab}u_b\frac{\partial}{\partial u_a}\right.$$
$$\left.-\frac{m}{2}t\left(u_1\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial u_2}\right)+t^2\lambda^{ab}u_b\frac{\partial}{\partial u_a}\right).$$

Note that symbols X_0 and D_0 has been defined in (42) and (25) and, further, ψ_Λ is an arbitrary solution of the homogeneous equation

$$\left(\frac{\partial}{\partial t}-\sum_{i=1}^{m}\frac{\partial^2}{\partial x_1^2}\right)\psi^j_\Lambda=\Lambda^{jk}\psi^k_\Lambda.$$

VI. EQUIVALENCE TRANSFORMATIONS

The solutions of the determining equations presented in Tables II–V are defined up to the equivalence transformations (26) which do not change the shape of Eqs. (1) for *arbitrary* f^k. However, for some *particular* f^k, it is possible to indicate more extended groups of equivalence transformations which include (26) as a subgroup. Here we discuss such transformations.

The most extended equivalence groups appear for the case of linear f^k presented in Table V. Let the related solutions have the following general form:

$$f^k=\Lambda^{kb}u^b, \tag{45}$$

where Λ^{kb} is a matrix which commutes with $(A^{-1})^{kb}$. So there exists an additional equivalence transformation

$$u_a \to \exp\left(-t\hat{\Lambda}^{cb} u_b \frac{\partial}{\partial u_c} u_a \right) = \exp(-t\hat{\Lambda}^{ab}) u_b , \tag{46}$$

where $\hat{\Lambda}^{cb}$ is a matrix which commutes with A^{ab} and Λ^{ab}. The transformed equation has the form (45) where $f'^k = (\Lambda^{kb} - \hat{\Lambda}^{kb}) u_b$. In particular, we can choose $\hat{\Lambda}^{kb} = \Lambda^{kb}$ and reduce the related f^k to zero.

For A diagonal there exists also the following equivalence transformation

$$u_1 \to u_1 \exp(-kt), \quad u_2 \to u_2 + nt, \tag{47}$$

$$u_1 \to u_1 - tu_2 + \frac{t^2}{2} p, \quad u_2 \to u_2 - tp, \tag{48}$$

$$u_1 \to u_1 + \frac{pt^2}{2}, \quad u_2 \to u_2 + pt. \tag{49}$$

Moreover, (48) is valid only for the case when A is proportional to the unit matrix.

Solutions present in Table V are defined up to equivalence transformations (26) and (46)–(49).

Using the transformation

$$u_1 \to \exp(nt) u_1, \quad u_2 \to \exp\left(-\frac{qn}{r} \right) u_2,$$

it is possible to reduce to zero the parameter n in Table III, item 1 (we will refer to this case as [T3.1]). The transformations $u_1 \to u_1, u_2 \to u_2 + \nu t + \mu x^2$ enable us to make zero parameters C_1 and C_2 in the cases when f^1 and f^2 have the form $f^1 = \varphi_1 + C_1, f^2 = \varphi_2 + C_2$ where φ_1 and φ_2 are given functions of u_1. Such transformations can be applied in the cases [T3.10] and [T3.8] (in the last case it is necessary to change roles of u_1 and u_2).

Transformations $u_2 \to \exp(-nt) u_2$ and $u_2 \to \exp(-bt) u_2$ give rise to new n and b in solutions 2 and 3 from Table IV, respectively. The transformation

$$u_1 \to u_1 \exp(-st), \quad u_2 \to u_2 + \frac{sr}{k} t$$

reduces to zero parameter s in nonlinearities [T3.6].

Consider further the scale transformation

$$u_1 \to \mu u_1, \quad u_2 \to \nu u_2, \quad t \to \lambda t \quad x \to \sqrt{\lambda} x. \tag{50}$$

Under obvious conditions for the parameters defining the functions f_1 and f_2 transformations (50) enable the reduction of nonzero coefficients p and q to zero coefficients for solutions 1, 8, and 9 from Table IV.

We see that using equivalence transformations it is possible to make ''cosmetic'' improvements to the solutions found for f^k. These transformations were not used systematically because they do not change the principal classes of solutions. Also in some cases their use would complicate the presentation of the results in standard form and make them less convenient for applications.

VII. DISCUSSION

In this article we have found all possible versions of systems of diffusion equations that admit a nontrivial Lie symmetry. These results can be used to construct mathematical models with required symmetry properties in, for example, physics, biology, and chemistry.

In the case when the matrix A is proportional to the unit matrix I Eq. (24) admits nontrivial symmetries for *all* f^1, f^2 given in Tables II–IV. In other words in this case we have obtained the richest spectrum of possible symmetries. If A is not proportional to I, the number of symmetries is sufficiently reduced by the requirement of commutativity of A^{-1} with the chosen matrices B and F in (43).

In the particular case when matrix A has the form Ib from (25) our results can be compared with those of Ref. 12. Our results are quite similar. However, a number of our solutions, namely, seven of those presented in Table IV, case 1 (which correspond to symmetries Z_N), solutions [T4.3] for $b=k=q=0$, [T5.2], [T3.8] for $p\neq 0$, [T3.11], and all solutions [T4.4] [T4.5], and [T4.7] are missing in Ref. 12. In addition, [T2.17] is presented in Ref. 12 incorrectly (see Table V, item 9 here).

Consider the examples of reaction diffusion equations mentioned earlier in Sec. I.

(i) The activator-inhibitor reaction equations[1] are given by

$$\dot{u}_1-\frac{\partial^2 u_1}{\partial x^2}=\frac{u_1^2}{u_2}-bu_1,\quad \dot{u}_2-a\frac{\partial^2 u_2}{\partial x^2}=u_1^2-u_2,$$

and these are a particular case of Eq. (24) with the nonlinearities given in [T2.5] with $d=2,k=0,\varphi_1=u_1^2/u_2-b,\varphi_2=u_1^2/u_2-1$, and so admits the symmetry

$$X=X_0+\alpha\left(u_1\frac{\partial}{\partial u_1}+2u_2\frac{\partial}{\partial u_2}\right).$$

(ii) The primitive predator-prey system can be defined by[1]

$$\dot{u}_1-D\frac{\partial^2 u_1}{\partial x_2}=-u_1u_2,\quad \dot{u}_2-\lambda D\frac{\partial^2 u_2}{\partial x^2}=u_1u_2.$$

This is a particular case of (24) with nonlinearities [T2.1] where $d=1,k=1,\varphi_2=-\varphi_1=u_2/u_1$, and so it admits the symmetry

$$X=X_0+\alpha\left(D_0-2u_1\frac{\partial}{\partial u_1}-2u_2\frac{\partial}{\partial u_2}\right).$$

(iii) The $\lambda-\omega$ reaction-diffusion system

$$\dot{u}_1=D\Delta u_1+\lambda(R)u_1-\omega(R)u_2,\quad \dot{u}_2=D\Delta u_2+\omega(R)u_1+\lambda(R)u_2, \tag{51}$$

where $R^2=u_1^2+u_2^2$ and Δ is the Laplacian operator, has symmetries that were analyzed in paper Ref. 2. Again we recognize that this system is a particular case of (24) with nonlinearities [T2.6] with $n=0$. Hence it admits the five-dimensional Lie algebra generated by

$$X=X_0+\alpha\left(u_1\frac{\partial}{\partial u_2}-u_2\frac{\partial}{\partial u_1}\right), \tag{52}$$

which is in accordance with results of Ref. 2 for the case when functions λ and ω are arbitrary. Moreover, using Table III, case [T3.2] we find that for the cases when

$$\lambda=\kappa_1R^r,\quad \omega=\kappa_2R^r, \tag{53}$$

Eq. (51) admits additional symmetry with respect to scaling transformations given by the operator

$$X=X_0+\alpha\left(u_1\frac{\partial}{\partial u_2}-u_2\frac{\partial}{\partial u_1}\right)+\nu D_5. \tag{54}$$

(iv) The nonlinear Schrödinger equation in m-dimensional space, is given by

$$\left(i\frac{\partial}{\partial t} - \sum_{i=1}^{m} \frac{\partial^2}{\partial x_i^2} \right) \psi = F(\psi, \psi^*)\psi, \tag{55}$$

also is a particular case of (24). If we denote

$$u_1 = \frac{1}{2}(\psi + \psi^*), \quad u_2 = \frac{1}{2i}(\psi - \psi^*), \tag{56}$$

then (55) reduces to the form (24) with $A = -\sigma_2$ and

$$f^1 = \frac{1}{2}(F^* + F)u_2 + \frac{1}{2i}(F - F^*)u_1, \quad f^2 = \frac{1}{2i}(F - F^*)u_2 - \frac{1}{2}(F + F^*)u_1. \tag{57}$$

In other words, any solution given in Table III–V with matrices belonging to classes I ($d = 0$) and II gives rise to the nonlinearity

$$F = \frac{1}{R^2}(u_2 f^1 - u_1 f^2 + i(u_2 f^2 + f^1 u^1)) \tag{58}$$

for the nonlinear Schrödinger equation (55) that admits a nontrivial Lie symmetry. In the cases [T3.7] with $n = 0$, [T3.2] for $s = l = q = 0$, $r \neq 4/m$ and $r = 4/m$, and [T4.8] for $k_1 = n_1 = k_0 = 0$, $p = q$, we recognize the well-known nonlinearities[11]

$$F = F(\psi^* \psi), \quad F = (\psi^* \psi)^k, \quad F = (\psi^* \psi)^{2/m}, \quad F = \ln(\psi^* \psi), \tag{59}$$

which correspond to extended symmetries. Our analysis makes it possible to describe all other possible versions of the nonlinear Schrödinger equation with a nontrivial symmetry. We plan to discuss these elsewhere.

Higher symmetries of the linear and nonlinear Schrödinger equations were investigated in Ref. 14; extended supersymmetries were studied in Ref. 15 The nonlinear Schrödinger equations and Eqs. (24) for diagonal A with *ad hoc* required symmetry with respect to the (extended) Galilei group were analyzed in Refs. 11 and 16. We notice that the algorithm used in the present article reduces such an analysis to routine and simple calculations. For example, to find all systems (1) *with arbitrary n* which are invariant with respect to the Galilei group it is sufficient to solve the system of homogeneous linear equations (31), which is easily integrated for any given invertable matrix A.

In the present article we have restricted ourselves to a complete description of all possible nonlinearities which generate Lie symmetry of Eq. (1). We have not analyzed nonclassical symmetries that may be found with using condition (13) nor have any symmetry reductions been presented. These problems will be a subject of further investigations. Finally, we remark that some of the results of this article have been presented in Ref. 17.

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Statistical turbulence suppression by a strong magnetic field: A Feynman path integral argument

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We show the suppression of the randomness of the magnetohydrodynamic flux (modeled by the Navier–Stokes equation) in the presence of a random stirring by a Feynman path integral one-loop and low viscosity argument. Additionally, we show exactly the above supressing turbulence phenomenon in the context of Beltrami fluxes. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1319858]

I. INTRODUCTION

One of the long-standing unsolved problems in turbulent magnetohydrodynamics going back to L. Landau (Ref. 1, p. 238) is to produce quantitative arguments for the charged fluid motion turbulence suppression by the presence of a strong magnetic field. In this article, we propose to present in Sec. II such an argument by using our Feynman path integral formulation for turbulence[2] at a low viscosity (turbulent) regime in the context of a background one-loop (Gaussian) approximation. Additionally, we show in Sec. III the above cited suppressing phenomena in the exactly soluble (nonperturbative) path integral context of Beltrami fluxes.

II. THE ONE-LOOP CASE

Let us start our analysis by considering the Navier–Stokes equation for a charged fluid flux in the presence of an uniform magnetic field $\mathbf{B}$ in the z direction and a uniform electric field $\mathbf{E}$ in the plane (x,y):

$$\frac{\partial \mathbf{V}(\mathbf{r},t)}{\partial t}+(\mathbf{V}\cdot\boldsymbol{\nabla})\mathbf{V}(\mathbf{r},t)=\left(e\mathbf{E}+\frac{1}{c}(\mathbf{V}(\mathbf{r},t)\times\mathbf{B})\right)+\nu\Delta\mathbf{V}(\mathbf{r},t)-(\mathbf{grad}P)(\mathbf{r},t)+\mathbf{F}^{\mathrm{ext}}(\mathbf{r},t). \quad (1)$$

Here, the random stirring force (caused by the fluid flux turbulent regime in the statistical-Langevin approach[2]) is such that it satisfies the white-noise Gaussian statistics with disorder strength $D>0$:

$$\langle (F^{\mathrm{ext}})_i(\mathbf{r},t)(F^{\mathrm{ext}})_j(\mathbf{r}',t')\rangle = D\,\delta_{ij}\delta^{(3)}(\mathbf{r},\mathbf{r}')\,\delta(t-t'). \quad (2)$$

It is worthwhile to remark that the presence of such external random fluctuations are considered in this statistical framework with the same conceptual role as used in the usual Langevin–Einstein approach for the study of Brownian motion. It is still missing a turbulence theory for first principles, leading to the master Eq. (1) with Eq. (2).

Now a functional integral shift[2] leads to the exact characteristic functional path integral expression for the random (turbulence) process defined by the magnetohydrodynamic (incompressible) fluid flux Eq. (1) after taking into account the fluid incompressibility condition on the fluid motion $\mathrm{div}\,\mathbf{V}(\mathbf{r},t)=0$ and disregarding the transverse part of the term $((\mathbf{V}\cdot\nabla)\mathbf{V})^{\mathrm{tr}}$ coming from the above mentioned incompressibility condition (see Ref. 2). We obtain, thus, the following Burger magnethydrodynamical turbulent path integral as the main object of our study:

$$Z[\mathbf{J}(\mathbf{r},t)]=\frac{1}{Z[0]}\int D^F[\mathbf{V}(\mathbf{r},t)]\exp\left\{-\frac{1}{2D}\int_{-\infty}^{+\infty}d^3\mathbf{r}\int_{-\infty}^{\infty}dt\left[\frac{\partial}{\partial t}\mathbf{V}-\nu\Delta\mathbf{V}+((\mathbf{V}\cdot\boldsymbol{\nabla})\mathbf{V})\right.\right.$$
$$\left.\left.-\left(e\mathbf{E}+\frac{1}{c}(\mathbf{V}(\mathbf{r},t)\times\mathbf{B})\right)\right]^2(\mathbf{r},t)\right\}\exp\left\{i\int_{-\infty}^{+\infty}d^3\mathbf{r}\int_{-\infty}^{\infty}dt\mathbf{J}(\mathbf{r},t)\cdot\mathbf{V}(\mathbf{r},t)\right\}. \quad (3)$$

Note that the square brackets in the above equation are the usual R^3-norm.

In order to show the randomness suppression of the fluid flux motion in the plane (x,y) normal to the magnetic field B at its strong field limit regime $B\to\infty$, we consider the background flux decomposition

$$\mathbf{V}(\mathbf{r},t)=\boldsymbol{\phi}+\sqrt{D}\mathbf{v}(\mathbf{r},t), \quad (4)$$

where the background flux $\boldsymbol{\phi}$ satisfies the steady-isotropic Ohm's law flux condition $(i=1,2,3)$

$$eE_i=-\frac{1}{c}\varepsilon_{ijk}\phi_jB\delta_{k3}. \quad (5)$$

As for the usual pertubative arguments in quantum field theories (Refs. 2 and Ref. 3, p. 29), we consider the usual one-loop Gaussian approximation for the path integral (3) with the following result:

$$S^{(\varepsilon)}_{\text{one loop}}[\mathbf{v}(\mathbf{r},t)]=\int d^3\mathbf{r}dt(v_1(\mathbf{r},t),v_2(\mathbf{r},t),v_3(\mathbf{r},t)$$

$$\begin{bmatrix} -\left(\frac{\partial}{\partial t}+\phi_i\frac{\partial}{\partial x_i}\right)^2+\frac{B^2}{c^2}+\nu^2\Delta^2 & \frac{2B}{c}\left(\frac{\partial}{\partial t}+\phi^i\frac{\partial}{\partial x_i}\right)+\frac{2\nu}{c}B\Delta & 0 \\ -\frac{2B}{c}\left(\frac{\partial}{\partial t}+\phi^i\frac{\partial}{\partial x_i}\right)-\frac{2}{c}(\nu+\varepsilon)B\Delta & -\left(\frac{\partial}{\partial t}+\phi_i\frac{\partial}{\partial x_i}\right)^2+\frac{B^2}{c^2}+\nu^2\Delta^2 & 0 \\ 0 & 0 & -\left(\frac{\partial}{\partial t}+\phi_i\frac{\partial}{\partial x_i}\right)^2 \end{bmatrix}$$

$$(v_1(\mathbf{r},t),v_2(\mathbf{r},t),v_3(\mathbf{r},t))^T, \quad (6)$$

where we have given a small ε-parameter to the viscosity term in the (2,1) entry of the Gaussian weight matrix associated to our mathematical one-loop theory [defined by just disregarding the nonlinear (cubic and quartic) terms]. Note that this parameter keeps the important interaction viscosity and magnetic field nonzero at this one-loop order.

Let us show the vanishing of the two-point correlation flux at the limit of the very strong magnetic field $B\to\infty$ in the plane (x,y) within the turbulent regime, which is defined phenomenologically in our approach by considering ν such that $B^2/c^2\Lambda^4\gg\nu^2$ and, by its turn, forces us to neglect the term $\nu^2(\Delta\mathbf{v})^2$ in relation to other terms in the matrix entry terms.

Let us use the following matrix inversion formulas to obtain the explicit expression for the flux two-point correlation functions,

$$\begin{bmatrix} a & b & 0 \\ -b+\delta & a & 0 \\ 0 & 0 & c \end{bmatrix}^{-1} = \begin{bmatrix} +\left(\dfrac{a}{a^2-b(-b+\delta)}\right) & -\left(\dfrac{b}{a^2-b(-b+\delta)}\right) & 0 \\ -\left(\dfrac{-b+\delta}{a^2-b(-b+\delta)}\right) & \left(\dfrac{a}{a^2-b(b+\delta)}\right) & 0 \\ 0 & 0 & +\left(\dfrac{1}{c}\right) \end{bmatrix}, \tag{7a}$$

where in momentum frequency space we have explicitly the following matrix entries:

$$\begin{aligned} a &= (w+\mathbf{k}\cdot\boldsymbol{\phi})^2+\frac{B^2}{c^2}, \\ b &= i\frac{2B}{c}(w+\mathbf{k}\cdot\boldsymbol{\phi})^2-\frac{2\nu}{c}B|\mathbf{k}|^2, \\ c &= (w+\mathbf{k}\cdot\boldsymbol{\phi})^2, \\ \delta &= -2\varepsilon\frac{B}{c}|\mathbf{k}|^2. \end{aligned} \tag{7b}$$

Since we are going to remove the parameter ε at the end of our calculations, we can safely use the approximation $\sqrt{b^2-\delta b}=b\sqrt{1-\delta/b^2}\cong b(1-\frac{1}{2}(\delta/b)=b-\delta/2$ in Eq. (7a).

We thus obtain the following structure for the (1,1) entry of the inverse matrix Eq. (7a):

$$\frac{a}{a^2+b^2-b\delta}=\frac{1}{2}\left(\frac{1}{a-i\sqrt{b^2-b\delta}}+\frac{1}{a+i\sqrt{b^2-b\delta}}\right)\cong\frac{1}{2}\left(\frac{1}{a+\frac{1}{2}i\delta-ib}+\frac{1}{a-\frac{1}{2}i\delta+ib}\right). \tag{7c}$$

As a consequence of Eq. (7c) we have the result below for the $x-x$ two-point correlation function in our one-loop approximation:

$$\begin{aligned} \langle v_1(\mathbf{r},t),v_1(\mathbf{r}',t')\rangle = \int_{|\mathbf{k}|<\Lambda} d^3\mathbf{k}\exp[i\mathbf{k}((\mathbf{r}-\mathbf{r}')-\boldsymbol{\phi}(t-t'))]\frac{1}{2}\int_{-\infty}^{+\infty}d\overline{w}e^{-i\overline{w}(t-t')} \\ \times\left\{\left(\frac{1}{\overline{w}^2+(2B/c)\overline{w}+(B^2/c^2-\frac{1}{2}i\delta+(2i\nu/c)B|\mathbf{k}|^2)}\right)\right. \\ \left.+\left(\frac{1}{\overline{w}^2-(2B/c)\overline{w}+(B^2/c^2-\frac{1}{2}i\delta-(2i\nu/c)B|\mathbf{k}|^2)}\right)\right\}. \end{aligned} \tag{8}$$

The first frequency $\overline{w}$-integral Eq. (8) may easily be evaluated by means of the residue theorem applied in the (causal) lower half-plane region $\mathrm{Im}(\overline{w})<0$ {after removing the regularizing parameter $\varepsilon\to 0$ [see Eq. (6)]}:

$$\overline{w}-\text{integral} = \lim_{\varepsilon\to 0}\left(\frac{2\pi\{-\exp[-i(-B/c-\sqrt{((2\nu-\varepsilon)/c)B}|\mathbf{k}|(-\sqrt{2}/2+i\sqrt{2}/2))(t-t')]\theta(t-t')\}}{2(-|\mathbf{k}|(\sqrt{(2\nu-\varepsilon)B/c})\sqrt{2}/2+i|\mathbf{k}|(\sqrt{2}/2)(\sqrt{(2\nu-\varepsilon)B/c}))}\right) \tag{9a}$$

or

$$\langle v_1(\mathbf{r},t),v_1(\mathbf{r}',t')\rangle$$

$$= -2\pi i \frac{\exp((iB/c)(t-t'))\times\theta(t-t')}{\sqrt{(2\nu/c)B}|(\mathbf{r}-\mathbf{r}')-\boldsymbol{\phi}(t-t')|(-\sqrt{2}/2+i(\sqrt{2}/2))}$$

$$\times\left[\frac{1}{2i}\left(\frac{1}{i(-|(\mathbf{r}'-\mathbf{r})-\boldsymbol{\phi}(t-t')-\sqrt{(2\nu/c)B}(\sqrt{2}/2)(t-t')\sqrt{(2\nu/c)B}(t-t'))}\right.\right.$$

$$\left.\left.-\text{complex conjugate}\right)\right]. \tag{9b}$$

Note that we have considered only the residue at the pole $w_+ = -B/c + |\mathbf{k}|\sqrt{[(2\nu-\varepsilon)/c]B} - i\sqrt{2/2}|\mathbf{k}|\sqrt{((2\nu-\varepsilon/c)B}$ in the lower half-plane which by its turn leads straightforwardly to the causal Fourier transform Eq. (9a) vanishing at $t\to\infty$. Now it is easy to see that at the large $B\to\infty$ limit with ν very small *but fixed*, the integral Eq. (9) vanishes. A similar result holds true for the second term of the $\overline{w}$-integral Eq. (8) and produces, thus, the suppression of the randomness at the limit of $B\to\infty$ within our one-loop leading small viscosity approximation, namely,

$$\lim_{B\to\infty}\langle v_1(\mathbf{r},t)v_1(\mathbf{r}',t')\rangle\to 0. \tag{10}$$

Analogously

$$\lim_{B\to\infty}\langle v_1(\mathbf{r},t)v_2(\mathbf{r}',t')\rangle = \lim_{B\to\infty}\langle v_2(\mathbf{r},t)v_2(\mathbf{r}',t)\rangle = 0. \tag{11}$$

However, the flux randomness in the B direction in this context is given exactly by the nonvanishing result (with $\Lambda\to\infty$)

$$\langle v_3(\mathbf{r},t),v_3(\mathbf{r},t)\rangle = \delta^{(3)}((\mathbf{r}-\mathbf{r}')-\boldsymbol{\phi}(t-t'))\frac{e^{-\nu(t-t')}}{\nu}\theta(t-t'). \tag{12}$$

At this point, it is very important to remark that the zero viscosity (full tubulent) regime is a *singular* limit never reached in our approach, a result opposite to those of the instanton calculations of Ref. 4.

Let us comment that our argument is not a theorem and is entirely based on a formal perturbative one-loop approximation for the path integral Eq. (3). Next-loop corrections for Eq. (3) are still an open problem in our framework since the usual renormalization program borrowed from relativistic quantum fields does not make sense in the turbulence context[5] (the usual power counting analysis and unitary conditions are meaningless here). Anyway, it is possible to evaluate ''next-loop corrections'' by introducing a cutoff $|\mathbf{k}|<\Lambda$ and the nonlinear terms in the functional integral weight in Eq. (3). An alternative proposal to analyze Eq. (3) is to devise scaling-decimation (nonperturbative) smearing of short wavelength modes in the momentum space as usually implemented in critical phenomena.[6]

Finally, let us make a strict mathematical comment. It is well known from the rigorous mathematical literature that the Navier–Stokes (NS) equation with completely delta-correlated noise in space cannot be studied rigorously in the sense that it is not possible to prove that it has a solution which is a random field. However, let us conjecture that the *integral equation* version of the NS equation may overcome the estimative problems involved in such unsuccessful mathematical attempts, namely,[2]

$$A_i[\mathbf{v}(\mathbf{r},t)] = B_i[\mathbf{F}(\mathbf{r},t)] \tag{13}$$

with

$$A_i[\mathbf{v}]=v_i(\mathbf{r},t)-\int_0^\infty ds\int_{R^3}d^3\mathbf{r}'O_{ijk}(\mathbf{r}-\mathbf{r}',t-t')\times(V_iV_k)(\mathbf{r}',t') \tag{14}$$

and

$$B_i[\mathbf{F}]=\int_0^\infty ds\int_{R^3}d^3\mathbf{r}'H_{(1)}(\mathbf{r}-\mathbf{r}',t-t')F_i(\mathbf{r}',t'). \tag{15}$$

Here the kernels O_{ijk} and $H_{(1)}$ are given respectively by

$$\begin{aligned} O_{ijk}(z,\xi)&=-\frac{1}{2}\left(\frac{\partial\overline{O}_{ik}}{\partial z_{\not j}}+\frac{\partial\overline{O}_{i\not j}}{\partial z_k}\right)(z,\xi),\\ \widetilde{O}_{pq}(z,\xi)&=\delta_{pq}\theta(\xi)H_0(|z|,\xi)+\frac{\partial^2}{\partial z_p\partial z_q}\left(\frac{2\nu\xi}{|z|}\int_0^{|z|}H_0(|z'|,\xi)dz'\right), \end{aligned} \tag{16}$$

$$H_{(0)}(|z|,\xi)=\frac{1}{(4\pi\nu|\xi)^{3/2}}\exp\left(-\frac{|z^2|}{4\pi\nu\xi}\right) \tag{17}$$

$$H_{(1)}(|z|,\xi)=\theta(\xi)H_{(0)}(|z|,\xi). \tag{18}$$

Anyway, we took the philosophy that the functional integral Eq. (3) is the main passive object to be analyzed mathematically (that functional integral should define the NS random equation!). It is very worthwhile to remark that the differential nonlinear NS equation does not make sense in principle for fluid configurations which are distributional objects as it must be expected with completely delta-correlated noise in space as we have shown in this article.

Note that in this path integral framework, the usual nonrandom NS equation is correctly obtained from the minimum functional point limit $D\to 0$ in Eq. (3). The objects that satisfy the differential Navier–Stokes equation with randomness are now the n-point correlation functions

$$\lim_{\mathbf{J}\to 0}\{\delta^N Z[\mathbf{J}(\mathbf{r},t)]/\delta J_1(\mathbf{r}_1,t_1)\cdots\delta J_N(\mathbf{r}_N,t_N)\}=\langle v_1(\mathbf{r}_1,t_1)\cdots v_N(\mathbf{r}_N,t_N)\rangle\times(-1)^N. \tag{19}$$

At this point we call to the reader's attention that this infinite-coupled set of classical equations must be shown to have a rigorous mathematical solution instead of the formal mathematical object in Eq. (1).

As a final comment on our perturbative argument presented here, let us point out that in the case *of not neglecting the term* $\nu^2\Delta^2$ in Eq. (7a), Eq. (8) now takes the following form (with $\Lambda=\infty$ and $\varepsilon=0$!):

$$\begin{aligned} \langle v_1(\mathbf{r},t)v_1(\mathbf{r}',t')\rangle=&\int_{-\infty}^{+\infty}d^3\mathbf{k}e^{i[\mathbf{k}((\mathbf{r}-\mathbf{r}')-\phi(t-t'))]}\times\frac{1}{2}\int_{-\infty}^{+\infty}d\overline{w}e^{-i\overline{w}(t-t')}\\ &\times\left\{\left(\frac{1}{\overline{w}^2+(2B/c)\,\overline{w}+(B^2/c^2+\nu^2|\mathbf{k}|^4+(2i\nu/c)\,B|\mathbf{k}|^2)}\right)\right.\\ &\left.\times\left(\frac{1}{\overline{w}^2-(2B/c)\overline{w}+(B^2/c^2+\nu^2|\mathbf{k}|^4-(2i\nu/c)\,B|\mathbf{k}|^2)}\right)\right\}. \end{aligned} \tag{20}$$

The same analysis implemented to Eq. (9) may be applied and leads to the same qualitative formal result. For instance, we have the behavior at large B

$$\lim_{B\to\infty}\int_{-\infty}^{+\infty} d\overline{w} e^{-\overline{w}(t-t')}\left(\frac{1}{\overline{w}^2+(2B/c)\overline{w}+(B^2/c^2+\nu^2|\mathbf{k}|^4-(2i\nu/c)B|\mathbf{k}|^2)}\right)$$
$$\times \lim_{B\to\infty}\exp\left\{-it\left(-\frac{B}{c}-\nu k^2\left(1+\frac{4B^2}{\nu^2c^2|\mathbf{k}|^4}\right)^{1/4}\left(i\frac{\sqrt{2}}{2}-\frac{\sqrt{2}}{2}\right)\right)\right\}$$
$$\simeq \lim_{B\to\infty}\exp\left\{-\left[\nu|\mathbf{k}|^2 t\frac{\sqrt{2}}{2}\left(1+\frac{4B^2}{\nu^2c^2|\mathbf{k}|^4}\right)^{1/4}\right]\right\}\sim 0, \tag{21}$$

which again indicates the randomness suppression at the limit of a very strong magnetic field for a charged fluid under the presence of an eletromagnetic field (laser) for any value of ν (including the case of physical turbulence phenomenologically modeled with very small ν).

III. A SOLUBLE MODEL OF TURBULENCE SUPPRESSION IN TURBULENT MAGNETOHYDRODYNAMICS

The celebrated Landau conjecture on the suppressing of turbulence (or randomness in the statistical approach) by a strong magnetic field, analyzed in Sec. II within the context of the path integral approximations stated there, can be displayed exactly in the following reduced degrees of freedom model of Beltrami fluxes in a turbulent regime defined analitically by $\mathrm{rot}\mathbf{v}(\mathbf{r},t)=\lambda\mathbf{v}(\mathbf{r},t)$.[7]

Let us, thus, start with the magnetohydrodynamical Navier–Stokes Eq. (1) in the following suitable form for Beltrami fluxes:

$$\frac{\partial\mathbf{v}(\mathbf{r},t)}{\partial t}+\left\{\frac{1}{2}\,\mathrm{grad}[(\mathbf{v}\cdot\mathbf{v})(\mathbf{r},t)]-(\mathbf{v}\times\mathrm{rot}\cdot\mathbf{v})(\mathbf{r},t)\right\}$$
$$=-\,\mathrm{grad}\,P(\mathbf{r},t)+\nu\Delta\mathbf{v}(\mathbf{r},t)+\mathbf{F}^{\mathrm{ext}}(\mathbf{r},t)+\frac{1}{c}(\mathbf{v}(\mathbf{r},t)\times\mathbf{B}). \tag{22}$$

It is important to remark that the wave vectors of the Beltrami hydrodynamical motions have eddies of a fixed scale $|\mathbf{k}|=\lambda$, as consequence of a Fourier (wave vector) transformation of the Beltrami condition.[7]

Let us, thus, suppose that the random stirring force in Eq. (23) satisfies the *spatially nonlocal* Gaussian statistics

$$\langle(F^{\mathrm{ext}})_i(\mathbf{r},t);(F^{\mathrm{ext}})_j(\mathbf{r}',t')\rangle_{|\mathbf{k}|=\lambda}=\lambda^2\delta_{ij}((\Delta^{-1})\delta(\mathbf{r}-\mathbf{r}')\delta(t-t'). \tag{23}$$

At this point, we remark that we assume implicity the same vector constraint $|\mathbf{k}|=\lambda$ in our random stirring equation (24), namely the exact expression for the right-hand side of Eq. (24) is given below:

$$\langle(F^{\mathrm{ext}})_i(\mathbf{r},t);(F^{\mathrm{ext}})_j(\mathbf{r}',t)\rangle=\frac{\delta_{ij}\cdot\lambda\cdot\mathrm{Sen}(\lambda|\mathbf{r}-\mathbf{r}'|)}{2\pi|\mathbf{r}-\mathbf{r}'|}\cdot\delta(t-t'). \tag{24}$$

At this point in our study, we consider the already mentioned Beltrami flux condition and its direct consequences, namely,

$$\lambda^2\mathbf{v}(\mathbf{r},t)=\mathrm{rot}(\mathrm{rot}\,\mathbf{v}(\mathbf{r},t))=-\Delta\mathbf{v}(\mathbf{r},t), \tag{25}$$

$$(\mathbf{v}\times\mathrm{rot}\,\mathbf{v})(\mathbf{r},t)=(\mathbf{v}\times\lambda\mathbf{v})(\mathbf{r},t)=0, \tag{26}$$

in order to replace the Navier–Stokes Eq. (23) by the exactly soluble Langevin-type fluid flux stirred by the external force $\mathbf{\Omega}^{\mathrm{ext}}(\mathbf{r},t)=\mathrm{rot}(\mathbf{F}^{\mathrm{ext}})(\mathbf{r},t)$:

$$\frac{\partial \mathbf{v}(\mathbf{r},t)}{\partial t}=(-\nu\lambda^2)\mathbf{v}(\mathbf{r},t)+\frac{1}{\lambda}\mathbf{\Omega}^{\mathrm{ext}}(\mathbf{r},t)+\frac{1}{c\lambda}(\mathbf{B}\cdot\mathbf{\Delta})\mathbf{v}(\mathbf{r},t). \tag{27}$$

Here the new external stirring $\mathbf{\Omega}^{\mathrm{ext}}(\mathbf{r},t)$ satisfies a Gaussian process with the following two-point correlation function (again with $|\mathbf{k}|=\lambda$!):

$$\langle \Omega_{\mathrm{l}}^{\mathrm{ext}}(\mathbf{r},t);\Omega_{\mathrm{l}'}^{\mathrm{ext}}(\mathbf{r}',t')\rangle=\lambda^2\delta^{\mathrm{ll}'}\delta^{(3)}(\mathbf{r}-\mathbf{r})\,\delta(t-t')-\lambda^2\partial_{\mathrm{l}}^{(r)}\partial_{\mathrm{l}'}^{(r')}(\Delta_r^{-1}\delta(\mathbf{r}-\mathbf{r}'))\,\delta(t-t'). \tag{28}$$

Now a simple functional integral shift leads to the following exactly soluble Feynman path integral for our Beltrami magnetohydrodynamic reduced model:

$$Z[\mathbf{j}(\mathbf{r},t)=\frac{1}{Z(0)}\times\int D^F[\mathbf{v}(\mathbf{r},t)]\exp\left\{-\frac{1}{2}\int_{-\infty}^{+\infty}dr^3\int_0^{\infty}dt\left[\frac{\partial\mathbf{v}}{\partial t}-\frac{1}{\lambda c}(\mathbf{B}\cdot\nabla)\mathbf{v}+\nu\lambda^2\mathbf{v}\right]^2(\mathbf{r},t)\right\}$$
$$\times\exp\left\{i\int_{-\infty}^{+\infty}d^3\mathbf{r}\int_0^{\infty}dt(\mathbf{j}\cdot\mathbf{v})(\mathbf{r},t)\right\}. \tag{29}$$

It is worthwhile remarking that we have used incompressible constraint $\partial_i^{(r)}v^i(\mathbf{r},t)=0$ to obtain that the spatially nonlocal piece of Eq. (29) does not contribute to the final path integral weight in Eq. (30).

Now the Fourier transformed expression for the correlation functions associated to the Beltrami magnetohydrodynamical model Eq. (30) are given exactly by (note again the wave vector constraint $|\mathbf{k}|=\lambda$ in the model formulas!)

$$\langle v_i(\mathbf{r},t)v_j(\mathbf{r}',t')\rangle=\delta_{ij}\times\frac{e^{-\nu\lambda^2|t-t'|}}{\nu\lambda^2}\times\left\{\int_{|\mathbf{k}|=\lambda}d^3\mathbf{k}e^{i\mathbf{k}[(\mathbf{r}-\mathbf{r}')-\mathbf{B}/c\lambda\,(t-t')|]}\right\}$$
$$=2\,\delta_{ij}\left(\frac{e^{\nu\lambda^2|t-t'|}}{\nu\lambda}\right)\frac{\mathrm{sen}[\lambda(|\mathbf{r}-\mathbf{r}')-(\mathbf{B}/c\lambda)\,(t-t')|)]}{|(\mathbf{r}-\mathbf{r}')-(\mathbf{B}/c\lambda)\,(t-t')|}. \tag{30}$$

It is a direct consequence of the exact expression of Eq. (29) that for the limit of strong magnetic field $|\mathbf{B}|\to\infty$, we get the vanishing of the correlation functions [Eq. (29)] and, thus, the exactly randomness suppression in our Beltrami magnetohydrodynamical model Eq. (28) and corroborate the Landau conjecture (Ref. 1) and the correctness of our one-loop calculations presented in the bulk of this article [Eqs. (10) and (11)].

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APPENDIX: THE ONE-LOOP ACTION

In this Appendix we show for completeness the Gaussian one-loop approximation for Eq. (3). Let us consider the complete functional integral weight

$$W[\mathbf{v}(\mathbf{r},t)]=\frac{1}{2D}\left[\frac{\partial v^i}{\partial t}+v^j\frac{\partial}{\partial x_j}v^i+(-\nu\Delta v^i)-eE^i-\frac{1}{c}\varepsilon^{ijk}v^jB^k\right]^2. \tag{A1}$$

By making the background field decomposition [Eq. (5)] on the manifold $\{\mathbf{v}(\mathbf{r},t)\}$ define the domain of the functional integral [Eq. (3)], one easily obtains the following result:

$$W[\mathbf{v}(\mathbf{r},t)]=\left(\frac{\partial v^i}{\partial t}\right)^2+\left(\phi_j\frac{\partial}{\partial x_j}v^i\right)^2+\nu^2(\Delta v^i)^2+\left(-\frac{1}{c}\varepsilon^{ijk}v^jB^k\right)^2+2\left(\frac{\partial v^i}{\partial t}\right)\left(\phi_j\frac{\partial}{\partial x_j}v^i\right)+2\left(\frac{\partial}{\partial t}v^i\right)$$
$$\times(-\nu\Delta v^i)+2\left(\frac{\partial v^i}{\partial t}\right)\left(-\frac{1}{c}\varepsilon^{ijk}v^jB^k\right)+2\phi_j\frac{\partial}{\partial\lambda_j}v^i(-\nu\Delta v^i)$$
$$+2\phi_j\frac{\partial}{\partial x_j}v^i\left(-\frac{1}{c}\varepsilon^{ijk}v^jB^k\right)+\frac{2\nu}{c}\Delta v^i\varepsilon_{ijk}v^jB^k+\text{nonquadratic terms.} \tag{A2}$$

Since under the integration on $R^3\times R$ the terms below are zero and since $\lim_{t\to\pm\infty}v^i(\mathbf{r},t)=\lim_{|\mathbf{r}|\to+\infty}v^i(\mathbf{r},t)=0$, namely

$$\int_{-\infty}^{+\infty}dt\int_{-\infty}^{+\infty}d^3\mathbf{r}\left(\frac{\partial v^i}{\partial t}\Delta v_i\right)(\mathbf{r},t)=\int_{-\infty}^{+\infty}d^3r\Delta\left(\int_{-\infty}^{+\infty}\frac{1}{2}\frac{\partial}{\partial t}(v^iv_i)=0\right), \tag{A3}$$

$$\int_{-\infty}^{+\infty}dt\int_{-\infty}^{+\infty}d^3\mathbf{r}\left(\left(\phi_j\frac{\partial}{\partial x_j}v^i\right)(\Delta v_i)\right)(\mathbf{r},t)=\int_{-\infty}^{+\infty}dt\int_{-\infty}^{+\infty}d^3\mathbf{r}\phi_jv^i\left(\left(\frac{\partial}{\partial x_j}v^i\right)\right)$$
$$=\int_{-\infty}^{+\infty}dt\int_{-\infty}^{+\infty}d^3\mathbf{r}\phi_j\Delta v^i\frac{\partial}{\partial x_j}v_i=0. \tag{A4}$$

Besides, we have kept a small ε-regularization of the important interaction term among viscosity and the magnetic field:

$$2\left(\frac{\nu}{c}\Delta v^i\right)(\varepsilon^{ijk}v^jB^k)\leftrightarrow\frac{2\nu}{c}\Delta v^i\cdot v_2B-\frac{2(\nu+\varepsilon)}{c}\Delta v^2\cdot v_1B. \tag{A5}$$

As a result we obtain the result shown in Eq. (6) under the form of an operator valued 3×3 matrix defining the Gaussian one-loop approximation of the full path integral weight Eq. (A1).

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New integrable equations of fourth order and higher degree related to Cosgrove's equation

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We give a general formulation of the algorithm of Fokas and Ablowitz, which then allows us to obtain transformations for nth order ordinary differential equations, to equations of the same order but perhaps of higher degree. Previously this algorithm has been used to obtain transformations for the six second order equations defining new transcendental functions discovered by Painlevé and co-workers, either to other equations in the Painlevé classification or to equations of second order and second degree. As an example of our approach we consider a new fourth order ordinary differential equation due to Cosgrove which is believed to define a new transcendent. We obtain transformations relating this equation to other fourth order ordinary differential equations, of degrees $\geqslant 2$. All of these transformations, as well as the corresponding higher degree differential equations, all of which have the Painlevé property, are new. © *2001 American Institute of Physics.*
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I. INTRODUCTION

As is well known, the six Painlevé equations ($P_I,\ldots,P_{VI}$) have for many years been the subject of much intensive research. One particular aspect of that research, of interest to many authors, has been the discovery of transformations relating a particular Painlevé equation either to itself (with possibly different values for any parameters appearing as coefficients), or to another second order ordinary differential equation (ODE). With this aim in mind, Fokas and Ablowitz[1] developed an algorithmic approach to obtaining transformations for second order ODEs in the Painlevé classification, either to second order ODEs linear in the second derivative (and so in the same Painlevé classification) or to ODEs of second order and second degree. In Ref. 1 the first of these two cases was investigated for P_{II}–P_V, and the second for P_{VI}. The second case has been investigated for P_I–P_{VI} in Refs. 2 and 3.

In the present article we give a general formulation of this algorithm, allowing us to obtain transformations for nth order ODEs of the form

$$V^{(n)}=F(V^{(n-1)},V^{(n-2)},\ldots,V;x), \tag{1}$$

where F is rational in $V^{(n-1)},\ldots,V$ with coefficients dependent on x, to ODEs of the same order but perhaps of higher degree. Thus we see that this algorithm can be applied to ODEs of order higher than 2, and can be used to obtain transformations to ODEs of degree greater than 2. As an example we apply this approach to a fourth order ODE recently found by Cosgrove, and which is believed to define a new transcendent.[4] We obtain transformations to a variety of fourth order ODEs, of degrees $\geqslant 2$. These transformations and the corresponding ODEs, all of which have the Painlevé property, are all new. We also indicate further possible extensions of this algorithm.

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II. THE FOKAS–ABLOWITZ ALGORITHM

Given an ODE of the form (1), we seek a transformation to an ODE in U, also of order n, defined by the relation

$$(dV^2+eV+f)U-(V'+aV^2+bV+c)=0, \tag{2}$$

where a, b, c, d, e and f are all functions of x only. Taking $n-1$ derivatives of this expression yields a polynomial in $U,\ldots,U^{(n-1)}$ and $V,\ldots,V^{(n)}$. Using (1) to replace $V^{(n)}$, and the jth derivative of (2) to replace $V^{(j+1)}$, $j=0,\ldots,n-2$, then gives a polynomial (say of degree N) in V with coefficients in $U,\ldots,U^{(n-1)}$,

$$\sum_{i=0}^{N}\alpha_i V^i=0. \tag{3}$$

In (3) each α_i is at most linear in $U^{(n-1)}$; in the case where F is a polynomial function of $V^{(n-1)},\ldots,V$, only α_0, α_1 and α_2 can depend on $U^{(n-1)}$.

In the general case, when $N>1$, we thus obtain V as an algebraic function of $U,\ldots,U^{(n-1)}$, and substitution into (2) then gives an ODE in U of order n related to (1) by the transformation (2). We could alternatively eliminate V between (2) and (3) by differentiating (3) and using (2) to replace V' in order to obtain a second polynomial in V, whose coefficients now also depend on $U^{(n)}$, and then successively eliminating leading order coefficients between this and (3), until we obtain an expression linear in V. Solving this for V and substituting back into (3)—or into one of the polynomials obtained during the elimination process—then gives an ODE in U of order n and of higher degree; the expression for V defines the inverse of (2).

However, of more interest than this general case is the case where, for certain choices of the coefficients a, b, c, d, e and f, the polynomial (3) reduces to a polynomial of degree less than N, say M,

$$\sum_{i=0}^{M}A_i V^i=0. \tag{4}$$

This occurs either when some leading order coefficients in (3) vanish, or when (3) factorizes, or both. We can explore the second of these cases by seeking a factorization of (3),

$$\sum_{i=0}^{N}\alpha_i V^i-\left(\sum_{i=0}^{N-M}g_i V^i\right)\left(\sum_{i=0}^{M}A_i V^i\right)=0, \tag{5}$$

where the coefficients A_i are functions of $U,\ldots,U^{(n-1)}$ and x, and the coefficients g_i are functions of x only, and $g_{N-M}=1$. [We proceed similarly if considering the factorization of (3) in the case where some leading order coefficients vanish.]

In the relation (5), we solve the coefficients of $V^N,\ldots,V^{N-M}$ for $A_M,\ldots,A_0$ (so $A_M=\alpha_N$). We then set the remaining coefficients of V identically to zero (as polynomials in $U,\ldots,U^{(n-1)}$) in order to determine g_i and any constraints on a, b, c, d, e and f. Provided that we are able to obtain a consistent solution, we then obtain a lower degree polynomial (4). In the case where $M=1$, V is easily determined from (4); substitution into (2) then gives an ODE of order n. In the case where $M>1$ we obtain the corresponding nth order ODE in U in the same way as discussed previously in the general case (3). [We note that obtaining an ODE of order n requires that at least one A_i in (4) depends on $U^{(n-1)}$; thus, for example, in the case where F is polynomial we must have $M=N-2$ or $N-1$.]

The above is a general statement of the algorithm presented in Refs. 1–3 for the case $n=2$ (second order) and $M=1$ or 2 (transformations to second order ODEs of degree 1 or 2). We note

that the requirement that all g_i are functions of x only is stronger than that usually made; we return to this point in the conclusions. We now consider the application of the above algorithm to a fourth order ODE.

III. APPLICATION TO COSGROVE'S EQUATION

We now consider a fourth order ODE due to Cosgrove,[4,5]

$$E[V] \equiv V'''' + 12VV'' + 6(V')^2 + \tfrac{32}{3}V^3 + p(V'' + 4V^2) - qX = 0, \tag{6}$$

where p and q are both constant. This ODE is of considerable interest, since it is believed to define a new transcendent.[4] Hierarchies of ODEs and partial differential equations (in $1+1$ and $2+1$ dimensions) related to the above ODE, together with their underlying linear problems, can be found in Refs. 6 and 7. Further generalizations can be found in Ref. 8.

Seeking a transformation for (6) as described above leads to a quintic in V [(3) with $N=5$],

$$\sum_{i=0}^{5} \alpha_i V^i = 0, \tag{7}$$

with α_0, α_1 and α_2 linear in U''', and with

$$\alpha_5 = 24(a - dU)^4. \tag{8}$$

Our analysis now consists of seeking lower degree polynomials (4). We consider two cases, according as to whether $\alpha_5 = 0$ or $\alpha_5 \neq 0$. We give full details in the first case, but for the second, for reasons of brevity, we restrict ourselves to writing down the final transformations (2) and the coefficients of the lower degree polynomial (4), i.e., we do not write down the inverse mapping giving V in terms of U, U', U''' and U''''.

A. Case 1: $\alpha_5 = 0$

In this case we have $a = d = 0$, for which values α_4 also vanishes, and (7) reduces to a cubic,

$$\sum_{i=0}^{3} \alpha_i V^i = 0, \tag{9}$$

with α_0 and α_1 linear in U''', and with

$$\alpha_3 = \tfrac{32}{3}. \tag{10}$$

Again rather than consider this general case, related to (6) by the transformation

$$U = \frac{V' + bV + c}{eV + f}, \tag{11}$$

wherein all coefficients are arbitrary, it is more interesting to seek a transformation to an ODE in U defined by a lower degree polynomial in V. Since in (9) we have $\alpha_3 \neq 0$, the only possibility is to seek a factorization of (9), i.e., to consider (5) with $N=3$ and $M=1$ or 2.

For $M=1$ we seek a factorization as

$$\sum_{i=0}^{3} \alpha_i V^i - (V^2 + gV + h)\left(\frac{32}{3}V + B\right) = 0, \tag{12}$$

from which we quickly determine B. However, requiring that the remaining coefficients of V in (12) (i.e., of V and V^0) vanish identically requires that $e = f = 0$. Thus we are unable to obtain a linear factor [see (11)].

For $M=2$ we seek a factorization as

$$\sum_{i=0}^{3}\alpha_i V^i-(V+g)\left(\frac{32}{3}V^2+BV+C\right)=0, \tag{13}$$

and again we easily determine B and C. We are then left with the coefficient of V^0, which we make vanish identically as a polynomial in U, U', U'' and U'''. One of the coefficients of this polynomial is $eg-f$, from which we see that if $e=0$ then we must also have $f=0$. Thus we must have $e\neq 0$. In this case we can assume (using a Möbius transformation) that $e=1$ and $b=0$. We thus obtain that $g=f$. From other coefficients in this polynomial we find that $c=f'$, and also that f defines a second solution of Cosgrove's equation, since $f=-w$ satisfies $E[w]=0$. In summary, we have a transformation

$$U=\frac{(V-w)'}{V-w}, \tag{14}$$

corresponding to which we have the quadratic in V

$$AV^2+BV+C=0, \tag{15}$$

where

$$A=\tfrac{32}{3}, \tag{16}$$

$$B=\tfrac{2}{3}(6p+27U^2+16w+18U'), \tag{17}$$

$$C=p(U'+U^2+4w)+U^4-6U^2w+(32/3)w^2+6U^2U' \tag{18}$$

$$+3(U')^2+12Uw'+4UU''+12w''+U'''', \tag{19}$$

and where w also satisfies (6). Elimination between (14) and (15) leads to an expression for V in terms of U [the inverse of (14)],

$$\begin{aligned}V=&[U''''+12w''+2UU''-12Uw''+10U'U''-2U^2U''+24U'w'+32ww'-12U^2w'\\&+6U(U')^2-24UU'w-8U^3U'-32Uw^2-6U^3w-2U^5+p(U''+8w'-12Uw-2U^3)]/\\&[2(2pU+9U^3+16Uw-12UU'-16w'-6U'')],\end{aligned} \tag{20}$$

and substitution into (15) then yields an ODE in U of fourth order and second degree, with coefficients depending on w, a second solution of Cosgrove's equation.

B. Case 2: $\alpha_5\neq 0$

In this case we assume that not both of a and d vanish, and we seek a factorization of the quintic (7). We quickly find that there is no factorization for $M=1$ and $M=2$. (Note also that for these choices of M, no A_i can depend on U'''.)

This then leaves us with the cases $M=3$ and $M=4$.

1. M=3

We seek a factorization of our quintic as

$$\sum_{i=0}^{5}\alpha_i V^i-(V^2+gV+h)[24(a-dU)^4V^3+BV^2+CV+D]=0, \tag{21}$$

from which we quickly obtain B, C, and D. We are then left with the coefficients of V and V^0 (polynomials in U, U', U'' and U'''), which we make vanish identically.

We find that if $d=0$, then both e and f must also vanish. We must therefore have $d\neq 0$, in which case we may assume (by use of a Möbius transformation) that $d=1$ and $a=0$. In this case we obtain $g=e$ and $h=f$, and $c=(be+e')/2$.

We then find that $b(e^2-4f)+(1/2)(e^2-4f)'=0$, and so our analysis splits into two cases: $e^2-4f=0$, and $e^2-4f\neq 0$.

Case 1: In this first case, we have $f=e^2/4$, and we find that our two remaining coefficients in the transformation (2), b and e, satisfy a pair of coupled ODEs. The second of these coefficients, e, defines a second solution of Cosgrove's equation; setting $e=-2w$, we find that $E[w]=0$. The coefficient b is then determined by the ODE

$$b'''-4bb''-3(b')^2+6b^2b'-b^4+(12w+p)(b'-b^2)+12w'b-4(3w''+8w^2+2pw)=0. \tag{22}$$

This equation is a special case of Chazy Class XII (N=2);[9] setting

$$b=\lambda(x)y(\zeta)+\mu(x), \quad \zeta=\zeta(x), \tag{23}$$

where $\zeta'=2\lambda$, $\mu=(3\lambda')/(2\lambda)$, and $\Lambda=\lambda'/\lambda$ satisfies the Riccati equation $\Lambda'-(1/2)\Lambda^2-(1/5)(12w+p)=0$, obtains

$$\dddot{y}-2y\ddot{y}-\tfrac{3}{2}(\dot{y})^2+\tfrac{3}{2}y^2\dot{y}-\tfrac{1}{8}y^4+\gamma=0, \tag{24}$$

wherein this last $\gamma(\zeta)$ is defined by

$$\gamma(\zeta(x))=\frac{1}{10\lambda^4}\left(\frac{9}{80}p^2-\frac{73}{10}pw-\frac{119}{5}w^2-\frac{21}{2}w''\right), \tag{25}$$

and $\dot{}$ denotes differentiation w.r.t. ζ. We recall[9,10] that the most general equation in this class with the Painlevé property (when put in canonical form) is

$$\dddot{y}-2y\ddot{y}-\tfrac{3}{2}(\dot{y})^2+\tfrac{3}{2}y^2\dot{y}-\tfrac{1}{8}y^4+\alpha y+\beta=0, \tag{26}$$

where α and β are two arbitrary functions of ζ. Thus we see that our Eq. (22) is equivalent to a special case of this last equation, with $\alpha=0$ and with β defined in terms of a solution of Cosgrove's equation. Equation (24) can be linearized [as can (26)] by the transformation $y=-2\dot{u}/u$.[9] Thus our Eq. (22) is linearizable.

Our final results in this case are therefore that we have a transformation defined by

$$U=\frac{(V-w)'+b(V-w)}{(V-w)^2}, \tag{27}$$

where w is a second solution of Cosgrove's equation, and where b satisfies (22), a linearizable equation with coefficients defined in terms of w. Corresponding to this transformation we have a cubic in V,

$$AV^3+BV^2+CV+D=0, \tag{28}$$

where

$$A=24U^4, \tag{29}$$

$$B=6U^2(5-10bU-12U^2w+6U'), \tag{30}$$

$$C=\tfrac{2}{3}(16-72bU+3pU^2+75b^2U^2-54U^2w+180bU^3w+108U^4w^2 \tag{31}$$

$$-30b'U^2+18U'-78bUU'-108U^2U'w+9(U')^2+12UU''), \tag{32}$$

$$D=\tfrac{1}{3}(12p+54b^2-9pbU-45b^3U+64w+36bUw-6pU^2w \tag{33}$$

$$-150b^2U^2w+18U^2w^2-180bU^3w^2-72U^4w^3-36b'+75bb'U \tag{34}$$

$$+60b'U^2w+3pU'+51b^2U'+156bUU'w+108U^2U'w^2-27b'U' \tag{35}$$

$$-18(U')^2w+36Uw'-15b''U-21bU''-24UU''w+3U'''). \tag{36}$$

Elimination of V between (27) and (28) then gives a fourth order ODE in U of degree three, with coefficients depending on w and b.

Case 2: We now assume $e^2-4f\neq 0$. We solve for b as $b=-(e^2-4f)'/(2(e^2-4f))$. In the resulting equations in e and f we make the change of variables $e=-(w+r)$ and $f=wr$ (so $w\neq r$), and we then find that both w and r satisfy Cosgrove's equation. Our final result in this case is that we have a transformation defined by

$$U=\frac{(rV'-r'V)+(wr'-w'r)+(Vw'-V'w)}{(r-V)(w-r)(V-w)}, \tag{37}$$

where both w and r are also solutions of Cosgrove's equation. In fact this transformation is a symmetric mapping of three different solutions (V, w and r) of Cosgrove's equation; we note also that the numerator consists of the the sum of the Wronskians of these three solutions. Corresponding to this transformation we have a cubic in V,

$$AV^3+BV^2+CV+D=0; \tag{38}$$

we give the coefficients A, B, C, D in Appendix A. Elimination of V between (37) and (38) then gives a fourth order ODE in U of degree three, with coefficients depending on w and r. [We could also, of course, obtain an ODE with coefficients depending on V and w, or V and r, by appropriate elimination between Cosgrove's equation (in r or w respectively) and the transformation (37).]

2. M=4

We now seek a factorization of our quintic as

$$\sum_{i=0}^{5}\alpha_iV^i-(V+g)[24(a-dU)^4V^4+BV^3+CV^2+DV+E]=0, \tag{39}$$

from which we easily obtain B, C, D and E. We are then left with the coefficient of V^0 (a polynomial in U, U', U'' and U'''), which we make vanish identically.

We find that we must have $f-eg+dg^2=0$. We consider this condition in the two cases $d=0$ or $d\neq 0$. We consider first the case $d=0$.

Case 1: We assume that $d=0$. We then have $f-eg=0$. When $e=0$, we find we must have $f=0$, which cannot be allowed. Thus we have $e\neq 0$, in which case (using a Möbius transformation) we may assume $e=1$ and $b=0$. We then solve for g as $g=f$. We then find $c=f'-af^2$, and that f defines a second solution of Cosgrove's equation; setting $f=-w$, we find that $E[w]=0$.

Thus our final results in this case are that we have a transformation defined by

$$U=\frac{(V-w)'+a(V^2-w^2)}{(V-w)}, \tag{40}$$

where w also satisfies Cosgrove's equation, and a is arbitrary. Corresponding to this transformation we have the quartic in V,

$$AV^4+BV^3+CV^2+DV+E=0, \tag{41}$$

where

$$A=24a^4, \tag{42}$$

$$B=6a^2(5-10aU+4a^2w-6a'), \tag{43}$$

$$\begin{aligned}C=&\tfrac{2}{3}(16+3pa^2-72aU+75a^2U^2+45a^2w-30a^3Uw-24a^4w^2-18a'+78aa'U\\&-54a^2a'w+9a'^2+30a^2U'-60a^3w'+12aa''),\end{aligned} \tag{44}$$

$$\begin{aligned}D=&\tfrac{1}{3}(12p-9paU+54U^2-45aU^3+32w+6pa^2w-36aUw-30a^2U^2w-18a^2w^2\\&+120a^3Uw^2-48a^4w^3-3pa'-51a'U^2-36a'w+42aa'Uw+36a^2a'w^2+18(a')^2w\\&+36U'-75aUU'+30a^2U'w-27a'U'-108aw'+150a^2Uw'-60a^3ww'+114aa'w'\\&-21a''U+24aa''w-15aU''+30a^2w''-3a'''),\end{aligned} \tag{45}$$

$$\begin{aligned}E=&\tfrac{1}{3}(3pU^2+3U^4+12pw-3paUw-18U^2w+21aU^3w+32w^2+36aUw^2-48a^2U^2w^2\\&-18a^2w^3+24a^3Uw^3-3pa'w+15a'U^2w-54aa'Uw^2+36a^2a'w^3+3pU'+18U^2U'\\&+3aUU'w-18a^2U'w^2-9a'U'w+9(U')^2-6paw'+36Uw'-36aU^2w'-36aww'\\&-6a^2Uww'+36a^3w^2w'-48a'Uw'+54aa'ww'-36aU'w'+36a^2(w')^2-3a''Uw\\&-18a''w'+12UU''-9aU''w+36w''-24aUw''+18a^2ww''-18a'w''-3a'''w+3U'''\\&-6aw'''),\end{aligned} \tag{46}$$

Elimination of V between (40) and (41) then gives a fourth order ODE in U of degree four, with coefficients depending on w and a. We note that in the case $a=0$ the transformation (40) becomes the transformation (14) and the quartic (41) becomes the quadratic (15).

Case 2: We now assume $d\neq 0$. We can then assume (using a Möbius transformation) that $d=1$ and $a=0$. We then have (see earlier) that $f=eg-g^2$. We then obtain that $(e-2g)(c-bg-g')=0$. However, taking $e=2g$ leads in any case to $(c-bg-g')=0$, and so we restrict our attention to the choice $c=bg+g'$. We then obtain that w defined by $g=-w$ is also a solution of Cosgrove's equation.

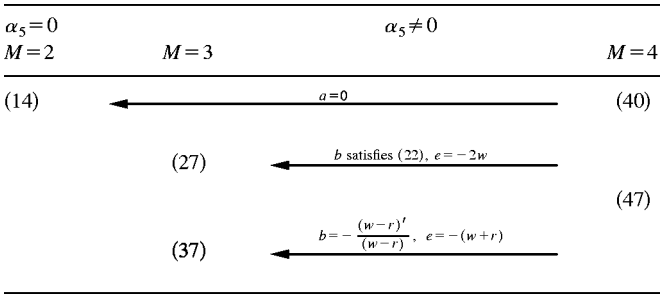
Our final results in this case are then that we have a transformation defined by

$$U=\frac{(V-w)'+b(V-w)}{V^2-w^2+e(V-w)}, \tag{47}$$

where w also satisfies Cosgrove's equation, and b and e are arbitrary. Corresponding to this transformation we have a quartic in V,

$$AV^4+BV^3+CV^2+DV+E=0; \tag{48}$$

TABLE I. Relations between transformations obtained.



we give the coefficients A, B, C, D, E in Appendix B. Elimination of V between (47) and (48) then gives a fourth order ODE in U of degree six, with coefficients depending on w, b and e. We note that taking $e=-2w$, and assuming that b satisfies (22), gives the transformation (27) together with the factorization of our quartic to yield the corresponding cubic factor (28) of (7). We note also that taking $b=-(w-r)'/(w-r)$ and $e=-(w+r)$, where r is also assumed to satisfy Cosgrove's equation, gives the transformation (37) together with the factorization of our quartic to yield the corresponding cubic factor (38) of (7).

We summarize relations between the different transformations obtained in this article in Table I. We see that there are two transformations from which the other three can be derived.

IV. CONCLUSIONS AND OUTLOOK

The Fokas–Ablowitz algorithm was originally phrased to obtain transformations for second order ODEs, to second order ODEs of degrees one or two. Here we have given a general formulation which can be applied to ODEs of order higher than 2, and which allows us to obtain transformations to ODEs of the same order but which may be of degree greater than 2. We have applied this to Cosgrove'e equation, an ODE believed to define a new transcendent, and which is therefore of as fundamental importance as the Painlevé equations themselves. This ODE has an underlying linear problem of third order,[6–8] and is likely to be the subject of much future research. We have obtained a variety of transformations relating this equation to other fourth order ODEs, of degrees $\geqslant 2$. These transformations and the corresponding ODEs, all of which have the Painlevé property, are all new. Of the transformations obtained, (40) and (47) can be understood to be master transformations, for transformations of the form (2), since all of our other transformations (14), (27) and (37) can be obtained from these two (see Table I). We note that all of our transformations hold also in the case $q=0$, in which case we may take the coefficient functions w and r to be any corresponding solution of Cosgrove's equation (hyperelliptic, elliptic, rational or zero; see Ref. 4).

In order to obtain further transformations for Eq. (6), we could consider a factorization (5) where the coefficients g_i are not restricted to be functions of x only, or we could alternatively consider generalizing the ansatz (2).

Let us consider generalizing the factorization (5). We note first that the aim of this factorization is to obtain restrictions on the coefficients a, b, c, d, e and f of the transformation (2) such that we obtain a lower degree polynomial (4) in V. That is, it is assumed that without any such restrictions on the coefficients of the transformation (2), the polynomial (3) is irreducible. The case where the polynomial (3) happens to factorize without making any restrictions on the coefficients of the transformation (2) is to be considered separately, with each factor then being used in the role played by Eq. (3). This possibility does not occur for (7).

Let us now consider the process of imposing restrictions on a, b, c, d, e and f such that (3) factorizes. In our description of this factorization process, we stated that the functions g_i are to be taken as functions of x only. This is a stronger requirement than is usually made (see, for example, Refs. 2 and 3). We now consider this factorization process more generally. The first factor can

always be assumed to be monic, and we can always proceed as described to obtain the coefficients A_i of the second factor. We are then left with the remaining coefficients of V, which must be made to vanish identically. At this stage some restriction needs to be made on the coefficients $g_0,\ldots,g_{N-M-1}$; we assumed that they depend only on x. However, more general assumptions can be made. For example, they could be assumed to be functions of $x,U,U',\ldots,U^{(n-2)}$; each coefficient of the terms $V^{N-M-1},\ldots,V^0$ is then to be made to vanish identically as a polynomial in $U^{(n-1)}$. We have checked that under such an assumption, no further results are obtained for Cosgrove's equation. Of course, more general assumptions can always be made, e.g., that each g_i be a polynomial in $U^{(n-1)}$ of some specified degree, or that each g_i be rational in $U^{(n-1)}$, again of some specified form.

In order to generalize the ansatz (2), we could, for example, seek transformations to fourth order ODEs defined by a relation of the form

$$U=\frac{(V')^2+(\Sigma_{i=0}^{2}a_iV^i)V'+\Sigma_{i=0}^{4}b_iV^i}{(\Sigma_{i=0}^{2}c_iV^i)V'+\Sigma_{i=0}^{4}d_iV^i}, \tag{49}$$

where all a_i, b_i, c_i and d_i are functions of x. This relation was used in Ref. 11 to obtain, for each of the Painlevé equations, transformations to previously unknown second order second degree equations having the Painlevé property. Furthermore, since we are now considering higher order equations with the Painlevé property, one might expect that the ansatz used for the form of the transformation could now be further generalized so as to include higher derivatives. Thus an obvious choice when considering fourth order ODEs with the Painlevé property would be an ansatz whereby U is expressed as a function linear in V''' and rational in V'', V' and V, with coefficients dependent on x, e.g., we may take

$$U=\frac{V'''+(\Sigma_{i=0}^{1}a_iV^i)V''+b_0(V')^2+(\Sigma_{i=0}^{2}c_iV^i)V'+\Sigma_{i=0}^{4}d_iV^i}{(\Sigma_{i=0}^{1}e_iV^i)V''+f_0(V')^2+(\Sigma_{i=0}^{2}g_iV^i)V'+\Sigma_{i=0}^{4}h_iV^i}. \tag{50}$$

Further generalizations, to the case where this function is a rational function of V''', can then be considered (and similarly when U depends on V, V' and V'' only). In cases such as these we then need to eliminate V between the expression for U and the original ODE in V (here Cosgrove's equation). Given the recent interest in higher order equations having the Painlevé property, and the corresponding interest in finding transformations for these, there seems to be much scope for future research.

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APPENDIX A: COEFFICIENTS OF THE CUBIC (38)

$$A=24U^4,$$

$$B=\frac{6U^2}{w-r}(6U^2r^2-5r+5w-6U^2w^2-10Ur'-6U'r+6U'w+10Uw'),$$

$$\begin{aligned}C=\frac{2}{3(w-r)^2}(&16r^2+3pU^2r^2-27U^2r^3+21U^4r^4-32wr-6pU^2wr+27U^2wr^2+24U^4wr^3\\&+16w^2+3pU^2w^2+27U^2w^2r-90U^4w^2r^2-27U^2w^3+24U^4w^3r+21U^4w^4+72Urr'\\&-90U^3r^2r'-72Uwr'+90U^3w^2r'+45U^2(r')^2+18U'r^2-54U^2U'r^3-36U'wr\end{aligned}$$

$$+54U^2U'wr^2+18U'w^2+54U^2U'w^2r-54U^2U'w^3+78UU'rr'-78UU'wr'$$
$$+9(U')^2r^2-18(U')^2wr+9(U')^2w^2-72Uw'r+90U^3w'r^2+72Uww'-90U^3w^2w'$$
$$-90U^2w'r'-78UU'w'r+78UU'ww'+45U^2(w')^2+30U^2rr''-30U^2wr''+12UU''r^2$$
$$-24UU''wr+12UU''w^2-30U^2w''r+30U^2ww''),$$

$$D=\frac{-1}{3(w-r)^2}(3pU^2r^3-12pr^2-32r^3+3U^4r^5+24pwr+32wr^2-3pU^2wr^2-18U^2wr^3$$
$$+27U^4wr^4-12pw^2+32w^2r-3pU^2w^2r+36U^2w^2r^2-30U^4w^2r^3-32w^3+3pU^2w^3$$
$$-18U^2w^3r-30U^4w^3r^2+27U^4w^4r+3U^4w^5-9pUrr'-30U^3r^3r'+9pUwr'$$
$$+36Uwrr'-90U^3wr^2r'-36Uw^2r'+90U^3w^2rr'+30U^3w^3r'-18(r')^2+45U^2r(r')^2$$
$$+45U^2w(r')^2-3pU'r^2-18U^2U'r^4+6pU'wr-36U^2U'wr^3-3pU'w^2$$
$$+108U^2U'w^2r^2-36U^2U'w^3r-18U^2U'w^4+78UU'r^2r'-78UU'w^2r'-24U'(r')^2$$
$$+9(U')^2r^3-9(U')^2wr^2-9(U')^2w^2r+9(U')^2w^3+9pUw'r-36Uw'r^2+30U^3w'r^3$$
$$-9pUww'+36Uww'r+90U^3ww'r^2-90U^3w^2w'r-30U^3w^3w'+36w'r'-90U^2w'rr'$$
$$-90U^2ww'r'-78UU'w'r^2+78UU'w^2w'+48U'w'r'-18(w')^2+45U^2(w')^2r$$
$$+45U^2w(w')^2-24U'(w')^2-36rr''+30U^2r^2r''+36wr''-30U^2w^2r''-30Ur'r''$$
$$-27U'rr''+27U'wr''+30Uw'r''+12UU''r^3-12UU''wr^2-12UU''w^2r+12UU''w^3$$
$$-21U''rr'+21U''wr'+21U''w'r-21U''ww'+36w''r-30U^2w''r^2-36ww''$$
$$+30U^2w^2w''+30Uw''r'+27U'w''r-27U'ww''-30Uw'w''-15Urr'''+15Uwr'''$$
$$-3U'''r^2+6U'''wr-3U'''w^2+15Uw'''r-15Uww''').$$

APPENDIX B: COEFFICIENTS OF THE QUARTIC (48)

$$A=24U^4,$$

$$B=6U^2(5-10bU+10eU^2+4U^2w+6U'),$$

$$C=\tfrac{2}{3}(16-72bU+3pU^2+75b^2U^2+72eU^2-150beU^3+75e^2U^4+45U^2w-30bU^3w$$
$$+30eU^4w-24U^4w^2-30b'U^2+30e'U^3+18U'-78bUU'+108eU^2U'+54U^2U'w$$
$$+9(U')^2+60U^3w'+12UU''),$$

$$D=\tfrac{1}{3}(12p+54b^2-9pbU-45b^3U-108beU+9peU^2+135b^2eU^2+54e^2U^2-135be^2U^3$$
$$+45e^3U^4+32w-36bUw+6pU^2w-30b^2U^2w+36eU^2w+60beU^3w-30e^2U^4w$$
$$-18U^2w^2+120bU^3w^2-120eU^4w^2-48U^4w^3-36b'+75bb'U-75b'eU^2-30b'U^2w$$
$$+36e'U-75be'U^2+75ee'U^3+30e'U^3w+3pU'+51b^2U'+36eU'-177beUU'$$
$$+126e^2U^2U'+36U'w-42bUU'w+72eU^2U'w-36U^2U'w^2-27b'U'+57e'UU'$$
$$+27e(U')^2+18(U')^2w+108Uw'-150bU^2w'+150eU^3w'+60U^3ww'+114UU'w'$$
$$-15b''U+15e''U^2-21bU''+36eUU''+24UU''w+30U^2w''+3U''').$$

$$
\begin{aligned}
E=\tfrac{1}{3}(&3pb^2+3b^4-6pbeU-12b^3eU+3pe^2U^2+18b^2e^2U^2-12be^3U^3+3e^4U^4+12pw\\
&-18b^2w-3pbUw+21b^3Uw+36beUw+3peU^2w-63b^2eU^2w-18e^2U^2w\\
&+63be^2U^3w-21e^3U^4w+32w^2+36bUw^2-48b^2U^2w^2-36eU^2w^2+96beU^3w^2\\
&-48e^2U^4w^2-18U^2w^3+24bU^3w^3-24eU^4w^3-3pb'-18b^2b'+36bb'eU-18b'e^2U^2\\
&-3bb'Uw+3b'eU^2w+18b'U^2w^2+9(b')^2+3pe'U+18b^2e'U-36bee'U^2\\
&+18e^2e'U^3+3be'U^2w-3ee'U^3w-18e'U^3w^2-18b'e'U+9(e')^2U^2+3peU'\\
&+18b^2eU'-36be^2UU'+18e^3U^2U'+3pU'w-15b^2U'w+33beUU'w-18e^2U^2U'w\\
&+54bUU'w^2-72eU^2U'w^2-36U^2U'w^3-18b'eU'-9b'U'w-24be'U'+42ee'UU'\\
&+27e'UU'w+9e^2(U')^2+9e(U')^2w-36bw'+6pUw'+36b^2Uw'+36eUw'\\
&-72beU^2w'+36e^2U^3w'+36Uww'+6bU^2ww'-6eU^3ww'-36U^3w^2w'-36b'Uw'\\
&+36e'U^2w'-48bU'w'+84eUU'w'+54UU'ww'+36U^2(w')^2+12bb''-12b''eU\\
&-9b''Uw-12be''U+12ee''U^2+9e''U^2w+9e''U'-12beU''+12e^2UU''-3bU''w\\
&+12eUU''w+9e'U''+18U''w'+36w''-24bUw''+24eU^2w''+18U^2ww''+18U'w''\\
&-3b'''+3e'''U+3eU'''+3U'''w+6Uw'''\big).
\end{aligned}
$$

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Conservation laws of semidiscrete Hamiltonian equations

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Many evolution partial differential equations (PDEs) can be cast into Hamiltonian form. Conservation laws of these equations are related to one-parameter Hamiltonian symmetries admitted by the PDEs [P. J. Olver, *Applications of Lie Groups to Differential Equations* (Springer, New York, 1986)]. In this paper we consider symmetries and Noether's theorem for semidiscrete Hamiltonian equations which are obtained by space discretization of Hamiltonian PDEs. Using symmetries, one can find conservation laws of these equations. Several applications including a transfer equation and the Korteweg–de Vries equation are presented. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1353184]

I. INTRODUCTION

Many partial differential equations (PDEs) possess conservation laws. Solutions of the equations of nondissipative continuum mechanics can often be presented as solutions of the Euler–Lagrange equations for the relevant functional. Conservation laws of such equations are given by Noether's theorem[1] if the admitted symmetries are known. The first discrete analog of Noether's theorem was presented by Maeda,[2,3] who considered transformations which do not change the independent variables and hence the mesh. Discrete versions of Noether's theorem for transformations which may also involve the independent variables have been developed by Dorodnitsyn.[4–6]

However, there are evolution equations without appropriate or natural Lagrangian formulation. For these equations one may prefer to use the Hamiltonian viewpoint. Much work has been done recently in preserving the structure and conservation laws of Hamiltonian PDEs under discretization. One approach is based on using the Hamiltonian formulation of PDEs on multisymplectic structures, which generalized the classical Hamiltonian structure by assigning a distinct symplectic operator for each space direction and time.[7] Variational integrators[8] generalize Veselov-type[9,10] discretizations of PDEs in variational form. They conserve the corresponding discrete multisymplectic form as well as the discrete momentum mappings corresponding to symmetries which do not transform the mesh. Different symplectic ordinary differential equation (ODE) solvers can also be used to build up multisymplectic integrators for PDEs[11–13] which preserve multisymplectic structure and may preserve some conservation laws.

In this paper we consider the Hamiltonian formulation of evolution equations based on the Poisson bracket approach. Conservation laws of these equations are related to one-parameter Hamiltonian symmetries admitted by the PDEs.[14,15] We introduce a discrete Poisson bracket, which provides us an infinite dimensional system of semidiscrete equations. Our main interest is to find conservation laws of such systems with the help of Noether's theorem in the Hamiltonian formulation. It will transpire that Noether's theorem can be carried over from the continuous case to the semidiscrete case so that one can use Hamiltonian symmetries of semidiscrete equations to find their conservation laws. As one can expect not all symmetries and conservation laws can be preserved under discretization of the bracket.

It is not known how to find all symmetries of a set of discrete equations. An overview of different methods and references can be found, for example, in Refs. 16 and 17. Some Lie point

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symmetries of the original continuous equations can be preserved under discretization. These symmetries are realized by the same vector field in the continuous and discrete cases.[5] Discrete equations can also have symmetries which have no continuous counterparts. Because our main interest is to see what happens to conservation laws of continuous equations under space discretization we do not consider symmetries which disappear in the continuous limit.

In the paper we consider semidiscrete Hamiltonian equations and their conservation laws. The space discretization of Hamiltonian PDEs can be viewed as a first step of discretization that leads from a PDE to a difference scheme. Therefore the consideration of semidiscrete Hamiltonian equations can explain how space discretizations affect the conservation laws.

The paper is organized as follows: In Sec. II we consider continuous and semidiscrete Hamiltonian equations. Symmetries and their connection with conservation laws are reviewed in Sec. III, where we construct the ideal of the Lie–Bäcklund operators on a uniform space mesh and present the Hamiltonian form of Noether's theorem. Section IV contains applications. Finally, we summarize the results of the paper in Sec. V.

II. HAMILTONIAN EQUATIONS

In what follows (except Sec. III B) we will consider the case of one dependent variable u and two independent variables: time t and space coordinate x. We assume that the solutions are sufficiently smooth all variational derivatives tend to zero as $u\to 0$ and that u and a number of space derivatives of u tend to zero as $|x|\to\infty$. For simplicity we suppose that the solution decays fast enough so that all integrals in the continuous case and all sums in the semidiscrete case make sense. All integrals are assumed to be taken over the whole real line.

A. Hamiltonian partial differential equations

Many evolution partial differential equations of the form

$$u_t = K(x,u^{(n)}), \tag{2.1}$$

where $u^{(n)}=(u,u_1,u_2,\ldots,u_n)$ represents u and a finite set of derivatives of u with respect to space coordinate x, can be represented in the Hamiltonian form

$$u_t = \mathcal{D}\left(\frac{\delta \mathcal{H}}{\delta u}\right), \quad \mathcal{H}[u]=\int H(x,u^{(n)})\mathrm{d}x \tag{2.2}$$

with the help of the Hamiltonian functional $\mathcal{H}[u]$, variational operator $\delta\cdot/\delta u$, and a linear operator $\mathcal{D}$.[14] Denote by $\mathcal{F}$ the space of functionals of the type

$$\int P(t,x,u^{(m)})\mathrm{d}x, \quad m\in\mathbb{N}.$$

The operator $\mathcal{D}$ is required to be Hamiltonian, i.e., it forms the Poisson bracket

$$\{P,\mathcal{L}\}=\int \frac{\delta \mathcal{P}}{\delta u}\mathcal{D}\left(\frac{\delta \mathcal{L}}{\delta u}\right)\mathrm{d}x \tag{2.3}$$

satisfying the conditions of *skew-symmetry*

$$\{\mathcal{P},\mathcal{L}\}=-\{\mathcal{L},\mathcal{P}\} \tag{2.4}$$

and the *Jacobi identity*

$$\{\{\mathcal{P},\mathcal{L}\},\mathcal{R}\}+\{\{\mathcal{R},\mathcal{P}\},\mathcal{L}\}+\{\{\mathcal{L},\mathcal{R}\},\mathcal{P}\}=0 \tag{2.5}$$

for all functionals $\mathcal{P},\mathcal{L},\mathcal{R}\in\mathcal{F}$.

The variational derivative of a functional can be found by the action of the Euler operator on the integrand

$$\frac{\delta \mathcal{H}}{\partial u}=E(H), \quad E=\frac{\partial \cdot}{\partial u}-D_x\left(\frac{\partial \cdot}{\partial u_1}\right)+D_x^2\left(\frac{\partial \cdot}{\partial u_2}\right)+\cdots+(-1)^n D_x^n\left(\frac{\partial \cdot}{\partial u_n}\right)+\cdots, \tag{2.6}$$

where D_x is the total differentiation operator:

$$D_x=\frac{\partial}{\partial x}+u_1\frac{\partial}{\partial u}+u_2\frac{\partial}{\partial u_1}+\cdots+u_{n+1}\frac{\partial}{\partial u_n}+\cdots. \tag{2.7}$$

Example 2.1: Let us illustrate the above-described approach on Korteweg–de Vries equation[14,18]

$$u_t=uu_x+u_{xxx}. \tag{2.8}$$

The Korteweg–de Vries equation can be presented in the Hamiltonian form (2.2) in several ways.[14] One of them is the following:

$$\mathcal{D}=D_x, \quad \mathcal{H}=\int\left(\frac{u^3}{6}-\frac{u_x^2}{2}\right)\mathrm{d}x. \tag{2.9}$$

Example 2.2: The same bracket can be used to cast the transfer equation

$$u_t=h''(u)u_x \tag{2.10}$$

in the the Hamiltonian form with the Hamiltonian functional

$$\mathcal{H}=\int h(u)\mathrm{d}x. \tag{2.11}$$

B. Semidiscrete Hamiltonian equations

Given a Hamiltonian PDE, it is desirable to discretize both the Poisson bracket and the Hamiltonian functional so that we preserve Poisson structure.

To do so let us introduce a two-dimensional mesh which is uniform (regular) in space and continuous in time. We denote the mesh points as $\{x_i(t)\}$, $i=0,\pm1,\pm2,...,t\geqslant 0$ and define the mesh by two conditions:

$$\begin{cases}\Omega_1=(x_{i+1}(t)-x_i(t))-(x_i(t)-x_{i-1}(t))=0, & i=0,\pm1,\pm2,..., \quad t\geqslant 0,\\ \Omega_2=x_i(t+\tau)-x_i(t)=0, & i=0,\pm1,\pm2,..., \quad t,\tau\geqslant 0.\end{cases} \tag{2.12}$$

We will use the short notation $\Omega=0$ for this mesh. The first equation means that for any fixed time the space mesh is uniform. The second equation requires that we consider only vertical mesh lines in the time–space plane. Figure 1 shows the type of the mesh we specified.

At the mesh points we introduce discrete space derivatives $\underset{h}{u_1}=\underset{+h}{D}u, \underset{h}{u_2}=\underset{-h\,h}{D}u_1$, $\underset{h}{u_{2k+1}}=\underset{+h\,h}{D}u_{2k}$, $\underset{h}{u_{2k+2}}=\underset{-h\,h}{D}u_{2k+1}$, $k=1,2,...$, where $\underset{+h}{D}$ and $\underset{-h}{D}$ are the right and left discrete differentiation operators. They can be defined with the help of the right shift S_+ and left shift S_- operators

$$S_+f(x)=f(x+h), \quad S_-f(x)=f(x-h) \tag{2.13}$$

as

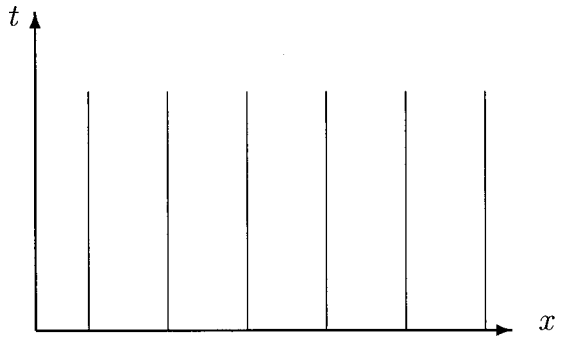

FIG. 1. The uniform mesh for the semidiscrete equations.

$$\underset{+h}{D}=\frac{S_+-1}{h},\quad \underset{-h}{D}=\frac{1-S_-}{h}. \tag{2.14}$$

We will consider the space of discrete derivatives $\underset{h}{u}^{(n)}=(u,\underset{h}{u}_1,\underset{h}{u}_2,\ldots,\underset{h}{u}_n)$ and corresponding functionals of the form

$$\underset{h}{\mathcal{P}}=\sum_{\Omega} \underset{h}{P}(t,x,h,\underset{h}{u}^{(n)})h, \tag{2.15}$$

where the summation is taken over all space points of the mesh Ω. We denote the space of such functionals as $\underset{h}{\mathcal{F}}$.

We assume that the Hamiltonian operator $\mathcal{D}$ can be approximated by an operator $\underset{h}{\mathcal{D}}$ such that the discrete bracket

$$\{\underset{h}{\mathcal{P}},\underset{h}{\mathcal{L}}\}_h=\sum_{\Omega} \frac{\delta \underset{h}{\mathcal{P}}}{\delta u}\underset{h}{\mathcal{D}}\left(\frac{\delta \underset{h}{\mathcal{L}}}{\delta u}\right)h \tag{2.16}$$

defines a Poisson bracket for functionals from $\underset{h}{\mathcal{F}}$. This means that $\{\cdot,\cdot\}_h$ is *skew-symmetric* and satisfies the Jacobi identity. We can choose some approximation $\underset{h}{\mathcal{H}}$ of the Hamiltonian functional $\mathcal{H}$ and get a set of Hamiltonian semidiscrete equations

$$\dot{u}=\underset{h}{\mathcal{D}}\left(\frac{\delta \underset{h}{\mathcal{H}}}{\delta u}\right), \tag{2.17}$$

which approximate Eq. (2.1) on the mesh (2.12).

Using the bracket notation, we can express a total time derivative of a functional $\underset{h}{\mathcal{P}}\in\underset{h}{\mathcal{F}}$ as

$$\frac{\mathrm{d}}{\mathrm{d}t}\underset{h}{\mathcal{P}}=\frac{\partial}{\partial t}\underset{h}{\mathcal{P}}+\{\underset{h}{\mathcal{P}},\underset{h}{\mathcal{H}}\}_h. \tag{2.18}$$

Definition: For a given Hamiltonian operator $\underset{h}{\mathcal{D}}$ a distinguished functional is a functional $\underset{h}{\mathcal{C}}(x,h,\underset{h}{u}^{(n)})$ such that

$$\underset{h}{\mathcal{D}}\left(\frac{\delta \underset{h}{\mathcal{C}}}{\delta u}\right)=0.$$

It follows that a functional is distinguished if and only if its Poisson bracket with every other functional is trivial:

$$\{\underset{h}{\mathcal{C}},\underset{h}{\mathcal{H}}\}_h=0 \quad \text{for any} \quad \underset{h}{\mathcal{H}}\in\mathcal{F}.$$

Example 2.3: Let us consider the bracket based on the central difference derivative operator

$$\underset{h}{D_0}=\frac{S_+-S_-}{2h}, \tag{2.19}$$

defined with the help of the right and left shift operators (2.13). It is easy to check that the bracket is *skew-symmetric* and satisfies the Jacobi identity. This bracket has two linearly independent distinguished functionals

$$\underset{h}{\mathcal{C}_1}=\sum_{i=-\infty}^{\infty} u_i h, \quad \underset{h}{\mathcal{C}_2}=\sum_{i=-\infty}^{\infty} (-1)^i u_i h. \tag{2.20}$$

In the continuous limit the first distinguished functional gives the only distinguished functional of the continuous bracket (2.3) generated by the total differentiation operator D_x (the continuous counterpart of $\underset{h}{D_0}$):

$$\underset{h}{\mathcal{C}_1}\to\int u\,\mathrm{d}x \quad \text{as} \quad h\to 0.$$

The second distinguished functional disappears in the continuous limit: $\underset{h}{\mathcal{C}_2}\to 0$ as $h\to 0$.

Alternatively, we can present the distinguished functionals as

$$\underset{h}{\tilde{\mathcal{C}}_1}=\sum_{i=-\infty}^{\infty} u_{2i} h, \quad \underset{h}{\tilde{\mathcal{C}}_2}=\sum_{i=-\infty}^{\infty} u_{2i+1} h.$$

These expressions indicate that conservations of mass for even and odd points of the mesh hold independently.

Remark: Approximating the first-order differential operator D_x by the second-order difference operator (2.19), we introduce stable spurious solutions into the semidiscrete framework. The resulting semidiscrete equations (2.17) possess two linearly independent solutions

$$u_i=C_1, \quad i\in\mathbb{Z}, \quad C_1=\text{const}, \tag{2.21}$$

$$u_i=C_2(-1)^i, \quad i\in\mathbb{Z}, \quad C_2=\text{const}. \tag{2.22}$$

However, the underlying Hamiltonian PDE possesses only the solution (2.21). The other solution is introduced into the semidiscrete equations by the space discretization.

Imposing the requirement $u_i \to 0$ as $i \to \infty$ for the solution and the initial data, we exclude all steady spurious solutions (except the trivial one $u_i \equiv 0$, $i \in \mathbb{Z}$) from the semidiscrete framework.

Example 2.4: We can choose a higher order approximation of the operator D_x (up to $O(h^4)$):

$$\hat{\mathcal{D}}_h = \frac{1}{3}(4\mathcal{D}_{0h} - \mathcal{D}_{02h}) = \frac{-S_+^2 + 8S_+ - 8S_- + S_-^2}{12h}, \tag{2.23}$$

The discrete bracket (2.16) based on $\hat{\mathcal{D}}_h$ has four linearly independent distinguished functionals:

$$\hat{\mathcal{C}}_{1h} = \sum_{i=-\infty}^{\infty} u_i h, \quad \hat{\mathcal{C}}_{2h} = \sum_{i=-\infty}^{\infty} (-1)^i u_i h,$$
$$\hat{\mathcal{C}}_{3h} = \sum_{i=-\infty}^{\infty} (4-\sqrt{15})^i u_i h, \quad \hat{\mathcal{C}}_{4h} = \sum_{i=-\infty}^{\infty} (4+\sqrt{15})^i u_i h. \tag{2.24}$$

Note that the functionals $\hat{\mathcal{C}}_{1h}$ and $\hat{\mathcal{C}}_{2h}$ are the same as in the previous example.

As a higher order approximation for the first-order operator D_x the operator (2.23) introduces steady spurious solutions. We do not investigate them since this operator will not be used further.

C. Discrete Euler operator

It is useful to have some practical formula to compute the variation derivatives of the discrete functionals. A discrete analog of the Euler operator (2.6) was introduced in order to study variations of discrete Lagrangian problems.[4–6] For Hamiltonian functionals of the form

$$\mathcal{H}_h = \sum_{\Omega} H(x,h,u,u_{1h},u_{2h},\ldots,u_{nh})h \tag{2.25}$$

the variational derivative can be found with the help of the discrete Euler operator E_h:

$$\frac{\delta \mathcal{H}_h}{\delta u} = E_h H, \tag{2.26}$$

where

$$E_h = \frac{\partial \cdot}{\partial u} - D_{-h}\left(\frac{\partial \cdot}{\partial u_{1h}}\right) + D_{+h-h}D_{+h-h}\left(\frac{\partial \cdot}{\partial u_{2h}}\right) + \cdots + (-1)^n (D_{-h})^{(n \bmod 2)} (D_{+h-h}D_{+h-h})^{\lfloor n/2 \rfloor}\left(\frac{\partial \cdot}{\partial u_{nh}}\right). \tag{2.27}$$

The function $\lfloor \cdot \rfloor$ denotes the integer part and $\cdot \bmod 2$ the remainder of the division by 2.

Another approach can be used for the Hamiltonian functionals of the form

$$\mathcal{H}_h = \sum_{i=-\infty}^{\infty} H[u_i]h = \sum_{i=-\infty}^{\infty} H(x_i,h,u_{i-m},\ldots,u_i,\ldots,u_{i+n})h \tag{2.28}$$

for some $m,n \in \mathbb{N}$. The variation derivative of the functional with respect to u_i is

$$\begin{aligned}\underset{h}{E}H &= \frac{\partial H[u_{i-n}]}{\partial u_i} + \cdots + \frac{\partial H[u_i]}{\partial u_i} + \cdots + \frac{\partial H[u_{i+m}]}{\partial u_i} \\ &= \left(\frac{\partial H[u_i]}{\partial u_{i+n}}\right)_{-n} + \cdots + \left(\frac{\partial H[u_i]}{\partial u_i}\right) + \cdots + \left(\frac{\partial H[u_i]}{\partial u_{i-m}}\right)_{m} \\ &= \sum_{k=-m}^{n} \left(\frac{\partial H[u_i]}{\partial u_{i+k}}\right)_{-k}, \end{aligned} \tag{2.29}$$

where $(\cdot)_k$ denotes that the quantity inside bracket is shifted on k steps. Thus in this case we get the following presentation of the discrete Euler operator:

$$\underset{h}{E} = \sum_{k=-m}^{n} \left(\frac{\partial \cdot}{\partial u_{i+k}}\right)_{-k}. \tag{2.30}$$

III. SYMMETRIES AND CONSERVATION LAWS

A. Invariance of semidiscrete equations

Let $\underset{h}{Z}$ be the space of sequences of variables $(t,x,h,u,\underset{h}{u_1},\underset{h}{u_2},\ldots)$ and $\underset{h}{\mathcal{A}}$ be the space of analytic functions of a finite number of variables z from $\underset{h}{Z}$.

Let us consider the infinite set of semidiscrete equations

$$\dot{u} = F(z), \quad F \in \underset{h}{\mathcal{A}} \tag{3.1}$$

defined at points of some two-dimensional mesh Ω. This equation is written on the finite number of points (stencil) of the difference mesh

$$\Omega(h_+, z) = 0, \quad h_+ = x_+ - x = (S_+ - 1)x, \tag{3.2}$$

which may be uniform or nonuniform. Then we say that the semidiscrete equation (3.1) on mesh (3.2) admits the group G if

$$\begin{cases} \dot{u} = F(z), \\ \Omega(h_+, z) = 0 \end{cases} \tag{3.3}$$

is an invariant manifold of the group G.

Symmetries of the systems of equation (3.3) are transformations generated by vector fields of the form

$$X = \xi^t(z)\frac{\partial}{\partial t} + \xi^x(z)\frac{\partial}{\partial x} + \eta(z)\frac{\partial}{\partial u}, \tag{3.4}$$

where $\xi^t,\ \xi^x,\ \eta \in \underset{h}{\mathcal{A}}$, which leave the system invariant. The infinitesimal criterion for invariance of Eq. (3.3) under a transformation generated by the operator (3.4) is given by the following conditions:

$$\mathbf{pr}\, X(\dot{u} - F(z))|_{\dot{u}=F,\Omega=0} = 0, \tag{3.5}$$

$$\mathbf{pr}\, X(\Omega)|_{\dot{u}=F,\Omega=0} = 0; \tag{3.6}$$

where the operator X is prolonged on all variables appearing in the system of Eq. (3.3)

$$\mathbf{pr}\,X = X + \zeta_1^t \frac{\partial}{\partial \dot{u}} + \underset{h}{\zeta_1^x} \frac{\partial}{\partial \underset{h}{u_1}} + \underset{h}{\zeta_2^x} \frac{\partial}{\partial \underset{h}{u_2}} + \cdots . \tag{3.7}$$

On the space-uniform grid (2.12) the coefficients of the prolonged operator are calculated through the prolongation formulas

$$\begin{gathered}\zeta_1^t = D_t(\eta) - \dot{u} D_t(\xi^t) - u_1 D_t(\xi^x), \quad \underset{h}{\zeta_1^x} = \underset{+h}{D}(\eta) - S_+(\dot{u}) \underset{+h}{D}(\xi^t) - \underset{h}{u_1} \underset{+h}{D}(\xi^x), \\ \underset{h}{\zeta_2^x} = \underset{-h+h}{D\,D}(\eta) - 2\underset{h}{u_2} \underset{+h}{D}(\xi^x) - \frac{1}{h} S_+(\dot{u}) \underset{+h}{D}(\xi^t) + \frac{1}{h} S_-(\dot{u}) \underset{-h}{D}(\xi^t), \ldots .\end{gathered} \tag{3.8}$$

These formulas are continuous for the time derivative $\dot{u}$[14,18–20] and discrete for the space derivatives.[5] Note that $u_1 = D_x(u)$ is the ''continuous'' derivative. It needs to be in some discrete representation, e.g., $\underset{h}{\tilde{D}_0}(u)$, which will be introduced in the following.

To check out the invariance one has to act by the prolonged operator $\mathbf{pr}\,X$ on the equation of system (3.3) and verify that the obtained expressions are annihilated on Eq. (3.3) and its difference consequences.

Conditions (3.5) and (3.6) require the invariance of the equations and of the mesh, correspondingly. For the mesh (2.12) the last condition can be split into two:

$$\underset{-h+h}{D\,D}(\xi^x)\big|_{\dot{u}=F,\Omega=0} = 0 \tag{3.9}$$

and

$$D_t(\xi^x)\big|_{\dot{u}=F,\Omega=0} = 0. \tag{3.10}$$

The bracket $\{\cdot,\cdot\}_h$ requires a space-uniform mesh that implies condition (3.9), which means the conservation of the space mesh uniformity under the group transformation.[21] Condition (3.10) has a clear geometrical meaning, it enforces that a vertical line of the time–space plane $x_i = \text{const}$, passing through a mesh point x_i, will remain vertical under the transformation. Let us note that in general the group transformation corresponding to the operator (3.4) destroys grid geometry.

Operators of the form (3.4) are called Lie–Bäcklund symmetries (they are also called *generalized* symmetries). An important subclass of the Lie–Bäcklund symmetries (3.4) is constituted by Lie point symmetries. They are given by the vector fields with coefficients ξ^t, ξ^x and η depending only on dependent and independent variables

$$X = \xi^t(t,x,u) \frac{\partial}{\partial t} + \xi^x(t,x,u) \frac{\partial}{\partial x} + \eta(t,x,u) \frac{\partial}{\partial u}. \tag{3.11}$$

Such symmetries are given by the same vector fields in the continuous and discrete cases.

Example 3.1: Groups satisfying invariance conditions.

If we require conditions (3.9) and (3.10) to be true for Lie point symmetries (3.11) independently of the considered equations, we find, as an example, that the transformations with generators

$$X = (ax + b) \frac{\partial}{\partial x} + \xi^t(t,x,u) \frac{\partial}{\partial t} + \eta(t,x,u) \frac{\partial}{\partial u}, \tag{3.12}$$

where a and b are constant, keep the mesh invariant.

Remark: In example 3.1 we require the mesh to be strongly invariant. For weak invariance of the semidiscrete equations we need the conditions (3.5), (3.9), and (3.10) to be satisfied on the

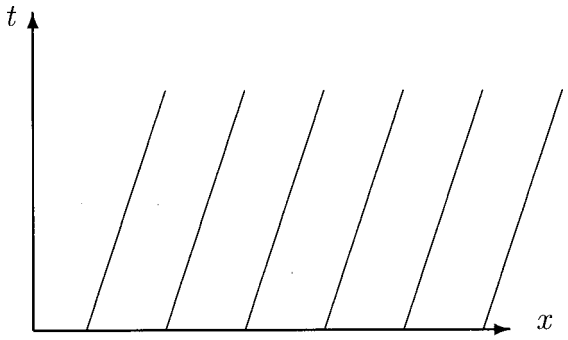

FIG. 2. Mesh deformation under the action of Galilean transformation.

solutions of the equations. Therefore a set of operators which keep equations invariant is broader than the set of operators which keep the mesh invariant independently of the considered equations.

Example 3.2: A group not satisfying invariance conditions.

Galilean transformation is central in models of Newton mechanics and is admitted by many equations. For example, the transfer equation (also known as nonviscous Burgers equation)

$$u_t = u u_x \tag{3.13}$$

and Korteweg–de Vries equation (2.8) are invariant with respect to the Galilean transformation

$$\begin{aligned} x^* &= x + t\alpha, \\ t^* &= t, \\ u^* &= u - \alpha, \end{aligned} \tag{3.14}$$

where α is a transformation parameter. Galilean transformation corresponds to the operator

$$X = t\frac{\partial}{\partial x} - \frac{\partial}{\partial u}.$$

The transformation does not keep vertical lines of the mesh [condition (3.10)]. Figure 2 shows that the vertical lines of the two-dimensional mesh (2.12) (see Fig. 1) become inclined under the transformation.

B. Factorization of the operators

In this point we overview factorization of operators both in continuous and discrete cases. The factorizations will be used to transfer the admitted symmetries into the canonical form. For simplicity we consider the space (x,u), where u is dependent variable and x is independent one.

(a) It is known that the Taylor group generated by the total differentiation operator D_x (2.7) provides a transition to the quotient algebra of the Lie–Bäcklund operators.[20] The operators $\xi(z)D_x$, where $\xi(z)$ is an analytic function of a finite number of variables in the space $(x,u,u_1,u_2,\ldots)$, form the ideal in the Lie algebra of operators

$$X = \xi(z)\frac{\partial}{\partial x} + \eta(z)\frac{\partial}{\partial u} + \cdots. \tag{3.15}$$

Thus instead of operator (3.15) one can consider the operator $\overline{X}$ in the canonical form

$$\overline{X}=X-\xi D_x=\overline{\eta}\frac{\partial}{\partial u}+\cdots, \quad \overline{\eta}=\eta-\xi u_x. \tag{3.16}$$

The representatives of this quotient algebra have independent variables as invariants and the extension formulas for them have simple and convenient form.

(b) Similar factorization can be done in the discrete case. Following Refs. 5 and 22 we consider the Lie–Bäcklund operator in the space $\underset{h}{Z}=(x,h,u,\underset{h}{u_1},\underset{h}{u_2},\ldots,\underset{h}{u_n},\ldots)$:

$$X=\xi(z)\frac{\partial}{\partial x}+\eta(z)\frac{\partial}{\partial u}+\underset{h}{\zeta_1}\frac{\partial}{\partial \underset{h}{u_1}}+\underset{h}{\zeta_2}\frac{\partial}{\partial \underset{h}{u_2}}+\cdots+h\underset{+h}{D}(\xi)\frac{\partial}{\partial h}, \tag{3.17}$$

where

$$\begin{gathered}\zeta_1=\underset{+h}{D}(\eta)-\underset{h}{u_1}\underset{+h}{D}(\xi), \quad \zeta_2=\underset{-h}{D}(\zeta_1)-\underset{h}{u_2}\underset{-h}{D}(\xi),\ \ldots,\\ \zeta_{2k+1}=\underset{+h}{D}(\zeta_{2k})-\underset{h}{u_{2k+1}}\underset{+h}{D}(\xi), \quad \zeta_{2k+2}=\underset{-h}{D}(\zeta_{2k+1})-\underset{h}{u_{2k+2}}\underset{-h}{D}(\xi),\ \ldots.\end{gathered} \tag{3.18}$$

Proposition 3.1: (*Dorodnitsyn*—Refs. 5 *and* 22) *The set of Lie–Bäcklund operators defined on the same uniform mesh forms a Lie algebra with multiplication*

$$[X_1,X_2]=X_1X_2-X_2X_1.$$

Let us consider the special operation of left multiplication of a Lie–Bäcklund operator by an analytic function $\underset{h}{\tilde{\xi}}(z)\in\mathcal{A}$:

$$\tilde{\xi}^*X=\overline{\tilde{\xi}\xi}\frac{\partial}{\partial x}+\overline{\tilde{\xi}\eta}\frac{\partial}{\partial u}+\left(\underset{+h}{D}(\tilde{\xi}\eta)-\underset{h}{u_1}\underset{+h}{D}(\tilde{\xi}\xi)\right)\frac{\partial}{\partial \underset{h}{u_1}}+\cdots+\underset{+h}{D}(\tilde{\xi}\xi)\frac{\partial}{\partial h}. \tag{3.19}$$

The first coordinates in the operator $\tilde{\xi}^*X$ are multiplied by $\tilde{\xi}(z)$ and the remaining coordinates are constructed according to the prolongation formulas (3.18).

Two representations for the operator of the Taylor group in the mesh space $\underset{h}{Z}$ were proposed in Refs. 5 and 22. They are the exact representations of the operator of total differentiation D_x in the space of difference variables

$$\begin{gathered}D^+=\frac{\partial}{\partial x}+\underset{+h}{\tilde{D}}(u)\frac{\partial}{\partial u}+\ldots, \quad \underset{+h}{\tilde{D}}=\sum_{n=1}^{\infty}\frac{(-h)^{n-1}}{n}\underset{+h}{D^n},\\ D^-=\frac{\partial}{\partial x}+\underset{-h}{\tilde{D}}(u)\frac{\partial}{\partial u}+\ldots, \quad \underset{-h}{\tilde{D}}=\sum_{n=1}^{\infty}\frac{h^{n-1}}{n}\underset{-h}{D^n},\end{gathered} \tag{3.20}$$

where $\underset{+h}{D}$ and $\underset{-h}{D}$ are right and left difference derivative operators on a uniform mesh.

It was shown in Refs. 5 and 22 that in the discrete case one can use ideals $\tilde{\xi}(z)*D^+$ and $\tilde{\xi}(z)*D^-$ for factorization of the operators (3.17). It is important to notice that every difference equation on a regular mesh admits the operators D^+ and D^-, which do not change the mesh, and that the representation (3.20) is true only for uniform meshes.

Another exact representation of the Taylor group operator in the mesh space $\underset{h}{Z}$ can be found with the help the central difference derivative (2.19). It is known that the finite transformations of a continuous groups have a one-to-one relation with infinitesimal transformations. This relation is expressed by a finite system of Lie equations for pointwise groups and by the unique recurrent sequence of coefficients of formal series for Lie–Bäcklund groups.[20] For both group types the solution of the system can be presented in the form of an exponential map. A finite transformation of any coordinate $z^i \in \underset{h}{Z}$ is generated by a vector field X,

$$(z^i)* = \exp(aX)(z^i) = \sum_{k=0}^{\infty} \frac{a^k}{k!} X^k(z^i).$$

Let us now invert the series, finding an infinitesimal transformation $aX(z^i)$ from the finite transformation $\exp(aX)(z^i)$:

$$aX(z^i) = \ln(\exp(aX))(z^i).$$

Taking the parameter value $a=h$, we can reconstruct the tangent field from the finite transformation of the Taylor group

$$\exp(a\underset{h}{\tilde{D}}_0)|_{a=h} = S_+$$

using the presentation of the right shift operator in terms of powers of $\underset{h}{D}_0$:

$$S_+ = h\underset{h}{D}_0 + \sqrt{1+h^2\underset{h}{D}_0^2} = h\underset{h}{D}_0 + \sum_{k=0}^{\infty} C_k^{1/2} h^{2k} \underset{h}{D}_0^{2k},$$

found from the relation

$$\underset{h}{D}_0 = \frac{S_+ - (S_+)^{-1}}{2h}.$$

We get

$$\underset{h}{\tilde{D}}_0 = \frac{1}{h}\sinh^{-1}(h\underset{h}{D}_0) = \frac{1}{h}\ln(h\underset{h}{D}_0 + \sqrt{1+h^2\underset{h}{D}_0^2}).$$

Using

$$\sinh^{-1}(x) = \ln(x+\sqrt{1+x^2}) = \sum_{k=0}^{\infty} \alpha_{2k+1} x^{2k+1}$$

with the expansion coefficients

$$\alpha_{2k+1}=(-1)^k\frac{1}{2}\frac{3}{4}\cdots\frac{2k-1}{2k}\frac{1}{2k+1}=\frac{(-1)^k}{2k+1}\frac{(2k-1)!!}{2^k k!},$$

where $(2k-1)!!=1\cdot 3\cdot 5\cdots(2k-1)$, we obtain the discrete representation of the operator D_x:

$$\underset{h}{\tilde{D}}_0=\sum_{k=0}^{\infty}\alpha_{2k+1}h^{2k}\underset{h}{D}_0^{2k+1}. \tag{3.21}$$

Finally, the infinitesimal operator of the Taylor group on $\underset{h}{Z}$ can be written as follows:

$$D^0=\frac{\partial}{\partial x}+\underset{h}{\tilde{D}}_0(u)\frac{\partial}{\partial u}+\underset{h}{\tilde{D}}_0(\underset{h}{u}_1)\frac{\partial}{\partial \underset{h}{u}_1}+\cdots+\underset{h}{\tilde{D}}_0(\underset{h}{u}_n)\frac{\partial}{\partial \underset{h}{u}_n}+\cdots, \tag{3.22}$$

where we used commutativity of the operators $\underset{+h}{D}$, $\underset{-h}{D}$ and $\underset{h}{D}_0$ on the uniform grid. One can also see that the operator D^0 satisfies conditions (3.18), i.e., the group generated by this operator is a nontrivial Lie–Bäcklund group.

Remark: The operators D^+ and D^- given in Eq. (3.20) use Newton series interpolation to the right and to the left, correspondingly. In the opposite directions they represent extrapolation. The operator D^0 represents interpolation on the whole real line.

Lemma 3.2: For any Lie–Bäcklund operators X and $\tilde{\xi}*D^0$, $\tilde{\xi}\in\underset{h}{\mathcal{A}}$ *defined on the same uniform mesh it is true that*

$$[\tilde{\xi}*D^0,X]=[\tilde{\xi}*D^0(\xi)-X(\tilde{\xi})]*D^0. \tag{3.23}$$

The proof of this Lemma is identical to the proof of the same result for the operators D^+ and D^-.[22] The Lemma provides us with the following result:

Theorem 3.3: The set of operators of the form

$$X_*=\tilde{\xi}(z)*D^0=\tilde{\xi}(z)\frac{\partial}{\partial x}+\tilde{\xi}(z)\underset{h}{\tilde{D}}_0(u)\frac{\partial}{\partial u}+\cdots \tag{3.24}$$

with arbitrary coefficients $\tilde{\xi}(z)$ *forms an ideal in the Lie algebra of all Lie–Bäcklund operators* $\{X\}$ *on the uniform grid.*

Consequently, instead of the Lie algebra of operators (3.17) we could consider the quotient algebra by the ideal $\tilde{\xi}(z)*D^0$. Although we can also use ideal $\tilde{\xi}(z)*D^+$ or $\tilde{\xi}(z)*D^-$ for factorization of the operators in the mesh space, the presence of the operator D_0 in the bracket suggests us to choose the ideal $\tilde{\xi}(z)*D^0$. As we will later see this choice is motivated by applications.

As representatives of the quotient algebra we shall consider the operators with the coordinate $\xi=0$:

$$\overline{X}=\overline{\eta}\frac{\partial}{\partial u}+\cdots,\quad \overline{\eta}=\eta-\xi\underset{h}{\tilde{D}}_0(u). \tag{3.25}$$

Let us note that the independent variable is invariant for the canonical operator (3.25). Furthermore it follows that the step of the mesh h is also invariant.

C. Conservation laws

For the system of Hamiltonian equations (2.17) considered on the grid (2.12) we have the following types of the conservation laws:

(1) If there are any distinguished functionals for the bracket (2.16), then they are conserved quantities. The distinguished functionals can be viewed as functionals corresponding to the symmetry $X_0 \equiv 0$.

(2) Hamiltonian form of Noether's theorem.

For the bracket based on the central difference derivative $\underset{h}{D}_0$ we can factorize the symmetries

$$X = \xi^t \frac{\partial}{\partial t} + \xi^x \frac{\partial}{\partial x} + \eta \frac{\partial}{\partial u} \tag{3.26}$$

by a combination of the discrete factorization (3.25) in space and continuous factorization (3.16) in time

$$\overline{X} = \overline{\eta} \frac{\partial}{\partial u}, \quad \overline{\eta} = \eta - \xi^t \underset{h}{\mathcal{D}} \left(\frac{\delta \underset{h}{\mathcal{H}}}{\delta u} \right) - \xi^x \underset{h}{\tilde{D}}_0(u), \tag{3.27}$$

where we substituted the expression for $\dot{u}$ from Eq. (2.17).

Definition: The Hamiltonian vector field associated with a functional $\underset{h}{\mathcal{P}}$ is the unique smooth vector field X_P satisfying

$$X_P(\underset{h}{\mathcal{F}}) = \{\underset{h}{\mathcal{F}}, \underset{h}{\mathcal{P}}\}_h. \tag{3.28}$$

In coordinate form it can be presented as the operator

$$X_P = \underset{h}{\mathcal{D}} \left(\frac{\delta \underset{h}{\mathcal{P}}}{\delta u} \right) \frac{\partial}{\partial u}. \tag{3.29}$$

Some symmetries (3.4) are given as Hamiltonian vector fields or are equivalent to Hamiltonian vector fields under factorization (3.27).

The Hamiltonian formulation of Noether's theorem provides the connection between symmetries and conservation laws.

Theorem 3.4: *For a Hamiltonian system of semidiscrete evolution equations (2.17) a Hamiltonian vector field X_P determines a generalized symmetry of the system if and only if there is an equivalent functional $\underset{h}{\tilde{\mathcal{P}}} = \underset{h}{\mathcal{P}} - \underset{h}{\mathcal{C}}$, differing only from $\underset{h}{\mathcal{P}}$ by a time-dependent distinguished functional $\underset{h}{\mathcal{C}}(t,x,h,u^{(n)})$, such that $\underset{h}{\tilde{\mathcal{P}}}$ determines a conservation law.*

The proof of this theorem is identical to that in the continuous case[14] and we will not reproduce it here.

Remark: The total derivative of the Hamiltonian is equal to its partial derivative

$$\frac{\mathrm{d}}{\mathrm{d}t} \underset{h}{\mathcal{H}} = \frac{\partial}{\partial t} \underset{h}{\mathcal{H}} + \{\underset{h}{\mathcal{H}}, \underset{h}{\mathcal{H}}\}_h = \frac{\partial}{\partial t} \underset{h}{\mathcal{H}} \tag{3.30}$$

because $\{\underset{h}{\mathcal{H}},\underset{h}{\mathcal{H}}\}_h=0$. Thus $\underset{h}{\mathcal{H}}$ is a conservation law if it is time independent. It is interesting to note that conservation of the time-independent Hamiltonian functional can be viewed as invariance of the equations with respect to time translation. Equations generated by time-independent Hamiltonian functionals are also time independent, that is they are invariant with respect to the operator

$$X_t=\frac{\partial}{\partial t}.$$

In the canonical form this operator can be presented as

$$\overline{X_t}=\dot{u}\frac{\partial}{\partial u}=\underset{h}{\mathcal{D}}\left(\frac{\delta\underset{h}{\mathcal{H}}}{\delta u}\right)\frac{\partial}{\partial u},$$

which shows that the Hamiltonian functional generates a symmetry and according to Theorem 3.4 it is a conservation law.

IV. EXAMPLES OF SEMIDISCRETE EQUATIONS WITH CONSERVATION LAWS

In this section we present several examples which demonstrate how Hamiltonian symmetries can be used to find conservation laws of the semidiscrete equations.

Example 4.1: Linear semidiscrete equations with infinitely many conservation laws.

Let us consider the Hamiltonian functional

$$\underset{h}{\mathcal{H}}=\sum_{\Omega} H[u]h,\quad H[u]=\frac{1}{2}(c_0u^2+c_1\underset{h}{u_1^2}+c_2\underset{h}{u_2^2}+\cdots+c_n\underset{h}{u_n^2}) \tag{4.1}$$

and the Poisson bracket based on the central difference derivative (2.19). They provide us the infinite set of ODEs

$$\dot{u}_i=c_0\frac{u_{i+1}-u_{i-1}}{2h}-c_1\frac{u_{i+2}-2u_{i+1}+2u_{i-1}-u_{i-2}}{2h^3}+\cdots+(-1)^n\underset{h}{c_n}\underset{h}{D_0}(\underset{h}{u_{2n}}) \tag{4.2}$$

with $i=0,\pm1,\pm2,\ldots$. In the continuous limit these equations correspond to the PDE

$$u_t=c_0u_1-c_1u_3+\cdots+(-1)^nc_nu_{2n+1}$$

for a function $u(t,x)$, $x\in\mathbb{R}$.

From the first glance we see that these equations conserve the distinguished functionals $\underset{h}{\mathcal{C}_1}$ and $\underset{h}{\mathcal{C}_2}$ given in Eq. (2.20) and the Hamiltonian functional (4.1). In addition to these evident conserved functionals we can construct conservation laws corresponding to the following symmetries:

(1) The admitted Hamiltonian operator

$$X_1=\frac{\partial}{\partial u} \tag{4.3}$$

corresponds to the functional

$$\underset{h}{\mathcal{P}_1}=\sum_{i=-\infty}^{\infty}x_iu_ih.$$

Because

$$\frac{\mathrm{d}}{\mathrm{d}t}\underset{h}{\mathcal{P}_1}=-c_0\sum_{i=-\infty}^{\infty}u_ih=-c_0\underset{h}{\mathcal{C}_1}$$

we obtain the conservation law

$$\underset{h}{\mathcal{P}_1}+tc_0\underset{h}{\mathcal{C}_1}=\sum_{i=-\infty}^{\infty}x_iu_ih+tc_0\sum_{i=-\infty}^{\infty}u_ih. \tag{4.4}$$

In the continuous limit we have

$$\underset{h}{\mathcal{P}_1}+tc_0\underset{h}{\mathcal{C}_1}\to\int xu\,\mathrm{d}x+tc_0\int u\,\mathrm{d}x.$$

(2) The symmetry

$$X_2=x\frac{\partial}{\partial u}$$

is admitted if $c_0=0$. It provides us the conservation law

$$\underset{h}{\mathcal{P}_2}=\frac{1}{2}\sum_{i=-\infty}^{\infty}x_i^2u_ih, \tag{4.5}$$

which goes into $\frac{1}{2}\int x^2u\,\mathrm{d}x$ in the continuous limit.

(3) The symmetry

$$X_3=x^2\frac{\partial}{\partial u} \tag{4.6}$$

is also admitted in the case $c_0=0$. Although it is not a Hamiltonian operator, the linear combination

$$X_3+\frac{h^2}{3}X_1=\left(x^2+\frac{h^2}{3}\right)\frac{\partial}{\partial u}$$

is. It is generated by the functional

$$\underset{h}{\mathcal{P}_3}=\frac{1}{3}\sum_{i=-\infty}^{\infty}x_i^3u_ih, \tag{4.7}$$

which lets us find the conservation law $\underset{h}{\mathcal{P}_3}+2tc_1\underset{h}{\mathcal{C}_1}$ which in the limit $h\to0$ becomes $\frac{1}{3}\int x^3u\,\mathrm{d}x+2tc_1\int u\,\mathrm{d}x$.

(4) Another Lie point symmetry admitted by the set of equations (4.2) is the translation in space presented by the operator

$$X_4=\frac{\partial}{\partial x}. \tag{4.8}$$

This operator is not canonical. Applying the factorization (3.27), we obtain the canonical symmetry

$$\overline{X}_4 = \underset{h}{\widetilde{D}}_0(u)\frac{\partial}{\partial u},$$

which is generated by the functional $\underset{h}{\mathcal{P}}_4$ satisfying

$$\underset{h}{D}_0\left(\frac{\delta \underset{h}{\mathcal{P}}_4}{\delta u}\right) = \underset{h}{\widetilde{D}}_0(u).$$

Further, with the help of the expression (3.21) we get

$$\left.\frac{\delta \underset{h}{\mathcal{P}}_4}{\delta u}\right|_i = \sum_{k=0}^{\infty} \alpha_{2k+1} h^{2k} \underset{h}{D}_0^{2k} u_i = \sum_{k=0}^{\infty} \alpha_{2k+1} \frac{(S_+ - S_-)^{2k}}{2^{2k}} u_i . \tag{4.9}$$

Applying

$$(S_+ - S_-)^{2k} = \sum_{j=0}^{2k} (-1)^j \frac{(2k)!}{j!(2k-j)!} S_{2(k-j)} = \sum_{p=-k}^{k} (-1)^{k-p} \frac{(2k)!}{(k-p)!(k+p)!} S_{2p},$$

where $S_i = S_{\mathrm{sign}(i)}^{|i|}$ represents a shift of indexes operator, to (4.9) and changing the order in the double sum, we arrive at

$$\left.\frac{\delta \underset{h}{\mathcal{P}}_4}{\delta u}\right|_i = \sum_{p=-\infty}^{\infty} b_{2p} S_{2p}(u_i) = \sum_{p=-\infty}^{\infty} b_{2p} u_{i+2p}, \tag{4.10}$$

where

$$b_{2p} = \sum_{k=|p|}^{\infty} \alpha_{2k+1} \frac{(-1)^{k-p}}{2^{2k}} \frac{(2k)!}{(k-p)!(k+p)!} = (-1)^p \sum_{k=|p|}^{\infty} \frac{1}{2k+1} \frac{1}{2^{2k}} \frac{((2k-1)!!)^2}{(k-p)!(k+p)!} \tag{4.11}$$

Let us note that $b_{-2p} = b_{2p}$.

Lemma 4.1: The series (4.11) defining coefficients b_{2p} for $p \in \mathbb{Z}$ are convergent.

Proof: Substituting $(k-p)!(k+p)! \geqslant (k!)^2$ into Eq. (4.11), we get

$$|b_{2p}| \leqslant \sum_{k=|p|}^{\infty} \frac{1}{2k+1} \frac{1}{2^{2k}} \left(\frac{(2k-1)!!}{k!}\right)^2 = \sum_{k=|p|}^{\infty} \frac{1}{2k+1} \left(\frac{(2k)!}{(2^k k!)^2}\right)^2 .$$

We use the bounds on the factorial provided by the Stirling's expansion

$$n^n \exp(-n)\sqrt{2\pi n} < n! < n^n \sqrt{2\pi n} \exp\left(-n + \frac{1}{12n}\right) \quad \text{for } n \in \mathbb{N}$$

to obtain the inequality

$$\frac{1}{2k+1}\left(\frac{(2k)!}{(2^k k!)^2}\right)^2 < \frac{1}{\pi k(2k+1)} \exp\left(\frac{1}{12}k\right) \quad \text{for } k \in \mathbb{N}$$

that ensures us that the series defining b_{2p} converges, moreover it can be shown that $|b_{2p}| \sim 1/|p|$ as $p \to \infty$.

A number of the first coefficients b_{2p} is given in Table I.

TABLE I. Some coefficients b_{2p}.

b_0	$b_{\pm 2}$	$b_{\pm 4}$	$b_{\pm 6}$	$b_{\pm 8}$	$b_{\pm 10}$	$b_{\pm 12}$	$b_{\pm 14}$
1.1662	−0.1070	0.0344	−0.0164	0.0095	−0.0061	0.0043	−0.0031

At this point we can construct the functional corresponding to the Hamiltonian symmetry $\overline{X}_4$. It is the conservation law of equations (4.2)

$$\mathop{\mathcal{P}_4}_h=\frac{1}{2}\sum_{i=-\infty}^{\infty} b_0u_i^2h+\sum_{p=1}^{\infty} b_{2p}\sum_{i=-\infty}^{\infty} u_iu_{i+2p}h=\frac{1}{2}\sum_{i=-\infty}^{\infty} u_i\sum_{p=-\infty}^{\infty} b_{2p}u_{i+2p}h. \tag{4.12}$$

For convergence of Eq. (4.12) it is essential that $u_i\to 0$ as $i\to\pm\infty$ fast enough.

Lemma 4.2: It is true that

$$\mathop{\mathcal{P}_4}_h\to\frac{1}{2}\int u^2\mathrm{d}x+O(h^2)\quad \text{as}\quad h\to 0.$$

Proof: Let us compare the functional $\mathop{\mathcal{P}_4}_h$ with the functional $1/2\sum_{i=-\infty}^{\infty} u_i^2h$:

$$\mathop{\mathcal{P}_4}_h-\frac{1}{2}\sum_{i=-\infty}^{\infty} u_i^2h=\frac{1}{2}\sum_{i=-\infty}^{\infty} u_i\left(\sum_{p=-\infty}^{\infty} b_{2p}u_{i+2p}-u_i\right)h$$

$$=\frac{1}{2}\sum_{i=-\infty}^{\infty} u_i\left(\sum_{k=0}^{\infty}\alpha_{2k+1}h^{2k}\mathop{D_0^{2k}}_h-1\right)u_ih=\frac{1}{2}\sum_{i=-\infty}^{\infty} u_i\sum_{k=1}^{\infty}\alpha_{2k+1}h^{2k}\mathop{D_0^{2k}}_h u_ih$$

$$=\frac{1}{2}\sum_{i=-\infty}^{\infty} u_i(\alpha_3h^2u''(x_i)+O(h^4))h=\frac{h^2}{2}\sum_{i=-\infty}^{\infty}\alpha_3u_iu''(x_i)h+O(h^4)=-\frac{h^2}{12}\int uu''\,dx+O(h^4).$$

On the other hand we have

$$\frac{1}{2}\sum_{i=-\infty}^{\infty} u_i^2h=\frac{1}{2}\int u^2\,\mathrm{d}x+O(h^2),$$

which combined with the previous result gives the statement of the lemma.

Let us note that in physical applications the integral (4.12) is referred as linear momentum.

(5) Equations (4.2) also admit the operators

$$Y_k=\mathop{D_0^{2k+1}}_h(u)\frac{\partial}{\partial u},\quad k=0,1,2,\ldots. \tag{4.13}$$

These operators are true Lie–Bäcklund symmetries, i.e., symmetries which are not equivalent to Lie point symmetries (3.11). All these operators are Hamiltonian with generating functionals

$$\underset{h}{\mathcal{R}}_k=\frac{1}{2}\sum_{i=-\infty}^{\infty} u_i D_0^{2k}(u_i)h=\frac{(-1)^k}{2}\sum_{i=-\infty}^{\infty}(\underset{h}{D}_0^k u_i)^2 h, \quad k=0,1,2,\ldots. \tag{4.14}$$

The functionals $\underset{h}{\mathcal{R}}_k$ are the conservation laws of (4.2), which in the continuous limit correspond to

$$\mathcal{R}_k=\frac{(-1)^k}{2}\int u_k^2\,dx, \quad k=0,1,2,\ldots.$$

It is interesting to note that the operators Y_k form the canonical operator $\overline{X}_4$ and that functionals $\underset{h}{\mathcal{R}}_k$ form the momentum functional (4.12) as the infinite series:

$$\overline{X}_4=\sum_{k=0}^{\infty}\alpha_{2k+1}h^{2k}Y_k, \quad \underset{h}{\mathcal{P}}_4=\sum_{k=0}^{\infty}\alpha_{2k+1}h^{2k}\underset{h}{\mathcal{R}}_k.$$

Example 4.2: In Examples 2.1 and 2.2 we saw that the Korteweg–de Vries equation and the transfer equation (2.10) can be rewritten as Hamiltonian PDEs. Let us now provide Hamiltonian semidiscretizations of these. We can take the operator $\underset{h}{D}_0$ for the discrete bracket and approximate the Hamiltonian functionals as

$$\underset{h}{\mathcal{H}}_1=\sum_{i=-\infty}^{\infty}\left(\frac{u_i^3}{6}-\frac{1}{2}\left(\frac{u_{i+1}-u_i}{h}\right)^2\right)h \tag{4.15}$$

and

$$\underset{h}{\mathcal{H}}_2=\sum_{i=-\infty}^{\infty}h(u_i)h, \tag{4.16}$$

leading to the semidiscrete equations

$$\dot{u}_i=\frac{u_{i+1}^2-u_{i-1}^2}{4h}+\frac{u_{i+2}-2u_{i+1}-2u_{i-1}-u_{i-2}}{2h^3} \tag{4.17}$$

and

$$\dot{u}_i=\frac{h'(u_{i+1})-h'(u_{i-1})}{2h}, \tag{4.18}$$

which approximate the original equations to order $O(h^2)$.

Some of the symmetries admitted by the original continuous equations[18] carry over to the semidiscretized equations. The invariance of Eqs. (4.17) and (4.18) on a uniform mesh with respect to translation in space provides us the conservation law (4.12). The equations also preserve the distinguished functionals (2.20) and their own Hamiltonian functionals.

That each of the above-found conservation laws is conserved can, of course, be proved directly. The advantage of the approach we used is that it is constructive and gives not only conservation laws, which we can expect (distinguished and Hamiltonian functionals), but also conservation laws of the form we would probably not try to find by ad hoc methods [see discrete momentum (4.12)]. We sum up the considered symmetries and their generating functionals in Table II.

TABLE II. Some symmetries and their generating functionals for the bracket given by the central difference derivative. The functionals (up to some distinguished functional) are conservation laws of the Hamiltonian semidiscrete equations constructed with the help of this bracket.

Operator	Operator in canonical form	Functional	Continuous limit of functional
	$0\,\frac{\partial}{\partial u}$	$\sum_{i=-\infty}^{\infty} u_i h, \quad \sum_{i=-\infty}^{\infty} (-1)^i u_i h$	$\int u\,\mathrm{d}x, \quad 0$
$\frac{\partial}{\partial t}$	$D_{0\,h}\left(\frac{\partial \mathcal{H}_h}{\delta u}\right)\frac{\partial}{\partial u}$	$\mathcal{H}_h$	$\mathcal{H}$
	$\frac{\partial}{\partial u}$	$\sum_{i=-\infty}^{\infty} x_i u_i h$	$\int xu\,\mathrm{d}x$
	$x\,\frac{\partial}{\partial u}$	$\frac{1}{2}\sum_{i=-\infty}^{\infty} x_i^2 u_i h$	$\frac{1}{2}\int x^2 u\,\mathrm{d}x$
	$\left(x^2+\frac{h^2}{3}\right)\frac{\partial}{\partial u}$	$\frac{1}{3}\sum_{i=-\infty}^{\infty} x_i^3 u_i h$	$\frac{1}{3}\int x^3 u\,\mathrm{d}x$
$\frac{\partial}{\partial x}$	$\sum_{k=0}^{\infty} \alpha_{2k+1} h^{2k} D_{0\,h}^{2k+1}(u)\,\frac{\partial}{\partial u}$	$\frac{1}{2}\sum_{i=-\infty}^{\infty} u_i \sum_{p=-\infty}^{\infty} b_{2p} u_{i+2p} h$	$\frac{1}{2}\int u^2\,\mathrm{d}x$
	$D_{0\,h}^{2k+1}(u)\,\frac{\partial}{\partial u}, \quad k=0,1,\ldots$	$\frac{(-1)^k}{2}\sum_{i=-\infty}^{\infty} (D_{0\,h}^k u_i)^2 h$	$\frac{(-1)^k}{2}\int u_k^2\,\mathrm{d}x$

V. CONCLUSIONS

In the paper we presented the Hamiltonian form of Noether's theorem for semidiscrete equations. The approach was illustrated on discretizations of Hamiltonian PDEs which preserve the Poisson bracket and some conservation laws of the original continuous equations. Using the connection between symmetries and conservation laws, we can point to two reasons why some conservation laws get lost after Poisson structure preserving space discretization. First, the symmetry can be lost because it is not admitted by the semidiscrete system on a uniform mesh (see Example 3.2). Second, there is a difference between continuous and discrete differentiation and some relations, which hold in the limit $h\to 0$, may not be true for finite steps h. One can easily see on the discrete Leibniz rule for the central discrete derivative

$$D_{0\,h}(FG)=\frac{G_+ + G_-}{2}D_{0\,h}(F)+\frac{F_+ + F_-}{2}D_{0\,h}(G)$$

or

$$D_{0\,h}(FG)=GD_{0\,h}(F)+FD_{0\,h}(G)+\frac{h^2}{2}(D\,D\,G)D_{0\,h}(F)+\frac{h^2}{2}(D\,D\,F)D_{0\,h}(G)$$

why some symmetries can be Hamiltonian in the continuous case, but lose this property under space discretization.

Although the necessity to have a discrete bracket satisfying *skew-symmetry* and Jacobi identity imposes limitations on the applications of the presented approach, extensions are possible in several ways. The results of the paper can be extended on the case of several dependent variables or several space variables. Work is in progress on conservation laws of the semidiscretized Schrödinger and wave equations, which can be presented as Hamiltonian equations with the help of the canonical bracket.[23] It is interesting to examine semidiscrete equations with periodic solutions, where the set of semidiscrete equations is finite. For such equations one can find first integrals

preserving time discretizations using first integral preserving discretization methods for Hamiltonian ODEs.[24–27] Note that, in general, it is impossible to preserve symplectic structure and all first integrals simultaneously.[28]

The present approach might also be applied to equations which have Lagrangian formulation. The consideration of semidiscrete equations with the Lagrangian formulation can take an intermediate position between the well-known continuous case and fully discrete case.[4–6] It can probably explain whether space or time discretization is the reason why particular conservation laws get lost under a discretization.

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Nonintegrability of Bianchi VIII Hamiltonian system

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In this paper we study the Bianchi VIII cosmological dynamical system. Our aim is to show that this system is nonintegrable. To show this we use an extension of Ziglin theory made by Morales-Ruiz and Ramis. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1351885]

I. INTRODUCTION

In certain cases cosmological models and relativistic systems can be represented as finite dimensional dynamical systems, i.e., as a set of ordinary differential equations. Such representation must be considered a great advantage. Usually the original model is represented as a coupled system of partial nonlinear differential equations arising from the field theory. Having a finite dimensional dynamical system, we have at hand a very rich theory and elaborated tools for its investigations.

It has to be mentioned, however, that dynamical systems of cosmological (or relativistic) origin have many special features which distinguish them from a ''typical'' dynamical system we meet in dynamical astronomy, classical mechanics or physics (see Ref. 1). These differences lead sometimes to controversies and long discussions. A good example is connected with the Bianchi IX [B(IX) or the Mixmaster] model and the presence of chaos in it. The numerically computed maximal Lapunov exponent for this system was equal to zero or different from zero depending on the time parametrization. Because an approximation of the Mixmaster model by a discrete map has strong chaotic properties,[2] it was natural to expect such behavior in the original system. However, as it was proved,[3] there exists no recurrence in the system and, thus, no form of standard deterministic chaos is present in it. Nevertheless, there were attempts to show that the dynamics of B(IX) contains some features characteristic for chaotic behavior. For example, in Refs. 4 and 5 one can find results of interesting numerical works where ''parametrization independent'' characteristics of chaos were used. Let us note, however, that this approach does not make big progress in understanding the system. The point is that in the cited works a certain approximation of the Mixmaster model was investigated, not the Mixmaster model itself. Moreover, one notices several notions used in these investigations which have no precise meaning.

A strict proof of the specific character of chaos in the Mixmaster system seems to be very difficult. That is why several authors tried to show that this system is not integrable. It must be mentioned that ''integrability'' here was understood differently by different authors. Several authors tested if the model passes the standard Painlevé integrability test in the form of the ARS

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algorithm.[6] In this approach the Mixmaster system is extended to a complex dynamical system. In Refs. 7 and 8 it was indicated that B(IX) model passes this test. This result was revised,[9] however, without any strict conclusions concerning integrability. Further studies[10] showed that the B(IX) model does not pass the so-called perturbative Painlevé test. The authors of this article suggest the existence of ''some chaotic regimes'' in the system, but, as the result of Cushman and Sniatycki shows, this claim without explanation of what ''chaotic regimes'' means is meaningless. The strongest result to this end was obtained in Ref. 11 where the authors show the existence of movable critical essential singularities in the B(IX) model. This kind of investigation connects a complicated behavior of the system with singularities of its solutions on the complex time plane. It should be mentioned, however, that the relation between Painlevé's test and integrability, in particular with complete integrability of Hamiltonian systems, is far from being clear.

The strongest and mathematically precise result concerning the Mixmaster model was obtained by J. J. Morales-Ruiz and J.-P. Ramis on the basis of their theory connecting Ziglin's method and differential Galois theory.[12] We state this result briefly. The Mixmaster model can be formulated as a Hamiltonian system. There exists a four dimensional invariant manifold $\mathcal{T}$ on which the system can be integrated explicitly. Solutions of the system restricted to $\mathcal{T}$ are known as Taub solutions. Studying variational equations around a selected Taub solution J. J. Morales-Ruiz proved that the Mixmaster model, considered as a complex Hamiltonian system, is not completely integrable (with meromorphic first integrals) in the sense of Liouville–Arnold theorem. As the system is homogeneous the meromorphic first integrals can be replaced by rational first integrals.

We make a few remarks about these results. First, it was not excluded that this system possesses one additional rational integral or is completely integrable in terms of nonrational integrals. Moreover, it can possess an additional integral only on the physically interesting zero energy level, or it can be integrable on it. Thus, by no means, does the result of Morales-Ruiz and Ramis close the subject.

In the sequel, when speaking about a completely integrable Hamiltonian system, we assume that all integrals are meromorphic.

In this article we apply Morales-Ruiz and Ramis approach to prove the nonintegrability of the Bianchi VIII model. To this end we study its dynamics carefully. We show that this system contains a four dimensional subsystem which is completely integrable. We demonstrate how to find an explicit form of solutions of this subsystem. Next, we consider particular solutions lying on the zero level of the Hamiltonian, and we investigate the normal variational equations for these solutions. Using the Kovacic algorithm, we determine the differential Galois group of these equations, and we prove the nonintegrability of the Bianchi VIII model.

II. DIFFERENTIAL GALOIS EXTENSION OF ZIGLIN THEORY

The fundamental papers of Ziglin[13,14] gave a formulation of a very basic theorem about the nonintegrability of analytic Hamiltonian systems. The idea of the Ziglin approach lies in a deep connection between properties of solutions on the complex time plane and the existence of first integral. This idea takes its origins from works of S. W. Kovalevskaya and A. M. Lapunov. Ziglin works found many continuations and many important applications (see, e.g., Refs. 15–27).

Here we give only the definitions needed for a formulation of the theorem we used to prove our main result.

We consider a complex Hamiltonian system with n degrees of freedom. It is defined on a complex analytic symplectic manifold M of complex dimension $2n$, and is given by a holomorphic Hamiltonian $\mathrm{H}: M \to \mathbb{C}$. The Hamiltonian vector field associated with H is denoted by X_{H}.

Let us assume that we know a nonequilibrium solution $z=\varphi(t)$, $t \in \mathbb{C}$, of Hamilton's equations of motion generated by X_{H} which is the maximal analytical continuation of a certain local solution. We associate a Riemannian surface Γ with it. Next, we consider the variational equations along $\varphi(t)$, and we restrict them to the normal bundle of Γ. These reduced variational equations are called the normal variational equations (NVE).

In the Ziglin approach the fundamental role is played by the monodromy group of NVE. Continuation along a close path γ with the base point $t_0 \in \mathbb{C}$ of a local fundamental solution of

NVE gives rise to a new fundamental solution of NVE defined in the same neighborhood of t_0. As NVE are linear and our system is Hamiltonian, there exists an element G_γ of symplectic group $\mathrm{Sp}(2(n-1),\mathbb{C})$ which transforms one solution to the other. In fact, G_γ depends on the homotopy class of γ, and map $\gamma \to G_\gamma$ gives a representation of the first homotopy group $\pi_1(\Gamma)$ of Γ in $\mathrm{Sp}(2(n-1),\mathbb{C})$. The image of this representation is called the monodromy group associated with NVE.

The Ziglin theory bases on two implications:

(i) If the considered Hamiltonian system possesses a first integral, then NVE also possess a first integral.
(ii) If NVE possess a first integral, then there exists a nonconstant function invariant with respect to the action of the monodromy group.

Now, it is clear that the existence of first integrals puts certain constraints onto the monodromy group and this fact was used by Ziglin to formulate his theorems.

J. J. Morales-Ruiz and J. P. Ramis modify the Ziglin approach in two respects. First, instead of answering the question of what restrictions to the monodromy group are imposed by the existence of certain numbers of independent first integrals, they ask what the consequences of complete integrability are. Next, instead of working with the monodromy group of NVE, they use the differential Galois group associated with NVE. This last group is bigger than the monodromy group and this fact makes a proof of complete nonintegrability easier. For a definition of differential Galois group, Liouvillian solutions and differential Galois theory (see Refs. 28–32).

We prove the main result of this article using the following theorem.

Theorem 1 (Morales-Ruiz, 1999): *Assume that there exist n first integrals of X_H which are meromorphic, in involution and functionally independent in a neighborhood of Γ. Then the identity component of the differential Galois group of NVE is Abelian.*

The main difficulty in application of the above theorem is connected with determination of the identity component of the differential Galois group of NVE. In fact, little is known about how to determine it for given equations. However, in our case, as it will be shown, we can reduce the investigated NVE to a second order linear equation with rational coefficients. This allows us to apply the Kovacic algorithm.[33] We describe it in the Appendix with some improvements compared to Refs. 34–36. Our description is self-contained and it can be useful in the study of other nonintegrability problems.

III. BIANCHI CLASS A HAMILTONIAN SYSTEMS

Homogeneous cosmological models are given by a four dimensional manifold $\mathcal{M}^4$ with a pseudo-Riemannian metric ds^2 satisfying Einstein equations. Homogeneity of a model means that metric ds^2 is invariant with respect to a certain three dimensional Lie group G acting on $\mathcal{M}^4$. It is assumed that orbits of this action are three dimensional. The most important are those models where the orbits of G action are spacelike, i.e., the metric restricted to an orbit is negative define. In such case $\mathcal{M}^4$ has the structure of Cartesian product of the form $\mathcal{M}^4=\mathbb{R}\times\mathcal{M}^3$ where $\mathcal{M}^3$ is an orbit of action of G. Vector fields X_i, $i=1,2,3$, which generate the action of group G, form a three dimensional Lie algebra. A simple classification of real three dimensional Lie algebras was done by Bianchi in 1897. It depends on a scalar $a\in\mathbb{R}$ and a vector (n_1,n_2,n_3), where $n_i\in\{+1,-1,0\}$ for $i=1,2,3$ in the following way:

$$[X_1,X_2]=n_3X_3,\ [X_2,X_3]=n_1X_1-aX_2,\ [X_3,X_1]=n_2X_2+aX_1.$$

Table I presents Bianchi classification. This classification, as well as the corresponding cosmological models, are naturally divided into two classes: to class A belong those models for which $a=0$, and to class B those for which $a\neq 0$. For a homogeneous model Einstein equations reduce to a certain dynamical system. In the case of a model belonging to class A this dynamical system is Hamiltonian. The Hamiltonian function for this system can be written in the following form:

TABLE I. Bianchi classification of three-dimensional Lie algebras.

Type	a	n_1	n_2	n_3	Type	a	n_1	n_2	n_3
I	0	0	0	0	III	1	1	-1	0
II	0	1	0	0	IV	1	1	0	0
VI_0	0	1	-1	0	V	1	0	0	0
VII_0	0	1	1	0	VI_a	$a\neq 1$	1	-1	0
VIII	0	1	1	-1	VII_a	$a\neq 0$	1	1	0
IX	0	1	1	1					

$$\mathrm{H}=g^{ij}p_ip_j+\frac{1}{2}\sum_{1\leqslant i<j\leqslant 3}n_iq_in_jq_j-\frac{1}{4}\sum_{i=1}^{3}(n_iq_i)^2, \tag{III.1}$$

where

$$[g^{ij}]=\begin{bmatrix}-q_1^2 & q_1q_2 & q_1q_3\\ q_2q_1 & -q_2^2 & q_2q_3\\ q_3q_1 & q_3q_2 & -q_3^2\end{bmatrix}.$$

From the physical interpretation it follows that variables q_i are non-negative. Thus our Hamiltonian system is defined on T^*Q, where $Q=\mathbb{R}_+^3$, where $\mathbb{R}_+$ is the positive real axis.

IV. PROPERTIES OF BIANCHI VIII HAMILTONIAN SYSTEM

From now on we will consider only the case of the Bianchi VIII model when $(n_1,n_2,n_3)=(1,1,-1)$. For short we called it a B(VIII) model.

For our investigation it is important to find a particular solution for the system. To this end we select an invariant set.

Lemma 1: For the B(VIII) *model a four dimensional manifold,*

$$\mathcal{T}=\{(q_1,q_2,q_3,p_1,p_2,p_3)\in T^*Q\,|\,q_1=q_2,\quad p_1=p_2\},$$

is invariant.

Proof: We make a symplectic change of variables

$$[q_1,q_2,q_3,p_1,p_2,p_3]^T=A[Q_1,Q_2,Q_3,P_1,P_2,P_3]^T,$$

where

$$A=\frac{1}{2}\begin{bmatrix}2 & 2 & 0 & 0 & 0 & 0\\ -2 & 2 & 0 & 0 & 0 & 0\\ 0 & 0 & 2 & 0 & 0 & 0\\ 0 & 0 & 0 & 1 & 1 & 0\\ 0 & 0 & 0 & -1 & 1 & 0\\ 0 & 0 & 0 & 0 & 0 & 2\end{bmatrix}. \tag{IV.1}$$

In the new variables the Hamiltonian of the B(VIII) model has the form

$$\mathrm{H}=-P_1^2Q_2^2-Q_1^2(1+P_2^2)-2Q_1P_1(Q_2P_2-Q_3P_3)+Q_2Q_3(2P_2P_3-1)-\tfrac{1}{4}Q_3^2(1+4P_3^2),$$

and thus Hamilton's equations read

$$\begin{aligned}
\dot{Q}_1 &= -2[P_1Q_2^2 + Q_1(Q_2P_2 - Q_3P_3)],\\
\dot{Q}_2 &= -2[Q_2(Q_1P_1 - Q_3P_3) + Q_1^2P_2],\\
\dot{Q}_3 &= 2Q_3[Q_1P_1 + Q_2P_2 - Q_3P_3],\\
\dot{P}_1 &= 2[Q_1(1+P_2^2) + P_1(Q_2P_2 - Q_3P_3)],\\
\dot{P}_2 &= Q_3(1-2P_2P_3) + 2P_1(Q_2P_1 + Q_1P_2),\\
\dot{P}_3 &= Q_2 + \tfrac{1}{2}Q_3 - 2P_3(Q_1P_1 + Q_2P_2 - Q_3P_3).
\end{aligned} \tag{IV.2}$$

Manifold $\mathcal{T}$ is defined in the new variables as

$$\mathcal{T} = \{(Q_1,Q_2,Q_3,P_1,P_2,P_3) \in T^*Q \,|\, Q_1 = 0, \quad P_1 = 0\}.$$

Direct inspection of the first and fourth equations in (IV.2) shows that indeed $\mathcal{T}$ is invariant. □

$\mathcal{T}$ is called Taub manifold and solutions lying on it are called Taub solutions. It is important to notice that the B(VIII) system restricted to $\mathcal{T}$ is integrable.

Lemma 2: The B(VIII) *model restricted to manifold* $\mathcal{T}$ *is a completely integrable Hamiltonian system*.

Proof: The B(VIII) model restricted to manifold $\mathcal{T}$ is given by the following system of differential equations:

$$\begin{aligned}
\dot{Q}_2 &= 2Q_2(Q_3P_3),\\
\dot{Q}_3 &= 2Q_3(Q_2P_2 - Q_3P_3),\\
\dot{P}_2 &= Q_3(1-2P_2P_3),\\
\dot{P}_3 &= Q_2 + \tfrac{1}{2}Q_3 - 2P_3(Q_2P_2 - Q_3P_3).
\end{aligned} \tag{IV.3}$$

Direct inspection shows that these equations are Hamiltonian with respect to the standard symplectic structure of $\mathbb{R}^4$, and that the Hamiltonian reads

$$\mathrm{H}_{\mathcal{T}} := \mathrm{H}_{|\mathcal{T}} = Q_2Q_3(2P_2P_3 - 1) - \tfrac{1}{4}Q_3^2(1+4P_3^2).$$

It is easy to verify that the function

$$F := Q_2Q_3 - (Q_2P_2)^2$$

is a first integral of system (IV.3). As $\mathrm{dH}_{\mathcal{T}} \wedge dF \not\equiv 0$, first integral $\mathrm{H}_{\mathcal{T}}$ and F are functionally independent. Thus system (IV.3) is completely integrable. □

There does not exist a direct ''recipe'' which allows us to obtain an explicit form of solutions of an integrable system. In fact, in general, it is a difficult task. Below, we demonstrate how to obtain an explicit form of a solution of system (IV.3). To this end, we first introduce noncanonical variables defined as follows:

$$z_i := \frac{\dot{q}_i}{q_i}, \quad i = 1,2,3.$$

In variables $(q_1,q_2,q_3,z_1,z_2,z_3)$ Bianchi class A models have the following form

$$\dot{q}_i = q_i z_i, \quad \dot{z}_i = (n_j q_j - n_k q_k)^2 - n_i^2 q_i^2,$$

where (i,j,k) runs all even permutations of $\{1,2,3\}$. In new variables Hamiltonian (III.1) reads

$$4\mathrm{H} = \sum_{1 \leqslant i < j \leqslant 3} (z_i z_j + 2 n_i n_j q_i q_j) - \sum_{i=1}^{3} (n_i q_i)^2.$$

Next we perform only for the B(VIII) model. We make a transformation

$$x := (q_1, q_2, q_3, z_1, z_2, z_3) \to X := (Q_1, Q_2, Q_3, Z_1, Z_2, Z_3),$$

given by $x = AX$, where matrix A is defined by (IV.1). The explicit form of equations of motion is the following:

$$\dot{Q}_1 = \tfrac{1}{2}(Q_1 Z_2 + Q_2 Z_1),$$

$$\dot{Q}_2 = \tfrac{1}{2}(Q_1 Z_1 + Q_2 Z_2),$$

$$\dot{Q}_3 = Q_3 Z_3,$$

$$\dot{Z}_1 = -4 Q_1 (2 Q_2 + Q_3),$$

$$\dot{Z}_2 = 2 Q_3 (2 Q_2 + Q_3),$$

$$\dot{Z}_3 = 4 Q_1^2 - Q_3^2,$$

and the first integral H reads

$$4\mathrm{H} = -4 Q_1^2 - Q_3 (4 Q_2 + Q_3) + Z_2 Z_3 + \tfrac{1}{4}(Z_2^2 - Z_1^2).$$

Now, invariant set $\mathcal{T}$ is defined as follows:

$$\mathcal{T} = \{(Q_1, Q_2, Q_3, Z_1, Z_2, Z_3) \,|\, Q_1 = 0, \quad Z_1 = 0\},$$

and the B(VIII) system restricted to $\mathcal{T}$ has the form

$$\dot{Q}_2 = \tfrac{1}{2} Q_2 Z_2, \tag{IV.4}$$

$$\dot{Q}_3 = Q_3 Z_3, \tag{IV.5}$$

$$\dot{Z}_2 = 2 Q_3 (2 Q_2 + Q_3), \tag{IV.6}$$

$$\dot{Z}_3 = -Q_3^2. \tag{IV.7}$$

This system possesses two functionally independent first integrals

$$H_{\mathcal{T}} = -Q_3 (4 Q_2 + Q_3) + Z_2 Z_3 + \tfrac{1}{4} Z_2^2, \quad G = Q_3^2 + Z_3^2.$$

Equations (IV.5) and (IV.7) form a closed subset which can be easily integrated explicitly if one takes into account that $Q_3^2 + Z_3^2$ is its first integral. The solution has the form

$$Q_3(t) = \frac{2Ak\mathrm{e}^{At}}{1 + k^2 \mathrm{e}^{2At}}, \quad Z_3(t) = A \frac{1 - k^2 \mathrm{e}^{2At}}{1 + k^2 \mathrm{e}^{2At}}, \tag{IV.8}$$

where $A \geqslant 0$ [because, as we already stated, the original phase space of the B(VIII) model is $T^*\mathbb{R}^3_+$], and $k \in \mathbb{R}$ are constants of integration. Thus, the main difficulty lies in explicit integrations of the subsystem formed by Eqs. (IV.4) and (IV.6). However, let us notice that, using first integral $\mathrm{H}_{\mathcal{T}}$, we can rewrite Eq. (IV.6) in the form

$$\dot{Z}_2 = \tfrac{1}{4} Z_2^2 + Z_3(t) Z_2 + Q_3(t)^2 - B, \tag{IV.9}$$

where B is the value of integral $\mathrm{H}_{\mathcal{T}}$. This is the Ricatti equation, and now the main difficulty of solving it lies in finding its particular solution. Equation (IV.9) depends on three parameters and thus we have to find a particular solution which is valid for all values of the parameters. It must be noted that there is no universal method for finding a particular solution of a Ricatti equation. However, in our case we can try to find it as a function of $Z_3(t)$. Direct calculations show that

$$U(t) = -2Z_3(t) + 2\sqrt{A^2 + B}$$

is a desired particular solution. In the above formula we assumed that $A^2 + B \geqslant 0$ because we look for real solutions, and we take the positive value of the square root. Now, using the standard procedure (see, e.g., Ref. 37), we obtain a general solution of (IV.9) in the form

$$Z_2(t) = Z(t)^{-1} + U(t), \tag{IV.10}$$

where

$$Z(t) = C \exp[-t\sqrt{A^2 + B}] - \frac{1}{4\sqrt{A^2 + B}},$$

and where C is an integration constant. Finally, integrating Eq. (IV.4) we obtain

$$Q_2(t) = D \frac{(1 + k^2 \exp 2tA) \exp[t(\sqrt{A^2 + B} - A)]}{(4C\sqrt{A^2 + B} - \exp[t\sqrt{A^2 + B}])^2}, \tag{IV.11}$$

where D is an integration constant.

Integrating system (IV.4)–(IV.7) we introduced five constants (A, B, C, D, k). However, only four of them can be independent. In fact, Eqs. (IV.8), (IV.10) and (IV.11) give a solution of system (IV.4)–(IV.7) if and only if the following condition is fulfilled:

$$2C(A^2 + B)^{3/2} = kAD. \tag{IV.12}$$

For further investigation we select only nonequilibrium solutions. As it is easy to verify Eqs. (IV.8), (IV.10) and (IV.11), define an equilibrium if and only if

$$A = B = 0, \quad \text{or} \quad A = D = C = 0, \quad \text{or} \quad k = D = A^2 + B = 0.$$

In our further investigations we plan to study those solutions which lie on the zero energy level. More precisely, we are interested in all real nonequilibrium solutions which lie on the invariant set $\mathrm{H}^{-1}(0) \cap \mathcal{T}$. For these solutions we have $B = 0$. Summarizing, all real nonequilibria solutions of system (IV.4)–(IV.7) which lie on the Taub manifold are given by (IV.8), (IV.10) and (IV.11) with $(A, B, C, D, k) \in \mathcal{P}$, where

$$\mathcal{P} := \{(A, B, C, D, k) \in \mathbb{R}_+ \times \mathbb{R}^4 \,|\, A > 0, \ B = 0, \ 2CA^2 = kD\}. \tag{IV.13}$$

V. NORMAL VARIATIONAL EQUATIONS

We can extend the B(VIII) Hamiltonian system to a complex one, i.e., as the phase space we can take $\mathbb{C}^6$. Moreover, we can take time as a complex variable. Solutions found in the previous section naturally extend to the complex time.

Let us take a solution $(Q_2(t),Q_3(t),Z_2(t),Z_3(t))$ which lies on invariant manifold $\mathcal{T}$, and let us write variational equations associated with this solution. They have the following form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\eta=\Lambda(t)\eta, \quad \eta\in\mathbb{C}^6,$$

where

$$\Lambda(t)=\frac{1}{2}\begin{bmatrix} Z_2(t) & 0 & 0 & Q_2(t) & 0 & 0 \\ 0 & Z_2(t) & 0 & 0 & Q_2(t) & 0 \\ 0 & 0 & 2Z_3(t) & 0 & 0 & 2Q_3(t) \\ \tilde{Q}(t) & 0 & 0 & 0 & 0 & 0 \\ 0 & 8Q_3(t) & 8Q(t) & 0 & 0 & 0 \\ 0 & 0 & -4Q_3(t) & 0 & 0 & 0 \end{bmatrix},$$

and $Q(t)=-8(2Q_2(t)+Q_3(t))$, $\tilde{Q}(t)=Q_2(t)+Q_3(t)$. From the definition of this manifold it follows that variations normal to $\mathcal{T}$ correspond to (η_1,η_4), and thus the normal variational equations are the following:

$$\frac{\mathrm{d}}{\mathrm{d}t}\eta_1=\frac{1}{2}Z_2(t)\eta_1+\frac{1}{2}Q_2(t)\eta_4,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\eta_4=-4[2Q_2(t)+Q_3(t)]\eta_1.$$

We transform this system to one equation of second order. To this end we determine η_4 from the first equation and we substitute it in the second. After simple calculations we obtain

$$\ddot{\xi}+a(t)\dot{\xi}+b(t)\xi=0, \tag{V.1}$$

where

$$a(t)=-Z_2(t), \quad b(t)=4Q_2(t)^2-Q_3(t)^2+\tfrac{1}{4}Z_2(t)^2,$$

and $\xi:=\eta_1$.

VI. MAIN RESULT

Generally, for a Taub solution given by (IV.8), (IV.10) and (IV.11) we do not know how to decide whether the identity component of the differential Galois group is Abelian or not. The reason is connected with the fact that we do not know how to transform Eq. (V.1) to an equation with rational coefficients. However, when such solution lies on the zero energy level $\mathrm{H}^{-1}(0)$ [it is equivalent to taking $(A,B,C,D,k)\in\mathcal{P}$ in (IV.8), (IV.10) and (IV.11)] then it is rational with respect to variable $z=\exp[At]$. This suggests making transformation $t\to z$ in (V.1). In order to minimize the number of parameters we distinguish two cases $k\neq 0$ and $k=0$, and we define

$$z(t):=\begin{cases} k\exp[At] & \text{for } k\neq 0, \\ \exp[At] & \text{for } k=0. \end{cases}$$

Let us note that the above transformation (which is a covering of the Riemannian surface) does not change the identity component of the differential Galois group of NVE. Now, after transformation $t\to z$ Eq. (V.1) has the form

$$\xi''+p(z)\xi'+q(z)\xi=0,$$

where

$$p(z)=\frac{A+a(t(z))}{Az},\quad q(z)=\frac{b(t(z))}{A^2z^2}.$$

Finally, putting

$$w:=\xi\exp\frac{1}{2}\int p(\tau)\,\mathrm{d}\tau,$$

we transform NVE to the reduced form

$$w''-r(z)w=0, \tag{VI.1}$$

where

$$r(z)=\frac{1}{2}\frac{dp(z)}{dz}+\frac{1}{4}p(z)^2-q(z).$$

For $k=0$ (in this case necessarily $C=0$) we have

$$r(z)=-\frac{c^2}{z^6}-\frac{1}{4z^2},\quad \text{where } c=\frac{2D}{A}. \tag{VI.2}$$

When $k\neq 0$ then

$$r(z)=\frac{s(z)}{z^2(z-c)^4},\quad c=4kAC, \tag{VI.3}$$

where

$$s(z)=-\tfrac{1}{4}(1+4c^2)z^4-cz^3+\tfrac{1}{2}c^2z^2-c^3z-c^2(1+\tfrac{1}{4}c^2).$$

We prove now that NVEs with $r(z)$ given by (VI.2) and (VI.3) have no Liouvillian solution.

Lemma 3: For $c\neq 0$ Eq. (VI.1) *with $r(z)$ given by* (VI.2) *has no Liouvillian solution.*

Proof: Let us use the Kovacic algorithm presented in the Appendix. We have $\Gamma'=\{0\}$, $\Gamma=\{0,\infty\}$, $\mathrm{ord}(0)=6$, $\mathrm{ord}(\infty)=2$, thus $m^+=6$ and $\gamma_2=\gamma=1$. Conditions 3, 4, 5 in the first step in the Appendix give $L=\{1\}$. It follows that we have $n=1$ and we proceed to the second step. Point 3 in this step gives $E_\infty=\{\frac{1}{2}\}$, and in point 5 we easily determine that $a_0=\mathrm{i}c$, $b_0=0$, and thus $E_0=\{\frac{3}{2}\}$. There is only one element in Cartesian product $E_0\times E_\infty$, namely $e=(e_0,e_\infty)=(\frac{3}{2},\frac{1}{2})$, and for it we have $d(e)=-1\notin\mathbb{N}_0$. Thus the equation considered has no Liouvillian solution. □

Lemma 4: For $c\neq 0$ Eq. (VI.1) *with $r(z)$ given by* (VI.3) *has no Liouvillian solution.*

Proof: As in the previous lemma we apply the Kovacic algorithm. We have $\Gamma'=\{0,c\}$, $\Gamma=\{0,c,\infty\}$, $\mathrm{ord}(0)=2$, $\mathrm{ord}(c)=4$, $\mathrm{ord}(\infty)=2$, thus $m^+=4$ and $\Gamma_2=\{0,\infty\}$, $\gamma_2=\gamma=2$. Conditions 3–5 in the first step give $L=\{1,2\}$. The partial fraction expansion for $r(z)$ has the form

$$r(z)=-\frac{4+c^2}{4c^2z^2}-\frac{2(2+c^2)}{c^3z}-\frac{(1+c^2)^2}{(z-c)^4}+\frac{2(1-c^4)}{c(z-c)^3}-\frac{2+(1+c^2)^2}{c^2(z-c)^2}+\frac{2(2+c^2)}{c^3(z-c)},$$

thus

$$\alpha_0=-\frac{4+c^2}{4c^2},\quad \Delta_0=\frac{2\mathrm{i}}{c}.$$

The Laurent series expansion of $r(z)$ at infinity has the form

$$r(z)=-\frac{1+4c^2}{4z^2}+O\left(\frac{1}{z^3}\right),$$

and thus

$$\alpha_\infty=-\tfrac{1}{4}-c^2,\quad \Delta_\infty=2\mathrm{i}c.$$

Now, we put $n=1$ and we go to the second step. We have

$$E_0=\left\{\frac{1}{2}\pm\frac{\mathrm{i}}{c}\right\},\quad E_\infty=\left\{\frac{1}{2}\pm\mathrm{i}c\right\}.$$

For pole $z=c$ we can find that

$$[\sqrt{r}]_c=\frac{\pm\mathrm{i}(1+c^2)}{(x-c)^2},\quad \text{thus}\quad a_c=-\mathrm{i}(1+c^2),$$

$$r-[\sqrt{r}]_c^2=\frac{2(1-c^4)}{c(z-c)^3}+O\left(\frac{1}{(z-c)^2}\right),\quad \text{thus}\quad b_c=2\,\frac{1-c^4}{c}.$$

From these calculations we find

$$E_c=\left\{1\pm\mathrm{i}\frac{1-c^2}{c}\right\}.$$

As $c\in\mathbb{R}\setminus\{0\}$, for $e\in E_0\times E_c\times E_\infty$ we have

$$\mathrm{Re}\sum_{p\in\Gamma}e_p=2\quad\text{and}\quad \mathrm{Re}\,d(e)=-1;$$

thus, it never happens that $d(e)\in\mathbb{N}_0$. It follows that we have to start from the second step of the algorithm with $n=2$. Now, we have

$$E_0=\{2(1-\Delta_0)+2j\Delta_0\,|\,j=0,1,2\}\cap\mathbb{Z}=2,$$

$$E_\infty=\{2(1-\Delta_\infty)+2j\Delta_\infty\,|\,j=0,1,2\}\cap\mathbb{Z}=2,$$

and $E_c=4$. Thus for unique $e=(2,4,2)$ we have $d(e)=-2\notin\mathbb{N}_0$, and we can conclude that the equation has no Liouvillian solution. □

Using the above two lemmas we prove the following.

Theorem 2: *The Hamiltonian system describing the* B(VIII) *model is not completely integrable in a neighborhood of a nonequilibrium Taub solution lying on the level* $\mathrm{H}^{-1}(0)$.

Proof: In fact, let us take a solution given by (IV.8), (IV.10) and (IV.11) with $(A,B,C,D,k)\in\mathcal{P}$. If $k=0$, then, by Lemma 3, NVE has no Liouvillian solution. Thus the identity component of the differential Galois group of NVE is $\mathrm{SL}(2,\mathbb{C})$, and from Theorem 1 it follows that the B(VIII) model is not completely integrable in a neighborhood of the selected solution. For $k\neq0$ we repeat the same arguments using Lemma 4. This ends the proof. □

VII. REMARKS AND COMMENTS

We proved that the B(VIII) model is not completely integrable in a neighborhood of an arbitrary nonequilibrium Taub solution lying on the zero level of the Hamiltonian. The method applied gives the nonintegrability result for all such solutions (note that they form a family parametrized by three parameters). As the theory used formulates only the necessary conditions for nonintegrability, one can expect that for specific values of parameters these conditions are not satisfied. For the system studied above it is not the case. It will be interesting and important to find examples where such phenomenon occurs. In fact, the applied theory gives only very limited insight into dynamical reasons of the nonintegrability, see Ref. 12. Thus, having examples for which this theory does not yield the nonintegrability for some parameters values we can numerically investigate a neighborhood of the particular solution. It seems that the obtained local phase portrait should show which dynamical phenomena are not ''sensed'' by the applied theory.

Let us stress that to relate the algebraic features of the system to geometry of its orbits is the main open problem in this domain.

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APPENDIX: KOVACIC ALGORITHM

The Kovacic algorithm gives an answer to the question if a linear second order differential equation with rational coefficients

$$w''+pw'+qw=0, \quad p, q\in\mathbb{C}(z), \quad '\equiv\frac{d}{dz}, \tag{A1}$$

possesses a Liouvillian solution. For definitions, details and proofs related to differential algebra, Refs. 29, 33, and 36. It is important that an answer to this question is connected with properties of the identity component of the differential Galois group of (A1).

It is known that when Eq. (A1) possesses a nonzero Liouvillian solution then all its solutions are Liouvillian. Making a change of variables

$$y=w\exp\frac{1}{2}\int p,$$

we transform (A1) to the reduced form

$$y''=ry, \tag{A2}$$

where

$$r=\tfrac{1}{2}p'+\tfrac{1}{4}p^2-q.$$

The new equation has the same identity component of differential Galois group as (A1). The logarithmic derivative $\omega:=y'/y$ of a solution y of Equation (A2) satisfies the Riccati equation

$$\omega'+\omega^2=r, \tag{A3}$$

and, according to Lie–Kolchin's theorem, Eq. (A2) has a Liouvillian solution if and only if the corresponding Riccati equation (A3) has an algebraic solution. Moreover, the degree n of the minimal polynomial for this algebraic solution belongs to

$$L_{\max} := \{1,2,4,6,12\}.$$

The differential Galois group G of (A2) is an algebraic subgroup of $\mathrm{SL}(2,\mathbb{C})$ and its identity component G^0 is of one of the following forms

Case 1: G^0 is triangularizable; for this case Eq. (A2) is reducible and has a solution of the form $y=\exp\int\omega$, where $\omega\in\mathbb{C}(z)$, i.e., Riccati equation (A3) has a rational solution $(n=1)$.

Case 2: G^0 is imprimitive; for this case Eq. (A2) has a solution of the form $y=\exp\int\omega$, where ω is algebraic over $\mathbb{C}(z)$ of degree 2, i.e., Riccati equation (A3) has an algebraic solution of degree $n=2$.

Case 3: G^0 is primitive and finite; for this case all solutions of Eq. (A2) are algebraic and Riccati equation (A3) has an algebraic solution of degree $n\in\{4,6,12\}$.

Case 4: $G^0=\mathrm{SL}(2,\mathbb{C})$ and Eq. (A2) has no Liouvillian solution, i.e. Riccati equation (A3) has no algebraic solution.

Now, we present the algorithm. First, we fix notation. The set of non-negative integers is denoted by $\mathbb{N}_0$. We define on $L_{\max}$ function h in the following way:

$$h(1)=1,\quad h(2)=2,\quad h(4)=3,\quad h(6)=2,\quad h(12)=1.$$

We write $r\in\mathbb{C}(z)$ in the form

$$r=\frac{s}{t},\quad s,t\in\mathbb{C}[z],$$

where s and t are relatively prime and t is monic. The algorithm consists of three steps.

First step

(1) Let $\Gamma' := \{c\in\mathbb{C}\mid t(c)=0\}$, $\Gamma := \Gamma'\cup\{\infty\}$. The order $\mathrm{ord}(c)$ of $c\in\Gamma'$ is equal to the multiplicity of c as a root of t; the order of infinity is defined by

$$\mathrm{ord}(\infty) := \max(0,4+\deg s-\deg t).$$

(2) Define

$$m^+ := \max_{c\in\Gamma}\mathrm{ord}(c).$$

For $i\in\mathbb{N}_0$ let

$$\Gamma_i := \{c\in\Gamma\mid \mathrm{ord}(c)=i\},$$

$$\Gamma_i' := \Gamma_i\setminus\{\infty\},\quad \gamma_i := \mathrm{card}\,\Gamma_i,\quad \text{and}\quad \gamma := \gamma_2+\sum_{\substack{\text{odd } k\\ 3\leqslant k\leqslant m^+}}\gamma_k.$$

(3) Define $L'\subset L_{\max}$ by the following rules:

$$1\in L'\Leftrightarrow \gamma=\gamma_2,$$

$$2\in L'\Leftrightarrow \gamma\geqslant 2,$$

$$4,6,12\in L'\Leftrightarrow m^+\leqslant 2.$$

(4) For each $c\in\Gamma_1\cup\Gamma_2$ find the Laurent series expansion of r around c in the form

$$r=\frac{\alpha_c}{(z-c)^2}+\frac{\beta_c}{z-c}+O(1),$$

for $c\in\Gamma_1'\cup\Gamma_2'$, and

$$r=\frac{\alpha_\infty}{z^2}+\frac{\beta_\infty}{z^3}+O\left(\frac{1}{z^4}\right),$$

for $c=\infty$. Put $\Delta_c:=\sqrt{1+4\alpha_c}$.

(5) If $m^+>2$, then $L=L'$. If $m^+\leqslant 2$ and $\forall c\in\Gamma_1\cup\Gamma_2\ \Delta_c\in\mathbb{Q}$, then $L=L'$ else $L=L'\setminus\{4,6,12\}$.

(6) If $L=\varnothing$, then go to **End** else assign n to the smallest element of L.

Second step

(1) If $\infty\in\Gamma_0$, then $E_\infty:=\{h(n)k\mid k=0,\ldots,n\}$.

(2) For each $c\in\Gamma_1$, define set $E_c:=\{nh(n)\}$.

(3) When $n=1$, for each $c\in\Gamma_2$, define the set

$$E_c:=\left\{\frac{1}{2}(1\pm\Delta_c)\right\}.$$

(4) When $n\geqslant 2$, for each $c\in\Gamma_2$, define the set

$$E_c:=\left\{\frac{h(n)}{2}(n-(n-2j)\Delta_c)\;\middle|\; j=0,\ldots,n\right\}\cap\mathbb{Z}.$$

If at least one set E_c is empty then go to **Continue**.

(5) When $n=1$, for each $c\in\Gamma_{2k}$, with $k\geqslant 2$, compute rational function $[\sqrt{r}]_c$ defined up to sign by the following conditions:

- for $c\in\Gamma_{2k}'$

$$[\sqrt{r}]_c=\frac{a_c}{(z-c)^k}+\sum_{2\leqslant j\leqslant k-1}\frac{s_{j,c}}{(z-c)^j},$$

$$r-[\sqrt{r}]_c^2=\frac{b_c}{(z-c)^{k+1}}+O\left(\frac{1}{(z-c)^k}\right),$$

- for $c=\infty$

$$[\sqrt{r}]_\infty=a_\infty z^{k-2}+\sum_{0\leqslant j\leqslant k-3}s_{j,\infty}z^j,$$

$$r-[\sqrt{r}]_\infty^2=-b_\infty z^{k-3}+O(z^{k-4}).$$

Now define the set E_c by

$$E_c:=\left\{\frac{1}{2}\left(k+\varepsilon\frac{b_c}{a_c}\right)\;\middle|\;\varepsilon=\pm 1\right\},$$

and function

$$\text{sign: } E_c\to\{+1,-1\},$$

$$\operatorname{sign}\left(\frac{1}{2}\left(k+\varepsilon\frac{b_c}{a_c}\right)\right):=\begin{cases}\varepsilon & \text{if} \quad b_c\neq 0,\\ +1 & \text{if} \quad b_c=0.\end{cases}$$

(6) When $n=2$ for each $c\in\Gamma_k$, with $k\geqslant 3$, define the set E_c by $E_c:=\{k\}$.

Third step

(1) For each $e=\{e_c\}_{c\in\Gamma}$ in Cartesian product $E:=\Pi_{c\in\Gamma}E_c$ compute

$$d(e)=n-\frac{1}{h(n)}\sum_{c\in\Gamma}e_c.$$

(2) Select elements e for which

(a) $d(e)\in\mathbb{N}_0$, and
(b) when $n=2$ or $n=6$, then e has an even number of components which are odd integers, and
(c) when $n=4$, then e has at least two components which are not divisible by 3 and the sum of all components which are not divisible by 3 is divisible by 3.

If no such element exists, then go to **Continue**.

(3) For each selected element e put

$$\theta=\frac{1}{h(n)}\sum_{c\in\Gamma'}\frac{e_c}{z-c}+\delta_n^1\sum_{\substack{c\in\Gamma_{2k}\\ k>1}}\operatorname{sign}(e_c)[\sqrt{r}]_c,$$

where δ_n^1 is the Kronecker symbol.

(4) For each (e,θ) decide if there exists a monic polynomial P of degree $d=d(e)$ satisfying the following system of equations,

$$P_n=-P,$$

$$P_{i-1}=-P_i'-\theta P_i-(i+1)(n-i)rP_{i+1},\quad \text{for}\quad n\geqslant i\geqslant 0,$$

$$P_{-1}=0,$$

and if so find it (in the above formulas P_i' denotes the derivative of P_i with respect to z).

Output: If a pair (θ,P) is found, then equation $y''=ry$ possesses the Liouvillian solution $\eta=\exp\int\omega$ where ω is a solution of the following irreducible algebraic equation

$$\sum_{i=1}^{n}\frac{P_i}{(n-i)!}\omega^i=0,$$

else

Continue: if n is not the greatest element in L then assign to n the next value in L and go to **Second step** else

End: equation $y''=ry$ has no Liouvillian solution.

1. Comments

A formulation of the Kovacic algorithm given in Ref. 38 is alternative to its original form and to that presented previously. It seems that it is much more convenient for computer implementation. However, for differential equations with simple structure of singularities, and depending on parameters it seems that the previous form of the algorithm is well suited. Let us note also that, as it was explained in Ref. 38, the polynomial P which appears in the point 4 of the third step satisfies a linear differential equation of order $n+1$ (this equation is isomorphic, as a differential operator, of the nth symmetric power of the investigated equation).

In the original formulation of the algorithm[23] consisting in fact, of three separated algorithms corresponding to cases 1, 2 and 3, each of them repeats similar steps. In Ref. 36 one can find a modification of the original formulation unifying and improving three algorithms in one. This form is very convenient for applications. However, there are errors in the algorithm. In fact, for

$$r(z)=-\frac{3}{16z^2}-\frac{2}{9(z-1)^2}+\frac{3}{16z(z-1)},$$

the equation $y''=r(z)y$ has a Liouvillian solution (see Ref. 33, Example 1, p. 23), but algorithm in Ref. 36 finds no such solution. Our analysis showed that there are three errors. Namely, we have the following.

(1) Conditions 5 in the first step of the algorithm (see Ref. 36, p. 215) are wrong. These conditions do not appear in earlier published versions of the algorithm[34,35]. However, when correctly stated they are important—they are necessary conditions for the existence of an algebraic solution (case 3). Their meaning is the following. If case 3 occurs, then poles $c\in\Gamma'$ have order not greater than 2 and for all $c\in\Gamma'$ we have $\Delta_c\in\mathbb{Q}$. Moreover, $c=\infty$ has order not greater then 2. This is equivalent to $\Sigma_{c\in\Gamma_1'\cup\Gamma_2'}\beta_c=0$. Finally, as it was shown in Ref. 33 (p. 11),

$$\alpha_\infty=\sum_{c\in\Gamma_2'}\alpha_c+\sum_{c\in\Gamma_1'\cup\Gamma_2'}c\beta_c.$$

Thus, the proper necessary condition is $\Delta_\infty\in\mathbb{Q}$.

(2) In the third step condition 2(b), $n=4$ in Ref. 36 (p. 216) is not correct. In fact, for

$$r(z)=-\frac{5z^2+27}{36(z^2-1)^2},$$

the equation $y''=r(z)y$ has an algebraic solution and case $n=4$ occurs (see Ref. 33, Example 2, p. 25). Applying the algorithm of Ref. 36 we find for $n=4$, $e=(4,4,4)\in E_1\times E_{-1}\times E_\infty$. For this e we have $d(e)=0$, but, according to the mentioned condition, we have to reject it from further calculations. However, exactly for this e, using the original algorithm we find the desired solution. This error appears also in the earlier version of the algorithm.[34,35]

(3) In the third step there is an additional condition for $n=4$ in 2(b). Namely, at least two components of e are divisible by 3. The example in the previous point shows that it is not a correct condition. In the earlier version of the algorithm the mentioned condition reads ''... at least two components of e are not multiples of 3,'' and this is the correct condition.

Let us explain how the proper condition for components of vectors e in the third step can be deduced. For $n=2$, 4 and 6 we can choose the fundamental solution (ξ,η) of the equation $y''=ry$ in such a way that $u_n^{h(n)}\in\mathbb{C}(z)$, where $u_2:=\xi\eta$, $u_4:=\eta^4+8\eta\xi^3$, and $u_6:=\xi\eta^5-\xi^5\eta$. Moreover, from the structure of differential Galois groups for the respective cases it follows that $u_n\notin\mathbb{C}(z)$ for $n=2$, 4 and 6. Thus writing

$$u_n^{h(n)}=\prod_{c\in\Gamma'}(z-c)^{e_c},\quad e_c\in\mathbb{Z},$$

we deduce that for $n=2$ and $n=6$ at least one e_c for $c\in\Gamma'$ is an odd integer, and for $n=4$ at least one e_c is not divisible by 3. Moreover, we have

$$d(e)=n-\frac{1}{h(n)}\sum_{c\in\Gamma}e_c,\quad e_c\in\mathbb{Z},$$

and this implies the necessary conditions in the presented algorithm.

Finally let us notice that in Ref. 39 necessary conditions for the existence of a Liouvillian solution of third and second order linear differential equations were formulated. This article gives also a clear explanation of the origin of arithmetic conditions which appear in the present formulation of the algorithm.

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Reduction of dispersionless coupled Korteweg–de Vries equations to the Euler–Darboux equation

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A quasilinear hyperbolic system of two first-order equations is introduced. The system is linearized by means of the hodograph transformation combined with Riemann's method of characteristics. In the process of linearization, the main step is to explicitly express the characteristic velocities in terms of the Riemann invariants. The procedure is shown to be performed by quadrature only for specific combinations of the parameters in the system. We then apply the method developed here to the dispersionless versions of the typical coupled Korteweg–de Vries (cKdV) equations including the Broer–Kaup, Ito, Hirota–Satsuma, and Bogoyavlenskii equations and show that these equations are transformed into the classical Euler–Darboux equation. A more general quasilinear system of equations is also considered with application to the dispersionless cKdV equations for the Jaulent–Miodek and Nutku–Öğuz equations. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1345500]

I. INTRODUCTION

In the development of soliton theory, a large number of nonlinear evolution equations have been found that can be solved by means of the inverse scattering transform (IST).[1–3] A remarkable feature of the IST is that it enables us to reduce essentially nonlinear problems to linear ones and this fact makes it possible to solve the initial value problem of a wide class of nonlinear evolution equations. The equations solved by the IST are now called soliton equations. Although the IST provides a general scheme for solving soliton equations, it is difficult to construct solutions analytically for arbitrary initial conditions. Exceptions are soliton solutions which can be obtained by purely algebraic means.

If one neglects dispersive terms, however, soliton equations are considerably simplified and they may sometimes be solved analytically without recourse to the IST. For a certain class of initial conditions, the solutions thus obtained would become multivalued functions after a finite time due to the effect of nonlinearity, namely wave-breaking occurs which usually accompanies shocks. While the properties of the solutions for the original dispersive equations in the small dispersion limit generally differ from those of the corresponding dispersionless equations, the latter provides useful information on wave characteristics such as the wave profile prior to wave-breaking and the time and location of shock formation.

The purpose of this paper is to show that typical dispersionless soliton equations are reducible to the linear equations whose solutions have been studied in detail. In particular, we are concerned here with the dispersionless coupled Korteweg–de Vries (cKdV) equations. It is demonstrated by means of the hodograph transformation combined with Riemann's method of characteristics that these equations can be transformed into either the Euler–Darboux (ED) equation or the Euler–Poisson–Darboux (EPD) equation which is a special case of the ED equation. The method of exact solution for both equations is now well known, mainly due to the original work of Riemann. This paper is organized as follows. In Sec. II, a quasilinear hyperbolic system of two first-order

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equations is introduced in two independent variables which are closely related to the dispersionless cKdV equations. The characteristic velocities and associated Riemann invariants are defined for this system. We regard the Riemann invariants as new independent variables and use the hodograph method to transform the quasilinear system of equations into a linear system of equations with respect to the time and space variables. Tsarev's method for solving the hodograph equations is also discussed. Then, we calculate the Riemann invariants by elementary integration and derive the conditions under which the characteristic velocities are represented explicitly by the Riemann invariants. In Sec. III, we exemplify various types of dispersionless cKdV equations which include the dispersionless versions of the Broer–Kaup, Ito, Hirota–Satsuma, and Bogoyavlenskii equations. It is shown that all these equations are transformed into the ED or EPD equations. In Sec. IV, we extend the method developed in Sec. II to a more general class of quasilinear system of equations and use it to linearize the dispersionless equations for the Jaulent-Miodek and Nutku–Öğuz equations. Section V is devoted to concluding remarks. In Appendix A, we derive an infinite number of conservation laws for the quasilinear system of equations considered in Sec. II. In Appendix B, the periodic-wave and soliton solutions for Ito's cKdV equation are presented which will suggest a hint for constructing general multisoliton solutions.

II. QUASILINEAR HYPERBOLIC SYSTEM

Let us introduce the following quasilinear system of first-order equations:

$$u_t = \alpha u u_x + \beta v v_x, \tag{2.1a}$$

$$v_t = \gamma v u_x + \delta u v_x, \tag{2.1b}$$

where $u=u(x,t)$ and $v=v(x,t)$ are real functions of x and t and α, β, γ, and δ are real parameters. We assume that $\beta \neq 0$ since the case $\beta=0$ decouples the equation for u from (2.1a). The notations $u_t=\partial u/\partial t, u_x=\partial u/\partial u_x$, etc. are used for convenience. The system of Eqs. (2.1) can be written compactly in a vector form as

$$\mathbf{u}_t = A\mathbf{u}_x, \quad \mathbf{u}=\begin{pmatrix} u \\ v \end{pmatrix}, \quad A=(A_{ij})=\begin{pmatrix} \alpha u & \beta v \\ \gamma v & \delta u \end{pmatrix}. \tag{2.2}$$

We consider here the hyperbolic system which is defined by the condition

$$\Delta \equiv (\alpha-\delta)^2 u^2 + 4\beta\gamma v^2 > 0. \tag{2.3}$$

As will be seen in Sec. III, typical dispersionless cKdV equations are reduced to (2.1) by appropriate change of dependent variables. In Appendix A, an infinite number of conservation laws are derived for Eq. (2.1).

A. Riemann invariants

In order to solve (2.1), we use the hodograph transformation combined with Riemann's method of characteristics. Although the method is well-known,[4,5] we shall summarize it in a form relevant to the present problem. The characteristic velocity c is defined by the solution of the following characteristic equation,

$$\det(A_{ij} - \delta_{ij} c) = 0, \tag{2.4}$$

where δ_{ij} is Kronecker's delta. Introducing A into (2.4), one obtains

$$c^{\pm} = \tfrac{1}{2}[(\alpha+\delta)u \pm \sqrt{(\alpha-\delta)^2 u^2 + 4\beta\gamma v^2}], \tag{2.5}$$

with the $\pm$ signs ordered vertically. The condition of hyperbolicity (2.2) assures that $c^{\pm}$ are real and distinct. Let $\mathbf{l}^{+}=(l_1^{+},l_2^{+})$ denotes a left eigenvector of A associated with the eigenvalue c^{+}, i.e., $\mathbf{l}^{+}\cdot A=c^{+}\mathbf{l}^{+}$. It then follows from (2.2) that $\mathbf{l}^{+}\cdot\mathbf{u}_t=\mathbf{l}^{+}\cdot A\mathbf{u}_x=c^{+}\mathbf{l}^{+}\cdot\mathbf{u}_x$. In terms of the components l_1^{+},l_2^{+}, this relation becomes

$$l_1^{+}\frac{du}{dt}+l_2^{+}\frac{dv}{dt}=0, \tag{2.6}$$

where $du/dt=u_t+(dx/dt)u_x=u_t-c^{+}u_x(dx/dt=-c^{+})$. If we rewrite (2.6) as $du/dv=-l_2^{+}/l_1^{+}$ and express l_1^{+} and l_2^{+} in terms of u and v, we can regard this equation as an ordinary differential equation for u with v being an independent variable. Its solution defines the Riemann invariant ϕ,

$$\phi(u,v)=\xi=\text{const. on}\frac{dx}{dt}=-c^{+}. \tag{2.7}$$

Similarly, one finds for c^{-},

$$l_1^{-}\frac{du}{dt}+l_2^{-}\frac{dv}{dt}=0, \tag{2.8}$$

where $\mathbf{l}^{-}=(l_1^{-},l_2^{-})$ is a left eigenvector corresponding to c^{-}. This equation yields another Riemann invariant ψ,

$$\psi(u,v)=\eta=\text{const. on}\frac{dx}{dt}=-c^{-}. \tag{2.9}$$

The Riemann invariants (2.7) and (2.9) play roles analogous to integrals for systems of ordinary differential equations.

B. Hodograph transformation

The hodograph transformation reverses the roles of the dependent and independent variables. In the present case, we regard x and t as functions of u and v. However, if we use (2.7) and (2.9), we can express u and v by the Riemann invariants ξ and η. Hence, it is more convenient to choose ξ and η as new independent variables, i.e., $x=x(\xi,\eta),t=t(\xi,\eta)$. Then, on the characteristic curve $dx/dt=-c^{+}$ ($\xi=$const.), one obtains $dx=x_{\eta}d\eta$ and $dt=t_{\eta}d\eta$. Introducing these relations into the equation $dx/dt=-c^{+}$ gives

$$x_{\eta}=-c^{+}t_{\eta}. \tag{2.10}$$

Similarly, on the characteristic curve $dx/dt=-c^{-}$ ($\eta=$const.), one obtains

$$x_{\xi}=-c^{-}t_{\xi}. \tag{2.11}$$

We can eliminate x from (2.10) and (2.11) to obtain the second-order linear equation for t,

$$t_{\xi\eta}=\frac{c_{\eta}^{-}}{c^{+}-c^{-}}t_{\xi}-\frac{c_{\xi}^{+}}{c^{+}-c^{-}}t_{\eta}. \tag{2.12}$$

Also, it is possible to find a single equation for x as

$$x_{\xi\eta}=\frac{c^{+}c_{\eta}^{-}}{c^{-}(c^{+}-c^{-})}x_{\xi}-\frac{c^{-}c_{\xi}^{+}}{c^{+}(c^{+}-c^{-})}x_{\eta}. \tag{2.13}$$

Note that to solve the above system of equations, one must express the characteristic velocities $c^{\pm}$ in terms of ξ and η explicitly. As will be shown in Sec. II C, this is always possible *in principle* for the system of equations with two dependent variables. However, in order to perform this procedure only by quadrature, certain conditions must be imposed on the parameters in (2.1). Equations (2.12) and (2.13) will play a central role in the reduction of the dispersionless cKdV equations.

Lastly, we shall introduce a new method developed by Tsarev.[6] Let w_1 and w_2 be the solutions of the following system of linear equations with $c^{\pm}$ being given functions of ξ and η,

$$\frac{w_{1,\eta}}{w_1-w_2}=\frac{c^+_\eta}{c^+-c^-},\ \frac{w_{2,\xi}}{w_1-w_2}=\frac{c^-_\xi}{c^+-c^-}, \tag{2.14}$$

and consider the system of linear algebraic equations for x and t, $x+c^+t=w_1$ and $x+c^-t=w_2$. Then, a direct calculation shows that the solutions for t and x given by

$$t=\frac{w_1-w_2}{c^+-c^-},\quad x=-\frac{c^-w_1-c^+w_2}{c^+-c^-}, \tag{2.15}$$

satisfy the system of Eqs. (2.10) and (2.11). We can derive from (2.14) a single linear equation for w_1,

$$w_{1,\xi\eta}=\frac{c^+_\eta}{c^+-c^-}w_{1,\xi}+\left(\frac{c^+_{\xi\eta}}{c^+_\eta}-\frac{c^+_\xi}{c^+-c^-}\right)w_{1,\eta}, \tag{2.16}$$

and for w_2,

$$w_{2,\xi\eta}=\left(\frac{c^-_{\xi\eta}}{c^-_\xi}+\frac{c^-_\eta}{c^+-c^-}\right)w_{2,\xi}-\frac{c^-_\xi}{c^+-c^-}w_{2,\eta}. \tag{2.17}$$

The Tsarev system of Eqs. (2.16) and (2.17) sometimes considerably simplifies the problem of finding solutions even when Eqs. (2.12) and (2.13) for t and x become too complicated to be solved analytically (see Secs. III and IV).

C. Calculation of the Riemann invariants

Following the method developed in Sec. II B, we shall now calculate the Riemann invariants and express the characteristic velocities in these terms. Three different cases arise according to values of the coefficients in (2.1).

(1) Case 1: $\alpha\neq\delta,\ \gamma\neq 0,\ \alpha-\gamma-\delta\neq 0$:

In this case, we first define the constant parameters a and b by

$$a=\frac{\beta}{\alpha-\gamma-\delta},\quad b=\frac{4\beta\gamma}{(\alpha-\delta)^2}. \tag{2.18}$$

In the following analysis, we consider the case $b/a\leqslant 1$, i.e., $4\gamma(\alpha-\gamma-\delta)\leqslant(\alpha-\delta)^2$.

For $c^+=\frac{1}{2}[(\alpha+\delta)u+\sqrt{\Delta}]$, one finds $\mathbf{l}^+=(l_1^+,l_2^+)=(1,-\{(\alpha-\delta)u-\sqrt{\Delta}\}/2\gamma v)$. Then, the equation that defines the Riemann invariant follows from (2.6) as

$$\frac{du}{dv}=\frac{1}{2\gamma v}\{(\alpha-\delta)u-\sqrt{\Delta}\}. \tag{2.19}$$

If we introduce a new dependent variable $\tilde{u}$ by $u=v\tilde{u}$, we can integrate (2.19) and obtain the Riemann invariants. The result is expressed compactly as follows:

$$(\sqrt{u^2+bv^2}+u)(\sqrt{u^2+bv^2}-\rho_1 u)^{\rho_1}v^{\rho_2}(u^2+av^2)^{\rho_3}=\xi, \tag{2.20a}$$

with

$$\rho_1=-\sqrt{1-\frac{b}{a}},\quad \rho_2=\mathrm{sgn}(\alpha-\delta)-1,\quad \rho_3=\frac{1}{2}\mathrm{sgn}(\alpha-\delta)-\frac{\gamma}{|\alpha-\delta|}+\frac{1}{2}\sqrt{1-\frac{b}{a}}. \tag{2.20b}$$

The corresponding Riemann invariant for $c^-=\frac{1}{2}[(\alpha+\delta)u-\sqrt{\Delta}]$ reads in the form

$$(\sqrt{u^2+bv^2}-u)(\sqrt{u^2+bv^2}+\rho_1 u)^{\rho_1}v^{\rho_2}(u^2+av^2)^{\rho_3}=\eta. \tag{2.21}$$

Now, we like to express $c^{\pm}$ in terms of the Riemann invariants. For this purpose, we divide (2.20a) by (2.21) and put $\sqrt{u^2+bv^2}=uz$ to define new variable z. We then find the equation that determines z,

$$\frac{z+1}{z-1}\left[\frac{z-\rho_1}{z+\rho_1}\right]^{\rho_1}=\frac{\xi}{\eta}. \tag{2.22}$$

By solving (2.22) together with (2.20) and (2.21), we can express u and v in terms of ξ and η. The expressions of $c^{\pm}$ then follow from (2.5). Equation (2.22) will become a transcendental equation for z. However, if the ratio b/a is chosen such that the factor ρ_1 becomes a rational number, (2.22) reduces to an algebraic equation for z. Of particular interest is the case for which the solutions of the algebraic equation can be obtained by quadrature. As is well-known, this situation occurs if the order of the algebraic equation is less than or equal to four. The corresponding values of b/a and ρ_1 are then given by

$$\frac{b}{a}=\frac{4\gamma(\alpha-\gamma-\delta)}{(\alpha-\delta)^2}=1,\frac{8}{9},\frac{3}{4},-3,-8,\quad \rho_1=0,-\frac{1}{3},-\frac{1}{2},-2,-3. \tag{2.23}$$

(2) Case 2: $\alpha\neq\delta,\ \gamma=0$:

This special case is particularly simple. Indeed, the characteristic velocities and corresponding Riemann invariants become

$$c^+=\alpha u,\quad c^-=\delta u, \tag{2.24}$$

$$u^2+\frac{\beta}{\alpha-\delta}v^2=\xi,\quad -\frac{\beta}{\alpha-\delta}v^2=\eta, \tag{2.25}$$

and $c^{\pm}$ are now written in the form

$$c^+=\alpha\sqrt{\xi+\eta},\quad c^-=\delta\sqrt{\xi+\eta}. \tag{2.26}$$

(3) Case 3: $\alpha=\delta,\gamma\neq 0$:

In this case, it follows from (2.5) that

$$c^{\pm}=\alpha u\pm\sqrt{\beta\gamma}v,\quad (\beta\gamma>0), \tag{2.27}$$

and the corresponding Riemann invariants are

$$u+\sqrt{\frac{\beta}{\gamma}}v=\xi,\quad -u+\sqrt{\frac{\beta}{\gamma}}v=\eta. \tag{2.28}$$

In terms of ξ and η, $c^{\pm}$ are expressed as

$$c^{\pm}=\tfrac{1}{2}(\alpha\pm|\gamma|)\xi+\tfrac{1}{2}(\alpha\mp|\gamma|)\eta. \tag{2.29}$$

D. Remark

Under certain condition, the equation for u is decoupled completely from that of v. To see this, we differentiate (2.1a) by t and use (2.1a) and (2.1b) to obtain

$$u_{tt}=\alpha^2(u^2u_x)_x+\beta(\alpha+\delta)(uv_{xx}+uv_x^2)+\beta(\alpha+2\gamma+\delta)vu_xv_x+\beta\gamma^2v^2u_{xx}. \tag{2.30}$$

Hence, if we put

$$\alpha+\delta=0,\ \gamma=0. \tag{2.31}$$

Equation (2.30) reduces to a second-order nonlinear equation for u,

$$u_{tt}=\alpha^2(u^2u_x)_x. \tag{2.32}$$

Exact solutions of Eq. (2.32) have been given by Zabusky[7] in his study of the vibrations of nonlinear string. A more general class of equations of the form $u_{tt}=(f(u)u_x)_x, f\in C^2(\mathbf{R})$, $f>0, f'\neq 0$ has been studied by Ames *et al.*[8]

III. REDUCTION OF DISPERSIONLESS COUPLED KDV EQUATIONS

In this section, we demonstrate that various types of dispersionless cKdV equations are transformed into second-order linear equations by employing the technique developed in Sec. II. In particular, we show that the resulting linear equations are reduced to the following ED equation:

$$f_{\xi\eta}=\frac{1}{\xi+\eta}(pf_\xi+qf_\eta),\quad f=f(\xi,\eta), \tag{3.1}$$

where p and q are arbitrary real constants. When $p=q$, this equation is called the Euler–Poisson–Darboux (EPD) equation. The method of exact solution for Eq. (3.1) is now established which originated from the work of Riemann. It consists of constructing the so-called Riemann–Green function which is defined by the solution of the boundary value problem of the adjoint equation to the ED equation.[9,10] The Riemann–Green function for Eq. (3.1) is actually given by the hypergeometric function (or the Legendre function in the case of the EPD equation). It is also remarked that a number of particular solutions of (3.1) have been obtained by investigating the symmetry group of the equation.[11,12]

We first define the dispersionless cKdV equation associated with the cKdV equation of the form $u_t=F(u,u_x,\ldots,v,v_x,\ldots), v_t=G(u,u_x,\ldots,v,v_x,\ldots)$, where F and G are real functions. Let us introduce new independent variables $T=\epsilon t$ and $X=\epsilon x$, where ϵ is a small parameter and rewrite the partial derivatives as $\partial/\partial t=\epsilon\partial/\partial T$ and $\partial/\partial x=\epsilon\partial/\partial X$. We substitute these into the cKdV equation and then take the limit $\epsilon\to 0$. Retaining the leading term in ϵ, we obtain the dispersionless cKdV equation. In the following analysis, we use the variables t and x in place of T and X, respectively.

A. Broer–Kaup equation

The first example that we consider here is the Broer–Kaup equation[13,14] given by

$$u_t+uu_x+h_x=0, \tag{3.2a}$$

$$h_t+u_x+(uh)_x\pm u_{xxx}=0. \tag{3.2b}$$

In accordance with the definition, the dispersionless Broer–Kaup equation can be written as

$$u_t=uu_x+2vv_x, \tag{3.3a}$$

$$v_t=\tfrac{1}{2}vu_x+uv_x, \tag{3.3b}$$

where we have put $h=-1+v^2$ and replaced t by $-t$. Comparing (3.3) with (2.1), one can see that (3.3) is a special case of (2.1) with

$$\alpha=1,\ \ \beta=2,\ \ \gamma=\tfrac{1}{2},\ \ \delta=1. \tag{3.4}$$

This choice of the parameters belongs to the case 3 in Sec. II C. The characteristic velocities and corresponding Riemann invariants are found from (2.27) and (2.28) as

$$c^{\pm}=u\pm v, \tag{3.5}$$

$$u+2v=\xi,\ \ -u+2v=\eta. \tag{3.6}$$

Using (3.6), $c^{\pm}$ are expressed in terms of ξ and η as

$$c^{+}=\tfrac{3}{4}\xi-\tfrac{1}{4}\eta,\ \ c^{-}=\tfrac{1}{4}\xi-\tfrac{3}{4}\eta. \tag{3.7}$$

The linear equations for t and x follow from (2.12) and (2.13). They read in the form,

$$t_{\xi\eta}=-\frac{3}{2(\xi+\eta)}(t_{\xi}+t_{\eta}), \tag{3.8}$$

$$x_{\xi\eta}=-\frac{3}{2(\xi+\eta)}\left(\frac{3\xi-\eta}{\xi-3\eta}x_{\xi}+\frac{\xi-3\eta}{3\xi-\eta}x_{\eta}\right). \tag{3.9}$$

Although Eq. (3.8) for t is an EPD equation, i.e., Eq. (3.1) with $p=q=-\frac{3}{2}$, that for x is not reduced to (3.1). However, following Tsarev's procedure summarized in Sec. II B, the reduction to the ED equation is possible. Indeed, if we introduce w_1 and w_2 by the relations

$$w_1=x+(\tfrac{3}{4}\xi-\tfrac{1}{4}\eta)t,\ \ w_2=x+(\tfrac{1}{4}\xi-\tfrac{3}{4}\eta)t, \tag{3.10}$$

the equations for these variables are derived immediately from (2.16) and (2.17) with $c^{\pm}$ given by (3.7). The result is

$$w_{1,\xi\eta}=-\frac{1}{2(\xi+\eta)}(w_{1,\xi}+3w_{1,\eta}), \tag{3.11}$$

$$w_{2,\xi\eta}=-\frac{1}{2(\xi+\eta)}(3w_{2,\xi}+w_{2,\eta}). \tag{3.12}$$

B. Ito equation

The second example is Ito's cKdV equation,[15]

$$u_t=6uu_x+2vv_x+u_{xxx}, \tag{3.13a}$$

$$v_t=2(uv)_x. \tag{3.13b}$$

The dispersionless Ito equation is written as

$$u_t=6uu_x+2vv_x, \tag{3.14a}$$

$$v_t=2(uv)_x. \tag{3.14b}$$

The above system of equations is equivalent to (2.1) with the choice of the parameters

$$\alpha=6,\quad \beta=2,\quad \gamma=2,\quad \delta=2. \tag{3.15}$$

Note that this corresponds to the case 1 in Sec. II C. The parameters a, b and ρ_1,ρ_2,ρ_3 defined, respectively, by (2.18) and (2.20b) become $a=b=1$ and $\rho_1=\rho_2=\rho_3=0$. It then follows from (2.5), (2.20), and (2.21) that

$$c^{\pm}=4u\pm 2\sqrt{u^2+v^2}, \tag{3.16}$$

$$\sqrt{u^2+v^2}+u=\xi,\quad \sqrt{u^2+v^2}-u=\eta. \tag{3.17}$$

Therefore,

$$c^{+}=3\xi-\eta,\quad c^{-}=\xi-3\eta. \tag{3.18}$$

Introducing (3.18) into (2.12), (2.13), (2.16), and (2.17), we find that the linear equations for t,x,w_1, and w_2 take exactly the same forms as those corresponding to the dispersionless Broer–Kaup equation described in Sec. II A. This fact would suggest the close relationship between dispersionless Broer–Kaup and dispersionless Ito equations. In fact, assuming that the Riemann invariants for both equations are proportional to each other, we put $4(\sqrt{u^2+v^2}+u)=\tilde{u}+2\tilde{v}$ and $4(\sqrt{u^2+v^2}-u)=-\tilde{u}+2\tilde{v}$ and rewrite (3.14) in terms of $\tilde{u}$ and $\tilde{v}$. We then find that $\tilde{u}$ and $\tilde{v}$ satisfy the dispersionless Broer–Kaup Eq. (3.3).

Remark: The Ito equation has been proven to be completely integrable, i.e., it exhibits an infinite number of conservation laws commuting each other with respect to an appropriate Poisson bracket.[15] Nevertheless, to the best of our knowledge, the multisoliton solutions have not as yet been explicitly constructed. In Appendix B, we shall present a periodic-wave and one-soliton solutions of the Ito equation which will suggest a hint in studying the structure of the multisoliton solutions.

C. Hirota–Satsuma equation

The third example is the Hirota–Satsuma equation,[16]

$$u_t=\tfrac{1}{2}(6uu_x+u_{xxx})+2vv_x, \tag{3.19a}$$

$$v_t=-3uv_x-v_{xxx}. \tag{3.19b}$$

The dispersionless Hirota–Satsuma equation takes the form

$$u_t=3uu_x+2vv_x, \tag{3.20a}$$

$$v_t=-3uv_x. \tag{3.20b}$$

The above system of equations is a special case of (2.1) with

$$\alpha=3,\quad \beta=2,\ \gamma=0,\quad \delta=-3, \tag{3.21}$$

which belongs to the case 2 in Sec. II C.

It follows from (2.24) and (2.25) that

$$c^{+}=3u,\quad c^{-}=-3u, \tag{3.22}$$

$$u^2+\frac{v^2}{3}=\xi,\quad -\frac{v^2}{3}=\eta. \tag{3.23}$$

Hence, $c^{\pm}$ may be expressed as

$$c^+=3\sqrt{\xi+\eta},\quad c^-=-3\sqrt{\xi+\eta}. \tag{3.24}$$

The linear equations for t and x reduce to the standard EPD equations. The final result is given as follows:

$$t_{\xi\eta}=-\frac{1}{4}\frac{1}{\xi+\eta}(t_\xi+t_\eta), \tag{3.25}$$

$$x_{\xi\eta}=\frac{1}{4}\frac{1}{\xi+\eta}(x_\xi+x_\eta). \tag{3.26}$$

Remark: The coefficients given by (3.21) satisfy the condition (2.31). It then follows from (2.32) that the equation for u is transformed into a single second-order nonlinear equation of the form $u_{tt}=9(u^2u_x)_x$.

D. Bogoyavlenskii equation

The last example is a cKdV equation proposed by Bogoyavlenskii,[17] which is

$$u_t=6uu_x+6v_x-u_{xxx}, \tag{3.27a}$$

$$v_t=-2uv_x+2v_{xxx}. \tag{3.27b}$$

The dispersionless version of this system of equations reduces, after replacing v by $v^2/6$, to

$$u_t=6uu_x+2vv_x, \tag{3.28a}$$

$$v_t=-2uv_x, \tag{3.28b}$$

which is a special case of Eq. (2.1) with

$$\alpha=6,\quad \beta=2,\ \gamma=0,\ \delta=-2. \tag{3.29}$$

Since this class belongs to case 2 in Sec. II C, one immediately finds from (2.20) and (2.25) the expressions

$$c^+=6u,\quad c^-=-2u, \tag{3.30}$$

$$u^2+\tfrac{1}{4}v^2=\xi,\quad -\tfrac{1}{4}v^2=\eta. \tag{3.31}$$

Hence, $c^\pm$ are written in the form

$$c^+=6\sqrt{\xi+\eta},\quad c^-=-2\sqrt{\xi+\eta}. \tag{3.32}$$

The linear equations for t and x are readily derived from (2.12) and (2.13) and they become the EP equation as follows:

$$t_{\xi\eta}=-\frac{1}{8(\xi+\eta)}(t_\xi+3t_\eta), \tag{3.33}$$

$$x_{\xi\eta}=\frac{1}{8(\xi+\eta)}(3x_\xi+x_\eta). \tag{3.34}$$

E. Remark

Here, we shall briefly discuss on a class of nonintegrable cKdV equations that reduces to the system of Eqs. (2.2). A variant of the famous Boussinesq system in the theory of shallow-water waves belongs to this class. In an appropriate dimensionless form, it reads[18]

$$h_t+(uh)_x=0, \tag{3.35a}$$

$$u_t+uu_x+h_x+h_{xxx}=0. \tag{3.35b}$$

If we put $h=v^2$, replace t by $-t$ and then take the dispersionless limit, we can see that the above system of equations reduces to the dispersionless Broer–Kaup Eq. (3.3). This example shows that the nonintegrability of the cKdV equation does not necessarily imply the nonintegrability of the corresponding dispersionless equation. This fact is almost trivial. Indeed, we can construct many examples of nonintegrable cKdV equations that reduce to the system of Eqs. (2.2) in the dispersionless limit. Our concern is rather the opposite problem, i.e., whether the integrable cKdV equations are always reducible to the integrable equations of the ED type or not in the dispersionless limit. The analysis developed in this section gives an affirmative answer as long as the typical integrable cKdV equations are concerned.

IV. EXTENSION

Here, we shall briefly discuss the following quasilinear system of equations which generalizes the system of Eqs. (2.1):

$$u_t=(\alpha_1u+\alpha_2v)u_x+(\beta_1u+\beta_2v)v_x, \tag{4.1a}$$

$$v_t=(\gamma_1u+\gamma_2v)u_x+(\delta_1u+\delta_2v)v_x, \tag{4.1b}$$

where $\alpha_j,\beta_j,\gamma_j$, and $\delta_j(j=1,2)$ are real parameters. Under certain conditions, the linear transformation of u and v makes it possible to transform (4.1) into (2.1). However, we exclude this special case below. Although we could develop the discussion analogous to that which has been done in Sec. II, we shall not enter into specific detail here. Instead, we will perform the reduction of (4.1) to the ED equation in two explicit examples.

A. Jaulent–Miodek equation

The Jaulent–Miodek equation[19] reads in the form

$$U_t+U_{xxx}+\tfrac{3}{2}QQ_{xxx}+\tfrac{9}{2}Q_xQ_{xx}-6UU_x-6UQQ_x-\tfrac{3}{2}U_xQ^2=0, \tag{4.2a}$$

$$Q_t+Q_{xxx}-6UQ_x-6U_xQ-\tfrac{15}{2}Q_xQ^2=0. \tag{4.2b}$$

The dispersionless Jaulent–Miodek equation now becomes

$$u_t=(u+v)u_x+uv_x, \tag{4.3a}$$

$$v_t=2vu_x+(u+v)v_x, \tag{4.3b}$$

where we have introduced new variables u and v by $U=\frac{1}{6}(u-(v/2))$ and $Q^2=v/3$, respectively. As is readily seen, the above system of equations is a special case of (4.1) with $\alpha_1=\alpha_2=1,\beta_1=1,\beta_2=0,\gamma_1=0,\gamma_2=2,\delta_1=\delta_2=1$. The characteristic velocities and corresponding Riemann invariants are easily calculated following the procedure developed in Sec. II. They are given by

$$c^+=u+v+\sqrt{2uv},\quad c^-=u+v-\sqrt{2uv}, \tag{4.4}$$

$$\sqrt{2u}+\sqrt{v}=\xi,\quad \sqrt{2u}-\sqrt{v}=\eta. \tag{4.5}$$

In terms of the Riemann invariants, $c^{\pm}$ are rewritten as

$$c^{+}=\tfrac{5}{8}\xi^2-\tfrac{1}{4}\xi\eta+\tfrac{1}{8}\eta^2,\quad c^{-}=\tfrac{1}{8}\xi^2-\tfrac{1}{4}\xi\eta+\tfrac{5}{8}\eta^2, \tag{4.6}$$

The equations for t and x now take the form,

$$t_{\xi\eta}=\frac{1}{2(\xi^2-\eta^2)}[(-\xi+5\eta)t_{\xi}-(5\xi-\eta)t_{\eta}], \tag{4.7}$$

$$x_{\xi\eta}=\frac{1}{2}\frac{(5\xi^2-2\xi\eta+\eta^2)(-\xi+5\eta)}{(\xi^2-2\xi\eta+5\eta^2)(\xi^2-\eta^2)}x_{\xi}-\frac{1}{2}\frac{(\xi^2-2\xi\eta+5\eta^2)(5\xi-\eta)}{(5\xi^2-2\xi\eta+\eta^2)(\xi^2-\eta^2)}x_{\eta}. \tag{4.8}$$

Although the reduction to the ED equation is difficult to perform in the t and x variables, Tsarev's method is applied successfully to transform (4.3) into the ED equation. Indeed, it is easy to show from (2.16), (2.17), and (4.6) that the variables $w_1=x+c^{+}t$ and $w_2=x+c^{-}t$ satisfy the following second-order equations of the ED type:

$$w_{1,\xi\eta}=-\frac{1}{2(\xi+\eta)}(w_{1,\xi}+3w_{1,\eta}), \tag{4.9}$$

$$w_{2,\xi\eta}=-\frac{1}{2(\xi+\eta)}(3w_{2,\xi}+w_{2,\eta}). \tag{4.10}$$

Remark: Levi *et al.*[20] introduced the system of equations

$$q_t=\tfrac{1}{4}(q_{xx}-3rq_x+3qr^2-3q^2)_x, \tag{4.11a}$$

$$r_t=\tfrac{1}{4}(r_{xx}+3rr_x+r^3-6rq)_x, \tag{4.11b}$$

which is the first member of the Lax hierarchy of the Broer–Kaup equation. If we take the dispersionless limit and then put $q=-2/3u$ and $r^2=\frac{4}{3}v$ in (4.11), the dispersionless equations for u and v reduce to (4.3). Note also that Eqs. (4.9) and (4.10) are the same equations as (3.11) and (3.12), respectively. One can see that the Lax hierarchy of the Broer–Kaup equation is mathematically equivalent to the Lax hierarchy of the Jaulent–Miodek equation.

B. Nutku–Öğuz equation

The Nutku–Öğuz equation[21] is written as

$$u_t=2\lambda uu_x+vv_x+(uv)_x+u_{xxx}, \tag{4.12a}$$

$$v_t=2\mu vv_x+uu_x+(uv)_x+v_{xxx}, \tag{4.12b}$$

where λ and μ are real constants satisfying the condition $\lambda+\mu=1$. Note that the above system of equations decouple for $\lambda=\mu=1/2$ and hence we consider the case $\lambda\neq\mu$ below. The dispersionless version of (4.12) becomes

$$u_t=(2\lambda u+v)u_x+(u+v)v_x, \tag{4.13a}$$

$$v_t=(u+v)u_x+\{u+2(1-\lambda)v\}v_x. \tag{4.13b}$$

The characteristic velocities and corresponding Riemann invariants are given by

$$c^{\pm}=[(\lambda+\tfrac{1}{2})u+(-\lambda+\tfrac{3}{2})v\pm\kappa(u+v)],\quad \kappa=\sqrt{\lambda^2-\lambda+\tfrac{5}{4}}, \tag{4.14}$$

$$u+(-\lambda+\tfrac{1}{2}+\kappa)v=\xi,\quad u+(-\lambda+\tfrac{1}{2}-\kappa)v=\eta. \tag{4.15}$$

Thus, $c^{\pm}$ are written in terms of ξ and η as

$$c^{+}=(\lambda+\tfrac{1}{2}+\kappa)\xi,\quad c^{-}=(\lambda+\tfrac{1}{2}-\kappa)\eta. \tag{4.16}$$

If we define new variables $\tilde{\xi}$ and $\tilde{\eta}$ according to $\tilde{\xi}=(\lambda+\frac{1}{2}+\kappa)\xi$ and $\tilde{\eta}=-(\lambda+\frac{1}{2}-\kappa)\eta$, the equations for x and t become

$$t_{\tilde{\xi}\tilde{\eta}}=-\frac{1}{\tilde{\xi}+\tilde{\eta}}(t_{\tilde{\xi}}+t_{\tilde{\eta}}), \tag{4.17a}$$

$$x_{\tilde{\xi}\tilde{\eta}}=\frac{\tilde{\xi}}{\tilde{\eta}(\tilde{\xi}+\tilde{\eta})}x_{\tilde{\xi}}+\frac{\tilde{\eta}}{\tilde{\xi}(\tilde{\xi}+\tilde{\eta})}x_{\tilde{\eta}}. \tag{4.17b}$$

The equation for x is not reducible to the ED equation. However, as seen from (4.16), each characteristic velocity depends only on a single Riemann invariant. In view of this observation, the Tsarev system of Eqs. (2.14) turns out to be the trivial equations $w_{1,\eta}=w_{2,\xi}=0$, which are integrated immediately to give the solutions $w_1=f_1(\xi)$ and $w_2=f_2(\eta)$, where f_1 and f_2 are arbitrary functions. The expressions (2.15) then yield the general solutions of Eq. (4.17) as follows:

$$t=\frac{f_1(\tilde{\xi})+f_2(\tilde{\eta})}{\tilde{\xi}+\tilde{\eta}}, \tag{4.18a}$$

$$x=-\frac{\tilde{\eta}f_1(\tilde{\xi})+\tilde{\xi}f_2(\tilde{\eta})}{\tilde{\xi}+\tilde{\eta}}. \tag{4.18b}$$

By direct calculation, one can easily confirm that (4.18) does indeed satisfy (4.17).

V. CONCLUDING REMARKS

In this paper, we demonstrated that a class of dispersionless cKdV equations can be linearized in the form of the EP or EPD equations by means of the hodograph transformation. In the process of linearization, the main step is to express the characteristic velocities in terms of the Riemann invariants. Although the Riemann invariants always exist for quasilinear hyperbolic systems of equations such as (2.2) and (4.1) with two dependent variables, the explicit expressions for the characteristic velocities are obtainable by quadrature only for special combinations of the parameters (Sec. II C). The present analysis shows that the procedure mentioned above can be performed completely in the case of the dispersionless versions for typical two-component cKdV equations (Secs. III and IV). It should be kept in mind that the cKdV equations exemplified here possess the completely integrable Hamiltonian structures. It will therefore be an interesting problem to apply the method developed in this paper to other types of integrable two-component nonlinear dispersive systems of equations and to investigate the relationship between the integrability of the original equations and the reducibility of the corresponding dispersionless equations to the ED or EPD equations.

APPENDIX A: CONSERVATION LAWS FOR EQ. (2.1)

We show that the system of Eqs. (2.1) exhibits an infinite number of conservation laws. By inspection, one can see that the conservation laws are represented by the integral of homogeneous polynomials of u and v as follows:

$$I_{2n}=\sum_{j=0}^{n} C_j^{(2n)}\int_{-\infty}^{\infty} u^{2(n-j)}v^{2j}dx,\quad (n=1,2,\dots), \tag{A1}$$

$$I_{2n+1}=\sum_{j=0}^{n} C_j^{(2n+1)}\int_{-\infty}^{\infty} u^{2(n-j)+1}v^{2j}dx,\quad (n=0,1,\dots). \tag{A2}$$

Here the integrand of $I_{2n}(I_{2n+1})$ is a polynomial of u and v of order $2n(2n+1)$.

We now derive the recursion relations that determine the coefficients $C_j^{(2n)}$ and $C_j^{(2n+1)}$.

1. Recursion relation for $C_j^{(2n)}$

Differentiating (A1) by t and using (2.1), we obtain, with integration by parts under appropriate boundary conditions, the relation

$$\frac{dI_{2n}}{dt}=\sum_{j=1}^{n}\left[\frac{2j\{2(\delta-\alpha)(n-j)-2\gamma j+\delta\}}{2(n-j)+1}C_j^{(2n)}+2\beta(n-j+1)C_{j-1}^{(2n)}\right]\times\int_{-\infty}^{\infty}u^{2(n-j)+1}v^{2j-1}v_x dx. \tag{A3}$$

Hence, the quantities I_{2n} are conserved if the following recursion relations hold for $C_j^{(2n)}$:

$$\frac{2j\{2(\delta-\alpha)(n-j)-2\gamma j+\delta\}}{2(n-j)+1}C_j^{(2n)}+2\beta(n-j+1)C_{j-1}^{(2n)}=0,\quad (j=1,2,\dots,n). \tag{A4}$$

Under the conditions

$$D_j^{(2n)}\equiv 2(\delta-\alpha)(n-j)-2\gamma j+\delta\neq 0,\quad (j=1,2,\dots,n), \tag{A5}$$

the coefficients $C_j^{(2n)}$ are determined successively by the relations,

$$C_j^{(2n)}=-\frac{\beta\{2(n-j)+1\}(n-j+1)}{j\{2(\delta-\alpha)(n-j)-2\gamma j+\delta\}}C_{j-1}^{(2n)},\quad (j=1,2,\dots,n), \tag{A6}$$

with $C_0^{(2n)}$ being an arbitrary constant.

If $D_j^{(2n)}=0$ for certain $j(=k)(k\leqslant n)$, then (A1) has the form

$$I_{2n}=\sum_{j=k}^{n} C_j^{(2n)}\int_{-\infty}^{\infty} u^{2(n-j)}v^{2j}dx,\quad (n=1,2,\dots), \tag{A7}$$

where $C_k^{(2n)}$ can be taken arbitrary and $C_j^{(2n)}\,(k+1\leqslant j\leqslant n)$ are determined by (A6).

2. Recursion relation for $C_j^{(2n+1)}$

Under the conditions,

$$D_j^{(2n+1)}\equiv 2(\delta-\alpha)(n-j)-2\gamma j-\alpha+2\delta\neq 0,\quad (j=0,1,\dots,n), \tag{A8}$$

one can determine $C_j^{(2n+1)}$ by the recursion relations,

$$C_j^{(2n+1)}=-\frac{\beta\{2(n-j)+3\}(n-j+1)}{j\{2(\delta-\alpha)(n-j)-2\gamma j-\alpha+2\delta\}}C_{j-1}^{(2n+1)},\quad (j=1,2,\dots,n), \tag{A9}$$

starting with an arbitrary constant $C_0^{(2n+1)}$.

If $D_j^{(2n+1)}=0$ for certain $j(=k)(k\leqslant n)$, then (A2) has the form

$$I_{2n+1}=\sum_{j=k}^{n} C_j^{(2n+1)}\int_{-\infty}^{\infty} u^{2(n-j)+1}v^{2j}dx,\quad (n=1,2,\dots), \tag{A10}$$

where $C_k^{(2n+1)}$ can be taken as arbitrary and $C_j^{(2n+1)}\,(k+1\leqslant j\leqslant n)$ are determined by (A9).

3. Examples

The conservation laws for the dispersionless cKdV equations discussed in Sec. II are constructed by using (A6) and (A9). We shall write down the first four of them for each equation.

a. Dispersionless Broer–Kaup Eq. (3.3)

$$I_1=\int_{-\infty}^{\infty} u dx,\quad I_2=\int_{-\infty}^{\infty} v^2 dx,\quad I_3=\int_{-\infty}^{\infty} uv^2 dx,\quad I_4=\int_{-\infty}^{\infty}(u^2v^2+v^4)dx. \tag{A11}$$

b. Dispersionless Ito Eq. (3.14)

$$\begin{gathered} I_1=\int_{-\infty}^{\infty} u dx,\quad I_2=\int_{-\infty}^{\infty}(u^2+v^2)dx,\\ I_3=\int_{-\infty}^{\infty}(u^3+uv^2)dx,\quad I_4=\int_{-\infty}^{\infty}\left(u^4+\frac{6}{5}u^2v^2+\frac{1}{5}v^4\right)dx. \end{gathered} \tag{A12}$$

c. Dispersionless Hirota–Satsuma Eq. (3.20)

$$\begin{gathered} I_1=\int_{-\infty}^{\infty} u dx,\quad I_2=\int_{-\infty}^{\infty}\left(u^2+\frac{2}{3}v^2\right)dx,\\ I_3=\int_{-\infty}^{\infty}\left(u^3+\frac{2}{3}uv^2\right)dx,\quad I_4=\int_{-\infty}^{\infty}\left(u^4+\frac{4}{5}u^2v^2+\frac{4}{15}v^4\right)dx. \end{gathered} \tag{A13}$$

d. Dispersionless Bogoyavlenskii Eq. (3.28)

$$\begin{gathered} I_1=\int_{-\infty}^{\infty} u dx,\quad I_2=\int_{-\infty}^{\infty}(u^2+v^2)dx,\\ I_3=\int_{-\infty}^{\infty}\left(u^3+\frac{3}{5}uv^2\right)dx,\quad I_4=\int_{-\infty}^{\infty}\left(u^4+\frac{2}{3}u^2v^2+\frac{1}{3}v^4\right)dx. \end{gathered} \tag{A14}$$

APPENDIX B: PERIODIC-WAVE AND SOLITON SOLUTIONS OF ITO'S CKDV EQUATION

In accordance with the exact solutions of Ito's cKdV and related equations, several references are now available.[22] Here, we shall derive the periodic-wave and soliton solutions and discuss their properties.

1. Periodic-wave solution

We shall first seek a periodic-wave solution of the Ito Eq. (3.13) of the form,

$$u=u(\zeta),\quad v=v(\zeta),\quad \zeta=x-ct,\quad (c>0). \tag{B1}$$

Introducing (B1) into Eq. (3.13) and integrating once, we obtain

$$-cu-u''-3u^2-v^2=k_1,\quad \left(u''=\frac{d^2u}{d\zeta^2}\right), \tag{B2}$$

$$-cv-2uv=k_2, \tag{B3}$$

where k_1 and k_2 are integration constants. In the following analysis, we assume that $k_2\neq 0$. Equation (B2) is once more integrated after eliminating v by (B3) to give

$$\frac{1}{2}(u')^2+u^3+\frac{c}{2}u^2-\frac{k_2^2}{4}\frac{1}{u+\frac{c}{2}}=-k_1u-k_3, \tag{B4}$$

with k_3 being an integration constant. It follows from (B3) that $u=-(cv+k_2)/2v$. If we substitute this expression into (B4) and define the new dependent variable g according to $v=-k_2g/c$, (B4) is transformed into the equation

$$\frac{(g')^2}{g}=\frac{4k_2^2}{c^3}g^4-\frac{4k_1}{c}(1-g)g^2-\frac{8k_3}{c^2}g^3-c(1-g)^2. \tag{B5}$$

Furthermore, we introduce the new independent variable η by

$$\frac{d\eta}{d\zeta}=\sqrt{\frac{4k_2^2g}{c^3}}, \tag{B6}$$

to recast (B5) into the form

$$\left(\frac{dg}{d\eta}\right)^2=(g-g_1)(g-g_2)(g-g_3)(g-g_4), \tag{B7}$$

where $g_j(j=1-4)$ are determined by the relations

$$\sum_{j=1}^{4}g_j=-\frac{c^2k_1}{k_2^2}+\frac{2ck_3}{k_2^2},\quad \sum_{j<k}g_jg_k=-\left(\frac{c^2k_1}{k_2^2}+\frac{c^4}{4k_2^2}\right),$$

$$\sum_{j<k<l}g_jg_kg_l=-\frac{c^4}{2k_2^2},\quad \prod_{j=1}^{4}g_j=-\frac{c^4}{4k_2^2}. \tag{B8}$$

The periodic-wave solution of (B7) is now given explicitly by Jacobi's elliptic functions $sn(\mu\eta,k)$ and $cn(\mu\eta,k)$ as follows:

$$g(\eta)=\frac{g_3-\lambda g_4\,\mathrm{sn}^2(\mu\eta,k)}{1-\lambda\,\mathrm{sn}^2(\mu\eta,k)}=\frac{g_3-\lambda g_4+\lambda g_4\,\mathrm{cn}^2(\mu\eta,k)}{1-\lambda+\lambda\,\mathrm{cn}^2(\mu\eta,k)}, \tag{B9}$$

where

$$\lambda=\frac{g_2-g_3}{g_2-g_4},\quad k^2=\frac{(g_2-g_3)(g_1-g_4)}{(g_1-g_3)(g_2-g_4)},$$
$$\mu^2=\tfrac{1}{4}(g_1-g_3)(g_2-g_4),\quad (g_4<g_3<g_2<g_1), \tag{B10}$$

and we have used the formula $\mathrm{sn}^2(\mu\eta,k)=1-\mathrm{cn}^2(\mu\eta,k)$. It follows from (B6) that

$$\zeta(\eta)=\int_0^{\eta}\sqrt{\frac{c^3}{4k_2^2 g(\eta')}}d\eta', \tag{B11}$$

where we have assumed $\zeta(0)=0$. Thus, the periodic-wave solution of Eq. (B7) is represented parametrically by (B9) and (B11). With g thus obtained, v is given by $v=-k_2 g/c$ and u is derived from (B3).

Remark: For appropriate choices of the integration constants k_1,k_2, and k_3, the real solutions of (B8) will exist which satisfy the condition $g_4<g_3<g_2<g_1$. If these constants take the values $k_1=-c^2\kappa_1, k_2=-c^2/\sqrt{\kappa_2}, k_3=c^3/(2\kappa_2), (\kappa_2>0)$ with κ_1 and κ_2 being arbitrary constants, the right-hand side of (B7) simplifies to $(g-1)(g^3-\kappa_1\kappa_2 g^2-(\kappa_2/4)g+(\kappa_2/4))$. Hence, $g_1=1$ and g_2,g_3, and g_4 are obtained by solving the cubic equation $g^3-\kappa_1\kappa_2 g^2-(\kappa_2/4)g+(\kappa_2/4)=0$. One can show that for certain ranges of κ_1 and κ_2, the real solutions of this equation exist which satisfy the condition $g_4<g_3<g_2<1$. Furthermore, if we put $\kappa_1=v_0^2/c^2$ and $\kappa_2=c^2/v_0^2$ to reduce this equation to $(g-1)(g^2-(c^2/4v_0^2))=0$, the periodic-wave solution derived here degenerates into the soliton solution as shown below.

2. Soliton solution

The soliton solution is simply obtained from the periodic-wave solution by taking an appropriate limit. First of all, we note that the relevant boundary conditions for the soliton solution should be $u,u',u''\to 0, g\to v_0(>0)$ as $|\zeta|\to\infty$. These conditions completely fix the integration constants k_1,k_2, and k_3. Indeed, it readily follows from (B2), (B3), and (B4) that

$$k_1=-v_0^2,\quad k_2=-v_0 c,\quad k_3=\frac{v_0^2 c}{2}. \tag{B12}$$

Substituting (B12) into (B8), we find

$$g_1=g_2=1,\quad g_3=-g_4=\frac{c}{2v_0}. \tag{B13}$$

To assure the positivity of μ^2 in (B10), we impose the condition $c/2v_0<1$. Then, the parameters in (B10) are reduced, with use of (B13), to

$$\lambda=\frac{1-\dfrac{c}{2v_0}}{1+\dfrac{c}{2v_0}},\quad k=1,\quad \mu=\frac{1}{2}\sqrt{1-\frac{c^2}{4v_0^2}}. \tag{B14}$$

In view of the relation $\mathrm{cn}^2(\mu\eta,1)=\mathrm{sech}^2\mu\eta=2/(\cosh 2\mu\eta+1)$, (B9) reduces to

$$g(\eta)=1-\frac{\dfrac{2v_0}{c}\left(1-\dfrac{c^2}{4v_0^2}\right)}{\cosh\left[\sqrt{1-\dfrac{c^2}{4v_0^2}}\,\eta\right]+\dfrac{2v_0}{c}}. \tag{B15}$$

Lastly, we substitute (B15) into (B11) and perform the integration, and we obtain

$$\zeta=\sqrt{\frac{c^2}{4v_0^2-c^2}}\left[\left(1+\frac{c}{2v_0}\right)\Pi\left(\phi,\frac{1}{1-\dfrac{c}{2v_0}},\frac{1}{\sqrt{2}}\right)+\frac{2v_0}{c}\left(1-\frac{c^2}{4v_0^2}\right)F\left(\phi,\frac{1}{\sqrt{2}}\right)\right], \tag{B16}$$

where

$$\phi=\sin^{-1}\sqrt{\left(1-\frac{c}{2v_0}\right)\frac{\cosh\left[\sqrt{1-\frac{c^2}{4v_0^2}}\eta\right]-1}{\cosh\left[\sqrt{1-\frac{c^2}{4v_0^2}}\eta\right]+\frac{c}{2v_0}}}. \tag{B17}$$

Here, F and Π are elliptic integrals of the first and third kinds defined, respectively, by

$$F(\phi,k)=\int_0^{\phi}\frac{d\alpha}{\sqrt{1-k^2\sin^2\alpha}},\quad \Pi(\phi,\nu,k)=\int_0^{\phi}\frac{d\alpha}{(1-\nu\sin^2\alpha)\sqrt{1-k^2\sin^2\alpha}}. \tag{B18}$$

Thus, (B15) and (B16) give a parametric representation of the solution of $v(=v_0 g)$. As seen from (B11) and (B15), ζ is a monotonically increasing function of η. In particular, $\zeta\to\sqrt{(c/4v_0^2)}\,\eta$ when $\eta\to\infty$. The solution u is then found from (B3) and (B12) as

$$u=\frac{v_0\left(1-\frac{c^2}{4v_0^2}\right)}{\cosh\left[\sqrt{1-\frac{c^2}{4v_0^2}}\eta\right]+\frac{c}{2v_0}}. \tag{B19}$$

If we denote the amplitude of u by a, we see from (B19) that $a\equiv u(0)=v_0(1-(c/2v_0))$. Hence, the propagation velocity c of the soliton is related to the soliton amplitude by the relation $c=2(v_0-a)$.

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Lie aspects of the dynamics of self-gravitating ellipsoids in *n* dimensions

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In this paper we study the dynamics of self-gravitating ellipsoids in n dimensions, from the point of view of the Poisson structure of the dual of a suitable Lie algebra. When $n=3$ this was done by Rosenteel. In this setting we describe explicitly the ring of invariant functions. In the two-dimensional case we apply a technique due to Pedersen to find globally defined Darboux coordinates on the coadjoint orbits. Finally we derive a characterization of tensors coming from potentials, and use it to exhibit the dynamical equations of the ellipsoid in the Hamiltonian form. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1316059]

I. INTRODUCTION

It was Rosensteel who pioneered[1] the Lie theoretical approach to the study of the dynamics of self-gravitating ellipsoids. His main idea was to view the dual of the Lie algebra $\mathrm{gcm}(3)=\mathrm{sym}(3)\ltimes \mathrm{gl}(3)$ as the phase space of these systems. In Sec. II we generalize this theory defining a n-dimensional ellipsoid introducing the Lie algebra $\mathrm{sym}(n)\times \mathrm{gl}(n)$ as the phase space for dynamical systems defined by ellipsoids in an arbitrary number of dimensions n. In Sec. III global Darboux coordinates are given explicitly for the two-dimensional problem. In Sec. IV the main result is the characterization of matrices of functions on the coordinates I_{ik} coming from a potential, then as a corollary we prove that the gravitational potential of a self-gravitating Riemman ellipsoid comes from potential in the sense we defined it.

II. CLASSIFICATION OF PHYSICAL ORBITS AND STRUCTURE OF THE ALGEBRA OF INVARIANTS

In this section we introduce the Lie algebra $\mathrm{sym}(n)\times \mathrm{gl}(n)$ as the phase space for dynamical systems defined by ellipsoids in an arbitrary number of dimensions n. The reduced phase space will then be the orbits under the coadjoint action. In general these orbits are the sets where the functions invariant under the coadjoint action take constant values. So it is important to classify the orbits and elucidate the structure of the algebra of functions invariant under the coadjoint action. This is what will be done in this section. For $n=3$ this has been done by Rosensteel.[1] Our results for general n include as special case his classification of orbits there, and his identification of orbits as level sets of the Kelvin circulation. It is interesting that the structure of the ring of invariants is a little more complicated when n is even than when n is odd.

Recall that $\mathrm{sym}(n)$ is the space of $n\times n$ real symmetric matrices, $\mathrm{gl}(n)$ is the group of $n\times n$ invertible matrices, and $\mathrm{gl}_+(n)$ is the subgroup of elements whose determinants are >0. Let $G=\mathrm{sym}(n)\times \mathrm{gl}_+(n)$ denote the group with multiplication law given by

$$(x,g)*(y,h)=(x+\psi_g(y),gh).$$

Lemma 1: The Lie algebra $\mathcal{G}$ of G is isomorphic with the space of matrices

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$$\begin{pmatrix} a & b \\ 0 & -a^t \end{pmatrix} \quad (a \in \mathrm{gl}(n), \quad b \in \mathrm{sym}(n)).$$

Proof: Immediate. □

Lemma 2: The following bilinear form on $\mathrm{sp}(n)\times\mathrm{sp}(n)$ is nondegenerate:

$$<,>:\mathrm{sp}(n)\times\mathrm{sp}(n)\to\mathbf{R}$$

$$<a,b>=\mathrm{tr}(ab).$$

In particular, this gives an identification $\mathrm{sp}(n)^*\sim\mathrm{sp}(n)$

Proof: Immediate. □

If we write (b,a) for the elements in $\mathcal{G}$, the adjoint action of G on $\mathcal{G}$ is given by

$$\mathrm{Ad}_{(x,g)}(b,a)=(gbg^t-\{a^g x+(a^g x)^t\},a^g).$$

Also the coadjoint action of G on $\mathcal{G}^*$ is given by

$$\mathrm{Ad}^*_{(x,g)}(c,a)=(\check{g}cg^{-1},a^g+x\check{g}cg^{-1}).$$

As was discussed in Ref. 1, the orbits in $\mathcal{G}^*$ related to physical phenomena are those where c is positive definite. This is the reason of defining the space $\mathcal{G}^+$ as

$$\mathcal{G}^+=\{(c,a)\in\mathcal{G}^*|c \text{ positive definite}\}.$$

Lemma 3: $\mathcal{G}^+$ is an open set in $\mathcal{G}^*$, invariant under the coadjoint action. Let $(c,a)\in\mathcal{G}^*$. Then $O_{(c,a)}$ contains an element of the form (I,a'), for some $a'\in gl(n)$, I being the identity matrix.

Proof: The result is a consequence of a classical theorem of Sylvester. □

From now on all the orbits that we consider, $O_{(c,a)}$ are orbits of elements in $\mathcal{G}^+$.

Theorem 4: If $n=2k+1$, every $O_{(c,a)}$ has a unique element $(I,\tilde{H})$, where

$$\tilde{H}=\begin{pmatrix} \begin{pmatrix} 0 & \lambda_1 \\ -\lambda_1 & 0 \end{pmatrix} & & & \\ & \ddots & & \\ & & \begin{pmatrix} 0 & \lambda_n \\ -\lambda_n & 0 \end{pmatrix} & \\ & & & 0 \end{pmatrix}$$

$$(\lambda_1\geqslant\lambda_2\geqslant\ldots\geqslant\lambda_n\geqslant 0).$$

If $n=2k$, it contains an element of the form

$$\tilde{H}=\begin{pmatrix} \begin{pmatrix} 0 & \lambda_1 \\ -\lambda_1 & 0 \end{pmatrix} & & \\ & \ddots & \\ & & \begin{pmatrix} 0 & \lambda_n \\ -\lambda_n & 0 \end{pmatrix} \end{pmatrix}$$

$$(\lambda_1\geqslant\lambda_2\geqslant\ldots\geqslant\lambda_n).$$

Proof: This is a consequence of the theory of compact Lie groups. We refer to Ref. 2, Theorem 4.12.2. □

Corollary 5: If $\lambda_1>\lambda_2>\ldots>\lambda_n>0$ then $O_{(c,a)}\simeq G/\mathrm{SO}(2)\times\mathrm{SO}(2)\times\ldots\times\mathrm{SO}(2)$.

Let $\mathcal{H}$ be the (CSA) of $\mathrm{SO}(n)$ given in Theorem 4. $\mathcal{W}$ the normalizer of $\mathcal{H}$ in $\mathrm{SO}(n)$, modulo its centralizer. It was proved by Chevalley[3] that the algebra of polynomials on $\mathrm{SO}(n)$ which are $\mathrm{SO}(n)$-invariant is isomorphic, via restriction to $\mathcal{H}$, with the algebra of polynomials on $\mathcal{H}$ that are $\mathcal{W}$-invariant. Let $I(\mathcal{H})$ denote this ring. Since every G orbit in $\mathcal{G}^+$ meets $\mathcal{H}$ in a $\mathcal{W}$ orbit in $\mathcal{H}$, it is clear that an invariant function on $\mathcal{G}^+$ is uniquely determined by its restriction to $\mathcal{H}$. Our aim now is to determine the ring of invariant functions on $\mathcal{G}^+$ whose restriction to $\mathcal{H}$ is all of $I(\mathcal{H})$. Let us denote this ring by $I(\mathcal{G}^+)$. It is interesting to note that unlike the theorem of Chevalley in the semisimple case, we need to go to the rational functions on $\mathcal{G}^+$ for $n=2k+1$, and algebraic functions on $\mathcal{G}^+$ for $n=2k$, to obtain all elements of $I(\mathcal{G}^+)$.

We begin with the determination of $\mathcal{W}$ and $I(\mathcal{H})$.

Lemma 6: $\mathcal{W}$ has the following determination.

(1) If $n=2k+1$, $\mathcal{W}$ consists of the group of all permutations of $(\lambda_1,\ldots,\lambda_k)$ followed by arbitrary changes of signs of the λ's.
(2) If $n=2k$, $\mathcal{W}$ consists of the group of all permutations of $(\lambda_1,\ldots,\lambda_n)$ followed by an even number of changes of sign of the λ's.

Proof: A proof is given in Ref. 2. □

Remark 7: It is very important to notice that when $n=2k$, $\mathcal{W}$ does not have arbitrary sign changes, because the only orthogonal matrix fixing $\gamma_s s\neq i$ and $\gamma_i\rightarrow-\gamma_i$ is the matrix K_i given in case $n=2k+1$ with last column and row deleted. However this matrix is not in $\mathrm{SO}(n)$ because its determinant is -1. The stabilizer of $\mathcal{H}$ in $O(n)$, the full orthogonal group, is the subgroup $\mathcal{W}'$ consisting in all the permutations followed by arbitrary sign changes. Therefore when n is odd $\mathcal{W}=\mathcal{W}'$ but when n is even $\mathcal{W}\subset\mathcal{W}'$, a normal subgroup.

Lemma 8: If $n=2k$, the ring of polynomial functions on $\mathcal{H}$, invariant under $\mathcal{W}$ is generated by

$$\sum_{1\leqslant i\leqslant k}\lambda_i^2,\quad \sum_{1\leqslant i\leqslant k}\lambda_i^4,\quad \ldots,\quad \sum_{1\leqslant i\leqslant k}\lambda_i^{2(k-1)},\quad \lambda_1,\ldots,\lambda_n.$$

If $n=2k+1$, it is generated by

$$\sum_{1\leqslant i\leqslant k}\lambda_i^2,\quad \sum_{1\leqslant i\leqslant k}\lambda_i^4,\quad \ldots,\quad \sum_{1\leqslant i\leqslant k}\lambda_i^{2(k-1)},\quad \sum_{1\leqslant i\leqslant k}\lambda_i^{2k}.$$

Proof: Let $\mathcal{W}'$ the group consisting in all permutations followed by arbitrary sign changes. Then $[\mathcal{W}',\mathcal{W}]=2$ and therefore $\mathcal{W}$ is normal in $\mathcal{W}'$. This can be proved as follows: when $n=2k+1$, $\mathcal{W}=\mathcal{W}'$, so there is nothing to prove. When $n=2k$ we take an element $\sigma\in\mathcal{W}'$, which has an odd number of sign changes; then $\mathcal{W}'=\mathcal{W}\cup\sigma\mathcal{W}$. Take an arbitrary polynomial $f(\lambda_1,\ldots,\lambda_k)$ invariant under $\mathcal{W}'$. Since S_n is a subgroup of $\mathcal{W}'$ all λ's can be interchanged, so f is symmetric. f has to be also invariant under arbitrary sign changes, what implies that $f=g(\lambda_1^2,\ldots,\lambda_k^2)$ showing that f is a polynomial in

$$\sum_{1\leqslant i\leqslant k}\lambda_i^2,\quad \sum_{1\leqslant i<j\leqslant k}\lambda_i^2\lambda_j^2,\ldots,\lambda_1^2,\ldots,\lambda_k^2. \tag{1}$$

Therefore when n is odd, the ring of polynomial invariants is generated by the polynomials in (1), because $\mathcal{W}=\mathcal{W}'$. Suppose n is even. Let s be any element of $\mathcal{W}'\setminus\mathcal{W}$. Since $\mathcal{W}$ is normal of index 2 in $\mathcal{W}'$, f^s is also $\mathcal{W}$-invariant. Write

$$f=\frac{f+f^s}{2}+\frac{f-f^s}{2}=f_1+f_2,$$

f_1 is $\mathcal{W}$ invariant and s-invariant. So it is $\mathcal{W}'$-invariant and so is a polynomial in (1). But $f_2^s = -f_2$ and hence $f_2^t = -f_2$ for any t that changes the sign of a single λ. So $f_2 = 0$ when $\lambda_j = 0$, showing that $\lambda_j | f_2$, hence that $\lambda_1, \ldots, \lambda_k | f_2$. So $f_2 = \lambda_1, \ldots, \lambda_k g(\lambda_1, \ldots, \lambda_k)$, where g is $\mathcal{W}'$-invariant and hence a polynomial in (1). Therefore f is a polynomial in

$$\sum_{1 \leqslant i \leqslant k} \lambda_i^2, \quad \sum_{1 \leqslant i < j \leqslant k} \lambda_i^2 \lambda_j^2, \ldots, \lambda_1, \ldots, \lambda_k.$$

To complete the proof we use the fact that if $x_1, \ldots, x_n$ are any set of variables, for any $r \leqslant N$,

$$\sum_{i_1 < \cdots < i_r} x_{i_1}, \ldots, x_{i_r}$$

is a polynomial in

$$\sum_i x_i, \sum_i x_i^2, \ldots, \sum_i x_i^r.$$

□

Theorem 9: For $m \geqslant 1$ the functions $f_m(a,c)$, given by the formula

$$f_m(a,c) = tr(((a^{c^{1/2}})_{sk})^{2m}) = \frac{1}{2^{2m}} \mathrm{tr}((cac^{-1} - a^t)^{2m})$$

are well defined and invariant under $\mathrm{ad}^*(G)$. Moreover for all m, f_m is a rational function in (c,a); and for $H \in \mathcal{H}$, $f_M(I,H) = \mathrm{tr}(H^{2m}) = (-1)^m \Sigma_{1 \leqslant i \leqslant k} \lambda_i^{2m}$.

Proof: This is a straightforward calculation. □

Theorem 10: For n odd, $I(\mathcal{G}^+)$ is the ring of invariant functions on $\mathcal{G}^*$ is generated by

$$f_1, f_2, \ldots, f_k, \quad k = \left[\frac{n}{2}\right].$$

Proof: By Theorem 9 the functions f_m restricted to $\mathcal{H}$ agree with the generators of the ring of invariant on $\mathcal{H}$. This proves the result. □

Remark 11: As we just proved in Theorem (10), when n is odd, the ring of invariant functions $I(\mathcal{G}^+)$ contains typically rational functions and not polynomials in (c,a) because of the presence of c^{-1}. When n is even the situation is quite different because the ring of invariants on $\mathcal{H}$ carries the additional polynomial $\lambda_1, \ldots, \lambda_k$. This polynomial gives rise to an additional function, the Pfaffian, which although a polynomial on $so(n)$, is not even rational on $\mathcal{G}^*$.

Let $n = 2k$, H a skew-symmetric $n \times n$ matrix. The Pfaffian of H is by definition

$$\mathrm{Pf}\{H\} = \frac{1}{k! 2^k} \sum \pm h_{(i_1 i_2)} \ldots h_{(i_{k-1} i_k)} \quad (H = (h_{ij})).$$

When $H \in \mathcal{H}$, $\mathrm{Pf}\{H\} = \lambda_1, \ldots, \lambda_k$. Also $\mathrm{Det}(H) = (\mathrm{Pf}\{H\})$.[2,4] We extend Pf to all $n \times n$ matrices by writing for any $n \times n$ matrix A,

$$\pi(A) = \mathrm{Pf}(\tfrac{1}{2}(A - A^t)).$$

Clearly π is a polynomial function, homogeneous of degree k, but has no general invariant properties. π is unique up to a sign since

$$\pi(A)^2 = \det(\tfrac{1}{2}(A - A^t))^2.$$

Lemma 12: Let $n=2k$. The invariant function Pf on $\mathcal{G}^+$ that coincides with Pf on SO(n) is given by

$$\mathrm{Pf}(c,a)=\pi(ca)\det(c)^{-1/2}=\pi(ac^{-1})\det(c)^{1/2}.$$

Proof: Direct computation. □

Theorem 13: For $n=2k$, the ring $I(\mathcal{G}^+)$ of invariant functions is generated by

$$f_1,\ldots,f_{k-1},\mathrm{Pf}.$$

In general Pf is not rational.

Proof: As we have seen in previous lemma the ring generated by the functions

$$f_1,\ldots,f_{k-1},\mathrm{Pf}$$

restricts to $I(\mathcal{H})$. It only remains to show that Pf is not a rational expression. Assume Pf $=P/Q$, then

$$\det(c)^{1/2}=\frac{P(c,a)}{Q(c,a)\pi(ac^{-1})}$$

is a rational function of c which is absurd. □

Theorem 14: The simultaneous level sets of the generators of $I(\mathcal{G}^+)$ are precisely the G-orbits in $\mathcal{G}^+$.

Proof: By Chevalley's theorem for SO(n), the $\mathcal{W}$-invariant functions on $\mathcal{H}$ separates the $\mathcal{W}$-orbits. Hence $I(\mathcal{G}^+)$ separate the G-orbits in $\mathcal{G}^+$. □

Proposition 15: For $n=3$, the square of the Kelvin circulation generates the ring $I(\mathcal{G}^+)$. It is defined as $f_1=\frac{1}{2}\mathrm{tr}(a^2)-\mathrm{tr}(cac^{-1}a^t)$.

Proof: By Theorem 10 the number of invariant functions is equal to $[n/2]$. Write the expression for f_1 and compare with the square of the lengths of the Kelvin circulation given in Ref. 1. □

The Riemann disks, the two-dimensional analogs of the Riemann S-type ellipsoids, where introduced by Weinberg in Refs. 5 and 6. There he considers this Riemann disks as models of galactic bar. The disks are compose of a two-dimensional fluid specified by a surface σ, and a pressure P, which acts only in the plane of the fluid. The surface density of the Riemann disk is obtained by collapsing a homogeneous ellipsoid with density ρ and principal axes $a\geqslant b\geqslant c$ and it is proved that the potential function in this case is given by the very simple formula

$$V=\frac{\pi G\sigma_0}{a}[A(\lambda)(x^2-a^2)+B(\lambda)(y^2-b^2)]$$

also the velocity field in the rotating frame may be written

$$u_x=\frac{a}{b}\Lambda y,\quad u_y=\frac{a}{b}\Lambda x.$$

Then he points out that with this form of u, each stream line is an ellipse similar to the boundary of the disk, and each fluid element conserves its density and pressure. Notice that this corresponds exactly with the orbits for the two-dimensional ellipsoids we defined here abstractly.

III. SYMPLECTIC STRUCTURE AND GLOBAL DARBOUX COORDINATES FOR COADJOINT ORBITS OF SO(2)⋉GL$_+$(2)

In this section we find global Darboux coordinates for the coadjoint orbits of sym(2)⋉gl$_+$(2) on the dual of its Lie algebra. If we denote by O any one of these orbits, then Darboux theorem

says that: for each point of O there is a local chart (σ,U), $\sigma=(q_1,\ldots,q_n;p_1,\ldots,p_n)$ such that the 2-form ω, defining the symplectic structure, restricted to U has the simple form

$$\omega|_U=\sum_{u=1}^{n} dp_u\wedge dq_u.$$

However, even locally, it is extremely difficult to find such coordinates for most of the symplectic manifolds known. Pedersen showed that for simply connected exponential solvable Lie groups, it is indeed possible to find such Darboux coordinates, not locally but globally defined. In his paper[7] he proves that such coordinates exist and develops a technique to find these coordinates. Even though our group is not solvable, we could adapt his proof to our case so that one can find explicit Darboux coordinates in the case of *physical orbits*.

Theorem 16: For every $(c,a)\in\mathcal{G}^+$, there exist global coordinates on $O_{(c,a)}$ so that $O_{(c,a)}$ is diffeomorphic to $\mathbf{R}^6$. Coordinates given by the map

$$\sigma:\ \hat{G}\sim O_{(c,a)}\to\mathbf{R}^6,$$

$$\left(\begin{pmatrix} u & v\\ v & w\end{pmatrix},\begin{pmatrix} e^{\alpha} & \gamma\\ 0 & e^{\beta}\end{pmatrix}\right)\to(u,v,w;\alpha,\beta,\gamma),$$

$$\hat{G}=\mathrm{sym}(2)\ltimes B_+(2).$$

Proof: The proof is immediate from Corollary 5 and the Iwasawa decomposition of $\mathrm{gl}_+(2)$ using the fact that in this case the stabilizer is isomorphic to $\mathrm{SO}(2)$. □

As was proved by Kirillov,[8] $O_{(c,a)}$ is a symplectic manifold. We are going to use the identification just given, $O_{(c,a)}\sim\hat{G}$, to compute its symplectic structure. First we would like to recall how this ''canonical'' symplectic structure is defined for coadjoint orbits of connected Lie groups.

For $g\in\mathcal{G}^*$ we define the skewsymmetric bilinear form $B_g:\ \mathcal{G}\times\mathcal{G}\to\mathbf{R}$ by $B_g(X,Y)=<g,[X,Y]>$. The radical of B_g is the Lie algebra $\mathcal{G}_g$ of the stabilizer G_g of g, and therefore we can define a symplectic form $\hat{B}_g:\ \mathcal{G}/\mathcal{G}_g\times\mathcal{G}/\mathcal{G}_g\to\mathbf{R}$ by factoring through $\mathcal{G}_g$.

Let $\omega=\omega_O$ be the canonical symplectic form on O. We recall how ω is defined: For $l\in O$, let $\alpha_l:\mathcal{G}/\mathcal{G}_g\to T_l(O)$ be the canonical vector space isomorphism, i.e., $\alpha_l(\dot{X})\varphi(l)=(d/dt)\,\varphi(\exp tX.l)|_{t=0}$, where $\dot{X}=X+\mathcal{G}_g$ and $\varphi\in\mathbf{C}^{\infty}(C)$. Then ω_l is defined to be the transport by α_l of $\hat{B}_l$, i.e., $\omega_l(\alpha_l(\hat{X}),\alpha(\hat{Y}))=B_l(X,Y)$. The form ω is then defined by moving ω_l by the elements of G to the points of O. Let us now return to our special situation where $\mathrm{gl}_l=\mathrm{SO}(2)$ and we have

$$\hat{G}\to O_l,\quad \hat{g}\to\hat{g}.l.$$

So if $\hat{\mathcal{G}}$ is the Lie algebra of $\hat{G}$, α_l is an isomorphism of $\hat{\mathcal{G}}$ with $T_l(O)$. Thus ω_l lifts to a symplectic form $\hat{\omega}$ on $\hat{G}$ characterized by

(1) $\hat{\omega}$ is invariant under left translations of $\hat{G}$;
(2) $\hat{\omega}_e(\hat{X},\hat{Y})=l([\hat{X},\hat{Y}]),\ \hat{X},\hat{Y}\in\hat{\mathcal{G}}$.

We have thus come down from G to $\hat{G}$; although G is not solvable, $\hat{G}$ is solvable, even exponential. For $\hat{\mathcal{G}}$ the elements are of the form

$$(s,b)\quad \left(s=\begin{pmatrix} u & v\\ v & w\end{pmatrix},\quad b=\begin{pmatrix} x & z\\ 0 & y\end{pmatrix}\right).$$

So we have a basis

$$S_1, S_2, S_3; B_1, B_2, B_3$$

for $\hat{\mathcal{G}}$ given by

$$S_1 = \left(\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, 0 \right), \quad S_2 = \left(\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, 0 \right), \quad S_3 = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right),$$

$$B_1 = \left(0, \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \right), \quad B_2 = \left(0, \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right), \quad B_3 = \left(0, \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \right).$$

The commutation rules are

$$[S_i, S_j] = 0, \quad [B_1, B_2] = 0, \quad [B_1, B_3] = B_3, \quad [B_2, B_3] = -B_3,$$

$$[B_1, S_1] = 2S_1, \quad [B_1, S_2] = 0, \quad [B_1, S_3] = S_3,$$

$$[B_2, S_1] = 0, \quad [B_2, S_2] = 2S_2, \quad [B_2, S_3] = S_3,$$

$$[B_3, S_1] = 0, \quad [B_3, S_2] = S_3, \quad [B_3, S_3] = 2S_1.$$

These are straightforward to check.

The element l we shall take to be $(I, r\left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right))$. So

$$<(s,b), l> = 2r \operatorname{tr}\left(b \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \right) + \operatorname{tr}(s) = 2rz + u + w,$$

where

$$b = \begin{pmatrix} x & z \\ 0 & y \end{pmatrix}, \quad s = \begin{pmatrix} u & w \\ w & v \end{pmatrix}.$$

Thus

$$l: \ S_1 \to 1, S_2 \to 1, S_3 \to 0, B_1 \to 0, B_2 = 0, B_3 \to 2r.$$

Moreover, at the identity element of $\hat{G}$,

$$S_1 = \frac{\partial}{\partial u}, \quad S_2 = \frac{\partial}{\partial v}, \quad S_3 = \frac{\partial}{\partial w},$$

$$B_1 = \frac{\partial}{\partial \alpha}, \quad B_2 = \frac{\partial}{\partial \beta}, \quad B_3 = \frac{\partial}{\partial \gamma}.$$

Theorem 17: In the coordinate system given in Theorem 16. $\hat{\omega}_e$ is equal to

$$\hat{\omega}_e = -(2r\, d\beta \wedge d\gamma + 2r\, d\gamma \wedge d\alpha + 2\, du \wedge d\alpha + 2\, dv \wedge d\beta + 2\, dw \wedge d\gamma).$$

Proof: Follows from the previous relations and the definition of $\hat{\omega}_e$. □

Theorem 18: The 2-form $\hat{\omega}$ on $\hat{G}$ is equal to

$$\begin{aligned} \omega = & -2e^{-2\alpha} du \wedge d\alpha - 2\gamma^2 e^{-2(\alpha+\beta)} dv \wedge d\alpha - 2(\gamma^2 e^{-2(\alpha+\beta)} + e^{2\beta}) dv \wedge d\beta \\ & + 2\gamma e^{-2(\alpha+\beta)} dv \wedge d\gamma - 2e^{-(2\alpha+\beta)} dw \wedge d\gamma - 2r\gamma e^{-\alpha} d\alpha \wedge d\beta \\ & + 2re^{-\alpha} d\alpha \wedge d\gamma - 2re^{-\alpha} d\beta \wedge d\gamma - 4\gamma e^{-(2\alpha+\beta)} d\alpha \wedge dw - 2\gamma e^{-(2\alpha+\beta)} d\beta \wedge dw. \end{aligned}$$

Proof: Since $\hat{\omega}$ is the left invariant extension of $\hat{\omega}_e$, Theorem 17 shows that

$$\hat{\omega} = -2r[d\beta]\wedge[d\gamma] + 2r[d\alpha]\wedge[d\gamma] + 2[d\alpha]\wedge[du] + 2[d\beta]\wedge[dv] + 2[d\gamma]\wedge[dw].$$

Now if we compute the left invariant 1-form that extend $d\alpha_e, \ldots, dw_e$ we get the result. □

We shall use Pedersen's[7] technique in the explicit construction of the global Darboux coordinates. If we denote by $\hat{\mathcal{S}} = \mathrm{sym}(2)$, view as a normal subgroup of $\mathcal{G}$, then the functions on $\hat{\mathcal{G}}/\hat{\mathcal{S}}$ are precisely those that are functions of α,β,γ only. We denote by $\mathcal{E}^O$ the space of all smooth functions on $\hat{G}/\hat{\mathcal{S}}$, i.e., smooth functions on α,β,γ. Our aim is to study $C^\infty(\hat{G})$ as a Poisson algebra under the Poisson bracket $\{.,.\}$ determined by $\hat{\omega}$. From classical results in symplectic manifolds we know that if $a_1, \ldots, a_n$ be a chart on a symplectic manifold M with symplectic form ω, and $\omega(\partial/\partial a_j, \partial/\partial a_k) = \omega_{jk}$ $(1 \leqslant j,k \leqslant n)$ then

$$\{a_j, a_k\} = \omega^{kj} \quad (1 \leqslant j,k \leqslant n),$$

where (ω^{kj}) is the inverse matrix of (ω_{kj}).

We now return to $\mathcal{G}$.

Theorem 19: In the coordinates $u,v,w,\alpha,\beta,\gamma$ the matrix of $\hat{\omega}$ is

$$\begin{pmatrix} 0 & \tilde{A} \\ -\tilde{A}^t & \tilde{B} \end{pmatrix},$$

where

$$\tilde{A} = \begin{pmatrix} -2e^{-2\beta} & 0 & \\ -2\gamma^2 e^{-2(\alpha+\beta)} & -2(e^{-2\beta} + \gamma^2 e^{-2(\alpha+\beta)}) & 0 \\ 4\gamma e^{-(2\alpha+\beta)} & 2\gamma e^{-(2\alpha+\beta)} & -2e^{-(2\alpha+\beta)} \end{pmatrix},$$

$$\tilde{B} = \begin{pmatrix} 0 & -2r\gamma e^{-\alpha} & 0 & -2re^{-\alpha} \\ 2r\gamma e^{\alpha} & 0 & -2re^{-\alpha} & \\ -2re^{-\alpha} & 2re^{-\alpha} & 0 & \end{pmatrix}.$$

Its inverse has the form

$$\begin{pmatrix} A & B \\ -B^t & 0 \end{pmatrix},$$

where A,B,C are 3×3 matrices. In particular

$$\{\alpha,\beta\} = \{\beta,\gamma\} = \{\gamma,\alpha\} = 0.$$

Proof: The matrix of ω has the form

$$\begin{pmatrix} 0 & X \\ -X^t & Y \end{pmatrix},$$

where X and Y are 3×3 matrices; and as $\hat{\omega}$ is invertible, X is invertible. Its inverse is

$$\begin{pmatrix} X^{-1t} Y X^{-1} & -X^{-1t} \\ X^{-1} & 0 \end{pmatrix}$$

as an easy calculation shows. □

We shall now give a brief description of Pedersen's work[7] and proceed to apply it in this case. Recall the isomorphism

$$\hat{G}\sim O, \quad \hat{g}\to \hat{g}.l$$

where

$$l=\left(I, r\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\right).$$

Let $\mathcal{E}^O(\hat{G})$ be the space of smooth functions on $\hat{G}/\hat{\mathcal{S}}$, i.e., smooth functions of α,β,γ. By theorem 19 this is an Abelian Lie algebra under $\{.,.\}$.

Following Pedersen we introduce $\mathcal{E}^1(\hat{G})$, the space of quantizable functions on $\hat{G}$, namely the space of smooth functions f on $\mathcal{G}$ such that

$$\{f,g\}\in \mathcal{E}^O(\mathcal{G}) \quad (g\in \mathcal{E}^O(\hat{G})).$$

Thus $\mathcal{E}^1(\hat{G})$ is the normalizer of $\mathcal{E}^O(\hat{G})$ with respect to $\{.,.\}$; consequently it is also a Lie algebra under $\{.,.\}$. Pederson now constructs a Lie algebra isomorphism

$$\delta:\ \mathcal{E}^1(\hat{G})\tilde{\to}\mathrm{Diff}^1(\hat{G}/\hat{\mathcal{S}}),$$

where $\mathrm{Diff}^1(\hat{G}/\hat{\mathcal{S}})$ is the Lie algebra of smooth differential operators in α,β,γ of degree $\leqslant 1$. It follows there will be elements

$$P_\alpha, P_\beta, P_\gamma \in \mathcal{E}^1(\hat{G})$$

such that

$$\delta(P_\alpha)=\frac{\partial}{\partial\alpha}, \quad \delta(P_\beta)=\frac{\partial}{\partial\beta}, \quad \delta(P_\gamma)=\frac{\partial}{\partial\gamma}.$$

Then we will have

$$\{P_\alpha, P_\beta\}=\{P_\beta, P_\gamma\}=\{P_\gamma, P_\alpha\}=0,$$

$$\{P_\alpha, \alpha\}=\{P_\beta, \beta\}=\{P_\gamma, \gamma\}=1,$$

$$\{P_\alpha, \beta\}=\{P_\alpha, \gamma\}=0,$$

etc. These relations then show that

$$\hat{\omega}=dP_\alpha\wedge d\alpha+dP_\beta\wedge d\beta+dP_\gamma\wedge d\gamma.$$

In other words

$$\alpha,\beta,\gamma,P_\alpha,P_\beta,P_\gamma$$

will be the global Darboux coordinates we are after.

It remains to describe the Pedersen isomorphism. Recall that

$$\mathcal{G}=\mathcal{S}\oplus\hat{b}(2), \quad \hat{b}(2)=\mathrm{Lie}(B_+(2)).$$

Let us now associate to $X\in\hat{b}$ the functions ψ^X on $\hat{G}$ by

$$\psi^X(\hat{g}) = <X, \hat{g}.l>.$$

Pedersen associates to ψ^X the differential operators $D(X)$ acting on functions on $\mathcal{G}/\hat{\mathcal{S}} \sim B_+(2)$

$$(D(X))(b) = \frac{d}{dt} u(\exp(-tX.b))|_{t=0};$$

thus

$$\delta(\psi^X) = D(X).$$

If φ is a smooth function on $\hat{G}/\hat{\mathcal{S}}$, Pedersen associates to φ the operator M_φ of multiplication by φ

$$\delta(\varphi) = M_\varphi, \quad M_\varphi u = \varphi u.$$

Since ψ^X and φ are functions on $\hat{G}$, $\{\psi^X, \varphi\}$ makes sense and it is not difficult to check that

$$\{\psi^X, \varphi\} = X\varphi,$$

$$[D(X), M_\varphi] = M_{X\varphi}.$$

The first relation shows that $\psi^X \in \mathcal{E}^1(\hat{G})$. Pedersen shows actually that the ψ^X and φ generate $\mathcal{E}^1(\hat{G})$ as an $\mathcal{E}^0(\hat{G})$-module and that δ defines a Lie algebra isomorphism

$$\delta: \ \mathcal{E}^1(\hat{G}) \tilde{\rightarrow} \mathrm{Diff}(\alpha, \beta, \gamma).$$

To construct the Darboux coordinates in our case it is not even necessary to assume Pedersen's theorem; it is enough to compute

$$\psi^{B_1}, \psi^{B_2}, \psi^{B_3}, D(B_1), D(B_2), D(B_3),$$

where $\{B_1, B_2, B_3\}$ is the basis of $\hat{b}(2)$ introduced earlier, and determine $P_\alpha, P_\beta, P_\gamma$.

We begin with $\gamma(B_j)$.

Lemma 20: We have

$$D(B_1) = -\frac{\partial}{\partial \alpha} - \gamma \frac{\partial}{\partial \gamma},$$

$$D(B_2) = -\frac{\partial}{\partial \beta},$$

$$D(B_3) = -e^\beta \frac{\partial}{\partial \gamma}.$$

Proof: We have, for any smooth function u of α, β, γ

$$(D(X)u)(b) = \frac{d}{dt} u(\exp(-tX.b))|_{t=0}$$

apply this formula when $X = B_1, B_2, B_3$ to get the result. □

Let

$$X=\begin{pmatrix}\xi & \zeta\\ 0 & \tau\end{pmatrix},\quad b=\begin{pmatrix}e^{\alpha} & \gamma\\ 0 & e^{\beta}\end{pmatrix},\quad s=\begin{pmatrix}u & w\\ w & v\end{pmatrix}.$$

Lemma 21: The function ψ^X is given by the formula

$$\psi^X(s,b)=2re^{-\alpha}(\xi\gamma+\zeta e^{\beta}-\tau\gamma)+2[(\xi u+\xi w)e^{-2\alpha}-\gamma e^{-(2\alpha+\beta)}(\xi w+\zeta v)$$
$$-\tau w\gamma e^{-(2\alpha+\beta)}+\tau v e^{-2\beta}(\gamma^2e^{-2\alpha}+1)].$$

Proof: We have

$$b^{-1}Xb=\begin{pmatrix}e^{-\alpha} & -\gamma e^{-(\alpha+\beta)}\\ 0 & e^{-\beta}\end{pmatrix}\begin{pmatrix}\xi & \zeta\\ 0 & \tau\end{pmatrix}\begin{pmatrix}e^{\alpha} & \gamma\\ 0 & e^{\beta}\end{pmatrix}=\begin{pmatrix}\xi & e^{-\alpha}(\xi\gamma+\zeta e^{\beta}-\tau\gamma)\\ 0 & \tau\end{pmatrix},$$

$$Xs\check{b}b^{-1}=\begin{pmatrix}\xi u+\zeta w & \xi w+\zeta v\\ \tau w & \tau v\end{pmatrix}\begin{pmatrix}e^{-2\alpha} & -\gamma e^{-(2\alpha+\beta)}\\ -\gamma e^{-(2\alpha+\beta)} & \gamma^2e^{-2(\alpha+\beta)}+e^{-2\beta}\end{pmatrix}.$$

From which the formula for ψ^X is immediate. □

Lemma 22: We have

$$\psi^{B_1}=2r\gamma e^{-\alpha}+2ue^{-2\alpha}-2\gamma we^{-(2\alpha+\beta)},$$

$$\psi^{B_2}=-2r\gamma e^{-\alpha}-2w\gamma e^{-(2\alpha+\beta)}+2ve^{-2\beta}(\gamma^2e^{-2\beta}+1),$$

$$\psi^{B_3}=2re^{\beta-\alpha}+2we^{-2\alpha}-2\gamma ve^{-(2\alpha+\beta)}.$$

Proof: Immediate. □

Lemma 23: Let

$$P_{\alpha}=-2r\gamma e^{-\alpha}-2ue^{-2\alpha}+2\gamma we^{-(2\alpha+\beta)}+\gamma e^{-\beta}(2we^{-2\alpha}-2\gamma ve^{-(2\alpha+\beta)}+2re^{\beta-\alpha}),$$

$$P_{\beta}=2r\gamma e^{-\alpha}+2w\gamma e^{-(2\alpha+\beta)}-2ve^{-2\beta}(\gamma^2e^{-2\beta}+1),$$

$$P_{\gamma}=-e^{-\beta}(2re^{\beta-\alpha}+2we^{-2\alpha}-2\gamma ve^{-(2\alpha+\beta)}),$$

then

$$\delta(P_{\alpha})=\frac{\partial}{\partial\alpha},\quad \delta(P_{\beta})=\frac{\partial}{\partial\beta},\quad \delta(P_{\gamma})=\frac{\partial}{\partial\gamma}.$$

Proof: From Lemmas 22 and 20 we get

$$\delta(-\psi^{B_1}+\gamma e^{-\beta}\psi^{B_3})=\frac{\partial}{\partial\alpha},$$

$$\delta(-\psi^{B_2})=\frac{\partial}{\partial\beta},$$

$$\delta(-e^{-\beta}\psi^{B_3})=\frac{\partial}{\partial\gamma}.$$

□

From this we get the following lemma.

Lemma 24: We have

$$\hat{\omega} = dP_\alpha \wedge d\alpha + dP_\beta \wedge d\beta + dP_\gamma \wedge d\gamma.$$

Proof: This is a straightforward computation. □

Theorem 25: The coordinates

$$\alpha, \beta, \gamma, P_\alpha, P_\beta, P_\gamma$$

are global Darboux coordinates on $\hat{G} \sim O$.

Proof: Immediate. □

IV. STRUCTURE OF POTENTIALS AND HAMILTONIAN FORM FOR ELLIPSOIDAL DYNAMICS

The equations of motion for a self-gravitating ellipsoid have been described in Ref. 1. They make sense for n-dimensional ellipsoids and take the following form. Let

$$\mathbf{I} = (I_{ij}), \quad \mathbf{S} = (S_{kl})$$

be, respectively, the inertia and shear tensor (in the laboratory frame). The motion of the ellipsoid is completely determined by the time evolution of **I** and **S**.

Let **T** the kinetic energy tensor. Then

$$\mathbf{T} = \tfrac{1}{2}\mathbf{S}^t\mathbf{I}^{-1}\mathbf{S}$$

and the differential equations are

$$\begin{aligned} \dot{\mathbf{I}} &= \mathbf{S} + \mathbf{S}^t \\ \dot{\mathbf{S}} &= 2\mathbf{T} + \mathbf{P} + \Pi, \end{aligned} \tag{2}$$

where $\Pi = p.v.\mathbf{1}$, $p =$ total pressure, $v =$ volume of the ellipsoid and **P** the gravitational tensor

$$\mathbf{P} = (P_{ij}).$$

We shall show in this section that Eqs. (2) can be expressed in the Hamiltonian form, i.e., for a suitable function H on the phase space,

$$\begin{aligned} \dot{I}_{ij} &= \{H, I_{ij}\}, \\ \dot{S}_{ij} &= \{H, S_{ij}\}. \end{aligned} \tag{3}$$

The main result that does this is Theorem 41. For the case $n = 3$ it was proved by Rosensteel.[1] It depends on a study of the conditions under which we may assert that a tensor $A = (a_{ij})$ is of the form

$$a_{ij} = \{V, S_{ij}\}$$

for a functions V of the I_{ik} that is SO(n)-invariant. Theorem 34 does this. Theorem 34 and its corollary Theorem 36 appear to be new. The method of proof of Rosensteel[1] was somewhat different from the one given here.

Lemma 26: The Poisson bracket of S_{ij} and I_{ij} is given by

$$\{I_{ij}, S_{rk}\} = -(\delta_{ik}I_{rj} + \delta_{jk}I_{ri}),$$

$$\{I_{ij}, I_{rk}\} = 0,$$

$$\{S_{ij},S_{rk}\}=\delta_{ik}S_{jr}-\delta_{rj}S_{ik}.$$

Proof: Refer to Ref. 1. □

Let's define the kinetic energy tensor

$$\mathbf{T}=\tfrac{1}{2}(S^tI^{-1}S),\quad T_{ij}=\tfrac{1}{2}S_{ki}I^{km}S_{mj}=T_{ji}. \tag{4}$$

Proposition 27: The following relations are satisfied:

$$\{T,I_{kl}\}=S_{kl}+S^t_{lk}, \tag{5}$$

$$\{T,S_{kl}\}=2T_{kl}. \tag{6}$$

Proof: This is a direct computation. □

It is now necessary to determine which matrices $A=(A_{ij})$ of functions of the I_{ij} can be written in the form $(\{V,S_{kl}\})$ for some rotation invariant function V of the I_{ij}.

Definition 28: Let $M_V=(\{V,S_{lj}\})$. A matrix, $A=(A_{lj})$, of functions on the coordinates $I_{ik}i\leqslant k$, is said to come from a potential if there exits a SO(n)-invariant function of the I_{ik} such that $A=M_V$, i.e., $A_{lj}=\{V,S_{lj}\}$ for all l,j.

Proposition 29: Let $V(I_{lk})=\mathrm{tr}(I^p)$, where I is the matrix whose components are the functions I_{ij} on $\mathcal{G}^*$; then $M_V=-2pI^p$.

Proof: The identity follows immediately from the formula

$$V=\sum_{i_1,\ldots,i_p} I_{i_1i_2}I_{i_2i_3},\ldots,I_{i_pi_1}.$$

□

Corollary 30: The matrix I comes from a potential.

Proof: Take $V=(-1/2)\,\mathrm{tr}(I)$ and apply the previous lemma. □

Lemma 31: Let $V_1,V_2,\ldots,V_n$ be SO(n)-invariant functions of the I_{ik}. Then for any smooth function $\Phi(V_1,\ldots,V_n)$ of the V_i the following equation is true:

$$M_{\Phi(V_1,\ldots,V_n)}=\sum_{1\leqslant i\leqslant n}\frac{\partial\Phi}{\partial V_i}M_{V_i}.$$

Proof:

$$M_{\Phi(V_1,\ldots,V_n)}=(\{\Phi(V_1,\ldots,V_n),S_{kl}\}).$$

Using the fact that $\{.,S_{kl}\}$ is a derivation we get

$$\{\Phi(V_1,\ldots,V_n),S_{kl}\}=\frac{\partial\Phi}{\partial V_1}\{V_1,S_{kl}\}+\ldots+\frac{\partial\Phi}{\partial V_n}\{V_n,S_{kl}\}.$$

This proves the lemma. □

Lemma 32: Let V be a function of the I_{ik}, invariant under SO(n). Then for all $g\in\mathrm{SO}(n)$,

$$(M_V)^g=g^tMg.$$

Proof: Notice that $(M_V)^g_{kl}=\{V,S_{kl}\}^g=\{V^g,S^g_{kl}\}=\{V,S^g_{kl}\}$. Using the pairing $<.,.>$ the lemma follows. □

For any smooth function F on the set of positive definite matrices define

$$\tilde{F}(a_1,\ldots,a_n)=F(\mathrm{diag}(a_1^2,\ldots,a_n^2)).$$

If $M=(F_{ij})$ is a matrix of such functions, we define

$$\tilde{M}=\widetilde{(F_{ij})}.$$

Finally let

$$\mathcal{D}=(D_{ij})$$

be the matrix of vector fields in the variables $a_1,\ldots,a_n$, with

$$D_{ij}=\delta_{ij}a_i\frac{\partial}{\partial a_i}(\text{no summation}).$$

Lemma 33: For any $\mathrm{SO}(n)$-invariant smooth function V on the set of positive definitive matrices,

$$\tilde{M}_V=\mathcal{D}\tilde{V}=\left(-\delta_{ij}a_i\frac{\partial}{\partial a_i}\tilde{V}\right).$$

Proof: Since both sides are smooth it is enough to verify this on the open set where the a_i are distinct. Moreover it is enough to do this locally.

Write

$$V_p(s)=\mathrm{tr}(s^p),\quad p=1,2,\ldots,n.$$

If V is $\mathrm{SO}(n)$-invariant, locally on U we have a representation

$$V(s)=\varphi(V_1(s),\ldots,V_n(s)),$$

where φ is smooth. Then

$$\tilde{M}_V=\sum_p\left(\frac{\widetilde{\partial\varphi}}{\partial V_p}\right)\tilde{M}_{V_p},$$

on the other hand, by Proposition 29

$$\tilde{M}_{V_p}(a_1,\ldots,a_n)=-2p\ \mathrm{diag}(a_1^{2p},\ldots,a_n^{2p})=(D_{ij}\tilde{V}_p(a_1,\ldots,a_n)),$$

hence

$$\tilde{M}_V=\sum_p\left(\frac{\widetilde{\partial\varphi}}{\partial V_p}\right)\tilde{M}_{V_p}=\sum_p\left(\frac{\widetilde{\partial\varphi}}{\partial V_p}\right)\mathcal{D}\tilde{V}=\mathcal{D}\varphi(\tilde{V}_1,\ldots,\tilde{V}_n)=\mathcal{D}\tilde{V}.$$

This proves the lemma. □

Theorem 34: Suppose

$$M=(M_{ij})$$

is a tensor of smooth functions on the open set of positive definite matrices with the following properties:

(1) $M^g=g^tMg\ \ (g\in\mathrm{SO}(n))$.
(2) There exist a smooth $\mathrm{SO}(n)$-invariant function V on the open positive definite matrices such that

$$\tilde{M}=\mathcal{D}\tilde{M}.$$

Then

$$M = M_V .$$

In particular M comes from a potential.

Remark 35: These conditions are obviously necessary. This theorem is very useful since it reduces the verification to the diagonal matrices.

Proof: By the lemma above,

$$\tilde{M} = \tilde{M}_V .$$

Since both M and M_V have the transformation properties (1), it follows that they are both uniquely determined by they restriction to the space of diagonal matrices. Since the restriction of M and M_V to the diagonal space are equal, we must have $M = M_V$. □

Theorem 36: Let f be a scalar smooth SO(n)-invariant function. Then the tensor

$$f.I = (\delta_{ij} f)$$

comes from a potential if and only if it is a function of the determinant. More precisely, if

$$f(s) = h((\det(s))^{1/2}),$$

then

$$f.I = M_g ,$$

where

$$g(s) = k((\det(s)^{\frac{1}{2}}), \quad k(x) = -\int^x \frac{h(t)}{t} dt.$$

Proof: Assume first that f is a smooth function of det. We can thus write

$$f(s) = h((\det)^{1/2}),$$

where h is a smooth function of a single variable $x > 0$. Select a function $k(x)$ $(x > 0)$, smooth, such that

$$h(x) = -xk'(x),$$

for instance

$$k(x) = -\int_1^x \frac{h(t)}{t} dt.$$

If

$$g(s) = k((\det(s))^{\frac{1}{2}})$$

we claim that

$$f.I = M_g .$$

In view of Theorem 36 it is enough to prove that

$$f(\mathrm{diag}(a_1^2,\ldots,a_n^2)) = -a_i \frac{\partial}{\partial a_i} g(\mathrm{diag}(a_1^2,\ldots,a_n^2)).$$

But

$$\begin{aligned} -a_i \frac{\partial}{\partial a_i} g(\mathrm{diag}(a_1^2,\ldots,a_n^2)) &= -a_i \frac{\partial}{\partial a_i} k(\mathrm{diag}(a_1,\ldots,a_n)) = -a_i k'(a_1,\ldots,a_n) \\ &\quad \times (a_1,\ldots,\hat{a}_i,\ldots,a_n) = -(a_1,\ldots,a_n)k'(a_1,\ldots,a_n) \\ &= h(a_1,\ldots,a_n) = f(\mathrm{diag}(a_1^2,\ldots,a_n^2)). \end{aligned}$$

We must now prove the converse. So we assume that for all $i=1,\ldots,n$

$$f(\mathrm{diag}(a_1^2,\ldots,a_n^2)) = -a_i \frac{\partial}{\partial a_i} g(\mathrm{diag}(a_1^2,\ldots,a_n^2))$$

for some smooth function g in the positive definite matrices.

Write

$$F(a_1,\ldots,a_n) = f(\mathrm{diag}(a_1^2,\ldots,a_n^2)), \quad G(a_1,\ldots,a_n) = -g(\mathrm{diag}(a_1^2,\ldots,a_n^2)).$$

Then

$$F(a_1,\ldots,a_n) = -a_i \frac{\partial G}{\partial a_1} \quad (1 \leqslant i \leqslant n, a_i > 0).$$

If we go to variables $b_1,\ldots,b_n$ where $b_1 = a_1 \ldots a_n$, $b_j = a_j$, $2 \leqslant j \leqslant n$, then

$$a_1 \frac{\partial G}{\partial a_1} = (a_1 \ldots a_n) \frac{\partial G}{\partial b_1},$$

$$a_j \frac{\partial G}{\partial a_j} = (a_1 \ldots a_n) \frac{\partial G}{\partial b_1} + a_j \frac{\partial G}{\partial b_j} \quad (2 \leqslant j \leqslant n).$$

As all the $a_j(\partial G/\partial a_j)$ are equal to F, we must have

$$\frac{\partial G}{\partial b_j} = 0, \quad 2 \leqslant j \leqslant n.$$

Hence G is a function of b_1 only, say

$$G(b_1,\ldots,b_n) = h(b_1) = h(a_1 \ldots a_n).$$

But then

$$F(a_1,\ldots,a_n) = a_1 h'(a_1,\ldots,a_n) a_2,\ldots,a_n = (a_1 \ldots a_n) h'(a_1 \ldots a_n).$$

Showing that F depends only on $a_1,\ldots,a_n$. So f is a function of det only. □

We begin by applying Theorem 34 to show that the gravitational potential tensor of an ellipsoid comes from a potential, and determine this potential. We observe that for any point $(c,a) \in \mathcal{G}^*$ (a symmetric) the corresponding ellipsoid is given by the equation

$$x^t a^{-1} x = 1.$$

For an ellipsoid with mass density $\rho(x)$, the analogue of the gravitational potential tensor is

$$P_{ij}(a)=k\int_{\Gamma}\int_{\Gamma'}\frac{\rho(x)\rho(x')(x_i-x_i')(x_j-x_j')}{\|x-x'\|^n}d^nx\,d^nx', \tag{7}$$

where k is a constant >0 and

$$\Gamma=\{x|x^ta^{-1}x\leqslant 1\},\quad \Gamma'=\{x'|x'^ta^{-1}x'\leqslant 1\}.$$

For a homogeneous ellipsoid, $\rho=$mass/volume. Hence, as the volume is $\det(a)^{\frac{1}{2}}$, we get for homogeneous ellipsoids

$$P_{ij}(a)=k.\det(a)^{-1}\int_{\Gamma}\int_{\Gamma'}\frac{(x_i-x_i')(x_j-x_j')}{\|x-x'\|^n}d^nx\,d^nx'.$$

Proposition 37: The following properties are valid for the tensor (P_{ij}):

(1) For any $g\in O(n)$, $P^g_{ij}(a)=(P_{ij}(g^tag))=g^tP_{ij}(a)g$,
(2) $P_{ij}(\mathrm{diag}(a_1^2,\ldots,a_n^2))=0\ (i\neq j)$,
(3) $P_{ij}(\mathrm{diag}(a_1^2,\ldots,a_n^2))=k(a_1^2,\ldots,a_n^2)^{-1}\int_{\Gamma}\int_{\Gamma'}\frac{(x_i-x_i')^2}{\|x-x'\|^3}d^nx\,d^nx'$.

Proof: All this properties are easy to verify. □

Theorem 38: Let $V=[1/(n-2)]\,\mathrm{tr}(P_{ij})$, where P_{ij} is the tensor defined as in Eq. (7). Then $P=(P_{ij})$ comes from a potential V, i.e.,

$$P_{ij}=\{V,S_{ij}\}.$$

Proof: Take $V=[1/(n-2)]\,\mathrm{tr}(P)$. We shall show that

$$M_V=P.$$

In view of Theorem 34 and Proposition 37 we must show that

$$P_{ij}(\mathrm{diag}(a_1^2,\ldots,a_n^2))=-a_i\frac{\partial}{\partial a_i}V(\mathrm{diag}(a_1^2,\ldots,a_n^2)).$$

But this equation follows after a change of variables on the region of integration. □

Remark 39: Even for $n=3$ *this proof is different from that on Ref. 1.*

Theorem 40: Finally,

$$\delta_{ij}\det{}^{1/2}=-\{\det{}^{1/2},S_{ij}\}.$$

Proof: We use Theorem 36. In the notation there $k(x)=x$, so $h(x)=-x$, proving what we want. □

We are thus able to prove that Eqs. (2) have the Hamiltonian form.

Theorem 41: Let

$$H=T+V-p.v,\quad V=\frac{1}{n-2}\mathrm{tr}(P)$$

then the equations of motion

$$\dot I=S_{ij}+S_{ji},\quad \dot S_{ij}=2T_{ij}+P_{ij}+p.v\,\delta_{ij}$$

can be written as

$$\dot{I}_{ij}=\{H,I_{ij}\},\quad \dot{S}_{ij}=\{H,S_{ij}\}.$$

Proof: We have

$$\{H,I_{ij}\}=\{T,I_{ij}\}+\{V-p.v,I_{ij}\}$$

the second term is 0 because it is a function of the I_{ij} only. The first is $S_{ij}+S_{ji}$ by Proposition 27. Further

$$\{H,S_{ij}\}=\{T,S_{ij}\}+\{V,S_{ij}\}-p\{v,S_{ij}\}.$$

The first term is $2T_{ij}$ by Proposition 27. The second term is P_{ij} by Theorem 38. Finally

$$\{p.v,S_{ij}\}=p\{\det^{1/2},S_{ij}\}=-p.\det^{1/2}\delta_{ij}=-\delta_{ij}p.v.$$

Hence

$$\{H,S_{ij}\}=2T_{ij}+P_{ij}+p.v\,\delta_{ij}.$$

□

Rosensteel, in case $n=3$, defines additional potential tensors that depend on the surface energy tensor

$$\mathcal{G}_{ij}=\frac{1}{2}\gamma_S\int_{\partial v}x_i.\boldsymbol{\nabla}.\mathbf{n}n_j\,dS,$$

where ∂E denotes the boundary of the ellipsoid, $\mathbf{n}$ denotes the outward normal vector. γ_S is the surface tension and dS denote the area element. Rosenkilde[9] has showed that $\mathcal{G}_{ij}$ is a symmetric tensor and simplifies to

$$\mathcal{G}_{ij}=\frac{1}{2}\gamma_S\int_{\partial v}(\delta_{ij}-n_in_j)dS.$$

It has been shown[1] that the matrix $(\mathcal{G}_{ij})$ also comes from a potential given by $V^{\Sigma}=\mathrm{tr}(\mathcal{G})$. We do not treat this case here.

Last remark: It is not clear at this moment what is, if there is any, correct physical interpretation for the energy functions and tensors defined here. This topic should be the subject of further studies.

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Towards the classification of static vacuum spacetimes with negative cosmological constant

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We present a systematic study of static solutions of the vacuum Einstein equations with negative cosmological constant which asymptotically approach the generalized Kottler (''Schwarzschild–anti-de Sitter'') solution, within (mainly) a conformal framework. We show connectedness of conformal infinity for appropriately regular such spacetimes. We give an explicit expression for the Hamiltonian mass of the (not necessarily static) metrics within the class considered; in the static case we show that they have a finite and well-defined Hawking mass. We prove inequalities relating the mass and the horizon area of the (static) metrics considered to those of appropriate reference generalized Kottler metrics. Those inequalities yield an inequality which is opposite to the conjectured generalized Penrose inequality. They can thus be used to prove a uniqueness theorem for the generalized Kottler black holes if the generalized Penrose inequality can be established. [DOI: 10.1063/1.1340869]

I. INTRODUCTION

Consider the families of metrics

$$ds^2=-\left(k-\frac{2m}{r}-\frac{\Lambda}{3}r^2\right)dt^2+\left(k-\frac{2m}{r}-\frac{\Lambda}{3}r^2\right)^{-1}dr^2+r^2\,d\Omega_k^2,\quad k=0,\pm 1, \tag{I.1}$$

$$ds^2=-(\lambda-\Lambda r^2)dt^2+(\lambda-\Lambda r^2)^{-1}\,dr^2+|\Lambda|^{-1}\,d\Omega_k^2,\quad k=\pm 1,\quad k\Lambda>0,\quad \lambda\in\mathbb{R}, \tag{I.2}$$

where $d\Omega_k^2$ denotes a metric of constant Gauss curvature k on a two-dimensional manifold ${}^2M$. (Throughout this work we assume that ${}^2M$ is compact.) These are well-known static solutions of the vacuum Einstein equation with a cosmological constant Λ; some subclasses of (I.1) and (I.2) have been discovered by de Sitter[1] [(I.1) with $m=0$ and $k=1$], by Kottler[2] [Eq. (I.1) with an arbitrary m and $k=1$], and by Nariai[3] [Eq. (I.2) with $k=1$]. As discussed in detail in Sec. V D, the parameter $m\in\mathbb{R}$ is related to the Hawking mass of the foliation $t=\text{const}$, $r=\text{const}$. We will refer to those solutions as the generalized Kottler and the generalized Nariai solutions. The constant Λ is an arbitrary real number, but in this paper we will mostly be interested in $\Lambda<0$, and this assumption will be made unless explicitly stated otherwise. There has been recently renewed interest in the black hole aspects of the generalized Kottler solutions.[4–7] The object of this paper is to initiate a systematic study of static solutions of the vacuum Einstein equations with a negative cosmological constant.

The first question that arises here is that of asymptotic conditions one wants to impose. In the present paper we consider metrics which tend to the generalized Kottler solutions, leaving the

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asymptotically Nariai case to future work. We present the following three approaches to asymptotic structure, and study their mutual relationships: three-dimensional conformal compactifications, four-dimensional conformal completions, and a coordinate approach. We show that under rather natural hypotheses the conformal boundary at infinity is connected.

The next question we address is that of the definition of mass for such solutions, *without assuming staticity* of the metrics. We review again the possible approaches that occur here: a naive coordinate approach, a Hamiltonian approach, a ''Komar-type'' approach, and the Hawking approach. We show that the Hawking mass converges to a finite value for the metrics considered here, and we also give conditions on the conformal completions under which the ''coordinate mass,'' or the Hamiltonian mass, are finite. Each of those masses come with different normalization factor, whenever all are defined, except for the Komar and Hamiltonian masses which coincide. We suggest that the correct normalization is the Hamiltonian one.

Returning to the static case, we recall that appropriately behaved vacuum black holes with $\Lambda=0$ are completely described by the parameter m appearing above,[8–10] and it is natural to enquire whether this remains true for other values of Λ. In fact, for $\Lambda<0$, Boucher, Gibbons, and Horowitz[11] have given arguments suggesting uniqueness of the anti-de Sitter solution within an appropriate class. As a step towards a proof of a uniqueness theorem in the general case we derive, under appropriate hypotheses (1) lower bounds on (loosely speaking) the area of cross sections of the horizon, and (2) upper bounds on the mass of static vacuum black holes with negative cosmological constant. When these inequalities are combined the result goes precisely the opposite way as a (conjectured) generalization of the Geroch–Huisken–Ilmanen–Penrose inequality[12–17] appropriate to spacetimes with nonvanishing cosmological constant. In fact, such a generalization was obtained by Gibbons[18] along the lines of Geroch,[13] and of Jang and Wald,[19] i.e., under the very stringent assumption of the global existence and smoothness of the inverse mean curvature flow, see Sec. VI. We note that it is far from clear that the arguments of Huisken and Ilmanen,[14,15] or those of Bray,[16,17] which establish the original Penrose conjecture can be adapted to the situation at hand. If this were the case, a combination of this inequality with the results of the present work would give a fairly general uniqueness result. In any case this part of our work demonstrates the usefulness of a generalized Penrose inequality, if it can be established at all.

To formulate our results more precisely, consider a static spacetime $(M,{}^4g)$ which might—but does not have to—contain a black hole region. In the asymptotically flat case there exists a well-established theory (see Ref. 20, or Ref. 10, Secs. 2 and 6 and references therein) which, under appropriate hypotheses, allows one to reduce the study of such spacetimes to the problem of finding all suitable triples (Σ,g,V), where (Σ,g) is a three-dimensional Riemannian manifold and V is a *non-negative* function on Σ. Further V is required to vanish precisely on the boundary of Σ, when nonempty:

$$V\geqslant 0, \quad V(p)=0\Leftrightarrow p\in\partial\Sigma. \tag{I.3}$$

Finally g and V satisfy the following set of equations on Σ:

$$\Delta V=-\Lambda V, \tag{I.4}$$

$$R_{ij}=V^{-1}D_iD_jV+\Lambda g_{ij} \tag{I.5}$$

($\Lambda=0$ in the asymptotically flat case). Here R_{ij} is the Ricci tensor of the (''three-dimensional'') metric g. We shall not attempt to formulate the conditions on $(M,{}^4g)$ which will allow one to perform such a reduction [some of the aspects of the relationship between (Σ,g,V) and the associated spacetime are discussed in Sec. III B], but we shall directly address the question of properties of solutions of (I.4)–(I.5). Our first main result concerns the topology of $\partial\Sigma$ (cf. Theorem IV.1, Sec. IV; compare Refs. 21 and 22):

Theorem I.1: Let $\Lambda<0$, consider a set (Σ,g,V) which is C^3 conformally compactifiable in the sense of Definition III.1 below, suppose that (I.3)–(I.5) hold. Then the conformal boundary at infinity $\partial_\infty\Sigma$ of Σ is connected.

Our second main result concerns the Hawking mass of the level sets of V, cf. Theorem V.2, Sec. V D:

Theorem I.2: Under the conditions of Theorem I.1, the Hawking mass m of the level sets of V is well defined and finite.

It is natural to enquire whether there exist static vacuum spacetimes with complete spacelike hypersurfaces and no black hole regions; it is expected that no such solutions exist when $\Lambda<0$ and $\partial_\infty\Sigma\neq S^2$. We hope that points (2) and (3) of the following theorem can be used as a tool to prove their nonexistence.

Theorem I.3: Under the conditions of Theorem I.1, suppose further that $\partial\Sigma=\varnothing$, and that the scalar curvature R' of the metric $g'=V^{-2}g$ is constant on $\partial_\infty\Sigma$. Then

(1) If $\partial_\infty\Sigma$ is a sphere, then the Hawking mass m of the level sets of V is nonpositive, vanishing if and only if there exists a diffeomorphism $\psi:\Sigma\to\Sigma_0$ and a positive constant λ such that $g=\psi^*g_0$ and $V=\lambda V_0\circ\psi$, with (Σ_0, g_0, V_0) corresponding to the anti-de Sitter space–time.
(2) If $\partial_\infty\Sigma$ is a torus, then the Hawking mass m is strictly negative.
(3) If the genus g_∞ of $\partial_\infty\Sigma$ is higher than or equal to 2, we have

$$m<-\frac{1}{3\sqrt{-\Lambda}}, \tag{I.6}$$

with $m=m(V)$ normalized as in Eq. (VI.7).

A mass inequality similar to that in point (1) above has been established in Ref. 11, and in fact we follow their technique of proof. However, our hypotheses are rather different. Further, the mass here is *a priori* different from the one considered in Ref. 11; in particular it is not clear at all whether the mass defined as in Ref. 11 is also defined for the metrics we consider, cf. Secs. III C and V A below.

We note that metrics satisfying the hypotheses of point (2) above, with arbitrarily large (strictly) negative mass, have been constructed in Ref. 23.

As a straightforward corollary of Theorem I.3 one has

Corollary I.4: Suppose that the generalized positive energy inequality $m\geqslant m_{\mathrm{crit}}(g_\infty)$ holds in the class of three-dimensional manifolds (Σ,g) which satisfy the requirements of point (1) of Definition III.1 with a connnected conformal infinity $\partial_\infty\Sigma$ of genus g_∞, and, moreover, the scalar curvature R of which satisfies $R\geqslant 2\Lambda$. Then

(1) If $m_{\mathrm{crit}}(g_\infty=0)=0$, then the only solution of Eqs. (I.4)–(I.5) satisfying the hypotheses of point (1) of Theorem I.3 are data for anti-de Sitter space–time.
(2) If $m_{\mathrm{crit}}(g_\infty>1)=-1/(3\sqrt{-\Lambda})$, then there exist no solutions of Eqs. (I.4)–(I.5) satisfying the hypotheses of point (3) of Theorem I.3.

When $\partial_\infty\Sigma=S^2$ one expects that the inequality $m\geqslant 0$, with m being the mass defined by spinorial identities can be established using Witten-type techniques (cf. Refs. 24 and 25), regardless of whether or not $\partial\Sigma=\varnothing$. (On the other hand, it follows from Ref. 26 that when $\partial_\infty\Sigma\neq S^2$ there exist no asymptotically covariantly constant spinors which can be used in the Witten argument.) This might require imposing some further restrictions on, e.g., the asymptotic behavior of the metric. To be able to conclude in this case that there are no static solutions without horizons, or that the only solution with a connected nondegenerate horizon is the anti-de Sitter one, requires working out those restrictions, and showing that the Hawking mass of the level sets of V coincides with the mass occuring in the positive energy theorem.

When horizons occur, our comparison results for mass and area read as follows.

Theorem I.5: Under the conditions of Theorem I.1, suppose further that the genus g_∞ of $\partial_\infty\Sigma$ satisfies $g_\infty\geqslant 2$, and that the scalar curvature R' of the metric $g'=V^{-2}g$ is constant on $\partial_\infty\Sigma$. Let $\partial_1\Sigma$ be any connected component of $\partial\Sigma$ for which the surface gravity κ defined by Eq. (VII.1) is largest, and assume that

$$0<\kappa\leqslant\sqrt{-\frac{\Lambda}{3}}. \tag{I.7}$$

Let m_0, respectively A_0, be the Hawking mass, respectively the area of $\partial\Sigma_0$, for that generalized Kottler solution (Σ_0,g_0,V_0), with the same genus g_∞, the surface gravity κ_0 of which equals κ. Then

$$m\leqslant m_0, \quad A_0(g_{\partial_1\Sigma}-1)\leqslant A(g_\infty-1), \tag{I.8}$$

where A is the area of $\partial_1\Sigma$ and $m=m(V)$ is the Hawking mass of the level sets of V. Further $m=m_0$ if and only if there exists a diffeomorphism $\psi:\Sigma\to\Sigma_0$ and a positive constant λ such that $g=\psi^* g_0$ and $V=\lambda V_0\circ\psi$.

The asymptotic conditions assumed in Theorems I.3 and I.5 are somewhat related to those of Refs. 27–29, 11. The precise relationships are discussed in Secs. III B and III C. Let us simply mention here that the condition that R' is constant on $\partial_\infty\Sigma$ is the (local) higher genus analog of the (global) condition in Refs. 28 and 29 that the group of conformal isometries of I coincides with that of the standard conformal completion of the anti-de Sitter space–time; the reader is referred to Proposition III.6 in Sec. III B for a precise statement.

We note that the hypothesis (I.7) is equivalent to the assumption that the generalized Kottler solution with the same value of κ has nonpositive mass; cf. Sec. II for a discussion. We emphasize, however, that we do not make any *a priori* assumptions concerning the sign of the mass of (Σ,g,V). Our methods do not lead to any conclusions for those values of κ which correspond to generalized Kottler solutions with positive mass.

With $m=m(V)$ normalized as in Eq. (VI.7), the inequality $m\leqslant m_0$ takes the following explicit form:

$$m\leqslant\frac{(\Lambda+2\kappa^2)\sqrt{\kappa^2-\Lambda}+2\kappa^3}{3\Lambda^2}, \tag{I.9}$$

while $A(g_\infty-1)\geqslant A_0(g_{\partial_1\Sigma}-1)$ can be explicitly written as

$$A(g_\infty-1)\geqslant 4\pi(g_{\partial_1\Sigma}-1)\left[\frac{\kappa+\sqrt{\kappa^2-\Lambda}}{\Lambda}\right]^2. \tag{I.10}$$

[The right-hand sides of Eqs. (I.9) and (I.10) are obtained by straightforward algebraic manipulations from (II.1) and (II.10).]

It should be pointed out that in Ref. 30 a lower bound for the area has also been established. However, while the bound there is sharp only for the generalized Kottler solutions with $m=0$, our bound is sharp for all Kottler solutions. On the other hand, in Ref. 30 it is not assumed that the space–time is static.

If the generalized Penrose inequality (which we discuss in some detail in Sec. VI) holds,

$$2M_{\mathrm{Haw}}(u)\geqslant\sum_{i=1}^{k}\left((1-g_{\partial_i\Sigma})\left(\frac{A_{\partial_i\Sigma}}{4\pi}\right)^{1/2}-\frac{\Lambda}{3}\left(\frac{A_{\partial_i\Sigma}}{4\pi}\right)^{3/2}\right) \tag{I.11}$$

(with the $\partial_i\Sigma$'s, $i=1,\ldots,k$, being the connected components of $\partial\Sigma$, the $A_{\partial_i\Sigma}$'s—their areas, and the $g_{\partial_i\Sigma}$'s—the genera thereof) we obtain uniqueness of solutions:

Corollary I.6: Suppose that the generalized Penrose inequality (I.11) holds in the class of three-dimensional manifolds (Σ,g) with scalar curvature R satisfying $R\geqslant 2\Lambda$, which satisfy the requirements of point (1) of Definition III.1 with a connnected conformal infinity $\partial_\infty\Sigma$ of genus $g_\infty>1$, and which have a compact connected boundary. Then the only static solutions of Eqs. (I.4)–(I.5) satisfying the hypotheses of Theorem I.5 are the corresponding generalized Kottler solutions.

II. THE GENERALIZED KOTTLER SOLUTIONS

We recall some properties of the solutions (I.1). Those solutions will be used as reference solutions in our arguments, so it is convenient to use a subscript 0 when referring to them. As already mentioned, we assume $\Lambda<0$ unless indicated otherwise. For $m_0\in\mathbb{R}$, let r_0 be the largest positive root of the equation[31]

$$V_0^2\equiv k-\frac{2m_0}{r}-\frac{\Lambda}{3}r^2=0. \tag{II.1}$$

We set

$$\Sigma_0=\{(r,v)|r>r_0,v\in{}^2M\},\quad g_0=\left(k-\frac{2m_0}{r}-\frac{\Lambda}{3}r^2\right)^{-1}dr^2+r^2\,d\Omega_k^2, \tag{II.2}$$

where, as before, $d\Omega_k^2$ denotes a metric of constant Gauss curvature k on a smooth two-dimensional compact manifold ${}^2M$. We denote the corresponding surface gravity by κ_0. [Recall that the surface gravity of a connected component of a horizon $N[X]$ is usually defined by the equation

$$(X^\alpha X_\alpha)_{,\mu}|_{N[X]}=-2\kappa X_\mu, \tag{II.3}$$

where X is the Killing vector field which is tangent to the generators of $N[X]$. This requires normalizing X; here we impose the normalization[32] that $X=\partial/\partial t$ in the coordinate system of (I.1).] We set

$$W_0(r)\equiv g_0^{ij}D_iV_0D_jV_0=\left(\frac{m_0}{r^2}-\frac{\Lambda r}{3}\right)^2. \tag{II.4}$$

When $m_0=0$ we note the relationship

$$W_0=-\frac{\Lambda}{3}(V_0^2-k), \tag{II.5}$$

which will be useful later on, and which holds regardless of the topology of ${}^2M$.

Suppose, now, that $k=-1$, and that m_0 is in the range

$$m_0\in[m_{\rm crit},0], \tag{II.6}$$

where

$$m_{\rm crit}\equiv-\frac{1}{3\sqrt{-\Lambda}}. \tag{II.7}$$

Here $m_{\rm crit}$ is defined as the smallest value of m_0 for which the metrics (I.1) can be extended across a Killing horizon.[5,7] Let us show that Eq. (II.6) is equivalent to

$$r_0\in\left[\frac{1}{\sqrt{-\Lambda}},\sqrt{-\frac{3}{\Lambda}}\right]. \tag{II.8}$$

In order to simplify notation it is useful to introduce

$$\frac{1}{l^2}\equiv-\frac{\Lambda}{3}. \tag{II.9}$$

Now, the equation $V_0(l/\sqrt{3})=0$ implies $m=m_{\rm crit}$. Next, an elementary analysis of the function r^3/l^2-r-2m_0 (recall that $k=-1$ in this section) shows that (1) V has no positive roots for $m<m_{\rm crit}$; (2) for $m=m_{\rm crit}$ the only positive root is $l/\sqrt{3}$; (3) if r_0 is the largest positive root of the equation $V_0(r_0)=0$, then for each $m_0>m_{\rm crit}$ the radius $r_0(m_0)$ exists and is a differentiable function of m_0. Differentiating the equation $r_0V_0(r_0)=0$ with respect to m_0 gives

$$\left(\frac{3r_0^2}{l^2}+k\right)\frac{\partial r_0}{\partial m_0}=\left(\frac{3r_0^2}{l^2}-1\right)\frac{\partial r_0}{\partial m_0}=2.$$

It follows that for $r\geqslant l/\sqrt{3}$ the function $r_0(m_0)$ is a monotonically increasing function on its domain of definition $[m_{\rm crit},\infty)$, which establishes our claim.

We note that the surface gravity κ_0 is given by the formula

$$\kappa_0=\sqrt{W_0(r_0)}=\frac{m_0}{r_0^2}+\frac{r_0}{l^2}, \tag{II.10}$$

which gives

$$\frac{\partial\kappa_0}{\partial m_0}=\frac{1}{r_0^2}+\left(\frac{1}{l^2}-\frac{2m_0}{r_0^3}\right)\frac{\partial r_0}{\partial m_0}.$$

Equation (II.10) shows that κ_0 vanishes when $m_0=m_{\rm crit}$.[33] Under the hypothesis that $m_0\leqslant 0$, it follows from what has been said above (a) that $\partial\kappa_0/\partial m_0$ is positive; (b) that we have

$$\kappa_0\in\left[0,\sqrt{-\frac{\Lambda}{3}}\right], \tag{II.11}$$

when (II.6) holds, and (c) that, under the current hypotheses on k and Λ, (II.6) is equivalent to (II.11) for the metrics (I.1). While this can probably be established directly, we note that it follows from Theorem I.5 that (II.11) is equivalent to (II.6) without having to assume that $m_0\leqslant 0$.

In what follows we shall need the fact that in the above ranges of parameters the relationship $V_0(r)$ can be inverted to define a smooth function $r(V_0):[0,\infty)\to\mathbb{R}$. Indeed, the equation $(dV_0/dr)(r_{\rm crit})=0$ yields $r_{\rm crit}^3=3m_0/\Lambda$; when $k=-1$, $\Lambda<0$, and when (II.6) holds one finds $V_0(r_{\rm crit})\leqslant 0$, with the inequality being strict unless $m=m_{\rm crit}$. Therefore, $V_0(r)$ is a smooth strictly monotonic function in $[r_0,\infty)$, which implies in turn that $r(V_0)$ is a smooth strictly monotonic function on $(0,\infty)$; further $r(V_0)$ is smooth up to 0 except when $m=m_{\rm crit}$.

III. ASYMPTOTICS

A. Three-dimensional formalism

As a motivation for the definition below, consider one of the metrics (I.1) and introduce a new coordinate $x\in(0,x_0]$ by

$$\frac{r^2}{l^2}=\frac{1-kx^2}{x^2} \tag{III.1}$$

with x_0 defined by substituting r_0 at the left-hand side of (III.1). It then follows that

$$g=l^2x^{-2}\left[(1-kx^2)^{-1}\left(1-\frac{2mx^3}{l\sqrt{1-kx^2}}\right)^{-1}dx^2+(1-kx^2)d\Omega_k^2\right].$$

Thus the metric

$$g' \equiv (l^{-2}x^2)g$$

is smooth up to boundary metric on the compact manifold with boundary $\overline{\Sigma}_0 \equiv [0,x_0]\times {}^2M$. Furthermore, xV_0 can be extended by continuity to a smooth up to boundary function on $\overline{\Sigma}_0$, with $xV_0=1$. This justifies the following definition.

Definition III.1: Let Σ be a smooth manifold (all manifolds are assumed to be Hausdorff, paracompact, and orientable throughout), with perhaps a compact boundary which we denote by $\partial\Sigma$ when non empty.[34] Suppose that g is a smooth metric on Σ, and that V is a smooth nonnegative function on Σ, with $V(p)=0$ if and only if $p\in\partial\Sigma$.

(1) (Σ,g) will be said to be C^i, $i\in\mathbb{N}\cup\{\infty\}$, conformally compactifiable or, shortly, compactifiable, if there exists a C^{i+1} diffeomorphism χ from $\Sigma\backslash\partial\Sigma$ to the interior of a compact Riemannian manifold with boundary $(\overline{\Sigma}\approx\Sigma\cup\partial_\infty\Sigma,\overline{g})$, with $\partial_\infty\Sigma\cap\Sigma=\varnothing$, and a C^i function $\omega:\overline{\Sigma}\to\mathbb{R}^+$ such that

$$g=\chi^*(\omega^{-2}\overline{g}). \tag{III.2}$$

We further assume that $\{\omega=0\}=\partial_\infty\Sigma$, with $d\omega$ nowhere vanishing on $\partial_\infty\Sigma$, and that $\overline{g}$ is of C^i differentiability class on $\overline{\Sigma}$.

(2) A triple (Σ,g,V) will be said to be C^i, $i\in\mathbb{N}\cup\{\infty\}$, compactifiable if (Σ,g) is C^i compactifiable, and if $V\omega$ extends by continuity to a C^i function on $\overline{\Sigma}$,

(3) with

$$\lim_{\omega\to 0} V\omega > 0. \tag{III.3}$$

We emphasize that Σ itself is allowed to have a boundary on which V vanishes,

$$\partial\Sigma=\{p\in\Sigma\,|\,V(p)=0\}$$

If that is the case we will have

$$\partial\overline{\Sigma}=\partial\Sigma\cup\partial_\infty\Sigma.$$

The conditions above are not independent when the ''static field equations'' [Eqs. (I.4)–(I.5)] hold:

Proposition III.2: Consider a triple (Σ,g,V) satisfying Eqs. (I.3)–(I.5).

(1) The condition that $|d\omega|_{\overline{g}}$ has no zeros on $\partial_\infty\Sigma$ follows from the remaining hypotheses of point 1 of Definition III.1, when those hold with $i\geqslant 2$.

(2) Suppose that (Σ,g) is C^i compactifiable with $i\geqslant 2$. Then $\lim_{\omega\to 0}V\omega$ exists. Further, one can choose a (uniquely defined) conformal factor so that ω is the $\overline{g}$ distance from $\partial_\infty\Sigma$. With this choice of conformal factor, when (III.3) holds a necessary condition that (Σ,g,V) is C^i compactifiable is that

$$(4\overline{R}_{ij}-\overline{R}\overline{g}_{ij})\overline{n}^i\overline{n}^j|_{\partial_\infty\Sigma}=0, \tag{III.4}$$

where $\overline{n}$ is the field of unit normals to $\partial_\infty\Sigma$.

(3) (Σ,g,V) is C^∞ compactifiable if and only if (Σ,g) is C^∞ compactifiable and Eqs. (III.3) and (III.4) hold.

Remarks: (1) When (Σ,g) is C^∞ compactifiable but Eq. (III.4) does not hold, the proof below shows that $V\omega$ is of the form $\alpha_0+\alpha_1\omega^2\log\omega$, for some smooth up-to-boundary functions α_0 and α_1. This is perhaps not so surprising because the nature of the equations satisfied by g and V

suggests that both $\overline{g}$ and $V\omega$ should be polyhomogeneous, rather than smooth. (''Polyhomogeneous'' means that $\overline{g}$ and $V\omega$ are expected to admit asymptotic expansions in terms of powers of ω and $\log\omega$ near $\partial_\infty\Sigma$ under some fairly weak conditions on their behavior at $\partial_\infty\Sigma$; cf., e.g., Ref. 36 for precise definitions and related results.) From this point of view the hypothesis that (Σ,g) is C^∞ compactifiable is somewhat unnatural and should be replaced by that of polyhomogeneity of $\overline{g}$ at $\partial_\infty\Sigma$.

(2) One can prove appropriate versions of point (3) above for (Σ,g)'s which are C^i compactifiable for finite i. This seems to lead to lower differentiability of $1/V$ near $\partial_\infty\Sigma$ as compared to $\overline{g}$, and for this reason we shall not discuss it here.

(3) We leave it as an open problem whether or not there exist solutions of (I.3)–(I.5) such that (Σ,g) is smoothly compactifiable, such that V can be extended by continuity to a smooth function on $\overline{\Sigma}$, while (III.3) does not hold.

(4) We note that (III.4) is a conformally invariant condition because ω and $\overline{g}$ are uniquely determined by g. However, it is not conformally covariant, in the sense that if $\overline{g}$ is conformally rescaled, then (III.4) will not be of the same form in the new rescaled metric. It would be of interest to find a form of (III.4) which does not have this drawback.

(5) The result above has counterparts for one-point compactifications in the asymptotically flat case (cf., e.g., the theorem in the Appendix of Ref. 35.)

Proof: Let $\alpha\equiv V\omega$. After suitable identifications we can without loss of generality assume that the map χ in (III.2) is the identity. Equations (I.4)–(I.5) together with the definition of $\overline{g}=\omega^2 g$ lead to the following:

$$\overline{\Delta}\alpha-3\frac{\overline{D}^i\omega\overline{D}_i\alpha}{\omega}+\left(\frac{\overline{\Delta}\omega}{\omega}+\frac{\overline{R}}{2}\right)\alpha=0, \tag{III.5}$$

$$\overline{D}_i\overline{D}_j\alpha-\frac{\overline{D}^k\omega\overline{D}_k\alpha}{\omega}\overline{g}_{ij}=\left(\overline{R}_{ij}+2\frac{\overline{D}_i\overline{D}_j\omega}{\omega}-\left(\frac{\overline{\Delta}\omega}{\omega}+\frac{\overline{R}}{2}\right)\overline{g}_{ij}\right)\alpha. \tag{III.6}$$

We have also used $R=2\Lambda$ which, together with the transformation law of the curvature scalar under conformal transformations, implies

$$\omega^2\overline{R}=6|d\omega|^2_{\overline{g}}+2\Lambda-4\omega\overline{\Delta}\omega. \tag{III.7}$$

In all the equations here barred quantities refer to the metric $\overline{g}$. Point (1) of the proposition follows immediately from Eq. (III.7).

To avoid factors of $-\Lambda/3$ in the remainder of the proof we rescale the metric g so that $\Lambda=-3$. Next, to avoid annoying technicalities we shall present the proof only for smoothly compactifiable (Σ,g), i.e., for $i=\infty$; the finite i cases can be handled using the results in Ref. 36, Appendix A and Ref. 37, Appendix A. Suppose, thus, that $i=\infty$. As shown in Ref. 38, Lemma 2.1 we can choose ω and $\overline{g}$ so that ω coincides with the $\overline{g}$ distance from $\partial_\infty\Sigma$ in a neighborhood of $\partial_\infty\Sigma$; we shall use the symbol x to denote this function. In this case we have

$$\overline{\Delta}\omega=\overline{p}, \tag{III.8}$$

where $\overline{p}$ is the mean curvature of the level sets of $\omega=x$. Further $|d\omega|^2_{\overline{g}}=1$ so that (III.8) together with (III.7) give $\overline{R}=-4\overline{p}/x$, in particular $\overline{p}|_{x=0}=0$. We can introduce Gauss coordinates (x^1,x^A) near $\partial_\infty\Sigma$ in which $x^1=x\in[0,x_0)$, while the $(x^A)=v$'s form local coordinates on $\partial_\infty\Sigma$, with the metric taking the form

$$\overline{g}=dx^2+\overline{h},\quad \overline{h}(\partial_x,\cdot)=0. \tag{III.9}$$

To prove point (2), from Eq. (III.6) we obtain

$$\omega\overline{D}^i\omega\overline{D}^j\omega\overline{D}_i(\omega^{-1}\overline{D}_j\alpha)=\overline{D}^i\omega\overline{D}^j\omega\left(\overline{R}_{ij}+2\frac{\overline{D}_i\overline{D}_j\omega}{\omega}-\left(\frac{\overline{\Delta}\omega}{\omega}+\frac{\overline{R}}{2}\right)\overline{g}_{ij}\right)\alpha. \tag{III.10}$$

Equations (III.8)–(III.10) lead to

$$x\partial_x(x^{-1}\partial_x\alpha)=\left(\overline{R}_{xx}-\frac{\overline{R}}{4}\right)\alpha. \tag{III.11}$$

At each $v\in\partial_\infty\Sigma$ this is an ODE of Fuchsian type for $\alpha(x,v)$. Standard results about such equations show that for each v the functions $x\to\alpha(x,v)$ and $x\to\partial_x\alpha(x,v)$ are bounded and continuous on $[0,x_0)$. Integrating (III.11) one finds

$$\partial_x\alpha=x\beta(v)+\left(\overline{R}_{xx}-\frac{\overline{R}}{4}\right)\alpha(0,v)x\ln x+O(x^2\ln x), \tag{III.12}$$

where $\beta(v)$ is a (v-dependent) integration constant. By hypothesis there exist no points at $\partial_\infty\Sigma$ such that $\alpha(0,v)=0$, Eqs. (III.11) and (III.12) show that $\partial_x^2\alpha$ blows up at $x=0$ unless (III.4) holds, and point (2) follows.

We shall only sketch the proof of point (3): Standard results about Fuchsian equations show that solutions of Eq. (III.11) will be smooth in x whenever $[\overline{R}_{xx}-(\overline{R}/4)](x=0,v)$ vanishes throughout $\partial_\infty\Sigma$. A simple bootstrap argument applied to Eq. (III.6) with $(ij)=(1A)$ shows that α is also smooth in v. Commuting Eq. (III.6) with $(x\partial_x)^i\partial_v^\beta$, where β is an arbitrary multi-index, and iteratively repeating the reasoning outlined above establishes smoothness of α jointly in v and x. □

A consequence of condition (3) of Definition III.1 is that the function

$$V'\equiv V^{-1},$$

when extended to $\overline{\Sigma}$ by setting $V'=0$ on $\partial_\infty\Sigma$, can be used as a compactifying conformal factor, at least away from $\partial\Sigma$: If we set

$$g'=V^{-2}g,$$

then g' is a Riemannian metric smooth up to boundary on $\overline{\Sigma}\setminus\partial\Sigma$. In terms of this metric Eqs. (I.4)–(I.5) can be rewritten as

$$\Delta' V'=3V'W+\Lambda V, \tag{III.13}$$

$$R'_{ij}=-2VD'_iD'_jV'. \tag{III.14}$$

Here R'_{ij} is the Ricci tensor of the metric g', D' is the Levi-Civita covariant derivative associated with g', while Δ' is the Laplace operator associated with g'. Taking the trace of (III.14) and using (III.13) we obtain

$$R'=-6W-2\Lambda V^2, \tag{III.15}$$

where

$$W\equiv D_iVD^iV. \tag{III.16}$$

Defining

$$W'\equiv g'^{ij}D'_iV'D'_jV'=(V')^2W, \tag{III.17}$$

Eq. (III.15) can be rewritten as

$$6W' = -2\Lambda - R'(V')^2. \tag{III.18}$$

If (Σ, g, V) is C^2 compactifiable then R' is bounded in a neighborhood of $\partial_\infty\Sigma$, and since V blows up at $\partial_\infty\Sigma$ it follows from Eq. (III.15) that so does W, in particular W is strictly positive in a neighborhood of $\partial_\infty\Sigma$. Further Eq. (III.18) implies that the level sets of V are smooth manifolds in a neighborhood of $\partial_\infty\Sigma$, diffeomorphic to $\partial_\infty\Sigma$ there.

Equations (I.4)–(I.5) are invariant under a rescaling $V \to \lambda V$, $\lambda \in \mathbb{R}^*$. This is related to the possibility of choosing freely the normalization of the Killing vector field in the associated space–time. Similarly the conditions of Definition III.1 are invariant under such rescalings with $\lambda > 0$. For various purposes—e.g., for the definition (VII.1) of surface gravity—it is convenient to have a unique normalization of V. We note that if (Σ, g, V) corresponds to a generalized Kottler solution (Σ_0, g_0, V_0), then (I.1) and (II.4) together with (III.16) give $6W'_0 = -2\Lambda(1-k(V'_0)^2) + O((V'_0)^3)$ so that from (III.15) one obtains

$$R'_0|_{\partial_\infty\Sigma} = -2\Lambda k. \tag{III.19}$$

We have the following:

Proposition III.3: Consider a C^i-compactifiable triple (Σ, g, V), $i \geqslant 3$, satisfying equations (I.4)–(I.5).

(1) We have
$$^2\mathcal{R}'|_{x=0} = \tfrac{1}{3}R'|_{x=0}, \tag{III.20}$$
where $^2\mathcal{R}'$ is the scalar curvature of the metric induced by $g' \equiv V^{-2}g$ on the level sets of V, and R' is the Ricci scalar of g'.

(2) If R' is constant on $\partial_\infty\Sigma$, replacing V by a positive multiple thereof if necessary we can achieve
$$R'|_{\partial_\infty\Sigma} = -2\Lambda k, \tag{III.21}$$
where $k = 0$, 1 or -1 according to the sign of the Gauss curvature of the metric induced by g' on $\partial_\infty\Sigma$.

Remark: When $k = 0$ Eq. (III.21) holds with an arbitrary normalization of V.

Proof: Consider a level set $\{V = \text{const}\}$ of V which is a smooth hypersurface in $\overline{\Sigma}$, with unit normal n_i, induced metric h_{ij}, scalar curvature $^2\mathcal{R}$, second fundamental form p_{ij} defined with respect to an inner pointing normal, mean curvature $p = h^{ij}p_{ij} = h^k_i h^m_j D_{(k}n_{m)}$; we denote by q_{ij} the trace-free part of p_{ij}: $q_{ij} = p_{ij} - 1/2 h_{ij}p$. Let R_{ijk}, respectively, R'_{ijk}, be the Cotton tensor of the metric g_{ij}, respectively, g'_{ij}; by definition

$$R_{ijk} = 2(R_{i[j} - \tfrac{1}{4}Rg_{i[j})_{;k]}, \tag{III.22}$$

where square brackets denote antisymmetrization with an appropriate combinatorial factor (1/2 in the equation above), and a semicolon denotes covariant differentiation. We note the useful identity due to Lindblom[39]

$$R'_{ijk}R'^{ijk} = V^6 R_{ijk}R^{ijk} = 8(VW)^2 q_{ij}q^{ij} + V^2 h^{ij}D_i W D_j W. \tag{III.23}$$

When (Σ, g, V) is C^3 compactifiable the function $R'_{ijk}R'^{ijk}$ is uniformly bounded on a neighborhood of $\overline{\Sigma}$, which gives

$$(VW)^2 q_{ij}q^{ij} \leqslant C \tag{III.24}$$

in that same neighborhood, for some constant C. Equations (III.24) and (III.17) give

$$|q|_g = O((V')^3). \tag{III.25}$$

Let q'_{ij} be the trace-free part of the second fundamental form p'_{ij} of the level sets of V' with respect to the metric g'_{ij}, defined with respect to an inner pointing normal; we have $q'_{ij} = q_{ij}/V$, so that

$$|q'|_{g'} = O((V')^2). \tag{III.26}$$

Throughout we use $|\cdot|_k$ to denote the norm of a tensor field with respect to a metric k.

Let us work out some implications of (III.26); Eqs. (III.13)–(III.15) lead to

$$\left(\Delta' + \frac{R'}{2}\right) V' = 0. \tag{III.27}$$

Equations (III.17) and (III.18) show that dV' is nowhere vanishing on a suitable neighborhood of $\partial_\infty \Sigma$. We can thus introduce coordinates there so that $V' = x$. If the remaining coordinates are Lie dragged along the integral curves of ∂_x the metric takes the form

$$g' = (W')^{-1}\, dx^2 + h', \quad h'(\partial_x, \cdot) = 0. \tag{III.28}$$

Equations (III.27)–(III.28) give then

$$p' = -\frac{1}{2\sqrt{W'}}\left(\frac{\partial W'}{\partial x} + R'x\right) = \frac{x}{12\sqrt{W'}}\left(4R' - x\frac{\partial R'}{\partial x}\right), \tag{III.29}$$

and in the second step we have used (III.18). Here $p' = \sqrt{W'}\partial_x(\sqrt{\det h'})/\sqrt{\det h'}$ is the mean curvature of the level sets of x measured with respect to the inner pointing normal $n' = \sqrt{W'}\partial_x$. Equation (III.14) implies

$$R'_{ij} n'^i n'^j = -2Vn'^i n'^j D'_i D'_j V' = -2\frac{D'^i V' D'^j V'}{V'W'} D'_i D'_j V' = -\frac{D'^i V' D'_i W'}{V'W'} = \frac{-\partial_x W'}{x}$$

in the coordinate system of Eq. (III.28). From (III.18) we get

$$R'_{ij} n'^i n'^j = \frac{R'}{3} + O(x). \tag{III.30}$$

From the Codazzi–Mainardi equation,

$$(-2R'_{ij} + R' g'_{ij}) n'^i n'^j = {}^2\mathcal{R}' + q'_{ij} q'^{ij} - \tfrac{1}{2} p'^2, \tag{III.31}$$

where ${}^2\mathcal{R}'$ is the scalar curvature of the metric induced by g' on $\partial_\infty \Sigma$, one obtains

$$(-2R'_{ij} + R' g'_{ij}) n'^i n'^j = {}^2\mathcal{R}' + O(x), \tag{III.32}$$

where we have used (III.26) and (III.29). This, together with Eq. (III.30), establishes Eq. (III.20). In particular $R'|_{\partial_\infty \Sigma}$ is constant if and only if ${}^2\mathcal{R}'$ is, and R' at $x = 0$ has the same sign as the Gauss curvature of the relevant connected component of $\partial_\infty \Sigma$. Under a rescaling $V \to \lambda V$, $\lambda > 0$, we have $W \to \lambda^2 V$; Eq. (III.15) shows that $R' \to \lambda^2 R'$, and choosing λ appropriately establishes the result. □

We do not know whether or not there exist smoothly compactifiable solutions of Eqs. (I.4)–(I.5) for which R' is not locally constant at $\partial_\infty \Sigma$, it would be of interest to settle this question.

B. Four-dimensional conformal approach

Consider a space–time $(M,{}^4g)$ of the form $M=\mathbb{R}\times\Sigma$ with the metric ${}^4g$

$$ {}^4g=-V^2\,dt^2+g,\quad g(\partial_t,\cdot)=0,\quad \partial_t V=\partial_t g=0. \tag{III.33}$$

By definition of a space–time ${}^4g$ has Lorentzian signature, which implies that g has signature $+3$; it then naturally defines a Riemannian metric on Σ which will still be denoted by g. Equations (I.4)–(I.5) are precisely the vacuum Einstein equations with cosmological constant Λ for the metric ${}^4g$. It has been suggested that an appropriate[28,29] framework for asymptotically anti-de Sitter space–times is that of conformal completions introduced by Penrose.[40] The work of Friedrich[41] has confirmed that it is quite reasonable to do that, by showing that a large class of space–times (not necessarily stationary) with the required properties exist; some further related results can be found in Refs. 42 and 43. In this approach one requires that there exists a space–time with boundary $(\overline{M},{}^4\overline{g})$ and a positive function $\Omega:\overline{M}\to\mathbb{R}^+$, with Ω vanishing precisely at $\mathrm{I}\subset\partial\overline{M}$, and with $d\Omega$ without zeros on I, together with a diffeomorphism $\Xi:M\to\overline{M}\backslash I$ such that

$$ {}^4g=\Xi^*(\Omega^{-2}\,{}^4\overline{g}). \tag{III.34}$$

The vector field $X=\partial_t$ is a Killing vector field for the metric (III.33) on M, and it is well known (cf., e.g., Ref. 44, Appendix B) that X extends as smoothly as the metric allows to I; we shall use the same symbol to denote that extension. We have the following trivial observation.

Proposition III.4: Assume that (Σ,g,V) is smoothly compactifiable, then $M=\mathbb{R}\times\Sigma$ with the metric (III.33) has a smooth conformal completion with I diffeomorphic to $\mathbb{R}\times\partial_\infty\Sigma$. Further $(M,{}^4g)$ satisfies the vacuum equations with a cosmological constant Λ if and only if Eqs. (I.4)–(I.5) hold.

The implication the other way around requires some more work.

Theorem III.5: Consider a space–time $(M,{}^4g)$ of the form $M=\mathbb{R}\times\Sigma$, with a metric ${}^4g$ of the form (III.33), and suppose that there exists a smooth conformal completion $(\overline{M},{}^4\overline{g})$ with nonempty I. Then

(1) X is timelike on I; in particular it has no zeros there;
(2) The hypersurfaces $t=\text{const}$ extend smoothly to I;
(3) (Σ,g,V) is smoothly compactifiable;
(4) there exists a (perhaps different) conformal completion of $(M,{}^4g)$, still denoted by $(\overline{M},{}^4\overline{g})$, such that $\overline{M}=\mathbb{R}\times\overline{\Sigma}$, where $(\overline{\Sigma},\overline{g})$ is a conformal completion of (Σ,g), with $X=\partial_t$ and with

$$ {}^4\overline{g}=-\alpha^2\,dt^2+\overline{g},\quad \overline{g}(\partial_t,\cdot)=0,\quad X(\alpha)=\mathcal{L}_X\overline{g}=0. \tag{III.35}$$

Remark: The new completion described in point (4) above will coincide with the original one if and only if the orbits of X are complete in the original completion.

Proof: As the isometry group maps M to M, it follows that X has to be tangent to I. On M we have ${}^4\overline{g}(X,X)>0$ hence ${}^4\overline{g}(X,X)\geqslant 0$ on I, and to establish point (1) we have to exclude the possibility that ${}^4\overline{g}(X,X)$ vanishes somewhere on I.

Suppose, first, that $X(p)=0$ for a point $p\in I$. Clearly X is a conformal Killing vector of ${}^4\overline{g}$. We can choose a neighborhood U of I so that X is strictly timelike on $U\backslash I$. There exists $\epsilon>0$ and a neighborhood $O\subset U$ of p such that the flow $\phi_t(q)$ of X is defined for all $q\in O$ and $t\in[-\epsilon,\epsilon]$. The ϕ_t's are local conformal isometries, and therefore map timelike vectors to timelike vectors. Since X vanishes at p the ϕ_t's leave p invariant. It follows that the ϕ_t's map causal curves through p into causal curves through p; therefore they map $\partial J^+(p)$ into itself. This implies that X is tangent to $\partial J^+(p)$. However this last set is a null hypersurface, so that every vector tangent to it is spacelike or null, which contradicts timelikeness of X on $\partial J^+(p)\cap U\neq\varnothing$. It follows that X has no zeros on I.

Suppose, next, that $X(p)$ is lightlike at p. There exists a neighborhood of p and a strictly positive smooth function ψ such that X is a Killing vector field for the metric ${}^4\overline{g}\psi^2$. Now the staticity condition

$$X_{[\alpha}\nabla_{\beta}X_{\gamma]}=0 \tag{III.36}$$

is conformally invariant, and therefore also holds in the ${}^4\overline{g}$ metric. We can thus use the Carter–Vishweshvara lemma[45,46] to conclude that the set $N=\{q\in\overline{M}|X(q)\neq 0\}\cap\partial\{{}^4\overline{g}(X,X)<0\}\neq\varnothing$ is a null hypersurface. By hypothesis there exists a neighborhood U of I in $\overline{M}$ such that $N\cap M\cap U=\varnothing$, hence $N\subset I$. This contradicts the fact[40] that the conformal boundary of a vacuum space–time with a strictly negative cosmological constant Λ is timelike. It follows that X cannot be lightlike on I either, and point (1) is established.

To establish point (2), we note that Eq. (III.36) together with point (1) show that the one-form

$$\lambda\equiv\frac{1}{{}^4\overline{g}_{\alpha\beta}X^{\alpha}X^{\beta}}\,{}^4\overline{g}_{\mu\nu}X^{\mu}\,dx^{\nu}$$

is a smooth closed one-form on a neighborhood O of I, hence on any simply connected open subset of O there exists a smooth function $\overline{t}$ such that $\lambda=d\overline{t}$. Now (III.33) shows that the restriction of λ to M is dt, which establishes our claim. From now on we shall drop the bar on $\overline{t}$, and write t for the corresponding time function on $\overline{M}$.

Let

$$\overline{\Sigma}=\overline{M}\cap\{t=0\},\quad \chi=\Xi|_{t=0},\quad \omega=\Omega|_{t=0},$$

where Ξ and Ω are as in (III.34); from Eq. (III.34) one obtains

$$g=\chi^*(\omega^{-2}\overline{g}),$$

which shows that $(\overline{\Sigma},\overline{g})$ is a conformal completion of (Σ,g). We further have $V^2\omega^2={}^4g(X,X)|_{t=0}\omega^2={}^4\overline{g}(X,X)|_{t=0}$, which has already been shown to be smoothly extendible to I^+ and strictly positive there, which establishes point (3).

There exists a neighborhood V of $\overline{\Sigma}$ in $\overline{M}$ on which a new conformal factor Ω can be defined by requiring $\Omega|_{t=0}=\omega$, $X(\Omega)=0$. Redefining ${}^4\overline{g}$ appropriately and making suitable identifications so that Ξ is the identity, Eq. (III.34) can then be rewritten on V as

$${}^4\overline{g}=-(V\Omega)^2\,dt^2+\Omega^2 g. \tag{III.37}$$

All the functions appearing in Eq. (III.37) are time independent. The new manifold $\overline{M}$ defined as $\overline{\Sigma}\times\mathbb{R}$ with the metric (III.37) satisfies all the requirements of point (4), and the proof is complete. □

In addition to the conditions described above, in Refs. 28 and 29 it was proposed to further restrict the geometries under consideration by requiring the group of conformal isometries of I to be the same as that of the anti-de Sitter space–time, namely the universal covering group of $O(2,3)$; cf. also Ref. 43 for further discussion. While there are various ways of adapting this proposal to our setup, we simply note that the requirement on the group of conformal isometries to be $O(2,3)$ or a covering thereof implies that the metric induced on I is locally conformally flat. Let us then see what are the consequences of the requirement of local conformal flatness of ${}^Ig$ in our context; this last property is equivalent to the vanishing of the Cotton tensor of the metric ${}^Ig$ induced by ${}^4\overline{g}$ on I. As has been discussed in detail in Sec. III A, we can choose the conformal factor Ω to coincide with V^{-1}, in which case Eq. (III.37) reads

$${}^4g'\equiv{}^4g/V^2=-dt^2+V^{-2}g=-dt^2+g', \tag{III.38}$$

with $g' \equiv V^{-2} g$ already introduced in Sec. III A. It follows that

$$ {}^I g \equiv {}^4 g'|_I = -dt^2 + h', \tag{III.39}$$

where h' is the metric induced on $\partial_\infty \Sigma \equiv I \cap \overline{\Sigma}$ by g'. Let ${}^I R_{ij}$ denote the Ricci tensor of ${}^I g$; from (III.39) we obtain

$$ {}^I R_{it} = 0, \quad {}^I R_{AB} = {}^2 \mathcal{R}_{AB}, \tag{III.40}$$

where ${}^2 \mathcal{R}_{AB}$ is the Ricci tensor of h'. In particular the xxA component of the Cotton tensor ${}^I R_{ijk}$ of ${}^I g$ satisfies

$$ {}^I R_{xxA} = -\frac{{}^2 \mathcal{R}_{,A}}{4}. $$

Point (1) of Proposition III.3, see Eq. (III.20), shows that the requirement of conformal flatness of ${}^I g$ implies that R' is constant on $\partial_\infty \Sigma$. Conversely, it is easily seen from (III.40) that a locally constant R'—or equivalently ${}^2 \mathcal{R}$—on $\partial_\infty \Sigma$ implies the local conformal flatness of ${}^I g$. We have therefore proved:

Proposition III.6: Let (Σ, g, V) be C^i conformally compactifiable, $i \geqslant 3$, and satisfy (I.3)–(I.5). The conformal boundary $\mathbb{R} \times \partial_\infty \Sigma$ of the space–time $(M = \mathbb{R} \times \Sigma, {}^4 g)$, ${}^4 g$ given by (III.33), is locally conformally flat if and only if the scalar curvature R' of the metric $V^{-2} g$ is locally constant on $\partial_\infty \Sigma$. This is equivalent to requiring that the metric induced by $V^{-2} g$ on $\partial_\infty \Sigma$ has locally constant Gauss curvature.

C. A coordinate approach

An alternative approach to the conformal one discussed above is by introducing preferred coordinate systems. As discussed in Ref. 27, Appendix D, coordinate approaches are often equivalent to conformal approaches when sufficiently strong hypotheses are made. We stress that this equivalence is a delicate issue when finite degrees of differentiability are assumed, as arguments leading from one approach to the other often involve constructions in which some differentiability is lost.

In any case, the coordinate approach has been used by Boucher, Gibbons, and Horowitz[11] in their argument for uniqueness of the anti-de Sitter metric within a certain class of static space–times. More precisely, in Ref. 11 one considers metrics which are asymptotic to generalized Kottler metrics with $k=1$ in the following strong sense: if g_0 denotes one of the metrics (I.1) with $k=1$, then one assumes that there exists a coordinate system (t, r, x^A) such that

$$\begin{aligned} g = g_0 &+ O(r^{-2}) dt^2 + O(r^{-6}) dr^2 + O(r) \,(\text{remaining differentials not involving } dr) \\ &+ O(r^{-1}) \,(\text{remaining differentials involving } dr). \end{aligned} \tag{III.41}$$

We note that in the uniqueness assertions of Ref. 11 one makes appeal to the positive energy theorem to conclude. Now we are not aware of a version of such a theorem which would hold without some further hypotheses on the behavior of the metric. For example, in such a theorem one is likely to require that the derivatives of the metric also fall off at some sufficiently high rates. In any case the argument presented in Ref. 11 seems to implicitly assume that the asymptotic behavior of g^{tt} described above is preserved under differentiation, so that the corrections terms in (III.41) give a vanishing contribution when calculating $|dV|_g^2 - |dV_0|_{g_0}^2$ and passing to the limit $r \to \infty$, with g_0—the anti-de Sitter metric. While it might well be possible that Eqs. (I.4)–(I.5) force the metrics satisfying (III.41) to have sufficiently good asymptotic properties to be able to justify this, or to apply a positive energy theorem,[47] this remains to be established.[48]

It is far from being clear whether or not a general metric of the form (III.41) has any well-behaved conformal completions. For example, the coordinate transformation (III.1) together

with a multiplication by the square of the conformal factor $\omega = x$ brings the metric (III.41) to one which can be continuously extended to the boundary, but if only (III.41) is assumed then the resulting metric will not be differentiable up to boundary on the compactified manifold in general. There could, however, exist coordinate systems which lead to better conformal behavior when Eqs. (I.4)–(I.5) are imposed.

In any case, it is natural to ask whether or not a metric satisfying the requirements of Sec. III A will have a coordinate representation similar to (III.41). A partial answer to this question is given by the following result; see Ref. 27 for a related discussion. While the conclusions in Ref. 27 appear to be weaker than ours, it should be stressed that in Ref. 27 staticity of the space–times under consideration is not assumed.

Proposition III.7: Let (Σ, g, V) be a C^i compactifiable solution of Eqs. (I.4)–(I.5), $i \geqslant 3$. Define a C^{i-2} function $\widetilde{k} = \widetilde{k}(x^A)$ on $\partial_\infty \Sigma$ by the formula

$$R'|_{\partial_\infty \Sigma} = -2\Lambda \widetilde{k}. \tag{III.42}$$

(1) Rescaling V by a positive constant if necessary, there exists a coordinate system (r, x^A) near $\partial_\infty \Sigma$ in which we have

$$V^2 = \frac{r^2}{l^2} + \widetilde{k}, \tag{III.43}$$

$$g = \left(\frac{r^2}{l^2} + \widetilde{k} - \frac{2\mu}{r} \right)^{-1} dr^2 + O(r^{-3}) dr\, dx^A + r^2 \check{h}_{AB} + O(r^{-1})) dx^A\, dx^B \tag{III.44}$$

(recall that $l^2 = -3\Lambda^{-1}$), for some r-independent smooth two-dimensional metric $\check{h}_{AB}$ with Gauss curvature equal to $\widetilde{k}$ and for some function $\mu = \mu(r, x^A)$. Further

$$\check{h}^{AB} g_{AB} = 2 \left(r^2 - \frac{\mu_\infty}{r} + O(r^{-2}) \right), \tag{III.45}$$

where $\check{h}^{AB}$ denotes the matrix inverse to $\check{h}_{AB}$ while

$$\mu_\infty \equiv \lim_{r \to \infty} \mu = \frac{l^3}{12} \left. \frac{\partial R'}{\partial x} \right|_{x=0}. \tag{III.46}$$

(2) If one moreover assumes that R' is locally constant on $\partial_\infty \Sigma$, then Eq. (III.44) can be improved to

$$g = \left(\frac{r^2}{l^2} + k - \frac{2\mu}{r} \right)^{-1} dr^2 + (r^2 \check{h}_{AB} + O(r^{-1})) dx^A\, dx^B, \tag{III.47}$$

with $\check{h}_{AB}$ having constant Gauss curvature $k = 0, \pm 1$ according to the genus of the connected component of $\partial_\infty \Sigma$ under consideration.

Remarks: (1) The function $(x, x^A) \to \mu(r = 1/x, x^A)$ is of differentiability class C^{i-3} on $\overline{\Sigma}$, with the function $(x, x^A) \to (\mu/r)(r = 1/x, x^A)$ being of differentiability class C^{i-2} on $\overline{\Sigma}$.

(2) In Eqs. (III.44) and (III.47) the error terms $O(r^{-j})$ satisfy

$$\partial_r^s \partial_{A_1} \cdots \partial_{A_t} O(r^{-j}) = O(r^{-j-s})$$

for $0 \leqslant s+t \leqslant i-3$.

(3) We emphasize that the function $\tilde{k}$ defined in Eq. (III.42) could *a priori* be x^A dependent. In such a case neither the definition of coordinate mass of Sec. V A nor the definition of Hamiltonian mass of Sec. V B apply.

(4) It seems that to be able to obtain (III.41), in addition to the hypothesis that R' is locally constant on $\partial_\infty \Sigma$ one would at least need the quantity appearing at the right-hand side of Eq. (III.46) to be locally constant on $\partial_\infty \Sigma$ as well. We do not know whether this is true in general; we have not investigated this question as this is irrelevant for our purposes.

Proof: Consider, near $\partial_\infty \Sigma$, the coordinate system of Eq. (III.28), from Eqs. (III.29) and (III.18) we obtain

$$\partial_x (\ln \sqrt{\det h'_{AB}}) = -2\tilde{k}x - \frac{3\mu_\infty}{l} x^2 + O(x^3), \tag{III.48}$$

l as in (II.9), $\tilde{k}$ as in (III.42), μ_∞ as in (III.46). This, together with Eq. (III.26), leads to

$$\frac{\partial h'_{AB}}{\partial x} = -2x\tilde{k} h'_{AB} + O(x^2) \Rightarrow h'_{AB} = (1-\tilde{k}x^2) l^2 \check{h}_{AB} + O(x^3),$$

where $\check{h}_{AB} \equiv (1/l^2)\, h'_{AB}|_{x=0}$. Proposition III.3 shows that $\tilde{k}$ is proportional to the Gauss curvature of $\check{h}_{AB}$. It follows now from (III.18) that

$$g = x^{-2} g' = \frac{l^2}{x^2}\left(1 - \frac{R' l^2 x^2}{6}\right)^{-1} dx^2 + \left\{ \frac{(1-\tilde{k}x^2)}{x^2} h'_{AB}|_{x=0} + O(x^3) \right\} dx^A\, dx^B.$$

The above suggests to introduce a coordinate r via the formula[49]

$$\frac{r^2}{l^2} = \frac{1-\tilde{k}x^2}{x^2}. \tag{III.49}$$

Suppose, first, that $\tilde{k}$ is locally constant on $\partial_\infty \Sigma$, then $\tilde{k}$ equals $k = 0, \pm 1$ according to the genus of the connected component of $\partial_\infty \Sigma$ under consideration, and one finds

$$\begin{aligned} g &= \left(\frac{r^2}{l^2} + k\right)^{-1} \left\{ 1 + \frac{l^2}{r^2}\left(k - \frac{R' l^2 x^2}{6}\right) \right\}^{-1} dr^2 + \left(\frac{r^2}{l^2} h'_{AB}|_{x=0} + O(r^{-1})\right) dx^A\, dx^B \\ &= \left(\frac{r^2}{l^2} + k - \frac{2\mu}{r}\right)^{-1} dr^2 + \left(\frac{r^2}{l^2} h'_{AB}|_{x=0} + O(r^{-1})\right) dx^A\, dx^B, \end{aligned}$$

where the ''mass aspect'' function $\mu = \mu(r, x^A)$ is defined as

$$\mu \equiv -\frac{r}{2}\left(1 + k\frac{l^2}{r^2}\right)\left(k - \frac{R' l^2 x^2}{6}\right) = -\frac{r}{2}\left(k - \frac{R' l^2}{6} + \frac{k^2 l^2}{r^2}\right) = \frac{r l^2}{2}\left(\frac{1}{6}(R' - R'|_{x=0}) - \frac{k^2}{r^2}\right). \tag{III.50}$$

This establishes Eqs. (III.43) and (III.47). When $\tilde{k}$ is not locally constant an identical calculation using the coordinate r defined in Eq. (III.49) establishes Eq. (III.44)—the only difference is the

occurrence of nonvanishing error terms in the $dr\,dx^A$ part of the metric, introduced by the angle dependence of $\tilde{k}$. It follows from Eq. (III.50)—or from the $\tilde{k}$ version thereof when $\tilde{k}$ is not locally constant—that

$$\mu=\frac{l^3}{12}\frac{\partial R'}{\partial x}\bigg|_{x=0}+O(r^{-1}),$$

which establishes Eq. (III.46). Equation (III.45) is obtained by integration of Eq. (III.48). □

IV. CONNECTEDNESS OF $\partial_\infty\Sigma$

The class of manifolds considered so far could in principle contain Σ's for which neither $\partial_\infty\Sigma$ nor $\partial\Sigma$ are connected. Under the hypothesis of staticity the question of connectedness of $\partial\Sigma$ is open; we simply note here the existence of dynamical (nonstationary) solutions of Einstein–Maxwell equations with a nonconnected black hole region with positive cosmological constant Λ.[50,51] As far as $\partial_\infty\Sigma$ is concerned, we have the following:

Theorem IV.1: Let (Σ,g,V) be a C^i compactifiable solution of Eqs. (I.4)–(I.5), $i\geqslant 3$. Then $\partial_\infty\Sigma$ is connected.

Proof: Consider the manifold $M=\mathbb{R}\times\Sigma$ with the metric (III.33); its conformal completion $\overline{M}=\mathbb{R}\times\overline{\Sigma}$ with the metric ${}^4g/V^2$ is a stably causal manifold with boundary. We wish to show that it is also globally hyperbolic in the sense of Ref. 4, namely that (1) it is strongly causal and (2) for each $p,q\in M$ the set $J^+(p)\cap J^-(q)$ is compact. The existence of the global time function t clearly implies strong causality, so it remains to verify the compactness condition. Now a path $\Gamma(s)=(t(s),\gamma(s))\in\mathbb{R}\times\Sigma$ is an achronal null geodesic from $p=(t(0),\gamma(0))$ to $q=(t(1),\gamma(1))$ if and only if $\gamma(s)$ is a minimizing geodesic between $\gamma(0)$ and $\gamma(1)$ for the ''optical metric'' $V^{-2}g$. Compactness of $J^+(p)\cap J^-(q)$ is then equivalent to compactness of the $V^{-2}g$ distance balls; this latter property will hold when $(\Sigma\cup\partial_\infty\Sigma,V^{-2}g)$ is a geodesically complete manifold (with boundary) by (an appropriate version of) the Hopf–Rinow theorem.

Let us thus show that $(\Sigma,V^{-2}g)$ is geodesically complete. Suppose, first, that $\partial\Sigma=\varnothing$; the hypothesis that Σ has compact interior together with the fact that V tends to infinity in the asymptotic regions implies that $V\geqslant V_0>0$ for some constant V_0. This shows that $(\Sigma,V^{-2}g)$ is a compact manifold with boundary $\partial_\infty\Sigma$, and the result follows. (When the metric induced by $V^{-2}g$ on $\partial_\infty\Sigma$ has positive scalar curvature connectedness of $\partial_\infty\Sigma$ can also be inferred from Ref. 21.)

Consider, next, the case $\partial\Sigma\neq\varnothing$. It is well known that $|dV|_g$ is a nonzero constant on every connected component of $\partial\Sigma$ [cf. the discussion around Eq. (VII.2)]; therefore we can introduce coordinates near $\partial\Sigma$ so that $V=x$, with the metric taking the form

$$V^{-2}g=x^{-2}((dx)^2+h_{AB}(x,x^A)dx^A\,dx^B), \tag{IV.1}$$

where the x^A's are local coordinates on $\partial\Sigma$. It is elementary to show now from (IV.1) that $(\Sigma\cup\partial_\infty\Sigma,V^{-2}g)$ is a complete manifold with boundary, as claimed.

When (Σ,g) is smoothly compactifiable we can now use Theorem 2.1 of Ref. 4 to infer connectedness of $\partial_\infty\Sigma$, compare Ref. 22, Corollary, Sec. III. For compactifications with finite differentiability we argue as follows: For small s let λ be the mean curvature of the sets $\{x=s\}$, where x is the coordinate of Eq. (III.9). In the coordinate system used there the unit normal to those sets pointing away from $\partial_\infty\Sigma$ equals $x\partial_x$; if (Σ,g,V) is C^3 compactifiable the tensor field $\overline{h}$ appearing in Eq. (III.9) will be C^1 so that[52]

$$\lambda=\frac{1}{\sqrt{\det g}}\partial_i(\sqrt{\det g}n^i)=\frac{x^3}{\sqrt{\det\overline{h}}}\partial_x(x^{-2}\sqrt{\det\overline{h}})=-2+O(x).$$

It follows that for s small enough the sets $\{x=s,t=\tau\}$ are trapped, with respect to the inward pointing normal, in the space–time $\mathbb{R}\times\Sigma$ with the metric (III.33). Suppose that $\partial_\infty\Sigma$ were not

connected, then those (compact) sets would be outer trapped with respect to every other connected component of $\partial_\infty\Sigma$. This is, however, not possible by the usual global arguments, cf., e.g., Refs. 53 and 54 or Ref. 37, Sec. 4 for details. □

V. THE MASS

A. A coordinate mass M_c

There exist several proposals how to assign a mass M to a space–time which is asymptotic to an anti-de Sitter space–time.[27,29,55,18,56] It seems that the simplest way to do that (as well as to extend the definition to the generalized Kottler context considered here) proceeds as follows: consider a metric defined on a coordinate patch covering the set

$$\Sigma_{\text{ext}}\equiv\{t=t_0, r\geqslant R, (x^A)\in {}^2M\} \tag{V.1}$$

(which we will call an ''end''), and suppose that in this coordinate system the functions $g_{\mu\nu}$ are of the form (I.1) plus lower order terms

$$\begin{gathered} g_{tt}=-\left(k-\frac{2m}{r}-\frac{\Lambda}{3}r^2\right)+\frac{o(1)}{r}, \quad g_{rr}=\left(k-\frac{2m}{r}-\frac{\Lambda}{3}r^2+\frac{o(1)}{r}\right)^{-1}, \\ g_{t\mu}=o(1), \quad \mu\neq t, \quad g_{r\mu}=o(1), \quad \mu\neq r, \quad g_{AB}-r^2h_{AB}=o(r^2), \end{gathered} \tag{V.2}$$

for some constant m, and for some constant curvature (t and r independent) metric $h_{AB}\,dx^A\,dx^B$ on ${}^2M$. Then we define the coordinate mass M_c of the end Σ_{ext} to be the parameter m appearing in (I.1). This procedure gives a unique prescription of how to assign a mass to a metric and a coordinate system on Σ_{ext}.

There is an obvious coordinate dependence in this definition when $k=0$: Indeed, in that case a coordinate transformation $r\to\lambda r$, $t\to t/\lambda$, $d\Omega_k^2\to\lambda^{-2}\,d\Omega_k^2$, where λ is a positive constant, does not change the asymptotic form of the metric, while m gets replaced by $\lambda^{-3}m$. When ${}^2M$ is compact this freedom can be removed, e.g., by requiring that the area of ${}^2M$ with respect to the metric $d\Omega_k^2$ be equal to 4π, or to 1, or to some other chosen constant. For $k=\pm 1$ this ambiguity does not arise because in this case such rescalings will change the asymptotic form of the metric, and are therefore not allowed.

It is far from being clear that the above definition will assign the same parameter M_c to every coordinate system satisfying our requirements: if that is the case, to prove such a statement one might perhaps need to further require that the coordinate derivatives of the coordinate components of g in the above described coordinate system have some appropriate decay properties; further one might perhaps have to replace the $o(1)$'s by $o(r^{-\sigma})$'s or $O(r^{-\sigma})$'s, for some appropriate σ's, perhaps as in (III.41); this is however irrelevant for our discussion at this stage.

A possible justification of this definition proceeds as follows: when ${}^2M=S^2$ and $\Lambda=0$ it is widely accepted that the mass of Σ_{ext} equals m, because m corresponds to the active gravitational mass of the gravitational field in a quasi-Newtonian limit. (It is also known in this case that the definition is coordinate independent.[57,58]) For $\Lambda\neq 0$ and/or ${}^2M\neq S^2$ one calls m the mass by analogy.

Consider, then, the metric (III.33), with V and g as in (III.43)–(III.44); suppose further that the limit

$$\mu_\infty\equiv\lim_{r\to\infty}\mu$$

exists and is a constant. To achieve the form of the metric ${}^4g$ just described one needs to replace the coordinate r of (III.43)–(III.44) with a new coordinate ρ defined as

$$r^2+k=\rho^2+k+\frac{\mu_\infty}{\rho}.$$

This leads to

$$
{}^4g = -\left(\frac{\rho^2}{l^2} + k + \frac{\mu_\infty}{\rho}\right) dt^2 + \left(\frac{\rho^2}{l^2} + k + \frac{\mu_\infty}{\rho} + O\left(\frac{1}{\rho^2}\right)\right)^{-1} d\rho^2
$$
$$
+ O(\rho^{-3}) d\rho\, dx^A + (\rho^2 \check{h}_{AB} + O(\rho^{-1})) dx^A\, dx^B, \tag{V.3}
$$

and therefore

$$
M_c \equiv -\frac{\mu_\infty}{2} = -\frac{l^3}{24} \left.\frac{\partial R'}{\partial x}\right|_{x=0}, \tag{V.4}
$$

where the second equality above follows from (III.46). We note that the approach described above does not give a definition of mass when $\lim_{r\to\infty}\mu$ does not exist, or is not a constant function on $\partial_\infty \Sigma$.

The above described dogmatic approach suffers from various shortcomings. First, when ${}^2M \neq S^2$, the arguments given are compatible with M_c being any function $M_c(m,\Lambda)$ with the property that $M_c(m,0)=m$. Next, the transition from $\Lambda \neq 0$ to $\Lambda = 0$ has dramatic consequences as far as global properties of the corresponding space–times are concerned, and one can argue that there is no reason why the function $M_c(m,\Lambda)$ should be continuous at zero. For example, according to Ref. 27, Eq. (III.8c), the mass of the metric (I.1) with ${}^2M = S^2$ should be $16\pi m l$, with l as in (II.9), which blows up when Λ tends to zero with m being held fixed. Finally, when ${}^2M \neq S^2$ the Newtonian limit argument does not apply because the metrics (I.1) with $\Lambda = 0$ and ${}^2M \neq S^2$ do not seem to have a Newtonian equivalent. In particular there is no reason why M_c should not depend upon the genus g_∞ of ${}^2M$ as well.

All the above arguments make it clear that a more fundamental approach to the definition of mass would be useful. It is common in field theory to define energy by Hamiltonian methods, and this is the approach we shall pursue in the next section.

B. The Hamiltonian mass M_{Ham}

The Hamiltonian approach allows one to define the energy from first principles. For a solution of the field equations, we can simply take as the energy the numerical value of the Hamiltonian. It must be recognized, however, that the Hamiltonians might depend on the choice of the phase space, if several such choices are possible, and they are defined only up to an additive constant on each connected component of the phase space. They also depend on the choice of the Hamiltonian structure, if more than one such structure exists.

Let us start by briefly recalling the results of the analysis of Ref. 59, based on the Hamiltonian approach of Kijowski and Tulczyjew,[60,61] see also Ref. 62. One assumes that a manifold M on which an (unphysical) background metric b is given, and one considers metrics ${}^4g$ which asymptote to b in the relevant asymptotic regions of M. We stress that the background metric is only a tool to prescribe the asymptotic boundary conditions, and does not have any physical significance. Let X be any vector field on M and let Σ be any hypersurface in M. By a well known procedure the motion of Σ along the flow of X can be used to construct a Hamiltonian dynamical system in an appropriate phase space of fields over Σ; the reader is referred to Refs. 60–63 for a geometric approach to this question. In Ref. 59 it is also assumed that X is a Killing vector field of the background metric; this is certainly not necessary (cf., e.g., Ref. 63 for general formulas), but is sufficient for our purposes, as we are going to take X to be equal to $\partial/\partial t$ in the coordinate system of Eq. (III.33). In the context of metrics which asymptote to the generalized Kottler metrics at large r, a rigorous functional description of the spaces involved has not been carried out so far, and lies outside the scope of this paper. Let us simply note that one expects, based on the results in Refs. 41, 42, and 63, to obtain a well-defined Hamiltonian system in this context. Therefore the formal calculations of Ref. 59 lead one to expect that on an appropriate space of fields, such that

the associated physical space–time metrics ${}^4g$ asymptote to the background metric b at a suitable rate, the Hamiltonian $H(X,\Sigma)$ will coincide with (or, at worse, will be closely related to) the one given by the formula derived in Ref. 59:

$$H(X,\Sigma)=\frac{1}{2}\int_{\partial\Sigma}\mathbb{U}^{\alpha\beta}\,dS_{\alpha\beta}, \tag{V.5}$$

where the integral over $\partial\Sigma$ should be understood as the limit as R tends to infinity of integrals of coordinate spheres $t=0$, $r=R$ on $\Sigma_{\rm ext}$. Here $dS_{\alpha\beta}$ is defined as

$$\frac{\partial}{\partial x^\alpha}\lrcorner\frac{\partial}{\partial x^\beta}\lrcorner \mathrm{d}x^0\wedge\cdots\wedge\mathrm{d}x^n,$$

with $\lrcorner$ denoting contraction, and $\mathbb{U}^{\alpha\beta}$ is given by

$$\mathbb{U}^{\nu\lambda}=\mathbb{U}^{\nu\lambda}{}_\beta X^\beta+\frac{1}{8\pi}\left(\sqrt{|\det g_{\rho\sigma}|}g^{\alpha[\nu}-\sqrt{|\det b_{\rho\sigma}|}b^{\alpha[\nu}\right)\delta^{\lambda]}_\beta X^\beta{}_{;\alpha}, \tag{V.6}$$

$$\mathbb{U}^{\nu\lambda}{}_\beta=\frac{2|\det b_{\mu\nu}|}{16\pi\sqrt{|\det g_{\rho\sigma}|}}g_{\beta\gamma}\left(e^2 g^{\gamma[\nu}g^{\lambda]\kappa}\right)_{;\kappa}. \tag{V.7}$$

Here, and *throughout this section*, g stands for the space–time metric ${}^4g$ unless explicitly indicated otherwise. Further, a semicolon denotes covariant differentiation *with respect to the background metric* b, while $e\equiv\sqrt{|\det g_{\rho\sigma}|}/\sqrt{|\det b_{\mu\nu}|}$. Some comments concerning Eq. (V.6) are in order: in Ref. 59 the starting point of the analysis is the Hilbert Lagrangian for vacuum Einstein gravity, $L=\sqrt{-\det g_{\mu\nu}}(g^{\alpha\beta}R_{\alpha\beta}/16\pi)$. As the normalization factors play an important role in giving a correct definition of mass, we recall that the factor $1/16\pi$ is determined by the requirement that the theory has the correct Newtonian limit (units $G=c=1$ are used throughout). With our signature $(-+++)$ the Einstein equations with a cosmological constant read

$$R_{\mu\nu}-\frac{g^{\alpha\beta}R_{\alpha\beta}}{2}g_{\mu\nu}=-\Lambda g_{\mu\nu},$$

so that one needs to repeat the analysis in Ref. 59 with L replaced by $(\sqrt{-\det g_{\mu\nu}}/16\pi)(g^{\alpha\beta}R_{\alpha\beta}-2\Lambda)$. The general expression for the Hamiltonian (V.5) in terms of X^μ, $g_{\mu\nu}$, and $b_{\mu\nu}$ ends up to coincide with that obtained with $\Lambda=0$, which can be seen either by direct calculations, or by the Legendre transformation arguments of Ref. 59, end of Sec. 3, together with the results in Ref. 62. Note that Eq. (V.6) does not exactly coincide with that derived in Ref. 59, as the formulas there do not contain the term $-\sqrt{|\det b_{\rho\sigma}|}b^{\alpha[\nu}\delta^{\lambda]}_\beta X^\beta{}_{;\alpha}$. However, this term does not depend on the metric g, and such terms can be freely added to the Hamiltonian because they do not affect the variational formula that defines a Hamiltonian. From an energy point of view such an addition corresponds to a choice of the zero point of the energy. We note that in our context $H(X,\Sigma)$ would not converge if the term $-\sqrt{|\det b_{\rho\sigma}|}b^{\alpha[\nu}\delta^{\lambda]}_\beta X^\beta{}_{;\alpha}$ were not present in (V.6).

In order to apply this formalism in our context, we let b be any t-independent metric on $M=\mathbb{R}\times\Sigma$ such that (with $0\neq\Lambda=-3/l^2$)

$$b=-\left(k+\frac{r^2}{l^2}\right)dt^2+\left(k+\frac{r^2}{l^2}\right)^{-1}dr^2+r^2\check{h} \tag{V.8}$$

on $\mathbb{R}\times\Sigma_{\rm ext}\approx\mathbb{R}\times[R,\infty)\times{}^2M$, for some $R\geqslant 0$, where $\check{h}=\check{h}_{AB}\,dx^A\,dx^B$ denotes a metric of constant Gauss curvature $k=0,\pm1$ on the two-dimensional connected compact manifold ${}^2M$.

Let us return to the discussion in Sec. V A concerning the freedom of rescaling the coordinate r by a positive constant λ. First, if k in Eq. (V.8) is any constant different from zero, then there

exists a (unique) rescaling of r and t which brings k to one, or to minus one. Next, if $k=0$ we can—without changing the asymptotic form of the metric—rescale the coordinate r by a positive constant λ, the coordinate t by $1/\lambda$, and the metric $\check{h}$ by λ^{-2}, so that there is still some freedom left in the coordinate system above; a unique normalization can then be achieved by asking, e.g., that the area

$$A_\infty \equiv \int_{^2M} d^2\mu_{\check{h}} \tag{V.9}$$

equals 4π—this will be the most convenient normalization for our purposes. Here $d^2\mu_{\check{h}}$ is the Riemannian measure associated with the metric $\check{h}$. We wish to point out that *regardless* of the value of k, the Hamiltonian $H(X,\Sigma)$ is *independent* of this scaling: this follows immediately from the fact that $\mathbb{U}^{\alpha\beta}$ behaves as a density under linear coordinate transformations. An alternative way of seeing this is that in the new coordinate system X equals $\lambda\partial/\partial t$, which accounts for a factor $1/\lambda$ in the transformation law of the coordinate mass, as discussed at the beginning of Sec. V A. The remaining factor $1/\lambda^2$ needed there is accounted for by a change of the area of $\partial_\infty\Sigma$ under the rescaling of the metric $\check{h}$ which accompanies that of r.

In order to evaluate H it is useful to introduce the following b-orthonormal frame:

$$e_{\hat{0}} = \left(k+\frac{r^2}{l^2}\right)^{-1/2}\partial_t, \quad e_{\hat{1}} = \left(k+\frac{r^2}{l^2}\right)^{1/2}\partial_r, \quad e_{\hat{A}} = \frac{1}{r}\check{e}_{\hat{A}}, \tag{V.10}$$

where $\check{e}_{\hat{A}}$ is an ON frame for the metric $\check{h}$. The connection coefficients, defined by the formula $\nabla_{e_{\hat{a}}} e_{\hat{b}} = \omega^{\hat{c}}{}_{\hat{b}\hat{a}} e_{\hat{c}}$, read

$$\omega_{\hat{0}\hat{1}\hat{0}} = -\frac{r}{l^2}\left(k+\frac{r^2}{l^2}\right)^{-1/2}, \quad \omega_{\hat{1}\hat{2}\hat{2}} = \omega_{\hat{1}\hat{3}\hat{3}} = -\frac{1}{r}\left(k+\frac{r^2}{l^2}\right)^{1/2},$$

$$\omega_{\hat{2}\hat{3}\hat{3}} = \begin{cases} -\dfrac{\coth\theta}{r}, & k=-1, \\ 0, & k=0, \\ -\dfrac{\cot\theta}{r}, & k=1. \end{cases} \tag{V.11}$$

Those connection coefficients which are not obtained from the above ones by permutations of indices are zero; we have used a coordinate system θ,φ on ^2M in which $\check{h}$ takes, locally, the form $d\theta^2+\sinh^2\theta\, d\varphi^2$ for $k=-1$, $d\theta^2+d\varphi^2$ for $k=0$, and $d\theta^2+\sin^2\theta\, d\varphi^2$ for $k=1$. We also have

$$X^{\hat{0}} = \sqrt{k+\frac{r^2}{l^2}} = \frac{r}{l}+O(r^{-1}), \quad e_{\hat{1}}(X^{\hat{0}}) = X^{\hat{0}}{}_{;\hat{1}} = -X_{\hat{0};\hat{1}} = X_{\hat{1};\hat{0}} = \frac{r}{l^2}, \tag{V.12}$$

all the remaining $X^{\hat{\mu}}$'s and $X_{\hat{\mu};\hat{\nu}}$'s are zero. Let the tensor field $e^{\mu\nu}$ be defined by the formula

$$e^{\mu\nu} \equiv g^{\mu\nu} - b^{\mu\nu}. \tag{V.13}$$

We shall use hatted indices to denote the components of a tensor field in the frame $e_{\hat a}$ defined in (V.10), e.g., $e^{\hat\alpha\hat c}$ denotes the coefficients of $e^{\mu\nu}$ with respect to that frame:

$$e^{\mu\nu}\partial_\mu\otimes\partial_\nu = e^{\hat\alpha\hat c} e_{\hat\alpha}\otimes e_{\hat c}\,.$$

Suppose that the metric ${}^4g$ is such that the $e^{\hat\alpha\hat c}$'s tend to zero as r tends to infinity. By a Gram–Schmidt procedure we can find a frame $f_{\tilde a}$, $\tilde a=0,\dots,3$, orthonormal *with respect to the metric* g, such that f_0 is proportional to e_0, and such that the $e_{\hat a}$ components of $f_0-e_0,\dots, f_3-e_3$ tend to zero as r tends to infinity:

$$f_{\tilde a} = f_{\tilde a}{}^{\hat a} e_{\hat a} \to_{r\to\infty} \delta^{\hat a}_{\tilde a} e_{\hat a}\,. \tag{V.14}$$

From (V.5) and (V.14) we expect that

$$H(X,\Sigma) = \lim_{R\to\infty}\int_{\Sigma\cap\{r=R\}} r^2 \mathbb{U}^{\hat1\hat0}\, d^2\mu_r\,, \tag{V.15}$$

where $d^2\mu_r$ is the Riemannian measure induced on $\Sigma\cap\{r=R\}$ by ${}^4g$. We wish to analyze when the above limit exists; we have

$$r^2\mathbb{U}^{\hat1\hat0}{}_\beta X^\beta = r^2\mathbb{U}^{\hat1\hat0}{}_{\hat0}X^{\hat0} \approx \frac{r^3}{l}\mathbb{U}^{\hat1\hat0}{}_{\hat0}\,,$$

hence we need to keep track of all the terms in $\mathbb{U}^{\hat1\hat0}{}_{\hat0}$ which decay as r^{-3} or slower. Similarly one sees from Eqs. (V.12) that only those terms in

$$\Delta^{\hat\alpha\hat\nu} \equiv \sqrt{|\det g_{\hat\rho\hat\sigma}|}\, g^{\hat\alpha\hat\nu} - \sqrt{|\det b_{\hat\rho\hat\sigma}|}\, b^{\hat\alpha\hat\nu}$$

which are $O(r^{-3})$, or which are decaying slower, will give a nonvanishing contribution to the term involving the derivatives of X in the integral (V.15). This suggests to consider metrics ${}^4g$ such that

$$e^{\hat\mu\hat\nu} = o(r^{-3/2}), \quad e_{\hat\rho}(e^{\hat\mu\hat\nu}) = o(r^{-3/2}). \tag{V.16}$$

The boundary conditions (V.16) ensure that one needs to keep track only of those terms in $\mathbb{U}^{\hat1\hat0}$ which are linear in $e^{\hat\mu\hat\nu}$ and $e_{\hat\rho}(e^{\hat\mu\hat\nu})$, when $\mathbb{U}^{\hat1\hat0}$ is Taylor expanded around b. For a generalized Kottler metric (I.1) we have

$$e^{\hat0\hat0} \approx e^{\hat1\hat1} \approx -\frac{2ml^2}{r^3}, \quad e_{\hat1}(e^{\hat0\hat0}) \approx e_{\hat1}(e^{\hat1\hat1}) \approx \frac{6ml}{r^3}, \tag{V.17}$$

with the remaining $e^{\hat\mu\hat\nu}$'s and $e_{\hat\sigma}(e^{\hat\mu\hat\nu})$'s vanishing, so that Eqs. (V.16) are satisfied. Under (V.16) one obtains

$$g_{\hat a\hat c} = \eta_{\hat a\hat c} - \eta_{\hat a\hat r}\eta_{\hat c\hat s}e^{\hat r\hat s} + o(r^{-3}),\ \sqrt{|\det g_{\mu\nu}|} = \sqrt{|\det b_{\mu\nu}|}\,(1+\tfrac12(e^{\hat0\hat0}-e^{\hat1\hat1}-e^{\hat A\hat A})+o(r^{-3})), \tag{V.18}$$

$$\begin{aligned}\mathbb{U}^{\hat1\hat0}{}_{\hat0} &= -\frac{1}{16\pi}(2e_{;\hat1}+e^{\hat1\hat\imath}{}_{;\hat\imath}-e^{\hat0\hat0}{}_{;\hat1}) + o(r^{-3})\\ &= \frac{1}{16\pi}\left(e_{\hat1}(e^{\hat A\hat A}) + \frac{1}{l}(e^{\hat A\hat A}-2e^{\hat1\hat1}) - \frac{1}{r}\check D_{\hat A}e^{\hat1\hat A}\right) + o(r^{-3}),\end{aligned}$$

$$\frac{1}{8\pi}\Delta^{\alpha[\hat{1}}X^{\hat{0}]}{}_{;\alpha}=\frac{1}{16\pi}(\Delta^{\hat{1}\hat{1}}-\Delta^{\hat{0}\hat{0}})X^{\hat{0}}{}_{;\hat{1}}=\frac{r}{16\pi l^2}(\Delta^{\hat{1}\hat{1}}-\Delta^{\hat{0}\hat{0}})+o(r^{-3})$$

$$=-\frac{r}{16\pi l^2}e^{\hat{A}\hat{A}}+o(r^{-3}). \tag{V.19}$$

The indices $\hat{\imath}$ run from 1 to 3 while the indices $\hat{A}$ run from 2 to 3; $\breve{D}_{\hat{A}}$ denotes the covariant derivative on ${}^2M$, and $\breve{D}_{\hat{A}}e^{\hat{1}\hat{A}}$ is understood to be the covariant derivative associated with the metric $\breve{h}$ of a vector field on ${}^2M$, with repeated $\hat{A}$ indices being summed over. In Eq. (V.18) $\eta_{\hat{\mu}\hat{\nu}}=\mathrm{diag}(-1,+1,+1,+1)$, while the $g_{\hat{\mu}\hat{\nu}}$'s are the components of the tensor $g_{\hat{\mu}\hat{\nu}}$ in a co-frame dual to (V.10). Inserting all this into (V.15) one is finally led to the simple expression

$$M_{\mathrm{Ham}}\equiv H\left(\frac{\partial}{\partial t},\{t=0\}\right)=\lim_{R\to\infty}\frac{r^3}{16\pi l^2}\int_{\Sigma\cap\{r=R\}}\left(r\frac{\partial e^{\hat{A}\hat{A}}}{\partial r}-2e^{\hat{1}\hat{1}}\right)d^2\mu_{\breve{h}}. \tag{V.20}$$

In particular if ${}^4g$ is the generalized Kottler metric (I.1) one obtains [cf. Eq. (V.17)]

$$M_{\mathrm{Ham}}=\frac{A_\infty m}{4\pi}, \tag{V.21}$$

A_∞ defined in (V.9). If ${}^2M=T^2$ with area normalized to 4π we obtain $M_{\mathrm{Ham}}=m$. For $k=\pm 1$ it follows from the Gauss–Bonnet theorem that $A_\infty=4\pi|1-g_\infty|$, where g_∞ is the genus of ${}^2M$, hence

$$M_{\mathrm{Ham}}=|1-g_\infty|m. \tag{V.22}$$

This gives again $M_{\mathrm{Ham}}=m$ for ${}^2M=S^2$, but this will not be true anymore for ${}^2M$'s of higher genus. We believe that the Hamiltonian approach is the one which provides *the* correct definition of mass in field theories, and therefore Eqs. (V.21)–(V.22) are the ones which provide the correct normalization of mass.

Let us finally consider static metrics ${}^4g$ of the form (III.33), and suppose that the hypotheses of point (2) of Proposition III.7 hold. We can then use the coordinates of that proposition to calculate M_{Ham}, and obtain

$$M_{\mathrm{Ham}}=-\frac{1}{8\pi}\int_{\partial_\infty\Sigma}\mu_\infty\, d^2\mu_{\breve{h}}. \tag{V.23}$$

If we further assume that μ_∞ is constant on $\partial_\infty\Sigma$, Eq. (V.23) gives

$$M_{\mathrm{Ham}}=-\frac{\mu_\infty}{2}=M_c$$

for ${}^2M=S^2$ and for an appropriately normalized T^2, while

$$M_{\mathrm{Ham}}=-|1-g_\infty|\frac{\mu_\infty}{2}=|1-g_\infty|M_c$$

for higher genus $\partial_\infty\Sigma$'s. Here M_c is the coordinate mass as defined in Sec. V A.

C. A generalized Komar mass

Recall that the Komar mass is a number which can be assigned to every stationary, asymptotically flat metric the energy-momentum tensor of which decays sufficiently rapidly:

$$M_K = \lim_{R\to\infty} \frac{1}{8\pi} \int_{S_{R,T}} \sqrt{|\det g_{\alpha\beta}|}\, \nabla^\mu X^\nu \, dS_{\mu\nu}, \tag{V.24}$$

where $X^\mu \partial_\mu$ is the Killing vector field which asymptotes to $\partial/\partial t$ in the asymptotically flat region, and the $S_{R,T} \equiv \{t=T, r=R\}$'s are coordinate spheres in that region. The normalization factor $1/(8\pi)$ has been chosen so that M_K reproduces the familiar mass parameter m when Schwarzschild metrics are considered. For metrics considered here with $\Lambda \neq 0$ the integral (V.24) diverges when $X^\mu \partial_\mu = \partial/\partial t$ and when the $S_{R,T}$'s are taken to be coordinate spheres in the region $\Sigma_{\rm ext}$ where the metric exhibits the generalized Kottler asymptotics. An obvious way to generalize M_K to the situation considered in this paper is to remove the divergent part of the integral using a background metric b:

$$M_K = \lim_{R\to\infty} \frac{1}{8\pi} \int_{S_{R,T}} (\sqrt{|\det g_{\alpha\beta}|}\, \nabla^\mu X^\nu - \sqrt{|\det b_{\alpha\beta}|}\, \overline{\nabla}^\mu X^\nu) dS_{\mu\nu}. \tag{V.25}$$

Here $\overline{\nabla}$ denotes a covariant derivative with respect to the background metric. More precisely, let $\Sigma_{\rm ext}$, b, $\check{h}$, etc., be as in Eq. (V.8), and consider time-independent metrics g which in the coordinate system of Eq. (V.8) are of the form (III.33) with

$$V^2 = \frac{r^2}{l^2} + \tilde{k} - \frac{2\beta}{r} + o\left(\frac{1}{r}\right), \quad \partial_r\left(V^2 - \frac{r^2}{l^2} - \tilde{k} + \frac{2\beta}{r}\right) = o\left(\frac{1}{r^2}\right), \quad g^{rr} = l^2 + \tilde{k} - \frac{2\gamma}{r} + o\left(\frac{1}{r}\right),$$

$$\sqrt{|\det g_{\alpha\beta}|} = \left(r^2 + \frac{2\delta l^2}{r} + o\left(\frac{1}{r}\right)\right) \sqrt{|\det \check{h}_{AB}|}, \tag{V.26}$$

for some r-independent differentiable functions $\tilde{k} = \tilde{k}(x^A)$, $\beta = \beta(x^A)$, $\gamma = \gamma(x^A)$, and $\delta = \delta(x^A)$ defined on a coordinate neigbhorhood of $\partial_\infty \Sigma$. [The conditions (V.26) roughly reflect the behavior of the metric in the coordinate system of Proposition III.7.] Under (V.26) the limit as R tends to infinity in the definition (V.25) of M_K exists, and one finds

$$\begin{aligned} M_K &= \lim_{R\to\infty} \frac{1}{4\pi} \int_{S_{R,T}} (\sqrt{|\det g_{\alpha\beta}|}\, g^{r\mu} g^{\nu t} \partial_{[\mu} g_{\nu]t} - \sqrt{|\det b_{\alpha\beta}|}\, b^{r\mu} b^{\nu t} \partial_{[\mu} b_{\nu]t}) dx^2\, dx^3 \\ &= \lim_{R\to\infty} \frac{1}{8\pi} \int_{S_{R,T}} (\sqrt{|\det g_{\alpha\beta}|}\, g^{rr} g^{tt} \partial_r g_{tt} - \sqrt{|\det b_{\alpha\beta}|}\, b^{rr} b^{tt} \partial_r b_{tt}) dx^2 dx^3 \\ &= \frac{1}{4\pi} \int_{\partial_\infty \Sigma} (3\beta - 2\gamma + 2\delta) d^2\mu_{\check{h}}. \end{aligned} \tag{V.27}$$

It turns out that the value of M_K so obtained depends on the background metric chosen. [Our definition of background, Eq. (V.8), is tied to the choice of a particular coordinate system, so another way of stating this is that the number M_K as defined so far is assigned to a metric *and* to a coordinate system, in a manner somewhat similar to the coordinate mass of Sec. V A.] Indeed, given any differentiable function $\alpha(x^A)$ there exists a neighborhood of $\partial_\infty \Sigma$ on which a new coordinate $\hat{r}$ can be introduced by the formula

$$\frac{\hat{r}^2}{l^2} - 2\frac{\alpha}{\hat{r}} = \frac{r^2}{l^2}. \tag{V.28}$$

We can then choose the new background to be

$$b=-\left(k+\frac{\hat{r}^2}{l^2}\right)dt^2+\left(k+\frac{\hat{r}^2}{l^2}\right)^{-1}d\hat{r}^2+\hat{r}^2\check{h},$$

and obtain a new M_K which will in general *not* coincide with the old one. [It is noteworthy that the coordinate transformation (V.28) with the associated change of background do *not* change the value of the Hamiltonian mass M_{Ham}.] For example, if α is constant, using hats to denote the corresponding functions appearing in the metric expressed in the new coordinate system we obtain

$$\hat{\beta}=\beta+\alpha,\quad \hat{\gamma}=\gamma+3\alpha,\quad \hat{\delta}=\delta-2\alpha\Rightarrow\hat{M}_K=M_K-\frac{7\alpha A_\infty}{4\pi},$$

where A_∞ is the area of $\partial_\infty\Sigma$ with respect to the metric $\check{h}$. It turns out that one can remove this coordinate dependence in an appropriate class of metrics, tailoring the prescription in such a way that Eq. (V.27) reproduces, up to a genus dependent factor, the coordinate mass M_c. In order to do that we shall suppose that the metric ${}^4g$ satisfies the hypotheses of point (2) of Proposition III.7 (in particular $\tilde{k}=k=0,\pm1$ according to the genus of the connected component of $\partial_\infty\Sigma$ under consideration), and we let the background be associated with a coordinate system (ρ,x^A) with ρ given by (III.43). It follows from Eqs. (V.3) and (III.45) that in this coordinate system it holds

$$\sqrt{|\det g_{\alpha\beta}|}=r^2+o\left(\frac{1}{r}\right),\tag{V.29}$$

where we have used the generic symbol r to denote the coordinate ρ. We then impose (V.29) as a restriction on the coordinate system in which the generalized Komar mass M_K has to be calculated. When this condition is imposed we obtain from (V.3) and (V.23)

$$M_K=-\frac{1}{8\pi}\int_{\partial_\infty\Sigma}\mu_\infty d^2\mu_{\check{h}}=M_{\mathrm{Ham}}.$$

We have thus proved

Proposition V.1: Consider a metric ${}^4g$ satisfying the hypotheses of point (2). of Proposition III.7, then the generalized Komar mass (V.25) associated to a background metric (V.8) such that (V.29) holds equals the Hamiltonian mass (V.20).

Proposition V.1 is the $\Lambda<0$ analogue of the theorem of Beig,[64] that for static $\Lambda=0$ vacuum metrics which are asymptotically flat in spacelike directions the ADM mass and the Komar masses coincide. Our treatment here is inspired by, and somewhat related to, the analysis of Ref. 43.

D. The Hawking mass $M_{\mathrm{Haw}}(\psi)$

Let ψ be a function defined on the asymptotic region Σ_{ext}, with Σ_{ext} defined as in (V.1), such that the level sets of ψ are smooth compact surfaces diffeomorphic to each other (at least for ψ large enough), with $\psi\to_{r\to\infty}\infty$. Following Hawking,[65] Gibbons [Ref. 18, Eq. (17)] assigns a mass $M_{\mathrm{Haw}}(\psi)$ to such a foliation via the formula

$$M_{\mathrm{Haw}}(\psi)\equiv\lim_{\epsilon\to0}\frac{\sqrt{A_{1/\epsilon}}}{32\pi^{3/2}}\int_{\{\psi=1/\epsilon\}}\left({}^2\mathcal{R}-\frac{1}{2}p^2-\frac{2}{3}\Lambda\right)dA,\tag{V.30}$$

where A_α is the area of the connected component under consideration of the level set $\{\psi=\alpha\}$.

By considering simple examples in Minkowski space–times it can be seen that this definition is ψ dependent. However, when ${}^2M=S^2$, $\Lambda=0$, and the coordinate system on Σ_{ext} is such that the ADM mass m_{ADM} (which equals m_H as defined in Sec. V B) of Σ_{ext} is well defined (see Refs. 58

and 57), then $M_{\mathrm{Haw}}(\psi)$ will be independent of ψ, in the class of ψ's singled out by the condition that the level sets of ψ approach round spheres at a suitable rate. No results of this kind are known when $\Lambda \neq 0$.

The definition (V.30) applied to the function $\psi = r$ and the metric (I.1) with $k \neq 0$ gives

$$M_{\mathrm{Haw}} = m|1-g_\infty|^{3/2}.$$

We have also used the Gauss–Bonnet theorem to calculate $\sqrt{A_{1/\epsilon}}$. Thus the definition (V.30) differs from the coordinate one by the somewhat unnatural factor $|1-g_\infty|^{3/2}$. It is not clear why such a factor should be included in the definition of mass.

Consider, next, the metrics (III.33) with V and g given by (III.43)–(III.44). Let $\psi = V$; from the Codazzi–Mainardi Eq. (III.31), Eq. (I.5), and the definition (III.16) of W we obtain, for V large enough so that $|dV| > 0$,

$$\begin{aligned} {}^2R - \frac{1}{2}p^2 - \frac{2}{3}\Lambda &= (-2R_{ij} + Rg_{ij})n^i n^j - |q_{ij}|_g^2 - \frac{2}{3}\Lambda \\ &= -2\frac{D^i V D^j V}{VW} D_i D_j V - |q_{ij}|_g^2 - \frac{2}{3}\Lambda \\ &= -\frac{D^i V D_i W}{VW} - |q_{ij}|_g^2 - \frac{2}{3}\Lambda. \end{aligned}$$

In the coordinate system of Eq. (III.28), where $V = 1/x$, one is led to

$${}^2R - \frac{1}{2}p^2 - \frac{2}{3}\Lambda = x^3\frac{\partial W}{\partial x} - \frac{2}{3}\Lambda + O(x^6) = -\frac{x^3}{6}\frac{\partial R'}{\partial x} + O(x^6),$$

and we have used (III.25) and (III.15). From $A_{1/\epsilon} \approx x^{-2} A'_{\partial_\infty \Sigma}$ we finally obtain

$$M_{\mathrm{Haw}}(V) = -\frac{\sqrt{A'_{\partial_\infty \Sigma}}}{32\pi^{3/2}} \int_{\partial_\infty \Sigma} \frac{1}{6}\frac{\partial R'}{\partial x} d^2\mu_{h'} = -\frac{\sqrt{A'_{\partial_\infty \Sigma}}}{32\pi^{3/2}} \int_{\partial_\infty \Sigma} l\frac{n'(R')}{6} d^2\mu_{h'}, \tag{V.31}$$

where $d^2\mu_{h'}$ is the Riemannian area element induced by g' on $\partial_\infty \Sigma$, and n' denotes the inward-pointing g'-unit normal to $\partial_\infty \Sigma$. We have thus proved the following result.

Theorem V.2: Let a triple (Σ, g, V) satisfying Eqs. (I.3)–(I.5) be C^i compactifiable, $i \geqslant 3$. Then the Hawking mass $M_{\mathrm{Haw}}(V)$ of the V-foliation is finite and well defined; it is given by the formula (V.31), with R'—the curvature scalar of the metric $g' = V^{-2}g$.

We can relate $M_{\mathrm{Haw}}(V)$ to the coordinate mass M_c if we assume in addition that the latter is well defined; recall that this required R' and $\partial_x R'$ to be constant on $\partial_\infty \Sigma$. In this case Eq. (V.4) gives

$$M_{\mathrm{Haw}}(V) = \left(\frac{A'_{\partial_\infty \Sigma}}{4\pi l^2}\right)^{3/2} M_c. \tag{V.32}$$

From Eq. (III.20) we have ${}^2\mathcal{R}'|_{x=0} = 2k/l^2$, and the Gauss–Bonnet theorem implies

$$\int_{\partial_\infty \Sigma} {}^2\mathcal{R}'\, d^2\mu_{h'} = \frac{2k}{l^2} A'_{\partial_\infty \Sigma} = 8\pi(1-g_\infty),$$

so that when $g_\infty \neq 1$ we obtain

$$M_{\mathrm{Haw}}(V) = |1-g_\infty|^{3/2} M_c. \tag{V.33}$$

We emphasize that $M_{\mathrm{Haw}}(V)$ is finite and well defined even when the conditions of Sec. V A, which we have set forth to define M_c, are not met.

Similarly, the Hamiltonian mass M_{Ham}, associated to the background singled out by the coordinate system of Proposition III.7, can be defined when R' is constant on $\partial_\infty\Sigma$. (This holds regardless of whether or not $\partial_x R'$ is constant on $\partial_\infty\Sigma$.) Proceeding as above, making use of Eqs. (III.42)–(III.47), one is led to

$$\begin{aligned} &g_\infty \neq 1 \Rightarrow M_{\mathrm{Haw}}(V) = |1-g_\infty|^{1/2} M_{\mathrm{Ham}}, \\ &g_\infty = 1, \quad A'_\infty = 4\pi l^2 \Rightarrow M_{\mathrm{Haw}}(V) = M_{\mathrm{Ham}}. \end{aligned} \tag{V.34}$$

VI. THE GENERALIZED PENROSE INEQUALITY

We recall here an argument of Geroch,[13] as extended by Jang and Wald,[19] and Gibbons,[18] for the validity of the Penrose inequality:[66]

Proposition VI.1: Assume we are given a three dimensional manifold (Σ, g) with connected boundary $\partial\Sigma$ such that:

(1) $R \geqslant 2\Theta$ for some strictly negative constant Θ.
(2) There exists a smooth, global solution of the inverse mean curvature flow without critical points, i.e., there exists a surjective function $u:\Sigma \to [0,\infty)$ such that du has no zeros and
$$\begin{aligned} &u|_{\partial\Sigma} = 0, \\ &\nabla_i \left(\frac{\nabla^i u}{|du|} \right) = |du|. \end{aligned} \tag{VI.1}$$
(3) The level sets of u
$$N_s = \{u(x) = s\}$$
are compact.
(4) The boundary $\partial\Sigma = u^{-1}(0)$ of Σ is minimal.
(5) The Hawking mass of the level sets of u as defined in (V.30) exists.

Then

$$2M_{\mathrm{Haw}}(u) \geqslant (1-g_{\partial\Sigma}) \left(\frac{A_{\partial\Sigma}}{4\pi} \right)^{1/2} - \frac{\Theta}{3} \left(\frac{A_{\partial\Sigma}}{4\pi} \right)^{3/2}. \tag{VI.2}$$

Here $A_{\partial\Sigma}$ is the area of $\partial\Sigma$ and $g_{\partial\Sigma}$ is the genus thereof.

Remarks: (1) The Proposition above can be applied to solutions of (I.4) and (I.5) with $\Theta = \Lambda$: in this case we have $R = 2\Lambda$; further Eq. (I.5) multiplied by V and contracted with two vectors tangent to $\partial\Sigma$ shows that the boundary $\{V=0\}$ is totally geodesic and hence minimal.

(2) Equation (VI.2) is sharp—the inequality there becomes an equality for the generalized Kottler metrics.

Proof: Let A_s denote the area of N_s, and define

$$\sigma(s) = \sqrt{A_s} \int_{N_s} \left({}^2R_s - \frac{1}{2} p_s^2 - \frac{2}{3}\Theta \right) d^2\mu_s, \tag{VI.3}$$

where ${}^2R_s$ is the scalar curvature of the metric induced on N_s, $d^2\mu_s$ is the Riemannian volume element associated to that same metric, and p_s is the mean curvature of N_s. The hypothesis that du is nowhere vanishing implies that all the objects involved are smooth in s. At $s=0$ we have

$$\sigma(0) = \sqrt{A_{\partial\Sigma}} \int_{\partial\Sigma} ({}^2R_0 - \tfrac{2}{3}\Theta) d^2\mu_0 = \sqrt{A_{\partial\Sigma}} (8\pi(1-g_{\partial\Sigma}) - \tfrac{2}{3}\Theta A_{\partial\Sigma}). \tag{VI.4}$$

On the other hand, $\lim_{s\to\infty}\sigma(s)=32\pi^{3/2}M_{\mathrm{Haw}}(u)$. The generalization in Ref. 18 of the classical calculation of Ref. 13 gives

$$\frac{\partial\sigma}{\partial s}\geqslant 0. \tag{VI.5}$$

This implies $\lim_{s\to\infty}\sigma(s)\geqslant\sigma(0)$, which gives (VI.2). □

To be able to carry out the above argument one had to assume that du had no zeros, which implies in particular that $\partial_\infty\Sigma$ is connected with $g_{\partial\Sigma}=g_\infty$. It is not known whether or not the other hypotheses of Proposition VI.1, or the conditions of Definition III.1 together with Eqs. (I.3)–(I.5), force $\partial\Sigma$ to be connected. If they do not, one is tempted to conjecture that the right inequality should be

$$2M_{\mathrm{Haw}}(u)\geqslant\sum_{i=1}^{k}\left((1-g_{\partial_i\Sigma})\left(\frac{A_{\partial_i\Sigma}}{4\pi}\right)^{1/2}-\frac{\Theta}{3}\left(\frac{A_{\partial_i\Sigma}}{4\pi}\right)^{3/2}\right). \tag{VI.6}$$

Here the $\partial_i\Sigma$'s, $i=1,\ldots,k$, are the connected components of $\partial\Sigma$, $A_{\partial_i\Sigma}$ is the area of $\partial_i\Sigma$, and $g_{\partial_i\Sigma}$ is the genus thereof. This would be the inequality one would obtain from the Geroch–Gibbons argument if it could be carried through for u's which are allowed to have critical points, on manifolds with $\partial_\infty\Sigma$ connected but $\partial\Sigma$ not necessarily connected.

We note that when $\Lambda=0$ there is a version of the proof of Proposition VI.1 due to Huisken and Ilmanen in which du is allowed to have zeros (with $\partial\Sigma$ connected).[67] Note that at points where du vanishes Eq. (VI.1) does not make sense classically, and has to be understood in a proper way. Further the monotonicity calculation of Ref. 13 breaks down at critical level sets of u, as those do not have to be smooth submanifolds. Nevertheless (when $\Lambda=0$) existence of appropriate functions u (perhaps with critical points) together with the monotonicity of σ can be established[14,15] when $\partial\Sigma$ is an outermost (necessarily connected) minimal sphere. It is conceivable that the argument of Huisken and Ilmanen can be modified to include the case $\Lambda\neq 0$. One of the difficulties here is to handle the possibly changing genus of the level sets of u.

Let us discuss some of the consequences of the (hypothetical) Eq. (VI.6). To proceed further it is convenient to introduce a mass parameter m defined as follows:

$$m=\begin{cases} M_{\mathrm{Haw}}, & \partial_\infty\Sigma=S^2,\\ M_{\mathrm{Haw}}, & \partial_\infty\Sigma=T^2, \text{ with the normalization } A'_\infty=4\pi l^2,\\ \dfrac{M_{\mathrm{Haw}}}{|g_{\partial_\infty\Sigma}-1|^{3/2}}, & g_{\partial_\infty\Sigma}>1. \end{cases} \tag{VI.7}$$

Strictly speaking, we should write $m(u)$ if $M_{\mathrm{Haw}}(u)$ is used above, $m(V)$ if $M_{\mathrm{Haw}}(V)$ is used, etc.; we shall do this when confusions are likely to occur. For generalized Kottler metrics the mass $m=m(u)$ so defined coincides with the mass parameter appearing in (I.1) when u is the radial solution $u=u(r)$ of the problem (VI.1); $m(V)$ coincides with the coordinate mass M_c for the metrics considered here when M_c is defined, cf. Eq. (V.32).

Note, first, that if all connected components of the horizon have spherical or toroidal topology, then the lower bound (VI.6) is strictly positive. For example, if $\partial\Sigma=T^2$, and $\partial_\infty\Sigma=T^2$ as well we obtain

$$2m\geqslant\frac{1}{l^2}\left(\frac{A_{\partial\Sigma}}{4\pi}\right)^{3/2}.$$

On the other hand, if $\partial\Sigma=T^2$ but $g_{\partial_\infty\Sigma}>1$ from Eq. (VI.6) one obtains

$$2m \geqslant \frac{1}{l^2|g_\infty - 1|}\left(\frac{A_{\partial\Sigma}}{4\pi}\right)^{3/2}.$$

Let us return to the case where Eqs. (I.3)–(I.5) hold;[68] we can then use the Galloway–Schleich–Witt–Woolgar inequality[4]

$$\sum_{i=1}^{k} g_{\partial_i\Sigma} \leqslant g_\infty . \tag{VI.8}$$

It implies that if $\partial_\infty\Sigma$ has spherical topology, then all connected components of the horizon must be spheres. Similarly, if $\partial_\infty\Sigma$ is a torus, then all components of the horizon are spheres, except perhaps for at most one which could be a torus. It follows that to have a component of the horizon which has genus higher than one we need $g_\infty > 1$ as well.

When some—or all—connected components of the horizon have genus higher than one the right-hand side of Eq. (VI.6) might become negative. Minimizing the generalized Penrose inequality (VI.6) with respect to the areas of the horizons gives the following interesting inequality:

$$M_{\mathrm{Haw}}(u) \geqslant -\frac{1}{3\sqrt{-\Lambda}} \sum_i |g_{\partial_i\Sigma} - 1|^{3/2}, \tag{VI.9}$$

where the sum is over those connected components $\partial_i\Sigma$ of $\partial\Sigma$ for which $g_{\partial_i\Sigma} \geqslant 1$. Equation (VI.9), together with the elementary inequality $\Sigma_{i=1}^N |\lambda_i|^{3/2} \leqslant (\Sigma_{i=1}^N |\lambda_i|)^{3/2}$, lead to

$$m \geqslant -\frac{1}{3\sqrt{-\Lambda}}. \tag{VI.10}$$

The Geroch–Gibbons argument establishing the inequality (VI.4) when a suitable u exists can also be *formally* carried through when $\partial\Sigma = \varnothing$. In this case one still considers solutions u of the differential equation that appears in Eq. (VI.1), however the Dirichlet condition on u at $\partial\Sigma$ is replaced by a condition on the behavior of u near some chosen point $p_0 \in \Sigma$. If the level set of u around p_0 approach distance spheres centered at p_0 at a suitable rate, then $\sigma(s)$ tends to zero when the N_s's shrink to p_0, which together with the monotonicity of σ leads to the positive energy inequality:

$$M_{\mathrm{Haw}}(u) \geqslant 0. \tag{VI.11}$$

It should be emphasized that the Horowitz–Myers solutions[23] with negative mass show that this argument breaks down when $g_\infty = 1$.

When $\partial_\infty\Sigma = S^2$ one expects that (VI.11), with $M_{\mathrm{Haw}}(u)$ replaced by the spinorially defined mass (which might perhaps coincide with $M_{\mathrm{Haw}}(u)$, but this remains to be established), can be proved by Witten-type techniques, compare Refs. 24 and 25. On the other hand it follows from Ref. 26 that when $\partial_\infty\Sigma \neq S^2$ there exist no asymptotically covariantly constant spinors which can be used in the Witten argument. The Geroch–Gibbons argument has a lot of ''ifs'' attached in this context, in particular if $\partial_\infty\Sigma \neq S^2$ then some level sets of u are necessarily critical and it is not clear what happens with σ when a jump of topology from a sphere to a higher genus surface occurs. We note that the area of the horizons does not occur in (VI.10) which, when $g_{\partial_\infty\Sigma} > 1$, suggests that the correct inequality is actually (VI.10) rather than (VI.11).

VII. MASS AND AREA INEQUALITIES

A. Preliminaries

Let (Σ,g,V) satisfy (I.3)–(I.5) together with the topological, the differential, and the asymptotic requirements spelled out in the statements of Theorems I.3 or I.5. (Lemma VII.3 below actually holds under more general conditions.) We first introduce the surface gravity κ of $\partial\Sigma$ to be the corresponding restriction of the function $\sqrt{W}$ defined by (III.16):

$$\kappa \equiv |dV|_g|_{\partial\Sigma}, \tag{VII.1}$$

where we have normalized V so that Eq. (III.21) holds, cf. Proposition III.3. By the strong maximum principle (Ref. 69, Lemma 3.4) W is nowhere vanishing on $\partial\Sigma$. Moreover, it is well known [and easily seen using Eq. (I.5)] that κ is locally constant on $\partial\Sigma$:

$$0 = n^j D_i D_j V|_{V=0} = \frac{D^j V}{\sqrt{W}} D_i D_j V|_{V=0} = \frac{1}{2\sqrt{W}} D_i W|_{V=0}. \tag{VII.2}$$

Here n^i is the unit normal to $\partial\Sigma$, where V vanishes. It is convenient to introduce the notion of a *reference solution* (RS): this is a generalized Kottler solution with the same genus g_∞ as (Σ,g,V). Moreover, if $\partial\Sigma\neq\emptyset$, the surface gravity κ of the RS is chosen to be equal to the maximum of the surface gravities of (Σ,g,V). On the other hand, if $\partial\Sigma=\emptyset$, the mass of the RS will be specified suitably below, in the proof of (I.3). It should be stressed, that we are *not* comparing manifolds and/or metrics, but we are only using the resulting scalar functions V and W:

We only consider RS with mass m_0 in the range (II.6) (if $\partial\Sigma\neq\emptyset$, this property follows from the restriction (I.7) on κ). Let $r(\cdot)$ be the function $V_0\to r(V_0)$ constructed at the end of Sec. II, composing r with V we obtain functions $r(V(\cdot))$ and $W_0(r(V(\cdot)))$ defined on Σ. By an abuse of notation we shall still denote those functions by r and W_0.

Remark: In the same manner, we can define a RS from other solutions with the property that W is a function of V only. (In Lemma VII.3 below we will also include the Nariai case.)

Following Ref. 70 we define $\psi(V)$ to be that unique solution of the equation

$$\psi^{-1}\frac{d\psi}{dV} = -VW_0^{-1}\frac{m_0}{r^3} \tag{VII.3}$$

which goes[71] to 1 as V goes to ∞. (In particular $\psi\equiv 1$ when $m_0=0$.) Here $r=r(V)$ is again the function defined at the end of Sec. II. Standard results on ODE's show that solutions of (VII.3) have no zeros unless identically vanishing, and that

$$\Psi \equiv \psi\circ V$$

can be extended by continuity to a smooth function on $\overline{\Sigma}$, still denoted by Ψ, which satisfies

$$\Psi>0, \quad \Psi|_{\partial_\infty\Sigma}=1.$$

We also define

$$\tilde{g}_{ij} = V^{-2}\Psi^4 g_{ij}, \quad \tilde{W}=\Psi^{-4}W, \quad \tilde{W}_0=\Psi^{-4}W_0. \tag{VII.4}$$

We proceed with a computation which is required in Lemma VII.1 as well as in Lemma VII.2. Consider a level set $\{V=\text{const}\}$ of V which is a smooth hypersurface in $\overline{\Sigma}$, with unit normal n_i, induced metric h_{ij}, scalar curvature ${}^2\mathcal{R}$, second fundamental form p_{ij} defined with respect to an inner pointing normal, mean curvature $p=h^{ij}p_{ij}$; we denote by q_{ij} the trace-free part of p_{ij}: $q_{ij}=p_{ij}-\frac{1}{2}h_{ij}p$. Using Eq. (II.4), the Eq. (I.4) with $g=g_0$ and $V=V_0$, together with the relation $dV_0/dr=\sqrt{W_0}/V_0$ we obtain

$$V^{-1}\frac{dW_0}{dV}=-\frac{2}{3}\Lambda-\frac{4m_0}{r^3}. \tag{VII.5}$$

To obtain (VII.6) we use, in this order, the definitions (VII.4), the Eqs. (I.4)–(I.5), Eqs. (VII.5) and (VII.3), and the Codazzi–Mainardi equation:

$$\begin{aligned}V^{-1}\tilde{W}^{-1}D^iVD_i(\tilde{W}-\tilde{W}_0)&=V^{-1}W^{-1}D^iV(D_iW)-V^{-1}\frac{dW_0}{dV}-4V^{-1}\Psi^{-1}\frac{d\Psi}{dV}(W-W_0)\\&=(2R_{ij}-Rg_{ij})n^in^j+\frac{2}{3}\Lambda+\frac{4m_0}{r^3}-\frac{4m_0}{r^3}(1-W_0^{-1}W)\\&=-{}^2\mathcal{R}-q_{ij}q^{ij}+\frac{1}{2}p^2+\frac{2}{3}\Lambda+\frac{4m_0}{r^3}-\frac{4m_0}{r^3}(1-W_0^{-1}W).\end{aligned} \tag{VII.6}$$

Lemma VII.1: Under the conditions of Theorem I.1, suppose further that the scalar curvature R' of the metric $g'=V^{-2}g$ is constant on $\partial_\infty\Sigma$. Let V be normalized so that (III.21) holds, with $A'_\infty=4\pi l^2$ when $\partial_\infty\Sigma=T^2$. If m is the Hawking mass parameter defined as in (VI.7), then

$$\int_{\partial_\infty\Sigma}D'_i(\tilde{W}-\tilde{W}_0)dS'^i=-\left(\frac{2\Lambda}{3}\right)^2A'_{\partial_\infty\Sigma}(m-m_0), \tag{VII.7}$$

where dS'^i denotes the outer-oriented area element of the metric $g'=V^{-2}g$, and $A'_{\partial_\infty\Sigma}$ is the area of $\partial_\infty\Sigma$ with respect to that metric.

Proof: Using

$$D'^i(\tilde{W}-\tilde{W}_0)n'_i=\frac{1}{\sqrt{W'}}D_i(\tilde{W}-\tilde{W}_0)D^iV \tag{VII.8}$$

and (VII.6), the left-hand side of (VII.7) reads

$$\int_{\partial_\infty\Sigma}\frac{V\tilde{W}}{\sqrt{W'}}\left[-{}^2\mathcal{R}-q_{ij}q^{ij}+\frac{1}{2}p^2+\frac{2}{3}\Lambda+\frac{4m_0}{r^3}-\frac{4m_0}{r^3}(1-W_0^{-1}W)\right]d^2\mu_{g'}, \tag{VII.9}$$

where $d^2\mu_{g'}$ is the two-dimensional surface measure associated with the metric g'. Chasing through the definitions one finds that $V\tilde{W}/\sqrt{W'}\approx\sqrt{-(\Lambda/3)}V^3$ near $\partial_\infty\Sigma$. From the definition of V_0 we further have $r\approx\sqrt{-(3/\Lambda)}V$, again near $\partial_\infty\Sigma$, so that $\lim_{V\to\infty}V\tilde{W}/(\sqrt{W'}r^3)=(-\Lambda/3)^2$. It follows that the second to last term in (VII.9) gives a contribution

$$\left(\frac{2\Lambda}{3}\right)^2A'_{\partial_\infty\Sigma}m_0, \tag{VII.10}$$

where $A'_{\partial_\infty\Sigma}$ denotes the g' area of the connected component of $\partial_\infty\Sigma$ under consideration. Equation (III.15) and its equivalent with W replaced by W_0 show that $(1-W_0^{-1}W)\to_{V\to\infty}0$ so that the last term drops out from (VII.9). Furthermore, by Eq. (III.25) we have $(V\tilde{W}/\sqrt{W'})\,q_{ij}q^{ij}=O(V^{-3})\to_{V\to\infty}0$, and it remains to analyze the contribution of $-V\tilde{W}({}^2\mathcal{R}-\frac{1}{2}p^2-\frac{2}{3}\Lambda)/\sqrt{W'}$ to the integral (VII.7). To do this, note that

$$A_{1/\epsilon}\equiv A(\{V=1/\epsilon\})=\int_{V'=\epsilon}d^2\mu_g=\int_{V'=\epsilon}V^2\,d^2\mu_{g'}\approx\epsilon^{-2}A'_{\partial_\infty\Sigma},$$

where $d^2\mu_g$ is the induced measure on $\partial_\infty\Sigma$ associated with the metric g. It follows that

$$
\begin{aligned}
&-\int_{V'=\epsilon}\frac{V\tilde{W}}{\sqrt{W'}}\left({}^2\mathcal{R}-\frac{1}{2}p^2-\frac{2}{3}\Lambda\right)d^2\mu_{g'}\\
&\quad\approx-\sqrt{-\frac{\Lambda}{3}}\frac{1}{\epsilon}\int_{V'=\epsilon}\left({}^2\mathcal{R}-\frac{1}{2}p^2-\frac{2}{3}\Lambda\right)d^2\mu_g\\
&\quad\approx-\sqrt{-\frac{\Lambda}{3}}\sqrt{\frac{A_{1/\epsilon}}{A'_{\partial_\infty\Sigma}}}\int_{V'=\epsilon}\left({}^2\mathcal{R}-\frac{1}{2}p^2-\frac{2}{3}\Lambda\right)d^2\mu_g\to_{\epsilon\to 0}-\left(\frac{2\Lambda}{3}\right)^2A'_{\partial_\infty\Sigma}m,
\end{aligned}
\tag{VII.11}
$$

where

$$
m\equiv\lim_{\epsilon\to 0}\frac{1}{4}\left(-\frac{\Lambda A'_{\partial_\infty\Sigma}}{3}\right)^{-3/2}\sqrt{A_{1/\epsilon}}\int_{\{V=1/\epsilon\}}\left({}^2\mathcal{R}-\frac{1}{2}p^2-\frac{2}{3}\Lambda\right)dA. \tag{VII.12}
$$

To finish the proof we need to show that m in (VII.12) is indeed the Hawking mass as defined in Eq. (VI.7). In the torus case this follows immediately from the normalization condition $A'_\infty=4\pi l^2$; for the remaining topologies this can be seen as follows: if V is normalized so that (III.21) holds, then (III.20) implies ${}^2\mathcal{R}'|_{x=0}=-\frac{2}{3}\Lambda k$. When $g_\infty\neq 1$ the Gauss–Bonnet theorem gives

$$
8\pi|1-g_\infty|=\left|\int {}^2\mathcal{R}'\,d^2\mu_{g'}\right|=-\tfrac{2}{3}\Lambda A'_{\partial_\infty\Sigma},
$$

which shows that the mass defined by Eq. (VII.12) coincides with that of (VI.7). □

For the subsequent lemma, recall from Theorem I.3 that $\partial_1\Sigma$ refers to the component of Σ with the largest surface gravity.

Lemma VII.2: Under the conditions of Theorem I.1, we have

$$
\int_{\partial_1\Sigma}\tilde{W}^{-1/2}\tilde{D}_i(\tilde{W}-\tilde{W}_0)d\tilde{S}^i=8\pi\left[(g_{\partial_1\Sigma}-1)-\frac{A_{\partial_1\Sigma}}{A_0}(g_\infty-1)\right]. \tag{VII.13}
$$

Proof: We integrate (VII.6) over $\partial_1\Sigma$. We note that Eq. (I.5) multiplied by V and contracted with two vectors tangent to $\partial\Sigma$ shows that $\partial\Sigma$ is totally geodesic; equivalently, $q_{ij}=0$. We introduce ${}^2\mathcal{R}_0=\frac{2}{3}\Lambda+(4m_0/r_0^3)$, the scalar curvature of the metric $d\Omega_k^2$. Using (VII.6) and the Gauss–Bonnet theorem, the left-hand side of (VII.13) can be written as

$$
\int_{\partial_1\Sigma}\left(-{}^2\mathcal{R}+\frac{2}{3}\Lambda+\frac{4m_0}{r_0^3}\right)dA=\int_{\partial_1\Sigma}(-{}^2\mathcal{R}+{}^2\mathcal{R}_0)dA=8\pi(g_{\partial_1\Sigma}-1)+{}^2\mathcal{R}_0A_{\partial_1\Sigma}. \tag{VII.14}
$$

Equation (VII.13) is then obtained by eliminating ${}^2\mathcal{R}_0$ from (VII.14), using the Gauss–Bonnet theorem for the generalized Kottler metrics: $8\pi(1-g_\infty)={}^2\mathcal{R}_0A_0$. □

The following elliptic equation for $\tilde{W}-\tilde{W}_0$ will be the crucial ingredient in the proof of the theorems. It is also useful for Lemma VII.3.

$$
(\tilde{\Delta}-a)(\tilde{W}-\tilde{W}_0)=\tfrac{1}{4}\tilde{W}^{-1}\tilde{R}_{ijk}\tilde{R}^{ijk}+\tfrac{3}{4}\tilde{W}^{-1}\tilde{D}_i(\tilde{W}-\tilde{W}_0)\tilde{D}^i(\tilde{W}-\tilde{W}_0), \tag{VII.15}
$$

with

$$a=\frac{5}{3r^3}m_0\Lambda V^4 W_0^{-2}\tilde{W}, \tag{VII.16}$$

$\tilde{\Delta}$ being the Laplace operator of the metric $\tilde{g}_{ij}$, and $\tilde{R}_{ijk}$—the Cotton tensor of $\tilde{g}_{ij}$. This equation is obtained by specializing[72] Eq. (V.4) of Ref. 70 (which has been used in that paper in the context of a uniqueness proof for static perfect fluid solutions) to the present case with $8\pi\rho=-8\pi p=\Lambda$.

It is important to stress that Eq. (VII.15), as it stands, makes only sense on the set $\{dV\neq 0\}$, because of the factors $\tilde{W}^{-1}$ appearing there. However, it follows from Eq. (I.4) that the set $\{dV=0\}$ has no interior: indeed, if dV vanishes on a connected open set then V is constant there, which is compatible with Eq. (I.5) only if V vanishes there. This contradicts our hypothesis that V vanishes only on $\partial\Sigma$. Hence Eq. (VII.15) holds on an open dense set of Σ. Since the left-hand side of Eq. (VII.15) is a smooth function on $\Sigma\backslash\partial\Sigma$, the right-hand side thereof is smoothly extendible by continuity to a smooth function on $\Sigma\backslash\partial\Sigma$, and Eq. (VII.15) holds everywhere on this set with the right-hand side being understood in the sense explained here.

Lemma VII.3: Let $\Lambda\in\mathbb{R}$, and let (Σ,g,V) be a solution of (I.3)–(I.5) such that

(a) either $W\equiv W_0$ for W_0 defined from the generalized Kottler or from the Nariai solution (I.2), or
(b) (Σ,g) is locally conformally flat.

Suppose further that Σ is a union of compact boundary-less level sets of V. Then

(1) Every connected component $\mathcal{V}$ of the set $\{p\in\Sigma\,|\,dV(p)\neq 0\}$ ''corresponds to'' one of the generalized Kottler solutions (I.1), or to one of the generalized Nariai solutions (I.2), or is flat. More precisely, there exists an interval $J\subset\mathbb{R}$, a two-dimensional compact Riemannian manifold $({}^2M,d\Omega_k^2)$, with $d\Omega_k^2$ an (r-independent) metric of constant Gauss curvature $k=0,\pm 1$, and a diffeomorphism $\psi:\mathcal{V}\to J\times{}^2M$ such that, transporting g and V to $J\times{}^2M$ using ψ, we have:

(i) Either there exists a constant $\lambda>0$ such that $V=\lambda V_0$ and
$$g=V_0^{-2}\,dr^2+r^2\,d\Omega_k^2,\quad r\in J,\quad V_0^2=k-\frac{2m}{r}-\frac{\Lambda}{3}r^2, \tag{VII.17}$$
(ii) or, when $k\Lambda>0$, there exists a constant $\lambda\in\mathbb{R}$ ($\lambda>0$ if $\Lambda>0$) such that
$$g=V^{-2}\,dz^2+|\Lambda|^{-1}\,d\Omega_k^2,\quad z\in J,\quad V^2=\lambda-\Lambda z^2, \tag{VII.18}$$
(iii) or, when $k=\Lambda=0$, there exists a constant $\lambda>0$ such that $V=\lambda z$ and
$$g=dz^2+d\Omega_k^2,\quad z\in J. \tag{VII.19}$$
(In each case the interval J is constrained by the condition that V and V^2 be non-negative).

(2) Under condition (a). above, if Σ is connected and if W_0 (considered as a function of V) has no zeros in the interval where V takes its values,
$$\forall p\in\Sigma\quad W_0(V(p))\neq 0, \tag{VII.20}$$
then $\mathcal{V}=\Sigma$, thus Eqs. (VII.18) or (VII.17) hold globally on Σ.

Remarks:

(1) Here we do not make any hypotheses on the sign of Λ.
(2) The result is local, in particular it is sufficient to be able to invert $r_0(V_0)$ locally on the range of the values of V under consideration to obtain $W_0(V)$.
(3) The set (Σ,g,V) corresponding to the metric (VII.19) arises from a boost Killing vector in suitably identified Minkowski space–time.
(4) We note that the set $\mathcal{V}$ could be empty, as is the case for $\mathbb{R}\times T^3$ with the obvious flat metric. Our analysis does not say anything about the metric on regions where dV vanishes.

(5) We note that the generalized Kottler and the generalized Nariai metrics also arise naturally in the generalized Birkhoff theorem, see Refs. 73 and 74, and also Ref. 75 for a very clear treatment in the $\Lambda>0$ case.
(6) The lemma can easily be reformulated by taking any conformally flat solution of (I.4)-(I.5) as a reference solution. The condition of conformal flatness is required to ensure that (VII.15) holds and excludes, in particular, the Horowitz–Myers solutions with a toroidal I^+ (Ref. 23) as RS.

Proof: The proof is an adaptation of an argument of Ref. 76 to the current setting. Suppose that $W=W_0$ for some W_0; Eq. (VII.15) shows then that $\tilde{R}_{ijk}\tilde{R}^{ijk}$ vanishes, so that (Σ,g) is locally conformally flat. It then follows that condition (b). holds in both cases.

We start by removing from Σ some undesirable points: set

$$\Sigma_{\text{sing}}\equiv\{p\in\Sigma\,|\,\text{the connected component of the set } \{q|V(q)=V(p)\} \text{ containing } p \text{ contains a point } r \text{ such that } dV(r)=0.\},$$

$$\Sigma'\equiv\Sigma\backslash\Sigma_{\text{sing}}.$$

Σ_{sing} is a closed subset of Σ, so that Σ' is still a manifold. It follows from Sard's theorem that $\Sigma'\neq\varnothing$. We note that Σ' still satisfies all the hypotheses of the lemma, except perhaps for being connected. By construction all the level sets of V are noncritical in Σ'. (Recall that a level set $\{V=c\}$ of V is noncritical if dV is nowhere vanishing on $\{V=c\}$.)

Let $\mathcal{U}$ to be any connected component of Σ'. Compactness of the level sets of V implies[77] that $\mathcal{U}$ is diffeomorphic to $I\times{}^2M$, for some two-dimensional compact connected manifold ${}^2M$ and some interval $I\subset\mathbb{R}$, with V equal to c on $\{c\}\times{}^2M$, $c\in I$, and that on $\mathcal{U}$ the function V can be used as a coordinate. Further we can introduce on ${}^2M$ a finite number of coordinate patches with coordinates x^A, $A=1,2$, so that on $\mathcal{U}$ the metric takes the form

$$g=W^{-1}\,dV^2+h_{AB}\,dx^A\,dx^B. \tag{VII.21}$$

Let, as before, $q_{AB}\,dx^A\,dx^B$ be the trace free part of the extrinsic curvature tensor of the level sets of V—in the coordinate system of (VII.21)

$$q_{AB}=\sqrt{W}\left(\frac{\partial h_{AB}}{\partial V}-\frac{1}{2}h^{CD}\frac{\partial h_{CD}}{\partial V}h_{AB}\right). \tag{VII.22}$$

Equations (VII.22) and (III.23) imply that q_{AB} vanishes hence $\partial h_{AB}/\partial V$ is pure trace, that $W=W(V)$, and that $\det\gamma_{AB}$ is a product of a function of V with a function of the remaining coordinates. We thus have

$$h=W(V)^{-1}\,dV^2+r(V)^2\,d\Omega^2 \tag{VII.23}$$

for some positive function $r(V)$, where $d\Omega^2$ is a V-independent metric on ${}^2M$. Next, from (I.5) and from the Codazzi–Mainardi equations (VII.24),

$$R'_{1a}=-D'_ap'+D'_bp'^b_a=-\tfrac{1}{2}D'_ap'+D'_bq'^b_a \tag{VII.24}$$

[here we are using the adapted coordinate system of Eq. (III.28) with $x^1=x$ and with the indices $a,b=2,3$ corresponding to the remaining coordinates; further D' denotes the Levi–Civita derivative associated with the metric h'], respectively (III.31), applied to ${}^2M\subset\mathcal{U}$, we find that the mean curvature p of all level surfaces, respectively, their Ricci scalars, are constant. Hence $({}^2M,d\Omega^2)$ is a space of constant curvature, and scaling r appropriately we can without loss of generality assume that the Gauss curvature k of the metric $d\Omega^2$ equals $0,\pm1$, as appropriate to the genus of ${}^2M$. We define

$$L=\frac{dW}{dV}+2\Lambda V. \tag{VII.25}$$

Evaluating (I.4) for the metric (VII.23), we find

$$\frac{dr}{dV}=-\frac{rL}{4W}. \tag{VII.26}$$

Equations (I.4)–(I.5) for the metric (VII.23) are equivalent to (VII.25)–(VII.26) together with

$$2W\left(\Lambda-\frac{k}{r^2}\right)=L\left(V^{-1}W-\frac{L}{8}\right), \tag{VII.27}$$

$$W\frac{dL}{dV}=\frac{3}{4}L^2+(V^{-1}W-\Lambda V)L. \tag{VII.28}$$

These equations arise, e.g., by adapting Eqs. (3.16) and (3.17) of Ref. 70 to the present case (namely by setting $8\pi\rho=-8\pi p=\Lambda$, $L_1=L$ and $C^2=k$, and allowing the constant k to take negative values). Suppose, first, that there exists V_* such that $L(V_*)=0$. Equation (VII.28) shows then that $L\equiv 0$, and from (VII.27) one obtains

$$\Lambda=\frac{k}{r^2}. \tag{VII.29}$$

If $k=0$ then Λ vanishes as well; further r is constant by Eq. (VII.26) and can therefore be absorbed into $d\Omega^2$. Integrating Eq. (VII.25) one finds that there exists a strictly positive constant λ such that $W=\lambda^2$, defining a coordinate z by the equation $z=V/\lambda$ proves point (iii) on $\mathcal{U}$. Next, if $k\neq 0$ Eq. (VII.29) gives $k\Lambda>0$ as desired, together with $r^2=-1/|\Lambda|$. Integrating Eq. (VII.25) one obtains $W=\Lambda(\lambda-V^2)$, for some constant $\lambda\in\mathbb{R}$. Introducing the coordinate z via the equation $V^2=\lambda-\Lambda z^2$ establishes point (1ii). on $\mathcal{U}$.

In the case of L without zeros we obtain, from (VII.25), (VII.26), and (VII.28), that $(d/dV)(V\sqrt{W}/rL)=0$, which implies that there exists a nonvanishing constant α such that

$$L=\alpha V\frac{\sqrt{W}}{r}. \tag{VII.30}$$

Using (VII.26) one is led to

$$\frac{dV}{dr}=-\frac{4\sqrt{W}}{\alpha V}. \tag{VII.31}$$

Next we define

$$m(V)=-\frac{\alpha}{4}r^2\sqrt{W}+\frac{\Lambda r^3}{3}; \tag{VII.32}$$

from (VII.25), (VII.30), and (VII.31) we obtain $dm/dV=0$, i.e., m is a constant. Equation (VII.27) gives $V^2=(16/\alpha^2)[k-(2m/r)-(\Lambda/3)r^2]$. Equation (VII.26) shows that we can use r as a coordinate, and Eq. (VII.31) implies that the metric is of the desired form (VII.17). This establishes point (1i) on $\mathcal{U}$.

Let $\mathcal{V}$ be the connected component of $\{dV\neq 0\}\subset\Sigma$ that contains $\mathcal{U}$. To establish point (1) of the lemma we need to show that $\mathcal{V}=\mathcal{U}$. We claim that $\mathcal{U}$ is open in V—and hence in Σ—which can be seen as follows: Let $p\in\mathcal{U}$, we thus have $dV(q)\neq 0$ for all q such that $V(p)=V(q)$. By

Eq. (VII.23) $|dV|_g=\sqrt{W}$ is constant on the intersection with $\mathcal{U}$ of the level set $V^{-1}(V(p))$ of V through p, so that $\inf_{V^{-1}(V(p))\cap\mathcal{U}}|dV|_g>0$, which easily implies that all nearby level sets in $\mathcal{U}\subset\Sigma'$ are noncritical.

Let us show now that $\mathcal{U}$ is closed in $\mathcal{V}$. To see that, consider a sequence $p_i\in\mathcal{U}$ such that $p_i\to p\in V$. By definition of $\mathcal{V}$ the function $|dV|_g$ has no zeros on V, hence $dV(p)\neq 0$. Now it follows from (III.23) that $|dV|_g$ is locally constant on smooth subsets of level sets of V, which easily implies (a) that the connected component of $V^{-1}(V(p))$ containing p is smooth and (b) that $|dV|_g$ is nowhere vanishing there. Compactness of the level sets of V implies that all the connected components of level sets intersecting a neighborhood of p are noncritical, and hence are in Σ'. It then follows that $p\in\mathcal{U}$.

We have thus shown that $\mathcal{U}$ is both open and closed in $\mathcal{V}$; connectedness of $\mathcal{V}$ shows that $\mathcal{U}=\mathcal{V}$, and point (1) is established.

To prove point (2), we note that the equality $W(p)=W_0(V(p))$ together with Eq. (VII.20) shows that V has no critical points on Σ; as Σ is connected the set $\mathcal{V}$ of point (1) coincides with Σ, and point (2) follows from point (1). □

B. Proofs

Proof of Theorem I.3: Suppose that $\partial\Sigma=\varnothing$. We first consider as RS a generalized Kottler solution with $m=0$ [see Eq. (II.5)]: This leads to

$$\Psi\equiv 1,\quad \widetilde{W}_0(V_0)=-\frac{\Lambda}{3}(V_0^2-k). \tag{VII.33}$$

We further normalize V as in Proposition III.3, so that by (III.15), (III.19), and (III.21) we have $\widetilde{W}-\widetilde{W}_0\to_{r\to\infty}0$. (Actually when $\partial_\infty\Sigma=T^2$, the normalization of V does not play any role, as we make claims only about the sign of m in this case.) Equation (VII.15) together with the maximum principle shows that

$$\widetilde{W}-\widetilde{W}_0\leqslant 0\quad \text{on } \Sigma, \tag{VII.34}$$

$$n'^i D'_i(\widetilde{W}-\widetilde{W}_0)|_{\partial_\infty\Sigma}\geqslant 0, \tag{VII.35}$$

where n' is the *outer* pointing g'-unit normal to $\partial_\infty\Sigma$. Further, equality is attained in (VII.34) or in (VII.35) if and only if $W\equiv W_0$ (Ref. 69, Theorems 3.5 and 3.6). Thus Lemma VII.1 together with Eq. (VII.35) shows that $m\leqslant 0$. Assume now that $m=0$ in the case $\partial_\infty\Sigma=S^2$; as an indirect argument, we also assume that $m=0$ in the T^2 case, or that $m\geqslant m_{\text{crit}}$ in the remaining cases. In the sphere or torus case from the strong maximum principle we obtain

$$W\equiv W_0. \tag{VII.36}$$

In the higher genus cases we consider (VII.15) again but take here as RS a generalized Kottler solution with the same mass as the given one, $m_0=m$. Equations (VII.34)–(VII.35) hold again; then Lemma VII.1 shows that equality must hold in (VII.35). Applying the maximum principle again yields Eq. (VII.36). We note that both point (a) as well as the structural hypotheses of Lemma VII.3 hold under the hypotheses of Theorem I.3. Equation (VII.36) and the discussion of Sec. II show that point (2) of that lemma applies, so that the given solution must be a member of the generalized Kottler family with m in the range (II.6) (the generalized Nariai metrics are excluded as they do not satisfy the asymptotic hypotheses of Theorem I.3). In the case $\partial_\infty\Sigma=S^2$ point (1) readily follows. In the remaining cases none of these solutions has the topology required in Theorem I.3, which gives a contradiction and establishes Theorem I.3. □

Proof of Theorem I.5: By choice of the RS we have $(\widetilde{W}-\widetilde{W}_0)|_{\partial\Sigma}=0$. We normalize V again so that $\lim_{\to\infty}(\widetilde{W}-\widetilde{W}_0)=0$ holds, cf. Proposition III.3 and Eq. (III.15). Negativity of m_0 implies

that a in (VII.15) is non-negative. The maximum principle applied to Eq. (VII.15) gives $\tilde{W}-\tilde{W}_0\leqslant 0$ on Σ, with equality being achieved somewhere if and only if $W\equiv W_0$. Moreover, as in the proof of point (2) the boundary version of the strong maximum principle (Ref. 69, Theorem 3.6) implies that $n^{i\prime}D_i'(\tilde{W}-\tilde{W}_0)>0$ on $\partial_\infty\Sigma$ unless $W=W_0$. Lemma VII.1 allows us to conclude that either $m<m_0$ or $W\equiv W_0$. In that last case point (2) of Lemma VII.3 implies that (Σ,g,V) corresponds to a generalized Kottler solution. In any case there holds $m\leqslant m_0$.

To prove the area inequality in (I.8) requires some care as the metric $\tilde{g}$ defined in Eq. (VII.4) is singular at Σ, so that standard maximum principle arguments such as Ref. 69, Theorem 3.6 do not apply. We proceed as follows. By choice of W_0 we have $\tilde{W}=\tilde{W}_0$ on $\partial_1\Sigma$. Further, Eq. (VII.2) shows that $n^iD_i(\tilde{W}-\tilde{W}_0)$ vanishes there. De l'Hospital's rule, the nonvanishing of dV at $\partial\Sigma$, and the requirement $\tilde{W}-\tilde{W}_0\leqslant 0$ lead to

$$n^jn^iD_iD_j(\tilde{W}-\tilde{W}_0)|_{\partial\Sigma}=\lim_{V\to 0}\frac{D^iVD_i(\tilde{W}-\tilde{W}_0)}{V}\leqslant 0.$$

It follows that the left-hand side of Eq. (VII.13) is nonpositive, which establishes the second part of (I.8). □

Proof of Corollary I.6: Assume that $\partial\Sigma$ is connected and that (VI.2) holds; we want to show that (I.8) implies an inequality inverse to (VI.2). In order to do this, note first that by (I.8) the mass m is nonpositive, and Eq. (VI.2) implies that $g_{\partial\Sigma}>1$. It is useful to introduce a genus-rescaled area radius $r_{\partial\Sigma}$ by the formula

$$r_{\partial\Sigma}=\sqrt{\frac{A_{\partial\Sigma}}{4\pi(g_{\partial\Sigma}-1)}}.$$

In terms of this object, the inequality (VI.2) reads

$$2m|g_\infty-1|^{3/2}+\left(r_{\partial\Sigma}+\frac{\Lambda}{3}r_{\partial\Sigma}^3\right)|g_{\partial\Sigma}-1|^{3/2}\geqslant 0. \tag{VII.37}$$

It follows that $r_{\partial\Sigma}+(\Lambda/3)r_{\partial\Sigma}^3\geqslant 0$, and the Galloway–Schleich–Witt–Woolgar inequality[4] $g_{\partial\Sigma}\leqslant g_\infty$ implies

$$2m+r_{\partial\Sigma}+\frac{\Lambda}{3}r_{\partial\Sigma}^3\geqslant 0. \tag{VII.38}$$

Let us denote by r_0 the $r_{\partial\Sigma}$ corresponding to the relevant generalized Kottler solution:

$$r_0=\sqrt{\frac{A_0}{4\pi(g_{\partial_\infty\Sigma}-1)}}.$$

The inequality (VII.38) is actually an equality for the generalized Kottler solutions, therefore it holds that $2m_0+r_0+(\Lambda/3)r_0^3=0$. We have $r_0\geqslant 1/\sqrt{-\Lambda}$ from (II.8), and $m\leqslant m_0$, $r_{\partial\Sigma}\geqslant r_0$ from (I.8), so that

$$\begin{aligned}2m+r_{\partial\Sigma}+\frac{\Lambda}{3}r_{\partial\Sigma}^3&=2m+r_{\partial\Sigma}+\frac{\Lambda}{3}r_{\partial\Sigma}^3-2m_0-r_0-\frac{\Lambda}{3}r_0^3\\&=2(m-m_0)+(r_{\partial\Sigma}-r_0)\left[1+\frac{\Lambda}{3}(r_{\partial\Sigma}^2+r_{\partial\Sigma}r_0+r_0^2)\right]\\&\leqslant(r_{\partial\Sigma}-r_0)(1+\Lambda r_0^2)\leqslant 0.\end{aligned} \tag{VII.39}$$

It follows from Eqs. (VII.38)–(VII.39) that $r_{\partial\Sigma}=r_0$, $m=m_0$, and the rigidity part of Theorem I.5 establishes Corollary I.6. □

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Magnification relations in gravitational lensing via multidimensional residue integrals

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We investigate the so-called magnification relations of gravitational lensing models. We show that multidimensional residue integrals provide a simple explanation for the existence of these relations, and an effective method of computation. We illustrate the method with several examples, thereby deriving new magnification relations for galaxy lens models and microlensing (point mass lensing). © *2001 American Institute of Physics.* [DOI: 10.1063/1.1347394]

I. INTRODUCTION

Gravitational lensing has proven to be not only important astrophysically, but intriguing mathematically as well. Mathematical investigations of gravitational lens theory have yielded important results and insights,[1–6] employing techniques and results from such disparate areas as catastrophe theory, differential geometry and Morse theory. In this paper, we illustrate how another seemingly unrelated subject, multidimensional residue calculus, applies to gravitational lensing, and specifically we explain the origin of certain ''magnification relations'' that have been discussed in the lensing literature.[7–10] We additionally demonstrate that calculations of these magnification relations are enormously simplified using residue techniques, and illustrate the method by deriving several new results.

This paper is organized as follows. In the remainder of this section, we introduce the relevant terminology of gravitational lensing, and describe the magnification relations. In Sec. II, we express the problem in terms of residue calculations at the image positions, and thereby relate it to a residue at infinity. Using one-dimensional residue calculus, we derive trace formulas for the magnification relations for a subset of lens models. In Sec. III, we consider a more general class of lens models, and describe how to perform the necessary multidimensional residue integrals. In Sec. IV, we apply this formalism and derive previously known results, as well as new results. In Sec. V, we summarize our results and discuss implications. The material discussed in Secs. II–IV may be unfamiliar to astronomers, and so we provide a simple procedure which may be applied to models to obtain their magnification relations, without requiring a detailed understanding of the underlying mathematics.

A. Gravitational lensing terminology

Numerous excellent introductions to gravitational lensing have been written, e.g., Refs. 1, 2; here we briefly summarize some of the results and terminology relevant to our discussion. The effects of gravitational lensing can perhaps best be understood by considering the time delay of trajectories connecting the lensed source to the observer.[1] The time delay is a simple sum of two terms, a ''geometrical'' piece, and a ''gravitational'' piece. Let ϕ_N be the three-dimensional (3-D) Newtonian potential, and $\psi=(2/Dc^2)\int \phi_N\, dl$ the projected 2-D potential, where D is a function of

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cosmology and the source and lens redshifts. Just as $\nabla^2\phi_N = 4\pi G\rho$, similarly $\nabla_\perp^2\psi \propto 4\pi G\Sigma$, where $\Sigma = \int \rho\, dl$ is the surface density. In the thin-screen, small deflection limit, the time delay can be written as

$$\tau = \tau_0(\tfrac{1}{2}|\vec{\Theta} - \vec{\beta}|^2 - \psi), \tag{1}$$

where the normalization τ_0 depends upon cosmology and the lens and source redshifts, $\vec{\Theta}$ is the image location on the sky and $\vec{\beta}$ is the location the source would have had, had not the lens intervened. Light rays follow null geodesics, which can be shown to obey Fermat's principle.[2] Plotting time delay as a function of the two angular coordinates on the sky, Fermat's principle demands that images arise at the stationary points of this time delay surface. Setting the gradient of the time delay to zero gives the so-called ''lens equations,'' the (real) solutions of which are the image positions. Since the time delay surface can have multiple stationary points, multiple images of a single source can arise, and the image multiplicity can depend on the source position relative to the lens. The curves on the source plane separating regions of different image multiplicity are called caustics. As a source crosses over a caustic, its image multiplicity generically changes by two, as a pair of images either merge together and annihilate, or are created and move apart. The magnification μ, which relates differential area elements of the unlensed source to area elements of the lensed images, is simply the inverse of the Jacobian J of the mapping from image coordinates $\vec{\Theta}$ to source coordinates $\vec{\beta}$. Since the orientation of an image can be inverted relative to the unlensed source, the magnification can have either sign. Much of the lensing literature adopts the convention of positive magnifications (i.e., defining $\mu = 1/|J|$); in this paper we always take the magnification to be signed, i.e., $\mu = 1/J$.

B. Lens models

Two astrophysically important types of lenses are compact objects (like stars or MACHOs) and galaxies. The former class are effectively point masses, and so have lensing potentials proportional to the Green's function for the 2-D Laplacian, i.e., $\psi = m \log r$ where m is proportional to the mass of the point lens. Only the weak-field regime is observationally relevant, so the potentials linearly superpose for multiple point masses (as long as they are not appreciably separated along the line of sight). Galaxies have more complicated, extended mass distributions with correspondingly complicated lens potentials. In principle, one may decompose the potential into eigenfunctions of the 2-D Laplacian,[11]

$$\psi = \sum_{m,n} (a_{mn}\cos m\theta + b_{mn}\sin m\theta) r^n. \tag{2}$$

This has the advantage that each term in the expansion relates to a corresponding multipole in the expansion of the surface density. In practice, it is necessary to truncate the series due to the limited observational constraints. Since galaxies are believed to have roughly ''isothermal'' $\rho \sim r^{-2}$ profiles, such truncated series generally consist of variations on the singular isothermal sphere (SIS) potential $\psi = br$. Two examples considered by Kochanek[11] are the SIS+elliptical potential $\psi = br(1 + \gamma\cos 2\theta)$ and the SIS+external shear $\psi = br + (\gamma/2)\, r^2 \cos 2\theta$. Another variation[12] is the singular isothermal ellipse (SIE) $\psi = bR = b\sqrt{x^2 + y^2/q^2}$ with axis ratio q. Other, more elaborate and more physically justified models have been employed in the lensing literature; here we will focus on simple models such as the above to avoid obfuscating the general method with heavy algebra. In Table I we list the models considered in this paper.

Given a model for the lens, the lensed images of a given source may be found by solving the lens equations as described above. For simple potentials, the solutions are often analytic. For example, consider the the SIS+external shear model. The stationarity equations become

TABLE I. Model lens potentials and results. The lth lens has mass m_l and position $\vec{\Theta}_l$. For the galaxy potentials, with only one lens, we choose coordinates centered on the lens and oriented along the ellipticity or shear axes. Here, the image position $\vec{\Theta}=(x,y)=(r\cos\theta, r\sin\theta)$ and source position $\vec{\beta}=(x_s,y_s)=(s\cos\theta_s,\ s\sin\theta_s)$. We use the complex notation (Ref. 3) $z=x+iy$, and similarly for z_s, z_l. Also, $R=\sqrt{x^2+y^2/q^2}$ is an elliptical radial coordinate, γ is the strength of the shear and q is the axis ratio. We reiterate that these results are physically meaningful only when all solutions to the lens equations are real.

Model	ψ	$\Sigma_i \mu_i$	$\Sigma_i \mu_i z_i$
point masses	$\Sigma_l m_l \log\lvert\vec{\Theta}-\vec{\Theta}_l\rvert$	1	$z_s+\Sigma_l \frac{m_l}{\bar{z}_s-\bar{z}_l}$
point masses+shear	$\psi_{\rm pm}+\frac{\gamma}{2}r^2\cos 2\theta$	$1/(1-\gamma^2)$	$\frac{1}{(1-\gamma^2)^2}(z_s+\gamma\bar{z}_s)$
SIE	bR	2	$2z_s$
SIS+elliptical	$br+\gamma br\cos 2\theta$	1	$z_s+2\gamma\bar{z}_s-\frac{\bar{z}_s^3}{32b^2\gamma^2}$
SIS+shear	$br+\frac{\gamma}{2}r^2\cos 2\theta$	$2/(1-\gamma^2)$	$\frac{2}{(1-\gamma^2)^2}(z_s+\gamma\bar{z}_s)$
SIE+shear	$bR+\frac{\gamma}{2}r^2\cos 2(\theta-\theta_\gamma)$	$2/(1-\gamma^2)$	$\frac{2}{(1-\gamma^2)^2}(z_s+\gamma e^{2i\theta_\gamma}\bar{z}_s)$

$$\frac{\partial\tau}{\partial r}=r-s\cos(\theta-\theta_s)-b-\gamma r\cos 2\theta=0, \tag{3}$$

$$\frac{1}{r}\frac{\partial\tau}{\partial\theta}=s\sin(\theta-\theta_s)+\gamma r\sin 2\theta=0, \tag{4}$$

where (r,θ) is the image position in polar coordinates, and (s,θ_s) is the source position. From this it is easy to show that the quantity $u=e^{i\theta}$ satisfies the fourth degree polynomial equation,

$$\gamma b u^4+\left(\gamma s v+\frac{s}{v}\right)u^3-\left(sv+\frac{\gamma s}{v}\right)u+\gamma b=0, \tag{5}$$

with $v=e^{i\theta_s}$. As a quartic equation in u, this can be solved analytically, and from u the image coordinates (r,θ) follow simply. For many models, it is possible to eliminate all but one variable in a similar fashion and thereby obtain analytic solutions, but for more realistic models, the lens equations must be solved numerically.

C. Magnification relations

As mentioned above, there are in general multiple lensed images for a given source. These images lie at the discrete positions satisfying the lens equations for a given source position, and the images have different magnifications and orientations. If we restrict ourselves to purely real solutions of the lens equations (i.e., the physically observable images) then the number of images changes when the source crosses over a caustic. The number of solutions, of course, does not change, but instead generically a pair of complex solutions become real (for a source crossing into a caustic) or a real pair become complex (for a source crossing out of a caustic).[5] For certain lens models, such as the simple potentials described above, there may exist certain parameter ranges such that *all* solutions to the lens equations are real. In such cases, it has been shown that there exist interesting and surprising relations among the image positions and magnifications. First, Witt and Mao[7] considered lensing by a binary microlensing system, involving two point masses, and derived the following result: when the image multiplicity is maximized, the sum of the signed magnifications of all the images is always 1. That is, $\Sigma_i \mu_i=1$, independent of quantities such as

the lens masses, separation, or source position (as long as the source is inside a caustic). This is quite an astonishing result, as the individual image magnifications can vary wildly as the source position changes, and even diverge as the source crosses a caustic. Witt and Mao derived this result by using resultants to obtain a monic polynomial equation satisfied by μ, and noted that the sum of the roots is given by the subleading coefficient. Rhie,[8] using similar reasoning, showed that a similar result is true for an arbitrary number of point mass lenses. Dalal[9] extended this work to galaxy potentials like those described above. Again, the magnification relations were obtained by using elimination theory (e.g., Gröbner bases) to obtain monic polynomial equations in μ; the ''total magnification'' was then given by the subleading coefficient. We summarize these results in Table I.

Subsequently, Witt and Mao[10] showed that for a particular class of power-law models, there exist additional magnification relations, involving not only μ but the image positions as well. They derived this result by separating the coupled lens equations into disjoint x and y equations, and then relating μ to the coefficients. Just as previous work had derived expressions for $\Sigma_i \mu_i$, Witt and Mao found expressions for $\Sigma_i \mu_i x_i^k$ and $\Sigma_i \mu_i y_i^k$. They called these the ''kth moments,'' and we adopt their terminology here. For example, they found that the first moment $\Sigma_i \mu_i \vec{\Theta}_i = 2\vec{\beta}$ for the SIE model.

The general pattern seen in previous work is that both the total magnification and the higher moments can be expressed in terms of the model parameters, and that progressively higher moments have progressively more complicated forms involving more of the parameters. The expressions' independence of certain parameters suggests some sort of invariant, but clearly not a topological invariant since certain models seemed not to obey any magnification relations whatsoever. Indeed, the origin of the magnification relations and their absence in certain models has been a mystery. In this paper, we provide an explanation of these relations, and additionally find a method easier than elimination theory to derive them.

D. Residue integrals

As noted above, the lens equations have multiple discrete solutions, both real and complex. While only the real solutions have a physical meaning, it is instructive to consider the complex solutions as well. In this paper, we will henceforth treat the image coordinates $\vec{\Theta}$ as complex variables. We are interested in the sum over these discrete points of various quantities, such as the signed magnification, or magnification times position, etc. From complex analysis, we know that one may relate a sum over discrete points to an integral over a contour encircling those points, by choosing an integrand which has poles at those points. For lensed images, which are stationary points of the time delay, there is an obvious class of integrands, namely rational functions of the form

$$f(x,y) = \frac{g(x,y)}{\partial_x \tau \, \partial_y \tau}. \tag{6}$$

There are complications, which we discuss later, due to the fact that the integrals here are multidimensional; however, the analogy to the one-dimensional case should be clear. We need only find the appropriate function g such that f will have a residue equaling the quantity we wish to sum over the images, and choose a contour large enough to enclose all the images. Now, converting a discrete sum to a contour integral would not seem to be much progress, however we can use another idea from one-dimensional complex analysis. Recall that by inverting coordinates (mapping the origin to infinity and vice versa) one can see that the sum of the residues of poles inside the contour is equal to the sum of the residues of poles outside the contour, but with opposite sign. In our case, we are summing over all the finite solutions, so the only pole outside the contour is at infinity. This is the essence of the method described in this paper: we relate the sum over the images to the behavior of the time delay at infinity, and we simply evaluate the residue at the

point(s) at infinity. The validity of the resulting magnification relations does not depend on the image coordinates being real, although of course their physical applicability does.

The methods presented in this paper apply when the lens equations are polynomial in the image variables. Lens equations containing algebraic functions, such as nth roots, can be put in this form by introducing an additional variable for each algebraic function along with the polynomial equation it satisfies. For example, if $\sqrt{x^3+1}$ appears, we introduce z satisfying $z^2=x^3+1$. In principle, these extra variables can then be eliminated to return to two equations in two variables. In Sec. II we discuss ''trace methods,'' which are based on ordinary one-dimensional complex analysis and apply when the lens equations can be conveniently reduced to one polynomial equation in one variable. In Sec. III we discuss residue methods which can be applied directly to two polynomial equations in two image variables. In Sec. IV we illustrate with specific examples. Possible extensions of our methods are discussed in Sec. V.

II. TRACE METHODS

Our method in this section is useful when all but one variable can be conveniently eliminated from the lens equations, e.g., Eq. (5). Of course, this is always possible in principle, but it may require computer implementation of Gröbner basis algorithms in practice. Thus, we assume that the x-coordinates of the images are the roots x_i of a polynomial equation of degree n,

$$f(x)=\sum_{i=0}^{n} a_i x^i=0. \tag{7}$$

We assume that the signed magnification $\mu(x)$ of an image at x is given by a rational function,

$$\mu=\frac{p(x)}{q(x)}, \tag{8}$$

where the denominator has no common roots with $f(x)$. This will necessarily be the case if the coordinates are chosen generically, since there will then be at most one image at a given x-coordinate, whose magnification must be a single-valued algebraic function of x. We wish to calculate the total magnification,

$$M=\sum_i \mu(x_i)\equiv \mathrm{Tr}\,\mu, \tag{9}$$

where the ''trace'' notation will be explained below. Generically, the roots x_i of $f(x)$ will be distinct; since M is determined by continuity when some roots coincide we will always consider the generic case.

Let $A=\mathbb{C}[x]$ be the ring of polynomials in x with complex coefficients. We call two polynomials g and h equivalent, writing $g\sim h$, if they differ by a polynomial multiple of $f(x)$. This sorts the polynomials into equivalence classes, and we denote the class containing g by $[g]$ and the set of all equivalence classes by A_f. This is of use for our problem because all polynomials in a given class take the same values at the x_i and therefore have the same trace. Addition and multiplication of classes are well-defined by $[g]+[h]=[g+h]$, $[g][h]=[gh]$, and A_f is itself a ring.

Now we observe that each class $[g]\in A_f$ contains a representative which has degree (at most) $n-1$. Indeed, the relation $f\sim 0$ implies

$$a_n x^n \sim -\sum_{i=0}^{n-1} a_i x^i, \tag{10}$$

and this can be used to eliminate all terms of degree n or greater from a polynomial g. The resulting polynomial is unique, being determined by its values at the n roots x_i. It follows that A_f is in fact a vector space of dimension n over $\mathbb{C}$.

Now consider, instead of polynomials, the set R of rational functions of x which are defined at the zeros of $f(x)$, and call two elements equivalent if their difference is $f(x)$ times another element. Then all elements of a class have the same trace, and the set R_f of equivalence classes is again a ring. In fact, it is isomorphic to A_f. An isomorphism is obtained by associating to a class $[g]$ in A_f the obvious class $[g]$ in R_f. To see that this mapping is invertible, we must find a polynomial representative g of an arbitrary class $[h]$ in R_f. To do so, simply let $g(x)$ be the unique polynomial of degree $n-1$ satisfying $g(x_i)=h(x_i)$ for all i. Then $g-h$ is a rational function vanishing at every x_i, so when expressed in lowest terms its numerator must be a multiple of $f(x)$. Therefore $g\in[h]$.

At this point we can explain the ''trace'' terminology for the sum over the roots x_i.[13] The vector space A_f has a basis consisting of (the classes of) the n polynomials δ_i of degree $n-1$ defined by $\delta_i(x_j)=\delta_{ij}$. Fix an element $g\in A_f$ and consider the linear operator on A_f given by multiplication by g. In the given basis, the matrix of this operator is diagonal, with entries $g(x_i)$. Hence the trace of this matrix, which is independent of the basis and coincides with the trace of the operator, is simply $\mathrm{Tr}\, g=\Sigma_i g(x_i)$. For example, consider $\mathrm{Tr}\, x$, which just gives the sum of the roots. Choosing the basis $\{1,x,x^2,\ldots,x^{n-1}\}$ for A_f, the matrix of the operator of multiplication by x has only one nonzero diagonal entry, $-a_{n-1}/a_n$, arising from the relation $x\cdot x^{n-1}\sim -(a_{n-1}/a_n)x^{n-1}+\cdots$. This recovers the standard result for the sum of the roots of a polynomial and shows how our method generalizes others based on that result.[7–10]

Returning to the problem of computing the total magnification, we see that $M=\mathrm{Tr}\,\mu=\mathrm{Tr}[\mu]$ can be computed using any element in its equivalence class. For example, we can choose the unique polynomial representative of degree $n-1$. Of course, we do not determine this polynomial from its values $\mu(x_i)$, since we do not know the x_i explicitly. Instead, we seek a polynomial solution of degree $n-1$ to the condition (8) defining $[\mu]$,

$$[\mu q(x)]=[p(x)]. \tag{11}$$

This is solved by using Eq. (10) to reduce the degree of each side to $n-1$, and then equating coefficients.

To compute the trace we use a formula due to Euler, which we derive by means of the residue theorem for complex contour integrals. A purely algebraic proof is not difficult,[14] but our derivation shows the relevance of residue methods and motivates the multivariable generalization which we describe in the following section. Consider the contour integral,

$$\frac{1}{2\pi i}\oint \frac{f'(x)\mu}{f(x)}dx, \tag{12}$$

where the contour is a large circle in the complex plane enclosing all the zeros x_i of $f(x)$. The integrand has a pole of residue $\mu(x_i)$ at x_i, and consequently the integral is $\mathrm{Tr}\,\mu$. However, we can also regard the contour as encircling the point at infinity and evaluate the integral in terms of the residue there, introducing if we wish the new variable $u=1/x$ to move the point at infinity to the origin. Furthermore, the integral is unchanged if $f'(x)\mu$ is replaced by any member of its equivalence class. By choosing the polynomial representative of degree $n-1$ we need only evaluate

$$\frac{1}{2\pi i}\oint \frac{x^k}{f(x)}dx=\frac{\delta_{k,n-1}}{a_n},\quad 0\leqslant k\leqslant n-1. \tag{13}$$

This proves Euler's formula,

$$\mathrm{Tr}\,\mu=\frac{\text{coefficient in degree } n-1 \text{ of } f'(x)\mu}{\text{coefficient in degree } n \text{ of } f(x)}, \tag{14}$$

where it is understood that the polynomial representative of degree $n-1$ is meant in the numerator. This makes it clear that the total magnification is determined by the leading behavior of $f(x)$ and $f'(x)\mu$ at infinity.

As an example, we consider a generalization of the SIS+elliptical potential ($n=1$ multipole) with an arbitrary harmonic, $\psi = br + \gamma br\cos m\theta$. As an aid to clarity, we shall depart from conventional notation, and instead rewrite the lens equations so that the variables are x,y, and parameters are denoted $a,b,c,\ldots$. In this case we define $x=e^{i\theta}$, $y=r$, $a=\gamma$, $b=b$, $c=s$, $d=e^{i\theta_s}$. The lens equations then take the form

$$f(x) = mabx^{2m} + c\,d^{-1}x^{m+1} - c\,dx^{m-1} - mab = 0, \tag{15}$$

$$2(y-b) - c(xd^{-1} + dx^{-1}) - ab(x^m + x^{-m}) = 0, \tag{16}$$

with the magnification satisfying

$$[m^2 ab(x^m + x^{-m}) + c(xd^{-1} + dx^{-1})]\mu = 2y. \tag{17}$$

Eliminating y results in

$$[m^2 abx^{2m} + c\,d^{-1}x^{m+1} + c\,dx^{m-1} + m^2 ab]\mu = abx^{2m} + cd^{-1}x^{m+1} + 2bx^m + c\,dx^{m-1} + ab. \tag{18}$$

Dividing through by x and replacing x^{-1} in the resulting equation with a polynomial equivalent via the relation $x^{-1}f(x) \sim 0$ produces

$$\begin{aligned}[2m^2 abx^{2m-1} + (m+1)c\,d^{-1}x^m - (m-1)c\,dx^{m-2}]\mu \\ \sim 2abx^{2m-1} + (1+m^{-1})c\,d^{-1}x^m + 2bx^{m-1} + (1-m^{-1})c\,dx^{m-2},\end{aligned} \tag{19}$$

where the left side is precisely in the Euler form $f'(x)\mu$. Then we immediately have the total magnification invariant as

$$M = \mathrm{Tr}\,\mu = \frac{2ab}{mab} = \frac{2}{m}. \tag{20}$$

It is no harder to verify that the total magnification is the same for a potential containing an arbitrary finite sum of harmonics $\Sigma_{k=1}^{m} b_k r\cos k\theta$; the highest harmonic determines M. Other models are amenable to this method as well.

In principle one can compute moments by this method, by replacing μ with $x^k\mu$ in the relevant equations, but we have preferred the residue methods of the next section for moment computations.

III. RESIDUE METHODS: THEORY

Let us review the key steps in our contour integral derivation of Euler's formula in the previous section. First, we expressed the total magnification as a complex contour integral of a function having poles at the image locations. Second, we converted this to an integral around the point at infinity. This amounts to viewing the complex plane as a subset of the Riemann sphere, or complex projective space $\mathbb{CP}^1$. Our change of variables $u=1/x$ connects two coordinate charts on $\mathbb{CP}^1$ centered at the origin and at infinity. Finally, we evaluated the residue at infinity, making it clear that the total magnification depends on the behavior of the integrand at infinity.

These steps all have multivariable analogs. In fact, there is a well-developed, if little-known, residue theory for meromorphic differential forms in several complex variables. This makes it possible to compute directly the total magnification and moments for lens models without reducing to one-variable lens equations. The theory is particularly effective in the situation of two

variables, and we describe it in this case. References include Refs. 15–18. An application to chemical reaction rate equations appears in Ref. 19, but we are not aware of other physical applications in the literature.

We consider a meromorphic two-form,

$$\omega = \frac{g(x,y)\,dx\,dy}{P_1(x,y)P_2(x,y)}, \tag{21}$$

on $\mathbb{C}^2$, which we view as a subset of the compact complex projective space $\mathbb{CP}^2$. Here P_1, P_2 are polynomials having finitely many common zeros (the image locations) of multiplicity one (as is generically the case), and g is also a polynomial. Such a form can be integrated over a 2-cycle, a compact two-dimensional real submanifold of $\mathbb{CP}^2$. Since ω is closed ($d\omega = 0$), the integral depends only on the homology class of the cycle. For example, in a small neighborhood of a common zero of the P_i, we can integrate over the ''torus'' T:$\{|P_1| = |P_2| = \epsilon\}$, defining the residue of ω at this zero:

$$\mathrm{Res}\,\omega = \left(\frac{1}{2\pi i}\right)^2 \int_T \omega. \tag{22}$$

[The standard orientation of T is that specified by the nonvanishing 2-form $d(\arg P_1)\,d(\arg P_2)$. That is, T is oriented so that $dP_1\,dP_2/(2\pi i)^2 P_1 P_2$ has a positive integral.] We will always denote by J the naive Jacobian of the mapping $(x,y) \mapsto [P_1(x,y), P_2(x,y)]$, namely,

$$J = \frac{\partial(P_1,P_2)}{\partial(x,y)} = \begin{vmatrix} \partial_x P_1 & \partial_y P_1 \\ \partial_x P_2 & \partial_y P_2 \end{vmatrix}. \tag{23}$$

This coincides with the physical Jacobian relating corresponding area elements in the source and image planes if x,y are rectangular coordinates, and P_1, P_2 are the corresponding lens equations, but requires a correction factor otherwise. The first key fact we need is that the residue at a nondegenerate zero (one where J does not vanish), located say at the origin, is given by[18]

$$\mathrm{Res}\,\frac{g\,dx\,dy}{P_1 P_2} = \frac{g(0)}{J(0)}, \tag{24}$$

which is equal to the magnification of the corresponding image if g is chosen appropriately ($g = 1$ for rectangular coordinates). Moments of magnification can be computed by including additional monomial factors in $g(x,y)$.

Next we need the Global Residue Theorem,[18] which states that the sum of all the residues of a meromorphic form, such as ω, on any compact manifold, such as $\mathbb{CP}^2$, vanishes. Note that this sum is over the common zeros of the P_i only, so that points where only one polynomial vanishes do not contribute; also the points summed over may depend on the choice of the factorization $P_1 P_2$ of the denominator of ω. The theorem makes it possible to replace the sum over the residues at the common zeros in $\mathbb{C}^2$ by minus the sum of residues at points at infinity in $\mathbb{CP}^2$. This is the fundamental explanation for the existence of magnification relations in general: compactness relates the sum of finite residues to the behavior of the lens equations at infinity, indeed to a finite number of terms in an expansion around infinity. It remains to explain how to locate the common zeros at infinity and compute their residues.

$\mathbb{CP}^2$ is conveniently described by homogeneous coordinates $[X,Y,U] \neq [0,0,0]$, where $[\lambda X, \lambda Y, \lambda U]$ is identified with $[X,Y,U]$ for all complex $\lambda \neq 0$. The points with $U \neq 0$ can be represented in the form $[x,y,1]$ and are viewed as the subset $\mathbb{C}^2$ of finite points. The polynomials $P_i(x,y)$ correspond to homogeneous polynomials $P_i^h(X,Y,U) \equiv U^{\deg P_i} P_i(X/U, Y/U)$. Their common zeros at infinity are those having $U = 0$. These also lie in coordinate charts diffeomorphic to

$\mathbb{C}^2$, described by $[1,y,u]$ or $[x,1,u]$. In these charts they can be treated just as are ''finite'' zeros. The meromorphic form ω is homogenized so as to have total degree zero, that is,

$$\omega^h = \frac{g(X/U,Y/U)\,d(X/U)\,d(Y/U)}{P_1(X/U,Y/U)P_2(X/U,Y/U)} = \frac{g^h U^{\deg P_1+\deg P_2-\deg g-3}(U\,dX\,dY - X\,dU\,dY - Y\,dX\,dU)}{P_1^h P_2^h}. \tag{25}$$

When $n \equiv \deg g - \deg P_1 - \deg P_2 + 3 > 0$, the denominator of ω^h takes the form $U^n P_1^h P_2^h$. This creates a subtlety in that the above theory applies to a chosen factorization of the denominator into two factors. Thus, we may factor it as $(U^n P_1^h)(P_2^h)$ and treat these as the two factors in applying the residue theorem. The common zeros then consist of all (finite and infinite) common zeros of the P_i^h, together with any zeros of P_2^h alone at infinity. The latter might have been overlooked in a naive application of the theorem. In the examples we will consider in detail, no such additional zeros exist, but we will point out a case where they do.

Unfortunately, the zeros at infinity are rarely nondegenerate, and their residues cannot be computed using Eq. (24). Instead, they typically lie at singular points of the curves $P_i = 0$, that is, at least one curve has multiple branches meeting at this point.[20] There is a classical method, dating back to Newton, for finding the branches of an algebraic curve $P(x,y)=0$ at a singular point, taken to be the origin. The branches are given as Puiseux series, or fractional power series, of the form

$$y = \sum_{i=0}^{\infty} a_i x^{\alpha_i}, \tag{26}$$

where the exponents α_i form an increasing sequence of rational numbers whose denominators eventually stabilize. The possibilities for the leading exponent α_0 are determined by requiring that at least two terms in the polynomial $P(x,a_0x^{\alpha_0})$ have the same degree, while the remaining terms have a higher degree. Then a_0 is found by demanding the vanishing of the terms of minimal degree. An elegant graphical method for identifying the possible exponents α_0 is provided by the Newton polygon, or diagram.[17,21] For each monomial $x^a y^b$ appearing in $P(x,y)$, plot the point (a,b) in the coordinate plane. Begin at the lowest of the leftmost points (minimize a, then minimize b) and draw a polygonal path with vertices at a subset of the points, terminating at the leftmost of the lowest points (minimize b, then minimize a), and choosing each successive segment to have the smallest possible slope (steepest possible negative slope). This is the Newton diagram of the polynomial $P(x,y)$. The points lying on any segment of the Newton diagram represent terms in P which will have minimal degree if α_0 is chosen as the negative reciprocal of the slope of that segment. The next term in the Puiseux series can be found by applying the same procedure to $P(x,a_0x^{\alpha_0}+\tilde{y})$, and so on. One term is often enough for computing the total magnification; higher moments require more terms in general. The denominators of the exponents stabilize at the stage where the Newton diagram has only a single segment. The curve $P(x,y)=0$ has at least as many branches at the origin as there are segments in the Newton diagram, and has more if there are multiple solutions to the equations for the coefficients a_i.

Consider one particular branch X of the curve $P_1(x,y)=0$ at a singular point, given by a Puiseux series $y = a_0x^{m/n} + \cdots$, with m,n relatively prime. On this branch draw a small circle C around the origin; its projection on the x-plane must wind n times around the origin. Now construct a 2-torus δC by ''thickening'' C: at any point p of C take a plane transverse to X and a small circle in this plane with center p. As p moves around C this circle sweeps out the torus δC. We may construct such a torus for each branch of the curve. These are called Leray tori, and the ''thickening'' operator δ is the Leray coboundary.

Our objective is to compute the residue integral $\int_T \omega$ at the origin. We can work entirely within a small ball B around the origin. The residue depends on the homology class of T in $H_2(B-\{P_1P_2=0\})$. As we explain in the Appendix, this class is, up to sign, the sum of the

classes of the Leray tori constructed on the branches of *either* of the curves $P_1=0$ or $P_2=0$. Therefore the residue is the sum of the integrals of ω over either set of Leray tori, with appropriate orientation.

The integral over a Leray torus δC lying on a branch of $P_1(x,y)=0$ given by a Puiseux series $y=p(x)$ is computed using the Leray residue formula. We give this formula under the assumption that $\partial_y P_1$ does not vanish on the given branch, which amounts to assuming that $y=p(x)$ is a branch of an irreducible factor of P_1 which appears to the first power only (the analog of a simple rather than multiple pole). The general formula can be found in Ref. 16. Our case reads as

$$\frac{1}{2\pi i}\int_{\delta C}\frac{g\,dx\,dy}{P_1P_2}=-\int_C\left.\frac{g\,dx}{P_2\,\partial_y P_1}\right|_{y=p(x)}, \tag{27}$$

which is proved as follows. To integrate over δC, we can integrate first over the circles in the planes transverse to C, then over C itself. Since these circles are centered at $P_1=0$, we can change variables from x,y to x,P_1 by means of $dP_1\,dx=-dx\,dy\,\partial_y P_1$ and then integrate over P_1 by means of the one-variable residue theorem. The evaluation of the residue at $P_1=0$ by substituting $y=p(x)$ leaves another one-variable residue integral to be performed. For this one must keep in mind that the cycle C may wind around the origin several times in the x-plane.

The Leray residue formula holds with obvious notational and possible sign changes if the Leray torus lies on a branch of $P_2(x,y)=0$, or if we choose to eliminate x rather than y in favor of a P_i.

IV. RESIDUE METHODS: EXAMPLES

In this section we apply the residue methods just developed to various lens models. The first is a generalized $n=2$ multipole model with potential $\psi=br+(\gamma/2)r^2\cos m\theta$. We again redefine notation to clarify the computation, writing the variables as x,y and the parameters as $a,b,c,\ldots$. Let $x=e^{i\theta}$, $y=r$, $a=\gamma$, $b=b$, $c=s$, $d=e^{i\theta_s}$. The lens equations then take the form

$$P_1=c\,d^{-1}x^{m+1}-c\,dx^{m-1}+\frac{m}{2}ay(x^{2m}-1)=0, \tag{28}$$

$$P_2=2(y-b)x^m-c\,d^{-1}x^{m+1}-c\,dx^{m-1}-ay(x^{2m}+1)=0. \tag{29}$$

Because x,y are not rectangular coordinates, there is an extra Jacobian factor in the magnification, and we find

$$\mu=\frac{4yx^{2m-1}}{J}. \tag{30}$$

Consequently the total magnification is given by the residue sum,

$$M=\sum_{\text{images}}\operatorname{Res}\frac{4yx^{2m-1}dx\,dy}{P_1P_2}. \tag{31}$$

The residue theorem relates this to the sum of the residues at points at infinity in $\mathbb{CP}^2$, which are found from the homogeneous forms of the P_i:

$$P_1^h=c\,d^{-1}X^{m+1}\,U^m-c\,dX^{m-1}\,U^{m+2}+\frac{m}{2}aY(X^{2m}-U^{2m}), \tag{32}$$

$$P_2^h=2X^m(YU^m-bU^{m+1})-c\,d^{-1}X^{m+1}\,U^m-c\,dX^{m-1}\,U^{m+2}-aY(X^{2m}+U^{2m}). \tag{33}$$

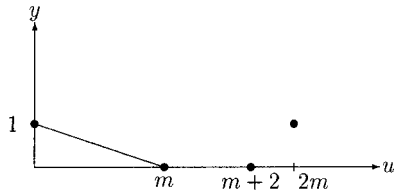

FIG. 1. The Newton diagram for $P_1^{X=1}$ in the $n=2$ multipole model. The degree of a monomial in y (u) is plotted vertically (horizontally). The case $m=3$ is shown.

The common roots at infinity are those with $U=0$, and there are two: $[X,Y,U]=[1,0,0]$, and $[0,1,0]$. The total magnification is minus the sum of the residues at these points of

$$\frac{4Y\,X^{2m-1}U^{2m+2}\,d(X/U)\,d(Y/U)}{P_1^h P_2^h}. \tag{34}$$

Consider first the point $[1,0,0]$, which we examine in the affine chart $[X,Y,U]=[1,y,u]$, where

$$P_1^{X=1}=c\,d^{-1}u^m-c\,du^{m+2}+\frac{m}{2}ay(1-u^{2m}), \tag{35}$$

$$P_2^{X=1}=2u^m(y-bu)-c\,d^{-1}u^m-c\,du^{m+2}-ay(1+u^{2m}), \tag{36}$$

and we need the residue at the origin of $4yu^{2m-1}\,du\,dy/P_1^{X=1}P_2^{X=1}$.

The Newton diagram for P_1 is shown in Fig. 1; there is a single branch on which to leading order $y\sim u^m$, as is easily verified by solving $P_1^{X=1}=0$ for y. The Leray formula evaluates the residue as the one-variable residue of

$$-\frac{4yu^{2m-1}\,du}{P_2^{X=1}\partial_y P_1^{X=1}}, \tag{37}$$

where $y\sim u^m$. But it is easily seen that the leading behavior of this 1-form near $u=0$ is $u^{2m-1}\,du$, so that there is no pole and no residue for $m>0$.

We examine the remaining root $[0,1,0]$ in the chart $[X,Y,U]=[x,1,u]$ where

$$P_1^{Y=1}=c\,d^{-1}x^{m+1}\,u^m-c\,dx^{m-1}u^{m+2}+\frac{m}{2}a(x^{2m}-u^{2m}), \tag{38}$$

$$P_2^{Y=1}=2x^mu^m(1-bu)-c\,d^{-1}x^{m+1}\,u^m-c\,dx^{m-1}\,u^{m+2}-a(x^{2m}+u^{2m}), \tag{39}$$

and we compute

$$\mathrm{Res}\,\frac{4x^{2m-1}u^{2m-1}\,dx\,du}{P_1^{Y=1}P_2^{Y=1}}. \tag{40}$$

The Newton diagram for $P_1^{Y=1}$ is shown in Fig. 2, and gives the leading behavior $u=lx+\cdots$. With this behavior, the lowest-order terms of $P_1^{Y=1}$ vanish iff $l^{2m}=1$, so that there are $2m$ branches with $l_p=\exp(ip\pi/m)$, $p=1,\ldots,2m$.

With the Leray formula, the total magnification becomes

$$\sum_{u=l_p x+\cdots} -\mathrm{Res}\,\frac{4x^{2m-1}u^{2m-1}\,dx}{P_2^{Y=1}\,\partial_u P_1^{Y=1}}. \tag{41}$$

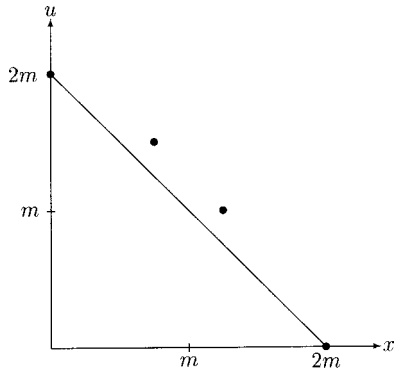

FIG. 2. The Newton diagram for $P_1^{Y=1}$ in the $n=2$ multipole model.

The leading terms are readily identified, and indeed the behavior is as dx/x, with residue

$$\sum_{p=1}^{2m} \frac{2}{m^2 a(l_p^m - a)} = \frac{2}{m^2 a} \sum_{p=1}^{2m} \frac{1}{(-1)^p - a} = \frac{4}{m(1-a^2)}. \tag{42}$$

In terms of the original parameters of the model,

$$M = \frac{4}{m(1-\gamma^2)}, \tag{43}$$

an attractive generalization of the known result[9] for $m=2$.

Once the branches of the P_i have been identified, it is easy to modify the calculation to compute moments rather than total magnification. For example, let us compute the first x-moment, $\mathrm{Tr}\, x\mu$. (We continue to use the Tr notation for the sum over the images.) Since $x=e^{i\theta}$ in terms of the physical variables of this model, from the real and imaginary parts of the result we can obtain the moments weighted by $\cos\theta$ and $\sin\theta$, in the case that all images are real. In homogeneous coordinates this simply gives an additional factor X/U in the residue in Eq. (34). At the point $[1,0,0]$ this adds a factor $1/u$ to the one-variable residue (37), changing the behavior to $u^{2m-2}\,du$. There is still no contribution for $m \geqslant 1$. At the point $[0,1,0]$, there is an extra factor $x/u = l^{-1} + \cdots$ in the residue (41), changing the contribution to

$$\sum_p \frac{2}{m^2 a l_p (l_p^m - a)} = \frac{2}{m^2 a} \sum_{p=1}^{2m} \frac{e^{-ip\pi/m}}{(-1)^p - a}, \tag{44}$$

which can be evaluated in closed form if desired.

From the real part of $\mathrm{Tr}\, yx\mu$ we can obtain the moment of $r\cos\theta$, the physical x-coordinate of the image. This leads to a factor YX/U^2, which worsens the singularity at $[0,1,0]$ to a double pole, requiring an additional term in the Puiseux expansion to obtain the residue. The result, for the true external shear model $m=2$, is

$$\mathrm{Tr}\, \mu r\cos\theta = -\frac{2x_s}{(1-\gamma)(1-\gamma^2)}. \tag{45}$$

This example illustrates the general situation. Higher moments produce extra monomial factors in the residue expression. In general this will worsen the singular behavior at points at infinity, although this may not occur for certain branches, such as those at $[0,1,0]$ in the example of $\mathrm{Tr}\, x\mu$. This will have two effects: points which do not contribute to the total magnification generally will

contribute to higher moments, and more terms in the Puiseux expansions will be required for higher moments. Both effects will result in higher moments being given by more complex expressions, with more model parameters contributing.

We turn to a second example, the Singular Isothermal Ellipse (SIE) potential.[10,12] For this model $\psi = bR = b\sqrt{x^2+y^2q^{-2}}$, where x,y are rectangular coordinates and b,q are parameters. The lens equations are

$$\tau_x = x - x_s - \frac{bx}{R} = 0, \tag{46}$$

$$\tau_y = y - y_s - \frac{by}{q^2 R} = 0, \tag{47}$$

and the magnification is given by

$$\mu^{-1} = \begin{vmatrix} \tau_{xx} & \tau_{xy} \\ \tau_{xy} & \tau_{yy} \end{vmatrix}. \tag{48}$$

Algebraic manipulation leads to the polynomial equations,

$$p_1 = q^2 x\tau_y - y\tau_x = q^2 x(y-y_s) - y(x-x_s) = 0, \tag{49}$$

$$p_2 = R^2\tau_x^2 - 2bRx\tau_x = (x-x_s)^2(x^2+y^2q^{-2}) - b^2x^2 = 0. \tag{50}$$

However, these equations have the extraneous solution $(x,y)=(0,0)$, which does not satisfy the original lens equations. This can be eliminated by substituting $y=wx$, and adopting the modified equations,

$$P_1 = p_1/q^2 x = wx - y_s - \eta w x + \eta w x_s, \tag{51}$$

$$P_2 = p_2/x^2 = b^2 - (x-x_s)^2(1+\eta w^2), \tag{52}$$

where we have set $\eta = q^{-2}$. Relating the naive Jacobian J of the P_i with respect to x,w to the Hessian of τ gives the magnification in the new variables,

$$\mu = \frac{2x(x-x_s)(1+\eta w^2)}{J}. \tag{53}$$

The moments of the magnification with respect to x are given by

$$\mathrm{Tr}\, x^k \mu = \sum \mathrm{Res} \frac{2x^{k+1}(x-x_s)(1+\eta w^2)\, dx\, dw}{P_1 P_2}. \tag{54}$$

In homogeneous coordinates we have

$$P_1^h = (1-\eta)XW - y_s U^2 + \eta x_s WU, \tag{55}$$

$$P_2^h = b^2 U^4 - (X - x_s U)^2(U^2 + \eta W^2), \tag{56}$$

and we need to compute

$$\mathrm{Tr}\, \mu x^k = \sum \mathrm{Res} \frac{2X^{k+1}U^{2-k}(X-x_sU)(U^2+\eta W^2)\, d(X/U)\, d(W/U)}{P_1^h P_2^h}. \tag{57}$$

There are two common zeros of the P_i^h at infinity, namely $[X,W,U]=[1,0,0]$, $[0,1,0]$, and in the corresponding affine charts we have

$$P_1^{X=1}=(1-\eta)w-y_s u^2+\eta x_s w u, \tag{58}$$

$$P_2^{X=1}=b^2u^4-(1-x_s u)^2(u^2+\eta w^2), \tag{59}$$

$$P_1^{W=1}=(1-\eta)x-y_s u^2+\eta x_s u, \tag{60}$$

$$P_2^{W=1}=b^2u^4-(x-x_s u)^2(u^2+\eta). \tag{61}$$

The residues at these zeros may be computed via the Leray formula applied to the branches of either P_1 or P_2; we have done both computations and the latter seems slightly simpler. In each case the branches can be determined directly without appealing to the Newton diagrams. At $[0,1,0]$, the equation $P_2^{W=1}=0$ is solved by

$$x=x_s u\pm b\,\eta^{-1/2}u^2\left(1+\frac{u^2}{\eta}\right)^{-1/2}, \tag{62}$$

giving one branch for each choice of sign. The contribution to $\mathrm{Tr}\,\mu x^k$ from one branch is

$$\mathrm{Res}\frac{2x^{k+1}(x-x_s u)(u^2+\eta)\,dx\,du}{u^{k+1}P_1^{W=1}P_2^{W=1}}. \tag{63}$$

Applying the Leray formula gives

$$\mathrm{Res}\frac{2x^{k+1}(x-x_s u)(u^2+\eta)\,du}{u^{k+1}P_1^{W=1}\,\partial_x P_2^{W=1}}, \tag{64}$$

which simplifies to

$$\mathrm{Res}\frac{x^{k+1}\,du}{u^{k+1}[x-y_s u^2-\eta(x-x_s u)]}=x_s^k, \tag{65}$$

where only the first term in the series expansion of x was required. The two branches at this point thus contribute $2x_s^k$ to the moment of x^k.

At the remaining point $[1,0,0]$, $P_2^{X=1}=0$ is solved by

$$w=\pm\frac{iu}{\sqrt{\eta}}\sqrt{1-\frac{b^2u^2}{(1-x_s u)^2}}=\pm\frac{iu}{\sqrt{\eta}}\left(1-\frac{1}{2}b^2u^2+\cdots\right), \tag{66}$$

and we need

$$\mathrm{Res}\frac{2(1-x_s u)(u^2+\eta w^2)\,du\,dw}{u^{k+1}P_1^{X=1}P_2^{X=1}}, \tag{67}$$

summed over the two branches. Integrating over w using the Leray residue formula and simplifying yields

$$\mathrm{Res}\frac{(u^2+\eta w^2)\,du}{\eta w u^{k+1}(1-x_s u)[(1-\eta)w+\eta x_s w u-y_s u^2]}, \tag{68}$$

where $u^2+\eta w^2=b^2u^4+\cdots$. Since $w\sim u$, there is no pole for $k<2$: the total magnification and first moment are simply given by the contributions from [0,1,0]. There is an additional contribution to the second moment given by $-2b^2/(1-\eta^2)=2b^2q^2/(1-q^2)$, which agrees with the result of Ref. 10.

We have verified the results of Witt and Mao[10] through the third moment. Those authors noted that the moments of x were independent of y_s to this order, and that ''this seems remarkable'' in view of the dependence of μ on this parameter. The explanation is that the term y_su^2 in $P_1^{X=1}$ does not contribute to the residue for low moments; indeed it *does* contribute to the residues for the third moment but its contribution cancels between the two branches. The fourth and higher moments do depend on y_s.

Last, we note that it is entirely straightforward, and no more work, to generalize the calculation to include an arbitrarily oriented external shear term. The first moment, for example, takes the form

$$\mathrm{Tr}\,\mu x=\frac{2}{(1-\gamma^2)^2}(x_s+\gamma_1x_s+\gamma_2y_s),\quad \mathrm{Tr}\,\mu y=\frac{2}{(1-\gamma^2)^2}(y_s+\gamma_2x_s-\gamma_1y_s), \tag{69}$$

where $\gamma_1\equiv\gamma\cos 2\theta_\gamma$, $\gamma_2\equiv\gamma\sin 2\theta_\gamma$, and θ_γ is the orientation angle of the shear (see Table I).

As our final example we consider microlensing due to a collection of N coplanar point masses. We adopt Witt's complex notation, writing $z=x+iy$ for the position of an image and w for the position of the source. The lenses have masses m_i and positions z_i. The lens equations are

$$z-w-\sum_{i=1}^{N}\frac{m_i}{\overline{z}-\overline{z}_i}=0, \tag{70}$$

and its complex conjugate; when we complexify the coordinates x,y of an image, z and $\overline{z}$ become independent variables and the conjugate equation becomes an independent condition as well. The observable (real) images are those for which $\overline{z}$ is the conjugate of z. Clearing denominators, we set

$$P_1=(z-w)\prod_i(\overline{z}-\overline{z}_i)-\sum_i m_i\prod_{j\neq i}(\overline{z}-\overline{z}_j), \tag{71}$$

$$P_2=(\overline{z}-\overline{w})\prod_i(z-z_i)-\sum_i m_i\prod_{j\neq i}(z-z_j). \tag{72}$$

For the magnification we find

$$\mu=J^{-1}\prod_i(z-z_i)(\overline{z}-\overline{z}_i), \tag{73}$$

where $J=\partial(P_1,P_2)/\partial(z,\overline{z})$. For the kth moment of magnification, we must compute

$$\mathrm{Tr}\,\mu z^k=\mathrm{Res}\frac{z^k\,\Pi_i(z-z_i)(\overline{z}-\overline{z}_i)\,dz\,d\overline{z}}{P_1P_2}. \tag{74}$$

The homogeneous polynomials are

$$P_1^h=(Z-wU)\prod_i(\overline{Z}-\overline{z}_iU)-\sum_i m_iU^2\prod_{j\neq i}(\overline{Z}-\overline{z}_jU), \tag{75}$$

$$P_2^h=(\overline{Z}-\overline{w}U)\prod_i(Z-z_iU)-\sum_i m_iU^2\prod_{j\neq i}(Z-z_jU). \tag{76}$$

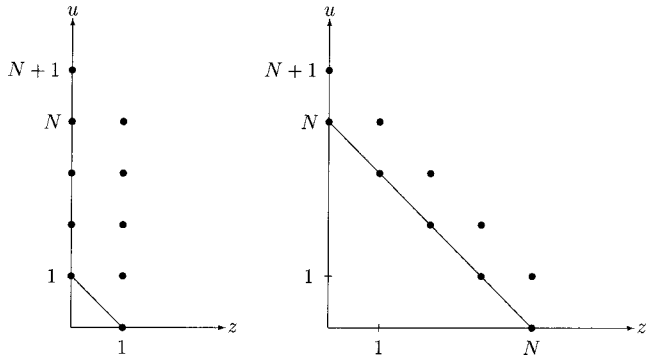

FIG. 3. The Newton diagrams for $P_1^{\overline{Z}=1}$ (left) and $P_2^{\overline{Z}=1}$ (right) for N point masses. The case $N=4$ is shown.

Setting $U=0$, we obtain $P_1^h=Z\overline{Z}^N$, $P_2^h=\overline{Z}Z^N$, so there are two common zeros at infinity, $[Z,\overline{Z},U]=[1,0,0],[0,1,0]$. However, we can say more: each of these zeros has multiplicity N. Since the homogeneous polynomials each have degree $N+1$, the number of finite common zeros will be $(N+1)^2-2N=N^2+1$, in agreement with previous results.[3]

Dehomogenizing the polynomials at these points, we find

$$P_1^{\overline{Z}=1}=(z-wu)\prod_i (1-u\overline{z_i})-u^2\sum_i m_i\prod_{j\neq i}(1-u\overline{z_j}), \tag{77}$$

$$P_2^{\overline{Z}=1}=(1-\overline{w}u)\prod_i (z-uz_i)-u^2\sum_i m_i\prod_{j\neq i}(z-uz_j), \tag{78}$$

$$P_1^{Z=1}=(1-wu)\prod_i (\overline{z}-u\overline{z_i})-u^2\sum_i m_i\prod_{j\neq i}(\overline{z}-u\overline{z_j}), \tag{79}$$

$$P_2^{Z=1}=(\overline{z}-\overline{w}u)\prod_i (1-uz_i)-u^2\sum_i m_i\prod_{j\neq i}(1-uz_j). \tag{80}$$

Because of the complex conjugation symmetry of these expressions, it suffices to examine the branches of, say, $P_i^{\overline{Z}=1}$ to deduce the others. The Newton diagrams of these are shown in Fig. 3. In each case, the Puiseux series are ordinary power series. For P_1 there is a single branch $u=z/w+\cdots$, while for P_2 there are N branches $u=z/z_i-(m_i/z_i^3)z^2+\cdots$.

It is now straightforward to compute the residues,

$$\mathrm{Res}\,\frac{Z^kU^{2-k}\Pi_i(Z-z_iU)(\overline{Z}-\overline{z_i}U)\,d(Z/U)\,d(\overline{Z}/U)}{P_1^hP_2^h}, \tag{81}$$

and determine the moments. The first two are $M=\mathrm{Tr}\,\mu=1$, and $\mathrm{Tr}\,z\mu=w+\Sigma_i[m_i/(\overline{w}-\overline{z_i})]$. The single branch contributes w^k to the kth moment, while the contribution of the N branches becomes progressively more complicated.

We have also considered a generalization of the model to include external shear. This brings the lens equations to the form[3]

$$z-w-\gamma\overline{z}-\sum_{i=1}^N\frac{m_i}{\overline{z}-\overline{z_i}}=0, \tag{82}$$

and its complex conjugate. Defining P_i^h as before, their zeros at infinity are $[1,0,0]$ and $[\gamma,1,0]$ for P_1^h, and $[0,1,0]$ and $[1,\gamma,0]$ for P_2^h. For $\gamma \neq 0,1$ there are no common zeros at infinity. Factoring the denominator of ω^h as $(U^n P_1^h)(P_2^h)$, the residue theorem gives the sum over the finite common roots as minus the sum of residues at the infinite roots of P_2^h. We find, for example, the total magnification $1/(1-\gamma^2)$, and the first moment,

$$\mathrm{Tr}\, z\mu = \frac{w+\gamma\overline{w}}{(1-\gamma^2)^2}. \tag{83}$$

Note that the first moment's dependence upon the lens' positions has vanished.

V. DISCUSSION

We have introduced in this paper a new framework for analyzing gravitational lens models. The use of residue integrals makes clear the origin of the magnification relations, and facilitates their computation for a wide class of model potentials. We have also applied this method to a series of models, confirmed and extended previous results, and provided new magnification relations for several models. Although multidimensional residue calculus may be unfamiliar to readers from astronomy, one may follow a simple procedure to perform the necessary integrals. Basically, the procedure is as follows.

(1) From the stationarity equations, construct two polynomials P_1, P_2 that simultaneously vanish at (and only at) the image positions.
(2) Define the ''Jacobian'' $J_P = \det[\partial(P_1,P_2)/\partial(x,y)]$, and define $g(x,y) = J_P(x,y)\mu(x,y)$ where μ is the magnification.
(3) Change to homogeneous coordinates: $(x,y) \to (X,Y,U)$ with $x = X/U, y = Y/U$ and homogenize the polynomials by multiplying each by the factor $U^{\deg P}$. Also, multiply g by $U^{\deg P_1 + \deg P_2}$.
(4) From the homogenized g, P_1, P_2, construct the 2-form $(g/P_1P_2)d(X/U)d(Y/U)$, and factor the denominator into two groups; usually, the grouping P_1, P_2 suffices. (Henceforth P_1, P_2 shall refer to the two groups, not the original polynomials.) If the denominator contains explicit factors of U then redefine one of the polynomials, say P_2, to contain these additional factors.
(5) For $U=0$, find the points (X,Y) where P_1, P_2 simultaneously vanish; these are the roots at infinity.
(6) Pick one of the polynomials—say P_1—and determine the behavior of $P_1 = 0$ in the vicinity of each common root. First define coordinates for the neighborhood of the root. For example, if the root is $Y=0$, $U=0$, then a good choice would be $(X,Y,U) = (1,y,u)$. As discussed, there are in general multiple branches of $P_1 = 0$ meeting at the root at infinity, each parametrized by a Puiseux series $y = \Sigma_i a_i u^{\alpha_i}$. The α_i's can be determined from the Newton diagram, and by substituting in the specified α_i's one may solve for the coefficients a_i. Usually, only the first one or two terms in the series are necessary.
(7) Construct the quantity

$$\frac{g(u, a_1 u^{\alpha_1} + a_2 u^{\alpha_2} + \cdots)}{\dfrac{\partial P_1}{\partial y}(u, a_1 u^{\alpha_1} + \cdots) P_2(u, a_1 u^{\alpha_1} + \cdots)},$$

and pick out the term $\sim u^{-1}$. The coefficient of u^{-1} is the contribution for this branch; summing over all the branches gives the residue for each root.
(8) Repeat this procedure for all the roots at infinity, and sum their residues. Negating this quantity gives the sum of the residues at finite poles (the images).

The above is of course just a rough outline; in Sec. III we describe the method in full detail. Following this procedure, the results listed in Table I can be reproduced with minimal effort.

As we have discussed, the methods presented in this paper apply when the two lens equations are polynomial in the two image variables. When algebraic functions of the image variables appear, we introduce new variables and equations to bring the whole set to polynomial form. In principle, the extra variables can be eliminated to return to a pair of polynomial equations to which our residue methods apply. A simple example of this was seen in our discussion of the SIE potential. In principle, however, the residue methods apply directly to any number of polynomial equations in the same number of variables. We have not investigated whether this can be turned into a practical computational scheme for dealing with algebraic functions. One would first require an analysis like that in the Appendix, determining the homology class of the torus T defining the residue integral. The Leray residue formula holds quite generally, but is less explicit without the machinery of algebraic curves and Puiseux series which we exploited in the two-variable case. Details can be found in Refs. 15, 16. We do not know how to extend our methods to equations involving transcendental functions.

Dalal[9] and Witt and Mao[10] have considered the applicability of such magnification relations to real gravitational lenses. For galaxies, Dalal[9] has shown that these relations can be an aid in fitting models to lensed objects, or can be used to rule out models *a priori*. Witt and Mao[10] have shown, however, that reliance upon simple galaxy models can be misleading, when applied to realistic galaxy potentials. This limits the applicability of magnification relations to making statements about models, as opposed to statements about the lenses themselves. For this reason, some authors have aimed at deriving magnification results that apply to generic lens models. For example, Petters[22] determines lower bounds on the total magnification using Morse theoretic methods. The residue integral method introduced here allows explicit results, for relatively little effort, by focusing on a specific class of models. The applicability of the derived relations then depends upon the validity of the model.

For microlensing, there is no doubt about the accuracy of the point mass model, and as such our derived magnification relations may be considered exact. The limitation of our results is that they have physical relevance only when the maximum number of images is attained. It is currently an open question whether there exist parameter ranges for which all solutions are real, e.g., Ref. 23. Nevertheless, such magnification relations have already proven themselves to have astrophysical value. Witt and Mao[7] have already shown how the total signed magnification (''zeroth moment'') can be used for binary microlensing to set lower limits on the overall unsigned magnification, useful for example for detecting source blending. Although the multiple images of a microlensing event cannot as yet be resolved, precluding the present-day experimental verification of our prediction regarding the first moment, we are hopeful that the future advent of space-based interferometers will allow our microlensing formulas to be tested observationally.

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APPENDIX: THE HOMOLOGY CLASS OF THE TORUS *T*

Here we explain why the torus T defining the local residue at a singular point, taken to be the origin, is homologous to the sum of the Leray tori constructed from the branches of *either* of the polynomials $P_i(x,y)$, and how to determine the correct orientations. We are grateful to Eduard Looijenga and Peter Teichner for explaining the topology to us. See also Sec. 2.2 of Dimca.[24]

We are working locally in a closed ball B around the origin, and we denote by X the zero locus $P_1P_2=0$ within B. The various tori define homology classes in $H_2(B-X)$. It is known that X is topologically a cone with vertex the origin and base $X\cap\partial B$, which is a linked collection of topological circles.[17,24] Denote the several branches of X as X_i, and the Leray torus built on a given branch as δC_i. Let σ_{ij} be a path running from the origin to ∂B along X_i, and returning to

the origin along branch X_j. A subset of these paths forms a basis for the relative homology group $H_1(X,\partial B)$. Furthermore, by Alexander duality,[16] an element of $H_2(B-X)$ is uniquely determined by its linking numbers with these paths (indeed, with those in a basis alone). [The linking number $l(c^1,c^2)$ of a 1-cycle with a 2-cycle in a 4-ball is the intersection number of c^1 with any 3-manifold having boundary c^2.]

The Leray tori have linking numbers,

$$l(\sigma_{ij},\delta C_k)=\delta_{ik}-\delta_{jk}. \tag{A1}$$

Indeed, the intersection of σ_{ij} with a solid torus bounded by δC_k is the intersection of σ_{ij} with C_k, which is one point if the outward segment of σ_{ij} lies on branch X_k, and one point (with opposite orientation) if the returning segment does.

The sum $\Sigma_{P_1}\delta C_k$ of Leray tori built on branches of $P_1=0$ therefore has linking number with σ_{ij} equal to $+1$ if X_i is a branch of P_1 and X_j is a branch of P_2, -1 if *vice versa*, and 0 if X_i and X_j are branches of the same polynomial. The sum $\Sigma_{P_2}\delta C_k$ has the negatives of these linking numbers and therefore represents the same homology class but with opposite orientation.

It remains to show that T has the linking numbers of $\Sigma_{P_1}\delta C_k$. A solid torus bounded by T is given by $\{|P_1|\leqslant\epsilon,|P_2|=\epsilon\}$. This meets any branch X_k of $P_1=0$ given by a Puiseux series $y=p(x)$ in the locus $|P_2(x,p(x))|=\epsilon$ on X_k. This set is topologically a circle around the origin, having intersection number $+1$ with a path radially outward from the origin. The solid torus meets no branch of $P_2=0$. Therefore, radially outward (inward) paths on any branch of P_1 contribute $+1$ (-1) to intersection numbers with this solid torus, while paths on branches of P_2 contribute nothing. This duplicates the linking numbers of $\Sigma_{P_1}\delta C_k$.

The orientation for T used in this argument is indeed the standard one prescribed in Sec. III. Using the Leray residue formula to evaluate

$$\left(\frac{1}{2\pi i}\right)^2\int_T\frac{dP_1\,dP_2}{P_1P_2} \tag{A2}$$

produces a positive contribution from every branch of P_1.

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Spherically symmetric space–times with constant curvature scalar

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In view of the geometrical importance of spaces with constant scalar curvature, a systematic study of spherically symmetric such space–time manifolds with respect to the eigenvalues of the Ricci tensor is made. The cases of two double or one quadruple eigenvalue are treated exhaustively. In the generic case of one double and two single eigenvalues, no conformally flat solutions, and only solutions with one arbitrary function of one variable are found. We also give all four-dimensional decomposable s.s. spaces with constant curvature scalar. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1339218]

I. INTRODUCTION

In this paper we study spherically symmetric solutions (s.s.s.) of the equation

$$R = R_0, \tag{1}$$

where R is the Ricci scalar of the four-dimensional pseudo-Riemannian metric $g_{\alpha\beta}$, and R_0 is a constant. The case $R_0 = 0$ was treated in a previous communication.[1] As expressed there, our original interests in s.s.s. of Eq. (1) was directed to their use as counterexamples for the validity of Birkhoff's theorem for a large class of gravitational theories derivable from a variational principle.[2] Equation (1), through the use of a scalar multiplier, is also derivable from a variational principle. The Lagrangian is given by

$$\sqrt{-g}(R-R_0)^2\phi,$$

where the scalar field ϕ acts as a multiplier and remains completely undetermined. Any solution of Eq. (1) with $R_0 = -4\Lambda$ solves also the field equations following from the Lagrangian $(-g)^{1/2}[R+2\Lambda+(8\Lambda)^{-1}R^2]$, where Λ is the cosmological constant. Moreover, any conformally flat solution of Eq. (1) with $R_0 = -4\Lambda$ satisfies the field equations following from the Lagrangian:

$$(-g)^{1/2}[R+2\Lambda+aR^2+3((8\Lambda)^{-1}-a)R^{\beta}_{\alpha}R^{\alpha}_{\beta}],$$

where $R_{\alpha\beta}$ is the contracted curvature (Ricci) tensor and a an arbitrary constant. Because Eq. (1) admits a multiplicity of solutions, as shown in this paper, no such field equation admits Birkhoff's theorem.

We were further motivated to look into the s.s.s. of Eq. (1) because they contain, as a subset, all s.s.s. of the Einstein–Maxwell field equations with a cosmological constant, and of the Yang–Kilmister (gauge-)theory of gravitation.[3] In this context, the solutions of the Bach–Treder-equation augmented with a cosmological constant term may be mentioned, because for them $R = R_0$ is implied.[4–6]

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TABLE I.

	Quadruple	Quadruple	Two double	Two double	One triple, one single	One double, two single canonical form	One double, two single canonical form
	$2C-R=0$	$2C-R\neq 0$	$2C-R=0$	$2C-R\neq 0$		(2)	(3)
$C=0$		De Sitter metric			(26a, b) Einstein cosmos (28a, b) (30a, c) (31) (incomplete) (79)	(no solution found)	(no solution found)
$C\neq 0$	(21)	(23)	(18)	(9) (14) (16a, b)	(no solution found)	(39a) with (41), (42),(44); (39b, c, d) with (41), and (47a, b, c); (52) with (30a, b), (31b, c); (54b, c, d) (56a, b, c) (57b, d)	(10) with (11); (63) with (65a, b, c); (72) with (68); (78a, b, c)

The prime interest in Eq. (1), however, is that this equation points to the possibility of a geometrization of many physical systems in the sense that their basic equations, or subcases of them, appear as special cases of (1). To name some: nonlinear wave equations as in the ϕ^4-theory and the 1-dimensional Landau–Ginzburg theory of superconduction, the Lane–Emden equation of stellar interiors and the Thomas–Fermi equation, particular cases of Boltzman's equation and the time-independent Schrödinger equation for special potentials. It is also known that, in Euclidean space, soliton equations may be derived by embedding 2-surfaces with the property (1); an example is given by surfaces with constant negative curvature: the corresponding Gauss–Codazzi equation is equivalent to the sine-Gordon equation.[7–9] Also for the Korteweg-de Vries equation a geometrical interpretation with the help of a surface of constant, nonvanishing Gaussian curvature has been suggested.[10]

The generic solution of Eq. (1) contains, at most, one arbitrary function of two variables and two further arbitrary functions of one variable each. In paper I, for $R_0=0$, we explicitly gave the general s.s.s. of Eq. (1) for certain specific values of the conformal invariant $C:=[3/4C_{\alpha\beta\gamma\delta}C^{\alpha\beta\gamma\delta}]^{1/2}$, e.g., for $C=0$, where $C_{\alpha\beta\gamma\delta}$ denotes the conformal curvature tensor, and implicitly reduced the problem to a linear equation. (For s.s. metrics $C=0$ and $C_{\alpha\beta\gamma\delta}=0$ are equivalent.) In the present case, $R_0\neq 0$, we have not been able to achieve as much, although we do obtain classes of solutions depending on one or even two arbitrary functions of one variable. This is due to the fact that none of the canonical forms of the metric considered in Sec. II linearizes Eq. (1) nor reduces it to a nonlinear partial differential equation whose solutions are known completely. Nevertheless, as in paper I, we display the general solution of Eq. (1) for metrics the Ricci tensor of which has a quadruple or two double eigenvalues. Also, all four-dimensional decomposable s.s. spaces with a constant curvature scalar are found.

After introducing, in Sec. II, the canonical forms for the metric we are using, in Sec. III we first deal with decomposable spaces. In Sec. IV we discuss all the metrics obtained by us with a degenerate eigenvalue structure of the corresponding Ricci tensor R_α^β. In Sec. V, s.s.s. of Eq. (1) with the most general eigenvalue structure of R_α^β are given. In Sec. VI a different canonical form for the metric is used in order to obtain further solutions. Those s.s.s. of the Yang–Kilmister theory found here are identified in Sec. VII. In Sec. VIII a brief discussion of the generation of s.s.s. of Eq. (1) from others or from s.s.s. of $R=0$ by conformal mappings is given. Our results are summarized in Table I and discussed in Sec. IX.

II. CANONICAL FORMS OF s.s. METRIC

As in paper I we use, alternatively, the canonical forms

$$ds^2=z^2(u,v)[2e^{w(u,v)}\,du\,dv-d\Omega^2] \tag{2}$$

and

$$ds^2=c^2(r,t)dt^2-a^4(r,t)[dr^2+r^2\,d\Omega^2], \tag{3a}$$

with $d\Omega^2:=d\theta^2+\sin^2\theta\,d\varphi^2$ for describing metrics with a Ricci tensor R_α^β of a nondegenerate eigenvalue structure. A canonical form equivalent to (3a) is

$$ds^2=c^2(\rho,t)dt^2-b^4(\rho,t)[d\rho^2+d\Omega^2]. \tag{3b}$$

Any s.s. metric can be brought into either form (2) or Eq. (3a).

For metrics the Ricci tensor of which has two double eigenvalues the following canonical forms are especially suited:[11]

$$ds^2=F(u,r)du^2+2\,du\,dr-r^2d\Omega^2, \tag{4}$$

with $R-2C\neq 0$ and

$$ds^2=F(u,r)du^2+2\,du\,dr-b_0^2d\Omega^2, \tag{5}$$

$$ds^2=2e^{2\alpha(u,v)}\,du\,dv-u^2d\Omega^2, \tag{6}$$

and the canonical form obtained from Eq. (6) by interchange of u and v. For both forms (5) and (6) $R-2C=0$ holds; b_0 is a constant.

We keep to the canonical forms (2)–(6) unless another form, obviously transformable into one of these forms, is more convenient for an explicit integration of (1). Such a transformation may not always be obtainable explicitly.

The equivalence problem arising from the use of different canonical forms is circumvented by a classification of the s.s.s. of Eq. (1) with regard to the eigenvalue structure of R_α^β and to the conformal invariant C.

Starting from the canonical form (2) we calculate the curvature invariants R and C. For convenience we repeat the resulting partial differential equations for $z(u,v)$ and $w(u,v)$ given in paper I, i.e.,

$$e^{-w}w_{,uv}+1-z^2C=0, \tag{7a}$$

$$z_{,uv}+\frac{1}{6}z^3e^w\left(C-\frac{1}{2}R\right)=0. \tag{7b}$$

III. DECOMPOSABLE SPHERICALLY SYMMETRIC SPACE–TIMES

Before entering the general discussion we shall first deal with a case of special geometric interest, the decomposable s.s.s. of Eq. (1). Two main subcases exist.

A. Two 2-dimensional subspaces

Here we take the canonical form

$$ds^2=2e^{w(u,v)}\,dv\,dv-b_0^2d\Omega^2. \tag{2′}$$

A constant Ricci scalar R_0 for (2′) can occur if and only if the $u-v$-space is of constant Gaussian curvature,

$$k=\frac{1}{b_0^2}-\frac{R_0}{2}. \tag{8}$$

Standard forms for such solutions of Eq. (1) are, for $k=1/a_0^2$,

$$ds^2=\left(1+\frac{uv}{4a_0^2}\right)^{-2}du\,dv-b_0^2d\Omega^2, \tag{9a}$$

and, for $k=-1/a_0^2$,

$$ds^2=\left(1-\frac{uv}{4a_0^2}\right)^{-2}du\,dv-b_0^2d\Omega^2. \tag{9b}$$

The case $k=0$ is represented by the canonical form

$$ds^2=du\,dv-b_0^2d\Omega^2.$$

Other canonical forms for the u, v-subspace of the metric (9a) are, for example,

$$d\sigma^2=dt^2-\sin^2(t/a_0)dr^2$$

or

$$d\sigma^2=\sinh^2(r/a_0)dt^2-dr^2.$$

However, the coordinates t, r chosen above cover only part of the range $-\infty<u<\infty$, $-\infty<v<\infty$, $vid.uv>0$ and $0<uv<4a_0^2$, respectively. From Eq. (6) we conclude $C=1/2R_0$ for the metrics (9). The Ricci tensor has two double (or one quadruple) eigenvalues $\lambda_{1,2}=\pm 1/a_0^2$, $\lambda_{3,4}=-1/b_0^2$. Moreover, the corresponding Riemannian space is symmetric. Equation (9) admits a two-dimensional isotropy group and a six-dimensional isometry group.[12] The metrics (9a) and (9b) have been discussed repeatedly[13] as solutions of Einstein's field equations with cosmological constant Λ and/or a constant nonsingular electromagnetic field. They also satisfy the field equations following from the Lagrangian:

$$(-g)^{1/2}[R+\Lambda+aR^2-(2a+R_0^{-1})R_\alpha^\beta R_\beta^\alpha],$$

to which a matter Lagrangian describing a constant, nonsingular electromagnetic field may be added. Wynne's solutions[14] of types XI, XII, XIII, XIV and XVI solving the field equations derived from the Lagrangian $R_\beta^\alpha R_\alpha^\beta+aR^2$ belong to this set.

B. One 1-dimensional and one 3-dimensional subspace

Here we use the canonical forms

$$ds^2=dt^2-A(r)dr^2-r^2\,d\Omega^2 \tag{10a}$$

and

$$ds^2=B(t)dt^2-t^2\,d\Omega^2-dr^2. \tag{10b}$$

Using the formulas of Takeno[15] one can show that a constant Ricci scalar R_0 occurs if and only if

$$A(r)=\left(1-\frac{R_0}{6}r^2+a_0/r\right)^{-1}, \tag{11a}$$

$$B(t)=\left(-1+\frac{R_0}{6}t^2+b_0/t\right)^2. \tag{11b}$$

For $a_0\neq 0$ ($b_0\neq 0$) the 3-dimensional subspace is not a space of constant curvature; $a_0=0$ leads to the Einstein cosmos. $b_0=0$, after a coordinate transformation, leads to the line element

$$ds^2=2\,du\,dv-\frac{6}{R_0}\cosh^2\left[\left(\frac{R_0}{12}\right)^{1/2}(u+v)\right]d\Omega^2. \tag{12}$$

For the decomposable spaces (10) and (11) the conformal invariant is given by

$$C=3a_0/2r^3 \quad \text{or} \quad 3b_0/2t^3, \quad \text{respectively.} \tag{13}$$

The eigenvalues of R^{α}_{β} for metric (10a) with (11a) are

$$\lambda_1=0,\ \lambda_2=\frac{R_0}{3}-\frac{a_0}{r^3},\ \lambda_3=\lambda_4=\frac{R_0}{3}+\frac{a_0}{2r^3}.$$

IV. s.s.s. WITH DEGENERATE EIGENVALUE STRUCTURE OF R^{β}_{α}

In general, the Ricci tensor of a s.s. spacetime admits one double and two single eigenvalues.

A. Two double eigenvalues

We first deal with the case of the metric not being conformally flat, i.e., $C\neq 0$. Two further subcases arise

1. $2C-R=0$

Here both canonical forms (5) and (6) must be considered. For (5), the general s.s.s. of Eq. (1) is given by

$$F(u,r)=a(u)+b(r)r+\left(\frac{1}{b_0^2}-\frac{R_0}{2}\right)r^2, \tag{14}$$

with arbitrary functions $a(u),b(u)$.

Among the metrics (5) with (14) we find the decomposable spaces (9) considered before, i.e., for $a(u)=\pm 1$, $b(u)=0$.

The eigenvalues of the Ricci tensor are

$$\lambda_{1,2}=\frac{R_0}{2}-\frac{1}{b_0^2},\ \lambda_{3,4}=1/b_0^2. \tag{15}$$

For the canonical form (6) the most general s.s.s. of Eq. (1) is given by

$$ds^2=z^2(u)\left\{\frac{4\,du\,dv}{(u-v)^2\left[1-\frac{R_0}{2}z^2(u)\right]}-d\Omega^2\right\}, \tag{16a}$$

with $z(u)$ arbitrary.

In this case the eigenvalues of R^{β}_{α} are

$$\lambda_{1,2}=\frac{R_0}{2}-\frac{1}{z^2(u)},\quad \lambda_{3,4}=\frac{1}{z^2(u)}. \tag{17}$$

Obviously, the interchange of u and v leads to another set of solutions,

$$ds^2=z^2(v)\left\{\frac{4\,du\,dv}{(u-v)^2\left[1-\frac{R_0}{2}z^2(v)\right]}-d\Omega^2\right\}. \tag{16b}$$

2. $2C-R\neq 0$

Here we must use the canonical form (4). The general s.s.s. of Eq. (1), in this case, then is given by

$$ds^2=\left(1-\frac{2m(u)}{r}+\frac{e^2(u)}{r^2}-\frac{\Lambda}{3}r^2\right)du^2+2\,du\,dr-r^2d\Omega^2, \tag{18}$$

where $e\cdot m\neq 0$ and

$$R_0=4\Lambda,\quad C=\frac{6m(u)}{r^3}-6\frac{e^2(u)}{r^4}, \tag{19}$$

$m(u),e(u)$ arbitrary functions.

The eigenvalues of R^β_α are

$$\lambda_{1,2}=\Lambda+e^2/r^4,\quad \lambda_{3,4}=\Lambda-e^2/r^4. \tag{20}$$

The solutions (18) include the Reissner–Nordström metric with cosmological term.

For conformally flat metrics, $C=0$, the canonical form (4) is the only possibility. However, from Eq. (19), in this case, we must have $m=e=0$ and thus Eq. (20) implies a quadruple eigenvalue of R^β_α. Hence, there are no conformally flat s.s.s. of Eq. (1) with two distinct double eigenvalues.

B. One quadruple eigenvalue

We follow the same subdivision as before.

1. $2C-R=0$

From Eqs. (14) and (15) we obtain

$$ds^2=[a(u)+b(u)r-r^2/b_0^2]du^2-2\,du\,dr-\frac{1}{b_0^2}d\Omega^2, \tag{21}$$

with the quadruple eigenvalue $\lambda=1/b_0^2$.

On the other hand we obtain from Eqs. (16a), (16b) and (17),

$$ds^2=-z_0^2\left[\frac{4\,du\,dv}{(u-v)^2}-d\Omega^2\right], \tag{22}$$

with the quadruple eigenvalues $\lambda=1/z_0^2$.

A coordinate transformation $u=2^{-1/2}(r-t)$, $v=2^{-1/2}(r+t)$ leads to

$$ds^2=\left(\frac{z_0}{t}\right)^2[dt^2-dr^2-t^2\,d\Omega^2].$$

Both (21) and (22) are decomposable spaces of type (9b), i.e., with negative Gaussian curvature $k=-2/b_0^2$ $(k=-1/z_0^2)$.

2. $2C-R\neq 0$

From Eqs. (18) and (20) we obtain

$$ds^2=\left(1-\frac{2m(u)}{r}-\frac{1}{3}\Lambda r^2\right)du^2+2\,dv\,dr-r^2\,d\Omega^2, \tag{23}$$

with $m\cdot\Lambda\neq 0$ and the quadruple eigenvalue $\lambda=\Lambda$.

The only conformally flat s.s.s. of Eq. (1) with the quadruple eigenvalue of R_α^β is the DeSitter metric (mentioned at the end of Sec. IV A) following from (23) by putting $m=0$, $\Lambda\neq 0$.

C. One triple and one single eigenvalue

In this case we were only able to find conformally flat solutions. For the canonical form (2), $C=0$ means

$$ds^2=z^2\left[\frac{4\,du\,dv}{(u-v)^2}-d\Omega^2\right], \tag{24}$$

and Eq. (1) then leads to

$$(u-v)^2z_{,uv}-\tfrac{1}{6}R_0z^3=0. \tag{25a}$$

In place of z we introduce a new dependent variable ϕ by $z=(u-v)\phi$. Equation (25a) is replaced by

$$\phi_{,uv}-\frac{R_0}{6}\phi^3+\frac{1}{(u-v)}[\phi_{,v}-\phi_{,u}]=0. \tag{25b}$$

We were able to find solutions of this equation with the following three special assumptions.

1. $\phi=A(u)\cdot B(v)$

A particular solution of Eq. (25b) is given by

$$A(u)=(a_0+a_1u+a_2u^2)^{-1/2},$$

$$B(v)=(a_0+a_1v+a_2v^2)^{-1/2},$$

where $4a_0a_2-a_1^2=2/3R_0$ must hold. The corresponding metric can be transformed into the forms

$$ds^2=2dUdV-\frac{6}{|R_0|}\sinh^2\left(\sqrt{\frac{|R_0|}{12}}(U-V)\right)d\Omega^2, \tag{26a}$$

for $R_0<0$, and

$$ds^2=2\,dU\,dV-\frac{6}{R_0}\sin^2\left(\sqrt{\frac{R_0}{12}}(U-V)\right)d\Omega^2, \tag{26b}$$

for $R_0>0$.

Both (26a) and (26b) are equivalent to the Einstein cosmos. The corresponding eigenvalues of the Ricci tensor, for (26a) and (26b) are

$$\lambda_1=0,\quad \lambda_2=\lambda_3=\lambda_4=R_0/3. \tag{27}$$

2. $\phi=\phi(u+v)$

This case always leads to a triple (or, possibly, quadruple) eigenvalue of R^{β}_{α}. Eq. (25b) reduces to

$$\phi''-\frac{R_0}{6}\phi^3=0. \tag{25c}$$

Solutions of Eq. (25c) with 0, 1 and 2 arbitrary parameters were given in Ref. 20, Sec. III. Examples in terms of Jacobian elliptic functions are, for $R_0<0$,

$$ds^2=\frac{12}{|R_0|}cn^2\left(u+v,\pm\frac{1}{\sqrt{2}}\right)\left[2\,du\,dv-\frac{(u-v)^2}{2}d\Omega^2\right], \tag{28a}$$

and, for $R_0>0$,

$$ds^2=\frac{12}{R_0}nc^2\left(u+v,\pm\frac{1}{\sqrt{2}}\right)\left[2\,du\,dv-\frac{(u-v)^2}{2}d\Omega^2\right]. \tag{28b}$$

The corresponding eigenvalues of the Ricci tensor are given by

$$\begin{aligned}\lambda_1&=\frac{|R_0|}{4}\left[-1-cn^{-4}\left(u+v,\pm\frac{1}{\sqrt{2}}\right)\right].\\ \lambda_2=\lambda_3=\lambda_4&=\frac{|R_0|}{12}\left[-3+cn^{-4}\left(u+v,\pm\frac{1}{\sqrt{2}}\right)\right],\end{aligned} \tag{29a}$$

and

$$\begin{aligned}\lambda_1&=\frac{R_0}{4}\left[1+nc^{-4}\left(u+v,\pm\frac{1}{\sqrt{2}}\right)\right],\\ \lambda_2=\lambda_3=\lambda_4&=\frac{R_0}{12}\left[3-nc^{-4}\left(u+v,\pm\frac{1}{\sqrt{2}}\right)\right],\end{aligned} \tag{29b}$$

respectively.

The only solution of this type with a quadruple eigenvalue is generated by $\phi=\sqrt{12/R_0}(u+v)^{-1}$ and this, according to Sec. IV B, is again the DeSitter space–time.

3. $\phi=(uv)^{-1/2}G(\ln(uv))$

A straightforward calculation shows that, again, a triple eigenvalue of R^{β}_{α} occurs. In this case, Eq. (25b) reduces to

$$\frac{d^2G}{(d\ln\eta)^2}-\frac{1}{4}G-\frac{R_0}{6}G^3=0, \tag{25d}$$

where $\eta:=u\cdot v$ and $G=G(\ln\eta)$ which was also solved in Ref. 16. The metric can be written, alternatively, in the forms

$$ds^2=\frac{2}{uv}G^2(\ln(uv))\left[2\,du\,dv-\frac{(u-v)^2}{2}d\Omega^2\right] \tag{30a}$$

and

$$ds^2=4G^2(U+V)\left[dU\,dV-\sinh^2\left(\frac{U-V}{2}\right)d\Omega^2\right], \tag{30b}$$

where $U:=\ln u$, $V:=\ln v$. The singular solution of (25d), i.e.,

$$G(\ln\eta)=\pm\left(\frac{3}{2R_0}\right)^{1/2}, \tag{31a}$$

leads back to (26b) for $R_0>0$.

On the other hand, the 2-parameter solutions of Eq. (25d) taken from Ref. 20, Sec. III, lead to new solutions of Eq. (1). They are given by

$$G(\ln\eta)=\alpha\left[-\frac{\varepsilon}{3}+\varepsilon\wp\left(\frac{1}{2}\ln\eta+\beta,g_2,g_3\right)\right]^{-1/2}, \tag{31b}$$

where $\wp(x)$ is the Weierstraß function with

$$g_2=\frac{4}{3}(1-R_0\alpha^2),\quad g_3=-\frac{8}{27}+\frac{4}{9}\varepsilon R_0\alpha^2,\quad \varepsilon=\pm1,$$

and α and β are arbitrary constants. Equation (31b) holds for an arbitrary sign of R_0. While we can go to the limit $R_0=0$ in (31b), this cannot be done with the further 2-parameter solution,

$$G(\ln\eta)=\sqrt{\frac{3}{R_0}}\left[-\frac{1}{3}+\wp\left(\frac{1}{2}\ln\eta+\beta,g_2,g_3\right)\right], \tag{31c}$$

where now $g_3=4/27-1/3g_2$ whereas g_2 and β are arbitrary constants. For (31c) $R_0>0$ must hold. The metric (30b) with (31b) or (31c) is conformally related to the metric (26a) (cf. Sec. VIII).

It is also possible to express the solutions of Eq. (25d) by Jacobian elliptic functions (cf. Ref. 20, Appendix E).

V. s.s.s. OF $R=R_0$ WITH GENERIC EIGENVALUE STRUCTURE OF R^{β}_{α}: CANONICAL FORM (2) OF THE METRIC

If the conformal invariant C is eliminated from Eqs. (7a) and (7b) we obtain the equation

$$z_{,uv}+\frac{1}{6}z(e^w+w_{,uv})-\frac{R_0}{12}z^3e^w=0. \tag{32}$$

In contrast to the case $R_0=0$ of paper I, for $w(u,v)$ arbitrarily given, Eq. (32) is a nonlinear partial differential equation for $z(u,v)$.

All the classes of solutions of Eqs. (32) found by us were obtained by assuming the following particular relation between the functions w and z:

$$e^w=z^a(u,v)g^2(u\pm v), \tag{33}$$

with integer a, while g satisfies the equation (37) whose solutions are (38a,...,e). The metric corresponding to (33) is

$$ds^2=2g^2(u\pm v)z^{a+2}(u,v)du\,dv-z^2(u,v)d\Omega^2, \tag{34}$$

while Eq. (32) with (33) goes over into

$$0=\left(1+\frac{a}{6}\right)zz_{,uv}-\frac{a}{6}z_{,u}z_{,v}\pm\frac{1}{3}z^2(\ln g)''+\frac{g^2}{6}\left[z^{a+2}-\frac{R_0}{2}z^{a+4}\right]. \tag{35}$$

The conformal invariant is given by

$$C=z^{-2}+z^{-(a+2)}g^{-2}\{\pm 2(\ln g)''+a(\ln z)_{,uv}\}. \tag{36}$$

If the additional restriction

$$(\ln g)''=\delta_0 g^2 \tag{37}$$

is introduced, we obtain from (35) and (37),

$$\left(1+\frac{a}{6}\right)zz_{,uv}-\frac{a}{6}z_{,u}z_{,v}\pm\frac{\delta_0}{3}g^2z^2+\frac{1}{6}g^2\left[z^{a+2}-\frac{R_0}{2}z^{a+4}\right]=0. \tag{35$'$}$$

For $\delta_0=0$, Eq. (37) is solved by

$$g=g_0e^{c_1(u\pm v)}, \tag{38a}$$

and for $\delta_0\neq 0$ by

$$\delta_0 g^2=(u\pm v+\delta_1)^{-2}, \tag{38b}$$

$$\delta_0 g^2=-\frac{c_1}{2}\cosh^{-2}\left(\sqrt{\frac{c_1}{2}}(u\pm v)+\delta_1\right), \tag{38c}$$

$$\delta_0 g^2=\frac{c_1}{2}\sinh^{-2}\left(\sqrt{\frac{c_1}{2}}(u\pm v)+\delta_1\right), \tag{38d}$$

$$\delta_0 g^2=\frac{c_1}{2}\cos^{-2}\left(\sqrt{\frac{c_1}{2}}(u\pm v)+\delta_1\right). \tag{38e}$$

As far as the corresponding metrics (34) are concerned, the choice $g_0=1$, $c_1=0$ in (38a) and $c_1=\pm 1$ in (38c) and (38d) is no restriction of generality. Thus the following metrics will occur:

$$ds^2=z^2[2z^a\,du\,dv-d\Omega^2], \tag{39a}$$

$$ds^2=z^2\left[2\frac{z^a}{\delta_0}\frac{du\,dv}{(u\pm v)^2}-d\Omega^2\right], \tag{39b}$$

$$ds^2=z^2\left[2\frac{z^a}{\delta_0}\frac{du\,dv}{\cosh^2\dfrac{u\pm v}{\sqrt{2}}}-d\Omega^2\right] \tag{39c}$$

and

$$ds^2=z^2\left[2\frac{z^a}{\delta_0}\frac{du\,dv}{\sinh^2\dfrac{u\pm v}{\sqrt{2}}}-d\Omega^2\right] \tag{39d}$$

and

$$ds^2=z^2\left[2\frac{z^a}{\delta_0}\frac{du\,dv}{\cos^2\frac{u\pm v}{\sqrt{2}}}-d\Omega^2\right]. \tag{39e}$$

For the solution of (35′) two essentially different cases can be distinguished.

A. $a=-6$

In this case (35′) reduces to a first-order nonlinear partial differential equation. By introducing $\varphi:=z^2$ as a new dependent variable, Eq. (35′) goes over into

$$\varphi_{,u}\varphi_{,v}+\tfrac{1}{3}g^2[\pm 4\delta_0\varphi^2+2\varphi^{-1}-R_0]=0. \tag{40}$$

By introducing, in place of φ, the variable

$$\chi(u,v)=\int^{\varphi}dx\,\frac{\sqrt{x}}{\sqrt{\mp 4\delta_0 x^3+R_0x-2}}, \tag{41}$$

Eq. (40) can be transformed into

$$\chi_{,u}\chi_{,v}=\mp\tfrac{1}{3}g^2. \tag{40′}$$

The integral in (41) can be evaluated in terms of elliptic integrals of the first and third kind of Legendre's canonical forms.[17] The problem of solving (35′) thus is reduced to finding solutions of Eq. (40′) for g^2 given by Eqs. (38a)–(38d). Then $z(u,v)$ can be determined as an implicit function of $u\pm v$ from Eq. (41).

(α) Let us start with (38a), that is $g=1$, $\delta_0=0$. Then

$$\chi=\frac{2}{\sqrt{3}}\sqrt{uv} \tag{42}$$

solves (40a) with the + sign on the right hand side. Apart from integration constants which are irrelevant for the corresponding metric (39a) this is the most general solution for which $\chi=A(u)\cdot B(v)$. Another solution is given by

$$\chi=\frac{1}{\sqrt{3}}(u\pm v). \tag{43}$$

In this case the integral in (41) can be carried through. We obtain

$$\chi=\frac{\varphi}{R_0}\sqrt{R_0-2\varphi^{-1}}-R_0^{3/2}\ln\frac{\sqrt{R_0-2\varphi^{-1}}-\sqrt{R_0}}{\sqrt{R_0-2\varphi^{-1}}+\sqrt{R_0}}, \tag{44a}$$

if $R_0>0$, and

$$\chi=\frac{\varphi}{R_0}\sqrt{R_0-2\varphi^{-1}}-2|R_0|^{3/2}\arctan\sqrt{\frac{R_0}{|R_0|}-2\frac{\varphi^{-1}}{|R_0|}}, \tag{44b}$$

if $R_0<0$. The three different eigenvalues of R_α^β corresponding to the solution (42) are given by:

$$\lambda_1=R_0-2\varphi^{-1}-\frac{1}{\sqrt{3}}\varphi\frac{\sqrt{R_0-2\varphi^{-1}}}{\sqrt{uv}},$$

$$\lambda_2 = -(2/3)\varphi^{-1}, \tag{45}$$

$$\lambda_3 = \lambda_4 = \frac{4}{3}\varphi^{-1} + \frac{1}{2\sqrt{3}}\varphi\frac{\sqrt{R_0 - 2\varphi^{-1}}}{\sqrt{uv}},$$

while the conformal invariant is

$$C = R_0 - 2\varphi^{-1} - \frac{1}{2}\sqrt{3}\varphi\frac{\sqrt{R_0 - 2\varphi^{-1}}}{\sqrt{uv}}. \tag{46}$$

(β) It is not difficult to obtain solutions of Eq. (40a) for the other values (38b)–(38d) of g^2. The solutions of Eq. (40a) corresponding to (38c), (38e), (38b) are, respectively,

$$\chi = \pm\frac{2}{\sqrt{-3\delta_0}}\arctan\left[\exp\sqrt{\frac{c_1}{2}}(u+v-\eta_0)\right], \tag{47a}$$

$$\chi = \frac{1}{2\sqrt{3\delta_0}}\ln\tan\left(\frac{\pi}{4} + \sqrt{\frac{|c_1|}{2}}(u+v-\eta_0)\right), \tag{47b}$$

$$\chi = \frac{1}{\sqrt{3\delta_0}}\ln(u+v-\eta_0). \tag{47c}$$

B. $a \neq -6$

In this case the substitution $z := \varphi^{1+a/6}$ transforms Eq. (35′) into

$$\left(1+\frac{a}{6}\right)^2\varphi_{,uv} + g^2\left[\pm\frac{1}{3}\delta_0\varphi + \frac{1}{6}\varphi^{1/6\,a^2+a+1} - \frac{R_0}{12}\varphi^{1/6\,a^2+4/3\,a+3}\right] = 0. \tag{48}$$

The canonical form of the metric now is

$$ds^2 = 2g^2(u \pm v)\varphi^{1/6(a+6)(a+2)}\,du\,dv - \varphi^{2+a/3}d\Omega^2. \tag{49}$$

For $g=1$, $a=0$, Eq. (48) reduces to the 2-dimensional nonlinear wave equation of the ϕ^4-theory,

$$\varphi_{,uv} + \left(\pm\frac{1}{3}\delta_0 + \frac{1}{6}\right)\varphi - \frac{R_0}{12}\varphi^3 = 0. \tag{50}$$

All known exact s.s. solutions of the ϕ^4-theory thus lead to spaces with constant curvature scalar (cf. Refs. 18–20).

(α) Again, we deal with the most simple case $g=1$, $\delta_0=0$ first, i.e., with (38a). The ansatz $\varphi = \varphi(Au+Bv)$, $AB \neq 0$ reduces Eq. (48) to an ordinary differential equation the integral of which is given by

$$\pm(Au+Bv+E) = \int^{\varphi}\frac{d\varphi}{\sqrt{2D + \dfrac{72}{AB(6+a)^2}\left[\dfrac{R_0}{2}\dfrac{\varphi^{((a+4)^2+8)/6}}{(a+4)^2+8} - \dfrac{\varphi^{((a+3)^2+3)/6}}{(a+3)^2+3}\right]}}. \tag{51}$$

For $a=0,-2,-3,-4$ the integral can be evaluated in terms of elliptical functions (cf. Appendix A). Specifically, for $a=0$ (and $g=1\cong\delta_0=0$) with $\varphi=\varphi(Au+Bv)$, Eq. (48) reduces to

$$\varphi'' + (6AB)^{-1}\left[\varphi - \frac{R_0}{2}\varphi^3\right] = 0. \tag{52}$$

Equation (51) is of the same type as Eq. (25d) solutions of which we presented in Eqs. (31a)–(31c). It is the 1-dimensional *Landau–Ginzburg* equation of a superconductor without an external magnetic field. While the functions appearing are the same the metrics are different, though. For $a=0$, from Eq. (39a),

$$ds^2 = \varphi^2(2\,du\,dv - d\Omega^2), \tag{53}$$

results which is not conformally flat in contradistinction to the metric, Eqs. (30), with (30a)–(30c). The singular solution with $\varphi=(2/R_0)^{1/2}$ admits two double eigenvalues; it was already found in Sec. III as a decomposable space [Eq. (9), $k=0$], and is among the metrics (5) with (14) discussed in Sec. IV. Solutions of (51) in terms of Jacobian elliptical functions were given by us in Appendix E of Ref. 20.

(β) Coming now to the values (38b)–(38d) for g^2 we must solve, for $a=0$, as the first particular case:

$$g^{-2}(u\pm v)\varphi_{,uv} + \left(\frac{1}{6} \pm \frac{\delta_0}{3}\right)\varphi - \frac{R_0}{12}\varphi^3 = 0. \tag{54a}$$

In Eqs. (B1), (B3), (B6) of Appendix B we display 1-parameter solutions of Eq. (54a) for certain fixed values of δ_0 and by assuming $\varphi=\varphi(u\pm v)$.

For the case (38b), $\delta_0=\mp 3/2$, and the corresponding metric (with the correct signature) is

$$ds^2 = \varphi^2\left[\frac{4}{3}\frac{du\,dv}{(u\pm v)^2} - d\Omega^2\right], \tag{54b}$$

with

$$\varphi = [1/2\sqrt{-R_0} + c_1(u\pm v)^{-1/3}]^{-1},$$

where $R_0 \leqslant 0$. For (38c) and (38d) we have $\delta_0=\mp 1/2$ and the solutions

$$ds^2 = \frac{6}{R_0}\cosh^2\frac{(u-v)}{\sqrt{2}}\left[\frac{2\,du\,dv}{\cosh^2\dfrac{u-v}{\sqrt{2}}} - d\Omega^2\right] \tag{54c}$$

and

$$ds^2 = \frac{6}{|R_0|}\cos^2\frac{u-v}{\sqrt{2}}\left[\frac{2\,du\,dv}{\cos^2\dfrac{u-v}{\sqrt{2}}} - d\Omega^2\right], \tag{54d}$$

where $R_0 \neq 0$.

Both metrics (54c) and (54d) have been met before in Eqs. (12) and (26b) (Einstein cosmos); they lead to degenerate eigenvalues of R_α^β.

For the particular value $a=-2$ we obtain from Eq. (48),

$$g^{-2}\varphi_{,uv} + \frac{3}{4}\left(\pm\delta_0 - \frac{R_0}{4}\right)\varphi + \frac{3}{8}\varphi^{-1/3} = 0. \tag{55}$$

Again, from Appendix B, we obtain the following solutions of (55) for the values (38b)–(38d) of g^2 if $\varphi=\varphi(u+v)$,

$$\varphi=\left[\pm\left(-\frac{6}{R_0}\right)^{1/2}+\tilde{c}_1(u\pm v+\delta_1)^{1/2}\right]^{3/2}, \tag{56a}$$

$$\varphi=\left[\frac{3}{5}\left(\mp 2\,\delta_0+\frac{R_0}{2}\right)\right]^{-3/4}\cosh^{-3/2}[\sigma(u\pm v)+\delta_1], \tag{56b}$$

and

$$\varphi=\left[\frac{3}{5}\left(\mp 2\,\delta_0+\frac{R_0}{2}\right)\right]^{-3/4}\cos^{-3/2}[\sigma(u\pm 4)+\delta_1], \tag{56c}$$

with

$$\sigma:=\left[-\frac{1}{5}\left(1\mp\frac{R_0}{4\,\delta_0}\right)\right]^{1/2}.$$

The corresponding metric, for (56a), is

$$ds^2=\frac{6}{|R_0|}\,\frac{du\,dv}{(u-v+\delta_1)^2}-\left[-\sqrt{\frac{6}{|R_0|}}+\tilde{c}_1(u+v+\delta_1)^{1/2}\right]^2 d\Omega^2, \tag{57}$$

for $R_0<0$.

If $\tilde{c}_1=c_1(12/|R_0|)^{1/4}$, $\delta_1=c_1^{-2}(3/|R_0|)^{1/2}$ the metric (57) can be transformed into

$$ds^2=\left(c_1-\sqrt{\frac{|R_0|}{6}}\,r\right)^4 dt^2-\frac{dr^2+r^2\,d\Omega^2}{\left(c_1-\sqrt{\frac{|R_0|}{6}}\,r\right)^2}.$$

For (56b) and (56c) we obtain metrics of the form

$$ds^2=4|\delta_0|\cosh^{-2}\left[\sqrt{\frac{c_1}{2}}(u\pm v)+\delta_1\right](2\,du\,dv-b_0^2\,d\Omega^2)$$

and

$$ds^2=4\,\delta_0\cos^{-2}\left[\sqrt{\frac{c_1}{2}}(u\pm v)+\delta_1\right](2\,du\,dv-b_0^2\,d\Omega^2),$$

i.e., essentially come back to the metric (52).

VI. s.s.s. of $R=R_0$ WITH GENERIC EIGENVALUE STRUCTURE OF R_α^β: CANONICAL FORM (3) OF THE METRIC

We now use a slightly altered form of the canonical form (3) of the metric,

$$ds^2=(\psi/\chi)^2\,dt^2-(\chi/r)^4[dr^2+r^2\,d\Omega^2], \tag{58}$$

with $\psi=\psi(r,t)$, $\chi=\chi(r,t)$.

We note that the change of radial coordinate $\rho=r^{-1}$ leads to

$$ds^2=(\psi/\chi)^2\,dt^2-\chi^4[d\rho^2+\rho^2\,d\Omega^2],$$

where now $\psi=\psi(\rho,t)$, $\chi=\chi(\rho,t)$.

While working with (58) permits us to find more s.s.s. of Eq. (1), we ought to check, in each case, if the solution is different from those given in Sec. V. In principle, (58) can be transformed into (2).

A straightforward calculation of the Ricci scalar R_0 and the conformal invariant gives

$$\psi''+\psi\left[3\chi''/\chi+\frac{R_0}{2}(\chi/r)^4\right]-\frac{6}{5}r^{-4}\chi[\psi^{-1}(\chi^5)^{\cdot\cdot}+(\chi^5)^{\cdot}(\psi^{-1})^{\cdot}]=0 \tag{59}$$

and

$$\begin{aligned} r^{-4}\chi^4 C=&-\chi^3[(\chi^{-3})''+3r^{-1}(\chi^{-3})'+2(\chi^{-3})' \\ &+2(\chi^{-3})'\psi^{-1}\psi']-3r^{-1}\psi^{-1}\psi'-\psi^{-1}\psi'', \end{aligned} \tag{60}$$

where $\psi':=d\psi/dr$, $\dot{\psi}:=d\psi/dt$.

Equations (59) and (60) hold for any s.s. metric as ψ and χ are arbitrary functions of two variables. In order to obtain solutions of (59) for given R_0 we add particular assumptions. Two main cases are discussed.

A.

$$\chi=\chi(r). \tag{61}$$

Now, Eq. (59) reduces to a linear equation for $\psi(r,t)$ and arbitrarily given $\chi(r)$. In principle we are thus led to s.s.s. of Eq. (1) with two free functions of the variable r and two more free functions of t. In fact, however, we succeeded in integrating (59) only for two subcases. In place of (59) we consider the system

$$\frac{\partial^2\psi(r,t)}{\partial r^2}+f(r)\psi(r,t)=0, \tag{62a}$$

$$\chi''-\frac{1}{3}f(r)\chi+\frac{R_0}{6}r^{-4}\chi^5=0, \tag{62b}$$

for $\psi(r,t)$ and $\chi(r)$ and discuss two choices for $f(r)$.

1. $f(r)=0$

From (62a),

$$\psi(r,t)=\omega(t)r+\nu(t). \tag{63}$$

One of the free functions $\omega(t),\nu(t)$ can be transformed to one in the metric (58), while $\chi(r)$ satisfies

$$\chi''+\frac{R_0}{6}r^{-4}\chi^5=0, \tag{64}$$

which is the *generalized Lane–Emden equation* of type $(0,R_0/6,-3,5)$. Its solutions (cf. Ref. 20) are given by

$$\chi=\left(\frac{3}{2R_0}\right)^{1/4}r^{1/2}, \tag{65a}$$

$$\chi = r d^{1/2}\left[1+\frac{1}{18}R_0\, d^2 r^2\right]^{-1/2}, \tag{65b}$$

and

$$\chi = c_1 r^{1/2}\left[-\frac{\varepsilon}{3}+\epsilon\wp\left(\mp\frac{1}{2}\ln r + c_2, g_2, g_3\right)\right]^{-1/2}, \tag{65c}$$

where in the Weierstraß function $\wp$ $g_2 = 4/3(1+c_1^2 R_0)$, $g_3 = -8/27 - 4/9\varepsilon c_1^2 R_0$, $\varepsilon^2 = 1, d, c_1, c_2$ arbitrary constants.

The singular solution (65a) is equivalent to the decomposable spaces (9) of Sec. III. The spatial sections of the metric (58) with (65a) are 3-spaces of constant curvature. The conformal invariant of this 1-parameter solution equals

$$C = 3\, d^{-2} r^{-2} + d^{-2} r^{-1}\left[1-\left(\frac{R_0\, d^2 r^2}{18}\right)^2\right]\omega(t)[\omega(t) r + \nu(t)]^{-1}. \tag{66}$$

2. $f(r) = 3\lambda(\lambda-1)r^{-2} + 1/2 R_0 \sigma^4 r^{4(\lambda-1)}$

A comparison of Eq. (62a) with this particular value of $f(r)$ with the differential equation

$$\frac{\partial^2 \psi}{\partial r^2} + \psi\left[\frac{1/4 - p^2\gamma^2}{r^2} + \delta^2\gamma^2 r^{2\gamma-2}\right] = 0, \tag{67}$$

for the Bessel functions, leads to the following solution:

$$\psi = r^{1/2}[\omega(t) I_p(\delta r^{\pm 2(4p^2+3)-1/2}) + \nu(t)\mathcal{N}_p(\delta r^{\pm 2(4p^2+3)^{-1/2}})], \tag{68}$$

where

$$\delta := \pm\sqrt{\frac{R_0}{2}}\,\frac{\sigma^2}{2}\sqrt{4p^2+3}, \quad p = \frac{\sqrt{1+12\lambda-12\lambda^2}}{2(2\lambda-1)}, \qquad \lambda \neq 1/2, \quad R_0 \gtrless 0. \tag{69}$$

Equation (62b) in this case looks difficult to solve:

$$r^4\chi'' - \left[\lambda(\lambda-1)r^2 + \frac{R_0}{6}\sigma^4 r^{4\lambda}\right]\chi + \frac{R_0}{6}\chi^5 = 0. \tag{70}$$

However, a particular solution,

$$\chi = \sigma r^{\lambda}, \tag{71}$$

with arbitrary λ is easily obtained.

The corresponding metric is

$$ds^2 = \psi^2\left(\frac{1}{\rho}, t\right)\sigma^{-2}\rho^{2\lambda}\, dt^2 - \sigma^2\rho^{-2\lambda}[d\rho^2 + \rho^2\, d\Omega^2], \tag{72}$$

with $\rho = r^{-1}$.

The conformal invariant belonging to (68) and (71) and calculated from Eq. (60) is

$$C = \frac{R_0}{2} + 3\sigma^{-4}(1-2\lambda)r^{2(1-2\lambda)}\left[\lambda - r + r\,\frac{\psi'}{\psi}\right].$$

The case $\lambda = 1/2$ excluded in (67), (68) again leads to the decomposable spaces (9) of Sec. III.

B. $\chi = \psi = A(r)B(t)$

For this case we obtain from Eqs. (59) and (60), respectively,

$$8r^4A^{-5}A'' + R_0B^4 - 3(B^4)^{\cdot\cdot} = 0 \tag{73}$$

and

$$C = -r^4B^{-4}A^{-2}[(A^{-2})'' + 3r^{-1}(A^{-2})'\,]. \tag{74}$$

By separation of variables, from Eq. (73),

$$A'' - \lambda_0/8r^{-4}A^5 = 0 \tag{75}$$

and

$$\ddot{y} - (R_0/3)y - \lambda_0/3 = 0, \tag{76}$$

where $y := B^4$ has been introduced. Equation (75) again is the generalized Lane–Emden equation (64); thus the solutions given in Eqs. (65a)–(65c) apply as well here if R_0 there is replaced by $-\lambda_0 \cdot 3/4$. Equation (76) is linear.

The corresponding metrics are conformal to decomposable spaces,

$$ds^2 = y(t)\left\{\frac{dt^2}{y(t)} - r^{-4}A^4(r)[dr^2 + r^2\,d\Omega^2]\right\}. \tag{77}$$

More precisely, the solutions corresponding to (65a) and (65c) are conformal to decomposable spaces of type (9) of Sec. III, i.e.,

$$ds^2 = dt^2 - \frac{9}{8}|\lambda_0|y(t)[d\rho^2 + d\Omega^2] \tag{78a}$$

and

$$ds^2 = dt^2 - y(t)\left[-\frac{\varepsilon}{3} + \varepsilon\wp(\pm\rho/2 + c_2, g_2, g_3)\right]^{-2}(d\rho^2 + d\Omega^2), \tag{78b}$$

where $\rho = \ln r$.

On the other hand (65b) leads to

$$ds^2 = y(t)\left\{\frac{dt^2}{y(t)} - \frac{dr^2 + r^2\,d\Omega^2}{[1 - \lambda_0/24r^2]^2}\right\} \tag{79}$$

which is conformally flat and gives a Ricci tensor with a triple eigenvalue. It thus belongs to the class of metrics (24) of Sec. IV C.

If $\lambda_0 = 0$ in Eqs. (75) and (76), we obtain $\chi = A_0 + B_0 r$ in place of Eq. (65a) and the metrics

$$ds^2 = dt^2 - (A_0r^{-1} + B_0)^4\left\{\begin{array}{l}\sinh\left(\sqrt{\dfrac{R_0}{3}}t + c_2\right)\\[2ex] \sin\left(\sqrt{\dfrac{|R_0|}{3}}t + c_2\right)\end{array}\right\}(dr^2 + r^2\,d\Omega^2). \tag{78c}$$

Finally, we mention a solution of Eq. (1) corresponding to the metric (78) but with coordinates r and t interchanged:

$$ds^2=-dr^2+y(r)[A(t)]^4(dt^2-d\Omega^2), \tag{80}$$

where

$$y=\begin{cases} c_1\sinh\left(\sqrt{\dfrac{|R_0|}{3}}r+c_2\right), & \text{if } R_0<0 \\ c_1\sin\left(\sqrt{\dfrac{R_0}{3}}r+c_2\right), & \text{if } R_0>0 \end{cases} \tag{81a}$$

and

$$A(t)=d_1\sin\left(\frac{t}{2}+d_2\right). \tag{81b}$$

VII. s.s.s. OF THE KILMISTER–YANG THEORY OF GRAVITATION

Kilmister and Yang have suggested the following field equations for a theory of gravitation:[3]

$$R_{\alpha[\beta;\gamma]}=0. \tag{82}$$

They are equivalent to[21]

$$C^{\kappa}_{\alpha\beta\gamma;\kappa}=0, \quad R=R_0=\text{const.} \tag{83}$$

If we write $d^{\alpha}_{\beta\gamma}:=C^{\kappa\alpha}{}_{\beta\gamma;\kappa}$ then, for a s.s. metric, the only nonvanishing components of $d^{\alpha}_{\beta\gamma}$ are

$$d^0_{01}=2d^2_{12}=2d^3_{13}=-C^{01}_{01,1}-3C^{01}_{01}\Gamma_{84}12^2 \tag{84a}$$

and

$$d^1_{01}=-2d^2_{02}=-2d^3_{03}=-C^{01}_{01,0}-3C^{01}_{01}\Gamma^2_{02}. \tag{84b}$$

For the further calculation we use Takeno's canonical form of the s.s. metric[15] with two redundant functions, that is,

$$ds^2=E\,dt^2-A\,dr^2+2D\,dr\,dt-B\,d\Omega^2. \tag{85}$$

Integration of $d^{\alpha}_{\beta\gamma}=0$ then leads to

$$C=c_0B(r,t)^{-3/2} \tag{86a}$$

where C is the conformal invariant and c_0 an arbitrary constant. Thus, for the canonical form (2),

$$C=c_0z^{-3}, \tag{86b}$$

while for (3) or (58), respectively,

$$C=c_0a^{-6}, \quad C=r^3\chi^{-6}, \tag{86c}$$

must hold in addition to (1) if the s.s. metric is to be a solution of Eq. (82). Equations (86) allow an easy inspection of the solutions of Eq. (1) presented in the previous sections. Of course all Einstein spaces and all conformally flat solutions with constant Ricci scalar are solutions of the Kilmister–Yang equations (82).[22] In paper I we have given the most general conformally flat

solution with $R=0$. Thus, it is of interest only, which solutions of Eq. (1) with $C\neq 0$ conform to Eqs. (86b) or (86c). Of all the solutions presented only the following three classes are solutions of the Yang–Kilmister equations:

$$ds^2=\left[a(u)+b(u)r+\left(\frac{1}{b_0^2}-\frac{R_0}{2}\right)r^2\right]du^2+2\,du\,dr-b_0^2\,d\Omega^2, \tag{87}$$

i.e., the s.s.s. of (1) with two double eigenvalues given in (14); the solution given by Ni,[23]

$$ds^2=dt^2-\left(1-\frac{a_0}{r}+b_0r^2\right)^{-1}dr^2-r^2\,d\Omega^2, \tag{88}$$

and the metric obtained from (88) by interchanging t and r,

$$ds^2=\left(-1+\frac{R_0}{6}t^2+\frac{b_0}{t}\right)^{-1}dt^2-t^2\,d\Omega^2.$$

The last two were found as decomposable spaces in Sec. III.

VIII. GENERATION OF SOLUTIONS BY CONFORMAL MAPPING

From the very start we used the fact that, locally, every s.s.s. metric is conformal to a decomposable s.s. space, built from two 2-dimensional subspaces. If in place of (2),

$$\overset{\star}{g}=z^2g, \tag{89}$$

is written, then Eqs. (7a) and (7b) can be recast into the form

$$e^{-w}z_{,uv}+\frac{1}{6}zC-\frac{\overset{\star}{R}}{12}z^3=0, \tag{90a}$$

$$\overset{\star}{C}-z^{-2}C=0, \tag{90b}$$

$$R-2C=0, \tag{90c}$$

where $R^\star, C^\star$ belong to the metric $g^\star$ while R, C are formed by g. If Eq. (90a) admits a solution $z(u,v)$ for arbitrarily given function $w(u,v)$ and fixed $R^\star=\text{const}$, then every s.s.s. of (1) is conformal to a s.s. metric,

$$ds^2=2e^{w(u,v)}\,du\,dv-d\Omega^2. \tag{91}$$

This is the local version, in the case of spherical symmetry of the problem of Yamabe for compact Riemannian manifolds, whether a conformal metric exist for which the scalar curvature is constant.[24,25] Now, Eq. (90a) is nonlinear and existence proofs for local (and global) solutions are available only for a number of very restricted choices of $w(u,v)$ such as, for example, $w=\text{const}$.[26]

In particular, Eq. (90a) can be used to generate s.s.s. of $R^\star=R_0$ from s.s. metrics with $R=0$, $R=R_0\neq 0$ and R not a constant, respectively. An example for the first case is given by Sec. IV C [$w=-2\log(u-v)$]; another one by solution (54b). On the other hand, $w=0$ leads to the metrics (53) of Sec. V B, with $R=1$. Finally, the rather peculiar choice of

$$w=\log 2-2\log(u-v)-\log\left[1-\frac{R_0}{2}z^2(u)\right]$$

with the arbitrary function $z(u)$ leads from $R=R_0z^2(u)$ to the class of metrics (16a) of Sec. IV A solving (1).

IX. DISCUSSION

In our investigation of s.s.s. with a constant Ricci scalar we obtained a number of explicitly given solutions depending on two free functions of one variable, at most. As far as we know, all s.s. metrics with a constant nonvanishing Ricci scalar presented in the literature are contained within the classes found in this paper and collected in Table I.

However, in contradistinction to the case $R_0=0$ of paper I we have found no way of transforming the relevant differential equation into a linear one for the case of metrics whose Ricci tensor has a nondegenerate eigenvalue structure. This explains, why, in this generic case, the solutions exhibited depend on just one arbitrary function of one variable and integration constants, or just on integration constants alone. Moreover, we have not been able to explicitly give a solution with nonvanishing conformal invariant and a triple eigenvalue of R_α^β nor a conformally flat solution with a generic eigenvalue structure, or to prove their nonexistence. However, we have exhausted all s.s.s. of Eq. (1) for which R_α^β has two double or one quadruple eigenvalue and all s.s. decomposable space–times. The set of solutions found in the other cases is general enough to be helpful for the construction of counterexamples to Birkhoff's theorem within large classes of gravitational theories. On the other hand, there exists a large class of gravitational theories which, for vanishing matter, coincides with the Einstein vacuum field equations, and which therefore admit a Birkhoff theorem just like Einstein's theory.[27]

Space–time manifolds with constant curvature have been investigated with the help of Killing–Yano symmetry;[28] they also occur in studies of conformal vector fields[29] and Kaehler metrics.[30] Also in this context it may well be an advantage to have a reservoir of exact solutions to play with, as presented here.

Their also exist investigations using constant scalar curvature within gauge theory,[31] supergravity,[32] and supergeometry.[33] However, the extension of the present investigation to higher-dimensional spaces is not as straightforward as one might expect. As listed in Appendix C, the equation replacing (7b) will contain an additional nonlinearity if the space–time-dimension $n>4$.

The case of plane symmetry which, in paper I, was completely solved can be dealt with only partial success for $R_0\neq 0$. If $R_0-2C=0$, the general solution of Eqs. (64a) and (64b) of paper I is given by

$$ds^2=\frac{16}{R_0}\frac{du\,dv}{(u+v)^2}-(u+v)^2(dx^2+dy^2). \tag{92}$$

For $2C-R_0\neq 0$ $z(u,v)$ is arbitrary while $w(u,v)$ must satisfy

$$w_{,uv}-\frac{R_0}{2}z^2e^w=-6\frac{z_{,uv}}{z}. \tag{93}$$

Even the case of conformally flat metrics resists *complete* integration. The cases of constant z or w are easily solved.

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APPENDIX A

The evaluation of Eq. (51). For $a=0$ we obtain the standard elliptic integral,

$$\int \frac{d\varphi}{\sqrt{2D+(6AB)^{-1}\left[\frac{R_0}{4}\varphi^4-\varphi^2\right]}},$$

which falls into one of the categories 251.00–259.00 of Ref. 17.

For $a=-2$ the substitution $u=\varphi^{2/3}$ leads to the integral

$$\int \frac{u^{1/2}\,du}{\sqrt{2D+9(8AB)^{-1}\left[\frac{R_0}{6}u^3-u\right]}},$$

i.e., to the cases 253.13–15 of Ref. 17. $a=-3$ with $u=\varphi^{+1/2}$ results in an integral

$$\int \frac{u\,du}{\sqrt{2D+8(3AB)^{-1}\left[\frac{R_0}{6}u^3-u\right]}},$$

of type 232.19–20 of Ref. 17 and, finally, $a=-4$ with $u=\varphi^{2/3}$ leads to

$$\int \frac{u^{1/2}\,du}{\sqrt{9R_0(8AB)^{-1}\left(u-\frac{2}{R_0}\right)^2+2D-9(2ABR_0)^{-1}}}.$$

APPENDIX B

Solutions to Eq. (54a). We list the following 1-parameter solutions of the relevant equations

$$\varphi=\left[-\varepsilon_1\varepsilon_2\frac{2}{3-n}\left(\frac{a}{b}\right)^2\right]^{1/(n-1)}\cosh^{2/(n-1)}(\sigma\eta+\delta_1), \tag{B1}$$

with

$$\sigma:=\left[\varepsilon_1 a^2\frac{(n-1)^2}{2(3-n)}\right]^{1/2}, \quad \varepsilon_1^2=\varepsilon_2^2=1,$$

solves

$$\cosh^2(\sigma\eta+\delta_1)\frac{d^2\varphi}{d\eta^2}+\varepsilon_1 a^2\varphi+\varepsilon_2 b^2\varphi^n=0, \tag{B2}$$

if $n\neq 3, a, b$ constants with $ab\neq 0$, δ_1 an integration constant,

$$\varphi=\left[\mp\varepsilon_1\varepsilon_2\frac{2}{3-n}\left(\frac{a}{b}\right)^2\right]^{1/(n-1)}\begin{Bmatrix}\cos^{2/(n-1)}(\sigma\eta+\delta_1)\\ \sinh^{2/(n-1)}(\sigma\eta+\delta_1)\end{Bmatrix}, \tag{B3}$$

with

$$\sigma:=\left[-\varepsilon_1 a^2\frac{(n-1)^2}{2(3-n)}\right]^{1/2},\quad \varepsilon_1^2=\varepsilon_2^2=1,$$

and the $\mp$ signs refer to cos and sinh, respectively, solves

$$\begin{Bmatrix}\cos^2(\sigma\eta+\delta_1)\\ \sinh^2(\sigma\eta+\delta_1)\end{Bmatrix}\frac{d^2\varphi}{d\eta^2}+\varepsilon_1 a^2\varphi+\varepsilon_2 b^2\varphi^n=0. \tag{B4}$$

Furthermore,

$$\varphi=\left[\pm|3+n|\left(-\frac{\varepsilon_2 b^2}{2(1+n)}\right)^{1/2}+\tilde{c}_1\eta^{(1-n)/(3+n)}\right]^{2/(1-n)}, \tag{B5}$$

solves

$$\eta^2\frac{d^2\varphi}{d\eta^2}+2\frac{1+n}{(3+n)^2}\varphi+\varepsilon_2 b^2\varphi^n=0, \tag{B6}$$

if $n\neq -3$, $\tilde{c}_1$ integration constant.

For $n=3$ we note the following results:

$$\varphi=[-\varepsilon_2 b^{-2}]^{1/2}\cosh(\eta+\delta_1), \tag{B7}$$

solves

$$\cosh^2\eta\frac{d^2\varphi}{d\eta^2}+\varepsilon_2 b^2\varphi^3=0, \tag{B8}$$

while

$$\varphi=[\varepsilon_2 b^{-2}]^{1/2}\cos(\eta+\delta_1), \tag{B9}$$

solves

$$\cos^2\eta\frac{d^2\varphi}{d\eta^2}+\varepsilon_2 b^2\varphi^3=0. \tag{B10}$$

APPENDIX C

Using the formulas given by Takeno[15] it is easy to see that, by a suitable change of the constant factor in the conformal invariant C (in the sense that it now depend on n), Eq. (7a) stays unchanged. On the other hand, in place of Eq. (7b) we get

$$z_{,uv}+\frac{1}{2(n-1)}z^3e^w\left(C-\frac{1}{2}R\right)+\frac{n-4}{4}(2z^{-1}z_u z_v+e^w z)=0. \tag{C1}$$

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Complete asymptotic expansions of the Fermi–Dirac integrals $\mathcal{F}_p(\eta)=1/\Gamma(p+1)\int_0^\infty[\epsilon^p/(1+e^{\epsilon-\eta})]d\epsilon$

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The complete asymptotic expansions, that is to say expansions which include any exponentially small terms lying beyond all orders of the asymptotic power series, are calculated for the Fermi–Dirac integrals. We present two methods to accomplish this, the first in the complex plane utilizing Mellin transforms and Hankel's representation of the gamma function, and the second on the real line using the known asymptotic expansions of the confluent hypergeometric functions. The complete expansions of $\mathcal{F}_p(\eta)$ are then used to investigate the effect that these traditionally neglected exponentially small terms have on physical systems. It is shown that for a 2 dimensional nonrelativistic ideal Fermi gas, the subdominant exponentially small series becomes dominant. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1350634]

I. INTRODUCTION

If one adheres to the conventional definition of the asymptotic series for a function given by Poincaré, all terms in the series are algebraic in the asymptotically small variable ϵ. This implies that transcendental exponentially small terms are not captured by the series in the limit $\epsilon\to 0$, and hence these transcendentally small terms have traditionally been neglected in asymptotics. These small terms are said to lie beyond all orders of the asymptotic expansion. By neglecting such terms in the asymptotic expansion of a given function, it is clear that the resultant series cannot give an exact representation of this function. It has been demonstrated however, most notably by Dingle[1] via his derivations of integral representations of the remainder terms of a wide class asymptotic series, that asymptotic series are capable of being precisely interpreted. Thus it became apparent in the late 1950s that the definition of Poincaré needed to be replaced. This led Dingle[1] to define the *complete asymptotic expansion* of a function $f(x)$ as an expansion constructed from asymptotic series, which formally exactly obeys—throughout a certain phase sector—all those relations satisfied by $f(x)$ which do not involve any finite numerical value of x. Dingle found that in practice a suitably rigorous analysis would yield, in a certain phase sector, the complete asymptotic expansion of a function, including any transcendentally small terms which may be present. Dingle's definition suggested that if methods were developed whereby the divergent sequence of late terms in an asymptotic expansion could be interpreted, then asymptotic expansions could become an exact representation of a function. The construction of such methods was pioneered by Dingle[1] with his theory of terminants, and has been further developed by Berry *et al.* in their work on *hyperasymptotics*.[2,3]

There has been an increasing amount of research undertaken in recent years which demonstrates the practical importance of obtaining complete asymptotic expansions as opposed to Poincaré expansions. For example, problems in crystal growth, viscous flow, quantum tunnelling, and optics[2,3] have demonstrated the physical manifestations of the terms lying beyond all orders in a complete asymptotic expansion; and work on ordinary differential equations and such problems as

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the Generalized Euler–Jacobi inversion formula[2] has reinforced their application to fundamental problems in classical analysis.

Our aim in this paper is to demonstrate that the transcendentally small terms appearing in a complete asymptotic expansion are capable of producing important physical effects, that can be manifest even when the expansion is truncated at an early order. In particular, we develop the complete asymptotic expansion of $\mathcal{F}_p(\eta)$, a function which is of fundamental importance in the statistical mechanics of Fermi systems. We then use this to demonstrate that exponentially small terms dominate the low temperature expansions of the thermodynamic functions of an ideal Fermi gas, when the number of spatial dimensions is even. We investigate the particular case of a two dimensional ideal Fermi gas in detail, and show that using our complete expansions we recover the exact result obtained by May[4] in which closed form solutions were obtained for the integrals occurring in the number equation, and internal energy.

As has been discussed by Dingle,[1,5] the commonly accepted Sommerfeld method of asymptotically expanding the Fermi–Dirac integrals (see, e.g., Refs. 6, 7), does not yield the complete asymptotic expansion and thus leads to erroneous conclusions regarding the exponentially small terms. For general p, the complete asymptotic expansion of $\mathcal{F}_p(\eta)$ consists of an asymptotic power series, as well as a subdominant exponentially small series which is traditionally neglected. In the particular case when p is an odd half integer, this exponentially small series vanishes identically, and so the usual assertion accompanying the Sommerfeld treatment that exponentially small terms are being neglected is, in this case, incorrect. When p is an integer, however, the asymptotic power series truncates into a finite sum, and the exponentially small terms then become dominant. This will be shown to be the cause of the aforementioned behavior of the even dimensional Fermi gas.

Although the complete asymptotic expansion of $\mathcal{F}_p(\eta)$ is known,[1,5] albeit not well known, we feel that our proofs being simultaneously both perspicuous, and rigorous and complete, elucidate the construction of this seemingly esoteric yet fundamentally important expansion. We present the derivations from two alternative angles. The first method is performed using contour integration, and highlights the mechanisms producing the various idiosyncrasies displayed by the expansion of $\mathcal{F}_p(\eta)$. We begin with the standard Mellin/inverse Mellin transform method, and use this to obtain a representation of $\mathcal{F}_p(\eta)$ along Hankel's contour. By paying careful attention to the various limits involved, we then show how the Hankel contour representation of $\mathcal{F}_p(\eta)$ is related to Hankel's representation of the gamma function. The second method makes use of standard hypergeometric theory, and the known asymptotic expansions of the confluent hypergeometric functions, and provides an expedient alternative construction.

II. THE COMPLETE ASYMPTOTIC EXPANSION OF $\mathcal{F}_p(\eta)$ USING MELLIN TRANSFORMS

We define $\mathcal{F}_p(\eta)$, following Dingle,[5] via

$$\mathcal{F}_p(\eta)=\frac{1}{\Gamma(p+1)}\int_0^\infty \frac{\epsilon^p}{1+e^{\epsilon-\eta}}d\epsilon. \tag{2.1}$$

We seek the complete asymptotic expansion for $\mathcal{F}_p(\eta)$ for the case of large positive real η, and $p>-1$.

To obtain a contour integral representation of $\mathcal{F}_p(\eta)$, we express it as the inverse Mellin transform of it's Mellin transform,[5,1] which results in

$$\mathcal{F}_p(\eta)=\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty}\frac{\pi e^{\eta s}\,ds}{s^{p+1}\sin(\pi s)},\quad 0<c<1. \tag{2.2}$$

By changing the sign of s in (2.2) and closing the contour to the right, we arrive at

$$\mathcal{F}_p(\eta)=\frac{1}{2i}\int_{\infty}^{(0+)}\frac{e^{-\eta s}\,ds}{(-s)^{p+1}\sin(\pi s)}, \tag{2.3}$$

where the integration is performed over Hankel's contour, viz. the contour begins at infinity in the first quadrant, encircles the origin in the positive direction and proceeds to infinity in the fourth quadrant in such a manner as to avoid enclosing any of the poles on the negative real axis.[8]

To proceed further, we shrink the curve onto the positive real axis from both above and below, indenting the curve around the simple poles at $s=1, 2, 3, \ldots$, and also about the origin which will either be a pole if p is an integer or both a pole and a branch point if p is a noninteger. In either case we can choose $-s=se^{-i\pi}$ on the top of the curve to ensure that the generally many valued function $(-s)^{-p-1}$ becomes definite. We choose the indentations of the curve around the simple poles, both above and below the real axis, to be semi-circles of radius ρ, centered at the poles. We denote the contour of the indentation at the simple pole $s=n$ above the real axis by $above_\rho(n)$, and that below the real axis by $below_\rho(n)$. The indentation around the origin is taken to be along the curve Ω_δ, where we define Ω_δ to be the circle of radius $\delta<1$ centered at the origin and traversed in the positive direction.[9]

The essence of the derivation that follows is to split up the $\int_\infty^{(0+)}$ integral so that we can deal with the simple poles, and the problem of the origin separately. Having dealt with the simple poles we will be left with integrals whose integrand is only nonanalytic at the origin, and we will then be in a position to identify these remaining pieces with Hankel's representation of the gamma function. To begin then, we split up (2.3) as follows:

$$\begin{aligned}\int_{\infty}^{(0+)}\frac{e^{-\eta s}\,ds}{2i(-s)^{p+1}\sin(\pi s)}=&\sum_{n=1}^{\infty}\int_{n+1-\rho}^{n+\rho}\frac{e^{-\eta s}\,ds}{2ie^{-i\pi(p+1)}s^{p+1}\sin(\pi s)}+\int_{1-\rho}^{\delta}\frac{e^{-\eta s}\,ds}{2ie^{-i\pi(p+1)}s^{p+1}\sin(\pi s)}\\&+\sum_{n=1}^{\infty}\int_{above_\rho(n)}\frac{e^{-\eta s}\,ds}{2ie^{-i\pi(p+1)}s^{p+1}\sin(\pi s)}\\&+\sum_{n=1}^{\infty}\int_{n+\rho}^{n+1-\rho}\frac{e^{-\eta s}\,ds}{2ie^{i\pi(p+1)}s^{p+1}\sin(\pi s)}+\int_{\delta}^{1-\rho}\frac{e^{-\eta s}\,ds}{2ie^{i\pi(p+1)}s^{p+1}\sin(\pi s)}\\&+\sum_{n=1}^{\infty}\int_{below_\rho(n)}\frac{e^{-\eta s}\,ds}{2ie^{i\pi(p+1)}s^{p+1}\sin(\pi s)}\\&+\int_{\Omega_\delta}\frac{e^{-\eta s}\,ds}{2i(-s)^{p+1}\sin(\pi s)}.\end{aligned} \tag{2.4}$$

The first and third lines of (2.4) are the contributions from along the real line from above and below, respectively.

We now take the limit $\rho\to 0$. The contribution of the indentations around the simple poles becomes

$$\frac{(e^{i\pi(p+1)}+e^{-i\pi(p+1)})}{2i}\sum_{l=1}^{\infty} i\pi\,\mathrm{Res}(e^{-\eta s}s^{-p-1}\mathrm{cosec}(\pi s)|s=l)=\cos(\pi p)\mathcal{F}_p(-\eta), \tag{2.5}$$

where $\mathrm{Res}(f(s)|s=l)$ signifies the residue of $f(s)$ at $s=l$, and where we have used

$$\mathcal{F}_p(-\eta)=\sum_{\nu=1}^{\infty}\frac{(-1)^{\nu+1}}{\nu^{p+1}}e^{-\nu\eta},\quad \eta>0. \tag{2.6}$$

For the contributions along the real axis we obtain

$$-\frac{\left[e^{i\pi(p+1)}-e^{-i\pi(p+1)}\right]}{2i}\lim_{\rho\to 0}\left[\sum_{l=1}^{\infty}\int_{l+\rho}^{l+1-\rho}\frac{e^{-\eta s}}{s^{p+1}\sin(\pi s)}ds+\int_{\delta}^{l-\rho}\frac{e^{-\eta s}}{s^{p+1}\sin(\pi s)}ds\right]$$

$$=\sin(\pi p)\mathcal{P}\int_{\delta}^{\infty}\frac{e^{-\eta s}ds}{s^{p+1}\sin(\pi s)}. \tag{2.7}$$

$\mathcal{P}$ signifies the Cauchy principal value of the integral.

Since $\delta<1$, we can substitute into the Ω_δ integral, the result[10]

$$\frac{\pi s}{\sin(\pi s)}=\sum_{\nu=0}^{\infty}2\tau_{2\nu}s^{2\nu},\quad |s|<1, \tag{2.8}$$

where

$$\tau_n\equiv\sum_{\nu=1}^{\infty}\frac{(-1)^{\nu+1}}{\nu^n}=(1-2^{1-n})\zeta(n), \tag{2.9}$$

and $\zeta(n)$ is the Riemann zeta function.

Adding these pieces together we see that (2.3) can be written in the following more illuminating form:

$$\mathcal{F}_p(\eta)=\cos(\pi p)\mathcal{F}_p(-\eta)+\sin(\pi p)\mathcal{P}\int_{\delta}^{\infty}\frac{e^{-\eta s}ds}{s^{p+1}\sin(\pi s)}$$

$$+\frac{i}{2\pi}\sum_{\nu=0}^{\infty}\frac{2\tau_{2\nu}}{\eta^{2\nu-p-1}}\int_{\Omega_\delta}(-s)^{2\nu-p-2}e^{-s}\,ds. \tag{2.10}$$

It is to be noted that no asymptotic analysis has yet been performed. In order to obtain the complete asymptotic expansion of $\mathcal{F}_p(\eta)$ for arbitrary $p>-1$, we need to asymptotically expand the contribution from (2.7).

In the special case when p is an integer, it will be noticed that the contribution from (2.7) vanishes, and it should be obvious that this is merely a result of the fact that $(-s)^{-p-1}$ is in fact single valued in this case. Also, the Ω_δ integral then simply yields the residues at the origin for the finite number of terms in which the integrand is meromorphic, and vanishes for the remainder of the terms since their integrands are analytic. Hence for integer p the asymptotic expansions to be derived will agree precisely with the exact results. This observation is in agreement with Dingle's definition of a complete asymptotic expansion, which requires that the correct asymptotic expansion should agree with exact result for those special special values of p in which direct integration of $\mathcal{F}_p(\eta)$ is possible.

If p is a noninteger, then the contribution from (2.7) must be asymptotically expanded. However, nothing in the following argument relies on p being a noninteger, and it is equally true for integer p; $p\in Z$ just happens to be a particularly simple special case of the general result to be now derived.

Consider then

$$\mathcal{P}\int_{\delta}^{\infty}\frac{e^{-\eta s}ds}{s^{p+1}\sin(\pi s)}, \tag{2.11}$$

and note that $s^{-p-1}e^{-\eta s}\to 0$ as $s\to\infty$. The dominant contribution obviously comes from the neighborhood of $s=\delta<1$. We develop the desired asymptotic power series then, by substituting

(2.8) into (2.11), and integrating term by term. By making this substitution we are essentially ignoring the poles of $\mathrm{cosec}(\pi s)$ at $s=1, 2, 3, \ldots$, and thus the resulting integrals are no longer of the Cauchy principle value type. We thus obtain

$$\mathcal{F}_p(\eta)\sim\sum_{\nu=0}^{\infty}\frac{2\tau_{2\nu}}{\eta^{2\nu-p-1}}\frac{i}{2\pi}\left[\int_{\Omega_\delta}(-t)^{2\nu-p-2}e^{-t}dt-2i\sin(\pi p)\int_{\delta}^{\infty}(-t)^{2\nu-p-2}e^{-t}dt\right]+\cos(\pi p)\mathcal{F}_p(-\eta). \tag{2.12}$$

The term in parentheses in the above power series will be recognized as the function $-2i\sin[(2\nu-p-1)\pi]\Gamma(2\nu-p-1)$,[11] viz. it is simply Hankel's expression for the gamma function. Inserting this result into (2.12), we arrive at

$$\mathcal{F}_p(\eta)\sim\sum_{\nu=0}^{\infty}2\tau_{2\nu}\frac{\sin[(2\nu-p-1)\pi]}{\pi}\Gamma(2\nu-p-1)\eta^{p+1-2\nu}+\cos(\pi p)\mathcal{F}_p(-\eta), \tag{2.13}$$

or upon utilizing the reflection formula for the gamma function,

$$\mathcal{F}_p(\eta)\sim\sum_{\nu=0}^{[(p+1)/2]}\frac{2\tau_{2\nu}}{\Gamma(p+2-2\nu)}\eta^{p+1-2\nu}+\frac{\sin(\pi p)}{\pi}\sum_{[(p+3)/2]}^{\infty}2\tau_{2\nu}\Gamma(2\nu-p-1)\times\eta^{p+1-2\nu}+\cos(\pi p)\mathcal{F}_p(-\eta), \tag{2.14}$$

$[x]$ represents the integer part of the real number x.

Expressed in this form, the behavior of $\mathcal{F}_p(\eta)$ in the special cases p an integer and p an odd half integer become obvious. The beauty of this derivation lies in the fact that it was not necessary to treat the integer and noninteger cases separately, and that it makes manifest the mechanism accounting for the structural differences of the expansions in these two cases, namely the single valued or many valuedness of the integrand, respectively.

III. THE COMPLETE ASYMPTOTIC EXPANSION OF $\mathcal{F}_p(\eta)$ USING CONFLUENT HYPERGEOMETRIC FUNCTIONS

The complete asymptotic expansion of $\mathcal{F}_p(\eta)$ can be obtained in a more expedient and less complicated, although less enlightening fashion by simply using the known asymptotic expansions for the confluent hypergeometric functions. By splitting the range of integration in (2.1) into $[0,\eta]$ and $[\eta,\infty]$, and inserting the binomial expansions of $(1+e^{x-\eta})^{-1}$ we obtain

$$\Gamma(p+1)\mathcal{F}_p(\eta)=\sum_{k=0}^{\infty}(-1)^k\int_0^{\eta}e^{-k(\eta-x)}x^p dx+\sum_{k=1}^{\infty}(-1)^{k+1}\int_{\eta}^{\infty}e^{-k(x-\eta)}x^p dx. \tag{3.1}$$

We then change the variable of integration to $t\equiv\pm(\eta-x)/\eta$ in the first and second summands, respectively, thus obtaining

$$\Gamma(p+1)\mathcal{F}_p(\eta)=\sum_{k=0}^{\infty}(-1)^k\eta^{p+1}\int_0^1 e^{(-\eta k)t}t^{1-1}(1-t)^{p+2-1-1}dt+\sum_{k=1}^{\infty}(-1)^{k+1}\eta^{p+1}\int_0^{\infty}e^{-(\eta k)t}t^{1-1}(1+t)^{p+2-1-1}dt. \tag{3.2}$$

The integrals in the first and second summands are then recognized as $[1/(p+1)]M(1,p+2,-\eta k)$ and $U(1,p+2,\eta k)$, respectively, where $M(a,b,z)\equiv{}_1F_1(a;b;z)\equiv\Phi(a,b,z)$ and

$U(a,b,z)\equiv z^{-a}\,{}_2F_0(a;1+a-b;-1/z)\equiv\Psi(a,b,z)$ are the two independent solutions of Kummer's equation discussed in Ref. 10. Hence $\mathcal{F}_p(\eta)$ can be written in terms of these confluent hypergeometric functions as

$$\mathcal{F}_p(\eta)=\frac{\eta^{p+1}}{\Gamma(p+2)}+\sum_{k=1}^{\infty}(-1)^{k+1}\frac{\eta^{p+1}}{\Gamma(p+1)}\left[U(1,p+2,\eta k)-\frac{1}{p+1}M(1,p+2,-\eta k)\right]. \tag{3.3}$$

To derive the complete asymptotic expansion for $\mathcal{F}_p(\eta)$ we then substitute into (3.3) the known asymptotic expansions for $M(1,p+2,-\eta k)$ and $U(1,p+2,\eta k)$,[10]

$$\frac{1}{p+1}M(1,p+2,-\eta k)\sim\sum_{n=0}^{\infty}\frac{(-p)_n}{k^{n+1}}\eta^{-n-1}-\frac{\Gamma(p+1)}{\eta^{p+1}}(-1)^{-p}\frac{e^{-\eta k}}{k^{p+1}}, \tag{3.4}$$

$$U(1,p+2,\eta k)\sim\sum_{n=0}^{\infty}(-1)^n\frac{(-p)_n}{k^{n+1}}\eta^{-n-1}, \tag{3.5}$$

where $(a)_n$ is Pochammer's symbol, defined by[10]

$$\begin{aligned}(a)_0&=1,\\ (a)_n&=a(a+1)(a+2)\cdots\ (a+n-1)=\frac{\Gamma(a+n)}{\Gamma(a)}.\end{aligned} \tag{3.6}$$

Interchanging the order of summation in the resultant double sum we thus obtain

$$\begin{aligned}\mathcal{F}_p(\eta)\sim&\frac{\eta^{p+1}}{\Gamma(p+2)}+\sum_{n=0}^{\infty}(-1)^n\frac{(-p)_n}{\Gamma(p+1)}\eta^{p-n}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^{n+1}}\\ &-\sum_{n=0}^{\infty}\frac{(-p)_n}{\Gamma(p+1)}\eta^{p-n}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^{n+1}}+(-1)^{-p}\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{k^{p+1}}e^{-\eta k}.\end{aligned} \tag{3.7}$$

Making use of (2.6) and (2.9) this becomes

$$\mathcal{F}_p(\eta)\sim(-1)^{-p}\mathcal{F}_p(-\eta)+\frac{\eta^{p+1}}{\Gamma(p+2)}+\sum_{n=1}^{\infty}2\tau_{2n}\left[\frac{-(-p)_{2n-1}}{\Gamma(p+1)}\right]\eta^{p+1-2n}. \tag{3.8}$$

Since $\mathcal{F}_p(\eta)$ and the above power series are real for real p and η, taking the real part of the above equation results in the correct exponential series in (2.14), $\cos(\pi p)\mathcal{F}_p(-\eta)$. We also note, using (3.6), that

$$\left[\frac{-(-p)_{2n-1}}{\Gamma(p+1)}\right]=\frac{1}{\Gamma(p+2-2n)}. \tag{3.9}$$

Hence we arrive at the following expression which is entirely equivalent to (2.13) and (2.14):

$$\mathcal{F}_p(\eta)\sim\cos(\pi p)\mathcal{F}_p(-\eta)+\sum_{\nu=0}^{\infty}\frac{2\tau_{2\nu}}{\Gamma(p+2-2\nu)}\eta^{p+1-2\nu}. \tag{3.10}$$

This method is certainly far more expedient than the previous method since all the genuine asymptotic analysis has already been performed for us in the tabulation of the complete asymptotic expansions of the functions U and M.

IV. LOW TEMPERATURE BEHAVIOR OF AN ARBITRARY DIMENSIONAL FERMI GAS

We proceed now to use our complete asymptotic expansion of $\mathcal{F}_p(\eta)$ to investigate the statistical mechanics of an ideal Fermi gas in d spatial dimensions. We will see that in even dimensions, the subdominant series in (3.10) produces very important physical effects in the expansions of the thermodynamic functions.

For an ideal nonrelativistic spin 1/2 Fermi gas at temperature T in d dimensions, the internal energy, U, and average number density, n, are expressed in terms of $\mathcal{F}_p$ via

$$n=\frac{2}{\lambda_T^d}\frac{1}{\Gamma\left(\frac{d}{2}+1\right)}\left(\frac{\epsilon_F}{kT}\right)^{d/2}=\frac{2}{\lambda_T^d}\mathcal{F}_{d/2-1}(\beta\mu), \tag{4.1}$$

$$\frac{U}{N\epsilon_{\mathrm{F}}}=\frac{d}{2}\Gamma(d/2+1)\left(\frac{kT}{\epsilon_{\mathrm{F}}}\right)^{d/2+1}\mathcal{F}_{d/2}(\beta\mu), \tag{4.2}$$

where ϵ_{F} is the Fermi energy, $\mu(T)$ is the chemical potential, k is Boltzmann's constant, $\lambda_T \equiv\sqrt{2\pi\hbar/mkT}$, and $\beta\equiv 1/kT$. The dependence of ϵ_{F} on n and d is stated implicitly in (4.1).

The convergent power series expansion of $\mathcal{F}_p(\eta)$, (2.6), can be used to examine the behavior of U and n for negative $\beta\mu$, i.e., in the classical region. We focus on the degenerate region in which $\beta\mu$ is large and positive. Using (2.14), we find in this case that n and U have the following expansions.

$$\frac{n\lambda_T^d}{2}\sim\sum_{\nu=0}^{[d/4]}\frac{2\tau_{2\nu}}{\Gamma(d/2+1-2\nu)}(\beta\mu)^{d/2-2\nu}-\sin(d\pi/2)\sum_{\nu=[(d+4)/4]}^{\infty}2\tau_{2\nu}\frac{\Gamma(2\nu-d/2)}{\pi}$$
$$\times(\beta\mu)^{d/2-2\nu}-\cos(d\pi/2)\sum_{\nu=1}^{\infty}\frac{(-1)^{\nu+1}}{\nu^{d/2}}e^{-\nu\beta\mu},\quad(\beta\mu)\to\infty \tag{4.3}$$

$$\frac{U}{N\epsilon_{\mathrm{F}}}\left(\frac{\epsilon_{\mathrm{F}}}{kT}\right)^{d/2+1}\frac{1}{\frac{d}{2}\Gamma(d/2+1)}\sim\sum_{\nu=0}^{[(d+2)/4]}\frac{2\tau_{2\nu}}{\Gamma(d/2+2-2\nu)}(\beta\mu)^{d/2+1-2\nu}+\sin(d\pi/2)$$
$$\times\sum_{\nu=[(d+6)/4]}^{\infty}2\tau_{2\nu}\frac{\Gamma(2\nu-d/2-1)}{\pi}(\beta\mu)^{d/2+1-2\nu}$$
$$+\cos(d\pi/2)\sum_{\nu=1}^{\infty}\frac{(-1)^{\nu+1}}{\nu^{d/2+1}}e^{-\nu\beta\mu},\quad(\beta\mu)\to\infty. \tag{4.4}$$

From these expansions we see clearly that n and U behave quite differently depending on whether the number of spatial dimensions is odd or even. For an odd number of dimensions the exponentially small series vanishes and we simply obtain a conventional asymptotic power series. For an even number of dimensions, however, the asymptotic power series truncates, and the exponentially small series thus dominates.

It is instructive to compare the expansions of n and U for the physically important cases $d=2$ and 3. The number density n goes like

$$d=2,\qquad\frac{n\lambda_T^2}{2}\sim\beta\mu+\sum_{\nu=1}^{\infty}\frac{(-1)^{\nu+1}}{\nu}e^{-\nu\beta\mu}, \tag{4.5}$$

$$d=3,\qquad\frac{n\lambda_T^3}{2}\sim\sum_{\nu=0}^{\infty}\frac{2\tau_{2\nu}}{\Gamma(5/2-2\nu)}(\beta\mu)^{3/2-2\nu}. \tag{4.6}$$

For the energy we obtain

$$d=2, \qquad \frac{U}{N\epsilon_{\mathrm{F}}}\left(\frac{\epsilon_{\mathrm{F}}}{kT}\right)^2 \sim \frac{(\beta\mu)^2}{2}+\frac{\pi^2}{6}-\sum_{\nu=1}^{\infty}\frac{(-1)^{\nu+1}}{\nu^2}e^{-\nu\beta\mu}, \tag{4.7}$$

$$d=3, \qquad \frac{U}{N\epsilon_{\mathrm{F}}}\left(\frac{\epsilon_{\mathrm{F}}}{kT}\right)^{5/2} \sim \frac{8}{9\sqrt{\pi}}\sum_{\nu=0}^{\infty}\frac{2\tau_{2\nu}}{\Gamma(7/2-2\nu)}(\beta\mu)^{5/2-2\nu}. \tag{4.8}$$

The $d=3$ result is simply the standard result first obtained by Sommerfeld,[7] but it is interesting to note that in this case the subdominant exponential series vanishes identically. The usual statement that this result neglects terms $O(e^{-\beta\mu})$, e.g., Ref. 6, is therefore incorrect. When $d=2$ it is the power series in (4.3) and (4.4) which vanish identically, leaving only a finite sum and the exponentially small series. Thus the subdominant exponentially small series which should have been neglected in strict adherence to Poincaré's definition has become dominant. We shall now investigate the physical effects of this dominance of the exponentially small series in the two dimensional Fermi gas in greater detail.

V. THE TWO DIMENSIONAL FERMI GAS

In 2 spatial dimensions we have seen that only the first term in the power series of the large $\beta\mu$ expansion of n is nonzero, and thus that the exponentially small series is dominant.

To obtain suitable asymptotic expansions in the ultra degenerate limit, $kT/\epsilon_F \ll 1$, for U and the heat capacity at constant volume, C_v, we invert (4.5) for $\beta\mu$ and substitute this into (4.7).

Inversion of (4.5) leads to an asymptotic expansion for the chemical potential,

$$\mu(T)=\epsilon_{\mathrm{F}}\left[1-\frac{e^{-\beta\epsilon_{\mathrm{F}}}}{\beta\epsilon_{\mathrm{F}}}-\frac{e^{-2\beta\epsilon_{\mathrm{F}}}}{2\beta\epsilon_{\mathrm{F}}}+O\left(\frac{e^{-3\beta\epsilon_{\mathrm{F}}}}{\beta\epsilon_{\mathrm{F}}}\right)\right]. \tag{5.1}$$

The first correction term to the chemical potential away from the Fermi energy is seen to be exponentially small in β, so that even as the system moves away from absolute zero the chemical potential stays essentially fixed at the Fermi energy. This demonstrates that this system is loath to move away from a perfect Fermi sphere configuration as T increases.

Substituting (5.1) into (4.7) we obtain

$$\begin{aligned} U=\frac{N\epsilon_{\mathrm{F}}}{2}\Bigg[1+\frac{\pi^2}{3}\left(\frac{kT}{\epsilon_{\mathrm{F}}}\right)^2-2\left(\frac{kT}{\epsilon_{\mathrm{F}}}+\left[\frac{kT}{\epsilon_{\mathrm{F}}}\right]^2\right)e^{-\epsilon_{\mathrm{F}}/kT} \\ -\left(\frac{kT}{\epsilon_{\mathrm{F}}}+\frac{1}{2}\left[\frac{kT}{\epsilon_{\mathrm{F}}}\right]^2\right)e^{-2(\epsilon_{\mathrm{F}}/kT)}\Bigg]+O\left(\frac{kT}{\epsilon_F}e^{-3\epsilon_F/kT}\right). \end{aligned} \tag{5.2}$$

Note that all the algebraic factors multiplying the exponential terms are in fact polynomials; they have not been truncated. Differentiating (5.2) we obtain the heat capacity at constant volume C_v,

$$\frac{C_v}{Nk}=\frac{\pi^2}{3}\frac{kT}{\epsilon_{\mathrm{F}}}-\left(\frac{\epsilon_F}{kT}+2+2\frac{kT}{\epsilon_{\mathrm{F}}}\right)e^{-\epsilon_{\mathrm{F}}/kT}-\left(\frac{\epsilon_{\mathrm{F}}}{kT}+1+\frac{1}{2}\frac{kT}{\epsilon_{\mathrm{F}}}\right)e^{-2(\epsilon_{\mathrm{F}}/kT)}+O\left(\frac{\epsilon_{\mathrm{F}}}{kT}e^{-3(\epsilon_{\mathrm{F}}/kT)}\right). \tag{5.3}$$

We see that to first order C_v vanishes linearly as $T\to 0$, as one would expect for a Fermi gas, just as in the 3 dimensional case. The interesting thing to note however is that unlike the 3 dimensional case, the small T behavior of C_v in 2 dimensions contains transcendental rather than algebraic correction terms. This lack of algebraic corrections to C_v is testament to the physical effects that the transcendentally small terms in a complete asymptotic expansion can have.

The results obtained here using the complete asymptotic expansion of $\mathcal{F}_p(\eta)$ are also seen to be in agreement with the closed form solutions obtained by May.[4] The reason for this is rather

obvious from the derivation in Sec. II, since it was pointed out there that in the case of integer p, our result for the asymptotic expansion of $\mathcal{F}_p(\eta)$ is actually the exact solution of the integral. In effect the complete asymptotic expansion thus simultaneously performs the Sommerfeld treatment, as well as an exact treatment for the case of integer p. By using the complete asymptotic expansions we are thus able to recover Sommerfeld's asymptotic result for $d=3$, and May's exact result for $d=2$. This provides a concrete physical example of the usefulness of obtaining the complete asymptotic expansions for a given function, as opposed to the traditional algebraic series.

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A unified framework for Lie and covariant differentiation (with application to tensor fields)

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A unified framework is provided in which Lie and covariant differentiation may be considered as special cases of a new operation, called ''*D* differentiation.'' The present article develops *D* differentiation of tensor fields, whereas the extension to spinor fields, called ''$\tilde{D}$ differentiation,'' is presented in a companion article. The concept of ''generalized curvature'' of *D* differentiation is introduced, and a bundle formulation of *D* differentiation is obtained. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1343091]

I. INTRODUCTION

In previous articles,[1–4] we investigated the problem of defining the Lie derivative $\tilde{\mathcal{L}}_{\mathbf{X}}\psi$ and the covariant derivative $\tilde{\nabla}_{\mathbf{X}}\psi$ of a spinor field ψ in full generality. We thus considered the operator $\tilde{\mathcal{L}}_{\mathbf{X}}$ when the differentiating vector field X is not restricted to being a Killing vector of the metric ($\mathcal{L}_{\mathbf{X}}g\neq 0$); analogously, we took into account, for $\tilde{\nabla}_{\mathbf{X}}$, the possibility of a metric-incompatible connection ($\nabla_{\mathbf{X}}g\neq 0$). Note that, here as in Ref. 2, we denote Lie (respectively, covariant) differentiation of a tensor field by $\mathcal{L}$ (respectively, ∇), and of a spinor field by $\tilde{\mathcal{L}}$ (respectively, $\tilde{\nabla}$).

In the first stage of this work,[1,2] we proposed a definition for $\tilde{\mathcal{L}}_{\mathbf{X}}\psi$ and for $\tilde{\nabla}_{\mathbf{X}}\psi$ based on heuristic analogies with tensor calculus. Then, we provided a bundle formalism[4] for the covariant derivative. In both treatments, we concentrated mainly on covariant differentiation, and obtained as by-products, results for Lie differentiation by making use of a ''translation rule'' exploiting similarities between Lie and covariant differentiation.[1,4]

In the present sequence of two articles, we are going to reanalyze Lie and covariant differentiation from the point of view of unifying them in one single operation, called ''*D* differentiation.'' This will put their respective properties in perspective, and justify the ''translation rule'' employed in Refs. 1 and 4. For the sake of clarity, we shall consider here exclusively *D* differentiation of tensor fields. The extension to spinor fields, under the name of ''$\tilde{D}$ differentiation,'' will appear in a companion article.[5]

We shall begin, in Sec. II, by constructing *D* differentiation, and determining its expression in coordinates. This operation will not require the presence of either a metric or a connection on the manifold M under consideration. If, however, M possesses a metric g, it will be possible to introduce a modified kind of *D* differentiation, denoted by ${}^{\mathbf{g}}D$, which preserves the metric.

Examples of *D* and modified *D* differentiation will then be given in Sec. III. It will be proved that both Lie and covariant differentiation are special cases of *D* differentiation. This observation will be the fundamental justification for the above-mentioned ''translation rule'' employed in Refs. 1 and 4. Furthermore, a special subclass of *D* differentiation, called ''restricted *D* differentiation,'' will be singled out and given special attention.

In Sec. IV, the concept of ''generalized curvature'' of *D* differentiation will be introduced. As

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the name suggests, it will play, for D differentiation, the role that curvature (in the traditional sense) plays for covariant differentiation. This investigation will shed light on the construction of $\tilde{D}$ differentiation of spinor fields in the companion article.[5]

A reformulation of D differentiation in terms of fiber bundles will then be obtained, in two stages, in Secs. V and VI. Its purpose will be twofold: first, it will provide a geometrical interpretation of D differentiation, and second, it will yield the appropriate language for the extension to spinor fields in Ref. 5.

II. CONSTRUCTION OF *D* DIFFERENTIATION

As explained in Sec. I, all our consideration will be based on a type of differentiation, called D differentiation, which is general enough to contain, as special cases, Lie and covariant differentiation, as well as other kinds described in the following. All throughout, we shall assume that M is a smooth (C^∞) manifold of dimension n. Moreover, the set of smooth functions, vector fields, and tensor fields defined on M will be denoted by $\mathcal{F}$, $\mathcal{X}$, and $\mathcal{T}$, respectively. A local basis of $\mathcal{X}$ will be written as $\{\vec{e}_{(\mathbf{i})}:1\leqslant i\leqslant n\}$, and $\{\underrightarrow{e}^{(\mathbf{i})}:1\leqslant i\leqslant n\}$ will be its dual basis. The Einstein summation convention will be adopted systematically.

The general operation of D differentiation associates with each vector field X of $\mathcal{X}$ an operator $D_{\mathbf{X}}:\mathcal{T}\to\mathcal{T}$ satisfying the axioms

$$D_{\mathbf{X}}(T+U)=D_{\mathbf{X}}T+D_{\mathbf{X}}U, \tag{2.1}$$

$$D_{\mathbf{X}}(kT)=kD_{\mathbf{X}}T, \tag{2.2}$$

$$D_{\mathbf{X}}(T\otimes U)=(D_{\mathbf{X}}T)\otimes U+T\otimes(D_{\mathbf{X}}U), \tag{2.3}$$

$$D_{\mathbf{X}}\text{ preserves tensor rank,} \tag{2.4}$$

$$D_{\mathbf{X}}\text{ commutes with tensor contractions,} \tag{2.5}$$

$$D_{\mathbf{X}}f=X(f)=\mathrm{d}f(X), \tag{2.6}$$

for all T, U in $\mathcal{T}$, all f in $\mathcal{F}$, and all constants k. By virtue of these conditions, the action of D differentiation on a tensor field of arbitrary rank is entirely determined[6] by its action on vector fields. Therefore, we shall henceforth restrict attention to vector fields, leaving the case of tensors to the reader.

For all vector fields X and Y, let $D_{\mathbf{X}}Y$ be given by

$$D_{\mathbf{X}}Y=D_{\mathbf{X}}(Y^{\mathbf{i}}\vec{e}_{(\mathbf{i})}) \tag{2.7}$$

$$=\{X(Y^{\mathbf{i}})+\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)Y^{\mathbf{j}}\}\vec{e}_{(\mathbf{i})}, \tag{2.8}$$

where $\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)$ is a collection of n^2 functions that characterize each particular operator of D differentiation. To ensure that the right-hand side of (2.8) is independent of the basis $\{\vec{e}_{(\mathbf{i})}\}$ chosen, $\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)$ must transform in a very special manner under a change of basis. To determine the transformation rule for $\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)$, we note that, under the frame change

$$\vec{e}\,'_{(\mathbf{i})}=\vec{e}_{(\mathbf{j})}N^{\mathbf{j}}{}_{\mathbf{i}}, \tag{2.9}$$

for a given matrix N, vector components transform as

$$X'^{\mathbf{i}}=M^{\mathbf{i}}{}_{\mathbf{j}}X^{\mathbf{j}},\quad MN=I, \tag{2.10}$$

so that the requirement of frame independence of the right-hand side of (2.8) may be written

$$\{X(Y^{\mathbf{i}})+\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)Y^{\mathbf{j}}\}\vec{e}_{(\mathbf{i})}=\{X(M^{\mathbf{a}}{}_{\mathbf{k}}Y^{\mathbf{k}})+\Lambda'^{\mathbf{a}}{}_{\mathbf{b}}(X)M^{\mathbf{b}}{}_{\mathbf{k}}Y^{\mathbf{k}}\}\vec{e}_{(\mathbf{i})}N^{\mathbf{i}}{}_{\mathbf{a}} \tag{2.11}$$

for all X and Y. Elementary algebra then yields $\Lambda'(X)$ in terms of $\Lambda(X)$ as

$$\Lambda'^{\mathbf{i}}{}_{\mathbf{j}}(X)=M^{\mathbf{i}}{}_{\mathbf{a}}\Lambda^{\mathbf{a}}{}_{\mathbf{b}}(X)N^{\mathbf{b}}{}_{\mathbf{j}}-X(M^{\mathbf{i}}{}_{\mathbf{a}})N^{\mathbf{a}}{}_{\mathbf{j}} \tag{2.12}$$

$$=M^{\mathbf{i}}{}_{\mathbf{a}}\Lambda^{\mathbf{a}}{}_{\mathbf{b}}(X)N^{\mathbf{b}}{}_{\mathbf{j}}-(dM^{\mathbf{i}}{}_{\mathbf{a}})(X)N^{\mathbf{a}}{}_{\mathbf{j}}. \tag{2.13}$$

So far, no assumption has been made on the relationship between $D_{\mathbf{X}}$ and $D_{\mathbf{fX}}$, for an arbitrary function f. This information is enciphered in the relationship between $\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)$ and $\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(fX)$, and we shall postulate, consistently with (2.12) and (2.13), that there exists a tensor $A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}}\vec{e}_{(\mathbf{i})}\otimes\underset{\rightarrow}{e}{}^{(\mathbf{j})}\otimes\vec{e}_{(\mathbf{a})}\otimes\underset{\rightarrow}{e}{}^{(\mathbf{b})}$, characterizing each particular operator D, such that

$$\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X+Y)=\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)+\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(Y) \tag{2.14}$$

$$\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(fX)=f\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)-A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}}\vec{e}_{(\mathbf{a})}(f)X^{\mathbf{b}} \tag{2.15}$$

$$=f\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)-A^{\mathbf{i}}{}_{\mathbf{j}}(\mathrm{d}f,X), \tag{2.16}$$

in which $A^{\mathbf{i}}{}_{\mathbf{j}}$ is an abbreviation for

$$A^{\mathbf{i}}{}_{\mathbf{j}}:=A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}}\vec{e}_{(\mathbf{a})}\otimes\underset{\rightarrow}{e}{}^{(\mathbf{b})}. \tag{2.17}$$

In terms of D, the expressions (2.14) and (2.15) read

$$D_{\mathbf{X+Y}}Z=D_{\mathbf{X}}Z+D_{\mathbf{Y}}Z, \tag{2.18}$$

$$D_{\mathbf{fX}}Z=fD_{\mathbf{X}}Z-A^{\mathbf{i}}{}_{\mathbf{j}}(\mathrm{d}f,X)Z^{j}\vec{e}_{(\mathbf{i})}, \tag{2.19}$$

for all X, Y, Z, and f.

For future reference, it is useful to note that, because of (2.14) and (2.15), it is now possible to express $\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)$ as a function of the components of X as follows:

$$\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)=\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X^{\mathbf{k}}\vec{e}_{(\mathbf{k})}) \tag{2.20}$$

$$=X^{\mathbf{k}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(\vec{e}_{(\mathbf{k})})-A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}}\vec{e}_{(\mathbf{a})}(X^{\mathbf{b}}) \tag{2.21}$$

$$=\lambda^{\mathbf{i}}{}_{\mathbf{jk}}X^{\mathbf{k}}-A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}}\vec{e}_{(\mathbf{a})}(X^{\mathbf{b}}), \tag{2.22}$$

where, in the last step, we have introduced the symbols $\lambda^{\mathbf{i}}{}_{\mathbf{jk}}$ given by

$$\lambda^{\mathbf{i}}{}_{\mathbf{jk}}:=\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(\vec{e}_{(\mathbf{k})}). \tag{2.23}$$

The transformation law (2.12) for $\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)$ translates then into the following one for $\lambda^{\mathbf{i}}{}_{\mathbf{jk}}$:

$$\lambda'^{\mathbf{i}}{}_{\mathbf{jk}}=M^{\mathbf{i}}{}_{\mathbf{a}}\lambda^{\mathbf{a}}{}_{\mathbf{bc}}N^{\mathbf{b}}{}_{\mathbf{j}}N^{\mathbf{c}}{}_{\mathbf{k}}-M^{\mathbf{i}}{}_{\mathbf{a}}N^{\mathbf{b}}{}_{\mathbf{j}}A^{\mathbf{a}}{}_{\mathbf{b}}{}^{\mathbf{c}}{}_{\mathbf{d}}\vec{e}_{(\mathbf{c})}(N^{\mathbf{d}}{}_{\mathbf{k}})+M^{\mathbf{i}}{}_{\mathbf{a}}\vec{e}_{(\mathbf{c})}(N^{\mathbf{a}}{}_{\mathbf{j}})N^{\mathbf{c}}{}_{\mathbf{k}}. \tag{2.24}$$

Moreover, after substitution of (2.22) into (2.8), the explicit form for $D_{\mathbf{X}}Y$ in terms of the components of X and Y becomes

$$D_{\mathbf{X}}Y=\{X(Y^{\mathbf{i}})+\lambda^{\mathbf{i}}{}_{\mathbf{jk}}X^{\mathbf{k}}Y^{\mathbf{j}}-A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}}Y^{\mathbf{j}}\vec{e}_{(\mathbf{a})}(X^{\mathbf{b}})\}\vec{e}_{(\mathbf{i})}. \tag{2.25}$$

The decompositions (2.22) and (2.25) will play an important role in the study of examples and properties of D differentiation in Secs. III and IV.

For the preceding developments, D differentiation has not required the presence of any metric on the manifold. Some authors (e.g., Ref. 7), however, have introduced a modified version of the Lie derivative, which involves the metric. (The purpose of that modification was to shed light on Ref. 8.) This construction may be adapted to D differentiation in general, and we shall present these considerations hereafter.

Let g denote the covariant metric on M:

$$g := g_{\mathbf{ij}} \underset{\rightarrow}{e}^{(\mathbf{i})} \otimes \underset{\rightarrow}{e}^{(\mathbf{j})}. \tag{2.26}$$

The definition (2.8), extended to a twice-covariant tensor, yields then the D derivative of g as

$$D_{\mathbf{X}} g = \{X(g_{\mathbf{ij}}) - \Lambda_{\mathbf{ij}}(X) - \Lambda_{\mathbf{ji}}(X)\} \underset{\rightarrow}{e}^{(\mathbf{i})} \otimes \underset{\rightarrow}{e}^{(\mathbf{j})} \tag{2.27}$$

$$= \{X(g_{\mathbf{ij}}) - 2\Lambda_{(\mathbf{ij})}(X)\} \underset{\rightarrow}{e}^{(\mathbf{i})} \otimes \underset{\rightarrow}{e}^{(\mathbf{j})}, \tag{2.28}$$

in which parentheses around indices indicate symmetrization, and the symbols $\Lambda_{\mathbf{ij}}$ are defined by

$$\Lambda_{\mathbf{ij}} = g_{\mathbf{ik}} \Lambda^{\mathbf{k}}{}_{\mathbf{j}}. \tag{2.29}$$

As a result of (2.28), given a vector field X, it is not true in general that $D_{\mathbf{X}} g = 0$. On the other hand, if, from $D_{\mathbf{X}}$, one constructs a new operator (denoted by ${}^{\mathbf{g}}D_{\mathbf{X}}$) as

$${}^{\mathbf{g}}D_{\mathbf{X}} Y = \{X(Y^{\mathbf{i}}) + {}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) Y^{\mathbf{j}}\} \vec{e}_{(\mathbf{i})}, \tag{2.30}$$

with

$${}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) := g^{\mathbf{ik}}\, {}^{\mathbf{g}}\Lambda_{\mathbf{kj}}(X) \tag{2.31}$$

$$:= g^{\mathbf{ik}} \{\Lambda_{[\mathbf{kj}]}(X) + \tfrac{1}{2} X(g_{\mathbf{kj}})\} \tag{2.32}$$

$$= g^{\mathbf{ik}} \{\Lambda_{[\mathbf{kj}]} + \tfrac{1}{2} d g_{\mathbf{kj}}\}(X), \tag{2.33}$$

where $2\Lambda_{[\mathbf{kj}]} := \Lambda_{\mathbf{kj}} - \Lambda_{\mathbf{jk}}$, then it is obvious that ${}^{\mathbf{g}}D_{\mathbf{X}} g = 0$, whatever X might be. In other words, given a vector field X and an operator of D differentiation that does not satisfy $D_{\mathbf{X}} g = 0$, it is always possible to construct the new operator ${}^{\mathbf{g}}D_{\mathbf{X}}$, which does satisfy ${}^{\mathbf{g}}D_{\mathbf{X}} g = 0$.

In order to determine the relationship between ${}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(fX)$ and ${}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)$, we return to (2.32), and use (2.15) and (2.29), to obtain

$$2\,{}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(fX) = g^{\mathbf{iu}} \{\Lambda_{\mathbf{uj}}(fX) - \Lambda_{\mathbf{ju}}(fX) + (fX)(g_{\mathbf{uj}})\} \tag{2.34}$$

$$= \Lambda^{\mathbf{i}}{}_{\mathbf{j}}(fX) - g^{\mathbf{iu}} g_{\mathbf{jv}} \Lambda^{\mathbf{v}}{}_{\mathbf{u}}(fX) + fX(g_{\mathbf{uj}}) g^{\mathbf{iu}} \tag{2.35}$$

$$= \{f\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) - A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}} \vec{e}_{(\mathbf{a})}(f) X^{\mathbf{b}}\} - g^{\mathbf{iu}} g_{\mathbf{jv}} \{f\Lambda^{\mathbf{v}}{}_{\mathbf{u}}(X) - A^{\mathbf{v}}{}_{\mathbf{u}}{}^{\mathbf{a}}{}_{\mathbf{b}} \vec{e}_{(\mathbf{a})}(f) X^{\mathbf{b}}\} + fX(g_{\mathbf{uj}}) g^{\mathbf{iu}} \tag{2.36}$$

$$= f \cdot \{\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) - g^{\mathbf{iu}} g_{\mathbf{jv}} \Lambda^{\mathbf{v}}{}_{\mathbf{u}}(X) + X(g_{\mathbf{uj}}) g^{\mathbf{iu}}\} - 2\,{}^{\mathbf{g}}A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}} \vec{e}_{(\mathbf{a})}(f) X^{\mathbf{b}} \tag{2.37}$$

$$= f 2\,{}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) - 2\,{}^{\mathbf{g}}A^{\mathbf{i}}{}_{\mathbf{j}}(df, X), \tag{2.38}$$

with

$$2\,{}^{\mathbf{g}}A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}} := A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}} - g^{\mathbf{iu}} g_{\mathbf{jv}} A^{\mathbf{v}}{}_{\mathbf{u}}{}^{\mathbf{a}}{}_{\mathbf{b}} = A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}} - A_{\mathbf{j}}{}^{\mathbf{ia}}{}_{\mathbf{b}}, \tag{2.39}$$

$$2\,{}^{\mathbf{g}}A^{\mathbf{i}}{}_{\mathbf{j}} := A^{\mathbf{i}}{}_{\mathbf{j}} - g^{\mathbf{iu}} g_{\mathbf{jv}} A^{\mathbf{v}}{}_{\mathbf{u}} = A^{\mathbf{i}}{}_{\mathbf{j}} - A_{\mathbf{j}}{}^{\mathbf{i}}. \tag{2.40}$$

These considerations show that, given an operation $D_{\mathbf{X}}$, the modified operator ${}^{\mathbf{g}}D_{\mathbf{X}}$ is also an operation of type D, and (2.39), (2.40) enable one to construct the tensors $A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}}$ and $A^{\mathbf{i}}{}_{\mathbf{j}}$ of ${}^{\mathbf{g}}D_{\mathbf{X}}$ in terms of those of $D_{\mathbf{X}}$. The modified operation ${}^{\mathbf{g}}D_{\mathbf{X}}$ will be seen, in the following section, to have a simple interpretation when particularized to covariant and Lie differentiation.

Remark: From the fact that $D_{\mathbf{X}}$ is a derivation, it follows[6] that, for all vector fields X and Y, the Lie derivative and $D_{\mathbf{X}}$ are related by

$$D_{\mathbf{X}} Y = \mathcal{L}_{\mathbf{X}} Y + S(Y), \tag{2.41}$$

where S is a vector-valued one-form (depending on X). Therefore, in some sense, studying general D differentiation amounts to investigating Lie differentiation and properties of the tensor S appearing in (2.41).

This is, however, not the point of view that we wish to adopt. We are going to construct a geometrical framework where all differentiations of D type will appear *on the same footing*, without giving particular emphasis to special cases. This is quite different from (2.41), which singles out Lie differentiation as the type in terms of which all other representatives of D differentiation are expressed.

III. EXAMPLES OF *D* DIFFERENTIATION

D differentiation contains, as special cases, some of the differential operators commonly used in differential geometry. The most important ones for our purposes are covariant differentiation $\nabla_{\mathbf{X}}$ and Lie differentiation $\mathcal{L}_{\mathbf{X}}$. Moreover, the modified version ${}^{\mathbf{g}}\mathcal{L}_{\mathbf{X}}$ of Lie differentiation introduced[7] for the investigation of Lie differentiation of *spinor* fields, also falls in the category of D differentiation. We are now going to consider each of these operators in turn, and relate them to D differentiation.

The coordinate expression for ∇, namely

$$\nabla_{\mathbf{X}} Y = \{X(Y^{\mathbf{i}}) + \gamma^{\mathbf{i}}{}_{\mathbf{j}}(X) Y^{\mathbf{j}}\} \vec{e}_{(\mathbf{i})} \tag{3.1}$$

$$= \{X(Y^{\mathbf{i}}) + \Gamma^{\mathbf{i}}{}_{\mathbf{jk}} X^{\mathbf{k}} Y^{\mathbf{j}}\} \vec{e}_{(\mathbf{i})}, \tag{3.2}$$

in which $\gamma^{\mathbf{i}}{}_{\mathbf{j}}$ and $\Gamma^{\mathbf{i}}{}_{\mathbf{jk}}$ denote the connection forms and the connection coefficients, enables one, after comparison with (2.8), (2.25), to identify $\Lambda^{\mathbf{i}}{}_{\mathbf{j}}$ and $\lambda^{\mathbf{i}}{}_{\mathbf{jk}}$ with $\gamma^{\mathbf{i}}{}_{\mathbf{j}}$ and $\Gamma^{\mathbf{i}}{}_{\mathbf{jk}}$, respectively. Furthermore, it also shows that $A^{\mathbf{i}}{}_{\mathbf{j}}$ and $A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}}$ vanish for ∇. Covariant differentiation is thus that particular D differentiation characterized by

$${}_{\nabla}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) = \gamma^{\mathbf{i}}{}_{\mathbf{j}}(X), \quad {}_{\nabla}\lambda^{\mathbf{i}}{}_{\mathbf{jk}} = \Gamma^{\mathbf{i}}{}_{\mathbf{jk}}, \tag{3.3}$$

$${}_{\nabla}A^{\mathbf{i}}{}_{\mathbf{j}} = 0, \quad {}_{\nabla}A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}} = 0, \tag{3.4}$$

where a prefixed subscript specifies that covariant differentiation is understood. In this context, the laws (2.13), (2.24) reduce to the well-known transformation laws for the connection forms and the connection coefficients.

To recognize Lie differentiation, one must recall its coordinate expression employed in Ref. 2:

$$\mathcal{L}_{\mathbf{X}} Y = \{X(Y^{\mathbf{i}}) - L^{\mathbf{i}}{}_{\mathbf{j}}(X) Y^{\mathbf{j}}\} \vec{e}_{(\mathbf{i})}, \tag{3.5}$$

$$L^{\mathbf{i}}{}_{\mathbf{j}}(X) := \vec{e}_{(\mathbf{j})}(X^{\mathbf{i}}) + D^{\mathbf{i}}{}_{\mathbf{jk}} X^{\mathbf{k}}, \tag{3.6}$$

where the symbols $D^{\mathbf{i}}{}_{\mathbf{jk}}$ denote the commutation coefficients of the basis:

$$D^{\mathbf{k}}{}_{\mathbf{ij}} \vec{e}_{(\mathbf{k})} = [\vec{e}_{(\mathbf{i})}, \vec{e}_{(\mathbf{j})}]. \tag{3.7}$$

It follows from (3.5) that, for Lie differentiation, the appropriate $\Lambda^{\mathbf{i}}{}_{\mathbf{j}}$ reads

$$\mathcal{L}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) = -L^{\mathbf{i}}{}_{\mathbf{j}}(X). \tag{3.8}$$

A simple calculation based on (2.17), (2.22), (3.6), (3.8) yields then

$$\mathcal{L}\lambda^{\mathbf{i}}{}_{\mathbf{jk}} = -D^{\mathbf{i}}{}_{\mathbf{jk}}, \quad \mathcal{L}A^{\mathbf{i}}{}_{\mathbf{j}} = \vec{e}_{(\mathbf{j})} \otimes \underset{\rightarrow}{e}{}^{(\mathbf{i})}, \quad \mathcal{L}A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}} = \delta^{\mathbf{i}}{}_{\mathbf{b}}\delta^{\mathbf{a}}{}_{\mathbf{j}}, \tag{3.9}$$

which fully characterize Lie differentiation within the class of D derivatives. Note that, as a result of (3.9), one has $\mathcal{L}_{\mathbf{f}\mathbf{X}} \neq f\mathcal{L}_{\mathbf{X}}$, in contrast with what happens for covariant differentiation.

Furthermore, a comparison of (3.3) and (3.8) reveals the origin of the ''translation rule''

$$\gamma^{\mathbf{i}}{}_{\mathbf{j}}(X) \rightarrow -L^{\mathbf{i}}{}_{\mathbf{j}}(X) \tag{3.10}$$

employed in Ref. 1 to ''convert'' statements about covariant differentiation into analogous ones for Lie differentiation: Both operations ∇ and $\mathcal{L}$ are special cases of D differentiation, and their symbols $\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)$ are interchanged under the substitution (3.10). In Ref. 1, the conversion (3.10) was performed in the context of differentiation of spinors; here we see its counterpart for tensors.

All this applies to D differentiation proper. In Sec. II, however, we also introduced, from D differentiation, a modified operation ${}^{\mathbf{g}}D$, which has the characteristic that ${}^{\mathbf{g}}D_{\mathbf{X}}g = 0$, where g is the metric. In the special case of covariant differentiation, the modified operation ${}^{\mathbf{g}}\nabla$ reads, by virtue of (2.30), (2.33), (3.3)

$${}^{\mathbf{g}}\nabla_{\mathbf{X}}Y = \{X(Y^{\mathbf{i}}) + {}^{\mathbf{g}}_{\nabla}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)Y^{\mathbf{j}}\}\vec{e}_{(\mathbf{i})} \tag{3.11}$$

with

$${}^{\mathbf{g}}_{\nabla}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) = g^{\mathbf{ik}}\{\gamma_{[\mathbf{kj}]} + \tfrac{1}{2}\mathrm{d}g_{\mathbf{kj}}\}(X). \tag{3.12}$$

The general construction (2.33) guarantees that ${}^{\mathbf{g}}\nabla_{\mathbf{X}}g = 0$, which is the main reason why one introduces the modified connection ${}_{\nabla}{}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)$. However, light is shed on (3.12) by pursuing the matter a little further. We begin by using the Cartan equation

$$\mathrm{d}g_{\mathbf{kj}} = \gamma_{\mathbf{kj}} + \gamma_{\mathbf{jk}} + h_{\mathbf{kj}}, \tag{3.13}$$

where $h_{\mathbf{kj}}$ denotes the nonmetricity one-forms:

$$h_{\mathbf{kj}}(X) := (\nabla_{\mathbf{X}}g)(\vec{e}_{(\mathbf{k})}, \vec{e}_{(\mathbf{j})}) = (\nabla_{\mathbf{X}}g)_{\mathbf{kj}}. \tag{3.14}$$

After substitution of (3.14) in (3.12), the latter implies

$${}^{\mathbf{g}}_{\nabla}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) = g^{\mathbf{ik}}(\gamma_{\mathbf{kj}} + \tfrac{1}{2}h_{\mathbf{kj}}) \tag{3.15}$$

$$= \gamma^{\mathbf{i}}{}_{\mathbf{j}} + \tfrac{1}{2}h^{\mathbf{i}}{}_{\mathbf{j}}, \tag{3.16}$$

so that (3.11) becomes

$${}^{\mathbf{g}}\nabla_{\mathbf{X}}Y = \nabla_{\mathbf{X}}Y + \tfrac{1}{2}h^{\mathbf{i}}{}_{\mathbf{j}}(X)Y^{\mathbf{j}}\vec{e}_{(\mathbf{i})} \tag{3.17}$$

$$= \nabla_{\mathbf{X}}Y + \tfrac{1}{2}(\nabla_{\mathbf{X}}g)^{\mathbf{i}}{}_{\mathbf{j}}Y^{\mathbf{j}}\vec{e}_{(\mathbf{i})}. \tag{3.18}$$

As one can see, the new covariant derivative ${}^{\mathbf{g}}\nabla_{\mathbf{X}}$ is obtained from the original one $\nabla_{\mathbf{X}}g$ by the adjunction of a linear transformation generated by $\frac{1}{2}\nabla_{\mathbf{X}}g$. The reason for the presence of that particular linear transformation becomes clear when ${}^{\mathbf{g}}\nabla_{\mathbf{X}}$ is applied to the metric g itself, rather than to a general vector field Y. A similar treatment to that leading to (3.18) yields then

$$ {}^{\mathbf{g}}\nabla_{\mathbf{X}} g = \nabla_{\mathbf{X}} g - \nabla_{\mathbf{X}} g = 0, \tag{3.19} $$

which confirms the interpretation suggested by (3.16), namely that, in the case of covariant differentiation ∇, the modified version ${}^{\mathbf{g}}\nabla_{\mathbf{X}}$ corresponds to covariant differentiation with respect to the metric-compatible part of the connection.

Let us now follow the same line of reasoning in the case of Lie differentiation. By virtue of (2.30), (2.33), (3.8), the modified operator ${}^{\mathbf{g}}\mathcal{L}_{\mathbf{X}}$ reads

$$ {}^{\mathbf{g}}\mathcal{L}_{\mathbf{X}} Y = \{ X(Y^{\mathbf{i}}) + {}_{\mathcal{L}}{}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) Y^{\mathbf{j}} \} \vec{e}_{(\mathbf{i})}, \tag{3.20} $$

with

$$ {}_{\mathcal{L}}{}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) = g^{\mathbf{ik}} \{ -L_{[\mathbf{kj}]} + \tfrac{1}{2} \mathrm{d} g_{\mathbf{kj}} \}(X). \tag{3.21} $$

Furthermore, as a result of (2.38), (2.40), and (3.9), ${}_{\mathcal{L}}{}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(fX)$ is related to ${}_{\mathcal{L}}{}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X)$ by

$$ {}_{\mathcal{L}}{}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(fX) = f\, {}_{\mathcal{L}}{}^{\mathbf{g}}\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X) - {}_{\mathcal{L}}{}^{\mathbf{g}}A^{\mathbf{i}}{}_{\mathbf{j}}(\mathrm{d}f, X), \tag{3.22} $$

where ${}_{\mathcal{L}}{}^{\mathbf{g}}A^{\mathbf{i}}{}_{\mathbf{j}}$ is given by

$$ 2\, {}_{\mathcal{L}}{}^{\mathbf{g}}A^{\mathbf{i}}{}_{\mathbf{j}} = \vec{e}_{(\mathbf{j})} \otimes \underset{\rightarrow}{e}{}^{(\mathbf{i})} - g^{\mathbf{iu}} g_{\mathbf{jv}} \vec{e}_{(\mathbf{u})} \otimes \underset{\rightarrow}{e}{}^{(\mathbf{v})}. \tag{3.23} $$

The last line may be simplified by introducing the two operations $\sharp$ and $\flat$ of metric dualization, as follows.

Let X be a vector field. Then, the one-form $X^{\flat}$, which g associates with X, is defined by

$$ (X^{\flat})(Y) := g(X,Y) = g_{\mathbf{ij}} X^{\mathbf{i}} Y^{\mathbf{j}}, \tag{3.24} $$

for all vector fields Y. The operator $\sharp$ is the inverse of $\flat$, and maps one-forms to vectors. With that notation, (3.23) becomes

$$ 2\, {}_{\mathcal{L}}{}^{\mathbf{g}}A^{\mathbf{i}}{}_{\mathbf{j}} = \vec{e}_{(\mathbf{j})} \otimes \underset{\rightarrow}{e}{}^{(\mathbf{i})} - (\underset{\rightarrow}{e}{}^{(\mathbf{i})})^{\sharp} \otimes (\vec{e}_{(\mathbf{j})})^{\flat}. \tag{3.25} $$

The main reason for introducing the modified version ${}^{\mathbf{g}}\mathcal{L}$ of Lie differentiation lies in the fact that, for an arbitrary X, ${}^{\mathbf{g}}\mathcal{L}_{\mathbf{X}} g$ vanishes (by construction), whereas $\mathcal{L}_{\mathbf{X}} g \neq 0$ in general. If one attempts to extend Lie differentiation to spinor fields, it is the fact that, in general, $\mathcal{L}_{\mathbf{X}} g \neq 0$ which creates difficulties. Therefore, one of the approaches[7] to spinorial Lie differentiation consists in extending ${}^{\mathbf{g}}\mathcal{L}$ to spinors, not $\mathcal{L}$ itself. The present article being devoted solely to tensors, we shall not elaborate further on Lie differentiation of spinor fields. The interested reader will find details in Ref. 5, where we shall investigate the spinorial analog of the material presented here.

Remark: In the case of covariant and Lie differentiation, the tensors $A^{\mathbf{i}}{}_{\mathbf{j}}$ appearing in (2.16) are very simple. By virtue of (3.4) and (3.9), it is possible to write both under the form

$$ \underset{\mathcal{L}}{\nabla} A^{\mathbf{i}}{}_{\mathbf{j}} = \alpha \vec{e}_{(\mathbf{j})} \otimes \underset{\rightarrow}{e}{}^{(\mathbf{i})}. \tag{3.26} $$

with $\alpha = 0$ or 1 according to whether the differentiation is of covariant or Lie type. This observation prompts us to give special attention to the subclass of D differentiation characterized by an arbitrary value of the constant α in (3.26), not just 0 or 1. Such kinds of D will be called ''restricted D derivatives,'' and they will be identified by a subscript R, as

$$ {}_{\mathbf{R}}A^{\mathbf{i}}{}_{\mathbf{j}} = \alpha \vec{e}_{(\mathbf{j})} \otimes \underset{\rightarrow}{e}{}^{(\mathbf{i})} \tag{3.27} $$

for an arbitrary α.

It must be emphasized that the class of restricted D derivatives contains much more than Lie and covariant differentiation because, even if (for instance) $\alpha=1$, the corresponding D derivative only reduces to Lie differentiation when the coefficients $\lambda^{\mathbf{i}}_{\mathbf{jk}}$ of (2.23) are given by (3.9). In other words, although restricted D differentiation uses the particular value (3.27) for the tensors ${}_{\mathbf{R}}A^{\mathbf{i}}_{\mathbf{j}}$, it nevertheless leaves the coefficients $\lambda^{\mathbf{i}}_{\mathbf{jk}}$ of (2.23) entirely unconstrained, but compatible with (2.24).

Note that the modified covariant derivative ${}^{\mathbf{g}}\nabla$ of (3.11), (3.12) also falls within the category of restricted D differentiation (with $\alpha=0$), as follows from (2.40) and (3.4). However, such is not the case for the modified Lie derivative ${}^{\mathbf{g}}\mathcal{L}$ of (3.20), (3.21), as shown by (3.23). This is why, when defining general D differentiation, we adopted the very weak assumption (2.15).

It is clear from (2.22) that (2.15) may be interpreted as the requirement that $\Lambda^{\mathbf{i}}_{\mathbf{j}}(X)$ be a general linear combination of the components $X^{\mathbf{k}}$ of X and all the directional derivatives $\vec{e}_{(\mathbf{a})}(X^{\mathbf{b}})$ of these components along the basic vectors $\vec{e}_{(\mathbf{a})}$. On the other hand, for restricted D differentiation (3.27), the relationship (2.16) between ${}_{\mathbf{R}}\Lambda^{\mathbf{i}}_{\mathbf{j}}(fX)$ and ${}_{\mathbf{R}}\Lambda^{\mathbf{i}}_{\mathbf{j}}(X)$ particularizes as

$$ {}_{\mathbf{R}}\Lambda^{\mathbf{i}}_{\mathbf{j}}(fX)=f\,{}_{\mathbf{R}}\Lambda^{\mathbf{i}}_{\mathbf{j}}(X)-\alpha\vec{e}_{(\mathbf{j})}(f)X^{\mathbf{i}}, \tag{3.28}$$

which implies, by (2.22),

$$ {}_{\mathbf{R}}\Lambda^{\mathbf{i}}_{\mathbf{j}}(X)=\lambda^{\mathbf{i}}_{\mathbf{jk}}X^{\mathbf{k}}-\alpha\vec{e}_{(\mathbf{j})}(X^{\mathbf{i}}). \tag{3.29}$$

Furthermore, the translation of (3.28) in terms of the operation D reads

$$ {}_{\mathbf{R}}D_{\mathbf{f}\,\mathbf{X}}Y=f\,{}_{\mathbf{R}}D_{\mathbf{X}}Y-\alpha X\,\mathrm{d}f(Y). \tag{3.30}$$

By providing the examples of covariant and Lie differentiation, as well as the modified versions of these operations, we have shown that the class of D derivatives (even the restricted subclass ${}_{\mathbf{R}}D$) unifies enough nontrivial material to justify its study. In Sec. IV, we are going to investigate some of the properties of D differentiation. Later, a geometrical interpretation of D differentiation will be developed.

IV. GENERALIZED CURVATURE OF *D* DIFFERENTIATION

As mentioned earlier, covariant and Lie differentiation satisfy the strikingly different properties $\nabla_{\mathbf{f}\,\mathbf{X}}=f\nabla_{\mathbf{X}}$ and $\mathcal{L}_{\mathbf{f}\,\mathbf{X}}\neq f\mathcal{L}_{\mathbf{X}}$. Another important difference is that

$$ \mathcal{L}_{\mathbf{X}}\mathcal{L}_{\mathbf{Y}}-\mathcal{L}_{\mathbf{Y}}\mathcal{L}_{\mathbf{X}}-\mathcal{L}_{[\mathbf{X},\mathbf{Y}]}=0, \tag{4.1}$$

whereas, in general,

$$ \nabla_{\mathbf{X}}\nabla_{\mathbf{Y}}-\nabla_{\mathbf{Y}}\nabla_{\mathbf{X}}-\nabla_{[\mathbf{X},\mathbf{Y}]}\neq 0. \tag{4.2}$$

This suggests that we study the same kind of operation for D differentiation. More precisely, let us define

$$ {}_{\mathbf{D}}\mathcal{R}(X,Y,Z):=(D_{\mathbf{X}}D_{\mathbf{Y}}-D_{\mathbf{Y}}D_{\mathbf{X}}-D_{[\mathbf{X},\mathbf{Y}]})Z, \tag{4.3}$$

for all vector fields X, Y, Z. It is at once obvious that

$$ {}_{\mathcal{L}}\mathcal{R}=0, \quad {}_{\nabla}\mathcal{R}=\text{curvature operator} \tag{4.4}$$

for Lie and covariant differentiation.

Owing to the properties of D, the mapping $Z\mapsto{}_{\mathbf{D}}\mathcal{R}(X,Y,Z)$ is a linear transformation, which enables us to reformulate (4.3) as

$$ {}_{\mathbf{D}}\mathcal{R}(X,Y,\cdot)={}_{\mathbf{D}}\Omega^{\mathbf{i}}_{\mathbf{j}}(X,Y)\vec{e}_{(\mathbf{i})}\otimes\underset{\rightarrow}{e}{}^{(\mathbf{j})}, \tag{4.5}$$

for a certain family of functions ${}_{\mathbf{D}}\Omega^{\mathbf{i}}{}_{\mathbf{j}}(X,Y)$. In the context of linear transformations, the interpretation of the tensor product appearing in (4.5) is

$$ {}_{\mathbf{D}}\mathcal{R}(X,Y,Z) = {}_{\mathbf{D}}\Omega^{\mathbf{i}}{}_{\mathbf{j}}(X,Y)\vec{e}_{(\mathbf{i})}\underset{\rightarrow}{e}{}^{(\mathbf{j})}(Z) \tag{4.6} $$

$$ = {}_{\mathbf{D}}\Omega^{\mathbf{i}}{}_{\mathbf{j}}(X,Y)Z^{\mathbf{j}}\vec{e}_{(\mathbf{i})}\,. \tag{4.7} $$

The expression of ${}_{\mathbf{D}}\Omega^{\mathbf{i}}{}_{\mathbf{j}}$, which generalizes to D differentiation what is, in the special case of covariant differentiation, the family of curvature two-forms, is tedious to evaluate in terms of the coefficients $\lambda^{\mathbf{i}}{}_{\mathbf{jk}}$ and the tensors $A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{a}}{}_{\mathbf{b}}$ of (2.15). This expression is established by employing repeatedly the definition (2.8) of D differentiation, the coordinate expansion (2.22), and the definition (3.7) of the commutation coefficients the basis, with the result

$$ \begin{aligned} {}_{\mathbf{D}}\Omega^{\mathbf{i}}{}_{\mathbf{j}}(X,Y) = {}& X^{\mathbf{a}}Y^{\mathbf{b}}{}_{D}R^{\mathbf{i}}{}_{\mathbf{jab}} + \{X^{\mathbf{a}}\vec{e}_{(\mathbf{u})}(Y^{\mathbf{b}}) - Y^{\mathbf{a}}\vec{e}_{(\mathbf{u})}(X^{\mathbf{b}})\}{}_{\mathbf{D}}S^{\mathbf{i}}{}_{\mathbf{ja}}{}^{\mathbf{u}}{}_{\mathbf{b}} \\ & + \{\vec{e}_{(\mathbf{u})}(X^{\mathbf{a}})\vec{e}_{(\mathbf{v})}(Y^{\mathbf{b}}) - \vec{e}_{(\mathbf{u})}(Y^{\mathbf{a}})\vec{e}_{(\mathbf{v})}(X^{\mathbf{b}})\}{}_{D}T^{\mathbf{i}}{}_{\mathbf{jab}}{}^{\mathbf{uv}}, \end{aligned} \tag{4.8} $$

where

$$ {}_{\mathbf{D}}R^{\mathbf{i}}{}_{\mathbf{jab}} = \vec{e}_{(\mathbf{a})}(\lambda^{\mathbf{i}}{}_{\mathbf{jb}}) - \vec{e}_{(\mathbf{b})}(\lambda^{\mathbf{i}}{}_{\mathbf{ja}}) + \lambda^{\mathbf{i}}{}_{\mathbf{ra}}\lambda^{\mathbf{r}}{}_{\mathbf{jb}} - \lambda^{\mathbf{i}}{}_{\mathbf{rb}}\lambda^{\mathbf{r}}{}_{\mathbf{ja}} - \lambda^{\mathbf{i}}{}_{\mathbf{jr}}D^{\mathbf{r}}{}_{\mathbf{ab}} + A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{r}}{}_{\mathbf{s}}\vec{e}_{(\mathbf{r})}(D^{\mathbf{s}}{}_{\mathbf{ab}}), \tag{4.9} $$

$$ {}_{\mathbf{D}}S^{\mathbf{i}}{}_{\mathbf{ja}}{}^{\mathbf{u}}{}_{\mathbf{b}} = A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{r}}{}_{\mathbf{b}}D^{\mathbf{u}}{}_{\mathbf{ra}} + A^{\mathbf{i}}{}_{\mathbf{r}}{}^{\mathbf{u}}{}_{\mathbf{b}}\lambda^{\mathbf{r}}{}_{\mathbf{ja}} - A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{u}}{}_{\mathbf{r}}D^{\mathbf{r}}{}_{\mathbf{ba}} - A^{\mathbf{r}}{}_{\mathbf{j}}{}^{\mathbf{u}}{}_{\mathbf{b}}\lambda^{\mathbf{i}}{}_{\mathbf{ra}} - \vec{e}_{(\mathbf{a})}(A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{u}}{}_{\mathbf{b}}), \tag{4.10} $$

$$ {}_{\mathbf{D}}T^{\mathbf{i}}{}_{\mathbf{jab}}{}^{\mathbf{uv}} = A^{\mathbf{i}}{}_{\mathbf{j}}{}^{\mathbf{u}}{}_{\mathbf{b}}\delta^{\mathbf{v}}{}_{\mathbf{a}} + A^{\mathbf{i}}{}_{\mathbf{r}}{}^{\mathbf{u}}{}_{\mathbf{a}}A^{\mathbf{r}}{}_{\mathbf{j}}{}^{\mathbf{v}}{}_{\mathbf{b}}\,. \tag{4.11} $$

These equations become a little less unmanageable for restricted D differentiation (3.27), and read

$$ \begin{aligned} {}_{\mathbf{R}}\Omega^{\mathbf{i}}{}_{\mathbf{j}}(X,Y) = {}& X^{\mathbf{a}}Y^{\mathbf{b}}{}_{\mathbf{R}}R^{\mathbf{i}}{}_{\mathbf{jab}} + \alpha\{X^{\mathbf{a}}\vec{e}_{(\mathbf{u})}(Y^{\mathbf{b}}) - Y^{\mathbf{a}}\vec{e}_{(\mathbf{u})}(X^{\mathbf{b}})\}\{\delta^{\mathbf{i}}{}_{\mathbf{b}}(D^{\mathbf{u}}{}_{\mathbf{ja}} + \lambda^{\mathbf{u}}{}_{\mathbf{ja}}) \\ & - \delta^{\mathbf{u}}{}_{\mathbf{j}}(D^{\mathbf{i}}{}_{\mathbf{ba}} + \lambda^{\mathbf{i}}{}_{\mathbf{ba}})\} + (\alpha - \alpha^{2})\{\vec{e}_{(\mathbf{j})}(X^{\mathbf{r}})\vec{e}_{(\mathbf{r})}(Y^{\mathbf{i}}) - \vec{e}_{(\mathbf{j})}(Y^{\mathbf{r}})\vec{e}_{(\mathbf{r})}(X^{\mathbf{i}})\}, \end{aligned} \tag{4.12} $$

with

$$ {}_{\mathbf{R}}R^{\mathbf{i}}{}_{\mathbf{jab}} = \vec{e}_{(\mathbf{a})}(\lambda^{\mathbf{i}}{}_{\mathbf{jb}}) - \vec{e}_{(\mathbf{b})}(\lambda^{\mathbf{i}}{}_{\mathbf{ja}}) + \lambda^{\mathbf{i}}{}_{\mathbf{ra}}\lambda^{\mathbf{r}}{}_{\mathbf{jb}} - \lambda^{\mathbf{i}}{}_{\mathbf{rb}}\lambda^{\mathbf{r}}{}_{\mathbf{ja}} - \lambda^{\mathbf{i}}{}_{\mathbf{jr}}D^{\mathbf{r}}{}_{\mathbf{ab}} + \alpha\vec{e}_{(\mathbf{j})}(D^{\mathbf{i}}{}_{\mathbf{ab}}). \tag{4.13} $$

We are now ready to investigate the question of the uniqueness of the operator of D differentiation that yields a vanishing ${}_{\mathbf{D}}\Omega^{\mathbf{i}}{}_{\mathbf{j}}(X,Y)$ for all X and Y in (4.8). Equivalently, we wish to decide to what extent the requirement

$$ D_{\mathbf{X}}D_{\mathbf{Y}}Z - D_{\mathbf{Y}}D_{\mathbf{X}}Z - D_{[\mathbf{X},\mathbf{Y}]}Z = 0, \tag{4.14} $$

for all X, Y, Z, determines D uniquely. As we shall see, (4.14) admits several nontrivial D operators, even of the restricted class (3.27).

Let us, initially, return to (4.12). For ${}_{\mathbf{R}}\Omega^{\mathbf{i}}{}_{\mathbf{j}}(X,Y)$ to vanish identically for all X and Y, one must have, as a necessary condition,

$$ \alpha - \alpha^{\mathbf{2}} = 0, \tag{4.15} $$

which implies that either $\alpha = 0$ or $\alpha = 1$. If $\alpha = 0$, then the second term on the right-hand side of (4.12) disappears automatically, whereas (4.13) becomes

$$ 0 = {}_{\mathbf{R}}R^{\mathbf{i}}{}_{\mathbf{jab}} = \vec{e}_{(\mathbf{a})}(\lambda^{\mathbf{i}}{}_{\mathbf{jb}}) - \vec{e}_{(\mathbf{b})}(\lambda^{\mathbf{i}}{}_{\mathbf{ja}}) + \lambda^{\mathbf{i}}{}_{\mathbf{ra}}\lambda^{\mathbf{r}}{}_{\mathbf{jb}} - \lambda^{\mathbf{i}}{}_{\mathbf{rb}}\lambda^{\mathbf{r}}{}_{\mathbf{ja}} - \lambda^{\mathbf{i}}{}_{\mathbf{jr}}D^{\mathbf{r}}{}_{\mathbf{ab}}\,. \tag{4.16} $$

The right-hand side of (4.16) is the usual expression of the Riemann tensor in terms of the connection coefficients $\lambda^{\mathbf{i}}{}_{\mathbf{jk}}$. Therefore, when $\alpha = 0$, the requirement (4.14) determines that D

differentiation be covariant differentiation with a flat connection. This, however, does not mean that the resulting D derivative is trivial, because the connection may still exhibit torsion or nonmetricity (or both).

On the other hand, when $\alpha=1$, the second term on the right-hand side of (4.12) no longer disappears automatically, but determines $\lambda^{\mathbf{i}}{}_{\mathbf{jk}}$ as

$$\lambda^{\mathbf{i}}{}_{\mathbf{jk}}=-D^{\mathbf{i}}{}_{\mathbf{jk}}, \tag{4.17}$$

which has been observed in (3.9) to identify Lie differentiation. Furthermore, when (4.17) holds, (4.13) vanishes identically, for $\alpha=1$, as a consequence of the Jacobi identity

$$[[\vec{e}_{(\mathbf{a})},\vec{e}_{(\mathbf{b})}],\vec{e}_{(\mathbf{j})}]+[[\vec{e}_{(\mathbf{b})},\vec{e}_{(\mathbf{j})}],\vec{e}_{(\mathbf{a})}]+[[\vec{e}_{(\mathbf{j})},\vec{e}_{(\mathbf{a})}],\vec{e}_{(\mathbf{b})}]=0. \tag{4.18}$$

The conclusion that we have reached is thus that, among all the operators ${}_{\mathbf{R}}D$ of restricted D differentiation, the only two operators satisfying (4.14) are either covariant differentiation in a flat manifold with, possibly, torsion and nonmetricitry (which is often called a ''tele-parallel'' space), or Lie differentiation. In the case of Lie differentiation, our result should not be confused with the well-known theorem[6]

$$[\mathcal{L}_{\mathbf{X}}Z,\mathcal{L}_{\mathbf{Y}}Z]=\mathcal{L}_{[\mathbf{X},\mathbf{Y}]}Z, \tag{4.19}$$

because (4.19) follows, as proved in Ref. 6, from

$$\mathcal{L}_{\mathbf{X}}Y=[X,Y] \tag{4.20}$$

and the Jacobi identity, whereas we have assumed the analog (4.14) of (4.19) for restricted D differentiation, and derived Lie differentiation as one of the possibilities. Obviously, (4.20) is special to the Lie derivative, and was not assumed to be a general property of D differentiation. Indeed, the analog of (4.20) for D differentiation is (2.25), and becomes, for the restricted class ${}_{\mathbf{R}}D$,

$${}_{\mathbf{R}}D_{\mathbf{X}}Y=\{X(Y^{\mathbf{i}})-\alpha Y(X^{\mathbf{i}})+\lambda^{\mathbf{i}}{}_{\mathbf{jk}}X^{\mathbf{k}}Y^{\mathbf{j}}\}\vec{e}_{(\mathbf{i})}, \tag{4.21}$$

which is different from (4.20), unless $\alpha=1$ and $\lambda^{\mathbf{i}}{}_{\mathbf{jk}}=-D^{\mathbf{i}}{}_{\mathbf{jk}}$.

Owing to the fact that the operator D of restricted type (3.27) fails to be uniquely determined by (4.14), it is also true, *a fortiori*, that D differentiation of general type is not determined by (4.14). It remains, at present, an open question to characterize the subclass of general D differentiation for which ${}_{\mathbf{D}}\Omega^{\mathbf{i}}{}_{\mathbf{j}}=0$. For our purposes, which are centered around covariant and Lie differentiation (of spinor fields, ultimately), it is not necessary to answer this question, because both covariant and Lie differentiation fall into the category of restricted D differentiation. As remarked in Sec. III, modified covariant differentiation ${}^{\mathbf{g}}\nabla$ belongs to D differentiation of restricted type as well. Moreover, modified Lie differentiation ${}^{\mathbf{g}}\mathcal{L}$, albeit not a member of the class of restricted D differentiation, does not lead to an identically vanishing $\Omega^{\mathbf{i}}{}_{\mathbf{j}}$, as one establishes by combining (3.23) with (4.8)–(4.11).

Our investigation of D differentiation has been conducted, up to now, in the language of tensors. Further light is shed on the construction by a reformulation in terms of fiber bundles. This will be done, in two stages, in Secs. V and VI.

V. BUNDLE FORMULATION OF *D* DIFFERENTIATION

The reason for recasting D differentiation in the framework of fiber bundles is twofold: first, we wish to provide a more geometrical interpretation of D differentiation, and second, bundles facilitate the extension of D differentiation to spinor fields, as we shall show in the companion article.[5] The initial stage of this reformulation, developed in the present section, will employ the

tangent bundle *TM* to the manifold *M*, as well as the principal bundle *PLM* of linear frames over *M*. A more powerful language, using the tangent bundle *TTM* to *TM*, will enable us to obtain further geometrical insight in Sec. VI.

Let P be a point of M, and X be a vector field over M. Consequently $X_{\mathbf{P}}$, the value of X at P, is a certain vector of the tangent space $T_{\mathbf{P}}M$ to M. Let $\varphi_{\mathbf{t}}(P)$ denote the integral curve of X passing through P at $t=0$. Let finally $y_{\mathbf{P}}$ denote a vector of $T_{\mathbf{P}}M$. Then, one may construct from $y_{\mathbf{P}}$ a vector field ${}^{\mathbf{D}}Y$, defined above $\varphi_{\mathbf{t}}(P)$, by requiring

$$0 = D_{\mathbf{X}}{}^{\mathbf{D}}Y, \tag{5.1}$$

$${}^{\mathbf{D}}Y_{\mathbf{P}} = y_{\mathbf{P}}. \tag{5.2}$$

In other words, one solves (5.1) for ${}^{\mathbf{D}}Y$, with initial condition (5.2). The vector field ${}^{\mathbf{D}}Y$ will be said to be ''*D*-transported'' along X. (This terminology is an obvious generalization of the phrases ''parallel-transported'' and ''Lie transported,'' which apply to covariant and Lie differentiation.)

To determine the explicit expression of ${}^{\mathbf{D}}Y$ in coordinates, we begin by selecting a field of bases $\{\vec{e}_{(\mathbf{i})}\}$ over M, so that $\{\vec{e}_{(\mathbf{i})\mathbf{P}}\}$ is a basis of $T_{\mathbf{P}}M$. The vector field ${}^{\mathbf{D}}Y$ may therefore be written, at the point $\varphi_{\mathbf{t}}(P)$, as

$${}^{\mathbf{D}}Y_{\varphi_{\mathbf{t}}(\mathbf{P})} = {}^{\mathbf{D}}Y^{\mathbf{i}}_{\varphi_{\mathbf{t}}(\mathbf{P})}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})}. \tag{5.3}$$

In the neighborhood of P, namely on the portion of the integral curve $\varphi_{\mathbf{t}}(P)$ near $t=0$, (5.3) becomes

$${}^{\mathbf{D}}Y_{\varphi_{\mathbf{t}}(\mathbf{P})} = \{{}^{\mathbf{D}}Y^{\mathbf{i}}_{\mathbf{P}} + tX_{\mathbf{P}}({}^{\mathbf{D}}Y^{\mathbf{i}}) + o(t^2)\}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})}. \tag{5.4}$$

By virtue of the hypothesis (5.1) that ${}^{\mathbf{D}}Y$ is *D*-transported, the quantities $X_{\mathbf{P}}({}^{\mathbf{D}}Y^{\mathbf{i}})$ of (5.4) may be replaced by their expressions coming from (2.8), with the result

$${}^{\mathbf{D}}Y_{\varphi_{\mathbf{t}}(\mathbf{P})} = \{{}^{\mathbf{D}}Y^{\mathbf{i}}_{\mathbf{P}} - t\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X_{\mathbf{P}}){}^{\mathbf{D}}Y^{\mathbf{j}}_{\mathbf{P}} + o(t^2)\}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})} \tag{5.5}$$

$$= \{y^{\mathbf{i}}_{\mathbf{P}} - t\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X_{\mathbf{P}})y^{\mathbf{j}}_{\mathbf{P}}\}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})} + o(t^2), \tag{5.6}$$

where, in the last step, use has been made of the initial condition (5.2).

The expression (5.6) enables one to calculate (at first order in t) the extension ${}^{\mathbf{D}}Y$ of the vector $y_{\mathbf{P}}$ over the integral curves of X. On the other hand, if Y is a vector field on M, then $Y_{\mathbf{P}}$ may be used as the vector $y_{\mathbf{P}}$ in the above, and ${}^{\mathbf{D}}Y_{\varphi\mathbf{t}(\mathbf{P})}$ reads, by (5.6):

$${}^{\mathbf{D}}Y_{\varphi_{\mathbf{t}}(\mathbf{P})} = \{Y^{\mathbf{i}}_{\mathbf{P}} - t\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X_{\mathbf{P}})Y^{\mathbf{j}}_{\mathbf{P}}\}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})} + \cdots. \tag{5.7}$$

Therefore, when dealing with a vector field Y, one has at one's disposal two objects that may be compared with one another, namely $Y_{\varphi_{\mathbf{t}}(\mathbf{P})}$ and ${}^{\mathbf{D}}Y_{\varphi_{\mathbf{t}}(\mathbf{P})}$. Let $\Delta_{\varphi_{\mathbf{t}(\mathbf{P})}}(X,Y)$ be the difference of these two quantities:

$$\Delta_{\varphi_{\mathbf{t}}(\mathbf{P})}(X,Y) := Y_{\varphi_{\mathbf{t}}(\mathbf{P})} - {}^{\mathbf{D}}Y_{\varphi_{\mathbf{t}}(\mathbf{P})} \tag{5.8}$$

$$= \{Y^{\mathbf{i}}_{\varphi_{\mathbf{t}}(\mathbf{P})} - Y^{\mathbf{i}}_{\mathbf{P}} + t\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X_{\mathbf{P}})Y^{\mathbf{j}}_{\mathbf{P}}\}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})} + \cdots \tag{5.9}$$

$$= \{[Y^{\mathbf{i}}_{\mathbf{P}} + tX_{\mathbf{p}}(Y^{\mathbf{i}})] - Y^{\mathbf{i}}_{\mathbf{P}} + t\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X_{\mathbf{P}})Y^{\mathbf{j}}_{\mathbf{P}}\}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})} + \cdots \tag{5.10}$$

$$= t(D_{\mathbf{X}}Y)_{\mathbf{P}} + \cdots. \tag{5.11}$$

As a consequence, we have established that

$$(D_{\mathbf{X}}Y)_{\mathbf{P}}=\lim_{\mathbf{t}\to\mathbf{0}}\frac{1}{t}\Delta_{\varphi_{\mathbf{t}}(\mathbf{P})}(X,Y) \tag{5.12}$$

$$=\lim_{\mathbf{t}\to\mathbf{0}}\frac{1}{t}\{Y_{\varphi_{\mathbf{t}}(\mathbf{P})}-{}^{D}Y_{\varphi_{\mathbf{t}}(\mathbf{P})}\}, \tag{5.13}$$

which yields a geometrical interpretation of D differentiation in terms of D transport of Y along the integral curves of X.

To go one step further, let us introduce the tangent bundle TM to the manifold M. We denote by π the projection from TM to M. In TM, the fiber $\pi^{-1}(P)$ above a point P of M is the tangent space $T_{\mathbf{P}}M$ to M at P, which is isomorphic to $\mathbf{R}^n$.

The vector $y_{\mathbf{P}}$ of $T_{\mathbf{P}}M$ employed previously may then be reinterpreted as a particular point of the fiber $\pi^{-1}(P)$ of TM above P. Moreover, the mapping (near $t=0$)

$$t\mapsto{}^{\mathbf{D}}Y_{\varphi_{\mathbf{t}}(\mathbf{P})}=\{y^{\mathbf{i}}_{\mathbf{P}}-t\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X_{\mathbf{P}})y^{\mathbf{j}}_{\mathbf{P}}\}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})} \tag{5.14}$$

$$=\{\delta^{\mathbf{i}}_{\mathbf{j}}-t\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X_{\mathbf{P}})\}y^{\mathbf{j}}_{\mathbf{P}}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})} \tag{5.15}$$

describes a curve in TM, which will be denoted by ${}^{\mathbf{D}}_{\mathbf{TM}}\varphi_{\mathbf{t}}(y_{\mathbf{P}})$, and will be called the ''D lift'' of the integral curve $\varphi_{\mathbf{t}}(P)$ of X to TM through $y_{\mathbf{P}}$. It follows from (5.15) that, when a field of bases has been selected, ${}^{\mathbf{D}}_{\mathbf{TM}}\varphi_{\mathbf{t}}(y_{\mathbf{P}})$ reads

$${}^{\mathbf{D}}_{\mathbf{TM}}\varphi_{\mathbf{t}}(y_{\mathbf{P}}=y^{\mathbf{i}}_{\mathbf{P}}\vec{e}_{(\mathbf{i})\mathbf{P}})=G^{\mathbf{i}}_{\mathbf{j}}(t,X)y^{\mathbf{j}}_{\mathbf{P}}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})}, \tag{5.16}$$

with

$$G^{\mathbf{i}}_{\mathbf{j}}(t,X):=\delta^{\mathbf{i}}_{\mathbf{j}}-t\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X_{\mathbf{P}}). \tag{5.17}$$

In (5.16), the object $y^{\mathbf{j}}_{\mathbf{P}}$ and $G^{\mathbf{i}}_{\mathbf{j}}(t,X)$ may be considered, respectively, as a column matrix and a square matrix of $GL(n)$, which reflects the fact that the fiber bundle TM has its fibers isomorphic to $\mathbf{R}^n$, and admits $GL(n)$ as its structure group. In the same context, the mapping

$$t\mapsto{}^{\mathbf{D}}_{\mathbf{GL(n)}}\varphi_{\mathbf{t}}(X):=G^{\mathbf{i}}_{\mathbf{j}}(t,X), \tag{5.18}$$

may be interpreted, given a field of bases $\{\vec{e}_{(\mathbf{i})}\}$, as the D lift to $GL(n)$ of the integral curve $\varphi_{\mathbf{t}}(P)$ of X.

What has been done to D-transport a vector $y_{\mathbf{P}}$ of $T_{\mathbf{P}}M$ along the integral curve $\varphi_{\mathbf{t}}(P)$ of a vector field X may also be applied to a set of n vectors forming a basis at P. In order to see this more clearly, one needs to introduce the principal bundle PLM of linear frames above M.

The fiber of PLM above a point P of M is constituted by all the possible bases of $T_{\mathbf{P}}M$. In other words, each particular point of the fiber above P is one particular basis of $T_{\mathbf{P}}M$. More precisely, let $\{\vec{e}_{(\mathbf{i})}\}$ denote again a field of bases over M. Let $\vec{e}_{(\underline{\mathbf{m}})\mathbf{P}}$ denote a particular point of the fiber above P, namely a particular basis of $T_{\mathbf{P}}M$, where we have underlined the index to distinguish $\vec{e}_{(\underline{\mathbf{m}})\mathbf{P}}$ from a member of the field of bases $\{\vec{e}_{(\mathbf{i})}\}$ at P. Because $\vec{e}_{(\underline{\mathbf{m}})\mathbf{P}}$ and $\{\vec{e}_{(\mathbf{i})\mathbf{P}}\}$ are bases of the same tangent space $T_{\mathbf{P}}M$, one may write

$$\vec{e}_{(\underline{\mathbf{m}})\mathbf{P}}:=E^{i}_{(\underline{\mathbf{m}})\mathbf{P}}\vec{e}_{(\mathbf{i})\mathbf{P}}, \tag{5.19}$$

where the scalars $E^{\mathbf{i}}_{(\underline{\mathbf{m}})\mathbf{P}}$ represent the components of $\vec{e}_{(\underline{\mathbf{m}})\mathbf{P}}$ in the basis $\{\vec{e}_{(\mathbf{i})\mathbf{P}}\}$, and form a $GL(n)$ matrix. [This reflects the fact that the fibres of PLM are isomorphic to $GL(n)$.]

Each of the vectors $\vec{e}_{(\underline{\mathbf{m}})\mathbf{P}}$ of (5.19) may now be D-transported along the integral curve $\varphi_{\mathbf{t}}(P)$ of a given vector field X, just as we did with the vector $y_{\mathbf{P}}$ in (5.16), (5.17), which yields a new basis ${}^{\mathbf{D}}\vec{e}_{(\underline{\mathbf{m}})\varphi_{\mathbf{t}}(\mathbf{P})}$, at the point $\varphi_{\mathbf{t}}(P)$, defined by

$$^{\mathbf{D}}\vec{e}_{(\underline{\mathbf{m}})\varphi_{\mathbf{t}}(\mathbf{P})}=G^{\mathbf{i}}{}_{\mathbf{j}}(t,X)E^{j}{}_{(\underline{\mathbf{m}})\mathbf{P}}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})}, \tag{5.20}$$

with $G^{\mathbf{i}}{}_{\mathbf{j}}$ as in (5.17). Therefore, the mapping

$$t\mapsto{}^{\mathbf{D}}_{\mathbf{PLM}}\varphi_{\mathbf{t}}(\vec{e}_{(\underline{\mathbf{m}})\mathbf{P}}=E^{\mathbf{i}}_{(\underline{\mathbf{m}})\mathbf{P}}\vec{e}_{(\mathbf{i})\mathbf{P}}):=G^{\mathbf{i}}{}_{\mathbf{j}}(t,X)E^{j}_{(\underline{\mathbf{m}})\mathbf{P}}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})} \tag{5.21}$$

may be interpreted as the D lift to the bundle PLM of the integral curve $\varphi_{\mathbf{t}}(P)$ of X through P.

As soon as one has at one's disposal the D lift to PLM of the integral curves of an arbitrary vector field X, it becomes possible to complete the circle, and rederive the formula (2.8) for D differentiation, which was our starting point. To this end, we employ Weyl's method, which exploits the fact that PLM and TM are associated bundles.

Let the field of frames $\{\vec{e}_{(\mathbf{i})}\}$ be fixed over M, and let P be a point of M. A vector $y_{\mathbf{P}}$ of $T_{\mathbf{P}}M$ is a linear combination of $\{\vec{e}_{(\mathbf{i})}\}$:

$$y_{\mathbf{P}}=y^{\mathbf{m}}_{\mathbf{P}}\vec{e}_{(\mathbf{m})\mathbf{P}}. \tag{5.22}$$

Given that $\vec{e}_{(\mathbf{m})\mathbf{P}}$ is a point in the fibre of PLM above P, one may apply (5.20), with $E^{\mathbf{j}}{}_{(\underline{\mathbf{m}})\mathbf{P}}=\delta^{\mathbf{j}}{}_{\mathbf{m}}$, to evaluate the D transport of $\vec{e}_{(\mathbf{m})\mathbf{P}}$ from P to $\varphi_{\mathbf{t}}(P)$ in PLM:

$$^{D}\vec{e}_{(\underline{\mathbf{m}})\varphi_{\mathbf{t}}(\mathbf{P})}=G^{\mathbf{i}}{}_{\mathbf{j}}(t,X)\,\delta^{\mathbf{j}}{}_{\mathbf{m}}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})} \tag{5.23}$$

$$=G^{\mathbf{i}}{}_{\mathbf{m}}(t,X)\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})}. \tag{5.24}$$

Weyl's method consists in defining the D transport of $y_{\mathbf{P}}$ from P to $\varphi_{\mathbf{t}}(P)$ as the vector of $T_{\varphi_{\mathbf{t}}(\mathbf{P})}M$ that has, in $^{\mathbf{D}}\vec{e}_{(\underline{\mathbf{m}})\varphi_{\mathbf{t}}(\mathbf{P})}$, the same components as $y_{\mathbf{P}}$ has in $\vec{e}_{(\mathbf{m})\mathbf{P}}$. Consequently, we put

$$^{\mathbf{D}}y_{\varphi_{\mathbf{t}}(\mathbf{P})}:=y^{\mathbf{m}}_{\mathbf{P}}G^{\mathbf{i}}{}_{\mathbf{m}}(t,X)\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})}. \tag{5.25}$$

This is as far as one can go with a vector $y_{\mathbf{P}}$. If, however, $y_{\mathbf{P}}$ is the value $Y_{\mathbf{P}}$ of the field Y at P, one has two vectors at one's disposal at $\varphi_{\mathbf{t}}(P)$, and one may compare them as in (5.8):

$$\Delta_{\varphi_{\mathbf{t}}(\mathbf{P})}(X,Y):=Y_{\varphi_{\mathbf{t}}(\mathbf{P})}-{}^{D}Y_{\varphi_{\mathbf{t}}(\mathbf{P})} \tag{5.26}$$

$$=\{Y^{\mathbf{i}}_{\varphi_{\mathbf{t}}(\mathbf{P})}-Y^{\mathbf{j}}_{\mathbf{P}}G^{\mathbf{i}}{}_{\mathbf{j}}(t,X)\}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})}+\cdots, \tag{5.27}$$

where (5.25) has been employed. A calculation similar to that leading from (5.8) to (5.11), using the definition (5.17) of $G^{\mathbf{i}}{}_{\mathbf{j}}$, yields then the expected result

$$\lim_{\mathbf{t}\to\mathbf{0}}\frac{1}{t}\Delta_{\varphi_{\mathbf{t}}(\mathbf{P})}(X,Y)=(D_{\mathbf{X}}Y)_{\mathbf{P}}. \tag{5.28}$$

It might seem that, in the present section, we have obtained no new results, and that, therefore, the reformulation of D differentiation in terms of the tangent bundle TM and the bundle PLM of linear forms was unnecessary. This, however, is not the case: In the companion article[5] about Lie and covariant differentiation of spinor fields, we shall exploit to a considerable extent the fact that a spinor field over M is a linear combination of the field of spinor frames over M, just as, above, a vector field was considered as a linear combination of the field of bases. The bundle of spinor frames will thus play, *mutatis mutandis*, the same role as the bundle PLM of linear frames. It will then be possible to adapt, quite simply, to spinor fields, the construction of D differentiation, and thus of Lie and covariant differentiation as special cases.

In addition to the TM and PLM bundle interpretations of D differentiation, another bundle formulation will prove enlightening, namely one involving the bitangent bundle TTM to the manifold, i.e., the tangent bundle to TM. Its construction will be presented in Sec. VI.

VI. BUNDLE FORMULATION OF GENERALIZED *D* DIFFERENTIATION

Let the manifold M admit a set of charts $\{\Phi_{\mathbf{i}}\}$. In the future, we shall assume that all our developments take place in a neighborhood of a point P of M entirely covered by one single chart, so that the index i of $\Phi_{\mathbf{i}}$ may be omitted.

Let the coordinates in M be denoted by $x^{\mathbf{i}}$. With a slight abuse of notation, we shall thus write

$$\Phi(P)=x^{\mathbf{i}}. \tag{6.1}$$

Let Γ denote a curve in M, with parameter t, passing through the point P at $t=0$:

$$\Gamma:\mathbf{R}\to M:t\mapsto\Gamma(t). \tag{6.2}$$

The derivative operator along Γ at $t=0$ is a vector belonging to $T_{\mathbf{P}}M$, which we write as

$$v_{\mathbf{P}}:=\left.\frac{d}{dt}\right|_{\mathbf{\Gamma}}^{\mathbf{t=0}}. \tag{6.3}$$

This operator acts on real-valued functions defined on M.

Let TM be the tangent bundle to M. A point of the fiber $\pi^{-1}(P)$ above P is a vector $v_{\mathbf{P}}$ of $T_{\mathbf{P}}M$. Consequently, the chart Φ' describing TM may be taken as

$$\Phi':TM\to\mathbf{R}^{\mathbf{2n}}:\Phi'(v_{\mathbf{P}}):=(\Phi(P),v^{\mathbf{j}}_{\mathbf{P}}) \tag{6.4}$$

$$=(x^{\mathbf{i}}_{\mathbf{P}},v^{\mathbf{j}}_{\mathbf{P}}), \tag{6.5}$$

where the components $v^{\mathbf{j}}_{\mathbf{P}}$ express $v_{\mathbf{P}}$ in a given field of bases $\{\vec{e}_{(\mathbf{i})\mathbf{P}}\}$:

$$v_{\mathbf{P}}=v^{\mathbf{j}}_{\mathbf{p}}\vec{e}_{(\mathbf{j})\mathbf{P}}. \tag{6.6}$$

Let Γ' denote a curve in TM, with parameter t', passing though the point $v_{\mathbf{P}}$ at $t'=0$:

$$\Gamma':\mathbf{R}\to TM:t'\mapsto\Gamma'(t'). \tag{6.7}$$

The derivative operator along Γ' at $t'=0$ is a vector of $T_{\mathbf{v_p}}TM$, which will be denoted by a boldface letter, as

$$\mathbf{u}_{\mathbf{v_p}}:=\left.\frac{d}{dt'}\right|_{\mathbf{\Gamma'}}^{\mathbf{t'=0}}. \tag{6.8}$$

This operator acts on real-valued functions defined on TM. (When there will be no danger of confusion, the subscript $v_{\mathbf{P}}$ will often be omitted, as well as the primes over t and Γ; sometimes the point $t'=0$ will also be omitted.)

One may then construct the *bitangent* bundle TTM, namely the tangent bundle to TM. The fiber $\pi'^{-1}(v_{\mathbf{P}})$ of TTM above a point $v_{\mathbf{P}}$ of TM is constituted by all the vectors of the tangent space $T_{\mathbf{v_p}}TM$. Furthermore, vector fields over TM are cross sections of TTM, just as vector fields over M are cross sections of TM. Vector fields over TM will be denoted by boldface capitals (for instance $\mathbf{X}$) to distinguish them from vector fields over M (such as X).

A special kind of vector $\mathbf{u}_{\mathbf{v_p}}$ of $T_{\mathbf{v_p}}TM$ will play an important role in our forthcoming constructions. It is based on the concept of a *fiber curve* in TM.

Let Γ' be a curve in TM, as in (6.7). If Γ' lies entirely in the fiber $\pi^{-1}(P)$ above P, in a neighborhood of $t'=0$, then Γ' will be called a *fiber curve* in that neighborhood. Moreover, the derivative operator $\mathbf{u}_{\mathbf{v_p}}$ of (6.8) will be called a *fiber vector*. Such vectors have a particular characteristic, when expressed in components, which we are now going to determine.

Let f be a function on TM. The coordinate expression ${}^{\mathbf{c}}f$ of f, defined by

$$^{\mathbf{c}}f = f \circ \Phi'^{-1}, \tag{6.9}$$

where Φ' is given by (6.5), is thus a function of $x^{\mathbf{i}}$ and $v^{\mathbf{j}}$. Therefore, a vector $\mathbf{u}_{\mathbf{w_P}}$ at $w_{\mathbf{P}}$ acts on f as

$$\mathbf{u}_{\mathbf{w_P}}[f] = \mathbf{u}^{\mathbf{i}}_{\mathbf{w_P}} \frac{\partial\, ^{\mathbf{c}}f}{\partial x^{\mathbf{i}}}(x^{\mathbf{k}} = x^{\mathbf{k}}_{\mathbf{P}}, v^l = w^l_{\mathbf{P}}) + \mathbf{u}^{\mathbf{j}}_{\mathbf{w_P}} \frac{\partial\, ^{\mathbf{c}}f}{\partial v^{\mathbf{j}}}(x^{\mathbf{k}} = x^{\mathbf{k}}_{\mathbf{P}}, v^l = w^l_{\mathbf{P}}), \tag{6.10}$$

for some scalars $\mathbf{u}^{\mathbf{i}}_{\mathbf{w_P}}$ and $\mathbf{u}^{\mathbf{j}}_{\mathbf{w_P}}$, which implies that

$$\left\{ \frac{\partial}{\partial x^{\mathbf{i}}}, \frac{\partial}{\partial v^{\mathbf{j}}} \right\}$$

forms a basis of $T_{\mathbf{v_P}}TM$. More generally, if $\{\vec{e}_{(\mathbf{i})\mathbf{P}}\}$ is an arbitrary basis (not necessarily holonomic) of $T_{\mathbf{P}}M$, one may extend it to act on functions defined on TM, the extension being denoted by $\{\vec{\mathbf{e}}_{(\mathbf{i})\mathbf{w_P}}\}$:

$$\vec{\mathbf{e}}_{(\mathbf{i})\mathbf{w_P}}[^{\mathbf{c}}f(x^{\mathbf{i}}, v^{\mathbf{j}})] := \vec{e}_{(\mathbf{i})}[^{\mathbf{c}}f(x^{\mathbf{i}}, v^{\mathbf{j}} = w^{\mathbf{j}}_{\mathbf{P}})]. \tag{6.11}$$

In other words, $\vec{\mathbf{e}}_{(\mathbf{i})\mathbf{w_P}}$ acts on $^{\mathbf{c}}f$ as $\vec{e}_{(\mathbf{i})\mathbf{P}}$ acts on the function obtained from $^{\mathbf{c}}f$ by fixing its fiber coordinates at the values $w^{\mathbf{j}}_{\mathbf{P}}$. A generic vector of $T_{\mathbf{v_P}}TM$ may thus be written

$$\mathbf{u}_{\mathbf{w_P}} = \mathbf{u}^{\mathbf{i}}_{\mathbf{w_P}} \vec{\mathbf{e}}_{(\mathbf{i})\mathbf{w_P}} + \mathbf{u}^{\mathbf{j}}_{\mathbf{w_P}} \left. \frac{\partial}{\partial v^{\mathbf{j}}} \right|_{\mathbf{v}^{\mathbf{k}} = \mathbf{w}^{\mathbf{k}}_{\mathbf{P}}}, \tag{6.12}$$

which generalizes (6.10).

If the curve Γ' along which $\mathbf{u}_{\mathbf{w_P}}$ differentiates is a fiber curve, the variables $x^{\mathbf{i}}$ of the coordinate expression $^{\mathbf{c}}\Gamma' = \Phi' \circ \Gamma'$ of Γ' remain constant, and the first term on the right-hand side of (6.12), when acting on a function $^{\mathbf{c}}f$, vanishes. As a consequence, a fiber vector $^{\mathbf{F}}\mathbf{u}_{\mathbf{w_P}}$ is of the form

$$^{\mathbf{F}}\mathbf{u}_{\mathbf{w_P}} = {}^{\mathbf{F}}\mathbf{u}^{\mathbf{j}}_{\mathbf{w_P}} \left. \frac{\partial}{\partial v^{\mathbf{j}}} \right|_{\mathbf{v}^{\mathbf{k}} = \mathbf{w}^{\mathbf{k}}_{\mathbf{P}}}, \tag{6.13}$$

for some scalars $^{\mathbf{F}}\mathbf{u}^{\mathbf{j}}_{\mathbf{w_P}}$.

The concept of a fiber vector leads to that of the *fiber lift* of a vector of $T_{\mathbf{P}}M$, which will play a fundamental role in what follows. Given two vectors $u_{\mathbf{P}}$ and $w_{\mathbf{P}}$ of $T_{\mathbf{P}}M$, let Γ' be the curve in TM defined by

$$\Gamma' : \mathbf{R} \to TM : t' \mapsto w_{\mathbf{P}} + t' u_{\mathbf{P}}. \tag{6.14}$$

It is clear that $\Gamma(0) = w_{\mathbf{P}}$ and that Γ' is a fiber curve. Therefore, the vector of $T_{\mathbf{w_P}}TM$ which is tangent to Γ' at $t' = 0$ is a fiber vector, and it will be written

$$\mathbf{u}^{\dagger}_{\mathbf{w_P}} = \left. \frac{d}{dt'} \right|^{\mathbf{t}' = \mathbf{0}}_{\mathbf{\Gamma}'}. \tag{6.15}$$

The vector $\mathbf{u}^{\dagger}_{\mathbf{w_P}}$ will be called the *fiber lift* of $u_{\mathbf{P}}$ to the point $w_{\mathbf{P}}$ of TM. Henceforth, a vector and its fiber lift will always be denoted by the same letter, the vector of $T_{\mathbf{P}}M$ in italics, and the lift in boldface (with a dagger).

By considering a function f on TM, and evaluating the differentiation that appears on the right-hand side of (6.15), one establishes that the fiber lift of a vector $u_{\mathbf{P}}$ decomposed as

$$u_{\mathbf{P}}=u^{\mathbf{i}}_{\mathbf{P}}\vec{e}_{(\mathbf{i})\mathbf{P}} \tag{6.16}$$

reads, in the language of (6.11) and (6.12),

$$\mathbf{u}^{\dagger}_{\mathbf{w_P}}=u^{\mathbf{j}}_{\mathbf{P}}\frac{\partial}{\partial v^{\mathbf{j}}}\bigg|_{\mathbf{v^k=w^k_P}}. \tag{6.17}$$

In order to geometrize the operation of D differentiation, we still need another type of lift, called the *generalized lift*. To introduce it, we proceed in a similar fashion as for the fiber lift, with, however, the fundamental difference that it is only possible to obtain the generalized lift of a vector *field* over M, but not of an isolated vector of $T_{\mathbf{P}}M$. To emphasize this difference, we shall denote the vector field to be lifted as X, instead of employing the symbol $u_{\mathbf{P}}$ as in (6.16).

Thus let X be a vector field over M, and let $w_{\mathbf{P}}$ be a vector of $T_{\mathbf{P}}M$. We saw, in Sec. V, how to obtain, from the integral curves $\varphi_{\mathbf{t}}$ of X, a family of curves $\overset{\mathbf{D}}{\mathbf{TM}}\varphi_{\mathbf{t}}$ in TM, which was called the D lift of $\varphi_{\mathbf{t}}$ to TM. By virtue of (5.16), (5.17), the curve passing through $w_{\mathbf{P}}$ at $t=0$ reads

$$t\mapsto\overset{\mathbf{D}}{\mathbf{TM}}\varphi_{\mathbf{t}}(w_{\mathbf{P}})=\{\delta^{\mathbf{i}}_{\mathbf{j}}-t\Lambda^{\mathbf{i}}_{\mathbf{j}}(X_{\mathbf{P}})\}w^{\mathbf{j}}_{\mathbf{P}}\vec{e}_{(\mathbf{i})\varphi_{\mathbf{t}}(\mathbf{P})}. \tag{6.18}$$

Owing to the fact that this curve lies in TM and passes through $w_{\mathbf{P}}$ at $t=0$, its tangent at $t=0$ is a vector of $T_{\mathbf{w_P}}TM$. This vector is called the *generalized lift* of X at the point $w_{\mathbf{P}}$ of TM, and is denoted by

$$\mathbf{X}^{\ddagger}_{\mathbf{w_P}}=\frac{d}{dt}\bigg|^{\mathbf{t=0}}_{\overset{\mathbf{D}}{\mathbf{TM}}\varphi_{\mathbf{t}}(\mathbf{w_P})}. \tag{6.19}$$

When the definition (6.19) of $\mathbf{X}^{\ddagger}_{\mathbf{w_P}}$ is combined with the expression (6.18) for the curve $\overset{\mathbf{D}}{\mathbf{TM}}\varphi_{\mathbf{t}}(w_{\mathbf{P}})$, the generalized lift becomes

$$\mathbf{X}^{\ddagger}_{\mathbf{w_P}}=X^{\mathbf{i}}_{\mathbf{P}}\mathbf{e}_{(\mathbf{i})\mathbf{w_P}}-\Lambda^{\mathbf{j}}_{\mathbf{i}}(X_{\mathbf{P}})w^{\mathbf{i}}_{\mathbf{P}}\frac{\partial}{\partial v^{\mathbf{j}}}\bigg|_{\mathbf{v^k=w^k_P}}. \tag{6.20}$$

The restricted proof of this result for the special case where the basis $\{\vec{e}_{(\mathbf{i})\mathbf{P}}\}$ is the holonomic one $\{\partial/\partial x^{\mathbf{i}}\}$ is simple. One considers a function f defined on TM, which, in coordinates, is expressed by (6.9). Moreover, the coordinate expression of the curve (6.18) along which $\mathbf{X}^{\ddagger}_{\mathbf{w_P}}$ differentiates reads (in a neighborhood of $t=0$)

$$t\mapsto(x^{\mathbf{i}}+tX^{\mathbf{i}}_{\mathbf{P}},\{\delta^{\mathbf{j}}_{\mathbf{k}}-t\Lambda^{\mathbf{j}}_{\mathbf{k}}(X_{\mathbf{P}})\}w^{\mathbf{k}}_{\mathbf{P}}). \tag{6.21}$$

Consequently, the definition (6.19) of $\mathbf{X}^{\ddagger}_{\mathbf{w_P}}$ becomes, when applied to f,

$$\mathbf{X}^{\ddagger}_{\mathbf{w_P}}[f]=\frac{d}{dt}\bigg|_{\mathbf{t=0}}f(x^{\mathbf{i}}+tX^{\mathbf{i}}_{\mathbf{P}},w^{\mathbf{j}}_{\mathbf{P}}-t\Lambda^{\mathbf{j}}_{\mathbf{k}}(X_{\mathbf{P}})w^{\mathbf{k}}_{\mathbf{P}}) \tag{6.22}$$

$$=X^{\mathbf{i}}_{\mathbf{P}}\frac{\partial f(x,v)}{\partial x^{\mathbf{i}}}\bigg|_{\mathbf{v^k=w^k_P}}-\Lambda^{\mathbf{j}}_{\mathbf{i}}(X_{\mathbf{P}})w^{\mathbf{i}}_{\mathbf{P}}\frac{\partial f(x,v)}{\partial v^{j}}\bigg|_{\mathbf{v^k=w^k_P}}, \tag{6.23}$$

which is the holonomic version of (6.20).

With this machinery at our disposal, we are in the position to define a new operation $\mathbf{D}$, called *generalized D differentiation*, which, from two vector fields X and Y over M, enables one to construct the vector field $\mathbf{D}_{\mathbf{X}}Y$ over TM. To emphasize that the vector field resulting from X and Y is a field over TM, rather than over M, we have employed a boldface letter $\mathbf{D}$ to denote it. (Generalized D differentiation will turn out to be deeply related to D differentiation, as we shall show.)

Let P be a point of M, and let $\varphi_{\mathbf{t}}(P)$ be the integral curve of the field X passing through P at $t=0$. Then, for every t fixed, the value $Y_{\varphi_{\mathbf{t}}(\mathbf{P})}$ of the field Y at the point $\varphi_{\mathbf{t}}(P)$ belongs to the fiber $\pi^{-1}(\varphi_{\mathbf{t}}(P))$ of TM above $\varphi_{\mathbf{t}}(P)$. One may thus apply the mapping $\overset{\mathbf{D}}{\mathbf{TM}}\varphi_{-\mathbf{t}}$ of (5.16) to $Y_{\varphi_{\mathbf{t}}(\mathbf{P})}$, and the result is an element of the fiber above $\varphi_{-\mathbf{t}}(\varphi_{\mathbf{t}}(P))=P$. Consequently, the mapping

$$t\mapsto \overset{\mathbf{D}}{\mathbf{TM}}\varphi_{-\mathbf{t}}(Y_{\varphi_{\mathbf{t}}(\mathbf{P})}) \tag{6.24}$$

is a curve in TM, lying in the fiber of TM above P (in the neighborhood of $t=0$). Therefore, the tangent to this curve is a fiber vector, and we define

$$(\mathbf{D}_{\mathbf{X}}Y)_{\mathbf{Y_P}} := \left.\frac{d}{dt}\right|^{\mathbf{t=0}}_{\overset{\mathbf{D}}{\mathbf{TM}}\varphi_{-\mathbf{t}}(Y_{\varphi_{\mathbf{t}}(\mathbf{P})})} . \tag{6.25}$$

To evaluate $\mathbf{D}_{\mathbf{X}}Y$ in coordinates, let us return to the definition (5.16), (5.17), of the mapping $\overset{\mathbf{D}}{\mathbf{TM}}\varphi_{-\mathbf{t}}$. One readily obtains then, at first order in t,

$$\overset{\mathbf{D}}{\mathbf{TM}}\varphi_{-\mathbf{t}}(Y_{\varphi_{\mathbf{t}}(\mathbf{P})}) = \{Y^{\mathbf{i}}_{\varphi_{\mathbf{t}}(\mathbf{P})} + t\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X_{\mathbf{P}})Y^{\mathbf{j}}_{\mathbf{P}}\}\vec{e}_{(\mathbf{i})\varphi_{-\mathbf{t}}(\varphi_{\mathbf{t}}(\mathbf{P}))} \tag{6.26}$$

$$= \{Y^{\mathbf{i}}_{\mathbf{P}} + tX_{\mathbf{P}}[Y^{\mathbf{i}}] + t\Lambda^{\mathbf{i}}{}_{\mathbf{j}}(X_{\mathbf{P}})Y^{\mathbf{j}}_{\mathbf{P}}\}\vec{e}_{(\mathbf{i})\mathbf{P}} \tag{6.27}$$

$$= \{Y^{\mathbf{i}}_{\mathbf{P}} + t(D_{\mathbf{X}}Y)^{\mathbf{i}}_{\mathbf{P}}\}\vec{e}_{(\mathbf{i})\mathbf{P}}, \tag{6.28}$$

where, in the last line, we have used the definition (2.8) of the D derivative. From (6.16), (6.17), (6.25), and (6.28), one easily establishes that

$$(\mathbf{D}_{\mathbf{X}}Y)_{\mathbf{Y_P}} = (D_{\mathbf{X}}Y)^{\mathbf{j}}_{\mathbf{P}}\left.\frac{\partial}{\partial v^{\mathbf{j}}}\right|_{\mathbf{v^k=Y^k_P}} \tag{6.29}$$

$$= (D_{\mathbf{X}}Y)^{\dagger}_{\mathbf{Y_P}}, \tag{6.30}$$

which establishes the relationship between generalized D differentiation and D differentiation, thus providing a geometrical interpretation of the latter in the language of fiber bundles.

Another relationship, this time between $\mathbf{D}$ and the generalized lift, sheds light on all this construction. To express it, one needs to recall that, given a mapping f from a manifold to itself, it is always possible to construct[6] the tangent mapping Tf, which transforms the tangent space $T_{\mathbf{P}}M$ at a point P into the tangent space $T_{\mathbf{f(P)}}M$ at $f(P)$. Furthermore, if Y is a vector field over M, it is also a cross section of TM, so that Y may be considered as a particular mapping from M to TM. Therefore, the tangent mapping TY transforms TM into TTM, and it follows that $(TY)(X_{\mathbf{P}})$, for any vector field X, belongs to TTM.

After these preparations, the operation $\mathbf{D}$ may be reformulated as

$$(\mathbf{D}_{\mathbf{X}}Y)_{\mathbf{Y_P}} = (TY)(X_{\mathbf{P}})_{\mathbf{Y_P}} - \mathbf{X}^{\ddagger}_{\mathbf{Y_P}}, \tag{6.31}$$

which shows the connection between $\mathbf{D}$ and the generalized lift $\mathbf{X}^{\ddagger}_{\mathbf{w_P}}$. The proof of (6.31) is simple, and only a few indications will suffice.

One begins by evaluating the tangent mapping TY, and calculates how the first term on the right-hand side of (6.31) acts on a function f. Then, one uses (6.20) for the generalized lift $\mathbf{X}^{\ddagger}_{\mathbf{w_P}}$. One thus constructs the complete right-hand side of (6.31) acting of f, and one observes that this action is identical to that of the right-hand side of (6.30).

We now have at our disposal various interpretations of the operation of D differentiation. It remains to put them all in perspective, which will be done in the conclusion.

VII. CONCLUSION

The purpose of this work has been to introduce a new operator of differentiation, called D differentiation, which contains, among others types, Lie and covariant differentiation. Our considerations have been restricted to D differentiation of tensor fields, but may be extended to spinor fields, as will be done in the companion article.[5]

We began, in Sec. II, by constructing D differentiation, and ascertaining that the definition is independent of the basis chosen on the manifold M. We also introduced a modified version of D differentiation, which is compatible with the metric g on M in the sense that, although $D_{\mathbf{X}}g$, in general, does not vanish for an arbitrary vector field X, the modified operation ${}^{\mathbf{g}}D$ satisfies ${}^{\mathbf{g}}D_{\mathbf{X}}g=0$ for all X.

In Sec. III, we established that Lie and covariant differentiation are special cases of a particular kind of D differentiation, called ''restricted'' D differentiation, defined in (3.27). We also saw that modified D differentiation ${}^{\mathbf{g}}D$, when specialized to D being covariant differentiation, falls into the category of restricted D differentiation as well. (It may then be interpreted as the covariant derivative with respect to the metric-compatible part of the connection.) On the other hand, modified D differentiation, in the case of Lie differentiation, does not belong to the subtype of restricted D differentiation.

The concept of ''generalized curvature'' of D differentiation was introduced in Sec. IV. We mainly discussed which kinds of D differentiation are compatible with an identically vanishing generalized curvature.

Finally, D differentiation was reformulated, in two stages, in terms of fiber bundles in Secs. V and VI. In the first stage, we defined the D transport of a vector y along the integral curves $\varphi_{\mathbf{t}}$ of a vector field X. This led to the concept of the lift of $\varphi_{\mathbf{t}}$ to the tangent bundle TM and to the bundle PLM of frames over M. Weyl's method enabled us then to obtain D differentiation from the bundle PLM.

In the second stage, we intoduced the notion of generalized D differentiation, which, from two vector fields X and Y over M, enables one to construct the vector field $\mathbf{D}_{\mathbf{X}}Y$, over the bundle TM. We proved that D differentiation is simply related to generalized D differentiation, through the concept of generalized lift of a vector field X over M to a vector field $\mathbf{X}^{\dagger}$ over TM. In addition to providing a geometrical interpretation of D differentiation, these bundle formulations constitute the appropriate language for the extension of our considerations to spinor fields in Ref. 5.

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The formulation of generalized D differentiation presented in Sec. VI was stimulated by the concepts of generalized Lie derivative and lift to the bitangent bundle employed in Refs. 7 and 9 in the context of spinor fields. More precisely, we realized that D differentiation could be given an enlightening interpretation by adapting and generalizing to D differentiation what had been done in Refs. 7 and 9 for Lie differentiation. It is a pleasure to thank Professor M. Godina for drawing our attention to Ref. 9. P. Campbell and T. Philbin are also gratefully acknowledged for interesting and useful discussions.

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Deformations of the metaplectic representations[a)]

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We describe all possible ''natural'' deformations of the metaplectic representation of the Lie superalgebras $\mathfrak{osp}(1,2n)$ and of its natural extension and show in particular that in most cases for the metaplectic representation itself, it is rigid. [DOI: 10.1063/1.1350637]

I. INTRODUCTION

As was shown by Flato and coworkers (see, e.g., Refs. 1, 2, 3), in anti-de Sitter space, massless particles are composite of two singletons, i.e., of the two representations of the universal covering of $SO_0(3,2)$ which decompose the metaplectic representation, the latter being actually an irreductible representation of the supersymmetry $\mathfrak{osp}(1,4)$. In view of the deformation philosophy of Flato (see, e.g., Ref. 4) it is therefore important to study deformations of the metaplectic representation, and of its natural extension, the so-called extended metaplectic representation. In order to make the problem amenable, we shall restrict our study to some natural categories of representations, essentially the following three: first, representations having the same weight structure as the initial one; second, representations which are still diagonal with respect to the Cartan subalgebra $\mathfrak{h}$; third (keeping in mind that both the metaplectic representation and its natural extension are representations of the Weyl algebra) representations of the second kind which are still representations of the Weyl algebra.

A main result of the present paper is the *rigidity of the metaplectic representation* in all these categories of representations [Theorem (4.7)]. So, in the $\mathfrak{osp}(1,4)$-supersymmetry framework, the metaplectic representation, i.e., the Di and Rac singletons, appears to be a completely isolated and really unique object. This result is also true for $\mathfrak{osp}(1,2n)$, for any $n\geqslant 2$. For $\mathfrak{osp}(1,2)$, the metaplectic representation is rigid in the first and third category, but not in the second one [Remarks (3.16) and (3.17)].

Now, what about the *extended metaplectic representation*? We start with the $\mathfrak{osp}(1,2)$-case, which is a necessary step and obtain a complete classification of all possible deformations which do exist in the three categories (Sec. III). Using these results we give, in the case of $\mathfrak{osp}(1,4)$, a complete description of the cohomology groups involved, corresponding to deformations in the three categories [Proposition (4.1) and Theorem (4.4)]. As a consequence, we show the *rigidity* in the first category, and give a complete classification of all deformations in the third [Proposition (4.2)]; infinitesimally, deformations in the second category belong to the third. Finally, we note that the results obtained in the case of $\mathfrak{osp}(1,4)$ generalize easily to $\mathfrak{osp}(1,2n), n\geqslant 2$ [Remark (4.8)]; as a consequence, there do not exist (nontrivial) deformations with unchanged weight structure, in contradistinction with the $\mathfrak{osp}(1,2)$-case, which happens to be very singular, probably due to its low dimension.

[a)]We dedicate this paper to the memory of Moshé Flato, our teacher, a permanent source of inspiration, and above all an irreplaceable friend.

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The results, and proofs, of the paper are given in details for the extended metaplectic representation. The results concerning the metaplectic representation itself are given in Remarks (3.16) and (3.17) for $\mathfrak{osp}(1,2)$, together with some applications to maximal primitive quotients of the enveloping algebra, and in Remark (4.6) in the case of $\mathfrak{osp}(1,4)$; we did not detail the proofs in that case because they are essentially a repetition (with some simplifications) of the arguments given in the extended metaplectic case. Also, we have not given the proofs in the case of $\mathfrak{osp}(1,2n), n \geqslant 2$, because they can be obtained by induction and application of exactly the same arguments as in the $\mathfrak{osp}(1,4)$-case, with some simplifications [$\mathfrak{osp}(1,4)$ is actually the most complicated case!].

II. DEFINITIONS AND NOTATIONS

In this section we recall some notions and notations from deformation theory; for more details, we refer to Refs. 5, 6, 7. Given a Lie superalgebra $\mathfrak{g}=\mathfrak{g}_{\bar{0}}\oplus\mathfrak{g}_{\bar{1}}$ and a representation π of $\mathfrak{g}$ in a space $\mathcal{H}=\mathcal{H}_{\bar{0}}\oplus\mathcal{H}_{\bar{1}}$, if we denote by $\mathcal{L}(\mathcal{H})=\mathcal{L}(\mathcal{H})_{\bar{0}}\oplus\mathcal{L}(\mathcal{H})_{\bar{1}}$ the space of linear maps from $\mathcal{H}$ into itself endowed with its natural Lie superalgebra structure, there is a representation R of $\mathfrak{g}$ in $\mathcal{L}(\mathcal{H})$ defined by

$$R_X(T)=\pi(X)\circ T-(-1)^{\deg X.\deg T}T\circ\pi(X)=[\pi(X),T].$$

For this representation, the spaces of cocycles Z^1 and of coboundaries B^1 are (respectively)

$$Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))=\{F:\mathfrak{g}\to\mathcal{L}(\mathcal{H})\,|\deg F=0,\ F([X,Y])=R_X(F_Y)-(-1)^{\deg X.\deg Y}R_Y(F_X)\},$$

$$B^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))=\{F_X=R_X(T), T\in\mathcal{L}(\mathcal{H})_{\bar{0}}\}.$$

Note that the corresponding cohomology $H^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))=Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))/B^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$ is 0-degree cohomology in the terminology of Ref. 7. Cocycles are canonically associated with extensions of π by itself, i.e., with representations on $\mathcal{H}\oplus\mathcal{H}$ of the type $\tilde{\pi}_X=\left(\begin{smallmatrix}\pi_X & C_X\\ 0 & \pi_X\end{smallmatrix}\right)$. Indeed such a formula defines a representation if and only if $C\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$, and this representation splits into the direct sum $\pi\oplus\pi$ if and only if $C\in B^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$ (see Refs. 5, 7 for more details). But they are also associated with deformations (or formal representations) of π, defined by $\pi^\lambda=\pi+\Sigma_{n\geqslant 1}\lambda^n C_n$, where C_n are 0-degree linear maps from $\mathfrak{g}$ into $\mathcal{L}(\mathcal{H})$, and λ is a formal parameter. In fact, π^λ can be interpreted as a $\mathbb{C}[[\lambda]]$-linear representation of $\mathfrak{g}$ in the space $\mathcal{L}(\mathcal{H})[[\lambda]]$ (see Ref. 6). If π^λ is a deformation of π, then $C_1\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$; if moreover $C_1\in B^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$, then π^λ is equivalent to a deformation without a λ-term and the λ^2-term is a cocycle. We recall that π^λ and π'^λ are equivalent if they are intertwined by a $T^\lambda=\mathrm{Id}+\Sigma_{n\geqslant 1}\lambda^n T^n, T^n\in\mathcal{L}(\mathcal{H})_{\bar{0}}$. Clearly, if $H^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))=\{0\}$, then π^λ can be reduced to π by a sequence of equivalences, and we shall say that π is rigid. So, in order to study deformations of π, the first step is the computation of $H^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$. To do that, it is often useful to extend the cocycles $C\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$ to the enveloping algebra $\mathcal{U}(\mathfrak{g})$; this is easily done using the corresponding extension $\tilde{\pi}$, which can obviously be extended to a representation of $\mathcal{U}(\mathfrak{g})$, so C can be extended to $\mathcal{U}(\mathfrak{g})$, and then it satisfies

$$C(1)=0,\ \text{and}\ \ C(uv)=\pi(u)\circ C(v)+C(u)\circ\pi(v),\ \ u,v\in\mathcal{U}(\mathfrak{g}).$$

If C is the coboundary defined by $T\in\mathcal{L}(\mathcal{H})$ we have $C(u)=\pi(u)\circ T-T\circ\pi(u)=[\pi(u),T], u\in\mathcal{U}$. Let $Z(\mathfrak{g})$ be the center of $\mathcal{U}(\mathfrak{g})$ and assume that π is Schur-irreducible, i.e., if $[\pi(X),T]=0$, with $T\in\mathcal{L}(\mathcal{H})_{\bar{0}}, \forall X\in\mathfrak{g}$, then $T=\lambda\,\mathrm{Id}_{|\mathcal{H}}$ (this is true for instance if π is irreducible by Quillen's lemma); if C is a coboundary, one has $C(Q)=0, \forall Q\in Z(\mathfrak{g})_{\bar{0}}$. For a general cocycle C, the identity $C(Q\cdot X)=C(X\cdot Q), Q\in Z(\mathfrak{g})_{\bar{0}}, X\in\mathfrak{g}$, gives $[\pi(X),C(Q)]=0$, so $C(Q)=\lambda(Q)\mathrm{Id}_{\mathcal{H}}, \lambda(Q)\in\mathbb{C}$; if we can find Q such that $\lambda(Q)\neq 0$, then, obviously, C is a nontrivial cocycle.

We now state a lemma which will prove very useful.

Lemma (2.1): Let $\mathfrak{h}$ *be an Abelian subalgebra of* $\mathfrak{g}$ *such that* $\mathfrak{h}\subset\mathfrak{g}_{\bar{0}}$. *Assume that* $\mathfrak{g}$ *splits as* $\mathfrak{g}=\oplus_{\alpha\in\Delta\subset\mathfrak{h}^*}\mathfrak{g}^{\alpha}$ *into weight spaces under* $ad\,\mathfrak{h}$; *let* π *be a representation of* $\mathfrak{g}$ *in* $\mathcal{H}$ *and assume that* $\mathcal{H}$ *splits as* $\mathcal{H}=\oplus_{p\in\mathcal{P}\subset\mathfrak{h}^*}\mathcal{H}^p$ *into weight spaces under* $\pi(\mathfrak{h})$. *Let* $C\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$. *Then if* $C(\mathfrak{h})(\mathcal{H}^p)\subset\mathcal{H}^p,\forall p\in\mathcal{P}$, *we have* $C(\mathfrak{g}^{\alpha})(\mathcal{H}^p)\subset\mathcal{H}^{p+\alpha},\forall p\in\mathcal{P},\alpha\in\Delta$.

Remark (2.2): Obviously, Lemma (2.1) can be applied if $C\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}$, the subspace of cocycles which vanish on $\mathfrak{h}$.

Proof: Let $X\in\mathfrak{g}^{\alpha}$. Relation $[H,X]=\alpha(H)X,\forall H\in\mathfrak{h}$, shows that $\pi(X)(\mathcal{H}^p)\subset\mathcal{H}^{p+\alpha}$. We decompose $C=A+B$, with $A(\mathfrak{g}^{\alpha})(\mathcal{H}^p)\subset\mathcal{H}^{p+\alpha}$, $\forall p$, α, and $B(\mathfrak{g}^{\alpha})(\mathcal{H}^p)\subset\oplus_{r\neq p+\alpha}\mathcal{H}^r$. It is easily seen that $A\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$, and $B\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}$. Then, if $X\in\mathfrak{g}^{\alpha},B([H,X])=[\pi(H),B(X)]=\alpha(H)B(X)$, so we deduce that $B(X)(\mathcal{H}^p)\subset\mathcal{H}^{p+\alpha},\forall p$, and then, from the definition of B, that $B=0$. □

Finally we want to stress that, when dealing with a Z_2-graded associative algebra A, we are using the notation $[a,b]$ for the super-bracket $[a,b]=ab-(-1)^{\deg a\cdot\deg b}ba$ while, for the Lie bracket, we write $[a,b]_{\mathcal{L}}=ab-ba$.

III. DEFORMATION OF THE EXTENDED METAPLECTIC REPRESENTATION OF $\mathfrak{g}=\mathfrak{osp}(1,2)$

Throughout this section, $\mathfrak{g}=\mathfrak{osp}(1,2),\mathfrak{g}_{\bar{0}}=\mathfrak{sl}(2)$. As in Ref. 8, we introduce a basis H, F, G for $\mathfrak{g}_{\bar{0}}$, and $E_{\pm}$ for $\mathfrak{g}_{\bar{1}}$, with commutation rules:

$$[H,F]=F,[H,G]=-G,[H,E_{\pm}]=\pm\tfrac{1}{2}E_{\pm},F=[E_+,E_+],G=-[E_-,E_-],$$

$$H=[E_+,E_-],[F,E_-]=-E_+ \text{ and } [G,E_+]=-E_-.$$

[3.1] Let $\mathcal{U}(\mathfrak{g})$ and $\mathcal{U}(\mathfrak{g}_{\bar{0}})$ be the respective enveloping algebras, and $Z(\mathfrak{g}),Z(\mathfrak{g}_{\bar{0}})$ their centers. Then $Z(\mathfrak{g})=\mathbb{C}[Q],Z(\mathfrak{g}_{\bar{0}})=\mathbb{C}[Q_0]$, where $Q_0=GF+H+H^2$, and $Q=Q_0-\frac{1}{2}[E_+,E_-]_{\mathcal{L}}$. If $\theta=\frac{1}{4}+[E_+,E_-]_{\mathcal{L}}$, it is shown in Ref. 8 (see also Ref. 9) that $\mathcal{U}(\mathfrak{g})$ is exactly the algebra with generators $E_{\pm}$ and θ and relations $[E_+,E_-]_{\mathcal{L}}=-\frac{1}{4}+\theta$, with θ anticommuting with $E_{\pm}$. Then $Q=-\frac{1}{16}+\theta^2$ and $Q_0=-\frac{3}{16}+\frac{1}{2}\theta+\theta^2$. $\mathcal{U}\theta$ is a two sided primitive ideal of $\mathcal{U}$, and the quotient $\mathcal{U}/\mathcal{U}\theta$ is the Weyl algebra W_1, i.e., the algebra with generators $E_{\pm}$ and relations $[E_+,E_-]_{\mathcal{L}}=-\frac{1}{4}$. The Weyl algebra has a natural Schur-irreducible representation on $\mathcal{H}=\mathbb{C}[z^{-1},z]$ defined by $\pi(E_+)=\frac{1}{2}(d/dz),\pi(E_-)=-\frac{1}{2}z$; using $W_1=\mathcal{U}/\mathcal{U}\theta$, we deduce a representation of $\mathfrak{g}$ on $\mathbb{C}[z^{-1},z]$, that we also denote by π. One has $\pi(H)=-\frac{1}{2}z(d/dz)-\frac{1}{4}$, $\pi(F)=\frac{1}{2}(d^2/dz^2)$, $\pi(G)=-\frac{1}{2}z^2$, $\pi(Q)=-\frac{1}{16}$ and $\pi(Q_0)=-\frac{3}{16}$. We call π the extended metaplectic representation (we shall explain why later).

At this stage, we shall interpret π as an extension of two irreducible representations of $\mathfrak{g}$: if $\mathcal{H}^+=\mathbb{C}[z]$ and $\mathcal{H}^-=(1/z)\mathbb{C}[1/z]$, then $\mathcal{H}^+$ is a subrepresentation of $\mathcal{H}$ that we denote π^+. In the notations of Ref. 7, π^+ is an irreducible representation of type $[-\frac{1}{4}]\downarrow$; let now π^- be the representation induced by π on $\mathcal{H}/\mathcal{H}^+$: then π^- is an irreducible representation of type $[\frac{1}{4}]\uparrow$, so that π^- is exactly the contragedient of π^+. There is an exact sequence: $0\to(\mathcal{H}^+,\pi^+)\to(\mathcal{H},\pi)\to(\mathcal{H}/\mathcal{H}^+,\pi^-)\to 0$, so π is an extension of π^+ by π^- (see Ref. 7). The restriction $\pi_{|\mathfrak{g}_{\bar{0}}}$ decomposes as $\pi_{\bar{0}}\oplus\pi_{\bar{1}}$ on $\mathcal{H}=\mathcal{H}_{\bar{0}}\oplus\mathcal{H}_{\bar{1}}$, the grading being defined by parity. We get two extensions: $0\to(\mathcal{H}_{\bar{0}}^+,\pi_{\bar{0}}^+)\to(\mathcal{H}_{\bar{0}},\pi_{\bar{0}})\to(\mathcal{H}_{\bar{0}}/\mathcal{H}_{\bar{0}}^+,\pi_{\bar{0}}^-)\to 0$ and $0\to(\mathcal{H}_{\bar{1}}^+,\pi_{\bar{1}}^+)\to(\mathcal{H}_{\bar{1}},\pi_{\bar{1}})\to(\mathcal{H}_{\bar{1}}/\mathcal{H}_{\bar{1}}^+,\pi_{\bar{1}}^-)\to 0$, and $\pi_{\bar{0}}^+=(-\frac{1}{4})\downarrow,\pi_{\bar{1}}^+=(-\frac{3}{4})\downarrow,\pi_{\bar{0}}^-=(\frac{3}{4})\uparrow,\pi_{\bar{1}}^-=(\frac{1}{4})\uparrow$. All these extensions are nontrivial.

Let now $\mathcal{F}=\mathbb{C}[[z,z^{-1}]]$ be the space of formal Laurent series, graded as $\mathcal{F}=\mathcal{F}_{\bar{0}}\oplus\mathcal{F}_{\bar{1}}$ by parity; we can extend π to a representation (denoted by the same symbol) of $\mathfrak{g}$ on $\mathcal{F}$. Note that $\mathcal{F}^+=\mathbb{C}[[z]]$ is a subrepresentation, that we denote by π^+. We define a scalar product by $\langle z^n,z^n\rangle=n!,\langle z^{-n},z^{-n}\rangle=1/(n-1)!$ if $n>0,\{z^n,n\in\mathbb{Z}\}$ being an orthogonal set, and denote by $\mathbf{H}$ the Hilbert space of series $f=\Sigma_{n\in\mathbb{Z}}a_nz^n\in\mathcal{F}$ such that $\Sigma_{n\geqslant 1}[|a_{-n}|^2/(n-1)!]<+\infty$ and $\Sigma_{n\geqslant 0}n!|a_n|^2<+\infty$. Let $\mathbf{H}^+=\mathcal{F}^+\cap\mathbf{H}$. If $f\in\mathbf{H}^+$, the two series $\Sigma\sqrt{n!}a_n$ and $\Sigma z^n/\sqrt{n!}$ are in l^2, so, by Schwarz inequality, one has

$$\left|\sum_{n\geqslant 0} a_n z^n\right| \leqslant \left[\sum_{n\geqslant 0} n!|a_n|^2\right]^{1/2}\left[\sum_{n\geqslant 0}\frac{z^{2n}}{n!}\right]^{1/2} = e^{|z|^2/2}\|f\|_{\mathbf{H}}.$$

In other words, $f(z)=\Sigma_{n\geqslant 0}a_n z^n$ is actually an entire function. Convergence in $\mathbf{H}^+$ implies pointwise convergence, and it is easily seen that $\mathbf{H}^+$ is exactly the space of entire functions such that $\int e^{-|z|^2}|f(z)|^2 dxdy<+\infty$; the scalar product on $\mathbf{H}^+$ is exactly $\langle f|g\rangle = 1/\pi\int e^{-|z|^2} f(z)\overline{g(z)}dxdy$.

We denote by $\mathbf{G}$ the twofold metaplectic covering of $SU(1,1)$: $\mathfrak{g}_0^-$ is its Lie algebra. $\mathbf{K}$ being the maximal compact subgroup of $\mathbf{G}$ we have the following.

Proposition (3.1): There exists a continuous representation U of $\mathbf{G}$ on $\mathbf{H}$ such that the space of $\mathbf{K}$-finite vectors of U is $\mathcal{H}$, and $dU_{|_{\mathcal{H}}}=\pi_{|_{\mathfrak{g}_0^-}}$.

Proof: Let $\pi^+=\pi^+_{|_{\mathfrak{g}_0^-}}$. The condition $\pi^+(F)^*=-\pi^+(G)$ is satisfied on $\mathcal{H}^+$, so by Nelson's criteria,[10] there exists a unitary representation U^+ of $\mathbf{G}$ in $\mathbf{H}^+$ such that $\mathcal{H}^+$ is the space of $\mathbf{K}$-finite vectors of U^+, and $dU^+|_{\mathcal{H}^+}=\pi^+$ (*a priori*, U^+ is a representation of the universal covering $\tilde{\mathbf{G}}$, but due to the weight structure, it is in fact a representation of $\mathbf{G}$). Now, let $\pi^-=\pi^-_{|_{\mathfrak{g}_0^-}}$, on $\mathcal{H}/_{\mathcal{H}^+}$; again, the condition $\pi^-(F)^*=-\pi^-(G)$ is satisfied, so there exists a unitary representation U^- of $\mathbf{G}$ in $\mathbf{H}/\mathbf{H}^+$ such that, if we identify the spaces $\mathcal{H}/\mathcal{H}^+$ and $\mathcal{H}^-$, $\mathcal{H}^-$ is the space of $\mathbf{K}$-finite vectors of U^- and $dU^-_{|_{\mathcal{H}^-}}=\pi^-$. In what follows, we identify the Hilbert spaces $\mathbf{H}/\mathbf{H}^+$ and $\mathbf{H}^-=\{f=\Sigma_{n\geqslant 1}a_n z^{-n}\in\mathcal{F}|\Sigma_{n\geqslant 1}[|a_{-n}|^2/(n-1)!]<\infty\}$, so U^- is a representation of $\mathbf{G}$ on $\mathbf{H}^-$. Let $Z_n(z)=z^n/\sqrt{n!}, Z_{-n}(z)=\sqrt{(n-1)!}z^{-n}, n\geqslant 0$; one has

$$\pi(F)Z_n=\tfrac{1}{2}\sqrt{n(n-1)}Z_{n-2},$$

$$\pi(G)Z_n=-\tfrac{1}{2}[\sqrt{(n+1)(n+2)}Z_{n+2}+\delta_{n+1,0}Z_1+\delta_{n+2,0}Z_0],\quad \forall n\in\mathbb{Z}.$$

So the representation π of $\mathfrak{g}_0^-$ on $\mathcal{H}=\mathcal{H}^+\oplus\mathcal{H}^-$ can be written as $\pi=\begin{pmatrix}\pi^+ & \xi\\ 0 & \pi^-\end{pmatrix}$, with an extension cocycle $\xi\in Z^1(\mathfrak{g}_0^-,\mathcal{L}(\mathcal{H}^-,\mathcal{H}^+))$ (see Ref. 5) defined by $\xi_H=\xi_F=0$, and $\xi_G(Z_n)=-\frac{1}{2}[\delta_{n+1,0}Z_1+\delta_{n+2,0}Z_0]$; it is obvious that $\xi(X), X\in\mathfrak{g}_0^-$, is always a continuous linear map from $\mathbf{H}^-$ into $\mathbf{H}^+$, so, by Ref. 5, there exists a representation U of $\mathbf{G}$ in $\mathbf{H}$ such that $dU|_{\mathcal{H}}=\pi_{|_{\mathfrak{g}_0^-}}$. □

Remark (3.2): Still identifying the spaces $\mathbf{H}/\mathbf{H}^+$ and $\mathbf{H}^-$, as in the proof of Proposition (3.1), we see that $U=\begin{pmatrix}U^+ & \tau\\ 0 & U^-\end{pmatrix}$ is an extension of U^+ by U^-, with extension cocycle τ (see Ref. 5), and actually a nontrivial extension (because its differential is a nontrivial extension). One has $U^+=U_0^+\oplus U_1^+=(-\frac{1}{4})\downarrow\oplus(-\frac{3}{4})\downarrow$, so U^+ is equivalent to the usual metaplectic representation of $\mathbf{G}$, which is obtained from the well-known harmonic oscillator representation of $\mathbf{G}$; moreover, one has $U^-=U_0^-\oplus U_1^-=(\frac{3}{4})\uparrow\oplus(\frac{1}{4})\uparrow$, so that U is a nontrivial (and therefore nonunitary) extension of the metaplectic representation of $\mathbf{G}$ by its own contragedient: this explains the name ''extended metaplectic representation.''

To end this subsection, we briefly explicit an isomorphism between U^+ and the usual metaplectic representation. Let $\phi_n(x)=H_n(x)e^{-x^2/2}/\pi^{1/4}2^{n/2}\sqrt{n!}$, with $H_n=(-1)^n e^{x^2}(d^n/dx^n)\times(e^{-x^2})$, be the orthonormal basis of Hermite functions in $L^2(\mathbb{R})$. Now $\theta_n(x)=\int(x+it)^n e^{-t^2/2}dt$ satisfies $\theta_{n+2}=x\theta_{n+1}-(n+1)\theta_n$; so, from Ref. 11, one has $\theta_n=\sqrt{2\pi}H_n(x/\sqrt{2})2^{-n/2}$ and $H_n(x)=2^n/\sqrt{\pi}\int(x+it)^n e^{-t^2}dt$. Hence $\phi_n(x)=e^{-x^2/2}/\pi^{3/4}\int Z_n(\sqrt{2}(x+it))e^{-t^2}dt$. Define an operator T by $T(f)=e^{-x^2/2}/\pi^{3/4}\int f(\sqrt{2}(x+it))e^{-t^2}dt$, $f\in\mathcal{H}^+$. One has $T(Z_n)=\phi_n$, so T extends to a unitary operator from $\mathbf{H}^+$ onto $L^2(\mathbb{R})$. It is easy to check that T maps the operator z (resp., d/dz) of $\mathbf{H}^+$ onto the operator $(1/\sqrt{2})(x-d/dx)$ [resp., $1/\sqrt{2}(x+d/dx)$] of $L^2(\mathbb{R})$, so it intertwines U^+ and the usual metaplectic representation of $\mathbf{G}$.

[3.2] In this subsection we shall deform the extended metaplectic representation π defined in subsection [3.1]. Note that π can be considered as a representation of $\mathfrak{g}$, hence also of $\mathfrak{g}_0^-$, but also as a representation of the Weyl algebra W_1. So we have to specify in what category of representations we want to deform π.

[*3.2.1*] We shall first deform π as a representation of the Lie algebra $\mathfrak{g}_0^-$ and assume that the weight structure of π is unchanged by the deformation. So if $\mathfrak{h}=\mathbb{C}H$ is the Cartan subalgebra, we have to compute $H^1(\mathfrak{g}_0^-,\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}$.

Proposition (3.3): One has $\dim H^1(\mathfrak{g}_0^-,\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}=2$; *any cocycle is equivalent to a cocycle such that* $C(H)=C(G)=0$, *and* $C(F)=(\alpha P+\beta\,\mathrm{Id})\pi(G)^{-1}$, *where* P *is the parity operator.*

Proof: If $C\in Z^1(\mathfrak{g}_0^-,\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}$, we deduce from Lemma (2.1) that $C(G)(\mathcal{H}_n)\subset\mathcal{H}_{n+2}(\mathcal{H}_n=\mathbb{C}z^n)$, so, up to a coboundary, we can assume that $C(G)=0$. $\forall X\in\mathfrak{g}_0^-$ we deduce from $C(Q_0X)=C(XQ_0)$ and $\pi(Q_0)=-\frac{3}{16}$ that $[\pi(X),C(Q_0)]=0$, so $C(Q_0)_{|_{\mathcal{H}_d}}=\alpha_d\,\mathrm{Id}_{\mathcal{H}_d},\alpha_d\in\mathbb{C}$, $d=\overline{0,1}$. If C is a coboundary, then $C(Q_0)=\pi(G)C(F)=0$, and since G is invertible, we get $C=0$. If $C(Q_0)\neq 0$,C cannot be a coboundary, and using $C(Q_0)=\pi(G)C(F)$, we deduce $C(F)_{|_{\mathcal{H}_d}}=\alpha_d\pi(G)^{-1}_{|_{\mathcal{H}_d}}$, $d=\overline{0,1}$. Now define $\alpha=\frac{1}{2}(\alpha_0^-\alpha_1^-)$, and $\beta=\frac{1}{2}(\alpha_0^-+\alpha_1^-)$. We get $C(F)=(\alpha\cdot P+\beta\,\mathrm{Id})\pi(G)^{-1}$. It is easy to check that these formulas define a cocycle. □

Let us now construct deformations associated with the cocycles of Proposition (3.3). Note that if C and C' are two such cocycles, one has $[C(X),C'(Y)]=0$, for every $X,Y\in\mathfrak{g}_0^-$. Thus if C_n is a sequence of such cocycles, then $\pi^\lambda=\pi+\Sigma_{n\geqslant 1}\lambda^nC_n$ defines a deformation of π. Using Lemma (2.1) and a sequence of equivalences, it is easily seen that any deformation of π such that the weight structure is unchanged (i.e., the cochains vanish on $\mathfrak{h}$) is equivalent to a deformation of the type described above, so we have the following.

Proposition (3.4): (1) *Any deformation of* π, *considered as a representation of* $\mathfrak{g}_0^-$, *with unchanged weight structure, is equivalent to a deformation* $\pi^\lambda_{f,g}$ *defined, given two formal series* $f(\lambda)$ *and* $g(\lambda)$ *such that* $f(0)=g(0)=0$, *by* $\pi^\lambda_{f,g}(H)=\pi(H)$, $\pi^\lambda_{f,g}(G)=\pi(G)$, $\pi^\lambda_{f,g}(F)=\frac{1}{2}(d^2/dz^2)-2(f(\lambda)P+g(\lambda))\cdot 1/z^2$. *One has* $\pi^\lambda_{f,g}(Q_0)=-\frac{3}{16}+(f(\lambda)P+g(\lambda))$; *as deformations* $\pi^\lambda_{f,g}\simeq\pi^\lambda_{f',g'}$, *if and only if* $f=f'$ *and* $g=g'$.

(2) *If* $\tilde{\pi}^\lambda$ *is a deformation of* π, *with unchanged weight structure, there exist* $f(\lambda),g(\lambda)\in\mathbb{C}[[\lambda]]$, *such that* $f(0)=g(0)=0$, *and* $\tilde{\pi}^\lambda(Q_0)=-\frac{3}{16}+(f(\lambda)P+g(\lambda))$; *as a deformation,* $\tilde{\pi}^\lambda\simeq\pi^\lambda_{f,g}$.

Proof: We have to prove the two last claims. Let $\pi^\lambda=\pi^\lambda_{f,g}$, and $\pi'^\lambda=\pi^\lambda_{f',g'}$. Assume that $T^\lambda\pi^\lambda=\pi'^\lambda T^\lambda$, with $T^\lambda=\mathrm{Id}+\Sigma_{n\geqslant 1}\lambda^nT_n$; since $\pi^\lambda(H)=\pi'^\lambda(H)=\pi(H)$, one has $[\pi(H),T^\lambda]=0$, so $T^\lambda(z^p)=t_p(\lambda)\cdot z^p$, with $t_p(0)=1$. Applying $T^\lambda\pi^\lambda(Q_0)=\pi'^\lambda(Q_0)T^\lambda$ on z^p, one gets $(-1)^pf(\lambda)+g(\lambda)=(-1)^pf'(\lambda)+g'(\lambda)$, so $g=g'$, and $f=f'$.

We know that $\tilde{\pi}^\lambda$ is equivalent to some $\pi^\lambda_{f,g}$; since $[Q_0,H]=0$, one has $\tilde{\pi}^\lambda(Q_0)(z^p)=q(\lambda)\cdot z^p$. Let $T^\lambda\tilde{\pi}^\lambda(Q_0)=\pi^\lambda_{f,g}(Q_0)T^\lambda$. As before, one sees that $T(z^p)=t_p(\lambda)\cdot z^p$, with $t_p(0)=1$, and $t_p(\lambda)q(\lambda)\cdot z^p=[-\frac{3}{16}+(-1)^pf(\lambda)+g(\lambda)]t_p(\lambda)z^p$, hence the formula for $\tilde{\pi}^\lambda(Q_0)$. □

Remark (3.5): A deformation of π with unchanged weight structure, when not trivial, can never be a representation of the Weyl algebra, because in the Weyl algebra, one has $Q_0=-\frac{3}{16}$. We shall see in the next section when it is possible to extend from $\mathfrak{g}_0^-$ to $\mathfrak{g}$.

[*3.2.2*] Here we deform π as a *representation of the superalgebra* $\mathfrak{g}$. We begin by assuming that the weight structure is unchanged (i.e., the cochains vanish on $\mathfrak{h}$), as was done in the case of $\mathfrak{g}_0^-$. So we have to compute $Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}$.

Proposition (3.6): $\mathrm{Dim}\,Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}=1$. *A nontrivial cocycle is defined by* $C(H)=C(E_-)=0$ *and* $C(E_+)=P\pi(E_-)^{-1}$, *where* P *is the parity operator.*

Proof: For simplicity, we write $X=\pi(X)$, for $X\in\mathfrak{g}$. Define the operators $E^\lambda_\pm$ by $E^\lambda_+=E_+ +\lambda P\cdot E_-^{-1}$ and $E^\lambda_-=E_-$. We get $[E^\lambda_+,E^\lambda_-]_{\mathcal{L}}=-\frac{1}{4}+2\lambda P$, and P anticommutes with E^λ_+ and E^λ_-. Therefore, from the definition of $\mathcal{U}(\mathfrak{g})$ by generators and relations (see Sec. [3.1]), there exists a formal representation π^λ of $\mathfrak{g}$ such that $\pi^\lambda(E_\pm)=E^\lambda_\pm$ and one has, $\forall X\in\mathfrak{g}$, $\pi^\lambda(X)=\pi(X)+\lambda C(X)+\lambda^2D(X)$ with $C\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}$. Now $\pi^\lambda(H)=[E^\lambda_+,E^\lambda_-]=\pi(H)$, so that $C(H)=C(E_-)=0$ and $C(E_+)=P\cdot E_-^{-1}$. This proves that the above definition of C gives indeed an element of $Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}$.

To prove the first assertion above, we take some $C \in Z^1(\mathfrak{g}, \mathcal{L}(\mathcal{H}))^\mathfrak{h}$. Since $C(H)=0$, by Lemma (2.1), one has $C(E_-)(\mathcal{H}_n) \subset \mathcal{H}_{n+1}$ ($\mathcal{H}_n = \mathbb{C}z^n$), so, up to a coboundary, we can assume that $C(E_-)=0$. From Sec. II, one has $C(Q)=\alpha\,\mathrm{Id}_\mathcal{H}$, and from the proof of Proposition (3.3), $C(Q_0)_{|_{\mathcal{H}_d}} = \alpha_d \cdot \mathrm{Id}_{\mathcal{H}_d}$, $d = \overline{0,1}$. Since $Q = Q_0 - \frac{1}{2}[E_+, E_-]_\mathcal{L}$, we deduce $C([E_+, E_-]_\mathcal{L})_{|_{\mathcal{H}_d}} = 2(\alpha_d - \alpha)\cdot \mathrm{Id}_{\mathcal{H}_d}$. But $H=[E_+, E_-]$, so $C(H)=[C(E_+), E_-]=0$ gives $C(E_+)E_- = -E_- C(E_+)$. Therefore $C(E_+)E_{-|_{\mathcal{H}_d}} = (\alpha_d - \alpha_d)\mathrm{Id}_{\mathcal{H}_d}$. But since E_- anticommutes with $(\frac{1}{4} + [E_+, E_-]_\mathcal{L})$ (see Sec. [3.1]), one has $E_- C([E_+, E_-]_\mathcal{L}) = -C([E_+, E_-]_\mathcal{L})E_-$. Applying on $f \in \mathcal{H}_0^-$, we get $(\alpha_0^- - \alpha)E_- f = -(\alpha_1^- - \alpha)E_- f$, and then $C(E_+)E_- = (\alpha_0^- - \alpha)P$, so $C(E_+) = (\alpha_0^- - \alpha)PE_-^{-1}$. □

We shall now classify our deformations up to equivalence. First, for $f \in \mathbb{C}[[\lambda]]$ and $f(0)=0$, we define a deformation π_f^λ by $\pi_f^\lambda(E_-) = \pi(E_-)$ and $\pi_f^\lambda(E_+) = \pi(E_+) + f(\lambda)P\pi(E_-)^{-1}$. It is indeed a deformation because, as in the proof of Proposition (3.6), $[\pi_f^\lambda(E_+), \pi_f^\lambda(E_-)]_\mathcal{L} = -\frac{1}{4} + 2f(\lambda)P$, and P anticommutes with $\pi_f^\lambda(E_\pm)$. One has $\pi_f^\lambda(H) = H$, so the weight structure is unchanged, as wanted. Moreover, one has $\pi_f^\lambda(Q_0) = -\frac{3}{16} + f(\lambda)P + 4f(\lambda)^2$, and $\pi_f^\lambda(Q) = -\frac{1}{16} + 4f(\lambda)^2$, using formulas given in (3.1). As in the proof of Proposition (3.4), it is easily proved that $\pi_f^\lambda \simeq \pi_{f'}^\lambda$ if and only if $f = f'$.

Proposition (3.7): Any deformation $\tilde{\pi}^\lambda$ of π, considered as a representation of $\mathfrak{g}$, with unchanged weight structure, is equivalent to some π_f^λ. In addition $\tilde{\pi}^\lambda(Q_0) = -\frac{3}{16} + f(\lambda)P + 4f(\lambda)^2$, and $\tilde{\pi}^\lambda(Q) = -\frac{1}{16} + 4f(\lambda)^2$.

We shall need the following technical lemma.

Lemma (3.8): Given $C_\pm \in \mathcal{L}(\mathcal{H})$ such that $[\pi(E_+), C_-]_\mathcal{L} + [C_+, \pi(E_-)]_\mathcal{L}$ anticommutes with $E_\pm$, and $[\pi(E_+), C_-] + [\pi(E_-), C_+] = 0$, there exists a cocycle $C \in Z^1(\mathfrak{g}, \mathcal{L}(\mathcal{H}))^\mathfrak{h}$ such that $C(E_\pm) = C_\pm$.

Proof: Define $\widetilde{E_\pm} = \begin{pmatrix} \pi(E_\pm) & C_\pm \\ 0 & \pi(E_\pm) \end{pmatrix} \in \mathcal{L}(\mathcal{H} \oplus \mathcal{H})$. Then $[\widetilde{E_+}, \widetilde{E_-}]_\mathcal{L} = -\frac{1}{4} + \tilde{T}$, where $\tilde{T}$ anticommutes with $\widetilde{E_\pm}$, so (see Sec. [3.1]), there exists a representation ρ of $\mathcal{U}(\mathfrak{g})$ on $\mathcal{H} \oplus \mathcal{H}$ such that $\rho(E_\pm) = \tilde{E}_\pm$ and one has $\rho(u) = \begin{pmatrix} \pi(u) & C(u) \\ 0 & \pi(u) \end{pmatrix}$ where C is a cocycle which satisfies $C(E_\pm) = C_\pm$. Since $H = [E_+, E_-]$, one has $C(H) = [\pi(E_+), C(E_-)] + [\pi(E_-), C(E_+)] = 0$. □

We now prove Proposition (3.7). From Sec. [3.1], we see that $\tilde{\pi}^\lambda$ is completely defined if one knows $\widetilde{E_\pm^\lambda} = \tilde{\pi}^\lambda(E_\pm)$, which have to satisfy $[\widetilde{E_+^\lambda}, \widetilde{E_-^\lambda}]_\mathcal{L} = -\frac{1}{4} + T^\lambda$, with T^λ anticommuting with $\widetilde{E_\pm^\lambda}$, and $[\widetilde{E_+^\lambda}, \widetilde{E_-^\lambda}] = H$.

Let $\widetilde{E_\pm^\lambda} = \pi(E_\pm) + \lambda C_\pm + o(\lambda^2)$. We know that there exists a cocycle $C \in Z^1(\mathfrak{g}, \mathcal{L}(\mathcal{H}))^\mathfrak{h}$ such that $C_\pm = C(E_\pm)$; by Proposition (3.6), C is equivalent to $\gamma_1 C_0$, where $\gamma_1 \in \mathbb{C}$, and C_0 is the cocycle of Proposition (3.6). Then, using an equivalence, we can replace $C_\pm$ by $\gamma_1 C_0(E_\pm)$. So we get new operators, that we still denote by $\tilde{E}_\pm^\lambda$, and which can be written as

$$\widetilde{E_+^\lambda} = \pi(E_+) + \lambda\gamma_1 P\pi(E_-)^{-1} + \lambda^2 D_+ + o(\lambda^3),$$

$$\widetilde{E_-^\lambda} = \pi(E_-) + \lambda^2 D_- + o(\lambda^3).$$

Now $D_\pm$ satisfies the assumptions of Lemma (3.8), so there exists $D \in Z^1(\mathfrak{g}, \mathcal{L}(\mathcal{H}))^\mathfrak{h}$ such that $D(E_\pm) = D_\pm$. By Proposition (3.6), D is equivalent to $\gamma_2 C_0, \gamma_2 \in \mathbb{C}$. So, via an equivalence of the form $(\mathrm{Id} + \lambda^2 T)$, we can replace $D_\pm$ by $\gamma_2 C_0(E_\pm)$ and get new operators, still denoted by $\widetilde{E_\pm^\lambda}$, which can be written as

$$\widetilde{E_+^\lambda} = \pi(E_+) + \lambda\gamma_1 P\pi(E_-)^{-1} + \lambda^2\gamma_2 P\pi(E_-)^{-1} + \lambda^3 J_+ + o(\lambda^4),$$

$$\widetilde{E_-^\lambda} = \pi(E_-) + \lambda^3 J_- + o(\lambda^4).$$

We can now repeat the argument for $J_\pm$, and so on. Eventually we obtain that, by equivalence, our operators $\widetilde{E_\pm^\lambda}$ can be written as

$$\widetilde{E_+^\lambda}=\pi(E_+)+\sum_{n\geqslant 1}\lambda^n\gamma_n P\pi(E_-)^{-1}=\pi(E_+)+f(\lambda)P\pi(E_-)^{-1}\ \text{ and }\ \widetilde{E_-^\lambda}=\pi(E_-),$$

which shows that $\tilde{\pi}^\lambda$ is equivalent to π_f^λ. Finally we obtain $\tilde{\pi}^\lambda(Q_0)=\pi_f^\lambda(Q_0)$ and $\tilde{\pi}^\lambda(Q)=\pi_f^\lambda(Q)$ as in the proof of Proposition (3.4).

Remark (3.9): (1) The deformations $\tilde{\pi}^\lambda$ of Proposition (3.7), when nontrivial, can never be representations of the Weyl algebra W_1 (where $Q=-\frac{1}{16}$).

(2) One has $\tilde{\pi}^\lambda(Q_0)=-\frac{3}{16}+f(\lambda)P+4f(\lambda)^2$, so $\tilde{\pi}^\lambda|_{\mathfrak{g}_0^-}$ is equivalent to $\pi_{f,4f^2}^\lambda$ by Proposition (3.4). In particular, $\pi_{f,g}^\lambda$ extends from $\mathfrak{g}_0^-$ to $\mathfrak{g}$ if and only if $g=4f^2$.

[3.3] From Sec. [3.2], we see that it is impossible to deform π nontrivially if one assumes that the weight structure and the Weyl structure are preserved. In this section, we study deformations of π, considered as a representation of $\mathfrak{g}$, such that the Weyl structure is preserved, i.e., which are still representations of the Weyl algebra. We then have to release our assumption about the weight structure: we shall assume only that our deformation is still H-diagonal on $\mathcal{H}=\oplus_{n\in\mathbb{Z}}\mathcal{H}_n$, $\mathcal{H}_n=\mathbb{C}z^n$, but the weights may change (and in fact will change, as we shall see). Writing such a deformation as $\pi^\lambda=\pi+\Sigma_{n\geqslant 1}\lambda^n C_n$, we must have $C_n([E_+,E_-]_{\mathcal{L}})=0$, $\forall n$, and $C_n(H)\times(\mathcal{H}_p)\subset\mathcal{H}_p,\forall_p$. The corresponding cohomology is defined by

$$Z_W^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))=\{C\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))\,|\,C([E_+,E_-]_{\mathcal{L}})=0,\ \text{and}\ C(H)(\mathcal{H}_p)\subset\mathcal{H}_p,\forall p\in\mathbb{Z}\},$$

$B_W^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))=B^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}$ (easy to check), and $H_W^1=Z_W^1/B_W^1$.

Proposition (3.10): $\dim H_W^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))=1$, *a nontrivial cocycle being defined by* $C(E_+)=\pi(E_-)^{-1}$, $C(E_-)=0$, *and one has* $C(H)=2\,\mathrm{Id}_{\mathcal{H}}$.

Proof: Again, we write $X=\pi(X),X\in\mathfrak{g}$, to simplify notations, and define two operators: $\tilde{E}_+^\lambda=E_++\lambda E_-^{-1}$, $\tilde{E}_-^\lambda=E_-$; one has $[\tilde{E}_+^\lambda,\tilde{E}_-^\lambda]=-\frac{1}{4}$ so that we can extend this to a formal representation of the Weyl algebra W_1. Since $W_1=\mathcal{U}(\mathfrak{g})/\mathcal{U}(\mathfrak{g})\theta$ (see Sec. [3.1]), it is actually a formal representation of $\mathfrak{g}$, which deforms π, so there exists $C\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$ such that $C(E_+)=E_-^{-1}$ and $C(E_-)=0$. One has $C(H)=C([E_+,E_-])=2\mathrm{Id}_{\mathcal{H}}$, so $C\in Z_W^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$.

Let us now consider a general $C\in Z_W^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$. Using Lemma (2.1), one has $C(E_-)\times(\mathcal{H}_n)\subset\mathcal{H}_{n+1}$, for every n, so up to a coboundary, we can assume that $C(E_-)=0$. By Lemma (2.1), one has $C(E_+)(z^n)=c_nz^{n-1}$, but since $C([E_+,E_-]_{\mathcal{L}})=[C(E_+),E_-]_{\mathcal{L}}=0$, and $E_-z^n=-\frac{1}{2}z^{n+1}$, we deduce that $c_{n+1}=c_n,\forall n$, so finally $C(E_+)=cE_-^{-1},c\in\mathbb{C}$. Since $C(H)=2c\,\mathrm{Id}_{\mathcal{H}}$, C is a coboundary if and only if $c=0$. □

Proposition (3.11): Let π^λ *be a deformation of* π, *as a representation of* $\mathfrak{g}$, *such that the Weyl structure is preserved* [*and that* $\pi^\lambda(H)$ *is still diagonal on* $\oplus_n\mathcal{H}_n$]. *Then* π^λ *is equivalent to a deformation* π_{Wf}^λ *defined, for* $f\in\mathbb{C}[[\lambda]]$ *with* $f(0)=0$, *by* $\pi_{Wf}^\lambda(E_+)=\pi(E_+)+f(\lambda)\pi(E_-)^{-1}$ *and* $\pi_{Wf}^\lambda(E_-)=\pi(E_-)$. *One has* $\pi^\lambda(H)=\pi_{Wf}^\lambda(H)=\pi(H)+2f(\lambda)\cdot\mathrm{Id}_{\mathcal{H}},\pi^\lambda(Q_0)=\pi_{Wf}^\lambda(Q_0)=-\frac{3}{16},\pi^\lambda(Q)=\pi_{Wf}^\lambda(Q)=-\frac{1}{16}$. *Two deformations* π_{Wf}^λ *and* $\pi_{Wf'}^\lambda$ *are equivalent if and only if* $f=f'$.

We need the following lemma, which is proved exactly as Lemma (3.8).

Lemma (3.12): Let $C_\pm\in\mathcal{L}(\mathcal{H})$, *we assume that* $[\pi(E_+),C_-]_{\mathcal{L}}-[\pi(E_-),C_+]_{\mathcal{L}}=0$, *and moreover that* $([\pi(E_+),C_-]+[\pi(E_-),C_+])(\mathcal{H}_n)\subset\mathcal{H}_n$; *then there exists* $C\in Z_W^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$ *such that* $C(E_\pm)=C_\pm$.

We can now prove Proposition (3.11). It is clear that π^λ is completely defined from $\tilde{E}_\pm^\lambda=\pi^\lambda(E_\pm)$, which must satisfy $[\tilde{E}_+^\lambda,\tilde{E}_-^\lambda]_{\mathcal{L}}=-\frac{1}{4}$, and $[\tilde{E}_+^\lambda,\tilde{E}_-^\lambda](\mathcal{H}_n)\subset\mathcal{H}_n$. Let $\pi^\lambda=\pi+\lambda C+O(\lambda^2)$; then $C\in Z_W^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$. Therefore, by Proposition (3.10), up to an equivalence, we can assume that $\pi^\lambda=\pi+\gamma_1C_0+O(\lambda^2)$, where C_0 is the cocycle defined in Proposition (3.10), and $\gamma_1\in\mathbb{C}$. So our operators $\tilde{E}_\pm^\lambda$ can be written as $\tilde{E}_+^\lambda=\pi(E_+)+\lambda\gamma_1\pi(E_-)^{-1}+\lambda^2D_++O(\lambda^3)$, and $\tilde{E}_-^\lambda=\pi(E_-)+\lambda^2D_-+O(\lambda^3)$. Now Lemma (3.12) can be applied to $D_\pm$: there exists $D\in Z_W^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))$ such that $D(E_\pm)=D_\pm$; by Proposition (3.10), D is equivalent to a cocycle $\gamma_2C_0,\gamma_2\in\mathbb{C}$, so, by an equivalence of the form $(\mathrm{Id}+\lambda^2T)$, we can assume that $\tilde{E}_+^\lambda=\pi(E_+)$

$+\lambda\gamma_1\pi(E_-)^{-1}+\lambda^2\gamma_2\pi(E_-)^{-1}+\lambda^3 J_+ + O(\lambda^4)$, and $\tilde{E}^\lambda_- = \pi(E_-)+\lambda^3 J_- + O(\lambda^4)$. We can repeat the same argument for $J_\pm$, and so on. Finally, up to an equivalence, we can write $\tilde{E}^\lambda_+ = \pi(E_+) + f(\lambda)\pi(E_-)^{-1}$, and $\tilde{E}^\lambda_- = \pi(E_-)$, so π^λ is equivalent to π^λ_{Wf}. It is easy to check that $\pi^\lambda(H) = \pi^\lambda_{Wf}(H) = \pi(H) + 2f(\lambda)\mathrm{Id}_{\mathcal{H}}$, and since the Weyl structure is preserved, one has $\pi^\lambda(Q_0) = -\frac{3}{16}$ and $\pi^\lambda(Q) = -\frac{1}{16}$. If π^λ_{Wf} and $\pi^\lambda_{Wf'}$ are equivalent, they have the same weight, so $f = f'$. □

[3.4] In this section, we shall compute those deformations of π, considered as a representation of $\mathfrak{g}$, which are still H-diagonal. This overlaps with Secs. [3.2] and [3.3], and we shall now show how the results of these two sections combine to describe the deformations we are dealing with. The cohomology associated with our problem is defined by

$$Z^1_H(\mathfrak{g},\mathcal{L}(\mathcal{H})) = \{C \in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H})) \,|\, C(H)(\mathcal{H}_n)\subset\mathcal{H}_n, \forall n\},$$

$$B^1_H(\mathfrak{g},\mathcal{L}(\mathcal{H})) = B^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}} \text{ (easy to check), and } H^1_H(\mathfrak{g},\mathcal{L}(\mathcal{H})) = Z^1_H/B^1_H.$$

$$\text{Obviously } H^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}} \subset H^1_H(\mathfrak{g},\mathcal{L}(\mathcal{H})) \text{ and } H^1_W(\mathfrak{g},\mathcal{L}(\mathcal{H})) \subset H^1_H(\mathfrak{g},\mathcal{L}(\mathcal{H})).$$

Proposition (3.13): $H^1_H(\mathfrak{g},\mathcal{L}(\mathcal{H})) = H^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}} \oplus H^1_W(\mathfrak{g},\mathcal{L}(\mathcal{H}))$.

Proof: Let $C \in Z^1_H(\mathfrak{g},\mathcal{L}(\mathcal{H}))$. By Lemma (2.1), $C(E_-)(\mathcal{H}_n)\subset\mathcal{H}_{n+1}$, so, up to a coboundary, we can assume that $C(E_-)=0$. Exactly as in the proof of Proposition (3.6) we now obtain $C([E_+,E_-]_{\mathcal{L}})_{|\mathcal{H}_d} = 2(\alpha_d-\alpha)\mathrm{Id}_{\mathcal{H}_d}, \alpha_d, \alpha \in \mathbb{C}$. Since E_- anticommutes with $(\frac{1}{4}+[E_+,E_-]_{\mathcal{L}})$, we deduce $E_- C([E_+,E_-]_{\mathcal{L}}) = -C([E_+,E_-]_{\mathcal{L}})E_-$, and thus $\alpha_1^- - \alpha = -(\alpha_0^- - \alpha)$. If we write $C(H)z^n = h_n \cdot z^n$, from $[H,E_-] = -\frac{1}{2}E_-$, we deduce $[C(H),E_-]=0$, and then $h_{n+1}=h_n, \forall n$, so $C(H)z^n = h\cdot z^n$. Since $H=[E_+,E_-]$, we obtain $[C(E_+),E_-] = h\cdot\mathrm{Id}$ and so $C([E_+,E_-]_{\mathcal{L}}) = [C(E_+),E_-]_{\mathcal{L}} = 2(\alpha_0^- - \alpha)\cdot P$, hence $C(E_+)E_- = (h/2)\mathrm{Id} + (\alpha_0^- - \alpha)\cdot P$. We conclude that $C(E_+) = (a\mathrm{Id}+bP)\cdot E_-^{-1}, C(E_-)=0$. Now if C_1 and C_2 are defined by $C_1(E_-)=C_2(E_-)=0$ and $C_1(E_+)=E_-^{-1}, C_2(E_+)=P\cdot E_-^{-1}$, then by Propositions (3.6) and (3.10), $C_1 \in Z^1_W(\mathfrak{g},\mathcal{L}(\mathcal{H}))$, $C_2 \in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}$, so we have proved that $H^1_H = H^{1\mathfrak{h}} + H^1_W$. But if C belongs to their intersection, we pick a representative of the cohomology class satisfying $C(E_+) = cE_-^{-1}$, $c\in\mathbb{C}$, $C(E_-)=0$ [Proposition (3.10)]: then $C(H) = 2c\mathrm{Id}$, but since the class is in $H^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}$, one has $c=0$, and thus $C=0$. □

We now construct deformations of π corresponding to the cocycles of Proposition (3.13). Define $E^\lambda_+ = \pi(E_+) + (f(\lambda)+g(\lambda)P)\pi(E_-)^{-1}$ and $E^\lambda_- = \pi(E_-)$ for $f,\ g \in \mathbb{C}[[\lambda]]$ with $f(0) = g(0) = 0$. Then $[E^\lambda_+, E^\lambda_-] = -\frac{1}{4} + 2g(\lambda)P$ and $[E^\lambda_+, E^\lambda_-] = \pi(H) + 2f(\lambda)$. Since P anticommutes with $\pi(E_\pm)$, there exists a deformation $\tilde{\pi}^\lambda_{f,g}$ of π such that $\tilde{\pi}^\lambda_{f,g}(E_\pm) = E^\lambda_\pm$ and we have $\tilde{\pi}^\lambda_{f,g}(H) = \pi(H) + 2f(\lambda)$, so H is still diagonal, with translated eigenvalues. One finds $\tilde{\pi}^\lambda_{f,g}(Q_0) = -\frac{3}{16} + g(\lambda)P + 4g(\lambda)^2$, and $\tilde{\pi}^\lambda_{f,g}(Q) = -\frac{1}{16} + 4g(\lambda)^2$. In particular, when $f=0$, $\tilde{\pi}_{0,g} = \pi^\lambda_g$, and when $g=0$, $\tilde{\pi}_{f,0} = \pi^\lambda_{Wf}$, we recover the deformations obtained in Secs. [3.2] and [3.3]. The proof of the next result is so similar to the proofs of Propositions (3.7) or (3.11) that we shall not repeat the arguments.

Proposition (3.14): Let π^λ be a deformation of a representation π of $\mathfrak{g}$; we assume that $\pi^\lambda(H)$ is still diagonal on $\oplus_{n\in\mathbb{Z}}\mathcal{H}_n$. Then there exist $f, g \in \mathbb{C}[[\lambda]]$ with $f(0)=g(0)=0$ such that π^λ is equivalent to $\tilde{\pi}^\lambda_{f,g}$. One has $\pi^\lambda(H) = \pi(H) + f(\lambda)$, $\pi^\lambda(Q_0) = -\frac{3}{16} + g(\lambda)P + 4g(\lambda)^2$, and $\pi^\lambda(Q) = -\frac{1}{16} + 4g(\lambda)^2$. Given a second deformation π'^λ, of the same type, with associated f' and g', then $\pi^\lambda \simeq \pi'^\lambda$ if and only if $f=f'$, and $g=g'$.

Remark (3.15): Given two functions $f(\lambda)$, and $g(\lambda)$, analytic for $|\lambda|<R$, such that $f(0) = g(0) = 0$, let us consider $\pi^\lambda = \tilde{\pi}^\lambda_{f,g|_{\mathfrak{g}_0^-}}$; it can be checked easily that the integrability conditions of (Ref. 6, Proposition 9) are satisfied, so π^λ is the differential of a deformation U^λ of U, as representations of the universal covering $\tilde{\mathbf{G}}$ of $\mathbf{G} = SU(1,1)$.

Remark (3.16): Define $\Delta_\pm$ by $\Delta_\pm(h)=1/z(h(z)\pm h(-z))$. Then $E^\lambda_+=\pi(E_+)+(f(\lambda)+g(\lambda)P)\pi(E_-)^{-1}=\frac{1}{2}(d/dz)-(f(\lambda)-g(\lambda))\Delta_+-(f(\lambda)+g(\lambda))\Delta_-$. Since $\Delta_{\pm|_{\mathcal{H}^{\bar{1}}_0}}=0$, this expression can be useful to solve the equation $E^\lambda_+(h)=0$.

Take for instance $f-g=\alpha\lambda$, $f+g=\beta\lambda$, $\alpha, \beta\in\mathbb{C}$. We obtain a family of representations of $\mathfrak{g}$ and it is easy to check that all $\mathfrak{h}$-diagonal modules appear, either directly, or as subquotients of that family (see Ref. 5 for the classification of such modules), by solving the equation $E^\lambda_+(h)=0$.

We shall give some details in the special case $\alpha=0$ and $\beta=1$, denoting by π^λ the corresponding representations. One has $\pi^\lambda(E_+)=\frac{1}{2}(d/dz)-\lambda\Delta_-$, $\pi^\lambda(E_-)=-\frac{1}{2}z$, $\pi^\lambda(H)=-\frac{1}{2}z(d/dz)-\frac{1}{4}+\lambda$, $\pi^\lambda(\theta)=\lambda P$, and $\pi^\lambda(Q)=\lambda^2-\frac{1}{16}$. Note that $\pi^\lambda(g)(\mathcal{H}_+)\subset\mathcal{H}_+$. Let $\rho^\lambda=\pi^\lambda_{|\mathcal{H}^+}$, and V_μ, $\mu\in\mathbb{C}$, be the $\mathfrak{g}$-Verma module with dominant weight μ. Then $\rho^\lambda\simeq V_{\lambda-1/4}$, so ρ^λ provides an explicit construction of all Verma modules, as a deformation of $\rho^0=V_{-1/4}$, which is the metaplectic representation.

There is an interesting direct consequence. First we recall some results of Ref. 8. The minimal primitive ideals of $\mathcal{U}=\mathcal{U}(\mathfrak{g})$ were determined in Ref. 8; they are the ideals $I_\nu=\mathcal{U}(Q-\nu)$, for $\nu\neq-\frac{1}{16}$, and the singular ideal $I=\mathcal{U}\theta$ (which is not generated by its intersection with the center of $\mathcal{U}$). The corresponding primitive quotients are the algebras $\mathcal{B}_\nu=\mathcal{U}/I_\nu$, $\nu\neq-\frac{1}{16}$, and, in the singular case, the Weyl algebra $W_1=\mathcal{U}/I$. Now ρ^λ is a faithful representation of $\mathcal{B}_{\lambda^2-1/16}$, $\lambda\neq0$, and ρ^0 is a faithful representation of the Weyl algebra. This is useful when $\lambda\neq0$, because one can deduce a very explicit description of the algebra $\mathcal{B}_{\lambda^2-1/16}$ as the algebra generated by the two operators $\rho^\lambda(E_+)=\frac{1}{2}(d/dz)-\lambda\Delta_-$ and $\rho^\lambda(E_-)=-\frac{1}{2}z$, acting on $\mathcal{H}_+=\mathbb{C}[z]$. As a consequence, $\mathcal{B}_{\lambda^2-1/16}$ can be described by generators and relations as the algebra generated by three elements $E^\lambda_\pm$ and P satisfying $[E^\lambda_+,E^\lambda_-]=-\frac{1}{4}+\lambda P$, $E_\pm P=-PE_\pm$, and $P^2=\mathrm{Id}$. When $\lambda=0$, these relations define an algebra which is an extension of the Weyl algebra by a parity and was introduced in Ref. 9, where it was shown that it is a quasi-simple and primitive algebra. It is not a quotient of the enveloping algebra of $\mathfrak{osp}(1,2)$, but rather a quotient of the enveloping algebra of $\mathfrak{sl}(2,1)$ (see Ref. 9).

Remark (3.17): For the metaplectic representation itself, i.e. $\pi_{|\mathcal{H}^+}$, one can define a cocycle $C\in Z^1_H(\mathfrak{g},\mathcal{L}(\mathcal{H}^+))$ by $C(E_+)=\Delta_-$, and $C(E_-)=0$. It is not difficult to prove [adapting the proof of Proposition (3.13)], that $H^1_H(\mathfrak{g},\mathcal{L}(\mathcal{H}^+))=\mathbb{C}\cdot C$, and $H^1(\mathfrak{g},\mathcal{L}(\mathcal{H}^+))^{\mathfrak{h}}=\{0\}$.

IV. DEFORMATIONS OF THE EXTENDED METAPLECTIC REPRESENTATION OF $\mathfrak{g}=\mathfrak{osp}(1,4)$

Throughout this section, $\mathfrak{g}$ is the Lie superalgebra $\mathfrak{osp}(1,4)$.

[4.1] Let us briefly recall some well-known facts about $\mathfrak{g}$ and the corresponding Weyl algebra W_2. The latter is the algebra generated by $E_\pm$, $E'_\pm$ with relations $[E_+,E_-]_\mathcal{L}=[E'_+,E'_-]_\mathcal{L}=-\frac{1}{4}$, $[E_\pm,E'_\pm]_\mathcal{L}=0$. The extended metaplectic representation π of W_2 is defined on $\mathcal{H}=\mathbb{C}[z,z',z^{-1},z'^{-1}]$ by $\pi(E_+)=\frac{1}{2}(\partial/\partial z)$, $\pi(E_-)=-\frac{1}{2}z$, $\pi(E'_+)=\frac{1}{2}(\partial/\partial z')$, $\pi(E'_-)=-\frac{1}{2}z'$.

It is a Schur-irreducible representation built from irreducible subquotients, which is obtained as follows: let $\mathcal{H}_{++}=\mathrm{span}\{z^n,z'^{n'},n,n'\geqslant0\}$, $\mathcal{H}_{-+}=\mathrm{span}\{z^{-n}z'^{n'},n>0,n'\geqslant0\}$, $\mathcal{H}_{+-}=\mathrm{span}\{z^nz'^{-n'},n\geqslant0,n'>0\}$, and $\mathcal{H}_{--}=\mathrm{span}\{z^{-n},z'^{-n'},n,n'>0\}$. Then $\mathcal{H}_{++}$, $\mathcal{H}_{-+}\oplus\mathcal{H}_{++}$, $\mathcal{H}_{+-}\oplus\mathcal{H}_{++}$, $\mathcal{H}_{-+}\oplus\mathcal{H}_{++}\oplus\mathcal{H}_{+-}$ are submodules. $\mathcal{H}_{++}$ is irreducible, and isomorphic with the metaplectic representation, the quotients $(\mathcal{H}_{-+}\oplus\mathcal{H}_{++})/\mathcal{H}_{++}$ and $(\mathcal{H}_{+-}\oplus\mathcal{H}_{++})/\mathcal{H}_{++}$ are irreducible, and so does the quotient $\mathcal{H}/(\mathcal{H}_{-+}\oplus\mathcal{H}_{++}\oplus\mathcal{H}_{+-})$, which is isomorphic with the contragedient to the metaplectic representation. All the extensions involved are nontrivial. So the extended metaplectic representation is, by definition, a triplet.

Now, we introduce $\mathfrak{g}=\mathfrak{osp}(1,4)$ as the sub-Lie superalgebra of W_2, generated, as a Lie superalgebra, by $\{E_\pm,E'_\pm\}$; one has $\mathfrak{g}=\mathfrak{g}_{\bar{0}}\oplus\mathfrak{g}_{\bar{1}}$, where $\mathfrak{g}_{\bar{1}}=\mathrm{span}\{E_\pm,E'_\pm\}$, and $\mathfrak{g}_{\bar{0}}=[\mathfrak{g}_{\bar{1}},\mathfrak{g}_{\bar{1}}]$. $\mathfrak{g}_{\bar{0}}$ acts on $\mathfrak{g}_{\bar{1}}$ by the adjoint action ad, and the form defined on $\mathfrak{g}_{\bar{1}}$ by $\langle X|Y\rangle=[X,Y]_\mathcal{L}$ is invariant. It is easy to see that ad is an isomorphism from $\mathfrak{g}_{\bar{0}}$ onto $\mathfrak{sp}(4)$. Let $\mathcal{U}(\mathfrak{g})$ be the enveloping algebra of $\mathfrak{g}$. The preceding construction shows that W_2 is a quotient of $\mathcal{U}(\mathfrak{g})$. Note that $\mathfrak{g}\subset W_2$, and also $\mathfrak{g}\subset\mathcal{U}(\mathfrak{g})$, which may lead to some misunderstanding if these inclusions are not properly inter-

preted: For instance E_+ and E'_+ commute when realized as elements of W_2, but do not commute when realized as elements of $\mathcal{U}(\mathfrak{g})$! Since W_2 is a quotient of $\mathcal{U}(\mathfrak{g})$, π is also a representation of $\mathcal{U}(\mathfrak{g})$. It has some interesting properties.

First, let $\rho=\pi_{|\mathfrak{g}_0^-}$ and $\rho^+=\rho_{|\mathcal{H}_{++}}$. Then ρ^+ decomposes, under parity, into $\rho^+=\rho_0^+\oplus\rho_1^+$, and one has: $\rho_0^+\simeq \mathrm{Rac}=D(\frac{1}{2},0)$, $\rho_1^+\simeq Di=D(1,\frac{1}{2})$, the two singleton representations (see Ref. 3, and also Refs. 1, 2) which appear in the usual metaplectic representation. Second, let $\mathfrak{l}$ (resp $\mathfrak{l}'$) be the sub-Lie superalgebra of $\mathfrak{g}$ with basis $E_\pm$, $H=[E_+,E_-]$, $F=[E_+,E_+]$, and $G=-[E_-,E_-]$ (resp., $E'_\pm$, $H'=[E'_+,E'_-]$, $F'=[E'_+,E'_+]$, and $G'=-[E'_-,E'_-]$). Then $\mathfrak{l}$ and $\mathfrak{l}'$ are isomorphic to $\mathfrak{osp}(1,2)$. Let $V_{n'}$ (resp., V'_n) be the subspace of $\mathcal{H}$ with basis $\{z^n\cdot z'^{n'}, n\in\mathbb{Z}\}$ (resp., $\{z^n\cdot z'^{n'}, n'\in\mathbb{Z}\}$), then $V_{n'}$ is stable under $\pi_{|\mathfrak{l}}$ (resp., V'_n is stable under $\pi_{|\mathfrak{l}'}$), and $\pi_{|\mathfrak{l}}$ (resp., $\pi_{|\mathfrak{l}'}$) acting on $V_{n'}$ (resp., V'_n) is isomorphic to the extended metaplectic representation. Obviously, $\mathcal{H}=\oplus_{n'\in\mathbb{Z}}V_{n'}=\oplus_{n\in\mathbb{Z}}V'_n$. Third, define $Z_+=-2[E'_+,E_-]$, $Z_-=-2[E_+,E'_-]$, $T=\frac{1}{2}[Z_+,Z_-]=-[E_+,E_-]+[E'_+,E'_-]$, $U=-([E_+,E_-]+[E'_+,E'_-])$. Then $\mathfrak{h}=\mathbb{C}T\oplus\mathbb{C}U=\mathbb{C}H\oplus\mathbb{C}H'$ is a Cartan subalgebra of $\mathfrak{g}$, and the subalgebra $\mathfrak{k}$ with basis $\{Z_\pm,T,U\}$ is isomorphic to $\mathfrak{sl}(2)\oplus\mathbb{C}$. One has

$$\pi(Z_+)=z\frac{\partial}{\partial z'},\quad \pi(Z_-)=z'\frac{\partial}{\partial z},\quad \pi(T)=\frac{1}{2}\left(z\frac{\partial}{\partial z}-z'\frac{\partial}{\partial z'}\right),\quad \pi(U)=\frac{1}{2}\left(z\frac{\partial}{\partial z}+z'\frac{\partial}{\partial z'}+1\right).$$

Now the subspace Ξ_r of $\mathcal{H}$ with basis $\{z^n,z'^{n'}, n+n'=r\}$ is stable under $\pi_{|\mathfrak{k}}$, and when acting on Ξ_r, $\pi_{|\mathfrak{k}}$ is an extension of a finite dimensional representation by two (up and down) representations. Obviously, $\mathcal{H}=\oplus_{r\in\mathbb{Z}}\Xi_r$, and $\mathcal{H}_{++}$ is the space of $\mathfrak{k}$-finite vectors of $\mathcal{H}$.

[4.2] Consider deformations of π which preserve the Weyl structure, and which are still $\mathfrak{h}$-diagonal on $\oplus_{n,n'\in\mathbb{Z}}\mathcal{H}_{n,n'}$, $\mathcal{H}_{n,n'}=\mathbb{C}z^nz'^{n'}$. The corresponding cohomology is $Z^1_W(\mathfrak{g},\mathcal{L}(\mathcal{H}))=\{C\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))|C(\mathfrak{h})\mathcal{H}_{n,n'}\subset\mathcal{H}_{n,n'}$ and $C([E_\pm,E'_\pm]_\mathcal{L})=C([E_+,E_-]_\mathcal{L})=C([E'_+,E'_-]_\mathcal{L})=0\}$, $B^1_W(\mathfrak{g},\mathcal{L}(\mathcal{H}))=B^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^\mathfrak{h}$ (easy to check), and $H^1_W(\mathfrak{g},\mathcal{L}(\mathcal{H}))=Z^1_W/B^1_W$.

Proposition (4.1): $\dim H^1_W(\mathfrak{g},\mathcal{L}(\mathcal{H}))=2$. *Any cocyle is equivalent to a cocycle defined, for* $\alpha,\beta\in\mathbb{C}$, *by* $C(E_-)=C(E'_-)=0$, $C(E_+)=\alpha\pi(E_-)^{-1}$, $C(E'_+)=\beta\pi(E'_-)^{-1}$, *and one has* $C(H)=2\alpha\,\mathrm{Id}_\mathcal{H}$, $C(H')=2\beta\,\mathrm{Id}_\mathcal{H}$.

Proof: Let $C\in Z^1_W(\mathfrak{g},\mathcal{L}(\mathcal{H}))$. By Lemma (2.1), $C(E_-)(\mathcal{H}_{n,n'})\subset\mathcal{H}_{n+1,n'}$, so up to a coboundary, we can assume that $C(E_-)=0$. Then $C(E'_-)(\mathcal{H}_{n,n'})\subset\mathcal{H}_{n,n'+1}$, and $C([E_-,E'_-]_\mathcal{L})=0$ leads to $[E_-,C(E'_-)]_\mathcal{L}=0$. Therefore $C(E'_-)z^nz'^{n'}=c_{n'}z^nz'^{n'+1}$, $\forall n$, n', $c_{n'}\in\mathbb{C}$, so there exists T such that $Tz^nz'^{n'}=t_{n'}z^nz'^{n'}$, and $C(E'_-)=[\pi(E'_-),T]$. But $[\pi(E_-),T]=0$, so, up to a coboundary, we can assume that $C(E_-)=C(E'_-)=0$. Since $C(\mathfrak{l})(V_{n'})\subset V_{n'}$, and $C(\mathfrak{l}')(V'_n)\subset V'_n$, $\forall n$, n', Proposition (3.10) gives $C(E_+)_{|V_{n'}}=c_{n'}\pi(E_-)^{-1}_{|V_{n'}}$ and $C(E'_+)_{|V_{n'}}=c'_n\pi(E'_-)^{-1}_{|V_{n'}}$, with $c_{n'}$, $c'_n\in\mathbb{C}$. In the Weyl algebra, one has $[E_+,E'_-]_\mathcal{L}=[E'_+,E_-]_\mathcal{L}=0$, so $[\pi(E'_-),C(E_+)]_\mathcal{L}=[\pi(E_-),C(E'_+)]_\mathcal{L}=0$. Acting on $z^nz'^{n'}$ we obtain $c_{n'}=c_{n'+1}$, and $c'_n=c'_{n+1}$, $\forall n$, n', so $C(E_+)=\alpha\pi(E_-)^{-1}$, $\alpha\in\mathbb{C}$, and $C(E'_+)=\beta\pi(E'_-)^{-1}$, $\beta\in\mathbb{C}$. To check that such a cocycle does exist, define $E^\lambda_+=\pi(E_+)+\lambda\alpha\pi(E_-)^{-1}$, $E^\lambda_-=\pi(E_-)$, $E'^\lambda_+=\pi(E'_+)+\lambda\beta\pi(E'_-)^{-1}$, and $E'^\lambda_-=\pi(E'_-)$. Then $[E^\lambda_+,E^\lambda_-]=-\frac{1}{4}$, $[E'^\lambda_+,E'^\lambda_-]=-\frac{1}{4}$, $[E^\lambda_\pm,E'^\lambda_\pm]=0$, so there exists a formal representation π^λ of the Weyl algebra such that $\pi^\lambda(E_\pm)=E^\lambda_\pm$, $\pi^\lambda(E'_\pm)=E'^\lambda_\pm$. Since the Weyl algebra is a quotient of $\mathcal{U}(\mathfrak{osp}(1,4))$, π^λ is a representation of $\mathfrak{g}$, and clearly a deformation of π. Writing $\pi^\lambda=\pi+\lambda C+\cdots$, we obtain the wanted cocycle. It cannot be a coboundary if α, or $\beta\neq0$ [see, e.g., Proposition (3.10)]. □

Exactly as at the end of the proof of Proposition (4.1), given $f,g\in\mathbb{C}[[\lambda]]$ with $f(0)=g(0)=0$, we can define a deformation of π by

$$\pi^\lambda_{f,g}(E^\lambda_+)=\pi(E_+)+f(\lambda)\pi(E_-)^{-1},\quad \pi^\lambda_{f,g}(E'_+)=\pi(E'_+)+g(\lambda)\pi(E'_-)^{-1},$$

$$\pi^\lambda_{f,g}(E_-)=\pi(E_-),\quad \pi^\lambda_{f,g}(E'_-)=\pi(E'_-).$$

One has $\pi^{\lambda}_{f,g}(H)=\pi(H)+2f(\lambda)\mathrm{Id}_{\mathcal{H}}$, and $\pi^{\lambda}_{f,g}(H')=\pi(H')+2g(\lambda)\mathrm{Id}_{\mathcal{H}}$. By Proposition (3.10), two such deformations are equivalent if and only if the associated formal series are the same. By a proof completely similar to that of Proposition (3.11), we obtain the following.

Proposition (4.2): Let π^{λ} be a deformation of π such that the Weyl structure is preserved, and $\mathfrak{h}$ is still diagonal on $\oplus_{n,n'\in Z}\mathcal{H}_{n,n'}$. Then π^{λ} is equivalent to some $\pi^{\lambda}_{f,g}$.

Remark (4.3): It is straightforward to compute the submodules of the representation $\pi^{\lambda}=\pi^{\lambda}_{f,g}$, e.g., when $f=\lambda\alpha$, $g=\lambda$, $\alpha\in\mathbb{C}$: it is enough to solve $\pi^{\lambda}(E_+)(h)=\pi^{\lambda}(E_-)(h)=0$. We shall not detail the complete results, but indicate only that, generically, π^{λ} is irreducible, and does not belong to the classes of irreducible classified up to now. In degenerate cases, π^{λ} is an extension of two irreducible representations, which are also new, and in the most degenerate cases, π^{λ} is isomorphic to the extended metaplectic representation, i.e., the representation with which we started

[4.3] We now turn to the more general problem of deformation which are still $\mathfrak{h}$-diagonal [as was done in Sec. [3.4] for $\mathfrak{osp}(1,2)$]. A subproblem is the case of deformations with unchanged weight structure. The corresponding cohomologies are defined by

$$Z^1_{\mathfrak{h}}(\mathfrak{g},\mathcal{L}(\mathcal{H}))=\{C\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))\,|\,C(\mathfrak{h})(\mathcal{H}_{n,n'})\subset\mathcal{H}_{n,n'}\},\quad \mathcal{H}_{n,n'}=\mathbb{C}z^n z'^{n'},$$

$$Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}=\{C\in Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))\,|\,C(\mathfrak{h})=0\},\quad B^1_{\mathfrak{h}}(\mathfrak{g},\mathcal{L}(\mathcal{H}))=B^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}},$$

$$H^1_{\mathfrak{h}}(\mathfrak{g},\mathcal{L}(\mathcal{H}))=Z^1_{\mathfrak{h}}(\mathfrak{g},\mathcal{L}(\mathcal{H}))/B^1_{\mathfrak{h}}(\mathfrak{g},\mathcal{L}(\mathcal{H})),$$

and

$$H^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}=Z^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}/B^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}.$$

It is clear that $H^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}$ and $H^1_W(\mathfrak{g},\mathcal{L}(\mathcal{H}))$ are contained in $H^1_{\mathfrak{h}}(\mathfrak{g},\mathcal{L}(\mathcal{H}))$. In the case of $\mathfrak{osp}(1,2)$, the last one was the direct sum of the first two, both of them being one dimensional and we constructed interesting deformations, with modified Casimir values [see, e.g., Propositions (3.13), (3.14) and Remark (3.16)]. The situation is very different here, for $\mathfrak{g}=\mathfrak{osp}(1,4)$, as shown by the next result.

Theorem (4.4): *$H^1(\mathfrak{g},\mathcal{L}(\mathcal{H}))^{\mathfrak{h}}=\{0\}$, and $H^1_{\mathfrak{h}}(\mathfrak{g},\mathcal{L}(\mathcal{H}))=H^1_W(\mathfrak{g},\mathcal{L}(\mathcal{H}))$.*

Remark (4.5): Theorem (4.4) shows that all deformations with unchanged weight structure are trivial. First order $\mathfrak{h}$-diagonal deformations are representations of the Weyl algebra, and there is no analog to the representations constructed in Remark (3.16).

Proof of Theorem (4.4): Starting with $C\in Z^1_{\mathfrak{h}}(\mathfrak{g},\mathcal{L}(\mathcal{H}))$, one has $C(E_-)(\mathcal{H}_{n,n'})\subset\mathcal{H}_{n+1,n'}$ by Lemma(2.1). So, up to a coboundary, we can assume that $C(E_-)=0$. We shall now prove that we can also assume, by a good choice of the coboundary, that $C(E'_-)=0$.

First, since $C(G')(\mathcal{H}_{n,n'})\subset\mathcal{H}_{n,n'+2}$, and $[E_-,G']=0$, so that $[E_-,C(G')]=0$, we can assume, up to a coboundary, that $C(G')=0$. Let $C(E'_-)z^n z'^{n'}=c_{n,n'}z^n z'^{n'+1}$. From $[G,E'_-]=0$, so that $[G,C(E'_-)]=0$, we deduce $c_{2p,n'}=c_{0,n'}$, and $c_{2p+1,n'}=c_{1,n'}$, so we can write $C(E'_-)z^{2p}z'^{n'}=c_{n'}z^{2p}z'^{n'+1}$, and $C(E'_-)z^{2p+1}z'^{n'}=d_{n'}z^{2p+1}z'^{n'+1}$. Now $[E'_-,E'_-]=-G'$, so that $[E'_-,C(E'_-)]=0$ and we get $c_{n'}=(-1)^{n'}c_0$, and $d_{n'}=(-1)^{n'}d_0$. Define T by $T(z^n z'^{n'})=z^n z'^{n'}$, if n' is even, and 0 if n' is odd. The coboundary $D=[\cdot,T]$ satisfies $D(E_-)=0$, and $D(E'_-)(z^n z'^{n'})=((-1)^{n'+1}/2)z^n z'^{n'+1}$. So the cocycle $\tilde{C}=C+2c_0D$ satisfies $\tilde{C}(E_-)=0$, $\tilde{C}(E'_-)z^n z'^{n'}=0$, if n is even, and $\tilde{C}(E'_-)z^n z'^{n'}=(d_0-c_0)(-1)^{n'}z^n z'^{n'+1}$, if n is odd. Let $d=d_0-c_0$.

It is clear that $\tilde{C}(\mathfrak{l}')(V'_n)\subset V'_n$, and, as a cocycle of $\mathfrak{l}'=\mathfrak{osp}(1,2)$, $\tilde{C}$ belongs to $Z^1_H(\mathfrak{l}',\mathcal{L}(V'_n))$, and V'_n is the extended metaplectic representation, so Proposition (3.13) can be applied. There are two cases: since $\tilde{C}(E'_-)=0$ on V'_{2p}, one has $\tilde{C}(E'_+)z^{2p}z'^{n'}=(\beta_{2p}+(-1)^{n'-1}\gamma_{2p})z^{2p}z'^{n'-1}$. But we can also use the cocycle $\hat{C}=C+2d_0D$, with $\hat{C}(E'_-)$ vanishing on V'_{2p+1}, to deduce

$$\tilde{C}(E'_+)z^{2p+1}z'^{n'}=(\hat{C}-2dD)(E'_+)z^{2p+1}z'^{n'}$$
$$=(\beta_{2p+1}+(-1)^{n'-1}\gamma_{2p+1}-(-1)^{n'}dn')z^{2p+1}z'^{n'-1}.$$

Now we use $[[E_-,E'_+],E'_-]=\frac{1}{2}E_-$, so that $[[E_-,E'_+],\tilde{C}(E'_-)]-[E'_-,\tilde{C}([E_-,E'_+])]=0$. Note that $\tilde{C}([E_-,E'_+])=[E_-,\tilde{C}(E'_+)]$. By a straightforward computation, acting on $z^{2p}z'^{n'}$, and then on $z^{2p+1}z'^{n'}$, we deduce $d=-2(\gamma_{2p}+\gamma_{2p+1})=2(\gamma_{2p+1}+\gamma_{2p+2})$, so that $\gamma_n=(-1)^n\,[\gamma_0+nd/2]$.

In order to decompose $\tilde{C}$ into $Z^{1\mathfrak{h}}+Z^1_W$ we have to evaluate $\tilde{C}(H')=[\tilde{C}(E'_+),E'_-]$ and $\tilde{C}(H)=[\tilde{C}(E_+),E_-]$. Acting on $z^{2p}z'^{n'}$ and $z^{2p+1}z'^{n'}$ we get $\tilde{C}(H')z^nz'^{n'}=-\beta_nz^nz'^{n'}$. Again Proposition (3.13) can be applied to $\tilde{C}_{|\mathfrak{l}}$ considered as an element of $Z^1_H(\mathfrak{l},\mathcal{L}(V_{n'}))$, so $\tilde{C}(E_+)z^nz'^{n'}=(\alpha_{n'}+(-1)^{n-1}\delta_{n'})z^{n-1}z'^{n'}(\alpha_{n'},\delta_{n'}\in\mathbb{C})$. Hence $\tilde{C}(H)z^nz'^{n'}=-\alpha_{n'}z^nz'^{n'}$. Since $[H,E'_-]=[H',E_-]=0$, we obtain $\alpha_{n'}=\alpha$ and $\beta_n=\beta(\alpha,\beta\in\mathbb{C})$ for every n, n'. Therefore $\tilde{C}$ can be written as the sum of a cocycle D in Z^1_W [according to Proposition (4.1)] and of $C_1=\tilde{C}-D$ in $Z^{1\mathfrak{h}}$, D being defined by $D(E_+)z^nz'^{n'}=\alpha z^{n-1}z'^{n'}$, $D(E'_+)z^nz'^{n'}=\beta z^nz'^{n'-1}$ and $D(E_-)=D(E'_-)=0$.

There remains to show that $\tilde{C}-D=0$ in order to prove $H^1_{\mathfrak{h}}=H^1_W$ and thus $H^{1\mathfrak{h}}=\{0\}$. Exactly as for (γ_n), using the relation $[[E'_-,E_+],E_-]=-\frac{1}{2}E'_-$, we have $d=2(-1)^{n'}(\delta_{n'}+\delta_{n'+1})$ and so $\delta_{n'}=(-1)^{n'}\,[\delta_0-n'(d/2)]$. Lengthy but straightforward calculations yield

$$C_1([E_+,E'_+])z^nz'^{n'}=-\tfrac{1}{2}[(-1)^nn'(\delta_{n'}+\delta_{n'-1})+(-1)^{n'}n(\gamma_n+\gamma_{n-1})$$
$$+(-1)^nnn'd]z^{n-1}z'^{n'}.$$

Since $[[E_+,E'_+],E_+]=0$, one has $[[E_+,E'_+],C_1(E_+)]-[E_+,C_1([E_+,E'_+])]=0$, so that $2\delta_0+d(n^2-2n+\frac{1}{2})=0$. Therefore $d=\delta_0=0$ and C_1 satisfies $C_1(E_-)=C_1(E'_-)=C_1(E_+)=0$ and $C_1(E'_+)z^nz'^{n'}=(-1)^{n+n'}\gamma z^nz'^{n'-1}$. Then $C_1([E_+,E'_+])=0$ and from $[[E_+,E'_+],[E_+,E'_-]]=-\frac{1}{2}[E'_+,E'_+]$ it follows that $C_1([E'_+,E'_+])=0$. So (acting on $z^nz'^{n'}$) $\gamma=0$. Thus $C_1=0$. □

Remark (4.6): The preceding results suggest that the metaplectic representation $\rho=\pi_{|\mathcal{H}_{++}}$ is rigid (in the category of $\mathfrak{h}$-diagonal deformations). This is indeed the case.

Theorem (4.7): $H^1_{\mathfrak{h}}(\mathfrak{g},\mathcal{L}(\mathcal{H}_{++}))=\{0\}$.

Proof: We start with $C\in Z^1_{\mathfrak{h}}(\mathfrak{g},\mathcal{L}(\mathcal{H}_{++}))$, following (with the same notations) the proof of Theorem (4.4), we can suppose, up to a coboundary, that C satisfies, $C(E_-)=0$, $C(E'_-)z^{2p}z'^{n'}=0$, $C(E'_-)z^{2p+1}z'^{n'}=(-1)^{n'}dz^{2p+1}z'^{n'+1}$ with $d\in\mathbb{C}$. Denoting by V'^{+}_n the subspace $V'_n\cap\mathcal{H}_{++}$, one has $C_{|\mathfrak{l}'}\in Z^1_H(\mathfrak{l}',\mathcal{L}(V'^{+}_n))$. Using Remark (3.17), $C(E'_+)$ on V'^{+}_n is given by $C(E'_+)z^{2p}z'^{n'}=\beta_{2p}(1+(-1)^{n'-1})z^{2p}z'^{n'-1}$ and $C(E'_+)z^{2p+1}z'^{n'}=[\beta_{2p+1}(1+(-1)^{n'-1})-dn'(-1)^{n'}]z^{2p+1}z'^{n'-1}$ if $n'\geqslant 1$ [$C(E'_+)z^nz'^{n'}$ vanishes if $n'=0$]. Considering $C_{|\mathfrak{l}}$ as an element of $Z^1_H(\mathfrak{l},\mathcal{L}(V^+_{n'}))$, we have $C(E_+)z^nz'^{n'}=\alpha_{n'}(1+(-1)^{n-1})z^{n-1}z'^{n'}$, if $n\geqslant 1$, and $C(E_+)z^nz'^{n'}=0$ if $n=0$. Again [see the proof of Theorem (4.4)] we have $\beta_n=(-1)^n\,[\beta_0+n(d/2)]$; since $[E_-,H']=0$ and $[E'_-,H]=0$, we have $\beta_n=\beta$ and $\alpha_{n'}=\alpha(\alpha,\beta\in\mathbb{C})$ for every n, $n'\in\mathbb{N}$, so that $\beta=d=0$. Now from the relation $[[E'_-,E_+],E_-]=-\frac{1}{2}E'_-$, acting on $z^nz'^{n'}$ with n even, we get, $\alpha=(-1)^{n'+1}(d/4)$, so $\alpha=0$. □

Remark (4.8): Theorems (4.4) and (4.7) are valid for $\mathfrak{osp}(1,2n)$, $n\geqslant 2$. The proofs are obtained by induction and the application of arguments completely similar to (and even simpler than) the arguments for $\mathfrak{osp}(1,4)$.

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On the concentration of the spectrum of integral-difference collision operator with Gaussian equilibrium distribution function in a vicinity of zero

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We study integral-difference collision operators with a truncated Gaussian equilibrium distribution function. We prove that the number of eigenvalues in an arbitrary small vicinity of zero goes to infinity when the truncation parameter goes to infinity. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1354643]

I. INTRODUCTION

We continue the study[1–3] of operators of the form

$$\mathcal{K}_\varphi : u(x) \mapsto \int_{-\infty}^{\infty} \frac{u(x)\varphi(s) - u(s)\varphi(x)}{|x-s|}\, ds, \tag{1}$$

acting originally in the Hilbert space $L_2(\mathbf{R}, dx)$. Here $\varphi(x)$ is the so-called equilibrium distribution function, having the following properties induced by its physical nature as a probability distribution:

$$\varphi(x) \geqslant 0; \quad \int_{-\infty}^{\infty} \varphi(x)\, dx = 1.$$

Such operators appear as collision operators in nonequilibrium statistical physics models.[4,5] In our previous papers[1–3] we have investigated spectral properties of operators $\mathcal{K}_\varphi$ under some additional conditions on function $\varphi(x)$. In particular, in the case when $\varphi(x)$ has compact support, the spectral analysis of the operator $\mathcal{K}_\varphi$ may be essentially reduced to the spectral analysis of the operator,

$$K_\varphi : u(x) \mapsto \int_{-1}^{1} \frac{u(x)\varphi(s) - u(s)\varphi(x)}{|x-s|}\, ds, \tag{2}$$

acting in the Hilbert space $L_2[-1,1]$. The spectral analysis of the operator K_φ is based on the following useful representation:[2,3]

$$K_\varphi = \varphi \circ K_0 - (K_0 \varphi), \tag{3}$$

where operator K_0 is defined as

$$K_0 : u \mapsto \int_{-1}^{1} \frac{u(x) - u(s)}{|x-s|}\, ds, \tag{4}$$

and $(K_0\varphi)$ stands for the operator of multiplication by function $K_0\varphi(x)$. The spectral problem for operator K_0 happened to be exactly solvable.[1] The eigenvalues are

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$$\mu_0=0; \quad \mu_n=2\sum_{j=1}^{n}\frac{1}{j}, \quad n=1,2,..., \tag{5}$$

and the correspondent eigenfunctions are Legendre polynomials $p_n(x)$.

However, physically important Gaussian equilibrium distributions have infinite support and there are not many results known concerning the spectral analysis of the corresponding collision operator. In our paper[3] we have considered a family of operators K_{φ_a} with a truncated Gaussian equilibrium distribution function,

$$\varphi(x)=C_a e^{-x^2}, \quad C_a^{-1}=\int_{-a}^{a} e^{-x^2}\,dx=\sqrt{\pi}\,\mathrm{erf}(a), \tag{6}$$

on the interval $[-a,a]$. We have proved[3] analytically that the first two eigenvalues λ_1, λ_2 of operator K_a go to zero $\sim a^{-1}$ when $a\to\infty$ and have confirmed it numerically for several other lower eigenvalues. In the present paper we shall prove analytically that zero becomes a point of spectral concentration when $a\to\infty$, i.e., the number of the eigenvalues in an arbitrary small vicinity of zero increases unlimitedly as $a\to\infty$.

II. RESULT

We study a family of operators,

$$K_{\varphi_a}: u(x)\mapsto\int_{-a}^{a}\frac{u(x)\varphi(s)-u(s)\varphi(x)}{|x-s|}\,ds, \tag{7}$$

on the interval $[-a,a]$ with the equilibrium distribution function $\varphi(x)$ given by Eq. (6). As we have shown in our paper,[3] a simple change of variables makes the spectral problem for operator K_{φ_a} equivalent to the spectral problem for the operator

$$K_a: u(x)\mapsto\int_{-1}^{1}\frac{u(x)\varphi_a(s)-u(s)\varphi_a(x)}{|x-s|}\,ds, \tag{8}$$

on the interval $[-1, 1]$, where

$$\varphi_a(x):=C_a e^{-a^2x^2}. \tag{9}$$

It is more convenient to study the spectral properties of our operator in the form (8).

We use notations

$$\langle u,v\rangle:=\int_{-1}^{1}u(x)\overline{v}(x)\,\frac{dx}{\varphi_a(x)},$$

for the inner product in space $L_2([-1,1],dx/\varphi_a(x))$ and

$$(u,v):=\int_{-1}^{1}u(x)\overline{v}(x)\,dx,$$

for the inner product in the space $L_2([-1,1],dx)$.

Let us denote by $E_a[-M,M]$ the spectral measure of the operator K_a on the interval $[-M,M]\subset\mathbf{R}$. By $\mathcal{H}_a=L_2([-1,1],dx/\varphi_a(x))$ we denote Hilbert space, where operator K_a acts as a self-adjoint operator.[1] The main result of this paper is the following.

Theorem: *For any* $M>0$,

$$\dim(E_a[-M,M]\mathcal{H}_a)\to\infty, \quad \text{as} \quad a\to\infty. \tag{10}$$

This theorem means that the number of eigenvalues (counted with multiplicity) of the operator K_a (and, consequently, of the operator K_{φ_a}) in an arbitrary small vicinity of zero increases to infinity when the truncation parameter a goes to infinity. Indeed, as it is shown in our previous papers,[2,3] the spectrum of the operators K_{φ_a} is purely discrete for all $a<\infty$. Hence, the increase of the spectral measure on the interval $[-M,M]$ can be caused only by the increase of the number of the eigenvalues (counted with multiplicity) on this interval. Therefore zero is a point of spectral concentration for the limit operator $\mathcal{K}_\infty=\lim_{a\to\infty} K_{\varphi_a}$.

We shall prove this theorem using the bilinear form approach. In order to prove our theorem it is enough[6,7] to construct for all $N>0$ a linear set $F_N^a\subset D(K_a)$, $\dim F_N^a=N$, such that for any $M>0$ there exists $a_0(N,M)$ such that for all $a>a_0(N,M)$ inequality,

$$|\langle K_a u,u\rangle|\leqslant M\langle u,u\rangle, \tag{11}$$

is true for all $u\in F_N^a$.

We construct F_N^a as a linear span,

$$F_N^a:=\bigvee_{k=0}^{N-1} u_k, \quad u_k(x):=p_k(x)\varphi_a^{1/2}(x),$$

where $p_k(x)$ are Legendre polynomials normalized in space $L_2([-1,1],dx)$ [the eigenfunctions of operator K_0 given by Eq. (4)].[1] Functions $u_k(x)$ are orthogonal in the space $L_2([-1,1], dx/\varphi_a(x))$, therefore $\dim F_N^a=N$ for all a.

Any function $u\in F_N^a$ can be represented as $u(x)=\Sigma_{k=0}^{N-1}\alpha_k u_k(x)$. Obviously,

$$\langle u,u\rangle=\sum_{k=0}^{N-1}\sum_{l=0}^{N-1}\alpha_k\overline{\alpha_l}(p_k,p_l)=\sum_{k=0}^{N-1}|\alpha_k|^2. \tag{12}$$

On the other hand, using representation (3), we have

$$\langle K_a u,u\rangle=(K_0 u,u)-\langle (K_0\varphi_a)u,u\rangle. \tag{13}$$

Let us first estimate the term

$$\begin{aligned}
|\langle (K_0\varphi_a)u,u\rangle| &= \left|\sum_{k=0}^{N-1}\sum_{l=0}^{N-1}\alpha_k\overline{\alpha_l}(K_0(\varphi_a)p_k,p_l)\right| \\
&= \left|\sum_{k=0}^{N-1}\sum_{l=0}^{N-1}\alpha_k\overline{\alpha_l}\int_{-1}^{1}\int_{-1}^{1}dx\,ds\,p_k(x)p_l(x)\,\frac{\varphi_a(x)-\varphi_a(s)}{|x-s|}\right| \\
&= \left|\sum_{k=0}^{N-1}\sum_{l=0}^{N-1}\alpha_k\overline{\alpha_l}\int_{-1}^{1}\int_{-1}^{1}dx\,ds\left[\frac{\varphi_a(x)p_k(x)p_l(x)}{|x-s|}-\frac{\varphi_a(x)p_k(s)p_l(s)}{|x-s|}\right]\right| \\
&= \left|\sum_{k=0}^{N-1}\sum_{l=0}^{N-1}\alpha_k\overline{\alpha_l}(\varphi_a,K_0(p_k p_l))\right|,
\end{aligned}$$

with a simple change of variables between x and s in the second term. Let us estimate terms $(\varphi_a,K_0(p_k p_l))$. As $p_k,p_l\in F_N^a$, then $k,l\leqslant N-1$, therefore the product of these Legendre polynomials is a polynomial of the power not higher than $2N-2$. Therefore one can represent

$$p_k(x)p_l(x)=\sum_{m=0}^{2N-2}\gamma_{kl}^m p_m(x),$$

where

$$\gamma_{kl}^m := \int_{-1}^{1} p_k(x)p_l(x)p_m(x)dx < \infty,$$

for all k,l,m. Therefore

$$|(\varphi_a, K_0(p_k p_l))| = \left| \sum_{m=0}^{2N-2} \gamma_{kl}^m (\varphi_a, K_0 p_m) \right| = \left| \sum_{m=0}^{2N-2} \gamma_{kl}^m \mu_m (\varphi_a, p_m) \right|.$$

Using the Laplace method[8] we find the asymptotics

$$(\varphi_a, p_m) = C_a \int_{-1}^{1} p_m(x) e^{-a^2 x^2} dx = C_a \sqrt{\pi} p_m(0) a^{-1}(1 + O(a^{-1})), \text{ as } a \to \infty.$$

Obviously $C_a < C_1$ for $a > 1$. Thus, we got the estimate at $a \to \infty$,

$$\left| \sum_{k=0}^{N-1} \sum_{l=0}^{N-1} \alpha_k \overline{\alpha_l} (\varphi_a, K_0(p_k p_l)) \right|$$
$$\leqslant 2C_1 \sum_{m=0}^{2N-2} \mu_m |p_m(0)| \max_{0 \leqslant k \leqslant N-1} \max_{0 \leqslant l \leqslant N-1} |\gamma_{kl}^m| \left| \sum_{k=0}^{N-1} \sum_{l=0}^{N-1} \alpha_k \overline{\alpha_l} \right| a^{-1}(1 + O(a^{-1})).$$

Obviously

$$|\alpha_k \overline{\alpha_l}| \leqslant \frac{(|\alpha_k| + |\alpha_l|)^2}{2};$$

therefore

$$\left| \sum_{k=0}^{N-1} \sum_{l=0}^{N-1} \alpha_k \overline{\alpha_l} \right| \leqslant 2N^2 \max_{0 \leqslant k \leqslant N-1} |\alpha_k|^2 \leqslant 2N^2 \sum_{k=0}^{N-1} |\alpha_k|^2.$$

Finally we have obtained the estimate

$$|((K_0 \varphi_a)u, u)| = \left| \sum_{k=0}^{N-1} \sum_{l=0}^{N-1} \alpha_k \overline{\alpha_l} (\varphi_a, K_0(p_k p_l)) \right|$$
$$\leqslant A(N) a^{-1} \sum_{k=0}^{N-1} |\alpha_k|^2 (1 + O(a^{-1})), \tag{14}$$

where the coefficient,

$$A(N) := 4C_1 N^2 \sum_{m=0}^{2N-2} \mu_m |p_m(0)| \max_{0 \leqslant k \leqslant N-1} \max_{0 \leqslant l \leqslant N-1} |\gamma_{kl}^m|,$$

does not depend on a and finite for any $N < \infty$.

Now let us estimate the term

$$(K_0 u, u) = \sum_{k=0}^{N-1} \sum_{l=0}^{N-1} \alpha_k \overline{\alpha_l} (K_0(p_k \varphi_a^{1/2}), p_l \varphi_a^{1/2}).$$

We have

$$(K_0(p_k\varphi_a^{1/2}),p_l\varphi_a^{1/2})=\int_{-1}^{1}dx\,p_l(x)\varphi_a^{1/2}(x)\int_{-1}^{1}ds\,\frac{p_k(x)\varphi_a(x)-p_k(s)\varphi_a(s)}{|x-s|}.$$

We split the domain of integration into two parts, one where $|x-s|<a^{-1/2}$, and the other one where $|x-s|\geqslant a^{-1/2}$. Then we can write

$$(K_0(p_k\varphi_a^{1/2}),p_l\varphi_a^{1/2})=\mathcal{I}_1+\mathcal{I}_2, \tag{15}$$

$$\mathcal{I}_1:=C_a\int\int_{|x-s|<a^{-1/2}}p_l(x)e^{-a^2x^2/2}\,\frac{p_k(x)e^{-a^2x^2/2}-p_k(s)e^{-a^2s^2/2}}{|x-s|}\,ds\,dx;$$

$$\mathcal{I}_2:=C_a\int\int_{|x-s|\geqslant a^{-1/2}}p_l(x)e^{-a^2x^2/2}\,\frac{p_k(x)e^{-a^2x^2/2}-p_k(s)e^{-a^2s^2/2}}{|x-s|}\,ds\,dx;$$

and estimate integrals $\mathcal{I}_1$ and $\mathcal{I}_2$ separately.

For $\mathcal{I}_1$ we have

$$|\mathcal{I}_1|\leqslant C_a\max_{x\in[-1,1]}|p_l(x)|\int\int_{|x-s|\leqslant a^{-1/2}}e^{-a^2x^2/2}\left|\frac{1}{x-s}\int_s^x(p_k(t)e^{-a^2t^2/2})'\,dt\right|ds\,dx$$

$$\leqslant C_a\max_{x\in[-1,1]}|p_l(x)|\max_{x\in[-1,1]}|(p_k(x)e^{-a^2x^2/2})'|\int\int_{|x-s|\leqslant a^{-1/2}}e^{-a^2x^2/2}\,ds\,dx. \tag{16}$$

One can estimate

$$\max_{x\in[-1,1]}|(p_k(x)e^{-a^2x^2/2})'|\leqslant\max_{x\in[-1,1]}|p_k'(x)|+a^2\max_{x\in[-1,1]}|p_k(x)|\max_{x\in[-1,1]}|xe^{-a^2x^2/2}|$$

$$=\max_{x\in[-1,1]}|p_k'(x)|+ae^{-1/2}\max_{x\in[-1,1]}|p_k(x)|. \tag{17}$$

Now we estimate

$$\int\int_{|s-x|\leqslant a^{-1/2}}e^{-a^2x^2/2}\,ds\,dx\leqslant\int_{-1}^{1}ds\int_{a-a^{-1/2}}^{s+a^{1/2}}dx\,e^{-a^2x^2/2}=\mathcal{I}_3+\mathcal{I}_4, \tag{18}$$

where

$$\mathcal{I}_3=\int_{2a^{-1/2}\leqslant|s|\leqslant1}ds\int_{s-a^{-1/2}}^{s+a^{1/2}}dx\,e^{-a^2x^2/2};$$

$$\mathcal{I}_4=\int_{-2a^{-1/2}}^{2a^{-1/2}}ds\int_{s-a^{-1/2}}^{s+a^{1/2}}dx\,e^{-a^2x^2/2}.$$

Everywhere in the domain of integration of $\mathcal{I}_3$ we have $|x|\geqslant a^{-1/2}$; therefore

$$\mathcal{I}_3\leqslant 2a^{-1/2}\max_{|x|\geqslant a^{-1/2}}e^{-a^2x^2/2}=2a^{-1/2}e^{-a/2}. \tag{19}$$

On the other hand,

$$\mathcal{I}_4\leqslant\int_{-2a^{-1/2}}^{2a^{-1/2}}ds\int_{-a^{-1/2}}^{a^{1/2}}dx\,e^{-a^2x^2/2}=4a^{-1/2}\int_{-a^{-1/2}}^{a^{1/2}}dxe^{-a^2x^2/2}.$$

Using the Laplace method[8] we get the asymptotics

$$\int_{-a^{-1/2}}^{a^{1/2}} dx\, e^{-a^2x^2/2} = a^{-1}\sqrt{\pi/2}(1+O(a^{-1/2})), \quad \text{as } a\to\infty;$$

therefore

$$\mathcal{I}_4 \leqslant a^{-3/2} 4\sqrt{\pi/2}(1+O(a^{-1/2})), \quad \text{as } a\to\infty. \tag{20}$$

Combining Eqs. (16)–(20) we get at $a\to\infty$:

$$|\mathcal{I}_1| \leqslant a^{-1/2} C_1 4\sqrt{\pi/2} e^{-1/2} \max_{x\in[-1,1]} |p_l(x)| \max_{x\in[-1,1]} |p_k(x)| (1+O(a^{-1/2})). \tag{21}$$

Now let us estimate $\mathcal{I}_2$:

$$|\mathcal{I}_2| \leqslant a^{1/2} C_a \int_{-1}^{1}\int_{-1}^{1} dx\, ds |p_l(x) e^{-a^2x^2/2}(p_k(x)e^{-a^2x^2/2} - p_k(s)e^{-a^2x^2/2})|$$

$$\leqslant a^{1/2} 2 C_a \max_{x\in[-1,1]} |p_l(x)| \max_{x\in[-1,1]} |p_k(x)| \int_{-1}^{1} e^{-a^2x^2/2}\, dx.$$

Again using the Laplace method[8] we have the asymptotics

$$\int_{-1}^{1} e^{-a^2x^2/2}\, dx = \sqrt{\pi} a^{-1}(1+O(a^{-1/2})), \quad \text{as } a\to\infty,$$

and therefore

$$|\mathcal{I}_2| \leqslant a^{-1/2} 2 C_1 \sqrt{\pi} \max_{x\in[-1,1]} |p_l(x)| \max_{x\in[-1,1]} |p_k(x)| (1+O(a^{-1})). \tag{22}$$

From Eqs. (15), (21), and (22) we see now that at $a\to\infty$,

$$|(K_0(p_k\varphi_a^{1/2}), p_l\varphi_a^{1/2})| \leqslant a^{-1/2} 2 C_1 \sqrt{\pi}(1+\sqrt{2}e^{-1/2}) \max_{x\in[-1,1]} |p_l(x)| \max_{x\in[-1,1]} |p_k(x)| (1+O(a^{-1}));$$

therefore at $a\to\infty$,

$$|(K_0 u, u)| = \left| \sum_{k=0}^{N-1} \sum_{l=0}^{N-1} \alpha_k \overline{\alpha_l} (K_0(p_k\varphi_a^{1/2}), p_l\varphi_a^{1/2}) \right|$$

$$\leqslant B(N) a^{-1/2} \sum_{k=0}^{N-1} |\alpha_k|^2 (1+O(a^{-1})), \tag{23}$$

where the coefficient

$$B(N) := 4N^2 C_1 \sqrt{\pi}(1+\sqrt{2}e^{-1/2}) \max_{0\leqslant k\leqslant N-1} \max_{x\in[-1,1]} |p_k(x)|^2$$

does not depend on a and finite for any $N<\infty$. Formulas (12)–(14), (23) mean that for any $N>0$, and $M>0$; and any function $u(x)=\Sigma_{k=0}^{N-1}\alpha_k u_k(x) \in F_N^a$, inequality (11) is satisfied for sufficiently large a, $a>a_0(N,M)$. Taking into account the normalization of the Legendre polynomials $p_k(x)$ in $L_2([-1,1],dx)$, we get a very rough estimate, $a_0(N,M) \leqslant N^6 M^{-2} 16\pi C_1^2 (1+\sqrt{2e^{-1/2}})^2$. The theorem is proved.

III. CONCLUSIONS

In the present paper we have proved that zero becomes a point of spectral concentration for collision operators with a truncated Gaussian equilibrium distribution function when the truncation parameter a goes to infinity. Nevertheless, other spectral properties of the limit operator are still unknown. In particular, it would be very interesting to clarify if the discrete spectrum of the truncated operators condenses into continuous one when $a \to \infty$.

As concerns physical conclusions, they have been discussed in our previous paper.[3]

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$\perp$-order automorphisms of Hilbert space effect algebras: The two-dimensional case

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It is well known that the $\perp$-order automorphisms of the effect algebra of a Hilbert space of dimension not less than three are implemented by unitary or antiunitary operators. The aim of this paper is to show that the same assertion also holds true in the two-dimensional case. © *2001 American Institute of Physics.*
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Let H be a (real or complex) Hilbert space. The effect algebra of H is the operator interval $[0,I]$ of all positive (self-adjoint, bounded linear) operators on H which are bounded by the identity I. Effect algebras play a very important role in the mathematical foundations of quantum mechanics (see, e.g., Ref. 1). It is well known that if the dimension of H is at least three, then the $\perp$-order automorphisms of $[0,I]$ (which are the bijective transformations of the effect algebra that preserve the order $\leqslant$ in both directions and also preserve the orthocomplementation $\perp: E \mapsto I - E$) are implemented by unitary or antiunitary operators on H (see Ref. 1, Sec. V 5 and Ref. 2). In fact, the proof is usually based on the fundamental theorem of projective geometry which holds true only in spaces of dimension not less than three. Because of the importance of effect algebras, it is a natural problem to clarify the situation in the two-dimensional case. In fact, Cassinelli *et al.* faced this issue in their paper[2] (it is trivial that the corresponding assertion fails to hold in one dimension). Moreover, in their recent work,[3] Lahti *et al.* showed that if the considered automorphism is induced via the functional calculus by a Borel function of the interval $[0,1]$, then it is necessarily the identity. The aim of this paper is to present the complete solution of the problem.

We have the following result.

Theorem: *Let H be a two-dimensional (real or complex) Hilbert space and let $[0,I]$ be the effect algebra of H. Let $\phi:[0,I]\to[0,I]$ be a bijective transformation with the property that*

$$E \leqslant F \Leftrightarrow \phi(E) \leqslant \phi(F) \quad \text{and} \quad \phi(I-E) = I - \phi(E)$$

hold for every $E,F \in [0,I]$. Then there exists an either unitary or antiunitary operator U on H such that

$$\phi(E) = UEU^* \quad (E \in [0,I]).$$

Proof: Several times in the proof we shall use the following easy observation: If A, B are positive (self-adjoint) operators, $B \leqslant A$, and A is of rank one, then $B = \lambda A$ for some scalar $\lambda \geqslant 0$.

We recall that every bijection of the effect algebra of a Hilbert space which preserves the order in both directions necessarily preserves the projections as well as their ranks in both directions (see [Ref. 1, Theorem 5.8, p. 219]). Clearly, we have $\phi(0)=0$, $\phi(I)=I$.

In what follows, let P be any rank-one projection on H and let Q be its orthogonal complement. Pick $\lambda \in [0,1]$. Since $0 \leqslant \phi(\lambda P) \leqslant \phi(P)$, it follows that $\phi(\lambda P) = f_P(\lambda)\phi(P)$ for some

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scalar $f_P(\lambda)\in[0,1]$. Clearly, $f_P:[0,1]\to[0,1]$ is a strictly monotone increasing bijection (observe that ϕ^{-1} has the same properties as ϕ). If $\lambda\in[0,1]$, then from the inequality

$$\phi(Q)\leqslant\phi(\lambda P+Q)\leqslant I=\phi(P)+\phi(Q)$$

we obtain

$$0\leqslant\phi(\lambda P+Q)-\phi(Q)\leqslant\phi(P).$$

This implies that

$$\phi(\lambda P+Q)=h_P(\lambda)\phi(P)+\phi(Q)$$

for some scalar $h_P(\lambda)\in[0,1]$. Similiary to the case of f_P, $h_P:[0,1]\to[0,1]$ is a strictly monotone increasing bijection. We show that $h_P=f_P$. Indeed, since

$$f_P(\lambda)\phi(P)=\phi(\lambda P)\leqslant\phi(\lambda P+Q)=h_P(\lambda)\phi(P)+\phi(Q),$$

it follows that $f_P\leqslant h_P$. Considering the inverse ϕ^{-1} of ϕ, it is easy to see that

$$\phi^{-1}(\lambda\phi(P))=f_P^{-1}(\lambda)P$$

and

$$\phi^{-1}(\lambda\phi(P)+\phi(Q))=h_P^{-1}(\lambda)P+Q.$$

Therefore, just as mentioned previously, we can deduce that $f_P^{-1}\leqslant h_P^{-1}$. Since the functions $f_P,h_P:[0,1]\to[0,1]$ are monotone increasing we then conclude that $f_P=h_P$. From the inequality

$$\begin{aligned}f_P(\lambda)\phi(P)=\phi(\lambda P)\leqslant\phi(\lambda I)=\phi(\lambda P+\lambda Q)\leqslant\phi(\lambda P+Q)\\ =h_P(\lambda)\phi(P)+\phi(Q)=f_P(\lambda)\phi(P)+\phi(Q)\end{aligned}$$

we infer that

$$0\leqslant\phi(\lambda I)-f_P(\lambda)\phi(P)\leqslant\phi(Q)$$

and this implies that

$$\phi(\lambda I)=f_P(\lambda)\phi(P)+k_P(\lambda)\phi(Q)$$

for some scalar $k_P(\lambda)\in[0,1]$. Since $\phi(P),\phi(Q)$ run through the set of all pairs of mutually orthogonal rank-one projections, it now follows that $\phi(\lambda I)$ is diagonizable with respect to every basis. This gives us that $\phi(\lambda I)$ is a scalar operator, that is, $\phi(\lambda I)=f(\lambda)I$ for some scalar $f(\lambda)\in[0,1]$. Clearly, $f:[0,1]\to[0,1]$ is a strictly monotone increasing bijection. Since

$$f_P(\lambda)\phi(P)=\phi(\lambda P)\leqslant\phi(\lambda I)=f(\lambda)I\leqslant\phi(\lambda P+Q)=f_P(\lambda)\phi(P)+\phi(Q),$$

it follows that $f=f_P=h_P$. So, we have

$$\phi(\lambda P)=f(\lambda)\phi(P)$$

and

$$\phi(\lambda P+Q)=f(\lambda)\phi(P)+\phi(Q).$$

The argument leading to this conclusion can also be applied to get

$$\phi(\lambda Q)=f(\lambda)\phi(Q)$$

and

$$\phi(P+\lambda Q)=\phi(P)+f(\lambda)\phi(Q).$$

For any $\lambda,\mu\in[0,1]$ we have

$$f(\lambda)\phi(P)=\phi(\lambda P)\leqslant\phi(\lambda P+\mu Q)\leqslant\phi(\lambda P+Q)=f(\lambda)\phi(P)+\phi(Q)$$

and

$$f(\mu)\phi(Q)=\phi(\mu Q)\leqslant\phi(\lambda P+\mu Q)\leqslant\phi(P+\mu Q)=\phi(P)+f(\mu)\phi(Q).$$

From the first inequality we infer that

$$\phi(\lambda P+\mu Q)=f(\lambda)\phi(P)+\alpha\phi(Q)$$

for some $\alpha\in[0,1]$, while from the second one we have

$$\phi(\lambda P+\mu Q)=\beta\phi(P)+f(\mu)\phi(Q)$$

for some $\beta\in[0,1]$. Comparing these equalities we get

$$\phi(\lambda P+\mu Q)=f(\lambda)\phi(P)+f(\mu)\phi(Q) \tag{1}$$

for every $\lambda,\mu\in[0,1]$.

Observe that f has the following symmetry property: $f(\lambda)+f(1-\lambda)=1$. Indeed, this follows from the equality $\phi(\lambda I)+\phi((1-\lambda)I)=I$.

Our next claim is to obtain a functional equation for f. In order to do this, we recall the following notation from Ref. 4. If E is an effect on a Hilbert space and φ is a unit vector, then let

$$\lambda(E,P_\varphi)=\sup\{\lambda\in[0,1]:\lambda P_\varphi\leqslant E\},$$

where P_φ is the orthogonal projection onto the subspace generated by φ. Suppose that $E\in[0,I]$. Then (Ref. 4, Theorem 4) tells us that

$$\lambda(E,P_\varphi)=\begin{cases}\|E^{-1/2}\varphi\|^{-2}, & \text{if } \varphi\in\mathrm{ran}(E^{1/2})\\ 0, & \text{else}\end{cases}.$$

Fix mutually orthogonal rank-one projections P, Q on H. Pick $\mu\in]0,1[$ and let $E=\mu P+Q$. Take any rank-one projection R on H which is neither equal to nor orthogonal to P. Similarly to the second step of the proof (Ref. 2, Lemma 3), it is easy to verify that

$$\lambda(E,R)=\frac{\mu}{\mu+(1-\mu)\mathrm{tr}\,PR}.$$

Indeed, if r is a unit vector in the range of R, then using the above-mentioned result from Ref. 4, we compute

$$\lambda(E,R)=\|((1/\sqrt{\mu})P+Q)r\|^{-2}=\frac{1}{(1/\mu)\|Pr\|^2+\|Qr\|^2}=\frac{\mu}{\|Pr\|^2+\mu\|Qr\|^2}$$

$$=\frac{\mu}{\mu\|Pr\|^2+\mu\|Qr\|^2+(1-\mu)\|Pr\|^2}=\frac{\mu}{\mu+(1-\mu)\|Pr\|^2}=\frac{\mu}{\mu+(1-\mu)\mathrm{tr}\,PR}.$$

By the definition of $\lambda(E,R)$, it is clear that

$$f(\lambda(E,R)) = \sup\{f(\lambda) : \lambda R \leqslant E\} = \sup\{f(\lambda) : \phi(\lambda R) \leqslant \phi(E)\}$$
$$= \sup\{f(\lambda) : f(\lambda)\phi(R) \leqslant \phi(E)\} = \lambda(\phi(E), \phi(R)).$$

Since $\phi(E) = \phi(\mu P + Q) = f(\mu)\phi(P) + \phi(Q)$, it follows that

$$f\left(\frac{\mu}{\mu + (1-\mu)\operatorname{tr} PR}\right) = \frac{f(\mu)}{f(\mu) + (1-f(\mu))\operatorname{tr}\phi(P)\phi(R)}.$$

As the quantities $\operatorname{tr} PR$ and $\operatorname{tr}\phi(P)\phi(R)$ do not depend on μ, it follows from this equality that $\operatorname{tr}\phi(P)\phi(R)$ can be uniquely expressed as a function of $\operatorname{tr} PR$. Denoting $g(\operatorname{tr} PR) = \operatorname{tr}\phi(P)\phi(R)$, we get a bijective function $g:]0,1[\to]0,1[$ for which

$$f\left(\frac{\mu}{\mu + (1-\mu)\nu}\right) = \frac{f(\mu)}{f(\mu) + (1-f(\mu))g(\nu)} \quad (\mu, \nu \in]0,1[)$$

holds true. Replacing μ by $1-\mu$ and ν by $1-\nu$ we have the following more aesthetic equality:

$$f\left(\frac{1-\mu}{1-\mu\nu}\right) = \frac{1-f(\mu)}{1-f(\mu)g(\nu)} \quad (\mu, \nu \in]0,1[). \tag{2}$$

Here we have used the fact that g has the same symmetry property as f. This follows from the following equality:

$$g(1-\operatorname{tr} PR) = g(\operatorname{tr} P - \operatorname{tr} PR) = g(\operatorname{tr}(P(I-R))) = \operatorname{tr}\phi(P)\phi(I-R) = \operatorname{tr}\phi(P)(I-\phi(R)) = \operatorname{tr}\phi(P)$$
$$-\operatorname{tr}\phi(P)\phi(R) = 1 - g(\operatorname{tr} PR).$$

Now, we turn to the solution of the functional equation (2). Our corresponding result is formulated in the following separate statement.

Proposition: Let $f,g:]0,1[\to]0,1[$ be functions. Suppose that f is a strictly monotone increasing bijection and that $f(1-x) = 1-f(x)$ and $g(1-y) = 1-g(y)$ hold for every $x,y \in]0,1[$. If

$$f\left(\frac{1-x}{1-xy}\right) = \frac{1-f(x)}{1-f(x)g(y)} \quad (x,y \in]0,1[), \tag{3}$$

then f and g are the identities on $]0,1[$.

Proof: The function f being continuous, Eq. (3) implies the continuity of g.

Observe that, with the notation

$$\alpha(t) := \frac{1}{1+e^t} \quad (t \in \mathbb{R}),$$

$$\beta(x) := \ln\frac{x}{1-x} \quad (x \in]0,1[),$$

$$\gamma(y) := \ln(1-y) \quad (y \in]0,1[),$$

we have the following identity:

$$\frac{1-x}{1-xy} = \frac{1}{1+\exp\left(\ln\frac{x}{1-x} + \ln(1-y)\right)} = \alpha(\beta(x) + \gamma(y))$$

for all $x,y \in]0,1[$. Therefore, Eq. (3) can be rewritten as

$$f\circ\alpha(\beta(x)+\gamma(y))=\alpha(\beta\circ f(x)+\gamma\circ g(y)) \quad (x,y\in]0,1[). \tag{4}$$

Substituting $x=\beta^{-1}(u)$ and $y=\gamma^{-1}(v)$ into Eq. (4) and applying the inverse function of α to both sides of Eq. (4), we get

$$\alpha^{-1}\circ f\circ\alpha(u+v)=\beta\circ f\circ\beta^{-1}(u)+\gamma\circ g\circ\gamma^{-1}(v) \tag{5}$$

for all $u\in\mathbb{R}$ and $v\in]-\infty,0[$. Thus the functions

$$F:=\alpha^{-1}\circ f\circ\alpha, \quad G:=\beta\circ f\circ\beta^{-1}, \quad H:=\gamma\circ g\circ\gamma^{-1}$$

satisfy the following so-called Pexider equation:

$$F(u+v)=G(u)+H(v) \quad (u\in\mathbb{R}, v\in]-\infty,0[).$$

Then, by known results of the theory of functional equations (cf. Ref. 5 or 6) and by the continuity of F, G, H, it follows that there exist constants $a,b,c\in\mathbb{R}$ such that

$$F(w)=cw+a+b \quad (w\in\mathbb{R}),$$

$$G(u)=cu+a \quad (u\in\mathbb{R}), \tag{6}$$

$$H(v)=cv+b \quad (v\in]-\infty,0[). \tag{7}$$

Using Eq. (6) and the definition of G, we get that $\beta\circ f(x)=c\beta(x)+a$, whence

$$f(x)=\frac{x^c}{x^c+e^{-a}(1-x)^c} \quad (x\in]0,1[).$$

Similarly, the definitions of H and γ, and Eq. (7) yield

$$g(y)=1-e^b(1-y)^c \quad (y\in]0,1[).$$

The function f being strictly increasing, G is also increasing whence we get that $c>0$. Thus f satisfies the identity $f(1-x)=1-f(x)$ if and only if $a=0$. The analogous identity for g is valid if and only if $b=0$, $c=1$. Therefore $f(x)=g(x)=x$ for all $x\in]0,1[$. □

Returning to the proof of our theorem, since the above-mentioned function g is the identity, we have $\mathrm{tr}\,PQ=\mathrm{tr}\,\phi(P)\phi(Q)$ for any rank-one projections P, Q on H. Hence, using Wigner's theorem on symmetry transformations we obtain that there exists an either unitary or antiunitary operator U on H such that

$$\phi(P)=UPU^*$$

for every rank-one projection P on H. As f is also the identity, from Eq. (1) we infer that

$$\phi(\lambda P+\mu Q)=\lambda\phi(P)+\mu\phi(Q)=\lambda UPU^*+\mu UQU^*=U(\lambda P+\mu Q)U^*,$$

which means that $\phi(E)=UEU^*$ holds for every effect E on H.

This completes the proof of our theorem. □

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On one class of exact Poisson structures

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We discuss some properties of a natural class of Poisson structures on Euclidean spaces and abstract manifolds. In particular it is proved that such structures are always exact and may be reconstructed from their Casimir functions. It is shown that in low dimensions they give the whole class of exact Poisson structures. The dimension of Poisson homology of these structures is computed in terms of the Milnor number of their Casimir functions. We also analyze some concrete examples of such structures in low dimensions and show that their centers are generated by Casimir functions. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Let M denote an affine algebraic variety and $F(M)$ denote an associative algebra of functions on M.

Definition 1: (cf. Refs. 1 and 2). A Poisson bracket on M is a bilinear mapping $\{\cdot,\cdot\}:F(M)\times F(M)\to F(M)$, *satisfying the following conditions:*

$$\text{antisymmetry}\quad \{f,g\}=-\{g,f\} \tag{1a}$$

$$\text{Leibniz rule}\quad \{f,gh\}=\{f,g\}h+\{f,h\}g, \tag{1b}$$

$$\text{Jacobi identity}\quad \{\{f,g\},h\}+\{\{g,h\},f\}+\{\{h,f\},g\}=0. \tag{1c}$$

For any field K of characteristic zero, let $K_n=K[x_1,\ldots,x_n]$ be the algebra of polynomials of n variables with coefficients in K (actually we will work only with fields of real or complex numbers).

We will be concerned with one class of Poisson brackets on K^n, which was introduced in (Ref. 3).

Definition 2: A Jacobian bracket on K^n *is defined as a bilinear map* $\{\cdot,\cdot\}:K_n\times K_n\to K_n$,

$$\{f,g\}=uJ(f,g,P_1,\ldots,P_{n-2}), \tag{2}$$

where $u,P_i\in K_n$, $i=1,\ldots,n-2$, *and* J *stands for the usual Jacobian* $J(h_1,\ldots,h_n)=\det(\partial h_i/\partial x_j)$.

As we will see in Sec. II, this formula actually defines a Poisson bracket on K^n. In the sequel we will establish some general properties of such brackets and explicate some results from (Refs. 3 and 4).

A Poisson structure defined by a Jacobian bracket will be called simply a Jacobian Poisson structure (JPS).

For the fields of real and complex numbers, the same formula defines a Poisson structure on $C^\infty(K^n)$. The polynomial context is chosen for simplicity.

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II. PROPERTIES OF JACOBIAN BRACKETS

Let us denote by $\chi(M)$ the vector space of vector fields being the sections of tangent bundle $T(M)\to M$, by $\chi^k(M)$ the space of k-vectors and by $\Omega^k(M)$ the space of differential k-forms on M, endowed with exterior differentiation $d:\Omega^k(M)\to\Omega^{k+1}(M)$. If the manifold M is endowed with a volume form Ω, then we can define the operation,

$$\Phi_k:\chi^k(M)\to\Omega^{n-k}(M), \tag{3}$$

$$\Phi_k:v\mapsto i(v)\Omega, \tag{4}$$

and using above we can define[5] $D=\Phi_{k-1}^{-1}\circ d\circ\Phi_k:\chi^k(M)\to\chi^{k-1}(M)$.

It will be convenient for further use to rewrite the bracket (2) in terms of a Poisson bivector. Let Λ denote the Poisson structure defined by the Jacobian Poisson bracket. Then

$$\Lambda=\omega^{ij}\frac{\partial}{\partial x^i}\wedge\frac{\partial}{\partial x^j}, \tag{5}$$

$$\omega^{ij}=\epsilon^{ijk_1\ldots k_{n-2}}\frac{\partial P_1}{\partial x^{k_1}}\cdots\frac{\partial P_{n-2}}{\partial x^{k_{n-2}}}, \tag{6}$$

$$\{f,g\}=\Lambda(df,dg)=\omega^{ij}\frac{\partial f}{\partial x^i}\frac{\partial g}{\partial x^j}. \tag{7}$$

Theorem 1: (cf. Ref. 3). *Any Jacobian bracket is a Poisson bracket.*

Proof: An antisymmetry and Leibniz rule follow directly from well-known properties of determinants. Proving the Jacobi identity requires more work.

One could obtain the Jacobi identity for a Jacobian Poisson bracket as a particular case of generalized Jacobi identity for the Nambu bracket,[6] but we prefer to give a short direct proof, which as we believe is illuminating.

A nontrivial case is if polynomials $P_1,\ldots,P_{n-2}$ are functionally independent,[7] otherwise the Jacobian bracket vanishes identically. Because the Jacobi identity is invariant with respect to changes of coordinates, we can prove it locally in a convenient system of local coordinates. Now when $P_1,\ldots,P_{n-2}$ are functionally independent, we can always choose locally a frame for which they are local coordinates, i.e., $\partial P_i/\partial x^j=\delta_{ij}$ for $i,j=1,\ldots,n-2$. Then the formula (6) gives that $\{f,g\}=\partial_{n-1}f\partial_n g-\partial_{n-1}g\partial_n f$, where $\partial_i f=\partial f/\partial x^i$. The rest of the proof now becomes trivial. □

In order to formulate the next important property of Jacobian brackets we need one general definition.

Definition 3 (Ref. 5): A Poisson structure Λ is called exact if $D(\Lambda)=0$.

Theorem 2: *Any Poisson structure defined by the Jacobian bracket is exact.*

Proof: As in Theorem 1 the proper choice of coordinate system simplifies the proof. Indeed, after choosing the coordinate system exactly as in Theorem 1, obviously $\omega^{ij}=\epsilon^{ij}$ is a constant tensor and

$$D(\Lambda)=\Phi^{-1}\circ d\circ\Phi^2(\Lambda)=\partial_j\omega^{ij}\partial_i-\partial_i\omega^{ij}\partial_j=2\partial_j\omega^{ij}\partial_i=2\partial_j\epsilon^{ij}\partial_i=0, \tag{8}$$

which finishes the proof. □

Remark 1: The property of exactness may be interpreted in terms of the modular vector field introduced in Ref. 8. Indeed, from the discusion in Ref. 8 it follows that our $D(\Lambda)$ actually coincides with the modular vector field of Poisson manifold (M,Λ). This, in turn, means that under the property of exactness, Ω is an invariant density for the flows of all Hamiltonian vector fields on M, i.e., $L_{X_f}\Omega=0$, where L_{X_f} denotes the Lie derivative with respect to X_f—Hamiltonian

vector field of $f \in \mathbf{C}^\infty(M)$, $(X_f := \{f, \cdot\})$, *and in such a case the Poisson manifold* (M, Λ) *is said to be unimodular.*[8] *Thus, we see that JPS on affine spaces are unimodular.*

It is obvious that functions $P_1, \ldots, P_{n-2}$ are Casimirs of the corresponding Jacobian Poisson bracket (2), i.e., $\{f, P_i\} = 0$, $\forall f \in K_n$, $i = 1, \ldots, n-2$.

It turns out that the existence of sufficiently many functionally independent Casimirs is a characteristic property of corresponding Jacobian Poisson structures.

Theorem 3: *A Poisson structure on* K^n *which has* $n-2$ *functionally independent Casimirs, is always a Jacobian Poisson structure.*

For simplicity of notation, we only present the proof for $n = 4$. The general case is completely analogous.

Proof: For $n = 4$, we have two Casimirs; let us name them P and Q. If our coordinates are x^1, x^2, x^3, x^4, then we have

$$\{x^i, P\} = \omega^{ij}\, \partial_j P = 0, \quad \{x^i, Q\} = \omega^{ij}\, \partial_j Q = 0; \quad i = 1,2,3,4.$$

First we observe that in this set of eight equations no more than five are linearly independent, because we always have

$\partial_i P\{x^i, P\} = 0$,
$\partial_i Q\{x^i, Q\} = 0$,
$\partial_i P\{x^i, Q\} + \partial_j Q\{x^j, P\} = 0$.

Actually the rank of the matrix of this system is exactly five. As a result we can take one of nonzero ω^{ij} as a parameter, and then, a standard procedure for solving linear equations gives us that components ω^{ij} are proportional to $\epsilon^{ijkl}\, \partial_k P\, \partial_l Q$, which exactly means that this is a Jacobian Poisson structure.

□

III. LOW-DIMENSIONAL ANALYSIS

In low dimensions we can establish further interesting properties of JPS. First of all it turns out that sometimes the exactness is an intrinsic property of JPS. More precisely, the converse of Theorem 2 holds true for dimension 3. Actually there are two curious facts about Poisson structures on K^3.

Theorem 4: *For any bivector* Λ *on* K^3, *the condition of its exactness* $[D(\Lambda) = 0]$ *implies a Jacobi identity.*

Proof: We will use one general formula from the calculus of bivectors (presented, e.g., in Ref. 3) which states that for any two bivector fields Λ_1, Λ_2 one has

$$D(\Lambda_1 \wedge \Lambda_2) = [\Lambda_1, \Lambda_2]_S + D(\Lambda_1) \wedge \Lambda_2 - \Lambda_1 \wedge D(\Lambda_2), \tag{9}$$

where $[\cdot, \cdot]_S$ denotes the Schouten bracket.[9]

In particular,

$$D(\Lambda \wedge \Lambda) = [\Lambda, \Lambda]_S + 2D(\Lambda) \wedge \Lambda. \tag{10}$$

Since for the dimension reasons $\Lambda \wedge \Lambda = 0$ on K^3, it becomes clear that $D(\Lambda) = 0$ implies $[\Lambda, \Lambda]_S = 0$, which is exactly equivalent to Jacobi identity.

□

Theorem 5: *For* $n = 3$, *an exact polynomial Poisson structure is always a Jacobian Poisson structure.*

Proof: Without losing generality we can consider Poisson bivectors with components given by homogeneous polynomials of the same degree. This enables us to obtain the proof by merely ''counting of parameters.'' We make no attempt to obtain coordinate free proofs because such counting of parameters is also helpful for dealing with the higher dimensional case.

In order to avoid complicated notations we present a proof for quadratic Poisson structures; the case of higher degree is completely similar.

Any quadratic Poisson structure on K^3 is of the form

$$\Lambda = c^{ij}_{st} x^s x^t \partial_i \wedge \partial_j ; \quad c^{ij}_{st} = -c^{ji}_{st}, \ c^{ij}_{st} = c^{ij}_{ts}, \tag{11}$$

and then using (9) we obtain

$$D(\Lambda) = 2c^{ij}_{st} \partial_j (x^s x^t) \partial_i = 4c^{is}_{st} x^t \partial_i , \tag{12}$$

and finally we have that $D(\Lambda)=0$ iff

$$c^{is}_{st} = 0, \quad i,t = 1,2,3. \tag{13}$$

As it follows from Theorem 4, we need not analyze conditions on c^{is}_{st} imposed by the Jacobi identity, so we work with conditions (13) alone.

Let us write down Λ explicitly, replacing (x^1,x^2,x^3) with (x,y,z),

$$\begin{aligned}\Lambda = &(c^{12}_{11}x^2 + c^{12}_{22}y^2 + c^{12}_{33}z^2 + 2c^{12}_{12}xy + 2c^{12}_{13}xz + 2c^{12}_{23}yz)\frac{\partial}{\partial x}\wedge\frac{\partial}{\partial y}\\ &+ (c^{23}_{11}x^2 + c^{23}_{22}y^2 + c^{23}_{33}z^2 + 2c^{23}_{12}xy + 2c^{23}_{13}xz + 2c^{23}_{23}yz)\frac{\partial}{\partial y}\wedge\frac{\partial}{\partial z}\\ &+ (c^{31}_{11}x^2 + c^{31}_{22}y^2 + c^{31}_{33}z^2 + 2c^{31}_{12}xy + 2c^{31}_{13}xz + 2c^{31}_{23}yz)\frac{\partial}{\partial z}\wedge\frac{\partial}{\partial x}.\end{aligned} \tag{14}$$

Any quadratic Jacobian Poisson bracket is defined by some homogenous polynomial of degree 3. Let P denote such a function, and Λ_P be the corresponding Jacobian Poisson structure. It is convenient to represent P in the form

$$P = 2c^{12}_{12}xyz + \tfrac{1}{3}c^{23}_{11}x^3 + \tfrac{1}{3}c^{31}_{22}y^3 + \tfrac{1}{3}c^{12}_{33}z^3 + c^{23}_{22}xy^2 + c^{23}_{33}xz^2 + c^{31}_{11}yx^2 + c^{31}_{33}yz^2 + c^{12}_{11}zx^2 + c^{12}_{22}zy^2. \tag{15}$$

Then clearly,

$$\begin{aligned}\Lambda_P = &(c^{12}_{11}x^2 + c^{12}_{22}y^2 + c^{12}_{33}z^2 + 2c^{12}_{12}xy + 2c^{23}_{33}xz + 2c^{31}_{33}yz)\frac{\partial}{\partial x}\wedge\frac{\partial}{\partial y}\\ &+ (c^{23}_{11}x^2 + c^{23}_{22}y^2 + c^{23}_{33}z^2 + 2c^{31}_{11}xy + 2c^{12}_{11}xz + 2c^{12}_{12}yz)\frac{\partial}{\partial y}\wedge\frac{\partial}{\partial z}\\ &+ (c^{31}_{11}x^2 + c^{31}_{22}y^2 + c^{31}_{33}z^2 + 2c^{23}_{22}xy + 2c^{12}_{12}xz + 2c^{12}_{22}yz)\frac{\partial}{\partial z}\wedge\frac{\partial}{\partial x}.\end{aligned} \tag{16}$$

Now it is easy to see that $\Lambda = \Lambda_P$ precisely when

$$c^{12}_{12} = c^{23}_{23} = c^{31}_{13}, \ c^{12}_{11} = c^{23}_{13}, \ c^{31}_{11} = c^{23}_{12}, \ c^{12}_{22} = c^{31}_{23}, \ c^{23}_{22} = c^{31}_{12}, \ c^{23}_{33} = c^{12}_{13}, \ c^{31}_{33} = c^{12}_{23}. \tag{17}$$

These relations evidently coincide with the conditions of exactness (13).

□

Remark 2: Analogs of these results do not hold in dimensions bigger than 4 as it may be seen by ''counting of parameters.'' Nevertheless they may hold for bivectors with components given by polynomials of low degree. For quadratic PS on $\mathbf{R}^4$ *this may be derived from the results of Ref. 5.*

Interesting examples of Jacobian Poisson structures are given by well-known Sklyanin brackets[4] defined as follows:

$$\{x^\alpha, x^0\} = 2J^{\beta\gamma}x^\beta x^\gamma, \quad \{x^\alpha, x^\beta\} = -2x^0 x^\gamma, \tag{18}$$

where $J^{\alpha\beta}=J^{\alpha}-J^{\beta}$; J^{α},J^{β} are some complex numbers, $\alpha,\beta=1,2,3$.

Thus Sklyanin brackets give examples of quadratic Poisson structures on $\mathbf{C}^4$ (cf. Ref. 5) and it is easy to observe that they are Jacobian Poisson brackets. Indeed if one takes in (2) $P=\Sigma_{i=0}^{3}a_i(x^i)^2$, $Q=\Sigma_{j=0}^{3}b_i(x^j)^2$ then the Jacobian Poisson structure generated by P and Q coincides with (18) if $J^{\alpha\beta}=(a_{\alpha}-a_{\beta})/a_0$ and $a_{\gamma}b_0-a_0b_{\gamma}=1/2$, for every $\alpha,\beta,\gamma=1,2,3$.

In Ref. 4 it was shown that the center of the Sklyanin bracket admits a complete description. We will generalize this fact to an arbitrary Jacobian Poisson bracket on K^n.

In order to give a complete description of the center let us denote by $K\{x^1,\ldots,x^n\}$ the algebra of convergent power series with coefficients from K.

Theorem 6: *For arbitrary n, the center of Jacobian Poisson bracket* (2) *in $K\{x^1,\ldots,x^n\}$ is the subalgebra generated by $P_1,\ldots,P_{n-2}$.*

Proof: The general case may be obtained by induction. For the sake of brevity we present a proof for dimension 4. The crucial point is that for the Jacobian Poisson bracket the rank $rk(\omega^{ij})=2$ for every dimension.

The Jacobian Poisson structure in dimension 4 has the form

$$\Lambda=\epsilon^{ijpq}\frac{\partial P}{\partial x^p}\frac{\partial Q}{\partial x^q}\partial_i\wedge\partial_j, \tag{19}$$

where $P=P_1$ and $Q=P_2$.

For any polynomial f, this structure defines a vector field $X_f\in\chi(M)$:

$$X_f=\Lambda(df,\cdot)=\{f,\cdot\}=\omega^{ij}\partial_i f\partial_j. \tag{20}$$

If g is another polynomial, then

$$(dg)(X_f)=(X_f)g=\Lambda(df,dg)=\{f,g\}. \tag{21}$$

Let $X_{x^i}\equiv X_i$ and let h be a Casimir. It is obvious that $(dh)(X_i)=0$, for $i=1,2,3,4$. We want to show that h is some algebraic function of Casimirs P and Q. Let us put $dh=h_1\,dx^1+h_2\,dx^2+h_3\,dx^3+h_4\,dx^4$. In the next step we want to find functions h_i solving the set of equations $(dh)(X_i)=0$, for $i=1,2,3,4$. Because only two of the vectors X_i are linearly independent $(rk(\omega^{ij})=2)$, we can choose two functions, for example h_3, h_4, as parameters, and we will obtain

$$h_1=\frac{1}{\omega^{12}}(\omega^{23}h_3+\omega^{24}h_4), \tag{22}$$

$$h_2=-\frac{1}{\omega^{12}}(\omega^{13}h_3+\omega^{14}h_4), \tag{23}$$

$$\omega^{ij}=\epsilon^{ijkl}\,\partial_k P\,\partial_l Q:=\epsilon^{ijkl}P_kQ_l. \tag{24}$$

For convenience we will rewrite these formulas as

$$\begin{pmatrix}\omega^{12}h_1\\ \omega^{12}h_2\\ \omega^{12}h_3\\ \omega^{12}h_4\end{pmatrix}=\begin{pmatrix}\omega^{23}h_3+\omega^{24}h_4\\ -\omega^{13}h_3-\omega^{14}h_4\\ \omega^{12}h_3\\ \omega^{12}h_4\end{pmatrix}=\begin{pmatrix}(Q_4h_3-Q_3h_4)P_1+(P_3h_4-P_4h_3)Q_1\\ (Q_4h_3-Q_3h_4)P_2+(P_3h_4-P_4h_3)Q_2\\ (Q_4h_3-Q_3h_4)P_3+(P_3h_4-P_4h_3)Q_3\\ (Q_4h_3-Q_3h_4)P_4+(P_3h_4-P_4h_3)Q_4\end{pmatrix}. \tag{25}$$

Finally, if we set

$$\alpha=\frac{1}{\omega^{12}}(Q_4h_3-Q_3h_4),\quad \beta=\frac{1}{\omega^{12}}(P_3h_4-P_4h_3), \tag{26}$$

then it is immediate that

$$dh=\alpha\, dP+\beta\, dQ, \tag{27}$$

which implies that h may be represented as an analytic function of P and Q.[7]

□

Remark 3: Some properties of Sklyanin structures may be extended to a more general class of Poisson structures. Let us say that a Poisson structure is of the Sklyanin type, if the bracket of any two variables is a function of the remaining $(n-2)$ *variables. For example, for quadratic structures, we have*

$$\{x^i,x^j\}=J^{ij}_{mn}x^m x^n, \tag{28}$$

where we use the usual summation convention and assume that both m and n avoid values i and j.

Counting of parameters suggests that all such structures on $\mathbf{R}^5$ may be defined by some Jacobian brackets, for example, by taking the Jacobian Poisson structure with polynomials P_i being proper Pham polynomials.[10]

For a quadratic structure like above, the proper choice of functions in dimension 5 is

$$P_1=\sum_{i=1}^{5} a_i x^i, \quad P_2=\sum_{i=1}^{5} b_i (x^i)^2, \quad P_3=\sum_{i=1}^{5} c_i (x^i)^2. \tag{29}$$

Then we obtain

$$\{x^i,x^j\}=\sum_{k,l,m} \epsilon^{ijklm} a_k b_l c_m x^l x^m. \tag{30}$$

IV. QUASI-HOMOGENEOUS POISSON STRUCTURES

It turns out that affine Poisson structures with certain homogeneity have especially nice properties. Below we give a precise definition and present two results about such structures.

Let us say that a collection $\mathbf{w}=(w_1,\ldots,w_n)$ of positive rational numbers w_i is a system of weights for variables $x_1,\ldots,x_n$. The $\mathbf{w}$-degree of a monomial $e=x_1^{k_1}\cdot\ldots x_n^{k_n}$ is defined as $\Sigma w_i k_i$. Recall that polynomial $P\in K_n$ is called quasi-homogeneous of $\mathbf{w}$-degree d if all monomials entering in P have the same $\mathbf{w}$-degree equal to d.[10]

Definition 4: A Poisson structure is called a quasi-homogeneous Poisson structure of $\mathbf{w}$*-degree d if components* ω^{ij} *of the corresponding bivector are quasi-homogeneous polynomials of the same* $\mathbf{w}$*-degree* $d+w_i+w_j$.

Let us also introduce the so-called Euler vector field $X_E=\Sigma w_i x^i \partial_i$ associated with weights $(w_1,\ldots,w_n)$. Then it is easy to check that for a quasi-homogeneous Poisson structure of $\mathbf{w}$-degree d one has $L_{X_E}\Lambda=d\Lambda$. Moreover, for homogeneous Poisson structures (all $w_i=1$) we obtain a useful decomposition theorem generalizing the decomposition theorem of Liu and Xu.[5]

Theorem 7: *If* Λ *is a homogeneous Poisson structure of degree d on* K^n*, then it may be decomposed as* $\Lambda=\Lambda_0-[1/(d+n-2)]X_\Lambda\wedge X_E$*, where* Λ_0 *is an exact Poisson structure,* $X_\Lambda=D(\Psi)$ *and* $X_E=\Sigma_i x^i\partial_i$.

Proof: First let us consider the general quasi-homogeneous case when $X_E=\Sigma w_i x^i\partial_i$ and let $\Lambda=\Lambda_0-(1/c)X_\Lambda\wedge X_E$ for some $c\in K$ with exact Λ_0. Then since $D(\Lambda_0)=0$ we will get

$$D\left(\Lambda-\frac{1}{c}X_\Lambda\wedge X_E\right)=X_\Lambda-\frac{1}{c}([X_E,X_\Lambda]+D(X_E)X_\Lambda-D(X_\Lambda)X_E) \tag{31}$$

$$=\frac{1}{c}\left(c-d+w_i+w_j-\sum_{k=1}^{n} w_k\right)X_\Lambda=0. \tag{32}$$

This equality may only hold when $w_i=w_j$ for every i,j. This means that only a homogeneous case is possible and then we can take $w_i=1$, which directly leads to $c=d+n-2$.

□

As is well known, Poisson structures may be restricted to level surfaces of Casimirs. It turns out that applying this procedure to a quasi-homogeneous Jacobian Poisson structure one comes to an interesting connection with singularity theory.

Let us consider a Jacobian Poisson structure (2) given by $(n-2)$ functionally independent polynomials $P_1,\ldots,P_{n-2}\in K_n$ each of which is quasi-homogeneous with respect to the same system of weights **w**. It is easy to see that in such case their common zero-set $X=\{P_1=\cdots=P_{n-2}=0\}$ in $\mathbf{C}^n$ is a so-called two-dimensional complete intersection with an isolated singularity at the origin of $\mathbf{C}^n$.[10] The Jacobian Poisson structure Λ_P (2) naturally defines a Poisson structure $\tilde{\Lambda}_P$ on the ring of regular functions on X which is just $A=\mathbf{C}_n/(P_1,\ldots,P_{n-2})$.[11] For this reduced structure $\tilde{\Lambda}_P$ one can define its Poisson homology in the usual way.[9]

In particular its zero-dimensional Poisson homology $H_0^\pi(X,\tilde{\Lambda}_P)$ is isomorphic to the factor space $A/\{A,A\}$, where $\{A,A\}$ defines the ideal in A generated by all pairwise brackets of elements of A.

Our last result shows that Poisson homology of $\tilde{\Lambda}_P$ is related to some important topological characteristic of X.

Recall that the Milnor number of a complete intersection germ X of complex dimension two is defined as $\dim H^2(X_\epsilon\cap B_\delta^{2n},\mathbf{Z})$, where X_ϵ is a small nonsingular deformation of X and B_δ^{2n} is a small ball centered at the origin.[12]

Theorem 8: *For any two-dimensional quasi-homogeneous complete intersection* $X=\{P_1=\cdots=P_{n-2}=0\}$ *in* $\mathbf{C}^n$, *the dimension of zero-dimensional Poisson homology*[9] *of* $\tilde{\Lambda}_P$ *on* X *is equal to the Milnor number of* X *at the origin.*

Proof: For simplicity we present a proof for $n=3$. As is known, the Milnor number μ always can be computed in a purely algebraic way.[10]

In particular for a hypersurface in three dimensions the Milnor number is equal to the dimension of local algebra of the singular point,[12] i.e., $\mu=\dim\mathbf{C}_3/(\partial_1P,\partial_2P,\partial_3P)$.

A simple algebraic verification shows that the theorem will be proved if we establish the following equality between ideals in $\mathbf{C}_3$:

$$\{\mathbf{C}_3,\mathbf{C}_3\}+(P)=(\partial_1P,\partial_2P,\partial_3P). \tag{33}$$

The fact that $\{\mathbf{C}_3,\mathbf{C}_3\}+(P)\supset(\partial_1P,\partial_2P,\partial_3P)$ is obvious since $\{x^i,x^j\}=\epsilon^{ijk}\partial_kP$, $\partial_iP\in\{\mathbf{C}_3,\mathbf{C}_3\}$.

The reverse inclusion is not true in general, but in the quasi-homogeneous case it may be proven using the Euler formula $P=(1/d)\,\Sigma_i x^i w_i\,\partial_iP$ and repeated application of the Leibniz rule.

Indeed, it is sufficient to prove that the bracket of arbitrary two monomials lies in the Jacobian ideal $(\partial_1P,\partial_2P,\partial_3P)$. For that one can proceed by induction over a **w**-degree of monomials and consider a bracket of the form $\{xe,ye'\}$ where e, e' are arbitrary monomials of the **w**-degree not exceeding a given number r which are all supposed to have brackets in the Jacobian ideal. Now we get $\{x^ie,x^je'\}=\{x^i,x^j\}ee'+\{e,e'\}x^ix^j+\{x^i,e'\}x^je+\{e,x^j\}x^ie'$. Apparently every member on the right hand side of the equation fulfils the induction assumption, which ends the proof.

□

In higher dimensions one makes use of the general formula $\mu=\dim(\mathbf{C}_n)^{n-2}/(\partial_1Q,\ldots,\partial_nQ)$, where $(\mathbf{C}_n)^{n-2}$ is the module of $n-2$ columns of polynomials from $\mathbf{C}_n$, ∂_iQ stands for column obtained by taking the i-th partial derivative of the column $Q=(P_1,\ldots,P_{n-2})^T$, and $(\partial_1Q,\ldots,\partial_nQ)$ denotes the submodule in $(\mathbf{C}_n)^{n-2}$ generated by columns ∂_iQ.[10]

The structure of the proof remains the same but computations become much more involved.

In conclusion we would like to notice that the natural problem of computing Poisson homology of JPS on the whole affine space seems to be very difficult. Using examples and technique presented in Ref. 13 it is possible to construct quadratic JPS on $\mathbf{R}^4$ with nontrivial second and third Poisson homology groups, but we were not able to calculate these groups explicitly. Some related results may be found in Ref. 14.

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An asymptotic expansion for the hypergeometric function ${}_2F_1(a,b;c;x)$

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Watson's treatise expresses the ordinary Bessel function as a limit of a hypergeometric function, where the first two parameters go to infinity, while simultaneously the argument goes to zero. We have extended Watson's method of proof to derive an asymptotic expression for the hypergeometric function to second order in the inverse of the first two parameters, with the ordinary Bessel function as its leading-order term. We show, as an example, that the use of this new result is pivotal in showing the correspondence between quantal and classical results of the differential cross section in Coulomb excitation. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1353185]

I. INTRODUCTION

The hypergeometric function ${}_2F_1(a,b;c;x)$[1,2] plays an important role in the solution of many physical problems. It is found, for example, in the quantal formulation of the differential cross section for excitation of atomic systems by the Coulomb field of charged particles.[3–6]

Historically, there have been two main approaches to modeling the electromagnetic interaction of two particles. In the *semiclassical approach*,[7] which has its roots in the classical study of radiation emitted by interacting charged particles,[8] the projectile is assumed to follow a classical hyperbolic trajectory, which determines the scattering angle, while the excitation of the target is caused by the resulting time-varying electric and magnetic fields. Results obtained through this technique provide both an intuitive physical picture of the scattering process and also serve as approximations to the quantal results for low-energy collisions.

In the *quantal approach*, and assuming the validity of first-order time-independent perturbation theory, the scattering process is described as a transition of the projectile between two Coulomb-distorted plane-wave states, while the target simultaneously undergoes a change in state. Both of these approaches have been reviewed by Alder *et al.*[5] and Biedenharn and Brussaard.[4]

In both approaches, expanding the interaction in multipoles and neglecting the penetration of the projectile into the target results, for each multipole order L, in a problem which factors into two parts—one solely dependent on the properties of the target in question, which controls the strength of the interaction, and a differential excitation function $\mathrm{d}f(\theta,\eta_i,\xi)/\mathrm{d}\Omega$, which determines the angular distribution of the scattered projectile. The angle θ is the deflection angle of the scattered particle, and the dimensionless Sommerfeld parameter η_i is defined by

$$\eta_i=\frac{Z_1Z_2e^2}{\hbar v_i}=Z_1Z_2\sqrt{\frac{M}{(E_i/\mathrm{Ry})}}, \tag{1.1}$$

where Z_1 and Z_2 are the charge numbers of the projectile and the atomic system, v_i their relative velocities, M the reduced mass of the system, in electron-mass units, and E_i is the initial kinetic energy of relative motion measured in rydbergs (13.8 eV). The dimensionless adiabaticity parameter ξ is defined by

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$$\xi = \eta_f - \eta_i = \eta_i \left[\left(1 - \frac{E_{if}}{E_i} \right)^{-1/2} - 1 \right]$$
$$= Z_1 Z_2 \sqrt{\frac{M}{(E_i/\mathrm{Ry})}} \left[\left(1 - \frac{E_{if}}{E_i} \right)^{-1/2} - 1 \right], \tag{1.2}$$

where the indices i and f refer to the initial and the final state, respectively, and $E_{if} = E_i - E_f$.

While, in general, the excitation function $\mathrm{d}f/\mathrm{d}\Omega$ can be expressed only as an infinite sum, in the special case where the organ of interaction is the dipole component of the electrostatic interaction ($E1$), the excitation functions in both the semiclassical and quantal derivations are soluble in terms of Bessel[7] and hypergeometric[9] functions, respectively.

By applying appropriate analytic continuations, we show, in Sec. III A, that the differential excitation function for θ bounded away from zero is left in terms of hypergeometric functions of the form

$$ {}_2F_1(\alpha \pm i\eta_i, \beta \mp i\eta_f; 1 \mp i\xi; t), \tag{1.3}$$

where α and β are integers and

$$t = \frac{\xi^2}{\xi^2 + 4\eta_i \eta_f \sin^2(\theta/2)}. \tag{1.4}$$

The usual procedure for obtaining a classical limit of a quantal result is to let η_i, $\eta_f \to \infty$ and assume ξ is finite.[4] Since our variable t becomes small as $\eta_i, \eta_f \to \infty$ and ξ is kept finite, it would seem to be the appropriate form of the quantal expression for investigating this correspondence between the semiclassical and quantal results directly.

Actually, demonstrating this result proves to be much more difficult than first thought, since it requires taking limits of hypergeometric functions whose first two parameters go to infinity, while the argument t goes to zero simultaneously. Further complicating the problem is the fact that, in many cases, the leading and first-order terms all cancel out in the subexpressions and a quadratic factor in η promotes the second-order correction terms in the asymptotic expressions to significance as $\eta \to \infty$.

For this reason, we have derived an asymptotic expansion for Gauss' hypergeometric function to second order in the inverses of the first two parameters and used the resulting expression to evaluate the limit.

The limiting case $E_i \to E_{if}$, in atomic collisions, needs special consideration and will be dealt with in a forthcoming paper. In this particular case, the parameters η_f, $\xi \to \infty$ simultaneously, whereas the parameter η_i remains finite and the argument $t \to 1$.

We used the symbolic computation program MAPLE VI[10] to help us with the algebraic manipulations in this work.

II. ASYMPTOTIC EXPANSION OF HYPERGEOMETRIC FUNCTION

Equation 5.7(1) of Watson's treatise[12] expresses the ordinary Bessel function as a limit of a hypergeometric function.

$$J_\nu(z) = \lim_{\lambda,\mu\to\infty} \frac{\left(\frac{1}{2}z\right)^\nu}{\Gamma(\nu+1)} {}_2F_1\left(\lambda, \mu; \nu+1; -\frac{z^2}{4\lambda\mu}\right). \tag{2.1}$$

${}_2F_1(a,b;c;x)$ is Gauss' hypergeometric function defined by

$$ {}_2F_1(a,b;c;x) = \sum_{n=0}^{\infty} \frac{(a)_n (b)_n}{n!(c)_n} x^n, \tag{2.2}$$

in the circle of convergence of this series ($|x|<1$) and by analytic continuation elsewhere.

We will extend Watson's method of proof to derive an asymptotic expression for the hypergeometric function with this result as its leading-order (constant) term. We believe this result has not been discussed before.

Expanding the right-hand side of the equation through the Gauss hypergeometric series (2.2) gives a summation whose $(m+1)$th term is

$$\frac{(-)^m(\frac{1}{2}z)^{\nu+2m}}{m!\Gamma(\nu+m+1)}\prod_{r=1}^{m-1}[(1+r\delta)(1+r\eta)], \tag{2.3}$$

where $\delta=\lambda^{-1}$ and $\eta=\mu^{-1}$. As is discussed in Ref. 11, Sec. 5.7, for $|\delta|<\delta_0<2|z|^{-1}$ and $\eta<\eta_0<2|z|^{-1}$, this term is smaller than the $(m+1)$th term in the absolutely convergent hypergeometric series, which represents

$$\frac{(\frac{1}{2}z)^{\nu}}{\Gamma(\nu+1)}\,{}_2F_1\left(\frac{1}{\delta_0},\frac{1}{\eta_0};\nu+1;\frac{z^2\delta_0\eta_0}{4}\right). \tag{2.4}$$

Since the Weierstrass test shows that the terms of this series are uniformly smaller than the terms of a convergent series of constants, for small enough δ and η in any circle around $z=0$, the series to which this term belongs is uniformly convergent for large enough λ and μ.

To extract higher-order corrections from this system, we require the product

$$\prod_{r=1}^{m-1}(1+r\delta)=(1+\delta)(1+2\delta)(1+3\delta)\cdots(1+(m-1)\delta) \tag{2.5}$$

in powers of δ. The constant term of this expression is obviously 1. The coefficient of the linear term is the sum of all possible integers between 1 and $(m-1)$, namely $m(m-1)/2$. The coefficient of the second-order term is zero for $m<2$ or the sum of all possible distinct products of two distinct integers between 1 and $(m-1)$ for $m\geqslant 2$. To derive a closed-form expression for this, we will first derive a closed-form expression for the sum of all possible multiplications of two (not necessarily distinct) integers between 1 and $(m-1)$. To obtain this, we use the following matrix.

$$\begin{array}{ccccc} 1\times1 & 1\times2 & 1\times3 & \cdots & 1\times(m-1) \\ 2\times1 & 2\times2 & 2\times3 & \cdots & 2\times(m-1) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (m-1)\times1 & (m-1)\times2 & (m-1)\times3 & \cdots & (m-1)\times(m-1) \end{array}. \tag{2.6}$$

We can use the result

$$\sum_{k=1}^{n}k=n(n+1)/2$$

to take the sum of each column and again to take the sum of all of the columns

$$[\tfrac{1}{2}m(m-1)+2\times\tfrac{1}{2}m(m-1)+\cdots+(m-1)\times\tfrac{1}{2}m(m-1)]=[\tfrac{1}{2}m(m-1)]^2=\tfrac{1}{4}m^2(m-1)^2. \tag{2.7}$$

In fact, this argument can be generalized by induction to products of any length

$$\sum_{k_1=1}^{m-1}\sum_{k_2=1}^{m-1}\cdots\sum_{k_n=1}^{m-1} k_1k_2\cdots k_n=\frac{1}{2}m(m-1)\sum_{k_1=1}^{m-1}\sum_{k_2=1}^{m-1}\cdots\sum_{k_{n-1}=1}^{m-1} k_1k_2\cdots k_{n-1}$$
$$=\left[\frac{1}{2}m(m-1)\right]^n. \tag{2.8}$$

This summation overcounts terms for our purposes, since it counts each product twice (once as $a\times b$ and once as $b\times a$) and also includes the squares, which are not obtained in our expansion. We therefore modify this expression somewhat and write

$$S=\frac{1}{2}\left[\left(\frac{m(m-1)}{2}\right)^2-\sum_{k=1}^{m-1}k^2\right]$$
$$=\frac{1}{2}\left[\left(\frac{m(m-1)}{2}\right)^2-\frac{m(m-1)(2m-2)}{6}\right]$$
$$=\frac{1}{24}m(m-1)(m-2)(3m-1), \tag{2.9}$$

which has the convenient property that it is 0 for $m<2$, thus eliminating the need to handle these cases separately.

Consequently, we now have an asymptotic expression for the $(m\text{-}1)$th term, viz.,

$$\frac{(-)^m(\frac{1}{2}z)^{\nu+2m}}{m!\Gamma(\nu+m+1)}\left[1+\frac{1}{2}m(m-1)\delta+\frac{1}{24}m(m-1)(m-2)(3m-1)\delta^2\right]$$
$$\times[1+\tfrac{1}{2}m(m-1)\eta+\tfrac{1}{24}m(m-1)(m-2)(3m-1)\eta^2]$$
$$=\frac{(-)^m\left(\frac{1}{2}z\right)^{\nu+2m}}{m!\Gamma(\nu+m+1)}\left[1+\frac{1}{2}m(m-1)(\delta+\eta)+\tfrac{1}{24}m(m-1)\right.$$
$$\left.\times(m-2)(3m-1)(\delta^2+\eta^2)+\frac{1}{4}m^2(m-1)^2\delta\eta\right], \tag{2.10}$$

and all that remains is to find a closed-form summation for each term in this expansion. The constant term is the one presented in Ref. 11, viz.,

$$\sum_{m=0}^{\infty}\frac{(-)^m(\frac{1}{2}z)^{\nu+2m}}{m!\Gamma(\nu+m+1)}=J_\nu(z). \tag{2.11}$$

To obtain the linear term, we notice that

$$\frac{1}{8}z^2J_{\nu+2}(z)=\frac{1}{2}\sum_{m=0}^{\infty}\frac{(-)^m(\frac{1}{2}z)^{\nu+4+2m}}{m!\Gamma(\nu+2+m+1)}$$
$$=\frac{1}{2}\sum_{n=2}^{\infty}\frac{(-)^n(\frac{1}{2}z)^{\nu+2n}}{(n-2)!\Gamma(\nu+n+1)}$$
$$=\frac{1}{2}\sum_{n=0}^{\infty}n(n-1)\frac{(-)^n(\frac{1}{2}z)^{\nu+2n}}{n!\Gamma(\nu+n+1)}, \tag{2.12}$$

where we have made use of the fact that the first two terms of the sum are 0 to extend the summation down to $n=0$. In obtaining the second-order terms, we use the generalized form of Eq. (2.12), namely,

$$(-)^k\left(\frac{1}{2}z\right)^k J_{\nu+k}(z)=\sum_{m=0}^{\infty}\frac{(-)^k\left(\frac{1}{2}z\right)^{\nu+2k+2m}}{m!\Gamma(\nu+k+m+1)}$$

$$=\sum_{n=0}^{\infty} n(n-1)\cdots(n-k+1)\frac{(-)^n\left(\frac{1}{2}z\right)^{\nu+2n}}{n!\Gamma(\nu+n+1)}. \tag{2.13}$$

Since the polynomials $\{1,m,m(m-1),m(m-1)(m-2),\cdots\}$ comprise a basis of all polynomials, we can sum the standard Bessel function expansion, with terms prefixed by any polynomial in the summation index, by expanding that polynomial over this basis and using the identity (2.13) to sum the sums from each component separately. Applying this to our present situation and writing $3m-1=8+3(m-3)$, we obtain

$$\frac{1}{24}\sum_{m=0}^{\infty} m(m-1)(m-2)(3m-1)\frac{(-)^m(\frac{1}{2}z)^{\nu+2m}}{m!\Gamma(\nu+m+1)}=-\frac{1}{24}z^3J_{\nu+3}(z)+\frac{1}{128}z^4J_{\nu+4}(z). \tag{2.14}$$

As well, using the identity $m(m-1)=2+4(m-2)+(m-2)(m-3)$, we get

$$\frac{1}{4}\sum_{m=0}^{\infty} m^2(m-1)^2\frac{(-)^m(\frac{1}{2}z)^{\nu+2m}}{m!\Gamma(\nu+m+1)}=\frac{1}{8}z^2J_{\nu+2}(z)-\frac{1}{8}z^3J_{\nu+3}(z)+\frac{1}{64}z^4J_{\nu+4}(z). \tag{2.15}$$

Combining the above gives the expansion

$$\frac{(\frac{1}{2}z)^{\nu}}{\Gamma(\nu+1)}{}_2F_1\left(\lambda,\mu;\nu+1;-\frac{z^2}{4\lambda\mu}\right)\sim J_{\nu}(z)+\frac{z^2}{8}J_{\nu+2}(z)\left(\frac{1}{\lambda}+\frac{1}{\mu}\right)$$
$$+\left[-\frac{1}{24}z^3J_{\nu+3}(z)+\frac{1}{128}z^4J_{\nu+4}(z)\right]\left(\frac{1}{\lambda^2}+\frac{1}{\mu^2}\right)$$
$$+\left[\frac{1}{8}z^2J_{\nu+2}(z)-\frac{1}{8}z^3J_{\nu+3}(z)+\frac{1}{64}z^4J_{\nu+4}(z)\right]\left(\frac{1}{\lambda\mu}\right), \tag{2.16}$$

for λ and μ large.

III. EXAMPLE: COULOMB EXCITATION AND HYPERGEOMETRIC FUNCTIONS

In the quantal expression for the E1 differential excitation function, we are bombarded with hypergeometric functions of the form

$${}_2F_1(\alpha+i\eta_i,\beta-i\eta_f;1-i\xi;t)={}_2F_1(\alpha+i\eta,\beta-i(\eta+\xi);1-i\xi;t), \tag{3.1}$$

or those of the form

$$ {}_2F_1(\alpha - i\eta_i, \beta + i\eta_f; 1 + i\xi; t) = {}_2F_1(\alpha - i\eta, \beta + i(\eta + \xi); 1 + i\xi; t). \tag{3.2} $$

In this section, we will use the variable name $\eta = \eta_i$ and express η_f as $\eta + \xi$, where convenient.

The hypergeometric function of form (3.1) may be converted to one of form (3.2) by making the substitution $\eta \to -\eta$ and $\xi \to -\xi$. For this reason, we will concern ourselves with expanding only the form (3.1) and will perform this transformation afterwards to handle form (3.2).

If we define $\lambda = \alpha + i\eta_i$ and $\mu = \beta - i\eta_f$, we may apply the asymptotic expression of Sec. II to these functions as $\eta \to \infty$. We define z by

$$ t = -\frac{z^2}{4\lambda\mu} \Rightarrow z = 2i\sqrt{\lambda\mu t}. \tag{3.3} $$

An additional complication arises, because z is a nonconstant function of η. Thus, in addition to the limiting process associated with the expansion of the hypergeometric function, there are additional terms associated with the variation in z as $\eta \to \infty$. We start by expanding z to second order in powers of η^{-1}:

$$ z = 2i\left[(\alpha + i\eta_i)(\beta - i\eta_f) \frac{\xi^2}{\xi^2 + 4\eta_i\eta_f \sin^2\left(\frac{\theta}{2}\right)} \right]^{1/2} \sim z_0 \left\{ 1 + c_1 \frac{1}{\eta} + c_2 \frac{1}{\eta^2} \right\}, \tag{3.4} $$

where

$$ \varepsilon = \frac{1}{\sin\left(\frac{\theta}{2}\right)}, \tag{3.5} $$

$$ z_0 = i|\xi|\varepsilon, \tag{3.6} $$

$$ c_1 = -\frac{i}{2}(\alpha - \beta), \tag{3.7} $$

$$ c_2 = \frac{(\alpha + \beta)^2 - 4i\xi\beta - \xi^2\varepsilon^2}{8}. \tag{3.8} $$

We want to expand the Bessel functions in the coefficients of the asymptotic expression of the hypergeometric function evaluated at z in powers of η^{-1}. Using the differentiation formula (9.1.30) of Ref. 2 and expanding the function $z^{-\nu}J_\nu(z)$ as a Taylor series about z_0, we find

$$ z^{-\nu}J_\nu(z) \sim z_0^{-\nu}J_\nu(z_0) - c_1 z_0^{-\nu+1}J_{\nu+1}(z_0)\frac{1}{\eta} - \left\{ c_2 z_0^{-\nu+1}J_{\nu+1}(z_0) + \frac{c_1^2}{2}[z_0^{-\nu+1}J_{\nu+1}(z_0) - z_0^{-\nu+2}J_{\nu+2}(z_0)] \right\}\frac{1}{\eta^2}. \tag{3.9} $$

Similarly, differentiating the Bessel function in the second coefficient gives

$$ \frac{\mathrm{d}}{\mathrm{d}z}[z^{-\nu+2}J_{\nu+2}(z)] = 4z^{-\nu+1}J_{\nu+2}(z) - z^{-\nu+2}J_{\nu+3}(z), \tag{3.10} $$

whence the linear approximation

$$z^{-\nu+2}J_{\nu+2}(z)=z_0^{2-\nu}J_{\nu+2}(z_0)+[4z_0^{-\nu+1}J_{\nu+2}(z_0)-z_0^{-\nu+2}J_{\nu+3}(z_0)]z_0c_1\frac{1}{\eta}. \tag{3.11}$$

Expanding the coefficients of the third and fourth term (beyond zeroth order) introduces only higher-order terms in η^{-1}. It suffices to use the ''constant'' approximation and evaluate them at z_0.

We now have the asymptotic expression

$$\begin{aligned}\frac{2^{-\nu}}{\Gamma(\nu+1)}{}_2F_1(\lambda,\mu;1+\nu;t)\sim{}&z_0^{-\nu}J_\nu(z_0)-c_1z_0^{-\nu+1}J_{\nu+1}(z_0)\frac{1}{\eta}\\&-\left\{c_2z_0^{-\nu+1}J_{\nu+1}(z_0)+\frac{c_1^2}{2}[z_0^{-\nu+1}J_{\nu+1}(z_0)-z_0^{-\nu+2}J_{\nu+2}(z_0)]\right\}\frac{1}{\eta^2}\\&+\left(\frac{1}{\lambda}+\frac{1}{\mu}\right)\{z_0^{2-\nu}J_{\nu+2}(z_0)-c_1[3z_0^{-\nu+2}J_{\nu+2}(z_0)-z_0^{-\nu+3}J_{\nu+3}(z_0)]\}\\&+\left(\frac{1}{\lambda^2}+\frac{1}{\mu^2}\right)\left\{-\frac{1}{24}z_0^{3-\nu}J_{\nu+3}(z_0)+\frac{1}{128}z_0^{4-\nu}J_{\nu+4}(z_0)\right\}+\left(\frac{1}{\lambda\mu}\right)\\&\times\left\{\frac{1}{8}z_0^{2-\nu}J_{\nu+2}(z_0)-\frac{1}{8}z_0^{3-\nu}J_{\nu+3}(z_0)+\frac{1}{64}z_0^{4-\nu}J_{\nu+4}(z_0)\right\}.\end{aligned} \tag{3.12}$$

Finally, we must expand the asymptotic variables λ and μ themselves in powers of η^{-1},

$$\frac{1}{\lambda}=\frac{1}{\alpha+i\eta}\sim-\frac{i}{\eta}+\frac{\alpha}{\eta^2}, \tag{3.13}$$

$$\frac{1}{\mu}=\frac{1}{\beta-i(\eta+\xi)}\sim\frac{i}{\eta}+\frac{\beta-i\xi}{\eta^2}, \tag{3.14}$$

$$\frac{1}{\lambda}+\frac{1}{\mu}\sim\frac{\alpha+\beta-i\xi}{\eta^2},\quad \frac{1}{\lambda^2}+\frac{1}{\mu^2}\sim-\frac{2}{\eta^2},\quad \frac{1}{\lambda\mu}\sim\frac{1}{\eta^2}. \tag{3.15}$$

With these expansions, the asymptotic expression becomes

$$\begin{aligned}{}_2F_1(\alpha+i\eta,\beta-i(\eta+\xi);1-i\xi;t)\sim{}&\Gamma(1-i\xi)\left(\frac{z_0}{2}\right)^{i\xi}\left\{J_{-i\xi}(z_0)-c_1z_0J_{1-i\xi}(z_0)\frac{1}{\eta}\right.\\&+\left[-c_2z_0J_{1-i\xi}(z_0)-\frac{c_1^2}{2}[z_0J_{1-i\xi}(z_0)-z_0^2J_{2-i\xi}(z_0)]\right.\\&\left.\left.+\frac{\alpha+\beta-i\xi+1}{8}z_0^2J_{2-i\xi}(z_0)-\frac{1}{24}z_0^3J_{3-i\xi}(z_0)\right]\frac{1}{\eta^2}\right\}.\end{aligned} \tag{3.16}$$

For the purposes of comparing with the semiclassical results, we express this asymptotic expansion in terms of the modified Bessel functions $I_\nu(z)$ (relation 9.6.3 of Ref. 2), and we obtain

$$
\begin{aligned}
&{}_2F_1(\alpha+i\eta,\beta-i(\eta+\xi);1-i\xi;t)\\
&\quad\sim\Gamma(1-i\xi)\left(\frac{x_0}{2}\right)^{i\xi}\Bigg\{I_{-i\xi}(x_0)-\frac{1}{2}i(\alpha-\beta)x_0I_{1-i\xi}(x_0)\frac{1}{\eta}\\
&\qquad-\Bigg\{\left[\frac{1}{12}(x_0^2-\xi^2-1-3\alpha(\alpha-1)-3\beta(\beta-1))+\frac{i\xi}{4}(\beta-\alpha)(\beta-\alpha-1)\right]x_0I_{1-i\xi}(x_0)\\
&\qquad+\left[\frac{1}{24}(3\alpha(\alpha-1)+3\beta(\beta-1)-6\alpha\beta+1)+\frac{i\xi}{24}\right]x_0^2I_{-i\xi}(x_0)\Bigg\}\frac{1}{\eta^2}\Bigg\},
\end{aligned}
\tag{3.17}
$$

where $x_0=|\xi|\varepsilon=|\xi|\sin(\theta/2)^{-1}$. Recurrence relations have been used to express all of the modified Bessel functions in terms of $I_{1-i\xi}$ and $I_{-i\xi}$.

Classical limit of the electric dipole differential excitation function. We begin our discussion with the excitation function expression,[9,12] but make explicit the distinction between the repulsive and attractive cases by writing ξ as $\mp|\xi|$. We can convert the repulsive case ($\eta_i>0$) to the attractive case ($\eta_i<0$) by simply switching the signs of η_i, η_f, and ξ. The total effect of this transformation is to replace the factor of $\exp(-\pi|\xi|)$, for repulsive potentials, by a factor of $\exp(+\pi|\xi|)$ for attractive potentials,

$$
\mathrm{d}f_{E1}=\frac{8\pi^3\eta_i\eta_f}{9\xi^2}\frac{e^{\mp\pi|\xi|}}{\sinh(\pi\eta_i)\sinh(\pi\eta_f)}\,\mathrm{d}/\mathrm{d}x\left(-x\frac{\mathrm{d}}{\mathrm{d}x}|\,{}_2F_1(-i\eta_i,-i\eta_f;1;x)|^2\right),
\tag{3.18}
$$

where

$$
x=-\frac{4\eta_i\eta_f}{\xi^2}\sin^2\left(\frac{\theta}{2}\right).
\tag{3.19}
$$

We will henceforth omit the subscripts and write ${}_2F_1(\ldots)$ simply as $F(\cdots)$. Expanding out the derivatives, and making use of the analytic continuations 15.3.15 and 15.3.6 of Ref. 2, we are left with

$$
\begin{aligned}
\mathrm{d}f_{E1}=&\frac{16\pi^3}{9}\frac{(\eta_i\eta_f)^2te^{\pm\pi|\xi|}}{\xi^2\sinh(\pi\eta_i)\sinh(\pi\eta_f)}\times\Bigg\{\frac{|\Gamma(i\xi)|^2}{|\Gamma(1+i\eta_i)|^2\Gamma(1+i\eta_f)|^2}[\mathrm{Im}(e1-e3)-\mathrm{Re}(e4)]\\
&+\mathrm{Im}\left(\frac{t^{-i\xi}\Gamma^2(i\xi)}{\Gamma^2(1-i\eta_i)\Gamma^2(1+i\eta_f)}(e2-e5)\right)-\mathrm{Re}\left(\frac{t^{-i\xi}\Gamma^2(i\xi)}{\Gamma^2(1-i\eta_i)\Gamma^2(1+i\eta_f)}(e6)\right)\\
&+t\Bigg[\frac{|\Gamma(i\xi)|^2}{|\Gamma(1+i\eta_i)|^2\Gamma(1+i\eta_f)|^2}[\mathrm{Im}(e3)+\mathrm{Re}(e4)]+\mathrm{Im}\left(\frac{t^{-i\xi}\Gamma^2(i\xi)}{\Gamma^2(1-i\eta_i)\Gamma^2(1+i\eta_f)}(e5)\right)\\
&+\mathrm{Re}\left(\frac{t^{-i\xi}\Gamma^2(i\xi)}{\Gamma^2(1-i\eta_i)\Gamma^2(1+i\eta_f)}(e6)\right)\Bigg]\Bigg\},
\end{aligned}
\tag{3.20}
$$

where

$$
\begin{aligned}
e1=&-\eta_iF(1+i\eta_i,1-i\eta_f;1-i\xi;t)F(1-i\eta_i,i\eta_f;1+i\xi;t)\\
&+\eta_fF(1+i\eta_i,1-i\eta_f;1-i\xi;t)F(-i\eta_i,1+i\eta_f;1+i\xi;t),
\end{aligned}
\tag{3.21}
$$

$$
\begin{aligned}
e2=&-\eta_fF(1+i\eta_i,1-i\eta_f;1-i\xi;t)F(i\eta_i,1-i\eta_f;1-i\xi;t)\\
&+\eta_iF(1+i\eta_i,1-i\eta_f;1-i\xi,t)F(1+i\eta_i,-i\eta_f;1-i\xi;t),
\end{aligned}
\tag{3.22}
$$

$$e3 = -\eta_i F(1+i\eta_i,2-i\eta_f;1-i\xi;t)F(1-i\eta_i,i\eta_f;1+i\xi;t) + \eta_f F(2+i\eta_i,1-i\eta_f;1-i\xi;t)F(-i\eta_i,1+i\eta_f;1+i\xi;t), \tag{3.23}$$

$$e4 = \eta_i\eta_f[F(1+i\eta_i,2-i\eta_f;1-i\xi;t)F(1-i\eta_i,i\eta_f;1+i\xi;t) + F(2+i\eta_i,1-i\eta_f;1-i\xi;t)F(-i\eta_i,1+i\eta_f;1+i\xi;t) - 2F(1-i\eta_i,1+i\eta_f;1+i\xi;t)F(1+i\eta_i,1-i\eta_f;1-i\xi;t)], \tag{3.24}$$

$$e5 = -\eta_f F(1+i\eta_i,2-i\eta_f;1-i\xi;t)F(i\eta_i,1-i\eta_f;1-i\xi;t) + \eta_i F(2+i\eta_i,1-i\eta_f;1-i\xi;t)F(1+i\eta_i,-i\eta_f;1-i\xi;t), \tag{3.25}$$

$$e6 = \eta_f^2 F(1+i\eta_i,2-i\eta_f;1-i\xi;t)F(i\eta_i,1-i\eta_f;1-i\xi;t) + \eta_i^2 F(2+i\eta_i,1-i\eta_f;1-i\xi;t)F(1+i\eta_i,-i\eta_f;1-i\xi;t) - 2\eta_i\eta_f F^2(1+i\eta_i,1-i\eta_f;1-i\xi;t), \tag{3.26}$$

t being given by Eq. (1.4).

Using the asymptotic expression (3.17), we see that as $\eta\to\infty$

$$A\,\mathrm{Im}(e1-e3)\to Cx_0\,\mathrm{Re}[I_{1-i\xi}(x_0)I_{i\xi}(x_0)], \tag{3.27}$$

$$\mathrm{Im}(B(e2-e5))\to -Cx_0\,\mathrm{Im}[iI_{1-i\xi}(x_0)I_{-i\xi}(x_0)], \tag{3.28}$$

$$A\,\mathrm{Re}(e4)\to -C\left[\frac{1}{2}x_0^2|I_{i\xi}(x_0)|^2+\frac{1}{2}x_0^2|I_{1+i\xi}(x_0)|^2-x_0\,\mathrm{Re}(I_{i\xi}(x_0)I_{1-i\xi}(x_0) - \xi x_0\,\mathrm{Im}(I_{i\xi}(x_0)I_{1-i\xi}(x_0))\right], \tag{3.29}$$

$$\mathrm{Re}(B(e6))\to -C[\xi^2\,\mathrm{Re}(I_{-i\xi}^2(x_0))-\tfrac{1}{2}x_0^2\,\mathrm{Re}(I_{-i\xi}^2(x_0))-\tfrac{1}{2}x_0^2\,\mathrm{Re}(I_{1-i\xi}^2(x_0)) + \xi x_0\,\mathrm{Re}(iI_{-i\xi}(x_0)I_{1-i\xi}(x_0))+x_0\,\mathrm{Re}(I_{-i\xi}(x_0)I_{1-i\xi}(x_0))], \tag{3.30}$$

where

$$A=\frac{|\Gamma(i\xi)|^2}{|\Gamma(1+i\eta_i)|^2|\Gamma(1+i\eta_f)|^2}, \tag{3.31}$$

$$B=\frac{t^{-i\xi}\Gamma^2(i\xi)}{\Gamma^2(1-i\eta_i)\Gamma^2(1+i\eta_f)}, \tag{3.32}$$

$$C=\frac{|\Gamma(1+i\xi)|^4}{\xi^2|\Gamma(1+i\eta_i)|^2|\Gamma(1+i\eta_f)|^2}, \tag{3.33}$$

and relation 6.1.31 of Ref. 2 defines

$$|\Gamma(1+i\eta)|^2=\frac{\pi\eta}{\sinh(\pi\eta)}. \tag{3.34}$$

This leaves the result

$$\mathrm{d}f_{E1}\rightarrow\frac{4\pi^3}{9}\frac{\varepsilon^2 e^{\pm|\xi|}}{\sinh^2(\pi|\xi|)}\times\left\{\frac{1}{2}x_0^2[|I_{i\xi}(x_0)|^2-\mathrm{Re}(I^2_{-i\xi}(x_0))+|I_{1-i\xi}(x_0)|^2-\mathrm{Re}(I^2_{1-i\xi}(x_0))]\right.$$
$$\left.+\mathrm{sgn}(\xi)x_0[\mathrm{Re}(iI_{-i\xi}(x_0)I_{1-i\xi}(x_0))-\mathrm{Im}(I_{i\xi}(x_0)I_{1-i\xi}(x_0))]+\xi^2\,\mathrm{Re}(I^2_{-i\xi}(x_0))\right\}. \tag{3.35}$$

To simplify this expression, we make use of the complex-number identity

$$\mathrm{Re}(z^2)=\mathrm{Re}^2(z^*)-\mathrm{Im}^2(z^*). \tag{3.36}$$

Thus, using relations (9.6.2) and (9.6.26) of Ref. 2, we obtain

$$\mathrm{d}f_{E1}\rightarrow\frac{4\pi^3}{9}\frac{\xi^2\varepsilon^2 e^{\pm\pi|\xi|}}{\sinh^2(\pi|\xi|)}\{(\varepsilon^2-1)\mathrm{Im}^2(I_{i\xi}(|\xi|\varepsilon))[\varepsilon\,\mathrm{Im}(I_{1-i\xi}(|\xi|\varepsilon))-\mathrm{sgn}(\xi)\mathrm{Re}(I_{i\xi}(|\xi|\varepsilon))]^2\}$$
$$=\frac{4\pi}{9}\xi^2\varepsilon^2 e^{\pm\pi|\xi|}\{(\varepsilon^2-1)K^2_{i\xi}(|\xi|\varepsilon)+\varepsilon^2K'^2_{i\xi}(|\xi|\varepsilon)\}, \tag{3.37}$$

as $\eta\rightarrow\infty$. $K_\nu(z)$ is the modified Bessel function of the second kind and $K'_\nu(z)$ is its derivative with respect to its argument and $\varepsilon=\sin(\theta/2)^{-1}$. This last expression is the semiclassical result quoted by Alder *et al.* [see Eqs. (II A.29) and (II E.57) of Ref. 3].

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Solutions of relativistic wave equations in superpositions of Aharonov–Bohm, magnetic, and electric fields

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We present new exact solutions (in $3+1$ and $2+1$ dimensions) of relativistic wave equations (Klein–Gordon and Dirac) in external electromagnetic fields of special form. These fields are combinations of Aharonov–Bohm solenoid field and some additional electric and magnetic fields. In particular, as such additional fields, we consider longitudinal electric and magnetic fields, some crossed fields, and some special nonuniform fields. The solutions obtained can be useful to study the Aharonov–Bohm effect in the corresponding electromagnetic fields. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1353182]

I. INTRODUCTION

The Aharonov–Bohm (AB) effect[1] plays an important role in quantum theory refining the status of electromagnetic potentials in this theory. First this effect was discussed in relation to a study of interaction between a nonrelativistic charged particle and an infinitely long and infinitesimally thin magnetic solenoid field (further the AB field) (a similar effect was discussed earlier by Ehrenberg and Siday[2]). It was discovered that particle wave functions vanish at the solenoid line. In spite of the fact that the magnetic field vanishes out of the solenoid, the phase shift in the wave functions is proportional to the corresponding magnetic flux.[3] A nontrivial particle scattering by the solenoid is interpreted as a possibility for quantum particles to ''feel'' potentials of the corresponding electromagnetic field. Indeed, potentials of the AB field do not vanish out of the solenoid. AB scattering for spinning particles was considered in Refs. 4 and 5 using exact solutions of the Dirac equation in the AB field. A number of theoretical works and convincing experiments were done to clarify the AB effect and to prove its existence (see, e.g., Refs. 6–9).

Progress in the study of the AB effect may be related to revealing new situations, where the effect takes place. For example, one can consider more complicated configurations of electromagnetic fields, different regimes of particle motions, different dimensions, and so on. To study these new possibilities one has to have exact solutions of the corresponding quantum equations in these configurations of electromagnetic fields. In this relation, we ought to mention exact solutions of the Schrödinger equation in a superposition of the AB field and a uniform magnetic field.[10] The latter solutions were analyzed in Refs. 11–13 from AB effect point of view. The corresponding coherent states were constructed in Ref. 12. Klein–Gordon and Dirac equations for particles moving in a superposition of the AB field, Coulomb field, and magnetic monopole field were found and analyzed in Refs. 14 and 15.

In this article we present new exact solutions (in $3+1$ and $2+1$ dimensions) of relativistic wave equations (Klein–Gordon and Dirac) in external electromagnetic fields of special form. These fields are combinations of the AB field and different types of electric and magnetic fields. In Sec. II we consider the AB field combined with longitudinal electromagnetic fields. In Sec. III superpositions of the AB, longitudinal, and crossed fields are studied. In Secs. IV and V we present solutions in the AB field combined with some nonuniform fields. Here we also discuss

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some relevant solutions in $2+1$ dimensional quantum electro dynamics (QED). Special functions and their properties, which are used in the article, are present in the Appendix.

Most of works, in which the AB effect was studied, are based on the use of exact solutions of the Schrödinger equation in the AB field.[1] Consider the latter a field in $3+1$ dimensions. If the magnetic solenoid is placed along the axis $z=x^3$, then the AB field can be given by potentials [we denote these potentials as $A^{(0)}_\mu(x)$, $x=(x^\mu,\mu=0,1,2,3)$] of the form

$$A^{(0)}_1=\frac{\Phi}{2\pi r^2}x^2,\quad A^{(0)}_2=-\frac{\Phi}{2\pi r^2}x^1,\quad A^{(0)}_0=A^{(0)}_3=0,\quad r^2=(x^1)^2+(x^2)^2. \tag{1.1}$$

The AB magnetic field has the form $\mathbf{H}^{(0)}=(0,0,H^{(0)})$, where $H^{(0)}$ is singular at $r=0$,

$$H^{(0)}=\Phi\,\delta(x^1)\,\delta(x^2). \tag{1.2}$$

The AB field creates a finite magnetic flux Φ along the axis z. It is convenient to define a quantity μ, which characterizes the magnetic flux Φ and is related to the latter as follows:

$$\Phi=(l_0+\mu)\Phi_0,\quad \Phi_0=2\pi c\hbar/|e|,\quad 0\leqslant\mu<1, \tag{1.3}$$

where l_0 is integer, and $e=-|e|$ is the charge of the electron. In what follows, we call μ the mantissa of the magnetic flux Φ. By definition μ is a positive fractional part of the magnetic flux if the latter is measured in units of quanta Φ_0. Cylindrical coordinates r,φ ($x^1=r\cos\varphi$, $x^2=r\sin\varphi$) are preferable for AB field consideration. In these coordinates

$$\frac{|e|}{c\hbar}A^{(0)}_1=\frac{l_0+\mu}{r}\sin\varphi,\quad \frac{|e|}{c\hbar}A^{(0)}_2=-\frac{l_0+\mu}{r}\cos\varphi. \tag{1.4}$$

In the present article, we are going to consider particle motion in electromagnetic fields A_μ that are a combination of the AB field and some additional fields with potentials $A^{(1)}_\mu$,

$$A_\mu=A^{(0)}_\mu+A^{(1)}_\mu. \tag{1.5}$$

Electromagnetic potentials enter in relativistic wave equations only via the operators of momenta $P_\mu=i\hbar\partial_\mu-(e/c)A_\mu$. Doing the transformation $\Psi(x)=e^{-il_0\varphi}\tilde{\Psi}(x)$ of wave functions, we can eliminate l_0 dependence of AB potentials in equations for $\tilde{\Psi}(x)$. Indeed, such equations already contain momentum operators of the form

$$\begin{gathered}e^{il_0\varphi}P_\mu e^{-il_0\varphi}=i\hbar\partial_\mu-\frac{e}{c}(\tilde{A}^{(0)}_\mu+A^{(1)}_\mu),\\ \frac{|e|}{ch}\tilde{A}^{(0)}_1=\frac{\mu}{r}\sin\varphi,\quad \frac{|e|}{ch}\tilde{A}^{(0)}_2=-\frac{\mu}{r}\cos\varphi,\quad \tilde{A}^{(0)}_0=\tilde{A}^{(0)}_3=0.\end{gathered} \tag{1.6}$$

Thus, all the matrix elements of any axial-symmetric operators depend on the mantissa of the magnetic flux only.

II. AHARONOV–BOHM FIELD COMBINED WITH LONGITUDINAL ELECTROMAGNETIC FIELDS

Here we consider particle motion in a superposition of the AB field and of some longitudinal electromagnetic fields. We call electric $\mathbf{E}$ and magnetic $\mathbf{H}$ fields longitudinal ones whenever they are parallel and are directed along the AB solenoid (along the axis z),

$$\mathbf{E}=E\mathbf{n},\quad \mathbf{H}=H\mathbf{n},\quad \mathbf{n}^2=1,\quad \mathbf{n}=(0,0,1). \tag{2.1}$$

It follows from Maxwell equations that in this case the functions E and H must obey the conditions

$$\begin{aligned} &E=E(x^0,x^3)=\partial_0 A_3-\partial_3 A_0, \quad A_0=A_0(x^0,x^3), \quad A_3=A_3(x^0,x^3), \\ &H=H(x^1,x^2)=\partial_2 A_1-\partial_1 A_2, \quad A_1=A_1(x^1,x^2), \quad A_2=A_2(x^1,x^2), \end{aligned} \tag{2.2}$$

where $A_0(x^0,x^3)$, $A_1(x^1,x^2)$, $A_2(x^1,x^2)$, $A_3(x^0,x^3)$ are arbitrary functions of the indicated arguments. Exact solutions of the relativistic wave equations in such fields (in the absence of the AB field) were studied in Refs. 16 and 17. As we show in the following, whenever the AB field is present, then exact solutions of the relativistic wave equations can be found only in the axially symmetric case with the magnetic field having the form $H=H(r)$. Thus, potentials of additional fields, which are considered in the present section, have the following form: $A_0^{(1)}=A_0^{(1)}(x^0,x^3)$, $A_3^{(1)}=A_3^{(1)}(x^0,x^3)$ arbitrary and

$$A_1^{(1)}=\frac{c\hbar}{|e|}\frac{A(r)}{r}\sin\varphi, \quad A_2^{(1)}=-\frac{c\hbar}{|e|}\frac{A(r)}{r}\cos\varphi, \quad H(r)=\frac{c\hbar}{|e|}\frac{A'(r)}{r}, \tag{2.3}$$

where $A(r)$ is an arbitrary function of r.

A. Classical description of radial motion

To interpret quantum numbers of wave functions, it is often useful to have a classical picture of the problem. That is why we present here a classical analysis of the particle motion in fields under consideration.

Consider classical trajectories that do not intersect the axis z, thus they do not ''feel'' the existence of the AB field. For such trajectories, the quantity P_r^2 is an integral of motion ($c^2P_r^2$ is said to be radial energy),

$$P_r^2=P_1^2+P_2^2=\hbar^2k_1^2, \quad m_0^2c^2+P_r^2=P_0^2-P_3^2, \tag{2.4}$$

where P_μ is the classical kinetic momentum (a classical analog of the operators P_μ) and m_0 is the rest mass. L_z is an integral of motion as well (L is the angular momentum),

$$L_z=\tilde{L}_z-\hbar(l_0+\mu)=\hbar(l-l_0), \quad \tilde{L}_z=x^1P^2-x^2P^1-\hbar A(r)=\hbar(l+\mu). \tag{2.5}$$

Here l is arbitrary (l will be an integer in quantum theory).

As will be seen in the following, exact solutions of relativistic wave equations can be found whenever the functions $A(r)$ in Eq. (2.3) have the form

$$(1) \quad A(r)=0, \tag{2.6}$$

$$(2) \quad A(r)=\frac{\gamma r^2}{2}, \quad \gamma>0, \tag{2.7}$$

$$(3) \quad A(r)=\gamma r, \quad \gamma>0. \tag{2.8}$$

The first case corresponds to the absence of an additional electromagnetic field, the second one corresponds to the additional constant uniform magnetic field H along the solenoid ($\gamma=|eH|/c\hbar$), and the third one corresponds to the additional constant magnetic field $H(r)=b/r$, ($\gamma=|eb|/c\hbar$). Consider classical motion in these cases.

(1) For $A(r)=0$, the momenta P_1 and P_2 are integrals of motion. Then the radial motion (the motion in x^1,x^2 plane) is parametrized by the proper time τ and can be presented as

$$x^1=\frac{P^1}{m_0c}\tau+x^1_{(0)}, \quad x^2=\frac{P^2}{m_0c}\tau+x^2_{(0)}, \tag{2.9}$$

where $x^1_{(0)}$, $x^2_{(0)}$ are integration constants. In this case

$$\tilde{L}_z=\hbar(l+\mu)=x^1_{(0)}P^2-x^2_{(0)}P^1. \tag{2.10}$$

Consider the quantity

$$\Delta R=P_r^{-1}(x^1_{(0)}P^2-x^2_{(0)}P^1)=\frac{l+\mu}{k_1}. \tag{2.11}$$

One can show that $|\Delta R|$ characterizes a minimal distance between the trajectory (2.9) and the axis x^3. All the classical trajectories are divided in two groups according to the sign of $l+\mu$. Trajectories with $l+\mu>0$ can be called right ones and those with $l+\mu<0$ can be called left ones. The reason is the following: Looking from the positive z direction, one can see that a minimal angle rotation from the vector $\mathbf{r}=(x^1,x^2,x^3)$ to the particle momentum is counterclockwise for the right trajectories and clockwise for left ones.

(2) For $A(r)=\gamma r^2/2$, the radial motion has the form

$$\begin{gathered} x^1=R\cos\kappa+x^1_{(0)}, \quad x^2=R\sin\kappa+x^2_{(0)}, \\ \kappa=\omega_0\tau+\varphi_0, \quad \omega_0=\frac{\gamma}{m}, \quad m=\frac{m_0c}{\hbar}. \end{gathered} \tag{2.12}$$

Here R, φ_0, $x^1_{(0)}$, $x^2_{(0)}$ are integration constants. The trajectories (2.12) are circles of radius R with centers having coordinates $x^1_{(0)}$, $x^2_{(0)}$,

$$(x^1-x^1_{(0)})^2+(x^2-x^2_{(0)})^2=R^2. \tag{2.13}$$

One can easily find

$$\begin{gathered} P_r=\hbar\gamma R, \quad l+\mu=\frac{\gamma}{2}(R^2-R_0^2), \quad (x^1_{(0)})^2+(x^2_{(0)})^2=R_0^2, \\ l+\mu\leqslant\frac{\gamma R^2}{2}=\frac{P_r^2}{2\hbar^2\gamma}=\frac{k_1^2}{2\gamma}. \end{gathered} \tag{2.14}$$

We can see that classical trajectories with $l\geqslant-\mu$ embrace the solenoid, and ones with $l<-\mu$ do not. In quantum theory these conditions are $l\geqslant 0$ and $l<0$, respectively. The quantity ΔR characterizes a minimal distance between the trajectory (2.12) and the solenoid,

$$\Delta R=|R-R_0|=\frac{2|l+\mu|}{\gamma(R+R_0)}. \tag{2.15}$$

(3) Consider finally $A(r)=\gamma r$. Here the radial motion depends essentially on values of constants a, ε,

$$a=\frac{P_r}{\hbar\gamma}=\frac{k_1}{\gamma}>0, \quad \varepsilon=(l+\mu). \tag{2.16}$$

For $\varepsilon=1$, the classical motion is possible only if $a>1$. For $\varepsilon=-1$, the classical motion is possible if $a>0$. Whenever $a\geqslant 1$ we get unbounded motion for r. For $0<a<1$, $\varepsilon=-1$, this motion is bounded. In the following we present the radial motion in s parametrization,

$$
\begin{gathered}
a>1:\ \ r=\frac{|l+\mu|(a\cosh s+\varepsilon)}{\gamma(a^2-1)},\quad \tau=\frac{|l+\mu|(a\sinh s+\varepsilon s)}{\gamma^2(a^2-1)^{3/2}},\\
\varphi-\varphi_0=\frac{s}{\sqrt{a^2-1}}+2\varepsilon\arctan\left(\sqrt{\frac{a-\varepsilon}{a+\varepsilon}}\tanh\frac{s}{2}\right),\\
a=1,\quad \varepsilon=-1:\ \ 2\gamma r=|l+\mu|(s^2+1),\quad 2\gamma^2\tau=|l+\mu|m\left(\frac{s^3}{3}+s\right),\\
\varphi-\varphi_0=s-2\arctan s,\\
a<1,\quad \varepsilon=-1:\ \ r=\frac{|l+\mu|(1-a\cos s)}{\gamma(1-a^2)},\quad \tau=\frac{|l+\mu|m(s-a\sin s)}{\gamma^2(1-a^2)^{3/2}},\\
\varphi-\varphi_0=s\left(\frac{1}{\sqrt{1-a^2}}-1\right)-2\arctan\left(\frac{a\sin s}{1+\sqrt{1-a^2}-a\cos s}\right).
\end{gathered}
\tag{2.17}
$$

In all the cases under consideration, the minimal distance between a trajectory and the solenoid is defined by

$$
\Delta R=\frac{|l+\mu|}{\gamma|a-\varepsilon|}. \tag{2.18}
$$

Thus, the quantity l has a clear classical interpretation.

B. Klein–Gordon equation in longitudinal fields

Here we consider solutions of the Klein–Gordon equation

$$
(P_\mu P^\mu-m_0^2c^2)\Psi(x)=0 \tag{2.19}
$$

in the superposition of the external fields (1.1) and (2.3). In this case, the operators (2.4) are integrals of motion. Whenever an additional field is axial-symmetric one (2.3), then the operator (2.5) is an integral of motion as well. Thus, we subject solutions of Eq. (2.19) to the following additional conditions:

$$
\hbar^{-2}(P_1^2+P_2^2)\Psi(x)=k_1^2\Psi(x),\quad \hbar^{-2}(P_0^2-P_3^2)\Psi(x)=(m^2+k_1^2)\Psi(x). \tag{2.20}
$$

Then such solutions can be presented in the form $\Psi(x)=\psi(x^1,x^2)\Phi(x^0,x^3)$, where the functions ψ and Φ obey

$$
\hbar^{-2}(P_1^2+P_2^2)\psi(x^1,x^2)=k_1^2\psi(x^1,x^2), \tag{2.21}
$$

$$
\hbar^{-2}(P_0^2-P_3^2)\Phi(x^0,x^3)=(m^2+k_1^2)\Phi(x^0,x^3). \tag{2.22}
$$

The AB field does not enter in Eq. (2.22). This equation can be solved for a large class of electromagnetic fields. All the corresponding solutions of Eq. (2.22) are described in detail in Refs. 16 and 17, that is why we do not present them here.

Let us turn to Eq. (2.21). As was mentioned previously, exact solutions of this equation can be found only in the superposition of the AB field and fields (2.6)–(2.8). In all these cases, the operator L_z is an integral of motion, thus we can search for solutions which are eigenvectors for the latter operator. In cylindrical coordinates, we get

$$L_z\psi(r,\varphi)=-i\hbar\partial_\varphi\psi(r,\varphi)=\hbar(l-l_0)\psi(r,\varphi),\quad \psi(r,\varphi)=\frac{\exp[i(l-l_0)\varphi]}{\sqrt{2\pi}}\psi(r). \tag{2.23}$$

Whenever additional fields have the structure (2.3), the radial function $\psi(r)$ obeys

$$\hat{R}\psi(r)=k_1^2\psi(r),\quad \hat{R}=\left(\frac{l+\mu+A(r)}{r}\right)^2-\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}-\frac{\mathrm{d}^2}{\mathrm{d}r^2}. \tag{2.24}$$

C. Solutions of the radial equation in the absence of additional fields

Consider Eq. (2.24) for $A(r)=0$,

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}\psi}{\mathrm{d}r}+\left[k_1^2-\frac{(l+\mu)^2}{r^2}\right]\psi=0. \tag{2.25}$$

A general solution of the equation can be written via Bessel functions $J_\nu(x)$, (Ref. 18, 8.402),

$$\psi(r)=\psi_{k_1,l}(r)=c_1J_\nu(k_1r)+c_2J_{-\nu}(k_1r),\quad \nu=|l+\mu|. \tag{2.26}$$

Solutions, which are bounded for all $r\geqslant 0$, must have $c_2=0$. In this case $\psi_{k_1,l}$ form an orthogonal and complete set of functions $(k_1,k_1'>0)$,

$$\int_0^\infty J_\nu(k_1'r)J_\nu(k_1r)r\,\mathrm{d}r=k_1^{-1}\delta(k_1-k_1'),\quad \int_0^\infty J_\nu(k_1r')J_\nu(k_1r)k_1\,\mathrm{d}k_1=\frac{\delta(r-r')}{r}. \tag{2.27}$$

Suppose $l=0,-1$, $\mu\neq 0$ (note that in this case the corresponding classical trajectories pass maximally close to the solenoid). Then we have a special case. Here there are solutions of the form (2.26) with $c_1=0$, $c_2\neq 0$ (of course they are unbounded), which obey relations (2.27). Moreover, there are solutions (2.26) with both $c_1\neq 0$ and $c_2\neq 0$, which are unbounded and not orthogonal,

$$\int_0^\infty J_\nu(k_1'r)J_{-\nu}(k_1r)r\,\mathrm{d}r=\frac{2\sin\nu\pi}{\pi(k_1'^2-k_1^2)}\left(\frac{k_1'}{k_1}\right)^\nu,\quad k_1>k_1',\quad |\nu|<1. \tag{2.28}$$

However, these solutions are quadratically integrable [due to (2.27)] and form a complete set of functions (in fact, an overcomplete set). Besides, Eq. (2.25) has solutions of the form

$$\psi(r)=K_\nu(qr),\quad k_1^2=-q^2, \tag{2.29}$$

where $K_\nu(r)$ are Macdonald functions (Ref. 18, 8.407). These functions have a finite norm ($\delta=\arg q$)

$$\int_0^\infty K_\nu^*(qr)K_\nu(qr)r\,\mathrm{d}r=\frac{\pi\sin 2\nu\delta}{2|q|^2\sin\nu\pi\sin 2\delta},\quad |\nu|<1,\quad -\pi/2<\delta<\pi/2\quad (\mathrm{Re}\,q>0). \tag{2.30}$$

But they are not orthogonal with respect to q,

$$\int_0^\infty K_\nu(q'r)K_\nu(qr)r\,\mathrm{d}r=\frac{\pi(q^{2\nu}-q'^{2\nu})}{2(q^2-q'^2)\sin\nu\pi},\quad |\nu|<1. \tag{2.31}$$

In particular, for $\nu=0$, we get

$$\int_0^\infty K_0^*(qr)K_0(qr)r\ \mathrm{d}r=\frac{\delta}{|q|^2\sin 2\delta},\quad \int_0^\infty K_0(q'r)K_0(qr)r\ \mathrm{d}r=\frac{\ln q-\ln q'}{q^2-q'^2}. \tag{2.32}$$

The above-mentioned peculiarities are related to the loss of hermicity of the operator $\hat{R}$ for $l=0,-1$, $\mu\neq 0$. A similar problem was discussed in Ref. 19.

D. Uniform magnetic field

Here we consider a superposition of AB field (1.1) and a uniform magnetic field (2.7). It is useful to introduce dimensionless operators a_k, a_k^+, $k=1,2$ by the following relations:

$$\begin{gathered}\hbar\sqrt{2\gamma}a_1=-iP_1-P_2,\quad \hbar\sqrt{2\gamma}a_1^+=iP_1-P_2,\quad \gamma=\frac{|eH|}{c\hbar},\\ \hbar\sqrt{2\gamma}a_2=-iP_1+P_2+\hbar\gamma(x^1+ix^2),\quad \hbar\sqrt{2\gamma}a_2^+=iP_1+P_2+\hbar\gamma(x^1-ix^2).\end{gathered} \tag{2.33}$$

Considering coordinates and momenta in these relations as classical quantities, we can get a representation for the classical motion (2.12) in terms of a_1 and a_2,

$$a_1=\sqrt{\frac{\gamma}{2}}\mathrm{Re}^{-i\kappa},\quad a_2=\sqrt{\frac{\gamma}{2}}(x_0^1+ix_0^2),\quad (x_0^1+ix_0^2)=R_0e^{i\delta}. \tag{2.34}$$

The following operator relations take place:

$$P_r^2=P_1^2+P_2^2=\hbar^2\gamma(a_1^+a_1+a_1a_1^+),\quad 2L_z=\hbar(a_1^+a_1+a_1a_1^+-a_2^+a_2-a_2a_2^+). \tag{2.35}$$

We introduce also a dimensionless coordinate ρ instead of r,

$$\rho=\frac{\gamma r^2}{2},\quad \mathrm{d}x^1\,\mathrm{d}x^2=\frac{1}{\gamma}\mathrm{d}\rho\ \mathrm{d}\varphi. \tag{2.36}$$

On the classical trajectories (2.12) ρ evolves as

$$2\rho=\gamma[R^2+R_0^2+2RR_0\cos(\kappa-\delta)]. \tag{2.37}$$

Being written in terms of the variables ρ,φ, the operators a_k,a_k^+ take the form

$$\begin{gathered}a_1=\sqrt{\rho}e^{-i\varphi}[(l_0+\mu+\rho-i\partial_\varphi)/2\rho+\partial_\rho],\\ a_1^+=\sqrt{\rho}e^{i\varphi}[(l_0+\mu+\rho-i\partial_\varphi)/2\rho-\partial_\rho],\\ a_2=-\sqrt{\rho}e^{i\varphi}[(l_0+\mu-\rho-i\partial_\varphi)/2\rho-\partial_\rho],\\ a_2^+=-\sqrt{\rho}e^{-i\varphi}[(l_0+\mu-\rho-i\partial_\varphi)/2\rho+\partial_\rho].\end{gathered} \tag{2.38}$$

Using the commutation relations for the momentum operators

$$P_\mu P_\nu-P_\nu P_\mu=-i\frac{e\hbar}{c}F_{\mu\nu},\quad F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu, \tag{2.39}$$

and definition of the magnetic field (1.2), we arrive at the following commutation relations for the operators a_k,a_k^+ :

$$[a_1,a_1^+]=1+f,\quad [a_2,a_2^+]=1-f,\quad [a_1,a_2]=-f,\quad [a_1,a_2^+]=0,$$
$$f=(\Phi/H)\,\delta(x^1)\,\delta(x^2)=2\,\frac{\Phi}{\Phi_0}\,\delta(\rho)=2(l_0+\mu)\,\delta(\rho). \tag{2.40}$$

These commutation relations contain a singular dimensionless function f. Whenever the AB field is absent ($f=0$), then the operators a_k,a_k^+ form two mutual commuting sets of creation and annihilation operators. It is not true in the presence of the AB field. However, as will be seen further, these operators behave as creation and annihilation ones when acting on functions that tend to zero (sufficiently rapidly) as $\rho\to 0$. Being written in the coordinates ρ,φ, the operators (2.35) have the form

$$P_r^2=2\gamma\hbar^2 Q,\quad L_z=-i\hbar\partial_\varphi,\quad Q=\frac{(l_0+\mu+\rho-i\partial_\varphi)^2}{4\rho}-\partial_\rho-\rho\partial_\rho^2. \tag{2.41}$$

In the case under consideration, the radial equation (2.24) reads

$$\overline{Q}\psi(\rho)=\left(\overline{n}+\frac{1}{2}\right)\psi(\rho),\quad \overline{Q}=\frac{(l+\mu+\rho)^2}{4\rho}-\partial_\rho-\rho\partial_\rho^2,\quad k_1^2=2\gamma\left(\overline{n}+\frac{1}{2}\right). \tag{2.42}$$

Bounded and quadratically integrable solutions of this equation are expressed via the Laguerre functions (A1) (see the Appendix). There are two types of solutions of the latter equation, we denote them as $\psi^{(j)}(\rho)$, $j=1,2$ (two types of states). The first one $j=1$ corresponds to $l\geqslant 0$ (classical trajectories embrace the solenoid),

$$\psi^{(1)}(\rho)=I_{n+\mu,n-l}(\rho),\quad 0\leqslant l\leqslant n,\quad n=0,1,2,\ldots,\quad \overline{n}=n+\mu. \tag{2.43}$$

The second type of solutions with $j=2$ corresponds to $l<0$ (classical trajectories do not embrace the solenoid),

$$\psi^{(2)}(\rho)=I_{n-l-\mu,n}(\rho),\quad l<0,\quad \overline{n}=n. \tag{2.44}$$

In these two cases radial momentum spectra are different,

$$(k_1^{(1)})^2=2\gamma(n+\mu+\tfrac{1}{2}),\quad 0\leqslant l\leqslant n,$$
$$(k_1^{(2)})^2=2\gamma(n+\tfrac{1}{2}),\quad l<0,\quad n=0,1,2,\ldots\ . \tag{2.45}$$

The spectrum for $j=2$ (which is a part of the total spectrum) corresponds exactly to the spectrum of a spinless particle in a uniform magnetic field (without the AB field). The spectrum for $j=1$ is shifted by $2\gamma\mu$ with respect to the one for $j=2$. It is important to note that the presence of the AB field partially lifts the degeneracy of the total spectrum in the quantum number l.

It is convenient to define effective quantum numbers $\overline{l}$ and $\overline{n}$ by

$$\overline{n}=n+\mu(2-j)=\begin{cases} n+\mu, & j=1,\quad \overline{l}=l+\mu,\quad \overline{l}\leqslant\overline{n} \\ n, & j=2,\quad n=0,1,2,\ldots\ . \end{cases} \tag{2.46}$$

Using these numbers, we introduce the functions

$$\psi_{n,l}^{(1)}(\rho,\varphi)=(-1)^{n-l}\frac{\exp[i(l-l_0)\varphi]}{\sqrt{2\pi}}I_{\overline{n},\overline{n}-\overline{l}}(\rho), \tag{2.47}$$

$$\psi^{(2)}_{n,l}(\rho,\varphi)=(-1)^n\frac{\exp[i(l-l_0)\varphi]}{\sqrt{2\pi}}I_{\overline{n}-\overline{l},\overline{n}}(\rho).$$

According to Eq. (A4), these functions can be expressed via the Laguerre polynomials. Thus, the orthonormality relation can be proved

$$\int_0^\infty \mathrm{d}\rho\int_0^{2\pi}\mathrm{d}\varphi\ \psi^{(j')}_{n',l'}{}^{*}(\rho,\varphi)\psi^{(j)}_{n,l}(\rho,\varphi)=\delta_{l.l'}\delta_{n,n'}. \tag{2.48}$$

The set of the Laguerre functions

$$I_{\alpha+n,n}(x),\quad n=0,1,2\ldots,\quad \alpha>-1 \tag{2.49}$$

is complete in the space of quadratically integrable functions of $x\geqslant 0$,

$$\sum_{n=0}^{\infty} I_{\alpha+n,n}(x)I_{\alpha+n,n}(y)=\delta(x-y). \tag{2.50}$$

Then the set $\psi^{(j)}_{n,l}(\rho,\varphi)$ is complete in the space of quadratically integrable functions of ρ,φ, ($\rho>0,0\leqslant\varphi\leqslant 2\pi$).

Using relations (A6)–(A11), one can get the action of the operators (2.38) on the functions $\psi^{(j)}_{n,l}(\rho,\varphi)$,

$$\begin{aligned} a_1\psi^{(j)}_{n,l}(\rho,\varphi)&=\sqrt{\overline{n}}\psi^{(j)}_{n-1,l-1}(\rho,\varphi),\quad a_1^+\psi^{(j)}_{n,l}(\rho,\varphi)=\sqrt{\overline{n+1}}\psi^{(j)}_{n+1,l+1}(\rho,\varphi),\\ a_2\psi^{(j)}_{n,l}(\rho,\varphi)&=\sqrt{\overline{n-l}}\psi^{(j)}_{n,l+1}(\rho,\varphi),\quad a_2^+\psi^{(j)}_{n,l}(\rho,\varphi)=\sqrt{\overline{n-l+1}}\psi^{(j)}_{n,l-1}(\rho,\varphi). \end{aligned} \tag{2.51}$$

These formulas show that the functions $\psi^{(1)}_{n,l}$ may be created by an action of the operators a_k^+ on $\psi^{(1)}_{0,0}$, and the functions $\psi^{(2)}_{n,l}$ may be created by an action of the operators a_k^+ on $\psi^{(2)}_{0,-1}$. Namely,

$$\psi^{(1)}_{n,l}=\sqrt{\frac{\Gamma(1+\mu)}{\Gamma(1+\overline{n})\Gamma(1+\overline{n}-\overline{l})}}(a_2^+)^{n-l}(a_1^+)^n\psi^{(1)}_{0,0}, \tag{2.52}$$

$$\psi^{(2)}_{n,l}=\sqrt{\frac{\Gamma(2-\mu)}{\Gamma(1+\overline{n})\Gamma(1+\overline{n}-\overline{l})}}(a_1^+)^n(a_2^+)^{n-l-1}\psi^{(2)}_{0,-1}. \tag{2.53}$$

It is natural to interpret $\psi^{(1)}_{0,0}$ as a vacuum state for the states $\psi^{(1)}_{n,l}$, and to interpret $\psi^{(2)}_{0,-1}$ as a vacuum state for the states $\psi^{(2)}_{n,l}$. Thus, for $\mu\neq 0$, we have two vacuum states in the problem. For $\mu=0$, the situations changes. By virtue of Eq. (A18)

$$I_{n,n-l}=(-1)^l I_{n-l,n}\rightarrow\psi^{(1)}_{n,l}=(-1)^l\psi^{(2)}_{n,l},\quad \mu=0, \tag{2.54}$$

and for any $l<n$, the function $\psi^{(1)}_{0,0}$ is connected to $\psi^{(2)}_{0,-1}$ as

$$a_2^+\psi^{(1)}_{0,0}=\psi^{(2)}_{0,-1},\quad a_2\psi^{(2)}_{0,-1}=\psi^{(1)}_{0,0}. \tag{2.55}$$

Thus, we have only one vacuum in the problem, one energy spectrum (2.45), and all the wave functions are created from the vacuum $\psi^{(1)}_{0,0}$.

One ought to stress that all the states obey the property $\psi^{(j)}_{n,l}(\rho=0,\varphi)=0$, which means that the scalar particle has zero probability to be found in the solenoid area. In fact, the existence of this property allows us to speak about the AB effect.

Definitions (2.51) can formally be considered for any values of indices n, l. In particular, we can consider the following relations:

$$a_1^+\psi^{(2)}_{n,-1}=\sqrt{n+1}\,\psi^{(2)}_{n+1,0}=(-1)^{n+1}(1+n)\sqrt{\frac{\Gamma(1+n)}{2\pi\Gamma(2-\mu+n)}}\exp\left[-il_0\varphi-\frac{\rho}{2}\right]\rho^{-\mu/2}L^{-\mu}_{n+1}(\rho),$$

$$\begin{aligned}a_1\psi^{(1)}_{n,0}&=\sqrt{n+\mu}\,\psi^{(1)}_{n-1,-1}\\&=(-1)^n(n+\mu)\sqrt{\frac{\Gamma(1+n)}{2\pi\Gamma(1+\mu+n)}}\exp\left[-i(1+l_0)\varphi-\frac{\rho}{2}\right]\rho^{-(1-\mu)/2}L^{\mu-1}_{n}(\rho),\\ a_2^+\psi^{(1)}_{n,0}&=\sqrt{n+1}\,\psi^{(1)}_{n,-1}\\&=(-1)^{n+1}(1+n)\sqrt{\frac{\Gamma(1+n)}{2\pi\Gamma(1+\mu+n)}}\exp\left[-i(1+l_0)\varphi-\frac{\rho}{2}\right]\rho^{-(1-\mu)/2}L^{\mu-1}_{n+1}(\rho),\end{aligned}\tag{2.56}$$

$$a_2\psi^{(2)}_{n,-1}=\sqrt{1-\mu+n}\,\psi^{(2)}_{n,0}=(-1)^n(1-\mu+n)\sqrt{\frac{\Gamma(1+n)}{2\pi\Gamma(2-\mu+n)}}\exp\left[-il_0\varphi-\frac{\rho}{2}\right]\rho^{-\mu/2}L^{-\mu}_{n}(\rho).$$

However, the functions $\psi^{(1)}_{n,-1}$, $\psi^{(2)}_{n,0}$ do not present any physical solutions of the problem, they are not in the set (2.47). Thus, in the general case $\mu\neq 0$, the action of the operators a_k^+, a_k on wave functions may lead them out of a class of physical solutions. The functions (2.56) are singular at $r=0$ (for $\mu\neq 0$), however they still remain quadratically integrable.

Thus, we see that $l=0,-1$ is a special case. Here there appear unbounded (but quadratically integrable) solution $\psi^{(1)}_{n,-1}$, $\psi^{(2)}_{n,0}$. Whenever $\mu\to 0$, these states either coincide with the corresponding states in the pure magnetic field or disappear. The states $\psi^{(1)}_{n,0}, \psi^{(2)}_{n,0}, \psi^{(1)}_{n,-1}, \psi^{(2)}_{n,-1}$ are not mutually orthogonal in spite of the fact that they belong to different eigenvalues of the operator P_r^2.

Equation (2.42) has additional solutions in the case $l=0,-1$. According to Eq. (A20) they have the form

$$\psi(\rho)=\psi_{\lambda\alpha}(\rho),\quad \alpha=\begin{cases}\mu, & l=0,\\ & 2\overline{n}=2\lambda+l+\mu-1,\\ 1-\mu, & l=-1,\end{cases}\tag{2.57}$$

where the functions $\psi_{\lambda\alpha}(\rho)$ are defined by Eqs. (A28) and (A29). Solutions (2.57) with any different complex λ are orthogonal and have finite norms according to the properties (A38)–(A40). These solutions are singular at $r=0$. For $l=0$ such solutions exist even in the pure magnetic field. Their existence is related to the loss of hermicity of the operator P_r^2.

E. Nonuniform magnetic field

Here we consider the radial equation (3.2.8) for $A(r)=\gamma r$,

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}r^2}+\frac{1}{r}\frac{\mathrm{d}\psi}{\mathrm{d}r}-\left(\frac{l+\mu+\gamma r}{r}\right)^2\psi+(\gamma a)^2\psi=0,\quad P_r^2=(\hbar\gamma a)^2,\quad k_1^2=(\gamma a)^2.\tag{2.58}$$

The constant a is defined in Eq. (2.16).

For $a\neq 1$ bounded solutions of this equation are expressed via the the Laguerre functions (A1) as

$$\psi(r)=\psi_{n,l}(r)=I_{\alpha+n,n}(x),\quad x=2\sqrt{1-a^2}\,\gamma r,\tag{2.59}$$

$$\alpha=2|l+\mu|, \quad 1+\alpha+2n=-\frac{2(l+\mu)}{\sqrt{1-a^2}}.$$

For $a>1$, there are solutions for any l (in complete accordance with the classical theory). In this case the Laguerre functions have imaginary arguments and complex indices.

For $a<1$, bounded solutions of the form (2.59) exist only for $l<0$ (also in accordance with the classical theory). Besides, in such a case

$$a^2=1-\frac{\alpha^2}{(1+\alpha+2n)^2}, \quad n=0,1,2,\ldots, \qquad x=\frac{2\alpha\gamma r}{1+\alpha+2n}. \tag{2.60}$$

Thus, n must be integer and a is quantized. Here the functions (2.59) can be expressed via the Laguerre polynomials by means of Eqs. (A4) and (A19).

For $a=1$, bounded solutions of the form (2.59) exist only for $l<0$, these functions can be expressed via the Bessel functions,

$$\psi(r)=J_\alpha(2\sqrt{\alpha\gamma r}), \quad a=1, \quad l<0. \tag{2.61}$$

One can see with the help of Eq. (A22) that the solutions (2.61) follow from Eq. (2.59) as $a\to 1$.

All the bounded solutions vanish at $r=0$.

It is interesting to note that there exist unbounded (but quadratically integrable solutions) of Eq. (2.58) for $l=0,-1$. For any complex a, the latter solutions are defined as

$$\psi(r)=\psi_{\lambda,\alpha}(2\sqrt{1-a^2}\gamma r), \quad a\neq 1, \quad \lambda=-\frac{l+\mu}{\sqrt{1-a^2}}, \quad \mathrm{Re}\sqrt{1-a^2}>0,$$
$$\psi(r)=K_\alpha(2\sqrt{\alpha\gamma r}), \quad a=1. \tag{2.62}$$

Here $K_\alpha(x)$ are Macdonald functions. The existence of such solutions is related to the loss of hermicity of the operator P_r^2.

F. Solutions of the Klein–Gordon equation that are not related to radial momentum conservation

As was demonstrated previously, selecting the radial momentum (2.21) as an integral of motion, we can separate variables and then consider two independent problems: a two-dimensional motion of the charge in the magnetic field (2.21) (the latter field includes the AB field), and a two-dimensional motion of the charge in an electric field, the latter problem does not depend on the AB field. However, there is a wide class of exact solutions, which are not eigenvectors for the radial momentum operator. They correspond to a superposition of the AB field and longitudinal running electric fields (potentials of such fields depend on $u^0=x^0-x^3$ only). Thus, here we will use light cone variables u^0,u^3,

$$u^0=x^0-x^3, \quad u^3=x^0+x^3. \tag{2.63}$$

Then the above-mentioned longitudinal running electric fields have the following potentials and strengths:

$$A_0^{(1)}=A_3^{(1)}=\tfrac{1}{2}B(u^0), \quad E=B'(u^0), \tag{2.64}$$

where $B(u^0)$ is an arbitrary function of u^0. Consider operators $\tilde{P}_0, \tilde{P}_3, \tilde{p}_3$,

$$2\tilde{P}_0 = P_0 - P_3, \quad 2\tilde{P}_3 = P_0 + P_3, \quad \tilde{P}_0 = i\hbar \frac{\partial}{\partial u^0},$$
$$\tilde{p}_3 = i\hbar \frac{\partial}{\partial u^3}, \quad \tilde{P}_3 = \tilde{p}_3 + \frac{\hbar g(u^0)}{2}, \quad g = \frac{|e|B(u^0)}{c\hbar}. \tag{2.65}$$

The operator $\tilde{p}_3$ commutes with the one L_z and both are integrals of motion. Thus, we can demand for solutions of Eq. (2.19) to be eigenvectors for these operators,

$$\tilde{p}_3 \Psi(x) = \frac{\hbar\lambda}{2}\Psi(x), \quad L_z\Psi(x) = \hbar(l - l_0)\Psi(x). \tag{2.66}$$

Such solutions have the form

$$\Psi(x) = [\lambda + g(u^0)]^{-1/2}\Phi(r,t)\exp i\left[(l-l_0)\varphi - m^2 t(u^0) - \frac{\lambda u^3}{2}\right],$$
$$t(u^0) = \frac{1}{2}\int \frac{du^0}{\lambda + g(u^0)}, \tag{2.67}$$

where the function $\Phi(r,t)$ obeys

$$\hat{R}_1\Phi(r,t) = 0, \quad \hat{R}_1 = i\partial_t + \partial_r^2 + \frac{\partial_r}{r} - \frac{[\overline{l} + A(r)]^2}{r^2}, \quad \overline{l} = l + \mu. \tag{2.68}$$

We recall that $A(r)$ was defined in Eq. (2.3).

Consider first the case $A(r) = 0$. Here we find a propagation function for Eq. (2.68) in the form [$J_\nu(x)$ are the Bessel functions]

$$G_0(r,r',t) = \frac{1}{2t} J_{|\overline{l}|}\left(\frac{rr'}{2t}\right) e^{iQ_0}, \quad Q_0 = \frac{r^2 + r'^2}{4t} - \frac{(|\overline{l}| + 1)\pi}{2},$$
$$\hat{R}_1|_{A=0} G_0(r,r',t) = 0, \quad \lim_{t\to 0} G_0(r,r',t) = \frac{1}{r}\delta(r - r'). \tag{2.69}$$

The case $A(r) = \rho = \gamma r^2/2$ can be considered in the same manner. Here the propagation function has the form

$$G(\rho,\rho',t) = \frac{1}{2\sin\tau} J_{|\overline{l}|}\left(\frac{\sqrt{\rho\rho'}}{\sin\tau}\right) e^{iQ}, \quad Q = \frac{\rho + \rho'}{\sin\tau} - \frac{(|\overline{l}| + 1)\pi}{2} - \overline{l}\,\tau,$$
$$\hat{R}_1 G(\rho,\rho',t) = 0, \quad \lim_{t\to 0} G(\rho,\rho',t) = \delta(\rho - \rho'), \quad \tau = \gamma t(u^0). \tag{2.70}$$

The functions $G_0(r,r',t)$ and $G(\rho,\rho',t)$ solve the Cauchy problem. For example,

$$\Phi(\rho,t) = \int_0^\infty G(\rho,\rho',t)\Phi(\rho')\,d\rho', \tag{2.71}$$

where $\Phi(\rho)$ is an arbitrary functions [an initial date for $\Phi(\rho,t)$].

For the field (2.8), the corresponding propagation function is quite complicated.[20]

G. Exact solutions of the Dirac equation

Here we are going to study the Dirac equation

$$(\gamma^{\mu}P_{\mu}-m_0c)\Psi(x)=0 \tag{2.72}$$

in the superposition of the AB field and field (2.1). We use a standard representation (see, e.g., Ref. 17) for γ matrices. In the case under consideration, we look for solutions with a definite radial momentum. The corresponding bispinors $\Psi(x)$ can be written in a block form

$$\Psi(x)=Q\begin{pmatrix}\psi_1(x^1,x^2)[m+F-ik_1\sigma_2]\\ \psi_2(x^1,x^2)[(m-F)\sigma_3-ik_1\sigma_1]\end{pmatrix}\upsilon\tilde{\Phi}(x^0,x^3),\quad F=\hbar^{-1}(P_0+P_3), \tag{2.73}$$

where υ is an arbitrary spinor; $\sigma_k(k=1,2,3)$ are Pauli matrices; the function $\tilde{\Phi}(x^0,x^3)$ obeys

$$\left[\hbar^{-2}(P_0^2-P_3^2)+i\frac{|e|E}{c\hbar}\right]\tilde{\Phi}(x^0,x^3)=0, \tag{2.74}$$

where $E=E(x^0,x^3)$ is electric field strength (2.2), and functions ψ_1,ψ_2 obey the following equations:

$$(P_1+iP_2)\psi_1(x^1,x^2)=\hbar k_1\psi_2(x^1,x^2),\quad (P_1-iP_2)\psi_2(x^1,x^2)=\hbar k_1\psi_1(x^1,x^2). \tag{2.75}$$

The presence of the arbitrary spinor υ in solutions (2.73) indicates that Eq. (2.72) does not fix the spin orientation. This orientation can be fixed by a choice of a spin operator.[16,17] One has to stress that Eq. (2.74) does not contain the AB field. All possible exact solutions of this equation were presented in Refs. 16 and 17, thus here we do not repeat these results.

Fields (2.3) are axially symmetric, thus J_z is an integral of motion in such a case (J is the total angular momentum operator). Let us consider solutions that are eigenvectors for this operator,

$$J_z\Psi=\hbar\left(l-l_0-\frac{1}{2}\right)\Psi,\quad J_z=L_z+\frac{\hbar}{2}\Sigma_3,\quad l=0,\pm1,\pm2,\ldots \tag{2.76}$$

[$\Sigma=\mathrm{diag}(\sigma,\sigma)$]. We obey equations (2.76) choosing

$$\psi_1(x^1,x^2)=\frac{\exp[i(l-l_0-1)\varphi]}{\sqrt{2\pi}}\psi_1(r),\quad \psi_2(x^1,x^2)=-i\frac{\exp[i(l-l_0)\varphi]}{\sqrt{2\pi}}\psi_2(r), \tag{2.77}$$

where the functions $\psi_k(r)$ satisfy a set of first-order differential equations

$$\left(\frac{\overline{l}+A(r)}{r}+\frac{\mathrm{d}}{\mathrm{d}r}\right)\psi_2(r)=k_1\psi_1(r),\quad \left(\frac{\overline{l}-1+A(r)}{r}-\frac{\mathrm{d}}{\mathrm{d}r}\right)\psi_1(r)=k_1\psi_2(r). \tag{2.78}$$

Consider solutions of the latter equations for fields (2.6)–(2.8).

For $A(r)=0$, we deal with the pure AB field. For $l\neq0$, all bounded solutions of Eq. (2.78) have the form

$$\psi_1(r)=J_{|\overline{l}-1|}(k_1r),\quad \psi_2(r)=\varepsilon J_{|\overline{l}|}(k_1r),\quad \varepsilon=\mathrm{sign}\,l, \tag{2.79}$$

where $J_{\mu}(x)$ are the Bessel functions. These solutions vanish at $r=0$. For $l=0,\mu\neq0$, the system of equations (2.78) has no bounded solutions. In such a case, a general solution of this system has the form

$$\psi_1(r)=c_1J_{\mu-1}(k_1r)+c_2J_{1-\mu}(k_1r),\quad \psi_2(r)=c_1J_{\mu}(k_1r)-c_2J_{-\mu}(k_1r), \tag{2.80}$$

where c_1, c_2 are arbitrary constants. In spite of the fact that these solutions are unbounded they still are quadratically integrable (as in the scalar case). Moreover, for any complex k_1 ($\mathrm{Re}\, k_1 > 0$) there exist unbounded solutions with a finite norm, they are expressed via the Macdonald functions,

$$\psi_1(r) = K_{1-\mu}(k_1 r), \quad \psi_2(r) = -K_\mu(k_1 r), \quad 0 < \mu < 1. \tag{2.81}$$

Similar to the scalar case, we can conclude that the operator $\gamma^\mu P_\mu$ is not self-conjugate anymore for $l=0$, $\mu \neq 0$. In contrast to the scalar case, there are no quadratically integrable unbounded solutions for $l=-1$, as well as for $l=0$, $\mu=0$.

Consider now the case of the uniform magnetic field (2.7). Using the operators (2.38), we can write Eq. (2.75) as

$$a_1 \psi_2(\rho,\varphi) = -i\sqrt{\bar{n}}\,\psi_1(\rho,\varphi), \quad a_1^+ \psi_1(\rho,\varphi) = i\sqrt{\bar{n}}\,\psi_2(\rho,\varphi), \quad k_1 = \sqrt{2\gamma\bar{n}}, \quad \rho = \frac{\gamma r^2}{2}.$$

Their solutions have the form [see Eqs. (2.51) and (2.47)]

$$\psi_1(\rho,\varphi) = \psi^{(j)}_{n-1,l-1}(\rho,\varphi), \quad \psi_2(\rho,\varphi) = -i\psi^{(j)}_{n,l}(\rho,\varphi). \tag{2.82}$$

As in the scalar case, there are two types of states (with $j=1,2$). These states are bounded at $l \neq 0$; they vanish at $r=0$. The states (2.82) are unbounded at $l=0$ but they still are quadratically integrable. Besides, there are unbounded solutions with finite norms for any complex $\bar{n}$. Such solutions are expressed via the functions $\psi_{\lambda,a}(x)$ [the latter are defined by Eqs. (A28) and (A29)] as

$$\psi_1(r) = \bar{n}^{3/4}\psi_{\lambda-1/2,1-\mu}(\rho), \quad \psi_2(r) = \bar{n}^{1/4}\psi_{\lambda,\mu}(\rho), \quad 2\bar{n} = 2\lambda + \mu - 1. \tag{2.83}$$

Thus, we see that the operator $\gamma^\mu P_\mu$ is not self-conjugate for $l=0, \mu \neq 0$ as well. All the above-mentioned singular solutions vanish or become nonsingular as $\mu \to 0$.

One ought also remark that ψ_1 (which correspond to $j=2$) from Eq. (2.82) vanish at $n=0$. Thus, the complete wave function (2.73) is an eigenvector for the operator Σ_3,

$$\Sigma_3 \Psi = -\Psi. \tag{2.84}$$

That means that in such states the electron spin has only one orientation, namely, opposite to the magnetic field.

Consider finally the case of nonuniform magnetic field (2.8). For $l \neq 0, a \neq 1$, the corresponding bounded solutions (they also vanish at $r=0$) have the form

$$\psi_1(r) = I_{n-1,n+1-2\bar{l}}(x), \quad \psi_2(r) = -I_{n,n-2\bar{l}}(x), \quad l > 0,$$

$$\psi_1(r) = I_{n+1-2\bar{l},n-1}(x), \quad \psi_2(r) = -I_{n-2\bar{l},n}(x), \quad l < 0, \tag{2.85}$$

$$x = 2\sqrt{1-a^2}\,\gamma r, \quad 1 - 2\bar{l} + 2n = \frac{1-2\bar{l}}{\sqrt{1-a^2}}, \quad \bar{l} = l + \mu,$$

where $I_{n,m}(x)$ are the Laguerre functions (A1), and we use the notation (2.16). Whenever $a^2 > 1$, any $l \neq 0$ are admissible in complete agreement with classical theory. Whenever $a^2 < 1$, only $l < 0$ are admissible. In such a case n is an integer and the functions (2.85) are expressed via the Laguerre polynomials according to Eq. (A19). At the same time, the following quantization takes place:

$$a^2=1-\frac{(1+2|\overline{l}|)^2}{(1+2|\overline{l}|+2n)^2},\quad n=0,1,2,\ldots. \tag{2.86}$$

For $a=1$, $l\neq 0$, the only bounded states can be found for $l<0$. They are expressed via the Bessel functions,

$$\psi_1(r)=J_{2|\overline{l}|+2}(2\sqrt{(1+2|\overline{l}|)\gamma r}),\quad \psi_2(r)=-J_{2|\overline{l}|}(2\sqrt{(1+2|\overline{l}|)\gamma r}). \tag{2.87}$$

Solutions (2.87) follow from Eq. (2.85) as $a\to 1$. That fact can be confirmed by the use of the limit (A22).

$l=0$ is a special case. Here there are only unbounded solutions. Some of them are quadratically integrable. Whenever $a^2>1$, such solutions have the form

$$\begin{aligned}\psi_1(r)&=c_1I_{n+1-2\mu,n-1}(x)+c_2I_{n-1,n+1-2\mu}(x),\\ \psi_2(r)&=-c_1I_{n-2\mu,n}(x)-c_2I_{n,n-2\mu}(x),\end{aligned} \tag{2.88}$$

where c_k are arbitrary constants, and for $a=1$ these solutions read

$$\psi_1(r)=J_{2-2\mu}(z),\quad \psi_2(r)=-J_{-2\mu}(z),\quad 0<\mu<\tfrac{1}{2},$$

$$\psi_1(r)=K_{2-2\mu}(z),\quad \psi_2(r)=K_{2\mu}(z),\quad \tfrac{1}{2}<\mu<1,\quad z=2\sqrt{|1-2\mu|\gamma r}. \tag{2.89}$$

Quadratically integrable solutions exist for $a^2<1$ as well. For example, for $0<\mu<\frac{1}{2}$ they have the form (2.88), where $c_2=0$. In such a case a^2 is quantized

$$a^2=1-\frac{(1-2\mu)^2}{(1-2\mu+2n)^2},\quad n=0,1,2,\ldots. \tag{2.90}$$

Moreover, for any complex a^2 (provided $\mathrm{Re}\sqrt{1-a^2}>0$) there exist unbounded solutions with a finite norm. They read

$$\psi_1(r)=a\,\psi_{\lambda,2(1-\mu)}(x),\quad \psi_2(r)=(1+\sqrt{1-a^2})\psi_{\lambda,2\mu}(x),\quad \lambda=\frac{1-2\mu}{2\sqrt{1-a^2}}. \tag{2.91}$$

All the above-mentioned solutions obey Eq. (2.84) for $n=0$.

Finally we present solutions, which do not have an analog in the Klein–Gordon case discussed in Sec. II F. These solutions are not eigenvectors of the radial momentum operator. With this aim in view we present Dirac wave functions in the following form:

$$\Psi(x)=\Psi_{(-)}(x)+\Psi_{(+)}(x),\quad \Psi_{(\pm)}(x)=P_{(\pm)}\Psi(x),\quad 2P_{(\pm)}=1\pm(\alpha\mathbf{n}), \tag{2.92}$$

where $\mathbf{n}$ is a unit vector, $\alpha=(\alpha_k=\gamma^0\gamma^k), k=1,2,3$, and $P_{(\pm)}$ are projection operators, $P_{(+)}+P_{(-)}=1$, $P_{(\pm)}^2=P_{(\pm)}$, $P_{(+)}P_{(-)}=P_{(-)}P_{(+)}=0$. Then we can always present $\Psi_{(\pm)}(x)$ in the following block form:

$$\Psi_{(+)}(x)=\begin{pmatrix}v(x)\\(\sigma\mathbf{n})v(x)\end{pmatrix},\quad \Psi_{(-)}(x)=\begin{pmatrix}u(x)\\-(\sigma\mathbf{n})u(x)\end{pmatrix}, \tag{2.93}$$

with $u(x)$, $v(x)$ being arbitrary spinors. Without loss of generality we can always choose $\mathbf{n}=(0,0,1)$. The Dirac equation (2.72) demands $u(x)$, $v(x)$ to obey

$$2\tilde{P}_0u=[m_0c-(\sigma\mathbf{B})\sigma_3]v,\quad 2\tilde{P}_3v=[m_0c+(\sigma\mathbf{B})\sigma_3]u, \tag{2.94}$$

$$2\tilde{P}_0 = P_0 - P_3, \quad 2\tilde{P}_3 = P_0 + P_3, \quad \mathbf{B} = (P_1, P_2, 0).$$

Suppose we consider external fields, for which the operator $\tilde{P}_3$ (2.65) is an integral of motion, and suppose we are looking for solutions that are eigenvectors of the latter operator. Then in accordance with Eq. (2.66)

$$2\tilde{P}_3 = \hbar(\lambda + g), \quad c\hbar g = |e|(A_0^{(1)} + A_3^{(1)}). \tag{2.95}$$

It follows from Eq. (2.94) that the spinor υ can be restored by the one u,

$$\hbar(\lambda + g)\upsilon = [m_0 c + (\sigma\mathbf{B})\sigma_3]u. \tag{2.96}$$

For external fields under consideration, the operator $\mathbf{B}$ commutes with $\lambda + g$, thus we get a closed equation for u,

$$2\hbar(\lambda + g)\tilde{P}_0 u = [m_0 c - (\sigma\mathbf{B})\sigma_3][m_0 c + (\sigma\mathbf{B})\sigma_3]u. \tag{2.97}$$

Considering eigenvectors for the operator J_z (2.76) in axial-symmetric external fields (2.3), we can write

$$u(x) = \begin{pmatrix} e^{-i\varphi}u_1(r,t) \\ u_{-1}(r,t) \end{pmatrix} \exp i\left[(l - l_0)\varphi - \frac{m^2}{2}\int \frac{du^0}{\lambda + g(u^0)} - \frac{\lambda u^3}{2}\right], \tag{2.98}$$

where the functions $u_\zeta(r,t)$, $\zeta = \pm 1$ obey the equations

$$\hat{R}_1^\zeta u_\zeta(r,t) = 0, \quad \hat{R}_1^\zeta = i\partial_t + \partial_r^2 + \frac{\partial_r}{r} - \frac{\left[l - \frac{1+\zeta}{2} + A(r)\right]^2}{r^2} - \zeta\frac{A'(r)}{r}, \tag{2.99}$$

which can be solved similar to the one (2.68).

III. SUPERPOSITION OF THE AHARONOV–BOHM, LONGITUDINAL, AND CROSSED FIELDS

We consider here the Klein–Gordon and Dirac equations in some superpositions of the AB field, longitudinal, and crossed fields. In fact, there are only two types of such fields, which admit exact solutions of these equations.

To define the first type of the fields, we introduce curvilinear coordinates u^μ by the relations

$$u^0 = x^0 - x^3, \quad u^1 = q(u^0)r^2, \quad u^2 = \varphi, \quad u^3 = x^0 + x^3 - u^0 u^1, \quad q(u^0) = [(u^0)^2 + a]^{-1}, \tag{3.1}$$

where a is a constant. In these coordinates, covariant components $A_\mu^{(1)}$ of electromagnetic potentials are given as

$$\begin{aligned} &\frac{|e|A_0^{(1)}}{c\hbar} = q(u^0)[f_1(u^1) + au^1 g_1(u^0)], \quad A_1^{(1)} = 0, \\ &\frac{|e|A_2^{(1)}}{c\hbar} = f_2(u^1) + u^1 g_2(u^0), \quad \frac{|e|A_3^{(1)}}{c\hbar} = \frac{g_1(u^0)}{2}. \end{aligned} \tag{3.2}$$

Here $g_s(u^0)$, $f_s(u^1)$ $(s = 1,2)$ are arbitrary functions of indicated arguments. The corresponding additional (to the AB field) electromagnetic field is given by its components in cylindrical reference frame

$$\frac{|e|E_r}{c\hbar}=\frac{|e|H_\varphi}{c\hbar}=qr[2q(f_1'+ag_1)+u^0g_1'],\quad \frac{|e|E_z}{c\hbar}=-g_1',$$
$$\frac{|e|E_\varphi}{c\hbar}=-\frac{|e|H_r}{c\hbar}=-qr[g_2'-2qu^0(g_2+f_2')],\quad \frac{|e|H_z}{c\hbar}=2q(g_2+f_2'). \tag{3.3}$$

Exact solutions in the field (3.3) were studied in Refs. 21 and 17.

In the case under consideration, the operators L_z (or J_z in the Dirac equation case) and $\tilde{P}_3$ (2.65) are integrals of motion. We are going to study solutions that are eigenvectors for such operators. Let us impose the following constraint on the functions $g_s(u^0)$, $f_s(u^1)$ $(s=1,2)$,

$$u^1(g_2^2-ag_1^2-b)+2g_2f_2-2g_1f_1=0,\quad b=\text{const}. \tag{3.4}$$

Then we can separate the variables u^0 and u^1 and present Klein–Gordon wave functions in the form

$$\Psi=\sqrt{\frac{q}{P}}e^{-i\Gamma}\psi(u^1),\quad P=\lambda+g_1(u^1),$$
$$\Gamma=\frac{\lambda}{2}u^3-(l-l_0)\varphi+\int[m^2+2q(2k_1+\overline{l}g_2)]\frac{du^0}{2P}. \tag{3.5}$$

The functions $\psi(u^1)$ obey

$$\psi''+\frac{1}{u^1}\psi'+R(u^1)\psi=0,\quad R(u^1)=\frac{2k_1+\lambda f_1}{2u^1}-\frac{a\lambda^2+b}{4}-\frac{(\overline{l}+f_2)^2}{4(u^1)}. \tag{3.6}$$

In the same case, Dirac wave functions have the form

$$\Psi=\frac{\sqrt{q}}{P}e^{-i\Gamma}KW[(1+\sigma_3)\psi_1(u^1)+(1-\sigma_3)\psi_{-1}(u^1)]\upsilon, \tag{3.7}$$

where υ is an arbitrary constant spinor, and

$$K=\begin{pmatrix} m+P-\sigma_3(\sigma\mathbf{F}) \\ (m-P)\,\sigma_3-(\sigma\mathbf{F})\end{pmatrix},\quad \mathbf{F}=\mathbf{e}_r\,qr(2i\partial_{u^1}-u^0P)+\mathbf{e}_\varphi\left(\frac{\overline{l}+f_2}{r}+qrg_2\right),$$
$$W=\cos\delta+i\sigma_3\sin\delta,\quad \delta=\int\frac{qg_2}{P}du^0. \tag{3.8}$$

The scalar functions $\psi_\zeta(u^1)(\zeta=\pm1)$ obey a set of independent equations

$$\psi_\zeta''+\frac{1}{u^1}\psi_\zeta'+\left[R(u^1)+\zeta\frac{f_2'}{2u^1}\right]\psi_\zeta=0. \tag{3.9}$$

Explicit solutions of Eqs. (3.6) and (3.9) can be written for

$$f_1(u^1)=\alpha u^1+\frac{\beta}{u^1},\quad f_2(u^1)=\gamma u^1,\quad \alpha,\,\beta,\,\gamma=\text{const}. \tag{3.10}$$

In such a case Eqs. (3.6) and (3.9) are reduced to the one (2.58). Solutions of the latter equation we have studied previously.

Let us return to the constraint (3.4). If $\beta\neq 0$, then $g_1=0, g_2=\text{const}$, and b can be found from Eq. (3.4) to be $b=g_2^2+2\gamma g_2$. If $\beta=0$, then g_1, g_2 are related by

$$(g_2+\alpha)^2=a\left(g_1+\frac{\gamma}{a}\right)^2+\alpha^2-\frac{\gamma^2}{a}+b. \tag{3.11}$$

Thus, one of the constants remains arbitrary. We see that there exist a wide class of fields, which admit exact solutions.

To define the second type of fields, which admit exact solutions, we introduce curvilinear coordinates u^μ by

$$u^0=x^0-x^3, \quad u^1=\frac{r^2}{u^0}, \quad u^2=\varphi, \quad u^3=x^0+x^3-\frac{r^2}{2u^0}. \tag{3.12}$$

Covariant components of electromagnetic potentials in the coordinates (3.12) are given by

$$\frac{|e|A_0^{(1)}}{c\hbar}=\frac{f_1(u^1)}{u^0}, \quad A_1^{(1)}=0, \quad \frac{|e|A_2^{(1)}}{c\hbar}=f_2(u^1), \quad A_3^{(1)}=0, \tag{3.13}$$

where $f_s(u^1)$ $(s=1,2)$ are arbitrary functions of u^1. The corresponding electromagnetic field is given by its components in the cylindrical reference frame

$$E_r=H_\varphi=\frac{2c\hbar r}{|e|(u^0)^2}f_1', \quad E_\varphi=-H_r=-\frac{2c\hbar r}{|e|(u^0)^2}f_2', \quad H_z=\frac{2c\hbar}{|e|u^o}f_2', \quad E_z=0. \tag{3.14}$$

In the absence of the AB field, exact solutions in such a field were studied in Refs. 22 and 17.

Here integrals of motion are the same as in the previous case. Klein–Gordon wave functions can be written in the form

$$\Psi=\frac{1}{\sqrt{u^0}}\psi(u^1)\exp\left\{-i\left[\frac{\lambda}{2}u^3-i(l-l_0)\varphi+m^2u^0+k_1\ln u^0\right]\right\}. \tag{3.15}$$

The functions $\psi(u^1)$ obey

$$\psi''+\frac{1}{u^1}\psi'+R(u^1)\psi=0, \quad R(u^1)=\frac{\lambda^2}{16}+\frac{k_1+2\lambda f_1}{4u^1}-\frac{(\overline{l}+f_2)^2}{4(u^1)^2}. \tag{3.16}$$

Dirac wave function can be presented in the form (3.7) and (3.8) with the following modifications:

$$P=\lambda, \quad q=\frac{1}{u^0}, \quad \mathbf{F}=\mathbf{e}_r\,\frac{r}{u^0}\left(2i\partial_1-\frac{\lambda}{2}\right)+\mathbf{e}_\varphi\frac{\overline{l}+f_2}{r}. \tag{3.17}$$

Besides, the functions $\psi_\zeta(u^1)$ have to obey Eq. (3.9) with $R(u^1)$ defined by Eq. (3.16). Solutions of the latter equations are available for $f_s(u^1)$ in the form (3.10). Thus, we have again returned to Eq. (2.58).

IV. SUPERPOSITION OF THE AHARONOV–BOHM FIELD AND SOME NONUNIFORM FIELDS

Consider now additional fields, which are given by potentials of the form

$$A_0^{(1)}=\frac{c\hbar}{|e|}f_1(r), \quad A_1^{(1)}=\frac{c\hbar}{|e|}\frac{A(r)}{r}\sin\varphi, \quad A_2^{(1)}=-\frac{c\hbar}{|e|}\frac{A(r)}{r}\cos\varphi, \quad A_3^{(1)}=\frac{c\hbar}{|e|}f_2(r). \tag{4.1}$$

Here $f_1(r), f_2(r), A(r)$ are arbitrary functions of r. The corresponding electromagnetic field components in cylindrical reference frame have the form

$$E_r=-\frac{c\hbar}{|e|}f_1'(r),\quad H_\varphi=\frac{c\hbar}{|e|}f_2'(r),\quad H_z=\frac{c\hbar}{|e|}\frac{A'(r)}{r},\quad E_\varphi=E_z=H_r=0. \tag{4.2}$$

Exact solutions of relativistic wave equations in such fields were studied in Refs. 23, and 17. Here we present exact solutions of the equations in the superposition of these fields and the AB field.

Stationary solutions of Klein–Gordon equation that are eigenvectors for the operators p_0, p_3, L_z can be written as

$$\Psi(x)=e^{-i\Gamma}\psi(r),\quad \Gamma=k_0x^o+k_3x^3-(l-l_0)\varphi. \tag{4.3}$$

Functions $\psi(r)$ obey

$$\psi''(r)+\frac{1}{r}\psi'(r)+R(r)\psi(r)+0,\quad R(r)=(k_0+f_1)^2-(k_3+f_2)^2-\frac{(\overline{l}+A)^2}{r^2}-m^2. \tag{4.4}$$

The corresponding solutions of the Dirac equation have the form $\Psi(x)=e^{-i\Gamma}M\psi$, where the matrix M reads $M=\mathrm{diag}(e^{-i\varphi},i,e^{-i\varphi},i)$, and the bispinor $\psi=(\psi_k)(k=1,2,3,4)$ obeys

$$\left[k_0+f_1-m\gamma^0-\frac{1}{r}\left(\overline{l}+A-\frac{1}{2}\right)\alpha_1-i\left(\frac{d}{dr}+\frac{1}{2r}\right)\alpha_2+(k_3+f_2)\alpha\right]\psi=0. \tag{4.5}$$

In some particular cases the latter equation can be reduced to the one (2.78) and thus solved explicitly. All such cases are described in Refs. 23, and 17.

V. AHARONOV–BOHM FIELD IN 2+1 QED

Consider Dirac equation in $2+1$ dimensions (see e.g., Refs. 24 and 25) ($x=(x^\mu)$, $\mu=0,1,2$, $\gamma^0=\sigma_3$, $\gamma^1=i\sigma_2$, $\gamma^3=-i\sigma_1$),

$$(\gamma^\mu P_\mu-m_0c)\,\Psi(x)=0,\quad \Psi(x)=\begin{pmatrix}\Psi_1(x)\\ \Psi_2(x)\end{pmatrix}. \tag{5.1}$$

For components of the spinor $\Psi(x)$ we get the following equations:

$$(P_0-m)\Psi_1+(P_1-iP_2)\Psi_2=0,\quad (P_0+m)\Psi_2+(P_1+iP_2)\Psi_1=0. \tag{5.2}$$

These equations can be solved exactly for a superposition of the AB field and an additional field described in the following. Potentials (1.6) of the latter field are given as

$$\frac{|e|}{c\hbar}A_0^{(1)}=B(r),\quad \frac{|e|}{c\hbar}A_1^{(1)}=\frac{A(r)}{r}\sin\varphi,\quad \frac{|e|}{c\hbar}A_2^{(1)}=-\frac{A(r)}{r}\cos\varphi, \tag{5.3}$$

where $A(r), B(r)$ are arbitrary functions of r. This field is an analog of field (4.1) in $3+1$ dimensions. Potentials $A_0^{(0)}$, $A_1^{(0)}$, $A_2^{(0)}$ of the AB field in $2+1$ dimensions are still given by the formulas (1.1). The operators

$$p_0=i\hbar\frac{\partial}{\partial x^0},\quad J_3=-i\hbar\frac{\partial}{\partial\varphi}+\frac{\hbar}{2}\sigma_3 \tag{5.4}$$

are integrals of motions in the external field under consideration. Thus, we can impose the following conditions on the spinor Ψ:

$$p_0\Psi=\hbar k_0\Psi,\quad J_3\Psi=\hbar\left(l-l_0-\tfrac{1}{2}\right)\Psi. \tag{5.5}$$

A solution of Eqs. (5.1) and (5.5) has the form

$$\Psi(x)=e^{-i\Gamma}\begin{pmatrix} e^{-i\varphi}\psi_1(r)\\ i\psi_2(r)\end{pmatrix},\quad \Gamma=k_0x^0-(l-l_0)\varphi, \tag{5.6}$$

where the functions $\psi_k(r)$ $(k=1,2)$ obey

$$\begin{aligned}\psi_1'(r)&=\frac{\overline{l}-1+A(r)}{r}\psi_1(r)-(k_0+B(r)+m)\psi_2(r),\\ \psi_2'(r)&=(k_0+B(r)-m)\psi_1(r)-\frac{\overline{l}+A(r)}{r}\psi_2(r).\end{aligned} \tag{5.7}$$

Explicit solutions of these equations can be found in three particular cases:

$$(1)\quad A(r)=B(r)=0, \tag{5.8}$$

$$(2)\quad A(r)=\rho=\frac{\gamma r^2}{2},\quad \gamma>0,\quad B(r)=0, \tag{5.9}$$

$$(3)\quad A(r)=\gamma r,\quad B(r)=\frac{b}{r},\quad \gamma>0. \tag{5.10}$$

In the following we consider each case in detail.

Case (5.8) corresponds to the pure AB field. For $l\neq 0$, there exist bounded solutions of the form

$$\begin{aligned}\psi_1(r)&=\sqrt{k_0+m}\;J_{|\overline{e}-1|}(kr),\quad k=\sqrt{k_0^2-m^2},\\ \psi_2(r)&=\varepsilon\sqrt{k_0+m}\,J_{|\overline{e}|}(kr),\quad \varepsilon=\operatorname{sign} l.\end{aligned} \tag{5.11}$$

Here $J_l(x)$ are Bessel functions. Solutions (5.11) vanish at $r=0$. They are orthogonal and normalized.

For $l=0$, $\mu\neq 0$, bounded solutions do not exist. However, there are unbounded at $r=0$ solutions. Some of them have the form

$$\begin{aligned}\psi_1(r)&=\sqrt{k_0+m}\;[c_1J_{\mu-1}(kr)+c_2J_{1-\mu}(kr)],\\ \psi(r)&=\sqrt{k_0-m}\;[c_1J_{\mu}(kr)-c_2J_{-\mu}(kr)].\end{aligned} \tag{5.12}$$

Here c_1,c_2 are arbitrary constants. Solutions (5.12) are still orthogonal and normalized. Another set of unbounded solutions (they are expressed via the Macdonald functions) reads

$$\begin{aligned}\psi_1(r)&=\sqrt{m+k_0}K_{1-\mu}(\sqrt{m^2-k_0^2}r),\quad \operatorname{Re}\sqrt{m^2-k_0^2}>0,\\ \psi_2(r)&=-\sqrt{m-k_0}K_{\mu}(\sqrt{m^2-k_0^2}r).\end{aligned} \tag{5.13}$$

As we see they are defined even for some complex k_0. It is interesting to remark that the latter solutions have finite norms.

The case (5.9) corresponds a combination of AB and uniform constant magnetic fields. Here we can introduce operators a_k^+,a_k $(k=1,2)$ by relations (2.33). Using the substitution

$$\psi_1(x)=e^{-ik_0x^0}\psi_1(\rho,\varphi),\quad \psi_2(x)=ie^{-ik_0x^0}\psi_2(\rho,\varphi), \tag{5.14}$$

we present (5.2) in the following form:

$$(k_0-m)\psi_1(\rho,\varphi)-\sqrt{2\gamma}a_1\psi_2(\rho,\varphi)=0,\quad (k_0+m)\psi_2(\rho,\varphi)-\sqrt{2\gamma}a_1^+\psi_1(\rho,\varphi)=0. \tag{5.15}$$

Now we can use the functions (2.47) and the relations (2.41).

Consider first states with $k_0^2\neq m^2$, $l\neq 0$. As in $3+1$ dimensions, these states can be divided in two types ($j=1,2$),

$$\psi_1(\rho,\varphi)=\sqrt{k_0+m}\,\psi^{(j)}_{n-1,\,l-1},\quad \psi_2(\rho,\varphi)=\sqrt{k_0-m}\,\psi^{(j)}_{n,l},\quad k_0^2=m^2+2\gamma\overline{n}, \tag{5.16}$$

where $\overline{n}$ was defined in Eq. (2.46). Solutions (5.16) vanish at $r=0$.

If $k_0^2\neq m^2$, $l=0$, $\mu\neq 0$, then solutions, which are formally defined by Eq. (5.16), are unbounded at $r=0$. However, they are still orthogonal and normalized. For $l=0$, $\mu\neq 0$, $k_0^2=m^2+\gamma(2\lambda+\mu-1)$ (λ is arbitrary complex), there exist other unbounded solutions. They have the form (5.6), with

$$\psi_1(r)=(k_0+m)\psi_{\lambda-1/2,\,1-\mu}(\rho),\quad \psi_2(r)=\sqrt{2\gamma}\psi_{\lambda,\mu}(\rho), \tag{5.17}$$

where the functions $\psi_{\lambda,\mu}(x)$ are defined by Eqs. (A28) and (A29). These solutions are orthogonal and normalized as well.

Consider now states with $k_0^2=m^2$. Suppose $k_0=m$; then a general solution of Eq. (5.7) reads

$$\begin{gathered}\psi_1(r)=Nf_l(\rho)+ce^{\rho/2}\rho^{[\overline{l}-1]/2},\quad \psi_2(r)=gNe^{-\rho/2}\rho^{-\overline{l}/2},\\ f_l(\rho)=e^{\rho/2}\rho^{[\overline{l}-1]/2}\int_\rho^\infty e^{-x}x^{-\overline{l}}dx,\quad g=\sqrt{\frac{\gamma}{2m^2}},\end{gathered} \tag{5.18}$$

where N, c are arbitrary constants. For $\mu\neq 0$ only some states with $l=0$ have a finite norm. Namely the states

$$\begin{gathered}\psi_1(r)=N\rho^{(\mu-1)/2}e^{\rho/2}\int_\rho^\infty e^{-x}x^{-\mu}\,dx,\quad \psi_2(r)=gN\,e^{-\rho/2}\rho^{-\mu/2},\\ N=\sqrt{\frac{\Gamma(1+\mu)\sin\mu\pi}{\pi[1+\mu\psi(1)-\mu\psi(1+\mu)+\mu g^2]}},\quad \int_0^\infty[\psi_1^2(r)+\psi_2^2]d\rho=1,\end{gathered} \tag{5.19}$$

where $\psi(x)$ is the logarithmic derivative of Γ-function (Ref. 18, 8.360). All the above-mentioned solutions are singular at $r=0$. One can see that $\lim_{\mu\to 0}N=0$. Thus, in $2+1$ dimensions, in pure magnetic field, the Dirac equation does not have solutions with $k_0=m$, in contrast to the corresponding $3+1$-dimensional case. For $\mu\neq 0$ (in the presence of the AB field) such solutions appear even in $2+1$ dimensions.

Suppose $k_0=-m$. Then, the functions

$$\psi_1(r)=0,\quad \psi_2(r)=[\Gamma(1-\overline{l})]^{-1/2}\rho^{-\overline{l}/2}e^{-\rho/2},\quad \int_0^\infty[\psi_1^2(r)+\psi_2^2]d\rho=1 \tag{5.20}$$

present solutions for $l\leqslant 0$. One can see that Eq. (5.20) is a particular case of Eq. (5.16). For $l<0$, the states (5.20) vanish at $r=0$. For $l=0$, $\mu\neq 0$, they are singular at $r=0$. If $\mu=0$, then this singularity disappears, however the states do not tend to zero as $r\to 0$.

Let us finally turn to case (5.10). Here it is enough to consider $b\neq 0$ only. Indeed, suppose $b=0$; then doing the change of functions ($\psi\to f$)

$$\psi_1(r)=\sqrt{k_0+m}\,f_1(r),\quad \psi_2(r)=\sqrt{k_0-m}f_2(r), \tag{5.21}$$

we can transform Eq. (5.7) to the form (2.78) with $k_1=\sqrt{k_0^2-m^2}$. Solutions of Eq. (2.78) are given by formulas (2.85)–(2.89). Thus, in the following we consider the case $b\neq 0$ only. We introduce the following notation:

$$g_1=\sqrt{|2\overline{l}-1|+2b},\quad g_{-1}=\sqrt{|2\overline{l}-1|-2b},\quad \varepsilon=\pm 1=\operatorname{sign} l. \tag{5.22}$$

Thus solutions of Eq. (5.7) have the form

$$\begin{gathered}\psi_1(r)=c_1 I_{\alpha+s,s}(y)+c_2 I_{\alpha+s-1,s+1}(y),\quad \psi_2(r)=c_3 I_{\alpha+s,s}(y)+c_4 I_{\alpha+s-1,s+1}(y),\\ y=2\sqrt{m^2+\gamma^2-k_0^2}\,r,\quad \alpha=1+g_1g_{-1},\quad 2+2s+g_1g_{-1}=\frac{2bk_0-(2\overline{l}-1)\gamma}{\sqrt{m^2+\gamma^2-k_0^2}},\end{gathered} \tag{5.23}$$

where

$$\begin{aligned}c_1&=(g_\varepsilon-\varepsilon g_{-\varepsilon})\sqrt{(2\overline{l}-1)k_0-2b\gamma-mg_1g_{-1}}=\frac{(g_\varepsilon-\varepsilon g_{-\varepsilon})}{(g_\varepsilon+\varepsilon g_{-\varepsilon})}c_3,\\ c_2&=-(g_\varepsilon+\varepsilon g_{-\varepsilon})\sqrt{(2\overline{l}-1)k_0-2b\gamma+mg_1g_{-1}}=\frac{(g_\varepsilon+\varepsilon g_{-\varepsilon})}{(g_\varepsilon-\varepsilon g_{-\varepsilon})}c_4,\end{aligned} \tag{5.24}$$

and relations (A6)–(A11) for the Laguerre functions $I_{n,m}$ were used. It follows from Eq. (5.22) that both g_1 and g_{-1} are real and positive for $(2\overline{l}-1)^2>4b^2$. If $(2\overline{l}-1)^2<4b^2$, then one of these quantities is real and positive and another one is imaginary. Suppose $(2\overline{l}-1)^2>4b^2$. Then for the energies $k_0^2<m^2+\gamma^2$ there exist bound states. In the latter case s is a positive integer and k_0^2 is quantized according to the last equation (5.23).

Another observation: For any b there exist a number l such that

$$1>g_1^2g_{-1}^2=(2\overline{l}-1)^2-4b^2>0. \tag{5.25}$$

For example, $b=0$ corresponds to $l=0$. Then one can choose two values for α,

$$\alpha_1=1+g_1g_{-1},\quad \alpha_2=1-g_1g_{-1}. \tag{5.26}$$

In both cases the solutions (5.23) have singularity at $r=0$ but still have finite norms.

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APPENDIX

(1) The Laguerre functions $I_{n,m}(x)$ are defined by

$$I_{n,m}(x)=\sqrt{\frac{\Gamma(1+n)}{\Gamma(1+m)}}\,\frac{\exp(-x/2)}{\Gamma(1+n-m)}x^{(n-m)/2}\Phi(-m,n-m+1;x). \tag{A1}$$

Here $\Phi(\alpha,\gamma;x)$ is the confluent hypergeometric function in a standard definition (see Ref. 18, 9.210). For $\gamma\neq -s$, where s is an integer and non-negative, the latter function can be presented by a series

$$\Phi(\alpha,\gamma;x)=\sum_{k=0}^{\infty}\frac{(\alpha)_k}{(\gamma)_k}\frac{x^k}{k!}=\frac{\Gamma(\gamma)}{\Gamma(\alpha)}\sum_{k=0}^{\infty}\frac{\Gamma(\alpha+k)}{\Gamma(\gamma+k)}\frac{x^k}{k!}. \tag{A2}$$

This series converges for any complex x. For any complex α, the Pochhammer symbols $(\alpha)_k$ are defined as follows:

$$2(\alpha)_k=\alpha(\alpha+1)\ldots(\alpha+k-1)=\frac{\Gamma(\alpha+k)}{\Gamma(\alpha)}. \tag{A3}$$

(2) Let m be a non-negative integer number; then the Laguerre functions are related to Laguerre polynomials $L_n^{\alpha}(x)$ (Ref. 18, 8.970, 8.972.1) by

$$I_{n,m}(x)=\sqrt{\frac{\Gamma(1+m)}{\Gamma(1+n)}}\exp(-x/2)x^{(n-m)/2}L_m^{n-m}(x),\quad m=0,1,2,\ldots, \tag{A4}$$

$$L_n^{\alpha}(x)=\frac{1}{n!}e^x x^{-\alpha}\frac{d^n}{dx^n}e^{-x}x^{n+\alpha}=\sum_{k=0}^{n}\binom{n+\alpha}{n-k}\frac{(-x)^k}{k!}=\binom{n+\alpha}{n}\Phi(-n,1+\alpha;x). \tag{A5}$$

Here n are non-negative integer numbers such that

$$\binom{\alpha}{n}=\frac{\Gamma(1+\alpha)}{\Gamma(1+n)\Gamma(1+\alpha-n)}=\frac{\alpha(\alpha-1)\ldots(\alpha-n+1)}{n!}.$$

(3) Using well-known properties of the confluent hypergeometric function (Ref. 18, 9.212; 9.213; 9.216), one can easily get both relations for the Laguerre functions

$$2\sqrt{x(n+1)}I_{n+1,m}(x)=(n-m+x)I_{n,m}(x)-2xI'_{n,m}(x), \tag{A6}$$

$$2\sqrt{x(m+1)}I_{n,m+1}(x)=(n-m-x)I_{n,m}(x)+2xI'_{n,m}(x), \tag{A7}$$

$$2\sqrt{xn}I_{n-1,m}(x)=(n-m+x)I_{n,m}(x)+2xI'_{n,m}(x), \tag{A8}$$

$$2\sqrt{xm}I_{n,m-1}(x)=(n-m-x)I_{n,m}(x)-2xI'_{n,m}(x), \tag{A9}$$

$$2\sqrt{nm}I_{n-1,m-1}(x)=(n+m-x)I_{n,m}(x)-2xI'_{n,m}(x), \tag{A10}$$

$$2\sqrt{(n+1)(m+1)}I_{n+1,m+1}(x)=(n+m+2-x)I_{n,m}(x)+2xI'_{n,m}(x), \tag{A11}$$

and a differential equation for these functions

$$4x^2I''_{n,m}(x)+4xI'_{n,m}(x)-[x^2-2x(1+n+m)+(n-m)^2]I_{n,m}(x)=0. \tag{A12}$$

Suppose $I_{n,m}(x)$ and $I_{m,n}(x)$ are linearly independent. Then, a general solution I of this equation has the form $I=AI_{n,m}(x)+BI_{m,n}(x)$. However, whenever condition (A18) holds, $I_{n,m}(x)$ and $I_{m,n}(x)$ are dependent. Formulas (A6)–(A11) and Eq. (A12) are valid for any complex n, m, x. One has to be careful applying formulas (A8)–(A10) for $n,m=0$. A straightforward calculation, which uses Eqs. (A1) and (A2), gives

$$\lim_{n\to 0}\sqrt{n}I_{n-1,m}(x)=-\frac{\sin m\pi}{\pi}\sqrt{\Gamma(1+m)}x^{-(1+m)/2}\exp(x/2),\quad \lim_{m\to 0}\sqrt{m}I_{n,m-1}(x)=0. \tag{A13}$$

A combination of Eqs. (A6)–(A9) results in the following relations:

$$2\sqrt{x}I'_{n,m}(x)=\sqrt{n}I_{n-1,m}(x)-\sqrt{n+1}I_{n+1,m}(x)=\sqrt{m+1}I_{n,m+1}(x)-\sqrt{m}I_{n,m-1}(x), \tag{A14}$$

$$\sqrt{x(n+1)}I_{n+1,m}(x)-(n-m+x)I_{n,m}(x)+\sqrt{xn}I_{n-1,m}(x)=0, \tag{A15}$$

$$\sqrt{x(m+1)}I_{n,m+1}(x)-(n-m-x)I_{n,m}(x)+\sqrt{xm}I_{n,m-1}(x)=0. \tag{A16}$$

(4) Using properties of the confluent hypergeometric function, one can get a representation

$$I_{n,m}(x)=\sqrt{\frac{\Gamma(1+n)}{\Gamma(1+m)}}\frac{\exp(x/2)}{\Gamma(1+n-m)}x^{(n-m)/2}\Phi(1+n,1+n-m;-x), \tag{A17}$$

and a relation (Ref. 18, 9.214)

$$I_{n,m}(x)=(-1)^{n-m}I_{m,n}(x), \quad n-m \ \text{integer}. \tag{A18}$$

(5) An asymptotic formula takes place

$$\Phi(a,c;x)\approx\frac{\Gamma(c)}{\Gamma(a)}e^{x}x^{a-c}, \quad \mathrm{Re}\,x\to\infty. \tag{A19}$$

Thus we obtain the following asymptotic behavior of $I_{n,m}(x)$ whenever m is not an integer:

$$I_{n,m}(x)=-\frac{\sin m\pi}{\pi}\sqrt{\Gamma(1+n)\Gamma(1+m)}x^{-(n+m+2)/2}\exp\,(x/2), \quad \mathrm{Re}\,x\to\infty, \tag{A20}$$

and

$$I_{n,m}(x)=(-1)^{m}\frac{x^{(n+m)/2}\exp(-x/2)}{\sqrt{\Gamma(1+n)\Gamma(1+m)}}, \quad \mathrm{Re}\,x\to\infty, \tag{A21}$$

whenever m is integer.

(6) One can prove the following asymptotic formula:

$$\lim_{p\to\infty} I_{p+\alpha,p+\beta}\left(\frac{x^2}{4p}\right)=J_{\alpha-\beta}(x), \tag{A22}$$

where $J_\nu(x)$ are Bessel functions.

(7) Taking into account Eqs. (A20) and (A21), one can see that only the functions $I_{\alpha+n,n}(x)$ with non-negative integer n and $\alpha>-1$ are quadratically integrable on the interval $(0,\infty)$. Such functions obey the orthonormality relation

$$\int_0^\infty I_{\alpha+n,n}(x)I_{\alpha+m,m}(x)\mathrm{d}x=\delta_{m,n}, \tag{A23}$$

which follows from the corresponding properties of the Laguerre polynomials (Ref. 18, 7.414.3). In such a case, the relation

$$I_{\alpha+n,n}(x)=\sqrt{\frac{n!}{\Gamma(n+\alpha+1)}}e^{-x/2}x^{\alpha/2}L_n^{\alpha}(x) \tag{A24}$$

follows from (A4).

(8) Consider a class of functions, which are closely related to Laguerre functions, and which appear often in various problems of mathematical physics.

As follows from Eq. (A12), the Laguerre functions are solutions of the following eigenvalue problem:

$$R_\alpha\psi=\lambda\psi, \quad R_\alpha=\frac{\alpha^2}{4x}+\frac{x}{4}-\frac{\mathrm{d}}{\mathrm{d}x}-x\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \quad 0<x<\infty, \quad \alpha=\mathrm{const}. \tag{A25}$$

A general solution of this problem has the form

$$\psi(x)=aI_{n,m}(x)+bI_{m,n}(x),\quad \alpha=n-m,\quad 2\lambda=n+m+1, \tag{A26}$$

where a, b are arbitrary constants. In the general case functions $\psi(x)$ vanish as $x\to\infty$ only if one of the numbers n or m is positive and an integer. However, one can provide such a behavior for any n,m, choosing some special values of a, b. Consider the functions

$$\psi_{\lambda,\alpha}(x)=x^{-1/2}W_{\lambda,\alpha/2}(x),\quad \psi_{\lambda,\alpha}(x)=\psi_{\lambda,-\alpha}(x), \tag{A27}$$

where $W_{\lambda,\mu}(x)$ are Whittaker functions (Ref. 18, 9.220.4). The functions $\psi_{\lambda,\alpha}(x)$ can be expressed via the confluent hypergeometric functions

$$\psi_{\lambda,\alpha}(x)=e^{-x/2}\left[\frac{\Gamma(-\alpha)x^{\alpha/2}}{\Gamma\left(\frac{1-\alpha}{2}-\lambda\right)}\Phi\left(\frac{1+\alpha}{2}-\lambda,1+\alpha;x\right)+\frac{\Gamma(\alpha)x^{-\alpha/2}}{\Gamma\left(\frac{1+\alpha}{2}-\lambda\right)}\Phi\left(\frac{1-\alpha}{2}-\lambda,1-\alpha;x\right)\right], \tag{A28}$$

or, using (A1), via the Laguerre functions

$$\psi_{\lambda,\alpha}(x)=\frac{\sqrt{\Gamma(1+n)\Gamma(1+m)}}{\sin(n-m)\pi}(\sin n\pi I_{n,m}(x)-\sin m\pi I_{m,n}(x)),$$
$$\alpha=n-m,\quad 2\lambda=1+n+m,\quad n=\lambda-\frac{1-\alpha}{2},\quad m=\lambda-\frac{1+\alpha}{2}. \tag{A29}$$

By the help of (A6)–(A16), the following properties of the functions $\psi_{\lambda,\alpha}(x)$ can be established:

$$\psi_{\lambda,\alpha}(x)=\sqrt{x}\psi_{\lambda-1/2,\alpha-1}(x)+\frac{1+\alpha-2\lambda}{2}\psi_{\lambda-1,\alpha}(x), \tag{A30}$$

$$\psi_{\lambda,\alpha}(x)=\sqrt{x}\psi_{\lambda-1/2,\alpha+1}(x)+\frac{1-\alpha-2\lambda}{2}\psi_{\lambda-1,\alpha}(x), \tag{A31}$$

$$2x\psi'_{\lambda,\alpha}(x)=(2\lambda-1-x)\psi_{\lambda,\alpha}(x)+\tfrac{1}{2}(2\lambda-1-\alpha)(2\lambda-1+\alpha)\psi_{\lambda-1,\alpha}(x), \tag{A32}$$

$$2x\psi'_{\lambda,\alpha}(x)=(\alpha-x)\psi_{\lambda,\alpha}(x)+(2\lambda-1-\alpha)\sqrt{x}\psi_{\lambda-1/2,\alpha+1}(x) \tag{A33}$$

$$=(x-2\lambda-1)\psi_{\lambda,\alpha}-2\psi_{\lambda+1,\alpha}. \tag{A34}$$

As a consequence of these properties we get

$$A_\alpha\psi_{\lambda,\alpha}(x)=\frac{2\lambda-1+\alpha}{2}\psi_{\lambda-1/2,\alpha-1}(x),\quad A^+_\alpha\psi_{\lambda-1/2,\alpha-1}(x)=\psi_{\lambda,\alpha}(x),$$
$$A_\alpha=\frac{x+\alpha}{2\sqrt{x}}+\sqrt{x}\frac{\mathrm{d}}{\mathrm{d}x},\quad A^+_\alpha=\frac{x+\alpha-1}{2\sqrt{x}}-\sqrt{x}\frac{\mathrm{d}}{\mathrm{d}x}. \tag{A35}$$

The operator R_α can be expressed via the operators A_α, A^+_α,

$$R_\alpha=A^+_\alpha A_\alpha+\frac{1-\alpha}{2},\quad R_{\alpha-1}=A_\alpha A^+_\alpha-\frac{\alpha}{2}. \tag{A36}$$

Since Eq. (A29) is a particular case of Eq. (A26), then $\psi_{\lambda,\alpha}(x)$ are also eigenfunctions for the operator R_α.

Using well-known asymptotics of the Whittaker function (Ref. 18, 9.227), we get

$$\psi_{\lambda,\alpha}(x)\sim x^{\lambda-1/2}e^{-x/2},\quad x\to\infty,\quad \psi_{\lambda,\alpha}(x)\sim\frac{\Gamma(|\alpha|)}{\Gamma\left(\frac{1+|\alpha|}{2}-\lambda\right)}x^{-|\alpha|/2},\quad \alpha\neq 0,\quad x\sim 0. \tag{A37}$$

The functions $\psi_{\lambda,0}(x)$ have a logarithmic singularity at $x\sim 0$. It is important to stress that the functions $\psi_{\lambda,\alpha}(x)$ are correctly defined and infinitely differentiable for $0<x<\infty$ and for any complex λ,α. In this respect one can mention that the Laguerre functions are not defined for negative integer n, m. In particular cases, when one of the numbers n, m is non-negative and an integer, the functions $\psi_{\lambda,\alpha}(x)$ coincide (up to a constant factor) with Laguerre functions. Thus, $\psi_{\lambda,\alpha}(x)$ are eigenfunctions (of the operator R_α), which vanish at $x\to\infty$.

According to Eq. (A37), the functions $\psi_{\lambda,\alpha}(x)$ are quadratically integrable on the interval $0<x<\infty$ whenever $|\alpha|<1$. It is not true for $|\alpha|\geqslant 1$. The corresponding integrals can be calculated (Ref. 18, 7.611),

$$\int_0^\infty \psi_{\lambda,\alpha}(x)\psi_{\lambda',\alpha}(x)\,dx=\frac{\pi}{(\lambda'-\lambda)\sin\alpha\pi}\left\{\left[\Gamma\left(\frac{1+\alpha-2\lambda'}{2}\right)\Gamma\left(\frac{1-\alpha-2\lambda}{2}\right)\right]^{-1}-\left[\Gamma\left(\frac{1-\alpha-2\lambda'}{2}\right)\Gamma\left(\frac{1+\alpha-2\lambda}{2}\right)\right]^{-1}\right\},\quad |\alpha|<1, \tag{A38}$$

$$\int_0^\infty |\psi_{\lambda,\alpha}(x)|^2\,dx=\frac{\pi}{\sin\alpha\pi}\,\frac{\psi\left(\frac{1+\alpha-2\lambda}{2}\right)-\psi\left(\frac{1-\alpha-2\lambda}{2}\right)}{\Gamma\left(\frac{1+\alpha-2\lambda}{2}\right)\Gamma\left(\frac{1-\alpha-2\lambda}{2}\right)},\quad |\alpha|<1, \tag{A39}$$

$$\int_0^\infty |\psi_{\lambda,0}(x)|^2\,dx=\frac{\psi'\left(\frac{1}{2}-\lambda\right)}{\Gamma^2\left(\frac{1}{2}-\lambda\right)},\quad \int_0^\infty \left|\psi_{n+1/2,0}(x)\right|^2\,dx=\Gamma^2(1+n). \tag{A40}$$

Here $\psi(x)$ is the logarithmic derivative of the Γ function (Ref. 18, 8.360).

For $|\alpha|\geqslant 1$, the situation is the following: the only quadratically integrable eigenfunctions of the operator R_α are Laguerre functions, they also form a complete set. The functions $\psi_{\lambda,\alpha}(x)$ are orthogonal whenever arguments of the Γ function in Eq. (A38) are integers and negative. That corresponds to n, m integer and non-negative. Thus, that is again the case of Laguerre functions according to Eq. (A29). If $|\alpha|<1$, then, in the general case, the functions $\psi_{\lambda,\alpha}(x)$ and $\psi_{\lambda',\alpha}(x)$, $\lambda'\neq\lambda$, are not orthogonal, as follows from Eq. (A38). That is a reflection of the fact that R_α is no longer a self-conjugate operator for such values of α.

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Double-scaling limit of a broken symmetry quantum field theory in dimensions $D<2$

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The Ising limit is a correlated limit in which two bare Lagrangian parameters, the coupling constant g and the *negative* mass squared $-m^2$, both approach infinity with the ratio $-m^2/g=\alpha>0$ held fixed. In a conventional Hermitian parity-symmetric scalar quantum field theory, with interaction term $g|\phi|^N/N$, the renormalized mass of the asymptotic theory is finite in this limit, and the limiting theory exhibits universality in N. For a non-Hermitian $\mathcal{PT}$-symmetric but parity-violating Lagrangian, with interaction term $-g(i\phi)^N/N$, the renormalized mass diverges in the same correlated limit. Nevertheless, the asymptotic theory still has interesting properties. In particular, the one-point Green's function approaches the value $-i\alpha^{1/(N-2)}$ independently of the space–time dimension D for $D<2$. Moreover, while the Ising limit of a conventional theory is dominated by a dilute instanton gas, the corresponding correlated limit of this $\mathcal{PT}$-symmetric theory is dominated by a constant-field configuration with corrections determined by a weak-coupling expansion in which the expansion parameter is proportional to an inverse power of g. We thus observe a weak-coupling/strong-coupling duality: the Ising limit itself is a strong-coupling limit, but the expansion about this limit takes the form of a conventional weak-coupling expansion. A possible generalization to dimensions $D<4$ is briefly discussed.
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I. $\mathcal{PT}$-SYMMETRIC QUANTUM FIELD THEORY

Conventional field-theoretic Hamiltonians possess two crucial symmetries, the continuous symmetry of the proper Lorentz group and the discrete symmetry of Hermiticity. While Lorentz invariance is a physical requirement, Hermiticity is a useful but rather mathematical constraint. However, assuming Lorentz invariance and positivity of the spectrum of the Hamiltonian one can prove the $\mathcal{PCT}$ theorem and thereby establish the physical discrete symmetry of $\mathcal{PCT}$ invariance. Recent papers have investigated the consequences of imposing only the physical symmetries of Lorentz invariance and $\mathcal{PCT}$ invariance in constructing a Hamiltonian. The constraint of $\mathcal{PCT}$ invariance is weaker than Hermiticity, so Hamiltonians having this property need not be Hermitian. In quantum mechanics and in scalar quantum field theory the $\mathcal{C}$ operator is unity, so $\mathcal{PCT}$ symmetry reduces to $\mathcal{PT}$ symmetry. While it has not yet been proved, there is strong analytical and

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numerical evidence supporting the conjecture that, except when $\mathcal{PT}$ symmetry is spontaneously broken, the energy levels of many such Hamiltonians are all real and positive. The reality and positivity of the spectrum are apparently a consequence of the $\mathcal{PT}$ symmetry of H. Hamiltonians having $\mathcal{PT}$ symmetry have been studied in quantum mechanics[1–14] and in quantum field theory.[15–20]

A simple example of such a quantum-mechanical Hamiltonian is $H=p^2+ix^3$. Hamiltonians of this form may be regarded as *complex deformations* of conventional Hermitian Hamiltonians. To illustrate this deformation we consider the Hamiltonian $H=p^2-(ix)^N$, where $N\geqslant 2$ is a real number that is *not necessarily an integer*. When $N=2$, we have the harmonic oscillator Hamiltonian, whose spectrum is real and positive. As N increases from 2, the entire spectrum of the Hamiltonian smoothly deforms as a function of N and remains real and positive for all values of $N>2$. Thus, these theories are in effect the analytic continuation of conventional quantum mechanics into the complex plane.

These non-Hermitian theories exhibit some remarkable properties. Most interesting is that the expectation value of the operator x in quantum mechanics and the field ϕ in the corresponding quantum field theory is *nonzero* when $N>2$. This is true even for the p^2-x^4 Hamiltonian that one obtains at $N=4$, and it is also true for the $-g\phi^4$ scalar quantum field theory. The $-g\phi^4$ quantum field theory is particularly surprising because it has a positive real spectrum and exhibits a nonzero value of $\langle\phi\rangle$, and in four-dimensional space–time has a dimensionless coupling constant, is renormalizable, and is asymptotically free (and thus nontrivial). It may thus provide a useful setting to describe the Higgs particle.[19]

In this article we investigate the Euclidean scalar quantum field theory in dimensions $D<2$ defined by the Lagrangian density

$$\mathcal{L}=\frac{1}{2}(\nabla\phi)^2+\frac{1}{2}m^2\phi^2-\frac{g}{N}(i\phi)^N \quad (N>2). \tag{1.1}$$

Our purpose here is to study this theory in the correlated limit in which two bare Lagrangian parameters, the coupling constant g and the *negative* mass squared $-m^2$, both approach infinity with the ratio

$$-m^2/g\equiv\alpha>0 \tag{1.2}$$

held fixed. In a conventional parity-symmetric scalar quantum field theory this limit is called the *Ising limit*. In this limit the renormalized mass of the asymptotic theory is finite. Moreover, the limiting theory exhibits universal properties that will be discussed in Sec. II. For the non-Hermitian $\mathcal{PT}$-symmetric Lagrangian Eq. (1.1) the renormalized mass diverges in this same limit. We will show, however, that the asymptotic theory exhibits intriguing properties. Of considerable interest is the fact that the one-point Green's function G_1 approaches the finite value $-i\alpha^{1/(N-2)}$. Furthermore, while the Ising limit of a parity-symmetric quantum field theory is dominated by a dilute instanton gas, the corresponding correlated limit of a $\mathcal{PT}$-symmetric quantum field theory lacking parity symmetry is dominated by a constant-field configuration with corrections determined by a weak-coupling expansion in which the lines represent propagators of the conventional weak-coupling form and the vertices are proportional to an inverse power of g.

This article is organized as follows. In Sec. II we review the Ising limit of a Hermitian parity-invariant self-interacting scalar quantum field theory and consider this same correlated limit in a $\mathcal{PT}$-symmetric quantum field theory. In Sec. III we examine Hermitian and non-Hermitian $\mathcal{PT}$-symmetric quantum field theories in the correlated limit of Eq. (1.2) for the special case of $D=0$. In Sec. IV we investigate the one-dimensional case of Eq. (1.1) in this correlated limit by using the correspondence between one-dimensional field theory and quantum mechanics. Finally, in Sec. V we study this correlated limit for a D-dimensional quantum field theory where $D<2$ and make some observations concerning the case $D\geqslant 2$.

II. CONVENTIONAL ISING LIMIT OF SCALAR QUANTUM FIELD THEORY

The *Ising limit* of a scalar quantum field theory is defined as follows. Given the Lagrangian density for a D-dimensional Euclidean space quantum field theory,

$$\mathcal{L}=\frac{1}{2}(\nabla\phi)^2+\frac{1}{2}m^2\phi^2+\frac{g}{N}|\phi|^N \quad (N>2), \tag{2.1}$$

take the limit as the bare coupling constant $g\to\infty$ but demand that the renormalized mass M (the pole of the two-point Green's function) remain fixed and finite. To satisfy this constraint the value of the bare mass squared m^2 must approach $-\infty$ so that the ratio $-m^2/g=\alpha$ is fixed. Thus, the Ising limit is a correlated limit. In this limit the renormalized Green's functions of Eq. (2.1) approach universal N-independent values.[21]

The terminology ''Ising limit'' is taken from statistical mechanics. The Ising model of statistical mechanics describes systems in which there are two equally likely spin states. By analogy, in the correlated limits $g\to\infty$ and $m^2\to-\infty$ the potential $\frac{1}{2}m^2\phi^2+(g/N)|\phi|^N$ develops a deep symmetric double well. In one Euclidean space–time dimension (quantum mechanics) the Lagrangian density $\mathcal{L}$ represents a particle that is equally likely to be in one of two possible states, the left well or the right well.

The Ising limit is a strong-coupling phenomenon and is not accessible by a conventional perturbative treatment. However, a nonperturbative semiclassical analysis in quantum mechanics can be used to calculate the amplitude for the particle to tunnel from one well to the other. This tunneling amplitude is exponentially small. The well is symmetric, so the splitting between the lowest energy state and the first excited state is also exponentially small and is proportional to this tunneling amplitude. The renormalized mass M is the difference between the energy of the (odd-parity) first excited state and the energy of the (even-parity) ground state. The Ising limit exists because M can remain fixed even though the double-well potential becomes infinitely deep and all of its energy levels approach negative infinity. The symmetry of the double well is crucial; if it were not symmetric, the renormalized mass could not remain finite as g and $-m^2$ become large.

To determine the dimensionless renormalized Green's functions of a D-dimensional Euclidean quantum field theory in the Ising limit, we follow a routine procedure. First, we construct the vacuum persistence amplitude in the presence of an external source:

$$\mathcal{Z}[J]=\int \mathcal{D}\phi\,\exp\left(-\int d^Dx\,[\mathcal{L}-J(x)\phi(x)]\right). \tag{2.2}$$

The connected unrenormalized n-point Green's functions are then usually obtained by repeated functional differentiation of $\mathcal{W}[J]\equiv\ln\mathcal{Z}[J]$ with respect to the source J:

$$G_n(x_1,x_2,x_3,\ldots,x_n)=\frac{\delta}{\delta J(x_1)}\frac{\delta}{\delta J(x_2)}\frac{\delta}{\delta J(x_3)}\cdots\frac{\delta}{\delta J(x_n)}\ln(\mathcal{Z}[J])\bigg|_{J=0}. \tag{2.3}$$

(If the Lagrangian is symmetric under $\phi\to-\phi$, then Green's functions having an odd number n of legs vanish.) In the Ising limit, as opposed to perturbation theory, the simpler objects to calculate are the n-point correlation functions

$$W_n(x_1,x_2,\ldots,x_n)\equiv\frac{1}{\mathcal{Z}}\int \mathcal{D}\phi\,\phi(x_1)\phi(x_2)\ldots\phi(x_n)\exp\left(-\int d^Dx\,\mathcal{L}\right), \tag{2.4}$$

and the G_n are then obtained by subtracting the disconnected parts according to the formulas for the cumulants according to

$$G_1(x_1)=W_1(x_1),$$

$$G_2(x_1,x_2)=W_2(x_1,x_2)-W_1(x_1)W_1(x_2), \tag{2.5}$$

$$G_3(x_1,x_2,x_3)=W_3(x_1,x_2,x_3)-W_1(x_1)W_2(x_2,x_3)-W_1(x_2)W_2(x_1,x_3)$$
$$-W_1(x_3)W_2(x_1,x_2)+2W_1(x_1)W_1(x_2)W_1(x_3),$$

and so on.

Second, we construct the one-particle-irreducible (1PI) connected Green's functions Γ_n. These are obtained by functional differentiation with respect to the classical field $\phi(x)$ of the effective action,

$$\Gamma[\phi]=\mathcal{W}[J]-\int d^Dx'\,[\phi(x')-G_1]J(x'), \tag{2.6}$$

where $\phi(x)$ is the expectation value of the field in the presence of the source $J(x)$:

$$\phi(x)=\frac{\delta\mathcal{W}[J]}{\delta J(x)}. \tag{2.7}$$

In an abbreviated notation, or in momentum space, the first few Γ_n are

$$\Gamma_1=G_1(G_2)^{-1},$$

$$\Gamma_2=-(G_2)^{-1}-G_1G_3(G_2)^{-3}, \tag{2.8}$$

$$\Gamma_3=G_3(G_2)^{-3}-G_1G_4(G_2)^{-4}+3G_1(G_3)^2(G_2)^{-5}.$$

One effect of these relations is to amputate the legs of the n-point unrenormalized Green's function by multiplying by $(G_2)^{-n}$.

Third, we construct the dimensionless renormalized 1PI Green's functions $\tilde{\Gamma}_n^{\mathrm{ren}}$. To do so we perform a (finite) wave-function renormalization by multiplying by $(\sqrt{Z})^n$, where Z is the wave-function renormalization constant. The *dimensionless* renormalized Green's functions are then obtained by multiplying by the appropriate power of the renormalized mass. Normally Z is defined as the residue of the pole of the two-point Green's function. However, in this article we use the simpler *intermediate renormalization scheme* in which the renormalization is performed in momentum space with the Green's functions evaluated at zero momentum on the external legs. In this scheme the value of Z is just the two-point Green's function in momentum space multiplied by the square of the renormalized mass.

The dimensionless renormalized 1PI Green's functions $\tilde{\Gamma}_n^{\mathrm{ren}}$ are the coefficients in the Taylor expansion of the renormalized effective action. In the Ising limit of the parity-symmetric Lagrangian density in Eq. (2.1) these coefficients are known analytically in the cases $D=0$ and $D=1$. In those cases the dimensionless renormalized $2n$-point momentum-space Green's functions $\tilde{\Gamma}_{2n}^{\mathrm{ren}}$ at zero external momentum have the form[21]

$$\tilde{\Gamma}_{2n}^{\mathrm{ren}}|_{D=0}=-\frac{n!}{2n(2n-1)},$$
$$\tilde{\Gamma}_{2n}^{\mathrm{ren}}(0,0,\ldots,0)|_{D=1}=-\frac{2^n\Gamma(n-\frac{1}{2})}{4\Gamma(\frac{1}{2})}. \tag{2.9}$$

Note that these results are independent of N; thus, apart from dimensional dependence, the Ising limit is evidently universal.

In this article we examine the Ising limit for the class of scalar quantum field theories defined in Eq. (1.1). While these theories are similar to those in Eq. (2.1), they do not possess parity symmetry. For such theories we will show that in this limit the Green's functions exhibit a remarkably simple structure even though in this limit the renormalized mass now diverges. Of course, when N is not an even integer, the spectrum of a quantum field theory whose interaction term is ϕ^N is not bounded below. Moreover, the functional-integral representation for the vacuum persistence amplitude

$$\mathcal{Z}=\int \mathcal{D}\phi \exp\left(-\int d^D x\, \mathcal{L}\right) \tag{2.10}$$

does not exist. However, for the strange looking non-Hermitian Lagrangian density in Eq. (1.1), which was discussed in detail in Ref. 15, it appears that for $N\geqslant 2$, the energy levels are all real and positive and that for this Lagrangian density the functional integral in Eq. (2.10) exists. (Note that for $N\geqslant 3$ the functional integral must be performed along a complex contour that begins *below* the negative-real axis and ends *below* the positive-real axis in the complex-ϕ plane. More precisely, the contour approaches infinity within asymptotic wedges whose opening angles are determined by the criterion that the functional integral in Eq. (2.10) exist. These wedges are described in detail in Ref. 15.) The $\mathcal{PT}$-symmetric Lagrangian density (1.1) is interesting because it provides a simple model of a quantum field theory with a broken symmetry. When $N=2$ the Lagrangian density represents a free theory, but as N increases from this value, the theory exhibits remarkable properties. For example, by direct calculation one can show that the value of $\langle\phi\rangle$ is nonzero (it has a negative-imaginary value) even if N is an even integer.[15]

III. CORRELATED LIMIT FOR $D=0$

In this section we discuss the Ising limit in the special case $D=0$. The vacuum persistence amplitude $\mathcal{Z}$ and correlation functions W_n are then expressible in terms of conventional Riemann integrals.

A. The parity-symmetric case

For the parity-symmetric theory the n-point correlation functions are

$$W_n=\frac{\int_{-\infty}^{\infty} dt\, t^n \exp(-\frac{1}{2}m^2t^2-(g/N)\,t^N)}{\int_{-\infty}^{\infty} dt \exp(-\frac{1}{2}m^2t^2-(g/N)\,t^N)}, \tag{3.1}$$

where N is an even integer greater than 2. Note that W_n vanishes when n is odd.

To evaluate the integrals in Eq. (3.1) in the limit of large g and $-m^2$, we substitute $-m^2=\alpha g$, where α is a positive constant, and use Laplace's method.[22] The Laplace points are the roots of $(d/dt)\,(\frac{1}{2}\alpha t^2-(1/N)\,t^N)=\alpha t-t^{N-1}=0$. Clearly, one Laplace point is always $t=0$, and expanding about this point gives the usual weak-coupling Feynman perturbation series. However, as $g\to\infty$, the contribution from this point vanishes exponentially relative to contributions from other Laplace points. Two real Laplace points located at $t=\pm\alpha^{1/(N-2)}$ dominate the asymptotic behavior of the integral representation for W_n. We thus obtain the leading asymptotic behavior

$$W_{2n}\sim\alpha^{2n/(N-2)} \quad (g\to\infty). \tag{3.2}$$

We then construct the connected Green's functions from the correlation functions W_n by using the zero-dimensional version of the cumulants in Eq. (2.5):

$$\begin{aligned} G_1&=W_1,\\ G_2&=W_2-(W_1)^2, \end{aligned} \tag{3.3}$$

$$G_3 = W_3 - 3W_1W_2 + 2(W_1)^3,$$

and so on. In the symmetric case these equations simplify enormously because $W_{2n+1}=0$.

We recover the first result in Eq. (2.9) by substituting Eq. (3.2) into Eq. (3.3) and then following the renormalization procedure described in Sec. II: we amputate the external legs, and then multiply by the appropriate power of the renormalized mass M, where $G_2 = M^{-2}$, to make the Green's functions dimensionless. In zero dimensions the wave-function renormalization constant Z can be chosen to be unity. Note that the dimensionless renormalized Green's functions in (2.9) are pure numbers independent of both N and α.

B. The parity-nonsymmetric case

Now consider the zero-dimensional version of the theory in Eq. (1.1). For this theory the n-point correlation functions W_n are

$$W_n = \frac{\int_{-\infty}^{\infty} dt\, t^n \exp[-\frac{1}{2}m^2t^2 + (g/N)(it)^N]}{\int_{-\infty}^{\infty} dt \exp[-\frac{1}{2}m^2t^2 + (g/N)(it)^N]}. \tag{3.4}$$

To evaluate W_n we split the range of integration in each of these integrals into two contributions:

$$\int_{-\infty}^{\infty} dt\, t^n \cdots = \int_{-\infty}^{0} dt\, t^n \cdots + \int_{0}^{\infty} dt\, t^n \cdots = 2\begin{pmatrix} \mathrm{Re(if}\ n\ \mathrm{even)} \\ i\ \mathrm{Im(if}\ n\ \mathrm{odd)} \end{pmatrix} \int_{0}^{\infty} dt\, t^n \cdots . \tag{3.5}$$

This integral exists if $1 < \mathrm{Re}\, N < 3$.

Note that W_n is an analytic function of N for $N \geqslant 0$ because the region inside of which the integration path in Eq. (3.4) lies *is an implicit function of N*. Indeed, as N ranges through real values, the paths of integration of the two integrals in Eq. (3.5) lie inside wedge-shaped regions that *rotate in opposite directions*.[23] It is convenient to take the paths of integration to lie at the center of the wedges. In this case, the path of integration of the first integral connects complex ∞ to 0 in the t plane along the straight line

$$\text{path 1:} \quad \arg t = -\pi/2 - \pi/N. \tag{3.6}$$

The second integration path runs from 0 to complex ∞ along

$$\text{path 2:} \quad \arg t = -\pi/2 + \pi/N. \tag{3.7}$$

The opening angle of each wedge is π/N.

When $N=2$ the wedges are centered about the positive and negative real axes and the opening angle of the wedges is 90°. In this case path 1 connects $-\infty$ to 0 and path 2 connects 0 to ∞ along the real-t axis. Here, W_n is *real* and parity symmetry is unbroken. As N increases, path 1 rotates anticlockwise and path 2 rotates clockwise. Integration along the real axis is no longer allowed when $N \geqslant 3$. The two paths slope downward at 45° angles when $N=4$. For all $N>2$ we find that $W_{2n+1} \neq 0$, demonstrating that parity symmetry is broken.

Now we discuss the Ising limit. To analyze the asymptotic behavior of the integrals in Eq. (3.4) we examine the expression

$$L(t) = \frac{1}{2}m^2t^2 - \frac{g}{N}(it)^N \quad (N>2). \tag{3.8}$$

The saddle points determining the asymptotic behavior are the zeros of $L'(t) = m^2t - ig(it)^{N-1}$. Remember that both g and $-m^2$ are large such that the ratio $\alpha = -m^2/g$ is fixed. There are many roots of $L'(t)=0$: First there is a root at $t=0$, which is the perturbative root, corresponding to

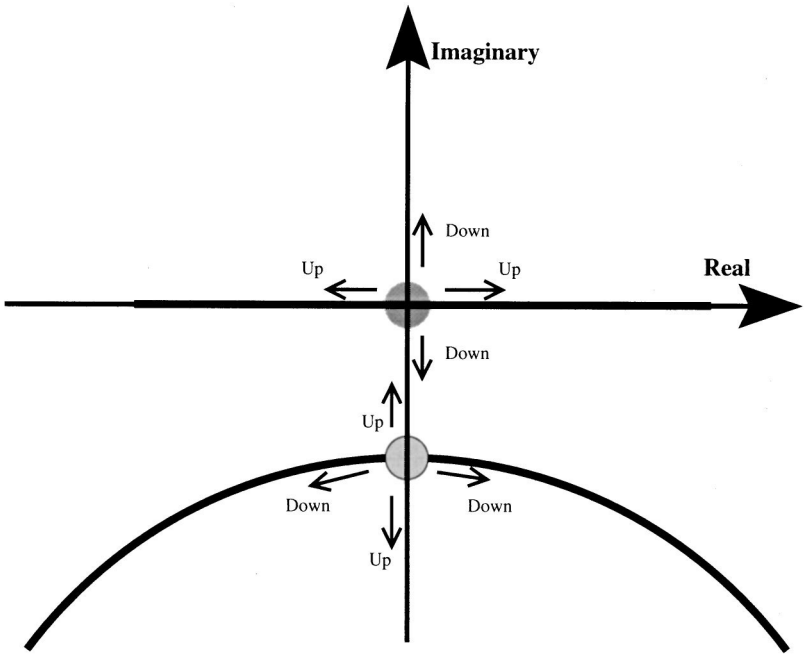

FIG. 1. Position of relevant saddle points and paths of stationary phase for the evaluation of Eq. (3.4) in the Ising limit.

expansions in powers of g. Second, there is a ring of roots surrounding the origin. The most important of these roots, and the one that determines the Ising limit of the theory, lies on the negative imaginary axis:

$$t_0 = -i\alpha^{1/(N-2)}. \tag{3.9}$$

To find the directions of the saddle points we calculate the second derivative of L: $L''(t) = m^2 + g(N-1)(it)^{N-2}$. Thus, $L''(0) = m^2$ and $L''(t_0) = -(N-2)m^2$, which is positive because m^2 is negative and $N > 2$. Hence, the down directions for the saddle point at $t = 0$ go vertically along the imaginary axis. The down directions for the saddle point t_0 are locally horizontal (see Fig. 1). As we trace the down paths away from the saddle point t_0 they curve downward and align with the directions in Eqs. (3.6) and (3.7). This verifies that t_0 is the saddle point that we should use.

It is straightforward to find the leading asymptotic behavior of the integrals in Eq. (3.4). The Gaussian corrections cancel and we obtain the leading-order result

$$W_n \sim (t_0)^n. \tag{3.10}$$

However, when we substitute this result into the formulas in Eq. (3.3), we find that except for G_1, each of the Green's functions *vanishes* to leading order. This happens because the sum of the numerical coefficients in each cumulant except the first is zero. (This does not happen in the parity-symmetric case because $W_n \equiv 0$ for odd n.)

Therefore, we are obliged to perform the asymptotic analysis to higher order. For example, to obtain the first nonvanishing contribution to G_2 we must calculate W_1 and W_2 to one order beyond the Gaussian approximation; to obtain G_3 we must calculate W_1, W_2, and W_3 to two orders beyond the Gaussian approximation; to obtain G_4 we must calculate W_1, W_2, W_3, and W_4 to three orders beyond the Gaussian approximation; and so on. To perform this calculation we need the kth derivative of $L(t)$ in (3.8):

$$L^{(k)}(t)=-\frac{i^k g\Gamma(N)}{\Gamma(N-k+1)}(it)^{N-k} \quad (k\geqslant 3). \tag{3.11}$$

Substituting the saddle point $t=t_0$ gives

$$L^{(k)}(t_0)=-\frac{i^k g\Gamma(N)}{\Gamma(N-k+1)}\alpha^{(N-k)/(N-2)} \quad (k\geqslant 3). \tag{3.12}$$

The expression for W_n then has the form

$$W_n\sim\frac{\int dt\, t^n \exp[\Sigma_{k=2}^{\infty}-(1/k!)\,L^{(k)}(t_0)(t-t_0)^k]}{\int dt \exp[\Sigma_{k=2}^{\infty}-(1/k!)\,L^{(k)}(t_0)(t-t_0)^k]}. \tag{3.13}$$

Note that $L(t_0)$ cancels from the numerator and denominator. Next, we make the translation $s=t-t_0$ and the scaling $s=v\epsilon\alpha^{1/(N-2)}$, where $\epsilon^2=\alpha^{-N/(N-2)}/[g(N-2)]$. The result is

$$W_n\sim(t_0)^n\frac{\int dv\,(1+iv\epsilon)^n e^{-(1/2)v^2}\exp\left[\Sigma_{k=3}^{\infty}\dfrac{v^k i^k\Gamma(N)\epsilon^{k-2}}{k!\Gamma(N+1-k)(N-2)}\right]}{\int dv\, e^{-(1/2)v^2}\exp\left[\Sigma_{k=3}^{\infty}\dfrac{v^k i^k\Gamma(N)\epsilon^{k-2}}{k!\Gamma(N+1-k)(N-2)}\right]}. \tag{3.14}$$

We expand the integrands in the numerator and denominator as series in powers of ϵ and perform the Gaussian integrals. We then substitute the result into Eq. (3.3) to obtain the small-ϵ leading asymptotic approximations to the unrenormalized connected Green's functions G_n:

$$\begin{aligned} G_1&\sim t_0,\\ G_2&\sim-(t_0)^2\epsilon^2, \end{aligned} \tag{3.15}$$

and

$$G_n\sim-(t_0)^n\epsilon^{2n-2}(N-1)(N-2)^{n-2}\Gamma\left[\frac{(n-2)(N-1)}{N-2}\right]\Big/\,\Gamma\left(\frac{n-2}{N-2}\right) \tag{3.16}$$

for $n>2$. To obtain the analogs of the first of Eqs. (2.9) we construct the coefficients of the effective action. Using the relations given in Eq. (2.8) we obtain

$$\begin{aligned} \Gamma_1&\sim-(t_0)^{-1}\epsilon^{-2},\\ \Gamma_2&\sim-(t_0)^{-2}\epsilon^{-2}(N-2), \end{aligned} \tag{3.17}$$

and so on. The general formula is

$$\Gamma_n\sim-(t_0)^{-n}\epsilon^{-2}\frac{1}{(N-2)}\left[\frac{(N-n-1)\Gamma(N)}{\Gamma(N-n+1)}+\delta_{n,2}\right]. \tag{3.18}$$

We construct the *dimensionless* renormalized coefficients $\tilde{\Gamma}_n^{\mathrm{ren}}$ by multiplying Γ_n by the appropriate power of the renormalized mass $M^2=1/G_2=-(\epsilon t_0)^{-2}=\alpha g(N-2)$ according to $\tilde{\Gamma}_n^{\mathrm{ren}}=\Gamma_n(M^2)^{-n/2}$. Thus, we have the result

$$\tilde{\Gamma}_n^{\mathrm{ren}}\sim-\epsilon^{n-2}\frac{i^n}{(N-2)}\left[\frac{(N-n-1)\Gamma(N)}{\Gamma(N-n+1)}+\delta_{n,2}\right], \tag{3.19}$$

independent of t_0. This is the analog of the first of Eqs. (2.9) for the $\mathcal{PT}$-symmetric theory.

IV. CORRELATED LIMIT FOR THE SCHRÖDINGER EQUATION

The Lagrangian in Eq. (1.1) is a field-theoretic generalization of the quantum-mechanical theory described by the non-Hermitian Hamiltonian

$$H=\frac{1}{2}p^2+\frac{1}{2}x^2-\frac{g}{N}(ix)^N. \tag{4.1}$$

This Hamiltonian is $\mathcal{PT}$-symmetric because under parity reflection $\mathcal{P}$: $p\to -p$ and $x\to -x$ and under time reversal, which is an antiunitary operation, $\mathcal{T}$: $p\to -p$, $x\to x$, and $i\to -i$. The Ising substitution $m^2=-\alpha g$ gives the Schrödinger equation

$$-\frac{1}{2}\psi''(x)+\left[-\frac{1}{2}\alpha g x^2-\frac{g}{N}(ix)^N-E\right]\psi(x)=0, \tag{4.2}$$

where $\alpha>0$. The eigenvalue problem is posed on a path in the complex-x plane whose endpoints lie in complex wedges similar to the wedges discussed earlier for the complex path integral. See Refs. 1 and 2.

We seek the large-g behavior of (4.2). In this limit the energy E scales like g because the potential scales like g (this will be verified shortly). Thus, we make the substitution

$$E=\lambda g. \tag{4.3}$$

We now can study $Q(x)=-\frac{1}{2}\alpha x^2-(1/N)(ix)^N-\lambda$ in the resulting Schrödinger equation

$$-\tfrac{1}{2}\psi''(x)+gQ(x)\psi(x)=0. \tag{4.4}$$

For large g it is the turning points [the zeros of $Q(x)$] that determine the physics of the problem. More precisely, it is the lowest-lying pair of turning points that control the physics. Near this pair of turning points, the polynomial $Q(x)$ can be approximated by a parabola. To construct the parabola, we locate the point on the imaginary axis midway between the pair of turning points by differentiating $Q(x)$ and setting $Q'(x)=-\alpha x-i(ix)^{N-1}=0$. The value of x on the negative imaginary axis that solves this equation is $x_0=-i\alpha^{1/(N-2)}$. At this value of x, we see that $Q(x)$ vanishes if

$$\lambda=\frac{N-2}{2N}\alpha^{N/(N-2)}, \tag{4.5}$$

which justifies the scaling of E used in (4.3).

Next, we expand the Schrödinger equation (4.4) around the point x_0 by substituting

$$x=-i\alpha^{1/(N-2)}+\epsilon t \quad \text{and} \quad \lambda=\frac{N-2}{2N}\alpha^{N/(N-2)}+\delta. \tag{4.6}$$

Here, we treat ϵ and δ as small parameters, whose size will be determined below. We obtain

$$-\frac{1}{2\epsilon^2}\psi''(t)+g\left[-\frac{N-2}{2}\alpha\epsilon^2t^2+i\frac{(N-1)(N-2)}{6}\alpha^{(N-3)/(N-2)}\epsilon^3t^3-\delta\right]\psi(t)=0. \tag{4.7}$$

The requirement of dominant balance[22] implies that we must choose

$$\epsilon=g^{-1/4} \quad \text{and} \quad \delta=\beta g^{-1/2}, \tag{4.8}$$

where $\beta=\mathrm{O}(1)$ is a constant. To leading order the resulting Schrödinger equation reads

$$-\frac{1}{2}\psi''(t)+\left[-\frac{N-2}{2}\alpha t^2+i\frac{(N-1)(N-2)}{6}\alpha^{(N-3)/(N-2)}g^{-1/4}t^3-\beta\right]\psi(t)=0. \tag{4.9}$$

As $g\to\infty$ this equation becomes the eigenvalue problem for the harmonic oscillator, whose nth eigenvalue is $\beta=(n+1/2)\sqrt{(N-2)\alpha}$, where $n=0,1,2,\ldots$ is an integer. Thus, for the Schrödinger equation (4.2) the nth eigenvalue in the Ising limit is

$$E_n=\frac{N-2}{2N}\alpha^{N/(N-2)}g+(n+1/2)\sqrt{(N-2)\alpha g}\quad(n=0,1,2,\ldots) \tag{4.10}$$

with higher-order corrections of order g^0.

From this formula we can determine the renormalized mass M_{R}:

$$M_{\mathrm{R}}\equiv E_1-E_0=\sqrt{(N-2)\alpha g}. \tag{4.11}$$

Observe that unlike the conventional Ising limit, the renormalized mass *diverges* as $g\to\infty$. Thus, the unrenormalized two-point Green's function, which behaves like M_{R}^{-2}, vanishes as $g\to\infty$ like $1/g$, in agreement with the result in (3.15) for the zero-dimensional case.

We can determine the one-point Green's function G_1 by calculating the expectation value of x in the ground-state wave function. Specifically,

$$G_1\equiv\frac{\int dx\, x[\psi_0(x)]^2}{\int dx\,[\psi_0(x)]^2}, \tag{4.12}$$

where we obtain the ground-state wave function ψ_0 by setting $g=\infty$ in (4.9). Because ψ_0 is a Gaussian in t and $x=x_0+\epsilon t$ from (4.6), we immediately have

$$G_1=x_0=-i\alpha^{1/(N-2)}. \tag{4.13}$$

This result is identical to that obtained in (3.15) for $D=0$.

To calculate G_1 to first order we need to solve $-\frac{1}{2}\psi''(s)+[-\frac{1}{2}+\frac{1}{2}s^2+i\eta s^3]\psi(s)=0$ as a perturbation series

$$\psi(s)=e^{-s^2/2}[1+\eta f(s)+\mathrm{O}(\eta^2)].$$

We find that $f(s)=-i(s+s^3/3)$. Finally, we use this result in the integral (4.12) to obtain

$$G_1=-i\alpha^{1/(N-2)}\left(1+\frac{N-1}{4\sqrt{N-2}}\alpha^{-(N+2)/(2N-4)}g^{-1/2}\right). \tag{4.14}$$

V. CORRELATED LIMIT FOR GENERAL $D<2$

In this section we use functional-integral techniques to study the Ising limit in a scalar Euclidean quantum field theory of space-time dimension $D<2$. We first focus on the calculation of the one-point Green's function:

$$G_1\equiv\frac{\int\mathcal{D}\phi\,\phi(0)\exp(-\int d^Dx\,\mathcal{L})}{\int\mathcal{D}\phi\exp(-\int d^Dx\,\mathcal{L})}, \tag{5.1}$$

where $\mathcal{L}$ is given in (1.1). Making the substitution in (1.2) and letting $x=s/\sqrt{g}$ gives

$$G_1=\frac{\int\mathcal{D}\phi\,\phi(0)\exp(-g^{1-D/2}S[\phi])}{\int\mathcal{D}\phi\exp(-g^{1-D/2}S[\phi])}, \tag{5.2}$$

where

$$S[\phi]=\int d^D s\left[\frac{1}{2}(\nabla\phi)^2-\frac{1}{2}\alpha\phi^2-\frac{1}{N}(i\phi)^N\right]\quad(N>2). \tag{5.3}$$

If we assume that $D<2$, then as $g\to\infty$ we can use saddle-point methods to determine the behavior of G_1 in (5.2) as $g\to\infty$ because the coefficient of $S[\phi]$ is large. We begin by taking the functional derivative of $S[\phi]$. The saddle points are determined by the equation

$$\frac{\delta}{\delta\phi(t)}S[\phi]=-\nabla^2\phi(t)-\alpha\phi(t)-i[i\phi(t)]^{N-1}=0. \tag{5.4}$$

The solution to this equation is a saddle point at $\phi=0$ and a ring of saddle points centered about 0. The dominant saddle point is the one on the negative imaginary axis:

$$\phi_0=-i\alpha^{1/(N-2)}. \tag{5.5}$$

The complex contour can be connected to this saddle point. If we substitute the value of ϕ_0, we get

$$G_1\sim-i\alpha^{1/(N-2)}\quad(g\to\infty). \tag{5.6}$$

We now calculate all higher-order corrections. To do so we substitute

$$\phi(s)=\phi_0+\eta(s)=-i\alpha^{1/(N-2)}+\eta(s), \tag{5.7}$$

$\eta(s)$ is treated as small; that is, $\eta(s)\ll 1$. To illustrate the procedure, we expand the functional S in (5.3) to third order in powers of $\eta(s)$. The result is

$$S_3[\eta]=\int d^D s\left[\frac{N-2}{2N}\alpha^{N/(N-2)}+\frac{1}{2}(\nabla\eta)^2+\frac{N-2}{2}\alpha\eta^2+\frac{(N-1)(N-2)}{6}\alpha^{(N-3)/(N-2)}i\eta^3\right]. \tag{5.8}$$

We can now rewrite (5.2) in the form

$$G_1=-i\alpha^{1/(N-2)}+\frac{\int\mathcal{D}\eta\,\eta(0)\exp(-g^{1-D/2}S_3[\eta])}{\int\mathcal{D}\eta\exp(-g^{1-D/2}S_3[\eta])}. \tag{5.9}$$

The constant term in S_3, which is proportional to the volume of Euclidean space-time, cancels from the exponentials in the numerator and the denominator in (5.9). We expand the cubic term in the exponential as a power series in η^3 and keep the first nontrivial term. In the denominator, the term proportional to η^3 vanishes by oddness, but in the numerator we must retain the cubic term because in this case the leading term vanishes for the same reason:

$$G_1\sim-i\alpha^{1/(N-2)}-i\frac{(N-1)(N-2)}{6}\alpha^{(N-3)/(N-2)}g^{1-D/2}\times\frac{\int\mathcal{D}\eta\,\eta(0)\int d^D t\,\eta^3(t)\exp(-g^{1-D/2}S_{\text{free}}[\eta])}{\int\mathcal{D}\eta\exp(-g^{1-D/2}S_{\text{free}}[\eta])}, \tag{5.10}$$

where $S_{\text{free}}[\eta]=\frac{1}{2}\int d^D s\,[(\nabla\eta)^2+(N-2)\alpha\eta^2]$.

We can evaluate this ratio of functional integrals *exactly*. To do so we introduce an external source function $J(s)$ in the integral in the numerator:

$$G_1 \sim -i\alpha^{1/(N-2)} - i\frac{(N-1)(N-2)}{6}\alpha^{(N-3)/(N-2)}g^{-3+3D/2} \times \frac{\delta}{\delta J(0)}\int d^D t\left[\frac{\delta}{\delta J(t)}\right]^3 \frac{\int \mathcal{D}\eta \exp(-g^{1-D/2}S_J[\eta])}{\int \mathcal{D}\eta \exp(-g^{1-D/2}S_{\text{free}}[\eta])}\Bigg|_{J=0}, \tag{5.11}$$

where $S_J[\eta] = \int d^D s\,(\frac{1}{2}([\nabla\eta(s)]^2 + \frac{1}{2}\alpha(N-2)[\eta(s)]^2 - J(s)\eta(s))$.

Next, we evaluate the Gaussian integral in the numerator by completing the square. Upon doing so, the integral in the denominator cancels and what remains is the formula

$$G_1 \sim -i\alpha^{1/(N-2)} - i\frac{(N-1)(N-2)}{6}\alpha^{(N-3)/(N-2)}g^{-3+3D/2} \times \frac{\delta}{\delta J(0)}\int d^D t\left[\frac{\delta}{\delta J(t)}\right]^3 \exp\left(\frac{1}{2}g^{1-D/2}\int\int dr\,ds\,J(r)J(s)\Delta(r,s)\right)\Bigg|_{J=0}, \tag{5.12}$$

where Δ is the coordinate-space propagator satisfying the Euclidean coordinate space Green's function equation

$$[\nabla^2 + \alpha(N-2)]\Delta(r,s) = \delta(r-s). \tag{5.13}$$

The final step is to expand the exponential containing the external source and to perform the indicated differentiations. The result is

$$G_1 \sim -i\alpha^{1/(N-2)} - i\frac{(N-1)(N-2)}{2}\alpha^{(N-3)/(N-2)}g^{-1+D/2}\int dr\,\Delta(r,0)\Delta(0,0). \tag{5.14}$$

This expression has a graphical interpretation: A propagator connects the origin to the point r, where there is a tadpole. The momentum-space propagator is $\tilde{\Delta}(p) = 1/[p^2 + \alpha(N-2)]$, so that

$$\Delta(r,s) = (2\pi)^{-D}\int d^D p\, e^{ip(r-s)}\frac{1}{p^2+\alpha(N-2)}. \tag{5.15}$$

Thus, $\tilde{\Delta}(0) = \int dr\,\Delta(r,0) = 1/\alpha(N-2)$ and $\Delta(0,0) = \Gamma(1-D/2)(4\pi)^{-D/2}[\alpha(N-2)]^{-1+D/2}$. The final result for G_1 is

$$G_1 \sim -i\alpha^{1/(N-2)}\left[1 + \frac{N-1}{2}[g(N-2)]^{-1+D/2}(4\pi)^{-D/2}\Gamma\left(1-\frac{D}{2}\right)\alpha^{(D/2)\,-\,N/(N-2)}\right], \tag{5.16}$$

which agrees exactly with (3.15) for the case $D=0$ and (4.14) for the case $D=1$.

The procedure we have used to calculate G_1 can be generalized to calculate any of the Green's functions G_n by taking advantage of the graphical methods developed above. For the two-point Green's function we immediately obtain

$$G_2(x,y) \sim g^{-1+D/2}\Delta(x\sqrt{g}, y\sqrt{g}) \tag{5.17}$$

to leading order, which in momentum space gives

$$G_2(p) \sim \frac{1}{p^2 + (N-2)\alpha g}. \tag{5.18}$$

From this equation we see that to leading order the renormalization constant $Z=1$ and that the renormalized mass M_{R} is given by

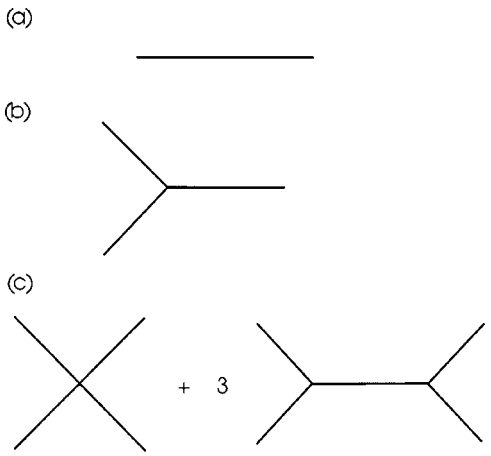

FIG. 2. Tree graphs contributing to G_2 through G_4 in the Ising limit.

$$M_{\mathrm{R}}^2=(N-2)\alpha g. \tag{5.19}$$

Observe that this result is independent of the dimension D and agrees with the result for $D=0$ and also with that in (4.11) for $D=1$, which was derived by quite different techniques. Figure 2 shows the tree graphs contributing to G_2 through G_4.

In fact, we find that the results in Eqs. (3.15) and (3.16) are valid for any dimension $D<2$, provided that they are interpreted as momentum space Green's functions evaluated at zero momentum on all external legs. The parameter ϵ^2 is, however, dimensional for $D\neq 0$. Equations (3.18) and (3.19) for the 1PI Green's functions are also valid with the same understanding.

Thus, we observe a form of universality; the expressions for the Green's functions are the same for all D and only depend on N, the exponent in the interaction term. This is quite different from the usual statement of universality, in which the Green's functions are independent of N but do depend on the value of D. However, Eq. (3.19) is D dependent insofar as the parameter ϵ must be replaced by its dimensionless version, given by

$$\tilde{\epsilon}^2=\frac{\alpha^{(D/2)\,-\,N/(N-2)}}{[(N-2)g]^{1-D/2}}. \tag{5.20}$$

This is the natural small parameter governing the asymptotic expansion, as in Eq. (5.16).

In the calculations performed so far it has been assumed implicitly that $D<2$. Indeed, D cannot exceed 2 if α is taken to be fixed, as in the original definition of the Ising limit in Eq. (1.2). However, if the restriction that α be fixed is relaxed and α is allowed to grow with g in such a way that $\tilde{\epsilon}$ in Eq. (5.20) remains small, then our results for the Green's functions in this modified Ising limit remain valid in the larger range $2<D<4$. Unfortunately, we still cannot extend the range of these results to the physically important case $D=4$.

Nevertheless, in the range of dimension $0\leqslant D<4$ with $D\neq 2$ we have the following picture. The scalar theory in this Ising-like regime is very simple. The only remnant of the theory is a renormalized mass M_{R}, which approaches infinity, and a one-point Green's function, which is the expectation value of the scalar field. The higher Green's functions are all negligible in this regime. If these results could be extended to $D=4$, we would have the equivalent of the Higgs phenomenon without requiring the existence of a (so-far unobserved) finite-mass Higgs particle.

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Casimir energy of a semi-circular infinite cylinder

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The Casimir energy of a semi-circular cylindrical shell is calculated by making use of the zeta function technique. This shell is obtained by crossing an infinite circular cylindrical shell by a plane passing through the symmetry axes of the cylinder and by considering only half of this configuration. All the surfaces, including the cutting plane, are assumed to be perfectly conducting. The zeta functions for scalar massless fields obeying the Dirichlet and Neumann boundary conditions on the semi-circular cylinder are constructed exactly. The sum of these zeta functions gives the zeta function for the electromagnetic field in question. The relevant plane problem is considered also. In all the cases the final expressions for the corresponding Casimir energies contain the pole contributions which are the consequence of the edges or corners in the boundaries. This implies that further renormalization is needed in order for the finite physical values for vacuum energy to be obtained for given boundary conditions. © *2001 American Institute of Physics.*
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I. INTRODUCTION

When calculating the ground state energy of a quantum field (the Casimir energy) the main problem is to single out a finite part of the vacuum energy which is initially divergent. Usually for this purpose a subtraction procedure is used with preliminary regularization of the divergent expressions (for example, by introducing ultraviolet cutoff). However, in quantum field theory treated with allowance for nontrivial boundary conditions or in the space–time with curvature, a complete renormalization procedure is not formulated explicitly. Therefore, for any specific problem the subtraction procedure should be invented anew. As a result, one succeeds in calculating the Casimir energy only in the problems with known spectra or at least implicitly known spectra. Practically it implies the boundary conditions of high symmetry[1,2] (parallel plates, sphere, cylinder).

In studies of the Casimir energy the zeta function technique,[3,4] which is also referred to as the zeta regularization or zeta renormalization, is widely used. In fact, the use of the zeta functions, as well as other regularizations, gives only regularized quantities for ground state energy, for effective potential and so on. The necessity to renormalize the expressions obtained in this way certainly remains. However, in some problems the zeta technique gives at once a finite result. Usually the latter is considered to be a renormalized physical answer though generally it is not the case.[5]

When using the zeta regularization in one or another problem, it is desirable to know beforehand whether the finite result can be obtained in this way. In order to answer this question the general analysis of the divergences in the problem at hand should be accomplished. This can be done by calculating the heat kernel coefficients[6] depending on the geometry of the manifold under

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consideration. For a large class of situations these coefficients have been obtained.[7] However, there are a number of problems (for example, boundaries with edges or corners) for which no general results regarding the heat trace are known.

In this situation it is undoubtedly worth carrying out, in the framework of the zeta function technique, the calculations of the Casimir energy for new configurations, the cases being interesting with both finite result and with pole contributions left in the final expression for the vacuum energy.

In the present article we address the calculation of the Casimir energy for boundaries with edges; more precisely, the vacuum energy of electromagnetic field will be calculated for a semi-circular cylindrical shell by making use of the relevant zeta functions. This shell is obtained by crossing an infinite circular cylindrical shell by a plane passing through the symmetry axes of the cylinder. All the surfaces, including the infinite cutting plane, are assumed to be perfectly conducting. Obviously it is sufficient to consider only a half of this configuration (left or right) which we shall refer to as a semi-circular cylindrical shell or, for the sake of shortening, as a semi-circular cylinder. The internal boundary value problem for this configuration is nothing other as a semi-cylindrical waveguide. In the theory of waveguides[8] it is well known that a semi-circular waveguide has the same eigenfrequencies as the cylindrical one but without degeneracy (without doubling) and safe for one frequency series (see later in this work). Notwithstanding the very close spectra, the zeta function technique does not give a finite result for a semi-circular cylinder unlike for a circular one. First the Casimir energy of an infinite perfectly conducting cylindrical shell was calculated in Ref. 9 by introducing ultraviolet cutoff and recently this result was derived by zeta function technique[10] (see also Refs. 11–13). As far as we know the asymmetric boundaries such as a semi-circular cylinder have not been considered in the Casimir problem.

The article is organized as follows. In Sec. II the electromagnetic spectra are considered in detail for cylindrical and semi-cylindrical shells. The general solution of the Maxwell equations for boundary conditions chosen is expressed in terms of two scalar functions, longitudinal components of the electric and magnetic Hertz vectors. These scalar functions are the eigenfunctions of the two-dimensional transverse Laplace operator and obey the Dirichlet and Neumann boundary conditions on the conducting surfaces. In Sec. III the spectral zeta function is constructed for the Dirichlet boundary value problem. To this end, the technique is used which has been elaborated before for representing the spectral zeta function, with given eigenfrequency equations, in terms of contour integral. When carrying out the analytic continuation of the zeta function into the physical region, the uniform asymptotic expansion for the modified Bessel functions is used. In the same way, in Sec. IV the zeta function is constructed for a scalar field obeying the Neumann boundary conditions given on the surface of a semi-circular cylindrical shell. Section V is concerned with the complete zeta function for an electromagnetic field with boundary conditions on the semi-circular cylinder. Transition to the relevant two-dimensional problem is also considered here. In the Conclusion (Sec. VI) the results obtained are summarized, and the origin of the pole singularities of the zeta functions at hand and their relation to the respective boundary value problem are briefly discussed.

II. EIGENMODES OF ELECTROMAGNETIC FIELD FOR CIRCULAR AND SEMI-CIRCULAR CYLINDERS

The construction of the solutions to the Maxwell equations with boundary conditions given on closed surfaces proves to be nontrivial problem. Mainly it is due to the vector character of the electromagnetic field.[8,14,15] In the case of cylindrical symmetry the electric $\mathbf{E}$ and magnetic $\mathbf{H}$ fields are expressed in terms of the electric ($\mathbf{\Pi}'$) and magnetic ($\mathbf{\Pi}''$) Hertz vectors having only one nonzero component

$$\mathbf{\Pi}' = \mathbf{e}_z \Phi(r,\varphi)\, e^{\pm i k_z' z}, \tag{2.1}$$

$$\mathbf{\Pi}'' = \mathbf{e}_z \Psi(r,\varphi)\, e^{\pm i k_z'' z}. \tag{2.2}$$

Here the cylindrical coordinate system r,φ,z is used with z axes directed along the cylinder axes. The common time-dependent factor $e^{i\omega t}$ is dropped. The scalar functions $\Phi(r,\varphi)$ and $\Psi(r,\varphi)$ are the eigenfunctions of the two-dimensional transverse Laplace operator and meet, respectively, the Dirichlet and Neumann conditions on the boundary $\partial\Gamma$

$$(\nabla_\perp^2+\gamma'^2)\Phi(r,\varphi)=0, \quad \Phi(r,\varphi)|_{\partial\Gamma}=0, \tag{2.3}$$

$$(\nabla_\perp^2+\gamma''^2)\Psi(r,\varphi)=0, \quad \left.\frac{\partial\Psi(r,\varphi)}{\partial n}\right|_{\partial\Gamma}=0, \tag{2.4}$$

where $\nabla_\perp^2$ is the transverse part of the Laplace operator

$$\nabla_\perp^2=\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2} \tag{2.5}$$

and

$$\gamma'^2=\omega^2-k_z'^2, \quad \gamma''^2=\omega^2-k_z''^2. \tag{2.6}$$

First we consider a cylindrical shell. In this case the functions $\Phi(r,\varphi)$ and $\Psi(r,\varphi)$ should be 2π-periodic in angular variable φ. As a result the Dirichlet boundary value problem (2.3) has the following unnormalized eigenfunctions (E-modes):

$$\Phi_{nm}(r,\varphi)=\begin{matrix}\sin\\ \cos\end{matrix}(n\varphi)\begin{cases}J_n(\gamma'_{nm}r), & r<a,\\ H_n^{(1)}(\overline{\gamma}'_{nm}r), & r>a,\end{cases} \tag{2.7}$$

where a is the cylinder radius, $J_n(x)$ are the Bessel functions, $H_n^{(1)}(x)$ are the Hankel functions of the first kind, and γ'_{nm}, $\overline{\gamma}'_{nm}$ stand for the roots of the frequency equations

$$J_n(\gamma'_{nm}a)=0, \quad H_n^{(1)}(\overline{\gamma}'_{nm}a)=0,$$
$$n=0,1,2,\ldots, \quad m=1,2,\ldots. \tag{2.8}$$

For the Neumann boundary value problem (2.4) we have the H-modes

$$\Psi_{nm}(r,\varphi)=\begin{matrix}\sin\\ \cos\end{matrix}(n\varphi)\begin{cases}J_n(\gamma''_{nm}r), & r<a,\\ H_n^{(1)}(\overline{\gamma}''_{nm}r), & r>a,\end{cases} \tag{2.9}$$

where γ''_{nm} and $\overline{\gamma}''_{nm}$ are the roots of the equations

$$\left.\frac{d}{dr}J_n(\gamma''_{nm}r)\right|_{r=a}=0, \quad \left.\frac{d}{dr}H^{(1)}(\overline{\gamma}''_{nm}r)\right|_{r=a}=0,$$
$$n=0,1,2,\ldots, \quad m=1,2,\ldots. \tag{2.10}$$

As usual, it is assumed that for $r>a$ the eigenfunctions should satisfy the radiation condition.

It is important to note that each root

$$\gamma'_{nm}, \quad \overline{\gamma}'_{nm}, \quad \gamma''_{nm}, \quad \overline{\gamma}''_{nm}, \quad n\geqslant 1, \quad m\geqslant 1, \tag{2.11}$$

is doubly degenerate since, according to Eqs. (2.7) and (2.9), there are two eigenfunctions which are proportional to either $\sin(n\varphi)$ or $\cos(n\varphi)$. The eigenfunctions for the roots with $n=0$

$$\gamma'_{0m}, \quad \overline{\gamma}'_{0m}, \quad \gamma''_{0m}, \quad \overline{\gamma}''_{0m}, \quad m=1,2,\ldots, \tag{2.12}$$

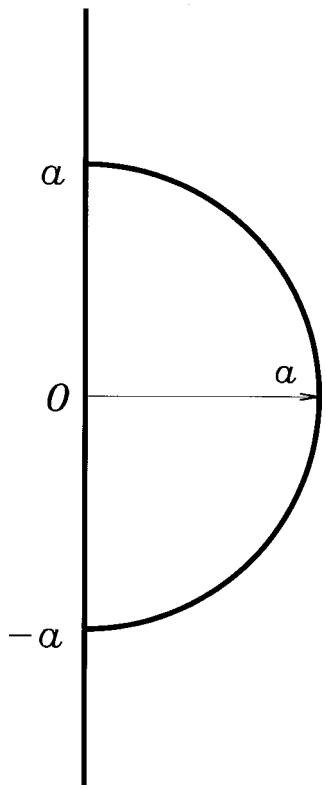

FIG. 1. The cross section of an infinite semi-circular cylindrical shell of radius a. All the surfaces (bold-faced lines) are assumed to be perfectly conducting. At the same time this picture presents the two-dimensional (plane) version of the problem under consideration, i.e., the semi-circular boundaries for massless fields defined on the plane.

are independent on φ, and the degeneracy disappears.

For given Hertz vectors $\mathbf{\Pi}'$ and $\mathbf{\Pi}''$ the electric and magnetic fields are constructed by the formulas

$$\begin{aligned} &\mathbf{E}=\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{\Pi}', \quad \mathbf{H}=-i\omega\boldsymbol{\nabla}\times\mathbf{\Pi}' \quad (E\text{-modes}),\\ &\mathbf{E}=i\omega\boldsymbol{\nabla}\times\mathbf{\Pi}'', \quad \mathbf{H}=\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{\Pi}'' \quad (H\text{-modes}). \end{aligned} \tag{2.13}$$

It has been proved[16] that the superposition of these modes gives the general solution to the Maxwell equations in the problem under consideration. An essential merit of using the Hertz polarization vectors is that in this approach the necessity to satisfy the gauge conditions does not arise.

Let us consider a waveguide which is obtained by cutting the infinite cylindrical shell by a plane passing through the symmetry axes of the cylinder (see Fig. 1). All the surfaces are assumed to be perfectly conducting. In this case the boundary value problems (2.3) and (2.4) for the Hertz electric ($\mathbf{\Pi}'$) and magnetic ($\mathbf{\Pi}''$) vectors have the following eigenfunctions:

$$\Phi_{nm}(r,\varphi)=\sin(n\varphi)\begin{cases} J_n(\gamma'_{nm}r), & r<a,\\ H_n^{(1)}(\overline{\gamma}'_{nm}r), & r>a, \end{cases} \tag{2.14}$$

$$n=1,2,\ldots, \quad m=1,2,\ldots$$

and

$$\Psi_{nm}(r,\varphi)=\cos(n\varphi)\begin{cases} J_n(\gamma''_{nm}r), & r<a, \\ H_n^{(1)}(\overline{\gamma}''_{nm}r), & r>a, \end{cases} \tag{2.15}$$

$$n=0,1,2,\ldots, \quad m=1,2,\ldots .$$

The frequencies γ'_{nm}, $\overline{\gamma}'_{nm}$, γ''_{nm}, and $\overline{\gamma}''_{nm}$ are determined by the same equations (2.8) and (2.10). However, the new spectral problem has two essential distinctions: (i) the frequencies (2.11) are now nondegenerate, and (ii) two series of eigenfrequencies

$$\gamma'_{0m}, \quad \overline{\gamma}'_{0m}, \quad m=1,2,\ldots, \tag{2.16}$$

are absent. At first sight one could expect that such a change of the spectrum cannot influence drastically the ultraviolet behavior of the relevant spectral density. However, as it will be shown below, the zeta function for a semi-circular cylinder, unlike for a circular one, does not provide a finite answer for the Casimir energy in the problem in question.

In view of all the above-mentioned the zeta function for the electromagnetic field obeying the boundary conditions on the surface of the semi-circular cylinder is the sum of two zeta functions for scalar massless fields satisfying the Dirichlet and Neumann conditions on the lateral of this cylinder.

III. ZETA FUNCTION FOR DIRICHLET BOUNDARY VALUE PROBLEM

First we consider the Dirichlet boundary conditions. We shall proceed from the following representation for the zeta function in terms of a contour integral for given frequency equations (2.8) with $n=1,2,\ldots$,

$$\zeta^{\mathrm{D}}_{\mathrm{cyl}}(s)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{dk_z}{2\pi}\sum_{n=1}^{\infty}\oint_C d\gamma\,(\gamma^2+k_z^2)^{-s/2}\frac{d}{d\gamma}\ln\frac{J_n(\gamma a)H_n^{(1)}(\gamma a)}{J_n(\infty)H_n^{(1)}(\infty)}. \tag{3.1}$$

The contour C consists of the imaginary axis $(-i\infty,i\infty)$ and a semi-circle of an infinite radius in the right half-plane of a complex variable γ. The details of obtaining this integral representation can be found in Refs. 10, 11, 17, and 18. Contribution into Eq. (3.1) of integration along a semi-circle of infinite radius vanishes. Therefore upon integration over k_z this formula acquires the form

$$\zeta^{\mathrm{D}}(s)=C(s)\sum_{n=1}^{\infty}\int_0^{\infty}dy\,y^{1-s}\frac{d}{dy}\ln[2yI_n(y)K_n(y)] \tag{3.2}$$

with

$$C(s)=\frac{a^{s-1}}{2\sqrt{\pi}\Gamma\left(\frac{s}{2}\right)\Gamma((3-s)/2)}. \tag{3.3}$$

In order to accomplish the analytic continuation of (3.2) into the physical region including the point $s=-1$, we shall use the uniform asymptotic expansion for the modified Bessel functions[19]

$$\ln[2ynI_n(ny)K_n(ny)]=\ln(yt)+\frac{t^2}{8n^2}(1-6t^2+5t^4)$$
$$+\frac{t^4}{64n^4}(13-284t^2+1062t^4-1356t^6+565t^8)+O(n^{-6}), \tag{3.4}$$

where $t=1/\sqrt{1+y^2}$. Following the usual procedure applied in the analogous calculations,[20–23] we add and subtract in the integrand in Eq. (3.2) the first two terms of the asymptotic expansion (3.3). After that we combine all the terms there in the following way:

$$\zeta_{\rm cyl}^{\rm D}(s)=C(s)[Z_1(s)+Z_2(s)+Z_3(s)], \tag{3.5}$$

$$Z_1(s)=\frac{1}{2}\sum_{n=1}^{\infty} n^{1-s}\int_0^{\infty} dy\, y^{1-s}\frac{d}{dy}\ln\left(\frac{y^2}{1+y^2}\right), \tag{3.6}$$

$$Z_2(s)=\frac{1}{8}\sum_{n=1}^{\infty} n^{-1-s}\int_0^{\infty} dy\, y^{1-s}\frac{d}{dy}[t^2(1-6\,t^2+5\,t^4)], \tag{3.7}$$

$$Z_3(s)=\sum_{n=1}^{\infty} n^{1-s}\int_0^{\infty} dy\, y^{1-s}\frac{d}{dy}\left[\ln(2yn\,I_n(yn)K_n(ny))-\ln\frac{y}{\sqrt{1+y^2}}-\frac{t^2(1-6t^2+5t^4)}{8n^2}\right]. \tag{3.8}$$

Analytic continuation of the function $Z_1(s)$ into vicinity of the point $s=-1$ can be accomplished in the same way as it has been done in Ref. 18. Therefore we write here only the final result of this continuation

$$Z_1(s)=\frac{1}{2}\zeta(s-1)\Gamma\left(\frac{3-s}{2}\right)\sum_{m=1}^{\infty}\frac{\Gamma(m-(1-s)/2)}{m\Gamma(m)}. \tag{3.9}$$

The integral in Eq. (3.6) converges when $-1<\mathrm{Re}\,s<3$, and the sum over n is finite for $\mathrm{Re}\,s>0$. Thus, the regions, where the integral and the sum exist, overlap, and this formula can be used for constructing the analytic continuation needed. For this aim we substitute the sum by the Riemann zeta function

$$\sum_{n=1}^{\infty} n^{-1-s}=\zeta(s+1) \tag{3.10}$$

and define the integral as an analytic function by making use of the formula[24]

$$\int_0^{\infty} dy\, y^{1-s}\frac{d}{dy}t^{2(\rho-1)}=(1-\rho)\frac{\Gamma((3-s)/2)\Gamma(\rho-(3-s)/2)}{\Gamma(\rho)},\quad 3-2\,\mathrm{Re}\,\rho<\mathrm{Re}\,s<3. \tag{3.11}$$

In view of the poles of the gamma functions on the right-hand side of this relation, the integral on the left-hand side of it is well defined, as a function of the complex variable s, only in the region indicated in Eq. (3.11). Doing the analytic continuation of this integral we define it outside this region also by this equation, keeping in mind that the gamma functions involved should be treated as the analytic functions over all the plane of the complex variable s safe for the known poles. This gives

$$Z_2(s)=\frac{1}{8}\zeta(s+1)\Gamma\left(\frac{3-s}{2}\right)\Gamma\left(\frac{1+s}{2}\right)\left[-1+3(1+s)-\frac{5}{8}(3+s)(1+s)\right]. \tag{3.12}$$

In order to investigate the convergence of the integral entering in Eq. (3.7) it makes sense to substitute in the integrand the logarithmic function by expansion (3.3). After that it is easy to be convinced that the integral under consideration converges when $-3<\mathrm{Re}\,s<3$. The sum over n in

this formula is finite for $\mathrm{Re}\, s > -2$. Hence, the function $Z_3(s)$ is an analytic function without singularities in the domain $-2 < \mathrm{Re}\, s < 3$. It is quiet enough for our purpose, and the analytic continuation is unnecessary.

Summarizing we conclude that Eqs. (3.3), (3.5), (3.8), (3.9), and (3.12) afford the analytic continuation needed and define the zeta function $\zeta^{\mathrm{D}}(s)$ as an analytic function in the region including the point $s=-1$.

Now we are able to calculate the value of the zeta function $\zeta^{\mathrm{D}}(s)$ at the point $s=-1$. For the coefficient $C(s)$ in Eq. (3.3) we have

$$C(-1) = -\frac{1}{4\pi a^2}. \tag{3.13}$$

From Eq. (3.9) it follows that

$$Z_1(-1) = \frac{1}{2} \lim_{s\to -1} \zeta(s-1) \left[\Gamma\left(\frac{1+s}{2}\right) + \sum_{m=2}^{\infty} \frac{1}{m(m-1)} \right]. \tag{3.14}$$

With allowance for the relations

$$\Gamma(x) = \frac{1}{x} - \gamma + O(x), \quad \sum_{m=2}^{\infty} \frac{1}{m(m-1)} = 1, \quad \zeta(-2) = 0, \tag{3.15}$$

where γ is the Euler constant, $\gamma = 0.577\,215\ldots$, one derives

$$\begin{aligned} Z_1(-1) &= \lim_{s\to -1} \frac{1}{2} [\zeta(-2) + \zeta'(-2)(s+1) + O((s+1)^2)] \left[\frac{2}{s+1} - \gamma + O(s+1) \right] \\ &= \zeta'(-2) = -0.030\,448. \end{aligned} \tag{3.16}$$

Using the values of the Riemann zeta function and its derivative at the origin,

$$\zeta(0) = -\tfrac{1}{2}, \quad \zeta'(0) = -\tfrac{1}{2}\ln(2\pi),$$

and taking into account the behavior of the gamma function near zero [see Eq. (3.15)] we deduce from Eq. (3.12)

$$\begin{aligned} Z_2(-1) &= \frac{1}{8} \lim_{s\to -1} [\zeta(0) + \zeta'(0)(s+1) + O((s+1)^2)] \left[\frac{2}{s+1} - \gamma + \mathcal{O}(s+1) \right] \cdot \left[-1 + \frac{7}{4}(s+1) \right] \\ &= -\frac{7}{32} - \frac{\gamma}{16} + \frac{1}{8}\ln(2\pi) + \frac{1}{8} \frac{1}{s+1} \Big|_{s\to -1}. \end{aligned} \tag{3.17}$$

When calculating $Z_3(-1)$ we shall use Eq. (3.8) for several first values of n, $n \leqslant n_0$, and for $n > n_0$ we substitute the asymptotic expansion (3.4) into (3.8) with the result

$$Z_3^{\mathrm{as}}(s)=\frac{1}{64}\left(\sum_{n=n_0+1}^{\infty} n^{-3-s}\right)\int_0^{\infty} dy\, y^{1-s}\frac{d}{dy}[t^4(13-284\,t^2+1062\,t^4-1356\,t^6+565\,t^8)]$$

$$=\frac{1}{64}\left(\sum_{n=n_0+1}^{\infty} n^{-3-s}\right)\Gamma\left(\frac{3-s}{2}\right)\left[-13\,\Gamma\left(\frac{3+s}{2}\right)+142\,\Gamma\left(\frac{5+s}{2}\right)\right.$$

$$\left.-\frac{532}{3}\Gamma\left(\frac{7+s}{2}\right)+\frac{113}{2}\Gamma\left(\frac{9+s}{2}\right)-\frac{113}{24}\Gamma\left(\frac{11+s}{2}\right)\right]. \tag{3.18}$$

The value of n_0 should be chosen so as to provide the accuracy needed. This algorithm with $n_0=6$ gives for $Z_3(-1)$

$$Z_3(-1)=0.022\,806. \tag{3.19}$$

Summing up Eqs. (3.16), (3.17), and (3.19) we obtain

$$\zeta^{\mathrm{D}}(-1)=-\frac{1}{4\pi a^2}\left(-\frac{7}{32}+0.022\,806-\frac{\gamma}{16}+\frac{1}{8}\ln(2\pi)+\zeta'(-2)+\frac{1}{8}\frac{1}{s+1}\bigg|_{s\to -1}\right)$$

$$=\frac{1}{a^2}\left(0.000\,523-0.009\,947\frac{1}{s+1}\bigg|_{s\to -1}\right). \tag{3.20}$$

Thus the zeta function $\zeta^{\mathrm{D}}(s)$ has a pole at the point $s=-1$, therefore it does not give the finite (renormalized) value for the respective Casimir energy

$$E^{\mathrm{D}}=\tfrac{1}{2}\zeta^{\mathrm{D}}(-1). \tag{3.21}$$

It implies that further renormalization is required.

IV. ZETA FUNCTION FOR NEUMANN BOUNDARY VALUE PROBLEM

When constructing the zeta function for the boundary value problem (2.4) with $\partial\Gamma$ being a semi-circular infinite cylinder, we shall again proceed from the frequency equations [now from Eq. (2.10)]. It should be taken into account that all these roots are not degenerate. Therefore we can write analogously to Eq. (3.1)

$$\zeta^{\mathrm{N}}(s)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{dk_z}{2\pi}\sum_{n=0}^{\infty}{}'\ \oint_C d\gamma\,(\gamma^2+k_z^2)^{-s/2}\frac{d}{d\gamma}\ln\frac{J_n'(\gamma a)H_n^{(1)\,\prime}(\gamma a)}{J_n'(\infty)H_n^{(1)\,\prime}(\infty)}. \tag{4.1}$$

The contour C is the same as in Eq. (3.1) and the prime on the Bessel and Hankel functions denotes differentiation with respect to the entire argument.

The product of the derivatives of the modified Bessel functions $I_n'(z)K_n'(z)$ has the following asymptotics when n is fixed and $|z|$ is large:[19]

$$I_n'(z)K_n'(z)=-\frac{1}{2z}\left[1+\frac{4n^2-3}{2(2z)^2}+\frac{(4n^2-1)(4n^2-45)}{8(2z)^4}+O(z^{-6})\right]. \tag{4.2}$$

Taking this into account in calculation of the denominator in Eq. (4.1), we obtain for $\zeta^{\mathrm{N}}(s)$ upon integration over k_z

$$\zeta^{\mathrm{N}}(s)=C(s)\sum_{n=0}^{\infty}{}'\ \int_0^{\infty} dy\, y^{1-s}\frac{d}{dy}\ln[-2yI_n'(y)K_n'(y)] \tag{4.3}$$

with the same function $C(s)$ as in Eq. (3.3).

Further we shall use the uniform asymptotic expansion for the derivatives of the Bessel functions:[19]

$$\ln[-2ynI_n'(ny)K_n'(ny)]=-\ln(yt)+\frac{t^2}{8n^2}(-3+10t^2-7t^4)+\frac{t^4}{n^4}\left(-\frac{27}{64}+\frac{109}{16}t^2-\frac{733}{32}t^4+\frac{441}{16}t^6-\frac{707}{64}t^8\right)+\mathcal{O}(n^{-6}). \tag{4.4}$$

In order to render the integral in the term with $n=0$ in Eq. (4.3) convergent we add and subtract the second term from the asymptotics (4.4). For $n\geqslant 1$ in Eq. (4.3) we add and subtract in respective intagrands the first two terms of the asymptotic expansion (4.4). After that we combine all the terms in the following way:

$$\zeta^{\mathrm{N}}(s)=C(s)[V_0(s)+V_1(s)+V_2(s)+V_3(s)], \tag{4.5}$$

$$V_0(s)=\int_0^\infty dy\, y^{1-s}\frac{d}{dy}\left\{\ln[-2yI_0'(y)K_0'(y)]-\frac{t^2}{8}(-3+10t^2-7t^4)\right\}, \tag{4.6}$$

$$V_1(s)=-\frac{1}{2}\sum_{n=1}^\infty n^{1-s}\int_0^\infty dy\, y^{1-s}\frac{d}{dy}\ln\left(\frac{y^2}{1+y^2}\right)=-Z_1(s), \tag{4.7}$$

$$V_2(s)=\frac{1}{8}\left(\sum_{n=1}^\infty n^{-1-s}+1\right)\int_0^\infty dy\, y^{1-s}\frac{d}{dy}[t^2(-3+10\,t^2-7\,t^4)], \tag{4.8}$$

$$V_3(s)=\sum_{n=1}^\infty n^{1-s}\int_0^\infty dy\, y^{1-s}\frac{d}{dy}\left\{\ln[-2ynI_n'(ny)K_n'(ny)]+\ln(yt)-\frac{t^2}{8n^2}(-3+10t^2-7t^4)\right\}. \tag{4.9}$$

Taking into account the behavior of the product $I_0'(y)K_0'(y)$ at the origin and at infinity,

$$\begin{aligned}-2yI_0'(y)K_0'(y)&=y+\tfrac{1}{8}(-1+4y-4\ln 2+\ln y)y^3+O(y^5\ln y),\\ -2yI_0'(y)K_0'(y)&=1-\frac{3}{8y^2}+\frac{45}{128y^4}+O(y^{-6}),\end{aligned} \tag{4.10}$$

it is easy to show that Eq. (4.6) defines $V_0(s)$ as an analytic function in the region $-3<\mathrm{Re}\,s<1$. Under this condition the integration by parts can be done here:

$$V_0(s)=-(1-s)\int_0^\infty dy\, y^{-s}\left\{\ln[-2yI_0'(y)K_0'(y)]-\frac{t^2}{8}(-3+10t^2-7t^4)\right\}. \tag{4.11}$$

The function $V_1(s)$ differs only in the sign of the function $Z_1(s)$ from the preceding section. The integral in Eq. (4.7) is convergent when $-1<\mathrm{Re}\,s<3$. The sum over n in this formula is finite when $\mathrm{Re}\ s>0$. Thus the regions, where the integral and the sum exist, overlap and this formula can be used for constructing the analytic continuation needed by making use of the substitutions (3.10) and (3.11). Substituting the sum in Eq. (4.8) by the Riemann zeta function and doing the integration according to Eq. (3.11) one obtains

$$V_2(s)=\frac{1}{8}[\zeta(1+s)+1]\Gamma\left(\frac{3-s}{2}\right)\Gamma\left(\frac{1+s}{2}\right)\left[3-5(1+s)+\frac{7}{8}(1+s)(3+s)\right]. \tag{4.12}$$

The convergence of the integral in Eq. (4.9) can be determined in the same line as it has been done for the function $Z_3(s)$ in the preceding section. This integral converges when $-3<\mathrm{Re}\,s<3$, and the sum encountered here is finite for $\mathrm{Re}\,s>-2$. Hence there is no need to do analytic continuation for $V_3(s)$.

Finally the zeta function $\zeta^{\mathrm{N}}(s)$ for the massless scalar field obeying the Neumann boundary conditions on a semi-circular cylinder is determined explicitly by Eqs. (4.5), (4.7), (4.11), and (4.12) in a finite domain of the complex plane s containing the closed interval of the real axis $-1\leqslant \mathrm{Re}\,s\leqslant 0$.

Now we turn to the calculation of the value of the function $\zeta^{\mathrm{N}}(s)$ at the point $s=-1$. Integration in Eq. (4.11) gives

$$V_0(-1)=-2\int_0^\infty dy\, y\left\{\ln[-2yI_0'(y)K_0'(y)]+\frac{3}{8}t^2\right\}+\frac{13}{16}$$
$$=2\cdot 0.475\,215+0.8123=1.763\,93. \tag{4.13}$$

From Eqs. (4.7) and (3.16) it follows that

$$V_1(-1)=-Z_1(-1)=-\zeta'(-2)=0.030\,44. \tag{4.14}$$

Developing the functions $\zeta(1+s)$ and $\Gamma((1+s)/2)$ in Eq. (4.12) near the point $s=-1$ one obtains

$$V_2(-1)=\frac{1}{8}[\zeta(0)+\zeta'(0)(s+1)+1+O((s+1)^2)]\cdot\left[\frac{2}{1+s}-\gamma+O(s+1)\right]\left[3-\frac{13}{4}(s+1)\right]$$
$$=-\frac{13}{32}-\frac{3}{16}\gamma+\frac{3}{4}\zeta'(0)+\frac{3}{8}\frac{1}{s+1}\bigg|_{s\to -1}. \tag{4.15}$$

When calculating $V_3(s)$ for $s=-1$ numerically we cannot use the method applied in the preceding section because it now requires us to take into account the next terms in the uniform asymptotic expansion (4.4). Instead of this we calculate numerically the first 30 terms in the sum (4.9) with the result[25]

$$V_3(-1)=-0.043\,66. \tag{4.16}$$

Substituting in Eq. (4.9) the logarithm by its uniform asymptotic expansion (4.4) we derive a rough estimation for $V_3(s)$ without numerical integration

$$V_3^{\mathrm{as}}(s)=\zeta(3+s)\int_0^\infty dy\, y^{1-s}\frac{d}{dy}\left[t^4\left(-\frac{27}{64}+\frac{109}{16}t^2-\frac{733}{32}t^4+\frac{441}{16}t^6-\frac{707}{64}t^8\right)\right]$$
$$=\zeta(3+s)\Gamma\left(\frac{3-s}{2}\right)\left[\frac{27}{64}\Gamma\left(\frac{3+s}{2}\right)-\frac{109}{32}\Gamma\left(\frac{5+s}{2}\right)+\frac{733}{192}\Gamma\left(\frac{7+s}{2}\right)-\frac{441}{384}\Gamma\left(\frac{9+s}{2}\right)\right.$$
$$\left.+\frac{707}{7680}\Gamma\left(\frac{11+s}{2}\right)\right]. \tag{4.17}$$

For $s=-1$ it gives

$$V_3^{\mathrm{as}}(-1)=-\frac{839}{2^6\cdot 3\cdot 5}\zeta(2)=-\frac{839}{960}\frac{\pi^2}{6}=-1.437\,60, \tag{4.18}$$

which is very far from Eq. (4.16) having only the right sign.

Summing up V_i, $i=0,1,2,3$, with allowance for Eq. (3.13) we arrive at the final result

$$\zeta^{\mathrm{N}}(-1)=-\frac{1}{4\pi a^2}\left[\frac{13}{32}+0.950\,43-\zeta'(-2)-\frac{3}{16}\gamma-\frac{3}{8}\ln(2\pi)-0.043\,66+\frac{3}{8}\frac{1}{s+1}\bigg|_{s\to-1}\right]$$
$$=\frac{1}{a^2}\left(-0.043\,45-0.0298\frac{1}{s+1}\bigg|_{s\to-1}\right). \tag{4.19}$$

Thus both the zeta functions for Dirichlet and Neumann boundary conditions have the pole at the point $s=-1$. Hence an additional renormalization is needed in order for a finite physical value of the relevant Casimir energies to be obtained.

V. VACUUM ENERGY OF ELECTROMAGNETIC FIELD WITH BOUNDARY CONDITIONS ON A SEMI-CIRCULAR CYLINDER

Analysis of the spectral problem for the electromagnetic field with boundary conditions on a semi-circular cylinder (see Sec. II) implies that the zeta function for this field is the sum of two zeta functions calculated in the preceding sections:

$$\zeta^{\mathrm{EM}}(s)=\zeta^{\mathrm{D}}(s)+\zeta^{\mathrm{N}}(s). \tag{5.1}$$

Substitution of Eqs. (3.20) and (4.17) into Eq. (5.1) gives

$$\zeta^{\mathrm{EM}}(-1)=-\frac{1}{4\pi a^2}\left[\frac{1}{4}+0.950\,43-\frac{\gamma}{4}-\frac{1}{4}\ln(2\pi)-0.043\,66+\frac{1}{2}\frac{1}{s+1}\bigg|_{s\to-1}\right]$$
$$=\frac{1}{a^2}\left(-0.044\,01-0.039\,78\frac{1}{s+1}\bigg|_{s\to-1}\right). \tag{5.2}$$

In both the zeta functions $\zeta^{\mathrm{D}}(s)$ and $\zeta^{\mathrm{N}}(s)$ the pole terms have the same sign. As a result the pole contribution in the sum (5.1) retains. Thus, the situation here proves to be analogous to that when calculating, in the framework of zeta technique, the vacuum energy for spheres in spaces of even dimensions.[21–23]

As was noted earlier, we have derived the exact expressions for the zeta functions in question which determine these functions as analytic functions of the complex variable s in a finite region of the plane s containing the closed interval of the real axis $-1\leqslant \mathrm{Re}\, s\leqslant 0$. It enables one to construct in a straightforward way the spectral zeta functions for relevant boundary value problem on the plane by making use of the relation[18]

$$\zeta_{\text{s-cir}}(s)=2\sqrt{\pi}\frac{\Gamma((s+1)/2)}{\Gamma(s/2)}\zeta_{\text{s-cyl}}(s), \tag{5.3}$$

where $\zeta_{\text{s-cir}}$ is the Dirichlet or the Neumann zeta function for a semi-circle, and $\zeta_{\text{s-cyl}}$ is the respective zeta function for semi-circular cylinder. We shall use this relation for calculating the values $\zeta^{\mathrm{D}}_{\text{s-cir}}(-1)$ and $\zeta^{\mathrm{N}}_{\text{s-cir}}(-1)$ which determine the vacuum energy of the massless scalar fields defined on the half-plane and obeying, respectively, the Dirichlet or Neumann boundary conditions on a semi-circle (see Fig. 1).

For $\zeta^{\mathrm{D}}_{\text{s-cir}}(-1)$ we get from Eqs. (5.3), (3.4), and (3.2)

$$\zeta^{\mathrm{D}}_{\text{s-cir}}(-1)=-\frac{1}{\pi a}\sum_{i=1}^{3}Z_i(0). \tag{5.4}$$

When $s=0$ integration in Eq. (3.6) can be done explicitly with the result

$$Z_1(0)=-\zeta(-1)\int_0^\infty dy\,\ln\frac{y}{\sqrt{1+y^2}}=\frac{1}{12}\left(-\frac{\pi}{2}\right)=-\frac{\pi}{24}. \tag{5.5}$$

From Eq. (3.12) it follows that

$$Z_2(0)=\frac{\pi}{128}\left(\frac{1}{s}\bigg|_{s\to 0}+\gamma\right). \tag{5.6}$$

Numerical integration in Eq. (3.8) with $s=0$ gives

$$Z_3(0)=-0.003\,04. \tag{5.7}$$

Summing up Eqs. (5.5)–(5.7) we arrive at the result

$$\zeta^{\mathrm{D}}_{\text{s-cir}}(-1)=\frac{1}{a}\left(\frac{1}{24}-\frac{\gamma}{128}+0.000\,97-\frac{1}{128}\frac{1}{s}\bigg|_{s\to 0}\right)=\frac{1}{a}\left(0.038\,127-\frac{1}{128}\frac{1}{s}\bigg|_{s\to 0}\right). \tag{5.8}$$

Following the same way one can write

$$\zeta^{\mathrm{N}}_{\text{s-cir}}(-1)=-\frac{1}{\pi a}\sum_{n=0}^{3}V_i(0). \tag{5.9}$$

Using Eq. (4.11) one gets

$$V_0(0)=-\int_0^\infty dy\left\{\ln[-2yI_0'(y)K_0'(y)]+\frac{3}{8}t^2\right\}-\frac{\pi}{64}=0.475\,175-\frac{\pi}{64}. \tag{5.10}$$

From Eqs. (4.7) and (5.5) it follows that

$$V_1(0)=-Z_1(0)=\frac{\pi}{24}. \tag{5.11}$$

Equation (4.12) gives

$$V_2(0)=\frac{5\pi}{128}\left(1+\gamma+\frac{1}{s}\bigg|_{s\to 0}\right). \tag{5.12}$$

For $V_3(0)$ numerical integration in Eq. (4.9) with $s=0$ gives

$$V_3(0)=-0.005\,659. \tag{5.13}$$

Finally, we have

$$\begin{aligned}\zeta^{\mathrm{N}}_{\text{s-cir}}(-1)&=\frac{1}{a}\left[-0.151\,32-\frac{5}{128}\left(\gamma+\frac{5}{3}\right)+0.001\,80-\frac{5}{128}\frac{1}{s}\bigg|_{s\to 0}\right]\\&=\frac{1}{a}\left(-0.237\,103-0.0124\frac{1}{s}\bigg|_{s\to 0}\right).\end{aligned} \tag{5.14}$$

Both the functions $\zeta^{\mathrm{D}}_{\text{s-cir}}(s)$ and $\zeta^{\mathrm{N}}_{\text{s-cir}}(s)$ have the pole at the point $s=-1$ with the coefficients of the same (negative) sign. For electromagnetic field defined on a plane the boundary conditions reduce to the Neumann conditions. Hence the relevant zeta function is $\zeta^{\mathrm{N}}_{\text{s-cir}}(s)$.

VI. CONCLUSION

In this article the spectral zeta functions are constructed for massless scalar fields obeying the Dirichlet and Neumann boundary conditions on a semi-circular infinite cylinder. Proceeding from this, the zeta function for electromagnetic field is also derived for such a configuration. In all three cases, the final expressions for the relevant Casimir energy contains the pole contribution. Hence for obtaining the physical result an additional renormalization is needed.

It is essential that for the zeta functions $\zeta(s)$ the exact formulas are derived which determine these functions in a finite region of the complex variable s but not at the vicinity of one point $s=-1$. This allowed one to get in a straightforward way the zeta functions for the two-dimensional (plane) version of the boundary value problem at hand, i.e., the zeta functions for scalar fields defined on a half-plane and obeying the Dirichlet and Neumann boundary conditions on a semi-circle. In this case the final expression for the vacuum energy contains the pole contributions also.

Notwithstanding the spectrum of a semi-circular cylinder is very close to the spectrum of circular one, the zeta function technique does not give a finite value for vacuum energy in the first case and does for the second configuration. In a recent paper[26] the divergences found in our consideration are attributed to the existence of edges or corners in the boundaries under investigation.

Closing, it is worth noting that, as far as we know, such boundary conditions with asymmetric geometry (semi-circular cylinder) has been considered in the Casimir problem for the first time.

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Perturbation theory and the energy spectrum of normal Fermi systems

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This paper is a study in a possible steady-state perturbation theory for arbitrary excited multiply degenerate states of a normal Fermi system in the statistical limit. An operator technique has been developed to transform the relevant Hamiltonian into an operator that is a function of occupation number operators only. The perturbation theory equations have been proved to be solvable in the space of quasinormal form operators and their formal solutions have been derived. It is shown that the operator series of perturbation theory can be transformed to a linked cluster expansion with the nonphysical powers of volume eliminated. Elimination of nonphysical terms is effected without use of the diagrams technique. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1357199]

I. INTRODUCTION

The perturbation theory for the energy of the ground state for a normal Fermi system was developed by Brueckner,[1] Goldstone,[2] and Hugenholtz[3] (see also Refs. 4–7) using diagram techniques. The main difficulty this procedure encounters is to transform a diagram series to a linked cluster expansion, which allows the contributions with nonphysical powers of volume to be eliminated. Van-Hove[8] examined the overall structure of the relevant perturbation theory series for the resolvent of the Schrödinger equation whose singular points are intimately related to the power spectrum.

The present paper is concerned with an operator technique in steady-state perturbation theory for calculating the entire spectrum of the perturbed Hamiltonian in the case in which the spectrum is strongly degenerate using the normal Fermi system as an example. The principal result is a (formal) proof of the statement that an invertible operator S can be found to transform the Hamiltonian of a normal Fermi system $H=H_0+\epsilon H_1$ to the form $\hat{E}=S^{-1}HS$, where the operator $\hat{E}$ is a functional of occupation number operators for eigenstates of the undisturbed Hamiltonian H_0. This operator technique was developed by one of us.[9] However, insuperable difficulties were encountered in the way of a solution for the equations involved owing to the small denominators. Our use of Keldysh's diagram technique to describe excited states[10] did not succeed in solving the problem fully either because of secular divergences that remained unsuppressed.

We prove that the resulting operator equations of the steady-state perturbation theory are solvable in the space of quasinormal form operators and construct their formal solutions. We show that the perturbation theory operator series can be transformed to a linked cluster expansion with the contributions involving nonphysical powers of the volume eliminated. Our development of the perturbation theory relies, not on the usual expansion into a series in the interaction parameter, but on a more general iterative scheme that avoids squares and higher powers of integrals defined in the principal value sense.

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II. ITERATIVE SCHEME

The Hamiltonian H under discussion has the following momentum representation:

$$H=\sum_{\sigma}\int d\overline{p}\frac{p^2}{2m}a_{\sigma}^{+}(\overline{p})a_{\sigma}(\overline{p})$$
$$+\varepsilon\frac{1}{2}\sum_{\sigma_1\sigma_2}\int d\overline{p_1}d\overline{p_2}d\overline{q}U(\overline{q})a_{\sigma_1}^{+}(\overline{p_1}+\overline{q})a_{\sigma_2}^{+}(\overline{p_2}-\overline{q})\times a_{\sigma_2}(\overline{p_2})a_{\sigma_1}(\overline{p_1})$$
$$\equiv H_0+\epsilon H_1. \tag{1}$$

This is defined for a set of N identical Fermi particles that are contained in a cube of volume $V=(2L)^3$. The limit $N/V\to n$ is assumed to exist and the equations are considered in the limit $N\to\infty$. The operators $a_{\sigma}(\overline{p}),a_{\sigma}^{+}(\overline{p'})$ anticommute to the delta-function and are Fourier transforms of secondary-quantized wave functions of the particle in the functions $\varphi_{\overline{p}}(\overline{x})=[1/(2\pi)^{3/2}]\cdot e^{i(\overline{p},\overline{x})}$, normalized to the delta-function. We define a linear space Π_λ as the space of eigenvectors of H_0 belonging to the eigenvalue λ. When $[H_0,\hat{E}]=H_0\hat{E}-\hat{E}H_0=0$ and $\varphi\in\Pi_\lambda$, one has $\hat{E}\varphi\subset\Pi_\lambda$, i.e., $\hat{E}\Pi_\lambda\subset\Pi_\lambda$. For this reason, when

$$S^{-1}HS=\hat{E} \text{ and } [H_0,\hat{E}]=0, \tag{2}$$

then the spectrum of H is known when the spectrum of $\hat{E}$ is defined on all Π_λ spaces. This remark shows that the solution of the problem under discussion must be sought by looking for a transform S that satisfies the requirements: $S^{-1}(H_0+\varepsilon H_1)S=\hat{E}, [H_0,\hat{E}]=0$, since the space Π_λ for H_0 is identical, as will be seen in what follows, with that of eigenvectors of operators that are functions of $a_{\sigma}^{+}(p)a_{\sigma}(\overline{p})$.

The basic device to solve the problem is to replace (2) with the equation

$$(H_0+\varepsilon H_1)(1+\varepsilon S_1+\varepsilon^2S_2+\cdots)=(1+\varepsilon S_1+\varepsilon^2S_2+\cdots)(H_0+\varepsilon\hat{E}_1+\varepsilon^2\hat{E}_2+\cdots), \tag{3}$$

where

$$S=1+\varepsilon S_1+\varepsilon^2S_2+\cdots,\quad \hat{E}=H_0+\varepsilon\hat{E}_1+\varepsilon^2\hat{E}_2+\cdots, \tag{4}$$

with the additional requirement.

$$[H_0,\hat{E}_n]=0,\quad n=1,2,\ldots. \tag{5}$$

Introducing the notations

$$H_{0n}=H_0+\varepsilon\hat{E}_1+\cdots+\varepsilon^n\hat{E}_n,\quad H_{11}=H_1-E_1,\quad H_{1k}=-\hat{E}_k\quad (k\geqslant 2), \tag{6}$$

rewriting (3) in the form

$$(H_{0n-1}+\varepsilon H_{11}+\varepsilon^2H_{12}+\cdots\varepsilon^nH_{1n}-\varepsilon^n\overline{E_n})(I+\varepsilon S_1+\cdots+\varepsilon^{n-1}S_{n-1}+\varepsilon^nS_n+\cdots+)$$
$$=(I+\varepsilon S_1+\cdots+\varepsilon^{n-1}S_{n-1}+\varepsilon^nS_n)(H_{0n-1}+\varepsilon^n\hat{E}_n), \tag{7}$$

and equating the coefficients of ε^n in (7), we obtain the following recurrence equation:

$$[H_{0n},S_n]+\sum_{k=1}^{n-1}H_{1k}S_{n-k}=\hat{E}_n,\quad [H_0,\hat{E}_n]=0\quad n\geqslant 2. \tag{8}$$

We now state the requirements for (8) to be solvable. Consider the linear space Π and the linear space T of operators defined on Π. We define the operator $A_0 \in T$ and the linear space $T_0 \subset T$ of operators that are permutable with this A_0. Suppose an operator B is given, and it is required to find operators S and M that satisfy equations like (8)

$$[A_0, S] = B + M, \quad [A_0, M] = 0, \quad \text{i.e.,} \quad M \in T_0. \tag{9}$$

Specify a linear operator P on T that transforms each element $\tau \in T$ to an element $P\tau \in T_0$, i.e., which is commutable with this A_0 and satisfies the following requirements: (a) $P^2 = P$; (b) $[A_0, PS] = 0$, $S \in T$; (c) if $PB = 0$ then Eq. (9) is solvable and a solution S exists such that $PS = 0$; (d) if $[A_0 S] = 0$, i.e., $S \in T_0$, then $PS = S$; (e) if $PH = h$ and $PS = 0$, then $P(hS) = 0$. Not all of these requirements are independent.

To solve (9), it is sufficient to define an operator P on T that satisfies (a)–(e), because, since $B = PB + QB$, where $Q = 1 - P$, then by assuming $M = -PB$ we obtain the result that Eq. (9) becomes $[A_0, S] = QB$, which is solvable in virtue of (c). Below we construct an operator P that satisfies (a)–(e) for (8).

III. QUASINORMAL FORMS

In the framework of secondary quantization any operator $\hat{A}$ can be written in a normal form[11]

$$\hat{A} = \sum_{n=1}^{\infty} \hat{A}_{nn},$$

$$\hat{A}_{nn} = \int dp_1 \cdots dp_n dp_1' \cdots dp_n' A_{nn}(p_1 \cdots p_n, p_1' \cdots p_n') a^+(p_1') \cdots a^+(p_n') a(p_n) \cdots a(p_1), \tag{10}$$

where $p' \equiv (\overline{p}, \sigma)$, $\int dp \equiv \int \prod_n d\overline{p}_j$. Since $a(p_i)$ and $a^+(p_i')$ are generalized operator functions,[12] one asks how their product in (10) is to be interpreted when p_i and p_i' are identical. They can produce a finite contribution in the statistical limit, even though an integration region of zero measure corresponds to the requirement $p_i = p_i'$. For such products to make sense, we shall understand (10) to be limits as $V \to \infty$ for the integral sums corresponding to a cube of volume V

$$\hat{A}_{nn}(V) \left(\frac{8\pi^3}{V} \right)^{2n} \sum_{\substack{p_1 \cdots p_n \\ p_1 \cdots p_p}} A_{nn}(p_1 \cdots p_n, p_1') a^+(p_1') \cdots a^+(p_n') a(p_n) \cdots a(p_1), \tag{11}$$

where $\overline{p} = (2\pi/L)\overline{n}$, $\overline{n}$ being a vector of integer components (n_1, n_2, n_3) taking on values between $-\infty$ and $+\infty$ which enumerates the nodes of a lattice with a cell of volume $\Delta\overline{p} = (2\pi/L)^3$ in the momentum space. We now carry out the following operation on (11):

(1) Decompose (11) in all different ways into subsums in which the arguments of a set of $a^+(p)$ operators are pairwise identical with those of the same number of $a(p)$ operators, all the other arguments along with those of the pairwise identical operators being different (it is only when the last requirement is satisfied that the decomposition is defined uniquely);
(2) Use commutation relations to juxtapose operators whose arguments are identical (that operation will be called pairing);
(3) Replace $a^+(p)a(p)$ with $[V/(2\pi)^3]\hat{n}_p$, where $\hat{n}_p = a_p^+ a_p$ is the occupation number operator for single-particle states with momentum $\overline{p}$ and spin σ; the operators a_p and a_p^+ anticommute to unity and are Fourier transforms of secondary-quantized functions of the particle $\hat{\psi}_\sigma(x), \hat{\psi}_\sigma^+(x)$ in functions $\varphi_p^v(\overline{x}) = (1/\sqrt{V}) e^{i(\overline{p}, \overline{x})}$ normalized to unity in volume V [although $\varphi_\sigma^\vartheta(\overline{x})$ and a_p vanish as $V \to \infty$, the operator $\hat{n}_p$ exists in the statistical limit];
(4) Pass to the limit $V \to \infty$ in each subsum.

As a result, (11) becomes

$$\hat{A}_{nn}=\sum_{m\geqslant 0,k\geqslant 0,m+k=n}\hat{A}_{m,kk};\hat{A}_{m,kk}=\int dq_1\cdots dq_m dp_1\cdots dp_k dp_1'\cdots dp_k'$$
$$\times A_{m,kk}(q_1\cdots q_m,p_1\cdots p_k,p_1'\cdots p_k')\hat{n}_{q_1}\cdots\hat{n}_{q_m}a^+(p_1')\cdots a^+(p_k')a(p_k)\cdots a(p_1). \quad (12)$$

All coefficient functions $A_{m,kk}(q_1\cdots q_m,p_1\cdots p_k,p_1'\cdots p_k')$ in (12) contain factors, which are functions $\sigma(q_1\cdots q_m,p_1\cdots p_k,p_1'\cdots p_k')$ vanishing when two arguments are identical; the function σ prohibit further pairing. Thus, one can consider all arguments different and all operators commutative in the integrals derived by pairing, because all pairings have been carried out. One especially important fact is that the integrals (12) contain a term that is a function of operators $\hat{n}_p$ only:

$$\hat{A}_{m,00}=\int dq_1\cdots dq_m A_{m,00}(q_1\cdots q_m)\hat{n}_{q_1}\cdots n_{q_m}, \quad (13)$$

which contains $n!$ integrals (11) in which all $a^+(p')$ are paired to all the $a(p)$. Operators like (13) will be called n-forms. Operators of the type $\hat{A}_{m,kk}$ with $k\geqslant 1$ will be called quasinormal forms. We thus obtain the result that any operator can be reduced to a sum of n-forms and quasinormal forms

$$\hat{A}=\sum_{m=1}^{\infty}\hat{A}_{m,00}+\sum_{m=0}^{\infty}\sum_{n=1}^{\infty}\hat{A}_{m,nn}. \quad (14)$$

The decomposition will be illustrated by using a simple example

$$\hat{A}_{11}=\int dp_1 dp_1' A_{11}(p_1p_1')a^+(p_1')a(p_1)$$
$$=\lim_{V\to\infty}\left(\frac{8\pi^3}{V}\right)^2\sum_{p_1p_1'}A_{11}(p_1p_1')a^+(p_1')a(p_1)$$
$$=\lim_{V\to\infty}\left\{\left(\frac{8\pi^3}{V}\right)^2\sum_{p_1\neq p_1'}A_{11}(p_1p_1')a^+(p_1')a(p_1)+\left(\frac{8\pi^3}{V}\right)^2\sum_{p_1=p_1'}A_{11}(p_1p_1)\frac{V}{(2\pi)^3}\hat{n}_{p_1}\right\}$$
$$=\int dp_1 A_{11}(p_1p_1)\hat{n}_{p_1}+\int dp_1 dp_1' A_{11}(p_1p_1')\sigma(p_1p_1')a^+(p_1')a(p_1)$$
$$\equiv\hat{A}_{1,00}+\hat{A}_{0,11}. \quad (15)$$

We shall make a remark that will be important for the subsequent argument: When an operator $\hat{A}$ commutes with the total momentum operator, then the coefficient functions in its normal form (10), $A_{nn}(p_1\cdots p_n,p_1'\cdots p_n')$, contain $\delta(\overline{p_1}+\cdots+\overline{p_n}-\overline{p_1'}-\cdots-\overline{p_n'})$. When we pass to the integral sum (11), that delta-function should be replaced with $[V/(2\pi)^3]\delta^{kr}_{\overline{p_1}+\cdots+\overline{p_n},\overline{p_1'}+\cdots+\overline{p_n'}}$, where $\delta^{kr}_{\overline{p},\overline{p'}}$ is the Kronecker delta. This will have the consequence that the coefficients in the n-form (13) in which all operators with momentums involved in the delta-function are paired, namely, the, $A_{n,00}(q_1\cdots q_n)$ will involve the factor $V/(2\pi)^3$ which is proportional to the volume. Products of such operators will obviously contain a factor with higher powers of the volume.

IV. SOLVING THE EQUATIONS

We attack Eq. (8) by considering the T-space of operators like (14). The space T_0 will be defined as the set of all operators τ that satisfy the requirement $[H_0,\tau]=0$. We are going to show

that T_0 consists of n-forms, i.e., of all operators like (13) that are functions of occupation number operators only. This can be seen as follows. From $[H_0,\hat{A}_{m,nn}]=0$ it follows that:

$$\int dq_1\cdots dq_m dp_1\cdots dp_n dp_1'\cdots dp_n' A_{m,nn}(q_1\cdots q_m,p_1\cdots p_n,{}_1p_1'\cdots p_n') \times\left(\sum_{k=1}^{n}\frac{\overline{p}_k^2}{2m}-\sum_{k=1}^{n}\frac{\overline{p}_k'^2}{2m}\right)\hat{n}_{q_1}\cdots\hat{n}_{q_m}a^+(p_n')a(p_n)\cdots a(p_1)=0.$$

In that case, however, $A_{m,nn}(q_1\cdots q_m,p_1\cdots p_n,p_1'\cdots p_n')$ must vanish throughout the entire space $p_1\cdots p_n,p_1'\cdots p_n'$, because $\Sigma_{k=1}^{n}[(\overline{p}_k^2/2m)-(\overline{p}_k'^2/2m)]$ vanishes only on a set of zero measure in that space. For this reason the operator $\hat{A}_{m,nn}$ which commutes with H_0 cannot be different from zero, unless it has the form (13), i.e., when $n=0$. We now introduce a linear operator P into T assuming $P\hat{A}=\Sigma_{m=1}^{\infty}\hat{A}_{m,00}$ by definition. Assume further that $Q=1-P$, hence $Q\hat{A}=\Sigma_{m=0}^{\infty}\Sigma_{n=1}^{\infty}\hat{A}_{m,nn}$. Thus, P separates an n-form in A, i.e., a sum of operators that are functions of $\hat{n}_p$ only, which are obtained by pairing from $\hat{A}$, while Q separates a quasinormal operator in $\hat{A}$, i.e., an operator each term of which involves products of $a^+(p')$ and $a(p)$ with different arguments after pairing. It follows that $PQ\hat{A}=0$. We now are going to verify that the operator P thus defined on T satisfies all of (a)–(e) for the case $A_0\equiv H_0$. Verification of (a), (b), (d), and (e) is trivial. It remains to show that (c) holds, i.e., to show that (9) with $A_0\equiv H_0$ is solvable. We have in fact proved a stronger statement, namely, that (8), i.e., equations of the type $[H_{0n},S_n]=B_n+M_n$, are solvable. We have constructed a space T_0 based on operators that commute with $A_0\equiv H_0$; however, since $\hat{E}_n$ has been assumed to commute with H_0, that very space T_0 corresponds to the operator $A_0=H_{0n}$ for any n. Consequently, P is independent of n. We begin by considering the equation

$$[H_{01},S_1]+H_1=\hat{E}_1,\quad \lfloor H_0,\hat{E}_1\rfloor=0. \tag{16}$$

We assume

$$\hat{E}_1=PH_1=\frac{1}{2}\sum_{\sigma_1\sigma_2}\frac{V}{(2\pi)^3}\int d\overline{p}_1 d\overline{p}_2 U(0).\hat{n}_{\overline{p}_1\sigma_1}\hat{n}_{\overline{p}_2\sigma_2} -\frac{1}{2}\sum_{\sigma_2}\frac{V}{(2\pi)^3}\int d\overline{p}_1 d\overline{p}_2 U(\overline{p}_1-\overline{p}_2).\hat{n}_{\overline{p}_1\sigma_1}\hat{n}_{\overline{p}_2\sigma_2}, \tag{17}$$

in order to be able to eliminate the n-form on the right-hand side of (16), so that we have to solve an equation whose right-hand side is quasinormal:

$$[H_{01},S_1]=-QH_1\equiv-\frac{1}{2}\sum_{\sigma_1\sigma_2}\int d\overline{p}_1 d\overline{p}_2 d\overline{q}U(\overline{q})\sigma(\overline{p}_1,\overline{p}_2,\overline{q})a_{\sigma_1}^+(\overline{p}_1+\overline{q}) \times a_{\sigma_1}^+(\overline{p}_2-\overline{q})a_{\sigma_2}(\overline{p}_2)a_{\sigma_1}(\overline{p}_1), \tag{18}$$

and in which the operator $H_{01}=H_0+\varepsilon\hat{E}_1$ is already known.

The integral (18) does not involve operators having pairwise identical arguments, because it is the limit of an integral sum with all pairings eliminated.

Making use of

$$[H_{01},UV]=[H_{01},U]V+U[H_{01},V] \quad \text{and} \quad [\hat{n}_p,a^+(p')]=\frac{(2\pi)^3}{V}\delta(p-p')a^+(p),$$

$$[\hat{n}_p,a(p')]=-\frac{(2\pi)^3}{V}\delta(p-p')a(p), \tag{19}$$

we calculate the commutator H_{01} with the right-hand side of (18)

$$[H_{01},QH_1]\equiv\frac{-1}{2}\sum_{\sigma_1\sigma_2}\int d\overline{p_1}d\overline{p_2}d\overline{q}\hat{\omega}_{01}(\overline{p_1},\overline{p_2},\overline{q},\sigma_1\sigma_2)U(\overline{q})\sigma(\overline{p_1},\overline{p_2},\overline{q})$$
$$\times a^+_{\sigma_1}(\overline{p_1}+\overline{q})a^+_{\sigma_2}(\overline{p_2}-\overline{q})a_{\sigma_2}(\overline{p_2})a_{\sigma_1}(\overline{p_1}), \tag{20}$$

where

$$\hat{\omega}_{01}(\overline{p_1},\overline{p_2},\overline{q},\sigma_1\sigma_2)=\frac{\overline{p_1}^2}{2m}+\frac{\overline{p_2}^2}{2m}-\frac{(\overline{p_1}\overline{q})^2}{2m}-\frac{(\overline{p_2}-q)^2}{2m}-\int d\overline{p}[U(\overline{p_1}-\overline{p})\hat{n}_{\overline{p}\sigma_1}+U(\overline{p_2}-\overline{p})\hat{n}_{\overline{p}\sigma_2}$$
$$-U(\overline{p_1}+q-\overline{p})\hat{n}_{\overline{p}\sigma_1}-U(\overline{p_2}-q-\overline{p})\hat{n}_{\overline{p}\sigma_2}]. \tag{21}$$

From (20) it follows that one of the solutions of (18) is

$$S_1=-\frac{1}{2}\sum_{\sigma_1\sigma_2}\oint d\overline{p_1}d\overline{p_2}d\overline{q}\frac{U(\overline{q})\sigma(\overline{p_1}\overline{p_2}\overline{q})}{\hat{\omega}_{01}(\overline{p_1}\overline{p_2}\overline{q},\sigma_1\sigma_2)}a^+_{\sigma_1}(\overline{p_1}+\overline{q})a^+_{\sigma_2}(\overline{p_2}-\overline{q})a_{\sigma_2}(\overline{p_2})a_{\sigma_1}(\overline{p_1}), \tag{22}$$

where $\oint$ denotes the principal value of the (multiple) integral in the sense of Cauchy. It is important to note that S_1 is a quasinormal operator and that $PS_1=0$. Equation (16) is thus proved to be solvable. It can now be discussed how the general equation (8) is to be solved. Suppose the quasinormal operators $S_1,S_2\cdots S_{n-1}$ are known. We begin by defining $\hat{E}_n=\Sigma_{k=1}^{n-1}PH_{1k}S_{n-k}=PH_1S_{n-1}$ because $P\hat{E}_kS_{n-k}=0$ in virtue of $PS_{n-k}=0$. The result is

$$[H_{0n},S_n]+\sum_{k=1}^{n-1}QH_{1k}S_{n-k}=0, \quad n\geqslant 2, \tag{23}$$

in which H_{0n} is known. The quasinormal operator $\Sigma_1^{n-1}QH_{1k}S_{n-k}$ contains terms $\hat{A}_{m,kk}$ in the form (12) with $k\geqslant 2$. The commutator H_{0n} with $\hat{A}_{m,kk}$ leads to the appearance, in the coefficient functions $A_{m,kk}(q_1\cdots q_m,p_1\cdots p_k,p_1'\cdots p_k')$, of the factor $\hat{\omega}_{0n}(p_1\cdots p_n,p_1'\cdots p_n')$ which is a function of occupation number operators only. It thus appears that one of the solutions of (23) is a quasinormal operator S_n containing the same terms as the operator $\Sigma_1^{n-1}QH_{1k}S_{n-k}$, but whose coefficient functions are

$$-\frac{P}{\hat{\omega}_{0n}(p_1\cdots p_n,p_1'\cdots p_n')}A_{m,kk}(q_1\cdots q_m,p_1\cdots p_k,p_1'\cdots p_k'),$$

where P means that the integrals are understood in the sense of the principal value. Consequently, Eq. (23) and the set of equations (8) have been proved to be solvable.

V. ELIMINATION OF CONTRIBUTIONS INVOLVING NONPHYSICAL POWERS OF VOLUME

We shall examine the structure of solutions of (23). To do this we write them in matrix form in the representation of occupation numbers $|n\rangle\equiv|\cdots n_p\cdots\rangle$

$$\langle n|S_1|n'\rangle = \frac{-1}{\hat{\omega}_{01}(n)}\langle n|H_{11}|n'\rangle;$$

$$\langle n|S_2|n'\rangle = \frac{1}{\hat{\omega}_{02}(n)}\sum_{n''}\langle n|H_{11}|n''\rangle\frac{1}{\hat{\omega}_{01}(n)}\langle n''|H_{11}|n'\rangle;$$

$$\langle n|S_3|n'\rangle = -\frac{1}{\hat{\omega}_{03}(n)}\sum_{\substack{n'',n'''\\ n''\neq n'}}\langle n|H_{11}|n''\rangle\frac{1}{\hat{\omega}_{02}(n'')}\langle n''|H_{11}|n'''\rangle\frac{1}{\hat{\omega}_{01}(n''')}\langle n'''|H_{11}|n'\rangle$$
$$-\frac{1}{\hat{\omega}_{03}(n)}E_2(n)\frac{1}{\hat{\omega}_{01}(n)}\langle n|H_{11}|n'\rangle;$$

$$\langle n|S_4|n'\rangle = \frac{1}{\hat{\omega}_{04}(n)}\sum_{\substack{n'',n''',n''''\\ n''\neq n',n''\neq n'}}\langle n|H_{11}|n''\rangle\frac{1}{\hat{\omega}_{03}(n'')}\langle n''|H_{11}|n'''\rangle$$
$$\times\frac{1}{\hat{\omega}_{02}(n''')}\langle n'''|H_{11}|n''''\rangle\frac{1}{\hat{\omega}_{01}(n'''')}\langle n''''|H_{11}|n'\rangle+\frac{1}{\hat{\omega}_{04}(n)}\sum_{n''}\langle n|H_{11}|n''\rangle$$
$$\times\frac{1}{\hat{\omega}_{03}(n'')}E_2(n'')\frac{1}{\hat{\omega}_{01}(n'')}\langle n''|H_{11}|n'\rangle+\frac{1}{\hat{\omega}_{04}(n)}E_2(n)\frac{1}{\hat{\omega}_{02}(n)}\sum_{n''}\langle n|H_{11}|n''\rangle$$
$$\times\frac{1}{\hat{\omega}_{01}(n'')}\langle n''|H_{11}|n'\rangle-\frac{1}{\hat{\omega}_{04}(n)}E_3(n)\frac{1}{\hat{\omega}_{01}(n)}\langle n|H_{11}|n'\rangle;\cdots 6. \tag{24}$$

Here, $1/\hat{\omega}_{0k}(n)$ is the symbolic form of the ''division by commutator'' operator, the inequalities in sums over intermediate states n'',n''',n'''' being due to Q in (23). In all of (24) we understand that $n\neq n'$, and the relation $\langle n|H_{11}|n\rangle=0$ has been used. One can see from (24) that the matrix elements $\langle n|S_2|n'\rangle$ do not contain factors that are diagonal elements of the operators in the representation of occupation numbers. In contrast to this, the second term in $\langle n|S_3|n'\rangle$ contains a diagonal factor, $E_2(n)$. The factor is proportional to the volume and gives a contribution proportional to the square of the volume when $\hat{S}_3$ is substituted into $\hat{E}_4$. We note however that the first term in $\langle n|S_3|n'\rangle$ in (24) contains a term with $n'''=n$, which exactly compensates the term with $E_2(n)$. As a result, we have

$$\langle n|S_3|n'\rangle = \frac{-1}{\hat{\omega}_{03}(n)}\sum_{\substack{n'',n'''\\ n''\neq n',n''\neq n}}\langle n|H_{11}|n''\rangle\frac{1}{\hat{\omega}_{02}(n'')}\langle n''|H_{11}|n'''\rangle\frac{1}{\hat{\omega}_{01}(n''')}\langle n'''|H_{11}|n'\rangle. \tag{25}$$

The expression (25) does not involve diagonal factors. We can see in a similar manner that the first term in $\langle n|S_4|n'\rangle$ contains terms with $n'''=n$, with $n''''=n''$ and with $n''''=n$ which compensate the second, third and fourth terms, respectively, in $\langle n|S_4|n'\rangle$; these terms contain the diagonal factors $E_2(n''),E_2(n),E_3(n)$. Accordingly, we derive an expression for $\langle n|S_4|n'\rangle$ with no diagonal factors

$$\langle n|S_4|n'\rangle = \frac{1}{\hat{\omega}_{04}(n)}\sum_{\substack{n'',n''',n''''\\ n''\neq n,n'''\neq n',n'''\neq n'',\\ n''''\neq n,n''\neq n'}}\langle n|H_{11}|n''\rangle\frac{1}{\hat{\omega}_{03}(n'')}\langle n''|H_{11}|n'''\rangle$$
$$\times\frac{1}{\hat{\omega}_{02}(n)}\langle n'''|H_{11}|n''''\rangle\frac{1}{\hat{\omega}_{01}(n'''')}\langle n''''|H_{11}|n'\rangle. \tag{26}$$

Continuing this process, which is in a sense similar to the separation of Van-Hove diagonal fragments,[8] we arrive at the conclusion that the matrix elements of S_k can be transformed so as to involve no diagonal factors. Accordingly, substituting $\langle n'|S_{k-1}|n\rangle$ into

$$E_k(n)=\sum_{n'}\langle n|H_{11}|n'\rangle\langle n'|S_{k-1}|n\rangle, \quad k\geqslant 2, \tag{27}$$

We see that (27) does not contain diagonal factors and that the matrix element E_k is proportional to the first power of the volume, namely, the desired result.

We shall prove these statements by induction. Suppose that for all $m\leqslant k$, where k is any given natural number, the following relation holds:

$$\langle n_m|S_m|n'\rangle=\frac{(-1)^m}{\hat{\omega}_{0m}(n_m)}\overrightarrow{\sum_{n_l\cdots n_{m-1}}}\langle n_m|H_{11}|n_{m-1}\rangle\frac{1}{\hat{\omega}_{0,m-1}(n_{m-1})}\langle n_{m-1}|H_{11}|n_{m-2}\rangle$$
$$\times\frac{1}{\hat{\omega}_{0,m-2}(n_{m-2})}\cdots\frac{1}{\hat{\omega}_{01}(n_1)}\langle n_1|H_{11}|n'\rangle, \tag{28}$$

where $\rightarrow$ at the sign of summation means that all indices $n_1\cdots n_m, n'$ are different, hence (28) involves no diagonal factors. We now prove that matrix elements of S_{k+1} have the same form. From (23)

$$\langle n|S_{k+1}|n'\rangle=\frac{-1}{\hat{\omega}_{0,k+1}(n)}\Bigg(\sum_{n_k}\langle n|H_{11}|n_k\rangle\langle n_k|S_k|n'\rangle-E_2(n)\langle n|S_{k-1}|n'\rangle-E_3(n)\langle n|S_{k-2}|n'\rangle$$
$$-\cdots-E_k(n)\langle n|S_1|n'\rangle\Bigg). \tag{29}$$

Using (28), we can write the sum over n_k contained in (29) in the form

$$\sum_{n_k}\langle n|H_{11}|n_k\rangle\langle n_k|S_k|n'\rangle=(-1)^k\overrightarrow{\sum_{n_1\cdots n_k}}\langle n|H_{11}|n_k\rangle$$
$$\times\frac{1}{\hat{\omega}_{0k}(n_k)}\langle n_k|H_{11}|n_{k-1}\rangle\frac{1}{\hat{\omega}_{0,k-1}(n_{k-1})}\langle n_{k-1}|H_{11}|n_{k-2}\rangle$$
$$\times\frac{1}{\hat{\omega}_{0,k-2}(n_{k-2})}\cdots\frac{1}{\hat{\omega}_{01}(n_1)}\langle n_1|H_{11}|n'\rangle. \tag{30}$$

The arrow here means that all indices $n_1\cdots n_k, n'$ are different. Now we separate in (30) successively those terms in which $n=n_{k-1}$, $n=n_{k-2}$, $n=n_1$. These terms will cancel with those containing the factors $E_2(n),E_3(n),\cdots E_k(n)$ on substituting (30) into (29). We finally find that the matrix element $\langle n|S_{k+1}|n'\rangle$ can be written in a form similar to (28)

$$\langle n|S_{k+1}|n'\rangle=\frac{(-1)^{k+1}}{\hat{\omega}_{0,k+1}(n)}\overrightarrow{\sum_{n_1\cdots n_k}}\langle n|H_{11}|n_k\rangle\frac{1}{\hat{\omega}_{0k}(n_k)}\langle n_k|H_{11}|n_{k-1}\rangle$$
$$\times\frac{1}{\hat{\omega}_{0,k-1}(n_{k-1})}\cdots\frac{1}{\hat{\omega}_{01}(n_1)}\langle n_1|H_{11}|n'\rangle, \tag{31}$$

where the arrow at the summation sign means that all indices $n, n_1 \cdots n_k, n'$ are different, hence (31) involves no diagonal factors, which is the desired result. The perturbation theory developed here for calculating excited multiply degenerate states is thus efficient enough for the many-body problem.

VI. CONCLUSION

As can be seen from (3), the operator S transforms eigenfunctions of the perfect gas Hamiltonian H_0 into the exact eigenfunctions of the interacting particle Hamiltonian H. The spectrum of the system is coincident with that of the operator $\hat{E}$, hence can be enumerated by occupation numbers for perfect gas states. As demonstrated in Ref. 9 (see also Ref. 10), the calculation of a statistical sum with $\hat{E}$ leads to an expression for free energy in the form of a functional of the Ballian–Dominicis distribution function of thermodynamical quasiparticles,[13] the entropy of the system being expressible in terms of the distribution function of quasiparticles through the same relation as is the case for perfect gas.

We wish to emphasize the fact that all results derived in this study hold only for normal systems in the statistical limit, i.e., for macroscopic systems with continuous spectra and without the long-range order. In that case the multiple degeneration of the power spectrum does not affect results in the statistical limit and does not prevent us from establishing a one-to-one correspondence between exact wave functions of the system of interacting particles and the wave functions of perfect gas enumerated by single-particle occupation numbers.

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Comprehensive analysis of conditionally exactly solvable models

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We study a quantum mechanical potential introduced previously as a conditionally exactly solvable (CES) model. Besides an analysis following its original introduction in terms of the point canonical transformation, we also present an alternative supersymmetric construction of it. We demonstrate that from the three roots of the implicit cubic equation defining the bound-state energy eigenvalues, there is always only one that leads to a meaningful physical state. Finally we demonstrate that the present CES interaction is, in fact, an exactly solvable Natanzon-class potential. [DOI: 10.1063/1.1362286]

I. INTRODUCTION

Exactly solvable models have attracted much attention since the early years of quantum mechanics. Some solvable potentials have become standard examples of textbooks, but a lot more have been discovered by various approaches. Systematic work has been done to generate and classify these potentials using the factorization method,[1] algebraic methods[2] and more recently, in terms of supersymmetric quantum mechanics (SUSYQM).[3] These approaches were found to be interrelated with each other.[4–6]

The most general family of solvable potentials is the six-parameter Natanzon class,[7] which contains potentials with solutions expressible in terms of a single (confluent) hypergeometric function. A rather important subclass of this is that of the shape-invariant potentials,[7–9] to which the most well-known potentials (such as the harmonic oscillator, Coulomb, Pöschl–Teller, etc.) potentials belong. Altogether 12 such potentials have been identified,[5,9] but some of these actually represent different forms of the same potentials, and their separate discussion is justified only for historical reasons. An important recent development was the introduction of SUSYQM, which can be considered a reinterpretation of the factorization method,[1] and which links basically isospectral potentials in a pairwise manner. Shape-invariant potentials are defined in terms of SUSYQM: The functional form of the SUSYQM partner potentials has to be the same, and only the parameters appearing in them can be different.

SUSYQM has been found to be rather useful in generating new solvable potentials as SUSYQM partners from known solvable ones. A rather wide potential class is obtained as the SUSYQM partner of Natanzon potentials, but these are not Natanzon potentials themselves (except in the case of shape invariance), since their solution is written as the linear combination of several (confluent) hypergeometric functions.[10] There are also further solvable potentials which are solved by functions other than the (confluent) hypergeometric type. Examples for this are the square well[11] and the exponential potential, which are solved by Bessel functions.

A different concept of solvability characterizes quasiexactly solvable (QES) potentials.[12] In

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this case only part of the eigenstates can be obtained, by requiring termination of a recursion relation defining the eigenfunctions in a polynomial form.

The most recent concept of solvability is related to conditionally exactly solvable (CES) potentials. The first models coined CES potentials[13,14] were characterized by the fact that the coupling constant of some potential term had to be fixed to a numerical constant value in order to obtain their solutions. These potentials were introduced by the point canonical transformation method.[15] Here we present the analysis of one of these CES potentials.[14] Our motivation is to clarify some inconsistencies in their treatment, and to determine their place in other classification schemes of solvable models. (We note that another class of CES potentials was also introduced using the techniques of SUSYQM,[16,17] but we do not extend our analysis on this class.)

In Sec. II we give a reinterpretation of the potential of Ref. 14 in a supersymmetric context, and derive the bound-state energies determined implicitly by a cubic equation. In Sec. III the procedure is placed in a more general context of methods based on variable transformations, and the potential is identified as an exactly solvable member of the Natanzon potential class.

II. THE MODEL OF DUTT, KHARE, AND VARSHNI

We start by presenting the potentials introduced by Dutt *et al.*[14] as CES models. The two potentials defined on the full axis $x\in(-\infty,\infty)$ can be written in a common form as

$$V^{(g_0,g_1,g_2,g_3)}(x)=\frac{g_0}{e^x z(x)}+\frac{g_1}{z(x)}+\frac{g_2}{z^2(x)}+\frac{g_3}{z^4(x)}, \tag{2.1}$$

with $z(x)=(1+e^{-2x})^{1/2}\in(1,\infty)$. The explicit form of these potentials[14] is

$$V_1^{(\mathrm{DKV})}(x)=V^{(0,-B,A,-3/4)}(x),\quad V_2^{(\mathrm{DKV})}(x)=V^{(-B,0,A,-3/4)}(x). \tag{2.2}$$

These potentials depend on two parameters (A and B) which define the potential shape. The coupling constant of the third potential term has to be fixed to a constant value ($-3/4$) in order to obtain exact solution of these models. This is why the authors of Ref. 14 identified these potentials as CES ones.

One can easily demonstrate that the two potentials, in fact, are equivalent in the sense that

$$V^{(0,-B,A,-3/4)}(x)=V^{(-D,0,C,-3/4)}(-x)+\epsilon, \tag{2.3}$$

where

$$\epsilon=-A+3/4,\quad C=-A+3/2,\quad D=B. \tag{2.4}$$

Thus, in what follows it is sufficient to deal with only one of the potentials, so we pick $V_1^{(\mathrm{DKV})}(x')$ for our analysis.

A. Conventional approach via the point canonical transformation

In Ref. 14 potentials (2.2) were introduced using the point canonical transformation method,[15] by which a Schrödinger-type differential equation can be transformed into another equation of this type, applying an invertible parametrization $r=r(x)$. With this change of variables, dating back to Liouville[18] a given asymptotically free equation

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+U(r)\right]\chi(r)=-\kappa^2\chi(r) \tag{2.5}$$

can be transformed into an apparently different bound state problem

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x)\right]\psi(x)=-k^2\psi(x). \tag{2.6}$$

After we denote the derivative by a prime $[x'(r)$, etc.], an extremely elementary correspondence between the potentials and/or energies is obtained,

$$U(r)+\kappa^2=[x'(r)]^2\{V[x(r)]+k^2\}+\left(\frac{3}{4}\frac{x''(r)}{x'(r)}\right)^2-\frac{1}{2}\frac{x'''(r)}{x'(r)}. \tag{2.7}$$

Obviously, the ''old'' energy eigenvalues are related to the parameters of the ''new'' potential, and vice versa. The formal definition of the new wave functions is also virtually trivial,

$$\psi(x)=(x'[r(x)])^{1/2}\chi[r(x)]. \tag{2.8}$$

In any situation of practical interest one may just pick up a suitable exactly solvable (ES) problem (2.5) and quickly derive its partner (2.6). Setting out from two shape-invariant[8] ES potentials defined on the positive half axis, Dutt *et al.*[14] used the variable transformation $x=\ln(\sinh r)$ to obtain potentials (2.2). The particular initial potentials and their energies were

$$U_1(r)=-2b\frac{\cosh r}{\sinh r}+a(a-1)\frac{1}{\sinh^2 r},\quad \kappa^2=\kappa_m^2=(a+n)^2+b^2/(a+n)^2 \tag{2.9}$$

[with $b>(a+n_{\max})^2$] and

$$U_2(r)=-(2a+1)b\frac{\cosh r}{\sinh^2 r}+[a(a+1)+b^2]\frac{1}{\sinh^2 r},\quad \kappa^2=\kappa_n^2=(a-n)^2 \tag{2.10}$$

(with $b>a>n_{\max}$).

Recalling the bound-state wave functions of potentials $U_j(r)$, the solutions to potentials $V_j^{(\mathrm{DKV})}(x)$ in (2.2) readily follow from Eq. (2.8). Without the loss of generality we can consider the $j=1$ case and recall the solutions of $U_1(r)$ (see, e.g., Refs. 9 and 5) in terms of Jacobi polynomials,

$$\chi(z)=(z-1)^{-(1/2)(a+n-s)}(z+1)^{-(1/2)(a+n+s)}P_n^{(-a-n+s,-a-n-s)}(z),\quad s=b/(a+n) \tag{2.11}$$

with $z=z(r)=\coth r$. Using this function in (2.8), substituting it into the Schrödinger equation, and matching parameters a and b with A and B appearing in $V_1^{(\mathrm{DKV})}(x)$ in (2.2), we find $B=2b$ and

$$A=n^2+1/2+(2n+1)\,a+b^2/(a+n)^2. \tag{2.12}$$

This equation will ultimately determine the energy eigenvalues of quantum number n, through a cubic equation as described also in Ref. 14. We postpone the analysis of this formula to Sec. II C, where our new results concerning the energy spectrum of the $V_j^{(\mathrm{DKV})}(x)$ potentials are presented. Before that, we present an alternative interpretation of the same problem in terms of a supersymmetric framework.

B. Supersymmetric construction

An interesting SUSY reinterpretation of the solvability of Schrödinger equations has been described by Nag *et al.*[19] They have employed the two Dutra's models[13] in order to illustrate their main idea. Unfortunately, the spectrum of states in the latter potentials can only be determined purely numerically.[20] Strictly speaking, the potentials do not belong to the CES class.[21,22] At best, only their incomplete (=quasiexact) non-numerical solution can be obtained at certain *exceptional* energies and couplings.[21,23] Within the SUSY methodical framework, they seem less suitable for illustrative purposes.

We shall now obtain the spectrum of the potential $V_1^{(\mathrm{DKV})}(x)$ in (2.2) in a manifestly supersymmetric fashion. Before doing this we recall that in supersymmetric quantum mechanics[9] a pair of Hamiltonians $H_\pm$ defined by

$$H_\pm = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V_\pm(x) = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + W^2(x) \pm W'(x) \tag{2.13}$$

are isospectral except for the zero energy ground state, which, for unbroken supersymmetry, exists only for one of the partner potentials, $V_-(x)$. The ground-state solution of H_- is related to the $W(x)$ superpotential through

$$W(x) = -\frac{\mathrm{d}}{\mathrm{d}x}\ln\psi_0^{(-)}(x). \tag{2.14}$$

One can also extend the concept of superpotential to the excited states of $V_-(x)$, simply using $\psi_n^{(-)}(x)$ in (2.14). In this case $W(x)$ has singularities at the nodes of $\psi_n^{(-)}(x)$, and one can talk about singular superpotentials.[9] [Note that such singularities cannot occur using the nodeless ground-state wave function $\psi_0^{(-)}(x)$.] Despite these singularities of $W(x)$, it can be shown[9] that $V_-(x)$ will be singularity free in this case too, and these will appear only for the partner potential $V_+(x)$. Our purpose is, however, to discuss only $V_-(x)$, which we identify with $V_1^{(\mathrm{DKV})}(x)$ in Eq. (2.2), in a supersymmetric form, therefore we shall avoid the problems arising due to the singularities of $W(x)$.

For this purpose, let us consider the superpotential

$$W(z) = \frac{B_1}{z} - \frac{1}{2z^2} - C_0 + \sum_{i=1}^{n} \frac{g_i'(z)}{g_i(z)}, \tag{2.15}$$

where $z = (1+\mathrm{e}^{-2x})^{1/2}$ as in (2.2) and (2.1), and $g_i(z)$ is given by

$$g_i(z) = \frac{1}{1+g_i z}, \quad C_0 = \epsilon_0^{1/2}, \tag{2.16}$$

where ϵ_n is related to the (negative) bound-state energies of potential $V_1^{(\mathrm{DKV})}(x)$ via $\epsilon_n = -E_n$. Note that the zero-energy wave function $\psi_0^{(-)}(x) = N_0 \exp[-\int W(x)\mathrm{d}x]$ is always normalizable for our choice of $W(x)$, irrespective of the values of g_i. It may be noted that if we had omitted the last term in (2.15), i.e.,

$$W_0(z) = \frac{B_1}{z} - \frac{1}{2z^2} - C_0, \tag{2.17}$$

we would have obtained only the ground state. Insertion of the last term containing the sum ensures that we would get the excited states also.

It is straightforward to show that $W(z)$ can be written in the form

$$W(z) = \frac{B_1 - \Sigma_{i=1}^n g_i}{z} - \frac{1}{2z^2} + C_0' + \frac{\Sigma_{i=1}^n (g_i^2 - 1)}{(1+g_i z)}, \tag{2.18}$$

where we have defined $C_0' = n - C_0$.

Using (2.18) we obtain

$$W^2(x)-W'(x)=\left[\left(B_1-\sum_{i=1}^{n} g_i\right)^2-C_0'-\sum_{i=1}^{n}(g_i^2-1)+1\right]\Big/ z^2$$
$$+\left[2\left(B_1-\sum_{i=1}^{n} g_i\right)C_0'+2\left(B_1-\sum_{i=1}^{n} g_i\right)\left(\sum_{i=1}^{n}(g_i^2-1)\right)-\left(B_1-\sum_{i=1}^{n} g_i\right)\right.$$
$$\left.+2g_i(g_i^2-1)\right]\Big/ z-\frac{3}{4z^4}+\sum_{i=1}^{n}\frac{1}{1+g_iz}\left[-2\left(B_1-\sum_{i=0}^{n} g_i\right)(g_i^2-1)g_i-g_i^2(g_i^2\right.$$
$$\left.-1)+2C_0'(g_i^2-1)-(g_i^4-1)+\sum_{j\neq i}\frac{(g_j^2-1)(g_i^2-1)g_i}{g_i-g_j}\right]+(C_0')^2. \tag{2.19}$$

We now make the following identification

$$W^2(x)-W'(x)=V_1^{(\mathrm{DKV})}(x)-E, \tag{2.20}$$

where E is the energy of the states in potential $V_1^{(\mathrm{DKV})}(x)$.

Then it follows that

$$-2\left(B_1-\sum_{i=1}^{n} g_i\right)g_i-g_i^2+2C_0'-(g_i^2+1)+2\sum_{i\neq j}\frac{(g_j^2-1)g_i}{g_i-g_j}=0, \tag{2.21}$$

$$2\left(B_1-\sum_{i=1}^{n} g_i\right)C_0'+2\left(B_1-\sum_{i=1}^{n} g_i\right)\left(\sum_{i=1}^{n}(g_i^2-1)\right)-\left(B_1-\sum_{i=1}^{n} g_i\right)+2\sum_{i=1}^{n} g_i(g_i^2-1)=-B, \tag{2.22}$$

$$\left(B_1-\sum_{i=1}^{n} g_i\right)^2-C_0'-\sum_{i=1}^{n}(g_i^2-1)+1=A, \tag{2.23}$$

$$(C_0')^2=-E. \tag{2.24}$$

Multiplying (2.21) by g_i and summing over i we obtain

$$-2\left(B_1-\sum_{i=1}^{n} g_i\right)\sum_{i=1}^{n} g_i-2\sum_{i=1}^{n} g_i^3+2\sum_{i=1}^{n} C_0'g_i-(2n-1)\sum_{i=1}^{n} g_i=0. \tag{2.25}$$

From (2.22) and (2.25) we get

$$B_1=\frac{B}{1+2C_0}=\frac{B}{1+2\epsilon_0^{1/2}}. \tag{2.26}$$

It can be verified by insertion that the wave functions $\psi_n^{(-)}(x)=N\exp[-\int W(x)\mathrm{d}x]$ are normalizable. Equations (2.21) and (2.23) also imply that

$$A=\frac{(B/2)^2}{\left(n+\frac{1}{2}+\epsilon_n^{1/2}\right)^2}+n^2+n+1+(2n+1)\epsilon_n^{1/2}, \tag{2.27}$$

where in obtaining the above-mentioned relation we have taken $C_0'=-\epsilon_n^{1/2}$. We can summarize that our supersymmetric construction reproduces exactly the results obtained in Ref. 14. Once we take $a=\epsilon_n^{1/2}$ it proves equivalent to Eq. (2.12) of Sec. II A.

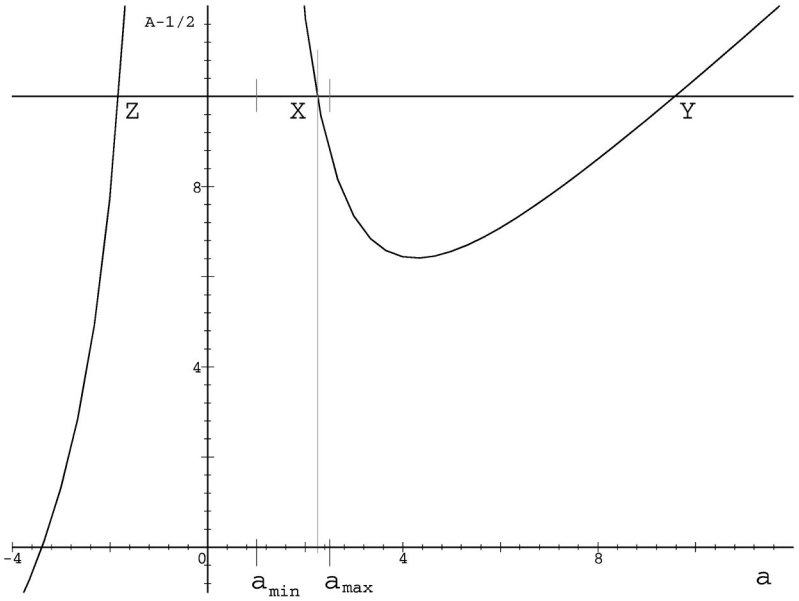

FIG. 1. Graphical solution of Eq. (2.12).

C. The allowed bound-state energies

Let us now continue with the analysis of the energy eigenvalues based on formula (2.12) and its equivalent form (2.27) obtained in two different ways. The key element of our approach is the strict observation of the constraints imposed on the parameters by the boundary conditions of the wave functions. By this we mean both the solutions of the ''old'' potential $U_1(r)$ (2.9) and those of the ''new'' one $V_1^{(\mathrm{DKV})}(x)$ (2.2).

The appropriate physical boundary condition for (2.11) near the threshold $r\to 0$ is standard, though a bit counterintuitive.[21,24] Its implementation implies that we have to choose $a>1/2$. Then, after the transition from r to x we get the wave functions still safely normalizable near the left infinity $x\to-\infty$. Similarly, our explicit wave functions remain asymptotically normalizable near the right infinities $r\to\infty$ and $x\to+\infty$ if and only if we have $a+n<b/(a+n)$. This means that the eligible quantum numbers $n=0,1,\ldots,M$ have to be such that $0\leqslant M<b^{1/2}-a$, i.e.,

$$(n+1/2)^2<(a+n)^2<b. \tag{2.28}$$

As mentioned in Sec. II A, for transition to the ''new'' potential $V_1^{(\mathrm{DKV})}(x)$ we have to reparametrize $g_1=-B\equiv-2b$ and define the ''new'' CES energy in terms of the ''old'' ES coupling, $k=a-1/2>0$. The second CES coupling $A>2(n+1/2)^2+3/4$ is then defined by (2.12), which is equivalent to (2.27) in Sec. II B. The n dependence of the ''new'' energy $a=a(n)=k_n+1/2>1/2$ is fully consistent with the n independence of the coupling A. For each level the CES potential $V(x)$ is a map of a *different* ES potential $U(r)$. The energies are determined by the cubic algebraic equation. In order to make this definition unique we have to tell which one of the three roots of Eq. (2.12) is ''physical.'' In Ref. 14 we find advice that ''from the three roots we can discard two by demanding that the spectrum must reduce to the standard one for $B=0$.'' Such a vague recipe is misleading since it is in manifest contradiction with the above-mentioned normalizability condition (2.28) which implies that $b=B/2>1/4$ cannot lie too close to zero.

The problem is not too difficult to disentangle. Equation (2.12) has very transparent graphical interpretation in terms of the intersection of the left-hand side horizontal line with the right-hand side curve with three branches. The latter shape is a sum of a growing linear term with a spike oriented upwards. Figure 1 indicates how one gets a triplet of roots in the $n=0$ ground state at

$b=6.25$ and $A=10.25$. Always, only one of them is compatible with the normalizability condition (2.28) and lies in the ''admissible'' interval $(0.5,2.5)$.

The general rule is that we always have to pick up the middle root as physical. Let us give a proof of this assertion. First we rename $b=\beta^2$ and rescale our three roots, $Z=[a_1(n)+n]/\beta < X=[a_2(n)+n]/\beta < Y=[a_3(n)+n]/\beta$. As long as $a(n)\in(1/2,\beta-n)$ we may rewrite Eq. (2.12) in the significantly simplified form

$$\tau=\mu X+\frac{1}{X^2}$$

(and, similarly for Y and Z) with abbreviations

$$\tau=\tau(A,b,n)\equiv\frac{A+n^2+n-1/2}{b},\quad 0<\mu=\frac{2n+1}{\beta}<2.$$

The leftmost root Z will always be negative and can be discarded immediately. Knowing that the acceptable root X is constrained, $X\in(T,1)$, $T=(n+1/2)/\beta\in(0,1)$, it is now sufficient to prove that the third root Y *always* violates our condition (2.28),

$$[X\in(T,1)\ \&\ T\in(0,1)]\Rightarrow Y>1. \tag{2.29}$$

For this purpose we eliminate τ and get the quadratic equation

$$\mu=\frac{X+Y}{X^2Y^2}.$$

We can skip the negative alternative and have the unique definition of the root Y,

$$Y=\frac{1+(1+4\mu X^3)^{1/2}}{2\,\mu X^2}.$$

As a smooth function of $\mu\in(0,2)$ and $X\in(T,1)$ it satisfies our rule (2.29) *everywhere* within a two-dimensional domain containing all points with $\mu<1$ and *not containing* any point of the sign-changing boundary. This is demonstrated quite easily. The boundary curve can be implicitly defined as a set $X=\xi(\mu)$,

$$1+(1+4\mu\,\xi^3)^{1/2}=2\,\mu\,\xi^2.$$

Only on it the sign of $Y-1$ can change. This set is a part of the curve defined by the square of the latter equation,

$$\mu\,\xi^2=\xi+1.$$

In the graphical language it is trivial to find that for the positive $\xi>0$ the right-hand side straight line intersects the left-hand side parabola in a point which is a decreasing function of μ. Hence, the curve touches the boundary of our open simplex of normalizability (with $\mu\in(0,2)$ and $X<1$) in a single point $(\mu=2,\xi=1)$. Q.E.D.

III. INTERPRETATION OF THE POTENTIAL

The potentials of Ref. 14 derived in two different ways in Sec. II can be placed into a more general context by realizing that both the point canonical transformation method[15] presented in Sec. II A and the supersymmetric construction of Sec. II B can be formulated in terms of a rather general approach based on the change of variables.[25,7,5] In this section we specify these connections with the formulation of Ref. 5, which can be considered a simplified treatment of the general Natanzon-class potentials.[7]

Following the discussion of Ref. 5 one considers the Schrödinger equation

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}+(E-V(x))\psi(x)=0 \tag{3.1}$$

and assumes that its solutions can be written in the form

$$\psi(x)=f(x)F(z(x)), \tag{3.2}$$

where $F(z)$ satisfies a second-order differential equation

$$\frac{\mathrm{d}^2F}{\mathrm{d}z^2}+Q(z)\frac{\mathrm{d}F}{\mathrm{d}z}+R(z)F(z)=0. \tag{3.3}$$

The function $F(z)$ can be any special function of mathematical physics, e.g., the (confluent) hypergeometric function,[26] or any other function satisfying a second-order differential equation of the type (3.3). Simple calculation shows[5] that the function $E-V(x)$ can be written as

$$E-V(x)=\frac{z'''(x)}{2z'(x)}-\frac{3}{4}\left(\frac{z''(x)}{z'(x)}\right)^2+(z'(x))^2\left[R(z(x))-\frac{1}{2}\frac{\mathrm{d}Q(z)}{\mathrm{d}z}-\frac{1}{4}Q^2(z(x))\right], \tag{3.4}$$

where the only unknown element is the function $z(x)$, which basically governs the change of variables connecting the two differential equations (3.1) and (3.3). Expressing $f(x)$ in (3.2) in terms of $z(x)$ and $Q(z)$, the solutions of the Schrödinger equation can be written[5] as

$$\psi(x)\sim(z'(x))^{-1/2}\exp\left(\frac{1}{2}\int^{z(x)}Q(z)\mathrm{d}z\right)F(z(x)). \tag{3.5}$$

We are left with the task of finding such a functional form of $z(x)$ which takes our Schrödinger equation (3.4) into an exactly and *completely* solvable problem.

Obviously, the transformation employed in Sec. II A (i.e., the point canonical transformation[15] or the Liouvillean method[18]) is a special case of the above-mentioned construction. Taking, in a way explained in detail in Ref. 27

$$Q(z)=0, \quad R(z)=-\kappa^2-U(z), \tag{3.6}$$

Eq. (3.4) reduces to the inverted version of Eq. (2.7) (with r and $-k^2$ there replaced with z and E here). Similarly, (3.5) also reduces to the equivalent of (2.8), where $\chi(r)$ is playing the role of $F(z)$.

From here the approaches applied in Refs. 25 and 5 and in the point canonical transformation[15] emphasize somewhat different strategies of deriving solvable potentials within the Natanzon potential class.[7] In Refs. 25 and 5 the main point is to identify some term on the right-hand side of Eq. (3.4), to account for the constant (i.e., the energy) term on the left-hand side. With this, a differential equation of the type

$$\left(\frac{\mathrm{d}z}{\mathrm{d}x}\right)^2\phi(z)=C \tag{3.7}$$

was obtained (see also Ref. 28), and this determined the function $z(x)$ describing the variable transformation. In some cases the $z(x)$ function could not be determined explicitly from (3.7), only the inverse $x(z)$ function, therefore a number of solvable models obtained this way turned out to be ''implicit'' potentials.[29,30] On the other hand, following the point canonical transformation method,[15] the $z(x)$ function is always available in an explicit form, however, it is not guaranteed that any $z(x)$ function would lead to a Schrödinger-like equation in which all the n dependence can be absorbed into the constant (energy) term. Equation (2.12) might turn out to have Sturm–Liouvillean form, where n typically appears in coordinate-dependent terms. Simply stated, the

approach of Ref. 5 focuses on having the energy in a simple form, even at the expense of leaving the solutions in a complicated (implicit) form, while in the point canonical transformation the preference is having the solutions in an explicit form, rather than getting the energy expression in a simple way. We stress that despite this difference, the two approaches are interrelated, and are special cases of deriving Natanzon-class potentials. We shall come back to this point later on.

A. Conventional construction

Let us now see how potential $V_1^{(\mathrm{DKV})}(x)$ in Eq. (2.2) can be obtained from the method described in Ref. 5. For this, $F(z)$ should be identified with a Jacobi polynomial: $F(z)=P_n^{(\alpha,\beta)}(z)$. Equation (4.2) in Ref. 5 is an explicit form for $E-V(x)$ in this case:

$$\begin{aligned} E-V(x)=&\frac{z'''(x)}{2z'(x)}-\frac{3}{4}\left(\frac{z''(x)}{z'(x)}\right)^2+\frac{(z'(x))^2}{1-z^2(x)}n(n+\alpha+\beta+1)\\ &+\frac{(z'(x))^2}{(1-z^2(x))^2}\left[\frac{1}{2}(\alpha+\beta+2)-\frac{1}{4}(\beta-\alpha)^2\right]\\ &+\frac{(z'(x))^2z(x)}{(1-z^2(x))^2}\,\frac{1}{2}(\beta-\alpha)(\beta+\alpha)+\frac{(z'(x))^2z^2(x)}{(1-z^2(x))^2}\left[\frac{1}{4}-\left(\frac{\alpha+\beta+1}{2}\right)^2\right]. \end{aligned} \tag{3.8}$$

As discussed in Ref. 5, one selects differential equations of the type (3.7) for $z(x)$ to get constant terms on the right-hand side of (3.8). In Ref. 5 the first two nontrivial terms were picked, leading to the PI and PII potential classes, typical representations of which are, for example, $U_2(r)$ and $U_1(r)$ in Eqs. (2.10) and (2.9), respectively. The defining differential equation of these is $(z')^2(1-z^2)^{-1}=C$ and $(z')^2(1-z^2)^{-2}=C$. Later in Ref. 30 the third ''PIII'' possibility, $z(z')^2(1-z^2)^{-2}=C$, was also discussed, resulting in an ''implicit potential.'' All these potentials are exactly solvable Natanzon-class potentials, furthermore, those discussed in Ref. 5 also have the property of shape invariance.

The fourth possibility,

$$z^2(z')^2(1-z^2)^{-2}=C \tag{3.9}$$

was not discussed in detail in Ref. 5, only the generic form of the solution was mentioned. However, it turns out that the function $z(x)=(1+\exp(2C^{1/2}x+D))^{1/2}$ satisfies (3.9), and it leads to the same variable transformation as that discussed in Ref. 14, if the $C^{1/2}=-1$ and $D=0$ choice is made. The actual form of (3.4) is now (in the ''PIV'' case)

$$\begin{aligned} E_n-V(x)=&-\left(n+\frac{\alpha+\beta+1}{2}\right)^2+\frac{1}{2}(\beta-\alpha)(\beta+\alpha)z^{-1}(x)+\frac{3}{4}z^{-4}(x)\\ &+\left[\left(n+\frac{\alpha+\beta+1}{2}\right)^2-\left(\frac{\alpha+\beta}{2}\right)^2-\frac{3}{4}-\frac{1}{4}(\beta-\alpha)^2\right]z^{-2}(x). \end{aligned} \tag{3.10}$$

This leads to a solvable potential if the n dependence can be canceled in the coordinate-dependent (i.e., potential) terms by a suitable change of the parameters. Comparing (3.10) with (2.2) we get

$$A=-\left[\left(n+\frac{\alpha+\beta+1}{2}\right)^2-\left(\frac{\alpha+\beta}{2}\right)^2-\frac{3}{4}-\frac{1}{4}(\beta-\alpha)^2\right], \tag{3.11}$$

$$B=\tfrac{1}{2}(\beta-\alpha)(\beta+\alpha), \tag{3.12}$$

and

$$E_n = -\left(n + \frac{\alpha+\beta+1}{2}\right)^2. \tag{3.13}$$

Obviously, α and β depend on n and also on the potential parameters A and B. Substituting (3.13) in (3.11) and combining it with (3.12) we arrive at (2.12), the equation defining the energy eigenvalues in the two approaches of Sec. II.

The bound-state wave functions are found to be

$$\psi(x) \sim z^{1/2}(x)(z(x)+1)^{\beta_n/2}(z(x)-1)^{\alpha_n/2}P_n^{(\alpha_n,\beta_n)}(z(x)), \tag{3.14}$$

which (apart from some misprints), corresponds to Eqs. (15), (16), and (18) in Ref. 14, if we substitute $\alpha_n = B/(2c) - c$ and $\beta_n = -B/(2c) - c$.

B. Supersymmetric connection

In the knowledge of the bound-state wave functions, constructing the superpotential $W(x)$ is a simple matter using Eq. (2.14). From (3.14) with $n=0$ one obtains

$$W(x) = \frac{1}{2}(\alpha_0+\beta_0+1) + \frac{\alpha_0-\beta_0}{2z(x)} - \frac{1}{2z^2(x)}. \tag{3.15}$$

In order to get closer to the methods described in Sec. II B, we also introduce the singular superpotentials obtained in a similar way to the wave functions with $n>0$. The Jacobi polynomial appearing in these functions is best expressed in a product form

$$P_n^{(\alpha_n,\beta_n)}(z) \sim \Pi_{i=1}^{n}(z-c_i), \tag{3.16}$$

where the c_i are at the roots (nodes) of the polynomial. Obviously, the logarithmic derivative of this product will reduce to a sum form

$$\frac{\mathrm{d}}{\mathrm{d}x}(\ln P_n^{(\alpha_n,\beta_n)}(z)) = \frac{\mathrm{d}z}{\mathrm{d}x}\frac{\mathrm{d}}{\mathrm{d}z}\sum_{i=1}^{n}\ln(z-c_i) = (z^{-1}-z)\sum_{i=1}^{n}\frac{1}{z-c_i}. \tag{3.17}$$

Here we used the differential equation (3.9) to express z' in terms of z. This explains the sum appearing in the superpotential (2.18) in Sec. II B. A similar construction can readily be presented for the superpotential used in Ref. 19 describing the potential of Ref. 13 in a supersymmetric framework. The polynomial there is of the Hermite type.

C. Relation to the Natanzon potentials

Our discussion in the present section was based on the approach of Ref. 5, which is general enough to incorporate both the conventional and the supersymmetric formulation of potential (2.2) in a relatively straightforward way. One can, however, put the whole subject into an even more general framework, that of the Natanzon potentials.[7] Although the discussion could have been presented using the formalism of this potential class, we decided to follow the easier route of Ref. 5 for several reasons. First, the general formalism was too heavy for demonstrative purposes, and second, its relation to the machinery of supersymmetric quantum mechanics[3,9] is less transparent. However, to conclude this section we present the essential facts about Natanzon potentials, and their relevance to the potentials we investigated.

The general families of the Natanzon[7] and Natanzon confluent[31] potentials are characterized by the feature that their solutions are expressed in terms of a single (confluent) hypergeometric function. The general Natanzon potential depends on six parameters, three of which (f, h_0, and h_1) appear explicitly in

$$V(x)=-\frac{z'''(x)}{2z'(x)}+\frac{3}{4}\left(\frac{z''(x)}{z'(x)}\right)^2+\frac{fz(x)(z(x)-1)+h_0(1-z(x))+h_1z(x)}{\mathcal{R}(z(x))}, \tag{3.18}$$

while three others (a, c_0, and c_1) enter implicitly through the $z(x)$ function determined by the differential equation

$$z'(x)\equiv\frac{dz}{dx}=\frac{2z(1-z)}{(\mathcal{R}(z))^{1/2}} \tag{3.19}$$

with

$$\mathcal{R}(z)=az(x)(z(x)-1)+c_0(1-z(x))+c_1z(x). \tag{3.20}$$

The construction of Ref. 5, when specified for the Jacobi polynomials (a special case of the hypergeometric function[26]) can easily be recognized as a particular reformulation of this change of variable method. (See also Ref. 32 and the Appendix of Ref. 28.) The energy spectrum is determined[7] by the implicit equation

$$2n+1=(f+1-aE_n)^{1/2}-(h_0+1-c_0E_n)^{1/2}-(h_1+1-c_1E_n)^{1/2}\equiv\alpha_n-\beta_n-\delta_n, \tag{3.21}$$

while the bound-state wave functions are written as

$$\psi(x)\sim\mathcal{R}^{1/4}(z(x))(1-z(x))^{\delta_n/2}(z(x))^{\beta_n/2}F(-n,\alpha_n-n;\beta_n+1;z(x)). \tag{3.22}$$

The form of (3.22) is again reminiscent of the construction of Ref. 5, while (3.21) is close to the implicit energy formula obtained for the potential of Ref. 14 in the point canonical transformation formalism.

Equations similar to those mentioned previously are valid for the Natanzon confluent potential class[31] too.

It is instructive to examine the role of the $3+3$ parameters appearing in the Natanzon potentials, as it is related to the concept of conditionally exact solvability. For the most commonly occurring potentials (like the shape-invariant ones[8]), the three parameters determining the $z(x)$ function via (3.19) and (3.20), usually only one appears, and even that one is a trivial scaling parameter of the coordinate and/or the energy scale. (Trivial coordinate shifts can also appear through them.) Usually they play a nontrivial role only in the case of some ''implicit'' potentials.[29]

The other three parameters appearing in (3.18) set the potential shape, and determine the relative strength of the individual potential terms. In most potentials only one or two of these parameters appear. The two parameters appearing in potential (2.2), A and B are of this type. (There could be one more parameter setting the length scale, but it is set to 1 in this case.) Obviously, when there are three potential terms, as in (2.2), and only two parameters, then the relative strength of the three potential terms cannot be arbitrary, and has to be constrained. This is why the third term of (2.2) is a numerical constant, i.e., $-3/4$. It is the presence of this numerical constant which earned potentials in Refs. 13 and 14 the name ''conditionally exactly solvable.'' In fact, based on the structure of their eigenfunctions, the potentials appearing in Ref. 14 are of the Natanzon type,[7] while those in Ref. 13 belong to the Natanzon confluent class.[31] There are, however, further considerations regarding normalizability and regularity, which might impose restrictions on the solvability of certain potentials. Not surprisingly, these may play a more important role in the case of the less ''trivial'' potentials.[33]

Finally, we note that the other class of CES potentials[16,17] has a completely different nature, and does not belong to the Natanzon class, rather it has features typical for SUSY partners of general Natanzon-class potentials. This again confirms our finding that the concept of conditionally exact solvability is not an alternative of exact solvability, rather it classifies potentials according to different principles.

IV. CONCLUSIONS

We analyzed the potentials introduced originally in Ref. 14 as conditionally exactly solvable (CES) potentials via the method of point canonical transformation. Our results concerned the following three areas.

(i) We gave a supersymmetric reinterpretation of this potential class.
(ii) We examined the cubic formula which determines implicitly the energy eigenvalues of the problem. We rigorously took into account boundary conditions of the eigenfunctions, and corrected certain inaccuracies presented in Ref. 14. We demonstrated that from the three roots of the cubic equation there is only one (the middle one) which can lead to physically acceptable eigenstates.
(iii) We interpreted this potential in the general framework of the Natanzon potential class, and demonstrated that this CES potential, in fact, belongs to this class, and therefore it is a *bona fide* exactly solvable problem.

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Berry's phase for compact Lie groups

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The methods of Kähler geometry are applied to generalize the results of Berry obtained for $SU(2)$ (namely, the existence of a geometrical part in the adiabatic phase) to any compact Lie group. We obtain explicit expressions for Berry's geometric phases, Berry's connections, and Berry's curvatures in terms of parameters of the corresponding Lie algebra valued Hamiltonian. It is demonstrated that the parameter space of the Hamiltonian in the general theory is essentially a homogeneous Kähler manifold. The fundamental Kähler potentials of this manifold completely determine Berry's phase. A general approach is exemplified by the Lie algebra Hamiltonians corresponding to $SU(2)$ and $SU(3)$ evolution groups. [DOI: 10.1063/1.1358879]

I. INTRODUCTION

A number of branches of physics make use of the geometric properties of Kähler coset spaces (a definition may be found in Kobayashi and Nomizu, Vol. 2[1]). For instance, in quantum field theory the Kähler coset spaces give rise to a broad class of supersymmetric nonlinear sigma models discussed in Zumino,[2] Alvarez-Gaumé and Freedman,[3] and Bando, Kuramoto, Maskawa, and Uehara[4] (among others). In quantization of dynamical systems with curved phase space with a nontrivial global geometry Kähler cosets serve as a model of such curved phase space (e.g., Beresin,[5] Bar-Moshe, and Marinov[6,7]). Kähler geometry is also used in relativity theory (for a review see Flaherty[8]).

In this work I show how geometric properties of Kähler coset spaces may be used in the ordinary nonrelativistic quantum mechanics. Knowledge of the fundamental Kähler potentials of these cosets enables me to generalize the result of Berry obtained for $SU(2)$ to essentially any compact Lie group.

Berry[9] was the first to discover the relation between the adiabatic phase acquired by the wave function under a slow variation of the Hamiltonian parameters and the geometry of the parameter space. Specifically, it has been demonstrated that the adiabatic phase includes a part of a pure geometrical origin (the geometric phase factor). Simon[10] has shown that the geometrical meaning of the geometric phase is the holonomy in a Hermitian line bundle over the parameter space of the Hamiltonian, and that the adiabatic theorem[11] (see also Messiah[12]) gives rise to a connection with such a bundle. When the parameter dependence of the Hamiltonian is determined by a closed curve C on the parameter space, the Berry geometrical factor Ω is expressed by the integral (Simon,[10] Berry[9])

$$\Omega(C)=\int_S F. \tag{1}$$

Here S is any oriented surface in the parameter space with $\partial S=C$, and F is a two-form given on this parameter space. As a consequence of Stokes' theorem the two-form F may be expressed in terms of the Berry vector potential[9] (or Berry's connection).

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However, explicit forms for the geometric phase factor Ω [Eq. (1)] and for the Berry connection in terms of the (local) coordinates of the parameter space have since been obtained only for a number of simple cases. The spin precession in a slowly time-dependent magnetic field when the parameter space is a two-dimensional sphere, and the Berry connection is expressed in terms of the spherical coordinates is the simplest example. After a suitable reparametrization of the time variable the Hamiltonian H for this case may be chosen as

$$H(s)=\mathbf{n}(s)\cdot\mathbf{J},|\mathbf{n}(s)|=1, \tag{2}$$

where $\mathbf{J}$ is the spin operator, and the vector $\mathbf{n}=(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)$. [It has been shown by Jakšić and Segert[13] that any two-level system may be described by the Hamiltonian (2) (with $\mathbf{J}=\boldsymbol{\sigma},\boldsymbol{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ are Pauli matrices) after a corresponding reparametrization of the time variable.] The corresponding Berry connection A_s induced by the adiabatic evolution of the spin state is

$$A_s=\frac{l}{2}(1-\cos\theta)\dot{\phi},\quad l=0,\pm1,\pm2\ldots\ . \tag{3}$$

The Berry geometrical phase is defined by Eq. (1), where the two-form F is

$$F=\frac{l}{2}\sin\theta d\phi\wedge d\theta,\quad l=0,\pm1,\pm2\ldots\ . \tag{4}$$

In this example the evolution operator acting on the spin state belongs to an irreducible representation of the $SU(2)$ group, the Hamiltonian $H(s)$ [Eq. (2)] determines a smooth curve in the Lie algebra $su(2)$, and the parameter space is the homogeneous space of the group $SU(2)$, $S^2=SU(2)/U(1)$.

It is my goal in the present paper to consider cases when the adiabatic evolution is determined by one-parameter Hamiltonians belonging to more complicated than $su(2)$ Lie algebras. I shall concentrate on one-parameter Hamiltonians which lead to compact evolution operators, and determine closed smooth curves in the semi-simple Lie algebras of arbitrary ranks. The aim is to generalize equations, Eq. (3), Eq. (4), and to find explicit expressions for Berry connections and Berry curvatures in terms of the coordinates of the corresponding parameter spaces.

This paper is organized as follows. Section II begins with an introduction of the relevant Lie algebra notations. We first obtain that the adiabatic phase is a scalar product of two vectors in the root space of the Lie algebra under consideration. We reveal that it is not always the case that the adiabatic phase depends on one integer only [as in the case of $su(2)$ Lie algebra, Eqs. (3), (4)]. Rather, it is dependent on a set of integers with a number equal to the rank of the Lie algebra [e.g., in the case of $su(2)$ the rank is equal to one; thus only one integer suffices]. We note that these integers determine irreducible representation in which quantum states form a basis.

In Sec. III we discuss the familiar example of Berry for $SU(2)$ while introducing the technique which enables generalization to any compact Lie group. In Sec. IV we introduce a complex parametrization of the parameter space by a Mackey-type decomposition for any element of the evolution group G. Applicability of this procedure is restricted to the cases when the parameter space of the Hamiltonian is a homogeneous Kähler manifold $\mathsf{G/H}$. Since in the cases under consideration this restriction is always satisfied, it becomes possible to apply this method to find explicit expressions for the adiabatic phase and the Berry potential in terms of the coordinates of the parameter space (Sec. V). We discover that the Berry potentials may be expressed in terms of the fundamental Kähler potentials of the homogeneous Kähler manifold $\mathsf{G/H}$. The Bando, Kuramoto, Maskawa, and Uehara[4] method is used to express the fundamental Kähler potentials in terms of the coordinates of the parameter space. Thus, the explicit expressions for the Berry connections in terms of the complex parameters are found. This result will be formulated as a theorem in Sec. V. It will be demonstrated in Sec. VI that the action of the group G on the Kähler manifold $\mathsf{G/H}$ induces the gauge transformation of the Berry potentials. Once explicit forms for

the Berry connections are obtained, the Berry curvature and the Berry geometrical phase are easily derived (Sec. VI). We illustrate the general procedure on a specific case of the $SU(3)$ group (Sec. VII). The paper is concluded in Sec. VIII.

II. PRELIMINARIES AND NOTATIONS

Assume that a matrix irreducible representation of a compact semi-simple Lie group G of order n and rank r is given. Let $\mathcal{G}$ be the Lie algebra of G in which $\mathcal{H}\in\mathcal{G}$ denotes its Cartan subalgebra. A canonical Cartan–Weyl basis $\{h_j, e_\alpha, e_{-\alpha}\}$ in $\mathcal{G}$ is introduced, where $j=1,\ldots,r \equiv \operatorname{rank}\mathcal{G}$, and $\{\alpha\}\in\mathbf{\Delta}^+_{\mathcal{G}}$ are the positive roots of $\mathcal{G}$. (The definitions and properties of semi-simple Lie algebras and Lie groups may be found in Gilmore.[14]) The number of the positive roots is $n_+=\frac{1}{2}[n-r]$. The canonical basis of the Lie algebra $\mathcal{G}$ may be chosen so that the commutation relations will be written in the following standard form:

$$\begin{gathered}[h_i h_j]=0 \quad , \quad [h_i, e_\alpha]=\alpha_i e_\alpha, \\ [e_\alpha, e_{-\alpha}]=\sum_{j=1}^{r} \alpha_i h_i \quad , \quad [e_\alpha, e_\beta]=\chi(\alpha,\beta) e_{\alpha+\beta}.\end{gathered} \tag{5}$$

Here $\chi(\alpha,\beta)$ is a function on the root lattice which vanishes if $\alpha+\beta\notin\Delta^+_{\mathcal{G}}$. Choosing primitive roots $\boldsymbol{\gamma}_j$, $j=1,\ldots,r$, the fundamental weights $\boldsymbol{\omega}_j$, $j=1,\ldots,r$ are determined from the equation

$$(\boldsymbol{\omega}_i\cdot\boldsymbol{\gamma}_i)=\frac{\delta_{ij}}{2}(\boldsymbol{\gamma}_i\cdot\boldsymbol{\gamma}_i). \tag{6}$$

For any unitary irreducible group representation its dominant weight $\mathbf{l}$ is given by a sum of the fundamental weights with non-negative integer coefficients:

$$\mathbf{l}=\sum_{j=1}^{r} l_j\boldsymbol{\omega}_j=\sum_{j=1}^{r} \tilde{l}_j\mathbf{x}_j, \tag{7}$$

where $(\tilde{l}_1,\ldots,\tilde{l}_r)$ are the coordinates of the dominant weight $\mathbf{l}$ in the root space of the Lie algebra in which an orthogonal coordinate system is chosen. (Here and afterwards boldface is used to denote vectors in the root space of the Lie algebra.) The set $\{\mathbf{x}_j, j=1,\ldots,r\}$ denotes the unit basis vector of this coordinate system.

We are interested in the cyclic adiabatic evolution of the weight eigenket $\psi_{\mathbf{l}}$ which is defined by the following equation:

$$h_j\psi_{\mathbf{l}}=\tilde{l}_j\psi_{\mathbf{l}}, \quad j=1,\ldots,r. \tag{8}$$

(For convenience we are dealing with the weight eigenket $\psi_{\mathbf{l}}$, corresponding to the dominant weight $\mathbf{l}$ here. The adiabatic evolution of an eigenket corresponding to an arbitrary weight may be considered in the same manner.) This adiabatic evolution will be determined by the Schrödinger equation with a Lie algebra valued Hamiltonian $b(s)\in\mathcal{G}$ given in the irreducible representation $(l_1,\ldots, l_r)$ of $\mathcal{G}$:

$$i\dot{\psi}(s)=\tau b(s)\psi(s), \quad \psi(0)=\psi_{\mathbf{l}}. \tag{9}$$

[The physical time t is replaced here by the scale time $s=t/\tau, s\in[0,1]$. The adiabatic limit is $\tau\to\infty$. The Hamiltonian $b(s)$ is assumed to depend smoothly on $s\in[0,1]$.] The cyclic evolution means that $b(s)$ takes the same values at the ends of the segment $[0,1]$. In order for the initial state $\psi_{\mathbf{l}}$ defined by Eq. (8) to be an eigenstate of the Hamiltonian $b(s)$, we demand that $b(0)=b(1)\in\mathcal{H}$.

The problem (9) can be written in terms of the Cartan–Maurer one-form:

$$dg\,g^{-1}=-i\tau b(s)ds,\quad g(s)\in \mathsf{G},\quad b(s)\in\mathcal{G}. \tag{10}$$

Here $g(s)$ is the evolution operator in the irreducible representation $(l_1,\ldots,l_r)$ of the Lie group G, $\psi(s)=g(s)\psi_{\mathbf{l}}$ and $g(0)=e$ is the unit element of the compact group G. Geometrically, the given Lie algebra Hamiltonian $b(s)$ determines a closed smooth curve in the Lie algebra $\mathcal{G}$ which begins and ends in the Cartan subalgebra $\mathcal{H}$ of $\mathcal{G}$. To solve Eq. (10) means to find the corresponding curve on the group manifold G.

For any given s the Hamiltonian $b(s)\in\mathcal{G}$ may be reduced to the Cartan subalgebra $\mathcal{H}$,

$$b(s)=g_1(s)\beta(s)g_1^{-1}(s),\quad \beta(s)\in\mathcal{H}. \tag{11}$$

It is useful to assume that the Cartan subalgebra element β does not depend on the parameter $s\in[0,1]$, i.e., the eigenvalues of the Hamiltonian $b(s)$ are constants on the segment under consideration. For example, the $su(2)$ Lie algebra Hamiltonian given by Eq. (2) has two constant eigenvalues ± 1 if $\mathbf{J}=\boldsymbol{\sigma}$, $(\sigma_1,\sigma_2,\sigma_3)$ are Pauli matrices. When $b(s)$ determines the closed curve that begins and ends in $\mathcal{H}$, $g_1(0)=g_1(1)=e$.

We look for an unknown group element as the following product:

$$g(s)=g_2(s)h(s),\quad h(s)\in\mathsf{H},\quad g_2(s)\in\mathsf{G}. \tag{12}$$

Inserting (12) to Eq. (10) we obtain

$$dh(s)h^{-1}(s)=-i\tau g_2^{-1}(s)g_1(s)\beta(s)g_1^{-1}(s)g_2(s)-dg_2(s)g_2^{-1}(s). \tag{13}$$

In the adiabatic limit $(\tau\to\infty)$ we neglect by the second part of the right-hand side of Eq. (13). It gives as a zeroth-order approximation,

$$h^{(0)}(s)=\exp(-i\tau\beta s),\quad \beta=\sum_{j=1}^{r}\beta^j h_j, \tag{14}$$

$$g_2^{(0)}(s)=g_1(s)h^{(1)}(s),\quad h^{(1)}(s)\in\mathsf{H}. \tag{15}$$

The element $h^{(1)}(s)$ (which is arbitrary in the zeroth-order approximation) should be chosen in such a way that the form $dg_2(s)g_2^{-1}(s)$ will be as minimal as possible. Then we find

$$h^{(1)}(s)=\exp(-i\mathcal{Q}(s)),\quad \mathcal{Q}(s)=\sum_{j=1}^{r}\mathcal{Q}^j(s)h_j, \tag{16}$$

$$\mathcal{Q}^j(s)=-i\int_0^s \mathrm{Tr}\left(g_1^{-1}(\tilde{s})\frac{dg_1(\tilde{s})}{d\tilde{s}}h_j\right)d\tilde{s}. \tag{17}$$

Equations (12), (14), (15), (16), (17) determine evolution operator $g(s)$ in the adiabatic limit:

$$g(s)=g_1(s)\exp(-i\tau\beta s)\exp(-i\mathcal{Q}(s)). \tag{18}$$

After a cyclic adiabatic evolution $(s=1)$, the eigenket $\psi_{\mathbf{l}}$ is transformed according to the formula

$$\psi_{\mathbf{l}}\rightsquigarrow g(1)\psi_{\mathbf{l}}=\exp(-i\tau\beta)\exp(-i\mathcal{Q}(1))\psi_{\mathbf{l}}, \tag{19}$$

where we have taken into account that $g_1(1)=e$. Let us introduce the r-dimensional vectors in the root space of the Lie algebra $\mathcal{G}$:

$$\boldsymbol{\beta}=\sum_{j=1}^{r}\beta^j\mathbf{x}_j,\quad \mathbf{Q}=\sum_{j=1}^{r}\mathcal{Q}^j(1)\mathbf{x}_j. \tag{20}$$

Using Eq. (8) and explicit forms for the elements β [Eq. (14)] and $\mathcal{Q}$ [Eq. (16)] we finally obtain that the adiabatic phase factor Θ acquired by the quantum state $\psi_{\mathbf{l}}$ is given by the scalar product of the dominant weight vector $\mathbf{l}$ [Eq. (7)] on the sum of the vectors $\mathbf{Q}$ and $\boldsymbol{\beta}$:

$$\psi_{\mathbf{l}} \to \exp(-i\Theta)\psi_{\mathbf{l}}, \quad \Theta = \mathbf{l}\cdot\boldsymbol{\beta} + \mathbf{l}\cdot\boldsymbol{\mathcal{Q}}. \tag{21}$$

While the first term in the above expression for the adiabatic phase Θ is associated with the dynamical phase, the second term $\mathbf{l}\cdot\boldsymbol{\mathcal{Q}}$ is the geometrical phase Ω, defined as

$$\Omega \equiv \mathbf{l}\cdot\boldsymbol{\mathcal{Q}}. \tag{22}$$

As we can see from Eq. (21), the Berry geometrical phase depends on integers $l_1, \ldots, l_r$ which determine the dominant weight $\mathbf{l}$ [Eq. (7)], and characterize the irreducible representation of the evolution group under consideration.

III. GEOMETRICAL PHASE FOR *SU*(2)

Let us discuss a familiar example of Berry[9] for a spin in a time-dependent magnetic field using the machinery that admits generalization to any compact Lie group. The Hamiltonian of Berry's example is given by

$$b(s) = \mu \mathbf{B}(s)\cdot\mathbf{J}, \tag{23}$$

where $\mathbf{B}(s) = B\mathbf{n}(s)$ is the vector of the magnetic field, μ is the particle magnetic momentum, and $\mathbf{J}$ is the angular momentum. This example can be understood as a case when the Hamiltonian $b(s)$ takes values on a closed curve in the Lie algebra of the $SU(2)$. The generators of the group $SU(2)$ are the Pauli matrices:

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{24}$$

The elements of the canonical basis of the Lie algebra $SU(2)$ in the fundamental (spinor) representation are

$$E_1 = \frac{1}{2}(\sigma_1 + i\sigma_2); \quad E_2 = \frac{1}{2}(\sigma_1 - i\sigma_2); \quad H = \frac{1}{\sqrt{2}}\sigma_3. \tag{25}$$

Correspondingly, the canonical commutation relations for the $SU(2)$ Lie algebra have the following form:

$$[e_1, e_2] = \sqrt{2}h, \quad [h, e_1] = \sqrt{2}e_1, \quad [h, e_2] = -\sqrt{2}e_2. \tag{26}$$

The rank of the Lie algebra $SU(2)$ is equal to one, $r=1$. The root space is one-dimensional, R^1, with two opposite roots $\pm\boldsymbol{\alpha} = \pm\sqrt{2}\mathbf{x}$, and the primitive root is $\boldsymbol{\gamma} = \boldsymbol{\alpha}$. The fundamental weight $\boldsymbol{\omega}$ is determined by Eq. (6), $\boldsymbol{\omega} = \frac{1}{2}\boldsymbol{\alpha}$. An arbitrary irreducible representation is defined by the dominant weight,

$$\mathbf{l} = l\boldsymbol{\omega} = \frac{l}{\sqrt{2}}\mathbf{x}, \quad l = 0, \pm 1, \pm 2, \ldots . \tag{27}$$

Consider the cyclic adiabatic evolution of the eigenket $\psi_{\mathbf{l}}$ which is the eigenvector of the following eigenvalue problem:

$$h\psi_{\mathbf{l}}=\frac{l}{\sqrt{2}}\psi_{\mathbf{l}},\quad l=0,\pm 1,\pm 2,\ldots\ . \tag{28}$$

The above equation means that the state $\psi_{\mathbf{l}}$ corresponds to the dominant weight $\mathbf{l}$. In accordance with Eq. (21) after the cyclic adiabatic evolution the state $\psi_{\mathbf{l}}$ acquires the geometrical phase factor Ω [Eq. (22)]. The geometric part of the adiabatic phase is determined by a scalar product of the dominant weight [Eq. (27)], and the vector $\boldsymbol{\mathcal{Q}}$ in the root space with the components given by Eq. (17). Thus, in order to obtain the geometrical phase we have to express the trace in Eq. (17) in terms of the Hamiltonian parameters. This trace depends on parameters of $g_1(s)$ only [see the decomposition of the Hamiltonian, Eq. (11)]. The parametrization of $g_1(s)\in SU(2)/U(1)$ should be introduced in such a way that the explicit calculation of the trace in Eq. (17) would be as simple as possible.

The desired (complex) parametrization of a representative $g_1(s)$ of the coset space $SU(2)/U(1)$ is obtained by the following decomposition:

$$g_1(s)=g_1(z(s),\overline{z}(s))=u(z)g_-(z,\overline{z}),\quad u(z)=\exp(ze_1). \tag{29}$$

The element $g_-(z,\overline{z})$ in the above expression is represented as the product,

$$g_-(z,\overline{z})=\exp(y(z,\overline{z})e_2)\exp(\kappa(z,\overline{z})h). \tag{30}$$

The explicit forms for the functions $y(z,\overline{z}),\kappa(z,\overline{z})$ are obtained from the condition that the element $g_1(z(s),\overline{z}(s))$ should be unitary. It gives

$$y(z,\overline{z})=-\frac{\overline{z}}{1+z\overline{z}},\quad \kappa(z,\overline{z})=\frac{1}{\sqrt{2}}\ln(1+z\overline{z}). \tag{31}$$

The explicit expression for the group element $g_1(z(s),\overline{z}(s))$ enables us to calculate the trace in the integral of Eq. (17):

$$\mathrm{Tr}\left(g_1^{-1}(s)\frac{dg_1(s)}{ds}h\right)=\dot{\overline{z}}\frac{\partial}{\partial\overline{z}}\kappa(z,\overline{z})-\dot{z}\frac{\partial}{\partial z}\kappa(z,\overline{z}). \tag{32}$$

In the above equation we have denoted $\dot{z}\equiv dz(s)/ds$,$\dot{\overline{z}}\equiv d\overline{z}(s)/ds$. The Berry connection A_s may be introduced and expressed in terms of the complex coordinates of the coset space $SU(2)/U(1)$:

$$A_s=\frac{il}{2}\left(\frac{\dot{z}\overline{z}-z\dot{\overline{z}}}{1+z\overline{z}}\right). \tag{33}$$

Using Stokes' theorem we determine the Berry geometrical phase factor [Eq. (22)]:

$$\Omega=-il\int\int\frac{dz\wedge d\overline{z}}{(1+z\overline{z})^2},\quad l=0,\pm 1,\pm 2,\ldots\ . \tag{34}$$

In order to compare Eq. (34) with the original Berry result[9] for the spin procession in the time-dependent magnetic field, use the stereographic projection of the two-dimensional sphere with the unit radius:

$$|z|=\cot\theta/2,\quad \arg z=\varphi. \tag{35}$$

Then the geometrical phase factor is equal to

$$\Omega=\frac{l}{2}\int\int\sin\theta\, d\theta\wedge d\varphi,\quad l=0,\pm 1,\pm 2,\ldots\ . \tag{36}$$

It is this result that was obtained by Berry.[9]

For a generalization to more complicated evolution groups the following two observations are important. First, the geometric phase is determined by the torus function $\kappa(z,\overline{z})$ only, appearing in the decomposition Equations (29), (30). The second is that the torus function $\kappa(z,\overline{z})$ is the Kähler potential of the Kähler manifold $SU(2)/U(1)$.

IV. COMPLEX PARAMETRIZATION OF THE HAMILTONIAN PARAMETER SPACE

The given Lie algebra valued Hamiltonian $b(s)\in\mathcal{G}$ varies adiabatically through a circuit C in the parameter space which is the homogeneous group manifold G/H. Indeed, $b(s)$ depends on s only through the group element $g_1(s)$ [Eq. (11)]. The Hamiltonian $b(s)$ decomposition, Eq. (11), is invariant under $g_1(s)\rightarrow g_1(s)h_1$, $\forall h_1\in\mathsf{H}$, so $g_1(s)$ must be chosen as a representative of the corresponding equivalence class. Thus, there is a gauge freedom in the diagonalization process [Eq. (11)], and the Cartan subgroup $\mathsf{H}\in\mathsf{G}$ is the group of the gauge transformations. Geometrically, G is described as a principal fiber bundle with the Cartan subgroup H as the standard fiber and G/H is the base coset space. According to Borel's theorem,[15] the necessary and sufficient condition for the coset space G/H (where G is a compact semi-simple group, and H is a closed subgroup of G) to be a homogeneous Kähler manifold is that H be the centralizer of a torus in G. A torus means a direct product of any $U(1)$ subgroup of H and the centralizer means a subgroup which consists of all G elements commutative with that torus elements. As it may be seen from Sec. II, in the case under consideration conditions of the Borel theorem are satisfied (H is a Cartan subgroup commuting with a torus), so the Hamiltonian parameter is a homogeneous Kähler manifold. Then the complex parametrization on G/H may be introduced, and the explicit expression for the geometrical factor Ω may be found in terms of the (complex) coordinates of the parameter space G/H.

The desired complex parametrization of the homogeneous group manifold G/H is introduced by the complex parametrization of the group element g_1, which determines decomposition of the Hamiltonian $b(s)$ [Eq. (11)]. Namely, given the canonical basis, the Lie algebra $\mathcal{G}$ is split into three subalgebras, $\mathcal{G}=\mathcal{H}\oplus\mathcal{B}_+\oplus\mathcal{B}_-$, ($\mathcal{B}_+,\mathcal{B}_-$ are called Borel subalgebras), corresponding to three subsets of the basis elements $\{e_{-\alpha}\},\{h_j\},\{e_\alpha\}$. Respectively, the Lie algebra $\mathcal{B}_+(\mathcal{B}_-)$ generates a nilpotent Borel subgroup $\mathsf{B}_+(\mathsf{B}_-)\subset\mathsf{G}^c$ (G^c means the complexification of the group G). The element g_1 has a unique (left) Mackey decomposition,

$$g_1=ug_-,\quad u\in\mathsf{B}_+,\quad g_-\in\mathsf{G}/\mathsf{B}_+. \tag{37}$$

(Note that in order to get u for any given g_1 one has to impose the condition that $g_-=u^{-1}g_1$ has no part in B_+. That would determine u completely.) The complex parameters which can be introduced in G/H correspond to the positive roots of $\mathcal{G}$,

$$u(z)=\exp\left(\sum_{\alpha\in\Delta_{\mathcal{G}}^+} z^\alpha e_\alpha\right),\quad z^\alpha\in\mathcal{C}. \tag{38}$$

$u(z)$ is an element of a nilpotent group and its matrix representions are polynomials of z^α. The local form (38) for $u(z)$ is valid in a neighborhood of the point $z^\alpha=0$, i.e., the origin of the coordinate system in G/H. The origin is related to the choice of coordinates. A transition to other domains of G/H covering the Kähler manifold G/H may be performed by the group transformation.

Given $u(z)$, $g_-(z,\overline{z})$ will acquire the following form:

$$g_-(z,\overline{z})=v^+(z,\overline{z})k(z,\overline{z}),\quad v(z,\overline{z})\in\mathsf{B}_+,\quad k(z,\overline{z})\in\mathsf{H}. \tag{39}$$

The elements $v^+(z,\overline{z})$, $k(z,\overline{z})$ are expressed as exponentials of the corresponding Lie algebra elements:

$$v^+(z,\overline{z})=\exp\left(\sum_{\alpha\in\Delta_{\mathcal{G}}^+} y^\alpha(z,\overline{z})e_{-\alpha}\right),\quad k(z,\overline{z})=\exp\left(\sum_{i=1}^{r}\kappa^i(z,\overline{z})h_i\right). \tag{40}$$

For a particular $u(z)\in \mathsf{B}_+$ the functions $y^\alpha(z,\overline{z})$ and $\kappa^i(z,\overline{z})$ may be determined when the group element g_1 is unitary:

$$g_1^+=g_1^{-1}\rightarrow v^+kk^+v=(u^+u)^{-1}. \tag{41}$$

v is obtained from the (right) Mackey decomposition of $(u^+u)^{-1}$, and the explicit forms for the functions $y_\alpha(z,\overline{z})$ may be found. As soon as v is given, one turns to the calculation of k from the equation

$$kk^+=(vu^+uv^+)^{-1}\in \mathsf{H}. \tag{42}$$

The functions $\kappa^i(z,\overline{z})$ are especially important as we shall see below. It will be shown in Sec. IV that the functions $\kappa^i(z,\overline{z})$ completely determine the Berry potentials when G is a compact evolution group, and the Hamiltonian parameter space is $\mathsf{G/H}$. These functions are linearly related with the fundamental Kähler potentials $K^i(z,\overline{z})$ of the Kähler manifold $\mathsf{G/H}$ under considerations:

$$K^i(z,\overline{z})=-2\sum_{j=1}^{r}\kappa^j(z,\overline{z})\mathrm{Tr}(h_j\eta_i). \tag{43}$$

The formula (43) was obtained by Itoh, Kugo, and Kunimoto.[16] Here η_i are the projection matrices introduced by Bando, Kuratomo, Maskawa, and Uehara.[4] The projection matrices exist in any matrix representation of G and correspond to elements of the Cartan subalgebra $h_j\in\mathcal{H}$. The basic properties of the projection matrices are[4]

$$\eta_j=\eta_j^+\quad \eta_j^2=\eta_j\quad \eta_j\hat{h}_k=\hat{h}_k\eta_j,\quad \forall j,k=1,\ldots,r,$$

$$\eta_j\hat{e}_{-\alpha}\eta_j=\hat{e}_{-\alpha}\eta_j,\quad \eta_j\hat{e}_\alpha\eta_j=\eta_j\hat{e}_\alpha. \tag{44}$$

(The overcaret stands for the matrix representation.) All η_j are commuting with each other. For any representation of G, where $\hat{h}_j$ are diagonal, all η_j are also diagonal. The explicit forms of η_j satisfying Eq. (44) may be found (Bando, Kuratomo, Maskawa, and Uehara[4]). For the irreducible representation under consideration the functions $\kappa^j(z,\overline{z}),j=1,\ldots,r$ may be expressed linearly in terms of the fundamental Kähler potentials $K^j(z,\overline{z}),j=1,\ldots,r$ [Eq. (43)]. In its turn a suitable method of construction of the fundamental Kähler potentials is given by Bando, Kuratomo, Maskawa, and Uehara[4] (see also Itoh, Kugo, and Kunitomo[16]). A number of particular examples is considered by Marinov and Bar-Moshe[6,7] in relation to the geometric quantization on homogeneous compact Kähler manifolds.

A technique for constructing the fundamental Kähler potentials may be described as follows. Once the projection matrices η_j are obtained from Eqs. (44), the projected determinant is defined for any matrix M as

$$\det{}_{\eta_j}M\equiv\det(\eta_jM\eta_j+I-\eta_j). \tag{45}$$

For any projection matrix η_j, a fundamental Kähler potential $K^j(z,\overline{z})$ is constructed from the fundamental represenation for the element $u(z)$ [Eq. (38)] of the nilpotent Borel subgroup B_+,

$$K^j(z,\overline{z})\equiv\ln\det{}_{\eta_j}(u(z)^+u(z)). \tag{46}$$

Note that the fundamental Kähler potential $K^j(z,\overline{z})$ is not a global function on $\mathsf{G/H}$, except for cases where $\mathsf{G/H}$ has a trivial topology. However, the manifold $\mathsf{G/H}$ may be covered with com-

plex coordinate neighborhoods. A transition from one neighborhood to another may be given by the group transformation. If the group G acts holomorphically on G/H, $z\to gz, \forall g\in \mathsf{G}$, the fundamental Kähler potentials (45) are transformed as

$$K^j(gz,\overline{gz})=K^j(z,\overline{z})+\Phi^j(z,g)+\overline{\Phi^j(z,g)}, \tag{47}$$

where $\Phi^j(z,g)$ are locally holomorphic functions of z^α, $\alpha=1,\ldots,(n-r)/2$. These functions must satisfy the following cocycle condition:

$$\Phi^j(z,g_2g_1)=\Phi^j(g_2z,g_1)+\Phi^j(z,g_2), \quad \forall g_1,g_2\in \mathsf{G}, \tag{48}$$

which results from the group property $z\to g_2(g_1z)=(g_2g_1)z$.

V. EXPRESSION OF BERRY'S CONNECTION IN TERMS OF THE FUNDAMENTAL KÄHLER POTENTIALS

With all the preliminary steps completed, we are in a position to formulate the main result of this work.

Theorem: Suppose that the cyclic adiabatic evolution of the dominant weight eigenket $\psi_{\mathbf{l}}$ defined by Eq. (8) is determined by the Schrödinger equation [Eq. (9)]. Let the Hamiltonian parameter space be a compact homogeneous Kähler manifold G/H, where G is the compact evolution group, and H its Cartan subgroup. Then the geometrical phase factor Ω acquired by the quantum state $\psi_{\mathbf{l}}$ is

$$\Omega=\int_0^1 A_s\,ds, \tag{49}$$

where the Berry connection A_s is completely determined in terms of the fundamental Kähler potentials of the parameter space G/H. Explicitly, when the local complex parametrization $\{z^\alpha,\overline{z^\alpha},\alpha=1,\ldots,(n-r)/2\}$ on G/H is introduced,

$$A_s=\mathbf{l}\cdot\mathbf{A}(z,\overline{z}), \quad \mathbf{A}(z,\overline{z})=\mathcal{L}_{z,\overline{z}}\boldsymbol{\kappa}(z,\overline{z}). \tag{50}$$

$\mathbf{A}(z,\overline{z})$ and $\boldsymbol{\kappa}(z,\overline{z})$ are the vectors in the root space of the Lie algebra of G given in the orthonormal basis $\{\mathbf{x}_j,j=1,\ldots,r\}$,

$$\boldsymbol{\kappa}(z,\overline{z})=\sum_{j=1}^{r}\kappa^j(z,\overline{z})\mathbf{x}_j, \quad \mathbf{A}(z,\overline{z})=\sum_{j=1}^{r}A^j(z,\overline{z})\mathbf{x}_j. \tag{51}$$

$\mathcal{L}_{z,\overline{z}}$ is the (Hermitian) differential operator:

$$\mathcal{L}_{z,\overline{z}}=i\sum_{\alpha,\overline{\alpha}=1}^{(n-r)/2}(\dot{z}^\alpha\partial_\alpha-\dot{z}^{\overline{\alpha}}\partial_{\overline{\alpha}}), \tag{52}$$

where $\dot{z}\equiv dz(s)/ds$, $z^{\overline{\alpha}}\equiv\overline{z^\alpha}$, $\partial_\alpha\equiv\partial/dz^\alpha$, $\partial_{\overline{\alpha}}\equiv\partial/dz^{\overline{\alpha}}$. The real functions $\kappa^j(z,\overline{z})$ define the Cartan subgroup element $k(z,\overline{z})\in \mathsf{H}$ [Eq. (40)] under (left) Mackey decomposition of a representative of the coset space G/H [Eqs. (37)–(40)]. These functions are linearly connected with the fundamental Kähler potentials $K^j(z,\overline{z})$ [Eq. (43)].

Proof: The geometric phase Ω is given by the scalar product of the dominant weight $\mathbf{l}$ and the vector $\boldsymbol{\mathcal{Q}}$ [Eq. (21)]. The coordinates of the vector $\boldsymbol{\mathcal{Q}}$ in the root space of the Lie algebra $\mathcal{G}$ corresponding to the evolution group G are determined by Eq. (17). When the local complex parametrization on the coset space G/H is introduced, the components $\mathcal{Q}^j$ of the vector $\boldsymbol{\mathcal{Q}}$ may be represented as a sum of two integrals:

$$\mathcal{Q}^j = -i \sum_{\alpha,\bar{\alpha}=1}^{(n-r)/2} \left\{ \int_C \mathrm{Tr}(g_1^{-1}\partial_\alpha g_1 h_j) dz^\alpha + \int_C \mathrm{Tr}(g_i^{-1}\partial_{\bar{\alpha}} g_1 h_j) dz^{\bar{\alpha}} \right\}. \tag{53}$$

The group element $g_1(z,\bar{z})$ which is the representative of the coset space G/H is decomposed (see Sec. III) as

$$g_1(z,\bar{z}) = u(z) v^+(z,\bar{z}) k(z,\bar{z}), \tag{54}$$

where $u(z) \in \mathsf{B}_+$, $v^+(z,\bar{z}) \in \mathbf{B}_-$, $k(z,\bar{z}) \in \mathsf{H}$ are given by Eqs. (38), (40). Let us recall that

$$k(z,\bar{z}) = \exp\left(\sum_{j=1}^{r} \kappa^j(z,\bar{z}) h_j \right).$$

It may be shown (see, for example, Itoh, Kugo, and Kunimoto[16]) that

$$\mathrm{Tr}\,(g_1^{-1}\partial_\alpha g_1 h_j) = -\partial_\alpha \kappa^j(z,\bar{z}), \quad \mathrm{Tr}(g_1^{-1}\partial_{\bar{\alpha}} g_1 h_j) = \partial_{\bar{\alpha}} \kappa^j(z,\bar{z}). \tag{55}$$

Indeed, noting that

$$\partial_{\bar{\alpha}} g_1(z,\bar{z}) = u(z)\partial_{\bar{\alpha}}(v^+(z,\bar{z}) k(z,\bar{z})), \tag{56}$$

we find that

$$\mathrm{Tr}\,(g_1^{-1}\partial_\alpha g_1 h_j) = \mathrm{Tr}(h_j (v^+(z,\bar{z}))^{-1} \partial_{\bar{\alpha}}(v^+(z,\bar{z}))) + \sum_{i=1}^{r} \partial_\alpha(\kappa^i(z,\bar{z}))\mathrm{Tr}(h_i h_j). \tag{57}$$

The expression $(v^+(z,\bar{z}))^{-1}\partial_{\bar{\alpha}}(v^+(z,\bar{z}))$ produces only terms belonging to the Borel subalgebra $\mathcal{B}_-$. As a consequence, the first term in the above equation equals zero. Using the orthogonality condition for the Cartan subalgebra canonic basis elements,

$$\mathrm{Tr}(h_i h_j) = \delta_{ij}, \tag{58}$$

we obtain

$$\mathrm{Tr}\,(g_1^{-1}\partial_{\bar{\alpha}} g_1 h_j) = \partial_{\bar{\alpha}} \kappa^j(z,\bar{z}). \tag{59}$$

In order to prove the first equation in (55) we use

$$\begin{aligned} g_1^{-1}\partial_\alpha g_1 = g_1^+ \partial_\alpha (g_1^+)^{-1} &= k^+ v u^+ \partial_\alpha ((u^+)^{-1} v^{-1} (k^+)^{-1}) \\ &= k^+ v \partial_\alpha (v^{-1}(k^+)^{-1}). \end{aligned} \tag{60}$$

Afterwards, we proceed with the proof as in the previous case.

From Eqs. (53), (55) we find

$$\mathcal{Q}^j = i \sum_{\alpha,\bar{\alpha}=1}^{(n-r)/2} \int_0^1 (\dot{z}^\alpha \partial_\alpha - \dot{z}^{\bar{\alpha}} \partial_{\bar{\alpha}}) \kappa^j(z,\bar{z}) ds \equiv \int_0^1 A^j(z,\bar{z}) ds. \tag{61}$$

Thus, the vector in the root space of $\mathcal{G}$,

$$\mathbf{A}(z,\bar{z}) = i \sum_{\alpha,\bar{\alpha}=1}^{(n-r)/2} (\dot{z}^\alpha \partial_\alpha - \dot{z}^{\bar{\alpha}} \partial_{\bar{\alpha}}) \boldsymbol{\kappa}(z,\bar{z}) \equiv \mathcal{L}_{z,\bar{z}} \boldsymbol{\kappa}(z,\bar{z}), \tag{62}$$

is introduced; the Berry connection and the Berry geometrical phase are determined by Eqs. (49), (50) respectively. □

In the next section we use this result to demonstrate that the holomorphic action of the evolution group G on the Hamiltonian parameter space G/H induces the gauge transformation of the Berry potentials. In addition, the Berry curvature and the Berry geometrical phase will be obtained.

VI. GAUGE TRANSFORMATION AND BERRY CURVATURE

Consider the transformation of the vector $\mathbf{A}(z,\overline{z})$ (in the root space) under the holomorphic action of the group G on the homogeneous Kähler G/H. As soon as the fundamental Kähler potentials $K^j(z,\overline{z}), j=1,\ldots,r$ are transformed in accordance with Eq. (47), the vector $\boldsymbol{\kappa}(z,\overline{z})$ changes in a similar fashion, i.e.,

$$\boldsymbol{\kappa}(z,\overline{z})\to\boldsymbol{\kappa}(gz,\overline{gz})=\boldsymbol{\kappa}(z,\overline{z})+\boldsymbol{\phi}(g,z)+\overline{\boldsymbol{\phi}(g,z)}. \tag{63}$$

Indeed, given the decomposition of the coset space representative [Eqs. (37)–(40)], the action of an arbitrary group element $g_2\in\mathsf{G}$ on the coset space G/H is defined (by Coleman, Wess, and Zumino[17]) as

$$g_2u(z)=u(g_2z)g_-(z,g_2), \tag{64}$$

and g_2z is a rational function of z. Once the nonlinear realization of the group action on the coset space G/H is determined [Eq. (64)], the transformation law (63) may be proved using the Mackey-type decomposition of the product $g_1\cdot g_2$ [where $g_1\in\mathsf{G/H}$ is given by Eqs. (37)–(40)] (for further details see Itoh, Kugo, and Kunimoto.[16] The change of the real vector $\boldsymbol{\kappa}(z,\overline{z})$ [Eq. (63)] under the holomorphic action of the group on its coset space leads to the gauge transformation of the vector $\mathbf{A}(z,\overline{z})$:

$$\mathbf{A}(z,\overline{z})=\mathcal{L}_{z,\overline{z}}\boldsymbol{\kappa}(z,\overline{z})\to\mathbf{A}(gz,\overline{gz})=\mathbf{A}(z,\overline{z})+d\mathbf{W}(z,\overline{z}), \tag{65}$$

where the real vector $\mathbf{W}(z,\overline{z})$ is defined in terms of the vectors $\boldsymbol{\phi}(g,z),\overline{\boldsymbol{\phi}(g,z)}$:

$$\mathbf{W}(z,\overline{z})\equiv i(\boldsymbol{\phi}(g,z)-\overline{\boldsymbol{\phi}(g,z)}). \tag{66}$$

Respectively, the Abelian Berry connection A_s defined by Eq. (50) is transformed as

$$\begin{gathered}A_s(z,\overline{z})\to A_s(gz,\overline{gz})=A_s(z,\overline{z})+dW(z,\overline{z}),\\ W(z,\overline{z})\equiv\mathbf{l}\cdot\mathbf{W}(z,\overline{z}).\end{gathered} \tag{67}$$

Note that the expression (49) for Ω may be rewritten as

$$\Omega=\sum_{\alpha=1}^{(n-r)/2}\int_C A_\alpha(z,\overline{z})dz^\alpha+\sum_{\alpha=1}^{(n-r)/2}\int_C A_{\overline{\alpha}}(z,\overline{z})dz^{\overline{\alpha}}, \tag{68}$$

where

$$\begin{gathered}A_\alpha(z,\overline{z})\equiv i\partial_\alpha(\mathbf{l}\cdot\boldsymbol{\kappa}(z,\overline{z})),\\ A_{\overline{\alpha}}(z,\overline{z})\equiv-i\partial_{\overline{\alpha}}(\mathbf{l}\cdot\boldsymbol{\kappa}(z,\overline{z})).\end{gathered} \tag{69}$$

Under the holomorphic action of the group G on the homogeneous Kähler manifold G/H, $A_\alpha(z,\overline{z})$, $A_{\overline{\alpha}}(z,\overline{z})$ transform as

$$A_\alpha(z,\overline{z})\to A_\alpha(gz,\overline{gz})=A_\alpha(z,\overline{z})+i\partial_\alpha(\mathbf{l}\cdot\boldsymbol{\phi}(g,z)),$$

$$A_{\bar{\alpha}}(z,\bar{z}) \to A_{\bar{\alpha}}(gz,\overline{gz}) = A_{\bar{\alpha}}(z,\bar{z}) - i\partial_{\bar{\alpha}}(\mathbf{l}\cdot\bar{\boldsymbol{\phi}}(g,z)). \tag{70}$$

Using the Stokes theorem, we obtain the expression for the Berry geometrical factor in terms of the surface integral,

$$\Omega = \int_S F, \quad F = \sum_{\alpha,\beta=1}^{(n-r)/2} \frac{\partial^2 K^{(\mathbf{l})}(z,\bar{z})}{\partial z^\alpha \partial \bar{z}^\beta} dz^\alpha \wedge d\bar{z}^\beta, \tag{71}$$

where

$$K^{(\mathbf{l})}(z,\bar{z}) = 2(\mathbf{l}\cdot\boldsymbol{\kappa}(z,\bar{z})), \tag{72}$$

and S is any oriented surface in the parameter space G/H with $\partial S = C$. As it may be seen from Eqs. (63), (71), the Berry curvature F is invariant under the gauge transformation [Eq. (67)] induced by the holomorphic group action on the parameter space G/H.

A simple way to calculate the vector $\boldsymbol{\kappa}(z,\bar{z})$ which determines the Berry connection and the Berry curvature is to use Eq. (43). This formula connects the vector $\boldsymbol{\kappa}(z,\bar{z})$ with the fundamental Kähler potentials given by Eqs. (44)–(46).

VII. *SU*(3) ADIABATIC EVOLUTION

The Cartan subgroup of the $SU(3)$ group is $U(1)\times U(1)$, so the Berry geometrical phase factor will be determined by the geometry of the Flag manifold $SU(3)/U(1)\times U(1)$. The canonical basis of $SU(3)$ Lie algebra is introduced with the help of the eight Gell-Mann generators:

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

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{73}$$

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

Then the elements of the canonical Cartan–Weyl basis in the fundamental three-dimensional representation are given by

$$E_{12} = 1/2(\lambda_1 + i\lambda_2); \quad E_{23} = 1/2(\lambda_6 + i\lambda_7); \quad E_{13} = 1/2(\lambda_4 + i\lambda_5);$$

$$E_{21} = 1/2(\lambda_1 - i\lambda_2); \quad E_{32} = 1/2(\lambda_6 - i\lambda_7); \quad E_{31} = 1/2(\lambda_4 - i\lambda_5); \tag{74}$$

$$H_1 = \frac{\sqrt{3}}{2}\lambda_3 + \frac{\lambda_8}{2}; \quad H_2 = -\frac{\lambda_3}{2} + \frac{\sqrt{3}}{2}\lambda_8.$$

The rank of the Lie algebra $SU(3)$ is equal to two, $r=2$. The root space is two-dimensional, R^2, and the canonical commutation relations determining the positive root vectors are

$$[h_1, e_{12}] = \frac{3}{\sqrt{6}} e_{12}; \quad [h_2, e_{12}] = -\frac{1}{\sqrt{2}} e_{12};$$

$$[h_1,e_{13}]=\frac{3}{\sqrt{6}}e_{13};\quad [h_2,e_{13}]=\frac{1}{\sqrt{2}}e_{13};\tag{75}$$

$$[h_1,e_{23}]=0;\quad [h_2,e_{23}]=-\sqrt{2}e_{23}.$$

From the commutation relations (75) we find six nonzero root vectors,

$$\pm\boldsymbol{\alpha_1}=\pm\left(\frac{3}{\sqrt{6}};-\frac{1}{\sqrt{2}}\right),\quad \pm\boldsymbol{\alpha_2}=\pm\left(\frac{3}{\sqrt{6}};\frac{1}{\sqrt{2}}\right),\quad \pm\boldsymbol{\alpha_3}=(0;-\sqrt{2}).\tag{76}$$

The root diagram is a hexagon, the two primitive roots are $\boldsymbol{\gamma_1}=\boldsymbol{\alpha_3}$, $\boldsymbol{\gamma_2}=\boldsymbol{\alpha_2}$. The fundamental weights are found to be

$$\boldsymbol{\omega_1}=\left(\frac{1}{\sqrt{6}};-\frac{1}{\sqrt{2}}\right),\quad \boldsymbol{\omega_2}=\left(\frac{2}{\sqrt{6}};0\right).\tag{77}$$

An arbitrary irreducible representation is defined by the (two-dimensional) dominant weight vector:

$$\mathbf{l}=l_1\boldsymbol{\omega_1}+l_2\boldsymbol{\omega_2},\quad l_1,l_2=0,\pm1,\pm2,\ldots\ .\tag{78}$$

The coordinates of this vector in the root space are

$$\tilde{l}_1=\frac{l_1}{\sqrt{6}}+\frac{2l_2}{\sqrt{6}},\quad \tilde{l}_2=-\frac{l_1}{\sqrt{2}}.\tag{79}$$

The eigenket $\psi_{\mathbf{l}}$ is an eigenvector of both Cartan Lie algebra elements h_1,h_2 with eigenvalues $\tilde{l}_1,\tilde{l}_2$. It follows from the Theorem (Sec. V) that in order to find the geometric phase factor Ω acquired by the dominant weight vector eigenket $\psi_{\mathbf{l}}$, one should determine the two-component vector $\mathbf{k}(z,\overline{z})$ in the root space of the Lie algebra $su(3)$. As it may be seen from Eq. (43) the components of this vector in the orthogonal basis of the root space are linear combinations of the fundamental Kähler potentials $K^1(z,\overline{z}),K^2(z,\overline{z})$ of the homogeneous Kähler manifold $SU(3)/U(1)\times U(1)$. The fundamental Kähler potentials $K^1(z,\overline{z}),K^2(z,\overline{z})$ are constructed using Eq. (46), where the element $u(z)$ is taken in the fundamental 3×3 representation:

$$u(z)\equiv\exp(z_1E_{12}+z_2E_{23}+z_3E_{13})=\begin{pmatrix}1 & z_1 & z_3^+\\ 0 & 1 & z_2\\ 0 & 0 & 1\end{pmatrix}.\tag{80}$$

We have denoted $z^{\pm}=z_3\pm\frac{1}{2}z_1z_2$, and the projection matrices found from Eqs. (44) are

$$\eta_1=\begin{pmatrix}0 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix},\quad \eta_2=\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 1\end{pmatrix}.\tag{81}$$

Knowing $u(z),\eta_1,\eta_2$ in the fundamental representation, the fundamental Kähler potentials are calculated, and we obtain

$$K^1(z,\overline{z})=\ln(1+z_1\overline{z_1}+z_3^-\overline{z_3^-}),\quad K^2(z,\overline{z})=\ln(1+z_2\overline{z_2}+z_3^+\overline{z_3^+}).\tag{82}$$

Finding the coefficients $\mathrm{Tr}(h_j\eta_i)$ (in the fundamental represenation $h_1\equiv H_1,h_2\equiv H_2$), we get the components of the vector $\boldsymbol{\kappa}(z,\overline{z})$ in the root space of $su(3)$ algebra:

$$\kappa^1(z,\bar{z})=\frac{\sqrt{6}}{4}K^1(z,\bar{z}),\quad \kappa^2(z,\bar{z})=\frac{1}{\sqrt{2}}K^2(z,\bar{z})-\frac{1}{2\sqrt{2}}K^1(z,\bar{z}). \tag{83}$$

[Note that the expressions for the components of the vector $\boldsymbol{\kappa}(z,\bar{z})$ in terms of the complex coordinates, Eqs. (82), (83), may be obtained also by the (left) Mackey decomposition of the coset space representative g_1, Eqs. (37)–(40)].

For the case of $SU(3)$ evolution group the Berry connection A_s given by Eq. (50) is (84):

$$A_s=\mathcal{L}_{z,\bar{z}}\{\mathbf{l}\cdot\boldsymbol{\kappa}(z,\bar{z})\},\quad \mathbf{l}\cdot\boldsymbol{\kappa}(z,\bar{z})=\frac{1}{2}[(l_1+l_2)K^1(z,\bar{z})-l_1K^2(z,\bar{z})],$$
$$\mathcal{L}=\sum_{\alpha,\bar{\alpha}=1}^{3}\left(\dot{z}^{\alpha}\frac{\partial}{\partial z^{\alpha}}-\dot{z}^{\bar{\alpha}}\frac{\partial}{\partial z^{\bar{\alpha}}}\right), \tag{84}$$

and the Berry curvature F [Eq. (71)] is

$$F=\sum_{\alpha,\bar{\beta}=1}^{3}\frac{\partial^2K^{(\mathbf{l})}(z,\bar{z})}{\partial z^{\alpha}\,\partial z^{\bar{\beta}}}dz^{\alpha}\wedge dz^{\bar{\beta}}, \tag{85}$$

where the real function $K^{(\mathbf{l})}(z,\bar{z})$ is a linear combination of the fundamental Kähler potentials $K_1(z,\bar{z})$, $K_2(z,\bar{z})$ with the integer coefficients:

$$K^{(\mathbf{l})}(z,\bar{z})=(l_1+l_2)K^1(z,\bar{z})-l_1K^2(z,\bar{z}),\quad l_1,l_2=0,\pm1,\pm2\ldots\ . \tag{86}$$

Note that a common approach to the $SU(3)$ group evolution is to use the Euler coordinates that are similar to the Euler angle parameters of $SU(2)$. Such a method has been used by Byrd,[18] Arvind, Mallesh, and Mukunda,[19] and Khanna, Mukhopadhaya, Simon, and Mukunda[20] in connection with the evolution of a three-level system. While the geometric phase factor for this case has been found, none of them noticed that in cases under their consideration there exists an intimate relation between the geometric phase factors, Berry connections and Berry curvature and the fundamental Kähler potentials of parameter spaces.

VIII. CONCLUSIONS

In this paper we have considered the adiabatic evolution determined by a compact Lie group taken in an arbitrary irreducible representation. It has been demonstrated that the parameter space of the Hamiltonian is essentially a homogeneous Kähler manifold and its fundamental Kähler potentials completely determine Berry geometrical phase. Besides, we have shown that the Berry geometrical factor and the Berry connections depend on a set of integers a number of which equals to the rank of the corresponding Lie algebra. These integers determine irreducible representation in which quantum states form a basis.

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Chaotic and irreversible properties of quantum scattering systems

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Recent results for a free particle are generalized to N-particle quantum systems. Chaotic and irreversible behavior occurs in scattering states that belong to a certain Hilbert space K^2 with a preferred time direction pointing to the future. At positive times the time evolution of positive observables exhibits quantum analogs of sensitive dependence on initial conditions, topological transitivity, and existence of a dense set of periodic points. A mixture of states in K^2 can be described in terms of a density operator with thermodynamical entropy that increases to its least upper bound when the time tends to infinity. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1345872]

I. INTRODUCTION

This paper is devoted to the quantum mechanics of N particles with two-body interactions that give rise to scattering. The objective is to generalize recent work on entropy increase[1] and chaotic observables[2] for a free particle. It is shown that chaotic and irreversible behavior occurs if wave functions belong to a certain Hilbert space K^2 with a preferred time direction pointing to the future.

It is assumed that the interaction between any two particles is reasonably smooth and tends to zero sufficiently fast when the distance between particles tends to infinity. As a result there are scattering states in which the N-particle system separates into bound clusters that eventually move away from one another and in the remote future are infinitely far apart. Associated with each mode of separation are wave operators that intertwine between the exact time evolution and the time evolution of bound clusters moving freely relative to one another. The intertwining property is true for long- as well as for short-range interactions. It is the feature that enables previous results for free particles to be generalized. For a function f to belong to K^2, it must be a wave function of a scattering state, hence it must be orthogonal to any bound states of the scattering system. Moreover, it must satisfy analyticity conditions generalizing the ones in Refs. 1 and 2.

The wave function for the motion of N particles relative to their center of mass is an element of $L^2(\mathbb{R}^{3N-3})$. Henceforth we refer to L^2. There is an orthogonal projection $\Pi: L^2 \to \Pi L^2$ onto scattering states. Let H be the Hamiltonian of the relative motion. In the Schrödinger picture the time evolution takes $f \in L^2$ into $f(t) := \exp(-iHt)f$. If $f \in K^2$, then $f(t) \in K^2$ if $t \geqslant 0$, but not necessarily if $t < 0$. This causes a time asymmetry that is essential in this paper. Unless stated otherwise, it is assumed throughout the following that $t \geqslant 0$.

The quantities with chaotic properties are operators representing observables in the Heisenberg picture. Given an operator A on L^2, the Heisenberg picture lets

$$A(t) := \exp(iHt)A \exp(-iHt)$$

act on time-independent wave functions f. The space K^2 has a central role in that we focus on

[a)]Deceased.

positive self-adjoint operators A on ΠL^2 with the property that $A^{1/2}$ maps K^2 into ΠL^2. Quadratic form techniques developed in Ref. 2 determine a topology for such operators A. The result is a topological space X with the property that $A(t) \in X$ if $A \in X$ and $t \geqslant 0$.

Once a topology is in place, we can formulate conditions for chaos. To this end, we follow Devaney's definition of chaos in classical dynamical systems.[3] Hence we investigate

(S) sensitive dependence on initial conditions,

(T) topological transitivity,

(P) existence of a dense set of periodic points.

Precise statements are provided by Theorems S, T, and P in Sec. VIII. Formally, these chaos theorems are the same as in Ref. 2, but they are of wider scope because a more general time evolution is being considered. The proof in the present paper can be reduced to the previous proof. This is an analog of the fact that chaos in classical dynamical systems is invariant under homeomorphisms.[3]

The chaos theorems show that the outcome of experiments is unpredictable, yet retains elements of regularity. As an illustration, let us consider a fixed operator $A \in X$ and compare this with $Z \in X$. To do so, we choose finite sets of wave functions $f_i, g_i \in K^2 (i = 1,2,...,j)$, then perform experiments to determine the matrix elements $\langle f_i|A|g_i\rangle$ and $\langle f_i|Z|g_i\rangle$. Suppose for each i the two matrix elements differ by less than the experimental error. We repeat the experiments at a later time with the same A, Z, and f_i, g_i. According to Theorem S, the expectation values $\langle f_i|A(t)|f_i\rangle$ and $\langle f_i|Z(t)|f_i\rangle$ may differ by any constant δ times $\|f_i\|^2$. Given any operator $B \in X$, Theorem T says that $\langle f_i|Z(t)|g_i\rangle$ may equal $\langle f_i|B|g_i\rangle$ within experimental errors, for each $i (i = 1,2,...,j)$. In this sense the space of chaotic operators is indecomposable. The system is not random, however. By Theorem P, the operator $Z(t)$ may be semiperiodic in the sense that τ exists such that $Z(t + n\tau) = Z(t)$ if $t \geqslant 0$, $n = 0,1,2,...$. This means that $\langle f_i|Z(t)|g_i\rangle$ is close to $\langle f_i|A|g_i\rangle$ at all times $t = n\tau$, for every i. The proofs of the theorems show that there are operators Z with these erratic behaviors in any neighborhood of any operator $A \in X$.

Chaos as defined in this paper is related to irreversible behavior because either phenomenon occurs if wave functions belong to the space K^2. First suppose that ρ is a positive operator in the trace class on ΠL^2. To study chaos, we use the Heisenberg picture with time-dependent observables $A(t)$. Irreversible behavior calls for the Schrödinger picture with time-dependent density operators $\rho(t)$ determined by

$$\rho(t) := \exp(-iHt)\rho \exp(iHt). \tag{1.1}$$

Following von Neumann, we define the quantum-mechanical entropy of $\rho(t)$ by

$$S[\rho(t)] := -\operatorname{Tr} \rho(t) \ln \rho(t). \tag{1.2}$$

Because H is self-adjoint, the entropy $S[\rho(t)]$ does not depend on the time t. Hence there is no irreversible behavior at this level.

Now assume that $t \geqslant 0$ and that the range of ρ belongs to K^2. The operator $\rho(t)$ then determines an operator $\tilde{\rho}(t)$ in the trace class on K^2. The time evolution on K^2 is represented by a semigroup $\{U(t)|0 \leqslant t < \infty\}$, not by a unitary group such as $\{\exp(-iHt)|-\infty < t < \infty\}$. This eliminates a major paradox of statistical mechanics, but, since $U(t)$ is an isometry on K^2, is not sufficient to produce entropy increase.

For further progress, we need to refer to an unbounded positive operator J introduced in Sec. V. A function $f \in \Pi L^2$ belongs to K^2 if and only if $Jf \in \Pi L^2$. In terms of the inner product $(\cdot, \cdot)$ on ΠL^2, the inner product $\langle \cdot, \cdot \rangle$ on K^2 is defined according to

$$\langle f,g\rangle = (f,g) + (Jf, Jg). \tag{1.3}$$

If Tr denotes the trace on ΠL^2 and $\langle \mathrm{Tr} \rangle$ the trace on K^2,

$$\langle \mathrm{Tr}\, \tilde{\rho}(t) \rangle = \mathrm{Tr}\, \rho(t) + \mathrm{Tr}\, J\rho(t)J. \tag{1.4}$$

This expression brings to mind a discussion by Mackey (Ref. 4; Ref. 5, Chap. 9) in which he showed that taking a factor of a classical dynamical system with invertible time evolution may give rise to a system with increasing entropy. The transformation $\rho(t) \to \sigma(t)$ with

$$\sigma(t) := \rho(t) + J\rho(t)J \quad (t \geqslant 0) \tag{1.5}$$

can be viewed as a quantum analog of taking a factor in the sense of Mackey. It is shown in Sec. XIII that $S[\sigma(t)]$ is not constant in time and increases to its least upper bound as $t \to \infty$. The irreversible feature at the heart of the proof is easy to visualize by looking at a scattering event. In the distant past the system was separated into clusters that approached the center of mass. In the remote future scattered clusters will move away from it. This history gives rise to Eqs. (13.7) and (13.8), generalizing corresponding relations in Ref. 1. As a result the proof that $S[\sigma(t)]$ increases is the same as in Ref. 1.

If ρ is of rank 1, it can be shown as in Ref. 1 that the entropy $S[\sigma(t)]$ is a monotone increasing function of t. It is an open problem whether $S[\sigma(t)]$ may exhibit fluctuations if ρ is of higher rank. The latter case is difficult to assess due to the fact that there are positive operators in the trace class on ΠL^2 that cannot occur as density operators σ because they are not generated by positive operators ρ. This problem is discussed in some detail in Ref. 1.

Let us write $\sigma(t) = L\rho(t)$. This defines a linear operator L taking $\rho(t)$ with finite $\langle \mathrm{Tr}\, \tilde{\rho}(t) \rangle$ into the trace class on ΠL^2. According to Sec. XIV, L is invertible and L^{-1} can be constructed explicitly. Given a bounded operator T on L^2, there is an operator TL^{-1} such that

$$\mathrm{Tr}\, T\rho(t) = \mathrm{Tr}(TL^{-1})\sigma(t). \tag{1.6}$$

In combination with the fact that $\mathrm{Tr}\sigma(t)$ does not depend on t, Eq. (1.6) indicates that $\sigma(t)$ can be used as a density operator to evaluate expectation values of observables.

The transformation $\rho(t),\ T \to \sigma(t),\ TL^{-1}$ can be viewed as a new example of the Λ-transformation advocated by Prigogine and co-workers[6,7] to show that irreversible behavior originates at the microscopic level. There is an overview of the Prigogine program in Ref. 1. Further references follow in Sec. XVI.

Section II describes our coordinate systems for N-body problems. Section III summarizes fundamental concepts in scattering theory. Section IV is devoted to a Hilbert space of analytic functions that serves as a building block to construct the space of wave functions K^2 in Sec. V. The topological space X is introduced in Sec. VI. An essential point about X is that operators $A(t) \in X$ are related to bounded operators $\tilde{A}(t)$ on K^2. Hence the time evolution on K^2 is investigated in Sec. VII. Devaney's definition of chaos is reviewed in Sec. VIII. Theorems S, T, and P in Sec. VIII state that the time evolution of operators $A \in X$ has chaotic properties that can be viewed as quantum transcriptions of Devaney's chaos conditions for maps on metric spaces. To prove the theorems, one needs to construct nets $\{Z_\tau\} \in X$ $(\tau \geqslant 0)$ that tend to $A \in X$ as $\tau \to \infty$, yet give rise to time evolutions $\{Z_\tau(t)\}$ with erratic behaviors. Section VIII sketches the construction, but formal proofs are omitted because they are the same as in Ref. 2. The time evolution on K^2 is reminiscent of K flows, often quoted as prototypes of chaotic systems. It is discussed in Sec. IX how the relation has helped to shape the present paper. Other chaos concepts are mentioned in Sec. X, including the notion of quantum chaos.

Comparing the trace classes on ΠL^2 and K^2, Sec. XI shows how the density operator ρ determines $\tilde{\rho}$. Constructing σ can be viewed as taking a partial trace of $\tilde{\rho}$. It is shown in Sec. XII that $\mathrm{Tr}\ \sigma(t)$ is constant and that $\mathrm{Tr}\ \sigma^2(t)$ is a decreasing function of t, provided $t \geqslant 0$. The entropy $S[\sigma(t)]$ increases to its least upper bound by Sec. XIII. The proof is the same as in Ref. 1. Section XIV describes how the usual density operator ρ can be reconstructed when σ is known. The density operator $\sigma(t)$ can be used to calculate expectation values of observables according to Sec.

XV. Section XVI relates the transformation $\rho(t)\to\sigma(t)$ to the Λ-transformation in many papers by Prigogine and co-workers. In certain cases applying Λ can be interpreted as taking a factor of a classical dynamical system. That this step may lead to a system with increasing entropy was the reason for us to introduce $\sigma(t)$ and the entropy $S[\sigma(t)]$.

II. COORDINATE SYSTEMS

Consider a system of n particles with masses m_j $(j=1,2,...,n)$ located at $\mathbf{X}_j$. Suppose the Schrödinger operator has the form

$$i\frac{\partial}{\partial t}=-\sum_{j=1}^{n}(2m_j)^{-1}\Delta(\mathbf{X}_j)+\sum_{i<j}V_{ij}(\mathbf{X}_i-\mathbf{X}_j).$$

It is convenient to introduce a standard notation that separates the relative and center-of-mass motions.

The total mass of particles $1,2,...,k$ is

$$M_k:=\sum_{j=1}^{k}m_j.$$

The center of mass of this set is located at

$$\boldsymbol{\eta}_k:=(M_k)^{-1}\sum_{j=1}^{k}m_j\mathbf{X}_j \quad (k=1,2,...,n).$$

The vector from $\boldsymbol{\eta}_k$ to $\mathbf{X}_{k+1}$ is

$$\boldsymbol{\xi}_k:=\mathbf{X}_{k+1}-\boldsymbol{\eta}_k=(M_k)^{-1}\sum_{j=1}^{k}m_j(\mathbf{X}_{k+1}-\mathbf{X}_j) \quad (k=1,2,...,n-1).$$

Imagine a particle of mass M_k at $\boldsymbol{\eta}_k$ and a particle of mass m_{k+1} at $\mathbf{X}_{k+1}$. The reduced mass is

$$\mu_k:=(M_{k+1})^{-1}M_k m_{k+1} \quad (k=1,2,...,n-1).$$

Hence we define

$$\mathbf{x}_k:=(2\mu_k)^{1/2}\boldsymbol{\xi}_k$$

$$=(M_kM_{k+1})^{-1/2}(2m_{k+1})^{1/2}\sum_{j=1}^{k}m_j(\mathbf{X}_{k+1}-\mathbf{X}_j) \quad (k=1,2,...,n-1),$$

$$\mathbf{x}_n:=(2M_n)^{1/2}\boldsymbol{\eta}_n=(2/M_n)^{1/2}\sum_{j=1}^{n}m_j\mathbf{X}_j.$$

It is easy to verify that

$$-\sum_{j=1}^{n}(2m_j)^{-1}\Delta(\mathbf{X}_j)=-\sum_{j=1}^{n}\Delta(\mathbf{x}_j). \tag{2.1}$$

If there were only j particles, the system could be described in terms of the coordinates $\mathbf{x}_k$ with $k=1,2,...,j-1$ plus the center -of-mass coordinate $\boldsymbol{\eta}_j$. If $i<j$, then $\mathbf{X}_i-\mathbf{X}_j$ does not depend on $\boldsymbol{\eta}_j$. Hence there exist constants d_{ij}^{k} such that

$$V_{ij}(\mathbf{X}_i-\mathbf{X}_j)=V_{ij}\left(\sum_{k=1}^{j-1} d_{ij}^k\mathbf{x}_k\right) \quad (i<j).$$

Now consider n multiparticle clusters. Denote the mass of cluster c by N_c and assume that the center of mass is located at $\mathbf{Y}_c$ $(c=1,2,...,n)$. Introduce internal coordinates in cluster c as in the previous paragraphs, but denote these by $\mathbf{y}_c$, where c is a cluster subscript, not a particle subscript. The interaction within cluster c depends on $\mathbf{y}_c$ only. The kinetic energy of cluster c relative to its center of mass is represented by $-\Delta(\mathbf{y}_c)$. The total kinetic energy is

$$-\sum_{c=1}^{n}\Delta(\mathbf{y}_c)-\sum_{c=1}^{n}(2N_c)^{-1}\Delta(\mathbf{Y}_c).$$

Now apply to N_c, $\mathbf{Y}_c$ $(c=1,2,...,n)$ the coordinate transformation that took m_j, $\mathbf{X}_j$ $(j=1,2,...,n)$ into $\mathbf{x}_k$ $(k=1,2,...,n)$. Denoting the new variables by $\mathbf{x}_k$ as before takes the kinetic energy of the relative motion of the clusters into $-\Sigma_{j=1}^{n-1}\Delta(\mathbf{x}_j)$. The interaction between clusters b and c depends on $\mathbf{y}_b,\mathbf{y}_c$, and some or all of the $\mathbf{x}_j$ $(j=1,2,...,n-1)$, but not on the overall center-of-mass coordinate $\mathbf{x}_n$. Thus we find that

$$i\frac{\partial}{\partial t}=-\sum_{c=1}^{n}\Delta(\mathbf{y}_c)+\sum_{c=1}^{n}V_{cc}(\mathbf{y}_c)-\sum_{j=1}^{n-1}\Delta(\mathbf{x}_j)+\sum_{b<c}V_{bc}(\mathbf{y}_b,\mathbf{y}_c,\mathbf{x}_1,\ldots,\mathbf{x}_{n-1})-\Delta(\mathbf{x}_n). \quad (2.2)$$

In an obvious notation, V_{cc} and V_{bc} are interactions within cluster c and between clusters b and c, respectively. The operator $-\Delta(\mathbf{x}_n)$ represents the kinetic energy of the center of mass. To simplify the notation, we combine the vectors $\mathbf{y}_c$ $(c=1,2,,...,n)$ into a vector $\mathbf{y}$ and the vectors $\mathbf{x}_j$ $(j=1,2,...,n-1)$ into a vector $\mathbf{x}$. This takes the relative Hamiltonian for cluster c into

$$H_c(\mathbf{y}):=-\Delta(\mathbf{y}_c)+V_{cc}(\mathbf{y}_c).$$

The relative kinetic energy of the clusters is denoted by

$$-\Delta(\mathbf{x}):=-\sum_{j=1}^{n-1}\Delta(\mathbf{x}_j).$$

In this notation the Hamiltonian for the relative motion is

$$H:=\sum_c H_c(\mathbf{y})-\Delta(\mathbf{x})+\sum_{b<c}V_{bc}(\mathbf{x},\mathbf{y}).$$

There are many ways to separate a system of N particles into clusters. By Eq. (2.1) all choices transform the kinetic energy into the negative Laplace operator. This indicates that the transformations between various sets of coordinates are orthogonal and allows us to use different coordinates in different parts of the same problem. Moreover, in case there are $n-1$ intercluster coordinates $\mathbf{x}$ as in Eq. (2.2), the transformation from $(2m_j)^{1/2}\mathbf{X}_j$ to $\mathbf{y}$, $\mathbf{x}$, $\mathbf{x}_n$ is orthogonal, so that

$$d^{3N}X=\prod_{j=1}^{N}(2m_j)^{-1/2}d^{3N-3n}y\,d^{3n-3}x\,d^3x_n.$$

The mass factor is a constant which should be taken into account if one wishes to calculate actual physical values of matrix elements. In the present context, however, an overall numerical factor is of no consequence. Hence we ignore the mass factor and work with normalized functions of $\mathbf{y}$, $\mathbf{x}$, $\mathbf{x}_n$. In fact, since all cluster decompositions arrive at the same center-of-mass coordinate $\mathbf{x}_n$ equal to $(2/M_N)^{1/2}\Sigma_{j=1}^{N}m_j\mathbf{X}_j$, the transformations among the relative coordinates $\mathbf{y}$, $\mathbf{x}$ are orthogonal,

even if we change cluster decompositions. In studying the relative motion, it is therefore sufficient to work in terms of the usual inner product $(\cdot,\cdot)$ and norm $\|\cdot\|$ of $L^2(\mathbb{R}^{3N-3})$-functions depending on $\mathbf{x}$, $\mathbf{y}$.

III. SCATTERING THEORY

This section reviews concepts from scattering theory[8–10] that are used throughout the paper.

Consider a specific decomposition into n clusters, hence $(3n-3)$-dimensional relative motion $-\Delta(\mathbf{x})$, and assume that each multiparticle cluster Hamiltonian $H_c(\mathbf{y})$ has a normalized eigenvector $\psi_c(\mathbf{y})$ with eigenvalue E_c. Denote the product $\Pi_c \psi_c(\mathbf{y})$ by $\psi(\mathbf{y})$ and the sum $\Sigma_c E_c$ by E. The vector $\mathbf{y}$ must have $3N-3n$ components. Since $\psi(\mathbf{y})$ is normalized by assumption, the operator Ψ on $L^2(\mathbb{R}^{3N-3})$ defined by

$$\Psi f(\mathbf{x},\mathbf{y}) := \psi(\mathbf{y}) \int f(\mathbf{x},\mathbf{z})\overline{\psi}(\mathbf{z}) d^{3N-3n}z \tag{3.1}$$

is an orthogonal projection. If $f \in L^2(\mathbb{R}^{3N-3})$ belongs to the domain of H,

$$H\Psi f(\mathbf{x},\mathbf{y}) = \left[E - \Delta(\mathbf{x}) + \sum_{b<c} V_{bc}(\mathbf{x},\mathbf{y}) \right] \Psi f(\mathbf{x},\mathbf{y}). \tag{3.2}$$

For a more general notation, we consider all possible cluster decompositions of N particles and in each decomposition allow all possible bound-state wave functions ψ. We refer to the possibilities as scattering channels and label these by a subscript α. The bound-state wave function in channel α is denoted by ψ_α. It is a function of $\mathbf{y}_\alpha$. Typically, ψ_α is a product of several cluster functions ψ_c. The projection operator determined by ψ_α as in Eq. (3.1) is denoted by Ψ_α. The operators $\Sigma_{b<c} V_{bc}$ and $E-\Delta(\mathbf{x})$ in Eq. (3.2) are replaced by V_α and

$$H_\alpha := E_\alpha - \Delta(\mathbf{x}_\alpha). \tag{3.3}$$

Hence

$$H\Psi_\alpha f = (H_\alpha + V_\alpha)\Psi_\alpha f.$$

If all interaction terms V_α are of short range, there exist wave operators $\Omega_{\alpha\pm}$ satisfying

$$\lim_{t \to \mp\infty} \|\exp(iHt)\exp(-iH_\alpha t)\Psi_\alpha f - \Omega_{\alpha\pm} f\| = 0. \tag{3.4}$$

As a result of this definition, $\Omega_{\alpha\pm}$ annihilates the orthogonal complement of the range of Ψ_α,

$$\Omega_{\alpha\pm}(1-\Psi_\alpha)f = 0.$$

A sufficient condition for $\Omega_{\alpha\pm}$ to exist is that each term $V_{ij}(\mathbf{X}_i - \mathbf{X}_j)$ in the sum V_α is of the form $V_{ij} = V_2 + V_p$, where $V_2 \in L^2(\mathbb{R}^3)$ and $V_p \in L^p(\mathbb{R}^3)$ with some p satisfying $2<p<3$ (Ref. 9, Theorem X1.34). Another sufficient condition is that $\epsilon>0$ exists such that

$$(1+|\mathbf{X}|^2)^{\epsilon+1/2} V_{ij}(\mathbf{X}) = V_{3/2} + V_\infty,$$

where $V_{3/2} \in L^{3/2}(\mathbb{R}^3)$ and $V_\infty \in L^\infty(\mathbb{R}^3)$, see Ref. 9, Theorem X1.35. Generally speaking, these conditions are satisfied if $V_{ij}(\mathbf{X})$ does not have serious singularities and at infinity tends to 0 like $|\mathbf{X}|^{-1-\delta}$ with some $\delta>0$.

If $V_{ij}(\mathbf{X})$ behaves at infinity like $|\mathbf{X}|^{-\mu}$ with $\mu \leqslant 1$, the interaction is said to be of long range. In this case the limits in Eq. (3.4) do not exist, but it may be possible to construct modified wave operators provided the factor $\exp(-iH_\alpha t)$ in Eq. (3.4) is replaced by one that better characterizes the time evolution of scattered clusters at large separations.[11] If $\sqrt{3}-1<\mu\leqslant 1$ and V_{ij} satisfies

suitable smoothness conditions, modified wave operators exist for any number of particles.[10,12] Even in cases where $\mu \leqslant \sqrt{3}-1$, there are results for two particles.[13] For such very slowly decaying interactions, modified wave operators have been shown to exist in larger systems[10,12] provided cluster wave functions $\psi(\mathbf{y})$ go to 0 sufficiently rapidly as $|\mathbf{y}| \to \infty$.

Whether the interaction is of short or long range, henceforth we simply refer to wave operators and denote these quantities by $\Omega_{\alpha\pm}$. They all satisfy the intertwining relation

$$\exp(-iHt)\Omega_{\alpha\pm} = \Omega_{\alpha\pm} \exp(-iH_\alpha t). \tag{3.5}$$

Denoting the orthogonal projection onto the range of $\Omega_{\alpha\pm}$ by $\Pi_{\alpha\pm}$, we have

$$\Omega_{\alpha\pm}^* \Omega_{\alpha\pm} = \Psi_\alpha, \quad \Omega_{\alpha\pm}\Omega_{\alpha\pm}^* = \Pi_{\alpha\pm}.$$

Since

$$\Omega_{\beta\pm}^* \Omega_{\alpha\pm} = \delta_{\alpha\beta}\Psi_\alpha, \tag{3.6}$$

the projections $\Pi_{\alpha+}$ commute and have mutually orthogonal ranges. The same applies to the projections $\Pi_{\alpha-}$. Summing over channels, we define the projections

$$\Pi_\pm := \sum_\alpha \Pi_{\alpha\pm}.$$

The sum has finitely many terms or converges strongly.

Let B be the projection onto any bound states of the N-particle system. If the wave operators exist, BL^2 is orthogonal to $\Pi_\pm L^2$. If

$$BL^2 + \Pi_+ L^2 = BL^2 + \Pi_- L^2 = L^2,$$

the scattering is said to be asymptotically complete. Under various smoothness assumptions on the interaction, asymptotic completeness has been proved for short-range interactions[14,15] and for long-range interactions[12] with $\sqrt{3}-1 < \mu \leqslant 1$. In two-particle problems asymptotic completeness is even known to be true in cases in which $\mu \leqslant \sqrt{3}-1$.[13]
Examples show that the existence of wave operators is not sufficient for asymptotic completeness.[16]

The important point in the following is the intertwining relation (3.5). It provides the link between time evolutions with and without interaction. In the present paper we can use operators $\Omega_{\alpha+}$ throughout. This gives rise to an operator J_+ and space K_+^2. Alternatively, we can use operators $\Omega_{\alpha-}$ giving rise to J_- and K_-^2. The restriction $t \geqslant 0$ applies in either case. If the projections Π_+ and Π_- are equal, the spaces K_+^2 and K_-^2 are isometrically isomorphic, operators $A_+^{1/2}(t)$ acting on K_+^2 are unitarily equivalent to operators $A_-^{1/2}(t)$ acting on K_-^2, and each operator $\sigma_+(t)$ defined in terms of J_+ by Eq. (1.4) is unitarily equivalent to an operator $\sigma_-(t)$ defined in terms of J_-. This will become clear once the operators $J_\pm$ are defined in Sec. V.

Since the theories with subscripts $+$ and $-$ run parallel, we omit the subscripts in the following, writing

$$\Omega_\alpha \Omega_\alpha^* = \Pi_\alpha, \quad \Pi = \sum_\alpha \Pi_\alpha.$$

Thus Ω_α is either $\Omega_{\alpha+}$ or $\Omega_{\alpha-}$, and similarly for the other operators. The projection Π is the projection onto scattering states meant in Sec. I. If asymptotic completeness holds, $\Pi_+ = \Pi_-$, so that Π is uniquely determined.

Recall that L^2 stands for $L^2(\mathbb{R}^{3N-3})$. If in channel α the system is separated into n clusters, a $(3n-3)$-dimensional coordinate $\mathbf{x}_\alpha$ refers to the relative motion of the clusters. The wave function of the clusters depends on a $(3N-3n)$-dimensional coordinate $\mathbf{y}_\alpha$. For any $f \in \Pi L^2$,

$$\exp(-iHt)f=\exp(-iHt)\sum_{\alpha}\ \Omega_{\alpha}\Omega_{\alpha}^{*}f=\sum_{\alpha}\ \Omega_{\alpha}\exp(-iH_{\alpha}t)\Omega_{\alpha}^{*}f. \tag{3.7}$$

Since $\Omega_{\alpha}^{*}f$ belongs to the range of Ψ_{α}, there must be a function f_{α} such that

$$\Omega_{\alpha}^{*}f=\psi_{\alpha}(\mathbf{y}_{\alpha})f_{\alpha}(\mathbf{x}_{\alpha}). \tag{3.8}$$

To calculate f_{α}, it suffices to multiply $\Omega_{\alpha}^{*}f$ by $\overline{\psi}(\mathbf{y}_{\alpha})$ and integrate with respect to $\mathbf{y}_{\alpha}$. Due to Eqs. (3.3) and (3.8)

$$\exp(-iH_{\alpha}t)\Omega_{\alpha}^{*}f=\exp(-iE_{\alpha}t)\psi_{\alpha}(\mathbf{y}_{\alpha})\exp[i\Delta(\mathbf{x}_{\alpha})t]f_{\alpha}(\mathbf{x}_{\alpha}).$$

In the following we mainly use the momentum representation. Hence we replace $\exp[i\Delta(\mathbf{x}_{\alpha})t]f_{\alpha}(\mathbf{x}_{\alpha})$ by $\exp(-ik_{\alpha}^{2}t)f_{\alpha}(\mathbf{k}_{\alpha})$. For f to belong to K^{2}, the functions $f_{\alpha}(\mathbf{k}_{\alpha})$ have to satisfy analyticity conditions introduced in Sec. IV.

IV. ANALYTIC FUNCTIONS

This section discusses functions $f(\mathbf{k})\in L^{2}(\mathbb{R}^{\nu})$ that are meant as prototypes of Fourier transforms of functions $f_{\alpha}(\mathbf{x}_{\alpha})$ in Eq. (3.8). We follow Ref. 1 closely, but in the process generalize previous results for $L^{2}(\mathbb{R}^{3})$ so that they become valid on $L^{2}(\mathbb{R}^{\nu})$.

Denoting $|\mathbf{k}|$ by k, we introduce $\nu-1$ spherical coordinates ω and replace $f(\mathbf{k})$ by $f(k,\omega)$. Hence $k^{(\nu-1)/2}f(k,\omega)$ is an element of $L^{2}(\mathbb{R}^{+}\times S^{\nu-1})$.

The Mellin transform

$$M_{\nu}f(k,\omega)=f^{\#}(u,\omega)$$

defined by

$$f^{\#}(u,\omega):=(2\pi)^{-1/2}\int_{0}^{\infty}k^{(\nu-1)/2}f(k,\omega)k^{iu-1/2}\,\mathrm{d}k$$

is a unitary map taking $L^{2}(\mathbb{R}^{+}\times S^{\nu-1})$ onto the space $L^{2}(\mathbb{R}\times S^{\nu-1})$ consisting of functions $f^{\#}(u,\omega)$ with inner product

$$(f^{\#},g^{\#})=\int_{S^{\nu-1}}\int_{-\infty}^{\infty}f^{\#}(u,\omega)\overline{g^{\#}}(u,\omega)\mathrm{d}u\,\mathrm{d}\omega.$$

The inverse Mellin transform is determined by

$$k^{(\nu-1)/2}f(k,\omega)=(2\pi)^{-1/2}\int_{-\infty}^{\infty}f^{\#}(u,\omega)k^{-iu-1/2}\,\mathrm{d}u.$$

If we define $z:=\ln k$ and

$$F(z,\omega):=e^{\nu z/2}f(e^{z},\omega),$$

it follows that

$$F(z,\omega)=(2\pi)^{-1/2}\int_{-\infty}^{\infty}f^{\#}(u,\omega)e^{-izu}\,\mathrm{d}u.$$

For starters we now assume that $f^{\#}(u,\omega)\in C_{0}^{\infty}(\mathbb{R}\times S^{\nu-1})$. This guarantees that F belongs to the domain of $\partial/\partial z$. Applying $i\partial/\partial z$ to F corresponds to multiplying $f^{\#}$ by u. Because $\partial/\partial z=k\partial/\partial k$,

$$i\frac{\partial}{\partial z}F(z,\omega)=k^{\nu/2}\left[ik\frac{\partial}{\partial k}+i\nu/2\right]f(k,\omega). \tag{4.1}$$

The operator in square brackets is among our major concepts. To give it a more transparent form, we examine the dilation operator D_ν, which is the self-adjoint operator on $L^2(\mathbb{R}^\nu)$ that acts on C_0^∞-functions $f(\mathbf{k})\in L^2(\mathbb{R}^\nu)$ as

$$D_\nu=\frac{i}{2}(\mathbf{k}\cdot\nabla_k+\nabla_k\cdot\mathbf{k}).$$

The differential operator D_ν is equal to $i\mathbf{k}\cdot\nabla_k+i\nu/2$. The components of $\mathbf{k}$ are of the form $k_j=k\cos\theta_j(\omega)$, with some set of functions $\theta_j(\omega)$ $(j=1,2,...,\nu)$. Hence

$$k\partial/\partial k=\sum_{j=1}^{\nu}k\frac{\partial k_j}{\partial k}\partial/\partial k_j=\sum_{j=1}^{\nu}k_j\partial/\partial k_j=\mathbf{k}\cdot\nabla_k.$$

It follows that the operator in square brackets in Eq. (4.1) is the dilation operator D_ν. Multiplying Eq. (4.1) by $k^{-1/2}$ gives

$$k^{(\nu-1)/2}D_\nu f(k,\omega)=(2\pi)^{-1/2}\int_{-\infty}^{\infty}uf^{\#}(u,\omega)k^{-iu-1/2}\,du.$$

Following Ref. 1, we now extend multiplication by u on $C_0^\infty(\mathbb{R}\times S^{\nu-1})$ to a self-adjoint operator u on $L^2(\mathbb{R}\times S^{\nu-1})$, then use the operator u so defined to extend the differential operator D_ν to the self-adjoint operator $D_\nu=M_\nu^{-1}uM_\nu$ on $L^2(\mathbb{R}^\nu)$. The spectra of u and D_ν are absolutely continuous and run from $-\infty$ to ∞.

The self-adjoint operator D_ν determines $\exp(\phi D_\nu)$. Taking $\phi=-\pi/2$ we define

$$J_\nu:=\exp(-\pi D_\nu/2)=M_\nu^{-1}\exp(-\pi u/2)M_\nu \tag{4.2}$$

and let the domain of J_ν be the set of all $f\in L^2(\mathbb{R}^\nu)$ with the property that $f^{\#}(u,\omega)\exp(-\pi u/2)$ belongs to $L^2(\mathbb{R}\times S^{\nu-1})$. The operator J_ν so defined is self-adjoint and positive. Henceforth the domain of J_ν is denoted by K_ν^2. Hence K_ν^2 is the set of all $f\in L^2(\mathbb{R}^\nu)$ with the property that $J_\nu f\in L^2(\mathbb{R}^\nu)$.

Functions in K_ν^2 have certain analyticity properties. This can be seen by examining the set of all functions $f(ke^{i\phi},\omega)$ which are analytic in the sector $-\pi/2<\phi<0$ for almost every $\omega\in S^{\nu-1}$ and have the property that

$$\int_{S^{\nu-1}}\int_0^\infty|(ke^{i\phi})^{(\nu-1)/2}f(ke^{i\phi},\omega)|^2dk\,d\omega$$

is bounded uniformly in the sector.[17,18] Functions in this set have mean-square boundary values $f(k,\omega)$ and $f(ke^{-i\pi/2},\omega)$. Under the inner product

$$\langle f,g\rangle=\int_{S^{\nu-1}}\int_0^\infty[f(k,\omega)\overline{g}(k,\omega)+f(ke^{-i\pi/2},\omega)\overline{g}(ke^{-i\pi/2},\omega)]k^{\nu-1}\,dk\,d\omega \tag{4.3}$$

the set is a Hilbert space which we denote by G_ν^2.

At this point we can adapt the reasoning for $\nu=3$ in Refs. 1 and 2 to general ν. On the basis of known properties[17,18] of Mellin transforms of functions in G_ν^2, it can be shown that $f\in L^2(\mathbb{R}^\nu)$ belongs to K_ν^2 if and only if $f(k,\omega)$ is the boundary value at $\phi=0$ of a function $f(ke^{i\phi},\omega)$ in G_ν^2. Moreover, for $-\pi/2\leqslant\phi\leqslant0$,

$$e^{\phi D_\nu}f(k,\omega)=e^{i\nu\phi/2}f(ke^{i\phi},\omega). \tag{4.4}$$

We now define an inner product $\langle \cdot, \cdot \rangle$ on K^2_ν by

$$\langle f,g\rangle := (f,g) + (J_\nu f, J_\nu g)$$

$$= \int_{S^{\nu-1}} \int_{-\infty}^{\infty} (1+e^{-\pi u}) f^{\#}(u,\omega)\overline{g^{\#}}(u,\omega)\mathrm{d}u\,\mathrm{d}\omega.$$

The term $(J_\nu f, J_\nu g)$ is equal to the second term on the right-hand side in Eq. (4.3). The fact that G^2_ν is a Hilbert space can now be used to show that K^2_ν is complete under the inner product $\langle \cdot, \cdot \rangle$, hence a Hilbert space.

If $-\pi/2 < \phi < 0$, then $\exp(-ik^2 e^{2i\phi}t)$ is bounded if and only if $t \geqslant 0$. Hence $f \in G^2_\nu$ yields $\exp(-ik^2e^{2i\phi}t) f \in G^2_\nu$ if $t \geqslant 0$, but not necessarily if $t<0$. In terms of boundary values at $\phi = 0$, it follows that $f \in K^2_\nu$ yields $\exp(-ik^2 t) f \in K^2_\nu$ if $t \geqslant 0$, but not necessarily if $t<0$. This is the reason why we assume that $t \geqslant 0$, unless stated otherwise. Due to Eq. (4.4) with $\phi = -\pi/2$,

$$J_\nu \exp(-ik^2 t) f(k,\omega) = \exp(ik^2 t) J_\nu f(k,\omega), \tag{4.5}$$

provided $f \in K^2_\nu$ and $t \geqslant 0$. Taking $\phi = -\pi/4$ gives

$$J^{1/2}_\nu \exp(-ik^2 t) f(k,\omega) = \exp(-k^2 t) J^{1/2}_\nu f(k,\omega). \tag{4.6}$$

V. THE SPACE OF WAVE FUNCTIONS

The time evolution of $f \in \Pi L^2$ can be represented by Eq. (3.7). In the momentum representation Eq. (3.8) takes the form

$$\Omega^*_\alpha f = \psi_\alpha(\mathbf{K}'_\alpha) f_\alpha(\mathbf{k}_\alpha), \tag{5.1}$$

where $\mathbf{k}'_\alpha$ and $\mathbf{k}_\alpha$ are the variables conjugate to $\mathbf{y}_\alpha$ and $\mathbf{x}_\alpha$, respectively. If channel α refers to a separation into n clusters, the vector $\mathbf{k}_\alpha$ has $3n-3$ components. We let $3n-3$ be the number ν in Sec. IV and assume that $f_\alpha(\mathbf{k}_\alpha)$ belongs to K^2_ν, but we change the notation and now refer to operators D_α and J_α and a space K^2_α. Using the notation $\|\cdot\|$ for norms on L^2-spaces, we denote the norm on K^2_α by $|||\cdot|||$. Thus, if $f_\alpha \in K^2_\alpha$, then $\langle f_\alpha, f_\alpha \rangle$ is denoted by $|||f_\alpha|||^2$.

Let K^2 be the set of $f \in \Pi L^2$ with the property that $\Sigma_\alpha |||f_\alpha|||^2 < \infty$. If $f \in K^2$, then

$$\left\| \sum_{\alpha=m}^{n} \Omega_\alpha J_\alpha \Omega^*_\alpha f \right\|^2 = \sum_{\alpha=m}^{n} \|\psi_\alpha J_\alpha f_\alpha\|^2 \leqslant \sum_{\alpha=m}^{n} |||f_\alpha|||^2.$$

Since $\Sigma^n_{\alpha=m} |||f_\alpha|||^2$ tends to 0 as $m,n \to \infty$, the sum $\Sigma_{\alpha \leqslant n} \Omega_\alpha J_\alpha \Omega^*_\alpha f$ tends to a limit as $n \to \infty$. We denote the limit by Jf. This defines the operator

$$J := \sum_\alpha \Omega_\alpha J_\alpha \Omega^*_\alpha \tag{5.2}$$

on ΠL^2 with domain K^2.

It is easy to verify that J is symmetric. We claim that the operator J with domain K^2 is self-adjoint on ΠL^2. To prove this, it is sufficient to show that $(J \pm i) f$ runs through ΠL^2 when f runs through K^2. By the definition of J,

$$(J \pm i) f = \sum_\alpha \Omega_\alpha (J_\alpha \pm i) \Omega^*_\alpha f.$$

Recall that $\Omega^*_\alpha f = \psi_\alpha f_\alpha$, where f_α belongs to a certain $L^2(\mathbb{R}^\nu)$-space. The operator J_α on $L^2(\mathbb{R}^\nu)$ is self-adjoint. Its domain is the set $K^2_\alpha \in L^2(\mathbb{R}^\nu)$. Hence $(J_\alpha \pm i)\psi_\alpha f_\alpha$ runs through $\psi_\alpha L^2(\mathbb{R}^\nu)$

when f_α runs through K_α^2. In the process, $\Omega_\alpha(J_\alpha \pm i)\Omega_\alpha^* f$ runs through $\Omega_\alpha \Omega_\alpha^* L^2$. When f runs through K^2, each f_α runs through its set K_α^2, hence $(J\pm i)f$ runs through $\Sigma_\alpha \Omega_\alpha \Omega_\alpha^* L^2$, as we wanted to show.

Now that we know that J is self-adjoint, we can be more specific about the convergence properties of the sum Σ_α in Eq. (5.2). If f runs through K^2,

$$\sum_{\alpha \leqslant n} \Omega_\alpha J_\alpha \Omega_\alpha^* f \pm i f$$

runs through a dense set in ΠL^2. It follows that K^2 is a core for $\Sigma_{\alpha \leqslant n} \Omega_\alpha J_\alpha \Omega_\alpha^*$, for every n. By Ref. 19, Theorem VIII.25

$$\lim_{n\to\infty} \left\| \left(\sum_{\alpha \leqslant n} \Omega_\alpha J_\alpha \Omega_\alpha^* \pm i \right)^{-1} f - (J \pm i)^{-1} f \right\| = 0 \tag{5.3}$$

for every $f \in \Pi L^2$. The sets $(J\pm i)^{-1}\Pi L^2$ are both equal to the domain of J, which can therefore be identified without prior knowledge of K^2. Instead of looking at $\Sigma_\alpha |||f_\alpha|||^2$ to define K^2, we can construct J via Eq. (5.3). Then we can let K^2 be the set of $f \in \Pi L^2$ with the property that $Jf \in \Pi L^2$. Either way J is self-adjoint on ΠL^2 with domain K^2, hence the two definitions of K^2 are equivalent.

Given J, the relation (1.3) defines an inner product on K^2. Denoting $\langle f, f\rangle$ by $|||f|||^2$, we proceed to show that the set K^2 is complete under the $|||\cdot|||$ norm.

Let $\{f_n\}$ $(n=1,2,...)$ be a sequence in K^2 with the property that $|||f_m - f_n||| \to 0$ as $m,n \to \infty$. Then $\|f_m - f_n\| \to 0$ and $\|Jf_m - Jf_n\| \to 0$, hence there are elements f and g in ΠL^2 such that $\|f_n - f\| \to 0$ and $\|Jf_n - g\| \to 0$. Since J is self-adjoint, J is closed. Hence f must belong to the domain of J and $Jf = g$. In other words, $f \in K^2$ and

$$|||f_n - f|||^2 = \|f_n - f\|^2 + \|Jf_n - Jf\|^2 \to 0.$$

This shows that a sequence $\{f_n\}$ in K^2 that converges in the $|||\cdot|||$-norm has a limit f in K^2. Equipped with the $|||\cdot|||$ norm, the set K^2 is a Hilbert space with inner product $\langle \cdot, \cdot \rangle$. It is easily verified that

$$\langle f, g\rangle = ([1+J^2]^{1/2} f, [1+J^2]^{1/2} g).$$

The adjoint on K^2 of an operator $S: K^2 \to K^2$ is denoted by $S^\dagger$. We continue to denote the adjoint on L^2 of an operator $T: L^2 \to L^2$ by T^*. Hence

$$\langle Sf, g\rangle = \langle f, S^\dagger g\rangle, \quad (Tf, g) = (f, T^* g).$$

The domains of operators S and T are denoted by $\mathrm{Dom}(S)$ and $\mathrm{Dom}(T)$, respectively.

If $f \in K^2$ and $t \geqslant 0$, then $\exp(-iHt)f \in K^2$. Indeed, with Eq. (3.3) for H_α, it follows from the intertwining relation (3.5) and Eq. (5.2) that

$$\begin{aligned} J \exp(-iHt) f &= \sum_\alpha \Omega_\alpha J_\alpha \exp(-iH_\alpha t) \Omega_\alpha^* f \\ &= \sum_\alpha \Omega_\alpha \exp(iH_\alpha t) \exp(-2iE_\alpha t) J_\alpha \Omega_\alpha^* f \\ &= \exp(iHt) \sum_\alpha \Omega_\alpha \exp(-2iE_\alpha t) J_\alpha \Omega_\alpha^* f. \end{aligned}$$

Defining

$$W(t) := \sum_\alpha \Omega_\alpha \exp(-2iE_\alpha t)\Omega_\alpha^*$$

gives

$$J\exp(-iHt)f = \exp(iHt)W(t)Jf. \tag{5.4}$$

The operator $W(t)$ is unitary on ΠL^2 and commutes with $\exp(-iHt)$. It follows that $\|J\exp(-iHt)f\| = \|Jf\|$, hence $|||\exp(-iHtf\|| = |||f|||$.

In much the same way as we defined the operator J, we can introduce the square root

$$J^{1/2} = \sum_\alpha \Omega_\alpha J_\alpha^{1/2}\Omega_\alpha^*.$$

If $f \in K^2$, it follows with Eq. (4.6) that

$$J^{1/2}\exp(-iHt)f = W^{1/2}(t)\sum_\alpha \Omega_\alpha \exp(-k_\alpha^2 t)J_\alpha^{1/2}\Omega_\alpha^* f. \tag{5.5}$$

The norm of this vector decreases as t increases.

We note for future reference that

$$\langle \exp(-iHt)f, g\rangle = \sum_\alpha \langle \exp(-ik_\alpha^2 t - iE_\alpha t)f_\alpha, g_\alpha\rangle, \tag{5.6}$$

where the left-hand side is an inner product on K^2, the terms on the right-hand side are inner products on spaces K_α^2.

Recall that Ω_α denotes either $\Omega_{\alpha+}$ or $\Omega_{\alpha-}$. Thus Eq. (5.2) actually defines operators

$$J_\pm := \sum_\alpha \Omega_{\alpha\pm} J_\alpha \Omega_{\alpha\pm}^*$$

giving rise to spaces $K_\pm^2$ with inner products $\langle\cdot,\cdot\rangle_\pm$. Now consider

$$\Theta := \sum_\alpha \Omega_{\alpha-}\Omega_{\alpha+}^*.$$

This operator commutes with $\exp(-iHt)$. Due to Eq. (3.6)

$$\Theta J_+ \Theta^* = J_-, \quad \Theta^* J_- \Theta = J_+.$$

If $\Pi_+ = \Pi_- = \Pi$, then $\Theta\Theta^* = \Theta^*\Theta = \Pi$, so that Θ is a unitary operator on ΠL^2. Under this assumption $\Theta K_+^2 = K_-^2$ and

$$\begin{aligned}\langle f,g\rangle_+ &= (f,g) + (J_+ f, J_+ g)\\ &= (\Theta f, \Theta g) + (\Theta J_+ \Theta^*\Theta f, \Theta J_+ \Theta^*\Theta g)\\ &= (\Theta f, \Theta g) + (J_-\Theta f, J_-\Theta g) = \langle \Theta f, \Theta g\rangle_-.\end{aligned}$$

Hence K_+^2 and K_-^2 are isometrically isomorphic. If $f \in K_+^2$ and $A^{1/2}(t)f \in \Pi L^2$, then $\Theta A^{1/2}(t)\Theta^*\Theta f \in \Pi L^2$. Thus if the expectation value of $A(t)$ is chaotic when wave functions belong to K_+^2, the expectation value of $\Theta A(t)\Theta^*$ is chaotic when wave functions belong to K_-^2.

Following Eq. (1.5) we write

$$\sigma_+(t)=\rho(t)+J_+\rho(t)J_+ .$$

If Θ is unitary, it follows that

$$\Theta\sigma_+(t)\Theta^*=\Theta\rho(t)\Theta^*+J_-\Theta\rho(t)\Theta^*J_- .$$

Hence the pair ρ, J_+ determines the same entropy as the pair $\Theta\rho\Theta^*, J_-$.

VI. THE OPERATOR TOPOLOGY

The operator J and the space K^2 are important for our purposes because the chaotic and irreversible behavior that we want to discuss, occurs precisely when states belong to K^2. The quantities with chaotic time evolution are positive self-adjoint operators A such that $A^{1/2}$ maps K^2 into ΠL^2. If A is not bounded, it may happen that (Af, g) is not well defined. Hence for $f,g \in K^2$, matrix elements of A are expressed in the form

$$\langle f|A|g\rangle := (A^{1/2}f, A^{1/2}g). \tag{6.1}$$

These are the quantities meant in Sec. I.

Because the operator J and the space K^2 have essential properties in common with the corresponding quantities in Refs. 1 and 2, many previous results can be copied unchanged. In this section we review the steps to construct a topology for the operators A that will later be shown to have chaotic time evolutions. As mentioned before, the domain of an operator T is denoted by $\mathrm{Dom}(T)$. The restriction to K^2 of an operator $T:\Pi L^2 \to \Pi L^2$ is denoted by $T\restriction K^2$.

Let T be a positive self-adjoint operator on ΠL^2 such that $\mathrm{Dom}(T^{1/2}) \supseteq K^2$. Consider the quadratic form

$$q[f,g] := (T^{1/2}f, T^{1/2}g) \tag{6.2}$$

on ΠL^2 with form domain $\mathrm{Dom}(q)=K^2$.

Since $T^{1/2}\restriction K^2$ is symmetric, the form is closed or closable. Denote the closure by $\overline{q}$ and its form domain by $\mathrm{Dom}(\overline{q})$. The form $\overline{q}$ determines a positive self-adjoint operator A on ΠL^2 with domain $\mathrm{Dom}(A) \subset \mathrm{Dom}(\overline{q})$ and $\mathrm{Dom}(A^{1/2}) = \mathrm{Dom}(\overline{q})$. For every $f,g \in \mathrm{Dom}(\overline{q})$,

$$\overline{q}[f,g] = (A^{1/2}f, A^{1/2}g).$$

Since K^2 is a core for $\overline{q}$, the set K^2 is a core for $A^{1/2}$.

The above-mentioned propositions follow from two representation theorems for quadratic forms,[20] see Chap. VI, Sec. II. That K^2 is a core for $A^{1/2}$ implies that $A^{1/2}=(A^{1/2}\restriction K^2)^*$. The theorems depend on the fact that $T^{1/2}\restriction K^2$ is closable, but do not make comparisons between any extensions of $T^{1/2}\restriction K^2$ and $A^{1/2}\restriction K^2$ to domains larger than K^2. As long as $f,g \in K^2$,

$$(T^{1/2}f, T^{1/2}g) = (A^{1/2}f, A^{1/2}g).$$

For the purpose of calculating expectation values of observables in states $f,g \in K^2$, all positive self-adjoint operators T with the same $T^{1/2}\restriction K^2$ are equivalent. Henceforth we select the particular operator A that is singled out by the representation theorems. We denote by Γ the set of all positive self-adjoint operators A on ΠL^2 with the property that K^2 is a core for $A^{1/2}$. On Γ one can define a sum as well as multiplication by a positive constant. Hence Γ is a cone, which includes all bounded positive operators on ΠL^2.

We now choose $A \in \Gamma$ and focus on the quadratic form

$$q[f,g] := (A^{1/2}f, A^{1/2}g)$$

with form domain $\mathrm{Dom}(q)=K^2$. Since A is a special case of the operator T in Eq. (6.2), the form is closed or closable. It is shown in Ref. 2 that $(1+J^2)^{-1/2}A^{1/2}$ is a bounded linear operator on K^2. Hence the operator $\tilde{A}$ defined by

$$\tilde{A}:=[(1+J^2)^{-1/2}A^{1/2}]^{\dagger}(1+J^2)^{-1/2}A^{1/2} \tag{6.3}$$

is a bounded positive operator on K^2 satisfying

$$(A^{1/2}f,A^{1/2}g)=\langle \tilde{A}f,g\rangle \tag{6.4}$$

for every $f,g\in K^2$.

Let us denote by Γ_q the set of positive closable forms on ΠL^2 with form domain K^2. The representation theorems do not require that $q\in\Gamma_q$ be given in terms of an operator $T^{1/2}$ as in Eq. (6.2). Any $q\in\Gamma_q$ determines $A\in\Gamma$ and $A\in\Gamma$ determines $\tilde{A}$. Hence $q\in\Gamma_q$ is of the form $\langle\tilde{A}f,g\rangle$ with some $\tilde{A}$.

Now consider a positive operator $\tilde{T}$ on K^2 with the property that the form $\langle\tilde{T}f,g\rangle$ on ΠL^2 with form domain K^2 is closable. Since $\langle\tilde{T}f,g\rangle$ must exist for every $f,g\in K^2$, the operator $\tilde{T}$ must be bounded on K^2. The form $\langle\tilde{T}f,g\rangle$ determines A and A determines the bounded linear operator $\tilde{A}$ on K^2 satisfying

$$\langle\tilde{T}f,g\rangle=\langle\tilde{A}f,g\rangle$$

for every $f,g\in K^2$. This requires that $\tilde{T}=\tilde{A}$. Hence the set Γ_q is associated with a set $\tilde{\Gamma}$ consisting of uniquely determined operators $\tilde{A}$. There is an invertible function $A=\gamma(\tilde{A})$ mapping $\tilde{\Gamma}$ onto Γ.

In order that we can define chaos, we need a topology on Γ. We begin with the topology on $\tilde{\Gamma}$ induced by the weak topology for bounded linear operators on K^2. This turns $\tilde{\Gamma}$ into a topology space $\tilde{X}$ with the property that a net $\{\tilde{Z}_\tau\}\in\tilde{X}(\tau\geqslant 0)$ tends to $\tilde{A}\in\tilde{X}$ as $\tau\to\infty$ if and only if $\langle\tilde{Z}_\tau f,g\rangle$ tends to $\langle\tilde{A}f,g\rangle$ for every fixed $f,g\in K^2$. Via the map γ, it follows that

$$\lim_{\tau\to\infty}(Z_\tau^{1/2}f,Z_\tau^{1/2}g)=(A^{1/2}f,A^{1/2}g). \tag{6.5}$$

Conversely, if Eq. (6.5) is true for every $f,g\in K^2$, then $\tilde{Z}_\tau$ tends to $\tilde{A}$ in $\tilde{X}$.

Since Eq. (6.5) says that the expectation value of Z_τ tends to the expectation value of A as $\tau\to\infty$, it represents a convergence concept that is suitable for our purpose. It implies that both γ and its inverse γ^{-1} are continuous. Given the topology of $\tilde{X}$ and the fact that γ maps $\tilde{\Gamma}$ onto Γ, there is one and only one topology on Γ that makes γ and γ^{-1} continuous. Details about the open sets that determine this topology are in Ref. 2. With the topology that recognizes Eq. (6.5) as convergence on Γ, the set Γ becomes a topological space denoted by X. This is our space of observables A.

By a transcription of Eq. (6.5), a net $\{Z_\tau\}\in X$ tends to $A\in X$ as $\tau\to\infty$ if and only if $f,g\in K^2$ and $\epsilon>0$ determine $T>0$ such that

$$|(A^{1/2}f,A^{1/2}g)-(Z_\tau^{1/2}f,Z_\tau^{1/2}g)|<\epsilon \quad \text{if} \quad \tau>T.$$

We denote this relation by $\lim_{\tau\to\infty}Z_\tau=A$.

VII. THE TIME EVOLUTION

Given an operator $A\in X$, our goal is to show that there exist nets $\{Z_\tau\}$ $(\tau\geqslant 0)$ that tend to A as $\tau\to\infty$ while the $Z_\tau(t)$ with $t>0$ have the special properties required by the chaos theorems S, T, and P in Sec. VIII. For the proof we construct nets $\{\tilde{Z}_\tau\}$ that tend to $\tilde{A}$. These determine $Z_\tau=\gamma(\tilde{Z}_\tau)$ as desired. To control $\tilde{Z}_\tau(t)$, we need to know how the time evolution acts on K^2. To

simplify the notation, we denote $\exp(-iHt)$ by $U(t)$. Whether f is viewed as an element of ΠL^2 or K^2, the time evolution takes f into $f(t)=U(t)f$. The adjoint of $U(t)$ on ΠL^2 is denoted by $U^*(t)$. It acts as $\exp(iHt)$. The adjoint of $U(t)$ on K^2 is denoted by $U^\dagger(t)$. This operator differs from $U^*(t)$. Due to Eq. (5.4)

$$\langle U(t)f,U(t)g\rangle=\langle f,g\rangle, \tag{7.1}$$

so that $U(t)$ is an isometry on K^2. As a result the set $U(t)K^2$ is a subspace of K^2 which is closed in the K^2-norm. If $Q(t)$ denotes the orthogonal projection of K^2 onto $U(t)K^2$, it follows from general properties of isometries (Ref. 2. see Chap. V, Sec. 2) that

$$U(t)U^\dagger(t)=Q(t). \tag{7.2}$$

To investigate $U^\dagger(t)$ and the projection $Q(t)$, we decompose $U(t)$ according to Eq. (3.7) and take advantage of the close connection between the space G^2_ν and the Hardy space H^2 of the lower half-plane.[17] When $ke^{i\phi}$ varies in the sector $-\pi/2<\phi<0$, then $(ke^{i\phi})^2$ runs through the lower half-plane. Hence we define

$$v+iw:=k^2e^{2i\phi},\quad F(v+iw,w):=2^{-1}(ke^{i\phi})^{(\nu-2)/2}f_\nu(ke^{i\phi},\omega),$$

and similarly for $G(v+iw,\omega)$ in terms of g_ν. If $f_\nu,g_\nu\in G^2_\nu$,

$$\langle f_\nu,g_\nu\rangle=\int_{S^{\nu-1}}\int_{-\infty}^{\infty}F(v-i0,\omega)\tilde{G}(\nu-i0,\omega)\mathrm{d}v\ \mathrm{d}\omega.$$

The Fourier transform of F is

$$\hat{f}_\nu(s,\omega)=(2\pi)^{-1/2}\int_{-\infty}^{\infty}\exp(ivs)F(v-i0,\omega)\mathrm{d}v.$$

The function $F(v+iw,\omega)$ belongs to the space H^2 of the $(v+iw)$-variable if and only if $f_\nu\in G^2_\nu$. By the Paley–Wiener theorem[21] $\hat{f}_\nu(s,\omega)=0$ if $s<0$, for almost every $\omega\in S^{\nu-1}$.

Since the Fourier transform is unitary,

$$\langle f_\nu,g_\nu\rangle=\int_{S^{\nu-1}}\int_0^{\infty}\hat{f}_\nu(s,\omega)\overline{\hat{g}}_\nu(s,\omega)\mathrm{d}s\ \mathrm{d}\omega. \tag{7.3}$$

We derived this relation assuming that $f_\nu,g_\nu\in G^2_\nu$. Now recall that $f_\nu(k,\omega)\in K^2_\nu$ if and only if $f_\nu(k,\omega)$ is the boundary value of $f_\nu(ke^{i\phi},\omega)\in G^2_\nu$. Whether f_ν and g_ν are viewed as elements of G^2_ν or K^2_ν, the inner product $\langle f_\nu,g_\nu\rangle$ is the same. Hence there is a unitary map taking $f_\nu(k,\omega)\in K^2_\nu$ into $\hat{f}_\nu(s,\omega)\in L^2(\mathbb{R}^+\times S^{\nu-1})$ and Eq. (7.3) applies whenever $f_\nu,g_\nu\in K^2_\nu$.

The time evolution multiplies $f_\nu\in K^2_\nu$ by $\exp(-ik^2t)$ and $f_\nu(ke^{i\phi},\omega)\in G^2_\nu$ by $\exp(-ik^2e^{2i\phi}t)$. In the process $F(v+i0,\omega)$ is multiplied by $\exp(-ivt)$, taking $\hat{f}_\nu(s,\omega)$ into

$$(2\pi)^{-1/2}\int_{-\infty}^{\infty}\exp(ivs-ivt)F(v-i0,\omega)dv=\hat{f}_\nu(s-t,\omega).$$

It follows that

$$\begin{aligned}\langle\exp(-ik^2t)f_\nu,g_\nu\rangle&=\int_{S^{\nu-1}}\int_t^{\infty}\hat{f}_\nu(s-t,\omega)\overline{\hat{g}}_\nu(s,\omega)\mathrm{d}s\ \mathrm{d}\omega\\&=\langle f_\nu,[\exp(-ik^2t)]^\dagger g_\nu\rangle=\int_{S^{\nu-1}}\int_0^{\infty}\hat{f}_\nu(s,\omega)\overline{\hat{g}}_\nu(s+t,\omega)\mathrm{d}s\ \mathrm{d}\omega.\end{aligned} \tag{7.4}$$

Replacing ν by the appropriate channel subscript α, we may use Eq. (5.6) on the right-hand side in Eq. (7.4). For $f,g\in K^2$ it follows that

$$\begin{aligned}\langle U(t)f,g\rangle &= \sum_\alpha \int_{S_\alpha}\int_t^\infty \exp(-iE_\alpha t)\hat{f}_\alpha(s-t,\omega)\overline{\hat{g}}_\alpha(s,\omega)\mathrm{d}s\,\mathrm{d}\omega \\ &= \langle f,U^\dagger(t)g\rangle \\ &= \sum_\alpha \int_{S_\alpha}\int_0^\infty \hat{f}_\alpha(s,\omega)\exp(-iE_\alpha t)\overline{\hat{g}}_\alpha(s+t,\omega)\mathrm{d}s\,\mathrm{d}\omega. \end{aligned} \tag{7.5}$$

Replacing f by $U^\dagger(t)f$ gives

$$\langle Q(t)f,g\rangle = \sum_\alpha \int_{S_\alpha}\int_t^\infty \hat{f}_\alpha(s,\omega)\overline{\hat{g}}_\alpha(s,\omega)\mathrm{d}s\,\mathrm{d}\omega.$$

Since $Q(t)$ is an orthogonal projection

$$\|\|Q(t)f\|\|^2 = \sum_\alpha \int_{S_\alpha}\int_t^\infty |\hat{f}_\alpha(s,\omega)|^2\mathrm{d}s\,\mathrm{d}\omega.$$

This is a nonincreasing function of t which tends to 0 as $t\to\infty$.

The family $\{U(t)|0\leqslant t<\infty\}$ is a semigroup of operators on K^2. As in Ref. 2, it follows from the semigroup property and Eq. (7.2) that

$$Q(s)U(t) = \begin{cases} U(t) & \text{if } 0\leqslant s\leqslant t \\ U(t)Q(s-t) & \text{if } 0\leqslant t<s, \end{cases} \tag{7.6}$$

$$Q(s)Q(t) = Q(\max s,t). \tag{7.7}$$

If $A\in\Gamma$, it can be shown as in Ref. 2 that the quadratic form

$$q_t[f,g] := (A^{1/2}U(t)f, A^{1/2}U(t)g) = \langle U^\dagger(t)\tilde{A}U(t)f,g\rangle$$

with form domain K^2 is closable, and hence determines an operator $A_t\in\Gamma$. Moreover, A_t is equal to the self-adjoint operator $U^*(t)AU(t)$ with domain $U^*(t)\mathrm{Dom}(A)$. It follows that $U^*(t)AU(t)\in\Gamma$. We denote this operator by $A(t)$. It represents the observable A in the Heisenberg picture. Given a form $q[f,g]\in\Gamma_q$, we can extract $A\in\Gamma$, then construct $A(t)\in\Gamma$. Or we can replace f, g by $U(t)f, U(t)g$ to find q_t, then determine $A_t\in\Gamma$. Since the two procedures give the same result, the Heisenberg picture can be used without ambiguity. The operator in $\tilde{\Gamma}$ determined by $A(t)\in\Gamma$ is

$$\tilde{A}(t) := U^\dagger(t)\tilde{A}U(t).$$

The set Γ contains unbounded operators such as J. In particular, the operators Z_τ in the proofs of the chaos theorems are not bounded. It may happen that the domain of $A\in\Gamma$ is a proper subset of K^2 and that the domain of $A(t)$ depends on t. In that case the intersection $\cap_{t\geqslant 0}\mathrm{Dom}[A(t)]$ could be very small, so that there would be few vectors f allowing $(A(t)f,g)$ to be followed over the entire interval $0\leqslant t<\infty$. On the other hand, the operator $[A(t)]^{1/2}$ can be applied to every $f\in K^2$ at all times $t\geqslant 0$. Hence the notation of Eq. (6.1) can be used at all positive times, expressing the matrix elements of $A(t)\in\Gamma$ in the form

$$\langle f|A(t)|g\rangle = ([A(t)]^{1/2}f, [A(t)]^{1/2}g).$$

VIII. CHAOTIC OBSERVABLES

The previous sections provide the framework to show that the time evolution of a large class of observables in quantum mechanics exhibits chaos in the spirit of Devaney's definition of chaos in classical dynamical systems.[3] Among the three components of chaos listed in Sec. I, properties (T) and (P) are strictly topological. According to Devaney[3] a map $F: X \to X$ on a topological space X is topologically transitive if for any pair of open sets $V,\ W \in X$ there exists $n>0$ such that $F^{(n)}(V) \cap W \neq 0$. We replace points $x \in X$ by operators $A \in X$. The iterated map $x \to F^{(n)}(x)$ is replaced by the time evolution $A \to A(t)$. Our results on topological transitivity and periodic points are as follows.

Theorem T: (Topological transitivity) Given $A, B \in X$, there is a net $\{Z_\tau\} \in X(\tau \geqslant 0)$ such that

$$\lim_{\tau \to \infty} Z_\tau = A, \quad \lim_{\tau \to \infty} Z_\tau(\tau) = B.$$

The interpretation is that the time evolution takes Z_τ in a neighborhood V of A into $Z_\tau(\tau)$ in a neighborhood W of B.

Theorem P: (Existence of a dense set of periodic points) Given $A \in X$, there is a net $\{Z_\tau\} \in X(\tau \geqslant 0)$ such that

$$\lim_{\tau \to \infty} Z_\tau = A,$$

$$Z_\tau(t + n\tau) = Z_\tau(t), \quad \text{if } t \geqslant 0,\ n = 0,1,2,\ldots.$$

This theorem states that there is an operator $Z_\tau \in X$ with semiperiodic $Z_\tau(t)$ in any neighborhood of any $A \in X$.

According to Devaney[3] a map $F: X \to X$ on a metric space X has sensitive dependence on initial conditions if there exists $\delta > 0$ such that, for any $x \in X$ and any neighborhood V of x, there exists $y \in V$ and $n \geqslant 0$ such that $|F^{(n)}(x) - F^{(n)}(y)| > \delta$. Given $x, y \in X$ and the map $F^{(n)}$, the distance $|F^{(n)}(x) - F^{(n)}(y)|$ is determined by the metric that defines the topology of Devaney's X. Typical examples allow scaling, so that the actual magnitude of δ is not important. In our transcription δ may be any positive number. Because our X is not a metric space, we have to introduce a distance between operators as an additional quantity. Since one would like the distance between $A \in X$ and $B \in X$ to be large when the difference between expectation values is large, regardless of the wave function $f \in K^2$, we define

$$|A - B| := \inf_{f \in K^2} \|f\|^{-2} |\|A^{1/2} f\|^2 - \|B^{1/2} f\|^2|.$$

Notice that $|A - B|$ does not satisfy the triangle inequality, and hence does not determine a metric.

Theorem S: (Sensitive dependence on initial conditions). Given $A \in X$ and $\delta > 0$, there is a net $\{Z_{\delta\tau}\} \in X(\tau \geqslant 0)$ such that

$$\lim_{\tau \to \infty} Z_{\delta\tau} = A,$$

$$|\|A^{1/2}(t) f\|^2 - \|Z_{\delta\tau}^{1/2}(t) f\|^2| > \delta \|f\|^2 \quad \text{if } t \geqslant \tau, \text{ for all } f \in K^2.$$

Assuming that τ and δ are sufficiently large, Theorem S says that the expectation values of $A(t)$ and $Z_{\delta\tau}(t)$ are very close at time $t = 0$, yet very different at times $t \geqslant \tau$.

According to Devaney's definition, a map $F: X \to X$ is chaotic on X if F has sensitive dependence on initial conditions, is topologically transitive, and has a dense set of periodic points. Due to Theorems S, T, and P, the time evolution of operators $A(t) \in X$ is chaotic in the sense of Devaney.

Among Devaney's conditions for chaos, sensitive dependence is probably best known, suggesting that it is the most important concept. In actual fact, if the map F is continuous and X is a metric space, the two topological conditions imply sensitive dependence.[22] Alternative definitions of chaos have been proposed by several authors. As shown in a recent review with a comparison table,[23] various definitions are not equivalent. On the other hand, all definitions are meant to capture the same set of essential features, and these have been retained in Theorems S, T, and P.

The wording of Theorems S, T, and P is the same as in Ref. 2, only the space X and the time evolution $U(t)$ are different. The proofs in Ref. 2 construct operators $\tilde{Z}_\tau$ with suitable properties, then invoke the map γ to find operators Z_τ that satisfy the theorems. The sole relation used in the construction of $\tilde{Z}_\tau$ is the counterpart in Ref. 2 of Eqs. (7.6) and (7.7) for the time evolution. Because this counterpart is the same as the current equations, the proofs in Ref. 2 may be copied unchanged. To illustrate how the theorems work, we quote the respective operators $\tilde{Z}_\tau$. Further details are in Ref. 2.

The proof of Theorem S uses

$$\tilde{Z}_{\delta\tau} := \tilde{A} + (1+\tau)^{-1} + \delta Q(\tau).$$

The term $(1+\tau)^{-1}$ guarantees that the form $\langle \tilde{Z}_{\delta\tau} f, g\rangle$ on ΠL^2 with form domain K^2 is closed for every δ; τ. When τ is sufficiently large and f is fixed, $|||Q(\tau)f|||$ is small so that $\langle \tilde{Z}_{\delta\tau} f, g\rangle$ is close to $\langle \tilde{A} f, g\rangle$. At time $t \geqslant \tau$ we have to examine $U^\dagger(t)\tilde{Z}_{\delta\tau}U(t)$. By Eqs. (7.1) and (7.6)

$$U^\dagger(t)Q(\tau)U(t) = \begin{cases} Q(\tau - t) & \text{if } 0 \leqslant t \leqslant \tau \\ I & \text{if } 0 \leqslant \tau \leqslant t, \end{cases}$$

where I is the identity operator. Hence

$$|\langle \tilde{A}(t)f, f\rangle - \langle \tilde{Z}_{\delta\tau}(t)f, f\rangle| > \delta |||f|||^2 \geqslant \delta |||f|||^2$$

$$\text{if } t \geqslant \tau, \text{ for all } f \in K^2.$$

Theorem S now follows easily. Moreover, we see that the error term $\delta\langle U^\dagger(t)Q(\tau)U(t)f, f\rangle$ is a nondecreasing function of $t \geqslant 0$ which reaches its maximum $\delta |||f|||^2$ at time $t = \tau$.

The proof of Theorem T uses

$$\tilde{Z}_\tau := [1 - Q(\tau)]\tilde{A}[1 - Q(\tau)] + U(\tau)\tilde{B}U^\dagger(\tau) + (1+\tau)^{-1}.$$

Since $|||U^\dagger(\tau)f||| = |||Q(\tau)f|||$, the matrix element $\langle \tilde{Z}_\tau f, g\rangle$ is close to $\langle \tilde{A} f, g\rangle$ if τ is large. On the other hand, at time $t = \tau$ the operator $\tilde{A}$ acts on $[1 - Q(\tau)]U(\tau) = 0$ while $\tilde{B}$ acts on $U^\dagger(\tau)U(\tau) = I$. As a result $\langle \tilde{Z}_\tau(\tau) f, g\rangle$ is close to $\langle \tilde{B} f, g\rangle$.

The proof of Theorem P uses

$$\tilde{Z}_\tau = \sum_{n=0}^{\infty} U(n\tau)[1 - Q(\tau)]\tilde{A}[1 - Q(\tau)]U^\dagger(n\tau) + (1+\tau)^{-1}.$$

Write this in the form

$$\tilde{Z}_\tau = \sum_{n=0}^{\infty} \tilde{Z}_{\tau n} + (1+\tau)^{-1}.$$

The sum converges in the strong operator topology. Since

$$Q(\tau)U(n\tau) = U(n\tau) \quad \text{if } n \geqslant 1,$$

the terms $\tilde{Z}_{\tau n}$ with $n \geqslant 1$ are equal to $Q(\tau)\tilde{Z}_{\tau n}Q(\tau)$, and hence tend strongly to 0 if $\tau \to \infty$. For any fixed f and sufficiently large τ the norm $\|\|\tilde{Z}_\tau f - \tilde{Z}_{\tau 0} f\|\|$ is close to 0. Hence $\langle \tilde{Z}_\tau f, g\rangle$ is close to $\langle \tilde{A} f, g\rangle$.

Now examine $\Sigma_n U^\dagger(\tau)\tilde{Z}_{\tau n}U(\tau)$. The term with $n=0$ contains a factor $[1-Q(\tau)]U(\tau)$. Since this vanishes $\tilde{Z}_{\tau 0}(\tau)=0$. In the term with $n=1$ the operator $\tilde{A}$ acts on

$$[1-Q(\tau)]U^\dagger(\tau)U(\tau)=1-Q(\tau).$$

Hence $\tilde{Z}_{\tau 1}(\tau)=\tilde{Z}_{\tau 0}$. By a similar reasoning $\tilde{Z}_{\tau n}(\tau)=\tilde{Z}_{\tau,n-1}$ $(n=1,2,...)$. Also $U^\dagger(\tau)(1+\tau)^{-1}U(\tau)=(1+\tau)^{-1}$. It follows that $\tilde{Z}_\tau(\tau)=\tilde{Z}_\tau$. The argument can be repeated to show that $\tilde{Z}_\tau(t+m\tau)=\tilde{Z}_\tau(t)$ if $t \geqslant 0$ and $m=0,1,2,...$. Hence the operator $\tilde{Z}_\tau(t)$ is semiperiodic.

IX. NOTES AND REMARKS

The chaos concept in this paper was developed with the idea in mind that *K*-maps and *K*-flows are classical dynamical systems with chaotic properties that are well understood. The proofs of Theorems S, T, and P are inspired by the symbolic dynamics used in chaos proofs for Bernoulli systems and other *K*-maps in which the dynamics can be represented by a shift on sequences of symbols.[24–28] Wave functions in this paper are assumed to belong to the space K^2 because the time evolution $\{U(t)|0 \leqslant t < \infty\}$ on K^2 is unitarily equivalent to a semigroup of shift operators, as shown by Eq. (7.5). The semigroup on K^2 is probably our best substitute for a *K*-flow. By a result due to Sinai[29] the nonequilibrium part of a *K*-flow can be represented in terms of Hilbert spaces N and $L^2(\mathbb{R})\otimes N$ and a unitary group $\{V(t)|-\infty<t<\infty\}$ such that $\hat{g}(s) \in L^2(\mathbb{R})\otimes N$ transforms according to

$$(V(t)\hat{g})(s)=\hat{g}(s-t). \tag{9.1}$$

The same canonical form is used extensively in the Lax–Phillips scattering theory for the wave equation.[30]

The group $\{V(t)\}$ in Eq. (9.1) has self-adjoint generator $-id/ds$ with spectrum $(-\infty, \infty)$. We want to contrast this with the semigroup $\{U(t)\}$ on K^2 generated by H. To this end, we apply the reasoning developed in Ref. 2 to the resolvent $(H-\lambda)^{-1}$. By Eq. (5.6)

$$\langle (H-\lambda)^{-1}f, g\rangle = \sum_\alpha \langle (k_\alpha^2 + E_\alpha - \lambda)^{-1} f_\alpha, g_\alpha\rangle. \tag{9.2}$$

A function $(k_\alpha^2+E_\alpha-\lambda)^{-1}f_\alpha$ belongs to K_α^2 if and only if it has a square-integrable analytic continuation taking the k_α^2-variable into the lower half-plane. It follows that each operator $(k_\alpha^2 + E_\alpha - \lambda)^{-1}$ on the right-hand side in Eq. (9.2) is bounded if and only if $\mathrm{Im}\,\lambda > 0$. Hence $(H-\lambda)^{-1}$ is bounded if and only if $\mathrm{Im}\,\lambda > 0$. The spectrum of H on K^2 is the half-plane $\mathrm{Im}\,\lambda \leqslant 0$.

The foregoing implies that H cannot represent the energy on K^2. If there is an energy operator $\tilde{H}$ on K^2, it must have the same spectrum as H on ΠL^2. To identify $\tilde{H}$, we examine the form

$$q[f,g] := (Hf,g) = \langle (1+J^2)^{-1}Hf, g\rangle$$

as a quadratic form on K^2 with form domain $\mathrm{Dom}\,(q)$ consisting of all $f \in K^2$ with the property that $Hf \in \Pi L^2$. Since $\mathrm{Dom}\,(q)$ contains all $f \in K^2$ that can be written as $\Sigma_\alpha \Omega_\alpha \psi_\alpha f_\alpha$ with functions $f_\alpha(k_\alpha, \omega) \in K_\alpha^2$ such that $k_\alpha^2 f_\alpha(k_\alpha, \omega) \in L^2(\mathbb{R}^\nu)$, properties of the spaces K_α^2 can be used to show that $\mathrm{Dom}\,(q)$ is dense in K^2. Now consider the operator $(1+J^2)^{-1}H$ on K^2 with domain $\mathrm{Dom}\,(q)$. This operator is symmetric and bounded below, due to properties of H on ΠL^2. Hence the form q has a well-defined closure $\overline{q}$ (Ref. 20, see Chap. VI, Sec. 1). The closed form $\overline{q}$ determines a self-adjoint operator $\tilde{H}$ on K^2 satisfying

$$\overline{q}[f,g]=\langle \tilde{H}f,g\rangle$$

for every $f\in \mathrm{Dom}\,(\tilde{H})\subset \mathrm{Dom}\,(\overline{q})$ and $g\in \mathrm{Dom}\,(\overline{q})$. The operator $\tilde{H}$ is the Friedrichs extension of $(1+J^2)^{-1}H$ (Ref. 20, see Chap. VI, Sec. 2). Since $\tilde{H}$ is an extension, $\mathrm{Dom}\,(\tilde{H})\supset \mathrm{Dom}\,(q)$. For $f,g\in \mathrm{Dom}\,(q)$,

$$(Hf,g)=\langle \tilde{H}f,g\rangle.$$

It is a significant property of the space K^2 that it gives rise to a time evolution whose generator H differs from the energy operator $\tilde{H}$.

If $A\in X$ is a bounded operator on ΠL^2, then $\tilde{A}$ defined by Eq. (6.3) equals $(1+J^2)^{-1}A$. By the same token, if $\tilde{A}\in\tilde{X}$ is the identity operator on K^2, then $A^{1/2}$ equals $(1+J^2)^{1/2}$, so that $A\in X$ equals $1+J^2$. It follows that the terms $(1+\tau)^{-1}$ in the operators $\tilde{Z}_\tau$ make unbounded contributions to the corresponding Z_τ on ΠL^2. The terms in question are included to guarantee that the form $\langle \tilde{Z}_\tau f,g\rangle$ on ΠL^2 with form domain K^2 is closed. It appears that we cannot avoid unbounded operators on ΠL^2. To take advantage of the special properties of the space K^2, we have to allow operators such as J whose domains are no larger than K^2. Such operators are not bounded on ΠL^2.

X. OTHER CHAOS CONCEPTS

Since operators in X have to be positive and are not necessarily bounded on ΠL^2, the elements of X do not give rise to an algebra. Hence the set of operators in this paper differs substantially from the operator algebras used by several authors to define noncommutative K-systems.[31–34] In an algebraic K-system[31,32,34] a sequence of operator-subalgebras replaces the σ-subalgebras of measurable sets that determine a classical K-system. An entropic K-system[33] is characterized in terms of its quantum dynamical entropy.[35] While these definitions are not equivalent,[36] all authors report mixing behavior characteristic of chaos.[31,32,37–42] In cases where spectral properties were investigated[31,32,39,41] there was agreement with Eq. (9.1).

Examples include a quantum version of the Arnold cat map.[39–42] Several statistical-mechanics models were shown[43] to be entropic K-systems. Because classically the Kolmogorov–Sinai entropy being positive indicates chaos, it was proposed[44] that quantum chaos is related to a positive quantum dynamical entropy. It was found, however,[44] that the quantum dynamical entropy vanishes in the case of a system of finitely many particles described by a density matrix with unitary time evolution. Such a system is therefore not chaotic from the dynamical-entropy point of view.

In typical papers on quantum chaos the question is not whether a system is chaotic in the sense of a mathematical definition. Starting from a chaotic classical system, one constructs a quantum counterpart and looks for characteristic features that would be different if the underlying classical system were integrable.[45–49] The distribution of energy-level spacings is an example. Computer calculations[50,51] show that the energy levels of a classically chaotic quantum billiard agree with a level-spacing distribution that is well established in nuclear physics[52] and in that context can be derived from random matrix theory.[53] If the billiard is classically integrable, a Poisson distribution applies.[54] That the classically chaotic case agrees with the predictions of random matrix theory has been explained[55] with the help of semiclassical path integrals that relate periodic orbits of a classical system to spectral properties of its quantum counterpart.[46] A more recent argument[56] arrives at the same conclusion on the basis of a supersymmetric field theory.[57]

Since a particle on a quantum billiard is confined to a bounded region in space, its energy spectrum is purely discrete. To investigate continuous spectra, several authors have developed scattering theories for classically chaotic systems in unbounded regions.[58–62] In this context random matrix theory was shown to apply to statistical properties of scattering amplitudes. These investigations are of practical interest because billiards with external leads are used as models for mesoscopic semiconductor devices.[49,63]

Since there is strong evidence that random matrix theory applies to nuclear physics[52] it might apply as well to a system of N distinguishable particles. One would like to know whether the results of this paper can be related to quantum chaos as studied in the literature.

XI. DENSITY OPERATORS

Whether chaos is related to irreversible behavior is a question with a long history. Boltzmann[64] implicitly invoked the assumption of molecular chaos in the 1872 proof of his H-theorem. Since K-systems are both chaotic and reversible, it is clear that chaos is not sufficient for irreversible behavior, yet many authors believe that chaos at the microscopic level promotes macroscopic irreversibility. Essentially, however, this is an open problem.

It is shown in the following sections that states in the space K^2 give rise to irreversible behavior that can be characterized in terms of an increasing entropy. Although chaos as such does not play a role in the proof, there is a connection in that the space K^2 provides the framework to describe chaotic as well as irreversible properties of scattering systems.

Let ρ be a positive operator in the trace class on ΠL^2 with time evolution $\rho(t)$ defined by Eq. (1.1). Since the entropy $S[\rho(t)]$ does not depend on t, we want to replace $\rho(t)$ by the density operator $\sigma(t)$ defined by Eq. (1.5) and show that $S[\sigma(t)]$ increases. With this objective in mind, we first examine the set of all positive operators R in the trace class on ΠL^2. Any R in this set acts on $f \in \Pi L^2$ according to

$$Rf = \sum_n \mu_n \phi_n (f, \phi_n),$$

where $\{\phi_n\}$ is an orthonormal set on ΠL^2 and the μ_n are positive numbers satisfying $\mathrm{Tr}\, R = \Sigma_n \mu_n < \infty$.

Given the set $\{\phi_n\}$ on ΠL^2, the set $\{(1+J^2)^{-1/2}\phi_n\}$ is orthonormal on K^2. Hence $\tilde{\rho}$ acting on $f \in K^2$ as

$$\tilde{\rho} f = \sum_n \mu_n (1+J^2)^{-1/2} \phi_n \langle f, (1+J^2)^{-1/2} \phi_n \rangle \tag{11.1}$$

belongs to the trace class on K^2, satisfying

$$\langle \mathrm{Tr}\, \tilde{\rho} \rangle = \mathrm{Tr}\, R. \tag{11.2}$$

Given R and $\tilde{\rho}$, we now consider ρ acting on $f \in \Pi L^2$ as

$$\rho f = \sum_n \mu_n (1+J^2)^{-1/2} \phi_n (f, [1+J^2]^{-1/2} \phi_n). \tag{11.3}$$

This operator satisfies

$$\rho = (1+J^2)^{-1/2} R (1+J^2)^{-1/2}. \tag{11.4}$$

It can be shown as in Ref. 1 that a density operator ρ on ΠL^2 is of the form (11.4) with some positive operator R in the trace class if and only if ρ and $J\rho$ belong to the trace class and ρJ and $J\rho J$ have closures in the trace class. The operator R is the closure of $(1+J^2)^{1/2}\rho(1+J^2)^{1/2}$, and

$$\mathrm{Tr}\, R = \mathrm{Tr}\, \rho + \mathrm{Tr}\, J\rho J. \tag{11.5}$$

The relation (1.4) follows from Eqs. (11.2) and (11.5). Henceforth we simply refer to $J\rho J$ when we actually mean its closure, and similarly for operators such as ρJ and $\rho(1+J^2)^{1/2}$.

If A is an operator in Γ, then $A^{1/2}(1+J^2)^{-1/2}$ is bounded. Assuming that ρ is of the form (11.4) we examine the operator

$$T := A^{1/2}(1+J^2)^{-1/2} R [A^{1/2}(1+J^2)^{-1/2}]^*.$$

Since R belongs to the trace class, so does T. When applied to an element of K^2, the operator T acts as $A^{1/2}\rho A^{1/2}$. Hence $A^{1/2}\rho A^{1/2}$ is closable with closure T. In the following we simply write $A^{1/2}\rho A^{1/2}$ when the closure is meant.

If ρ is normalized so that $\mathrm{Tr}\,\rho = 1$, then $\mathrm{Tr}(A^{1/2}\rho A^{1/2})$ is the expectation value of the observable A in the state ρ. To show this, we assume that ρ has orthonormal eigenvectors r_n with eigenvalues λ_n. If ρ is of the form (11.4) each r_n belongs to K^2. Hence for any $f \in \Pi L^2$,

$$A^{1/2}\rho A^{1/2} f = \sum_n \lambda_n A^{1/2} r_n (f, A^{1/2} r_n).$$

It follows easily that

$$\mathrm{Tr}(A^{1/2}\rho A^{1/2}) = \sum_n \lambda_n (A^{1/2} r_n, A^{1/2} r_n).$$

The eigenvalue λ_n is the probability that the system is in the state r_n. The expectation value of A in this state is $(A^{1/2} r_n, A^{1/2} r_n)$. Hence $\mathrm{Tr}(A^{1/2}\rho A^{1/2})$ can be interpreted as the expectation value of A in the mixed state ρ.

Let $\{\chi_m\}$ be a complete orthonormal set on ΠL^2. If we expand ρ as in Eq. (11.3), the expectation value of A takes the form

$$\begin{aligned}
\mathrm{Tr}(A^{1/2}\rho A^{1/2}) &= \sum_m (A^{1/2}\rho A^{1/2}\chi_m, \chi_m) \\
&= \sum_m \sum_n \mu_n |(A^{1/2}[1+J^2]^{-1/2}\phi_n, \chi_m)|^2 \\
&= \sum_n \mu_n \|A^{1/2}(1+J^2)^{-1/2}\phi_n\|^2 \\
&= \sum_n \mu_n \|\,|(1+J^2)^{-1/2} A^{1/2}(1+J^2)^{-1/2}\phi_n|\,\|^2 \\
&= \sum_n \mu_n \langle \tilde{A}(1+J^2)^{-1/2}\phi_n, (1+J^2)^{-1/2}\phi_n\rangle = \langle \mathrm{Tr}\,\tilde{A}\tilde{\rho}\rangle.
\end{aligned}$$

This generalizes Eq. (6.4) and indicates that $\tilde{\rho}$ is the density operator on K^2 that matches ρ of the form (11.4) on ΠL^2.

Our problem is that the entropy $S[\rho(t)]$ does not depend on t if ρ is a density operator on ΠL^2. The time evolution on K^2 replaces $(1+J^2)^{-1/2}\phi_n$ by $U(t)(1+J^2)^{-1/2}\phi_n$. As a result $\tilde{\rho}$ is replaced by $U(t)\tilde{\rho}U^\dagger(t)$. Since $U(t)$ is an isometry on K^2, the entropy $-\langle \mathrm{Tr}\tilde{\rho}(t)\ln\tilde{\rho}(t)\rangle$ does not depend on $t \geqslant 0$ either. In Sec. XII we therefore take a partial trace of $\tilde{\rho}$ as in Eq. (1.5). This defines the density operator $\sigma(t)$ with increasing entropy $S[\sigma(t)]$.

XII. THE DENSITY OPERATOR σ

If ρ is of the form (11.4) and $t > 0$, there is an operator $R(t)$ in the trace class on ΠL^2 such that $\rho(t)$ satisfies Eq. (11.4) with $R(t)$ instead of R. Moreover,

$$J\rho(t)J = \exp(iHt) W(t) J\rho J W^*(t) \exp(-iHt). \tag{12.1}$$

These properties follow from Eq. (5.4). A formal proof with attention to all domain questions can be conducted as in Ref. 1. Since $W(t)$ is unitary, $\mathrm{Tr}\, J\rho(t)J$ does not depend on t. Hence $\mathrm{Tr}\,\sigma(t)$ does not depend on t.

While $\mathrm{Tr}\,\rho^2(t)$ does not depend on t either, $\mathrm{Tr}\,\sigma^2(t)$ is a decreasing function of $t \geqslant 0$,

$$\mathrm{Tr}\,\sigma^2(s) > \mathrm{Tr}\,\sigma^2(t) \quad \text{if} \quad 0 \leqslant s < t. \tag{12.2}$$

To show this, we deduce from Eq. (5.5) that

$$\Omega_\alpha \Omega_\alpha^* J^{1/2} \exp(-iHt) f = W^{1/2}(t)\Omega_\alpha \exp(-k_\alpha^2 t) J_\alpha^{1/2} \Omega_\alpha^* f$$

for every $f \in K^2$. This relation can be used to prove that

$$\Omega_\alpha \Omega_\alpha^* J^{1/2} \rho(t) J^{1/2} \Omega_\beta \Omega_\beta^* = W^{1/2}(t)\Omega_\alpha \exp(-k_\alpha^2 t) T_{\alpha\beta} \exp(-k_\beta^2 t) \Omega_\beta^* [W^{1/2}(t)]^*,$$

where we have used the abbreviation

$$T_{\alpha\beta} := J_\alpha^{1/2} \Omega_\alpha^* \rho \Omega_\beta J_\beta^{1/2}.$$

As in Ref. 1,

$$\mathrm{Tr}\,\rho(t)J\rho(t)J = \mathrm{Tr}[J^{1/2}\rho(t)J^{1/2}][J^{1/2}\rho(t)J^{1/2}]. \tag{12.3}$$

Let us define

$$\Pi_n := \sum_{\alpha \leqslant n} \Omega_\alpha \Omega_\alpha^*. \tag{12.4}$$

Even if the number of channels is not finite, Π_n tends strongly to the identity operator on ΠL^2 as $n \to \infty$. Hence it follows from known properties of the trace class (Ref. 65, Chap III, Theorem 6.3) that

$$\mathrm{Tr}\,\Pi_n [J^{1/2}\rho(t)J^{1/2}]\Pi_n [J^{1/2}\rho(t)J^{1/2}]\Pi_n \tag{12.5}$$

tends to the right-hand side of Eq. (12.3) when $n \to \infty$. We want to prove that $\mathrm{Tr}\,\rho(t)J\rho(t)J$ is a decreasing function of t. For this it is sufficient to show that

$$\mathrm{Tr}\,\Omega_\alpha \exp(-k_\alpha^2 t) T_{\alpha\beta} \exp(-k_\beta^2 t) \Omega_\beta^* \Omega_\beta \exp(-k_\beta^2 t) T_{\beta\alpha} \exp(-k_\alpha^2 t) \Omega_\alpha^* \tag{12.6}$$

is decreasing for every fixed α, β.

The projection operator $\Omega_\beta^* \Omega_\beta$ commutes with $\exp(-k_\beta^2 t)$ and with the operator $J_\beta^{1/2}$ included in $T_{\beta\alpha}$. Hence it can be absorbed in $T_{\beta\alpha}$. With a similar procedure for $\Omega_\alpha^* \Omega_\alpha$, it follows that expression (12.6) is equal to

$$\mathrm{Tr} \exp(-k_\alpha^2 t) T_{\alpha\beta} \exp(-2k_\beta^2 t) T_{\beta\alpha} \exp(-k_\alpha^2 t).$$

In an obvious notation, we denote this quantity by $\mathrm{Tr}\,\Theta_{\alpha\beta\alpha}(t)$. It is equal to $\mathrm{Tr}\,\Theta_{\beta\alpha\beta}(t)$.

Now suppose $0 \leqslant s < t$ and examine

$$\begin{aligned}
&\mathrm{Tr}\,\Theta_{\alpha\beta\alpha}(s) + \mathrm{Tr}\,\Theta_{\beta\alpha\beta}(s) - \mathrm{Tr}\,\Theta_{\alpha\beta\alpha}(t) - \mathrm{Tr}\,\Theta_{\beta\alpha\beta}(t) \\
&\quad = \mathrm{Tr} \exp(-k_\alpha^2 s) T_{\alpha\beta} [\exp(-2k_\beta^2 s) - \exp(-2k_\beta^2 t)] T_{\beta\alpha} \exp(-k_\alpha^2 s) \\
&\qquad + \mathrm{Tr} \exp(-k_\beta^2 s) T_{\beta\alpha} [\exp(-2k_\alpha^2 s) - \exp(-2k_\alpha^2 t)] T_{\alpha\beta} \exp(-k_\beta^2 s) \\
&\qquad + \mathrm{Tr} \exp(-k_\alpha^2 t) T_{\alpha\beta} [\exp(-2k_\beta^2 s) - \exp(-2k_\beta^2 t)] T_{\beta\alpha} \exp(-k_\alpha^2 t) \\
&\qquad + \mathrm{Tr} \exp(-k_\beta^2 t) T_{\beta\alpha} [\exp(-2k_\alpha^2 s) - \exp(-2k_\alpha^2 t)] T_{\alpha\beta} \exp(-k_\beta^2 t).
\end{aligned} \tag{12.7}$$

If $s<t$, the operators $\exp(-2k_\beta^2 s)-\exp(-2k_\beta^2 t)$ and $\exp(-2k_\alpha^2 s)-\exp(-2k_\alpha^2 t)$ are strictly positive. Since $T_{\beta\alpha}=T_{\alpha\beta}^*$, expression (12.7) vanishes if and only if $T_{\alpha\beta}=0$. If $T_{\alpha\beta}\neq 0$, the traces in Eq. (12.7) are positive. Repeating this reasoning for all α, β, we see that expression (12.5) is a decreasing function of t unless $T_{\alpha\beta}=0$ for all $\alpha,\beta\leqslant n$. Since any positive ρ gives rise to some nonvanishing operators $T_{\alpha\beta}$, it follows with Eq. (12.3) that

$$\operatorname{Tr}\rho(s)J\rho(s)J>\operatorname{Tr}\rho(t)J\rho(t)J \quad \text{if} \quad 0\leqslant s<t,$$

whenever ρ is of the form (11.4) with a positive trace-class operator R.

By Eq. (12.1) $\operatorname{Tr}[J\rho(t)J][J\rho(t)J]$ does not depend on t. Hence

$$\operatorname{Tr}\sigma^2(t)=\operatorname{Tr}\rho^2+\operatorname{Tr}\rho(t)J\rho(t)J+\operatorname{Tr}J\rho(t)J\rho(t)+\operatorname{Tr}(J\rho J)(J\rho J).$$

Two terms on the right do not depend on t while the remaining two are decreasing. Hence $\operatorname{Tr}\sigma^2(t)$ is decreasing, as we wanted to show.

Let $v(t)$ be a positive operator satisfying $\operatorname{Tr}v(t)=1$. The quantities

$$S_\alpha[v(t)]:=(1-\alpha)^{-1}\ln\operatorname{Tr}[v(t)]^\alpha \quad (\alpha>0;\alpha\neq 1)$$

are called Rényi entropies or α-entropies. [Ref. 66, Definition 2.2.2, Remark 2.2.5; Ref. 67, Eq. (7.14).] Taking $\alpha=2$ and $v(t)=\sigma(t)/\operatorname{Tr}\sigma(t)$, we have an increasing Rényi entropy $S_2[\sigma(t)/\operatorname{Tr}\sigma(t)]$.

XIII. THE ENTROPY

If T is any positive compact operator, we denote by $\gamma_n(T)$ the nth largest eigenvalue of T, counting multiplicity. If ρ and $J\rho J$ belong to the trace class

$$\sum_n \gamma_n(\rho)<\infty, \quad \sum_n \gamma_n(J\rho J)<\infty. \tag{13.1}$$

With a view to the entropy, we define

$$s(\gamma):=\begin{cases}-\gamma\ln\gamma & \text{if} \quad \gamma>0\\ 0 & \text{if} \quad \gamma=0\end{cases}$$

and assume

$$\begin{aligned}S(\rho)&:=\sum_n s[\gamma_n(\rho)]<\infty,\\ S(J\rho J)&:=\sum_n s[\gamma_n(J\rho J)]<\infty.\end{aligned} \tag{13.2}$$

Due to Eq. (5.4) and the fact that $\exp(iHt)$ and $W(t)$ are unitary, $S[\rho(t)]$ and $S[J\rho(t)J]$ do not depend on t.

By general entropy inequalities[68]

$$S[\sigma(t)]\leqslant S[\rho(t)]+S[J\rho(t)J] \tag{13.3}$$

with equality if and only if

$$\rho(t)J\rho(t)J=0, \quad J\rho(t)J\rho(t)=0.$$

The sum $S(\rho)+S(J\rho J)$ is finite by Eq. (13.2). It is an upper bound for $S[\sigma(t)]$ by Eq. (13.3). We claim that

$$\lim_{t\to\infty} S[\sigma(t)] = S(\rho) + S(J\rho J). \tag{13.4}$$

Typically, $\rho J\rho J \neq 0$, hence $S[\sigma(t)]$ has to increase, approaching its least upper bound as $t\to\infty$.

The relations (13.3) and (13.4) are compatible due to the fact that $\rho(t)J\rho(t)J$ and its adjoint $J\rho(t)J\rho(t)$ tend to 0 in the trace norm as $t\to\infty$. To show this, we denote the trace norm of an operator T in the trace class by $\|T\|_1$. By Eq. (5.4)

$$\begin{aligned}\|J\rho(t)J[\Pi_n\rho(t)-\rho(t)]\|_1 &= \|\exp(iHt)W(t)J\rho JW^*(t)\exp(-2iHt)(\Pi_n\rho-\rho)\exp(iHt)\|_1 \\ &\leqslant \|J\rho J\|\|\Pi_n\rho-\rho\|_1,\end{aligned}$$

where Π_n is the projection defined by Eq. (12.4). Since the right-hand side tends to 0 as $n\to\infty$, uniformly in t, it is sufficient to show that $J\rho(t)J\Omega_\alpha\Omega_\alpha^*\rho(t)$ tends to 0 in the trace norm as $t\to\infty$, for every fixed α. Since $J^{1/2}$ commutes with $\Omega_\alpha\Omega_\alpha^*$, it follows with Eq. (5.5) that

$$\begin{aligned}J\rho(t)J\Omega_\alpha\Omega_\alpha^*\rho(t) &= J\rho(t)J^{1/2}\Omega_\alpha\Omega_\alpha^*J^{1/2}\rho(t) \\ &= \exp(iHt)W(t)J\rho\Omega_\alpha J_\alpha^{1/2}\exp(-2k_\alpha^2 t)J_\alpha^{1/2}\Omega_\alpha^*\rho\exp(iHt) \\ &= \exp(iHt)W(t)J\rho J^{1/2}\Omega_\alpha\exp(-2k_\alpha^2 t)\Omega_\alpha^*J^{1/2}\rho\exp(iHt).\end{aligned} \tag{13.5}$$

The operator $\exp(-2k_\alpha^2 t)$ tends strongly to 0 as $t\to\infty$. Since $\Omega_\alpha^*J^{1/2}\rho$ belongs to the trace class and $J\rho J^{1/2}\Omega_\alpha$ is bounded, the expression on the right in Eq. (13.5) tends to 0 in the trace norm, as we wanted to show.

The proof of Eq. (13.4) rests on a fundamental concept of physics. To explain this, we have to go back to the dilation operator D_ν of Sec. IV. Let $P_{\nu+}$ and $P_{\nu-}$ be the spectral projections onto the subspaces of $L^2(\mathbb{R}^\nu)$ in which D_ν is positive and negative, respectively. The important equations are[69]

$$\begin{aligned}\lim_{t\to\infty}\|P_{\nu-}\exp(-ik^2t)f\| &= 0, \\ \lim_{t\to-\infty}\|P_{\nu+}\exp(-ik^2t)f\| &= 0\end{aligned} \tag{13.6}$$

for every $f(\mathbf{k})\in L^2(\mathbb{R}^\nu)$. If $f\in K_\nu^2$, it follows with Eq. (4.5) that

$$\lim_{t\to\infty}\|P_{\nu+}J_\nu\exp(-ik^2t)f\| = 0.$$

Hence $\exp(-ik^2t)f$ and $J_\nu\exp(-ik^2t)f$ become mutually orthogonal as $t\to\infty$.

The dilation operator is the quantum analog of $\mathbf{x}\cdot\mathbf{k}$, where $\mathbf{x}$ represents the position relative to the center of mass and $\mathbf{k}$ is proportional to the momentum of a multiparticle system. One expects that $\mathbf{x}\cdot\mathbf{k}$ was negative in the distant past and will be positive in the remote future. This is confirmed by Eq. (13.6). It is the irreversible aspect of the time evolution that causes $S[\sigma(t)]$ to tend to its least upper bound.

The generalization to a scattering system goes as follows. Depending on the channel being considered, D_ν is denoted by D_α, giving rise to the generalized dilation operator

$$D := \sum_\alpha \Omega_\alpha D_\alpha \Omega_\alpha^*.$$

For any $f\in K^2$, it is easy to show that $Jf = \exp(-\pi D/2)f$. The projection operators $P_{\nu\pm}$ are denoted by $P_{\alpha\pm}$. They determine orthogonal projections

$$P_{\pm} := \sum_{\alpha} \Omega_{\alpha} P_{\alpha\pm} \Omega_{\alpha}^{*}$$

satisfying $P_{+} + P_{-} = \Sigma_{\alpha} \Omega_{\alpha} \Omega_{\alpha}^{*} = \Pi$. By Eq. (5.1) and the intertwining relation (3.5), any $f \in \Pi L^2$ satisfies

$$\lim_{t\to\infty} \| P_{-} \exp(-iHt) f \| = 0,$$
$$\lim_{t\to-\infty} \| P_{+} \exp(-iHt) f \| = 0. \tag{13.7}$$

If $f \in K^2$, if follows from Eq. (5.4) that

$$\lim_{t\to\infty} \| P_{+} J \exp(-iHt) f \| = 0. \tag{13.8}$$

Given the interpretation of the dilation operators D_{α}, Eq. (13.7) expresses the fact that clusters in a scattering experiment moved in the direction of the center of mass in the distant past and will move away from the center of mass in the remote future.

The above-mentioned relations are the key ingredients in proving Eq. (13.4). Since the proof is the same as in Ref. 1, we sketch the general idea, referring to Ref. 1 for details.

The first step defines

$$\pi_{+}(t) := P_{+} \rho(t) P_{+}, \quad \pi_{-}(t) := P_{-} J \rho(t) J P_{-}$$

and shows that

$$\lim_{t\to\infty} \| \pi_{+}(t) + \pi_{-}(t) - \sigma(t) \|_1 = 0.$$

It follows that

$$\lim_{t\to\infty} \gamma_k[\pi_{+}(t) + \pi_{-}(t)] = \lim_{t\to\infty} \gamma_k[\sigma(t)].$$

By a separate argument

$$\lim_{t\to\infty} \gamma_k[\pi_{+}(t) + \pi_{-}(t)] = \lambda_k,$$

where λ_k ($k = 1,2,...$) is the kth largest number, counting multiplicity, in the set consisting of all nonvanishing eigenvalues $\gamma_n(\rho)$ and $\gamma_m(J\rho J)$ ($m,n = 1,2,...$).

We want to compare the entropies

$$S(\rho) + S(J\rho J) = \sum_{k} s(\lambda_k) = \sum_{k} \lim_{t\to\infty} s\{\gamma_k[\sigma(t)]\} \tag{13.9}$$

and

$$\lim_{t\to\infty} S[\sigma(t)] = \lim_{t\to\infty} \sum_{k} s\{\gamma_k[\sigma(t)]\}. \tag{13.10}$$

To prove that $S[\sigma(t)]$ tends to $S(\rho) + S(J\rho J)$, it is sufficient to show that the limit and the summation in Eq. (13.10) may be interchanged. In this context, it can be shown that

$$0 \leqslant s\{\gamma_{k+1}[\sigma(t)]\} \leqslant s(2\lambda_k)$$

whenever $2\lambda_k \leqslant 1/e$. Since $\Sigma_k s(2\lambda_k)$ converges absolutely by Eqs. (13.1) and (13.2), the right-hand sides of Eqs. (13.9) and (13.10) are equal by the dominated convergence theorem. This completes the proof of Eq. (13.4). The result is summarized in the following theorem.

Theorem E: (Entropy increase) If ρ is of the form (11.4), $\sigma(t)$ and $S[\sigma(t)]$ are defined by Eqs. (1.5) and (1.2), and Eq. (13.2) is satisfied, the entropy $S[\sigma(t)]$ tends to its maximum possible value $S(\rho)+S(J\rho J)$ as $t \to \infty$.

XIV. RECONSTRUCTING THE DENSITY OPERATOR ρ

With the help of the Mellin transform, it is possible to recover ρ when σ is known. For the reconstruction procedure to be meaningful, σ has to be of the form $\rho + J\rho J$ with a positive trace-class operator ρ satisfying Eq. (11.4). It was shown in Ref. 1 that not all positive operators in the trace class satisfy the conditions on σ. In particular, there are examples of positive τ in the trace class that would yield nonpositive ρ. This paper is not meant for such operators τ. They cannot occur as operators σ.

Given ρ, let us first examine $\Omega_\alpha^* \rho \Omega_\beta$. Since ρ belongs to the trace class on ΠL^2, both ρ and $\Omega_\alpha^* \rho \Omega_\beta$ are integral operators. In the notation of Eq. (5.1), the integral kernel of $\Omega_\alpha^* \rho \Omega_\beta$ is of the form

$$\psi_\alpha(\mathbf{k}'_\alpha)\rho_{\alpha\beta}(\mathbf{k}_\alpha;\mathbf{l}_\beta)\overline{\psi}_\beta(\mathbf{l}'_\beta).$$

It is convenient to write $\Omega_\alpha^* \rho \Omega_\beta = \psi_\alpha \rho_{\alpha\beta} \overline{\psi}_\beta$. Expressing $\mathbf{k}_\alpha, \mathbf{l}_\beta$ in terms of spherical polar coordinates replaces $\rho_{\alpha\beta}(\mathbf{k}_\alpha;\mathbf{l}_\beta)$ by $\rho_{\alpha\beta}(k_\alpha,\omega_\alpha;l_\beta,\omega'_\beta)$. The Mellin transform M_α acting on k_α commutes with $\psi_\alpha(\mathbf{k}'_\alpha)$. Henceforth we omit the variable $\mathbf{k}'_\alpha$. Thus

$$M_\alpha \Omega_\alpha^* \rho \Omega_\beta M_\beta^{-1} = \psi_\alpha M_\alpha \rho_{\alpha\beta} M_\beta^{-1} \overline{\psi}_\beta = \psi_\alpha \rho^\#_{\alpha\beta} \overline{\psi}_\beta$$

has integral kernel

$$\psi_\alpha \rho^\#_{\alpha\beta}(u,\omega_\alpha;v,\omega^*_\beta)\overline{\psi}_\beta. \tag{14.1}$$

By Eq. (4.2) $M_\alpha J_\alpha M_\alpha^{-1}$ acts as multiplication by $\exp(-\pi u/2)$. Hence $M_\alpha J_\alpha \Omega_\alpha^* \rho \Omega_\beta J_\beta M_\beta^{-1}$ has integral kernel

$$\psi_\alpha \exp(-\pi u/2)\rho^\#_{\alpha\beta}(u,\omega_\alpha;v,\omega'_\beta)\exp(-\pi v/2)\overline{\psi}_\beta. \tag{14.2}$$

Adding expressions (14.1) and (14.2) shows that $M_\alpha \Omega_\alpha^* \sigma \Omega_\beta M_\beta^{-1}$ has integral kernel

$$\psi_\alpha\{1+\exp[-\pi(u+v)/2]\}\rho^\#_{\alpha\beta}(u,\omega_\alpha;v,\omega'_\beta)\overline{\psi}_\beta. \tag{14.3}$$

Conversely, suppose σ is known. Construct the integral operator $M_\alpha \Omega_\alpha^* \sigma \Omega_\beta M_\beta^{-1}$. By the reasoning for ρ, the integral kernel is of the form

$$\psi_\alpha \sigma^\#_{\alpha\beta}(u,\omega_\alpha;v,\omega'_\beta)\overline{\psi}_\beta.$$

This quantity must be equal to expression (14.3). Hence

$$\rho^\#_{\alpha\beta}(u,\omega_\alpha;v,\omega'_\beta) = \{1+\exp[-\pi(u+v)/2]\}^{-1}\sigma^\#_{\alpha\beta}(u,\omega_\alpha;v,\omega'_\beta), \tag{14.4}$$

showing that there is a bounded transformation taking $\sigma^\#_{\alpha\beta}$ into $\rho^\#_{\alpha\beta}$.

Once $\rho^{\#}_{\alpha\beta}$ is known, the inverse Mellin transform determines $M_\alpha^{-1}\rho^{\#}_{\alpha\beta}M_\beta=\rho_{\alpha\beta}$, hence $\Omega^*_\alpha\rho\Omega_\beta$. Denoting $\Sigma_{\alpha\leqslant n}\,\Omega_\alpha\Omega^*_\alpha$ by Π_n as in Eq. (12.4), we can find $\Pi_n\rho\Pi_n$. This quantity tends to ρ in the trace norm as $n\to\infty$ (Ref. 65, Chap. III, Theorem 6.3). Hence, even if the number of channels is infinite, σ completely determines ρ.

If ρ is of the form (11.4) then $\rho(t)$ is of this form for all $t\geqslant 0$. Since neither the transformation taking ρ into σ, nor the Mellin transform depends on t, the reasoning that proved Eq. (14.4) can be repeated for every $t>0$. Summarizing, we have a linear transformation $L:\sigma(t)=L\rho(t)$ whose domain consists of all operators ρ of the form (11.4). This operator is invertible. Defined on the range of L, the inverse is a linear operator $L^{-1}:\rho(t)=L^{-1}\sigma(t)$.

XV. OBSERVABLES IN THE σ REPRESENTATION

If T is a bounded self-adjoint operator, its expectation value is $\mathrm{Tr}\,T\rho(t)$. In this section we construct a set of operators $(TL^{-1})_{\beta\alpha}$ with the property that

$$\lim_{n\to\infty}\sum_{\alpha,\beta\leqslant n}\mathrm{Tr}\,\Omega_\beta(TL^{-1})_{\beta\alpha}\Omega^*_\alpha\sigma(t)=\mathrm{Tr}\,T\rho(t), \tag{15.1}$$

provided $\sigma(t)$ is of the form (1.5). This result means that $\sigma(t)$ can be used as a density operator to calculate expectation values of bounded observables.

We first consider

$$\begin{aligned}&(M_\beta\Omega^*_\beta T\Omega_\alpha M_\alpha^{-1})(M_\alpha\Omega^*_\alpha\rho\Omega_\beta M_\beta^{-1})\\&\quad=(M_\beta\Omega^*_\beta T\Omega_\alpha M_\alpha^{-1})(\psi_\alpha\rho^{\#}_{\alpha\beta}\overline{\psi}_\beta)\\&\quad=(M_\beta\Omega^*_\beta T\Omega_\alpha M_\alpha^{-1})\{1+\exp[-\pi(u+v)/2]\}^{-1}\psi_\alpha\sigma^{\#}_{\alpha\beta}\overline{gw_\beta},\end{aligned} \tag{15.2}$$

where u and v are variables in the integral kernel of $\sigma^{\#}_{\alpha\beta}$, as in Eq. (14.4). Now we define

$$(TL^{-1})^{\#}_{\beta\alpha}:=(M_\beta\Omega^*_\beta T\Omega_\alpha M_\alpha^{-1})\{1+\exp[-\pi(u+v)/2]\}^{-1}. \tag{15.3}$$

This is an operator that acts on trace-class operators with kernels $\psi_\alpha\sigma^{\#}_{\alpha\beta}(u,\omega_\alpha;v,\omega'_\beta)\overline{\psi}_\beta$. It cannot act on elements of ΠL^2. We can define

$$(TL^{-1})_{\beta\alpha}:=M_\beta^{-1}(TL^{-1})^{\#}_{\beta\alpha}M_\alpha. \tag{15.4}$$

This operator acts on trace-class operators

$$M_\alpha^{-1}\psi_\alpha\sigma^{\#}_{\alpha\beta}\overline{\psi}_\beta M_\beta=\psi_\alpha\sigma_{\alpha\beta}\overline{\psi}_\beta=\Omega^*_\alpha\sigma\Omega_\beta.$$

Due to Eqs. (15.2)–(15.4)

$$(TL^{-1})_{\beta\alpha}\Omega^*_\alpha\sigma\Omega_\beta=\Omega^*_\beta T\Omega_\alpha\Omega^*_\alpha\rho\Omega_\beta.$$

Hence

$$\mathrm{Tr}\,\Omega_\beta(TL^{-1})_{\beta\alpha}\Omega^*_\alpha\sigma=\mathrm{Tr}\,\Omega_\beta\Omega^*_\beta T\Omega_\alpha\Omega^*_\alpha\rho.$$

Summing over $\alpha,\beta\leqslant n$ on the right gives $\mathrm{Tr}\,\Pi_nT\Pi_n\rho$. In terms of the trace norm

$$\|\Pi_nT\Pi_n\rho-T\rho\|_1=\|\Pi_nT\Pi_n\rho-\Pi_nT\rho+\Pi_nT\rho-T\rho\|_1\leqslant\|T\|\|\Pi_n\rho-\rho\|_1+\|\Pi_nT\rho-T\rho\|_1.$$

Since Π_n tends strongly to the identity on ΠL^2 as $n\to\infty$, each term on the right-hand side tends to 0 as $n\to\infty$. Hence

$$\lim_{n\to\infty}|\mathrm{Tr}\,\Pi_n T\Pi_n\rho-\mathrm{Tr}\,T\rho|\leqslant\lim_{n\to\infty}\|\Pi_n T\Pi_n\rho-T\rho\|_1=0.$$

This proves Eq. (15.1) at time $t=0$. The proof can be repeated at all later times.

The foregoing can be generalized to unbounded operators $A\in\Gamma$ by taking advantage of the fact that $A^{1/2}(1+J^2)^{-1/2}$ is bounded. Instead of $\mathrm{Tr}\,T\rho$ we consider $\mathrm{Tr}(A^{1/2}\rho A^{1/2})$. If ρ is of the form (11.4) it is not difficult to prove that

$$\sum_{\alpha,\beta\leqslant n}\mathrm{Tr}\,A^{1/2}(1+J^2)^{-1/2}\Omega_\alpha\Omega_\alpha^*R\Omega_\beta\Omega_\beta^*[A^{1/2}(1+J^2)^{-1/2}]^* \tag{15.5}$$

tends to $\mathrm{Tr}(A^{1/2}\rho A^{1/2})$ as $n\to\infty$. We want to express this quantity in terms of σ instead of R or ρ.

It is easy to see that

$$(1+J^2)^{-1/2}\Omega_\alpha\Omega_\alpha^*=\Omega_\alpha\Omega_\alpha^*(1+J^2)^{-1/2}=\Omega_\alpha(1+J_\alpha^2)^{-1/2}\Omega_\alpha^*.$$

Hence define

$$(AL^{-1})_\alpha^{1/2}:=A^{1/2}\Omega_\alpha M_\alpha^{-1}\{1+\exp[-\pi(u+v)/2]\}^{-1/2}M_\alpha.$$

This operator is not bounded, but the range of $\Omega_\alpha^*\sigma\Omega_\beta$ is in its domain. The closure of

$$(AL^{-1})_\alpha^{1/2}\Omega_\alpha^*\sigma\Omega_\beta[(AL^{-1})_\beta^{1/2}]^*$$

is equal to the operator in expression (15.5). Taking the trace and summing over α, β gives $\mathrm{Tr}(A^{1/2}\rho A^{1/2})$ as desired.

XVI. THE PRIGOGINE PROGRAM

It has long been advocated by Prigogine and co-workers[6,7] that irreversible behavior originates at the microscopic level. Their strategy for proving this calls for a transformation Λ that breaks the time-reversal symmetry in the sense that $\Lambda\rho(t)$ is defined only for $t\geqslant 0$ and evolves in time according to a semigroup. In quantum mechanics the quantity

$$\Omega(t):=\mathrm{Tr}\,\rho^*(t)\Lambda^*\Lambda\rho(t)\quad(t\geqslant 0) \tag{16.1}$$

should be a decreasing function of t. The classical counterpart of $\Omega(t)$ is obtained if the trace in Eq. (16.1) is replaced by integration over the phase space.

It was predicted early on that any Λ-operator in quantum mechanics would have to act on operators and could not act on the elements of the Hilbert space on which ρ operates.[70] The authors referred to a superoperator. They also observed that one would have to introduce a time evolution that is not generated by the Hamiltonian.[70] Our transformation $\rho(t)\to L\rho(t)=\sigma(t)$ agrees with the above-mentioned requirements. The operator $\sigma(t)$ is defined for $t\geqslant 0$ only. Due to Eq. (1.1) for $\rho(t)$ and Eq. (12.1) for $J\rho(t)J$, the time evolution of $\sigma(t)$ is described by a semigroup. To define σ, we have to start from an operator ρ on ΠL^2, an element $f\in\Pi L^2$ will not do. This is the superoperator aspect. According to Eq. (12.2) $\mathrm{Tr}\,\sigma^2(t)$ is a monotone decreasing function of t, as is $\Omega(t)$ in Eq. (16.1). Since $\mathrm{Tr}\,\sigma(t)$ is the same as $\langle\mathrm{Tr}\,\tilde{\rho}(t)\rangle$, the Prigogine observation about the time evolution agrees with the discussion in Sec. IX, which shows that the time evolution of $\tilde{\rho}(t)$ on K^2 is not generated by the Hamiltonian $\tilde{H}$ on K^2.

In the early years of the Prigogine program, Λ-operators were constructed explicitly for several classical dynamical systems, including the baker map[71] and other Bernoulli systems,[72] as well as K-flows.[73] The focus has since shifted to large nonintegrable Hamiltonian systems with many resonances. Since this part of the program is not directly related to the present paper, we

merely refer to recent papers on classical[74] and quantum systems.[75] A brief overview of earlier work by Prigogine and co-workers can be found in Ref. 1. There are no previous results on Λ-operators for N-particle quantum systems.

The classical dynamical systems for which Λ-operators were constructed have a compact phase space and a uniform equilibrium density $\rho_0=1$. The norm $\|\Lambda\rho(t)-1\|$ is a monotone decreasing function of t which tends to 0 as $t\to\infty$, for all initial densities $\rho(0)\neq 1$. This is necessary and sufficient in order that the entropy associated with $\Lambda\rho(t)$ is a nondecreasing function of t that tends to its maximal value of 0 as $t\to\infty$ (Ref. 4, Ref. 5, Corollary 7.8).

If a classical dynamical system allows an invertible Λ-operator, it has to be mixing.[76] If Λ is a projection and $\|\Lambda\rho(t)-1\|$ is monotone decreasing to 0, it is necessary[77,78] and sufficient[79] that the underlying invertible system is a K-system.

The inverse problem of finding the K-system when $\Lambda\rho(t)$ is known was investigated in recent papers.[80–82] With a slight change of notation, the authors considered measure preserving Markov semigroups $\{M_t|0\leqslant t<\infty\}$ satisfying $\|M_t\rho-1\|\to 0$ as $t\to\infty$, with the understanding that $M_t\Lambda\rho=\Lambda\rho(t)$ in our earlier notation. Their question was whether the semigroup $\{M_t\}$ can be lifted to an invertible time evolution. Assuming that Λ was a projection[80] they showed that the semigroup $\{M_t\}$ is the Frobenius–Perron semigroup of an exact dynamical system. Let this be $\{S_t\}$ with phase space Y. By a result due to Rohlin[83] the system $\{S_t\}$ is a factor of a K-system $\{K_t\}$ with phase space X. This means that there is a transformation $F:X\to Y$ such that $S_t\circ F=F\circ K_t$. The Rohlin theory provides a natural extension mechanism by which the K-system $\{K_t\}$ was constructed explicitly.[80]

Since the Λ-operators referred to previously[71–73] are invertible, the assumption that Λ is a projection does not cover all possibilities. With more general methods than used in Ref. 80 it was shown[81,82] that any measure preserving Markov semigroup can arise as a projection of a K-system, be it that the projection is not necessarily the Λ-operator that was used to find the Markov semigroup in the first place.

The prevalence of K-systems in the foregoing suggest that a Λ-operator for a classical dynamical system is most likely to exist when the time evolution can be represented by a group of shift operators $\{V(t)|-\infty<t<\infty\}$ as in Eq. (9.1). In quantum mechanics the semigroup $\{U(t)|0\leqslant t<\infty\}$ is our best analog of $\{V(t)\}$. Although the Rohlin theory does not apply to this situation, it suggests the follow point of view.

Given ρ and $\tilde{\rho}$ satisfying Eqs. (11.3) and (11.1), and $f,g\in K^2$,

$$\langle\tilde{\rho}f,g\rangle=(\rho f,g)+(\rho J^2 f,g)+(J\rho f,Jg)+(J\rho J^2 f,Jg).$$

To express this equation in a different form, we define the two-component vector $\tilde{f}$ with components $\tilde{f}_0:=f$, $\tilde{f}_1:=Jf$, and inner product

$$\sum_{i=0,1}(\tilde{f}_i,\tilde{g}_i)=\langle f,g\rangle.$$

Next, we define the 2×2 matrix $\tilde{\rho}$ with elements

$$\tilde{\rho}_{00}:=\rho,\quad \tilde{\rho}_{01}:=\rho J,$$

$$\tilde{\rho}_{10}:=J\rho,\quad \tilde{\rho}_{11}:=J\rho J.$$

It follows that

$$\sum_{i,j}(\tilde{\rho}_{ij}\tilde{f}_j,\tilde{g}_i)=\langle\tilde{\rho}f,g\rangle.$$

Now we take the trace of the 2×2 matrix $\tilde{\rho}$ and let this operation be the transformation F,

$$F\rho := \sum_{i=0,1} \tilde{\rho}_{ii} = \sigma.$$

Hence F is the operator that was denoted by L before. The time evolution takes ρ into $\rho(t)$ and $\tilde{\rho}$ into $\tilde{\rho}(t)$. This replaces the Rohlin transformation K_t. Instead of $F \circ K_t$ we consider $\rho \to \rho(t) \to \sigma(t)$. Alternatively, we first take the step $\rho \to \sigma$. The time evolution $\sigma \to \sigma(t)$ replaces S_t. Instead of $S_t \circ F$ we find $\rho \to \sigma \to \sigma(t)$, producing the same net result as $\rho \to \rho(t) \to \sigma(t)$. In this sense, replacing $\rho \to \rho(t)$ by $\sigma \to \sigma(t)$ is like taking a factor of a classical dynamical system.

The idea to introduce $\sigma(t)$ came from publications by Mackey (Ref. 4, Ref. 5, Chap. 9) in which he pointed out that taking a factor of a classical dynamical system with constant entropy may give rise to an entropy that increases. Quoting the Rohlin theorem,[83] Mackey referred to papers on Λ-operators[71,79] as an illustration. If Λ is a projection, it is an example of a transformation F that yields a factor with increasing entropy. In Mackey's terminology, a factor is a specific type of trace. This suggested taking the sum of the diagonal elements of the matrix $\tilde{\rho}$. Since the transformation $\rho(t) \to \sigma(t)$ is invertible, it is not a projection, yet it does have the property of leading to an increasing entropy $S[\sigma(t)]$.

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On mathematical structure of effective observables

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We decompose the Hilbert space of wave functions into two subspaces, and assign to a given observable two effective representatives that act in the model space. The first serves to determine some of the eigenvalues of the full observable, while the second serves to determine its matrix elements, in any basis in one of the subspaces, in terms of quantities pertaining to the model space. We also show that if the Hamiltonian of a physical system possesses symmetries then these symmetries continue to hold for its effective representatives of the first type. Maximum information about the system can be obtained in terms of two sets of effective representatives. The first set of representatives is complete. Other observables that do not commute with all members of the complete set have only one type of representative. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1286034]

I. INTRODUCTION

Effective operators are often used in nuclear, atomic, and molecular physics. The general scheme aims to construct from the Hamiltonian of the system, acting on the Hilbert space of wave functions, an operator that acts on a low-dimensional space, so that the eigenvalues of the latter operator are also eigenvalues of the full Hamiltonian of the given system.[1–9] The low-dimensional space we have mentioned is called a model space and the operator acting on it to produce some of the eigenvalues of the full Hamiltonian is called an effective Hamiltonian, or an effective representative of the Hamiltonian. The latter requirement does not determine an effective representative uniquely. A general class of effective representatives was obtained by Suzuki[10] who also delineated forms according to the role of an arbitrary parameter, the starting energy, in the iterative method of solution,[4] or according to their Hermiticity. Hermitian forms have been introduced or adopted by many researchers.[10–17] A standard non-Hermitian form[2,18,19] is relatively simple, and is commonly used for implementing the scheme of effective representatives.

Our present work, which is concerned with the effective representation of any observable in the standard non-Hermitian scheme, has the following objectives:

(1) To establish the equivalence between the decoupling condition on the transformed observable and a corresponding condition on its transformed eigenfunctions.
(2) To show that the decoupling equation always has solutions and to specify the maximum number of inequivalent solutions.
(3) Starting from a complete set of observables associated with the physical system, we construct a complete set of effective representatives, and prove accordingly that the symmetries of the Hamiltonian are carried over to the effective representatives.
(4) Two effective representatives can be constructed associated with every observable. The first representative corresponds to the standard non-Hermitian form and gives some of the eigenvalues of the original observable. The second representative is Hermitian and has the property that the matrix elements of the original observable, in any basis of the subspace that is mapped onto the model space, can be calculated in terms of this representative and the projected basis in the model space.

II. THE MODEL SPACE

The truncated Hilbert space of square integrable functions associated with the system, denoted by H_N, consists of all N-columns with complex entries. H_N is just the unitary space of complex numbers C^N through the isomorphism $\psi \in H_N \leftrightarrow \psi^t \in C^N$, where (t) denotes the transpose. The standard basis in H_N will be denoted by $e_i (i=1,...,N)$, so that

$$e_1=(1,0,....,0)^t, e_2=(0,1,....,0)^t, \ldots\ldots\ldots, e_N=(0,....,0,1)^t. \tag{1}$$

Let K be a distinct subset of d elements of the set $\{1,2,...,N\}$. The subspace generated by the subset of basis elements $\{e_k : k \in K\}$ will be denoted by Π_K, and will be called a model space. The projection on Π_K will be denoted by P_K, whereas Q_K will denote the projection on the orthogonal complement $\Pi_K^{\perp} = H_N \ominus \Pi_K$. It follows that $P_K + Q_K = I$, $P_K Q_K = Q_K P_K = 0$. If it is desired, one may rearrange the order of the basis elements (1) so that the vectors $e_i (i \in K)$ are placed first. We shall assume that such reordering is done whenever it is necessary, and drop the index K, if no ambiguity arises. The symbol P accordingly, will denote a projection on some model space Π. The reordering operation is particularly useful when we have to represent vectors and operators in matrix form.

Let S be an operator in H_N such that

$$S = QSP. \tag{2}$$

It follows that $S^2 = 0$, and hence $e^{\pm S} = 1 \pm S$. Equation (2) implies also that

$$S = \begin{pmatrix} 0_d & 0 \\ s & 0 \end{pmatrix}, \tag{3}$$

where 0_d is the nil $d \times d$ matrix. Consider the transformation

$$e^{-S} : H_N \to H_N, \quad \psi \to \tilde{\psi} = (1-S)\psi. \tag{4}$$

Setting $\psi = \binom{\alpha}{\beta}$ where $\alpha^t \in C^d$, we write

$$\tilde{\psi} \equiv \begin{pmatrix} \tilde{\alpha} \\ \tilde{\beta} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -s & 1 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta - s\alpha \end{pmatrix}. \tag{5}$$

It is apparent that the mapping e^{-S} is determined by S given by (3), which in turn is determined by $s : \Pi \to \Pi^{\perp}$.

Through an obvious isomorphism we may overlook Π as being a subspace of H_N and consider it as a space on its own right. Hence, and whenever it is convenient, we may set $P\psi = \alpha$, $P\tilde{\psi} = \tilde{\alpha}$, and thus consider $P\psi, P\tilde{\psi}$ as d-vectors instead of being N-vectors with vanishing components in $\Pi^{\perp}$. A similar statement is applicable to $\Pi^{\perp}$ and to the vectors $Q\psi, Q\tilde{\psi}$, and hence we may set $Q\psi = \beta$, $Q\tilde{\psi} = \tilde{\beta}$. It is evident from (5) that if $\alpha = 0$ then $\psi = \tilde{\psi}$, and hence every point in the invariant subspace $\{\binom{0}{\beta} : \beta^t \in C^{N-d}\}$ is a fixed point of the transformation e^{-S}.

Let $\Psi = \{\psi_i \in H_N : i = 1,...,d\}$ be a linearly independent set of vectors. Hence there exists at least one subspace Π_K in which the set of projections of these vectors is linearly independent. This last statement is equivalent to say that the rank of the matrix $[\langle e_j | \psi_i \rangle]$, $(i=1,...,d; j=1,...,N)$ is d. The symbol $\langle | \rangle$ designates the inner product.

We shall choose the matrix S such that

(i) $Q\tilde{\psi}_i = 0, \quad (i=1,...,d)$;

(ii) The set of vectors $P\Psi = \{P\psi_i : i=1,...,d\}$, where P is the projection corresponding to $\{1,2,...,d\}$, is linearly independent.

Requirement (ii) can always be satisfied through reordering the basis if necessary. By (5), requirement (i) implies $s\alpha_i-\beta_i=0 (i=1,...,d)$, or

$$sP\psi_i-Q\psi_i=0 \quad (i=1,...,d). \tag{6}$$

We write (6) collectively as a matrix equation $s[P\Psi]-[Q\Psi]=0$, in which $[P\Psi]=[P\psi_1 \vdots ..... \vdots P\psi_d]$, $[Q\Psi]=[Q\psi_1 \vdots ..... \vdots Q\psi_d]$. As its columns are linearly independent the matrix $[P\Psi]$ is invertible, and hence

$$s=[Q\psi][P\Psi]^{-1}. \tag{7}$$

Therefore requirements (i) and (ii) yield Eq. (7). It is easy to see that Eq. (7), which embodies in it that the matrix $[P\Psi]$ is invertible, is in fact equivalent to conditions (i) and (ii).

With s so-chosen, the matrix S given by (3) has the property: e^{-S} projects every vector of the d-dimensional space $\mathrm{Lin}\,\Psi$, generated by the set of vectors $\Psi=\{\psi_1,\ldots,\psi_d\}$, onto the model space $\mathrm{Lin}\{\alpha_1,\ldots,\alpha_d\}\equiv\Pi$. This follows immediately from requirement (i) and linearity of e^{-S}. In other words, an arbitrary vector

$$\begin{pmatrix} \alpha \\ s\alpha \end{pmatrix} \in \mathrm{Lin}\,\psi$$

is mapped by e^{-S} to

$$\begin{pmatrix} \alpha \\ 0 \end{pmatrix} \in \Pi.$$

The operator e^{-S} is not a projection operator as implied by the mathematical definition of a projection operator. The word ''project'' however is used here in a geometrical sense to describe an operation in which every vector of a certain subspace (visualized as hyperplane) is mapped to a vector that has the same first d-components, whereas its remaining components are zeros (visualized as a vector in a coordinate hyperplane). Also if $\phi\notin\mathrm{Lin}\,\Psi$, then its image $\tilde{\phi}$ is not in the model space. The proof of the last fact relies on the regularity of e^{-S}, which implies that the image of the independent set $\{\psi_1,.....,\psi_d,\phi\}$ namely $\{\alpha_1,.....,\alpha_d,\tilde{\phi}\}$ is linearly independent, and hence $\phi\notin\mathrm{Lin}\{\alpha_1,.....,\alpha_d\}=\Pi$. The vector $\tilde{\phi}$ therefore has at least one nonvanishing component outside the space Π.

The operator e^{-S}, with s given by (7), as projects the subspace $\mathrm{Lin}\,\Psi$ orthogonally on Π, is thus determined solely by $\mathrm{Lin}\,\Psi$ and Π, and is independent of the particular choice of a set of d-independent vectors in $\mathrm{Lin}\,\Psi$. Indeed if $\Psi'=\{\psi_1',...,\psi_d'\}$ is another set of independent vectors in $\mathrm{Lin}\,\Psi$, then

$$\psi_i'=\sum_{j=1}^{d} c_{ji}\psi_j \quad (i=1,...,d), \tag{8}$$

where c_{ji} are constants. Denoting the matrix whose elements are c_{ji} $(i,j=1,...,d)$ by C, and the matrices whose columns are ψ_i and ψ_i' by $[\Psi]$ and $[\Psi']$, respectively, we write the last relation as $[\Psi']=[\Psi]C$. Equivalently we have $[P\Psi']=[P\Psi]C$ and $[Q\Psi']=[Q\Psi]C$. Substituting from these equations for $[P\Psi]$ and $[Q\Psi]$ in (7) we get $s=[Q\Psi'][P\Psi']^{-1}$, which proves our assertion.

We finally note that as e^{-S} is invertible, the inverse image of every vector $\alpha\in\Pi$, which also is identifiable with $\binom{\alpha}{0}$, is retrievable as $\binom{\alpha}{s\alpha}$.

III. LEE AND SUZUKI TRANSFORMATION

Let O be a Hermitian $N\times N$ matrix, with an independent set of eigenvectors $\{\psi_i : i=1,....,N\}$, and consider the eigenequation

$$O\psi_i = E_i\psi_i \quad (i=1,...,N). \tag{9}$$

Applying the Lee and Suzuki similarity transformation[5] to the matrix O and to the truncated space H_N, we obtain

$$\tilde{O}\tilde{\psi}_i = E_i\tilde{\psi}_i \quad (i=1,...,N), \tag{10}$$

where we have used tilde to designate transformed quantities so that

$$\tilde{O} = e^{-S}Oe^{S}, \quad \tilde{\psi} = e^{-S}\psi. \tag{11}$$

Our work will be distinguished from that of Lee and Suzuki through our identification of additional freedom in the choice of S. Multiplying both sides of (10) by P and injecting $I=P+Q$ conveniently in the right-hand side we get

$$P\tilde{O}P\tilde{\psi}_i + P\tilde{O}Q\tilde{\psi}_i = E_iP\tilde{\psi}_i \quad (i=1,...,N). \tag{12}$$

In a similar way we get

$$Q\tilde{O}P\tilde{\psi}_i + Q\tilde{O}Q\tilde{\psi}_i = E_iQ\tilde{\psi}_i \quad (i=1,...,N). \tag{13}$$

We shall choose the transformation (11) such that there exists a subset $J\subset\{1,...,N\}$ with *card* $J=d$, for which (i) the set of vectors $\{P\tilde{\psi}_i : i\in J\}$ is linearly independent, and (ii) $Q\tilde{\psi}_i = 0 (i\in J)$. Such a choice, as we have seen in the previous section, is certainly possible.

Proposition 1: Let $J\subset\{1,...,N\}$ be such that the set $\{P\psi_i : i\in J\}$ is linearly independent. The following assertions concerning the Lee and Suzuki transformation are equivalent:

A1. $Q\tilde{\psi}_i = 0\ (i\in J)$

A2. $s_J = [Q\Psi_J][P\Psi_J]^{-1}$

A3. (i) the decoupling equation $Q\tilde{O}P=0$ holds, and

(ii) $P\psi_i (i\in J)$ are eigenvectors of $P\tilde{O}P$.

Proof: We have seen in Sec. II that the assertions A1 and A2 are equivalent (this expression of s_J was first given by Navratil and Barrett).[17] To prove that assertion A1 implies A3, we set $Q\tilde{\psi}_i = 0 (i\in J)$ in (12) and (13) to find that $P\tilde{\psi}_i (i\in J)$ are eigenvectors of $P\tilde{O}P$, and $Q\tilde{O}P\tilde{\psi}_i = 0\ (i\in J)$. Due to the linear independence of $P\psi_i (i\in J)$, the later d-equations imply that $Q\tilde{O}P=0$. Conversely, if $\alpha_k\,(i=1,...,d)$ are linearly independent eigenvectors of $P\tilde{O}P$ then the N-vectors $\binom{\alpha_k}{0}$ $(k=1,...,d)$ are eigenvectors of $\tilde{O}$. It follows that the inverse image of these vectors $\{e^S\binom{\alpha_k}{0} : k=1,...,d\}$ coincides with a subset $\Psi_J=\{\psi_i : i\in J\}$ of eigenvectors of O. The subset Ψ_J clearly fulfills assertion 1. Hence A1 is equivalent to A3.

IV. THE EFFECTIVE FORM

When the transformed operator $\tilde{O}$ is such that $Q_K\tilde{O}P_K=0$, for some subset $K\subset\{1,...,N\}$, with *card* $K=d$, we refer to the operator $O_{\text{eff}}\equiv P_K\tilde{O}P_K$ as an effective representative of the operator O corresponding to the model space Π_K, and to the form taken by $\tilde{O}$ as an effective form. When $\tilde{O}$ is in an effective form corresponding to the model space Π, the matrix elements $(O_{\text{eff}})_{ij}$ are all zero except those for which $i,j\leqslant d$, and consequently we make the identification $O_{\text{eff}}:\Pi\to\Pi$, in which O_{eff} is considered a $d\times d$ matrix. In a similar way we treat $Q\tilde{O}Q$ as an $(N-d)\times(N-d)$ matrix.

We elaborate here on the effective form and develop a more explicit framework. We write the eigenequation (9) as

$$\begin{pmatrix} a & b \\ b^+ & f \end{pmatrix}\begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix} = E_i \begin{pmatrix} \alpha_i \\ \beta_i \end{pmatrix} \quad (i=1,.....,N), \tag{14}$$

where the matrix O has been partitioned to submatrices corresponding to Π and $\Pi^{\perp}$, with a is a $d\times d$ matrix. By (11) the last equation is transformed to

$$\begin{pmatrix} a+bs & b \\ -s(a+bs)+b^+ +fs & f-sb \end{pmatrix}\begin{pmatrix} \alpha_i \\ \beta_i - s\alpha_i \end{pmatrix} = E_i \begin{pmatrix} \alpha_i \\ \beta_i - s\alpha_i \end{pmatrix}. \tag{15}$$

The later equation is equivalent to (12) and (13) together. It is easy to check that every s_J, given as in proposition 1, puts $\tilde{O}$ into an effective form corresponding to some model space Π. In other words, every s_J is a solution to the decoupling equation

$$Q\tilde{O}P \equiv -s(a+bs)+b^+ +fs=0. \tag{16}$$

To demonstrate the converse we assume that the later equation is satisfied by some s, and hence the action of $Q\tilde{O}P$ on any vector in Π is zero. In particular this action is zero for all vectors α_i such that $\psi_i=\binom{\alpha_i}{\beta_i}$, $(i=1,....,N)$ are eigenvectors of O, and hence

$$-s(a+bs)\alpha_i + b^+\alpha_i + fs\alpha_i = 0 \quad (i=1,....,N). \tag{17}$$

Making use of (14) we reduce the last equation to the eigenequation

$$(f-sb)(s\alpha_i-\beta_i) = E_i(s\alpha_i-\beta_i) \quad (i=1,....,N), \tag{18}$$

which is the same as embodied in Eq. (15) but now extended to all i. However, not all vectors $s\alpha_i-\beta_i$ can be eigenvectors of $(f-sb)$ because the later operator has only $N-d$ eigenvectors. It follows that there exists a subset J consisting of d elements of $\{1,....,N\}$ such that $s\alpha_i-\beta_i=0$ $(i\in J)$, which implies that $s=s_J$, as given in proposition 1.

We list here the following comments on the effective form assuming from now on that $\tilde{O}$ is in such a form, i.e., the transformation (10) is such that $Q\tilde{O}P=0$.

(1) If $\tilde{O}$ is the effective form corresponding to the model space Π then the right-hand side of the secular (characteristic) equation $\det(O-EI_N)=0$ can be factorized to a product of two polynomials; one of which is of degree d in E

$$\det(O_{\text{eff}}-EI_d)\cdot\det(Q\tilde{O}Q-EI_{N-d})=0. \tag{19}$$

The eigenvalues of O is the set of zeros of these two polynomials. In practical problems the secular equation of O_{eff} can be solved numerically as it is of low degree in E, whereas that of $Q\tilde{O}Q$ is of high degree in E and it is often hopeless to approach it for direct solution. One may apply the method of effective form described in the previous section afresh to the operator $Q\tilde{O}Q$. Or alternatively one may pick up a new set of eigenvectors, say $\Psi_{J'}$, determine $s_{J'}$, and consequently a new effective form. Alternatively the matrix s could be determined by iterative methods.[4,12,7]

(2) If $P\psi_i$ is an eigenvector of O_{eff} corresponding to E_i then by (12) $P\tilde{O}Q\tilde{\psi}_i=0$ which implies that the $(N-d)$-vector $Q\tilde{\psi}_i$ is complex orthogonal to the rows of $d\times(N-d)$ matrix $P\tilde{O}Q$, and the vector $Q\tilde{\psi}_i$ is not necessarily zero. Therefore, if α is an eigenvector of O_{eff} then, though $\binom{\alpha}{0}$ is an eigenvector of $\tilde{O}$ belonging to the eigenvalue E_i, there may exist another

eigenvector $\binom{\alpha}{\gamma}$ of $\tilde{O}$ that belongs to the same eigenvalue E_i. In the latter case $b\gamma=0$ and γ is an eigenvector of $Q\tilde{O}Q$ belonging to the eigenvalue E_i. It is clear that $\binom{0}{\gamma}$ is an eigenvector of $\tilde{O}$ that belongs to the eigenvalue E_i. We summarize the latter observations by the following proposition

Proposition 2: Let ϕ be an eigenvector of $\tilde{O}$ belonging to the eigenvalue E.
(i) If $Q\phi=0$ then E is an eigenvalue of O_{eff} to which the eigenvector $P\phi$ belongs.
(ii) if $Q\phi\neq 0$ then $Q\phi$ is an eigenvector of $Q\tilde{O}Q$ belonging to the eigenvalue E. If in addition, $P\phi\neq 0$, then $P\phi$ is not an eigenvector of O_{eff} unless $bQ\phi=0$. In the latter case E is a common eigenvalue of O_{eff} and $Q\tilde{O}Q$ to which the independent eigenvectors $\binom{P\phi}{0}$ and $\binom{0}{Q\phi}$ belong. In the latter case the spectra of O_{eff} and $Q\tilde{O}Q$ intersect.
(iii) $P\phi$ is an eigenvector of O_{eff} does not necessitate that $Q\phi=0$. However if the spectra of O_{eff} and $Q\tilde{O}Q$ do not intersect in E, then $Q\phi=0\Leftrightarrow P\phi$ is an eigenvector of O_{eff} belonging to the eigenvalue E.

(3) If the matrix $[P\Psi_J]$ is singular for some choice of model space, say Π, then we have to replace it by another Π' such that the matrix $[P'\Psi_J]$ is invertible. There certainly exists such a new choice of model space, otherwise the set Ψ_J would be linearly dependent.

We demonstrate here that for a given set of eigenvectors Ψ_J, two legitimate choices of model spaces lead to two effective representatives which are related by a similarity transformation. Let Π and Π' be two legitimate choices and denote the projections on the corresponding model spaces by P and P', respectively. This leads to two distinct s, say s and s', and hence to two distinct effective representatives $O_{\text{eff}}=P\tilde{O}P$ and $O'_{\text{eff}}=P'\tilde{O}'P'$. If $\{E_i:i\in J\}$ is the set of eigenvalues to which Ψ_J belong, then

$$O_{\text{eff}}[P\Psi_J]=[P\Psi_J]\Lambda_J, \quad O'_{\text{eff}}[P'\Psi_J]=[P'\Psi_j]\Lambda_J, \tag{20}$$

where Λ_J is a diagonal matrix with diagonal elements $(E_i:i\in J)$. From (20) we deduce that

$$O_{\text{eff}}=[P\Psi_J][P'\Psi_J]^{-1}O'_{\text{eff}}[P'\Psi_J][P\Psi_J]^{-1}, \tag{21}$$

which proves our claim.

Each independent set of eigenvectors Ψ_J provide at least one model space Π_K. The number of possible choices of Π_K is not less than one and not greater than $\binom{N}{d}$, which is of course the number of independent sets of projections $\{P_K\Psi_J:card\ K=d,\ K\subset\{1,....,N\}\}$. All such choices lead of course to the same set of eigenvalues Λ_J.

If the eigenvalues of O are nondegenerate then different choices of Ψ_J out of the set of N-independent eigenvectors Ψ, result in effective representatives with different spectra. The total choices of inequivalent effective representatives corresponding to O is $\binom{N}{d}$; and within each of these there are a maximum number of $\binom{N}{d}$ equivalent representatives.

The above-identified freedoms are new and extend the work of Lee and Suzuki.

V. SPECTRAL REPRESENTATION OF O_{eff}

Let O_{eff} be an effective representative of the operator O in the model space Π, and let $\{E_i:i\in J\}$ be the spectrum of O_{eff}, to which the vectors $P\Psi_i(i\in J)$ belong, so that $O_{\text{eff}}P\psi_i=E_iP\psi_i(i\in J)$. Since each $P\psi_i$ lies in the model space we have

$$P\psi_i=\sum_{\mu=1}^{d} c_{i\mu}e_\mu \quad (i\in J), \tag{22}$$

$$\langle P\psi_i|P\psi_j\rangle=\sum_{\mu=1}^{d} c^*_{i\mu}c_{j\mu}\equiv\gamma_{ij} \quad (i,j\in J). \tag{23}$$

The matrix γ is clearly Hermitian, and determines the overlap the eigenvector of O_{eff} one with respect to another. Let

$$\chi=\sum_{j\in J} b_j P\psi_j \tag{24}$$

be an arbitrary vector in the model space, then

$$\langle P\psi_i|\chi\rangle=\sum_{j\in J} \gamma_{ij}b_j \quad (i\in J). \tag{25}$$

Hence

$$\sum_{i\in J} \gamma_{ki}^{-1}\langle P\psi_i|\chi\rangle=b_k \quad (k\in J), \tag{26}$$

where γ^{-1} is the inverse of the matrix γ. It is clear that γ^{-1} always exists since $P\psi_i\,(i\in J)$ are linearly independent. Applying O_{eff} to χ where b_k are given by (26) we get

$$O_{\text{eff}}|\chi\rangle=\sum_{i,k\in J} \gamma_{ki}^{-1}\langle P\psi_i|\chi\rangle E_k P\psi_k\,. \tag{27}$$

This yields

$$O_{\text{eff}}=\sum_{i,k\in J} E_i\gamma_{ik}^{-1}|P\psi_i\rangle\langle P\psi_k|,$$

which expresses O_{eff} in terms of quantities pertaining to the model space.

VI. A COMPLETE SET OF EFFECTIVE REPRESENTATIVES

Let $O_1\equiv H$ be the Hamiltonian of a physical system and $O^2,\ldots\ldots,O^c$ be a set of observables pertaining to the system so that the set of observables $\Gamma=\{O^1,O^2,\ldots,O^c\}$ is complete. It follows from the latter assumption that

$$[O^\rho,O^\sigma]=0 \quad (\rho,\sigma=1,....,c). \tag{28}$$

The energy eigenvectors $\{e_i:i=1,2,...\}$ of a suitably chosen Hamiltonian could be taken as a basis for the Hilbert space of wave functions of the physical system. For example, these could be the energy eigenstates of the simple harmonic oscillator, when one considers the bound states of the nucleus. Observables pertaining to the system are represented by Hermitian matrices in terms of this basis. Unless the matrices representing observables are given by recurrence formulas, we have to be content with finite matrix approximations, which imply truncating the infinite basis $\{e_i\}_1^\infty$ at some sufficiently large term N. The space generated by the truncated basis $[e_1,\ldots,e_N]\equiv H_N$ will hopefully contain good approximations of all states of interest to the problem we consider.

It must be noted that, whenever the eigenvalue problem is to be solved numerically, which is usually the case in physically interesting problems, truncation is an inevitable task. It is true that if $\{e_i\}_1^\infty$ is a basis of the Hilbert space of square integrable functions H_∞, the sequence (e_N) tends weakly to zero as N tends to infinity.[20,21] This means that for every $\psi\in H_\infty$ the sequence of numbers $(\langle e_N|\psi\rangle)$ tends to zero as N tends to infinity. However one cannot be confident that the space H_N resulting from a specific choice of N will contain, to a good approximation, the physical states of interest unless a skillful choice of basis is made. Only in the latter case an upper cutoff can be safely applied without seriously changing the low-lying properties.

It is noted that all the algebra carried out in the previous sections, or to be carried out in the forthcoming discussion, is valid for infinite matrices as much as it is valid for finite ones, and hence we may replace N by ∞ without affecting the validity of these results.

The Hermitian commuting set of matrices Γ is complete, and there exists accordingly a complete set of simultaneous eigenfunctions ψ_i of the observables O^σ such that

$$O^\sigma \psi_i = E_i^\sigma \psi_i \quad (i=1,...,N;\sigma=1,....,c), \tag{29}$$

where E_i^σ are the eigenvalues of the observable O^σ to which the eigenvector ψ_i belongs. The eigenvectors given by (29) are preserved when the similarity transformation (11) is applied to the Hilbert space of wave functions H_N and to the operators acting on H_N, and hence

$$\tilde{O}^\sigma \tilde{\psi}_i = E_i^\sigma \tilde{\psi}_i \quad (i=1,...,N;\sigma=1,...,c). \tag{30}$$

Assume that the eigenvectors $\tilde{\psi}_1,....,\tilde{\psi}_d$ are such that the set $\{P\tilde{\psi}_1,.....,P\tilde{\psi}_d\}$ is linearly independent, and take

$$s=[Q\tilde{\psi}_1.....Q\tilde{\psi}_d][P\tilde{\psi}_1.....P\tilde{\psi}_d]^{-1}. \tag{31}$$

The matrix s is the same for observables forming the complete set Γ, for it is constructed of the same subset of the simultaneous eigenvectors of $\tilde{O}^\sigma(\sigma=1,...,c)$. The resulting transformed observables $\tilde{O}^\sigma$, have the same effective form, and hence have $P\tilde{\psi}_i(i=1,...,d)$ as a common subset of eigenvectors $\{\tilde{\psi}_i : i=1,...,N\}$. Define a set of effective representatives

$$\sigma_{\text{eff}}^\sigma = P\tilde{O}^\sigma P \quad (\sigma=1,....,c), \tag{32}$$

and hence

$$O_{\text{eff}}^\sigma P\tilde{\psi}_i = E_i^\sigma P\tilde{\psi}_i \quad (i=1,....,d;\sigma=1,....,c). \tag{33}$$

It follows, and since the set $\{P\psi_i : i=1,...,d\}$ is complete in the model space Π, that

$$[O_{\text{eff}}^\rho, O_{\text{eff}}^\sigma]=0 \quad (\sigma,\rho=1,...,c). \tag{34}$$

The effective Hamiltonian $H_{\text{eff}} \equiv O_{\text{eff}}^1$ and the effective representatives $O_{\text{eff}}^\sigma(\sigma=2,...,c)$ we have constructed have the virtue that the symmetries exhibited by the original Hamiltonian H are carried over to H_{eff} with the effective representatives $O_{\text{eff}}^\sigma(\sigma=2,...,c)$ playing the role of generators of symmetry for H_{eff}.

The matrices (32) are obviously non-Hermitian and, consequently, the expectation value of an effective representative in a state $P\psi$ in the model space is generally a complex number. An exception to this fact is that when $P\psi$ is an eigenvector $P\psi_i$ of O_{eff}. In this case

$$\langle O_{\text{eff}} \rangle_{P\psi_i} = \langle P\psi_i | O_{\text{eff}} | P\psi_i \rangle / \|P\psi_i\|^2 = E_i. \tag{35}$$

VII. A SECOND TYPE OF EFFECTIVE REPRESENTATIVE

The role of an effective operator seems limited to producing some of the eigenvalues of the original observable. However, we may enhance the scheme of ''effectiveness'' and make a further step as follows: The matrix S which is determined by iterative methods[4,7,18] and utilized to construct the effective representative O_{eff} can also be utilized to construct an effective representative of a second type $\overline{O}_{\text{eff}}$ that satisfy the property

$$\langle \psi | O | \phi \rangle = \langle P\psi | \overline{O}_{\text{eff}} | P\phi \rangle, \tag{36}$$

for all $\psi,\phi\in \mathrm{Lin}\{\psi_1,\ldots,\psi_d\}$. Using (11) and the definition of the adjoint operator, we have

$$\begin{aligned}\langle\psi|O|\phi\rangle&=\langle e^{-S}\tilde{\psi}|O|e^{-S}\tilde{\phi}\rangle\\&=\langle\tilde{\psi}|e^{-S^+}Oe^{-S}|\tilde{\phi}\rangle\\&=\langle P\tilde{\psi}|e^{-S^+}Oe^{-S}|P\tilde{\phi}\rangle\\&=\langle P\psi|Pe^{-S^+}Oe^{-S}P|P\phi\rangle.\end{aligned}\tag{37}$$

The requirement (36) is fulfilled on taking

$$\tilde{O}_{\mathrm{eff}}=Pe^{-S^+}Oe^{-S}P.\tag{38}$$

In particular $\langle\psi_i|O|\psi_j\rangle=\langle\alpha_i|\overline{O}_{\mathrm{eff}}|\alpha_j\rangle$.

We therefore associate with every observable $O^\sigma\in\Gamma$ two effective representatives. The first, O_{eff}, serves to determine some of the eigenvalues of O^σ and the projection of the corresponding eigenvectors on the model space; the second $\overline{O}^\sigma_{\mathrm{eff}}$ has the important property: the matrix elements of the original operator O^σ with respect to any basis in the space $\mathrm{Lin}\{\psi_1,\ldots,\psi_d\}$ is given in terms of $\overline{O}^\sigma_{\mathrm{eff}}$ and the projected basis in the model space. It is evident that the last matrix can be calculated easily since $\overline{O}^\sigma_{\mathrm{eff}}$ is known whenever S is known, and since the basis elements of the model space have finite components. We mention that the matrix $\langle P\psi_i|\overline{O}_{\mathrm{eff}}|P\psi_j\rangle$ is not the matrix of $\overline{O}_{\mathrm{eff}}$ since $\{P\psi_i\}_{i=1}^d$ is not orthogonal. In particular, and if $\psi\in\mathrm{Lin}\,\Psi$ then

$$\langle O\rangle_\psi=\langle P\psi|\overline{O}_{\mathrm{eff}}|P\psi\rangle=\|P\psi\|^2\langle\overline{O}_{\mathrm{eff}}\rangle_{P\psi}.$$

Expressed in words, the expectation value of the observable O in the state $\psi\in\mathrm{Lin}\,\Psi$ is equal to the expectation value of its representative of the second type in the projection of the given state on the model space times the square norm of this projection.

For observables O that do not commute with all elements of the complete set Γ we can define only one effective representative, that is the effective representative of the second type $\overline{O}_{\mathrm{eff}}$. This serves to give a portion of the transition matrix of O, namely that which corresponds to a basis of $\mathrm{Lin}\,\Psi$.

A systematic study of the system is achieved by decomposing the space H_N into linear subspaces $\mathrm{Lin}\,\Psi_{J_r}$ $(r=1,2,\ldots,a)$, with $J_r\cap J_s=\varnothing$ if $(r\neq s)$, so that

$$H_N=\mathrm{Lin}\,\Psi_{J_1}\oplus\ldots\oplus\mathrm{Lin}\,\Psi_{J_a}.\tag{39}$$

Now in each subspace $\mathrm{Lin}\,\Psi_{J_r}$ we assign to every observable O in a complete set of observables an effective representative of the first type $O_{r\,\mathrm{eff}}$ and an effective observable of the second type $\overline{O}_{r\,\mathrm{eff}}$. These effective representatives, of first or second type, differ from one subspace to another as does s_J. If representatives of the first type are all obtained, all eigenvalues of the full observable O become known. Also if $\chi,\chi'\in\mathrm{Lin}\,\Psi_{J_r}$ then we have $\langle\chi|O|\chi'\rangle=\langle P_r\chi|\overline{O}_{r\,\mathrm{eff}}|P_r\chi'\rangle$ where P_r denotes the projection on the model space corresponding to the subspace $\mathrm{Lin}\,\Psi_{J_r}$. Although similar relations are valid for every two vectors in the same subspace, one cannot express $\langle\chi|O|\chi'\rangle$ in terms of representatives of second type when χ and χ' belong to different subspaces, and consequently when they are arbitrary vectors in H_N.

VIII. TOWARDS PRACTICAL APPLICATIONS

Following the traditional lines of thinking for many-body problems, we suggest that S is developed for small subsystems and used as an approximation for the full S. For example two- and three-body problems may be solved with high precision using current numerical techniques.[17,18] A

set of solutions $P\psi_i\ (i=1,...,d)$ is selected, S is evaluated, and the resulting H_{eff} is then used in many-body problems within the appropriately restricted model space. Detailed tests will be needed for specific Hamiltonians to determine the efficacy of this approach and the utility of the various freedoms we have identified within the present work.

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Variable separation for natural Hamiltonians with scalar and vector potentials on Riemannian manifolds

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The additive variable separation in the Hamilton–Jacobi equation is studied for a natural Hamiltonian with scalar and vector potentials on a Riemannian manifold with positive–definite metric. The separation of this Hamiltonian is related to the separation of a suitable geodesic Hamiltonian over an extended Riemannian manifold. Thus the geometrical theory of the geodesic separation is applied and the geometrical characterization of the separation is given in terms of Killing webs, Killing tensors, and Killing vectors. The results are applicable to the case of a nondegenarate separation on a manifold with indefinite metric, where no null essential separable coordinates occur. © *2001 American Institute of Physics.*
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I. INTRODUCTION

A smooth real function V and a smooth vector field $\mathbf{A}$ on a Riemannian n-manifold $(Q,\mathbf{g})$ define a Hamiltonian function on the cotangent bundle T^*Q,

$$H=\tfrac{1}{2}g^{ij}(p_i+A_i)(p_j+A_j)+V=\tfrac{1}{2}g^{ij}p_ip_j+A^ip_i+U, \tag{1.1}$$

where the function on Q

$$U=V+\tfrac{1}{2}A^iA_i=V+\tfrac{1}{2}\mathbf{A}\cdot\mathbf{A} \tag{1.2}$$

is extended to T^*Q as a function constant on the fibers. Hamiltonians of this kind appear in many classical problems of analytical mechanics and physics, and for this reason they are called *natural*. The Hamiltonian (1.1) corresponds to a Lagrangian $L:TQ\to\mathbb{R}$ of the form

$$L=\tfrac{1}{2}g_{ij}\dot{q}^i\dot{q}^j-A_i\dot{q}^i-V, \tag{1.3}$$

where $\frac{1}{2}g_{ij}\dot{q}^i\dot{q}^j$ is the *kinetic energy* and V and $\mathbf{A}$ play the role of *scalar* and *vector potentials*, respectively, generating Lagrangian forces

$$F_i=(\partial_jA_i-\partial_iA_j)\dot{q}^j-\partial_iV. \tag{1.4}$$

Here we denote by $(\underline{q},\underline{p})=(q^i,p_i)$ and by $(\underline{q},\underline{\dot{q}})=(q^i,\dot{q}^i)$ the coordinate systems on T^*Q and TQ, associated with a coordinate system $\underline{q}=(q^i)$ on Q. We denote by ∂_i the partial derivative with respect to the variable q^i. In the following we shall use the symbol ∂^i for the partial derivative with respect to p_i.

A natural Hamiltonian is called separable if there are coordinates $\underline{q}$ on Q such that the Hamilton–Jacobi equation

$$H(\underline{q},\underline{p})=h, \quad p_i=\partial_iW \tag{1.5}$$

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admits a *separated complete solution* of the form

$$W(\underline{q},\underline{c})=W_1(q^1,\underline{c})+\cdots W_n(q^n,\underline{c}), \tag{1.6}$$

where $\underline{c}=(c_i)$ is a set of n constants satisfying the *completeness condition*

$$\det\left[\frac{\partial^2 W}{\partial q^i \partial c_j}\right]\neq 0. \tag{1.7}$$

The interest of separable Hamiltonians lies essentially on two facts: (1) in separable coordinates $\underline{q}$ the integration of the Hamilton–Jacobi equation is reduced to (at most n) simple integrals (i.e., involving single variables); (2) the separation of variables is characterized by the existence of n first integrals in involution, quadratic or linear in the conjugate momenta $\underline{p}$. Hence, separable Hamiltonians give rise to a particular but wide class of completely integrable Hamiltonian systems. In the theory of separation of variables a basic role is played by the geodesic Hamiltonian

$$G=\tfrac{1}{2}g^{ij}p_i p_j\,. \tag{1.8}$$

Indeed, as pointed out by Levi-Civita,[1] a necessary condition for the separability of a natural Hamiltonian (1.1) is the separability of the corresponding geodesic Hamiltonian (1.8). Moreover, it is known that the separability of G is characterized by the existence of Killing vectors and Killing 2-tensors on the Riemannian manifold Q (which generate quadratic and linear first integrals in involution) satisfying suitable properties.[2–9] This shows that the separability is not simply a local property concerning with coordinates but it is in fact related to the existence of intrinsic objects satisfying coordinate-independent properties. As a consequence, the intrinsic characterization of the separability (by means of algebraic objects like Killing vectors and tensors[4–8] and geometrical objects like ''Killing webs''[9,10]) provide a useful and effective tool for finding and constructing separable Hamiltonian systems. While the theory of the geodesic separability can be easily extended to natural Hamiltonians of the kind

$$G=\tfrac{1}{2}g^{ij}p_i p_j+V, \tag{1.9}$$

involving a scalar potential only, the extension to the general Hamiltonian (1.1) with a vector potential meets some difficulties, as explained below. However, several important results are already present in the literature, but all concerning the general form of the functions (g^{ij},A^i,V) in separable coordinates[11–14] (also in the time-dependent case). The aim of the present paper is to revisit all this matter at the light of the more recent progress in the geometrical characterization of the separation.[10] As it has been done for a pure geodesic Hamiltonian G, for investigating on the intrinsic properties of the objects $(\mathbf{g},\mathbf{A},V)$ underlying the separation, a starting point could be the fundamental *Levi-Civita separability conditions*[1]

$$\partial^i\partial^j H\partial_i H\partial_j H+\partial_i\partial_j H\partial^i H\partial^j H-\partial^i\partial_j H\partial_i H\partial^j H-\partial_i\partial^j H\partial^i H\partial_j H=0 \tag{1.10}$$

(no sum over the indices $i\neq j$) which yield second-order differential equations on the functions (g^{ij},A^i,V). But these equations turn out to be of such a complexity that this way seems to be hopeless. An alternative method could be the analysis of the known expressions[11,12] of the functions (g^{ij},A^i,V) in separable coordinates (as done for instance in Ref. 15, for the orthogonal separation, on the basis of previous results by Steigeberger[13]). But also this method appears to be rather difficult and, moreover, it does not provide a good and complete understanding of the intrinsic meaning of the separation, where a basic and simplifying role is played by particular classes of coordinates, called *normal separable coordinates*.[7–10] Instead, we propose here a direct and geometrical method which makes the problem clear and easily solvable from the very beginning. The basic (and very simple) idea of this method is the following: we replace the original Hamiltonian (1.1) by an ''equivalent'' geodesic Hamiltonian on the ''extended manifold'' Q

$\times\mathbb{R}$ endowed with a suitable ''extended metric'' (Sec. IV); then, we apply to this new Hamiltonian the well-known methods of the theory of the geodesic separability.[7,8,10]

In the present paper we consider, for simplicity, only the case of a positive–definite metric. This makes the discussion considerably easier, since we avoid the cases of degenerate separation where the so-called second-class null coordinates occur. However, all results hold for the nondegenerate separation in a metric of any signature. The case of a Lorentzian metric will be considered in detail in a further paper.

II. NOTATION

We denote by $\langle \mathbf{X}, \varphi \rangle = X^i \varphi_i$ the evaluation between a vector field $\mathbf{X}$ and a 1-form φ. In particular, $\langle \mathbf{X}, dV \rangle = X^i \partial_i V$ is the derivative of the function V with respect to the vector $\mathbf{X}$. We denote by $\mathbf{u} \cdot \mathbf{v}$ the scalar product of two vectors, $\mathbf{u} \cdot \mathbf{v} = \mathbf{g}(\mathbf{u}, \mathbf{v}) = g_{ij} u^i v^j$. The canonical Poisson–Lie brackets of functions over a cotangent bundle are defined by

$$\{f, g\} = \partial^i f \partial_i g - \partial^i g \partial_i f. \tag{2.1}$$

We consider the natural identification between contravariant symmetric tensors $\mathbf{K} = (K^{i_1 \cdots i_k})$ on Q and the homogeneous polynomial functions on the cotangent bundle T^*Q, defined by

$$P(\mathbf{K}) = P_{\mathbf{K}} = K^{i_1 \cdots i_k} p_{i_1} \cdots p_{i_k}. \tag{2.2}$$

For a function f on Q (tensor of order 0) P_f is its natural extension to T^*Q constant on the fibers. Then the Poisson brackets induce Nijenhuis–Lie brackets between contravariant symmetric tensors on Q by setting

$$\{P_{\mathbf{K}}, P_{\mathbf{L}}\} = P_{[\mathbf{K}, \mathbf{L}]}. \tag{2.3}$$

If $\mathbf{K}$ and $\mathbf{L}$ are of order k and l, respectively, then $[\mathbf{K}, \mathbf{L}]$ is of order $k + l - 1$. In particular, for two vector fields, $[\mathbf{X}, \mathbf{Y}]$ are the ordinary Lie brackets, and $[\mathbf{X}, \mathbf{K}]$ is the Lie derivative of the tensor field $\mathbf{K}$ with respect to the vector field $\mathbf{X}$. We say that two (symmetric) tensors are *in involution* (or that they *commute*) if $[\mathbf{K}, \mathbf{L}] = 0$. This means that the corresponding polynomial functions are in involution: $\{P_{\mathbf{K}}, P_{\mathbf{L}}\} = 0$. Killing vectors and Killing tensors are defined by the *Killing equations*

$$[\mathbf{X}, \mathbf{G}] = 0, \quad [\mathbf{K}, \mathbf{G}] = 0, \tag{2.4}$$

where

$$\mathbf{G} = (g^{ij})$$

is the contravariant metric tensor. This means that the corresponding functions $P_{\mathbf{X}}$ and $P_{\mathbf{K}}$ are first integrals of the geodesic flow. As for any symmetric 2-tensor on a Riemannian manifold, a Killing tensor $\mathbf{K}$ can be interpreted as a linear operator over 1-forms or vector fields; we shall denote by $\mathbf{K}\varphi$ and by $\mathbf{K}\mathbf{X}$, respectively, the images by $\mathbf{K}$ of a 1-form φ and of a vector $\mathbf{X}$, whose local representations, in any coordinate system $\underline{q}$, are

$$\mathbf{K}\varphi = g_{ij} K^{jh} \varphi_h \, dq^i, \quad \mathbf{K}\mathbf{X} = K^{ih} g_{hj} X^j \partial_i. \tag{2.5}$$

The contravariant metric tensor $\mathbf{G}$ corresponds to the identity mapping,

$$\mathbf{G}\varphi = \varphi, \quad \mathbf{G}\mathbf{X} = \mathbf{X}.$$

We denote by $\flat$ the bijective mapping from vector fields to 1-forms on Q, defined by the equivalent equations

$$\langle \mathbf{Y}, \mathbf{X}^\flat \rangle = \mathbf{Y} \cdot \mathbf{X}, \quad \mathbf{G}(\mathbf{X}^\flat, \varphi) = \langle \mathbf{X}, \varphi \rangle. \tag{2.6}$$

III. AN OUTLINE ON THE GEODESIC SEPARATION

In order to make this paper self-contained we recall in this section, with suitable adaptations, the basic definitions and results of the geometrical theory of the separation of the geodesic Hamilton–Jacobi equation.

(A) An *orthogonal web* on a Riemannian manifold Q_n is a set $(\mathcal{S}^a)$ $(a=1,...,m)$ of $m \leqslant n$ pairwise transversal and orthogonal foliations of leaves of codimension 1. In a positive–definite metric the orthogonality implies the transversality, and moreover, the intersections of all the leaves of $(\mathcal{S}^a)$ form a foliation $\mathcal{O}$ of submanifolds of dimension $r=n-m$. If these submanifolds are the orbits of a r-dimensional space D of commuting Killing vectors, then we say that the set

$$(\mathcal{S}^a, D) = (\mathcal{S}^1, \ldots, \mathcal{S}^m, D) \tag{3.1}$$

is a *Killing web*. The orbits of D are locally flat submanifolds.

(B) If the foliations $(\mathcal{S}^a)$ are, respectively, orthogonal to m eigenvectors $(\mathbf{X}_a)$ of a Killing 2-tensor $\mathbf{K}$ associated with m pointwise distinct eigenvalues (λ^a), and if $\mathbf{K}$ is D-invariant $([\mathbf{X}, \mathbf{K}]=0, \forall \mathbf{X} \in D)$ then we say that the set

$$(\mathcal{S}^1, \ldots, \mathcal{S}^m, D, \mathbf{K}) \tag{3.2}$$

is a *separable Killing web* and that $\mathbf{K}$ is a *characteristic Killing tensor* of the web. Since only the eigenvectors (or eigenforms) orthogonal to the foliations $(\mathcal{S}^a)$ are relevant for the separation, we call them *main eigenvectors* (or *main eigenforms*) of $\mathbf{K}$. Points of Q where these objects are not defined or do not satisfy the above requirements are called *singular points* of the web. They form the *singular set* of the web.

(C) From a purely algebraic point of view a separable Killing web is then completely determined by a pair

$$(D, \mathbf{K}) \tag{3.3}$$

which we call *characteristic Killing pair*, made of a r-dimensional linear space $(r \leqslant n)$ D of commuting Killing vectors and of a Killing 2-tensor $\mathbf{K}$ satisfying the following requirements: (i) the vectors of D span a regular distribution Δ of rank r (i.e., a subbundle $\Delta \subseteq TQ$ such that $\dim(\Delta)=n+r$); (ii) $\mathbf{K}$ is D-invariant; (iii) $\mathbf{K}$ has $m=n-r$ *normal* (i.e., orthogonally integrable) eigenvectors $(\mathbf{X}_a)$ $(a=1,...,m)$ (the *main eigenvectors*) orthogonal to D and associated with m pointwise distinct eigenvalues (λ^a).

(D) In a neighborhood of a nonsingular point a Killing web $(\mathcal{S}^a, D)$ generates coordinate systems (q^a, q^α) $(a=1,...,m;\ \alpha=m+1,...,n)$ such that each dq^a is a characteristic 1-form of the corresponding foliation $\mathcal{S}^a$ (q^a is constant on the leaves of $\mathcal{S}^a$) and (q^α) are the affine parameters of the integral curves of r vector fields $(\mathbf{X}_\alpha)$ forming a basis of D, with zero values on a chosen submanifold $\mathcal{Z}$ of codimension r, transversal to the orbits of D. It follows that the coordinates (q^a) are orthogonal, $g^{ab}=\mathbf{G}(dq^a, dq^b)=0$ for $a \neq b$, and their coordinate hypersurfaces are open submanifolds of the leaves of the web. Moreover, the coordinates (q^α) are ignorable, $\partial_\alpha g^{ij}=0$, since they are generated by Killing vectors. We say that such a coordinate system is *adapted* to or *generated* by the Killing web, and *based on the section* $\mathcal{Z}$ (Fig. 1).

(E) It can be shown that[10] the coordinates adapted to a Killing web are separable for the geodesic Hamiltonian G if and only if there exists a Killing 2-tensor $\mathbf{K}$ satisfying conditions of item (B), i.e., if and only if $(\mathcal{S}^a, D, \mathbf{K})$ is a separable Killing web. This is equivalent to say that the geodesic Hamiltonian G is separable if and only if there exists a characteristic Killing pair $(D, \mathbf{K})$ [see item (C)].

(F) It can be proved that[9,10] in a separable Killing web the distribution $\Delta^\perp$ orthogonal to D is completely integrable, so that there exists a foliation of m-dimensional manifolds orthogonal to the

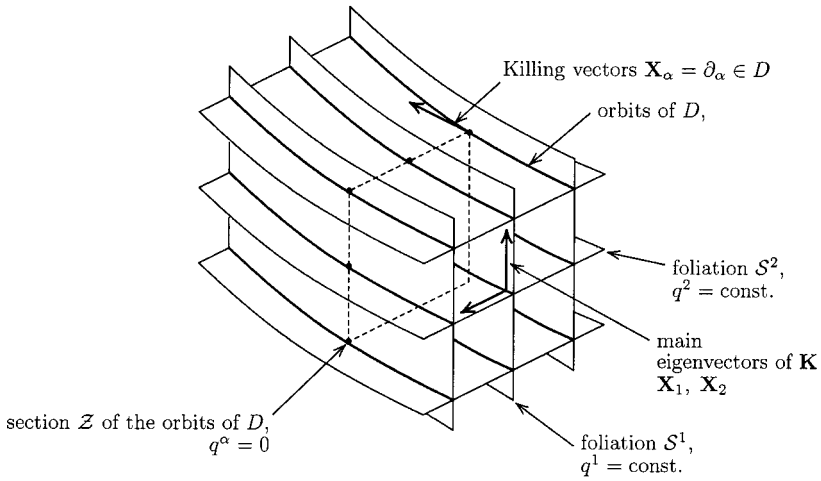

FIG. 1. Illustration of the elements of a separable Killing web $(\mathcal{S}^a, D, \mathbf{K})$ (for $a=1,2$).

orbits of D. The separable coordinates adapted to a separable Killing web and based on a section $\mathcal{Z}$ orthogonal to D are called *normal separable coordinates*. In these coordinates the contravariant metric assumes the semidiagonal *standard form*

$$[g^{ij}] = \left[\begin{array}{ccc|c} g^{11} & & & \\ & \ddots & 0 & \\ & g^{aa} & & 0 \\ & 0 & \ddots & \\ & & g^{mm} & \\ \hline & 0 & & g^{\alpha\beta} \end{array}\right]. \tag{3.4}$$

(G) There are two extreme cases of the above description: (i) $m=n$, $r=0$; in this case the space of Killing vectors D vanishes, the Killing web is simply an orthogonal web of n foliations of codimension 1; (ii) $m=0$, $r=n$; in this case the foliations $\mathcal{S}^a$ disappear, and only the n-dimensional space D of commuting K-vectors is present; such a K-web is always separable, with $\mathbf{K}=0$. There is a further particular case: (iii) $m=1$, $r=n-1$; in this case we have a single foliation of codimension 1 made of the orbits of $n-1$ commuting K-vectors; such a K-web is always separable, with $\mathbf{K}=\mathbf{G}$.

(H) Separable coordinate systems occur in equivalence classes: two separable systems are equivalent if the corresponding complete integrals generate the same Lagrangian foliation in T^*Q. A separable Killing web is the geometrical counterpart of an equivalence class of separable coordinates for the geodesic Hamiltonian. According to Levi-Civita,[1] the coordinates (q^i) of a separable system are divided into two classes: a coordinate q^i is of *first class* if the fraction $\partial_i H/\partial^i H$ is linear (homogeneous) in the momenta (p_j). Otherwise, it is of *second class*. Second-class coordinates are also called *essential separable coordinates*. They are usually labeled by indices $a,b,\ldots$ running from 1 to $m \leqslant n$. The first-class coordinates are labeled by indices $\alpha, \beta, \ldots$ running from $m+1$ to n. The numbers (r, m) of coordinates of first and second class, respectively, are the same for two equivalent separable systems and moreover, a separable systems is always equivalent to a normal separable system, see item (F), in which the first-class coordinates are ignorable and the metric tensor has the standard form (2.1).[7,8] In the transformation from a generic separable coordinate system to a normal one, the second-class coordinates remain essentially unchanged (they are related by a separated transformation, whose Jacobian is diagonal) so that their coordinate surfaces are invariant; these surfaces span the foliations $\mathcal{S}^a$ of the underlying

separable Killing web. Moreover, the partial derivatives (∂_α) with respect to the first-class coordinates (ignorable or not), interpreted as vector fields, span the space D of the underlying separable Killing web.

(I) The nonvanishing metric components (3.4) in normal separable coordinates have the form

$$g^{aa}=\varphi^a_{(m)}, \quad g^{\alpha\beta}=g^{aa}\phi_a^{\alpha\beta}, \tag{3.5}$$

where $\phi_a^{\alpha\beta}$ are functions of q^a only and $\varphi^a_{(m)}$ is the mth row of the inverse of a $m\times m$ *Stäckel matrix* $[\varphi_a^{(b)}]$: this is a matrix of functions depending only on the coordinate q^a corresponding to the lower index.

(J) A characteristic Killing pair $(D,\mathbf{K})$ generates an m-dimensional space $\mathcal{K}$ of Killing 2-tensors which are (i) D-invariant, (ii) in involution, and (iii) with m eigenvectors in common orthogonal to D (the main eigenvectors of the characteristic tensor $\mathbf{K}$). The components of an element of $\mathcal{K}$ in normal separable coordinates form a matrix similar to that of the metric (3.4). By formulas similar to (3.5), the rows of the inverse Stäckel matrix generate the components of a basis $(\mathbf{K}_b)$ of $\mathcal{K}$, $b=1,...,m$, with $\mathbf{K}_m=\mathbf{G}$,

$$K_b^{aa}=\varphi^a_{(b)}, \quad K_b^{\alpha\beta}=\varphi^a_{(b)}\phi_a^{\alpha\beta}. \tag{3.6}$$

This space includes $\mathbf{K}$ and the contravariant metric tensor $\mathbf{G}$. We call $\mathcal{K}$ the separable Killing algebra generated by $(D,\mathbf{K})$. If $\mathbf{K}^0$ is an element of $\mathcal{K}$ with distinct eigenvalues corresponding to the main eigenvectors, then the pairs $(D,\mathbf{K}^0)$ and $(D,\mathbf{K})$ are said to be equivalent (the define the same $\mathcal{K}$). The m quadratic functions

$$G_b=\tfrac{1}{2}P(\mathbf{K}_b)=\tfrac{1}{2}K_b^{ij}p_ip_j=\tfrac{1}{2}\varphi^a_{(b)}(p_a^2+\phi_a^{\alpha\beta}p_\alpha p_\beta) \tag{3.7}$$

together with the r linear functions

$$G_\alpha=P(\mathbf{X}_\alpha)=p_\alpha$$

associated with a basis $(\mathbf{X}_\alpha)$ of D, form a system of n independent first integrals in involution of the geodesic flow. Moreover, from the eigenform equations

$$\mathbf{K}_b\,dq^a=\lambda_b^a\,dq^a, \tag{3.8}$$

we derive the following relation between the main eigenvalues of $\mathbf{K}_b$ (corresponding to the main eigenvectors of the characteristic tensor $\mathbf{K}$) and the inverse Stäckel matrix,

$$\lambda_b^a=\frac{\varphi^a_{(b)}}{\varphi^a_{(m)}}, \tag{3.9}$$

so that

$$G_b=\tfrac{1}{2}\lambda_b^a g^{aa}(p_a^2+\phi_a^{\alpha\beta}p_\alpha p_\beta). \tag{3.10}$$

In this last formula, the quadratic first integrals in involution are expressed in terms of the main eigenvalues of the Killing tensors forming a basis of $\mathcal{K}$, without any reference to the Stäckel matrix.

(K) It can be shown that[10] a natural Hamiltonian $H=G+V$ is separable if and only if there exists a characteristic Killing pair $(D,\mathbf{K})$ such that

$$D(V)=0, \quad d(\mathbf{K}\,dV)=0. \tag{3.11}$$

The first of these two conditions means that V is D-invariant, $\langle \mathbf{X}, dV\rangle = 0$, $\forall \mathbf{X} \in D$, the second one that the 1-form $\mathbf{K}\,dV$ (image of dV by $\mathbf{K}$) is closed, hence locally exact. We call the second equation (3.11) the *characteristic equation of a separable potential*. Moreover,[7,8] a function V satisfies conditions (3.11) if and only if in a normal separable coordinate system is of the form

$$V = g^{aa}\phi_a = \varphi^a_{(m)}\phi_a\,, \tag{3.12}$$

where each ϕ_a is a function of q^a only. Functions of this kind are called *Stäckel multipliers*.[6] We observe that the first-class metric components $g^{\alpha\beta}$ (3.5) are Stäckel multipliers. It is remarkable that if V satisfies equations (3.11) then the characteristic equation holds for all elements of the algebra $\mathcal{K}$ generated by the characteristic Killing pair $(D,\mathbf{K})$. Hence, with a basis $(\mathbf{K}_b)$ of $\mathcal{K}$, we can associate (at least locally) m D-invariant functions (V_b) such that

$$\mathbf{K}_b\, dV = dV_b\,. \tag{3.13}$$

These *associated potentials* have a form similar to (3.12),

$$V_b = K_b^{aa}\phi_a = \varphi^a_{(b)}\phi_a\,. \tag{3.14}$$

The n functions

$$\begin{gathered} H_b = G_b + V_b = \tfrac{1}{2}\varphi^a_{(b)}(p_a^2 + \phi_a^{\alpha\beta}p_\alpha p_\beta + 2\phi_a) = \tfrac{1}{2}\lambda^a_b g^{aa}(p_a^2 + \phi_a^{\alpha\beta}p_\alpha p_\beta + 2\phi_a), \\ H_\alpha = P(\mathbf{X}_\alpha) = p_\alpha \end{gathered} \tag{3.15}$$

are independent first integrals in involution.

(L) It is useful to remark that, from an intrinsic point of view, a Stäckel multiplier is always the sum of scalar products of gradients of functions constant on the leaves of the web.

IV. THE EXTENDED METRIC

Let Q be a differentiable manifold with local coordinates (q^i) and let $\hat{Q} = Q \times \mathbb{R}$ be the *extended manifold* with local coordinates $(q^A) = (q^i, q^0)$ (q^0 is the natural coordinate over the real line). Let us consider on Q a positive–definite contravariant metric tensor $\mathbf{G} = (g^{ij})$, a vector field $\mathbf{A} = (A^i)$, and a function U. The triple

$$\hat{\mathbf{G}} = (\mathbf{G}, \mathbf{A}, U)$$

generates a contravariant symmetric 2-tensor $\hat{\mathbf{G}}$ on $\hat{Q}$ by setting

$$\hat{G}^{AB} = \begin{bmatrix} \hat{G}^{ij} & \hat{G}^{i0} \\ \hat{G}^{0j} & \hat{G}^{00} \end{bmatrix} = \begin{bmatrix} g^{ij} & A^i \\ A^j & 2U \end{bmatrix}. \tag{4.1}$$

In matrix notation,

$$\hat{\mathbf{G}} = \begin{bmatrix} \mathbf{G} & \mathbf{A} \\ \mathbf{A}^\tau & 2U \end{bmatrix}. \tag{4.2}$$

If $\det \hat{\mathbf{G}} > 0$, then $\hat{\mathbf{G}}$ is a positive–definite metric tensor, which we call *extended metric tensor*. Since $\det \mathbf{G} > 0$ and the determinant of the matrix (4.2) is a sum containing the term $2U \cdot \det \mathbf{G}$, the regularity condition $\det \hat{\mathbf{G}} > 0$ can be locally satisfied by adding to the function U a suitable positive constant. Because of the physical meaning of the function U (1.2) any additional constant

is inessential. If the function U has a lower bound, then this process of regularization is global. However, the local definition of the extended metric when U has no lower bound is not an obstruction to our purposes, since we shall use it as a local device.

Remark 4.1: In order to get a globally regular metric we could extend the manifold Q by two real axes, $\hat{Q}=Q\times\mathbb{R}\times\mathbb{R}$, and consider the contravariant metric

$$\hat{\mathbf{G}}=\begin{bmatrix}\mathbf{G} & \mathbf{A} & 0\\ \mathbf{A}^{\intercal} & 2U & 1\\ 0 & 1 & 0\end{bmatrix} \tag{4.3}$$

for which $\det\hat{\mathbf{G}}=-\det\mathbf{G}$. However, this metric is Lorentzian. Both the extensions (4.2) and (4.3) are contravariant. The metric (4.2) is a sort of Kaluza–Klein metric. Metrics similar to (4.2) and (4.3), with $\mathbf{A}=0$, have been considered by Eisenhart[16] in his interpretation of the dynamical trajectories of a holonomic system, with time-dependent constraints and potentials, as geodesics on a Riemannian manifold.

Remark 4.2: Any real function f on Q has a natural extension to $\hat{Q}=Q\times\mathbb{R}$ (constant along the fiber $\mathbb{R}$). For the sake of simplicity we denote this extension by the same symbol f. From the definition (4.2) it follows that the extended metric is characterized by the following equations, where (f, g) are arbitrary functions on Q:

$$\begin{aligned}\hat{\mathbf{G}}(df,dg)&=\mathbf{G}(df,dg),\\ \hat{\mathbf{G}}(df,dq^0)&=\langle\mathbf{A},df\rangle,\\ \hat{\mathbf{G}}(dq^0,dq^0)&=2U.\end{aligned} \tag{4.4}$$

Remark 4.3: The extended geodesic Hamiltonian is

$$\hat{G}=\tfrac{1}{2}P(\hat{\mathbf{G}})=\tfrac{1}{2}\hat{G}^{AB}p_Ap_B=\tfrac{1}{2}g^{ij}p_ip_j+A^ip_ip_0+Up_0^2 \tag{4.5}$$

(with indices $A=0,1,...,n$; $i, j=1,...,n$). Since q^0 is ignorable, the corresponding momentum p_0 is a first integral. As a consequence, the integral curves with $p_0=1$ of the Hamilton equations of $\hat{G}$ reduce to the integral curves of the Hamilton equations of H (1.1). In other words, the geodesic flow of the extended metric is projectable onto the Hamiltonian flow of H.

Remark 4.4: Let $W(\underline{q},\underline{c})$ be a complete solution of the Hamilton–Jacobi equation (1.5). Then the function

$$\hat{W}(\underline{q},q^0,\underline{c},c_0)=c_0(W(\underline{q},\underline{c})+q^0) \tag{4.6}$$

is a complete solution of the Hamilton–Jacobi equation associated with $\hat{G}$:

$$\tfrac{1}{2}g^{ij}\partial_i\hat{W}\partial_j\hat{W}+A^i\partial_i\hat{W}\partial_0\hat{W}+U(\partial_0\hat{W})^2=k.$$

Indeed, this equation reduces to

$$c_0^2(\tfrac{1}{2}g^{ij}\partial_iW\partial_jW+A^i\partial_iW+U)=k,$$

i.e., to Eq. (1.5) with $h=k/c_0^2$. Furthermore,

$$\begin{bmatrix} \dfrac{\partial^2 \hat{W}}{\partial q^i \partial c_j} & \dfrac{\partial^2 \hat{W}}{\partial q^i \partial c_0} \\ \dfrac{\partial^2 \hat{W}}{\partial q^0 \partial c_j} & \dfrac{\partial^2 \hat{W}}{\partial q^0 \partial c_0} \end{bmatrix} = \begin{bmatrix} c_0 \dfrac{\partial^2 W}{\partial q^i \partial c_j} & \dfrac{\partial W}{\partial q^i} \\ 0 & 1 \end{bmatrix}$$

and the completeness condition, i.e., the regularity of this matrix, is satisfied for $c_0 \neq 0$. By (4.6) we observe that if W is a separated complete solution of the form (1.6), then also $\hat{W}$ is separated. In other words, if (q^i) are separable coordinates for the Hamiltonian H, then (q^i, q^0) are also separable for the geodesic extended Hamiltonian $\hat{G}$. This shows that the separation of $\hat{G}$ is a necessary condition for the separation of H, and this is the reason why we shall analyze the separation in the extended space (Sec. V). However, as we shall see, the converse is not always true: the separation of $\hat{G}$ does not imply the separation of H, unless we consider a more general kind of separation, the *gauge separation* (see Definition 5.9 below).

Let us look at some properties of the fundamental objects defined on the extended manifold: vectors, 1-forms and 2-tensors. A vector field on $\hat{Q}$ is represented by a pair

$$\hat{\mathbf{X}} = (\mathbf{X}, \xi), \tag{4.7}$$

where $\mathbf{X}$ is a q^0-dependent vector field on Q and ξ a function on $\hat{Q}$. Its components are

$$(\hat{X}^A) = (X^i, \xi), \quad \hat{X}^i = X^i, \quad \hat{X}^0 = \xi,$$

so that, as a derivation,

$$\hat{\mathbf{X}} = X^i \frac{\partial}{\partial q^i} + \xi \frac{\partial}{\partial q^0} = X^i \partial_i + \xi \partial_0 .$$

A vector field $\hat{\mathbf{X}}$ is *horizontal* if $\xi = 0$, *vertical* if $\mathbf{X} = 0$. If we introduce the *fundamental vertical* vector field

$$\hat{\mathbf{X}}_0 = (0,1) = \partial_0 \tag{4.8}$$

then the expression (4.7) can be replaced with

$$\hat{\mathbf{X}} = \mathbf{X} + \xi \hat{\mathbf{X}}_0 . \tag{4.9}$$

We say that a vector field $\hat{\mathbf{X}}$ on $\hat{Q}$ is *vertically invariant* if $[\hat{\mathbf{X}}, \hat{\mathbf{X}}_0] = 0$. A vector field is vertically invariant iff both components $(\mathbf{X}, \xi)$ are q^0-independent. In this case, $\mathbf{X}$ is a vector field on Q and ξ is a function on Q. We call $\mathbf{X}$ the *basic component* of $\hat{\mathbf{X}}$ and ξ the *vertical component*.

Proposition 4.5: Two vertically invariant vector fields $\hat{\mathbf{X}} = (\mathbf{X}, \xi)$ and $\hat{\mathbf{Y}} = (\mathbf{Y}, \eta)$ commute, $[\hat{\mathbf{X}}, \hat{\mathbf{Y}}] = 0$, iff

$$\begin{gathered} \langle \mathbf{X}, d\eta \rangle = \langle \mathbf{Y}, d\xi \rangle, \\ [\mathbf{X}, \mathbf{Y}] = 0. \end{gathered} \tag{4.10}$$

Proof: Since all components do not depend on q^0, we have

$$[\hat{\mathbf{X}}, \hat{\mathbf{Y}}]^i = \hat{X}^A \partial_A Y^i - \hat{Y}^A \partial_A X^i = \hat{X}^j \partial_j Y^i - \hat{Y}^j \partial_j X^i = [\mathbf{X}, \mathbf{Y}]^i .$$

$$[\hat{\mathbf{X}}, \hat{\mathbf{Y}}]^0 = \hat{X}^A \partial_A \hat{Y}^0 - \hat{Y}^A \partial_A \hat{X}^0 = X^j \partial_j \hat{Y}^0 - Y^j \partial_j \hat{X}^0 = \langle \mathbf{X}, d\eta \rangle - \langle \mathbf{Y}, d\xi \rangle .$$

■

Proposition 4.6: A vertically invariant vector field $\hat{\mathbf{X}}=(\mathbf{X},\xi)$ is a Killing vector iff

$$\langle \mathbf{A}, d\xi\rangle = \langle \mathbf{X}, dU\rangle,$$

$$[\mathbf{X},\mathbf{A}] = \nabla\xi, \tag{4.11}$$

$$[\mathbf{X},\mathbf{G}] = 0.$$

Proof: The Killing equation $[\hat{\mathbf{X}},\hat{\mathbf{G}}]=0$ is equivalent to

$$\{\xi p_0 + X^i p_i, \tfrac{1}{2} g^{ij} p_i p_j + A^i p_i p_0 + U p_0^2\} = 0,$$

that is to

$$X^i(\tfrac{1}{2}\partial_i g^{hk} p_h p_k + \partial_i A^h p_h p_0 + \partial_i U p_0^2) - (\partial_i \xi p_0 + \partial_i X^h p_h)(g^{ik} p_k + A^i p_0) = 0.$$

The coefficients of p_0^2, $p_0 p_k$, and $p_h p_k$ generate equations

$$X^i \partial_i U - A^i \partial_i \xi = 0,$$

$$X^i \partial_i A^k - g^{ik}\partial_i \xi - A^i \partial_i X^k = 0,$$

$$(\tfrac{1}{2} X^i \partial_i g^{hk} - g^{ik}\partial_i X^h) p_h p_k = 0,$$

which are the coordinate representations of Eqs. (4.11).

■

The last equation (4.11) means that the basic component $\mathbf{X}$ of $\hat{\mathbf{X}}$ is a Killing vector. We notice that the fundamental vertical vector $\hat{\mathbf{X}}_0$ is a Killing vector. As for the contravariant metric, a contravariant symmetric 2-tensor on $\hat{Q}$ is represented by a triple

$$\hat{\mathbf{K}} = (\mathbf{K},\mathbf{C},F), \tag{4.12}$$

where $\mathbf{K}=(K^{ij})$ is a contravariant symmetric 2-tensor, $\mathbf{C}=(C^i)$ is a vector field, and F is a function on Q (all these objects may be q^0-dependent). In components,

$$\hat{K}^{AB} = \begin{bmatrix} K^{ij} & K^{i0} \\ K^{0j} & K^{00} \end{bmatrix} = \begin{bmatrix} K^{ij} & C^i \\ C^j & 2F \end{bmatrix}. \tag{4.13}$$

In matrix notation,

$$\hat{\mathbf{K}} = \begin{bmatrix} \mathbf{K} & \mathbf{C} \\ \mathbf{C}^{\intercal} & 2F \end{bmatrix}. \tag{4.14}$$

With this tensor we associate the Hamiltonian

$$\tfrac{1}{2} P(\hat{\mathbf{K}}) = \tfrac{1}{2}\hat{K}^{AB} p_A p_B = \tfrac{1}{2} K^{ij} p_i p_j + C^i p_i p_0 + F p_0^2. \tag{4.15}$$

This tensor is vertically invariant, $[\hat{\mathbf{X}}_0,\hat{\mathbf{K}}]=0$, iff all components are q^0-independent. In this case $\mathbf{K}$, $\mathbf{C}$, and F are objects on Q.

Proposition 4.7: A vertically invariant 2-tensor $\hat{\mathbf{K}}=(\mathbf{K},\mathbf{C},F)$ is a Killing tensor iff

$$
\begin{gathered}
[\mathbf{G},\mathbf{K}]=0,\\
[\mathbf{C},\mathbf{G}]=[\mathbf{A},\mathbf{K}],\\
[\mathbf{C},\mathbf{A}]=\nabla F-\mathbf{K}\nabla U,\\
\langle\mathbf{C},dU\rangle=\langle\mathbf{A},dF\rangle.
\end{gathered}
\tag{4.16}
$$

Proof: The Killing equation $[\hat{\mathbf{K}},\hat{\mathbf{G}}]=0$ is equivalent to $\{P_{\hat{\mathbf{G}}},P_{\hat{\mathbf{K}}}\}=0$,

$$
\begin{aligned}
&(g^{il}p_l+A^i p_0)(\tfrac{1}{2}\partial_i K^{hk}p_h p_k+\partial_i C^k p_k p_0+\partial_i F p_0^2)\\
&\quad-(K^{il}p_l+C^i p_0)(\tfrac{1}{2}\partial_i g^{hk}p_h p_k+\partial_i A^k p_k p_0+\partial_i U p_0^2)=0.
\end{aligned}
$$

The first equation (4.16) is determined by the coefficient of $(p_h p_k p_l)$. The coefficients of $p_0 p_h p_k$, $p_k p_0^2$, and p_0^3 give rise, respectively, to equations

$$
\begin{gathered}
(g^{ih}\partial_i C^k+\tfrac{1}{2}A^i\partial_i K^{hk}-K^{ih}\partial_i A^k-\tfrac{1}{2}C^i\partial_i g^{hk})p_h p_k=0,\\
g^{ik}\partial_i F+A^i\partial_i C^k-K^{ik}\partial_i U-C^i\partial_i A^k=0,\\
A^i\partial_i F-C^i\partial_i U=0,
\end{gathered}
$$

which are the coordinate representations of the last three equations (4.16). ■

We notice that the first equation (4.16) means that the basic component $\mathbf{K}$ is a Killing tensor.

Remark 4.8: As for any Riemannian manifold, the bijective mapping $\flat$ from 1-forms to vector fields on $\hat{Q}$ is defined by, see (2.6),

$$
\langle\hat{\mathbf{X}},df\rangle=\hat{\mathbf{G}}(df,\hat{\mathbf{X}}^{\flat}),
\tag{4.17}
$$

where f is a function on $\hat{Q}$. Since

$$
df=\frac{\partial f}{\partial q^i}dq^i+\frac{\partial f}{\partial q^0}dq^0,
$$

it follows that

$$
\hat{\mathbf{G}}(df,dq^0)=\frac{\partial f}{\partial q^i}\hat{G}^{i0}+\frac{\partial f}{\partial q^0}\hat{G}^{00}=A^i\frac{\partial f}{\partial q^i}+2U\frac{\partial f}{\partial q^0}.
$$

This shows that

$$
dq^0=(\mathbf{A},2U)^{\flat}.
\tag{4.18}
$$

Remark 4.9: A 1-form $\hat{\varphi}$ on $\hat{Q}$ is represented by a pair (φ,φ_0), where φ is a q^0-dependent 1-form on Q and φ_0 is a function on $\hat{Q}$. In local coordinates (q^i,q^0) we have $\hat{\varphi}=\hat{\varphi}_A\,dq^A=\varphi_i\,dq^i+\varphi_0\,dq^0$, where $\varphi=\varphi_i\,dq^i$. For any vector field $\hat{\mathbf{X}}=(\mathbf{X},\xi)$,

$$
\langle\hat{\mathbf{X}},\hat{\varphi}\rangle=\langle\mathbf{X},\varphi\rangle+\xi\varphi_0.
\tag{4.19}
$$

We say that $\hat{\varphi}$ is a *basic 1-form* if

$$
\varphi_0=\langle\hat{\mathbf{X}}_0,\hat{\varphi}\rangle=0.
\tag{4.20}
$$

The contravariant components of the image of a 1-form $\hat{\varphi}$ by a symmetric 2-tensor $\hat{\mathbf{K}}$ are

$$\begin{aligned}\hat{K}^{AB}\hat{\varphi}_B &= (\hat{K}^{ij}\varphi_j + \hat{K}^{i0}\varphi_0, \hat{K}^{0i}\varphi_i + \hat{K}^{00}\varphi_0)\\ &= (\hat{K}^{ij}\varphi_j + C^i\varphi_0, C^i\varphi_i + 2F\varphi_0).\end{aligned} \tag{4.21}$$

This shows that the eigenform equation $\hat{\mathbf{K}}\hat{\varphi} = \lambda\hat{\varphi}$ is equivalent to equations

$$\begin{aligned}&\mathbf{K}\varphi + \varphi_0\mathbf{C}^\flat = \lambda(\varphi + \varphi_0\mathbf{A}^\flat),\\ &\langle \mathbf{C}, \varphi\rangle + 2F\varphi_0 = \lambda(\langle \mathbf{A}, \varphi\rangle + 2U\varphi_0).\end{aligned} \tag{4.22}$$

For a basic eigenform these equations become

$$\begin{aligned}&\mathbf{K}\varphi = \lambda\varphi,\\ &\langle \mathbf{C}, \varphi\rangle = \lambda\langle \mathbf{A}, \varphi\rangle.\end{aligned} \tag{4.23}$$

V. SEPARABLE KILLING WEBS IN THE EXTENDED METRIC

Assume that the extended geodesic Hamiltonian $\hat{G}$ is separable. According to the general theory of the geodesic separability, this fact is characterized by the existence of a separable Killing web,

$$(\hat{\mathcal{S}}^a, \hat{D}, \hat{\mathbf{K}}), \tag{5.1}$$

where (I) $\hat{\mathcal{S}}^a$ is a set of m orthogonal foliations of submanifolds of codimension 1 ($a = 1,...,m$); (II) $\hat{D}$ is a $r+1$-dimensional linear space of commuting Killing vectors ($m + r = n$). These Killing vectors are tangent to the orbits of $\hat{D}$, and these orbits coincide with the complete intersections of the leaves of the foliations $\hat{\mathcal{S}}^a$; (III) $\hat{\mathbf{K}}$ is a Killing tensor of order 2. (III.a) $\hat{\mathbf{K}}$ is $\hat{D}$-invariant (it commutes with all elements of $\hat{D}$); (III.b) $\hat{\mathbf{K}}$ has m main eigenvectors orthogonal to the leaves of $\hat{\mathcal{S}}^a$, corresponding to distinct eigenvalues. It follows that locally on $\hat{Q}$ there are m independent functions $(\hat{q}^a)$ such that $(d\hat{q}^a)$ are characteristic 1-forms of the web, so that

$$\hat{\mathbf{K}}\, dq^a = \lambda^a\, dq^a, \quad \langle \hat{\mathbf{X}}, d\hat{q}^a\rangle = 0, \quad \forall \hat{\mathbf{X}} \in \hat{D}, \tag{5.2}$$

and

$$\hat{\mathbf{G}}(d\hat{q}^a, d\hat{q}^b) = 0, \quad a \neq b. \tag{5.3}$$

As it will be justified below, it is interesting to consider the particular case in which the fundamental vertical vector field $\hat{\mathbf{X}}_0$ is an element of $\hat{D}$.

Proposition 5.1: A separable Killing web $(\hat{\mathcal{S}}^a, \hat{D}, \hat{\mathbf{K}})$ on the extended manifold $\hat{Q}$, such that $\hat{\mathbf{X}}_0 \in \hat{D}$, is reducible to a separable Killing web on Q,

$$(\mathcal{S}^a, D, \mathbf{K}). \tag{5.4}$$

The meaning of the term ''reducible'' is explained in the following proof.

Proof: Since the second equation (5.2) implies in particular

$$\langle \hat{\mathbf{X}}_0, d\hat{q}^a\rangle = 0, \tag{5.5}$$

the functions $(\hat{q}^a)$ are vertically invariant and reduce to functions (q^a) on Q, so that, according to Remark 4.2, we can use the simplified notation $\hat{q}^a = q^a$. As a consequence, the web $(\hat{\mathcal{S}}^a)$ reduces to a web $(\mathcal{S}^a)$ with characteristic 1-forms (dq^a). Because of (4.4) and (5.3),

$$\mathbf{G}(dq^a, dq^b) = \hat{\mathbf{G}}(dq^a, dq^b) = 0 \quad (a \neq b) \tag{5.6}$$

and the reduced web is orthogonal. According to Propositions 4.5 and 4.6, the Killing vectors $\hat{\mathbf{X}} = (\mathbf{X}, \xi) \in \hat{D}$ reduce to commuting Killing vectors $\mathbf{X}$ on Q and form a space D of dimension $r = n - m$ (one dimension is lost by the vertical vector $\hat{\mathbf{X}}_0 \in \hat{D}$, which projects onto the zero vector field of Q). Since (dq^a) are basic 1-forms, from (4.19) it follows that

$$\langle \mathbf{X}, dq^a \rangle = \langle \hat{\mathbf{X}}, dq^a \rangle = 0. \tag{5.7}$$

Thus, the reduced Killing vectors are tangent to the leaves of the reduced web. The Killing tensor $\hat{\mathbf{K}}$ reduces to a Killing tensor $\mathbf{K}$ on Q (Proposition 4.7). The reduced Killing tensor commutes with all the reduced Killing vectors of D; the proof that $[\hat{\mathbf{X}}, \hat{\mathbf{K}}] = 0$ implies $[\mathbf{X}, \mathbf{K}] = 0$ is similar to that in the proof of Proposition 4.6. Finally, because of (4.23), the eigenform equation (5.2) reduces to equation

$$\mathbf{K}\, dq^a = \lambda^a\, dq^a,$$

and this shows that the reduced characteristic 1-forms (dq^a) are eigenforms of $\mathbf{K}$ corresponding to the distinct eigenvalues (λ^a). Since these eigenvalues are vertically invariant, they reduce to functions on Q.

■

Remark 5.2: If we choose a local basis $(\hat{\mathbf{X}}_\alpha, \hat{\mathbf{X}}_0)$ of $\hat{D}$ including the fundamental vertical vector field and a local section $\hat{\mathcal{Z}}$ orthogonal to the orbits of $\hat{D}$, then normal separable coordinates $(\hat{q}^A) = (\hat{q}^a, \hat{q}^\alpha, \hat{q}^0)$ are defined on $\hat{Q}$ such that $\hat{q}^a = q^a$,

$$\frac{\partial}{\partial \hat{q}^\alpha} = \hat{\mathbf{X}}_\alpha, \quad \frac{\partial}{\partial \hat{q}^0} = \hat{\mathbf{X}}_0, \tag{5.8}$$

and

$$\langle \hat{\mathbf{X}}_0, d\hat{q}^0 \rangle = 1, \quad \langle \hat{\mathbf{X}}_0, d\hat{q}^\alpha \rangle = 0, \quad \langle \hat{\mathbf{X}}_\alpha, d\hat{q}^0 \rangle = 0, \quad \langle \hat{\mathbf{X}}_\alpha, d\hat{q}^\beta \rangle = \delta^\beta_\alpha. \tag{5.9}$$

According to the general theory of the geodesic separation, the m separable coordinates (q^a) are essential, the $r+1$ coordinates $(\hat{q}^\alpha, \hat{q}^0)$ are ignorable, and the contravariant components of the extended metric

$$\hat{G}^{AB} = \hat{\mathbf{G}}(d\hat{q}^A, d\hat{q}^B), \tag{5.10}$$

have a form similar to (3.4) and (3.5), with one additional line and row with index 0 (index of first-class),

$$\begin{gathered} \hat{G}^{ab} = 0 \quad (a \neq b), \quad \hat{G}^{a\alpha} = 0, \quad \hat{G}^{a0} = 0, \\ \hat{G}^{aa} = \varphi^a_{(m)}, \quad \hat{G}^{00} = \phi_a \hat{G}^{aa}, \quad \hat{G}^{\alpha 0} = \phi^\alpha_a \hat{G}^{aa}, \quad \hat{G}^{\alpha\beta} = \phi^{\alpha\beta}_a \hat{G}^{aa}, \end{gathered} \tag{5.11}$$

where ϕ_a, ϕ^α_a, $\phi^{\alpha\beta}_a$ are functions of the coordinate corresponding to the lower index only. Furthermore, since all the elements of $\hat{D}$ commute, we have in particular $[\hat{\mathbf{X}}_0, \hat{\mathbf{X}}_\alpha] = 0$, and, due to (5.9), also the coordinates $(\hat{q}^\alpha)$ reduce to coordinates (q^α) on Q, so that we can use the simpler notation q^α instead of $\hat{q}^\alpha$. It follows that (q^a, q^α) is a normal separable coordinate system asso-

ciated with the reduced separable Killing web (5.4). However, as we shall see below, these coordinates are not separable with respect to the complete Hamiltonian H (1.1). For the separability of H further conditions are required. From the first characteristic equation of the extended metric (4.4) it follows that

$$\begin{aligned}\hat{G}^{ab}&=\hat{\mathbf{G}}(dq^a,dq^b)=\mathbf{G}(dq^a,dq^b)=g^{ab},\\ \hat{G}^{a\alpha}&=\hat{\mathbf{G}}(dq^a,dq^\alpha)=\mathbf{G}(dq^a,dq^\alpha)=g^{a\alpha},\\ \hat{G}^{\alpha\beta}&=\hat{\mathbf{G}}(dq^\alpha,dq^\beta)=\mathbf{G}(dq^\alpha,dq^\beta)=g^{\alpha\beta}.\end{aligned} \tag{5.12}$$

Hence, the comparison with (5.11) shows that the metric components (g^{ij}) maintain the same expressions (3.4) and (3.5),

$$\begin{aligned}&g^{ab}=0 \quad (a\neq b), \quad g^{aa}=\varphi^a_{(m)},\\ &g^{a\alpha}=0, \quad g^{\alpha\beta}=g^{aa}\phi_a^{\alpha\beta}=\varphi^a_{(m)}\phi_a^{\alpha\beta}.\end{aligned} \tag{5.13}$$

Remark 5.3: The natural coordinate q^0 of $\hat{Q}$ does not coincide with the separable coordinate $\hat{q}^0$ determined by $\hat{\mathbf{X}}_0$ in the basis of $\hat{D}$. As for any function of $\hat{Q}$, we can consider the differential of q^0 in the coordinates $(\hat{q}^A)=(q^a,q^\alpha,\hat{q}^0)$, written in the form

$$dq^0=f\,d\hat{q}^0+f_\alpha\,dq^\alpha+\xi_a\,dq^a.$$

Since we have $\langle\hat{\mathbf{X}}_0,dq^0\rangle=1$ because of the definition of $\hat{\mathbf{X}}_0$, from (5.9) and (5.5) (where $\hat{q}^\alpha=q^\alpha$, $\hat{q}^a=q^a$) it follows that $f=1$. Moreover, by applying to both sides of this equation the Killing vector $\hat{\mathbf{X}}_\alpha=(\mathbf{X}_\alpha,\xi_\alpha)$, due again to (5.9) and to (5.2) we get

$$\langle\hat{\mathbf{X}}_\alpha,d\hat{q}^0+f_\alpha\,dq^\alpha+\xi_a\,dq^a\rangle=f_\alpha, \quad \langle\hat{\mathbf{X}}_\alpha,dq^0\rangle=\langle\mathbf{X}_\alpha+\xi_\alpha\hat{\mathbf{X}}_0,dq^0\rangle=\xi_\alpha,$$

so that $f_\alpha=\xi_\alpha$. Hence,

$$dq^0=d\hat{q}^0+\xi_\alpha\,dq^\alpha+\xi_a\,dq^a, \tag{5.14}$$

where (ξ_α) are just the vertical components of the Killing vectors $(\hat{\mathbf{X}}_\alpha)$. Since the Killing vectors commute with $\hat{\mathbf{X}}_0$, these components reduce to functions on Q. By developing the commutation relations

$$\begin{aligned}0&=\left[\frac{\partial}{\partial\hat{q}^a},\frac{\partial}{\partial\hat{q}^\alpha}\right]=\left[\frac{\partial}{\partial\hat{q}^a},\hat{\mathbf{X}}_\alpha\right]\\ &=\left[\frac{\partial}{\partial\hat{q}^a},\mathbf{X}_\alpha+\xi_\alpha\hat{\mathbf{X}}_0\right]=\left[\frac{\partial}{\partial q^a},\mathbf{X}_\alpha\right]+\frac{\partial\xi_\alpha}{\partial q^a}\hat{\mathbf{X}}_0\\ &=\partial_a\xi_\alpha\hat{\mathbf{X}}_0,\end{aligned}$$

we find that

$$\partial_a\xi_\alpha=0. \tag{5.15}$$

By differentiating Eq. (5.14), we find equation

$$d\xi_\alpha\wedge dq^\alpha+d\xi_a\wedge dq^a=0.$$

Due to (5.15) and the q^0-independence of ξ_α, we obtain

$$\partial_\beta \xi_\alpha \, dq^\beta \wedge dq^\alpha + \partial_\alpha \xi_a \, dq^\alpha \wedge dq^a + \partial_b \xi_a \, dq^b \wedge dq^a + \partial_0 \xi_a \, dq^0 \wedge dq^a = 0.$$

It follows that

$$\partial_\alpha \xi_\beta = \partial_\beta \xi_\alpha, \quad \partial_\alpha \xi_a = 0, \quad \partial_a \xi_b = \partial_b \xi_a, \quad \partial_0 \xi_a = 0. \tag{5.16}$$

The last equation (5.16) shows that also the functions (ξ_a) appearing in (5.14) are q^0-independent. The remaining equations show that on Q there exist local functions $S_1(q^a)$ and $S_2(q^\alpha)$ depending on the essential coordinates (q^a) and on the ignorable coordinates (q^α), respectively, such that

$$\xi_a = \partial_a S_1, \quad \xi_\alpha = \partial_\alpha S_2. \tag{5.17}$$

Thus, the link (5.14) between q^0 and $\hat{q}^0$ takes the form

$$d\hat{q}^0 = dq^0 - d(S_1 + S_2), \quad S_1 = S_1(q^a), \quad S_2 = S_2(q^\alpha). \tag{5.18}$$

Remark 5.4: From Eqs. (4.4) it follows that

$$\begin{gathered}\hat{\mathbf{G}}(dq^a, dq^0) = \langle \mathbf{A}, dq^a \rangle = A^a, \\ \hat{\mathbf{G}}(dq^\alpha, dq^0) = \langle \mathbf{A}, dq^\alpha \rangle = A^\alpha, \\ \hat{\mathbf{G}}(dq^0, dq^0) = 2U.\end{gathered} \tag{5.19}$$

On the other hand, from (5.14), using (5.11) and (5.12), and recalling that $\hat{q}^a = q^a$, $\hat{q}^\alpha = q^\alpha$, we derive

$$\begin{aligned}\hat{\mathbf{G}}(dq^a, dq^0) &= \hat{\mathbf{G}}(dq^a, d\hat{q}^0) + \hat{\mathbf{G}}(dq^a, dq^\alpha)\xi_\alpha + \hat{\mathbf{G}}(dq^a, dq^b)\xi_b \\ &= \hat{G}^{a0} + \hat{G}^{a\alpha}\xi_\alpha + \hat{G}^{ab}\xi_b = \hat{G}^{aa}\xi_a = g^{aa}\xi_a, \\ \hat{\mathbf{G}}(dq^\alpha, dq^0) &= \hat{\mathbf{G}}(dq^\alpha, d\hat{q}^0) + \hat{\mathbf{G}}(dq^\alpha, dq^\beta)\xi_\beta + \hat{\mathbf{G}}(dq^\alpha, dq^b)\xi_b \\ &= \hat{G}^{\alpha 0} + \hat{G}^{\alpha\beta}\xi_\beta + \hat{G}^{ab}\xi_b = \hat{G}^{aa}\phi_a^\alpha + \hat{G}^{\alpha\beta}\xi_\beta = g^{aa}\phi_a^\alpha + g^{\alpha\beta}\xi_\beta, \\ \hat{\mathbf{G}}(dq^0, dq^0) &= \hat{\mathbf{G}}(d\hat{q}^0, d\hat{q}^0) + \hat{\mathbf{G}}(dq^\alpha, dq^\beta)\xi_\alpha\xi_\beta + \hat{\mathbf{G}}(dq^a, dq^b)\xi_a\xi_b \\ &\quad + 2\hat{G}(d\hat{q}^0, dq^\alpha)\xi_\alpha + 2\hat{\mathbf{G}}(d\hat{q}^0, dq^a)\xi_a + 2\hat{\mathbf{G}}(dq^\alpha, dq^a)\xi_\alpha\xi_a \\ &= \hat{G}^{00} + \hat{G}^{\alpha\beta}\xi_\alpha\xi_\beta + \hat{G}^{ab}\xi_a\xi_b + 2\hat{G}^{\alpha 0}\xi_\alpha = g^{aa}(\phi_a + \phi_a^{\alpha\beta}\xi_\alpha\xi_\beta + \xi_a^2 + 2\phi_a^\alpha\xi_\alpha).\end{aligned} \tag{5.20}$$

The comparison of Eqs. (5.19) and (5.20) shows that

$$\begin{gathered}A^a = g^{aa}\xi_a, \\ A^\alpha = g^{aa}\phi_a^\alpha + g^{\alpha\beta}\xi_\beta = g^{aa}(\phi_a^\alpha + \phi_a^{\alpha\beta}\xi_\beta), \\ 2U = g^{aa}(\phi_a + \phi_a^{\alpha\beta}\xi_\alpha\xi_\beta + \xi_a^2 + 2\phi_a^\alpha\xi_\alpha).\end{gathered} \tag{5.21}$$

We can summarize the preceding remarks in the following.

Proposition 5.5: If the extended metric admits a separable Killing web $(\hat{\mathcal{S}}^a, \hat{D}, \hat{\mathbf{K}})$ with $\hat{\mathbf{X}}_0 \in \hat{D}$, then on Q there exists a coordinate system (q^a, q^α) such that the components of $\mathbf{G}$ and $\mathbf{A}$ and the function U assume the form (5.13), (5.21), with $(\phi_a^\alpha, \phi_a^{\alpha\beta}, \phi_a)$ functions of the coordinate corresponding to the lower index only, and $\xi_i = \partial_i(S_1 + S_2)$, with $S_1(q^a)$ and $S_2(q^\alpha)$ functions of the essential coordinates (q^a) and of the ignorable coordinates (q^α), respectively.

Remark 5.6: From Eqs. (5.21) we observe that the vector field $\mathbf{A}$ is a sum of three vectors:

$$\mathbf{A}=\mathbf{A}_{(1)}+\mathbf{A}_{(2)}+\mathbf{A}_{(3)},$$

$$\mathbf{A}_{(1)}=g^{aa}\xi_a\mathbf{X}_a=\nabla S_1, \qquad \mathbf{A}_{(2)}=g^{\alpha\beta}\xi_\beta\mathbf{X}_\alpha=\nabla S_2=g^{aa}\phi_a^{\alpha\beta}\xi_\beta\mathbf{X}_\alpha, \tag{5.22}$$

$$\mathbf{A}_{(3)}=g^{aa}\phi_a^\alpha\mathbf{X}_\alpha,$$

where

$$\mathbf{X}_a=\partial_a=\frac{\partial}{\partial q^a}, \quad \mathbf{X}_\alpha=\partial_\alpha=\frac{\partial}{\partial q^\alpha}. \tag{5.23}$$

Since $\mathbf{X}_a\cdot\mathbf{X}_\alpha=0$, both vectors $\mathbf{A}_{(2)}$ and $\mathbf{A}_{(3)}$ are orthogonal to $\mathbf{A}_{(1)}$:

$$\mathbf{A}_{(1)}\cdot\mathbf{A}_{(2)}=0, \quad \mathbf{A}_{(1)}\cdot\mathbf{A}_{(3)}=0. \tag{5.24}$$

From the last equation (5.21) we get the following decomposition for the function U:

$$U=\tfrac{1}{2}\mathbf{A}_{(1)}\cdot\mathbf{A}_{(1)}+\tfrac{1}{2}\mathbf{A}_{(2)}\cdot\mathbf{A}_{(2)}+\mathbf{A}_{(2)}\cdot\mathbf{A}_{(3)}+V^0, \tag{5.25}$$

where

$$V^0=g^{aa}\phi_a \tag{5.26}$$

is a Stäckel multiplier. From (1.2), (5.22), (5.24), and (5.25) we derive the following expression for the (physical) scalar potential:

$$V=U-\tfrac{1}{2}\mathbf{A}\cdot\mathbf{A}=V^0-\tfrac{1}{2}\mathbf{A}_{(3)}\cdot\mathbf{A}_{(3)}. \tag{5.27}$$

Remark 5.7: Let us consider the reduced separable Killing web $(\mathcal{S}^a,D,\mathbf{K})$ of Proposition 5.1. Each foliation $\mathcal{S}^a$ is locally represented by equation $q^a=\text{const}$, the vectors $\mathbf{X}_\alpha=\partial_\alpha$ form a local basis of D, and the vectors $\mathbf{X}_a=\partial_a$ are eigenvectors of $\mathbf{K}$ orthogonal to D. Then the function S_1 is constant on the orbits of D, since it depends on the coordinates (q^a) only, while the function S_2 is constant on the submanifolds orthogonal to the orbits of D, since $\langle\mathbf{X}_a,dS_2\rangle=\partial_aS_2=0$. Hence, the vectors of the decomposition (5.22) are completely characterized by the following properties:

$$\begin{gathered}\mathbf{A}_{(1)} \text{ is a gradient of the orbits of } D,\\ \mathbf{A}_{(2)} \text{ is a gradient of the foliation orthogonal to the orbits of } D,\\ \mathbf{A}_{(3)} \text{ is tangent to the orbits of } D \text{ and its components in any}\\ \text{basis of } D \text{ are Stäckel multipliers.}\end{gathered} \tag{5.28}$$

Here, by *gradient of a foliation* we mean a vector field which is the gradient of a function constant on the leaves of the foliation (i.e., the corresponding 1-form is the differential of a function constant on the leaves). It follows in particular that $\mathbf{A}_{(1)}$ and $\mathbf{A}_{(3)}$ are D-invariant.

Remark 5.8: As a consequence of the expressions (5.13) and (5.21), the Hamilton–Jacobi equation (1.5) can be written in the form

$$\tfrac{1}{2}\varphi^a_{(m)}(\overline{p}_a^2+\phi_a^{\alpha\beta}\overline{p}_\alpha\overline{p}_\beta+2\phi_a^\alpha\overline{p}_\alpha+\phi_a)=h, \tag{5.29}$$

by setting

$$\overline{p_i}=p_i+\xi_i=p_i+\partial_i(S_1+S_2)\Leftrightarrow\begin{cases}\overline{p_a}=p_a+\xi_a=p_a+\partial_a S_1,\\ \overline{p_\alpha}=p_\alpha+\xi_\alpha=p_\alpha+\partial_\alpha S_2.\end{cases}\tag{5.30}$$

We can consider this equation as the last one of the following system of m equations:

$$\varphi^a_{(b)}(\overline{p}^2_a+\phi^{\alpha\beta}_a\overline{p}_\alpha\overline{p}_\beta+2\phi^\alpha_a\overline{p}_\alpha+\phi_a)=c_b,\tag{5.31}$$

where (c_b) are m arbitrary constants, and $c_m=2h$. By applying the Stäckel matrix $[\varphi^{(b)}_a]$ we get the equivalent system

$$\overline{p}^2_a+\phi^{\alpha\beta}_a\overline{p}_\alpha\overline{p}_\beta+2\phi^\alpha_a\overline{p}_\alpha+\phi_a=\varphi^{(b)}_a c_b.\tag{5.32}$$

By setting $\overline{p}_\alpha=c_\alpha=\text{const}$, this system splits into m separated equations:

$$(p_a+\partial_a S_1)^2=\Phi_a(q^a,\underline{c}),\quad p_\alpha=c_\alpha-\partial_\alpha S_2,\tag{5.33}$$

where

$$\Phi_a(q^a,\underline{c})=\varphi^{(b)}_a c_b-\phi^{\alpha\beta}_a c_\alpha c_\beta-2\phi^\alpha_a c_\alpha-\phi_a\tag{5.34}$$

are functions of the coordinate corresponding to the index only, and (in general) of all the n constants $\underline{c}=(c_b,c_\alpha)$. If we consider the integrals (with any choice of the signs)

$$W_a(q^a,\underline{c})=\pm\int\sqrt{\Phi_a(q^a,\underline{c})}dq^a,\tag{5.35}$$

then we build a complete solution of the Hamilton–Jacobi equation of the form

$$W=c_\alpha q^\alpha+\sum_a W_a-S,\quad S=S_1+S_2.\tag{5.36}$$

We observe that this is not a separated complete solution, due to the presence of the function S, which is not in general a sum of functions of single coordinates. However, this function does not contain the constants $\underline{c}$.

Hence, we are led to consider a more general kind of separation.

Definition 5.9: A Hamiltonian is *gauge-separable* if the corresponding Hamilton–Jacobi equation admits a complete solution of the form

$$W(\underline{q},\underline{c})=\sum_{i=1}^n W_i(q^i,\underline{c})-S(\underline{q}).\tag{5.37}$$

The gauge-separation is also called *R-separation* in connection with the multiplicative separation of the Helmholtz equation.[17]

Thus, we have proved

Proposition 5.10: If the extended metric admits a separable Killing web with $\hat{\mathbf{X}}_0\in\hat{D}$, then the Hamiltonian H (1.1) is gauge separable.

Remark 5.11: We have the ordinary separation of the Hamiltonian H if and only if (ξ_a) and (ξ_α) are functions of the coordinate corresponding to the index only, i.e.,

$$\partial_b\xi_a=0\quad(a\neq b),\quad\partial_\beta\xi_\alpha=0\quad(\alpha\neq\beta).\tag{5.38}$$

Since these functions are the covariant components of the vectors $\mathbf{A}_{(1)}$ and $\mathbf{A}_{(2)}$, it follows that the first equation (5.38) and the second equation (5.38) are, respectively, equivalent to the following two conditions:

$$\begin{aligned}&(1)\ \mathbf{A}_{(1)}\ \text{is the sum of gradients of the foliations } S^a,\\ &(2)\ \text{there is a basis } (\mathbf{X}_\alpha)\ \text{of } D\ \text{such that } \langle \mathbf{X}_\alpha, d(\mathbf{A}_{(2)}\cdot\mathbf{X}_\beta)\rangle = 0\ \text{ for }\ \alpha\neq\beta.\end{aligned} \tag{5.39}$$

Furthermore, going back to (5.14), we remark that conditions (5.38) are necessary and sufficient for the separability of the coordinate system (q^a,q^α,q^0), which in this case is equivalent to the coordinate system $(q^a,q^\alpha,\hat{q}^0)$ associated with the separable Killing web on the extended manifold.

VI. FINAL STATEMENTS AND REMARKS

From the discussion in the preceding section we can derive the following theorem on the intrinsic characterization of the separation of a natural Hamiltonian with scalar and vector potential.

Theorem 6.1: The Hamiltonian (1.1) is separable if and only if (i) on Q there exists a separable Killing web $(\mathcal{S}^a,D,\mathbf{K})$; (ii) the vector field $\mathbf{A}$ is a sum of three vectors,

$$\mathbf{A}=\mathbf{A}_{(1)}+\mathbf{A}_{(2)}+\mathbf{A}_{(3)},$$

where (ii.1) $\mathbf{A}_{(1)}$ is locally the sum of gradients of the foliations $\mathcal{S}^a$, (ii.2) $\mathbf{A}_{(2)}$ is locally a gradient of the foliation orthogonal to the orbits of D, and there exists a basis $(\mathbf{X}_\alpha)$ of D $(\alpha=m+1,\ldots,n)$ such that

$$\langle \mathbf{X}_\alpha, d(\mathbf{A}_{(2)}\cdot\mathbf{X}_\beta)\rangle = 0 \quad \text{for}\ \ \alpha\neq\beta;$$

(ii.3) $\mathbf{A}_{(3)}$ is tangent to the orbits of D and its components $A^\alpha_{(3)}$ with respect to any basis $(\mathbf{X}_\alpha)$ of D are Stäckel multipliers,

$$\langle \mathbf{X}, dA^\alpha_{(3)}\rangle = 0,\ \ \forall \mathbf{X}\in D, \quad d(\mathbf{K}\,dA^\alpha_{(3)})=0;$$

(iii) the function V is a sum

$$V=V^0-\tfrac{1}{2}\mathbf{A}_{(3)}\cdot\mathbf{A}_{(3)},$$

where V^0 is a Stäckel multiplier,

$$\langle \mathbf{X}, dV^0\rangle = 0, \quad \forall \mathbf{X}\in D, \quad d(\mathbf{K}\,dV^0)=0.$$

Proof: Assume that the Hamiltonian (1.1) is separable in a coordinate system (q^i). Then (Remark 4.4) the extended metric is separable in the coordinate system (q^i,q^0), with q^0 ignorable. As a consequence, on $\hat{Q}$ there exists a separable Killing web (5.1). Since q^0 is ignorable, the vector field ∂_0 belongs to $\hat{D}$. But this vector coincides with the fundamental vector field $\hat{\mathbf{X}}_0$. Thus, we are in the situation considered in Sec. V, and because of Proposition 5.5, Remarks 5.6–5.7, Proposition 5.10, and Remark 5.11, the conditions (i)–(iii) are fulfilled. Conversely, assume that these conditions are satisfied. Then, because of Remarks 5.7, 5.8, and 5.11, the Hamilton–Jacobi equation admits a separated solution.

■

Remark 6.2: The separable coordinates (q^α) are ignorable (hence, of first class) with respect to both the geodesic Hamiltonians $\hat{G}$ and G but in general they could be nonignorable and of second class for the Hamiltonian H, due to the presence of the functions ξ_α in the components of the vector potential. More precisely, an ignorable coordinate q^α is also of first class and ignorable in the whole Hamiltonian H if and only if the corresponding function ξ_α is constant. To see this, we consider the Hamiltonian written in the form

$$H=\tfrac{1}{2}g^{\alpha\beta}(p_\alpha+A_\alpha)(p_\beta+A_\beta)+\tfrac{1}{2}g^{aa}(p_a+A_a)^2+V.$$

The coordinates (q^α) appear only in the components (A_α). Because of (5.21),

$$A_\alpha = \xi_\alpha + g^{aa} g_{\alpha\beta} \phi_a^\beta,$$

so that $\partial_\alpha A_\beta = \partial_\alpha \xi_\beta = \delta_{\alpha\beta} \xi_\alpha^0$, where $\xi_\alpha^0 = \partial_\alpha \xi_\alpha$. Thus,

$$\frac{\partial_\alpha H}{\partial^\alpha H} = \frac{g^{\beta\gamma}(p_\beta + A_\beta)\partial_\alpha \xi_\gamma}{g^{\alpha\beta}(p_\beta + A_\beta)} = \xi_\alpha^0,$$

and this fraction becomes a linear (homogeneous) function in the momenta if and only if $\xi_\alpha^0 = 0$; in this case, $\partial_\alpha H = 0$.

Remark 6.3: The only physically interesting component of the vector potential $\mathbf{A}$ is $\mathbf{A}_{(3)}$, since the other two components are gradients and do not influence the motion of the system in the configuration space. Since the orbits in the configuration space are determined, via the Jacobi method, by the partial derivatives of W with respect to the constants $\underline{c}$, the independence of the motions from the gradient components can also be observed by the expressions of the separated solution (5.34)–(5.36), where the covariant components (ξ_a) and (ξ_α) of $\mathbf{A}_{(1)}$ and $\mathbf{A}_{(2)}$ do not appear explicitly. It follows, in particular, that there are no physically interesting separable systems with a vector potential $\mathbf{A}$, without the occurrence of symmetries (Killing vectors), since in this case $\mathbf{A}_{(3)}$ vanishes.

After this last remark we can confine our interest to the case $\mathbf{A}_{(1)} = \mathbf{A}_{(2)} = 0$, that is $\mathbf{A} = \mathbf{A}_{(3)}$, and consider the following simplified version of Theorem 6.1.

Theorem 6.4: The Hamiltonian (1.1) is separable if and only if (i) on Q there exists a characteristic Killing pair $(D, \mathbf{K})$, (ii) up to a gauge transformation the vector potential $\mathbf{A}$ is D-invariant, tangent to the orbits of D and its components (A^α) with respect to any basis $(\mathbf{X}_\alpha)$ of D are Stäckel multipliers,

$$\langle \mathbf{X}, dA^\alpha \rangle = 0, \quad \forall \mathbf{X} \in D, \quad d(\mathbf{K}\, dA^\alpha) = 0; \tag{6.1}$$

(iii) the scalar potential V is a sum

$$V = U - \tfrac{1}{2}\mathbf{A}\cdot\mathbf{A} \tag{6.2}$$

where U is a Stäckel multiplier,

$$\langle \mathbf{X}, dU \rangle = 0, \quad \forall \mathbf{X} \in D, \quad d(\mathbf{K}\, dU) = 0. \tag{6.3}$$

Remark 6.5: In (ii) the condition that $\mathbf{A}$ is D-invariant is redundant, since it follows from the other requirements. However, in view of the applications, it is convenient to mention it explicitly in the statement. We also observe that the Stäckel multiplier U in (6.2) is just the scalar part of the Hamiltonian (1.1). The expression (6.2) exhibits a relation of the ''physical'' potential energy V with the vector potential $\mathbf{A}$. This represents a very strong restriction for the separability of a physical system with $\mathbf{A} \neq 0$.

Remark 6.6: According to Theorem 6.4, the separation of a Hamilton–Jacobi equation always occurs in coordinates (q^a, q^α) for which (i) the metric tensor components assume the form (3.4)–(3.5); (ii) up to a gauge transformation the components of the vector potential have the form

$$A^a = 0, \quad A^\alpha = g^{aa} \phi_a^\alpha; \tag{6.4}$$

(iii) the scalar potentials have the form

$$U = g^{aa} \phi_a, \quad V = U - \tfrac{1}{2} g^{aa} g^{bb} \phi_a^\alpha \phi_b^\beta g_{\alpha\beta}, \tag{6.5}$$

where ϕ_a^α and ϕ_a are functions depending on the coordinate corresponding to the lower index only. All these expressions are derived from (5.21), with $\xi_a = 0$ and $\xi_\alpha = 0$. From (1.4) it follows that the Lagrangian forces are

$$F_a = -\partial_a V - \partial_a A_\alpha \dot{q}^\alpha, \quad F_\alpha = \partial_a A_\alpha \dot{q}^a. \tag{6.6}$$

In the case of a vanishing scalar potential, $V=0$, also the scalar product

$$\mathbf{A}\cdot\mathbf{A} = g^{aa} g^{bb} \phi_a^\alpha \phi_b^\beta g_{\alpha\beta} \tag{6.7}$$

must be a Stäckel multiplier. This is a further very strong restriction for the separability, which, however, disappears in the case $m=1$.

Remark 6.7: Theorem 6.4 has another interesting consequence. Let $(\mathbf{K}_b)$ $(b=1,...,m)$ be a basis of the Killing algebra $\mathcal{K}$ generated by the characteristic Killing pair $(D,\mathbf{K})$, with $\mathbf{K}_1=\mathbf{K}$ and $\mathbf{K}_m=\mathbf{G}$ [see item (J) of Sec. III]. Then, besides the $r=n-m$ linear first integrals $H_\alpha = P(\mathbf{X}_\alpha)$ associated with a basis of D, we have m independent quadratic (nonhomogeneous) first integrals in involution of the form

$$H_b = \tfrac{1}{2} P_{\mathbf{K}_b} + P_{\mathbf{A}_b} + U_b, \tag{6.8}$$

where $\mathbf{A}_b = A_b^\alpha \mathbf{X}_\alpha$ are m vector fields and U_b are m functions such that

$$\mathbf{K}_b\, dA^\alpha = dA_b^\alpha, \quad \mathbf{K}_b\, dU = dU_b. \tag{6.9}$$

Note that $\mathbf{A}_m=\mathbf{A}$ and $U_m=U$. In the separable coordinates (q^a,q^α), these objects have the following expressions, involving the inverse Stäckel matrix $[\varphi^a_{(b)}]$:

$$A_b^\alpha = \varphi^a_{(b)} \phi_a^\alpha, \quad U_b = \varphi^a_{(b)} \phi_a, \tag{6.10}$$

so that the final coordinate expressions of the first integrals are

$$\begin{aligned} H_\alpha &= p_\alpha, \\ H_b &= \tfrac{1}{2}\varphi^a_{(b)}(p_a^2 + \phi_a^{\alpha\beta} p_\alpha p_\beta + 2\phi_a^\alpha p_\alpha + 2\phi_a) \\ &= \tfrac{1}{2}\lambda^a_{(b)} g^{aa}(p_a^2 + \phi_a^{\alpha\beta} p_\alpha p_\beta + 2\phi_a^\alpha p_\alpha + 2\phi_a), \end{aligned} \tag{6.11}$$

where λ_b^a are the eigenvalues of the Killing tensors [see (3.9)]. For the case $\mathbf{A}=0$ they reduce to the expressions (3.15). These first integrals correspond to the constants of integration (c_b,c_α) of the separated Hamilton–Jacobi equations of the kind (5.31) (in the present case $\overline{p_\alpha}=p_\alpha=c_\alpha$). Thus, due to the Jacobi theorem, they are certainly first integrals in involution. However, it is interesting to prove that functions (6.8) are first integrals in involution, in a direct and intrinsic way, from their defining equations (6.8) and (6.9) and from the D-invariance, by analyzing their Poisson brackets with the Hamiltonian

$$H = H_m = \tfrac{1}{2} P_{\mathbf{G}} + P_{\mathbf{A}} + U.$$

We get

$$\begin{aligned} \{H_b,H\} = {} & \tfrac{1}{4}\{P_{\mathbf{K}_b}, P_{\mathbf{G}}\} + \tfrac{1}{2}\{P_{\mathbf{K}_b}, P_{\mathbf{A}}\} + \tfrac{1}{2}\{P_{\mathbf{A}_b}, P_{\mathbf{G}}\} + \tfrac{1}{2}\{P_{\mathbf{K}_b}, U\} \\ & + \{P_{\mathbf{A}_b}, P_{\mathbf{A}}\} + \tfrac{1}{2}\{U_b, P_{\mathbf{G}}\} + \{P_{\mathbf{A}_b}, U\} + \{U_b, P_{\mathbf{A}}\}. \end{aligned} \tag{6.12}$$

The terms in (6.12) are, in the order, polynomials of third, second, first, and 0th degree in the momenta. Thus, the Poisson brackets vanish iff these polynomials vanish separately. This gives rise to equations similar to (4.16),

$$
\begin{aligned}
&[\mathbf{G},\mathbf{K}_b]=0,\\
&[\mathbf{A}_b,\mathbf{G}]=[\mathbf{A},\mathbf{K}_b],\\
&[\mathbf{A}_b,\mathbf{A}]=\nabla U_b-\mathbf{K}_b\nabla U,\\
&\langle \mathbf{A}_b, dU\rangle=\langle \mathbf{A}, dU_b\rangle.
\end{aligned}
\tag{6.13}
$$

This shows, in other words, that the fact that (H_b) are first integrals in involution is equivalent to the fact that the 2-tensors $\hat{\mathbf{K}}_b=(\mathbf{K}_b,\mathbf{A}_b,U_b)$ in the extended manifold are Killing tensors in involution and form the Killing algebra $\hat{\mathcal{K}}$ associated with the characteristic Killing pair $(\hat{D},\hat{\mathbf{K}})$, where $\hat{D}$ is spanned by the vectors $\hat{\mathbf{X}}_\alpha=(\mathbf{X}_\alpha,0)$ and by $\hat{\mathbf{X}}_0$. The first equation (6.13) is just the Killing equation for $\mathbf{K}_b$. If we assume that all these objects, in particular the functions U_b (including $U_m=U$), are D-invariant (which is equivalent to assume that H_b and H_α are in involution) and that the vector fields $\mathbf{A}_b$ are tangent to D, then both terms on the right-hand side of the third equation (6.13) are orthogonal to D, while the Lie bracket at the left one is tangent to D. Hence, both sides vanish identically and we get the second equation (6.9) together with $[\mathbf{A}_b,\mathbf{A}]=0$. Under the same assumptions, both sides of the fourth equation (6.13) vanish identically. The second remaining equation (6.13) is equivalent to the first equation (6.9). The fact that all (H_b) are in involution can be proved in a similar way. We remark that all the vector potentials commute, $[\mathbf{A}_b,\mathbf{A}_a]=0$.

VII. ILLUSTRATIVE EXAMPLES

Let us apply the above results to the Euclidean three-space $Q=\mathbb{E}_3$. In the following examples we give only the expressions of separable scalar and vectors potentials, without entering in the details of the integration of the corresponding Hamilton–Jacobi equations. In $\mathbb{E}_3$ the Lagrangian forces (1.4) are the components of the Lorentz force

$$\mathbf{F}=\mathbf{B}\times\mathbf{v}-\nabla V,\quad \mathbf{B}=\nabla\times\mathbf{A},$$

where $\mathbf{v}$ is the velocity of the particle, ∇ is the gradient operator, $\nabla\times$ is the curl operator, and $\times$ is the cross product of vectors. We shall use the well-known formula

$$\nabla\times(f\mathbf{V})=\nabla f\times\mathbf{V}+f\nabla\times\mathbf{V},$$

for any smooth function f and vector field $\mathbf{V}$. We consider on $\mathbb{E}_3$ Cartesian rectangular coordinates (x, y, z) with origin at a point O and denote by $(\mathbf{X}, \mathbf{Y}, \mathbf{Z})$ the corresponding unit vectors. Due to Remark 6.3, only the cases of separable webs with symmetries (rotational or translational) are interesting for the separation of a vector potential. We consider for brevity and simplicity the cylindrical and the spherical web only (although the remaining two rotational webs, the prolate and oblate spheroidal ones, could be of some interest for the applications).

Example 1. The cylindrical web. In this first example we consider the cylindrical web around the z axis, made of cylinders around the axis, half-planes issued from the axis (the *meridian planes*) and planes orthogonal to the axis (the *equatorial planes*). These surfaces are, respectively, orthogonal to the vectors

$$(\mathbf{u}_z,\mathbf{R}_z,\mathbf{Z}),$$

where

$$\mathbf{u}_z=\frac{\mathbf{r}_z}{|\mathbf{r}_z|}$$

is the unit vector determined by the radius vector orthogonal to the z axis,

$$\mathbf{r}_z=\mathbf{r}-z\mathbf{Z}, \quad \mathbf{r}=x\mathbf{X}+y\mathbf{Y}+z\mathbf{Z}=r\mathbf{u},$$

and

$$\mathbf{R}_z=\mathbf{Z}\times\mathbf{r}$$

is the rotational vector around the z axis. The standard cylindrical coordinates are (ρ, θ, z), where ρ is the distance from the z axis, $\rho=|\mathbf{r}_z|$, and θ is the rotation angle around it, oriented as $\mathbf{R}_z$ and starting (for instance) from the (x, z) plane. Thus we have

$$\nabla\rho=\mathbf{u}_z, \quad |\mathbf{u}_z|=1,$$

$$\nabla\theta=\rho^{-2}\mathbf{R}_z, \quad |\mathbf{R}_z|=\rho=|\mathbf{r}_z|,$$

$$\nabla z=\mathbf{Z}, \quad |\mathbf{Z}|=1,$$

and from

$$\mathbf{p}=\mathbf{v}=p_\rho\nabla\rho+p_\theta\nabla\theta+p_z\nabla z=p_\rho\mathbf{u}_z+p_\theta\rho^{-2}\mathbf{R}_z+p_z\mathbf{Z},$$

we get the well-known expression of the geodesic Hamiltonian

$$G=\tfrac{1}{2}\mathbf{p}\cdot\mathbf{p}=\tfrac{1}{2}(p_\rho^2+\rho^{-2}p_\theta^2+p_z^2).$$

The curls of all vectors above are zero, with the exception of

$$\nabla\times\mathbf{R}_z=2\mathbf{Z}.$$

We have three inequivalent characteristic Killing pairs $(D,\mathbf{K})$ associated with this web.

Case 1. $r=\dim(D)=2$:

$$D=\mathrm{span}(\mathbf{Z},\mathbf{R}_z), \quad \mathbf{K}=\mathbf{G}.$$

With respect to this Killing pair, (θ, z) are first-class (ignorable), and ρ is the essential (second-class) coordinate, so that a Stäckel multiplier is any function $U(\rho)$. Thus in this case the most general separable vector potential has the form

$$\mathbf{A}=\phi(\rho)\mathbf{Z}+\psi(\rho)\mathbf{R}_z.$$

It follows that

$$\begin{aligned}\mathbf{B}=\nabla\times(\phi\mathbf{Z}+\psi\mathbf{R}_z)&=\nabla\phi\times\mathbf{Z}+\nabla\psi\times\mathbf{R}_z+2\psi\mathbf{Z}\\&=\phi'\mathbf{u}_z\times\mathbf{Z}+\psi'\mathbf{u}_z\times\mathbf{R}_z+2\psi\mathbf{Z}\\&=\phi'\rho^{-1}\mathbf{r}\times\mathbf{Z}+\psi'\rho\mathbf{Z}+2\psi\mathbf{Z},\end{aligned}$$

that is

$$\mathbf{B}=-\rho^{-1}\phi'\mathbf{R}_z+(\rho\psi'+2\psi)\mathbf{Z}=f(\rho)\mathbf{R}_z+h(\rho)\mathbf{Z},$$

where $f=-\rho^{-1}\phi'$, $h=\rho\psi'+2\psi$ are two independent functions. Since

$$\mathbf{A}\cdot\mathbf{A}=\phi^2(\rho)+\rho^2\psi(\rho)$$

is a function of ρ only, the most general separable scalar potential (6.2) is any function $V(\rho)$. Thus the Hamiltonian is

$$H=\tfrac{1}{2}\mathbf{p}^2+\mathbf{A}\cdot\mathbf{p}+U=\tfrac{1}{2}(p_\rho^2+\rho^{-2}p_\theta^2+p_z^2)+\phi(\rho)p_z+\rho^{-2}\psi(\rho)p_\theta+U(\rho).$$

Note that the Coriolis and centrifugal forces, appearing in a frame rotating around the z axis with constant angular velocity $\boldsymbol{\omega}=\omega\mathbf{Z}$ with respect to an inertial one, fits with this scheme, being

$$V=\tfrac{1}{2}\omega^2\rho^2,\quad \mathbf{A}=-\omega\mathbf{R}_z,\quad \omega\in\mathbb{R},$$

so that

$$\mathbf{F}=-2\omega\mathbf{Z}\times\mathbf{v}+\omega^2\rho\mathbf{u}_z.$$

Case 2. $r=1$:

$$D=\mathrm{span}(\mathbf{Z}),\quad \mathbf{K}=\mathbf{R}_z\otimes\mathbf{R}_z.$$

Note that $\mathbf{K}$ has eigenvectors $(\mathbf{u}_z,\mathbf{R}_z)$ orthogonal to D, with distinct eigenvalues $(0,\rho^2)$ (they coincide on the z axis, which is the singular set of the web). In this case only z is ignorable, while (ρ,θ) are essential coordinates, so that any Stäckel multiplier is of the kind

$$U=f(\rho)+\rho^{-2}h(\theta),$$

where $f(\rho)$ is any smooth function and $h(\theta)$ is any periodic smooth function (the same is understood for any function of θ considered below). Thus, a separable vector potential has the form

$$\mathbf{A}=(\phi(\rho)+\rho^{-2}\psi(\theta))\mathbf{Z},$$

and consequently

$$\mathbf{B}=\rho^{-1}(2\psi(\theta)\rho^{-3}-\phi'(\rho))\mathbf{R}_z+\psi'(\theta)\rho^{-3}\mathbf{u}_z.$$

The corresponding Hamiltonian is

$$H=\tfrac{1}{2}\mathbf{p}^2+\mathbf{A}\cdot\mathbf{p}+U=\tfrac{1}{2}(p_\rho^2+\rho^{-2}p_\theta^2+p_z^2)+(\phi(\rho)+\rho^{-2}\psi(\theta))p_z+f(\rho)+\rho^{-2}\psi(\theta).$$

Since

$$\mathbf{A}\cdot\mathbf{A}=\phi^2(\rho)+\rho^{-4}\psi^2(\theta)-2\rho^{-2}\psi(\rho)\psi(\theta),$$

the separable scalar potential (6.2) has the form

$$V=f(\rho)+\rho^{-2}h(\theta)-\tfrac{1}{2}\phi^2(\rho)-\tfrac{1}{2}\rho^{-4}\psi^2(\theta)-\rho^{-2}\phi(\rho)\psi(\theta),$$

i.e.,

$$V=f(\rho)+\rho^{-2}(h(\theta)-\phi(\rho)\psi(\theta))-\tfrac{1}{2}\rho^{-4}\psi^2(\theta),$$

where $f(\rho)$ and $h(\theta)$ are arbitrary functions, while $\phi(\rho)$ and $\psi(\theta)$ are the functions entering in the expressions of $\mathbf{A}$ and $\mathbf{B}$. In this case we have a quadratic first integral

$$H_1=\tfrac{1}{2}P_{\mathbf{K}_1}+P_{\mathbf{A}_1}+U_1,\quad \mathbf{K}_1=\mathbf{K}.$$

We compute its elements U_1 and $\mathbf{A}_1$ as follows: for any Stäckel multiplier U

$$\nabla U=(f'(\rho)-2\rho^{-3}h(\theta))\mathbf{u}_z+\rho^{-4}h'(\theta)\mathbf{R}_z$$

and

$$\mathbf{K}\nabla U=\rho^{-2}h'(\theta)\mathbf{R}_z,$$

since $\mathbf{R}_z \cdot \mathbf{u}_z = 0$ and $\mathbf{R}_z^2 = \rho^2$. It follows that

$$U_1 = h(\theta),$$

since $\nabla U_1 = h'(\theta)\nabla\theta = h'(\theta)\rho^{-2}\mathbf{R}_z$. By applying the same method to the component of $\mathbf{A}$ (which is a Stäckel multiplier) we find

$$\mathbf{A}_1 = \psi(\theta)\mathbf{Z}.$$

Thus the quadratic first integral is

$$H_1 = \tfrac{1}{2}(\mathbf{R}_z \cdot \mathbf{p})^2 + \mathbf{A}_1 \cdot \mathbf{p} + U_1 = \tfrac{1}{2}p_\theta^2 + \psi(\theta)p_z + h(\theta).$$

Case 3. $r = 1$:

$$D = \mathrm{span}(\mathbf{R}_z), \quad \mathbf{K} = \mathbf{Z} \otimes \mathbf{Z}.$$

The Killing tensor $\mathbf{K} = \mathbf{Z} \otimes \mathbf{Z}$ has eigenvectors $(\mathbf{Z}, \mathbf{u_z})$ orthogonal to D, with distinct eigenvalues (1, 0). In this case θ is ignorable, while (ρ, z) are essential coordinates. Thus any Stäckel multiplier has the form

$$U = f(\rho) + h(z),$$

and the most general separable vector potential is

$$\mathbf{A} = (\phi(\rho) + \psi(z))\mathbf{R}_z.$$

As a consequence,

$$\mathbf{B} = (\rho\phi'(\rho) + 2\phi(\rho) + 2\psi(z))\mathbf{Z} - \psi'(z)\rho\mathbf{u}_z.$$

The corresponding Hamiltonian is

$$H = \tfrac{1}{2}\mathbf{p}^2 + \mathbf{A} \cdot \mathbf{p} + U = \tfrac{1}{2}(p_\rho^2 + \rho^{-2}p_\theta^2 + p_z^2) + (\phi(\rho) + \psi(z))p_\theta + f(\rho) + h(z).$$

Since

$$\mathbf{A} \cdot \mathbf{A} = \rho^2(\phi^2(\rho) + \psi^2(z) + 2\phi(\rho)\psi(z)),$$

the separable scalar potential (6.2) has the form

$$V = f(\rho) + h(z) - \tfrac{1}{2}\rho^2(\phi^2(\rho) + \psi^2(z) + 2\phi(\rho)\psi(z)),$$

i.e.,

$$V = f(\rho) + h(z) - \rho^2(\tfrac{1}{2}\psi^2(z) + \phi(\rho)\psi(z)),$$

where $f(\rho)$, $h(z)$ are arbitrary functions, while $\psi(z)$, $\phi(\rho)$ are the functions entering in the expressions of $\mathbf{A}$ and $\mathbf{B}$. Also in this case we have a quadratic first integral H_1. Since

$$\nabla U = f'(\rho)\mathbf{u}_z + h'(z)\mathbf{Z}, \quad \mathbf{K}\nabla U = h'(z)\mathbf{Z},$$

we find $U_1 = h(z)$, and in a similar way, $\mathbf{A}_1 = \psi(z)\mathbf{R}_z$. Thus the quadratic first integral is

$$H_1 = \tfrac{1}{2}(\mathbf{Z} \cdot \mathbf{p})^2 + \mathbf{A}_1 \cdot \mathbf{p} + U_1 = \tfrac{1}{2}p_z^2 + \psi(z)p_\theta + h(z).$$

Example 2. The spherical web. This web is made of spheres around the origin, meridian half-planes (issued from the z axis), and circular cones around the axis with vertex at the origin. These surfaces are, respectively, orthogonal to the vectors

$$(\mathbf{r},\mathbf{R}_z,\mathbf{l}),$$

where $\mathbf{l}$ is the unit vector

$$\mathbf{l}=\frac{\mathbf{r}\times\mathbf{R}_z}{|\mathbf{r}\times\mathbf{R}_z|}=\frac{\mathbf{r}\times\mathbf{R}_z}{r\rho}$$

tangent to the meridian planes and to the spheres. The standard spherical coordinates are (r,θ,ϕ), where ϕ is the latitude, so that

$$\nabla r=\mathbf{u},\quad \nabla\theta=\rho^{-2}\mathbf{R}_z,\quad \mathbf{p}=p_r\mathbf{u}+p_\theta\rho^{-2}\mathbf{R}_z+r^{-1}p_\phi\mathbf{l},\quad \nabla\phi=r^{-1}\mathbf{l},$$

with $\rho=r\cos\phi$, and the geodesic Hamiltonian assumes the standard form

$$G=\tfrac{1}{2}(p_r^2+\rho^{-2}p_\theta^2+r^{-2}p_\phi^2).$$

Up to equivalences, there is only one characteristic Killing pair characterizing this web, with $r=1$:

$$D=\mathrm{span}(\mathbf{R}_z),\quad \mathbf{K}=r^2\mathbf{G}-\mathbf{r}\otimes\mathbf{r}.$$

The vectors $(\mathbf{r},\mathbf{l})$ are eigenvectors of $\mathbf{K}$ orthogonal to $\mathbf{R}_z$, with distinct eigenvalues $(0,r^2)$. The coordinates (r,ψ) are essential, θ is ignorable, and a Stäckel multiplier is a function

$$U=f(r)+r^{-2}h(\phi).$$

Thus the separable vector potential is

$$\mathbf{A}=(\alpha(r)+r^{-2}\beta(\phi))\mathbf{R}_z,$$

and

$$\mathbf{B}=(\alpha'-2\beta r^{-3})\rho\mathbf{l}-\beta' r^{-3}\rho\mathbf{u}+2(\alpha+\beta r^{-2})\mathbf{Z}.$$

The Hamiltonian is

$$H=\tfrac{1}{2}(p_r^2+\rho^{-2}p_\phi^2)+(\alpha(r)+r^{-2}\beta(\phi))p_\theta+f(r)+r^{-2}h(\phi).$$

Since

$$\nabla U=(f'-2r^{-3}h)\mathbf{u}+r^{-3}h'\mathbf{l},\quad \mathbf{K}\nabla U=h'(\phi)\nabla\phi=\nabla h,$$

we find $U_1=h(\phi)$ and, in a similar way, $\mathbf{A}_1=\beta(\phi)\mathbf{R}_z$. It follows that the associated quadratic first integral is

$$H_1=r^2G-\tfrac{1}{2}(\mathbf{p}\cdot\mathbf{r})^2+\mathbf{A}_1\cdot\mathbf{p}+U_1=\tfrac{1}{2}r^2(\rho^{-2}p_\theta^2+r^{-2}p_\phi^2)+\beta(\phi)p_\theta+h(\phi).$$

Example 3. Rotational surfaces in $\mathbb{E}_3$. For a particle moving on a regular surface S in $\mathbb{E}_3$ only the restriction of the scalar potential V to S and the tangent component of the vector potential $\mathbf{A}$ have influence on the motion, as well as the orthogonal part of $\mathbf{B}$. Only the case of a surface with symmetry (translational or rotational) is relevant for the separation of a vector potential. Let us consider the case of a rotational surface around the z axis. Then the dynamics of the point on this

surface is separable for any scalar and vector potential in $\mathbb{E}_3$ invariant under the rotation $\mathbf{R}_z$. Indeed, let us consider the cylindrical web of Example 1 and the cylindrical coordinates (ρ,θ,z). Let us consider the decomposition of the vector potential,

$$\mathbf{A}=\alpha\mathbf{u}_z+\beta\mathbf{R}_z+\gamma\mathbf{Z},$$

where, due to the rotational invariance, the functions (α,β,γ) do not depend on the rotation angle θ. It follows that

$$\mathbf{B}=\nabla\alpha\times\mathbf{u}_z+\nabla\beta\times\mathbf{R}_z+2\beta\mathbf{Z}+\nabla\gamma\times\mathbf{Z}.$$

But the first and the last terms are vectors parallel to $\mathbf{R}_z$, since the gradients of θ-invariant functions are tangent to the meridian half-planes, thus they are tangent to the surface and can be disregarded. The relevant potential is then

$$\mathbf{A}=\beta(\rho,z)\mathbf{R}_z,$$

which is tangent to the surface and orthogonal to the meridian planes. On the surface (ρ,z) can be represented as functions of a parameter u, so that the scalar and vector potentials are

$$V=f(u),\quad \mathbf{A}=\phi(u)\mathbf{R}_z.$$

The coordinates on the surfaces are then (θ,u), with θ ignorable and u essential coordinate.

Example 4. The Euclidean plane $\mathbb{E}_2$. We consider $\mathbb{E}_2$ as the (x,y) plane in the three-dimensional Euclidean space $\mathbb{E}_3$. In the rectangular Cartesian web the only interesting case is $m=1$, $D=\mathrm{span}(\mathbf{X})$, $\mathbf{K}=\mathbf{G}$, so that

$$\mathbf{A}=A(y)\mathbf{X},\quad V=V(y).$$

It follows that

$$\mathbf{B}=A'(y)\mathbf{Y}\times\mathbf{X}=-A'(y)\mathbf{Z},\quad \mathbf{F}=-A'(y)\mathbf{Z}\times\mathbf{v}-V'(y)\mathbf{Y}.$$

For the polar web we have $r=1$, $D=\mathrm{span}(\mathbf{R}_z)$, $\mathbf{K}=\mathbf{G}$, and

$$\mathbf{A}=A(r)\mathbf{R}_z,\quad V=V(r).$$

It follows that

$$\begin{aligned}\mathbf{B}=\nabla\times(A\mathbf{R}_z)&=\nabla A\times\mathbf{R}+2A\mathbf{Z}\\&=A'(r)\nabla r\times\mathbf{R}+2A\mathbf{Z}\\&=A'(r)r^{-1}\mathbf{r}\times(\mathbf{Z}\times\mathbf{r})+2A\mathbf{Z}\\&=(rA'+2A)\mathbf{Z},\end{aligned}$$

and the corresponding separable force is

$$\mathbf{F}=B(r)\mathbf{Z}\times\mathbf{v}-V'(r)\mathbf{u},\quad B(r)=rA'+2A,\quad \mathbf{r}=r\mathbf{u}.$$

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k-cosymplectic manifolds and Lagrangian field theories

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A geometrical description of classical field theories of first order is given. The underlying k-cosymplectic structure permits to derive the corresponding field equations. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1360997]

I. INTRODUCTION

As is well-known, the natural arena to study mechanics is symplectic geometry. One interesting problem is to extend this geometric framework for the case of classical field theories. Several different approaches were developed in the past forty years, and according to them, the field equations are presented in different geometric formats: jet fields, Ehresmann connections, or multivector fields (we refer the reader to Refs. 1–5 and the references therein; see also Refs. 6–21 for recent developments).

In a recent paper[22] we have constructed a geometric description of classical field theories in terms of k-cosymplectic manifolds. A k-cosymplectic manifold is a natural generalization of a cosymplectic manifold, which is the geometrical setting for nonautonomous mechanical systems (see Refs. 23–25).

In the present paper, which can be viewed as a natural extension of Ref. 22, we consider the Lagrangian description of first order classical field theories. The field equations are then derived by using the canonical almost stable k-tangent structure on the stable k-tangent bundle $\mathbf{R}^k \times T^1_k Q$ of a manifold Q. From the Lagrangian function L, we construct in an intrinsical way the Poincaré–Cartan forms $(\omega_L)_A$, $1 \leqslant A \leqslant k$, which determine a k-cosymplectic structure if L is regular. The k-cosymplectic structure provides us a k-vector field whose integral sections are the solutions of the field equations. The integrability is not assured, but it can be checked in terms of an arbitrary solution.

If the Lagrangian is not regular, then we develop a constraint algorithm which, if the field equations are compatible, yields a final constraint submanifold where a solution exists. This algorithm is very similar to that constructed in Ref. 25.

This Lagrangian description is of course completely equivalent to the Hamiltonian one developed in our precedent paper by means of a convenient Legendre transformation.

II. *k*-VECTOR FIELDS

Let M be a differentiable manifold of dimension m and $\mathbf{R^k}$ the k-dimensional Euclidean space with coordinates $t=(t^A)=(t^1,\ldots,t^k)$. Let $J^1_0(\mathbf{R^k},M)$ be the $(k+1)m$-dimensional manifold of one jet of mappings from $\mathbf{R^k}$ to M at the origin of $\mathbf{R^k}$ with elements denoted by $j^1_0\sigma$. $J^1_0(\mathbf{R^k},M)$ is called the tangent bundle of k^1-velocities in Ref. 26.

Let $\{\mathbf{r_1},\ldots,\mathbf{r_k}\}$ be the canonical basis of $\mathbf{R^k}$. The manifold $J^1_0(\mathbf{R^k},M)$ can be canonically identified with the Whitney sum $T^1_k M = TM \oplus \cdots \oplus TM$ of k copies of TM via the diffeomorphism,

$$J^1_0(\mathbf{R^k},M) \to T^1_k M = TM \oplus \cdots \oplus TM$$

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$$j_0^1\sigma \to (v_1,\ldots,v_k)$$

defined by

$$v_A = \left.\frac{d\sigma_A}{ds}\right|_{s=0}, \quad s\in\mathbf{R}, \quad 1\leqslant A\leqslant k,$$

where $\sigma_A(s)=\sigma(s\mathbf{r_A})$.

Let $\tau_M : T_k^1M \to M$ be the canonical projection. If (x^i) are local coordinates on $U\subseteq M$ then the induced local coordinates (x^i,x_A^i), $1\leqslant i\leqslant m$, $1\leqslant A\leqslant k$, on $\tau_M^{-1}(U)\equiv T_k^1U$ are given by

$$x^i(j_0^1\sigma)=x^i(\sigma(0)), \quad x_A^i(j_0^1\sigma)=\frac{d}{ds}(x^i\circ\sigma^A)_{|s=0}=v_A(x^i). \tag{1}$$

Definition II.1: A section $\mathbf{X}:M\to T_k^1M$ *of the projection* $\tau_M:T_k^1M\to M$ *will be called a k-vector field on M.*

Since T_k^1M is the Whitney sum of k copies of TM we deduce that a k-vector field $\mathbf{X}$ defines k vector fields $\{X_1,\ldots,X_k\}$ on M by projecting $\mathbf{X}$ onto every factor. We shall identify $\mathbf{X}$ with the k-tuple $(X_1,\ldots,X_k)$.

Definition II.2: An integral section of the k-vector field $(X_1,\ldots,X_k)$ *passing through a point* $x\in M$ *is a map* $\sigma:U_0\subset\mathbf{R}^k\to M$, *defined on some neighborhood* U_0 *of* $0\in\mathbf{R^k}$, *and satisfying*

$$\sigma(0)=x, \quad d\sigma(t)\left(\left.\frac{\partial}{\partial t^A}\right|_t\right)=X_A(\sigma(t)), \quad 1\leqslant A\leqslant k, \quad \text{for all} \quad t\in U_0.$$

We say that a k-vector field $(X_1,\ldots,X_k)$ *on M is integrable if there is an integral section passing through each point of M.*

Remark II.3: Let us consider the trivial bundle $\pi:E=R^k\times M\to R^k$. A jet field γ on π (see Ref. 5) is a section of the projection $\pi_{1,0}:J^1\pi\equiv\mathbf{R}^k\times T_k^1M\to E\equiv\mathbf{R}^k\times M$. We identify each k-vector field $\mathbf{X}$ on M with the jet field $\gamma=(id_{\mathbf{R}^k},\mathbf{X})$, that is $\gamma(t,x)=(t,X_1(x),\ldots,X_k(x))$. The integral sections of the jet field γ (see Ref. 5) correspond to the solutions of the k-vector field $\mathbf{X}$ (see Ref. 27). For this reason the *solutions* of $\mathbf{X}$ are called its *integral sections*.

Let us remark that if σ is an *integral section* of a k-vector field $(X_1,\ldots,X_k)$ then each curve on M defined by $\sigma_A=\sigma(s\,\mathbf{r_A})$ is an integral curve of the vector field X_A on M.

Howewer, given k integral curves of $X_1,\ldots,X_k$, respectively, it is not possible in general to reconstruct an integral section of $(X_1,\ldots,X_k)$.

Proposition II.4: Assume that the vector fields $\{X_1,\ldots,X_k\}$ *on M are linearly independent. Then, the k-vector field* $(X_1,\ldots,X_k)$ *is integrable if and only if the distribution generated by* $\{X_1,\ldots,X_k\}$ *is integrable.*

III. THE CANONICAL STABLE *k*-TANGENT STRUCTURE

Let Q be a manifold of dimension n with local coordinates (q^i) and let (q^i,v_A^i) be the induced coordinates on T_k^1Q. Let F be a tensor field of type (1,1) on Q such that $F=\Sigma_{i,j}F_j^i(\partial/\partial q^i)\otimes dq^j$. Then the A-lift F^A of F to T_k^1Q is the (1,1)-tensor field with local expression:

$$F^A=\sum_{i,j} F_j^i\left(\frac{\partial}{\partial v_A^i}\right)\otimes dq^j$$

(see Ref. 26 for further details about the intrinsic construction). If $I_M=\Sigma_i(\partial/\partial q^i)\otimes dq^i$ is the identity tensor field on M then for each $A\in\{1,2,\ldots k\}$, its A-lifting defines the tensor field $\tilde{J}_A=I^A$ locally given by

$$\tilde{J}_A = \sum_i \frac{\partial}{\partial v_A^i} \otimes dq^i. \tag{2}$$

The family $(\tilde{J}_1,\ldots,\tilde{J}_k)$ is called the *canonical k-tangent structure* of $T_k^1 M$ (see Ref. 28).

Let $J^1(\mathbf{R^k},Q)$ be the $k+(k+1)n$-dimensional manifold of one jets from $\mathbf{R^k}$ to Q, with elements denoted by $j_t^1\phi$. This manifold can be identified with the manifold $J^1\pi$ of one jets of sections of the trivial bundle $\pi:\mathbf{R^k}\times Q\to\mathbf{R^k}$.

$J^1\pi$ is diffeomorphic to $\mathbf{R^k}\times T_k^1 Q$ by composing the following diffeomorphisms:

$$J^1\pi \to \mathbf{R^k}\times J_0^1(\mathbf{R^k},Q)\to \mathbf{R^k}\times T_k^1 Q,$$

$$j_t^1\phi \to (t, j_0^1\phi_t)\to (t,v_1,\ldots,v_k),$$

where

$$\phi_t(t')=\phi(t+t'),\quad t'\in\mathbf{R^k},\quad v_A=\frac{d}{ds}(\phi_t^A)_{|s=0},\quad s\in\mathbf{R},\quad 1\leqslant A\leqslant k,$$

and $\phi_t^A(s)=\phi_t(s\,\mathbf{r_A})$.

Let $\tau:\mathbf{R^k}\times T_k^1 Q\to Q$ be the canonical projection. If (q^i) are local coordinates on $U\subseteq Q$ then the induced local coordinates (t^A,q^i,v_A^i), $1\leqslant i\leqslant n$, $1\leqslant A\leqslant k$, on $\tau^{-1}(U)\equiv\mathbf{R^k}\times T_k^1 U$ are given by

$$t^A(j_t^1\phi)=t^A,\quad q^i(j_t^1\sigma)=q^i(\phi_t(0)),\quad v_A^i(j_t^1\phi)=\frac{d}{ds}(q^i\circ\phi_t^A)_{|s=0}=v_A(q^i).$$

Therefore we obtain $\tau(t^A,q^i,v_A^i)=(q^i)$.

On $\mathbf{R^k}\times T_k^1 Q$ there exist a family of k tensor fields J_A of type (1,1) defined by

$$J_A=\frac{\partial}{\partial t^A}\otimes dt^A+\tilde{J}_A=\frac{\partial}{\partial t^A}\otimes dt^A+\sum_{i=1}^n \frac{\partial}{\partial v_A^i}\otimes dq^i,\quad 1\leqslant A\leqslant k,$$

where we have transported the canonical k-tangent structure $(\tilde{J}_1,\ldots,\tilde{J}_k)$ of $T_k^1 Q$ to $\mathbf{R^k}\times T_k^1 Q$.

If we set $\overline{\eta}_A=dt^A$ and $\xi_A=\partial/\partial t^A$, then the family $(J_A,\overline{\eta}_A,\xi_A;1\leqslant A\leqslant k)$ is called the *canonical stable k-tangent structure* on $\mathbf{R^k}\times T_k^1 Q$, and $\mathbf{R^k}\times T_k^1 Q$ is the *stable k-tangent bundle of Q*.

IV. SECOND ORDER PARTIAL DIFFERENTIAL EQUATIONS

In this section we characterize the k-vector fields on $\mathbf{R}^k\times T_k^1 Q$ such that their integral sections are canonical prolongations of maps from $\mathbf{R}^k$ to Q.

Let C be the *canonical vector field* of the vector bundle $\pi_{1,0}:\mathbf{R}^k\times T_k^1 Q\to\mathbf{R^k}\times Q$. This vector field C is the infinitesimal generator of the following flow:

$$\mathbf{R}\times(\mathbf{R}^k\times T_k^1 Q)\to\mathbf{R}^k\times T_k^1 Q$$

$$(s,(t,q^i,v_A^i))\to(t,q^i,e^s v_A^i),$$

and in local coordinates it has the form

$$C=\sum_{i,A} v_A^i\frac{\partial}{\partial v_A^i}. \tag{3}$$

C is a sum of vector fields,

$$C=\sum_{A=1}^{k} C_A,$$

where each C_A is the infinitesimal generator of the following flow:

$$\mathbf{R}\times(\mathbf{R}^k\times T_k^1Q)\to\mathbf{R}^k\times T_k^1Q$$

$$(s,(t,q^i,v_A^i))\to(t,q^i,v_1^i,\ldots,v_{A-1}^i,e^s v_A^i,v_{A+1}^i,\ldots,v_k^i).$$

In local coordinates they have the form

$$C_A=\sum_{i=1}^{n} v_A^i\frac{\partial}{\partial v_A^i},\quad 1\leqslant A\leqslant k. \tag{4}$$

Let us consider on $\mathbf{R}^k\times T_k^1Q$ the tensor fields $\hat{J}_1,\ldots,\hat{J}_k$ of type (1,1), defined as follows:

$$\hat{J}_A=\tilde{J}_A-C_A\otimes dt^A,\quad 1\leqslant A\leqslant k.$$

Definition IV.1: A k-vector field $\zeta=(\zeta_1,\ldots,\zeta_k)$ on $\mathbf{R}^k\times T_k^1Q$ is said to be a second order partial differential equation (SOPDE for short) if

$$\hat{J}_A(\zeta_A)=0,\quad \overline{\eta}_A(\zeta_B)=\delta_{AB},$$

for all $1\leqslant A,B\leqslant k$.

From a direct computation in local coordinates we obtain that the local expression of a SOPDE $\zeta=(\zeta_1,\ldots,\zeta_k)$ on $\mathbf{R}^k\times T_k^1Q$ is

$$\zeta_A=\frac{\partial}{\partial t^A}+v_A^i\frac{\partial}{\partial q^i}+(\zeta_A)_B^i\frac{\partial}{\partial v_B^i},\quad 1\leqslant A\leqslant k, \tag{5}$$

where $(\zeta_A)_B^i$ are functions on $\mathbf{R}^k\times T_k^1Q$.

As a direct consequence of the above local expressions, we deduce that the familiy of vector fields $\{\zeta_1,\ldots,\zeta_k\}$ are linearly independent.

Definition IV.2: Let $\phi:\mathbf{R}^k\to Q$ be a map, we define the first prolongation $\phi^{(1)}$ of ϕ as the map

$$\phi^{(1)}:\mathbf{R}^k\to J^1\pi\equiv\mathbf{R}^k\times T_k^1Q,$$

$$t\to j_t^1\phi\equiv(t,j_0^1\phi_t).$$

In local coordinates:

$$\phi^{(1)}(t^1,\ldots,t^k)=\left(t^1,\ldots,t^k,\phi^i(t^1,\ldots,t^k),\frac{\partial\phi^i}{\partial t^A}(t^1,\ldots,t^k)\right),\quad 1\leqslant A\leqslant k,1\leqslant i\leqslant n. \tag{6}$$

From (5) it follows that an integral section σ of a SOPDE ζ is the first prolongation $\phi^{(1)}$ of a map ϕ from $\mathbf{R}^k$ to Q.

Definition IV.3: $\phi:\mathbf{R}^k\to Q$ is called a solution of the SOPDE ζ on $\mathbf{R}^k\times T_k^1Q$ if the first prolongation $\phi^{(1)}$ of ϕ is an integral section of ζ.

From (5) and (6) we have the following.

Proposition IV.4: $\phi:\mathbf{R}^k\to Q$ is a solution of the SOPDE $\zeta=(\zeta_1,\ldots,\zeta_k)$, locally given by (5), if and only if

$$\frac{\partial\phi^i}{\partial t^A}=v_A^i,\quad \frac{\partial^2\phi^i}{\partial t^A\,\partial t^B}=(\zeta_A)_B^i.$$

Remark IV.5: Let us consider the trivial bundles $\pi: E = R^k \times Q \to R^k$ and $\pi_1: \mathbf{R^k} \times T^1_k Q \to \mathbf{R^k}$. We identify each SOPDE $(\zeta_1, \ldots, \zeta_k)$ with the following *semi-holonomic second order jet field:*

$$J^1\pi \equiv \mathbf{R^k} \times T^1_k Q \to J^1\pi_1 \equiv \mathbf{R^k} \times T^1_k (T^1_k Q),$$

$$(t^A, q^i, v^i_A) \to (t^A, q^i, v^i_A, v^i_A, (\zeta_A)^i_B).$$

If the SOPDE ζ on $\mathbf{R}^k \times T^1_k Q$ is integrable, then its integral sections are canonical prolongations of maps from $\mathbf{R^k}$ to Q and then ζ defines a second order jet field Γ on π whose coordinate representation of the corresponding connection $\tilde{\Gamma}$ is

$$\tilde{\Gamma} = dt^A \otimes \left(\frac{\partial}{\partial t^A} + v^i_A \frac{\partial}{\partial q^i} + (\zeta_A)^i_B \frac{\partial}{\partial v^i_B} \right),$$

since $(\zeta_A)^i_B = (\zeta_B)^i_A$ (see Ref. 5).

The integrability of the SOPDE is equivalent to the condition given by $\mathcal{R} = 0$, where $\mathcal{R}$ is the curvature tensor of the above connection (see Ref. 13 and 5).

V. *k*-COSYMPLECTIC STRUCTURES

The keystone of the nonautonomous Lagrangian formalism of classical mechanics is the cosymplectic structure on the phase space $\mathbf{R} \times TQ$. For field theory we shall show that this statement remains true, provided the two- forms that define the cosymplectic structure are replaced by two vector valued forms.

Let $J^1(Q, \mathbf{R^k})_0$ be the manifold of one jets of maps from Q to $\mathbf{R^k}$ with target at $0 \in \mathbf{R^k}$.

The manifold $J^1(Q, \mathbf{R^k})_0$ can be canonically identified with the Whitney sum $(T^1_k)^* Q$ of k copies of T^*Q, that is

$$J^1(Q, \mathbf{R^k})_0 \to (T^1_k)^* Q = T^*Q \oplus \cdots \oplus T^*Q,$$

$$j^1_{q,0}\sigma \equiv (p^1_q, \ldots, p^k_q),$$

where $p^A_q = d(\pi_A \circ \sigma)(q)$ being $\pi_A: \mathbf{R^k} \to \mathbf{R}$ the canonical projection.

Let $J^1(Q, \mathbf{R^k})$ be the $k + (k+1)n$-dimensional manifold of one jets from Q to $\mathbf{R^k}$, with elements denoted by $j^1_{q,t}\sigma$. We recall that one jets of mappings from Q to $\mathbf{R^k}$ can be identified with the manifold $J^1\rho$ of one jets of sections of the trivial bundle $\rho: \mathbf{R^k} \times Q \to Q$.

$J^1\rho$ is diffeomorphic to $\mathbf{R^k} \times (T^1_k)^* Q$, via the diffeomorphism given by

$$j^1_q \alpha \in J^1\rho \to (\sigma(q), j^1_{q,0}\sigma_q) \in \mathbf{R^k} \times (T^1_k)^* Q,$$

where $\sigma_q(\tilde{q}) = \sigma(\tilde{q}) - \sigma(q)$ and $\tilde{q}$ denotes an arbitrary point in Q.

Let us denote by $\tau^*: \mathbf{R^k} \times (T^1_k)^* Q \to Q$ the canonical projection. If (q^i) are local coordinates on $U \subseteq Q$ then the induced local coordinates $(t^A, q^i, p^A_i), 1 \leq i \leq n, 1 \leq A \leq k$, on $(\tau^*)^{-1}(U) \equiv \mathbf{R^k} \times (T^1_k)^* U$ are given by

$$t^A(j^1_q\sigma) = t^A(\sigma(q)), \quad q^i(j^1_q\sigma) = q^i(q), \quad p^A_i(j^1_q\sigma) = d(\sigma^A_q)(q)\left(\frac{\partial}{\partial q^i}_{|q} \right),$$

where $\sigma^A_q = \pi_A \circ \sigma_q$.

An $\mathbf{R^k}$-valued one-form η_0 and a $\mathbf{R^k}$-valued two-form ω_0 on $\mathbf{R^k} \times (T^1_k)^* Q$ are defined by

$$\eta_0 = \sum_{A=1}^{m} (\eta_0)_A \, \mathbf{r_A} = \sum_{A=1}^{k} ((\pi^1_A)^* dt) \mathbf{r_A}, \quad \omega_0 = \sum_{A=1}^{k} (\omega_0)_A \, \mathbf{r_A} = \sum_{A=1}^{m} (\pi^2_A)^* (\omega_Q) \, \mathbf{r_A}, \tag{7}$$

where $\pi_A^1:\mathbf{R^k}\times(T_k^1)^*Q\to\mathbf{R}$ and $\pi_A^2:\mathbf{R^k}\times(T_k^1)^*Q\to T^*Q$ are the projections defined by

$$\pi_A^1((t^B),(p^B))=t^A,\quad \pi_A^2((t^B),(p^B))=p^A,$$

and ω_Q is the canonical symplectic form on T^*Q.

In local coordinates we have

$$(\eta_0)_A=dt^A,\quad (\omega_0)_A=\sum_{i=1}^{n} dq^i\wedge dp_i^A\quad 1\leqslant A\leqslant k. \tag{8}$$

Moreover, let be $V=\ker T\mu^*$, where $\mu^*:\mathbf{R^k}\times(T_k^1)^*Q\to\mathbf{R^k}\times Q$. A simple inspection in local coordinates shows that the forms $(\eta_0)_A$ and $(\omega_0)_A$ are closed and the following relations hold:

(i) $(\eta_0)_1\wedge\cdots\wedge(\eta_0)_k\neq 0$, $(\eta_0)_{A_{|V}}=0$, $\omega_{A_{|V\times V}}=0$,

(ii) $(\cap_{A=1}^n\ker(\eta_0)_A)\cap(\cap_{A=1}^n\ker(\omega_0)_A)=\{0\}$, $\dim(\cap_{A=1}^n\ker(\omega_0)_A)=k$.

Inspired in the above geometrical model we have introduced in Ref. 22 the following definition.

Definition V.1: Let M be a differentiable manifold of dimension $(k+1)n+k$. A family $(\eta_A,\omega_A,V;1\leqslant A\leqslant k)$, where each η_A is a closed 1-form, each ω_A is a closed 2-form and V is an nk-dimensional integrable distribution on M, such that

(i) $\eta_1\wedge\cdots\wedge\eta_k\neq 0$, $\eta_{A_{|V}}=0$, $\omega_{A_{|V\times V}}=0$,

(ii) $(\cap_{A=1}^k\ker\eta_A)\cap(\cap_{A=1}^k\ker\omega_A)=\{0\}$, $\dim(\cap_{A=1}^k\ker\omega_A)=k$,

is called a k-cosymplectic structure, and the manifold M a k-cosymplectic manifold.

The canonical model for these geometrical structures is $(\mathbf{R^k}\times(T_k^1)^*Q,\eta_0,\omega_0,V)$.

For any k-cosymplectic structure (η_A,ω_A,V) on M, there exists a family of k vector fields $(\xi_1,\ldots,\xi_k)$ characterized by the conditions

$$\eta_A(\xi_B)=\delta_{AB},\quad \iota_{\xi_B}\omega_A=0,$$

for all $1\leqslant A,B\leqslant k$. These vector fields are called the Reeb vector fields associated to the k-cosymplectic structure.

If (M,η,ω,V) is a k-cosymplectic manifold we can define the vector bundle morphism,

$$\begin{gathered}\Omega^\sharp:T_k^1M\to T^*M\\ (X_1,\ldots,X_k)\to\Omega^\sharp(X_1,\ldots,X_k)=\sum_{A=1}^{k}\iota_{X_A}\omega_A+\eta_A(X_A)\,\eta_A.\end{gathered} \tag{9}$$

Remark V.2: If $k=1$ then $\Omega^\sharp$ is defined from TM onto T^*M and it is in fact the isomorphism $\chi_{\eta,\omega}$ defined on the cosymplectic manifold (M,η,ω) by (see Ref. 23, 24)

$$\chi_{\eta,\omega}(X)=\iota_X\omega+\eta(X)\,\eta.$$

Let (M,η_A,ω_A,V) be a k-cosymplectic manifold, $H:M\to\mathbf{R}$ a Hamiltonian function and ξ_A are the Reeb vector fields determined by (η_A,ω_A,V). In Ref. 22 we have proved that if an integrable k-vector field $\mathbf{X}=(X_1,\ldots,X_k)$ satisfies the equations

$$\begin{gathered}\eta_A(X_B)=\delta_{AB},\quad \forall A,B,\\ \Omega^\sharp(X_1,\ldots,X_k)=dH+\sum_{A=1}^{k}(1-\xi_A(H))\,\eta_A,\end{gathered} \tag{10}$$

then its integral sections ϕ are solutions of the Hamiltonian field equations corresponding to H:

$$\frac{\partial H}{\partial x^i}=-\sum_{A=1}^{k}\frac{\partial \phi_i^A}{\partial s^A},\quad \frac{\partial H}{\partial x_i^A}=\frac{\partial \phi^i}{\partial s^A}.$$

The existence of canonical coordinates (s^A,x^i,x_i^A) is ensured by the corresponding Darboux theorem (see Ref. 22).

VI. THE LAGRANGIAN FORMALISM

Given a Lagrangian function of the form $L=L(t^A,q^i,v_A^i)$ one obtains, by using a variational principle, the *Euler–Lagrange equations* for L:

$$\sum_{A=1}^{k}\frac{d}{dt^A}\left(\frac{\partial L}{\partial v_A^i}\right)-\frac{\partial L}{\partial q^i}=0,\quad v_A^i=\frac{\partial q^i}{\partial t^A}. \tag{11}$$

First of all, one realizes that such a L can be considered as a function $L:\mathbf{R^k}\times T_k^1Q\to\mathbf{R}$.

In this section we shall give a geometrical description of the above equations (11) using a k-cosymplectic structure on $\mathbf{R^k}\times T_k^1Q$ associated to the regular Lagrangian L. This k-cosymplectic structure shall be constructed using the canonical stable k-tangent structure of $\mathbf{R^k}\times T_k^1Q$.

For each $1\leqslant A\leqslant k$, we define the following.

• The vertical derivation ι_{J_A} of forms on $\mathbf{R^k}\times T_k^1Q$ by

$$\iota_{J_A}f=0,\ (\iota_{J_A}\alpha)(X_1,\ldots,X_p)=\sum_{j=1}^{p}\alpha(X_1,\ldots,J_AX_j,\ldots,X_p),$$

for any function f and any p-form α on $\mathbf{R^k}\times T_k^1Q$;

• the vertical differentation d_{J_A} of forms on $\mathbf{R^k}\times T_k^1Q$ by

$$d_{J_A}=[\iota_{J_A},d]=\iota_{J_A}\circ d-d\circ\iota_{J_A},$$

where d denotes the usual exterior differentation.

Let us consider the 1-forms,

$$(\beta_L)_A=d_{J_A}L-\xi_A(L)\,\overline{\eta}_A,\ 1\leqslant A\leqslant k.$$

In bundle coordinates (t^A,q^i,v_A^i) we have

$$(\beta_L)_A=\sum_{i=1}^{n}\frac{\partial L}{\partial v_A^i}dq^i,\ 1\leqslant i\leqslant k. \tag{12}$$

Definition VI.1: A Lagrangian L is called regular if and only if the Hessian matrix,

$$\left(\frac{\partial^2 L}{\partial v_A^i\,\partial v_B^j}\right), \tag{13}$$

is nonsingular.

Now, we introduce the following 2-forms:

$$(\omega_L)_A=-d(\beta_L)_A,\ 1\leqslant A\leqslant k.$$

Proposition VI.2: Let $L:\mathbf{R^k}\times T_k^1Q\to\mathbf{R}$ be a regular Lagrangian, and V_0 the vertical distribution of the bundle $\pi_{1,0}:\mathbf{R^k}\times T_k^1Q\to\mathbf{R^k}\times Q$. Then, L is regular if and only if $(\mathbf{R^k}\times T_k^1Q,\overline{\eta}_A,(\omega_L)_A,V_0)$ is a k-cosymplectic manifold.

Proof: Assume that L is a regular Lagrangian. We shall prove that $(\mathbf{R}^k \times T^1_k Q, \overline{\eta}_A, (\omega_L)_A, V_0)$ is a k-cosymplectic manifold.

Conditions (i) are rather obvious. Now, we shall prove condition (ii) in Definition V.1. Let X be a vector field with the local expression

$$X = X^A \frac{\partial}{\partial t^A} + X^i \frac{\partial}{\partial q^i} + X^i_A \frac{\partial}{\partial v^i_A},$$

such that

$$\imath_X (\omega_L)_A = 0, \text{ and } \overline{\eta}_A(X) = 0, \quad \text{for all } 1 \leqslant A \leqslant k.$$

The second condition implies that $X^A = 0$, for all A, and then the first condition yields

$$X^i \frac{\partial^2 L}{\partial v^i_A \partial v^j_B} = 0, \tag{14}$$

and

$$X^i \frac{\partial^2 L}{\partial v^i_A \partial q^j} - X^i \frac{\partial^2 L}{\partial v^j_A \partial q^i} - X^i_B \frac{\partial^2 L}{\partial v^j_A \partial v^i_B} = 0. \tag{15}$$

Since L is regular, from (14) we deduce that $X^i = 0$, for all i, so that (15) implies $X^i_A = 0$, for all i and A. Therefore, we conclude that $X = 0$.

Next, we shall prove the second part of condition (ii) in Definition V.1. Let Y be a vector field with the local expression

$$Y = Y^A \frac{\partial}{\partial t^A} + Y^i \frac{\partial}{\partial q^i} + Y^i_A \frac{\partial}{\partial v^i_A},$$

such that

$$\imath_X (\omega_L)_A = 0, \quad \text{for all } 1 \leqslant A \leqslant k.$$

We then have

$$Y^j \frac{\partial^2 L}{\partial v^i_A \partial v^j_B} = 0, \tag{16}$$

and

$$- Y^B \frac{\partial^2 L}{\partial v^i_A \partial t^B} + Y^j \frac{\partial^2 L}{\partial v^j_A \partial q^i} - Y^j \frac{\partial^2 L}{\partial v^i_A \partial q^j} - Y^j_B \frac{\partial^2 L}{\partial v^i_A \partial v^j_B} = 0. \tag{17}$$

From (16) and the regularity of L we deduce that $Y^j = 0$, for all j, so that (17) reduces to

$$- Y^B \frac{\partial^2 L}{\partial v^i_A \partial t^B} - Y^j_B \frac{\partial^2 L}{\partial v^i_A \partial v^j_B} = 0. \tag{18}$$

Since the matrix $(\partial^2 L / \partial v^i_A \partial v^j_B)$ is regular, (18) implies that

$$Y^j_B = \mathcal{A}^j_{BD} Y^D,$$

for some matrix $\mathcal{A}^j_{BD}$. Therefore, we get

$$Y = Y^B\left(\frac{\partial}{\partial t^B} + \mathcal{A}^j_{CB}\frac{\partial}{\partial v^j_C}\right).$$

Thus, $\cap_{A=1}^n \ker(\omega_L)_A$ is locally spanned by the family of k independente local vector fields $\{\partial/\partial t^B + \mathcal{A}^j_{CB}(\partial/\partial v^j_C)\}$.

Then we have proved that $(\mathbf{R^k}\times T^1_kQ, (\eta_0)_A, (\omega_L)_A, V_0)$ is a k-cosymplectic manifold.

The converse is proved by reversing the above arguments. ■

Let $L:\mathbf{R^k}\times T^1_kQ\to\mathbf{R}$ be a regular Lagrangian and $(\overline{\eta}_A, (\omega_L)_A, V_0)$ the associated k-cosymplectic structure on $\mathbf{R^k}\times T^1_kQ$.

The equations,

$$\overline{\eta}_A((\xi_L)_B) = \delta^A_B, \quad \iota_{(\xi_L)_A}(\omega_L)_B = 0, \quad 1\leqslant A,B\leqslant k, \tag{19}$$

define the Reeb vector fields $\{(\xi_L)_1,\ldots,(\xi_L)_k\}$ on $\mathbf{R^k}\times T^1_kQ$ which are locally given by

$$(\xi_L)_A = \frac{\partial}{\partial t^A} + ((\xi_L)_A)^i_B\frac{\partial}{\partial v^i_B}, \tag{20}$$

where the functions $((\xi_L)_A)^i_B$ satisfy

$$\frac{\partial^2 L}{\partial t^A\,\partial v^j_C} + \frac{\partial^2 L}{\partial v^i_B\,\partial v^j_C}((\xi_L)_A)^i_B = 0, \tag{21}$$

for all $1\leqslant A,B,C\leqslant k$ and $1\leqslant i,j\leqslant n$.

Since L is regular, from the local conditions (21) we can define, in a neighborhood of each point of $\mathbf{R^k}\times T^1_kQ$, a k-vector field that satisfies (19). Next, one can construct a global k-vector field ξ_L, which is a solution of (19), by using a partition of unity.

Let L be a regular Lagrangian and let $\Omega^\sharp_L$ be the $\sharp$-morphism defined by the k-cosymplectic structure $(\overline{\eta}_A, (\omega_L)_A, V_0)$, as in (9):

$$\begin{gathered}\Omega^\sharp_L : T^1_k(\mathbf{R^k}\times T^1_kQ)\to T^*(\mathbf{R^k}\times T^1_kQ)\\ (X_1,\ldots,X_k)\to\Omega^\sharp_L(X_1,\ldots,X_k) = \sum_{A=1}^k \iota_{X_A}(\omega_L)_A + \overline{\eta}_A(X_A)\,\overline{\eta}_A.\end{gathered} \tag{22}$$

Theorem VI.3: *Let L be a regular Lagrangian and let $\mathbf{X}=(X_1,\ldots,X_k)$ be a k-vector field such that*

$$\begin{gathered}\overline{\eta}_A(X_B) = \delta_{AB}, \quad 1\leqslant A,B\leqslant k,\\ \Omega^\sharp_L(X_1,\ldots,X_k) = dE_L + \sum_{A=1}^k (1-(\xi_L)_A(E_L))\,\overline{\eta}_A,\end{gathered} \tag{23}$$

where $E_L = C(L) - L$. Then $\mathbf{X}=(X_1,\ldots,X_k)$ is a SOPDE. In addition, if $\mathbf{X}=(X_1,\ldots,X_k)$ is integrable then its solutions satisfy the Euler–Lagrange equations (11).

Proof: It should be noticed that in general Eqs. (23) have not a unique solution. In fact, the solutions of (23) are given by $(X_1,\ldots,X_k) + (\ker\Omega^\sharp)$, where $(X_1,\ldots,X_k)$ is a particular solution. Nevertheless, we shall show now that there exist always solutions of equations (23) when L is assumed to be regular. In this case, from (3) and (20) we obtain

$$(\xi_L)_A(E_L) = -\frac{\partial L}{\partial t^A}. \tag{24}$$

Let $(X_1,\ldots,X_k)$ be a solution of (23) locally given by

$$X_A(t,q^i,v_A^i)=\frac{\partial}{\partial t^A}+(X_A)^i\frac{\partial}{\partial q^i}+(X_A)_B^j\frac{\partial}{\partial v_B^j}.$$

Then, from (24) we obtain

$$\sum_{A,B,j}\left(-\frac{\partial^2 L}{\partial t^A\partial v_A^i}+(X_A)^j\left(\frac{\partial^2 L}{\partial q^i\partial v_A^j}-\frac{\partial^2 L}{\partial q^j\partial v_A^i}\right)-(X_A)_B^j\frac{\partial^2 L}{\partial v_B^j\partial v_A^i}\right)=\sum_{A,j}\left(v_A^j\frac{\partial^2 L}{\partial q^i\partial v_A^j}-\frac{\partial L}{\partial q^i}\right), \tag{25}$$

$$\sum_{A,i}(X_A)^i\frac{\partial^2 L}{\partial v_B^j\,\partial v_A^i}=\sum_{A,i}v_A^i\frac{\partial^2 L}{\partial v_B^j\,\partial v_A^i}, \tag{26}$$

and since L is regular, from (26) we deduce that the solutions of Eqs. (23) are SOPDE's, that is, each X_A has the form

$$X_A(t,q^i,v_A^i)=\frac{\partial}{\partial t^A}+v_A^i\frac{\partial}{\partial q^i}+(X_A)_B^j\frac{\partial}{\partial v_B^j}. \tag{27}$$

From (25) we deduce that the functions $(X_A)_B^j$ satisfy the equations

$$\sum_A\frac{\partial^2 L}{\partial t^A\,\partial v_A^i}+\sum_{j,B}\left(v_B^j\frac{\partial^2 L}{\partial q^j\,\partial v_B^i}+\sum_A(X_A)_B^j\frac{\partial^2 L}{\partial v_B^j\,\partial v_A^i}\right)=\frac{\partial L}{\partial q^i},\quad 1\leqslant i\leqslant n. \tag{28}$$

Since L is regular, (28) leads us to define local solutions of (23) in a neigborhood of each point of $\mathbf{R^k}\times T_k^1Q$. Using a partition of unity one can easily obtain a global solution of (23).

Now, let

$$\phi:\mathbf{R^k}\to Q,$$

$$(t^B)\to(\phi^i(t^1,\ldots,t^k)),$$

be a solution of $(X_1,\ldots,X_k)$. From Proposition IV.4 and Eq. (27) we deduce that

$$\frac{\partial\phi^i}{\partial t^A}=v_A^i,\quad \frac{\partial^2\phi_A^i}{\partial t^A\,\partial t^B}=(X_A)_B^i.$$

Replacing in (28) we get

$$\sum_A\frac{\partial^2 L}{\partial t^A\,\partial v_A^i}+\sum_{j,B}\left(\frac{\partial\phi^j}{\partial t^B}\frac{\partial^2 L}{\partial q^j\,\partial v_B^i}+\sum_A\frac{\partial^2\phi^j}{\partial t^A\,\partial t^B}\frac{\partial^2 L}{\partial v_B^j\,\partial v_A^i}\right)=\frac{\partial L}{\partial q^i},\quad 1\leqslant i\leqslant n, \tag{29}$$

which shows that ϕ is a solution of the Euler–Lagrange equations (11). ■

In conclussion, we can consider Eqs. (23) as a *geometric version* of the Euler–Lagrange field equations.

Remark VI.4: We have given a geometric version of the Euler–Lagrange equations for a nonautonomous Lagrangian constructing a k-cosymplectic structure on $\mathbf{R^k}\times T_k^1Q$ defined from the Lagrangian and the canonical stable k-tangent structure on $\mathbf{R^k}\times T_k^1Q$. We can also construct this k-cosymplectic structure using the *Legendre tranformation* $\mathcal{F}L$ of L which is the map

$$\mathcal{F}L:\mathbf{R^k}\times T_k^1Q\to\mathbf{R^k}\times(T_k^1)^*Q,$$

defined as follows: if $(t,\mathbf{v})=(t^1,\ldots,t^k,v_1,\ldots,v_k)\in\mathbf{R^k}\times(T_k^1Q)_q$ with $q\in Q$ and $v_A\in T_qQ$, then

$$\mathcal{FL}(t,y)=(t^1,\ldots,t^k,p^1,\ldots p^k)\in \mathbf{R^k}\times(T^1_kQ)^*_q,\quad p^A\in T^*_qQ$$

is given by

$$p^A(v_q)=(\beta_L)_A(\overline{v_q}),\quad 1\leqslant A\leqslant k,$$

for any $v_q\in T_qQ$, where $\overline{v_q}\in T_v(T^1_kQ)$ is any tangent vector such that $d\tau_Q(v)(\overline{v_q})=v_q$, with $\tau_Q:T^1_kQ\to Q$ the canonical projection. In induced coordinates we have

$$\mathcal{FL}:(t^A,q^i,v^i_A)\to\left(t^A,q^i,\frac{\partial L}{\partial v^i_A}\right). \tag{30}$$

The Jacobian matrix of $\mathcal{FL}$ is

$$\begin{pmatrix} I_k & & 0 & 0 & \ldots & 0\\ 0 & & I_n & 0 & \ldots & 0\\ & \mathcal{B} & & & \mathcal{C} & \end{pmatrix}, \tag{31}$$

where I_k e I_n are the identity matrices of order k and n, respectively, $\mathcal{B}$ is a matrix $nk\times(k+n)$ and $\mathcal{C}$ is the matrix

$$\left(\frac{\partial^2 L}{\partial v^i_A\,\partial v^j_B}\right).$$

Now, from (12) and (30) we deduce the following.

Lemma VI.5: We have

$$(\omega_L)_A=\mathcal{FL}^*((\omega_0)_A),\quad \overline{\eta}_A=\mathcal{FL}^*((\eta_0)_A),$$

for all A.

Next, from (31) we obtain the following proposition.

Proposition VI.6: The following conditions are equivalent:

(1) L is regular.

(2) $\mathcal{FL}$ is a local diffeomorphism.

(3) $(\overline{\eta}_1,\ldots,\overline{\eta}_k,(\omega_L)_1,\ldots,(\omega_L)_k,V_0)$ is a k-cosymplectic structure on $\mathbf{R}^k\times T^1_kQ$.

VII. SINGULAR CASE

When the Lagrangian function L is not regular, the family $(\overline{\eta}_A,(\omega_L)_A,V_0,1\leqslant A\leqslant k)$ is no longer a k-cosymplectic structure. Even in this case, from (24), we deduce that if $\mathbf{X}=(X_1,\ldots,X_k)$ is an integrable SOPDE such that

$$\begin{aligned}&\overline{\eta}_A(X_B)=\delta_{AB},\\ &\Omega^\sharp_L(X_1,\ldots,X_k)=dE_L+\sum_{A=1}^{k}\left(1+\frac{\partial}{\partial t^A}(L)\right)\overline{\eta}_A,\end{aligned} \tag{32}$$

then its solutions satisfy the Euler–Lagrange equations.

But we cannot assure that such a solution exists. Therefore we shall develop a constraint algorithm inspired in the well-known one for singular Lagrangians in mechanics in order to obtain a final constraint submanifold where such a solution exists.

We put $P_1=\mathbf{R}^k\times T^1_kQ$. Next, let P_2 be the subset of P_1 which consists of those points where there exists solution of (32), that is,

$$P_2=\{z\in P_1/\exists \mathbf{X}\in (T^1_k(\mathbf{R}^k\times(T^1_k)^*Q))_z \text{ satisfying the SOPDE condition and being a solution of (32)}\}.$$

If P_2 is a submanifold of P_1, then there exists a section of $\tau_{\mathbf{R}^k\times T^1_kQ}$ over P_2. This section is not in general a k-vector field on P_2. To find solutions taking values into $T^1_kP_2$ we construct a new subset P_3 of P_2 as follows:

$$P_3=\{z\in P_2/\exists \mathbf{X}\in (T^1_kP_2)_z \text{satisfying the SOPDE condition and being a solution of (32)}\}.$$

If P_3 is a submanifold of P_2, there exists a section of τ_{P_2} over P_3 which is solution of (23), but that not defines, in general, a k-vector field on P_3.

Proceeding further, we get a family of constraint manifolds,

$$\cdots\to P_3\to P_2\to P_1=\mathbf{R}^k\times T^1_kQ.$$

In the most favorable case, this constraint algorithm stabilizes at some step, say $P_{h+1}=P_h$ and $\dim P_h>0$. In this case, we call $P_f=P_h$ the final constraint manifold. On P_f there exists a SOPDE solution of (32).

Of course, this solution would not be unique as in the regular case. It should be noticed that, in addition, the solutions on P_f shall not be in principle integrable. To guarantee the existence of an integrable solution one has to develop an additional constraint algorithm taking the brackets of the vector fields which compose a SOPDE solution. Doing that we shall obtain an integrable SOPDE solution on a (smaller, in general) submanifold S of P_f; its solutions shall satisfy the Euler–Lagrange equations (11) (see Ref. 13).

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Miura map between lattice Kadomtsev–Petviashvili and its modification is canonical

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We consider the Miura map between the lattice Kadomtsev–Petviashvili hierarchy and the lattice modified KP hierarchy and prove that the map is canonical not only between the first Hamiltonian structures, but also between the second Hamiltonian structures. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1359416]

I. INTRODUCTION

It is well known that the Miura map, a transformation between the Korteweg–de Vries (KdV) equation and modified KdV (MKdV) equation, plays a central role in the development of soliton theory. Indeed, the celebrated inverse scattering method for solving nonlinear equations starts with the Miura map.[1] This type of transformation turns out to exist in the context of other integrable equations (see Refs. 2–13, and references therein).

Kupershmidt, in a recent paper,[9] considered the canonical properties of Miura maps between Kadomtsev–Petviashvili and MKP hierarchies. He shows that, both in continuous and discrete cases, Miura transformations are canonical between the first Hamiltonian structures. For the ordinary or continuous KP and its modification, Shaw and Tu[12] generalized the results of Kupershmidt and proved that the very Miura map is also canonical between the second Hamiltonian structures.

We will consider the canonical property of the Miura map between the lattice MKP (LMKP) and the lattice KP (LKP) hierarchies. The LKP hierarchy is a bi-Hamiltonian system and two Hamiltonian structures were constructed by using the residue calculus in Ref. 8. For the LMKP hierarchy, the first Hamiltonian structure was also found in Ref. 9. A slightly different version of the LMKP hierarchy was proposed by Oevel and he further obtained the bi-Hamiltonian description for this hierarchy by means of an *r*-matrix approach.[14] By introducing a parameter, we unify Kupershmidt's version of the LMKP hierarchy and Oevel's version into a single system. Our main purpose of the paper is to prove that Kupershmidt's Miura map is a canonical map not only between the first Hamiltonian structures of LKP and LMKP, but also between the second Hamiltonian structures.

The paper is organized as follows. In Sec. II, we introduce notations and recall the relevant formulas such as bi-Hamiltonian structures of the LKP and LMKP hierarchies. In Secs. III and IV, we show that Kupershmidt's Miura map is a canonical transformation for the first Hamiltonian structures and the second Hamiltonian structures, respectively. Section V is intended for a summary and discussions.

II. BACKGROUND AND NOTATIONS

To introduce the LKP and LMKP hierarchies, we consider the algebra of shift operators

$$g=\{u_N(n)T^N+u_{N-1}(n)T^{N-1}+\cdots+u_0(n)+u_{-1}(n)T^{-1}+\cdots\},$$

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where u_j are scalar functions of integer n. The shift operator T is given by

$$(Tf)(n)=f^{(1)}(n):=f(n+1),$$

and for arbitrary integer k, $(T^k f)(n)=f^{(k)}(n)=f(n+k)$.

For any operator $\xi=\Sigma_j u_j T^j \in g$, the projections to various shift orders are denoted by

$$\xi_j=u_j T^j, \quad \xi_{\geqslant k}=\sum_{j\geqslant k} u_j T^j, \quad \xi_{<k}=\sum_{j<k} u_j T^j,$$

$$\xi_{>k}=\sum_{j>k} u_j T^j, \quad \xi_{\leqslant k}=\sum_{j\leqslant k} u_j T^j.$$

From the shift operator T, we also have the difference operator

$$\Delta=T-1,$$

and its formal inverse

$$\Delta^{-1}=\sum_{j\geqslant 1} T^{-j}.$$

Another important notation is the so-called trace, which is defined as

$$\mathrm{tr}\left(\sum_i u_i T^i\right)=\sum_n u_0(n),$$

this permits us to identify g and its dual by the metric $g^*:\langle u^*,u\rangle=\mathrm{tr}(u^*u)$. It can be shown that the metric is bi-invariant.

The LKP hierarchy is defined by the following Lax operator:

$$L=T+\sum_{i=0}^{\infty} A_i T^{-i}, \tag{1}$$

and the flow equations are constructed as

$$L_{t_n}=[(L^n)_{\geqslant 0},L]. \tag{2}$$

The LKP hierarchy (2) is a bi-Hamiltonian system. Its two Hamiltonian structures are constructed by means of the residue calculus in Ref. 8. Recently, Oevel proposed an r-matrix setting for these Hamiltonian structures. The two Hamiltonian structures are given by the following Poisson tensors:

$$P_1(\nabla H)=[\nabla H,L]_{\leqslant 0}, \tag{3}$$

$$P_2(\nabla H)=(L\nabla H)_{\geqslant 1}L-L(\nabla HL)_{\geqslant 1}+\tfrac{1}{2}[(L\nabla H+\nabla HL)_0,L]+\tfrac{1}{2}[\rho([\nabla H,L]_0),L], \tag{4}$$

where ρ is a skew-symmetric linear map on the algebra g_0 given explicitly by

$$\rho=\frac{T+1}{T-1}, \tag{5}$$

and

$$\nabla H = \frac{\delta H}{\delta A_0} + T\frac{\delta H}{\delta A_1} + \cdots . \tag{6}$$

As for the LMKP hierarchy, we consider the following Lax operator:

$$\mathcal{L} = qT + \sum_{i=0}^{\infty} a_i T^{-i}, \tag{7}$$

and the flow equations are represented by

$$\mathcal{L}_{t_n} = [(\mathcal{L}^n)_{\geqslant 1} + \alpha(\mathcal{L}^n\Delta^{-1})_0, \mathcal{L}], \tag{8}$$

where α is a constant.

The case $\alpha=0$ and the case $\alpha=1$ were considered by Kupershmidt and Oevel, respectively. In these two cases, the MLKP hierarchy (8) is a bi-Hamiltonian system. When $\alpha=0$, the first Hamiltonian structure of (8) is found by Kupershmidt in the context of the residue calculus, it is not clear how to construct the second one this way. Oevel, in the case $\alpha=1$, gives the bi-Hamiltonian structures by means of an *r*-matrix approach.

Consider the linear operator on g,

$$r(\xi) = \xi_{\geqslant 1} - \xi_{<1} - 2\alpha(\xi\Delta^{-1})_0,$$

by direct calculations it is found that the above-mentioned r solves the modified Yang–Baxter equation only and only if $\alpha=0$ or $\alpha=1$. As we mentioned previously, these are exactly the two cases studied by Kupershmidt and by Oevel. In the following, our parameter α will take the value either one or zero. The above-mentioned *r*-matrix leads to the first Hamiltonian structure for the LMKP hierarchy.

To get the second Poisson tensor, one may use Suris's construction[15] by considering the following linear operators:

$$\mathcal{A}_1(\xi) = \xi_{\geqslant 1} - \xi_{<0} - 2\alpha(\xi\Delta^{-1})_0 - \rho(\xi_0) + 2\alpha\Delta^{-1}\xi_0,$$

$$\mathcal{A}_2(\xi) = \xi_{\geqslant 1} - \xi_{<0} + \rho(\xi_0),$$

$$\mathcal{S}(\xi) = \rho(\xi_0) - \xi_0 - 2\alpha\Delta^{-1}\xi_0,$$

$$\mathcal{S}^{\dagger}(\xi) = -\rho(\xi_0) - \xi_0 - 2\alpha(\xi\Delta^{-1})_0.$$

When $\alpha=1$, the above-mentioned operators are those presented by Oevel and lead to the second Poisson tensor for this case. It can be proved that in the case $\alpha=0$, these operators satisfy the conditions of Suris's theorem (or the theorem 1 of Oevel[14]), therefore they also lead to a Poisson tensor, this time for Kupershmidt's case. Unifying both Kupershmidt's case and Oevel's case, we have the following two Poisson tensors:

$$\widetilde{\mathcal{P}}_1(\nabla H) = [(\nabla H)_{\geqslant 1}, \mathcal{L}] - [\nabla H, \mathcal{L}]_{\geqslant 0} - \alpha[(\nabla H\Delta^{-1})_0, \mathcal{L}] - \alpha\Delta^{-1}[\nabla H, \mathcal{L}]_0, \tag{9}$$

$$\begin{aligned}\widetilde{\mathcal{P}}_2(\nabla H) = {} & (\mathcal{L}\nabla H)_{\geqslant 1}\mathcal{L} - \mathcal{L}(\nabla H\mathcal{L})_{\geqslant 1} + \tfrac{1}{2}[\mathcal{L}, \nabla H]_0\mathcal{L} + \tfrac{1}{2}\mathcal{L}[\mathcal{L}, \nabla H]_0 + \alpha\Delta^{-1}[\mathcal{L}, \nabla H]_0\mathcal{L} \\ & + \alpha[\mathcal{L}, (\mathcal{L}\nabla H\Delta^{-1})_0] + \tfrac{1}{2}[\rho([\nabla H, \mathcal{L}]_0), \mathcal{L}],\end{aligned} \tag{10}$$

where ρ is the one defined by (5) and ∇H is parametrized as

$$\nabla H = T^{-1}\frac{\delta H}{\delta q} + \frac{\delta H}{\delta a_0} + T\frac{\delta H}{\delta a_1} + \cdots . \tag{11}$$

In the remaining part of this section, we introduce the Miura map between LKP hierarchy and LMKP hierarchy following Kupershmidt. With the aid of a new field w, we introduce a map between LKP and MLKP hierarchies via the conjugacy

$$L=e^{w}\mathcal{L}e^{-w}=e^{w}qTe^{-w}+\sum_{i=0}^{\infty}e^{w}a_{i}T^{-i}e^{-w},$$

comparing the coefficients of different power of the shift operator of two sides leads to a transformation

$$q=e^{w^{(1)}-w},\quad A_{i}=a_{i}e^{w-w^{(-i)}}\quad (i\geqslant 0).$$

Let us introduce the new notations

$$R_{i}=R_{i}(q):=\prod_{s=0}^{i}q^{(-s)}/q\quad (i\geqslant 0).$$

By eliminating the intermediate variable w, we reach the Miura map between the two sets of variables

$$M:\quad A_{0}=a_{0},\quad A_{i}=R_{i}a_{i}\quad (i>0). \tag{12}$$

This is the Miura map constructed in Ref. 9.

Now we prove that if $\mathcal{L}$ solves the MLKP hierarchy, $L=e^{w}\mathcal{L}e^{-w}$ solves the LKP hierarchy. From $q=e^{w^{(1)}-w}$, we obtain $q_{t}=q(T-1)w_{t}$. On the other hand, the time evolution of q can be read from the MLKP hierarchy, that is $q_{t}=q(T-1)((\mathcal{L}^{n})_{0}+\alpha(\mathcal{L}^{n}\Delta^{-1})_{0})$, so $w_{t}=(\mathcal{L}^{n})_{0}+\alpha(\mathcal{L}^{n}\Delta^{-1})_{0}$. Now

$$\begin{aligned}L_{t}&=[w_{t},L]+e^{w}[(\mathcal{L}^{n})_{\geqslant 1}-\alpha(\mathcal{L}^{n}\Delta^{-1})_{0},\mathcal{L}]e^{-w}\\&=[w_{t},L]+[e^{w}(\mathcal{L}^{n})_{\geqslant 1}e^{-w},L]-\alpha[(\mathcal{L}^{n}\Delta^{-1})_{0},L]=[(L^{n})_{\geqslant 0},L],\end{aligned}$$

where we used $(\mathcal{L}^{n})_{0}=(L^{n})_{0}$ and $e^{w}(\mathcal{L}^{n})_{\geqslant 1}=(L^{n})_{\geqslant 1}e^{w}$. Thus the Miura map (12) indeed converts the LMKP hierarchy into the LKP hierarchy.

III. CANONICAL PROPERTIES FOR FIRST HAMILTONIAN STRUCTURES

In this section, we prove that the Miura map is canonical between the first Hamiltonian structures. First we calculate the Hamiltonian matrices from the Poisson tensors (3) and (9). By substituting (6) into P_{1} and (11) into P_{2}, it is straightforward to get

$$B_{1}^{\mathrm{LKP}}=(B_{ij}),B_{ij}=T^{j}A_{i+j}-A_{i+j}T^{-i}\quad (i,j\geqslant 0), \tag{13}$$

and

$$B_{1}^{\mathrm{LMKP}}=\begin{array}{c}\\ q\\ a_{0}\\ a_{i>0}\end{array}\begin{array}{c}\begin{array}{ccc}q & a_{0} & a_{j>0}\end{array}\\ \begin{pmatrix}0 & q(T-1) & \alpha q(T-1)T^{j}\\ (1-T^{-1})q & 0 & 0\\ \alpha T^{-i}(1-T^{-1})q & 0 & B_{ij}^{(\mathrm{LMKP})}\end{pmatrix}\end{array}, \tag{14}$$

where

$$B_{ij}^{(\mathrm{LMKP})}=T^{j}a_{i+j}-a_{i+j}T^{-i}+\alpha(a_{i}T^{j-i}-T^{j-i}a_{j}+T^{-i}a_{j}-a_{i}T^{j}), \tag{15}$$

The Jacobian matrix of the Miura map (12) is easily calculated as

$$q \qquad a_0 \qquad a_{i>0}$$

$$J = A_n(a_n D_n \quad R_n\delta_n^0 \quad R_n\delta_n^i), \tag{16}$$

where δ_j^i is the standard Kronecker symbol and D_n is the abbreviated notation for the Fréchet derivative given by

$$D_n := D(R_n) = R_n \frac{1-T^{-n}}{T-1} q^{-1}, \quad D_n^\dagger = q^{-1}\frac{1-T^n}{T^{-1}-1} R_n . \tag{17}$$

We need to calculate the matrix operator $JB_1^{\mathrm{LMKP}}J^\dagger$, but first it is easy to find that

$$q \qquad\qquad a_0 \qquad\qquad a_{j>0}$$

$$JB_1^{\mathrm{LMKP}} = \begin{matrix} A_0 \\ A_{i>0} \end{matrix}\begin{pmatrix} (1-T^{-1})q & 0 & 0 \\ \alpha R_i T^{-i}(1-T^{-1})q & a_i D_i q(T-1) & \alpha a_i D_i q(T-1)T^j + R_i B_{ij}^{(\mathrm{LMKP})} \end{pmatrix},$$

now the entries of the first row of the $JB_1^{\mathrm{LMKP}}J^\dagger$ are seen as

$$(JB_1^{\mathrm{LMKP}}J^\dagger)_{0,m} = (1-T^{-1})qD_m^\dagger a_m = -(1-T^m)R_m a_m = (T^m-1)A_m ,$$

which coincide with the $(B_1^{\mathrm{LKP}})_{0,m}$. It is noticed that we have used the second formula of (17). Therefore, for the first row and the first column, two matrix operators B_1^{LKP} and $JB_1^{\mathrm{LMKP}}J^\dagger$ are just the same as expected. We turn our attention to other entries of matrices. We find that

$$\begin{aligned}(JB_1^{\mathrm{LMKP}}J^\dagger)_{mn} &= \alpha R_m T^{-m}(1-T^{-1})qD_n^\dagger a_n + \alpha a_m D_m q(T-1)T^n R_n + \alpha R_m(a_m T^{n-m} - T^{n-m}a_n \\ &\quad + T^{-m}a_n - a_m T^n)R_n + R_m(T^n a_{m+n} - a_{n+m}T^{-m})R_n \\ &= \alpha R_m T^{-m}(T^n-1)R_n a_n + \alpha a_m R_m(1-T^{-m})T^n R_n + \alpha R_m(a_m T^{n-m} - T^{n-m}a_n \\ &\quad + T^{-m}a_n - a_m T^n)R_n + R_m(T^n a_{m+n} - a_{n+m}T^{-m})R_n \\ &= R_m(T^n a_{m+n} - a_{n+m}T^{-m})R_n .\end{aligned}$$

Now we use the formula in Ref. 9,

$$R_n T^m R_m = T_m R_{n+m} ,$$

and obtain the desired the results $(JB_1^{\mathrm{LMKP}}J^\dagger)_{mn} = (B_1^{\mathrm{LKP}})_{mn}$. Thus, the Miura map is indeed canonical.

IV. CANONICAL PROPERTY FOR SECOND HAMILTONIAN STRUCTURES

We now show that the Miura map (12) is also canonical between the second Hamiltonian structure of the LKP hierarchy and the second Hamiltonian structure of the LMKP hierarchy. As in Sec. III, we first calculate the Hamiltonian matrix operators from the Poisson tensors (4) and (10). The calculation in the present case is a bit cumbersome although it is straightforward. For the LKP hierarchy we have

$$A_{k,t} = \sum_{\ell=0}^{\infty} (B_2^{\mathrm{LKP}})_{k\ell}\frac{\delta H}{\delta A_\ell}, \quad k \geqslant 0, \quad t \equiv t_n, \quad H \equiv H_n = \frac{1}{n}\mathrm{tr}(L^n),$$

where

$$(B_2^{\mathrm{LKP}})_{k\ell} = \sum_{j=1}^{\ell+1}(A_{\ell-j}T^j A_{k+j} - A_{k+j}T^{\ell-k-j}A_{\ell-j}) + A_k(1-T^{-k})(1+T+\cdots+T^\ell)A_\ell ,$$

$$A_{-1}\equiv 1,\quad k\geqslant 0,\quad \ell\geqslant 0.$$

For the MLKP hierarchy, we have

$$B_2^{\mathrm{LMKP}} \begin{matrix} q \\ a_{k\geqslant 0} \end{matrix} = \begin{matrix} q & a_{m\geqslant 0} \end{matrix} \begin{pmatrix} q(T-T^{-1})q & \alpha q(T-1)\sum_{i=1}^{m+1} a_{m-i}T^i + q(T-T^m)a_m \\ \alpha\sum_{j=1}^{k+1} T^{-j}a_{k-j}(1-T^{-1})q + a_k(T^{-k}-T^{-1})q & B_{km}^{\mathrm{LMKP}} \end{pmatrix}$$

with

$$B_{km}^{\mathrm{LMKP}} = \sum_{i=1}^{m+1}(a_{m-i}T^i a_{k+i} - a_{k+i}T^{m-k-i}a_{m-i}) + a_k\frac{(1-T^{-k+1})(1-T^m)}{1-T}a_m + \alpha a_k(T^{-k}-1)\sum_{i=1}^{m+1} a_{m-i}T^i + \alpha\sum_{j=1}^{k+1} T^{-j}a_{k-j}(1-T^m)a_m,$$

$$a_{-1}\equiv q.$$

Thus, the matrix operator JB_2^{LMKP} reads as

$$JB_2^{\mathrm{LMKP}} = \begin{matrix} A_0 \\ A_{k\geqslant 0} \end{matrix} \begin{matrix} q & a_{m\geqslant 0} \end{matrix} \begin{pmatrix} (a_0+\alpha T^{-1}q)(1-T^{-1})q & qT^{m+1}a_{m+1} - a_{m+1}T^{-1}q + \alpha T^{-1}q(1-T^m)a_m \\ a_kD_kq(T-T^{-1})q + a_kR_k(T^{-k}-T^{-1})q + \alpha R_k\sum_{j=1}^{k+1} T^{-j}a_{k-j} \times (1-T^{-1})q & a_kD_k(q(T-T^{-m})a_m + \alpha R_kq(T-1) \times \sum_{i=1}^{m+1} a_{m-i}T^i) + R_kB_{km}^{\mathrm{LMKP}} \end{pmatrix}.$$

With all these formulas in hand, we find that the entries of the first row of $JB_2^{\mathrm{LMKP}}J^\dagger$ are

$$\begin{aligned}(JB_2^{\mathrm{LMKP}}J^\dagger)_{0,n} &= (a_0+\alpha T^{-1}q)(1-T^{-1})qD_n^\dagger a_n \\ &\quad + (qT^{n+1}a_{n+1} - a_{n+1}T^{-1}q + \alpha T^{-1}q(1-T^n)a_n)R_n \\ &= -(a_0+\alpha T^{-1}q)(1-T^n)A_n + qT^{n+1}a_{n+1}R_n - a_{n+1}T^{-1}qR_n + \alpha T^{-1}q(1-T_n)A_n \\ &= -a_0(1-T^n)A_n + qT^{n+1}a_{n+1}R_n - a_{n+1}T^{-1}qR_n \\ &= A_0(T^n-1)A_n + T^{n+1}A_{n+1} - A_{n+1}T^{-1} = (B_2^{\mathrm{LKP}})_{0,n},\end{aligned}$$

where we used

$$q^{(-n-1)}R_n = R_{n+1},\quad q^{-1}R_n^{(-1)} = R_{n+1},$$

which hold identically. For the remaining entries, we have

$$(JB_2^{\mathrm{LMKP}}J^{\dagger})_{mn}=a_mD_mq(T-T^{-1})qD_n^{\dagger}a_n+R_ma_m(T^{-m}-T^{-1})qD_n^{\dagger}a_n \tag{18}$$

$$+a_mD_mq(T-T^n)a_n+R_ma_m\frac{(1-T^{-m+1})(1-T^n)}{1-T}a_nR_n \tag{19}$$

$$+\alpha R_m\sum_{j=1}^{m+1}T^{-j}a_{m-j}((1-T^{-1})qD_n^{\dagger}a_n+(1-T^n)a_nR_n) \tag{20}$$

$$+\alpha(a_mD_mq(T-1)+R_ma_m(T^{-m}-1))\sum_{j=1}^{n+1}a_{n-j}T^jR_n \tag{21}$$

$$+R_m\left(\sum_{l=1}^{n+1}(a_{n-l}T^la_{m+l}-a_{m+l}T^{n-m-l}a_{n-l})\right)R_n, \tag{22}$$

so we need to prove that the above-mentioned expression is $(B_2^{\mathrm{LKP}})_{mn}$.

It is easy to see that $(20)=(21)=0$ in terms of D_m.

Since $T-T^{-1}=-(1+T)(T^{-1}-1)$, we obtain

$$(18)+(19)=-A_m\frac{1-T^{-m}}{T-1}(1+T)(1-T^n)A_n+A_m(T^{-m}-T^{-1})\frac{1-T^n}{T^{-1}-1}A_n$$

$$+A_m\frac{1-T^{-m}}{T-1}(T-T^n)A_n+A_m\frac{(1-T^{-m+1})(1-T^n)}{1-T}A_n$$

$$=A_m\frac{1-T^{-m}-T^{n+1}+T^{n-m+1}}{1-T}A_n=A_m\frac{(1-T^{-m})(1-T^{n+1})}{1-T}A_n.$$

Thus to complete the proof, we need to show that

$$R_m\left(\sum_{i=1}^{n+1}a_{n-i}T^ia_{m+i}-a_{m+i}T^{n-m-i}a_{n-i}\right)R_n=\sum_{j=1}^{n+1}(A_{n-j}T^jA_{m+j}-A_{m+j}T^{n-m-j}A_{n-j}),$$

this amounts to the identity

$$R_mT^jR_n=R_{n-j}T^jR_{m+j},\quad 1\leqslant j\leqslant n+1,$$

which can be seen as follows:

$$\begin{aligned}R_mT^jR_n&=q^{(-1)}\cdots q^{(-m)}q^{(-1+j)}\cdots q^{(-n+j)}\\&=q^{(-1)}\cdots q^{(-m)}q^{(-1+j)}\cdots qq^{(-1)}\cdots q^{(-n+j)}\\&=q^{(-1)}\cdots q^{(-n+j)}q^{(-1+j)}\cdots qa^{(-1)}\cdots q^{(-m)}\\&=R_{n-j}T^jR_{m+j}.\end{aligned}$$

Thus, we conclude that the Miura map is canonical in the sense of the second Hamiltonian structures.

V. CONCLUSIONS AND DISCUSSIONS

We have proved that the canonical property of the Miura map holds between the LKP hierarchy and the LMKP hierarchy, that is, it maps the bi-Hamiltonian structures of the LMKP hierarchy to those of the LKP hierarchy. In Ref. 9, the lattice KP hierarchy is extended and it turns

out that the extended lattice KP hierarchy is isomorphic to the lattice MKP hierarchy. Since we are dealing with a slightly generalized version of the LMKP hierarchy here (8), we have a different extended LKP hierarchy.

Introducing a new field u and defining the following invertible transformation

$$u=q, \quad A_0=a_0, \quad A_i=R_i a_i,$$

it is easy to see that the first Hamiltonian matrix operator for our extended LKP hierarchy reads

$$B_1^{\mathrm{ELKP}}=\begin{array}{c} \\ u \\ A_0 \\ A_{n>0} \end{array}\begin{array}{c} \begin{array}{ccc} u & A_0 & A_{m>0} \end{array} \\ \begin{pmatrix} 0 & u(T-1) & \alpha u(T-1)T^m R_m \\ (1-T^{-1})u & 0 & (T^m-1)A_m \\ \alpha R_n T^{-n}(1-T^{-1})u & A_n(1-T^{-n}) & T^m A_{n+m}-A_{n+m}T^{-n} \end{pmatrix} \end{array}, \tag{23}$$

and the flow equations are given

$$u_t=u(T-1)\frac{\delta H}{\delta A_0}+\alpha\sum_{m=1}^{\infty} u(T-1)T^m\frac{\delta H}{\delta A_m},$$

$$A_{i,t}=\alpha R_n T^{-n}(1-T^{-1})u\frac{\delta H}{\delta u}+\sum_{j=0}^{\infty}(B_1^{\mathrm{ELKP}})_{ij}\frac{\delta H}{\delta A_j}, \quad H\equiv H_{n+1}=\frac{1}{n+1}\mathrm{tr}(L^{n+1}),$$

where the Hamiltonian H is the seam as in the LKP case. We could have a second Hamiltonian structure for the extended LKP hierarchy, but it is in a rather complicated form. So we omit it.

To conclude the paper, we point out that it seems interesting to prove the canonical property of the Miura map on the level of the Poisson tensors since that will hopefully make the proof more concise. For the Gelfand–Dickey hierarchy, such proof was given by Dickey[4] and for the continuous KP hierarchy and the constrained KP hierarchy, it is provided in Ref. 12 and in Refs. 11, 13, respectively.

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Two binary Darboux transformations for the KdV hierarchy with self-consistent sources

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Two binary (integral type) Darboux transformations for the KdV hierarchy with self-consistent sources are proposed. In contrast with the Darboux transformation for the KdV hierarchy, one of the two binary Darboux transformations provides non-auto-Bäcklund transformation between two nth KdV equations with self-consistent sources with different degrees. The formula for the m-times repeated binary Darboux transformations are presented. This enables us to construct the N-soliton solution for the KdV hierarchy with self-consistent sources. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1357826]

I. INTRODUCTION

The soliton equations with self-consistent sources have important physical applications (see Refs. 1–11), for example, the KdV equation with self-consistent source describes the interaction of long and short capillary-gravity waves.[5] There are some ways to derive the integrable nonlinear evolution equations with self-consistent sources.[1–3,12,13] In recent years soliton equations with self-consistent sources (SESCS) were studied based on the constrained flows of soliton equations which are just the stationary equations of SESCSs.[14–19] Since the Lax representations for the constrained flows of soliton equations can always be deduced from the adjoint representations of the Lax representations for soliton equations, this approach provides a simple and natural way to derive both the SESCSs and their Lax representations.[15–17] The SESCS is an infinite-dimensional integrable Hamiltonian system possessing t-type Hamiltonian or bi-Hamiltonian formulation[20] and can be solved by the inverse scattering method.[1–3,21–23]

The Darboux transformation is a power tool for solving soliton equations (see Ref. 24 for a review). The Darboux transformation for KdV hierarchy was widely studied (see, for example, Refs. 24–27). In the present paper we will generalize these results to the KdV hierarchy with self-consistent sources. We construct one Darboux transformation and two binary (integral type) Darboux transformations for the KdV hierarchy with self-consistent sources. The Darboux transformations usually present auto-Bäcklund transformations for soliton equations. In contrast with the case of soliton equations, one binary Darboux transformation in our case is proved to be a non-auto-Bäcklund transformation between two nth KdV equations with self-consistent sources with different degrees. This provides an interesting example for constructing non-auto-Bäcklund transformations by means of Darboux transformations. Furthermore we present the formula for the m-times repeated binary Darboux transformations and construct the N-soliton solution for the KdV hierarchy with self-consistent sources.

The paper is organized as follows. In the next section we recall the KdV hierarchy with self-consistent sources and briefly describe how to derive their Lax representation from the adjoint

representation of the Lax representation for the KdV hierarchy. In Sec. III, we briefly review Darboux transformations for the KdV hierarchy and present two binary Darboux transformations. Based on these results, in Sec. IV, we propose one Darboux transformation and two binary Darboux transformations for the KdV hierarchy with self-consistent sources and show that the first binary Darboux transformation gives the auto-Bäcklund transformation for the KdV hierarchy with self-consistent sources, and the second binary Darboux transformation leads to a non-auto-Bäcklund transformation relating two nth KdV equations with self-consistent sources with different degrees. Finally in the last section we present the m-times repeated binary Darboux transformations and construct the N-soliton solution for the nth KdV equation with self-consistent sources.

II. THE KdV HIERARCHY WITH SELF-CONSISTENT SOURCES

To make the paper self-contained, we first recall the high-order constrained flows of the KdV hierarchy and briefly describe how to derive the Lax representation for the KdV hierarchy with self-consistent sources.

Consider the Schrödinger equation

$$\phi_{xx}+(\lambda+u)\phi=0. \tag{2.1}$$

In order to derive the Lax representation for the KdV hierarchy with self-consistent sources, we rewrite Eq. (2.1) in the matrix form

$$\begin{pmatrix}\phi\\ \phi_x\end{pmatrix}_x=U\begin{pmatrix}\phi\\ \phi_x\end{pmatrix},\quad U=\begin{pmatrix}0 & 1\\ -\lambda-u & 0\end{pmatrix}. \tag{2.2}$$

The adjoint representation of (2.2) reads[28]

$$V_x=[U,V]\equiv UV-VU. \tag{2.3}$$

Set

$$V=\sum_{i=0}^{\infty}\begin{pmatrix}a_i & b_i\\ c_i & -a_i\end{pmatrix}\lambda^{-i}. \tag{2.4}$$

Equation (2.3) yields

$$a_0=b_0=0,\quad c_0=-1,\quad a_1=0,\quad b_1=1,\quad c_1=-\tfrac{1}{2}u,$$

$$a_2=\tfrac{1}{4}u_x,\quad b_2=-\tfrac{1}{2}u,\quad c_2=\tfrac{1}{8}(u_{xx}+u^2),\ldots,$$

and in general for $k=1,2,\ldots,$

$$a_k=-\tfrac{1}{2}b_{k,x},\quad b_{k+1}=Lb_k=-\tfrac{1}{2}L^{k-1}u,\quad c_k=-\tfrac{1}{2}b_{k,xx}-b_{k+1}-b_ku, \tag{2.5}$$

where

$$L=-\tfrac{1}{4}\partial^2-u+\tfrac{1}{2}\partial^{-1}u_x,\quad \partial=\frac{\partial}{\partial x},\quad \partial\partial^{-1}=\partial^{-1}\partial=1.$$

Set

$$V^{(n)}=\sum_{i=0}^{n+1}\begin{pmatrix}a_i & b_i\\ c_i & -a_i\end{pmatrix}\lambda^{n+1-i}+\begin{pmatrix}0 & 0\\ b_{n+2} & 0\end{pmatrix}, \tag{2.6}$$

and take

$$\begin{pmatrix} \phi \\ \phi_x \end{pmatrix}_{t_n} = V^{(n)}(u,\lambda)\begin{pmatrix} \phi \\ \phi_x \end{pmatrix}, \tag{2.7}$$

or equivalently

$$\phi_{t_n} = A^{(n)}(u,\lambda)\phi, \quad A^{(n)}(u,\lambda) \equiv \sum_{i=0}^{n+1} (a_i + b_i\partial)\lambda^{n+1-i}. \tag{2.8}$$

Then the compatibility condition of Eqs. (2.1) and (2.8) or (2.2) and (2.7) gives rise to the KdV hierarchy

$$u_{t_n} = K_n[u] \equiv \partial \frac{\delta H_n}{\delta u} \equiv -2b_{n+2,x}, \quad n = 0,1,\ldots, \tag{2.9}$$

where $H_n = 4b_{n+3}/2n+3$. We have

$$\frac{\delta\lambda}{\delta u} = \phi^2, \quad L\phi^2 = \lambda\phi^2. \tag{2.10}$$

The high-order constrained flows of the KdV hierarchy consist of the equations obtained from the spectral problem (2.1) for N distinct λ_j and the restriction of the variational derivatives for the conserved quantities H_n and λ_j,[29]

$$D\left[\frac{\delta H_n}{\delta u} - 2\alpha\sum_{j=1}^{N}\frac{\delta\lambda_j}{\delta u}\right] \equiv D\left[-2b_{n+2} - 2\alpha\sum_{j=1}^{N}\phi_j^2\right] = 0, \tag{2.11a}$$

$$\phi_{j,xx} + (\lambda_j + u)\phi_j = 0, \quad j = 1,\ldots,N, \tag{2.11b}$$

where $n = 0,1,\ldots$. According to Eqs. (2.5), (2.10), and (2.11), we may define

$$\tilde{a}_i = a_i, \quad \tilde{b}_i = b_i, \quad \tilde{c}_i = c_i, \quad i = 0,1,\ldots,n+1,$$

$$\tilde{b}_{n+2+i} = -\alpha\sum_{j=1}^{N}\lambda_j^i\phi_j^2, \quad \tilde{a}_{n+2+i} = -\tfrac{1}{2}\tilde{b}_{n+2+i,x} = \alpha\sum_{j=1}^{N}\lambda_j^i\phi_j\phi_{j,x}, \quad i = 0,1,2,\ldots,$$

$$\tilde{c}_{n+2+i} = -\frac{1}{2}\tilde{b}_{n+2+i,xx} - \tilde{b}_{n+3+i} - \tilde{b}_{n+2+i}u = \alpha\sum_{j=1}^{N}\lambda_j^i\phi_{j,x}^2.$$

Then the construction of $\tilde{a}_i, \tilde{b}_i, \tilde{c}_i$ ensures that

$$\begin{aligned} N^{(n)} &= \lambda^{n+1}\sum_{k=0}^{\infty}\begin{pmatrix} \tilde{a}_k & \tilde{b}_k \\ \tilde{c}_k & -\tilde{a}_k \end{pmatrix}\lambda^{-k} + \begin{pmatrix} \eta & 0 \\ 0 & \eta \end{pmatrix} \\ &= \sum_{k=0}^{n+1}\begin{pmatrix} a_k & b_k \\ c_k & -a_k \end{pmatrix}\lambda^{n+1-k} + \begin{pmatrix} \eta & 0 \\ 0 & \eta \end{pmatrix} + \alpha\sum_{j=1}^{N}\frac{1}{\lambda-\lambda_j}\begin{pmatrix} \phi_j\phi_{j,x} & -\phi_j^2 \\ \phi_{j,x}^2 & -\phi_j\phi_{j,x} \end{pmatrix}, \end{aligned}$$

where η is a constant, also satisfies the adjoint representation (2.3), i.e.,

$$N_x^{(n)} = [U, N^{(n)}], \tag{2.12}$$

which gives rise to the Lax representation of the constrained flow (2.11).

The KdV hierarchy with self-consistent sources is given by[16,17]

$$u_{t_n}=D\left[\frac{\delta H_n}{\delta u}-2\alpha\sum_{j=1}^{N}\frac{\delta\lambda_j}{\delta u}\right]\equiv D\left[-2b_{n+2}-2\alpha\sum_{j=1}^{N}\phi_j^2\right], \tag{2.13a}$$

$$\phi_{j,xx}+(\lambda_j+u)\phi_j=0,\quad j=1,\ldots,N. \tag{2.13b}$$

Since the high-order constrained flows (2.11) are just the stationary equations of the KdV hierarchy with self-consistent sources (2.13), it is obvious that the zero-curvature representation for the KdV hierarchy with self-consistent sources (2.13) is given by

$$U_{t_n}-N_x^{(n)}+[U,N^{(n)}]=0, \tag{2.14}$$

with the auxiliary linear problems

$$\begin{pmatrix}\psi\\ \psi_x\end{pmatrix}_x=U\begin{pmatrix}\psi\\ \psi_x\end{pmatrix},\quad \begin{pmatrix}\psi\\ \psi_x\end{pmatrix}_{t_n}=N^{(n)}\begin{pmatrix}\psi\\ \psi_x\end{pmatrix}, \tag{2.15}$$

or equivalently

$$\psi_{xx}+(\lambda+u)\psi=0, \tag{2.16a}$$

$$\psi_{t_n}=A^{(n)}\psi+\eta\psi+\alpha\sum_{j=1}^{N}\frac{1}{\lambda-\lambda_j}\phi_j(\phi_{j,x}\psi-\phi_j\psi_x). \tag{2.16b}$$

Let's assume that all products $\phi_j\psi$ decay at $x=-\infty$ and that $\partial^{-1}=\int_{-\infty}^{x}dx$. It is easy to find from (2.13b) and (2.16a) that

$$\frac{1}{\lambda-\lambda_j}(\phi_{j,x}\psi-\phi_j\psi_x)=\partial^{-1}\phi_j\psi. \tag{2.17}$$

Let's denote

$$B_N=\alpha\sum_{j=1}^{N}\phi_j\partial^{-1}\phi_j.$$

Then Eq. (2.16b) can be rewritten as

$$\psi_{t_n}=Q^{(n,N)}\psi\equiv A^{(n)}\psi+\eta\psi+B_N\psi. \tag{2.18}$$

When $n=1$, the Eq. (2.13) gives the KdV equation with self-consistent sources

$$u_{t_1}=-\frac{1}{4}(6uu_x+u_{xxx})-2\alpha D\sum_{j=1}^{N}\phi_j^2, \tag{2.19a}$$

$$\phi_{j,xx}+(\lambda_j+u)\phi_j=0,\quad j=1,\ldots,N, \tag{2.19b}$$

and the auxiliary linear problem reads

$$\psi_{xx}+(\lambda+u)\psi=0, \tag{2.20a}$$

$$\psi_{t_1}=\left(\frac{1}{4}u_x+\eta\right)\psi+\left(\lambda-\frac{1}{2}u\right)\psi_x+\alpha\sum_{j=1}^{N}B_j\psi. \tag{2.20b}$$

III. THE DARBOUX TRANSFORMATION FOR THE KdV HIERARCHY

In this section we recall the Darboux transformation for the KdV hierarchy (see Ref. 24 for a review[25–27]).

(1) The Darboux transformation for the KdV hierarchy.

Assume that u be the solution of the nth KdV equation (2.9) and denote the fixed solution of (2.1) and (2.8) with $\lambda=\xi$ by $f=f(x,t,\xi)$. The Darboux transformation (DT) is defined by

$$\tilde{\phi}=\phi_x-\frac{f_x}{f}\phi, \tag{3.1a}$$

$$\tilde{u}=u+2\partial^2\ln f. \tag{3.1b}$$

It is known that the Schrödinger equations (2.1) and (2.8) are covariant with respect to the action of the Darboux transformation (3.1), namely $\tilde{\phi},\tilde{u}$ satisfy

$$\tilde{\phi}_{xx}+(\lambda+\tilde{u})\tilde{\phi}=0, \tag{3.2}$$

$$\tilde{\phi}_{t_n}=\tilde{A}^{(n)}\tilde{\phi}\equiv A^{(n)}(\tilde{u},\lambda)\tilde{\phi}, \tag{3.3}$$

and $\tilde{u}$ satisfies the nth KdV equation (2.9). Equations (2.8), (3.1), and (3.3) imply that

$$\tilde{\phi}_{t_n}=\left[\phi_x-\frac{f_x}{f}\phi\right]_{t_n}=(A^{(n)}\phi)_x-\left(\frac{A^{(n)}f}{f}\right)_x\phi-\frac{f_x}{f}A^{(n)}\phi=\tilde{A}^{(n)}\tilde{\phi}. \tag{3.4}$$

So the covariance of (2.1) and (2.8) with respect to the action of DT (3.1) leads to the following lemma.

Lemma 3.1: If u is the solution of the nth KdV equation (2.9) and f is a solution of (2.1) and (2.8) with $\lambda=\xi$ and the Darboux transformation is given by (3.1), then formula (3.4) holds.

We now construct the binary Darboux transformation.

(2) The first binary Darboux transformation.

Also, it is known that the linearly independent solution of (2.1) and (2.8) with $\lambda=\xi$ is given by the Liouville formula

$$g=f\partial^{-1}\frac{1}{f^2}. \tag{3.5}$$

The DT (3.1) implies that

$$\tilde{g}=g_x-\frac{f_x}{f}g=\frac{1}{f} \tag{3.6}$$

is one of the solutions of (3.2) and (3.3) with $\lambda=\xi$ and $\tilde{u}$ given by (3.1b). The linearly independent solution $\tilde{g}_1$ of (3.2) and (3.3) with $\lambda=\xi$ is once more given by the Liouville formula

$$\tilde{g}_1=\tilde{g}\partial^{-1}\frac{1}{\tilde{g}^2}=\frac{1}{f}\partial^{-1}f^2. \tag{3.7}$$

By using f and $\tilde{g}_1$, performing two-times repeated DT of (3.1) [notice that the right-hand side of (3.1a) can be added to a constant factor] and using (2.17) gives rise to the binary Darboux transformation

$$\overline{\phi}=\frac{1}{\xi-\lambda}\left[\tilde{\phi}_x-\frac{\tilde{g}_{1x}}{\tilde{g}_1}\tilde{\phi}\right]=\frac{1}{\xi-\lambda}\left[\xi\phi-\lambda\phi+\frac{f}{\partial^{-1}f^2}(f_x\phi-f\phi_x)\right]=\phi-\frac{f}{\partial^{-1}f^2}\partial^{-1}(f\phi), \tag{3.8a}$$

$$\overline{u}=\tilde{u}+2\partial^2\ln\tilde{g}_1=u+2\partial^2\ln(\partial^{-1}f^2). \tag{3.8b}$$

Obviously, the equations (2.1) and (2.8) are covariant with respect to the action of the binary DT (3.8), namely $\overline{\phi},\overline{u}$ satisfy

$$\overline{\phi}_{xx}+(\lambda+\overline{u})\overline{\phi}=0, \tag{3.9}$$

$$\overline{\phi}_{t_n}=\overline{A^{(n)}}\overline{\phi}\equiv A^{(n)}(\overline{u},\lambda)\overline{\phi}, \tag{3.10}$$

and this $\overline{u}$ satisfies the nth KdV equation (2.9). It is found from (3.8), (2.8), and (3.10) that

$$\overline{\phi}_{t_n}=\overline{A^{(n)}}\overline{\phi}=\left[\phi-\frac{f}{\partial^{-1}f^2}\partial^{-1}(f\phi)\right]_{t_n}=A^{(n)}\phi-\frac{1}{\partial^{-1}f^2}\left\{\left[A^{(n)}f-\frac{2f}{\partial^{-1}f^2}\partial^{-1}(fA^{(n)}f)\right]\partial^{-1}(f\phi)\right.$$
$$\left.+f\partial^{-1}[fA^{(n)}\phi+\phi A^{(n)}f]\right\}. \tag{3.11}$$

So the covariance of (2.1) and (2.8) with respect to the action of binary DT (3.8) leads to the following lemma.

Lemma 3.2: If u is the solution of the nth KdV equation (2.9) and f is a solution of (2.1) and (2.8) with $\lambda=\xi$ the binary DT is given by (3.8), then formula (3.11) holds.

(3) The second binary Darboux transformation.

Also the combination of $\tilde{g}$ and $\tilde{g}_1$ gives a solution of (3.2) and (3.3) with $\lambda=\xi$

$$\tilde{g}_2=\tilde{g}+\tilde{g}_1=\frac{1}{f}(1+\partial^{-1}f^2). \tag{3.12}$$

By using f and $\tilde{g}_2$, performing two-times repeated DT (3.1) leads to second binary Darboux transformation

$$\overline{\phi}=\frac{1}{\xi-\lambda}\left[\tilde{\phi}_x-\frac{\tilde{g}_{2x}}{\tilde{g}_2}\tilde{\phi}\right]=\frac{1}{\xi-\lambda}\left[\xi\phi-\lambda\phi+\frac{f}{1+\partial^{-1}f^2}(f_x\phi-f\phi_x)\right]=\phi-\frac{f}{1+\partial^{-1}f^2}\partial^{-1}(f\phi), \tag{3.13a}$$

$$\overline{u}=\tilde{u}+2\partial^2\ln\tilde{g}_2=u+2\partial^2\ln(1+\partial^{-1}f^2). \tag{3.13b}$$

Also the equation (2.1) and (2.8) are covariant with respect to the action of the binary DT (3.13), namely $\overline{\phi},\overline{u}$ satisfy (3.9) and (3.10), $\overline{u}$ satisfies the nth KdV equation (2.9). Similarly, the covariance of (2.1) and (2.8) with respect to the action of binary DT (3.13) leads to the following lemma.

Lemma 3.3: If u is a solution of the nth KdV equation (2.9) and f is a solution of (2.1) and (2.8) with $\lambda=\xi$ and the binary DT is given by (3.13), then the following formula holds:

$$\overline{\phi}_{t_n}=\overline{A^{(n)}}\overline{\phi}=\left[\phi-\frac{f}{1+\partial^{-1}f^2}\partial^{-1}(f\phi)\right]_{t_n}=A^{(n)}\phi-\frac{1}{1+\partial^{-1}f^2}\left\{\left[A^{(n)}f\right.\right.$$
$$\left.\left.-\frac{2f}{1+\partial^{-1}f^2}\partial^{-1}(fA^{(n)}f)\right]\partial^{-1}(f\phi)+f\partial^{-1}[fA^{(n)}\phi+\phi A^{(n)}f]\right\}. \tag{3.14}$$

IV. THE DARBOUX TRANSFORMATION FOR THE KdV HIERARCHY WITH SELF-CONSISTENT SOURCES

Based on the Darboux transformation for the KdV hierarchy, we now construct Darboux transformation and two binary Darboux transformations for the KdV hierarchy with self-consistent sources. The first binary Darboux transformation is an auto-Bäcklund transformation for the nth KdV equation with self-consistent sources (2.13). The second one is a Bäcklund transformation relating two nth KdV equations with self-consistent sources (2.13) with degree N and $N+1$, respectively.

(1) Darboux transformation for the KdV hierarchy with sources.

Theorem 4.1: *Assume that $u,\phi_1,\ldots,\phi_N$ be the solution of the nth KdV equation with self-consistent sources (2.13) and f_1 satisfies (2.16a) and (2.18) with $\lambda=\xi_1$, then the Darboux transformation is defined by*

$$\overline{\psi}=\psi_x-\frac{f_{1,x}}{f_1}\psi, \tag{4.1a}$$

$$\overline{u}=u+2\partial^2\ln f_1, \tag{4.1b}$$

$$\overline{\phi}_j=\frac{1}{\sqrt{\lambda_j-\xi_1}}\left[\phi_{j,x}-\frac{f_{1,x}}{f_1}\phi_j\right],\quad j=1,\ldots,N, \tag{4.1c}$$

the Lax representation (2.16a) and (2.18) are covariant with respect to the Darboux transformation (4.1). Namely $\overline{u},\overline{\psi},\overline{\phi}_j, j=1,\ldots,N$, satisfy

$$\overline{\psi}_{xx}+(\lambda+\overline{u})\overline{\psi}=0, \tag{4.2}$$

$$\overline{\psi}_{t_n}=\overline{Q}^{(n,N)}\overline{\psi}=\overline{A}^{(n)}\overline{\psi}+\eta\overline{\psi}+\overline{B}_N\overline{\psi}\equiv A^{(n)}(\overline{u},\lambda)\overline{\psi}+\eta\overline{\psi}+\alpha\sum_{j=1}^{N}\overline{\phi}_j\partial^{-1}(\overline{\phi}_j\overline{\psi}), \tag{4.3}$$

and $\overline{u},\overline{\phi}_1,\ldots,\overline{\phi}_N$ satisfy the nth KdV equation with self-consistent sources (2.13),

$$\overline{u}_{t_n}=D\left[-2\overline{b}_{n+2}-2\alpha\sum_{j=1}^{N}\overline{\phi}_j^2\right], \tag{4.4a}$$

$$\overline{\phi}_{j,xx}+(\lambda_j+\overline{u})\overline{\phi}_j=0,\quad j=1,\ldots,N. \tag{4.4b}$$

Proof: Based on the results in the previous section, it is obvious that (4.2) and (4.4b) hold. In order to prove (4.3) we need to show the following equality:

$$\tilde{\psi}_{t_n}=\left[\psi_x-\frac{f_{1,x}}{f_1}\psi\right]_{t_n}=(Q^{(n,N)}\psi)_x-\left(\frac{Q^{(n,N)}f_1}{f_1}\right)_x\psi-\frac{f_{1,x}}{f_1}Q^{(n,N)}\psi=\tilde{Q}^{(n,N)}\tilde{\psi}. \tag{4.5}$$

The Lemma 3.1 implies that equality (3.4) with ϕ replaced by ψ holds. So we only need to check the terms containing $\phi_1,\ldots,\phi_N$ in the equality (4.5), i.e., to show the following equality:

$$(B_N\psi)_x-\left(\frac{B_Nf_1}{f_1}\right)_x\psi-\frac{f_{1,x}}{f_1}B_N\psi=\overline{B}_N\overline{\psi}. \tag{4.6}$$

Using (4.1) and (2.17), we have

$$\begin{aligned}\overline{B}_N\overline{\psi}&=\alpha\sum_{j=1}^{N}\overline{\phi}_j\partial^{-1}\left[\frac{1}{\sqrt{\lambda_j-\xi_1}}\left(\phi_{j,x}-\frac{f_{1,x}}{f_1}\phi_j\right)\left(\psi_x-\frac{f_{1,x}}{f_1}\psi\right)\right]\\&=\alpha\sum_{j=1}^{N}\frac{1}{\sqrt{\lambda_j-\xi_1}}\overline{\phi}_j\left[\phi_{j,x}\psi-\partial^{-1}(\phi_{j,xx}\psi)-\frac{f_{1,x}}{f_1}\phi_j\psi+\partial^{-1}\left(\frac{f_{1,xx}}{f_1}\phi_j\psi\right)\right]\\&=\alpha\sum_{j=1}^{N}\frac{1}{\sqrt{\lambda_j-\xi_1}}\overline{\phi}_j\left[\phi_{j,x}\psi-\frac{f_{1,x}}{f_1}\phi_j\psi+(\lambda_j-\xi_1)\partial^{-1}(\phi_j\psi)\right]\end{aligned}\tag{4.7}$$

and

$$\begin{aligned}\text{the left terms in (4.6)}=\alpha\sum_{j=1}^{N}&\left[\phi_{j,x}\partial^{-1}(\phi_j\psi)-\frac{1}{f_1}\psi\phi_{j,x}\partial^{-1}(f_1\phi_j)\right.\\&\left.+\frac{f_{1,x}}{f_1^2}\psi\phi_j\partial^{-1}(f_1\phi_j)-\frac{f_{1,x}}{f_1}\phi_j\partial^{-1}(\phi_j\psi)\right]\\=\alpha\sum_{j=1}^{N}&\sqrt{\lambda_j-\xi_1}\overline{\phi}_j\left[\partial^{-1}(\phi_j\psi)-\frac{1}{f_1}\psi\partial^{-1}(f_1\phi_j)\right]\\=\alpha\sum_{j=1}^{N}&\sqrt{\lambda_j-\xi_1}\overline{\phi}_j\left[\partial^{-1}(\phi_j\psi)+\frac{1}{f_1(\lambda_j-\xi_1)}\psi(f_1\phi_{j,x}-f_{1,x}\phi_j)\right].\end{aligned}\tag{4.8}$$

Comparing (4.7) with (4.8), it is immediately found that equality (4.6) holds. The equations (4.2) and (4.3) lead to (4.4a). This completes the proof.

(2) The first binary Darboux transformation for the KdV hierarchy with sources.

Theorem 4.2: *Assume that $u,\phi_1,\ldots,\phi_N$ be the solution of the n*th *KdV equation with self-consistent sources (2.13) and f_1 satisfies (2.16a) and (2.18) with $\lambda=\xi_1$, then the first binary Darboux transformation is defined by*

$$\overline{\psi}=\psi-\frac{f_1}{\partial^{-1}f_1^2}\partial^{-1}(f_1\psi),\tag{4.9a}$$

$$\overline{u}=u+2\partial^2\ln(\partial^{-1}f_1^2),\tag{4.9b}$$

$$\overline{\phi}_j=\phi_j-\frac{f_1}{\partial^{-1}f_1^2}\partial^{-1}(f_1\phi_j),\quad j=1,\ldots,N,\tag{4.9c}$$

*the Lax representation (2.16a) and (2.18) are covariant with respect to the binary Darboux transformation (4.9). Namely $\overline{u},\overline{\psi},\overline{\phi}_j, j=1,\ldots,N$, satisfy (4.2), (4.3) and the n*th *KdV equation with self-consistent sources (4.4).*

Proof: It is obvious that (4.2) and (4.4b) hold. Similarly, in order to prove (4.3) we need to show the equality (3.11) with $\phi,A^{(n)}$ replaced by $\psi,Q^{(n,N)}$. In fact, using Lemma 3.2, we only need to check the terms containing $\phi_1,\ldots,\phi_N$ in the equality, i.e., to show the following equality:

$$B_N\psi-\frac{1}{\partial^{-1}f_1^2}\left[B_Nf_1-2\frac{1}{\partial^{-1}f_1^2}f_1\partial^{-1}(f_1B_Nf_1)\right]\partial^{-1}(f_1\psi)-\frac{f_1}{\partial^{-1}f_1^2}\partial^{-1}[f_1B_N\psi+\psi B_Nf_1]=\overline{B}_N\overline{\psi}.\tag{4.10}$$

Notice that

$$\partial^{-1}\left[\frac{f_1^2}{(\partial^{-1}f_1^2)^2}(\partial^{-1}(f_1\phi_j))(\partial^{-1}(f_1\psi))\right]=-\frac{1}{\partial^{-1}f_1^2}(\partial^{-1}(f_1\phi_j))(\partial^{-1}(f_1\psi))$$
$$+\partial^{-1}\left[\frac{f_1\phi_j}{\partial^{-1}f_1^2}\partial^{-1}(f_1\psi)+\frac{f_1\psi}{\partial^{-1}f_1^2}\partial^{-1}(f_1\phi_j)\right]. \tag{4.11}$$

Using (4.9) and (4.11), we have

$$\begin{aligned}\overline{B_N}\overline{\psi}&=\alpha\sum_{j=1}^{N}\overline{\phi}_j\partial^{-1}(\overline{\phi}_j\overline{\psi})\\&=\alpha\sum_{j=1}^{N}\overline{\phi}_j\partial^{-1}\left[\left(\phi_j-\frac{f_1}{\partial^{-1}f_1^2}\partial^{-1}(f_1\phi_j)\right)\left(\psi-\frac{f_1}{\partial^{-1}f_1^2}\partial^{-1}(f_1\psi)\right)\right]\\&=\alpha\sum_{j=1}^{N}\overline{\phi}_j\left[\partial^{-1}(\phi_j\psi)-\frac{1}{\partial^{-1}f_1^2}(\partial^{-1}(f_1\phi_j))(\partial^{-1}(f_1\psi))\right],\end{aligned} \tag{4.12}$$

and

$$\begin{aligned}\text{the left terms in (4.10)}=\alpha\sum_{j=1}^{N}\Bigg\{&\phi_j\partial^{-1}(\phi_j\psi)-\frac{1}{\partial^{-1}f_1^2}\Bigg[\phi_j(\partial^{-1}(f_1\phi_j))(\partial^{-1}(f_1\psi))\\&-2\frac{f_1}{\partial^{-1}f_1^2}\partial^{-1}(f_1\phi_j\partial^{-1}(f_1\phi_j))(\partial^{-1}(f_1\psi))+f_1\partial^{-1}(f_1\phi_j\partial^{-1}(\phi_j\psi))\\&+f_1\partial^{-1}(\phi_j\psi\partial^{-1}(\phi_jf_1))\Bigg]\Bigg\}\\=\alpha\sum_{j=1}^{N}\Bigg[&\phi_j\partial^{-1}(\phi_j\psi)-\frac{\phi_j}{\partial^{-1}f_1^2}(\partial^{-1}(f_1\phi_j))(\partial^{-1}(f_1\psi))\\&+\frac{f_1}{(\partial^{-1}f_1^2)^2}(\partial^{-1}(f_1\phi_j))^2(\partial^{-1}(f_1\psi))-\frac{f_1}{\partial^{-1}f_1^2}(\partial^{-1}(f_1\phi_j))\\&\times(\partial^{-1}(\phi_j\psi))\Bigg].\end{aligned} \tag{4.13}$$

By substituting (4.9c) into (4.12) and comparing it with (4.13), it is immediately found that equality (4.10) holds. The equations (4.2) and (4.3) lead to (4.4a). This completes the proof.

(3) The second binary Darboux transformation for the KdV hierarchy with sources.

Theorem 4.3: *Assume that $u,\phi_1,\ldots,\phi_N$ is the solution of the n*th *KdV equation with self-consistent sources (2.13), $f_1\equiv\phi_{N+1}$ satisfies (2.16a) and (2.18) with $\lambda=\lambda_{N+1}$ and $\eta=-\frac{1}{2}\alpha$, then the second binary Darboux transformation is defined by*

$$\overline{\psi}=\psi-\frac{f_1}{1+\partial^{-1}f_1^2}\partial^{-1}(f_1\psi)=\psi-\overline{\phi}_{N+1}\partial^{-1}(f_1\psi), \tag{4.14a}$$

$$\overline{u}=u+2\partial^2\ln(1+\partial^{-1}f_1^2), \tag{4.14b}$$

$$\overline{\phi}_j=\phi_j-\frac{f_1}{1+\partial^{-1}f_1^2}\partial^{-1}(f_1\phi_j)=\phi_j-\overline{\phi}_{N+1}\partial^{-1}(f_1\phi_j),\quad j=1,\ldots,N, \tag{4.14c}$$

where

$$\overline{\phi}_{N+1}=\frac{f_1}{1+\partial^{-1}f_1^2},\quad f_1=\phi_{N+1}, \tag{4.14d}$$

and the binary Darboux transformation (4.14) transforms the Lax representation (2.16a) and (2.18) with $\eta=-\frac{1}{2}\alpha$ *into the following Lax representation:*

$$\overline{\psi}_{xx}+(\lambda+\overline{u})\overline{\psi}=0, \tag{4.15}$$

$$\overline{\psi}_{t_n}=\overline{Q}^{(n,N+1)}\overline{\psi}=\overline{A}^{(n)}\overline{\psi}-\frac{1}{2}\alpha\overline{\psi}+\overline{B}_{N+1}\overline{\psi}\equiv A^{(n)}(\overline{u},\lambda)\overline{\psi}-\frac{1}{2}\alpha\overline{\psi}+\alpha\sum_{j=1}^{N+1}\overline{\phi}_j\partial^{-1}(\overline{\phi}_j\overline{\psi}), \tag{4.16}$$

and $\overline{u},\overline{\phi}_1,\ldots,\overline{\phi}_{N+1}$ *satisfies the n*th *KdV equation with self-consistent sources (2.13) with degree* $N+1$

$$\overline{u}_{t_n}=D\left[-2\overline{b}_{n+2}-2\alpha\sum_{j=1}^{N+1}\overline{\phi}_j^2\right], \tag{4.17a}$$

$$\overline{\phi}_{j,xx}+(\lambda_j+\overline{u})\overline{\phi}_j=0,\quad j=1,\ldots,N+1. \tag{4.17b}$$

Proof: It is easy to see that (4.14c) holds for $j=N+1$. So, based on the results in the previous section, it is obvious that (4.15) and (4.17b) hold. Similarly, in order to prove (4.16), by using Lemma 3.3 one only needs to check the terms containing $\phi_1,\ldots,\phi_N,\overline{\phi}_{N+1}$ in the equality (3.14) with $\phi,A^{(n)}$ replaced by $\psi,Q^{(n,N)}$, i.e., to show the following equality:

$$\begin{aligned}&B_N\psi-\frac{1}{1+\partial^{-1}f_1^2}\left[B_Nf_1-\frac{1}{2}\alpha\overline{\phi}_{N+1}(1-\partial^{-1}f_1^2)-2\overline{\phi}_{N+1}\partial^{-1}(f_1B_Nf_1)\right]\partial^{-1}(f_1\psi)\\&\quad-\overline{\phi}_{N+1}\partial^{-1}\left[\psi B_Nf_1-\frac{1}{2}\alpha f_1\psi+f_1B_N\psi\right]=\overline{B}_{N+1}\overline{\psi}.\end{aligned} \tag{4.18}$$

Notice that

$$\partial^{-1}(\overline{\phi}_{N+1}\overline{\psi})=\partial^{-1}\left[\frac{f_1}{1+\partial^{-1}f_1^2}\psi-\left(\frac{f_1}{1+\partial^{-1}f_1^2}\right)^2\partial^{-1}(f_1\psi)\right]=\frac{1}{1+\partial^{-1}f_1^2}\partial^{-1}(f_1\psi). \tag{4.19}$$

By means of (4.11) and (4.12) with $\partial^{-1}f_1^2$ replaced by $(1+\partial^{-1}f_1^2)$ one gets

$$\begin{aligned}\overline{B}_{N+1}\overline{\psi}&=\alpha\sum_{j=1}^{N+1}\overline{\phi}_j\partial^{-1}(\overline{\phi}_j\overline{\psi})\\&=\alpha\sum_{j=1}^{N}\overline{\phi}_j\left[\partial^{-1}(\phi_j\psi)-\frac{1}{1+\partial^{-1}f_1^2}(\partial^{-1}(f_1\phi_j))\partial^{-1}(f_1\psi)\right]+\frac{\alpha\overline{\phi}_{N+1}}{1+\partial^{-1}f_1^2}\partial^{-1}(f_1\psi).\end{aligned} \tag{4.20}$$

Using (4.13) with $\partial^{-1}f_1^2$ replaced by $(1+\partial^{-1}f_1^2)$ it is found that

$$\text{the left terms in (4.18)} = \alpha \sum_{j=1}^{N} \left\{ \phi_j \partial^{-1}(\phi_j \psi) - \frac{1}{1+\partial^{-1} f_1^2} [\phi_j (\partial^{-1}(f_1 \phi_j)) \partial^{-1}(f_1 \psi) - \overline{\phi}_{N+1} (\partial^{-1}(f_1 \phi_j))^2 \partial^{-1}(f_1 \psi)] - \overline{\phi}_{N+1} (\partial^{-1}(f_1 \phi_j)) \partial^{-1}(\phi_j \psi) \right\} + \frac{\alpha \overline{\phi}_{N+1}}{1+\partial^{-1} f_1^2} \partial^{-1}(f_1 \psi). \tag{4.21}$$

By substituting (4.14c) into (4.20) and comparing it with (4.21), it is easy to see that equality (4.18) holds. The equations (4.15) and (4.16) yield (4.17). This completes the proof.

Remark: The binary Darboux transformation defined by (4.14) is a non-auto-Bäcklund transformation relating the two nth KdV equations with self-consistent sources (2.13) and (4.17). This Darboux transformation can be used to construct the soliton solution for (2.13).

For example, in order to find one soliton solution for the KdV equation with self-consistent sources (2.19) with $N=1$, we start from the solution $u=0$ for the KdV equation with self-consistent sources (2.19) with $N=0$. The solution for (2.20) with $N=0, u=0, \lambda=-k^2, k>0$, $\eta=-\frac{1}{2}\alpha$ reads

$$\phi_1 = c e^{kx-k^3 t-1/2\,\alpha t}.$$

Then one finds from (4.14) that

$$\overline{u} = 2k^2 \operatorname{sech}^2(kx-k^3 t-\tfrac{1}{2}\alpha t + x_0),$$

$$\phi_1 = \frac{1}{2}\sqrt{2k}\operatorname{sech}\left(kx-k^3 t-\frac{1}{2}\alpha t + x_0\right),$$

which is the one soliton solution for the KdV equation with self-consistent sources (2.19) with $N=1$.

V. THE *m*-TIMES REPEATED BINARY DARBOUX TRANSFORMATION FOR THE KdV HIERARCHY WITH SELF-CONSISTENT SOURCES

It is evident that the Darboux transformation can be applied to (4.2), (4.3), and (4.15), (4.16) once more to produce some new solutions for the KdV hierarchy with self-consistent sources.

(1) The m-times repeated second binary Darboux transformation.

Assume that $f_1, \ldots, f_m$ be solution of (2.16a) and (2.18) with $\lambda = \lambda_{N+1}, \ldots, \lambda_{N+m}$, respectively. We use $u[i], \psi[i], f_j[i], \phi_j[i]$ to denote the action of i-times repeated binary Darboux transformation of (4.14) on the initial solution u, ψ, f_j, ϕ_j. We have

$$f_j[i]_{xx} + (\lambda_j + u[i]) f_j[i] = 0, \tag{5.1}$$

$$f_{j,t_n}[i] = Q^{(n,N+i)}[i] f_j[i]. \tag{5.2}$$

We define two integral types of the Wronskian determinant of k functions $g_1, \ldots, g_k$ in a similar way as in Ref. 27 by

$$W_1(g_1, \ldots, g_k) = \det F, \quad W_2(g_1, \ldots, g_k) = \det G,$$

where

$$F_{ij} = \delta_{ij} + \partial^{-1}(g_i g_j), \quad i,j = 1, \ldots, k,$$

$$G_{ij}=\delta_{ij}+\partial^{-1}(g_ig_j),\quad i=1,\ldots,k-1,\quad j=1,\ldots,k,\quad G_{kj}=g_j,\quad j=1,\ldots,k.$$

Lemma 5.1: For arbitrary integers $l,k(1\leqslant l\leqslant m-1,1\leqslant k\leqslant m-l)$, we have

$$W_1(f_{l+1}[l],\ldots,f_{l+k}[l])=\frac{W_1(f_l[l-1],f_{l+1}[l-1],\ldots,f_{l+k}[l-1])}{1+\partial^{-1}f_l^2[l-1]},\tag{5.3}$$

$$W_2(f_{l+1}[l],\ldots,f_{l+k}[l],\psi[l])=\frac{W_1(f_l[l-1],f_{l+1}[l-1],\ldots,f_{l+k}[l-1],\psi[l-1])}{1+\partial^{-1}f_l^2[l-1]}.\tag{5.4}$$

Proof: According to (4.14), we have

$$f_{l+j}[l]=f_{l+j}[l-1]-\frac{f_l[l-1]}{1+\partial^{-1}f_l^2[l-1]}\partial^{-1}(f_l[l-1]f_{l+j}[l-1]),\tag{5.5}$$

so using (4.11)

$$\begin{aligned}F_{ij}&=\delta_{ij}+\partial^{-1}(f_{l+i}[l]f_{l+j}[l])\\&=\delta_{ij}+\partial^{-1}(f_{l+i}[l-1]f_{l+j}[l-1])\\&\quad-\frac{1}{1+\partial^{-1}f_l^2[l-1]}(\partial^{-1}f_{l+i}[l-1]f_l[l-1])(\partial^{-1}f_l[l-1]f_{l+j}[l-1])\\&\equiv\delta_{ij}+a_{ij}-ba_{i0}a_{0j},\end{aligned}\tag{5.6}$$

where

$$a_{ij}=\partial^{-1}(f_{l+i}[l-1]f_{l+j}[l-1]),\quad b=\frac{1}{1+\partial^{-1}f_l^2[l-1]}.$$

Then

$$\begin{aligned}&W_1(f_{l+1}[l],\ldots,f_{l+k}[l])\\&\quad=\det(F_{ij})\\&\quad=\begin{pmatrix}1+a_{11}-ba_{10}a_{01}&a_{12}-ba_{10}a_{02}&a_{13}-ba_{10}a_{03}&\cdots&a_{1k}-ba_{10}a_{0k}\\a_{21}-ba_{20}a_{01}&1+a_{22}-ba_{20}a_{02}&a_{23}-ba_{20}a_{03}&\cdots&a_{2k}-ba_{20}a_{0k}\\\vdots&\vdots&\vdots&\ddots&\vdots\\a_{k1}-ba_{k0}a_{01}&a_{k2}-ba_{k0}a_{02}&a_{k3}-ba_{k0}a_{03}&\cdots&1+a_{kk}-ba_{k0}a_{0k}\end{pmatrix}\\&\quad=\begin{pmatrix}1+a_{11}&a_{12}&\cdots&a_{1k}\\a_{21}&1+a_{22}&\cdots&a_{2k}\\\vdots&\vdots&\ddots&\vdots\\a_{k1}&a_{k2}&\cdots&1+a_{kk}\end{pmatrix}-ba_{01}\begin{pmatrix}a_{10}&a_{12}&a_{13}&\cdots&a_{1k}\\a_{20}&1+a_{22}&a_{23}&\cdots&a_{2k}\\\vdots&\vdots&\vdots&\ddots&\vdots\\a_{k0}&a_{k2}&a_{k3}&\cdots&1+a_{kk}\end{pmatrix}\end{aligned}$$

$$-ba_{02}\begin{pmatrix} 1+a_{11} & a_{10} & a_{13} & \cdots & a_{1k} \\ a_{21} & a_{20} & a_{23} & \cdots & a_{2k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{k1} & a_{k0} & a_{k3} & \cdots & 1+a_{kk} \end{pmatrix}-\cdots$$

$$-ba_{0k}\begin{pmatrix} 1+a_{11} & a_{12} & \cdots & a_{1(k-1)} & a_{10} \\ a_{21} & 1+a_{22} & \cdots & a_{2(k-1)} & a_{20} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ a_{k1} & a_{k2} & \cdots & a_{k(k-1)} & a_{k0} \end{pmatrix}$$

$$=\frac{1}{1+a_{00}}\begin{pmatrix} 1+a_{00} & a_{01} & a_{02} & \cdots & a_{0k} \\ a_{10} & 1+a_{11} & a_{12} & \cdots & a_{1k} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{k0} & a_{k1} & a_{k2} & \cdots & 1+a_{kk} \end{pmatrix}$$

$$=\frac{W_1(f_l[l-1],\ldots,f_{l+k}[l-1])}{1+\partial^{-1}f_l^2[l-1]}.$$

In the similar way the formula (5.4) can be proved. This completes the proof.

Theorem 5.1: *Assume that $u,\phi_1,\ldots,\phi_N$ is the solution of the n*th *KdV equation with self-consistent sources (2.13), $f_1,\ldots,f_m$ is the solution of (2.16a) and (2.18) with $\lambda=\lambda_{N+1},\ldots,\lambda_{N+m}$, respectively, and $\eta=-\frac{1}{2}\alpha$. Then the m-times repeated binary Darboux transformation of (4.14) is given by*

$$\psi[m]=\frac{W_2(f_1,\ldots,f_m,\psi)}{W_1(f_1,\ldots,f_m)}, \tag{5.7a}$$

$$u[m]=u+2\partial^2\ln W_1(f_1,\ldots,f_m), \tag{5.7b}$$

$$\phi_j[m]=\frac{W_2(f_1,\ldots,f_m,\phi_j)}{W_1(f_1,\ldots,f_m)},\quad j=1,\ldots,N, \tag{5.7c}$$

$$\phi_{N+j}[m]=\frac{W_2(f_1,\ldots,f_m,f_j)}{W_1(f_1,\ldots,f_m)}=\frac{W_2(f_1,\ldots,f_{j-1},f_{j+1},\ldots,f_m,f_j)}{W_1(f_1,\ldots,f_m)},\quad j=1,\ldots,m, \tag{5.7d}$$

and $u[m],\psi[m],\phi_1[m],\ldots,\phi_{N+m}[m]$ satisfy

$$\psi_{xx}[m]+(\lambda+u[m])\psi[m]=0, \tag{5.8}$$

$$\psi_{t_n}[m]=Q^{(n,N+m)}[m]\psi[m]=A^{(n)}(u[m],\lambda)\psi[m]-\frac{1}{2}\alpha\psi[m]+\alpha\sum_{j=1}^{N+m}\phi_j[m]\partial^{-1}(\phi_j[m]\psi[m]), \tag{5.9}$$

and

$$u_{t_n}[m]=D\left[-2b_{n+2}(u[m])-2\alpha\sum_{j=1}^{N+m}\phi_j^2[m]\right], \tag{5.10a}$$

$$\phi_{j,xx}[m]+(\lambda_j+u[m])\phi_j[m]=0, \quad j=1,\ldots,N+m. \tag{5.10b}$$

Proof: Using (4.14), (5.3), and (5.4), one obtains

$$\begin{aligned}
\psi[m]&=\psi[m-1]-\frac{f_m[m-1]}{1+\partial^{-1}f_m^2[m-1]}\partial^{-1}(f_m[m-1]\psi[m-1])\\
&=\frac{1}{1+\partial^{-1}f_m^2[m-1]}W_2(f_m[m-1],\psi[m-1])\\
&=\frac{W_2(f_m[m-1],\psi[m-1])}{W_1(f_m[m-1])}\\
&=\frac{W_2(f_{m-1}[m-2],f_m[m-2],\psi[m-2])}{1+\partial^{-1}f_{m-1}^2[m-2]}\frac{1+\partial^{-1}f_{m-1}^2[m-2]}{W_1(f_{m-1}[m-2],f_m[m-2])}\\
&=\cdots=\frac{W_2(f_1,\ldots,f_m,\psi)}{W_1(f_1,\ldots,f_m)},
\end{aligned} \tag{5.11}$$

$$\begin{aligned}
u[m]&=u[m-1]+2\partial^2\ln(1+\partial^{-1}f_m^2[m-1])\\
&=u[m-1]+2\partial^2\ln W_1(f_m[m-1])\\
&=u[m-2]+2\partial^2\ln(1+\partial^{-1}f_{m-1}^2[m-2])+2\partial^2\ln\frac{W_1(f_{m-1}[m-2],f_m[m-2])}{1+\partial^{-1}f_{m-1}^2[m-2]}\\
&=u[m-2]+2\partial^2\ln W_1(f_{m-1}[m-2],f_m[m-2])\\
&=\cdots=u+2\partial^2\ln W_1(f_1,\ldots,f_m).
\end{aligned} \tag{5.12}$$

Similarly we can prove the (5.7c) and (5.7d). It is easy to find (5.8), (5.9), and (5.10) from the Proposition 4.3.

The m-times repeated binary Darboux transformation (5.8) provides a Bäcklund transformation relating two nth KdV equations with self-consistent sources (2.13) with degree N and $N+m$, respectively. We now use the N-times repeated binary Darboux transformation (5.6) to construct the N-soliton solution for the nth KdV equation with self-consistent sources (2.13) with $\lambda_j=-k_j^2<0,k_j>0,j=1,\ldots,N$. We start from (2.13) with $N=0$. Taking $N=0,u=0,\lambda=-k_j^2,\eta=-\frac{1}{2}\alpha$, then (2.16a) and (2.18) reduce to

$$\psi_{xx}-k_j^2\psi=0,$$

$$\psi_{t_n}=(-1)^n k_j^{2n}\psi_x-\tfrac{1}{2}\alpha\psi,$$

which solution is given by

$$f_j=e^{k_jx+(-1)^n k_j^{2n+1}t_n-\frac{1}{2}\alpha t_n+x_{0,j}}, \quad j=1,\ldots,N. \tag{5.13}$$

Then according to Proposition 5.1, the N-soliton solution for the nth KdV equation with self-consistent sources (2.13) with $\lambda_j=-k_j^2<0,k_j>0,j=1,\ldots,N$, is given by

$$u=2\partial^2\ln W_1(f_1,\ldots,f_N), \tag{5.14}$$

$$\phi_j=\frac{W_2(f_1,\ldots,f_N,f_j)}{W_1(f_1,\ldots,f_N)}=\frac{W_2(f_1,\ldots,f_{j-1},f_{j+1},\ldots,f_N,f_j)}{W_1(f_1,\ldots,f_N)},\quad j=1,\ldots,N, \tag{5.15}$$

where f_j is given by (5.13).

(2) The m-times repeated first binary Darboux transformation.

We define

$$W_1(g_1,\ldots,g_k)=\det F,\qquad W_2(g_1,\ldots,g_k)=\det G, \tag{5.16}$$

where

$$F_{ij}=\partial^{-1}(g_ig_j),\quad i,j=1,\ldots,k,$$

$$G_{ij}=\partial^{-1}(g_ig_j),\quad i=1,\ldots,k-1,\quad j=1,\ldots,k,\quad G_{kj}=g_j,\quad j=1,\ldots,k.$$

In exactly the same way we can prove the following theorem.

Theorem 5.2: *Assume that $u,\phi_1,\ldots,\phi_N$ is the solution of the n*th *KdV equation with self-consistent sources (2.13), $f_1,\ldots,f_m$ is the solution of (2.16a) and (2.18) with $\lambda=\xi_1,\ldots,\xi_m$, respectively. Then the m-times repeated binary Darboux transformation of (4.9) is given by*

$$\psi[m]=\frac{W_2(f_1,\ldots,f_m,\psi)}{W_1(f_1,\ldots,f_m)}, \tag{5.17a}$$

$$u[m]=u+2\partial^2\ln W_1(f_1,\ldots,f_m), \tag{5.17b}$$

$$\phi_j[m]=\frac{W_2(f_1,\ldots,f_m,\phi_j)}{W_1(f_1,\ldots,f_m)},\quad j=1,\ldots,N, \tag{5.17c}$$

and $u[m],\psi[m],\phi_1[m],\ldots,\phi_N[m]$ satisfy

$$\psi_{xx}[m]+(\lambda+u[m])\psi[m]=0, \tag{5.18}$$

$$\psi_{t_n}[m]=Q^{(n,N)}[m]\psi[m], \tag{5.19}$$

and

$$u_{t_n}[m]=D\left[-2b_{n+2}(u[m])-2\alpha\sum_{j=1}^{N}\phi_j^2[m]\right], \tag{5.20a}$$

$$\phi_{j,xx}[m]+(\lambda_j+u[m])\phi_j[m]=0,\quad j=1,\ldots,N. \tag{5.20b}$$

(3) The m-times repeated Darboux transformation of (4.1).

We define the Wronskian determinant W by

$$W_1(g_1,\ldots,g_k)=\det F,\quad F_{ij}=\frac{\partial^{i-1}g_j}{\partial x^{i-1}},\quad i,j=1,\ldots,k. \tag{5.21}$$

In exactly the same way we can prove the following theorem.

Theorem 5.3: *Assume that $u,\phi_1,\ldots,\phi_N$ is the solution of the n*th *KdV equation with self-consistent sources (2.13), $f_1,\ldots,f_m$ is the solution of (2.16a) and (2.18) with $\lambda=\xi_1,\ldots,\xi_m$, respectively. Then the m-times repeated Darboux transformation of (4.1) is given by*

$$\psi[m]=\frac{W(f_1,\ldots,f_m,\psi)}{W(f_1,\ldots,f_m)}, \tag{5.22a}$$

$$u[m]=u+2\partial^2 \ln W(f_1,\ldots,f_m), \tag{5.22b}$$

$$\phi_j[m]=\frac{W(f_1,\ldots,f_m,\phi_j)}{W(f_1,\ldots,f_m)}, \quad j=1,\ldots,N, \tag{5.22c}$$

and $u[m],\psi[m],\phi_1[m],\ldots,\phi_N[m]$ *satisfy (5.18), (5.19), and (5.20).*

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Conformally flat anisotropic spheres in general relativity

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The condition for the vanishing of the Weyl tensor is integrated in the spherically symmetric case. Then, the resulting expression is used to find new, conformally flat, interior solutions to Einstein equations for locally anisotropic fluids. The slow evolution of these models is contrasted with the evolution of models with similar energy density or radial pressure distribution but nonvanishing Weyl tensor, thereby bringing out the different role played by the Weyl tensor, the local anisotropy of pressure, and the inhomogeneity of the energy density in the collapse of relativistic spheres. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In the study of self-gravitating systems there are three factors whose relevance has been recurrently and separately stressed in the literature. These are, the Weyl tensor, the local anisotropy of pressure, and the inhomogeneity of energy density distribution (density contrast).

The Weyl tensor[1] or some functions of it,[2] have been proposed to provide a gravitational arrow of time. The rationale behind this idea being that tidal forces tend to make the gravitating fluid more inhomogeneous as the evolution proceeds, thereby indicating the sense of time. However, some works have thrown doubts on this proposal.[3] Also, as it will be seen below, it is worth noticing that the relation between the Weyl tensor and the density contrast is affected by the presence of local anisotropy of pressure.

The role of density inhomogeneities in the collapse of dust[4] and in particular in the formation of naked singularities,[5] has been extensively discussed in the literature.

Finally, the assumption of local anisotropy of pressure, has proved to be very useful in the study of relativistic compact objects (see Ref. 6, and references therein).

A hint pointing to the relevance of the above mentioned three factors in the fate of spherical collapse is also provided by the expression of the active gravitational mass in terms of those factors.[7,8]

These three factors are usually considered separately, their relationship being omitted from discussion, even though they are related by a simple expression, which we shall present below.[7,8]

The purpose of this work is twofold. On the one hand we shall integrate the vanishing Weyl tensor condition, which will allow us to construct conformally flat models (with anisotropic pressure). The obtained solutions represent static or slowly evolving (in the quasistatic approximation) spheres, which could serve for the modeling of compact self-gravitating objects. On the other hand, we want to study, comparatively, the effects of the above mentioned parameters on the (slow) evolution of relativistic spheres. For doing this we shall contrast the evolution of the conformally flat models with the evolution of models with the same energy density or radial

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pressure distribution, but nonvanishing Weyl tensor. With this purpose it will be useful to calculate the active gravitational mass and the fluid velocity for each model.

The paper is organized as follows: In the next section all relevant equations and conventions are given. The condition for the vanishing of the Weyl tensor is integrated in Sec. III and the models are described in Sec. IV. Finally a discussion of results is presented in the last section.

II. RELEVANT EQUATIONS AND CONVENTIONS

A. The field equations

We consider a spherically symmetric distribution of collapsing fluid, which we assume to be locally anisotropic and bounded by a spherical surface Σ. The line element is given in Schwarzschild-type coordinates by

$$ds^2=e^{\nu}dt^2-e^{\lambda}dr^2-r^2(d\theta^2+\sin^2\theta d\phi^2), \tag{1}$$

where ν and λ are functions of t and r. The coordinates are $x^0=t$; $x^1=r$; $x^2=\theta$; $x^3=\phi$.

The metric (1) has to satisfy Einstein field equations

$$G^{\mu}_{\nu}=-8\pi T^{\mu}_{\nu}, \tag{2}$$

which in our case read[9]

$$-8\pi T^0_0=-\frac{1}{r^2}+e^{-\lambda}\left(\frac{1}{r^2}-\frac{\lambda'}{r}\right), \tag{3}$$

$$-8\pi T^1_1=-\frac{1}{r^2}+e^{-\lambda}\left(\frac{1}{r^2}+\frac{\nu'}{r}\right), \tag{4}$$

$$-8\pi T^2_2=-8\pi T^3_3=-\frac{e^{-\nu}}{4}(2\ddot{\lambda}+\dot{\lambda}(\dot{\lambda}-\dot{\nu}))+\frac{e^{-\lambda}}{4}\left(2\nu''+\nu'^2-\lambda'\nu'+2\frac{\nu'-\lambda'}{r}\right), \tag{5}$$

$$-8\pi T_{01}=-\frac{\dot{\lambda}}{r}, \tag{6}$$

where dots and primes stand for partial differentiation with respect to t and r, respectively.

In order to give physical significance to the T^{μ}_{ν} components we apply the Bondi approach,[9] i.e., we introduce local Minkowski coordinates (τ,x,y,z), defined by

$$d\tau=e^{\nu/2}dt, \quad dx=e^{\lambda/2}dr, \quad dy=rd\theta, \quad dz=r\sin\theta d\phi.$$

Then, denoting the Minkowski components of the energy tensor by a bar, we have

$$\overline{T^0_0}=T^0_0, \quad \overline{T^1_1}=T^1_1, \quad \overline{T^2_2}=T^2_2, \quad \overline{T^3_3}=T^3_3, \quad \overline{T_{01}}=e^{-(\nu+\lambda)/2}T_{01}.$$

Next we suppose that, when viewed by an observer moving relative to these coordinates with velocity ω in the radial direction, the physical content of space consists of an anisotropic fluid of energy density ρ, radial pressure P_r, and tangential pressure $P_{\perp}$. Thus, when viewed by this moving observer, the covariant energy-momentum tensor in Minkowski coordinates is

$$\begin{pmatrix} \rho & 0 & 0 & 0 \\ 0 & P_r & 0 & 0 \\ 0 & 0 & P_{\perp} & 0 \\ 0 & 0 & 0 & P_{\perp} \end{pmatrix}.$$

Then a Lorentz transformation readily shows that

$$T_0^0=\overline{T}_0^0=\frac{\rho+P_r\omega^2}{1-\omega^2}, \tag{7}$$

$$T_1^1=\overline{T}_1^1=-\frac{P_r+\rho\omega^2}{1-\omega^2}, \tag{8}$$

$$T_2^2=T_3^3=\overline{T}_2^2=\overline{T}_3^3=-P_\perp, \tag{9}$$

$$T_{01}=e^{(\nu+\lambda)/2}\overline{T}_{01}=-\frac{(\rho+P_r)\omega e^{(\nu+\lambda)/2}}{1-\omega^2}. \tag{10}$$

Note that the velocity in the (t,r,θ,ϕ) system, dr/dt, is related to ω by

$$\omega=\frac{dr}{dt}e^{(\lambda-\nu)/2}. \tag{11}$$

Outside of the fluid, the spacetime is Schwarzschild,

$$ds^2=\left(1-\frac{2M}{r}\right)dt^2-\left(1-\frac{2M}{r}\right)^{-1}dr^2-r^2(d\theta^2+\sin^2\theta d\phi^2). \tag{12}$$

In order to match the two metrics smoothly on the boundary surface $r=r_\Sigma(t)$, we require continuity of the first and second fundamental forms across that surface. As a result of this matching we obtain the well known result

$$[P_r]_\Sigma=0. \tag{13}$$

Next, the radial component of the conservation law,

$$T^\mu_{\nu;\mu}=0 \tag{14}$$

gives

$$(-8\pi T_1^1)'=\frac{16\pi}{r}(T_1^1-T_2^2)+4\pi\nu'(T_1^1-T_0^0)+\frac{e^{-\nu}}{r}\left(\ddot{\lambda}+\frac{\dot{\lambda}^2}{2}-\frac{\dot{\lambda}\dot{\nu}}{2}\right), \tag{15}$$

which in the static case becomes

$$P_r'=-\frac{\nu'}{2}(\rho+P_r)+\frac{2(P_\perp-P_r)}{r}, \tag{16}$$

representing the generalization of the Tolman–Oppenheimer–Volkof equation for anisotropic fluids.[6]

In this work we shall consider exclusively static or slowly evolving (quasistatic) systems. By this we mean that our sphere either does not change or changes slowly on a time scale that is very long compared to the typical time in which the sphere reacts to a slight perturbation of hydrostatic equilibrium (this typical time scale is called hydrostatic time scale). Thus our system is always very close to or in hydrostatic equilibrium and its evolution may be regarded as a sequence of static models linked by (6). This assumption is very sensible because the hydrostatic time scale is very small for almost any phase of the life of the star. It is of the order of 27 min for the Sun, 4.5 s for a white dwarf, and 10^{-4} s for a neutron star of one solar mass, and 10 km radius. It is well

known that any of the stellar configurations mentioned above, change on a time scale that is very long compared to their respective hydrostatic time scales. Let us now translate this assumption in conditions to ω and metric functions.

First of all, slow contraction means that the radial velocity ω as measured by the Minkowski observer is always much smaller than the velocity of light ($\omega \ll 1$). Therefore we shall neglect terms of the order $O(\omega^2)$.

Then (15) yields

$$\ddot{\lambda} + \frac{\dot{\lambda}^2}{2} - \frac{\dot{\nu}\dot{\lambda}}{2} = 8\pi r e^{\nu}\left[P_r' + (\rho + P_r)\frac{\nu'}{2} - 2\frac{P_\perp - P_r}{r}\right]. \tag{17}$$

Since, by assumption, our system is always (not only at a given time t) in equilibrium (or very close to), (16) and (17) imply then, for an arbitrary slowly evolving configuration,

$$\ddot{\lambda} \approx \dot{\nu}\dot{\lambda} \approx \dot{\lambda}^2 \approx 0, \tag{18}$$

and of course, time derivatives of any order of the left-hand side of the hydrostatic equilibrium equation must also vanish, for otherwise the system will deviate from equilibrium. This condition implies, in particular, that we must demand

$$\ddot{\nu} \approx 0.$$

Finally, from the time derivative of (6), and using (10), it follows that

$$\dot{\omega} \approx O(\ddot{\lambda}, \dot{\lambda}\omega, \dot{\nu}\omega), \tag{19}$$

which implies that we shall also neglect terms linear in the acceleration. On purely physical considerations, it is obvious that the vanishing of $\dot{\omega}$ is required to keep the system always in equilibrium.

Thus, from now on, we shall always assume

$$O(\omega^2) = \dot{\lambda}^2 = \dot{\nu}^2 = \dot{\lambda}\dot{\nu} = \ddot{\lambda} = \ddot{\nu} = 0, \tag{20}$$

implying that the system remains in (or very close to) equilibrium.

B. The Weyl tensor

We can now calculate the components of the Weyl tensor. Neglecting terms of order $\dot{\lambda}\dot{\nu}, \dot{\lambda}^2, \dot{\nu}^2, \ddot{\lambda}$, and $\ddot{\nu}$, we find that all nonvanishing components can be expressed through C^3_{232}. Thus,

$$W \equiv \frac{r}{2}C^3_{232} = \frac{r^3 e^{-\lambda}}{6}\left(\frac{e^{\lambda}}{r^2} + \frac{\nu'\lambda'}{4} - \frac{1}{r^2} - \frac{\nu'^2}{4} - \frac{\nu''}{2} - \frac{\lambda' - \nu'}{2r}\right). \tag{21}$$

Next, defining the mass function as usual

$$m(r,t) = 4\pi \int_0^r T^0_0 r^2 dr, \tag{22}$$

the following relations may be established:[7,8]

$$W = -\frac{4}{3}\pi \int_0^r r^3 (T^0_0)' dr + \frac{4}{3}\pi r^3 (T^2_2 - T^1_1), \tag{23}$$

$$m(r,t)=\frac{4}{3}\pi r^3 T_0^0-\frac{4}{3}\pi\int_0^r r^3(T_0^0)'dr. \tag{24}$$

Both, (23) and (24) are valid in the general (dynamic) case. However only in the static or the quasistatic case T_0^0 and T_1^1 denote the proper energy density and the radial pressure, respectively.

C. The Tolman–Whittaker mass

The Tolman–Whittaker mass[10] within a sphere of radius r inside Σ, is defined as[8]

$$m_{\mathrm{TW}}(r,t)=4\pi\int_0^r r^2 e^{(\nu+\lambda)/2}(T_0^0-T_1^1-2T_2^2)dr. \tag{25}$$

Two alternative expressions, easily obtained from the field equations (see Ref. 8 for details) are

$$m_{\mathrm{TW}}=e^{(\nu+\lambda)/2}(m+4\pi P_r r^3) \tag{26}$$

and

$$m_{\mathrm{TW}}=\tfrac{1}{2}e^{(\nu-\lambda)/2}\nu' r^2. \tag{27}$$

The interpretation of m_{TW} as the active gravitational mass follows at once from (27) and (16). Indeed, the first term on the right-hand side of (16) (the ''gravitational force'' term) is the product of the passive gravitational mass density $(\rho+P_r)$ and a term proportional to m_{TW}/r^2. A similar conclusion can be obtained if we recall that the gravitational acceleration of a test particle, instantaneously at rest in a static gravitational field, as measured with standard rods and coordinate clocks is given by[11]

$$a=-\frac{e^{(\nu-\lambda)/2}\nu'}{2}=-\frac{m_{\mathrm{TW}}}{r^2}. \tag{28}$$

D. The velocity of a fluid element

For the comparative study of the (slow) evolution of different solutions, it will be useful to plot the velocity (ω) profiles for different pieces of material. A simple expression for ω, may be obtained as follows: from (3) and (22), it results

$$e^{-\lambda}=1-\frac{2m}{r}, \tag{29}$$

and from (29),

$$\dot{m}=\frac{\dot{\lambda}re^{-\lambda}}{2}, \tag{30}$$

then using (6),

$$\omega=-\frac{\dot{m}e^{(\lambda-\nu)/2}}{4\pi r^2(\rho+P_r)}. \tag{31}$$

III. THE VANISHING WEYL CONDITION

We shall now proceed to integrate the condition,

$$W=0, \tag{32}$$

which, using (21), may be written as

$$\left(\frac{e^{-\lambda}\nu'}{2r}\right)'+e^{-(\nu+\lambda)}\left(\frac{e^{\nu}\nu'}{2r}\right)'-\left(\frac{e^{-\lambda}-1}{r^2}\right)'=0. \tag{33}$$

Introducing new variables,

$$y=e^{-\lambda}; \quad \frac{\nu'}{2}=\frac{u'}{u}, \tag{34}$$

Eq. (33) is cast into

$$y'+\frac{2y[u''-u'/r+u/r^2]}{[u'-u/r]}-\frac{2u}{r^2[u'-u/r]}=0, \tag{35}$$

whose formal solution is

$$y=e^{-\int k(r)dr}\left[\int e^{\int k(r)dr}f(r)dr+C_1\right], \tag{36}$$

where C_1 is a constant of integration, and

$$k(r)=2\frac{d}{dr}\left[\ln\left(u'-\frac{u}{r}\right)\right], \tag{37}$$

$$f(r)=\frac{2u}{r^2(u'-u/r)}, \tag{38}$$

changing back to the original variables, Eq. (36) becomes

$$\frac{\nu'}{2}-\frac{1}{r}=\frac{e^{\lambda/2}}{r}\sqrt{1-c^2r^2e^{-\nu}} \tag{39}$$

with $c^2\equiv -C_1$.

Next, (39) may be formally integrated, to obtain

$$e^{\nu}=c^2r^2\cosh^2\left[\int\frac{e^{\lambda/2}}{r}dr+\tilde{C}\right], \tag{40}$$

where $\tilde{C}$ is a constant of integration (a function of t, in the slowly evolving case). The reader may check that (40) satisfies (39) and (32) [or (33)].

In the next section we shall present some models satisfying (39) [or (40)].

IV. THE MODELS

A simple counting of Eqs. (3)–(6) and unknowns $(\nu,\lambda,\rho,P_r,P_\perp,\omega)$ indicates that we have to provide two additional relations (in the form of equations of state and/or restrictions on metric variables), in order to integrate the system (3)–(6).

If one assumes that the fluid is locally isotropic ($P_r=P_\perp$) then, demanding $W=0$, we are driven to a unique solution (the Schwarzschild interior solution), a fact also obvious from (23). However, if $P_r\neq P_\perp$, then the condition $W=0$, does not single out a unique model.

In what follows we shall construct two models with $W=0$. One of them characterized by $P_r=0$, and for the other we prescribe a given energy density distribution which is similar to the one proposed by Gokhroo and Mehra.[12] Additionally, we present two other models with $W\neq 0$. One is characterized by $P_r=0$ and $\rho=\rho(t)$, (Refs. 8, 13) and the other has the same energy density distribution as one of the conformally flat solutions.

A. Model I

Our first model is characterized by

$$W=0 \tag{41}$$

and

$$P_r=0. \tag{42}$$

Then, from (4) and (39), it follows

$$e^{-\nu}=\frac{g}{c^2r^2}\frac{(4-9g)}{(1-2g)} \tag{43}$$

with

$$g\equiv\frac{m(r,t)}{r}, \tag{44}$$

and where (29) has been used.

Next, taking r-derivative of (43), and using

$$\nu'=\frac{2m}{r^2(1-2m/r)}\equiv\frac{2g}{r(1-2g)}, \tag{45}$$

easily derived from (4), we obtain

$$g'=\frac{54g^3-42g^2+8g}{r(18g^2-18g+4)}, \tag{46}$$

which after integration yields

$$Dr=\frac{g^{1/2}}{(4-9g)^{1/6}}, \tag{47}$$

where D is a constant (a function of t in the slowly evolving case) of integration. Solving (47) for g, one obtains

$$g=a^{1/3}\{[2+(27a+4)^{1/2}]^{1/3}+[2-(27a+4)^{1/2}]^{1/3}\} \tag{48}$$

with

$$(Dr)^6=a\equiv\left(\frac{r}{r_\Sigma}\right)^6\frac{g_\Sigma^3}{4-9g_\Sigma}, \tag{49}$$

where subscript Σ indicates that the quantity is evaluated at the boundary surface $r=r_\Sigma$.

The remaining variables are now easily obtained from the field equations and (43), (48). Thus,

$$\rho=\frac{3g}{2\pi r^2}\frac{(1-2g)}{(2-3g)}, \tag{50}$$

$$P_\perp=\frac{3g^2}{4\pi r^2}\frac{1}{(2-3g)}, \tag{51}$$

$$e^{-\lambda}=1-2g. \tag{52}$$

For the Tolman–Whittaker mass we obtain, using either (26) or (27),

$$m_{\mathrm{TW}}=g\left(\frac{r}{r_\Sigma}\right)r\left[\frac{g_\Sigma\left(1-\frac{9}{4}g_\Sigma\right)}{g\left(1-\frac{9}{4}g\right)}\right]^{1/2}, \tag{53}$$

or, using the dimensionless varibles,

$$x\equiv\frac{r}{r_\Sigma};\quad n=\frac{m_\Sigma}{r_\Sigma}\equiv\frac{M}{r_\Sigma}=g_\Sigma, \tag{54}$$

$$m_{\mathrm{TW}}=\frac{Mx^3(Z_1+Z_2)^{1/2}(4-9n)^{1/2}}{[4(4-9n)^{1/2}-9nx^2(Z_1+Z_2)]^{1/2}}, \tag{55}$$

with

$$Z_{1,2}=[2(4-9n)^{1/2}\pm(27x^6n^3+16-36n)^{1/2}]^{1/3}. \tag{56}$$

It is worth noticing that from the requirement $\rho\geqslant 0$, it follows, using (50),

$$g<\tfrac{1}{2}, \tag{57}$$

a stronger restriction appears from the condition

$$\rho\geqslant P_\perp \tag{58}$$

which requires

$$g<\tfrac{2}{5}. \tag{59}$$

Finally, the velocity ω of any fluid element is given by

$$\omega=\frac{\omega_\Sigma n^{1/2}x^2(2-3g)(4-9g)^{1/2}(1-2n)}{g^{1/2}(4-9n)^2(1-2g)^2}\times\left\{2(Z_1+Z_2)+\frac{3nx^2(Z_2^2-Z_1^2)}{(27x^6n^3+16-36n)^{1/2}}\right\}, \tag{60}$$

where (11), (31), (48)–(50), (54), and (56) have been used.

B. Model II

The second model we shall consider, is well known. It is characterized by

$$P_r=0, \tag{61}$$

$$\rho=\rho(t), \tag{62}$$

and is not conformally flat.

A static version of this model was studied by Florides.[13] Models with vanishing radial pressure have been discussed in the past,[14] and more recently in relation with the formation of naked singularities.[15]

The corresponding variables are (see Ref. 8 for details),

$$\rho=\rho(t); \quad P_r=0, \tag{63}$$

$$P_\perp=\frac{2\pi r^2\rho^2}{3\left(1-\frac{8\pi}{3}r^2\rho\right)}, \tag{64}$$

$$e^{\nu}=\frac{\left(1-\frac{8\pi}{3}r_\Sigma^2\rho\right)^{3/2}}{\left(1-\frac{8\pi}{3}r^2\rho\right)^{1/2}}, \tag{65}$$

$$e^{-\lambda}=1-\frac{8\pi}{3}r^2\rho, \tag{66}$$

$$W=-\frac{8\pi^2r^5\rho^2}{9\left(1-\frac{8\pi}{3}r^2\rho\right)}, \tag{67}$$

$$m_{\mathrm{TW}}=\frac{4\pi}{3}r^3\rho\left(\frac{1-\frac{8\pi}{3}r_\Sigma^2\rho}{1-\frac{8\pi}{3}r^2\rho}\right)^{3/4}, \tag{68}$$

$$\omega=\omega_\Sigma\left(\frac{r}{r_\Sigma}\right)\left(\frac{1-\frac{8\pi}{3}r_\Sigma^2\rho}{1-\frac{8\pi}{3}r^2\rho}\right)^{1/4}. \tag{69}$$

C. Model III

This model is conformally flat and is further characterized by

$$e^{-\lambda}=\left(1-\frac{r^2}{b^2}\right)^2, \tag{70}$$

where b is a constant (a function of t in the slowly evolving case).

Then, from (40) one obtains

$$e^{\nu}=\frac{c^2}{4B^2}\,\frac{[B^2r^2+b^2-r^2]^2}{(b^2-r^2)} \tag{71}$$

with

$$\tilde{C}=\ln B. \tag{72}$$

From the field equations, (70) and (71), we can now obtain the expressions for ρ, P_r, and $P_\perp$,

$$\rho=\frac{3}{4\pi b^2}\left(1-\frac{5r^2}{6b^2}\right), \tag{73}$$

$$8\pi P_r=-\frac{1}{r^2}+\frac{(b^2-r^2)^2}{b^4}\left[\frac{1}{r^2}+\frac{4B^2b^2-2[B^2r^2+b^2-r^2]}{(b^2-r^2)[B^2r^2+b^2-r^2]}\right], \tag{74}$$

$$8\pi(P_r-P_\perp)=-\frac{2r^2}{b^4}. \tag{75}$$

b, c, and B are related to the total mass and the radius of the sphere through the boundary conditions

$$e^{-\lambda_\Sigma}=1-\frac{2M}{r_\Sigma}, \tag{76}$$

$$e^{\nu_\Sigma}=1-\frac{2M}{r_\Sigma}, \tag{77}$$

$$P_{r_\Sigma}=0, \tag{78}$$

the corresponding expressions are

$$b=\frac{r_\Sigma}{\left[1-\left(1-\frac{2M}{r_\Sigma}\right)^{1/2}\right]^{1/2}}, \tag{79}$$

$$c=\frac{1}{r_\Sigma}\left[\frac{4M}{r_\Sigma}-\frac{9M^2}{r_\Sigma^2}\right]^{1/2}, \tag{80}$$

$$B=\frac{(1-2M/r_\Sigma)^{1/4}[(1-2M/r_\Sigma)^{1/2}+(3M/r_\Sigma-1)]}{[1-(1-2M/r_\Sigma)^{1/2}]^{1/2}[4M/r_\Sigma-9M^2/r_\Sigma^2]^{1/2}}. \tag{81}$$

For the Tolman–Whittaker mass the obtained expression is

$$m_{\mathrm{TW}}=\frac{cr^3}{2Bb^2(b^2-r^2)^{1/2}}[2B^2b^2-B^2r^2-b^2+r^2], \tag{82}$$

or, using (79)–(81) and (54),

$$m_{\mathrm{TW}}=\frac{Mx^3(1-2n)^{1/4}}{[1-x^2+x^2(1-2n)^{1/2}]^{1/2}}\left\{3-2x^2-\frac{(1-x^2)}{n}[1-(1-2n)^{1/2}]\right.$$
$$\left.\times\left[1+\frac{4n-9n^2}{2(1-2n)^{1/2}[(1-2n)^{1/2}+3n-1]}\right]\right\}, \tag{83}$$

and the expression for ω in this model, results in

$$\omega=\frac{4\dot{b}Bx[1-(1-2n)^{1/2}]}{(4n-9n^2)^{1/2}(1-x^2[1-(1-2n)^{1/2}])^{1/2}}$$
$$\times\frac{1}{[2B^2+B^2x^2[1-(1-2n)^{1/2}]+1-x^2[1-(1-2n)^{1/2}]]}, \tag{84}$$

where $\dot{b}$ is easily obtained from (79),

$$\dot{b}=\frac{\omega_\Sigma n(1-2n)^{1/2}\left(5-\frac{2}{n}[1-(1-2n)^{1/2}]\right)}{2[1-(1-2n)^{1/2}]^{3/2}}. \tag{85}$$

D. Model IV

This model has the same energy density distribution as the previous one (same λ), but is not conformally flat ($W\neq 0$). Instead, the model is further characterized by

$$P_r=0. \tag{86}$$

Then, from (70), (86) and field equations, we obtain

$$\rho=\frac{3}{4\pi b^2}\left(1-\frac{5r^2}{6b^2}\right), \tag{87}$$

$$e^{\nu}=\frac{\beta}{(b^2-r^2)^{1/2}}e^{b^2/2(b^2-r^2)}, \tag{88}$$

$$P_\perp=\frac{(2b^2r^2-r^4)(6b^2-5r^2)}{32\pi b^4(b^2-r^2)^2}, \tag{89}$$

with

$$\beta\equiv b\left(1-\frac{2M}{r_\Sigma}\right)^{5/4}e^{-[1/2(1-2M/r_\Sigma)^{1/2}]}, \tag{90}$$

and b is given by (79).

For the active gravitational mass, we obtain, after some lengthy calculations,

$$m_{\mathrm{TW}}=M(1-2n)^{5/8}x^3(1-(1-2n)^{1/2})\frac{\left[1-\frac{x^2}{2}(1-(1-2n)^{1/2})\right]}{n(1-x^2[1-(1-2n)^{1/2}])^{5/4}}$$
$$\times\exp\frac{1}{4}\left[\frac{(x^2-1)(1-(1-2n)^{1/2})}{(1-2n)^{1/2}[1-x^2(1-(1-2n)^{1/2})]}\right], \tag{91}$$

where n and x are defined by Eq. (54). Observe that condition $\rho\geqslant 0$ is satisfied for all n, however if we demand $\rho\geqslant P_\perp$, then

$$n\leqslant 0.4. \tag{92}$$

Finally, the expression for the velocity takes the form

$$\omega=\frac{2\omega_\Sigma x[1-x^2+x^2(1-2n)^{1/2}]^{1/4}[5n-2+2(1-2n)^{1/2}]}{(1-2n)^{1/8}[6-5x^2+5x^2(1-2n)^{1/2}][1-(1-2n)^{1/2}]}$$
$$\times\exp\tfrac{1}{4}\left[\frac{(1-x^2)[1-(1-2n)^{1/2}]}{(1-2n)^{1/2}[1-x^2+x^2(1-2n)^{1/2}]}\right]. \tag{93}$$

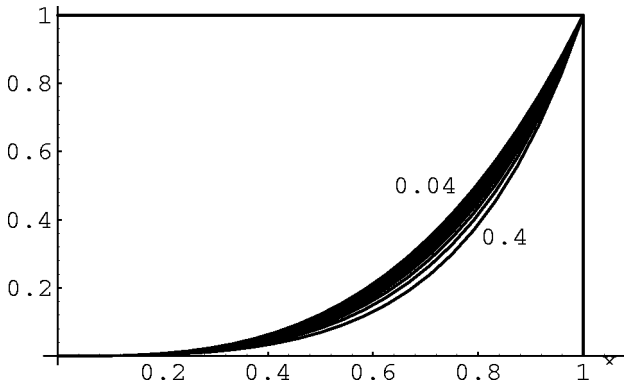

FIG. 1. m_{TW}/M as function of x for the model I, and ten values of n, from 0.04 to 0.4.

V. DISCUSSION

We have integrated the vanishing Weyl condition. The resulting expression (39) [and (40)] allows us to find conformally flat models in a very simple way, once an additional condition on physical or metric variables is imposed. Specifically we have found two conformally flat models (I, III). In order to bring out the role of Weyl tensor in its slow evolution, we have also presented two other models (II, IV) with the nonvanishing Weyl tensor. Model II, as model I has vanishing radial pressure, whereas model IV has the same energy density distribution as model III. This will allow us to see the effect of the three abovementioned factors (local anisotropy, Weyl tensor, density contrast) on the Tolman–Whittaker mass distribution within the sphere, and on the velocity profile of different pieces of matter. With this purpose, all models are considered with the same total mass M and surface velocity ω_{Σ}.

Figure 1 exhibits the evolution of m_{TW}/M as function of x, in the process of slow contraction (increasing n), for model I. For all other models the behavior is qualitatively the same, i.e., as the contraction proceeds, the active gravitational mass within the sphere decreases. However, the absolute value of m_{TW} is different for different models (for same n and x) as can be seen from Figs. 2–4, which display the ratio $m_{\mathrm{TW}}/m_{\mathrm{TW}}(\mathrm{II})$ for the three models (I, III, IV).

As it can be seen, for any $r<r_{\Sigma}$ (for the same total mass M), we have

$$m_{\mathrm{TW}}(\mathrm{III})>m_{\mathrm{TW}}(\mathrm{I})>m_{\mathrm{TW}}(\mathrm{IV})>m_{\mathrm{TW}}(\mathrm{II}),$$

the differences being larger for more compact (larger n) configurations. Parenthetically, the two conformally flat models present the largest TW masses.

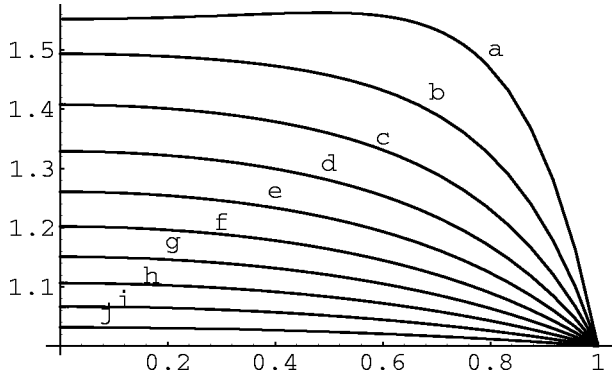

FIG. 2. $m_{\mathrm{TW}}(\mathrm{I})/m_{\mathrm{TW}}(\mathrm{II})$ as function of x, curves a–j correspond to $n=0.4$, 0.36, 0.32, 0.28, 0.24, 0.20, 0.16, 0.12, 0.08, 0.04.

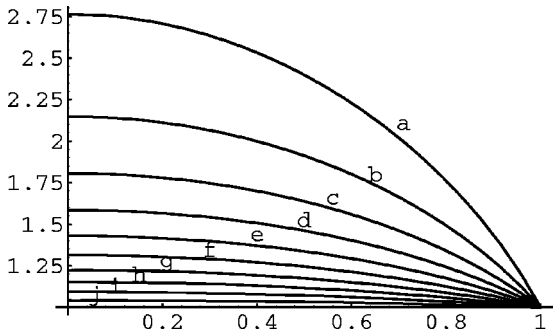

FIG. 3. $m_{TW}(III)/m_{TW}(II)$ as a function of x, for the same values of n as in Fig. 2.

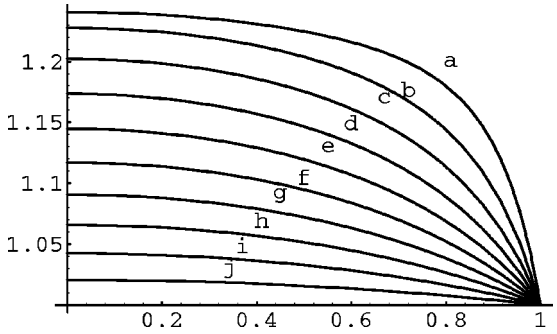

FIG. 4. $m_{TW}(IV)/m_{TW}(II)$ as function of x, for the same values of n as in Fig. 2.

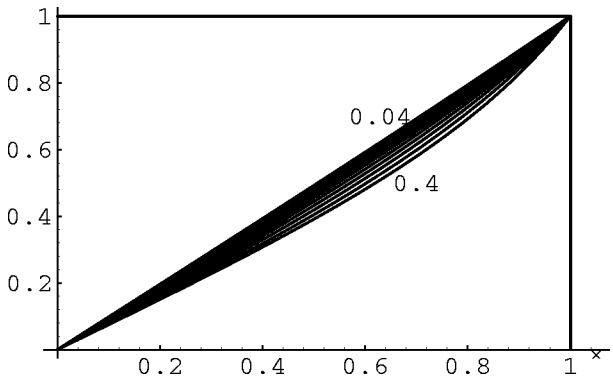

FIG. 5. ω/ω_Σ as function of x for model III, and ten values of n, from 0.04 to 0.4.

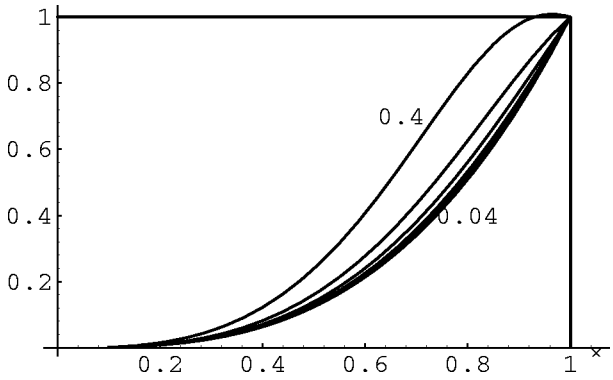

FIG. 6. Same as Fig. 5 for model I.

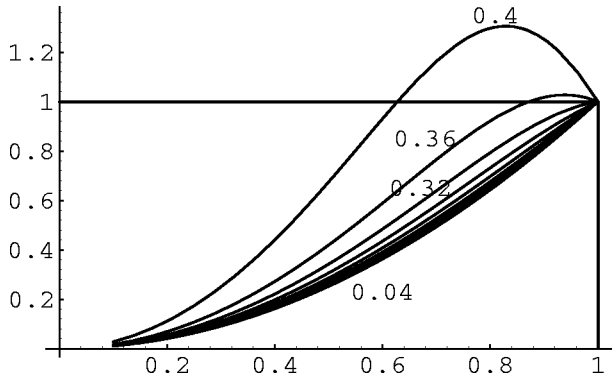

FIG. 7. The ratio $\omega(\mathrm{I})/\omega(\mathrm{II})$ as function of x, for ten values of n from 0.04 to 0.4.

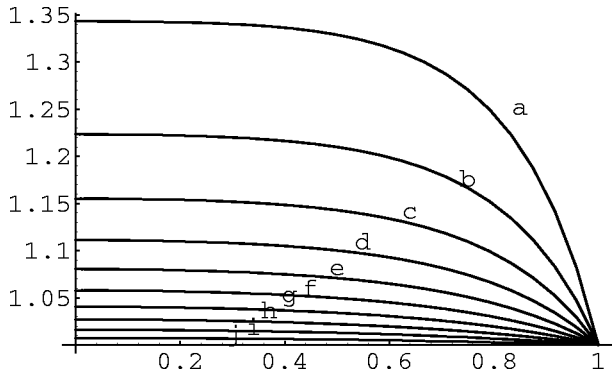

FIG. 8. The ratio $\omega(\mathrm{IV})/\omega(\mathrm{II})$ as function of x, curves a–j correspond to $n=0.4$, 0.36, 0.32, 0.28, 0.24, 0.20, 0.16, 0.12, 0.08, 0.04.

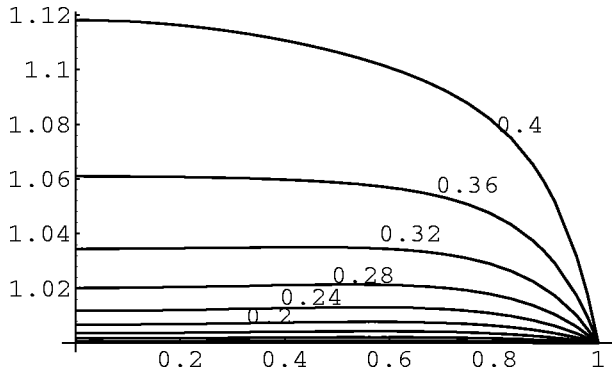

FIG. 9. The ratio $\omega(\mathrm{III})/\omega(\mathrm{II})$ as function of x, for ten values of n from 0.04 to 0.4.

For models II, III, and IV the collapse proceeds in a quasihomologous (quasilinear) regime as indicated in Fig. 5 for model III (for models II and IV the figures are similar), deviating from that regime as n increases.

However for model I, the contraction is not homologous even for small n as indicated in Fig. 6.

Figures 7–9 display the ratio $\omega/\omega(\mathrm{II})$ for the three models (I, III, IV).

Except for extremely high fields in model I, we see that

$$\omega(\mathrm{IV})>\omega(\mathrm{III})>\omega(\mathrm{II})>\omega(\mathrm{I}),$$

which indicate that for the same energy density distribution (III, IV) or radial pressure distribution (I, II), the slow contraction of interior shells proceeds slower in the conformally flat case.

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Closed constraint algebras and path integrals for loop group actions

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In this paper we study systems with a closed algebra of second class constraints. We describe a construction of the reduced theory that resembles the conventional treatment of first class constraints. It suggests, in particular, to compute the symplectic form on the reduced space by a fiber integral of the symplectic form on the original space. This approach is then applied to a class of systems with loop group symmetry. The chiral anomaly of the loop group action spoils the first class character of the constraints but not their closure. Proceeding along the general lines described above, we obtain a 2-form from a fiber (path) integral. This form is not closed as a relict of the anomaly. Examples of such reduced spaces are provided by *D*-branes on group manifolds with WZW action. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1330730]

I. INTRODUCTION

According to Dirac's classification, constraints in Hamiltonian mechanics split into first-class and second-class. The theory of the first-class constraints is well developed because it is a major tool in gauge theories. Second-class constraints naturally arise in gauge theories with anomalies: quantum corrections may cause first-class constraints of the classical system to become second-class.[1,2]

We reconsider Dirac's approach to second-class constraints and provide a new realization of the reduced phase space which is more in line with the reduction procedure for the first-class constraints (see also Ref. 1). In this framework the Liouville form (the exponential of the symplectic form) on the reduced phase space can be obtained by fiber integration from the Liouville form on the original phase space of the system. The procedure can suffer from possible global difficulties similar to the Gribov problems one often encounters in the context of ordinary (anomaly-free) gauge theories.

Our main interest is to apply this formalism to loop group actions on symplectic manifolds. If the Poisson bracket of the symmetry generators contains a Schwinger term (for instance, this is the case in the WZW model), the constraints become second-class. Such a situation was considered in the mathematical literature.[3,4] We use a fiber integration procedure to derive the Liouville form on the reduced phase space. As a new manifestation of the anomaly it turns out that this form is not closed (see also Ref. 4)!

''Anomalous'' reduced spaces of this type naturally arise in the theory of D-branes on group manifolds.[5] It is an interesting problem to develop a consistent quantization theory for such

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spaces. Because of the connection between deformation quantization and open strings (see, e.g., Refs. 6–8) one expects valuable insights from open string theory. For the case of D-branes on group manifolds this was analyzed in Ref. 9.

II. DIRAC BRACKETS FROM FIBER INTEGRATION

Our aim in the present section is to reformulate the symplectic reduction for a system of constraints which form a closed algebra. To begin with we shall briefly recall the standard theory of reduction. This is used as a starting point for presenting an alternative formulation, applicable to closed constraint algebras under certain additional conditions. For the case of a purely second-class constraint system the approach suggests we construct the symplectic two-form and its associated Liouville form through a fiber integral. The material within this section serves as a toy model for the discussion of infinite dimensional phase spaces with an anomalous loop group action in Secs. 3 and 4.

Let us denote the original, unconstrained phase space by N and let x^i, $i=1,\ldots,2n$, be local coordinates. Their Poisson bracket is denoted by $P^{ij}=\{x^i,x^j\}$ and its associated symplectic form by

$$\Omega=\tfrac{1}{2}\Omega_{ij}dx^i\,dx^j.$$

$\Phi^\alpha=\Phi^\alpha(x)$, $\alpha=1,\ldots,2m$, are constraints in this phase space. According to our assumptions they form a closed algebra, i.e.,

$$\{\Phi_\alpha,\Phi_\beta\}=\Pi_{\alpha\beta}(\Phi), \tag{1}$$

with a matrix Π that is a function of the constraints Φ_α only. For simplicity we also assume that the constraints are independent from one another (*irreducible* constraints) and that they are all *regular* so that they may be used as local coordinates in phase space, at least in a neighborhood of the constraint surface $\Phi(x)=0$. Details and further results used in the text below can be found, e.g., in Ref. 10.

The standard procedure of symplectic reduction proceeds as follows: First the symplectic form Ω is pulled back to the constraint surface, which we denote by N_0. The resulting two-form Ω_0 on N_0 is degenerate in general. Its kernel is surface-forming, however, and the quotient of N_0 with respect to the orbits (''gauge orbits'') is the reduced phase space M. By construction, the induced two-form ω on M is nondegenerate.

In the case of mere second-class constraints, i.e., $\det\Pi\neq 0$ on N_0 in our context, the last step does not arise, since Ω_0 is nondegenerate already. The Poisson bracket associated with Ω_0 may be obtained directly from the Poisson bracket on N by the following prescription:

$$\{f,g\}_D:=\{f,g\}-\{f,\Phi^\alpha\}(\Pi^{-1})_{\alpha\beta}\{\Phi^\beta,g\},$$

which is defined at least in some neighborhood of the constraint surface $N_0\subset N$. As a bivector-field this bracket, known as the Dirac bracket, is *tangential* to the constraint surface $\Phi(x)=0$ (in contrast to the original Poisson bracket). Hence, it has a push-forward to N_0, and this coincides with the inverse of Ω_0.

Due to the closedness of our constraint algebra (1), the Hamiltonian vector fields,

$$v^\alpha:=\{\Phi^\alpha,\cdot\}\equiv P^{ij}\frac{\partial\Phi^\alpha}{\partial x_i}\frac{\partial}{\partial x_j},$$

are surface-forming everywhere in N. In fact, one can easily show that

$$[v^\alpha,v^\beta]=\frac{\partial\Pi^{\alpha\beta}}{\partial\Phi^\gamma}v^\gamma.$$

Thus the v^α's generate orbits in *all* of N and this is true even if the set (Φ^α) contains second-class constraints.

The last observation opens new possibilities for performing the symplectic reduction, viewing the reduced phase space M as an appropriate orbit space. The difference to the standard Dirac procedure outlined above lies primarily in the treatment of the second-class constraints, which are dealt with very analogously to first-class constraints in their standard reduction. Consequently, our main focus in the remainder of this section will be on second-class constraints. We will briefly comment on the extension to more general cases with the simultaneous presence of first- and second-class constraints towards the end of the section.

For the case of pure second-class constraints, the matrix (1) is nondegenerate on the constraint surface, i.e., at $\Phi=0$. In what follows we will strengthen this requirement by assuming that $\det\Pi(\Phi)\neq 0$ not only at the value zero, but for all values of Φ adopted. This permits us to regard the image C of the constraint map $\phi: N\to C\subset\mathbb{R}^{2m}$, $x\mapsto\Phi^\alpha(x)$, as a symplectic manifold; indeed $C\equiv \mathrm{Im}\,\phi$ is endowed naturally with the symplectic form

$$\varpi=\tfrac{1}{2}(\Pi^{-1})_{\alpha\beta}d\Phi^\alpha\, d\Phi^\beta. \tag{2}$$

By construction, the map ϕ is Poisson.

In contrast to the standard approaches in which the reduced phase space M is regarded as a restriction of the original phase space N to the constraint surface $\Phi(x)=0$, we propose to view M as the *space of orbits* generated by the second-class constraints Φ^α. Since the constraints are second-class, their Hamiltonian vector fields v^α are nowhere tangential to the constraint surface. Thus, at least locally, any point of the constraint surface, i.e., of the reduced phase space M, corresponds to an orbit (namely the one that is generated by the v^αs through the point in question).

Before we follow this general idea, we shall pause for a moment and comment on the possible global difficulties. The full equivalence between the reduced phase space M and the orbit space requires any orbit to intersect the constraint surface once and once only. Despite the fact that we required Π to be nondegenerate everywhere, the orbits do not necessarily have this property in general. The situation we meet here is similar to the one of choosing gauge conditions for a set of first-class constraints, with $\det\Pi$ playing the role of the Faddeev–Popov determinant. Note that the combined system of first-class constraints and gauge-conditions forms a set of second-class constraints. It is known that even for a nonvanishing Faddeev–Popov determinant (along the intersection of the constraint surface with the gauge conditions) the chosen gauge conditions may show global deficiencies, in which case they are referred to as having a Gribov problem.[11]

By analogy, we call the orbits generated by the v^α's to have a *Gribov problem*, if they do not intersect the constraint surface precisely once. To conclude these remarks, let us illustrate such problems through the following simple example where we take $N=T^*\mathbb{R}\backslash(0,0)$ with standard symplectic form $\Omega=dq\wedge dp$. Now let us choose the constraints,

$$\Phi^1:=\frac{(q^2-p^2)}{2\sqrt{q^2+p^2}}-\frac{1}{2}\quad\text{and}\quad\Phi^2:=\frac{qp}{2\sqrt{q^2+p^2}}.$$

Their Poisson bracket is given by $\Pi^{12}=1$ and one can easily establish that there is just *one* orbit in $T^*\mathbb{R}\backslash(0,0)$. On the other hand, $T^*\mathbb{R}\backslash(0,0)$ contains *two* points of the reduced phase space: $(q,p)=(\pm 1,0)$. In fact, the map from $N=T^*\mathbb{R}\backslash(0,0)$ to $C=\mathbb{R}^2\backslash(-\frac{1}{2},0)$ defines a two-fold covering (as one may see most easily in polar coordinates). These constructions are easily extended to obtain examples with an arbitrary number of Gribov copies.

In the absence of a Gribov problem,[12] however, the reduced phase space M may be fully identified with the space of orbits. Let π denote the projection from N to M along the orbits. In its spirit related to Ref. 1, we make the following proposition: The symplectic two-form ω on M satisfies

$$\pi^*\omega=\Omega-\phi^*\varpi. \tag{3}$$

The proof proceeds in several steps. First, we show that the form $(\Omega-\phi^*\varpi)$ descends to the space of leaves of the foliation. Indeed, it is horizontal,

$$\Omega(v^\alpha,\cdot)-\phi^*\varpi(u^\alpha,\cdot)=d\Phi_\alpha(x)-\phi^*d\Phi_\alpha=0. \tag{4}$$

Here u^α denotes the projection of the vector fields v^α to C (which is well-defined since the v^α's are tangential to the orbits): $u^\alpha=\{\Phi^\alpha,\cdot\}_C$, the index C being used to make clear that the bracket corresponds to (2). For later use we remark here that by assumption on the determinant of Π, the vector fields u^α—and thus also the vector fields v^α—are nonzero everywhere; correspondingly, the action generated by the constraints is free.

Equation (4) implies that, since the form in question is closed, it is also invariant with respect to the flows generated by the constraints. Hence, it is a pullback of some two-form on M, which we denote by ω.

Next, we show that ω coincides with the inverse of Dirac's bracket. For this purpose we consider two functions f and g on N which are constant on the leaves of the foliation. This implies that their Poisson brackets with the constraints vanish, yielding $\{f,g\}_D=\{f,g\}$. Denote the corresponding Hamiltonian vector fields by v_f and v_g. Note that one can use either the original Poisson bracket or the Dirac bracket to define them. We would like to show that

$$\omega(\pi_*v_f,\pi_*v_g)=\{f,g\}_D.$$

Indeed,

$$\{f,g\}_D=\{f,g\}=\Omega(v_f,v_g)=\omega(\pi_*v_f,\pi_*v_g).$$

Here we have used that the vector fields v_f and v_g project to zero by ϕ. Thus we have fully established our formula (3) above.

In the presence of a Gribov problem with nonvanishing number of Gribov copies the map ϕ restricted to an orbit is not injective. For the following constructions we shall assume that the restriction of ϕ is a bijection. Note that this property is not guaranteed by the absence of a Gribov problem, since ϕ may still fail to be surjective after restriction to an orbit. As an example we take N to be $T^*\mathbb{R}^2$ with the standard symplectic form and choose the constraints $\Phi^1:=\exp(q^2)[\exp(q^1)-1]$, $\Phi^2:=\exp(-q^1-q^2)p_1$, which again leads to $\Pi^{12}=1$. Now, $C\equiv\mathrm{Im}\,\phi=T^*\mathbb{R}$, but an orbit characterized by a fixed value of q^2 maps only to the parts of C with $\Phi^1>-\exp(q^2)$.

If the map ϕ restricted to any orbit is surjective and there is no Gribov problem, the original phase space is a fiber bundle with typical fiber C and base manifold M. In this case there is an alternative way to express the relation between the form Ω on N and ω on M: Let us consider the Liouville forms of mixed degree $L:=\exp(\Omega)$ on N and $l:=\exp(\omega)$ on M. The top degree components of L and l are the Liouville volume forms on N and M, respectively. We define the normalized fiber integral (or push forward map) π_* over the leaves of our foliation by the formula

$$\pi_*\alpha:=\frac{1}{\mathrm{Vol}\,C}\int_{\mathrm{fiber}}\alpha. \tag{5}$$

Here α is a differential form on N and Vol C is a (possibly infinite) symplectic volume of the constraint space C. If C is compact, π_* is just the ordinary push-forward map to M. Otherwise, the normalization factor $(\mathrm{Vol}\,C)^{-1}$ is reminiscent of the infinite normalization constants in the definitions of path integrals. By applying the fiber integral (5) to the Liouville form L, we obtain

$$\pi_* L = \frac{1}{\mathrm{Vol}\, C} \int_{\mathrm{fiber}} \exp(\Omega) = \frac{1}{\mathrm{Vol}\, C} \exp(\omega) \int_{\mathrm{fiber}} \exp(\Phi^* \varpi)$$

$$= \frac{\int_C \exp(\varpi)}{\mathrm{Vol}\, C} \exp(\omega) = l. \tag{6}$$

In the next section we shall generalize Eq. (3) to an infinite dimensional context where Ω is given by a symplectic form on some space of fields. There will be one major difference in comparison to the considerations in the present section: the forms ω and ϖ will no longer be closed! The fiber integral (5) (which becomes a path integral) will then provide a prescription of how to define the Liouville form l for a nonclosed form ω.

Before turning to this, however, we briefly extend the above considerations to the general setting of a closed algebra of constraints, where there are both first- and second-class constraints. Note in this context that although one may always replace a set of constraints by an equivalent set of constraints where first- and second-class constraints are split,[10] this splitting is achieved only on-shell (i.e., in a ''weak sense''). On the full phase space of the original theory, however, it may be impossible to find a splitting for which the second-class constraints do not generate first-class constraints upon Poisson commutation.

In the case of a closed constraint algebra containing first-class constraints, the matrix $\Pi(\Phi)$ is degenerate. Consequently, the manifold $C = \mathrm{Im}\, \phi$ is no longer symplectic but only a Poisson manifold. Hence, C foliates into symplectic leaves. Let C_0 denote the symplectic leaf containing the origin $\Phi = 0$ and $\tilde{N}_0$ be the pre-image of C_0, i.e., $\tilde{N}_0 = \phi^{-1}(C_0)$. ($\tilde{N}_0$ may be obtained equivalently through the action on N_0 of the flow generated by the constraints.) The reduced phase space may now be regarded as the space of orbits in $\tilde{N}_0$, at least in the absence of a Gribov problem. A formula of the type (3) is true, if in the right-hand side Ω is the restriction of the symplectic form on the original space N to $\tilde{N}_0$ and ϖ is the symplectic form on C_0. By means of such a formula one may, however, no more relate the Liouville forms on N and M such as in (6). The reason is that the fiber integration over Ω restricted to $\tilde{N}_0$ yields zero, since in the presence of first-class constraints this differential form has a kernel along the fibers.

III. HAMILTONIAN SYSTEMS WITH LOOP GROUP SYMMETRY

Now we turn to the infinite dimensional situation of interest. Our phase space N is a field space with symplectic form Ω. By assumption, it has a Hamiltonian action of the loop group LG of some Lie group G, which we take to be compact, simple, and simply connected for simplicity. To an algebra element $\varepsilon(s) \in L\mathcal{G}$ we associate a Hamiltonian vector field,

$$v_\varepsilon = \{J_\varepsilon, \cdot\}, \tag{7}$$

on N, where

$$J_\varepsilon = \mathrm{tr} \int_0^1 \varepsilon(s) J(s) ds, \tag{8}$$

and $J(s)$ is a field giving rise to the moment map for the loop group action.

Using an orthonormal basis t^a in the Lie algebra $\mathcal{G}$, we can write the Poisson brackets of the components of $J(s)$ in the form

$$\{J^a(s), J^b(s')\} = k \delta^{ab} \delta'(s - s') + f_c^{ab} \delta(s - s') J^c(s). \tag{9}$$

Here k is a coefficient in front of the anomalous term in the bracket. We would like to use the currents $J^a(s)$ as constraints in our Hamiltonian system. If k vanishes, they are first-class constraints and can be treated by the standard procedure. Our main interest is to deal with the case of nonvanishing k. To simplify notations we will set $k = 1$ for the rest of the paper.

According to Eq. (9), the currents $J(s)$ form a closed algebra of both first- and second-class constraints. The zero modes of the currents $J_0^a := \int J^a(s)ds$ are first-class. All the remaining modes in a Fourier decomposition of $J(s)$ are second-class. The latter do not close among themselves since Poisson brackets of J_n with J_{-n} have J_0-contributions. Hence, the Fourier modes J_n do not allow us to split off a closed algebra of pure second-class constraints. As we remarked above, such a splitting into closed first-class and closed second-class constraints need not even exist.

In the present case, however, we can split the constraints into first- and second-class. To see this, we return to the loop group LG, whose Lie algebra elements enter the Hamiltonians (8). LG may be written as a semidirect product of the group of based loops ΩG, formed by the loops with property $g(0)=e$, and the group G: Any $g(s)\in LG$ can be written uniquely as $g(s)=\tilde{g}(s)\hat{g}$ with $\tilde{g}(s)\in\Omega G$ and $\hat{g}\in G$. On the Lie algebra level this corresponds to the unique splitting of any $\varepsilon(s)\in L\mathcal{G}$ into the sum of a constant Lie algebra element $\varepsilon(0)$ and an $\tilde{\varepsilon}(s)\in\Omega\mathcal{G}$: $\varepsilon(s)=\varepsilon(0)+\tilde{\varepsilon}(s)$ with $\tilde{\varepsilon}(0)=0$. Re-expressing the relations (9) in terms of the Hamiltonians (8), one finds

$$\{J_\varepsilon, J_\eta\} = \mathrm{tr}\int_0^1 \varepsilon(s)\,\eta'(s)ds + J_{[\varepsilon,\eta]}. \tag{10}$$

Since $\delta'(s-s')$ is an invertible operator on test-functions vanishing on the end-points of the interval, these relations become second-class upon restriction to $\Omega\mathcal{G}$. Moreover, the algebra of this subclass of Hamiltonians is obviously closed now.

So, following the ideas of Sec. II, we should now be able to forget the first-class constraints and just restrict our attention to the subclass of second-class constraints so as to perform the pushforward integral (6) we are after. However, at this point we have to fight with the infinite dimensionality of the space of constraints and with the properties of an (appropriately defined) dual for the Lie algebra of the group ΩG. [Recall that the moment(um) map yields elements in the *dual* space of the Lie algebra of the group action in question; cf., e.g., Ref. 13 for details.]

In this paper, we do not intend to go into the functional analytical details that would be necessary to fully and rigoroulsy *extend* the approach of the previous section to the present infinite dimensional case (although this might yield interesting insights). Instead we will make use of a (mathematically rigorous) formula which is of the *form* of Eq. (3) with a (weakly) nondegenerate ϖ, which, however, is not closed and thus not symplectic.

For this purpose we return to the action of the group ΩG. As follows from Eq. (9), this group (or also LG) acts on the space of currents by standard gauge transformation,

$$J^g(s) = g^{-1}Jg + g^{-1}\partial_s g.$$

This action has no fixed points (here the restriction to ΩG becomes relevant!), similar to the flows of the vector fields u_α on C in Sec. II. Hence, the action of ΩG on N is also free. Then, one can form the space of orbits, $M := N/\Omega G$ which replaces the space of leaves of the foliation of Sec. II. The projection from N to M is denoted by π.

Similar to Eq. (3) we may decompose the symplectic form Ω on the original phase space according to (cf. Theorem 8.3 in Ref. 3)

$$\Omega = \pi^*\omega + J^*\varpi, \tag{11}$$

where ω is a two-form on M and ϖ lives on the space of currents (for a more precise definition of this space cf. Ref. 3). The explicit formula for ϖ looks as follows. Denote by Ψ the solution of the equation

$$\partial_s\Psi\Psi^{-1} = J(s),$$

with the boundary condition $\Psi(0)=e$. In other words, $\Psi(s)$ is a path ordered exponential of $J(s)$ and $\Psi(1)$ is the holonomy map, which takes values in the group G. Obviously, the holonomy map descends to M and we shall denote the induced map by $\psi: M\to G$.

The form ϖ is given by

$$\varpi := \frac{1}{2}\mathrm{tr}\int_0^1 (\Psi^{-1}d\Psi\,\partial_s(\Psi^{-1}d\Psi))ds. \tag{12}$$

As remarked above, it is not closed,

$$d\varpi = \tfrac{1}{6}\mathrm{tr}(\Psi^{-1}(1)d\Psi(1))^3.$$

As a consequence of formula (11), the form ω is also not closed,

$$d\omega = -\tfrac{1}{6}\mathrm{tr}(\psi^{-1}d\psi)^3.$$

Note, however, that the right-hand side of the last two formulas is proportional to the coefficient k in (9), which we have set to one thereafter. Thus, these forms become closed in the absence of the anomalous term in the current algebra. This observation will become relevant when interpreting the final result of the calculation in Sec. 4.

Although ϖ is not symplectic, it comes very close to an inverse of the Poisson brackets (10) between the second-class constraints. By straightforward calculation one verifies the two relations:

$$\iota(v_{\tilde{\varepsilon}})\varpi \equiv \varpi(v_{\tilde{\varepsilon}},\cdot) = -dJ_{\tilde{\varepsilon}}, \quad \varpi(v_{\tilde{\varepsilon}},v_{\tilde{\eta}}) = \{J_{\tilde{\varepsilon}},J_{\tilde{\eta}}\}. \tag{13}$$

For these relations to hold it is essential that one restricts the Lie algebra elements to $\Omega\mathcal{G}$ (for the corrections appearing otherwise cf. Proposition 8.1 in Ref. 3). In the finite dimensional setting, equations of the form (13) for a complete set of Hamiltonian vector fields are already sufficient to ensure that ϖ is the sought-for symplectic form; the closedness would then follow automatically by validity of the Jacobi identity for the Poisson bracket.

In the present infinite dimensional setting, the form ϖ yielding relations of the form (13) is even not unique. Indeed, one can change the splitting (11) by an arbitrary 2-form β on the group G,

$$\tilde{\omega} = \omega + \psi^*\beta, \quad \tilde{\varpi} = \varpi - \Psi^*\beta,$$

without affecting the relations (13) where ϖ is replaced by $\tilde{\varpi}$. Note that because the 3-form $\mathrm{tr}(\psi^{-1}\,d\psi)^3$ belongs to a nontrivial cohomology class on G, also the 2-form $\tilde{\omega}$ is not closed,

$$d\tilde{\omega} = d\omega + \psi^*\,d\beta \neq 0.$$

The phase space N is symplectic and carries the Liouville form $L = \exp(\Omega)$. The (formal) top degree part of L gives the measure of the Hamiltonian path integral. Inspired by Eq. (6), we would like to (formally) *define* the Liouville form l on M by the formula

$$l := \pi_* L = \frac{1}{\mathrm{Vol}\,\Omega G}\int_{\Omega G}\exp\Omega \equiv \frac{\int_{\Omega G}\exp(\varpi)}{\mathrm{Vol}\,\Omega G}\exp(\omega), \tag{14}$$

where we made use of the definition (5) as well as of the relation (11). In the next section we compute the path integral,

$$I(\psi) := \frac{1}{\mathrm{Vol}\,\Omega G}\int_{\Omega G}\exp(\varpi),$$

where $\psi = \Psi(1)$ is an element of G. Note that the resulting integral will be a differential form of mixed degree rather than a function on G (or its pullback to M).

IV. EVALUATION OF THE PATH INTEGRAL

We want to integrate $\exp(\varpi)$ over the group of based loops ΩG. Therefore we split the field $\Psi(s)$ in formula (12) into a product of an element $h \in \Omega G$ and an extra factor $\exp(\alpha s)$, i.e.,

$$\Psi(s) = h(s)\exp(\alpha s),$$

where $h(s) \in G$ is a periodic G-valued function and $\alpha \in \mathcal{G}$ is sent to the group element $\Psi(1) = \exp(\alpha) \in G$ by the exponential mapping.

A short and elementary computation allows us to reexpress the form ϖ in terms of the variables $h(s)$ and α. The result is

$$\varpi = \frac{1}{2}\mathrm{tr}\int_0^1 ds((h^{-1}dh)D_\alpha(h^{-1}\,dh) + 2h^{-1}dh\,d\alpha + d(e^{\alpha s})e^{-\alpha s}\,d\alpha).$$

D_α denotes the covariant derivative $D_\alpha = \partial_s - \mathrm{ad}_\alpha$ where $\mathrm{ad}_\alpha(\cdot) = [\alpha, \cdot]$. The last term in ϖ can be evaluated with the help of the following formula:

$$\theta(s) := d(e^{\alpha s})e^{-\alpha s} = \frac{1}{\mathrm{ad}_\alpha}(e^{s\mathrm{ad}_\alpha} - 1)d\alpha. \tag{15}$$

Here, $1/\mathrm{ad}_\alpha = (\mathrm{ad}_\alpha)^{-1}$ is the inverse of the adjoint action ad_α with α. Note that the function $(1/x)(1-e^{sx}) = \Sigma_{n\geqslant 1} s^n x^{n-1}/n!$ is regular even at $x=0$ so that the right-hand side of formula (15) is well-defined. To establish Eq. (15) we differentiate the function $\theta(s)$ with respect to s to find

$$\partial_s\theta(s) = d\alpha + [\alpha, \theta(s)].$$

If the ansatz $\theta(s) = \exp(s\,\mathrm{ad}_\alpha)\,\vartheta(s)$ is inserted into the expression for $\partial_s\theta(s)$, we deduce

$$\partial_s\vartheta(s) = e^{-s\ \mathrm{ad}_\alpha}d\alpha.$$

This equation can easily be integrated to give the claimed formula for $\theta(s)$.

Formula (15) actually allows us to perform the integral over s for the third term in ϖ. This results in

$$\varpi = \frac{1}{2}\mathrm{tr}\int_0^1 ds(\phi D_\alpha\phi + 2\phi\,d\alpha) - \frac{1}{2}\mathrm{tr}\left(d\alpha\frac{1}{(\mathrm{ad}_\alpha)^2}(e^{\mathrm{ad}_\alpha} - 1 - \mathrm{ad}_\alpha)d\alpha\right). \tag{16}$$

Again, the argument of the second trace is well-defined on the kernel of ad_α. In this expression for the form ϖ we also introduced the field $\phi(s) = h^{-1}(s)dh(s)$. By construction, $\phi(s)$ is a fermionic field subject to the constraint $\phi(0) = 0 = \phi(1)$. The integral over the exponential of the two-form ϖ is now reinterpreted as a fermionic ''path integral'' $\int \mathcal{D}\phi\exp(\varpi)$.

From the proof of Eq. (15) above it is obvious that $D_\alpha\theta(s) = d\alpha$. Therefore one can rewrite the form ϖ also as

$$\varpi = \frac{1}{2}\mathrm{tr}\int_0^1 ds(\phi + \theta)D_\alpha(\phi + \theta).$$

This may lead one to conclude that the integration of $\exp\varpi$ over ϕ merely results in the Pfaffian of D_α. However, $(\phi+\theta)(s)$ does not vanish at $s=1$ and a change of variables to $\phi+\theta$ is illegitimate.

We therefore proceed with integrating $\exp(\varpi)$ in the form of Eq. (16). As the last term does not depend on ϕ (resp. h) and as, being a two-form, it commutes with the first two terms, we can split the exponential into two parts, the second one of which we may pull out of the integral, i.e., we shall write $\varpi = \varpi_1 - \varpi_2$ with

$$\varpi_1=\frac{1}{2}\mathrm{tr}\int_0^1 ds(\phi D_\alpha\phi+2\phi\, d\alpha), \tag{17}$$

$$\varpi_2=\frac{1}{2}\mathrm{tr}\left(d\alpha\frac{1}{(\mathrm{ad}_\alpha)^2}(e^{\mathrm{ad}_\alpha}-1-\mathrm{ad}_\alpha)d\alpha\right), \tag{18}$$

and compute the Integral $I=\int\mathcal{D}\phi\exp(\varpi_1)$, leaving out the extra factor $\exp(-\varpi_2)$ for the moment.

The field $\phi(s)$ is a periodic fermionic field which admits a Fourier decomposition: $\phi(s)=\Sigma_n\phi_n\exp(2\pi ins)$. In terms of the Fourier modes ϕ_n, the constraint $\phi(0)=0$ becomes $\Sigma_n\phi_n=0$. To turn the integral into a Gaussian one over *unrestricted* variables, we introduce a Lagrange multiplier λ. This leaves us with the computation of the following integral:

$$I=\int\prod_n d\phi_n\, d\lambda\,\exp\mathrm{tr}\left(\frac{1}{2}\sum_m\ \phi_{-m}D_m\phi_m+\phi_0\, d\alpha+\lambda\sum_m\ \phi_m\right),$$

where $D_n\equiv 2\pi in-\mathrm{ad}_\alpha$ and λ is again a fermionic variable. A product over the Lie algebra indices of ϕ_n and λ in the integration measure is understood, furthermore. Defining $J_n=\lambda+\delta_{n,0}\,d\alpha$, the second and third terms in the exponent may be combined into $\Sigma_m\phi_{-m}J_m$.

We would like to remark that the last reformulation of our integral involves the choice of some particular (anti)self-adjoint extension for the operator D_α: on its original domain of definition which consists of sections vanishing at both ends of the interval $[0,1]$, iD_α is symmetric only, while on sections satisfying periodic boundary conditions it becomes self-adjoint.

The operator D_α is not invertible in the space of periodic sections. Its kernel is the ''diagonal part'' of the constant section. By ''diagonal'' we mean the subspace of the Lie algebra that commutes with α, thus being in the kernel of ad_α. We therefore integrate over ϕ_0^{diag} first. This produces a delta function $\delta(J_0^{\mathrm{diag}})\equiv\delta(\lambda^{\mathrm{diag}}+(d\alpha)^{\mathrm{diag}})$, which fixes the diagonal part of λ. On the remaining space the operator is invertible and we can perform the fermionic Gaussian integration, using

$$\int\ \mathcal{D}\psi\exp\left(\frac{1}{2}\psi_i\mathcal{O}_{ij}\psi_j+\psi_iJ_i\right)=\mathrm{Pf}(\mathcal{O})\exp\left(\frac{1}{2}J_i\mathcal{O}^{-1}_{ij}J_j\right). \tag{19}$$

Here, ψ and J have been taken fermionic, the operator $\mathcal{O}$ was assumed to satisfy $\psi\mathcal{O}\psi=-(\mathcal{O}\psi)\psi$, and $Pf(\mathcal{O})$ denotes the Pfaffian of $\mathcal{O}$. We get

$$I=\mathrm{Pf}(D_\alpha)\int d\tilde{\lambda}\,\exp\mathrm{tr}\left(\frac{1}{2}\sum_n\ J_{-n}D_n^{-1}J_n\right), \tag{20}$$

where the Pfaffian is taken over the space of periodic sections without a kernel and $\tilde{\lambda}$ denotes the nondiagonal part of λ. Note that $J_0^{\mathrm{diag}}\equiv 0$ so that the expression in the exponent is well-defined. Actually, since D_n becomes merely the number $2\pi in$ on diagonal elements, all of the diagonal parts of J_n drop out due to $J_{-n}=J_n$ and the fermionic character of J_n. We indicate this again by means of tildes. Inserting the definition of J_n, Eq. (20) becomes

$$I=\mathrm{Pf}(D_\alpha)\int d\tilde{\lambda}\,\exp\mathrm{tr}\left[\frac{1}{2}\tilde{\lambda}\left(\sum_n\ D_n^{-1}\right)\tilde{\lambda}+\tilde{\lambda}(\mathrm{ad}_\alpha)^{-1}\widetilde{d\alpha}+\frac{1}{2}\widetilde{d\alpha}(\mathrm{ad}_\alpha)^{-1}\widetilde{d\alpha}\right].$$

This is again a Gaussian integral for the variable $\tilde{\lambda}$ and we assume that α is sufficiently ''generic'' for $\Sigma_nD_n^{-1}$ to possess an inverse. We may again apply Eq. (19) to obtain

$$I=\mathrm{Pf}(D_\alpha)\mathrm{Pf}\left(\sum_n\ D_n^{-1}\right)\exp\mathrm{tr}\left[-\frac{1}{2}\widetilde{d\alpha}\frac{(\Sigma_nD_n^{-1})^{-1}}{ad_\alpha^2}\widetilde{d\alpha}+\frac{1}{2}\widetilde{d\alpha}(ad_\alpha)^{-1}\widetilde{d\alpha}\right],$$

where use of the ad-invariance of the trace (Killing metric) has been made.

This result for $I=\int \mathcal{D}\exp(\varpi_1)$ may now be combined with the expression for ϖ_2 in Eq. (18) to yield

$$\int \mathcal{D}\phi \exp(\varpi)=\mathrm{Pf}(D_\alpha)\mathrm{Pf}\left(\sum_n D_n^{-1}\right)\exp\left[-\frac{1}{2}\mathrm{tr}\,\widetilde{d\alpha}\frac{(\Sigma_n D_n^{-1})^{-1}+e^{\mathrm{ad}_\alpha}}{\mathrm{ad}_\alpha^2}\widetilde{d\alpha}\right].$$

Here we made use of the fact that the diagonal parts of $d\alpha$ drop out in (18) and that $\mathrm{tr}(\widetilde{d\alpha}f(\mathrm{ad}_\alpha)\widetilde{d\alpha})$ vanishes for any function f with $f(x)=f(-x)$. We are left with the computation of the operator $\Sigma_n D_n^{-1}$ and the two Pfaffians.

We start with $\mathrm{Pf}(D_\alpha)$. Denote by $i\alpha_r$ the nonvanishing eigenvalues of ad_α, which are purely imaginary as G is taken compact. The index r runs over all roots in the Lie algebra of G; with $r>0$ $(r<0)$ labeling the positive (negative) roots, one has $\alpha_r=-\alpha_{-r}$, furthermore. In this notation one finds the following formal expression for the Pfaffian:

$$\mathrm{Pf}(D_\alpha)=\left(\prod_{r>0} i\alpha_r\right)\prod_{n>0}\left((2\pi i\, n)^{\mathrm{rank}G}\prod_{r'}(2\pi i\, n+i\alpha_{r'})\right).$$

Clearly this is not well-defined. However, integrating $\exp\varpi$ over all of ΩG we cannot expect to obtain a finite result as the volume of the ''gauge group'' ΩG is infinite. So we should divide (again formally) by this volume. The group of (based) loops is a group of even cohomology, $H^{2k+1}(\Omega G)=0$, $\varepsilon=\int_0^1 ds\,\mathrm{tr}(h^{-1}dh\partial_s h^{-1}dh)$ being the generator of $H^2(\Omega G)$. So, formally the Haar measure of ΩG is given by the infinite product of ε's multiplied by the Haar measure on G (since the zero mode drops out from ε). Using our previous notation and Fourier decomposition, ε may be rewritten as $\mathrm{tr}\Sigma_{n\neq 0}(2\pi i\, n)d\phi_{-n}\,d\phi_n$. Thus we are led to *define*

$$\mathrm{Pf}(D_\alpha)/\mathrm{Vol}\,\Omega G:=\left(\prod_{r>0}\alpha_r\right)\prod_{n>0}\prod_{r'}\left(1+\frac{\alpha_{r'}}{2\pi n}\right).$$

By means of $\sin x=x\Pi_{n=1}^{\infty}(1-x^2/n^2\pi^2)$ we then obtain

$$\mathrm{Pf}(D_\alpha)/\mathrm{Vol}\,\Omega G=\prod_{r>0}\left(\sin\left(\frac{\alpha_r}{2}\right)\right). \tag{21}$$

We remark that the square of this result agrees with the expression obtained for $\det D_\alpha$ obtained in Ref. 14 by means of zeta function regularization.

We now come to the operator $\Sigma_n D_n^{-1}$, $D_n\equiv 2\pi i\, n-\mathrm{ad}_\alpha$, acting in that part of the Lie algebra that does not commute with α. Here we may use the simple formula,

$$\sum_n \frac{1}{2\pi i n-x}=\frac{1}{2}\coth\left(\frac{x}{2}\right),$$

to conclude that

$$\sum_n D_n^{-1}=\frac{1}{2}\coth(\mathrm{ad}_\alpha/2)\quad\text{and thus}\quad\left(\sum_n D_n^{-1}\right)^{-1}=2\tanh(\mathrm{ad}_\alpha/2).$$

Putting all this together, we arrive at the following result:

$$\frac{\int\mathcal{D}\phi\exp(\varpi)}{\mathrm{Vol}\,\Omega G}=\prod_{r>0}\cos\left(\frac{\alpha_r}{2}\right)\exp\left[-\mathrm{tr}\,d\alpha\frac{\sinh^3(\mathrm{ad}_\alpha/2)}{ad_\alpha^2\cosh(\mathrm{ad}_\alpha/2)}d\alpha\right].$$

Again, we have replaced $\widetilde{d\alpha}$ by $d\alpha$ as the extra contributions involving $(d\alpha)^{\mathrm{diag}}$ cancel anyway. We can finally rewrite the two-form in the exponent in terms of the group element $\psi=\exp(\alpha)$. First, we remark that

$$\prod_{r>0}\cos\left(\frac{\alpha_r}{2}\right)=\det{}^{1/2}\left(\frac{1+\mathrm{Ad}_\psi}{2}\right),$$

where $\det^{1/2}$ denotes the unique positive square root of the matrix $(1+\mathrm{Ad}_\psi)/2$. Next, formula (15) can be evaluated at $s=1$ to give $d\psi\,\psi^{-1}=\mathrm{ad}_\alpha^{-1}(1-e^{\mathrm{ad}_\alpha})d\alpha$. This may be inserted into our previous result for the integral and leads to

$$I(\psi)=\frac{\int\mathcal{D}\phi\exp(\varpi)}{\mathrm{Vol}\,\Omega G}=\det{}^{1/2}\left(\frac{1+\mathrm{Ad}_\psi}{2}\right)\exp\frac{1}{4}\left(\mathrm{tr}\,d\psi\,\psi^{-1}\frac{\mathrm{Ad}_\psi-1}{\mathrm{Ad}_\psi+1}\,d\psi\,\psi^{-1}\right).\tag{22}$$

V. RESULTS AND DISCUSSION

Combining Eqs. (14) and (22), we obtain the expression

$$l=\det{}^{1/2}\left(\frac{1+\mathrm{Ad}_\psi}{2}\right)\exp\left(\omega+\frac{1}{4}\,\mathrm{tr}\,d\psi\,\psi^{-1}\frac{\mathrm{Ad}_\psi-1}{\mathrm{Ad}_\psi+1}\,d\psi\,\psi^{-1}\right),\tag{23}$$

for the Liouville form l on the orbit space M. The same expression was previously used in Ref. 4 [formula (21)]. Our path integral consideration gives a natural derivation of Eq. (23), and shows its relation to the Liouville form L on the field space N.

Let us recall on this occasion that there was some freedom in our computation associated with the choice of an anti-self-adjoint extension for D_α. Instead of the periodic boundary conditions we introduced in the paragraph below Eq. (18), we could have extended the antisymmetric operator D_α also to sections with different (only quasi-periodic) behavior at the boundary. The final formula for $I(\psi)$ does depend on this choice of boundary conditions. It is expected, however, that the top degree part of the Liouville form l is insensitive to this freedom in the computation.

The space M arises as a result of reduction from the field space N with respect to second-class constraints. The residual first-class constraints J_0^a generate vector fields v_a on N which descend to M. According to Ref. 4, Proposition 4.1, the Liouville form l satisfies the following interesting equation:

$$(d+\tfrac{1}{24}f_{abc}\iota(v_a)\iota(v_b)\iota(v_c))l=0.\tag{24}$$

Note that in the finite dimensional case of Sec. II, $l=\exp(\omega)$ is a closed form. In the infinite dimensional situation we obtain an extra term $(1/24)f_{abc}\iota(v_a)\iota(v_b)\iota(v_c)$ on the left-hand side of Eq. (24), which modifies the exterior differential and should be interpreted as yet another manifestation of the chiral anomaly. It is a very interesting open question to trace the nature of this anomaly back to properties of the path integral in Sec. IV.

Simple examples of spaces M are given by D-branes in the WZW model.[5] There, the reduced spaces are conjugacy classes in a group manifold, and the form ω is given by the formula [see Eq. (7) in Ref. 5),

$$\omega=-\frac{1}{4}\mathrm{tr}\left(d\psi\,\psi^{-1}\frac{\mathrm{Ad}_\psi+1}{\mathrm{Ad}_\psi-1}\,d\psi\,\psi^{-1}\right).$$

Formula (23) shows that the form ω should be corrected by the extra term arising from the path integral to yield

$$\tilde{\omega}=-\mathrm{tr}\left(d\psi\,\psi^{-1}\frac{1}{\mathrm{Ad}_\psi-\mathrm{Ad}_\psi^{-1}}\,d\psi\,\psi^{-1}\right).$$

Note that in this case, the linear map $(\mathrm{Ad}_\psi - 1)(\mathrm{Ad}_\psi + 1)^{-1}$ representing the correction term in Eq. (23) is inverse to the element $B = (\mathrm{Ad}_\psi + 1)(\mathrm{Ad}_\psi - 1)^{-1}$ that appears in ω. Hence, their difference $\tilde{\omega}$ is represented by $B - B^{-1}$. Surprisingly, the same combination shows up in the expression for the effective B-field derived in Ref. 8 in the analysis of D-branes on the flat background. It is another challenging question to understand why the formula of Ref. 8 applies to group manifolds and to establish the relation with the path integral of Sec. III.

In this paper we did not touch the issue of quantization of the spaces N and M. While one can attempt to quantize N using the symplectic form Ω, it is not clear what it means to quantize M because the form ω is not closed. In the case of the D-branes in the WZW model one can use the link between string theory and noncommutative geometry to obtain an answer to this question.[9] The general case, however, remains an open problem.

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The braiding for representations of q-deformed affine sl_2

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We compute the braiding for the ''principal gradation'' of $U_q(\widehat{sl_2})$ for $|q|=1$ from first principles, starting from the idea of a rigid braided tensor category. It is not necessary to assume either the crossing or the unitarity condition from S-matrix theory. We demonstrate the uniqueness of the normalization of the braiding under certain analyticity assumptions, and show that its convergence is critically dependent on the number theoretic properties of the number τ in the deformation parameter $q=e^{2\pi i\tau}$. We also examine the convergence using probability, assuming a uniform distribution for q on the unit circle. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1357197]

I. INTRODUCTION

The sine-Gordon S-matrix for the quantum scattering of solitons was solved initially in the literature in Ref. 1, by imposing conditions on the S-matrix called crossing and unitarity. These conditions were previously observed in other S-matrices found using perturbative techniques in quantum field theory,[2] and were subsequently taken to be axioms for the nonperturbative result.

The bootstrap methods use the $U_q(\widehat{sl_2})$ Hopf algebra,[3] and its spin half representation W, which is a space of functions taking values in $\mathbb{C}^2$, where the first component corresponds to ''solitons'' and the second to ''anti-solitons.'' Then $W\otimes W$ corresponds to a two soliton system, which can interact by collision. There is an initial two soliton quantum state in $W\otimes W$, and after the collision process we have a final quantum state in $W\otimes W$. The scattering matrix gives a map $W\otimes W\to W\otimes W$, which sends the initial to the final state. In terms of the Hopf algebra, this map is a braiding.[4]

This scattering matrix is fairly easy to find up to a multiplication by a scalar function, but the scalar function itself is more difficult. We denote this scalar function by $a(z)$ where $z\in\mathbb{C}$. The crossing condition in terms of this function becomes

$$a(z)=a\left(-\frac{q}{z}\right)\frac{(z-z^{-1})}{(zq^{-1}-z^{-1}q)}, \tag{1}$$

and the unitarity condition is $a(z)a(z^{-1})=1$.

The crossing condition arises from physics by equating a scattering process with the same scattering process after rotating the space–time diagram of the collision by a right-angle. This rotation involves a time reversal of one of the incoming and one of the outgoing solitons, which implies that these are turned into anti-solitons. The rotation of the diagram also implies that z, which corresponds roughly to the relative momentum of the colliding solitons (conserved in the collision), is transformed to $-z^{-1}q$. The interested reader can refer to the comprehensive book[2] for a complete discussion. The article[1] is also an excellent review.

Zamolodchikov–Zamolodchikov[1] solved these equations (1) to get a formula for $a(z)$ in terms of a double infinite product of gamma functions. It was thought that this product probably

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converged for all physical values of z, and all values of q where $|q|=1$. However no proof of this was provided. The convergence of this function has also not been treated in subsequent papers in the literature.

Here, in this paper, we find an alternative formula which is more amenable to a convergence analysis. We find that the convergence is highly delicate, and the function converges with probability one, for q on the unit circle, i.e., $q=e^{2\pi i\tau}$, including convergence for all irrational algebraic values of τ, and diverges for certain transcendental values of τ.

Another alternative formula for $a(z)$ was found in Johnson,[5] as an integral, or as a combination of ''regularized'' quantum dilogarithms. This was done to make contact with semiclassical results for the scattering which involve integrating classical time delays. However, the convergence of this formula, or of the individual quantum dilogarithms, was also difficult to analyze because the contour integrals which one has to do are difficult to perform, involving sums over an infinite double set of poles.

In this paper we shall consider the problem purely in terms of braidings of the representations of a Hopf algebra, rather than invoking the crossing and unitarity conditions of S-matrix theory. We begin with the loop group of analytic functions used in the classical inverse scattering procedure for sine-Gordon,[6] and deform this by inclusion of a parameter q.[7]

II. THE UNIVERSAL ENVELOPING ALGEBRA $\mathcal{H}$

We begin with the loop group of analytic functions from $\mathbb{C}^*$ to $SL_2(\mathbb{C})$ which obey the symmetry condition $U\phi(-z)U^{-1}=\phi(z)$, where

$$U=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}.$$

The Lie algebra for this group has generators $X_{\pm 1}$, $X_{\pm 2}$, and H, given by

$$X_{+1}(z)=\begin{pmatrix}0 & 0\\ z & 0\end{pmatrix},\quad X_{-1}(z)=\begin{pmatrix}0 & 1/z\\ 0 & 0\end{pmatrix},\quad H(z)=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$

$$X_{+2}(z)=\begin{pmatrix}0 & z\\ 0 & 0\end{pmatrix},\quad X_{-2}(z)=\begin{pmatrix}0 & 0\\ 1/z & 0\end{pmatrix}. \tag{2}$$

These generators obey the usual coproduct rule for the universal enveloping algebra of a Lie algebra, namely $\Delta(X_{\pm 1})=X_{\pm 1}\otimes 1+1\otimes X_{\pm 1}$, etc. This rule can be deformed by the inclusion of a parameter $q\in\mathbb{C}$ to give

$$\Delta H=1\otimes H+H\otimes 1,\quad \Delta X_{\pm 1}=X_{\pm 1}\otimes q^{-H/2}+q^{H/2}\otimes X_{\pm 1},$$

$$\Delta X_{\pm 2}=X_{\pm 2}\otimes q^{H/2}+q^{-H/2}\otimes X_{\pm 2}. \tag{3}$$

The Lie algebra structure remains the same, with the exception of an alteration in the Serre relation.[3,4] If in addition we define a counit ϵ (which kills all the generators) and an antipode S [which has $S(H)=-H$ and $S(X_{\pm n})=-q^{\pm 1}X_{\pm n}$] we can make the universal enveloping algebra into a Hopf algebra, which we denote $\mathcal{H}$. This is the so-called ''principal gradation'' of $U_q(\widehat{sl_2})$, which is actually a subalgebra of $U_q(\widehat{sl_2})$. We use the convention that $r=\sqrt{q}$ in the terms $q^{\pm H/2}$.

III. RIGID BRAIDED TENSOR CATEGORIES

Here we shall give a highly abbreveiated, specialized, and incomplete account of rigid braided tensor categories, for a full account see Ref. 4.

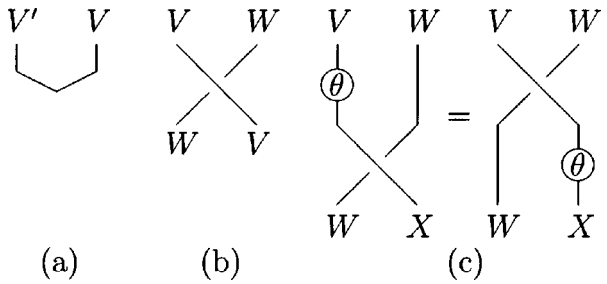

FIG. 1. Diagrams for braided categories.

The representations of a Hopf algebra $\mathcal{H}$ form a category, with objects the representations, and the morphisms $\rho: V \to W$ are intertwining maps for the representations V and W. This means that ρ is linear and that $\rho(h(v)) = h(\rho(v))$ for all $h \in \mathcal{H}$.

The tensor product of two representations is also a representation. The action on $V \otimes W$ is given by the coproduct $\Delta: \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}$. If we write $\Delta h = \Sigma h_{(1)} \otimes h_{(2)}$, then $h(v \otimes w) = \Sigma h_{(1)}(v) \otimes h_{(2)}(w)$. The category contains an ''identity object,'' the representation $\mathbb{C}$ with all generators having zero action. This means that category of representations forms a tensor or monoidal category. (Technically we should also say that the associator is trivial.)

If the category is *rigid*, for an object V there is a dual object V', and an ''evaluation'' morphism $\mathrm{eval}: V' \otimes V \to \mathbb{C}$ given by $\mathrm{eval}(\alpha, v) = \alpha(v)$.

If the category is *braided*, for two objects V and W there is a morphism $\Psi_{VW}: V \otimes W \to W \otimes V$. The braiding is functorial, which means that if there is a morphism $\theta: V \to X$, then the maps $(I \otimes \theta)\Psi_{VW}: V \otimes W \to W \otimes X$ and $\Psi_{XW}(\theta \otimes I): V \otimes W \to W \otimes X$ are the same.

Figure 1 shows the standard diagramatic notation used for braided categories. Elements of representations are denoted by vertical lines. For Fig. 1(a), note that $\mathbb{C}$ is traditionally denoted by an invisible line. The braiding $\Psi_{VW}: V \otimes W \to W \otimes V$ is shown in Fig. 1(b), and the rule for the functoriality of the braiding in Fig. 1(c).

The finite dimensional representations of a quasitriangular Hopf algebra form a rigid braided tensor category. We shall assume that the representations of our Hopf algebra $\mathcal{H}$ also form a rigid braided tensor category, and this will allow us to explicitly calculate the braiding.

IV. THE ''STANDARD'' REPRESENTATION OF $\mathcal{H}$

Take W to be a vector space of analytic functions: $\mathbb{C}^* \to \mathbb{C}^2$ (or at least analytic in a neighborhood of zero and a neighborhood of infinity), which obeys the condition $Uw(-z) = w(z)$ for all $w \in W$. The algebra $\mathcal{H}$ acts on W using matrix multiplication, $(hw)(z) = h(z)w(z)$, for the five generators listed in (2).

We can consider a dual space W' to W, which shall consist of analytic functions: $\mathbb{C}^* \to \mathbb{C}^2$ which are defined for $|z|$ sufficiently small and sufficiently large. Now define an evaluation map $\mathrm{eval}: W' \otimes W \to \mathbb{C}$ by

$$\mathrm{eval}\left(\begin{pmatrix} f \\ g \end{pmatrix} \otimes \begin{pmatrix} u \\ v \end{pmatrix}\right) = \frac{1}{4\pi i} \oint_\gamma (f(z)\, u(z) + g(z)\, v(z)) \frac{dz}{z}, \tag{4}$$

where γ consists of two anticlockwise circular contours about 0, one of large radius, and one of small radius. To find the action of $\mathcal{H}$ on W' we use the fact that the action commutes with $\mathrm{eval}: W' \otimes W \to \mathbb{C}$, and that the action of the generators is zero on $\mathbb{C}$. This means that

$$0=H\left(\operatorname{eval}\left(\begin{pmatrix}f\\g\end{pmatrix}\otimes\begin{pmatrix}u\\v\end{pmatrix}\right)\right)$$
$$=\operatorname{eval}\left(H\left(\begin{pmatrix}f\\g\end{pmatrix}\otimes\begin{pmatrix}u\\v\end{pmatrix}\right)\right)$$
$$=\operatorname{eval}\left(H\begin{pmatrix}f\\g\end{pmatrix}\otimes\begin{pmatrix}u\\v\end{pmatrix}+\begin{pmatrix}f\\g\end{pmatrix}\otimes H\begin{pmatrix}u\\v\end{pmatrix}\right),$$

so we get

$$\operatorname{eval}\left(H\begin{pmatrix}f\\g\end{pmatrix}\otimes\begin{pmatrix}u\\v\end{pmatrix}\right)=-\operatorname{eval}\left(\begin{pmatrix}f\\g\end{pmatrix}\otimes\begin{pmatrix}u\\-v\end{pmatrix}\right)$$
$$=-\frac{1}{4\pi i}\oint\left(f(z)\,u(z)-g(z)\,v(z)\right)\frac{dz}{z},$$

so we deduce that

$$H\begin{pmatrix}f\\g\end{pmatrix}(z)=\begin{pmatrix}-1&0\\0&1\end{pmatrix}\begin{pmatrix}f(z)\\g(z)\end{pmatrix}.$$

Now we continue with the generator X_{+1}

$$0=\operatorname{eval}\left(X_{+1}\left(\begin{pmatrix}f\\g\end{pmatrix}\otimes\begin{pmatrix}u\\v\end{pmatrix}\right)\right)$$
$$=\operatorname{eval}\left(X_{+1}\begin{pmatrix}f\\g\end{pmatrix}\otimes\begin{pmatrix}u/r\\vr\end{pmatrix}+\begin{pmatrix}f/r\\gr\end{pmatrix}\otimes X_{+1}\begin{pmatrix}u\\v\end{pmatrix}\right),$$

from which we get

$$\operatorname{eval}\left(X_{+1}\begin{pmatrix}f\\g\end{pmatrix}\otimes\begin{pmatrix}u/r\\vr\end{pmatrix}\right)=-\operatorname{eval}\left(\begin{pmatrix}f/r\\gr\end{pmatrix}\otimes\begin{pmatrix}0\\zu\end{pmatrix}\right)=-\frac{r}{4\pi i}\oint z\,g(z)\,u(z)\frac{dz}{z}.$$

From this, and the corresponding calculations for the other generators, we see that the action on W' is given by the matrix multiplication

$$\left(h\begin{pmatrix}f\\g\end{pmatrix}\right)(z)=\tilde{h}(z)\begin{pmatrix}f(z)\\g(z)\end{pmatrix},\tag{5}$$

where the matrices $\tilde{h}(z)$ are given by

$$\tilde{X}_{+1}(z)=-q\begin{pmatrix}0&z\\0&0\end{pmatrix},\quad \tilde{X}_{-1}(z)=-q^{-1}\begin{pmatrix}0&0\\1/z&0\end{pmatrix},\quad \tilde{H}(z)=-\begin{pmatrix}1&0\\0&-1\end{pmatrix},$$

$$\tilde{X}_{+2}(z)=-q\begin{pmatrix}0&0\\z&0\end{pmatrix},\quad \tilde{X}_{-2}(z)=-q^{-1}\begin{pmatrix}0&1/z\\0&0\end{pmatrix}.\tag{6}$$

There is a morphism $\theta: W\to W'$ given by

$$\theta(k)(z)=\begin{pmatrix}0&1\\1&0\end{pmatrix}k(-zq).\tag{7}$$

To verify this we check that it commutes with the actions of the generators, for example;

$$\left(X_{+1}\theta\left(\begin{pmatrix}u\\v\end{pmatrix}\right)\right)(z)=-\begin{pmatrix}0&qz\\0&0\end{pmatrix}\theta\left(\begin{pmatrix}u\\v\end{pmatrix}\right)(z)=-\begin{pmatrix}0&qz\\0&0\end{pmatrix}\begin{pmatrix}v(-zq)\\u(-zq)\end{pmatrix},$$

$$\theta\left(X_{+1}\begin{pmatrix}u\\v\end{pmatrix}\right)(z)=\begin{pmatrix}0&1\\1&0\end{pmatrix}\left(X_{+1}\begin{pmatrix}u\\v\end{pmatrix}\right)(-zq)=\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&0\\-qz&0\end{pmatrix}\begin{pmatrix}u(-zq)\\v(-zq)\end{pmatrix},$$

which are equal as required.

V. THE BRAIDINGS

We use the convention for tensor products that $\mathbb{C}^2\otimes\mathbb{C}^2\cong\mathbb{C}^4$ and $M_2\otimes M_2\cong M_4$, where

$$\begin{pmatrix}u\\v\end{pmatrix}\otimes\begin{pmatrix}u'\\v'\end{pmatrix}\cong\begin{pmatrix}uu'\\uv'\\vu'\\vv'\end{pmatrix},\quad\begin{pmatrix}a&b\\c&d\end{pmatrix}\otimes\begin{pmatrix}a'&b'\\c'&d'\end{pmatrix}\cong\begin{pmatrix}aa'&ab'&ba'&bb'\\ac'&ad'&bc'&bd'\\ca'&cb'&da'&db'\\cc'&cd'&dc'&dd'\end{pmatrix}. \tag{8}$$

Then we can consider $W\otimes W$ or $W'\otimes W$ as a space of analytic maps from a subset of $\mathbb{C}^*\times\mathbb{C}^*$ to $\mathbb{C}^4$. Now if $k\in W'\otimes W$ we have

$$\mathrm{eval}(k)=\frac{1}{4\pi i}\oint(1\ \ 0\ \ 0\ \ 1)\,k(x,x)\,\frac{dx}{x}.$$

By the coproduct rule H and (for example) X_{+1} act on $W\otimes W$ by matrix multiplication

$$(Hk)(x,y)=(H(x)\otimes I_2+I_2\otimes H(y))k(x,y),$$

$$(X_{+1}k)(x,y)=(X_{+1}(x)\otimes q^{-H(y)/2}+q^{H(x)/2}\otimes X_{+1}(y))\,k(x,y),$$

and they act on $W'\otimes W$ by

$$(Hk)(x,y)=(\tilde{H}(x)\otimes I_2+I_2\otimes H(y))k(x,y),$$

$$(X_{+1}k)(x,y)=(\tilde{X}_{+1}(x)\otimes q^{-H(y)/2}+q^{\tilde{H}(x)/2}\otimes X_{+1}(y))\,k(x,y).$$

The braiding $\Psi_{WW}:W\otimes W\to W\otimes W$ will be assumed to have the form $(\Psi_{WW}k)(x,y)=M(x,y)k(y,x)$, where $M(x,y)$ is a 4×4 matrix. Since the braiding is a morphism we must have $\Psi_{WW}(hk)=h(\Psi_{WW}k)$ for the five generators h and all $k\in W\otimes W$. The cases for $h=H$ and X_{+1} are given below:

$$M(x,y)(H(y)\otimes I_2+I_2\otimes H(x))=(H(x)\otimes I_2+I_2\otimes H(y))\,M(x,y),$$

$$M(x,y)\,(X_{+1}(y)\otimes q^{-H(x)/2}+q^{H(y)/2}\otimes X_{+1}(x))=(X_{+1}(x)\otimes q^{-H(y)/2}+q^{H(x)/2}\otimes X_{+1}(y))\,M(x,y).$$

A simple calculation will show that these five conditions determine the matrix $M(x,y)$ up to a complex multiple, and we find

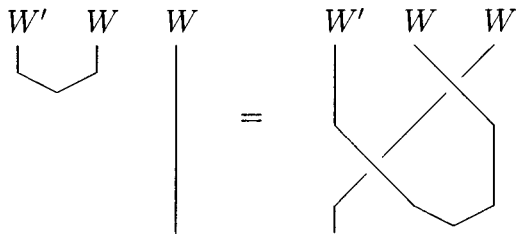

FIG. 2. Moving the evaluation map.

$$(\Psi_{WW}k)(x,y)=a(x,y)\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & \dfrac{xy(q^2-1)}{q^2x^2-y^2} & \dfrac{q(x^2-y^2)}{q^2x^2-y^2} & 0\\ 0 & \dfrac{q(x^2-y^2)}{q^2x^2-y^2} & \dfrac{xy(q^2-1)}{q^2x^2-y^2} & 0\\ 0 & 0 & 0 & 1\end{pmatrix}k(y,x),$$

where $a(x,y)$ is complex valued. Note that $(\Psi_{WW}^2k)(x,y)=a(x,y)a(y,x)k(x,y)$. In the same manner we can determine the braiding $\Psi_{W'W}:W'\otimes W\to W\otimes W'$ to be $(\Psi_{W'W}k)(x,y)=N(x,y)k(y,x)$, where the matrix $N(x,y)$ is given by

$$(\Psi_{W'W}k)(x,y)=\frac{c(x,y)}{q^2y^2-x^2}\begin{pmatrix}q^2y^2-x^2 & 0 & 0 & (q^2-1)xy\\ 0 & 0 & q(y^2-x^2) & 0\\ 0 & q(y^2-x^2) & 0 & 0\\ (q^2-1)xy & 0 & 0 & q^2y^2-x^2\end{pmatrix}k(y,x),$$

where $c(x,y)$ is another complex valued function.

Now we use the fact that as the braiding is functorial, it must commute with the evaluation morphism. We see that the maps $(I\otimes\mathrm{eval})(\Psi_{W'W}\otimes I)(I\otimes\Psi_{WW})$ and $\mathrm{eval}\otimes I:W'\otimes W\otimes W\to W$ are the same. In terms of the standard pictures, this is Fig. 2.

Now, identifying $W'\otimes W\otimes W$ with maps from subsets of $(\mathbb{C}^*)^3$ to $\mathbb{C}^2\otimes\mathbb{C}^2\otimes\mathbb{C}^2$, we get

$$\begin{aligned}((\Psi_{W'W}\otimes I)(I\otimes\Psi_{WW})k)(x,y,z)&=(N(x,y)\otimes I_2)((I\otimes\Psi_{WW})k)(y,x,z)\\&=(N(x,y)\otimes I_2)\,(I_2\otimes M(x,z))\,k(y,z,x),\end{aligned}\tag{9}$$

and applying $I\otimes\mathrm{eval}$ to this gives

$$\frac{1}{4\pi i}\oint(I_2\otimes(1\,0\,0\,1))\,(N(x,z)\otimes I_2)\,(I_2\otimes M(x,z))\,k(z,z,x)\,\frac{dz}{z},$$

and some matrix multiplication shows that this is

$$\frac{1}{4\pi i}\oint a(x,z)\,c(x,z)\,((1\,0\,0\,1)\otimes I_2)\,k(z,z,x)\,\frac{dz}{z}.$$

Just applying $\mathrm{eval}\otimes I$ to k gives

$$\frac{1}{4\pi i}\oint((1\,0\,0\,1)\otimes I_2)\,k(z,z,x)\,\frac{dz}{z},$$

and since these must be the same for all choices of k we deduce that $c(x,z)=1/a(x,z)$.

Now use the fact that the braiding commutes with the morphism $\theta: W \to W'$ in (7), so $(I \otimes \theta)\Psi_{WW}$ and $\Psi_{W'W}(\theta \otimes I): W \otimes W \to W \otimes W'$ are the same. Then

$$((I \otimes \theta)\Psi_{WW}k)(x,y) = \left(I_2 \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right)(\Psi_{WW}k)(x,-qy)$$

$$= \left(I_2 \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\right) M(x,-qy)\, k(-qy,x),$$

$$(\Psi_{W'W}(\theta \otimes I)k)(x,y) = N(x,y)\,((\theta \otimes I)k)(y,x),$$

$$= N(x,y) \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes I_2\right) k(-qy,x). \tag{10}$$

From some more matrix multiplication, this is true if

$$\frac{1}{a(x,y)} = a(x,-qy)\,\frac{x^2 - q^2y^2}{q(x^2-y^2)}. \tag{11}$$

VI. THE NORMALIZATION OF THE BRAIDING, $|q|=1$

In this section we find the normalization $a(x,y)$. For the moment we shall suppose that the value of x is fixed. Suppose that a solution $a(x,y)$ of (11) is an analytic function of y (except for isolated singularities) in some annulus centered on zero contained in the region $|y|>|x|$. We can narrow the annulus down until it no longer contains any isolated singularities or zeros. For convenience we set $z=x/y$ (so $|z|<1$), and $f(z)=a(x,x/z)$. Then $f(z)$ satisfies the equation

$$f(z)f(-z/q) = q\,\frac{z^2-1}{z^2-q^2}. \tag{12}$$

Now $f(z)$ will have a winding number $\omega \in \mathbb{Z}$ around zero as z winds once around zero. The function $c(z)=z^{-\omega}f(z)$ will have zero winding number, so its log, $b(z)=\log(c(z))$, will be analytic (and single valued) in the annulus. Now $c(z)$ obeys the equation $c(z)c(-z/q)=q(-z^2/q)^{-\omega}(z^2-1)/(z^2-q^2)$, so we must have

$$b(z)+b(-z/q) = \log(1-z^2) - \log(1-z^2/q^2) - \log(q) - \omega \log(-z^2/q),$$

as $-z/q$ is in the annulus if z is, because $|q|=1$. Since all the other functions are single valued in the annulus, we must have $\omega=0$. Now we can take the Laurent expansion of both sides in the annulus, and compare coefficients, to get the *unique* solution (up to the addition of a multiple of πi)

$$b(z) = -\tfrac{1}{2}\log(q) + \sum_{n>0} \frac{1}{n}\,\frac{1-q^{2n}}{1+q^{2n}} z^{2n}, \quad |z|<1, \quad z \in \text{annulus}. \tag{13}$$

By the uniqueness of analytic continuation, the exponential of this formula must coincide with $f(z)$ in a disk from zero up to the radius of convergence of the series. We also conclude that $f(z)$ did in fact not have any zeros or isolated singularities in this disk.

In the same manner, if $f(z)$ were analytic (except for isolated singularities) in some annulus centered on zero outside the unit disk, we could conclude that on that annulus (again up to the addition of a multiple of πi)

$$b(z) = \tfrac{1}{2}\log(q) - \sum_{n>0} \frac{1}{n}\,\frac{1-q^{2n}}{1+q^{2n}} z^{-2n}, \quad |z|>1. \tag{14}$$

We can now see explicitly from the series (on the assumption that the series converge anywhere) that $b(z)=-b(1/z)$ plus a multiple of πi, i.e., that $1/f(z)=\pm f(1/z)$.

Now we can look at different values of x. As a consequence of the analyticity condition we assumed for $a(x,y)$, it can be seen that $a(x,y)$ in fact only depends on $z=x/y$. We shall abuse our previous notation by referring to $a(z)$.

VII. THE CONVERGENCE OF THE SERIES BY NUMBER THEORY, $|q|=1$

The radius of convergence R of the series (13) is given by

$$R^{-1}=\limsup_{n\to+\infty}\left|\frac{1}{n}\cdot\frac{1-q^{2n}}{1+q^{2n}}\right|^{1/(2n)}=\limsup_{n\to+\infty}\left|\frac{1-q^{2n}}{1+q^{2n}}\right|^{1/(2n)}. \tag{15}$$

We see that the series is not even defined if q is an even root of -1. For any other root of unity the series has radius of convergence 1, except for $q=\pm 1$, when the series terminates. Now consider the case $q=e^{2\pi i\tau}$, where τ is irrational.

Call $n\in\mathbb{N}$ type 1 if $|1-q^{2n}|<1$, which implies that $|1+q^{2n}|\geqslant 1$. Then

$$\limsup_{n\to+\infty,\ \text{type 1}}\left|\frac{1-q^{2n}}{1+q^{2n}}\right|^{1/(2n)}\leqslant\limsup_{n\to+\infty,\ \text{type 1}}1=1.$$

Call $n\in\mathbb{N}$ type 2 if $|1-q^{2n}|\geqslant 1$, in which case

$$\limsup_{n\to+\infty,\ \text{type 2}}\left|\frac{1-q^{2n}}{1+q^{2n}}\right|^{1/(2n)}\geqslant\limsup_{n\to+\infty,\ \text{type 2}}\left|\frac{1}{1+q^{2n}}\right|^{1/(2n)}\geqslant 1,$$

and we deduce that

$$R^{-1}=\limsup_{n\to+\infty,\ \text{type 2}}\left|\frac{1-q^{2n}}{1+q^{2n}}\right|^{1/(2n)}.$$

Then we find

$$\limsup_{n\to+\infty,\ \text{type 2}}\left|\frac{1}{1+q^{2n}}\right|^{1/(2n)}\leqslant R^{-1}\leqslant\limsup_{n\to+\infty,\ \text{type 2}}\left|\frac{2}{1+q^{2n}}\right|^{1/(2n)},$$

which implies

$$R^{-1}=\limsup_{n\to+\infty,\ \text{type 2}}\left|\frac{1}{1+q^{2n}}\right|^{1/(2n)}=\limsup_{n\to+\infty}\left|\frac{1}{1+q^{2n}}\right|^{1/(2n)}. \tag{16}$$

If we let $d(\tau,n)$ be the minimum distance from $4\pi in\tau$ to an odd multiple of πi, then $d(\tau,n)\geqslant|1+q^{2n}|\geqslant(2/\pi)\,d(\tau,n)$, so

$$R=\liminf_{n\to+\infty}\left(\min_{p\ \text{odd}}|4\pi in\tau-p\pi i|\right)^{1/(2n)}=\liminf_{n\to+\infty}\left(\min_{p\ \text{odd}}\left|\tau-\frac{p}{4n}\right|\right)^{1/(2n)}\leqslant 1. \tag{17}$$

We see that the radius of convergence of the power series is dependent on how well τ can be approximated by rational numbers. Fortunately many results are known in this area,[8] and we shall use one of these now.

Suppose that the irrational number $\tau\in\mathbb{R}$ is *algebraic* of degree $k>1$ (this means that it is a root of a polynomial of degree k with integer coefficients). Then there is a constant $K>0$ so that for all n and all $p\in\mathbb{Z}$

$$\left|\tau-\frac{p}{4n}\right|\geqslant\frac{K}{(4n)^k}.$$

From the formula for R above (17)

$$R\geqslant\liminf_{n\to+\infty}\left(\frac{K}{2^k(2n)^k}\right)^{1/(2n)}=1,$$

so we conclude that for any irrational algebraic number τ, the radius of convergence is 1.

To get a radius of convergence less than 1, we shall have to create an irrational number with very good rational approximations. Let

$$\tau=\sum_{s\geqslant 1}\frac{1}{4m_s}, \tag{18}$$

where the strictly positive integers m_s have the property that $4m_s$ divides m_{s+1} for all $s\geqslant 1$. If we set $n=m_t$, then

$$\frac{n}{m_{t+1}}\leqslant|l-4n\tau|\leqslant\frac{2n}{m_{t+1}},$$

for $l=\Sigma_{t\geqslant s\geqslant 1}m_t/m_s$ an odd integer, so

$$\frac{1}{4m_{t+1}}\leqslant\min_{p\ \text{odd}}\left|\tau-\frac{p}{4n}\right|\leqslant\frac{1}{2m_{t+1}}.$$

Then by (17)

$$R\leqslant\liminf_{t\to+\infty}\left(\frac{1}{m_{t+1}}\right)^{1/(2m_t)}.$$

If we set $m_1=1$ and $m_{s+1}=2^{2sm_s}$ for all $s\geqslant 1$, then the radius of convergence of the series (13) for τ given by (18) is zero. Also τ is too closely approximated by nonequal rational numbers to be rational itself.

VIII. THE CONVERGENCE OF THE SERIES BY PROBABILITY, $|q|=1$

We consider the probability that the radius of convergence R of the series (13) is 1, given that q has a uniform distribution on the circle (equivalently, τ has a uniform distribution on [0,1]). From (17), for $0<s<1$

$$P[R>s]=P\left[\liminf_{n\to+\infty}\min_{p\ \text{odd}}\left|\tau-\frac{p}{4n}\right|^{1/(2n)}>s\right]=\lim_{m\to\infty}P\left[\inf_{n\geqslant m}\min_{p\ \text{odd}}\left|\tau-\frac{p}{4n}\right|^{1/(2n)}>s\right]. \tag{19}$$

For any random variable X_n and $s<t<1$,

$$(\forall n\geqslant m\ \ X_n>t)\Rightarrow\inf_{n\geqslant m}X_n>s,$$

or alternatively

$$P[X_n>t\ \ \forall n\geqslant m]\leqslant P[\inf_{n\geqslant m}X_n>s].$$

Then from (19),

$$P[R>s]\geqslant \lim_{m\to\infty} P\left[\min_{p\ \text{odd}}\left|\tau-\frac{p}{4n}\right|^{1/(2n)}>t \quad \forall n\geqslant m\right].$$

If we define

$$A_n(x)=\left\{\tau\in[0,1]:\min_{p\ \text{odd}}\left|\tau-\frac{p}{4n}\right|\leqslant x\right\},$$

then (with superscript c denoting complement)

$$P[R>s]\geqslant \lim_{m\to\infty} P[\cap_{n\geqslant m}A_n(t^{2n})^c].$$

Then by taking complements

$$P[R\leqslant s]\leqslant \lim_{m\to\infty} P[\cup_{n\geqslant m}A_n(t^{2n})]\leqslant \lim_{m\to\infty}\sum_{n\geqslant m} P[A_n(t^{2n})],$$

so if the series

$$\sum_{n\geqslant 1} P[A_n(t^{2n})], \tag{20}$$

converges, then $R>s$ with probability one. If we write

$$A_n(x)=\{\tau\in[0,1]:\min_{p\ \text{odd}}|4n\tau-p|\leqslant 4nx\},$$

then, if $4nx\leqslant 1$, in the interval $[0,4n]$ there are $2n$ odd integers p, and each has a disjoint interval of length $8nx$ about it satisfying the inequality above. From this we find $P[A_n(x)]=4nx$, so the sum (20) becomes (with the exception of a finite number of terms at the beginning),

$$\sum_{n\geqslant 1} 4n\,t^{2n},$$

which converges since $|t|<1$. We conclude that $P[R>s]=1$, and so $R=1$ with probability one. Since the algebraic numbers have measure zero, the series must have $R=1$ for many transcendental (nonalgebraic) τ.

IX. THE CASE $|q|\neq 1$

In this case we would get the same unique series *if* the annulus in which $a(z)$ was analytic and free of zeros or singularities was sufficiently wide. We would need to have both z and $-z/q$ in the same annulus, so the ratio of the outer and inner radii of the annulus would have to be greater than the larger of $|q|$ and $1/|q|$. If this condition was satisfied, we would have the solutions (13) or (14). However there may be other solutions to the normalization which would always have zeros or singularities in such wide annuli.

Let us examine the series (13) for $|q|\neq 1$. Here $\lim_{n\to+\infty}|(1-q^{2n})/(1+q^{2n})|=1$, so the series has radius of convergence 1. However, now we can make an analytic continuation of the series. In the case $|q|<1$ we write, for any integer $k\geqslant 1$

$$\frac{1-q^{2n}}{1+q^{2n}}=1+2\sum_{m=1}^{k}(-1)^m q^{2mn}-\frac{2(-1)^k q^{2(k+1)n}}{1+q^{2n}}, \tag{21}$$

and substituting this into (13) gives

$$b(z)=-\frac{1}{2}\log(q)-\log(1-z^2)-2\sum_{m=1}^{k}(-1)^m\log(1-z^2q^{2m})-\sum_{n\geqslant 1}\frac{2(-1)^k q^{2(k+1)n}z^{2n}}{n(1+q^{2n})}.$$

The last term in the formula tends to zero uniformly on any bounded set as $k\to\infty$, allowing us to take the limit as $k\to\infty$ of the other terms. We then get the infinite product expansion, valid everywhere in $\mathbb{C}^*$,

$$a_+(z)=\frac{1}{r}\cdot\frac{1}{(1-z^2)}\cdot\prod_{\text{odd } m\geqslant 1}\frac{(1-z^2q^{2m})^2}{(1-z^2q^{2(m+1)})^2},\quad |q|<1. \tag{22}$$

A similar rearrangement to (21) for $|q|>1$ would give

$$a_+(z)=\frac{(1-z^2)}{r}\cdot\prod_{\text{odd } m\geqslant 1}\frac{(1-z^2q^{-2(m+1)})^2}{(1-z^2q^{-2m})^2},\quad |q|>1. \tag{23}$$

These are the *unique* (up to a sign) solutions of (12) which are analytic for z in a neighborhood of zero in $\mathbb{C}^*$. In the same way we can analytically extend the series (14) to obtain $a_-(z)=\pm 1/a_+(1/z)$, the *unique* solutions of (11) which are analytic for z in a neighborhood of infinity in $\mathbb{C}^*$.

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Numerical evidence that the perturbation expansion for a non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian is Stieltjes

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Recently, several studies of non-Hermitian Hamiltonians having $\mathcal{PT}$ symmetry have been conducted. Most striking about these complex Hamiltonians is how closely their properties resemble those of conventional Hermitian Hamiltonians. This paper presents further evidence of the similarity of these Hamiltonians to Hermitian Hamiltonians by examining the summation of the divergent weak-coupling perturbation series for the ground-state energy of the $\mathcal{PT}$-symmetric Hamiltonian $H=p^2+\frac{1}{4}x^2+i\lambda x^3$ recently studied by Bender and Dunne. For this purpose the first 193 (nonzero) coefficients of the Rayleigh–Schrödinger perturbation series in powers of λ^2 for the ground-state energy were calculated. Padé-summation and Padé-prediction techniques recently described by Weniger are applied to this perturbation series. The qualitative features of the results obtained in this way are indistinguishable from those obtained in the case of the perturbation series for the quartic anharmonic oscillator, which is known to be a Stieltjes series.
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I. INTRODUCTION

Hamiltonians describing fundamental interactions traditionally possess two symmetries, the continuous symmetry of the proper Lorentz group and the discrete symmetry of Hermiticity. Lorentz invariance is a physical requirement. Hermiticity is a useful mathematical constraint that guarantees that the spectrum is real, although recent work shows that Hermiticity is only a sufficient condition and is not necessary for the reality of eigenvalues. From the assumptions of Lorentz invariance and positivity of the spectrum of the Hamiltonian one can prove the $\mathcal{PCT}$ theorem and thereby establish the physical symmetry of $\mathcal{PCT}$ invariance.

What happens if we impose only the more physical symmetries of Lorentz invariance and $\mathcal{PCT}$ invariance when we construct a Hamiltonian? The constraint of $\mathcal{PCT}$ invariance is weaker than Hermiticity, so Hamiltonians having this property need not be Hermitian. While it has not been proved, there is compelling analytical and numerical evidence supporting the conjecture that, except when $\mathcal{PCT}$ symmetry is spontaneously broken, the energy levels of such Hamiltonians are all real and positive.[1,2] The reality and positivity of the spectrum is apparently a consequence of the $\mathcal{PCT}$ symmetry of H.

Many examples of $\mathcal{PCT}$-symmetric Hamiltonians in quantum field theory have been studied.[3–8] In quantum mechanics, where the $\mathcal{C}$ operator is unity, many examples of $\mathcal{PT}$-symmetric Hamiltonians have also been studied.[9–19] A simple example of such a quantum-mechanical Hamiltonian is $H=p^2+ix^3$. Hamiltonians such as this may be regarded as *complex deformations* of conventional Hermitian Hamiltonians. To understand this deformation we consider the Hamiltonian

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$$H = p^2 - (ix)^{2+\epsilon},$$

where $\epsilon \geqslant 0$. When $\epsilon = 0$, we have the conventional harmonic oscillator Hamiltonian, whose spectrum is real and positive. As ϵ increases from 0, the entire spectrum of the Hamiltonian smoothly deforms as a function of ϵ and remains real and positive for all positive values of ϵ. Thus, these theories are in effect the analytic continuation of conventional quantum mechanics into the complex plane.

These non-Hermitian theories exhibit some remarkable properties. Most interesting is that the expectation value of the operator x in quantum mechanics (and of the field ϕ in quantum field theory) is *nonzero* when $\epsilon > 0$. This is true even for the $p^2 - x^4$ Hamiltonian that one obtains at $\epsilon = 2$ and it is also true for the $-g\phi^4$ scalar quantum field theory. The $-g\phi^4$ quantum field theory is particularly surprising because it has a positive real spectrum and exhibits a nonzero value of $\langle \phi \rangle$. In four-dimensional space–time it has a dimensionless coupling constant, is renormalizable, and is asymptotically free (and thus nontrivial). It may thus provide a useful setting to describe the Higgs particle.[7]

We are struck by the close similarity between the properties of non-Hermitian $\mathcal{PT}$-symmetric quantum-mechanical Hamiltonians and conventional Hermitian Hamiltonians. Moreover, in mathematical terms, we are struck by the strong resemblance between self-adjoint Sturm–Liouville problems and these new complex Sturm–Liouville problems. The purpose of this paper is to present further evidence of this strong similarity by investigating various aspects of Padé summation and Padé prediction of the Rayleigh–Schrödinger perturbation series for the ground-state energy of the complex $\mathcal{PT}$-symmetric Hamiltonian

$$H(\lambda) = p^2 + \tfrac{1}{4}x^2 + i\lambda x^3. \tag{1}$$

Note that this Hamiltonian is $\mathcal{PT}$ symmetric because under parity reflection $\mathcal{P}: p \to -p$ and $\mathcal{P}: x \to -x$ and under time reversal, which is an antiunitary operation, $\mathcal{T}: p \to -p$, $\mathcal{T}: x \to x$, and $\mathcal{T}: i \to -i$.

The Schrödinger equation for the Hamiltonian in (1) reads

$$-\psi''(x) + (\tfrac{1}{4}x^2 + i\lambda x^3)\psi(x) = E\psi(x),$$

where the wave function obeys the boundary conditions $\lim_{|x|\to\infty} \psi(x) = 0$. Note that this Schrödinger equation is obeyed on the *real axis* in the complex-x plane. The wave function vanishes exponentially as $\exp(-2\sqrt{\lambda}|x|^{5/2}/5)$ as $x \to \pm\infty$ on the real axis.

The large-order behavior of the divergent Rayleigh–Schrödinger perturbation series,

$$E_0(\lambda) \sim \frac{1}{2} + \sum_{n=1}^{\infty} b_n \lambda^{2n} \quad (\lambda \to 0^+), \tag{2}$$

for the ground-state energy eigenvalue of the Hamiltonian in (1) has already been examined in Ref. 20, where the first 46 terms of the perturbation expansion had been generated using recursion formulas. It was observed there that the coefficients b_n are all integers, that they alternate in sign, and that their magnitude grows rapidly with n. The first 10 coefficients are listed in Table I.

To calculate the coefficients b_n we make the *ansatz* that the wave function is a formal series in powers of the coupling constant λ and that the coefficient of λ^n has the form of a Gaussian $\exp(-x^2/4)$ times a polynomial of degree $3n$ in the variable x. The eigenvalue $E_0(\lambda)$ automatically appears as a series in powers of λ^2. Thus, for each additional coefficient in the series for E_0 it is necessary to calculate *two* orders in powers of λ for the wave function.

In Ref. 20 it was pointed out that the Hamiltonian (1) describes a $0+1$ dimensional ϕ^3 field theory and that ϕ^3 theories were the first quantum field theories in which the divergences of

TABLE I. The first ten coefficients b_n in the perturbation expansion (2) for the ground state energy of the complex $\mathcal{PT}$-symmetric Hamiltonian (1).

n	b_n
1	11
2	−930
3	158 836
4	−385 016 10
5	117 779 675 16
6	−430 004 827 146 0
7	181 521 520 337 834 4
8	−868 277 986 898 581 530
9	464 025 598 165 231 889 260
10	−274 145 574 452 876 905 074 540

perturbation theory were studied.[21] Using the standard methods for determining the large-order behavior of perturbation theory[22,23] it can be shown that the leading large-n behavior of the coefficients b_n is given by

$$b_n=(-1)^{n+1}60^{n+1/2}(2\pi)^{-3/2}\Gamma(n+1/2)[1+O(1/n)] \quad (n\to\infty). \tag{3}$$

This asymptotic behavior was verified numerically in Ref. 20. There, it was also shown that the first correction term to this leading asymptotic behavior, which is proportional to $1/n$, is negative. Although divergent, the series in (2) is Borel summable.[24–27] If the factor of i were absent from the Hamiltonian (1), then the perturbation coefficients b_n would not alternate in sign and the perturbation series would not be Borel summable.

It is interesting that to derive the asymptotic formula in (3) one must use dispersion-relation techniques that rely on crucial assumptions about the analyticity of the function $E_0(\lambda)$. These assumptions are justified for the Hermitian Hamiltonian of the anharmonic oscillator,[28,29]

$$\mathcal{H}(\beta)=p^2+x^2+\beta x^4. \tag{4}$$

However, the validity of these assumptions is unproved for the non-$\mathcal{PT}$-symmetric λx^3 oscillator.

The eigenvalues $\mathcal{E}(\beta)$ of the quartic anharmonic oscillator possess several other properties which closely resemble those of the eigenvalues $E(\lambda)$ of the $\mathcal{PT}$-symmetric Hamiltonian (1). For example, the ground-state energy eigenvalue $\mathcal{E}_0(\beta)$ of the quartic anharmonic oscillator possesses a divergent weak-coupling perturbation expansion, which also diverges factorially:[22,30]

$$\mathcal{E}_0(\beta)\sim 1+\sum_{n=1}^{\infty}\mathcal{B}_n\beta^n \quad (\beta\to 0^+), \tag{5}$$

$$\mathcal{B}_n=(-1)^{n+1}\frac{4}{\pi^{3/2}}\left(\frac{3}{2}\right)^{n+1/2}\Gamma(n+1/2)[1+O(1/n)] \quad (n\to\infty). \tag{6}$$

A comparison of the large-order asymptotics (3) and (6) shows that the two perturbation expansions (2) and (5) possess the same rate of divergence if we choose

$$\beta=40\lambda^2. \tag{7}$$

In view of these striking similarities between the ground-state eigenvalues $E_0(\lambda)$ and $\mathcal{E}_0(\beta)$ it should be interesting to investigate what other similarities do exist. In particular, we are interested in similarities that could provide evidence that the Padé summation of the divergent perturbation series (2) for the ground-state energy of the $\mathcal{PT}$-symmetric Hamiltonian (1) converges.

In the case of the ground-state energy shift $\Delta\mathcal{E}_0(\beta)$ of the quartic anharmonic oscillator, which is defined by

$$\mathcal{E}_0(\beta) = 1 + \beta\Delta\mathcal{E}_0(\beta), \tag{8}$$

it was shown rigorously by Simon (Theorem IV.2.1 of Ref. 28) that the corresponding perturbation series is a Stieltjes series. This has some far-reaching consequences. In the case of the Stieltjes series, Padé approximants possess a highly developed convergence theory, as we discuss in detail in Sec. II. In particular, the Stieltjes nature of the perturbation series (5) guarantees that certain subsequences of the Padé table converge to a uniquely determined Stieltjes function.

Although we cannot prove it rigorously, we believe that for the $\mathcal{PT}$-symmetric Hamiltonian (1) the ground-state energy shift $\Delta E_0(\lambda^2)$ defined by

$$E_0(\lambda) = \tfrac{1}{2} + \lambda^2\Delta E_0(\lambda^2), \tag{9}$$

in which E_0 is considered as a function of λ^2, is also a Stieltjes function. This implies that the corresponding perturbation series is a Stieltjes series.

It is the intention of this paper to provide numerical evidence supporting this conjecture. We do this by comparing Padé summations and Padé predictions (see Ref. 31, and references therein) of the perturbation expansions for the ground-state energy shift $\Delta E_0(\lambda^2)$ and for the analogous ground-state energy shift $\Delta\mathcal{E}_0(\beta)$ of the quartic anharmonic oscillator.

Here, one might argue that one should also investigate the summation of the perturbation expansion for the ground-state energy shift $\Delta E_0(\lambda^2)$ with the help of the sequence transformations that were described in Secs. 7 and 8 of Ref. 32 and which produced very good results in the case of the anharmonic oscillators.[30,33,34] However, the convergence theory of these sequence transformations, which in the case of power series also produce rational approximants, is still very much in its infancy and no theoretical results concerning the transformation of the Stieltjes series are known so far. Consequently, we would only produce numbers without gaining any further mathematical insight.

In Sec. II, we present the relevant details of Padé approximants, the computation of Padé approximants by means of Wynn's recursive epsilon algorithm,[35] and we discuss the Stieltjes series and their associated Stieltjes functions. In Sec. III, we show that the Padé summation of the perturbation expansions for $\Delta E_0(\lambda^2)$ and $\Delta\mathcal{E}_0(\beta)$, respectively, produces results of identical quality if the two coupling constants λ and β satisfy (7). In Sec. IV, we discuss the prediction of unknown perturbation coefficients with the help of Wynn's epsilon algorithm, and we show that the coefficients of the perturbation expansions for either $\Delta E_0(\lambda^2)$ or $\Delta\mathcal{E}_0(\beta)$ can be predicted equally well. Finally, in Sec. V we give a brief summary.

Here, we would like to emphasize that we are fully aware that our approach, which uses only a *finite* number of perturbation series coefficients, has obvious limitations. While it is in this way possible to disprove the Stieltjes nature of a given series, it is not possible to prove rigorously its Stieltjes nature. Nevertheless, we believe that our numerical results are interesting and provide some insight into the nature of the $\mathcal{PT}$-symmetric Hamiltonian (1) and of its associated divergent Rayleigh–Schrödinger perturbation series (2).

II. PADÉ APPROXIMANTS, WYNN'S EPSILON ALGORITHM, AND STIELTJES SERIES

In recent years, Padé approximants have become the standard tool in theoretical physics to overcome problems with slowly convergent or divergent power series. Accordingly, there is a vast literature on the mathematical properties of Padé approximants as well as on their applications in theoretical physics. Any attempt to provide a reasonably complete bibliography would be beyond the scope of this paper (see, e.g., the extensive bibliography compiled by Brezinski[36]). We just mention that the popularity of Padé approximants in theoretical physics can be traced back to a review by Baker,[37] that the first specialized monograph on Padé approximants is due to Baker,[38] and that currently the most complete source of information is the second edition of the monograph

by Baker and Graves-Morris.[39] In addition to treatments in more mathematically oriented books on continued fractions and related topics,[40–43] Padé approximants are also discussed in books on mathematical and theoretical physics, e.g., in Sec. 8 of the book by Bender and Orszag,[26] or in Part III of a book by Baker on critical phenomena.[44] Then, there is a book by Pozzi[45] on the use of Padé approximants in fluid dynamics. Finally, there is even a monograph[46] and two articles[47,48] on the history of Padé approximants and related topics.

A Padé approximant $P_m^l(z)$ to a function f possessing a (formal) power series expansion

$$f(z)=\sum_{\nu=0}^{\infty}\gamma_\nu z^\nu, \tag{10}$$

which may converge or diverge, is the ratio of two polynomials $A_l(z)$ and $B_m(z)$ of degrees l and m in z (p. 383 of Ref. 26):

$$P_m^l(z)=\frac{A_l(z)}{B_m(z)}=\frac{a_0+a_1z+a_2z^2+\cdots a_lz^l}{1+b_1z+b_2z^2+\cdots b_mz^m}. \tag{11}$$

An alternative notation for Padé approximants, which is used in the books by Baker and Graves-Morris,[38,39] is $P_m^l(z)=[l/m]_f(z)$. This notation is usually simplified further to $P_m^l(z)=[l/m]$ if explicit references to f and z are not necessary.

The coefficients a_λ and b_μ of the polynomials $A_l(z)$ and $B_m(z)$ in (11) are chosen in such a way that the Taylor expansion of $f(z)$ and of its Padé approximant agree as far as possible:

$$f(z)-P_m^l(z)=O(z^{l+m+1})\quad(z\to 0). \tag{12}$$

This asymptotic error estimate leads to a system of linear equations by means of which the coefficients $a_0,\ a_1,\ldots,\ a_l$ and $b_1,\ b_2,\ldots,\ b_m$ in (11) can be computed.[38,39] Moreover, several algorithms are known which permit a recursive computation of Padé approximants. A discussion of the merits and weaknesses of the various computational schemes can for instance be found in Sec. II.3 of the book by Cuyt and Wuytack.[49]

Probably, the best known recursive algorithm for Padé approximants is Wynn's epsilon algorithm:[35]

$$\varepsilon_{-1}^{(n)}=0,\quad \varepsilon_0^{(n)}=s_n\quad(n\in\mathbb{N}_0), \tag{13a}$$

$$\varepsilon_{k+1}^{(n)}=\varepsilon_{k-1}^{(n+1)}+1/[\varepsilon_k^{(n+1)}-\varepsilon_k^{(n)}]\quad(k,n\in\mathbb{N}_0). \tag{13b}$$

A compact FORTRAN program for the epsilon algorithm as well as the underlying computational algorithm is described in Sec. 4.3 of Ref. 32.

If the input data $\varepsilon_0^{(n)}=s_n$ of Wynn's epsilon algorithm are the partial sums

$$f_n(z)=\sum_{\nu=0}^{n}\gamma_\nu z^\nu \tag{14}$$

of the formal power series (10) according to $\varepsilon_0^{(n)}=f_n(z)$, then the elements $\varepsilon_{2k}^{(n)}$ with *even* subscripts are Padé approximants to $f(z)$ according to[35]

$$\varepsilon_{2k}^{(n)}=P_k^{k+n}(z). \tag{15}$$

The elements $\varepsilon_{2k+1}^{(n)}$ with *odd* subscripts are only auxiliary quantities, which diverge if the whole transformation process converges.

The epsilon algorithm is a useful numerical algorithm that is applied successfully in a large variety of different fields. Accordingly, there is an extensive literature dealing with it. A fairly complete coverage of the older literature can be found in a book by Brezinski.[50] It may be

interesting to note that the epsilon algorithm is not restricted to scalar sequences but can be generalized to cover vector sequences. A recent review of these developments can be found in Ref. 51.

If one tries to sum a divergent power series by converting its partial sums (14) to Padé approximants, it is usually a good idea to use *diagonal* Padé approximants, whose numerator and denominator polynomials have equal degrees. If this is not possible one should use Padé approximants with numerator and denominator polynomials whose degrees differ as little as possible. If we use the epsilon algorithm for the computation of the Padé approximants, then (15) implies that we should use the elements of the following staircase sequence in the Padé table as approximations to $f(z)$ [see Eq. (4.3-7) of Ref. 32]:

$$P_0^0(z),P_0^1(z),P_1^1(z),\ldots,P_\nu^\nu(z),P_\nu^{\nu+1}(z),P_{\nu+1}^{\nu+1}(z),\ldots. \tag{16}$$

This staircase sequence exploits the available information optimally if the partial sums $f_n(z)$ with $n\geqslant 0$ are computed successively and if, after the computation of each new partial sum, the element of the epsilon table with the highest possible *even* subscript is computed. With the help of the notation $[\![x]\!]$ for the integral part of x, this staircase sequence can be written compactly as follows:

$$\varepsilon_{2[\![n/2]\!]}^{(n-2[\![n/2]\!])}=P_{[\![n/2]\!]}^{n-[\![n/2]\!]}(z) \quad (n=0,1,2,\ldots). \tag{17}$$

As remarked previously, Padé approximants are now used almost routinely to overcome problems with slowly convergent or divergent power series. Hence, their practical usefulness is beyond question. However, from a theoretical point of view, the situation is not so good. So far, a completely satisfactory *general* convergence theory of Padé approximants for essentially arbitrary power series does not exist.

Nevertheless, there is a special class of series, the so-called *Stieltjes* series, which possess a highly developed and elegant convergence theory. In this section we will only discuss those properties of Stieltjes series and Stieltjes functions that are needed to provide numerical evidence that the perturbation expansion for the ground-state energy shift $\Delta E_0(\lambda^2)$ of the complex $\mathcal{PT}$-symmetric Hamiltonian (1), considered as a function of λ^2, is a Stieltjes series. Detailed discussions of the properties of Stieltjes series and their special role in the theory of Padé approximants can be found in Sec. 8.6 of Ref. 26 or in Sec. 5 of Ref. 39.

A function $F(z)$ with $z\in\mathbb{C}$ is called a *Stieltjes* function if it can be expressed as a Stieltjes integral according to

$$F(z)=\int_0^\infty \frac{d\Phi(t)}{1+zt} \quad (|\arg(z)|<\pi). \tag{18}$$

Here, $\Phi(t)$ is a bounded, nondecreasing function taking infinitely many different values on $0\leqslant t<\infty$. Moreover, the moment integrals

$$\mu_n=\int_0^\infty t^n\, d\Phi(t) \quad (n\in\mathbb{N}_0) \tag{19}$$

must be real and finite for all finite values of n. A Stieltjes function can be expressed by its corresponding *Stieltjes* series:

$$F(z)=\sum_{\nu=0}^{\infty} (-1)^\nu \mu_\nu z^\nu. \tag{20}$$

Whether this series converges or diverges depends on the behavior of the Stieltjes moments μ_n as $n\to\infty$.

In a typical Stieltjes summation problem, as it occurs in the context of divergent perturbation expansion, only the numerical values of a finite number of Stieltjes moments μ_n are known. Thus, one has to find a way of constructing an approximation to the unknown Stieltjes function $F(z)$ from a finite string of moments.

Of course, one would also like to have some theoretical evidence that $F(z)$ exists and is uniquely determined by the Stieltjes moments $\{\mu_n\}_{n=0}^{\infty}$. Many necessary and sufficient conditions that guarantee this are known in literature.

Unfortunately, it is normally by no means easy to apply them. For example, a necessary condition that the series (20) is indeed a Stieltjes series is that the Hankel determinants

$$D(m,n)=\begin{vmatrix} \mu_m & \mu_{m+1} & \cdots & \mu_{m+n} \\ \mu_{m+1} & \mu_{m+2} & \cdots & \mu_{m+n+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{m+n} & \mu_{m+n+1} & \cdots & \mu_{m+2n} \end{vmatrix} \tag{21}$$

are positive for all $m,n\geqslant 0$ (see Theorem 5.1.2 on p. 197 of Ref. 39). A straightforward evaluation of such a Hankel determinant is in particular for larger values of n computationally very unattractive. However, these determinants can be evaluated recursively with the help of the Frobenius formula [see Eq. (4.10) on p. 23 of Ref. 39].

Then, there is a sufficient criterion, the so-called Carleman condition (see p. 410 of Ref. 26 or pp. 239 and 240 of Ref. 39), which requires that the series $\Sigma_{j=1}^{\infty}(\mu_j)^{-1/(2j)}$ diverges and thus limits the admissible growth of the moments μ_n as $n\to\infty$.[52] If the condition $D(m,n)>0$ on the determinants as well as the Carleman condition are both satisfied, then the Padé approximants $P_m^{m+j}(z)$ constructed from the partial sums of the moment expansion (20) converge for every $j\geqslant -1$ to the corresponding Stieltjes function $F(z)$ as $m\to\infty$ [see for example Theorem 5.5.1 on p. 240 of Ref. 39].

If only a finite number of moments are known, it is impossible to prove that $D(m,n)>0$ holds for all $m,n\geqslant 0$, and it is also not possible to prove rigorously that the Carleman condition is satisfied, although we would like to emphasize that the large-order formula (3), which was verified numerically in Ref. 20, is in agreement with the Carleman condition.

In this paper, we prefer to use an indirect approach in order to provide evidence that the perturbation series for the energy shift $\Delta E_0(\lambda^2)$ of the $\mathcal{PT}$-symmetric Hamiltonian (1) is indeed a Stieltjes series. For that purpose, let us assume that the moment expansion (20), whose Stieltjes nature we want to establish, is a Stieltjes series. Padé approximants to Stieltjes series possess a highly developed convergence theory, and many conditions and inequalities are known that Padé approximants to a Stieltjes series must satisfy. For example, Padé approximants constructed from the partial sums

$$F_n(z)=\sum_{\nu=0}^{n}(-1)^{\nu}\mu_{\nu}z^{\nu} \tag{22}$$

of the moment expansion (20) for a Stieltjes function $F(z)$ satisfy for $z>0$ the following inequalities (Theorem 15.2 on p. 215 of Ref. 38):

$$(-1)^{j+1}\{P_{m+1}^{m+j+1}(z)-P_m^{m+j}(z)\}\geqslant 0, \tag{23}$$

$$(-1)^{j+1}\{P_m^{m+j}(z)-P_{m-1}^{m+j+1}(z)\}\geqslant 0, \tag{24}$$

$$P_m^m(z)\geqslant F(z)\geqslant P_m^{m-1}(z). \tag{25}$$

It follows from inequality (23) that the Padé sequence $\{P_m^{m+j}(z)\}_{m=0}^{\infty}$ is *increasing* for $z>0$ if j is *odd*, and it is *decreasing* if j is *even*. Moreover, if we set $j=-1$ in (24) and replace m by $m+1$, we obtain the inequality

$$P_{m+1}^{m}(z)\geqslant P_m^{m+1}(z) \quad (m\in\mathbb{N}_0). \tag{26}$$

Thus, if we use Wynn's epsilon algorithm (13) to convert the partial sums (22) to Padé approximants and choose the approximants to $F(z)$ according to (17), then it follows from inequalities (25) and (26) that these Padé approximants satisfy the following inequality if the moment expansion (20) for $F(z)$ is a Stieltjes series:

$$P_m^{m+1}(z)\leqslant F(z)\leqslant P_{m+1}^{m+1}(z) \quad (z>0,\ m\in\mathbb{N}_0). \tag{27}$$

Thus, the approximants (17) produced by Wynn's epsilon algorithm yield for $z>0$ two nesting sequences $P_m^{m+1}(z)=\varepsilon_{2m}^{(1)}$ and $P_{m+1}^{m+1}(z)=\varepsilon_{2m+2}^{(0)}$ of lower and upper bounds to $F(z)$ if the moment expansion (20) is a Stieltjes series.

If only the numerical values of a finite number of Stieltjes moments are available, then it is of course not possible to prove rigorously that the series under consideration is a Stieltjes series. Nevertheless, we can provide considerable evidence that this hypothesis is true if inequality (27) is valid in all cases that can be checked.

III. SUMMATION RESULTS

In this section we want to show that the Padé summation of the perturbation expansion

$$\Delta E_0(\lambda^2)=\sum_{\nu=0}^{\infty} b_{\nu+1}\lambda^{2\nu} \tag{28}$$

for the ground-state energy shift of the $\mathcal{PT}$-symmetric Hamiltonian (1) and of the perturbation expansion

$$\Delta \mathcal{E}_0(\beta)=\sum_{\nu=0}^{\infty} \mathcal{B}_{\nu+1}\beta^{\nu} \tag{29}$$

for the ground-state energy shift of the quartic anharmonic oscillator yield results of virtually identical quality if the two coupling constants λ and β satisfy (7). Moreover, we want to demonstrate numerically that inequality (27), which is satisfied in the case of the Padé summation of a Stieltjes series, is apparently also satisfied. In our summation calculations, we used all coefficients b_ν and $\mathcal{B}_\nu$ with $0\leqslant\nu\leqslant 193$ which had been computed recursively.

In this paper, we compute all Padé approximants with the help of Wynn's epsilon algorithm (13). Thus, the partial sums

$$s_n(\lambda^2)=\sum_{\nu=0}^{n} b_{\nu+1}\lambda^{2\nu} \tag{30}$$

and

$$\sigma_n(\beta)=\sum_{\nu=0}^{n} \mathcal{B}_{\nu+1}\beta^{\nu} \tag{31}$$

are used as input data for Wynn's epsilon algorithm according to $\varepsilon_0^{(n)}=s_n(\lambda^2)$ or $\varepsilon_0^{(n)}=\sigma_n(\beta)$, respectively, and the approximations to the energy shifts are chosen according to (17).

In Table II we present illustrative results of the Padé summation of the perturbation expansion (28) for the ground-state energy shift $\Delta E_0(\lambda^2)$ with $\lambda=1/7$ and of the perturbation expansion (29)

TABLE II. Padé summation of the perturbation expansions (28) and (29) for the ground-state energy shifts $\Delta E_0(\lambda^2)$ and $\Delta\mathcal{E}_0(\beta)$ with $\lambda=1/7$ and $\beta=40/49$, respectively.

n	$s_n(\lambda^2)$	$\sigma_n(\beta)$	$P^{n-[\![n/2]\!]}_{[\![n/2]\!]}(\lambda^2)$	$P^{n-[\![n/2]\!]}_{[\![n/2]\!]}(\beta)$
0	0.110×10^{002}	0.750×10^{000}	11.00 000 000 000 000	0.750 000 000 000 000
1	-0.798×10^{001}	-0.321×10^{000}	−7.97 959 183 673 469	−0.321 428 571 428 571
2	0.582×10^{002}	0.315×10^{001}	6.76 871 520 405 468	0.497 075 017 205 781
3	-0.269×10^{003}	-0.133×10^{002}	3.14 452 476 154 168	0.283 471 705 042 096
4	0.177×10^{004}	0.861×10^{002}	5.92 770 890 838 469	0.444 962 648 249 413
5	-0.134×10^{005}	-0.639×10^{003}	4.84 920 642 167 536	0.379 736 282 027 717
50	0.153×10^{072}	0.684×10^{070}	5.52 416 958 165 793	0.419 249 574 461 710
51	-0.964×10^{073}	-0.432×10^{072}	5.52 416 451 428 038	0.419 249 241 261 250
52	0.620×10^{075}	0.278×10^{074}	5.52 416 888 260 688	0.419 249 527 748 761
53	-0.407×10^{077}	-0.182×10^{076}	5.52 416 531 636 255	0.419 249 293 076 390
54	0.272×10^{079}	0.122×10^{078}	5.52 416 839 738 891	0.419 249 495 310 895
101	-0.210×10^{172}	-0.939×10^{170}	5.52 416 721 141 847	0.419 249 415 925 473
102	0.263×10^{174}	0.118×10^{173}	5.52 416 721 422 990	0.419 249 416 112 202
103	-0.334×10^{176}	-0.149×10^{175}	5.52 416 721 178 460	0.419 249 415 949 529
104	0.427×10^{178}	0.191×10^{177}	5.52 416 721 397 212	0.419 249 416 094 862
105	-0.552×10^{180}	-0.247×10^{179}	5.52 416 721 206 667	0.419 249 415 968 069
150	0.318×10^{279}	0.142×10^{278}	5.52 416 721 306 531	0.419 249 416 033 824
151	-0.590×10^{281}	-0.264×10^{280}	5.52 416 721 305 477	0.419 249 416 033 119
152	0.110×10^{284}	0.493×10^{282}	5.52 416 721 306 436	0.419 249 416 033 760
153	-0.207×10^{286}	-0.928×10^{284}	5.52 416 721 305 579	0.419 249 416 033 187
154	0.392×10^{288}	0.175×10^{287}	5.52 416 721 306 359	0.419 249 416 033 708
188	0.371×10^{367}	0.166×10^{366}	5.52 416 721 306 035	0.419 249 416 033 489
189	-0.860×10^{369}	-0.385×10^{368}	5.52 416 721 306 009	0.419 249 416 033 472
190	0.201×10^{372}	0.898×10^{370}	5.52 416 721 306 033	0.419 249 416 033 488
191	-0.471×10^{374}	-0.211×10^{373}	5.52 416 721 306 011	0.419 249 416 033 474
192	0.111×10^{377}	0.496×10^{375}	5.52 416 721 306 031	0.419 249 416 033 487

for the ground-state energy shift $\Delta\mathcal{E}_0(\beta)$ with $\beta=40/49$. Thus, the two coupling constants λ and β satisfy (7). This implies that the two perturbation expansions, whose partial sums are displayed in columns 2 and 3, should show the same rate of divergence.

Here, we must remember that the larger-order estimates (3) and (6), respectively, imply that the partial sums (30) for the ground-state energy shift $\Delta E_0(\lambda^2)$ of the $\mathcal{PT}$-symmetric Hamiltonian (1) are for all $n\geqslant 0$ at least one order of magnitude greater than the partial sums (31) for the ground-state energy shift $\Delta\mathcal{E}_0(\beta)$ of the quartic anharmonic oscillator. Otherwise, the observed rates of divergence in columns 2 and 3 are virtually identical.

Moreover, the Padé approximants in columns 4 and 5 apparently satisfy inequality (27), which holds if the series to be transformed is a Stieltjes series. If the index n in column 1 is even ($n=2m$), then the diagonal Padé approximants $P^m_m(\lambda^2)$ and $P^m_m(\beta)$ provide upper bounds that strictly decrease with increasing m and, if n is odd ($n=2m+1$), then the Padé approximants $P^{m+1}_m(\lambda^2)$ and $P^{m+1}_m(\beta)$ provide lower bounds that strictly increase with increasing m.

We have done analogous summation calculations also for many other values of the coupling constants λ and β. Of course, the performance of the Padé summations depend very much on the size of the coupling constants. For smaller values of λ and the corresponding β, convergence is better than in Table II, whereas for $\lambda=1$ and $\beta=40$ only the first digit of the summation results stabilize. For larger values of λ and β, Padé summation produces only relatively crude upper and lower bounds. However, we emphasize that the typical qualitative features of the summation results in Table II—the same rate of divergence of two perturbation series and the occurrence of strictly decreasing upper bounds P^m_m and strictly increasing lower bounds P^{m+1}_m—were consistently observed in all cases considered.

Thus, Wynn's epsilon algorithm is apparently unable to detect any substantial difference

between the perturbation series (29) for $\Delta\mathcal{E}_0(\beta)$, whose Stieltjes nature was established rigorously by Simon (Theorem IV.2.1 of Ref. 28), and the perturbation series (28) for $\Delta E_0(\lambda^2)$, whose Stieltjes nature we conjecture.

IV. PADÉ PREDICTIONS

As shown by countless articles from all branches of physics, Padé approximants have become the standard tool to overcome problems with slowly convergent or divergent power series. However, Padé approximants have other useful features that are not as well known yet. For example, Padé approximants can be used to make predictions for higher-order series coefficients that were not used for the construction of the approximant.

On a heuristic level the prediction capability of Padé approximants, which was apparently first noted and used by Gilewicz,[53] can be explained quite easily. Let us assume that the partial sums (14) of the power series for some function $f(z)$ are to be converted to Padé approximants. Then, the *accuracy-through-order* relationship (12) implies that a Padé approximant $P_m^l(z)$ to $f(z)$ can be expressed as the partial sum $f_{l+m}(z)$ from which it was constructed plus a term $z^{l+m+1}\mathcal{R}_m^l(z)$, which was generated by the transformation of the partial sum to the rational approximant:

$$P_m^l(z)=\sum_{\nu=0}^{l+m}\gamma_\nu z^\nu+z^{l+m+1}\mathcal{R}_m^l(z)=f_{l+m}(z)+z^{l+m+1}\mathcal{R}_m^l(z). \tag{32}$$

Similarly, the power series (10) can be expressed as follows:

$$f(z)=\sum_{\nu=0}^{l+m}\gamma_\nu z^\nu+z^{l+m+1}\sum_{\nu=0}^{\infty}\gamma_{l+m+\nu+1}z^\nu=f_{l+m}(z)+z^{l+m+1}\mathcal{F}_{l+m+1}(z). \tag{33}$$

Let us now assume that the indices l and m are so large that the Padé approximant $P_m^l(z)$ provides a sufficiently accurate approximation to $f(z)$. Then, the Padé transformation term $\mathcal{R}_m^l(z)$ must also provide a sufficiently accurate approximation to the truncation error $\mathcal{F}_{l+m+1}(z)$ of the power series. In general, we have no reason to assume that

$$\mathcal{R}_m^l(z)=\mathcal{F}_{l+m+1}(z) \tag{34}$$

might hold *exactly* for finite values of l and m. Consequently, Taylor expansions of $\mathcal{R}_m^l(z)$ and $\mathcal{F}_{l+m+1}(z)$, respectively, will in general produce different results. Nevertheless, the *leading* coefficients of the Taylor expansion for $\mathcal{R}_m^l(z)$ should in such a case provide sufficiently accurate approximations to the corresponding coefficients of the Taylor series for $\mathcal{F}_{l+m+1}(z)$.

It is important to note that this prediction capability of Padé approximants does not depend on the convergence of the power series expansions for $\mathcal{R}_m^l(z)$ and $\mathcal{F}_{l+m+1}(z)$, respectively, which was used implicitly in our heuristic reasoning given previously. Padé approximants are able to make predictions about series coefficients even if the power series (10) for f as well as the power series expansions for $\mathcal{R}_l^m$ and $\mathcal{F}_{l+m+1}(z)$ are only asymptotic as $z\to 0$. This fact explains why the prediction capability of Padé approximants can be so very useful in the case of violently divergent perturbation expansions (see Refs. 31, 54–72, and references therein).

Theoretically, very little is known about the prediction of series coefficients that were not used for the construction of the Padé approximant. A notable exception are again Stieltjes series for which inequalities are known.

Let us assume that the partial sums (22) of the moment expansion for some Stieltjes function $F(z)$ are to be converted to Padé approximants. Such a Padé approximant $P_m^l(z)$ possesses the following power series expansion:

$$P_m^l(z)=\sum_{\nu=0}^{\infty}(-1)^\nu\mu_\nu^{[l/m]}z^\nu. \tag{35}$$

In Theorem 5.2.7 on p. 220 of Ref. 39 it was shown that for all $n \in \mathbb{N}_0$ and for all $l \geqslant m-1$ the coefficients $\mu_n^{[l/m]}$ in (35) are bounded in magnitude by the Stieltjes moments μ_n in (20) according to

$$0 \leqslant \mu_n^{[l/m]} \leqslant \mu_n . \tag{36}$$

This inequality can be used to analyze the Stieltjes nature of a moment expansion of the type of (20). With the help of computer algebra systems like MAPLE or MATHEMATICA it is possible to construct Padé approximants $P_m^l(z)$ in an unspecified symbolic variable z, and this can even be done free of rounding errors if the coefficients of the series to be transformed are exact integers like the coefficients b_n in (2) or exact rational numbers like the coefficients $\mathcal{B}_n$ in (5). In the next step, a leading part of a power series expansion of the Padé approximant must be constructed. The resulting series coefficients can then be compared with the corresponding coefficients of the moment expansion.

Again, this poses no principal problems for computer algebra systems like MAPLE and MATHEMATICA. However, the accuracy-through-order relationship (12) implies that inequality (36), which is to be checked, is by default satisfied for all indices $n \leqslant l+m$, and only for $n \geqslant l+m+1$ we obtain useful information about the Stieltjes nature of the moment expansion, from which the Padé approximant was constructed. Thus, if $l+m$ becomes large, the brute-force approach based on computer algebra systems becomes very demanding both with respect to computer time and memory because it requires both the symbolic construction of complicated Padé approximants and also symbolic differentiations of very high orders.

These computational problems can be simplified considerably with the help of a recently derived recursive scheme (Sec. 3 of Ref. 31) that permits a direct calculation of the transformation term $\mathcal{R}_m^l(z)$ in (32) if the corresponding Padé approximant $P_m^l(z)$ can be computed with the help of Wynn's epsilon algorithm according to (15); that is, for Padé approximants of the type $P_k^{k+n}(z)$ with $k, n \in \mathbb{N}_0$.

It follows from the accuracy-through-order relationship (12) in combination with (15) that $\varepsilon_{2k}^{(n)}$ can be expressed as follows if the partial sums (14) of the power series for some function $f(z)$ are used as input data for Wynn's epsilon algorithm (13):

$$\varepsilon_{2k}^{(n)} = f_{n+2k}(z) + z^{n+2k+1} \varphi_{2k}^{(n)}(z). \tag{37}$$

The quantities $\varphi_{2k}^{(n)}(z)$ can be computed with the help of the recursive scheme in Eq. (3.15) of Ref. 31, which uses the coefficients γ_n of the power series (10) for $f(z)$ as input data, as follows:

$$\varphi_0^{(n)}(z) = 0, \quad n \in \mathbb{N}_0, \tag{38a}$$

$$\varphi_2^{(n)}(z) = \frac{[\gamma_{n+2}]^2}{\gamma_{n+1} - \gamma_{n+2} z}, \quad n \in \mathbb{N}_0, \tag{38b}$$

$$\varphi_{2k+2}^{(n)}(z) = \varphi_{2k}^{(n+2)}(z) + \frac{\alpha_{2k+2}^{(n)}(z)}{\beta_{2k+2}^{(n)}(z)}, \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0, \tag{38c}$$

$$\alpha_{2k+2}^{(n)}(z) = \frac{\gamma_{n+2k+2} + \delta\varphi_{2k}^{(n+1)}(z)}{\gamma_{n+2k+1} + \delta\varphi_{2k}^{(n)}(z)} - \frac{\gamma_{n+2k+2} + \delta\varphi_{2k}^{(n+1)}(z)}{\gamma_{n+2k+1} + z\varphi_{2k}^{(n+1)}(z) - \varphi_{2k-2}^{(n+2)}(z)}, \tag{38d}$$

$$\beta_{2k+2}^{(n)}(z) = \frac{1}{\gamma_{n+2k+2} + \delta\varphi_{2k}^{(n+1)}(z)} - \frac{z}{\gamma_{n+2k+1} + \delta\varphi_{2k}^{(n)}(z)} + \frac{z}{\gamma_{n+2k+1} + z\varphi_{2k}^{(n+1)}(z) - \varphi_{2k-2}^{(n+2)}(z)}, \tag{38e}$$

where

TABLE III. Predictions $b_n^{(0,66)}$ for the coefficients b_{n+68} of the perturbation series (28) for $\Delta E_0(\lambda^2)$ with $0 \leqslant n \leqslant 15$.

n	$b_n^{(0,66)}$	b_{n+68}
0	$-0.118\,625\,502\,281\,564\,111\,353\times 10^{217}$	$-0.118\,625\,502\,281\,564\,111\,358\times 10^{217}$
1	$0.487\,707\,952\,691\,623\,584\,397\times 10^{220}$	$0.487\,707\,952\,691\,623\,585\,158\times 10^{220}$
2	$-0.203\,437\,822\,070\,101\,216\,978\times 10^{224}$	$-0.203\,437\,822\,070\,101\,222\,504\times 10^{224}$
3	$0.860\,803\,267\,021\,875\,481\,138\times 10^{227}$	$0.860\,803\,267\,021\,875\,756\,369\times 10^{227}$
4	$-0.369\,393\,498\,548\,727\,222\,559\times 10^{231}$	$-0.369\,393\,498\,548\,728\,279\,960\times 10^{231}$
5	$0.160\,732\,212\,082\,002\,560\,522\times 10^{235}$	$0.160\,732\,212\,082\,005\,901\,209\times 10^{235}$
6	$-0.709\,026\,471\,212\,486\,114\,145\times 10^{238}$	$-0.709\,026\,471\,212\,576\,489\,701\times 10^{238}$
7	$0.317\,020\,667\,799\,578\,470\,271\times 10^{242}$	$0.317\,020\,667\,799\,793\,728\,631\times 10^{242}$
8	$-0.143\,648\,198\,373\,426\,854\,924\times 10^{246}$	$-0.143\,648\,198\,373\,887\,496\,043\times 10^{246}$
9	$0.659\,514\,281\,085\,804\,565\,498\times 10^{249}$	$0.659\,514\,281\,094\,798\,452\,336\times 10^{249}$
10	$-0.306\,750\,687\,264\,795\,900\,309\times 10^{253}$	$-0.306\,750\,687\,281\,012\,588\,650\times 10^{253}$
11	$0.144\,514\,693\,689\,642\,646\,364\times 10^{257}$	$0.144\,514\,693\,716\,909\,093\,737\times 10^{257}$
12	$-0.689\,498\,329\,409\,437\,387\,151\times 10^{260}$	$-0.689\,498\,329\,840\,371\,816\,155\times 10^{260}$
13	$0.333\,104\,548\,293\,054\,144\,923\times 10^{264}$	$0.333\,104\,548\,937\,521\,023\,558\times 10^{264}$
14	$-0.162\,924\,769\,352\,053\,020\,131\times 10^{268}$	$-0.162\,924\,770\,269\,205\,895\,837\times 10^{268}$
15	$0.806\,654\,532\,549\,091\,198\,441\times 10^{271}$	$0.806\,654\,545\,029\,445\,531\,410\times 10^{271}$

$$\delta\varphi_{2k}^{(n)}(z) = z\varphi_{2k}^{(n+1)}(z) - \varphi_{2k}^{(n)}(z). \tag{39}$$

The rational function $\varphi_{2k}^{(n)}(z)$ can be expressed as a power series in z according to

$$\varphi_{2k}^{(n)}(z) = g_0^{(n,2k)} + g_1^{(n,2k)}z + g_2^{(n,2k)}z^2 + \cdots + g_\nu^{(n,2k)}z^\nu + \cdots. \tag{40}$$

The coefficients $g_\nu^{(n,2k)}$ of this series expansion can be used to predict the coefficients $\gamma_{n+2k+\nu+1}$ with $\nu \geqslant 0$ of the power series expansion (10) for $f(z)$ that were not used for the construction of either $\varepsilon_{2k}^{(n)}$ or $\varphi_{2k}^{(n)}(z)$.

Thus, we can compute the rational function $\varphi_{2k}^{(n)}$ with the help of the recursive scheme (38) in the case of the perturbation series (28) for $\Delta E_0(\lambda^2)$ and (29) for $\Delta\mathcal{E}_0(\beta)$. In the case of the $\mathcal{PT}$-symmetric perturbation series we obtain the expansion

$$\varphi_{2k}^{(n)}(\lambda^2) = b_0^{(n,2k)} + b_1^{(n,2k)}\lambda^2 + b_2^{(n,2k)}\lambda^4 + \cdots + b_\nu^{(n,2k)}\lambda^{2\nu} + \cdots, \tag{41}$$

and in the case of the perturbation series for the quartic anharmonic oscillator we obtain

$$\varphi_{2k}^{(n)}(\beta) = \mathcal{B}_0^{(n,2k)} + \mathcal{B}_1^{(n,2k)}\beta + \mathcal{B}_2^{(n,2k)}\beta^2 + \ldots + \mathcal{B}_\nu^{(n,2k)}\beta^\nu + \cdots. \tag{42}$$

The coefficients $b_\nu^{(n,2k)}$ and $\mathcal{B}_\nu^{(n,2k)}$ with $\nu \geqslant 0$ can be used to obtain predictions for the coefficients $b_{n+2k+\nu+2}$ and $\mathcal{B}_{n+2k+\nu+2}$, respectively, that were not used for the construction of the Padé approximants $\varepsilon_{2k}^{(n)} = P_k^{k+n}$ or the transformation terms $\varphi_{2k}^{(n)}$.

In Table III we compute the rational function $\varphi_{66}^{(0)}(\lambda^2)$ corresponding to the diagonal Padé approximant $\varepsilon_{66}^{(n)} = P_{33}^{33}(\lambda^2)$ with the help of the recursive scheme (38) from the coefficients b_ν with $1 \leqslant \nu \leqslant 67$. The resulting expansion coefficients $b_\nu^{(0,66)}$ defined in (41) with $\nu \geqslant 0$ provide predictions to the coefficients $b_{\nu+68}$ of the perturbation series (28). All calculations for Table III were done free of rounding errors using the exact rational arithmetics of MAPLE. Only in the final step the coefficients were converted to floating point numbers for the sake of readability.

The results in Table III show that the expansion coefficients $b_\nu^{(0,66)}$ with $\nu \geqslant 0$ provide already remarkably accurate predictions to the corresponding coefficients $b_{\nu+68}$. Moreover, the Stieltjes inequality (36) is satisfied in all cases.

In Table IV we do the same calculations as in Table III, but this time for the ground-state energy shift $\Delta\mathcal{E}_0(\beta)$ of the quartic anharmonic oscillator. Thus, the expansion of the rational function $\varphi_{66}^{(0)}(\beta)$, which is computed from the coefficients $\mathcal{B}_\nu$ with $1 \leqslant \nu \leqslant 67$ of the perturbation series (29), provides predictions $\mathcal{B}_\nu^{(0,66)}$ to the coefficients $\mathcal{B}_{\nu+68}$.

TABLE IV. Predictions $\mathcal{B}_n^{(0,66)}$ for the coefficients $\mathcal{B}_{n+66}$ of the perturbation series (29) for $\Delta E_0(\beta)$ with $0 \leqslant n \leqslant 15$.

n	$\mathcal{B}_n^{(0,66)}$	$\mathcal{B}_{n+68}$
0	$-0.243\,941\,384\,991\,118\,295\,771\times 10^{108}$	$-0.243\,941\,384\,991\,118\,295\,782\times 10^{108}$
1	$0.250\,725\,042\,695\,070\,353\,544\times 10^{110}$	$0.250\,725\,042\,695\,070\,353\,955\times 10^{110}$
2	$-0.261\,457\,030\,278\,874\,510\,535\times 10^{112}$	$-0.261\,457\,030\,278\,874\,517\,978\times 10^{112}$
3	$0.276\,569\,040\,522\,183\,341\,803\times 10^{114}$	$0.276\,569\,040\,522\,183\,434\,367\times 10^{114}$
4	$-0.296\,701\,814\,375\,736\,021\,569\times 10^{116}$	$-0.296\,701\,814\,375\,736\,909\,442\times 10^{116}$
5	$0.322\,749\,390\,515\,363\,534\,568\times 10^{118}$	$0.322\,749\,390\,515\,370\,538\,244\times 10^{118}$
6	$-0.355\,923\,577\,678\,312\,610\,650\times 10^{120}$	$-0.355\,923\,577\,678\,359\,918\,630\times 10^{120}$
7	$0.397\,845\,013\,388\,761\,856\,087\times 10^{122}$	$0.397\,845\,013\,389\,043\,208\,304\times 10^{122}$
8	$-0.450\,670\,140\,529\,734\,425\,361\times 10^{124}$	$-0.450\,670\,140\,531\,237\,820\,183\times 10^{124}$
9	$0.517\,267\,603\,130\,982\,724\,472\times 10^{126}$	$0.517\,267\,603\,138\,312\,496\,560\times 10^{126}$
10	$-0.601\,463\,530\,952\,366\,420\,452\times 10^{128}$	$-0.601\,463\,530\,985\,369\,171\,801\times 10^{128}$
11	$0.708\,383\,831\,448\,709\,420\,419\times 10^{130}$	$0.708\,383\,831\,587\,280\,706\,922\times 10^{130}$
12	$-0.844\,934\,259\,800\,460\,726\,512\times 10^{132}$	$-0.844\,934\,260\,347\,380\,950\,714\times 10^{132}$
13	$0.102\,047\,769\,191\,033\,928\,036\times 10^{135}$	$0.102\,047\,769\,395\,298\,233\,145\times 10^{135}$
14	$-0.124\,779\,572\,617\,585\,209\,351\times 10^{137}$	$-0.124\,779\,573\,343\,562\,971\,244\times 10^{137}$
15	$0.154\,446\,315\,576\,951\,606\,777\times 10^{139}$	$0.154\,446\,318\,044\,174\,985\,350\times 10^{139}$

A comparison of Tables III and IV shows that their qualitative features are identical. In this context it is quite remarkable that although the coefficients b_n grow significantly more rapidly in magnitude than the coefficients $\mathcal{B}_n$, which follows from the large-order estimates (3) and (6), Padé prediction nevertheless yields results of virtually identical quality.

The Padé prediction of unknown series coefficients based on the recursive scheme (38) is certainly computationally simpler than the straightforward symbolic computation and expansion of Padé approximants. The rational function $\varphi_{2k}^{(n)}(z)$ has a simpler structure than $\varepsilon_{2k}^{(n)} = P_k^{k+n}(z)$, and the first $n+2k$ symbolic differentiations can be avoided. Nevertheless, the recursive symbolic computation of the rational function $\varphi_{2k}^{(n)}(z)$ from the coefficients $\gamma_0, \gamma_1, \ldots, \gamma_{n+2k}$ of the power series (10) can become quite demanding, in particular if k becomes large.

The problems connected with the computation of $\varphi_{2k}^{(n)}(z)$ can largely be avoided if one only tries to compute a prediction

$$g_{2k}^{(n)} = g_0^{(n,2k)} \tag{43}$$

for the *first* term γ_{n+2k+1} not used for the construction of either $\varepsilon_{2k}^{(n)}$ or $\varphi_{2k}^{(n)}(z)$. For that purpose, we have only to set $z=0$ in (38). This yields the following recursive scheme [Eq. (3.17) of Ref. 31]:

$$g_0^{(n)} = 0, \quad n \in \mathbb{N}_0, \tag{44a}$$

$$g_2^{(n)} = \frac{[\gamma_{n+2}]^2}{\gamma_{n+1}}, \quad \in \mathbb{N}_0, \tag{44b}$$

$$g_{2k+2}^{(n)} = g_{2k}^{(n+2)} + \frac{[\gamma_{n+2k+2} - g_{2k}^{(n+1)}]^2}{\gamma_{n+2k+1} - g_{2k}^{(n)}} - \frac{[\gamma_{n+2k+2} - g_{2k}^{(n+1)}]^2}{\gamma_{n+2k+1} - g_{2k-2}^{(n+2)}}, \quad k \in \mathbb{N}, \quad n \in \mathbb{N}_0. \tag{44c}$$

The main advantage of this recursive scheme over the recursive scheme (38), from which it was derived, is that it only involves numbers but no symbolic expressions.

In Table V we present selected results for the Padé predictions of the *first* coefficients of the perturbation expansion (28) for $\Delta E_0(\lambda^2)$ and (29) for $\Delta \mathcal{E}_0(\beta)$, which were not used in the Padé approximants $\varepsilon_{2[\![n/2]\!]}^{(n-2[\![n/2]\!])} = P_{[\![n/2]\!]}^{n-[\![n/2]\!]}$ for $2 \leqslant n \leqslant 191$. The first predictions $b_0^{(n-2[\![n/2]\!],2[\![n/2]\!])}$ to b_{n+2} and $\mathcal{B}_0^{(n-2[\![n/2]\!],2[\![n/2]\!])}$ to $\mathcal{B}_{n+2}$ were computed with the help of the recursive scheme (44). For the sake of readability, we present in Table V only the relative errors

TABLE V. Relative errors R_n and $\mathcal{R}_n$ defined in (45) and (46) of the Padé predictions for the first coefficients of the perturbation series (28) and (29) not used for the construction of the rational approximants.

n	R_n	$\mathcal{R}_n$
2	$-0.295\,410\,699$	$-0.316\,117\,394$
3	$-0.207\,610\,910$	$-0.218\,823\,682$
4	$-0.759\,683\,860\times10^{-1}$	$-0.833\,341\,229\times10^{-1}$
5	$-0.483\,909\,816\times10^{-1}$	$-0.522\,231\,970\times10^{-1}$
6	$-0.197\,254\,000\times10^{-1}$	$-0.218\,362\,310\times10^{-1}$
7	$-0.120\,176\,754\times10^{-1}$	$-0.130\,908\,858\times10^{-1}$
50	$-0.258\,379\,657\times10^{-14}$	$-0.273\,374\,025\times10^{-14}$
51	$-0.134\,007\,443\times10^{-14}$	$-0.141\,313\,446\times10^{-14}$
52	$-0.658\,949\,507\times10^{-15}$	$-0.696\,514\,376\times10^{-15}$
53	$-0.341\,294\,856\times10^{-15}$	$-0.359\,600\,798\times10^{-15}$
54	$-0.167\,932\,626\times10^{-15}$	$-0.177\,342\,673\times10^{-15}$
100	$-0.327\,674\,717\times10^{-29}$	$-0.341\,449\,758\times10^{-29}$
101	$-0.166\,900\,610\times10^{-29}$	$-0.173\,636\,626\times10^{-29}$
102	$-0.827\,630\,688\times10^{-30}$	$-0.862\,097\,827\times10^{-30}$
103	$-0.421\,400\,183\times10^{-30}$	$-0.438\,256\,801\times10^{-30}$
104	$-0.208\,999\,229\times10^{-30}$	$-0.217\,623\,211\times10^{-30}$
140	$-0.354\,821\,178\times10^{-41}$	$-0.367\,523\,224\times10^{-41}$
141	$-0.179\,775\,658\times10^{-41}$	$-0.186\,000\,741\times10^{-41}$
142	$-0.893\,606\,384\times10^{-42}$	$-0.925\,378\,776\times10^{-42}$
143	$-0.452\,675\,070\times10^{-42}$	$-0.468\,247\,723\times10^{-42}$
144	$-0.225\,028\,932\times10^{-42}$	$-0.232\,976\,269\times10^{-42}$
187	$-0.295\,089\,701\times10^{-55}$	$-0.304\,045\,084\times10^{-55}$
188	$-0.146\,895\,157\times10^{-55}$	$-0.151\,456\,461\times10^{-55}$
189	$-0.741\,750\,230\times10^{-56}$	$-0.764\,148\,505\times10^{-56}$
190	$-0.369\,259\,543\times10^{-56}$	$-0.380\,666\,936\times10^{-56}$
191	$-0.186\,438\,979\times10^{-56}$	$-0.192\,040\,968\times10^{-56}$

$$R_n=\frac{b_0^{(n-2\llbracket n/2\rrbracket,2\llbracket n/2\rrbracket)}-b_{n+2}}{b_{n+2}} \tag{45}$$

and

$$\mathcal{R}_n=\frac{\mathcal{B}_0^{(n-2\llbracket n/2\rrbracket,2\llbracket n/2\rrbracket)}-\mathcal{B}_{n+2}}{\mathcal{B}_{n+2}}. \tag{46}$$

If the input data of the recursive scheme (44) are exact rational numbers as the coefficients b_n or $\mathcal{B}_n$, then the predictions can be computed free of rounding errors. However, it turned out that the predictions computed in this way were *huge* rational numbers which slowed down computation considerably. Therefore, we used the floating-point arithmetics of MAPLE with an accuracy of 600 decimal digits for the computation of results presented in Table V.

The results in Table V show that the first coefficients not used for the construction of the Padé approximants $\varepsilon_{2\llbracket n/2\rrbracket}^{(n-2\llbracket n/2\rrbracket)}=P_{\llbracket n/2\rrbracket}^{n-\llbracket n/2\rrbracket}$ can be predicted with remarkable accuracy by the recursive scheme (44) if n is sufficiently large. Moreover, the agreement of the relative errors R_n and $\mathcal{R}_n$ is stunning. However, for our purposes most important is the observation that all relative errors in Table V are negative which is in agreement with the Stieltjes inequality (36).

Thus, the prediction results of this section show that there is no significant difference between the prediction of coefficients b_n of the perturbation series (28), whose Stieltjes nature we want to establish, and the prediction of the coefficients $\mathcal{B}_n$ of the analogous quartic anharmonic oscillator perturbation series (29), whose Stieltjes nature was established rigorously by Simon (Theorem

IV.2.1 of Ref. 28). Accordingly, these results provide further numerical evidence that the perturbation series (28) for the ground-state energy shift $\Delta E_0(\lambda^2)$ is indeed a Stieltjes series.

V. SUMMARY AND CONCLUSIONS

As shown by countless monographs or articles, the mathematical theory of the conventional Hermitian Hamiltonians of quantum mechanics is well established and has reached a high degree of sophistication. Moreover, the divergence and the summation of the perturbation expansions resulting from these Hamiltonians is also comparatively well understood, in particular in the case of the Padé summation of Stieltjes series. In contrast, the rigorous mathematical theory of non-Hermitian, $\mathcal{PT}$-symmetric Hamiltonians is virtually nonexistent. It is not known whether divergent perturbation expansions resulting from such Hamiltonians can be summed to yield a uniquely determined result. Consequently, the best we can do for the moment is to perform numerical studies from which we can try to draw general qualitative conclusions.

The main intention of this paper is to provide numerical evidence that the perturbation series (28) for the ground-state energy shift $\Delta E_0(\lambda^2)$ is a Stieltjes series, because this would guarantee that certain subsequences of the Padé table constructed from the partial sums of this perturbation series converge to a uniquely determined summation result, as discussed in Sec. II.

If the Padé approximants are computed with the help of Wynn's recursive algorithm (13) according to (15) and (17)—as it is done in this paper—and if the series to be transformed is the moment expansion of a Stieltjes function, then the Padé approximants must satisfy inequality (27). As shown in Table II, the Padé summation results for the perturbation series (28) for the ground-state energy shift $\Delta E_0(\lambda^2)$ as well as for the analogous perturbation series (29) for the ground-state energy shift $\Delta \mathcal{E}_0(\beta)$ of the quartic anharmonic oscillator, which is known to be a Stieltjes series, satisfy this inequality. Moreover, the divergence of the two perturbation expansions (28) and (29) as well as as the convergence of their Padé summation results is virtually indistinguishable if the two coupling constants λ and β satisfy (7).

If a Padé approximant $P_m^l(z)$ constructed from the partial sums (22) of the moment expansion for a Stieltjes function $F(z)$ is expanded in power series around $z=0$ according to (35), then this series must be strictly alternating for $z>0$ just like the Stieltjes series for $F(z)$. Moreover, the coefficients $\mu_n^{[l/m]}$ of this expansion are bounded in magnitude by the Stieltjes moments μ_n according to inequality (36).

Thus, via inequality (36) it can be checked whether a moment expansion of the type of (20) is a Stieltjes series. However, the accuracy-through-order relationship (12) implies that this inequality is by default satisfied for all indices $n \leqslant l+m$, and only for $n \geqslant l+m+1$ do we obtain useful information. In particular for large values of l and m, the symbolic construction of Padé approximants and their subsequent expansion may become quite demanding both with respect to time and memory.

These computational problems can to some extent be overcome by expressing the Padé approximants $P_k^{k+n}(z)$, that can be computed with the help of Wynn's epsilon algorithm, according to (37) by the partial sum from which it was constructed plus the transformation term $z^{n+2k+1}\varphi_{2k}^{(n)}(z)$. The quantities $\varphi_{2k}^{(n)}(z)$ can be computed recursively with the help of (38), and their computation is less demanding than the recursive computation of the corresponding Padé approximants $P_k^{k+n}(z)$. Moreover, the Taylor expansion of $\varphi_{2k}^{(n)}(z)$ according to (40) yields the desired coefficients $\mu_{n+2k+\nu+1}^{[k+n/k]}$ with $\nu \geqslant 0$.

In Tables III and IV, we proceed as described previously and confirm the validity of the Stieltjes inequality (36) in the case of the first 15 coefficients of the quantities $\varphi_{66}^{(0)}(\lambda^2)$ and $\varphi_{66}^{(0)}(\beta)$ corresponding to the Padé approximants $P_{33}^{33}(\lambda^2)$ and $P_{33}^{33}(\beta)$, respectively. In this context, it is remarkable that the quality of the predictions is virtually indistinguishable although the coefficients b_n of the $\mathcal{PT}$-symmetric perturbation series grow much more rapidly than the coefficients $\mathcal{B}_n$ for the quartic anharmonic oscillator.

For larger values of n and k the symbolic computation of the quantities $\varphi_{2k}^{(n)}(z)$ via the recursive scheme (38) becomes quite demanding. In such a case, it is much simpler to compute

only the prediction for the first series coefficient not used for the computation of $\varphi_{2k}^{(n)}(z)$. This can be done with the help of the recursive scheme (44). In Table V we show that all first predictions, which we can compute from the coefficients b_ν and $\mathcal{B}_\nu$ with $1 \leqslant \nu \leqslant 192$, satisfy the Stieltjes inequality (36). Moreover, the quality of the prediction results is again virtually identical.

We are of course aware that numerical results cannot replace rigorous mathematical proofs. Nevertheless, we believe that our numerical experiments are both interesting and useful, and that they provide considerable evidence that the perturbation series (28) for the ground-state energy shift $\Delta E_0(\lambda^2)$ of the $\mathcal{PT}$-symmetric Hamiltonian (1) is indeed a Stieltjes series, which would imply that the Padé summation of this divergent perturbation series converges.

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Wave equations with point interactions in finite energy spaces

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Given the abstract wave equation $\ddot{\phi}-\Delta_\alpha\phi=0$, where Δ_α is the Laplace operator with a point interaction of strength α, we define and study $\overline{W}_\alpha$, the associated wave generator in the phase space of finite energy states. We prove the existence of the phase flow generated by $\overline{W}_\alpha$, and describe its most relevant properties with a particular emphasis on the associated symplectic structure and scattering theory.
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I. INTRODUCTION

To introduce the problem we begin with a well known example. Given the free scalar, *zero mass*, wave equation,

$$\ddot{\phi}-\Delta\phi=0, \tag{1}$$

the usual attitude in the literature is to search the solutions in the real Sobolev–Hilbert space $H^2(\mathsf{R}^3)$; in order to fix the notations we recall that $H^s(\mathsf{R}^3)$, $s\in\mathsf{R}$, is defined as the set of tempered distributions with a Fourier transform which is square integrable w.r.t. the measure with density $(1+|k|^2)^s$. This is a standard mathematical choice but not the more natural one. In fact, Eq. (1) can be written in the first order form

$$\dot{\psi}=W\psi, \tag{2}$$

where the linear operator,

$$W:H^2(\mathsf{R}^3)\oplus H^1(\mathsf{R}^3)\to H^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3),$$

is defined as

$$W\begin{pmatrix}\phi\\ \dot{\phi}\end{pmatrix}=\begin{pmatrix}0 & 1\\ \Delta & 0\end{pmatrix}\begin{pmatrix}\phi\\ \dot{\phi}\end{pmatrix}. \tag{3}$$

Here Δ is the usual Laplace operator viewed as a self-adjoint operator on $L^2(\mathsf{R}^3)$. It is well known that Eq. (2) generates a strongly continuous one parameter group of evolution,

$$U^t:H^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)\to H^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3).$$

This group is energy preserving, i.e., there exists an energy form

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$$\mathcal{E}(\phi,\dot{\phi})=\tfrac{1}{2}(\|\dot{\phi}\|_2^2+\|\sqrt{-\Delta}\,\phi\|_2^2),$$

coinciding with the Hamiltonian of the system, preserved by the flow. Moreover U^t constitutes a group of canonical transformations w.r.t. the symplectic form

$$\omega((\phi,\dot{\phi}),(\varphi,\dot{\varphi})):=\langle\phi,\dot{\varphi}\rangle-\langle\varphi,\dot{\phi}\rangle$$

[$\langle\cdot,\cdot\rangle$ denoting the usual scalar product on $L^2(\mathsf{R}^3)$] and W is nothing but the Hamiltonian vector field corresponding, via ω, to $\mathcal{E}$.

As the form of Hamiltonian $\mathcal{E}$ suggests, a more natural domain for the study of the system described by (3) is the space of the finite energy states, which is larger than the original one, because the first component ϕ of such a state is not necessarily square integrable, as instead is implicit in the standard Sobolev environment recalled above. This more suitable description goes as follows.

Let us define (general and more complete definitions will be given in the following section) $\overline{H}^1(\mathsf{R}^3)$ as the completion of the space $C_0^\infty(\mathsf{R}^3)$ in the norm $\|\sqrt{-\Delta}\,\phi\|_2$. Now it is possible to define the new operator $\overline{W}$ on $\overline{H}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)$, the Hilbert space of finite energy states, by

$$\overline{W}:\overline{H}^2(\mathsf{R}^3)\oplus H^1(\mathsf{R}^3)\to\overline{H}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3),\quad \overline{W}(\phi,\dot{\phi}):=(\dot{\phi},\mathbf{\Delta}\phi),\tag{4}$$

where

$$\overline{H}^2(\mathsf{R}^3):=\{\phi\in\overline{H}^1(\mathsf{R}^3):\mathbf{\Delta}\phi\in L^2(\mathsf{R}^3)\}.$$

It is an easy matter to verify that $\overline{W}$ is a skew-adjoint operator (see, e.g., Ref. 1, Thm. 2.1.2, Ref. 2, Sec. XI.10) so that due to the Stone theorem it defines a strongly continuous one parameter group of evolution,

$$\overline{U}^t:\overline{H}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)\to\overline{H}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3),$$

which is trivially energy preserving, just because the energy coincides with the norm of the Hilbert space, and the flow is given by a group of isometric operators. This procedure generalizes to the case in which one considers an abstract wave equation with a positive self-adjoint operator in the place of $-\Delta$ (see Ref. 3 and Ref. 4, Sec. 8).

Here we consider and study in detail the case in which $-\Delta$ is replaced by $-\Delta_\alpha$, the Laplace operator with a point interaction of strength α (see Sec. II for its precise definition), and construct the corresponding wave generator $\overline{W}_\alpha$; since $-\Delta_\alpha$ is not positive when $\alpha<0$ one cannot directly use the results appearing in Refs. 3 and 4.

The abstract wave equation corresponding to Δ_α, i.e.,

$$\ddot{\phi}-\Delta_\alpha\phi=0,\tag{5}$$

was introduced for the first time in Ref. 5. There, when ϕ is vector-valued and when $\alpha=-mc/e$ (m the phenomenological mass, c the velocity of light, e the electric charge), it is shown that (5) describes the evolution of the electromagnetic field self-interacting with a point particle in the dipole approximation (the so called linearized Pauli–Fierz model). Another model connected with the wave equation (5), often studied in the 1950s and 1960s literature on exact models in quantum field theory, is the so called ''pair theory'' (see Refs. 6–8 and references therein). The classical version of this model is the regularized version of the one we study here, and many at the time unanswered questions about its behavior in the ultraviolet limit find their rigorous collocation in the present work.

In Refs. 5, 9, and 10 it is also shown that the Cauchy problem is well posed on the phase space $D^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)$, $D^1(\mathsf{R}^3)\simeq H^1(\mathsf{R}^3)\oplus\mathsf{R}$, [refer to Sec. II for the definition of $D^1(\mathsf{R}^3)$] and that the corresponding strongly continuous one parameter group of evolution,

$$U_\alpha^t : D^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)\to D^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3),$$

preserves the energy,

$$\mathcal{E}_\alpha(\phi,\dot\phi) := \tfrac{1}{2}(\|\dot\phi\|_2^2 + F_\alpha(\phi,\phi)),$$

where F_α denotes the bilinear form corresponding to the self-adjoint operator $-\Delta_\alpha$. Therefore, analogously to the case of the free wave equation, the problem of defining (5) on the larger space of finite energy states naturally arises. The theory of delta point interactions was originally developed in the context of nonrelativistic quantum mechanics (see Ref. 11 and references therein); this made it natural to use $L^2(\mathsf{R}^3)$ as the underlying Hilbert space and so, in order to define the dynamics on the space of finite energy states, one has to modify the original definition of $-\Delta_\alpha$, to allow the elements of its domain being not square integrable. This is done in Sec. III where we also show (Thm. 3.1) that the operators $\overline{W}_\alpha$ here constructed generate an evolution group $\overline{U}_\alpha^t$, a fact that, in the case $\alpha\leqslant 0$, is not immediately evident. So, as an aside result, a conserved energy form exists; this form however is not positive when $\alpha<0$, and therefore it is not suitable to define the norm of the appropriate phase space.

In Sec. IV we treat the Hamiltonian formulation of the wave equations with delta interactions. Here we solve the problem by giving a complex structure $\mathcal{J}_\alpha$ commuting with the operator $\overline{W}_\alpha$. This leads to an equivalent Schrödinger-like first order formulation which, also in view of a future quantization of the dynamical system under study, plays a key role. The complex structure before mentioned is obtained considering separately the case $\alpha\leqslant 0$ from the other case: in the strictly negative case we obtain an invariant splitting of the phase space and the complex structure in such a way that the Hamiltonian vector field appears separately as a Schrödinger equation both on the stable and unstable part of the phase space; in particular, on the unstable subspace, which is finite dimensional, the Hamiltonian is that of a harmonic repulsor, and the Schrödinger equation is the corresponding ordinary differential equation, as expected.

The last topic treated (see Sec. V) is the scattering theory for the pair of operators $(\overline{W}_\alpha,\overline{W})$. The Hilbert phase spaces for $\overline{W}_\alpha$ and $\overline{W}$ being different, a resort has to be made to the two Hilbert space scattering theory introduced by Kato in Ref. 4. Using the Birman invariance principle and the trace condition of the Birman–Kuroda theorem, we are able to prove the existence of the Möller wave operators and their completeness (Thms. 5.1 and 5.2). As a consequence of the machinery needed for the definition of wave operators, one obtains a relation [see (12)–(14)] between the evolution group (acting on the real Hilbert space of states with finite energy) generated by $\overline{W}_\alpha$ and the unitary group [acting on the complex Hilbert space $L^2_{\mathsf{C}}(\mathsf{R}^3)$, the complexification of $L^2(\mathsf{R}^3)$] generated by $\sqrt{-\Delta_\alpha}$ (in the case $\alpha<0$ one considers only the positive part of the operator). This can be seen as a variation of the procedure applied in Sec. III in case one uses the standard complex structure on $L^2_{\mathsf{C}}(\mathsf{R}^3)$: indeed the two structures are related in a simple way [see (10) and (11)]. The relations (12)–(14) could also be used to define the group $\overline{U}_\alpha^t$, the generator of which is easily seen to be $\overline{W}_\alpha$, providing an alternative proof of the existence of the dynamics.

II. PRELIMINARIES

We start by giving definitions and main properties of the Sobolev type spaces needed in the sequel, and to which we made reference in the Introduction. We define the family of pre-Hilbert spaces $\tilde H^s(\mathsf{R}^3)$, $s\in\mathsf{R}$, as the set of tempered distributions with a Fourier transform (denoted by $\hat{}$ or by $\mathcal{F}$) which is square integrable w.r.t. the measure with density $|k|^{2s}$. The scalar product is defined as

$$\langle \phi_1, \phi_2 \rangle_s := \int_{\mathbb{R}^3} dk\, |k|^{2s} \hat{\phi}_1(k)\, \hat{\phi}_2(k).$$

Note that, when $s>0$, $H^s(\mathbb{R}^3) \subset \tilde{H}^s(\mathbb{R}^3)$ and $\tilde{H}^{-s}(\mathbb{R}^3) \subset H^{-s}(\mathbb{R}^3)$, the embeddings being continuous. Since $|k|^{-2s}$ is locally integrable for any $s<3/2$,

$$\forall s < \tfrac{3}{2}, \quad L^2(\mathbb{R}^3, |x|^{2s}\, dx) \subset \mathcal{S}'(\mathbb{R}^3), \quad \tilde{H}^s(\mathbb{R}^3) \equiv \mathcal{F}^{-1}(L^2(\mathbb{R}^3, |k|^{2s}\, dk)),$$

and thus $\tilde{H}^s(\mathbb{R}^3)$ is complete for any $s<3/2$ and coincides with the usual Riesz potential spaces (see, e.g., Ref. 12, Sec. 7.1.2).

We can then define the isomorphism $(r-s<3/2)$,

$$(-\overline{\Delta})^{s/2}: \tilde{H}^r(\mathbb{R}^3) \to \tilde{H}^{r-s}(\mathbb{R}^3), \quad \mathcal{F}((-\overline{\Delta})^{s/2}\phi)(k) := |k|^s \hat{\phi}(k).$$

Our notation is justified by observing that, in the case $0<r=s<3/2$, $(-\overline{\Delta})^{s/2}$ coincides with the closure of $(-\Delta)^{s/2}: H^s(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$.

Since, contrary to what happens for the usual Sobolev chain $H^s(\mathbb{R}^3)$, $\tilde{H}^r(\mathbb{R}^3)$ is not included in $\tilde{H}^s(\mathbb{R}^3)$ when $r>s$, we also define the sequence of spaces,

$$\overline{H}^n(\mathbb{R}^3) := \bigcap_{k=1}^{n} \tilde{H}^k(\mathbb{R}^3) \equiv \mathcal{F}^{-1}\Big(\bigcap_{k=1}^{n} L^2(\mathbb{R}^3, |x|^{2k}\, dx)\Big).$$

Obvioulsy $\overline{H}^n(\mathbb{R}^3)$ is a Hilbert space with norm

$$\|\phi\|_{\overline{H}^n} := \left(\sum_{k=1}^{n} \|(-\overline{\Delta})^{k/2}\phi\|_2^2 \right)^{1/2}.$$

We come now to point interactions; for their general theory of we refer to Ref. 11; here we confine ourselves to the essential definitions and results. The operator $-\Delta_\alpha$ describing a standard point interaction at the origin with strength α is defined as follows. Let us introduce the dense linear subspace of $L^2(\mathbb{R}^3)$,

$$D^2_\alpha(\mathbb{R}^3) := \left\{ \phi \in L^2(\mathbb{R}^3) : \phi = \phi_\lambda + Q_\phi G_\lambda, \ \ \phi_\lambda \in H^2(\mathbb{R}^3), \left(\alpha + \frac{\sqrt{\lambda}}{4\pi} \right) Q_\phi = \phi_\lambda(\mathbf{0}) \right\},$$

where $0<\lambda \neq -\mathrm{sign}(\alpha)\ (4\pi\alpha)^2$ and

$$G_\lambda(x) = \frac{e^{-\sqrt{\lambda}|x|}}{4\pi|x|}.$$

The Laplacian with a point interaction with strength α is the operator,

$$-\Delta_\alpha : D^2_\alpha(\mathbb{R}^3) \to L^2(\mathbb{R}^3), \quad -\mathbf{\Delta}_\alpha \phi := -\mathbf{\Delta}\phi_\lambda - \lambda Q_\phi G_\lambda .$$

Its resolvent is given by

$$(-\Delta_\alpha + \lambda)^{-1} = (-\Delta + \lambda)^{-1} + \left(\alpha + \frac{\sqrt{\lambda}}{4\pi} \right)^{-1} G_\lambda \otimes G_\lambda ,$$

where $G_\lambda \otimes G_\lambda(\phi) := \langle G_\lambda, \phi \rangle\, G_\lambda$.

The bilinear form corresponding to $-\Delta_\alpha$ has domain $D^1(\mathbb{R}^3) \times D^1(\mathbb{R}^3)$,

$$D^1(\mathbb{R}^3) := \{ \phi \in L^2(\mathbb{R}^3) : \phi = \phi_\lambda + Q_\phi G_\lambda, \phi_\lambda \in H^1(\mathbb{R}^3), \ \ Q_\phi \in \mathbb{R} \},$$

and is defined by

$$F_\alpha(\phi,\varphi) := \langle (-\Delta+\lambda)^{1/2}\phi_\lambda, (-\Delta+\lambda)^{1/2}\varphi_\lambda\rangle - \lambda\langle \phi,\varphi\rangle + \left(\alpha + \frac{\sqrt{\lambda}}{4\pi}\right) Q_\phi Q_\varphi$$

(see Ref. 13). Both the expressions for F_α and $-\Delta_\alpha$ contain the arbitrary parameter λ, but contrary to the appearance, they do not depend on it. Indeed (following Ref. 14, Sec. 2) the operator and form domain can be defined in the following alternative, and more useful, way. Note that, since for any $\lambda>0$,

$$G_\lambda \in L^2(\mathbb{R}^3), \quad G-G_\lambda \in \overline{H}^2(\mathbb{R}^3), \quad (G-G_\lambda)(\mathbf{0}) = \frac{\sqrt{\lambda}}{4\pi},$$

where

$$G(x) = \frac{1}{4\pi|x|},$$

defining

$$\phi_{\mathrm{reg}} := \phi_\lambda + Q_\phi(G_\lambda - G) \in \overline{H}^2(\mathbb{R}^3),$$

we have equivalently,

$$D^2_\alpha(\mathbb{R}^3) = \{\phi \in L^2(\mathbb{R}^3) : \phi = \phi_{\mathrm{reg}} + Q_\phi G, \phi_{\mathrm{reg}} \in \overline{H}^2(\mathbb{R}^3), \quad Q_\phi \in \mathbb{R}, \alpha\, Q_\phi = \phi_{\mathrm{reg}}(\mathbf{0})\}.$$

Correspondingly, the form domain is

$$D^1(\mathbb{R}^3) = \{\phi \in L^2(\mathbb{R}^3) : \phi = \phi_{\mathrm{reg}} + Q_\phi G, \phi_{\mathrm{reg}} \in \overline{H}^1(\mathbb{R}^3), Q_\phi \in \mathbb{R}\},$$

so that, with this definition, the singular part of the field is exactly Coulombian. However such a singular field G *is not in the configuration space* $D^1(\mathbb{R}^3)$. The removal of this incongruence will lead, in the following section, to the introduction of the operator $\overline{W}_\alpha$.

With the domains so given we can redefine the operator and the form as

$$-\Delta_\alpha \phi = -\overline{\Delta}\phi_{\mathrm{reg}}$$

and

$$F_\alpha(\phi,\varphi) = \langle (-\overline{\Delta})^{1/2}\phi_{\mathrm{reg}}, (-\overline{\Delta})^{1/2}\varphi_{\mathrm{reg}}\rangle + \alpha\, Q_\phi Q_\varphi .$$

Now it is well known (see Ref. 11, Chap. I.1) that $-\Delta_\alpha$ is a self-adjoint operator in $L^2(\mathbb{R}^3)$. An important property is that $-\Delta_\alpha$ is positive only for $\alpha \geqslant 0$, whereas for $\alpha<0$ it is only bounded from below; more precisely if $\alpha \geqslant 0$ (*repulsive* delta interactions) the spectrum of the operator is absolutely continuous and coinciding with $[0,+\infty)$; if $\alpha<0$ (*attractive* delta interactions) the spectrum is given by $\{-\lambda_0\}\cup[0,+\infty)$, where $-\lambda_0 = -(4\pi\alpha)^2$ is an isolated negative eigenvalue, and the remaining part of the spectrum is absolutely continuous. In the Schrödinger case this eigenvalue corresponds to a bound state, while in the wave case where one has a second order equation in time, it leads to unstable solutions exponentially running away in the past or in the future (see Refs. 5, 9, 10 and reference therein for the meaning of these well known runaway solutions in classical electrodynamics).

We now come to the wave generator associated to the standard delta operator. Its domain and action are given by

$$W_\alpha : D^2_\alpha(\mathbb{R}^3) \oplus D^1(\mathbb{R}^3) \to D^1(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3),$$

$$W_\alpha \begin{pmatrix} \phi \\ \dot{\phi} \end{pmatrix} = \begin{pmatrix} 0 & \mathbf{1} \\ \Delta_\alpha & 0 \end{pmatrix} \begin{pmatrix} \phi \\ \dot{\phi} \end{pmatrix}. \tag{6}$$

By considering the Hilbert space structure given by $D^1(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \simeq H^1(\mathbb{R}^3) \oplus \mathbb{R} \oplus L^2(\mathbb{R}^3)$ this operator is the generator of a strongly continuous group of operators,

$$U^t_\alpha : D^1(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \to D^1(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3).$$

In the case $\alpha \geqslant 0$ this is an immediate consequence of the skew-adjointness of W_α with respect to the positive energy scalar product on the phase space given by

$$\langle\langle (\phi, \dot{\phi}), (\varphi, \dot{\varphi}) \rangle\rangle_\alpha := \langle \dot{\phi}, \dot{\varphi} \rangle + F_\alpha(\phi, \varphi). \tag{7}$$

More precisely one has the following result (the proof being a straighforward calculation).

Theorem 2.1: *For any $\alpha \in \mathbb{R}$, with respect to the scalar product $\langle\langle \cdot, \cdot \rangle\rangle_\beta$, $\beta \geqslant 0$, one has*

$$D(W^*_\alpha) = D(W_\beta)$$

and

$$W^*_\alpha(\phi, \dot{\phi}) = -\left(\dot{\phi}_{\mathrm{reg}} + \frac{\alpha}{\beta} Q_{\dot{\phi}} G, \overline{\Delta} \phi_{\mathrm{reg}} \right), \quad \beta > 0,$$

$$W^*_\alpha(\phi, \dot{\phi}) = -(\dot{\phi}_{\mathrm{reg}} + Q_{\dot{\phi}} G, \overline{\Delta} \phi_{\mathrm{reg}}) \equiv W_\beta(\phi, \dot{\phi}), \quad \beta = 0 = \alpha.$$

In the case $\alpha < 0$ the operator W_α is readily proven to be a generator by considering the operator

$$W_{\alpha,\lambda}(\phi, \dot{\phi}) := (\dot{\phi}, (\Delta_\alpha - \lambda)\phi_{\mathrm{reg}}),$$

where $\lambda > \lambda_0$. This, being now $-\Delta_\alpha + \lambda$ positive, is skew-adjoint with respect to the scalar product,

$$\langle\langle (\phi, \dot{\phi}), (\varphi, \dot{\varphi}) \rangle\rangle_{\alpha,\lambda} := \langle \dot{\phi}, \dot{\varphi} \rangle + F_\alpha(\phi, \varphi) + \lambda \langle \phi, \varphi \rangle, \tag{8}$$

and so it generates a group of isometries [w.r.t. the Hilbert structure given by (8)]. The original operator W_α, being a perturbation of the previous one by a bounded operator, also generates a strongly continuous group of operators on the phase space (which however are no longer isometries).

We now describe an alternative way to prove that W_α, $\alpha < 0$, is a generator. Such a different method will play a key role in the next sections. As we already said before in the case $\alpha < 0$ the self-adjoint operator $-\Delta_\alpha$ has a negative eigenvalue $-\lambda_0$ (with corresponding normalized eigenvector $4\pi\sqrt{-2\alpha}\, G_{\lambda_0}$) which gives rise to the runaway solutions of the wave equation associated to W_α. Proceeding as in Ref. 10, Sec. 4 (note that there we worked with the different decomposition $\phi = \phi_{\lambda_0} + Q_\phi G_{\lambda_0}$) we consider the linear operator

$$W^{\mathrm{nr}}_\alpha : [D^2_\alpha(\mathbb{R}^3)]_{\mathrm{nr}} \oplus [D^1(\mathbb{R}^3)]_{\mathrm{nr}} \to [D^1(\mathbb{R}^3)]_{\mathrm{nr}} \oplus [L^2(\mathbb{R}^3)]_{\mathrm{nr}},$$

$$W_\alpha \begin{pmatrix} \phi \\ \dot{\phi} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ \Delta^{\mathrm{nr}}_\alpha & 0 \end{pmatrix} \begin{pmatrix} \phi \\ \dot{\phi} \end{pmatrix},$$

where, given any vector subspace $\mathcal{V} \subseteq L^2(\mathbb{R}^3)$, we have defined the corresponding ''nonrunaway'' subspace $[\mathcal{V}]_{\mathrm{nr}}$ by

$$[\mathcal{V}]_{\mathrm{nr}} := \{\phi \in \mathcal{V} : \langle \phi, G_{\lambda_0} \rangle = 0\},$$

and

$$\Delta_\alpha^{\mathrm{nr}} := (\Delta_\alpha)_{|[D^2_\alpha(\mathsf{R}^3)]_{\mathrm{nr}}} \equiv P_{\mathrm{nr}} \cdot (\Delta_\alpha)_{|[D^2_\alpha(\mathsf{R}^3)]_{\mathrm{nr}}},$$

P_{nr} being the orthogonal projector onto $[L^2(\mathsf{R}^3)]_{\mathrm{nr}}$. By simple calculations one has (see Ref. 10, Sec. 4])

$$[D^1(\mathsf{R}^3)]_{\mathrm{nr}} = \{\phi \in D^1(\mathsf{R}^3) : Q_\phi = -4\pi\sqrt{\lambda_0}\,\langle \phi_{\mathrm{reg}}, G_{\lambda_0} \rangle\},$$

$$[D^2_\alpha(\mathsf{R}^3)]_{\mathrm{nr}} = \{\phi \in D^2_\alpha(\mathsf{R}^3) : \phi_{\mathrm{reg}}(0) = \lambda_0\,\langle \phi_{\mathrm{reg}}, G_{\lambda_0} \rangle\},$$

and

$$\begin{aligned}
\Delta_\alpha^{\mathrm{nr}}\phi &= \overline{\Delta}\phi_{\mathrm{reg}} - 8\pi\sqrt{\lambda_0}\,\langle \overline{\Delta}\phi_{\mathrm{reg}}, G_{\lambda_0} \rangle G_{\lambda_0} \\
&= \overline{\Delta}\phi_{\mathrm{reg}} + 8\pi\sqrt{\lambda_0}\,\langle (-\overline{\Delta} + \lambda_0)\phi_{\mathrm{reg}}, G_{\lambda_0} \rangle G_{\lambda_0} - 8\pi\sqrt{\lambda_0}\,\lambda_0\,\langle \phi_{\mathrm{reg}}, G_{\lambda_0} \rangle G_{\lambda_0} \\
&= \overline{\Delta}\phi_{\mathrm{reg}}.
\end{aligned}$$

The *non-negative* bilinear form associated to $-\Delta_\alpha^{\mathrm{nr}}$ is then

$$F_\alpha^{\mathrm{nr}}(\phi, \varphi) = \langle (-\overline{\Delta})^{1/2}\phi_{\mathrm{reg}}, (-\overline{\Delta})^{1/2}\varphi_{\mathrm{reg}} \rangle - 4\pi\,\lambda_0^{3/2}\langle \phi_{\mathrm{reg}}, G_{\lambda_0} \rangle \langle \varphi_{\mathrm{reg}}, G_{\lambda_0} \rangle$$

and W_α^{nr} is skew-adjoint w.r.t. the scalar product

$$\langle\langle (\phi, \dot{\phi}), (\varphi, \dot{\varphi}) \rangle\rangle_\alpha^{\mathrm{nr}} := \langle \dot{\phi}, \dot{\varphi} \rangle + F_\alpha^{\mathrm{nr}}(\phi, \varphi).$$

The strongly continuous one parameter group of evolution generated by W_α^{nr} preserves the *non-negative* energy,

$$\mathcal{E}_\alpha^{\mathrm{nr}}(\phi, \dot{\phi}) := \tfrac{1}{2}(\langle \dot{\phi}, \dot{\phi} \rangle + F_\alpha^{\mathrm{nr}}(\phi, \phi)),$$

which coincides with the Hamiltonian of the system w.r.t. the symplectic form ω (see Ref. 10, Thm. 4.2] for an alternative Hamiltonian picture).

Since $\Delta_\alpha G_{\lambda_0} = \lambda_0 G_{\lambda_0}$, and

$$D^2_\alpha(\mathsf{R}^3) \simeq [D^2_\alpha(\mathsf{R}^3)]_{\mathrm{nr}} \oplus \mathsf{R},$$

$$D^1(\mathsf{R}^3) \simeq [D^1(\mathsf{R}^3)]_{\mathrm{nr}} \oplus \mathsf{R},$$

$$L^2(\mathsf{R}^3) \simeq [L^2(\mathsf{R}^3)]_{\mathrm{nr}} \oplus \mathsf{R},$$

we can write

$$W_\alpha = W_\alpha^{\mathrm{nr}} \times \Lambda_0,$$

where

$$\Lambda_0 : \mathsf{R}^2 \to \mathsf{R}^2, \quad \mathbf{\Lambda}_0(x, \dot{x}) := (\dot{x}, \lambda_0 x).$$

Therefore W_α, $\alpha < 0$, is a generator and

$$U_\alpha^t \equiv e^{tW_\alpha} = e^{tW_\alpha^{\mathrm{nr}}} \times e^{t\Lambda_0}.$$

Here and below, given two linear operators $A_1 : D(A_1) \to H_1$ and $A_2 : D(A_2) \to H_2$, $A_1 \times A_2 : D(A_1) \times D(A_2) \to H_1 \oplus H_2$ denotes the linear operator defined by

$$A_1 \times A_2 (\phi_1, \phi_2) := (A_1 \phi_1, A_2 \phi_2).$$

In conclusion, for any $\alpha \in \mathsf{R}$, U_α^t is a group of canonical transformation w.r.t. the symplectic form ω, and W_α is the Hamiltonian vector field corresponding to the energy

$$\mathcal{E}_\alpha(\phi, \dot{\phi}) = \frac{1}{2}\left(\|\dot{\phi}\|_2^2 + F_\alpha(\phi, \phi) \right) \equiv \mathcal{E}(\phi_{\mathrm{reg}}, \dot{\phi}) + \frac{\alpha}{2} Q_\phi^2.$$

Let us remark that the flow U_α^t can be explicitly calculated (see Ref. 5, Thm. 3.1).

III. THE OPERATOR $\overline{W}_\alpha$

Now we would like to mimic the construction of the energy space for the usual wave generator and the extension of the operator itself, to the case of delta point interactions. To this end, let us define the linear operator,

$$\overline{W}_\alpha : \overline{D}_\alpha^2(\mathsf{R}^3) \oplus D^1(\mathsf{R}^3) \to \overline{D}^1(\mathsf{R}^3) \oplus L^2(\mathsf{R}^3), \quad \overline{W}_\alpha(\phi, \dot{\phi}) := (\dot{\phi}, \overline{\mathbf{\Delta}} \phi_{\mathrm{reg}}),$$

where

$$\overline{D}_\alpha^2(\mathsf{R}^3) := \{ \phi = \phi_{\mathrm{reg}} + Q_\phi G, \phi_{\mathrm{reg}} \in \overline{H}^2(\mathsf{R}^3), Q_\phi \in \mathsf{R}, \alpha\, Q_\phi = \phi_{\mathrm{reg}}(0) \},$$

$$\overline{D}^1(\mathsf{R}^3) := \{ \phi = \phi_{\mathrm{reg}} + Q_\phi G, \phi_{\mathrm{reg}} \in \overline{H}^1(\mathsf{R}^3), Q_\phi \in \mathsf{R} \}.$$

Analogously to the free case, $\overline{D}^1(\mathsf{R}^3) \oplus L^2(\mathsf{R}^3)$ describes now the space of finite energy states. Moreover the Coulombian singularity G *is now in the configuration space* $\overline{D}^1(\mathsf{R}^3)$.

Introducing the Hilbert space structure given by $\overline{D}^1(\mathsf{R}^3) \oplus L^2(\mathsf{R}^3) \simeq \overline{H}^1(\mathsf{R}^3) \oplus \mathsf{R} \oplus L^2(\mathsf{R}^3)$ we want now to show that also in this case $\overline{W}_\alpha$ generates a strongly continuous one parameter group of evolution. When $\alpha > 0$, considering, similarly to the case of W_α, the scalar product,

$$\langle\langle (\phi, \dot{\phi}), (\varphi, \dot{\varphi}) \rangle\rangle_\alpha := \langle \dot{\phi}, \dot{\varphi} \rangle + \langle (-\overline{\Delta})^{1/2} \phi_{\mathrm{reg}}, (-\overline{\Delta})^{1/2} \varphi_{\mathrm{reg}} \rangle + \alpha\, Q_\phi Q_\varphi,$$

one can prove that $\overline{W}_\alpha$ is skew-adjoint and so it is a generator. Note that when $\alpha = 0$, contrary to the situation discussed in the previous section, $\langle\langle \cdot, \cdot \rangle\rangle_\alpha$ is no more a scalar product, being annihilated by the zero energy eigenvector $(G, 0)$ (this fact has to be compared with the presence of a zero energy resonance for $-\Delta_0$). In order to show that also in the case $\alpha \leqslant 0$ $\overline{W}_\alpha$ is a generator one cannot use the same strategy as before consisting in a translation, since the scalar product (8) is now ill-defined, $\overline{D}^1(\mathsf{R}^3)$ being not a subset of $L^2(\mathsf{R}^3)$. So the perturbation argument fails and we are forced to proceed in an alternative way. The decomposition of W_α, $\alpha < 0$, introduced at the end of the previous section is our starting point: we simply extend it to the case of $\overline{W}_\alpha$. Therefore we define, when $\alpha < 0$,

$$[\overline{D}_\alpha^2(\mathsf{R}^3)]_{\mathrm{nr}} = \{ \phi \in \overline{D}_\alpha^2(\mathsf{R}^3) : \phi_{\mathrm{reg}}(\mathbf{0}) = \lambda_0 \langle \phi_{\mathrm{reg}}, G_{\lambda_0} \rangle \}$$

$$[\overline{D}^1(\mathsf{R}^3)]_{\mathrm{nr}} = \{ \phi \in \overline{D}^1(\mathsf{R}^3) : Q_\phi = -4\pi \sqrt{\lambda_0} \langle \phi_{\mathrm{reg}}, G_{\lambda_0} \rangle \},$$

and

$$\overline{W}_\alpha^{\mathrm{nr}}:[\overline{D}_\alpha^2(\mathsf{R}^3)]_{\mathrm{nr}}\oplus[D^1(\mathsf{R}^3)]_{\mathrm{nr}}\to[\overline{D}^1(\mathsf{R}^3)]_{\mathrm{nr}}\oplus[L^2(\mathsf{R}^3)]_{\mathrm{nr}},$$

$$\overline{W}_\alpha^{\mathrm{nr}}(\phi,\dot\phi):=(\dot\phi,\overline{\Delta}_\alpha^{\mathrm{nr}}\phi),$$

where

$$\overline{\Delta}_\alpha^{\mathrm{nr}}:[\overline{D}_\alpha^2(\mathsf{R}^3)]_{\mathrm{nr}}\to[L^2(\mathsf{R}^3)]_{\mathrm{nr}},$$

$$\overline{\Delta}_\alpha^{\mathrm{nr}}\phi:=\overline{\Delta}\phi_{\mathrm{reg}}.$$

With such definitions $\overline{W}_\alpha^{\mathrm{nr}}$ results skew-adjoint with respect to the scalar product on $[\overline{D}^1(\mathsf{R}^3)]_{\mathrm{nr}}\oplus[L^2(\mathsf{R}^3)]_{\mathrm{nr}}$ given by

$$\langle\langle(\phi,\dot\phi),(\varphi,\dot\varphi)\rangle\rangle_\alpha^{\mathrm{nr}}:=\langle\dot\phi,\dot\varphi\rangle+\langle(-\overline{\Delta})^{1/2}\phi_{\mathrm{reg}},(-\overline{\Delta})^{1/2}\varphi_{\mathrm{reg}}\rangle-4\pi\lambda_0^{3/2}\langle\phi_{\mathrm{reg}},G_{\lambda_0}\rangle\langle\varphi_{\mathrm{reg}},G_{\lambda_0}\rangle.$$

Moreover, since

$$\overline{D}_\alpha^2(\mathsf{R}^3)\simeq[\overline{D}_\alpha^2(\mathsf{R}^3)]_{\mathrm{nr}}\oplus\mathsf{R},\quad \overline{D}^1(\mathsf{R}^3)\simeq[D^1(\mathsf{R}^3)]_{\mathrm{nr}}\oplus\mathsf{R},$$

similarly to the case of W_α, we have

$$\overline{W}_\alpha=\overline{W}_\alpha^{\mathrm{nr}}\times\Lambda_0.$$

For the case $\alpha=0$ a similar decomposition is possible by using the projection onto the subspace orthogonal to the eigenvector $(G,0)$. Indeed, defining

$$\overline{W}_{(0)}:\overline{H}_0^2(\mathsf{R}^3)\oplus D^1(\mathsf{R}^3)\to\overline{H}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3),\quad \overline{W}_{(0)}(\phi,\dot\phi):=(\dot\phi_{\mathrm{reg}},\overline{\boldsymbol{\Delta}}\phi),$$

where $\overline{H}_0^2(\mathsf{R}^3):=\{\phi\in\overline{H}^2(\mathsf{R}^3):\phi(\mathbf{0})=\mathbf{0}\}$, the operator $\overline{W}_{(0)}$ is skew-adjoint with respect to the scalar product

$$\langle\langle(\phi,\dot\phi),(\varphi,\dot\varphi)\rangle\rangle_{(0)}:=\langle\dot\varphi,\dot\varphi\rangle+\langle(-\overline{\Delta})^{1/2}\phi,(-\overline{\Delta})^{1/2}\varphi\rangle$$

and, since $\overline{D}^1(\mathsf{R}^3)\simeq\overline{H}^1(\mathsf{R}^3)\oplus\mathsf{R}$, the following decomposition holds:

$$\overline{W}_0=\overline{W}_{(0)}\times 0.$$

We can now state our result regarding the existence of dynamics.

Theorem 3.1: *$\overline{W}_\alpha$ is a closed operator coinciding with the closure of W_α. It generates a strongly continuous group of evolution,*

$$\overline{U}_\alpha^t:\overline{D}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)\to\overline{D}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3),$$

which can be defined as

$$\overline{U}_\alpha^t(\phi,\dot\phi)=\lim_{n\uparrow\infty}U_\alpha^t(\phi_n,\dot\phi),$$

where $\{\phi_n\}_1^\infty\subset D^1(\mathsf{R}^3)$ is any sequence such that $\phi_n\to\phi$ in $\overline{D}^1(\mathsf{R}^3)$.

Proof: $\overline{W}_\alpha$ is a generator since it is skew-adjoint when $\alpha>0$ and $\overline{W}_0=\overline{W}_{(0)}\times 0$, $\overline{W}_\alpha=\overline{W}_\alpha^{\mathrm{nr}}\times\Lambda_0$, $\alpha<0$, where both $\overline{W}_{(0)}$ and $\overline{W}_\alpha^{\mathrm{nr}}$ are skew-adjoint. Therefore $\overline{W}_\alpha$ is closed. By its definition $\overline{W}_\alpha$ is equal to W_α on $D_\alpha^2(\mathsf{R}^3)\oplus D^1(\mathsf{R}^3)$ and so it coincides with the closure of W_α if $D_\alpha^2(\mathsf{R}^3)\oplus D^1(\mathsf{R}^3)$ is a core. This is proven as follows:

analogously to the case of W_α, any $\phi \in \overline{D^2_\alpha}(\mathsf{R}^3)$ admits the representation

$$\phi = \phi_\lambda + Q_\phi G_\lambda ,$$

where

$$\phi_\lambda = \phi_{\mathrm{reg}} - Q_\phi (G_\lambda - G) \in \overline{H^2}(\mathsf{R}^3)$$

and

$$\left(\alpha + \frac{\sqrt{\lambda}}{4\pi} \right) Q_\phi = \phi_\lambda(0).$$

Consider then a sequence ϕ^n_λ in $H^2(\mathsf{R}^3)$ and define

$$\phi_n := \phi^n_\lambda + Q_n G_\lambda \in D^2_\alpha(\mathsf{R}^3),$$

where

$$Q_n := \left(\alpha + \frac{\sqrt{\lambda}}{4\pi} \right)^{-1} \phi^n_\lambda(0).$$

Now if ϕ^n_λ converges in $\overline{H^2}(\mathsf{R}^3)$ to ϕ_λ, we have that Q_n converges to Q_ϕ, thanks to the continuous embedding of $\overline{H^2}(\mathsf{R}^3)$ in $C^0_b(\mathsf{R}^3)$ (see, e.g., Ref. 12, Sec. 5.6.2).

$\overline{W}_\alpha$ being equal to W_α on $D^2_\alpha(\mathsf{R}^3) \oplus D^1(\mathsf{R}^3)$, the same is true for the corresponding groups of evolution. Since $D^2_\alpha(\mathsf{R}^3) \oplus D^1(\mathsf{R}^3)$ is dense in $D^1(\mathsf{R}^3) \oplus L^2(\mathsf{R}^3)$ which is continuously embedded in $\overline{D^1}(\mathsf{R}^3) \oplus L^2(\mathsf{R}^3)$, one has the equality $\overline{U^t_\alpha}(\phi, \dot\phi) = U^t_\alpha(\phi, \dot\phi)$ for any $\phi \in D^1(\mathsf{R}^3)$. The proof is then concluded by the denseness of $D^1(\mathsf{R}^3)$ in $\overline{D^1}(\mathsf{R}^3)$. □

Let us remark, that since $\overline{W}_\alpha$ is the closure of W_α, our construction coincides, in the case $\alpha \geqslant 0$, with the abstract one given in Ref. 3 (see also Ref. 4, Sec. 8 for a similar construction). Moreover, since $W_\alpha = W^{\mathrm{nr}}_\alpha \times \Lambda_0$ when $\alpha < 0$, one has that $\overline{W}^{\mathrm{nr}}_\alpha$ is the closure of W^{nr}_α.

IV. THE SYMPLECTIC STRUCTURE

The standard symplectic structure recalled in the Introduction,

$$\omega((\phi, \dot\phi), (\varphi, \dot\varphi)) := \langle \phi, \dot\varphi \rangle - \langle \varphi, \dot\phi \rangle,$$

it is not well defined on the phase space of finite energy states, i.e., $\overline{D^1}(\mathsf{R}^3) \oplus L^2(\mathsf{R}^3)$. This requires a different approach to the Hamiltonian description of the dynamical system described in the previous paragraph. The problem shows up already in the case of the free wave equation, with the phase space $\overline{H^1}(\mathsf{R}^3) \oplus L^2(\mathsf{R}^3)$; usually in the standard literature on infinite dimensional Hamiltonian systems (see, e.g., Ref. 15) only the easier case of the free field with strictly positive mass is explicitly discussed.

We recall that (see Refs. 16, 15) when the Hilbert space carries a complex structure $\mathcal{J}$, it is possible to complexify the space in such a way that the imaginary part of the complex scalar product turns out to be a symplectic form, while the real part is the old (real) scalar product, coinciding with the energy. Any skew-adjoint operator A *commuting* with $\mathcal{J}$ remains skew-adjoint within the complex Hilbert space, so that $iA := \mathcal{J} \cdot A$ is self-adjoint. Therefore, since $e^{tA} \equiv e^{-it(iA)}$, A generates a strongly continuous group of unitary (hence symplectic) transformations. More precisely, collecting the known results on the subject (see, e.g., Ref. 15, Sec. 2.6, Sec. 2.7, Ref. 16, Chap. II), we state the following.

Theorem 4.1: *Let A be an injective skew-adjoint operator on the real Hilbert space H with inner product $\langle\cdot,\cdot\rangle$. Then the closure of the densely defined linear operator,*

$$A\cdot(-A^2)^{-1/2}:\mathrm{Range}\,(A)\to H,$$

defines a complex structure $\mathcal{J}$ commuting with A. Defining, for any $\psi\in H$, the multiplication by the complex number i as

$$i\,\psi:=\mathcal{J}\psi,$$

H becomes a complex Hilbert space with a Hermitian inner product,

$$[\psi_1,\psi_2]:=\langle\psi_1,\psi_2\rangle+i\,\langle\psi_1,\mathcal{J}\psi_2\rangle.$$

The strongly continuous one parameter group $U^t:=e^{tA}$ is a group of symplectic transformations relative to the symplectic form

$$\Omega(\psi_1,\psi_2):=\mathrm{Im}\,[\psi_1,\psi_2],$$

and the linear vector field,

$$A:D(A)\to H$$

is Hamiltonian with an associated densely defined Hamiltonian function

$$\mathcal{H}:D(\mathcal{Q})\to\mathsf{R},\quad \mathcal{H}(\psi):=\tfrac{1}{2}\,\mathcal{Q}(\psi),$$

where $\mathcal{Q}$ denotes the quadratic form associated to the self-adjoint operator $\mathcal{J}\cdot A$.

A wide class of examples is obtained by the following construction, which is a simple consequence of the above theorem. Let us consider an injective non-negative self-adjoint operator,

$$B:D(B)\to K$$

on the Hilbert space K and let us consider the closure of

$$\begin{pmatrix} 0 & 1 \\ -B^2 & 0 \end{pmatrix}$$

on the Hilbert space $H=\overline{D}(B)\oplus K$, where $\overline{D}(B)$ is the completion of $D(B)$ with respect to the norm $\|u\|_B:=\|Bu\|_K$. In the case in which this closure is injective, the complex structure $\mathcal{J}$ given by the previous theorem is

$$\mathcal{J}_B:\overline{D}(B)\oplus K\to\overline{D}(B)\oplus K,\quad \mathcal{J}_B(u,v)=(\overline{B}^{-1}v,\overline{B}u),$$

where $\overline{B}$ and $\overline{B}^{-1}$ are the closures, respectively, of B and its inverse $B^{-1}:\mathrm{Range}\,(B)\to\overline{D}(B)$. This allows us to endow H with the structure of a complex Hilbert space, which we continue to call H; precisely, defined a generic element as $w:=(u,v)\in\overline{D}(B)\oplus K$, the Hermitian scalar product in H is

$$[w_1,w_2]_B:=\langle\langle w_1,w_2\rangle\rangle_B+i\,\langle\langle w_1,\mathcal{J}_B w_2\rangle\rangle_B,$$

where

$$\langle\langle w_1,w_2\rangle\rangle_B:=\langle\overline{B}u_1,\overline{B}u_2\rangle+\langle v_1,v_2\rangle.$$

On the product $H\times H$ we have the symplectic form

$$\Omega_B : \overline{D}(B) \oplus K \times \overline{D}(B) \oplus K \to \mathsf{R}, \quad \mathbf{\Omega}_B(w_1, w_2) = \langle\langle w_1, \mathcal{J}_B w_2 \rangle\rangle.$$

With respect to the complex variable w, the wave equation,

$$\ddot{u} = -\overline{B^2} u, \tag{9}$$

assumes the Schrödinger-like form,

$$-i\,\dot{w} = \overline{B} w.$$

Moreover such an equation is Hamiltonian w.r.t. the symplectic form Ω_B and the densely defined Hamiltonian function,

$$\mathcal{H}_B : D(\overline{B}^{3/2}) \times D(\overline{B}^{1/2}) \to \mathsf{R}, \quad \mathcal{H}_B(w) = \tfrac{1}{2}(\|\overline{B}^{1/2} v\|^2 + \|\overline{B}^{3/2} u\|^2),$$

where the operator $\overline{B^s}$ is defined as the closure of B^s.

The strongly continuous symplectic group of operators obtained by solving Eq. (9) preserves the energy $\mathcal{E}_B(u,v) := \frac{1}{2}[w,w]_B$.

An immediate example is given by the choice $B = \sqrt{-\Delta} : H^1(\mathsf{R}^3) \to L^2(\mathsf{R}^3)$, corresponding to the standard wave equation and leading to the complex structure

$$\mathcal{J} : \overline{H}^1(\mathsf{R}^3) \oplus L^2(\mathsf{R}^3) \to \overline{H}^1(\mathsf{R}^3) \oplus L^2(\mathsf{R}^3),$$

$$\mathcal{J}(\phi, \dot{\phi}) := ((-\overline{\Delta})^{-1/2} \dot{\phi}, -(-\overline{\Delta})^{1/2} \phi).$$

Other concrete examples are obtained when the operator B^2 is a point interaction, more precisely $B = \sqrt{-\Delta_\alpha} : D^1(\mathsf{R}^3) \to L^2(\mathsf{R}^3)$ with $\alpha > 0$. In this case the corresponding complex structure is given by

$$\mathcal{J}_\alpha : \overline{D}^1(\mathsf{R}^3) \oplus L^2(\mathsf{R}^3) \to \overline{D}^1(\mathsf{R}^3) \oplus L^2(\mathsf{R}^3),$$

$$\mathcal{J}_\alpha(\phi, \dot{\phi}) := ((-\overline{\Delta}_\alpha)^{-1/2} \dot{\phi}, -(-\overline{\Delta}_\alpha)^{1/2} \phi).$$

The same procedure is not directly applicable to the cases $\alpha \leqslant 0$, due to the lack of skew-adjointness and injectivity for the operator $\overline{W}_\alpha$. A natural way out is to project the operator on the subspace of absolute continuity and to apply the abstract scheme to this projection. This works well for the case $\alpha < 0$, whereas the case $\alpha = 0$ deserves a different treatment. Here are the details of the two constructions.

In the case $\alpha < 0$ we have seen in Sec. III that $\overline{W}_\alpha^{\mathrm{nr}}$ is skew-adjoint, w.r.t. the scalar product $\langle\langle \cdot, \cdot \rangle\rangle_\alpha^{\mathrm{nr}}$, and one-to-one. Therefore we can apply to it Thm. 4.1 (or better the successive example with $B = \sqrt{-\Delta_\alpha^{\mathrm{nr}}}$) obtaining the complex structure $\mathcal{J}_\alpha$ commuting with W_α, $\alpha < 0$, defined as

$$\mathcal{J}_\alpha := \mathcal{J}_\alpha^{\mathrm{nr}} \times j,$$

where

$$\mathcal{J}_\alpha^{\mathrm{nr}} : [\overline{D}^1(\mathsf{R}^3)]_{\mathrm{nr}} \oplus [L^2(\mathsf{R}^3)]_{\mathrm{nr}} \to [\overline{D}^1(\mathsf{R}^3)]_{\mathrm{nr}} \oplus [L^2(\mathsf{R}^3)]_{\mathrm{nr}},$$

$$\mathcal{J}_\alpha^{\mathrm{nr}}(\phi, \dot{\phi}) = ((-\overline{\Delta}_\alpha^{\mathrm{nr}})^{-1/2} \dot{\phi}, -(-\overline{\Delta}_\alpha^{\mathrm{nr}})^{1/2} \phi)$$

and

$$j : \mathsf{R}^2 \to \mathsf{R}^2, \quad \mathrm{j}(x, \dot{x}) := (\dot{x}, -x).$$

Here, analogously to the case $\alpha>0$, the linear operators,

$$(-\overline{\Delta}_\alpha^{\mathrm{nr}})^{1/2}:[\overline{D^1}(\mathsf{R}^3)]_{\mathrm{nr}}\to[L^2(\mathsf{R}^3)]_{\mathrm{nr}},$$

and

$$(-\overline{\Delta}_\alpha^{\mathrm{nr}})^{-1/2}:[L^2(\mathsf{R}^3)]_{\mathrm{nr}}\to[\overline{D^1}(\mathsf{R}^3)]_{\mathrm{nr}},$$

are defined as the closures of

$$(-\Delta_\alpha^{\mathrm{nr}})^{1/2}:[D^1(\mathsf{R}^3)]_{\mathrm{nr}}\subset[\overline{D^1}(\mathsf{R}^3)]_{\mathrm{nr}}\to[L^2(\mathsf{R}^3)]_{\mathrm{nr}}$$

and

$$(-\Delta_\alpha^{\mathrm{nr}})^{-1/2}:\mathrm{Range}\,((-\Delta_\alpha^{\mathrm{nr}})^{1/2})\subset[L^2(\mathsf{R}^3)]_{\mathrm{nr}}\to[\overline{D^1}(\mathsf{R}^3)]_{\mathrm{nr}},$$

respectively.

We have then the complex Hilbert space of the couples,

$$(\psi,z):=((\phi,\dot\phi),(x,\dot x))\in[\overline{D^1}(\mathsf{R}^3)]_{\mathrm{nr}}\oplus[L^2(\mathsf{R}^3)]_{\mathrm{nr}}\oplus\mathsf{R}^2,$$

with the Hermitian scalar product

$$[(\psi_1,z_1),(\psi_2,z_2)]_\alpha:=[\psi_1,\psi_2]_\alpha^{\mathrm{nr}}+[z_1,z_2],$$

where

$$[\psi_1,\psi_2]_\alpha^{\mathrm{nr}}:=\langle\langle\psi_1,\psi_2\rangle\rangle_\alpha^{\mathrm{nr}}+i\,\langle\langle\psi_1,\mathcal{J}_\alpha^{\mathrm{nr}}\psi_2\rangle\rangle_\alpha^{\mathrm{nr}},$$

and

$$[z_1,z_2]:=(z_1,z_2)+i\,(z_1,jz_2),\quad (z_1,z_2):=\dot x_1\dot x_2+x_1x_2.$$

The associated symplectic form is

$$\Omega_\alpha:[\overline{D^1}(\mathsf{R}^3)]_{\mathrm{nr}}\oplus[L^2(\mathsf{R}^3)]_{\mathrm{nr}}\oplus\mathsf{R}^2\to\mathsf{R},$$

$$\Omega_\alpha((\psi_1,z_1),(\psi_2,z_2))=\langle\langle\psi_1,\mathcal{J}_\alpha^{\mathrm{nr}}\psi_2\rangle\rangle_\alpha^{\mathrm{nr}}+(z_1,jz_2).$$

With respect to the complex variables (ψ,z) the wave equation corresponding to W_α takes the Schrödinger-like form

$$\begin{cases}-i\,\dot\psi=(-\overline{\Delta}_\alpha^{\mathrm{nr}})^{1/2}\psi,\\ -i\,\dot z=L_0z,\end{cases}\qquad L_0:=\begin{pmatrix}-\lambda_0 & 0\\ 0 & 1\end{pmatrix},$$

and such an equation is Hamiltonian w.r.t. the symplectic form Ω_α and the densely defined Hamiltonian function

$$\mathcal{H}_\alpha:D(\mathcal{Q}_\alpha^{\mathrm{nr}})\oplus\mathsf{R}^2\to\mathsf{R},\quad \mathcal{H}_\alpha(\psi,z)=\tfrac12\,\mathcal{Q}_\alpha^{\mathrm{nr}}(\psi)+\tfrac12\,(L_0z,z),$$

where

$$\mathcal{Q}_\alpha^{\mathrm{nr}}(\phi,\dot\phi)=\tfrac12\,(\|(-\overline{\Delta}_\alpha^{\mathrm{nr}})^{1/4}\dot\phi\|_2^2+\|(-\overline{\Delta}_\alpha^{\mathrm{nr}})^{3/4}\phi\|_2^2)$$

is the quadratic form associated to the self-adjoint operator $\mathcal{J}_\alpha^{\mathrm{nr}}\cdot W_\alpha^{\mathrm{nr}}$.

If $(\phi,\dot{\phi})\in \overline{D}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)$ has the orthogonal decomposition $(\phi,\dot{\phi})\equiv\psi+z\tilde{G}$, where $\tilde{G}$ denotes the normalized eigenvector corresponding to λ_0, then

$$\mathcal{E}_\alpha(\phi,\dot{\phi})=\tfrac{1}{2}[\psi,\psi]^{\mathrm{nr}}_\alpha+\tfrac{1}{2}(L_0 z,z).$$

Therefore, being

$$\overline{U}^t_\alpha=e^{t\overline{W}^{\mathrm{nr}}_\alpha}\times e^{t\Lambda_0},$$

a strongly continuous group of unitary and symplectic transformations, the energy is conserved by the flow.

We come now to the case $\alpha=0$. In this case, in order to apply Thm. 4.1, which requires injectivity, it is necessary to project onto the subspace orthogonal to the eigenvector $(G,0)$. Being $\overline{W}_{(0)}$ one-to-one and skew-adjoint w.r.t. the scalar product $\langle\langle\cdot,\cdot\rangle\rangle_{(0)}$, one can then apply Thm. 4.1 thus obtaining a one parameter group $\overline{U}^t_{(0)}$ of symplectic transformations such that

$$\overline{U}^t_0=\overline{U}^t_{(0)}\times 1,$$

and so $\overline{U}^t_0$ preserves the energy $\mathcal{E}_0(\phi,\dot{\phi})=\mathcal{E}(\phi_{\mathrm{reg},},\dot{\phi})$.

Since $(-\Delta_0)^{1/2}\phi=(-\overline{\Delta})^{1/2}\phi_{\mathrm{reg}}$ (note that this equality holds true only in the case $\alpha=0$) one has

$$\phi_{\mathrm{reg}}=(-\overline{\Delta})^{-1/2}\cdot(-\Delta_0)^{1/2}\phi,$$

and so, when $(\phi,\dot{\phi})\in\overline{H}^2_0(\mathsf{R}^3)\oplus D^1(\mathsf{R}^3)$,

$$\mathcal{J}\cdot\overline{W}_{(0)}(\phi,\dot{\phi})=((-\overline{\Delta})^{1/2}\phi,(-\Delta_0)^{1/2}\dot{\phi})\equiv((-\overline{\Delta}_0)^{1/2}\phi,(-\Delta_0)^{1/2}\dot{\phi}).$$

Moreover, $\mathcal{J}$ commutes with $\overline{W}_{(0)}$ [see (15) in the next section] and so $\mathcal{J}$ coincides with the complex structure associated to $\overline{W}_{(0)}$ by Thm. 4.1. With respect to the complex variable $\psi=(\phi,\dot{\phi})$ the wave equation corresponding to $\overline{W}_{(0)}$ assumes the Schrödinger-like form

$$-i\dot{\psi}=(-\overline{\Delta}_0)^{1/2}\psi.$$

We summarize the results obtained in the following.

Theorem 4.2: *For every $\alpha\in\mathsf{R}\backslash\{\mathbf{0}\}$ there exists a symplectic form,*

$$\Omega_\alpha:\overline{D}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)\times\overline{D}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)\to\mathsf{R},$$

with respect to which the vector field

$$\overline{W}_\alpha:\overline{D}^2_\alpha(\mathsf{R}^3)\times D^1(\mathsf{R}^3)\to\overline{D}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)$$

is Hamiltonian. Moreover for $\alpha\leqslant 0$ the analogous result occurs for the reduced vector fields,

$$\overline{W}^{\mathrm{nr}}_\alpha:[\overline{D}^2_\alpha(\mathsf{R}^3)]_{\mathrm{nr}}\times[\overline{D}^1(\mathsf{R}^3)]_{\mathrm{nr}}\to[\overline{D}^1(\mathsf{R}^3)]_{\mathrm{nr}}\oplus[L^2(\mathsf{R}^3)]_{\mathrm{nr}}$$

and

$$\overline{W}_{(0)}:\overline{H}^2_0(\mathsf{R}^3)\oplus D^1(\mathsf{R}^3)\to\overline{H}^1(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3).$$

For every $\alpha\in\mathsf{R}$ the evolution group $\overline{U}^t_\alpha$ preserves the energy,

$$\mathcal{E}_\alpha(\phi,\dot\phi)=\tfrac{1}{2}(\|\dot\phi\|_2^2+F_\alpha(\phi,\phi)).$$

V. SCATTERING THEORY

The Hilbert spaces where the operators $\overline{W}_\alpha$ and $\overline{W}$ act on, respectively, $\overline{D^1}(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)$ and $\overline{H^1}(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)$, are different (also as sets), and so one is forced to use a two Hilbert space formulation to treat scattering theory for the pair $(\overline{W}_\alpha,\overline{W})$. We refer to the seminal paper by Kato[4] for the relevant constructions and results in scattering theory with two Hilbert spaces. Our approach will follow the lines of the construction given in Ref. 4, Secs. 8–9 (also see Ref. 17, Sec. 3.5).

From now on, given the real vector space $L^2(\mathsf{R}^3)$, we will denote by $L^2_{\mathsf{C}}(\mathsf{R}^3)$ the complex vector space,

$$L^2_{\mathsf{C}}(\mathsf{R}^3):=\{\phi_1+i\phi_2,\phi_1,\phi_2\in L^2(\mathsf{R}^3)\}.$$

We begin introducing the isometries

$$C:\overline{H^1}(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)\to L^2_{\mathsf{C}}(\mathsf{R}^3),$$

$$C(\phi,\dot\phi)\equiv C_0(\phi,\dot\phi):=(-\overline{\Delta})^{1/2}\phi-i\dot\phi,$$

$$C_\alpha:\overline{D^1}(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)\to L^2_{\mathsf{C}}(\mathsf{R}^3),\quad \alpha>0,$$

$$C_\alpha(\phi,\dot\phi):=(-\overline{\Delta}_\alpha)^{1/2}\phi-i\dot\phi,$$

$$C_\alpha:[\overline{D^1}(\mathsf{R}^3)]_{\mathrm{nr}}\oplus[L^2(\mathsf{R}^3)]_{\mathrm{nr}}\to[L^2_{\mathsf{C}}(\mathsf{R}^3)]_{\mathrm{nr}},\quad \alpha<0,$$

$$C_\alpha((\phi,\dot\phi)):=(-\overline{\Delta}^{\mathrm{nr}}_\alpha)^{1/2}\phi-i\dot\phi.$$

These isometries lead to the following relations:

$$\mathcal{J}=C^{-1}\cdot iC, \tag{10}$$

$$\mathcal{J}_\alpha=C_\alpha^{-1}\cdot i\,C_\alpha,\quad \alpha>0,\quad \mathcal{J}^{\mathrm{nr}}_\alpha=C_\alpha^{-1}\cdot i\,C_\alpha,\quad \alpha<0, \tag{11}$$

$$\overline{U}^t=C^{-1}\cdot e^{it\sqrt{-\Delta}}\cdot C,$$

$$\overline{U}^t_0=C^{-1}\cdot e^{it\sqrt{-\Delta_0}}\cdot C\times 1, \tag{12}$$

$$\overline{U}^t_\alpha=C_\alpha^{-1}\cdot e^{it\sqrt{-\Delta_\alpha}}\cdot C_\alpha,\quad \alpha>0, \tag{13}$$

$$\overline{U}^t_\alpha=C_\alpha^{-1}\cdot e^{it\sqrt{-\Delta^{\mathrm{nr}}_\alpha}}\cdot C_\alpha\times e^{t\Lambda_0},\quad \alpha<0. \tag{14}$$

Note that the two equalities,

$$\mathcal{J}=C^{-1}\cdot i\,C,\quad \overline{U}^t_{(0)}=C^{-1}\cdot e^{it\sqrt{-\Delta_0}}\cdot C, \tag{15}$$

imply, as we stated in the previous section, that $\mathcal{J}$ commutes with $\overline{W}_{(0)}$.

Moreover the relations (12)–(14) provide an alternative construction of the dynamics generated by $\overline{W}_\alpha$. In fact one could use such relations as definitions of $\overline{U}^t_\alpha$ and then check by differentiating with respect to the time parameter that this evolution group is generated by the operator $\overline{W}_\alpha$.

We introduce now the identification operators,

$$J_\alpha : \overline{D}^1(\mathbf{R}^3) \oplus L^2(\mathbf{R}^3) \to \overline{H}^1(\mathbf{R}^3) \oplus L^2(\mathbf{R}^3),$$

$$J_\alpha(\phi, \dot{\phi}) := \begin{cases} ((-\overline{\Delta})^{-1/2} \cdot (-\overline{\Delta}_\alpha)^{1/2} \phi, \dot{\phi}), & \text{for } \alpha > 0, \\ (\phi_{\mathrm{reg}}, \dot{\phi}) \equiv ((-\overline{\Delta})^{-1/2} \cdot (-\overline{\Delta}_0)^{1/2} \phi, \dot{\phi}), & \text{for } \alpha = 0, \\ ((-\overline{\Delta})^{-1/2} \cdot (-\overline{\Delta}_\alpha^{\mathrm{nr}})^{1/2} \cdot \Pi_{\mathrm{nr}} \phi, \dot{\phi}), & \text{for } \alpha < 0, \end{cases}$$

where Π_{nr} denotes the projection

$$\Pi_{\mathrm{nr}} : \overline{D}^1(\mathbf{R}^3) \to [\overline{D}^1(\mathbf{R}^3)]_{\mathrm{nr}},$$

and

$$J'_\alpha : \overline{H}^1(\mathbf{R}^3) \oplus L^2(\mathbf{R}^3) \to \overline{D}^1(\mathbf{R}^3) \oplus L^2(\mathbf{R}^3),$$

$$J'_\alpha(\phi, \dot{\phi}) := \begin{cases} ((-\overline{\Delta}_\alpha)^{-1/2} \cdot (-\overline{\Delta})^{1/2} \phi, \dot{\phi}), & \text{for } \alpha > 0 \\ (\phi, \dot{\phi}), & \text{for } \alpha = 0 \\ ((-\overline{\Delta}_\alpha^{\mathrm{nr}})^{-1/2} \cdot P_{\mathrm{nr}} \cdot (-\overline{\Delta})^{1/2} \phi, \dot{\phi}), & \text{for } \alpha < 0. \end{cases}$$

We can then define the Möller wave operators,

$$\Omega_\pm(\overline{W}, \overline{W}_\alpha; J_\alpha) := \text{s-} \lim_{t \to \pm\infty} \overline{U}^{-t} \cdot J_\alpha \cdot \overline{U}_\alpha^t \cdot P_{\mathrm{ac}}(\overline{W}_\alpha),$$

$$\Omega_\pm(\overline{W}_\alpha, \overline{W}; J'_\alpha) := \text{s-} \lim_{t \to \pm\infty} \overline{U}_\alpha^{-t} \cdot J'_\alpha \cdot \overline{U}^t,$$

where

$$P_{\mathrm{ac}}(\overline{W}_\alpha) : \overline{D}^1(\mathbf{R}^3) \oplus L^2(\mathbf{R}^3) \to \overline{D}^1(\mathbf{R}^3) \oplus L^2(\mathbf{R}^3),$$

$$P_{\mathrm{ac}}(\overline{W}_\alpha)(\phi, \dot{\phi}) := \begin{cases} (\phi, \dot{\phi}), & \text{for } \alpha > 0, \\ (\phi_{\mathrm{reg}}, \dot{\phi}), & \text{for } \alpha = 0, \\ (\Pi_{\mathrm{nr}} \phi, P_{\mathrm{nr}} \dot{\phi}), & \text{for } \alpha < 0. \end{cases}$$

Concerning the existence of such wave operators, we have the following

Theorem 5.1: *The Möller wave operators,*

$$\Omega_\pm(\overline{W}, \overline{W}_\alpha; J_\alpha) := \text{s-} \lim_{t \to \pm\infty} \overline{U}^{-t} \cdot J_\alpha \cdot \overline{U}_\alpha^t \cdot P_{\mathrm{ac}}(\overline{W}_\alpha),$$

$$\Omega_\pm(\overline{W}_\alpha, \overline{W}; J'_\alpha) := \text{s-} \lim_{t \to \pm\infty} \overline{U}_\alpha^{-t} \cdot J'_\alpha \cdot \overline{U}^t,$$

exist, are complete and are mutually adjoint isometries, i.e.,

$$\mathrm{Range}\, \Omega_+(\overline{W}, \overline{W}_\alpha; J_\alpha) = \mathrm{Range}\, \Omega_-(\overline{W}, \overline{W}_\alpha; J_\alpha) = \overline{H}^1(\mathbf{R}^3) \oplus L^2(\mathbf{R}^3),$$

$$\mathrm{Range}\, \Omega_+(\overline{W}_\alpha, \overline{W}; J'_\alpha) = \mathrm{Range}\, \Omega_-(\overline{W}_\alpha, \overline{W}; J'_\alpha) = \mathrm{Range}\, P_{\mathrm{ac}}(\overline{W}_\alpha),$$

$$\Omega_{\pm}(\overline{W},\overline{W}_{\alpha};J_{\alpha})^{*}\cdot\Omega_{\pm}(\overline{W},\overline{W}_{\alpha};J_{\alpha})=P_{\mathrm{ac}}(\overline{W}_{\alpha}),$$

$$\Omega_{\pm}(\overline{W}_{\alpha},\overline{W};J'_{\alpha})^{*}\cdot\Omega_{\pm}(\overline{W}_{\alpha},\overline{W};J'_{\alpha})=1_{\overline{H^{1}}(\mathbb{R}^{3})\oplus L^{2}(\mathbb{R}^{3})},$$

$$\Omega_{\pm}(\overline{W},\overline{W}_{\alpha};J_{\alpha})^{*}=\Omega_{\pm}(\overline{W}_{\alpha},\overline{W};J'_{\alpha}).$$

Proof: With the above definitions one has

$$\Omega_{\pm}(\overline{W},\overline{W}_{\alpha};J_{\alpha})=C^{-1}\cdot\Omega_{\pm}(\sqrt{-\Delta},\sqrt{H_{\alpha}};I_{\alpha})\cdot C_{\alpha}\cdot P_{\mathrm{ac}}(\overline{W}_{\alpha}),$$

$$\Omega_{\pm}(\overline{W}_{\alpha},\overline{W};J'_{\alpha})=C_{\alpha}^{-1}\cdot\Omega_{\pm}(\sqrt{H_{\alpha}},\sqrt{-\Delta};I'_{\alpha})\cdot C,$$

where

$$\Omega_{\pm}(\sqrt{-\Delta},\sqrt{H_{\alpha}};I_{\alpha}):=\text{s-}\lim_{t\to\pm\infty}e^{-it\sqrt{-\Delta}}\cdot I_{\alpha}\cdot e^{it\sqrt{H_{\alpha}}},$$

$$\Omega_{\pm}(\sqrt{H_{\alpha}},\sqrt{-\Delta};I'_{\alpha}):=\text{s-}\lim_{t\to\pm\infty}e^{-it\sqrt{H_{\alpha}}}\cdot I'_{\alpha}\cdot e^{it\sqrt{-\Delta}}.$$

Here $I'_{\alpha}:=P_{\mathrm{ac}}(-\Delta_{\alpha})$, I_{α} is its left inverse, and

$$H_{\alpha}:=\begin{cases}-\Delta_{\alpha}, & \text{for } \alpha\geqslant 0\\ -\Delta_{\alpha}^{\mathrm{nr}}, & \text{for } \alpha<0.\end{cases}$$

By Birman invariance principle one has

$$\Omega_{\pm}(\sqrt{-\Delta},\sqrt{H_{\alpha}};I_{\alpha})=\Omega_{\pm}(-\Delta,H_{\alpha};I_{\alpha})$$

and

$$\Omega_{\pm}(\sqrt{H_{\alpha}},\sqrt{-\Delta};I'_{\alpha})=\Omega_{\pm}(H_{\alpha},-\Delta;I'_{\alpha}).$$

Therefore one has the identities

$$\Omega_{\pm}(\sqrt{-\Delta},\sqrt{H_{\alpha}};I_{\alpha})=\text{s-}\lim_{t\to\pm\infty}e^{it\Delta}\cdot I_{\alpha}\cdot e^{itH_{\alpha}}=\text{s-}\lim_{t\to\pm\infty}e^{it\Delta}\cdot e^{-it\Delta_{\alpha}}\cdot P_{\mathrm{ac}}(-\Delta_{\alpha})=\Omega_{\pm}(-\Delta,-\Delta_{\alpha})$$

and

$$\begin{aligned}\Omega_{\pm}(\sqrt{H_{\alpha}},\sqrt{-\Delta};I'_{\alpha})&=\text{s-}\lim_{t\to\pm\infty}e^{-itH_{\alpha}}\cdot I'_{\alpha}\cdot e^{-it\Delta}\\&=\text{s-}\lim_{t\to\pm\infty}P_{\mathrm{ac}}(-\Delta_{\alpha})\cdot e^{it\Delta_{\alpha}}\cdot e^{-it\Delta}\\&=P_{\mathrm{ac}}(-\Delta_{\alpha})\cdot\Omega_{\pm}(-\Delta_{\alpha},-\Delta)=\Omega_{\pm}(-\Delta_{\alpha},-\Delta).\end{aligned}$$

In conclusion one obtains the equalities

$$\Omega_{\pm}(\overline{W},\overline{W}_{\alpha};J_{\alpha})=C^{-1}\cdot\Omega_{\pm}(-\Delta,-\Delta_{\alpha})\cdot C_{\alpha}\cdot P_{\mathrm{ac}}(\overline{W}_{\alpha}),$$

$$\Omega_{\pm}(\overline{W}_{\alpha},\overline{W};J'_{\alpha})=C_{\alpha}^{-1}\cdot\Omega_{\pm}(-\Delta_{\alpha},-\Delta;)\cdot C,$$

and the proof is concluded since the wave operators $\Omega_{\pm}(-\Delta,-\Delta_\alpha)$, and $\Omega_{\pm}(-\Delta_\alpha,-\Delta)$ exist, are complete and are mutually adjoint isometries. This is proven (see Ref. 11, Appendix E) by the Birman–Kuroda theorem being the resolvent difference,

$$(-\Delta_\alpha+z)^{-1}-(-\Delta+z)^{-1},$$

a rank one (hence trace class) operator. □

The previous theorem holds true also with the different (α-independent and much simpler and natural) couple of identification operators defined by

$$J:\overline{D^1}(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)\to\overline{H^1}(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3),\quad J(\phi,\dot\phi):=(\phi_{\mathrm{reg}},\dot\phi),$$

$$J':\overline{H^1}(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3)\to\overline{D^1}(\mathsf{R}^3)\oplus L^2(\mathsf{R}^3),\quad J'(\phi,\dot\phi):=(\phi,\dot\phi).$$

This is true by Ref. 4, Thms. 10.3 and 10.5 since the condition 10.1 in Ref. 4 is verified with $m=M=1$. In our situation such a condition simply reads as

$$\forall\,\phi\in H^1(\mathsf{R}^3)\cap\mathrm{Range}\,P_{\mathrm{ac}}(-\mathbf{\Delta}_\alpha),\quad \|\sqrt{H_\alpha}\,\phi\|_{L^2}=\|\sqrt{-\mathbf{\Delta}}\,\phi\|_{L^2}.$$

In more detail one has the following.

Theorem 5.2: *J is $(\overline{U}^t_\alpha,\pm)$-equivalent to J_α, i.e.,*

$$\text{s-}\lim_{t\to\pm\infty}(J_\alpha-J)\cdot\overline{U}^t_\alpha\cdot P_{\mathrm{ac}}(\overline{W}_\alpha)=0.$$

Therefore

$$\Omega_{\pm}(\overline{W},\overline{W}_\alpha;J):=\text{s-}\lim_{t\to\pm\infty}\overline{U}^{-t}\cdot J\cdot\overline{U}^t_\alpha\cdot P_{\mathrm{ac}}(\overline{W}_\alpha)$$

exist and are equal to $\Omega_{\pm}(\overline{W},\overline{W}_\alpha;J_\alpha)$.

J' is a $(\overline{U}^t_\alpha,\pm)$-asymptotic left-inverse to J, i.e.,

$$\text{s-}\lim_{t\to\pm\infty}(J'\cdot J-1)\cdot\overline{U}^t_\alpha\cdot P_{\mathrm{ac}}(\overline{W}_\alpha)=0,$$

thus

$$\Omega_{\pm}(\overline{W}_\alpha,\overline{W};J'):=\text{s-}\lim_{t\to\pm\infty}\overline{U}^{-t}_\alpha\cdot J'\cdot\overline{U}^t$$

exist and are equal to $\Omega_{\pm}(\overline{W},\overline{W}_\alpha;J)^*\equiv\Omega_{\pm}(\overline{W}_\alpha,\overline{W};J'_\alpha)$.

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Fractional differential forms

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A generalization of exterior calculus is considered by allowing the partial derivatives in the exterior derivative to assume fractional orders. That is, a fractional exterior derivative is defined. This is found to generate new vector spaces of finite and infinite dimension, fractional differential form spaces. The definitions of closed and exact forms are extended to the new fractional form spaces with closure and integrability conditions worked out for a special case. Coordinate transformation rules are also computed. The transformation rules are different from those of the standard exterior calculus due to the properties of the fractional derivative. The metric for the fractional form spaces is given, based on the coordinate transformation rules. All results are found to reduce to those of standard exterior calculus when the order of the coordinate differentials is set to one. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1364688]

I. INTRODUCTION

In recent years exterior calculus has been generalized by basing it on various graded algebras, see, e.g., Refs. 1 and 2. Other attempts at generalization are based on nonassociative geometries, see, e.g., Refs. 3 and 4. In this paper another attempt at generalization is made using fractional derivatives in the definition of the exterior derivative. That is, a fractional exterior derivative is defined. Having a fractional exterior derivative gives rise to the notion of coordinate differentials of fractional order. These in turn can be used to define vector spaces of fractional differential forms. This formalism is found to produce an infinite number of finite and infinite dimensional vector spaces associated with each point $P \in E^n$ (n dimensional Euclidean space).

In Secs. II and III a brief review of exterior calculus and fractional calculus will be given to fix notation and provide a convenient reference. They are by no means complete, but are sufficient for the purposes of this paper. Section IV defines fractional form spaces based on the fractional exterior derivative. Basis sets are given for the new vector spaces and notation is fixed. In Sec. V the definitions of closed and exact are expanded to include the fractional form case. Once defined, the notions of closed and exact forms are examined for these new vector spaces. In both cases the results reduce to those found in standard exterior calculus when the order of the coordinate differentials is set equal to one. Coordinate transformations are worked out for the fractional form spaces in Sec. VI. The transformation rules are somewhat more complicated than for standard exterior calculus. They do, however, reduce to the usual transformation rules when the order or the coordinate differentials is set to one. Having found the coordinate transformation rule, a metric for the fractional form spaces is constructed. Metrical properties of these new vector spaces will be investigated in a later paper.

The convention in the literature is that the coordinate index is a superscript. For the topics presented in this paper it is more convenient for the coordinate index to be a subscript rather than the traditional superscript. To avoid confusion with this, the summation convention will not be used in this paper.

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II. BRIEF REVIEW OF DIFFERENTIAL FORMS

The calculus of differential forms is an elegant branch of pure mathematics and a powerful tool in applied mathematics. A clear introduction to the field, with emphasis on applications, is given in Flanders.[5] Vector spaces at a point $P \in E^n$ (n dimensional Euclidean space) can be constructed out of expressions of the following type:

$$\text{one forms,} \quad \alpha = \sum_{i=1}^{n} a_i \, dx_i , \tag{1}$$

$$\text{two forms,} \quad \beta = \sum_{i,j=1}^{n} b_{ij} \, dx_i \wedge dx_j , \tag{2}$$

$$\vdots$$

$$\text{``}n\text{''} \text{ forms,} \quad \omega = w \, dx_1 \wedge dx_2 \wedge \cdots \wedge dx_n , \tag{3}$$

where the $\{x_i\}$ are the Cartesian coordinates of E^n. The above sums are taken over all possible values of the indices with the constraint that

$$dx_i \wedge dx_j = - dx_j \wedge dx_i . \tag{4}$$

The functions a_i , b_{ij}, etc., depend only on P and may be real or complex depending on the application. If a k form, γ, is multiplying an m form, μ, the following would be true:

$$\gamma \wedge \mu = (-1)^{km} \mu \wedge \gamma. \tag{5}$$

The result would be zero if $k+m>n$. The exterior product, $\wedge$, is distributive, associative, and antisymmetric. The dimension of the vector space of k forms over $P \in E^n$ is

$$\binom{n}{k} = \frac{n!}{k!(n-k)!},$$

which is zero if $k>n$. For the purposes of this paper let $F(k,k,n)$ denote the vector space of k forms over $P \in E^n$. The apparently redundant ''k'' in the above notation will be needed later for the fractional form case, as there is some additional freedom.

The exterior derivative is defined as

$$d = \sum_{i=1}^{n} dx_i \frac{\partial}{\partial x_i}. \tag{6}$$

The exterior derivative maps k forms into $k+1$ forms and has the following algebraic properties. Let γ and λ be k forms, and μ be an m form, then

$$d(\gamma + \lambda) = d\gamma + d\lambda, \tag{7}$$

$$d(\gamma \wedge \mu) = (d\gamma) \wedge \mu + (-1)^k \gamma \wedge d\mu, \tag{8}$$

$$d(d\gamma) = 0. \tag{9}$$

The last identity is called the Poincaré lemma. A form, γ, is called closed if $d\gamma = 0$. A form, γ, is called exact if there exists a form, μ, such that $d\mu = \gamma$. The order of μ is one less than the order of γ. Exact forms are always closed. Closed forms are not always exact. The interested reader should consult Flanders[5] or Lovelock and Rund[6] for further details.

III. BRIEF OVERVIEW OF FRACTIONAL CALCULUS

There are many books that develop fractional calculus and the various definitions of fractional integration and differentiation. The reader should consult Refs. 7–9 for further details and applications. For the purposes of this paper the Riemann–Liouville definition of fractional integration and differentiation will be used. $\Gamma(q)$ is the gamma function (generalized factorial) of the parameter ''q'' [i.e., $\Gamma(n+1)=n!$ for all whole numbers, ''n''],

$$\frac{\partial^q f(x)}{(\partial(x-a))^q}=\frac{1}{\Gamma(-q)}\int_a^x \frac{f(\xi)\mathrm{d}\xi}{(x-\xi)^{q+1}}, \quad \mathrm{Re}(q)<0, \tag{10}$$

$$\frac{\partial^q f(x)}{(\partial(x-a))^q}=\frac{\partial^n}{\partial x^n}\left[\frac{1}{\Gamma(n-q)}\int_a^x \frac{f(\xi)\mathrm{d}\xi}{(x-\xi)^{q-n+1}}\right], \quad \frac{\mathrm{Re}(q)\geqslant 0}{n>q(n \text{ is whole})}. \tag{11}$$

The parameter q is the order of the integral or derivative and is allowed to be complex. Positive real values of q represent derivatives and negative real values represent integrals.

Equation (10) is a fractional integral and Eq. (11) is a fractional derivative. In this paper only real and positive values of q will be considered. Notice that the derivative written in this form becomes a nonlocal object. Fractional derivatives have many interesting properties. For example the derivative of a constant need not be zero (the initial point a in the above-given definition is set to zero in the following),

$$\frac{\partial^q 1}{(\partial x)^q}=\frac{x^{-q}}{\Gamma(1-q)}. \tag{12}$$

The derivative of powers of x is

$$\frac{\partial^q x^p}{(\partial x)^q}=\frac{\Gamma(p+1)}{\Gamma(p-q+1)}x^{p-q}, \quad \frac{p>-1}{q\geqslant 0}. \tag{13}$$

Composition and product rules for fractional derivatives are given in the following. In the following, n is a whole number and q is a complex number whose real part is greater than zero,

$$\frac{\partial^n}{\partial x^n}\frac{\partial^q}{(\partial(x-a))^q}f(x)=\frac{\partial^{n+q}}{(\partial(x-a))^{n+q}}f(x), \tag{14}$$

$$\frac{\partial^q}{(\partial(x-a))^q}\frac{\partial^{-q}}{(\partial(x-a))^{-q}}f(x)=f(x), \tag{15}$$

$$\frac{\partial^{-q}}{(\partial(x-a))^{-q}}\frac{\partial^q}{(\partial(x-a))^q}f(x)\neq f(x). \tag{16}$$

Composing derivatives where both have fractional order is given by the following formula:

$$\frac{\partial^p}{(\partial(x-a))^p}\frac{\partial^q}{(\partial(x-a))^q}f(x)=\frac{\partial^{p+q}}{(\partial(x-a))^{p+q}}f(x)-\sum_{j=1}^{k}\frac{\partial^{q-j}}{(\partial(x-a))^{q-j}}f(x)\bigg|_{x=a}\frac{(x-a)^{-p-j}}{\Gamma(1-p-j)}, \tag{17}$$

where $0\leqslant k-1\leqslant q\leqslant k$, $p\geqslant 0$, and k is a whole number. The product rule is

$$\frac{\partial^q}{(\partial x)^q}(fg)=\sum_{j=0}^{\infty}\binom{q}{j}\left(\frac{\partial^{q-j}f}{(\partial x)^{q-j}}\right)\left(\frac{\partial^j g}{\partial x^j}\right). \tag{18}$$

The above-mentioned formula and definitions can be found in Refs. 7–9.

IV. FRACTIONAL FORM SPACES

If the partial derivatives in the definition of the exterior derivative are allowed to assume fractional orders, a fractional exterior derivative can be defined

$$\mathrm{d}^{\nu}=\sum_{i=1}^{n}\mathrm{d}x_i^{\nu}\frac{\partial^{\nu}}{(\partial(x_i-a_i))^{\nu}}. \tag{19}$$

Note that the subscript i denotes the coordinate number, the superscript ν denotes the order of the fractional coordinate differential, and a_i is the initial point of the derivative.

Sometimes the notation ∂_i^{ν} will be used to denote

$$\frac{\partial^{\nu}}{(\partial(x_i-a_i))^{\nu}}.$$

In two dimensions (x,y), the fractional exterior derivative of order ν of x^p, with the initial point taken to be the origin, is given by

$$\mathrm{d}^{\nu}x^p=\mathrm{d}x^{\nu}\frac{\Gamma(p+1)}{\Gamma(p-\nu+1)}x^{p-\nu}+\mathrm{d}y^{\nu}\frac{x^p}{y^{\nu}\Gamma(1-\nu)}. \tag{20}$$

For specific values of the derivative parameter the following results are obtained:

$$\nu=0,\quad \mathrm{d}^0x^p=2x^p, \tag{21}$$

$$\nu=1,\quad \mathrm{d}^1x^p=\mathrm{d}x^1px^{p-1}, \tag{22}$$

$$\nu=2,\quad \mathrm{d}^2x^p=\mathrm{d}x^2\,p(p-1)x^{p-2}. \tag{23}$$

By analogy with standard exterior calculus, vector spaces can be constructed using the $\mathrm{d}x_i^{\nu}$. Let $\mathrm{F}(\nu,m,n)$ be a vector space at $P\in E^n$. ν denotes the sum of the fractional differential orders of the basis elements, m denotes the number of coordinate differentials appearing in the basis elements, n the number of coordinates, and $\{x_i\}$ are the Cartesian coordinates for E^n. For example, a basis set for $\mathrm{F}(\nu,1,n)$ would be $\{\mathrm{d}x_1^{\nu},\mathrm{d}x_2^{\nu},\ldots,\mathrm{d}x_n^{\nu}\}$ and arbitrary element of $F(\nu,1,n)$ would be expressed as

$$\alpha=\sum_{i=1}^{n}\alpha_i\,\mathrm{d}x_i^{\nu}. \tag{24}$$

For a fixed ν this is an n dimensional vector space. Also note that there is a different vector space for each value of ν. For $\nu=1$ the one forms from exterior calculus are recovered. Now suppose that the basis elements are made up of two coordinate differentials, $F(\nu,2,n)$. In this case the basis set is more complicated,

$$\{\mathrm{d}x_1^{\mu_{11}}\wedge\mathrm{d}x_1^{\mu_{21}},\mathrm{d}x_1^{\mu_{11}}\wedge\mathrm{d}x_2^{\mu_{31}},\ldots,\mathrm{d}x_n^{\mu_{n-1m}}\wedge\mathrm{d}x_n^{\mu_{\mathrm{nm}}}|\,\mu_{ij}+\mu_{kj}=\nu\}. \tag{25}$$

Note that $\mathrm{d}x_1^{\mu_{11}}\wedge\mathrm{d}x_1^{\mu_{21}}$ would be zero if and only if $\mu_{11}=\mu_{21}$, etc. An arbitrary element of $F(\nu,2,n)$ would be expressed as a sum of the form

$$\beta=\sum_{i=1}^{n}\sum_{j=1}^{n}\int_0^{\nu}(\beta_{ij}(\nu_1,\nu-\nu_1)\mathrm{d}x_i^{\nu_1}\wedge\mathrm{d}x_j^{\nu-\nu_1})\mathrm{d}\nu_1, \tag{26}$$

where $\beta_{ii}(\mu,\mu)=0$. Unlike the previous vector space, $F(\nu,1,n)$, this is clearly infinite dimensional for any value of ν. Not only is it infinite but it is uncountably infinite. An arbitrary element of $F(\nu,3,n)$ would be expressed as an integral of the form

$$\beta=\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n}\int_0^{\nu}\int_0^{\nu-\nu_1}(\beta_{ijk}(\nu_1,\nu-\nu_2,\nu-\nu_1-\nu_2)\mathrm{d}x_i^{\nu_1}\wedge\mathrm{d}x_j^{\nu_2}\wedge\mathrm{d}x_k^{\nu-\nu_1-\nu_2})\mathrm{d}\nu_2\,\mathrm{d}\nu. \tag{27}$$

With each step up on the middle index of $F(\nu,m,n)$ another integral and summation is included. A basis set for this vector space would be

$$F(\nu,m,n)=\left\{\mathrm{d}x_{\nu_1}^{\mu_{i_k i}}\wedge\mathrm{d}x_{\mu_2}^{\mu_{2}1}\wedge\ldots\wedge\mathrm{d}x_{i_m}^{\mu_{m^i}},\cdots\middle|\sum_{k=1}^{m}\mu_{i_k j}=\nu\right\}. \tag{28}$$

The basis elements range over all possible combinations of the fractional coordinate differentials and all possible choices for the μ's. Note that m need not be less than or equal to n.

Let $P\in E^n$, and let $A\in F(\nu,m,n)$ and $B\in F(\mu,k,n)$ at the point P. Then the exterior product of A and B maintains the antisymmetry property of Eq. (5),

$$A\wedge B=(-1)^{km}B\wedge A\in F(\mu+\nu,k+m,n). \tag{29}$$

If $k+m>n$, $A\wedge B$ need not be zero. Equation (7) is also maintained due to the linearity of the fractional derivative. Equation (8) is not maintained due to the product rule for the fractional derivative [see Eq. (18)]. Note also that d^{ν} maps $F(\mu,k,n)$ into $F(\mu+\nu,k+1,n)$.

V. CLOSED AND EXACT FRACTIONAL FORMS

By analogy with exterior calculus the notions of closed and exact can be extended to fractional forms.

Let $g\in F(\mu,k,n)$ then g is ν-exact if $\exists$ and $f\in F(\mu-\nu,k-1,n)$ such that $\mathrm{d}^{\nu}f=g$.

Let $g\in F(\nu,k,n)$ then g is μ closed if $\mathrm{d}^{\mu}g=0$.

To examine the notion of exactness (integrability conditions) in the fractional form case the kernel is needed for the fractional derivative operator. This will be denoted by $\mathrm{Ker}(\partial_i^{\nu})$. In the following the initial point of the derivative will be taken to be the origin. Solve

$$\partial_i^{\nu}(h)=0. \tag{30}$$

Equation (30) is solved using Eq. (11). Let m be the first whole number greater than or equal to ν then

$$h=(x_i)^{\nu-m}\sum_{k=0}^{m-1}c_k(x_i)^k. \tag{31}$$

This is basically the result from Oldham (Ref. 7, p. 155). The c_k's can be functions of the other coordinates. The kernel for the operator, d^{ν} (when restricted to act only on scalar functions), is similarly constructed, $\mathrm{Ker}(\mathrm{d}^{\nu})$.

$$\mathrm{d}^{\nu} f = \sum_{i=1}^{m} \mathrm{d}x_i^{\nu} \frac{\partial^{\nu} f}{(\partial x_i)^{\nu}} = 0 \tag{32}$$

$$\Rightarrow f = \left(\prod_{i=1}^{n} x_i \right)^{\nu - m} \left(\sum_{k_1=0}^{m-1} \cdots \sum_{k_n=0}^{m-1} C_{k_1 \cdots k_n} (x_1)^{k_1} \cdots (x_n)^{k_n} \right). \tag{33}$$

The $C_{k_1,\ldots k_n}$ are now constants and m is once again the first whole number greater than or equal to ν.

The fractional integrability conditions can now be constructed for the following restricted case. Let g be a ν form in $F(\nu,1,\mathrm{n})$,

$$g = \sum_{i=1}^{n} \alpha_i \, \mathrm{d}x_i^{\nu}. \tag{34}$$

When can a 0 form, f, be found such that $\mathrm{d}^{\nu} f = g$? If such an f exists it will be contained in the family of functions given by

$$f = \partial_i^{-\nu}(\alpha_i) + (x_i)^{\nu - m} \sum_{k=0}^{m-1} c_k (x_i)^k. \tag{35}$$

Recall that there is no sum over the repeated indices, except where a summation symbol is encountered. This solution must satisfy, $\partial_j^{\nu} f = \alpha_j$,

$$\partial_j^{\nu} \left(\partial_i^{-\nu}(\alpha_i) + (x_i)^{\nu - m} \sum_{k=0}^{m-1} c_k (x_i)^k \right) = \alpha_j. \tag{36}$$

Equation (36) is to be solved to determine the unknown functions c_k, and must be true for all values of i. Equation (36) can be rearranged to give

$$\sum_{k=0}^{m-1} (\partial_j^{\nu} c_k)(x_i)^k = \frac{\alpha_j - \partial_j^{\nu}(\partial_i^{-\nu} \alpha_i)}{(x_i)^{\nu - m}}. \tag{37}$$

The left-hand side of (37) is a polynomial of order $m-1$ in the variable x_i, hence it can only be solved for the c_k if the following is true:

$$\frac{\partial^m}{\partial x_i^m} \left(\frac{\alpha_j - \partial_j^{\nu}(\partial_i^{-\nu} \alpha_i)}{(x_i)^{\nu - m}} \right) = 0. \tag{38}$$

Equation (38) is the integrability condition for fractional forms of type $F(\nu,1,n)$. Note that if $\nu = m = 1$ the usual integrability conditions from exterior calculus are recovered.

Consider the second definition and examine what it takes to be closed for fractional forms. Let

$$\alpha = \sum_{i=1}^{n} \alpha_i \, \mathrm{d}x_i^{\nu} \in F(\nu,1,n)$$

and consider its fractional exterior derivative,

$$\mathrm{d}^{\mu} \alpha = \sum_{i=1}^{n} \mathrm{d}^{\mu}(\alpha_i \, \mathrm{d}x_i^{\nu}), \tag{39}$$

$$d^{\mu}\alpha=\sum_{i=1}^{n}\sum_{j=1}^{n} dx_j^{\mu}\wedge\sum_{k=0}^{\infty}\binom{\mu}{k}\left(\frac{\partial^{\mu-k}}{(\partial x_j)^{\mu-k}}\alpha_j\right)\left(\frac{\partial^k}{\partial x_j^k}dx_i^{\nu}\right). \tag{40}$$

In the last sum of Eq. (40) k takes on only whole number values hence

$$\frac{\partial^k}{\partial x_j^k}(dx_i^{\nu})=0 \quad \forall \quad k\geqslant 1. \tag{41}$$

This reduces Eq. (40) to the following:

$$d^{\mu}\alpha=\sum_{i=1}^{n}\sum_{j=1}^{n} dx_j^{\mu}\wedge dx_i^{\nu}\binom{\mu}{0}\left(\frac{\partial^{\mu}}{(\partial x_j)^{\mu}}\alpha_i\right). \tag{42}$$

Since dx_j^{μ} and dx_i^{ν} are linearly independent, provided $\mu\neq\nu$ or $i\neq j$, $d^{\mu}\alpha=0$ if and only if

$$\frac{\partial^{\mu}}{(\partial x_j)^{\mu}}\alpha_i=0. \tag{43}$$

In other words $\alpha_i\in\mathrm{Ker}(\partial_j^{\mu})$. For the special case of $\mu=\nu$ the symmetry from Eq. (29) can be used to obtain

$$\frac{\partial^{\nu}}{(\partial x_i)^{\nu}}\alpha_j+(-1)\frac{\partial^{\nu}}{(\partial x_j)^{\nu}}\alpha_i=0. \tag{44}$$

For $\nu=1$ the usual result from exterior calculus is recovered,

$$\frac{\partial}{\partial x_i}\alpha_j-\frac{\partial}{\partial x_j}\alpha_i=0. \tag{45}$$

VI. TRANSITION TO CURVILINEAR COORDINATES

When coordinate transformation rules are worked out for exterior or tensor calculus (see Refs. 5 and 6) the following construction can be used. Let $\{x_i\}$ and $\{y_i\}$ be two coordinate systems with a one to one mapping between them in some neighborhood of $P\in E^n$. Take $\{x_i\}$ to again be Cartesian coordinates and $\{y_i\}$ to be curvilinear coordinates. Assume the $\{x_i\}$ can be written smoothly in terms of the $\{y_i\}$,

$$x_i=x_i(y). \tag{46}$$

The exterior derivative is then applied to the Eq. (46) giving the following:

$$dx_i=dx_i(y), \tag{47}$$

$$\sum_{k=1}^{n} dx_k\frac{\partial x_i}{\partial x_k}=\sum_{l=1}^{n} dy_l\frac{\partial x_i}{\partial y_l}, \tag{48}$$

$$\sum_{k=1}^{n} dx_k\,\delta_i^k=\sum_{l=1}^{n} dy_l\frac{\partial x_i}{\partial y_l}, \tag{49}$$

$$dx_i=\sum_{l=1}^{n} dy_l\frac{\partial x_i}{\partial y_l}. \tag{50}$$

This is very straightforward and can be adapted to the fractional from case. In the two coordinate systems the fractional exterior derivative d^ν takes the following forms:

$$\mathrm{d}^\nu = \sum_{i=1}^{n} \mathrm{d}x_i^\nu \frac{\partial^\nu}{(\partial(x_i - a_i))^\nu}, \tag{51}$$

and

$$\mathrm{d}^\nu = \sum_{i=1}^{n} \mathrm{d}y_i^\nu \frac{\partial^\nu}{(\partial(y_i - \tilde{a}_i))^\nu}, \tag{52}$$

where a_i is the initial point of the derivative in the Cartesian system and $\tilde{a}_i$ is the same point but in the curvilinear coordinates. Recall that x_i is in the kernel for the operator $\partial/\partial x_k$ for $k \neq i$, and when $k = i$ the result is one. For the fractional case the same type of object is needed. Consider a function α_k that maps points in E^n into the complex numbers

$$\alpha_k = \frac{\Gamma(1)}{\Gamma(\nu+1)} \left(\prod_{i=1/i\neq k}^{n} (x_i - a_i) \right)^{\nu-m} (x_k - a_k)^\nu, \tag{53}$$

where a_i is the initial point for the fractional derivative. The function α_k was chosen so that it would be in the kernel of

$$\frac{\partial^\nu}{(\partial(x_i - a_i))^\nu}$$

for $i \neq k$, and for $i = k$,

$$\frac{\partial^\nu \alpha_k}{(\partial(x_k - a_k))^\nu} = 1. \tag{54}$$

If the fractional exterior derivative is applied to α_k in the two different coordinate systems the following coordinate transformation rule can be obtained [where all quantities on the right-hand side of (55) must be expressed in terms of the $\{y_i\}$ coordinates]:

$$\mathrm{d}x_k^\nu = \sum_{i=1}^{n} \frac{\mathrm{d}y_i^\nu}{\Gamma(\nu+1)} \frac{\partial^\nu}{(\partial(y_i - \tilde{a}_i))^\nu} \left(\left(\prod_{j=1/j\neq k}^{n} (x_j - a_j) \right)^{\nu-m} (x_k - a_k)^\nu \right). \tag{55}$$

Note that for $\nu = m = 1$ the usual coordinate transformation rule is recovered. The coordinate transformation matrix for the fractional forms will be denoted by

$$J_i^k(x,y,\nu) = \frac{1}{\Gamma(\nu+1)} \frac{\partial^\nu}{(\partial(y_i - \tilde{a}_i))^\nu} \left(\left(\prod_{j=1/j\neq k}^{n} (x_j - a_j) \right)^{\nu-m} (x_k - a_k)^\nu \right), \tag{56}$$

$$\mathrm{d}x_k^\nu = \sum_{i=1}^{n} \mathrm{d}y_i^\nu \, J_i^k(x,y,\nu). \tag{57}$$

A fractional form,

$$A = \sum_{k=1}^{n} A_k(x) \mathrm{d}x_k^\nu, \tag{58}$$

written in the $\{x_i\}$ coordinates would be transformed into the $\{y_i\}$ coordinates according to

$$A=\sum_{k=1}^{n}\sum_{i=1}^{n}A_k(x(y))J_i^k(x,y,\nu)\mathrm{d}y_i^{\nu}. \tag{59}$$

Reversing the coordinate transformation yields

$$A=\sum_{k=1}^{n}\sum_{i=1}^{n}\sum_{j=1}^{n}A_k(x)J_i^k(x,y,\nu)J_j^i(y,x,\nu)\mathrm{d}x_j^{\nu} \tag{60}$$

$$\Rightarrow\delta_j^k=\sum_{i=1}^{n}J_j^i(y,x,\nu)J_i^k(x,y,\nu). \tag{61}$$

As an example consider the coordinate transformation for two-dimensional Cartesian coordinates to polar coordinates. The initial point for the fractional derivatives is taken to be the origin

$$x_1=r\cos(\theta),\quad x_2=r\sin(\theta). \tag{62}$$

The coordinate transformations for the fractional differentials are then

$$\mathrm{d}x_1^{\nu}=\frac{\Gamma(2\nu-m+1)}{\Gamma(\nu+1)\Gamma(\nu-m+1)}\frac{\cos^{\nu}(\theta)}{\sin^{m-\nu}(\theta)}r^{\nu-m}\,\mathrm{d}r^{\nu}+\frac{r^{2\nu-m}}{\Gamma(\nu+1)}\frac{\partial^{\nu}}{(\partial\theta)^{\nu}}\left(\frac{\cos^{\nu}(\theta)}{\sin^{m-\nu}(\theta)}\right)\mathrm{d}\theta^{\nu}, \tag{63}$$

$$\mathrm{d}x_2^{\nu}=\frac{\Gamma(2\nu-m+1)}{\Gamma(\nu+1)\Gamma(\nu-m+1)}\frac{\sin^{\nu}(\theta)}{\cos^{m-\nu}(\theta)}r^{\nu-m}\,\mathrm{d}r^{\nu}+\frac{r^{2\nu-m}}{\Gamma(\nu+1)}\frac{\partial^{\nu}}{(\partial\theta)^{\nu}}\left(\frac{\sin^{\nu}(\theta)}{\cos^{m-\nu}(\theta)}\right)\mathrm{d}\theta^{\nu}. \tag{64}$$

For $\nu=m=1$ the transformation equations from exterior calculus are recovered,

$$\mathrm{d}x_1=\cos(\theta)\mathrm{d}r-r\sin(\theta)\mathrm{d}\theta, \tag{65}$$

$$\mathrm{d}x_2=\sin(\theta)\mathrm{d}r+r\cos(\theta)\mathrm{d}\theta. \tag{66}$$

Having found the coordinate transformation rule a metric for $F(\nu,1,n)$ can be constructed just as is done in exterior calculus (see Ref. 6, p. 46)

$$g_{ij}(y,\nu)=\sum_{k=1}^{n}J_i^k(x,y,\nu)J_j^k(x,y,\nu), \tag{67}$$

which can be used to give a fractional line element

$$\mathrm{d}s^{2\nu}=\sum_{i,j=1}^{n}g_{ij}(y,\nu)\mathrm{d}y_i^{\nu}\otimes\mathrm{d}y_j^{\nu} \tag{68}$$

or

$$\mathrm{d}s^{\nu}=\sqrt{\sum_{i,j=1}^{n}g_{ij}(y,\nu)\mathrm{d}y_i^{\nu}\otimes\mathrm{d}y_j^{\nu}}, \tag{69}$$

where $\otimes$ is the symmetric product for coordinate differentials.

VII. CONCLUSION

In this paper a natural extension of the exterior derivative to a fractional exterior derivative was considered. It was found to generate some new vector spaces, both finite and infinite in dimension. Of particular interest is the observation that at each point $P\in E^n$ there is an infinite

number of n dimensional vector spaces. Due to their similarity with tangent spaces, perhaps an appropriate name for these new vector spaces should be fractional tangent spaces. Notions of closed and exact were also defined for these fractional form spaces. Integrability and closure conditions were investigated for the special case of $F(\nu,1,n)$. The results produced were found to reduce to the standard results from exterior calculus when the order of the fractional exterior derivative was set equal to one. Coordinate transformation rules were also worked out for $F(\nu,1,n)$. The transformation rules are somewhat more complicated than for traditional exterior calculus. They do, however, reduce to the usual formula when the order of the coordinate differentials is set equal to one. Coordinate transformation rules give rise to a metric for $F(\nu,1,n)$. Properties of the metric, such as its associated covariant derivative, will be investigated in a later paper.

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Structure and representation theory for the double group of the four-dimensional cubic group

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Hypercubic groups in any dimension are defined and their conjugate classifications and representation theories are derived. Double group and spinor representation are introduced. A detailed calculation is carried out on the structures of four-dimensional cubic group O_4 and its double group, as well as all inequivalent single-valued representations and spinor representations of O_4. All representations are derived adopting Clifford theory of decomposition of induced representations. Based on these results, single-valued and spinor representations of the orientation-preserved subgroup of O_4 are calculated. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1358880]

I. INTRODUCTION

It is well known that electrons stay in spinor representations of the symmetry group of a given lattice in condensed matter physics; it is reasonable to assume that quarks, leptons, as well as baryons, should reside in *spinor representations* of the symmetry group of a four-dimensional lattice in lattice field theory (the concept of ''spinor representation'' will be clarified in Sec. II). Accordingly, to explore the structure and representations (spinor representations especially) of such groups has important significance in high energy physics.

In this paper, we concentrate on the case of hypercubic lattices, though they are not the maximum symmetric lattices in four dimension.[1] In history, the first representation-theoretical consideration of a symmetry group of such lattices was given by Young.[2] Then mathematicians worked in this field due to interest in the wreath product[3,4] to which Kerber gave a thorough review in his book.[5] Physicists became involved after Wilson introduced lattice gauge theory.[6] Baake *et al.* first gave an explicit description of characters of the four-dimensional cubic group;[7] Mandula *et al.* derived the same results using a different method.[8] As for spinor representations, Mandula *et al.* resolved this problem for what we call the *orientation-preserved* four-dimensional cubic-group in Ref. 9.

In this paper, the power of Clifford theory on decomposition of induced representations (Sec. II A) is fully applied. A systematic and schematic description of conjugate classification and representation theory of the generalized cubic group O_n, as well as the concept of the orientation-preserved subgroup of them SO_n, is given in Sec. II B. The double group is introduced in Sec. II C to clarify the terms ''single-valued representation'' and ''two-valued representation (spinor representation).'' Then specifying these general results to four dimension, we give a detailed description of structure and conjugate classification of O_4 (Sec. III A), its double $\overline{O_4}$ (Sec. III B), and those of SO_4, $\overline{SO_4}$ (Sec. V). We derive all inequivalent single-valued representations as well as spinor representations of O_4, adopting Clifford theory (Sec. IV). Based on these results, we reproduce representation theory of $\overline{SO_4}$ in Sec. VI.

It should be pointed out that the ''spinor'' part for O_4 of our work is completely new and that although other results are well known, our method to derive them is much more tidy and system-

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atic than that used by other authors who gave the same results, thanks to the power of Clifford theory.

II. CONCEPTUAL FOUNDATIONS

A. Clifford theory on decomposition of induced representations

Two results of Clifford theory, a powerful method for decomposing induced representations of a given group E with a normal subgroup N,[10–13] will be applied in this paper. We will use $\mathcal{C}[E]$ for the group algebra of E in complex field and G for E/N in the following. The first result is

Theorem 1: *(Clifford—Refs. 14 and 10.) Let M be a simple $\mathcal{C}[E]$-module, and L a simple $\mathcal{C}[N]$-submodule of M_N s.t. L is stable relative to E, i.e., L is isomorphic to all of its conjugates. Then*

$$M \cong L \otimes_{\mathcal{C}} I$$

for a left ideal I in $End_{\mathcal{C}[E]} L^E$. The E-action on $L \otimes_{\mathcal{C}} I$ is given by

$$x \mapsto U(x) \otimes V(x), x \in E,$$

where $U: E \to GL(L)$ is a projective representation of E on L, and $V: E \to GL(I)$ is a projective representation of G, that is, $V(x)$ depends only on the coset xN of x in G, for each $x \in E$. The factor sets associated with U and V are inverse of each other.

The second result can be regarded as a special case of Theorem 1. Let $E = N \rtimes G, |E| < \infty$ and N be Abelian, then adjoint action of G upon N makes N a G-module. This G-action can be extended naturally to a G-action upon $\mathcal{C}[N]$ by linearity. Define $\Pi(N) := \{\pi_\mu\} \subset \mathcal{C}[N]$,

$$\pi_\mu := \sum_{a \in N} \chi_\mu(a^{-1}) a, \tag{1}$$

where χ_μ are all irreducible representations of N. The G-action on $\Pi(N)$ is closed and thus $\Pi(N)$ is separated into orbits $\Pi(N) = \amalg_{o \in \mathcal{I}} \Pi_o$ where $\mathcal{I}$ is an index set to label different orbits. For each Π_o, choose one of its elements and denote it as $\pi_{o,e}$. The stabilizer of each $\pi_{o,e}$ in G (*little group*) is denoted as S_o. There is a bijection from $G/S_o = \{hS_o\}$ to Π_o defined by

$$\mathrm{Ad}_h(\pi_{o,e}) = h \pi_{o,e} h^{-1} =: \pi_{o,h}, \tag{2}$$

where $\{h\}$ is a system of representatives of left cosets G/S_o. Define

$$\Pi_{o,h;\eta,i} \equiv \pi_{o,h} h \otimes_{S_o} e^o_{\eta,i} \tag{3}$$

in which $\{e^o_{\eta,i} | i = 1,2,\ldots,d^o_\eta\}$ with fixed o, η, and η is the ηth irreducible representation of S_o whose dimension is d^o_η, then

Proposition 1 (Little group method—Refs. 11–13):

(1) For each fixed (o,η), $\{\Pi_{o,h;\eta,i}\}$ induces an irreducible representation of E, denoted as $D_{o,\eta}$.
(2) If $(o,\eta) \neq (o',\eta')$, then $D_{o,\eta}$ and $D_{o',\eta'}$ are inequivalent.
(3) $\{D_{o,\eta}\}$ gives all inequivalent irreducible representations of E.

B. Cubic group in any dimension

The symmetry group of a cube including inversions in three-dimensional Euclidean space, which is denoted as O_h in the theory of point groups,[15] can be generalized into any n-dimensional Euclidean space E^n, along two different approaches whose results are equivalent. The first approach of generalization, which is very natural and straightforward, is geometrical. An *n-cube* (or *hypercube in E^n*) C_n is defined to be a subset of E^n, $C_n = \{p | x^i(p) = \pm 1\}$, where $x^i: E^n \to \mathcal{R}, i = 1,2,\ldots,n$ are coordinate functions of E^n, together with the distance inherited from E^n. *n-cubic*

group (*hypercubic group of degree n*) O_n consists of all isometries of E^n which stabilize C_n. While the second approach of generalization is algebraic. O_h has a semidirect product structure as $Z_2^3 \rtimes S_3$;[11] we generalize this to $Z_2^n \rtimes S_n$, which is just a *wreath product* $Z_2 \wr S_n$ of Z_2 with S_n. We point out that these two generalizations are identical. Let $\{e_i\}$ be a standard orthogonal basis of E^n, namely $x^j(e_i)=\delta_i^j$. Define $n+1$ points in C_n to be $p_0=(-1,-1,\ldots,-1), p_i=p_0+2e_i$.

Lemma 1: $\forall \epsilon \in O_n$, ϵ *is entirely determined by images* $\epsilon(p_i), i=0,1,2,\ldots,n$.

Proof: The fact that ϵ is an isometry of E^n ensures the equality of Euclidean distances $d(p,p_i)=d(\epsilon(p),\epsilon(p_i))$, $i=0,1,\ldots,n$ for any other p in C_n. If all $\epsilon(p_i)$ are given, $\epsilon(p)$ will be fixed for any other p accordingly due to the fundamental lemma of Euclidean geometry (lemma A1 in the Appendix). In fact, the existence of solution in lemma A1 is guaranteed by the fact that ϵ stablizes C_n and lemma A1 itself ensures the uniqueness. □

To fix $\epsilon(p_0)$, there are 2^n ways; while for a fixed $\epsilon(p_0)$, there are $n!$ possibilities to fix $\epsilon(p_i), i=1,2,\ldots,n$. Therefore, $|O_n|=2^n \cdot n!$.

Proposition 2 (*Structure of* O_n)*:*

$$O_n \cong Z_2^n \rtimes S_n. \tag{4}$$

Proof: Introduce a class of isometries in E^n:

$$\sigma(e_i)=e_{\sigma(i)}, \quad I_i(e_j)=(1-2\delta_{ij})e_j, \quad i=1,2,\ldots,n, \tag{5}$$

where $\sigma \in S_n$ permutes the axes and I_i inverts the ith axis. Subjected to the relations

$$I_i^2=e, \quad I_iI_j=I_jI_i, \quad i,j=1,2,\ldots,n, \quad \sigma I_i=I_{\sigma(i)}\sigma, \sigma \in S_n \tag{6}$$

these isometries generate a subgroup of C_n isomorphic to $Z_2^n \rtimes S_n$ whose order is $2^n n! = |O_n|$. So Eq. (4) follows. □

Kerber gave a detailed introduction on the conjugate classification and representation theory of a general wreath product $N \wr G$ in Ref. 5. We specify his general results to our case $Z_2^n \rtimes S_n \cong Z_2 \wr S_n$.

Some fundamental facts about symmetrical groups S_n should be recalled.[15] Each element $\sigma \in S_n$ has a cycle decomposition

$$\sigma=\begin{pmatrix} 1 & 2 & \ldots & n \\ \sigma(1) & \sigma(2) & \ldots & \sigma(n) \end{pmatrix}=\prod_{k=1}^{n}\prod_{\alpha=1}^{\nu_k}\tau_{k\alpha}, \tag{7}$$

where $\tau_{k\alpha}$ are independent k cycles, which can be expressed as $(a_1a_2\ldots a_k)$, and write $n(k,\alpha)=\{a_1,a_2,\ldots,a_n\}$. The cycle structure of σ can be represented formally as

$$(\nu)=\prod_{k=1}^{n}(k^{\nu_k}), \tag{8}$$

where $\{\nu_k\}$ satisfies $\Sigma_{k=1}^n k\cdot\nu_k=n$. Two elements in S_n are conjugate equivalent, iff they have the same cycle structure. The number of elements in class (ν) is equal to $N_{(\nu)}=n!/\Pi_{k=1}^n(k^{\nu_k}\nu_k!)$. Each cycle structure (ν) can be visualized by one unique Young diagram which is denoted also by (ν). There is a one-to-one correspondence between all inequivalent irreducible representations of S_n and all Young diagrams, which enable us to represent each irreducible representation by the corresponding Young diagram (ν). We write the basis of one of these representations (ν) in $d_{(\nu)}$ dimension as $e_{(\nu)i}, i=1,2,\ldots,d_{(\nu)}$.

We point out that the conjugate classification of O_n has a deep relation to that of S_n. A generic element in $Z_2 \wr S_n$ can be written as

$$\sigma\cdot\prod_i I_i^{s_i}=\begin{pmatrix} 1 & 2 & \ldots & n \\ (-)^{s_1}\sigma(1) & (-)^{s_2}\sigma(2) & \ldots & (-)^{s_n}\sigma(n) \end{pmatrix} \tag{9}$$

in which $s_i \in \mathcal{Z}/2\mathcal{Z}$. We call the right-hand side of Eq. (9) by *permutation with signature*. $\sigma\Pi_i I_i^{s_i}$ can be decomposed according to Eq. (7), i.e.,

$$\prod_i I_i^{s_i} = \prod_{k=1}^{n} \prod_{\alpha=1}^{\nu_i} \prod_{a \in n(k,\alpha)} I_a^{s_a}$$

and

$$\sigma \prod_i I_i^{s_i} = \prod_{k=1}^{n} \prod_{\alpha=1}^{\nu_i} \left(\tau_{k\alpha} \prod_{a \in n(k,\alpha)} I_a^{s_a} \right). \tag{10}$$

The *cycle with signature* is defined to be

$$\tau_{k\alpha} \prod_{a \in n(k,\alpha)} I_a^{s_a} = \begin{pmatrix} a_1 & a_2 & \dots & a_k \\ (-)^{s_{a_1}} a_2 & (-)^{s_{a_2}} a_3 & \dots & (-)^{s_{a_k}} a_1 \end{pmatrix}.$$

For two independent $(k,\alpha),(k',\alpha')$, it is easy to verify that

$$\tau_{k\alpha}\tau_{k'\alpha'} = \tau_{k'\alpha'}\tau_{k\alpha}, \quad \prod_{a \in n(k,\alpha)} I_a^{s_a} \tau_{k'\alpha'} = \tau_{k'\alpha'} \prod_{a \in n(k,\alpha)} I_a^{s_a}, \quad \prod_{a \in n(k',\alpha')} I_a^{s_a} \tau_{k\alpha} = \tau_{k\alpha} \prod_{a \in n(k',\alpha')} I_a^{s_a}.$$

Proposition 3 (Refs. 3–5): We use $\sim$ to denote conjugate equivalent.
(1) Descent rule:

$$\sigma \prod_i I_i^{s_i} \sim \sigma' \prod_i I_i^{s_i'} \Rightarrow \sigma \sim \sigma'. \tag{11}$$

(2) Permutation rule: Let

$$\tilde{\sigma} = \begin{pmatrix} 1 & 2 & \dots & n \\ \tilde{\sigma}(1) & \tilde{\sigma}(2) & \dots & \tilde{\sigma}(n) \end{pmatrix} = \begin{pmatrix} \sigma(1) & \sigma(2) & \dots & \sigma(n) \\ \sigma'(1) & \sigma'(2) & \dots & \sigma'(n) \end{pmatrix}$$

then

$$\tilde{\sigma} \left(\sigma \prod_i I_i^{s_i} \right) \tilde{\sigma}^{-1} = \begin{pmatrix} \tilde{\sigma}(1) & \tilde{\sigma}(2) & \dots & \tilde{\sigma}(n) \\ (-)^{s_1}\sigma'(1) & (-)^{s_2}\sigma'(2) & \dots & (-)^{s_n}\sigma'(n) \end{pmatrix}. \tag{12}$$

(3) Signature rule within one cycle: Let $\tau_{k\alpha}$ be a k-cycle and a_0 be a given number in $n(k,\alpha)$, then

$$\tau_{k\alpha} \prod_{a \in n(k,\alpha)} I_a^{s_a} \sim \tau_{k\alpha} \prod_{a \in n(k,\alpha)} I_a^{s_a + \delta_{aa_0} + \delta_{a,\tau_{k\alpha}(a_0)}}. \tag{13}$$

Note that $\tau_{k\alpha}(a_0)$ is calculated modulo k (the subscripts of I_a are always understood in this way).

(4) Signature rule between two cycles: Let $\tau_{k\alpha}, \tau_{k\beta}$ be two independent k-cycles and we define a bijection $\theta: n(k,\alpha) \to n(k,\beta), a_i \mapsto b_i$. Then

$$\tau_{k\alpha} \prod_{a \in n(k,\alpha)} I_a^{s_a} \cdot \tau_{k\beta} \prod_{b \in n(k,\beta)} I_b^{s_b} \sim \tau_{k\alpha} \prod_{a \in n(k,\alpha)} I_a^{s_{\theta(a)}} \cdot \tau_{k\beta} \prod_{b \in n(k,\beta)} I_b^{s_{\theta^{-1}(b)}}. \tag{14}$$

This theorem ensures conjugate classification of $Z_2 \wr S_n$ is totally determined by the structure of cycles with signature. We verify this statement by generalizing Young diagram technology. First, draw a *Young diagram with numbers and signatures* for each element

$$\sigma \Pi_i I_i^{s_i} \in Z_2 \wr S_n$$

according to the decomposition Eq. (10) by the following rules:

(1) Plot Young diagram of the class in S_n to which σ belongs and fill each column of this Young diagram with numbers in corresponding cycle by cyclic ordering from the upmost box to the downmost box.
(2) Draw a *slash* in the Young box if the number in this box is mapped to a minus-signed number.

Secondly, partition elements in $Z_2 \wr S_n$ by their cycle structure in S_n and Eq. (11) guarantees that elements belonging to different partitions cannot be conjugate equivalent. Equation (12) implies that all the numbers that we filled by rule (1) are unnecessary, so smear them out and leave boxes and *slash*es only. Within each column, Eq. (13) says that the positions of *slash*es make no difference. What's more, only the fact that the total number of *slash*es is even or odd distinguishes different classes. Therefore we regulate each column to contain zero or one *slash* at the bottom box. Equation (14) shows that we cannot distinguish the case where one column without any *slash* (Mr. Zero) is put to the left of another column with one *slash* (Mr. One) from that Mr. Zero is to the right of Mr. One, if they have same cyclic length; thus we regulate that Mr. Zero shall always stand left to Mr. One. Therefore, conjugate classes of $Z_2 \wr S_n$ can be uniquely characterized by generalizing Young diagrams containing *slash*es. Following Eq. (8), we represent conjugate classes by

$$(\nu^+, \nu^-) = \prod_{k=1}^{n} (k^{\nu_k^+ + \nu_k^-}), \tag{15}$$

where ν_k^+ is the number of Mr. Zero-type k-cycles and ν_k^- is that of Mr. One-type k-cycles, which satisfy $\nu_k^+ + \nu_k^- = \nu_k$. It is not difficult to check some numerical properties of conjugate classes of $Z_2 \wr S_n$.

Corollary 1: (1) Given a class (ν) *in* S_n, *there are*

$$\prod_{k=1}^{n} (1 + \nu_k) \tag{16}$$

classes in $Z_2 \wr S_n$ *which descend to* (ν).
(2) The number of elements in a class (ν^+, ν^-) *is*

$$N_{(\nu^+,\nu^-)} = N_{(\nu)} \prod_{k=1}^{n} \left(C_{\nu_k}^{\nu_k^+} \left(\sum_{i=0}^{[k/2]} C_k^{2i} \right)^{\nu_k^+} \left(\sum_{j=1}^{[(k+1)/2]} C_k^{2j-1} \right)^{\nu_k^-} \right), \tag{17}$$

where C_m^n *is combinatorial number defined to be* $m!/(n!(m-n)!)$.
(3) The order of a class (ν^+, ν^-) *is*

$$lcm(\{k \cdot 2^{\delta(\nu_k^-)} | \nu_k \neq 0\}), \tag{18}$$

where $\delta(\nu_k^-) = 0$, *if* $\nu_k^- = 0$; $\delta(\nu_k^-) = 1$, *if* $\nu_k^- > 0$.
(4) Determinant (signature, parity) of a class

$$\det((\nu^+, \nu^-)) = (-1)^{\sum_{k=1}^{n} \nu_k^-} \cdot \det((\nu)), \tag{19}$$

where $\det((\nu))$ *is the determinant of* (ν) *in* S_n.
All inequivalent irreducible representations of Z_2^n can be expressed as

$$\chi_{(s)} := \bigotimes_{p=1}^{n} \chi_{(-)^{s_p}} \tag{20}$$

in which $s_p \in \mathcal{Z}/2\mathcal{Z}, p=1,2,\ldots,n$ and $\chi_{(-)}, \chi_{(+)}$ are two irreducible representations of Z_2 with $\chi_{(+)}$ being the unit representation. Thus $\pi_{(s)}$ can be defined by Eq. (1) and $\Pi(Z_2^n)=\{\pi_{(s)}\}$. Note that $\pi_{(s)}$ satisfy $\pi_{(s)}\pi_{(s')}=\pi_{(s\cdot s')}$ where $(s\cdot s')(p)=s(p)s'(p)$. $\Pi(Z_2^n)$ is divided into $n+1$ orbits under the S_n-action, namely $\Pi(Z_2^n)=\amalg_{p=0}^{n}\Pi_p$. For a given p, Π_p consists of those $\pi_{(s)}$ that have p components in (s) equal to 1, other $n-p$ components equal to 0; hence $|\Pi_p|=C_n^p$. Each $\pi_{p,e}$ is specified to a $\pi_{(s)}$ with $s_p=0, p=1,2,\ldots,n-p; s_p=1, p=n-p+1,\ldots,n$, whose stationary subgroup is just $S_{(n-p)}\otimes S_p$, denoted as F_p. Representatives of left-cosets in S_n/F_p are written as σ_r, then according to Eqs. (2) and (3) and Theorem 1,

Proposition 4 (*Representation theory of $Z_2 \wr S_n$*)*:*

$$\Pi_{p,\sigma_r;(\mu)i,(\nu)j} = \pi_{p,\sigma_r}\sigma_r \otimes_{F_p} (e_{(\mu)i}\otimes e_{(\nu)j})$$

give all inequivalent irreducible representations of $Z_2 \wr S_n$ when $(p,(\mu),(\nu))$ runs over its domain. where $\pi_{p,\sigma_r}=Ad_{\sigma_r}(\pi_{p,e})$ whose (s) will be denoted as $(s^{(p\sigma_r)})$.

Corollary 2: (1) Burside formula. $\Sigma_{(p,(\mu),(\nu))}(C_n^p d_{(\mu)} d_{(\nu)})^2 = 2^n n!$

(2) The number of conjugate classes is $\Sigma_{(p,(\mu),(\nu))} 1$.

(3) Representation matrix element. Given $\sigma \Pi_q I_q^{t_q} \in Z_2 \wr S_n$,

$$D_{(p,(\mu),(\nu))}\left(\sigma \prod_q I_q^{t_q}\right)_{\sigma_r ij}^{\sigma_r' i' j'} = \delta^{\sigma'}_{\tilde{\sigma}_r(\sigma\sigma_r)} D_{(\mu)}(\sigma_{(n-p)}(\sigma\sigma_r))_i^{i'} D_{(\nu)}(\sigma_p(\sigma\sigma_r))_j^{j'} \prod_q (-)^{s_q^{(p\sigma_r)} t_q}.$$

(4) Character:

$$\chi_{(p,(\mu),(\nu))}\left(\sigma \prod_q I_q^{t_q}\right) = \delta^{\sigma'}_{\tilde{\sigma}_r(\sigma\sigma_r)} \chi_{(\mu)}(\sigma_{(n-p)}(\sigma\sigma_r)) \chi_{(\nu)}(\sigma_p(\sigma\sigma_r)) \prod_q (-)^{s_q^{(p\sigma_r)} t_q},$$

where $\tilde{\sigma}_r, \sigma_{(n-p)}, \sigma_p$ map an element in S_n to its decompositions according to S_n/F_p, S_{n-p}, and S_p, respectively.

At the end of this section, we introduce the *orientation-preserved* n-cubic group SO_n which is a normal subgroup of O_n,

$$SO_n := (O_n \cap SO(n)) \lhd O_n. \tag{21}$$

Define $Z_2^n|_e$ as a subgroup of Z_2^n generated by $I_i I_j, i \neq j$ and $Z_2^n|_o := Z_2^n \setminus Z_2^n|_e$. Then

$$SO_n = (Z_2^n|_e \cdot A_n) \sqcup (Z_2^n|_o \cdot (S_n \setminus A_n)) \tag{22}$$

in which $\cdot$ is the product of two subsets in a group, A_n stands for the alternative subgroup in S_n. Thus, $|SO_n| = (2^n \cdot (n)!)/2$.

C. Double group and spinor representation

Some fundamental facts of Clifford algebra are necessary for giving the definition and properties of double groups. Denote the Clifford algebra upon Euclidean space V as $\mathrm{Cl}(V)$; the isometry $x \mapsto -x$ on V extends to an automorphism of $\mathrm{Cl}(V)$ denoted by $x \mapsto \tilde{x}$ and referred to as the canonical automorphism of $\mathrm{Cl}(V)$. We use $\mathrm{Cl}^*(V)$ to denote the multiplicative group of invertible elements in $\mathrm{Cl}(V)$ and the Pin group is the subgroup of $\mathrm{Cl}^*(V)$ generated by unit vectors in V, i.e.,

$$\mathrm{Pin}(V) := \{a \in \mathrm{Cl}^*(V) : a = u_1 \cdots u_r, u_j \in V, \|u_j\| = 1\}.$$

Proofs of the following four statements can be found in Ref. 16.

Lemma 2: If $u \in V$ is non-null, then R_u, reflection along u, is given in terms of Clifford multiplication by

$$R_u x = -uxu^{-1}, \quad \forall x \in V.$$

Theorem 2: *The sequence*

$$0 \to Z_2 \to \mathrm{Pin}(V) \xrightarrow{\widetilde{Ad}} O(V) \to 1$$

is exact, in which

$$\widetilde{\mathrm{Ad}}_a(x) := \tilde{a}xa^{-1}, \quad \forall x \in \mathrm{Cl}(V), \quad a \in \mathrm{Pin}(V).$$

We will usually write $\widetilde{\mathrm{Ad}}$ just by π as a surjective homomorphism.

Proposition 5: $\mathrm{Cl}(E^4)$, *as an associative algebra with unit, is isomorphic to* $M_2(\mathbf{H})$ *where* $\mathbf{H}$ *denotes quaternions.*

Lemma 3: Under the above-given algebra isomorphism, the image of $\mathrm{Pin}(E^4)$ *is a subset of* $SU(4)$.

Now we give the main definition of this paper.

Definition 1: Let ϵ be an injective homomorphism from a group G to $O(n)$, then the double group or the spin-extension of G with respect to ϵ is defined to be $D_n(G,\epsilon) := \pi^{-1}(\epsilon(G))$.

An introduction to double groups in three dimension can be found in Ref. 17. Following elementary facts in the theory of group extension,[18] this diagram

$$\begin{array}{ccccccccc} 0 & \to & Z_2 & \to & \mathrm{Pin}(E^n) & \xrightarrow{\pi} & O(n) & \to & 1 \\ & & \| & & \uparrow & & \uparrow \epsilon & & \\ 0 & \to & Z_2 & \to & \pi^{-1}(\epsilon(G)) & \to & G & \to & 1 \end{array}$$

is commutative. If $\epsilon_1(G) \sim \epsilon_2(G)$, there is

$$\begin{array}{ccccccccc} 0 & \to & Z_2 & \xrightarrow{i} & \pi^{-1}(\epsilon_1(G)) & \xrightarrow{\pi} & \epsilon_1(G) & \to & 1 \\ & & \| & & \downarrow & & \downarrow & & \\ 0 & \to & Z_2 & \xrightarrow{i'} & \pi^{-1}(\epsilon_2(G)) & \xrightarrow{\pi'} & \epsilon_2(G) & \to & 1. \end{array}$$

Note that the double group is not a universal object for a given abstract group G but a special type of Z_2-central extension of G subjected to the embedding ϵ. For example, the results of doubling two Z_2 subgroups in $O(2)$, $I := \{1,\sigma\}, R := \{1, R(\pi)\}$, where σ denotes reflection along y axis and $R(\pi)$ is the rotation over π, are $\pi^{-1}(I) \cong Z_2 \otimes Z_2$ while $\pi^{-1}(R) \cong Z_4$. Nevertheless, we will use the symbol $\overline{G}$ to denote the double group at most cases where n and ϵ are fixed, and will not distinguish G from $\epsilon(G)$. Meanwhile, the symbol $\overline{e}$ is adopted to refer -1 in Clifford algebra and is called *central element.*

Let $s: G \to \overline{G}, s.t. \pi s = Id_G$, namely s is a cross section of π. There is a property of the conjugate classes of $\overline{G}$ which is easy to verify.

Lemma 4: Let C be a conjugate class in G, then either $\pi^{-1}(C)$ will be one conjugate class in $\overline{G}$ satisfying $\forall g \in C, s(g) \sim -s(g)$; or it will split into two conjugate classes C_1, C_2 in $\overline{G}$ s.t. $\forall g \in C, s(g) \in C_1 \Leftrightarrow -s(g) \in C_2$.

We will give a more in-depth result on the splitting of conjugate classes when doubling G to $\overline{G}$ in another paper.

Let r be an irreducible representation of $\overline{G}$ on L, then $r(-1) = \pm \mathbf{1}$.

Definition 2: An irreducible representation of $\overline{G}$ *with* $r(-1)=\mathbf{1}$ *is called a single-valued representation of* G *while an irreducible representation with* $r(-1)=-\mathbf{1}$ *is called a spinor representation or two-valued representation of* G.

Proposition 6: Let $\mathrm{IRR}_{\mathcal{C}}(G)$ *be the class of all inequivalent irreducible representations of* G *and* $\mathrm{IRR}_{\mathcal{C}}(G)^s$ *be the class of all inequivalent single-valued representations of* G, *define* $\phi:\mathrm{IRR}_{\mathcal{C}}(G)\to\mathrm{IRR}_{\mathcal{C}}(G)^s, r\mapsto r\circ\pi$. *Then* ϕ *is a bijection.*

Proof: One can check: $r\circ\pi$ is a representation of $\overline{G}$; if $r\cong r'$, then $r\circ\pi\cong r'\circ\pi$; that r is irreducible implies that $r\circ\pi$ is irreducible and $r\circ\pi$ is single valued. Therefore, ϕ is well defined. If r and r' are inequivalent, then $r\circ\pi$ and $r'\circ\pi$ are two elements in $\mathrm{IRR}_{\mathcal{C}}(G)^s$, namely ϕ is injective. To prove that ϕ is a surjection, consider any $\tilde{r}\in\mathrm{IRR}_{\mathcal{C}}(G)^s:\overline{G}\to L$. Define $r:G\to L, g\mapsto\tilde{r}(s(g))$ where $s(g)$ is any element in $\pi^{-1}(g)$. One can check: r is a well-defined map since $\tilde{r}$ is single valued; r is an irreducible representation of G on L, accordingly $r\in\mathrm{IRR}_{\mathcal{C}}(G)$ and lastly, $\phi(r)=\tilde{r}$. So the result follows. □

This proposition says that all single-valued representations of G which are part of inequivalent irreducible representations of $\overline{G}$ are completely determined by the representation theory of G.

III. STRUCTURE OF $\overline{O_4}$

A. Structure of O_4

It follows Proposition 2, that $O_4\cong Z_2^4\rtimes S_4$; hence $|O_4|=384$. In point group theory, the rotation subgroup of O_h is denoted as O; on the other hand, $S_4\cong Z_2^2\rtimes S_3\cong O$.[11] We write the isomorphism explicitly. The structure of $Z_2^2\rtimes S_3$ is given by four generators α,β,η,t and the relations

$$\alpha^2=e,\quad \beta^2=e,\quad \alpha\beta=\beta\alpha, \tag{23}$$

$$t^3=e,\quad \eta^2=e,\quad \eta t=t^2\eta, \tag{24}$$

$$t\alpha=\alpha\beta t,\quad t\beta=\alpha t,\quad \eta\alpha=\beta\eta, \tag{25}$$

and the isomorphisms are defined to be

$$(12)(34)\leftrightarrow\alpha\leftrightarrow\mathrm{diag}(-1,-1,1),(13)(24)\leftrightarrow\beta\leftrightarrow\mathrm{diag}(1,-1,-1)$$

$$(234)\leftrightarrow t\leftrightarrow\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix},(23)\leftrightarrow\eta\leftrightarrow\begin{pmatrix}0&0&-1\\0&-1&0\\-1&0&0\end{pmatrix}.$$

The structure of $Z_2^4\rtimes S_4$ is given by Eqs. (23)–(25) together with [see Eq. (6)]

$$I_i^2=e,\quad I_iI_j=I_jI_i,\quad i,j=1..4,\quad i\neq j, \tag{26}$$

$$\begin{gathered}\alpha I_1=I_2\alpha,\quad \alpha I_3=I_4\alpha,\\ \beta I_1=I_3\beta,\quad \beta I_2=I_4\beta,\\ tI_1=I_1t,\quad tI_2=I_4t,\quad tI_3=I_2t,\quad tI_4=I_3t,\\ \eta I_1=I_1\eta,\quad \eta I_2=I_3\eta,\quad \eta I_4=I_4\eta.\end{gathered} \tag{27}$$

The matrix representations of above generators are given by [see Eq. (5)]

$$(I_i)^j_k=\delta^j_k(1-2\delta^j_i),\quad i,j,k=1,2,3,4, \tag{28}$$

TABLE I. Conjugate classes of $Z_2^4 \rtimes S_4$. ''SplitNo'' reflects the relation between the classes of $Z_2 \wr S_4$ and those of S_4. ''Ord'' means order of each class. ''Num'' is the number of elements in each class. ''Det'' is the signature of each class. See. Eqs. (16)–(19).

No	SplitNo	YoungDiagram	ord	num	det	No	SplitNo	YoungDiagram	ord	num	det
1	1-1		1	1	1	2	1-2		2	4	-1
3	1-3		2	6	1	4	1-4		2	4	-1
5	1-5		2	1	1						
6	2-1		2	12	-1	7	2-2		2	24	1
8	2-3		4	12	1	9	2-4		2	12	-1
10	2-5		4	24	-1	11	2-6		4	12	1
12	3-1		2	12	1	13	3-2		4	24	-1
14	3-3		4	12	1						
15	4-1		3	32	1	16	4-2		6	32	-1
17	4-3		6	32	-1	18	4-4		6	32	1
19	5-1		4	48	-1	20	5-2		8	48	1

$$\alpha \mapsto \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \beta \mapsto \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad t \mapsto \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \eta \mapsto \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{29}$$

In fact, if we introduce

$$\gamma \mapsto \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

then the generators of O_4 can be reduced to a smaller set $\{I_i, \gamma, t | i = 1,2,3,4\}$ whose generating relations are Eqs. (26) and (27) together with

$$\gamma^2 = e, \quad t^3 = e, \quad (t\gamma)^4 = e, \tag{30}$$

$$\gamma I_1 = I_3 \gamma, \quad \gamma I_2 = I_2 \gamma, \quad \gamma I_4 = I_4 \gamma, \tag{31}$$

while $\alpha = (t^2\gamma)^2, \beta = t\gamma t^2 \gamma t, \eta = \gamma t \gamma t^2 \gamma$.

Applying the general results on conjugate classification of O_n Eqs. (15)–(19), we give the table of conjugate classes of O_4 (see Table I).

B. Construction of $\overline{O_4}$

We will denote $s(g)$ still as g for all $g \in G$. $\overline{O_4}$ is generated by the following equations.

Proposition 7:

$$I_i^2 = -1, \quad I_i I_j = -I_j I_i, \quad i,j = 1..4, \quad i \neq j, \tag{32}$$

$$\gamma^2 = -1, \quad t^3 = -1, \quad (t\gamma)^4 = -1, \tag{33}$$

$$\underline{\gamma I_1 = -I_3 \gamma}, \quad \gamma I_2 = -I_2 \gamma, \gamma I_4 = -I_4 \gamma, \tag{34}$$

$$tI_1 = I_1 t, \quad \underline{tI_2 = I_4 t}, \quad \underline{tI_3 = I_2 t}, \quad \underline{tI_4 = I_3 t}. \tag{35}$$

Proof: First, Eqs. (32)–(35) are valid. In fact, the standard orthogonal bases in E^4 satisfy Clifford relations $e_i e_j + e_j e_i = -2\delta_{ij}$, which is equivalent to Eq. (32); therefore, one can take $I_i = e_i$. Following lemma 2, we set

$$\gamma = \frac{1}{\sqrt{2}}(e_3 - e_1)$$

and check that Eq. (34) is satisfied. Let $t = 1/2\,(1 - e_2 e_3 + e_2 e_4 - e_3 e_4)$, which is the product of

$$\frac{1}{\sqrt{2}}(e_2 - e_3) \text{ and } \frac{1}{\sqrt{2}}(e_4 - e_2),$$

and Eq. (35) can be verified. Finally, one can check that Eq. (33) is also satisfied.

Second, notice that the above-mentioned equations are just Eqs. (26), (27), (30), and (31), which generate $\underline{O_4}$, twisted by a Z_2 factor set. So due to the validity of the above-mentioned equations, $\forall g \in \overline{O_4}$, either g or $-g$ will be generated. But -1 can be generated. Therefore, the above-mentioned equation set generations $\overline{O_4}$. □

We can give another proof of this result by proposition 5. In fact, we introduce γ-matrices in E^4 as

$$\gamma_i = \begin{pmatrix} \mathbf{0}_{2\times 2} & i\sigma_i \\ i\sigma_i & \mathbf{0}_{2\times 2} \end{pmatrix}, \quad i = 1,2,3; \quad \gamma_4 = \begin{pmatrix} \mathbf{0}_{2\times 2} & -\mathbf{1}_{2\times 2} \\ \mathbf{1}_{2\times 2} & \mathbf{0}_{2\times 2} \end{pmatrix}$$

in which σ_i stand for three Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Note that σ_2 in our convention is different from the usual definition in physics. $\gamma_i (i = 1..4)$ satisfy Clifford relations $\gamma_i \gamma_j + \gamma_j \gamma_i = -2\delta_{ij}\mathbf{1}_{4\times 4}$ and $\gamma_i^\dagger = -\gamma_i, \gamma_i \gamma_i^\dagger = \mathbf{1}_{4\times 4}, \det(\gamma_i) = 1$.

We use $S(g)$ as the image of $s(g)$ in $M_2(\mathbf{H})$. Let

$$S(I_i) = \gamma_i, \quad S(\gamma) = \frac{i}{\sqrt{2}} \cdot \begin{pmatrix} 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & -1 \\ 1 & -1 & 0 & 0 \\ -1 & -1 & 0 & 0 \end{pmatrix}, \quad S(t) = \frac{e^{i(7\pi/4)}}{\sqrt{2}} \cdot \begin{pmatrix} 1 & -i & 0 & 0 \\ 1 & i & 0 & 0 \\ 0 & 0 & i & 1 \\ 0 & 0 & -i & 1 \end{pmatrix}, \tag{36}$$

then one can check that these matrices give correct images under $\widetilde{\mathrm{Ad}}$ and satisfy the corresponding relations in Eqs. (32)–(35). It should be noticed that the $\widetilde{\mathrm{Ad}}$-map condition can fix these matrices

TABLE II. Conjugate classes of $\overline{O_4}$. The labels of classes are descended from those of O_4 with the ($'$) for those classes split when lifted into $\overline{O_4}$.

No.	1	1′	2	3	4	5	6	7	8	8′	9	10	11	12	13	14	14′	15	15′	16	17	18	19	20	20′
Num.	1	1	8	12	8	2	24	48	12	12	24	48	24	24	48	12	12	32	32	64	64	64	96	48	48
Ord.	1	2	4	4	2	2	4	4	8	8	2	8	8	4	8	4	4	6	3	12	6	6	4	8	8

up to a nonvanishing scalar and that by using lemma 3, the scalar can be fixed up to a Z_4 uncertainty, namely if one searches out an $S(g)$ then $iS(g), -S(g), -iS(g)$ will also work. One can figure out two of them by calculating the projections on the basis of $\mathrm{Cl}(E^4)$ and ruling out those whose projections are purely imaginary.

We point out that the generating relations in proposition 7 are not unique, due to the canonical automorphism of $\mathrm{Cl}(E^4)$. In fact from the second proof of this proposition, we have noticed that at last there is still a Z_2 uncertainty. Consequently, we can change the cross section s to another one s' by a ''local'' Z_2 transformation and the underlined equations in Eqs. (32)–(35) may gain or lose some (-1)-factors accordingly. Anyway, they are equivalent to the former ones.

To classify the elements in $\overline{O_4}$, Lemma 4 will enable us to use the same symbols for the conjugate classes of O_4 and to use a ($'$) for those splitting classes. Except for classes 1,8,14,15,20, which split into two classes for each, any other class in O_4 is lifted to one class. Therefore, there are totally 25 classes in $\overline{O_4}$ (see Table II).

IV. REPRESENTATIONS OF $\overline{O_4}$

A. Single-valued representations of O_4

Due to Theorem 6, there are totally 20 inequivalent single-valued representations of O_4 corresponding to the 20 inequivalent irreducible representations of O_4; the representation theory of O_4 can be systematically solved by applying little group method (Proposition 1).

All inequivalent irreducible characters of Z_2^4 are listed in Table III. Following Theorem 4, $\Pi(Z_2^4)$ are partitioned into orbits with index set defined in a physical convention $\mathcal{I} := \{S,P,V,A,T\}$.

$$\Pi_S = \{\pi_{0000}\}, \quad F_S \cong S_4; \quad \Pi_P = \{\pi_{1111}\}, \quad F_P \cong S_4,$$

TABLE III. Character table of Z_2^4. $I_{i_1 i_2 \ldots I_a} := I_{i_1} \cdot I_{i_2} \cdot \ldots \cdot I_{i_a}$. Irreducible characters are labeled as $\chi_{s_1 s_2 s_3 s_4}, s_i \in \mathcal{Z}/2\mathcal{Z}$ [see Eq. (20)].

$\overline{Z_2^4}$	$[e]$	$[I_1]$	$[I_2]$	$[I_3]$	$[I_4]$	$[I_{12}]$	$[I_{13}]$	$[I_{14}]$	$[I_{23}]$	$[I_{24}]$	$[I_{34}]$	$[I_{234}]$	$[I_{134}]$	$[I_{124}]$	$[I_{123}]$	$[I_{1234}]$
χ_{0000}	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
χ_{0001}	1	1	1	1	−1	1	1	−1	1	−1	−1	−1	−1	−1	1	−1
χ_{0010}	1	1	1	−1	1	1	−1	1	−1	1	−1	−1	−1	1	−1	−1
χ_{0100}	1	1	−1	1	1	−1	1	1	−1	−1	1	−1	1	−1	−1	−1
χ_{1000}	1	−1	1	1	1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
χ_{0011}	1	1	1	−1	−1	1	−1	−1	−1	−1	1	1	1	−1	−1	1
χ_{0101}	1	1	−1	1	−1	−1	1	−1	−1	1	−1	1	−1	1	−1	1
χ_{1001}	1	−1	1	1	−1	−1	−1	1	1	−1	−1	−1	1	1	−1	1
χ_{0110}	1	1	−1	−1	1	−1	−1	1	1	−1	−1	1	−1	−1	1	1
χ_{1010}	1	−1	1	−1	1	−1	1	−1	−1	1	−1	−1	1	−1	1	1
χ_{1100}	1	−1	−1	1	1	1	−1	−1	−1	−1	1	−1	−1	1	1	1
χ_{1110}	1	−1	−1	−1	1	1	1	−1	1	−1	−1	1	1	1	−1	−1
χ_{1101}	1	−1	−1	1	−1	1	−1	1	−1	1	−1	1	1	−1	1	−1
χ_{1011}	1	−1	1	−1	−1	−1	1	1	−1	−1	1	1	−1	1	1	−1
χ_{0111}	1	1	−1	−1	−1	−1	−1	−1	1	1	1	−1	1	1	1	−1
χ_{1111}	1	−1	−1	−1	−1	1	1	1	1	1	1	−1	−1	−1	−1	1

$$\Pi_V=\{\pi_{0001},\pi_{0010},\pi_{0100},\pi_{1000}\},\quad F_V\cong S_3,$$

$$\Pi_A=\{\pi_{1110},\pi_{1101},\pi_{1011},\pi_{0111}\},\quad F_A\cong S_3,$$

$$\Pi_T=\{\pi_{0011},\pi_{0101},\pi_{1001},\pi_{0110},\pi_{1010},\pi_{1100}\},\quad F_T\cong Z_2^2.$$

We will use $[\lambda]$ instead of (ν) to denote Young diagrams where $[\lambda]=[\lambda_1\lambda_2\ldots\lambda_n],\lambda_k=\sum_{i=k}^{n}\nu_i$.

1. Orbit S

All inequivalent irreducible representations of S_4 are labeled by $[4],[31],[2^2],[21^2],[1^4]$; accordingly,

$$\Pi_S\cdot([4],[31],[2^2],[21^2],[1^4])$$

provide two one-dimensional, one two-dimensional, and two three-dimensional representations. As for representation matrices, all $I_i,i=1,..,4$ are mapped to identity, while α,β,t,η take the same matrix form as they have in S_4, i.e., $\Pi_S\cdot[4]:I_i,\alpha,\beta,t,\eta\to 1$; $\Pi_S\cdot[1^4]:I_i,\alpha,\beta,t\to 1$, $\eta\to -1$;

$$\Pi_S\cdot[2^2]:I_i,\alpha,\beta\to\mathbf{1}_{2\times 2},t\to\begin{pmatrix} e^{i\frac{2\pi}{3}} & 0\\ 0 & e^{i\frac{4\pi}{3}}\end{pmatrix},\quad \eta\to\begin{pmatrix}0&1\\1&0\end{pmatrix},$$

$$\Pi_S\cdot[31]:I_i\to\mathbf{1}_{3\times 3},\alpha\to\begin{pmatrix}-1&0&0\\0&1&0\\0&0&-1\end{pmatrix},\quad \beta\to\begin{pmatrix}-1&0&0\\0&-1&0\\0&0&1\end{pmatrix},\quad t\to\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix},$$

$$\eta\to\begin{pmatrix}1&0&0\\0&0&1\\0&1&0\end{pmatrix};$$

$\Pi_S\cdot[21^2]$: I_i,α,β,t take the same form of $\Pi_S\cdot[31]$ and η gains a minus sign compared to $\Pi_S\cdot[31]$.

2. Orbit P

$$\Pi_P\cdot([4],[31],[2^2],[21^2],[1^4]).$$

The only difference from *orbit S* is that I_i are mapped to $-\mathbf{1}$.

3. Orbit V

All inequivalent irreducible representations of S_3 can be written as $[3],[21],[1^3]$ and it has no difficulty, using our generating relations, to check

$$\alpha\pi_{1000}\alpha^{-1}=\pi_{0100},\quad \eta\pi_{0100}\eta^{-1}=\pi_{0010},\quad \alpha\pi_{0010}\alpha^{-1}=\pi_{0001}.$$

Hence, this orbit gives two four-dimensional representations and one eight-dimensional representation,

$$\Pi_V\cdot([3],[21],[1^3])=(e,\alpha,\beta\eta,\alpha\beta\eta)\cdot\pi_{1000}\cdot([3],[21],[1^3]).$$

The representation matrices of $\Pi_V\cdot[3]$ are coincident with those in Eqs. (28) and (29). Representation matrices of $\Pi_V\cdot[1^3]$ are the same as those in $\Pi_V\cdot[3]$, except that η picking on a minus sign. $\Pi_V\cdot[21]$:

$$e_i\rightarrow\begin{pmatrix}\Pi_V\cdot[3](e_i) & \mathbf{0}_{4\times4}\\ \mathbf{0}_{4\times4} & \Pi_V\cdot[3](e_i)\end{pmatrix},$$

$$\alpha\rightarrow\begin{pmatrix}\Pi_V\cdot[3](\alpha) & \mathbf{0}_{4\times4}\\ \mathbf{0}_{4\times4} & \Pi_V\cdot[3](\alpha)\end{pmatrix},\quad \beta\rightarrow\begin{pmatrix}\mathbf{0}_{4\times4} & \Pi_V\cdot[3](\beta)\\ \Pi_V\cdot[3](\beta) & \mathbf{0}_{4\times4}\end{pmatrix},$$

$$t\rightarrow\begin{pmatrix}e^{i\frac{2\pi}{3}}\cdot\Pi_V\cdot[3](t) & \mathbf{0}_{4\times4}\\ \mathbf{0}_{4\times4} & e^{i\frac{4\pi}{3}}\cdot\Pi_V\cdot[3](t)\end{pmatrix},\quad \eta\rightarrow\begin{pmatrix}\mathbf{0}_{4\times4} & \Pi_V\cdot[3](\eta)\\ \Pi_V\cdot[3](\eta) & \mathbf{0}_{4\times4}\end{pmatrix}.$$

4. Orbit A

Similar to *orbit V*, there are two four-dimensional representations and one eight-dimensional representation,

$$\Pi_A\cdot([3],[21],[1^3])=(e,\alpha,\beta\eta,\alpha\beta\eta)\cdot\pi_{0111}\cdot([3],[21],[1^3])$$

while the representation matrices for I_i pick on a minus sign, without changing the others.

5. Orbit T

The stationary subgroup F_T leaving π_{0110} invariant is $\{e,\eta,\alpha\beta,\alpha\beta\eta\}$ with four one-dimensional irreducible representations, denoted by $\pi_{(a,b)},a,b=0,1$. Therefore, there are four six-dimensional representations given by this orbit. Notice that

$$\alpha\pi_{0110}\alpha^{-1}=\pi_{1001},\quad t\pi_{1001}t^{-1}=\pi_{1010},\quad t\pi_{1010}t^{-1}=\pi_{1100},$$

$$\alpha\pi_{1010}\alpha^{-1}=\pi_{0101},\quad \beta\pi_{1100}\beta^{-1}=\pi_{0011},$$

the four representations can be labeled as

$$\Pi_T\cdot(\pi_{00},\pi_{01},\pi_{10},\pi_{11})=(e,\alpha,\alpha\beta t,\beta t^2,\beta t,t^2)\cdot\pi_{0110}\cdot(\pi_{00}+\pi_{01}+\pi_{10}+\pi_{11}).$$

Then we enumerate the matrices for the four representations,

$$\Pi_T\cdot\pi_{00}:I_1\rightarrow\mathrm{diag}(1,-1,-1,-1,1,1),\quad I_2\rightarrow\mathrm{diag}(-1,1,1,-1,-1,1),$$

$$I_3\rightarrow\mathrm{diag}(-1,1,-1,1,1,-1),\quad I_4\rightarrow\mathrm{diag}(1,-1,1,1,-1,-1),$$

$$\alpha\rightarrow\begin{pmatrix}0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&0&0&1&0\\0&0&0&1&0&0\\0&0&1&0&0&0\\0&0&0&0&0&1\end{pmatrix},\quad \beta\rightarrow\begin{pmatrix}0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&1&0&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0\\0&0&0&1&0&0\end{pmatrix},$$

$$t\to\begin{pmatrix}0&0&0&0&0&1\\0&0&0&1&0&0\\0&1&0&0&0&0\\0&0&1&0&0&0\\1&0&0&0&0&0\\0&0&0&0&1&0\end{pmatrix},\quad \eta\to\begin{pmatrix}1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&0&1&0&0\\0&0&1&0&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0\end{pmatrix},$$

$$\Pi_T\cdot\pi_{01}: I_1\to\Pi_2\cdot\pi_{00}(I_1),\quad I_2\to\Pi_T\cdot\pi_{00}(I_2),\quad I_3\to\Pi_T\cdot\pi_{00}(I_3),\quad I_4\to\Pi_T\cdot\pi_{00}(I_4),$$

$$\alpha\to\begin{pmatrix}0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&0&0&1&0\\0&0&0&-1&0&0\\0&0&1&0&0&0\\0&0&0&0&0&-1\end{pmatrix},\quad \beta\to\begin{pmatrix}0&-1&0&0&0&0\\-1&0&0&0&0&0\\0&0&-1&0&0&0\\0&0&0&0&0&1\\0&0&0&0&-1&0\\0&0&0&1&0&0\end{pmatrix},$$

$$t\to\begin{pmatrix}0&0&0&0&0&1\\0&0&0&1&0&0\\0&1&0&0&0&0\\0&0&1&0&0&0\\-1&0&0&0&0&0\\0&0&0&0&-1&0\end{pmatrix},\quad \eta\to\begin{pmatrix}1&0&0&0&0&0\\0&-1&0&0&0&0\\0&0&0&-1&0&0\\0&0&-1&0&0&0\\0&0&0&0&0&-1\\0&0&0&0&-1&0\end{pmatrix},$$

$$\Pi_T\cdot\pi_{10}: I_1\to\Pi_T\cdot\pi_{00}(I_1),\quad I_2\to\Pi_T\cdot\pi_{00}(I_2),\quad I_3\to\Pi_T\cdot\pi_{00}(I_3),\quad I_4\to\Pi_T\cdot\pi_{00}(I_4),$$

$$\alpha\to\Pi_T\cdot\pi_{00}(\alpha),\quad \beta\to\Pi_T\cdot\pi_{00}(\beta),\quad t\to\Pi_T\cdot\pi_{00}(t),\quad \eta\to(-1)\cdot\Pi_T\cdot\pi_{00}(\eta),$$

$$\Pi_T\cdot\pi_{11}: I_1\to\Pi_T\cdot\pi_{01}(I_1),\quad I_2\to\Pi_T\cdot\pi_{01}(I_2),\quad I_3\to\Pi_T\cdot\pi_{01}(I_3),\quad I_4\to\Pi_T\cdot\pi_{01}(I_4),$$

$$\alpha\to\Pi_T\cdot\pi_{01}(\alpha),\quad \beta\to\Pi_T\cdot\pi_{01}(\beta),\quad t\to\Pi_T\cdot\pi_{01}(t),\quad \eta\to(-1)\cdot\Pi_T\cdot\pi_{01}(\eta).$$

Here we find all 20 inequivalent irreducible representations corresponding to the 20 conjugate classes of O_4, which satisfy Burside formula

$$2\times(1^2+1^2+2^2+3^2+3^2)+2\times(4^2+4^2+8^2)+4\times6^2=384.$$

Following Proposition 6, we have found all of the single-valued representations of O_4.

B. Spinor representations of O_4

Notice the following facts that $\overline{Z_2^4}\lhd\overline{O_4}$, $\overline{O_4}/\overline{Z_2^4}\cong S_4$ and Eq. (36) generates a spinor representation of O_4 which is still denoted as S; what's more, its restriction to $\overline{Z_2^4}$ is also a two-valued representation of Z_2^4. These facts ensure two conditions in Theorem 1. To apply Theorem 1 to deduce spinor representations of O_4, we develop a calculation method. The matrices of a spinor representation of O_4 for I_i,γ,t, denoted as $\tilde{S}(I_i),\tilde{S}(\gamma),\tilde{S}(t)$, can be decomposed as

$$\tilde{S}(I_i)=S(I_i)\otimes\mathbf{1},\quad i=1,3,4,\quad \tilde{S}(I_2)=-S(I_2)\otimes\mathbf{1};$$

$$\tilde{S}(\gamma)=\Gamma\otimes\tilde{\gamma};\quad \tilde{S}(t)=T\otimes\tilde{t},$$

where Γ, T and $S(I_i)$ act on the same module, $\tilde{\gamma}, \tilde{t}$ have *the same texture (zero matrix elements) of the representation matrices of five inequivalent irreducible representations of* S_4 [the minus added before $S(I_2)$ is for a physical convention]. There are five spinor representations of dimension 4,4,8,12, and 12, respectively, and the second half of Burside formula is satisfied

$$4^2+4^2+8^2+12^2+12^2=384.$$

Corresponding to the generating equations (32)–(35), there are a system of matrix equations

$$\tilde{S}(\gamma)^2=\tilde{S}(t)^3=-\mathbf{1}, \quad (\tilde{S}(\gamma)\tilde{S}(t))^4=-\mathbf{1}, \tag{37}$$

$$\tilde{S}(\gamma)\tilde{S}(I_2)=-\tilde{S}(I_2)\tilde{S}(\gamma), \quad \tilde{S}(\gamma)\tilde{S}(I_4)=-\tilde{S}(I_4)\tilde{S}(\gamma), \quad \tilde{S}(\gamma)\tilde{S}(I_1)=-\tilde{S}(I_3)\tilde{S}(\gamma), \tag{38}$$

$$\tilde{S}(t)\tilde{S}(I_1)=\tilde{S}(I_1)\tilde{S}(t), \quad \tilde{S}(t)\tilde{S}(I_2)=-\tilde{S}(I_4)\tilde{S}(t), \quad \tilde{S}(t)\tilde{S}(I_3)=-\tilde{S}(I_2)\tilde{S}(t),$$

$$\tilde{S}(t)\tilde{S}(I_4)=\tilde{S}(I_3)\tilde{S}(t), \tag{39}$$

plus a unitary condition

$$\tilde{S}(\gamma)^{\dagger}\tilde{S}(\gamma)=\mathbf{1}, \quad \tilde{S}(t)^{\dagger}\tilde{S}(t)=\mathbf{1}. \tag{40}$$

Note that we add a minus sign to the second and the third equations in Eq. (39) compared with Eq. (35) according to the same physics convention, though they are completely equivalent.

Solving Eqs. (37)–(40) for the four-dimensional case gives two solutions:

$$\underline{4}_+ : \tilde{S}(\gamma)=\Gamma\cdot\tilde{\gamma}_+, \quad \Gamma=\frac{1}{\sqrt{2}}\cdot\begin{pmatrix} 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & -1 \\ 1 & -1 & 0 & 0 \\ -1 & -1 & 0 & 0 \end{pmatrix}, \quad \tilde{\gamma}_+=i,$$

$$\tilde{S}(t)=T\cdot\tilde{t}, \quad T=\frac{1}{\sqrt{2}}\cdot\begin{pmatrix} 1 & -i & 0 & 0 \\ 1 & i & 0 & 0 \\ 0 & 0 & i & 1 \\ 0 & 0 & -i & 1 \end{pmatrix}, \quad \tilde{t}=e^{i(7\pi/4)},$$

$$\underline{4}_- : \tilde{S}(\gamma)=\Gamma\cdot\tilde{\gamma}_-, \quad \tilde{\gamma}_-=-i, \quad \tilde{S}(t)=T\cdot\tilde{t}.$$

Note that $\underline{4}_+$ is just the representation S with $\tilde{S}(I_2)=-S(I_2)$.

As for the eight-dimensional case we can suppose

$$\tilde{\gamma}=\begin{pmatrix} 0 & \tilde{c} \\ \tilde{d} & 0 \end{pmatrix}, \quad \tilde{t}=\begin{pmatrix} \tilde{a} & 0 \\ 0 & \tilde{d} \end{pmatrix}.$$

The solution $\underline{8}$ is given by

$$\tilde{c}=e^{i(\pi/3)}, \quad \tilde{d}=e^{i(2\pi/3)}, \quad \tilde{a}=e^{i(5\pi/12)}, \quad \tilde{d}=e^{i(13\pi/12)}.$$

Finally, we set for the twelve-dimensional case

$$\tilde{\gamma}=\begin{pmatrix} 0 & 0 & \tilde{z} \\ 0 & \tilde{y} & 0 \\ \tilde{x} & 0 & 0 \end{pmatrix}, \quad \tilde{t}=\begin{pmatrix} 0 & 0 & \tilde{n} \\ \tilde{l} & 0 & 0 \\ 0 & \tilde{m} & 0 \end{pmatrix},$$

such that

$$\underline{12}_+ : \tilde{x}=1, \quad \tilde{y}=i, \quad \tilde{z}=-1, \quad \tilde{l}=1, \quad \tilde{m}=1, \quad \tilde{n}=e^{i(5\pi/4)},$$

$$\underline{12}_- : \tilde{x}=1, \quad \tilde{y}=-i, \quad \tilde{z}=-1, \quad \tilde{l}=1, \quad \tilde{m}=-1, \quad \tilde{n}=e^{i(\pi/4)}.$$

So far, we obtain all inequivalent irreducible representations of $\overline{O_4}$ and we summarize our results in Table IV.

V. STRUCTURE OF $\overline{SO_4}$

Specify $n=4$ in Eq. (21). Then we know immediately that $|SO_4|=192$. Introduce

$$\eta=\gamma t\gamma t^2\gamma, \tag{41}$$

$$\alpha=(t^2\gamma)^2, \quad \beta=t\gamma t^2\gamma t, \tag{42}$$

$$x=e_1\eta, \quad y=e_4\eta, \quad q=e_2\eta. \tag{43}$$

Then the structure of SO_4 can be summarized as

$$x^2=y^2=q^4=e, \quad yx=xy, \quad qx=xq^3, \quad qy=yq^3, \tag{44}$$

$$\alpha^2=\beta^2=t^3=e, \quad \beta\alpha=\alpha\beta, \quad t\alpha=\alpha\beta t, \quad t\beta=\alpha t, \tag{45}$$

$$\alpha x=q\beta, \quad \alpha y=q^3\beta, \quad \alpha q=x\beta, \tag{46}$$

$$\beta x=q^3\alpha, \quad \beta y=q\alpha, \quad \beta q=y\alpha, \tag{47}$$

$$tx=xt^2, \quad ty=q^3t^2, \quad tq=yt^2, \tag{48}$$

together with

$$x\alpha=\beta q^3, \quad xt=t^2x, \quad y\beta=\alpha q^3, \quad yt=t^2q^3, \quad qt=t^2y. \tag{49}$$

Accordingly, each group element can be expressed as a ''normal ordering'' product of $x,y\rightarrow q\rightarrow\alpha,\beta\rightarrow t$ and their powers from left to right. Throwing away all classes which belong to O_4 but not to SO_4, there are 11 left which are 1,3,5,7,8,11,12,14,15,18,20 in Table I. The 14th and the 20th will part into two classes with equal numbers of elements each under adjoint action of SO_4 which are denoted as $14,\underline{14'},20,\underline{20'}$. Therefore, there are 13 conjugate classes in SO_4.

Due to the fact that $\overline{SO_4}\lhd\overline{O_4}$, the diagram

$$\begin{array}{ccccccccc} 0 & \rightarrow & Z_2 & \rightarrow & \overline{O_4} & \overset{\pi}{\rightarrow} & O_4 & \rightarrow & 1 \\ & & \| & & \uparrow & & \uparrow & & \\ 0 & \rightarrow & Z_2 & \rightarrow & \overline{SO_4} & \rightarrow & SO_4 & \rightarrow & 1 \end{array}$$

is commutative. We can lift generating relations (44), (45)–(49) to

$$x^2=y^2=q^4=-1, \quad yx=-xy, \quad qx=-xq^3, \quad qy=-yq^3,$$

TABLE IV. Character table of $\overline{O_4}$. Character is labeled by a superscript showing its dimension where an underline shows a spinor representation and a subscript distinguishing different representations with same dimension.

	Π_S					Π_P					Π_V			Π_A			Π_T				Spinor rep				
	$[4]$ $\chi_1^{(1)}$	$[1^4]$ $\chi_3^{(1)}$	$[2^2]$ $\chi_1^{(2)}$	$[31]$ $\chi_1^{(3)}$	$[21^2]$ $\chi_3^{(3)}$	$[4]$ $\chi_2^{(1)}$	$[1^4]$ $\chi_4^{(1)}$	$[2^2]$ $\chi_2^{(2)}$	$[31]$ $\chi_2^{(3)}$	$[21^2]$ $\chi_4^{(3)}$	$[3]$ $\chi_1^{(4)}$	$[1^3]$ $\chi_3^{(4)}$	$[21]$ $\chi_1^{(8)}$	$[3]$ $\chi_4^{(4)}$	$[1^3]$ $\chi_2^{(4)}$	$[21]$ $\chi_2^{(8)}$	π_{00} $\chi_3^{(6)}$	π_{01} $\chi_2^{(6)}$	π_{10} $\chi_4^{(6)}$	π_{11} $\chi_1^{(6)}$	$\underline{4}_+$ $\chi_1^{(4)}$	$\underline{4}_-$ $\chi_2^{(4)}$	$\underline{8}$ $\chi^{(8)}$	12_+ $\chi_1^{(12)}$	12_- $\chi_2^{(12)}$
1	1	1	2	3	3	1	1	2	3	3	4	4	8	4	4	8	6	6	6	6	4	4	8	12	12
$1'$	1	1	2	3	3	1	1	2	3	3	4	4	8	4	4	8	6	6	6	6	−4	−4	−8	−12	−12
2	1	1	2	3	3	−1	−1	−2	−3	−3	2	2	4	−2	−2	−4	0	0	0	0	0	0	0	0	0
3	1	1	2	3	3	1	1	2	3	3	0	0	0	0	0	0	−2	−2	−2	−2	0	0	0	0	0
4	1	1	2	3	3	−1	−1	−2	−3	−3	−2	−2	−4	2	2	4	0	0	0	0	0	0	0	0	0
5	1	1	2	3	3	1	1	2	3	3	−4	−4	−8	−4	−4	−8	6	6	6	6	0	0	0	0	0
6	1	−1	0	1	−1	1	−1	0	1	−1	2	−2	0	2	−2	0	2	0	−2	0	0	0	0	0	0
7	1	−1	0	1	−1	−1	1	0	−1	1	0	0	0	0	0	0	0	2	0	−2	0	0	0	0	0
8	1	−1	0	1	−1	−1	1	0	−1	1	2	−2	0	−2	2	0	0	−2	0	2	$-2\sqrt{2}$	$2\sqrt{2}$	0	$-2\sqrt{2}$	$2\sqrt{2}$
$8'$	1	−1	0	1	−1	−1	1	0	−1	1	2	−2	0	−2	2	0	0	−2	0	2	$2\sqrt{2}$	$-2\sqrt{2}$	0	$2\sqrt{2}$	$-2\sqrt{2}$
9	1	−1	0	1	−1	1	−1	0	1	−1	−2	2	0	−2	2	0	2	0	−2	0	0	0	0	0	0
10	1	−1	0	1	−1	1	−1	0	1	−1	0	0	0	0	0	0	−2	0	2	0	0	0	0	0	0
11	1	−1	0	1	−1	−1	1	0	−1	1	−2	2	0	2	−2	0	0	−2	0	2	0	0	0	0	0
12	1	1	2	−1	−1	1	1	2	−1	−1	0	0	0	0	0	0	2	−2	2	−2	0	0	0	0	0
13	1	1	2	−1	−1	−1	−1	−2	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	1	1	2	−1	−1	1	1	2	−1	−1	0	0	0	0	0	0	−2	2	−2	2	2	2	4	−2	−2
$14'$	1	1	2	−1	−1	1	1	2	−1	−1	0	0	0	0	0	0	−2	2	−2	2	−2	−2	−4	2	2
15	1	1	−1	0	0	1	1	−1	0	0	1	1	−1	1	1	−1	0	0	0	0	2	2	−2	0	0
$15'$	1	1	−1	0	0	1	1	−1	0	0	1	1	−1	1	1	−1	0	0	0	0	−2	−2	2	0	0
16	1	1	−1	0	0	−1	−1	1	0	0	−1	−1	1	1	1	−1	0	0	0	0	0	0	0	0	0
17	1	1	−1	0	0	−1	−1	1	0	0	1	1	−1	−1	−1	1	0	0	0	0	0	0	0	0	0
18	1	1	−1	0	0	1	1	−1	0	0	−1	−1	1	−1	−1	1	0	0	0	0	0	0	0	0	0
19	1	−1	0	−1	1	1	−1	0	−1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	1	−1	0	−1	1	−1	1	0	1	−1	0	0	0	0	0	0	0	0	0	0	$\sqrt{2}$	$-\sqrt{2}$	0	$-\sqrt{2}$	$\sqrt{2}$
$20'$	1	−1	0	−1	1	−1	1	0	1	−1	0	0	0	0	0	0	0	0	0	0	$-\sqrt{2}$	$\sqrt{2}$	0	$\sqrt{2}$	$-\sqrt{2}$

TABLE V. Conjugate classes of $\overline{SO_4}$.

No.	1	$\overline{1}$	3	5	$\overline{5}$	7	8	$\overline{8}$	11	$\overline{11}$	12	14	$\overline{14}$	$14'$	$\overline{14'}$	15	$\overline{15}$	18	$\overline{18}$	20	$\overline{20}$	$20'$	$\overline{20'}$
Num	1	1	12	1	1	48	12	12	12	12	24	6	6	6	6	32	32	32	32	24	24	24	24
Ord	1	2	4	2	2	4	8	8	8	8	4	4	4	4	4	6	3	6	6	8	8	8	8

$$\alpha^2=\beta^2=t^3=-1, \quad \beta\alpha=-\alpha\beta, \quad t\alpha=-\alpha\beta t, \quad t\beta=\alpha t,$$

$$\alpha x=q\beta, \quad \alpha y=q^3\beta, \quad \alpha q=x\beta,$$

$$\beta x=q^3\alpha, \quad \beta y=q\alpha, \quad \beta q=y\alpha,$$

$$tx=-xt^2, \quad ty=q^3t^2, \quad tq=yt^2,$$

$$x\alpha=\beta q^3, \quad xt=-t^2x, \quad y\beta=\alpha q^3, \quad yt=t^2q^3, \quad qt=t^2y$$

by definitions (41)–(43). As to the conjugate classification, 1,5,8,11,14,15,18,20,$14'$,$20'$ violate relation $-g\sim g$, so that $\overline{SO_4}$ is partitioned into 23 classes, suggesting that there are altogether 23 inequivalent irreducible representations in which 13 representations are single valued to SO_4. We summarize the conjugate classes of $\overline{SO_4}$ in Table V.

VI. REPRESENTATION THEORY OF $\overline{SO_4}$

All inequivalent irreducible representations of $\overline{SO_4}$ can be reduced from those of $\overline{O_4}$. Table VI gives the characters of all inequivalent irreducible representations of $\overline{O_4}$, with respect to the classes of $\overline{SO_4}$. A brief observation gives some important information. First, $1_1\cong 1_4, 1_2\cong 1_3, 2_1\cong 2_2, 3_1\cong 3_4, 3_2\cong 3_3, 4_1\cong 4_4, 4_2\cong 4_3, 8_1\cong 8_2, 6_1\cong 6_3$. Second, omitting equivalence, 1_1, 1_2, 2_1, 3_1, 3_1, 4_1, 4_2, 8_1, 6_1, remain irreducible within $\overline{SO_4}$, while other seven become reducible. Third, as for each of these reducible ones, the inner product of the character with itself equals 2, implying that it can be reduced to two inequivalent irreducible representations; thus there are 13 single-valued and 10 spinor representations as we expected. Finally, it is one possible solution to the Burside theorem that each of these seven reducible representations splits into two inequivalent irreducible representations with equal dimensions. We conjecture that it is the solution to our representation theory of $\overline{SO_4}$ and try to verify it in the following.

Summarily speaking, there are nine single-valued inequivalent irreducible representations inherited from $\overline{O_4}$,

$$1_1, 1_2, 2\equiv 2_1, 3_1, 3_2, 4_1, 4_2, 8\equiv 8_1, 6\equiv 6_1$$

and we conjecture the splitting relations

$$6_2, 6_4 \to 3_\alpha, 3_\beta, 3_\gamma, 3_\delta,$$

$$\underline{4}_1, \underline{4}_2 \to 2_\alpha, 2_\beta, 2_\gamma, 2_\delta,$$

$$\underline{8} \to 4_\alpha, 4_\beta,$$

$$\underline{12}_1, \underline{12}_2 \to 6_\alpha, 6_\beta, 6_\gamma, 6_\delta.$$

TABLE VI. Character table of $\overline{O_4}$ (with respect to the classes of $\overline{SO_4}$). (χ,χ) evaluates the inner product of a character with itself.

	1	$\overline{1}$	3	5	$\overline{5}$	7	8	$\overline{8}$	11	$\overline{11}$	12	14	$\overline{14}$	$14'$	$\overline{14}'$	15	$\overline{15}$	18	$\overline{18}$	20	$\overline{20}$	$20'$	$\overline{20}'$	(χ,χ)
$\chi_1^{(1)}$	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	**1**
$\chi_2^{(1)}$	1	1	1	1	1	−1	−1	−1	−1	−1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	**1**
$\chi_1^{(2)}$	2	2	2	2	2	0	0	0	0	0	2	2	2	2	2	−1	−1	−1	−1	0	0	0	0	**1**
$\chi_1^{(3)}$	3	3	3	3	3	1	1	1	1	1	−1	−1	−1	−1	−1	0	0	0	0	−1	−1	−1	−1	**1**
$\chi_2^{(3)}$	3	3	3	3	3	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	0	0	0	0	1	1	1	1	**1**
$\chi_3^{(1)}$	1	1	1	1	1	−1	−1	−1	−1	−1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	**1**
$\chi_4^{(1)}$	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	**1**
$\chi_2^{(2)}$	2	2	2	2	2	0	0	0	0	0	2	2	2	2	2	−1	−1	−1	−1	0	0	0	0	**1**
$\chi_3^{(3)}$	3	3	3	3	3	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	0	0	0	0	1	1	1	1	**1**
$\chi_4^{(3)}$	3	3	3	3	3	1	1	1	1	1	−1	−1	−1	−1	−1	0	0	0	0	−1	−1	−1	−1	**1**
$\chi_1^{(4)}$	4	4	0	−4	−4	0	2	2	−2	−2	0	0	0	0	0	1	1	−1	−1	0	0	0	0	**1**
$\chi_2^{(4)}$	4	4	0	−4	−4	0	−2	−2	2	2	0	0	0	0	0	1	1	−1	−1	0	0	0	0	**1**
$\chi_1^{(8)}$	8	8	0	−8	−8	0	0	0	0	0	0	0	0	0	0	−1	−1	1	1	0	0	0	0	**1**
$\chi_3^{(4)}$	4	4	0	−4	−4	0	−2	−2	2	2	0	0	0	0	0	1	1	−1	−1	0	0	0	0	**1**
$\chi_4^{(4)}$	4	4	0	−4	−4	0	2	2	−2	−2	0	0	0	0	0	1	1	−1	−1	0	0	0	0	**1**
$\chi_2^{(8)}$	8	8	0	−8	−8	0	0	0	0	0	0	0	0	0	0	−1	−1	1	1	0	0	0	0	**1**
$\chi_1^{(6)}$	6	6	−2	6	6	0	0	0	0	0	2	−2	−2	−2	−2	0	0	0	0	0	0	0	0	**1**
$\chi_2^{(6)}$	6	6	−2	6	6	2	−2	−2	−2	−2	−2	2	2	2	2	0	0	0	0	0	0	0	0	**2**
$\chi_3^{(6)}$	6	6	−2	6	6	0	0	0	0	0	2	−2	−2	−2	−2	0	0	0	0	0	0	0	0	**1**
$\chi_4^{(6)}$	6	6	−2	6	6	−2	2	2	2	2	−2	2	2	2	2	0	0	0	0	0	0	0	0	**2**
$\chi_1^{(4)}$	4	−4	0	0	0	0	$-2\sqrt{2}$	$2\sqrt{2}$	0	0	0	2	−2	2	−2	2	−2	0	0	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	**2**
$\chi_2^{(4)}$	4	−4	0	0	0	0	$2\sqrt{2}$	$-2\sqrt{2}$	0	0	0	2	−2	2	−2	2	−2	0	0	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	**2**
$\chi^{(8)}$	8	−8	0	0	0	0	0	0	0	0	0	4	−4	4	−4	−2	2	0	0	0	0	0	0	**2**
$\chi_1^{(12)}$	12	−12	0	0	0	0	$-2\sqrt{2}$	$2\sqrt{2}$	0	0	0	−2	2	−2	2	0	0	0	0	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	**2**
$\chi_2^{(12)}$	12	−12	0	0	0	0	$2\sqrt{2}$	$-2\sqrt{2}$	0	0	0	−2	2	−2	2	0	0	0	0	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	**2**

A. Hidden single-valued representations

The representation matrices of x, y, q in 6_2 are written as

$$x\mapsto\begin{pmatrix}1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&0&1&0&0\\0&0&1&0&0&0\\0&0&0&0&0&-1\\0&0&0&0&-1&0\end{pmatrix},\quad y\mapsto\begin{pmatrix}1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&0&-1&0&0\\0&0&-1&0&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0\end{pmatrix},$$

$$q\mapsto\begin{pmatrix}-1&0&0&0&0&0\\0&-1&0&0&0&0\\0&0&0&-1&0&0\\0&0&1&0&0&0\\0&0&0&0&0&1\\0&0&0&0&-1&0\end{pmatrix}.$$

The textures of these matrices inspire us to such hypotheses that in $3_{\alpha,\beta,\gamma,\delta}$, x,y,q take on a form like

$$x,y\mapsto\begin{pmatrix}\pm1&\\&\pm H\end{pmatrix},\quad q\mapsto\begin{pmatrix}\pm1&\\&\pm Q\end{pmatrix},$$

where

$$H\equiv\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad Q\equiv\begin{pmatrix}0&-1\\1&0\end{pmatrix}.$$

After taking account of the conjugate equivalence, only four possibilities survive from the totally 64, i.e.,

$$\text{I:}x\to\begin{pmatrix}1&\\&H\end{pmatrix},\quad y\to\begin{pmatrix}1&\\&-H\end{pmatrix},\quad q\to\begin{pmatrix}-1&\\&Q\end{pmatrix},\tag{50}$$

$$\text{II:}x\to\begin{pmatrix}-1&\\&H\end{pmatrix},\quad y\to\begin{pmatrix}-1&\\&-H\end{pmatrix},\quad q\to\begin{pmatrix}1&\\&Q\end{pmatrix},\tag{51}$$

$$\text{III:}x\to\begin{pmatrix}1&\\&-H\end{pmatrix},\quad y\to\begin{pmatrix}1&\\&H\end{pmatrix},\quad q\to\begin{pmatrix}-1&\\&Q\end{pmatrix},\tag{52}$$

$$\text{IV:}x\to\begin{pmatrix}-1&\\&-H\end{pmatrix},\quad y\to\begin{pmatrix}-1&\\&H\end{pmatrix},\quad q\to\begin{pmatrix}1&\\&Q\end{pmatrix},\tag{53}$$

which also satisfy Eq. (44). Then we regard α,β,t as unknowns, Eqs. (45)–(49) as constraints, and solve these matrix equations. Modulo similarity, each of Eqs. (50)–(53) gives two solutions, labeled as I, I′, II, II′, III, III′, IV, IV′; however, there is no difficulty to find out that I≅III, I′≅III′, II≅IV, II′≅IV′. Thus I, I′, II, II′ are what we need:

$$3_\alpha \equiv \mathrm{I}{:}\alpha \to \mathrm{diag}(-1,1,-1),\quad \beta \to \mathrm{diag}(1,-1,-1),\quad t \to \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

$$3_\beta \equiv \mathrm{I}'{:}\alpha \to \mathrm{diag}(1,-1,-1),\quad \beta \to \mathrm{diag}(-1,-1,1),\quad t \to \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

$$3_\gamma \equiv \mathrm{II}{:}\alpha \to \mathrm{diag}(-1,1,-1),\quad \beta \to \mathrm{diag}(1,-1,-1),\quad t \to \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix},$$

$$3_\delta \equiv \mathrm{II}'{:}\alpha \to \mathrm{diag}(1,-1,-1),\quad \beta \to \mathrm{diag}(-1,-1,1),\quad t \to \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}.$$

B. Spinor representations

It is more straightforward to reduce out the spinor representations. We recall that the spinor representation matrices of O_4 are of the form of tensor product

$$S_i(g) = S(g) \otimes s_i(g),\quad \forall g \in \overline{O_4}, i = \underline{4}_1, \underline{4}_2, \underline{8}, \underline{12}_1, \underline{12}_2,$$

where S is given by the algebraic isomorphism from $\mathrm{Cl}(E^4)$ to $M_2(\mathbf{H})$ and s_i has the same texture (zero matrix element positions) of irreducible representation i of S_4. Additionally, for g in $\overline{SO_4}$, $S(g)$ takes on a 2-by-2 block diagonal form

$$S(g) = \begin{pmatrix} S_{\mathrm{up}}(g) & 0 \\ 0 & S_{\mathrm{down}}(g) \end{pmatrix}. \tag{54}$$

So it is just what we want

$$S_{\mathrm{up}}(x) = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} e^{i(3/4)\pi} & e^{i(-3/4)\pi} \\ e^{i(1/4)\pi} & e^{i(-1/4)\pi} \end{pmatrix},\quad S_{\mathrm{up}}(y) = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} e^{i(3/4)\pi} & e^{i(1/4)\pi} \\ e^{i(-3/4)\pi} & e^{i(-1/4)\pi} \end{pmatrix}, \tag{55}$$

$$S_{\mathrm{up}}(q) = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} e^{i(1/4)\pi} & e^{i(3/4)\pi} \\ e^{i(3/4)\pi} & e^{i(1/4)\pi} \end{pmatrix},\quad S_{\mathrm{up}}(t) = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}, \tag{56}$$

$$S_{\mathrm{up}}(\alpha) = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix},\quad S_{\mathrm{up}}(\beta) = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}, \tag{57}$$

$$S_{\mathrm{down}}(x) = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} e^{i(3/4)\pi} & e^{i(-3/4)\pi} \\ e^{i(1/4)\pi} & e^{i(-1/4)\pi} \end{pmatrix},\quad S_{\mathrm{down}}(y) \to \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} e^{i(-1/4)\pi} & e^{i(-3/4)\pi} \\ e^{i(1/4)\pi} & e^{i(3/4)\pi} \end{pmatrix}, \tag{58}$$

$$S_{\mathrm{down}}(q) = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} e^{i(1/4)\pi} & e^{i(3/4)\pi} \\ e^{i(3/4)\pi} & e^{i(1/4)\pi} \end{pmatrix},\quad S_{\mathrm{down}}(t) = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} i & 1 \\ -i & 1 \end{pmatrix}, \tag{59}$$

$$S_{\mathrm{down}}(\alpha) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix},\quad S_{\mathrm{down}}(\beta) = \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}. \tag{60}$$

Keeping the second factor unchanged, each spinor representation in $\overline{O_4}$ splits into two spinor representations in $\overline{SO_4}$, denoted as 2_α, 2_β, 2_γ, 2_δ, 4_α, 4_β, 6_α, 6_β, 6_γ, 6_δ.

TABLE VII. Character table of $\overline{SO_4}$.

	1	$\overline{1}$	3	5	$\overline{5}$	7	8	$\overline{8}$	11	$\overline{11}$	12	14	$\overline{14}$	14′	$\overline{14}'$	15	$\overline{15}$	18	$\overline{18}$	20	$\overline{20}$	20′	$\overline{20}'$
Num.	1	1	12	1	1	48	12	12	12	12	24	6	6	6	6	32	32	32	32	24	24	24	24
$\chi_1^{(1)}$	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
$\chi_2^{(1)}$	1	1	1	1	1	−1	−1	−1	−1	−1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1
$\chi^{(2)}$	2	2	2	2	2	0	0	0	0	0	2	2	2	2	2	−1	−1	−1	−1	0	0	0	0
$\chi_1^{(3)}$	3	3	3	3	3	1	1	1	1	1	−1	−1	−1	−1	−1	0	0	0	0	−1	−1	−1	−1
$\chi_2^{(3)}$	3	3	3	3	3	−1	−1	−1	−1	−1	−1	−1	−1	−1	−1	0	0	0	0	1	1	1	1
$\chi_1^{(4)}$	4	4	0	−4	−4	0	2	2	−2	−2	0	0	0	0	0	1	1	−1	−1	0	0	0	0
$\chi_2^{(4)}$	4	4	0	−4	−4	0	−2	−2	2	2	0	0	0	0	0	1	1	−1	−1	0	0	0	0
$\chi^{(8)}$	8	8	0	−8	−8	0	0	0	0	0	0	0	0	0	0	−1	−1	1	1	0	0	0	0
$\chi^{(6)}$	6	6	−2	6	6	0	0	0	0	0	2	−2	−2	−2	−2	0	0	0	0	0	0	0	0
$\chi_\alpha^{(3)}$	3	3	−1	3	3	1	−1	−1	−1	−1	−1	−1	−1	3	3	0	0	0	0	−1	−1	1	1
$\chi_\beta^{(3)}$	3	3	−1	3	3	1	−1	−1	−1	−1	−1	3	3	−1	−1	0	0	0	0	1	1	−1	−1
$\chi_\gamma^{(3)}$	3	3	−1	3	3	−1	1	1	1	1	−1	−1	−1	3	3	0	0	0	0	1	1	−1	−1
$\chi_\delta^{(3)}$	3	3	−1	3	3	−1	1	1	1	1	−1	3	3	−1	−1	0	0	0	0	−1	−1	1	1
$\chi_\alpha^{(2)}$	2	−2	0	2	−2	0	$-\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	0	2	−2	0	0	1	−1	1	−1	0	0	$\sqrt{2}$	$-\sqrt{2}$
$\chi_\beta^{(2)}$	2	−2	0	2	−2	0	$\sqrt{2}$	$-\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	0	2	−2	0	0	1	−1	1	−1	0	0	$-\sqrt{2}$	$\sqrt{2}$
$\chi_\gamma^{(2)}$	2	−2	0	−2	2	0	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	−2	2	1	−1	−1	1	$\sqrt{2}$	$-\sqrt{2}$	0	0
$\chi_\delta^{(2)}$	2	−2	0	−2	2	0	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	−2	2	1	−1	−1	1	$-\sqrt{2}$	$\sqrt{2}$	0	0
$\chi_\alpha^{(4)}$	4	−4	0	4	−4	0	0	0	0	0	0	4	−4	0	0	−1	1	−1	1	0	0	0	0
$\chi_\beta^{(4)}$	4	−4	0	−4	4	0	0	0	0	0	0	0	0	−4	4	−1	1	1	−1	0	0	0	0
$\chi_\alpha^{(6)}$	6	−6	0	6	−6	0	$-\sqrt{2}$	$\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	0	−2	2	0	0	0	0	0	0	0	0	$-\sqrt{2}$	$\sqrt{2}$
$\chi_\beta^{(6)}$	6	−6	0	6	−6	0	$\sqrt{2}$	$-\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	0	−2	2	0	0	0	0	0	0	0	0	$\sqrt{2}$	$-\sqrt{2}$
$\chi_\gamma^{(6)}$	6	−6	0	−6	6	0	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	0	0	0	2	−2	0	0	0	0	$-\sqrt{2}$	$\sqrt{2}$	0	0
$\chi_\delta^{(6)}$	6	−6	0	−6	6	0	$\sqrt{2}$	$-\sqrt{2}$	$\sqrt{2}$	$-\sqrt{2}$	0	0	0	2	−2	0	0	0	0	$\sqrt{2}$	$-\sqrt{2}$	0	0

In fact, $S(g)$ falls in the so-called ''chiral''-representation of $\mathrm{Cl}(E^4)$ in physical language. Due to $\mathrm{Cl}(V)=\mathrm{Cl}(V)_e\oplus\mathrm{Cl}(V)_o$, and the choice of chiral-representation, there are

$$\mathrm{Cl}(E^4)_e\cong\begin{pmatrix}\mathbf{H} & O\\ 0 & \mathbf{H}\end{pmatrix},\quad \mathrm{Cl}(E^4)_o\cong\begin{pmatrix}0 & \mathbf{H}\\ \mathbf{H} & 0\end{pmatrix}.$$

Notice that $\overline{SO_4}<\mathrm{Spin}(4)\subset\mathrm{Cl}(E^4)_e$, so our reducing process for spinor representations roots in the structure of Clifford algebra.

Conclusively, our conjecture gives all inequivalent irreducible representations of $\overline{SO_4}$ whose characters are summarized in Table VII.

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APPENDIX: FUNDAMENTAL LEMMA OF *n*-DIMENSIONAL EUCLIDEAN GEOMETRY

Lemma A1 (Weak form): Let $p_i, i=0,1,2,\ldots,n$ be $n+1$ *points in n-dimensional Euclidean space* E^n *which are noncollinear and give* $n+1$ *non-negative real numbers* $d_i, i=0,1,2,\ldots,n$, *then there exists at most one point* $p\in E^n$ *s.t.* $d(p,p_i)=d_i$.

Proof: Without losing generality, set $p_0=(0,0,\ldots,0)$ and understand $p,p_i, i=1,2,\ldots,n$ as vectors in E^n. Consider equation set

$$(p-p_i,p-p_i)=d_i^2,\quad i=1,2,\ldots,n, \tag{A1}$$

$$(p,p)=d_0^2, \tag{A2}$$

where $(,)$ is the standard inner product of E^n.

Substitute Eq. (A2) into Eq. (A1)

$$(p_i,p)=\tfrac{1}{2}(d_0^2-d_i^2+(p_i,p_i)),\quad i=1,2,\ldots,n. \tag{A3}$$

The noncollinearity implies that Eq. (A3) has a solution p. The weak form of *fundamental lemma of Euclidean geometry* follows. □

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Quaternionic differential operators

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Motivated by a quaternionic formulation of quantum mechanics, we discuss quaternionic and complex linear differential equations. We touch only a few aspects of the mathematical theory, namely the resolution of the second order differential equations with constant coefficients. We overcome the problems coming out from the loss of the fundamental theorem of the algebra for quaternions and propose a practical method to solve quaternionic and complex linear second order differential equations with constant coefficients. The resolution of the complex linear Schrödinger equation, in the presence of quaternionic potentials, represents an interesting application of the mathematical material discussed in this paper. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1360195]

I. INTRODUCTION

There is substantial literature analyzing the possibility to discuss quantum systems by adopting quaternionic wave functions.[1–14] This research field has been attacked by a number of people leading to substantial progress. In the last years, many articles,[15–31] review papers[32–34] and books[35–37] provided a detailed investigation of group theory, eigenvalue problem, scattering theory, relativistic wave equations, Lagrangian formalism and variational calculus within a quaternionic formulation of quantum mechanics and field theory. In this context, by observing that the formulation of physical problems in mathematical terms often requires the study of partial differential equations, we develop the necessary theory to solve quaternionic and complex linear differential equations. The main difficulty in carrying out the solution of quaternionic differential equations is obviously represented by the noncommutative nature of the quaternionic field. The standard methods of resolution break down and, consequently, we need to modify the classical approach. It is not our purpose to develop a complete quaternionic theory of differential equations. This exceeds the scope of this paper. The main objective is to include what seemed to be most important for an introduction to this subject. In particular, we restrict ourselves to second order differential equations and give a practical method to solve such equations when quaternionic constant coefficients appear.

Some of the results given in this paper can be obtained by translation into a complex formalism.[15,16,31] Nevertheless, many subtleties of quaternionic calculus are often lost by using the translation trick. See, for example, the difference between quaternionic and complex geometry in quantum mechanics,[32,34] generalization of variational calculus,[9,10] the choice of a one-dimensional quaternionic Lorentz group for special relativity,[21] the new definitions of transpose and determinant for quaternionic matrices.[29] A wholly quaternionic derivation of the general solution of second order differential equations requires a detailed discussion of the fundamental theorem of algebra for quaternions, a revision of the resolution methods and a quaternionic generalization of the complex results.

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The study of quaternionic linear second order differential equations with constant coefficients is based on the explicit resolution of the characteristic quadratic equation.[38–41] We shall show that the loss of fundamental theorem of the algebra for quaternions does not represent a problem in solving quaternionic linear second order differential equations with constant coefficients. From there, we introduce more advanced concepts, like diagonalization and Jordan form for quaternionic and complex linear matrix operators, which are developed in detail in the recent literature[22–31] and we apply them to solve quaternionic and complex linear second order differential equations with constant coefficients.

As an application of the mathematical material presented in this paper, we discuss the complex linear Schrödinger equation in the presence of quaternionic potentials and solve such an equation for stationary states and constant potentials. We also calculate the relation between the reflection and transmition coefficients for the step and square potential and give the quaternionic solution for bound states.

This work was intended as an attempt at motivating the study of quaternionic and complex linear differential equations in view of their future applications within a quaternionic formulation of quantum mechanics. In particular, our future objective is to understand the role that such equations could play in developing nonrelativistic quaternionic quantum dynamics[4] and the meaning that quaternionic potentials[15,16] could play in discussing CP violation in the kaon system.[36]

In order to give a clear exposition and to facilitate access to the individual topics, the sections are rendered as self-contained as possible. In Sec. II, we review some of the standard concepts used in quaternionic quantum mechanics, i.e., state vector, probability interpretation, scalar product and left/right quaternionic operators.[29,35,42–45] Section III contains a brief discussion of the momentum operator. In Sec. IV, we summarize without proofs the relevant material on quaternionic eigenvalue equations from Ref. 31. Section V is devoted to the study of the one-dimensional Schrödinger equation in quaternionic quantum mechanics. Sections VI and VII provide a detailed exposition of quaternionic and complex linear differential equations. In Sec. VIII, we apply the results of previous sections to the one-dimensional Schrödinger equation with quaternionic constant potentials. Our conclusions are drawn in the final section.

II. STATES AND OPERATORS IN QUATERNIONIC QUANTUM MECHANICS

In this section, we give a brief survey of the basic mathematical tools used in quaternionic quantum mechanics.[32–37] The quantum state of a particle is defined, at a given instant, by a quaternionic wave function interpreted as a probability amplitude given by

$$\Psi(\mathbf{r})=[f_0+\mathbf{h}\cdot\mathbf{f}](\mathbf{r}), \tag{1}$$

where $\mathbf{h}=(i,j,k)$, $\mathbf{f}=(f_1,f_2,f_3)$ and $f_m:\mathbb{R}^3\to\mathbb{R}$, $m=0,1,2,3$. The probabilistic interpretation of this wave function requires that it belong to the Hilbert vector space of square-integrable functions. We shall denote by $\mathcal{F}$ the set of wave functions composed of sufficiently regular functions of this vector space. The same function $\Psi(\mathbf{r})$ can be represented by several distinct sets of components, each one corresponding to the choice of a particular basis. With each pair of elements of $\mathcal{F}$, $\Psi(\mathbf{r})$, and $\Phi(\mathbf{r})$, we associate the quaternionic scalar product,

$$(\Psi,\Phi)=\int d^3r\overline{\Psi}(\mathbf{r})\Phi(\mathbf{r}), \tag{2}$$

where

$$\overline{\Psi}(\mathbf{r})=[f_0-\mathbf{h}\cdot\mathbf{f}](\mathbf{r}) \tag{3}$$

represents the quaternionic conjugate of $\boldsymbol{\Psi}(\mathbf{r})$.

A quaternionic linear operator, $\mathcal{O}_{\mathbb{H}}$, associates with every wave function $\Psi(\mathbf{r})\in\mathcal{F}$ another wave function $\mathcal{O}_{\mathbb{H}}\Psi(\mathbf{r})\in\mathcal{F}$, the correspondence being linear from the right on $\mathbb{H}$,

$$\mathcal{O}_{\mathbb{H}}[\Psi_1(\mathbf{r})q_1+\Psi_2(\mathbf{r})q_2]=[\mathcal{O}_{\mathbb{H}}\Psi_1(\mathbf{r})]q_1+[\mathcal{O}_{\mathbb{H}}\Psi_2(\mathbf{r})]q_2,$$

$q_{1,2}\in\mathbb{H}$. Due to the noncommutative nature of the quaternionic field we need to introduce complex and real linear quaternionic operators, respectively, denoted by $\mathcal{O}_{\mathbb{C}}$ and $\mathcal{O}_{\mathbb{R}}$, the correspondence being linear from the right on $\mathbb{C}$ and $\mathbb{R}$

$$\mathcal{O}_{\mathbb{C}}[\Psi_1(\mathbf{r})z_1+\Psi_2(\mathbf{r})z_2]=[\mathcal{O}_{\mathbb{C}}\Psi_1(\mathbf{r})]z_1+[\mathcal{O}_{\mathbb{C}}\Psi_2(\mathbf{r})]z_2,$$

$$\mathcal{O}_{\mathbb{R}}[\Psi_1(\mathbf{r})\lambda_1+\Psi_2(\mathbf{r})\lambda_2]=[\mathcal{O}_{\mathbb{H}}\Psi_1(\mathbf{r})]\lambda_1+[\mathcal{O}_{\mathbb{H}}\Psi_2(\mathbf{r})]\lambda_2,$$

$z_{1,2}\in\mathbb{C}$ and $\lambda_{1,2}\in\mathbb{R}$.

As a concrete illustration of these operators let us consider the case of a finite, say n-dimensional, quaternionic Hilbert space. The wave function $\Psi(\mathbf{r})$ will then be a column vector,

$$\Psi=\begin{pmatrix}\Psi_1\\ \Psi_2\\ \vdots\\ \Psi_n\end{pmatrix},\quad \Psi_{1,2,\ldots,n}\in\mathcal{F}.$$

Quaternionic, complex and real linear operators will be represented by $n\times n$ quaternionic matrices $M_n[\mathcal{A}\otimes\mathcal{O}]$, where $\mathcal{O}$ represents the space of real operators acting on the components of Ψ and $\boldsymbol{\mathcal{A}}=(\mathcal{A}_{\mathbb{H}},\mathcal{A}_{\mathbb{C}},\mathcal{A}_{\mathbb{R}})$ denote the real algebras,

$$\mathcal{A}_{\mathcal{H}}\ :\ \{\mathbf{1},\ \mathbf{L},\ \mathbf{R},\ \mathbf{L}*\mathbf{R}\}_{16},$$

$$\mathcal{A}_{\mathbb{C}}\ :\ \{\mathbf{1},\ \mathbf{L},\ R_i,\ \mathbf{L}R_i\}_8,$$

$$\mathcal{A}_{\mathbb{R}}\ :\ \{\mathbf{1},\ \mathbf{L}\}_4,$$

generated by the left and right operators,

$$\mathbf{L}:=(L_i,L_j,L_k),\quad \mathbf{R}:=(R_i,R_j,R_k),\tag{4}$$

and by the mixed operators,

$$\mathbf{L}*\mathbf{R}:=\{L_pR_q\},\quad p,q=i,j,k.\tag{5}$$

The action of these operators on the quaternionic wave function Ψ is given by

$$\mathbf{L}\Psi\equiv\mathbf{h}\Psi,\quad \mathbf{R}\Psi\equiv\Psi\mathbf{h}.$$

The operators $\mathbf{L}$ and $\mathbf{R}$ satisfy the left/right quaternionic algebra,

$$L_i^2=L_j^2=L_k^2=L_iL_jL_k=R_i^2=R_j^2=R_k^2=R_kR_jR_i=-\mathbf{1},$$

and the following commutation relations:

$$[L_p,R_q]=0.$$

III. SPACE TRANSLATIONS AND QUATERNIONIC MOMENTUM OPERATOR

Space translation operators in quaternionic quantum mechanics are defined in the coordinate representation by the real linear anti-Hermitian operator,[36]

$$\boldsymbol{\partial}\equiv(\partial_x,\partial_y,\partial_z).\tag{6}$$

To construct an observable momentum operator we must look for a Hermitian operator that has all the properties of the momentum expected by analogy with the momentum operator in complex quantum mechanics. The choice of the quaternionic linear operator,

$$\boldsymbol{\mathcal{P}}_L = -L_i \hbar \boldsymbol{\partial}, \tag{7}$$

as a Hermitian momentum operator, would appear completely satisfactory, until we consider the translation invariance for quaternionic Hamiltonians, $\mathcal{H}_q$. In fact, due to the presence of the left acting imaginary unit i, the momentum operator (7) does not commute with the j/k-part of $\mathcal{H}_q$. Thus, although this definition of the momentum operator gives a Hermitian operator, we must return to the anti-Hermitian operator $\boldsymbol{\partial}$ to get a translation generator, $[\boldsymbol{\partial}, \mathcal{H}_q] = 0$. A second possibility to be considered is represented by the complex linear momentum operator, introduced by Rotelli in Ref. 44,

$$\boldsymbol{\mathcal{P}}_R = -R_i \hbar \boldsymbol{\partial}. \tag{8}$$

The commutator of $\boldsymbol{\mathcal{P}}_R$ with a quaternionic linear operator $\mathcal{O}_{\mathbb{H}}$ gives

$$[\boldsymbol{\mathcal{P}}_R, \mathcal{O}]\Psi = \hbar[\mathcal{O}, \boldsymbol{\partial}]\Psi i.$$

Taking $\mathcal{O}_{\mathbb{H}}$ to be a translation invariant quaternionic Hamiltonian $\mathcal{H}_q$, we have

$$[\boldsymbol{\mathcal{P}}_R, \mathcal{H}_q] = 0.$$

However, this second definition of the momentum operator has the following problem: the complex linear momentum operator $\boldsymbol{\mathcal{P}}_R$ does not represent a quaternionic Hermitian operator. In fact, by computing the difference

$$(\Psi, \boldsymbol{\mathcal{P}}_R \Phi) - \overline{(\Phi, \boldsymbol{\mathcal{P}}_R \Psi)},$$

which should vanish for a Hermitian operator $\boldsymbol{\mathcal{P}}_R$, we find

$$(\Psi, \boldsymbol{\mathcal{P}}_R \Phi) - (\boldsymbol{\mathcal{P}}_R \Psi, \Phi) = \hbar[i, (\Psi, \boldsymbol{\partial}\Phi)], \tag{9}$$

which is in general nonvanishing. There is one important case in which the right-hand side of Eq. (9) does vanish. The operator $\boldsymbol{\mathcal{P}}_R$ gives a satisfactory definition of the Hermitian momentum operator when restricted to a *complex geometry*,[45] that is a *complex projection* of the quaternionic scalar product, $(\Psi, \boldsymbol{\mathcal{P}}_R \Phi)_{\mathbb{C}}$. Note that the assumption of a complex projection of the quaternionic scalar product does not imply complex wave functions. The state of quaternionic quantum mechanics with complex geometry will be again described by vectors of a quaternionic Hilbert space. In quaternionic quantum mechanics with complex geometry observables can be represented by the quaternionic Hermitian operator, H, obtained taking the *spectral decomposition*[31] of the corresponding anti-Hermitian operator, A, or simply by the complex linear operator, $-AR_i$, obtained by multiplying A by the operator representing the right action of the imaginary unit i. These two possibilities represent equivalent choices in describing quaternionic observables within a quaternionic formulation of quantum mechanics based on complex geometry. In this scenario, the complex linear operator $\boldsymbol{\mathcal{P}}_R$ has all the expected properties of the momentum operator. It satisfies the standard commutation relations with the coordinates. It is a translation generator. Finally, it represents a *quaternionic observable*. A review of quaternionic and complexified quaternionic quantum mechanics by adopting a complex geometry is found in Ref. 34.

IV. OBSERVABLES IN QUATERNIONIC QUANTUM MECHANICS

In a recent paper,[31] we find a detailed discussion of eigenvalue equations within a quaternionic formulation of quantum mechanics with quaternionic and complex geometry. Quaternionic eigen-

value equations for quaternionic and complex linear operators require eigenvalues from the right. In particular, without loss of generality, we can reduce the eigenvalue problem for quaternionic and complex linear anti-Hermitian operators $A \in M_n[\mathcal{A}_{\mathrm{H}} \otimes \mathcal{C}]$ to

$$A\Psi_m = \Psi_m \lambda_m i, \quad m = 1,2,\ldots,n, \tag{10}$$

where λ_m are real eigenvalues.

There is an important difference between the structure of Hermitian operators in complex and quaternionic quantum mechanics. In complex quantum mechanics we can always trivially relate an anti-Hermitian operator, A, to a Hermitian operator, H, by removing a factor i, i.e., $A = iH$. In general, due to the noncommutative nature of the quaternionic field, this does not apply to quaternionic quantum mechanics.

Let $\{\Psi_m\}$ be a set of normalized eigenvectors of A with complex imaginary eigenvalues $\{i\lambda_m\}$. The anti-Hermitian operator A is then represented by

$$A = \sum_{r=1}^{n} \Psi_r \lambda_r i \Psi_r^{\dagger}, \tag{11}$$

where $\Psi^{\dagger} := \overline{\Psi^t}$. It is easy to verify that

$$A\Psi_m = \sum_{r=1}^{n} \Psi_r \lambda_r i \Psi_r^{\dagger} \Psi_m = \sum_{r=1}^{n} \Psi_r \lambda_r i \delta_{rm} = \Psi_m \lambda_m i.$$

In quaternionic quantum mechanics with quaternionic geometry,[36] the observable corresponding to the anti-Hermitian operator A is represented by the following Hermitian quaternionic linear operator:

$$H = \sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^{\dagger}. \tag{12}$$

The action of these operators on the eigenvectors Ψ_m gives

$$H\Psi_m = \Psi_m \lambda_m.$$

The eigenvalues of the operator H are real and eigenvectors corresponding to different eigenvalues are orthogonal.

How to relate the Hermitian operator H to the anti-Hermitian operator A? A simple calculation shows that the operators $L_i H$ and HL_i does not satisfy the same eigenvalue equation of A. In fact,

$$L_i H \Psi_m = \left[L_i \left(\sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^{\dagger} \right) \right] \Psi_m = i \sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^{\dagger} \Psi_m = i \Psi_m \lambda_m$$

and

$$HL_i \Psi_m = \left[\left(\sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^{\dagger} \right) L_i \right] \Psi_m = \sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^{\dagger} i \Psi_m.$$

These problems can be avoided by using the right operator R_i instead of the left operator L_i. In fact, the operator HR_i satisfies the same eigenvalue equation of A,

$$HR_i \Psi_m = \left[\left(\sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^{\dagger} \right) R_i \right] \Psi_m = \sum_{r=1}^{n} \Psi_r \lambda_r \Psi_r^{\dagger} \Psi_m i = \Psi_m \lambda_m i.$$

The eigenvalues of the operator $-AR_i$ are real and eigenvectors corresponding to different eigenvalues are orthogonal. The right hermiticity of this operator is recovered within a quaternionic formulation of quantum mechanics based on complex geometry.[34]

When the space state is finite-dimensional, it is always possible to form a basis with the eigenvectors of the operators H and $-AR_i$. When the space state is infinite-dimensional, this is no longer necessarily the case. So, it is useful to introduce a new concept, that of an observable. By definition, the Hermitian operators H or $-AR_i$ are observables if the orthonormal system of vectors forms a basis in the state space.

In quaternionic quantum mechanics with quaternionic geometry, the Hermitian operator corresponding to the anti-Hermitian operator A of Eq. (11) is thus given by the operator H of Eq. (12). By adopting a complex geometry, observables can also be represented by complex linear Hermitian operators obtained by multiplying the corresponding anti-Hermitian operator A by $-R_i$. We remark that for complex eigenvectors, the operators L_iH, HL_i, HR_i and A reduce to the same complex operator,

$$iH = i\sum_{r=1}^{n} \lambda_r \Psi_r \Psi_r^{\dagger}.$$

We conclude this section by giving an explicit example of quaternionic Hermitian operators in a finite two-dimensional space state. Let

$$A = \begin{pmatrix} -i & 3j \\ 3j & i \end{pmatrix} \tag{13}$$

be an anti-Hermitian operator. An easy computation shows that the eigenvalues and the eigenvectors of this operator are given by

$$\{2i,4i\} \quad \text{and} \quad \left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} i \\ j \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} k \\ 1 \end{pmatrix} \right\}.$$

It is immediate to verify that iA and Ai are characterized by complex eigenvalues and so cannot represent quaternionic observables. In quaternionic quantum mechanics with quaternionic geometry, the quaternionic observable corresponding to the anti-Hermitian operator of Eq. (13) is given by the Hermitian operator,

$$H = \Psi_1 2 \Psi_1^{\dagger} + \Psi_2 4 \Psi_2^{\dagger} = \begin{pmatrix} 3 & k \\ -k & 3 \end{pmatrix}. \tag{14}$$

Within a quaternionic quantum mechanics with complex geometry, a second equivalent definition of the quaternionic observable corresponding to the anti-Hermitian operator of Eq. (13) is given by the complex linear Hermitian operator,

$$\tilde{H} = \begin{pmatrix} -i & 3j \\ 3j & i \end{pmatrix} R_i. \tag{15}$$

V. THE QUATERNIONIC SCHRÖDINGER EQUATION

For simplicity, we shall assume a one-dimensional description. In the standard formulation of quantum mechanics, the wave function of a particle whose potential energy is $V(x,t)$ must satisfy the Schrödinger equation,

$$i\hbar\, \partial_t \Phi(x,t) = \mathcal{H}\, \Phi(x,t) = \left(-\frac{\hbar^2}{2m} \partial_{xx} + V(x,t) \right) \Phi(x,t). \tag{16}$$

Let us modify the previous equation by introducing the quaternionic potential,

$$[V+\mathbf{h}\cdot\mathbf{V}](x,t).$$

The i-part of this quaternionic potential violates the norm conservation. In fact,

$$\partial_t \int_{-\infty}^{+\infty} dx\, \overline{\Phi}\,\Phi = \int_{-\infty}^{+\infty} dx \left[\frac{\hbar}{2m}\overline{\Phi}\, i\, \partial_{xx}\Phi - \frac{\hbar}{2m}(\partial_{xx}\overline{\Phi}) i\,\Phi - \frac{1}{\hbar}\overline{\Phi}\{i,\mathbf{h}\}\cdot\mathbf{V}\Phi \right]$$

$$= \frac{2}{\hbar}\int_{-\infty}^{+\infty} dx\, \overline{\Phi}\, V_1 \Phi.$$

The j/k-part of $\mathbf{h}\cdot\mathbf{V}$ is responsible for T-violation.[4] To show that, we briefly discuss the time reversal invariance in quaternionic quantum mechanics. The quaternionic Schrödinger equation in the presence of a quaternionic potential which preserves norm conservation, is given by[4,15,16,36]

$$i\,\hbar\,\partial_t \Phi(x,t) = [\mathcal{H} - j\,W]\Phi(x,t), \tag{17}$$

where $W \in \mathbb{C}$. Evidently, quaternionic conjugation,

$$-\hbar\,\partial_t \overline{\Phi}(x,t) i = \mathcal{H}\,\overline{\Phi}(x,t) + \overline{\Phi}(x,t) j\, W,$$

does not yield a time-reversed version of the original Schrödinger equation

$$-i\,\hbar\,\partial_t \Phi_{\mathrm{T}}(x,-t) = [\mathcal{H} - j\,W]\Phi_{\mathrm{T}}(x,-t). \tag{18}$$

To understand why the T-violation is proportional to the j/k-part of the quaternionic potential, let us consider a real potential W. Then, the Schrödinger equation has a T-invariance. By multiplying Eq. (17) by j from the left, we have

$$-i\,\hbar\,\partial_t\, j\,\Phi(x,t) = [\mathcal{H} - j\,W] j\,\Phi(x,t), \quad W \in \mathbb{R},$$

which has the same form of Eq. (18). Thus,

$$\Phi_{\mathrm{T}}(x,-t) = j\,\Phi(x,t).$$

A similar discussion applies for imaginary complex potential $W \in i\,\mathbb{R}$. In this case, we find

$$\Phi_{\mathrm{T}}(x,-t) = k\,\Phi(x,t).$$

However, when both V_2 and V_3 are nonzero, i.e., $W \in \mathbb{C}$, this construction does not work, and the quaternionic physics is T-violating. The system of neutral kaons is the natural candidate to study the presence of *effective* quaternionic potentials, $V+\mathbf{h}\cdot\mathbf{V}$. In studying such a system, we need of V_1 and $V_{2,3}$ in order to include the decay rates of $K_{\mathrm{S}}/K_{\mathrm{L}}$ and CP-violation effects.

A. Quaternionic stationary states

For stationary states,

$$V(x,t) = V(x) \quad \text{and} \quad W(x,t) = W(x),$$

we look for solutions of the Schrödinger equation of the form

$$\Phi(x,t) = \Psi(x)\zeta(t). \tag{19}$$

Substituting (19) in the quaternionic Schrödinger equation, we obtain

$$i\,\hbar\,\Psi(x)\dot{\zeta}(t) = [\mathcal{H} - j\,W(x)]\Psi(x)\zeta(t). \tag{20}$$

Multiplying by $-\overline{\Psi}(x)i$ from the left and by $\overline{\zeta}(t)$ from the right, we find

$$\hbar\,\dot{\zeta}(t)\overline{\zeta}(t)/|\zeta(t)|^2=\overline{\Psi}(x)[-i\,\mathcal{H}+k\,W(x)]\Psi(x)/|\Psi(x)|^2. \tag{21}$$

In this equation we have a function of t on the left-hand side and a function of x on the right-hand side. The previous equality is only possible if

$$\hbar\,\dot{\zeta}(t)\overline{\zeta}(t)/\,|\zeta(t)|^2=\overline{\Psi}(x)[-i\,\mathcal{H}+k\,W(x)]\Psi(x)/|\Psi(x)|^2=q, \tag{22}$$

where q is a quaternionic constant. The energy operator $-i\,\mathcal{H}+k\,W(x)$ represents an anti-Hermitian operator. Consequently, its eigenvalues are purely imaginary quaternions, $q=\mathbf{h}\cdot\mathbf{E}$. By applying the unitary transformation u,

$$\overline{u}\,\mathbf{h}\cdot\mathbf{E}\,u=-\,i\,E,\quad E=\sqrt{E_1^2+E_2^2+E_3^2},$$

Eq. (22) becomes

$$\hbar\,\overline{u}\,\dot{\zeta}(t)\overline{\zeta}(t)u/|\zeta(t)|^2=\overline{u}\,\overline{\Psi}(x)[-i\,H+k\,W(x)]\Psi(x)u/|\Psi(x)|^2=-i\,E. \tag{23}$$

The solution $\Phi(x,t)$ of the Schrödinger equation is not modified by this similarity transformation. In fact,

$$\Phi(x,t)\rightarrow\Psi(x)u\,\overline{u}\,\zeta(t)=\Psi(x)\zeta(t).$$

By observing that $|\Phi(x,t)|^2=|\Psi(x)|^2|\zeta(t)|^2$, the norm conservation implies $|\zeta(t)|^2$ constant. Without loss of generality, we can choose $|\zeta(t)|^2=1$. Consequently, by equating the first and the third term in Eq. (23) and solving the corresponding equation, we find

$$\zeta(t)=\exp[-iEt/\hbar]\zeta(0), \tag{24}$$

with $\zeta(0)$ unitary quaternion. Note that the position of $\zeta(0)$ in Eq. (24) is very important. In fact, it can be shown that $\zeta(0)\exp[-iEt/\hbar]$ is not solution of Eq. (23). Finally, to complete the solution of the quaternionic Schrödinger equation, we must determine $\Psi(x)$ by solving the following second order (right complex linear) differential equation,

$$\left[i\,\frac{\hbar^2}{2m}\,\partial_{xx}-i\,V(x)+k\,W(x)\right]\Psi(x)=-\Psi(x)i\,E. \tag{25}$$

B. Real potential

For $W(x)=0$, Eq. (25) becomes

$$\left[\frac{\hbar^2}{2m}\,\partial_{xx}-V(x)\right]\{[\Psi(x)]_{\mathrm{C}}-j[j\Psi(x)]_{\mathrm{C}}\}=i\,\{[\Psi(x)]_{\mathrm{C}}-j[j\Psi(x)]_{\mathrm{C}}\}i\,E. \tag{26}$$

Consequently,

$$\left[\frac{\hbar^2}{2m}\,\partial_{xx}-V(x)\right][\Psi(x)]_{\mathrm{C}}=-[\Psi(x)]_{\mathrm{C}}E,$$

and

$$\left[\frac{\hbar^2}{2m}\,\partial_{xx}-V(x)\right][j\Psi(x)]_{\mathrm{C}}=[j\Psi(x)]_{\mathrm{C}}E.$$

By solving these complex equations, we find

$$\Psi(x)=\exp\left[\sqrt{\frac{2m}{\hbar^2}(V-E)}\,x\right]k_1+\exp\left[-\sqrt{\frac{2m}{\hbar^2}(V-E)}\,x\right]k_2+j$$
$$\times\left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}(V+E)}\,x\right]k_3+\exp\left[-\sqrt{\frac{2m}{\hbar^2}(V+E)}\,x\right]k_4\right\},$$

where k_n, $n=1,\ldots,4$, are complex coefficients determined by the initial conditions.

C. Free particles

For free particles, $V(x)=W(x)=0$, the previous solution reduces to

$$\Psi(x)=\exp\left[i\frac{p}{\hbar}x\right]k_1+\exp\left[-i\frac{p}{\hbar}x\right]k_2+j\left\{\exp\left[\frac{p}{\hbar}x\right]k_3+\exp\left[-\frac{p}{\hbar}x\right]k_4\right\},$$

where $p=\sqrt{2mE}$. For scattering problems with a wave function incident from the left on quaternionic potentials, we have

$$\Psi(x)=\exp\left[i\frac{p}{\hbar}x\right]+r\exp\left[-i\frac{p}{\hbar}x\right]+j\,\tilde{r}\exp\left[\frac{p}{\hbar}x\right], \tag{27}$$

where $|r|^2$ is the standard coefficient of reflection and $|\tilde{r}\exp[(p/\hbar)x]|^2$ represents an additional evanescent probability of reflection. In our study of quaternionic potentials, we shall deal with the rectangular potential barrier of width a. In this case, the particle is free for $x<0$, where the solution is given by (27), and $x>a$, where the solution is

$$\Psi(x)=t\exp\left[i\frac{p}{\hbar}x\right]+j\,\tilde{t}\exp\left[-\frac{p}{\hbar}x\right]. \tag{28}$$

Note that, in Eqs. (27) and (28), we have, respectively, omitted the complex exponential solution $\exp[-(p/\hbar)x]$ and $\exp[(p/\hbar)x]$ which are in conflict with the boundary condition that $\Psi(x)$ remain finite as $x\to-\infty$ and $x\to\infty$. In Eq. (28), we have also omitted the complex exponential solution $\exp[-i(p/\hbar)x]$ because we are considering a wave incident from the left.

VI. QUATERNIONIC LINEAR DIFFERENTIAL EQUATION

Consider the second order quaternionic linear differential operator,

$$\mathcal{D}_{\mathbb{H}}=\partial_{xx}+(a_0+\mathbf{L}\cdot\mathbf{a})\partial_x+b_0+\mathbf{L}\cdot\mathbf{b}\in\mathcal{A}_{\mathbb{H}}\otimes\mathcal{O}.$$

We are interested in finding the solution of the quaternionic linear differential equation,

$$\mathcal{D}_{\mathbb{H}}\,\varphi(x)=0. \tag{29}$$

In analogy to the complex case, we look for solutions of exponential form

$$\varphi(x)=\exp[qx],$$

where $q\in\mathbb{H}$ and $x\in\mathbb{R}$. To satisfy Eq. (29), the constant q has to be a solution of the quaternionic quadratic equation,[38–41]

$$q^2+(a_0+\mathbf{h}\cdot\mathbf{a})q+b_0+\mathbf{h}\cdot\mathbf{b}=0. \tag{30}$$

A. Quaternionic quadratic equation

To simplify our discussion, it is convenient to modify Eq. (30) by removing the real constant a_0. To do this, we introduce a new quaternionic constant p defined by $p=q+a_0/2$. The quadratic equation (30) then becomes

$$p^2+\mathbf{h}\cdot\mathbf{a}\,p+c_0+\mathbf{h}\cdot\mathbf{c}=0, \tag{31}$$

where $c_0=b_0-a_0^2/4$ and $\mathbf{c}=\mathbf{b}-(a_0/2)\mathbf{a}$. We shall give the solution of Eq. (31) in terms of real constant c_0 and of the real vectors $\mathbf{a}$ and $\mathbf{c}$. Let us analyze the following cases:

- $\mathbf{a}\neq 0$, $\mathbf{c}\neq 0$:
  - **(i)** $\mathbf{a}\times\mathbf{c}=0$,
  - **(ii)** $\mathbf{a}\cdot\mathbf{c}=0$,
  - **(iii)** $\mathbf{a}\times\mathbf{c}\neq 0\neq\mathbf{a}\cdot\mathbf{c}$;
- $\mathbf{a}=0$, $\mathbf{c}\neq 0$;
- $\mathbf{a}\neq 0$, $\mathbf{c}=0$;
- $\mathbf{a}=\mathbf{c}=0$.

• **(i)** $\mathbf{a}\times\mathbf{c}=0$. In this case $\mathbf{a}$ and $\mathbf{c}$ are parallel vectors, so Eq. (31) can be easily reduced to a complex equation. In fact, by introducing the imaginary unit $\mathcal{I}=\mathbf{h}\cdot\mathbf{a}/|\mathbf{a}|$ and observing that $\mathbf{h}\cdot\mathbf{c}=\mathcal{I}\alpha$, with $\alpha\in\mathbb{R}$, we find

$$p^2+\mathcal{I}|\mathbf{a}|p+c_0+\mathcal{I}\alpha=0,$$

whose *complex* solutions are immediately found.

• **(ii)** $\mathbf{a}\cdot\mathbf{c}=0$. By observing that $\mathbf{a}$, $\mathbf{c}$ and $\mathbf{a}\times\mathbf{c}$ are orthogonal vectors, we can rearrange the imaginary part of p, $\mathbf{h}\cdot\mathbf{p}$, in terms of the new basis $(\mathbf{a},\mathbf{c},\mathbf{a}\times\mathbf{c})$, i.e.,

$$p=p_0+\mathbf{h}\cdot(x\,\mathbf{a}+y\,\mathbf{c}+z\,\mathbf{a}\times\mathbf{c}). \tag{32}$$

Substituting (32) in Eq. (31), we obtain the following system of equations for the real variables p_0, x, y and z:

$$\begin{aligned}
&\mathbb{R}: && p_0^2-(x^2+x)|\mathbf{a}|^2-y^2|\mathbf{c}|^2-z^2|\mathbf{a}|^2|\mathbf{c}|^2+c_0=0,\\
&\mathbf{h}\cdot\mathbf{a}: && p_0(1+2x)=0,\\
&\mathbf{h}\cdot\mathbf{c}: && 1+2p_0y-z|\mathbf{a}|^2=0,\\
&\mathbf{h}\cdot\mathbf{a}\times\mathbf{c}: && y+2p_0z=0.
\end{aligned}$$

The second equation, $p_0(1+2x)=0$, implies $p_0=0$ and/or $x=-\frac{1}{2}$. For $p_0=0$, it can be shown that the solution of Eq. (31), in terms of p_0, x, y and z, is given by

$$p_0=0,\quad x=-\frac{1}{2}\pm\sqrt{\Delta},\quad y=0,\quad z=\frac{1}{|\mathbf{a}|^2}, \tag{33}$$

where

$$\Delta=\frac{1}{4}+\frac{1}{|\mathbf{a}|^2}\left(c_0-\frac{|\mathbf{c}|^2}{|\mathbf{a}|^2}\right)\geqslant 0.$$

For $x=-\frac{1}{2}$, we find

$$y=-\frac{2p_0}{4p_0^2+|\mathbf{a}|^2},\quad z=\frac{1}{4p_0^2+|\mathbf{a}|^2}, \tag{34}$$

and

$$p_0^2=\tfrac{1}{4}[\pm 2\sqrt{c_0^2+|\mathbf{c}|^2}-2c_0-|\mathbf{a}|^2].$$

It is easily verified that

$$\Delta\leqslant 0\Rightarrow\sqrt{c_0^2+|\mathbf{c}|^2}-c_0\geqslant\frac{|\mathbf{a}|^2}{2};$$

thus

$$p_0=\pm\tfrac{1}{2}\sqrt{2(\sqrt{c_0^2+|\mathbf{c}|^2}-c_0)-|\mathbf{a}|^2}. \tag{35}$$

Summarizing, for $\Delta\neq 0$, we have two quaternionic solutions, $p_1\neq p_2$,

$$\Delta>0\ :\quad p_0=0,$$

$$x=-\tfrac{1}{2}\pm\sqrt{\Delta},$$

$$y=0,$$

$$z=\frac{1}{|\mathbf{a}|^2}; \tag{36}$$

$$\Delta<0\ :\quad p_0=\pm\tfrac{1}{2}\sqrt{2(\sqrt{c_0^2+|\mathbf{c}|^2}-c_0)-|\mathbf{a}|^2},$$

$$x=-\tfrac{1}{2},$$

$$y=-\frac{2p_0}{4p_0^2+|\mathbf{a}|^2},$$

$$z=\frac{1}{4p_0^2+|\mathbf{a}|^2}. \tag{37}$$

For $\Delta=0$, these solutions tend to the same solution $p_1=p_2$ given by

$$\Delta=0\ :\quad p_0=0,\quad x=-\frac{1}{2},\quad y=0,\quad z=\frac{1}{|\mathbf{a}|^2}. \tag{38}$$

• **(iii)** $\mathbf{a}\times\mathbf{c}\neq 0\neq\mathbf{a}\cdot\mathbf{c}$. In discussing this case, we introduce the vector $\mathbf{d}=\mathbf{c}-d_0\,\mathbf{a}$, $d_0=\mathbf{a}\cdot\mathbf{c}/|\mathbf{a}|^2$ and the imaginary part of p in terms of the orthogonal vectors $\mathbf{a}$, $\mathbf{d}$ and $\mathbf{a}\times\mathbf{d}$,

$$p=p_0+\mathbf{h}\cdot(x\,\mathbf{a}+y\,\mathbf{d}+z\,\mathbf{a}\times\mathbf{d}). \tag{39}$$

By using this decomposition, from Eq. (31) we obtain the following system of real equations:

$$\begin{array}{ll}\mathbb{R}: & p_0^2-(x^2+x)|\mathbf{a}|^2-y^2|\mathbf{d}|^2-z^2|\mathbf{a}|^2|\mathbf{d}|^2+c_0=0,\\ \mathbf{h}\cdot\mathbf{a}: & p_0(1+2x)+d_0=0,\\ \mathbf{h}\cdot\mathbf{d}; & 1+2p_0y-z|\mathbf{a}|^2=0,\\ \mathbf{h}\cdot\mathbf{a}\times\mathbf{d}: & y+2p_0z=0.\end{array}$$

The second equation of this system, $p_0(1+2x)+d_0=0$, implies $p_0\neq 0$ since $d_0\neq 0$. Therefore, we have

$$x=-\frac{p_0+d_0}{2p_0},\quad y=-\frac{2p_0}{4p_0^2+|\mathbf{a}|^2},\quad z=\frac{1}{4p_0^2+|\mathbf{a}|^2},\tag{40}$$

and

$$16\,w^3+8[|\mathbf{a}|^2+2c_0]w^2+4\left[|\mathbf{a}|^2(c_0-d_0^2)+\frac{|\mathbf{a}|^4}{4}-|\mathbf{d}|^2\right]w-d_0^2|\mathbf{a}|^4=0,\tag{41}$$

where $w=p_0^2$. By using the Descartes rule of signs it can be proved that Eq. (41) has only one real positive solution,[38] $w=\alpha^2$, $\alpha\in\mathbb{R}$. This implies $p_0=\pm\,\alpha$. Thus, we also find two quaternionic solutions.

• $\mathbf{a}=0$ and $\mathbf{c}\neq 0$. By introducing the imaginary *complex* unit $\mathcal{I}=\mathbf{h}\cdot\mathbf{c}/|\mathbf{c}|$, we can reduce Eq. (31) to the following *complex* equation:

$$p^2+c_0+\mathcal{I}|\mathbf{c}|=0.$$

• $\mathbf{a}\neq 0$ and $\mathbf{c}=0$. This case is similar to the previous one. We introduce the imaginary *complex* unit $\mathcal{I}=\mathbf{h}\cdot\mathbf{a}/|\mathbf{a}|$ and reduce Eq. (31) to the *complex* equation,

$$p^2+\mathcal{I}\,|\mathbf{a}|p+c_0=0.$$

• $\mathbf{a}=\mathbf{c}=0$. Equation (31) becomes

$$p^2+c_0=0.$$

For $c_0=-\alpha^2$, $\alpha\in\mathbb{R}$, we find two real solutions. For $c_0=\alpha^2$, we obtain an *infinite* number of quaternionic solutions, i.e., $p=\mathbf{h}\cdot\mathbf{p}$, where $|\mathbf{p}|=|\alpha|$.

Let us resume our discussion on a quaternionic linear quadratic equation. For $\mathbf{a}=0$ and/or $\mathbf{c}=0$ and for $\mathbf{a}\times\mathbf{c}=0$ we can reduce quaternionic linear quadratic equations to *complex* equations. For non null vectors satisfying $\mathbf{a}\cdot\mathbf{c}=0$ or $\mathbf{a}\times\mathbf{c}\neq 0\neq\mathbf{a}\cdot\mathbf{c}$, we have *effective* quaternionic equations. In these cases, we always find two quaternionic solutions (36), (37) and (40)–(41). For $\mathbf{a}\cdot\mathbf{c}=0$ and $\Delta=0$, these solutions tend to the same solution (38). Finally, the fundamental theorem of algebra is lost for a *restricted* class of quaternionic quadratic linear equations, namely

$$q^2+\alpha^2=0,\quad \alpha\in\mathbb{R}.$$

B. Second order quaternionic differential equations with constant coefficients

Due to the quaternionic linearity from the right of Eq. (29), we look for general solutions which are of the form

$$\varphi(x)=\varphi_1(x)c_1+\varphi_2(x)c_2,$$

where $\varphi_1(x)$ and $\varphi_2(x)$ represent two linear independent solutions of Eq. (29) and c_1 and c_2 are quaternionic constants fixed by the initial conditions. In analogy to the complex case, we can distinguish between quaternionic linear dependent and independent solutions by constructing a Wronskian functional. To do this, we need to define a quaternionic determinant. Due to the noncommutative nature of quaternions, the standard definition of the determinant must be revised. The study of quaternionic, complex and real functionals, extending the complex determinant to quaternionic matrices, has been extensively developed in quaternionic linear algebra.[46–49] In a recent paper,[50] we find an interesting discussion on the impossibility to obtain a quaternionic functional with the main properties of the complex determinant. For quaternionic matrices, M, a *real positive* functional, $|\det M|=\sqrt{\det[MM^{\dagger}]}$, which reduces to the absolute value of the standard

determinant for complex matrices, was introduced by Study[51] and its properties axiomatized by Dieudonné.[52] The details can be found in the excellent survey paper of Aslaksen.[53] This functional allows us to construct a real positive Wronskian,[31]

$$\begin{aligned}\mathcal{W}(x) &= \left| \det\begin{pmatrix} \varphi_1(x) & \varphi_2(x) \\ \dot{\varphi}_1(x) & \dot{\varphi}_2(x) \end{pmatrix} \right| \\ &= |\varphi_1(x)\| \dot{\varphi}_2(x) - \dot{\varphi}_1(x)\varphi_1^{-1}(x)\varphi_2(x)| \\ &= |\varphi_2(x)\| \dot{\varphi}_1(x) - \dot{\varphi}_2(x)\varphi_2^{-1}(x)\varphi_1(x)| \\ &= |\dot{\varphi}_1(x)\| \varphi_2(x) - \varphi_1(x)\dot{\varphi}_1^{-1}(x)\dot{\varphi}_2(x)| \\ &= |\dot{\varphi}_2(x)\| \varphi_1(x) - \varphi_2(x)\dot{\varphi}_2^{-1}(x)\dot{\varphi}_1(x)|.\end{aligned}$$

Solutions of Eq. (29),

$$\varphi_{1,2}(x) = \exp[q_{1,2}\, x] = \exp\left[\left(p_{1,2} - \frac{a_0}{2}\right)x\right],$$

are given in terms of the solutions of the quadratic equation (31), $p_{1,2}$, and of the real variable x. In this case, the Wronskian becomes

$$\mathcal{W}(x) = |p_1 - p_2\| \exp[q_1 x]\| \exp[q_2 x]|.$$

This functional allows us to distinguish between quaternionic linear dependent ($\mathcal{W}=0$) and independent ($\mathcal{W}\neq 0$) solutions. A generalization for quaternionic second order differential equations with nonconstant coefficients should be investigated.

For $p_1 \neq p_2$, the solution of Eq. (29) is then given by

$$\varphi(x) = \exp\left[-\frac{a_0}{2}x\right]\{\exp[p_1\, x]c_1 + \exp[p_2\, x]c_2\}. \tag{42}$$

As observed at the end of the previous subsection, the fundamental theorem of algebra is lost for a *restricted* class of quaternionic quadratic equation, i.e., $p^2 + \alpha^2 = 0$ where $\alpha \in \mathbb{R}$. For these equations we find an infinite number of solutions, $p = \mathbf{h}\cdot\boldsymbol{\alpha}$ with $|\boldsymbol{\alpha}|^2 = \alpha^2$. Nevertheless, the general solution of the second order differential equation,

$$\ddot{\varphi}(x) + \alpha^2\, \varphi(x) = 0, \tag{43}$$

is also expressed in terms of *two* linearly independent exponential solutions,

$$\varphi(x) = \exp[i\, \alpha\, x]c_1 + \exp[-i\, \alpha\, x]c_2. \tag{44}$$

Note that any other exponential solution, $\exp[\mathbf{h}\cdot\boldsymbol{\alpha}\, x]$, can be written as a linear combination of $\exp[i\,\alpha\, x]$ and $\exp[-i\,\alpha\, x]$,

$$\exp[\mathbf{h}\cdot\boldsymbol{\alpha}\, x] = \frac{1}{2\alpha}\{\exp[i\, \alpha\, x](\alpha - i\, \mathbf{h}\cdot\boldsymbol{\alpha}) + \exp[-i\, \alpha\, x](\alpha + i\, \mathbf{h}\cdot\boldsymbol{\alpha})\}.$$

As a consequence, the loss of the fundamental theorem of algebra for quaternions does *not*

represent an obstacle in solving second order quaternionic linear differential equations with constant coefficients. To complete our discussion, we have to examine the case $p_1=p_2$. From Eq. (38) we find

$$p_1=p_2=-\frac{\mathbf{h}\times\mathbf{a}}{2}+\frac{1}{|\mathbf{a}|^2}\mathbf{h}\cdot\mathbf{a}\times\left(\mathbf{b}-\frac{a_0}{2}\mathbf{a}\right),$$

Thus, a first solution of the differential equation (29) is

$$\xi(x)=\exp\left\{\left[\mathbf{h}\cdot\left(\frac{\mathbf{a}\times\mathbf{b}}{|\mathbf{a}|^2}-\frac{\mathbf{a}}{2}\right)-\frac{a_0}{2}\right]x\right\}.$$

For $\mathbf{a}\times\mathbf{b}=0$, we can immediately obtain a second linearly independent solution by multiplying $\exp[-(a/2)x]$ by x, $\eta(x)=x\,\xi(x)$. For $\mathbf{a}\times\mathbf{b}\neq 0$, the second linearly independent solution takes a more complicated form, i.e.,

$$\eta(x)=\left(x+\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}\right)\xi(x). \tag{45}$$

It can easily be shown that $\eta(x)$ is a solution of the differential equation (29),

$$\begin{aligned}
&\ddot{\eta}(x)+a\,\dot{\eta}(x)+b\,\eta(x)\\
&\quad=\left[x(q^2+a\,q+b)+2\,q+a+\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}(q^2+a\,q)+b\,\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}\right]\xi(x)\\
&\quad=\left(2\,q+a+\left[b,\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}\right]\right)\xi(x)\\
&\quad=\left(2\,\mathbf{h}\cdot\frac{\mathbf{a}\times\mathbf{b}}{|\mathbf{a}|^2}+\left[\mathbf{h}\cdot\mathbf{b},\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}\right]\right)\xi(x)=0.
\end{aligned}$$

Thus, for $p_1=p_2=p=\mathbf{h}\cdot((\mathbf{a}\times\mathbf{b})/|\mathbf{a}|^2-\mathbf{a}/2$, the general solution of the differential equation (29) is given by

$$\varphi(x)=\exp\left[-\frac{a_0}{2}x\right]\left\{\exp[p\,x]c_1+\left(x+\frac{\mathbf{h}\cdot\mathbf{a}}{|\mathbf{a}|^2}\right)\exp[p\,x]c_2\right\}. \tag{46}$$

C. Diagonalization and Jordan form

To find the general solution of linear differential equations, we can also use quaternionic formulations of eigenvalue equations, matrix diagonalization and Jordan form. The quaternionic linear differential equation (29) can be written in matrix form as follows:

$$\dot{\Phi}(x)=M\,\Phi(x), \tag{47}$$

where

$$M=\begin{pmatrix}0 & 1\\ -b & -a\end{pmatrix}\quad\text{and}\quad\Phi(x)=\begin{bmatrix}\varphi(x)\\ \dot{\varphi}(x)\end{bmatrix}.$$

By observing that x is real, the formal solution of the matrix equation (47) is given by

$$\Phi(x)=\exp[M\,x]\Phi(0), \tag{48}$$

where $\Phi(0)$ represents a constant quaternionic column vector determined by the initial conditions $\varphi(0)$, $\dot{\varphi}(0)$ and $\exp[Mx]=\Sigma_{n=0}^{\infty}[(Mx)^n/n!]$. In the sequel, we shall use right eigenvalue equations for quaternionic linear matrix operators equations,

$$M\,\Phi=\Phi\,q. \tag{49}$$

Without loss of generality, we can work with *complex* eigenvalue equations. By setting $\Psi=\Phi u$, from the previous equation, we have

$$M\,\Psi=M\,\Phi u=\Phi\,q\,u=\Phi u\,\bar{u}qu=\Psi\,z, \tag{50}$$

where $z\in\mathbb{C}$ and u is a unitary quaternion. In a recent paper,[31] we find a complete discussion of the eigenvalue equation for quaternionic matrix operators. In such a paper was shown that the complex counterpart of the matrix M has an eigenvalue spectrum characterized by eigenvalues which appear in conjugate pairs $\{z_1,\bar{z}_1,z_2,\bar{z}_2\}$. Let Ψ_1 and Ψ_2 be the quaternionic eigenvectors corresponding to the complex eigenvalues z_1 and z_2,

$$M\,\Psi_1=\Psi_1\,z_1 \quad \text{and} \quad M\,\Psi_2=\Psi_2\,z_2.$$

It can be shown that for $|z_1|\neq|z_2|$, the eigenvectors Ψ_1 and Ψ_2 are linearly independent on $\mathbb{H}$ and consequently there exists a 2×2 quaternionic matrix $S=[\Psi_1\,\Psi_2]$ which diagonalizes M,

$$\exp[M\,x]=S\exp\left[\begin{pmatrix} z_1 & 0\\ 0 & z_2\end{pmatrix}x\right]S^{-1}=S\begin{pmatrix}\exp[z_1x] & 0\\ 0 & \exp[z_2x]\end{pmatrix}S^{-1}.$$

In this case, the general solution of the quaternionic differential equation can be written in terms of the elements of the matrices S and S^{-1} and of the complex eigenvalues z_1 and z_2,

$$\begin{bmatrix}\varphi(x)\\ \dot{\varphi}(x)\end{bmatrix}=\begin{pmatrix}S_{11}\exp[z_1x] & S_{12}\exp[z_2x]\\ S_{21}\exp[z_1x] & S_{22}\exp[z_2x]\end{pmatrix}\begin{bmatrix}S_{11}^{-1}\,\varphi(0)+S_{12}^{-1}\,\dot{\varphi}(0)\\ S_{21}^{-1}\,\varphi(0)+S_{22}^{-1}\,\dot{\varphi}(0)\end{bmatrix}.$$

Hence,

$$\begin{aligned}\varphi(x)&=S_{11}\exp[z_1\,x][S_{11}^{-1}\,\varphi(0)+S_{12}^{-1}\,\dot{\varphi}(0)]\\ &\quad+S_{12}\exp[z_2\,x][S_{21}^{-1}\,\varphi(0)+S_{22}^{-1}\,\dot{\varphi}(0)]\\ &=\exp[S_{11}\,z_1(S_{11})^{-1}\,x]S_{11}[S_{11}^{-1}\,\varphi(0)+S_{12}^{-1}\,\dot{\varphi}(0)]\\ &\quad+\exp[S_{12}\,z_2(S_{12})^{-1}\,x]S_{12}[S_{21}^{-1}\,\varphi(0)+S_{22}^{-1}\,\dot{\varphi}(0)]\\ &=\exp[S_{21}(S_{11})^{-1}\,x]S_{11}[S_{11}^{-1}\,\varphi(0)+S_{12}^{-1}\,\dot{\varphi}(0)]\\ &\quad+\exp[S_{22}(S_{12})^{-1}\,x]S_{12}[S_{21}^{-1}\,\varphi(0)+S_{22}^{-1}\,\dot{\varphi}(0)].\end{aligned} \tag{51}$$

We remark that a different choice of the eigenvalue spectrum does *not* modify the solution (51). In fact, by taking the following quaternionic eigenvalue spectrum:

$$\{q_1,q_2\}=\{\bar{u}_1z_1u_1,\bar{u}_2z_2u_2\},\quad |q_1|\neq|q_2|, \tag{52}$$

and observing that the corresponding linearly independent eigenvectors are given by

$$\{\,\Phi_1=\Psi_1u_1,\Phi_2=\Psi_2u_2\}, \tag{53}$$

we obtain

$$
\begin{aligned}
M &= [\Phi_1\, \Phi_2]\mathrm{diag}\{q_1, q_2\}[\Phi_1\, \Phi_2]^{-1} \\
&= [\Psi_1 u_1\, \Psi_2 u_2]\mathrm{diag}\{\overline{u_1} z_1 u_1, \overline{u_2} z_2 u_2\}[\Psi_1 u_1\, \Psi_2 u_2]^{-1} \\
&= [\Psi_1\, \Psi_2]\mathrm{diag}\{z_1, z_2\}[\Psi_1\, \Psi_2]^{-1}.
\end{aligned}
$$

Let us now discuss the case $|z_1| = |z_2|$. If the eigenvectors $\{\Psi_a, \Psi_b\}$, corresponding to the eigenvalue spectrum $\{z, z\}$, are linearly independent on $\mathbb{H}$, we can obviously repeat the previous discussion and diagonalize the matrix operator M by the 2×2 quaternionic matrix $U = [\Psi_1\, \Psi_2]$. Then, we find

$$
\begin{aligned}
\varphi(x) &= \exp[U_{11} z (U_{11})^{-1} x] U_{11} [U_{11}^{-1} \varphi(0) + U_{12}^{-1} \dot{\varphi}(0)] \\
&\quad + \exp[U_{12} z (U_{12})^{-1} x] U_{12} [U_{21}^{-1} \varphi(0) + U_{22}^{-1} \dot{\varphi}(0)] \\
&= \exp[U_{21} (U_{11})^{-1} x] U_{11} [{}_{11}^{-1} \varphi(0) + U_{12}^{-1} \dot{\varphi}(0)] \\
&\quad + \exp[U_{22} (U_{12})^{-1} x] U_{12} [U_{21}^{-1} \varphi(0) + U_{22}^{-1} \dot{\varphi}(0)].
\end{aligned} \tag{54}
$$

For linearly dependent eigenvectors, we cannot construct a matrix which diagonalizes the matrix operator M. Nevertheless, we can transform the matrix operator M to Jordan form,

$$
M = J \begin{pmatrix} z & 1 \\ 0 & z \end{pmatrix} J^{-1}. \tag{55}
$$

It follows that the solution of our quaternionic differential equation can be written as

$$
\Phi(x) = J \exp\left[\begin{pmatrix} z & 1 \\ 0 & z \end{pmatrix} x\right] J^{-1} \Phi(0) = \begin{pmatrix} J_{11} & x J_{11} + J_{12} \\ J_{21} & x J_{21} + J_{22} \end{pmatrix} \exp[zx] \begin{bmatrix} J_{11}^{-1} \varphi(0) + J_{12}^{-1} \dot{\varphi}(0) \\ J_{21}^{-1} \varphi(0) + J_{22}^{-1} \dot{\varphi}(0) \end{bmatrix}.
$$

Thus,

$$
\begin{aligned}
\varphi(x) &= J_{11} \exp[z\, x][J_{11}^{-1} \varphi(0) + J_{12}^{-1} \dot{\varphi}(0)] \\
&\quad + (x J_{11} + J_{12}) \exp[z\, x][J_{21}^{-1} \varphi(0) + J_{22}^{-1} \dot{\varphi}(0)] \\
&= \exp[J_{11} z (J_{11})^{-1} x] J_{11} [J_{11}^{-1} \varphi(0) + J_{12}^{-1} \dot{\varphi}(0)] \\
&\quad + [x + J_{12} (J_{11})^{-1}] \exp[J_{11} z (J_{11})^{-1} x] \\
&\quad \times J_{11} [J_{21}^{-1} \varphi(0) + J_{22}^{-1} \dot{\varphi}(0)] \\
&= \exp[J_{21} (J_{11})^{-1} x] J_{11} [J_{11}^{-1} \varphi(0) + J_{12}^{-1} \dot{\varphi}(0)] \\
&\quad + [x + J_{12} (J_{11})^{-1}] \exp[J_{21} (J_{11})^{-1} x] \\
&\quad \times J_{11} [J_{21}^{-1} \varphi(0) + J_{22}^{-1} \dot{\varphi}(0)].
\end{aligned} \tag{56}
$$

The last equality in the previous equation follows from the use of Eq. (55) and the definition of M.

Finally, the general solution of the quaternionic differential equation (29) can be given by solving the corresponding eigenvalue problem. We conclude this section by observing that the quaternionic exponential solution, $\exp[q\, x]$, can also be written in terms of complex exponential solutions, $u \exp[z\, x] u^{-1}$, where $q = u\, z\, u^{-1}$. The elements of the similarity transformations S, U or J and the complex eigenvalue spectrum of M determine the quaternion u and the complex number z. This form for exponential solutions will be very useful in solving complex linear differential equations with constant coefficients. In fact, due to the presence of the right acting operator R_i, we cannot use quaternionic exponential solutions for complex linear differential equations.

VII. COMPLEX LINEAR QUATERNIONIC DIFFERENTIAL EQUATIONS

Consider now the second order complex linear quaternionic differential operator,

$$\begin{aligned}\mathcal{D}_{\mathbb{C}}=&[a_{02}+\mathbf{L}\cdot\mathbf{a}_2+(b_{02}+\mathbf{L}\cdot\mathbf{b}_2)R_i]\partial_{xx}\\&+[a_{01}+\mathbf{L}\cdot\mathbf{a}_1+(b_{01}+\mathbf{L}\cdot\mathbf{b}_1)R_i]\partial_x\\&+a_{00}+\mathbf{L}\cdot\mathbf{a}_0+(b_{00}+\mathbf{L}\cdot\mathbf{b}_0)R_i\\&\in\mathcal{A}_{\mathbb{C}}\otimes\mathcal{O},\end{aligned}$$

and look for solutions of the complex linear quaternionic differential equation,

$$\mathcal{D}_{\mathbb{C}}\,\varphi(x)=0. \tag{57}$$

Due to the presence of R_i in (57), the general solution of the complex linear quaternionic differential equation cannot be given in terms of quaternionic exponentials. In matrix form, Eq. (57) reads as

$$\dot{\Phi}(x)=M_{\mathbb{C}}\Phi(x), \tag{58}$$

where

$$M_{\mathbb{C}}=\begin{pmatrix}0 & 1\\ -b_{\mathbb{C}} & -a_{\mathbb{C}}\end{pmatrix}\quad\text{and}\quad\Phi(x)=\begin{bmatrix}\varphi(x)\\ \dot{\varphi}(x)\end{bmatrix}.$$

The complex counterpart of complex linear quaternionic matrix operator $M_{\mathbb{C}}$ has an eigenvalue spectrum characterized by four complex eigenvalues $\{z_1,z_2,z_3,z_4\}$. It can be shown that $M_{\mathbb{C}}$ is diagonalizable if and only if its complex counterpart is diagonalizable. For diagonalizable matrix operator $M_{\mathbb{C}}$, we can find a complex linear quaternionic linear similarity transformation $S_{\mathbb{C}}$ which reduces the matrix operator $M_{\mathbb{C}}$ to diagonal form,[31]

$$M_{\mathbb{C}}=S_{\mathbb{C}}\begin{pmatrix}\dfrac{z_1+\overline{z_2}}{2}+\dfrac{z_1-\overline{z_2}}{2i}R_i & 0\\ 0 & \dfrac{z_3+\overline{z_4}}{2}+\dfrac{z_3-\overline{z_4}}{2i}R_i\end{pmatrix}S_{\mathbb{C}}^{-1}.$$

It is immediate to verify that

$$\left\{\begin{pmatrix}1\\0\end{pmatrix},\ \begin{pmatrix}j\\0\end{pmatrix},\ \begin{pmatrix}0\\1\end{pmatrix},\ \begin{pmatrix}0\\j\end{pmatrix}\right\}$$

are eigenvectors of the diagonal matrix operator,

$$\begin{pmatrix}\dfrac{z_1+\overline{z_2}}{2}+\dfrac{z_1-\overline{z_2}}{2i}R_i & 0\\ 0 & \dfrac{z_3+\overline{z_4}}{2}+\dfrac{z_3-\overline{z_4}}{2i}R_i\end{pmatrix},$$

with right complex eigenvalues z_1, z_2, z_3 and z_4. The general solution of the differential equation (57) can be given in terms of these complex eigenvalues,

$$\varphi(x)=S_{\mathrm{C}\,11}\exp\left[\left(\frac{z_1+\overline{z_2}}{2}+\frac{z_1-\overline{z_2}}{2i}R_i\right)x\right][S_{\mathrm{C}\,11}^{-1}\varphi(0)+S_{\mathrm{C}\,12}^{-1}\dot{\varphi}(0)]$$
$$+S_{\mathrm{C}\,12}\exp\left[\left(\frac{z_3+\overline{z_4}}{2}+\frac{z_3-\overline{z_4}}{2i}R_i\right)x\right][S_{\mathrm{C}\,21}^{-1}\varphi(0)+S_{\mathrm{C}\,22}^{-1}\dot{\varphi}(0)]$$
$$=u_1\exp[z_1x]k_1+u_2\exp[z_2x]k_2$$
$$+u_3\exp[z_3x]k_3+u_4\exp[z_4x]k_4, \tag{59}$$

where k_n are complex coefficients determined by the initial conditions. This solution holds for diagonalizable matrix operator M_{C}. For nondiagonalizable matrix operators we need to find the similarity transformation J_{C} which reduces M_{C} to the Jordan form. For instance, it can be shown that for equal eigenvalues, $z_1=z_2$, the general solution of the differential equation (57) is

$$\varphi(x)=u\exp[zx]k_1+(ux+\tilde{u})\exp[zx]k_2+u_3\exp[z_3x]k_3+u_4\exp[z_4x]k_4. \tag{60}$$

A. Schrödinger equation

Let us now examine the complex linear Schrödinger equation in the presence of a constant quaternionic potential,

$$\left[\frac{\hbar^2}{2m}\partial_{xx}-V+jW\right]\Psi(x)=i\Psi(x)iE. \tag{61}$$

In this case, the complex linear matrix operator,

$$M_{\mathrm{C}}=\begin{pmatrix}0 & 1\\ -b_{\mathrm{C}} & 0\end{pmatrix},\quad b_{\mathrm{C}}=V-jW+iER_i,$$

represents a diagonalizable operator. Consequently, the general solution of the Schrödinger equation is given by

$$\varphi(x)=u_1\exp[z_1x]k_1+u_2\exp[z_2x]k_2+u_3\exp[z_3x]k_3+u_4\exp[z_4x]k_4. \tag{62}$$

The quaternions u_n and the complex eigenvalues z_n are obtained by solving the eigenvalue equation for the complex linear operator M_{C}. We can also obtain the general solution of Eq. (61) by substituting $u\exp[\sqrt{2m/\hbar^2}\,zx]$ in the Schrödinger equation. We find the following quaternionic equation:

$$uz^2-(V-jW)u-iEui=0,$$

where $u=z_u+j\tilde{z}_u$. This equation can be written as two complex equations:

$$[z^2-(V-E)]z_u-\overline{W}\tilde{z}_u=[z^2-(V+E)]\tilde{z}_u+Wz_u=0.$$

An easy calculation shows that z satisfies the complex equation,

$$z^4-2Vz^2+V^2+|W|^2-E^2=0, \tag{63}$$

whose roots are

$$z_{1,2}=\pm\sqrt{V-\sqrt{E^2-|W|^2}}=\pm z_-\quad\text{and}\quad z_{3,4}=\pm\sqrt{V+\sqrt{E^2-|W|^2}}=\pm z_+. \tag{64}$$

By setting $(u_{1,2})_{\mathrm{C}}=(-ju_{3,4})_{\mathrm{C}}=1$, we find

$$u_- = \left(1 + j\frac{W}{E+\sqrt{E^2-|W|^2}}\right) \quad \text{and} \quad u_+ = \left(\frac{\overline{W}}{E+\sqrt{E^2-|W|^2}} + j\right). \tag{65}$$

The solution of the complex linear quaternionic Schrödinger equation is then given by

$$\Psi(x) = u_- \left\{ \exp\left[\sqrt{\frac{2m}{\hbar^2}} z_- x \right] k_1 + \exp\left[-\sqrt{\frac{2m}{\hbar^2}} z_- x \right] k_2 \right\} + u_+ \left\{ \exp\left[\sqrt{\frac{2m}{\hbar^2}} z_+ x \right] k_3 + \exp\left[-\sqrt{\frac{2m}{\hbar^2}} z_+ x \right] k_4 \right\}. \tag{66}$$

Equation (63) can also be obtained by multiplying the complex linear Schrödinger equation (61) from the left by the operator,

$$\frac{\hbar^2}{2m}\partial_{xx} - V - j\,W.$$

This gives

$$\left[\left(\frac{\hbar^2}{2m}\right)^2 \partial_{xxxx} - 2\frac{\hbar^2}{2m} V \partial_{xx} + V^2 + |W|^2\right]\Psi(x) = i\left[\frac{\hbar^2}{2m}\partial_{xx} - V + j\,W\right]\Psi(x) i\,E = E^2\,\Psi(x).$$

By substituting the exponential solution $u \exp[\sqrt{2m/\hbar^2}\, z\, x]$ in the previous equation, we immediately re-obtain Eq. (63).

VIII. QUATERNIONIC CONSTANT POTENTIALS

Of all Schrödinger equations the one for a constant potential is mathematically the simplest. The reason for resuming the study of the Schrödinger equation with such a potential is that the qualitative features of a physical potential can often be approximated reasonably well by a potential which is pieced together from a number of constant portions.

A. The potential step

Let us consider the quaternionic potential step,

$$V(x) - j\,W(x) = \begin{cases} 0, & x<0, \\ V - j\,W, & x>0, \end{cases}$$

where V and W represent constant potentials. For scattering problems with a wave function incident from the left on the quaternionic potential step, the complex linear quaternionic Schrödinger equation has the solution

$$\Psi(x) = \begin{cases} x<0: \quad \exp\left[i\frac{p}{\hbar}x \right] + r\exp\left[-i\frac{p}{\hbar}x \right] + j\,\tilde{r}\exp\left[\frac{p}{\hbar}x \right]; & \\ x>0: \quad u_- t \exp\left[\sqrt{\frac{2m}{\hbar^2}} z_- x \right] + u_+ \tilde{t} \exp\left[-\sqrt{\frac{2m}{\hbar^2}} z_+ x \right] & [E > \sqrt{V^2+|W|^2}], \\ u_- t \exp\left[-\sqrt{\frac{2m}{\hbar^2}} z_- x \right] + u_+ \tilde{t} \exp\left[-\sqrt{\frac{2m}{\hbar^2}} z_+ x \right] & [E < \sqrt{V^2+|W|^2}], \end{cases} \tag{67}$$

where r, $\tilde{r}$, t and $\tilde{t}$ are complex coefficients to be determined by matching the wave function $\Psi(x)$ and its slope at the discontinuity of the potential $x=0$.

For $E>\sqrt{V^2+|W|^2}$, the complex exponential solutions of the quaternionic Schrödinger equation are characterized by

$$z_-=i\sqrt{\sqrt{E^2-|W|^2}-V}\in i\,\mathbb{R} \quad \text{and} \quad z_+=\sqrt{\sqrt{E^2-|W|^2}+V}\in\mathbb{R}.$$

The complex linearly independent solutions,

$$u_-\exp\left[-\sqrt{\frac{2m}{\hbar^2}}z_-x\right] \quad \text{and} \quad u_+\exp\left[\sqrt{\frac{2m}{\hbar^2}}z_+x\right],$$

have been omitted, $k_2=k_3=0$ in (66), because we are considering a wave incident from the left and because the second complex exponential solution, $\exp[\sqrt{2m/\hbar^2}\,z_+x]$, is in conflict with the boundary condition that $\Psi(x)$ remain finite as $x\to\infty$. The standard result of complex quantum mechanics are immediately recovered by considering $W=0$ and taking the complex part of the quaternionic solution.

For $E<\sqrt{V^2+|W|^2}$, the complex exponential solutions of the quaternionic Schrödinger equation are characterized by

$$z_-=\sqrt{V-\sqrt{E^2-|W|^2}}, \quad z_+=\sqrt{V+\sqrt{E^2-|W|^2}} \quad \in\mathbb{R} \quad [E>|W|],$$

$$z_\pm=(V^2+|W|^2-E^2)^{1/4}\exp\left[\pm\,i\frac{\theta}{2}\right], \quad \tan\theta=\frac{\sqrt{|W|^2-E^2}}{V} \quad \in\mathbb{C} \quad [E<|W|].$$

The complex linearly independent solutions,

$$u_-\exp\left[\sqrt{\frac{2m}{\hbar^2}}z_-x\right] \quad \text{and} \quad u_+\exp\left[\sqrt{\frac{2m}{\hbar^2}}z_+x\right],$$

have been omitted, $k_1=k_3=0$ in (66), because they are in conflict with the boundary condition that $\Psi(x)$ remain finite as $x\to\infty$.

A relation between the complex coefficients of reflection and transmission can immediately be obtained by the continuity equation,

$$\partial_t\rho(x,t)+\partial_xJ(x,t)=0, \tag{68}$$

where

$$\rho(x,t)=\overline{\Phi}(x,t)\Phi(x,t),$$

and

$$J(x,t)=\frac{\hbar}{2m}\{[\partial_x\overline{\Phi}(x,t)]i\,\Phi(x,t)-\overline{\Phi}(x,t)i\,\partial_x\Phi(x,t)\}.$$

Note that, due to the noncommutative nature of the quaternionic wave functions, the position of the imaginary unit i in the probability current density $J(x,t)$ is important to recover a continuity equation in quaternionic quantum mechanics. For stationary states, $\Phi(x,t)=\Psi(x)\exp[-i\,(E/\hbar)t]\zeta(0)$, it can easily be shown that the probability current density,

$$J(x,t)=\frac{\hbar}{2m}\overline{\zeta}(0)\exp\left[\,i\frac{E}{\hbar}t\,\right]\{[\partial_x\overline{\Psi}(x)]i\,\Psi(x)-\overline{\Psi}(x)i\,\partial_x\Psi(x)\}\exp\left[-i\frac{E}{\hbar}t\,\right]\zeta(0),$$

must be independent of x, $J(x,t)=f(t)$. Hence,

$$\frac{\hbar}{2m}\{[\partial_x\overline{\Psi}(x)]i\,\Psi(x)-\overline{\Psi}(x)i\,\partial_x\Psi(x)\}=\exp\left[-i\frac{E}{\hbar}t\right]\zeta(0)f(t)\overline{\zeta}(0)\exp\left[i\frac{E}{\hbar}t\right]=\alpha,$$

where α is a real constant. This implies that the quantity

$$\mathcal{J}=\frac{p}{2m}\{[\partial_x\overline{\Psi}(x)]i\,\Psi(x)-\overline{\Psi}(x)i\,\partial_x\Psi(x)\},$$

has the same value at all points x. In the free potential region, $x<0$, we find

$$\mathcal{J}_-=\frac{p}{m}(1-|r|^2).$$

In the potential region, $x>0$, we obtain

$$\mathcal{J}_+=\begin{cases}\sqrt{\dfrac{2}{m}(\sqrt{E^2-|W|^2}-V)}\left[1-\left(\dfrac{|W|}{E+\sqrt{E^2-|W|^2}}\right)^2\right]|t|^2 & [E>\sqrt{V^2+|W|^2}],\\ 0 \quad [E<\sqrt{V^2+|W|^2}].\end{cases}$$

Finally, for stationary states, the continuity equation leads to

$$\begin{gathered}|r|^2+\frac{\sqrt{E^2-|W|^2}-V}{E}\left[1-\left(\frac{|W|}{E+\sqrt{E^2-|W|^2}}\right)^2\right]|t|^2=1 \quad [E>\sqrt{V^2+|W|^2}],\\ |r|^2=1 \quad [E<\sqrt{V^2+|W|^2}].\end{gathered} \tag{69}$$

Thus, by using the concept of a probability current, we can define the following coefficients of transmission and reflection:

$$R=|r|^2,\quad T=\frac{\sqrt{E^2-|W|^2}-V}{E}\left[1-\left(\frac{|W|}{E+\sqrt{E^2-|W|^2}}\right)^2\right]|t|^2 \quad [E>\sqrt{V^2+|W|^2}],$$

$$R=|r|^2,\quad T=0 \quad [E<\sqrt{V^2+|W|^2}].$$

These coefficients give the probability for the particle, arriving from $x=-\infty$, to pass the potential step at $x=0$ or to turn back. The coefficients R and T depend only on the ratios E/V and $|W|/V$. The predictions of complex quantum mechanics are recovered by setting $W=0$.

B. The rectangular potential barrier

In our study of quaternionic potentials, we now reach the rectangular potential barrier,

$$V(x)-j\,W(x)=\begin{cases}0, & x<0,\\ V-j\,W, & 0<x<a,\\ 0, & x>a.\end{cases}$$

For scattering problems with a wave function incident from the left on the quaternionic potential barrier, the complex linear quaternionic Schrödinger equation has the solution

$$\Psi(x)=\begin{cases} x<0: \quad \exp\left[i\frac{p}{\hbar}x \right]+r\exp\left[-i\frac{p}{\hbar}x \right]+j\,\tilde{r}\exp\left[\frac{p}{\hbar}x \right]; \\ 0<x<a: \quad u_-\left\{ \exp\left[\sqrt{\frac{2m}{\hbar^2}}z_- x \right] k_1+\exp\left[-\sqrt{\frac{2m}{\hbar^2}}z_- x \right] k_2 \right\} \\ \qquad\qquad +u_+\left\{ \exp\left[\sqrt{\frac{2m}{\hbar^2}}z_+ x \right] k_3+\exp\left[-\sqrt{\frac{2m}{\hbar^2}}z_+ x \right] k_4 \right\}; \\ x>a: \quad t\exp\left[i\frac{p}{\hbar}x \right]+j\,\tilde{t}\exp\left[-\frac{p}{\hbar}x \right]. \end{cases} \tag{70}$$

The complex coefficients r, $\tilde{r}$, t and $\tilde{t}$ are determined by matching the wave function $\Psi(x)$ and its slope at the discontinuity of the potential $x=0$ and will depend on $|W|$.

By using the continuity equation, we immediately find the following relation between the transmission, $T=|t|^2$, and reflection, $R=|r|^2$, coefficients

$$R+T=1. \tag{71}$$

C. The rectangular potential well

Finally, we briefly discuss the quaternionic rectangular potential well,

$$V(x)-j\,W(x)=\begin{cases} 0, & x<0, \\ -V+j\,W, & 0<x<a, \\ 0, & x>a. \end{cases}$$

In the potential region, the solution of the complex linear quaternionic Schrödinger equation is then given by

$$\begin{aligned} \Psi(x)=&u_-\left\{ \exp\left[\sqrt{\frac{2m}{\hbar^2}}z_- x \right] k_1+\exp\left[-\sqrt{\frac{2m}{\hbar^2}}z_- x \right] k_2 \right\} \\ &+u_+\left\{ \exp\left[\sqrt{\frac{2m}{\hbar^2}}z_+ x \right] k_3+\exp\left[-\sqrt{\frac{2m}{\hbar^2}}z_+ x \right] k_4 \right\}, \end{aligned} \tag{72}$$

where

$$u_-=\left(1-j\frac{W}{E+\sqrt{E^2-|W|^2}} \right), \quad u_+=\left(j-\frac{\overline{W}}{E+\sqrt{E^2-|W|^2}} \right),$$

and

$$z_-=i\sqrt{\sqrt{E^2-|W|^2}+V}, \quad z_+=\sqrt{\sqrt{E^2-|W|^2}-V}.$$

Depending on whether the energy is positive or negative, we distinguish two separate cases. If $E>0$, the particle is unconfined and is scattered by the potential; if $E<0$, it is confined and in a bound state. We limit ourselves to discussing the case $E<0$. For $|W|<|E|<\sqrt{V^2+|W|^2}$, solution (72) becomes

$$u_-\left\{\exp\left[i\sqrt{\frac{2m}{\hbar^2}}\sqrt{\sqrt{E^2-|W|^2}+V}\,x\right]k_1+\exp\left[-i\sqrt{\frac{2m}{\hbar^2}}\sqrt{\sqrt{E^2-|W|^2}+V}\,x\right]k_2\right\}$$
$$+u_+\left\{\exp\left[i\sqrt{\frac{2m}{\hbar^2}}\sqrt{V-\sqrt{E^2-|W|^2}}\,x\right]k_3+\exp\left[-i\sqrt{\frac{2m}{\hbar^2}}\sqrt{V-\sqrt{E^2-|W|^2}}\,x\right]k_4\right\}. \tag{73}$$

For $|E|<|W|$, the solution is given by

$$u_-\left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}}\rho\exp\left[i\frac{\theta+\pi}{2}x\right]\right]k_1+\exp\left[-\sqrt{\frac{2m}{\hbar^2}}\rho\exp\left[i\frac{\theta-\pi}{2}x\right]\right]k_2\right\}$$
$$+u_+\left\{\exp\left[\sqrt{\frac{2m}{\hbar^2}}\rho\exp\left[i\frac{\pi-\theta}{2}\right]x\right]k_3+\exp\left[-\sqrt{\frac{2m}{\hbar^2}}\rho\exp\left[-i\frac{\theta+\pi}{2}x\right]\right]k_4\right\}, \tag{74}$$

where $\rho=\sqrt{V^2+|W|^2-E^2}$ and $\tan\theta=\sqrt{|W|^2-E^2}/V$. In the region of zero potential, by using the boundary conditions at large distances, we find

$$\Psi(x)=\begin{cases}x<0: & \exp\left[\sqrt{\frac{2m}{\hbar^2}|E|}\,x\right]c_1+j\exp\left[-i\sqrt{\frac{2m}{\hbar^2}|E|}\,x\right]c_4;\\ x>a: & \exp\left[-\sqrt{\frac{2m}{\hbar^2}|E|}\,x\right]d_2+j\exp\left[i\sqrt{\frac{2m}{\hbar^2}|E|}\,x\right]d_3.\end{cases} \tag{75}$$

The matching conditions at the discontinuities of the potential yield the energy eigenvalues.

IX. CONCLUSIONS

In this paper, we have discussed the resolution of quaternionic, $\mathcal{D}_{\mathbb{H}}\varphi(x)=0$, and complex, $\mathcal{D}_{\mathbb{C}}\varphi(x)=0$, linear differential equations with constant coefficients within a quaternionic formulation of quantum mechanics. We emphasize that the only *quaternionic quadratic* equation involved in the study of second order linear differential equations with constant coefficients is given by Eq. (30) following from $\mathcal{D}_{\mathbb{H}}\varphi(x)=0$. Due to the right action of the factor i in complex linear differential equations, we cannot factorize a quaternionic exponential and consequently we are not able to obtain a *quaternionic quadratic* equation from $\mathcal{D}_{\mathbb{C}}\varphi(x)=0$. Complex linear differential equations can be solved by searching for quaternionic solutions of the form $q\exp[zx]$, where $q\in\mathbb{H}$ and $z\in\mathbb{C}$. The complex exponential factorization gives a *complex quartic* equation. A similar discussion can be extended to real linear differential equations, $\mathcal{D}_{\mathbb{R}}\varphi(x)=0$. In this case, the presence of left/right operators **L** and **R** in $\mathcal{D}_{\mathbb{R}}$ requires quaternionic solutions of the form $q\exp[\lambda x]$, where $q\in\mathbb{H}$ and $\lambda\in\mathbb{R}$. A detailed discussion of real linear differential equations deserves a further investigation.

The use of quaternionic mathematical structures in solving the complex linear Schrödinger equation could represent an important direction for the search of new physics. The open question of whether quaternions could play a significant role in quantum mechanics is strictly related to the whole understanding of resolutions of quaternionic differential equations and eigenvalue problems. The investigation presented in this work is only a first step towards a whole theory of quaternionic differential, integral and functional equations. Obviously, due to the great variety of problems in using a noncommutative field, it is very difficult to define the precise limit of the subject.

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APPENDIX A: QUATERNIONIC LINEAR QUADRATIC EQUATIONS

In this appendix, we give some examples of quaternionic linear quadratic equations; see cases (i)–(iii) and find their solutions.

• **(i):** $p^2+\sqrt{2}(i+j)p-1-2\sqrt{2}(i+j)=0$.

In solving such an equation we observe that $\mathbf{a}=(\sqrt{2},\sqrt{2},0)$ and $\mathbf{c}=-(2\sqrt{2},2\sqrt{2},0)$ are parallel vectors, $\mathbf{c}=-2\,\mathbf{a}$. Consequently, by introducing the *complex* imaginary unit $\mathcal{I}=(i+j)/\sqrt{2}$, we can reduce the quadratic quaternionic equation to the following *complex* equation:

$$p^2+2\,\mathcal{I}\,p-1-4\,\mathcal{I}=0,$$

whose solutions are $p_{1,2}=-\mathcal{I}\pm 2\,\sqrt{\mathcal{I}}$. It follows that the quaternionic solutions are

$$p_{1,2}=\pm\sqrt{2}-(1\mp\sqrt{2})\,\frac{i+j}{\sqrt{2}}.$$

• **(ii):** $p^2+i\,p+\frac{1}{2}k=0, \quad \Delta=0$.

We note that $\mathbf{a}=(1,0,0)$ and $\mathbf{c}=(0,0,\frac{1}{2})$ are orthogonal vectors and $\mathbf{\Delta}=0$. So, we find two coincident quaternionic solutions given by

$$p=-\frac{1}{2}\mathbf{h}\cdot\mathbf{a}+\mathbf{h}\cdot\mathbf{a}\times\mathbf{c}=-\frac{i+j}{2}.$$

• **(ii):** $p^2+j\,p+1-k=0, \quad \Delta>0$.

In this case, $\mathbf{a}=(0,1,0)$ and $\mathbf{c}=(0,0,-1)$ are orthogonal vectors, $c_0=1$ and $\Delta=1/4$. So,

$$p_0=0, \quad x=-\tfrac{1}{2}\pm\tfrac{1}{2}, \quad y=0, \quad z=1.$$

By observing that

$$\mathbf{h}\cdot\mathbf{a}=j, \quad \mathbf{h}\cdot\mathbf{c}=-k, \quad \mathbf{h}\cdot\mathbf{a}\times\mathbf{c}=-i,$$

we find the following quaternionic solutions:

$$p_1=-i \quad \text{and} \quad p_2=-(i+j).$$

• **(ii):** $p^2+k\,p+j=0, \quad \mathbf{\Delta}<0$.

We have $\mathbf{a}=(0,0,1)$, $\mathbf{c}=(0,1,0)$ and $c_0=0$. Then $\mathbf{a}\cdot\mathbf{c}=0$ and $\Delta=-3/4$. So,

$$p_0=\pm\tfrac{1}{2}, \quad x=-\tfrac{1}{2}, \quad y=\mp\tfrac{1}{2}, \quad z=\tfrac{1}{2}.$$

In this case,

$$\mathbf{h}\cdot\mathbf{a}=k, \quad \mathbf{h}\cdot\mathbf{c}=j, \quad \mathbf{h}\cdot\mathbf{a}\times\mathbf{c}=-i;$$

thus, the solutions are given by

$$p_{1,2}=\tfrac{1}{2}(\pm 1-i\mp j-k).$$

• **(iii):** $p^2+i\,p+1+i+k=0$.

We have $\mathbf{a}=(1,0,0)$, $\mathbf{c}=(1,0,1)$ and $c_0=1$. In this case $\mathbf{a}\cdot\mathbf{c}\neq 0$, so we introduce the quaternion $d_0+\mathbf{h}\cdot\mathbf{d}=1+k$, whose vectorial part $\mathbf{d}=\mathbf{c}-d_0\mathbf{a}=(0,0,1)$ is orthogonal to $\mathbf{a}$. The imaginary part of our solution will be given in terms of the imaginary quaternions,

$$\mathbf{h}\cdot\mathbf{a}=i, \quad \mathbf{h}\cdot\mathbf{d}=k, \quad \mathbf{h}\cdot\mathbf{a}\times\mathbf{d}=-j.$$

The real part of p is determined by solving the equation

$$16\,p_0^6+24\,p_0^4-3\,p_0^2-1=0.$$

The real positive solution is given by $p_0^2=\frac{1}{4}$. Consequently,

$$p_0=\pm\tfrac{1}{2}, \quad x=-\tfrac{1}{2}\mp 1, \quad y=\mp\tfrac{1}{2}, \quad z=\tfrac{1}{2}.$$

The quaternionic solutions are

$$p_1=\tfrac{1}{2}(1-3i-j-k) \quad \text{and} \quad p_2=-\tfrac{1}{2}(1-i+j-k).$$

APPENDIX B: QUATERNIONIC LINEAR DIFFERENTIAL EQUATIONS

We solve quaternionic linear differential equations whose characteristic equations are given by examples **(i)**–**(iii)** in Appendix A.

• **(i):** $\ddot{\varphi}(x)+\sqrt{2}(i+j)\dot{\varphi}(x)-[1+2\sqrt{2}(i+j)]\varphi(x)=0, \quad \varphi(0)=i, \quad \dot{\varphi}(0)=\dfrac{1+k}{\sqrt{2}}.$

The exponential $\exp[p\,x]$ is solution of the previous differential equation if and only if the quaternion p satisfies the following quadratic equation:

$$p^2+\sqrt{2}(i+j)p-1-2\sqrt{2}(i+j)=0,$$

whose solutions are given by

$$p_{1,2}=\pm\sqrt{2}-(1\mp\sqrt{2})\frac{i+j}{\sqrt{2}}.$$

Consequently,

$$\varphi(x)=\exp\left\{\left[\sqrt{2}-(1-\sqrt{2})\frac{i+j}{\sqrt{2}}\right]x\right\}c_1+\exp\left\{\left[-\sqrt{2}-(1+\sqrt{2})\frac{i+j}{\sqrt{2}}\right]x\right\}c_2.$$

By using the initial conditions, we find

$$\varphi(x)=\exp\left[-\frac{i+j}{\sqrt{2}}x\right]\cosh\left[\left(\sqrt{2}+\frac{i+j}{\sqrt{2}}\right)x\right]i.$$

• **(ii):** $\ddot{\varphi}(x)+(1+i)\dot{\varphi}(x)+\dfrac{2+i+k}{4}\varphi(x)=0, \quad \varphi(0)=0, \quad \dot{\varphi}(0)=-\dfrac{1+i+j}{2}.$

We look for exponential solutions of the form $\varphi(x)=\exp[q\,x]=\exp[(p-\frac{1}{2})x]$. The quaternion p must satisfy the quadratic equation,

$$p^2+i\,p+\tfrac{1}{2}k=0.$$

This equation implies

$$p_1 = p_2 = -\frac{i+j}{2}.$$

Thus,

$$\varphi_1(x) = \exp\left[-\frac{1+i+j}{2}x\right].$$

The second linearly independent solution is given by

$$\varphi_2(x) = (x+i)\exp\left[-\frac{1+i+j}{2}x\right].$$

By using the initial conditions, we find

$$\varphi(x) = \{\exp[q\,x] + (x+i)\exp[\,qx]i\}[1+q^{-1}(1+i\,q)i]^{-1},$$

where $q = -(1+i+j)/2$.

- **(ii):** $\ddot{\varphi}(x) + (2+j)\dot{\varphi}(x) + (2+j-k)\varphi(x) = 0,\ \varphi(0) = \dfrac{1-i}{2},\ \dot{\varphi}(0) = j.$

  The exponential solution $\varphi(x) = \exp[q\,x] = \exp[(p-1)x]$ leads to

$$p^2 + j\,p + 1 - k = 0,$$

whose solutions are

$$p_1 = -i \quad \text{and} \quad p_2 = -(i+j).$$

Consequently,

$$\varphi(x) = \exp[-x]\{\exp[-i\,x]c_1 + \exp[-(i+j)x]c_2\}.$$

The initial conditions yield

$$\varphi(x) = \exp[-x]\left\{\exp[-i\,x]\frac{3-i-2j}{2} + \exp[-(i+j)x](j-1)\right\}.$$

- **(ii):** $\ddot{\varphi}(x) + k\,\dot{\varphi}(x) + j\,\varphi(x) = 0,\ \varphi(0) = i+k,\ \dot{\varphi}(0) = 1.$

  The characteristic equation is

$$p^2 + k\,p + j = 0,$$

whose solutions are

$$p_{1,2} = \tfrac{1}{2}(\pm 1 - i \mp j - k).$$

Thus, the general solution of our differential equation reads as

$$\varphi(x) = \exp\left[\frac{1-i-j-k}{2}x\right]c_1 + \exp\left[-\frac{1+i-j+k}{2}x\right]c_2.$$

By using the initial conditions, we obtain

$$\varphi(x)=\left\{ \exp\left[\frac{1-i-j-k}{2}x\right]+\exp\left[-\frac{1+i-j+k}{2}x\right]\right\}\frac{i+k}{2}.$$

• **(iii):** $\ddot{\varphi}(x)+(i-2)\dot{\varphi}(x)+(2+k)\varphi(x)=0$, $\varphi(0)=0$, $\dot{\varphi}(0)=j$.
By substituting $\varphi(x)=\exp[q\,x]=\exp[(p+1)x]$ in the previous differential equation, we find

$$p^2+i\,p+1+i+k=0.$$

The solutions of this quadratic quaternionic equation are

$$p_1=\tfrac{1}{2}(1-3i-j-k) \quad \text{and} \quad p_2=-\tfrac{1}{2}(1-i+j-k).$$

So, the general solution of the differential equation is

$$\varphi(x)=\exp\left[\frac{1-3i-j-k}{2}x\right]c_1+\exp\left[-\frac{1-i+j-k}{2}x\right]c_2.$$

By using the initial conditions, we obtain

$$\varphi(x)=\left\{\exp\left[\frac{1-3i-j-k}{2}x\right]-\exp\left[-\frac{1-i+j-k}{2}x\right]\right\}\frac{j-i+2k}{6}.$$

APPENDIX C: DIAGONALIZATION AND JORDAN FORM

In this appendix, we find the solution of quaternionic and complex linear differential equations by using diagonalization and Jordan form.

1. Quaternionic linear differential equation

By using the discussion about quaternionic quadratic equation, it can immediately be shown that the solution of the following second order equation:

$$\ddot{\varphi}(x)+(k-i)\dot{\varphi}(x)-j\,\varphi(x)=0,$$

with initial conditions

$$\varphi(0)=\frac{k}{2}, \quad \dot{\varphi}(0)=1+\frac{j}{2},$$

is given by

$$\varphi(x)=\left(x+\frac{k}{2}\right)\exp[i\,x].$$

Let us solve this differential equation by using its matrix form (47), with

$$M=\begin{pmatrix}0 & 1\\ j & i-k\end{pmatrix}.$$

This quaternionic matrix can be reduced to its Jordan form,

$$M=J\begin{pmatrix}i & 1\\ 0 & i\end{pmatrix}J^{-1},$$

by the matrix transformation

$$J=\begin{pmatrix} 1 & \dfrac{k}{2} \\ i & 1+\dfrac{j}{2} \end{pmatrix}, \quad J^{-1}=\begin{pmatrix} \dfrac{3+j}{4} & -\dfrac{i+k}{4} \\ -\dfrac{i+k}{2} & \dfrac{1-j}{2} \end{pmatrix}.$$

The solution of the quaternionic linear quaternionic differential equation is then given by

$$\begin{aligned}\varphi(x)&=J_{11}\exp[i\,x][J_{11}^{-1}\,\varphi(0)+J_{12}^{-1}\,\dot{\varphi}(0)]\\&\quad+(x\,J_{11}+J_{12})\exp[i\,x][J_{21}^{-1}\,\varphi(0)+J_{22}^{-1}\,\dot{\varphi}(0)]\\&=(x\,J_{11}+J_{12})\exp[i\,x]\\&=\left(x+\frac{k}{2}\right)\exp[i\,x].\end{aligned}$$

2. Complex linear differential equations

Let us now consider the complex linear quaternionic differential equation,

$$\ddot{\varphi}(x)-j\,\varphi(x)i=0,$$

with initial conditions

$$\varphi(0)=j, \quad \dot{\varphi}(0)=k.$$

To find particular solutions, we set $\varphi(x)=q\exp[z\,x]$. Consequently,

$$q\,z^2-j\,q\,i=0.$$

The solution of the complex linear second order differential equation is

$$\varphi(x)=\tfrac{1}{2}[(i+j)\exp[-ix]+(j-i)\cosh x+(k-1)\sinh x].$$

This solution can also be obtained by using the matrix

$$M_{\mathrm{C}}=\begin{pmatrix} 0 & 1 \\ j\,R_i & 0 \end{pmatrix},$$

and its diagonal form

$$M_{\mathrm{C}}=S_{\mathrm{C}}\begin{pmatrix} -i\,R_i & 0 \\ 0 & i \end{pmatrix}S_{\mathrm{C}}^{-1},$$

where

$$S_{\mathrm{C}}=\begin{pmatrix} \dfrac{1-i-j-k}{2}+\dfrac{1-i+j+k}{2}R_i & \dfrac{1+i-j+k}{2}-\dfrac{1+i+j-k}{2}R_i \\ \dfrac{1+i+j-k}{2}-\dfrac{1+i-j+k}{2}R_i & -\dfrac{1-i-j-k}{2}+\dfrac{1-i+j+k}{2}R_i \end{pmatrix}$$

and

$$S_{\mathrm{C}}^{-1}=\frac{1}{4}\begin{pmatrix} \dfrac{1+i+j+k}{2}-\dfrac{1+i-j-k}{2}R_i & \dfrac{1-i-j+k}{2}+\dfrac{1-i+j-k}{2}R_i \\ \dfrac{1-i+j-k}{2}+\dfrac{1-i-j+k}{2}R_i & -\dfrac{1+i+j+k}{2}-\dfrac{1+i-j-k}{2}R_i \end{pmatrix}.$$

The solution of the complex linear quaternionic differential equation is then given by

$$\begin{aligned}\varphi(x)&=S_{\mathrm{C}\,11}\exp[-iR_ix][S_{\mathrm{C}\,11}^{-1}\varphi(0)+S_{\mathrm{C}\,12}^{-1}\dot{\varphi}(0)]\\&\quad+S_{\mathrm{C}\,12}\exp[ix][S_{\mathrm{C}\,21}^{-1}\varphi(0)+S_{\mathrm{C}\,22}^{-1}\dot{\varphi}(0)]\\&=\frac{1}{4}\{(1-i+j-k)\exp[-x]-(1+i-j-k)\exp[x]\}\\&\quad+\frac{i+j}{2}\exp[-ix].\end{aligned}$$

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The holonomy Lie algebras of neutral metrics in dimension four

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The Lie algebra isomorphism between $su(1,1)\times su(1,1)$ and $o(2,2)$ is used to obtain a list of subalgebras of the latter. The resulting list of 32 subalgebras is then examined on a case by case basis to see if each can be the Lie algebra of the holonomy group of a neutral metric in four dimensions. The conclusions, taken in conjunction with previously known results, furnish a classification of such Lie subalgebras of $o(2,2)$, with only one case remaining unresolved. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1362284]

I. INTRODUCTION

In this article we shall study and indeed classify the subalgebras of $o(2,2)$ that can occur as holonomy Lie algebras of a neutral metric in dimension four. By a *neutral* metric we mean one that has signature (2,2). The notion of holonomy is due to E. Cartan. In two encyclopaedic articles Berger[1,2] in the 1950s succeeded in classifying the holonomy groups of irreducible Riemannian spaces apart from a few exceptional cases which were resolved later. See Ref. 3 for a discussion of the most difficult cases G_2 and Spin(7). Actually Berger's work even extends to the case of indefinite metrics and symmetric linear connections but all the time under the assumption that the holonomy representation is irreducible.

Let us turn our attention now to the case of indefinite metrics. In the book by Besse[4] the reader can see a discussion of the possible holonomy groups that can occur for Lorentz metrics in dimensions two through four and the corresponding geometric interpretation. We should mention here that Besse considers exclusively the local solution so that one may as well work at the Lie algebra rather than the Lie group level. Likewise in this article all considerations will be local. Another treatment of four-dimensional Lorentzian manifolds and the significance of holonomy in general relativity may be found in a series of papers by Hall and co-workers.[5–9] It is important to appreciate that our classification pertains to subalgebras of $o(2,2)$ under the adjoint representation. For a classification of low-dimensional abstract Lie algebras we refer to the work of Patera *et al.*[10] Finally we should mention the work of Berard-Bergery and Ikemakhen[11] who considered the possible holonomy groups of neutral metrics in dimension four. Their work may be seen as complementary to ours: putting the results together gives almost a complete classification of which Lie algebras can occur as holonomy Lie algebras of a neutral metric in dimension four.

We begin in Sec. II by obtaining a classification of all possible Lie subalgebras of $o(2,2)$ exploiting the fact that $o(2,2)$ is isomorphic to $su(1,1)\times su(1,1)$ and give the isomorphisim explicitly. We obtain a list of 32 classes of Lie subalgebras and they are displayed in Table I. Remarkably all but 2 of these 32 subalgebras are reducible.

The principal concern of our article has been throughout to decide whether there exists at least one metric that gives rise to a particular subalgebra in our list of 32. For certain subalgebras we are able to write down a metric directly in which case we move on to the next subalgebra. In the more difficult cases we actually construct metrics by integrating the conditions imposed upon them by the curvature and its covariant derivatives. We do not claim to have described the most general

TABLE I. The subalgebras of o(2,2).

No.	Basis for the Lie subalgebra	Dimension
1	$\begin{bmatrix} 0 & \alpha & 0 & 0 \\ -\alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & \beta \\ 0 & 0 & -\beta & 0 \end{bmatrix}$	1
2	$\begin{bmatrix} 0 & 0 & \alpha & 0 \\ 0 & 0 & 0 & \beta \\ \alpha & 0 & 0 & 0 \\ 0 & \beta & 0 & 0 \end{bmatrix}$	1
3	$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & -1 & 0 \end{bmatrix}$	1
4	$\begin{bmatrix} 0 & -\beta & \alpha & 0 \\ \beta & 0 & 0 & -\alpha \\ \alpha & 0 & 0 & \beta \\ 0 & -\alpha & -\beta & 0 \end{bmatrix}$	1
5	$\begin{bmatrix} 0 & 1-\alpha & 0 & 1 \\ \alpha-1 & 0 & 1 & 0 \\ 0 & 1 & 0 & \alpha+1 \\ 1 & 0 & -(\alpha+1) & 0 \end{bmatrix}$	1
6	$\begin{bmatrix} 0 & -\alpha & 0 & 0 \\ \alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & \alpha \\ 0 & 0 & -\alpha & 0 \end{bmatrix}$	1
7	$\begin{bmatrix} 0 & 0 & \alpha & 0 \\ 0 & 0 & 0 & \alpha \\ \alpha & 0 & 0 & 0 \\ 0 & \alpha & 0 & 0 \end{bmatrix}$	1
8	$\begin{bmatrix} 0 & 1 & -\alpha & 1 \\ -1 & 0 & 1 & -\alpha \\ -\alpha & 1 & 0 & 1 \\ 1 & -\alpha & -1 & 0 \end{bmatrix}$	1
9	$\begin{bmatrix} 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & 0 & -1 & 0 \end{bmatrix}$	1
10	$\begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}, \begin{bmatrix} -J & J \\ -J & J \end{bmatrix}$	2
11	$\begin{bmatrix} 0 & I+\alpha K \\ I+\alpha K & 0 \end{bmatrix}, \begin{bmatrix} -J & J \\ -J & J \end{bmatrix}$	2
12	$\begin{bmatrix} -J & J \\ -J & J \end{bmatrix}, \begin{bmatrix} \alpha J & I \\ I & \alpha J \end{bmatrix} (\alpha \neq 0)$	2
13	$\begin{bmatrix} J & I+L \\ I+L & J \end{bmatrix}, \begin{bmatrix} -J & J \\ -J & J \end{bmatrix}$	2
14	$\begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}, \begin{bmatrix} 0 & K \\ K & 0 \end{bmatrix}$	2

TABLE I. (*Continued.*)

No.	Basis for the Lie subalgebra	Dimension
15	$\begin{bmatrix}0 & I\\ I & 0\end{bmatrix}, \begin{bmatrix}J & 0\\ 0 & J\end{bmatrix}$	2
16	$\begin{bmatrix}-J & 0\\ 0 & J\end{bmatrix}, \begin{bmatrix}J & 0\\ 0 & J\end{bmatrix}$	2
17	$\begin{bmatrix}-J & J\\ -J & J\end{bmatrix}, \begin{bmatrix}J & L\\ L & J\end{bmatrix}$	2
18	$\begin{bmatrix}-J & J\\ -J & J\end{bmatrix}, \begin{bmatrix}0 & K\\ K & 0\end{bmatrix}$	2
19	$\begin{bmatrix}-J & J\\ -J & J\end{bmatrix}, \begin{bmatrix}J & 0\\ 0 & J\end{bmatrix}$	2
20	$\begin{bmatrix}0 & I+K\\ I+K & 0\end{bmatrix}, \begin{bmatrix}(\beta-1)J & J+\beta L\\ -J+\beta L & (\beta+1)J\end{bmatrix} (\beta=\pm 1)$	2
21	$\begin{bmatrix}0 & I\\ I & 0\end{bmatrix}, \begin{bmatrix}-J & 0\\ 0 & J\end{bmatrix}, \begin{bmatrix}0 & J\\ -J & 0\end{bmatrix}$	3
22	$\begin{bmatrix}0 & I+K\\ I+K & 0\end{bmatrix}, \begin{bmatrix}0 & 0\\ 0 & 2J\end{bmatrix}, \begin{bmatrix}0 & J+L\\ -J+L & 0\end{bmatrix}$	3
23	$\begin{bmatrix}0 & I\\ I & 0\end{bmatrix}, \begin{bmatrix}-J & J\\ -J & J\end{bmatrix}, \begin{bmatrix}0 & K\\ K & 0\end{bmatrix}$	3
24	$\begin{bmatrix}0 & I\\ I & 0\end{bmatrix}, \begin{bmatrix}-J & J\\ -J & J\end{bmatrix}, \begin{bmatrix}J & 0\\ 0 & J\end{bmatrix}$	3
25	$\begin{bmatrix}0 & I+\alpha L\\ I+\alpha L & 0\end{bmatrix}, \begin{bmatrix}-J & J\\ -J & J\end{bmatrix}, \begin{bmatrix}J & L\\ L & J\end{bmatrix}$	3
26	$\begin{bmatrix}0 & I+\alpha K\\ I+\alpha K & 0\end{bmatrix}, \begin{bmatrix}-J & J\\ -J & J\end{bmatrix}, \begin{bmatrix}J & L\\ L & J\end{bmatrix}$	3
27	$\begin{bmatrix}0 & I\\ I & 0\end{bmatrix}, \begin{bmatrix}-J & 0\\ 0 & J\end{bmatrix}, \begin{bmatrix}0 & J\\ -J & 0\end{bmatrix}, \begin{bmatrix}0 & K\\ K & 0\end{bmatrix}$	4
28	$\begin{bmatrix}0 & I\\ I & 0\end{bmatrix}, \begin{bmatrix}-J & 0\\ 0 & J\end{bmatrix}, \begin{bmatrix}0 & J\\ -J & 0\end{bmatrix}, \begin{bmatrix}J & 0\\ 0 & J\end{bmatrix}$	4
29	$\begin{bmatrix}0 & I\\ I & 0\end{bmatrix}, \begin{bmatrix}-J & 0\\ 0 & J\end{bmatrix}, \begin{bmatrix}0 & J\\ -J & 0\end{bmatrix}, \begin{bmatrix}J & L\\ L & J\end{bmatrix}$	4
30	$\begin{bmatrix}0 & I\\ I & 0\end{bmatrix}, \begin{bmatrix}-J & J\\ -J & J\end{bmatrix}, \begin{bmatrix}0 & K\\ K & 0\end{bmatrix}, \begin{bmatrix}J & L\\ L & J\end{bmatrix}$	4
31	$\begin{bmatrix}0 & I\\ I & 0\end{bmatrix}, \begin{bmatrix}-J & 0\\ 0 & J\end{bmatrix}, \begin{bmatrix}0 & J\\ -J & 0\end{bmatrix}, \begin{bmatrix}J & L\\ L & J\end{bmatrix}, \begin{bmatrix}0 & K\\ K & 0\end{bmatrix}$	5
32	$\begin{bmatrix}-J & 0\\ 0 & J\end{bmatrix}, \begin{bmatrix}J & 0\\ 0 & J\end{bmatrix}, \begin{bmatrix}0 & I\\ I & 0\end{bmatrix}, \begin{bmatrix}0 & K\\ K & 0\end{bmatrix}, \begin{bmatrix}0 & J\\ -J & 0\end{bmatrix}, \begin{bmatrix}0 & L\\ L & 0\end{bmatrix}$	6

metric corresponding to every subalgebra. We shall come back to this question in a future project.

The are two main differential geometric tools that we shall use in our analysis, of which the first is the Ambrose–Singer[12] theorem, which says that the holonomy algebra can be computed from successive derivatives of the curvature tensor.[4,7,12,13] The second tool is a coordinate normal form due to A. G. Walker[14] for a metric that leaves invariant a null distribution. As a result of this normal form, in trying to construct metrics of this type, instead of dealing potenially with ten unknown functions, we only have three unknowns. Walker's normal form is all the more impor-

tant because of the following easily proved fact about the holonomy representation of neutral geometries, again to be understood in a purely local sense: whenever a null line is left invariant so is a null plane containing the line. Thus Walker's theorem is applicable to 27 of the subalgebras that appear in Table I.

In Sec. IV we turn our attention to one-dimensional algebras which forms a self-contained story. In Sec. V we give a second table which displays the geometric properties that a metric would have to have if its holonomy is to correspond to one of the algebras in our list of 32. Actually we exclude the first nine algebras in Table I, because they are accounted for already in Sec. IV, as well the two irreducible cases.

In Sec. VI we eliminate several easy cases by elementary arguments. In the remaining sections we consider in turn various classes of subalgebras within which the geometric properties of the putative metrics are similar. In every case but one the existence question is answered definitively.

We shall use a minimum of notation. The curvature tensor of a connection will be thought of as type (1,3) tensor field with components R^i_{jkl} in some coordinate system. The components of the covariant derivative of R^i_{jkl} will be similarly denoted by $R^i_{jkl;m}$. The summation convention on repeated indices applies unless the contrary is specified.

II. CLASSIFICATION OF THE LIE SUBALGEBRAS OF o(2,2)

In this section we shall obtain a classification of the Lie subalgebras of o(2,2). We exploit the fact that o(2,2) is isomorphic to $\mathrm{su}(1,1)\oplus\mathrm{su}(1,1)$. Such an isomorphism is mentioned by Helgason[15] but he does not give details. In fact at the group level we have an epimorphism f of $\mathrm{SU}(1,1)\times\mathrm{SU}(1,1)$ onto $\mathrm{SO}_\circ(2,2)$ whose kernel is isomorphic to $\mathbb{Z}_2$. Since the formulas are rather complicated and will not be needed later we refrain from giving them and refer the reader to Ref. 16.

In order to describe the isomorphism f_* at the Lie algebra level we shall introduce the following notation for certain 2×2 real matrices:

$$J=\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \quad K=\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad L=\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{2.1}$$

The matrices iK, iJ and L then constitute a basis for su(1,1) and under the adjoint representation every element of su(1,1) is conjugate to one of $\alpha iJ, \beta iK$ or $iK+L$ where $\alpha,\beta\in\mathbb{R}$ and the latter $iK+L$ is nilpotent.

An explicit form of f_* mapping generators to generators is as follows:

$$f_*\begin{bmatrix} iK & 0 \\ 0 & 0 \end{bmatrix}=\begin{bmatrix} -J & 0 \\ 0 & J \end{bmatrix}, \quad f_*\begin{bmatrix} 0 & 0 \\ 0 & iK \end{bmatrix}=\begin{bmatrix} J & 0 \\ 0 & J \end{bmatrix},$$

$$f_*\begin{bmatrix} iJ & 0 \\ 0 & 0 \end{bmatrix}=\begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}, \quad f_*\begin{bmatrix} 0 & 0 \\ 0 & iJ \end{bmatrix}=\begin{bmatrix} 0 & K \\ K & 0 \end{bmatrix},$$

$$f_*\begin{bmatrix} L & 0 \\ 0 & 0 \end{bmatrix}=\begin{bmatrix} 0 & J \\ -J & 0 \end{bmatrix}, \quad f_*\begin{bmatrix} 0 & 0 \\ 0 & L \end{bmatrix}=\begin{bmatrix} 0 & L \\ L & 0 \end{bmatrix}.$$

At this stage we consider $\mathbb{R}^4$ to be equipped with the neutral inner product $\left[\begin{smallmatrix} I & 0 \\ 0 & -I \end{smallmatrix}\right]$. Subsequently we shall find it convenient to change this representation.

To obtain the classification of the subalgebras of o(2,2) we now have the apparently simple task of finding subalgebras in $\mathrm{su}(1,1)\oplus\mathrm{su}(1,1)$ and pushing forward with f_*. The following elementary fact should be noted:

Lemma 2.1: There is a two-dimensional Lie subalgebra of su(1,1) *with generators* iJ *and* $iK+L$ *and this subalgebra is unique up to isomorphism.*

We obtained the classification by considering elements of $\mathrm{su}(1,1)\oplus\mathrm{su}(1,1)$ as 2×2 block diagonal matrices and letting the restriction of a subalgebra to each block have dimensions m and n, respectively. Of course the primary invariant of a subalgebra is its dimension which can vary

from zero to six. We note also that the matrix $\left[\begin{smallmatrix} K & 0 \\ 0 & I \end{smallmatrix}\right]$ defines an automorphism of o(2,2) which maps $\left[\begin{smallmatrix} -J & 0 \\ 0 & J \end{smallmatrix}\right]$ to $\left[\begin{smallmatrix} J & 0 \\ 0 & J \end{smallmatrix}\right]$, $\left[\begin{smallmatrix} 0 & I \\ I & 0 \end{smallmatrix}\right]$ to $\left[\begin{smallmatrix} 0 & K \\ K & 0 \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} 0 & J \\ -J & 0 \end{smallmatrix}\right]$ to $\left[\begin{smallmatrix} 0 & L \\ L & 0 \end{smallmatrix}\right]$, respectively. It follows that the cases (m,n) and (n,m) give rise to isomorphic subalgebras in o(2,2).

The classification for one-dimensional algebras is obtained immediately and, allowing for change of basis, agrees with results obtained previously in Ref. 17. For the remaining algebras, one simply checks for a given dimension d, with $2 \leqslant d \leqslant 5$, all the possible subalgebras of $\mathrm{su}(1,1) \oplus \mathrm{su}(1,1)$ that can arise for particular values of m and n such that $m \geqslant n$ and $2 \leqslant m+n \leqslant 5$ and one realizes the corresponding subalgebra of o(2,2) by applying f_*.

Let us outline the method for three-dimensional sualgebras. First of all (3,0) corresponds to $\mathrm{su}(1,1) \oplus \{0\}$ and the algebra in o(2,2) has generators $\left[\begin{smallmatrix} 0 & I \\ I & 0 \end{smallmatrix}\right]$, $\left[\begin{smallmatrix} -J & 0 \\ 0 & J \end{smallmatrix}\right]$, $\left[\begin{smallmatrix} -J & 0 \\ 0 & J \end{smallmatrix}\right]$. For the case (3,1) we may assume that our generators are of the form $\left[\begin{smallmatrix} iJ & 0 \\ 0 & aN \end{smallmatrix}\right]$, $\left[\begin{smallmatrix} iK & 0 \\ 0 & bN \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} L & 0 \\ 0 & cN \end{smallmatrix}\right]$ where $a,b,c \in \mathbb{R}$ and the precise form of N is unknown. The Lie bracket of the first two must be twice the third, which implies that $c=0$. Likewise from the brackets of the first and third and second and third, respectively, we deduce that $a=b=0$, and hence no such algebra of this kind is possible.

Similarly one may argue that the case (3,2) is impossible and that (3,3) corresponds precisely to the diagonal subalgebra in $\mathrm{su}(1,1) \oplus \mathrm{su}(1,1)$. For the case (2,1) we may assume that the generators have the form $\left[\begin{smallmatrix} iJ & 0 \\ 0 & aM \end{smallmatrix}\right]$, $\left[\begin{smallmatrix} iK+L & 0 \\ 0 & bM \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} 0 & 0 \\ 0 & M \end{smallmatrix}\right]$ where $a,b \in \mathbb{R}$. We can now put M into canonical form and we obtain three classes of algebras in o(2,2) depending on a parameter α. Similarly for the case (2,2) we obtain a single class of Lie algebras in o(2,2) that depends on a parameter α. Table I gives our list of the subalgebras of o(2,2) in terms of a basis for each subalgebra. We state the dimension of the subalgebra and have numbered the subalgebras from 1 to 32 for future reference, though certain of these numbers pertain to classes of subalgebras depending on parameters α and β.

III. DIFFERENTIAL GEOMETRIC PRELIMINARIES

For the moment M will denote a C^∞ manifold of dimension n. Also ∇ will denote a C^∞ symmetric linear connection on M. A tensor field T on M is said to be *parallel* if $\nabla_X T = 0$ for all vector fields X on M. On the other hand T is said to be *recurrent* if $\nabla_X T = \theta(X)T$ for some one-form θ on M or equivalently $\nabla T = \theta \otimes T$. An r-dimensional distribution D on M will be said to be parallel if for all Y in D and all vector fields X on M, the vector field $\nabla_X Y$ also belongs to D. If ∇ is a symmetric connection, then D is necessarily integrable. Even if D is parallel it may contain no parallel or recurrent vector fields itself.

We will assume that the reader is familiar with the basic idea of holonomy and refer to Refs. 4 and 13. A good reference also is Ref. 7 which is concerned with four-dimensional Lorentzian manifolds as opposed to the neutral metrics which is the subject of the present article. There are a number of technical difficulties associated with holonomy which we shall ignore. Specifically we shall have occasion to solve linear systems of equations and we shall need to assume that the rank of these systems is constant. We also need to know that the Lie algebra of the holonomy group can be computed pointwise from the curvature R of ∇ and the covariant derivatives of R. Therefore, we shall make the assumption that the manifolds, metrics and connections concerned are real analytic. We shall be working infinitesimally at the Lie algebra rather that the group level throughout.

From now on ∇ will be the Levi-Civita connection of a metric g on M and the holonomy group of g will be denoted by $\mathrm{Hol}(g)$ and its Lie algebra by $\mathrm{hol}(g)$. We say that $\mathrm{Hol}(g)$ is *nondegenerately reducible* if on each tangent space $T_x M$ to M the group $\mathrm{Hol}(g)$ leaves invariant a proper *nondegenerate* subspace. The local de Rham theorem asserts that if $\mathrm{Hol}(g)$ [or even $\mathrm{hol}(g)$] acts nondegenerately reducibly, then M and g split locally as a product manifold and product metric.

We turn now to a theorem of A. G. Walker[14] that will be fundamental to much of our analysis.

Theorem 3.1:[14] Let (M,g) *be a pseudo-Riemannian manifold of class* C^∞. *If* g *admits a parallel, null* r*-distribution, then there is a system of coordinates* (x^i) *relative to which* g *assumes the following form,*

$$g_{ij}=\begin{bmatrix} 0 & 0 & I \\ 0 & A & H \\ I & H^t & B \end{bmatrix},$$

where I is the $r\times r$ identity matrix and A,B,H and H^t are matrix functions of the same class as M, satisfying the following conditions but otherwise arbitrary:

(i) *A and B are symmetric, A is of order $(n-2r)\times(n-2r)$ and nonsingular, B is of order $r\times r$, H is of order $(n-2r)\times r$ and H^t is the transpose of H.*

(ii) *A and H are independent of the coordinates $x^1,x^2,\ldots,x^r$.* □

As a footnote to Theorem 3.1 we note that if in addition B is independent of, say, x^k, for a fixed k with $1\leqslant k\leqslant r$, then $\partial/\partial x^k$ is a parallel vector field for g.

The special case of Walker's theorem that we shall need is when $n=4$ and $r=2$. In that case A and H are zero and we denote the 2×2 matrix B by $\left[\begin{smallmatrix} a & c \\ c & b \end{smallmatrix}\right]$. We shall also use (x,y,z,w) for the coordinate system rather than (x^1,x^2,x^3,x^4). We record next the geodesic equations as an efficient means of the encoding the components Γ^i_{jk} of the Levi-Civita connection of g:

$$\ddot{x}+a_x\dot{x}\dot{z}+c_x\dot{x}\dot{w}+a_y\dot{y}\dot{z}+c_y\dot{y}\dot{w}+\tfrac{1}{2}(aa_x+ca_y+a_z)(\dot{z})^2$$

$$+(ac_x+cc_y+a_w)\dot{z}\dot{w}+\tfrac{1}{2}(ab_x+cb_y+2c_w-b_z)(\dot{w})^2=0,$$

$$\ddot{y}+c_x\dot{x}\dot{z}+b_x\dot{x}\dot{w}+c_y\dot{y}\dot{z}+b_y\dot{y}\dot{w}+\tfrac{1}{2}(ca_x+ba_y+2c_z-a_w)(\dot{z})^2$$

$$+(cc_x+bc_y+b_z)\dot{z}\dot{w}+\tfrac{1}{2}(cb_x+bb_y+b_w)(\dot{w})^2=0,$$

$$\ddot{z}-\tfrac{1}{2}a_x(\dot{z})^2-c_x\dot{z}\dot{w}-\tfrac{1}{2}b_x(\dot{w})^2=0,$$

$$\ddot{w}-\tfrac{1}{2}a_y(\dot{z})^2-c_y\dot{z}\dot{w}-\tfrac{1}{2}b_y(\dot{w})^2=0.$$

One finds also that the nonzero components (allowing for symmetry) of the totally covariant curvature tensor are given by

$$R_{1313}=-\tfrac{1}{2}a_{xx},$$

$$R_{1314}=-\tfrac{1}{2}c_{xx},$$

$$R_{1323}=-\tfrac{1}{2}a_{xy},$$

$$R_{1324}=-\tfrac{1}{2}c_{xy},$$

$$R_{1334}=\tfrac{1}{2}a_{xw}-\tfrac{1}{2}c_{xz}-\tfrac{1}{4}b_xa_y+\tfrac{1}{4}c_xc_y,$$

$$R_{1414}=-\tfrac{1}{2}b_{xx},$$

$$R_{1423}=-\tfrac{1}{2}c_{xy},$$

$$R_{1424}=-\tfrac{1}{2}b_{xy},$$

$$R_{1434}=\tfrac{1}{2}c_{xw}-\tfrac{1}{2}b_{xz}-\tfrac{1}{4}(c_x)^2+\tfrac{1}{4}b_xa_x-\tfrac{1}{4}b_xc_y+\tfrac{1}{4}c_xb_y,$$

$$R_{2323}=-\tfrac{1}{2}a_{yy},$$

$$R_{2324}=-\tfrac{1}{2}c_{yy},$$

$$R_{2334}=\tfrac{1}{2}a_{yw}-\tfrac{1}{2}c_{yz}+\tfrac{1}{4}c_xa_y-\tfrac{1}{4}a_xc_y-\tfrac{1}{4}c_ya_y+\tfrac{1}{4}(c_y)^2,$$

$$R_{2424}=-\tfrac{1}{2}b_{yy},$$

$$R_{2434}=\tfrac{1}{2}c_{yw}-\tfrac{1}{2}b_{yz}+\tfrac{1}{4}b_xa_y-\tfrac{1}{4}c_xc_y,$$

$$\begin{aligned}R_{3434}=&c_{zw}-\tfrac{1}{2}a_{ww}-\tfrac{1}{2}b_{zz}+\tfrac{1}{4}ab_xa_x-\tfrac{1}{4}a(c_x)^2-\tfrac{1}{2}cc_xc_y\\&+\tfrac{1}{4}ca_xb_y-\tfrac{1}{2}c_xa_w+\tfrac{1}{2}a_xc_w-\tfrac{1}{4}a_xb_z+\tfrac{1}{4}cb_xa_y+\tfrac{1}{4}bb_ya_y\\&-\tfrac{1}{4}b(c_y)^2-\tfrac{1}{2}c_yb_z+\tfrac{1}{4}a_yb_w+\tfrac{1}{4}b_xa_z+\tfrac{1}{2}b_yc_z-\tfrac{1}{4}b_ya_w.\end{aligned}$$

From the formulas for the geodesic equations we obtain the following facts.

Corollary 3.2: Suppose the neutral metric g on $\mathbb{R}^4$ admits a parallel null two-distribution. Then g has the following extra properties:

(1) *g possesses a parallel null vector field iff there exists a coordinate system (x,y,z,w) in which a, b and c are independent of x.*
(2) *g possesses a null recurrent vector field iff there exists a coordinate system (x,y,z,w) in which b and c are independent of x.*
(3) *g possesses two parallel orthogonal null vector fields iff there exists a coordinate system (x,y,z,w) in which a, b and c are independent of x and y.*
(4) *g possesses orthogonal null recurrent and null parallel vector fields iff there exists a coordinate system (x,y,z,w) in which a, b and c are independent of y and b and c are independent of x.*
(5) *g possesses two orthogonal null recurrent vector fields iff there exists a coordinate system (x,y,z,w) in which b and c are independent of x and a and b are independent of y.*

We record another useful result in this section.

Proposition 3.3: Suppose on the n-dimensional manifold M with symmetric connection ∇ there exists a vector field Δ that is recurrent, nowhere vanishing, and satisfies

$$R(X,Y)\Delta=0$$

for all vector fields X and Y on M and R is the type (1,3) *Riemann tensor. Then Δ may be rescaled locally so as to give a parallel vector field.*

Proof: Since Δ is recurrent we find by calculation that

$$R(X,Y)\Delta=d\theta(X,Y)\Delta.$$

It follows that θ is closed. Write locally $\theta=df$ for some function on M and define

$$\overline{\Delta}=e^{-f}\Delta.$$

Then $\overline{\Delta}$ is parallel. □

We finish up this section with two results that will be used several times in the analysis of the more difficult cases. As before g denotes a neutral metric on the four-dimensional space M and g has a parallel and of course integrable distribution D. The quotient space M/D assumed to be a smooth manifold will be denoted by Q.

Lemma 3.4: If the Levi-Civita connection of g is projectable to the quotient space Q, then the Ricci tensor of the projected connection is symmetric.

Proof: Assuming that the connection of g projects to Q to show that induced connection of Q has symmetric Ricci tensor, it is sufficient to show that

$$R^1_{341}+R^2_{342}+R^3_{343}-R^1_{431}-R^2_{432}-R^4_{434}=0. \tag{3.1}$$

We replace the third term in (3.1) by R^1_{134}, the sixth term by R^2_{234} and apply the Bianchi identity to the fourth term. Thus the left hand side of (3.1) becomes

$$R^1_{341}+R^2_{342}+R^1_{134}-R^1_{143}+R^1_{314}-R^2_{432}+R^2_{234}=R^2_{342}+R^2_{234}+R^2_{423}=0$$

by the Bianchi identity. □

Proposition 3.5: If the Levi-Civita connection of g is projectable to Q and the connection on Q has one-dimensional holonomy group, then either it is a Levi-Civita connection or else g has a parallel vector field.

Proof: By Lemma 3.4 the connection on Q is symmetric. Furthermore, since the holonomy group is one-dimensional, the Ricci tensor, which embodies the entire curvature tensor, is recurrent. There are now two possibilities according as the Ricci tensor on Q is nondegenerate or degenerate. In the former case Ricci may be scaled so as to produce a metric on Q for which the induced connection on Q is its Levi-Civita connection.[18] In the latter case the connection on Q possesses a parallel one-form.[19] It follows by pullback that g on M possesses a parallel one-form and hence, by duality, a parallel vector field. □

We remark that in Theorem 3.1, in the case where the projected connection is Levi-Civita, g is not necessarily of the form of a complete lift of a metric on Q but differs from it by the pullback of a quadratic form on Q. This point is fully discussed in Ref. 19 where it is explained how M may be identified locally as the tangent bundle of Q.

IV. ONE-DIMENSIONAL HOLONOMY ALGEBRAS

The case of the Lie algebras that are one-dimensional will be discussed in this section. The argument in this case is self-contained and closely resembles the the Lorentzian situation. The following results are based on lemmas of Hall and McIntosh[8] in the Lorentzian case.

Lemma 4.1: If G and F are a pair of two forms on a finite dimensional vector space V such that

$$F(X,Y)G(Z,W)=F(Z,W)G(X,Y)$$

for all $X,Y,Z,W, \in V$ and F is nonzero, then there exists $\lambda \in \mathbb{R}$ such that $G=\lambda F$.

Proof: If we assume $F_{12}\neq 0$, then in some basis of V we have $G_{ij}F_{12}=G_{12}F_{ij}$ and therefore $G_{ij}=(G_{12}/F_{12})F_{ij}$. Take $\lambda=(G_{12}/F_{12})$ then $G_{ij}=\lambda F_{ij}$ for all i and j. □

Proposition 4.2: Suppose that the dimension of the ambient manifold M is at least four. The curvature tensor cannot be spanned by a single nondegenerate form, in the sense that if $R=\theta \otimes F$ where θ is an endomorphism field and F is a two-form, then F cannot be of maximal rank.

Proof: Relative to a not necessarily coordinate frame field we have in components that

$$R_{ijkl}=g_{in}\theta^n_j F_{kl}=G_{ij}F_{kl},$$

where $G_{ij}=g_{in}\theta^n_j$. Since $R_{ijkl}=R_{klij}$ then we find that

$$G_{ij}F_{kl}=G_{kl}F_{ij},$$

and by Lemma 4.1 we conclude that for some function λ

$$G_{ij}=\lambda F_{ij}.$$

Thus

$$R_{ijkl}=\lambda F_{ij}F_{kl}.$$

Since $R^{i}_{[jkl]}=0$ the above condition gives $F_{i[j}F_{kl]}=0$ which implies that F is decomposable hence singular. □

Corollary 4.3: None of $A_1(\alpha\beta\neq 0), A_2(\alpha\beta\neq 0), A_4, A_5(\alpha\neq 0), A_6, A_7, A_8(\alpha\neq 0)$ *are holonomy Lie algebras.*

Note also that the cases $A_1(\alpha=0)$ and $A_2(\alpha=0)$ are obviously holonomy algebras: take respectively the product of flat and nonflat two-dimensional Riemannian spaces (with signs adjusted to obtain neutral signature) and, after effecting the permutation switching the second and third basis vectors, the product of flat and nonflat two-dimensional Lorentzian spaces. □

Proposition 4.4: A_3 *is a holonomy algebra*

Proof: We take the metric to be the product of a special three-dimensional Lorentzian metric $2dxdz+dy^2+b(y,z)dz^2$ where b_{zz} in nonzero and $-dw^2$. The three-dimensional Lorentzian metric has a one-dimensional algebra[4] and ∂_x is a parallel null vector field. Thus the metric $-dw^2+2dxdz+dy^2+b(y,z)dz^2$ has one-dimensional holonomy with the algebraic type of A_3. □

Finally, note that the cases $A_5(\alpha=0)$ and $A_8(\alpha=0)$ are identical. Furthermore, this case is equivalent to A_9 by means of making the transformation on $\mathbb{R}^4$ that has matrix $\left[\begin{smallmatrix} I & 0 \\ 0 & K \end{smallmatrix}\right]$.

Proposition 4.5: A_9 *is a holonomy algebra.*

Proof: In this case there must be two orthogonal null parallel vector fields. We apply Corollary 3.2 (5) and deduce that the Riemann curvature [as a type (1,3) tensor] components R^{i}_{jkl} for fixed k and l are multiples of $\left[\begin{smallmatrix} 0 & J \\ 0 & 0 \end{smallmatrix}\right]$. Note that because $\partial/\partial x$ and $\partial/\partial x$ are parallel we have that

$$\nabla_W R(X,Y)\frac{\partial}{\partial x}=0$$

and

$$\nabla_W R(X,Y)\frac{\partial}{\partial y}=0$$

for arbitrary W,X and Y, which proves that the holonomy algebra is indeed one-dimensional. To obtain the generator in the form given in A_9 it is necessary to apply the transformation with matrix $1/\sqrt{2}\left[\begin{smallmatrix} I & I \\ I & -I \end{smallmatrix}\right]$ to $\mathbb{R}^4$. □

The entire situation for one-dimensional holonomy can be summarized very neatly by means of the following theorem.

Theorem 4.6: *The holonomy Lie algebra is one-dimensional if and only if the metric possesses two parallel vector fields.*

V. GEOMETRIC STRUCTURE OF THE SUBALGEBRAS

Of the algebras listed in Table I only A_{28} and A_{32} act irreducibly. Berger[1] classified the irreducible holonomy groups of pseudo-Riemannian manifolds. Actually there are a number of exceptions to Berger's list, but the dimensions of these groups are too high to concern us here. Furthermore, Berger assumes that the spaces concerned are not pseudo-Riemannian symmetric spaces which he discussed separately in Ref. 2. In a recent paper Berard-Bergery and Ikemakhen[11] listed all symmetric spaces for neutral metrics in dimension four. Of these spaces, $SO_{\circ}(2,3)/SO_{\circ}(2,2)$ gives an example where the holonomy algebra is A_{32}. Likewise $SU(1,1)/U(1,1)$ being irreducible must correspond to A_{28}.

TABLE II. The geometric structure of the subalgebras.

Geometric structure	Lie subalgebras
A null two-dimensional distribution D	$A_{12}, A_{19}, A_{24}, A_{29}, A_{31}$
Two null two-dimensional complementary distributions D_1, D_2	A_{15}, A_{21}, A_{27}
Two nondegenerate two-dimensional orthogonal distributions D_1, D_2	A_{14}, A_{16}
Two null two-dimensional distributions D_1, D_2 D_1 containing a parallel vector field and D_2 a recurrent vector field	A_{11}(with $\alpha=\pm 1$)
Two null two-dimensional distributions D_1 and D_2 each containing a recurrent vector field	$A_{10}, A_{11}(\alpha=\pm 1), A_{18}, A_{23}$
A null two-dimensional distribution D containing a recurrent vector field	$A_{13}, A_{25}, A_{26}, A_{30}$
A null two-dimensional distribution D containing one parallel vector field	A_{17}, A_{26}(with $\alpha=-1$)
One-dimensional and three-dimensional nondegenerate distributions D_1, D_2, with D_2 containing a null recurrent vector field.	$A_{20}(\beta=\pm 1)$

Since all the algebras except A_{28} and A_{32} in Table I are reducible the existence of such an algebra as a holonomy algebra implies that the associated metric will preserve various geometric structures. Since we have already considered A_1-A_9 we list below in Table II the geometric properties that a metric with a reducible holonomy algebra must have in the remaining cases, *provided it exists*.

VI. ELIMINATION OF SOME EASY CASES

In this section we shall discuss some of the cases in Table I where we can decide easily whether or not the algebra comes from a metric.

Proposition 6.1: $A_{14}, A_{16}, A_{20}(\beta=\pm 1)$ *and* A_{22} *are holonomy algebras.*

Proof: For A_{16} an equivalent pair of generators is $\left[\begin{smallmatrix} J & 0 \\ 0 & 0 \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} 0 & 0 \\ 0 & J \end{smallmatrix}\right]$. The existence of a metric follows from the local de Rham theorem: use a pair of nonflat two-dimensional Riemannian metrics with the signs adjusted so as to produce a neutral four-dimensional metric.

For A_{14} apply the permutation $e_2 \leftrightarrow e_3$ on $\mathbb{R}^4$. We then obtain the generators $\left[\begin{smallmatrix} L & 0 \\ 0 & 0 \end{smallmatrix}\right]$ and $\left[\begin{smallmatrix} 0 & 0 \\ 0 & L \end{smallmatrix}\right]$ for A_{14} and the inner product is $\left[\begin{smallmatrix} K & 0 \\ 0 & K \end{smallmatrix}\right]$. This time the de Rham theorem implies that we have a product of nonflat two-dimensional Lorentzian manifolds. Similarly A_{22} corresponds to the product of an irreducible three-dimensional Lorentzian metric and a one-dimensional flat factor adjusted so as to obtain a neutral signature.

In the case of $A_{20}(\beta=1)$ we have the product of a three-dimensional Lorentzian manifold, which has a recurrent null vector field that cannot be scaled so as to give a parallel field, and a one-dimensional factor with negative squared length. Similarly for $A_{20}(\beta=-1)$ we have the product of such a Lorentzian manifold and a one-dimensional factor with positive squared length. □

Proposition 6.2: A_{18}, A_{19} *are holonomy algebras.*

Proof: Consider the following metric on $\mathbb{R}^2$,

$$g = a dx^2 + 2c dx dy + b dy^2,$$

where a, b and c are functions of x and y. Now define

$$\overline{g} = 2a dx dz + 2c dz dy + 2b dw dy + (z a_x + w a_y) dx^2 + (z b_x + w b_y) dy^2 + 2(z c_x + w c_y) dx dy$$

on $\mathbb{R}^4 = T\mathbb{R}^2$ where (x,y,z,w) is the induced coordinate system. Then $\overline{g}$ is the complete lift of g.[20] It turns out that the curvature $\overline{R}$ of $\overline{g}$ is the complete lift of the curvature R of g. Furthermore, because g is two-dimensional, R is recurrent and hence so is $\overline{R}$. Assuming that g is not flat its

holonomy group is one-dimensional and the holonomy group of $\bar{g}$ is two-dimensional being in fact the tangent group of the group of g. For details see Ref. 20. It follows immediately that if g is Riemannian the holonomy algebra type of $\bar{g}$ is A_{19}.

If, however, g is Lorentzian and we assume that g is represented in some frame by the matrix L, then $\bar{g}$ is represented by $\left[\begin{smallmatrix}0 & L\\ L & 0\end{smallmatrix}\right]$ and the holonomy algebra has a basis consisting of $\left[\begin{smallmatrix}K & 0\\ 0 & K\end{smallmatrix}\right]$ and $\left[\begin{smallmatrix}0 & K\\ 0 & 0\end{smallmatrix}\right]$. The latter algebra is equivalent to A_{18} by means of the transformation of $\mathbb{R}^4$ whose matrix is $1/\sqrt{2}\left[\begin{smallmatrix}L & L\\ I & -I\end{smallmatrix}\right]$. □

We now consider the algebras $A_{10}, A_{11}, A_{15}, A_{21}, A_{23}$ and A_{27}. In each of these algebras there are two 'null, complementary invariant subspaces. This situation has been studied in Ref. 11. The authors use a normal form for such a metric, which was actually obtained by one of the present authors in Ref. 21. The normal form is valid in $2n$ dimensions for a metric with two null, complementary invariant distributions and comes down to the fact that the components of the metric are the second order derivatives of a single function. Berard-Bergery and Ikhemaken exhibit metrics for cases which correspond in our classification to $A_{10}, A_{11}, A_{12}, A_{15}, A_{18}, A_{23}$ and A_{27}. They also mention that the existence of a metric in case A_{21} follows from general results of Bryant.[3]

We conclude this section with examples for A_{30} and A_{31}. These examples are actually easy to find because they are generic cases within the class of metrics possessing the corressponding geometric structure. Furthermore, in both cases the curvature by itself generates the full holonomy algebra, the dimension of which is maximal given that the metrics in question possess that particular geometric structure.

Proposition 6.3: $A_{26}(\alpha=-1)$, A_{30} *and* A_{31} *are holonomy algebras.*

Proof: The algebra A_{31} can be obtained by a generic metric that satisfies the condition of Theorem 3.1 with $n=4$ and $r=2$. As a specific example take

$$g = dxdz + dydw + e^{2x}(dz^2 + dw^2).$$

It is easy to check that the five curvature matrices derived from g are linearly independent. Similarly generic metrics that satisfy the conditions of Corollary 3.2 (1) and (2) provide examples of the algebras $A_{26}(\alpha=-1)$ and A_{30}, respectively. □

Proposition 6.4: A_{17} *is a holonomy algebra.*

Proof: In this case we have an invariant null distribution containing a parallel null vector field and so we are in the situation of part 1 of Corollary 3.2. The corresponding nonzero curvature matrices are

$$R^i_{j24} = \begin{bmatrix} 0 & C_{yy} & 2CC_{yy} & R_{3424}+2CB_{yy} \\ 0 & B_{yy} & 2BC_{yy}-R_{3424} & 2BB_{yy} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -C_{yy} & -B_{yy} \end{bmatrix},$$

$$R^i_{j23} = \begin{bmatrix} 0 & A_{yy} & 2CA_{yy} & 2CC_{yy}+R_{3423} \\ 0 & C_{yy} & 2BA_{yy}-R_{3423} & 2BC_{yy} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -A_{yy} & -C_{yy} \end{bmatrix},$$

$$R^i_{j34} = \begin{bmatrix} 0 & -R_{2334} & -2CR_{2334} & -2CR_{2434}+R_{3434} \\ 0 & -R_{2434} & -2BR_{2334}-R_{3434} & -2BR_{2434} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & R_{2334} & R_{2434} \end{bmatrix},$$

where $A=\frac{1}{2}a, B=\frac{1}{2}b$ and $C=\frac{1}{2}c$.

All the matrices in A_{17} are nilpotent and so we must have that $B_{yy}=C_{yy}=C_{yw}-B_{yz}=0$, as a result of which R^i_{j24} becomes zero. In order to realize A_{17} as a holonomy algebra all that is needed now is that the covariant derivatives $R^i_{jkl;m}$ should bring in no new holonomy generators; and in order for that situation to occur all that is needed is for the components $R^2_{2kl;m}$ to vanish. One can easily check that in view of all the preceding hypotheses these conditions are satisfied identically. To summarize: A_{17} will be produced by generic metrics of the form given by part (1) of Corollary 3.2 for which in addition

$$b_{yy}=c_{yy}=c_{yw}-b_{yz}=0.$$

□

VII. THE ALGEBRAS A_{12} AND A_{24}

Proposition 7.1: Neither A_{12} nor A_{24} is a holonomy algebra.

Proof: In both cases we change the inner product to $\left[\begin{smallmatrix}0 & I\\ I & 0\end{smallmatrix}\right]$. The generators for A_{12} become $\left[\begin{smallmatrix}\alpha J+I & 0\\ 0 & \alpha J-I\end{smallmatrix}\right]$ and $\left[\begin{smallmatrix}0 & J\\ 0 & 0\end{smallmatrix}\right]$ and for A_{24} $\left[\begin{smallmatrix}J & 0\\ 0 & J\end{smallmatrix}\right]$, $\left[\begin{smallmatrix}I & 0\\ 0 & -I\end{smallmatrix}\right]$ and $\left[\begin{smallmatrix}0 & J\\ 0 & 0\end{smallmatrix}\right]$, respectively. In both cases $\left[\begin{smallmatrix}J & 0\\ 0 & J\end{smallmatrix}\right]$ commutes with each generator. It follows that we must in each case be looking at a pseudo-Kähler metric that keeps a null two-dimensional distribution D invariant.

We apply Walker's normal form to the five nonzero generators of the curvature. It is then easy to see that we can obtain A_{12} only in the case where all the second order derivatives of A, B and C with respect to x and y vanish and that we can never obtain A_{24}. Indeed each upper left hand 2×2 block in the generators must be a linear combination of I and J. In the case of A_{12} there are at least two dependence relations among the generators $R^i_{i13}, R^i_{j24}, R^i_{j23}$ and R^i_{j34} which implies that all the stated second order derivatives are zero. In the case of A_{24} it is easy to see that if any of the 2×2 blocks is zero, so are all the above-mentioned second derivatives. Hence there are again at least two dependence relations among the 2×2 blocks which again implies the vanishing of $A_{xx}, A_{xy}, A_{yy}, B_{xx}, B_{xy}, B_{yy}, C_{xx}$, C_{xy} and C_{yy}. Thus the curvature matrices span at most a two-dimensional subspace.

Given that the stated second order derivatives of A, B and C are zero we see that the connection of g is projectable via the submersion $(x,y,z,w)\mapsto(z,w)$. We can now apply Proposition 3.5 to conclude that both A_{12} and A_{24} are excluded as holonomy algebras. In the former case the generator $\alpha J-I$ on Q does not correspond to the holonomy of a two-dimensional metric. In the latter case we would have a two-dimensional holonomy algebra on Q isomorphic to $\mathrm{gl}(1,\mathbb{C})$. Thus the connection would correspond to the real and imaginary parts of a scalar holomorphic connection. Such a connection has Ricci symmetric only when it reduces to a metric connection and thus its holonomy algebra cannot be two-dimensional. □

VIII. THE ALGEBRAS $A_{13}, A_{25}, A_{26}(\alpha\neq -1)$

In this section we investigate the case where we have a single recurrent vector field that cannot be scaled so as to give a parallel field. We are thus looking at A_{13}, A_{25} and $A_{26}(\alpha\neq -1)$, the case A_{30} already having been dealt with.

Proposition 8.1: A_{13} is not a holonomy algebra in the cases where (i) $a_{xx}=a_{yy}=0$ or (ii) $b=a_{xw}=0$. (The generic case as explained below remains undecided.)

Proof: In this case following the notation of Corollary 3.2 we have that $b_x=c_x=0$. We now record the form of the curvature matrices that are possibly nonzero and write $\frac{1}{2}a, \frac{1}{2}b$ and $\frac{1}{2}c$ as A, B and C, respectively. Thus

$$R^i_{j13}=\begin{bmatrix} A_{xx} & A_{xy} & 2(AA_{xx}+CA_{xy}) & A_{xw}\\ 0 & 0 & 2CA_{xx}+2BA_{xy}-A_{xw} & 0\\ 0 & 0 & -A_{xx} & 0\\ 0 & 0 & -A_{xy} & 0\end{bmatrix}, \tag{8.1}$$

$$R^i_{j24}=\begin{bmatrix} 0 & C_{yy} & 2CC_{yy} & 2CB_{yy}+C_{yw}-B_{yz} \\ 0 & B_{yy} & 2BC_{yy}-C_{yw}+B_{yz} & 2BB_{yy} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -C_{yy} & -B_{yy} \end{bmatrix}, \tag{8.2}$$

$$R^i_{j23}=\begin{bmatrix} A_{xy} & A_{yy} & 2(AA_{xy}+CA_{yy}) & 2CC_{yy}+R_{3423} \\ 0 & C_{yy} & 2(CA_{xy}+BA_{yy})-R_{3423} & 2BC_{yy} \\ 0 & 0 & -A_{xy} & 0 \\ 0 & 0 & -A_{yy} & -C_{yy} \end{bmatrix}, \tag{8.3}$$

$$R^i_{j34}=\begin{bmatrix} -A_{xw} & -R_{2334} & -2(AA_{xw}+CR_{2334}) & 2C(B_{yz}-C_{yw})+R_{3434} \\ 0 & B_{yz}-C_{yw} & -2(CA_{xw}+BR_{2334})-R_{3434} & 2B(B_{yz}-C_{yw}) \\ 0 & 0 & A_{xw} & 0 \\ 0 & 0 & R_{2334} & C_{yw}-B_{yz} \end{bmatrix}. \tag{8.4}$$

The algebra A_{13} has a generator, unique up to scaling, that is singular and in fact nilpotent. It follows that

$$A_{xx}=B_{yy}=0. \tag{8.5}$$

Furthermore, any nonsingular generator in A_{13} has doubly degenerate eigenvalues which implies

$$A_{xy}=\pm C_{yy}, \tag{8.6}$$

$$A_{xw}=\pm(C_{yw}-B_{yz}). \tag{8.7}$$

It follows that R^i_{j13} and R^i_{j24} are proportional. Since the order of nilpotence of the singular generator is 2 we can distinguish two subcases

$$A_{xy}=0 \tag{8.8}$$

or

$$BA_{xy}-A_{xw}=0. \tag{8.9}$$

Note both A_{xy} and A_{xw} can be zero or else $\partial/\partial x$ would be parallel. If (8.9) holds, then to obtain A_{13} we must also have that

$$B^2A_{yy}-2BR_{2334}-R_{3434}=0, \tag{8.10}$$

whereas if (8.8) holds, then we must have that

$$A_{yy}=0. \tag{8.11}$$

Let us assume now that (8.9) holds and we use R^i_{j13} and R^i_{j34} as generators of A_{13}. Now one may check that $R^1_{113;m}$ vanishes in view of the given hypotheses. In order to obtain A_{13} we can therefore posit the existence of one-forms λ, μ and ν such that

$$R^i_{j13m}=\nu_m R^i_{j13} \tag{8.12}$$

and

$$R^i_{j34m}=\lambda_m R^i_{j13}+\mu_m R^i_{j34}. \tag{8.13}$$

In fact, by applying the second (differential) Bianchi identity to (8.12) and using (8.9) we can deduce that

$$\nu_m = \mu_m \tag{8.14}$$

and also that μ_1 is zero.

It turns out that (8.12) is satisfied identically and that (8.13) holds for $m=1$. The remaining conditions in (8.13) give three third order partial differential equation (PDE) conditions which have to be adjoined to (8.5)–(8.7), (8.9) and (8.10) as well as the vanishing of B_x and C_x. Analyzing this PDE system presents a considerable challenge and is probably best formulated as an exterior differential system. We hope to return to this problem at a later stage.

We now take up the case given by (8.8). We find now that the Levi-Civita connection projects via the submersion $(x,y,z,w)\mapsto(z,w)$. The curvature will also project to and so too will the Ricci tensor. The holonomy group of the projected connection must be one-dimensional since one of the generators for A_{13} is annihilated in the projection and so the projected Ricci tensor is recurrent and symmetric. Now according to Proposition 3.5 the two-dimensional connection is either a Levi-Civita connection or has a parallel vector field. However, the generator of the holonomy algebra on the quotient space is not semi-simple, and so the connection is not Levi-Civita and also A_{13} corresponds to the situation where g has no parallel vector field.

To finish Proposition 3.5 it remains to take care of the case where B and A_{xw} vanish. This situation is similar to the preceding paragraph but this time the connection projects via $(x,y,z,w)\mapsto(y,z)$. Again the connection on the quotient space cannot be Levi-Civita because it leaves a direction invariant. □

Proposition 8.2: A_{26} is a holonomy algebra.

Proof: Again A_{26} corresponds to the case where $\partial/\partial x$, say, is a recurrent vector field and we select our generators for A_{26} as combinations of $R^i_{j13}, R^i_{j23}, R^i_{j24}$ and R^i_{j34} given in (8.1)–(8.4). Now A_{26} has a semi-simple generator and two nilpotent ones. Furthermore, we cannot have all of A_{xx}, A_{xy}, and A_{xw} zero or else $\partial/\partial x$ will be parallel. Likewise if all of B_{yy}, C_{yy} and $C_{yw}-B_{yz}$ are zero, every generator will be singular and we must be in the case $\alpha=\pm 1$. Now the case $\alpha=-1$ has been discussed in Proposition 6.3. The case $\alpha=1$ will be discussed later. To obtain the algebra A_{26} we can assume then that

$$A_{xx}=B_{yy}=A_{xy}(C_{yz}-B_{yy})+A_{xw}C_{yy}=0. \tag{8.15}$$

Notice that R^i_{j24} is proportional to R^i_{j13} so our assumptions imply that the curvature spans A_{26}. We have to ensure now that the covariant derivatives $R^i_{jkl;m}$ produce no new generators and it is sufficient to show that no new generators with *semi-simple* parts occur. However, an easy calculation shows that any covariant derivative of the form $R^i_{ikl;m}$ (i fixed and no sum) is simply the ordinary derivative $R^i_{ikl,m}$. It follows that in considering the introduction of new generators from the derivatives $R^i_{jkl;m}$ we need only take into account $R^i_{j23;m}$ and $R^i_{j34;m}$. Thus the following conditions, in addition to the ones previously imposed, are necessary and sufficient to obtain the algebra A_{26}:

$$R^1_{123}R^2_{223;m}-R^2_{223}R^1_{123;m}=0, \tag{8.16}$$

$$R^1_{123}R^2_{234;m}-R^2_{223}R^1_{134;m}=0. \tag{8.17}$$

However, we can be even more explicit in this case. In fact, (8.17) can be written compactly as

$$\left(\frac{A_{xy}}{C_{yy}}\right),m=0, \tag{8.18}$$

where m denotes derivative with respect to each if the four coordinates x,y,z,w. Thus

$$A_x = kC_y + F(x,z,w), \tag{8.19}$$

where $k \in \mathbb{R}$ and F is a smooth function of its three arguments.

Turning next to (8.16) the first two conditions corresponding to $m=1$ and $m=2$ are already satisfied so that (8.16) gives in addition only

$$A_{xy}(C_{yw} - B_{yz})_z - C_{yy}A_{xzw} = 0, \tag{8.20}$$

$$A_{xy}(C_{yw} - B_{yz})_w - C_{yy}A_{xww} = 0. \tag{8.21}$$

However, note that in view of (8.15) and (8.19) both (8.20) and (8.21) will be satisfied identically. Note that if $A_{xy}=0$, then since A_{xw} cannot also vanish we must have that $C_{yy}=0$. Clearly all the conditions in (8.16) and (8.17) are satisfied in this case. We shall summarize all of these possibilities below.

We now come back to the other possibility at the beginning of the proof, namely, that all of B_{yy}, C_{yy} and $C_{yw} - B_{yz}$ are zero. If now the matrix M where

$$M = \begin{bmatrix} A_{xx} & A_{xy} & -A_{xw} \\ A_{xy} & A_{yy} & R_{2334} \\ -A_{xw} & R_{2334} & R_{3434} \end{bmatrix} \tag{8.22}$$

is nonsingular, then the curvature will determine the algebra A_{26}. But the same argument about the covariant derivatives of diagonal elements $R^i_{ikl;m}$ holds equally as above and so no additional semi-simple generator can be produced by the covariant derivatives $R^i_{jkl;m}$. Thus without any further conditions we can be sure that we will have A_{26} as the holonomy algebra.

The possibilities for obtaining the algebra A_{26} can be summarized by the following formulas: either

$$A = xH_y(y,z,w) + K(y,z,w), \tag{8.23}$$

$$kB = yN_w(x,z,w) + L(x,z,w), \tag{8.24}$$

$$kC = yN_z(x,z,w) + G(x,z,w) + H(y,z,w), \tag{8.25}$$

or

$$A = A(x,y,z,w) \tag{8.26}$$

with $\det(M) \neq 0$, where M is given by (8.22),

$$B = yN_w(x,z,w) + L(x,z,w), \tag{8.27}$$

$$kC = yN_z(x,z,w) + G(x,z,w), \tag{8.28}$$

where $k \in \mathbb{R}$ and the notion indicates the functions concerned are arbitrary smooth functions of the arguments indicated. □

Proposition 8.3: A_{25} is a holonomy algebra.

Proof: This case is very similar to A_{26}. Again starting from (8.1)–(8.4) to obtain A_{25} we shall need the following conditions to be satisfied:

$$A_{xx} = 0, \tag{8.29}$$

$$B_{yy} = 0, \tag{8.30}$$

$$A_{xy} - C_{yy} = 0, \tag{8.31}$$

$$A_{xw}-C_{yw}+B_{yz}=0. \tag{8.32}$$

Again when covariant derivatives of R^i_{jkl} are considered no new generators with a semi-simple part independent of the one already obtained can be produced and so the stated conditions are sufficient to obtain A_{25}. The conditions we have found to obtain A_{25} have the following solution in terms of arbitrary smooth functions:

$$A=xg_y(y,z,w)+h(y,z,w), \tag{8.33}$$

$$B=yf(w)-yk_w(z,w)+l(x,z,w), \tag{8.34}$$

$$C=g(y,z,w)-yk_z(z,w). \tag{8.35}$$

□

IX. THE ALGEBRAS A_{21} AND A_{29}

In this section we consider the algebras A_{29} and A_{21}

Proposition 9.1: A_{29} is not a holonomy algebra.

Proof: A metric g that has A_{29} as its holonomy algebra is characterized by the property that it keeps invariant a two-dimensional null distribution and that the upper left hand block 2×2 in the algebra is trace-free. We shall argue first of all that these conditions force the Levi-Civita connection to project via the submersion $(x,y,z,w)\mapsto(z,w)$ referring to Theorem 3.1. Recalling A, B and C stand for $\frac{1}{2}a$, $\frac{1}{2}b$ and $\frac{1}{2}c$, respectively, these conditions on the curvature matrices may be written as

$$A_{xx}+C_{xy}=0, \tag{9.1}$$

$$A_{xy}+C_{yy}=0, \tag{9.2}$$

$$C_{xy}+B_{yy}=0, \tag{9.3}$$

$$C_{xx}+B_{xy}=0, \tag{9.4}$$

$$R_{1334}+R_{2434}=0. \tag{9.5}$$

Now the covariant derivatives of the curvature $R^i_{jkl;m}$ must have the same trace-free property. We thus obtain precisely the following conditions:

$$C_yC_{xx}-B_xA_{xy}=0, \tag{9.6}$$

$$C_yB_{xy}-C_{yy}B_x=0, \tag{9.7}$$

$$C_yC_{xy}-A_{yy}B_x=0, \tag{9.8}$$

$$C_yB_{xx}-C_{xy}B_x=0, \tag{9.9}$$

$$C_yR_{1434}-B_xR_{2334}=0, \tag{9.10}$$

$$A_yC_{xx}-A_{xy}C_x=0, \tag{9.11}$$

$$A_xB_{xy}-C_{yy}C_x=0, \tag{9.12}$$

$$A_yC_{xy}-A_{yy}C_x=0, \tag{9.13}$$

$$A_yB_{xx}-C_{xy}C_x=0, \tag{9.14}$$

$$A_y R_{1434} - C_x R_{2334} = 0. \tag{9.15}$$

The argument now depends on whether the quantity $C_x C_y - A_y B_x$ is zero or nonzero. In the latter case it is easy to see from (9.1)–(9.4), (9.6)–(9.9) and (9.11)–(9.14) that all second order derivatives of A, B and C, respectively, vanish and hence the connection of g is projectable.

Now suppose that $C_x C_y - A_y B_x$ is zero. Then using the condition itself and (9.7), (9.9), (9.11) and (9.13) we deduce that

$$B_x = \theta(z,w) C_y, \tag{9.16}$$

$$A_y = \theta(z,w) C_x \tag{9.17}$$

for some smooth function θ of z and w. Again because $C_x C_y - A_y B_x$ is zero we find from (9.16) and (9.17) that

$$\theta = \pm 1. \tag{9.18}$$

In what follows we shall take the positive value in (9.18). We shall come back to the negative value later.

From (9.16) and (9.17) with θ having the value unity we can assert the existence of a function ρ such that

$$A = \rho_{xx}, \tag{9.19}$$

$$B = \rho_{yy}, \tag{9.20}$$

$$C = \rho_{xy}. \tag{9.21}$$

One can now see that (9.6)–(9.9) and (9.11)–(9.14) are satisfied identically and that (9.1)–(9.4) imply precisely that ρ satisfies

$$\Delta \rho = \theta(z,w) x + \varphi(z,w) y + \psi(z,w) \tag{9.22}$$

for some functions θ, φ and ψ of z and w where Δ denotes the Laplacian operator with respect to the x,y variables. It remains to satisfy (9.5), (9.10) and (9.15). Condition (9.5) implies that there exists a function σ such that

$$\theta = \sigma_z,$$

$$\varphi = \sigma_w.$$

Equation (9.22) may be integrated twice to give

$$8\rho = (\theta(z,w) x + \varphi(z,w) y)(x^2 + y^2) + p(x,y), \tag{9.23}$$

where $p(x,y)$ is a a quadratic polynomial in x and y. Finally we come to (9.10), (9.15) being essentially the same as (9.10). In terms of ρ (9.10) reads

$$(\rho_{xxy})^2 - \rho_{xxx}\rho_{xyy} + (\rho_{xyy})^2 - \rho_{xxy}\rho_{yyy} = 0. \tag{9.24}$$

When (9.23) is substituted into (9.24) we find finally that

$$\theta^2 + \varphi^2 = 0, \tag{9.25}$$

and hence both θ and φ vanish. Thus ρ is quadratic in x and y and A, B and C are independent of x and y. It follows that the Levi-Civita connection of g projects via the submersion $(x,y,z,w)\mapsto(z,w)$ to a flat connection, there are two parallel one-forms associated to g and we certainly do not obtain algebra A_{29}.

We return now to (9.18) and take θ to be -1. The analysis is very similar to the case where θ is 1 so we shall proceed quickly using similar notation. Thus we now have

$$A=\rho_{xx}, \tag{9.26}$$

$$B=\rho_{yy}, \tag{9.27}$$

$$C=-\rho_{xy}. \tag{9.28}$$

The analog of (9.23) now is

$$\rho=\tfrac{1}{2}(x\sigma_w+y\sigma_z)xy+q(x,y), \tag{9.29}$$

where $q(x,y)$ is a quadratic polynomial in x and y. The analog of (9.24) reads

$$\rho_{xxx}\rho_{xyy}-\rho_{yyy}\rho_{xxy}+(\rho_{xyy})^2-(\rho_{xxy})^2=0. \tag{9.30}$$

When (9.29) is substituted in (9.30) we find in contradiction to (9.25) that

$$\sigma_z^2=\sigma_w^2, \tag{9.31}$$

so the solution for A, B and C is given by

$$A=y\tau, \tag{9.32}$$

$$B=x\tau, \tag{9.33}$$

$$C=-(x+y)\tau, \tag{9.34}$$

where $\tau=\sigma'$ is a function of $z+w$. Now the connection corresponding to (9.32)–(9.34) is clearly projectable via the submersion $(x,y,z,w)\mapsto(z,w)$ and the projected connection is given by

$$\ddot{z}=\tau(\dot{w}^2-2\dot{z}\dot{w}), \tag{9.35}$$

$$\ddot{w}=\tau(\dot{z}^2-2\dot{z}\dot{w}). \tag{9.36}$$

The Ricci tensor of the connection corresponding to (9.35) and (9.36) is symmetric only in the case where τ is a function of $z+w$. However, in that case the connection is Levi-Civita with metric given by

$$\overline{g}=e^{\tau}(dz^2-dzdw+dw^2). \tag{9.37}$$

It follows that the holonomy algebra of g is two-dimensional and so A_{29} cannot occur as a holonomy algebra. □

Corollary 9.2: A_{21} cannot occur as a holonomy algebra.

Proof: We note that A_{21} is a three-dimensional subalgebra of A_{29} and so has the same characteristic trace-free property. Thus the argument is the same as in Proposition 9.1. □

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Yangian construction of a centrally extended Lie algebra of a diffeomorphism group of a torus

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I. INTRODUCTION

Recently, Lie algebras of an area preserving diffeomorphism group of two-dimensional regions received a lot of attention.

Algebras of an area preserving diffeomorphisms play an important role in the theory of a classical and quantum W-gravity,[1] W-string theory.[2]

In Ref. 3 based on a special deformation method applied to an area preserving diffeomorphism algebra of a two dimensional region it was obtained a centralles realization of W_∞ algebra.

In Ref. 4 Arnold studied a model of ideal liquid on a two dimensional region D. The area preserving diffeomorphism group of the region D is a configuration space for the model. In Ref. 4 it was given a detailed analysis of an algebraic structure of the Lie algebra of an area preserving diffeomorphism group of a torus $\mathrm{diff}(T^2)$.

In this paper we construct a Yangian algebra of a centrally extended Lie algebra of an area preserving diffeomorphism group of a two dimensional torus $Y(\mathrm{diff}(T^2)_c)$.

Yangian algebra is example of noncommutative, noncocommutative Hopf algebra (quantum group) and was introduced by Drinfeld in Ref. 5 as a deformation of a universal enveloping algebra $U(g[\lambda])$ of a loop extended simple Lie algebra g.

Yangian algebras are related to a rational solution of a classical Yang–Baxter equation. Each solution of a classical Yang–Baxter equation on a given Lie algebra g determines a Lie bialgebra structure on g. Lie bialgebras may be thought of as a classical limit for quantum groups. A general method of quantization of Lie bialgebras was given in Ref. 5.

In this paper we will follow Drinfeld's method of quantization of Lie bialgebras and apply it to the construction of a Yangian algebra for the $\mathrm{diff}(T^2)_c$ algebra. Yangian algebra $Y(\mathrm{diff}(T^2)_c)$ is a deformation of loop extended $\mathrm{diff}(T^2)_c$ algebra, i.e., a set of all polynomial mappings

$$g: S^1 \to \mathrm{diff}(T^2)_c,$$

where S^1 is a unit circle.

A Lie bialgebra structure on $\mathrm{diff}(T^2)_c[\lambda]$ is determined by a cocommutator mapping ϕ

$$\phi: \mathrm{diff}(T^2)_c[\lambda] \to \mathrm{diff}(T^2)_c[\lambda] \otimes \mathrm{diff}(T^2)_c[\lambda],$$

satisfying a 1-cocycle condition

$$ad_x \phi(y) - ad_y \phi(x) = \phi([x,y]), \tag{1}$$

for $x,y,z \in \mathrm{diff}(T^2)_c[\lambda]$, $ad_x(y \otimes z) = [x \otimes 1 + 1 \otimes x, y \otimes z]$.

In Sec. II we construct a cocommutator mapping ϕ with the help of a new solution of classical Yang–Baxter equation on $\mathrm{diff}(T^2)_c[\lambda]$.

In Sec. III we quantize constructed Lie bialgebra. As a result, we obtain a Yangian algebra $Y(\mathrm{diff}(T^2)_c[\lambda])$ and its quantum double $DY(\mathrm{diff}(T^2)_c[\lambda])$. We give also an asymptotic form of a quantum R-matrix for $DY(\mathrm{diff}(T^2)_c[\lambda])$.

II. LIE BIALGEBRA STRUCTURE ON $\mathrm{diff}(T^2)_c[\lambda]$

Let us denote by $\mathrm{diff}(T^2)'_c[\lambda]$ an algebra generated by $g_{\bar{m}}\lambda^M$, $c\lambda^M$, $\bar{m}\in Z\times Z$, $M\in Z$ satisfying the following commutation relations:

$$[q_{\bar{m}}\lambda^M, q_{\bar{n}}\lambda^N] = \omega(\bar{m},\bar{n}) q_{\bar{m}+\bar{n}}\lambda^{M+N} + |\bar{m}|\,\delta_{\bar{m}+\bar{n},0} c\lambda^{M+N}, \tag{2}$$

$$[c\lambda^M, q_{\bar{m}}\lambda^N] = 0, \tag{3}$$

where $\omega(\bar{m},\bar{n}) := m_1 n_2 - n_1 m_2$, $|\bar{m}| := m_1 + m_2$, and $\delta_{\bar{m}+\bar{n},0} := \delta_{m_1+n_1,0}\,\delta_{m_2+n_2,0}$. To the algebra $\mathrm{diff}(T^2)'_c[\lambda]$ we add a set of new generators $d\lambda^M$, $M\in Z$ satisfying

$$[d\lambda^M, q_{\bar{m}}\lambda^N] = |\bar{m}| q_{\bar{m}}\lambda^{M+N} \quad [c\lambda^M, d\lambda^N] = 0. \tag{4}$$

The algebra defined by (2), (3), and (4) is a centrally extended Lie algebra of a diffeomorphism group of a torus. We denote it by $\mathrm{diff}(T^2)_c[\lambda]$.

We define an operator $r(\lambda,\mu)\in \mathrm{diff}(T^2)_c[\lambda]\otimes\mathrm{diff}(T^2)_c[\lambda] \equiv \mathrm{diff}(T^2)_c\otimes\mathrm{diff}(T^2)_c[\lambda,\mu]$ in the following way:

$$r(\lambda,\mu) = \frac{1}{\lambda-\mu}\left(\sum_{\bar{m}\in Z\times Z} q_{-\bar{m}}\otimes q_{\bar{m}} + d\otimes c + c\otimes d\right).$$

It is easy to check that $r(\lambda,\mu)$ satisfies a classical Yang–Baxter equation

$$[r_{12}(\lambda,\mu), r_{13}(\lambda,\nu)] + [r_{12}(\lambda,\mu), r_{23}(\mu,\nu)] + [r_{13}(\lambda,\nu), r_{23}(\nu,\mu)] = 0,$$

where $r_{12}(\lambda,\mu) = r(\lambda,\mu)\otimes 1$, $r_{23}(\mu,\nu) = 1\otimes r(\mu,\nu)$ $r_{13}(\lambda,\nu) = 1/\lambda-\nu\,(\Sigma_{\bar{m}\in Z\times Z} q_{-\bar{m}}\otimes 1\otimes q_{\bar{m}} + d\otimes 1\otimes c + c\otimes 1\otimes d)$.

The cocommutator mapping ϕ determined by $r(\lambda,\mu)$ has the form

$$\phi(q_{\bar{m}}\lambda^M) = [r(\lambda,\mu), q_{\bar{m}}\lambda^M\otimes 1 + 1\otimes q_{\bar{m}}\mu^M],$$

$$\phi(d\lambda^M) = [r(\lambda,\mu), d\lambda^M\otimes 1 + 1\otimes d\mu^M],$$

$$\phi(c\lambda^M) = 0.$$

It is straightforward to verify that ϕ satisfies a 1-cocycle condition (1). This means that a pair $(\mathrm{diff}(T^2)_c[\lambda],\phi)$ is a Lie bialgebra.

Quantization of the $(\mathrm{diff}(T^2)_c[\lambda],\phi)$ Lie bialgebra we perform in three steps.

First, we quantize the $(\mathrm{diff}(T^2)'_c[\lambda]_+,\phi)$ Lie bialgebra, generated by $g_{\bar{m}}\lambda^M$, $c\lambda^M$, $\bar{m}\in Z\times Z$, $M\geqslant 0$. As a result we obtain a Yangian algebra $Y(\mathrm{diff}(T^2)'_c[\lambda])$.

In the second step we quantize the $(\mathrm{diff}(T^2)'_c[\lambda]_-,\phi)$ Lie bialgebra generated by $g_{\bar{m}}\lambda^M$, $c\lambda^M$, $\bar{m}\in Z\times Z$, $M<0$. Quantization of this Lie bialgebra we denote by $Y^*(\mathrm{diff}(T^2)'_c[\lambda])$.

Separately we will discuss quantization of the $d\lambda^M$, $\in Z$ generators.

III. YANGIAN ALGEBRA $Y(\mathrm{diff}(T^2)'_c)$

The algebra $Y(\mathrm{diff}(T^2)'_c)$ is generated by $Q_{\bar{m},}$ M, c_M, $\bar{m}\in Z\times Z$, $M\geqslant 0$ which depend on a quantum parameter h such that

$$\lim_{h\to 0}(Q_{\bar{m},M}, c_M) = (q_{\bar{m}}\lambda^M, c\lambda^M).$$

The algebra $Y(\mathrm{diff}(T^2)'_c)$ is endowed with a counit $\varepsilon(Q_{\bar{m},M})=0$, $\varepsilon(c_M)=0$, and a coassociative comultiplication Δ which in classical limit gives the cocommutator ϕ

$$\lim_{h\to 0}\frac{1}{h}(\Delta-\Delta')=\phi,$$

where Δ' denotes the transposed comultiplication, i.e., for $\Delta(a)=b\otimes c$, $\Delta'(a)=c\otimes b$. Unfortunately an antipodal mapping S does not exist for the $Y(\mathrm{diff}(T^2)'_c[\lambda])$ algebra. It means that quantization of the $(\mathrm{diff}(T^2)'_c[\lambda]_+,\phi)$ Lie bialgebra leads to a noncommutative, noncocommutative bialgebra.

The classical algebra $\mathrm{diff}(T^2)'_c[\lambda]_+$ can be generated by $q_{\bar{m}}$, c, $q_{\bar{m}}\lambda$, $c\lambda$, $\bar{m}\in Z\times Z$. We describe quantization of the $(\mathrm{diff}(T^2)'_c[\lambda]_+,\phi)$ Lie bialgebra in terms of quantum generators $Q_{\bar{m},0}=g_{\bar{m}}$, $c_0=c$, $Q_{\bar{m},1}$, c_1.

Lemma: An algebra $Y(\mathrm{diff}(T^2)'_c)$ generated by $q_{\bar{m}},Q_{\bar{m},1}$ having the following properties:

$$[q_{\bar{m}},q_{\bar{n}}]=\omega(\bar{m},\bar{n})q_{\bar{m}+\bar{n}}+|\bar{m}|\,\delta_{\bar{m}+\bar{n},0}c, \tag{5}$$

$$[q_{\bar{m}},Q_{\bar{n},1}]=\omega(\bar{m},\bar{n})Q_{\bar{m}+\bar{n},1}+|\bar{m}|\,\delta_{\bar{m}+\bar{n},0}c_1, \tag{6}$$

$$[Q_{\bar{m},1},[Q_{\bar{n},1},q_{\bar{k}}]]-[q_{\bar{m}},[Q_{\bar{n},1},Q_{\bar{k},1}]$$

$$=\frac{1}{12}h^2\sum_{\bar{l},\bar{f}\in Z\times Z}\alpha^{\bar{f},\bar{l}}_{\bar{m},\bar{n},\bar{k}}\{q_{\bar{m}+\bar{n}+\bar{k}-\bar{l}-\bar{f}},q_{\bar{f}},q_{\bar{l}}\}_+ +\frac{1}{16}h^2\sum_{\bar{l}\in Z\times Z}\tilde{\alpha}^{\bar{l}}_{\bar{m},\bar{n},\bar{k}}\{q_{\bar{m}+\bar{n}+\bar{k}-\bar{l}},q_{\bar{l}}\}_+c$$
$$+\frac{1}{4}h^2\tilde{\alpha}_{\bar{m},\bar{n},\bar{k}}q_{\bar{m}+\bar{n}+\bar{k}}c^2+\frac{1}{12}h^2|\bar{m}||\bar{n}||\bar{k}|(\omega(\bar{m},\bar{n})+\omega(\bar{n},\bar{k})+\omega(\bar{k},\bar{m}))\,\delta_{\bar{m}+\bar{n}+\bar{k},0}c^3, \tag{7}$$

with a comultiplication

$$\Delta(q_{\bar{m}})=q_{\bar{m}}\otimes 1+1\otimes q_{\bar{m}},$$

$$\Delta(c)=c\otimes 1+1\otimes c,\quad \Delta(c_1)=c_1\otimes 1+1\otimes c_1,$$

$$\Delta(Q_{\bar{m},1})=Q_{\bar{m},1}\otimes 1+1\otimes Q_{\bar{m},1}+\frac{1}{2}h\sum_{\bar{k}\in Z\times Z}\omega(\bar{m},\bar{k})q_{\bar{m}-\bar{k}}\otimes q_{\bar{k}}+\frac{1}{2}h|\bar{m}|(q_{\bar{m}}\otimes c-c\otimes q_{\bar{m}})$$

and a counit

$$\varepsilon(q_{\bar{m}})=0,\quad \varepsilon(Q_{\bar{m},1})=0,\quad \varepsilon(c)=0,\quad \varepsilon(c_1)=0$$

is a bialgebra.

In (7), $\{q_{\bar{m}_1},\ldots,q_{\bar{m}_n}\}_+=1/n!\,\Sigma_{\sigma\in S_n}q_{\sigma(\bar{m}_1)},\ldots,q_{\sigma(\bar{m}_n)}$, where S_n is a permutation group of n elements $(\bar{m}_1,\ldots,\bar{m}_n)$. Exact form of the coefficients $\alpha^{\bar{f},\bar{l}}_{\bar{m},\bar{n},\bar{k}}$, $\tilde{\alpha}^{\bar{l}}_{\bar{m},\bar{n},\bar{k}}$, $\tilde{\alpha}_{\bar{m},\bar{n},\bar{k}}$ is given in the appendix.

The formula (7) can be obtained from (5), and (6), Jacobi identity and the relation

$$[Q_{\bar{m},1},Q_{\bar{n},1}]=\omega(\bar{m},\bar{n})Q_{\bar{m}+\bar{n},2}+|\bar{m}|\,\delta_{\bar{m}+\bar{n},0}c_2+\frac{1}{12}h^2\underline{\sum_{k,l\in Z\times Z}}\beta^{\bar{k},\bar{l}}_{\bar{m},\bar{n}}\{q_{\bar{m}+\bar{n}-\bar{k}-\bar{l}},q_{\bar{k}},q_{\bar{l}}\}_+$$
$$-\frac{1}{8}h^2(|\bar{m}|-|\bar{n}|)\underline{\sum_{k\in Z\times Z}}\omega(\bar{m},\bar{k})\omega(\bar{n},\bar{k})\{q_{\bar{m}+\bar{n}-\bar{k}},q_{\bar{k}}\}_+c$$
$$-\frac{1}{8}h^2\omega(\bar{m},\bar{n})\underline{\sum_{k\in Z\times Z}}(\omega(\bar{m},\bar{k})|\bar{m}|+\omega(\bar{n},\bar{k})|\bar{n}|)\{q_{\bar{m}+\bar{n}-\bar{k}},q_{\bar{k}}\}_+c$$
$$-\frac{1}{4}h^2\omega(\bar{m},\bar{n})|\bar{m}||\bar{n}|q_{\bar{m}+\bar{n}}c^2-\frac{1}{12}h^2|\bar{m}|^3\delta_{\bar{m}+\bar{n},0}c^3. \tag{8}$$

Another way to obtain (7) is to use (5), and (6) and

$$[q_{\bar{m}},Q_{\bar{n},2}]=\omega(\bar{m},\bar{n})Q_{\bar{m}+\bar{n},2}+|\bar{m}|\,\delta_{\bar{m}+\bar{n},0}c_2+\frac{1}{12}h^2\underline{\sum_{k,l\in Z\times Z}}\tilde{\beta}^{\bar{k},\bar{l}}_{\bar{m},\bar{n}}\{q_{\bar{m}+\bar{n}-\bar{k}-\bar{l}},q_{\bar{k}},q_{\bar{l}}\}_+$$
$$+\frac{1}{8}h^2\underline{\sum_{k\in Z\times Z}}\tilde{\tilde{\beta}}_{\bar{m},\bar{n},\bar{k}}\{q_{\bar{m}+\bar{n}-\bar{k}},q_{\bar{k}}\}_+c$$
$$+\frac{1}{8}h^2\omega(\bar{m},\bar{n})|\bar{m}||\bar{n}|q_{\bar{m}+\bar{n}}c^2-\frac{1}{12}h^2|\bar{m}|^3\delta_{\bar{m}+\bar{n},0}c^3. \tag{9}$$

Explicit form of the coefficients $\beta^{\bar{k},\bar{l}}_{\bar{m},\bar{n}}$, $\tilde{\beta}^{\bar{k},\bar{l}}_{\bar{m},\bar{n}}$, $\tilde{\tilde{\beta}}_{\bar{m},\bar{n},\bar{k}}$ is given in the appendix.

The comultiplication for the elements $Q_{\bar{m},2}$ has the following form:

$$\Delta(Q_{\bar{m},2})=Q_{\bar{m},2}\otimes 1+1\otimes Q_{\bar{m},2}+\frac{1}{2}h\underline{\sum_{k\in Z\times Z}}\omega(\bar{m},\bar{k})(Q_{\bar{m}-\bar{k},1}\otimes q_{\bar{k}}-q_{\bar{k}}\otimes Q_{\bar{m}-\bar{k},1})$$
$$+\frac{1}{2}h|\bar{m}|(Q_{\bar{m},1}\otimes c-c\otimes Q_{\bar{m},1}+q_{\bar{m}}\otimes c_1-c_1\otimes q_{\bar{m}})$$
$$-h^2\frac{1}{8}\underline{\sum_{k,l\in Z\times Z}}\gamma^{\bar{k},\bar{l}}_{\bar{m}}(\{q_{\bar{k}},q_{\bar{l}}\}_+\otimes q_{\bar{m}-\bar{k}-\bar{l}}+q_{\bar{m}-\bar{k}-\bar{l}}\otimes\{q_{\bar{k}},q_{\bar{l}}\}_+)$$
$$+\frac{1}{8}h^2|\bar{m}|\underline{\sum_{k\in Z\times Z}}\omega(\bar{m},\bar{k})(q_{\bar{m}-\bar{k}}\otimes cq_{\bar{k}}+q_{\bar{k}}c\otimes q_{\bar{m}-\bar{k}})$$
$$+\frac{1}{16}h^2\underline{\sum_{k\in Z\times Z}}\omega(\bar{m},\bar{k})(2|\bar{k}|-|\bar{m}|)(\{q_{\bar{m}-\bar{k}},q_{\bar{k}}\}_+\otimes c+c\otimes\{q_{\bar{m}-\bar{k}},q_{\bar{k}}\}_+)$$
$$-\frac{1}{4}h^2|\bar{m}|^2(c\otimes cq_{\bar{m}}+q_{\bar{m}}c\otimes c), \tag{10}$$

where $\gamma^{\bar{k},\bar{l}}_{\bar{m}}$ is given in the appendix.

Relations (5), (6), and (7) uniquely determine commutation relations and comultiplication for all $Q_{\bar{m},M}$, $\bar{m}\in Z\times Z$, $M\geqslant 0$.

Quantization of the $(\mathrm{diff}(T^2)'_c[\lambda]_-,\phi)$ Lie bialgebra is much more complicated. We denote the algebra generated by $Q_{\bar{m},-M}$, c_{-M}, $\bar{m}\in Z\times Z$, $M>0$ by $Y^*(\mathrm{diff}(T^2)'_c)$. The comultiplication $\Delta(Q_{\bar{m},-M})$, $\bar{m}\in Z\times Z, M>0$, and commutation relations for $Q_{\bar{m},-M}$ are an infinite power series in quantum parameter h and defining relations for $Y^*(\mathrm{diff}(T^2)'_c)$, similar to (7) cannot be given. All formulas, i.e., comultiplication and commutation relations can be given only asymptotically.

Up to second order terms in h the algebra $Y^*(\mathrm{diff}(T^2)'_c)$ is defined by the following commutation relations:

$$[Q_{\overline{m},-M},Q_{\overline{n},-N}]=\omega(\overline{m},\overline{n})Q_{\overline{m}+\overline{n},-M-N}+|\overline{m}|\,\delta_{\overline{m}+\overline{n},0}c_{-M-N}+O(h^2),$$

$\overline{m},\ \overline{n}\in Z\times Z,\ M,\ N>0$. The bialgebra structure on $Y^*(\mathrm{diff}(T^2)'_c)$ is given by the counit

$$\varepsilon(Q_{\overline{m},-M})=0,\quad \varepsilon(c_{-M})=0$$

and the comultiplication $\Delta(Q_{\overline{m},-M})$, $\overline{m}\in Z\times Z,\ M>0$,

$$\Delta(Q_{\overline{m},-M})=Q_{\overline{m},-M}\otimes 1+1\otimes Q_{\overline{m},-M}-\frac{1}{2}h\sum_{i=0}^{M-1}\sum_{\overline{k}\in Z\times Z}\omega(\overline{m},\overline{k})Q_{\overline{m}-\overline{k},-i-1}\otimes Q_{\overline{k},i-M}$$
$$-\frac{1}{2}h|\overline{m}|\sum_{i=0}^{M-1}(Q_{\overline{m},-i-1}\otimes c_{i-M}-c_{-i-1}\otimes Q_{\overline{m},i-M})+O(h^2).$$

It is possible to determine commutation relations between elements of $Y(\mathrm{diff}(T^2)'_c)$ and $Y^*(\mathrm{diff}(T^2)'_c)$. The simplest formulas read

$$[q_{\overline{m}},Q_{\overline{n},-1}]=\omega(\overline{m},\overline{n})Q_{\overline{m}+\overline{n},-1}+|\overline{m}|\,\delta_{\overline{m}+\overline{n},0}c_{-1}+O(h^3)$$

or

$$Q_{\overline{m},1},Q_{\overline{n},-1}]=\omega(\overline{m},\overline{n})q_{\overline{m}+\overline{n}}+|\overline{m}|\,\delta_{\overline{m}+\overline{n},0}c+O(h^2).$$

Quantum generators d_M, $M\in Z$, which in classical limit are equal to $d\lambda^M$ cannot be written as a commutator of elements of $Y(\mathrm{diff}(T^2)_c)$ or $Y^*(\mathrm{diff}(T^2)_c)$. This implies that there is no general formula for comultiplication and commutation relations for quantum generators d_M, $M\in Z$. From $\phi(d)=0$ follows that the comultiplication $\Delta(d)$ is undeformed,

$$\Delta(d)=d\otimes 1+1\otimes d,$$

where $d=d_0$. The comultiplication $\Delta(d_M)$ $M>0$ up to linear terms in the quantum parameter h has the form

$$\Delta(d_M)=d_M\otimes 1+1\otimes d_M+\frac{1}{2}h\sum_{i=0}^{M-1}\sum_{\overline{k}\in Z\times Z}|\overline{k}|Q_{-\overline{k},M-i-1}\otimes Q_{\overline{k},i}+O(h^2),\tag{11}$$

and is a finite power series in h. For example, for $M=1$ formula (11) is exact

$$\Delta(d_1)=d_1\otimes 1+1\otimes d_1+\frac{1}{2}h\sum_{\overline{k}\in Z\times Z}|\overline{k}|q_{-\overline{k}}\otimes q_{\overline{k}}.$$

The comultiplication $\Delta(d_M)$, $M<0$ is an infinite power series in the quantum parameter h. Up to the linear terms it has the following form:

$$\Delta(d_{-M})=d_{-M}\otimes 1+1\otimes d_{-M}-\frac{1}{2}h\sum_{i=0}^{M-1}\sum_{\overline{k}\in Z\times Z}|\overline{k}|Q_{-\overline{k},-i-1}\otimes Q_{\overline{k},i-M}+O(h^2).$$

The commutation relations for d_M, $M\in Z$ asymptoticaly can be written as

$$[d_M,d_N]=0+O(h^2)$$

and

$$[d_M, Q_{\bar{m},N}] = |\bar{m}| Q_{\bar{m},M+N} + O(h^2).$$

Quantization of the $(\mathrm{diff}(T^2)'_c[\lambda]_-, \phi)$ Lie bialgebra is equivalent to a construction of an algebra called a quantum double for $Y(\mathrm{diff}(T^2)_c)$. If we introduce in the quantum space spanned by $Q_{\bar{m},M}, c_M, d_M$, $\bar{m} \in Z \times Z, M \in Z$ the following scalar product

$$< Q_{\bar{m},M}, Q_{\bar{n},N} > = \delta_{\bar{m},\bar{n}} \delta_{M+N+1,0},$$

$$< d_M, c_N > = \delta_{M+N+1,0},$$

then with respect to this scalar product the algebras $Y(\mathrm{diff}(T^2)_c)$ and $Y^*(\mathrm{diff}(T^2)_c)$ are dual. The pair $(Y(\mathrm{diff}(T^2)_c), Y^*(\mathrm{diff}(T^2)_c))$ is called a quantum double $DY(\mathrm{diff}(T^2)_c)$.

Having defined the Yangian algebra $Y(\mathrm{diff}(T^2)_c)$ and its quantum double $DY(\mathrm{diff}(T^2)_c)$ we would like to discuss existence of a quantum R-matrix for $DY(\mathrm{diff}(T^2)_c)$. A comultiplication defined on the quantum algebra $DY(\mathrm{diff}(T^2)_c)$ can be replaced by a transposed comultiplication Δ'. In this way we obtain another bialgebra structure on $DY(\mathrm{diff}(T^2)_c)$. These two structures are connected by a transformation called quantum R-matrix,

$$R\Delta = \Delta' R.$$

It has an asymptotic form

$$R = 1 \otimes 1 - h \sum_{M=0}^{\infty} \left(\sum_{\bar{k} \in Z \times Z} Q_{-\bar{k},-M-1} \otimes Q^{\bar{}}_{\bar{k},M} + d_{-M-1} \otimes c_M + c_{-M-1} \otimes d_M \right) + O(h^2).$$

IV. CONCLUDING REMARKS

In this paper we discussed a quantization of a loop extended Lie algebra of a diffeomorphism group of a two dimensional torus with a central extension. We found a new solution of a classical Yang–Baxter equation $r(\lambda, \mu)$ on the $\mathrm{diff}(T^2)_c[\lambda]$ Lie algebra. Using this solution we constructed a Lie bialgebra structure on $\mathrm{diff}(T^2)_c[\lambda]$ and quantized it by applying Drinfeld's method of quantization of Lie bialgebras. As a result, we obtained a Yangian algebra $Y(\mathrm{diff}(T^2)_c)$ and its dual $Y^*(\mathrm{diff}(T^2)_c)$.

The main result of this paper is formulated in the lemma, Sec. III. According to this lemma $Y(\mathrm{diff}(T^2)'_c)$ is a bialgebra. It means that on $Y(\mathrm{diff}(T^2)'_c)$ is defined a coassociative comultiplication Δ and a counit ε. Unfortunately the antipodal mapping S, defined by the formula

$$m(S \otimes 1)\Delta = \varepsilon \tag{12}$$

does not exist, i.e., there is no Hopf algebra structure on the $Y(\mathrm{diff}(T^2)'_c)$ algebra. In (12) m denotes a multiplication in the algebra $Y(\mathrm{diff}(T^2)'_c)$, i.e., for $a, b \in Y(\mathrm{diff}(T^2)'_c)$, $m(a \otimes b) = ab$. By applying the formula (12) to the generator $Q_{\bar{m},2}$ it is easy to see that the expression $S(Q_{\bar{m},2})$ is divergent.

There are some interesting, unsolved problems connected with the quantum algebra $DY(\mathrm{diff}(T^2)_c)$. The main unsolved problem is to construct a representation theory for $DY(\mathrm{diff}(T^2)_c)$. It is also important to find the full expression for a quantum R-matrix. We would like to discuss these problems in future publications.

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This paper is dedicated to Professor B. Mróz.

APPENDIX

In this appendix we give explicit expressions of the coefficients $\alpha^{\overline{f,l}}_{\overline{m,n,k}}$, $\tilde{\alpha}^{\overline{l}}_{\overline{m,n,k}}$, $\tilde{\tilde{\alpha}}_{\overline{m,n,k}}$, $\beta^{\overline{k,l}}_{\overline{m,n}}$, $\tilde{\beta}^{\overline{k,l}}_{\overline{m,n}}$, $\tilde{\tilde{\beta}}_{\overline{m,n,k}}$, and $\gamma^{\overline{k,l}}_{\overline{m}}$ from Eqs. (7), (8), (9), and (10).

Coefficients from Eq. (7) have the following form:

$$
\begin{aligned}
\alpha^{\overline{f,l}}_{\overline{m,n,k}} = {} & \tfrac{1}{4}\omega(\overline{n},\overline{k})(2\omega(\overline{m},\overline{n})+2\omega(\overline{m},\overline{k})-\omega(\overline{m},\overline{f})-\omega(\overline{m},\overline{l})+\omega(\overline{n},\overline{f})+\omega(\overline{n},\overline{l})+\omega(\overline{k},\overline{f})\\
& +\omega(\overline{k},\overline{l}))[(|\overline{m}||\overline{f}|-g(\overline{m},\overline{f}))(|\overline{n}||\overline{l}|+|\overline{k}||\overline{l}|-g(\overline{n},\overline{l})-g(\overline{k},\overline{l}))\\
& +\omega(\overline{m},\overline{f})\omega(\overline{n},\overline{l})+\omega(\overline{m},\overline{f})\omega(\overline{k},\overline{l})]+\tfrac{1}{4}\omega(\overline{k},\overline{m})(2\omega(\overline{n},\overline{m})+2\omega(\overline{n},\overline{k})\\
& -\omega(\overline{n},\overline{f})-\omega(\overline{n},\overline{l})+\omega(\overline{m},\overline{f})+\omega(\overline{m},\overline{l})+\omega(\overline{k},\overline{f})+\omega(\overline{k},\overline{l}))[(|\overline{n}||\overline{f}|\\
& -g(\overline{n},\overline{f}))(|\overline{m}||\overline{l}|+|\overline{k}||\overline{l}|-g(\overline{m},\overline{l})-g(\overline{k},\overline{l}))+\omega(\overline{n},\overline{f})\omega(\overline{m},\overline{l})\\
& +\omega(\overline{n},\overline{f})\omega(\overline{k},\overline{l})]+\tfrac{1}{4}\omega(\overline{m},\overline{n})(2\omega(\overline{k},\overline{m})+2\omega(\overline{k},\overline{n})-\omega(\overline{k},\overline{f})-\omega(\overline{k},\overline{l})\\
& +\omega(\overline{m},\overline{f})+\omega(\overline{n},\overline{f})+\omega(\overline{m},\overline{l})+\omega(\overline{n},\overline{l}))[(|\overline{k}||\overline{f}|-g(\overline{k},\overline{f}))(|\overline{m}||\overline{l}|+|\overline{n}||\overline{l}|\\
& -g(\overline{m},\overline{l})-g(\overline{n},\overline{l}))+\omega(\overline{k},\overline{f})\omega(\overline{m},\overline{l})+\omega(\overline{k},\overline{f})\omega(\overline{n},\overline{l})]+\tfrac{1}{4}(|\overline{f}||\overline{l}|\\
& -g(\overline{f},\overline{l}))[(|\overline{m}|^2-g(\overline{m},\overline{m}))\{\omega(\overline{n},\overline{k})(\omega(\overline{n}+\overline{k},\overline{f})+\omega(\overline{n}+\overline{k},\overline{l}))\\
& -\omega(\overline{k},\overline{m})\omega(\overline{n},\overline{f}+\overline{l})-\omega(\overline{m},\overline{n})\omega(\overline{k},\overline{f}+\overline{l})\}+(|\overline{n}|^2-g(\overline{n},\overline{n}))\{\omega(\overline{k},\overline{m})\\
& \times(\omega(\overline{m}+\overline{k},\overline{f})+\omega(\overline{m}+\overline{k},\overline{l}))-\omega(\overline{n},\overline{k})\omega(\overline{m},\overline{f}+\overline{l})-\omega(\overline{m},\overline{n})\omega(\overline{k},\overline{f}+\overline{l})\}\\
& +(|\overline{k}|^2-g(\overline{k},\overline{k}))\{\omega(\overline{m},\overline{n})(\omega(\overline{m}+\overline{n},\overline{f})+\omega(\overline{m}+\overline{n},\overline{l}))\\
& -\omega(\overline{k},\overline{m})\omega(\overline{n},\overline{f}+\overline{l})-\omega(\overline{n},\overline{k})\omega(\overline{m},\overline{f}+\overline{l})\}],
\end{aligned}
$$

$$
\begin{aligned}
\tilde{\alpha}^{\overline{l}}_{\overline{m,n,k}} = {} & \omega(\overline{n},\overline{k})(\omega(\overline{m},\overline{n})+\omega(\overline{m},\overline{k}))^2(|\overline{k}|+|\overline{n}|-|\overline{m}|)+(|\overline{n}-|\overline{k}|)\\
& \times\{\omega(\overline{n},\overline{k})\omega(\overline{m},\overline{n})(\omega(\overline{m},\overline{k})+\omega(\overline{n},\overline{k}))+\omega(\overline{m},\overline{n})\omega(\overline{m},\overline{k})(\omega(\overline{m},\overline{n})+\omega(\overline{m},\overline{k}))\\
& +\omega(\overline{n},\overline{k})\omega(\overline{m},\overline{k})(\omega(\overline{n},\overline{k})+\omega(\overline{n},\overline{m}))\}+2(|\overline{n}|+|\overline{k}|-|\overline{m}|)\omega(\overline{n},\overline{k})\omega(\overline{m},\overline{l})(\omega(\overline{n},\overline{l})\\
& +\omega(\overline{k},\overline{l}))+2(|\overline{n}|-|\overline{k}|)\omega(\overline{m},\overline{n})\omega(\overline{k},\overline{l})(\omega(\overline{m},\overline{l})+\omega(\overline{n},\overline{l}))+2(|\overline{n}|-|\overline{k}|)\omega(\overline{m},\overline{k})\\
& \times\omega(\overline{n},\overline{l})(\omega(\overline{k},\overline{l})+\omega(\overline{m},\overline{l}))-2|\overline{m}|\omega(\overline{n},\overline{k})\omega(\overline{m},\overline{l})(\omega(\overline{m},\overline{l})+\omega(\overline{n},\overline{l})+\omega(\overline{k},\overline{l}))\\
& +|\overline{m}|[(|\overline{n}|^2-g(\overline{n},\overline{n}))\omega(\overline{m},\overline{k})+(|\overline{k}|^2-g(\overline{k},\overline{k}))\omega(\overline{m},\overline{n})][|\overline{l}||\overline{n}|+|l||\overline{m}|+|\overline{l}||\overline{k}|-|\overline{l}|^2\\
& -g(\overline{l},\overline{n})-g(\overline{l},\overline{m})-g(\overline{l},\overline{k})+g(\overline{l},\overline{l})]-|\overline{m}|\omega(\overline{n},\overline{k})[(|\overline{m}||\overline{l}|\\
& -g(\overline{m},\overline{l}))(|\overline{n}|^2+|\overline{k}|^2+|\overline{n}||\overline{m}|+2|\overline{n}||\overline{k}|-|\overline{n}||\overline{l}|+|\overline{k}||\overline{m}|-|\overline{k}||\overline{l}|-2g(\overline{n},\overline{k})-g(\overline{n},\overline{n})\\
& -g(\overline{m},\overline{n})+g(\overline{n},\overline{l})-g(\overline{m},\overline{k})+g(\overline{k},\overline{l})-g(\overline{k},\overline{k}))+\omega(\overline{m},\overline{l})(\omega(\overline{n},\overline{m})-\omega(\overline{n},\overline{l})\\
& +\omega(\overline{k},\overline{m})-\omega(\overline{k},\overline{l}))]-|\overline{m}|(\omega(\overline{m},\overline{n})+\omega(\overline{k},\overline{m}))[(|\overline{k}||\overline{l}|\\
& -g(\overline{k},\overline{l}))(|\overline{n}|^2+|\overline{n}||\overline{m}|+|\overline{n}||\overline{k}|-|\overline{n}||\overline{l}|-g(\overline{n},\overline{n})-g(\overline{m},\overline{n})-g(\overline{n},\overline{k})+g(\overline{n},\overline{l}))\\
& +\omega(\overline{k},\overline{l})(\omega(\overline{n},\overline{k})+\omega(\overline{n},\overline{m})-\omega(\overline{n},\overline{l}))],
\end{aligned}
$$

$$\tilde{\alpha}_{\overline{m,n,k}}=|\overline{m}||\overline{k}|\omega(\overline{m},\overline{n})(\omega(\overline{k},\overline{m})+\omega(\overline{k},\overline{n}))+|\overline{m}||\overline{n}|\omega(\overline{m},\overline{k})(\omega(\overline{m},\overline{n})+\omega(\overline{k},\overline{n}))+|\overline{n}||\overline{k}|\omega(\overline{n},\overline{k})$$
$$\times(\omega(\overline{m},\overline{n})+\omega(\overline{m},\overline{k}))-|\overline{m}|(|\overline{n}|+|\overline{k}|)\omega(\overline{n},\overline{k})(\omega(\overline{m},\overline{n})+\omega(\overline{m},\overline{k})),$$

where $\omega(\overline{m},\overline{n}):=m_1n_2-m_2n_1$, $|\overline{m}|:=m_1+m_2$, and $g(\overline{m},\overline{n}):=m_1n_1+m_2n_2$. Coefficients from Eqs. (8) and (9) have the form

$$\beta_{\overline{m,n}}^{\overline{k,l}}=\tfrac{1}{4}(2\omega(\overline{m},\overline{n})-\omega(\overline{m},\overline{k})-\omega(\overline{m},\overline{l})+\omega(\overline{n},\overline{k})+\omega(\overline{n},\overline{l}))[(|\overline{m}||\overline{k}|-g(\overline{m},\overline{k}))(|\overline{n}||\overline{l}|-g(\overline{n},\overline{l}))$$
$$+\omega(\overline{m},\overline{k})\omega(\overline{n},\overline{l})]+\tfrac{1}{4}(|\overline{k}||\overline{l}|-g(\overline{k},\overline{l}))[(|\overline{m}|^2-g(\overline{m},\overline{m}))(\omega(\overline{m},\overline{n})+\omega(\overline{n},\overline{k})+\omega(\overline{n},\overline{l}))$$
$$-(|\overline{n}|^2-g(\overline{n},\overline{n}))(\omega(\overline{n},\overline{m})+\omega(\overline{m},\overline{k})+\omega(\overline{m},\overline{l}))],$$

$$\tilde{\beta}_{\overline{m,n}}^{\overline{k,l}}=\tfrac{1}{4}(\omega(\overline{m},\overline{n})-\omega(\overline{m},\overline{k})-\omega(\overline{m},\overline{l}))[(|\overline{k}||\overline{l}|-g(\overline{k},\overline{l}))(|\overline{m}||\overline{n}|+|\overline{m}|^2-g(\overline{m},\overline{n})-g(\overline{m},\overline{m}))$$
$$-(|\overline{m}||\overline{k}|-g(\overline{m},\overline{k}))(|\overline{m}||\overline{l}|-g(\overline{m},\overline{l}))-\omega(\overline{m},\overline{k})\omega(\overline{m},\overline{l})]+\tfrac{1}{4}(|\overline{n}|^2+|\overline{m}||\overline{n}|$$
$$-|\overline{n}||\overline{k}|-|\overline{n}||\overline{l}|-g(\overline{n},\overline{n})-g(\overline{m},\overline{n})+g(\overline{n},\overline{k})+g(\overline{n},\overline{l}))[(|\overline{m}||\overline{k}|-g(\overline{m},\overline{k}))\omega(\overline{m},\overline{l})$$
$$+(|\overline{m}||\overline{l}|-g(\overline{m},\overline{l}))\omega(\overline{m},\overline{k})]+\tfrac{1}{4}\omega(\overline{m},\overline{n})(|\overline{k}||\overline{l}|-g(\overline{k},\overline{l}))(|\overline{m}|^2+|\overline{m}||\overline{n}|$$
$$-|\overline{m}||\overline{k}|-|\overline{m}||\overline{l}|-g(\overline{m},\overline{m})-g(\overline{m},\overline{n})+g(\overline{m},\overline{k})+g(\overline{m},\overline{l})),$$

$$\tilde{\tilde{\beta}}_{\overline{m,n,k}}=|\overline{m}|(\omega(\overline{m},\overline{k})-\omega(\overline{m},\overline{n}))(\omega(\overline{m},\overline{k})+\tfrac{1}{2}\omega(\overline{n},\overline{k}))+\tfrac{1}{2}|\overline{m}|(|\overline{m}||\overline{k}|-g(\overline{m},\overline{k}))(|\overline{n}|^2$$
$$+|\overline{m}||\overline{n}|-|\overline{n}||\overline{k}|+g(\overline{n},\overline{k})-g(\overline{m},\overline{n})-g(\overline{n},\overline{n})).$$

Coefficient $\gamma_{\overline{m}}^{\overline{k,l}}$ from Eq. (10) has the form

$$\gamma_{\overline{m}}^{\overline{k,l}}=\tfrac{1}{2}(|\overline{k}||\overline{l}|-g(\overline{k},\overline{l}))(|\overline{m}|^2-|\overline{m}||\overline{k}|-|\overline{m}||\overline{l}|+g(\overline{m},\overline{k})+g(\overline{m},\overline{l})-g(\overline{m},\overline{m}))$$
$$+\tfrac{1}{2}\omega(\overline{k},\overline{l})(\omega(\overline{m},\overline{l})-\omega(\overline{m},\overline{k})-2\omega(\overline{k},\overline{l})).$$

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Quantum toroidal algebra $U_q(sl_{2,\mathrm{tor}})$ and R matrices

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We show the existence of R matrices acting on the tensor product of a certain class of representations of the quantum toroidal algebra $U_q(sl_{2,\mathrm{tor}})$. In particular, the explicit expressions of R matrices acting on the tensor product of level 1 integrable highest weight representations of $U_q(\widehat{sl_2})$ are obtained. Our approach is based on the work of Chari and Pressley. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In Ref. 1, based on the work of Chari and Pressley,[2,3] we studied representations of the quantum toroidal algebra $U_q(sl_{n+1,\mathrm{tor}})$ and proved the existence of R matrices acting on the tensor product of a certain class of representations. In this analysis, we used an isomorphism of $U_q'(sl_{n+1,\mathrm{tor}})$ obtained in Ref. 4. Since this result had been proved only for the case $n \geqslant 2$, the analysis in Ref. 4 was restricted to this case.

In this paper, for the algebra $U_q(sl_{2,\mathrm{tor}})$ we prove the existence of a similar isomorphism and show that R matrices exist if we consider tensor product representations via similar comultiplications used in Ref. 1. This part is essentially the same as the results in Refs. 1 and 4. Moreover we show that R matrices exist for other comultiplications of $U_q(sl_{2,\mathrm{tor}})$. (This result is not restricted to the case $n=1$.) In particular, we obtain the explicit expressions of the latter R matrices acting on the tensor product of level 1 integrable highest weight representations of $U_q(\widehat{sl_2})$ as trigonometric R matrices were obtained as intertwiners of the tensor products of finite dimensional representations of the quantum affine algebras in Ref. 5.

II. MAIN RESULTS

A. Definition of algebras

Throughout this paper, we fix a complex number q which is transcendental over $\mathbf{Q}$. Let $(a_{ij})_{0\leqslant i,j\leqslant 1}$ be the Cartan matrix of type $A_1^{(1)}$. Set $\mathfrak{h}=\mathbf{C}h_0\oplus\mathbf{C}h_1\oplus\mathbf{C}d$, and let α_i and $\Lambda_i (i=0,1)$ be the elements of $\mathfrak{h}^*$ determined by

$$\langle h_i,\alpha_j\rangle = a_{ij}, \quad \langle d,\alpha_j\rangle = 1, \quad \langle h_i,\Lambda_j\rangle = \delta_{ij}, \quad \langle d,\Lambda_j\rangle = 0. \tag{2.1}$$

We set $Q^+=\mathbf{Z}_{\geqslant 0}\alpha_0\oplus\mathbf{Z}_{\geqslant 0}\alpha_1$ and define a partial order $\leqslant$ on $\mathfrak{h}^*$ by $\mu\leqslant\lambda$ if and only if $\lambda-\mu\in Q^+$.

Following Refs. 7 and 8, we define $U_q(sl_{2,\mathrm{tor}})$ to be the $\mathbf{C}$ algebra with generators $x_{i,k}^{\pm}$, $h_{i,r}$, $k_i^{\pm 1}$, $C^{\pm 1}$ and $\tilde{D}^{\pm 1} (i=0,1, k\in\mathbf{Z}, r\in\mathbf{Z}\backslash\{0\})$ and relations

$$\tilde{D}^{\pm 1}\tilde{D}^{\mp 1}=1, \quad \tilde{D}k_i=k_i\tilde{D}, \tag{2.2}$$

$$\tilde{D}x_{i,k\pm\delta_{i0}}^{\pm}\tilde{D}^{-1}=q^{2k\pm 1}x_{i,k\pm\delta_{i0}}^{\pm}, \quad \tilde{D}h_{i,r}\tilde{D}^{-1}=q^{2r}h_{i,r}, \tag{2.3}$$

$$C^{\pm 1} \text{ central}, \quad k_i^{\pm 1} k_i^{\mp 1} = C^{\pm 1} C^{\mp 1} = 1, \tag{2.4}$$

$$[k_i, k_j] = [k_i, h_{j,r}] = 0, \tag{2.5}$$

$$[h_{i,r}, h_{j,s}] = \delta_{r+s,0} \frac{[ra_{ij}]}{r} \frac{C^r - C^{-r}}{q - q^{-1}}, \tag{2.6}$$

$$k_i x_{j,k}^{\pm} k_i^{-1} = q^{\pm a_{ij}} x_{j,k}^{\pm}, \tag{2.7}$$

$$[h_{i,r}, x_{j,k}^{\pm}] = \pm \frac{[ra_{ij}]}{r} C^{(r \mp |r|)/2} x_{j,r+k}^{\pm}, \tag{2.8}$$

$$[x_{i,k}^{+}, x_{j,l}^{-}] = \frac{\delta_{ij}}{q - q^{-1}} (C^{-l} \phi_{i,k+l}^{(-)} - C^{-k} \phi_{i,k+l}^{(+)}), \tag{2.9}$$

$$[x_{i,k+1}^{\pm}, x_{i,l}^{\pm}]_{q^{\pm 2}} + [x_{i,l+1}^{\pm}, x_{i,k}^{\pm}]_{q^{\pm 2}} = 0, \tag{2.10}$$

$$[x_{i,0}^{\pm}, [x_{i,0}^{\pm}, [x_{i,0}^{\pm}, x_{j,0}^{\pm}]_{q^2}]]_{q^{-2}} = 0 \quad (i \neq j). \tag{2.11}$$

Here $[m] = (q^m - q^{-m})/(q - q^{-1})$, $[x,y]_p = xy - pyx$, and $\phi_{i,\mp r}^{(\pm)} (r \geqslant 0)$ is expressed in terms of $k_i^{\pm 1}$ and $h_{i,r}$'s by

$$\sum_{r \geqslant 0} \phi_{i,\mp r}^{(\pm)} z^{\pm r} = k_i^{\mp 1} \exp\left(\mp (q - q^{-1}) \sum_{r > 0} h_{i,\mp r} z^{\pm r} \right). \tag{2.12}$$

For later purpose, we introduce generating series $x_i^{\pm}(z)$ and $\phi_i^{(\pm)}(z)$ by

$$x_i^{\pm}(z) = \sum x_{i,k}^{\pm} z^{-k},$$

and the left hand side of (2.12), respectively.

Let $U_q(\widehat{sl}_2)$[6] be the **C** algebra defined by generators $x_k^{\pm}, h_r, k^{\pm 1}, C^{\pm 1}, \tilde{D}^{\pm 1} (k \in \mathbf{Z}, r \in \mathbf{Z} \backslash \{0\})$ and relations (2.2)–(2.10) with $i = j = 1$ and $x_{1,k}^{\pm}, h_{1,r}, k_1$ replaced by $x_k^{\pm}, h_r, k$, respectively.

We shall denote $U_q(sl_{2,\mathrm{tor}})$ and $U_q(\widehat{sl}_2)$ by $\tilde{\mathcal{U}}$ and U, respectively. Let $\tilde{v}$ be the homomorphism $U \to \tilde{\mathcal{U}}$ such that

$$x_k^{\pm} \mapsto x_{1,k}^{\pm}, \quad h_r \mapsto h_{1,r}, \quad k \mapsto k_1, \quad C \mapsto C, \quad \tilde{D} \mapsto \tilde{D}. \tag{2.13}$$

B. $\tilde{\mathcal{U}}$ modules and their tensor products

In this paper, we shall consider only irreducible $\tilde{\mathcal{U}}$ modules satisfying the following condition (*) and their tensor products.

(*) The element $k_0 k_1$ acts as 1 on a $\tilde{\mathcal{U}}$ module V, and if regarded as a U module via the map $\tilde{v}$, the $\tilde{\mathcal{U}}$ module V satisfies the following three conditions:

(i) V is a direct sum of integrable highest weight modules of type **1**;
(ii) each weight space of V is finite dimensional;
(iii) the set of weights of V has a maximal element.

Let V be an irreducible $\tilde{\mathcal{U}}$ module satisfying the above condition (*) and λ a maximal element of the set of weights of V. Then by Theorem 2 in the next section and the remark after it, we can

see that V_λ, the weight space of V of weight λ, is one dimensional. Since V is irreducible, V is generated as a $\tilde{\mathcal{U}}$ module by a nonzero vector in this space. We shall call such a vector a highest weight vector of V.

For $a\in\mathbf{C}^\times$, let γ_a be the automorphism of $\tilde{\mathcal{U}}$ such that

$$x_{i,k}^{\pm}\mapsto a^{\pm\delta_{i0}}x_{i,k}^{\pm},\quad h_{i,r}\mapsto h_{i,r},\quad k_i\mapsto k_i,\quad C\mapsto C,\quad \tilde{D}\mapsto\tilde{D}. \tag{2.14}$$

For a representation (ρ,V) of $\tilde{\mathcal{U}}$, we denote the representation $(\rho\circ\gamma_a,V)$ by $V(a)$.

Let $\tilde{\Delta}_1$ and $\tilde{\Delta}_2$ be the comultiplications $\tilde{\mathcal{U}}\to\tilde{\mathcal{U}}\otimes\tilde{\mathcal{U}}$ such that

$$\begin{aligned}
&\tilde{\Delta}_1(C)=\tilde{\Delta}_2(C)=C\otimes C,\quad \tilde{\Delta}_1(D)=\tilde{D}_2(D)=D\otimes D,\\
&\tilde{\Delta}_1(\phi_i^{(+)}(z))=\tilde{\Delta}_2(\phi_i^{(+)}(z))=\phi_i^{(+)}(z/C_2)\otimes\phi_i^{(+)}(z),\\
&\tilde{\Delta}_1(\phi_i^{(-)}(z))=\tilde{\Delta}_2(\phi_i^{(-)}(z))=\phi_i^{(-)}(z)\otimes\phi_i^{(-)}(z/C_1),\\
&\tilde{\Delta}_1(x_i^{+}(z))=x_i^{+}(z)\otimes 1+\phi_i^{(-)}(z)\otimes x_i^{+}(z/C_1),\\
&\tilde{\Delta}_1(x_i^{-}(z))=1\otimes x_i^{-}(z)+x_i^{-}(z/C_2)\otimes\phi_i^{(+)}(z),\\
&\tilde{\Delta}_2(x_i^{+}(z))=x_i^{+}(z)\otimes 1+\phi_i^{(+)}(C_1z)\otimes x_i^{+}(C_1z),\\
&\tilde{\Delta}_2(x_i^{-}(z))=1\otimes x_i^{-}(z)+x_i^{-}(C_2z)\otimes\phi_i^{(-)}(C_2z),
\end{aligned} \tag{2.15}$$

where $C_1=C\otimes 1$ and $C_2=1\otimes C$. [These comultiplications are similar to those by Drinfeld for the quantum affine algebras. To check relations (2.11) (or (4.17) below), we need Lemma 4 and its corollary in Sec. IV.] For $\tilde{\mathcal{U}}$ modules V_1 and V_2 satisfying condition (*), we regard the tensor product $V_1\otimes V_2$ as a $\tilde{\mathcal{U}}$ module via the comultiplication $\tilde{\Delta}_j$ and denote it by $V_1\tilde{\otimes}_jV_2$ $(j=1,2)$.

C. Main results

Our main results in this paper are Theorem 1 and Proposition 2 below.

Theorem 1: *Let $V_\alpha(\alpha=1,2,3)$ be an irreducible $\tilde{\mathcal{U}}$ module satisfying condition (*) and v_α its highest weight vector. Then for each $i=0,1$, the following hold.*

(1) There exists a unique $\mathrm{Hom}_{\mathbf{C}}(V_\alpha\otimes V_\beta,V_\beta\otimes V_\alpha)$ *valued rational function $R^{(\alpha\beta)}(x)$ such that $R^{(\alpha\beta)}(a/b):V_\alpha(a)\tilde{\otimes}_iV_\beta(b)\to V_\beta(b)\tilde{\otimes}_iV_\alpha(a)$ is a homomorphism sending $v_\alpha\otimes v_\beta$ to $v_\beta\otimes v_\alpha$.*

(2) *The $R^{(\alpha\beta)}(x)$ satisfy the Yang–Baxter equation*

$$\begin{aligned}
&(I^{(3)}\otimes R^{(12)}(a))(R^{(13)}(ab)\otimes I^{(2)})(I^{(1)}\otimes R^{(23)}(b))\\
&\quad=(R^{(23)}(b)\otimes I^{(1)})(I^{(2)}\otimes R^{(13)}(ab))(R^{(12)}(a)\otimes I^{(3)}),
\end{aligned} \tag{2.16}$$

where $I^{(\alpha)}=id_{V_\alpha}$.

Remark: A similar result holds also for $U_q(sl_{n+1,\mathrm{tor}})$ with $n\geqslant 2$.

Leaving the proof of this theorem to the next section, we give some result on the explicit expression of the R matrix.

For $j=0,1$, set $V_j=W_j\otimes\mathcal{H}$ where $W_0=\mathbf{C}[e^{\pm\alpha}]$, $W_1=e^{\alpha/2}\mathbf{C}[e^{\pm\alpha}]$ and $\mathcal{H}=\mathbf{C}[a_{-1},a_{-2},\ldots]$. Define $\partial_\alpha,a_r(r\in\mathbf{Z}_{>0}),\bar{D}\in\mathrm{End}\ V_j$ by

$$\partial_\alpha(e^{m\alpha}\otimes x)=2me^{m\alpha}\otimes x,\quad a_r(e^{m\alpha}\otimes x)=\frac{[r][2r]}{r}e^{m\alpha}\otimes\frac{\partial x}{\partial a_{-r}}, \tag{2.17}$$

$$\overline{D}(e^{m\alpha}\otimes x)=q^{-(2m^2-m)-2\Sigma m_r r}e^{m\alpha}\otimes x\left(x=\prod_{r>0}a_{-r}^{m_r}\right).$$

Proposition 1: (Ref. 9) *For each* $j=0,1$, *the assignment*

$$x_i^+(z)\mapsto ze^{s_i\alpha}z^{s_i\partial_\alpha}\exp\left(s_i\sum_{r>0}\frac{a_{-r}}{[r]}z^r\right)\exp\left(-s_i\sum_{r>0}\frac{a_r}{[r]}(qz)^{-r}\right),$$

$$x_i^-(z)\mapsto ze^{-s_i\alpha}z^{-s_i\partial_\alpha}\exp\left(-s_i\sum_{r>0}\frac{a_{-r}}{[r]}(qz)^r\right)\exp\left(s_i\sum_{r>0}\frac{a_r}{[r]}z^{-r}\right),$$

$$\phi_i^{(\pm)}(z)\mapsto q^{\mp s_i\partial_\alpha}\exp\left(\mp s_i(q-q^{-1})\sum_{r>0}a_{\mp r}z^{\pm r}\right),$$

$$C\mapsto q,\quad \tilde{D}\mapsto\overline{D},$$

with $s_1=1$ *and* $s_0=-1$ *defines a* $\tilde{\mathcal{U}}$ *action on* V_j. *This is the irreducible highest weight module with highest weight* Λ_j *if regarded as a* $U_q(\widehat{sl}_2)$ *module via the map* $\tilde{v}$.

Remark: This proposition was proved in Ref. 9. But contrary to the claim there, the $x_{i,k}^{\pm}$ do not satisfy the relation

$$[x_{1,k+1}^{\pm},x_{0,l}^{\pm}]_{q^{\mp 2}}+[x_{0,l+1}^{\pm},x_{1,k}^{\pm}]_{q^{\mp 2}}=0.$$

We do not include the above among the relations of the algebra. This is consistent with the $q=1$ case.[10]

Set

$$\psi^{(\pm)}(w)=w(e^{\pm\alpha/2}\otimes e^{\mp\alpha/2})w^{\pm\partial_\alpha\otimes 1\mp|\otimes\partial_\alpha}\exp\left(\pm\sum_{r>0}\frac{b_{-r}}{[2r]}w^{2r}\right)\exp\left(\mp\sum_{r>0}\frac{b_r}{[2r]}w^{-2r}\right),\tag{2.18}$$

where

$$b_r=a_r^{(1)}-q^{-r}a_r^{(2)},\quad b_{-r}=q^r a_{-r}^{(1)}-a_{-r}^{(2)},$$

$$(r>0,\quad a_s^{(1)}=a_s\otimes 1,\quad a_s^{(2)}=1\otimes a_s).$$

Define $c_r^{\pm}\in\oplus_j\mathrm{Hom}_{\mathbf{C}}(V_j\otimes V_j,V_{1-j}\otimes V_{1-j})(r\in\mathbf{Z}+\frac{1}{2})$ and $c_r^{\pm}\in\oplus_j\mathrm{Hom}_{\mathbf{C}}(V_j\otimes V_{1-j},V_{1-j}\otimes V_j)$ $(r\in\mathbf{Z})$ by

$$\sum_r c_r^{\pm}/w^{2r}=\psi^{(+)}(w)\pm\psi^{(-)}(q^{\mp 1}w).\tag{2.19}$$

The $c_r^{\pm}$ satisfy

$$\{c_r^{\pm},c_s^{\pm}\}=\pm\delta_{r+s,0}(q^{2r}+q^{-2r}),\quad \{c_r^+,c_s^-\}=0,$$
$$(\overline{D}\otimes\overline{D})c_r^{\pm}(\overline{D}\otimes\overline{D})^{-1}=q^{2r}c_r^{\pm}.\tag{2.20}$$

where $\{x,y\}=xy+yx$.

Proposition 2: For the $\tilde{\mathcal{U}}$ *modules* V_j *in Proposition 1, the explicit expression of the intertwiner* $R(a/b):V_j(a)\tilde{\otimes}_1V_k(b)\to V_k(b)\tilde{\otimes}_1V_j(a)$ *is given by*

$$R(x)=\prod_{\substack{r>0\\ r\in\mathbf{Z}+1/2}}\left(1+\frac{x-1}{q^{2r}x-q^{-2r}}c_{-r}^{-}c_{r}^{-}\right)\quad\text{if}\quad j=k,$$

$$R(x)=(-1)^{(\partial_\alpha\otimes 1-1\otimes\partial_\alpha-1)/2}c_0^{-}\prod_{\substack{r>0\\ r\in\mathbf{Z}}}\left(1+\frac{x-1}{q^{2r}x-q^{-2r}}c_{-r}^{-}c_{r}^{-}\right)\quad\text{if}\quad j\neq k.$$

Proof: First note that the vectors $v_0=1\otimes 1$ and $v_1=e^{\alpha/2}\otimes 1$ are higheset weight vectors of V_0 and V_1, respectively, and that on the tensor product $V_j(a)\widetilde{\otimes}_1V_k(b)$, $\widetilde{\mathcal{U}}$ acts as follows:

$$\phi_i^{(\pm)}(z)=q^{\mp s_i\partial_+}\exp\left(\mp s_i(q-q^{-1})\sum_{r>0}h_{\mp r}z^{\pm r}\right),$$

$$\begin{aligned}x_i^{+}(w^2)&=we^{s_i\alpha_+}w^{s_i\partial_+}\exp\left(s_i\sum_{r>0}\frac{h_{-r}}{[2r]}w^{2r}\right)\exp\left(-s_i\sum_{r>0}\frac{q^{-2r}h_r}{[2r]}w^{-2r}\right)\\&\quad\times(a^{\delta_{i0}}\psi^{(s_i)}(w)+b^{\delta_{i0}}\psi^{(-s_i)}(w/q)),\\x_i^{-}(w^2)&=we^{-s_i\alpha_+}w^{-s_i\partial_+}\exp\left(-s_i\sum_{r>0}\frac{q^{2r}h_{-r}}{[2r]}w^{2r}\right)\exp\left(s_i\sum_{r>0}\frac{h_r}{[2r]}w^{-2r}\right)\\&\quad\times(b^{-\delta_{i0}}\psi^{(s_i)}(w)+a^{-\delta_{i0}}\psi^{(-s_i)}(w/q)),\\\widetilde{D}&=\overline{D}\otimes\overline{D},\quad C=q^2\end{aligned}\tag{2.21}$$

where

$$h_r=a_r^{(1)}+q^ra_r^{(2)},\quad h_{-r}=q^{-r}a_{-r}^{(1)}+a_{-r}^{(2)}\ (r>0),$$

$$e^{\pm\alpha_+}=e^{\pm\alpha/2}\otimes e^{\pm\alpha/2},\quad \partial_+=\partial_\alpha\otimes 1+1\otimes\partial_\alpha.$$

Since

$$\begin{aligned}&c_r^{-}v_j\otimes v_k=0\quad\text{for}\quad r>0,\quad r\in\mathbf{Z}+\delta_{j,k}/2,\\&c_0^{-}v_j\otimes v_k=(-1)^jv_k\otimes v_j\quad\text{for}\quad j\neq k,\end{aligned}\tag{2.22}$$

the expression for $R(x)$ maps $v_j\otimes v_k$ to $v_k\otimes v_j$. So it is sufficient to prove that the expression is an intertwiner. Noting $[h_r,b_s]=0$, it is easy to show that the $c_r^{\pm}$ commute with h_r, ∂_+ and $e^{\pm\alpha_+}$, so the expression commutes with h_r, ∂_+, $e^{\pm\alpha_+}$ and $\overline{D}\otimes\overline{D}$. Therefore we only have to show that

$$\begin{aligned}&[R(x),\psi^{(+)}(w)+\psi^{(-)}(w/q)]=0,\\&R(x)(x\psi^{(-)}(w)+\psi^{(+)}(w/q))=(\psi^{(-)}(w)+x\psi^{(+)}(w/q))R(x).\end{aligned}\tag{2.23}$$

This is equivalent to

$$[R(x),c_r^{+}]=0,\quad R(x)(q^{2r}-q^{-2r}x)c_r^{-}=(q^{2r}x-q^{-2r})c_r^{-}R(x)\tag{2.24}$$

and easily checked, using (2.20). □

Remark: The expression of the intertwiner $R(a/b):V_j(a)\widetilde{\otimes}_2V_k(b)\to V_k(b)\widetilde{\otimes}_2V_j(a)$ is also similarly obtained.

III. PROOF OF THEOREM 1

A. Notations

First we introduce more notations.

1. Algebra U

The algebra U is well known to be described by generators e_i, f_i, $t_i^{\pm 1}$, $D^{\pm 1}$ $(i=0,1)$ and relations

$$D^{\pm 1}D^{\mp 1}=1, \quad Dt_i=t_iD, \tag{3.1}$$

$$De_iD^{-1}=qe_i, \quad Df_iD^{-1}=q^{-1}f_i, \tag{3.2}$$

$$t_i^{\pm 1}t_i^{\mp 1}=1, \quad t_it_j=t_jt_i, \tag{3.3}$$

$$t_ie_jt_i^{-1}=q^{a_{ij}}e_j, \quad t_if_jt_i^{-1}=q^{-a_{ij}}f_j, \tag{3.4}$$

$$[e_i,f_j]=\frac{\delta_{ij}}{q-q^{-1}}(t_i-t_i^{-1}), \tag{3.5}$$

$$[e_i,[e_i,[e_i,e_j]_{q^2},],]_{q^{-2}}=0 \quad (i\neq j), \tag{3.6}$$

$$[f_i,[f_i,[f_i,f_j]_{q^2},],]_{q^{-2}}=0 \quad (i\neq j). \tag{3.7}$$

We take the following correspondence of the generators:[11]

$$\begin{aligned} &e_1=x_0^+, \quad f_1=x_0^-, \quad t_1=k, \quad D=\tilde{D}, \\ &e_0=Ck^{-1}x_1^-, \quad f_0=x_{-1}^+kC^{-1}, \quad t_0=Ck^{-1}. \end{aligned} \tag{3.8}$$

We let U' denote the subalgebra of U generated by e_i, f_i and $t_i^{\pm 1}$ $(i=0,1)$. The defining relations of this subalgebra are (3.3)–(3.7). Let σ be the anti-automorphism of U determined by

$$e_i\mapsto e_i, \quad f_i\mapsto f_i, \quad t_i\mapsto t_i^{-1}, \quad D\mapsto D^{-1}. \tag{3.9}$$

Since σ preserves the subalgebra U', it defines an anti-automorphism of U', which we denote by the same letter σ.

2. Algebras $\mathcal{U}$ and $\tilde{\mathcal{U}}$

We need the $\mathbf{C}$ algebra defined by the same generators as those of $U_q(sl_{2,\mathrm{tor}})$ ($\tilde{D}^{\pm 1}$ replaced by $D^{\pm 1}$) and relations (2.4)–(2.11) and

$$D^{\pm 1}D^{\mp 1}=1, \quad Dk_i=k_iD, \tag{3.10}$$

$$Dx_{i,k}^{\pm}D^{-1}=q^{\pm 1}x_{i,k}^{\pm}, \quad Dh_{i,r}D^{-1}=h_{i,r}. \tag{3.11}$$

We shall denote this algebra by $\mathcal{U}$.

We let $\mathcal{U}'$ (resp. $\tilde{\mathcal{U}}'$) signify the subalgebra of $\mathcal{U}$ (resp. $\tilde{\mathcal{U}}$) generated by $x_{i,k}^{\pm}$, $h_{i,r}$, $k_i^{\pm 1}$ and $C^{\pm 1}$ $(i=0,\ 1,\ k\in\mathbf{Z},\ r\in\mathbf{Z}\backslash\{0\})$. As easily shown, these two subalgebras are isomorphic and their defining relations are (2.4)–(2.11). We shall identify these two subalgebras.

Let $\mathcal{X}_j$ $(j=0,1)$, δ_a $(a\in\mathbf{C}^{\times})$ and ζ be the automorphisms of $\mathcal{U}$ determined by

$$\mathcal{X}_j \ : \ x_{i,k}^{\pm}\mapsto(-1)^{j\delta_{ij}}x_{i,k\mp\delta_{ij}}^{\pm}, \quad h_{i,r}\mapsto h_{i,r}, \quad k_i\mapsto C^{-\delta_{ij}}k_i, \tag{3.12}$$

$$C\mapsto C,\quad D\mapsto D,$$

$$\delta_a\ :\ x^{\pm}_{i,k}\mapsto a^k x^{\pm}_{i,k},\quad h_{i,r}\mapsto a^r h_{i,r},\quad k_i\mapsto k_i, \tag{3.13}$$

$$C\mapsto C,\quad D\mapsto D,$$

$$\zeta\ :\ x^{\pm}_{i,k}\mapsto q^{\pm 2\delta_{i0}}x^{\mp}_{i,-k},\quad h_{i,r}\mapsto -h_{i,-r},\quad k_i\mapsto k_i^{-1}, \tag{3.14}$$

$$C\to C^{-1},\quad D\to D^{-1}.$$

(The existence of $\mathcal{X}_j$ is guaranteed by Lemma 3 in Sec. IV.) We also need the anti-automorphism η of $\mathcal{U}$ such that

$$x^{\pm}_{i,k}\mapsto x^{\pm}_{i,-k},\quad h_{i,r}\mapsto -C^r h_{i,-r},\quad k_i\mapsto k_i^{-1}, \tag{3.15}$$

$$C\mapsto C,\quad D\mapsto D^{-1}.$$

Since these (anti-)automorphisms preserve the subalgebra $\mathcal{U}'$, they define (anti)-automorphisms of $\mathcal{U}'$, which we denote by the same letters.

We define an automorphism $\tilde{\zeta}$ and an anti-automorphism $\tilde{\eta}$ of $\tilde{\mathcal{U}}$ so that they map the generators other than $\tilde{D}^{\pm 1}$ as ζ and η do, and send $\tilde{D}$ to $\tilde{D}^{-1}$ and $\tilde{D}k_1^{-1}$, respectively.

3. $\mathcal{U}$ modules

Let λ be a dominant integral weight of $\widehat{sl}_2$ and $\mathbf{P}=(P_0,P_1)$ a pair of polynomials with constant term 1 and $\deg P_i=\langle h_i,\lambda\rangle$. By $V(\lambda,\mathbf{P})$, we denote an irreducible $\mathcal{U}$ module genenated by a simultaneous eigenvector v_+ annihilated by the $x^+_{i,k}$ of C, D, and the $\phi^{(\pm)}_{i,\mp r}$ such that

$$Cv_+=v_+,\quad Dv_+=q^{\langle d,\lambda\rangle}v_+,$$

$$\sum_{r\geqslant 0}\phi^{(\pm)}_{i,\mp r}u^{\mp r}v_+=q^{\deg P_i}P_i(q^{-2}u)/P_i(u)v_+, \tag{3.16}$$

where the right-hand side of the last equality should be understood as a Laurent expansion around $u=\infty$ (resp. 0) for the $\phi^{(+)}_{i,-r}$ (resp. the $\phi^{(-)}_{i,r}$). The existence and uniqueness of $V(\lambda,\mathbf{P})$ are proven in the standard manner. (See Refs. 1–3). We call v_+ a highest weight vector of $V(\lambda,\mathbf{P})$.

For a representation (ρ,V) of $\mathcal{U}$, we let V_a signify the representation $(\rho\circ\delta_a,V)$.

B. Results in Refs. 1 and 4 for $U_q(sl_{2,\mathrm{tor}})$

Most of the results in Refs. 1 and 4 hold also for $U_q(sl_{2,\mathrm{tor}})$. We state them in this section. We will give the proof of Proposition 3 and Lemma 1 in the next section. The remaining claims are proven as in Ref. 1, using Lemmas 3 and 4 in the next section.

1. Isomorphisms ψ and π

Let $h:U\to\mathcal{U}$, $v:U'\to\mathcal{U}$ and $\tilde{h}:U'\to\tilde{\mathcal{U}}$ be the homomorphisms determined by

$$h\ :\ e_i\mapsto x^+_{i,0},\quad f_i\mapsto x^-_{i,0},\quad t_i\mapsto k_i,\quad D\mapsto D, \tag{3.17}$$

$$v\ :\ x^{\pm}_k\mapsto x^{\pm}_{1,k},\quad h_r\mapsto h_{1,r},\quad k\mapsto k_1,\quad C\mapsto C, \tag{3.18}$$

$$\tilde{h}\ :\ e_i\mapsto x^+_{i,0},\quad f_i\mapsto x^-_{i,0},\quad t_i\mapsto k_i. \tag{3.19}$$

Proposition 3: There exist isomorphisms $\psi:\mathcal{U}\to\tilde{\mathcal{U}}$ and $\pi:\mathcal{U}\to\tilde{\mathcal{U}}$ determined by

$$\psi v=\tilde{h},\quad \psi h=\tilde{\eta}\tilde{v}\sigma \text{ and } \pi h=\tilde{v},\quad \pi\eta v\sigma=\tilde{h},$$

respectively.

Lemma 1: The isomorphisms ψ and π satisfy the following identities:

(1) $\pi=\tilde{\eta}\psi\eta$,
(2) $\tilde{\zeta}\psi=\psi\zeta$,
(3) $\gamma_{a^{-1}}\pi=\pi\delta_a$.

2. $\mathcal{U}$ modules and $\tilde{\mathcal{U}}$ modules

We shall regard a $\tilde{\mathcal{U}}$ module as a $\mathcal{U}$ module via the map π. Then thanks to Lemma 1 (3) we can see that

$$V(a^{-1})\simeq V_a, \tag{3.20}$$

as a $\mathcal{U}$ module. Moreover condition (*) for an irreducible $\tilde{\mathcal{U}}$ module can be rewritten as a condition for an irreducible $\mathcal{U}$ module as follows.

Theorem 2: *An irreducible $\tilde{\mathcal{U}}$ module satisfies condition (*) if and only if it is isomorphic to one of the $V(\lambda,\mathbf{P})$ as a $\mathcal{U}$ module.*

Noting $\pi(D)=\tilde{v}(D)$, $\pi(k_i)=\tilde{v}(t_i)$ $(i=0,1)$, and the fact that $V(\lambda,\mathbf{P})$ is spanned by the vectors $x^{-}_{i_1,k_1}\cdots x^{-}_{i_m,k_m}v_+$, we find from this theorem that the notions of highest weight vectors for both modules coincide.

3. Tensor product of $\mathcal{U}$ modules and R matrices

Letting $\psi'=\psi\mathcal{X}_0^{-1}$, set

$$\Delta_i=(\psi'\otimes\psi')^{-1}\circ\tilde{\Delta}_i\circ\psi',\quad \Delta_i'=(\pi\otimes\pi)^{-1}\circ\tilde{\Delta}_i\circ\pi\ \ (i=1,2). \tag{3.21}$$

For $\mathcal{U}$ modules $V_\alpha=V(\lambda_\alpha,\mathbf{P}_\alpha)$ $(\alpha=1,2)$, we regard the tensor product $V_1\otimes V_2$ as a $\mathcal{U}$ module via the comultiplication Δ_i (resp. Δ_i') and denote it by $V_1\otimes_i V_2$ (resp. $V_1\otimes_i' V_2$) $(i=1,2)$.

Theorem 3: *Set $V_\alpha=V(\lambda_\alpha,\mathbf{P}_\alpha)$ $(\alpha=1,2,3)$ and let v_α's be their highest weight vectors. Then for each $i=0,1$, the following hold.*

(1) There exists a unique $\mathrm{Hom}_{\mathbf{C}}(V_\alpha\otimes V_\beta,V_\beta\otimes V_\alpha)$ *valued rational function $\mathcal{R}^{(\alpha\beta)}(x)$ such that $\mathcal{R}^{(\alpha\beta)}(a/b):V_{\alpha,b}\otimes_i V_{\beta,a}\to V_{\beta,a}\otimes_i V_{\alpha,b}$ is a homomorphism sending $v_\alpha\otimes v_\beta$ to $v_\beta\otimes v_\alpha$;*

(2) the $\mathcal{R}^{(\alpha\beta)}(x)$ satisfy the Yang–Baxter equation (2.16).

C. Proof of Theorem 1

Now we turn to the proof of Theorem 1.

Lemma 2: Set $\phi=\mathcal{X}_0\zeta\eta$. Then the following hold:

$$(\Delta_i^{\phi})^{\mathrm{op}}=\Delta_j' \ \text{ for } \ (i,j)=(1,2),(2,1).$$

Proof: For a comultiplication Δ and (anti-)automorphism p, set $\Delta^p=(p\otimes p)^{-1}\circ\Delta\circ p$. Since $\tilde{\Delta}_i^{\tilde{\zeta}}=\tilde{\Delta}_i^{\mathrm{op}}$ and $\tilde{\Delta}_i^{\tilde{\eta}}=\tilde{\Delta}_j$, it is sufficient to show that $\tilde{\zeta}\psi'\phi=\tilde{\eta}\pi$. Thanks to Lemma 1 (1) and $\tilde{\eta}^2=1=\zeta^2$, this is equivalent to Lemma 1 (2). □

Proposition 4: Set $V=V(\lambda,\mathbf{P})$ and let v_+ be its highest weight vector. There exists a bilinear form $(\cdot,\cdot)$ on V uniquely determined by

$$(v_+,v_+)=1,\quad (xv,v')=(v,\phi(x)v')\ \ (v,v'\in V,x\in\mathcal{U}). \tag{3.22}$$

This bilinear form is nondegenerate and symmetric.

Proof: First we show the existence. For $V=\oplus_{\mu\in Q^+}V_{\lambda-\mu}$, set $V^{\mathrm{res}*}=\oplus_{\mu\in Q^+}V^*_{\lambda-\mu}$ and regard this space as a $\mathcal{U}$ module by

$$\langle xf,v\rangle=\langle f,\phi(x)v\rangle \quad (f\in V^{\mathrm{res}*},v\in V,x\in\mathcal{U}). \tag{3.23}$$

Then since

$$\begin{aligned}&\phi(x^{\pm}_{i,k})=q^{\pm 2\delta_{i0}}x^{\mp}_{i,k\pm\delta_{i0}},\quad \phi(h_{i,r})=C^{-r}h_{i,r},\\ &\phi(k_i)=C^{-\delta_{i0}}k_i,\quad \phi(D)=D,\quad \phi(C)=C^{-1},\end{aligned} \tag{3.24}$$

there exists an isomorphism $g:V\tilde{\to}V^{\mathrm{res}*}$. A scalar multiple of the bilinear form determined by

$$(v,v')=\langle g(v),v'\rangle \quad (v,v'\in V), \tag{3.25}$$

satisfies conditions (3.22).

The uniqueness follows from (3.22) and (3.24). Since V is irreducible and $\phi^2=1$, the form is nondegenerate and symmetric. □

Now we are in a position to give the following proof.

Proof of Theorem 1.

In this proof, we let $i\neq j\in\{1,2\}$. Set $V_\alpha=V(\lambda_\alpha,\mathbf{P}_\alpha)$ $(\alpha=1,2,3)$ and $E_{\alpha\beta}=\Pi_\mu\mathrm{Hom}_{\mathbf{C}}((V_\alpha\otimes V_\beta)_{\lambda_\alpha+\lambda_{\beta-\mu}},(V_\beta\otimes V_\alpha)_{\lambda_\alpha+\lambda_{\beta-\mu}})$. For $f\in E_{\alpha\beta}$, define $\overline{f}\in E_{\alpha\beta}$ by

$$(f(u_\alpha\otimes u_\beta),u'_\beta\otimes u'_\alpha)=(u_\beta\otimes u_\alpha,\overline{f}(u'_\alpha\otimes u'_\beta)) \quad (u_\gamma,u'_\gamma\in V_r). \tag{3.26}$$

Let $\mathcal{R}^{(\alpha\beta)}(a/b)$ signify the intertwiner $V_{\alpha,b}\otimes_i V_{\beta,a}\to V_{\beta,a}\otimes_i V_{\alpha,b}$ in Theorem 3. Proposition 4 gives

$$(\Delta_i(x)u_\alpha\otimes u_\beta,u'_\alpha\otimes u'_\beta)=(u_\alpha\otimes u_\beta,\Delta_i^{\phi}(\phi(x))u'_\alpha\otimes u'_\beta) \quad (x\in\mathcal{U},u_\gamma,u'_\gamma\in V_\gamma). \tag{3.27}$$

This fact and Lemma 2 show that $\overline{\mathcal{R}}^{(\alpha\beta)}(a/b)$ is an intertwiner $V_{\alpha,b}\otimes'_j V_{\beta,a}\to V_{\beta,a}\otimes'_j V_{\alpha,b}$. Thanks to Eq. (3.20) and the definition of Δ'_j, this implies that $\overline{\mathcal{R}}^{(\alpha\beta)}(a/b)$ is an intertwiner $V_\alpha(a)\tilde{\otimes}'_j V_\beta(b)\to V_\beta(b)\tilde{\otimes}'_j V_\alpha(a)$. Clearly the $\overline{\mathcal{R}}^{(\alpha,\beta)}(x)$ send $v_\alpha\otimes v_\beta$ to $v_\beta\otimes v_\alpha$ and satisfy the Yang–Baxter equation. Therefore the theorem follows from Theorem 2. □

IV. PROOF OF PROPOSITION 3 AND LEMMA 1

Proposition 3 follows from Proposition 7 below as in Ref. 1. Lemma 1 follows from Proposition 7 (1) and its corollary since $\psi|_{\mathcal{U}'}=f$ and $\pi|_{\mathcal{U}'}=f^{-1}$. Therefore, in this section we shall prove Proposition 7.

A. Presentations of $\mathcal{U}'$

First we prove the following proposition.

Proposition 5: (1) The algebra $\mathcal{U}'$ admits a presentation in terms of generators $x^{\pm}_{i,0},x^{\pm}_{i,1},x^{\pm}_{i,-1},k_i^{\pm1}$ $(i=0,1)$, $C^{\pm1}$ and relations

$$k_i^{\pm1}k_i^{\mp1}=C^{\pm1}C^{\mp1}=1, \tag{4.1}$$

$$C \text{ central},\quad k_ik_j=k_jk_i, \tag{4.2}$$

$$k_ix^{\pm}_{j,k}k_i^{-1}=q^{\pm a_{ij}}x^{\pm}_{j,k}, \tag{4.3}$$

$$[x^+_{i,k},x^-_{i,-k}]=\frac{C^k k_i-C^{-k}k_i^{-1}}{q-q^{-1}}, \tag{4.4}$$

$$[x^+_{i,\pm 1},x^-_{i,0}]=C[x^+_{i,0},x^-_{i,\pm 1}], \tag{4.5}$$

$$[x^\pm_{i,0},x^\pm_{i,-1}]_{q^{\pm 2}}=[x^\pm_{i,1},x^\pm_{i,0}]_{q^{\pm 2}}=0, \tag{4.6}$$

$$[x^+_{i,-1},X^+_{i-2}]_{q^2}=[X^-_{i,2},x^-_{i,1}]_{q^{-2}}=0, \tag{4.7}$$

$$[x^+_{i,k},x^-_{j,l}]=0 \quad (i\neq j), \tag{4.8}$$

$$[x^\pm_{i,0},[x^\pm_{i,0},[x^\pm_{i,0},x^\pm_{j,0}]_{q^2}]]_{q^{-2}}=0 \quad (i\neq j). \tag{4.9}$$

For $i\neq j$ the following elements are central

$$[x^\pm_{i,0},x^\pm_{j,-1}]_{q^{\mp 2}}+[x^\pm_{j,0},x^\pm_{i,-1}]_{q^{\mp 2}}, \tag{4.10}$$

$$[x^\pm_{i,1},x^\pm_{j,0}]_{q^{\mp 2}}+[x^\pm_{j,1},x^\pm_{i,0}]_{q^{\mp 2}}, \tag{4.11}$$

$$[x^+_{i,-1},x^+_{j,-1}]_{q^{-2}}+[x^+_{j,0},X^+_{i,-2}]_{q^{-2}}, \tag{4.12}$$

$$[x^-_{i,1},x^-_{j,1}]_{q^2}+[X^-_{j,2},x^-_{i,0}]_{q^2}, \tag{4.13}$$

where

$$X^\pm_{i,\mp 2}=\pm\frac{C^{\pm 1}}{[2]}[H_{i,\mp 1},x^\pm_{i\mp 1}],$$

with

$$H_{i,1}=Ck_i^{-1}[x^+_{i,0},x^-_{i,1}](=k_i^{-1}[x^+_{i,1},x^-_{i,0}]),$$

$$H_{i,-1}=C^{-1}k_i[x^+_{i,-1},x^-_{i,0}](=k_i[x^+_{i,0},x^-_{i,-1}]).$$

(2) Relations (4.7), (4.12), and (4.13) can be replaced by

$$[X^+_{i,2},x^+_{i,1}]_{q^2}=[x^-_{i,-1},X^-_{i,-2}]_{q^{-2}}=0, \tag{4.14}$$

$$[x^+_{i,1},x^+_{j,1}]_{q^{-2}}+[X^+_{j,2},x^+_{i,0}]_{q^{-2}}, \tag{4.15}$$

$$[x^-_{i,-1},x^-_{j,-1}]_{q^2}+[x^-_{j,0},X^-_{i,-2}]_{q^2}. \tag{4.16}$$

where

$$X^\pm_{i,\pm 2}=\pm\frac{1}{[2]}[H_{i,\pm 1},x^\pm_{i,\pm 1}].$$

Hereafter we shall denote the algebra defined by the generators and relations in the proposition (1) [resp. (2)] by A [resp. B].

First we prove the following two lemmas.

Lemma 3: In $\mathcal{U}'$, the following equalities hold:

$$\mathrm{Sym}_{m_1,m_2,m_3}[x^\pm_{i,m_1},[x^\pm_{i,m_2},[x^\pm_{i,m_3},x^\pm_{j,n}]_{q^2}]]_{q^{-2}}=0 \quad (i\neq j). \tag{4.17}$$

Proof: Set

$$I_{ij}^{\pm}(n)=[x_{i,0}^{\pm},[x_{i,0}^{\pm},[x_{i,0}^{\pm},x_{j,n}^{\pm}]_{q^2}]]_{q^{-2}} \quad (i\neq j). \tag{4.18}$$

Then, as easily checked, the following equalities hold:

$$[3]q^2[x_{i,0}^{+},[x_{i,0}^{+},[x_{i,1}^{+},x_{j,m}^{+}]_{q^{-2}}]]_{q^{-2}}-I_{ij}^{+}(m+1)=\frac{1}{[2]}[h_{i,1},I_{ij}^{+}(m)], \tag{4.19}$$

$$[x_{i,0}^{+},[x_{i,1}^{+},x_{j,m}^{+}]_{q^{-2}}]-q^{-2}[x_{i,0}^{+},[x_{i,0}^{+},x_{j,m+1}^{+}]_{q^2}]=\frac{C}{[3][2]}[I_{ij}^{+}(m),x_{i,1}^{-}]. \tag{4.20}$$

Since $I_{ij}^{+}(0)=0$, we can see that $I_{ij}^{+}(m)=0$ for $m\geqslant 0$ by combining (4.19) and (4.20) with $m\geqslant 0$. Applying η and ζ to this result, we get $I_{ij}^{\pm}(m)=0$ for any m.

From $[h_{i,m_1},I_{ij}^{\pm}(n)]=0$, relations (4.17) with $m_2=m_3=0$ follow. Considering the commutator of these relations with h_{i,m_2}, we find that relations (4.17) with $m_3=0$ hold. From the commutator of these relations with h_{i,m_3}, the assertion follows. □

Lemma 4: We have

$$[x_{1,k+1}^{\pm},x_{0,l}^{\pm}]_{q^{\mp 2}}+[x_{0,l+1}^{\pm},x_{1,k}^{\pm}]_{q^{\mp 2}}\in Z(\mathcal{U}').$$

Proof: Set $X=[x_{1,1}^{+},x_{0,0}^{+}]_{q^{-2}}+[x_{0,1}^{+},x_{1,0}^{+}]_{q^{-2}}$. It is straightforward to show that X commutes with $x_{i,m}^{-}$, k_i and C $(i=0,1,\ m=0,\pm 1)$. From (4.20) with $m=0$, it follows that X also commutes with $x_{i,0}^{+}$ $(i=0,1)$. From these we find $X\in Z(\mathcal{U}')$. Applying $\mathcal{X}_i^{\pm 1}$ $(i=0,1)$ repeatedly to X, we get the claim for the $x_{i,k}^{+}$. The claim for the $x_{i,k}^{-}$ can be proven by the use of the automorphism ζ. □

By considering the commutator of the central elements in the lemma with $h_{1,1}$, we obtain

Corollary 1: In $\mathcal{U}'$, the following equalities hold:

$$(z-w)((z-q^{\mp 2}w)x_1^{\pm}(z)x_0^{\pm}(w)+(w-q^{\mp 2}z)x_0^{\pm}(w)x_1^{\pm}(z))=0.$$

Next assuming Lemma 5 below for a while, we give the following proof.

Proof of Proposition 5

(1) By Lemma 4, we can see that there exists a homomorphism $A\to\mathcal{U}'$ determined by

$$x_{i,k}^{\pm}\mapsto x_{i,k}^{\pm} \quad (k=0,\pm 1), \quad k_i\mapsto k_i, \quad C\mapsto C. \tag{4.21}$$

We shall show the existence of the inverse mapping of this homomorphism.

First we note that for each $i=0$, 1, there exists a homomorphism $\rho_i:U'\to A$ determined by

$$\begin{gathered} e_1\mapsto x_{i,0}^{+}, \quad f_1\mapsto x_{i,0}^{-}, \quad t_1\mapsto k_i, \\ e_0\mapsto Ck_i^{-1}x_{i,1}^{-}, \quad f_0\mapsto x_{i,-1}^{+}k_iC^{-1}, \quad t_0\mapsto Ck_i^{-1}. \end{gathered} \tag{4.22}$$

For example, since $[e_0,e_1]_{q^{-2}}\mapsto k_i^{-1}[x_{i,0}^{-},x_{i,1}^{+}]$, we get $[[e_0,e_1]_{q^{-2}},e_1]\mapsto -[2]x_{i,1}^{+}$. Therefore relation (3.6) with $i=1$ and $j=0$ is preserved. Set

$$X_{i,k}^{\pm}=\rho_i(x_k^{\pm}) \ \text{ and } \ H_{i,r}=\rho_i(h_r). \tag{4.23}$$

Then by the definition of ρ_i we have $X_{i,0}^{\pm}=x_{i,0}^{\pm}$ and $X_{i,\mp 1}^{\pm}=x_{i,\mp 1}^{\pm}$. This implies that $H_{i,\pm 1}$ and $X_{i,\mp 2}^{\pm}$ defined above coincide with those in the proposition. Moreover we have $X_{i,\pm 1}^{\pm}=x_{i,\pm 1}^{\pm}$ since the following equalities hold:

$$[H_{i,r},x_{i,0}^{\pm}]=\pm[2]C^{(r\mp|r|)/2}x_{i,r}^{\pm} \ \text{ for } \ r=\pm 1. \tag{4.24}$$

Next we prove that the assignment

$$x_{i,k}^{\pm}\mapsto X_{i,k}^{\pm},\quad h_{i,r}\mapsto H_{i,r},\quad k_i\mapsto k_i,\quad C\mapsto C, \tag{4.25}$$

defines the desired homomorphism $\mathcal{U}'\to A$. Since the ρ_i's are homomorphisms, the relations of $\mathcal{U}'$ among the generators with the same subscript $i=j$ are clearly preserved. Relations (2.5) and (2.7) with $i\neq j$ are checked by using the fact $k_0k_1\in Z(A)$. Relation (2.11) is clearly preserved. Relations (2.6) and (2.8) [resp. (2.9)] with $i\neq j$ are checked, using Lemma 5 (1) [resp. (2)] below. This completes the proof of the existence of the map. Since $X_{i,k}^{\pm}=x_{i,k}^{\pm}$ for $k=0,\pm1$, this map is the inverse mapping of the one in the first paragraph.

(2) Since $A\simeq\mathcal{U}'$, relations (4.14) hold and the elements (4.15) and (4.16) are central in A. So we can see the existence of a homomorphism $B\to A$.

Clearly there exists an anti-homomorphism $A\to B$ such that

$$x_{i,k}^{\pm}\mapsto x_{i,-k}^{\pm},\quad k_i\mapsto k_i^{-1},\quad C\mapsto C. \tag{4.26}$$

The composition of this map and the anti-automorphism η of $A(\simeq\mathcal{U}')$ gives the inverse mapping of the preceding homomorphism. □

Finally, to complete the proof of Proposition 5, we prove the following lemma.

Lemma 5: In A, the following hold:

(1) $H_{0,r}+H_{1,r}\in Z(A)$ *for any* $r(\neq0)$.

(2) $[X_{i,k}^{+},X_{j,l}^{-}]=0$ *for* $i\neq j$ *and any k,l.*

Proof: Throughout this proof let $i\neq j\in\{0,1\}$. We prove in three steps.

(i) Proof of (1) with $|r|=1,2$. First we consider the case $|r|=1$. It is easy to check the equalities $[x_{i,0}^{\pm},X_{j,\pm2}^{\mp}]=0(i\neq j)$. Using these, we can show that $H_{0,r}+H_{1,r}$ commutes with the elements $x_{i,0}^{\pm}$, $x_{i,\mp1}^{\pm}$, $k_i(i=0,1)$ and C. Recalling the definition of $H_{i,\pm1}$ and using (4.24), we find from the above that $H_{0,r}+H_{1,r}$ also commutes with $H_{i,\pm1}$ and $x_{i,\pm1}^{\pm}$. This completes the proof. Clearly $H_{0,r}+H_{1,r}$ commutes with k_i and C. The fact $H_{0,\pm1}+H_{1,\pm1}\in Z(A)$ implies

$$[H_{0,r}+H_{1,r},H_{i,\pm1}]=[H_{i,r},H_{i,\pm1}]-[H_{j,r},H_{j,\pm1}]=0.$$

Therefore, noting (4.24), we can see that to prove (1) for $|r|>1$ it is sufficient to show that $H_{0,r}+H_{1,r}$ commutes with $x_{i,0}^{\pm}(i=0,1)$. Noting this remark and using

$$H_{i,\pm2}=C^{\pm1}k_i^{\mp1}[x_{i,\pm1}^{+},x_{i,\pm1}^{-}]\mp\frac{q-q^{-1}}{2}H_{i,\pm1}^{2},$$

it is easy to prove the case $|r|=2$.

(ii) Proof of (2). Comparing

$$[H_{i,\pm1},[H_{i,\pm1},[X_{i,k}^{+},X_{j,l}^{-}]]]\ \text{ and }\ [H_{i,\pm2},[X_{i,k}^{+},X_{j,l}^{-}]],$$

we find that $[X_{i,k\pm1}^{+},X_{j,l\pm1}^{-}]=0$ follows from $[X_{i,k}^{+},X_{j,l}^{-}]=0$ (†). So it is sufficient to prove the assertion with $l=0$. We show that $[X_{i,k}^{+},X_{j,0}^{-}]=0$ for $0\leqslant|k|\leqslant m$ by induction on m. The case $m=1$ holds thanks to (4.8) and the fact $X_{i,k}^{\pm}=x_{i,k}^{\pm}$ $(k=0,\pm1)$. Suppose that the case $m(\geqslant1)$ holds. Then

$$0=\frac{C^{(1\mp1)/2}}{[2]}[H_{i,\pm1},[X_{i,\pm m}^{+},X_{j,0}^{-}]]=[X_{i,\pm(m+1)}^{+},X_{j,0}^{-}]+C[X_{i,\pm m}^{+},X_{j,\pm1}^{-}]$$

and the second term on the right-most side vanishes thanks to the induction assumption and (†). So we get the case $m+1$.

(iii) Proof of (1) with $|r|\geqslant3$. We prove the case $r\geqslant3$. The proof of the case $r\leqslant-3$ is similar. Set

$$P_{i,0}=1,\quad P_{i,k}=(q-q^{-1})C^l k_i^{-1}[X^+_{i,k-l},X^-_{i,l}]\ \text{ for }\ k>0,$$
$$Q_{ij,m}=\sum_{\substack{s+t=m\\ s,t\geqslant 0}} P_{i,s}P_{j,t}\ \text{ for }\ m\geqslant 0, \tag{4.27}$$

where l is any integer. Using (4.6) and (4.11), calculate the commutator of $P_{i,k+1}$ (with $l=k$) with $x^+_{m,0}$ and that of $P_{i,k+1}$ (with $l=1$) with $x^-_{m,0}$ $(m=0,1)$. Then we get

$$[P_{i,k+1},x^\pm_{j,0}]=C^{(1\mp 1)/2}(q^{\mp 2}P_{i,k}x^\pm_{j,1}-q^{\pm 2}x^\pm_{j,1}P_{i,k}),$$
$$[P_{i,k+1},x^\pm_{i,0}]=C^{(1\mp 1)/2}(q^{\pm 2}P_{i,k}x^\pm_{i,1}-q^{\mp 2}x^\pm_{i,1}P_{i,k}), \tag{4.28}$$

for $k\geqslant 0$. From this we obtain

$$[Q_{ij,m+1},x^\pm_{i,0}]=q^{\mp 2}C^{(1\mp 1)/2}[Q_{ij,m},x^\pm_{i,1}], \tag{4.29}$$

for $m\geqslant 0$.

Now we prove that $H_{0,r}+H_{1,r}\in Z(A)$ for $0<r\leqslant m$ by induction on m. We have already proved this for $m=2$. Suppose that the case $m(\geqslant 2)$ holds. Then

$$[H_{i,r},H_{j,s}]=-[H_{i,r},H_{i,s}]=0\ \text{ for }\ 0<r,s\leqslant m.$$

Noting this and

$$P_i(u):=\sum_{k\geqslant 0} P_{i,k}u^k=\exp\left((q-q^{-1})\sum_{l>0} H_{i,l}u^l\right), \tag{4.30}$$

we find that

$$\sum_{k\geqslant 0} Q_{ij,k}u^k(=P_i(u)P_j(u))\ \text{ and }\ \exp\left((q-q^{-1})\sum_{l>0}(H_{0,l}+H_{1,l})u^l\right)$$

coincide mod $O(u^{m+2})$, so

$$Q_{ij,k}\in Z(A)\ \text{ for }\ 0\leqslant k\leqslant m,$$
$$Q_{ij,m+1}-(q-q^{-1})(H_{0,m+1}+H_{1,m+1})\in Z(A). \tag{4.31}$$

Using this and (4.29), we find that $H_{0,m+1}+H_{1,m+1}$ commutes with $x^\pm_{i,0}$ $(i=0,1)$. Thanks to the remark in (i), this proves the case $m+1$. □

B. Braid group action on $\mathcal{U}'$

Next we show the existence of a braid group action on $\mathcal{U}'$.

Define an automorphism $T_1{}^{12}$ of U' by

$$T_1:\ e_1\mapsto -f_1t_1,\quad f_1\mapsto -t_1^{-1}e_1,\quad t_1\mapsto t_1^{-1},\quad t_0\mapsto t_0t_1^2,$$
$$e_0\mapsto\frac{1}{[2]}[e_1,[e_1,e_0]_{q^{-2}}],\quad f_0\mapsto\frac{1}{[2]}[[f_0,f_1]_{q^2},f_1]. \tag{4.32}$$

Let S denote the automorphism of $\mathcal{U}'$ determined by

$$x^\pm_{i,k}\mapsto(-1)^k x^\pm_{1-i,k},\quad h_{i,r}\mapsto(-1)^r h_{1-i,r},\quad k_i\mapsto k_{1-i},\quad C\mapsto C. \tag{4.33}$$

Let $\mathcal{B}$ be the group defined by generators $\mathcal{T}$, $\mathcal{Y}$, Q and relations

$$\mathcal{T}^{-1}\mathcal{Y}\mathcal{T}^{-1}=\mathcal{Y}^{-1},\quad Q\mathcal{Y}Q^{-1}=\mathcal{Y}^{-1},\quad Q^2=1. \tag{4.34}$$

Let $^-$ denote the automorphism of $\mathcal{B}$ such that

$$\overline{\mathcal{T}}=\mathcal{T},\quad \overline{\mathcal{Y}}=Q\mathcal{T},\quad \overline{Q}=\mathcal{Y}^{-1}\mathcal{T}. \tag{4.35}$$

Proposition 6: (1) There exist automorphisms $\mathcal{T}_0$ and $\mathcal{T}_1$ of $\mathcal{U}'$ determined by

$$\mathcal{T}_1 v=vT_1,\quad \mathcal{T}_1 h=hT_1,\quad \mathcal{T}_0=S\mathcal{T}_1S^{-1}.$$

The inverse $\mathcal{T}_i^{-1}$ is given by $\eta\mathcal{T}_i\eta$.

(2) The automorphisms $\mathcal{T}_i$, $\mathcal{X}_i$ $(i=0,1)$ and S satisfy

$$\mathcal{X}_0\mathcal{X}_1=\mathcal{X}_1\mathcal{X}_0,$$

$$\mathcal{T}_i\mathcal{X}_{1-i}=\mathcal{X}_{1-i}\mathcal{T}_i,$$

$$\mathcal{T}_i^{-1}\mathcal{X}_i\mathcal{T}_i^{-1}=\mathcal{X}_{1-i}^2\mathcal{X}_i^{-1},$$

$$S\mathcal{T}_iS^{-1}=\mathcal{T}_{1-i},\quad S\mathcal{X}_iS^{-1}=\mathcal{X}_{1-i}.$$

Corollary 2: The mapping $\mathcal{T}\mapsto\mathcal{T}_1$, $\mathcal{Y}\mapsto\mathcal{X}_1\mathcal{X}_0^{-1}$, $Q\mapsto S$ defines a $\mathcal{B}$ action on $\mathcal{U}'$.

Proof: We show only the existence of the homomorphism $\mathcal{T}_1$. The remaining claims are proven as in Ref. 4.

Since

$$x_1^+=-T_1^{-1}e_0,\quad x_{-1}^-=-T_1^{-1}f_0,$$

it is easy to show that the automorphism T_1 maps as follows:

$$\begin{gathered}x_0^+\mapsto -x_0^-k,\quad x_0^-\mapsto -k^{-1}x_0^+,\quad k\mapsto k^{-1},\\ x_1^+\mapsto -Ck^{-1}x_1^-,\quad x_{-1}^-\mapsto -x_{-1}^+kC^{-1},\quad C\mapsto C,\\ x_{-1}^+\mapsto\frac{k^2}{[2]}[[x_{-1}^+,x_0^-]_{q^4},x_0^-]_{q^2},\quad x_1^-\mapsto[x_0^+,[x_0^+,x_1^-]_{q^{-4}}]_{q^{-2}}\frac{k^{-2}}{[2]}.\end{gathered} \tag{4.36}$$

Thanks to this, (4.32) and Proposition 5 (2), it is sufficient to show that the assignment

$$\begin{gathered}x_{1,0}^+\mapsto -x_{1,0}^-k_1,\quad x_{1,0}^-\mapsto -k_1^{-1}x_{1,0}^+,\quad k_1\mapsto k_1^{-1},\\ x_{1,1}^+\mapsto -Ck_1^{-1}x_{1,1}^-,\quad x_{1,-1}^-\mapsto -x_{1,-1}^+k_1C^{-1},\quad C\mapsto C,\\ x_{1,-1}^+\mapsto\frac{k_1^2}{[2]}[[x_{1,-1}^+,x_{1,0}^-]_{q^4},x_{1,0}^-]_{q^2},\quad x_{1,1}^-\mapsto[x_{1,0}^+,[x_{1,0}^+,x_{1,1}^-]_{q^{-4}}]_{q^{-2}}\frac{k_1^{-2}}{[2]},\\ x_{0,k}^+\mapsto\frac{1}{[2]}[x_{1,0}^+,[x_{1,0}^+,x_{0,k}^+]_{q^{-2}}],\quad x_{0,k}^-\mapsto\frac{1}{[2]}[[x_{0,k}^-,x_{1,0}^-]_{q^2},x_{1,0}^-]\ \ (k=0,\pm1),\\ k_0\mapsto k_0k_1^2\end{gathered} \tag{4.37}$$

defines a homomorphism $B\to\mathcal{U}'$.

Nearly half of the relations of B are easily shown to be preserved by noting that vT_1 and hT_1 are homomorphisms. For example, $[x^+_{1,0},x^+_{1,-1}]_{q^2}$ is mapped to $vT_1([x^+_0,x^+_{-1}]_{q^2})=0$. The rest of the relations are checked by tedious but straightforward calculations. Here we only note the following two facts:

(i) The above assignment sends $X^{\pm}_{0,\pm 2}$ as

$$X^+_{0,2}\mapsto\frac{1}{[2]}[x^+_{1,0},[x^+_{1,0},x^+_{0,2}]_{q^{-2}}],\quad X^-_{0,-2}\mapsto\frac{1}{[2]}[[x^-_{0,-2},x^-_{1,0}]_{q^2},x^-_{1,0}],$$

and maps the elements (4.10), (4.11), (4.15), and (4.16) to their counterparts in $\mathcal{U}'$.

(ii) To check (4.6) and (4.14) with $i=0$, and (4.8), we need the following simple fact. If X, Y, and Z are elements of an algebra such that

$$[X,[X,[X,Y]_{q^2}]]_{q^{-2}}=0,\quad [X,[X,[X,Z]_{q^2}]]_{q^{-2}}=0,\quad [Y,Z]_{q^2}=0$$

then they satisfy

$$[[X,[X,Y]_{q^{-2}}],[X,[X,Z]_{q^{-2}}]]_{q^2}=0.$$

□

C. Isomorphism *f*

Now we can prove the following proposition:

Proposition 7: (1) There exists an automorphism f of $\mathcal{U}'$ determined by

$$f\upsilon=\tilde{h},\quad f\tilde{h}=\eta\upsilon\sigma.$$

The inverse f^{-1} is given by $\eta f\eta$.

(2) The automorphism f and the $\mathcal{B}$ action in Corollary 2 satisfy

$$f(x\cdot u)=\overline{x}\cdot f(u)\quad (x\in\mathcal{B},u\in\mathcal{U}').$$

Proof: Define elements $\mathbf{x}^{\pm}_{i,k}$ and $\mathbf{k}_i$ $(i=0,1,\ k=0,\pm 1)$ of $\mathcal{U}'$ by

$$\begin{aligned}&\mathbf{x}^{\pm}_{1,k}=(-1)^k\overline{\mathcal{Y}^{\mp k}}x^{\pm}_{1,0},\quad \mathbf{k}_1=k_1,\\ &\mathbf{x}^{\pm}_{0,k}=(-1)^k\overline{Q}\mathbf{x}^{\pm}_{1,k},\quad \mathbf{k}_0=\overline{Q}\mathbf{k}_1.\end{aligned}\tag{4.38}$$

The explicit expressions are

$$\begin{aligned}&\mathbf{x}^{\pm}_{1,0}=x^{\pm}_{1,0},\quad \mathbf{k}_1=k_1,\\ &\mathbf{x}^+_{1,-1}=x^-_{0,0}k_0,\quad \mathbf{x}^+_{1,1}=-\frac{1}{[2]}[[x^+_{0,0},x^+_{1,0}]_{q^{-2}},x^+_{1,0}],\\ &\mathbf{x}^+_{0,0}=x^-_{1,-1}k_1C,\quad \mathbf{k}_0=C^{-1}k_1^{-1},\\ &\mathbf{x}^+_{0,1}=x^+_{0,-1},\quad \mathbf{x}^+_{0,-1}=-\frac{1}{[2]}[x^-_{1,0},[x^-_{1,0},x^-_{0,-1}]_{q^2}]k_0k_1^2C,\\ &\mathbf{x}^{\mp}_{i,k}=q^{\mp 2\delta_{i0}}\zeta\mathbf{x}^{\pm}_{i,-k}.\end{aligned}\tag{4.39}$$

and it is easy to show that they satisfy

$$\mathbf{x}^{\pm}_{1,k}=h(x^{\pm}_k),\quad \mathbf{k}_1=h(k).\tag{4.40}$$

Using the above, we can show that the mapping

$$x_{i,k}^{\pm} \mapsto \mathbf{x}_{i,k}^{\pm}, \quad k_i \mapsto \mathbf{k}_i, \quad C \mapsto k_0 k_1 (= h(C)), \tag{4.41}$$

defines a homomorphism $f : B \to \mathcal{U}'$. We omit the details. The remaining claims of (1) and (2) are proven as in Ref. 4. □

From Eqs. (4.39) and (4.41), we can easily obtain the following corollary.

Corollary 3: (*of the proof*)

The automorphism f satisfies the following identities:

(1) $f\zeta = \zeta f$;
(2) $f\gamma_{a^{-1}} = \delta_a f$.

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The Hausdorff entropic moment problem

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Our aim in this paper is twofold. First, to find the necessary and sufficient conditions to be satisfied by a given sequence of real numbers $\{\omega_n\}_{n=0}^{\infty}$ to represent the ''entropic moments'' $\int_{[0,a]}[\rho(x)]^n dx$ of an unknown non-negative, decreasing and differentiable (*a.e.*) density function $\rho(x)$ with a finite interval support. These moments are called entropic moments because they are closely connected with various information entropies (Renyi, Tsallis, ...). Second, we outline an efficient method for the reconstruction of the density function from the knowledge of its first N entropic moments. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The problem of moments[1,2] asks when a given sequence of complex numbers may be represented as the moments around the origin of a non-negative measure, defined on the line (Hamburger), on a half-line (Stieltjes), on a finite interval (Hausdorff) or on the unit circumference (the trigonometric moment problem).

This is a classical topic in analysis which has illuminated an extraordinary number of scientific subjects from both standpoints, theoretical and applied. Indeed, it has facilitated many developments[3] in function theory, in functional analysis, in spectral representations of operators, in Fourier analysis as well as in probability and statistics. Also, it has numerous applications not only in approximation theory, in numerical mathematics and for the prediction of stochastic processes, but also in linear prediction, in inverse scattering, in digital filtering and for the determination of rigorous relationships among physical quantities of many-particle systems within the framework of the density functional theory as well as in the design of algorithms for simulating physical systems. The latter should not surprise anybody since the own terminology ''problem of moments'' was taken by Stieltjes from Mechanics. Moreover, he used very often physical concepts (mass, stability, electrostatic properties, ...) in solving analytical problems.[1,4]

In this paper, we shall focus our attention on the problem of entropic moments, which differs from the ordinary moment problem above mentioned in that it does not consider the moments-around-the-origin of a density function $\rho(x)$ defined by

$$\mu_n = \int_K x^n \rho(x) dx, \tag{1}$$

but the quantities

$$\omega_n = \int_K [\rho(x)]^n dx, \tag{2}$$

which are called frequency moments of $\rho(x)$, $x \in K$, in probability and statistics.[5–9] The study of these quantities was initiated by Yule following a suggestion of Pearson. Then Sichel[6,7] usefully employed them for the fitting of certain frequency curves. It happens that estimators based on

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frequency moments are, at times, much better than the ordinary moment estimates. Moreover, the frequency moments are fairly efficient in the range where the ordinary moments are very inefficient.[10] This is so in some cases where the range K is unlimited and the density is poorly known.[8]

It is interesting to remark that the frequency moments ω_n are location independent when $K=\mathbb{R}$ (Hamburger case); that is, two densities differing only in location have identical frequency moments. In these cases, the location parameter can be provided by the mode, the median or any other appropriate quantity.[9]

We shall call the quantities ω_n the ''entropic'' moments of the density function $\rho(x)$, because they are closely connected to the so-called Renyi and Tsallis entropies of $\rho(x)$ defined[11,12] by

$$S_q^R := \frac{1}{1-q}\ln\int_K [\rho(x)]^q\,dx; \quad q>0, \quad q\neq 1, \quad \int_K \rho(x)dx=1, \tag{3}$$

and

$$S_q^T := \frac{1}{q-1}\left[1-\int_K [\rho(x)]^q\,dx\right]; \quad q>0, \quad q\neq 1, \quad \int_K \rho(x)dx=1, \tag{4}$$

respectively. The entropic adjective allows us to identify more appropriately the moments ω_n from the other type of moments[8] (moments around the origin, central moments, factorial moments, absolute moments, ...) of a frequency distribution.

In addition, the entropic moments ω_α have various physical meanings depending on the nature of the associated density function ρ (charge density, momentum density, ...). Indeed, they characterize some density functionals which describe certain physical quantities of fundamental and/or experimentally accessible character such as, up to a constant factor, the Thomas–Fermi kinetic energy ($\omega_{5/3}$), the Dirac exchange energy ($\omega_{4/3}$) and the electron average density (ω_2) of the many-electron systems; see, e.g., Ref. 24.

This paper has a twofold aim. First we solve the Hausdorff entropic moment problem in Sec. II, which allows us to characterize a density function by means of its entropic moments. Then, in Sec. III, we describe a practical procedure to reconstruct the density from its entropic moments.

II. THE HAUSDORFF ENTROPIC MOMENT PROBLEM

Let $K=[0,a]$ with $a>0$, and $\mathcal{M}(K)$ the set of real density functions $f(x)$ bounded on K and such that $f(0)=1$ and $f(a)=0$. We have obtained the following result for this set of functions.

Theorem 1: *The necessary and sufficient conditions which the given sequence of positive numbers $\omega_0,\omega_1,\ldots,\omega_n,\ldots$, must satisfy in order that a positive, decreasing and differentiable (a.e.) density function $f(x), x\in K$, having these entropic moments (2) may exist, are given by*

$$\Sigma^k \frac{\omega_{m+1}}{m+1}\geqslant 0 \quad \text{and} \quad \Sigma^k\omega_m\geqslant 0, \tag{5}$$

for $k,m=0,1,2,\ldots$, and being

$$\Sigma^k\omega_m=\omega_m-\binom{k}{1}\omega_{m+1}+\ldots+(-1)^k\omega_{m+k}.$$

Proof: Let us first prove the sufficiency condition. For convenience we adopt the notations

$$\mu_m\equiv\frac{\omega_{m+1}}{m+1}, \quad \nu_m\equiv\omega_m; \quad m=0,1,2,\ldots,$$

so that $\nu_m = m\mu_{m-1}$ for $m=1,2,\ldots$, and $\mu_{-1}\equiv a$. If conditions (5) are fulfilled, the Hausdorff theorem for the ordinary moment problem on the interval $[0,1]$ allows us to state[1] that

$$\exists! z(t)\geqslant 0 \quad \text{on } [0,1], \quad \text{such that } \int_0^1 t^m z(t)\,dt = \nu_m$$

and

$$\exists! g(t)\geqslant 0 \quad \text{on } [0,1], \quad \text{such that } \int_0^1 t^m g(t)\,dt = \mu_m .$$

On the other hand, let us define

$$h(t) = \int_t^1 z(s)\,ds, \quad t\in[0,1].$$

So, $h'(t) = -z(t)$. Moreover, $h(t)$ has the same ordinary moments as $g(t)$; then, they are equal. Thus $g(t)$ is a decreasing function since $g'(t) = -z(t)$. We can define $f(x)$ as its inverse with $x\in[g(1)=0, g(0)=a]$, which will be positive, decreasing and differentiable (*a.e.*). One should realize that in case that $g(t)$ is a constant $c>0$ on some subintervals, this would provoke a jump discontinuity for $f(x)$ in $x=c$ and *vice versa*. Then, it is straightforward to obtain that

$$\int_0^a [f(x)]^m\,dx = \nu_m = \omega_m; \quad m=0,1,2,\ldots \quad .$$

To prove necessity, we define the inverse of $f(x)$ as $h(t)$, $t\in[0,1]$, which is decreasing and differentiable (*a.e.*). A simple change of variable $t=f(x)$ allows us to find the following relationship between the entropic moments of $f(x)$ and the ordinary moments of $h(t)$:

$$m\int_0^a t^m h(t)\,dt = \frac{\omega_{m+1}}{m+1}, \quad m=0,1,2,\ldots \quad .$$

Now we consider the function $z(t) = -h'(t)$, $t\in[0,1]$, and we realize that its ordinary moments are given by ω_m. Then, the direct application of the classical Hausdorff moment above mentioned leads us to the relations (5). □

III. DENSITY RECONSTRUCTION

Associated to any moment problem there exists an inverse problem, namely that of the reconstruction of the corresponding density function. Moreover, in practical purposes we have at our disposal only a finite number of moments. The inverse Hausdorff (ordinary) moment problem (1), that is the determination of the density $\rho(x)$ from the moments around the origin $\{\mu_n\}_{n=0}^{\infty}$, was first proposed by Pafnuty Chebyshev.[13] It is a severely ill-conditioned problem because of the lack of *a priori* information and the large involved numerical instabilities.[14–19] To avoid these instabilities, various regularization methods (Tikhonov, maximum-entropy methods, orthogonal-polynomials based methods,...) have been proposed; see Ref. 16 for a brief survey. The maximum-entropy method has been widely and efficiently used for scientific applications.[16,20–22] It consists in maximizing an entropic functional, and it allows us to find a density estimate which converges to the solution of the problem when the number of the involved moments increases.

Here we shall use a maximum entropy method to solve the inverse Hausdorff entropic moment problem discussed in the previous section when the number of known entropic moments is finite. Based on the proof of Theorem 1, this method first computes the maximum-entropy estimate to the solution $z(t)$ of the inverse Hausdorff problem related to the sequence $\{\mu_n\}_{n=0}^{\infty}$ with $\mu_n \equiv \omega_{n+1}/n+1$. Then, the inverse of the estimated $z(t)$ is the desired approximated solution of

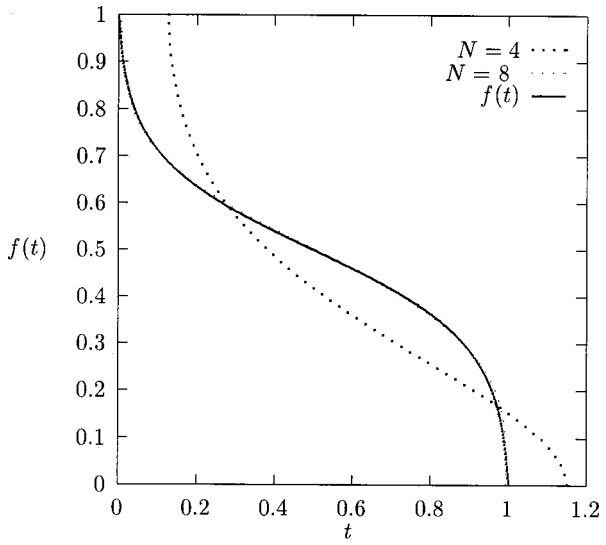

FIG. 1. Graphical representation of the function $f(t)=\frac{1}{2}+\frac{1}{10}\ln[1/(At+B)-1]$ and its estimates from the entropic moments ω_n, $n=0,1,\ldots,N$ with $N=4$ and $N=8$.

our problem. Let us notice that, although we know that the asymptotic ($N\to\infty$) approach to $z(t)$ is inversible, the different Nth estimates to $z(t)$ may not have this property. In the case that there is not any inversible approach, our method is not applicable.

Although we may use any entropic functional to be maximized, we have chosen the Fisher information measure defined by

$$E_f \equiv \int_{[0,a]} \frac{[f'(x)]^2}{f(x)}\,dx,$$

if $f(x)>0$, and $E_f=0$ if $f(x)\equiv 0$. Contrary to other entropic functionals (e.g., Boltzmann–Shannon information entropy, Burg entropy, positive L^2 entropy), this choice has the advantage of taking into account information from the derivative of the function, what is expected to have a strong smoothing effect on the estimate. In doing so we follow the operation lines of Borwein, Limber, and Noll[23] to which we refer for further details.

To illustrate the method and the rate of convergence of the Fisher-information estimates for a function $f(t)$ from its first $N+1$ entropic moments $\omega_n=\int_0^1[f(t)]^n dt$, $n=0,1,\ldots,N$, we have represented in Fig. 1 the exact values and the Fisher estimates for the cases $N=4$ and $N=8$ of a specific function, namely,

$$f(t)=\frac{1}{2}+\frac{1}{10}\ln\left(\frac{1}{At+B}-1\right),\quad \text{with}\quad A=\frac{1}{1+e^5}\quad \text{and}\quad B=\frac{1}{1+e^{-5}}-\frac{1}{1+e^5}. \tag{6}$$

We visually notice in the figure the fast convergence of the method for this function as well as the good precision reached with nine entropic moments.

Finally we show in Fig. 2 the reconstruction of the function $f(t)$ given by (6) from the first $N+1$ moments around the origin $\mu_n=\int_0^1 f(t)t^n\,dt$ in the cases $N=4$ and 8. The comparison of the two figures for the two corresponding Nth cases illustrates that there are functions that may be better estimated or reconstructed from the entropic moments (2) that from the ordinary moments (1). Needless to say that there exist other functions where the reciprocal situation occurs; consider, for example, the inverse of the function $f(t)$ given by Eq. (6).

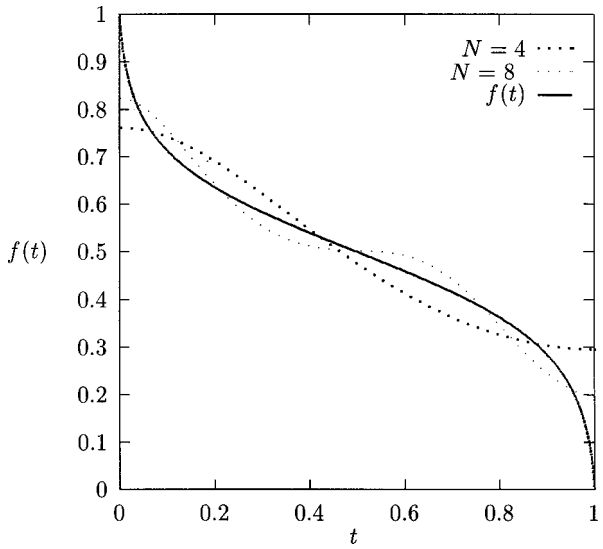

FIG. 2. Graphical representation of the function $f(t)=\frac{1}{2}+\frac{1}{10}\ln[1/(At+B)-1]$ and its estimates from the moments μ_n, $n=0,1,\ldots,N$ with $N=4$ and $N=8$.

IV. CONCLUSIONS

In this paper we have posed the entropic moment problem, whose elements are information measures of an unknown density function. Physically, the entropic moments may also describe some fundamental and/or experimentally accessible quantities of quantum-mechanical systems as already pointed out. Then, we have solved the Hausdorff entropic moment problem by use of some specific properties of the inverse function of the density according to the lines of a recent work of the authors.[24] Moreover, our strategy has let us outline a maximum-entropy method based on an algorithm of minimization of the Fisher information measure[23] which allows one to solve the inverse finite Hausdorff entropic moment problem; that is, to determine the density function from its first few entropic moments. We realize that other density reconstruction procedures which do not include the previous determination of the inverse density function (which would avoid the requirement of decreasing behavior for the density) would be desirable.

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Asymptotic limits of SU(2) and SU(3) Wigner functions

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Asymptotic limits are given for the SU(2) Wigner $\mathcal{D}^j_{mn}$ functions as $j\to\infty$ for three domains of m and n. Similar asymptotic limits are given for the SU(3) Wigner functions of an irrep with highest weight $(\lambda,0)$ as $\lambda\to\infty$. The results are shown to be relevant to the analysis of experiments with quantum interferometers. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1358305]

I. INTRODUCTION

The asymptotic properties of Wigner functions provide a classical interpretation of these functions. This is of interest, for example, for the design and interpretation of quantum interferometer experiments. It is known that a passive optical element which linearly transforms two input modes (beams) into two output modes, is represented by a U(2) transformation.[1–4] Similarly, a three-mode passive element is represented by a U(3) transformation.[5,6] Typically, the input modes in multimode interferometry are minimal uncertainty wave packets containing large photon numbers;[7] as a result, the relevant U(2) and U(3) transformations are close to corresponding classical limits.

We show that different asymptotic limits correspond to different classical situations and/or to group (and Lie algebra) contractions. For example, in one limit, the group SU(2) contracts to the Euclidean group E(2) and, in another, it contracts to the Heisenberg–Weyl group HW(2) of the two-dimensional harmonic oscillator. Thus, the SU(2) Wigner functions, in the corresponding limits, approach those of E(2) and HW(2), respectively. Similar contractions apply to SU(3).

Some asymptotic limits of the SU(2) Wigner functions are known.[8–14] Others can be inferred from known limits of the Jacobi polynomials $\{P_n^{(\alpha,\beta)}\}$ to which the reduced SU(2) Wigner d functions are related.[15] In particular, the following limits can be found in Szegö's book[8] and elsewhere:

$$H_n(x)=n!\lim_{\lambda\to\infty}\lambda^{-n/2}P_n^{(\lambda)}(x/\lambda), \tag{1}$$

$$L_n^{(\alpha)}(x)=\lim_{\beta\to\infty}P_n^{(\alpha,\beta)}(1-2x/\beta), \tag{2}$$

$$J_\alpha(x)=\lim_{n\to\infty}\left(\frac{x}{2n}\right)^\alpha P_n^{(\alpha,\beta)}(\cos(x/n)), \tag{3}$$

where $P_n^{(\lambda)}$ is an ultraspherical polynomial, H_n is a Hermite polynomial, $L_n^{(\alpha)}$ is a Laguerre polynomial, and J_α is a Bessel function. These classical limits hold for any finite value of the variable x. Hence, they give the asymptotic limits of the SU(2) d functions for values of their

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arguments close to 0 or $\pi/2$. For the applications we have in mind, the asymptotic behavior of d functions is required over most of the range of its argument. This is not given by the classical limits of Eqs. (1)–(3). For example, it would be wrong to conclude from Eq. (1) that the value of $P_n^{(\lambda)}(x)$ approaches the value $\lambda^{n/2}H_n(\lambda x)/n!$ as $\lambda\to\infty$.

An example of the kind of classical limit we seek has been derived by Arecchi *et al.*[11] who show that, for finite $l+m$, the values $d^l_{0m}(\beta)$ of the d functions that are proportional to spherical harmonics become proportional to $u_{l+m}(\sqrt{l}(\beta-\pi/2))$ as $l\to\infty$, where u_n is a harmonic oscillator wave function. It is shown in this paper, that asymptotic expressions of this kind can be extended to arbitrary $d^j_{m,\pm(j-\nu)}$ for finite m and ν. We also give asymptotic expressions for d^j_{mn} that apply when m and n are both finite and other expressions that apply when $j\pm m$ and $j\pm n$ are both finite. We also show by numerical examples that the limits are approached rapidly with increasing j and that, between them, the three sets of expressions given cover the range of possible m and n values for a given set of d^j_{mn} functions.

The asymptotic expressions derived for SU(2) in Sec. II are applied, in Sec. III, to give corresponding limits for the SU(3) Wigner functions for an irrep of highest weight $(\lambda,0)$.

Applications to quantum interferometers are considered briefly in the concluding section.

II. LIMITS OF SU(2) WIGNER FUNCTIONS

The complex extension of the SU(2) Lie algebra is spanned by 2×2 complex matrices $\{J_0,J_+,J_-\}$ which satisfy the commutation relations

$$[J_0,J_\pm]=\pm J_\pm,\quad [J_+,J_-]=2J_0. \tag{4}$$

We consider an irrep in which these elements are represented by operators $\{\hat J_0,\hat J_+,\hat J_-\}$ which act, in the usual way, on a $(2j+1)$-dimensional Hilbert space spanned by vectors $\{|jm\rangle; m=-j,\ldots,+j\}$:

$$\begin{aligned}\hat J_0|jm\rangle&=m|jm\rangle,\\ \hat J_\pm|jm\rangle&=\sqrt{(j\mp m)(j\pm m+1)}\ \ |jm\pm1\rangle.\end{aligned} \tag{5}$$

Wigner functions for SU(2) are defined by

$$\mathcal{D}^j_{mn}(\alpha,\beta,\gamma)=e^{-im\alpha}d^j_{mn}(\beta)e^{-in\gamma}, \tag{6}$$

where

$$d^j_{mn}(\beta)=\langle jm|e^{-i\beta\hat J_y}|jn\rangle, \tag{7}$$

with $\hat J_y=-\frac{1}{2}i(\hat J_+-\hat J_-)$, is the so-called reduced Wigner function. We consider asymptotic expressions for $d^j_{mn}(\beta)$ as $j\to\infty$, in three situations: (i) when $n\approx j$ and $m^2\ll j^2$, (ii) when $m\approx n$ and $m^2\approx j^2$, and (iii) when $m\approx n$ and $m^2\ll j^2$.

A. Harmonic oscillator limits

For $n=j$, the reduced Wigner function, d^j_{mn}, is given by

$$d^j_{mj}(\beta)=\sqrt{\frac{(2j)!}{(j+m)!(j-m)!}}(\cos\beta/2)^{j+m}(\sin\beta/2)^{j-m}. \tag{8}$$

The derivative of this function vanishes when $\beta=\beta_m$, where β_m is the semiclassical angle for which $\cos\beta_m=m/j$. For this angle

$$\cos(\beta_m/2)=\sqrt{\frac{j+m}{2j}},\quad \sin(\beta_m/2)=\sqrt{\frac{j-m}{2j}}, \tag{9}$$

and the substitutions

$$\beta-\beta_m=2\phi,\quad j+m=s,\quad j-m=d, \tag{10}$$

give

$$\begin{aligned}(\cos\beta/2)^{j+m}&=(s/2j)^{s/2}[\cos\phi-\sqrt{d/s}\sin\phi]^s,\\ (\sin\beta/2)^{j+m}&=(d/2j)^{d/2}[\cos\phi+\sqrt{s/d}\sin\phi]^d.\end{aligned} \tag{11}$$

Defining the two functions

$$X(\phi)=\cos\phi-\sqrt{\frac{d}{s}}\sin\phi,\quad Y(\phi)=\cos\phi+\sqrt{\frac{s}{d}}\sin\phi, \tag{12}$$

then gives

$$d^j_{mj}(\beta)=\sqrt{\frac{(2j)!}{s!d!}\frac{s^s d^d}{(2j)^{2j}}}X(\phi)^s\,Y(\phi)^d. \tag{13}$$

The functions $X(\phi)$ and $Y(\phi)$ satisfy

$$\frac{dX(\phi)}{d\phi}=-\sqrt{\frac{d}{s}}Y(\phi),\quad \frac{dY(\phi)}{d\phi}=\sqrt{\frac{s}{d}}X(\phi), \tag{14}$$

so that

$$f(\phi)=X(\phi)^sY(\phi)^d \tag{15}$$

satisfies the equation

$$\frac{df}{d\phi}=\sqrt{sd}\frac{X^2-Y^2}{XY}f. \tag{16}$$

For small values of ϕ,

$$\sqrt{sd}\,(X^2-Y^2)\approx-4j\sin\phi\cos\phi,\quad XY\approx\cos^2\phi. \tag{17}$$

Thus

$$\frac{df}{d\phi}\approx-4j\frac{\sin\phi}{\cos\phi}f(\phi), \tag{18}$$

with solution

$$X(\phi)^s\,Y(\phi)^d=f(\phi)\approx(\cos\phi)^{4j}. \tag{19}$$

When $s=j+m$ and $d=j-m$ are both large, the asymptotic expression for the factorials[16]

$$z!\to\sqrt{\frac{2\pi}{z}}e^{-z}z^{z+1}, \tag{20}$$

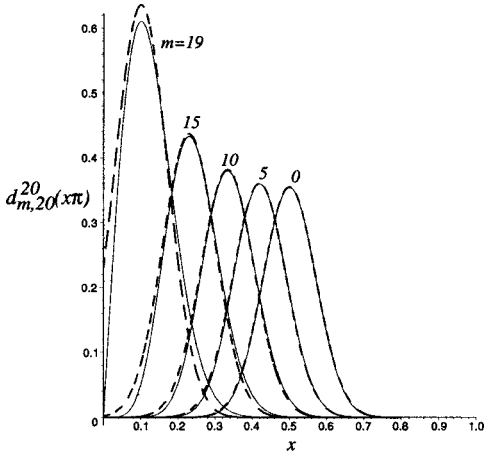

FIG. 1. The reduced Wigner function $d^j_{mj}(x\pi)$ for $j=20$ and various values of m. Exact values are shown as thin continuous lines and asymptotic values, given by Eq. (22), as broken heavy lines.

gives

$$\sqrt{\frac{(2j)!}{s!d!}\frac{s^s d^d}{(2j)^{2j}}} \to \left(\frac{j}{\pi s d}\right)^{1/4}. \tag{21}$$

Combining this expression with Eq. (19) gives the asymptotic expression, for large values of $j+m$ and $j-m$

$$\begin{aligned} d^j_{mj}(\beta) = (-1)^{j-m} d^j_{jm}(\beta) &\to \left(\frac{1}{\sqrt{j\,\pi}\sin\beta_m}\right)^{1/2} [\cos((\beta-\beta_m)/2)]^{4j} \\ &\to \left(\frac{1}{\sqrt{j\,\pi}\sin\beta_m}\right)^{1/2} \exp[-j(\beta-\beta_m)^2/2]. \end{aligned} \tag{22}$$

This asymptotic expression is compared with the exact result for a range of values of m for $j=20$ in Fig. 1. It is seen to be remarkably accurate even for m close to j. It breaks down for $m=\pm j$ but then we have

$$\begin{aligned} d^j_{jj}(\beta) &= [\cos(\beta/2)]^{2j} \to \exp[-j\beta^2/4], \\ d^j_{-jj}(\beta) &= [\sin(\beta/2)]^{2j} \to \exp[-j(\beta-\pi)^2/4]. \end{aligned} \tag{23}$$

These results have a simple classical interpretation. A state with angular momentum j and z component $m=j$ is a minimal uncertainty state. It has a density function $|\psi_{jj}(\theta,\varphi)|^2$ that is independent of φ and concentrated about the $\theta=0$ direction (the z axis). The rate of falloff of the density with increasing angle is indicated by

$$\langle jj|e^{-i\beta\hat{J}_y}|jj\rangle = d^j_{jj}(\beta), \tag{24}$$

which, as seen from Eq. (23), decreases rapidly with increasing β, for large values of j. This is what one would expect from classical mechanics where the angular momentum vector is directed along the z axis when $m=j$. By the same token, a classical angular-momentum vector with z-component m makes an angle β_m with the z axis with $\cos\beta_m = m/j$. Thus, the rotated state $e^{-i\beta_m\hat{J}_y}|jj\rangle$ is expected to have maximum overlap with the state $|jm\rangle$ and conversely the overlap

$$\langle jm|e^{-i\beta\hat{J}_y}|jj\rangle = d^j_{mj}(\beta) \tag{25}$$

is expected to peak at a value of β equal to β_m, as indeed it does.

A significant property of the above asymptotic limits are that they are all simple harmonic oscillator coherent states; i.e., harmonic oscillator ground-state wave functions centered about β_m. We now show that, in the $j\to\infty$ limit, the other d^j_{mn} functions, for m small and $n\approx j$, approach excited harmonic oscillator coherent states.

Consider first the d^l_{0n} function, which for integer values of l, is proportional to a spherical harmonic

$$d^l_{0n}(\theta) = (-1)^n \sqrt{\frac{4\pi}{2l+1}}\, Y_{ln}(\theta,0). \tag{26}$$

For $l\to\infty$, we have, from Eq. (22), the limit

$$d^l_{0l}(\theta)\to\left(\frac{1}{\sqrt{l\pi}}\right)^{1/2} \exp[-l(\theta-\pi/2)^2/2]; \tag{27}$$

which is a harmonic oscillator ground-state wave function centered about $\theta=\pi/2$. Let $n=l-\nu$, so that $\nu\ll l$ when $n\approx l$. Thus, if $\psi_{l\nu}$ denotes the function

$$\psi_{l\nu}(\theta) = (-1)^\nu d^l_{0,l-\nu}(\theta+\pi/2) = (-1)^l \sqrt{\frac{4\pi}{2l+1}}\, Y_{l,l-\nu}(\theta+\pi/2,0), \tag{28}$$

then, in the $l\to\infty$ limit,

$$\psi_{l0}(\theta)\to\left(\frac{1}{\sqrt{l\pi}}\right)^{1/2} e^{-l\theta^2/2} = l^{-1/4} u_0(\sqrt{l}\,\theta), \tag{29}$$

where u_0 is the harmonic oscillator ground-state wave function.

For $l\gg\nu$ and $l\to\infty$, the limits

$$\begin{aligned} \hat{J}_+ Y_{l,l-\nu} &= \sqrt{\nu(2l-\nu+1)}\, Y_{l,l-\nu+1} \to \sqrt{2l\nu}\, Y_{l,l-\nu+1}, \\ \hat{J}_- Y_{l,l-\nu} &= \sqrt{(2l-\nu)(\nu+1)}\, Y_{l,l-\nu-1} \to \sqrt{2l(\nu+1)}\, Y_{l,l-\nu-1}, \end{aligned} \tag{30}$$

imply that the angular momentum raising and lowering operators contract to harmonic oscillator lowering and raising operators, respectively. From the explicit expression for the actions of the $\hat{J}_\pm$ operators on spherical harmonic oscillators, we also have

$$[\hat{J}_\pm Y_{l,l-\nu}](\theta+\pi/2,0) = \left[(l-\nu)\tan\theta \pm \frac{d}{d\theta}\right] Y_{l,l-\nu}(\theta+\pi/2,0) \tag{31}$$

so that, for small θ and $l\gg\nu$,

$$[\hat{J}_\pm Y_{l,l-\nu}](\theta+\pi/2,0) \to \left(l\theta \pm \frac{d}{d\theta}\right) Y_{l,l-\nu}(\theta+\pi/2,0). \tag{32}$$

It follows that, in the $l\to\infty$ limit,

$$\psi_{l,\nu+1}(\theta) = \frac{1}{\sqrt{2l(\nu+1)}}\left(l\theta - \frac{d}{d\theta}\right)\psi_{l\nu}(\theta) = \frac{1}{\sqrt{(\nu+1)}}\,\frac{1}{\sqrt{2}}\left(\sqrt{l}\,\theta - \frac{1}{\sqrt{l}}\,\frac{d}{d\theta}\right)\psi_{l\nu}(\theta), \tag{33}$$

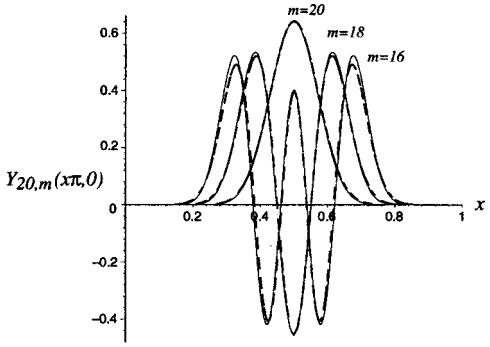

FIG. 2. Spherical harmonics $Y_{20,m}(\theta,\varphi)$ for $m=20$, 18, and 16 plotted as a function of θ for $\varphi=0$. Exact values are shown as fine continuous lines and asymptotic values, given by Eq. (37), as heavy dashed lines.

thereby providing a recursion relation for the $\psi_{l\nu}$ functions. Since ψ_{l0} is a harmonic oscillator ground-state wave function, the recursion relation is easily solved to give

$$\psi_{l\nu}(\theta)\rightarrow l^{-1/4}u_{\nu}(\sqrt{l}\,\theta), \tag{34}$$

where u_{ν} is the harmonic oscillator wave function

$$u_{\nu}(x)=\left(\frac{1}{\sqrt{\pi}2^{\nu}\nu!}\right)^{1/2}H_{\nu}(x)\,e^{-x^2/2} \tag{35}$$

with H_{ν} a Hermite polynomial. Thus, we obtain the asymptotic limit of the Wigner function for $\nu\ll l$ and $l\rightarrow\infty$,

$$d^{l}_{0,l-\nu}(\beta)\rightarrow(-1)^{\nu}l^{-1/4}u_{\nu}(\sqrt{l}\,(\beta-\pi/2)), \tag{36}$$

and the corresponding asymptotic expression for a spherical harmonic

$$Y_{l,m}(\theta,0)=(-1)^{m}\sqrt{\frac{2l+1}{4\pi}}\,d^{l}_{0,m}(\theta)\rightarrow(-1)^{l}\sqrt{\frac{2l+1}{4\pi}}\,l^{-1/4}u_{l-m}(\sqrt{l}(\theta-\pi/2)), \tag{37}$$

when $m\approx l$. The latter expression accords with the result obtained by Arecchi *et al.*[11] after correction for what are presumed to be typographical errors.

The asymptotic expression for Y_{lm} is compared with exactly computed spherical harmonics for $l=20$ and $m=20$, 18, and 16, in Fig. 2. Comparisons for $l=20$ and $m=19$, 17, and 15 are

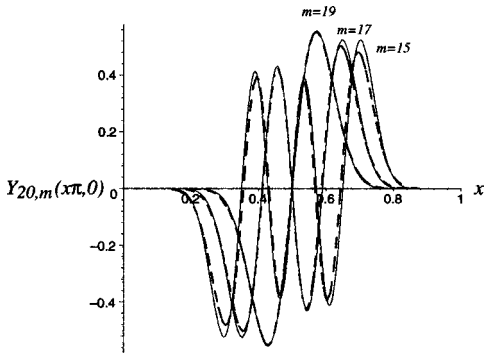

FIG. 3. Spherical harmonics $Y_{20,m}(\theta,\varphi)$ for $m=19$, 17, and 15 plotted as a function of θ for $\varphi=0$. Exact values are shown as fine continuous lines and asymptotic values, given by Eq. (37), as heavy dashed lines.

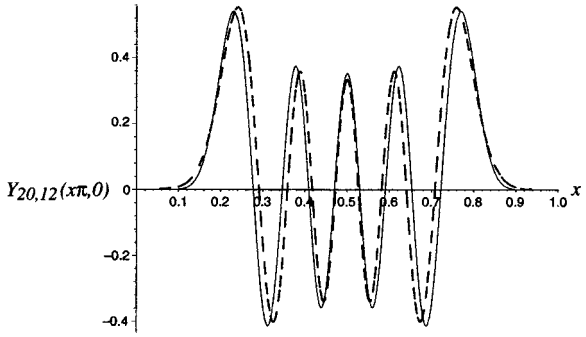

FIG. 4. The spherical harmonic $Y_{20,12}(\theta,\varphi)$. Exact values are shown as a fine continuous line and asymptotic values, given by Eq. (37) multiplied by a factor $1/\sqrt{\sin\theta}$, are shown as a heavy dashed line.

shown in Fig. 3. Even for finite values of l the agreement is excellent for θ near $\pi/2$. It deteriorates as θ approaches 0 or π. This can be attributed in part to the fact that the volume element for the spherical harmonics is $\sin\theta d\theta$ whereas the corresponding harmonic oscillator wave functions are normalized without the factor $\sin\theta$. Thus, one expects better agreement if the asymptotic expressions are renormalized by a factor $1/\sqrt{\sin\theta}$. This indeed turns out to be the case. Figure 4 shows that, with this adjustment, quite good agreement can be obtained even for $m=12$.

A similar analysis can be applied to other d functions. For $l\gg\nu$ and $j\to\infty$, the equations

$$\begin{aligned}\hat{J}_+ d^j_{m,j-\nu} &= \sqrt{\nu(2j-\nu+1)}\, d^j_{m,j-\nu+1} \to \sqrt{2j\nu}\, d^j_{m,j-\nu+1},\\ \hat{J}_- d^j_{m,j-\nu} &= \sqrt{(2j-\nu)(\nu+1)}\, d^j_{m,j-\nu-1} \to \sqrt{2j(\nu+1)}\, d^j_{m,j-\nu-1}\end{aligned} \tag{38}$$

imply that $\hat{J}_\pm$ can again be interpreted as harmonic oscillator raising and lowering operators. Starting with the shifted harmonic oscillator wave functions

$$d^j_{mj}(\beta) \to \left(\frac{1}{\sqrt{j\pi}\sin\beta_m}\right)^{1/2} e^{-j(\beta-\beta_m)^2/2} = \left(\frac{1}{\sqrt{j}\sin\beta_m}\right)^{1/2} u_0(\sqrt{j}\,(\beta-\beta_m)), \tag{39}$$

we find, for small values of ν that

$$d^j_{m,j-\nu}(\beta) \to (-1)^\nu \left(\frac{1}{\sqrt{j}\sin\beta_m}\right)^{1/2} u_\nu(\sqrt{j}(\beta-\beta_m)) \tag{40}$$

as $j\to\infty$, and

$$d^j_{j-\nu,m}(\beta) \to (-1)^{j-m} \left(\frac{1}{\sqrt{j}\sin\beta_m}\right)^{1/2} u_\nu(\sqrt{j}(\beta-\beta_m)). \tag{41}$$

Similarly, from the symmetry properties of the d-functions,

$$d^j_{m,\nu-j}(\beta) \to (-1)^{j+m} \left(\frac{1}{\sqrt{j}\sin\beta_m}\right)^{1/2} u_\nu(\sqrt{j}\,(\beta-\beta_m)) \tag{42}$$

and

$$d^j_{\nu-j,m}(\beta) \to (-1)^\nu \left(\frac{1}{\sqrt{j}\sin\beta_m}\right)^{1/2} u_\nu(\sqrt{j}(\beta-\beta_m)). \tag{43}$$

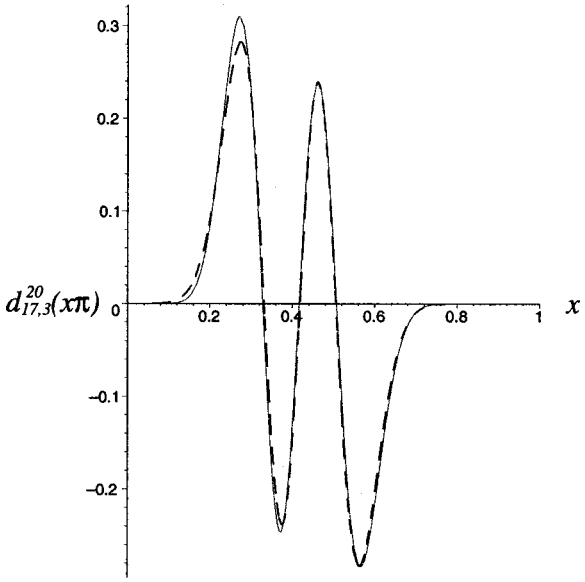

FIG. 5. The Wigner function $d^{20}_{17,3}$ compared to its asymptotic harmonic oscillator limit. Exact values are shown as a fine continuous line and asymptotic values, given by Eq. (41), as a dashed line.

Figure 5 shows the function $d^{20}_{17,3}$ compared to its asymptotic harmonic oscillator limit. Again further improvement in the limit can be obtained by dividing the asymptotic expression by $\sqrt{\sin\beta}$.

B. The SU(2)→HW(2) contraction

The above harmonic oscillator limits for d^j_{mn} apply when m is small and n is close to $\pm j$ (or vice versa). They are at their best, for finite values of j, when β is close to the appropriate semiclassical angle and deteriorate as β approaches 0 or π. When $m\approx n$, there are other asymptotic limits which derive from contractions of the SU(2) Lie algebra.

We consider here a HW(2) contraction of SU(2) which follows from the Holstein–Primakoff[17] representation in which the angular momenta are realized as the operators

$$\hat{J}_0=j-\hat{n},\quad \hat{J}_+=\sqrt{2j-\hat{n}}\,a,\quad \hat{J}_-=a^\dagger\sqrt{2j-\hat{n}}; \tag{44}$$

$a^\dagger$ and a are the raising and lowering operators of a simple harmonic oscillator with commutation relation

$$[a,a^\dagger]=I, \tag{45}$$

and $\hat{n}=a^\dagger a$ is the number operator. In this representation, a state $|jm\rangle$ becomes a simple harmonic oscillator state $|\mu\rangle$ having $\mu=j-m$ quanta, for which $\hat{n}|\mu\rangle=\mu|\mu\rangle$. It follows that, when acting on states for which m is close to some value $\bar{m}\gg -j$, the angular momentum operators approach the asymptotic forms

$$\hat{J}_0\to jI-a^\dagger a,\quad \hat{J}_+\to\sqrt{j+\bar{m}}\,a,\quad \hat{J}_-\to\sqrt{j+\bar{m}}\,a^\dagger. \tag{46}$$

Likewise $\hat{J}_y\to\frac{1}{2}i\sqrt{j+\bar{m}}(a^\dagger-a)$ and, for m and n both close to $\bar{m}=\frac{1}{2}(m+n)$,

$$d^j_{mn}(\beta)\to\langle j-m|e^{(1/2)\,\beta\sqrt{j+\bar{m}}\,(a^\dagger-a)}|j-n\rangle. \tag{47}$$

The last expression, derived from a contraction limit of the SU(2) Lie algebra, is at its best for small values of β and for m and n far from $-j$. A similar expression holds for m and n far from $+j$.

From the identity

$$e^{\alpha(a^\dagger - a)} = e^{\alpha a^\dagger} e^{-\alpha^2/2} e^{-\alpha a}, \tag{48}$$

it follows that

$$\begin{aligned}\langle \mu | e^{\alpha(a^\dagger - a)} | \nu \rangle &= \frac{1}{\sqrt{\mu!\,\nu!}} \langle 0 | a^\mu e^{\alpha a^\dagger} e^{-\alpha a} (a^\dagger)^\nu | 0 \rangle e^{-\alpha^2/2} \\ &= \frac{1}{\sqrt{\mu!\,\nu!}} \langle 0 | (a+\alpha)^\mu (a^\dagger - \alpha)^\nu | 0 \rangle e^{-\alpha^2/2} \\ &= \sqrt{\frac{\nu!}{\mu!}} \sum_p \binom{\mu}{p} \frac{(-\alpha^2)^{\nu-p}}{(\nu-p)!} \alpha^{\mu-\nu} e^{-\alpha^2/2}.\end{aligned} \tag{49}$$

Now recall[16] that, for $\mu - \nu > -1$,

$$\sum_p \binom{\mu}{p} \frac{(-\alpha^2)^{\nu-p}}{(\nu-p)!} = L_\nu^{(\mu-\nu)}(\alpha^2), \tag{50}$$

where $L_\nu^{(\mu-\nu)}$ is a generalized Laguerre polynomial. Thus, for $\mu - \nu > -1$, we obtain the identity

$$\langle \mu | e^{\alpha(a^\dagger - a)} | \nu \rangle = \sqrt{\frac{\nu!}{\mu!}}\, \alpha^{\mu-\nu} L_\nu^{(\mu-\nu)}(\alpha^2)\, e^{-\alpha^2/2} \tag{51}$$

and, with $\alpha = \frac{1}{2}\beta\sqrt{j+(m+n)/2}$, we obtain the asymptotic expression

$$d^j_{mn}(\beta) \to \sqrt{\frac{(j-n)!}{(j-m)!}} (a_{jmn}\beta)^{n-m} L_{j-n}^{(n-m)}(a_{jmn}^2\beta^2)\, e^{-a_{jmn}^2\beta^2/2}, \quad \text{for } m \leqslant n, \tag{52}$$

where $a_{jmn} = \frac{1}{2}\sqrt{(2j+m+n)/2}$. This expression is valid for small values of β and $j+\overline{m} \gg n-m$. For $m \geqslant n$ and $j+\overline{m} \gg m-n$, the identity $d^j_{mn}(\beta) = d^j_{nm}(-\beta)$ gives

$$d^j_{mn}(\beta) \to \sqrt{\frac{(j-m)!}{(j-n)!}} (-a_{jmn}\beta)^{m-n} L_{j-m}^{(m-n)}(a_{jmn}^2\beta^2)\, e^{-a_{jmn}^2\beta^2/2}, \quad \text{for } m \geqslant n. \tag{53}$$

The asymptotic expression (53) for $d^{20}_{18,15}$ is compared with the exactly computed function in Fig. 6.

Other expressions are obtained from the symmetry properties of the d^j_{mn} functions. For example, an asymptotic expression for m close to $-j$ and n close to $+j$ is obtained from the identity

$$d^j_{mn}(\beta) = (-1)^{j-m} d^j_{-mn}(\beta + \pi). \tag{54}$$

These limits are approached for the largest range of β when m and n are similar and close to $\pm j$. This is because the SU(2)$\to$HW(2) contraction is valid to within some specified accuracy over the largest span of $\{|jm\rangle\}$ states when $|m|$ is close to j.

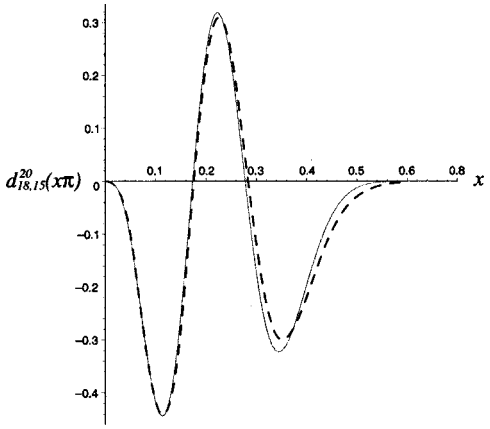

FIG. 6. The reduced Wigner function $d^{20}_{18,15}(x\pi)$. Exact values are shown as a fine continuous line and asymptotic values, given by Eq. (53), as a dashed line.

C. The SU(2)→E(2) contraction limit

For m close to n and both far from $\pm j$, a more appropriate contraction is the one in which SU(2)→E(2), where E(2) is the Euclidean group of transformations of the two-dimensional plane. This limit is obtained from the observation that, as $j^2-m^2\to\infty$, the right-hand sides of Eq. (5) approach values given by

$$\hat{J}_0|jm\rangle = m\,|jm\rangle,$$
$$\hat{J}_\pm|jm\rangle \to \sqrt{j^2-m^2}\,|jm\pm1\rangle = j\sin\beta_m\,|jm\pm1\rangle. \tag{55}$$

With $\cos\beta_{\overline{m}}=\overline{m}/j$, $\sqrt{j^2-\overline{m}^2}=j\sin\beta_{\overline{m}}$, and, for values of m close to $\overline{m}$, the SU(2) states are represented, in the $j^2-\overline{m}^2\to\infty$ limit, as functions on the circle, i.e., $|jm\rangle\to\psi_m$ with

$$\psi_m(\theta) = \frac{e^{im\theta}}{\sqrt{2\pi}}, \tag{56}$$

and the angular momentum operators are represented

$$\hat{J}_0 \to -i\frac{d}{d\theta}, \quad \hat{J}_\pm \to j\sin\beta_{\overline{m}} e^{\pm i\theta}. \tag{57}$$

It follows that $\hat{J}_y\to j\sin\beta_{\overline{m}}\sin\theta$ and, for m and n both close to $\overline{m}=\frac{1}{2}(m+n)$,

$$d^j_{mn}(\beta)\to\frac{1}{2\pi}\int_0^{2\pi} e^{-i(m-n)\theta}\,e^{-i\beta j\sin\beta_{\overline{m}}\sin\theta}\,d\theta = (-1)^{m-n}J_{m-n}(j\beta\sin\beta_{\overline{m}}), \tag{58}$$

where J_m is a Bessel function and we have used a known[16,10] integral expression for J_m. This expression is a generalization to finite values of the d-function's argument of the known asymptotic limit, for infinitesimal β/j,[12,13]

$$\lim_{j\to\infty} d^j_{mn}(\beta/j) = (-1)^{m-n}J_{m-n}(\beta). \tag{59}$$

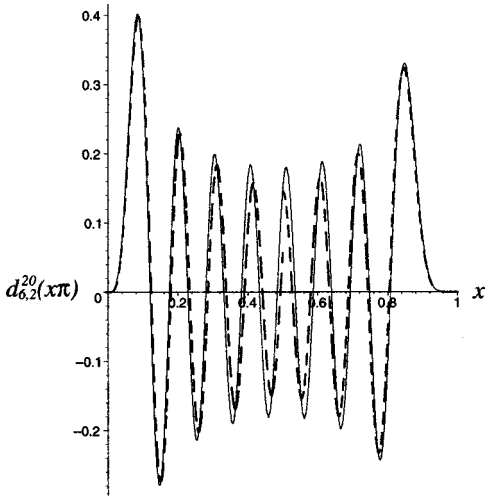

FIG. 7. The reduced Wigner function $d^{20}_{6,2}(x\pi)$. Exact values are shown as a fine continuous line and asymptotic values as a dashed heavy line. For $0<x<0.5$ the asymptotic values are given by Eq. (58) and for $0.5<x<1$ they are given by Eq. (61).

The expressions given by Eq. (57) are the limits of a general coherent state representation of the SU(2) algebra carried by functions on the circle. Note, however, that since it is derived from a contraction of the Lie algebra, it is only valid locally. Thus, the asymptotic limit of Eq. (58) is only expected to be good for relatively small values of β and $m-n$.

The asymptotic expression (58) for the reduced Wigner function $d^{20}_{6,2}$ is compared, for $0\leqslant\beta\leqslant\pi/2$, with the exact function in Fig. 7. It is seen to be an excellent approximation for small values of its argument. It is appropriate to restrict the use of Eq. (58) to $0\leqslant\beta\leqslant\pi/2$ because, for β in the range $\pi/2\leqslant\beta\leqslant\pi$, a better limit is obtained by use of the identity

$$d^j_{mn}(\beta)=(-1)^{j+m}d^j_{m,-n}(\pi-\beta), \tag{60}$$

which, for $\pi/2\leqslant\beta\leqslant\pi$, leads to the asymptotic expression

$$d^j_{mn}(\beta)\rightarrow(-1)^{j+m}J_{m+n}(j(\beta-\pi)\sin\beta_{(m-n)/2}). \tag{61}$$

Comparison of the exact expression with Eq. (58) for β in the range $0\leqslant\beta\leqslant\pi/2$ and with (61) for $\pi/2\leqslant\beta\leqslant\pi$ is shown in Fig. 7.

For small values of β it turns out that a remarkable improvement in accuracy is obtained by the *ad hoc* replacement $j\rightarrow j+1/2$ in the argument of the Bessel function of the asymptotic expression. This replacement has also been found by other authors to increase numerical accuracy; to first order, it can be regarded as a substitution of j by $\sqrt{j(j+1)}$, which is the appropriate classical value of the magnitude of the angular momentum. The modified estimate is compared with the exact expression for $d^{20}_{6,2}(x\pi)$ in Fig. 8.

The above results have a natural interpretation in terms of an SU(2)→E(2) contraction. If we define

$$x=\frac{1}{2j\sin\beta_{\bar{m}}}(J_++J_-),\quad y=-\frac{i}{2j\sin\beta_{\bar{m}}}(J_+-J_-),\quad J_z=J_0, \tag{62}$$

we obtain the commutation relations

$$[J_z,x]=\mathrm{i}y,\quad [J_z,y]=-\mathrm{i}x,\quad [x,y]=\frac{i}{j^2\sin^2\beta_{\bar{m}}}J_z\rightarrow 0, \tag{63}$$

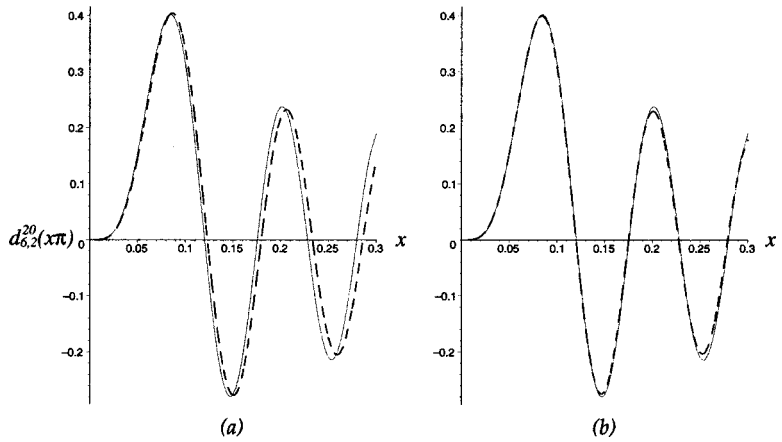

FIG. 8. The reduced Wigner function $d^{20}_{6,2}(x\pi)$. Exact values are shown as a fine continuous line and asymptotic values as a dashed line. The asymptotic expression in (a) is given by Eq. (58) and in (b) it is given by (58) with j replaced by $j+1/2$.

as $j \sin \beta_{\overline{m}} \to \infty$. They are the commutation relations of the infinitesimal generators of the Euclidean group in two dimensions. Moreover, the SU(2) representation with highest weight j contracts to a representation of the Euclidean group E(2) in which

$$x \to \cos\theta, \quad y \to \sin\theta, \quad J_z \to -i\frac{d}{d\theta}. \tag{64}$$

This contraction limit makes sense geometrically if one considers the manifold of SU(2) coherent states in the Hilbert space generated by applying all SU(2) transformations to a fixed state $|jm\rangle$. This manifold has the geometry of a sphere and one knows that small neighborhoods on a sphere look locally like neighborhoods of a two-dimensional Euclidean plane.

D. Summary of SU(2) Wigner function limits in a U(2) basis

In summarizing the limits for d^j_{mn}, it is useful to characterize the value of m as being central if $m \approx 0$ and extremal if $m \approx \pm j$. The various asymptotic limits for d^j_{mn} are then at their best in the following situations: (i) Harmonic oscillator limits; when m is central and n is extremal, (ii) HW(2) contraction limits; when m and n are both extremal, and (iii) E(2) contraction limits; when m and n are both central.

For application of the above results to SU(3), the results are most usefully expressed in a U(2) weight basis in which a state $|jm\rangle$ is identified with the U(2) weight state $|sd\rangle$ with $s=j+m$ and $d=j-m$. A reduced SU(2) Wigner function is then expressed

$$d^j_{mn}(\beta) = \langle s_1 d_1 | \beta | s_2 d_2 \rangle, \tag{65}$$

with $s_1=j+m$, $d_1=j-m$, $s_2=j+n$, and $d_2=j-n$. The above asymptotic limits are summarized as follows.

1. Harmonic oscillator limits

If m is central then $s=j+m \gg 0$ and $d=j-m \gg 0$ in the $j \to \infty$ limit. Equations (40) and (41) are then expressed

$$\langle sd|\beta|2j-n,n\rangle = (-1)^{n-d}\langle 2j-n,n|\beta|sd\rangle \to \delta_{s+d,2j}\,(-1)^n \left(\frac{j}{sd}\right)^{1/4} u_n(\sqrt{j}(\beta-\beta_{sd})), \tag{66}$$

where $j=(s+d)/2$ and

$$\cos\beta_{sd}=\frac{s-d}{s+d} \quad \Rightarrow \quad \sin\beta_{sd}=\sqrt{\frac{sd}{j}}, \tag{67}$$

and u_n is given by Eq. (35). This limit is valid for small values of n.

2. HW(2) contraction limits

If m and n are both close to j, then $s_1 \gg d_1$ and $s_2 \gg d_2$. Substituting the expression

$$a^2_{jmn}=\tfrac{1}{8}(2j+m+n)=\tfrac{1}{8}(s_1+s_2) \tag{68}$$

for a^2_{jmn} into Eqs. (52) and (53) then gives, in this limit,

$$\langle s_1 d_1|\beta|s_2 d_2\rangle \to \delta_{s_1+d_1,s_2+d_2}\sqrt{\frac{d_2!}{d_1!}}\left(\frac{\beta}{2}\sqrt{\frac{s_1+s_2}{2}}\right)^{s_2-s_1} L_{d_2}^{(s_2-s_1)}(\beta^2(s_1+s_2)/8)e^{-\beta^2(s_1+s_2)/16} \tag{69}$$

for $s_1 \leqslant s_2$ and

$$\langle s_1 d_1|\beta|s_2 d_2\rangle \to \delta_{s_1+d_1,s_2+d_2}\sqrt{\frac{d_1!}{d_2!}}\left(-\frac{\beta}{2}\sqrt{\frac{s_1+s_2}{2}}\right)^{s_1-s_2} L_{d_1}^{(s_1-s_2)}(\beta^2(s_1+s_2)/8)e^{-\beta^2(s_1+s_2)/16} \tag{70}$$

for $s_1 \geqslant s_2$.

If m is close to j and n is close to $-j$, so that $s_1 \gg d_1$ and $s_2 \ll d_2$, the identity $d^j_{mn}(\beta)=(-1)^{j-n}d^j_{m,-n}(\beta+\pi)$ interchanges the coefficients s_2 and d_2 to give

$$\langle s_1 d_1|\beta|s_2 d_2\rangle=(-1)^{d_2}\langle s_1 d_1|\beta+\pi|d_2 s_2\rangle \tag{71}$$

for which Eqs. (69) and (70) continue to apply. Similarly, for $s_1 \ll d_1$ and $s_2 \gg d_2$,

$$\langle s_1 d_1|\beta|s_2 d_2\rangle=(-1)^{d_1}\langle d_1 s_1|\beta+\pi|s_2 d_2\rangle, \tag{72}$$

and, for $s_1 \ll d_1$ and $s_2 \ll d_2$, the identity $d^j_{mn}(\beta)=(-1)^{m-n}d^j_{-m,-n}(\beta)$ gives

$$\langle s_1 d_1|\beta|s_2 d_2\rangle=(-1)^{s_1-s_2}\langle d_1 s_1|\beta|d_2 s_2\rangle. \tag{73}$$

3. E(2) contraction limits

When m and n are both small and j is large, $s_1 \gg 0$, $d_1 \gg 0$, $s_2 \gg 0$, and $d_2 \gg 0$. Replacing $2j\sin\beta_{\overline{m}}$ by $\sqrt{(s_1+s_2)(d_1+d_2)}$ in Eq. (58) then gives

$$\langle s_1 d_1|\beta|s_2 d_2\rangle \to \delta_{s_1+d_1,s_2+d_2}(-1)^{s_1-s_2}J_{s_1-s_2}(\sqrt{(s_1+s_2)(d_1+d_2)}\beta/2). \tag{74}$$

III. $(\lambda,0)$ SU(3) WIGNER FUNCTIONS

The complex extension of the U(3) Lie algebra is spanned by 3×3 matrices $\{C_{ij}\}$ which satisfy the commutation relations

$$[C_{ij},C_{kl}]=\delta_{jk}C_{il}-\delta_{il}C_{kj}. \tag{75}$$

The $SU(3)\subset U(3)$ subalgebra is spanned by the subset $\{C_{11}-C_{22},C_{22}-C_{33},C_{ij};i\neq j\}$.

A. Representations of the U(3) Lie algebra

We consider a U(3) irrep of highest weight $(\lambda,0,0)$ in which the $\{C_{ij}\}$ matrices are represented by operators $\{\hat{C}_{ij}\}$ on a Hilbert space spanned by a weight basis $\{|\nu\rangle\}$. The components of a weight $\nu\equiv(\nu_1,\nu_2,\nu_3)$ are the eigenvalues of the $\hat{C}_{ii}$ operators, viz.

$$\hat{C}_{ii}|\nu\rangle=\nu_i|\nu\rangle, \quad i=1,2,3, \tag{76}$$

and sum to give $\nu_1+\nu_2+\nu_3=\lambda$. For a $(\lambda,0,0)$ irrep, the weight basis states are defined uniquely, to within phase factors. Such an irrep restricts to an SU(3) irrep of highest weight $(\lambda,0)$.

The basis states $\{|\nu\rangle\}$ are conveniently realized within the space of a three-dimensional harmonic oscillator. Thus, if $\{c_i^\dagger,c_i;i=1,2,3\}$ denotes a triplet of harmonic oscillator raising and lowering operators, the (orthonormal) weight states are

$$|\nu\rangle=\frac{(c_1^\dagger)^{\nu_1}(c_2^\dagger)^{\nu_2}(c_3^\dagger)^{\nu_3}}{\sqrt{\nu_1!\,\nu_2!\,\nu_3!}}|0\rangle, \quad \nu_1+\nu_2+\nu_3=\lambda, \tag{77}$$

where $|0\rangle$ is the harmonic oscillator lowest-weight (vacuum) state, and the U(3) operators are expressed

$$\hat{C}_{ij}=a_i^\dagger a_j\,. \tag{78}$$

It follows that the $i\neq j$ operators act on the weight states according to the equation

$$\hat{C}_{ij}|\nu_1,\nu_2,\nu_3\rangle=\sqrt{(\nu_i+1)\nu_j}\sum_{\nu'}\delta_{\nu_i',\nu_i+1}\delta_{\nu_j',\nu_j-1}\delta_{\nu_k',\nu_k}|\nu_1',\nu_2',\nu_3'\rangle, \tag{79}$$

for $i\neq k\neq j$.

The above (weight) basis reduces the $SU(2)_{23}\subset SU(3)$ subalgebra spanned by the I-spin operators

$$\hat{I}_+=\hat{C}_{23}, \quad \hat{I}_-=\hat{C}_{32}, \quad \hat{I}_0=\tfrac{1}{2}(\hat{C}_{22}-\hat{C}_{33}). \tag{80}$$

The corresponding I-spin quantum numbers are identified by setting

$$\nu_1=\lambda-2I, \quad \nu_2=I+N, \quad \nu_3=I-N, \tag{81}$$

and writing

$$|\nu\rangle\equiv|IN\rangle=\frac{(c_1^\dagger)^{\lambda-2I}}{\sqrt{(\lambda-2I)!}}\frac{(c_2^\dagger)^{I+N}(c_3^\dagger)^{I-N}}{\sqrt{(I+N)!(I-N)!}}|0\rangle. \tag{82}$$

The action of the $SU(2)_{23}$ operators is then expressed in the usual way by

$$\hat{I}_0|IN\rangle=N|IN\rangle, \quad \hat{I}_\pm|IN\rangle=\sqrt{(I\mp N)(I\pm N+1)}\,|IN\pm1\rangle. \tag{83}$$

Similarly, the $SU(2)_{12}$ and $SU(2)_{13}$ subalgebras are spanned by U-spin and V-spin operators, respectively,

$$\hat{U}_+=\hat{C}_{12}, \quad \hat{U}_-=\hat{C}_{21}, \quad \hat{U}_0=\tfrac{1}{2}(\hat{C}_{11}-\hat{C}_{22}), \tag{84}$$

$$\hat{V}_+=\hat{C}_{13}, \quad \hat{V}_-=\hat{C}_{31}, \quad \hat{V}_0=\tfrac{1}{2}(\hat{C}_{11}-\hat{C}_{33}). \tag{85}$$

Thus, we have the identifications $|\nu\rangle\equiv|IN\rangle\equiv|UM\rangle\equiv|VP\rangle$ with

$$\nu_1=\lambda-2I=U+M=V+P,$$

$$\nu_2=I+N=U-M=\lambda-2V, \tag{86}$$

$$\nu_3=I-N=\lambda-2U=V-P.$$

It is important to note that, for a $(\lambda,0)$ irrep, the above weight basis becomes identical to the basis $\{|jIN\rangle\}$ constructed, for a general $SU(3)\supset SU(2)_{23}$ irrep, by VCS methods[18] and used in the computation of SU(3) Clebsch–Gordan coefficients.[19] [For a $(\lambda,0)$ irrep the extra label j in $\{|jIN\rangle\}$ is redundant and can be dropped.] The bases are identified explicitly as follows. First observe that the highest weight state of the SU(3) $(\lambda,0)$ irrep is the state

$$|\phi\rangle=\frac{(c_1^\dagger)^\lambda}{\sqrt{\lambda!}}|0\rangle. \tag{87}$$

Thus, with the observation that

$$(c_1)^{\lambda-\nu_1}(c_1^\dagger)^\lambda|0\rangle=\frac{\lambda!}{\nu_1!}(c_1^\dagger)^{\nu_1}|0\rangle, \tag{88}$$

we obtain the expression of the $U(3)\supset SU(3)$ basis states

$$|\nu\rangle=\sqrt{\frac{\nu_1!}{\lambda!\,\nu_2!\,\nu_3!}}(\hat{C}_{21})^{\nu_2}(\hat{C}_{31})^{\nu_3}|\phi\rangle. \tag{89}$$

This basis is identical to that of VCS theory,

$$|IN\rangle=\sqrt{\frac{(\lambda-2I)!}{\lambda!}}\frac{(\hat{C}_{21})^{I+N}(\hat{C}_{31})^{I-N}}{\sqrt{(I+N)!(I-N)!}}|\phi\rangle, \tag{90}$$

with the relationship between ν and IN given by Eq. (81). It is also identical to the Gel'fand basis $\{|\nu I\rangle\}$ used for a $(\lambda,0)$ irrep in Ref. 20 with $I=\frac{1}{2}(\nu_2+\nu_3)$ (cf. appendix of Ref. 19).

B. $(\lambda,0)$ Wigner functions for finite λ

As shown recently,[20] an SU(3) element can be expressed as a product of SU(2) subgroup elements in the form

$$g(\alpha_1,\beta_1,\gamma_1,\alpha_2,\beta_2,\alpha_3,\beta_3,\gamma_3)=R_{23}(\alpha_1,\beta_1,\gamma_1)R_{12}(\alpha_2,\beta_2,\alpha_2)R_{23}(\alpha_3,\beta_3,\gamma_3). \tag{91}$$

This is a particularly convenient parametrization because, in the above basis, the matrices of the $SU(2)_{23}$ rotations are given by standard SU(2) Wigner functions; viz.

$$\langle I'N'|\hat{R}_{23}(\alpha,\beta,\gamma)|IN\rangle=\delta_{I'I}\mathcal{D}^I_{N'N}(\alpha,\beta,\gamma) \tag{92}$$

or, in terms of weights,

$$\langle\nu|\hat{R}_{23}(\alpha,\beta,\gamma)|\mu\rangle=\delta_{\nu_1,\mu_1}\mathcal{D}^{(\lambda-\nu_1)/2}_{(\nu_2-\nu_3)/2,(\mu_2-\mu_3)/2}(\alpha,\beta,\gamma). \tag{93}$$

Similarly, for the $SU(2)_{12}$ matrix elements

$$\langle\mu|\hat{R}_{12}(\alpha,\beta,\gamma)|\mu'\rangle=\delta_{\mu_3,\mu_3'}\mathcal{D}^{(\lambda-\mu_3)/2}_{(\mu_1-\mu_2)/2,(\mu_1'-\mu_2')/2}(\alpha,\beta,\gamma). \tag{94}$$

The expressions are simplified by writing the SU(2) Wigner functions in a U(2) basis [cf. Eq. (65)] in which

$$\mathcal{D}^{j}_{mn}(\alpha,\beta,\gamma)=\langle j+m,j-m|\beta|j+n,j-n\rangle e^{-i(m\alpha+n\gamma)}. \tag{95}$$

Then

$$\begin{aligned}\langle \nu|\hat{R}_{23}(\alpha,\beta,\gamma)|\mu\rangle&=\delta_{\nu_1,\mu_1}\langle \nu_2\nu_3|\beta|\mu_2\mu_3\rangle e^{-i[(\nu_2-\nu_3)\alpha+(\mu_2-\mu_3)\gamma]/2},\\ \langle \mu|\hat{R}_{12}(\alpha,\beta,\gamma)|\mu'\rangle&=\delta_{\mu_3,\mu_3'}\langle \mu_1\mu_2|\beta|\mu_1'\mu_2'\rangle e^{-i[(\mu_1-\mu_2)\alpha+(\mu_1'-\mu_2')\gamma]/2},\end{aligned} \tag{96}$$

and

$$\begin{aligned}&D^{(\lambda,0)}_{\nu,\nu'}(\alpha_1,\beta_1,\gamma_1,\alpha_2,\beta_2,\alpha_3,\beta_3,\gamma_3)\\ &\quad=e^{-i[(\nu_2-\nu_3)\alpha_1+(\lambda-\nu_1)\gamma_1+2(\nu_1+\nu_1'-\lambda)\alpha_2+(\lambda-\nu_1')\alpha_3+(\nu_2'-\nu_3')\gamma_3]/2}\\ &\qquad\times\sum_{n=0}^{n_{\max}}e^{in(\gamma_1-\alpha_2+\alpha_3)}\langle \nu_2\nu_3|\beta_1|\lambda-\nu_1-n,n\rangle\\ &\qquad\times\langle \nu_1,\lambda-\nu_1-n|\beta_2|\nu_1',\lambda-\nu_1'-n\rangle\langle \lambda-\nu_1'-n,n|\beta_3|\nu_2'\nu_3'\rangle,\end{aligned} \tag{97}$$

where $n_{\max}=\mathrm{Min}(\lambda-\nu_1,\lambda-\nu_1')$.

Expressions for the SU(3) Wigner functions of other irreps are given in Ref. 20.

IV. $(\lambda,0)$ WIGNER FUNCTIONS FOR $\lambda\to\infty$

Wigner functions for an SU(3) $(\lambda,0)$ irrep have a number of asymptotic expressions which can be obtained by substituting the corresponding limits for the SU(2) Wigner functions into Eq. (97). The appropriate limits depend on the location of the weights ν and ν' in the weight diagram. A weight can be characterized as extremal if it is close to a vertex, or central, if it is far from a vertex.

A. Limits of $(\lambda,0)$ Wigner functions for ν central and ν' close to a highest weight

When ν' is of highest weight, i.e., $\nu'=(\lambda,0,0)$, the expression for the SU(3) Wigner function of Eq. (97) reduces to

$$\begin{aligned}D^{(\lambda)}_{\nu,(\lambda)}(\alpha_1,\beta_1,\gamma_1,\alpha_2,\beta_2,\alpha_3,\beta_3,\gamma_3)&=e^{-i[(\nu_2-\nu_3)\alpha_1+(\lambda-\nu_1)\gamma_1+2\nu_1\alpha_2]/2}\\ &\quad\times\langle \nu_2\nu_3|\beta_1|\lambda-\nu_1,0\rangle\langle \nu_1,\lambda-\nu_1|\beta_2|\lambda 0\rangle,\end{aligned} \tag{98}$$

where, to simplify the notation, we have identified the weights $(\lambda)\equiv(\lambda,0)\equiv(\lambda,0,0)$. The reduced SU(2) Wigner functions in this expression are of the type with asymptotic limits given by Eq. (22). Thus, we obtain

$$\begin{aligned}D^{(\lambda)}_{\nu,(\lambda)}(\alpha_1,\beta_1,\gamma_1,\alpha_2,\beta_2,\alpha_3,\beta_3,\gamma_3)&\to\left(\frac{\lambda}{4\pi^2\nu_1\nu_2\nu_3}\right)^{1/4}e^{-i[(\nu_2-\nu_3)\alpha_1+(\nu_2+\nu_3)\gamma_1+2\nu_1\alpha_2]/2}\\ &\quad\times e^{-[(\nu_2+\nu_3)(\beta_1-\beta_{\nu_2\nu_3})^2+\lambda(\beta_2-\beta_{\nu_1,\nu_2+\nu_3})^2]/4}\end{aligned} \tag{99}$$

with $\beta_{\nu_2\nu_3}$ defined by Eq. (35).

More generally, for ν' close to the highest weight, the use of the harmonic oscillator limits of Eq. (66) give

$$
\begin{aligned}
&D^{(\lambda)}_{\nu,\nu'}(\alpha_1,\beta_1,\gamma_1,\alpha_2,\beta_2,\alpha_3,\beta_3,\gamma_3)\\
&\quad\to e^{-i[(\nu_2-\nu_3)\alpha_1+(\lambda-\nu_1)\gamma_1+2(\nu_1+\nu_1'-\lambda)\alpha_2+(\lambda-\nu_1')\alpha_3+(\nu_2'-\nu_3')\gamma_3]/2}\\
&\qquad\times(-1)^{\lambda-\nu_1'}\left(\frac{\lambda-\nu_1}{4\nu_1\nu_2\nu_3}\right)^{1/4}\sum_{n=0}^{\lambda-\nu_1'}e^{in(\gamma_1-\alpha_2+\alpha_3)}\left(\frac{\lambda-n}{\lambda-\nu_1-n}\right)^{1/4}\\
&\qquad\times u_n\left(\sqrt{\tfrac{1}{2}(\lambda-\nu_1)}\,(\beta_1-\beta_{\nu_2,\nu_3})\right)\\
&\qquad\times u_{2I-n}\left(\sqrt{\tfrac{1}{2}(\lambda-n)}(\beta_2-\beta_{\nu_1,\lambda-\nu_1-n})\right)d^I_{I-n,N}(\beta_3),
\end{aligned}
\tag{100}
$$

where $I=\frac{1}{2}(\nu_2'+\nu_3')$ and $N=\frac{1}{2}(\nu_2'-\nu_3')$. It can be seen that this expression reduces to that of Eq. (99) when $I=0$ and $\nu'=(\lambda,0,0)$.

This limiting expression for the $\lambda=60$ SU(3) Wigner function is compared with the exact expression for a range of values of some of its arguments in Fig. 9.

B. Limits of $(\lambda,0)$ Wigner functions for ν and ν' both close to vertices

If ν and ν' are both close to the highest weight, then the first and last SU(2) Wigner functions in Eq. (97) are those of small-dimensional SU(2) irreps, while, for the middle function, the limit given by Eqs. (69) and (70) applies. Thus, for $\nu_1'\geqslant\nu_1$,

$$
\begin{aligned}
&D^{(\lambda)}_{\nu,\nu'}(\alpha_1,\beta_1,\gamma_1,\alpha_2,\beta_2,\alpha_3,\beta_3,\gamma_3)\\
&\quad\to\sum_{n=0}^{\lambda-\nu_1'}e^{-i(\nu_1+\nu_1'-\lambda+n)\alpha_2}\sqrt{\frac{(\lambda-\nu_1'-n)!}{(\lambda-\nu_1-n)!}}\left(\frac{\beta_2}{2}\sqrt{\frac{\nu_1+\nu_1'}{2}}\right)^{\nu_1'-\nu_1}\\
&\qquad\times\mathcal{D}^{(\lambda-\nu_1)/2}_{(\nu_2-\nu_3)/2,(\lambda-\nu_1-2n)/2}(\alpha_1,\beta_1,\gamma_1)\,\mathcal{D}^{(\lambda-\nu_1')/2}_{(\lambda-\nu_1'-2n)/2,(\nu_2'-\nu_3')/2}(\alpha_3,\beta_3,\gamma_3)\\
&\qquad\times L^{(\nu_1'-\nu_1)}_{\lambda-\nu_1'-n}(\beta_2^2(\nu_1+\nu_1')/8)e^{-\beta_2^2(\nu_1+\nu_1')/16}
\end{aligned}
\tag{101}
$$

and, for $\nu_1'\leqslant\nu_1$,

$$
\begin{aligned}
&D^{(\lambda)}_{\nu,\nu'}(\alpha_1,\beta_1,\gamma_1,\alpha_2,\beta_2,\alpha_3,\beta_3,\gamma_3)\\
&\quad\to\sum_{n=0}^{\lambda-\nu_1}e^{-i(\nu_1+\nu_1'-\lambda+n)\alpha_2}\sqrt{\frac{(\lambda-\nu_1-n)!}{(\lambda-\nu_1'-n)!}}\left(-\frac{\beta_2}{2}\sqrt{\frac{\nu_1+\nu_1'}{2}}\right)^{\nu_1-\nu_1'}\\
&\qquad\times\mathcal{D}^{(\lambda-\nu_1)/2}_{(\nu_2-\nu_3)/2,(\lambda-\nu_1-2n)/2}(\alpha_1,\beta_1,\gamma_1)\,\mathcal{D}^{(\lambda-\nu_1')/2}_{(\lambda-\nu_1'-2n)/2,(\nu_2'-\nu_3')/2}(\alpha_3,\beta_3,\gamma_3)\\
&\qquad\times L^{(\nu_1-\nu_1')}_{\lambda-\nu_1-n}(\beta_2^2(\nu_1+\nu_1')/8)e^{-\beta_2^2(\nu_1+\nu_1')/16}.
\end{aligned}
\tag{102}
$$

This limiting expression for the $\lambda=60$ SU(3) Wigner function is compared with the exact expression for a range of values of some of its arguments in Fig. 10.

If ν is near $(\lambda,0,0)$ and ν' near $(0,\lambda,0)$, then the matrix element $\langle\nu_2\nu_3|\beta_1|\lambda-\nu_1-n,n\rangle$ in Eq. (97) is a reduced Wigner function for a low-dimensional SU(2) irrep. The second matrix element $\langle\nu_1,\lambda-\nu_1-n|\beta_2|\nu_1',\lambda-\nu_1'-n\rangle$ is one for which $\nu_1\gg\lambda-\nu_1-n$ and $\nu_1'\ll\lambda-\nu_1'-n$. Thus, by Eq. (71), it is re-expressed in the form

$$
\langle\nu_1,\lambda-\nu_1-n|\beta_2|\nu_1',\lambda-\nu_1'-n\rangle=(-1)^{\lambda-\nu_1'-n}\langle\nu_1,\lambda-\nu_1-n|\beta_2+\pi|\lambda-\nu_1'-n,\nu_1'\rangle
\tag{103}
$$

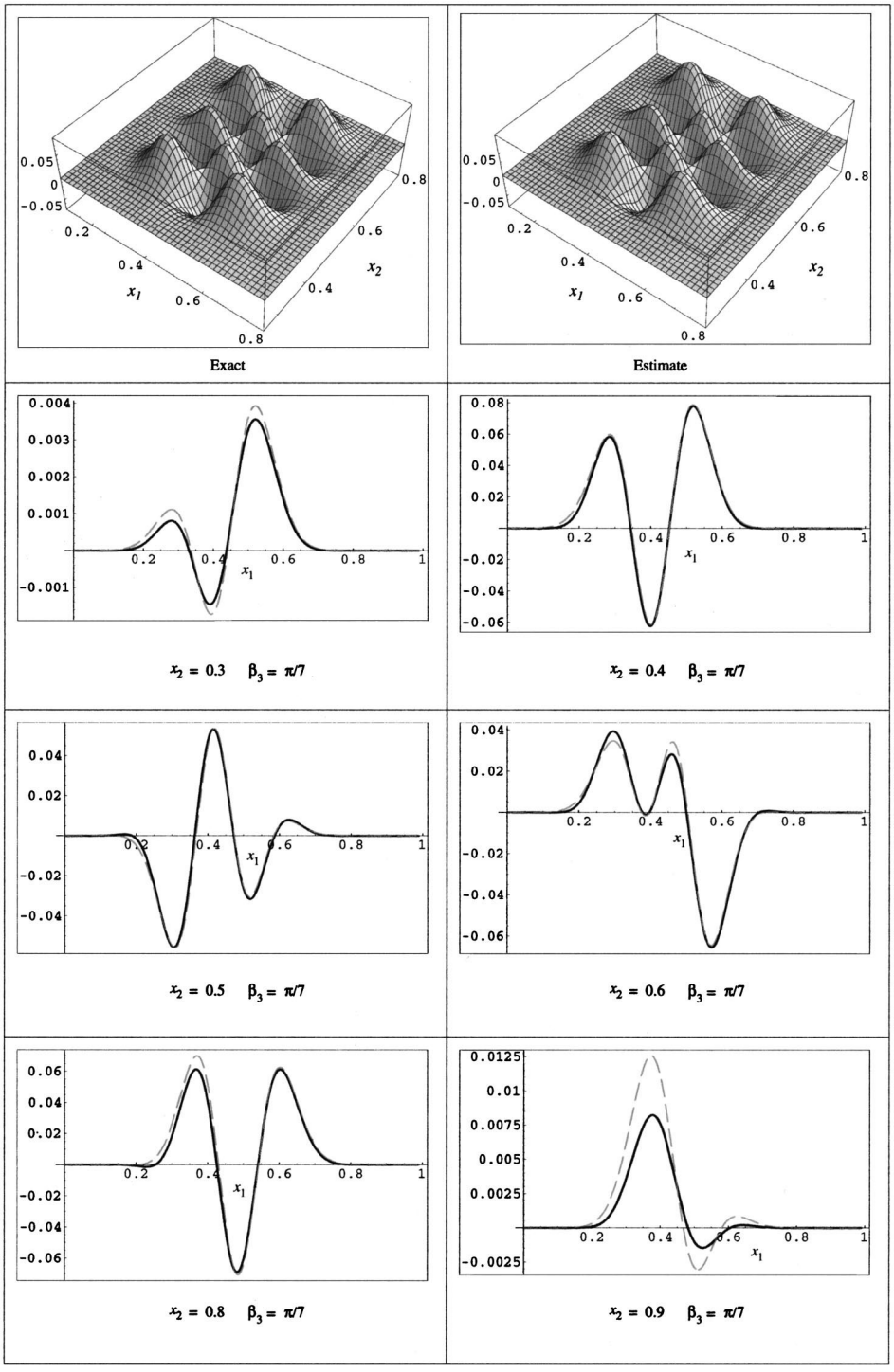

FIG. 9. The SU(3) Wigner function $\mathcal{D}^{(\lambda)}_{\nu,\nu'}(0,\beta_1=x_1\pi,0,0,\beta_2=x_2\pi,0,\beta_3=\pi/7,0)$ for $(\lambda)=(60,0,0)$, $\nu=(24,21,15)$, $\nu'=(54,4,2)$. The top graphs show, respectively, the surfaces for the exact function and its estimate using Eq. (100). The sequence of slices provide a detailed comparison between the exact function (full line) and its estimate (dashed line) for the sequence of values of $\beta_2=0.3\pi,0.4\pi,\ldots,0.8\pi$.

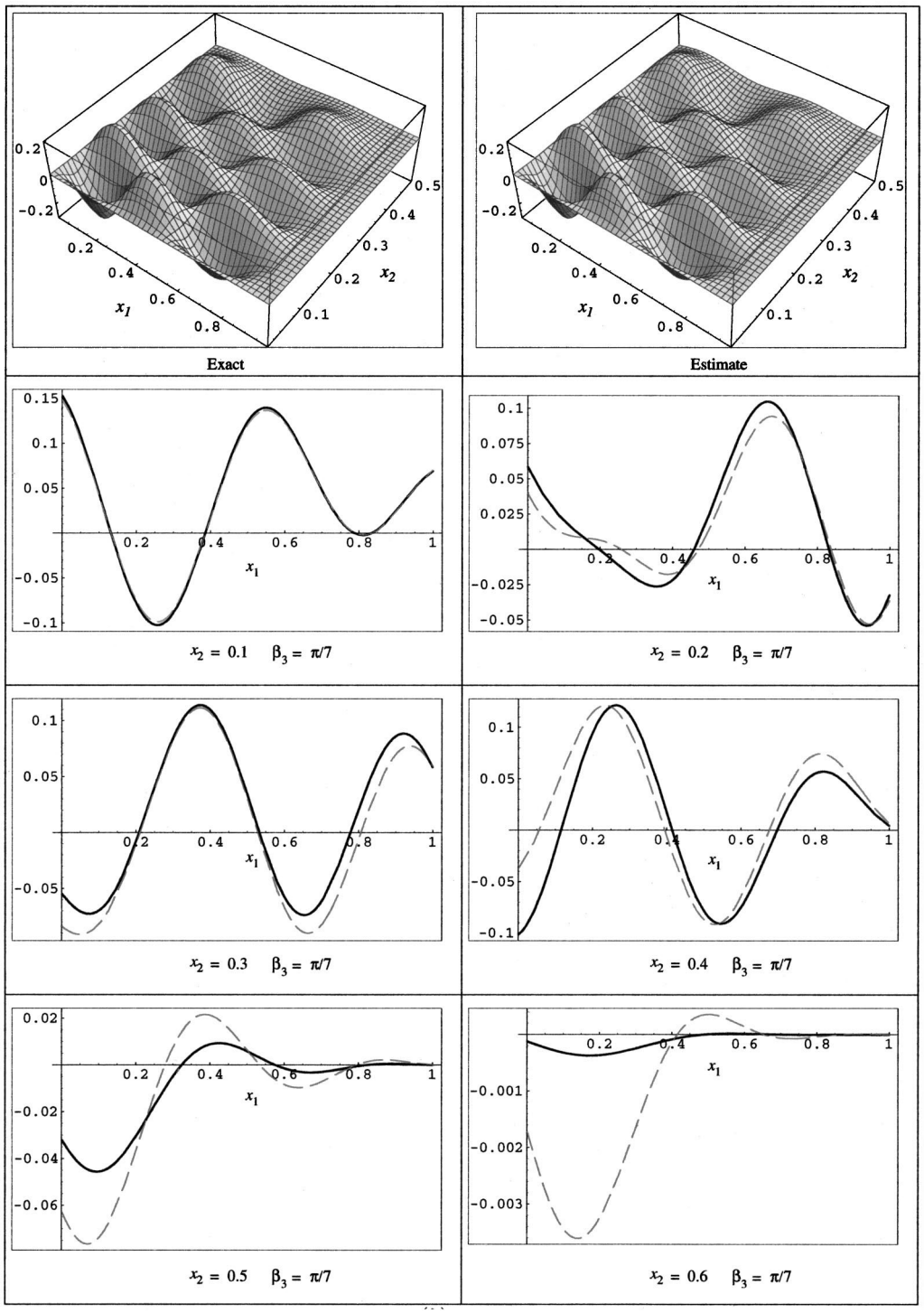

FIG. 10. The SU(3) Wigner function $\mathcal{D}^{(\lambda)}_{\nu,\nu'}(0,\beta_1=x_1\pi,0,0,\beta_2=x_2\pi,0,\beta_3=\pi/7,0)$ for $(\lambda)=(60,0,0)$, $\nu=(52,6,2)$, $\nu'=(50,7,3)$. The top graphs show, respectively, the surfaces for the exact function and its estimate using Eq. (102). The sequences of slices provide a detailed comparison between the exact function (full line) and its estimate (dashed line) for the sequence of values of $\beta_2=0.1\,\pi,0.2\,\pi,\ldots,0.6\,\pi$.

for which Eqs. (69) and (70) apply. The third matrix element, $\langle \lambda-\nu_1'-n,n|\beta_3|\nu_2'\nu_3'\rangle$, is one for which $\lambda-\nu_1'-n \gg n$ and $\nu_2' \gg \nu_3'$ and for which Eqs. (69) and (70) apply directly.

Asymptotic expressions are similarly found for ν and ν' near other vertices. Thus, for instance, if ν and ν' are both close to $(0,\lambda,0)$, then each of the three SU(2) Wigner functions in Eq. (97) will be approximated by the limit given by Eqs. (69) or (70).

C. $(\lambda,0)$ Wigner functions for ν and ν' both central

If ν and ν' are both central weights of a $(\lambda,0)$ irrep and $\lambda\to\infty$, then the E(2) limit of Eq. (74) applies. If we replace the SU(2) matrix elements in Eq. (97) by their E(2) limits, we obtain

$$\begin{aligned} D^{(\lambda)}_{\nu,\nu'}&(\alpha_1,\beta_1,\gamma_1,\alpha_2,\beta_2,\alpha_3,\beta_3,\gamma_3) \\ &\to e^{-i[(\nu_2-\nu_3)\alpha_1+(\lambda-\nu_1)\gamma_1+2(\nu_1+\nu_1'-\lambda)\alpha_2+(\lambda-\nu_1')\alpha_3+(\nu_2'-\nu_3')\gamma_3]/2} \\ &\quad\times\sum_{n=0}^{n_{\max}} e^{in(\gamma_1-\alpha_2+\alpha_3)} J_{\nu_3-n}\left(\sqrt{(2\nu_2+\nu_3-n)(\nu_3+n)}\,\beta_1/2\right) \\ &\quad\times J_{\nu_1'-\nu_1}\left(\sqrt{(\nu_1+\nu_1')(2\lambda-\nu_1-\nu_1'-2n)}\,\beta_2/2\right) \\ &\quad\times J_{n-\nu_3'}\left(\sqrt{(2\nu_2'+\nu_3'-n)(\nu_3'+n)}\,\beta_3/2\right). \end{aligned} \tag{104}$$

It is important to note that this expression presumes the E(2) limit to be applicable for all values of n that occur in the summation. The following considerations show that this presumption is valid for sufficiently small values of β_1 and β_3.

Consider the matrix element

$$\langle \nu_2\nu_3|\beta_1|\lambda-\nu_1-n,n\rangle = d^{(\lambda-\nu_1)/2}_{(\nu_2-\nu_3)/3,(\lambda-\nu_1-2n)/2}(\beta_1). \tag{105}$$

For $\nu_2=\nu_3=\lambda/3$, for example, this matrix element becomes

$$d^{\lambda/3}_{0,\lambda/3-n}(\beta_1) = \sqrt{\frac{12\pi}{2\lambda+3}}\,Y_{\lambda/3,\lambda/3-n}(\beta_1,0). \tag{106}$$

For small β_1, it takes its largest values when $n\approx\lambda/3$. Moreover, Figs. 2 and 3 show that, for $\lambda=60$, the value of this matrix element becomes negligible for $\beta_1<\pi/5$ as n approaches 0. A similar result holds for the matrix element $\langle \lambda-\nu_1'-n,n|\beta_3|\nu_2'\nu_3'\rangle$ for $\nu_2'\approx\nu_3'\approx\lambda/3$.

The limiting expression (104) for the $\lambda=150$ SU(3) Wigner function is compared with the exact expression for a range of values of some of its arguments in Fig. 11.

V. APPLICATIONS TO QUANTUM INTERFEROMETRY

Quantum interferometers are important in quantum information theory and for precision measurements of phases shifts, e.g., for the detection of gravitational waves.[21] The accuracies obtainable with such devices are naturally expressed in terms of Wigner functions—SU(2) Wigner functions for two-channel interferometers and SU(3) Wigner functions for three-channel interferometers.

A. Two-channel interferometry

A two-channel interferometer is an optical device, such as a beam splitter or a Mach–Zehnder interferometer, that transforms a two-channel input state of the electromagnetic field into a two-channel output state. If the device consists of passive optical elements that conserve photon number (i.e., the sum of the photon numbers in the output channels equals the sum in the input channels), then it is characterized by a U(2) transformation.[1]

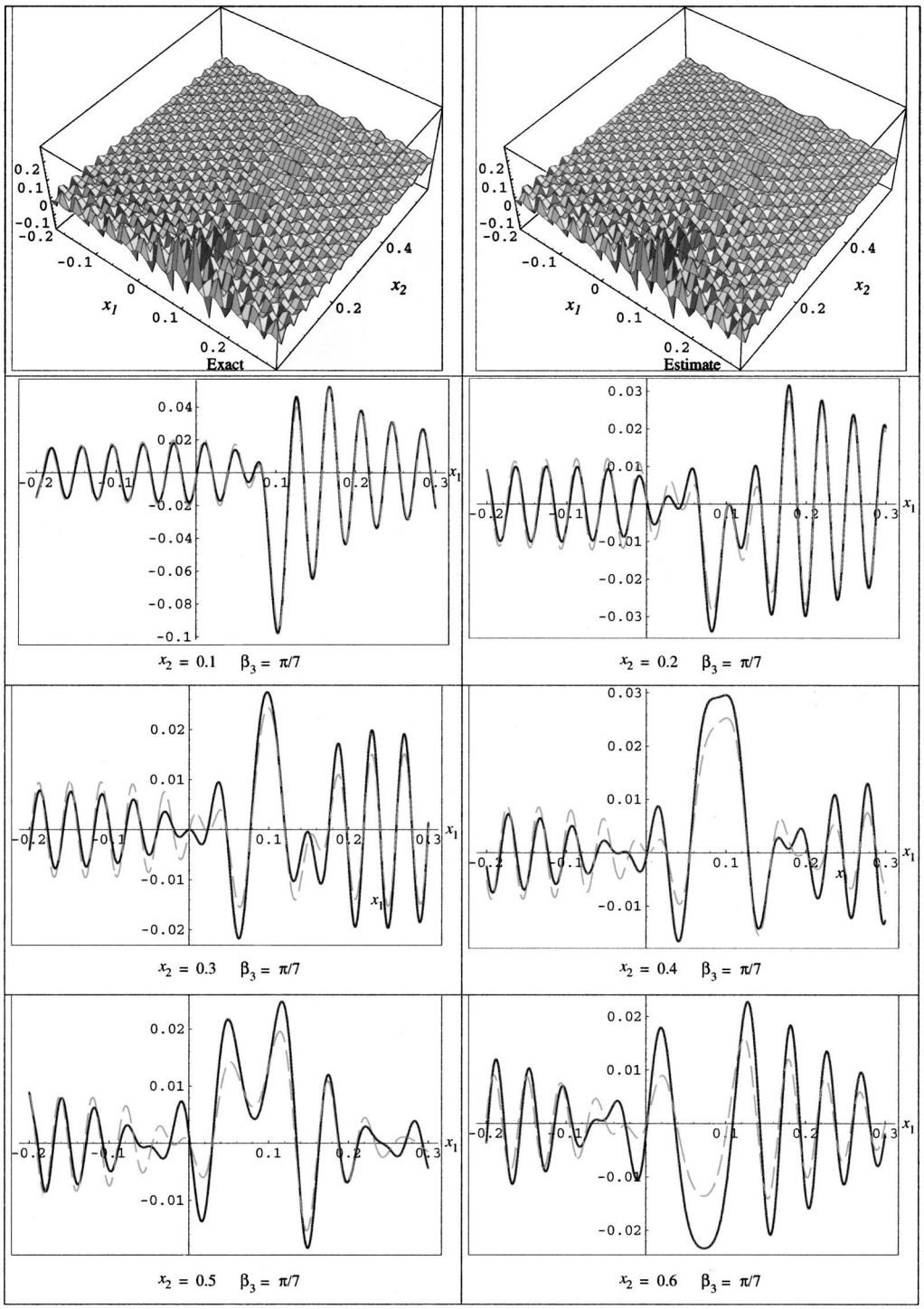

FIG. 11. The SU(3) Wigner function $\mathcal{D}^{(\lambda)}_{\nu,\nu'}(0,\beta_1=x_1\pi,0,0,\beta_2=x_2\pi,0,\beta_3=-\pi/9,0)$ for $(\lambda)=(150,0,0)$, $\nu=(46,44,49)$, $\nu'=(47,52,51)$. The top graphs show, respectively, the surfaces for the exact function and its estimate using Eq. (104). The sequences of slices provide a detailed comparison between the exact function (full line) and its estimate (dashed line) for the sequence of values of $\beta_2=0.1\,\pi,0.2\,\pi,\ldots,0.6\,\pi$.

In a classical description of two-channel interferometry, the electromagnetic field is represented by a two-component complex vector $\alpha=(\alpha_1,\alpha_2)$, where α_1 and α_2 are the amplitudes of the fields in the two channels. The interferometer effects a U(2) transformation

$$\alpha^{\text{in}}\rightarrow\alpha^{\text{out}}=\omega\alpha^{\text{in}}, \tag{107}$$

where

$$\omega=\begin{pmatrix} u & v \\ -v^* & u^* \end{pmatrix}, \quad \text{with } |u|^2+|v|^2=1, \tag{108}$$

is a U(2) matrix. For example, a beam splitter effects a U(2) transformation with $u=e^{i\phi_{\text{tr}}}\cos\theta$ and $v=e^{i\phi_{\text{ref}}}\sin\theta$ where ϕ_{tr} is the phase shift due to transmission, ϕ_{ref} is the phase shift due to reflection, and $\cos\theta$ is the amplitude transmissivity of the beam splitter.[2] A lossless two-path interferometer, such as a Mach–Zehnder interferometer, is also described by a U(2) transformation; in effect a lossless two-path interferometer is equivalent to a number-conserving beam splitter.

In quantum mechanics, a closest-to-classical two-channel field is a two-component coherent state of a two-dimensional harmonic oscillator

$$|\alpha\rangle\equiv|(\alpha_1,\alpha_2)\rangle=e^{\alpha_1 a_1^\dagger-\alpha_1^* a_1}e^{\alpha_2 a_2^\dagger-\alpha_2^* a_2}|0\rangle, \tag{109}$$

where $|0\rangle$ is the harmonic oscillator ground state and $a_1^\dagger$ and $a_2^\dagger$ are harmonic oscillator raising operators. The raising operators transform under $\omega\in$ U(2) according to the equation

$$\begin{aligned} a_1^\dagger&\rightarrow\hat{U}(\omega)a_1^\dagger\hat{U}^\dagger(\omega)=ua_1^\dagger-v^*a_2^\dagger, \\ a_2^\dagger&\rightarrow\hat{U}(\omega)a_2^\dagger\hat{U}^\dagger(\omega)=u^*a_2^\dagger+va_1^\dagger, \end{aligned} \tag{110}$$

from which it follows that $\hat{U}(\omega)|\alpha\rangle=|\omega\alpha\rangle$ and that the transformation of a coherent input is given by

$$|\alpha^{\text{in}}\rangle\rightarrow|\alpha^{\text{out}}\rangle=|\omega\alpha^{\text{in}}\rangle. \tag{111}$$

These relationships express the correspondence between classical and quantal coherent states. More importantly, they show that an interferometer transforms any input state by a map $|\psi\rangle\rightarrow\hat{U}(\omega)|\psi\rangle$. An arbitrary input state $|\psi\rangle$ is a superposition $\Sigma_{jm}c_{jm}|jm\rangle$ of basis states defined in a Schwinger representation by

$$|jm\rangle=\frac{(a_1^\dagger)^{j+m}(a_2^\dagger)^{j-m}}{\sqrt{(j+m)!(j-m)!}}|0\rangle, \quad m=-j,\ldots,+j. \tag{112}$$

Such states are identified with fields having a fixed number, $2j$, of photons; an input state $|jm\rangle$ is one with $j+m$ photons in channel one and $j-m$ in channel two. Thus the transformation of an arbitrary state is expressed in terms of SU(2) Wigner functions

$$\hat{U}(\omega):|\psi\rangle\rightarrow|\psi'\rangle=\hat{U}(\omega)|\psi\rangle=\sum_{jmn}c_{jm}|jn\rangle\,\mathcal{D}^j_{nm}(\omega), \quad \omega\in\text{SU(2)}. \tag{113}$$

It is interesting to note that a minimal uncertainty state entering channel one

$$|(\alpha,0)\rangle=e^{\alpha a_1^\dagger-\alpha^* a_1}|0\rangle, \tag{114}$$

is a coherent state of the Heisenberg–Weyl group, whereas the state

$$\hat{U}(\omega)|jm=j\rangle \tag{115}$$

is a coherent state of the group U(2), according to the generalized definition of coherent states by Perelomov and others.[22] Thus a state emerging from a quantum interferometer when the input is the state $|(\alpha,0)\rangle$ is a combined Heisenberg–Weyl–U(2) coherent state

$$|\omega(\alpha,0)\rangle=\hat{U}(\omega)e^{\alpha a_1^\dagger-\alpha^* a_1}|0\rangle. \tag{116}$$

Some of the interesting questions in quantum interferometry concern the measurement of phase shifts of specially prepared quantum input states. Consider, for example, the phase shift

$$\alpha_1\rightarrow e^{-i\theta}\alpha_1, \quad \alpha_2\rightarrow\alpha_2, \tag{117}$$

of a classical input. With the understanding that only relative phase shifts of the two components (α_1,α_2) are measured, such a phase shift is equivalent to

$$\alpha_1\rightarrow e^{-i\theta/2}\alpha_1, \quad \alpha_2\rightarrow e^{i\theta/2}\alpha_2. \tag{118}$$

Thus the equivalent transformations of quantum mechanical states are generated by

$$a_1^\dagger\rightarrow e^{-i\theta/2}a_1^\dagger, \quad a_2^\dagger\rightarrow e^{i\theta/2}a_2^\dagger. \tag{119}$$

It is then seen that the corresponding transformation $|jm\rangle\rightarrow e^{-im\theta}|jm\rangle$ of an SU(2) weight state is an overall phase change and undetectable. However, the transformation becomes detectable in a symmetric quantum interferometer in which the beams pass through beam splitters immediately before and immediately after they are phase shifted. If the first beam splitter effects an SU(2) transformation $e^{-i\hat{J}_x\pi/2}$ and the second reverses the transformation of the first, then the net result of the quantum interferometer is a detectable transformation in which

$$|jm\rangle\rightarrow e^{i\hat{J}_x\pi/2}e^{-i\theta\hat{J}_z}e^{-i\hat{J}_x\pi/2}|jm\rangle=e^{-i\theta\hat{J}_y}|jm\rangle=\sum_n |jn\rangle\, d^j_{nm}(\theta). \tag{120}$$

In such an interferometer, a minimal uncertainty input $|(\alpha,0)\rangle$ is transformed to an output $|(\alpha\cos(\theta/2),\alpha\sin(\theta/2))\rangle$. Thus, the ratio $\tan(\theta/2)$ of the output amplitudes provides a measure of θ; if only intensities are measured it provides a measure of θ modulo π. Measurements of phase shifts can also be made with other input states and it is of interest to consider choices with the greatest potential for accuracy.

The potential accuracy of a phase shift measurement is given by the width of the distribution function

$$N_\theta(\varphi)=|\langle\psi(\theta)|e^{-i\varphi\hat{J}_y}|\psi\rangle|^2=|\langle\psi|e^{-i(\varphi-\theta)\hat{J}_y}|\psi\rangle|^2. \tag{121}$$

It follows that $N_\theta(\varphi)=P(\varphi-\theta)$ where

$$P(\theta)=|\langle\psi|e^{-\theta\hat{J}_y}|\psi\rangle|^2. \tag{122}$$

For example, if $|\psi\rangle$ is the highest weight state $|jm=j\rangle$ then $P(\theta)$ is given by Eq. (23),

$$P_1(\theta)=|d^j_{jj}(\theta)|^2=\exp[-j\theta^2/2]. \tag{123}$$

On the other hand, if $|\psi\rangle$ is the state $|j\,m=0\rangle$, then $P(\theta)$ has the asymptotic expression given by Eq. (58),

$$P_2(\theta)=|d^j_{00}(\theta)|^2\sim|J_0(j\theta)|^2. \tag{124}$$

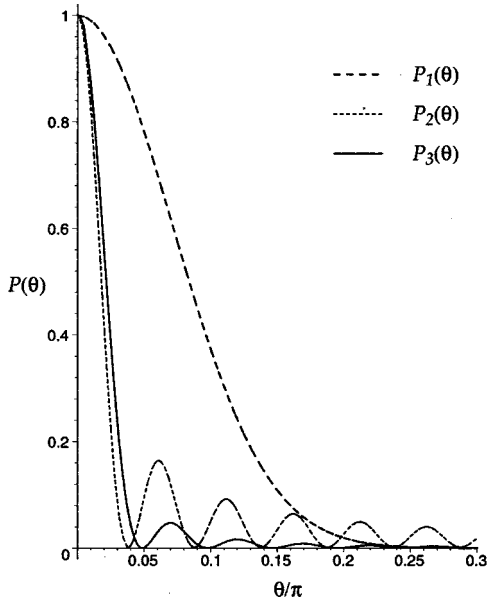

FIG. 12. The distribution functions given by Eqs. (123), (124), and (127) for $j=20$.

Thus, in spite of the fact that the highest weight state $|jj\rangle$ is a minimal uncertainty state, the variance in θ when the input state is $|jj\rangle$ is proportional to $1/\sqrt{j}$, whereas for a $|j\,m=0\rangle$ input state, it is proportional to $1/j$. This can be understood as follows. The density distribution of a spherical harmonic $|Y_{jj}(\theta,\varphi)|^2$ is concentrated about the $\theta=0$ pole whereas the density $|Y_{j0}(\theta,\varphi)|^2$ is spread uniformly about the $\theta=\pi/2$ equatorial circumference. Thus, the variance in θ can be much smaller for the latter distribution without violation of the uncertainty principle. This raises the question as to whether or not there might exist states with even less uncertainty relative to the $\hat{J}_y$ orientation than the state $|j0\rangle$. One candidate is the so-called SU(2) phase states[3,6,23]

$$|j\varphi\rangle=(2j+1)^{-1/2}\sum_{\mu=-j}^{j}e^{i\mu\varphi}|y;j\mu\rangle, \tag{125}$$

where $|y;j\mu\rangle$ is an eigenstate of $\hat{J}_y$ with eigenvalue μ. Putting $|\psi\rangle$ equal to $|j\varphi\rangle$ in Eq. (122) gives

$$P_3(\theta)=|\langle j\varphi|e^{-i\theta\hat{J}_y}|j\varphi\rangle|^2=(2j+1)^{-2}\left|\sum_{\mu}e^{i\mu\theta}\right|^2=(2j+1)^{-2}|\chi_j(\theta)|^2, \tag{126}$$

where χ_j is the well-known character of the SU(2) irrep of angular momentum j. Thus,

$$P_3(\theta)=\frac{\sin^2[(2j+1)\theta/2]}{(2j+1)^2\sin^2[\theta/2]}. \tag{127}$$

The function P_3 is also familiar in diffraction theory. The variance of φ for this function is proportional to $1/(j+0.5)$.

The distribution function $P(\theta)$ is shown in Fig. 12 for each of the three input states $|jj\rangle$, $|j0\rangle$, and $|j\theta\rangle$. The figure shows that the phase state and the $m=0$ state gives much more accurate measurements than the highest weight state. The down side is that these states are much more difficult to prepare and measure than a coherent mixture of $m=j$ minimal uncertainty states. (Another candidate for improving the estimation of phase is the so-called intelligent state,[24] which is also difficult to prepare.)

The advantage of using $|jm=0\rangle$ or SU(2) phase states over $|jm=j\rangle$ states for precision measurements is an example of the greater potential for acquiring or transmitting information by quantal states than is possible with classical states. A highest weight state $|jj\rangle$ is a state with all photons in channel one. A classical-like coherent state

$$|(\alpha,0)\rangle = e^{\alpha a_1^\dagger - \alpha^* a_1}|0\rangle, \tag{128}$$

is a superposition of many highest weight states:

$$|(\alpha,0)\rangle = e^{-|\alpha|^2/2}\sum_j \frac{\alpha^{2j}}{\sqrt{(2j)!}}|jj\rangle. \tag{129}$$

The distribution function for a coherent state is given by

$$|\langle(\alpha,0)|e^{-i\theta\hat{J}_y}|(\alpha,0)\rangle|^2 = |\langle(\alpha,0)|(\alpha\cos(\theta/2),\alpha\sin(\theta/2))\rangle|^2 = e^{-|\alpha|^2(1-\cos(\theta/2))}. \tag{130}$$

Thus, if $|\alpha|^2$ is set equal to the average number of photons, $2j$, then as $j\to\infty$ this distribution function approaches the value $\exp[-j\theta^2/2]$ that it has for the number state $|jj\rangle$ as one would expect.

In contrast, the state $|j\,m=0\rangle$ is unlike any classical state. In quantum mechanics it is a state

$$|j0\rangle = \frac{(a_1^\dagger)^j(a_2^\dagger)^j}{j!}|0\rangle, \tag{131}$$

having an equal number of photons in each channel. Whereas the preparation of such a state has not been performed, a compromise state is the coherent linear superposition of such states given[25] by a two-mode squeezed coherent state

$$e^{\beta(a_1^\dagger a_2^\dagger - a_1 a_2)}|0\rangle = \operatorname{sech}\beta\sum_{j=0}^{\infty}(\tanh\beta)^j\,|j\,m=0\rangle. \tag{132}$$

This state produces the desired $1/\langle j\rangle$ scaling of the phase uncertainty[26] for the appropriately weighted average value of j. However, apart from the problems of producing such a squeezed state, it is also noted that the distribution of j values is heavily weighted in favor of low-j values. Thus, it is doubtful that much could be gained by the use of such squeezed states.[3]

One might suppose that a classical-like input

$$|(\alpha,\alpha)\rangle = e^{\alpha a_1^\dagger - \alpha^* a_1}e^{\alpha a_2^\dagger - \alpha^* a_2}|0\rangle, \tag{133}$$

with equal amplitudes in each of the two ports might have some advantages. Such a state corresponds to an equal distribution of photon numbers in each port with a relatively narrow spread about some mean value. However, it follows from Eq. (111) that

$$|(\alpha,\alpha)\rangle = e^{-i\hat{J}_y\pi/2}\,|(\sqrt{2}\,\alpha,0)\rangle. \tag{134}$$

Hence

$$P(\theta) = |\langle(\alpha,\alpha)|e^{-i\theta\hat{J}_y}|(\alpha,\alpha)\rangle|^2 = |\langle(\sqrt{2}\,\alpha,0)|e^{-i\theta\hat{J}_y}|(\sqrt{2}\,\alpha,0)\rangle|^2, \tag{135}$$

and the variance is precisely the same as for the input state $|(\sqrt{2}\,\alpha,0)\rangle$. It should be noted that, whereas the state $|(\alpha,\alpha)\rangle$ can be obtained by an SU(2) rotation of the state $|(\sqrt{2}\,\alpha,0)\rangle$, it is impossible to rotate a highest weight state $|jj\rangle$ into the state $|jm=0\rangle$.

The optimization of the inputs to an interferometer in order to yield the most precise phase shift information possible with a limited number of photons is important; e.g., for the detection of

gravitational waves.[21] Caves has suggested injecting a standard coherent state into one channel and a squeezed vacuum state into the other. Another suggestion is to put a squeezed input into one channel and an antisqueezed input into the other.[27] Clearly an expansion of such inputs in an SU(2) basis will make it possible to analyze the precisions obtainable with such inputs in the large photon number limit using the asymptotic SU(2) Wigner functions given in this paper.

B. Three-channel interferometry

Similar considerations apply to a three-channel interferometer which transforms input states by a U(3) transformation

$$T(g):|\psi\rangle \rightarrow T(g)|\psi\rangle, \quad g \in \mathrm{U}(3). \tag{136}$$

The transformation is analogous to the U(2) transformation discussed in the preceding section, but with $T(g)$ a unitary representation of a matrix $g \in \mathrm{U}(3)$. The U(3) transformation can be factorized into a sequence of SU(2) transformations and an overall phase factor; physically, this corresponds to a realization of a three-channel interferometer as a combination of two-channel devices (phase shifters, mirrors and beam splitters).

The infinitesimal generators of the unitary transformation $T(g)$ are given in a generalized Schwinger representation in Eq. (78). In such a representation, basis states for an SU(3) irrep of highest weight $(\lambda,0)$ are weight states $|\nu\rangle \equiv |\nu_1 \nu_2 \nu_3\rangle$; they can be regarded as triplet Fock number states with ν_i photons in channel i of the interferometer and fixed total photon number.

Many of the results for two-channel interferometry, discussed in the preceding section, carry forward to the three-channel case in an intuitively clear manner. For instance, the state in which all photons enter through channel one is the minimal uncertainty (highest weight) state $|(\lambda)\rangle \equiv |\lambda,0,0\rangle$. For analysis of experiments with such an input state, the SU(3) Wigner function $D^{(\lambda)}_{\nu,(\lambda)}$ and its asymptotic limit is relevant. On the other hand, the Wigner functions for central weights are relevant for balanced input states.

Whereas the two-channel interferometer is suited to the measurement of phase difference between two channels of propagation, it may be desirable to measure multiple phase shifts simultaneously, e.g., because the phase shifts are transient or the mean particle flux of the source is limited. Moreover, the most efficient use of photons for precision measurement is to divide them up and measure relative phases between multiple paths.[7,6] The SU(N) interferometer is ideally suited for this purpose. The SU(3) interferometer allows the measurement of two phase shifts simultaneously.

D'Ariano and Paris[7] have shown that much improved accuracy is already obtained with an easily produced coherent state input by suitably dividing the input into the many channels of a multichannel interferometer. They show that with a mean number λ of photons, the variance of the phase shift estimation scales as $\Delta\theta^2 \propto 1/N^2\lambda$ for an N-channel interferometer. In contrast, if the fixed input of λ photons were to be split between $N-1$ two-channel interferometers, then the variance of each would be proportional to $(N-1)/\lambda$ and, with the estimate of θ given by the mean of the θ_i obtained in the two-channel interferometers, the variance would be independent of N (assuming the spread of measured phase shifts is small compared to the range 0 to 2π). Thus, nothing is gained by splitting the λ photons over many two-channel interferometers but a huge gain results from appropriate use of a multichannel interferometer.

Still further gains can, in principle, be achieved by use both of exotic inputs and multichannel interferometers. The balanced input state is a preferred input state for phase-shift determination but it is hard to generate. Also, it is just one of many inputs which can, in principle, improve the precision of phase-shift estimation. The generalization to SU(3) of the SU(2) phase state considered in the preceding section,[6] could also yield superior scaling laws for the phase-shift estimation in terms of λ. The precision of two simultaneously measured phase shifts is rigorously expressed in terms of the covariance matrix for the two phases. This 2×2 matrix includes the variance for each phase and the covariance between the two phases. Detailed analyses of the results achievable

with various techniques and three-channel inputs is in principle possible by expanding the inputs in an SU(3) basis and using the asymptotic Wigner functions to infer variances as done for two-channel interferometers in Sec. V A.

VI. CONCLUDING REMARKS

In this paper, we have derived several previously unknown asymptotic limits of SU(2) Wigner d^j_{mn} functions which converge rapidly as $j\to\infty$ and are shown to be accurate over a wide range of their arguments. We have also shown how SU(3) Wigner functions for multiplicity-free irreps of highest weight $(\lambda,0)$ can be factored into products of SU(2) Wigner functions so that their limits can be inferred from those of SU(2). This kind of inference is not limited to SU(3) and can be generalized to SU(N) irreps of highest weight $(\lambda,0,...)$ for $N>3$.

Explicit limiting expressions have been given for some representative classes of SU(3) Wigner functions. In particular, we have considered Wigner functions for states whose weights are either extremal or central in the terminology of Sec. IV. Other expressions can be derived by variations of the methods given. For example, useful asymptotic SU(3) Wigner functions can be determined for which one weight is extremal and the other is close to a side. Depending on the domains of the initial and final states of a Wigner function, it will often happen that the expressions are much simpler in some other set of SU(3) Euler angles than those given. This is a simple reflection of the fact that a given SU(3) transformation may be simple when expressed as one sequence of SU(2) transformations but seemingly complex when expressed in some other way. Thus, by choosing the most appropriate sequence the number of summations over products of SU(2) Wigner functions can be minimized.

Asymptotic limits of Wigner functions are of interest for many reasons. In situations where they are valid, they can facilitate computations and provide quick estimates of the behaviors of quantum systems. In this way they give physical insight into the ways quantal systems approach classical limits. This has been illustrated in this paper by using the limits to estimate variances in phase shift measurements by quantum interferometry and to determine the ways they scale with the number of photons. Asymptotic limits may also be important in quantum information theory for identifying quantum states that behave in very nonclassical and potentially useful ways.

Our initial hope was to derive asymptotic expressions for the Wigner functions of generic SU(3) irreps. However, while we did succeed in deriving some expressions, they proved under numerical investigation to be accurate only over narrow ranges of their arguments. Thus, while of some mathematical interest, they are of limited practical value. Clearly further investigation is needed before any results are presented.

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Erratum: "η-invariants and determinant lines" [J. Math. Phys. 35, 5155 (1994)]

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There are two errors in Ref. 1 which we would like to set straight. The first affects some of the equations, but none of the results. The second is more serious, and was noticed in the course of writing the paper.[3]

The first error, which is in some sense a matter of convention, comes in the computation of the boundary operator associated to the Dirac operator, for example, in the second equation of Appendix A. Namely, if X is a manifold with boundary whose metric is a product near the boundary, then near the boundary we write the Dirac operator on X as

$$D_X = J(\partial_\mu + B_{\partial X}),$$

where the boundary is cut out by $\mu = 0$, the coordinate μ is negative on the interior of X, the 1-form $d\mu$ has unit length, and J is Clifford multiplication by $d\mu$. We call $B_{\partial X}$ the boundary operator associated to D_X. In the familiar case where X is even-dimensional, if D_X is the chiral Dirac operator mapping plus spinor fields to minus spinor fields, then the boundary operator $B_{\partial X}$ may be identified with the ordinary Dirac operator on ∂X. (Both the plus spinors and minus spinors restricted to the boundary may be identified with $S_{\partial X}$, and J is an isomorphism between the two restrictions.) However, if X is odd-dimensional, as in the paper, then near the boundary $J = \left(\begin{smallmatrix} -\sqrt{-1} & 0 \\ 0 & \sqrt{-1} \end{smallmatrix}\right)$ relative to the decomposition of spinors on the boundary $S_{\partial X} = S^+_{\partial X} \oplus S^-_{\partial X}$, and we have

$$B_{\partial X} = J^{-1} D_{\partial X}.$$

In the paper we left off the factor J^{-1}, and so factors of $\sqrt{-1}$ are missing in formulas sprinkled throughout the paper, though they do not affect the main results. For example, the basic boundary condition in Eq. (1.2) should read as

$$W_{(a,T)} = \left\{ \langle \phi^+, \phi^- \rangle \in H_{\partial X} : \phi^- - \sqrt{-1}\left(T \oplus \frac{D_{\partial X}(a)}{\sqrt{D_{\partial X}(a)^2}} \right) \phi^+ = 0 \right\}. \tag{1.2$'$}$$

Other affected formulas include (1.5), (2.16), and many formulas in Sec. IV and Appendix A. For example, Eq. (4.8) should be replaced by

$$\tau_C(a,T) = (-\sqrt{-1})^{\dim K^+ + \dim K^-} \det T. \tag{4.8$'$}$$

Although explicit formulas for $\tau_X(a,T)$ are changed, the main conclusions about the invariant τ_X are unchanged by these factors.

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These factors are also important in understanding what happens when we reverse orientation. For any manifold X we identify spinors on the manifold X with spinors on the oppositely oriented manifold $-X$:

$$S_{-X} \cong S_X .$$

[See the text following (2.14) in the paper.] The Dirac operator changes sign under this identification:

$$D_{-X} = -D_X .$$

However, if Y is even-dimensional (for example, the boundary of an odd-dimensional manifold), then $S^{\pm}_{-Y} \cong S^{\mp}_{Y}$ and the boundary operators are identified:

$$B_{-Y} = B_Y .$$

A more substantial correction occurs in the formula after (2.18) for the τ-invariant of the orientation-reversed manifold:

$$\tau_{-X} = (-1)^{\binom{k}{2}} \tau_X^{-1}, \qquad (*)$$

where k is the number of components of ∂X on which the boundary Dirac operator has odd index. (Of course, $k=0$ if ∂X is connected.) This was applied in Ref. 3 to the double X^d of a manifold X to conclude

$$\tau_{X^d} = (-1)^{\binom{k}{2}}. \qquad (**)$$

As a simple example, let X be the closed interval $[0, 1]$. Then the double X^d is the circle with the nonbounding spin structure. In this case $k=2$ and formula $(**)$ is correct.

To understand $(*)$ one should be aware that the pairing in the statement of the gluing formula Theorem 2.20 depends on the gluing map. For example, one can glue together two disjoint closed intervals into a single circle or into two disjoint circles, depending on the choice of gluing map. For circles with the nonbounding spin structure, the τ-invariants differ by a sign in the two cases. The equality in Eq. $(*)$ refers to the identification of the inverse determinant line of $\partial(-X)$ with the dual of the determinant line of ∂X under which boundary components are not permuted; the formula states that τ_X and τ_{-X} pair to $(-1)^{\binom{k}{2}}$. If we choose a boundary condition (a,T) for X, then with the boundary condition $(a,-T^{-1})$ for $-X$ we see easily that $\tau_{-X}(a,-T^{-1}) = \tau_X(a,T)^{-1}$. But if $L_1,\ldots,L_n$ are the inverse determinant lines of the components of ∂X, then to pair $L_1 \otimes \cdots \otimes L_n$ with $L_1^{-1} \otimes \cdots \otimes L_n^{-1}$ we must permute the latter tensor product to $L_n^{-1} \otimes \cdots \otimes L_1^{-1}$, and this accounts for the sign.

Finally, we remark that an improved argument deriving the holonomy theorem for determinant line bundles (see Sec. V of the paper) appears in Ref. 2.

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Erratum: "Three flavor neutrino oscillations in matter" [J. Math. Phys. 41, 2768 (2000)]

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On p. 2779, Eq. (73), should be

$$\theta_3^M \equiv \arctan\frac{U_{e2}^M}{U_{e1}^M} = \arctan\sqrt{\left(\frac{U_{e2}^M}{U_{e1}^M}\right)^2} = \arctan\sqrt{\frac{U_{e2}^M U_{e2}^M}{U_{e1}^M U_{e1}^M}}$$

$$= \arctan\sqrt{\frac{\lambda_2^2 + c_1 + \lambda_2 \tilde{T}_{ee} + (\tilde{T}^2)_{ee}}{\lambda_1^2 + c_1 + \lambda_1 \tilde{T}_{ee} + (\tilde{T}^2)_{ee}} \frac{3\lambda_1^2 + c_1}{3\lambda_2^2 + c_1}}.$$

Note that Eq. (80) on p. 2781 is correct and that Figs. 2 and 4 have been generated with this equation.

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Temporally stable coherent states for infinite well and Pöschl–Teller potentials

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This article is a direct illustration of a construction of coherent states which has been recently proposed by two of us (JPG and JK). We have chosen the example of a particle trapped in an infinite square-well and also in Pöschl–Teller potentials of the trigonometric type. In the construction of the corresponding coherent states, we take advantage of the simplicity of the solutions, which ultimately stems from the fact they share a common SU(1,1) symmetry *à la* Barut-Girardello. Many properties of these states are then studied, both from mathematical and from physical points of view. © *2001 American Institute of Physics*.
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I. INTRODUCTION

Despite its relevance for the understanding of the most elementary parts of quantum mechanics, the problem of a particle trapped in an infinite square-well (Fig. 1) usually deserves no more than a few pages in most physics textbooks.[1–3] Solutions are straightforward to derive, energy is nicely quantized and trigonometric wave functions afford an immediate intuition of quantum behavior. The model is widely used to give a fair idea of many body systems in atomic or molecular physics. However, very soon one may become puzzled by less trivial problems pertaining to the mathematics of quantum mechanics: domain of self-adjointness for the operators involved, possible nonuniqueness of self-adjoint extensions (see in particular the very instructive examples in Chapters VIII.I, VIII.2, and X.1 of Ref. 4), explicit kernel of the evolution operator, crucial role played by the boundary conditions, semiclassical behavior and the classical limit, and other limiting situations such as a very large or a vanishingly small width of the well.

Actually all these questions can be considered through a nice analytic regularization of the infinite well potential. Indeed, consider the continuously indexed family of potentials

$$V(x)\equiv V_{\lambda,\kappa}(x)=\frac{1}{2}V_0\left(\frac{\lambda(\lambda-1)}{\cos^2/2a}+\frac{\kappa(\kappa-1)}{\sin^2 x/2a}\right),\quad 0\leqslant x\leqslant \pi a, \tag{1.1}$$

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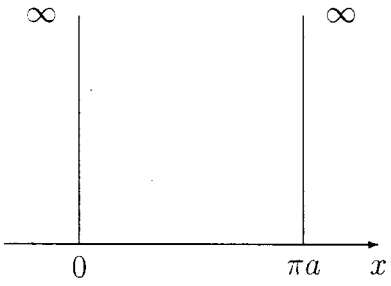

FIG. 1. The infinite square-well potential.

for $\lambda,\kappa>1$ ($V_0>0$ is a coupling constant). Clearly this is a smooth approximation, for $\lambda,\kappa \to 1^+$, of the infinite square-well over the interval $[0,\pi a]$. These potentials, called the Pöschl–Teller (PT) potentials,[3,5] are shown in Fig. 2 for the values $(\lambda,\kappa)=(4,4),(4,8),(4,16)$, respectively. In order to make contact with standard quantum mechanics on the whole line, there are two possibilities. Either one requires that $V(x)=\infty$ outside the interval $[0,\pi a]$, or one periodizes the potential, with period πa, and one imposes periodic boundary conditions at the points $\{n\pi a, n\in\mathbb{Z}\}$. But, since the walls separating the successive cells are impenetrable, one may also simply ignore these extensions and consider only the interval $[0,\pi a]$, which we shall do in the present article.

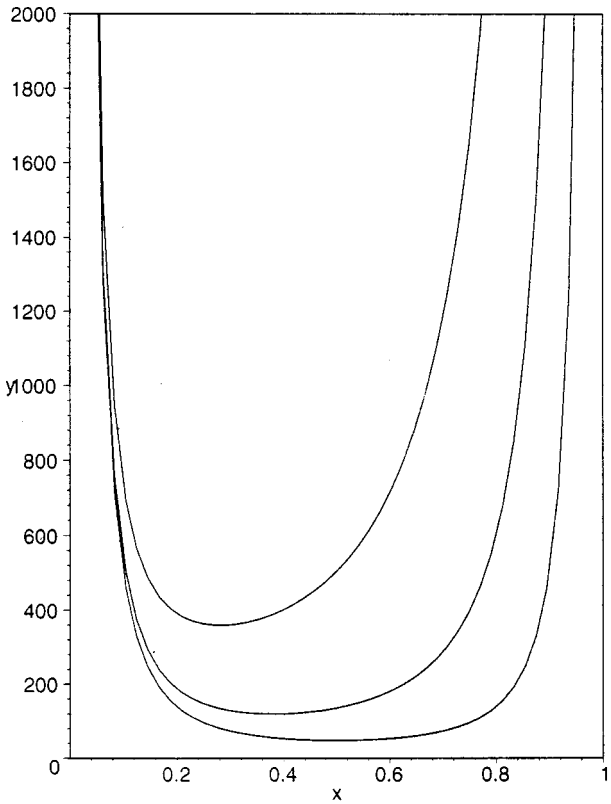

FIG. 2. The Pöschl–Teller potential $V(x)=1/2V_0[\lambda(\lambda-1)\cos^{-2}x/2a+\kappa(\kappa-1)\sin^{-2}x/2a]$, with $a=\pi^{-1}$ and for $(\lambda,\kappa)=(4,4),(4,8),(4,16)$ (from bottom to top).

The Pöschl–Teller potentials share with their infinite well limit the nice property of being analytically integrable. The reason behind this can be understood within a group-theoretical context: The family of potentials (1.1) possesses an underlying dynamical algebra, namely $\mathfrak{su}(1,1)$ and the discrete series representations of the latter. We recall that the discrete series unitary irreducible representations (UIRs) of $\mathfrak{su}(1,1)$ are labeled by a parameter η, which takes its values in $\{1/2,1,3/2,2,...\}$ for the discrete series *stricto sensu*, and in $[1/2,+\infty)$ for the extension to the universal covering of the group SU(1, 1). The relation between the Pöschl–Teller parameters and η is given by

$$2\eta-1=\lambda+\kappa,$$

and the limit case $\lambda,\kappa\rightarrow 1^{+}$ corresponds to $\eta=3/2$.

Other approaches in the past led to the group SU(2) as the dynamical group for the Pöschl–Teller potentials, when $\lambda+\kappa$ is an integer.[6] We emphasize here the fact that the SU(1, 1) approach seems more natural, for it extends easily and naturally to noninteger values of $\lambda+\kappa$.

In fact, the Pöschl–Teller potential (1.1), sometimes called PT of the first type, is closely related to several other potentials, widely used in molecular and solid state physics.

- The symmetric Pöschl–Teller potential well, given by $\lambda=\kappa\geqslant 1$, is

$$V_{\lambda}(x)=2V_0\frac{\lambda(\lambda-1)}{\sin^2 x/a}. \tag{1.2}$$

  This potential may be periodized with period $\pi a/2$, instead of πa.

- The same potential, for $1/2\leqslant\lambda<1$, is known as the Scarf potential.[7] This is no longer a well, but an inverted well, that is, a peak between two infinite negative wells. When periodized over the whole line, this is a good model for a 1-D crystal (as a smooth substitute to the well-known Kronig–Penney model), since the spectrum of the corresponding Hamiltonian has a band structure. The nonsymmetric extension of the Scarf potential has similar properties.[8] Interestingly, both cases admit SU(1, 1) as a dynamical group, although the representations underlying the band part are those of the complementary series.
- There exists also the so-called scattering (or modified) Pöschl–Teller potentials, obtained by replacing the trigonometric functions in (1.1) by their hyperbolic counterparts.[5] A special case is the Rosen-Morse potential,[9] which is simply the symmetric version of the previous one. These potentials are widely used in molecular physics, and they have the same dynamical group SU(1, 1) (but again other representations are involved). For a review of this case and its applications, we refer to Refs. 10–12.

In this article we present and study families of coherent states (CSs) adapted to the infinite well and to the Pöschl–Teller potentials. We call these states *adapted* and *coherent* because they are a direct generalization of the standard ones corresponding to the harmonic oscillator[13] (for an extensive and up-to-date bibliography see, for instance, Ref. 14). We recall that the Schrödinger-Klauder-Glauber CS reads

$$|z\rangle=e^{-|z|^2/2}\sum_{n\geqslant 0}\frac{z^n}{\sqrt{n!}}|n\rangle. \tag{1.3}$$

We extend them in a sense already explained in Refs. 15–17 and briefly sketched in the following. We first consider in (1.3) the kets $|n\rangle$ as the eigenstates of the infinite well (resp. Pöschl–Teller) Hamiltonian H corresponding to the eigenvalue $\hbar\omega e_n$, $n\geqslant 0$, $e_0=0$. Next, analogous to the pioneering work of Jackson,[18] we replace in the square root the factorial $n!$ by the generalized factorial $[e_n]!=e_1\ldots e_n$, to get the so-called action identity[16]

$$\langle z|H|z\rangle=\hbar\omega|z|^2. \tag{1.4}$$

Note that similar factorial ''deformations'' in the construction of coherent states already appear in Refs. 19 and 20. We finally require (temporal) stability for our new family of coherent states under the action of the evolution operator $e^{-iHt/\hbar}$ (see Ref. 16 and Sec. VII of this work for details). Our interest in these infinite well and Pöschl–Teller coherent states lies mostly in the simplicity of the formulas involved. We have here at our disposal a nice tool for examining many quantum features, such as probability densities, autocorrelation, mean values of observables, Heisenberg inequalities, semiclassical limits, and others.

The article is organized as follows. In Sec. II, we describe the classical motion in an infinite square-well potential and in a Pöschl–Teller potential. In our opinion, it is essential to recall this elementary (and pedagogical!) material for the subsequent discussions on a quantum level. Sections III and IV are devoted to the quantum infinite well and Pöschl–Teller potentials, respectively. In particular, we give here an up-to-date survey of the nontrivial questions of self-adjointness for some of the most familiar physical observables. We examine in Sec. V the questions related to various limits: semiclassical $\hbar \to 0$, $n\hbar = \text{const}$, infinite narrowness $a \to 0$, infinite width $a \to \infty$, Pöschl–Teller→infinite well, and others. We describe in Sec. VI the dynamical symmetry algebra $\mathfrak{su}(1,1)$ common to both models and underlying their integrability. In Sec. VII we first review the general construction of ''action-angle'' or rather ''energy-time'' coherent states before giving their explicit form and their most immediate mathematical properties in the infinite well case, and in the Pöschl–Teller case (Sec. VIII). Section IX is devoted to the most interesting physical properties of our states, and in particular to the revival features they present, which are well illustrated by the large number of figures shown there. Finally. Sec. X summarizes the discussion about the role of coherent states when expressed in terms of action-angle variables.

A final lesson of the article is that a comprehensive study of quantum mechanics requires not only algebra, or numerical simulations, but also a precise use of functional analysis. The fine points of the latter are not mathematical pedantry; they express deep physical properties.

II. THE CLASSICAL PROBLEM

A. Classical infinite well

It is worthwhile to start out this article with a short pedagogical review of the classical behavior of a particle of mass m trapped in an infinite well of width πa.

For a nonzero energy

$$E = \tfrac{1}{2} m v^2, \tag{2.1}$$

there corresponds a speed

$$v = \sqrt{\frac{2E}{m}} \tag{2.2}$$

for a position $0 < x < \pi a$. There are perfect reflections at the boundaries of the well. So the motion is periodic with period (the ''round trip time'') T equal to

$$T = \frac{2\pi a}{v} = 2\pi a \sqrt{\frac{m}{2E}}. \tag{2.3}$$

With the initial condition $x(0) = 0$, the time behavior of the position is then given by (see Fig. 3)

$$\begin{aligned} 0 \leqslant t \leqslant \tfrac{1}{2} T: &\quad x = v t, \\ \tfrac{1}{2} T \leqslant t \leqslant T: &\quad x = 2\pi a - v t, \end{aligned} \tag{2.4}$$

and of course

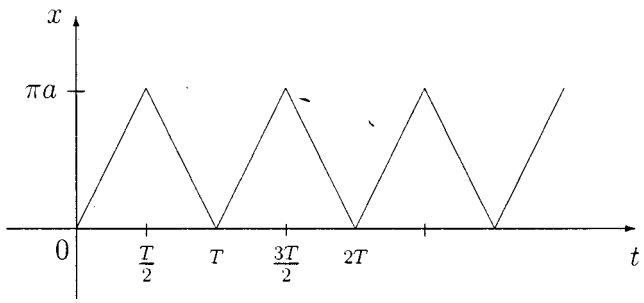

FIG. 3. The position $x(t)$ of the particle trapped in the infinite square-well of width πa, as a function of time.

$$x(t+nT)=x(t). \tag{2.5}$$

Consequently the velocity is a periodized Haar function (Fig. 4):

$$\mathbf{v}=v\sum_{n=0}^{+\infty}[\mathbb{1}_{[nT,(n+1/2)T]}-\mathbb{1}_{[(n+1/2)T,(n+1)T]}] \tag{2.6}$$

(here $\mathbb{1}_B$ denotes the characteristic function of a set $B\in\mathbb{R}$), whereas the acceleration is the superposition of two Dirac combs on the half-line (Fig. 5):

$$\gamma=\sum_{n=0}^{+\infty}[\delta_{nT}-\delta_{(n+1/2)T}]. \tag{2.7}$$

The average position and average velocity of the particle are then

$$\overline{x}=\frac{1}{T}\int_0^T x(t)dt=\frac{\pi a}{2},\quad \overline{v}=0, \tag{2.8}$$

whereas the mean square dispersions are

$$\sqrt{\overline{x^2}-\overline{x}^2}=\frac{\pi a}{2\sqrt{3}},\quad \sqrt{\overline{v^2}-\overline{v}^2}=\sqrt{\frac{2E}{m}}. \tag{2.9}$$

Note the standard Fourier expansion for the position and the velocity, respectively,

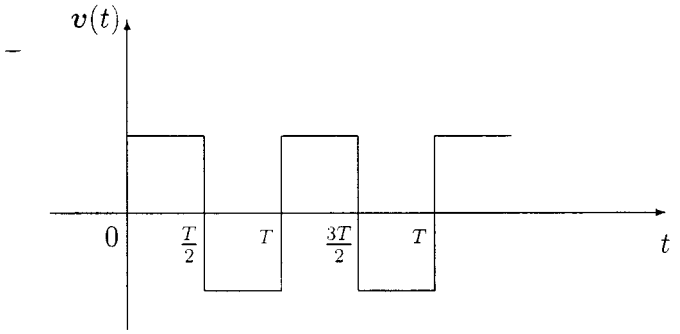

FIG. 4. The velocity $\mathbf{v}(t)$ of the particle in the infinite square-well: periodized Haar function.

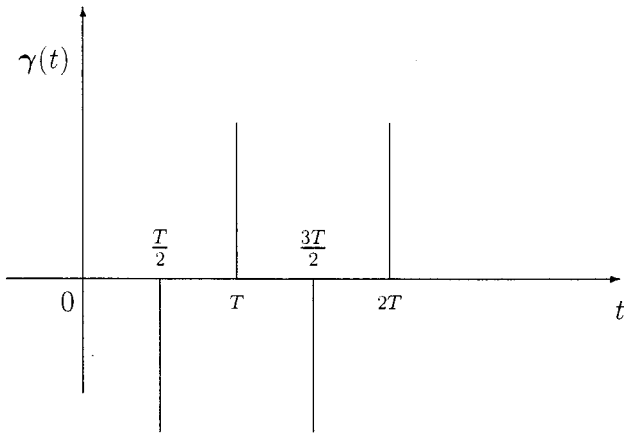

FIG. 5. The acceleration $\gamma(t)$ of the particle of the particle in the infinite square-well.

$$x(t)=\frac{\pi a}{2}-\frac{4a}{\pi}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\cos\frac{2\pi}{T}(2n+1)t, \tag{2.10}$$

$$\mathbf{v}(t)=4\frac{v}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}\sin\frac{2\pi}{T}(2n+1)t. \tag{2.11}$$

Figure 6 shows the phase trajectory of the system. This trajectory encircles a surface of area equal to the action variable

$$A=\frac{1}{2\pi}\oint pdq=mva, \tag{2.12}$$

where $q=x$ and $p=mv$ are canonically conjugate. Note the other expressions for A:

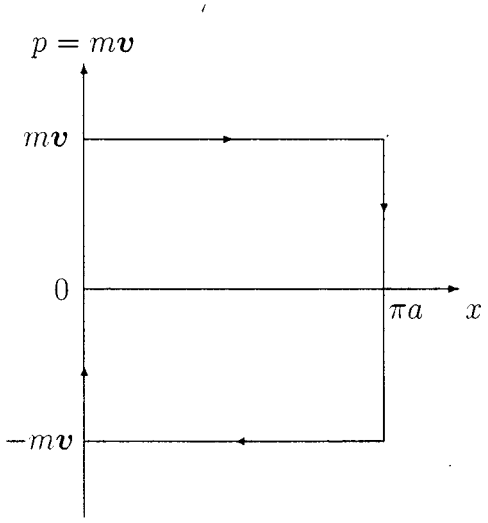

FIG. 6. Phase trajectory of the particle in the infinite square-well.

$$A=\frac{2\pi a^2 m}{T}=\frac{mv^2 T}{2\pi}=a\sqrt{2mE}. \tag{2.13}$$

The action-angle variables (A,φ) are obtained through the canonical transformation (ϑ denotes the step function)

$$\varphi=\mathrm{sgn}(p)\frac{q}{a}+\vartheta(-p)2\pi \pmod{2\pi}, \tag{2.14}$$

$$A=|p|a, \tag{2.15}$$

with generating function equal to the Maupertuis action, as should be expected:

$$\begin{aligned} S_0&=2\pi nA+S_0^{\mathrm{princ}},\\ S_0^{\mathrm{princ}}&=A\varphi=pq+|p|\vartheta(-p)a, \quad \varphi\in(0,2\pi). \end{aligned} \tag{2.16}$$

Finally, note the time evolution of the angle variable:

$$\varphi=\frac{\mathbf{v}}{a}t+\varphi_0\equiv\alpha t+\varphi_0. \tag{2.17}$$

B. Pöschl–Teller potentials

The solution to the equations of motion with the potentials (1.1) is straightforward, in spite of the rather heavy expression of the latter. The turning points $x_\pm$ of the periodic motion at a given energy E are given by

$$x_\pm=a\arccos\left[\frac{\alpha-\beta}{2}\pm\sqrt{\Delta}\right], \tag{2.18}$$

where $\Delta=(1-1/2(\sqrt{\alpha}+\sqrt{\beta})^2)(1-1/2(\sqrt{\alpha}-\sqrt{\beta})^2)$, $\alpha=(V_0/E)\lambda(\lambda-1)$, $\beta=(V_0/E)\kappa(\kappa-1)$.

So, the motion is possible only if

$$E>\frac{V_0}{2}(\sqrt{\lambda(\lambda-1)}+\sqrt{\kappa(\kappa-1)})^2. \tag{2.19}$$

The time evolution of the position is given by

$$\begin{aligned} x(t)&=a\arccos\left[\frac{\alpha-\beta}{2}+\sqrt{\Delta}\cos\left(\sqrt{\frac{2E}{m}}\frac{t}{a}\right)\right],\\ x(0)&=x_-. \end{aligned} \tag{2.20}$$

Hence the period is

$$T=2\pi a\sqrt{\frac{m}{2E}}. \tag{2.21}$$

It is remarkable that the period T does not depend on the strength V_0, nor on λ and κ.

The action variable A satisfies the relation $dA/dE=T/2\pi$, and thus

$$A=\alpha\sqrt{2mE}+\mathrm{const.} \tag{2.22}$$

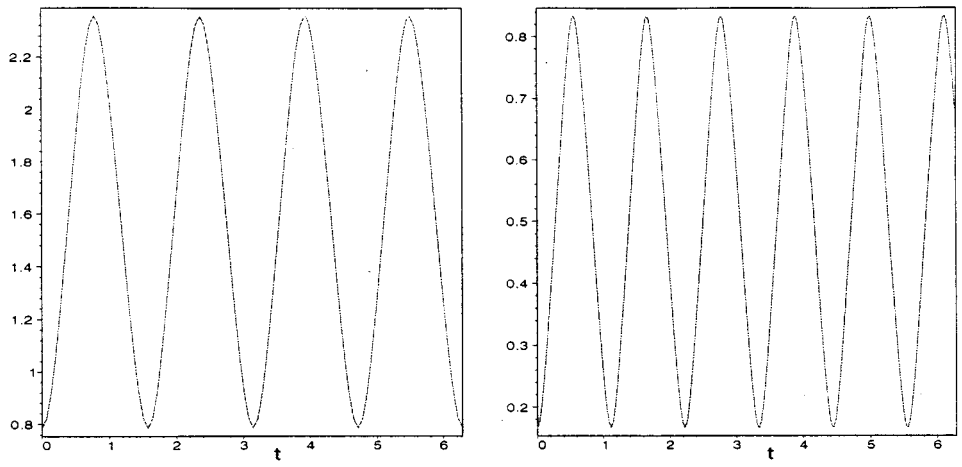

FIG. 7. The position $x(t)$ of the particle in the symmetric Pöschl–Teller potential $\lambda=\kappa=2$: (a) $E=8V_0$, $T=\pi/2$; and (b) $E=16V_0$, $T=\pi/2\sqrt{2}$ (compare Fig. 3).

The constant is determined by the condition that $A=0$ for $E=V_{\min}$, that is, const $=-a\sqrt{2mV_{\min}}$. The Pöschl–Teller potential $V(x)$ reaches its minimum at the location x_0 defined by

$$\tan^2\frac{x_0}{2a}=\sqrt{\frac{\kappa(\kappa-1)}{\lambda(\lambda-1)}}. \tag{2.23}$$

So we have, in agreement with (2.19),

$$V_{\min}=V(x_0)=\frac{V_0}{2}[\sqrt{\lambda(\lambda-1)}+\sqrt{\kappa(\kappa-1)}]^2, \tag{2.24}$$

and, consequently,

$$A=a\sqrt{2mE}-a\sqrt{mV_0}[\sqrt{\lambda(\lambda-1)}+\sqrt{\kappa(\kappa-1)}]. \tag{2.25}$$

It is worthwhile to compare (2.21) and (2.25) with their respective infinite well counterparts (2.3) and (2.13). We should also check that the time behavior (2.20) of $x(t)$ goes into (2.4) at the limits $\alpha,\beta\to 0$. We give in Figures 7–9 the curves for $x(t)$, $\mathbf{v}(t)$ and $\boldsymbol{\gamma}(t)$, respectively, in the particular symmetric case $\lambda=\kappa=2$, for two different values of the energy, namely, $E=8V_0$ and $E=16V_0$. Figure 10 shows the corresponding phase trajectory in the plane $(q=x,\ p=mv)$. Note that, in the general case, the equation for the latter reads (at energy E)

$$p=\pm\frac{\sqrt{2mE}}{\sin q/a}\left[1-(\alpha+\beta)+(\alpha-\beta)\cos\frac{q}{a}-\cos^2\frac{q}{a}\right]^{1/2}. \tag{2.26}$$

Finally, let us give the canonical transformation leading to the action-angle variables

$$\varphi=\arccos\frac{1}{\sqrt{\Delta}}\left[\cos\frac{q}{a}-\frac{\alpha-\beta}{2}\right], \tag{2.27}$$

$$A=a[p^2+2mV(q)]^{1/2}. \tag{2.28}$$

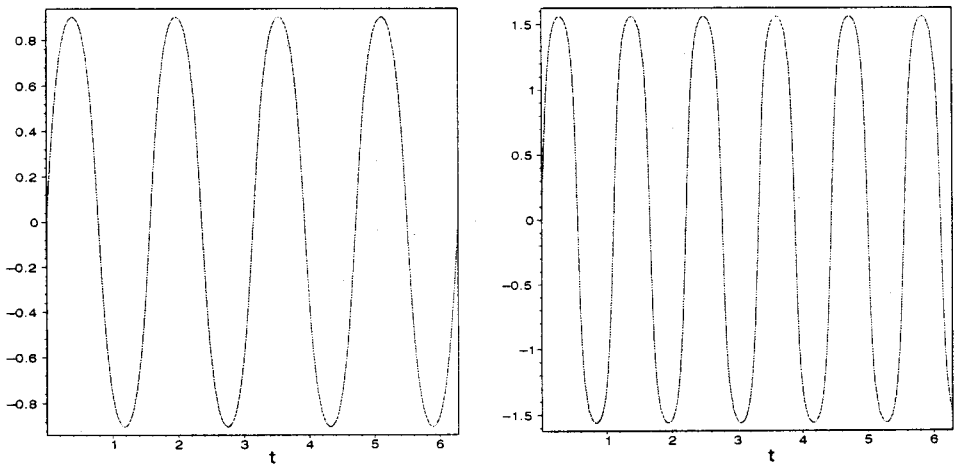

FIG. 8. The velocity $\mathbf{v}(t)$ of the particle in the symmetric (2,2) Pöschl–Teller potential, for the same values of E and T as in Fig. 7 (compare Fig. 4).

The Maupertuis action generating (2.25) is given by

$$S_0(u) = 2\pi nA + S_0^{\text{princ}}(u),$$

$$S_0^{\text{princ}}(u) = -a\sqrt{2mE}\int_{u_-}^{u} [1-(\alpha+\beta)+(\alpha-\beta)s-s^2]^{1/2}\frac{ds}{1-s^2}$$

with $u = \cos x/a$. The last integral may be calculated explicitly, but the result is not illuminating.

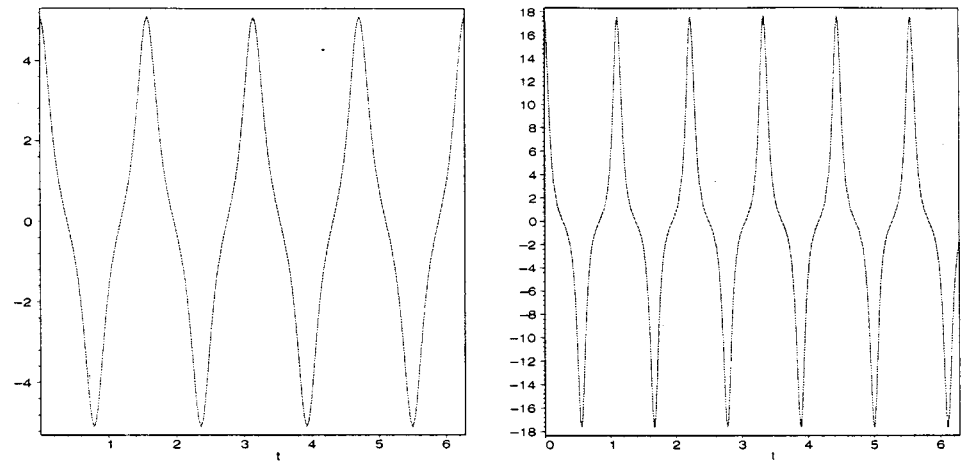

FIG. 9. The acceleration $\gamma(t)$ of the particle in the symmetric (2,2) Pöschl–Teller potential, for the same values of E and T as in Fig. 7 (compare Fig. 5).

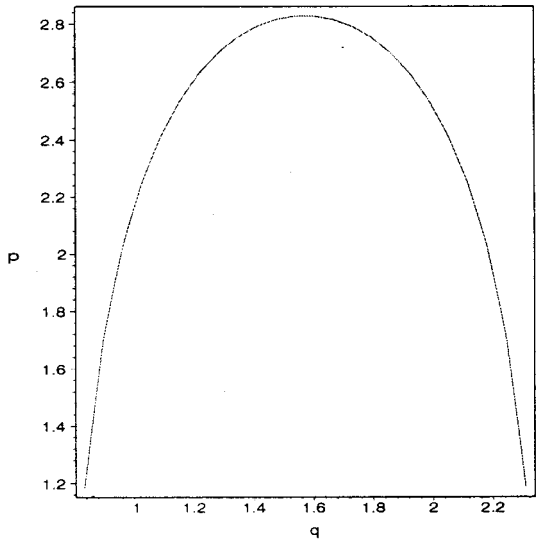

FIG. 10. Upper part of the phase trajectory of the particle the symmetric (2,2) Pöschl–Teller system, for the same values of E and T as in Fig. 7 (compare Fig. 6).

III. THE QUANTUM PROBLEM FOR THE INFINITE WELL

Any quantum system trapped inside the infinite well $0 \leqslant x \leqslant \pi a$ must have its wave function equal to zero outside the well. It is thus natural to impose on the wave functions the boundary conditions

$$\psi(x) = 0, \quad x \geqslant \pi a \quad \text{and} \quad x \leqslant 0. \tag{3.1}$$

Since the movement takes place only inside the interval $[0, \pi a]$, we may as well ignore the rest of the line and replace the conditions (3.1) by the following ones:

$$\psi \in L^2([0, \pi a], dx), \quad \psi(0) = \psi(\pi a) = 0. \tag{3.2}$$

Alternatively, one may consider the periodized well and impose the same periodic boundary conditions, namely, $\psi(n\pi a) = 0$, $\forall n \in \mathbb{Z}$.

In either case, stationary states of the trapped particle of mass m are easily found from the eigenvalue problem for the Schrödinger operator. For reasons to be justified in the sequel, we choose the shifted Hamiltonian:

$$H \equiv H_w = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - \frac{\hbar^2}{2ma^2}. \tag{3.3}$$

Then

$$\Psi(x,t) = e^{-iHt/\hbar}\Psi(x,0), \tag{3.4}$$

where $\Psi(x,0) \equiv \psi(x)$ obeys the eigenvalue equation

$$H\psi(x) = E\psi(x), \tag{3.5}$$

together with the boundary conditions (3.1). Normalized eigenstates and corresponding eigenvalues are then given by

$$\psi_n(x)=\sqrt{\frac{2}{\pi a}}\sin(n+1)\frac{x}{a}\equiv\langle x|n\rangle,\quad 0\leqslant x\leqslant \pi a, \tag{3.6}$$

$$H|n\rangle=E_n|n\rangle,\quad n=0,1,..., \tag{3.7}$$

$$E_n=\frac{\hbar^2}{2ma^2}n(n+2)\equiv\hbar\omega e_n, \tag{3.8}$$

with

$$\omega=\frac{\hbar}{2ma^2}\equiv\frac{2\pi}{T_r}\quad\text{and}\quad e_n=n(n+2),\quad n=0,1,...,$$

where T_r is the ''revival'' time to be compared with the purely classical round trip time given in (2.3). Now the Bohr–Sommerfeld quantization rule applied to the classical action gives

$$a\sqrt{2mE}=A=(n+1)\hbar, \tag{3.9}$$

so

$$E=(n+1)^2\frac{\hbar^2}{2ma^2}=E_n+\frac{\hbar^2}{2ma^2},\quad n=0,1,\ldots. \tag{3.10}$$

Thus here the Bohr–Sommerfeld quantization is exact,[2] despite the presence of the extra term $\hbar^2/2ma^2$ which follows from our particular choice of zero in the energy scale [see (3.3)].

After these elementary considerations, let us have a closer look at the functional analysis of our problem, following mostly Refs. 4 and 21. We shall denote by $\mathcal{H}$ the state space of the infinite well, that is, the closure of the linear span of the orthonormal set $\{|n\rangle, n\in\mathbb{N}\}$. In the x-representation, of course, $\mathcal{H}=L^2([0,\pi a],dx)$. We also denote by $AC(0,\pi a)$ the set of absolutely continuous functions on $[0,\pi a]$ whose derivatives belong to $L^2([0,\pi a],dx)$ and by $AC^2(0,\pi a)$ the set of functions in $L^2([0,\pi a],dx)$ whose weak derivatives are in $AC(0,\pi a)$ [we recall that, roughly speaking, a function is absolutely continuous iff it is the indefinite (Lebesgue) integral of an integrable function].

We begin with the Hamiltonian (3.3). More precisely, we define the infinite well Hamiltonian as the unbounded operator $H\equiv H_w$ in $L^2([0,\pi a],dx)$, acting as (3.3), on the dense domain

$$\mathcal{D}(H_w)=\{\psi\in AC^2(0,\pi a)\,|\,\psi(0)=\psi(\pi a)=0\}. \tag{3.11}$$

On this domain, H_w is self-adjoint, with purely discrete, nondegenerate spectrum $\{E_n=\hbar\omega e_n, n=0,1,...\}$, and the corresponding eigenfunctions $\{\psi_n, n=0,1,...\}$ form an orthonormal basis. Furthermore, the resolvent

$$R_w(-\hbar\omega)\equiv(H_w+\hbar\omega)^{-1}=\frac{1}{\hbar\omega}\sum_{n=0}^{\infty}\frac{1}{(n+1)^2}|n\rangle\langle n|$$

is a trace-class operator, with trace norm and Hilbert–Schmidt norm, respectively:

$$\|R_w(-\hbar\omega)\|_1=\frac{1}{\hbar\omega}\sum_{n=0}^{\infty}\frac{1}{(n+1)^2}=\frac{\pi^2}{6}\frac{1}{\hbar\omega},$$

$$\|R_w(-\hbar\omega)\|_2=\frac{1}{\hbar\omega}\left[\sum_{n=0}^{\infty}\frac{1}{(n+1)^4}\right]^{1/2}=\frac{\pi^2}{\sqrt{90}}\frac{1}{\hbar\omega}.$$

At this stage, it is instructive to compare the Hamiltonian of the infinite well with that of a free particle constrained on a circle of radius $a/2$. Here also, the Hilbert space is $L^2([0,\pi a],dx)$. The Hamiltonian H_c has the same expression as $H_w \equiv H$, but on the domain

$$\mathcal{D}(H_c)=\{\psi\in AC^2(0,\pi a)\,|\,\psi(0)=\psi(\pi a),\psi'(0)=\psi'(\pi a)\}, \tag{3.12}$$

and it is also self-adjoint on its domain. The spectrum is again purely discrete, the eigenvalues coincide with half of those of H_w, namely, $E_{2n-1}=\hbar\omega e_{2n-1}$, $n=1,2,...$, but each of them is doubly degenerate, and there is the additional, simple eigenvalue corresponding to $n=0$, namely, $e_{-1}=-1$. The eigenfunctions are

$$\left\{\sqrt{\frac{2}{\pi a}}\sin 2n\frac{x}{a},n=1,2,...;\sqrt{\frac{2}{\pi a}}\cos 2n\frac{x}{a},n=0,1,2,...\right\}, \tag{3.13}$$

and they constitute another orthonormal basis of $L^2([0,\pi a],dx)$. Thus, there exists a unitary correspondence between the two bases (3.6) and (3.13). However, the explicit form of this map rests on the full Hilbert space structure and not only on simple trigonometric identities (see also later in this work).

This is another instance of the well-known fact that the physics is determined by the boundary conditions, not only by the differential expression of the operator.

Now we turn to the canonical position and momentum operators. The position operator is $Q=x$, acting on $L^2([0,\pi a],dx)$. It is bounded and self-adjoint. As for the momentum, the natural choice is the operator $P_0=-id/dx$, acting on the dense domain

$$\mathcal{D}(P_0)=\{\psi\in AC(0,\pi a)\,|\,\psi(0)=\psi(\pi a)=0\}. \tag{3.14}$$

This operator is closed and symmetric, but *not* self-adjoint. Since its defect indices are (1,1), P_0 has self-adjoint extensions, in fact an infinite number of them, indexed by the points of a unit circle, namely $P_\alpha=-i\hbar d/dx$, acting on the dense domain

$$\mathcal{D}(P_\alpha)=\{\psi\in AC(0,\pi a)\,|\,\psi(\pi a)=\alpha\psi(0),\ \ |\alpha|=1\}. \tag{3.15}$$

For simplicity, we choose $\alpha=1$, that is, periodic boundary conditions. Any other choice $P_\alpha,\alpha\neq 1$, is physically acceptable, and yields similar results.

The operator $P\equiv P_1$ is a valid candidate for the momentum observable. Its spectrum is purely discrete and nondegenerate, $\sigma(P)=\{2n\hbar/a,n=0,\pm 1,\pm 2,...\}$, with corresponding eigenfunctions $\chi_n(x)=1/\sqrt{\pi a}\exp(i2nx/a)$. The trouble is that none of these belongs to the domain of the Hamiltonian H_w! And indeed, one has

$$\frac{P^2}{2m}\neq H_w+\frac{\hbar^2}{2ma^2}, \tag{3.16}$$

since

$$\mathcal{D}(P^2)=\{\psi\in AC^2(0,\pi a)\,|\,\psi(0)=\psi(\pi a),\psi'(0)=\psi'(\pi a)\},$$

so that, up to the constant $\hbar^2/2ma^2$, $P^2/2m$ coincides with the Hamiltonian H_c of a particle on a circle, not H_w!

To conclude, we evaluate the canonical commutation relations (CCRs), which take the standard form

$$[Q,P]=i\hbar I, \tag{3.17}$$

on the domain $\mathcal{D}(QP)\cap\mathcal{D}(PQ)=\mathcal{D}(P_0)$, as given in (3.14). Correspondingly, we obtain the uncertainty relations in the eigenstates ψ_n of the Hamiltonian H_w [compare with the classical case, (2.8) and (2.9)]:

$$\begin{aligned}\langle Q\rangle_n&=\frac{\pi a}{2},\\ \langle Q^2\rangle_n&=a^2\left(\frac{\pi^2}{3}-\frac{1}{2(n+1)^2}\right),\\ \langle P\rangle_n&=0,\\ \langle P^2\rangle_n&=\frac{1}{a^2}\hbar^2(n+1)^2,\end{aligned}\tag{3.18}$$

where $\langle\cdot\rangle_n\equiv\langle\psi_n|\cdot|\psi_n\rangle$. Note that, in the last relation, $\psi_n\in\mathcal{D}(P)$, but $\psi_n\notin\mathcal{D}(P^2)$, so that we really mean $\langle P^2\rangle_n\equiv\|P\psi_n\|^2$. Also, according to Ref. 3, the relation $\langle P\rangle_n=0$ expresses the fact that the current associated to the particle vanishes identically.

Taking all these relations together, we obtain the uncertainties

$$\langle\Delta Q\rangle_n^2=\langle Q^2\rangle_n-\langle Q\rangle_n^2=a^2\left(\frac{\pi^2}{12}-\frac{1}{2(n+1)^2}\right)\geqslant a^2\left(\frac{\pi^2}{12}-\frac{1}{2}\right),$$

$$\langle\Delta P\rangle_n^2=\langle P^2\rangle_n-\langle P\rangle_n^2=\frac{1}{a^2}\hbar^2(n+1)^2\geqslant\frac{\hbar^2}{a^2},$$

and the uncertainty relations

$$\langle\Delta Q\rangle_n\langle\Delta P\rangle_n=\hbar\left(\frac{(n+1)^2\pi^2}{12}-\frac{1}{2}\right)^{1/2}\geqslant\hbar\left(\frac{\pi^2}{12}-\frac{1}{2}\right)^{1/2}\simeq 0.57\hbar>\frac{1}{2}\hbar,\tag{3.19}$$

as expected for a quantum state which is *not* of minimal uncertainty. We will make similar considerations in Sec. IX for the case of coherent states.

However, although the CCRs (3.17) look perfectly normal, they still lead to inconsistencies, because of the unbounded character of the operators. The problem arises, for instance, when one tries to prove the absence of condensation in a one-dimensional interacting Bose gas,[22] by first putting the system in a finite box of length Λ with periodic boundary conditions, and then taking the thermodynamic limit $\Lambda\to\infty$. The key ingredient is the Bogoliubov inequality, namely

$$\tfrac{1}{2}\beta\langle AA^*+A^*A\rangle_\beta\langle[[C,H],C^*]\rangle_\beta\geqslant|\langle[C,A]\rangle_\beta|^2,\tag{3.20}$$

where H is the Hamiltonian, and $\langle X\rangle_\beta=\mathrm{Tr}(e^{-\beta H}X)/\mathrm{Tr}(e^{-\beta H})$ denotes the thermal average of the observable X with respect to the temperature $T=(k\beta)^{-1}$ and the Hamiltonian H. In the relation (3.20), A and C are observables of the system which are to be chosen in a convenient way for a specific application. The inequality (3.20) is perfectly valid for bounded operators, but some care must be exercised with domains in the case of unbounded ones, lest absurdities follow!

In the present case, there are two possibilities. The first one[22] consists in keeping the CCR (3.17), introducing a generalized notion of state as a quadratic form and generalizing the Bogoliubov inequality (3.20) in a corresponding way. This indeed allows one to prove the absence of condensation in the Bose gas for a reasonable class of interactions, including of course a gas of free particles.

An alternative[23] consists in keeping (3.20) unchanged, but generalizing the usual algebraic formalism to the quasi-*algebra generated by the operators Q, P. By this we mean the following. Define the dense domain

$$\mathcal{D}=\{\psi\in C^{\infty}(0.\pi a)\,|\,\psi^{(k)}(0)=\psi^{(k)}(\pi a),k=0,1,\ldots\}. \tag{3.21}$$

Then it is easy to see that

$$\mathcal{D}=\bigcap_{k=0}^{\infty}\mathcal{D}(P^k),$$

and this gives to $\mathcal{D}$ a natural structure of Fréchet space. From this one gets a rigged Hilbert space

$$\mathcal{D}\subset L^2([0,\pi a],dx)\subset\mathcal{D}',$$

where $\mathcal{D}'$ denotes the strong dual of $\mathcal{D}$. Define $\mathfrak{A}=\mathcal{L}(\mathcal{D},\mathcal{D}')$ as the space of all continuous linear maps from $\mathcal{D}$ into $\mathcal{D}'$. This space then carries a natural structure of quasi-*algebra in the sense of Ref. 24. Roughly speaking, this means that $\mathfrak{A}$ obeys the usual rules of algebra, except that the product AB of two elements of $\mathfrak{A}$ is well defined iff one of them leaves the domain $\mathcal{D}$ invariant. But then the canonical commutator $[Q,P]$, when viewed as an element of $\mathfrak{A}$, becomes

$$[Q,P]=i\hbar(I-\pi a\,\hat{\delta}(x)), \tag{3.22}$$

where $\hat{\delta}(x)$ denotes the multiplication operator $\mathcal{D}\ni\varphi\mapsto\delta(x)\varphi\in\mathcal{D}'$, an element of $\mathfrak{A}$. Then, with the modified CCR (3.22), the usual Bogoliubov inequality (3.20) holds on $\mathfrak{A}$ and the standard argument for proving the absence of condensation applies. The same reasoning can be made with any other momentum observable P_α $\alpha\neq 1$, only the r.h.s. of (3.22) becomes slightly more complicated.[23]

This somewhat long digression should convince the reader that the infinite well problem is really singular, and therefore formal considerations, in particular with respect to boundary conditions, may be misleading (see, for instance, Ref. 25 or 26)!

In the light of the preceding results, the time evolution (3.4) is trivial. On one hand, we can expand $\Psi(x,0)\equiv\psi(x)$ in terms of the basis of eigenvectors ψ_n given in (3.6):

$$\Psi(x,0)=\sum_{n=0}^{\infty}c_n\psi_n(x),$$

and thus

$$\Psi(x,t)=\sum_{n=0}^{\infty}c_n e^{-iHt/\hbar}\psi_n(x)=\sum_{n=0}^{\infty}c_n e^{-iE_nt/\hbar}\psi_n(x)=\sum_{n=0}^{\infty}c_n\psi_n(x,t).$$

Alternatively, one may obtain the same result[27] with help of the propagator (Green function) $G(x-x_0,t)$:

$$\Psi(x,t)=\int_0^{\pi a}G(x-x_0,t)\Psi(x_0,0)dx_0. \tag{3.23}$$

Since the Green function is the solution with initial condition $\delta(x-x_0)$ at $t=0$ [we must take, of course, $x_0\in(0,\pi a)$], we may write

$$
\begin{aligned}
G(x-x_0,t) &= e^{-iHt/\hbar}\delta(x-x_0) \\
&= e^{-iHt/\hbar}\sum_{n=0}^{\infty}\overline{\psi_n(x_0)}\psi_n(x) \\
&= \sum_{n=0}^{\infty}\overline{\psi_n(x_0)}e^{-iE_nt/\hbar}\psi_n(x) \\
&= \sum_{n=0}^{\infty}\overline{\psi_n(x_0)}\psi_n(x,t).
\end{aligned}
$$

Here we have used the relation

$$
\delta(x-x_0)=\sum_{n=0}^{\infty}\overline{\psi_n(x_0)}\psi_n(x) \Leftrightarrow \langle x_0|x\rangle=\sum_{n=0}^{\infty}\langle x_0|n\rangle\langle n|x\rangle,
$$

which expresses the completeness of the basis $\{|n\rangle\}$.

Inserting the value of $G(x-x_0,t)$ into (3.23), we get indeed

$$
\begin{aligned}
\Psi(x,t) &= \int_0^{\pi a}\sum_{n=0}^{\infty}\overline{\psi_n(x_0)}\psi_n(x,t)\Psi(x_0,0)dx_0 \\
&= \sum_{n=0}^{\infty}\psi_n(x,t)\int_0^{\pi a}\overline{\psi_n(x_0)}\Psi(x_0,0)dx_0 \\
&= \sum_{n=0}^{\infty}c_n\psi_n(x,t).
\end{aligned}
$$

Next we turn to the momentum representation. Since the spectrum of the operator P is discrete, the Hilbert space in the momentum representation reduces to the space l^2 of square summable sequences. This is just a reformulation of the theory of Fourier series, as opposed to the Fourier integral that makes the transition between the position and the momentum representation for quantum mechanics on the full line $\mathbb{R}$. This fact has been overlooked, for instance, in Ref. 26 [nothing, of course, forbids one to take the Fourier integral transform of the infinite well wave function $\Psi(x,t)$, but the result is just a mathematically equivalent version of the same object, *not* the momentum representation wave function]. Thus an arbitrary state $\psi\in\mathcal{H}$ is expressed in terms of the eigenstates χ_n of P,

$$
\psi=\sum_{n=-\infty}^{\infty}a_n\chi_n, \quad a_n=\langle\chi_n|\psi\rangle, \quad \text{thus} \quad \hat{\psi}\equiv\{a_n\}\in l^2.
$$

For instance, we obtain for the energy eigenstates

$$
\psi_{2k+1}(x)=-\frac{i}{\sqrt{2}}[\chi_{k+1}(x)-\chi_{-k-1}(x)], \tag{3.24}
$$

$$
\psi_{2k}(x)=-\frac{4}{\pi}\sum_{n=-\infty}^{\infty}\frac{2k+1}{4n^2-(2k+1)^2}\chi_n(x). \tag{3.25}
$$

These relations constitute in fact the unitary correspondence between two different orthonormal bases, as discussed after (3.13), and the map is indeed nontrivial.

A last topic that would deserve to be discussed is the solution of the infinite well problem in the path integral formalism. However, this is treated in full detail in Ref. 28, so we will refrain from reproducing it here.

IV. THE SAME FOR PÖSCHL–TELLER

Pöschl–Teller potentials were originally introduced in a molecular physics context. The energy eigenvalues and corresponding eigenstates are solutions to the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{V_0}{2}\left(\frac{\lambda(\lambda-1)}{\cos^2 x/2a}+\frac{\kappa(\kappa-1)}{\sin^2 x/2a}\right)-\frac{\hbar^2}{8ma^2}(\lambda+\kappa)^2\right]\psi(x)=E\psi(x),\quad 0\leqslant x\leqslant \pi a, \tag{4.1}$$

where we have also shifted the Hamiltonian of the trapped particle of mass m by an amount equal to $-(\hbar^2/8ma^2)(\lambda+\kappa)^2$. Here, too, as for the infinite well, we have the choice of putting the potential equal to infinity outside the interval $[0,\pi a]$, or periodizing the problem, with period $2\pi a$.

Since the potential strength is overdetermined by specifying V_0, λ and κ simultaneously, we can freely put for convenience, as in Refs. 3 and 5,

$$V_0=\frac{\hbar^2}{4ma^2}. \tag{4.2}$$

With this choice, and the boundary conditions (BC) $\psi(0)=\psi(\pi a)=0$, the normalized eigenstates and the corresponding eigenvalues, all of them simple, are given by

$$\Psi_n(x)=[c_n(\kappa,\lambda)]^{-1/2}\left(\cos\frac{x}{2a}\right)^{\lambda}\left(\sin\frac{x}{2a}\right)^{\kappa}{}_2F_1\left(-n,n+\lambda+\kappa;\kappa+\frac{1}{2};\sin^2\frac{x}{2a}\right), \tag{4.3}$$

where $c_n(\kappa,\lambda)$ is a normalization factor that can be given analytically when κ and λ are positive integers, ${}_2F_1$ is a hypergeometric function, and

$$E_n=\frac{\hbar^2}{2ma^2}n(n+\lambda+\kappa)\equiv\hbar\omega e_n,\quad n=0,1,..., \tag{4.4}$$

with

$$\omega=\frac{\hbar}{2ma^2},\quad e_n=n(n+\lambda+\kappa),\quad \lambda,\kappa>1. \tag{4.5}$$

Note that the Bohr–Sommerfeld rule applied to the canonical action (2.25) yields [here we do *not* impose the normalization (4.2)]:

$$a\sqrt{2mE}-a\sqrt{mV_0}[\sqrt{\lambda(\lambda-1)}+\sqrt{\kappa(\kappa-1)}]=\hbar(n+\tfrac{1}{2}),$$

that is,

$$E_n=\frac{\hbar^2}{2ma^2}\left(n+\frac{1}{2}\right)^2+\frac{\hbar}{ma}\sqrt{mV_0}\left(n+\frac{1}{2}\right)[\sqrt{\lambda(\lambda-1)}+\sqrt{\kappa(\kappa-1)}]$$
$$+\frac{V_0}{2}[\sqrt{\lambda(\lambda-1)}+\sqrt{\kappa(\kappa-1)}]^2. \tag{4.6}$$

This formula is interesting on two counts at least.

(a) The first term in (4.6) gives, apart from the term 1/2 in $(n+1/2)$, the exact spectrum of the infinite well. More precisely, these values of the energy may be obtained simply by letting $V_0 \to 0$ in $V(x)$ and keeping in mind that $V=\infty$ outside $[0,\pi a]$.

(b) In the limit $V_0 \to \infty$, the first term in (4.6) can be neglected and one is left, up to a global, V_0 dependent, shift, with the spectrum of a harmonic oscillator with elementary quantum

$$\hbar\omega = \hbar \sqrt{\frac{V_0}{ma^2}} [\sqrt{\lambda(\lambda-1)} + \sqrt{\kappa(\kappa-1)}].$$

Hence, the Pöschl–Teller potential interpolates between the square-well and the harmonic oscillator.

As we did in the case of the infinite well, let us examine now the functional-analytic properties of the Pöschl–Teller Hamiltonian. The Schrödinger equation (4.1) is an eigenvalue equation for an ordinary differential Sturm–Liouville operator, which is singular at both ends of the interval $[0,\pi a]$ (see, for instance, Ref. 29). The situation now depends on the values of λ and κ, as follows from the thorough analysis of Gesztesy *et al.*[30] In particular, there exist critical values λ, $\kappa = \frac{3}{2}$, although one would naively expect the value 1 to play that role.

Let $\dot{T}$ be the minimal differential operator, that is, the operator defined by the differential expression (4.1) on the space $C_0^\infty(0,\pi a)$ of C^∞ functions with (compact) support strictly contained in the open interval $(0,\pi a)$. Then, we have the following.

- If λ, $\kappa \geqslant \frac{3}{2}$, the operator $\dot{T}$ is in the limit point case at both ends $x=0$, πa, thus it is essentially self-adjoint and its closure H_{PT} automatically satisfies Dirichlet BCs at $x=0$ and $x=\pi a$, i.e., $\psi(0)=\psi(\pi a)=0$.
- If $\lambda \geqslant \frac{3}{2} > \kappa$, the operator $\dot{T}$ is in the limit point case at $x=\pi a$, but in the limit circle case at $x=0$; hence the defect indices of its closure are (1,1) and we need a BC at $x=0$ for defining a self-adjoint extension; quite naturally, we choose the Dirichlet BC, the one at $x=\pi a$ being automatic.
- If $\kappa \geqslant \frac{3}{2} > \lambda$, the operator $\dot{T}$ is in the limit point case at $x=0$, but in the limit circle case at $x=\pi a$; again we impose a Dirichlet BC at $x=\pi a$, the one at $x=0$ being automatic.
- If $\frac{1}{2} < \lambda$, $\kappa < \frac{3}{2}$, the operator $\dot{T}$ is in the limit circle case at both ends $x=0$, πa, the defect indices are (2,2), and we have to impose two BCs, again chosen as Dirichlet. Notice that the Dirichlet BC may be written as $\psi(0)=\psi(\pi a)=0$ in the first, regular, case, but it takes a more complicated form in the singular cases.[30] Clearly this choice of boundary conditions is dictated by physics, namely, it is the same as for the infinite well. One may also say that the chosen self-adjoint extension of $\dot{T}$ is obtained by analytic extension from large positive values λ, $\kappa \geqslant \frac{3}{2}$, since, in this context, everything depends analytically on λ, κ.

In all four cases, we define the Pöschl–Teller Hamiltonian as the self-adjoint operator H_{PT} in $L^2([0,\pi a],dx)$, acting as the left-hand side of (4.1), on the dense domain

$$\mathcal{D}(H_{\mathrm{PT}}) = \{\psi \in AC^2(0,\pi a) \,|\, V_{\mathrm{PT}}\psi \in L^2([0,\pi a],dx) \ \text{ and } \ \psi \text{ satisfies a Dirichlet BC at } x=0,\pi a\}, \tag{4.7}$$

where V_{PT} is the Pöschl–Teller potential. The Pöschl–Teller Hamiltonian has pure point spectrum, without multiplicity, and given by $E_n = (\hbar^2/2ma^2)n(n+\lambda+\kappa) \equiv \hbar\omega e_n$, $n=0,1,...$, as given in (4.4), with corresponding eigenvectors (4.3). Notice that these eigenfunctions belong to the domain $\mathcal{D}(H_{\mathrm{PT}})$, since they satisfy the boundary conditions (by assumption[5]).

Several remarks are in order at this point.

(1) First, the case $\frac{1}{2} < \lambda$, $\kappa < 1$ (the mixed cases have no physical relevance) corresponds to the inverted well, yet the spectrum of H_{PT} remains unchanged, that is, pure point and positive.

Although the potential is now attractive, it is too close to the walls to allow negative energy bound states. This counterintuitive situation follows, of course, from the Dirichlet BC that make the walls impenetrable and thus confine the particle inside of the interval. On the other hand, for λ or $\kappa<\frac{1}{2}$, the problem is of a different nature and the analysis of Ref. 30 does not apply any more (presumably, here one faces again the ''fall towards the center'' phenomenon[2]).

(2) Next, one may choose different BCs for defining a self-adjoint extension of $\dot{T}$. An interesting choice is to take the full periodicity interval $[-\pi a,\pi a]$, that is, $(-\pi a,0)\cup(0,\pi a)$, and to impose to both ψ and ψ' continuity conditions at $x=0$ and periodic BCs at $x=\pm\pi a$. The resulting self-adjoint Hamiltonian $H_{\mathrm{PT}}^{\mathrm{per}}$ also has a pure point spectrum, namely $\{n(n+\lambda+\kappa),(n+1)(n+1-\lambda-\kappa),n=0,1,2,...\}$, with all eigenvalues simple. For $\lambda=\kappa=1$, one indeed recovers the doubly degenerate spectrum of the circle Hamiltonian H_c of Sec. III.

(3) Finally, the real difference with respect to the values of λ, κ comes when one periodizes the Pöschl–Teller Hamiltonian over the whole line, that is, on $\mathbb{R}\backslash\pi a\mathbb{Z}$, with continuity BCs at $x\in\pi a\mathbb{Z}$. Then, if $\lambda\geqslant\frac{3}{2}$ or $\kappa\geqslant\frac{3}{2}$, the periodized Hamiltonian $H_{\mathbb{R}}^{\mathrm{per}}$ is self-adjoint, and has a pure point spectrum, with each eigenvalue of infinite multiplicity. On the contrary, if $\frac{1}{2}<\lambda$, $\kappa\leqslant\frac{3}{2}$, then $H_{\mathbb{R}}^{\mathrm{per}}$ really looks as the Hamiltonian of a 1-D crystal, and, indeed, it has no eigenvalue and its spectrum has a band structure, that is, it is purely continuous with infinitely many gaps.[7,8,30]

Coming back to the interval $[0,\pi a]$, the resolvent of the Pöschl–Teller Hamiltonian H_{PT} reads

$$R_{\mathrm{PT}}\left(-\frac{1}{4}\hbar\omega(\lambda+\kappa)^2\right)\equiv\left(H_{\mathrm{PT}}+\frac{1}{4}\hbar\omega(\lambda+\kappa)^2\right)^{-1}=\frac{1}{\hbar\omega}\sum_{n=0}^{\infty}\frac{1}{\left[n+\frac{1}{2}(\lambda+\kappa)\right]^2}|n,\lambda,\kappa\rangle\langle n,\lambda,\kappa|,$$

where $|n,\lambda,\kappa\rangle$ denotes the eigenfunction Ψ_n of (4.3). As before, it is a trace-class operator, with trace norm:

$$\left\|R_{\mathrm{PT}}\left(-\frac{1}{4}\hbar\omega(\lambda+\kappa)^2\right)\right\|_1=\frac{1}{\hbar\omega}\sum_{n=0}^{\infty}\frac{1}{\left[n+\frac{1}{2}(\lambda+\kappa)\right]^2}.$$

Note that the Hilbert space and the momentum observable P remain the same as in the case of the infinite well. Thus, the previous discussion remains valid and the same difficulties are present. For instance, as for (3.16), $P^2/2m$ does *not* coincide with the first term of H_{PT}. Also one can calculate, at least in principle, the analogs of (3.24) and (3.25), which are simply the Fourier series expansion of the Pöschl–Teller energy eigenstates Ψ_n.

V. THE LIMITS

In this section, we shall investigate various limiting cases. Let us begin with the infinite square-well. Since the natural dimensionless variable is $y=x/a$, we may rewrite the Hamiltonian (3.3) in terms of y, and we get the scaling equation

$$H_{\mathrm{W}}\equiv H_{\mathrm{W}}[a]=\frac{1}{a^2}H_{\mathrm{W}}[1]. \tag{5.1}$$

The operator $H_{\mathrm{W}}[1]$ is self-adjoint in $L^2([0,\pi],dy)$, its eigenvalues are $E_n[1]=(\hbar^2/2m)n(n+2)$, and one has the scaling law $E_n[a]=(1/a^2)E_n[1]$. From these relations, the two limits $a\to0$ (infinitely narrow well) and $a\to\infty$ (infinitely large well) are trivial. The spectrum keeps the same shape, only the eigenvalues scale as $1/a^2$.

The same considerations apply to the Pöschl–Teller Schrödinger equation (4.1). If we do not impose the normalization relation (4.2), we get the scaling relation

$$H_{\mathrm{PT}} \equiv H_{\mathrm{PT}}[a, V_0] = \frac{1}{a^2} H_{\mathrm{PT}}[1, a^2 V_0]. \tag{5.2}$$

With (4.2), this becomes, exactly as for the infinite well,

$$H_{\mathrm{PT}}[a] = \frac{1}{a^2} H_{\mathrm{PT}}[1], \tag{5.3}$$

and the same for the eigenvalues. Thus, when the well gets narrower as $a \to 0$, the eigenvalues increase as $1/a^2$, but the spectrum keeps the same shape. Similarly, $a \to \infty$ implies $V_0 \to 0$, and the spacing between successive eigenvalues goes to zero: in the limit, we recover a free particle, with continuous energy spectrum $[0, \infty)$.

Next we analyze the limit $\lambda, \kappa \to 1$, that is, the limit Pöschl–Teller→infinite square-well. For simplicity, we take the symmetric case $\lambda = \kappa$, with Pöschl–Teller potential (1.2). As in the case of the infinite square-well, the symmetric Pöschl–Teller Hamiltonian is self-adjoint and its resolvent

$$R_{\mathrm{PT}}(-\hbar\omega\lambda^2) \equiv (H_{\mathrm{PT}} + \hbar\omega\lambda^2)^{-1} = \frac{1}{\hbar\omega} \sum_{n=0}^{\infty} \frac{1}{(n+\lambda)^2} |n,\lambda\rangle\langle n,\lambda|$$

is a trace-class operator, with trace norm:

$$\| R_{\mathrm{PT}}(-\hbar\omega\lambda^2) \|_1 = \frac{1}{\hbar\omega} \sum_{n=0}^{\infty} \frac{1}{(n+\lambda)^2}.$$

As for the limit Pöschl–Teller→infinite square-well, the exact statement is that $H_{\mathrm{PT}} \to H_{\mathrm{W}}$ in strong resolvent sense as $\lambda \to 1$, that is, $R_{\mathrm{PT}}(z) \to R_{\mathrm{W}}(z)$ strongly, for all nonreal z. This follows from Ref. 4, Theorem VIII.25 (a), as we now prove. The domain $C_0^\infty(0, \pi a)$ is dense in $L^2([0, \pi a], dx)$ and it is a core both for H_{W} and for $H_{\mathrm{PT}}[\lambda]$, for any $\lambda \geqslant \frac{3}{2}$.[21] Then, we obtain a core for $H_{\mathrm{PT}}[\lambda]$, $1 < \lambda < \frac{3}{2}$, by taking the set $\mathcal{D}_{\mathrm{PT}} = \{\psi = \phi + c_1\psi_1 + c_2\psi_2, \phi \in C_0^\infty(0, \pi a)\}$, where ψ_1 and ψ_2 are two solutions of $H_{\mathrm{PT}}\chi = k^2\chi$, $\mathrm{Im}\, k \geqslant 0$, chosen in such a way that ψ obeys the boundary conditions that define H_{PT}. In our case of Dirichlet BC, this implies[30] that $c_1 = 0$ and $\psi_2 = \Psi_n$, the eigenfunction (4.3), taken for $\lambda = \kappa$.

Choose any decreasing sequence $\{\lambda_j, j = 1,2,...; \lambda_j > 1, \lambda_j \to 1 \text{ as } j \to \infty\}$. Then, $H_{\mathrm{PT}}[\lambda_j]\psi \to H_{\mathrm{W}}\psi$, for each $\psi = \phi + c\psi_2 \in \mathcal{D}_{\mathrm{PT}}$. Indeed,

$$\begin{aligned} \| H_{\mathrm{PT}}[\lambda_j]\psi - H_{\mathrm{W}}\psi \| &= \left\| V_{\lambda_j}(x)\psi - \frac{\hbar^2}{2ma^2}(\lambda_j^2 - 1)\psi \right\| \\ &= \frac{\hbar^2}{ma^2} \left\| \lambda_j(\lambda_j - 1) \left[\sin\frac{x}{a} \right]^{-2} \psi - \frac{1}{2}(\lambda_j^2 - 1)\psi \right\| \\ &= (\lambda_j - 1)\frac{\hbar^2}{ma^2} \left(\lambda_j \left\| \left[\sin\frac{x}{a} \right]^{-2} \psi \right\| + \frac{1}{2}(\lambda_j + 1)\|\psi\| \right) \to 0 \quad \text{as} \quad j \to \infty, \end{aligned}$$

since both $\phi \in C_0^\infty(0, \pi a)$ and $\psi_2 = \Psi_n$ belong to the domain of $[\sin x/a]^{-2}$. By the theorem quoted, this implies that $H_{\mathrm{PT}} \to H_{\mathrm{W}}$ in a strong resolvent sense. As a consequence, by Ref. 4, Theorem VIII.24, for each eigenvalue $E_n = \hbar\omega n(n+2)$ of the limiting operator H_{W}, there is, for each j, an eigenvalue $E_n[\lambda_j] = \hbar\omega n(n + 2\lambda_j)$ of $H_{\mathrm{PT}}[\lambda_j]$ such that $E_n[\lambda_j] \to E_n$ as $j \to \infty$. Put in a simpler way, the eigenvalues $E_n[\lambda]$ are continuous in λ and $E_n[\lambda] \to E_n$ as $\lambda \to 1$, for each $n = 0,1,2,....$

Finally, there is the semiclassical limit $\hbar \to 0$, $n\hbar = \text{const}$, but this problem is fully treated in the literature, for instance, in Ref. 2, so we omit it.

VI. THE DYNAMICAL ALGEBRA $\mathfrak{su}(1,1)$

Behind the spectral structure of the infinite well or Pöschl–Teller Hamiltonians, there exists a dynamical algebra generated by lowering and raising operators.[17,31] The latter are defined by

$$a|n\rangle = \sqrt{e_n}|n-1\rangle, \tag{6.1}$$

$$a^\dagger|n\rangle = \sqrt{e_{n+1}}|n+1\rangle, \tag{6.2}$$

with

$$e_n = n(n+2), \text{ for the infinite well,}$$

$$e_n = n(n+\lambda+\kappa), \text{ for the Pöschl-Teller potential, } n = 0,1,2,\ldots.$$

Then we note that the operator

$$X_N = a^\dagger a \tag{6.3}$$

is diagonal with eigenvalues e_n:

$$X_N|n\rangle = e_n|n\rangle. \tag{6.4}$$

Note that the number operator N,

$$N|n\rangle = n|n\rangle, \tag{6.5}$$

is given in terms of X_N by

$$N = -\tfrac{1}{2}(\lambda+\kappa) + (X_N + \tfrac{1}{4}(\lambda+\kappa)^2)^{1/2}. \tag{6.6}$$

For any diagonal operator Δ with eigenvalues δ_n,

$$\Delta|n\rangle = \delta_n|n\rangle, \tag{6.7}$$

we denote its finite difference by Δ'. The latter is defined as the diagonal operator with eigenvalues $\delta'_n \equiv \delta_{n+1} - \delta_n$,

$$\Delta'|n\rangle = \delta'_n|n\rangle. \tag{6.8}$$

More generally, the mth finite difference $\Delta^{(m)}$ will be recursively defined by

$$\Delta^{(m)} = (\Delta^{(m-1)})'. \tag{6.9}$$

Now, from the infinite matrix representation (in the basis $|n\rangle$) of the operators a and $a^\dagger$,

$$a = \begin{pmatrix} 0 & \sqrt{e_1} & 0 & 0 & \ldots \\ 0 & 0 & \sqrt{e_2} & 0 & \ldots \\ 0 & 0 & 0 & \sqrt{e_3} & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix}, \tag{6.10}$$

$$a^{\dagger}=\begin{pmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{e_1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{e_2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{e_3} & 0 & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}, \tag{6.11}$$

it is easy to check that

$$[a,a^{\dagger}]=\begin{pmatrix} e_1-e_0 & 0 & 0 & \cdots \\ 0 & e_2-e_1 & 0 & \cdots \\ 0 & 0 & e_3-e_2 & 0 \\ \cdots & \cdots & \cdots & \cdots \end{pmatrix}=X_N', \tag{6.12}$$

$$X_N'|n\rangle=e_n'|n\rangle,\ \ e_n'=e_{n+1}-e_n=2n+3,\ \text{resp. } 2n+1+\lambda+\kappa. \tag{6.13}$$

We also check that, for any diagonal operator Δ, we have

$$\begin{aligned} [a,\Delta]&=\Delta' a, \\ [a^{\dagger},\Delta]&=-a^{\dagger}\Delta'. \end{aligned} \tag{6.14}$$

Therefore,

$$[a,X_N']=X_N''a,$$

with

$$X_N''|n\rangle=e_n''|n\rangle=(e_{n+1}'-e_n')|n\rangle=2|n\rangle. \tag{6.15}$$

So

$$X_N''=2I,\ \ X_N'''=0, \tag{6.16}$$

and

$$[a,X_N']=2a. \tag{6.17}$$

Similarly,

$$[a^{\dagger},X_N']=-2a^{\dagger}. \tag{6.18}$$

In summary, there exists a ''dynamical'' Lie algebra, which is generated by $\{a,a^{\dagger},X_N'\}$. Then the commutation rules

$$[a,a^{\dagger}]=X_N',\ \ [a,X_N']=2a,\ \ [a^{\dagger},X_N']=-2a^{\dagger} \tag{6.19}$$

clearly indicate that it is isomorphic to

$$\mathfrak{su}(1,1)\sim\mathfrak{sl}(2,\mathbb{R})\sim\mathfrak{so}(2,1). \tag{6.20}$$

A more familiar basis for (6.20) is given [in $\mathfrak{so}(2,1)$ notation] by

$$L^{-}=\frac{1}{\sqrt{2}}a,\ \ L^{+}=\frac{1}{\sqrt{2}}a^{\dagger},\ \ L_{12}=\frac{1}{2}X_N', \tag{6.21}$$

where L_{12} is the generator of the compact subgroup SO(2), namely,

$$[L^{\pm},L_{12}]=\mp L^{\pm},\ \ [L^{-},L^{+}]=L_{12}. \tag{6.22}$$

Note that if we add the operator X_N (i.e., the Hamiltonian H) to the set $\{a,a^{\dagger},X_N'\}$, we obtain an infinite-dimensional Lie algebra contained in the enveloping algebra. Indeed

$$\begin{gathered}[a,X_N]=X_N'a,\ \ [a^{\dagger},X_N]=-a^{\dagger}X_N',\\ [a,X_N'a]=2a^2,\ \ [a^{\dagger},X_N'a]=-X_N'^2-2X_N,\end{gathered} \tag{6.23}$$

etc. Note also the relation between X_N and X_N':

$$X_N=\tfrac{1}{4}(X_N'^2-2X_N'-3),\ \ \text{resp.}\ \ \tfrac{1}{4}(X_N'^2-2X_N'-(\lambda+\kappa+1)(\lambda+\kappa)). \tag{6.24}$$

In the same vein, we note that the condition $X_N'''=0$ is necessary for obtaining a genuine Lie algebra (instead of a subset of the enveloping algebra). Therefore, $\mathfrak{su}(1,1)$ is the *only* dynamical Lie algebra that can arise in such a problem.

It follows from the considerations above that the space $\mathcal{H}$ of states $|n\rangle$ carries some representation of $\mathfrak{su}(1,1)$. The latter is found by examining the formulas for the $\mathfrak{su}(1,1)$ discrete series representation.[32–34]

Given $\eta=1/2,1,3/2,...$ the discrete series UIR U_η is realized on the Hilbert space $\mathcal{H}_\eta$ with basis $\{|\eta,n\rangle, n\in\mathbb{N}\}$ through the following actions of the Lie algebra elements:

$$L_{12}|\eta,n\rangle=(\eta+n)|\eta,n\rangle, \tag{6.25}$$

$$L^{-}|\eta,n\rangle=\frac{1}{\sqrt{2}}\sqrt{(2\eta+n-1)n}\,|\eta,n-1\rangle, \tag{6.26}$$

$$L^{+}|\eta,n\rangle=\frac{1}{\sqrt{2}}\sqrt{(2\eta+n)(n+1)}\,|\eta,n+1\rangle. \tag{6.27}$$

The representation U_η fixes the Casimir operator

$$Q=-L_{12}(L_{12}-1)+2L^{+}L^{-} \tag{6.28}$$

to the following value:

$$Q\mathcal{H}_\eta=\eta(\eta-1)\mathcal{H}_\eta. \tag{6.29}$$

Using (6.21) and (6.26), and comparing with (6.1), (6.2), and (6.13), we obtain the specific value of η for the infinite well problem, namely, $\eta=3/2$, so that we can make the identifications $\mathcal{H}_{3/2}\equiv\mathcal{H}$,$|3/2,n\rangle\equiv|n\rangle$. On the other hand, we obtain a continuous range of values for the Pöschl–Teller potentials:

$$\eta=\frac{\lambda+\kappa+1}{2}>\frac{3}{2}, \tag{6.30}$$

and we shall denote the corresponding Hilbert spaces and states (3.6) by $\mathcal{H}_\eta$ and $|\eta,n\rangle$, respectively. The relation (6.30) simply means that we are here in the presence of the (abusively called) discrete series representations of the universal covering of SU(1, 1), except for the interval $\eta\in(1/2,3/2)$.

VII. COHERENT STATES FOR THE INFINITE WELL

In a general setting, consider a strictly increasing sequence of positive numbers

$$0=e_0<e_1<e_2\ldots<e_n<\ldots, \tag{7.1}$$

which are eigenvalues of a self-adjoint positive operator X_N in some Hilbert space $\mathcal{H}$,

$$X_N|n\rangle=e_n|n\rangle, \tag{7.2}$$

where the set $\{|n\rangle, n\in\mathbb{N}\}$ is an orthonormal basis of $\mathcal{H}$.[16,31]

There corresponds to (7.1) a (generically infinite) dynamical Lie algebra with basis $\{a,a^\dagger,X'_N,\ldots\}$, with the notation of the previous section. There also corresponds a continuous family $\{|z\rangle, z\in C(0,R)\subset\mathbb{C}\}$ [$C(0,R)$ is the open disk of center 0 and radius R] of normalized coherent states, eigenvectors of the operator a:

$$a|z\rangle=z|z\rangle. \tag{7.3}$$

The explicit form of those coherent states is

$$|z\rangle=\frac{1}{N(|z|^2)}\sum_{n\geqslant 0}\frac{z^n}{\sqrt{\rho_n}}|n\rangle, \tag{7.4}$$

where

$$\rho_0=1,\ \ \rho_n=e_1e_2\cdots e_n,\ \ n>0. \tag{7.5}$$

$N(|z|^2)$ is a normalization factor:

$$\langle z|z\rangle=1\Leftrightarrow(N(|z|^2))^2=\sum_{n=0}^{+\infty}\frac{|z|^{2n}}{\rho_n}. \tag{7.6}$$

Of course, these coherent states exist only if the radius of convergence

$$R=\limsup_{n\to+\infty}\sqrt[n]{\rho_n} \tag{7.7}$$

is nonzero. In fact, different specific choices of ρ_n give rise to many different families of coherent states, as illustrated in a series of recent works.[35–38]

Now suppose that X_N is (up to a factor) the Hamiltonian for a quantum system,

$$H=\hbar\omega X_N. \tag{7.8}$$

Then the coherent states (7.4) evolve in time as

$$e^{-iHt/\hbar}|z\rangle=\frac{1}{N(|z|^2)}\sum_{n\geqslant 0}\frac{z^n}{\sqrt{\rho_n}}e^{-i\omega e_n t}|n\rangle. \tag{7.9}$$

If $e_n\propto n$, i.e., in the case of the harmonic oscillator, the temporal evolution of the coherent state $|z\rangle$ reduces to a rotation in the complex plane, namely, $e^{-iHt/\hbar}|z\rangle=|ze^{-i\omega t}\rangle$. In general, however, we will lose the temporal stability of our family of coherent states (7.4). Hence, in order to restore it, we must extend our original definitions to the entire orbits

$$\{e^{-iHt/\hbar}|z\rangle,\ \ z\in C(0,R),\ \ t\in I\}. \tag{7.10}$$

The interval I is the whole real line when e_n is generic, whereas it can be restricted to a period, that is, a finite interval $[a, b]$,

$$b-a=\frac{2\pi}{\omega\alpha} \tag{7.11}$$

if $e_n \in \alpha\mathbb{N}$. A straightforward calculation now shows that

$$\langle z|H|z\rangle=\langle z|\hbar\omega X_N|z\rangle=\hbar\omega|z|^2. \tag{7.12}$$

Therefore the quantity $|z|^2$ is the average energy evaluated in the elementary quantum unit $\hbar\omega$. Note that

$$\hbar|z|^2\equiv J \tag{7.13}$$

is simply the action variable in the case where H is the Hamiltonian of the harmonic oscillator and the variable z is given the meaning of a classical state in the phase space $\mathbb{C}$. Indeed, the given choice of ρ_n in (7.5) ensures that $\langle z|H|z\rangle=\omega J$ for a general Hamiltonian.

On the other hand, introducing the dimensionless number

$$\gamma=\omega t, \quad \gamma\in\omega I, \tag{7.14}$$

we are naturally led to study the continuous family of states

$$|z,\gamma\rangle=\frac{1}{N(J)}\sum_{n\geqslant 0}\frac{z^n e^{-i\gamma e_n}}{\sqrt{\rho_n}}|n\rangle. \tag{7.15}$$

These states, parametrized by $(z,\gamma)\in C(0,R)\times I$, may be called ''coherent'' for several reasons. First they are, by construction, eigenvectors of the operator

$$a(\gamma)\equiv e^{-i\gamma H/\hbar\omega}a e^{i\gamma H/\hbar\omega}, \tag{7.16}$$

namely,

$$a(\gamma)|z,\gamma\rangle=z|z,\gamma\rangle. \tag{7.17}$$

They obey the temporal stability condition

$$e^{-iHt/\hbar}|z,\gamma\rangle=|z,\gamma+\omega t\rangle. \tag{7.18}$$

Again, if we consider the harmonic oscillator case, we do not make any distinction between the argument of the complex parameter z and the angle variable γ, since then $e_n=n$ and $z^n e^{-i\gamma n}=(ze^{-i\gamma})^n$, so that the only parameters we need are $J=|z|^{1/2}$ and γ. The latter are easily identified with the classical action-angle variables. We shall stick to the minimal parametrization set in the present generalization and shall denote from now on our coherent states by

$$|J,\gamma\rangle=\frac{1}{N(J)}\sum_{n\geqslant 0}\frac{J^{n/2}e^{-i\gamma e_n}}{\sqrt{\rho_n}}|n\rangle. \tag{7.19}$$

In a suitable way[16] (see also the discussion in Sec. X), it is also acceptable to regard the parametrization (J, γ) as ''action-angle'' variables, and it is convenient to refer to them as such, even when keeping in mind the possibility of extending $\sqrt{J}$ to the complex plane, i.e., replacing $\sqrt{J}$ by z.

Let us now make those things explicit in our problem of the infinite well. In that case,

$$\rho_n = e_1 e_2 \ldots e_n = \frac{n!(n+2)!}{2}, \tag{7.20}$$

$$|J,\gamma\rangle = \frac{1}{N(J)} \sum_{n\geqslant 0} \frac{J^{n/2} e^{-i\gamma n(n+2)}}{\sqrt{n!(n+2)!/2}} |n\rangle. \tag{7.21}$$

The normalization factor is easily calculated in terms of the modified Bessel function I_ν:[39]

$$(N(J))^2 = 2\sum_{n=0}^{+\infty} \frac{J^n}{n!(n+2)!} \tag{7.22}$$

$$= \frac{2}{J} I_2(2\sqrt{J}). \tag{7.23}$$

The radius of convergence $R = \limsup_{n\to+\infty} \sqrt[n]{n!(n+2)!/2}$ is of course infinite. Moreover, since the e_n's here are natural numbers, the interval of variation of the evolution parameter γ can be chosen as $I=[0,2\pi]$.

The positive constants ρ_n arise as moments of a probability distribution $\rho(u)$,

$$\rho_n = \int_0^\infty u^n \rho(u) du. \tag{7.24}$$

Also, $\rho(u)$ is explicitly given in terms of the other modified Bessel function K_ν,[39]

$$\rho(u) = u K_2(2\sqrt{u}). \tag{7.25}$$

It is then immediate to check that the family $\{|J,\gamma\rangle, J\in\mathbb{R}^+, \gamma\in[0,2\pi]\}$ resolves the unit operator, i.e.,

$$I = \int |J,\gamma\rangle\langle J,\gamma| d\mu(J,\gamma), \tag{7.26}$$

with

$$\int (\cdot) d\mu(J,\gamma) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\gamma \int_0^{+\infty} k(J)(\cdot) dJ, \tag{7.27}$$

where

$$k(J) = N(J)^2 \rho(J) = 2 I_2(2\sqrt{J}) K_2(2\sqrt{J}). \tag{7.28}$$

As it is well known, the overlap of two coherent states does not vanish in general. Explicitly, we have

$$\langle J',\gamma'|J,\gamma\rangle = \frac{2}{N(J)N(J')} \sum_{n\geqslant 0} \frac{(JJ')^{n/2}}{n!(n+2)!} e^{-in(n+2)(\gamma-\gamma')}. \tag{7.29}$$

If $\gamma=\gamma'$, we obtain a Bessel function

$$\langle J',\gamma|J,\gamma\rangle = \frac{2}{(JJ')^{1/2} N(J)N(J')} I_2(2(JJ')^{1/4}). \tag{7.30}$$

If $\gamma\neq\gamma'$, we can give an integral representation of (7.29) in terms of a theta function and Bessel functions:[39]

$$\langle J',\gamma'|J,\gamma\rangle=\frac{e^{i(\gamma-\gamma')/4}}{i\pi N(J)N(J')}\int_0^\pi d\varphi\,\theta_1\left(\frac{\varphi}{\pi},-\frac{\gamma-\gamma'}{\pi}\right)$$
$$\times\left[\frac{-e^{-i(\varphi-\gamma+\gamma')}}{(JJ')^{1/2}}I_2(2(JJ')^{1/4}e^{i(\varphi-(\gamma-\gamma')/2+\pi/2)})\right.$$
$$\left.+\frac{e^{i(\varphi+\gamma-\gamma')}}{(JJ')^{1/2}}I_2(2(JJ')^{1/4}e^{-i(\varphi+(\gamma-\gamma')/2-\pi/2)})\right]. \tag{7.31}$$

VIII. COHERENT STATES FOR THE PÖSCHL–TELLER POTENTIALS

The relations (7.20) and (7.21) of the previous section are easily generalized to the present case. We shall list them without unnecessary comments.

From the energies $E_n=\hbar\omega e_n$ given by (4.4), we get the moments

$$\rho_n=e_1e_2\ldots e_n=n!\,\frac{\Gamma(n+\nu+1)}{\Gamma(\nu+1)} \tag{8.1}$$

with $\nu=\lambda+\kappa>2$.

Thus, the coherent states read

$$|J,\gamma\rangle=\frac{[\Gamma(\nu+1)]^{1/2}}{N(J)}\sum_{n\geqslant 0}\frac{J^{n/2}e^{-i\gamma n(n+\nu)}}{[n!\Gamma(n+\nu+1)]^{1/2}}|n\rangle. \tag{8.2}$$

The normalization is then given by

$$N(J)^2=\Gamma(\nu+1)\sum_{n\geqslant 0}\frac{J^n}{n!\Gamma(n+\nu+1)}=\frac{\Gamma(\nu+1)}{J^{\nu/2}}I_\nu(2\sqrt{J}). \tag{8.3}$$

The radius of convergence R is infinite. The interval of variation of the evolution parameter γ is generically the whole real line, unless the parameter ν is an integer.

The numbers ρ_n are moments of a probability distribution $\rho(u)$ involving the modified Bessel function K_ν:

$$\rho_n=\int_0^\infty u^n\rho(u)du, \tag{8.4}$$

with [compare with (7.25)]

$$\rho(u)=\frac{2}{\Gamma(\nu+1)}u^{\nu/2}K_\nu(2\sqrt{u}). \tag{8.5}$$

It might be useful to recall here the well-known relation between modified Bessel functions,[39]

$$K_\nu(z)=\frac{\pi}{2\sin\pi\nu}[I_{-\nu}(z)-I_\nu(z)],\quad \nu\notin\mathbb{Z}. \tag{8.6}$$

The resolution of the unity is then explicitly given by

$$I=\int|J,\gamma\rangle\langle J,\gamma|d\mu(J,\gamma), \tag{8.7}$$

with

$$\int (\cdot)d\mu(J,\gamma)=\lim_{\Gamma\to\infty}\frac{1}{2\Gamma}\int_{-\Gamma}^{\Gamma}d\gamma\left[\int_{0}^{+\infty}k(J)(\cdot)dJ\right], \tag{8.8}$$

where

$$k(J)=N(J)^2\rho(J)=2I_\nu(2\sqrt{J})K_\nu(2\sqrt{J}).$$

Finally, the overlap between two coherent states is given by the series

$$\langle J',\gamma'|J,\gamma\rangle=\frac{\Gamma(\nu+1)}{N(J)N(J')}\sum_{n\geqslant 0}\frac{(JJ')^{n/2}}{n!\Gamma(n+\nu+1)}e^{-in(n+\nu)(\gamma-\gamma')}, \tag{8.9}$$

which reduces to a Bessel function for $\gamma=\gamma'$:

$$\langle J',\gamma|J,\gamma\rangle=\frac{\Gamma(\nu+1)}{N(J)N(J')}\frac{I_\nu(2(JJ')^{1/4})}{(JJ')^{\nu/4}}. \tag{8.10}$$

At this point, we should emphasize the fact that, when $\gamma=0$ and J is taken as a complex parameter, our temporally stable families of coherent states (7.21) and (8.2) are nothing else but the temporal evolution orbits of the well-known Barut-Girardello coherent states for SU(1, 1).[40] It seems that this connection between infinite square-well/Pöschl–Teller potentials and the latter CS has not been pointed out so far.

In addition, we should also quote Nieto and Simmons,[41] who have considered the infinite square-well and the Pöschl–Teller potentials as examples of their construction of coherent states. The latter are required to minimize an uncertainty relation or, equivalently, to be eigenvectors of some ''lowering operator'' A^- (*à la* Barut-Girardello[40]). However, those states have a totally different meaning and should be considered only in the semiclassical limit.

IX. PHYSICAL FEATURES OF THE COHERENT STATES

In this section, we shall study the spatial and temporal features of the coherent states, treating together the infinite well CS (7.19) and the Pöschl–Teller CS (8.2), the former being obtained from the latter simply by putting $\nu=\lambda+\kappa=2$. As (infinite) superposition of stationary states which are spatially and temporally periodic for integer values of ν, they should display nonambiguous revivals and fractional revivals. Quantum revivals have recently attracted the interest of many authors and some of them have considered the infinite square-well as a toy-model for preparing more realistic studies. But let us first recall the main definitions concerning the notion of revival, as given in Ref. 42. For other related works, see Refs. 43–48; for updated references, see also Ref. 26.

A *revival* of a wave function occurs when a wave function evolves in time to a state closely reproducing its initial form. A *fractional revival* occurs when the wave function evolves in time to a state that can be described as a collection of spatially distributed subwave functions, each of which closely reproduces the shape of the initial wave function. If a revival corresponds to phase alignments of nearest-neighbor energy eigenstates that constitute the wave function, it can be asserted that a fractional revival corresponds to phase alignments of nonadjacent energy eigenstates that constitute this wave function.

For a general wave packet of the form

$$|\psi(t)\rangle=\sum_{n\geqslant 0}c_n e^{-iE_n t/\hbar}|n\rangle, \tag{9.1}$$

with $\Sigma_{n\geqslant 0}|c_n|^2=1$, the concept of revival arises from the weighting probabilities $|c_n|^2$. Suppose that the expansion (9.1) is strongly weighted around a mean value $\langle n\rangle$ for the number operator N, $N|n\rangle=n|n\rangle$:

$$\langle\psi|N|\psi\rangle=\sum_{n\geqslant 0} n|c_n|^2\equiv\langle n\rangle. \tag{9.2}$$

Let $\overline{n}\in\mathbb{N}$ be the closest integer to $\langle n\rangle$. Assuming that the spread $\sigma\approx\Delta n\equiv[\langle n^2\rangle-\langle n\rangle^2]^{1/2}$ is small compared with $\langle n\rangle\approx\overline{n}$, we expand the energy E_n in a Taylor series in n around the centrally excited value $\overline{n}$:

$$E_n\simeq E_{\overline{n}}+E'_{\overline{n}}(n-\overline{n})+\tfrac{1}{2}E''_{\overline{n}}(n-\overline{n})^2+\tfrac{1}{6}E'''_{\overline{n}}(n-\overline{n})^3+\ldots, \tag{9.3}$$

where each prime on $E_{\overline{n}}$ denotes a derivative. These derivatives define distinct time scales,[43] namely the *classical period* $T_{\rm cl}=2\pi\hbar/|E'_{\overline{n}}|$; the *revival time* $t_{\rm rev}=2\pi\hbar/(1/2|E''_{\overline{n}}|)$; the *superrevival time* $t_{\rm sr}=2\pi\hbar/(1/6|E'''_{\overline{n}}|)$; and so on. Inserting this expansion into the evolution factor $e^{-iE_nt/\hbar}$ of (9.1) allows us to understand the possible occurrence of a quasiperiodic revival structure of the wave packet (9.1) *according* to the weighting probability $n\mapsto|c_n|^2$. In the present case, we have

$$E_n=\frac{\hbar}{2ma^2}n(n+\nu)=\frac{\hbar}{2ma^2}[\overline{n}(\overline{n}+\nu)+(2\overline{n}+\nu)(n-\overline{n})+(n-\overline{n})^2]. \tag{9.4}$$

So the first characteristic time is the ''classical'' period

$$T_{\rm cl}=\frac{2\pi\hbar}{2\overline{n}+\nu}\,\frac{2ma^2}{\hbar^2}=\frac{2\pi ma^2}{\hbar(\overline{n}+\nu/2)}, \tag{9.5}$$

which should be compared with the actual classical (Bohr–Sommerfeld) counterpart deduced from (2.21) and (2.25),

$$T=\frac{2\pi ma^2}{A+a\sqrt{mV_0}[\sqrt{\lambda(\lambda-1)}+\sqrt{\kappa(\kappa-1)}]}. \tag{9.6}$$

The second characteristic time is the revival time

$$t_{\rm rev}=\frac{4\pi ma^2}{\hbar}=(2\overline{n}+\nu)T_{\rm cl}. \tag{9.7}$$

There is no superrevival time here, because the energy is a quadratic function of n.

With these definitions, the wave packet (9.1) reads in the present situation (up to a global phase factor):

$$|\psi(t)\rangle=\sum_{n\geqslant 0} c_n e^{-2\pi i[(n-\overline{n})t/T_{\rm cl}+(n-\overline{n})^2t/t_{\rm rev}]}|n\rangle. \tag{9.8}$$

Hence, it will undergo motion with the classical period, modulated by the revival phase.[49] Since $T_{\rm cl}\ll t_{\rm rev}$ for large $\overline{n}$, the classical period dominates for small values of t (mod $t_{\rm rev}$), and the motion is then periodic with period $T_{\rm cl}$. As t increases from 0 and becomes nonnegligible with respect to $t_{\rm rev}$, the revival term $(n-\overline{n})^2t/t_{\rm rev}$ in the phase of (9.8) causes the wave packet to spread and collapse. The latter gathers into a series of subsidiary waves, the fractional revivals, which move periodically with a period equal to a rational fraction of $T_{\rm cl}$. Then, a full revival obviously occurs at each multiple of $t_{\rm rev}$.

In order to put into evidence these revival structures for a given wave packet $\psi(x,t)=\langle x|\psi(t)\rangle$, an efficient method is to calculate its autocorrelation function[49]

$$A(t)=\langle\psi(x,0)|\psi(x,t)\rangle=\sum_{n\geqslant 0}|c_n|^2e^{-iE_nt/\hbar}. \tag{9.9}$$

Numerically, $|A(t)|^2$ varies between 0 and 1. The maximum $|A(t)|^2=1$ is reached when $\psi(x,t)$ exactly matches the initial wave packet $\psi(x,0)$, and the minimum 0 corresponds to nonoverlapping: $\psi(x,t)$ is far from the initial state. On the other hand, fractional revivals and fractional ''superrevivals'' appear (in the general case) as periodic peaks in $|A(t)|^2$ with periods that are rational fractions of the classical round trip time $T_{\rm cl}$ and the revival time $t_{\rm rev}$.

Since the weighting distribution $|c_n|^2$ is crucial for understanding the temporal behavior of the wave packet (9.1), it is worthwhile to give also some general precisions of a statistical nature[20,50,51] before examining the special case of our coherent states. It is clear that the revival features will be more or less apparent, depending on the value of the deviation $(n-\overline{n})$ (relatively to n) that is effectively taken into account in the construction of the wave packet. In this respect, it is interesting to compare $|c_n|^2$ with the Poissonian case $\langle n\rangle^n e^{-\langle n\rangle}/n!$ and with the Gaussian case, $(2\pi(\Delta n)^2)^{-1/2}\exp[-(n-\langle n\rangle)^2/2(\Delta n)^2]$.

A quantitative estimate is given by the so-called Mandel parameter Q[20,50] defined as follows:

$$Q=\frac{(\Delta n)^2}{\langle n\rangle}-1. \tag{9.10}$$

In the Poissonian case, we have $Q=0$, i.e., $\Delta n=\langle n\rangle^{1/2}$. We say that the weighting distribution is sub-Poissonian (resp. super-Poissonian) if $Q<0$ (resp. $Q>0$). In the super-Poissonian case, i.e., $\Delta n>\langle n\rangle^{1/2}$, the set of states $|n\rangle$ which contribute significantly to the wave packet can be rather widely spread around $n\simeq\langle n\rangle$, and this may have important consequences for the properties of localization and temporal stability of the wave packet.

When the wave packets are precisely our coherent states

$$|J,\gamma\rangle=\frac{1}{N(J)}\sum_{n\geqslant 0}\frac{J^{n/2}e^{-ie_n\gamma}}{\sqrt{\rho_n}}|n\rangle, \tag{9.11}$$

the weighting distribution depends on J,

$$|c_n|^2=\frac{J^n}{N(J)^2\rho_n}, \tag{9.12}$$

and we can see the interesting statistical interplay with the probability distribution $\rho(J)$ of which the ρ_n are the moments [see (7.24)].

To simplify, we put

$$E(J)\equiv N(J)^2=\sum_{n\geqslant 0}\frac{J^n}{\rho_n}=\frac{\Gamma(\nu+1)}{J^{\nu/2}}I_\nu(2\sqrt{J}),\quad \nu\geqslant 2. \tag{9.13}$$

The following mean values are easily computed, together with their asymptotic values for large J:[39]

$$\langle n\rangle=\frac{J}{E(J)}\frac{d}{dJ}E(J)=J\frac{d}{dJ}\ln E(J)=\sqrt{J}\frac{I_{\nu+1}(2\sqrt{J})}{I_\nu(2\sqrt{J})}=\sqrt{J}-\frac{\nu}{2}-\frac{1}{4}+O\left(\frac{1}{\sqrt{J}}\right). \tag{9.14}$$

$$\begin{aligned}\langle n^2\rangle &= \frac{J}{E(J)}\frac{d}{dJ}J\frac{d}{dJ}E(J)\\ &= \sqrt{J}\frac{I_{\nu+1}(2\sqrt{J})}{I_\nu(2\sqrt{J})}+J\frac{I_{\nu+2}(2\sqrt{J})}{I_\nu(2\sqrt{J})}\\ &= \langle n\rangle + J\frac{I_{\nu+2}(2\sqrt{J})}{I_\nu(2\sqrt{J})}\\ &\approx \sqrt{J}(\sqrt{J}+1)\quad (J\gg 1).\end{aligned} \tag{9.15}$$

So, the dispersion is

$$\begin{aligned}(\Delta n)^2 &= J\frac{I_{\nu+2}(2\sqrt{J})}{I_\nu(2\sqrt{J})}+\langle n\rangle-\langle n\rangle^2\\ &= \frac{J}{[I_\nu(2\sqrt{J})]^2}(I_{\nu+2}(2\sqrt{J})I_\nu(2\sqrt{J})-[I_{\nu+1}(2\sqrt{J})]^2)+\sqrt{J}\frac{I_{\nu+1}(2\sqrt{J})}{I_\nu(2\sqrt{J})}\\ &\approx \frac{\sqrt{J}}{2},\quad \text{for } J \text{ large.}\end{aligned} \tag{9.16}$$

Finally, the Mandel parameter is given explicitly by

$$Q = J\frac{d}{dJ}\ln\frac{d}{dJ}\ln E(J) = \sqrt{J}\left[\frac{I_{\nu+2}(2\sqrt{J})}{I_{\nu+1}(2\sqrt{J})}-\frac{I_{\nu+1}(2\sqrt{J})}{I_\nu(2\sqrt{J})}\right]. \tag{9.17}$$

It is easily checked that $(I_{\nu+1}(x))^2 \geqslant I_\nu(x)I_{\nu+2}(x)$, for any $x\geqslant 0$, and thus, $Q\leqslant 0$ for any $J\geqslant 0$. Note that $Q\simeq 0$ for large J, while $Q\simeq -J$ for small J. Therefore, $|c_n|^2$ is sub-Poissonian in the case of our coherent states, whereas a quasi-Poissonian behavior is restored at high J. This fact is important for understanding the curves presented in Fig. 11(a), which show the distributions

$$D(n,J,\nu)\equiv|c_n|^2=\frac{1}{n!\Gamma(n+\nu+1)}\frac{J^{n+\nu/2}}{I_\nu(2\sqrt{J})} \tag{9.18}$$

for $\nu=2$ and different values of J. For the sake of comparison, we show in Fig. 11(b) the corresponding distribution $|c_n|^2=(1/n!)|\alpha|^{2n}e^{-|\alpha|^2}$ for the harmonic oscillator. Exactly as in the latter case, it can be shown easily that the distribution $D(n,J,\nu)$ tends for $J\to\infty$ to a Gaussian distribution. This Gaussian is centered at $\sqrt{J}-\nu/2-1/4$ and has a half-width equal to $(1/\sqrt{2})J^{1/4}$:

$$D(n,J,\nu)\approx\frac{1}{\sqrt{\pi\sqrt{J}}}e^{-[n-(\sqrt{J}-\nu/2-1/4)]^2/\sqrt{J}}\quad (n\gg 1). \tag{9.19}$$

We consider now the probability density $|\langle x|J,\gamma\rangle|^2$ as a function of the evolution parameter $\gamma=\omega t$ for increasing values of J. This evolution is shown in Fig. 12 in the case of the infinite square-well, for $J=2$, 10, and 50. We can see here at $\gamma=\pi=1/2t_{\text{rev}}$ a perfect revival of the initial shape at $\gamma=0$. This revival takes place near the opposite wall, as expected from the symmetry with respect to the center of the well. On the other hand, the ruling of the wave packet evolution by the classical period $T_{\text{cl}}=t_{\text{rev}}/(2\bar{n}+\nu)=\pi/(\bar{n}+1)$ becomes more and more apparent as J increases. We also note that, at multiples of the half reversal time $1/2t_{\text{rev}}=\pi$, the probability of localization near the walls increases with the energy J.

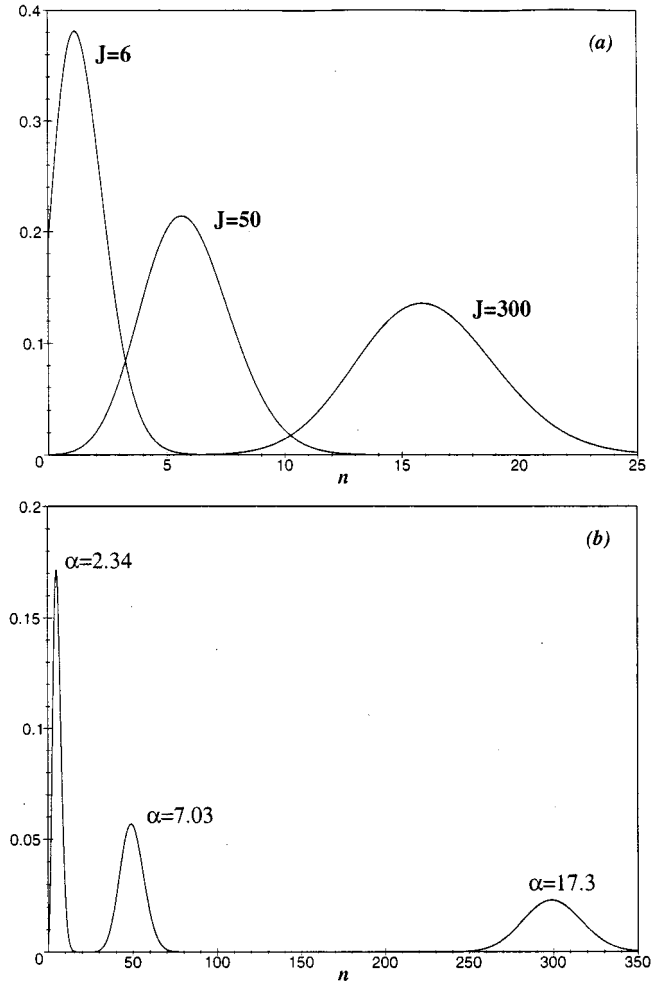

FIG. 11. (a) The weighting distribution $|c_n|^2 \equiv D(n,J,\nu)$ given in (9.18) for the infinite square-well $\nu=2$ and different values of J. Note the almost Gaussian shape at $J=300$, centered at $n=\langle n\rangle=\sqrt{J}-\nu/2-1/4\simeq 16$, with a width equal to $2\Delta n=\sqrt{2}J^{1/4}\simeq 5.9$. (b) The same for for the harmonic oscillator: $|c_n|^2=(1/n!)|\alpha|^{2n}e^{-|\alpha|^2}$. The values of α are chosen so as to get essentially the same mean energy values as in (a): $\alpha=\sqrt{J}$.

In Fig. 13, we show the squared modulus

$$|\langle J,0|e^{-iHt/\hbar}|J,0\rangle|^2=|\langle J,0|J,\omega t\rangle|^2 \tag{9.20}$$

$$=\frac{\Gamma(\nu+1)}{N(J)^2}\left|\sum_{n\geqslant 0}\frac{J^n}{n!\Gamma(n+\nu+1)}e^{-i\omega n(n+\nu)t}\right|^2 \tag{9.21}$$

of the autocorrelation versus $\gamma=\omega t$ for the infinite well, for $J=2$, 10, 50. Like in Fig. 12, we draw the attention on the large J regime. Here fractional revivals occur as intermediate peaks at rational multiples of the classical period $T_{\rm cl}=\pi/(\overline{n}+1)\approx\pi/\sqrt{J}$, $J\gg 1$, and they tend to diminish as J increases, which is clearly the mark of a quasiclassical behavior. The same quantity is shown in Fig. 14 for the Pöschl–Teller potential, for $J=20$ and 40. Note that, in actual calculations like this, one has to choose a finite number of orthonormal eigenstates of the Pöschl–Teller potential, denoted here by $n_{\max}$. Correspondingly, the normalization of the coherent state $|J,\gamma\rangle$ has then to be modified as

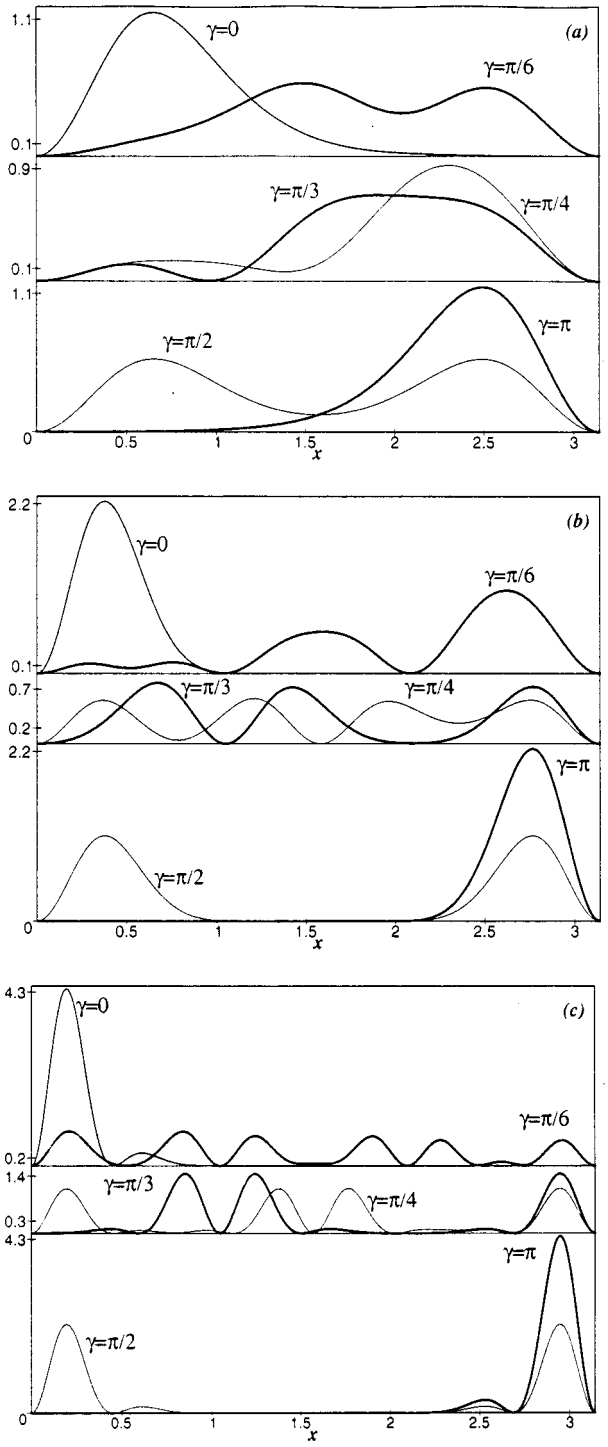

FIG. 12. The evolution (vs γ) of the probability density $|\langle x|J,\gamma\rangle|^2$, in the case of the infinite square-well for (a) $J=2$; (b) $J=10$; and (c) $J=50$. We note the perfect revival at $\gamma=\pi=1/2t_{\text{rev}}$ (in suitable units), symmetric with respect to the center of the well.

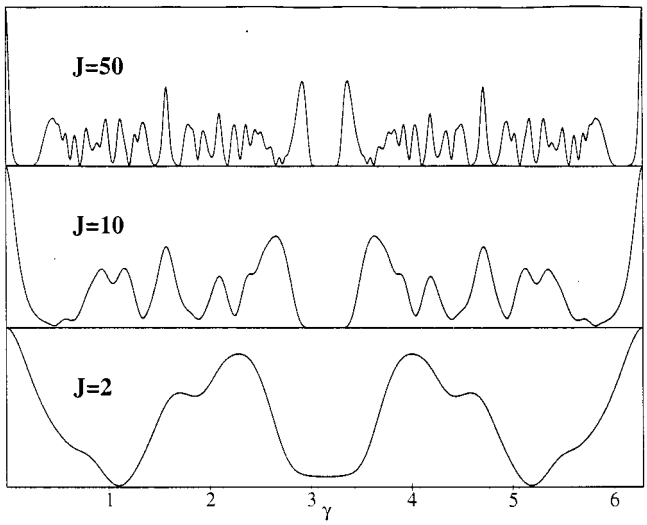

FIG. 13. Squared modulus $|\langle J,0|J,\omega t\rangle|^2$ of the autocorrelation vs $\gamma=\omega t$ for the infinite square-well, for $J=2$, 10, 50. As in Fig. 12, the large J regime is characterized by the occurrence of fractional revivals.

$$\sum_{p=0}^{n_{\max}} \frac{J^p}{p!\Gamma(p+\kappa+\lambda)} = \frac{I_{\kappa+\lambda-1}(2\sqrt{J})}{J^{1/2(\kappa+\lambda-1)}} - \frac{J^{n_{\max}+1}\,{}_1F_2(1;n_{\max}+2,n_{\max}+1+\kappa+\lambda;J)}{(n_{\max}+1)!\Gamma(n_{\max}+1+\kappa+\lambda)}, \quad (9.22)$$

where ${}_1F_2$ is a hypergeometric function.

Most interesting is the temporal behavior of the average position $\langle Q\rangle$ and of the average momentum $\langle P\rangle$ in such coherent states:

$$\langle J,0|A(t)|J,0\rangle = \langle J,0|e^{iHt/\hbar}Ae^{-iHt/\hbar}|J,0\rangle = \langle J,\omega t=\gamma|A|J,\omega t=\gamma\rangle \quad (9.23)$$

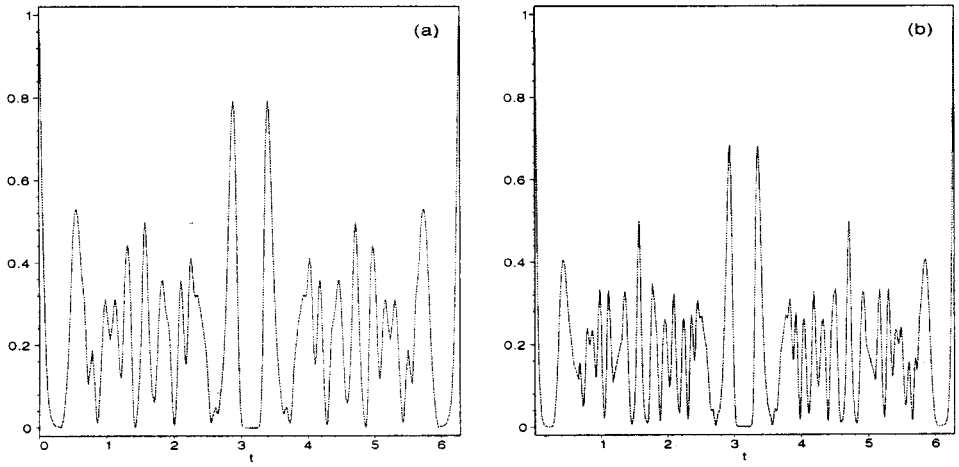

FIG. 14. Squared modulus $|\langle J,0|J,\omega t\rangle|^2$ of the autocorrelation for the Pöschl–Teller potential with $n_{\max=10}$, for (a) $J=20$; (b) $J=40$.

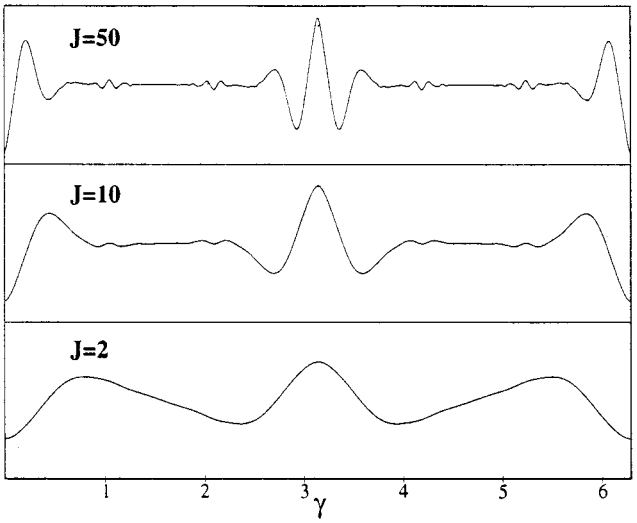

FIG. 15. Temporal behavior of the average position of the particle in the infinite square-well (in the Heisenberg picture), $\langle J,0|Q(t)|J,0\rangle=\langle J,\omega t=\gamma|Q|J,\omega t=\gamma\rangle$, as a function of $\gamma=\omega t$, for $J=2$, 10, 50.

for $A=Q$ or $A=P\equiv P_1$. This temporal behavior is shown in Fig. 15 for the average position in the infinite square-well, for $J=2$, 10, 50. We note the tendency to stability around the classical mean value $1/2\pi a$, except for strong oscillations of ultrashort duration between the walls near $\gamma=n\pi$. The latter increase with J as expected when one approaches the classical regime. For the sake of comparison, we show in Fig. 16 the temporal behavior of the average position in the asymmetric Pöschl–Teller potential $(\kappa,\lambda)=(4,8)$, for $J=20$ and 50.

Figure 17 shows the temporal behavior of the average momentum $\langle J,0|P(t)|J,0\rangle$ in the case of the infinite square-well, for $J=2$, 10, 50. Like in Fig. 15, we note the presence of strong ultrashort oscillations at $\gamma=n\pi$, whereas a tendency to perfect stability (around the classical mean value 0) exists at intermediate values of γ (this tendency is, however, less marked than for the average position).

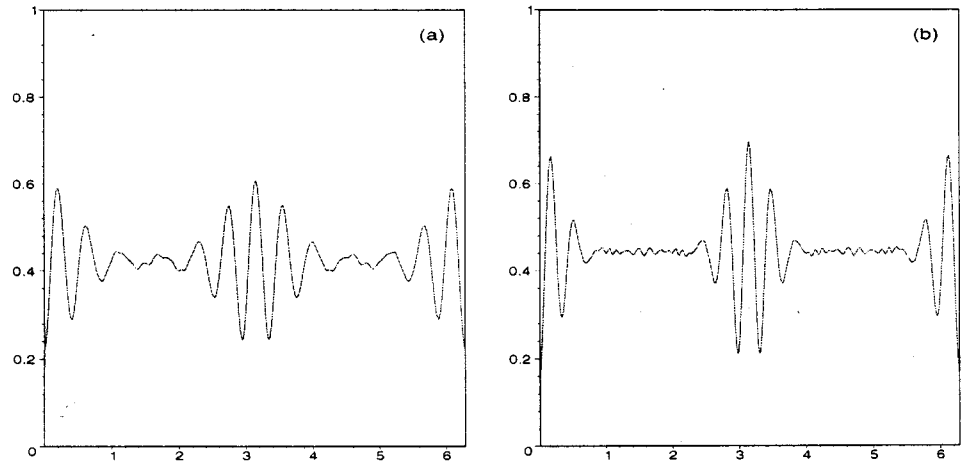

FIG. 16. Temporal behavior of the average position for the asymmetric Pöschl–Teller potential $(\lambda,\kappa)=(4,8)$ with $n_{\max=10}$, for (a) $J=20$ and (b) $J=50$.

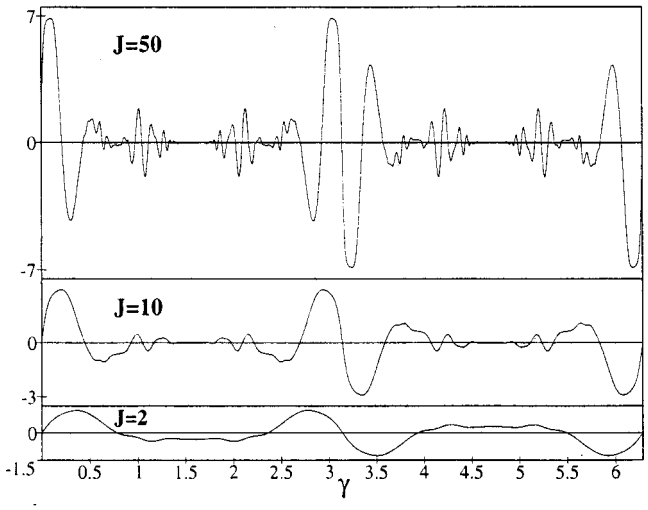

FIG. 17. Temporal behavior of the average momentum $\langle J,0|P(t)|J,0\rangle$ in the case of the infinite square-well, for $J=2$, 10, 50.

Next, we examine the uncertainty in position and momentum, in order to evaluate how close these CS come to saturating the uncertainty relations. Figure 18 shows the temporal behavior of the squared uncertainty in position, $(\Delta Q)^2$, for the infinite square-well, again for $J=2$, 10, 50. Figure 19 does the same for momentum, $(\Delta P)^2$, and Fig. 20 shows the product of the two, $(\Delta Q)^2(\Delta P)^2$. We note here that the product approaches the limit value 1/4 (saturation of the Heisenberg inequality) for a longer time at small J. This is consistent with (3.19), since at small J the wave packet is centered near the ground state, for which we reach the minimal value $(0.57)^2$. On the other hand, we also note the strong oscillations of $(\Delta Q)^2(\Delta P)^2$ at half the revival time, a fact which is consistent with the previous figures, showing the average position and momentum.

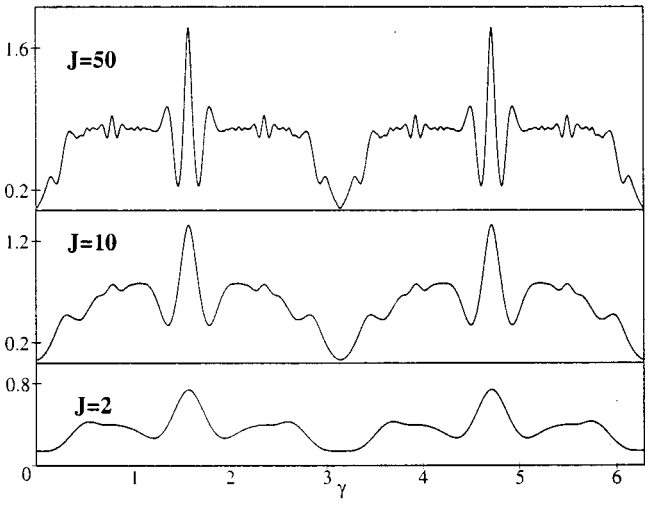

FIG. 18. Temporal behavior of the squared uncertainty in position $(\Delta Q)^2$, in the case of the infinite square-well, for $J=2$, 10, 50.

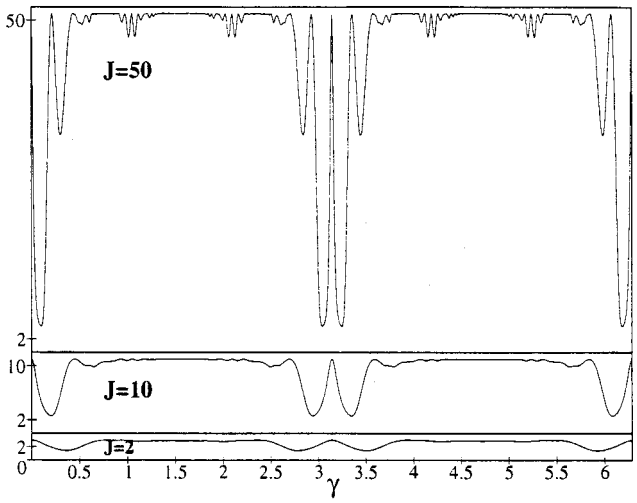

FIG. 19. Temporal behavior of the squared uncertainty in momentum $(\Delta P)^2$, in the case of the infinite square-well, for $J=2$, 10, 50.

At $1/2t_{\mathrm{rev}}$, the quantum interferences are dominant and they enforce the spreading of the wave packet for a relatively long duration.

As a last bit of information (but not the least!), we exhibit in Fig. 21 the temporal behavior of the average position $\langle J,0|Q(t)|J,0\rangle$ for the infinite square-well, for a very high value $J=10^6$, near $\gamma=\omega t=0$. Here the quasiclassical behavior is striking in the range of values considered for γ. These temporal oscillations are clearly governed by $T_{\mathrm{cl}}\simeq\pi/\sqrt{J}=3\times10^{-3}$ and should be compared with their purely classical counterpart of Fig. 3.

X. DISCUSSION

Coherent states have many roles to play in quantum theory. Among those roles is included the Hilbert space representation that coherent states induce, which is largely kinematical in nature, and

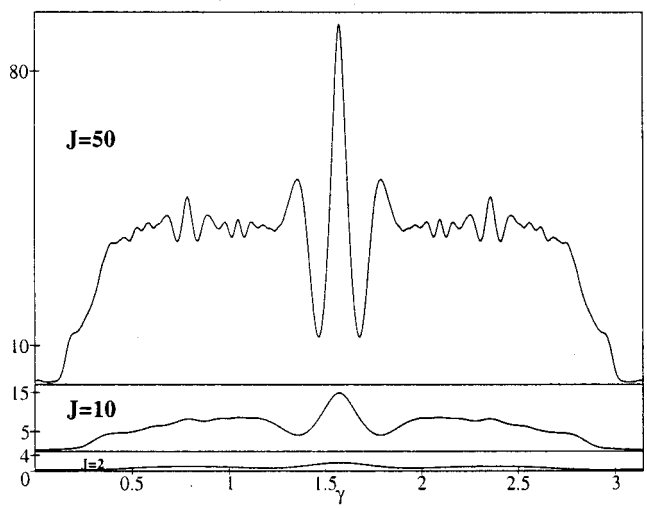

FIG. 20. Temporal behavior of the product of the squared uncertainties $(\Delta Q)^2(\Delta P)^2$, in the case of the infinite square-well, for $J=2$, 10, 50.

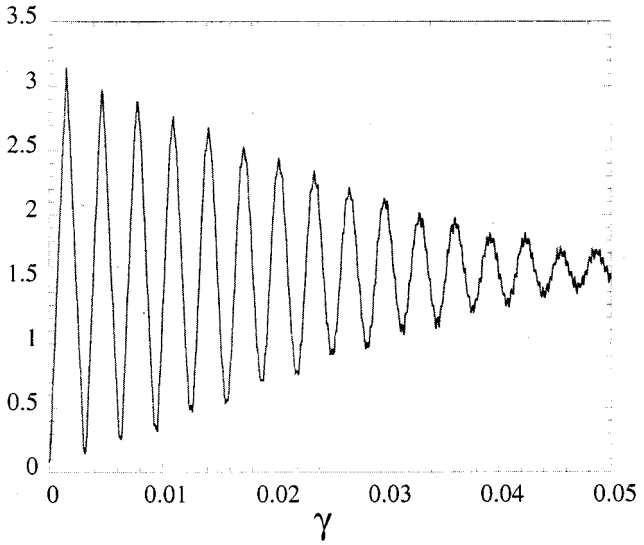

FIG. 21. Temporal behavior of the average position in the case of the infinite square-well, for a very high value $J=10^6$.

the adaption of the coherent states themselves to some particular dynamics and the possible description that ensues. To accommodate these goals, the definition of what constitutes a ''set of coherent states'' has been increasingly broadened over the years. Widening the scope of coherent states also widens the range of potential applications. This basic principle lies behind the developments in this article.

The minimal definition of a set of coherent states involves continuity of labeling and a resolution of unity, and, therefore, holomorphic representations and/or definitions via groups are just a small subset of the possibilities. In the present article, we have exploited this diversity in coherent state definition to study the motion of a particle in Pöschl–Teller potentials as well as in the closely related infinite square-well potential.

The specific choices we have made for the set of coherent states are based on two additional guiding principles besides continuity and resolution of unity.[15,16] The first of these is ''temporal stability,'' which in words asserts that the temporal evolution of any coherent state always remains a coherent state. The second of these, referred to as the ''action identity'' in Ref. 16, chooses variables for the coherent state labels that have as close a connection as possible with classical ''action-angle'' variables. In particular, for a single degree of freedom, the label pair (J,γ) is used to identify the coherent state $|J,\gamma\rangle$. Temporal stability means that, under the chosen dynamics, temporal evolution proceeds according to $|J,\gamma+\omega t\rangle$, for some fixed parameter ω. To ensure that (J,γ) describes action-angle variables, it is sufficient to require that the symplectic potential induced by the coherent states themselves is of Darboux form, or specifically that

$$i\hbar\langle J,\gamma|d|J,\gamma\rangle = J\,d\gamma,$$

where $d|J,\gamma\rangle \equiv |J+dJ,\gamma+d\gamma\rangle - |J,\gamma\rangle$. Temporal stability is what fixes the *phase* behavior of the coherent states, i.e., the factor $e^{-i\gamma e_n}$ [cf. (7.15)], while ensuring that (J,γ) are canonical action-angle variables is what fixes the *amplitude* behavior of the coherent states, i.e., $1/N\sqrt{[e_n]!}$ [cf. (7.19) and (7.20)]. The given amplitude behavior may be arrived at by other means,[20] but requiring that J and γ be canonical classical coordinates is equivalent and tends to stress the physics of the situation.

In order for coherent states to interpolate well between quantum and classical mechanics, it is necessary for values of the action $J \gg \hbar$ that the quantum motion be well approximated by the

classical motion. In particular, for a classical system with closed, localized trajectories, a suitable wave packet should, if possible, remain ''coherent'' for a number of classical periods. For the systems under study in this article, we have demonstrated the tendency for improved packet coherence with increasing J values within the range studied. For significantly larger values of J, we notice that the packet coherence substantially improves. Interesting results have been obtained independently in a related study by Fox and Choi,[52] who found a similar packet coherence for ten or more classical periods for an infinite square-well, even though they used a different amplitude prescription for their coherent states. In both works, however, the probability distribution shows a Gaussian behavior for large values of J, and this explains the similarity of the results.

It would appear that allowing for generalized phase and amplitude behavior in the definition of coherent states has led us closer to the idealized goal of a set of coherent states adapted to a chosen system and having a large number of properties in common with the associated classical system, despite being fully quantum in their characteristics.

Note added. After completion of the present article, an article by Crawford[53] has come to the authors' attention. This paper studies the dependence of various coherent states on the weighting parameters $\{\rho_n\}$ and how they effect various correlation functions of interest regarding general systems, and particularly for the hydrogen atom. The studies reported in Ref. 53 offer a good complement to those of the present article.

Note added in proof. As this article was going to press, an article by Bonneau *et al.*[54] appeared, in which the authors discuss in a pedagogical way some of the functional analysis of the infinite well problem, in the same spirit as in Sec. III and with similar results.

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Stereographic variables for multidimensional quantum group covariant *q*-oscillators

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In this paper, we study the unitary matrix representation of quantum group $SU_q(2)$ in terms of stereographic coordinates z and z^* and a central unitary phase u. The fractional linear transformation of z and z^* gives the action of $SU_q(2)$ on the quantum sphere $SU_q(2)/U(1)$ with coordinates z and z^*. We then extend this action to $SU_q(2)$ and derive the transformation law of u. Finally, we construct the two-dimensional covariant q-oscillators in terms of stereographic variables and then we generalize it to d-dimensional case. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1370953]

I. INTRODUCTION

Over the last decade, a great deal of attention has been paid to quantum groups both in the mathematical and the physical literature. An algebraic structure for a quantum group, called the q-deformation algebra, is the generalization of its corresponding Lie algebra. Deformations of Lie algebras were first introduced in the context of group contractions,[1] where a Lie algebra is deformed into another Lie algebra. The q-oscillator which is the simplest deformation of the oscillator algebra was introduced by Coon and collaborators[2] and by Kuryshkin.[3] Quantum groups and quantum algebras entailing a Hopf Algebra structure were formulated by Faddeev,[4] Jimbo,[5] Drinfeld,[6] and Woronowicz.[7] For the quantum algebra $SU_q(2)$, Macfarlane[8] and Biedenharn[9] achieved a new realization where they constructed the quantum enveloping algebra in terms of the two independent new q-deformed harmonic oscillators. They used the Schwinger approach[10] of quantum theory of angular momentum and they also generalized the Schwinger construction used in the quantum theory of $SU(2)$ angular momentum.

As is know from previous studies;[11–13] a 2×2 unitary matrix can be parametrized in terms of a phase and a stereographic complex coordinate z which can be used as the coordinates of $SU(2)/U(1)=CP^1$. We also know that a 2×2 quantum unitary matrix can be parametrized in terms of a central unitary phase u and the operator z such that this z is the stereographic quantum coordinate of the quantum sphere $SU_q(2)/U(1)$. Here the operator z which describes the complex sphere S_q^2 satisfies the following commutation relation:

$$zz^*-q^{-2}z^*z=q^{-2}-1, \quad 0<q<1. \tag{1}$$

The action of $SU_q(2)$ on the quantum sphere is given by a fractional linear transformation on z and z^*.

In this paper, we consider the action of $G=SU_q(2)$ on $M=SU_q(2)$ where we consider M to be given in terms of coordinates z, z^* and a central phase u and we derive the transformation law of u. Moreover, we construct the d-dimensional covariant q-oscillators in terms of stereographic variables. The plan of this paper is as follows: In Sec. II we consider a 2×2 unitary matrix. A coset representation of this matrix in terms of stereographic variables z and z^* is given. This yields an equation which determines the linear fractional transformation of z. In Sec. III we discuss the unitary quantum group $SU_q(2)$. The quantum sphere is described in terms of stereographic variables z and z^*.[14] The coset representation of $SU_q(2)/U(1)=CP_q^1$ is obtained. Then we show that the commutation relation between z and z^* is as in Eq. (1) and we find quantum linear fractional transformation equations for z, z^*z, and u. In Sec. IV by starting with the consideration

of the commutation relation satisfied by a and a^* which are quantum coordinates of $SU_q(2)/U(1)$, we get the covariant q-oscillators in two-dimensions. Then we change the variables into stereographic variables and we generalize this two-dimensional covariant q-oscillators to d-dimensional ones. Finally, in Sec. V we present our conclusion.

II. THE UNITARY GROUP SU(2) AND THE COSET SU(2)/U(1)=CP[1]

We start by writing elements of unitary group SU(2) in terms of 2×2 matrices. If A is a 2×2 unitary matrix, then its elements can be represented as

$$A=\begin{pmatrix} a & -\overline{c} \\ c & \overline{a} \end{pmatrix}, \quad a,c\in C. \tag{2}$$

It is clear that elements of matrix A also satisfies the equality of $a\overline{a}+c\overline{c}=1$.

Since we want to show that this matrix A can be parametrized in terms of a phase and stereographic complex coordinate z first we write A as the product of two matrices,

$$A=ZU=\begin{pmatrix} a' & -r \\ r & \overline{a}' \end{pmatrix}\begin{pmatrix} u & 0 \\ 0 & \overline{u} \end{pmatrix}, \quad a',u\in C; r\geqslant 0; u\overline{u}=1. \tag{3}$$

This representation is well known in the nonlinear realization[15] language. The matrix Z is called an SU(2)/U(1) coset representative, which here is fixed by choosing r real. Z is also a unitary matrix. Therefore, we can easily say that its elements also satisfy the following equality:

$$\overline{a}'a'+r^2=1 \tag{4}$$

which describes the upper half of the sphere. Starting from this point of view, we can write

$$a'=z(1+z\overline{z})^{-1/2}, \tag{5}$$

$$r=(1+z\overline{z})^{-1/2}. \tag{6}$$

If we rewrite the elements of the matrix Z by using equalities (5) and (6); our coset representation of Z becomes

$$Z=(1+z\overline{z})^{-1/2}\begin{pmatrix} z & -1 \\ 1 & \overline{z} \end{pmatrix} \tag{7}$$

such that Z describes an element of S^2.

In order to write a linear fractional transformation for z; we first consider the unitary matrix M which can be written as follows:

$$M=\begin{pmatrix} \alpha & -\overline{\gamma} \\ \gamma & \overline{\alpha} \end{pmatrix}, \quad \alpha,\gamma\in C; \alpha\overline{\alpha}+\gamma\overline{\gamma}=1. \tag{8}$$

Then, by multiplying this matrix M with matrix Z and equating the product to matrix Z', we attain the fractional transformation

$$z'=\frac{\alpha z-\overline{\gamma}}{\gamma z+\overline{\alpha}}. \tag{9}$$

III. THE QUANTUM UNITARY GROUP $SU_q(2)$ AND QUANTUM LINEAR FRACTIONAL TRANSFORMATIONS FOR STEREOGRAPHIC COORDINATES z AND UNITARY PHASE u

In this section we will discuss the unitary quantum group $SU_q(2)$ by using its matrix representation. If $A=\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$ is an element of $SU_q(2)$, then in addition to the $GL_q(2)$ commutation relations, the equalities $d=a^*$, $b=-qc^*$, and $ad-qbc=1$ hold. Therefore, matrix A can be rewritten as

$$A=\begin{pmatrix} a & -qc^* \\ c & a^* \end{pmatrix}. \tag{10}$$

Here elements of matrix A are noncommuting quantities such that they satisfy the following commutation relations:

$$ac=qca, \tag{11}$$

$$c^*a^*=qa^*c^*, \tag{12}$$

$$ac^*=qc^*a, \tag{13}$$

$$ca^*=qa^*c, \tag{14}$$

$$aa^*+q^2c^*c=1, \tag{15}$$

$$a^*a+cc^*=1, \tag{16}$$

$$cc^*=c^*c. \tag{17}$$

By using Eqs. (15), (16), and (17); we can easily attain the commutation relation for a and a^*

$$aa^*-q^2a^*a=1-q^2, \quad 0<q<1. \tag{18}$$

When a is rescaled by $(1-q^2)^{-1/2}$, we get precisely the q^2-oscillator commutation relation[2,3] such that if $a/(1-q^2)^{1/2}$ is defined as b, then

$$bb^*-q^2b^*b=1, \quad 0<q<1. \tag{19}$$

As in Sec. II, if we want to express the $SU_q(2)$ matrices in terms of stereographic coordinates z and z^*, which describe the complex sphere S^2, we should use the following transformations

$$a=z(1+z^*z)^{-1/2}, \tag{20}$$

$$c=u(1+z^*z)^{-1/2}, \tag{21}$$

where u is a central unitary phase such that $u^{-1}=u^*$. Inverse ''coordinate transformation'' equations can also be written as follows:

$$z=a(c^*c)^{-1/2}, \tag{22}$$

$$z^*=(c^*c)^{-1/2}a^*. \tag{23}$$

In the above equalities, we should be careful which variables commute with each other. From relations (11)–(17), it follows[11] that u commutes with z and z^*, which means it commutes with everything, but of course z and z^* do not commute with each other. To find the commutation

relation between z and z^*, we can use the commutation relation between a and a^*. If we write $(1+z^*z)^{-1/2}z^*$ and $z(1+z^*z)^{-1/2}$ instead of a^* and a, respectively, in Eq. (18), then we get

$$zz^*-q^{-2}z^*z=q^{-2}-1. \tag{24}$$

Since $0<q<1$, $q^{-2}-1>0$ and rescaling z by $w=z/(q^{-2}-1)^{1/2}$ gives

$$ww^*-q'w^*w=1, \quad q'=q^{-2}>1 \tag{25}$$

which is again a q-oscillator relation. Thus whereas (19) is a $q<1$ q-oscillator, (25) is a $q'>1$ q-oscillator. Hence, we saw that from the point of view of $SU_q(2)$ the q-oscillator ($q<1$) and the q^{-1}-oscillator ($q^{-1}>1$) are just different ''coordinates'' of the same algebraic structure.

Now let us rewrite the matrix A by using z and z^*,

$$A=ZU=\begin{pmatrix} u^*z(1+z^*z)^{-1/2} & -q(1+z^*z)^{-1/2} \\ (1+z^*z)^{-1/2} & (1+z^*z)^{-1/2}z^*u \end{pmatrix}\begin{pmatrix} u & 0 \\ 0 & u^* \end{pmatrix}. \tag{26}$$

In the above equality, matrix U is an element of U(1) which is a subgroup of $SU_q(2)$ and the matrix Z is the coset representative of $CP_q^1=SU_q(2)/U(1)$.

Let us redefine z and z^* such that $z\to u^*z$ and $z^*\to z^*u$. Notice that this redefinition of z and z^* leaves Eq. (24) invariant. By using this equation we can rearrange Z matrix as follows:

$$Z=\begin{pmatrix} z(1+z^*z)^{-1/2} & -(1+zz^*)^{-1/2} \\ (1+z^*z)^{-1/2} & z^*(1+zz^*)^{-1/2} \end{pmatrix}. \tag{27}$$

Now we can derive the transformation laws for z, z^*z, and u, respectively. By following the steps in Sec. I, we can write the following equality:

$$\begin{pmatrix} \tilde{z}(1+\tilde{z}^*\tilde{z})^{-1/2}\tilde{u} & -(1+\tilde{z}\tilde{z}^*)^{-1/2}\tilde{u}^* \\ (1+\tilde{z}^*\tilde{z})^{-1/2}\tilde{u} & \tilde{z}^*(1+\tilde{z}\tilde{z}^*)^{-1/2}\tilde{u}^* \end{pmatrix}=\begin{pmatrix} a & -qc^* \\ c & a^* \end{pmatrix}\begin{pmatrix} z(1+z^*z)^{-1/2}u & -(1+zz^*)^{-1/2}u^* \\ (1+z^*z)^{-1/2}u & z^*(1+zz^*)^{-1/2}u^* \end{pmatrix} \tag{28}$$

This equality is the key point. Because, only by looking at corresponding elements of the right-hand side and the left-hand side matrices, we can easily find the transformation laws.

For $z \xrightarrow{SU_q(2)} \tilde{z}$; we consider the (1,1) elements and (2,1) elements of the matrices in the RHS and LHS. Equating these elements gives the following equalities:

$$\tilde{z}(1+\tilde{z}^*\tilde{z})^{-1/2}\tilde{u}=(az-qc^*)(1+z^*z)^{-1/2}u, \tag{29}$$

$$(1+\tilde{z}^*\tilde{z})^{-1/2}\tilde{u}=(cz+a^*)(1+z^*z)^{-1/2}u. \tag{30}$$

If Eq. (29) is divided by (30), then we will get the fractional linear transformation equation for z,

$$\tilde{z}=(az-qc^*)(cz+a^*)^{-1}=(qcz+a^*)^{-1}(az-c^*). \tag{31}$$

In order to find the transformation law for z^*z, first we should find the transformation law of z^* by considering (1,2) and (2,2) matrix elements of Eq. (28). Then by multiplying the transformation of z^* with Eq. (31), we get the following one:

$$\tilde{z}^*\tilde{z}=((-c+a^*z^*)(az-q^2c^*))((cz+a^*)(a+q^2c^*z^*))^{-1}. \tag{32}$$

Considering (1,2) and (2,1) elements of RHS and LHS matrices in (28) gives the following equality:

$$\tilde{u}^2=(cz+a^*)(a+qc^*z^*)^{-1}u^2 \tag{33}$$

which is the linear fractional transformation equation for u^2. As a result, since u is central, it is clear that we can write the transformation law of u as

$$\tilde{u}=[(cz+a^*)(a+qc^*z^*)^{-1}]^{1/2}u, \tag{34}$$

$$\tilde{u}=vu, \quad \text{where} \quad v=[(cz+a^*)(a+qc^*z^*)^{-1}]^{1/2}. \tag{35}$$

It can be verified that v is unitary by using the relation

$$(a+qc^*z^*)(cz+a^*)^{-1}=(a^*+qcz)^{-1}(c^*z^*+a) \tag{36}$$

which follows from (11)–(17) and (24). The transformation given by (31) and (34) completely define the action of $\mathrm{SU}_q(2)$ on the ''coordinates'' z and u of $\mathrm{SU}_q(2)$. For $q\to 1$ these transformations reduce to their classical form.

IV. MULTIDIMENSIONAL QUANTUM GROUP COVARIANT *q*-OSCILLATORS WITH STEREOGRAPHIC VARIABLES

In this section, first we will consider the two-dimensional q-oscillators, then we generalize it to the d-dimensional case. For two-dimensional q-oscillators we have two copies of the one-dimensional q-oscillator such that

$$a_i a_i^*-q^2 a_i^* a_i=1-q^2, \tag{37}$$

$$[a_i,a_j]=0, \quad i\neq j$$

$$[a_i,a_j^*]=0, \quad i\neq j \quad \text{where} \quad i,j=1,2. \tag{38}$$

From previous studies, we also know that the basic number[16,17] $[n]$ for this system can be written, respectively, as

$$[n_1]=a_1^* a_1=1-q^{2n_1}, \tag{39}$$

$$[n_2]=a_2^* a_2=1-q^{2n_2}, \tag{40}$$

and the spectrum degeneracy of the basic number operator for two copies of the q-oscillator can be achieved as

$$[n_1+n_2]=1-q^{2(n_1+n_2)}=[n_1]+q^{2n_1}[n_2] \tag{41}$$

which implies that we can redefine our annihilation operators

$$c_1=a_1, \tag{42}$$

$$c_2=q^{n_1}a_2. \tag{43}$$

Thus, (41) becomes

$$H=[n_1+n_2]=a_1^* a_1+q^{2n_1}a_2^* a_2=c_1^* c_1+c_2^* c_2, \tag{44}$$

c_i and c_i^* are quantum group covariant oscillator creation and annihilation operators.[18] H is invariant under the quantum group $\mathrm{U}_q(2)$. Its expression in terms of c_i^* and c_i is the same as the expression of the multidimensional quantum harmonic oscillator in terms of the undeformed creation and annihilation operators. In this sense it can be called a Hamiltonian. By considering the above redefinition, the commutation relations satisfied by these operators c_i's can be written as

$$c_1 c_2 = q c_2 c_1, \tag{45}$$

$$c_1 c_2^* = q c_2^* c_1, \tag{46}$$

$$c_1 c_1^* - q^2 c_1^* c_1 = 1 - q^2, \tag{47}$$

$$c_2 c_2^* - q^2 c_2^* c_2 = c_1 c_1^* - c_1^* c_1. \tag{48}$$

With the consideration of (20), we can also write our new creation and annihilation operators c_i^* and c_i in terms of stereographic variables as

$$c_1 = a_1 = z_1 (1 + z_1^* z_1)^{-1/2}, \tag{49}$$

$$c_2 = q^{n_1} a_2 = q^{n_1} z_2 (1 + z_2^* z_2)^{-1/2}. \tag{50}$$

Thus our H can be rewritten as

$$H = \frac{z_1^* z_1}{1 + z_1^* z_1} + q^{2n_1} \frac{z_2^* z_2}{1 + z_2^* z_2}. \tag{51}$$

In order to find the covariant multidimensional generalization of $H = [z^* z/(1 + z^* z)]$, we try an expression for H which corresponds to the replacement $z^* z \to w_1^* w_1 + w_2^* w_2 + \cdots + w_d^* w_d$. Hence for two dimensions

$$H = \frac{w_1^* w_1 + w_2^* w_2}{1 + w_1^* w_1 + w_2^* w_2} \tag{52}$$

such that for the one-dimensional case $w_1 = z$, $w_2 = 0$.

Then we can write

$$H = \frac{K}{1 + K}, \tag{53}$$

where $K = w_1^* w_1 + w_2^* w_2$, thus operator c_i's can be written as

$$c_i = w_i \sqrt{1 - H}. \tag{54}$$

By considering equations (44) to (48), we can obtain

$$c_1 f(H) = f(1 - q^2 + q^2 H) c_1, \tag{55}$$

$$c_2 f(H) = f(1 - q^2 + q^2 H) c_2. \tag{56}$$

Thus, with the help of Eqs. (45)–(48) and (54)–(56), we can easily find the commutation relations satisfied by w_i's as

$$w_1 w_2 = q w_2 w_1, \tag{57}$$

$$w_1 w_2^* = q^{-1} w_2^* w_1, \tag{58}$$

$$w_1 w_1^* - q^{-2} w_1^* w_1 = w_2 w_2^* - w_2^* w_2, \tag{59}$$

$$w_2 w_2^* - q^{-2} w_2^* w_2 = q^{-2} - 1. \tag{60}$$

Up to now, although we consider the two-dimensional q-oscillator, its generalization to the d-dimensional case is straightforward. In order to see this, let us consider operator a_i's ($i=1,2,\ldots,d$) which satisfy the following commutation relation:

$$a_i a_i^* - q^2 a_i^* a_i = 1 - q^2,$$

$$[a_i, a_j] = 0, \quad i \neq j, \tag{61}$$

$$[a_i, a_j^*] = 0, \quad i \neq j, \quad \text{where } i,j = 1,2,\ldots,d$$

and the basic number operator

$$\begin{aligned}[n] &= [n_1 + n_2 + \cdots + n_d] \\ &= [n_1] + q^{2n_1}[n_2] + q^{2(n_1+n_2)}[n_3] + \cdots + q^{2(n_1+n_2+\cdots+n_{d-1})}[n_d].\end{aligned} \tag{62}$$

Thus, annihilation operator can be redefined

$$c_i = q^{n_1+n_2+\cdots+n_{i-1}} a_i, \quad i = 2,3,\ldots,d, \tag{63}$$

whereas $c_1 = a_1$ and the Hamiltonian becomes

$$H = c_1^* c_1 + c_2^* c_2 + \cdots + c_d^* c_d. \tag{64}$$

Here, unlike operator a_i's which commute operator c_i's satisfy the following commutation relation:

$$c_i c_j = q c_j c_i, \quad i < j \tag{65}$$

$$c_i c_j^* = q c_j^* c_i, \quad i \neq j, \quad \text{where } i,j = 1,2,\ldots,d, \tag{66}$$

$$c_1 c_1^* - q^2 c_1^* c_1 = 1 - q^2, \tag{67}$$

$$c_i c_i^* - q^2 c_i^* c_i = c_{i-1} c_{i-1}^* - c_{i-1}^* c_{i-1}, \quad i = 2,3,\ldots,d. \tag{68}$$

As in the two-dimensional case, operator c_i's can be written in terms of w_i's as in (54). By considering this equation with (55), (56) and (65) to (68), commutation relations which are satisfied by w_i's can be written as

$$w_i w_j = q w_j w_i, \quad i < j, \tag{69}$$

$$w_i w_j^* = q^{-1} w_j^* w_i, \quad i \neq j, \quad \text{where } i,j = 1,2,\ldots,d, \tag{70}$$

$$w_{i-1} w_{i-1}^* - q^{-2} w_{i-1}^* w_{i-1} = w_i w_i^* - w_i^* w_i, \quad i = 2,3,\ldots,d, \tag{71}$$

$$w_d w_d^* - q^{-2} w_d^* w_d = q^{-2} - 1, \tag{72}$$

whereas the Hamiltonian H (64) now becomes

$$H = K(1+K)^{-1}, \tag{73}$$

where $K = w_1^* w_1 + w_2^* w_2 + \cdots + w_d^* w_d$.

V. CONCLUSION

We have shown that there are three most useful oscillator representations of the d-dimensional q-oscillator. One of these is simply given by d commuting copies of the one dimensional

q-oscillator. This set of quantum coordinates for the q-oscillator is simple, though not very useful since the invariance of the d-dimensional q-oscillator under the action of the quantum group $SU_q(d)$ is hidden. To see the action of $SU_q(d)$ one has to make a (nonlinear) transformation from these oscillator creation and annihilation operators into Pusz–Woronowicz creation and annihilation operators on which the quantum group $SU_q(2)$ acts linearly. Similarly the set of stereographic q-oscillators given by (69)–(72) we have constructed in this paper transform linearly under the quantum group $SU_q(d)$. Their commutation relations are remarkably similar to the commutation relations of Pusz–Woronowicz oscillators. The one-dimensional restriction of all three realizations of the d-dimensional q-oscillator are the same.

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Generating all Wigner functions

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In the context of phase-space quantization, matrix elements and observables result from integration of c-number functions over phase space, with Wigner functions serving as the quasiprobability measure. The complete sets of Wigner functions necessary to expand all phase-space functions include off-diagonal Wigner functions, which may appear technically involved. Nevertheless, it is shown here that suitable generating functions of these complete sets can often be constructed, which are relatively simple, and lead to compact evaluations of matrix elements. New features of such generating functions are detailed and explored for integer-indexed sets, such as for the harmonic oscillator, as well as continuously indexed ones, such as for the linear potential and the Liouville potential. The utility of such generating functions is illustrated in the computation of star functions, spectra, and perturbation theory in phase space. © *2001 American Institute of Physics.*
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I. INTRODUCTION

General phase-space functions $f(x,p)$ and $g(x,p)$ compose noncommutatively through Groenewold's $\star$-product,[1] which is the unique associative pseudodifferential deformation[2] of ordinary products:

$$\star \equiv e^{i\hbar(\overleftarrow{\partial}_x\overrightarrow{\partial}_p-\overleftarrow{\partial}_p\overrightarrow{\partial}_x)/2}. \tag{1}$$

This product is the cornerstone of deformation (phase-space) quantization,[2–5] as well as applications of matrix models and noncommutative geometry ideas in M-physics.[6] Its mechanics, however, is not always straightforward.

The practical Fourier representation of this product as an integral kernel has been utilized widely since Baker's[7] early work,

$$f\star g=\frac{1}{\hbar^2\pi^2}\int \mathrm{d}p'\,\mathrm{d}p''\,\mathrm{d}x'\,\mathrm{d}x''\,f(x',p')g(x'',p'')$$
$$\times\exp\left(\frac{-2i}{\hbar}(p(x'-x'')+p'(x''-x)+p''(x-x'))\right). \tag{2}$$

The determinantal nature of the star product controls the properties of the phase-space trace,[8,9]

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$$\int \mathrm{d}p\,\mathrm{d}x\, f\star g=\int \mathrm{d}p\,\mathrm{d}x\, fg=\int \mathrm{d}p\,\mathrm{d}x\, g\star f. \tag{3}$$

The above-mentioned $\star$-product and phase-space integrals provide the multiplication law and, respectively, the trace in phase-space quantization,[3] the third autonomous and logically complete formulation of quantum mechanics beyond the conventional formulations based on operators in Hilbert space or path integrals. (This formulation is reviewed in Refs. 2 and 5.) Properly ordered operators (e.g., Weyl-ordered) correspond uniquely to phase-space c-number functions (referred to as ''classical kernels'' of the operators in question); operator products correspond to $\star$-products of their classical kernels; and operator matrix elements, conventionally consisting of traces thereof with the density matrix, correspond to phase-space integrals of the classical kernels with the Wigner function (WF), the Weyl correspondent of the density matrix.[5,10] The celebrated $\star$-genvalue functional equations determining the Wigner functions[8,11] and their spectral properties (e.g., projective orthogonality[12]) are reviewed and illustrated in Ref. 4.

The functions introduced by Wigner[10] and Szilard correspond to diagonal elements of the density matrix, but quantum mechanical applications (such as perturbation theory), as well as applications in noncommutative soliton problems[13] often require the evaluation of off-diagonal matrix elements; they therefore utilize the complete set of diagonal and off-diagonal generalized Wigner functions introduced by Moyal.[3] For instance, in noncommutative soliton theory, the diagonal WFs are only complete for radial phase-space functions (functions $\star$-commuting with the harmonic oscillator Hamiltonian—the radius squared), whereas deviations from radial symmetry necessitate the complete off diagonal set.

As for any representation problem, the particular features of the $\star$-equations under consideration frequently favor an optimal basis of WFs; but, even in the case of the oscillator, the equations are technically demanding. It is pointed out here, however, that suitable generating functions for them, acting as a transform of these basis sets, often result in substantially simpler and more compact objects, which are much easier to use, manipulate, and intuit. In the following, after some elementary overview of the Weyl correspondence formalism (Sec. II), we illustrate such functions for the harmonic oscillator (Sec. III), which serves as the archetype of WF bases indexed discretely; it turns out that these generating functions amount to the phase-space coherent states for WFs, and also the WFs of coherent state wave functions (Appendix A). Direct applications to first-order perturbation theory are illustrated in Appendix B.

For sets indexed continuously, the generating function may range from a mere Fourier transform, illustrated by the linear potential (Sec. IV), to a less trivial continuous transform we provide for the Liouville potential problem (Sec. V), where the advantage of the transform method comes to cogent evidence.

Throughout our discussion, we provide the typical $\star$-composition laws of such generating functions, as well as applications such as the evaluation of $\star$-exponentials of phase-space functions (Appendix C), or $\star$-versions of modified Bessel functions (technical aspects of integral transforms of which are detailed in Appendix D). Appendix E provides the operator (Weyl-) correspondent to the generating function for the Liouville diagonal WF introduced in Sec V.

II. OVERVIEW OF GENERAL RELATIONS IN THE WEYL REPRESENTATION

Without loss of generality, we review basic concepts in two-dimensional phase space, (x,p), as the extension to higher dimensions is straightforward. In addition, we first address discrete spectra, E_n, $n=0,1,2,3,\ldots$, and will only later generalize to continuous spectra.

In the Weyl correspondence,[14] c-number phase-space kernels $a(x,p)$ of suitably ordered operators $\mathcal{A}(\mathcal{X},\mathcal{P})$ are defined by

$$a(x,p)\equiv\frac{1}{2\pi}\int \mathrm{d}y\, e^{-iyp}\left\langle x-\frac{\hbar}{2}y\right|\mathcal{A}(\mathcal{X},\mathcal{P})\left|x+\frac{\hbar}{2}y\right\rangle. \tag{4}$$

Conversely, the ordering of these operators is specified through

$$\mathcal{A}(\mathcal{X},\mathcal{P})=\frac{1}{(2\pi)^2}\int \mathrm{d}\tau\,\mathrm{d}\sigma\,\mathrm{d}x\,\mathrm{d}p\;a(x,p)\exp(i\tau(\mathcal{P}-p)+i\sigma(\mathcal{X}-x)). \tag{5}$$

An operator product then corresponds to a star-composition of these kernels,[1]

$$a(x,p)\star b(x,p)=\frac{1}{2\pi}\int \mathrm{d}y\,e^{-iyp}\left\langle x-\frac{\hbar}{2}y\right|\mathcal{A}(\mathcal{X},\mathcal{P})\mathcal{B}(\mathcal{X},\mathcal{P})\left|x+\frac{\hbar}{2}y\right\rangle. \tag{6}$$

Moyal[3] appreciated that the density matrix in this phase-space representation is a Hermitean generalization of the Wigner function:

$$\begin{aligned} f_{mn}(x,p)&\equiv\frac{1}{2\pi}\int \mathrm{d}y\,e^{-iyp}\left\langle x-\frac{\hbar}{2}y\right|\psi_n\rangle\langle\psi_m\left|x+\frac{\hbar}{2}y\right\rangle \\ &=\frac{1}{2\pi}\int \mathrm{d}y\,e^{-iyp}\psi_m^*\left(x-\frac{\hbar}{2}y\right)\psi_n\left(x+\frac{\hbar}{2}y\right)=f_{nm}^*(x,p), \end{aligned} \tag{7}$$

where the $\psi_m(x)$'s are (ortho-)normalized solutions of a Schrödinger problem. (Wigner[10] mainly considered the diagonal elements of the density matrix (pure states), usually denoted as $f_m \equiv f_{mm}$.) As a consequence, matrix elements of operators are produced by mere phase-space integrals,[3]

$$\langle\psi_m|\mathcal{A}|\psi_n\rangle=\int \mathrm{d}x\,\mathrm{d}p\;a(x,p)f_{mn}(x,p). \tag{8}$$

The standard machinery of density matrices then is readily transcribed in this language, e.g., the trace relation,[3]

$$\int \mathrm{d}x\,\mathrm{d}p\;f_{mn}(x,p)=\int \mathrm{d}x\;\psi_n^*(x)\psi_m(x)=\delta_{mn}; \tag{9}$$

and[8]

$$f_{mn}\star f_{kl}=\frac{1}{2\pi\hbar}\,\delta_{ml}f_{kn}=\frac{1}{h}\,\delta_{ml}f_{kn}. \tag{10}$$

Given (3), it follows from Eqs. (9) and (10) that[3]

$$\int \mathrm{d}x\,\mathrm{d}p\;f_{mn}(x,p)f_{lk}^*(x,p)=\frac{1}{2\pi\hbar}\,\delta_{ml}\delta_{nk}. \tag{11}$$

For complete sets of input wave functions, it also follows that[3]

$$\sum_{m,n} f_{mn}(x,p)f_{mn}^*(x',p')=\frac{1}{2\pi\hbar}\,\delta(x-x')\,\delta(p-p'). \tag{12}$$

An arbitrary phase-space function $\varphi(x,p)$ can thus be expanded as

$$\varphi(x,p)=\sum_{m,n} c_{mn}f_{mn}(x,p), \tag{13}$$

the coefficients being specified through (11),

$$c_{mn}=2\pi\hbar\int \mathrm{d}x\,\mathrm{d}p\;f_{mn}^*(x,p)\varphi(x,p). \tag{14}$$

Further note the resolution of the identity,[3]

$$\sum_n f_{nn}(x,p)=\frac{1}{2\pi\hbar}=\frac{1}{h}. \tag{15}$$

For instance, for eigenfunctions of the Hamiltonian $\mathcal{H}(\mathcal{X},\mathcal{P})$ with eigenvalues E_n, the corresponding WFs satisfy the following star-genvalue equations[8] (also see Refs. 11 and 4), with $H(x,p)$, the phase-space kernel of $\mathcal{H}(\mathcal{X},\mathcal{P})$:

$$H\star f_{mn}=E_n f_{mn}, \quad f_{mn}\star H=E_m f_{mn}. \tag{16}$$

The time dependence of a pure state WF is given by Moyal's dynamical equation:[3]

$$i\hbar\frac{\partial}{\partial t}f(x,p;t)=H\star f(x,p;t)-f(x,p;t)\star H. \tag{17}$$

By virtue of the $\star$-unitary evolution operator (a "$\star$-exponential"[2]),

$$U_\star(x,p;t)=e_\star^{itH/\hbar}\equiv 1+(it/\hbar)H(x,p)+\frac{(it/\hbar)^2}{2!}H\star H+\frac{(it/\hbar)^3}{3!}H\star H\star H+\cdots, \tag{18}$$

the time-evolved WF is obtained formally in terms of the WF at $t=0$,

$$f(x,p;t)=U_\star^{-1}(x,p;t)\star f(x,p;0)\star U_\star(x,p;t). \tag{19}$$

(These associative combinatoric operations completely parallel those of operators in the conventional formulation of quantum mechanics in Hilbert space.[15]) Just like any star-function of H, this $\star$-exponential can be computed,[16]

$$\exp_\star(itH/\hbar)=\exp_\star(itH/\hbar)\star 1=\exp_\star(itH/\hbar)\star 2\pi\hbar\sum_n f_{nn}=2\pi\hbar\sum_n e^{itE_n/\hbar}f_{nn}. \tag{20}$$

(Of course, for $t=0$, the obvious identity resolution is recovered.)

For continuous spectra, the sums in the above-mentioned relations extend to integrals over a continuous parameter (the energy), and the Kronecker δ_{mn}'s into δ-functions (these last ones reflecting the infinite normalizations of unnormalizable states). For example, Eqs. (9) and (11) extend to

$$\int \mathrm{d}x\,\mathrm{d}p\, f_{E_1E_2}(x,p)=\delta(E_1-E_2), \tag{21}$$

$$\int \mathrm{d}x\,\mathrm{d}p\, f_{E_1E_2}(x,p)f^*_{E_1'E_2'}(x,p)=\frac{1}{2\pi\hbar}\,\delta(E_1-E_1')\,\delta(E_2-E_2'). \tag{22}$$

Completeness (12) extends to

$$\int \mathrm{d}E_1\,\mathrm{d}E_2\, f_{E_1E_2}(x,p)f^*_{E_1E_2}(x',p')=\frac{1}{2\pi\hbar}\,\delta(x-x')\,\delta(p-p'). \tag{23}$$

More generally, (10) extends to

$$f_{E_1E_2}\star f_{E_1'E_2'}=\frac{1}{2\pi\hbar}\,\delta(E_1-E_2')f_{E_1'E_2}. \tag{24}$$

Finally, Eq. (15) extends to

$$\frac{1}{2\pi\hbar}=\frac{1}{2\pi}\int \mathrm{d}y\, e^{-ipy}\int \mathrm{d}E\left\langle x-\frac{\hbar y}{2}\middle|E\right\rangle\left\langle E\middle|x+\frac{\hbar y}{2}\right\rangle=\int \mathrm{d}E\, f_{EE}(x,p), \tag{25}$$

and hence (20) extends to

$$\exp_\star(itH/\hbar)=2\pi\hbar\int \mathrm{d}E\, e^{itE/\hbar} f_{EE}(x,p). \tag{26}$$

III. GENERATING FUNCTIONS FOR THE HARMONIC OSCILLATOR

Consider the harmonic oscillator,

$$H(x,p)=\tfrac{1}{2}(p^2+x^2), \tag{27}$$

where, without loss of generality, parameters have been absorbed in the phase space variables: $m=1$, $\omega=1$. Further recall that the normalized eigenfunctions of the corresponding operator Hamiltonian $\mathcal{H}$ are $\psi_n(x)=(\sqrt{\pi}2^n n!)^{-1/2}e^{-(1/2)x^2}H_n(x)$, for the eigenvalues $E_n=\hbar(n+1/2)$. Define a radial and an angular variable,

$$z\equiv 4H=2(x^2+p^2),\quad \tan\theta=\frac{p}{x}, \tag{28}$$

so that

$$a\sqrt{2}\equiv(x+ip)=|x+ip|e^{i\theta}=\left(\frac{z}{2}\right)^{1/2}e^{i\theta}. \tag{29}$$

Groenewold,[1] as well as Bartlett and Moyal,[17] have worked out the complete sets of solutions to Moyal's time-evolution equation (17), which are all linear combinations of terms $\exp(it(m-n))f_{mn}$. They solved that equation indirectly, by evaluating the integrals (7) for time-dependent Hermite wave functions, which yield generalized Laguerre polynomial-based functions. More directly, Fairlie[8] dramatically simplified the derivation of the solution by relying on his fundamental equation (16). He thus confirmed Groenewold's WFs,[1,17]

$$f_{mn}(x,p)=\frac{(-1)^m}{\pi}\sqrt{\frac{m!}{n!}}z^{(n-m)/2}e^{-z/2}e^{i(n-m)\theta}L_m^{n-m}(z). \tag{30}$$

The special case of diagonal elements,

$$f_n\equiv f_{nn}=\frac{(-1)^n}{\pi}e^{-z/2}L_n(z), \tag{31}$$

constitutes the time-independent ''$\star$-genfunctions'' of the oscillator hamiltonian kernel[4] [i.e., the complete set of solutions of the time-independent Moyal equation $H\star f-f\star H=0$, where $H\star f_n=E_n f_n$. Incidentally, (10) restricted to diagonal WFs closes them under $\star$-multiplication,[12] $f_m\star f_n=\delta_{mn}f_m/(2\pi\hbar)$.] That is to say, ''radially symmetric'' phase-space functions, i.e., functions that only depend on z but not θ, can be expanded in terms of merely these diagonal elements—unlike the most general functions in phase space which require the entire set of off-diagonal f_{mn} above for a complete basis. Note, however, that all $\star$-products of such radially symmetric functions are commutative, since, manifestly,

$$\sum_n c_n f_n\star\sum_m d_m f_m=\sum_m d_m f_m\star\sum_n c_n f_n. \tag{32}$$

Moreover, the $\star$-exponential (20) for this set of $\star$-genfunctions is directly seen to amount to

$$\exp_\star(itH/\hbar)=\left(\cos\left(\frac{t}{2}\right)\right)^{-1}\exp\left(\frac{2i}{\hbar}H\tan\left(\frac{t}{2}\right)\right), \tag{33}$$

which is, to say, a Gaussian in phase space.[2] As an application, note that the hyperbolic tangent $\star$-composition law of Gaussians follows trivially, since these amount to $\star$-exponentials with additive time intervals, $\exp_\star(tf)\star\exp_\star(Tf)=\exp_\star((t+T)f)$,[2]

$$\exp\left(-\frac{a}{\hbar}(x^2+p^2)\right)\star\exp\left(-\frac{b}{\hbar}(x^2+p^2)\right)=\frac{1}{1+ab}\exp\left(-\frac{a+b}{\hbar(1+ab)}(x^2+p^2)\right). \tag{34}$$

We now introduce the following generating function for the entire set of generalized Wigner functions:

$$G(\alpha,\beta;x,p)\equiv\sum_{m,n}\frac{\alpha^m}{\sqrt{m!}}\frac{\beta^n}{\sqrt{n!}}f_{mn}=\frac{1}{\pi}\sum_n\ \beta^n\frac{1}{n!}z^{n/2}e^{-z/2}e^{in\theta}\sum_m\ (-z^{-1/2}e^{-i\theta}\alpha)^m L_m^{n-m}(z). \tag{35}$$

Utilizing the identity[18] 8.975.2,

$$\sum_{m=0}^{\infty}L_m^{n-m}(z)k^m=e^{-zk}(1+k)^n, \tag{36}$$

we obtain

$$\begin{aligned}G(\alpha,\beta;x,p)&=\frac{1}{\pi}e^{-z/2}\sum_n\ \frac{1}{n!}(\beta\sqrt{z}e^{i\theta})^n e^{-z(-z^{-1/2}e^{-i\theta}\alpha)}(1-z^{-1/2}e^{-i\theta}\alpha)^n\\&=\frac{1}{\pi}e^{-z/2}\sum_n\ \frac{1}{n!}(\beta\sqrt{z}e^{i\theta}-\alpha\beta)^n e^{\sqrt{z}e^{-i\theta}\alpha}=\frac{1}{\pi}e^{-z/2}e^{\beta\sqrt{z}e^{i\theta}-\alpha\beta}e^{\sqrt{z}e^{-i\theta}\alpha}.\end{aligned} \tag{37}$$

Thus,

$$G(\alpha,\beta;x,p)=\frac{1}{\pi}\exp\left(\sqrt{z}\,(\alpha e^{-i\theta}+\beta e^{i\theta})-\alpha\beta-\frac{z}{2}\right). \tag{38}$$

Since

$$\sqrt{z}\,(\alpha e^{-i\theta}+\beta e^{i\theta})=\sqrt{2}(\alpha+\beta)x-\sqrt{2}ip(\alpha-\beta), \tag{39}$$

one can re-express:

$$G(\alpha,\beta;x,p)=G^*(\beta,\alpha;x,p)=\frac{1}{\pi}\exp\left(\alpha\beta-\left(x-\frac{\alpha+\beta}{\sqrt{2}}\right)^2-\left(p+i\frac{\alpha-\beta}{\sqrt{2}}\right)^2\right). \tag{40}$$

As the name implies, from $G(\alpha,\beta;x,p)$, the f_{mn}'s are generated by

$$f_{mn}(x,p)=\frac{1}{\sqrt{m!n!}}\frac{\partial^m}{\partial\alpha^m}\frac{\partial^n}{\partial\beta^n}G(\alpha,\beta;x,p)\bigg|_{\alpha=\beta=0}. \tag{41}$$

These functions $\star$-compose as

$$G(\alpha,\beta)\star G(\epsilon,\zeta)=\frac{e^{\alpha\zeta}}{2\pi\hbar}G(\epsilon,\beta). \tag{42}$$

The phase-space trace is

$$\int \mathrm{d}x\,\mathrm{d}p\,G(\alpha,\beta)=e^{\alpha\beta}. \tag{43}$$

By (16), the action of the Hamiltonian kernel on this function is

$$H\star G=\hbar\left(\frac{1}{2}+\beta\frac{\partial}{\partial\beta}\right)G=\hbar\left(\frac{1}{2}-\alpha\beta+\beta\sqrt{z}e^{i\theta}\right)G, \tag{44}$$

and

$$G\star H=\hbar\left(\frac{1}{2}+\alpha\frac{\partial}{\partial\alpha}\right)G=\hbar\left(\frac{1}{2}-\alpha\beta+\alpha\sqrt{z}e^{-i\theta}\right)G. \tag{45}$$

Consequently,

$$\int \mathrm{d}x\,\mathrm{d}p\,H\star G(\alpha,\beta)=\hbar\left(\frac{1}{2}+\beta\frac{\partial}{\partial\beta}\right)e^{\alpha\beta}=\hbar\left(\frac{1}{2}+\alpha\beta\right)e^{\alpha\beta}. \tag{46}$$

The spectrum then follows by operating on both sides of this equation,

$$E_n=\frac{1}{n!}\frac{\partial^n}{\partial\alpha^n}\frac{\partial^n}{\partial\beta^n}\int \mathrm{d}x\,\mathrm{d}p\,H\star G(\alpha,\beta)\Big|_{\alpha=\beta=0}=\frac{\hbar}{n!}\frac{\partial^n}{\partial\alpha^n}\frac{\partial^n}{\partial\beta^n}\left(\frac{1}{2}+\alpha\beta\right)e^{\alpha\beta}\Big|_{\alpha=\beta=0}=\hbar\left(\frac{1}{2}+n\right). \tag{47}$$

In general, matrix elements of operators may be summarized compactly through this generating function in phase space.

This generating function could be interpreted as a phase-space coherent state, or the off-diagonal WF of coherent states, as discussed in Appendix A,[19]

$$G(\alpha,\beta;x,p)=\exp_\star(\beta a^\dagger)f_0\exp_\star(\alpha a), \tag{48}$$

$$\begin{aligned} &a\star G(\alpha,\beta)=\hbar\beta G(\alpha,\beta),\quad a^\dagger\star G(\alpha,\beta)=\frac{\partial}{\partial\beta}G(\alpha,\beta),\\ &G(\alpha,\beta)\star a=\frac{\partial}{\partial\alpha}G(\alpha,\beta),\quad G(\alpha,\beta)\star a^\dagger=\hbar\alpha G(\alpha,\beta), \end{aligned} \tag{49}$$

and hence Eqs. (44) and (45) amount to

$$\begin{aligned} H\star G(\alpha,\beta)&=\left(a^\dagger\star a+\frac{\hbar}{2}\right)\star G(\alpha,\beta)=\hbar\left(\beta\frac{\partial}{\partial\beta}+\frac{1}{2}\right)G(\alpha,\beta),\\ G(\alpha,\beta)\star H&=G(\alpha,\beta)\star\left(a^\dagger\star a+\frac{\hbar}{2}\right)=\hbar\left(\alpha\frac{\partial}{\partial\alpha}+\frac{1}{2}\right)G(\alpha,\beta). \end{aligned} \tag{50}$$

This formalism finds application in, e.g., perturbation theory in phase space, cf. Appendix B.

IV. GENERATING FUNCTIONS FOR THE LINEAR POTENTIAL

The linear potential in phase space has been addressed[11] (also see Refs. 19 and 4). We shall adopt the simplified conventions of Ref. 4, i.e., $m=1/2$, $\hbar=1$. The Hamiltonian kernel is then

$$H(x,p)=p^2+x, \tag{51}$$

and the eigenfunctions of $\mathcal{H}$ are Airy functions,

$$\psi_E(x)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}X\, e^{iX(E-x-X^2/3)}=\mathrm{Ai}(x-E), \tag{52}$$

indexed by the continuous energy E. The spectrum being continuous, the Airy functions are not square integrable, but have continuum normalization, $\int \mathrm{d}x\, \psi^*_{E_1}(x)\psi_{E_2}(x)=\delta(E_1-E_2)$, instead. Thus, (21) *et seq.* are now operative. The generalized WFs are[11]

$$\begin{aligned} f_{E_1E_2}(x,p)&=\frac{1}{4\pi^2}\int \mathrm{d}z \exp\left(iz\left(\frac{E_1+E_2}{2}-x-p^2-z^2/12\right)\right)\exp(ip(E_1-E_2))\\ &=\exp(ip(E_1-E_2))\frac{2^{2/3}}{2\pi}\mathrm{Ai}\left(2^{2/3}\left(x+p^2-\frac{E_1+E_2}{2}\right)\right). \end{aligned} \tag{53}$$

The $\star$-exponential (26) then is again a plain exponential of the shifted Hamiltonian kernel,

$$\exp_\star(it(x+p^2))=2\pi\int_{-\infty}^{\infty}\mathrm{d}E\, e^{iEt}\frac{2^{2/3}}{2\pi}\mathrm{Ai}\left(2^{2/3}\left(x+p^2-\frac{E_1+E_2}{2}\right)\right)=\exp(it(x+p^2+t^2/12)). \tag{54}$$

(This could also be derived directly, as the CBH expansion simplifies dramatically in this case, cf. Appendix C.) As before, the $\star$-composition law for plain exponentials of the hamiltonian kernel function follows,

$$\exp(a(x+p^2))\star\exp(b(x+p^2))=\exp((a+b)(x+p^2-\tfrac{1}{4}ab)). \tag{55}$$

Since the complete basis Wigner functions are now indexed continuously, a generating function for them must rely on an integral instead of an infinite sum. The simplest transform is possibly a double Fourier transform with respect to the energy indices [but note the transform factors $\exp(iE_1X)$, $\exp(-iE_2Y)$ may also be regarded as plane waves]. Suitably normalized,

$$\begin{aligned} G(X,Y;x,p)&\equiv 2\pi\int_{-\infty}^{+\infty}\mathrm{d}E_1\int_{-\infty}^{+\infty}\mathrm{d}E_2\left(\frac{1}{\sqrt{2\pi}}e^{iE_1X}\right)f_{E_1E_2}(x,p)\left(\frac{1}{\sqrt{2\pi}}e^{-iE_2Y}\right)\\ &=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}E_1\int_{-\infty}^{+\infty}\mathrm{d}E_2\, e^{i(E_1-E_2)\,p+iE_1X-iE_2Y}2^{2/3}\mathrm{Ai}\left(2^{2/3}\left(x+p^2-\frac{E_1+E_2}{2}\right)\right)\\ &=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}E\int_{-\infty}^{+\infty}\mathrm{d}\omega\, e^{i\omega\, p+i(E+\omega/2)X-i(E-\omega/2)Y}2^{2/3}\mathrm{Ai}(2^{2/3}(x+p^2-E))\\ &=\delta\left(p+\frac{X+Y}{2}\right)\int_{-\infty}^{+\infty}\mathrm{d}E\, e^{iE(X-Y)}2^{2/3}\mathrm{Ai}(2^{2/3}(x+p^2-E))\\ &=\delta\left(p+\frac{X+Y}{2}\right)\int_{-\infty}^{+\infty}\mathrm{d}E\, e^{iE(X-Y)}\frac{1}{2\pi}\int \mathrm{d}z\, e^{iz(E-x-p^2-z^2/12)} \end{aligned}$$

$$= \delta\left(p + \frac{X+Y}{2}\right) e^{i(X-Y)(x+p^2+(X-Y)^2/12)}. \tag{56}$$

The phase-space trace is

$$\int \mathrm{d}x\, \mathrm{d}p\, G(X,Y;x,p) = 2\pi\delta(X-Y), \tag{57}$$

and, given (24) for these functions, $f_{E_1E_2} \star f_{E_1'E_2'} = (1/2\pi)\,\delta(E_1-E_2')f_{E_1'E_2}$, the $\star$-composition law for these G's is

$$G(X,Y;x,p) \star G(W,Z;x,p) = \delta(X-Z)G(W,Y;x,p). \tag{58}$$

V. GENERATING FUNCTIONS FOR THE LIOUVILLE POTENTIAL

A less trivial system with a continuous spectrum is the Hamiltonian with the Liouville potential.[20,21] In the conventions of Ref. 4 ($\hbar=1$, $m=1/2$), the Hamiltonian kernel is

$$H = p^2 + e^{2x}, \tag{59}$$

and the eigenfunctions of the corresponding $\mathcal{H}$ are

$$\psi_E(x) = \psi_E^*(x) = \frac{1}{\pi}\sqrt{\sinh(\pi\sqrt{E})}K_{i\sqrt{E}}(e^x), \tag{60}$$

with continuum normalizations $\int \mathrm{d}x\, \psi_{E_1}^*(x)\psi_{E_2}(x) = \delta(E_1-E_2)$. The modified Bessel function (Ref. 22, Chap. VI, Sec. 6.22) can be written in the Heine–Schläfli form,

$$K_{ip}(e^x) = \frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}X\, \exp(-e^x\cosh X + iXp) = K_{-ip}(e^x). \tag{61}$$

The nondiagonal WF is then

$$f_{E_1E_2}(x,p) = \frac{1}{\pi^3}\int \mathrm{d}y\, e^{-2ipy}\sqrt{\sinh(\pi\sqrt{E_1})}K^*_{i\sqrt{E_1}}(e^{x-y})\sqrt{\sinh(\pi\sqrt{E_2})}K_{i\sqrt{E_2}}(e^{x+y}). \tag{62}$$

This Wigner function amounts to Meijer's G function,

$$f_{E_1E_2}(x,p) = \frac{1}{8\pi^3}\sqrt{\sinh(\pi\sqrt{E_1})\sinh(\pi\sqrt{E_2})} \times G^{40}_{04}\left(\frac{e^{4x}}{16}\middle| \frac{ip+i\sqrt{E_1}}{2}, \frac{ip-i\sqrt{E_1}}{2}, \frac{-ip+i\sqrt{E_2}}{2}, \frac{-ip-i\sqrt{E_2}}{2}\right). \tag{63}$$

Alternatively, the WF may be written as a double integral representation,

$$f_{E(k)\,E(q)}(x,p) = \frac{1}{2\pi^3}\sqrt{\sinh(\pi\sqrt{E(k)})\sinh(\pi\sqrt{E(q)})} \times \int \mathrm{d}X\, \mathrm{d}Y\, e^{ikX}\, e^{iqY}\left(\frac{\cosh Y}{\cosh X}\right)^{ip} K_{2ip}(e^x\sqrt{4\cosh X\cosh Y}), \tag{64}$$

where $E(k)\equiv k^2$, $E(q)\equiv q^2$. This is an inverse integral transform, as in Sec. IV, of a generating function

$$G(X,Y;x,p)\equiv\int_{-\infty}^{\infty}\frac{\mathrm{d}k}{\sqrt{\sinh(\pi\sqrt{E(k)})}}\int_{-\infty}^{\infty}\frac{\mathrm{d}q}{\sqrt{\sinh(\pi\sqrt{E(q)})}}e^{-ikX}e^{-iqY}f_{E(k)\,E(q)}(x,p)$$
$$=\frac{2}{\pi}\left(\frac{\cosh Y}{\cosh X}\right)^{ip}K_{2ip}(e^{x}\sqrt{4\cosh X\cosh Y})=G^{*}(Y,X;x,p). \tag{65}$$

The form and construction of this G are consequences of (61), as detailed in Appendix D.

However, the $\star$-composition law of this particular generating function is not so straightforward. It is singular, as a consequence of the general relation (24) and the behavior of the integrand in (65) as $k,q\to 0$.

The singularity may be controlled by regulating the $\star$-product through imaginary shifts in the momenta,

$$G\left(X,Y;x,p-\frac{i\epsilon}{2}\right)\star G\left(W,Z;x,p+\frac{i\epsilon}{2}\right)=\frac{1}{2\pi}G(W,Y;x,p)\Gamma(\epsilon)\left(e^{x}\sqrt{\frac{\cosh Y\cosh W}{\cosh X\cosh Z}}(\cosh X+\cosh Z)\right)^{-\epsilon}.$$

It follows that one derivative with respect to either of X or Z suffices to eliminate the divergence at $\epsilon=0$,

$$\lim_{\epsilon\to 0}\partial_{X}G\left(X,Y;x,p-\frac{i\epsilon}{2}\right)\star G\left(W,Z;x,p+\frac{i\epsilon}{2}\right)$$
$$=\frac{1}{2\pi}G(W,Y;x,p)(-\partial_{X})\ln\left(e^{x}\sqrt{\frac{\cosh Y\cosh W}{\cosh X\cosh Z}}(\cosh X+\cosh Z)\right)$$
$$=\frac{1}{2\pi}G(W,Y;x,p)\left(\frac{1}{2}\tanh X-\frac{\sinh X}{\cosh X+\cosh Z}\right).$$

Unlike the situation in (58), here the right-hand side vanishes at $X=Z$. More symmetrically,

$$\lim_{\epsilon\to 0}\partial_{X}G\left(X,Y;x,p-\frac{i\epsilon}{2}\right)\star\partial_{W}G\left(W,Z;x,p+\frac{i\epsilon}{2}\right)=\frac{1}{2\pi}\partial_{W}G(W,Y;x,p)\left\{\frac{1}{2}\tanh X-\frac{\sinh X}{\cosh X+\cosh Z}\right\}.$$

By some contrast to the above, Eq. (65), an alternate generating function for just the diagonal WFs, $f_{EE}\equiv f_{E}$, could be defined through the spectral resolution of the $\star-K$ function,

$$\mathcal{G}(z;x,p)\equiv K_{\star\, i\sqrt{H(x,p)}}(e^{z})=2\pi\int_{0}^{\infty}\mathrm{d}E\,K_{i\sqrt{E}}(e^{z})\,f_{E}(x,p). \tag{66}$$

This can be evaluated by reliance on Macdonald's trilinear identity,[22,23]

$$\int_{0}^{\infty}\mathrm{d}E\,K_{i\sqrt{E}}(e^{z})\psi_{E}(x)\,\psi_{E}^{*}(y)=\frac{1}{2}\exp\left(-\frac{1}{2}(e^{x+y-z}+e^{x-y+z}+e^{-x+y+z})\right). \tag{67}$$

$\mathcal{G}$ then is obtained by replacing $x\to x+Y$ and $y\to x-Y$, and Fourier transforming by $(1/\pi)\int\mathrm{d}Y\,e^{-2ipY}$,

$$\int_0^\infty \mathrm{d}E\, K_{i\sqrt{E}}(e^z)\, f_E(x,p) = \frac{1}{2\pi}\int \mathrm{d}Y\, e^{-2ipY} \exp\left(-\frac{1}{2}(e^{2x-z}+e^{z+2Y}+e^{z-2Y})\right). \tag{68}$$

Finally, simplifying the right-hand side gives

$$\begin{aligned} 2\pi\int_0^\infty \mathrm{d}E\, K_{i\sqrt{E}}(e^z)\, f_E(x,p) &= \exp\left(-\frac{1}{2}e^{2x-z}\right)\int \mathrm{d}Y\, e^{-2ipY}\exp\left(-\frac{1}{2}e^z(e^{2Y}+e^{-2Y})\right) \\ &= \exp(-\tfrac{1}{2}e^{2x-z})K_{ip}(e^z) = \mathcal{G}(z;x,p). \end{aligned} \tag{69}$$

As a side check of this expression, (69), note that it must satisfy

$$H\star\mathcal{G}(z;x,p) = \mathcal{G}(z;x,p)\star H = (-\partial_z^2+e^{2z})\mathcal{G}(z;x,p), \tag{70}$$

which follows from the spectral resolution evident in (66). Indeed, since $e^{-z}\partial_z K_{ip}(e^z) = ipe^{-z}K_{ip}(e^z) - K_{ip+1}(e^z)$, and $(-\partial_z^2+e^{2z})K_{ip}(e^z) = p^2K_{ip}(e^z)$, these relations are satisfied,

$$\begin{aligned} (p^2+e^{2x})\star(\exp(-\tfrac{1}{2}e^{2x-z})K_{ip}(e^z)) &= (\exp(-\tfrac{1}{2}e^{2x-z})K_{ip}(e^z))\star(p^2+e^{2x}) \\ &= \exp(-\tfrac{1}{2}e^{2x-z})(-e^{2x-z}\,\partial_z K_{ip}(e^z)) \\ &\quad + (p^2+\tfrac{1}{2}e^{2x-z}-\tfrac{1}{4}e^{4x-2z})\exp(-\tfrac{1}{2}e^{2x-z})K_{ip}(e^z) \\ &= (-\partial_z^2+e^{2z})(\exp(-\tfrac{1}{2}e^{2x-z})K_{ip}(e^z)). \end{aligned} \tag{71}$$

Parenthetically, as an alternative to the ordinary product form in (69), the phase-space kernel $\mathcal{G}$ may also be represented as an integral either of a $\star$-exponential or of a single $\star$-product (Note: Do not shift the integration parameter y by the phase-space variable x before the star products are evaluated.),

$$\begin{aligned} \mathcal{G}(z;x,p) &= \frac{1}{2}\int \mathrm{d}y\, \exp_\star\left(-\frac{y}{2\sinh y}e^{2x-z}+iyp-e^z\cosh y\right) \\ &= \frac{1}{2}\int \mathrm{d}y\, \exp\left(-\frac{1}{2}e^{y-z}e^{2x}\right)\star\exp(iyp-e^z\cosh y). \end{aligned} \tag{72}$$

This follows from the identities (cf. Appendix C)

$$\exp_\star\left(-\frac{y}{2\sinh y}e^{2x-z}+iyp\right) = \exp\left(-\frac{1}{2}e^{y-z}e^{2x}\right)\star\exp(iyp) = \exp\left(-\frac{1}{2}e^{2x-z}+iyp\right). \tag{73}$$

The ordinary product form in (69) and the $\star$-exponential form in (72) reveal that $\mathcal{G}(z;x,p) = \mathcal{G}(z;x,-p)$, so one may replace $\exp(iyp)$ by $\cos(yp)$ in the second line of (72). Given these, there are several ways to verify (70). These relations and the star-product expressions for the kernel in (72) are isomorphic to those of the corresponding operators, as discussed in Appendix E.

The $\star$-composition law of these generating functions follows from (24) and Macdonald's identity,

$$\mathcal{G}(u;x,p)\star\mathcal{G}(v;x,p) = \frac{1}{2}\int \mathrm{d}w\, \exp\left(-\frac{1}{2}(e^{u+v-w}+e^{u-v+w}+e^{-u+v+w})\right)\mathcal{G}(w;x,p). \tag{74}$$

This also follows directly from the explicit form (69). Again, this is isomorphic to the corresponding operator composition law given in Appendix E.

From the orthogonality of the ψ_E's, the diagonal WFs may be recovered by inverse transformation,

$$f_E(x,p)=\int \mathrm{d}z\,\frac{\sinh(\pi\sqrt{E})}{2\pi^3}K_{i\sqrt{E}}(e^z)\mathcal{G}(z;x,p). \tag{75}$$

This representation and the specific factorized x,p-dependence of $\mathcal{G}$ can be of considerable use, e.g., in systematically computing diagonal matrix elements in phase space.

In illustration of the general pattern, consider the first-order energy shift effected by a perturbation Hamiltonian kernel H_1. It is, cf. Appendix B, Eq. (B11),

$$\Delta E=\int \mathrm{d}z\,\mathrm{d}x\,\mathrm{d}p\,H_1\frac{\sinh(\pi\sqrt{E})}{2\pi^3}K_{i\sqrt{E}}(e^z)\mathcal{G}(z;x,p). \tag{76}$$

Choosing

$$H_1=e^{2nx}e^{isp/2}, \tag{77}$$

yields

$$\Delta E=\frac{\sinh(\pi\sqrt{E})}{2\pi^3}\int \mathrm{d}z\,K_{i\sqrt{E}}(e^z)\left(\int \mathrm{d}x\,e^{2nx}\exp\left(-\frac{1}{2}e^{2x-z}\right)\right)\left(\int \mathrm{d}p\,K_{ip}(e^z)\,e^{isp/2}\right). \tag{78}$$

Now,

$$\int \mathrm{d}x\,e^{2nx}\exp\left(-\frac{1}{2}e^{2x-z}\right)=2^{n-1}\Gamma(n)\,e^{nz}, \tag{79}$$

and hence (Ref. 18, 6.576.4, $a=b$),

$$\begin{aligned}\int \mathrm{d}z\,K_{i\sqrt{E}}(e^z)\,K_{ip}(e^z)\,e^{nz}=&\frac{2^{n-3}}{\Gamma(n)}\Gamma\left(\frac{n+i\sqrt{E}+ip}{2}\right)\Gamma\left(\frac{n+i\sqrt{E}-ip}{2}\right)\\&\times\Gamma\left(\frac{n-i\sqrt{E}+ip}{2}\right)\Gamma\left(\frac{n-i\sqrt{E}-ip}{2}\right).\end{aligned} \tag{80}$$

Thus,

$$\begin{aligned}\Delta E=&\frac{\sinh(\pi\sqrt{E})}{2\pi^3}4^{n-2}\int \mathrm{d}p\,e^{isp/2}\Gamma\left(\frac{n+i\sqrt{E}+ip}{2}\right)\\&\times\Gamma\left(\frac{n+i\sqrt{E}-ip}{2}\right)\Gamma\left(\frac{n-i\sqrt{E}+ip}{2}\right)\Gamma\left(\frac{n-i\sqrt{E}-ip}{2}\right).\end{aligned} \tag{81}$$

Finally (Ref. 18, 6.422.19),

$$\begin{aligned}&\int \mathrm{d}p\,e^{isp/2}\Gamma\left(\frac{n+i\sqrt{E}+ip}{2}\right)\Gamma\left(\frac{n+i\sqrt{E}-ip}{2}\right)\Gamma\left(\frac{n-i\sqrt{E}+ip}{2}\right)\Gamma\left(\frac{n-i\sqrt{E}-ip}{2}\right)\\&=4\pi\,G^{22}_{22}\left(e^s\left|\begin{matrix}\frac{2-n+i\sqrt{E}}{2},\frac{2-n-i\sqrt{E}}{2}\\ \frac{n+i\sqrt{E}}{2},\frac{n-i\sqrt{E}}{2}\end{matrix}\right.\right).\end{aligned} \tag{82}$$

To sum up, the perturbed energy shift is a Meijer function,

$$\Delta E = \frac{4^n \sinh(\pi\sqrt{E})}{8\pi^2} G^{22}_{22}\left(e^s \left| \begin{matrix} \frac{2-n+i\sqrt{E}}{2}, \frac{2-n-i\sqrt{E}}{2} \\ \frac{n+i\sqrt{E}}{2}, \frac{n-i\sqrt{E}}{2} \end{matrix} \right. \right). \tag{83}$$

In principle, any polynomial perturbation in either x or p can be obtained from this, by differentiation with respect to n and s. (Retaining a bit of exponential in x would be helpful to suppress the region of large negative x).

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APPENDIX A: ⋆-FOCK SPACE AND COHERENT STATES

Dirac's Hamiltonian factorization method for algebraic solution of the harmonic oscillator carries through (cf. Ref. 2) intact in ⋆-space. Indeed,

$$H = \frac{1}{2}(x-ip)\star(x+ip) + \frac{\hbar}{2}, \tag{A1}$$

motivating definition of

$$a \equiv \frac{1}{\sqrt{2}}(x+ip), \quad a^\dagger \equiv \frac{1}{\sqrt{2}}(x-ip). \tag{A2}$$

Thus, noting

$$a\star a^\dagger - a^\dagger \star a = \hbar, \tag{A3}$$

and also that, by above,

$$a\star f_0 = \frac{1}{\sqrt{2}}(x+ip)\star e^{-(x^2+p^2)} = 0, \tag{A4}$$

provides a ⋆-Fock vacuum, it is evident that associativity of the ⋆-product permits the entire ladder spectrum generation to go through as usual. The ⋆-genstates of the Hamiltonian, such that $H\star f = f\star H$, are thus

$$f_{nn} = f_n = \frac{1}{n!}(a^\dagger\star)^n f_0 (\star a)^n. \tag{A5}$$

These states are real, like the Gaussian ground state, and are thus left-right symmetric ⋆-genstates. They are also transparently ⋆-orthogonal for different eigenvalues; and they project to themselves, as they should, since the Gaussian ground state does, $f_0\star f_0 = f_0/2\pi\hbar$.

The complete set of generalized WFs can thus be written as

$$f_{mn} = \frac{1}{\sqrt{n!m!}}(a^\dagger\star)^n f_0 (\star a)^m, \quad m,n = 0,1,2,3,\cdots. \tag{A6}$$

The standard combinatoric features of conventional Fock space apply separately to left and right (its adjoint) $\star$-multiplication:

$$a\star f_n \equiv a\star f_{nn} = \hbar\sqrt{n} f_{n,n-1}, \quad a^\dagger\star a\star f_n = \hbar\sqrt{n} a^\dagger\star f_{n,n-1} = \hbar n f_n,$$

$$a^\dagger\star f_n \equiv a^\dagger\star f_{nn} = \sqrt{n+1} f_{n,n+1}, \tag{A7}$$

$$a\star a^\dagger\star f_n = \sqrt{n+1} a\star f_{n,n+1} = \hbar(n+1) f_n,$$

$$f_n\star a = \sqrt{n+1} f_{n+1,n},$$

$$f_n\star a\star a^\dagger = \hbar(n+1) f_n, \tag{A8}$$

$$f_n\star a^\dagger = \hbar\sqrt{n} f_{n-1,n}, \quad f_n\star a^\dagger\star a = \hbar n f_n.$$

Furthermore, a left/right (non-self-adjoint) coherent state is naturally defined[19,24]

$$\Phi(\alpha,\beta) = \exp_\star(\alpha a^\dagger) f_0 \exp_\star(\beta a), \quad a\star\Phi(\alpha,\beta) = \alpha\Phi(\alpha,\beta), \quad \Phi(\alpha,\beta)\star a^\dagger = \beta\Phi(\alpha,\beta). \tag{A9}$$

Up to a factor of $\exp((|\alpha|^2+|\beta|^2)/2)$, this is also the WF of coherent states $|\alpha\rangle$ and $\langle\beta|$.[24] As indicated in the text, this coherent state is identifiable with the generating function G for the harmonic oscillator.

APPENDIX B: STATIONARY PERTURBATION THEORY

Perturbation theory could be carried out in Hilbert space and its resulting wave functions utilized to evaluate the corresponding WF integrals. However, in the spirit of logical autonomy of Moyal's formulation of quantum mechanics in phase space, the perturbed Wigner functions may also be computed *ab initio* in phase space,[17,25] without reference to the conventional Hilbert space formulation. The basics are summarized in the following.

As usual, the Hamiltonian kernel decomposes into free and perturbed parts,

$$H = H_0 + \lambda H_1. \tag{B1}$$

Fairlie's stationary, real, $\star$-genvalue equations[8,4] for the full Hamiltonian,

$$H(x,p)\star f_n(x,p) = f_n(x,p)\star H(x,p) = E_n(\lambda) f_n(x,p), \tag{B2}$$

are solved upon expansion of their components E and f in powers of λ, the perturbation strength,

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots, \tag{B3}$$

$$f_n = f_n^0 + \lambda f_n^1 + \lambda^2 f_n^2 + \cdots. \tag{B4}$$

Note the superscripts on E and f are order indices and not exponents. Resolution into individual powers of λ yields the real equations:

$$H_0\star f_n^0 = f_n^0\star H_0 = E_n^0 f_n^0, \tag{B5}$$

$$H_0\star f_n^1 + H_1\star f_n^0 = f_n^1\star H_0 + f_n^0\star H_1 = E_n^0 f_n^1 + E_n^1 f_n^0, \tag{B6}$$

$$H_0\star f_n^2 + H_1\star f_n^1 = f_n^2\star H_0 + f_n^1\star H_1 = E_n^0 f_n^2 + E_n^1 f_n^1 + E_n^2 f_n^0. \tag{B7}$$

Left multiplication of (B6) by $f_n^0\star$ yields

$$f_n^0\star H_0\star f_n^1 + f_n^0\star H_1\star f_n^0 = E_n^0 f_n^0\star f_n^1 + E_n^1 f_n^0\star f_n^0, \tag{B8}$$

and, by (B5),

$$f_n^0 \star H_1 \star f_n^0 = E_n^1 f_n^0 \star f_n^0; \tag{B9}$$

by (11), (10), and the cyclicity of the trace (3),

$$\int \mathrm{d}x\, \mathrm{d}p\, E_n^1 f_n^0 \star f_n^0 = \int \mathrm{d}x\, \mathrm{d}p (f_n^0 \star H_1 \star f_n^0) = \int \mathrm{d}x\, \mathrm{d}p (H_1 \star f_n^0 \star f_n^0) = \frac{1}{2\pi\hbar} \int \mathrm{d}x\, \mathrm{d}p H_1 \star f_n^0. \tag{B10}$$

Hence,

$$E_n^1 = \int \mathrm{d}x\, \mathrm{d}p\, H_1 f_n^0, \tag{B11}$$

the diagonal element of the perturbation. For the off-diagonal elements, similarly left-$\star$-multiply (B6) by f_m^0,

$$f_m^0 \star H_0 \star f_n^1 + f_m^0 \star H_1 \star f_n^0 = E_n^0 f_m^0 \star f_n^1 + E_n^1 f_m^0 \star f_n^0. \tag{B12}$$

By completeness, f_n^i, $i \neq 0$, resolves to

$$f_n^i = \sum_{k,l} a_{n,kl}^i f_{kl}^0, \tag{B13}$$

the reality condition dictating

$$a_{n,kl}^i = a_{n,lk}^{*i}. \tag{B14}$$

Consequently, by (10),

$$E_m^0 \sum_{k,l} a_{n,kl}^1 f_m^0 \star f_{kl}^0 + f_m^0 \star H_1 \star f_n^0 = E_n^0 \sum_{k,l} a_{n,kl}^1 f_m^0 \star f_{kl}^0 + E_n^1 \frac{1}{2\pi\hbar} f_n^0 \delta_{mn}, \tag{B15}$$

and hence

$$E_m^0 \sum_{k} a_{n,km}^1 f_{km}^0 + 2\pi\hbar f_m^0 \star H_1 \star f_n^0 = E_n^0 \sum_{k} a_{n,km}^1 f_{km}^0 + E_n^1 f_n^0 \delta_{mn}. \tag{B16}$$

For $m \neq n$,

$$(E_n^0 - E_m^0) \sum_{l} a_{n,lm}^1 f_{lm}^0 = 2\pi\hbar (f_m^0 \star H_1 \star f_n^0), \tag{B17}$$

so that

$$\sum_{l} a_{n,lm}^1 f_{lm}^0 = \frac{2\pi\hbar (f_m^0 \star H_1 \star f_n^0)}{E_n^0 - E_m^0}. \tag{B18}$$

Finally, use of (11), yields

$$a^1_{n,lm}=(2\pi\hbar)^2\int \mathrm{d}x\,\mathrm{d}p\,\frac{f^0_{ml}\star f^0_m\star H_1\star f^0_n}{E^0_n-E^0_m}$$
$$=(2\pi\hbar)^2\int \mathrm{d}x\,\mathrm{d}p\,\frac{1}{2\pi\hbar}\,\frac{f^0_{ml}\star H_1\star f^0_n}{E^0_n-E^0_m}$$
$$=(2\pi\hbar)\int \mathrm{d}x\,\mathrm{d}p\,\frac{H_1\star f^0_n\star f^0_{ml}}{E^0_n-E^0_m}$$
$$=\frac{\delta_{nl}}{E^0_n-E^0_m}\int \mathrm{d}x\,\mathrm{d}p\,H_1 f^0_{mn},\quad (m\neq n). \tag{B19}$$

We also have the similar equation for $l\neq n$. Consequently, $a^1_{n,lm}$ is proportional to the matrix element of the perturbation, and it vanishes unless l or m is equal to n. [Note: This differs from Ref. 25, Eq. (45).] To sum up,

$$f^1_n=\sum_{m\neq n}\frac{1}{E^0_n-E^0_m}\Bigg(f^0_{nm}\Bigg(\int \mathrm{d}x'\,\mathrm{d}p'\,H_1(x',p')f^0_{mn}(x',p')\Bigg)$$
$$+f^0_{mn}\Bigg(\int \mathrm{d}x'\,\mathrm{d}p'\,H_1(x',p')f^0_{nm}(x',p')\Bigg)\Bigg). \tag{B20}$$

By (8), it can be seen that the same result may also follow from evaluation of the WF integrals of perturbed wave functions obtained in standard perturbation theory in Hilbert space.

For example, consider $H_1=\sqrt{2}\,x=a+a^\dagger$. It follows that $E^1_0=0$, and

$$a^1_{n,lm}=\frac{\delta_{n,l}}{(E^0_n-E^0_m)}\int\int \mathrm{d}x\,\mathrm{d}p\,f^0_{mn}\star(a+a^\dagger)$$
$$=\frac{\delta_{n,}}{(E^0_n-E^0_m)}\int\int \mathrm{d}x\,\mathrm{d}p(\sqrt{m+1}\,f^0_{m+1,n}+\sqrt{n+1}\,f^0_{m,n+1})$$
$$=\delta_{n,l}(\sqrt{m+1}\,\delta_{m+1,n}-\sqrt{n+1}\,\delta_{m,n+1}), \tag{B21}$$

for $m\neq n$, and the $(m\leftrightarrow l)$ expression for $l\neq n$. Hence,

$$f^1_n=\sqrt{n}\,(f^0_{n-1,n}+f^0_{n,n-1})-\sqrt{n+1}\,(f^0_{n,n+1}+f^0_{n+1,n}). \tag{B22}$$

APPENDIX C: COMBINATORIC DERIVATION OF IDENTITIES (54) AND (73)

The $\star$-exponential (54) of the Hamiltonian kernel for the linear potential is also easy to work out directly, since the combinatorics in $\star$-space are identical to the combinatorics of any associative algebra. In particular, the Campbell-Baker-Hausdorff expansion also holds for $\star$-exponentials,

$$\exp_\star(A)\star\exp_\star(B)=\exp_\star(A+B+\tfrac{1}{2}[A,B]_\star+\tfrac{1}{12}[A,[A,B]_\star]_\star+\tfrac{1}{12}[[A,B]_\star,B]_\star+C), \tag{C1}$$

where C represents a sum of triple or more nested $\star$-commutators (Moyal Brackets, $[A,B]_\star\equiv A\star B-B\star A$). Now, choosing $A=itx$ and $B=itp^2+it^2p+\frac{1}{3}it^3$, yields $[A,B]_\star=-2it^2p-it^3$, $[A,[A,B]_\star]_\star=2it^3$, $[[A,B]_\star,B]_\star=0$, and hence $C=0$.

Consequently,

$$\exp_\star(itx)\star\exp_\star(itp^2+it^2p+\tfrac{1}{3}it^3)=\exp_\star(itx+itp^2). \tag{C2}$$

But further note $\exp_\star(ax)=\exp(ax)$, and also $\exp_\star(bp^2+cp+d)=\exp(bp^2+cp+d)$. This reduces the $\star$-product to a mere translation,

$$\begin{aligned}\exp_\star(ax)\star\exp_\star(bp^2+cp+d)&=\exp(ax)\star\exp(bp^2+cp+d)\\&=\exp(ax+\tfrac{1}{2}ia\partial_p)\exp(bp^2+cp+d)\\&=\exp(ax+b(p+\tfrac{1}{2}ia)^2+c(p+\tfrac{1}{2}ia)+d)\\&=\exp(ax+bp^2+(c+iab)p+d-\tfrac{1}{4}a^2b+\tfrac{1}{2}iac).\end{aligned}\tag{C3}$$

Consequently,

$$\exp_\star(itx)\star\exp_\star(itp^2+it^2p+\tfrac{1}{3}it^3)=\exp(it(x+p^2+t^2/12)),\tag{C4}$$

and the identity

$$\exp_\star(it(x+p^2))=\exp(it(x+p^2+t^2/12))\tag{54′}$$

follows.

The proof of

$$\exp_\star\left(-\frac{y}{2\sinh y}e^{2x-z}+iyp\right)=\exp\left(-\frac{1}{2}e^{y-z}e^{2x}\right)\star\exp(iyp)=\exp\left(-\frac{1}{2}e^{2x-z}+iyp\right)\tag{73}$$

is similar. Choosing now $A=-\frac{1}{2}e^{y-z}e^{2x}$ and $B=iyp$, it follows that $[A,B]_\star=-2yA$, so that only those multiple Moyal commutators survive which are linear in A. This means, then, that in the Hausdorff expansion[26] for $Z(A,B)\equiv\ln_\star(\exp_\star(A)\star\exp_\star(B))$, only B and terms *linear* in A survive. Hence, Z reduces to merely

$$Z=B+A\left(\frac{B]_\star}{1-e^{-B]_\star}}\right).\tag{C5}$$

The Hadamard expansion in $B]_\star$ means successive right $\star$-commutation with respect to B as many times as the regular power expansion of the function in the parenthesis dictates. Consequently,

$$\exp\left(-\frac{1}{2}e^{y-z}e^{2x}\right)\star\exp(iyp)=\exp_\star\left(-\frac{1}{2}e^{y-z}e^{2x}\right)\star\exp_\star(iyp)=\exp_\star\left(-\frac{y}{2\sinh y}e^{2x-z}+iyp\right).\tag{C6}$$

On the other hand,

$$\exp(-\tfrac{1}{2}e^{y-z}e^{2x})\star\exp(iyp)=\exp(-\tfrac{1}{2}e^{y-z+2x})\exp(iy(p+i\tilde{\partial}_x/2))=\exp(-\tfrac{1}{2}e^{2x-z}+iyp),\tag{C7}$$

and the identity is proven.

APPENDIX D: CONSTRUCTION OF THE GENERATING FUNCTION FOR THE LIOUVILLE WFS

From (60) and (61), it is evident that the Liouville wave functions can be generated by

$$\exp(-e^x\cosh X)=\int_{-\infty}^{\infty}\frac{dk}{\sqrt{\sinh(\pi\sqrt{E(k)})}}e^{-ikX}\,\psi_{E(k)}(x),\tag{D1}$$

where $E(k)\equiv k^2$. Therefore, the usual wave function bilinears appearing in the WFs are generated by (recalling that the ψ's are real)

$$\exp(-e^{x-y}\cosh X)\exp(-e^{x+y}\cosh Y)=\int_{-\infty}^{\infty}\frac{dk}{\sqrt{\sinh(\pi\sqrt{E(k)})}}\int_{-\infty}^{\infty}\frac{dq}{\sqrt{\sinh(\pi\sqrt{E(q)})}}$$
$$\times e^{-ikX-iqY}\psi_{E(k)}(x-y)\psi_{E(q)}(x+y). \tag{D2}$$

Consequently, Fourier transforming this produces a generating function for WFs,

$$\frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}y\, e^{-2ipy}\exp(-e^{x-y}\cosh X)\exp(-e^{x+y}\cosh Y)$$
$$=\int_{-\infty}^{\infty}\frac{\mathrm{d}k}{\sqrt{\sinh(\pi\sqrt{E(k)})}}\int_{-\infty}^{\infty}\frac{\mathrm{d}q}{\sqrt{\sinh(\pi\sqrt{E(q)})}}e^{-ikX-iqY}f_{E(k)\,E(q)}(x,p). \tag{D3}$$

Evaluation of this expression yields just a factor multiplying a modified Bessel function,

$$\int_{-\infty}^{\infty}\mathrm{d}y\, e^{-2ipy}\exp(-e^{x-y}\cosh X-e^{x+y}\cosh Y)$$
$$=\int_{-\infty}^{\infty}\mathrm{d}y\exp\left(-2ip\left(y+\frac{1}{2}\ln(\cosh X/\cosh Y)\right)\right)\exp(-(e^{x}\sqrt{4\cosh X\cosh Y})\cosh y)$$
$$=2\left(\frac{\cosh Y}{\cosh X}\right)^{ip}K_{2ip}(e^{x}\sqrt{4\cosh X\cosh Y}). \tag{D4}$$

Thus, a generating function for the complete set of Liouville Wigner functions is

$$\frac{2}{\pi}\left(\frac{\cosh Y}{\cosh X}\right)^{ip}K_{2ip}(e^{x}\sqrt{4\cosh X\cosh Y})=\int_{-\infty}^{\infty}\frac{\mathrm{d}k}{\sqrt{\sinh(\pi\sqrt{E(k)})}}\int_{-\infty}^{\infty}\frac{\mathrm{d}q}{\sqrt{\sinh(\pi\sqrt{E(q)})}}$$
$$\times e^{-ikX-iqY}f_{E(k)\,E(q)}(x,p), \tag{65$'$}$$

as in the text.

APPENDIX E: OPERATOR ORDERING AND EQ. (69)

Given the factorized phase-space generating function

$$\mathcal{G}(z;x,p)=\exp(-\tfrac{1}{2}e^{2x-z})K_{ip}(e^{z}), \tag{69$'$}$$

what is the operator corresponding to it? According to Weyl's prescription, Eq. (5), the associated operator is

$$\mathfrak{G}(z;\mathcal{X},\mathcal{P})=\frac{1}{(2\pi)^2}\int \mathrm{d}\tau\,\mathrm{d}\sigma\,\mathrm{d}x\,\mathrm{d}p\,\mathcal{G}(z;x,p)\exp(i\tau(\mathcal{P}-p)+i\sigma(\mathcal{X}-x))$$
$$=\frac{1}{(2\pi)^2}\int \mathrm{d}\tau\,\mathrm{d}\sigma\,\mathrm{d}x\,\mathrm{d}p\exp(i\tau\mathcal{P}+i\sigma\mathcal{X})\exp\left(-\frac{1}{2}e^{2x-z}-i\sigma x\right)K_{ip}(e^{z})\exp(-i\tau p). \tag{E1}$$

The integrals over x and p may be evaluated separately, if the σ contour is first shifted slightly above the real axis, $\sigma\to\sigma+i\epsilon$, thereby suppressing contributions to the x-integral as $x\to-\infty$. Now $s\equiv\frac{1}{2}e^{2x-z}$ gives

$$\int_{-\infty}^{+\infty} dx \exp\left(-\frac{1}{2} e^{2x-z} - i(\sigma + i\epsilon)x \right) = \int_0^\infty \frac{ds}{2s} (2se^z)^{-i(\sigma+i\epsilon)/2} \exp(-s)$$
$$= \tfrac{1}{2} e^{-i(z+\ln 2)\sigma/2} \Gamma(-i(\sigma+i\epsilon)/2). \tag{E2}$$

By (61),

$$\int dp\, K_{ip}(e^z) \exp(-i\tau p) = \frac{1}{2} \int_{-\infty}^{\infty} dX\, e^{-e^z \cosh X}\, 2\pi \delta(X-\tau) = \pi\, e^{-e^z \cosh \tau}. \tag{E3}$$

So

$$\mathfrak{G}(z;\mathcal{X},\mathcal{P}) = \frac{1}{8\pi} \int d\tau\, d\sigma\, e^{-i(z+\ln 2)\sigma/2} \Gamma(-i(\sigma+i\epsilon)/2)\, e^{-e^z \cosh \tau} \exp(i\tau\mathcal{P} + i\sigma\mathcal{X}). \tag{E4}$$

The shifted σ contour avoids the pole in Γ at the origin.

Ordering with all $\mathcal{P}$'s to the right, thereby departing from Weyl ordering, yields $\exp(i\tau\mathcal{P} + i\sigma\mathcal{X}) = \exp(i\sigma\mathcal{X})\exp(i\sigma\pi/2)\exp(i\tau\mathcal{P})$. Performing the σ integration before the τ integration, permits taking the limit $\epsilon \to 0$ to obtain

$$\mathfrak{G}(z;\mathcal{X},\mathcal{P}) = \frac{1}{8\pi} \int d\tau \left(\int d\sigma \Gamma(-i(\sigma+i\epsilon)/2) \exp(i\sigma\mathcal{X} + i\sigma\tau/2 - i\sigma(z+\ln 2)/2) \right)$$
$$\times e^{-e^z \cosh \tau} \exp(i\tau\mathcal{P})$$
$$= \frac{1}{8\pi} \int d\tau (4\pi \exp(-e^{2\mathcal{X}+\tau-(z+\ln 2)})) e^{-e^z \cosh \tau} \exp(i\tau\mathcal{P})$$
$$= \frac{1}{2} \int d\tau \exp\left(-\frac{1}{2} e^{2\mathcal{X}+\tau-z} - \frac{1}{2} e^{z+\tau} - \frac{1}{2} e^{z-\tau} \right) \exp(i\tau\mathcal{P}). \tag{E5}$$

This is the operator correspondent to (72); it reflects the Weyl correspondence through which it was originally defined (although, technically, it was taken out of Weyl ordering above, merely as a matter of convenience, not a bona-fide change of representation).

This form leads to a more intuitive Hilbert space representation. Acting to the right of a position eigen-bra, $\langle x|\mathcal{X} = \langle x|x$, while the subsequent exponential of the momentum operator just translates, $\langle x|\exp(i\tau\mathcal{P}) = \langle x+\tau|$. So the full right-operation of $\mathfrak{G}$ is

$$\langle x|\mathfrak{G}(z;\mathcal{X},\mathcal{P}) = \frac{1}{2} \int d\tau \langle x+\tau| \exp\left(-\frac{1}{2} e^{2x+\tau-z} - \frac{1}{2} e^{z+\tau} - \frac{1}{2} e^{z-\tau} \right)$$
$$= \frac{1}{2} \int dy \langle y| \exp\left(-\frac{1}{2} e^{x+y-z} - \frac{1}{2} e^{z+y-x} - \frac{1}{2} e^{z-y+x} \right). \tag{E6}$$

Inserting $1 = \int dx\, |x\rangle\langle x|$ gives $\mathfrak{G}(z;\mathcal{X},\mathcal{P}) = \int dx\, |x\rangle\langle x|\mathfrak{G}(z;\mathcal{X},\mathcal{P})$, and leads to a coordinate space realization of the operator involving an x,y-symmetric kernel,

$$\mathfrak{G}(z;\mathcal{X},\mathcal{P}) = \frac{1}{2} \int dx\, dy\, |x\rangle\langle y| \exp\left(-\frac{1}{2} e^{x+y-z} - \frac{1}{2} e^{x-y+z} - \frac{1}{2} e^{-x+y+z} \right). \tag{E7}$$

This operator is diagonal on energy states: by Macdonald's identity (67), and the reality and orthogonality of the wave functions,

$$\langle E_1|\mathfrak{G}(z;\mathcal{X},\mathcal{P})|E_2\rangle = \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\;\psi^*_{E_1}(x)\;\psi_{E_2}(y)\exp\left(-\frac{1}{2}e^{x+y-z}-\frac{1}{2}e^{z+y-x}-\frac{1}{2}e^{z-y+x}\right)$$
$$= \delta(E_1-E_2)\,K_{i\sqrt{E_1}}(e^z). \tag{E8}$$

This is in agreement with the corresponding phase-space expression, (66).

The composition law of this operator also parallels its phase-space isomorph, (74),

$$\mathfrak{G}(u)\mathfrak{G}(v) = \frac{1}{2}\int \mathrm{d}w\exp\left(-\frac{1}{2}(e^{u+v-w}+e^{u-v+w}+e^{-u+v+w})\right)\mathfrak{G}(w). \tag{E9}$$

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Exact solution of the Dirac equation for a spin-$\frac{1}{2}$ charged particle in two-dimensional and three-dimensional Euclidean spaces with shape invariance symmetry

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It is shown that two types of shape invariance with respect to quantum numbers n and m lead us to solve Dirac equation for a spin-$\frac{1}{2}$ charged particle in two-dimensional and three-dimensional Euclidean spaces in the presence of magnetic fields. Also, we introduce supersymmetry algebra and shape invariance symmetry represented by two bunches of spinors obtained from the above solutions. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1350635]

I. INTRODUCTION

The study of supersymmetry in quantum mechanics was first done by Nicolai,[1] then, a few years later, Witten introduced the concept of supersymmetry breaking in quantum field models.[2] Over the last few years it has been shown that supersymmetry in quantum mechanics plays an important role in deriving exact solutions of quantum mechanical problems.[3–6] A certain class of exactly solvable potentials is characterized by a property known as shape invariance.[7–12] It has been shown that the Schrödinger equation with shape invariant potentials[4,5,9–12] can be exactly solved by an algebraic procedure or elementary calculation. Also, there have been some attempts to solve the Schrödinger equation for 2-dimensional potentials from the shape invariance approach.[13,14]

In Ref. 15, with the help of the master function together with the corresponding weight function, and using from the solvable quantum models, obtained from shape invariance on secondary quantum number m, we derived solutions of the Dirac equation on the real forms of homogeneous manifold $SL(2,c)/GL(1,c)$ in the presence of a magnetic monopole field. Now, in the present paper our aim is to use the formalism of supersymmetric quantum mechanics and shape invariance symmetry to study the motion of a spin-$\frac{1}{2}$ charged particle in the presence of different magnetic fields in two-dimensional (2D) and three-dimensional (3D) Euclidean spaces. Therefore, it seems appropriate to mention first some of the results obtained so far.

In our previous works[11,16] we introduced the master function $A(x)$ as a polynomial of at most degree two, and also, the non-negative weight function $W(x)$ depending on the master function in the interval (a,b). For a given master function $A(x)$, the weight function $W(x)$ is chosen so that $(1/W(x))(d/dx)(A(x)W(x))$ is at most a first order polynomial, and also, the interval (a,b) is fixed by letting $A(x)W(x)$ and its derivatives vanish at both ends. It is shown that polynomials $\Phi_n(x)$ of order n with the Rodrigues representation,

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$$\Phi_n(x)=\frac{a_n}{W(x)}\left(\frac{d}{dx}\right)^n(A^n(x)W(x)), \tag{1}$$

are orthogonal with respect to the defined scalar product by weight function $W(x)$ in the interval (a,b), where constants a_n depend on the selection of normalization; n is a natural number. These orthogonal polynomials which are the special functions used in mathematical physics, such as Jacobi functions, hypergeometric functions, satisfy the second order differential equation,

$$A(x)\Phi_n''(x)+\frac{(A(x)W(x))'}{W(x)}\Phi_n'(x)-\left[n\left(\frac{A(x)W'(x)}{W(x)}\right)'+\frac{n(n+1)}{2}A''(x)\right]\Phi_n(x)=0,\quad n=0,1,2,\ldots, \tag{2}$$

where the prime means a derivative with respect to x. Also, a new second order differential equation has been associated to the differential equation corresponding to classical orthogonal functions $\Phi_n(x)$ just by differentiating the differential equation (2) m times then multiplying it by $(-1)^m A^{m/2}(x)$:

$$A(x)\Phi_{n,m}''(x)+\frac{(A(x)W(x))'}{W(x)}\Phi_{n,m}'(x)+\left[-\frac{1}{2}(n^2+n-m^2)A''(x)+(m-n)\left(\frac{A(x)W'(x)}{W(x)}\right)'-\frac{m^2}{4}\frac{A'^2(x)}{A(x)}-\frac{m}{2}\frac{A'(x)W'(x)}{W(x)}\right]\Phi_{n,m}(x)=0,\quad m=0,1,2,\ldots,n. \tag{3}$$

Equation (3) has the following solution as the Rodrigues formula, and the so-called associated special function related to the master function $A(x)$ and weight function $W(x)$:

$$\Phi_{n,m}(x)=\frac{a_n(-1)^m}{A^{m/2}(x)W(x)}\left(\frac{d}{dx}\right)^{n-m}(A^n(x)W(x)). \tag{4}$$

In Ref. 12 using a differential equation (2) and the procedure of factorization introduced in Ref. 16 with respect to the parameter n, we have obtained the following shape invariance equations:

$$B(n)A(n)\psi_n(x)=E(n)\psi_n(x),$$
$$A(n)B(n)\psi_{n-1}(x)=E(n)\psi_{n-1}(x), \tag{5}$$

with

$$E(n)=\frac{n}{4\left[\left(\frac{A(x)W'(x)}{W(x)}\right)'+nA''(x)\right]^2}\left\{4\left(\frac{A(x)W'(x)}{W(x)}\right)'^2\left(nA'^2(0)-A(0)\left(\frac{A(x)W'(x)}{W(x)}\right)'\right)-\left(\frac{AW'}{W}\right)(0)\left(A''(x)\left(\frac{AW'}{W}\right)(0)-2A'(0)\left(\frac{A(x)W'(x)}{W(x)}\right)'\right)\times\left(2\left(\frac{A(x)W'(x)}{W(x)}\right)'+nA''(x)\right)+n^2A''(0)(A'^2(0)-2A''(0)A(0))\times\left(nA''(0)+4\left(\frac{A(x)W'(x)}{W(x)}\right)'\right)-10nA(0)A''(x)\left(\frac{A(x)W'(x)}{W(x)}\right)'^2\right\}. \tag{6}$$

The 1-dimensional wavefunctions $\psi_n(x)$ are expressed in terms of a multiple of orthogonal polynomials $\Phi_n(x)$ as

$$\psi_n(x)=W^{1/2}(x)\Phi_n(x), \tag{7}$$

where n is named the main quantum number. The raising and the lowering operators of the main quantum number n, i.e., $B(n)$ and $A(n)$ that are adjoint of each other, have the following explicit form:

$$B(n)=A(x)\frac{d}{dx}+\frac{1}{2}\left[nA'(x)+\frac{A(x)W'(x)}{W(x)}+n\frac{A'(0)\left(\frac{A(x)W'(x)}{W(x)}\right)'-A''(x)\left(\frac{AW'}{W}\right)(0)}{\left(\frac{A(x)W'(x)}{W(x)}\right)'+nA''(x)}\right], \tag{8}$$

$$A(n)=-A(x)\frac{d}{dx}+\frac{1}{2}\left[nA'(x)+\frac{A(x)W'(x)}{W(x)}+n\frac{A'(0)\left(\frac{A(x)W'(x)}{W(x)}\right)'-A''(x)\left(\frac{AW'}{W}\right)(0)}{\left(\frac{A(x)W'(x)}{W(x)}\right)'+nA''(x)}\right].$$

One can easily show that the shape invariance relations (5) are written as follows:

$$\begin{aligned} B(n)\psi_{n-1}(x)&=E_n\psi_n(x),\\ A(n)\psi_n(x)&=E_n\psi_{n-1}(x), \end{aligned} \tag{9}$$

in which we have defined

$$E_n:=\sqrt{E(n)}. \tag{10}$$

Also, we are reminded that in Ref. 11 the differential equation (3) was factorized with respect to parameter m, and that we obtained the shape invariant equations with respect to secondary quantum number m as

$$\begin{aligned} B(m)A(m)\psi_{n,m}(x)&=E(n,m)\psi_{n,m}(x),\\ A(m)B(m)\psi_{n,m-1}(x)&=E(n,m)\psi_{n,m-1}(x), \end{aligned} \tag{11}$$

with

$$E(n,m)=-(n-m+1)\left[\left(\frac{A(x)W'(x)}{W(x)}\right)'+\frac{1}{2}(n+m)A''(x)\right]. \tag{12}$$

Thus, the 1-dimensional wavefunctions $\psi_{n,m}(x)$ were expressed in terms of a multiple of associated special functions as

$$\psi_{n,m}(x)=A^{1/4}(x)W^{1/2}(x)\Phi_{n,m}(x). \tag{13}$$

The raising and the lowering operators of the secondary quantum number m, i.e., $B(m)$ and its adjoint $A(m)$ are

$$B(m)=\sqrt{A(x)}\frac{d}{dx}-\frac{\frac{A(x)W'(x)}{2W(x)}+\frac{2m-1}{4}A'(x)}{\sqrt{A(x)}},$$
$$A(m)=-\sqrt{A(x)}\frac{d}{dx}-\frac{\frac{A(x)W'(x)}{2W(x)}+\frac{2m-1}{4}A'(x)}{\sqrt{A(x)}}. \tag{14}$$

The shape invariance relations (11) can be written as relations of raising and lowering of the wavefunctions $\psi_{n,m}(x)$ with respect to the secondary quantum number m,

$$B(m)\psi_{n,m-1}(x)=E_{n,m}\psi_{n,m}(x),$$
$$A(m)\psi_{n,m}(x)=E_{n,m}\psi_{n,m-1}(x), \tag{15}$$

with

$$E_{n,m}:=\sqrt{E(n,m)}. \tag{16}$$

II. SOLUTION OF THE DIRAC EQUATION IN 1+2 SPACE–TIME WITH THE EUCLIDEAN SPATIAL PART

Now, we use the usual polar coordinates for the flat spatial part of the 1+2 space–time, i.e., $0\leqslant r<+\infty$ and $0\leqslant\theta<2\pi$. Thus the Minkowskian space–time metric can be written as

$$g_{\mu\nu}=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-r^2\end{pmatrix}, \tag{17}$$

where μ and ν denote rows and columns by t, r and θ. Naturally, the 3-bein $E_a{}^\mu$ and its inverse, i.e., $e_\mu{}^a$, establish a connection between the Minkowskian diagonal metric $\eta^{ab}:=(1,-1,-1)$ with the space–time metric $g_{\mu\nu}$:

$$E_a{}^\mu\eta^{ab}E_b{}^\nu=g^{\mu\nu},$$
$$E_a{}^\mu g_{\mu\nu}E_b{}^\nu=\eta_{ab}, \tag{18a}$$
$$e_\mu{}^a g^{\mu\nu}e_\nu{}^b=\eta^{ab},$$
$$e_\mu{}^a\eta_{ab}e_\nu{}^b=g_{\mu\nu}. \tag{18b}$$

Indices a and b take the values 0, 1 and 2 due to the generators of Clifford algebra, and $g^{\mu\nu}$ and η^{ab} are inverse of metrics $g_{\mu\nu}$ and η_{ab}, respectively. Using Eqs. (18) we obtain the following 3-beins for the metric (17):

$$E_a{}^\mu=(e_\mu{}^a)^{-1}=\begin{pmatrix}1&0&0\\0&1&0\\0&0&\frac{1}{r}\end{pmatrix}. \tag{19}$$

The nonvanishing components of Christoffel symbols $\Gamma^\lambda_{\mu\nu}$ for the space–time metric (17) are calculated as

$$\Gamma^{r}_{\theta\theta}=-r, \quad \Gamma^{\theta}_{r\theta}=\frac{1}{r}. \tag{20}$$

Of course, it is evident that just for the spatial part of the 1+2 space–time the nonvanishing Christoffel symbols are calculated the same as (20), thus describing a 2-dimensional space with zero Ricci scalar curvature, i.e., $R=0$.

The Dirac equation for the space–time corresponding to the metric (17) is

$$D\Psi(t;r,\theta)=0, \tag{21}$$

in which the Dirac operator D is defined as[17]

$$D=-i\gamma^{a}E_{a}{}^{\mu}(\partial_{\mu}-iA_{\mu}+\tfrac{1}{8}\omega_{\mu ab}[\gamma^{a},\gamma^{b}]). \tag{22}$$

Here, A_t is a scalar potential corresponding to an electric field, and A_r and A_θ are components of a gauge potential corresponding to a magnetic field. The generators of Clifford algebra, i.e., the matrices γ^a are

$$\gamma^{0}=\sigma^{3}, \quad \gamma^{1}=i\sigma^{2}, \quad \gamma^{2}=-i\sigma^{1}, \tag{23}$$

where σ^1, σ^2 and σ^3 are the known Pauli matrices. The generators of Clifford algebra generate the Minkowskian diagonal metric η^{ab} by the following equation:

$$\gamma^{a}\gamma^{b}=\eta^{ab}I_{2\times 2}-i\epsilon^{abc}\gamma_{c}. \tag{24}$$

The components of the spin connection $\omega_{\mu}{}^{a}{}_{b}$ satisfy

$$\partial_{\mu}e_{\nu}{}^{a}-\Gamma^{\lambda}_{\mu\nu}e_{\lambda}{}^{a}+\omega_{\mu}{}^{a}{}_{b}e_{\nu}{}^{b}=0. \tag{25}$$

Then, with the help of Eqs. (19) and (20) we calculate the nonvanishing components of the spin connection as

$$\omega_{\theta\ 12}=-\omega_{\theta\ 21}=1. \tag{26}$$

Using the relation (24), for the space–time 1+2 with the flat spatial part with spin connections given in Eqs. (26), evidently we can calculate contribution of the last term in the Dirac operator D is zero. Substituting Eqs. (19) and (23) in Eq. (21), we obtain the Dirac matrix equation (21) as follows:

$$\begin{pmatrix} \partial_t-iA_t & \partial_r-\dfrac{i}{r}\partial_\theta-iA_r+\dfrac{1}{2r}-\dfrac{1}{r}A_\theta \\ -\partial_r-\dfrac{i}{r}\partial_\theta+iA_r-\dfrac{1}{2r}-\dfrac{1}{r}A_\theta & -\partial_t+iA_t \end{pmatrix}\Psi(t;r,\theta)=0. \tag{27}$$

In this paper we assume that the electric field does not exist, i.e., $A_t=0$, and that the magnetic field is static, i.e., $\partial_t A_\mu=0$, with radial symmetry $A_\mu=A_\mu(r)$ for $\mu=r$ and θ. There are two approaches to solve Eq. (27).

A. The first approach for solving the Dirac equation in 2D Euclidean space

The first approach uses the shape invariance with respect to the main quantum number n, where we assume time evolution spinors as e^{-iE_nt}, in which the spectrum E_n is defined as in Eq. (10). Then, for

$$\Psi(t;r,\theta)=e^{-iE_nt}\Psi(r,\theta)=e^{-iE_nt}\begin{pmatrix}\psi_1(r,\theta)\\ i\psi_2(r,\theta)\end{pmatrix}, \tag{28}$$

from the Dirac equation (27) we obtain the following two equations:

$$\left(\frac{\partial}{\partial r}-\frac{i}{r}\frac{\partial}{\partial\theta}-iA_r+\frac{1}{2r}-\frac{1}{r}A_\theta\right)\psi_2(r,\theta)=E_n\psi_1(r,\theta),$$
$$\left(-\frac{\partial}{\partial r}-\frac{i}{r}\frac{\partial}{\partial\theta}+iA_r-\frac{1}{2r}-\frac{1}{r}A_\theta\right)\psi_1(r,\theta)=E_n\psi_2(r,\theta). \tag{29}$$

We assume angular functionality as phase factor for functions $\psi_1(r,\theta)$ and $\psi_2(r,\theta)$, and it is easy to conclude that existence of the difference of phase between functions $\psi_1(r,\theta)$ and $\psi_2(r,\theta)$ has no effect on the determination of the magnetic field. Thus, we choose the same phase factor as follows:

$$\psi_a(r,\theta)=e^{ik\theta}\psi_a(r),\quad a=1,2. \tag{30}$$

We establish the relation between variable x and radial coordinate r as

$$\frac{dx}{A(x)}=dr. \tag{31}$$

Also we substitute Eqs. (30) into Eqs. (29) and then we reduce the equations with respect to θ in order to compare the obtained results with Eqs. (9). Then, we find that

$$B(n)=\frac{d}{dr}+\frac{k}{r}-iA_r(n)+\frac{1}{2r}-\frac{1}{r}A_\theta(n),$$
$$A(n)=-\frac{d}{dr}+\frac{k}{r}+iA_r(n)-\frac{1}{2r}-\frac{1}{r}A_\theta(n), \tag{32}$$

with

$$A_r(n)=\frac{-i}{2r},$$
$$A_\theta(n)=k-\frac{r}{2}\left[nA'(x)+\frac{A(x)W'(x)}{W(x)}+n\frac{A'(0)\left(\frac{A(x)W'(x)}{W(x)}\right)'-A''(x)\left(\frac{AW'}{W}\right)(0)}{\left(\frac{A(x)W'(x)}{W(x)}\right)'+nA''(x)}\right]_{x=x(r)}, \tag{33}$$

where $x=x(r)$ is obtained from Eq. (31). It is necessary to limit the variable x such that one can restrict the interval of r to $0\leqslant r<+\infty$. The 2-form of the magnetic field is calculated as

$$B_n(r)=-\frac{1}{2}\left[\left(nA''(x)+\left(\frac{A(x)W'(x)}{W(x)}\right)'\right)rA(x)+nA'(x)+\frac{A(x)W'(x)}{W(x)}\right.$$
$$\left.+n\frac{A'(0)\left(\frac{A(x)W'(x)}{W(x)}\right)'-A''(x)\left(\frac{AW'}{W}\right)(0)}{\left(\frac{A(x)W'(x)}{W(x)}\right)'+nA''(x)}\right]_{x=x(r)}dr\wedge d\theta. \tag{34}$$

In general, magnetic fields described by Eq. (34) are quantized by the main quantum number n, except for $A(x)=1$ (see Appendix A). Also, from the above comparison, it obviously becomes clear that the first bunch spinors describing a spin-$\frac{1}{2}$ charged particle in the presence of magnetic field (34) on the flat surface, labeled by n, are

$$\Psi_n(t;r,\theta)=e^{-iE_nt}\begin{pmatrix}\psi_n(r,\theta)\\ i\psi_{n-1}(r,\theta)\end{pmatrix}=e^{-iE_nt}\Psi_n(r,\theta), \tag{35}$$

where we have used the following notation:

$$\psi_n(r,\theta)=e^{ik\theta}\psi_n(x(r))=:e^{ik\theta}\psi_n(r). \tag{36}$$

In this approach, by accepting the results (33) and (35), the equations

$$\begin{aligned} b(n)\psi_{n-1}(r,\theta)&=E_n\psi_n(r,\theta),\\ a(n)\psi_n(r,\theta)&=E_n\psi_{n-1}(r,\theta),\end{aligned} \tag{37}$$

with

$$\begin{aligned} b(n)&=\frac{\partial}{\partial r}-\frac{i}{r}\frac{\partial}{\partial\theta}-\frac{1}{r}A_\theta(n),\\ a(n)&=-\frac{\partial}{\partial r}-\frac{i}{r}\frac{\partial}{\partial\theta}-\frac{1}{r}A_\theta(n),\end{aligned} \tag{38}$$

describe the matrix components of the Dirac equation (27). However, Eqs. (37) together with the change of variable (31) represent a 2-dimensional shape invariance equations on the flat space (r,θ), where the shape invariance parameter is the main quantum number n. In Appendix A for different choices of the master function $A(x)$, we have introduced the solvable Dirac equations on the flat surface in the presence of the related magnetic fields (quantized by n) with the spinors expressed in terms of the special orthogonal polynomials. An example is the case in which $A(x)=1$ together with $\beta=0$, where the magnetic field has a constant value along the z-axis perpendicular to the flat surface. In Appendix A for the sake of brevity, we have not introduced the explicit form of the raising and the lowering operators $b(n)$ and $a(n)$, and also, have written the components of the spinors in terms of the special functions without phase factor $e^{ik\theta}$.

Now, we show that the first bunch of the spinors, i.e., Eq. (35), represents a supersymmetry algebra and also a shape invariance symmetry in terms of the quantum number n. With attention to Eqs. (36), one can easily rewrite the Dirac equation for the spinors $\Psi_n(r,\theta)$ as the following by using Eqs. (37):

$$D_2(n)\Psi_n(r,\theta)=E_n\Psi_n(r,\theta), \tag{39}$$

where time-independent Dirac operator $D_2(n)$ is defined as

$$D_2(n):=\begin{pmatrix}0 & -ib(n)\\ ia(n) & 0\end{pmatrix}. \tag{40}$$

It is obvious that the square of the Dirac operator $D_2(n)$ becomes

$$D_2^2(n)=\begin{pmatrix}b(n)a(n) & 0\\ 0 & a(n)b(n)\end{pmatrix}=:H(n), \tag{41}$$

which leads to the Schrödinger equations in the flat surface. Let us define the chiral fermionic creation and annihilation operators as[18]

$$Q_+(n)=Q_+b(n), \tag{42a}$$

$$Q_-(n)=Q_-a(n), \tag{42b}$$

with $Q_\pm=\mp(i/2(\sigma_1\pm i\sigma_2)$, where $D_2(n)=Q_+(n)+Q_-(n)$. It is clear that these operators are nilpotent, i.e., $Q_\pm^2(n)=0$. Also, we have

$$H(n)=\{Q_+(n),Q_-(n)\},\quad [Q_\pm(n),H(n)]=0, \tag{43}$$

therefore, two fermionic operators $Q_+(n)$ and $Q_-(n)$ together with the square of the time-independent Dirac operator, i.e., the bosonic generator $H(n)$ satisfy the supersymmetry algebra. The representation of the supersymmetry algebra by the spinors $\Psi_n(r,\theta)$ is

$$\begin{aligned} Q_+(n)\Psi_n(r,\theta)&=E_n\begin{pmatrix}\psi_n(r,\theta)\\0\end{pmatrix},\\ Q_-(n)\Psi_n(r,\theta)&=E_n\begin{pmatrix}0\\ i\psi_{n-1}(r,\theta)\end{pmatrix},\\ H(n)\Psi_n(r,\theta)&=E(n)\Psi_n(r,\theta).\end{aligned} \tag{44}$$

The appropriate operators for representing the shape invariance symmetry by the spinors $\Psi_n(r,\theta)$ are

$$\mathcal{B}(n):=\begin{pmatrix} b(n) & 0\\ 0 & \dfrac{E_n}{E_{n-1}}b(n-1)\end{pmatrix}, \tag{45a}$$

$$\mathcal{A}(n):=\begin{pmatrix} a(n) & 0\\ 0 & \dfrac{E_n}{E_{n-1}}a(n-1)\end{pmatrix}. \tag{45b}$$

One can readily conclude the raising and the lowering relations of the spinors $\Psi_n(r,\theta)$ as

$$\begin{aligned}\mathcal{B}(n)\Psi_{n-1}(r,\theta)&=E_n\Psi_n(r,\theta),\\ \mathcal{A}(n)\Psi_n(r,\theta)&=E_n\Psi_{n-1}(r,\theta).\end{aligned} \tag{46}$$

Also, with the help of Eqs. (46) one can obtain the shape invariant equations on the flat surface for the spinors $\Psi_n(r,\theta)$ as

$$\begin{aligned}\mathcal{B}(n)\mathcal{A}(n)\Psi_n(r,\theta)&=E(n)\Psi_n(r,\theta),\\ \mathcal{A}(n)\mathcal{B}(n)\Psi_{n-1}(r,\theta)&=E(n)\Psi_{n-1}(r,\theta).\end{aligned} \tag{47}$$

In this discussion of supersymmetry algebra and shape invariance symmetry, angular functionality of the spinors $\Psi_n(r,\theta)$ does not play any essential role, and in fact, the solvable models related to the first approach represent supersymmetry and shape invariance properties just by restricting on the radial part.

B. The second approach for solving the Dirac equation in 2D Euclidean space

The second approach uses the shape invariance symmetry with respect to the secondary quantum number m. Thus, in order to solve the Dirac equation (27), we take time evolution

spinors as $e^{-iE_{n,m}t}$; then instead of E_n, $A_r(n)$ and $A_\theta(n)$ we arrive at Eqs. (29) with $E_{n,m}$ given in Eq. (16), $A_r(m)$ and $A_\theta(m)$, respectively. After reducing $e^{ik\theta}$, by comparing components of the obtained Dirac equation with Eqs. (15), we get

$$\begin{aligned} B(m)&=\frac{d}{dr}+\frac{k}{r}-iA_r(m)+\frac{1}{2r}-\frac{1}{r}A_\theta(m),\\ A(m)&=-\frac{d}{dr}+\frac{k}{r}+iA_r(m)-\frac{1}{2r}-\frac{1}{r}A_\theta(m). \end{aligned} \tag{48}$$

This time the radial coordinate r is related to variable x by the following relation:

$$\frac{dx}{\sqrt{A(x)}}=dr, \tag{49}$$

and also, the scalar potential and components of the gauge potential become

$$\begin{aligned} A_r(m)&=\frac{-i}{2r},\\ A_\theta(m)&=k+\frac{r}{2}\left[\frac{\dfrac{A(x)W'(x)}{W(x)}+\dfrac{2m-1}{2}A'(x)}{\sqrt{A(x)}}\right]_{x=x(r)}. \end{aligned} \tag{50}$$

The end points of the interval (a,b) for variable x must be chosen such that the interval of radial coordinate r can be restricted to $0\leqslant r<+\infty$. In order to define the radial coordinate as in Eq. (49), we must clearly choose the master function $A(x)$ positive in the interval (a,b). The 2-form magnetic field, in this approach, is quantized by the secondary quantum number m as

$$\begin{aligned} B_m(r)=\frac{1}{2}\Bigg[&\frac{1}{\sqrt{A(x)}}\frac{A(x)W'(x)}{W(x)}+\frac{2m-1}{2}\frac{A'(x)}{\sqrt{A(x)}}+\left(\left(\frac{A(x)W'(x)}{W(x)}\right)'+\frac{2m-1}{2}A''(x)\right)r\\ &-\frac{1}{4}\left(2\frac{A'(x)W'(x)}{W(x)}+(2m-1)\frac{A'^2(x)}{A(x)}\right)r\Bigg]_{x=x(r)} dr\wedge d\theta, \end{aligned} \tag{51}$$

where, we have used relation (49) to express the relations (50) and (51). The second bunch spinors describing the states of a spin-$\frac{1}{2}$ charged particle in the presence of the magnetic field (51), labeled by two quantum numbers n and m, are

$$\Psi_{n,m}(t;r,\theta)=e^{-iE_{n,m}t}\begin{pmatrix}\psi_{n,m}(r,\theta)\\ i\psi_{n,m-1}(r,\theta)\end{pmatrix}=e^{-iE_{n,m}t}\Psi_{n,m}(r,\theta), \tag{52}$$

in which we have used the following notation using the change of variable (49):

$$\psi_{n,m}(r,\theta)=e^{ik\theta}\psi_{n,m}(x(r))=e^{ik\theta}\psi_{n,m}(r). \tag{53}$$

In the second approach, while admitting the gauge potentials and the spinors as in Eqs. (50) and (52), respectively, the following equations:

$$\begin{aligned} b(m)\psi_{n,m-1}(r,\theta)&=E_{n,m}\psi_{n,m}(r,\theta),\\ a(m)\psi_{n,m}(r,\theta)&=E_{n,m}\psi_{n,m-1}(r,\theta), \end{aligned} \tag{54}$$

with

$$b(m)=\frac{\partial}{\partial r}-\frac{i}{r}\frac{\partial}{\partial_\theta}-\frac{1}{r}A_\theta(m),$$
$$a(m)=-\frac{\partial}{\partial r}-\frac{i}{r}\frac{\partial}{\partial_\theta}-\frac{1}{r}A_\theta(m), \tag{55}$$

express the matrix components of the Dirac equation (27). In this case, Eqs. (54) describe shape invariance symmetry on the flat surface (r,θ), such that the shape invariance parameter is the secondary quantum number m. Possible different choices for the master function $A(x)$, some of the solvable Dirac equations on the flat surface in the presence of corresponding magnetic fields (quantized by m) with the spinors that are described in terms of associated special functions are included in Appendix B, where we have not added the explicit form of the raising and the lowering operators $b(m)$ and $a(m)$ for the sake of brevity.

Now we show the second bunch of the spinors, i.e. (52), representing a supersymmetry algebra and a shape invariance symmetry. Using Eqs. (54) and omitting time-dependence, we can rewrite the Dirac equation (27) as

$$D_2(m)\Psi_{n,m}(r,\theta)=E_{n,m}\Psi_{n,m}(r,\theta), \tag{56}$$

with time-independent Dirac operator $D_2(m)$ as

$$D_2(m):=\begin{pmatrix}0 & -ib(m)\\ ia(m) & 0\end{pmatrix}. \tag{57}$$

The square of the Dirac operator $D_2(m)$ leads to the Schrödinger Hamiltonians on the flat surface with a shape invariant parameter of secondary quantum number m,

$$D_2^2(m)=\begin{pmatrix}b(m)a(m) & 0\\ 0 & a(m)b(m)\end{pmatrix}=:H(m). \tag{58}$$

Choosing the chiral fermionic creation and annihilation operators as

$$Q_+(m)=Q_+b(m), \tag{59a}$$
$$Q_-(m)=Q_-a(m), \tag{59b}$$

one evidently gets for the nilpotent operators $Q_\pm(m)$ of order two and the bosonic operator $H(m)$ the supersymmetry algebra (43) but with m instead of n. The spinors $\Psi_{n,m}(r,\theta)$ on the flat surface represent supersymmetry algebra as

$$Q_+(m)\Psi_{n,m}(r,\theta)=E_{n,m}\begin{pmatrix}\psi_{n,m}(r,\theta)\\ 0\end{pmatrix},$$
$$Q_-(m)\Psi_{n,m}(r,\theta)=E_{n,m}\begin{pmatrix}0\\ i\psi_{n,m-1}(r,\theta)\end{pmatrix}, \tag{60}$$
$$H(m)\Psi_{n,m}(r,\theta)=E(n,m)\Psi_{n,m}(r,\theta).$$

The matrix and differential operators for describing the shape invariance symmetry by the second bunch of spinors, i.e., $\Psi_{n,m}(r,\theta)$ on the flat surface are

$$\mathcal{B}(m):=\begin{pmatrix}b(m) & 0\\ 0 & \dfrac{E_{n,m}}{E_{n,m-1}}b(m-1)\end{pmatrix}, \tag{61a}$$

$$\mathcal{A}(m) := \begin{pmatrix} a(m) & 0 \\ 0 & \dfrac{E_{n,m}}{E_{n,m-1}} a(m-1) \end{pmatrix}. \tag{61b}$$

The raising and the lowering relations and the shape invariant equations of the spinors $\Psi_{n,m}(r,\theta)$ are obtained as

$$\begin{aligned} \mathcal{B}(m)\Psi_{n,m-1}(r,\theta) &= E_{n,m}\Psi_{n,m}(r,\theta), \\ \mathcal{A}(m)\Psi_{n,m}(r,\theta) &= E_{n,m}\Psi_{n,m-1}(r,\theta), \end{aligned} \tag{62}$$

$$\begin{aligned} \mathcal{B}(m)\mathcal{A}(m)\Psi_{n,m}(r,\theta) &= E(n,m)\Psi_{n,m}(r,\theta), \\ \mathcal{A}(m)\mathcal{B}(m)\Psi_{n,m-1}(r,\theta) &= E(n,m)\Psi_{n,m-1}(r,\theta). \end{aligned} \tag{63}$$

Once again we see that in the properties of supersymmetry algebra and the shape invariance described by the spinors $\Psi_{n,m}(r,\theta)$, the angular functionality of the spinors do not have any important role.

III. SOLUTION OF THE DIRAC EQUATION IN 1+3 SPACE–TIME WITH THE EUCLIDEAN SPATIAL PART

The metric that describes 1+3 space–time with the flat spatial part is

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -r^2 & 0 \\ 0 & 0 & 0 & -r^2 \sin^2\theta \end{pmatrix}, \tag{64}$$

here, μ and ν take symbols t, r, θ and ϕ with intervals $0 \leqslant r < +\infty$, $0 \leqslant \theta \leqslant \pi$ and $0 \leqslant \phi < 2\pi$. The variables r, θ and ϕ are the usual global spherical coordinates. We also emphasize that in this section the spherical radial coordinate r is different from the polar coordinate r in the previous section. The nonvanishing components of the Christoffel symbols $\Gamma^{\lambda}_{\mu\nu}$ corresponding to the space–time metric (64) are

$$\Gamma^{r}_{\theta\theta} = -r, \quad \Gamma^{\theta}_{r\theta} = \Gamma^{\phi}_{r\phi} = \frac{1}{r}, \quad \Gamma^{r}_{\phi\phi} = -r\sin^2\theta, \quad \Gamma^{\phi}_{\theta\phi} = \cot\theta, \quad \Gamma^{\theta}_{\phi\phi} = -\frac{1}{2}\sin 2\theta. \tag{65}$$

Also, the generators γ^a of the Clifford algebra,

$$\{\gamma^a, \gamma^b\} = 2I_{4\times 4}\eta^{ab}, \tag{66}$$

are chosen as

$$\gamma^0 = \begin{pmatrix} I_{2\times 2} & 0 \\ 0 & -I_{2\times 2} \end{pmatrix}, \quad \gamma^1 = i\begin{pmatrix} 0 & \sigma^2 \\ \sigma^2 & 0 \end{pmatrix}, \quad \gamma^2 = -i\begin{pmatrix} 0 & \sigma^1 \\ \sigma^1 & 0 \end{pmatrix}, \quad \gamma^3 = -i\begin{pmatrix} 0 & \sigma^3 \\ \sigma^3 & 0 \end{pmatrix}, \tag{67}$$

where η^{ab} are components of the 1+3 diagonal Minkowskian space–time metric, i.e., $\eta^{ab} = (1, -1, -1, -1)$. The 4-beins for the Minkowskian space–time metric (64) are calculated as

$$E_a{}^{\mu}=(e_{\mu}{}^{a})^{-1}=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{r} & 0 \\ 0 & 0 & 0 & \frac{1}{r\sin\theta} \end{pmatrix}. \tag{68}$$

Using Eqs. (25), (65) and (68) we derive the nonvanishing components of the spin connection $\omega_{\theta ab}$ as

$$\omega_{\theta\ 12}=-\omega_{\theta\ 21}=1, \quad \omega_{\phi\ 13}=-\omega_{\phi\ 31}=\sin\theta, \quad \omega_{\phi\ 23}=-\omega_{\phi\ 32}=\cos\theta. \tag{69}$$

Now, we use the Dirac operator introduced in Eq. (22) in the following equation:

$$D\Psi(t;r,\theta,\phi)=0, \tag{70}$$

for the 1+3 space–time. Substituting the results obtained in Eqs. (67)–(69), for the Dirac equation (70) we obtain the following explicit form:

$$\begin{pmatrix} I_{2\times2}(\partial_t-iA_t) & i\sigma^2\left(\partial_r-iA_r+\frac{1}{r}\right)-\frac{i}{r}\sigma^1(\partial_\theta-iA_\theta \\ & +\frac{1}{2}\cot\theta)-\frac{i}{r\sin\theta}\sigma^3(\partial_\phi-iA_\phi) \\ i\sigma^2\left(\partial_r-iA_r+\frac{1}{r}\right)-\frac{i}{r}\sigma^1(\partial_\theta-iA_\theta & \\ +\frac{1}{2}\cot\theta)-\frac{i}{r\sin\theta}\sigma^3(\partial_\phi-iA_\phi) & -I_{2\times2}(\partial_t-iA_t) \end{pmatrix}\Psi(t;r,\theta,\phi)=0. \tag{71}$$

There exist two approaches for solving the Dirac matrix equation (71) by using shape invariance symmetry with respect to the main and secondary quantum numbers n and m, respectively, as of the previous section. For this purpose, we take the scalar potential equal to zero, i.e. $A_t=0$, and also, we assume that 2-form of the static magnetic field has the spherical radial symmetry.

A. The first approach for solving the Dirac equation in 3D Euclidean space

In the first approach due to the shape invariance symmetry with respect to the main quantum number n, we introduce the spinors $\Psi(t;r,\theta,\phi)$ as

$$\Psi(t;r,\theta,\phi)=e^{-iE_nt}\Psi(r,\theta,\phi)=e^{-iE_nt}\begin{pmatrix} \psi_1(r,\theta,\phi) \\ \psi_2(r,\theta,\phi) \\ i\psi_1(r,\theta,\phi) \\ i\psi_2(r,\theta,\phi) \end{pmatrix}. \tag{72}$$

If we choose the functionality of the spinors from the angular variables θ and ϕ as phase factors in the following form:

$$\psi_a(r,\theta,\phi)=e^{ik_\theta\theta+ik_\phi\phi}\psi_a(r), \quad a=1,2; \tag{73}$$

then, by choosing $A_\phi=k_\phi$ in the Dirac equation (71), one can obtain the following equations:

$$\left(\frac{\partial}{\partial r}-\frac{i}{r}\frac{\partial}{\partial\theta}-\frac{i}{r\sin\theta}\frac{\partial}{\partial\phi}-iA_r-\frac{A_\theta-1}{r}-\frac{A_\phi}{r\sin\theta}-\frac{i}{2r}\cot\theta\right)\psi_2(r,\theta,\phi)=E_n\psi_1(r,\theta,\phi),$$
$$\left(-\frac{\partial}{\partial r}-\frac{i}{r}\frac{\partial}{\partial\theta}-\frac{i}{r\sin\theta}\frac{\partial}{\partial\phi}+iA_r-\frac{A_\theta+1}{r}-\frac{A_\phi}{r\sin\theta}-\frac{i}{2r}\cot\theta\right)\psi_1(r,\theta,\phi)=E_n\psi_2(r,\theta,\phi). \tag{74}$$

Reducing the equations (74) with respect to the variables θ and ϕ and by changing the variable as given in (31), we can compare the derived results with Eqs. (9), to get the spinors (72) as

$$\Psi_n(t;r,\theta,\phi)=e^{-iE_nt}\begin{pmatrix}\psi_n(r,\theta,\phi)\\ \psi_{n-1}(r,\theta,\phi)\\ i\psi_n(r,\theta,\phi)\\ i\psi_{n-1}(r,\theta,\phi)\end{pmatrix}=e^{-iE_nt}\Psi_n(r,\theta,\phi), \tag{75}$$

with the following convention:

$$\psi_n(r,\theta,\phi)=e^{ik_\theta\theta+ik_\phi\phi}\psi_n(x(r))$$
$$=:e^{ik_\theta\theta+ik_\phi\phi}\psi_n(r). \tag{76}$$

Also, from the latter comparison we lead to the following values for the components of the gauge potential:

$$A_r(n)=-\frac{i}{r},$$

$$A_\theta(n)=k_\theta-\frac{i}{2}\cot\theta-\frac{r}{2}$$
$$\times\left[nA'(x)+\frac{A(x)W'(x)}{W(x)}+n\frac{A'(0)\left(\frac{A(x)W'(x)}{W(x)}\right)'-A''(x)\left(\frac{AW'}{W}\right)(0)}{\left(\frac{A(x)W'(x)}{W(x)}\right)'+nA''(x)}\right]_{x=x(r)},$$

$$A_\phi(n)=k_\phi, \tag{77}$$

where $x=x(r)$ is the solution of Eq. (31). It is obvious that the 2-form of the magnetic field is calculated as Eq. (34). Thus the operators that describe shape invariance symmetry on components of the spinors are

$$b(n)=\frac{\partial}{\partial r}-\frac{i}{r}\frac{\partial}{\partial\theta}-\frac{i}{r\sin\theta}\frac{\partial}{\partial\phi}-iA_r(n)-\frac{A_\theta(n)-1}{r}-\frac{A_\phi(n)}{r\sin\theta}-\frac{i}{2r}\cot\theta,$$
$$a(n)=-\frac{\partial}{\partial r}-\frac{i}{r}\frac{\partial}{\partial\theta}-\frac{i}{r\sin\theta}\frac{\partial}{\partial\phi}+iA_r(n)-\frac{A_\theta(n)+1}{r}-\frac{A_\phi(n)}{r\sin\theta}-\frac{i}{2r}\cot\theta, \tag{78}$$

with the relations of raising and lowering of the spinors components $\psi_n(r,\theta,\phi)$ as

$$b(n)\psi_{n-1}(r,\theta,\phi)=E_n\psi_n(r,\theta,\phi),$$
$$a(n)\psi_n(r,\theta,\phi)=E_n\psi_{n-1}(r,\theta,\phi). \tag{79}$$

The information given in Appendix A includes the solutions of this subsection, too. It must be noted that the raising and the lowering operators $b(n)$ and $a(n)$ act in 3D Euclidean space with coordinates (r,θ,ϕ), and the functionality of the spinors to angles of θ and ϕ have no role in expressing shape invariance symmetry.

The spinors obtained in this subsection represent the supersymmetry algebra and the shape invariance symmetry with respect to the main quantum number n. From the results of the Dirac equation as Eqs. (78) we can define time-independent Dirac operator $D_3(n)$ in the following form:

$$D_3(n) := \begin{pmatrix} 0 & Q_+ b(n) - Q_- a(n) \\ Q_- a(n) - Q_+ b(n) & 0 \end{pmatrix}, \tag{80}$$

where it has the following eigenvalue equation:

$$D_3(n)\Psi_n(r,\theta,\phi) = E_n \Psi_n(r,\theta,\phi). \tag{81}$$

Now, one can check that the chiral fermionic creation and annihilation operators defined as

$$\begin{aligned} Q_+(n) &:= \begin{pmatrix} 0 & Q_+ b(n) - Q_- a(n) \\ 0 & 0 \end{pmatrix}, \\ Q_-(n) &:= \begin{pmatrix} 0 & 0 \\ Q_- a(n) - Q_+ b(n) & 0 \end{pmatrix}, \end{aligned} \tag{82}$$

together with the square of the time-independent Dirac operator, i.e. bosonic operator $H(n) = D_3^2(n)$, satisfy the supersymmetry algebra (43). The supersymmetry algebra (43) is represented by the chiral fermionic creation and annihilation operators, together with the square of the time-independent Dirac operator in 3D Euclidean space as

$$\begin{aligned} Q_+(n)\Psi_n(r,\theta,\phi) &= E_n \begin{pmatrix} \psi_n(r,\theta,\phi) \\ \psi_{n-1}(r,\theta,\phi) \\ 0 \\ 0 \end{pmatrix}, \\ Q_-(n)\Psi_n(r,\theta,\phi) &= E_n \begin{pmatrix} 0 \\ 0 \\ i\psi_{n-1}(r,\theta,\phi) \\ i\psi_{n-1}(r,\theta,\phi) \end{pmatrix}, \\ H(n)\Psi_n(r,\theta,\phi) &= E(n)\Psi_n(r,\theta,\phi). \end{aligned} \tag{83}$$

The spinors themselves $\Psi_n(r,\theta,\phi)$ in 3D Euclidean space represent a shape invariance symmetry as

$$\begin{aligned} \mathcal{B}(n)\Psi_{n-1}(r,\theta,\phi) &= E_n \Psi_n(r,\theta,\phi), \\ \mathcal{A}(n)\Psi_n(r,\theta,\phi) &= E_n \Psi_{n-1}(r,\theta,\phi), \end{aligned} \tag{84}$$

or

$$\begin{aligned} \mathcal{B}(n)\mathcal{A}(n)\Psi_n(r,\theta,\phi) &= E(n)\Psi_n(r,\theta,\phi), \\ \mathcal{A}(n)\mathcal{B}(n)\Psi_{n-1}(r,\theta,\phi) &= E(n)\Psi_{n-1}(r,\theta,\phi), \end{aligned} \tag{85}$$

in which the operators $\mathcal{B}(n)$ and $\mathcal{A}(n)$ are the raising and the lowering operators, respectively:

$$\mathcal{B}(n) := \frac{1}{2}\left((I_{2\times 2}+\sigma^3)b(n) + \frac{E_n}{E_{n-1}}(I_{2\times 2}-\sigma^3)b(n-1)\right)\otimes I_{2\times 2},$$
$$\mathcal{A}(n) := \frac{1}{2}\left((I_{2\times 2}+\sigma^3)a(n) + \frac{E_n}{E_{n-1}}(I_{2\times 2}-\sigma^3)a(n-1)\right)\otimes I_{2\times 2}. \tag{86}$$

B. The second approach for solving the Dirac equation in 3D Euclidean space

The second approach is obtained by using the shape invariance symmetry with respect to the secondary quantum number m, again. For this purpose one can take the spinors $\Psi(t;r,\theta,\phi)$ as in Eqs. (72), but with $E_{n,m}$ instead of E_n. Choosing the time-independent components of spinors as Eqs. (73), the Dirac equation (71) is transformed to two equations given in (74), but with $E_{n,m}$ instead of E_n. Thus, by comparing the derived results with those of Eqs. (15), the solution of the Dirac equation (70) is obtained as the following spinors:

$$\Psi_{n,m}(t;r,\theta,\phi) = e^{-iE_{n,m}t}\begin{pmatrix} \psi_{n,m}(r,\theta,\phi) \\ \psi_{n,m-1}(r,\theta,\phi) \\ i\psi_{n,m}(r,\theta,\phi) \\ i\psi_{n,m-1}(r,\theta,\phi)\end{pmatrix} = e^{-iE_{n,m}t}\Psi_{n,m}(r,\theta,\phi), \tag{87}$$

in which the components $\psi_{n,m}(r,\theta,\phi)$ are

$$\psi_{n,m}(r,\theta,\phi) = e^{ik_\theta\theta+ik_\phi\phi}\psi_{n,m}(x(r)) =: e^{ik_\theta\theta+ik_\phi\phi}\psi_{n,m}(r). \tag{88}$$

Here, $x=x(r)$ is the solution of differential equation related to the change of variable (49). Also, in this approach, the components of the gauge potential are

$$A_r(m) = -\frac{i}{r},$$
$$A_\theta(m) = k_\theta - \frac{i}{2}\cot\theta + \frac{r}{2}\left[\frac{\frac{A(x)W'(x)}{W(x)} + \frac{2m-1}{2}A'(x)}{\sqrt{A(x)}}\right]_{x=x(r)}, \tag{89}$$
$$A_\phi(m) = k_\phi.$$

One can conclude the 2-form of the magnetic field as Eq. (51). Consequently, information obtained in Appendix B describes solvability of the Dirac equation in the 3D Euclidean space due to the shape invariance symmetry with respect to the secondary quantum number m.

It is easy to show that with definitions of the time-independent Dirac operator $D_3(m)$, the fermionic creation $Q_+(m)$, and the annihilation $Q_-(m)$ operators as

$$D_3(m) := \begin{pmatrix} 0 & Q_+b(m)-Q_-a(m) \\ Q_-a(m)-Q_+b(m) & 0\end{pmatrix}, \tag{90}$$

$$Q_+(m) := \begin{pmatrix} 0 & Q_+b(m)-Q_-a(m) \\ 0 & 0\end{pmatrix},$$
$$Q_-(m) := \begin{pmatrix} 0 & 0 \\ Q_-a(m)-Q_+b(m) & 0\end{pmatrix}, \tag{91}$$

the bosonic operator $H(m) \coloneqq D_3^2(m)$ and the fermionic operators $Q_{\pm}(m)$ satisfy the supersymmetry algebra (43). One can consider that the spinors $\Psi_{n,m}(r,\theta,\phi)$ represent shape invariance symmetry by the raising and the lowering operators $\mathcal{B}(m)$ and $\mathcal{A}(m)$ as

$$\begin{aligned}\mathcal{B}(m) &\coloneqq \frac{1}{2}\left((I_{2\times 2}+\sigma^3)b(m)+\frac{E_{n,m}}{E_{n,m-1}}(I_{2\times 2}-\sigma^3)b(m-1)\right)\otimes I_{2\times 2},\\ \mathcal{A}(m) &\coloneqq \frac{1}{2}\left((I_{2\times 2}+\sigma^3)a(m)+\frac{E_{n,m}}{E_{n,m-1}}(I_{2\times 2}-\sigma^3)a(m-1)\right)\otimes I_{2\times 2}.\end{aligned} \tag{92}$$

IV. CONCLUSION

Using the master function $A(x)$ we have obtained two bunches of solutions for the Dirac equation of a spin-$\frac{1}{2}$ charged particle in 2D and 3D Euclidean spaces in the presence of the magnetic fields (34) and (51), where they are quantized by the main quantum number n and the secondary quantum number m, respectively. The first bunch spinors, i.e. $\Psi_n(r,\theta)$ and $\Psi_n(r,\theta,\phi)$, are expressed in terms of orthogonal polynomials $\Phi_n(x(r))$ via the change of variable (31) and the second bunch spinors, i.e. $\Psi_{n,m}(r,\theta)$ and $\Psi_{n,m}(r,\theta,\phi)$, are expressed in terms of the associated special functions $\Phi_{n,m}(x(r))$ via the change of variable (49). Both of these spinors represent supersymmetry algebra and shape invariance symmetry.

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APPENDIX A: SHAPE INVARIANCE APPROACH OF THE MAIN QUANTUM NUMBER *n* TO THE SOLUTION OF DIRAC EQUATION IN 2D AND 3D EUCLIDEAN SPACES

$$\mathbf{A}(\mathbf{x})=\mathbf{1}, \quad \mathbf{W}(\mathbf{x})=e^{(-1/2)\,\alpha\mathbf{x}^2+\beta\mathbf{x}},$$

$$-\infty<x<+\infty, \quad \alpha>0, \quad -\infty<\beta<+\infty,$$

$$H_n^{(\alpha,\beta)}(x)=\frac{a_n}{e^{(-1/2)\,\alpha x^2+\beta x}}\left(\frac{d}{dx}\right)^n(e^{(-1/2)\,\alpha x^2+\beta x}),$$

$$x=r,$$

$$B_n(r)=\frac{-1}{2}[\beta-2\alpha r]dr\wedge d\theta,$$

$$\psi_n(r)=e^{(-1/4)\,\alpha r^2(+1/2)\,\beta r}H_n^{(\alpha,\beta)}(r),$$

$$E_n=\sqrt{n\alpha};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{x} \quad \mathbf{W}(\mathbf{x})=\mathbf{x}^{\alpha}\mathbf{e}^{-\beta\mathbf{x}},$$

$$0<x<+\infty, \quad \alpha>-1, \quad \beta>0,$$

$$L_n^{(\alpha,\beta)}(x)=\frac{a_n}{x^{\alpha}e^{-\beta x}}\left(\frac{d}{dx}\right)^n(x^{n+\alpha}e^{-\beta x}),$$

$$x=e^r,$$

$$B_n(r)=\tfrac{1}{2}[n-\alpha+\beta(1+r)e^r]dr\wedge d\theta,$$

$$\psi_n(r)=e^{(1/2)\,\alpha r(-1/2)\,\beta e^r}L_n^{(\alpha,\beta)}(e^r),$$

$$E_n=\sqrt{n(n+\alpha)};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{x^2},\quad \mathbf{W}(\mathbf{x})=\mathbf{x}^{\alpha}\mathbf{e}^{-\beta/\mathbf{x}},$$

$$-\infty<x<0,\quad \alpha<-2,\quad \beta>0,$$

$$\overline{F}_n^{(\alpha,\beta)}(x)=\frac{a_n}{x^{\alpha}e^{-\beta/x}}\left(\frac{d}{dx}\right)^n(x^{2n+\alpha}e^{-\beta/x}),$$

$$x=-\frac{1}{r},$$

$$B_n(r)=\beta\left[\frac{n}{2n+\alpha}-\frac{1}{2}\right]dr\wedge d\theta,$$

$$\psi_n(r)=(-1)^{\alpha/2}r^{-\alpha/2}e^{(1/2)\,\beta r}\overline{F}_n^{(\alpha,\beta)}\left(-\frac{1}{r}\right),$$

$$E_n=\sqrt{-\frac{n(n+\alpha)\beta^2}{(2n+\alpha)^2}};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{1}-\mathbf{x^2},\quad \mathbf{W}(\mathbf{x})=(\mathbf{1}-\mathbf{x})^{\alpha}(\mathbf{1}+\mathbf{x})^{\beta},$$

$$-1<x<+1,\quad \alpha>-1,\quad \beta>-1,$$

$$P_n^{(\alpha,\beta)}(x)=\frac{a_n}{(1-x)^{\alpha}(1+x)^{\beta}}\left(\frac{d}{dx}\right)^n((1-x)^{n+\alpha}(1+x)^{n+\beta}),$$

$$x=\tanh r,$$

$$B_n(r)=\frac{1}{2}\left[\frac{\beta^2-\alpha^2}{2n+\alpha+\beta}+(2n+\alpha+\beta)\frac{r}{\cosh^2 r}+(2n-\alpha-\beta)\tanh r\right]dr\wedge d\theta,$$

$$\psi_n(r)=(1-\tanh r)^{\alpha/2}(1+\tanh r)^{\beta/2}P_n^{(\alpha,\beta)}(\tanh r),$$

$$E_n=\sqrt{\frac{4n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta)^2}};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{x^2}-\mathbf{1},\quad \mathbf{W}(\mathbf{x})=(\mathbf{x}-\mathbf{1})^{\alpha}(\mathbf{x}+\mathbf{1})^{\beta},$$

$$-\infty<x<-1,\quad \beta>-1,\quad \alpha+\beta<-2,$$

$$\mathcal{P}_n^{(\alpha,\beta)}(x)=\frac{a_n}{(x-1)^{\alpha}(x+1)^{\beta}}\left(\frac{d}{dx}\right)^n((x-1)^{n+\alpha}(x+1)^{n+\beta}),$$

$$x=-\coth r,$$

$$B_n(r)=\frac{1}{2}\left[\frac{\alpha^2-\beta^2}{2n+\alpha+\beta}-(2n+\alpha+\beta)\frac{r}{\sinh^2 r}+(2n-\alpha-\beta)\coth r\right]dr\wedge d\theta,$$

$$\psi_n(r)=(-1)^{\alpha/2}(1+\coth r)^{\alpha/2}(1-\coth r)^{\beta/2}\mathcal{P}_n^{(\alpha,\beta)}(-\coth r),$$

$$E_n=\sqrt{\frac{4n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta)^2}};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{1}+\mathbf{x^2},\quad \mathbf{W}(\mathbf{x})=(\mathbf{1}+\mathbf{x^2})^{\alpha}\mathbf{e}^{\beta\tan^{-1}\mathbf{x}},$$

$$-\infty<x<+\infty,\quad \alpha<-1,\quad \beta<0,$$

$$J_n^{(\alpha,\beta)}(x)=\frac{a_n}{(1+x^2)^{\alpha}e^{\beta\tan^{-1}x}}\left(\frac{d}{dx}\right)^n((1+x^2)^{n+\alpha}e^{\beta\tan^{-1}x}),$$

$$x=\tan r$$

$$B_n(r)=-\left[\frac{\alpha\beta}{2(n+\alpha)}+(n+\alpha)\frac{r}{\cos^2 r}+(n+\alpha)\tan r\right]dr\wedge d\theta,$$

$$\psi_n(r)=\cos^{-\alpha}re^{(1/2)\beta r}J_n^{(\alpha,\beta)}(\tan r),$$

$$E_n=\sqrt{-n(n+2\alpha)\left(1+\frac{\beta^2}{4(n+\alpha)^2}\right)};$$

$$\mathbf{A}(\mathbf{x})=-\mathbf{1}-\mathbf{x^2},\quad \mathbf{W}(\mathbf{x})=(\mathbf{1}+\mathbf{x^2})^{\alpha}\mathbf{e}^{\beta\cot^{-1}\mathbf{x}},$$

$$-\infty<x<+\infty,\quad \alpha<-1,\quad \beta<0,$$

$$\overline{\mathcal{F}}_n^{(\alpha,\beta)}(x)=\frac{a_n(-1)^n}{(1+x^2)^{\alpha}e^{\beta\cot^{-1}x}}\left(\frac{d}{dx}\right)^n((1+x^2)^{n+\alpha}e^{\beta\cot^{-1}x}),$$

$$x=\cot r,$$

$$B_n(r)=-\left[\frac{\alpha\beta}{2(n+\alpha)}+(n+\alpha)\frac{r}{\sin^2 r}-(n+\alpha)\cot r\right]dr\wedge d\theta,$$

$$\psi_n(r)=\sin^{-\alpha}re^{(1/2)\beta r}\overline{\mathcal{F}}_n^{(\alpha,\beta)}(\cot r),$$

$$E_n=\sqrt{-n(n+2\alpha)\left(1+\frac{\beta^2}{4(n+\alpha)^2}\right)};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{x}(\mathbf{1}-\mathbf{x}),\quad \mathbf{W}(\mathbf{x})=\mathbf{x}^{\alpha}(\mathbf{1}-\mathbf{x})^{\beta},$$

$$0<x<+1,\quad \alpha>-1,\quad \beta>-1,$$

$$F_n^{(\alpha,\beta)}(x)=\frac{a_n}{x^{\alpha}(1-x)^{\beta}}\left(\frac{d}{dx}\right)^n(x^{n+\alpha}(1-x)^{n+\beta}),$$

$$x=\frac{e^r}{1+e^r},$$

$$B_n(r)=\frac{1}{2}\left[\frac{n(\alpha-\beta)}{2n+\alpha+\beta}-\frac{n+\alpha-(n+\beta)e^r}{1+e^r}+(2n+\alpha+\beta)\frac{re^r}{(1+e^r)^2}\right]dr\wedge d\theta,$$

$$\psi_n(r)=e^{(1/2)\,\alpha r}(1+e^r)^{(-1/2)(\alpha+\beta)}F_n^{(\alpha,\beta)}\left(\frac{e^r}{1+e^r}\right),$$

$$E_n=\sqrt{\frac{n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta)^2}};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{x}(\mathbf{1}+\mathbf{x}),\quad \mathbf{W}(\mathbf{x})=\mathbf{x}^{\alpha}(\mathbf{1}+\mathbf{x})^{\beta},$$

$$-1<x<+\infty,\quad \beta>-1,\quad \alpha+\beta<-2,$$

$$\mathcal{F}_n^{(\alpha,\beta)}(x)=\frac{a_n}{x^{\alpha}(1+x)^{\beta}}\left(\frac{d}{dx}\right)^n(x^{n+\alpha}(1+x)^{n+\beta}),$$

$$x=\frac{e^r}{1-e^r},$$

$$B_n(r)=\frac{1}{2}\left[\frac{n(\alpha-\beta)}{2n+\alpha+\beta}-\frac{n+\alpha+(n+\beta)e^r}{1-e^r}-(2n+\alpha+\beta)\frac{re^r}{(1-e^r)^2}\right]dr\wedge d\theta,$$

$$\psi_n(r)=e^{(1/2)\,\alpha r}(1-e^r)^{(-1/2)(\alpha+\beta)}\mathcal{F}_n^{(\alpha,\beta)}\left(\frac{e^r}{1-e^r}\right),$$

$$E_n=\sqrt{\frac{n(n+\alpha)(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta)^2}}.$$

APPENDIX B: SHAPE INVARIANCE APPROACH OF THE SECONDARY QUANTUM NUMBER *m* TO THE SOLUTION OF DIRAC EQUATION IN 2D AND 3D EUCLIDEAN SPACES

$$\mathbf{A}(\mathbf{x})=\mathbf{1},\quad \mathbf{W}(\mathbf{x})=\mathbf{e}^{(-1/2)\,\alpha\mathbf{x}^2+\beta\mathbf{x}},$$

$$-\infty<x<+\infty,\quad \alpha>0,\quad -\infty<\beta<+\infty,$$

$$H_{n,m}^{(\alpha,\beta)}(x)=\frac{a_n(-1)^m}{e^{(-1/2)\,\alpha x^2+\beta x}}\left(\frac{d}{dx}\right)^{n-m}(e^{(-1/2)\,\alpha x^2+\beta x}),$$

$$x=r,$$

$$B_m(r)=\tfrac{1}{2}[\beta-2\alpha r]dr\wedge d\theta,$$

$$\psi_{n,m}(r)=e^{(-1/4)\,\alpha r^2+(1/2)\,\beta r}H_{n,m}^{(\alpha,\beta)}(r),$$

$$E_{n,m}=\sqrt{\alpha(n-m+1)};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{x},\quad \mathbf{W}(\mathbf{x})=\mathbf{x}^{\alpha}\mathbf{e}^{-\beta\mathbf{x}},$$

$$0<x<+\infty,\quad \alpha>-1,\quad \beta>0,$$

$$L_{n,m}^{(\alpha,\beta)}(x)=\frac{a_n(-1)^m}{x^{\alpha+m/2}e^{-\beta x}}\left(\frac{d}{dx}\right)^{n-m}(x^{n+\alpha}e^{-\beta x}),$$

$$x=\tfrac{1}{4}r^2,$$

$$B_m(r)=-\tfrac{1}{2}\beta r\,dr\wedge d\theta,$$

$$\psi_{n,m}(r)=\left(\frac{r^2}{4}\right)^{(1/2)(\alpha+1/2)}e^{(-1/8)\beta r^2}L_{n,m}^{(\alpha,\beta)}\left(\frac{1}{4}r^2\right),$$

$$E_{n,m}=\sqrt{\beta(n-m+1)};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{x^2},\quad \mathbf{W}(\mathbf{x})=\mathbf{x}^{\alpha}\mathbf{e}^{-\beta/\mathbf{x}},$$

$$0<x<+\infty,\quad \alpha<-2,\quad \beta>0,$$

$$\overline{F}_{n,m}^{(\alpha,\beta)}(x)=\frac{a_n(-1)^m}{x^{\alpha+m}e^{-\beta/x}}\left(\frac{d}{dx}\right)^{n-m}(x^{2n+\alpha}e^{-\beta/x}),$$

$$x=e^r,$$

$$B_m(r)=\tfrac{1}{2}[\alpha+2m-1+\beta(1-r)e^{-r}]dr\wedge d\theta,$$

$$\psi_{n,m}(r)=e^{(1/2)(1+\alpha)r}e^{(-1/2)\beta e^{-r}}\overline{F}_{n,m}^{(\alpha,\beta)}(e^r),$$

$$E_{n,m}=\sqrt{-(n-m+1)(n+m+\alpha)};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{1}-\mathbf{x^2},\quad \mathbf{W}(\mathbf{x})=(\mathbf{1}-\mathbf{x})^{\alpha}(\mathbf{1}+\mathbf{x})^{\beta},$$

$$-1<x<+1,\quad \alpha>-1,\quad \beta>-1,$$

$$P_{n,m}^{(\alpha,\beta)}(x)=\frac{a_n(-1)^m}{(1-x)^{\alpha+m/2}(1+x)^{\beta+m/2}}\left(\frac{d}{dx}\right)^{n-m}((1-x)^{n+\alpha}(1+x)^{n+\beta}),$$

$$x=-\cos r,$$

$$B_m(r)=\frac{1}{2}\left[\frac{\beta-\alpha}{\sin r}(1-r\cot r)-(\alpha+\beta+2m-1)(r\cot^2 r-\cot r+r)\right]dr\wedge d\theta,$$

$$\psi_{n,m}(r)=(1+\cos r)^{(1/2)(\alpha+1/2)}(1-\cos r)^{(1/2)(\beta+1/2)}P_{n,m}^{(\alpha,\beta)}(-\cos r),$$

$$E_{n,m}=\sqrt{(n-m+1)(n+m+\alpha+\beta)};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{x^2}-\mathbf{1},\quad \mathbf{W}(\mathbf{x})=(\mathbf{x}-\mathbf{1})^{\alpha}(\mathbf{x}+\mathbf{1})^{\beta},$$

$$+1<x<+\infty,\quad \alpha>-1,\quad \alpha+\beta<-2,$$

$$\mathcal{P}_{n,m}^{(\alpha,\beta)}(x)=\frac{a_n(-1)^m}{(x-1)^{\alpha+m/2}(x+1)^{\beta+m/2}}\left(\frac{d}{dx}\right)^{n-m}((x-1)^{n+\alpha}(x+1)^{n+\beta}),$$

$$x=\cosh r,$$

$$B_m(r)=\frac{1}{2}\left[\frac{\alpha-\beta}{\sinh r}(1-r\coth r)-(\alpha+\beta+2m-1)(r\coth^2 r-\coth r-r)\right]dr\wedge d\theta,$$

$$\psi_{n,m}(r)=(\cosh r-1)^{(1/2)(\alpha+1/2)}(\cosh r+1)^{(1/2)(\beta+1/2)}\mathcal{P}_{n,m}^{(\alpha,\beta)}(\cosh r),$$

$$E_{n,m}=\sqrt{-(n-m+1)(n+m+\alpha+\beta)};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{1}+\mathbf{x^2},\quad \mathbf{W}(\mathbf{x})=(\mathbf{1}+\mathbf{x^2})^{\alpha}\mathbf{e}^{\beta\tan^{-1}\mathbf{x}},$$

$$-\infty<x<+\infty,\quad \alpha<-1,\quad -\infty<\beta<+\infty,$$

$$\mathcal{T}_{n,m}^{(\alpha,\beta)}(x)=\frac{a_n(-1)^m}{(1+x^2)^{\alpha+m/2}e^{\beta\tan^{-1}x}}\left(\frac{d}{dx}\right)^{n-m}((1+x^2)^{n+\alpha}e^{\beta\tan^{-1}x}),$$

$$x=\sinh r,$$

$$B_m(r)=\frac{1}{2}\left[\frac{\beta}{\cosh r}(1-r\tanh r)-(2\alpha+2m-1)(r\tanh^2 r-\tanh r-r)\right]dr\wedge d\theta,$$

$$\psi_{n,m}(r)=\cosh^{\alpha+1/2}r e^{(1/2)\,\beta\tan^{-1}\sinh r}\mathcal{T}_{n,m}^{(\alpha,\beta)}(\sinh r),$$

$$E_{n,m}=\sqrt{-(n-m+1)(n+m+2\alpha)};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{x}(\mathbf{1}-\mathbf{x}),\quad \mathbf{W}(\mathbf{x})=\mathbf{x}^{\alpha}(\mathbf{1}-\mathbf{x})^{\beta},$$

$$0<x<+1,\quad \alpha>-1,\quad \beta>-1,$$

$$F_{n,m}^{(\alpha,\beta)}(x)=\frac{a_n(-1)^m}{x^{\alpha+m/2}(1-x)^{\beta+m/2}}\left(\frac{d}{dx}\right)^{n-m}(x^{n+\alpha}(1-x)^{n+\beta}),$$

$$x=\frac{1+\sin r}{2},$$

$$B_m(r)=\frac{1}{2}\left[\frac{\alpha-\beta}{\cos r}(1+r\tan r)-(\alpha+\beta+2m-1)(r\tan^2 r+\tan r+r)\right]dr\wedge d\theta,$$

$$\psi_{n,m}(r)=\left(\frac{1+\sin r}{2}\right)^{(1/2)(\alpha+1/2)}\left(\frac{1-\sin r}{2}\right)^{(1/2)(\beta+1/2)}F_{n,m}^{(\alpha,\beta)}\left(\frac{1+\sin r}{2}\right),$$

$$E_{n,m}=\sqrt{(n-m+1)(n+m+\alpha+\beta)};$$

$$\mathbf{A}(\mathbf{x})=\mathbf{x}(\mathbf{1}+\mathbf{x}),\quad \mathbf{W}(\mathbf{x})=\mathbf{x}^{\alpha}(\mathbf{1}+\mathbf{x})^{\beta},$$

$$0<x<+\infty,\quad \alpha>-1,\quad \alpha+\beta<-2,$$

$$\mathcal{F}_{n,m}^{(\alpha,\beta)}(x)=\frac{a_n(-1)^m}{x^{\alpha+m/2}(1+x)^{\beta+m/2}}\left(\frac{d}{dx}\right)^{n-m}(x^{n+\alpha}(1+x)^{n+\beta}),$$

$$x=\frac{\cosh r-1}{2},$$

$$B_m(r)=\frac{1}{2}\left[\frac{\alpha-\beta}{\sinh r}(1-r\coth r)-(\alpha+\beta+2m-1)(r\coth^2 r-\coth r-r)\right]dr\wedge d\theta,$$

$$\psi_{n,m}(r)=\left(\frac{\cosh r-1}{2}\right)^{(1/2)(\alpha+1/2)}\left(\frac{\cosh r+1}{2}\right)^{(1/2)(\beta+1/2)}\mathcal{F}_{n,m}^{(\alpha,\beta)}\left(\frac{\cosh r-1}{2}\right),$$

$$E_{n,m}=\sqrt{-(n-m+1)(n+m+\alpha+\beta)}.$$

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Noncommutative Bloch theory

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For differential operators which are invariant under the action of an Abelian group Bloch theory is the preferred tool to analyze spectral properties. By shedding some new noncommutative light on this we motivate the introduction of a noncommutative Bloch theory for elliptic operators on Hilbert C*-modules. It relates properties of C*-algebras to spectral properties of module operators such as band structure, weak genericity of cantor spectra, and absence of discrete spectrum. It applies, e.g., to differential operators invariant under a projective group action, such as Schrödinger, Dirac, and Pauli operators with periodic magnetic field, as well as to discrete models, such as the almost Matthieu equation and the quantum pendulum.
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I. INTRODUCTION

Bloch (or Floquet) theory in its usual form has a long history already. Basically it starts from the fact that partial differential equations with constant coefficients are mapped into algebraic equations by means of the Fourier or Laplace transform. Now, if the coefficients are not constant but just periodic under an Abelian (locally compact topological) group one still has the Fourier transform on such groups, mapping functions on the group Γ into functions on the dual group $\hat{\Gamma}$; the original spectral problem on a noncompact manifold is mapped into a (continuous) sum of spectral problems on a compact manifold (see Sec. II).

This is what makes Bloch theory an indispensable tool especially for solid state physics, where one describes the motion of noninteracting electrons in a periodic solid crystal by a Schrödinger operator $-\Delta+V$ on $L^2(\mathbb{R}^d)$. The potential function V is the gross electric potential generated by all the crystal ions and thus is periodic under the lattice given by the crystal symmetry. Bloch theory shows that the spectrum of the periodic Schrödinger operator has band structure in the following sense:

Definition 1 (band structure): A subset of the real line has band structure if it is a locally finite union of closed intervals.

Band structure is an essential ingredient of electronic transport in metals and semi-conductors. By exploiting Bloch theory and the structure of the Schrödinger operator further one can see that the spectrum is purely absolutely continuous, which is sometimes included in the definition of band structure.

Measurements of crystals often require magnetic fields b (2-form). In quantum mechanics, they are described by a vector potential (1-form) a such that $b=da$ ($B=\operatorname{curl} A$ for the corresponding vector fields). The magnetic Schrödinger operator then reads

$$H=-(\nabla-ia)^2+V.$$

But, although b is periodic or even constant, a need not be so, and H will not be periodic. It is therefore necessary to use magnetic translations under which H still is invariant.[1] But now, these translations do not commute with each other in general. Therefore ordinary (commutative) Bloch theory does not apply.

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Basically, the reason for this failure is that a non-Abelian group has no ''good'' group dual: the set of (equivalence classes of) irreducible representations has no natural group structure whereas the set of one-dimensional representations is too small to describe the group—otherwise it would be Abelian.

But although $\hat{\Gamma}$ does not exist anymore, the algebra $C(\hat{\Gamma})$ of continuous functions continues to exist in some sense: It is given by the reduced group C^*-algebra of Γ which is just the C^*-algebra generated by Γ in its regular representation on itself [on $l^2(\Gamma)$].

Section III shows how one can reformulate ordinary Bloch theory in a way which refrains from using the points of $\hat{\Gamma}$ and relies just on the role of $C(\hat{\Gamma})$. From a technical point of view this requires switching from measurable fields of Hilbert spaces to continuous fields which then can be described as Hilbert C^*-modules over the commutative C^*-algebra $C(\hat{\Gamma})$.

Having done this one can retain the setup but omit the condition of commutativity for the C^*-algebra $C(\hat{\Gamma})$. Thus one is lead to noncommutative Bloch theory (Sec. IV) dealing with elliptic operators on Hilbert C^*-modules over noncommutative C^*-algebras. The basic task is now to relate properties of the C^*-algebra to spectral properties of ''periodic'' operators. Thus one generalizes spectral results for elliptic operators on compact manifolds as well as results of ordinary Bloch theory:

Theorem 1: *Isolated eigenvalues of $\mathcal{A}$-elliptic operators have $\mathcal{A}$-finite eigenprojections, their eigenspaces have finite τ-dimension.*

Under certain assumptions they have essential spectrum only (isolated eigenvalues have infinite multiplicity).

See Theorem 6 for exact assumptions (they are fulfilled by Schrödinger operators with periodic magnetic field).

Noncommutative Bloch theory allows to treat continuous and discrete models, i.e., differential and difference operators, on equal footing. It opens the way to apply a result of Choi and Elliott[2] on weak genericity of Cantor spectra in discrete models to the continuous models also, i.e., to the phenomenon opposite to the band structure:

Definition 2 (Cantor set): A Cantor set is a subset of a topological space which is nowhere dense (the closure has empty interior) and has no isolated points.

Now the C^*-algebras of symmetries determines which of the two opposite spectral types is present:

Definition 3 (Kadison property): The Kadison constant K of a C^*-algebra $\mathcal{A}$ together with a trace τ is defined by

$$K = \inf\{\tau(P) \,|\, 0 \neq P \in \mathcal{A} \text{ projection}\}. \tag{1}$$

We say the pair $(\mathcal{A}, \tau)$ has the Kadison property if $K > 0$.

Theorem 2 (band structure): *If $(\mathcal{A}, \tau)$ has the Kadison property, then the spectrum of every symmetric $\mathcal{A}$-elliptic operator has a band structure.*

(See Theorem 7.) This applies, e.g., to magnetic Schrödinger operators in the case of rational magnetic flux.

Opposite to the Kadison property is the property RRI_0 (see Definition 4), and it is a criterion for the opposite spectral type:

Theorem 3 (Cantor spectrum): *If $(\mathcal{A}, \tau)$ has the property RRI_0, then every $\mathcal{A}$-elliptic operator can be approximated arbitrarily well (in norm resolvent sense) by one which has Cantor spectrum.*

(See Theorem 8.) The important issue here is that the approximation takes place within a natural C^*-algebra generated by symmetries connected to the operator. Approximation within a von Neumann algebra would be pointless, of course. This theorem applies, e.g., to magnetic Schrödinger operators on $\mathbb{R}^2$ in the case of irrational flux.

In Sec. V we list examples where noncommutative Bloch theory applies: gauge-periodic

elliptic differential operators (Schrödinger, Pauli, Dirac with periodic magnetic field) and difference operators (almost Matthieu, quantum pendulum).

For the convenience of the reader we add an appendix on continuous fields of Hilbert spaces and on Hilbert C^*-modules and their GNS representation.

A short overview of this paper appeared in Ref. 3.

II. COMMUTATIVE BLOCH THEORY

In this section we recall the basic elements of Bloch theory for periodic operators in the geometric context of vector bundles, since even in the scalar case of a magnetic Schrödinger operator one is lead to consider possibly nontrivial complex line bundles.[4] The standard reference for the theory of direct integrals is Ref. 5, Chap. II; for the Bloch theory in Euclidean space see Ref. 6, Chap. XIII.16.

Our general assumptions are: X is an oriented smooth Riemannian manifold without boundary, Γ a discrete abelian group acting on X freely, isometrically, and properly discontinuously. Furthermore, we assume the action to be cocompact in the sense that the quotient $M:=X/\Gamma$ is compact.

Next, let E be a smooth Hermitian vector bundle over X.

Example 1 (solid crystals): The main motivating example for our setting comes from solid state physics. Here, $X=\mathbb{R}^n$ is the configuration space of a single electron $(n=2,3)$. It is supposed to move in a crystal whose translational symmetries are described by a lattice $\mathbb{Z}^n\simeq\Gamma\subset\mathbb{R}^n$, which acts on X by translations, of course. Note that this does not take into account the point symmetries. Γ could be extended by them but the action would not be free any more. Considering just the translations is enough to achieve the compactness of the quotient $M\simeq T^n$.

Wave functions of electrons are just complex-valued functions on $\mathbb{R}^n$, so we can set $E=\mathbb{R}^n\times\mathbb{C}$. One may also include the spin of the electrons into the picture by choosing the appropriate trivial spinor bundle $E=\mathbb{R}^n\times\mathbb{C}^k$.

Definition 4 (periodic operator): Assume there is an isometric lift γ_* of the action of γ from X to E in the following sense:

$$\gamma_*:E_x\to E_{\gamma x} \quad \text{for} \quad x\in X,\gamma\in\Gamma. \tag{2}$$

This defines an action T_γ on the sections: For $s\in C_c^\infty(E)$ we define

$$(T_\gamma s)(x):=\gamma_* s(\gamma^{-1}x) \quad \text{for} \quad x\in X,\gamma\in\Gamma. \tag{3}$$

$(T_\gamma)_{\gamma\in\Gamma}$ induces a unitary representation of Γ in $L^2(E)$ since γ_* acts isometrically and $T_\gamma^*=(T_\gamma)^{-1}$.

A differential operator D on $\mathcal{D}(D):=C_c^\infty(E)$ is called periodic if, on $\mathcal{D}(D)$, we have

$$\forall\,\gamma\in\Gamma:[T_\gamma,D]=0. \tag{4}$$

Example 2 (periodic Schrödinger operator): Given a manifold as described above, we may lift the action to any trivial vector bundle $E:=X\times\mathbb{C}^k$ canonically. If D is a periodic operator on X (for example any geometric operator, i.e., defined by the metric on X) and $V\in C^\infty(X,M(k,\mathbb{C}))$ a periodic field of endomorphisms, then $D+V$ is a periodic operator on E.

In the case of a crystal, we choose the Laplacian (which describes the kinetic energy quantum mechanically) and a periodic potential $V\in C^\infty(\mathbb{R}^n,\mathbb{R})$ (which describes the electric field of the ions at the lattice sites) to get the periodic Schrödinger operator $\Delta+V$.

Example 3 (Schrödinger operator with exact periodic magnetic field): Let $b\in\Omega^2(X)$ be a magnetic field 2-form. In dimension 3 this corresponds (by the Hodge star) to a vector field B, in dimension 2 to a scalar function which may be thought of as the length and orientation of a normal vector B. From physical reasons one has $\operatorname{div}B=0$, *i.e., $db=0$. For simplicity we assume that b is not only closed but exact, so there is $a\in\Omega^1(X)$ with $b=da$ ($B=\operatorname{curl}A$ for the corresponding vector fields). This defines a magnetic Hamiltonian operator*

$$\Delta^a := (d-\imath a)^*(d-\imath a) \tag{5}$$

(the minimally coupled Hamiltonian), where d is the ordinary differential (corresponding to the gradient) and $*$ the adjoint of an operator between the Hilbert spaces of L^2-functions $L^2(X)$ and of L^2-1-forms $L^2(X,\Lambda T^*X)$.

For later convenience we set, for $\gamma\in\Gamma$ and $\omega\in\Omega(X)$, $\gamma^*\omega := (\gamma^{-1})^*\omega$, considering γ^{-1} as a map $X\to X$ and using the usual pullback of forms. This puts the action on forms in a notation compatible with the action in sections (3) from the preceding definition.

Now, if b is periodic, a does not need to be so: If $b\in\Omega^2(\mathbb{R}^n)$ is constant then a is affine linear. So the translations are no symmetries for the magnetic Hamiltonian. Reference 1 was the first to define the so-called magnetic translations: Since $d(a-\gamma^*a)=da-\gamma^*da=b-\gamma^*b=0$, one can [at least if $H^1(X)=0$] find a function χ_γ with $d\chi_\gamma=a-\gamma^*a$. One may define such a function explicitly by

$$\chi_\gamma(x) := \int_{x_0}^{x}(a-\gamma^*a)$$

which is well-defined if $H_1(X)=0$. If we now define a gauge function $s_\gamma := e^{\imath\chi_\gamma}$ then

$$\begin{aligned}(d-\imath a)(s_\gamma\gamma^*f) &= s_\gamma\gamma^*df+\imath(a-\gamma^*a)s_\gamma\gamma^*f-\imath a s_\gamma\gamma^*f\\ &= s_\gamma\gamma^*df-\imath\gamma^*a\gamma^*f\\ &= s_\gamma\gamma^*df-\imath s_\gamma\gamma^*(af)\\ &= s_\gamma\gamma^*((d-\imath a)f).\end{aligned}$$

So we have found symmetries of the magnetic Hamiltonian operator, the gauged translations

$$T_\gamma : C^\infty(X)\to C^\infty(X),\quad (T_\gamma s)(x)=s_\gamma(x)(\gamma^*s)(x)$$

coming from the lifted action,

$$\gamma_* : X\times\mathbb{C}\to X\times\mathbb{C},\quad \gamma_*(x,c)=(\gamma x, s_\gamma(x)c).$$

The commutation relation for the magnetic translations is

$$\begin{aligned}(T_{\gamma_1}T_{\gamma_2}s)(x) &= s_{\gamma_1}(x)s_{\gamma_2}(\gamma_1^{-1}x)s(\gamma_2^{-1}\gamma_1^{-1}x)\\ &= \exp\left(\imath\left(\int_{x_0}^{x}a-\gamma_1^*a+\int_{x_0}^{\gamma_1^{-1}x}a-\gamma_2^*a\right)\right)s(\gamma_2^{-1}\gamma_1^{-1}x)\\ &= \exp\left(\imath\left(\int_{x_0}^{x}a-\gamma_1^*a+\int_{\gamma_1x_0}^{x}\gamma_1^*a-(\gamma_1\gamma_2)^*a\right)\right)s(\gamma_2^{-1}\gamma_1^{-1}x)\\ &= \exp\left(\imath\left(\int_{x_0}^{\gamma_1x_0}(\gamma_1\gamma_2)^*a-\gamma_1^*a+\int_{x_0}^{x}a-(\gamma_1\gamma_2)^*a\right)\right)s(\gamma_2^{-1}\gamma_1^{-1}x)\\ &= \exp\left(\imath\left(\int_{x_0}^{\gamma_1x_0}(\gamma_1\gamma_2)^*a-\gamma_1^*a\right)\right)s_{\gamma_1\gamma_2}(x)s(\gamma_2^{-1}\gamma_1^{-1}x)\\ &= \Theta(\gamma_1,\gamma_2)s_{\gamma_1\gamma_2}(x)s(\gamma_2^{-1}\gamma_1^{-1}x)\\ &= \Theta(\gamma_1,\gamma_2)(T_{\gamma_1\gamma_2}s)(x)\end{aligned} \tag{6}$$

with $\Theta(\gamma_1,\gamma_2)\in S^1$. In general this is just a projective representation of Γ. If a itself is periodic, then $\chi_\gamma=0$ for $\gamma\in\Gamma$, i.e., there is no gauge, and we have just ordinary translations forming a proper representation.

But even if a is not periodic it can happen that the magnetic translations commute with each other. This is called the case of integral flux since the term occurring in the exponential in line (6) is just the magnetic flux through one lattice face. A periodic a obviously gives rise to zero magnetic flux.

Furthermore, if $V\in C^\infty(X,\mathbb{R})$ is Γ-periodic it commutes with the magnetic translations as well, so Δ^a+V is a (symmetric elliptic) periodic operator.

Finally, the very same magnetic translations can be used for the Pauli Hamiltonian and the magnetic Dirac operator.

Remark 1 (integral flux): In the case of the integral flux mentioned above quite the opposite spectral phenomena can occur: Periodic Schrödinger operators have an absolutely continuous band spectrum, whereas the Landau Hamiltonian on $\mathbb{R}^2$ (constant magnetic field, no electric potential) exhibits a pure point spectrum of infinite degeneracy. In Ref. 7 we show that these are indeed the only phenomena that can occur (although possibly combined) in the case of integral flux.

Remark 2 (nonintegral flux): If the magnetic flux is rational one can find a superlattice of Γ, i.e., a subgroup of finite index, such that the flux is integral. The quotient will still be compact, of course, so that the rational case can be completely reduced to the integral.

If the magnetic flux is irrational there is no such superlattice. Still, one may try to make use of the projective representation defined above. There are several approaches, similar in the objects which are used, different in the objectives that are aimed at and accordingly in the results. Our approach will mimic Bloch theory noncommutatively, see Sec. III.

Remark 3 (nonexact magnetic field): If b is closed but not exact one first has to agree upon the quantization procedure used. (5) may be identified as a Bochner Laplacian for a connection with curvature b, and such a connection exists if and only if b defines an integral cohomology class, i.e., $[b]\in H^2(X,\mathbb{Z})$. There may exist different quantizations for the same magnetic field. This is connected to the Bloch decomposition again. For this and the construction of the magnetic translations in this case, see Ref. 8.

Lemma 1 (associated bundle): E is the lift π^*E' of a Hermitian vector bundle E' over M by the projection $\pi:X\to M$. E and X are Γ-principal fiber bundles over E' resp. M.

To every Γ-principal fiber bundle and every character $\chi\in\hat{\Gamma}$ we associate a line bundle. This gives the relations depicted in the following diagram ("$\rightsquigarrow$" denotes association of line bundles.),

$$\begin{array}{ccccccc}
 & \mathbb{C}^N & & \mathbb{C}^N & & \mathbb{C}^N & & \mathbb{C}^N \\
 & \downarrow & & \downarrow & & \downarrow & & \downarrow \\
\Gamma & \hookrightarrow & E & \longrightarrow & E' & \rightsquigarrow & \mathbb{C} \hookrightarrow E_\chi & \longrightarrow & E' \\
 & \downarrow{\scriptstyle \pi^E} & & \downarrow{\scriptstyle \pi^{E'}} & & & \downarrow & & \downarrow \\
\Gamma & \hookrightarrow & X & \xrightarrow{\pi} & M & \rightsquigarrow & \mathbb{C} \hookrightarrow F_\chi & \longrightarrow & M
\end{array}$$

principal fiber bundles and associated line bundles.

In this situation we have $E_\chi\simeq E'\otimes F_\chi$.

For proofs of this and the following, basically well-known material in this section: see e.g., Ref. 8.

Example 4 (magnetic bundles): Consider again the case of the magnetic translations for a periodic magnetic 2-form $b \in \Omega^2(X)$, E being a complex line bundle with curvature b ($b \in H^2(X,\mathbb{Z})$). Hence we have $c_1(E)=[b]$ for the Chern class (up to factors of 2π, depending on the convention). Since b is periodic we may restrict it to a form $b_M \in \Omega^2(M)$ on the quotient. The existence of the lifted action, i.e., the fact that E can be written as a pull-back $E=\pi^*E'$, corresponds to the integrality of b_M from $c_1(E')=[b_M] \in H^2(M,\mathbb{Z})$. Tensoring E' with the flat line bundle F_χ does not change the Chern class (up to torsion). In particular, in dimension 2 the integrality of b_M is equivalent to the integrality of the flux, and E' is trivial only for zero flux.

Next we want to decompose the Hilbert space $L^2(E)$ of square-integrable sections of E into a direct integral over the character space $\hat{\Gamma}$. On $\hat{\Gamma}$ we use the Haar measure. From the theory of representations of locally compact groups we need the following character relations for abelian discrete Γ, i.e., for Abelian, compact $\hat{\Gamma}$ (see Ref. 9, Sec. I E):

Lemma 2 (character relations): For $\gamma \in \Gamma$,

$$\int_{\hat{\Gamma}} \chi(\gamma)\, d\chi = \begin{cases} 1, & \gamma = e, \\ 0, & \gamma \neq e. \end{cases} \tag{7}$$

For $\chi, \chi' \in \hat{\Gamma}$,

$$\sum_{\gamma \in \Gamma} \overline{\chi}(\gamma)\chi'(\gamma) = \delta(\chi - \chi') \tag{8}$$

in the distributional sense, i.e., for $f \in C(\hat{\Gamma})$,

$$\sum_{\gamma \in \Gamma} \int_{\hat{\Gamma}} \overline{\chi}(\gamma)\chi'(\gamma) f(\chi)\, d\chi = f(\chi').$$

We define for every character $\chi \in \hat{\Gamma}$ a mapping $\Phi_\chi : C_c^\infty(E) \ni s \mapsto \tilde{s}_\chi \in C^\infty(E)$ by

$$\tilde{s}_\chi(x) := \sum_{\gamma \in \Gamma} \chi(\gamma)\, \gamma_* s(\gamma^{-1}x). \tag{9}$$

Since

$$\begin{aligned} \tilde{s}_\chi(\gamma' x) &= \sum_{\gamma \in \Gamma} \chi(\gamma)\, \gamma s(\gamma^{-1}\gamma' x) \\ &= \sum_{\gamma \in \Gamma} \chi(\gamma' \gamma'^{-1}\gamma)(\gamma' \gamma'^{-1}\gamma)_* s((\gamma'^{-1}\gamma)^{-1}x) \\ &= \chi(\gamma')\, \gamma'_* \tilde{s}_\chi(x), \end{aligned}$$

we have

$$\tilde{s}_\chi \in C^\infty(E)^{\Gamma,\chi} = \{ r \in C^\infty(E) \mid \forall_{\gamma \in \Gamma} T_\gamma r = \chi(\gamma) r \}$$

which defines a section $s_\chi \in C^\infty(E_\chi)$.

Let $\mathcal{D}$ be a fundamental domain for the Γ-action, i.e., an open subset of X such that $\cup_{\gamma \in \Gamma} \gamma \mathcal{D} = X$ up to a set of measure 0 and $\gamma \mathcal{D} \cap \mathcal{D} = \varnothing$ for $\gamma \neq e$. Then,

$$\int_{\hat{\Gamma}} \|s_\chi\|^2_{L^2(E_\chi)} d\chi = \int_{\hat{\Gamma}} \int_{\mathcal{D}} |\tilde{s}_\chi(x)|^2 dx\, d\chi$$

$$= \int_{\mathcal{D}} \int_{\hat{\Gamma}} \sum_{\gamma_1, \gamma_2 \in \Gamma} \chi(\gamma_1^{-1}\gamma_2) \langle \gamma_{1*} s(\gamma_1^{-1}x) | \gamma_{2*} s(\gamma_2^{-1}x) \rangle_E d\chi\, dx$$

$$= \int_{\mathcal{D}} \sum_{\gamma \in \Gamma} |s(\gamma^{-1}x)|^2 dx$$

$$= \|s\|^2_{L^2(E)}.$$

On the one hand, this shows that we can define a measurable structure on $\Pi_{\chi \in \hat{\Gamma}} L^2(E_\chi)$ by choosing a sequence in $C_c^\infty(E)$ which is the total in $L^2(E)$. On the other hand, we can see that the direct integral $\int_{\hat{\Gamma}}^{\oplus} L^2(E_\chi)\, d\chi$ is isomorphic to $L^2(E)$ via the isometry Φ, whose inverse is given by

$$\Phi^*: (s_\chi)_{\chi \in \hat{\Gamma}} \mapsto \int_{\hat{\Gamma}} \tilde{s}_\chi(x)\, d\chi,$$

as is easily seen from the character relations (7) and (8).

This shows

Lemma 3 (direct integral): The mapping defined by (9) can be extended continuously to a unitary,

$$\Phi: L^2(E) \to \int_{\hat{\Gamma}}^{\oplus} L^2(E_\chi)\, d\chi. \tag{10}$$

For the direct integral of Hilbert spaces $H = \int_{\hat{\Gamma}}^{\oplus} H_\chi d\chi$ the set of decomposable bounded operators $L^\infty(\hat{\Gamma}, \mathcal{L}(H))$ is given by the commutant $(L^\infty(\hat{\Gamma}, \mathbb{C}))'$ in $\mathcal{L}(H)$. Since commutants are weakly closed and $C(\hat{\Gamma}, \mathbb{C})$ is weakly dense in $L^\infty(\hat{\Gamma}, \mathbb{C})$ one has $(L^\infty(\hat{\Gamma}, \mathbb{C}))' = (C(\hat{\Gamma}, \mathbb{C}))'$. Therefore, in order to determine the decomposable operators one has to determine the action of $C(\hat{\Gamma})$ on $L^2(E)$. This is easily done using the explicit form of Φ:

Proposition 1 $[C(\hat{\Gamma})\text{-}action]$: *$f \in C(\hat{\Gamma})$ acts on $s \in C_c^\infty(E)$ by*

$$M_f s := \Phi^* f \Phi s, \tag{11}$$

and one has

$$(M_f s)(x) = \sum_{\gamma \in \Gamma} \hat{f}(\gamma^{-1}) T_\gamma s(x), \tag{12}$$

where

$$\hat{f}(\gamma) := \int_{\hat{\Gamma}} f(\chi) \overline{\chi}(\gamma)\, d\chi \tag{13}$$

is the Fourier transform of f. M_f is a bounded operator with norm $\|f\|_\infty$.

Corollary 1 (decomposable operators): Conjugation by Φ defines an isomorphism between decomposable bounded operators on $\int_{\hat{\Gamma}}^{\oplus} L^2(E_\chi)\, d\chi$ and Γ-periodic bounded operators on $L^2(E)$.

An unbounded operator is decomposable if and only if its (bounded) resolvent is decomposable. For a periodic symmetric elliptic operator D we have a domain of definition $\mathcal{D}(D)$

$=C_c^\infty(X)$ on which D is essentially self-adjoint. This domain is invariant for D as well as for the Γ-action, and one has $[D,\gamma]=0$ for all $\gamma\in\Gamma$. Thus all bounded functions of D commute with the Γ-action, and one has

Theorem 4 (decomposition of periodic operators): *The closure $\overline{D}$ of every periodic symmetric elliptic operator D is decomposable with respect to the direct integral of Hilbert spaces $\int_{\hat\Gamma}^{\oplus} L^2(E_\chi)\,d\chi$. A core for the domain of $\overline{D}_\chi$ is given by $C^\infty(E_\chi)$, and the action of D_χ on $C^\infty(E_\chi)\simeq C^\infty(E)^{\Gamma,\chi}$ is just the action of D as differential operator on $C^\infty(E)^{\Gamma,\chi}$. We have $\overline{D}_\chi=\overline{D_\chi}$, where*

$$D_\chi := D|_{C^\infty(E)^{\Gamma,\chi}} \tag{14}$$

and the closures are to be taken as operators in $L^2(E_\chi)$.

Proof: Given the remark above we have shown the decomposability already.

$C_c^\infty(X)$ is a core for $\overline{D}$, its image under Φ_χ is contained in $C^\infty(E)^{\Gamma,\chi}$ and is a core for $\overline{D}_\chi$, since Φ is an isometry. On this domain (9) gives the action of $\overline{D}_\chi$ as asserted in the theorem. Since D_χ is a symmetric elliptic operator on the compact manifold M it is essentially self-adjoint. $\overline{D}_\chi$ is a fiber of $\overline{D}$ (which is self-adjoint by, e.g., Ref. 10) and therefore self-adjoint, thus both define the same unique self-adjoint extension $\overline{D_\chi}$ of D_χ. □

In passing we harvest a corollary which we will not use in the sequel, but which is well known in the Euclidean setting:

Corollary 2 (reverse Bloch property): Every symmetric elliptic Abelian periodic operator has the reverse Bloch property, i.e., to every $\lambda\in\operatorname{spec}\overline{D}$ there is a bounded generalized eigensection $s\in C^\infty(E)$ with $Ds=\lambda s$.

Proof: If $\lambda\in\operatorname{spec}\overline{D}$ then, by the general theory for direct integrals,

$$\{\chi\in\hat\Gamma\,|\,(\lambda-\varepsilon,\lambda+\varepsilon)\cap\operatorname{spec}\overline{D}_\chi\neq\varnothing\}$$

has positive measure for every $\varepsilon>0$. The fibers $\overline{D}_\chi$ are elliptic operators on a compact manifold and thus have discrete spectrum; the eigenvalues depend continuously on χ (even piecewise real-analytically; see below). We choose a sequence $(\chi_n)_{n\in\mathbb{N}}$ with $(\lambda-1/n,\lambda+1/n)\cap\operatorname{spec}\overline{D}_{\chi_n}\neq\varnothing$, so that there is an accumulation point χ_∞ ($\hat\Gamma$ is compact), and $\lambda\in\operatorname{spec}\overline{D}_{\chi_\infty}$ due to continuity.

Since $\operatorname{spec}\overline{D}_{\chi_\infty}$ is discrete λ is an eigenvalue of $\overline{D}_{\chi_\infty}$. The lift of an eigensection (which is smooth due to ellipticity) lies in $C^\infty(E)^{\Gamma,\chi}$ and therefore is bounded. Furthermore the lift satisfies the same eigenvalue equation because of (14). □

III. COMMUTATIVE BLOCH THEORY FROM A NONCOMMUTATIVE POINT OF VIEW

By Gelfand's representation theorem every commutative C^*-algebra $\mathcal{A}$ is isomorphic to $C_\infty(X)$, the continuous functions vanishing at infinity of a topological Hausdorff space X, where X is the spectrum $\hat{\mathcal{A}}$ of $\mathcal{A}$, i.e., the set of equivalence classes of irreducible unitary representations;[11] C^*-norm is given by the supremum norm, the involution by pointwise complex conjugation. Hilbert $\mathcal{A}$-modules are given by the sections $C_\infty(\mathcal{H})$ of a continuous field of Hilbert spaces over X, finitely generated projective $\mathcal{A}$-modules are given by the sections $C_\infty(E)$ of a vector bundle E over X.[12] In this section we describe the corresponding structures in the case of periodic elliptic differential operators, so that we can find a formulation of Bloch theory that avoids using the points of the space $\hat\Gamma$ and relies solely on the algebraic structures with respect to $C(\hat\Gamma)$.

In Proposition 1 we already determined the action of $C(\hat{\Gamma})$ on $L^2(E)$. Now we use the scalar product that is given in each fiber by the direct integral to define a $C(\hat{\Gamma})$-values scalar product:

Definition and proposition 1 [pre-Hilbert $C(\hat{\Gamma})$-module]: For $s_1, s_2 \in C_c^\infty(E)$ we define by

$$\langle s_1 | s_2 \rangle(\chi) := \langle (\Phi s_1)_\chi | (\Phi s_2)_\chi \rangle_{L^2(E_\chi)}, \tag{15}$$

a $C(\hat{\Gamma})$-valued scalar product that makes $C_c(E)$ into a pre-Hilbert C^*-module over $C(\hat{\Gamma})$; it is a submodule of the $C(\hat{\Gamma})$-module $L^2(E)$.

Proof: $C_c(E)$ is obviously a $C(\hat{\Gamma})$-submodule of $L^2(E)$. Furthermore, by definition the scalar product is

$$\begin{aligned}
\langle s_1 | s_2 \rangle(\chi) &= \langle (\Phi s_1)_\chi | (\Phi s_2)_\chi \rangle_{L^2(E_\chi)} \\
&= \sum_{\gamma, \gamma' \in \Gamma} \overline{\chi}(\gamma) \chi(\gamma') \int_{\mathcal{D}} \langle \gamma_* s_1(\gamma^{-1} x) | \gamma'_* s_2(\gamma'^{-1} x) \rangle_{E_x} \, dx \\
&= \sum_{\gamma, \gamma'' \in \Gamma} \chi(\gamma'') \int_{\gamma^{-1}\mathcal{D}} \langle s_1(y) | \gamma''_* s_2(\gamma''^{-1} y) \rangle_{E_y} \, dy \\
&= \sum_{\gamma'' \in \Gamma} \chi(\gamma'') \langle s_1 T_{\gamma''} s_2 \rangle_{L^2(E)}, \qquad (16)
\end{aligned}$$

and therefore continuous in χ, since the last sum in (16) is finite. The $*$-property is immediately clear, and the $C(\hat{\Gamma})$-linearity of the scalar product follows from

$$\begin{aligned}
\langle s_1 | M_f s_2 \rangle(\chi) &= \langle (\Phi s_1)_\chi | (f \Phi s_2)_\chi \rangle_{L^2(E_\chi)} \\
&= \langle (\Phi s_1)_\chi | f(\chi) (\Phi s_2)_\chi \rangle_{L^2(E_\chi)} \\
&= \langle (\Phi s_1)_\chi | (\Phi s_2)_\chi \rangle_{L^2(E_\chi)} f(\chi).
\end{aligned}$$

□

(16) is the Fourier transform of the map $\gamma \mapsto \langle s_1 T_\gamma s_2 \rangle$ and will lead us on the right track for the construction of a suitable Hilbert C^*-module in the noncommutative example of gauge-periodic elliptic operators (see Lemma 8).

In Appendix B we describe how—for arbitrary (i.e., noncommutative) C^*-algebras—a C^*-valued scalar product on an $\mathcal{A}$-module together with the C^*-norm on $\mathcal{A}$ defines a Banach norm on the $\mathcal{A}$-module. The C^*-norm on $C(\hat{\Gamma})$ is the supremum norm, so that in this case the Banach norm $\|\cdot\|'_{\mathcal{E}}$ on $\mathcal{E}' := C_c(E) \ni s$ is given by

$$\|s\|_{\mathcal{E}'} := \sup_{\chi \in \hat{\Gamma}} \langle s | s \rangle(\chi).$$

We can take the closure $\mathcal{E}'$ with respect to this norm, and hence make $\mathcal{E}'$ into a C^*-module over $\hat{\Gamma}$:

Definition and proposition 2 [Hilbert $C(\hat{\Gamma})$-module and GNS representation]: We denote the closure of $C_c(E)$ as Hilbert $C(\hat{\Gamma})$- module by $\mathcal{E}$. $\mathcal{E}$ is a submodule of the $C(\hat{\Gamma})$-module $L^2(E)$. The Haar measure on $\hat{\Gamma}$ defines a faithful trace τ on $C(\hat{\Gamma})$, and the corresponding GNS representation π_τ (see appendix B) of $\mathcal{E}$ is just the original $C(\hat{\Gamma})$-action on $L^2(E)$.

Proof: Since

$$\|\langle s_1|s_2\rangle_{\mathcal{E}}\|_{L^\infty(\hat{\Gamma})} \geqslant \|\langle s_1|s_2\rangle_{\mathcal{E}}\|_{L^1(\hat{\Gamma})} \geqslant |\langle s_1|s_2\rangle_{L^2(E)}|,$$

the closure of $C_c(E)$ in the $\mathcal{E}$-norm is a subspace of $L^2(E)$, and by definition a $C(\hat{\Gamma})$-module.

The integral with respect to a measure defines a trace. Since $\hat{\Gamma}$ is compact (Γ is discrete) it has finite volume with respect to Haar measure, so that the trace is finite, and all $f \in C(\hat{\Gamma}) \subset L^1(\hat{\Gamma})$ are trace class. Since $\hat{\Gamma}$ has no open subsets of Haar measure zero the trace is faithful. We can compute the scalar product that is defined by τ for $s_1, s_2 \in \mathcal{E}$ as follows:

$$\begin{aligned}\langle s_1|s_2\rangle_\tau &\overset{\text{defi}}{=} \tau\langle s_1|s_2\rangle_{\mathcal{E}} \\ &\overset{(17)}{=} \int_{\hat{\Gamma}} \sum_{\gamma\in\Gamma} \chi(\gamma)\langle s_1 T_\gamma s_2\rangle_{L^2(E)}\, d\chi \\ &\overset{(7)}{=} \langle s_1|s_2\rangle_{L^2(E)}.\end{aligned}$$

Since $\mathcal{E} \supset C_c(E)$ is dense in $L^2(E)$ with respect to the L^2-norm and therefore with respect to the norm generated by τ, the GNS representation space for τ is $L^2(E)$. Hence, the module structures coincide. □

Proposition 2 (continuous field of Hilbert spaces over $\hat{\Gamma}$): The continuous field of Hilbert spaces over $\hat{\Gamma}$ that corresponds to $\mathcal{E}$ (see Appendix A) has the fiber $L^2(E_\chi)$ over χ, the continuity structure is defined by $\mathcal{E}$.

Proof: We get the fiber at χ as GNS representation space of the state $\pi_\chi : C(\hat{\Gamma}) \ni f \mapsto f(\chi)$. For the continuity structure, see Appendix A. □

To sum up: We have replaced the decomposition of $L^2(E)$ into a direct integral of Hilbert spaces over the space $\hat{\Gamma}$ by a Hilbert C^*-module over the C^*-algebra $C(\hat{\Gamma})$, endowed with a faithful trace whose GNS representation gives us back the original Hilbert space $L^2(E)$. In Proposition 1 we determined the $C(\hat{\Gamma})$-action and noticed that decomposable bounded operators with respect to the direct integral are just the ones commuting with this action (the periodic operators). Thus, decomposable operators are just the module maps on the $C(\hat{\Gamma})$-module $L^2(E)$. This includes especially the images (under the GNS representation) of module maps on $\mathcal{E}$. To conclude this section we cite a special case of Theorem 11 from Sec. V that shows that periodic elliptic differential operators define indeed regular unbounded module maps (see, e.g., Ref. 13, Chap. 9 for these notions) on $\mathcal{E}$, so that the resolvent of such operators belongs to the image of the GNS representation.

Theorem 5 (decomposition of periodic operators): *Let D be a periodic symmetric elliptic differential operator. Then D defines a regular operator $D_{\mathcal{E}}$ with domain of definition $\mathcal{D}(D_{\mathcal{E}}) = C_c^\infty(E)$ in $\mathcal{E}$. For $\lambda \in \mathbb{R}$ we have*

$$\pi_\tau((\lambda \mathbb{1}_{\mathcal{E}} + \overline{D_{\mathcal{E}}})^{-1}) = (\lambda \mathbb{1}_{L^2(E)} + \overline{D})^{-1}. \tag{17}$$

IV. NONCOMMUTATIVE BLOCH THEORY

Motivated by the noncommutative insight gained in the previous section, we will now define a general class of abstract elliptic operators that allows for a noncommutative version of Bloch theory. This will let us read off spectral properties from properties of the C^*-algebras that are involved.

Definition 5 ($\mathcal{A}$-elliptic operator): Let $\mathcal{A}$ be a unital C^*-algebra, $\mathcal{E}$ a Hilbert C^*-module over $\mathcal{A}$. An unbounded operator D on $\mathcal{E}$ is called $\mathcal{A}$-elliptic if

(1) D is densely defined;
(2) D is regular in the sense that D has a densely defined adjoint D^* with range $\mathrm{ran}(1+D^*D) \overset{\text{dense}}{\subset} \mathcal{E}$*; and*
(3) D has $\mathcal{A}$-compact resolvent, i.e., $(1+D^*D)^{-1} \in \mathcal{K}_{\mathcal{A}}(\mathcal{E})$.

We will explain the name $\mathcal{A}$-compact resolvent in the proof of Lemma 7. Hilbert modules are understood to be Hilbert right modules, as described in Appendix B. Hilbert spaces are Hilbert $\mathbb{C}$-modules, therefore our scalar products are complex linear in the second entry and complex antilinear in the first entry, corresponding to the convention in Mathematical Physics.

Remark 4 (module and Hilbert space operators): Given a normalized faithful trace τ on $\mathcal{A}$ we can define, as described in Appendix B, a Hilbert space scalar product on $\mathcal{E}$ by

$$\langle e_1|e_2\rangle_\tau := \tau(\langle e_1|e_2\rangle_{\mathcal{E}})$$

for $e_1, e_2 \in \mathcal{E}$. Let H_τ be the completion of $\mathcal{E}$ with respect to $\langle\cdot|\cdot\rangle_\tau$, i.e., the corresponding GNS representation space. We write $\langle\cdot|\cdot\rangle_{H_\tau}$ for $\langle\cdot|\cdot\rangle_\tau$. $\mathcal{L}_{\mathcal{A}}(\mathcal{E})$ is represented faithfully on H_τ. Thus the spectrum of an element a of the C^*-algebra $\mathcal{L}_{\mathcal{A}}(\mathcal{E})$ coincides (as a set) with the spectrum of the operator $\pi_\tau(a)$ on the Hilbert space H_τ:

Lemma 4 (spectrum of module and Hilbert space operators): If $a \in \mathcal{L}_{\mathcal{A}}(\mathcal{E})$, then

$$\mathrm{spec}\, a = \mathrm{spec}\, \pi_\tau(a).$$

In the sequel we will identify $\mathcal{E}$ resp. $\mathcal{L}_{\mathcal{A}}(\mathcal{E})$ with the images in H_τ resp. $\mathcal{L}(H_\tau)$.

Definition and proposition 3 (tr_τ-trace): The $\mathcal{A}$-finite operators $\mathcal{F}_{\mathcal{A}}$ are defined by

$$\mathcal{F}_{\mathcal{A}}(\mathcal{E}) = \mathrm{span}\{\pi^{\mathcal{E}}_{x,y} | x,y \in \mathcal{E}\}$$

with

$$\pi^{\mathcal{E}}_{x,y}(z) = x\langle y|z\rangle_{\mathcal{E}} \quad \text{for} \quad z \in \mathcal{E},$$

so that $\mathcal{K}_{\mathcal{A}}(\mathcal{E}) = \overline{\mathcal{F}_{\mathcal{A}}(\mathcal{E})}$. On $\mathcal{F}_{\mathcal{A}}(\mathcal{E})$ we define a faithful trace by

$$\mathrm{tr}_\tau(\pi^{\mathcal{E}}_{x,y}) = \tau(\langle y|x\rangle_{\mathcal{E}}), \tag{18}$$

the trace associated to τ in the GNS representation. We denote the corresponding trace class ideal in $\mathcal{L}_{\mathcal{A}}(\mathcal{E})$ by $\mathcal{L}^1_{\mathcal{A}}(\mathcal{E}, \mathrm{tr}_\tau)$.

Proof: For the generators of $\mathcal{F}_{\mathcal{A}}(\mathcal{E})$ one can easily show the relations,

$$(\pi^{\mathcal{E}}_{x,y})^* = \pi^{\mathcal{E}}_{y,x}, \pi^{\mathcal{E}}_{xa,y} = \pi^{\mathcal{E}}_{x,ya^*},$$

$$T\pi^{\mathcal{E}}_{x,y} = \pi^{\mathcal{E}}_{Tx,y}, \pi^{\mathcal{E}}_{x,y}T = \pi^{\mathcal{E}}_{x,T^*y}$$

for $x,y \in \mathcal{E}, a \in \mathcal{A}, T \in \mathcal{L}_{\mathcal{A}}(\mathcal{E})$. Thus, from the trace property of τ we have

$$\mathrm{tr}_\tau((\pi^{\mathcal{E}}_{x,y})^*) = \tau(\langle x|y\rangle_{\mathcal{E}}) = (\mathrm{tr}_\tau \pi^{\mathcal{E}}_{x,y})^*,$$

$$\mathrm{tr}_\tau(T\pi^{\mathcal{E}}_{x,y}) = \tau(\langle y|Tx\rangle_{\mathcal{E}}) = \tau(\langle T^*y|x\rangle_{\mathcal{E}}) = \mathrm{tr}_\tau(\pi^{\mathcal{E}}_{x,y}T).$$

For all $z,t \in \mathcal{E}$ we have

$$\begin{aligned}\mathrm{tr}_\tau(\pi^{\mathcal{E}}_{x,y}\pi^{\mathcal{E}}_{z,t}) &= \mathrm{tr}_\tau(\pi^{\mathcal{E}}_{x\langle y|z\rangle_{\mathcal{E}},t}) \\ &= \tau(\langle t|x\langle y|z\rangle_{\mathcal{E}}\rangle_{\mathcal{E}}) \\ &= \tau(\langle t|\pi^{\mathcal{E}}_{x,y}(z)\rangle_{\mathcal{E}})\end{aligned}$$

so that $\mathrm{tr}_{\mathcal{E}}$ is faithful: Set $t=\pi^{\mathcal{E}}_{x,y}(z)$, and note that τ is a faithful trace on $\mathcal{A}$. □

Remark 5 ($\mathrm{tr}\,\pi^{H_\tau}_{x,y}$ *vs* $\mathrm{tr}_\tau\,\pi^{\mathcal{E}}_{x,y}$)*: By Definition 3, we have*

$$\mathrm{tr}_\tau\,\pi^{\mathcal{E}}_{x,y}=\tau(\langle y|x\rangle_{\mathcal{E}})=\langle y|x\rangle_{H_\tau}=\mathrm{tr}\,\pi^{H_\tau}_{x,y}$$

with the usual canonical Hilbert space trace tr *and the usual rank 1 operators,*

$$\pi^{H_\tau}_{x,y}:H_\tau\ni z\mapsto x\langle y|z\rangle_{H_\tau}\in H_\tau$$

on the Hilbert space H_τ*. However,* $\pi^{\mathcal{E}}_{x,y}$ *and* $\pi^{H_\tau}_{x,y}$ *are different operators,*

$$\pi^{\mathcal{E}}_{x,y}(z)=x\langle y|z\rangle_{\mathcal{E}},$$

whereas

$$\pi^{H_\tau}_{x,y}(z)=x\langle y|z\rangle_{H_\tau}=x\,\tau(\langle y|z\rangle_{\mathcal{E}}).$$

Thus, in general tr_τ *and* tr *are indeed different traces.*

Remark 6 ($\mathrm{tr}\,\pi^{\mathcal{E}}_{x,y}$ *vs* $\mathrm{tr}_\tau\,\pi^{\mathcal{E}}_{x,y}$)*: Let* $(e_n)_{n\in\mathbb{N}}$ *be an orthonormal base of* H_τ*. To simplify matters we assume* $e_n\in\mathcal{E}$ *for all* $n\in\mathbb{N}$*. Since* $\mathcal{E}$ *is dense in* H_τ *this can always be achieved. Then,*

$$\begin{aligned}\mathrm{tr}_\tau\,\pi^{\mathcal{E}}_{x,y}=\mathrm{tr}\,\pi^{H_\tau}_{x,y} &= \sum_{n\in\mathbb{N}}\langle e_n|\pi^{H_\tau}_{x,y}(e_n)\rangle_{H_\tau} \\ &= \sum_{n\in\mathbb{N}}\langle e_n x\langle y|e_n\rangle_{H_\tau}\rangle_{H_\tau} \\ &= \sum_{n\in\mathbb{N}}\langle e_n|x\rangle_{H_\tau}\langle y|e_n\rangle_{H_\tau} \\ &= \sum_{n\in\mathbb{N}}\tau(\langle e_n|x\rangle_{\mathcal{E}})\,\tau(\langle y|e_n\rangle_{\mathcal{E}}),\end{aligned}$$

$$\begin{aligned}\mathrm{tr}\,\pi^{\mathcal{E}}_{x,y}=\sum_{n\in\mathbb{N}}\langle e_n\rangle|\pi^{\mathcal{E}}_{x,y}(e_n)\rangle_{H_\tau} &= \sum_{n\in\mathbb{N}}\langle e_n|x\langle y|e_n\rangle_{\mathcal{E}}\rangle_{H_\tau} \\ &= \sum_{n\in\mathbb{N}}\tau(\langle e_n|x\langle y|e_n\rangle_{\mathcal{E}}\rangle_{\mathcal{E}}) \\ &= \sum_{n\in\mathbb{N}}\tau(\langle e_n|x\rangle_{\mathcal{E}}\langle y|e_n\rangle_{\mathcal{E}}).\end{aligned}$$

So, $\mathrm{tr}\,\pi^{H_\tau}_{x,y}$ *and* $\mathrm{tr}\,\pi^{\mathcal{E}}_{x,y}$ *coincide if* τ *is multiplicative. But in this case* τ*, being a multiplicative faithful trace, is a* $*$*- isomorphism* $\mathcal{A}\to\mathbb{C}$ *already, so that we just reproduce the Hilbert space trace.*

In general tr *will be larger than* tr_τ *because*

$$\begin{aligned}\operatorname{tr}\pi^{\mathcal{E}}_{e_m,e_m}&=\sum_{n\in\mathbb{N}}\tau(\langle e_n|e_m\rangle_{\mathcal{E}}\langle e_m|e_n\rangle_{\mathcal{E}})=\sum_{n\in\mathbb{N}}\tau(\langle e_m|e_n\rangle^*_{\mathcal{E}}\langle e_m|e_n\rangle_{\mathcal{E}})\\&\geqslant\tau(\langle e_m|e_m\rangle^*_{\mathcal{E}}\langle e_m|e_m\rangle_{\mathcal{E}})\\&\geqslant(\tau(\langle e_m|e_m\rangle_{\mathcal{E}}))^2\\&=\|e_m\|^2_{H_\tau}\\&=1\\&=\operatorname{tr}\pi^{H_\tau}_{e_m,e_m}\\&=\operatorname{tr}_\tau\pi^{\mathcal{E}}_{e_m,e_m}.\end{aligned}$$

Here we used the Cauchy–Schwarz inequality $\tau(a^*b)\leqslant\sqrt{\tau(a^*a)\tau(b^*b)}$ *and the fact that the trace is normalized.*

To sum up: The tr_τ*-trace is defined only on the image of the adjointable module operators in the GNS representation, and on these it is in general smaller than the Hilbert space trace, so that the corresponding trace class ideal is larger,*

$$\pi_\tau(\mathcal{L}^1_{\mathcal{A}}(\mathcal{E},\operatorname{tr}_\tau))\supset\pi_\tau(\mathcal{L}_{\mathcal{A}}(\mathcal{E}))\cap\mathcal{L}^1(H_\tau,\operatorname{tr}).$$

Remark 7 (tr_τ *for standard Hilbert modules): If* $\mathcal{E}$ *is a standard* $\mathcal{A}$*-module* $H\otimes\mathcal{A}$ *(tensor product of Hilbert modules) with a Hilbert space* H*, then the GNS representation space* H_τ *of* $\mathcal{E}$ *is given by* $H_\tau=H\hat{\otimes}Xh_\tau$ *(tensor product of Hilbert spaces), where* h_τ *is the GNS representation space of* $\mathcal{A}$*. Therefore we have for the elementary tensors* $x\otimes a,y\otimes b\in\mathcal{E}$*,*

$$\langle y\otimes b|x\otimes a\rangle_{\mathcal{E}}=\langle y|x\rangle_H\,b^*a,$$

$$\pi^{H_\tau}_{x\otimes a,y\otimes b}=\pi^H_{x,y}\otimes\pi^{h_\tau}_{a,b},$$

$$\pi^{\mathcal{E}}_{x\otimes a,y\otimes b}=\pi^H_{x,y}\otimes\pi^{\mathcal{A}}_{a,b}=\pi^H_{x,y}\otimes ab^*.$$

With the standard traces $\operatorname{tr}_H,\operatorname{tr}_{h_\tau}$ *on the Hilbert spaces* H,h_τ *we get*

$$\operatorname{tr}\pi^{H_\tau}_{x\otimes a,y\otimes b}=\operatorname{tr}_\tau\pi^{\mathcal{E}}_{x\otimes a,y\otimes b}=\langle y|x\rangle_H\,\tau(b^*a)=\operatorname{tr}_H(\pi^H_{x,y})\operatorname{tr}_{h_\tau}(\pi^{h_\tau}_{a,b}).$$

Thus we arrive at

$$\operatorname{tr}=\operatorname{tr}_H\otimes\operatorname{tr}_{h_\tau},\quad \operatorname{tr}_\tau=\operatorname{tr}_H\otimes\tau.$$

Lemma 5 (tr *for* tr_τ*-trace class): Let* $\mathcal{E}=H\otimes\mathcal{A}$ *be as above. If* $\mathcal{A}$ *is infinite dimensional with a unitary orthonormal basis for* h_τ*, then* 0 *is the only* tr_τ*-trace class operator with finite standard trace. In particular, all Hilbert* $\mathcal{A}$*-submodules are infinite dimensional vector spaces.*

Proof: Let $(x_n)_{n\in\mathbb{N}}$ be an orthonormal basis of h_τ, consisting of unitary elements of $\mathcal{A}$. Then,

$$\operatorname{tr}_{h_\tau}\pi^{\mathcal{A}}_{a,b}=\sum_{n\in\mathbb{N}}\langle x_nab^*x_n|ab^*x_n\rangle_{h_\tau}=\sum_{n\in\mathbb{N}}\tau(x_n^*ab^*x_n)=\sum_{n\in\mathbb{N}}\tau(ab^*).$$

□

Lemma 6 (nonexistence of finite dimensional modules): If $\mathcal{A}$ *is infinite dimensional with a unitary orthonormal basis for* h_τ*, then every projective* $\mathcal{A}$*-module is an infinite dimensional vector space.*

Proof: If $\mathcal{E}$ is a projective Hilbert $\mathcal{A}$-module, then $\mathcal{E}$ is a direct summand of a free module $H\otimes\mathcal{A}$ for a suitable Hilbert space H, and we can apply Lemma 5. □

Lemma 7 (spectral projections): Let D be a self-adjoint $\mathcal{A}$-elliptic operator and let $\lambda_1,\lambda_2 \in \mathbb{R}\backslash\operatorname{spec} D$, $\lambda_1 \leqslant \lambda_2$. Then the corresponding spectral projection $P_{[\lambda_1,\lambda_2]}$ on the interval $[\lambda_1,\lambda_2]$ is $\mathcal{A}$-compact. If $e^{-tD^2} \in \mathcal{L}^1_{\mathcal{A}}(\mathcal{E},\mathrm{tr}_\tau)$ for $t>0$ then the spectral projections are tr_τ-trace class.

Proof: Reduction to $D \geqslant 0$: If $\operatorname{spec} D = \mathbb{R}$ there is nothing to prove. So, let $\lambda_0 \in \mathbb{R}\backslash\operatorname{spec} D$. We show that we can assume $D \geqslant 0$ for the proof of $\mathcal{A}$-compactness, Let,

$$D' := f(D)$$

with

$$f(x) := x - \lambda_0 \quad \text{for} \quad x \in \mathbb{R}.$$

Then $0 \notin \operatorname{spec} D'$. We set $g(x) := (1+x^2)^{-1}$ so that

$$(1+D'^2)^{-1} = g \circ f(D) = g(D)b(D)$$

with

$$b(x) = \frac{g \circ f(x)}{g(x)} = \frac{1+(x-\lambda_0)^2}{1+x^2}.$$

Since b is continuous and bounded $b(D) \in \mathcal{L}_{\mathcal{A}}(\mathcal{E})$. If D is $\mathcal{A}$-elliptic, i.e., $g(D) \in \mathcal{K}_{\mathcal{A}}(\mathcal{E})$, then we get $g(D)b(D) \in \mathcal{K}_{\mathcal{A}}(\mathcal{E})$, i.e., D' is $\mathcal{A}$-elliptic. Denote the spectral projections of D' with P'. Then obviously $P'(\lambda) = P(\lambda+\lambda_0)$, so that it suffices to test P' for $\mathcal{A}$-compactness.

Finally, we set $D'' := |D'|$. Then D'' is $\mathcal{A}$-elliptic by definition, positive by construction, and strictly positive because $0 \notin \operatorname{spec} D'$. If we denote the spectral projections of D'' by P'', then

$$P''(\lambda) = 1_{(-\infty,\lambda]}(D'') = (1_{(-\infty,\lambda]^\circ}|\cdot|)(D') = 1_{[-\lambda,\lambda]}(D') = P'_{[-\lambda,\lambda]}.$$

Therefore we get for $0 \leqslant \lambda_1 \leqslant \lambda_2$,

$$P''_{(\lambda_1,\lambda_2]} = P''(\lambda_2) - P''(\lambda_1) = P'_{[-\lambda_2,\lambda_2]} - P'_{[-\lambda_1,\lambda_1]} = P'_{[-\lambda_2,-\lambda_1)\cup(\lambda_1,\lambda_2]}.$$

By assumption $0 \notin \operatorname{spec} D'$ and therefore $P'_{[0,\infty)}, P'_{(-\infty,0]} \in \mathcal{L}_{\mathcal{A}}(\mathcal{E})$, so that

$$P'_{(\lambda_1,\lambda_2]} = P''_{(\lambda_1,\lambda_2]} P'_{[0,\infty)} \in \mathcal{K}_{\mathcal{A}}(\mathcal{E}) \tag{19}$$

and

$$P'_{[-\lambda_2,-\lambda_1)} = P''_{(\lambda_1,\lambda_2]} P'_{(-\infty,0]} \in \mathcal{K}_{\mathcal{A}}(\mathcal{E}), \tag{20}$$

if $P''_{(\lambda_1,\lambda_2]} \in \mathcal{K}_{\mathcal{A}}(\mathcal{E})$. If $\lambda_1 \leqslant 0 \leqslant \lambda_2$ we write

$$P'_{[\lambda_1,\lambda_2]} = P'_{[\lambda_1,0)} + P'_{(0,\lambda_2]}$$

and apply Eqs. (19) and (20). Hence it suffices to test P'' for $\mathcal{A}$-compactness.

$\mathcal{A}$-compactness: We show that every spectral projection $P_{[\lambda_1,\lambda_2]}$ for $\lambda_1,\lambda_2 \in \mathbb{R}\backslash\operatorname{spec} D$ can be produced by continuous functional calculus from $S := (1+D^2)^{-1}$, so that it belongs to $\mathcal{K}_{\mathcal{A}}(\mathcal{E})$. For this we note that $S^{-1} = D^2+1$ is densely defined (D is regular), self-adjoint and bounded below by 1. Thus $\sqrt{S^{-1}-1}$ exists, is positive and self-adjoint. By the spectral mapping theorem we have

$$z \in \operatorname{spec}\sqrt{S^{-1}-1} \Leftrightarrow (z^2+1)^{-1} \in \operatorname{spec} S \Leftrightarrow z \in \operatorname{spec} D.$$

Therefore, the operator

$$R_z := (z - \sqrt{S^{-1} - 1})^{-1}$$

exists for all z in the resolvent set of D. Since the function

$$\lambda \mapsto (z - \sqrt{\lambda^{-1} - 1})^{-1}$$

is continuous and bounded on every closed set not containing $(z^2+1)^{-1}$, R_z belongs to the C^*-algebra generated by S for every $z \in \mathbb{C} \backslash \operatorname{spec} D$ and therefore belongs to $\mathcal{K}_{\mathcal{A}}(\mathcal{E})$, i.e., it is $\mathcal{A}$-compact. Since

$$P_{[\lambda_1,\lambda_2]} = \frac{1}{2\pi\imath} \oint_c R_z \, dz$$

for a suitable closed path c in $\mathbb{C} \backslash \operatorname{spec} D$ with winding number 1 fulfilling $c \cap \mathbb{R} = \{\lambda_1, \lambda_2\}$, $P_{[\lambda_1,\lambda_2]}$ belongs to the C^*-algebra generated by all R_z.

Trace class property: Let e^{-tD^2} be tr_τ-trace class. (We do not assume positivity of D any more.) Since

$$\begin{aligned} P_{[\lambda_1,\lambda_2]} = \int_{\lambda_1}^{\lambda_2} dP(\lambda) &\leqslant e^{t(\lambda_2-\lambda_1)^2} \int_{\lambda_1}^{\lambda_2} e^{-t(\lambda-\lambda_1)^2} dP(\lambda) \\ &\leqslant e^{t(\lambda_2-\lambda_1)^2} \int_{\mathbb{R}} e^{-t(\lambda-\lambda_1)^2} dP(\lambda) \\ &= e^{t(\lambda_2-\lambda_1)^2} e^{-tD^2}, \end{aligned}$$

the spectral projections inherit the trace class property from e^{-tD^2}. □

If λ is an isolated eigenvalue then for sufficiently small $\varepsilon > 0$ $P_\lambda := P_{[\lambda-\varepsilon,\lambda+\varepsilon]}$ is the projection on the eigenspace of λ, independent of ε. So P_λ fulfills the hypotheses of Lemma 7, and we can determine the dimension of the eigenspace.

Theorem 6 (isolated eigenvalue): *If λ is an isolated eigenvalue of a self-adjoint $\mathcal{A}$-elliptic operator D, then the corresponding eigenspace E_λ is an (algebraically) finitely generated projective Hilbert $\mathcal{A}$-module, and the projection P_λ is $\mathcal{A}$-finite. If e^{-tD^2} is tr_τ-trace class then so is P_λ, i.e., E_λ has finite τ-dimension $\mathrm{tr}_\tau P_\lambda$.*

If $\mathcal{E}, \mathcal{A}$ fulfill the hypotheses of Lemma 6, then E_λ has infinite Hilbert dimension $\mathrm{tr}\, P_\lambda$ for every isolated eigenvalue λ of D. In particular, D has essential spectrum only.

Proof: P_λ is the spectral projection of a self-adjoint operator and therefore self-adjoint, and $\mathcal{A}$-compact by Lemma 7. Thus the eigenspace E_λ is the image of a closed adjointable projection P_λ and therefore a closed complementable $\mathcal{A}$-module. Since the projection $P_\lambda|_{E_\lambda} = \mathbb{1}$ is $\mathcal{A}$-compact E_λ is algebraically finitely generated and projective, because algebraically finitely generated $\mathcal{A}$-modules E are just the ones with unital $\mathcal{K}_{\mathcal{A}}(E)$ and automatically projective (see Ref. 14, Theorem 15.4.2 and Corollary 15.4.8).

If $e^{-tD^2} \in \mathcal{L}_{\mathcal{A}}{}^1(\mathcal{E}, \mathrm{tr}_\tau)$ then so is P_λ by Lemma 7, and under the same hypotheses we can apply Lemma 6. □

The main idea of the following proof goes back to Ref. 15:

Theorem 7 (band structure): *Assume that $\mathcal{K}_{\mathcal{A}}(\mathcal{E})$ has the Kadison property with respect to tr_τ (see Definition 3). Then the spectrum of every self-adjoint $\mathcal{A}$-elliptic operator D with $e^{-tD^2} \in \mathcal{L}^1_{\mathcal{A}}(\mathcal{E}, \mathrm{tr}_\tau)$ has band structure.*

Proof: Let $a = \lambda_0 < \cdots < \lambda_n = b \in \mathbb{R} \backslash \operatorname{spec} D$, so that $P_{[\lambda_i,\lambda_{i+1}]} \neq 0$ for $0 \leqslant i \leqslant n-1$, i.e., $\operatorname{spec} D$ has at least n components in $[a,b]$. Then,

$$P_{[a,b]}=\sum_{i=0}^{n-1} P_{[\lambda_i,\lambda_{i+1}]}$$

and therefore

$$\mathrm{tr}_\tau P_{[a,b]}=\sum_{i=0}^{n-1} \mathrm{tr}_\tau P_{[\lambda_i,\lambda_{i+1}]}\geqslant nc_K$$

$$\Leftrightarrow n\leqslant \frac{1}{c_K}\mathrm{tr}_\tau P_{[a,b]},$$

since all projections occurring in this sum are tr_τ-trace class by Lemma 7. □

If $c_K=0$ then we cannot apply Theorem 7. Instead, spectra with the structure of a Cantor set seem possible. Examples show that the opening of gaps which are allowed depends heavily on the specific structure of the operator and cannot easily be controlled globally. To get generic results we therefore have to make sure that not only $c_K=0$, but also that the trace can be arbitrarily small on ''many'' projections. This is accomplished by the following theorem by Choi and Elliott:[2]

Theorem 8 (Cantor spectrum): *Let $\mathcal{A}$ be a C*-algebra with a faithful state Φ. Assume that every self-adjoint element can be approximated arbitrarily well by an element with finite spectrum on whose minimal spectral projections Φ is arbitrarily small. Then the self-adjoint elements with Cantor spectrum are dense in all self-adjoint elements.*

In particular, the algebras in Theorem 8 have real rank zero, i.e., the invertible self-adjoint elements are dense in all self-adjoint ones:

Definition and proposition 4 (real rank): Let $\mathcal{A}$ be a unital C-algebra. The real rank of $\mathcal{A}$ is defined by*

$$\mathrm{RR}(\mathcal{A})=\min\{m\in\mathbb{N}_0|\forall n\geqslant m+1:\mathrm{RR}_n(\mathcal{A})\},\tag{21}$$

where

$$\mathrm{RR}_n(\mathcal{A})=\left\langle \forall x\in\mathcal{A}_{sa}^n:\forall\varepsilon>0:\exists y\in\mathcal{A}_{sa}^n:\sum_{k=1}^n y_k^2\in\mathcal{A}^\times\wedge\left\|\sum_{k=1}^n (y_k-x_k)^2\right\|<\varepsilon\right\rangle.\tag{22}$$

For all $n\in\mathbb{N}_0$ we have $\mathrm{RR}_n(\mathcal{A})\Rightarrow\mathrm{RR}_{n+1}(\mathcal{A})$. The following conditions are equivalent:

(1) $\mathrm{RR}(\mathcal{A})=0$;
(2) $\mathcal{A}_{sa}^\times\subset\mathcal{A}_{sa}$ dense;
(3) The self-adjoint elements with finite spectrum are dense in $\mathcal{A}_{sa}$.

We say $\mathcal{A}$ has real rank 0 with infinitesimal state (RRI_0) if $\mathcal{A}$ fulfills the assumptions of Theorem 8.

For the convenience of the reader we include a proof of these equivalences which are well known in the C^*-community.

Proof: This well-known result can be proven as an exercise in continuous functional calculus. □

Remark 8 (Kadison property and RRI_0):

(1) Kadison property and property RRI_0 are mutually exclusive since the first forbids existence of projections with arbitrarily small trace whereas the latter requires this.
(2) C-algebras $\mathcal{A}$ with RRI_0 can contain operators with band structure: If $\mathcal{A}$ is the irrational rotation algebra (see below) then $\mathcal{A}$ has RRI_0 by Theorem 9. But $\mathcal{A}$ contains a subalgebra isomorphic to $C(S^1)$, consisting of operators with band spectrum only.*
(3) On the other hand, a C-algebra $\mathcal{A}$ with the Kadison property cannot contain self-adjoint elements with Cantor spectrum: If $x\in\mathcal{A}_{sa}$ has Cantor spectrum, then every point in* spec x *is*

an accumulation point of $\operatorname{spec} x$ *and* $\mathbb{R}\backslash\operatorname{spec} x$, *so that* x *has no band spectrum in contradiction to Theorem 7.*

(4) If $\mathcal{A}_1$ *has the Kadison property and* $\mathcal{A}_2$ *has property* RRI_0, *then* $\mathcal{A}:=\mathcal{A}_1\oplus\mathcal{A}_2$ *has neither of these properties.*

Remark 9 (real rank and dimension):

(1) If $\mathcal{A}$ *is commutative so that* $\mathcal{A}=C(X)$ *for a topological space* X *then* $\mathrm{RR}(\mathcal{A})=\dim X$ *with the usual definition of dimension.*

(2) Therefore, C-algebras with real rank 0 are (noncommutative) zero-dimensional spaces. This includes finite discrete spaces. However, the additional trace condition in Theorem 8 excludes finite spaces: By the Riesz–Kakutani theorem every state on* $C(X)$ *is given by an integral with respect to a normalized measure* μ, *i.e.,* $\Phi(f)=\int f\,d\mu$ *and* $\mu(X)=1$. *Such states are faithful if and only if every open set has strictly positive measure. The trace condition requires that* X *has connected components with arbitrary small measure.*

(3) Every W-algebra has real rank 0, since the measurable functional calculus (as opposed to the continuous one) allows us to ''cut out'' points from the spectrum arbitrarily close.*

(4) Property RR_0 *is preserved under inductive limits, in particular* $\mathcal{A}\otimes\mathcal{K}$ *has real rank 0 if* $RR(\mathcal{A})=0$.

Example 5 (rotation algebra): The rotation algebra $\mathcal{A}_\theta$ *is the C*-algebra generated by two unitaries* U,V *and the relation*

$$VU=e^{2\pi\imath\theta}UV$$

for a given $\theta\in\mathbb{R}$. *It also arises as a reduced twisted group C*-algebra* $C_r^*(\mathbb{Z}_2,\Theta)$ *for the cocycle* Θ *given by* $e^{2\pi\imath\theta}$ *since* $H^2(\mathbb{Z}^2,S^1)\simeq S^1$. *It carries a canonical trace defined by*

$$\tau(1)=1,\tau(U)=\tau(V)=0.$$

The properties of this algebra depend strongly on the nature of θ:

Theorem 9 (properties of the rotation algebra):

(1) If $\theta=p/q$ *with* $p\in\mathbb{Z},q\in\mathbb{N}$ *co-prime then the Kadison constant of* $\mathcal{A}_\theta$ *and of* $\mathcal{A}_\theta\otimes\mathcal{K}$ *is* $1/q$.

(2) If θ *is irrational then* $\mathcal{A}_\theta$ *and* $\mathcal{A}_\theta\otimes\mathcal{K}$ *(together with the canonical trace) have real rank 0 with infinitesimal state.*

Proof:

(1) As is well known, the spectrum of $\mathcal{A}_\theta$ *is* T^2, *and all irreducible representations* π_z *have dimension* q. *The canonical trace of* $a\in\mathcal{A}_\theta$ *is*

$$\tau(a)=\frac{1}{q}\int_{T^2}\mathrm{tr}\,\pi_z(a)\,dz$$

with the canonical trace tr *on* $M(q,\mathbb{C})$. *Minimal projections have rank 1 in the fiber, and so the Kadison constant is* $1/q$.

(2) $\mathcal{A}_\theta$ *has real rank zero.*[16] *Since* $\mathcal{A}_\theta$ *is simple and nonelementary we also get* RRI_0 (Ref. 2, Corollary 8).

□

Theorem 10 (Cantor spectrum): *Assume the C*-algebra* $\mathcal{K}_{\mathcal{A}}(\mathcal{E})$ *has real rank 0 with an infinitesimal state. Then every self-adjoint* $\mathcal{A}$*-elliptic operator can be approximated arbitrarily close in norm resolvent sense by a self-adjoint operator with Cantor spectrum.*

Proof: Lemma 7 and Theorem 8. □

V. APPLICATIONS

A. Discrete models

Example 6 (generalized Harper operators): Sunada[17] *defines magnetic Schrödinger Operators on graphs: Let X be a connected locally finite graph, χ a $\mathbb{C}^\times$-valued (i.e., nonvanishing complex-valued) map (a weight) on the oriented edges $E(X)$, $o,t:E(X)\to X$ the origin and termination point mappings. We define a symmetric operator on $l^2(X)$ by*

$$(H_\chi f)(x)=\sum_{\substack{e\in E(X)\\ o(e)=x}}\chi(e)f(t(e))$$

for $f\in l^2(X)$. Two weights χ_1,χ_2 are called cohomologous if there is a function $s:X\to S^1$ with

$$\chi_1(e)=\chi_2(e)\frac{s(o(e))}{s(t(e))}$$

for $e\in E(X)$.

Furthermore, let Γ be a group with a properly discontinuous free action on X and such that the quotient graph is finite (say n points). A weight χ is called gauge-invariant if $\gamma^*\chi$ is cohomologous to χ for all $\gamma\in\Gamma$. Then χ defines a cocycle $\Theta\in Z^2(\Gamma,S^1)$ such that H_χ commutes with the corresponding twisted right translations $[R^\Theta_\gamma f(\gamma')=\Theta(\gamma',\gamma)f(\gamma'\gamma)]$. Referemce 17 constructs an injective $*$-homomorphismus,

$$C_r^*(\Gamma,\Theta)\otimes M(n,\mathbb{C})\to\mathrm{End}(l^2(X)),$$

whose image contains H_χ. On the other hand,

$$\mathcal{A}\otimes M(n,\mathbb{C})=\mathcal{K}_\mathcal{A}(\mathcal{A}\otimes\mathbb{C}^n)$$

for the Hilbert $\mathcal{A}$-module $\mathcal{A}\otimes\mathbb{C}^n$ which is the tensor product of the canonical module $\mathcal{A}=C_r^*(\Gamma,\Theta)$ and the Hilbert $\mathbb{C}$-module $\mathbb{C}^n$. As in Theorem 7, Ref. 17 proves band structure.

All spectral characterizations of this section apply as soon as the corresponding C-algebra $C_r^*(\Gamma,\Theta)\otimes M(n,\mathbb{C})$ fulfills the corresponding assumptions.*

We get the ordinary Harper operator for $E(X)=\Gamma=\mathbb{Z}^2$ and a suitable graph X with coordination number 4 (square lattice), the hexagonal Harper operator and the quantum pendulum for graphs with coordination numbers 6 resp. 8. The corresponding C-algebras are rotation algebras, so that we have band structure for rational flux, and weak genericity of Cantor spectrum for irrational flux.*

For another approach to the Harper operator, properties of the density of states, and for necessary (though yet unverified) conditions for Cantor spectrum see the beautiful paper by Shubin on discrete magnetic Laplacians.[18]

B. Continuous models

Example 7 (gauge-periodic elliptic operators): In this case $\mathcal{A}$ will be a twisted group C-algebra (left translations), and the Hilbert module will be a tensor product $\mathcal{E}=\mathcal{A}\otimes\mathcal{H}$ with a Hilbert space $\mathcal{H}$ such that $\mathcal{K}_\mathcal{A}(\mathcal{E})\simeq\mathcal{A}\otimes\mathcal{K}(\mathcal{H})$. The operator D will be a differential operator which is invariant under a projective representation of a group, such as Schrödinger, Dirac, and Pauli operators with periodic magnetic and electric fields.*

The geometric situation we consider is similar to the case of Abelian periodic operators (see Definition 4) from the Introduction. Now we allow the group to be noncommutative, and we allow the action to be represented projectively only on the bundle.

Definition and proposition 5 (gauge-periodic operator): Let X be a smooth oriented Riemannian manifold without boundary, Γ a discrete group acting on X from the left freely, isometrically,

and properly discontinuously. Furthermore, we assume the action to be cocompact in the sense that the quotient $M:=X/\Gamma$ *is compact. This defines, as in the Abelian case, a left action of* $\gamma \in \Gamma$ *on smooth functions* $f \in C^\infty(X)$ *by*

$$\gamma^* f(x) := f(\gamma^{-1}x) \tag{23}$$

for $x \in X$. *As before, this extends to a unitary action on* $L^2(X)$.

Next, let E be a smooth Hermitian vector bundle over X. Let U be a projective representation of Γ *in the unitary operators* $\mathcal{U}(L^2(E))$ *in the following sense:*

$$\forall \gamma_1, \gamma_2 \in \Gamma: \exists \Theta(\gamma_1, \gamma_2) \in C(X, S^1): U_{\gamma_1} U_{\gamma_2} = \Theta(\gamma_1, \gamma_2) U_{\gamma_1 \gamma_2}. \tag{24}$$

Assume that U is a (projective) lift of the Γ*-action on* $C^\infty(X)$, i.e.,

$$\forall \varphi \in C_c^\infty(X): \forall s \in L^2(E): \forall \gamma \in \Gamma: U_\gamma(\varphi s) = (\gamma^* \varphi) U_\gamma(s). \tag{25}$$

Assume that U is smooth, i.e., $\forall \gamma \in \Gamma: U_\gamma(C^\infty(E) \cap L^2(E)) \subset C^\infty(E)$. *Then* U_γ *is* γ*-local, i.e.,*

$$\forall s \in C^\infty(E): \operatorname{supp}(U_\gamma s) \subset \gamma \operatorname{supp} s, \tag{26}$$

and it leaves the domain $\mathcal{D}(D) = C_c^\infty(E)$ *of any differential operator D on E invariant. We call D* **gauge-periodic** *if, on* $\mathcal{D}(D)$, *one has*

$$\forall \gamma \in \Gamma: [U_\gamma, D] = 0. \tag{27}$$

Proof: Let $x \in X \backslash \operatorname{supp} s$. Since $\operatorname{supp} s$ is closed there is a neigborhood $O \subset X$ of x and $\varphi \in C_c^\infty(X)$ with $\varphi|O = 1$, $\varphi|_{\operatorname{supp} s} = 0$. Then $(1-\varphi)s = s$ and therefore

$$U_\gamma s = U_\gamma((1-\varphi)s) = (1 - \gamma^* \varphi) U_\gamma s = 0 \text{ on } \gamma O.$$

Since U is smooth also, it leaves $C_c^\infty(E)$ invariant. □

Proposition 3 (cocycle property): Θ *fulfills the cocycle property,*

$$\forall \gamma_1, \gamma_2, \gamma_3 \in \Gamma: \Theta(\gamma_1, \gamma_2)\Theta(\gamma_1\gamma_2, \gamma_3) = \Theta(\gamma_1, \gamma_2\gamma_3)\gamma_1^*[\Theta(\gamma_2, \gamma_3)]. \tag{28}$$

Proof: This follows from associativity $U_{\gamma_1}(U_{\gamma_2}U_{\gamma_3}) = (U_{\gamma_1}U_{\gamma_2})U_{\gamma_3}$ and the projectivity condition (24),

$$\begin{aligned} U_{\gamma_1}(U_{\gamma_2}U_{\gamma_3}) = U_{\gamma_1}\Theta(\gamma_2, \gamma_3)U_{\gamma_2\gamma_3} &= \gamma_1^*[\Theta(\gamma_2, \gamma_3)]U_{\gamma_1}U_{\gamma_2\gamma_3} \\ &= \Theta(\gamma_1, \gamma_2\gamma_3)\gamma_1^*[\Theta(\gamma_2, \gamma_3)]U_{\gamma_1\gamma_2\gamma_3}, \end{aligned}$$

$$\begin{aligned} (U_{\gamma_1}U_{\gamma_2})U_{\gamma_3} &= \Theta(\gamma_1, \gamma_2)U_{\gamma_1\gamma_2}U_{\gamma_3} \\ &= \Theta(\gamma_1, \gamma_2)\Theta(\gamma_1\gamma_2, \gamma_3)U_{\gamma_1\gamma_2\gamma_3}. \end{aligned}$$

□

Remark 10 (exact cocycle and representation): Θ *therefore defines a class in the group cohomology* $H^2(\Gamma, C(X, S^1))$.[19] *Exact 2-cocycles have the form,*

$$\Theta(\gamma, \gamma') = \sigma(\gamma)\gamma^*[\sigma(\gamma')]\sigma(\gamma\gamma')^{-1} \tag{29}$$

with a 1-cocycle σ, *so they define a proper representation of* Γ *by*

$$\tilde{U}_\gamma := \sigma(\gamma)^{-1} U_\gamma, \tag{30}$$

which also commutes with D if the cocycle is constant in $x \in X$. Without loss of generality we assume that Θ is normalized, i.e., $\Theta(e,e)=1$.

Proposition 4 (bundle morphisms): U defines a family u of vector bundle morphisms on E, $u_\gamma : E_x \to E_{\gamma x}$. u is a projective lift of the Γ-action from X to E, i.e.,

$$\forall \gamma_1 \gamma_2 \in \Gamma : u_{\gamma_1} u_{\gamma_2} = \Theta(\gamma_1, \gamma_2) u_{\gamma_1 \gamma_2} \tag{31}$$

with the same cocycle Θ as for U. u induces U via

$$(U_\gamma s)(x) := u_\gamma s(\gamma^{-1} x). \tag{32}$$

If t is a (proper) lift of the Γ-action from X to E and T the induced action

$$(T_\gamma s)(x) := t_\gamma s(\gamma^{-1} x) \tag{33}$$

on $C^\infty(X)$, then u and U can be expressed as $u=mt$ and $U=MT$, where m is a family of (strict) vector bundle isomorphisms.

Proof: Let $v \in E_x$. We choose $s \in C^\infty(E)$ with $s(x)=v$ and set—*a priori* depending on s $-u^s_\gamma(v) := (U_\gamma(s))(\gamma x) \in E_{\gamma x}$. If $\varphi \in C^\infty(x)$, $\varphi(x)=1$, we get

$$u^{\varphi s}_\gamma(v) = (\gamma^* \varphi)(\gamma x)(U_\gamma(s))(\gamma x) = u^s_\gamma(v),$$

i.e., $u^s_\gamma(v)$ depends on the value of s at the point x only; hence we omit s in the notation. The morphism property follows from the corresponding property of U_γ, and from $(u_\gamma)^{-1} = u_{\gamma^{-1}}$.

u induces U by construction.

If there is a proper lift t then $m := u t^{-1}$ defines the strict morphism we look for

$$\begin{array}{ccccc} E & \xrightarrow{t_\gamma^{-1}} & E & \xrightarrow{u_\gamma} & E \\ \downarrow & & \downarrow & & \downarrow \\ X & \xrightarrow{\gamma^{-1}} & X & \xrightarrow{\gamma} & X \end{array}$$

□

Remark 11 (lift of the action): If Θ is exact and $\tilde{u}$ the family of vector bundle isomorphisms belonging to $\tilde{U}$ by remark 10 then $\tilde{u}$ is a proper lift of the Γ-action from X to E.

Proposition 5 (properties of the cocycle): (1) $\forall \gamma \in \Gamma : \Theta(\gamma, e) = \Theta(e, \gamma) = 1$; (2) $\forall \gamma \in \Gamma : \Theta(\gamma, \gamma^{-1}) = \Theta(\gamma^{-1}, \gamma)$.

Proof: Easy consequences of the cocycle property. □

For the case of a bicharacter Θ Brüning and Sunada[20,21] describe how to construct a parametrix for elliptic gauge-periodic differential operator by lifting and translating a parametrix for a fundamental domain. The same construction works for the slightly more general case of a 2-cocycle.

From this one concludes as in the cited work:

Theorem 11 (self-adjointness): *Every symmetric elliptic gauge-periodic differential operator is essentially self-adjoint on $C^\infty_c(E)$.*

Similarly, a trivial extension of Refs. 20 and 21 shows how to construct the heat kernel:

Theorem 12 (heat kernel): *Let D be a symmetric elliptic gauge-periodic differential operator, bounded below, of order $p > d = \dim X$. Then $e^{-t\overline{D}}$ has, for $t>0$, a smooth integral kernel $K_t(x,y) \in E_x \otimes E_y^*$ such that*

$$|K_t(x,y)| \leq C_1 t^{-d/p} \exp(-C_2 \operatorname{dist}(x,y)^{p/(p-1)} t^{-1/(p-1)}) \tag{34}$$

with $C_1, C_2 > 0$, *uniformly on* $(0,T] \times X \times X$.

Again following 20 we construct a suitable decomposition of $L^2(E)$. For that we choose a fundamental domain $\mathcal{D}$ for the Γ-action, set $\mathcal{H} = L^2(E|_{\mathcal{D}})$ and define a unitary map by

$$\Phi: L^2(E) \to l^2(\Gamma, \mathcal{H}) \simeq l^2(\Gamma) \otimes \mathcal{H}, \quad \Phi(s)(\gamma) = (U_\gamma(s))|_{\mathcal{D}}.$$

Then we have for $f \in l^2(\Gamma) \otimes \mathcal{H}$,

$$\begin{aligned}(\Phi U_\gamma \Phi^* f)(\gamma') &= (U_{\gamma'} U_\gamma \Phi^* f)|_{\mathcal{D}} = \Theta(\gamma', \gamma)(U_{\gamma' \gamma} \Phi^* f)|_{\mathcal{D}} \\ &= \Theta(\gamma', \gamma)(\Phi \Phi^* f)(\gamma' \gamma) = \Theta(\gamma', \gamma) f(\gamma' \gamma) \\ &=: \Theta(\gamma', \gamma) R_\gamma f(\gamma') = R^\Theta_\gamma f(\gamma')\end{aligned}$$

with the right translation R_γ and twisted right translation $R^\Theta_\gamma f(\gamma')$.

So it is natural to try and define a $C^*_r(\Gamma, \Theta)$-action on $L^2(E)$ by

$$R^\Theta_\gamma(s) = U_\gamma(s)$$

for $s \in L^2(E)$. Here, the cocycle Θ can in general depend on $x \in X$ so that we have to find the gauge-translations in $C(X, S^1) \times_{\alpha, \theta} \Gamma$. This C^*-algebra has interesting structural properties but is not suitable for the applications on spectral theory developed in the previous section.

If Θ is periodic in $x \in X$ then we get a field of twisted reduced group C^*-algebras $C^*_r(\Gamma, \Theta_x), x \in M$ over M. In general this field is still too ''large.''

Therefore we require the cocycle to be constant in $x \in X$, so that we have to deal with the reduced twisted group C^*-algebra $C^*_r(\Gamma, \Theta)$ only. This is still general enough for the applications we are interested in: magnetic Schrödinger operators (and their Pauli and Dirac analogs).

Now note that $l^2(\Gamma)$ is the GNS representation space of $\mathcal{A} := C^*_r(\Gamma, \Theta)$ with respect to the canonical trace given by

$$\tau(R^\Theta_\gamma) = \begin{cases} 1, & \gamma = e, \\ 0, & \text{else}, \end{cases}$$

and that $l^1(\Gamma) \subset C^*_r(\Gamma, \Theta) \subset l^2(\Gamma)$. The action is naturally a left action since it is given by endomorphisms on a vector space. Therefore it's natural to view the left Hilbert-$\mathcal{A}$ module as $\mathcal{E} := \mathcal{H} \otimes \mathcal{A}$ so that $L^2(E)$ is the Hilbert-GNS representation space of $\mathcal{E}$. To define the scalar product we use the observations made in the commutative case (see Definition and Proposition 1),

$$\langle s_1 | s_2 \rangle_{\mathcal{E}} = \sum_{\gamma \in \Gamma} \langle U_\gamma s_2 | s_1 \rangle_{L^2(E)} R^\Theta_\gamma. \tag{35}$$

Lemma 8 (left pre-Hilbert $\mathcal{A}$-module): for $s_1, s_2 \in C_c(E)$ *defines the structure of a left pre-Hilbert $\mathcal{A}$-module on* $C_c(E)$*; under the isomorphism* Φ *it coincides with the left tensor Hilbert $\mathcal{A}$-module structure of* $\mathcal{H} \otimes \mathcal{A}$.

Proof: For $f_1, f_2 \in \mathcal{H}, a_1, a_2 \in \mathcal{A}$ we have by definition

$$\langle a_1 \otimes f_1 | a_2 \otimes f_2 \rangle_{\mathcal{A} \otimes \mathcal{H}} = \langle f_2 | f_1 \rangle_{\mathcal{H}} a_1 a_2^*,$$

since a left Hilbert-$\mathbb{C}$-module is a Hilbert space with conjugated scalar product (complex linear in the first argument, antilinear in the second). For $s_1, s_2 \in C_c(E)$ we get after identifying $\delta_{\gamma^{-1}}$ with $\overline{\Theta}(\gamma, \gamma^{-1}) R^\Theta_\gamma$,

$$\langle \Phi(s_1)|\Phi(s_2)\rangle_{\mathcal{A}\otimes\mathcal{H}} = \sum_{\gamma,\gamma'\in\Gamma} \langle \delta_\gamma \otimes \Phi(s_1)(\gamma)|\delta_{\gamma'}\otimes\Phi(s_2)(\gamma')\rangle_{\mathcal{A}\otimes\mathcal{H}}$$

$$= \sum_{\gamma,\gamma'\in\Gamma} \langle \Phi(s_2)(\gamma')\Phi(s_1)(\gamma)\rangle_{\mathcal{H}} \overline{\Theta}(\gamma^{-1},\gamma)\Theta(\gamma'^{-1},\gamma') R^{\Theta}_{\gamma^{-1}}(R^{\Theta}_{\gamma'^{-1}})^*$$

$$= \sum_{\gamma,\gamma'\in\Gamma} \langle \Phi(s_2)(\gamma')|\Phi\Phi(s_1)(\gamma)\rangle_{\mathcal{H}} \overline{\Theta}(\gamma^{-1},\gamma) R^{\Theta}_{\gamma^{-1}} R^{\Theta}_{\gamma'}$$

$$= \sum_{\gamma,\gamma'\in\Gamma} \langle (U_{\gamma'}s_2)|_{\mathcal{D}}(U_\gamma s_1)|_{\mathcal{D}}\rangle_{\mathcal{H}} \overline{\Theta}(\gamma^{-1},\gamma)\Theta(\gamma^{-1},\gamma') R^{\Theta}_{\gamma^{-1}\gamma'}$$

$$= \sum_{\gamma,\gamma'\in\Gamma} \langle (U_{\gamma\gamma'}s_2)|_{\mathcal{D}}|(U_\gamma s_1)|_{\mathcal{D}}\rangle_{\mathcal{H}} \overline{\Theta}(\gamma^{-1},\gamma)\Theta(\gamma^{-1},\gamma\gamma') R^{\Theta}_{\gamma'}$$

$$= \sum_{\gamma,\gamma'\in\Gamma} \langle (U_\gamma U_{\gamma'}s_2)|_{\mathcal{D}}|(U_\gamma s_1)|_{\mathcal{D}}\rangle_{\mathcal{H}} \Theta(\gamma,\gamma')\overline{\Theta}(\gamma^{-1},\gamma)\Theta(\gamma^{-1},\gamma\gamma') R^{\Theta}_{\gamma'}$$

$$= \sum_{\gamma,\gamma'\in\Gamma} \langle (U_\gamma U_{\gamma'}s_2)|_{\mathcal{D}}|(U_\gamma s_1)|_{\mathcal{D}}\rangle_{\mathcal{H}} R^{\Theta}_{\gamma'}$$

$$= \sum_{\gamma'\in\Gamma} \langle U_{\gamma'}s_2|s_1\rangle_{L^2(E)} R^{\Theta}_{\gamma'}.$$

This shows that the structures coincide. □

Lemma 9 (left Hilbert $\mathcal{A}$-module): The completion of the left pre-Hilbert $\mathcal{A}$ -module $C_c(E)$ is isomorphic to $\mathcal{E}=\mathcal{H}\otimes\mathcal{A}$. The GNS representation of $\mathcal{E}$ with respect to the canonical trace τ on $\mathcal{A}$ is isomorphic to $L^2(E)$.

Proof: By Eq. (35) we have for $s\in C_c(E)$,

$$\|s\|^2_{\mathcal{E}} = \|\langle s|s\rangle_{\mathcal{E}}\|_{\mathcal{A}} \geqslant \langle s|s\rangle_{L^2(E)}.$$

Therefore, the completion of $C_c(E)$ with respect to $\|\cdot\|_{\mathcal{E}}$ is contained in the one with respect to $\|\cdot\|_{L^2(E)}$, i.e. in $L^2(E)$. But $C_c(E)$ is dense in $\mathcal{E}$.

We get the scalar product of the GNS representation with respect to τ for $s_1, s_2\in C_c(E)$ from

$$\langle s_1|s_2\rangle_\tau = \tau(\langle s_2|s_1\rangle_{\mathcal{E}}) = \tau\left(\sum_{\gamma\in\Gamma}\langle U_\gamma s_1|s_2\rangle_{L^2(E)} R^{\Theta}_{\gamma}\right),$$

$$= \sum_{\gamma\in\Gamma}\langle U_\gamma s_1|s_2\rangle_{L^2(E)}\tau(\tilde{\rho}(\delta_\gamma))$$

$$= \langle s_1|s_2\rangle_{L^2(E)}.$$

Since $C_c(E)\subset\mathcal{E}\subset L^2(E)$ is dense the GNS representation space is exactly $L^2(E)$. □

Lemma 10 ($\mathcal{A}$-compact operators): The $\mathcal{A}$-compact operators on $\mathcal{E}$ are given by

$$\mathcal{K}_{\mathcal{A}}(\mathcal{E}) \simeq \mathcal{A}^{op}\otimes\mathcal{K}. \tag{36}$$

Here $\mathcal{K}$ denotes the compact operators on $\mathcal{H}=L^2(E|_{\mathcal{D}})$, and $\mathcal{A}^{op}$ is the C-algebra $C^*_r(\Gamma,\theta)^L$ generated by the left translations twisted with θ.*

Proof: For tensor products of left Hilbert modules we have in general,

$$\mathcal{K}_{\mathcal{A}}(\mathcal{A}\otimes\mathcal{H})\simeq\mathcal{K}_{\mathcal{A}}(\mathcal{A})\otimes\mathcal{K}_{\mathbb{C}}(\mathcal{H}) \quad \simeq\mathcal{A}^{\mathrm{op}}\otimes\mathcal{K}.$$

The statement about $\mathcal{A}^{\mathrm{op}}$ is well known in the untwisted case since the opposite of left multiplication is right multiplication. It is easy to check that this holds in the twisted case also. □

Following our rationale from Sec. IV we define a trace tr_τ and identify bounded module operators in $\mathcal{L}_{\mathcal{A}}(\mathcal{E})$ with their images in $\mathcal{L}(L^2(E))$ under the faithful representation with respect to τ.

As in Refs. 22 and 21, one shows, using Theorem 12:

Theorem 13 (gauge-periodic operators): *Let D be a symmetric gauge-periodic differential operator. Then the resolvent of $\overline{D}$ is $\mathcal{A}$-compact, and $e^{-t\overline{D}^2}$ is tr_τ-trace class.*

Theorem 14 (gauge-periodic module operators): *Let D be a symmetric gauge-periodic differential operator. Then D defines an $\mathcal{A}$-elliptic operator T such that the resolvents of $\overline{D}$ and $\overline{T}$ coincide (under the GNS representation).*

Proof: Set $\mathcal{D}(T):=\mathcal{D}(D)=C_c^\infty(E)$. Then $\mathcal{D}(T)\subset\mathcal{E}$ dense, we set $T:=D$ as operators on vector spaces.

T is adjointable since D is symmetric and gauge-periodic: For $s_1,s_2\in C_c^\infty(E)$ we have

$$\begin{aligned}\langle s_1|Ds_2\rangle_{\mathcal{E}}&=\sum_{\gamma\in\Gamma}\langle U_\gamma s_1|Ds_2\rangle_{L^2(E)}R_\gamma^\theta\\&=\sum_{\gamma\in\Gamma}\langle DU_\gamma s_1|s_2\rangle_{L^2(E)}R_\gamma^\theta\\&=\sum_{\gamma\in\Gamma}\langle U_\gamma Ds_1|s_2\rangle_{L^2(E)}R_\gamma^\theta\\&=\langle Ds_1|s_2\rangle_{\mathcal{E}}.\end{aligned}$$

Finally, $\mathrm{ran}(1+D^*D)$ is dense in $L^2(E)$ because D is essentially self-adjoint; therefore, T is regular. □

This allows us to apply all of the spectral characterizations from the previous section.

Example 8 (periodic elliptic operator): A gauge-periodic operator is called periodic if the corresponding cocycle fulfills $\Theta\equiv 1$. If the group Γ is Abelian then we are back in the commutative case (see Definition 4) where ordinary Bloch theory applies. If Γ is not Abelian then it does not apply, although the cocycle is trivial. But it is still covered by noncommutative Bloch theory, of course.

Example 9 (magnetic Schrödinger operator): In example 3 and Remark 3 we saw that the magnetic Schrödinger operator with a magnetic field $b\in\Omega^2(X), db=0, [(1/2\pi)\,b]\in H^2(X,\mathbb{Z})$ is given by a (symmetric elliptic) Bochner–Laplace operator on a Hermitian line bundle L over X with curvature b. It is gauge-periodic with possibly nonconstant cocycle if $H^1(X,S^1)=0$ (see Remark 3 and the work cited there in). If b is exact then the cocycle can be chosen to be constant. If the magnetic flux is integral $[b_M\in H^2(M,\mathbb{Z})$, see Example 3], then the operator is periodic. If there is a periodic magnetic potential a for $b=da$ (i.e., if the magnetic flux is 0) then the operator is strictly periodic in the usual sense of ordinary Bloch theory, i.e., it is a periodic operator on $L^2(X)$ (no magnetic translations, no bundles).

Example 10 (magnetic Schrödinger operator on $\mathbb{R}^2$): In the Euclidean case, if $\Gamma=\mathbb{Z}^2$ we end up with a rotation algebra $\mathcal{A}_\theta$, where θ is given by the magnetic flux. So, from Theorem 9 we get band structure in the case of rational flux and weak genericity of Cantor spectra in the case of irrational flux. Since it is a criterion inside the algebra of symmetries it applies to the corresponding Pauli and Dirac operators as well.

Example 11 (magnetic Schrödinger operator on $\mathbb{H}^2$): To investigate the importance of the geometry it is interesting to study the hyperbolic analog, since the corresponding cocompact

groups (Fuchsian groups) are nonamenable and therefore ''opposite'' to the amenable groups in the Euclidean case. The analog of a constant magnetic field is a constant multiple of the volume form. References 23, 24 compute K-groups and Kadison constants for twisted Fuchsian groups: Again, one has Kadison property if and only if the magnetic flux is rational.

References 25 and 26 study similar questions for good orbifolds.

Example 12 (gauge-periodic point perturbations): In Euclidean space, point perturbations provide explicitly solvable models for periodic Schrödinger operators. References 27 and 28 show how to define these types of operators more generally in our given geometric context (manifold with cocompact group action). If the point perturbation is gauge-periodic, then the perturbed operator is gauge-periodic in our sense, so that noncommutative Bloch theory applies. In particular, periodic point perturbations of the magnetic Schrödinger operator with rational flux have band structure.

C. Elliptic operators on Hilbert module bundles

Example 13: Ref. 29 extended the usual notion of an index of an operator by replacing Hilbert spaces by Hilbert modules: Let $\mathcal{A}$ be a C^*-algebra, M a compact Riemannian manifold and E a bundle over M of Hilbert $\mathcal{A}$-modules (a Hilbert module bundle). On can define Sobolev norms as usual, now coming from an $\mathcal{A}$-scalar product. Thus one gets a scale of Sobolev–Hilbert $\mathcal{A}$-modules for which the Sobolev lemma holds. Instead of the usual pseudo-differential operators whose coefficients are vector space endomorphisms one has $\mathcal{A}$-pseudo-differential operators with coefficients in the bundle $\mathcal{L}_{\mathcal{A}}(E)\cup_{x\in M}\mathcal{L}_{\mathcal{A}}(E_x)$. They act in the usual way on the Sobolev–Hilbert modules. Symbols of $\mathcal{A}$-pseudo-differential operators are represented by section of $\mathcal{L}_{\mathcal{A}}(E)$. As in the scalar case, an elliptic operator has an $\mathcal{A}$-compact resolvent, hence it is $\mathcal{A}$-elliptic in the sense of Definition 5. Furthermore, elliptic operators are $\mathcal{A}$-Fredholm and therefore have an index in $K_0(\mathcal{A})$.

A special case are the periodic elliptic operators: Let X be a Riemannian manifold with properly discontinuous, isometric, cocompact action of a group Γ, and D a Γ-periodic operator as in Example 8, $M:=\Gamma\backslash X$. Let ρ be the right regular representation of Γ on $\mathcal{A}:=C_r^*(\Gamma)$. [Usually one studies the right regular representation on the vector space $\mathbb{C}\Gamma\subset C_r^*(\Gamma)$ or on the Hilbert space $l^2(\Gamma)\supset C_r^*(\Gamma)$; but $C_r^*(\Gamma)$ is a Γ-invariant subspace of $l^2(\Gamma)$.] Then $X\times_\rho\mathcal{A}$ is an $\mathcal{A}$-bundle over M on which D acts. Besides, $\mathcal{A}$ carries the structure of a standard Hilbert-$\mathcal{A}$ module. If D is elliptic then D determines an elliptic operator on $X\times_\rho\mathcal{A}$.

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APPENDIX A: CONTINUOUS FIELDS OF HILBERT SPACES

We follow the classic Ref. 30.

Definition 6 (continuous fields of Banach and Hilbert spaces): Let B be a topological space, $(E(z))_{z\in B}$ a family of Banach spaces. The linear space $\Pi:=\Pi_{z\in B}E(z)$ is called space of all vector fields. A continuity structure on Π is defined by a subspace $\Lambda\subset\Pi$ such that:

(1) Λ is a $C_\infty(B)$-submodule of Π;
(2) $\forall z\in B:\forall\xi\in E(z):\exists x\in\Lambda:x(z)=\xi$;
(3) $\forall x\in\Lambda:(z\mapsto\|x(z)\|)\in C_\infty(B)$;
(4) $\forall x\in\Pi:\langle\forall\varepsilon>0:\forall z\in B:\exists x'\in\Lambda,$ neighborhood $U\ni z:\ \forall z'\in U:\|x(z')-x'(z')\|<\varepsilon\rangle\Rightarrow x\in\Lambda\rangle$;

$\mathcal{E}:=((E(z))_{z\in B},\Lambda)$ *is called continuous field of Banach spaces. If the fibers* $E(z)$ *are Hilbert spaces we have a continuous field of Hilbert spaces. The scalar product is automatically continuous.*

Condition 4 is a completeness condition: If a vector field $x\in\Pi$ can be locally approximated arbitrarily well by continuous vector fields then it is continuous.

Proposition 6 (defining submodule): Let B,Π *be as above and* $\Lambda\subset\Pi$ *a subspace with*

(1) $\forall z\in B:\{x(z)|x\in\Lambda\}=:\Lambda(z)$ *dense in* $E(z)$*; and*
(2) $\forall x\in\Lambda:(z\mapsto\|x\|)\in C_\infty(B)$.

Then there is a unique continuity structure $\tilde{\Lambda}$ *on* Π *with* $\tilde{\Lambda}\supset\Lambda$. $\tilde{\Lambda}$ *is given by*

$$\tilde{\Lambda}=\{x\in\Pi|\forall z\in B:\varepsilon>0\,\exists\ neighborhood\ U\ni z,x'\in\bar{\Lambda}:\forall z'\in U:\|x(z')-x'(z')\|<\varepsilon\}.$$

Lemma 11 (continuous fields and Banach space bundles): A continuous field of Banach spaces $\mathcal{E}$ *defines a Banach space bundle* E *over* B *so that the continuous sections* $C(E)$ *are the continuous vector fields of* $\mathcal{E}$.

Proof: As a set $E:=\Pi_{z\in B}E(z)$. We choose the topology so that the natural projection $\pi:E\to B$ is continuous and open: The topology is generated by the tubular neighborhoods

$$T(U,x,\varepsilon):=\{\xi\in E|\pi(\xi)\in U\wedge\|\xi-x(\pi(\xi))\|<\varepsilon\}$$

for open sets $U\subset B$, continuous fields $x\in\mathcal{E}$ and $\varepsilon>0$. It is easy to check that the tubular neighborhoods generate a topology on E with the desired properties. On the fibers $E(z)$ it induces the strong topology since the intersections $E(z)\cap T(U,x,\varepsilon)$ of the fibers with the tubular neighborhoods are just norm balls in the fiber. □

Remark 12 (local triviality): A bundle has a continuous open surjection onto the base, but is not necessarily locally trivial. However, for a locally compact base and finite dimensional fibers this follows from the existence of the projection.

Lemma 12 (continuous field as the Hilbert C-module): A continuous field of Hilbert spaces* $\mathcal{E}=((E(z))_{z\in B},\Lambda)$ *over* B *defines a Hilbert* $C_\infty(B)$*-module structure on* Λ. *Vice versa: A Hilbert* $C_\infty(B)$*-module defines a continuous field of Hilbert spaces, and this correspondence is one-to-one.*

APPENDIX B: HILBERT *C**-MODULES

Usually Hilbert C^*-modules are defined to be right modules. We define these and the left modules and list basic properties and objects connected to them.

Definition 7 [(right) Hilbert module]: Let $\mathcal{A}$ *be a* C^**-algebra. A right* $\mathcal{A}$*-module* $\mathcal{E}$ *is called (right) pre-Hilbert* $\mathcal{A}$*-module if it is endowed with a map* $\langle\cdot|\cdot\rangle:\mathcal{E}\times\mathcal{E}\to\mathcal{A}$ *with the following properties:*

(1) $\langle e|f+g\rangle=\langle e|f\rangle+\langle e|g\rangle$ *for* $e,f,g\in\mathcal{E}$;
(2) $\langle e|f\lambda\rangle=\langle e|f\rangle\lambda$ *for* $e,f\in\mathcal{E},\lambda\in\mathbb{C}$;
(3) $\langle e|fa\rangle=\langle e|f\rangle a$ *for* $e,f\in\mathcal{E},a\in\mathcal{A}$;
(4) $\langle f|e\rangle=\langle e|f\rangle^*$ *for* $e,f\in\mathcal{E}$;
(5) $\langle e|e\rangle\geqslant 0$ *in* $\mathcal{A}$ *for* $e\in\mathcal{E}$, *and* $\langle e|e\rangle=0\Leftrightarrow e=0$.

Then the map $\mathcal{E}\ni e\mapsto\sqrt{\|\langle e|e\rangle\|_{\mathcal{A}}}$ *defines a norm on* $\mathcal{E}$. *The closure of* $\mathcal{E}$ *is defined as the completion of* $\mathcal{E}$ *as Banach space with this norm.*

$\mathcal{E}$ *is called (right) Hilbert* $\mathcal{A}$*-module if* $\mathcal{E}$ *is complete in this norm.*

An operator $T\in\mathcal{L}(\mathcal{E})$ *is called adjointable if there is* $T^*\in\mathcal{L}(\mathcal{E})$ *such that for all* $e,f\in\mathcal{E}$: $\langle e|Tf\rangle=\langle T^*e|f\rangle$. *The set of adjointable operators is denoted by* $\mathcal{L}_{\mathcal{A}}(\mathcal{E})$.

For $e,f\in\mathcal{E}$ *we define an operator* $\pi_{e,f}$ *by*

$$\pi_{e,f}:\mathcal{E}\ni x\mapsto e\langle f|x\rangle\in\mathcal{E}.$$

We set $\mathcal{F}_{\mathcal{A}}(\mathcal{E}):=\mathrm{span}\{\pi_{e,f}|e,f\in\mathcal{E}\}$ *and call this the set of* $\mathcal{A}$*-finite operators. The set* $\mathcal{K}_{\mathcal{A}}(\mathcal{E})$ *of* $\mathcal{A}$*-compact operators is the closure of* $\mathcal{F}_{\mathcal{A}}(\mathcal{E})$ *in* $\mathcal{L}_{\mathcal{A}}(\mathcal{E})$.

The brackets indicate that by Hilbert module we mean a right Hilbert module.

Definition 8 (left Hilbert module): Let $\mathcal{A}$ *be a C*-algebra. A left* $\mathcal{A}$*-module* $\mathcal{E}$ *is called left pre-Hilbert* $\mathcal{A}$*-module if it is endowed with a map* $\langle\cdot|\cdot\rangle:\mathcal{E}\times\mathcal{E}\to\mathcal{A}$ *with the following properties:*

(1) $\langle e+f|g\rangle=\langle e|g\rangle+\langle f|g\rangle$ *for* $e,f,g\in\mathcal{E}$;
(2) $\langle\lambda e|f\rangle=\lambda\langle e|f\rangle$ *for* $e,f\in\mathcal{E},\lambda\in\mathbb{C}$;
(3) $\langle ae|f\rangle=a\langle e|f\rangle$ *for* $e,f\in\mathcal{E},a\in\mathcal{A}$;
(4) $\langle f|e\rangle=\langle e|f\rangle^*$ *for* $e,f\in\mathcal{E}$;
(5) $\langle e|e\rangle\geqslant 0$ *in* $\mathcal{A}$ *for* $e\in\mathcal{E}$, *and* $\langle e|e\rangle=0\Leftrightarrow e=0$.

Then the map $\mathcal{E}\ni e\mapsto\sqrt{\|\langle e|e\rangle\|_{\mathcal{A}}}$ *defines a norm on* $\mathcal{E}$. *The closure of* $\mathcal{E}$ *is defined as the completion of* $\mathcal{E}$ *as Banach space with this norm.*

$\mathcal{E}$ *is called left Hilbert* $\mathcal{A}$*-module if* $\mathcal{E}$ *is complete in this norm.*

An operator $T\in\mathcal{L}(\mathcal{E})$ *is called adjointable if there is* $T^*\in\mathcal{L}(\mathcal{E})$ *such that for all* $e,f\in\mathcal{E}$: $\langle e|Tf\rangle=\langle T^*e|f\rangle$. *The set of adjointable operators is denoted by* $\mathcal{L}_{\mathcal{A}}(\mathcal{E})$.

For $e,f\in\mathcal{E}$ *we define an operator* $\pi^L_{e,f}$ *by*

$$\pi^L_{e,f}:\mathcal{E}\ni x\mapsto\langle x|e\rangle f\in\mathcal{E}.$$

We set $\mathcal{F}_{\mathcal{A}}(\mathcal{E}):=\mathrm{span}\{\pi^L_{e,f}|e,f\in\mathcal{E}\}$ *and call this the set of* $\mathcal{A}$*-finite operators. The set* $\mathcal{K}_{\mathcal{A}}(\mathcal{E})$ *of* $\mathcal{A}$*-compact operators is the closure of* $\mathcal{F}_{\mathcal{A}}(\mathcal{E})$ *in* $\mathcal{L}_{\mathcal{A}}(\mathcal{E})$.

Remark 13 (basic properties):

(1) If $\mathcal{E}$ *is a pre-Hilbert* $\mathcal{A}$*-module,* $e\in\mathcal{E}$, *then Definition 7.4 implies* $\langle e|e\rangle\in\mathcal{A}_{sa}$ *so that the condition* $\langle e|e\rangle\geqslant 0$ *in 7.5 makes sense indeed;*
(2) If $\mathcal{E}$ *is a pre-Hilbert* $\mathcal{A}$*-module,* $e,f\in\mathcal{E},a\in\mathcal{A}$ *then we have*

$$\langle ea|f\rangle=\langle f|ea\rangle^*=(\langle f|e\rangle a)^*=a^*\langle f|e\rangle^*=a^*\langle e|f\rangle,$$

i.e., we have $\mathbb{C}$*- and* $\mathcal{A}$*-sesqui-linearity;*
(3) The $\mathbb{C}$*-sesqui-linearity follows for unital* $\mathcal{A}$ *from the* $\mathcal{A}$*-sesqui-linearity.*
(4) For $e,f\in\mathcal{E}$ *we have* $\pi^*_{e,f}=\pi_{f,e}$ *so that indeed* $\mathcal{F}_{\mathcal{A}}(\mathcal{E})\subset\mathcal{L}_{\mathcal{A}}(\mathcal{E})$;
(5) $\mathcal{L}_{\mathcal{A}}(\mathcal{E})$ *and* $\mathcal{K}_{\mathcal{A}}(\mathcal{E})$ *are C*-algebras, the former is the multiplier algebra of the latter (Ref. 14, Chap. 15);*
(6) Everything analogous for left Hilbert modules;
(7) $\mathcal{A}\times\mathcal{A}\ni(a,b)\mapsto a^*b\in\mathcal{A}$ *together with multiplication of* $\mathcal{A}$ *on* $\mathcal{A}$ *on the right gives the standard Hilbert* $\mathcal{A}$*-module structure on* $\mathcal{A}$;
(8) $\mathcal{A}\times\mathcal{A}\ni(a,b)\mapsto ab^*\in\mathcal{A}$ *together with multiplication of* $\mathcal{A}$ *on* $\mathcal{A}$ *on the left gives the standard left Hilbert* $\mathcal{A}$*-module structure on* $\mathcal{A}$;

Definition 9 (free and projective Hilbert modules): A Hilbert $\mathcal{A}$*-module is called free if it is a free module over* $\mathcal{A}$. *It is called projective if it is a direct summand of a free module.*

Lemma 13 (left and right Hilbert modules): Let $\mathcal{A}$ *be a C*-*algebra *and* $(\mathcal{E},\langle\cdot|\cdot\rangle)$ *a left pre-Hilbert* $\mathcal{A}$*-module over* $\mathcal{A}$. *Then,*

$$\langle\cdot|\cdot\rangle^{\mathcal{E}^{\mathrm{op}}}:\mathcal{E}^{\mathrm{op}}\times\mathcal{E}^{\mathrm{op}}\to\mathcal{A}^{\mathrm{op}},\quad(e^{\mathrm{op}},f^{\mathrm{op}})\mapsto(\langle f|e\rangle)^{\mathrm{op}}\tag{B1}$$

defines on $\mathcal{E}=\mathcal{E}^{\mathrm{op}}$ *(equality as vector spaces) the structure of a pre-Hilbert* $\mathcal{A}^{\mathrm{op}}$*-module.*

Furthermore, for a left Hilbert $\mathcal{A}$*-module* $(\mathcal{E},\langle\cdot|\cdot\rangle)$ *we have* $\mathcal{F}_{\mathcal{A}}(\mathcal{E})\simeq\mathcal{F}_{\mathcal{A}^{\mathrm{op}}}(\mathcal{E}^{\mathrm{op}})$ *and therefore* $\mathcal{K}_{\mathcal{A}}(\mathcal{E})\simeq\mathcal{K}_{\mathcal{A}^{\mathrm{op}}}(\mathcal{E}^{\mathrm{op}})$ *and* $\mathcal{L}_{\mathcal{A}}(\mathcal{E})\simeq\mathcal{L}_{\mathcal{A}^{\mathrm{op}}}(\mathcal{E}^{\mathrm{op}})$.

Proof: It is well known that right $\mathcal{A}$-modules $\mathcal{E}$ and left $\mathcal{A}^{\mathrm{op}}$-modules $\mathcal{E}^{\mathrm{op}}$ are in one-to-one correspondence. So we just have to verify the corresponding Hilbert module structures: Let e^{op}, $f^{\mathrm{op}} \in \mathcal{E}^{\mathrm{op}}$, $a^{\mathrm{op}} \in \mathcal{A}^{\mathrm{op}}$. We denote by a^{op} and a corresponding elements in $\mathcal{A}^{\mathrm{op}}$ resp. $\mathcal{A}$. ($\mathcal{A}^{\mathrm{op}}$ and $\mathcal{A}$ are identical as Banach spaces, and in this sense $a^{\mathrm{op}}=a$.) Then,

$$\langle e^{\mathrm{op}}|f^{\mathrm{op}}a^{\mathrm{op}}\rangle^{\mathcal{E}^{\mathrm{op}}}=(\langle e^{\mathrm{op}}|(af)^{\mathrm{op}}\rangle)^{\mathrm{op}}=\langle af|e\rangle=a\langle f|e\rangle=(\langle f|e\rangle)^{\mathrm{op}}a^{\mathrm{op}}=\langle e^{\mathrm{op}}|f^{\mathrm{op}}\rangle^{\mathcal{E}^{\mathrm{op}}}a^{\mathrm{op}}.$$

Since $\mathcal{E}=\mathcal{E}^{\mathrm{op}}$ as Banach space we have $\mathcal{L}(\mathcal{E})\simeq\mathcal{L}(\mathcal{E}^{\mathrm{op}})$. Furthermore, for $e,f,x\in\mathcal{E}$,

$$\pi_{e,f}(x)=e\langle f|x\rangle=(\langle f|x\rangle)^{\mathrm{op}}e^{\mathrm{op}}=\langle x^{\mathrm{op}}|f^{\mathrm{op}}\rangle^{\mathcal{E}^{\mathrm{op}}}e^{\mathrm{op}}=\pi^{L}_{f^{\mathrm{op}},e^{\mathrm{op}}},$$

so that $\mathcal{F}_{\mathcal{A}}(\mathcal{E})$ and $\mathcal{F}_{\mathcal{A}^{\mathrm{op}}}(\mathcal{E}^{\mathrm{op}})$ are isomorphic, and so are the corresponding closures and multiplier algebras. □

Remark 14 (standard module): For the standard Hilbert $\mathcal{A}$-module structure on $\mathcal{A}$ it is well known that $\mathcal{F}_{\mathcal{A}}(\mathcal{A})=\mathcal{A}$, $\mathcal{K}_{\mathcal{A}}(\mathcal{A})=\mathcal{A}$ and $\mathcal{L}_{\mathcal{A}}(\mathcal{A})=\mathcal{M}(\mathcal{A})$. If we denote by $\mathcal{A}^{L}$ the standard left Hilbert $\mathcal{A}$-module then Lemma 13 shows: $\mathcal{F}_{\mathcal{A}}(\mathcal{A}^{L})\simeq\mathcal{F}_{\mathcal{A}^{\mathrm{op}}}(\mathcal{A}^{\mathrm{op}})=\mathcal{A}^{\mathrm{op}}$.

APPENDIX C: GNS REPRESENTATION FOR HILBERT *C**-MODULES

Let $\mathcal{A}$ be a C^*-algebra, τ a state on $\mathcal{A}$ and $\mathcal{E}$ a Hilbert $\mathcal{A}$-module. Analogously to the well know GNS representation of Banach $*$-algebras we define a scalar product on $\mathcal{E}$ by

$$\langle x|y\rangle_{\tau}:=\tau(\langle x|y\rangle_{\mathcal{E}}) \quad \text{for} \quad x,y\in\mathcal{E}. \tag{C1}$$

$N_{\tau}:=\{x\in\mathcal{E}|\langle x|x\rangle_{\tau}=0\}$ is the corresponding null space. Then the GNS representation space $\mathcal{E}_{\tau}$ is given by the completion of $\mathcal{E}/N_{\tau}$ with respect to $\langle\cdot|\cdot\rangle_{\tau}$. $L\in\mathcal{L}_{\mathcal{A}}(\mathcal{E})$ acts continuously on $x\in\mathcal{E}_{\tau}$ because

$$\begin{aligned}\|Lx\|_{\tau}^2=\langle Lx|Lx\rangle_{\tau}&=\tau(\langle Lx|Lx\rangle_{\mathcal{E}})\\&=\tau(\langle x|L^*Lx\rangle_{\mathcal{E}})\\&\leqslant\tau(\langle x|x\rangle_{\mathcal{E}})\|L^*L\|\\&=\|x\|_{\tau}^2\|L\|^2.\end{aligned}$$

Thus we have a $*$-representation of $\mathcal{L}_{\mathcal{A}}(\mathcal{E})$ in $\mathcal{L}(\mathcal{E}_{\tau})$.

If τ is faithful then $N_{\tau}=0$ so that the representation is faithful.

If $\mathcal{E}=\mathcal{A}$ with $\langle a|b\rangle_{\mathcal{E}}=a^*b$ is the standard Hilbert $\mathcal{A}$-module then we get back the usual GNS representation of the multiplier algebra $\mathcal{L}_{\mathcal{A}}(\mathcal{A})=\mathcal{M}(\mathcal{A})$ and, by restriction, the GNS representation of $\mathcal{K}_{\mathcal{A}}(\mathcal{A})=\mathcal{A}$.

For left Hilbert modules the scalar product must be reversed so that one gets complex linearity on the correct entry.

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Coordinate Bethe ansatz for the one-dimensional SU(n) Hubbard model with open boundary conditions

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The one-dimensional (1D) SU(n) Hubbard model with open boundary condition is solved by using the coordinate Bethe ansatz method. The energy and integrable boundary conditions are obtained. At the same time, the corresponding Bethe ansatz equations are achieved by diagonalizing the inhomogeneous transfer matrix of the open SU($2n-2$) XXX vertex model. When $n=2$, our result comes back to that of the 1D Hubbard model given by Deguchi and Yue (con-mat/9704138). © *2001 American Institute of Physics.* [DOI: 10.1063/1.1368368]

I. INTRODUCTION

In the integrable models to describe the strongly correlated electron system, the one-dimensional (1D) Hubbard model is one of the well studied models. It was proposed in Refs. 1 and 2 in order to describe electrons hopping on a D-dimension lattice while experiencing an on-site interaction. Although much work has been done on the Hubbard model since Lieb-Wu's work,[3] the integrability was not shown until 1986 by Shastry,[4] Olmedilla and Wadati.[5] Moreover, the eigenvalue of the transfer matrix related to the Hubbard model was suggested in Ref. 4 and proved through different methods.[6,7] Based on the Lie algebra knowledge, Maassarani succeeded in generalizing Shastry's method to construct an SU(n) Hubbard model[8] by considering two coupled SU(n) XX models.[9] Furthermore, he found the related R-matrix which ensures the integrability of the one-dimensional SU(n) Hubbard model.[10] (It was also proved by Martins for $n=3,4$,[11] and by Yue and Sasaki for general n in terms of Lax-pair formalism.[12]) The exact solution for the SU(3) and SU(n) Hubbard model with period boundary condition was also given in Refs. 13 and 14, respectively.

Recently, the integrable models with open boundary and impurities boundary have attracted a lot of interest.[15–30] On the 1D Hubbard model with open boundary conditions, the integrability and the exact solution have been investigated by several authors.[22–24] However, for the SU(n) Hubbard model, due to the noninvertibility of the partial transposition of the R matrix, the generalized algebraic method[15] does not work on the model with open boundary conditions. At the same time, the exact solution for the model with open boundary conditions has not been obtained yet. In this paper, we will apply the coordinate Bethe ansatz method to solve the SU(n) Hubbard model with open boundary conditions.

This paper is organized as following. In Sec. II, we will describe the open boundary SU(n) Hubbard model and present the integrable boundary conditions. In Sec. III, we will diagonalize the transfer matrix of open boundary SU($2n-2$) XXX vertex model by using the nested Bethe ansatz method to obtain the Bethe ansatz equations for the open boundary SU(n) Hubbard model. Some discussions are included in Sec. IV.

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II. COORDINATE BETHE ANSATZ FOR SU(n) HUBBARD

The Hamiltonian of the open SU(n) Hubbard model is

$$H=\sum_{k=1}^{\tilde{L}-1}\sum_{\alpha=1}^{n-1}\left(E_{\sigma,k}^{n\alpha}E_{\sigma,k+1}^{\alpha n}+E_{\sigma,k}^{\alpha n}E_{\sigma,k+1}^{n\alpha}+E_{\tau,k}^{n\alpha}E_{\tau,k+1}^{\alpha n}+E_{\tau,k}^{\alpha n}E_{\tau,k+1}^{n\alpha}\right)$$
$$+\frac{n^2U}{4}\sum_{k=1}^{\tilde{L}}C_{\sigma,k}C_{\tau,k}+\sum_{\alpha=1}^{n}\left(p_{\sigma\alpha}E_{\sigma,\tilde{L}}^{\alpha\alpha}+p_{\tau\alpha}E_{\tau,\tilde{L}}^{\alpha\alpha}+q_{\sigma\alpha}E_{\sigma,1}^{\alpha\alpha}+q_{\tau\alpha}E_{\tau,1}^{\alpha\alpha}\right), \tag{1}$$

where U is the Coulomb coupling constant and $E_{\rho,k}^{\alpha\beta}(\rho=\sigma,\tau)$ is a matrix with zeros everywhere except for a one at the intersection of row α and column β. The subscripts ρ and k stand for two different E operators at site $k(k=1,2,...,\tilde{L})$. The $(2n-2)\times(2n-2)$ diagonal matrix C is defined by $C=\Sigma_{\alpha=1}^{n-1}E^{\alpha\alpha}-E^{nn}$.

As in Ref. 13, we introduce the following particle state $|1\rangle_j,\cdots,|n-1\rangle_j$ and vacuum state $|0\rangle_j$ of the jth site:

$$|1\rangle_j=\begin{Bmatrix}1\\0\\\vdots\\0\\0\end{Bmatrix}_j,\quad |2\rangle_j=\begin{Bmatrix}0\\1\\\vdots\\0\\0\end{Bmatrix}_j,\quad\cdots,\quad |n-1\rangle_j=\begin{Bmatrix}0\\0\\\vdots\\1\\0\end{Bmatrix}_j,\quad |0\rangle_j=|n\rangle_j=\begin{Bmatrix}0\\0\\\vdots\\0\\1\end{Bmatrix}_j. \tag{2}$$

One can prove that $E_j^{\alpha n}$ and $E_j^{n\alpha}$ act as a creating and destroying operators of $|\alpha\rangle_j$, respectively.

In the coordinate Bethe ansatz method, the N particle eigenstates of the Hamiltonian can be assumed as

$$|\psi\rangle=\sum_{x_1\leqslant x_2\leqslant\cdots\leqslant x_N}f_{\rho_1\rho_2\cdots\rho_N}^{\alpha_1\alpha_2\cdots\alpha_N}E_{\rho_1x_1}^{\alpha_1n}E_{\rho_2x_2}^{\alpha_2n}\cdots E_{\rho_Nx_N}^{\alpha_Nn}|0\rangle. \tag{3}$$

Here $|0\rangle$ is the vacuum state of the total chain defined by $|0\rangle=\Pi_{j=1}^{\tilde{L}}\otimes|0\rangle_j$ and

$$f_{\rho_1\rho_2\cdots\rho_N}^{\alpha_1\alpha_2\cdots\alpha_N}=\sum_{Q,P}\epsilon_P\epsilon_QA_{\rho_{Q_1}\rho_{Q_2}\cdots\rho_{Q_N}}^{\alpha_{Q_1}\alpha_{Q_2}\cdots\alpha_{Q_N}}(k_{P_1},k_{P_2},\cdots,k_{P_N})\exp\left\{i\sum_{j=1}^{N}k_{P_j}x_{Q_j}\right\}\times\theta(x_{Q_1}\leqslant x_{Q_2}\leqslant\cdots\leqslant x_{Q_N}) \tag{4}$$

with

$$\theta(x_1\leqslant x_2\leqslant\cdots\leqslant x_N)=\begin{cases}1, & x_1<x_2<\cdots<x_N\\ \frac{1}{2}, & x_i=x_j(i\neq j,i,j=1,2,\cdots,N)\\ 0, & \text{others,}\end{cases} \tag{5}$$

where $\alpha_i\in[1,n-1](i\in[1,N])$ stands for different particle states, x_i the position of the particle, and $\rho_i=\sigma,\tau$ the type of the ith particle. The Q runs over S_N, the permutation group of N coordinates x_j, and P over all the permutations and the ways of negations of N momenta k_j. There are $N!\times2^N$ possibilities for P, while $N!$ for Q. ϵ_Q, ϵ_P denotes the sign of Q and P, respectively. For the permutation of P, if the permutation is even, P makes $\epsilon_P=-1$ for odd number of k's negative and $\epsilon_P=1$ for even number of k's negative. Substituting the wave function into the Schrödinger equation

$$H|\psi_N\rangle=E|\psi_N\rangle, \tag{6}$$

we have the following results:

$$A^{\cdots\alpha_i,\alpha_j,\cdots}_{\cdots\rho_i,\rho_j,\cdots}(\cdots,k_i,k_j,\cdots)=S^{\alpha_i\rho_i\ \ \alpha_j\rho_j}_{\alpha_i'\rho_i'\ \ \alpha_j'\rho_j'}(\sin k_i,\sin k_j)A^{\cdots\alpha_j',\alpha_i',\cdots}_{\cdots\rho_j',\rho_i'\cdots}(\cdots,k_j,k_i,\cdots), \tag{7}$$

$$A^{\alpha_1,\cdots}_{\rho_1,\cdots}(k_{P_1},\cdots)=M^{\alpha_1}_{\rho_1}(k_{P_1})A^{\alpha_1,\cdots}_{\rho_1,\cdots}(-k_{P_1},\cdots), \tag{8}$$

$$A^{\cdots,\alpha_N}_{\cdots,\rho_N}(\cdots,k_{P_N})=V^{\alpha_N}_{\rho_N}(-k_{P_N})A^{\cdots,\alpha_N}_{\cdots,\rho_N}(\cdots,-k_{P_N}) \tag{9}$$

with $S_{ij}(\sin k_i,\sin k_j)$ being the two-particle scattering matrix

$$S_{ij}(\sin k_i,\sin k_j)=\frac{(\sin k_i-\sin k_j)\tilde{I}+i\gamma\tilde{P}_{ij}}{\sin k_i-\sin k_j+i\gamma}, \tag{10}$$

where $\gamma=n^2U$, $\tilde{I}_{ij}=I^{\rho}_{ij}\otimes I^{\alpha}_{ij}$, $\tilde{P}_{ij}=P^{\rho}_{ij}\otimes P^{\alpha}_{ij}$ is the direct product of two kinds of permutation operators and permutes the particle styles and particle states simultaneously,

$$M^{\alpha_i}_{\rho_i}(k)=\frac{1+q^{\alpha_i}_{\rho_i}e^{-ik}}{1+q^{\alpha_i}_{\rho_i}e^{ik}}, \tag{11}$$

$$V^{\alpha_i}_{\rho_i}(k)=\frac{1+p^{\alpha_i}_{\rho_i}e^{-ik}}{1+p^{\alpha_i}_{\rho_i}e^{ik}}e^{2i(\tilde{L}+1)k} \tag{12}$$

with $q^{\alpha_i}_{\rho_i}=q_{\rho_i,n}-q_{\rho_i,\alpha_i}$, $p^{\alpha_i}_{\rho_i}=p_{\rho_i,n}-p_{\rho_i,\alpha_i}$. The energy of the Hamiltonian is

$$E=2\sum_{i=1}^{N}\cos k_i+\frac{\gamma}{2}(\tilde{L}-2N)+p_{\sigma n}+p_{\tau n}+q_{\sigma n}+q_{\tau n}. \tag{13}$$

From Eqs. (7)–(9), we can find that the amplitudes A satisfy

$$A^{\alpha_1,\cdots,\alpha_N}_{\rho_1,\cdots,\rho_N}(k_{P_1},\cdots k_{P_N})=\sum_{\{\rho_i',\alpha_i'\}}\{M(k_{P_1})X_{\hat{1}2}X_{\hat{1}3}\cdots X_{\hat{1}N}V(k_{P_1})\times X_{N1}X_{N-11}\cdots X_{21}\}^{\alpha_1\rho_1\cdots\alpha_N\rho_N}_{\alpha_1'\rho_1'\cdots\alpha_N'\rho_N'}A^{\alpha_1',\cdots,\alpha_N'}_{\rho_1',\cdots,\rho_N'}(k_{P_1},\cdots k_{P_N}), \tag{14}$$

where $X_{\hat{ij}}=S_{ij}(-\sin k_i,\sin k_j)$, $X_{ij}=S_{ij}(\sin k_i,\sin k_j)$,

$$M(k)=\mathrm{diag}(M^1_{\sigma}(k),\cdots,M^{n-1}_{\sigma}(k),M^1_{\tau}(k),\cdots,M^{n-1}_{\tau}(k)), \tag{15}$$

$$V(k)=\mathrm{diag}(V^1_{\sigma}(k),\cdots,V^{n-1}_{\sigma}(k),V^1_{\tau}(k),\cdots,V^{n-1}_{\tau}(k)). \tag{16}$$

From the point of the vertex model's view, the scattering matrix S_{ij} can be viewed as a SU($2n-2$) vertex model R_{ij}, which are defined by

$$R_{ij}(\sin k_i,-\sin k_j)=\frac{(\sin k_i-\sin k_j)I+\eta P_{ij}}{\sin k_i-\sin k_j+\eta}, \tag{17}$$

where $\eta=i\gamma$, I and P_{ij} are $(2n-2)^2\times(2n-2)^2$ identy matrix and permutation matrix, respectively. The notations $R_{ij}(u)=R_{ij}(u,0)$, $R_{ij}(u+v)=R_{ij}(u,v)$ will be used later. The R-matrix defined by (17) satisfies the Yang–Baxter equation

$$R_{12}(u-v)R_{13}(u)R_{23}(v)=R_{23}(v)R_{13}(u)R_{12}(u-v), \tag{18}$$

it also fulfills the following properties

$$P\text{-}T \text{ invariance:} \quad P_{12}R_{12}(u)P_{12}=R_{12}^{t_1t_2}(u), \tag{19}$$

$$\text{unitarity:} \quad R_{12}(u)R_{21}(-u)=1\cdot \mathrm{id}, \tag{20}$$

$$\text{crossing symmetry:} \quad R_{12}^{t_1}(u)R_{12}^{t_2}(-u-2(n-1)\eta)=\frac{u(u+2(n-1)\eta)}{(u+\eta)(u+(2n-3)\eta)}\cdot \mathrm{id}. \tag{21}$$

In order to diagonalize Eq. (14), we introduce the following operator $t(u)$:

$$t(u)=\mathrm{tr}_0\, K_0^+(u)T(u,\{-\sin k_i\})K_0^-(u)T(-u,\{-\sin k_i\})^{-1}, \tag{22}$$

where

$$T(u,\{-\sin k_i\})=L_{01}(u,-\sin k_1)L_{02}(u,-\sin k_2)\cdots L_{0N}(u,-\sin k_N) \tag{23}$$

with $L_{0j}(u,v)=R_{0j}(u,v)$. $K_0^+(u)$ and $K_0^-(u)$ are all $2(n-1)\times 2(n-1)$ diagonal matrices. If we choose

$$K_0^-(-\sin k)=\mathrm{diag}(V_\sigma^1(k),\cdots,V_\sigma^{n-1}(k),V_\tau^1(k),\cdots,V_\tau^{n-1}(k)), \tag{24}$$

$$K_0^+(-\sin k)=\mathrm{diag}(M_1^1(k),\cdots,M_1^{n-1}(k),M_2^1(k),\cdots,M_2^{n-1}(k)), \tag{25}$$

where

$$\begin{aligned} M_1^i(k)&=[-2\sin k+2(n-1)i\gamma]M_\sigma^i(k)-i\gamma\sum_{j=1}^{n-1}(M_\sigma^j(k)+M_\tau^j(k)),\\ M_2^i(k)&=[-2\sin k+2(n-1)i\gamma]M_\tau^i(k)-i\gamma\sum_{j=1}^{n-1}(M_\sigma^j(k)+M_\tau^j(k)), \end{aligned} \tag{26}$$

in terms of the operator $t(u)$ (22), Eq. (14) is given by the form

$$t(-\sin k_{P_1})\vec{A}(k_{P_1},\cdots,k_{P_N})=\frac{-2\sin k_{P_1}(-2\sin k_{P_1}+2(n-1)i\gamma)}{-2\sin k_{P_1}+i\gamma}\vec{A}(k_{P_1},\cdots,k_{P_N}), \tag{27}$$

where the eigenvalue is given by $-2\sin k_{P_1}(-2\sin k_{P_1}+2(n-1)i\gamma)/(-2\sin k_{P_1}+i\gamma)$. Now our attention is paid to the diagonalizing operator $t(u)$ (22), which is similar to the transfer matrix in the vertex model with open boundary conditions. If we know the eigenvalue $\Lambda(u)$ of $t(u)$, we will obtain the Bethe equations for the energy (13), which is

$$\Lambda(-\sin k_{P_1})=\frac{-2\sin k_{P_1}(-2\sin k_{P_1}+2(n-1)i\gamma)}{-2\sin k_{P_1}+i\gamma}. \tag{28}$$

The diagonalization of the $t(u)$ requires that $[t(u),t(v)]=0$ for arbitrary u, v, which means that the model is integrable. One can prove that only R matrix satisfy the unitary, crossing unitary properties, and $K^-(u)$,$K^+(u)$, respectively, satisfy the following reflection equations:[17]

$$R_{12}(u-v)K_1^-(u)R_{21}(u+v)K_2^-(v)=K_2^-(v)R_{12}(u+v)K_1^-(u)R_{21}(u-v), \tag{29}$$

$$R_{12}(-u+v)K_1^+(u)^{t_1}R_{21}(-u-v-2(n-1)\eta)K_2^+(v)^{t_2}$$
$$=K_2^+(v)^{t_2}R_{12}(-u-v-2(n-1)\eta)K_1^+(u)^{t_1}R_{21}(-u+v), \tag{30}$$

where $t(u)$ can be diagonalized. Solving the reflection equations (29) and (30), we have the following diagonal solution:

$$K^-(u,\xi)=\mathrm{diag}(P_1^A,P_2^A,\cdots,P_{2n-2}^A), \tag{31}$$

where

$$P_a^A(u,\xi)=\begin{cases}\xi+u, & 1\leqslant a\leqslant A\\ \xi-u, & A<a\leqslant 2n-2\end{cases} \tag{32}$$

and

$$K^+(u,\tilde{\xi})=\mathrm{diag}(P_1^B,P_2^B,\cdots,P_{2n-2}^B) \tag{33}$$

with

$$P_a^B(u,\tilde{\xi})=\begin{cases}\tilde{\xi}-u-(n-1)\eta, & 1\leqslant a\leqslant B\\ \tilde{\xi}+u+(n-1)\eta, & B<a\leqslant 2n-2.\end{cases} \tag{34}$$

In Eqs. (32) and (34), ξ and $\tilde{\xi}$ both are free parameters. The integer numbers A and B are also free parameters which take values from 1 to $2n-2$. Comparing Eq. (24) with Eq. (31), and Eq. (25) with Eq. (32), we can get the constraint relation between ξ, $\tilde{\xi}$ and $p_{\rho,\alpha}$, $q_{\rho,\alpha}$. The relations are given as follows:

$$\begin{gathered}p_\sigma^1=\cdots=p_\sigma^A=p,\\ p_\sigma^{A+1}=\cdots=p_\sigma^{n-1}=p_\tau^1=\cdots=p_\tau^{n-1}=-p,\quad A\in[1,n-1],\\ p_\sigma^1=\cdots=p_\sigma^{n-1}=p_\tau^1=\cdots=p_\tau^{A-n+1}=p,\\ p_\tau^{A-n+2}=\cdots=p_\tau^{n-1}=-p,\quad A\in[n,2n-2],\end{gathered} \tag{35}$$

$$\begin{gathered}q_\sigma^1=\cdots=q_\sigma^B=q,\\ q_\sigma^{B+1}=\cdots=q_\sigma^{n-1}=q_\tau^1=\cdots=q_\tau^{n-1}=-q,\quad B\in[1,n-1]\\ q_\sigma^1=\cdots=q_\sigma^{n-1}=q_\tau^1=\cdots=q_\tau^{B-n+1}=q,\\ q_\tau^{B-n+2}=\cdots=q_\tau^{n-1}=-q,\quad B\in[n,2n-2]\end{gathered} \tag{36}$$

with

$$\xi=\begin{cases}\infty & \text{for } A=2n-2\\ \dfrac{1-p^2}{2ip} & \text{for } A\in[1,2n-3],\end{cases}\qquad \tilde{\xi}=\begin{cases}\infty & \text{for } B=2n-2\\ -\dfrac{1-q^2}{2iq}-i(n-1-B)\gamma & \text{for } B\in[1,2n-3].\end{cases} \tag{37}$$

In Sec. III we will diagonalize Eq. (22) with K^- and K^+ taking the form of Eqs. (31) and (33), respectively.

III. NESTED BETHE ANSATZ

Let

$$U(u)=T(u)K^{-}(u)T^{-1}(u), \tag{38}$$

one can prove that double-row monodromy matrix $U(u)$ satisfies the reflection equation

$$R_{12}(u-v)U_1(u)R_{21}(u+v)U_2(v)=U_2(v)R_{12}(u+v)U_1(u)R_{21}(u-v). \tag{39}$$

Rewriting Eq. (39) in the component form

$$R_{12}(u_-)^{a_1a_2}_{c_1c_2}U(u)_{c_1d_1}R_{21}(u_+)^{d_1c_2}_{b_1d_2}U(v)_{d_2b_2}=U(v)_{a_2c_2}R_{12}(u_+)^{a_1c_2}_{c_1d_2}U(u)_{c_1d_1}R_{21}(u_-)^{d_1d_2}_{b_1b_2}, \tag{40}$$

where the repeated indices sum over 1 to $2n-2$, $u_-=u-v$, $u_+=u+v$ and introducing a set of notations for convenience:

$$\begin{gathered}A(v)=U(v)_{11},\quad B_a(v)=U(v)_{1a},\quad C_a(v)=U(v)_{a1},\\ D_{ab}(v)=U(v)_{ab},2\leqslant a,b\leqslant 2n-2\end{gathered} \tag{41}$$

we have the commutation relations from Eq. (40)

$$B_{b_1}(u_1)B_{b_2}(u_2)=R_{12}(u_1-u_2)^{d_2d_1}_{b_2b_1}B_{d_2}(u_2)B_{d_1}(u_1), \tag{42}$$

$$\begin{aligned}A(v)B_b(u)=&\frac{a(u-v)b(u+v)}{a(u+v)b(u-v)}B_b(u)A(v)-\frac{b(2u)c(u-v)}{a(2u)b(u-v)}B_b(v)A(u)\\&-\frac{c(u+v)}{a(u+v)}B_c(v)\tilde{D}_{cb}(u),\end{aligned} \tag{43}$$

$$\begin{aligned}\tilde{D}_{a_1b_1}(u)B_{b_2}(v)=&\frac{a(u-v)a(u+v+\eta)}{b(u-v)b(u+v+\eta)}R_{12}(u+v+\eta)^{a_1c_2}_{c_1d_2}R_{21}(u-v)^{d_1d_2}_{b_1b_2}B_{c_2}(v)\tilde{D}_{c_1d_1}(u)\\&-\frac{a(2u+\eta)c(u-v)}{b(2u+\eta)b(u-v)}R_{12}(2u+\eta)^{a_1d_1}_{d_2b_1}B_{d_1}(u)\tilde{D}_{d_2b_2}(v)\\&+\frac{a(2u+\eta)}{b(2u+\eta)}\frac{c(u+v)b(2v)}{a(u+v)a(2v)}R_{12}(2u+\eta)^{a_1d_2}_{b_2b_1}B_{d_2}(u)A(v),\end{aligned} \tag{44}$$

where all indices take values from 2 to $2n-2$, and the repeated indices sum over 2 to $2n-2$. The notations $a(u)=u+\eta$, $b(u)=u$, $c(u)=\eta$ are used. The new operators $\tilde{D}$ are defined by

$$\tilde{D}_{ab}(v)=D_{ab}(v)-\delta_{ab}\frac{R_{12}(2v)^{a1}_{1a}}{R_{12}(2v)^{11}_{11}}A(v). \tag{45}$$

Introducing the vacuum state,

$$|\mathrm{vac}\rangle=\prod^{\otimes N}(1,0,...,0)^t, \tag{46}$$

where t denotes the transposition and $(1,0,\cdots,0)$ is a $1\times 2(n-1)$ matrix. The action of the double-row monodromy matrix on the vacuum state is

$$A(u)|\mathrm{vac}\rangle = K_1^-(u)|\mathrm{vac}\rangle = \alpha^{(1)}(u)|\mathrm{vac}\rangle,$$

$$\tilde{D}_{ab}(u)|\mathrm{vac}\rangle = \delta_{ab}\left(K_a^-(u) - \frac{c(2u)}{a(2u)}K_1^-(u)\right)\frac{a(2u)}{b(2u)}\beta^{(1)}(u)|\mathrm{vac}\rangle,$$

$$C_a(u)|\mathrm{vac}\rangle = 0, \quad B_a(u)|\mathrm{vac}\rangle \neq 0, \tag{47}$$

where $\alpha^{(1)}(u)$ and $\beta^{(1)}(u)$ are defined by Eqs. (58) and (59), respectively. Note that the action of $B_a(u)$ on the vacuum state is not proportional to the vacuum state. Now we construct the eigenvectors of transfer matrix $t(u)$. It takes the form

$$\Psi(v_1,\cdots,v_L) = B_{b_1}(v_1)\cdots B_{b_L}(v_L)|\mathrm{vac}\rangle F^{b_1\cdots b_L}. \tag{48}$$

Using Eq. (22), we then obtain the action of $t(u)$ on Ψ,

$$\begin{aligned}
t(u)\Psi = {} & \alpha^{(1)}(u)S_1(u)\prod_{j=1}^{L}\frac{a(v_j-u)b(v_j+u)}{b(v_j-u)a(v_j+u)}\times F^{b_1\cdots b_L}B_{b_1}(v_1)\cdots B_{b_L}(v_L)|\mathrm{vac}\rangle \\
& + \prod_{j=1}^{L}\frac{a(u-v_j)a(u+v_j+\eta)}{b(u-v_j)b(v_j+u+\eta)}\beta^{(1)}(u)\tau^{(2)}(\tilde{u},\{\tilde{v}_i\})_{b_1\cdots b_L}^{d_1\cdots d_L} \\
& \times F^{b_1\cdots b_L}B_{d_1}(v_1)\cdots B_{d_L}(v_L)|\mathrm{vac}\rangle \\
& + \sum_{k=1}^{L}\left(\frac{-c(v_k-u)}{b(v_k-u)}S_1(u) + \frac{c(v_k+u)a(2u+\eta)}{a(v_k+u)b(2u+\eta)}T_1(u)\right)\frac{b(2v_k)}{a(2v_k)} \\
& \cdot \prod_{j=1,\neq k}^{L}\frac{a(v_j-v_k)b(v_j+v_k)}{b(v_j-v_k)a(v_j+v_k)}\alpha^{(1)}(v_k)S(v_k,\{v_i\})_{b_1\cdots b_L}^{d_1\cdots d_L}F^{b_1\cdots b_L} \\
& \cdot B_{d_1}(u)b_{d_2}(v_1)\cdots B_{d_k}(v_{k-1})B_{d_{k+1}}(v_{k+1})\cdots B_{d_L}(v_L)|\mathrm{vac}\rangle \\
& - \sum_{k=1}^{L}\left(\frac{c(u+v_k)}{a(u+v_k)}S_1(u) + \frac{c(u-v_k)a(2u+\eta)}{b(u-v_k)b(2u+\eta)}T_1(u)\right) \\
& \times \frac{\beta^{(1)}(v_k)}{T_1(v_k)}\prod_{j=1,\neq k}^{L}\frac{a(v_k-v_j)a(v_j+v_k+\eta)}{b(v_k-v_j)b(v_j+v_k+\eta)}\times S(v_k,\{v_i\})_{c_1\cdots c_L}^{d_1\cdots d_L}\tau^{(2)} \\
& \times(\tilde{v}_k,\{\tilde{v}_i\})_{b_1\cdots b_L}^{c_1\cdots c_L}F^{b_1\cdots b_L}\times B_{d_1}(u)b_{d_2}(v_1)\cdots B_{d_k}(v_{k-1})B_{d_{k+1}}(v_{k+1})\cdots B_{d_L}(v_L)|\mathrm{vac}\rangle,
\end{aligned} \tag{49}$$

where

$$\begin{aligned}
\tau^{(2)}(\tilde{u},\{\tilde{v}_i\})_{b_1\cdots b_L}^{c_1\cdots c_L} &= \sum_{a=2}^{m+n}K_a^+(u)\{(L^{(1)}(\tilde{u},\tilde{v}_1)\cdots L^{(1)}(\tilde{u},\tilde{v}_L)K^-(\tilde{u},\xi^{(1)}) \\
&\quad \cdot L^{(1)}(-\tilde{u},\tilde{v}_L)^{-1}\cdots L^{(1)}(-\tilde{u},\tilde{v}_1)^{-1})_{b_1\cdots b_L}^{c_1\cdots c_L}\}_{aa} \\
&= \sum_{a=2}^{m+n}K_a^+(u)\{(T^{(1)}(\tilde{u},\{\tilde{v}_i\})K^-(\tilde{u},\xi^{(1)})T^{(1)}(-\tilde{u},\{\tilde{v}_i\})^{-1})_{b_1\cdots b_L}^{c_1\cdots c_L}\}_{aa}
\end{aligned} \tag{50}$$

with $\tilde{u}=u+\eta/2$, $\xi^{(1)}=\xi-\eta/2$, $\tilde{v}_i=v_i+\eta/2$. $S_1(u)$ is defined by Eq. (56), $T_1(u)$ is defined by Eq. (57) and

$$S(v_k,\{v_i\})^{d_1\cdot d_L}_{b_1\cdots b_L}=\prod_{j=1+k}^{L}\delta_{b_jd_j}R_{12}(v_1-v_k)^{d_1d_2}_{c_2b_1}R_{12}(v_2-v_k)^{c_2d_3}_{c_3b_2}\times\cdots R_{12}(v_{k-1}-v_k)^{c_{k-1}d_k}_{b_kb_{k-1}}. \tag{51}$$

From Eq. (49), one can see that the function Ψ is not the eigenstate of $t(u)$ unless F's are the eigenstates of $\tau^{(2)}$ and the sum of the third and the fourth term in Eq. (49) is zero, which will give a restriction on the L spectrum parameters $\{v_i\}$. So, we arrive at the following results.

If F is the eigenstate of $\tau^{(2)}$ with the eigenvalue $\Lambda^{(2)}$ satisfying Eq. (53), then Ψ is the eigenstate of $t(u)$ with the eigenvalue $\Lambda^{(1)}$,

$$\begin{aligned}\Lambda^{(1)}(u)=&\alpha^{(1)}(u)S_1(u)\prod_{j=1}^{L}\frac{a(v_j-u)b(v_j+u)}{b(v_j-u)a(v_j+u)}\\&+\beta^{(1)}(u)\prod_{j=1}^{L}\frac{a(u-v_j)a(u+v_j+\eta)}{b(u-v_j)b(v_j+u+\eta)}\Lambda^{(2)}(u,\{v_i\}),\end{aligned} \tag{52}$$

where

$$\begin{aligned}&\tau^{(2)}(u,\{v_i\})F=\Lambda^{(2)}(u,\{v_i\})F,\\&\Lambda^{(2)}(v_k,\{v_i\})=\frac{\alpha^{(1)}(v_k)b(2v_k)T_1(v_k)}{\beta^{(1)}(v_k)a(2v_k)}\prod_{j=1,\neq k}^{L}\frac{b(v_j+v_k)a(v_j-v_k)}{-a(v_k-v_j)a(v_k+v_j+\eta)}.\end{aligned} \tag{53}$$

Therefore, the diagonalization of $t(u)$ is reduced to finding the eigenvalue of $\tau^{(2)}$. The explicit expression of $\tau^{(2)}$ [see Eq. (49)] implies that $\tau^{(2)}$ can be considered as the transfer matrix of an L-sites quantum chain, in which every spin takes $2n-3$ values. The related Yang–Baxter equation is the same as the one of $t(u)$, except R being an $(2n-3)^2\times(2n-3)^2$ matrix. Hence, we can use the same method to find the eigenvalue of $\tau^{(2)}$. Repeating the procedure $2n-4$ times again, we have the following result:

$$\begin{aligned}\Lambda^{(k)}(u,\{v_i^{(k-1)}\},\{v_i^{(k)}\})=&S_k(u)\alpha^{(k)}(u,\{v_i^{(k-1)}\})\cdot\prod_{j=1}^{L_k}\frac{a(v_j^{(k)}-u)b(u+v_j^{(k)}+(k-1)\eta)}{b(v_j^{(k)}-u)a(u+v_j^{(k)}+(k-1)\eta)}\\&+\beta^{(k)}(u,\{v_i^{(k-1)}\})\prod_{j=1}^{L_k}\frac{a(u-v_j^{(k)})a(u+v_j^{(k)}+k\eta)}{b(u-v_j^{(k)})b(u+v_j^{(k)}+k\eta)}\\&\cdot\Lambda^{(k+1)}(u,\{v_i^{(k)}\},\{v_i^{(k+1)}\})\quad(1\leqslant k\leqslant 2n-3)\end{aligned} \tag{54}$$

and

$$\begin{aligned}\Lambda^{(k+1)}(v_l^{(k)},\{v_i^{(k)}\},\{v_i^{(k+1)}\})=&\frac{\alpha^{(k)}(v_l^{(k)},\{v_i^{(k-1)}\})2v_l^{(k)}+(k-1)\eta}{\beta^{(k)}(v_l^{(k)},\{v_i^{(k-1)}\})}\frac{2v_l^{(k)}+(k-1)\eta}{2v_l^{(k)}+k\eta}T_k(v_l^{(k)})\\&\cdot\prod_{j=1,\neq l}^{L_k}\frac{(v_l^{(k)}+v_j^{(k)}+(k-1)\eta)(v_l^{(k)}-v_j^{(k)}-\eta)}{(v_l^{(k)}+v_j^{(k)}+(k+1)\eta)(v_l^{(k)}-v_j^{(k)}+\eta)},(1\leqslant k\leqslant 2n-3)\end{aligned} \tag{55}$$

where

$$S_k(u)=\begin{cases}(\tilde{\xi}+(n-1)\eta-B\eta-u)\dfrac{2u+2(n-1)\eta}{2u+k\eta}, & 1\leqslant k\leqslant B\\ (\tilde{\xi}+(n-1)\eta+u)\dfrac{2u+2(n-1)\eta}{2u+k\eta}, & B<k\leqslant 2n-2\end{cases} \tag{56}$$

and

$$T_k(u)=\begin{cases}(\tilde{\xi}+(n-1)\eta-B\eta-u)\dfrac{2u+2(n-1)\eta}{2u+(k+1)\eta}, & 1\leqslant k\leqslant B\\ (\tilde{\xi}+(n-1)\eta+u)\dfrac{2u+2(n-1)\eta}{2u+(k+1)\eta}, & B<k\leqslant 2n-3,\end{cases} \tag{57}$$

$$\alpha^{(k)}(u,\{v_i^{(k-1)}\})=\begin{cases}\xi+u, & 1\leqslant k\leqslant A\\ \xi-A\eta-u, & A<k\leqslant 2n-2,\end{cases} \tag{58}$$

$$\beta^{(k)}(u,\{v_i^{(k-1)}\})=\prod_{j=1}^{L_{k-1}}\frac{(u+v_j^{(k-1)}+(k-1)\eta)(u-v_j^{(k-1)})}{(u+v_j^{(k-1)}+k\eta)(u-v_j^{(k-1)}+\eta)}\frac{2u+(k-1))\eta}{2u+k\eta}. \tag{59}$$

In the above-mentioned representation, $v_j^{(1)}=v_j$, $v_j^{(0)}=-\sin k_{P_j}$, $L_0=N$, $L_1=L$, $L_{2n-2}=0$, and $\Lambda^{(2n-1)}=0$, $\Pi^0=1$ are assumed. Notice that $\beta^{(k)}(u,\{v_i^{k-1}\})$ vanishes at the special points $v_i^{(k-1)}$ due to the factor $u-v_i^{(k-1)}$ appearing in $\beta^{(k)}$. Taking $u=v_i^{(k-1)}$ in formula (54), we can get another kind of constraints on $\Lambda^{(k)}$,

$$\begin{aligned}\Lambda^{(k)}(v_l^{(k-1)},\{v_i^{(k-1)}\},\{v_i^{(k)}\})=&\alpha^{(k)}(v_l^{(k-1)},(v_i^{(k-1)}\})S_k(v_l^{k-1})\\ &\cdot\prod_{j=1}^{L_k}\frac{(v_j^{(k)}-v_l^{(k-1)}+\eta)(v_j^{(k)}+v_l^{(k-1)}+(k-1)\eta)}{(v_j^{(k)}-v_l^{(k-1)})(v_j^{(k)}+v_l^{(k-1)}+k\eta)},\\ &1\leqslant k\leqslant 2n-3.\end{aligned} \tag{60}$$

Now, changing the index k into $k+1$ in the above formula (60), we can obtain constrains on $\Lambda^{(k+1)}$. Comparing these with Eq. (55), one can derive out the following Bethe ansatz equations

$$\begin{aligned}&\prod_{j=1}^{L_{k-1}}\frac{(v_l^{(k)}-v_j^{(k-1)}+\eta)(v_l^{(k)}+v_j^{(k-1)}+k\eta)}{(v_l^{(k)}-v_j^{(k-1)})(v_l^{(k)}+v_j^{(k-1)}+(k-1)\eta)}\cdot\prod_{j=1}^{L_{k+1}}\frac{(v_l^{(k)}-v_j^{(k+1)})(v_l^{(k)}+v_j^{(k+1)}+(k+1)\eta)}{(v_l^{(k)}-v_j^{(k+1)}-\eta)(v_l^{(k)}+v_j^{(k+1)}+(k\eta)}\\ &\cdot\prod_{j=1,\neq l}^{L_k}\frac{(v_l^{(k)}-v_j^{(k)}-\eta)(v_l^{(k)}+v_j^{(k)}+(k-1)\eta)}{(v_l^{(k)}-v_j^{(k)}+\eta)(v_l^{(k)}+v_j^{(k)}+(k+1)\eta)}=\frac{S_{k+1}(v_l^{(k)})\alpha^{(k+1)}(v_l^{(k)})}{T_k(v_l^{(k)})\alpha^{(k)}(v_l^{(k)})},\quad 1\leqslant k\leqslant 2n-3.\end{aligned} \tag{61}$$

The function $\Lambda^{(1)}(u,\ldots)$ must not be singular at $u=v_j^{(k)}$ $(1\leqslant j\leqslant L_k,\ 1\leqslant k\leqslant 2n-3)$ since the transfer matrix $t(u)$ is an analytic function of u. In fact, Eq. (53) comes from the condition under which the unwanted term vanishes. One can understand this constraint from another point of view: From Eq. (52), we know that $u=v_j=v_j^{(1)}$ is a pole of $\Lambda^{(1)}(u)$. In order to keep the analyticity of $\Lambda^{(1)}(u)$, one should need the residue of $\Lambda^{(1)}(u)$ at v_j vanishing, which also gives the constraint (53). So, $\Lambda^{(1)}(u)$ is analytic at v_j. Similarly, Eq. (64) ensures the anlayticity of $\Lambda^{(1)}(u)$ at all $v_j^{(k)}$. Therefore, the eigenvalues of the transfer matrix are analytic functions if the previous Bethe ansatz equations are satisfied. Substituting

$$\Lambda(-\sin k)=\frac{-2\sin kM_\sigma^1(k)V_\sigma^1(k)}{(\tilde{\xi}+\sin k+(n-1-B)i\gamma)(\xi-\sin k)}\Lambda^{(1)}(-\sin k) \tag{62}$$

into Eq. (28), we then obtain all the Bethe ansatz equations for the SU(n) Hubbard model with open boundary conditions which take the following forms:

$$\frac{(1+qe^{ik_{P_1}})(p+e^{-ik_{P_1}})}{(1+qe^{-ik_{P_1}})(p+e^{ik_{P_1}})}e^{-2i\tilde{L}k_{P_1}}=\prod_{j=1}^{L_1}\frac{(w_j^{(1)}+\sin k_{P_1}+\eta/2)(w_j^{(1)}-\sin k_{P_1}-\eta/2)}{(w_j^{(1)}+\sin k_{P_1}-\eta/2)(w_j^{(1)}-\sin k_{P_1}+\eta/2)}, \tag{63}$$

$$\prod_{j=1}^{L_{k-1}}\frac{(w_l^{(k)}-w_j^{(k-1)}-\eta/2)(w_l^{(k)}+w_j^{(k-1)}-\eta/2)}{(w_l^{(k)}-w_j^{(k-1)}+\eta/2)(w_l^{(k)}+w_j^{(k-1)}+\eta/2)}\cdot\prod_{j=1}^{L_{k+1}}\frac{(w_l^{(k)}-w_j^{(k+1)}-\eta/2)(w_l^{(k)}+w_j^{(k+1)}-\eta/2)}{(w_l^{(k)}-w_j^{(k+1)}+\eta/2)(w_l^{(k)}+w_j^{(k+1)}+\eta/2)}$$
$$\times\prod_{j=1,\neq l}^{L_k}\frac{(w_l^{(k)}-w_j^{(k)}+\eta)(w_l^{(k)}+w_j^{(k)}+\eta)}{(w_l^{(k)}-w_j^{(k)}-\eta)(w_l^{(k)}+w_j^{(k)}-\eta)}=\frac{T_k(w_l^{(k)}-k\eta/2)\alpha^{(k)}(w_l^{(k)}-k\eta/2)}{S_{k+1}(w_l^{(k)}-k\eta/2)\alpha^{(k+1)}(w_l^{(k)}-k\eta/2)},$$
$$(1\leqslant k\leqslant 2n-3). \tag{64}$$

In the above representations Eqs. (63) and (64), $v_j^{(k)}=w_j^{(k)}-k\eta/2$, $v_j^{(0)}=-\sin k_{P_j}$.

IV. SUMMARY

We obtain the energy and the integrable open boundary conditions for the open boundary SU(n) Hubbard model by using the coordinate Bethe ansatz method. The Bethe ansatz equations are achieved by diagonalizing the inhomogeneous transfer matrix of the open SU($2n-2$) XXX vertex model. Using these Bethe ansatz equations one can study the boundary contributions to the thermodynamical quantities such as special heat and magnetic susceptibility. When $n=2$, our result coincides with that obtained by Deguchi and Yue.[23]

However, there is a shortage in our results. We only get the eigenvalue of the Hamiltonian instead of all the conserved quantities. There may be other alternative ways to deal with this problem.

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On the observables describing a quantum reference frame

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A reference frame F is described by the element g of the Poincaré group $\mathcal{P}$ which connects F with a given fixed frame F_0. If F is a quantum frame, defined by a physical object following the laws of quantum physics, the parameters of g have to be considered as quantum observables. However, these observables are not compatible and some of them, namely the coordinates of the origin of F, cannot be represented by self-adjoint operators. Both these difficulties can be overcome by considering a positive-operator-valued measure on $\mathcal{P}$, covariant with respect to the left translations of the group, namely a covariance system. We develop a construction procedure for this kind of mathematical structure. The formalism is also used to discuss the quantum observables measured with respect to a quantum reference frame. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1370395]

I. INTRODUCTION

As Mach remarked at the end of the nineteenth century,[1] from the physical point of view a frame of reference is defined by a material object of the same nature as the objects that form the system under investigation and the measuring instruments. Such an idea does not conflict with classical mechanics: for example a rigid body can define a spatial origin and an orientation. The situation becomes more complicated in quantum mechanics: Heisenberg's uncertanty relations forbid the exact determination of the position and the velocity of a frame. As noted by some authors,[2] such an analysis not only contributes to remove a classical concept from quantum mechanics, but also reveals some surprising physical consequences, such as the ''paradox of the quantum frames.'' That is, if we have three frames of reference, F_1,F_2 and F_3, the observables that describe the relation between F_1 and F_2 may not be compatible with the observables that describe the relation between F_2 and F_3, even if the systems do not interact.

We follow an operational approach: the mathematical structures involved should have a direct physical meaning. From this point of view, a frame is determined by the procedures that transform an initial frame into the chosen one. The set of the transformations allowed by a relativistic theory is represented by the proper orthochronous Poincaré group $\mathcal{P}$. Each element of $\mathcal{P}$ can be identified by means of ten indipendent parameters, indicating the coordinates of the new origin in the Minkowsky space–time, the three components of the velocity and three angles of orientation. From a physical point of view these ten variables can be determined by their measurement performed on the physical object defining the frame: They have to be considered observables. Unfortunately spectral measures, the mathematical structures traditionally associated to the physical concept of observables in quantum mechanics, cannot describe either simultaneous measurements of position and velocity or measurements of time (Pauli's theorem). According to Gleason's theorem, the natural generalization of spectral measures, compatible with the ''Copenhagen interpretation,'' is given by the so-called *positive operator value measures* (POVMs).[3–5]

An observable is often characterized by its transformation properties under a particular symmetry group. We can define a *system of covariance* as a POVM endowed with its covariance properties under some symmetry group.[6–8] If a POVM reduces to a spectral measure, the structure so defined is called a system of imprimitivity.[9]

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Following some hints that can be found in Ref. 8, in Sec. II we illustrate a general construction procedure for covariant observables, which allows one to assign the statistical distribution of the outcomes to the state vector of the system on which the measurement is performed. The cornerstones of our procedure are three theorems. The first one (covariant dilatation) asserts that any system of covariance can be derived from a suitable system of imprimitivity to which it is linked by means of a suitable ''intertwining operator.'' The second theorem is Mackey's imprimitivity theorem, which allows us to find the most general form of a system of imprimitivity. The third one is the ''intertwining operator theorem,'' which we derived in order to find the most general intertwining operator connecting the systems of imprimitivity to the unknown system of covariance. Its application is possible when the unitary representations of the symmetry group acting on the involved Hilbert spaces are decomposed into irreducible unitary representations.

We stress that our results are very general and allow one to describe all the possible measurements of a given observable, defined by its spectrum and its transformation properties under a relevant symmetry group, performed on a physical system which is identified by its covariance properties under the same group. We do not introduce any model, but use general symmetry properties of the measurement, to get all the POVMs describing a chosen observable.

In Sec. III, the developed procedure is used for a new derivation of the most general POVM on Minkowsky space–time which is covariant with respect to the Poincaré group, found in Ref. 10 by means of a different method.

Coming back to quantum frames in Sec. IV, their description can be given by a system of covariance on the proper orthochronous Poincaré group, which is in this case both the parameter space and the symmetry group. Harmonic analysis on $\mathrm{SL}(2C)$ and on the group of translations of $\mathbf{R}^4$ allows the decomposition of the most general unitary representation of $\mathcal{P}$ into irreducible unitary representations. In this way, the intertwining operator theorem can be applied and the most general probability distribution can be found.

A comparison with the Poincaré covariant POVM on Minkowsky space–time indicates the existence of some constraints. In particular the so-called baricentric measures cannot be obtained: In other words one cannot require that the coordinates of the origin coincide with the coordinates of the center of mass of the physical system defining the frame. Moreover through an analysis of our results, one realizes that, for a complete description of a quantum reference frame, kinematical variables are not sufficient and internal degrees of freedom of the system have to be involved.

Finally, the formalism we adopted also allows an alternative derivation of the paradox of the quantum frames. Indeed, in Sec. V, we derive the form of the POVMs describing the relative observables between a generical quantum object and a quantum reference frame. The observables describing the relations between noninteracting quantum frames are just a particular case.

We hope that an analysis of the variances of the probability distributions we have found will give a new class of indeterminacy relations.

II. MATHEMATICAL TOOLS

In the traditional framework of quantum mechanics, the states of a system are described by rays in a complex separable Hilbert space, or by normalized positive trace class operators, while observables are described by self-adjoint operators or, equivalentely, by spectral measures. It is well known that the last ones cannot describe either joint measurements of incompatible observables, or measurements of time, indeed Pauli's theorem[11,12] forbids the description by means of a self-adjoint operator of an observable canonically conjugate to a Hamiltonian with a semibounded spectrum. Nevertheless, as noted by some authors,[8,13,14] the description of some measuring instruments requires a different mathematical structure, which can be recognized as a generalization of spectral measures: the so-called POVMs. Gleason's theorem assures us that they are the most general mathematical structures describing observables compatible with the probabilistic interpretation of quantum mechanics.

The analysis of the proof of Pauli's theorem, shows that it is based on the covariance of time measurements with respect to time translations. This is not accidental, but shows the importance of

symmetry in our discussion. Indeed, the requirement of precise covariance properties of the quantum measurement under some symmetry group $\mathcal{G}$ leads to the following definition of covariance systems.[6]

Notation: From now on:

(1) S will indicate a topological space that is locally compact and has a countable base of its topology. S is called the ''space of the possible results of the measurement.''
(2) $\mathcal{H}$ will indicate a complex separable Hilbert space. $\mathcal{H}$ is called ''the space of states (of the quantum system).''
(3) $\mathcal{G}$ will indicate a locally compact topological group which has a countable base of its topology. $\mathcal{G}$ is called the ''symmetry group of the theory.''

Definition 1: Let $\mathcal{H}$ be a space of states and S be a space of possible results. A POVM on S is a class $\tau := \{\tau(I)\}_{I\in\mathcal{B}(S)}$, where $\mathcal{B}$ is the σ-algebra of Borel sets of S and each $\tau(I):\mathcal{H}\to\mathcal{H}$ is a positive bounded operator such that:
(1) $\tau(I)\geqslant\tau(\varnothing)=0 \quad \forall I\in\mathcal{B}$,
(2) $\tau(\cup I_i)=\Sigma\tau(I_i)$,
(3) $\tau(S)=1$,

where $\{I_i\}$ is a countable collection of disjoint elements of $\mathcal{B}$ and the convergence is in the weak topology.

Given a space of states $\mathcal{H}$, a space of possible results S and a POVM $\{\tau(I)\}_{I\in\mathcal{B}(S)}$, for any pure state of the system determined by a normalized vector $\phi\in\mathcal{H}$, the probability that the outcome of the measurement of the observable described by $\{\tau(I)\}_{I\in\mathcal{B}(S)}$ belongs to the Borel set I is

$$P(\phi,I)=\langle\phi,\tau(I)\phi\rangle. \tag{1}$$

More generally, for any mixed state of the system determined by a normalized positive trace class operator ρ on $\mathcal{H}$, the probability above is given by

$$P(\rho,I)=\mathrm{Tr}[\rho\tau(I)]. \tag{2}$$

Note: If $\tau(I_1\cap I_2)=\tau(I_1)\cdot\tau(I_2)$ for all $I_1,I_2\in\mathcal{B}$, then τ is a spectral measure.

The physical requirement that two observers, related by a transformation of the symmetry group $\mathcal{G}$ and performing the same experiment, get the same statistical distribution of the outcomes of the measurement, leads to a natural covariance condition and, eventually, to the following definition:

Definition 2: Let *$\mathcal{H}$ be a space of states, S be a space of possible results and $\mathcal{G}$ a symmetry group of the theory. Suppose that $\mathcal{G}$ acts on S by means of a representation $\Lambda:g\to\Lambda(g),g\in\mathcal{G}$, where $\Lambda(g):S\to S$ are Borel mappings. Suppose $\mathcal{G}$ acts on $\mathcal{H}$ by means of a strongly continuous unitary representation $U:g\to U(g)$. Let $\{\tau(I)\}_{I\in\mathcal{B}(S)}$ a POVM on S, with the property.*

$$U(g)\tau(I)U(g)^{\dagger}=\tau(\Lambda(g)I) \tag{3}$$

for any $I\in\mathcal{B}(S),g\in\mathcal{G}$. In this case the structure $(\mathcal{H},S,\mathcal{G},\Lambda,U,\tau)$ so defined is called the system of covariance. Furthermore, if τ is a spectral measure, it is called the system of imprimitivity.[6–9,15]

While spectral measures represent a ''property'' of the system on which the measurement is performed, generic POVMs can't describe ''definite observables,'' but we have to prefer them because they are able to describe simultaneous measurements of incompatible observables and measurements of time.

While there is a unified treatment of imprimitivity systems, mainly due to Mackey, we cannot say the same for covariance systems. Anyway we can overcome this difficulty by means of the following theorem, which may be recognized as a covariant version of Naimark's dilatation theorem.[7,8]

Proposition 1: Let $(\mathcal{H},S,\mathcal{G},\Lambda,U,\tau)$ *be a system of covariance. Then there is an imprimitivity system* $(\mathcal{H}',S,\mathcal{G},\Lambda,V,E)$*, where* $\mathcal{H}'$ *is a Hilbert space,* V *a strongly continuous unitary representation of the symmetry group* $\mathcal{G}$ *acting on* $\mathcal{H}'$*,* E *is a spectral measure on the Borel* σ *algebra* $\mathcal{B}$ *of* S*, and there is an ''intertwining operator'' A*:$\mathcal{H}\to\mathcal{H}'$*, with the property* $AU(g)=V(g)A$*, for any* $g\in\mathcal{G}$*, so that the following relation connects the spectral measure* E *to the POVM* τ*:*

$$\tau(I)=A^{+}E(I)A. \tag{4}$$

Moreover, τ *is normalized* (i.e., $\tau(S)=1$) *if and only if* $A^{+}A=1$*, namely if* A *is isometric.*

Finally Mackey's imprimitivity theorem allows one to find the most general form of a system of imprimitivity.

Proposition 2: Let $(\mathcal{H}',S,\mathcal{G},\Lambda,V,E)$ *be a transitive system of imprimitivity. Let* $q\in S$ *be a generical element of* S*, for any* $x\in S$ *let* $g_x\in\mathcal{G}$ *be an element of* $\mathcal{G}$ *with the property* $x=\Lambda(g_x)q$*. Let* H_q *be ''the little group,'' namely the closed subgroup of* $\mathcal{G}$ *defined by*

$$g\in H_q\Leftrightarrow\Lambda(g)q=q. \tag{5}$$

Then one can represent $\mathcal{H}'$ *as direct integral of Hilbert spaces on* S

$$\mathcal{H}'=\int_S^{\oplus}\mathcal{H}'(x)d\mu(x), \tag{6}$$

where $d\mu(x)$ *is a measure on* $\mathcal{B}(S)$ *having the same null sets as the spectral measure* E*. The vectors* $\phi\in\mathcal{H}'$ *can be represented by ''wave functions''* $\psi(x)$ *and the projectors* $E(I)$ *as diagonal operators*:

$$(E(I)\psi)(x)=f_I(x)\psi(x), \tag{7}$$

where $f_I(x)$ *is the characteristic function of the Borel set* $I\in\mathcal{B}$*. Moreover the unitary representation* V *of* $\mathcal{G}$ *takes the form of an ''induced representation:''*

$$[V(g)\psi](x)=\left[\frac{d\mu(x')}{d\mu(x)}\right]^{1/2}R(g_x^{-1}gg_{x'})\psi(x'),\quad x'=\Lambda(g^{-1})x, \tag{8}$$

where $g_x^{-1}gg_{x'}\in H_q$ *and* R *is a unitary representation of* H_q*.*

The introduction of a system of imprimitivity is very advantageous: in this way the probability that the result of the measurement, performed on the state ϕ, belongs to the Borel set $I\in S$ takes the following simple form:

$$\begin{aligned}P(\phi,I)&=\langle\phi,\tau(I)\phi\rangle\\&=\langle A\phi,E(I)A\phi\rangle\\&=\int_S f_I(x)\|\psi(x)\|^2d\mu(x),\quad \psi=A\phi.\end{aligned} \tag{9}$$

In other words the usual concept of *probability density*, which can be found in the traditional formulation of quantum mechanics, can be reestablished even if spectral measures are replaced by generic POVMs.

The last step of our construction procedure is the description of the most general intertwining operator joining the imprimitivity system found by means of Mackey's theorem to the unknown covariance system. The following theorem allows one to know when such an operator exists and what its general form is. It is based on a generalization of an argument given in Ref. 16 and on Schur's lemma.

Proposition 3: Let $\mathcal{G}$ be a locally compact topological group with a countable base of open sets and of type I. Let $\hat{\mathcal{G}}$ be its dual space, namely the space of equivalence classes of its irriducible representations. Let U and V be two unitary representations of its, defined by their central decompositions:

$$U(g)=\int_{\hat{\mathcal{G}}}^{\oplus}(U_\lambda(g)\otimes 1_\lambda)d\mu(\lambda),\quad V(g)=\int_{\hat{\mathcal{G}}}^{\oplus}(U_\lambda(g)\otimes 1'_\lambda)d\mu'(\lambda), \tag{10}$$

acting, respectively, on Hilbert spaces

$$\mathcal{H}=\int_{\hat{\mathcal{G}}}^{\oplus}\mathcal{H}_\lambda\otimes\mathcal{K}_\lambda d\mu(\lambda),\quad \mathcal{H}'=\int_{\hat{\mathcal{G}}}^{\oplus}\mathcal{H}_\lambda\otimes\mathcal{K}'_\lambda d\mu'(\lambda), \tag{11}$$

where U_λ are irreducible representation and 1_λ and $1'_\lambda$ are the unity operators acting on the Hilbert spaces $\mathcal{K}_\lambda$ or $\mathcal{K}'_\lambda$.

An isometric intertwining operator $A:\mathcal{H}\to\mathcal{H}'$

$$AU(g)=V(g)A,\quad \forall g\in\mathcal{G},\quad A^+A=1 \tag{12}$$

exists if and only if μ is absolutely continuous with respect to μ' and

$$\dim(\mathcal{K}'_\lambda)\geqslant\dim(\mathcal{K}_\lambda) \tag{13}$$

almost everywhere with respect to μ. In this case it will assume the following form:

$$[A\phi]_\lambda=\left(\frac{d\mu}{d\mu'}\right)^{1/2}(1_\lambda\otimes A_\lambda)\phi_\lambda,\quad A_\lambda^+A_\lambda=1, \tag{14}$$

where 1_λ is the unity operator in $\mathcal{H}_\lambda$ and $A_\lambda:\mathcal{K}_\lambda\to\mathcal{K}'_\lambda$ is an isometry defined almost everywhere with respect to μ.

The theorem reduces all our efforts, once we have the imprimitivity system, to the decomposition of *V* into irreducible unitary representations of the symmetry group *G*, that, from now on, will be denoted by I.U.R.s. The conditions for the applicability of the theorem are not too restrictive, since most of the groups of physical interest have the required properties, namely they are locally compact with a countable base of open sets and of type I. However we shall see that the absolute continuity of the measure μ on $\hat{\mathcal{G}}$ with respect to μ' leads to interesting physical consequences, namely to a series of constraints on the realizability of some measurements on particular physical systems.

III. LOCALIZATION OF EVENTS IN SPACE–TIME

The first step necessary for the description of a realistic quantum reference frame is the definition of its origin. From an operational point of view this is the description of the way in which a microscopical object can localize a point of the Minkowsky space–time manifold, namely an instant indicating the beginning of the time scale and a point in space with respect to which position measurements are referred. In other words, how a quantum system can point at a particular event, in a relativistic covariant way. This kind of measurement can be described by a POVM on the Minkowsky space–time $\mathcal{M}$ covariant with respect to the universal covering of the proper orthochronous Poincaré group, which will be indicated by $\mathcal{P}$. The problem has already been studied in Ref. 10 with a different method. We are going to rederive those results by means of the above developed construction procedure.

The first step is the construction of the most general imprimitivity system on $\mathcal{M}$ covariant with respect to $\mathcal{P}$, whose action $\tilde{\Lambda}$ on $\mathcal{M}$ is given by

$$\tilde{\Lambda}(y,a)(x)=y+\Lambda(a)x,\quad (y,a)\in\mathcal{P},\quad y\in\mathcal{T}_4,\quad a\in \mathrm{SL}(2C), \tag{15}$$

where $\Lambda: a \to \Lambda(a)$ is the representation of SL$(2C)$ acting on $\mathcal{M}$ by means of the Lorentz matrices.

The system of imprimitivity is transitive. If we choose as a representative point of the only orbit in $\mathcal{M}$ under the action of $\mathcal{P}$ the origin $O=(0,0,0,0)$, we can recognize the little group in the Lorentz group, or more precisely in SL$(2C)$, its universal covering. According to the imprimitivity theorem the unitary representation V has the form of an induced representation

$$[V(y,a)\psi](x) = D(a)\psi(x'), \quad x,x' \in \mathcal{M}, \tag{16}$$

where ψ takes its values in a Hilbert space $\tilde{\mathcal{H}}$, $D(a)$ is a unitary representation (not necessarily irreducible) of SL$(2C)$ and

$$x' = \Lambda(a^{-1})(x-y). \tag{17}$$

The projection-valued measure E on the homogeneous space $\mathcal{M}$ allows one to represent the vectors ψ belonging to the Hilbert space $\mathcal{H}'$ as square-integrable vector-value function defined on $\mathcal{M}$. The Lebesgue measure d^4x on $\mathcal{M}$, canonically associated to Minkowsky coordinates, is invariant under the action of $\mathcal{P}$ and the norm of ψ assumes the simple form:

$$\|\psi\|^2 = \int_{\mathcal{M}} \|\psi(x)\|^2 d^4x, \tag{18}$$

while the spectral measure E on the Borel σ algebra B of $\mathcal{M}$ assumes the diagonal form:

$$[E(I)\psi](x) = f_I(x)\psi(x), \quad I \in \mathcal{B}. \tag{19}$$

The second step is the decomposition of V into I.U.R.s of the Poincaré group $\mathcal{P}$. We perform a Fourier transform on $\mathcal{M}$ and pass from the coordinate representation to the momentum representation:

$$\tilde{\psi}(k) = (2\pi)^{-2} \int_{\mathcal{M}} \exp(ik\cdot x)\psi(x) d^4x, \quad k\cdot x = x^\alpha k_\alpha, \tag{20}$$

$$\|\psi\|^2 = \int \|\tilde{\psi}(k)\|^2 d^4k. \tag{21}$$

V takes the following form:

$$[V(y,a)\tilde{\psi}](k) = \exp(ik\cdot y) D(a)\tilde{\psi}(k'), \quad k' = \Lambda(a^{-1})k. \tag{22}$$

The physical states of $\mathcal{H}$ contain only non-negative energy representations, it follows that if A is an intertwining operator between U and V, then $A\mathcal{H} \subseteq \mathcal{H}'' \subseteq \mathcal{H}'$, where $\mathcal{H}''$ is the invariant subspace of $\mathcal{H}'$ which contains the vectors with non-negative energy, namely the wave functions $\tilde{\psi}(k)$ with support in the future cone V_+. We may disregard the values taken by $\tilde{\psi}(k)$ on the boundary of the cone, which has vanishing Lebesgue measure. In what follows we consider the subrepresentation V'' of V acting on $\mathcal{H}''$.

Now we introduce for any k in the open future cone an element $a_k \in$ SL$(2C)$ defined by

$$k = \Lambda(a_k)(M,0,0,0), \quad k^{02} - \mathbf{k}^2 = M^2, \tag{23}$$

and the new wave function ψ', defined by

$$\tilde{\psi}(k) = D(a_k)\psi'(k). \tag{24}$$

The representation V'' takes the following form:

$$[V''(y,a)\psi'](k)=\exp(ik\cdot y)D(a_k^{-1}aa_{k'})\psi'(k'), \tag{25}$$

where $a_k^{-1}aa_{k'}=u\in \mathrm{SU}(2)$. We can now consider the decomposition of D into I.U.R.s of $\mathrm{SL}(2C)$, whose matrix elements we indicate with $D^{\rho n}_{jmj'm'}(a)$. They are identified by two parameters: $\chi=(\rho,n)$. Two different I.U.R.s identified by (ρ,n) and $=(\rho',n')$ are equivalent if and only if either $(\rho,n)=(\rho',n')$, or $(\rho,n)=(-\rho',-n')$. There are two series of I.U.R.s: the principal series with ρ real and n integer, and the supplementary series with ρ imaginary and $n=0$.[17–20] Moreover one should not forget the trivial one-dimensional representation. The restriction of these representations to the subgroup SU(2) is given by

$$D^{\chi}_{jmj'm'}(u)=\delta_{jj'}R^{j}_{mm'}(u), \tag{26}$$

where $R^{j}_{mm'}(u)$ stands for the matrix elements of the I.U.R. of SU(2), labeled by the integer or half-integer index j, with

$$j=\left|\frac{n}{2}\right|,\left|\frac{n}{2}\right|+1,\ldots \quad m=-j,-j+1,\ldots,j-1,j. \tag{27}$$

Every unitary representation of SL(2C) can be decomposed uniquely into primary representations, which are direct sums of I.U.R.s, as SL(2C) is a type I group. We consider the direct integral decomposition of the Hilbert space $\tilde{\mathcal{H}}$ into irreducible spaces labeled by the variable $\chi=(\rho,n)$, and introduce an index α, which distinguishes the spaces where equivalent I.U.R.s operate:

$$\tilde{\mathcal{H}}=\int_{\widehat{\mathrm{SL}(2C)}}^{\oplus}\bigoplus_{\alpha}\tilde{\mathcal{H}}^{\chi}_{\alpha}d\omega(\chi), \tag{28}$$

$$\|\psi\|^2=\int_{\widehat{\mathrm{SL}(2C)}\times V_+}\sum_{\alpha}\|\psi_{\alpha}(k,\chi)\|^2 d\omega(\chi)d^4k, \tag{29}$$

where ω is a generic measure on $\widehat{\mathrm{SL}(2C)}$.

For fixed values of α,M,χ the Poincaré group $\mathcal{P}$ acts in the way described by Wigner[21]

$$[V''(y,a)\psi']_{\alpha,jm}(k,\chi)=\exp(ik\cdot y)\sum_{m'}R^{j}_{mm'}(a_k^{-1}aa_{k'})\psi'_{\alpha,jm'}(k',\chi), \tag{30}$$

as

$$a_k^{-1}aa_{k'}=u\in \mathrm{SU}(2). \tag{31}$$

Every I.U.R. of $\mathcal{P}$ with positive mass, identified by the variables (M,j), appears in the direct integral decomposition of V'' with a given multiplicity (defined almost everywhere on the positive real axis, i.e., on the M axis). The multiplicity of a particular representation (M,j) is strictly positive if the subset of $\widehat{\mathrm{SL}(2C)}$, whose elements are the I.U.R.s $\chi=(\rho,n)$ of $\mathrm{SL}(2C)$ with $n\leqslant 2j$, has nonvanishing measure ω. Then one can always assume that the multiplicity is as large as one needs, allowing the index α to take a sufficient number of different values.

As we have seen in Sec. II the intertwining operator theorem can be applied once U, the unitary representation of $\mathcal{P}$ acting on the Hilbert space $\mathcal{H}$, is decomposed into direct integral of spaces where I.U.R.s of $\mathcal{P}$ operate:

$$[U(y,a)\phi]_{\alpha jm}(k)=\exp(ik\cdot y)\sum_{m'}R^{j}_{mm'}(u)\phi_{\alpha jm'}(k'), \tag{32}$$

with

$$\|\phi\|^2 = \int \sum_{\alpha,j} \|\phi_\alpha(k,j)\|^2 d\mu(k). \tag{33}$$

The discrete index α distinguishes the spaces where equivalent I.U.R.s operate. Note that the range of the sum on the indices α and j may depend on M. The measure $d\mu(k)$ gives some information about the mass spectrum of the system on which the measurement is performed. According to our third theorem, an isometric intertwining operator A between U and V'' exists only if $\mu(k)$ (and therefore the corresponding measure on the range of M) is absolutely continuous with respect to the Lebesgue measure d^4k. This is possible if and only if the physical system on which the measurement is performed has a continuous mass spectrum, so we have to disregard the vacuum state and the one-particle states, whose mass spectrum has a vanishing Lebesgue measure. Moreover, if a value j appears in the decomposition, the measure ω of the set $I \in \mathcal{B}(\widehat{\mathrm{SL}(2C)})$ with $I = (\{\chi = (\rho,n) \in \widehat{\mathrm{SL}(2C)}, n \leqslant 2j\})$ has to be strictly positive. Eventually, if these conditions are satisfied the most general intertwining operator takes the following form:

$$\psi'_{\alpha jm}(k,\chi) = \sum_{\alpha'} A^j_{\alpha\alpha'}(M,\chi)\phi_{\alpha' jm}(k), \tag{34}$$

assuming that $d\mu(k)/d^4k = 1$ when M belongs to the mass spectrum, with

$$\int \sum_{\alpha} \overline{A^j_{\alpha\alpha'}(M,\chi)} A^j_{\alpha\alpha''}(M,\chi) d\omega(\chi) = \delta_{\alpha'\alpha''}. \tag{35}$$

Finally the most general density of probability on the Minkowsky space–time, describing the measurement of the coordinates of an event individuated by a quantum state described by a vector $\phi \in \mathcal{H}$ takes the following form:

$$\rho(x) = \sum_{\alpha} \int_{\widehat{\mathrm{SL}(2C)}} \|\psi_\alpha(x,\chi)\|^2 d\omega(\chi), \tag{36}$$

where

$$\psi_{\alpha pl}(x,\chi) = (2\pi)^{-2} \int \exp(-ik\cdot x) \sum_{\alpha',jm} D^\chi_{pljm}(a_k) A^j_{\alpha\alpha'}(M,\chi)\phi_{\alpha' jm}(k) d^4k. \tag{37}$$

This is the main result of Ref. 10.

IV. QUANTUM FRAMES OF REFERENCE

From an operational point of view a reference frame F can be defined by the operations which allow one to connect it to an initially fixed frame F_0. In a relativistic theory the set of the allowed transformation is represented by the Poincaré group $\mathcal{P}$. Every element of $\mathcal{P}$ individuates the translation in the Minkowsky space–time and the Lorentz transformation which cause the origin and the axes of the two frames coincide. We can also recognize in the four-vector individuating the translation the coordinates of the new origin with respect to the old one, while in the columns of the Lorentz matrix one finds the components of the new four orthogonal axes, relative to the old orthogonal basis. The ten indipendent parameters individuating the Poincaré transformation can also be recognized as relative observables of the two frames, namely relative position, time, velocity and spatial orientation. Their description can be given by a POVM on $\mathcal{P}$, covariant with respect to $\mathcal{P}$ itself. In other words the Poincaré group is in this case both the symmetry group and the measured space, endowed with the invariant Haar measure ν. The description is simplified by the assumption of the classical nature of the frame F_0, in other words it will be considered an

abstract mathematical tetrad with well-defined position, velocity and orientation. In this case the Poincaré group acts just on the system F by means of left translation and the covariance condition assumes the following form:

$$U(g)\tau(I)U(g)^{-1}=\tau(gI), \quad g\in\mathcal{P}, I\subseteq\mathcal{P}. \tag{38}$$

As shown in the previous sections, the starting point is the application of Mackey's imprimitivity theorem. In this case it is particulary simple: there is only one orbit and, if we choose, for example, as a representative point the identity $e\in\mathcal{P}$, the little group is reduced to the identity and the induced representation is simply the left regular representation or the direct sum of several representations equivalent to the left regular one and distinguished by the index α:

$$[V(g')\psi]_\alpha(g)=\psi_\alpha(g'^{-1}g), \tag{39}$$

$$[V(y,a)\psi]_\alpha(x,b)=\psi_\alpha(\Lambda(a^{-1})(x-y),a^{-1}b). \tag{40}$$

It can be decomposed into I.U.R.s of $\mathcal{P}$ by means of the harmonic analysis on $\mathcal{P}$, defined by

$$\tilde{\psi}(\gamma)=\int \psi(g)D^\gamma(g)d\nu(g), \tag{41}$$

where γ stands for (M,j). The inversion formula is given by

$$\psi(g)=\int_{\hat{\mathcal{P}}}\mathrm{Tr}[\tilde{\psi}(\gamma)D^\gamma(g^{-1})]d\hat{\nu}(\gamma), \tag{42}$$

where $d\hat{\nu}(\gamma)$ is the Plancherel measure on $\hat{\mathcal{P}}$. On the new ''wave function,'' defined on $\hat{\mathcal{P}}$, the space of equivalence classes of I.U.R.s of $\mathcal{P}$, the group action assumes the following form:

$$[V(g)\tilde{\psi}]_\alpha(\gamma)=D^\gamma(g)\tilde{\psi}_\alpha(\gamma). \tag{43}$$

This procedure can be repeated whenever the action of the symmetry group $\mathcal{G}$ on the measure space S is free and transitive, namely if for all $x,y\in S$ exists one and only one $g\in\mathcal{G}$ so that $y=\Lambda(g)x$. In this way, for example, we can construct time measurements covariant with respect to time translations and position measurements covariant with respect to space displacements.

In our case we just have to combine the usual Fourier transform on R^4 and the harmonis analysis on $\mathrm{SL}(2C)$, which give

$$\tilde{\psi}_{\alpha,jmj'm'}(k,\rho,n)=(2\pi)^{-2}\int \exp(ikx)D^{\rho n}_{jmj'm'}(a)\psi_\alpha(x,a)d\mu(a)d^4x, \tag{44}$$

and

$$\|\psi\|^2=\int_{\hat{T}\times\widehat{\mathrm{SL}(2C)}}\sum_\alpha \mathrm{Tr}[\psi^+_\alpha(k,\chi)\psi_\alpha(k,\chi)]d^4k\,d\hat{\mu}(\chi), \tag{45}$$

where $d\hat{\mu}(\chi)$ is the Plancherel measure on $\widehat{\mathrm{SL}(2C)}$, which is concentrated on the principal series only.

As in Sec. III we consider only $\mathcal{H}''$, the invariant subspace of $\mathcal{H}'$ which contains only the vectors with non-negative energy, and the subrepresentation V'' acting on $\mathcal{H}''$. For every k belonging to the open future cone V_+ we introduce an element $a_k\in\mathrm{SL}(2C)$ defined by Eq. (23) and the new wave function ψ', given by

$$\tilde{\psi}_{\alpha,plj'm'}(k,\chi)=\sum_{qs} D^\chi_{plqs}(a_k)\psi'_{\alpha,qsj'm'}(k,\chi). \tag{46}$$

In this way the action of $\mathcal{P}$ on $\mathcal{H}''$ for fixed values of α, M, χ, j', m' assumes the form introduced by Wigner[21]

$$[V''(y,a)\psi']_{\alpha,jmj'm'}(k,\chi) = \exp(ik\cdot y)\sum_{m'} R^{j}_{mn}(a_k^{-1}aa_{k'})\psi'_{\alpha,jnj'm'}(k',\chi), \tag{47}$$

because of Eqs. (31) and (26) Once we have introduced the primary decomposition of U shown in Eq. (32), the most general intertwining operator can be found if and only if the measure $d\mu(k)$, defining the mass spectrum of the physical system on which the measurement is performed, is absolutely continuous with respect to d^4k. In this case, redefining if necessary the normalization of the wave function $\phi \in \mathcal{H}$ so that $d\mu(k)/d^4k = 1$ when M belongs to the mass spectrum, we can write:

$$\psi'_{\alpha jmqs}(k,\chi) = \sum_{\alpha'} A^{j}_{qs,\alpha\alpha'}(M,\chi)\phi_{\alpha' jm}(k), \tag{48}$$

with

$$\int \sum_{\alpha} \sum_{q=|n/2|}^{\infty} \sum_{s=-q}^{q} \overline{A^{j}(M,\chi)_{\alpha\alpha' qs}} A^{j}(M,\chi)_{\alpha\alpha'' qs} d\hat{\mu}(\chi) = \delta_{\alpha'\alpha''}. \tag{49}$$

Finally the density of probability assumes the following form:

$$\rho(x,b) = \sum_{\alpha} |\psi_{\alpha}(x,b)|^2, \tag{50}$$

where

$$\begin{aligned}\psi_{\alpha}(x,b) &= (2\pi)^{-2}\int \exp(-ik\cdot x)\mathrm{Tr}[D^{\chi}(b^{-1}a_k)\psi'_{\alpha}(k,\chi)]d^4k\,d\hat{\mu}(\chi)\\ &= (2\pi)^{-6}\int d^4k \exp(-ik\cdot x)\int_0^{+\infty} d\rho \sum_{n=-\infty}^{+\infty}(n^2+\rho^2)\\ &\quad\times \sum_{j,q=|n/2|}^{\infty}\sum_{m=-j}^{j}\sum_{s=-q}^{q} D^{(\rho,n)}_{qsjm}(b^{-1}a_k)\psi'_{\alpha jmqs}(k,\chi).\end{aligned} \tag{51}$$

It is quite interesting to compare the density of probability on the Minkowsky space–time, which is described by equations (36) and (37), which was found indpendently in Sec. III, and the density of probability which can be found from Eqs. (50) and (51) by integration on $\mathrm{SL}(2C)$:

$$\rho(x) = \int_{\mathrm{SL}(2C)} \rho(x,a)d\mu(a), \tag{52}$$

which after some calculations assumes the following form:

$$\rho(x) = \sum_{\alpha} \int \mathrm{Tr}[\psi'_{\alpha}(x,\chi)^{+}\psi'_{\alpha}(x,\chi)]d\hat{\mu}(\chi), \tag{53}$$

with

$$\hat{\psi}_{\alpha}(x,\chi) = (2\pi)^{-2}\int \exp(-ik\cdot x)\tilde{\psi}_{\alpha}(k,\chi)d^4k, \tag{54}$$

where $d\hat{\mu}(\chi)$ is the Plancherel measure on the principal series of the I.U.R.s of SL$(2C)$.

As Eqs. (36) and (37) show, the most general density of probability on the Minkowsky space–time admits a generic measure $d\omega(\chi)$ on the space of I.U.R.s of SL$(2C)$. From these considerations one can guess there are some constraints on the realizability of some measurement, whose properties can be found through an analysis of the physical meaning of the parameters $\chi=(\rho,n)$ in this context. For example, as shown in Ref. 10 one can recognize as ''baricentric'' a measurement of events such that the measure ω on $\mathcal{B}(\widehat{\mathrm{SL}(2C)})$ appearing in Eq. (36) is concentrated on the trivial representation $D(a)=1$. Our results show that such a requirement cannot be compatible with the measurement of the further parameters fully describing a reference frame. In other words the origin of the quantum reference frame can never be localized on the world line of the center of mass of the microscopical system defining it. Moreover, as the same author suggested in a previous paper,[22] for a complete description of a quantum reference frame kinematical variables are not sufficient, but internal degree of freedom must be involved. We can see, for example, that neither the invariant mass of the system nor its spatial distribution, namely the center of mass position, can be arbitrarily fixed and disregarded, but have a fundamental role in the whole description.

V. THE OBSERVABLES RELATIVE TO A QUANTUM REFERENCE FRAME

The quantum picture is complete if every classical element is disregarded and every kinematical variable of a quantum system F_j is referred to a quantum reference frame F_i, namely a microscopical system with continuous mass spectrum. This can be simply obtained in two steps if the quantum systems F_i and F_j do not mutually interact.

First of all let us introduce as a preliminary tool a classical frame F_0, with respect to which the parameters of the Poincaré tranformation connecting it to the quantum frame F_i and a cinematical variable of the system F_j are referred. The first ones are described by a POVM τ_i on the universal covering of the Poincaré group $\mathcal{P}$, acting on the Hilbert space $\mathcal{H}_i$, while the second ones are described by a POVM τ_j on a measure space S acting on the Hilbert space $\mathcal{H}_j$. If there is no interaction the POVMs τ_i and τ_j and the unitary representation of $\mathcal{P}$ can be extended to the whole Hilbert space $\mathcal{H}=\mathcal{H}_j\otimes\mathcal{H}_i$ by the relations:

$$U(g)=U_j(g)\otimes U_i(g), \quad g\in\mathcal{P}, \tag{55}$$

$$\hat{\tau}_i(I)=I\otimes\tau_i(I) \quad \hat{\tau}_j(J)=\tau_j(J)\otimes I, \tag{56}$$

for all Borel subsets $I\subseteq\mathcal{P}$ and $J\subseteq S$. One can easily see that $\hat{\tau}_i$ and $\hat{\tau}_j$ are endowed with the right covariance properties with respect to Poincaré transformations

$$U(g)\hat{\tau}_i(I)U(g^{-1})=\hat{\tau}_i(gI) \quad U(g)\hat{\tau}_j(J)U(g^{-1})=\hat{\tau}_j(\Lambda(g)J) \quad \forall g\in\mathcal{P}. \tag{57}$$

Moreover the operators in their ranges are mutually commuting

$$[\hat{\tau}_i(I),\hat{\tau}_j(J)]=0, \quad I\subseteq\mathcal{P}, \quad J\subseteq S. \tag{58}$$

If these condition are satisfied the *convolution*[23,24] τ_{ij} of the two POVMs $\hat{\tau}_i$ and $\hat{\tau}_j$ can be defined by the relation

$$\tau_{ij}(J)=\int f_J(\Lambda(g^{-1})x)d\hat{\tau}_i(g)d\hat{\tau}_j(x), \quad g\in\mathcal{P}, \quad x\in S, \quad J\subseteq S. \tag{59}$$

It is suitable for the description of the relative observables of the system F_j with respect to the quantum frame F_i. Indeed τ_{ij} is endowed with the properties of a POVM acting on the Hilbert space $\mathcal{H}$, namely positivity, σ additivity and normalization. Moreover, as we expected, it is invariant under the action of the Poincaré group $\mathcal{P}$:

$$U(\tilde{g})\tau_{ij}(J)U(\tilde{g}^{-1})=\int f_J(\Lambda(g^{-1}\tilde{g})\Lambda(\tilde{g}^{-1})x)d\hat{\tau}_i(g)d\hat{\tau}_j(x)=\tau_{ij}(J), \tag{60}$$

in fact a Poincaré transformation will act on both F_i and F_j, changing the ''absolute'' cinematical variables of the two systems but leaving invariant the relative ones.

The mathematical description of the relations connecting two noninteracting quantum frames F_i and F_j can be obtained as a special case of this formalism. If in the previous discussion the quantum system F_j has a continuous mass spectum, while the measure space S coincides with the Poincaré group again, τ_{ij} describes the measurement of the ten parameters of the transformation connecting the two frames. It assumes the following form:

$$\tau_{ij}(I)=\int f_I(g^{-1}g')d\hat{\tau}_i(g)d\hat{\tau}_j(g'), \quad J\subseteq\mathcal{P}. \tag{61}$$

The intuition can be helped by a calculation of the density of probability describing the statistics of the measurement, defined by

$$\langle\phi_i\otimes\phi_j,\tau_{ij}(I)\phi_i\otimes\phi_j\rangle=\int_{\mathcal{P}}f_I(g)\rho_{ij}(g)d\mu(g), \tag{62}$$

which assumes the following form:

$$\rho_{ij}(g)=\int_{\mathcal{P}}\rho_i(\phi_i,g')\rho_j(\phi_j,g'g)d\mu(g'), \tag{63}$$

where $\rho_i(\phi_i,g')$ and $\rho_j(\phi_j,g'g)$ are the densities of probability describing a measurement of the ''absolute'' parameters g' and $g'g$, namely relative to a classical reference frame F_0, which were calculated in Sec. IV. In other words if the Poincaré transformations identified by the elements g' and $g'g$ connect the classical frame to the quantum frames F_i and F_j, respectively, then the transformation from F_i to F_j will be individuated by the element $g\in\mathcal{P}$, whatever g' may be.

The introduction of a third quantum frame F_k in the description leads to some surprising consequences, which are commonly called ''the paradox of quantum frames.'' While the relative observables of F_i and F_j, or of F_i and F_k, can be described, respectively, by $\tau_{ij}=\tilde{\tau}_i*\tau_j$ or by $\tau_{ik}=\tau_i*\tau_k$, the relative observables of F_j and F_k cannot be obtained by the convolution $\widetilde{\tau_{ik}}*\tau_{ij}$ as it does not own the necessary properties. The operators in its range could be positive if and only if the POVMs τ_{ik} and τ_{ij} commute, but it cannot be required and it is not generally true. One can easily see that the commutativity of the POVM $\{\tau_i(I)\}_{I\in\mathcal{B}(\mathcal{P})}$ is a sufficient condition for the commutativity of τ_{ik} and τ_{ij}:

$$[\hat{\tau}_i(I),\hat{\tau}_i(I')]=0\Rightarrow[\tau_{ik}(I),\tau_{ij}(I')]=0, \quad I,I'\subseteq\mathcal{P}, \tag{64}$$

however the first condition cannot be required. Note that the commutativity of the projectors in the range of the spectral measure $\{E_i(I)\}_{I\in\mathcal{B}(\mathcal{P})}$ does not involve the commutativity of the POVM $\tau_i(I)=A^+E_i(I)A$, unless the range of the intertwining operator $\mathcal{H}''=A\mathcal{H}$ is an invariant subspace under the action of the projectors $E_i(I)$. One can easily see that in this case the positive operators in the range of the POVM τ_i would be projectors too, but this is forbidden by Pauli's theorem and by the noncompatibility of the observables describing a reference frame. In other words sequential measurement of the relative parameters of two quantum frames F_j and F_k with respect to a third quantum frame F_i are not compatible, even if they do not mutually interact.[2,22]

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Perturbation of a lattice spectral band by a nearby resonance

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A soluble model of weakly coupled ''molecular'' and ''nuclear'' Hamiltonians is studied in order to exhibit explicitly the mechanism leading to the enhancement of fusion probability in case of a narrow near-threshold nuclear resonance. We, further, consider molecular cells of this type being arranged in lattice structures. It is shown that if the real part of the narrow nuclear resonance lies within the molecular band generated by the intercellular interaction, an enhancement, proportional to the inverse width of the nuclear resonance, is to be expected. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1371264]

I. INTRODUCTION

Molecules are usually treated as purely Coulombic systems, while the strong interaction between their nuclear constituents is assumed to play a negligible role. However, at least in principle, any Coulombic molecular level lying above the lower threshold of the nuclear subsystem, is embedded in the continuous spectrum of the nuclear sub-Hamiltonian. The coupling between the molecular and nuclear channels, hence, turns this level into a resonance (see, e. g., Refs. 1–5 and references cited therein). Of course, due to the wide Coulombic barrier between the nuclei and the short-range character of the nuclear interaction, this coupling, and thus the width of the resonance, which determines the fusion probability of the nuclear constituents of the molecule, is in general extremely small.

However, as pointed out in Refs. 6 and 7 the situation is rather different if the nuclear subsystem of a molecule has a sufficiently narrow near-threshold resonance. Examples of such nuclear systems may be read off from the data presented in Ref. 8. Among them are even customary systems like $p\,p\,{}^{16}\mathrm{O}$ and $p\,{}^{17}\mathrm{O}$,[9,10] i.e., the nuclear constituents of the water molecule H_2O or the hydroxyl ion OH^- with O being the isotope ^{17}O. For LiD and H_2O the influence of near-threshold nuclear resonances on the molecular properties has been studied in Refs. 11–13 by estimating the overlap integrals between the corresponding molecular and nuclear wave functions. The best known example of such phenomena is the muon catalyzed fusion of deuteron and triton in the $dt\,\mu$ molecule, where the near-threshold nuclear resonance $^5\mathrm{He}(3/2^+)$ plays a decisive role.[14]

Being motivated by the above special cases, we deal in this paper with a rather general model Hamiltonian related to the ones considered by Friedrichs in Ref. 15. This Hamiltonian consists of a ''nuclear'' part, a ''molecular'' part with eigenvalues embedded in the continuous spectrum of the nuclear part, and a weak coupling term which turns these unperturbed eigenvalues into ''molecular'' resonances. Since the model is explicitly solvable, the mechanism of formation of the resonances becomes clearly visible.

The following property pointed out in Refs. 6 and 7 appears, in particular, as a general feature: if the ''nuclear'' channel itself has a narrow resonance with a position close to the ''molecular''

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energy, then the width (the imaginary part) of the resulting ''molecular'' resonance is found to be inversely proportional to the ''nuclear'' width. In other words, a large increase of the decay rate of the ''molecular'' state, i.e., of the fusion probability, is observed in this case. Such a coincidence of nuclear and molecular energies is, of course, a rather rare phenomenon in nature.

A further goal of the present work is to show that the decay rate may be considerably enhanced when arranging molecular clusters of this type within a crystalline structure. The reason is that in such a configuration the original discrete molecular energy turns into a band, i.e., into a whole interval of the continuous spectrum. (Note that in the models under consideration, the spectral band generated by the ''molecular'' level is shifted finally, after switching on the coupling between the ''nuclear'' and ''molecular'' channels, into the unphysical sheet.) That is, even if the position of the ''nuclear'' resonance differs from the original ''molecular'' level, it can get into this band. This allows for a fine tuning by exciting the crystalline structure to energies as close as possible to the energy of the ''nuclear'' resonance. We show that the lattice states, which correspond to such an initial choice of their quasimomentum distribution, decay exponentially with a rate which is again inversely proportional to the width of the ''nuclear'' resonance.

Concluding this introduction, we would like to mention the papers Refs. 16 and 17 which develop approaches of the direct spectral modelling resembling the one employed in the present work. Reference 16 is devoted, in particular, to the study of a one-electron model of a solid having a cubic crystalline lattice (see Sec. 3.2 in Ref. 16). This model exibits a mechanism of the formation of gaps in the absolutely continuous spectrum of the total Hamiltonian due to the resonance coupling between the electron and lattice sub-Hamiltonians, while the absolutely continuous spectra of the sub-Hamiltonians do not have the corresponding gaps. Reference 17 discusses a similar effect of formation of gaps in the absolutely continuous spectrum of a self-adjoint operator defined in a Hilbert space associated with a periodically ''decorated'' periodic graph. The gaps are produced by the resonance interaction between the basic graph and the attached (''decorating'') graphs.

Notice that the phenomena we discuss in the present paper also arise partly due to the resonance coupling between the sub-Hamiltonians. In particular, some resonances and resonance bands are formed of an eigenvalue or spectral band of one of the sub-Hamiltonians embedded into the absolutely continuous spectrum of another sub-Hamiltonian. We refer, however, not to details of the structure of the resulting (real) spectrum of the total Hamiltonian like the spectral gaps of Refs. 16 and 17 but study an interplay between the arising resonances (or resonance bands) and the resonances which occurred before coupling.

The paper is organized as follows.

In Sec. II we introduce the explicitly soluble model designed to demonstrate the interplay of the molecular and nuclear resonance widths. It is also shown that in a wide time interval the decay of the ''molecular'' state is indeed of the standard exponential character.[19] This transition will take place primarily into the open nuclear channels and its rate is determined by the inverse width of the nuclear resonance. In Sec. III we consider the case where molecular Hamiltonians of the type considered in Sec. II are arranged in form of an infinite one-dimensional lattice. Section IV is devoted to the generalization to multi-dimensional lattices. In both these sections, the time evolution of originally pure molecular states, extended to a spectral band within a lattice, is studied. It is shown that if the real part of the ''nuclear'' resonance lies within such a spectral band, then there exist molecular states which decay exponentially, with a rate inversely proportional to the ''nuclear'' width.

II. TWO-CHANNEL MOLECULAR RESONANCE MODEL

A. Description of the model Hamiltonian

Let us consider a two-channel Hilbert space $\mathcal{H}=\mathcal{H}_1\oplus\mathcal{H}_2$ consisting of a ''nuclear'' Hilbert space $\mathcal{H}_1$ (channel 1) and a one-dimensional ''molecular'' space $\mathcal{H}_2=\mathbb{C}$ (channel 2). The elements

of $\mathcal{H}$ are represented as vectors $u=\binom{u_1}{u_2}$ where $u_1\in\mathcal{H}_1$ and $u_2\in\mathcal{H}_2$, with u_2 being a complex number. The inner product $\langle u,v\rangle_{\mathcal{H}}=\langle u_1,v_1\rangle+u_2\overline{v_2}$ in $\mathcal{H}$ is naturally defined via the inner products $\langle u_1,v_1\rangle$ in $\mathcal{H}_1$ and $u_2\overline{v_2}$ in $\mathcal{H}_2$.

As a Hamiltonian in $\mathcal{H}$ we consider the 2×2 operator matrix

$$A=\begin{pmatrix} h_1 & b \\ \langle\,\cdot\,,b\rangle & \lambda_2 \end{pmatrix}, \tag{2.1}$$

where h_1 is the (self-adjoint) ''nuclear Hamiltonian'' in $\mathcal{H}_1$, and $\lambda_2\in\mathbb{R}$ a trial ''molecular'' energy. A vector $b\in\mathcal{H}_1$ provides the coupling between the channels. It should be mentioned that the Hamiltonian (2.1) resembles one of the well-known Friedrichs models[15] (for a discussion of the other Friedrichs-type models see, e.g., Ref. 18 and the references cited therein).

If there is no coupling between the channels, i.e., for $b=0$, the spectrum of A consists of the spectrum of h_1 and the additional discrete eigenvalue λ_2. We assume that the continuous spectrum $\sigma_c(h_1)$ of the Hamiltonian h_1 is not empty and that the eigenvalue λ_2 is embedded in $\sigma_c(h_1)$. It is also assumed that λ_2 is not a threshold point of $\sigma_c(h_1)$, and that this spectrum is absolutely continuous in a sufficiently wide neighborhood of λ_2.

A nontrivial coupling ($b\neq 0$) between the channels will, in general, shift the eigenvalue λ_2 into an unphysical sheet of the energy plane. The resulting perturbed energy appears as a resonance, i.e., as a pole of the analytic (or, more precisely, meromorphic) continuation of the resolvent $r(z)=(A-z)^{-1}$ taken between suitable states (see, e.g., Ref. 5). In the present paper we assume that such a continuation through the absolutely continuous spectrum of h_1 in some neighborhood of λ_2 is possible at least for the matrix element $\langle r_1(z)b,b\rangle$ of the resolvent $r_1(z)=(h_1-z)^{-1}$. Then one infers a meromorphic continuability at least for the compressed resolvent $P_2(A-z)^{-1}|_{\mathcal{H}_2}$ where P_2 denotes the orthogonal projection onto the space $\mathcal{H}_2$. Indeed, the explicit representation for the resolvent $r(z)$ is easily seen to be

$$r(z)=\begin{pmatrix} r_1(z)+\dfrac{r_1(z)b\langle\,\cdot\,,b\rangle r_1(z)}{M_2(z)} & -\dfrac{r_1(z)b}{M_2(z)} \\ -\dfrac{\langle\,\cdot\,,b\rangle r_1(z)}{M_2(z)} & \dfrac{1}{M_2(z)} \end{pmatrix}, \tag{2.2}$$

where the transfer function $M_2(z)$ reads $M_2(z)=\lambda_2-z-\beta(z)$ with $\beta(z)=\langle r_1(z)b,b\rangle$. Thus, if $\beta(z)$ admits a meromorphic continuation through an interval of the absolutely continuous spectrum of the ''nuclear'' Hamiltonian h_1, then the function $P_2(A-z)^{-1}|_{\mathcal{H}_2}=M_2^{-1}(z)$ admits such a continuation, too.

Evidently the poles of $r(z)$ on the physical sheet are either due to zeros of the function $M_2(z)$ or due to poles of the resolvent $r_1(z)$. The latter correspond to the discrete spectrum of the operator h_1 which may determine part of the point spectrum of A. This is true, in particular, for the multiple eigenvalues of h_1. In any case it is obvious that the perturbation of the eigenvalue λ_2 only corresponds to solutions of the equation $M_2(z)=0$, i.e., of

$$z=\lambda_2-\beta(z). \tag{2.3}$$

This equation has no roots z with $\operatorname{Im} z\neq 0$ on the physical sheet. For, being eigenvalues of the selfadjoint operator A, they have, of course, to be real. Thus, Eq. (2.3) may have solutions only on the real axis and in the unphysical sheet(s) of the Riemann surface of the resolvent $r_1(z)$.

We start with a brief discussion of the case where the ''nuclear'' channel Hamiltonian h_1 generates no resonances close to λ_2 in a domain $\mathcal{D}$ of the unphysical sheet which adjoins the physical sheet from below the cut. This assumption implies that for a wide set of unit vectors $\hat{b}$

$=b/\|b\|$ the quadratic form $\beta(z)=\|b\|^2\langle r_1(z)\hat{b},\hat{b}\rangle$ can be analytically continued in $\mathcal{D}$. Moreover, under certain smallness conditions for $\|b\|$, Eq. (2.3) is uniquely solvable[22] in $\mathcal{D}$ providing in first order perturbation theory (see, e.g., Refs. 20 and 21)

$$z_2 =_{\|b\|\to 0} \lambda_2 - \langle r_1(\lambda_2+\mathrm{i}0)b,b\rangle + o(\|b\|^2). \tag{2.4}$$

The real and imaginary parts of the resonance $z_2=E_R^{(2)}-\mathrm{i}(\Gamma_R^{(2)}/2)$, thus, are given by

$$\begin{aligned} E_R^{(2)} &= \lambda_2 - \mathrm{Re}\langle r_1(\lambda_2+\mathrm{i}0)b,b\rangle + o(\|b\|^2), \\ \Gamma_R^{(2)} &= 2\,\mathrm{Im}\langle r_1(\lambda_2+\mathrm{i}0)b,b\rangle + o(\|b\|^2). \end{aligned} \tag{2.5}$$

B. Perturbation of the ''molecular'' resonance by a nearby ''nuclear'' resonance

Our main interest concerns the opposite case of a ''nuclear'' resonance $z_1=E_R^{(1)}-\mathrm{i}(\Gamma_R^{(1)}/2)$, $\Gamma_R^{(1)}>0$, with a real part $E_R^{(1)}$ close to λ_2. For the sake of simplicity we assume the corresponding pole of $r_1(z)$ to be of first order. Let the element $b\in\mathcal{H}_1$ be such that the function $\beta(z)$ admits an analytic continuation into a domain $\mathcal{D}$ which contains both points λ_2 and z_1. This domain, moreover, is assumed to belong to the unphysical sheet which adjoins the physical sheet along the upper rim of the cut. In $\mathcal{D}$ the function $\beta(z)$, thus, can be written as

$$\beta(z)=\frac{a}{z_1-z}+\beta^{\mathrm{reg}}(z) \tag{2.6}$$

with $\beta^{\mathrm{reg}}(z)$ being a holomorphic function. For a fixed ''structure function'' $\hat{b}=b/\|b\|$ we have $|a|=C_a\|b\|^2$ with a constant C_a determined by the residue of $r_1(z)$ at $z=z_1$. Note that this residue is usually expressed in terms of resonance (Gamow) functions (see, for example, Ref. 23). In fact, we assume that the resonance corresponds to an ''almost eigenstate'' of h_1. That is, in principle a limiting procedure $\Gamma_R^{(1)}\to 0$ is possible so that the resonance turns into a usual eigenvalue with an eigenvector $\psi_1\in\mathcal{H}_1$. More precisely, we assume

$$C_a=C_a^{(0)}+o(1) \quad \text{as} \quad \Gamma_R^{(1)}\to 0 \tag{2.7}$$

with $C_a^{(0)}\equiv\langle\hat{b},\psi_1\rangle\langle\psi_1,\hat{b}\rangle\neq 0$. This can be achieved, e.g., if the Hamiltonian h_1 itself has a matrix representation of the form (2.1) and the resonance z_1 is generated by a separated one-dimensional channel. In such a case, according to (2.2) and (2.4), we would have $C_a^{(0)}=1$ (for details see Ref. 7, Sec. II).

Let

$$\mathrm{Re}\,a>0 \quad \text{and} \quad \mathrm{Im}\,a\ll\mathrm{Re}\,a \tag{2.8}$$

and, for $z\in\mathcal{D}$,

$$|\mathrm{Im}\,\beta^{\mathrm{reg}}(z)|\geqslant c_{\mathcal{D}}\|b\|^2 \quad \text{and} \quad |\beta^{\mathrm{reg}}(z)|\leqslant C_{\mathcal{D}}\|b\|^2$$

with constants $c_{\mathcal{D}}>0$ and $C_{\mathcal{D}}>0$. Furthermore, the coupling between the channels in the Hamiltonian (2.1) is assumed to be so weak that

$$|\beta^{\mathrm{reg}}(z)|\leqslant C_{\mathcal{D}}\|b\|^2\ll\Gamma_R^{(1)} \quad \text{while} \quad |a|=C_a\|b\|^2\ll(\Gamma_R^{(1)})^2. \tag{2.9}$$

It can be expected that these conditions are fulfilled in specific molecular systems even under the supposition that the ''nuclear'' width $\Gamma_R^{(1)}$ itself is very small.

After inserting (2.6) for $\beta(z)$, Eq. (2.3) turns into the ''quadratic'' equation

$$(\lambda_2-z)(z_1-z)-a+(z_1-z)\beta^{\mathrm{reg}}(z)=0$$

which can be ''solved,'' i.e., can be rewritten in form of two equations:

$$z=\frac{\lambda_2+z_1-\beta^{\rm reg}(z)}{2}\pm\sqrt{\left(\frac{\lambda_2-z_1-\beta^{\rm reg}(z)}{2}\right)^2+a}. \tag{2.10}$$

Under conditions (2.9) the existence of solutions of (2.10), and thus of Eq. (2.3), is guaranteed, analogously to the proof in Ref. 22, by Banach's fixed point theorem. Each of the equations (2.10) has only one solution in the domain $\mathcal{D}$. In case of the sign ''$-$'' we denote the root of (2.10) by $z_{\rm nucl}$, in case of the sign ''$+$'' by $z_{\rm mol}$.

The inequalities (2.9) imply

$$\frac{|a|}{|\lambda_2-z_1-\beta^{\rm reg}(z)|_{z\in\mathcal{D}}|^2}\approx\frac{|a|}{|\lambda_2-E_R^{(1)}|^2+\left(\frac{\Gamma_R^{(1)}}{2}\right)^2}\leqslant\frac{4C_a\|b\|^2}{(\Gamma_R^{(1)})^2}\ll 1. \tag{2.11}$$

For $z\in\mathcal{D}$ the value of

$$\varepsilon(z)=\frac{4a}{[\lambda_2-z_1-\beta^{\rm reg}(z)]^2} \tag{2.12}$$

is very small, $|\varepsilon(z)|\ll 1$. Thus, to separate the main terms of the solutions of Eqs. (2.10), one can apply the asymptotic relation $\sqrt{1+\varepsilon}=1+\varepsilon/2+O(\varepsilon^2)$. As a result we find

$$z=\frac{\lambda_2+z_1-\beta^{\rm reg}(z)}{2}\pm\frac{\lambda_2-z_1-\beta^{\rm reg}(z)}{2}\left(1+\frac{2a}{(\lambda_2-z_1-\beta^{\rm reg}(z))^2}+O(\varepsilon^2)\right). \tag{2.13}$$

In other words, the roots $z_{\rm nucl}$ and $z_{\rm mol}$ of (2.10) are essentially given by

$$z_{\rm nucl}\cong z_1-\frac{a}{\lambda_2-z_1-\beta^{\rm reg}(z_1)}\cong z_1-\frac{a}{\lambda_2-z_1}, \tag{2.14}$$

$$z_{\rm mol}\cong\lambda_2-\beta^{\rm reg}(\lambda_2+{\rm i}0)+\frac{a}{\lambda_2-z_1-\beta^{\rm reg}(\lambda_2+{\rm i}0)}\cong\lambda_2+\frac{a}{\lambda_2-z_1}. \tag{2.15}$$

From the second condition (2.9) follows $|a/(\lambda_2-z_1)|\ll\Gamma_R^{(1)}$. Consequently, this term provides in $z_{\rm nucl}$ a very small perturbation of the initial ''nuclear'' resonance z_1. As compared to $\Gamma_R^{(1)}$ it represents also in $z_{\rm mol}$ a very weak perturbation of the ''molecular'' energy λ_2. However, as compared to the result (2.4), valid in case of a missing nearby ''nuclear'' resonance, it can be rather large. In particular, if the ''molecular'' energy λ_2 coincides with the real part $E_R^{(1)}$ of the ''nuclear'' resonance z_1, then $z_{\rm mol}=E_R^{(m)}-i\,(\Gamma_R^{(m)}/2)$ with

$$E_R^{(m)}\cong\lambda_2-2\,\frac{{\rm Im}\,a}{\Gamma_R^{(1)}}\quad\text{and}\quad\Gamma_R^{(m)}\cong 4\,\frac{{\rm Re}\,a}{\Gamma_R^{(1)}}. \tag{2.16}$$

The width of the ''molecular'' resonance $z_{\rm mol}$ in the presence of a nearby ''nuclear'' resonance z_1, thus, turns out to be inversely proportional to the ''nuclear'' width $\Gamma_R^{(1)}$.

Let us contrast the results (2.4) and (2.16) in some more detail. Since such a comparison is necessarily of a qualitative character, we simulate the situation of a missing nearby nuclear resonance simply by dropping the pole term in the representation (2.6) of $\beta(z)$. After this removal we get $\beta(z)\equiv\beta^{\rm reg}(z)$ and for ${\rm Im}\,z\leqslant 0$ the eigenvalue λ_2 generates the resonance (2.4) having the width $\Gamma_R^{(2)}\approx 2\,{\rm Im}\,\beta^{\rm reg}(\lambda_2+{\rm i}0)$. The latter satisfies the inequalities $c_{\mathcal{D}}\|b\|^2\leqslant\Gamma_R^{(2)}/2\leqslant C_{\mathcal{D}}\|b\|^2$. Substituting $|{\rm Re}\,a|\sim C_a\|b\|^2\sim(C_a/c_{\mathcal{D}})\,\Gamma_R^{(2)}$ in (2.16) we find the following approximate estimate of $\Gamma_R^{(m)}$ relative to $\Gamma_R^{(2)}$:

$$\Gamma_R^{(m)} \sim \Gamma_R^{(2)} \cdot \frac{C_a / c_{\mathcal{D}}}{\Gamma_R^{(1)}}. \tag{2.17}$$

The second inequality (2.9), chosen as a condition for $\|b\|$ reflects the fact that the ''usual'' molecular width $\Gamma_R^{(2)}$ is much smaller than the width of a usual ''nuclear'' resonance $\Gamma_R^{(1)}$,

$$C_a \Gamma_R^{(2)} \ll c_{\mathcal{D}} (\Gamma_R^{(1)})^2. \tag{2.18}$$

This can practically always be assumed for concrete molecules.

Under condition (2.7) the value of $C_a = |a|/\|b\|^2$ differs from zero, $C_a \geqslant C > 0$, as $\Gamma_R^{(1)} \to 0$. Therefore the estimates (2.16) and (2.17) imply that in the presence of a narrow ($\Gamma_R^{(1)} \ll C_a / c_{\mathcal{D}}$) ''nuclear'' resonance close to λ_2 the ''molecular'' width $\Gamma_R^{(m)}$ is much larger than the ''molecular'' width $\Gamma_R^{(2)}$ observed in absence of such a resonance. In fact, according to (2.17) this ratio is determined by the large quotient $(C_a / c_{\mathcal{D}} / \Gamma_R^{(1)})$.

Finally we note that if the conditions (2.9), and hence the condition (2.18) are not fulfilled, i.e., if the coupling between the channels in the Hamiltonian (2.1) is not small compared with the ''nuclear'' width, then it follows from (2.10) that the molecular width $\Gamma_R^{(m)}$ achieves itself an order of $\Gamma_R^{(1)}$. We do not discuss this case since such a situation can hardly be assumed to exist.

C. Exponential decay of the ''molecular'' state

Let us suppose that an initial state of the system described by the Hamiltonian A corresponds exactly to the pure ''molecular'' wave function $\varphi = \binom{1}{0}$. Then, the time evolution of the system is described by the solution $\psi(t)$ of the Cauchy problem

$$i \frac{d\psi}{dt} = A\psi, \quad \psi|_{t=0} = \varphi. \tag{2.19}$$

The probability of finding the system at the time t still in the molecular state φ is given by

$$P_{\mathrm{mol}}(t) = |\langle \psi(t), \varphi \rangle|^2.$$

The remainder $1 - P_{\mathrm{mol}}(t)$, hence, determines the probability for the state φ to decay into open channels of the continuous spectrum of the ''nuclear'' sub-Hamiltonian h_1.

To estimate the probability $P_{\mathrm{mol}}(t)$, we use the standard integral representation of a function of an operator via its resolvent. In the case considered this means

$$\exp\{-\mathrm{i}At\} = -\frac{1}{2\pi \mathrm{i}} \oint_\gamma dz\, \mathrm{e}^{-\mathrm{i}zt} (A - z)^{-1}. \tag{2.20}$$

The integration in (2.20) is performed in the physical sheet along a contour γ going counterclockwise around the spectrum of the matrix A. Recall that, due to the self-adjointness of the operator A, this spectrum is real. Taking into account the representations (2.2) and (2.20) one finds

$$\langle \psi(t), \varphi \rangle = -\frac{1}{2\pi \mathrm{i}} \oint_\gamma dz\, \frac{\exp(-\mathrm{i}zt)}{\lambda_2 - z - \beta(z)}. \tag{2.21}$$

This leads to the following important result. Under the conditions of Sec. II B the behavior of the integral (2.21) for $t > 0$ is described by the formula

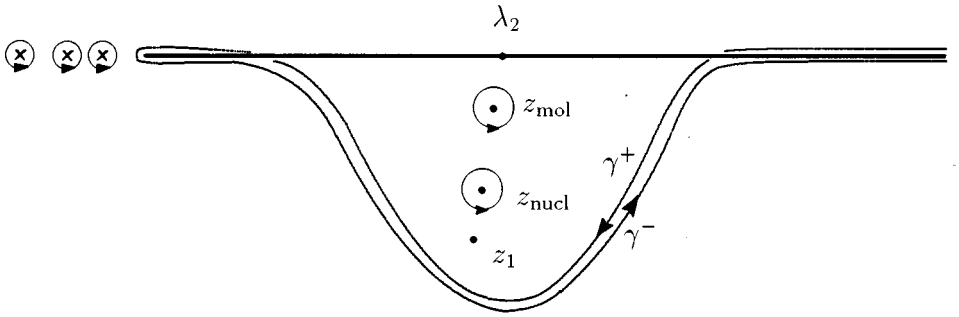

FIG. 1. A scheme showing the deformation of the integration path γ. The part γ^+ of the resulting contour belongs to the unphysical sheet, part γ^- to the physical sheet. The crosses ''×'' denote the discrete eigenvalues of the Hamiltonian A while the solid line corresponds to the continuous spectrum.

$$\langle \psi(t),\varphi\rangle = \exp\{-\mathrm{i}z_{\rm mol}t\}\left[1-\frac{a}{(\lambda_2-z_1-\beta^{\rm reg}(\lambda_2+\mathrm{i}0))^2}+O(\varepsilon^4(\lambda_2+\mathrm{i}0))\right] + \exp\{-\mathrm{i}z_{\rm nucl}t\}\left[\frac{a}{(\lambda_2-z_1-\beta^{\rm reg}(z_1))^2}+O(\varepsilon^4(z_1))\right]+\tilde{\varepsilon}(t), \tag{2.22}$$

where the value of $\varepsilon(z)$ is given by Eq. (2.12). The background term $\tilde{\varepsilon}(t)=O(\|b\|^2)$ is small, $|\tilde{\varepsilon}(t)|\ll 1$, for all $t>0$. In particular, if $E_R^{(1)}=\lambda_2$ we have

$$\langle \psi(t),\varphi\rangle \approx \exp\{-\mathrm{i}z_{\rm mol}t\}\left[1+\frac{4a}{(\Gamma_R^{(1)})^2}+\cdots\right]+\exp\{-\mathrm{i}z_{\rm nucl}t\}\left[-\frac{4a}{(\Gamma_R^{(1)})^2}+\cdots\right]. \tag{2.23}$$

The proof of the asymptotic relation (2.22) is carried out by estimating the contribution of the resonance poles $z_{\rm mol}$ and $z_{\rm nucl}$ to the integral (2.21). This is done by deforming parts of the contour γ situated in a neighborhood of the molecular energy λ_2 (see Fig. 1). A part γ^+ of γ, situated initially on the upper rim of the cut, is shifted into the neighboring unphysical sheet. Having done such a deformation one finds explicitly the residues of the integrand in (2.21) at $z=z_{\rm mol}$ and $z=z_{\rm nucl}$. An analogous deformation of a part γ^- of γ, situated initially on the lower rim, is performed in a domain $\mathrm{Im}\,z<0$ of the physical sheet. It is assumed that, though the parts γ^+ and γ^- belong to different energy sheets, their positions on these sheets coincide. It is also assumed that for any $z\in\gamma^\pm$ the estimate $|\beta^\pm(z)|\ll|\lambda_2-z|$ holds. Thus, the integration in (2.21) around the continuous spectrum of A, except the residues at $z=z_{\rm mol}$ and $z=z_{\rm nucl}$, gives

$$-\frac{1}{2\pi\mathrm{i}}\int_{\gamma^+}dz\,\exp(-\mathrm{i}zt)\left(\frac{1}{\lambda_2-z-\beta^+(z)}-\frac{1}{\lambda_2-z-\beta^-(z)}\right) = -\frac{1}{2\pi\mathrm{i}}\int_{\gamma^+}dz\,\exp(-\mathrm{i}zt)\,\frac{\beta^+(z)-\beta^-(z)}{[\lambda_2-z-\beta^+(z)][\lambda_2-z-\beta^-(z)]}. \tag{2.24}$$

Here we have used the specific notation $\beta^+(z)$ for the values of the function $\beta(z)$ at points z belonging to the curve γ^+ (i.e., lying in the unphysical sheet), and $\beta^-(z)$ for the values of $\beta(z)$ at the same points of the curve γ^- (i.e., lying in the physical sheet). Both $\beta^-(z)$ and $\beta^+(z)$ are of the order of $O(\|b\|^2)$, and $|\beta^\pm(z)|\ll|\lambda_2-z|$, while the exponential $\exp(-\mathrm{i}zt)$ at $\mathrm{Im}\,z<0$ is decreasing for $t>0$. The value of the function (2.24), thus, is always small, having an order of $O(\|b\|^2)$, and is even decreasing (in general nonexponentially) with increasing t. We include the contribution of this function in the background term $\tilde{\varepsilon}(t)$. The summand $\tilde{\varepsilon}(t)$ also includes a

contribution to (2.21) from the residues at the discrete eigenvalues of A. Apart from factors oscillating when t changes, the value of this contribution remains practically the same for all $t \geqslant 0$.

The formulas (2.22) and (2.23) show explicitly that in a large time interval $0 \leqslant t < T$, $T \sim (2/\Gamma_R^{(m)})\,|\ln \max|\tilde{\varepsilon}(t)||$, the decay of a ''molecular'' state φ in the presence of a narrow ''nuclear'' resonance is indeed of exponential character. The rate of this decay is determined mainly by the width $\Gamma_R^{(m)}$ of the ''molecular'' resonance z_{mol}, i.e., by the ratio $|\mathrm{Re}\, a|/\Gamma_R^{(1)}$,

$$P_{\mathrm{mol}}(t) \cong \exp\{-\Gamma_R^{(m)} t\} \cong \exp\left\{-\frac{4|\mathrm{Re}\, a|}{\Gamma_R^{(1)}} t\right\}. \tag{2.25}$$

III. ''MOLECULAR'' RESONANCES IN A ONE-DIMENSIONAL LATTICE

Let us assume that the ''molecules'' described by the Hamiltonian (2.1) are arranged in form of an infinite one-dimensional (linear) crystalline structure. To describe such a crystal we introduce the lattice Hilbert space

$$\mathcal{G} = \bigoplus_{i=-\infty}^{+\infty} \mathcal{H}^{(i)}$$

representing an orthogonal sum of the Hilbert spaces associated with the individual cells

$$\mathcal{H}^{(i)} = \mathcal{H}_1^{(i)} \oplus \mathcal{H}_2^{(i)}. \tag{3.1}$$

Here the subspaces $\mathcal{H}_1^{(i)} \equiv \mathcal{H}_1$ and $\mathcal{H}_2^{(i)} \equiv \mathcal{H}_2 \equiv \mathbb{C}$ are exactly the same ones as in Sec. II and, thus, $\mathcal{H}^{(i)} \equiv \mathcal{H}$. The elements of the total Hilbert space $\mathcal{G}$ are represented by the sequences $u = (\ldots, u^{(-2)}, u^{(-1)}, u^{(0)}, u^{(1)}, u^{(2)}, \ldots)$ with components $u^{(i)} = \binom{u_1^{(i)}}{u_2^{(i)}}$ where $u_1^{(i)} \in \mathcal{H}_1$ and $u_2^{(i)} \in \mathcal{H}_2 = \mathbb{C}$. The inner product in $\mathcal{H}$ is defined by $\langle u, v \rangle_{\mathcal{H}} = \Sigma_{i=-\infty}^{+\infty} \langle u^{(i)}, v^{(i)} \rangle_{\mathcal{H}(i)}$. The subspaces $\mathcal{G}_1 = \oplus_{i=-\infty}^{+\infty} \mathcal{H}_1^{(i)}$ and $\mathcal{G}_2 = \oplus_{i=-\infty}^{+\infty} \mathcal{H}_2^{(i)}$, with $\mathcal{G} = \mathcal{G}_1 \oplus \mathcal{G}_2$, are called pure nuclear and pure molecular channels, respectively.

In the present section we deal with the Hamiltonian H acting in $\mathcal{H}$ according to

$$(Hu)^{(i)} = W u^{(i-1)} + A u^{(i)} + W u^{(i+1)}, \tag{3.2}$$

where only the interaction between neighboring cells is taken into account and the interaction operator W is chosen in the simplest form

$$W = \begin{pmatrix} 0 & 0 \\ 0 & w \end{pmatrix} \tag{3.3}$$

with w being a positive number. Such a choice of the interaction corresponds to the natural assumption that the cells interact between each other via the molecular states, while the direct interaction between nuclear constituents belonging to different cells is negligible. We assume that the closed interval $[\lambda_2 - 2w, \lambda_2 + 2w]$ is totally embedded in the continuous spectrum $\sigma_c(h_0)$ of h_0 and, moreover, that no thresholds of $\sigma_c(h_0)$ belong to this interval. For the sake of simplicity we also assume that the interval belongs to the domain $\mathcal{D}$ introduced in Sec. II and that for any $\mu \in [\lambda_2 - 2w, \lambda_2 + 2w]$

$$\mathrm{Im}\langle r_0(\mu \pm \mathrm{i}0)\hat{b}, \hat{b} \rangle \neq 0. \tag{3.4}$$

Obviously, the Hamiltonian (3.2) represents a special case of the infinite Jacobi operator matrix (regarding the properties of some infinite scalar Jacobi matrices see, e.g., Refs. 24 and 25 and references cited therein). It is a self-adjoint operator on the domain $\mathcal{D}(H)=\oplus_{i=-\infty}^{+\infty}\mathcal{D}^{(i)}$ with $\mathcal{D}^{(i)}=\mathcal{D}(h_1)\oplus\mathbb{C}$.

The resolvent $R(z)=(H-z)^{-1}$ of H possesses a natural block structure, $R(z)=\{R(j,k;z)\}$, $j,k=0,\pm1,\pm2,\ldots,\pm\infty$. The blocks $R(j,k;z)$, providing the mapping $\mathcal{H}^{(k)}\to\mathcal{H}^{(j)}$, satisfy the equations

$$WR(j-1,k;z)+(A-z)R(j,k;z)+WR(j+1,k;z)=\delta_{jk}I, \tag{3.5}$$

where δ_{jk} stands for the Kronecker delta and I for the identity operator in the Hilbert space $\mathcal{H}$ of cells. Hereafter we assume $\operatorname{Im} z\neq0$ so that the value of z automatically belongs to the resolvent set of the operator H. The blocks $R(j,k;z)$ themselves possess a 2×2 matrix structure, $R(j,k;z)=\{R_{mn}(j,k;z)\}$, $m,n=1,2$, corresponding to the decomposition $\mathcal{H}=\mathcal{H}_1\oplus\mathcal{H}_2$.

The Fourier transform

$$(Fu)(p)=\frac{1}{\sqrt{2\pi}}\sum_{j=-\infty}^{+\infty}u^{(j)}\exp(\mathrm{i}pj) \tag{3.6}$$

in $\mathcal{G}$ reduces Eq. (3.5) to

$$(A-z)R(p,p';z)+2\cos p\,WR(p,p';z)=\delta(p-p')I, \tag{3.7}$$

where the quasimomentum p runs through the interval $[-\pi,\pi]$ and the function $R(p,p';z)$ represents the kernel of the resolvent $R(z)$ in this representation. From (3.7) follows immediately

$$R(p,p';z)=G(p;z)\,\delta(p-p'), \tag{3.8}$$

where

$$G(p;z)=\begin{pmatrix} r_1(z)+\dfrac{r_1(z)b\langle\cdot,b\rangle r_1(z)}{\widetilde{M}_2(p;z)} & -\dfrac{r_1(z)b}{\widetilde{M}_2(p;z)} \\ -\dfrac{\langle\cdot,b\rangle r_1(z)}{\widetilde{M}_2(p;z)} & \dfrac{1}{\widetilde{M}_2(p;z)} \end{pmatrix}. \tag{3.9}$$

This corresponds to the representation (2.2) of the resolvent of the cell Hamiltonian A, the only difference being that the transfer function $M_2(z)$ is replaced by the expression

$$\widetilde{M}_2(p;z)=\lambda_2-z+2w\cos p-\beta(z). \tag{3.10}$$

The factorization (3.8) implies

$$R(j,k;z)=\frac{1}{2\pi}\int_{-\pi}^{\pi}dp\,\mathrm{e}^{-\mathrm{i}p(j-k)}G(p;z)$$

and with the representation (3.9) we, thus, obtain

$$R(j,k;z)=\begin{pmatrix} \delta_{jk}r_1(z)+r_1(z)b\,R_{22}(j,k;z)\langle\cdot,b\rangle r_1(z) & -r_1(z)b\,R_{22}(j,k;z) \\ -R_{22}(j,k;z)\langle\cdot,b\rangle r_1(z) & R_{22}(j,k;z) \end{pmatrix}, \tag{3.11}$$

where

$$R_{22}(j,k;z)=\frac{1}{2\pi}\int_{-\pi}^{\pi}dp\,\frac{e^{-ip(j-k)}}{\lambda_2-z+2w\cos p-\beta(z)}. \tag{3.12}$$

Introducing the new variable $\zeta=e^{-ip}$, this integral is reduced to

$$R_{22}(j,k;z)=\frac{1}{2\pi i}\oint_{\gamma}d\zeta\,\frac{\zeta^{j-k}}{w\zeta^2+M_2(z)\zeta+w}.$$

Here, γ stands for the unit circle centered at the origin, the integration over γ being performed in the counterclockwise sense. Further, applying the residue theorem and taking into account the sign of the difference $j-k$ one finds

$$R_{22}(j,k;z)=\frac{\left\{\frac{1}{2w}[\sqrt{[M_2(z)-2w][M_2(z)+2w]}-M_2(z)]\right\}^{|j-k|}}{\sqrt{[M_2(z)-2w][M_2(z)+2w]}}. \tag{3.13}$$

It is assumed here that the branch $\sqrt{(\xi-2w)(\xi+2w)}$ of the function $((\xi-2w)(\xi+2w))^{1/2}$ is defined in the plane of the complex parameter ξ, cut along the interval $[-2w,2w]$, and that $\mathrm{Im}\,\xi>0$ implies $\mathrm{Im}\sqrt{(\xi-2w)(\xi+2w)}>0$, while $\mathrm{Im}\,\xi<0$ implies $\mathrm{Im}\sqrt{(\xi-2w)(\xi+2w)}<0$.

From Eqs. (3.11) and (3.13) it follows that all the nontrivial singularities of the resolvent $R(z)$, differing from those of the cell ''nuclear'' channel resolvent $r_1(z)$, are determined by the properties of the function

$$D(z)=\sqrt{[M_2(z)-2w][M_2(z)+2w]}.$$

First, we note that if $\|b\|=0$, and thus $M_2(z)=\lambda_2-z$, then the ''molecular'' and ''nuclear'' channels in the Hamiltonian H decouple. In this case the eigenvalue λ_2 generates for H an additional branch of the absolutely continuous spectrum which occupies the interval $[\lambda_2-2w,\lambda_2+2w]$. Second, even if $\|b\|\neq 0$ then the function $D(z)$ cannot have roots z with $\mathrm{Im}\,z\neq 0$ in the physical sheet. Otherwise such roots would generate for H a complex spectrum. But this is impossible because of the selfadjointness of H. Also, under the condition (3.4) this function cannot have real roots within the interval $[\lambda_2-2w,\lambda_2+2w]$ since for $\lambda_2-2w\leqslant\mu\leqslant\lambda_2+2w$ the imaginary part

$$\mathrm{Im}[M_2(\mu\pm i0)-2w]=\mathrm{Im}[M_2(\mu\pm i0)+2w]=-\|b\|^2\,\mathrm{Im}\langle r_1(\mu\pm i0)\hat{b},\hat{b}\rangle$$

is nonzero by the assumption (3.4). Thus, in a close neighborhood of the interval $[\lambda_2-2w,\lambda_2+2w]$ the equation $D(z)=0$ may only have roots in the unphysical sheet. In fact, assuming the conditions (2.9) and repeating literally the considerations which led to (2.13), one can rewrite this relation in form of the four equations,

$$z=\frac{\lambda_2-2w+z_1-\beta^{\mathrm{reg}}(z)}{2}\pm\frac{\lambda_2-2w-z_1-\beta^{\mathrm{reg}}(z)}{2}\left[1+\frac{2a}{(\lambda_2-2w-z_1-\beta^{\mathrm{reg}}(z))^2}+O(\varepsilon_-^2)\right], \tag{3.14}$$

$$z=\frac{\lambda_2+2w+z_1-\beta^{\mathrm{reg}}(z)}{2}\pm\frac{\lambda_2+2w-z_1-\beta^{\mathrm{reg}}(z)}{2}\left[1+\frac{2a}{(\lambda_2+2w-z_1-\beta^{\mathrm{reg}}(z))^2}+O(\varepsilon_+^2)\right], \tag{3.15}$$

where $\varepsilon_\pm=4a/(\lambda_2\pm 2w-z_1-\beta^{\mathrm{reg}}(z))$. In that part of the domain $\mathcal{D}$ which belongs to the unphysical sheet, equation $D(z)=0$ has four solutions being given essentially by

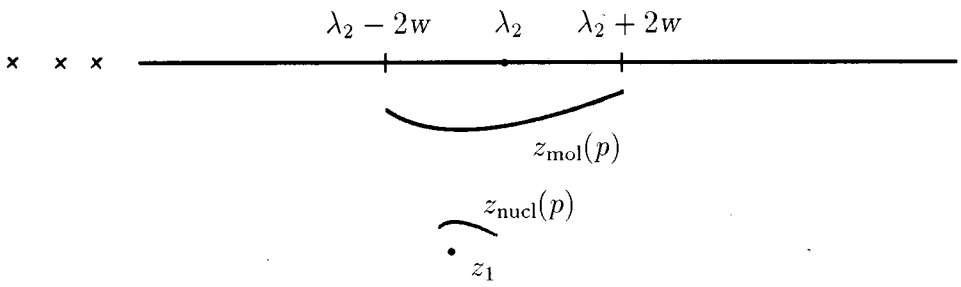

FIG. 2. A scheme showing the position of the resonance bands generated in the unphysical sheet by the ''molecular'' eigenvalue λ_2 and the ''nuclear'' resonance z_1. These bands are generated, respectively, by the points $z_{\rm mol}(p)$ and $z_{\rm nucl}(p)$ with the quasimomentum p running through the interval $[-\pi,\pi]$.

$$z_{\rm nucl}^{(\pm)} \cong z_1 - \frac{a}{\lambda_2 \pm 2w - z_1 - \beta^{\rm reg}(z_1)} \cong z_1 - \frac{a}{\lambda_2 \pm 2w - z_1}, \tag{3.16}$$

$$z_{\rm mol}^{(\pm)} \cong \lambda_2 \pm 2w - \beta^{\rm reg}(\lambda_2 \pm 2w + {\rm i}0) + \frac{a}{\lambda_2 \pm 2w - z_1 - \beta^{\rm reg}(\lambda_2 \pm 2w + {\rm i}0)}$$

$$\cong \lambda_2 \pm 2w + \frac{a}{\lambda_2 \pm 2w - z_1}. \tag{3.17}$$

Obviously, each of the roots $z_{\rm nucl}^{(\pm)}$ and $z_{\rm mol}^{(\pm)}$ represents an additional square-root branching point of the Riemann surface of the functions $R_{22}(j,k;z)$. Consequently, these roots are also the branching points of the Riemann surface of the total resolvent $R(z)$. Thus, one has to introduce the ''resonance'' cuts in the unphysical sheet considered. The cuts can be made, say, between $z_{\rm nucl}^{(-)}$ to $z_{\rm nucl}^{(+)}$ and between $z_{\rm mol}^{(-)}$ and $z_{\rm mol}^{(+)}$. Evidently, these cuts are to be interpreted as the resonance spectral bands generated by the initial ''molecular'' level λ_2 and the ''nuclear'' resonance z_1 (see Fig. 2).

Consider now the time evolution of the system described by the Hamiltonian H starting from a pure molecular state $\varphi = \varphi_1 \oplus \varphi_2$, $\|\varphi_n\| \in \mathcal{G}_n$, $n=1,2$, with $\varphi_1 = 0$ and $\|\varphi\| = \|\varphi_2\| = 1$. The probability to find the system at a time $t \geqslant 0$ in the molecular channel is given by

$$P_{\rm mol}(\varphi,t) = \|\mathsf{P}_2 {\rm e}^{-{\rm i}Ht}\varphi\|^2, \tag{3.18}$$

where P_2 is the orthogonal projection in $\mathcal{G}$ on the pure molecular subspace $\mathcal{G}_2$.

As in (2.20) we represent the time evolution operator $\exp(-{\rm i}Ht)$ in terms of the resolvent $R(z) = (H-z)^{-1}$,

$$\exp\{-{\rm i}Ht\} = -\frac{1}{2\pi{\rm i}} \oint_\gamma dz\, e^{-{\rm i}zt}(H-z)^{-1}, \tag{3.19}$$

where the integration is performed along a counterclockwise contour γ in the physical sheet encircling the spectrum of the Hamiltonian H. Recall that this spectrum is real since H is a self-adjoint operator.

According to Eqs. (3.8) and (3.10) the operator $\mathsf{P}_2 R(z)|_{\mathcal{G}_2}$ acts in quasimomentum representation as the multiplication operator

$$G_{22}(p,z) = [\tilde{M}_2(p;z)]^{-1} \tag{3.20}$$

and, thus,

$$(\mathsf{P}_2 R(z)\varphi)(p) = \frac{1}{\tilde{M}_2(p;z)}\,\varphi_2(p), \quad p \in [-\pi,\pi].$$

Here $\varphi_2(p)$ stands for the values of the Fourier transform (3.6) of the vector $\varphi_2 = (\ldots,\varphi_2^{(-2)},\varphi_2^{(-1)},\varphi_2^{(0)},\varphi_2^{(1)},\varphi_2^{(2)},\ldots)$, which means

$$(\mathsf{P}_2 \mathrm{e}^{-\mathrm{i}Ht}\varphi)(p) = -\frac{1}{2\pi\mathrm{i}}\,\varphi_2(p)\,J(p,t) \tag{3.21}$$

with

$$J(p,t) = \oint_\gamma dz\,\frac{\exp(-\mathrm{i}zt)}{\tilde{\lambda}_2(p) - z - \beta(z)}. \tag{3.22}$$

This expression has exactly the same form as the integral (2.21). The only difference consists in the replacement of λ_2 by the sum

$$\tilde{\lambda}_2(p) = \lambda_2 + 2w\cos p. \tag{3.23}$$

Thus, to estimate the function $J(p,t)$ one can immediately use the relation (2.22) in order to find

$$\begin{aligned} J(p,t) = {} & \exp\{-\mathrm{i}z_{\mathrm{mol}}(p)t\}\left[1 - \frac{a}{(\tilde{\lambda}_2(p) - z_1 - \beta^{\mathrm{reg}}(\tilde{\lambda}_2(p)+\mathrm{i}0))^2} + O(\varepsilon^4(p,\tilde{\lambda}_2(p)+\mathrm{i}0))\right] \\ & + \exp\{-\mathrm{i}z_{\mathrm{nucl}}(p)t\}\left[\frac{a}{(\tilde{\lambda}_2(p) - z_1 - \beta^{\mathrm{reg}}(z_1))^2} + O(\varepsilon^4(p,z_1))\right] + \tilde{\varepsilon}(p,t), \end{aligned} \tag{3.24}$$

where

$$\varepsilon(p,z) = \frac{a}{[\tilde{\lambda}_2(p) - z_1 - \beta^{\mathrm{reg}}(z)]^2}. \tag{3.25}$$

The function $\tilde{\varepsilon}(p,t) = O(\|b\|^2)$ is always small, $|\tilde{\varepsilon}(p,t)| \ll 1$. In accordance with Eqs. (2.14) and (2.15) we, hence, obtain for the positions of the poles

$$z_{\mathrm{nucl}}(p) \cong z_1 - \frac{a}{\lambda_2 + 2w\cos p - z_1}, \tag{3.26}$$

$$z_{\mathrm{mol}}(p) \cong \lambda_2 + 2w\cos p + \frac{a}{\lambda_2 + 2w\cos p - z_1}. \tag{3.27}$$

The resonance bands representing the ranges of the functions $z_{\mathrm{nucl}}(p)$ and $z_{\mathrm{mol}}(p)$, with p running through the interval $[-\pi,\pi]$, are schematically depicted in Fig. 2.

The asymptotics (3.24) implies

$$P_{\mathrm{mol}}(\varphi,t) = \int_{-\pi}^{\pi} dp\,|J(p,t)|^2\,|\varphi_2(p)|^2 = \int_{-\pi}^{\pi} dp\,\exp\{-\Gamma_R^{(m)}(p)\,t\}\,|\varphi_2(p)|^2 + \tilde{\varepsilon}(t), \tag{3.28}$$

where

$$\Gamma_R^{(m)}(p) = -2\,\mathrm{Im}\,z_{\mathrm{mol}}(p) \cong -2\,\mathrm{Im}\,\frac{a}{\lambda_2 + 2w\cos p - z_1}. \tag{3.29}$$

The background term $\tilde{\varepsilon}(t)$ in (3.28) is small for any $t\geqslant 0$, $\tilde{\varepsilon}(t)=O(\|b\|^2)$ and $|\tilde{\varepsilon}(t)|\ll 1$.

Further, let us assume that the real part $E_R^{(1)}$ of the ''nuclear'' resonance z_1 belongs to the interval $[\lambda_2-2w,\lambda_2+2w]$, that is $|E_R^{(1)}-\lambda_2|\leqslant 2w$. Then, one can always prepare an initial ''molecular'' state φ which decays via the ''nuclear'' channel with a rate as close as possible to the desired maximal value. Under the assumption (2.8), this maximum is given by

$$\max_{-\pi\leqslant p\leqslant\pi}\Gamma_R^{(m)}(p)\cong 4\frac{\operatorname{Re} a}{\Gamma_R^{(1)}}$$

[cf. formula (2.16)]. The correspondingly prepared ''molecular'' state φ has an almost monochromatic component $\varphi_2(p)$ being localized in a close neighborhood of the quasimomenta

$$p=\pm\arccos\frac{E_R^{(1)}-\lambda_2}{2w}.$$

For example, if the function $\varphi_2(p)$ is nonzero only for quasimomenta p restricted by $|\cos p-(E_R^{(1)}-\lambda_2)/2w|\leqslant\delta\Gamma_R^{(1)}/(4w)$ with some small $\delta>0$, then the width $\Gamma_R^{(m)}$ given by the relation (3.29) varies in an interval lying approximately between $[1/(1+\delta^2)]4\operatorname{Re} a/\Gamma_R^{(1)}$ and $4\operatorname{Re} a/\Gamma_R^{(1)}$.

IV. ''MOLECULAR'' RESONANCES IN A MULTIDIMENSIONAL LATTICE

In this section we consider the case where the ''molecules'' described by the Hamiltonians (2.1) form an infinite N-dimensional crystalline structure. To label the cells of the respective lattice we use the multi-index $i\in\mathbb{Z}^N$, i.e., $i=(i_1,i_2,\ldots,i_N)$ with $i_k=\ldots,-2,-1,0,1,2,\ldots$, $k=1,2,\ldots,N$. The Hilbert space of the system considered is in this case $\mathcal{G}=\oplus_{i\in\mathbb{Z}^N}\mathcal{H}^{(i)}$, where the individual cell spaces are given by (3.1), with $\mathcal{H}_1^{(i)}\equiv\mathcal{H}_1$ and $\mathcal{H}_2^{(i)}\equiv\mathcal{H}_2\equiv\mathbb{C}$ being the spaces introduced in Sec. II. For the components $u^{(i)}\in\mathcal{H}^{(i)}$ of the elements u of the total Hilbert space $\mathcal{G}$ we again use the column representation $u^{(i)}=\binom{u_1^{(i)}}{u_2^{(i)}}$ with $u_1^{(i)}\in\mathcal{H}_1$ and $u_2^{(i)}\in\mathcal{H}_2=\mathbb{C}$. The inner product in $\mathcal{H}$ is defined as $\langle u,v\rangle_{\mathcal{H}}=\Sigma_{i\in\mathbb{Z}^N}\langle u^{(i)},v^{(i)}\rangle_{\mathcal{H}^{(i)}}$. The subspaces $\mathcal{G}_1=\oplus_{i\in\mathbb{Z}^N}\mathcal{H}_1^{(i)}$ and $\mathcal{G}_2=\oplus_{i\in\mathbb{Z}^N}\mathcal{H}_2^{(i)}$, with $\mathcal{G}_1\oplus\mathcal{G}_2=\mathcal{G}$, represent pure nuclear and pure molecular channels, respectively.

The Hamiltonian is defined in $\mathcal{G}$ by the expression

$$(Hu)^{(i)}=Au^{(i)}+\sum_{j\in\mathbb{Z}^n,j\neq i}W(i,j)u^{(j)},\tag{4.1}$$

where the interaction matrices

$$W(i,j)=\begin{pmatrix}w_{11}(i,j) & w_{12}(i,j)\\ w_{21}(i,j) & w_{22}(i,j)\end{pmatrix}$$

consist of the block components $w_{mn}(i,j)$ providing the mappings $\mathcal{H}_n\to\mathcal{H}_m$, $m,n=1,2$. These components describe the direct interaction between the mth and nth channels of the different cells i and j, respectively. The matrices $W(i,j)$ are assumed to be bounded operators in $\mathcal{H}$ which depend only on the difference $i-j=(i_1-j_1,i_2-j_2,\ldots,i_N-j_N)$, i.e., $W(i,j)=W(i-j)$ and, thus, the same holds for the block components, $w_{mn}(i,j)=w_{mn}(i-j)$. Moreover, the series of $W(j)$ is assumed to be convergent with respect to the operator norm topology, i.e.,

$$\sum_{j\in\mathbb{Z}_N,j\neq 0}\|W(j)\|<+\infty\tag{4.2}$$

and the property

$$W(j-i)=[W(i-j)]^*\tag{4.3}$$

is assumed. With such $W(i,j)$ the Hamiltonian (4.1) is a self-adjoint operator on the domain $\mathcal{D}(H)=\oplus_{i\in\mathbb{Z}^N}\mathcal{D}^{(i)}$ with $\mathcal{D}^{(i)}=\mathcal{D}(h_1)\oplus\mathbb{C}$. Note that, since $\mathcal{H}_2=\mathbb{C}$, the quantities $w_{22}(i-j)$ are complex numbers. The $w_{12}(i-j)$ are vectors in $\mathcal{H}_1$, the $w_{21}(i-j)$ are continuous linear forms on $\mathcal{H}_1$, and the $w_{11}(i-j)$ are bounded operators in $\mathcal{H}_1$.

Let us denote by $\mathbb{T}^N$ the Cartesian product $\mathbb{T}^N=\underbrace{\mathbb{T}\times\mathbb{T}\times\ldots\times\mathbb{T}}_{N}$ of the N intervals $\mathbb{T}=[-\pi,\pi]$ and by p the points of $\mathbb{T}^N$, $p=(p_1,p_2,\ldots,p_N)$, $p_k\in\mathbb{T}$. The assumption (4.2) implies that the operator-valued function

$$\Omega(p)=\sum_{j\in\mathbb{Z}_n,j\neq 0} W(j)\exp(\mathrm{i}\langle p,j\rangle),\quad \Omega(p):\mathcal{H}\to\mathcal{H},\quad p\in\mathbb{T}^N, \tag{4.4}$$

where $\langle p,j\rangle=\Sigma_{k=1}^{N}p_kj_k$ is continuous and bounded on $\mathbb{T}^N$. Due to Eq. (4.3), the values

$$\Omega(p)=\begin{pmatrix}\omega_{11}(p) & \omega_{12}(p)\\ \omega_{21}(p) & \omega_{22}(p)\end{pmatrix}$$

of this function represent selfadjoint operators in $\mathcal{H}$ for any $p\in\mathbb{T}^N$, with

$$\omega_{mn}(p):\mathcal{H}_n\to\mathcal{H}_m;\quad [\omega_{11}(p)]^*=\omega_{11}(p),\quad \omega_{22}(p)\in\mathbb{R},\quad \text{and}\quad [\omega_{21}(p)]^*=\omega_{12}(p).$$

The quantity $\tilde{b}(p)=\omega_{12}(p)$ can be considered as a vector of $\mathcal{H}_1$ while $\omega_{21}(p)=\langle\cdot,\tilde{b}(p)\rangle$ [cf. definition (2.1) of the Hamiltonian A].

The blocks $R(j,k;z)$, $R(j,k;z):\mathcal{H}^{(k)}\to\mathcal{H}^{(j)}$, $j,k\in\mathbb{Z}^N$, of the resolvent $R(z)=(H-z)^{-1}$ satisfy the equation

$$(A-z)R(j,k;z)+\sum_{j'\in\mathbb{Z}_N,j'\neq j} W(j-j')R(j',k;z)=\delta_{jk}I. \tag{4.5}$$

After Fourier transformation in $\mathcal{G}$,

$$(Fu)(p)=\frac{1}{(2\pi)^{N/2}}\sum_{j\in\mathbb{Z}^N} u^{(j)}\exp(\mathrm{i}\langle p,j\rangle),\quad p\in\mathbb{T}^N,$$

the system (4.5) takes the form

$$(A-z)R(p,p';z)+\Omega(p)\,R(p,p';z)=\delta(p-p')I, \tag{4.6}$$

where the quasimomenta p,p' run through the set $\mathbb{T}^N$ and $R(p,p';z)$ stands for the transformed resolvent $R(z)$. Thus, the factorization (3.8) holds with

$$G(p;z)=[A+\Omega(p)-z]^{-1}. \tag{4.7}$$

First, let us consider the specific case where intercellular interactions $W(i-j)$ in the Hamiltonian (4.1) have the simple form

$$W(i-j)=\begin{pmatrix}0 & 0\\ 0 & w_{22}(i-j)\end{pmatrix}, \tag{4.8}$$

i.e., where the cells interact with each other only via the molecular channels. Obviously, in this case the factor $G(p;z)$ is still given by (3.9). As compared to this expression the only difference is that now $p\in\mathbb{T}^N$ and

$$\widetilde{M}_2(p;z)=\lambda_2-z+\omega_{22}(p)-\beta(z). \tag{4.9}$$

Let $\omega_{22}^{\min}=\min_{p\in\mathbb{T}^N}\omega_{22}(p)$ and $\omega_{22}^{\max}=\max_{p\in\mathbb{T}^N}\omega_{22}(p)$. Similarly to the analogous assumption in Sec. III we assume that the closed interval $[\lambda_2+\omega_{22}^{\min},\lambda_2+\omega_{22}^{\max}]$ is totally embedded in the absolutely continuous spectrum $\sigma_c(h_1)$ of h_1, and no thresholds of this spectrum belong to $[\lambda_2+\omega_{22}^{\min},\lambda_2+\omega_{22}^{\max}]$. We also assume that this interval belongs to the holomorphy domain $\mathcal{D}$ of the function $\beta(z)$, and that for $\mu\in[\lambda_2+\omega_{22}^{\min},\lambda_2+\omega_{22}^{\max}]$ the inequality (3.4) holds.

Let us consider the time evolution of the system described by the Hamiltonian (4.1) with the simple intercellular interactions (4.8) subject to the above conditions. We start again from a pure molecular state $\varphi=\varphi_1\oplus\varphi_2$, $\|\varphi_n\|\in\mathcal{G}_n$, $n=1,2$, with $\varphi_1=0$ and $\|\varphi\|=\|\varphi_2\|=1$. The probability $P_{\mathrm{mol}}(\varphi,t)$ to find the system at a time $t\geqslant 0$ in the molecular channel is given by the analog of (3.18). As in Sec. III one finds the quasimomentum representation

$$(\mathsf{P}_2R(z)\varphi)(p)=G_{22}(p;z)\varphi_2(p)=\frac{1}{\widetilde{M}_2(p;z)}\,\varphi_2(p),\quad p\in\mathbb{T}^N,$$

and relations (3.21), (3.22) and (3.24) are still valid with the only difference that instead of (3.23) $\widetilde{\lambda}_2(p)$ is now of the form

$$\widetilde{\lambda}_2(p)=\lambda_2+\omega_{22}(p),\quad p\in\mathbb{T}^N.$$

According to Eqs. (2.14) and (2.15) the main terms of the roots $z_{\mathrm{nucl}}(p)$ and $z_{\mathrm{mol}}(p)$ of the function (4.9) in the unphysical sheet read

$$z_{\mathrm{nucl}}(p)\cong z_1-\frac{a}{\lambda_2+\omega_{22}(p)-z_1}, \tag{4.10}$$

$$z_{\mathrm{mol}}(p)\cong\lambda_2+\omega_{22}(p)+\frac{a}{\lambda_2+\omega_{22}(p)-z_1}. \tag{4.11}$$

The asymptotic equation (3.24) now implies

$$P_{\mathrm{mol}}(\varphi,t)=\int_{\mathbb{T}^N}dp\,|J(p,t)|^2\,|\varphi_2(p)|^2=\int_{\mathbb{T}^N}dp\,\exp\{-\Gamma_R^{(m)}(p)t\}|\varphi_2(p)|^2+\widetilde{\varepsilon}(t) \tag{4.12}$$

with

$$\Gamma_R^{(m)}(p)=-2\,\mathrm{Im}\,z_{\mathrm{mol}}(p)\cong-2\,\mathrm{Im}\frac{a}{\lambda_2+\omega_{22}(p)-z_1}.$$

As in Sec. III the background term $\widetilde{\varepsilon}(t)$ is small for any $t\geqslant 0$, $\widetilde{\varepsilon}(t)=O(\|b\|^2)$ and $|\widetilde{\varepsilon}(t)|\ll 1$.

Thus, if the real part $E_R^{(1)}$ of the ''nuclear'' resonance z_1 belongs to the interval $[\lambda_2+\omega_{22}^{\min},\lambda_2+\omega_{22}^{\max}]$ then there are ''molecular'' states φ which decay via the ''nuclear'' channel with a rate as close as possible to the maximal value (2.16). In this case the components $\varphi_2(p)$ are localized in a close neighborhood of the manifold

$$\lambda_2+\omega_{22}(p)=E_R^{(1)} \tag{4.13}$$

in the quasimomentum space $\mathbb{T}^N$. In particular, if the initial state φ is prepared such that the component $\varphi_2(p)$ is nonzero only for the quasimomenta p lying in the domain $|\lambda_2+\omega_{22}(p)-E_R^{(1)}|\leqslant\delta\Gamma_R^{(1)}/2$ with some small $\delta>0$, then one should only integrate over this domain in the

integral (4.12). In such a case, under the condition (2.8), a lower estimate for the decay rate $\Gamma_R^{(m)}$ is given, as in Sec. III, by $[1/(1+\delta^2)]4\,\mathrm{Re}\,a/\Gamma_R^{(1)}$. Thus, by varying δ one can get a rate as close as possible to the maximum (2.16).

Now, let us consider briefly the case of more general intercellular interactions $W(i-j)$ where all the components $\omega_{mn}(p)$, $m,n=1,2$, of the matrix $\Omega(p)$, $p\in\mathbb{T}^N$, can be nontrivial. In this case the component $G_{22}(p;z)$ of the factor (4.7) is given again by Eqs. (3.20) and (4.9). However, the function $\beta(z)$ in (4.9) is to be replaced by the modified function

$$\tilde{\beta}(p;z)=\langle[h_1+\omega_{11}(p)-z]^{-1}[b+\tilde{b}(p)],[b+\tilde{b}(p)]\rangle,$$

where $\tilde{b}(p)=\omega_{12}(p)$. We make the natural assumption that the direct intercellular interactions in nuclear channels $w_{11}(i-j)$ are so weak that the term $\omega_{11}(p)$ produces only a very small perturbation of the initial ''nuclear'' resonance z_1 generated by the Hamiltonian h_1. More precisely, we assume that the resonance $\tilde{z}_1(p)$ generated by the perturbed Hamiltonian $h_1+\omega_{11}(p)$ has the property

$$|\tilde{z}_1(p)-z_1|\ll\Gamma_R^{(1)}\quad\text{for any}\quad p\in\mathbb{T}^N \tag{4.14}$$

and that no other resonances arise in the domain $\mathcal{D}$. Another natural assumption is that the strength of the interactions $w_{12}(i-j)$ and $w_{21}(i-j)$, $i\neq j$, between ''nuclear'' and ''molecular'' channels of different cells is much weaker than the one of a single cell. This is why we can assume $\|\tilde{b}(p)\|/\|b\|\lesssim 1$ and the following features. The elements $\tilde{b}(p)\in\mathcal{H}_1$ are such that for any $p\in\mathbb{T}^n$ the function $\tilde{\beta}(p;z)$ admits an analytic continuation into the domain $\mathcal{D}$ of the unphysical sheet and in $\mathcal{D}$ a representation of the type (2.6) holds for $\tilde{\beta}(p;z)$,

$$\tilde{\beta}(p;z)=\frac{\tilde{a}(p)}{\tilde{z}_1(p)-z}+\tilde{\beta}^{\mathrm{reg}}(p;z), \tag{4.15}$$

with an explicitly separated pole term $\tilde{a}(p)/(\tilde{z}_1(p)-z)$ and a holomorphic remainder $\tilde{\beta}^{\mathrm{reg}}(p;z)$. As in Sec. II B we assume that $|\tilde{a}(p)|=C_a(p)\|b\|^2$, and that for any $p\in\mathbb{T}^N$ the limiting procedure (2.7) is possible for $C_a(p)$ while $\mathrm{Im}\,\tilde{a}(p)\ll\mathrm{Re}\,\tilde{a}(p)$. For the remainder $\tilde{\beta}^{\mathrm{reg}}(p;z)$, $p\in\mathbb{T}^N$, $z\in\mathcal{D}$, the same statements are assumed to be valid as for the function $\beta^{\mathrm{reg}}(z)$. Under these assumptions one can repeat almost literally the study of the probability $P_{\mathrm{mol}}(\varphi,t)$ as performed above in case of the interactions (4.8). We find again that the asymptotics of $P_{\mathrm{mol}}(\varphi,t)$ is given by (4.12) with

$$\Gamma_R^{(m)}(p)\cong -2\,\mathrm{Im}\frac{\tilde{a}(p)}{\lambda_2+\omega_{22}(p)-\tilde{z}_1(p)}.$$

Let us denote by $(\mathrm{Re}\,\tilde{a})_{\max}$ the maximal value of the function $\mathrm{Re}\,\tilde{a}(p)$ on the manifold (4.13). It is obvious that if one prepares the initial pure ''molecular'' state φ such that its component $\varphi_2(p)$ is localized in a close neighborhood of the subset of the manifold (4.13), where $\mathrm{Re}\,\tilde{a}(p)=(\mathrm{Re}\,\tilde{a})_{\max}$, then for the probability $P_{\mathrm{mol}}(\varphi,t)$ the main qualitative result remains practically the same as in case of the interactions (4.8). Namely, varying the support of the component $\varphi_2(p)$ in $\mathbb{T}^N$ one can achieve a decay rate of the state φ as close as possible to the maximal value of the width $\Gamma_R^{(m)}(p)$ in (4.13). The main term $4(\mathrm{Re}\,\tilde{a})_{\max}/\Gamma_R^{(1)}$ of this value is again inversely proportional to the ''nuclear'' width $\Gamma_R^{(1)}$.

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A uniqueness theorem for entanglement measures

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We obtain a mathematically simple characterization of all functionals coinciding with the von Neumann reduced entropy on pure states based on the Khinchin–Faddeev axiomatization of Shannon entropy and give a physical interpretation of the axioms in terms of entanglement. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The characterization and classification of entanglement in quantum mechanics is one of the cornerstones of the emerging field of quantum information theory. This note is devoted to the study of entanglement measures. Entanglement measures are positive real-valued functionals defined on the joint state space of two or more quantum systems (subject to further requirements). A number of entanglement measures have been discussed in the literature, such as the von Neumann reduced entropy, the relative entropy of entanglement,[1] the so-called entanglement of distillation and the entanglement of formation.[2] Several authors proposed physically motivated postulates to characterize entanglement measures (see, e.g., Refs. 1, 3, and 4). These postulates (although they vary from author to author in the details) have in common that they are based on the concepts of the operational formulation of quantum mechanics.[5] Mathematically, the list of postulates for entanglement measures serves as the definition of the notion of entanglement measure. Many authors agree that the only physically reasonable entanglement measure on pure states is given by the von Neumann reduced entropy. Indeed, it is a known fact that there are important entanglement measures which do coincide with the von Neumann reduced entropy on pure states, for instance the relative entropy of entanglement.[1] Accordingly, it is generally seen as a desirable property of the axiomatic characterization of entanglement measures that it allows only for entanglement measures which coincide with the von Neumann reduced entropy on pure states. This point of view is supported by an argument by Popescu and Rohrlich[6] who claimed to have identified a list of physically reasonable axioms which ensure the uniqueness of entanglement measures on pure states. A mathematically exact statement and proof of this *operational* uniqueness theorem remained so far elusive but will be given in a forthcoming paper.[7]

In this paper we present an alternative list of physically reasonable and mathematically simple postulates for entanglement measures such that all entanglement measures satisfying these postulates coincide with the von Neumann reduced entropy on pure states. Mathematically our postulates are just an adaptation of the Khinchin–Faddeev characterization of Shannon entropy[8] and all proofs in this paper are elementary. The main purpose of this paper is not to communicate new mathematical methods but rather that physically the Khinchin-Faddeev postulates admit a natural interpretation in terms of entanglement rather than information or lack of information. What is also interesting about the present result is first that our axiomatization can be formulated without resorting to the mathematical apparatus and the physical concepts of the theory of local quantum operations and second that the technical asymptotic requirements which are so central to the Popescu–Rohrlich argument (see Refs. 6 and 7) can be eliminated as well. It turns out that they can be replaced basically by a single intuitive and comparably weak requirement which fixes the value of entanglement measures on pure states.

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II. PRELIMINARIES

In this section we collect some basic definitions and results which are used in the course of this paper.

In the present paper we restrict ourselves mainly to the situation of a composite quantum system consisting of two subsystems with Hilbert space $\mathcal{H}_1\otimes\mathcal{H}_2$ where $\mathcal{H}_1$ and $\mathcal{H}_2$ denote the Hilbert spaces of the subsystems. The states of the system are identified with the density operators on $\mathcal{H}_1\otimes\mathcal{H}_2$. A density operator is a positive trace class operator with trace one.

Definition 1: Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces of arbitrary dimension. A density operator ρ on the tensor product $\mathcal{H}_1\otimes\mathcal{H}_2$ is called separable *or* disentangled *if there exist a family $\{\omega_i\}$ of positive real numbers, a family $\{\rho_i^{(1)}\}$ of density operators on $\mathcal{H}_1$ and a family $\{\rho_i^{(2)}\}$ of density operators on $\mathcal{H}_2$ such that*

$$\rho=\sum_i \omega_i\rho_i^{(1)}\otimes\rho_i^{(2)}, \tag{1}$$

where the sum converges in trace class norm.

The set of states is a convex set and its extreme points, which are also called *pure states*, are the projection operators. Every pure state obviously corresponds to a unit vector ψ in $\mathcal{H}_1\otimes\mathcal{H}_2$. We denote the projection operator onto the subspace spanned by the unit vector ψ by P_ψ.

The Schmidt decomposition (see also Ref. 9) is of central importance in the characterization and quantification of entanglement associated with pure states.

Lemma 2: Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces of arbitrary dimension and let $\psi\in\mathcal{H}_1\otimes\mathcal{H}_2$. Then there exist a family of non-negative real numbers $\{p_i\}_i$ and orthonormal bases $\{a_i\}_i$ and $\{b_i\}_i$ of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, such that

$$\psi=\sum_i \sqrt{p_i}a_i\otimes b_i.$$

The family of positive numbers $\{p_i\}_i$ is called the family of *Schmidt coefficients* of ψ. For pure states the family of Schmidt coefficients of a state completely characterizes the amount of entanglement of that state. A pure state ψ is separable if and only if $\psi=a\otimes b$ for some $a\in\mathcal{H}_1$ and $b\in\mathcal{H}_2$. With every vector ψ in $\mathcal{H}_1\otimes\mathcal{H}_2$ we associate a closed subspace $M(\psi)$ of $\mathcal{H}_1\otimes\mathcal{H}_2$: let $\psi=\Sigma_i\sqrt{p_i}a_i\otimes b_i$ be the Schmidt decomposition of ψ as in Lemma 2, then $M(\psi)$ is defined as the subspace of $\mathcal{H}_1\otimes\mathcal{H}_2$ spanned by all simple product states $a_i\otimes b_i$ with nonzero Schmidt coefficient in the Schmidt decomposition of ψ. We call $M(\psi)$ the *Schmidt subspace* associated with ψ. The dimension of $M(\psi)$ is called the *Schmidt rank* of ψ. Moreover, we call two states ψ and ϕ *Schmidt orthogonal* if $M(\psi)$ and $M(\phi)$ are orthogonal.

The *von Neumann reduced entropy* for density operators σ on a tensor product Hilbert space $\mathcal{H}_1\otimes\mathcal{H}_2$ is defined as

$$S_{\mathrm{vN}}(\sigma):=-\mathrm{Tr}_{\mathcal{H}_1}(\mathrm{Tr}_{\mathcal{H}_2}\sigma\ln(\mathrm{Tr}_{\mathcal{H}_2}\sigma)), \tag{2}$$

where $\mathrm{Tr}_{\mathcal{H}_1}$ and $\mathrm{Tr}_{\mathcal{H}_2}$ denote the partial traces over $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. In the case of pure states $\sigma=P_\psi$, it can be shown that $-\mathrm{Tr}_{\mathcal{H}_1}(\mathrm{Tr}_{\mathcal{H}_2}P_\psi\ln(\mathrm{Tr}_{\mathcal{H}_2}P_\psi))=-\mathrm{Tr}_{\mathcal{H}_2}(\mathrm{Tr}_{\mathcal{H}_1}P_\psi\ln(\mathrm{Tr}_{\mathcal{H}_1}P_\psi))$ $=-\Sigma_i p_i\ln p_i$ where $\{p_i\}_i$ denotes the family of Schmidt coefficients of ψ. However, for a general mixed state σ we have $\mathrm{Tr}_{\mathcal{H}_1}(\mathrm{Tr}_{\mathcal{H}_2}\sigma\ln(\mathrm{Tr}_{\mathcal{H}_2}\sigma))\neq\mathrm{Tr}_{\mathcal{H}_2}(\mathrm{Tr}_{\mathcal{H}_1}\sigma\ln(\mathrm{Tr}_{\mathcal{H}_1}\sigma))$.

The Khinchin–Faddeev axiomatization of Shannon entropy can be formulated as follows (taken from Ref. 10)

Lemma 3: Let Π denote the set of all probability distributions $(p_1,\ldots,p_n)$ $(p_i\geqslant 0,\Sigma_i p_i=1)$. Let $S:\Pi\to\mathbb{R}$ be a function satisfying

Continuity: $p\mapsto S(p,1-p)$ is continuous on $[0,1]$.

Normalization: $S(1/2,1/2)=\log 2$.

Symmetry: $S(p_{\kappa(1)},\ldots,p_{\kappa(n)})=S(p_1,\ldots,p_n)$ *for all permutations* κ *of* $\{1,\ldots,n\}$.

Recursion: For every $0\leqslant\eta\leqslant 1$ *we have* $S(p_1,\ldots,p_{n-1},\eta p_n,(1-\eta)p_n)=S(p_1,\ldots,p_n)+p_n S(\eta,1-\eta)$.

Then S is equal to the Shannon entropy, i.e., $S(p_1,\ldots,p_n)=-\Sigma_{i=1}^n p_i\log p_i$.

III. KHINCHIN–FADDEEV-TYPE POSTULATES FOR ENTANGLEMENT MEASURES

A. Entanglement measures on pure states

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. For the moment we restrict ourselves to the problem of characterizing entanglement measures defined on pure states, i.e., functionals $E:\mathcal{H}_1\otimes\mathcal{H}_2\to\mathbb{R}^+$. The discussion in this section starts from the question: what are the minimal conditions we want to impose on a mathematically satisfactory measure of entanglement? It is reasonable to require that E is defined and continuous on the tensor product of the Hilbert spaces of any given two systems. Moreover, we have argued above that the sequence of Schmidt coefficients fully characterizes the entanglement of a pure state. Therefore we expect $E(\psi)$ to depend only on the Schmidt coefficients of ψ. Equivalently, we require that for any given system $\mathcal{H}_1\otimes\mathcal{H}_2$ the entanglement measure $E:\mathcal{H}_1\otimes\mathcal{H}_2\to\mathbb{R}^+$ is invariant under unitary operations of the form $U\otimes V$, where U and V are unitaries on $\mathcal{H}_1$ and on $\mathcal{H}_2$, respectively. We also require that E is invariant under embeddings into larger Hilbert spaces.

(P1) An entanglement measure is a positive real-valued functional E which for any given two systems is well defined on the tensor product of the Hilbert spaces of the two systems. For any given two systems corresponding to Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ the function $\mathcal{H}_1\otimes\mathcal{H}_2\ni\psi\mapsto E(\psi)$ is continuous in the norm topology.

(P2) For any given two systems with Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ the function $E:\mathcal{H}_1\otimes\mathcal{H}_2\to\mathbb{R}^+$ satisfies

$$E(U\otimes V\psi)=E(\psi)$$

for all $\psi\in\mathcal{H}_1\otimes\mathcal{H}_2$ and all unitaries U,V acting on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively.

(P3) Whenever $\psi\in\mathcal{H}_1\otimes\mathcal{H}_2\subset\mathsf{H}_1\otimes\mathsf{H}_2$ with embeddings $\mathcal{H}_1\hookrightarrow\mathsf{H}_1$ and $\mathcal{H}_2\hookrightarrow\mathsf{H}_2$ of $\mathcal{H}_1$ and $\mathcal{H}_2$ into larger Hilbert spaces H_1 and H_2, respectively, then $E|_{\mathcal{H}_1\otimes\mathcal{H}_2}(\psi)=E|_{\mathsf{H}_1\otimes\mathsf{H}_2}(\psi)$.

We exclude the identically vanishing functional $E\equiv 0$. It is an immediate consequence of (P2) and (P3), that for every pure state ψ the value $E(\psi)$ does only depend on the nonzero Schmidt coefficients of ψ. We will therefore also write $E(\lambda_1,\ldots,\lambda_n)$ for $E(\psi)$ where $\{\lambda_1,\ldots,\lambda_n\}$ denotes the family of (nonvanishing) Schmidt coefficients of ψ.

Hilbert spaces are linear spaces, and therefore, trivially, all normalized linear combinations of pure states are pure states themselves. Consider for instance $\phi=\Sigma_m\sqrt{p_m}\psi_m$ where $\{p_m\}$ is a probability distribution and where $\psi_m\in\mathcal{H}_1\otimes\mathcal{H}_2$. Naively one might hope that the entanglement $E(\phi)$ of ϕ is a weighted sum of the entanglement of the ψ_m plus the entanglement associated with the superposition $E(p_1,\ldots,p_m)$. It is easy to see that this is not true in general, and that on the contrary superpositions of maximally entangled states can even be unentangled. Mathematically this can be traced back to the fact that the Schmidt spaces of the superimposed states are not orthogonal. Generally, superposing a family $\psi_1,\ldots,\psi_m$ of pure states whose Schmidt spaces are not mutually orthogonal may increase as well as decrease entanglement. However, in the case of superpositions of mutually Schmidt orthogonal pure states no term in the Schmidt decomposition of one state can cancel terms in the Schmidt decomposition of another state. Therefore for the special case of a superposition $\phi=\Sigma_m\sqrt{p_m}\psi_m$ of a family $\{\psi_1,\ldots,\psi_m\}$ of mutually Schmidt orthogonal pure states (where $\{p_1,\ldots,p_m\}$ is a probability distribution), what we expect physically is that the entanglement of the superposed state equals the averaged entanglement of the $\{\psi_i\}$ plus the entanglement $E(p_1,\ldots,p_n)$ associated with the superposition. More formally we require

(P4) Let $\{\psi_1,\ldots,\psi_m\}$ be a family of mutually Schmidt orthogonal pure states and $\{\lambda_1,\ldots,\lambda_m\}$ be a distribution of probability amplitudes, i.e., a sequence of complex numbers with $\Sigma_{i=1}^m|\lambda_i|^2=1$, then

$$E(\lambda_1\psi_1+\cdots+\lambda_m\psi_m)=E(|\lambda_1|^2,\ldots,|\lambda_m|^2)+\sum_{i=1}^{m}|\lambda_i|^2E(\psi_i).$$

We note the following:

Lemma 4: Let E be an entanglement measure on pure states satisfying (P1), (P2), (P3), and (P4). Then $E(\psi)=0$ *for all separable pure states.*

Proof: Let ψ_1,ψ_2 be two separable orthogonal pure states. Then by (P4) $E(1\psi_1+0\psi_2)=E(1,0)=1E(\psi_1)+0E(\psi_2)+E(1,0)$. Thus $E(\psi_1)=0$. □

Lemma 5: The von Neumann reduced entropy S_{vN} *satisfies (P1), (P2), (P3), and (P4).*

Proof: Straightforward. □

We show that the requirements (P1)–(P4) already fix the von Neumann reduced entropy up to a multiplicative constant.

Proposition 6: Let E be an entanglement measure on pure states satisfying the postulates (P1), (P2), (P3), and (P4). Then there exist a positive real constant c such that $E=cS_{\mathrm{vN}}$.

Proof: Let $\psi_1,\ldots,\psi_{n+1}$ be a collection of mutually orthogonal separable pure states and $\{\lambda_1,\ldots,\lambda_n\}$ be a distribution of complex probability amplitudes and $\eta\in[0,1]$. Then

$$\begin{aligned}E(\lambda_1\psi_1+\ldots+\lambda_{n-1}\psi_{n-1}+\sqrt{\eta}\lambda_n\psi_n+\sqrt{1-\eta}\lambda_n\psi_{n+1})\\ =|\lambda_n|^2E(\sqrt{\eta}\psi_n+\sqrt{1-\eta}\psi_{n+1})+(1-|\lambda_n|^2)E\left(\frac{1}{1-|\lambda_n|^2}(\lambda_1\psi_1+\cdots+\lambda_{n-1}\psi_{n-1})\right)\\ +E(|\lambda_n|^2,1-|\lambda_n|^2).\end{aligned}$$

Moreover,

$$\begin{aligned}E(\lambda_1\psi_1+\cdots+\lambda_n\psi_n)=|\lambda_n|^2E(\psi_n)+(1-|\lambda_n|^2)E\left(\frac{1}{1-|\lambda_n|^2}(\lambda_1\psi_1+\cdots+\lambda_{n-1}\psi_{n-1})\right)\\ +E(|\lambda_n|^2,1-|\lambda_n|^2).\end{aligned}$$

Thus

$$E(|\lambda_1|^2,\ldots,|\lambda_{n-1}|^2,\eta|\lambda_n|^2,(1-\eta)|\lambda_n|^2)=E(|\lambda_1|^2,\ldots,|\lambda_n|^2)+|\lambda_n|^2E(\eta,1-\eta).$$

Therefore E considered as a function of the Schmidt coefficients satisfies all conditions of the Khinchin–Faddeev characterization of Shannon's entropy. Therefore $E(p_1,\ldots,p_n)=-c\Sigma_{i=1}^{n}p_i\ln p_i$ for some positive real constant c. □

B. Entanglement measures for mixed states

An entanglement measure on mixed states is a functional defined on the state space of any given two quantum systems. If the Hilbert spaces of the two systems are $\mathcal{H}_1$ and $\mathcal{H}_2$, then the state space is the set of density operators on $\mathcal{H}_1\otimes\mathcal{H}_2$, denoted by $\mathcal{D}(\mathcal{H}_1\otimes\mathcal{H}_2)$. An entanglement measure is then a functional satisfying the obvious generalizations of (P1)–(P3).

(M1) An entanglement measure is a positive real-valued functional E which for any given two systems is well defined on the set of density operators on the tensor product of the Hilbert spaces of the two systems. For any given two systems corresponding to Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ the function $\mathcal{D}(\mathcal{H}_1\otimes\mathcal{H}_2)\ni\rho\mapsto E(\rho)$ is continuous with respect to the trace class norm.

(M2) For any given two systems with Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ the function $E:\mathcal{D}(\mathcal{H}_1\otimes\mathcal{H}_2)\to\mathbb{R}^+$ satisfies

$$E(U\otimes V\rho U^\dagger\otimes V^\dagger)=E(\rho)$$

for all $\rho\in\mathcal{D}(\mathcal{H}_1\otimes\mathcal{H}_2)$ and all unitaries U,V acting on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively.

(M3) whenever $\rho \in \mathcal{D}(\mathcal{H}_1 \otimes \mathcal{H}_2) \subset \mathcal{D}(\mathsf{H}_1 \otimes \mathsf{H}_2)$ with embeddings $\mathcal{H}_1 \hookrightarrow \mathsf{H}_1$ and $\mathcal{H}_2 \hookrightarrow \mathsf{H}_2$ of $\mathcal{H}_1$ and $\mathcal{H}_2$ into larger Hilbert spaces H_1 and H_2 respectively, then $E|_{\mathcal{H}_1 \otimes \mathcal{H}_2}(\rho) = E|_{\mathsf{H}_1 \otimes \mathsf{H}_2}(\rho)$.
Moreover we require that (P4) is satisfied without change and that mixing of states does not increase entanglement.

(M4) Let $\{\psi_1, \ldots, \psi_m\}$ be a family of mutually Schmidt orthogonal pure states and $\{\lambda_1, \ldots, \lambda_m\}$ be a distribution of probability amplitudes, then

$$E(P_\psi) = E(|\lambda_1|^2, \ldots, |\lambda_m|^2) + \sum_{i=1}^{m} |\lambda_i|^2 E(P_{\psi_i}),$$

where $\psi \equiv \lambda_1 \psi_1 + \cdots + \lambda_m \psi_m$ and where P_ψ and P_{ψ_i} denote the projection operators onto the subspace spanned by ψ and ψ_i, respectively.

(M5) Mixing of states does not increase entanglement, i.e., E is convex

$$E(\eta\sigma + (1-\eta)\tau) \leqslant \eta E(\sigma) + (1-\eta) E(\tau)$$

for all $0 \leqslant \eta \leqslant 1$ and all $\sigma, \tau \in \mathcal{D}(\mathcal{H}_1 \otimes \mathcal{H}_2)$.

Lemma 7: Let E be an entanglement measure on mixed states satisfying (M1), (M2), (M3), (M4), and (M5). Then $E(\rho) = 0$ for all separable states ρ.

Proof: By Lemma 4 E vanishes for all separable pure states. Every separable state ρ is a statistical mixture $\rho = \Sigma_{i=1}^{n} p_i P_{\psi_i}$ where $\{\psi_i\}_{i=1}^{n}$ is a family of separable pure states and where $(p_1, \ldots, p_n)$ is a probability distribution with n possibly infinite. Thus, by (M5) and (M1)

$$E(\rho) \leqslant \sum_{i=1}^{n} p_i E(P_{\psi_i}) = 0.$$

Hence $E(\rho) = 0$ for all separable states ρ. □

Example 8: Let H and K be finite dimensional Hilbert spaces. The greatest cross norm on the space of trace class operators $T(\mathsf{H} \otimes \mathsf{K})$ on $\mathsf{H} \otimes \mathsf{K}$ is defined by

$$\|\sigma\|_\gamma := \inf\left\{ \sum_{i=1}^{n} \|x_i\|_1 \|y_i\|_1 \;\middle|\; \sigma = \sum_{i=1}^{n} x_i \otimes y_i \right\}, \tag{3}$$

where $\sigma \in T(\mathsf{H} \otimes \mathsf{K})$, where the infimum runs over all finite decompositions of σ into elementary tensors and where $\|\cdot\|_1$ denotes the trace class norm. For projection operators P_ψ the value of $\|\cdot\|_\gamma$ has been computed in Ref. 11: *$\|P_\psi\|_\gamma = (\Sigma_i \sqrt{p_i})^2$ where $\{p_i\}$ denotes the family of Schmidt coefficients of the unit vector ψ. The entanglement measure introduced in Ref. 11,*

$$E(\sigma) \equiv \|\sigma\|_\gamma \ln \|\sigma\|_\gamma,$$

does not satisfy (P4).

IV. DISCUSSION

In this work we gave a mathematical characterization of all functionals defined on the state space of composite quantum systems which coincide with von Neumann reduced entropy on pure states: a functional on pure states coincides with the von Neumann reduced entropy if and only if it satisfies the conditions (P1)–(P4). Mathematically the axioms (P1)–(P4) are just a version of the Khinchin–Faddeev characterization of Shannon entropy but physically we have seen that they admit an interpretation in terms of entanglement.

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On the eigenproblems of $\mathcal{PT}$-symmetric oscillators

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We consider the non-Hermitian Hamiltonian $H=-d^2/dx^2+P(x^2)-(ix)^{2n+1}$ on the real line, where $P(x)$ is a polynomial of degree at most $n\geqslant 1$ with all non-negative real coefficients (possibly $P\equiv 0$). It is proved that the eigenvalues λ must be in the sector $|\arg\lambda|\leqslant \pi/(2n+3)$. Also for the cubic case $H=-d^2/dx^2-(ix)^3$, we establish a zero-free region of the eigenfunction u and its derivative u' and we find some other interesting properties of eigenfunctions. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1366328]

I. INTRODUCTION

We are considering the eigenproblem

$$-u''(x)+[P(x^2)-(ix)^{2n+1}]u(x)=\lambda u(x), \quad \text{for } -\infty<x<\infty, \tag{1}$$

with $u(\pm\infty)=0$, where $P(x)$ is a polynomial of degree at most $n\geqslant 1$ with all non-negative real coefficients (possibly $P\equiv 0$).

This is an example of a class of problems, the so-called $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian problems, which have arisen in recent years in a number of physical contexts.[1–3] Bessis conjectured the following in 1995.

Conjecture: *Eigenvalues of $H=-d^2/dx^2-(ix)^3$ are all real and positive.*

Many numerical and asymptotic results[4–7] support this conjecture. And later for $n>1$ it was conjectured that the equation (1) also has positive real eigenvalues, under different boundary conditions.[8] However, there is no rigorous proof of this to date.

This paper is organized as follows: In Sec. II, we prove that eigenvalues of the equation (1) lie in the sector

$$|\arg\lambda|\leqslant\frac{\pi}{2n+3}.$$

This goes part way to proving that the eigenvalues are real and positive. We generalize this result to $H=-d^2/dx^2+[P(x^2)+ixQ(x^2)]$ for some real polynomials P and Q. In particular, for the potentials $-(ix)^3$ and x^2+igx^3 with any real g, we have that $|\arg\lambda|\leqslant\pi/5$. Then next in Sec. III, for the case $H=-d^2/dx^2-(ix)^3$, we fairly precisely locate the zeros of the eigenfunctions and their first derivatives in the complex plane. Conversely we find a large zero-free region. In Sec. IV, still with $H=-d^2/dx^2-(ix)^3$, we find a large class of polynomials that are orthogonal to $|u|^2$ on each horizontal line. And finally in the last section, we discuss related open problems.

For the rest of the Introduction, we provide some more background information on (1). First, a $\mathcal{PT}$-symmetric Hamiltonian is a Hamiltonian which is invariant under the product of the parity operation $\mathcal{P}(:x\mapsto -x)$ and the time reversal operation $\mathcal{T}(:i\mapsto -i)$. Certainly (1) is $\mathcal{PT}$-symmetric while, for example, $-d^2/dx^2+x-(ix)^3$ is not $\mathcal{PT}$-symmetric. If $H=-d^2/dx^2+V(x)$ is $\mathcal{PT}$-symmetric, then $\overline{V(-x)}=V(x)$ (an overbar denotes the complex conjugate) and so $\mathrm{Re}\,V(x)$ is an even function and $\mathrm{Im}\,V(x)$ is an odd function. Hence if $V(x)$ is a polynomial, then $V(x)=P(x^2)+ixQ(x^2)$ for some real polynomials P and Q.

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Next by the work of Caliceti *et al.*,[9,10] it is known that the $\mathcal{PT}$-symmetric Hamiltonian $H=-d^2/dx^2+x^2-g(ix)^3$ has a discrete spectrum, for g real, and these eigenvalues are positive real if g is small enough. However, there are some $\mathcal{PT}$-symmetric Hamiltonians that have no eigenvalues,[11] or nonreal eigenvalues.[12]

Last, for any $\lambda\in\mathbb{C}$ there are two linearly independent solutions of (1), if the boundary conditions are not imposed. In generic cases, the solutions blow up at both $+\infty$ and $-\infty$, while in exceptional cases, the solutions decay to zero as x approaches $+\infty$ or $-\infty$. Only in very exceptional cases (when λ is an eigenvalue!) one does find a solution that decays to zero at both $+\infty$ and $-\infty$ (see Lemma 1 for details).

II. THE EIGENVALUES LIE IN A SECTOR

In this section, we prove that the eigenvalues λ of (1) lie in the sector $|\arg\lambda|\leqslant\pi/2n+3$ and we extend this result for more general cases. To do this we will use results in Sec. 7.4 of Hille.[13]

A. Definitions and set-up

For any $\lambda\in\mathbb{C}$ Eq. (1) without the boundary conditions allows two linearly independent solutions. Also if $u(x)$ solves the ODE (1), then since $P(z^2)-(iz)^{2n+1}$ is an entire function (analytic in the whole complex plane), there exists an entire function $u(z)$ which agrees with $u(x)$ on the real line and satisfies $-u''(z)+[P(z^2)-(iz)^{2n+1}]u(z)=\lambda u(z)$. Now we begin by describing the asymptotic behavior of u near infinity. Recall that deg $P\leqslant n$.

Definition: Let

$$\theta_j=2\pi\frac{j}{2n+3}-\frac{\arg(i^{2n+1})}{2n+3}=\begin{cases}\dfrac{2\pi j-\dfrac{\pi}{2}}{2n+3}, & \text{if } n \text{ is even;}\\[2ex] \dfrac{2\pi j+\dfrac{\pi}{2}}{2n+3}, & \text{if } n \text{ is odd.}\end{cases}$$

We define *Stokes regions*,

$$S_j=\{z\in\mathbb{C}:\theta_j<\arg z<\theta_{j+1}\},$$

for $j=0,1,2,\ldots,2n+2$. And for notational convenience, we define $S_{j+2n+3}=S_j$ for all j. Also we denote

$$S_{j,\epsilon}=\{z\in\mathbb{C}:\theta_j+\epsilon<\arg z<\theta_{j+1}-\epsilon\},$$

for $0<\epsilon<\pi/(2n+3)$.

Notice θ_j is neither 0 nor π. Thus the negative and the positive real axes lie within two of the Stokes regions (see Fig. 1). We call these the *left-* and the *right-hand* Stokes regions, respectively. Also we call the rays $\{\arg z=\theta_j\}$ ''critical rays.''

Lemma 1: Every solution of $-u''(z)+[P(z^2)-(iz)^{2n+1}]u(z)=\lambda u(z)$ *is asymptotic to*

$$(\text{const})z^{-(2n+1)/4}\exp\left[\pm\frac{2}{2n+3}(iz)^{(2n+3)/2}(1+o(1))\right], \tag{2}$$

as $z\to\infty$ *in* $S_{j,\epsilon}$, *for each* $0<\epsilon<\pi/(2n+3)$. *The error* $o(1)$ *is uniform in* $\arg z$ *in the sense that* $\lim_{r\to\infty}\sup\{|o(1)|:z\in S_{j,\epsilon},|z|=r\}=0$.

Also u *has infinitely many zeros in* $\mathbb{C}$ *but only finitely many in* $\cup_j S_{j,\epsilon}$, *for each* $0<\epsilon<\pi/(2n+3)$.

The asymptotic expressions imply in particular that in each Stokes region, $u(z)$ either decays to 0 or blows up, as z approaches infinity in $S_{j,\epsilon}$.

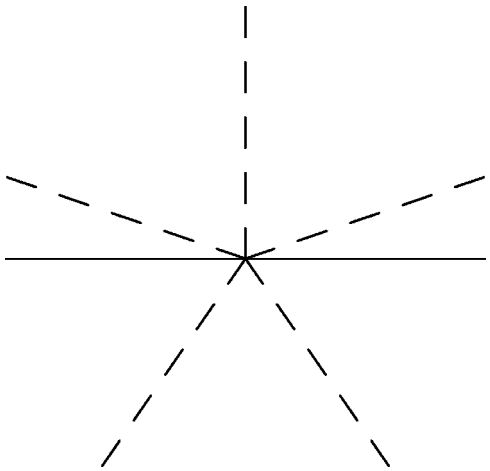

FIG. 1. For $n=1$; the solid line is the real axis and the dotted rays are the critical rays, $\arg z=\theta_j=\pi/10$, $\pi/2$, $9\pi/10$, $13\pi/10$ and $17\pi/10$.

Proof: See Sec. 7.4 of Hille[13] for a proof of a more general result. An outline of the proof is as follows: Hille first transforms the equation into another complex Z-plane by using the Liouville transform. And then he compares u with the solutions of the sine equation $w''(Z)+w(Z)=0$ and finally transforms back to the original complex z-plane. The above asymptotic expressions are the asymptotic expressions for solutions of the sine equation (in the Z-variable) expressed in terms of the original z-variable. The Stokes regions are determined by the Liouville transformation.

Also one can deduce the last assertion of this lemma from Sec. 7.4 of Hille.[13] This is proved in Theorem 5 of Gundersen[14] for more general equations. □

Remark 1: Under the Liouville transformation, a neighborhood of infinity in each Stokes region in the complex z-plane maps to a neighborhood of infinity in either the upper or lower half Z-plane. Thus if u decays in a Stokes region S_j for some j, then u must blow up in the Stokes regions S_{j+1} and S_{j-1}. Otherwise, there would be a solution of the sine equation in the Z-plane which decays to zero in all directions. This is a contradiction. However, u might blow up in many consecutive Stokes regions (even in all Stokes regions) (see Sec. 7.4 of Hille[13]).

Definition: Let $\lambda \in \mathbb{C}$ and let $u(z)\not\equiv 0$ be an analytic function on $\mathbb{C}$ that satisfies (1). We say u is an *eigenfunction* and λ is an *eigenvalue*, for (1), if $u(z)$ decays to zero along rays to infinity in the left- and right-hand Stokes regions [that is, if u has decaying asymptotics in (2), in these two regions].

Remark 2: Given a Stokes region S_j, there always exists a solution of $-u''(z)+[P(z^2)-(iz)^{2n+1}]u(z)=\lambda u(z)$ that blows up in S_j by Sec. 7.4 of Hille.[13] If there were two linearly independent eigenfunctions with the same eigenvalue, then all the solutions of $-u''(z)+[P(z^2)-(iz)^{2n+1}]u(z)=\lambda u(z)$ would satisfy $u(\pm\infty+0i)=0$ and there would be no solutions that blow up in the left- and right-hand Stokes regions. Thus there are no repeated eigenvalues, and all eigenvalues are simple.

Remark 3: Note that if $u(z)$ is an eigenfunction with eigenvalue λ, then $\overline{u}(-\overline{z})$ is an eigenfunction with eigenvalue $\overline{\lambda}$. If an eigenvalue is real then $u(z)=c\overline{u}(-\overline{z})$ by Remark 2, and clearly $|c|=1$. Writing $c=e^{-2i\phi}$ and replacing u by $e^{i\phi}u$, we get that eigenfunctions with real eigenvalues are symmetric with respect to the imaginary axis.

B. The main results

The main result of this paper is the following.

Theorem 2: *If λ is an eigenvalue of (1), then, $\lambda\neq 0$ and $|\arg\lambda|\leqslant \pi/(2n+3)$.*

According to Mezincescu,[11] that the eigenvalues have a positive real part was known already;[15] our proof below includes a very simple argument for this fact. In the proof and elsewhere, we will use the following.

Since $u(z)$ decays exponentially along rays to infinity in the left- and right-hand Stokes regions, so does u' by the Cauchy integral formula. Therefore $p(r)|u(re^{i\theta})|^2$ and $p(r)|u'(re^{i\theta})|^2$ are integrable along the line $\{re^{i\theta}: -\infty<r<\infty\}$ for any polynomial $p(r)$, provided $|\theta|<\pi/2(2n+3)$ (if $|\theta|$ is larger than this, then one end of the line will be outside the decaying Stokes regions).

Proof of Theorem 2: Let u be an eigenfunction with eigenvalue λ, so that

$$u''(z)+[-P(z^2)+(iz)^{2n+1}]u(z)=-\lambda u(z),$$

where $P(z)=\Sigma_{k=0}^{n}a_k z^k$ for some $a_k\geqslant 0$, $k=0,1,2,\ldots,n$.

Write

$$\lambda=\alpha+i\beta, \quad \alpha,\beta\in\mathbb{R}.$$

Fix θ with $|\theta|<\pi/2(2n+3)$ and let $v(r)=u(re^{i\theta})$. Then $v'(r)=u'(re^{i\theta})e^{i\theta}$ and $v''(r)=u''(re^{i\theta})e^{2i\theta}$. Thus our ODE becomes

$$v''(r)+\{[\alpha+i\beta-P(r^2e^{2i\theta})]e^{2i\theta}+i^{2n+1}r^{2n+1}e^{i(2n+3)\theta}\}v(r)=0.$$

Then we multiply this by $e^{-i(2n+3)\theta}\overline{v(r)}$, integrate and use integration by parts to obtain

$$e^{-i(2n+3)\theta}\int_{-\infty}^{\infty}|v'|^2\,dr=(\alpha+i\beta)e^{-i(2n+1)\theta}\int_{-\infty}^{\infty}|v|^2\,dr-\int_{-\infty}^{\infty}e^{-i(2n+1)\theta}P(r^2e^{2i\theta})|v|^2\,dr$$

$$+i^{2n+1}\int_{-\infty}^{\infty}r^{2n+1}|v|^2\,dr, \tag{3}$$

for all $|\theta|<\pi/2(2n+3)$. We note that for these θ the line $re^{i\theta}$ stays in the left- and right-hand Stokes regions where u (and hence u') decays exponentially to zero as r approaches $\pm\infty$.

Taking the real part of (3) yields [since $|\theta|<\pi/2(2n+3)$]

$$0<\cos(2n+3)\theta\int_{-\infty}^{\infty}|v'|^2\,dr$$

$$=\{\alpha\cos(2n+1)\theta+\beta\sin(2n+1)\theta\}\int_{-\infty}^{\infty}|v|^2\,dr-\int_{-\infty}^{\infty}\mathrm{Re}[e^{-i(2n+1)\theta}P(r^2e^{2i\theta})]|v|^2\,dr. \tag{4}$$

But $\mathrm{Re}[e^{-i(2n+1)\theta}P(r^2e^{2i\theta})]=\Sigma_{k=0}^{n}a_k r^{2k}\cos(2n-2k+1)\theta\geqslant 0$ if $a_k\geqslant 0$ and $|\theta|<\pi/2(2n+1)$ [certainly true if $|\theta|<\pi/2(2n+3)$]. Thus it follows from (4) that

$$\alpha\cos(2n+1)\theta+\beta\sin(2n+1)\theta>0,$$

for all $|\theta|<\pi/2(2n+3)$. That is,

$$\alpha>|\beta|\tan(2n+1)\theta,$$

for all $0\leqslant\theta<\pi/2(2n+3)$.

Then with $\theta=0$ we have $\alpha>0$, in particular $\lambda\neq 0$ and by letting $\theta\to\pi/2(2n+3)$ we get

$$\alpha\geqslant|\beta|\tan\frac{(2n+1)\pi}{2(2n+3)}.$$

Finally using $\tan\phi=\cot(\pi/2-\phi)$, we conclude that

$$\tan\frac{\pi}{2n+3}\geqslant\frac{|\beta|}{\alpha}.$$

That is, $|\arg\lambda|\leqslant\pi/(2n+3)$. □

Remark 4: We can extend Theorem 2 by allowing P to have some negative coefficients as long as P satisfies $\mathrm{Re}[e^{-i(2n+1)\theta}P(r^2e^{2i\theta})]\geqslant 0$ for $|\theta|<\pi/2(2n+3)$. For example, with $n=3$ and $c\in\mathbb{R}$, let $P(z)=z^3+cz^2+z$; then $\mathrm{Re}[e^{-7i\theta}P(r^2e^{2i\theta})]=r^2[r^4\cos\theta+cr^2\cos(3\theta)+\cos(5\theta)]$. Thus if $c^2\cos^2(3\theta)-4\cos\theta\cos(5\theta)\leqslant 0$ for $|\theta|<\pi/18$, i.e., $|c|\leqslant\sqrt{\frac{16}{3}}\cos(\pi/18)\cos(5\pi/18)\approx 1.837$, then $\mathrm{Re}[e^{-7i\theta}P(r^2e^{2i\theta})]\geqslant 0$. Therefore, the theorem holds for this P provided $c\geqslant-\sqrt{\frac{16}{3}}\cos(\pi/18)\cos(5\pi/18)$.

Also by a simple change of variables, we get the same result for $H=-d^2/dz^2+[P(z^2)-g(iz)^{2n+1}]$ for any nonzero real g.

Moreover, by translations in $\mathbb{C}$, we have the same result for $H=-d^2/dz^2+P((z-\xi)^2)-gi^{2n+1}(z-\xi)^{2n+1}$ for any $\xi\in\mathbb{C}$. For instance, if u solves $u''(z)-iz^3u(z)=-\lambda u(z)$, then $v(z)=u(z+ai)$ solves $v''(z)+[(3az^2-a^3)-iz(z^2-3a^2)]v(z)=-\lambda v(z)$ for any real number a. Observe that v still satisfies the boundary conditions $v(\pm\infty+0i)=u(\pm\infty+ai)=0$.

Remark 5: The readers should notice that our boundary conditions are different, for $n\geqslant 2$, from those Bender *et al.*[8] take. Bender *et al.*[8] impose the zero boundary conditions of the problems $-u''-(iz)^Nu=\lambda u$ for $N\geqslant 4$ not on Stokes regions containing the real axis but instead on Stokes regions which are near the negative imaginary axis for large N.

The next theorem extends Theorem 2.

Theorem 3: *Let $\lambda\in\mathbb{C}$ and $n\geqslant 1$. Suppose that u solves the ODE,*

$$u''-[P(z^2)+izQ(z^2)]u=-\lambda u,\quad u(\pm\infty+0i)=0, \tag{5}$$

for some real polynomials $P(z)=\Sigma_{k=0}^{n}a_kz^k$ and $Q(z)=\Sigma_{k=0}^{n}b_kz^k$ with all non-negative a_k and with $b_n\in\mathbb{R}-\{0\}$. If for all $k<n$ the coefficients a_k,b_k satisfy

$$\frac{\sin^2(2n-2k)\theta}{\cos(2n-2k+1)\theta\cos(2n-2k-1)\theta}b_k^2\leqslant\begin{cases}4a_ka_{k+1}, & \text{if } n=1 \text{ and } k=0;\\ 2a_ka_{k+1}, & \text{if } n>1 \text{ and } k=0,\ n-1;\\ a_ka_{k+1}, & \text{if } n>1 \text{ and } 1\leqslant k\leqslant n-2;\end{cases} \tag{6}$$

at $\theta=\pi/2(2n+3)$, then $|\arg\lambda|\leqslant\pi/(2n+3)$.

For $n=3$, the coefficients of b_k^2 in (6) are approximately 3.41,0.74 and 0.14 for $k=0,1,2$, respectively.

Theorem 3 contains Theorem 2, just by taking $b_k=0$ for $k=0,1,\ldots,n-1$ [in which case (6) is trivially satisfied].

Proof: The main idea of the proof is the same as that of the proof of Theorem 2. Even if the equation (5) is little different from the equation for (2), Stokes regions for (5) are the same as for (2) [if b_n has the same sign as $(-1)^{n+1}$] or else are rotated by 180° (if b_n has the opposite sign). See Sec. 7.4 of Hille[13] for details. Thus in either case, the lines $r\mapsto re^{i\theta}$ with $|\theta|<\pi/2(2n+3)$ lie within the left- and right-hand Stokes regions, where we impose the zero boundary conditions. And this gives the integrabilities in the proof.

Let $v(r)=u(re^{i\theta})$. Then like we derived (4) in the proof of Theorem 2 we have

$$\{\alpha\cos(2n+1)\theta+\beta\sin(2n+1)\theta\}\int_{-\infty}^{\infty}|v|^2\,dr$$

$$=\int_{-\infty}^{\infty}\{\cos[(2n+3)\theta]|v'|^2+\Sigma_{k=0}^{n}a_k\cos[(2n-2k+1)\theta]r^{2k}|v|^2$$

$$+\Sigma_{k=0}^{n-1}b_k\sin[(2n-2k)\theta]r^{2k+1}|v|^2\}dr,\quad \text{for } |\theta|<\frac{\pi}{2(2n+3)}. \tag{7}$$

Since $a_k\geqslant 0$ for all k, we get $\alpha>0$ by letting $\theta=0$ in (7). (This is true for any Q with real coefficients and deg $Q=n$.)

If we find conditions on a_k and b_k such that

$$\Sigma_{k=0}^{n}a_k\cos[(2n-2k+1)\theta]r^{2k}+\Sigma_{k=0}^{n-1}b_k\sin[(2n-2k)\theta]r^{2k+1}\geqslant 0, \tag{8}$$

for every $r\in\mathbb{R}$ and $|\theta|<\pi/2(2n+3)$, then it follows from (7) with $\theta\to\pm\pi/2(2n+3)$, that

$$\alpha\cos\frac{(2n+1)\pi}{2(2n+3)}\pm\beta\sin\frac{(2n+1)\pi}{2(2n+3)}\geqslant 0.$$

Therefore, $|\arg\lambda|\leqslant\pi/(2n+3)$ as desired, like in the proof of Theorem 2.

When $n\geqslant 3$, we can rewrite the expression in (8) as

$$\left\{a_0\cos(2n+1)\theta+rb_0\sin 2n\theta+r^2\frac{a_1}{2}\cos(2n-1)\theta\right\}$$

$$+\Sigma_{k=1}^{n-2}\left\{\frac{a_k}{2}\cos(2n-2k+1)\theta+rb_k\sin(2n-2k)\theta+r^2\frac{a_{k+1}}{2}\cos(2n-2k-1)\theta\right\}r^{2k}$$

$$+\left\{\frac{a_{n-1}}{2}\cos 3\theta+rb_{n-1}\sin 2\theta+r^2a_n\cos\theta\right\}r^{2n-2}. \tag{9}$$

Now (9) is non-negative if each quadratic in r has a nonpositive discriminant:

$$b_0^2\sin^2 2n\theta-2a_0a_1\cos(2n+1)\theta\cos(2n-1)\theta\leqslant 0,$$

$$b_k^2\sin^2(2n-2k)\theta-a_ka_{k+1}\cos(2n-2k+1)\theta\cos(2n-2k-1)\theta\leqslant 0,\quad \text{for } 1\leqslant k\leqslant n-2,$$

$$b_{n-1}^2\sin^2 2\theta-2a_{n-1}a_n\cos 3\theta\cos\theta\leqslant 0,$$

which is (6). The coefficients of b_k^2 in (6) are all increasing functions of $0\leqslant\theta<\pi/2(2n+3)$, and so it suffices that (6) hold at $\theta=\pi/2(2n+3)$.

Now when $n=1,2$, it is easy to see similarly that the theorem holds. This completes the proof. □

Remark 6: In (7), the sign of $\int_{-\infty}^{\infty}r^{2k+1}|v|^2\,dr$ is difficult to determine because r can be negative as well as positive. However, we were able to estimate the right-hand side of (7) by using properties of quadratic functions. Certainly, as it is clear from the proof, the conditions in Theorem 3 are sufficient but not necessary. For example, in the proof of Theorem 2 we used $a_k=a_k/2+a_k/2$ to get (9) from (7). If we use $a_k=\delta_ka_k+(1-\delta_k)a_k$ for some $0<\delta_k<1$, we will obtain new sufficient conditions for the theorem.

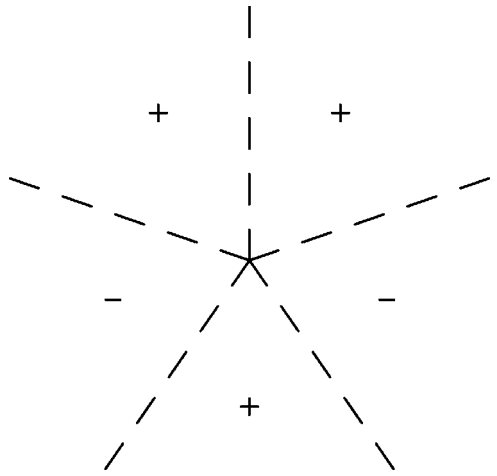

FIG. 2. In this figure, rays are $\arg z = \pi/10,\ \pi/2,\ 9\pi/10,\ 13\pi/10$ and $17\pi/10$. A ''+'' indicates that the eigenfunction is blowing up while a ''−'' indicates that the eigenfunction is decaying to zero as z approaches infinity.

III. THE ZERO-FREE REGION FOR u AND u', FOR THE CUBIC POTENTIAL

The results in the previous section are based on the eigenfunction u decaying to zero as z approaches infinity on the left- and the right-hand Stokes regions. Hence consideration of the *finite* zeros of u may be useful for further results on our eigenproblem.

For the next two sections, we will suppose $H = -d^2/dz^2 - (iz)^3$. See Fig. 2 for the asymptotic behavior of the eigenfunction u. In this section, we provide a zero-free region for the eigenfunction u of

$$u'' - iz^3 u = -\lambda u, \quad \text{with } u(\pm\infty + 0i) = 0, \tag{10}$$

and for its derivative u'. And we give some answers on how zeros of the eigenfunction should be arranged in $\mathbb{C}$.

It is obvious that u and u' do not share a common zero. Otherwise, by (10), all the derivatives of u and u itself would vanish at zero, and so $u \equiv 0$.

The following lemma is needed for our argument. Recall $\lambda = \alpha + i\beta$.

Lemma 4: Let $z:[c,d] \to \mathbb{C}$ be a smooth curve with $z'(t) \neq 0$ for $t \in [c,d]$. If u solves (10), then writing $z(t) = x(t) + iy(t)$,

$$\operatorname{Re}(u'\overline{u})\big|_{z(c)}^{z(d)} = \int_c^d x' |u_x(z(t))|^2\, dt + \int_c^d [x' \operatorname{Re}(iz^3(t) - \lambda) - y' \operatorname{Im}(iz^3(t) - \lambda)] |u(z(t))|^2\, dt, \tag{11}$$

and

$$\operatorname{Im}(u'\overline{u})\big|_{z(c)}^{z(d)} = -\int_c^d y' |u_x(z(t))|^2\, dt + \int_c^d [y' \operatorname{Re}(iz^3(t) - \lambda) + x' \operatorname{Im}(iz^3(t) - \lambda)] |u(z(t))|^2\, dt. \tag{12}$$

Hille calls this lemma the Green's transform,[13] and he uses it to get information on zero-free regions of solutions of linear second order equations (mainly with coefficient functions that are real on the real line).

Proof: Let $f(t) = u(z(t))$ for $t \in [c,d]$. Then $f'(t) = z'(t)u'(z(t))$ and

$$\left(\frac{f'(t)}{z'(t)}\right)' = z'(t)u''(z(t)) = z'(t)[iz^3(t) - \lambda] f(t).$$

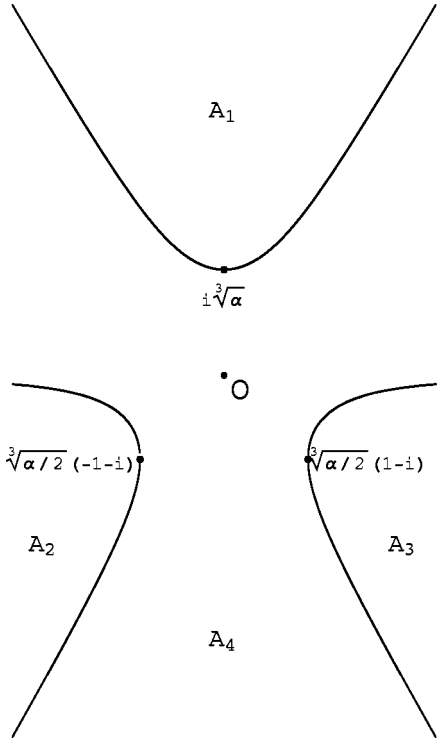

FIG. 3. The level curves $\mathrm{Re}(iz^3-\lambda)=0$. Here $\mathrm{Re}(iz^3-\lambda)$ is negative in A_4 since $\alpha>0$, while it is positive in A_1, A_2 and A_3.

Hence by integration by parts,

$$\left(\frac{f'(t)}{z'(t)}\right)\overline{f}(t)\Big|_c^d=\int_c^d\frac{|f'|^2}{z'}dt+\int_c^d z'[iz^3-\lambda]|f|^2\,dt. \tag{13}$$

Now by the formula $f'(t)=z'(t)u'(z(t))$ and splitting real and imaginary parts of the above, we get the lemma. □

Now we examine the consequences of this lemma. First, if $\mathrm{Re}(u'\overline{u})$ were not one-to-one on the imaginary axis, that would imply that the eigenvalue would be real by (11) with $z(t)=it$.

Remark 7: Second, another immediate consequence of Lemma 4 is that on any vertical line segments on which $\mathrm{Im}(iz^3-\lambda)$ does not change its sign, $\mathrm{Re}(u_x\overline{u})$ as a function of y is one-to-one. On horizontal line segments on which $\mathrm{Im}(iz^3-\lambda)$ does not change its sign, $\mathrm{Im}(u_x\overline{u})$ as a function of x is one-to-one (Mezincescu[11] observed this last fact on the real axis, where $y\equiv 0$). These observations are special cases of Theorem 11.3.3 of Hille.[13]

A. Case of nonreal eigenvalues

Next, let us define open regions A_j and B_j, $j=1,2,3,4$ as in Figs. 3 and 4. The following two theorems provide a large zero-free region for an eigenfunction u of (10) and its derivative u', assuming λ is nonreal. Perhaps these theorems might help show that λ must actually be real. The underlying ideas of the proofs are taken from Sec. 11.3 of Hille's book.[13]

Theorem 5: *If* $\beta:=\mathrm{Im}\,\lambda>0$ *then* $\mathrm{Im}(u'\overline{u})<0$ *on*

$$B_1\cup\{z\in B_4:\mathrm{Re}\,z\leqslant-\sqrt[3]{\beta/2}\}\cup\{z\notin A_1:\mathrm{Im}\,z\geqslant-\sqrt[3]{\beta/2}\};\quad \text{see Fig. 5.}$$

Mezincescu[11] has previously observed that the eigenfunction has no zeros on the real axis, which obviously lies in the shaded region of Fig. 5. Moreover, we see that all the zeros of u and u' in $\mathrm{Im}\,z\geqslant 0$ must be in A_1.

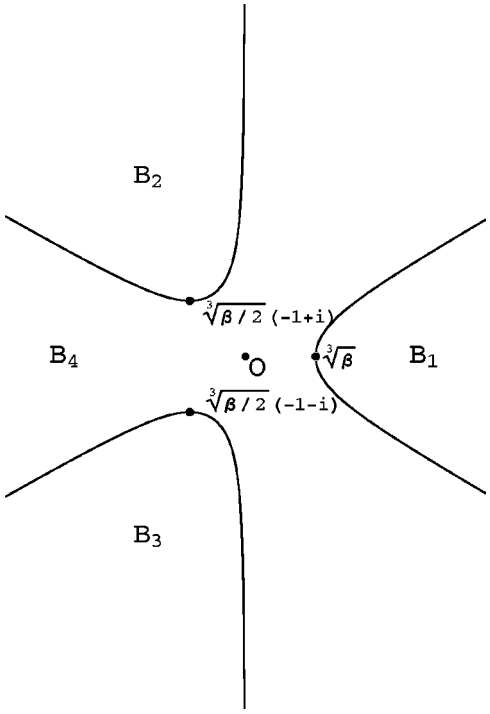

FIG. 4. The level curves $\mathrm{Im}(iz^3-\lambda)=0$ with $\beta>0$ fixed. Here $\mathrm{Im}(iz^3-\lambda)$ is negative in B_4 while it is positive in B_1, B_2 and B_3.

Note that the lowest point in the closure $cl(B_2)$ of B_2 is $-\sqrt[3]{\beta/2}+i\sqrt[3]{\beta/2}$.

Proof of Theorem 5: For any fixed $y_0\in\mathbb{R}$, by (12) with $z(t)=t+iy_0$ and by $u(\pm\infty+iy_0)=0=u'(\pm\infty+iy_0)$, it follows that

$$\mathrm{Im}[u'(x+iy_0)\overline{u}(x+iy_0)]=\int_{-\infty}^{x}\mathrm{Im}(iz(t)^3-\lambda)|u|^2\,dt,$$

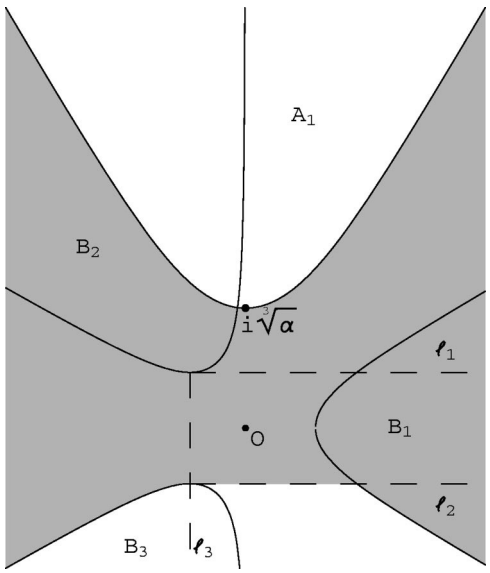

FIG. 5. $\mathrm{Im}(u'\overline{u})<0$ in the shaded area. The lines l_1,l_2,l_3 are $l_1:\mathrm{Im}\,z=\sqrt[3]{\beta/2}$, $l_2:\mathrm{Im}\,z=-\sqrt[3]{\beta/2}$ and $l_3:\mathrm{Re}\,z=-\sqrt[3]{\beta/2}$.

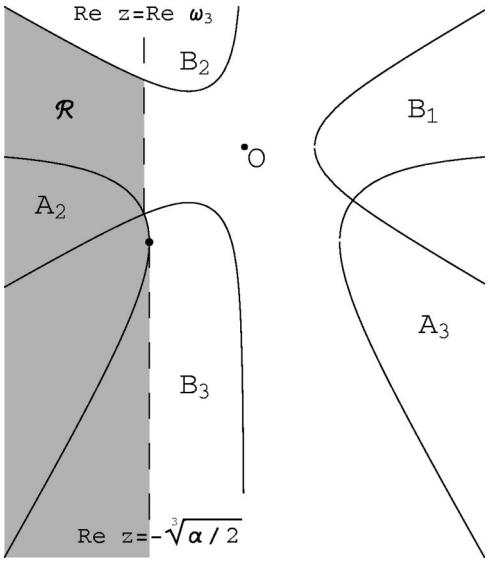

FIG. 6. $\mathrm{Re}(u'\overline{u})>0$ in the shaded area.

and this is negative for $x+iy_0\in B_4$ with $|y_0|\leqslant\sqrt[3]{\beta/2}$, because then $z(t)=t+iy_0\in B_4$ for all $-\infty<t<x$ and so $\mathrm{Im}(iz(t)^3-\lambda)<0$.

This argument also implies that $\mathrm{Im}(u'\overline{u})<0$ in $\{z\in B_4:\mathrm{Re}\,z\leqslant-\sqrt[3]{\beta/2}\}$; see Fig. 5.

Similarly in B_1, for all y_0 we have that $\mathrm{Im}(u'\overline{u})=-\int_x^\infty\mathrm{Im}(iz(t)^3-\lambda)|u(t+iy_0)|^2\,dt<0$.

For $z\notin A_1$ with $\mathrm{Im}\,z\geqslant\sqrt[3]{\beta/2}$ (so that $z\in A_4$), we use (12) along vertical line segments starting from points on the line $\mathrm{Im}\,z=\sqrt[3]{\beta/2}$ to conclude that $\mathrm{Im}(u'\overline{u})<0$ in this region. □

Note that $\mathrm{Im}(u'\overline{u})=-\frac{1}{2}(\partial/\partial y)|u(x+iy)|^2$. Hence in the region in Theorem 5, $|u(x+iy)|$ is an increasing function of y.

Theorem 6: *Assume* $\beta>0$. *Then*

(i) $\mathrm{Re}(u'\overline{u})>0$ *on the union of the regions* A_2, *the region below* A_2 *and the region* $\mathcal{R}\subset B_4$ *between* A_2 *and* B_2 *with the real part less than or equal to that of the zero* ω_3 *of* $iz^3-\lambda$ *in the third quadrant. See Fig. 6.*

(ii) $\mathrm{Re}(u'\overline{u})<0$ *on the union of the regions* A_3, *the region below* A_3 *and the region in* B_1 *with the real part greater than or equal to that of the zero* ω_4 *of* $iz^3-\lambda$ *in the fourth quadrant. See Fig. 7.*

Obviously $iz^3-\lambda$ has three zeros. When $\beta>0$, one of the zeros is in the second quadrant, one ω_3 in the third and one ω_4 in the fourth quadrant. Certainly these are the three points at which the boundaries of the A_i and B_i intersect.

Theorem 2 with $n=1$ shows that $|\beta|/\alpha\leqslant\tan(\pi/5)\approx0.73$. And it is easy to see that the rightmost point of $cl(A_2)$ is $\sqrt[3]{\alpha/2}\,(-1-i)$, at which $\mathrm{Im}(iz^3-\lambda)=x^3-3xy^2-\beta>0$ by $0<\beta<\alpha$. Thus the rightmost point of $cl(A_2)$ lies inside B_3 as shown in Fig. 6. Similarly, the leftmost point of $cl(A_3)$ is $\sqrt[3]{\alpha/2}\,(1-i)$, at which $\mathrm{Im}(iz^3-\lambda)=x^3-3xy^2-\beta<0$. Hence the leftmost point of $cl(A_3)$ lies outside B_1 as shown in Fig. 7.

Proof of Theorem 6: In regions A_2 and A_3, we use (11) with horizontal lines to infinity to get the statements in parts (i) and (ii) of this theorem. In the region $\mathcal{R}$ between A_2 and B_2 with the real part less than or equal to that of the zero ω_3 of $iz^3-\lambda$ in the third quadrant (see Fig. 6), we use (11) with vertical lines $z(t)=x_0+it$ to show that $\mathrm{Re}(u'\overline{u})>0$. That is, we use $\mathrm{Re}(u'\overline{u})|_{x_0+ic}^{x_0+id}$ $=-\int_c^d\mathrm{Im}(iz(t)^3-\lambda)|u(x_0+it)|^2\,dt$. If $x_0+id\in\mathcal{R}$, we can find $x_0+ic\in cl(A_2\cap B_3^c)$, so that $\mathrm{Re}\,[u'(x_0+ic)\overline{u}(x_0+ic)]>0$, and $-\mathrm{Im}(iz(t)^3-\lambda)>0$. Hence, the above integral is an increasing function of d. Therefore we have the desired result in this region $\mathcal{R}$.

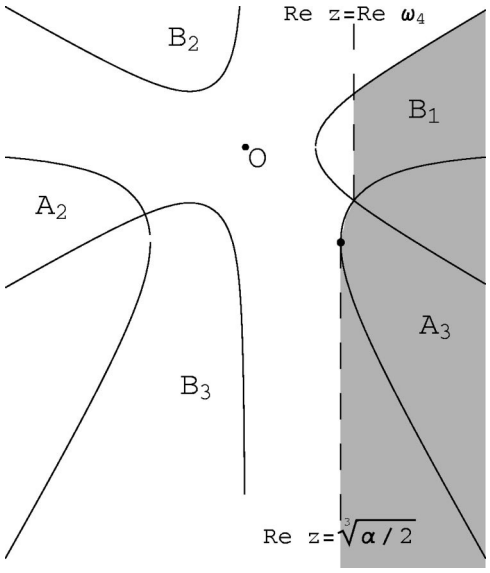

FIG. 7. $\mathrm{Re}(u'\overline{u})<0$ in the shaded area.

The region below A_2 is contained in B_3 since the rightmost point of $cl(A_2)$ lies in B_3 (see Fig. 6). Thus a similar argument implies that $\mathrm{Re}(u'\overline{u})>0$ in the region below A_2. Also, the region below A_3 is contained in B_4 (see Fig. 7) and so modified arguments show that the other statements of this theorem in part (ii) hold. □

Corollary 7: When $\mathrm{Im}\,\lambda=\beta>0$, *the zero-free region of u and u′ contains the union of the three shaded regions in Figs. 5, 6 and 7.*

Note that in case $\mathrm{Im}\,\lambda=\beta<0$ we can get similar theorems corresponding to the above two, since $\overline{u}(-\overline{z})$ is an eigenfunction with eigenvalue $\overline{\lambda}$. The regions involved are simply the reflections of the above with respect to the imaginary axis.

B. Case of real eigenvalues

In case $\beta=0$, so that λ is real and $\lambda=\alpha>0$, the regions B_1,B_2,B_3 degenerate to the sectors $\{-\pi/6<\arg z<\pi/6\},\{\pi/2<\arg z<5\pi/6\},\{-5\pi/6<\arg z<-\pi/2\}$, respectively, and we obtain the following theorem on zero-free regions.

Theorem 8: *Suppose* λ *is real. Then* $\mathrm{Im}(u'\overline{u})<0$ *on* $\{-\pi/6\leqslant\arg z\leqslant 7\pi/6\}-A_1$ (*which is a degenerate case of Fig. 5), while* $\mathrm{Re}(u'\overline{u})$ *behaves as in Figs. 6 and 7 with* B_1,B_2,B_3 *being sectors as above*.

Also $\mathrm{Re}(u'\overline{u})<0$ *in* $cl(A_1)\cap\{\mathrm{Re}\,z<0\}$ *and* $\mathrm{Re}(u'\overline{u})>0$ *in* $cl(A_1)\cap\{\mathrm{Re}\,z>0\}$.

Corollary 9: When λ *is real, the zero-free region of u and u′ contains the union of all regions in Theorem 8; see Fig. 8. That is, u and u′ can only have zeros in* $\{iy:y>\sqrt[3]{\lambda}\}$

$$\cup\left\{z\in A_4:-\frac{5\pi}{6}<\arg z<-\frac{\pi}{6},\mathrm{Im}\,z>-\sqrt[3]{\lambda/2}\right\}\cup\{z:|\mathrm{Re}\,z|<\sqrt[3]{\lambda/2},\mathrm{Im}\,z\leqslant-\sqrt[3]{\lambda/2}\}.$$

Remark 8: Bender *et al.*[16] find numerically that u has some zeros along an ''arch'' within the unshaded region in Fig. 8, when λ is real.

In proving Theorem 8, we will use the following lemma.

Lemma 10: Suppose $\zeta\in A_1$, $\mathrm{Re}(u'\overline{u})=0$ at ζ. *Then* $\mathrm{Re}(u'\overline{u})<0$ *at all* $\zeta-t\in A_1,t>0$ *and* $\mathrm{Re}(u'\overline{u})>0$ *at all* $\zeta+t\in A_1,t>0$.

Note that there is no restriction on the sign of $\mathrm{Im}\,\lambda$, in this lemma.

Proof: On horizontal line segments $z(t)=t+iy_0$ in A_1, (11) becomes

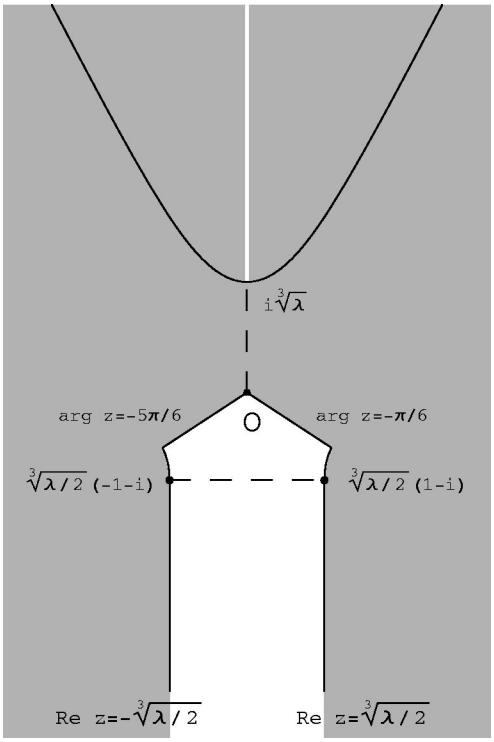

FIG. 8. When λ is real, the shaded area is the zero-free region of u and u'.

$$\mathrm{Re}(u'\overline{u})\Big|_{c+iy_0}^{d+iy_0}=\int_c^d |u_x(z(t))|^2\,dt+\int_c^d \mathrm{Re}(iz^3(t)-\lambda)|u(z(t))|^2\,dt.$$

Since $\mathrm{Re}(iz^3(t)-\lambda)>0$ in A_1, $\mathrm{Re}(u'\overline{u})$ is a strictly increasing function of x on each horizontal line segment in A_1. □

Proof of Theorem 8: The proofs of Theorems 5 and 6 give everything except the last statement of the theorem. For that, recall that we can take $u(z)=\overline{u}(-\overline{z})$ by Remark 3; this implies that $\mathrm{Re}(u'\overline{u})$ is an odd function with respect to reflection in the imaginary axis, and so $\mathrm{Re}(u'\overline{u})=0$ on the whole imaginary axis. Now we use Lemma 10 to complete the proof. □

C. Arrangement of the zeros

In the previous two subsections, we find zero-free regions of eigenfunctions and their first derivatives. We now examine the locations of zeros of such functions. For this purpose, mainly we will use Lemma 4 and make use of Fig. 2.

By the last statement of Lemma 1, in the sector $S_{-1,\pi/20}$ that contains the negative imaginary axis, the eigenfunction u has only finitely many zeros. Now with the zero-free region in Corollaries 7 and 9, we see that u has only finitely many zeros in $\mathrm{Im}\,z<0$. Since u has infinitely many zeros, u has infinitely many zeros in $\mathrm{Im}\,z\geqslant 0$. When $\beta>0$ (hence when $\beta<0$ as well), by Theorem 5, u must have infinitely many zeros in A_1. Also when $\beta=0$, by Theorem 8, u has infinitely many zeros on the positive imaginary axis.

The next theorem gives some information on how zeros of u and u' in A_1 should be arranged, when $\beta>0$. Note that all the zeros of u and u' in $\mathrm{Im}\,z\geqslant 0$ lie in A_1 by Theorem 5.

Theorem 11: *Suppose $u(z)$ is an eigenfunction of (10) with eigenvalue $\lambda\in\mathbb{C}$, with $\mathrm{Im}\,\lambda=\beta>0$. Then*

(i) $\mathrm{Re}(u'\overline{u})\geqslant 0$ *for some point on the imaginary axis if and only if* uu' *has infinitely many zeros in* $A_1\cap B_2$ *and at most finitely many zeros in* $A_1\cap B_2^c$; *and*

(ii) $\mathrm{Re}(u'\overline{u})<0$ *for every point on the imaginary axis if and only if* uu' *has no zeros in* $\{z\in A_1:\mathrm{Re}\,z\leqslant 0\}$ *and infinitely many in* $\{z\in A_1:\mathrm{Re}\,z>0\}$.

We will use the following lemma along with Lemma 10.

Lemma 12: Assume $\mathrm{Im}\,\lambda=\beta>0$. *Suppose* $\mathrm{Re}\,\zeta_1\leqslant\mathrm{Re}\,\zeta_2$ *and* $\mathrm{Re}(u'\overline{u})=0$ *at* ζ_1, ζ_2 (*where* $\zeta_1\neq\zeta_2$). *Then*

(i) $\zeta_1,\zeta_2\in cl(A_1\cap B_2)\Rightarrow \mathrm{Re}\,\zeta_1<\mathrm{Re}\,\zeta_2$ *and* $\mathrm{Im}\,\zeta_1<\mathrm{Im}\,\zeta_2$, *and*

(ii) $\zeta_1,\zeta_2\in cl(A_1\cap B_2^c)\Rightarrow \mathrm{Re}\,\zeta_1<\mathrm{Re}\,\zeta_2$ *and* $\mathrm{Im}\,\zeta_1>\mathrm{Im}\,\zeta_2$.

Proof of part (i): We will first prove this for $\zeta_1,\zeta_2\in A_1\cap B_2$. Suppose that $\mathrm{Re}\,\zeta_1=\mathrm{Re}\,\zeta_2$. Then we could find a vertical line segment $z(t)$ in $A_1\cap B_2$ whose end points are ζ_1 and ζ_2. We now apply (11) to this line segment to get

$$0=-\int_c^d \mathrm{Im}(iz^3(t)-\lambda)|u(z(t))|^2\,dt.$$

This would imply $u\equiv 0$ on the curve $z(t)$ since $\mathrm{Im}(iz^3(t)-\lambda)>0$ in B_2. Then since u is analytic, $u\equiv 0$ in $\mathbb{C}$. This is a contradiction. Hence $\mathrm{Re}\,\zeta_1<\mathrm{Re}\,\zeta_2$.

Similarly, suppose that $\mathrm{Im}\,\zeta_1\geqslant\mathrm{Im}\,\zeta_2$. Then we could find a smooth curve $z(t)=x(t)+iy(t)$ in $A_1\cap B_2$ such that $z(c)=\zeta_1$, $z(d)=\zeta_2$, $x'(t)>0$ and $y'(t)\leqslant 0$. Note that $\mathrm{Im}(iz^3(t)-\lambda)>0$ and $\mathrm{Re}(iz^3(t)-\lambda)>0$ in $A_1\cap B_2$. This contradicts (11) like for the case of $\mathrm{Re}\,\zeta_1=\mathrm{Re}\,\zeta_2$. We now see that the above argument still holds for $\zeta_1,\zeta_2\in cl(A_1\cap B_2)$.

Proof of part (ii): We use (11) again and a similar argument like in the proof of part (i). □

Proof of Theorem 11: Suppose $u(z)$ is an eigenfunction of (10) with eigenvalue $\lambda\in\mathbb{C}$, with $\mathrm{Im}\,\lambda=\beta>0$. Since u has infinitely many zeros in A_1 (by the paragraph shortly before Theorem 11), certainly uu' also has infinitely many zeros in A_1.

Proof of part (i): Suppose that $\mathrm{Re}(u'\overline{u})\geqslant 0$ for some point iy_0 on the imaginary axis. From (11) with $z(t)=it$, it follows that

$$\mathrm{Re}(u'\overline{u})|_{ic}^{id}=\beta\int_c^d |u(it)|^2\,dt. \tag{14}$$

Since $\beta>0$, $\mathrm{Re}(u'\overline{u})>0$ at every point iy for $y>y_0$. Now by Lemma 10, we obtain that $\mathrm{Re}(u'\overline{u})>0$ at every $x+iy\in A_1$ for $y>y_0$ and $x\geqslant 0$. Thus uu' does not have any zeros in $\{z\in A_1\cap B_2^c:\mathrm{Re}\,z\geqslant 0,\mathrm{Im}\,z>y_0\}$.

The entire function uu' does not have infinitely many zeros in any bounded region. If uu' had infinitely many zeros in $A_1\cap B_2^c$, then uu' would have infinitely many zeros in $\{z\in A_1\cap B_2^c:\mathrm{Re}\,z<0\}$ (see Fig. 9). But if uu' has a zero z_1 in $\{z\in A_1\cap B_2^c:\mathrm{Re}\,z<0\}$, then by Lemma 12 (ii), uu' has no zeros in $\{z\in A_1\cap B_2^c:\mathrm{Re}\,z_1\leqslant\mathrm{Re}\,z<0\}$. This requires that uu' would have infinitely many zeros in a bounded region. This is a contradiction. Thus uu' has infinitely many zeros in $A_1\cap B_2$ and at most finitely many zeros in $A_1\cap B_2^c$.

Conversely, suppose that uu' has infinitely many zeros in $A_1\cap B_2$ and at most finitely many zeros in $A_1\cap B_2^c$. Choose a zero z_0 in $A_1\cap B_2$. Then it follows from Lemma 10 that $\mathrm{Re}(u'\overline{u})>0$ at $i\,\mathrm{Im}\,z_0$ since $\mathrm{Re}\,z_0<0$.

Proof of part (ii): Suppose that $\mathrm{Re}(u'\overline{u})<0$ for every point on the imaginary axis. Then by Lemma 10, $\mathrm{Re}(u'\overline{u})<0$ for every point in $\{z\in A_1:\mathrm{Re}\,z\leqslant 0\}$. This implies that uu' has no zeros in $\{z\in A_1:\mathrm{Re}\,z\leqslant 0\}$. Now since we know that uu' has infinitely many zeros in A_1, uu' must have infinitely many zeros in $\{z\in A_1:\mathrm{Re}\,z>0\}$.

Conversely, suppose that $\mathrm{Re}(u'\overline{u})\geqslant 0$ for some point on the imaginary axis. Then uu' would have at most finitely many zeros in $\{z\in A_1:\mathrm{Re}\,z>0\}$ by the argument as in the proof of part (i). This completes the proof. □

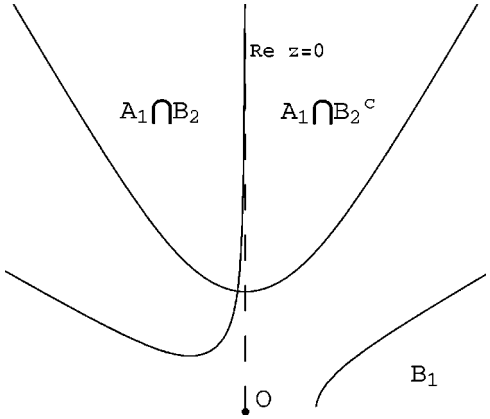

FIG. 9. The relative positions of $A_1 \cap B_2$, $A_1 \cap B_2^c$ and the imaginary axis with $\beta > 0$.

Remark 9: Since the negative imaginary axis is in the middle of a blowing-up Stokes region (see Fig. 2), $u(iy)$ blows up as y tends to $-\infty$. On the other hand, the positive imaginary axis is a critical ray. We can show that $|u(iy)|^2 \leqslant (\text{const}) y^{-3/2}$ for all y near positive infinity, by Theorem 7.4.4 of Hille.[13]

Since the right-hand side of (14) approaches $+\infty$ as c tends to $-\infty$ (while d is fixed), we see that $\mathrm{Re}[u'(ic)\overline{u}(ic)] < 0$ for all c near negative infinity. However, the right-hand side of (14) is convergent as d tends to $+\infty$ (while c is fixed). Thus $\mathrm{Re}(u'\overline{u})$ may or may not become positive near infinity along the positive imaginary axis.

The next lemma gives some information on the locations of zeros of u and u' in $\mathrm{Im}\, z < 0$, if any exist. There can only be finitely many such zeros of u, by the paragraph shortly before Theorem 11. One can show that u' also has at most finitely many zeros in $\mathrm{Im}\, z < 0$. Indeed, using (12) along each vertical half-line in the Stokes region containing the negative imaginary axis, one can show that $\mathrm{Im}(u'\overline{u}) = 0$ at some point z_0 on each vertical half-line in $\mathrm{Im}\, z < 0$ by an argument similar to that in Remark 9. This with the next lemma implies that uu' has at most finitely many zeros in $\mathrm{Im}\, z < 0$.

Lemma 13: Assume $\mathrm{Im}\,\lambda = \beta \geqslant 0$. *Suppose* $\mathrm{Im}\,\zeta_1 \leqslant \mathrm{Im}\,\zeta_2$ *and* $\mathrm{Im}(u'\overline{u}) = 0$ *at* ζ_1, ζ_2 *(where* $\zeta_1 \neq \zeta_2$*). Then*

(i) $\zeta_1, \zeta_2 \in cl(A_4 \cap B_3) \Rightarrow \mathrm{Im}\,\zeta_1 < \mathrm{Im}\,\zeta_2$ *and* $\mathrm{Re}\,\zeta_1 < \mathrm{Re}\,\zeta_2$, *and*

(ii) $\zeta_1, \zeta_2 \in cl(A_4 \cap B_4) \Rightarrow \mathrm{Im}\,\zeta_1 < \mathrm{Im}\,\zeta_2$ *and* $\mathrm{Re}\,\zeta_1 > \mathrm{Re}\,\zeta_2$.

Proof: We omit the proof because it is very similar to the proof of Lemma 12. We use (12) instead of (11), and also make use of Figs. 6 and 7. □

Roughly speaking, then, the zeros move up and to the right in the third quadrant, and down and to the right in the fourth quadrant. This observation supports that when λ is real, zeros of u in $\mathrm{Im}\, z < 0$ lie on an arch-shaped curve as in Figs. 5 and 6 of the paper by Bender *et al.*[16]

IV. OTHER PROPERTIES OF EIGENFUNCTIONS

In this section, we present a possible way of proving the conjecture that the eigenvalues λ of $H = -d^2/dz^2 - (iz)^3$ are positive real. Given an eigenfunction u with eigenvalue λ, Theorem 14 below gives a class $\mathcal{O}$ of polynomials $p(x,y)$ which are orthogonal to $|u|^2$ in the sense that $\int_{-\infty}^{\infty} p(x,y)|u(x+iy)|^2\, dx = 0$ for all y. One can perhaps prove the conjecture as follows. Suppose $\mathrm{Im}\,\lambda \neq 0$; if $\mathcal{O}$ is large enough then $|u|^2 \equiv 0$, giving a contradiction, so that $\mathrm{Im}\,\lambda = 0$.

Let u be an eigenfunction of $H = -d^2/dz^2 - (iz)^3$ with eigenvalue $\lambda = \alpha + i\beta$.

Theorem 14: *Let* $\mathcal{O} = \{\text{polynomials } p(\cdot,\cdot) : \int_{-\infty}^{\infty} p(x,y)|u(x+iy)|^2\, dx = 0 \text{ for all } y\}$. *Then:*

(i) $x^3 - 3xy^2 - \beta \in \mathcal{O}$,

(ii) for all $m \geqslant 0$,

$$\tilde{p}(x,y) := \frac{4}{m+1}\left(\frac{x^{m+5}}{m+5} - 3y^2\frac{x^{m+3}}{m+3} - \beta\frac{x^{m+2}}{m+2}\right)(x^3 - 3y^2x - \beta) - m(m-1)x^{m-2}$$
$$-4x^m(3x^2y - y^3 + \alpha) - \frac{12}{m+1}yx^{m+2} \in \mathcal{O},$$

(iii) if $p \in \mathcal{O}$ *then* $p_y + 2(x^3 - 3xy^2 - \beta)\int_0^x p(t,y)\,dt \in \mathcal{O}$, *and*
(iv) if $p \in \mathcal{O}$ *then* $p_{xx} + p_{yy} + 12x^2yp + 4(x^3 - 3xy^2 - \beta)\int_0^x p_y(t,y)\,dt \in \mathcal{O}$.

For example the following polynomials are in $\mathcal{O}$:

$$p_3(x,y) = x^3 - 3xy^2 - \beta, \text{ by } (i),$$

$$p_7(x,y) = x^7 - 9x^5y^2 - 5x^4\beta + 18x^3y^4 + 18x^2y^2\beta + 4x(\beta^2 - 3y),$$

by applying (iii) to p_3 and multiplying by 2,

$$p_8(x,y) = 2x^8 - 16x^6y^2 - 7x^5\beta + 30x^4y^4 + 25x^3y^2\beta + 5x^2(\beta^2 - 12y) + 10y^3 - 10\alpha,$$

by applying (ii) with $m = 0$ and multiplying by $\frac{5}{2}$,

$$p_9(x,y) = 2x^9 - 15x^7y^2 - 6x^6\beta + 27x^5y^4 + 4x^3(\beta^2 - 27y) + 24xy^3 + 21x^4y^2\beta - 24x\alpha,$$

by applying (ii) with $m = 1$ and multiplying by 6, and

$$p_{10}(x,y) = 20x^{10}y - 144x^8y^3 - 55x^7y\beta + 252x^6y^5 + 189x^5y^3\beta + x^4(-1680y^2 + 35y\beta^2)$$
$$-35x^3\beta + x^2(420y^4 - 420y\alpha) + 105xy^2\beta + 35\beta^2 - 210y,$$

by applying (iv) to p_8 and multiplying by $\frac{7}{2}$.

We do not know whether Theorem 14 generates all the polynomials in $\mathcal{O}$.

Proof of Theorem 14: It is useful to have the following two formulas, which follow from multiplying (10) by $\overline{u}$ and separating real and imaginary parts:

$$\mathrm{Im}[u_x(x+iy)\overline{u}(x+iy)]_x = (x^3 - 3xy^2 - \beta)|u(x+iy)|^2 \tag{15}$$

and

$$\mathrm{Re}[u_x(x+iy)\overline{u}(x+iy)]_x = |u_x|^2 + (-3x^2y + y^3 - \alpha)|u|^2. \tag{16}$$

Also, it can be shown that the exponential decay of u and its derivatives at $\pm\infty + iy$ allows us to differentiate through the integrals that follow.

Proof of part (i): This is clear by integrating (15), using the zero boundary conditions in the left- and right-hand Stokes regions.

Proof of part (ii): Suppose m is a non-negative integer. Then

$$\frac{d^2}{dy^2}\int_{-\infty}^{\infty} x^m|u|^2\,dx = \frac{d}{dy}\int_{-\infty}^{\infty} x^m\frac{\partial}{\partial y}|u|^2\,dx$$

$$= -2\frac{d}{dy}\int_{-\infty}^{\infty} x^m\,\mathrm{Im}(u_x\overline{u})dx$$

$$= \frac{2}{m+1}\frac{d}{dy}\int_{-\infty}^{\infty} x^{m+1}\,\mathrm{Im}(u_x\overline{u})_x dx \quad \text{by integration by parts,} \tag{17}$$

$$= \frac{2}{m+1}\frac{d}{dy}\int_{-\infty}^{\infty} x^{m+1}(x^3-3xy^2-\beta)|u|^2\,dx, \quad \text{by (15)}$$

$$= \frac{2}{m+1}\int_{-\infty}^{\infty}[-2(x^{m+4}-3x^{m+2}y^2-\beta x^{m+1})\mathrm{Im}(u_x\overline{u})-6x^{m+2}y|u|^2]dx$$

$$= \frac{2}{m+1}\int_{-\infty}^{\infty} 2\left(\frac{x^{m+5}}{m+5}-3y^2\frac{x^{m+3}}{m+3}-\beta\frac{x^{m+2}}{m+2}\right)(x^3-3xy^2-\beta)|u|^2\,dx$$

$$-\frac{12}{m+1}\int_{-\infty}^{\infty} x^{m+2}y|u|^2\,dx, \tag{18}$$

where the last step is by integration by parts and (15).

Also we have

$$\frac{d^2}{dy^2}\int_{-\infty}^{\infty} x^m|u|^2\,dx = -2\int_{-\infty}^{\infty} x^m[\mathrm{Re}(u_x\overline{u})_x-2|u_x|^2]dx, \quad \text{by differentiating through (17);} \tag{19}$$

$$= -2\int_{-\infty}^{\infty} x^m[(-3x^2y+y^3-\alpha)|u|^2-|u_x|^2]dx, \quad \text{by (16);} \tag{20}$$

$$= -m(m-1)\int_{-\infty}^{\infty} x^{m-2}|u|^2\,dx+4\int_{-\infty}^{\infty} x^m|u_x|^2\,dx, \tag{21}$$

where the last step is from (19) with integration by parts.

Now use (21) to eliminate $\int_{-\infty}^{\infty} x^m|u_x|^2\,dx$ from (20), and then equate the resulting expression to (18). This yields $\int_{-\infty}^{\infty}\tilde{p}(x,y)|u|^2\,dx=0$, which is (ii).

Proof of part (iii): Suppose that $\int_{-\infty}^{\infty} p(x,y)|u|^2\,dx=0$ for all y. Then

$$0 = \frac{d}{dy}\int_{-\infty}^{\infty} p(x,y)|u|^2\,dx$$

$$= \int_{-\infty}^{\infty}[p_y(x,y)|u|^2-2p(x,y)\mathrm{Im}(u_x\overline{u})]dx$$

$$= \int_{-\infty}^{\infty}\left[p_y(x,y)|u|^2+2\left\{\int_0^x p(t,y)dt\right\}\mathrm{Im}(u_x\overline{u})_x\right]dx, \tag{22}$$

by integration by parts. This with (15) gives (iii).

Proof of part (iv): Suppose $\int_{-\infty}^{\infty} p(x,y)|u|^2\,dx=0$ for all y. Then we differentiate through (22) with respect to y again to get

$$
\begin{aligned}
0 &= \int_{-\infty}^{\infty} [p_{yy}(x,y)|u|^2 - 4p_y(x,y)\mathrm{Im}(u_x\overline{u}) - 2p(x,y)\mathrm{Im}(iu_{xx}\overline{u} - i|u_x|^2)]dx \\
&= \int_{-\infty}^{\infty} \left[p_{yy}(x,y)|u|^2 + 4\left\{ \int_0^x p_y(t,y)dt \right\} \mathrm{Im}(u_x\overline{u})_x - 2p(x,y)(\mathrm{Re}(u_x\overline{u})_x - 2|u_x|^2) \right] dx \\
&= \int_{-\infty}^{\infty} \left[p_{yy}(x,y) + 4\left\{ \int_0^x p_y(t,y)dt \right\} (x^3 - 3xy^2 - \beta) \right] |u|^2\, dx - 2\int_{-\infty}^{\infty} p(x,y)[-\mathrm{Re}(u_x\overline{u})_x \\
&\quad + 2(-3x^2y + y^3 - \alpha)|u|^2]dx, \quad \text{by (15) and (16);} \\
&= \int_{-\infty}^{\infty} \left[p_{yy}(x,y) + 4\left\{ \int_0^x p_y(t,y)dt \right\} (x^3 - 3xy^2 - \beta) - 4p(x,y)(-3x^2y + y^3 - \alpha) \right] |u|^2\, dx \\
&\quad - \int_{-\infty}^{\infty} p_x(x,y) 2\,\mathrm{Re}(u_x\overline{u})dx.
\end{aligned}
$$

But $(y^3-\alpha)\int_{-\infty}^{\infty} p|u|^2\,dx = 0$, and so applying integration by parts again to the last term gives (iv). □

Corollary 15: Let $u(z)$ be an eigenfunction of (2). Then $\int_{-\infty}^{\infty}|u(x+iy)|^2\,dx$ is a convex function.

Proof: This is a consequence of (21) with $m=0$, or it can be proved using the subharmonicity of $|u|^2$. □

V. CONCLUSIONS

Using path integrations, we were able to prove that eigenvalues of (1) lie in the sector $|\arg\lambda| \leqslant \pi/(2n+3)$ and we extended the result for some more general Hamiltonians. Also we provided zero-free regions of eigenfunctions and their first derivatives, for the potential $-(ix)^3$. Then finally we had the set $\mathcal{O}$ of polynomials $p(x,y)$ which are orthogonal to $|u|^2$ in the sense that $\int_{-\infty}^{\infty} p(x,y)|u|^2\,dx = 0$ for all y.

In a recent communication with Mezincescu, he pointed out that for the potential $-(ix)^3$, the formula (13) with $z(t) = y_0 + (t - y_0\cos\theta)e^{i\theta}$ together with the harmonic oscillator inequality implies $\alpha \geqslant \max_{0<\theta<\pi/10}\{|\beta|\sin 3\theta + 5(\cos 5\theta/12)^{3/5}\}/\cos 3\theta$. This is a slight improvement over our estimate $|\arg\lambda| \leqslant \pi/5$, and gives an almost sharp lower bound of 1.1258 on the real part of the first eigenvalue for the potential $-(ix)^3$ (numerically $\lambda_1 \approx 1.1562$ by Bender *et al.*[8]).

In this paper we consider only polynomial potentials with odd degrees. However, a number of other authors have worked on even degree potentials, particularly quartic[17,18] and sextic[19,20] polynomial potentials. Our techniques in proving Theorems 2 and 3 can be used to obtain information on eigenvalues for even degree potentials if both ends of a line passing through the origin stay in decaying Stokes regions.

Obvious open problems are to narrow the eigenvalue sectors closer to the positive real axis, and finally to prove that the eigenvalues are real. Since some $\mathcal{PT}$-symmetric non-Hermitian Hamiltonians do not have all real eigenvalues, one might further want to classify $\mathcal{PT}$-symmetric non-Hermitian Hamiltonians which do have positive real eigenvalues.

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Symmetry transformations in extended irreversible thermodynamics

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In this paper we consider symmetry transformations that preserve the first law and the second law of thermodynamics, as well as the pseudo-Riemannian structure of the Legendre manifold defined in terms of the second derivative matrix of the entropy function in extended irreversible thermodynamics. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1368844]

I. INTRODUCTION

In 1973 Hermann[1] suggested that equilibrium thermodynamics (ET) might be formulated in terms of a contact manifold M with coordinate cover (x,u,y), $x=(x^1,\ldots,x^n)$, $y=(y_1,\ldots,y_n)$. This contact manifold M is equipped with a contact one-form $w=\mathrm{d}u-\Sigma_{i=1}^{n} y_i\,\mathrm{d}x^i=\mathrm{d}u-y_i\,\mathrm{d}x^i$ (summation over repeated indices), where the fundamental equation of states in ET is a Legendre submanifold $\mathcal{L}$ of M. Later, Weinhold[2] suggested that the second derivative matrix elements of the total internal energy might be used to define a metric structure on the set of thermodynamic states. In 1983 Salamon *et al.*[3] constructed a group of coordinate transformations that preserve the structure of w and the metric structure of Weinhold. In this paper we further generalize and clarify the work of Salamon *et al.* to extended irreversible thermodynamics (EIT). First we consider symmetry transformations that preserve the first law and the second law in $\mathcal{L}$. We then generalize these results to the contact manifold M such that the contact structure of M as well as the pseudometric structure of $\mathcal{L}$ are preserved. Finally as an illustration of our results, we consider the transformations that carry the entropy surface to the energy surface, the coordinate transformations of Salamon *et al.*, and the partial Legendre involutions.

Consider a system of molecules in r components contained in a volume V, where no chemical reactions take place. Let E be the total internal energy of the system, N_i the number of particles of species i, Φ_i^α the generalized fluxes such as the mass flux, heat flux, etc.,[4] P the hydrostatic pressure, μ_i the chemical potential conjugate to N_i, and X_i^α the generalized potential conjugate to Φ_i^α.[4] Here $i=1,2,\ldots,r$, and $\alpha=1,2,\ldots,k$, represent the order of the tensor variables Φ_i^α. For simplicity we denote the set of extensive thermodynamic variables $\{E,V,N_i,\Phi_i^\alpha : i=1,2,\ldots,r;\alpha=1,2,\ldots,k\}$ by $x=(x^1,\ldots,x^N)$, where the x^i's are the global thermodynamic variables. Thus x^i's are differentiable functions of time t. Depending on the nonequilibrium system under consideration we can take k as large as necessary so that a sufficient number of the generalized fluxes are included in the system. To this end we consider an irreversible path γ in the thermodynamic base space B_N with coordinate cover $x=(x^1,\ldots,x^N)$. Assume that P, μ_i, and X_i^α are C^1 functions defined on an open subset of B_N with compact support. Consider an infinitesimal portion of the irreversible process along γ. Let $\Delta W=-P\Delta V+\mu_i\Delta N_i-X_i^\alpha\Delta\Phi_i^\alpha$ be the infinitesimal change of work, ΔQ the net amount of heat exchanged between the system and its surroundings, and ΔQ_d the change of dissipative energy (loss of available energy). Define the work one form

$$\xi=-P\,\mathrm{d}V+\mu_i\mathrm{d}N_i-X_i^\alpha\mathrm{d}\Phi_i^\alpha, \tag{1}$$

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and the heat one-form $\Omega = dE - \xi$. The first law and the second law of thermodynamics can be formulated as[5]

$$\Delta E = \Delta W + \Delta Q + \Delta Q_d, \tag{2a}$$

and

$$\Omega \wedge d\Omega = 0, \quad \Delta Q_d \geqslant 0, \tag{2b}$$

where we have assumed that ΔQ_d is semipositive definite and vanishes only at thermodynamic equilibrium. Notice that the second law formulated in (2b) is equivalent to the Clausius principle[5] as well as the Kelvin's principle.[6]

By solving the Pfaffian equation $\Omega = 0$ under the Frobenius integrability condition $\Omega \wedge d\Omega = 0$[7] (or Caratheodory's inaccessibility condition[8]) we can obtain the generalized Gibbs relation:[5]

$$\Omega = T\,dS = dE + P\,dV - \mu_i\,dN_i + X_i^\alpha\,d\Phi_i^\alpha, \tag{3}$$

where T is the thermodynamic temperature and S is the entropy function of the system. Let $u = S = f(x)$ be the integral surface of the Pfaffian equation $\Omega = 0$ under the integrability condition (2b). Denote $y = (T^{-1}, PT^{-1}, -\mu_i T^{-1}, X_i^\alpha T^{-1}) = (y_1, \ldots, y_N)$. As a consequence of the Gibbs relation we have $y_i = \partial_i f$. Thus the entropy surface $u = f(x)$ can be used to define the one graph space

$$\mathcal{L} = \left\{ (x,u,y) \,\middle|\, u = f(x), y_i = \frac{\partial f}{\partial x^i} = \partial_i f \right\}. \tag{4}$$

In Sec. II we consider symmetry transformations that preserve the Pfaffian equation together with the integrability condition (2b).

II. SYMMETRY TRANSFORMATIONS PRESERVING THE FIRST LAW AND THE SECOND LAW

The change of dissipative energy ΔQ_d depends on the irreversible process under consideration. Based on the expression of Q_d in local theory of EIT, Q_d cannot be expressed as a function of x alone in B_N.[5] From a physical point of view the semipositive definite property of ΔQ_d must be invariant under symmetry transformations that preserve the Pfaffian equation $\Omega = 0$ together with the integrability condition (2b). Otherwise it leads to violation of the second law. On the other hand, symmetry transformations preserving the structure of the Pfaffian equation together with condition (2b) are equivalent to the invariance of the integral surface $u = S = f(x)$ with the contact condition $du = y_i\,dx^i$. Therefore the invariance of the first law and the second law is equivalent to the invariance of the integral surface $u = f(x)$ together with the contact condition $du = y_i\,dx^i$.

Let B_N^* be a replica of B_N with coordinate cover x^*. Let U and U^* be open subsets of $B_N \times R$ and $B_N^* \times R$, respectively. Consider the transformations $\varphi: (x,u) \in U \to (x^*, u^*) \in U^*$ given by

$$\begin{gathered} x^* = F(x,u), \quad F = (F^1, \ldots, F^N) \\ u^* = G(x,u), \end{gathered} \tag{5}$$

where φ is a one-to-one (1–1) and onto mapping from U onto U^*, and F, G are C^1 functions defined on U. Further, we assume that the matrix A with matrix elements $D_j F^i = \partial_j F^i + y_j \partial_u F^i$ is nonsingular. Now

$$du^* - y_i^* d(x^*)^i = (\partial_u G - y_i^* \partial_u F^i)[du - y_i\,dx^i] + [D_j G - y_i^* D_j F^i]dx^j, \tag{6}$$

it is evident that $du^*=y_i^*\mathrm{d}(x^*)^i$, if and only if,

$$D_jG=y_i^*(D_jF^i),\ \text{ or }\ y^*=A^{-1}\cdot DG\ \text{ with }\ DG=\begin{bmatrix}D_1G\\ \vdots\\ D_NG\end{bmatrix}. \tag{7}$$

Since φ is 1–1 onto, thus $u^*=g(x^*)$ and

$$y_i^*=\partial_i^*g=\frac{\partial}{\partial(x^*)^i}g.$$

Let

$$\mathcal{L}^*=\{(x^*,u^*,y^*)|u^*=g(x^*),y_i^*=\partial_i^*g\}.$$

Then $\varphi\mathcal{L}=\mathcal{L}^*$. Hence the first law and the second law are invariant under the transformations (5) if and only if (7) is satisfied. So far F and G are arbitrary differentiable functions defined on U. The transformations (5) can be reformulated as

$$x^*=F(x,u),\quad u^*=G(x,y), \tag{8}$$

$$y^*=H(x,u,y)=A^{-1}DG.$$

The second derivative matrix D^2u of the entropy function $u=f(x)$ is symmetric and nondegenerate. However, it is not positive definite. Thus D^2u can be considered as a nondegenerate tensor field of type (0, 2). Following Ruppeiner[9] we define a pseudometric d^2s on $\mathcal{L}$ by $d^2s=(\partial_i\partial_ju)\mathrm{d}x^i\,\mathrm{d}x^j=g_{ij}\mathrm{d}x^i\,\mathrm{d}x^j=\mathrm{d}x^i\,\mathrm{d}y_i=\langle\mathrm{d}x,\mathrm{d}y\rangle$, where $\langle,\rangle$ denotes scalar product of vectors in R^N. The entropy surface $u=f(x)$ becomes a pseudo-Riemannian manifold when it is endowed with the pseudometric d^2s. The physical significance of d^2s has been investigated by Salamon and Berry.[10] They showed that d^2s was related to the dissipative availability of energy. On the other hand, Casas-Vazquez and Jou[11] have computed the Gaussian curvature of the thermodynamic metric for a nonequilibrium system. They found that the presence of heat flux increased the thermodynamic curvature. In this paper we only concentrate on the geometric aspect of the pseudometric d^2s.

By (8) we can obtain

$$\begin{aligned}\langle\mathrm{d}x^*,\mathrm{d}y^*\rangle=&\{\langle\partial_jF,\partial_kH\rangle+\langle\partial_jF,\partial_uH\rangle y_k+\langle\partial_uF,\partial_jH\rangle y_k+\langle\partial_uF,\partial_uH\rangle y_jy_k\}\mathrm{d}x^j\,\mathrm{d}x^k\\&+\langle D_kF,\partial^jH\rangle\mathrm{d}x^k\,\mathrm{d}y_j\,.\end{aligned} \tag{9}$$

Hence $\langle\mathrm{d}x^*,\mathrm{d}y^*\rangle=B(x,u,y)\langle\mathrm{d}x,\mathrm{d}y\rangle$ provided the following conditions are satisfied:

$$\langle\partial_jF,\partial_kH\rangle=0,\quad\langle\partial_jF,\partial_uH\rangle=0,\quad j,k=1,2,...,N. \tag{9a}$$

$$\langle\partial_uF,\partial_kH\rangle=0,\quad\langle\partial_uF,\partial_uH\rangle=0,\quad k=1,2,...,N. \tag{9b}$$

$$B(x,u,y)=\delta_{jk}\langle D_jF,\partial^kH\rangle. \tag{9c}$$

As an example we consider the following transformations:

$$x^*=F(x,u)=(u,x^2,\ldots,x^N),\quad u^*=G(x,u)=x^1. \tag{10}$$

Then $du^*=y_i^*\mathrm{d}(x^*)^i$ if and only if $y^*=H(x,u,y)=A^{-1}DG=(y_1^{-1},-y_1^{-1}y_2,\ldots,-y_1^{-1},y_N)$. We can easily check that (9a) and (9b) are satisfied, while (9c) yields $B(x,u,y)=-y_1^{-1}=-T$. Furthermore we have $\partial_uG-y_i^*(\partial_uF^i)=-y_1^{-1}=\lambda$. Therefore $\mathrm{d}u^*-y_i^*\mathrm{d}(x^*)^i=\lambda(\mathrm{d}u-y_i\,\mathrm{d}x^i)$ and $\langle\mathrm{d}x^*,\mathrm{d}y^*\rangle=\lambda\langle\mathrm{d}x,\mathrm{d}y\rangle$.

We notice that (8) is the transformation from the entropy surface $u=\mathcal{S}=f(x)$ to the energy surface $u^*=E=g(x^*)$. Except for the negative sign, the pseudo-Riemannian structures of $\mathcal{L}$ and $\mathcal{L}^*$ are (conformal) equivalent.[12] This example cannot be obtained from the work of Salamon *et al.*

III. CONTACT TRANSFORMATIONS

In this section we generalize the transformations defined on $B_N\times R$ to the $(2N+1)$-dimensional contact manifold M with coordinate cover (x,u,y), where x, u, y are independent variables. Define the one-form $\omega=\mathrm{d}u-y_i\,\mathrm{d}x^i$ in M. For every $x\in B_N$, the vector space

$$\Delta_x=\{v\in T_xM\,|\langle\omega(x),v(x)\rangle=\omega_i v^i=0;\omega(x)=\omega_i(x)\mathrm{d}x^i,v(x)=v^i(x)\partial_i\}$$

is called the contact hyperplane to M at x, where T_xM is the tangent bundle to M at x. Since $\omega\wedge(\mathrm{d}\omega)^N\neq 0$ and $\omega\wedge(\mathrm{d}\omega)^{N+1}=0$, the one-form ω defines a nondegenerate hyperplane distribution $x\to\Delta_x$ with Δ_x as the kernel of ω. This distribution of hyperplanes is called the contact structure of M. If λ is a function defined on M which does not vanish at any point of M, then $\lambda\omega$ defines the same contact structure of M. The differentiable manifold M equipped with such a one-form (contact one-form) ω is called a contact manifold.[13] Notice that M can be identified with $T^*(B_N)\times R$, where $T^*(B_N)$ is the cotangent bundle of B_N. On the other hand, M can also be identified with the one-jet space $J^1(B_N,R)$ from B_N into R, which is a vector bundle with base B_N. The fiber at $x\in B_N$ is $R\times T^*(B_N)$. The jet j^1_xf is the pair $(f(x),\mathrm{d}f(x))$, and the canonical projection $\pi:M\to B_N$ is the mapping $j^1_xf\to x$. A section of M is a mapping $\sigma:B_N\to M$ such that $\pi\circ\sigma(x)=x$ for every $x\in B_N$. Hence the mapping $j^1f:x\to j^1_xf$ defines a section of M such that $(j^1f)^*\omega=0$, where $(j^1f)^*$ is the pull-back of j^1f. The image of B_N under j^1f is the one-graph space

$$\mathcal{L}=\{(x,u,y)\,|u=f(x),y_i=\partial_i f\},$$

which is the N-dimensional Legendre submanifold of M.

We now consider the 1–1 onto mapping $\varphi:M\to M^*$ given by

$$\begin{aligned} x^*&=F(x,u),\quad u^*=G(x,u),\\ y^*&=H(x,u,y), \end{aligned}\tag{11}$$

where F, G are arbitrary functions of class C^1 defined at every $(x,u)\in U$, U an open subset of $B_N\times R$. Let $\omega^*=\mathrm{d}u^*-y_i^*\,\mathrm{d}(x^*)^i$. By (10) we have

$$\omega^*=[\partial_uG-(\partial_uF^i)y_i^*]\omega+[D_jG-(D_jF^i)y_i^*]\mathrm{d}x^j.$$

Set $\lambda=\partial_uG-(\partial_uF^i)y_i^*$. Since F and G are arbitrary functions of (x,u), without loss of generality, we can assume that λ is nowhere vanishing in M. Hence $\omega^*=\lambda\omega$ if and only if

$$D_jG=(D_jF^i)y_i^*,\quad \text{or}\quad H(x,u,y)=A^{-1}\cdot DG.\tag{12}$$

As $\mathrm{d}\omega=\mathrm{d}\lambda\wedge\omega+\lambda\,\mathrm{d}\omega$, the contact ideal[14] generated by $(\omega,\mathrm{d}\omega)$ is invariant under φ. By examining (5), (8), and (11), we notice that (11) is the lift of (5) from $\mathcal{L}$ into M, while (5) is the projection of (11) onto $\mathcal{L}$. Hence

$$\mathcal{L}^*=\{(x^*,u^*,y^*)\,|u^*=g(x^*),y_i^*=\partial_i^*g\}$$

is the image of $\mathcal{L}$ under φ, where $\omega|_{\mathcal{L}}=\omega^*|_{\mathcal{L}^*}=0$. The first law and the second law are therefore invariant under φ if and only if (12) is satisfied. Next we calculate $\langle\mathrm{d}x^*,\mathrm{d}y^*\rangle$. By (11) we obtain

$$\langle dx^*, dy^* \rangle = \{\langle \partial_j F, \partial_k H \rangle dx^j\, dx^k + \langle \partial_j F, \partial_u H \rangle dx^j\, du + \langle \partial_u F, \partial_k H \rangle du\, dx^k\}$$
$$+ \langle \partial_u F, \partial_u H \rangle du\, du + \langle \partial_u F, \partial^k H \rangle du\, dy_k\} + \langle \partial_j F, \partial^k H \rangle dx^j dy_k . \tag{13}$$

Since dx^i, du, and dy_k are independent, $\langle dx^*, dy^* \rangle = B(x,u,y)\langle dx, dy \rangle$ if and only if the following conditions are satisfied:

$$\langle \partial_j F, \partial_k H \rangle = 0, \quad \langle \partial_i F, \partial_u H \rangle = 0, \tag{14a}$$

$$\langle \partial_u F, \partial_k H \rangle = 0, \quad \langle \partial_u F, \partial_u H \rangle = 0, \quad \langle \partial_u F, \partial^k H \rangle = 0, \tag{14b}$$

$$B(x,u,y) = \delta_{jk} \langle \partial_j F, \partial^k H \rangle \tag{14c}$$

for $j,k = 1,2,...,N$.

Suppose $\langle dx^*, dy^* \rangle = B(x,u,y)\langle dx, dy \rangle$. Then $\langle dx^*, dy^* \rangle|_{\mathcal{L}^*}$ and $\langle dx, dy \rangle|_{\mathcal{L}}$ are conformal equivalent pseudometrices on $\mathcal{L}$ and $\mathcal{L}^*$, respectively. However, the converse is not necessarily true. Comparing (9) and (13) we observe that (9) is the projection of (13) on $\mathcal{L}^*$. Consequently (14a)–(14c) become (9a)–(9c), respectively, if we impose the condition

$$\langle dx^*, dy^* \rangle|_{\mathcal{L}^*} = B(x,u,y)|_{\mathcal{L}} \langle dx, dy \rangle|_{\mathcal{L}} . \tag{15}$$

Therefore the transformations in (11) preserve the contact structure of M and the pseudometric structure on $\mathcal{L}$ if conditions (12), (14a), (9b), and (9c) are satisfied.

Suppose the transformations in (11) define a one-parameter Lie group of transformations,

$$x^* = F(x,u,\epsilon), \quad u^* = G(x,u,\epsilon), \quad y^* = H(x,u,y,\epsilon). \tag{16a}$$

Consider the infinitesimal transformations of (16a):

$$(x^*)^i = x^i + \xi^i(x,u)\epsilon + 0(\epsilon^2),$$
$$u^* = u + \eta(x,u)\epsilon + 0(\epsilon^2), \tag{16b}$$
$$y_i^* = y_i + \eta_i(x,u,y)\epsilon + 0(\epsilon^2).$$

To the first order of ϵ we have the following results:

$$\omega^* = \{1 + \epsilon \partial_u(\eta - y_i \xi^i)\}\omega + \epsilon[D_j(\eta - y_i \xi^i) - \eta_j] dx^j, \tag{17a}$$

$$\langle dx^*, dy^* \rangle|_{\mathcal{L}^*} = \langle dx, dy \rangle|_{\mathcal{L}} + \epsilon[D_j \eta_i\, dx^i\, dx^j + (D_j \xi^i + \partial^i \eta_j) dx^j\, dy_i]|_{\mathcal{L}} . \tag{17b}$$

Let $\alpha = \partial_u(\eta - y_i \xi^i)$. Then $\omega^* = (1 + \epsilon\alpha)\omega$ if and only if

$$\eta_j = D_j(\eta - y_i \xi^i). \tag{18}$$

On the other hand, $\langle dx^*, dy^* \rangle|_{\mathcal{L}^*}$ and $\langle dx, dy \rangle|_{\mathcal{L}}$ are conformal equivalent pseudometrices if

$$D_j \eta_i|_{\mathcal{L}} = 0 \quad B(x,u,y)|_{\mathcal{L}} = \delta_{ij}(D_j \xi^i + \partial^i \eta_j)|_{\mathcal{L}} . \tag{19}$$

Therefore the infinitesimal transformations in (16b) with generator

$$X = \xi^i(x,u)\partial_i + \eta(x,u)\partial_u + \eta_i(x,u,y)\partial^i$$

preserve the contact structure as well as the pseudometric structure if conditions (18) and (19) are satisfied.

Next we consider the coordinate transformations that satisfy (12), (14a), (9b), and (9c). For simplicity we set $\partial_j G = b_j(x,u)$, $\partial_u G = b(x,u)$, $\partial_j F^i = a_{ij}(x,u)$, $\partial_u F^i = a^i(x,u)$, where we have abused the notation for a_{ij}. Then (12) can be rewritten as

$$b_j(x,u) + b(x,u)y_j = y_i^*[a_{ij}(x,u) + a^i(x,u)y_j]. \tag{20a}$$

Assume that matrix A with elements $(A)_{ij} = a_{ij}$ is nonsingular. Since F and G are arbitrary C^1 functions, we can choose b_j, b, a_{ij} and a^i in (20a) such that (14a) and (9b) are satisfied. To this end we set $a_{ij}(x,u) = a_{ij} = \text{const}$, $a^i(x,u) = a^i = \text{const}$. In order to satisfy (14a) we must have $b_j(x,u) = b_j = \text{const}$, and $b(x,u) = b = \text{const}$. Thus (20a) becomes

$$(a_{ij} + a^i y_j)y_i^* = b_j + by_j. \tag{20b}$$

This equation can be solved for y_i^* such that $y_i^* = H_i(x,u,y) = H_i(y)$. Thus, by assumption we have

$$\begin{aligned} (x^*)^i &= F^i(x,u) = a^i u + a_{ij}x^j + \alpha^i, \alpha^i \in R, \\ u^* &= G(x,u) = bu + b_j x^j + c, c \in R, \\ y_i^* &= H_i(y). \end{aligned} \tag{21}$$

In the following discussions we consider two special solutions of (21).

(i) Without loss of generality we set $a^i = a$ for $i = 1$ and $a^i = 0$ for $i \geqslant 2$. Then (20b) becomes

$$a_{ij}y_i^* + ay_j y_1^* = b_j + by_j. \tag{22}$$

Since a, b, b_j, and a_{ij} are arbitrary, we can solve this equation in many different ways, where the simplest solution can be obtained by setting $b = 0$, $a = 1$, $b_1 = 1$, $b_j = 0$ for $j \geqslant 2$, $a_{1j} = 0$ for all j and $a_{ij} = \delta_{ij}$ for $i,j \geqslant 2$. Then $y^* = (y_1^{-1}, -y_1^{-1}y_2, \ldots, -y_1^{-1}y_N)$. This is exactly what we have in example 1.

(ii) We set $a^i = 0$ for all i. Then

$$F^i(x,u) = a_{ij}x^j + \alpha^i, \quad G(x,u) = bu + b_j x^j + c.$$

Equation (20b) becomes $a_{ij}y_i^* = b_j + by_j$, which has the solution

$$y_i^* = [(A^T)^{-1}]_{ij}(b_j + by_j). \tag{23}$$

Notice that

$$\begin{aligned} F(x,u) &= A(x+\alpha), \quad \alpha = (\alpha^1, \ldots, \alpha^N), \\ G(x,u) &= bu + b_j x^j + c, \\ H(x,u,y) &= (A^T)^{-1}(by + r), \quad r = (b_1, \ldots b_N) \end{aligned}$$

are the coordinate transformations considered by Salamon *et al.*

IV. FURTHER GENERALIZATIONS

In order to consider partial Legendre involutions[15] we generalize (11) as follows:

$$x^* = F(x,u,y), \quad u^* = G(x,u,y), \quad y^* = H(x,u,y), \tag{24}$$

where F, G, H are functions of class C^1 defined in M. Thus

$$\omega^*=[\partial_u G-(\partial_u F^i)y_i^*]\omega+[D_j G-(D_j F^i)y_i^*]\mathrm{d}x^j+[\partial^j G-(\partial^j F^i)y_i^*]\mathrm{d}y_j. \tag{25}$$

Let $\lambda=\partial_u G-(\partial_u F^i)y_i^*$. Then $\omega^*=\lambda\omega$ if and only if

$$D_j G=(D_j F^i)y_i^*, \tag{26a}$$

$$\partial^i G=(\partial^j F^i)y_i^*. \tag{26b}$$

Furthermore, as an extension of (14a)–(14c) we obtain $\langle \mathrm{d}x^*,\mathrm{d}y^*\rangle=B(x,u,y)\langle \mathrm{d}x,\mathrm{d}y\rangle$ if and only if the following conditions are satisfied:

$$\langle \partial_j F,\partial_k H\rangle=0,\quad \langle \partial_j F,\partial_u H\rangle=0, \tag{27a}$$

$$\langle \partial_u F,\partial_k H\rangle=0,\quad \langle \partial_u F,\partial_u H\rangle=0,\quad \langle \partial_u F,\partial^k H\rangle=0, \tag{27b}$$

$$\langle \partial^j F,\partial^k H\rangle=0,\quad \langle \partial^j F,\partial_u H\rangle=0 \tag{27c}$$

and

$$B(x,u,y)=\delta_{jk}[\langle \partial_j F,\partial^k H\rangle+\langle \partial^j F,\partial_k H\rangle]. \tag{27d}$$

It should be noted that (26a) and (26b) are complementary conditions. By examining (27a)–(27c) we conclude that both F^i and H_i are independent of u. For simplicity we assume

$$F^i(x,u)=\sum_{j=1}^{N}(a_{ij}x^j+b_{ij}y_j)+\alpha^i. \tag{28a}$$

This implies that G can be written as

$$G=au+c\sum_{i=1}^{N}x^i y_i+d. \tag{28b}$$

By (26a) and (26b) we obtain

$$cx^j=\sum_{i=1}^{N}b_{ij}y_i^*, \tag{29a}$$

$$(a+c)y_j=\sum_{i=1}^{N}a_{ij}y_i^*. \tag{29b}$$

We now solve (29a) and (29b) for y_i^*. Since $\langle \partial_j F,\partial_k H\rangle=\langle \partial^j F,\partial^k H\rangle=0$, without loss of generality we choose b_{ij} and a_{ij} such that

$$\sum_{i=1}^{N}b_{ij}y_i^*=\begin{cases}cx^j, & j\leqslant m\\ 0, & i,j\geqslant m+1,\end{cases} \tag{30a}$$

$$\sum_{i=1}^{N}a_{ij}y_i^*=\begin{cases}0, & i,j\leqslant m\\ (a+c)y_j, & i,j\geqslant m+1.\end{cases} \tag{30b}$$

In order to obtain a unique solution for y_i^*, both matrices A and B must be nonsingular with matrix elements $(A)_{ij}=a_{ij}$ and $(B)_{ij}=b_{ij}$. Thus A is $(N-m)$ by $(N-m)$ and B is m by m. Furthermore, $a=-c$ so that the sum in (28b) is restricted to $i\leqslant m$. Consequently (30a) and (30b) yield the following solution for y_i^*:

$$y_i^* = \begin{cases} -a[(B^T)^{-1}]_{ij}x^j, & i,j \leqslant m \\ a^{-1}[(A^T)^{-1}]_{ij}y_j, & i,j \geqslant m+1. \end{cases} \tag{31}$$

By (28a) and (31) we finally obtain

$$\langle dx^*, dy^* \rangle = -a\left\{ \sum_{i=1}^{m} dx^i\, dy_i - a^{-2} \sum_{i=m+1}^{N} dx^i\, dy_i \right\}. \tag{32}$$

Hence $\langle dx^*, dy^* \rangle|_{\mathcal{L}^*}$ is a pseudo-Riemannian metric with signature $(m, N-m)$ if $a=-1$. To summarize, the following transformations

$$(x^*)^i = F^i(x,u) = \begin{cases} \sum_{j=1}^{m} b_{ij}y_j + \alpha^i, & i \leqslant m \\ \sum_{j=m+1}^{N} a_{ij}x^j + \alpha^i, & i \geqslant m+1, \end{cases} \tag{33a}$$

$$u^* = G(x,u,y) = -u + \sum_{i=1}^{m} x^i y_i + d, \tag{33b}$$

$$y_i^* = H_i(x,y) = \begin{cases} \sum_{j=1}^{m} [(B^T)^{-1}]_{ij}x^j, & i \leqslant m \\ -\sum_{j=m+1}^{N} [(A^T)^{-1}]_{ij}y_j, & i \geqslant m+1 \end{cases} \tag{33c}$$

preserve the contact structure in M and the pseudometric structure in $\mathcal{L}$. It is interesting to note that the Legendre involution

$$x^* = (y_1, \ldots, y_m, x^{m+1}, \ldots, x^N),$$

$$u^* = -u + \sum_{i=1}^{m} x^i y_i,$$

$$y^* = (x^1, \ldots, x^m, -y_{m+1}, \ldots, -y_N)$$

is a special example of (33a)–(33c).

V. CONCLUSION

In this paper we consider symmetry transformations that preserve the first law and the second law of thermodynamics. These symmetry transformations form a group of contact transformations on a contact manifold M, where the entropy surface (or energy surface) is a Legendre submanifold $\mathcal{L}$ of the contact manifold M. These contact transformations depend on $N+1$ arbitrary differentiable functions $F=(F^1,\ldots,F^N)$ and G [or $\xi=(\xi^1,\ldots,\xi^N)$ and η]. Under some specific conditions on F and G (ξ and η) we show that these contact transformations preserve the contact structure of M as well as the pseudometric structure of $\mathcal{L}$ defined by the second derivative matrix of the entropy function (or the energy function). Finally, as an illustration of our results, we consider three examples, the transformations between the entropy surface and the energy surface, the group of coordinate transformations by Salamon *et al.*, and the partial Legendre involutions.

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Free energies based on generalized entropies and H-theorems for nonlinear Fokker–Planck equations

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The relationship between H-theorems and free energies is studied on the basis of generalized entropies. Two kinds of nonlinear Fokker–Planck equations with different nonlinear diffusion terms that exhibit the power-law-type equilibrium distributions of Tsallis thermostatistics are investigated from the viewpoint of nonequilibrium free energies and stability analysis of their solutions. Using the generalized entropies Liapunov functions are constructed to show H-theorems, which ensure uniqueness of and convergence to the equilibrium distributions of the nonlinear Fokker–Planck equations. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Recently Tsallis proposed use of a nonextensive entropy that is obtained by generalizing the Boltzmann entropy and developed generalized thermostatistics.[1–3] Tsallis' thermostatistics, which is characterized by power-law-type equilibrium probability distributions[1–3] unlike Boltzmann statistics with exponential type distributions and also is closely related with fractal-inspired statistics based on Renyi entropy,[4] has aroused great interest in various research areas because of its potential applicability in a variety of physical systems. Among them are systems exhibiting Levy-type anomalous diffusion[5] and self-gravitating systems.[6] Tsallis' equilibrium probability distributions are obtained by maximizing, with respect to probabilities $\{p_i\}$, the generalized entropies S_q with a real parameter q representing nonextensivity:[1–3,7]

$$S_q=\frac{k(1-\Sigma_i p_i^q)}{q-1} \tag{1}$$

(k stands for a constant corresponding to the Boltzmann constant k_B in the limit $q\to 1$) under the constraints of normalization of a probability distribution $\Sigma_{i=1} p_i=1$ and conservation of internal energy.[1–3]

According to averaging procedures for the energy constraint, Tsallis' thermostatistics has been so far classified into three versions or choices.[3]

In the so-called first choice,[1] the energy constraint takes the standard form

$$\sum_{i=1} p_i \epsilon_i=\langle \epsilon\rangle^{(1)} \tag{2}$$

with ϵ_i representing the energy of ith state of a system and $\langle \epsilon\rangle^{(1)}$ a given constant. Solving the variational problem for the well known MaxEnt principle $\delta(S_q-\lambda_1\Sigma_{i=1} p_i-\lambda_2\Sigma_{i=1} p_i\epsilon_i)=0$ (λ_1 and λ_2 represent Lagrange multipliers) yields the equilibrium distribution of the form

$$p_i^{(1)}=\frac{1}{Z_q^{(1)}}[1-\beta^{(1)}(q-1)\epsilon_i]^{1/(q-1)}, \tag{3}$$

where $Z_q^{(1)}$ stands for the normalization constant (i.e., partition function) and $\beta^{(1)}$ the Lagrange multiplier related constant.

In the second choice,[1,2] the energy constraint is given by

$$\sum_{i=1} p_i^q \epsilon_i = \langle \epsilon \rangle^{(2)} \tag{4}$$

and the corresponding MaxEnt principle yields the equilibrium distribution

$$p_i^{(2)} = \frac{1}{Z_q^{(2)}} [1 - \beta^{(2)}(1-q)\epsilon_i]^{1/(1-q)}, \tag{5}$$

where $\beta^{(2)}$ represents a constant that is proportional to the Lagrange multiplier associated to the energy constraint (4) and $Z_q^{(2)}$ normalization constant.

In the third choice,[3] one adopts

$$\frac{\Sigma_{i=1} p_i^q \epsilon_i}{\Sigma_{i=1} p_i^q} = \langle \epsilon \rangle_q \tag{6}$$

as an energy constraint to have the equilibrium distribution

$$p_i = \frac{1}{Z_q} \left[1 - \frac{\beta(1-q)}{C(q)} (\epsilon_i - \langle \epsilon \rangle_q) \right]^{1/(1-q)} \tag{7}$$

with

$$C(q) = \sum_{i=1} p_i^q, \tag{8}$$

$$Z_q = \sum_{i=1} \left[1 - \frac{\beta(1-q)}{C(q)} (\epsilon_i - \langle \epsilon \rangle_q) \right]^{1/(1-q)}, \tag{9}$$

$$\langle \epsilon \rangle_q = \sum_{i=1} \frac{p_i^q}{C(q)} \epsilon_i, \tag{10}$$

where β represents a constant that is proportional to the Lagrange multiplier associated to the energy constraint (6) and Z_q normalization constant.

Most of the papers published so far have concerned formal arguments on equilibrium properties of the novel statistics. The nature and physical implications of the nonextensive generalized entropies of Tsallis (hereafter referred to as Tsallis entropy) are still far less understood. The study of dynamical aspects of the Tsallis entropies is considered to be useful to get deeper insights into its physical meaning.

The Tsallis entropies themselves are known to play a Liapunov function of a certain type of nonlinear diffusion equations[8] that exhibit super or subdiffusion phenomena.[9–12] Recently a nonlinear Fokker–Planck equation (NFPE) that is obtained by adding a linear streaming term based on the introduction of a quadratic potential to the above mentioned nonlinear diffusion equations has been proposed by Plastino and Plastino[13] to investigate dynamical behaviors of the temporal solutions. They showed that the equilibrium probability distributions of Tsallis can be given as a fixed-point-type solution of the nonlinear Fokker–Planck equation and that a special version of H-theorem holds with the entropy chosen as an H-functional: the Tsallis entropy itself becomes a Liapunov functional of the NFPE. A microscopic derivation of the NFPE was studied by Borland[14] and also by Kaniadakis and Lapenta,[15] who investigated the relationships between the

linear Fokker–Planck equation, the NFPE with a quadratic potential, and the nonlinear porous media equation exhibiting the same equilibrium probability distribution of Tsallis' thermostatistics to show their equivalence.

An H-theorem is well known to be quite useful to ensure convergence to equilibrium probability distribution(s) of any temporal solution of a master equation.[16–23] The H-function (functional) associated with an H-theorem usually takes the form of difference of nonequilibrium free energies between two states of a system[23] as in the case of the Kullback Leibler divergence[24] or relative entropy for standard linear Markovian master equations.

Previously I proposed, within the framework of Markovian stochastic processes, generalized relative entropies,[23] which are a natural extension of the relative entropy of Boltzmann statistics, together with generalized nonequilibrium free energies based on the Tsallis entropies. The generalized relative entropies $H_q(\{p_i\},\{g_i\})$ defined as a function of two arbitrary probabilities $\{p_i\}$ and $\{g_i\}$ $(p_i>0, g_i>0)$, which were also proposed independently by Tsallis,[25] are given by

$$H_q(\{p_i\},\{g_i\})=\frac{1}{(q-1)}\left[\sum_{i=1} p_i\left(\frac{p_i}{g_i}\right)^{q-1}-1\right]. \tag{11}$$

I showed that an H-theorem holds for an arbitrary linear master equation, when the generalized relative entropies are chosen as its H-function (see also Ref. 26):

$$\begin{aligned}&\frac{d}{dt}H_q(\{p_i(t)\},\{g_i(t)\})\leq 0 \quad \text{for} \quad q>0,\ q\neq 1\\ &\frac{d}{dt}H_q(\{p_i(t)\},\{g_i(t)\})\geq 0 \quad \text{for} \quad q<0,\end{aligned} \tag{12}$$

where the two probabilities $\{p_i(t)\}$ and $\{g_i(t)\}$ are assumed to obey a given linear master equation of a Markovian dynamics.

The generalized nonequilibrium free energies that were studied in Ref. 23 in connection with the above mentioned generalized relative entropies, however, have a drawback that they do not physically make sense, since the construction of them is based on the second choice of Tsallis statistics, where the average of unity differs from unity.[2,3] I also note here that in the generalized relative entropy (11) as an H-function of the H-theorem of Ref. 23, the equilibrium probability distribution (when dealing with the case of $\{g_i\}=\{g_i^{\rm eq}\}$) exhibited by a given linear master equation need not be the Tsallis distribution. Although such an H-theorem with an H-function that makes sense for an arbitrarily given linear master equation will be useful in some engineering problems where the generalized relative entropies, if chosen as a target function of a certain computational task, may improve efficiencies of computations involved, it will not be helpful for understanding underlying concepts or physical meaning of the Tsallis entropies as well as Tsallis statistics.

I would like to be concerned with finding free energies appropriately defined based on the Tsallis entropies that play the role of a Liapunov function exclusively for such a master equation as exhibiting equilibrium probability distributions of Tsallis' thermostatistics (3), (5), or (7). I consider the NFPE of Plastino and Plastino[13] to be a nice candidate for dealing with dynamical behaviors of its solution in terms of an H-theorem. An example of free energy as a Liapunov functional of a nonlinear master equation was studied previously by the author[27] for a different type of NFPE, which exhibits mean field-type phase transitions.[27,28]

The aims of this article are twofold. First, I want to show that NFPE studied in Ref. 13, which exhibits the Tsallis distribution of the first choice as a fixed point solution, has a Liapunov functional taking the form of free energy involving the Tsallis entropies and an H-theorem holds. Second, I want to extend the above-mentioned H-theorem so as to adapt to the case with the third choice of Tsallis statistics,[3] where the escort probability[3,29] manifests itself and the generalized entropies expressed in terms of the escort probability take a modified form.

In the following section I define a free energy based on the Tsallis entropy for the system described by the NFPE of Ref. 13 to show that the free energy functional is bounded from below and it decreases monotonically with time (H-theorem), provided that $0<q<1$ with the natural boundary condition imposed. In Sec. III, I propose another kind of NFPE that has a fixed-point-type solution associated with the Tsallis equilibrium distribution of the third choice and construct a free energy using a modified Tsallis entropy that is expressed in terms of the escort probability. With this free energy functional being chosen as a Liapunov functional I show an H-theorem to hold, provided that $0<1/q<1$ with the natural boundary condition imposed. A brief summary and discussion is given in Sec. IV. A preliminary result of the present work was reported in the workshop proceedings of the 5th International Workshop on Similarity and Diversity.

II. H-THEOREM FOR A NONLINEAR FOKKER-PLANCK EQUATION AND THE GENERALIZED ENTROPY

The nonlinear Fokker-Planck equation (NFPE) we deal with in this section reads

$$\frac{\partial p}{\partial t}=-\frac{\partial}{\partial x}(A(x)p)+D\frac{\partial^2}{\partial x^2}p^q, \tag{13}$$

where q is a real number, D a positive constant, and $A(x)$ an arbitrary function. This equation was studied previously for the temporal behavior of its time dependent solution $p(t,x)$ (Refs. 13, 30, and 31) and for a microscopic derivation of the NFPE itself.[14,15] Introducing the probability current j,

$$j=A(x)p-D\frac{\partial}{\partial x}p^q, \tag{14}$$

one can transform the NFPE into the equation describing the conservation law of probability:

$$\frac{\partial p}{\partial t}+\frac{\partial j}{\partial x}=0. \tag{15}$$

Indeed, with the natural boundary condition of the present system,

$$p(t,\pm\infty)=0, \quad \frac{\partial p^q}{\partial x}(t,\pm\infty)=0, \tag{16}$$

it follows

$$\frac{d}{dt}\int_{-\infty}^{\infty}p\,dx=j(t,-\infty)-j(t,\infty)=0. \tag{17}$$

Since $\partial p/\partial t=0$ implies $j=0$, the equilibrium distribution $P_{\mathrm{eq}}(x)$ satisfies

$$A(x)=qDp^{q-2}\frac{\partial p}{\partial x}. \tag{18}$$

Integrating this equation yields

$$p^{q-1}=\frac{-(q-1)\phi(x)}{Dq}+(Dq\beta)^{-1} \tag{19}$$

with

$$\phi(x)=-\int^{x}A(x)dx, \tag{20}$$

where the integration constant is set to be $(Dq\beta)^{-1}$.

When $\phi(x)\to\infty$ as $|x|\to\infty$, Eq. (19) implies $0<q<1$, because $P_{\rm eq}^{q-1}>0$. Then it follows that $P_{\rm eq}\to 0(|x|\to\infty)$. Assuming that $0<q<1$ and $\phi(x)\approx|x|^m$ with $m>0(|x|\to\infty)$, one also has $\partial P_{\rm eq}^q/\partial x\approx|x|^{mq/(q-1)-1}\to 0(|x|\to\infty)$. In what follows we deal with the relevant case with $0<q<1$, where the natural boundary condition (16) makes sense.

We now see that the equilibrium distribution takes the form that appears in Tsallis statistics as a result of optimizing the generalized entropy under the constraints called the first choice:[1,13]

$$P_{\rm eq}(x)=[(Dq\beta)^{-1}(1-\beta(q-1)\phi(x))]^{1/(q-1)}, \tag{21}$$

where β is determined by normalization of $P_{\rm eq}(x)$. We note that β uniquely exists with $\beta>0$ when the potential is bounded from below: $\phi(x)>^{\exists}d$. Defining the partition function $Z^{(1)}$ as

$$Z^{(1)}=\int_{-\infty}^{\infty}(1-\beta(q-1)\phi(x))^{1/(q-1)}dx, \tag{22}$$

one has

$$\beta=\frac{Z^{(1)q-1}}{Dq} \tag{23}$$

with the above equilibrium distribution being rewritten as

$$P_{\rm eq}(x)=\frac{1}{Z^{(1)}}\left[1-\frac{Z^{(1)q-1}(q-1)\phi(x)}{Dq}\right]^{1/(q-1)}. \tag{24}$$

We proceed to define a Liapunov functional taking the form of a free energy based on Tsallis entropy as

$$F\equiv U-\frac{D}{k}S \tag{25}$$

with

$$U\equiv\int\phi p\,dx,\quad S\equiv\frac{k}{q-1}\left[1-\int p^q dx\right], \tag{26}$$

where integrability for each quantity is assumed. When $P=P_{\rm eq}$ and $\phi(x)\approx|x|^m$ (for large $|x|$), the condition of integrability becomes $1/(m+1)<q<1$.

A. Boundedness from below

The Liapunov functional F satisfies the following inequality:

$$F(p(\cdot))\geqslant F(P_{\rm eq}(\cdot)),\quad 0<q<1. \tag{27}$$

Proof: First we note that $\phi(x)$ can be expressed in terms of $P_{\rm eq}(x)$ as

$$\phi(x)=\frac{Dq\beta P_{\rm eq}^{q-1}-1}{(1-q)\beta}, \tag{28}$$

which follows from Eq. (21). Then F is rewritten as

$$F(p(\cdot))=\int\phi p\,dx-\frac{D}{q-1}\left[1-\int p^q dx\right]=\frac{D}{q-1}\int(p^q-qpP_{\rm eq}^{q-1})dx+\frac{1}{q-1}\left(\frac{1}{\beta}-D\right) \tag{29}$$

with

$$F(P_{\rm eq}(\cdot))=-D\int P_{\rm eq}^{q}dx+\frac{1}{q-1}\left(\frac{1}{\beta}-D\right). \tag{30}$$

Then one has

$$F(p(\cdot))-F(P_{\rm eq}(\cdot))=\frac{D}{q-1}\int (p^{q}-qpP_{\rm eq}^{q-1}+(q-1)P_{\rm eq}^{q})dx. \tag{31}$$

Since

$$\begin{aligned} P^{q}-qpP_{\rm eq}^{q-1}+(q-1)P_{\rm eq}^{q}&=P_{\rm eq}^{q}(y^{q}-qy+q-1)\geqslant 0, \quad q>1,\ q<0,\\ &\leqslant 0, \quad 0<q<1, \end{aligned} \tag{32}$$

with $y\equiv p/P_{\rm eq}$, it follows that for $0<q<1$ one has $F(p(\cdot))\geqslant F(P_{\rm eq}(\cdot))$.

B. H-theorem

An H-theorem with the Liapunov functional (i.e., H-functional) defined earlier holds for $0<q<1$:

$$\frac{dF}{dt}\leqslant 0. \tag{33}$$

Proof: Differentiating F with respect to t one obtains

$$\begin{aligned} \frac{dF}{dt}&=\int\left(\phi+\frac{Dq}{q-1}p^{q-1}\right)\left[-\frac{\partial}{\partial x}(-\phi_{x}(x)p)+D\frac{\partial^{2}}{\partial x^{2}}p^{q}\right]dx\\ &=-\int\phi_{x}^{2}pdx+2D\int\phi_{xx}p^{q}dx-D^{2}q^{2}\int p^{2q-3}\left(\frac{\partial p}{\partial x}\right)^{2}dx, \end{aligned} \tag{34}$$

where integration by parts was used. We assume the existence of each integral on the rhs of Eq. (34):

$$\int p^{2q-3}\left(\frac{\partial p}{\partial x}\right)^{2}dx<\infty, \qquad \int pP_{\rm eq}^{2q-4}\left(\frac{\partial P_{\rm eq}}{\partial x}\right)^{2}dx<\infty. \tag{35}$$

Using (28), dF/dt is further rewritten as

$$\frac{dF}{dt}=\int\left[B_{1}\left(\frac{\partial p}{\partial x}\right)^{2}+B_{2}\frac{\partial p}{\partial x}\frac{\partial P_{\rm eq}}{\partial x}+B_{3}\left(\frac{\partial P_{\rm eq}}{\partial x}\right)^{2}\right]dx, \tag{36}$$

where

$$\begin{aligned} B_{1}&=-D^{2}q^{2}p^{2q-3}, \quad B_{2}=2D^{2}q^{2}p^{q-1}P_{\rm eq}^{q-2},\\ B_{3}&=-D^{2}q^{2}pP_{\rm eq}^{2q-4}. \end{aligned} \tag{37}$$

Then it follows that

$$\frac{dF}{dt}=-D^{2}q^{2}\int p\left(p^{q-2}\frac{\partial p}{\partial x}-P_{\rm eq}^{q-2}\frac{\partial P_{\rm eq}}{\partial x}\right)^{2}dx=-\frac{D^{2}q^{2}}{(q-1)^{2}}\int p\left[\frac{\partial}{\partial x}(p^{q-1}-P_{\rm eq}^{q-1})\right]^{2}dx\leqslant 0. \tag{38}$$

We see that equality is implied by $p^{q-1}-P_{\mathrm{eq}}^{q-1}=c(\mathrm{const})$. It can easily be shown that $dF/dt=0$ is attained, if and only if $p=P_{\mathrm{eq}}(c=0)$: noting that, with $\tilde{c}$ representing some constant,

$$p^{q-1}=P_{\mathrm{eq}}^{q-1}+c=(Dq\beta)^{-1}(\tilde{c}-\beta(q-1)\phi(x)) \tag{39}$$

and $\beta>0$, $q<1$, and $\phi(x)>^{\exists}d(\mathrm{const})$, we see that $p(x;\tilde{c})$ is a monotonically decreasing function of $\tilde{c}$. With the normalization condition $\int p(x;\tilde{c})dx=1$, it follows $p=P_{\mathrm{eq}}$. When $0<q<1$, inequality (33) together with (27) implies that the equilibrium distribution (21) is the unique equilibrium solution of the NFPE (13) and that the free energy (25) continues to decrease until it approaches $F(P_{\mathrm{eq}}(\cdot))$.

III. ANOTHER H-THEOREM BASED ON THE MODIFIED GENERALIZED ENTROPIES

In this section I propose another kind of NFPE to study an H-theorem based on the modified generalized entropies that arise within the framework of Tsallis statistics of the third choice.

A. Escort probability and modified generalized entropy in Tsallis statistics of third choice

Since it follows from the equilibrium probability distribution in Tsallis statistics of the third choice (7) that

$$\sum_{i=1}\frac{p_i^q}{C(q)}p_i^{1-q}Z_q^{1-q}=\sum_{i=1}\frac{p_i^q}{C(q)}\left[1-\frac{\beta(1-q)}{C(q)}(\epsilon_i-\langle\epsilon\rangle_q)\right]=1, \tag{40}$$

one has

$$C(q)=Z_q^{1-q}. \tag{41}$$

We note that the β used in this section should be independent of the β used in Sec. II. Then the equilibrium distribution (7) can be rewritten as

$$p_i=C(q)^{1/(q-1)}\left[1-\frac{\beta(1-q)}{C(q)}(\epsilon_i-\langle\epsilon\rangle_q)\right]^{1/(1-q)}, \tag{42}$$

where the parameters $C(q)$ and $\langle\epsilon\rangle_q$ are determined by (8) and (10).

In general, the escort probability[3,29] is defined as

$$\tilde{p}_i=\frac{p_i^q}{C(q)}. \tag{43}$$

Then the equilibrium distribution (42) can be rewritten as

$$\tilde{p}_i=C(q)^{1/(q-1)}\left[1-\frac{\beta(1-q)}{C(q)}(\epsilon_i-\langle\epsilon\rangle_q)\right]^{q/(1-q)}. \tag{44}$$

Introducing

$$Q=\frac{1}{q} \tag{45}$$

and noting

$$C(q)=\sum_{i=1}p_i^q=\sum_{i=1}\left(\frac{\tilde{p}_i^{1/q}}{\Sigma_{i=1}\tilde{p}_i^{1/q}}\right)^q=\frac{1}{(\Sigma_{i=1}\tilde{p}_i^{1/q})^q}\sum_{i=1}\tilde{p}_i=\left(\sum_{i=1}\tilde{p}_i^{1/q}\right)^{-q}, \tag{46}$$

we define

$$\tilde{C}(Q)=\left(\sum_{i=1}\tilde{p}_i^{Q}\right)^{-1/Q}, \tag{47}$$

to have

$$\tilde{C}(Q)=C(q). \tag{48}$$

Then the escort probability (43) can be rewritten as

$$\tilde{p}_i=\tilde{C}(Q)^{Q/(1-Q)}\left[1-\frac{\beta(Q-1)}{\tilde{C}(Q)Q}(\epsilon_i-\langle\epsilon\rangle)\right]^{1/(Q-1)} \tag{49}$$

with $\langle\epsilon\rangle=\Sigma_{i=1}\tilde{p}_i\epsilon_i$. The introduction of Q (45) together with considering the escort probability (49) make the theoretical treatment presented below quite smart.

Note that Tsallis entropy S_q can be rewritten in terms of $\{\tilde{p}_i\}$ as

$$S_q=\frac{1-\Sigma_i p_i^q}{q-1}=\frac{1-C(q)}{q-1}=\frac{1-\tilde{C}(Q)}{q-1}=\frac{1-(\Sigma_{i=1}\tilde{p}_i^{Q})^{-1/Q}}{(1/Q)-1}=\tilde{S}_Q, \tag{50}$$

where we have defined the transformed entropy $\tilde{S}_Q$ that takes a modified form of generalized entropy as a function of $\{\tilde{p}_i\}$.

B. Nonlinear Fokker–Planck equation with nonlocal diffusion coefficient

We propose a nonlinear Fokker–Planck equation that will turn out to be closely related to Tsallis statistics of the third choice:[3]

$$\frac{\partial p}{\partial t}=-\frac{\partial}{\partial x}(A(x)p)+\frac{1}{\beta}\left(\int p^Q\,dx\right)^{-(Q+1)/Q}\frac{\partial^2}{\partial x^2}p^Q, \tag{51}$$

where β is a positive constant and the coefficient of the diffusion term is a time varying nonlocal quantity instead of a constant D of the NFPE of Sec. II. Introducing the probability current j,

$$j=A(x)p-D_p(Q)\frac{\partial}{\partial x}p^Q \tag{52}$$

with

$$D_p(Q)=\frac{1}{\beta}\tilde{C}(Q)^{Q+1}, \tag{53}$$

$$\tilde{C}(Q)=\left(\int p^Q dx\right)^{-1/Q}, \tag{54}$$

one can transform the NFPE (51) into the equation describing the conservation law of probability:

$$\frac{\partial p}{\partial t}+\frac{\partial j}{\partial x}=0,$$

which implies, as in the previous section, $(d/dt)\int_{-\infty}^{\infty}p\,dx=j(t,-\infty)-j(t,\infty)=0$ when the natural boundary condition $p(t,\pm\infty)=0$, $(\partial p^Q/\partial x)(t,\pm\infty)=0$ is imposed.

Since $\partial p/\partial t=0$ implies $j=0$, one has

$$A(x)=QD_{p_{\rm eq}}(Q)P_{\rm eq}^{Q-2}\frac{\partial P_{\rm eq}}{\partial x}. \tag{55}$$

Integrating this equation yields

$$P_{\rm eq}^{Q-1}=\frac{-(Q-1)(\phi(x)-\langle\phi(x)\rangle)}{D_{p_{\rm eq}}(Q)Q}+\theta \tag{56}$$

with $\phi(x)=-\int^x A(x)dx$,

$$\langle\phi(x)\rangle=\int \phi(x)p_{\rm eq}dx, \tag{57}$$

where the integration constant is set to be $(Q-1)\langle\phi(x)\rangle/D_{p_{\rm eq}}(Q)Q+\theta$.

The θ is a constant which will be identified later. Since it follows from Eq. (56) that

$$\int P_{\rm eq}^{Q}dx=\theta, \tag{58}$$

one has

$$\theta=\tilde{C}_0(Q)^{-Q} \tag{59}$$

with

$$\tilde{C}_0(Q)=\left(\int P_{\rm eq}^{Q}dx\right)^{-1/Q}. \tag{60}$$

We now see that the equilibrium distribution takes the form of the escort probability that appears in Tsallis statistics of the third choice Eq. (49):

$$P_{\rm eq}(x)=\tilde{C}_0(Q)^{-Q/(Q-1)}\left[1-\frac{\beta(Q-1)}{\tilde{C}_0(Q)Q}(\phi(x)-\langle\phi\rangle)\right]^{1/(Q-1)}, \tag{61}$$

where $\langle\phi(x)\rangle$ and $\tilde{C}_0(Q)$ are determined by Eq. (57) and normalization of $P_{\rm eq}(x)$. The existence of the equilibrium probability distribution $P_{\rm eq}(x)$ with the self-consistently determined $\langle\phi\rangle$ and $\tilde{C}_0$ can be confirmed in the course of our analysis. Defining the partition function $\tilde{Z}_Q$ as

$$\tilde{Z}_Q=\int_{-\infty}^{\infty}\left[1-\frac{\beta(Q-1)}{\tilde{C}_0(Q)Q}(\phi(x)-\langle\phi\rangle)\right]^{1/(Q-1)}dx, \tag{62}$$

one can rewrite the above equilibrium distribution as

$$P_{\rm eq}(x)=\frac{1}{\tilde{Z}_Q}\left[1-\frac{\tilde{Z}_Q^{Q-1}(Q-1)}{\tilde{C}_0(Q)^{Q+1}Q1/\beta}(\phi(x)-\langle\phi\rangle)\right]^{1(Q-1)}. \tag{63}$$

Note that as far as equilibrium distributions are concerned, $(1/\beta)\tilde{C}_0(Q)^{Q+1}$ corresponds to D of the NFPE (13). We then find that the above expression of the equilibrium distribution (63) takes a form similar to the Tsallis equilibrium distribution of the first choice (24) exhibited by the NFPE of Sec. II except for the appearance of $\langle\phi\rangle$.

C. Free energy and H-theorem

We define a Liapunov functional taking the form of a free energy based on the modified Tsalliis entropy (50) as

$$F \equiv U - \frac{1}{\beta}\tilde{S} \tag{64}$$

with

$$U \equiv \int \phi p dx, \quad \tilde{S} \equiv \frac{1}{1/Q-1}\left[1-\left(\int p^Q dx\right)^{-1/Q}\right]. \tag{65}$$

Assuming the existence of the equilibrium distribution $P_{\mathrm{eq}}(x)$ for the sake of simplicity, we show that the Liapunov functional F satisfies the following inequality:

$$F(p(\cdot)) \geqslant F(P_{\mathrm{eq}}(\cdot)) \quad (0<Q<1). \tag{66}$$

Proof: First we note that ϕ can be expressed in terms of P_{eq} as

$$\phi = \langle \phi \rangle + \frac{\tilde{C}_0(Q) Q (1-\tilde{C}_0(Q)^Q P_{\mathrm{eq}}^{Q-1})}{(Q-1)\beta}, \tag{67}$$

which follows from Eq. (56). Then $F(p(\cdot))$ is rewritten as

$$\begin{aligned} F(p(\cdot)) &= \int \phi p dx - \frac{1}{\beta(1/Q-1)}\left[1-\left(\int p^Q dx\right)^{-1/Q}\right] \\ &= \langle \phi \rangle - \frac{\tilde{C}_0(Q)^{Q+1} Q}{\beta(Q-1)} \int p P_{\mathrm{eq}}^{Q-1} dx - \frac{Q}{\beta(Q-1)}\left(\int p^Q dx\right)^{-1/Q} + \frac{Q(\tilde{C}_0(Q)+1)}{\beta(Q-1)} \end{aligned} \tag{68}$$

with

$$F(P_{\mathrm{eq}}(\cdot)) = \langle \phi \rangle + \frac{Q(1-\tilde{C}_0(Q))}{\beta(Q-1)}. \tag{69}$$

Then one has

$$F(p(\cdot)) - F(P_{\mathrm{eq}}(\cdot)) = \frac{Q}{\beta(Q-1)}\left[2\tilde{C}_0(Q) - \tilde{C}(Q) - \tilde{C}_0(Q)^{Q+1}\int p P_{\mathrm{eq}}^{Q-1} dx\right]. \tag{70}$$

Using a Hölder inequality one has

$$\left[\int (P_{\mathrm{eq}}^{(Q-1)/b} p^{1/b})^b dx\right]^{1/b}\left[\int (P_{\mathrm{eq}}^{Q/b'})^{b'} dx\right]^{1/b'} \geqslant \int p^{1/b} dx \tag{71}$$

with $b = 1/Q$, $b' = 1/(1-Q)$ $(1/b + 1/b' = 1)$.

Accordingly it follows that

$$\int P_{\mathrm{eq}}^{Q-1} p dx \left[\int P_{\mathrm{eq}}^Q dx\right]^{(1-Q)/Q} \geqslant \left(\int p^Q dx\right)^{1/Q}. \tag{72}$$

Substituting this into Eq. (70) one obtains inequality (66) implying that $F(p(\cdot))$ is bounded from below:

$$F(p(\cdot))-F(P_{\rm eq}(\cdot))\geqslant \frac{Q}{\beta(1-Q)}[-2\tilde{C}_0(Q)+\tilde{C}(Q)+\tilde{C}_0(Q)^2\tilde{C}(Q)^{-1}]$$
$$=\frac{Q}{\beta(1-Q)}(\tilde{C}_0(Q)-\tilde{C}(Q))^2\tilde{C}(Q)^{-1}\geqslant 0. \tag{73}$$

It is worth noting that the result that $F(p(\cdot))$ is bounded from below can be obtained without assuming the existence of the equilibrium probability distribution $P_{\rm eq}(x)$, which requires the self-consistent determining of $\langle\phi\rangle$ and $\tilde{C}_0$ in Eq. (61). In the above proof we have essentially used Eq. (67) to represent $\phi(x)$ in terms of a function that suffices to satisfy $\partial p/\partial t=0$ in Eq. (51) alone. Then also note that time independent terms in $F(p(\cdot))$ has no contribution to the boundedness of the $F(p(\cdot))$.

Assuming again the existence of the equilibrium distribution $P_{\rm eq}(x)$ for the sake of simplicity, we can show that an H-theorem with the H-functional given by the Liapunov functional (64) holds for $0<Q<1$:

H-Theorem:

$$\frac{dF}{dt}\leqslant 0. \tag{74}$$

Proof: Differentiating F with respect to t one obtains

$$\frac{dF}{dt}=\int\left(\phi-\frac{\tilde{C}(Q)^{Q+1}}{\beta(1/Q-1)}p^{Q-1}\right)\frac{\partial p}{\partial t}dx$$
$$=\int\left(\phi-\frac{\tilde{C}(Q)^{Q+1}}{\beta(1/Q-1)}p^{Q-1}\right)\left[-\frac{\partial}{\partial x}(-\phi_x(x)p)+\frac{1}{\beta}\tilde{C}(Q)^{Q+1}\frac{\partial^2}{\partial x^2}p^Q\right]dx$$
$$=-\int\phi_x^2 p\,dx-\frac{2}{\beta}Q\tilde{C}(Q)^{Q+1}\int\phi_x p^{Q-1}\frac{\partial p}{\partial x}dx-\frac{Q^2}{\beta^2}\tilde{C}(Q)^{2Q+2}\int p^{2Q-3}\left(\frac{\partial p}{\partial x}\right)^2 dx, \tag{75}$$

where integration by parts was used. Noting

$$\phi_x=-\frac{Q}{\beta}\tilde{C}_0(Q)^{Q+1}P_{\rm eq}^{Q-2}\frac{\partial p_{\rm eq}}{\partial x}, \tag{76}$$

dF/dt is further rewritten as

$$\frac{dF}{dt}=-\frac{Q^2}{\beta^2}\int p\left[\tilde{C}_0(Q)^{2(Q+1)}P_{\rm eq}^{2(Q-2)}\left(\frac{\partial P_{\rm eq}}{\partial x}\right)^2-2\tilde{C}_0(Q)^{Q+1}\tilde{C}(Q)^{Q+1}P_{\rm eq}^{Q-2}p^{Q-2}\frac{\partial p}{\partial x}\frac{\partial P_{\rm eq}}{\partial x}\right]dx$$
$$-\frac{Q^2}{\beta^2}\int p\tilde{C}(Q)^{2(Q+1)}p^{2(Q-2)}\left(\frac{\partial p}{\partial x}\right)^2 dx$$
$$=-\frac{Q^2}{\beta^2}\int p\left[\tilde{C}_0(Q)^{Q+1}P_{\rm eq}^{Q-2}\frac{\partial P_{\rm eq}}{\partial x}-\tilde{C}(Q)^{Q+1}p^{Q-2}\frac{\partial p}{\partial x}\right]^2 dx. \tag{77}$$

Then it follows that

$$\frac{dF}{dt}=-\frac{Q^2}{\beta^2(Q-1)^2}\int p\left[\frac{\partial}{\partial x}(\tilde{C}(Q)^{Q+1}p^{Q-1}-\tilde{C}_0(Q)^{Q+1}P_{\rm eq}^{Q-1})\right]^2 dx\leqslant 0. \tag{78}$$

We see that equality is implied by

$$\tilde{C}(Q)^{Q+1}p^{Q-1}-\tilde{C}_0(Q)^{Q+1}P_{\rm eq}^{Q-1}=c(\text{const}). \tag{79}$$

We can prove that $dF/dt=0$ is attained, if and only if $p=P_{\rm eq}$ $(c=0)$ as follows. Multiplying both hands of Eq. (79) by p and performing integration, one obtains

$$\tilde{C}(Q)-\tilde{C}_0(Q)^{Q+1}\int pP_{\rm eq}^{Q-1}dx=c. \tag{80}$$

Using inequality (72) one has

$$\int P_{\rm eq}^{Q-1}pdx\geqslant\left(\int p^Q dx\right)^{1/Q}\left[\int P_{\rm eq}^Q dx\right]^{-(1-Q)/Q}=\tilde{C}(Q)^{-1}\tilde{C}_0(Q)^{1-Q}. \tag{81}$$

Hence it follows from (80) and (81) that

$$c\tilde{C}(Q)\leqslant\tilde{C}(Q)^2-\tilde{C}_0(Q)^2. \tag{82}$$

On the other hand, one also obtains, by multiplying both hands of Eq. (79) by $P_{\rm eq}$ and by performing integration,

$$\tilde{C}(Q)^{Q+1}\int P_{\rm eq}p^{Q-1}dx-\tilde{C}_0(Q)=c. \tag{83}$$

Noting inequality similar to (72),

$$\int P_{\rm eq}p^{Q-1}dx\geqslant\tilde{C}_0(Q)^{-1}\tilde{C}(Q)^{1-Q}. \tag{84}$$

It follows from (83) that

$$c\tilde{C}_0(Q)\geqslant\tilde{C}(Q)^2-\tilde{C}_0(Q)^2. \tag{85}$$

Accordingly one has from (82) and (85)

$$c\tilde{C}_0(Q)\geqslant\tilde{C}(Q)^2-\tilde{C}_0(Q)^2\geqslant c\tilde{C}(Q). \tag{86}$$

Now we can see that assuming $c\neq 0$ leads to contradiction. Let $c>0$. One immediately obtains from the above inequality

$$\tilde{C}_0(Q)\geqslant\tilde{C}(Q)>0 \tag{87}$$

as well as

$$\tilde{C}(Q)^2-\tilde{C}_0(Q)^2>0 \tag{88}$$

which are in contradiction.

Assuming $c<0$ also leads to contradiction.

Accordingly one has

$$c=0, \tag{89}$$

which implies

$$p=\left[\frac{\tilde{C}_0(Q)}{\tilde{C}(Q)}\right]^{(Q+1)/(Q-1)}P_{\rm eq}. \tag{90}$$

Since both p and $P_{\rm eq}$ satisfy the normalization condition, it follows $p=P_{\rm eq}$. This concludes the proof of the H-theorem.

When $0<Q<1$, inequality (74) together with (66) implies that the equilibrium distribution (61) is the unique equilibrium solution of the NFPE (51), which is approached for long times from any initial condition, and that the free energy (64) continues to decrease until it approaches $F(P_{\rm eq}(\cdot))$.

We here note that inequality (78) together with the equality condition given by Eq. (79) would hold without the assumption for the existence of the equilibrium distribution $P_{\rm eq}(x)$ that satisfies the normalization condition: With regard to $P_{\rm eq}$ appearing in Eqs. (78) and (79) it suffices to use Eq. (56) or Eq. (76), which is obtained from the equilibrium condition $\partial p/\partial t=0$ of Eq. (51) alone. Given a function $P_{\rm eq}(x)$ satisfying Eq. (56), the equality condition (79) of the H-theorem (74) implies

$$p^{Q-1}=\frac{-(Q-1)\phi(x)}{(Q/\beta)\tilde{C}(Q)^{Q+1}}+\omega', \tag{91}$$

where ω' is some constant. Then, noting Eq. (56) the p given by (91) is seen to satisfy the equilibrium condition $\partial p/\partial t=0$ of Eq. (51). Since $\int p(t,x)dx=1$ holds for any $t>0$ for some initial condition $\int p(0,x)dx=1$, there must exist ω' such that the p given by Eq. (91) satisfy $\int p dx=1$. This implies the existence of the legitimate equilibrium distribution $P_{\rm eq}(x)$ given by Eq. (61) for the NFPE (51).

Finally, it is noted that whereas the correspondence between D and $(1/\beta)\tilde{C}_0(Q)^{Q+1}$ in the diffusion terms of the two NFPEs (13) and (51) under the equilibrium conditions turns out to hold with respect to the equilibrium distributions (24) and (63), it should not be the case dynamically. Comparing between the expressions of the nonequilibrium free energies (25) and (64), we see that $1/\beta$ in the NFPE (51) simply corresponds to D in the NFPE (13) putting aside the difference of the definitions of the entropies S and $\tilde{S}$.

IV. SUMMARY AND DISCUSSION

We have studied two different types of nonlinear master equations (13) and (51) taking the form of nonlinear Fokker–Planck equations exhibiting equilibrium distributions of Tsallis statistics respectively with the first and third choices. We have proven H-theorems by constructing Liapunov functions that take the form of free energy based on Tsallis entropies. The H-theorems in this case ensure uniqueness of as well as convergence to the equilibrium distribution. It is important to note that although the equilibrium distributions of Tsallis statistics of the third choice take a form with a self-reference style that must be determined in a self-consistent manner from Eqs. (7)–(10), no multiple distributions are possible with a single equilibrium distribution being uniquely determined for a given set of parameters q and β.

When defining the free energy, we incorporated the ordinarily used average of the internal energy exhibiting extensivity instead of q-averaged internal energy exhibiting nonextensivity, which was used in Tsallis statistics of the second choice[2,3] and was also incorporated to construct a free energy associated with the H-function (11) of the H-theorem (12) for a linear master equation.[23] It is worth noting that when the q-averaged internal energy is used, we can no longer prove H-theorems for our NFPEs.

In proving the H-theorems of the present systems I have assumed that the support of the equilibrium distribution extends to infinity for the sake of simplicity. It is straightforward to prove that our H-theorems also hold true in the case where the equilibrium distribution has a compact support and a boundary condition analogous to the natural boundary condition (16) is imposed. For instance, in the case of the NFPE (13) of Sec. II the restriction $0<q<1$ can be lifted and the H-theorem (33) together with inequality (27) can be extended to the case with $q>1$ where the equilibrium distribution (21) must be subjected to a high-energy cutoff [the Tsallis cutoff, i.e., $P_{\rm eq}(x)=0$ for x satisfying $1-\beta(q-1)\phi(x)<0$].

The present study reveals that understanding physical meaning of Tsallis entropies may be reduced to that of the nonlinear Fokker–Planck equations investigated. Our results have clarified the relationship between Tsallis' thermostatistics of the first and third choices from the view point of dynamical processes. The two choices of Tsallis' thermostatistics yield similar equilibrium distributions similar to each other, when the escort probabilities are considered instead of the original probabilities. The dynamics underlying the equilibrium distributions, however, are governed by different nonlinear evolution equations associated with different entropies. In this regard, it might well be understood that Tsallis statistics of the third choice follows from the modified form of the generalized entropy (50) rather than from using such an unfamiliar averaging procedure for the energy constraint as (6) for optimizing the original form of Tsallis entropy (1). Parameters D and $1/\beta$, characterizing, respectively, the equilibrium distributions of the first (24) and third (63) choices, are given a meaning within the dynamics level, that is, the constant coefficients of the nonlinear diffusion terms of the NFPEs. Furthermore, those parameters play the role of ''temperature'' in each expression of the free energies.

For more detailed knowledge about the physical meaning of Tsallis entropies, research of microscopic mechanisms underlying the appearance of the nonlinear diffusion terms of the NFPEs will be required, without introducing phenomenology.

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A simple treatment of the sine-Gordon equation

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To avoid difficulties due to the complexity of the Lax pair of the sine-Gordon equation, the orthogonality relations of the squared Jost solutions is derived simply using the $1+1$ dimensional Green's theorem. The direct perturbation theory for sine-Gordon in the laboratory reference is re-developed, correcting some numerical coefficients in published orthogonality relationships. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1329342]

I. INTRODUCTION

The pioneering work on direct theory for the perturbed sine-Gordon equation by McLaughlin and Scott[1] has deep meaning not only in physical applications but also in mathematical substance. It is the first example of the perturbed nonlinear equation of second derivative in time that is essentially different from that for the perturbed equations involving only first derivative in time. They transformed the linearized equation of second derivative in time to an equivalent equation just containing the first derivative in time. Then they treated the equation with the idea of the usual Green's function theory for the linear partial differential equations. Since the linearized equation is very complicated and its potential is often defined by some of its functional properties rather than given explicitly, development of the theory is very laborious.

At that time the perturbation theory based on the inverse scattering transform(IST) was generally accepted. In order to emphasize the special meaning of the direct perturbation theory, the authors[1] inclined to avoid using the results of the inverse scattering transform and developed the direct theory based on a particular method of variation with respect to the potential. However, avoiding results of IST is obviously unnecessary. A recent work[2,3] on direct perturbation theory for dark solitons do use the results of IST to construct a rigorous complete set of squared Jost solutions, overcoming the long frustrating difficulty caused by the nonvanishing boundary conditions.

In Ref. 1, although the authors inclined to avoid using results of IST, a set of squared Jost solutions was still given in the appendix in which we find one biorthogonality relationship contains an incorrect numerical coefficient because they can not be verified via explicit expressions of Jost solutions of the one-kink case. Since a complete set of solutions for the linearized equation is fundamental to the direct perturbation theory, it is reasonable to develop a direct theory for perturbed sine-Gordon equation along a similar procedure for the perturbed NLS equation,[2–4] that is, first, to construct a rigorous complete set of solutions for the linearized equation via results of the IST.

In this paper work all of these difficulties are overcome by using $1+1$ dimensional Green's theorem and the direct theory for the perturbed sine-Gordon equation is exactly developed. For simplicity and to emphasize essential points, we are restricted mainly to a single soliton (kink) case, however, almost all of the formulas can be extended to the multisoliton case.

II. THE PERTURBED EQUATION

For physical applications it is necessary to develop a direct approach to the perturbed sine-Gordon equation in the laboratory reference in which it takes the form

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$$\alpha_{xx}-\alpha_{tt}-\sin\alpha=\epsilon r[\alpha], \tag{1}$$

where x, t are the space–time, ϵ is a small parameter, and $r[\alpha]$ is a functional of α. When ϵ vanishes, (1) tends to the unperturbed sine-Gordon equation. Since (1) has a second-order derivative in t, the initial condition also is included $\alpha_t(x,0)$, in addition to $\alpha(x,0)$. For example, we assume

$$\alpha(x,0)=\theta(x,0), \quad \alpha_t(x,0)=\theta_t(x,0), \tag{2}$$

where $\theta(x,t)$ is usually a soliton solution of the unperturbed sine-Gordon equation.

Soliton solutions of the unperturbed sine-Gordon equation are easily found in the light-cone coordinates where its Lax pair takes a standard Zakharov–Shabat form. Soliton solutions in the laboratory reference can then be obtained by a simple coordinate transformation.[5] However, the initial condition (2) can not be expressed in the light-cone coordinates, hence the direct approach to the perturbed sine-Gordon was developed in the laboratory reference in the pioneering work of McLaughlin and Scott.[1]

Suppose

$$\alpha=\theta^a+\epsilon q, \tag{3}$$

where θ^a is the adiabatic solution in the usual sense[1,4,6–8] and ϵq is the remaining term of the order of ϵ. Substitution of it into (1) yields

$$\{\partial_{xx}-\partial_{tt}-\cos\theta\}q=R, \tag{4}$$

where the operator on the left hand side is called the linearized operator and

$$R=r[\theta]-s[\theta], \quad s[\theta]=\frac{1}{\epsilon}\{\theta_{xx}-\theta_{tt}-\sin\theta\}. \tag{5}$$

(4) is of the order of ϵ, the θ in the left hand side and in the term $r[\theta]$ is the exact soliton solution while θ in the term $s[\theta]$ is the adiabatic solution. The initial condition (2) turns to

$$q(x,0)=0, \quad q_t(x,0)=0. \tag{6}$$

To solve (4) with the initial condition (6) by the Green's function method, we must first find solutions of the homogeneous version of (4), i.e., (4) with a vanishing right hand side.

III. A SINGLE SOLITON CASE

To explain the essential points of the direct perturbation theory, we take the simplest case, i.e., a single soliton (kink) case as an example. The kink solution of the unperturbed sine-Gordon equation is known as[1,5]

$$\theta=4\arctan e^X, \tag{7}$$

where

$$X=-i[\kappa_1(x-x_1)+\lambda_1 t], \tag{8}$$

x_1 is a real constant

$$\kappa=\tfrac{1}{2}(\zeta-\zeta^{-1}), \quad \lambda=\tfrac{1}{2}(\zeta+\zeta^{-1}), \quad \lambda^2-\kappa^2=1, \tag{9}$$

ζ is a spectral parameter[2] and ζ_1 lies on the upper imaginary axis of the complex ζ-plane, $\zeta_1=i|\zeta_1|$. Substituting the expression of $\cos\theta=1-2\,\mathrm{sech}^2 X$ obtained from (8) into (4) we have

$$\{\partial_{xx}-\partial_{tt}-(1-2\,\mathrm{sech}^2 X)\}q=R. \tag{10}$$

To construct the Green's function theory for (10), we must find all eigenfunctions of the linearized operator with zero eigenvalue in advance. Suppose $\Psi(x,t,\zeta)$ is one of such solutions, then

$$\{\partial_{xx}-\partial_{tt}-(1-2\,\mathrm{sech}^2 X)\}\Psi(x,t,\zeta)=0. \tag{11}$$

Setting

$$\Psi(x,t,\zeta)=\theta(x,t,\zeta)e^{i(\kappa x+\lambda t)}, \tag{12}$$

where the form of the exponential is chosen to ensure the $1+1$ dimensional Lorentz invariance, (11) becomes

$$\{i2\lambda\partial_t-i2\kappa\partial_x+\partial_{tt}-\partial_{xx}-2\,\mathrm{sech}^2 X\}\theta(x,t,\zeta)=0, \tag{13}$$

here we have used (9). We may assume $\theta(x,t,\zeta)$ depends on t and x via X, then

$$\partial_{tt}-\partial_{xx}=-\partial_{XX},\quad i2\lambda\partial_t-i2\kappa\partial_x=(\zeta\zeta_0^{-1}+\zeta^{-1}\zeta_0)\partial_X. \tag{14}$$

Hence (13) becomes

$$\{\xi^2\partial_X+\xi L+\partial_X\}\theta=0, \tag{15}$$

where

$$\xi=\frac{\zeta}{\zeta_0},\quad L=\partial_{XX}+2(1-\tanh^2 X). \tag{16}$$

Expanding $\theta(X,\zeta)$ into a power series of ξ whose coefficients $\theta_n(X)$ are functions of X only, $\theta=\theta_0+\xi\theta_1+\xi^2\theta_2+\cdots$, then equating the coefficients of each power of ξ, from (15) we obtain recursion equations:

$$\theta_{0X}=0,\quad \theta_{1X}=L\theta_0,\quad \theta_{2X}=L\theta_1,\quad \theta_{3X}=L\theta_2-\theta_{1X},\ldots. \tag{17}$$

It is easy to solve (17) successively, we finally obtain an eigenfunction of (11)

$$\Psi(x,t,\zeta)=\frac{e^{i(\kappa x+\lambda t)}}{(\zeta-\overline{\zeta_1})^2}(\zeta^2-2\zeta\overline{\zeta_1}\tanh X+\overline{\zeta_1^2}), \tag{18}$$

where the constant factor $(\zeta-\overline{\zeta_1})^{-2}$ is introduced for later convenience. Similarly, another eigenfunction of (11) is

$$\Phi(x,t,\zeta)=\frac{e^{-i(\kappa x+\lambda t)}}{(\zeta-\overline{\zeta_1})^2}(\zeta^2+2\zeta\overline{\zeta_1}\tanh X+\overline{\zeta_1^2}). \tag{19}$$

$\Psi(x,t,\zeta)$ and $\Phi(x,t,\zeta)$ are analytic in the upper half plane, but have different asymptotic behaviors

$$\begin{aligned}&\Psi(x,t,\zeta)\to e^{i(\kappa x+\lambda t)},\\ &\Phi(x,t,\zeta)\to a(\zeta)^2 e^{-i(\kappa x+\lambda t)},\end{aligned}\quad \text{as } x\to\infty \tag{20}$$

and

$$\begin{aligned}\Psi(x,t,\zeta)&\to e^{i(\kappa x+\lambda t)},\\ \Phi(x,t,\zeta)&\to a(\zeta)^2 e^{-i(\kappa x+\lambda t)},\end{aligned}\quad \text{as } x\to-\infty, \tag{21}$$

where

$$a(\zeta)=\frac{\zeta-\zeta_1}{\zeta-\bar{\zeta}_1}. \tag{22}$$

Different asymptotic behaviors of $\Psi(x,t,\zeta)$ and $\Phi(x,t,\zeta)$ show the linear independence between them.

IV. GREEN'S THEOREM

The next step of development is to choose an adequate adjoint function for the eigenfunction of (11) and to define the corresponding inner product. We now derive a general integral relation by using the $1+1$ dimensional Green's theorem. Because both $\Psi(x,t,\zeta)$ and $\Phi(x,t,\zeta)$ are eigenfunctions of (11), we have

$$\begin{aligned}&i\partial_t\{\Phi(x,t,\zeta')\Psi(x,t,\zeta)_t-\Phi(x,t,\zeta')_t\Psi(x,t,\zeta)\}\\ &\quad=i\partial_x\{\Phi(x,t,\zeta')\Psi(x,t,\zeta)_x-\Phi(x,t,\zeta')_x\Psi(x,t,\zeta)\}.\end{aligned} \tag{23}$$

Integration upon each side with respect to t and x in a domain of Ω where x runs from $-\infty$ to ∞ and t from 0 to t, by Green's theorem,[9] we obtain

$$\begin{aligned}&i\int_{-\infty}^{\infty}dx\{\Phi(x,t,\zeta')\Psi(x,t,\zeta)_t-\Phi(x,t,\zeta')_t\Psi(x,t,\zeta)\}\Big|_{t=0}^{t=t}\\ &\quad=i\int_0^t dt\{\Phi(x,t,\zeta')\Psi(x,t,\zeta)_x-\Phi(x,t,\zeta')_x\Psi(x,t,\zeta)\}\Big|_{x=-\infty}^{x=\infty}.\end{aligned} \tag{24}$$

The integrand of the right hand side, $A(x,t,\zeta',\zeta)$, tends to

$$\begin{aligned}A(L,t,\zeta',\zeta)&=-a(\zeta')^2(\kappa'+\kappa)e^{-i(\kappa'-\kappa)L}e^{-i(\lambda'-\lambda)t},\\ A(-L,t,\zeta',\zeta)&=a(\zeta)^2(\kappa'+\kappa)e^{i(\kappa'-\kappa)L}e^{-i(\lambda'-\lambda)t},\end{aligned} \tag{25}$$

in the limit of $L\to\infty$. In (25), only the factors $e^{-i(\lambda'-\lambda)t}$ is dependent of t. The integration on the right hand side of (25) is equal to the integrand divided by $i(\lambda-\lambda')$, hence we obtain

$$i\int_{-\infty}^{\infty}dx\{\Phi(x,t,\zeta')\Psi(x,t,\zeta)_t-\Phi(x,t,\zeta')_t\Psi(x,t,\zeta)\}=\lim_{L\to\infty}\frac{1}{-i(\lambda'-\lambda)}B(L.t,\zeta',\zeta), \tag{26}$$

where

$$B(L,t,\zeta',\zeta)=A(L,t,\zeta',\zeta)-A(-L,t,\zeta',\zeta). \tag{27}$$

Noticing

$$\begin{aligned}\lambda-\lambda'&=\tfrac{1}{2}(\zeta-\zeta')(1-\zeta^{-1}\zeta'^{-1}),\\ \kappa-\kappa'&=\tfrac{1}{2}(\zeta-\zeta')(1+\zeta^{-1}\zeta'^{-1}),\end{aligned} \tag{28}$$

and ζ and ζ' should be considered as $\zeta+i0$ and $\zeta'+i0$, we have

$$\lim_{L\to\infty} P\frac{1}{-i(\lambda'-\lambda)}e^{-i(\kappa'-\kappa)L}=\frac{2}{(1-\zeta^{-2})}\pi\delta(\zeta-\zeta')=\frac{\zeta}{\kappa}\pi\delta(\zeta-\zeta'). \tag{29}$$

Finally, (26) becomes

$$i\int_{-\infty}^{\infty}dx\{\Phi(x,t,\zeta')\Psi(x,t,\zeta)_t-\Phi(x,t,\zeta')_t\Psi(x,t,\zeta)\}=-4\pi\zeta a(\zeta)^2\delta(\zeta-\zeta'). \tag{30}$$

V. THE LINEARIZED OPERATOR WITH THE FIRST DERIVATIVE IN *t*

Since (4) has a second-order derivative in t, in the direct approach it is necessary to transform it into an equivalent equation having first-order derivatives in t only.[1] (4) is obviously equivalent to

$$\begin{pmatrix} i\partial_t & -1 \\ \partial_{xx}-\cos\theta & i\partial_t \end{pmatrix}\begin{pmatrix} q \\ iq_t \end{pmatrix}=\begin{pmatrix} 0 \\ R \end{pmatrix}. \tag{31}$$

We can simply write it as

$$\{i\partial_t-\mathbf{L}\}\mathbf{q}=\mathbf{R}, \tag{32}$$

where

$$\mathbf{L}=-\begin{pmatrix} 0 & -1 \\ \partial_{xx}-(1-2\,\mathrm{sech}^2\,X) & 0 \end{pmatrix}, \tag{33}$$

$$\mathbf{q}=\begin{pmatrix} q \\ iq_t \end{pmatrix},\quad \mathbf{R}=\begin{pmatrix} 0 \\ R \end{pmatrix}. \tag{34}$$

Now we write (11) as

$$\{i\partial_t-\mathbf{L}\}\mathbf{\Psi}(x,t,\zeta)=\mathbf{0}, \tag{35}$$

where $\mathbf{0}=(0,0)^T$ and

$$\mathbf{\Psi}(x,t,\zeta)=\begin{pmatrix} \Psi(x,t,\zeta) \\ i\Psi(x,t,\zeta)_t \end{pmatrix}. \tag{36}$$

Taking (30) into account, we define the adjoint function for $\mathbf{\Psi}(x,t,\zeta)$ by

$$\mathbf{\Psi}(x,t,\zeta)^A=\mathbf{\Phi}(x,t,\zeta)^T(-i\sigma_2)=(-i\Phi(x,t,\zeta)_t\ \ \Phi(x,t,\zeta)), \tag{37}$$

and the inner product by

$$\langle\mathbf{\Psi}(t,\zeta')|\mathbf{\Psi}(t,\zeta)\rangle=\int_{-\infty}^{\infty}dx\mathbf{\Psi}(x,t,\zeta')^A\mathbf{\Psi}(x,t,\zeta). \tag{38}$$

(26) and (30) turn to

$$\langle\mathbf{\Psi}(t,\zeta')|\mathbf{\Psi}(t,\zeta)\rangle=\lim_{L\to\infty}\frac{1}{-i(\lambda'-\lambda)}B(L,t,\zeta',\zeta)=-4\pi\zeta a(\zeta)^2\delta(\zeta-\zeta'). \tag{39}$$

Noticing time-independence of the right hand side of (39), it is convenient to introduce

$$\Psi(x,\zeta)=e^{-i\lambda t}\Psi(x,t,\zeta),\quad \Psi'(x,\zeta)=e^{-i\lambda t}i\Psi(x,t,\zeta)_t, \tag{40}$$

namely

$$\Psi(x,\zeta)=\frac{e^{i\kappa x}}{(\zeta-\bar{\zeta}_1)^2}(\zeta^2-2\zeta\zeta_1\tanh X+\zeta_1^2), \tag{41}$$

and

$$\Psi'(x,\zeta)=-\lambda\Psi(x,\zeta)+\lambda_1\frac{e^{i\kappa x}}{(\zeta-\bar{\zeta}_1)^2}2\zeta\zeta_1(1-\tanh^2 X). \tag{42}$$

From (35) we obtain

$$\{i\partial_t-\mathbf{L}\}\mathbf{\Psi}(x,\zeta)=\lambda\mathbf{\Psi}(x,\zeta), \tag{43}$$

where

$$\mathbf{\Psi}(x,\zeta)=\begin{pmatrix}\Psi(x,\zeta)\\ \Psi'(x,\zeta)\end{pmatrix}. \tag{44}$$

Since the right hand side of (39) is independent of t, and involves $\delta(\zeta-\zeta')$, we define the inner product of $\mathbf{\Psi}(x,\zeta)$ with its adjoint such that

$$\langle\mathbf{\Psi}(\zeta')|\mathbf{\Psi}(\zeta)\rangle=\int_{-\infty}^{\infty}dx\mathbf{\Psi}(x,\zeta')^A\mathbf{\Psi}(x,\zeta), \tag{45}$$

where the adjoint is

$$\mathbf{\Psi}(x,\zeta)^A=\mathbf{\Phi}(x,\zeta)^T(-i\sigma_2)=(-\Phi'(x,\zeta),\ \Phi(x,\zeta)). \tag{46}$$

We then obtain

$$\langle\mathbf{\Psi}(\zeta')|\mathbf{\Psi}(\zeta)\rangle=\lim_{L\to\infty}\frac{1}{-i(\lambda'-\lambda)}B(L,0,\zeta',\zeta)=-4\pi\zeta a(\zeta)^2\delta(\zeta-\zeta'). \tag{47}$$

For $\zeta=\zeta_1$, from (43) we have

$$\{i\partial_t-\mathbf{L}\}\mathbf{\Psi}(x,\zeta_1)=\lambda_1\mathbf{\Psi}(x,\zeta_1) \tag{48}$$

and

$$\{i\partial_t-\mathbf{L}\}\dot{\mathbf{\Psi}}(x,\zeta_1)=\lambda_1\dot{\mathbf{\Psi}}(x,\zeta_1)+\zeta_1^{-1}\kappa_1\mathbf{\Psi}(x,\lambda_1), \tag{49}$$

where

$$\dot{\Psi}(x,\zeta_1)=\frac{d}{d\zeta}\Psi(x,\zeta)|_{\zeta=\zeta_1}. \tag{50}$$

But for $\zeta=\zeta_1$, which is a double zero of $a(\zeta)^2$, we have

$$\langle\mathbf{\Psi}(\zeta_1)|\mathbf{\Psi}(\zeta_1)\rangle=0. \tag{51}$$

From (47) we have

$$-i(\lambda'-\lambda)\langle\mathbf{\Psi}(\zeta')|\mathbf{\Psi}(\zeta)\rangle=B(\infty,0,\zeta',\zeta). \tag{52}$$

Applying an operator $d/d\zeta^2$ to (52), then setting $\zeta=\zeta'=\zeta_1$, we obtain

$$\langle \mathbf{\Psi}(\zeta_1)|\dot{\mathbf{\Psi}}(\zeta_1)\rangle = -i2\zeta_1\dot{a}(\zeta_1)^2. \tag{53}$$

Applying an operator $\{d^3/d\zeta^3+3(d/d\zeta' d^2/d\zeta^2\}$ to (52), setting $\zeta=\zeta'=\zeta_1$, we obtain

$$\langle \dot{\mathbf{\Psi}}(\zeta_1)|\dot{\mathbf{\Psi}}(\zeta_1)\rangle = -i2\zeta_1\dot{a}(\zeta_1)\ddot{a}(\zeta_1) - i2\dot{a}(\zeta_1)^2. \tag{54}$$

(47), (53), and (54) are desired orthogonality relations. These agree with the orthogonality relations published in Ref. 1 (after proper normalization of the eigenfunctions), except for Eq. (54) for which an incorrect numerical coefficient appears in Ref. 1.

VI. THE EXPANSION OF THE UNITY

Assume $\mathbf{q}(x)$ in (32) be expanded as

$$\mathbf{q}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\zeta f(\zeta)\mathbf{\Psi}(x,\zeta) + f_1\mathbf{\Psi}(x,\zeta_1) + g_1\dot{\mathbf{\Psi}}(x,\zeta_1). \tag{55}$$

By using the orthogonality relations, we obtain

$$f(\zeta) = -\frac{1}{2\zeta a(\zeta)^2}\langle \mathbf{\Psi}(\zeta)|\mathbf{f}\rangle, \quad g_1 = i\frac{1}{2\zeta_1\dot{a}(\zeta_1)^2}\langle \mathbf{\Psi}(\zeta_1)|\mathbf{f}\rangle, \tag{56}$$

and

$$f_1 = i\frac{1}{2\zeta_1\dot{a}(\zeta_1)^2}\langle \dot{\mathbf{\Psi}}(\zeta_1)|\mathbf{f}\rangle - i\frac{1}{2\zeta_1\dot{a}(\zeta_1)^2}\left\{\frac{1}{\zeta_1}+\frac{\ddot{a}(\zeta_1)}{\dot{a}(\zeta_1)}\right\}\langle \mathbf{\Psi}(\zeta_1)|\mathbf{f}\rangle. \tag{57}$$

Substituting them back to (55) yields

$$\begin{aligned}\delta(x-y) = &-\frac{1}{2\pi}\int_\Gamma d\zeta \frac{1}{2\zeta a(\zeta)^2}\mathbf{\Psi}(x,\zeta)\mathbf{\Psi}(y,\zeta)^A \\ &+ i\frac{1}{2\zeta_1\dot{a}(\zeta_1)^2}\{\dot{\mathbf{\Psi}}(x,\zeta_1)\mathbf{\Psi}(y,\zeta_1)^A + \mathbf{\Psi}(x,\zeta_1)\dot{\mathbf{\Psi}}(y,\zeta_1)^A\} \\ &- i\frac{1}{2\zeta_1\dot{a}(\zeta_1)^2}\left\{\frac{1}{\zeta_1}+\frac{\ddot{a}(\zeta_1)}{\dot{a}(\zeta_1)}\right\}\mathbf{\Psi}(x,\zeta_1)\mathbf{\Psi}(y,\zeta_1)^A.\end{aligned} \tag{58}$$

Here, as noted, real ζ should be considered as $\zeta+i0$, the factor ζ^{-1} in the integrand is replaced by $(\zeta+i0)^{-1}$, its pole $\zeta=0-i0$ is in the lower half plane. Hence, the integral path Γ is along the real axis from $-\infty$ to ∞ and runs above the origin when approaches it. This integral path is denoted by Γ. (59) is the expansion of the unity.

VII. PROOF OF COMPLETENESS RELATION

To prove (58), it is necessary to show that the right hand side is equal to $\delta(x-y)$ by using an independent approach. $\mathbf{\Psi}(x,\zeta)$ and $\mathbf{\Phi}(x,\zeta)$ are analytical on the upper half-plane of complex ζ, as seen from their explicit expressions (18) and (19). It can be shown[5] that

$$-\frac{1}{2\pi}\int_\Gamma d\zeta\frac{1}{2\zeta}B(x,y,\zeta) = \delta(x-y), \tag{59}$$

where

$$B(x,y,\zeta)=\begin{pmatrix}1\\-\lambda\end{pmatrix}(-\lambda\,1)e^{i\kappa(x-y)}. \tag{60}$$

In the case of $x>y$, the first term in the right hand side of (58) minus the left hand side of (59) is

$$-\frac{1}{2\pi}\int_\Gamma d\zeta\frac{1}{2\zeta}\left\{\frac{1}{a(\zeta)^2}\mathbf{\Psi}(x,\zeta)\mathbf{\Psi}(y,\zeta)^A-B(x,y,\zeta)\right\}. \tag{61}$$

In the limit of $|\zeta|\to\infty$, the integrand of (61) approaches $O(|\zeta|^{-1})e^{i\kappa(x-y)}$.

As $x>y$, a vanishing integral on an upper semicircle with an extremely large radius can be added to the integral in (61). Thus the integral in (61) becomes a clockwise contour integral. The pole $\zeta=-i0$, locating on the lower half-plane, lies out of the contour.

Near ζ_1, we have

$$\frac{1}{a(\zeta)^2}=\frac{1}{\dot a(\zeta_1)^2(\zeta-\zeta_1)^2}-\frac{\ddot a(\zeta_1)}{\dot a(\zeta_1)^3(\zeta-\zeta_1)}+\cdots. \tag{62}$$

Evaluating the contour integral, the contribution due to ζ_1 just cancels the second in the right hand side of (58). Hence the right hand side of (58) is indeed equal to $\delta(x-y)$ when $x\geqslant y$.

As $x\leqslant y$, we can show

$$\begin{aligned}\delta(x-y)=&-\frac{1}{2\pi}\int_\Gamma d\zeta\frac{1}{2\zeta\tilde a(\zeta)^2}\tilde{\mathbf{\Phi}}(x,\zeta)\tilde{\mathbf{\Phi}}(y,\zeta)^A\\&-i\frac{1}{2\overline{\zeta_1}\dot{\tilde a}(\overline{\zeta_1})^2}\{\dot{\tilde{\mathbf{\Phi}}}(x,\overline{\zeta_1})\tilde{\mathbf{\Phi}}(y,\overline{\zeta_1})^A+\tilde{\mathbf{\Phi}}(x,\overline{\zeta_1})\dot{\tilde{\mathbf{\Phi}}}(y,\overline{\zeta_1})^A\}\\&+i\frac{1}{2\overline{\zeta_1}\dot{\tilde a}(\overline{\zeta_1})^2}\left\{\frac{1}{\overline{\zeta_1}}+\frac{\ddot{\tilde a}(\overline{\zeta_1})}{\dot{\tilde a}(\overline{\zeta_1})}\right\}\mathbf{\Psi}(x,\overline{\zeta_1})\mathbf{\Psi}(y,\overline{\zeta_1})^A.\end{aligned} \tag{63}$$

Here

$$\tilde a(\zeta)=a(\zeta)^{-1}=\frac{\zeta-\overline{\zeta_1}}{\zeta-\zeta_1}, \tag{64}$$

and

$$\tilde{\mathbf{\Phi}}(x,\zeta)=\tilde a(\zeta)^2\mathbf{\Psi}(x,\zeta),\quad \tilde{\mathbf{\Psi}}(x,\zeta)=\tilde a(\zeta)^2\mathbf{\Phi}(x,\zeta) \tag{65}$$

are analytical on the lower half-plane of complex ζ.

Noting (64) and (65), we can transform (61) into

$$-\frac{1}{2\pi}\int_\Gamma d\zeta\frac{1}{2\zeta}\left\{\frac{1}{\tilde a(\zeta)^2}\tilde{\mathbf{\Phi}}(x,\zeta)\tilde{\mathbf{\Phi}}(y,\zeta)^A-B(x,y,\zeta)\right\}. \tag{66}$$

When $x<y$, in the limit of $|\zeta|\to\infty$, the integrand of (66) approaches $O(|\zeta|^{-1})e^{i\kappa(x-y)}$. A vanishing integral on a lower semicircle with an extremely large radius can be added to the integral in (66). Thus the integral in (66) becomes an anti-clockwise contour integral. The pole $\zeta=-i0$, locating on the lower half plane, lies inside of the contour.

As $\zeta\to-i0$, we have $i\kappa\to\infty$ and $e^{i\kappa(x-y)}\to0$, that is, the contribution of this pole vanishes.

Near $\overline{\zeta_1}$, we have

$$\frac{1}{\tilde{a}(\zeta)^2}=\frac{1}{\dot{\tilde{a}}(\bar{\zeta}_1)^2(\zeta-\bar{\zeta}_1)^2}-\frac{\ddot{\tilde{a}}(\bar{\zeta}_1)}{\dot{\tilde{a}}(\bar{\zeta}_1)^3(\zeta-\bar{\zeta}_1)}+\cdots. \tag{67}$$

Evaluating the contour integral, the contribution due to $\bar{\zeta}_1$ just cancels the second in the right hand side of (63). Hence the right hand side of (63) is indeed equal to $\delta(x-y)$ when $x\geqslant y$.

VIII. VERIFICATION IN A SINGLE SOLITON CASE

We have shown (58) for $x\geqslant y$ and (63) for $x\leqslant y$. If we can show that the right hand sides of these two equations are equal to each other for arbitrary x and y, then the right hand side of (58) and that of (63) are equal to $\delta(x-y)$ in general. From (22), we have

$$\zeta_1\ddot{a}(\zeta_1)+\dot{a}(\zeta_1)=0,\quad \bar{\zeta}_1\ddot{\tilde{a}}(\bar{\zeta}_1)+\dot{\tilde{a}}(\bar{\zeta}_1)=0 \tag{68}$$

and

$$i\zeta_1\dot{a}(\zeta_1)^2=-i\bar{\zeta}_1\dot{\tilde{a}}(\bar{\zeta}_1)=\frac{1}{4|\zeta_1|}. \tag{69}$$

Hence, comparing (58) with (63), it is necessary to show the following equation for arbitrary x and y:

$$\dot{\mathbf{\Psi}}(x,\zeta_1)\mathbf{\Psi}(y,\zeta_1)^A+\mathbf{\Psi}(x,\zeta_1)\dot{\mathbf{\Psi}}(y,\zeta_1)^A=\dot{\tilde{\mathbf{\Phi}}}(x,\bar{\zeta}_1)\tilde{\mathbf{\Phi}}(y,\bar{\zeta}_1)^A+\tilde{\mathbf{\Phi}}(x,\bar{\zeta}_1)\dot{\tilde{\mathbf{\Phi}}}(y,\bar{\zeta}_1)^A. \tag{70}$$

From (41), we have

$$\mathbf{\Psi}(x,\zeta_1)=\tilde{\mathbf{\Phi}}(x,\bar{\zeta}_1)=h_1\frac{1}{2}\operatorname{sech}X\begin{pmatrix}1\\ \lambda_1\tanh X\end{pmatrix}, \tag{71}$$

where $h_1=e^{i\kappa_1x_1-\lambda_1t}$. Similarly, we have

$$\mathbf{\Phi}(x,\zeta_1)=\tilde{\mathbf{\Psi}}(x,\bar{\zeta}_1)=h_1^{-1}\frac{1}{2}\operatorname{sech}X\begin{pmatrix}1\\ -\lambda_1\tanh X\end{pmatrix}. \tag{72}$$

From (42), we have

$$\dot{\mathbf{\Psi}}(x,\zeta_1)=\dot{\tilde{\mathbf{\Phi}}}(x,\bar{\zeta}_1)=-h_1\zeta_1\kappa_1\frac{1}{2}\operatorname{sech}X\begin{pmatrix}0\\ 1\end{pmatrix}+h_1i\zeta_1\lambda_1x\frac{1}{2}\operatorname{sech}X\begin{pmatrix}1\\ \lambda_1\tanh X\end{pmatrix}. \tag{73}$$

Similarly, we have

$$\dot{\mathbf{\Phi}}(x,\zeta_1)=\dot{\tilde{\mathbf{\Psi}}}(x,\bar{\zeta}_1)=h_1^{-1}\zeta_1\kappa_1\frac{1}{2}\operatorname{sech}X\begin{pmatrix}0\\ 1\end{pmatrix}-h_1^{-1}i\zeta_1\lambda_1x\frac{1}{2}\operatorname{sech}X\begin{pmatrix}1\\ -\lambda_1\tanh X\end{pmatrix}. \tag{74}$$

Substituting these formula into (70), we can see the validity of (70). Therefore, (68) is correct, and the completeness relation is proved.

IX. SECULARITY CONDITIONS

Substituting the expansion (55) into (32), and evaluating the inner products of $\mathbf{\Psi}(x,\zeta)^A$, $\mathbf{\Psi}(x,\zeta_1)^A$ and $\dot{\mathbf{\Psi}}(x,\zeta_1)^A$ with the resulted equation, respectively, we obtain

$$-4\pi\zeta a(\zeta)^2\{ig_t(\zeta)+\lambda f(\zeta)\}=\langle\mathbf{\Psi}(\zeta)|\mathbf{R}\rangle, \tag{75}$$

$$-i2\zeta_1\dot{a}(\zeta_1)^2\{ig_{1t}+\lambda_1 g_1\}=\langle\mathbf{\Psi}(\zeta_1)|\mathbf{R}\rangle, \tag{76}$$

and

$$-i2\zeta_1\dot{a}(\zeta_1)^2\{if_{1t}+\lambda_1 f_1+\zeta_1\kappa_1 g_1\}-i2\dot{a}(\zeta_1)\{\zeta_1\ddot{a}(\zeta_1)+\dot{a}(\zeta_1)\}\{ig_{1t}+\lambda_1 g_1\}=\langle\dot{\mathbf{\Psi}}(\zeta_1)|\mathbf{R}\rangle. \tag{77}$$

Although the initial value of $g_1(0)$ and $f_1(0)$ vanishes, the values of $g_1(t)$ and $f_1(t)$ will grow in time unless we impose the secularity condition[4,6,7,10–12]

$$\langle\mathbf{\Psi}(\zeta_1)|\mathbf{R}\rangle=0, \quad \langle\dot{\mathbf{\Psi}}(\zeta_1)|\mathbf{R}\rangle=0. \tag{78}$$

By means of these secularity conditions the adiabatic solution can be determined. That is, the time dependence of the parameters characterizing soliton solution of order of ϵ can be determined. Then from (75) one can determine the time dependence of $f(\zeta)$, because the right hand side has been found.

X. ADIABATIC TERMS

In the case of a single soliton (kink), the solution is characterized by two parameters $\zeta_1=i|\zeta_1|$ and the center position x_1, it is necessary to determine their time dependence of order of ϵ. We write

$$X=-i\kappa_1 z, \quad z=x-\hat{x}, \quad \hat{x}=x_1-\frac{\lambda_1}{\kappa_1}t, \quad \frac{d}{dt}\hat{x}=-\frac{\lambda_1}{\kappa_1}. \tag{79}$$

We then have

$$s[\theta]=-i2\lambda_{1\tau}\operatorname{sech}X+4\lambda_1\{\kappa_{1\tau}z-\kappa_1\hat{x}_\tau\}\operatorname{sech}X\tanh X, \tag{80}$$

where $\tau=\epsilon t$.

Because of the vanishing of the first component of $\mathbf{R}$, and the integrands depend on x via z, the secularity conditions reduce to

$$\int_{-\infty}^{\infty}dz\Phi(z,\zeta_1)s[\theta]=\int_{-\infty}^{\infty}dz\Phi(z,\zeta_1)r[\theta] \tag{81}$$

and

$$\int_{-\infty}^{\infty}dz\dot{\Phi}(z,\zeta_1)s[\theta]=\int_{-\infty}^{\infty}dz\dot{\Phi}(z,\zeta_1)r[\theta]. \tag{82}$$

Substituting (80), we obtain

$$\int_{-\infty}^{\infty}dz\Phi(z,\zeta_1)s[\theta]=2\frac{1}{\kappa_1}\lambda_{1\tau}-2\frac{\lambda_1}{\kappa_1^2}\kappa_{1\tau}=2\left(\frac{\lambda_1}{\kappa_1}\right)_\tau \tag{83}$$

and

$$\int_{-\infty}^{\infty}dz\dot{\Phi}(z,\zeta_1)s[\theta]=-i\zeta_1^{-1}\lambda_1\frac{\lambda_1}{\kappa_1}\hat{x}_\tau. \tag{84}$$

XI. VISCOSITY, AN EXAMPLE

Considering a kink under viscosity, the perturbation term is expressed as $-\eta\alpha_t$, where η is the coefficient of viscosity. In this case, η is our small parameter ϵ and

$$r[\theta]=\theta_t=-i2\lambda_1 \operatorname{sech} X. \tag{85}$$

We then obtain

$$\int_{-\infty}^{\infty} dz\Phi(z,\zeta_1)r[\theta]=-2\frac{\lambda_1}{\kappa_1} \tag{86}$$

and

$$\int_{-\infty}^{\infty} dz\dot{\Phi}(z,\zeta_1)r[\theta]=0. \tag{87}$$

The secularity conditions up to the order of ϵ are

$$2\left(\frac{\lambda_1}{\kappa_1}\right)_t=-2\eta\frac{\lambda_1}{\kappa_1}, \quad \hat{x}_t=-\frac{\lambda_1}{\kappa_1}. \tag{88}$$

From (88) we have

$$\ln\left(\frac{\lambda_1}{\kappa_1}\right)\Big|_0^t=-\eta t, \quad \frac{\lambda_1(t)}{\kappa_1(t)}=\frac{\lambda_1(0)}{\kappa_1(0)}e^{-\eta t}, \tag{89}$$

and

$$\frac{d}{dt}\hat{x}=-\frac{\lambda_1(0)}{\kappa_1(0)}e^{-\eta t}, \quad \hat{x}(t)=-\frac{\lambda_1(0)}{\kappa_1(0)}\frac{1}{\eta}(1-e^{-\eta t})+x_0. \tag{90}$$

When $\eta\to 0$, (90) tends to the last formula of (79).

XII. EXTENSION TO MULTISOLITON CASE

Now we discuss the problem of how to extend the above theory to the multisoliton case. In the multisoliton case, we must use the inverse scattering transform. The corresponding Lax equations of the unperturbed sine-Gordon equation are

$$\partial_x w(x,t,\zeta)=L(x,t,\zeta)w(x,t,\zeta), \quad \partial_t w(x,t,\zeta)=M(x,t,\zeta)w(x,t,\zeta), \tag{91}$$

with

$$L(x,t,\zeta)=\frac{1}{4}\begin{pmatrix} -i\zeta+i\frac{1}{\zeta}\cos\theta & -\{\theta_x-\theta_t\}+i\frac{1}{\zeta}\sin\theta \\ \{\theta_x-\theta_t\}+i\frac{1}{\zeta}\sin\theta & i\zeta-i\frac{1}{\zeta}\cos\theta \end{pmatrix} \tag{92}$$

and

$$M(x,t,\zeta)=\frac{1}{4}\begin{pmatrix} i\zeta+i\frac{1}{\zeta}\cos\theta & \{\theta_x-\theta_t\}+i\frac{1}{\zeta}\sin\theta \\ -\{\theta_x-\theta_t\}+i\frac{1}{\zeta}\sin\theta & -i\zeta-i\frac{1}{\zeta}\cos\theta \end{pmatrix}. \tag{93}$$

The function satisfying two Lax equations is called the full Jost solution.

Under boundary condition

$$\cos\theta\to 1, \quad \text{as}|x|\to\infty. \tag{94}$$

As $|x|\to\infty$,

$$L(x,t,\zeta)\to -i\,\tfrac{1}{2}\kappa\sigma_3, \quad M(x,t,\zeta)\to i\,\tfrac{1}{2}\lambda\sigma_3. \tag{95}$$

In the inverse scattering transform, the Jost solutions $\psi(x,\zeta)$ and $\varphi(x,\zeta)$ are defined only by the first Lax equation and by the asymptotic behaviors

$$\psi(x,\zeta)\to\begin{pmatrix}0\\1\end{pmatrix}e^{i1/2\,\kappa x}, \quad \text{as } x\to\infty,$$

$$\varphi(x,\zeta)\to\begin{pmatrix}1\\0\end{pmatrix}e^{-i\,1/2\,\kappa x}, \quad \text{as } x\to-\infty. \tag{96}$$

By introducing a t-dependent factor $h(t,\zeta)=e^{-i(1/2)\lambda t}$ which is determined by the second Lax equation, we obtain the full Jost solutions

$$\psi(x,t,\zeta)=h(t,\zeta)^{-1}\psi(x,t), \quad \varphi(x,t,\zeta)=h(t,\zeta)\varphi(x,t), \tag{97}$$

for example.

From Lax equations it can be shown that

$$\{\partial_{xx}-\partial_{tt}-\cos\theta\}W(x,t,\zeta)=0, \tag{98}$$

which corresponds to (11) for a single soliton case, where $W=w_1^2+w_2^2$, and $w=(w_1\ w_2)^T$ is a full Jost solution. We write

$$\Psi(x,t,\zeta)=\psi_1(x,t,\zeta)^2+\psi_2(x,t,\zeta)^2, \quad \Psi(x,\zeta)=\psi_1(x,\zeta)^2+\psi_2(x,\zeta)^2, \tag{99}$$

and similar expressions for $\Phi(x,t,\zeta)$ and $\Phi(x,\zeta)$. It is obvious that

$$\Psi(x,t,\zeta)=h(t,\zeta)^{-2}\Psi(x,t), \quad \Phi(x,t,\zeta)=h(t,\zeta)^2\Phi(x,t). \tag{100}$$

With these squared Jost solutions as solutions of the linearized equation, our previous derivations can be easily extended to multisoliton case, except those in Sec. VIII. It is obvious that the verification of the completeness in multisoliton case can not be based on the explicit expressions of the squared Jost solutions. It may be shown by using Marchenko equation for the sine-Gordon equation in the laboratory Ref. 5 which will be discussed elsewhere.

XIII. DISCUSSION

As we have seen, owing to the complexity of the Lax pair of the sine-Gordon equation, the orthogonality relations of the squared Jost solutions is not easy to derive. Moreover, derivation of the orthogonality relation by using the $1+1$ dimensional Green's theorem is suitable for perturbed

nonlinear equations whose unperturbed counterparts are not completely integrable, such as the perturbed φ^4 equation, the perturbed driven sine-Gordon equation,[13] and other perturbed relativistic nonlinear Klein–Gordon equations.

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On bidirectional fifth-order nonlinear evolution equations, Lax pairs, and directionally dependent solitary waves

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In this paper, Lax pairs are constructed for two fifth-order nonlinear evolution equations of ''Boussinesq''-type which govern wave propagation in two opposite directions. One of the equations is related to the well-known Sawada–Kotera (SK) equation and, through its bilinear form, is identified with the Ramani equation. The second equation—about which very little seems to be known—may be considered a *bidirectional* version of the Kaup–Kupershmidt (KK) equation and is the main focus of this study. The ''anomalous'' solitary wave of this latter equation is derived and is found to possess the remarkable property that *its profile depends on the direction of propagation*. This type of directional dependence would appear to be quite unusual and, to our knowledge, has not been reported in the literature before now. By taking an appropriate undirectional (long wave) limit, it is shown that neither the Ramani, nor the bidirectional Kaup–Kupershmidt (bKK) equation can be classified as truly ''Boussinesq'' in character (a distinction that is made precise in the study). Recursion formulas are given for generating an infinity of conserved densities for both equations. These are used to obtain the first few conservation laws of the bKK and Ramani equations explicitly; not surprisingly, they exhibit the same lacunary behavior as their unidirectional counterparts. In conclusion, a canonical interpretation of the *N*-soliton solution of the bKK equation is proposed which provides a basis for constructing these anomalous solitons in a future work. [DOI: 10.1063/1.1354642]

I. INTRODUCTION

Nonlinear partial differential equations (PDEs) that describe wave propagation (in both one and two spatial dimensions) have been studied extensively since Korteweg and de Vries[1] first proposed their celebrated equation,

$$u_t - 6uu_x + u_{3x} = 0 \tag{1}$$

(the subscripts denote partial derivatives), as a model for small-amplitude gravity waves on shallow water. The continued interest in the Kortewg–de Vries (KdV) equation (1) stems, in large measure, from its exact solvability (for suitably restricted initial data) by the inverse scattering transform (IST).[2,3] The equation is now considered generic among completely integrable equations that govern the propagation of *unidirectional* weakly nonlinear, weakly dispersive waves (both because of its simple structure and the important rôle it plays in many different areas of mathematical physics).[4–9] By virtue of their derivation (from the ''full'' governing physical equations), the plethora of nonlinear PDEs that have been reported over the last thirty years or so describe, in the main, wave propagation in a *single* spatial direction. Additionally—and quite astonishingly—a significant number of these equations have turned out to be *completely integrable*[10] and, consequently, possess all the remarkable properties that characterize this very special class of evolution equations.[11,12] Chief among these distinguishing properties is the existence of multisoliton solu-

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tions which describe the ''elastic'' collisions of mutually interacting solitary waves. Yet—by their very construction—the KdV and other unidirectional nonlinear evolution equations (NEEs) are relevant to waves that progress in only one direction, and *de facto* permit only *overtaking* solitons.

However, in many physical situations, it is often preferable (and more satisfactory) to have an equation which allows us to model waves that propagate in *opposite* directions. In the context of soliton theory, the NEE would then admit solutions which represent the *head-on* collisions between solitary waves, as well as overtaking ones. For modeling small-amplitude shallow water waves, the relevant equation (in $1+1$ dimensions) is the well-known Boussinesq equation[13] which, in its familiar normalized form, may be written

$$u_{tt}-u_{xx}+3(u^2)_{xx}-u_{4x}=0. \tag{2}$$

We note that u_{xx} term in Eq. (2) can be removed by a simple translation of u, though we shall not do so here. Boussinesq's equation (*singular*) should not be confused with the classical Boussinesq equations (*plural*), a pair of coupled shallow water equations that were first reported by Boussinesq in Ref. 13, though they too describe both left- and right-traveling waves. Although Boussinesq was able to obtain Eq. (2) by simplifying the coupled equations, his derivation is in fact contradictory and strictly incorrect. A discussion of this paradox and an appreciation of the historical importance of Boussinesq's somewhat neglected contribution to shallow water wave theory can be found in Refs. 14–17. Equation (2) can be derived directly from the underlying Euler equations using precisely the same asymptotic assumptions that lead to the KdV Eq. (1), except that one allows for propagation in both the positive and negative x directions (see, e.g., Ref. 18). Remarkably, it turns out that the Boussinesq Eq. (2) is also completely integrable[19,20] just like its unidirectional cousin the KdV Eq. (1). [Lest this outcome be thought less than remarkable, it is as well to recall that the exactly comparable asymptotic derivation of the Boussinesq version of the two-dimensional KdV or Kadomtsev–Petviashvili (KP) equation yields a bidirectional nonlinear wave equation that is *not* completely integrable![21]] Thus, the Boussinesq equation (2) has all the special properties that we normally attribute to integrable equations. In particular, its left- and right-running soliton solutions have profiles that are identical to their unidirectional KdV counterparts[22] and so—and this is the important point—these profiles are the *same* regardless of the direction of propagation [a property that is implicit in Eq. (2)]. In other words, the Boussinesq equation *is* the bidirectional equivalent of the KdV equation: Put more precisely, Eq. (2) subsumes the KdV equation in the sense that we can recover Eq. (1) and its solutions by restricting to waves traveling in only one direction (either to the left or right; see Sec. V).

Bearing in mind the preceding remarks, we now wish to be more precise in our use of terminology. Though we intend the descriptive term Boussinesq to imply that an equation is *bidirectional* (i.e., supports wave propagation in two opposite directions), the converse may not be the case. A NEE may be bidirectional and yet not be strictly Boussinesq in character because the equation cannot be reduced to a corresponding *uni*directional integrable equation (in some suitably chosen approximation). In this study, a bidirectional NEE will be deemed to be of *Boussinesq* form if it possesses the following properties: (1) The equation reduces to a completely integrable unidirectional equation when propagation is restricted to one direction; (2) The *two* reduced equations—and hence their solutions—that are obtained in the left- and rightward running limits are essentially the same. Where (1) and (2) are not satisfied, then we will use the looser designation ''bidirectional'' to describe the equation. Until now, this subtle but important distinction seems to have attracted little or no attention; yet, as we shall see, it is of some relevance to the fifth-order equations that concern us here.

Before proceeding, a further comment on our use of terminology and notation is necessary. In the context of this study, we will use the order of the *uni*directional equation to fix the ''order'' of its bidirectional counterpart. Thus, the Boussinesq equation is taken to be *third*-order—the order of the KdV equation—rather than the fourth-order implied by Eq. (2). The reason for doing so becomes clearer when we rewrite Eq. (2) in its nonlocal form

$$\partial_x^{-1}u_{tt}-u_x+6uu_x-u_{3x}=0,$$

which reduces the order by one and makes transparent its connection with the KdV Eq. (1). Similarly, the ''fifth-order'' of the title is intended to preserve the genealogy of the bidirectional equations with the more familiar fifth-order unidirectional NEEs that form the starting point for this study. [Here, and in general, $\partial_x^{-1}f=\int^x f(x',t)\mathrm{d}x'$ denotes the indefinite integral of $f(x,t)$ with respect to x (and contains an arbitrary function of t). However, if $f\to 0$ sufficiently rapidly as $x\to-\infty$ or $+\infty$ (as, for example, when ''soliton'' boundary conditions are imposed), then we intend $\partial_x^{-1}f=\int_{-\infty}^x f(x',t)\mathrm{d}x'$ or $-\int_x^{\infty}f(x',t)\mathrm{d}x'$, respectively.]

The foregoing considerations lead us to suspect that we should be able to find a bidirectional counterpart of a given unidirectional nonlinear evolution equation, which may or may not be of Boussinesq form. (Under our strict definition, Johnson's 2D bidirectional equation[21] would not be classified as Boussinesq since it is not completely integrable). One obvious place to look for such equations is the classification of integrable equations based on Sato theory and the τ-function that was developed by the Kyoto school.[23] Yet it is often far from apparent—particularly from the standpoint of wave propagation—which, if any, of the equations in an integrable hierarchy would be the appropriate choice of bidirectional equation (much less identify *the* Boussinesq generalization). This lack of transparency stems from the fact that the equations in Ref. 23 are, for the most part, expressed in Hirota's bilinear formalism.[24] Other than the more easily recognizable equations of lower-order, the bilinear equations in Ref. 23 are far removed from any obvious physical interpretation (which, at the very least, would require knowledge of the ''correct'' transformation from the τ-function to the dependent physical variable). A further complication may arise where the equation being sought happens to be a reduction of one of the bilinear forms listed. Nevertheless, the Jimbo–Miwa[23] scheme is thought to provide a broad classification of integrable systems and, as we shall see, can be helpful in identifying a NEE that has been obtained by other means.

Now, two important unidirectional NEEs that have been studied extensively over the last two decades are the Sawada–Kotera (SK) (or Caudrey–Dodd–Gibbon) equation[25,26]

$$u_t+45u^2u_x-15u_xu_{xx}-15uu_{3x}+u_{5x}=0, \tag{3}$$

and the Kaup–Kupershmidt (KK) equation[27,28]

$$u_t+45u^2u_x-\tfrac{75}{2}u_xu_{xx}-15uu_{3x}+u_{5x}=0. \tag{4}$$

The close connection between these two completely integrable fifth-order equations is well-documented;[27,29–33] nevertheless, despite their evident duality, Eqs. (3) and (4) are fundamentally different.[29] One might anticipate that both equations will have bidirectional (possibly Boussinesq) counterparts; yet, as far as we can tell, these have not been ''identified'' specifically.

In this paper, we present a procedure for constructing bidirectional generalizations of known unidirectional NEEs. The method proceeds by generating a Lax pair for the putative bidirectional equation from the Lax pair of its unidirectional cousin, and does so by exploiting the connection between the prototype KdV and Boussinesq equations. Aside from its intuitive appeal, the other advantages of this approach are that it is equation specific and, by construction, provides us with a Lax pair which ensures the complete integrability of the resulting bidirectional equation. We shall describe the procedure in the next section, and then use it to construct bidirectional versions of the SK Eq. (3) and the KK Eq. (4), together with their Lax pairs. As both these NEEs are associated with fifth-order scattering problems, solving them by the IST method[2,3] will, we suspect, prove extremely difficult. Rather, we shall make use of Hirota's bilinear transform method[24,34] which is an effective tool for obtaining exact solutions of NEEs using only ''elementary'' means. In Sec. III, we construct two quite distinct bilinear forms for the bidirectional SK equation; one of them comprises a *single* bilinear equation which identifies it with the well-known Ramani[35] equation. The second bilinear form is a coupled system that is given in Ref. 23, where

it appears as a special reduction of the KP hierarchy of the *B*-type (BKP) (though no mention is made there of its connection with Ramani's equation). On the other hand, the bidirectional counterpart of the KK equation constructed here has two bilinear representations which appear to be equally complicated coupled systems. It is this completely integrable equation—which we designate the bidirectional Kaup–Kupershmidt (bKK) equation—that is the main focus of this study. Not surprisingly, the bKK equation is also listed in Ref. 23 (as a special reduction in the KP hierarchy of *C*-type (CKP)), though there is no intimation of its specific relation to the KK equation. Nevertheless, as far as we can tell, very little is known about this equation and the Lax pair constructed here would, therefore, appear to be a new result.

In Sec. IV, we derive the solitary wave of the bKK equation by exploiting the duality between the bilinear forms of the Ramani and bKK equations [in much the same way that one of us (A.P.) has done for the SK and KK equations (3) and (4)[32]]. Remarkably, the profile of this solitary wave *depends on its direction of propagation*, a property that we have not encountered before now. According to the definition formulated earlier, this would imply that the bKK equation is not the Boussinesq form of the KK equation. This is indeed the case; in Sec. V we show that the bKK equation cannot be reduced to the KK equation by restricting wave propagation to only one direction. [Incidentally, this result justifies the designation bKK (*small* b) for the equation.] In the same way, we demonstrate that the Ramani equation is not truly Boussinesq since it cannot be reduced to the Sawada–Kotera equation in a unidirectional approximation.

It is well-known that the sequence of conservation laws for both the SK and KK equations exhibit the unusual behavior whereby every third conserved density is absent.[26,27,36] In Sec. VI, we show that, not unexpectedly, this same lacunary pattern is shared by both the Ramani and bKK equations. We formulate their first few conservation laws explicitly, and give recursion formulas for generating an infinity of conserved densities for each equation. (Although Hu[37] has previously investigated the conservation laws of Ramani's equation, there would appear to be a small but significant error in this work.) Finally, just like its unidirectional cousin the KK Eq. (4),[32,33] we show how the anomalous character of the multisoliton solutions of the bKK equation arises quite naturally within the bilinear formalism. This leads us to a canonical interpretation of its *N*-soliton that paves the way for constructing these somewhat complicated solutions explicitly in a future study. Some bilinear identities that facilitate the analysis are given in Appendix A.

II. LAX PAIRS AND BIDIRECTIONAL EVOLUTION EQUATIONS

We recall that the Lax operators[38] for the KdV Eq. (1) may be written

$$L^{\mathrm{KdV}}=\partial_x^2-u,$$
$$M^{\mathrm{KdV}}=-4\partial_x^3+6u\partial_x+3u_x \tag{5}$$

(where ∂_x^n denotes the nth partial derivative with respect to x). Then the Lax equation $L_t^{\mathrm{KdV}}+[L^{\mathrm{KdV}},M^{\mathrm{KdV}}]=0$ leads to Eq. (1), while $L^{\mathrm{KdV}}\psi=\lambda\psi$, $\psi_t=M^{\mathrm{KdV}}\psi$ constitute the classical IST scheme for the KdV equation. On the other hand, Eq. (2) has the Lax pair[19]

$$L^{\mathrm{B}}=-4\partial_x^3-\partial_x+6u\partial_x+3u_x+i\sqrt{3}\partial_x^{-1}u_t,$$
$$M^{\mathrm{B}}=\partial_x^2-u, \tag{6}$$

so that the IST for the Boussinesq equation comprises the third-order scattering problem $L^{\mathrm{B}}\psi=\lambda\psi$. (This inverse spectral problem was solved by Deift *et al.*[20]) Now, if we compare Eqs. (5) and (6), we observe that the Lax pair of the Boussinesq equation can be recast in terms of the KdV operators as

$$L^{\mathrm{B}}=M^{\mathrm{KdV}}-\partial_x+i\sqrt{3}\partial_x^{-1}u_t,\quad M^{\mathrm{B}}=L^{\mathrm{KdV}}. \tag{7}$$

Written in this way, the Lax pair (7) mirrors the intimate connection between the KdV and Boussinesq equations that is apparent at the physical level where the equations describe equivalent models for shallow water waves that propagate in one and two opposite directions, respectively. In effect, Eq. (7) uses the Lax pair of the *uni*directional KdV Eq. (1) to generate the Lax pair of its *bi*directional cousin, Eq. (2), by exchanging the rôles of the KdV scattering and time evolution operators L^{KdV} and M^{KdV}. The first of the two extra terms in L^{B} is simply required to give the u_{xx} term of the Boussinesq Eq. (2) (but note our earlier comment regarding the elimination of this term), whereas the second term ensures that its Lax equation $(i/\sqrt{3})L^{\mathrm{B}}_t+[L^{\mathrm{B}},M^{\mathrm{B}}]=0$ is purely multiplicative. This exchange mechanism suggests a general procedure for constructing bidirectional versions of unidirectional NEEs which we will now exploit to obtain bidirectional counterparts of the SK and KK equations.

A. A bidirectional Sawada–Kotera equation

We start with the Lax pair of the SK Eq. (3)[36]

$$\begin{aligned} L^{\mathrm{SK}}&=\partial_x^3-3u\partial_x,\\ M^{\mathrm{SK}}&=9\partial_x^5-45u\partial_x^3-45u_x\partial_x^2+(45u^2-30u_{xx})\partial_x. \end{aligned} \tag{8}$$

Following the exchange procedure outlined above, we define new operators

$$L^{\mathrm{bSK}}=M^{\mathrm{SK}}+K,\quad M^{\mathrm{bSK}}=L^{\mathrm{SK}}, \tag{9}$$

which give the putative Lax pair for our *bi*directional Sawada–Kotera (bSK) equation. The unknown differential operator K must be chosen so as to eliminate any unwanted terms from the compatibility condition on L^{bSK} and M^{bSK}: One easily shows that K must have the form

$$K=a(x,t)\partial_x+b(x,t), \tag{10}$$

where $a(x,t)$, $b(x,t)$ are functions to be found. Direct substitution of Eqs. (9) and (10) into the Lax equation $L^{\mathrm{bSK}}_t+[L^{\mathrm{bSK}},M^{\mathrm{bSK}}]=0$ yields the defining equations

$$15u_t+a_x=0,\quad 15u_{xt}+a_{xx}+b_x=0,\quad b_t=0,$$

from which we obtain $a=-15\partial_x^{-1}u_t$ and $b=$constant (which may be set to zero without loss of generality). The Lax operators (9) now read

$$\begin{aligned} L^{\mathrm{bSK}}&=9\partial_x^5-45u\partial_x^3-45u_x\partial_x^2+(45u^2-30u_{xx}-15\partial_x^{-1}u_t)\partial_x\\ M^{\mathrm{bSK}}&=\partial_x^3-3u\partial_x, \end{aligned} \tag{11}$$

and their compatibility leads to the completely integrable equation

$$5\partial_x^{-1}u_{tt}+5u_{xxt}-15uu_t-15u_x\partial_x^{-1}u_t-45u^2u_x+15u_xu_{xx}+15uu_{3x}-u_{5x}=0. \tag{12}$$

Though we have been able to construct a bidirectional version of the SK Eq. (3), the NEE (12), in its present form at least, is not readily identifiable. Moreover, if we were to use the IST method to obtain its soliton solutions, we must solve the *fifth*-order inverse spectral problem, $L^{\mathrm{bSK}}\psi=\lambda\psi$, which, we suspect, will be considerably more difficult than the corresponding third-order scattering problem for the SK equation.[27] Rather, we shall make use of Hirota's direct method[24] which, additionally, will allow us to recognize Eq. (12) by its bilinear form. Now that we have shown that the exchange method works for the SK equation, we turn to our main purpose: To find a bidirectional counterpart of the Kaup–Kupershmidt equation (4).

B. A bidirectional Kaup–Kupershmidt equation

Repeating the procedure of Sec. II A for the KK Eq. (4), its Lax representation[27]

$$L^{\mathrm{KK}}=\partial_x^3-3u\partial_x-\tfrac{3}{2}u_x,$$
$$M^{\mathrm{KK}}=9\partial_x^5-45u\partial_x^3-\tfrac{135}{2}u_x\partial_x^2+(45u^2-\tfrac{105}{2}u_{xx})\partial_x+45uu_x-15u_{3x}, \tag{13}$$

is replaced by

$$L^{\mathrm{bKK}}=M^{\mathrm{KK}}+A(x,t)\partial_x+B(x,t),\quad M^{\mathrm{bKK}}=L^{\mathrm{KK}}, \tag{14}$$

which gives a putative Lax pair for the *bi*directional Kaup–Kupershmidt (bKK) equation. The unknown functions $A(x,t)$, $B(x,t)$ are determined by requiring that the operators (14) constitute a legitimate Lax pair: Proceeding on this basis, we get

$$15u_t+A_x=0,\quad \tfrac{45}{2}u_{xt}+A_{xx}+B_x=0.$$

Integrating these equations once, we find that $A=-15\partial_x^{-1}u_t$ and $B=-\frac{15}{2}u_t$ (where the arbitrary function of integration in the last expression has been set to zero, with no loss in generality). Combining these results with Eqs. (13) and (14), we finally obtain the Lax pair

$$L^{\mathrm{bKK}}=9\partial_x^5-45u\partial_x^3-\tfrac{135}{2}u_x\partial_x^2+(45u^2-\tfrac{105}{2}u_{xx}-15\partial_x^{-1}u_t)\partial_x+45uu_x-15u_{3x}-\tfrac{15}{2}u_t,$$
$$M^{\mathrm{bKK}}=\partial_x^3-3u\partial_x-\tfrac{3}{2}u_x, \tag{15}$$

whose compatibility yields the integrable bKK equation

$$5\partial_x^{-1}u_{tt}+5u_{xxt}-15uu_t-15u\partial_x^{-1}u_t-45u^2u_x+\tfrac{75}{2}u_xu_{xx}+15uu_{3x}-u_{5x}=0. \tag{16}$$

Although we have succeeded in constructing a bidirectional version of the KK Eq. (4) by using the exchange procedure, the resulting fifth-order NEE (16) is not new. As we anticipated, the bKK equation can be found in the Jimbo–Miwa classification as a special reduction of the CKP hierarchy of integrable equations (see Ref. 23, p. 969). Yet no mention is made there of its connection with the KK equation or of its bidirectional character; furthermore, the Lax pair (15) is not given in Ref. 23 and would appear to be new. Even so, to the best of our knowledge, Eq. (16) has not been studied in any detail and is the main interest of the remainder of this paper. In the next section, we shall obtain the bilinear form of the bKK equation with a view to finding its soliton solutions. (This avoids solving the associated *fifth*-order inverse spectral problem which lies outside the scope of the present study).

One further comment is warranted before we proceed. The bidirectional NEEs (12) and (16) differ only in the coefficients of the nonlinear term u_xu_{xx} [cf. Eqs. (3) and (4)]. Yet, just like their unidirectional cousins, the bSK and bKK equations are fundamentally different: There is no scaling that transforms one equation into the other. We shall say more about this distinction later.

III. BILINEAR FORMS

As an alternative to the IST[2,3]—which, in this instance, would mean solving a fifth-order inverse spectral problem—Hirota's bilinear transform method[24,34] is arguably the most straightforward technique for finding exact solutions of NEEs. In this section, we construct bilinear forms of both the bSK and bKK equations, Eqs. (12) and (16), primarily with a view to obtaining multisoliton solutions. Yet, here, the bilinear formalism confers further advantages. Thus, the bSK Eq. (12) has a bilinear form that allows us to identify it with a well-known integrable equation and which, by virtue of its simple structure, is easily solved for soliton solutions. Additionally, we can

exploit the duality between the bSK and bKK equations to develop a strategy for solving the more complicated bilinear form of the latter equation (in much the same way as has been done for the SK and KK equations[32,33]).

A. Bilinearization of the bidirectional Sawada–Kotera equation

Following Hirota's method,[24,34] we make a change of dependent variable

$$u(x,t)=\alpha\partial_x^2 \ln f(x,t), \tag{17}$$

where α is a constant. Integrating the bSK Eq. (12) with respect to x, we obtain

$$5\alpha(\ln f)_{tt}+5u_{xt}-15\alpha u(\ln f)_{xt}-G(u)=0, \tag{18}$$

where we have used (17) and put

$$G(u)=15u^3-15uu_{xx}+u_{4x}. \tag{19}$$

The arbitrary function of integration in (18) has been set to zero by imposing soliton (i.e., rapidly decaying) boundary conditions as $x\to\pm\infty$.

The first term of (18) can be cast into bilinear form by using the identity

$$(\ln f)_{tt}=(\mathrm{D}_t^2 f\cdot f)/2f^2, \tag{20}$$

where the Hirota derivatives D_x, D_t are defined by[34]

$$\mathrm{D}_x\mathrm{D}_t a(x,t)\cdot b(x,t)=(\partial_x-\partial_{x'})(\partial_t-\partial_{t'})a(x,t)b(x',t')\big|_{x'=x,\ t'=t}.$$

We can bilinearize the next pair of terms in (18) by first noting the identity (A3) (with $u\to u/\alpha$)

$$u_{xt}+6u(\ln f)_{xt}=\alpha(\mathrm{D}_x^3\mathrm{D}_t f\cdot f)/2f^2. \tag{21}$$

Combining the identities (A1) and (A6), we also deduce the relation

$$[\partial_{xt}^2+2(\ln f)_{xt}](g/f)=(\mathrm{D}_x\mathrm{D}_t f\cdot g)/f^2,$$

where $g(x,t)$ is an arbitrary function. But if we define g by

$$g/f=u, \tag{22}$$

then the last result yields the identity

$$u_{xt}+2u(\ln f)_{xt}=(\mathrm{D}_x\mathrm{D}_t f\cdot g)/f^2. \tag{23}$$

Using Eqs. (21) and (23), we can now bilinearize the next two terms of Eq. (18) through the linear combination

$$5u_{xt}-15\alpha u(\ln f)_{xt}=\lambda\frac{\mathrm{D}_x\mathrm{D}_t f\cdot g}{f^2}+\alpha\mu\frac{\mathrm{D}_x^3\mathrm{D}_t f\cdot f}{2f^2}, \tag{24}$$

provided that λ and μ satisfy $\lambda+\mu=5$, $2\lambda+6\mu=-15\alpha$, in which case

$$\lambda=\tfrac{15}{4}(\alpha+2),\quad \mu=-\tfrac{5}{4}(3\alpha+2). \tag{25}$$

It only remains to bilinearize the expression $G(u)$. We first make use of (A5) (with $u\to u/\alpha$), which gives

$$120u^3+60\alpha uu_{xx}+2\alpha^2u_{4x}=\alpha^3(\mathrm{D}_x^6f\cdot f)/f^2. \tag{26}$$

By combining the identities (A7) and (A8), and substituting (A2), (A4), and (22), we get the further relation between the three terms of G

$$12u^3+14\alpha uu_{xx}+\alpha^2u_{4x}=\alpha^2(\mathrm{D}_x^4f\cdot g)/f^2. \tag{27}$$

The bilinearization of $G(u)$ follows from (26) and (27) if we can find constants γ and ν such that

$$G(u)=\gamma(12u^3+14\alpha uu_{xx}+\alpha^2u_{4x})+\nu(120u^3+60\alpha uu_{xx}+2\alpha^2u_{4x}). \tag{28}$$

Comparing (19) with (28), we require

$$12\gamma+120\nu=15,\quad \alpha(14\gamma+60\nu)=-15,\quad \alpha^2(\gamma+2\nu)=1,$$

which are compatible if $\alpha^2+3\alpha+2=0$, i.e., $\alpha=-1$ or $\alpha=-2$.

Solving for γ and ν, and substituting from Eqs. (20), (24)–(28) into Eq. (18), we finally obtain the bilinear form of the bSK Eq. (12)

$$[80\alpha\mathrm{D}_t^2-20\alpha(3\alpha+2)\mathrm{D}_x^3\mathrm{D}_t-\alpha^2(7\alpha+6)\mathrm{D}_x^6]f\cdot f+(\alpha+2)[120\mathrm{D}_x\mathrm{D}_t+30\alpha\mathrm{D}_x^4]f\cdot g=0, \tag{29a}$$

$$\alpha\mathrm{D}_x^2f\cdot f-2\,f\cdot g=0, \tag{29b}$$

where the last equation is just a restatement of Eq. (22) [using the bilinear identity (A2)]. There are two cases to consider: (i) $\alpha=-1$. The bilinear form (29) reads

$$(80\mathrm{D}_t^2+20\mathrm{D}_x^3\mathrm{D}_t-\mathrm{D}_x^6)f\cdot f-(120\mathrm{D}_x\mathrm{D}_t-30\mathrm{D}_x^4)f\cdot g=0, \tag{30a}$$

$$\mathrm{D}_x^2f\cdot f+2\,f\cdot g=0. \tag{30b}$$

(ii) $\alpha=-2$. In this case Eqs. (29a) and (29b) decouple, thus making the auxiliary function g redundant and reducing the bilinear form to the single equation

$$(5\mathrm{D}_t^2+5\mathrm{D}_x^3\mathrm{D}_t-\mathrm{D}_x^6)f\cdot f=0. \tag{31}$$

Using the transformation (17), we have shown that it is possible to construct *two* bilinear forms of the bidirectional Sawada–Kotera equation (12). The first of these, Eq. (30), has u and f related by $u=-\partial_x^2\ln f$, and is a coupled bilinear system that is given in Ref. 23. This shows that the bSK Eq. (12) is, in fact, a reduction of the BKP hierarchy of integrable equations. The alternative bilinear representation, Eq. (31), with $u=-2\partial_x^2\ln f$, identifies the bSK Eq. (12) with the well-known Ramani equation.[35] The latter equation has attracted considerable attention in the literature and is widely held to be completely integrable.[23,35,37,39,40] In particular, the Lax representation (11) that has been obtained here through the exchange procedure, agrees with the Lax pair of the Ramani equation that was found previously by other means.[39] Hitherto, the designation ''Ramani equation'' appears to have been used only in connection with the bilinear form (31). However, we shall also use it to refer to the bidirectional Sawada–Kotera Eq. (12) and invoke the alternative description ''bSK equation'' whenever we wish to emphasize its bidirectional character and genealogy with the Sawada–Kotera equation, Eq. (3).

B. Bilinearization of the bidirectional Kaup–Kupershmidt equation

Proceeding as above, we obtain the integrated form of the bKK Eq. (16)

$$5\alpha(\ln f)_{tt}+5u_{xt}-15\alpha u(\ln f)_{xt}-H(u)=0, \tag{32}$$

where u and f are related by Eq. (17) and

$$H(u)=15u^3-\tfrac{45}{4}u_x^2-15uu_{xx}+u_{4x}. \tag{33}$$

Since the first three terms in Eq. (32) are identical to those of Eq. (18), they can be bilinearized exactly as in Sec. III A [using an auxiliary function g, Eq. (22)]. Moreover, the expression $H(u)$ differs from $G(u)$, Eq. (19), by just a single term. Thus, to complete the bilinearization of the bKK equation, we need only find a further bilinear relation between the terms of $H(u)$ in addition to (26) and (27) (and containing the extra u_x^2 term).

To this end, we first make use of (A4) (with $u\to u/\alpha$) to deduce the two identities

$$\alpha^2 u\left(\frac{\mathrm{D}_x^4 f\cdot f}{f^2}\right)=12u^3+2\alpha uu_{xx},\quad \alpha^2\frac{\partial^2}{\partial x^2}\left(\frac{\mathrm{D}_x^4 f\cdot f}{f^2}\right)=24(uu_{xx}+u_x^2)+2\alpha u_{4x}, \tag{34}$$

which taken together involve all four terms of $H(u)$. We also have

$$2u\left(\frac{h}{f}\right)+\alpha\frac{\partial^2}{\partial x^2}\left(\frac{h}{f}\right)=\alpha\frac{\mathrm{D}_x^2 f\cdot h}{f^2}, \tag{35}$$

which follows directly from (A2), (A7), and (17), for any ancillary function $h(x,t)$. But if we define h by [cf. (29b)]

$$\frac{h}{f}=\alpha\frac{\mathrm{D}_x^4 f\cdot f}{2f^2}, \tag{36}$$

and use (34), then Eq. (35) yields the additional bilinear relation

$$12u^3+14\alpha uu_{xx}+12\alpha u_x^2+\alpha^2 u_{4x}=\alpha^2(\mathrm{D}_x^2 f\cdot h)/f^2. \tag{37}$$

The bilinearization of H now follows from Eqs. (26), (27), and (37) provided we can find constants σ, γ, and ν such that

$$\begin{aligned}H(u)=&\sigma(12u^3+14\alpha uu_{xx}+12\alpha u_x^2+\alpha^2u_{4x})+\gamma(12u^3+14\alpha uu_{xx}+\alpha^2u_{4x})\\&+\nu(120u^3+60\alpha uu_{xx}+2\alpha^2u_{4x}).\end{aligned} \tag{38}$$

As before, this is possible only if $\alpha=-1$ or $\alpha=-2$, and then

$$\sigma=-\frac{15}{16\alpha},\quad \gamma=-\frac{15(\alpha+1)}{16\alpha},\quad \nu=\frac{7\alpha+6}{32\alpha}. \tag{39}$$

Every term in Eq. (32) has now been bilinearized: The resulting bilinear form of the bKK Eq. (16) is

$$\begin{gathered}\alpha(5\mathrm{D}_t^2+\mu\mathrm{D}_x^3\mathrm{D}_t-2\alpha^2\nu\mathrm{D}_x^6)f\cdot f+2(\lambda\mathrm{D}_x\mathrm{D}_t-\alpha^2\gamma\mathrm{D}_x^4)f\cdot g-2\alpha^2\sigma\mathrm{D}_x^2 f\cdot h=0,\\ \alpha\mathrm{D}_x^2 f\cdot f-2f\cdot g=0,\\ \alpha\mathrm{D}_x^4 f\cdot f-2f\cdot h=0,\end{gathered} \tag{40}$$

where λ, μ, σ, γ, and ν are given by Eqs. (25) and (39) [and the last equation is simply a restatement of Eq. (36)]. Once again, there are two possibilities: (i) $\alpha=-1$. The bilinear form (40) becomes

$$(80D_t^2+20D_x^3D_t-D_x^6)f\cdot f-120D_xD_tf\cdot g+30D_x^2f\cdot h=0, \tag{41a}$$

$$D_x^2f\cdot f+2\,f\cdot g=0, \tag{41b}$$

$$D_x^4f\cdot f+2\,f\cdot h=0, \tag{41c}$$

with $u=-\partial_x^2\ln f$. (ii) $\alpha=-2$. In this case, we have $u=-2\partial_x^2\ln f$ and the bilinear form (40) reads

$$16(5D_t^2+5D_x^3D_t-D_x^6)f\cdot f-30D_x^4f\cdot g+30D_x^2f\cdot h=0,$$

$$D_x^2f\cdot f+f\cdot g=0, \tag{42}$$

$$D_x^4f\cdot f+f\cdot h=0.$$

Although the bKK equation appears in Ref. 23 in its normal form (16), the bilinear forms (41) and (42) are not listed there and, as far as we can tell, are new results.

For our part, the crucial observation is the following one: Although we have been able to construct two bilinear forms for the bKK equation [under the transformation (17)], neither of these systems can be reduced to a *single* bilinear equation [comparable to Eq. (31) for the Ramani equation]. As we shall see, this distinguishing feature of the bKK Eq. (16) has consequences for obtaining its soliton solutions. Indeed, both the bilinear forms (41) and (42) involve three field variables [cf. Eq. (30)]; thus, in spite of their duality, the bKK equation would seem to be a more complicated system than Ramani's equation.

Not surprisingly, the results that we have obtained here for the Ramani and bKK equations mirror those given in Ref. 32 for their unidirectional cousins, the SK Eq. (3) and KK Eq. (4), with one notable exception. The assertion in Ref. 32 that the KK equation possesses a *single* bilinear form [under (17)] is incorrect. There, the author did not take account of the relation (27) when constructing its bilinear form, and so missed a second bilinear representation [akin to (42) for the bKK equation]. However, as there is no simple way of solving this alternative bilinear form of the KK equation for soliton solutions [the same comment applies to Eq. (42) incidentally; see Sec. IV], the results and conclusions of Ref. 32 remain valid.

IV. SOLITARY WAVES

Now that we have found bilinear forms of the bidirectional NEEs (12) and (16), we would like to be able to solve them for exact solutions. For the Ramani equation this is comparatively straightforward since we can employ the simpler bilinear form (31) as opposed to the coupled equations (30a) and (30b). More particularly, we can make use of Hirota's celebrated formula[24] to obtain the explicit N-soliton solution of Eq. (31). Hereafter, we shall dub this generic form the ''*regular*'' N-soliton solution. Understandably, the alternate and more complicated bilinear form of Ramani's equation, Eq. (30), has largely been ignored for analytic purposes. Yet its multisoliton solutions are easily inferred from the corresponding solutions of Eq. (31) and this provides the key to solving the bilinear form of the bKK equation, Eq. (41), for which there is no obvious ansatz. In this section, we shall pursue this line of reasoning with a view to deriving the solitary wave of the bKK equation.

The ''regular'' solitary wave has the form[24]

$$f(x,t)=1+e^{\theta},\quad \theta=px+\omega t+\eta, \tag{43}$$

which solves the Ramani bilinear form (31) if $\omega(p)$ satisfies the dispersion relation

$$5\omega^2+5\omega p^3-p^6=0. \tag{44}$$

Transforming to the ''physical'' variable u, we get

$$u(x,t) = -2\partial_x^2 \ln f = -\tfrac{1}{2}p^2 \operatorname{sech}^2 \tfrac{1}{2}(px+\omega t+\eta), \tag{45}$$

where p, η are arbitrary (real) parameters and ω is given by Eq. (44). This is the familiar sech^2 solitary wave of the Ramani Eq. (12) which propagates to the left or right depending on the sign of ω. However, it is important to emphasize that the left- and right-going solitary waves have *identical* bell-shaped profiles (for a given wave number p) but travel with different speeds.

Evidently, the bilinear forms (30) and (31) are equivalent under the transformation $f \leftrightarrow f^2$ (we omit the formal demonstration here which makes use of various bilinear identities; but see Ref. 32 for a similar argument). It follows that the corresponding solitary-wave solution of the alternative bilinear form (30) is given by squaring Eq. (43); i.e.,

$$f(x,t) = 1 + 2e^{\theta} + e^{2\theta}, \tag{46}$$

which is a solution of Eqs. (30a) and (30b) provided that ω satisfies the dispersion law (44) (and $g = -2p^2 e^{\theta}$).

The situation for the bKK equation is not quite so simple: At first glance, there seems little to choose between the bilinear forms (41) and (42). However, on closer scrutiny, we see that (modulo the ancillary equations) the bilinear forms of the Ramani Eq. (30) and bKK Eq. (41)—corresponding to $\alpha = -1$—bear a marked resemblance to one another: Ditto the bilinear forms (31) and (42) for which $\alpha = -2$. This is hardly surprising: These bilinear forms echo the intimate connection between the Ramani and bKK equations that is evident from their normalized forms, Eqs. (12) and (16). We can expect this duality to be manifested in their analytic properties and, importantly, in the structure of their soliton solutions. In particular, we anticipate that the solitary wave of the bilinearized bKK Eq. (41) will mimic the corresponding solution of the Ramani Eq. (30). This suggests that we seek a solitary-wave solution of Eqs. (41a)–(41c) in the form [cf. Eq. (46)]

$$f(x,t) = 1 + e^{\theta} + be^{2\theta}, \quad \theta = px + \omega t + \eta, \tag{47}$$

where b is a constant (and the coefficient of e^{θ} has been set to unity without loss of generality). We will take this as a working hypothesis, choosing to work with the bilinear form (41) rather than (42).

For a general bilinear operator $F(\mathrm{D}_x, \mathrm{D}_t)$, we have the fundamental result[34]

$$F(\mathrm{D}_x, \mathrm{D}_t) e^{\theta_1} \cdot e^{\theta_2} = F(\mathbf{p}_1 - \mathbf{p}_2) e^{\theta_1 + \theta_2}, \quad \theta_i = p_i x + \omega_i t + \eta_i, \quad i = 1,2, \tag{48}$$

where for brevity we write $F(\mathbf{p}) = F(p,\omega)$. Then, with f given by Eq. (47), we obtain

$$F(\mathrm{D}_x, \mathrm{D}_t) f \cdot f = 2e^{\theta}[F(\mathbf{p}) + bF(2\mathbf{p})e^{\theta} + bF(\mathbf{p})e^{2\theta}], \tag{49}$$

whenever F is even and $F(\mathbf{0}) = 0$.

We first solve the ancillary equations (41b) and (41c) for g and h, respectively. Setting $F = \mathrm{D}_x^2$ in Eq. (49), and substituting into Eq. (41b), we deduce

$$g = -p^2 e^{\theta}\left[1 + (4b-1)\frac{e^{\theta}}{f}\right]. \tag{50}$$

Similarly, we solve Eq. (41c) to obtain

$$h = -p^4 e^{\theta}\left[1 + (16b-1)\frac{e^{\theta}}{f}\right]. \tag{51}$$

There is good reason to write the auxiliary functions in this way. First and foremost, they will simplify the computations needed to solve the third bilinear equation (41a). But they also identify two special values of b. When $b = 1/4$, Eq. (50) simplifies to $g = -p^2 e^{\theta}$ and (47) becomes f

$=(1+\frac{1}{2}e^{\theta})^2$; in the absence of h, this would recover the solitary-wave solution of the Ramani bilinear form (30) noted above [a similar result holds for the SK Eq. (3)[32]]. On the other hand, if $b=1/16$, then Eq. (51) reduces to $h=-p^4e^{\theta}$ and $f=(1+e^{\theta}+\frac{1}{16}e^{\theta})$ which is just the anomalous solitary wave of the KK Eq. (4) (with g now absent).[32]

For the bKK equation, however, we cannot simplify *both* Eqs. (50) and (51) simultaneously, and this complicates matters. It is clear that direct substitution of g and h into Eq. (41a) may present difficulties since the last two bilinear terms would then involve quotients. However, we can avoid these by making use of the identities (A9) and (A10) which, together with Eqs. (48) and (49), give

$$\mathrm{D}_x\mathrm{D}_t f\cdot g=-\omega p^3e^{\theta}\left[(1+be^{2\theta})+\frac{4(4b-1)}{f^2}e^{\theta}(1-be^{2\theta})^2\right]$$

and

$$\mathrm{D}_x^2 f\cdot h=-p^6e^{\theta}\left[(1+be^{2\theta})+\frac{4(16b-1)}{f^2}e^{\theta}(1-be^{2\theta})^2\right].$$

Then, using Eq. (49) once more with $F=80\mathrm{D}_t^2+20\mathrm{D}_x^3\mathrm{D}_t-\mathrm{D}_x^6$, Eq. (41a) becomes

$$\{[F(\mathbf{p})+15(4\omega p^3-p^6)](1+be^{2\theta})+bF(2\mathbf{p})e^{\theta}\}f^2$$
$$+60p^3[4(4b-1)\omega-(16b-1)p^3]e^{\theta}(1-be^{2\theta})^2=0.$$

But, bearing in mind the form of f, Eq. (47), we must have

$$F(\mathbf{p})+15(4\omega p^3-p^6)=0,\quad F(2\mathbf{p})=0,\quad 4(4b-1)\omega-(16b-1)p^3=0.$$

Substituting the expression for F, the first and second equations both yield the dispersion relation (44). The last equation determines the constant b as

$$b=\frac{1}{16}\left(\frac{4\omega-p^3}{\omega-p^3}\right), \tag{52}$$

and completes the derivation of the solitary-wave solution of the bKK Eq. (16). And now we have a surprise: The parameter b depends on the dispersion relation ω and, therefore, on the direction of travel! This is quite different from the result for the bidirectional SK Eq. (12), which has $b=1/4$ independent of the direction of propagation. Before we go on to consider the consequences for the solitary wave itself, it will pay us to take a closer look at the expression (52).

Now, using the dispersion relation (44), one easily shows that $b>0$ for all real $p\neq 0$. To emphasize this, we write $b=\frac{1}{16}a^2$ where

$$a^2=\frac{4\omega-p^3}{\omega-p^3},\quad a>0. \tag{53}$$

The solitary wave of the bKK Eq. (16) that is generated by f, Eq. (47), is therefore,

$$u(x,t)=-\partial_x^2\ln f(x,t)=-\partial_x^2\ln(1+e^{\theta}+\tfrac{1}{16}a^2e^{2\theta}),$$

which may be written

$$u(x,t)=-\partial_x^2\ln(a\cosh\theta+2)=-ap^2\frac{a+2\cosh\theta}{(a\cosh\theta+2)^2}. \tag{54}$$

As far as we are aware, this solution was not previously known (although it bears comparison with the anomalous solitary wave of its unidirectional cousin, the KK Eq. (4)[27,32]). To pin down the directional dependence of the solitary wave (54), we first solve the dispersion equation (44); this has the two real roots

$$\omega = -\Omega_{\pm} p^3, \quad \Omega_{\pm} = \frac{1}{2}\left(1 \pm \frac{3}{\sqrt{5}}\right). \tag{55}$$

Substituting for ω in (53) and simplifying, we get

$$a(\Omega_+) = \tfrac{1}{2}(\sqrt{5}+1), \quad a(\Omega_-) = \tfrac{1}{2}(\sqrt{5}-1). \tag{56}$$

The parameter a plays a crucial rôle in distinguishing the left- and right-running solitary waves; before we examine this in greater detail, we wish to make one or two more general observations. Evidently, the bKK solitary wave (54) has a symmetrical profile that decays rapidly to zero, but not as fast as the sech^2 solitary wave (45) of the companion Ramani Eq. (12). Further, it is clear that $u(x,t)$ is invariant under the parity transformation $p \to -p$ and we may, therefore, take $p > 0$ in what follows, without loss of generality.

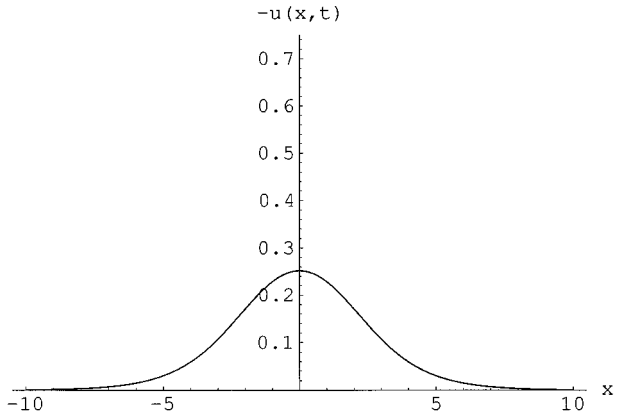
Yet the most striking feature of the bKK solitary wave is that *its shape depends on the direction of propagation*, a property that we have not come across before. The rightward travelling wave is parameterized by Ω_+ in Eqs. (55) and (56). In this case, the solitary wave (54) is a single bell-shaped hump which propagates in the positive x direction with speed $c = \Omega_+ p^2$ and amplitude $A_+ = 1/\sqrt{5}\, p^2$. Figure 1 shows three typical solitary waves with wave numbers $p = 0.75$, 1, 1.25 [where in all figures we plot the physical wave $-u(x,t)$ in its rest frame]. They exhibit the characteristic soliton properties whereby taller waves are narrower and travel faster than short, fat waves.

The left-going solitary wave is given by taking the negative parameter Ω_- in Eq. (55). And now we have another surprise: Its wave profile is strikingly different to that of the right-going solitary wave, it being comprised of two symmetrically positioned peaks! Figure 2 shows three of these double-humped solitary waves which, typically, increase in amplitude as the wavelength shortens and speed $c = |\Omega_-| p^2$ increases. The shape of this twin-peaked solitary wave merits further scrutiny. Its amplitude

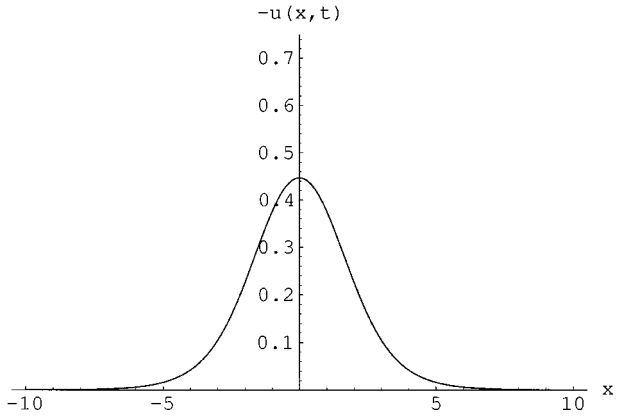
$$A_- = \left(\frac{5-\sqrt{5}}{10}\right) p^2 = a(\Omega_-) A_+ ,$$

is significantly smaller than the amplitude of its right-moving counterpart. This is clearly illustrated in Figs. 1 and 2 where, for the purpose of comparison, we have chosen the same wave numbers for left- and right-going waves. More precisely, for any prescribed wave number p, the amplitude A_- is a *fixed* fraction $a(\Omega_-) \approx 0.618$ of the amplitude A_+. This should not surprise us: both solitary waves transport the same ''mass'' $(= 2p)$, but for the left-traveling wave it is distributed equally over the two humps. Also, the trough that is formed by the two peaks is relatively shallow and, significantly, *never vanishes* even in the long wavelength limit $(p \to 0)$. In fact, one can easily show that the depth of the trough is a constant proportion (≈ 0.146) of the wave amplitude A_- for all wave numbers p.

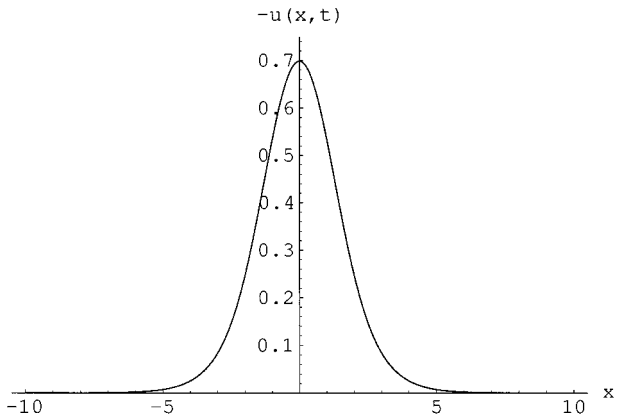
We mention that a solitary wave with a similar double-hump profile has been reported by Sasa and Satsuma[41] for a higher-order nonlinear Schrödinger equation. However, this NEE describes *uni*directional propagation, and its solitary wave possesses quite different properties; most notably, this twin-peaked wave can be reduced to a single-hump (sech) profile in a suitable limit. Contrast this with the bKK solitary wave (54) whose profile changes from a double to a single hump simply by switching direction from left to right (and vice versa). This type of *directionally dependent solitary wave* is quite unusual and, as far as we know, has not been reported before now. Moreover, this remarkable property has an important consequence: According to our strict



(a)



(b)



(c)

FIG. 1. The right-traveling single-humped solitary wave of the bKK equation: (a) $p=0.75$, (b) $p=1$, and (c) $p=1.25$.

definition, the bidirectional Kaup–Kupershmidt Eq. (16) cannot be *the* Boussinesq version of the Kaup–Kupershmidt Eq. (4). Similarly, Ramani's equation (12) is not the Boussinesq counterpart of the SK Eq. (3), even though the solitary wave in this case has the same profile irrespective of its direction of propagation. Before we proceed to verify these assertions in the next section, a last remark is in order. The reason for solving the bilinear form (41) instead of (42) is, with hindsight, now clear. To generate the solitary wave of Eq. (42) would require the ansatz

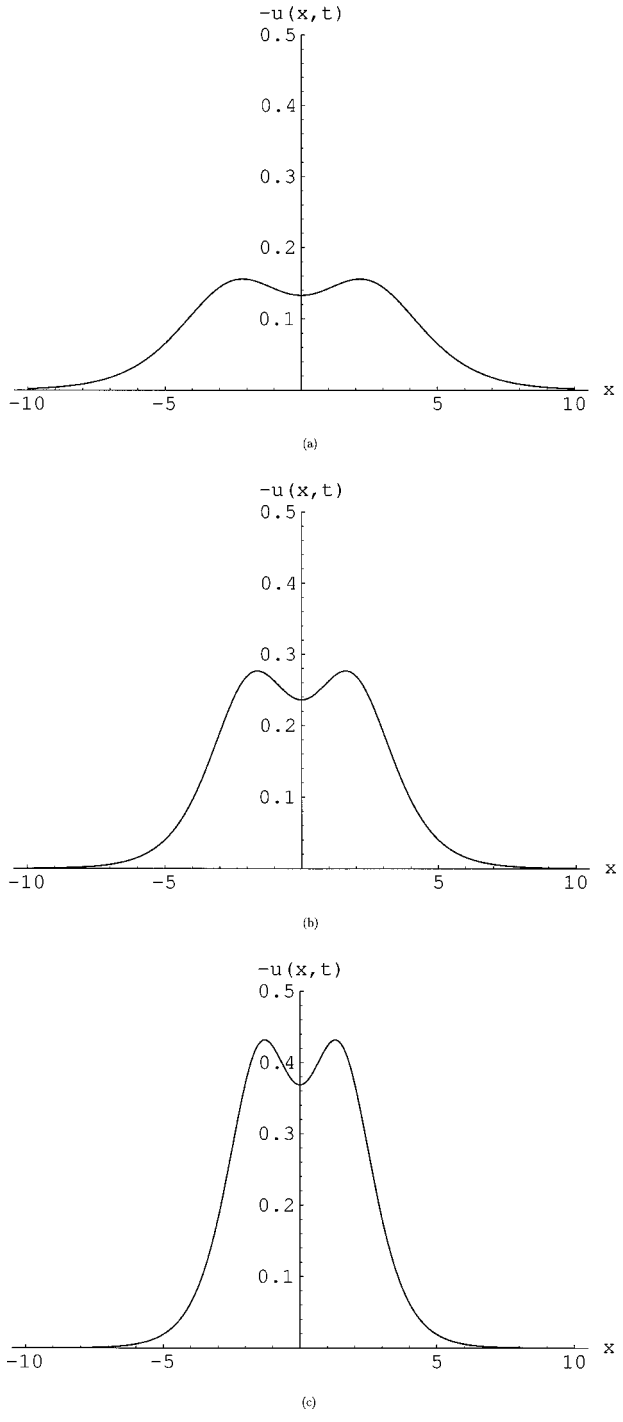


FIG. 2. The left-traveling double-humped solitary wave of the bKK equation: (a) $p=0.75$, (b) $p=1$, and (c) $p=1.25$.

$f=(1+e^{\theta}+be^{2\theta})^{1/2}$; but this form of f cannot be easily handled within the bilinear formalism, whether expressed in this way or otherwise formulated as an *infinite* series in e^{θ}.

V. UNIDIRECTIONAL APPROXIMATIONS

We stated earlier that the Boussinesq Eq. (2) may considered the bidirectional equivalent of the KdV Eq. (1): We shall now make this equivalence more precise. Let us introduce new far-field variables

$$\xi=\epsilon(x\pm t),\quad \tau=\tfrac{1}{2}\epsilon^3 t,\quad u=\epsilon^2 U(\xi,\tau),$$

where $\epsilon>0$ is a constant parameter. The choice of the characteristic variable ξ restricts wave propagation to one direction only: To the left $(+)$ or right $(-)$. Then, to leading order as $\epsilon\to 0$ with $U=O(1)$, the Boussinesq Eq. (2) transforms to the KdV equation

$$\pm U_\tau+3(U^2)_\xi-U_{3\xi}=0,$$

in *both* the left- and right-running limits. Thus, the Boussinesq equation subsumes the KdV equation in the unidirectional (long wave) approximation. Similarly, one easily shows that the solitary wave and multisoliton solutions of the Boussinesq equation transform to their KdV counterparts travelling to the left $(+)$ or right $(-)$. Hence, and not unexpectedly, Eq. (2) does satisfy the two requirements that characterize this equation as the *Boussinesq* form of the KdV Eq. (1).

We repeat this procedure with a view to deriving unidirectional approximations for both Ramani and bKK equations. By writing Eqs. (12) and (16) in the form

$$5\partial_x^{-1}u_{tt}+5u_{xxt}-15uu_t-15u_x\partial_x^{-1}u_t-45u^2u_x+15\rho u_x u_{xx}+15uu_{3x}-u_{5x}=0, \tag{57}$$

we can deal with both equations simultaneously. With $\rho=1$ we obtain Ramani's Eq. (12), while $\rho=5/2$ yields the bKK Eq. (16). Incidentally, written in this way, Eq. (57) also serves to emphasize the close connection between these two bidirectional equations. As before, we introduce a unidirectional transformation

$$\xi=\epsilon x+\kappa t,\quad \tau=\delta t,\quad u=\beta U(\xi,\tau),\quad (\delta,\epsilon>0), \tag{58}$$

that allows us to track left- or right-running waves according to the sign of κ. After transforming the variables in Eq. (57), and simplifying, we get

$$\begin{aligned}5\kappa^2U_\xi+10\kappa\delta U_\tau+5\delta^2\partial_\xi^{-1}U_{\tau\tau}+\epsilon\kappa(5\epsilon^2U_{3\xi}-30\beta UU_\xi)+\epsilon\delta(5\epsilon^2U_{\xi\xi\tau}-15\beta UU_\tau\\ -15\beta U_\xi\partial_\xi^{-1}U_\tau)-\epsilon^2(45\beta^2U^2U_\xi-15\beta\epsilon^2\rho U_\xi U_{\xi\xi}-15\beta\epsilon^2UU_{3\xi}+\epsilon^4U_{5\xi})=0.\end{aligned}$$

But if we are to obtain the SK Eq. (3) and KK Eq. (4) as the unidirectional approximations for the Ramani and bKK equations, respectively, then we must take $\beta=\epsilon^2$ and $\kappa\delta=O(\epsilon^6)$. We now have

$$\begin{aligned}\epsilon^6(\zeta U_\tau-45U^2U_\xi+15\rho U_\xi U_{\xi\xi}+15UU_{4\xi}-U_{5\xi})+5\kappa^2U_\xi+5\delta^2\partial_\xi^{-1}U_{\tau\tau}\\ +\epsilon^3\kappa(5U_{3\xi}-30UU_\xi)+\epsilon^3\delta(5U_{\xi\xi\tau}-15UU_\tau-15U_\xi\partial_\xi^{-1}U_\tau)=0,\end{aligned}$$

where the constant ζ has the sign of κ. Evidently, we will obtain the SK and KK equations to leading order as $\epsilon\to 0$ only if the remaining terms have order greater than ϵ^6. But this would require the order of both κ and δ to exceed ϵ^3 which contradicts the requirement that $\kappa\delta=O(\epsilon^6)$.

In other words, we have shown that neither the SK nor KK equation can be recovered from their bidirectional cousins in a suitable unidirectional approximation. This justifies our contention that, contrary to appearances, the Ramani Eq. (12) and bKK Eq. (16) are not *the* Boussinesq forms of the SK Eq. (3) and KK Eq. (4), respectively. This conclusion is borne out when we attempt to retrieve the solitary waves of the SK and KK equations from their bidirectional counterparts Eqs. (45) and (54), respectively. For, under the transformation (58), there is no way of deriving the correct dispersion relation $(\omega=-p^5)$ from the bidirectional counterpart (44) in the unidirectional limit $(\epsilon\to 0)$.

VI. CONSERVATION LAWS

One of the many remarkable properties that are deemed to characterize soliton equations is the existence of an infinite sequence of conservation laws. These are of the form

$$\frac{\partial T_n}{\partial t}+\frac{\partial X_n}{\partial x}=0, \quad n=1,2,..., \tag{59}$$

where T_n denotes the nth conserved density and X_n is the corresponding flux. Then, with suitable boundary conditions, Eq. (59) yields a corresponding sequence of integrals of motion $\int T_n dx$. Conservation laws play an important rôle in soliton theory. It is often the case that the first few conservation laws of a NEE have a physical interpretation. They can also be used to investigate both quantative and qualitative aspects of solutions, particularly soliton solutions.[5,18,22,38,42–44] Not least, the possession of infinitely many conserved densities may predict, or at least confirm, the integrability of an equation.

The conservation laws of the SK Eq. (3) have been obtained in one way or another by a number of authors,[26,27,36,37,45] while those of the KK Eq. (4) were reported in Refs. 27 and 45. Both sequences have the unusual property whereby every third conserved density is missing; specifically T_2, T_5, T_8,... are absent. In this section, we show that, not surprisingly, this same lacunary pattern is shared by their bidirectional cousins the Ramani Eq. (12) and bKK Eq. (16). We present recursion formulas for generating an infinite sequence of conservation laws for each equation, and formulate the first few conserved densities and associated flux explicitly. We should add that Hu[37] has investigated the conservation laws of Ramani's equation, but his results contain a slight error. The author gives only the first two nontrivial conserved densities [Eqs. (61) and (62) below] and no recursion formula, and so missed the lacunary behavior. On the other hand, the results given here for the bKK equation are, we believe, entirely new.

We begin by adopting an elementary approach; i.e., we search for conservation laws of the Ramani equation by just manipulating Eq. (12). This has the advantage of identifying the appropriate variables in which to express the conserved densities, and highlights the more complicated scenario that obtains for bidirectional NEEs over unidirectional equations. To this end, we rewrite Eq. (12) as the system [cf. the Boussinesq Eq. (2)[19,22]]

$$u_t+v_x=0, \tag{60a}$$

$$v_t+(3u^3-3uv-3uu_{xx}+v_{xx}+\tfrac{1}{5}u_{4x})_x=0, \tag{60b}$$

where the auxiliary field variable $v(x,t)$ is effectively defined by Eq. (60a) as $v=-\partial_x^{-1}u_t$. Both these equations are in the conservation form (59) and so, by inspection, we deduce the first two conserved densities and associated flux of Ramani's equation

$$T_1=u, \quad X_1=v, \tag{61}$$

$$T_2=v, \quad X_2=3u^3-3uv-3uu_{xx}+v_{xx}+\tfrac{1}{5}u_{4x}. \tag{62}$$

They have ranks $R(T_1)=1$ and $R(T_2)=2$, and may be identified with the conservation of mass and momentum, respectively. [Note that the corresponding flux has rank $R(X_n)=n+1$]. Clearly, little further progress is possible using this direct approach: Indeed, we anticipate that T_3 will be missing and there is no obvious way to formulate T_4.

Various techniques are available for obtaining an infinity of conservation laws for completely integrable equations. We shall employ the systematic method that was developed by Satsuma[46,47] to derive the conserved densities of a NEE from its Bäcklund transformation (BT). This procedure was used by Hu[37] and we shall broadly follow his development for the Ramani equation.

Following the standard procedure,[36] we introduce the potential $w(x,t)$ defined by

$$u=-2w_x, \tag{63}$$

and consider the BT equation for the Ramani Eq. (12)

$$(w'-w)_t-[(w'-w)_{xx}+3(w'-w)(w'+w)_x+(w'-w)^3]_x=0, \tag{64}$$

where w' is a second solution. This is the corrected version of the BT that was reported by Hu.[37] The lengthy derivation of Eq. (64), along with the more complex second half of the BT (which we will not need), can be found in Ref. 37. It is a complicating feature of bidirectional NEEs that the BT does not separate neatly into spatial and temporal equations (unlike their unidirectional counterparts): Both parts of the BT contain time derivatives. Nonetheless, it is worth noting that Eq. (64) has the form of a conservation law in which the flux is precisely the *spatial* part of the BT of its unidirectional cousin, the SK Eq. (3). In this sense, we may regard Eq. (64) as the ''spatial'' half of the BT of Ramani's equation. We shall find that the BT for the bKK Eq. (16) has exactly the same type of structure.

To proceed, we introduce the expansion[36]

$$w'-w=k+\sum_{n=1}^{\infty}\frac{J^{(n)}}{k^n}, \quad (k>0), \tag{65}$$

where $J^{(n)}(n=1,2,...)$ is the sequence of ''generalized'' conserved densities (that also includes any trivial ones). We now substitute Eq. (65) into Eq. (64) and equate coefficients of powers k^{-n} to zero. Then, using Eqs. (60a) and (63), we get for the first four $J^{(n)}$'s

$$\begin{aligned} J^{(1)}&=u,\\ J^{(2)}&=-J_x^{(1)}=-u_x,\\ J^{(3)}&=\tfrac{1}{3}\partial_x^{-1}J_t^{(1)}+\tfrac{2}{3}u_{xx}=-\tfrac{1}{3}(v-2u_{xx}),\\ J^{(4)}&=\tfrac{1}{3}\partial_x^{-1}J_t^{(2)}+\tfrac{1}{3}v_x-\tfrac{1}{3}u_{3x}=\tfrac{1}{3}(2v-u_{xx})_x, \end{aligned} \tag{66}$$

and the general recursion relation

$$\begin{aligned} J^{(n+2)}=&\tfrac{1}{3}\partial_x^{-1}J_t^{(n)}-\tfrac{1}{3}J_{xx}^{(n)}-J_x^{(n+1)}+uJ^{(n)}-\sum_{m=1}^{n-1}J^{(n-m)}J_x^{(m)}\\ &-\sum_{m=1}^{n}J^{(n-m+1)}J^{(m)}-\tfrac{1}{3}\sum_{m=1}^{n-2}\sum_{p=1}^{n-m-1}j^{(n-m-p)}J^{(m)}J^{(p)}, \end{aligned} \tag{67}$$

for $n\geqslant 3$.

Now, $J^{(n)}$ has rank $R(J^{(n)})=\frac{1}{2}(n+1)$. When n is even, the generalized density $J^{(n)}$ has fractional rank and is trivial (i.e., it can be expressed as an x-derivative). The conserved densities $T_n(n=1,2,...)$ are generated by the odd $J^{(2n-1)}$ and have integer rank $R(T_n)=n$. Thus, from Eq. (66) we see that $J^{(1)}$, $J^{(3)}$ reproduce the first two conserved densities T_1, T_2, Eqs. (61)–(62), whereas $J^{(2)}$, $J^{(4)}$ give trivial results. To obtain T_3 we set $n=3$ in the recursion formula (67): This yields

$$J^{(5)}=-\tfrac{2}{3}(v-\tfrac{1}{5}u_{xx})_{xx},$$

which shows that T_3 is trivial. Proceeding in the same way, we deduce the conserved densities of ranks 4–6

$$T_4=v^2-3u^2v-3uu_x^2-2u_xv_x-\tfrac{4}{5}u_{xx}^2, \tag{68}$$

$$T_5=9u^5+10uv^2+90u^2u_x^2-5vu_x^2+10uu_xv_x+25uu_{xx}^2+5v_x^2+2u_{xx}v_{xx}+2u_{3x}^2, \tag{69}$$

$$T_6=0. \tag{70}$$

As expected, the sequence of conservation laws of Ramani's equation exhibits the same lacunary behavior as the SK equation, with every third one missing. However, we note that the SK Eq. (3) has its densities of ranks 2, 5, 8,... absent, whereas the bSK Eq. (12) has those of ranks 3, 6, 9,... missing! Hu[37] only reported $J^{(1)}$, $J^{(2)}$, $J^{(3)}$, so was unable to spot this lacunary pattern.

The recursion relation (67) for Ramani's equation was not previously known and merits further scrutiny. In order to compute the next generalized density $J^{(n+2)}$ one certainly needs to know all $n+1$ densities of lower rank. But there is a further consideration: Unfortunately, the first term on the right-hand side of (67) involves $\partial_x^{-1}J_t^{(n)}$ which can only be integrated *directly* for those $J^{(n)}$ which are trivial. For any $J^{(n)}$ which corresponds to a nontrivial conserved density, T_m say, one is faced with evaluating $\partial_x^{-1}(T_m)_t$ and this evidently requires knowledge of the associated flux X_m. This underlines the extra complexity that is involved in deriving the conservation laws of a bidirectional equation as compared with its unidirectional counterpart (where knowledge of the flux is not required; cf. the SK equation[36]). The expressions for the flux become increasingly intricate and unwieldy, and we have, therefore, chosen to omit X_4 and X_5 here; they are listed in Appendix B, Eqs. (B1) and (B2).

We can repeat the entire procedure to obtain the sequence of conservation laws of the bidirectional KK equation. The ''spatial'' part of the BT for the bKK Eq. (16) is

$$(w'-w)_t-[(w'-w)_{xx}+3(w'-w)(w'+w)_x+(w'-w)^3+3w_{xx}]_x=0. \tag{71}$$

Notice that this is again in conservation form with the flux now given by the spatial half of the BT for the KK Eq. (4).[48] Substituting the series (65) into (71), and collecting powers of k, we deduce

$$J^{(1)}=u, \quad J^{(2)}=-\tfrac{1}{2}u_x,$$

$$J^{(3)}=-\tfrac{1}{3}(v-\tfrac{1}{2}u_{xx}), \quad J^{(4)}=\tfrac{1}{2}(v-\tfrac{1}{2}u^2)_x,$$

where $v=-\partial_x^{-1}u_t$, as before. The BT (71) differs from Eq. (64) by the single extra term $3w_{xx}=-\frac{3}{2}u_x$ which contributes to the term of $O(k^0)$. It follows that the recursion relation for the bKK Eq. (16) is identical to the recursion formula (67) obtained above for Ramani's Eq. (12). The additional term kicks in at $J^{(2)}$ and we get the first six conservation laws for the bKK equation

$$\begin{gathered}
T_1=u, \quad X_1=v,\\
T_2=v, \quad X_2=3u^3-3uv-\tfrac{9}{4}u_x^2-3uu_{xx}+v_{xx}+\tfrac{1}{5}u_{4x},\\
T_3=0, \quad X_3=0,\\
T_4=v^2-3u^2v-\tfrac{3}{4}uu_x^2-\tfrac{1}{2}u_xv_x-\tfrac{1}{20}u_{xx}^2,\\
T_5=36u^5+40uv^2+180u^2u_x^2+10vu_x^2-20uu_xv_x+25uu_{xx}^2+10v_x^2-2u_{xx}v_{xx}+u_{3x}^2,\\
T_6=0, \quad X_6=0.
\end{gathered} \tag{72}$$

The flux X_4 and X_5 are given in Appendix C, Eqs. (C1) and (C2). The lacunary pattern is again evident with every third conserved density absent: Those of ranks 3, 6, 9,... are missing whereas its undirectional cousin the KK Eq. (4) has ranks 2, 5, 8,... missing.

VII. SUMMARY AND PROSPECTUS

A method has been described for finding bidirectional versions of unidirectional nonlinear evolution equations. Specifically, we are able to construct a Lax pair for the bidirectional NEE from the Lax pair of its unidirectional cousin by using a novel exchange procedure (Sec. II). This

has the advantage of assuring that the ''new'' equation is completely integrable. In this study, the method was used to obtain bidirectional versions of the well-known Sawada–Kotera equation (3) and Kaup–Kupershmidt equation (4). We make no claim to originality of these fifth-order Bousinesq-type NEEs. Indeed, we identified the bidirectional counterpart of the SK equation, Eq. (12), with the familiar Ramani equation through its bilinear form (31). Similarly, the bidirectional KK equation (16) that is constructed here appears in the Jimbo–Miwa classification[23] as a reduction of the CKP hierarchy.[49] Yet very little is known about the bKK equation; to the best of our knowledge, its Lax pair (15) and bilinear forms (41) and (42) are reported here for the first time.

The close resemblance between the bSK-Ramani Eq. (12) and the bKK Eq. (16) belies the fact that they are fundamentally different integrable equations. Nevertheless, we were able to take advantage of their duality to derive the anomalous solitary wave of the bKK equation. This solitary wave, Eq. (54), has the remarkable property that its shape depends on the direction of propagation. This type of *directionally dependent solitary wave* is quite unusual in soliton theory and, as far as we know, has not been observed till now. Moreover, this special feature of the bKK equation distinguishes it from the bSK–Ramani equation whose solitary wave, Eq. (45), has the *same* classical bell-shaped profile whether traveling to the left or right.

Though they admit solutions that can propagate in two opposite directions, the bSK–Ramani and bKK equations are *not* the bidirectional equivalents of the SK and KK equations, respectively. We found that neither the bSK–Ramani nor bKK equation could be reduced to its unidirectional counterpart in a suitable unidirectional (far-field) approximation. In other words, we can assert that the bidirectional NEEs (12) and (16) constructed here are not of truly Boussinesq form (a distinguishing feature that was made precise in Sec. I). This justified our usage of the *small* ''b'' in the designations bSK and bKK for these bidirectional NEEs.

Finally, we presented Bäcklund transformations for the bSK–Ramani and bKK equations [the first of these, Eq. (64), being a corrected version of the BT given by Hu[37]]. Using these BTs we were able to obtain recursion formulas for generating an infinite sequence of conservation laws for both equations. The first six conserved densities of each equation—and their associated flux—were formulated explicitly and found to possess the same lacunary pattern as their unidirectional cousins; namely, that every third conservation law in the sequence is missing.

Naturally, our study raises further questions which deserve investigation. We shall consider these briefly, and offer some thoughts on future work. The most obvious unanswered question concerns the derivation of the multisoliton solutions of the bKK Eq. (16). Of course, for the related bSK–Ramani Eq. (12) we are free to solve the simpler bilinear form (31)—rather than the coupled system (30a) and (30b)—for which the N-soliton solution is given by Hirota's celebrated generic formula.[24] For the bKK equation, however, no reduction to a single bilinear equation is possible and we must, therefore, solve one or other of the two coupled bilinear forms (41) or (42). This is an altogether more difficult problem: Both bilinear forms involve three field variables and, more to the point, there is no prescribed ansatz akin to Hirota's regular N-soliton for solving Eqs. (41) or (42).

Nevertheless, let us consider this problem in the light of our successful derivation of the bKK solitary wave (in Sec. IV). To generate the regular two-soliton of the bSK–Ramani equation, we take[24]

$$f(x,t)=1+e^{\theta_1}+e^{\theta_2}+A_{12}e^{\theta_1+\theta_2},\quad \theta_i=p_ix+\omega_it+\eta_i,\quad i=1,2, \tag{73}$$

and solve the Ramani bilinear form (31) for the dispersion relations $\omega_i(p_i)$ [cf. Eq. (44)] and the interaction coefficient A_{12}. [The calculations, which make use of Eq. (48), are quite routine and we omit the details here.] Now, the analysis in Sec. IV shows that the equivalent two-soliton solution of the alternative coupled bilinear form (30a) and (30b) is given by squaring (73); i.e., we set

$$\begin{aligned} f(x,t)=1&+2e^{\theta_1}+2e^{\theta_2}+e^{2\theta_1}+e^{2\theta_2}+2(A_{12}+1)e^{\theta_1+\theta_2}\\ &+2A_{12}(e^{2\theta_1+\theta_2}+e^{\theta_1+2\theta_2})+A_{12}^2e^{2(\theta_1+\theta_2)}. \end{aligned} \tag{74}$$

But, if we exploit the duality between the bSK–Ramani and bKK equations through their bilinear forms (30) and (41) (just as we did for the solitary wave), then we can conjecture that the structure of the two-soliton solution of the bKK equation (41) will mimic (74). Clearly, we can apply this same reasoning to the *N*-soliton solution: This suggests a possible strategy for deriving the *N*-soliton by the bilinear transform method. As a first step, and to confirm the efficacy of this strategy, we were able to deduce the directionally dependent solitary wave of the bKK equation. Furthermore, we would expect the multisoliton solutions to have this same directional dependence: This holds out the prospect of studying multiple head-on collisions between single- and double-humped solitary waves.

A last remark on the soliton solutions is germane. We notice that, on setting $\theta_1=\theta_2$ in Eq. (73), we get the correct form of the anomalous solitary wave (47) of the bKK equation (modulo a phase shift $\eta\rightarrow\eta-\ln 2$). Similarly, if we were to put $\theta_1=\theta_3$ and $\theta_2=\theta_4$ in the regular four-soliton solution,[24] the resulting expression would give the form of the putative two-soliton solution of the bKK equation [cf. Eq. (74)]. Put another way, we may consider the *two*-soliton solution of the bKK equation to be a degenerate regular *four*-soliton solution. By the same token, the *N*-soliton would be a degenerate regular $2N$-soliton (obtained by setting the phase variables equal in pairs). This interpretation accords with that given by Date *et al.*[49] who described the *N*-soliton of those equations in the CKP hierarchy in a similar manner (albeit *implicitly* and from an entirely different perspective). For our own part, the anomalous character of the bKK solitons (like those of its close relative the KK equation[32,33]) arises quite naturally within the bilinear formalism as a *squared* regular *N*-soliton. This canonical interpretation of the *N*-soliton provides a basis on which one might construct these somewhat complicated solutions explicitly and work on this is currently in progress.

In Ref. 29, Fordy and Gibbons (and, independently, Hirota and Ramani[50]) established the deep relation between the SK Eq. (3) and KK Eq. (4) by obtaining Miura-type transformations linking them to an ''intermediate'' fifth-order NEE (the Fordy–Gibbons equation). The question then arises as to whether there exist similar transformations connecting their bidirectional cousins the bSK–Ramani Eq. (12) and bKK Eq. (16). We have attempted but failed to find Miura transformations relating these equations; but this should not be taken to imply that no comparable link exists. Indeed, we have already exploited their close relation in deriving the bKK solitary wave. This strongly suggests that it should be possible to construct a Bäcklund transformation between Eqs. (12) and (16), either linking the equations directly or via some intermediary NEE (which, presumably, would be a bidirectional counterpart to the unidirectional Fordy–Gibbons equation). These are open questions worthy of attention.

Lastly, but certainly not least, we have concluded that the bSK–Ramani Eq. (12) and bKK Eq. (16), are not truly *Boussinesq* in character. This begs the obvious question: What, then, are the Boussinesq versions of the SK Eq. (3) and KK Eq. (4)? We can be quite confident that they will belong to the generic BKP and CKP hierarchies of NEEs,[23,49] respectively. But is it possible to construct these Boussinesq equations specifically, along with their Lax pairs, by means of the exchange procedure described here? These, and other questions concerning their properties, merit investigation.

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APPENDIX A: BILINEAR FORMULAS

If $u=\partial_x^2\ln f$ and $u_{nx}=\partial^n u/\partial_x^n$, then

$$\mathrm{D}_x\mathrm{D}_t f\cdot f/f^2=2(\ln f)_{xt}, \tag{A1}$$

$$\mathrm{D}_x^2 f\cdot f/f^2=2u, \tag{A2}$$

$$\mathrm{D}_x^3\mathrm{D}_t f\cdot f/f^2 = 2u_{xt} + 12u(\ln f)_{xt}, \tag{A3}$$

$$\mathrm{D}_x^4 f\cdot f/f^2 = 12u^2 + 2u_{xx}, \tag{A4}$$

$$\mathrm{D}_x^6 f\cdot f/f^2 = 120u^3 + 60uu_{xx} + 2u_{4x}. \tag{A5}$$

For arbitrary functions f and g

$$\frac{\mathrm{D}_x\mathrm{D}_t f\cdot g}{f^2} = \frac{g}{f}\left(\frac{\mathrm{D}_x\mathrm{D}_t f\cdot f}{f^2}\right) + \frac{\partial^2}{\partial x\partial t}\left(\frac{g}{f}\right), \tag{A6}$$

$$\frac{\mathrm{D}_x^2 f\cdot g}{f^2} = \frac{g}{f}\left(\frac{\mathrm{D}_x^2 f\cdot f}{f^2}\right) + \frac{\partial^2}{\partial x^2}\left(\frac{g}{f}\right), \tag{A7}$$

$$\frac{\mathrm{D}_x^4 f\cdot g}{f^2} = \frac{g}{f}\left(\frac{\mathrm{D}_x^4 f\cdot f}{f^2}\right) + 6\left(\frac{\mathrm{D}_x^2 f\cdot f}{f^2}\right)\left(\frac{\mathrm{D}_x^2 f\cdot g}{f^2}\right) - 6\frac{g}{f}\left(\frac{\mathrm{D}_x^2 f\cdot f}{f^2}\right)^2 + \frac{\partial^4}{\partial x^4}\left(\frac{g}{f}\right), \tag{A8}$$

$$\mathrm{D}_x\mathrm{D}_t\left(f\cdot\frac{g}{f}\right) = \frac{1}{f^2}(\mathrm{D}_x\mathrm{D}_t f^2\cdot g - g\mathrm{D}_x\mathrm{D}_t f\cdot f), \tag{A9}$$

$$\mathrm{D}_x^2\left(f\cdot\frac{g}{f}\right) = \frac{1}{f^2}(\mathrm{D}_x^2 f^2\cdot g - g\mathrm{D}_x^2 f\cdot f). \tag{A10}$$

APPENDIX B: THE RAMANI EQUATION: THE FLUX X_4 AND X_5

$$\begin{aligned}X_4 = &-\tfrac{27}{5}u^5 + 9u^3v - 6uv^2 - 18u^2u_x^2 + 3vu_x^2 + 6uu_xv_x - 2v_x^2 + 9u^3u_{xx} - 6uvu_{xx} + \tfrac{24}{5}u_x^2u_{xx}\\ &- \tfrac{18}{5}uu_{xx}^2 - 3u^2v_{xx} + 2vv_{xx} + \tfrac{2}{5}u_{xx}v_{xx} + \tfrac{36}{5}uu_xu_{3x} - \tfrac{2}{5}v_xu_{3x} - \tfrac{1}{5}u_{3x}^2 - 2u_xv_{3x}\\ &- \tfrac{3}{5}u^2u_{4x} + \tfrac{2}{5}vu_{4x} + \tfrac{2}{5}u_{xx}u_{4x} - \tfrac{2}{5}u_xu_{5x},\end{aligned} \tag{B1}$$

$$\begin{aligned}X_5 = &\,45u^4v - 30u^2v^2 + \tfrac{10}{3}v^3 + 45u^3u_x^2 + 15uvu_x^2 + 9u_x^4 + 150u^2u_xv_x - 30vu_xv_x - 20uv_x^2\\ &- 60u^2vu_{xx} + 15uu_x^2u_{xx} - 22u_xv_xu_{xx} + 24u^2u_{xx}^2 - vu_{xx}^2 - \tfrac{20}{3}u_{xx}^3 + 20uvv_{xx} - 15u_x^2v_{xx}\\ &+ 34uu_{xx}v_{xx} - 4v_{xx}^2 - 30u^2u_xu_{3x} - 4vu_xu_{3x} - 34uv_xu_{3x} - 4u_xu_{xx}u_{3x} + 4uu_{3x}^2 + 10uu_xv_{3x}\\ &+ 10v_xv_{3x} + 2u_{3x}v_{3x} + 4uvu_{4x} - 3u_x^2u_{4x} - 8uu_{xx}u_{4x} - 2v_{xx}u_{4x} + \tfrac{1}{5}u_{4x}^2 + 2u_{xx}v_{4x}\\ &+ 2uu_xu_{5x} + 2v_xu_{5x} - \tfrac{2}{5}u_{3x}u_{5x} + \tfrac{2}{5}u_{xx}u_{6x}.\end{aligned} \tag{B2}$$

APPENDIX C: THE bKK EQUATION: THE FLUX X_4 AND X_5

$$\begin{aligned}X_4 = &-\tfrac{27}{5}u^5 + 9u^3v - 6uv^2 - \tfrac{9}{2}u^2u_x^2 - \tfrac{15}{4}vu_x^2 + 6uu_xv_x - \tfrac{5}{4}v_x^2 + 9u^3u_{xx} - 6uvu_{xx} + \tfrac{51}{20}u_x^2u_{xx}\\ &- \tfrac{27}{20}uu_{xx}^2 - 3u^2v_{xx} + 2vv_{xx} + \tfrac{2}{5}u_{xx}v_{xx} + \tfrac{27}{10}uu_xu_{3x} - \tfrac{2}{5}v_xu_{3x} - \tfrac{1}{20}u_{3x}^2 - \tfrac{1}{2}u_xv_{3x}\\ &- \tfrac{3}{5}u^2u_{4x} + \tfrac{2}{5}vu_{4x} + \tfrac{1}{10}u_{xx}u_{4x} - \tfrac{1}{10}u_xu_{5x},\end{aligned} \tag{C1}$$

$$\begin{aligned}X_5 = &\,180u^4v - 120u^2v^2 + \tfrac{40}{3}v^3 - 90u^3u_x^2 - 30uvu_x^2 - \tfrac{171}{4}u_x^4 + 420u^2u_xv_x - 60vu_xv_x - 80uv_x^2\\ &- 240u^2vu_{xx} + 60uu_x^2u_{xx} - 118u_xv_xu_{xx} - 39u^2u_{xx}^2 + 11vu_{xx}^2 + \tfrac{46}{3}u_{xx}^3 + 80uvv_{xx} + 30u_x^2v_{xx}\\ &+ 76uu_{xx}v_{xx} - 11v_{xx}^2 + 60u^2u_xu_{3x} - 16vu_xu_{3x} - 76uv_xu_{3x} + 5u_xu_{xx}u_{3x} - 5uu_{3x}^2 - 20uu_xv_{3x}\end{aligned}$$

$$+20v_xv_{3x}+4u_{3x}v_{3x}+16uvu_{4x}+6u_x^2u_{4x}+10uu_{xx}u_{4x}-4v_{xx}u_{4x}-\tfrac{1}{5}u_{4x}^2-2u_{xx}v_{4x}$$
$$-4uu_xu_{5x}+4v_xu_{5x}+\tfrac{2}{5}u_{3x}u_{5x}-\tfrac{2}{5}u_{xx}u_{6x}. \quad \text{(C2)}$$

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On the variational principle for dust shells in General Relativity

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The variational principle for a thin dust shell in General Relativity is constructed. The principle is compatible with the boundary-value problem of the corresponding Euler–Lagrange equations, and leads to ''natural boundary conditions'' on the shell. These conditions and the gravitational field equations which follow from an initial variational principle, are used for elimination of the gravitational degrees of freedom. The transformation of the variational formula for spherically-symmetric systems leads to two natural variants of the effective action. One of these variants describes the shell from a stationary interior observer's point of view, another from the exterior one. The conditions of isometry of the exterior and interior faces of the shell lead to the momentum and Hamiltonian constraints. The canonical equivalence of the mentioned systems is shown in the extended phase space. Some particular cases are considered. © *2001 American Institute of Physics.*
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I. INTRODUCTION

A thin spherically-symmetric dust shell is among the simplest popular models of collapsing gravitating configurations. The equations of motion of these objects are obtained in Refs. 1 and 2. The construction of a variational principle for such systems was discussed from different points of view in Refs. 3–7. There are a number of problems here, most basic of which is the dependence on the choice of the evolution parameter (internal, external, proper). The choice of time coordinate, in turn, affects the choice of a particular quantization scheme, leading, in general, to quantum theories which are not unitarily equivalent.

In most of these papers the variational principle for shells is usually constructed in a comoving frame of reference, or in one of variants of freely falling frames of reference. However, use of such frames of reference frequently leads to effects unrelated to the object under consideration. The essential physics involves a picture of a gravitational collapse from the point of view of an infinitely remote stationary observer. In quantum theory this point of view enables us to treat bound states in terms of asymptotic quantities and to build the relevant scattering theory correctly. On the other hand, to treat primordial black holes in the theory of self-gravitating shells it is convenient to take the viewpoint of a central stationary observer. In the approach related to proper time of the shell reduction of the system leads to complicated Lagrangians and Hamiltonians which creates difficulties on quantization. In particular it leads to theories with higher derivatives or to finite difference equations.

In our opinion, the choice of the exterior or interior stationary observers is most natural and corresponds to the real physics. To provide the necessary properties of invariance, specification of the canonical transformations in an extended phase space which translate the corresponding dynamical systems into one another enough. In addition the action for a shell should satisfy some natural requirements. In the absence of self-forces it should pass into the action for a geodesic motion. Further, according to the correspondence principle, at small velocities and masses of the

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shell, and also in the absence of other sources of the gravitational field, we should obtain the action for a self-gravitating Newtonian shell (see Appendix C).

The natural Hamiltonian formulation of a self-gravitating shell was considered in works.[8,9] However, this formulation was not obtained by a variational procedure from some initial action containing the standard Einstein–Hilbert term. The action for such a self-gravitating spherical shell of mass m can be introduced with the help of a naive ''relativization'' of the Newtonian action. It is carried out by simple replacement of the kinetic energy $mv^2/2$ by the relativistic expression $-mc\sqrt{(1-v^2/c^2)}$ [see below Lagrangians (C17) and (4.3)]. If there is an exterior gravitational field then the kinetic and potential energy of the shell have as their general relativistic analog the geodesic Lagrangian $-mc\,{}^{(2)}ds_{\pm}/dt_{\pm}$. The subsigns ''$_{\pm}$'' correspond to exterior and interior observers. The gravitational self-action of the shell is the same for all cases, and its sign depends on whether stationary observer can exist inside and outside the shell.

The above Hamiltonian formulation for the shell, as well as the procedure of ''relativization'' follows from the Lagrange formalism of dust shells constructed in the present paper. We view the system as a compound configuration consisting of two vacuum regions with a spatially-closed boundary surface formed by the shell. The initial action we take as the sum of actions of York type for either region and the action for dust matter. For the complete action introduced in this way the variational principle is compatible with the boundary-value problem of the corresponding Euler–Lagrange equations for either region of the configuration, and leads to ''natural boundary conditions'' on the shell. The missing boundary conditions are obtained by consideration of the variations with respect to normal displacements of the shell. The obtained conditions coincide with the known Israel matching conditions at singular hypersurfaces and are considered as constraints. Together with the equations of the gravitational field they are used to eliminate of the gravitational degrees of freedom. The tangential variations of thus-obtained action with constraints lead to the known equations of motion of the Israel.[1]

The problem of the complete reduction of the action is solved for spherically-symmetric systems. By transforming the variational formula and using the constraints the obtained action is reduced to two variants of the effective action. One of these variants describes the shell from an interior stationary observer's point of view, and the other from the exterior one. Then we go over from the Lagrangian to the Hamiltonian description. The conditions of isometry of the exterior and interior sides of the shell lead to the momentum and Hamiltonian constraints. The canonical equivalence of these two variants of the description of the shells in the extended phase space indicates the existence of a ''discrete gauge'' transformation associated with the transition from the interior observer to the exterior one.

The paper is organized as follows: In Sec. II the full action is constructed for a compound, piecewise smooth Lorentz manifold with a four-dimensional spatially-closed boundary surface between two vacuum regions, corresponding to the world sheet of the shell. From here the Einstein equations for regions outside the shell and surface equations follow. Further, the action for the shell and the equations of motion are constructed.

In Sec. III spherically-symmetric relativistic dust shells are considered. The Lagrangians and Hamiltonians describing the shell from the point of view of the interior or exterior observer are obtained. Then momentum and Hamiltonian constraints are found. They emerge from independent consideration of the interior and exterior faces of the shell using the conditions of isometry of its two faces. In Sec. IV special cases of dust shells and configurations of several shells are briefly considered.

In Appendix A it is shown that the surface equations, obtained in Sec. II, reduce to the known equations for jumps of the extrinsic curvature tensor of the shell. In Appendix B we show the canonical equivalence of the actions for the dust spherically-symmetric shell written relative to the interior and exterior observers. This equivalence is thought of as operating in the extended phase space of the corresponding dynamical system. In Appendix C the action for an arbitrary nonrelativistic gravitating dust shell is constructed. The Lagrangian for the spherical gravitating nonrelativistic dust shell is found. It was deemed worthwhile to consider the nonrelativistic case because

it clarifies the interpretation of the results and allows comparisons with the general relativistic approach.

In this work we consider both relativistic and nonrelativistic systems. In this connection, we shall keep all the dimensional constants. Here c is the velocity of light, γ is the gravitational constant, $\chi=8\pi\gamma/c^2$, $\hbar$ is Planck's constant. The metric tensor $g_{\mu\nu}$ ($\mu,\nu=0, 1, 2, 3$) has the signature $(+\,-\,-\,-)$.

II. THE VARIATIONAL PRINCIPLE AND EQUATIONS OF MOTION FOR RELATIVISTIC DUST SHELLS

Consider a timelike spatially-closed hypersurface $\Sigma_t^{(3)}$ into some region $D^{(4)}$ of the space–time $V^{(4)}$. Let it be the world sheet of the infinitely thin dust shell with the surface density of dust σ. This shell divides the region $D^{(4)}$ into the interior and exterior ones, $D_-^{(4)}$ and $D_+^{(4)}$. Introduce the general coordinate map x^μ on our compound manifold $D^{(4)}=D_-^{(4)}\cup\Sigma_t^{(3)}\cup D_+^{(4)}$ and the metrics $g_{\mu\nu}^{\pm}$ on $D_\pm^{(4)}$, so that $g_{\mu\nu}^-|_{\Sigma_t^{(3)}}=g_{\mu\nu}^+|_{\Sigma_t^{(3)}}$.

One defines the elements of the four-volume $d^4\Omega$ on $D_\pm^{(4)}$ and three-volume $d^3\Omega$ on $\Sigma_t^{(3)}$ according to the formulas,

$$d^4\Omega=\sqrt{-g}d^4x=\sqrt{-g}dx^0\wedge dx^1\wedge dx^2\wedge dx^3, \tag{2.1}$$

$$d^3\Omega=-\sqrt{-g}n^\mu d\Sigma_\mu=\sqrt{-g}d\Sigma, \tag{2.2}$$

where n^μ is the unit normal to $\Sigma_t^{(3)}$, directed from $D_-^{(4)}$ to $D_+^{(4)}$ ($n_\mu n^\mu=-1, u_\mu n^\mu=0$), $g=\det|g_{\mu\nu}|$. Three-forms $d\Sigma_\mu$ and $d\Sigma$ are determined by the relations,

$$dx^\mu\wedge d\Sigma_\nu=\delta^\mu_\nu d^4x,\quad \eta\wedge d\Sigma=d^4x\quad (d\Sigma_\mu=n_\mu d\Sigma), \tag{2.3}$$

where "$\wedge$" denotes the exterior product, and $\eta=n_\mu dx^\mu$ is a normal covector.

Now let us fix coordinate system x^μ so that the coordinates $x^a(a=2, 3)$ be Lagrange coordinates of particles on the shell $\Sigma_t^{(3)}$. Then $u^\mu x^a{}_{,\mu}=n^\mu x^a{}_{,\mu}=0$, where "$,\mu$" is derivative with respect to the coordinate x^μ. Hence it follows $u^a=n^a=0$. The equations $x^a=\text{const}$ determine the world line γ of some particle of dust on $\Sigma_t^{(3)}$. The set $\{\gamma\}=\{x^a, x^a+dx^a\}$ of the world lines forms the elementary stream tube of dust. On the shell $\Sigma_t^{(3)}$ we shall introduce the basis of one-forms,

$$\{e^0\equiv\omega=u_\mu dx^\mu,\quad e^a=dx^a\}\quad (a,b=2,3) \tag{2.4}$$

and the dual vector basis,

$$\{e_0\equiv u=u^\mu\partial_\mu,\quad e_a\},\quad e^i(e_k)=\delta^i_k\quad (i,k=0,2,3). \tag{2.5}$$

In the basis $\{e^i\}=\{\omega, dx^a\}$ the metric tensor and three-form of volume on $\Sigma_t^{(3)}$ are

$${}^{(3)}g=\omega\otimes\omega-q_{ab}dx^a\otimes dx^b, \tag{2.6}$$

$$d^3\Omega=-\omega\wedge d^2\Omega,\quad d^2\Omega=\sqrt{q}dx^2\wedge dx^3. \tag{2.7}$$

Here "$\otimes$" is the sign of a tensor product, $d^2\Omega$ is the surface element of the area for the section which is orthogonal to the elementary stream tube of dust, q_{ab} is the metric on these sections, $q=\det|q_{ab}|$. In the neighborhood of the hypersurface $\Sigma_t^{(3)}$ the metric tensor ${}^{(4)}g$ and four-form of volume $d^4\Omega$ can be expressed in the form

$${}^{(4)}g={}^{(3)}g-\eta\otimes\eta, \tag{2.8}$$

$$d^4\Omega=\eta\wedge d^3\Omega=\omega\wedge\eta\wedge d^2\Omega. \tag{2.9}$$

We introduce the two-form of mass on $\Sigma_t^{(3)}$ by the formula $d^2m=\sigma d^2\Omega$, then $\sigma d^3\Omega=\omega \wedge d^2m$.

Now we take the full action of the compound configuration in the form,

$$I_{\rm tot}^{(g)}=I_{\rm EH}-c\int_{\Sigma_t^{(3)}}\left(\sigma n^\mu+\frac{1}{2\chi}[\omega^\mu]\right)\sqrt{-g}d\Sigma_\mu+I_{\partial D^{(4)}}+I_0. \tag{2.10}$$

It is the functional of the metric $g_{\mu\nu}$, density of the dust σ and hypersurface $\Sigma_t^{(3)}$: $I_{\rm tot}^{(g)}\equiv I_{\rm tot}^{(g)}(g_{\mu\nu},\sigma,\Sigma_t^{(3)})$. The first term in the right-hand side of (2.10),

$$I_{\rm EH}=-\frac{c}{2\chi}\int_{D_-^{(4)}\cup D_+^{(4)}}{}^{(4)}R d^4\Omega \tag{2.11}$$

is the Einstein–Hilbert action for the regions $D_\pm^{(4)}$, where ${}^{(4)}R$ is the curvature scalar.

The second term in the right-hand side (2.10) contains the matter term $c\sigma d^3\Omega$ and matching term. The symbol $[\omega^\mu]=\omega^\mu|_+-\omega^\mu|_-$ denotes the jump of the quantity,

$$\omega^\mu=g^{\sigma\rho}\Gamma^\mu_{\sigma\rho}-g^{\mu\rho}\Gamma^\sigma_{\sigma\rho}, \tag{2.12}$$

$$\Gamma^\mu_{\sigma\rho}=\tfrac{1}{2}g^{\mu\nu}(g_{\nu\rho,\sigma}+g_{\nu\sigma,\rho}-g_{\rho\sigma,\nu}), \tag{2.13}$$

on Σ_t. The sign ''$|_+$'' or ''$|_-$'' indicates the marked values to be calculated as a limiting magnitude when approaching the boundary Σ_t from outside or inside, respectively. In Appendix A it will be shown, that the relation

$$[\omega^\mu]n_\mu=2[K] \tag{2.14}$$

takes place. Here $K=g^{\mu\nu}K_{\mu\nu}$ is the trace of the extrinsic curvature tensor

$$K_{\mu\nu}=-n_{\mu;\rho}h^\rho_\nu \quad (h^\rho_\nu=\delta^\rho_\nu+n^\rho n_\nu), \tag{2.15}$$

where $_{;\rho}$ is covariant derivative with respect to the coordinate x^μ. The third term

$$I_{\partial D^{(4)}}=\frac{c}{2\chi}\int_{\partial D^{(4)}}\omega^\mu\sqrt{-g}d\Sigma_\mu \tag{2.16}$$

contains the surface terms which are introduced to fix the metric on the boundary $\partial D^{(4)}$ of the region $D^{(4)}$. Note, that the boundary $\partial D^{(4)}$ consists of the pieces of timelike as well as spacelike hypersurfaces. The last term I_0 in (2.10) contains the boundary terms on the timelike infinitely remote hypersurfaces, necessary for normalization of the action.

The relation

$$\sqrt{-g}\,{}^{(4)}R=\sqrt{-g}G+(\sqrt{-g}\omega^\mu)_{,\mu} \tag{2.17}$$

takes place, where

$$G=g^{\mu\nu}(\Gamma^\rho_{\mu\sigma}\Gamma^\sigma_{\nu\rho}-\Gamma^\sigma_{\mu\nu}\Gamma^\rho_{\rho\sigma}) \tag{2.18}$$

contains only the first derivatives of the metric. Therefore the action (2.10) can be rewritten in a more compact form

$$I_{\rm tot}^{(g)}=I_g+I_m+I_0, \tag{2.19}$$

where

$$I_g=-\frac{c}{2\chi}\int_{D_-^{(4)}\cup D_+^{(4)}}\sqrt{-g}G d^4x=\int_{D_-^{(4)}\cup D_+^{(4)}}L_g d^4x \tag{2.20}$$

is the gravitational action of the first order, and

$$I_m=c\int_{\Sigma_t^{(3)}}\sigma d^3\Omega=-c\int_{S_t^{(2)}}d^2m\int_\gamma\omega \tag{2.21}$$

is the action for the dust.

The first and the penultimate terms in (2.10) form the action which can be ascribed to that of the York's type $I_Y=I_{\mathrm{EH}}+I_{\partial D^{(4)}}$.[10] It is used in variational problems with the fixed metric on the boundary $\partial D^{(4)}$ of the region $D^{(4)}$. It can also be used in variational problems with the general relativistic version of ''natural boundary conditions'' for ''free edge.''[11] In this case the metric on the boundary is arbitrary and the corresponding momenta vanishes. Together with I_0 it forms the York–Gibbons–Hawking action $I_{\mathrm{YGH}}=I_Y+I_0$ for a free gravitational field.

In our case of the compound configuration we also fix the metric on boundary $\partial D^{(4)}$, as it was done in variational problem for action I_Y. In addition, inside the system there is the boundary surface $\Sigma_t^{(3)}$, with singular distribution of matter on it. One can interpret this configuration as the two vacuum regions $D_\pm^{(4)}$ with a common ''loaded edge'' (or with a ''massive edge''). The sum of the actions of type I_Y for these regions and of the action for matter I_m and normalizing term I_0 do leads to the action $I_{\mathrm{tot}}^{(g)}$.

If there is no dust, $\sigma=0$, the common boundary is not ''loaded.'' Then, the requirement $\delta I_{\mathrm{tot}}^{(g)}=0$, at arbitrary, everywhere continuous variations of the metric, gives generalization of the above ''natural boundary conditions'' for free hypersurface $\Sigma_t^{(3)}$. They coincide with the condition of continuity for the extrinsic curvature on $\Sigma_t^{(3)}$, i.e., with ordinary matching conditions. If the edge, being matched, is ''loaded'' by some surface distribution of matter, then we obtain the corresponding surface equation or the boundary conditions for $D_\pm^{(4)}$. They are the analog of the generalized ''natural boundary conditions'' for ''loaded edges.'' The initial action is chosen so, that the surface equations on $\Sigma_t^{(3)}$ following from the requirement $\delta I_{\mathrm{tot}}^{(g)}=0$, coincide with the matching conditions on singular hypersurfaces.[1] In this case, the variational principle for the action $I_{\mathrm{tot}}^{(g)}$ will be compatible with the boundary-value problem of the corresponding Euler–Lagrange equations.[12,13]

Note, that, as a rule, the boundary terms are formulated in terms of the extrinsic curvature of the corresponding hypersurfaces. For the configuration which contains the boundary hypersurface dividing the domain $D^{(4)}$ into parts and the whole boundary consisting of several pieces of edge, initial, and eventual hypersurfaces, it is more convenient to use the covariant approach. In order to calculate $\delta I_{\mathrm{tot}}^{(g)}$ we use the complete action in the form (2.10). According to Ref. 14 we have

$$\delta(\sqrt{-g}\,{}^{(4)}R)=-\sqrt{-g}\,{}^{(4)}G^{\mu\nu}\delta g_{\mu\nu}+(\sqrt{-g}\Omega^\mu)_{,\,\mu}, \tag{2.22}$$

where

$$\Omega^\mu=g^{\sigma\rho}\delta\Gamma^\mu_{\sigma\rho}-g^{\mu\rho}\delta\Gamma^\sigma_{\sigma\rho}, \tag{2.23}$$

and ${}^{(4)}G^{\mu\nu}={}^{(4)}R^{\mu\nu}-\frac{1}{2}{}^{(4)}Rg^{\mu\nu}$ is the Einstein tensor. In addition, we shall use the following conditions: the boundary of the configuration $\partial D^{(4)}$, the metric on it, and the normal vector are fixed. Then $\delta d\Sigma_\mu|_{\partial D^{(4)}}=0$, $\delta g_{\mu\nu}|_{\partial D^{(4)}}=0$, $\delta n_\mu|_{\partial D^{(4)}}=0$. The hypersurface $\Sigma_t^{(3)}$ is fixed, and the metric and its variations are continuous on $\Sigma_t^{(3)}$: $[g_{\mu\nu}]_{\Sigma_t^{(3)}}=0$, $[\delta g_{\mu\nu}]_{\Sigma_t^{(3)}}=0$, $[n_\mu]_{\Sigma_t^{(3)}}=0$, $[\delta n_\mu]_{\Sigma_t^{(3)}}=0$.

For the variation δI_m according to the formula (2.21) we have $\delta I_m=-c\int d^2m\int\delta\omega=-c\int d^2m\int\delta\omega_\gamma$. Here, the quantity d^2m is considered as a stationary value at variations of the metric.[15] The sign ''$|_\gamma$'' designates restriction of the one-forms on the world line γ so, that

$$\delta\omega_{|\gamma}=\delta ds=\tfrac{1}{2}u^{\mu}u^{\nu}ds\ \delta g_{\mu\nu}=-\tfrac{1}{2}u_{\mu}u_{\nu}\omega_{|\gamma}\delta g^{\mu\nu}. \tag{2.24}$$

If all these conditions are satisfied, then from the requirement $\delta I^{(g)}_{\rm tot}=0$ one obtains the vacuum Einstein equations

$$^{(4)}G^{\mu\nu}=0,\quad \forall D^{(4)}_{\pm} \tag{2.25}$$

and the surface equations on $\Sigma^{(3)}_t$,

$$Q_{\mu\nu}-\tfrac{1}{2}Qg_{\mu\nu}=-\chi\sigma u_{\mu}u_{\nu}, \tag{2.26}$$

where $Q=g^{\mu\nu}Q_{\mu\nu}$, and

$$Q_{\sigma\rho}=n_{\mu}[\Gamma^{\mu}_{\sigma\rho}]-\tfrac{1}{2}(n_{\sigma}[\Gamma^{\mu}_{\mu\rho}]+n_{\rho}[\Gamma^{\mu}_{\mu\sigma}]). \tag{2.27}$$

It is shown in Appendix A that the surface equations (2.26) reduce to the known equations for the jump discontinuity of the extrinsic curvature tensor of the hypersurface $\Sigma^{(3)}_t$,[1]

$$[K_{\mu\nu}]-[K]h_{\mu\nu}=-\chi\sigma u_{\mu}u_{\nu}, \tag{2.28}$$

where $h_{\mu\nu}=g_{\mu\nu}+n_{\mu}n_{\nu}$ is the metric on $\Sigma^{(3)}_t$. From the relations (2.28) it follows

$$[K_{\mu\nu}]u^{\mu}u^{\nu}=-\frac{\chi}{2}\sigma, \tag{2.29}$$

The missing equation for the average tensor of the extrinsic curvature

$$\overline{K^{\mu}_{\nu}}=\tfrac{1}{2}(K^{\mu}_{\nu|_+}+K^{\mu}_{\nu|_-}) \tag{2.30}$$

can be obtained by considering the variations of $I^{(g)}_{\rm tot}$ with respect to normal displacements of the hypersurface $\Sigma^{(3)}_t$. For this purpose we define some one-parameter family of timelike hypersurfaces in a neighborhood of $\Sigma^{(3)}_t$ so that $\Sigma^{(3)}_t$ is included in this family. The family induces $(3+1)$-decomposition of the objects in the neighborhood of $\Sigma^{(3)}_t$. Thus for the four-curvature scalar one has

$$^{(4)}R=\,^{(3)}R+K^{\mu}_{\nu}K^{\nu}_{\mu}-K^2+\frac{2}{\sqrt{-g}}\{\sqrt{-g}(Kn^{\mu}-a^{\mu})\}_{,\mu}, \tag{2.31}$$

where $a^{\mu}=n^{\mu}_{;\nu}n^{\nu}$ and $^{(3)}R$ is the curvature scalar of hypersurfaces of the family. Substituting (2.31) into (2.11) and taking into account the relations $a^{\mu}n_{\mu}=0$ and (2.14), one obtains the action (2.10) in the form

$$I^{(g)}_{\rm tot}=\hat{I}_g+I_m+\hat{I}_{\partial D^{(4)}}+I_0, \tag{2.32}$$

where

$$\hat{I}_g=\int_{D^{(4)}_-\cup D^{(4)}_+}\hat{L}_g d^4x=-\frac{c}{2\chi}\int_{D^{(4)}_-\cup D^{(4)}_+}(^{(3)}R+K^{\mu}_{\nu}K^{\nu}_{\mu}-K^2)\sqrt{-g}d^4x \tag{2.33}$$

is the gravitational action, containing normal derivatives up to the first order, and $\hat{I}_{\partial D^{(4)}}$ and I_0 contain the boundary terms, which are unessential here.

Now let every point $p\in\Sigma^{(3)}_t$ be translated at a coordinate distance $\delta x^{\mu}(p)=n^{\mu}\delta\lambda(p)$ in the normal direction. As a result of the displacement one gets a new hypersurface $\tilde{\Sigma}^{(3)}_t$. The initial

and eventual positions of a shell are fixed, therefore $\delta\lambda(p)=0$, $\forall p\in\Sigma_t^{(3)}\cap\partial D^{(4)}=\tilde{\Sigma}_t^{(3)}\cap\partial D^{(4)}$. In addition, we fix the metric $g_{\mu\nu}$ and all the quantities on $\Sigma_t^{(3)}$, so that $\delta I_m=0$.

As a result of the displacement of the hypersurface $\Sigma_t^{(3)}$, the initial regions $D_+^{(4)}$ and $D_-^{(4)}$ are transformed into new ones $\tilde{D}_+^{(4)}$ and $\tilde{D}_-^{(4)}$, so that, $\tilde{D}_-^{(4)}\cup\tilde{\Sigma}_t^{(3)}\cup\tilde{D}_+^{(4)}=D_-^{(4)}\cup\Sigma_t^{(3)}\cup D_+^{(4)}=D^{(4)}$. Then, for example, the variation of the region $D_-^{(4)}$ can be expressed in the form $\delta D_-^{(4)}=\tilde{D}_-^{(4)}\setminus D_-^{(4)}=D_+^{(4)}\setminus\tilde{D}_+^{(4)}$. The variation of the action (2.33), under the above conditions, proves to be equal,

$$\delta I_{\rm tot}^{(g)}=\delta\hat{I}_g=\int_{\tilde{D}_-^{(4)}\cup\tilde{D}_+^{(4)}}\hat{L}_g d^4x-\int_{D_-^{(4)}\cup D_+^{(4)}}\hat{L}_g\,d^4x\cong-\int_{\delta D_-^{(4)}}(\hat{L}_g^+-\hat{L}_g^-)d^4x. \tag{2.34}$$

Here $\hat{L}_g^+$ and $\hat{L}_g^-$ are Lagrangians defined by the relation (2.33) and calculated as a limiting magnitude when approaching the hypersurface $\Sigma_t^{(3)}$ from outside or inside, respectively. Under the infinitesimal normal displacement of the hypersurface $\Sigma_t^{(3)}$, the full action is variated by the formula,

$$\delta I_{\rm tot}^{(g)}=-\int_{\Sigma_t^{(3)}}(\hat{L}_g^+-\hat{L}_g^-)\,\delta x^\mu d\Sigma_\mu=\int_{\Sigma_t^{(3)}}[\hat{L}_g]\delta\lambda\,d\Sigma. \tag{2.35}$$

Hence, from arbitrariness of $\delta\lambda(p)$ and the requirement $\delta I_{\rm tot}^{(g)}=0$, one finds

$$[\hat{L}_g]=\hat{L}_g^+-\hat{L}_g^-=[K_\nu^\mu K_\mu^\nu-K^2]=2\overline{K}_\nu^\mu([K_\mu^\nu]-[K]\delta_\mu^\nu)=0. \tag{2.36}$$

Here we considered that $[{}^{(3)}R]=0$ on $\Sigma_t^{(3)}$. Then, using (2.28), from (2.36) we obtain

$$\overline{K}_{\mu\nu}u^\mu u^\nu=0. \tag{2.37}$$

The relations (2.28) and (2.37) form the necessary complete set of algebraic conditions or constraints for the extrinsic curvature tensor $K_{\nu|_\pm}^\mu$ of the hypersurface $\Sigma_t^{(3)}$.

Now we can eliminate gravitational degrees of freedom in the action $I_{\rm tot}^{(g)}$ and construct the action for the shell. For this purpose it is necessary to calculate $I_{\rm tot}^{(g)}$ on the solutions of the vacuum Einstein equations (2.25) taking into account the constraints (2.28) and (2.37). Note, first, that on this stage we use explicitly only the following results of these equations:

$${}^{(4)}R=0,\quad [\omega^\mu]n_\mu=2[K]=\chi\sigma. \tag{2.38}$$

Substituting these relations for the corresponding terms in (2.10) one finds

$$I_{\rm tot}^{(g)}{}_{|\{\text{Eqs. (2.38)}\}}=I_{\rm sh}+I_{\partial D^{(4)}}+I_0, \tag{2.39}$$

where

$$I_{\rm sh}=\frac{1}{2}\int_{\Sigma_t^{(3)}}c\sigma d^3\Omega=-\frac{c}{2}\int_{S_t^{(2)}}d^2m\int_\gamma\omega \tag{2.40}$$

is the reduced action for the dust shell. This action must be considered together with constraints (2.28) and (2.37). The action $I_{\rm sh}^{(g)}$ is quite certain if the gravitational fields in the neighborhood of $\Sigma_t^{(3)}$ are determined as the solutions of the vacuum Einstein equations (2.25) which satisfy the boundary conditions (2.28) and (2.37). That is the finding of these fields that completes the construction of the action for the shell. At this stage all the equations (2.25) and constraints (2.28), (2.37) are already used.

Note, that one usually comes to the action for the shell in the other form. In our approach the action can be obtained at the partial reduction of initial action $I^{(g)}_{\rm tot}$, when the constraint in (2.38) is not taken into account. As a result we come to the action of the type,

$$\tilde{I}_{\rm sh}=-c\int_{\Sigma^{(3)}_t}\left(\sigma-\frac{1}{\chi}[K]\right)\omega\wedge d^2\Omega, \tag{2.41}$$

or to some its modification. In the spherically-symmetric case from here follows the Lagrangian of the shell in a frame of reference of the comoving observer. However, quantity $[K]$ contains second derivatives with respect to proper time of the shell. When eliminating them, through the integration by parts, one comes to rather complicated Lagrangians and Hamiltonians.

To find the equations of motion for particles of the shell from action $I_{\rm sh}$ (2.40) one should introduce the independent coordinates $x^\mu_\pm$ in each of the regions $D^{(4)}_\pm$, and the interior coordinates $y^i\,(i,k=0,2,3)$ on $\Sigma^{(3)}_t$. Let the equations of embedding of $\Sigma^{(3)}_t$ into $D^{(4)}_\pm$ have the form $x^\mu_\pm=x^\mu_\pm(y^i)$. Then we can write the relations,

$$^{(4)}ds^2_\pm=g^\pm_{\mu\nu}dx^\mu_\pm dx^\nu_\pm,\quad {}^{(3)}ds^2=g^\pm_{\mu\nu}x^\mu_{\pm,i}x^\mu_{\pm,k}dy^i dy^k=h_{ik}dy^i dy^k, \tag{2.42}$$

$$\omega=\omega^\pm=u^\pm_\mu dx^\mu_\pm,\quad \omega^\pm_{|\gamma}=ds_\pm,\quad u^\mu_\pm=dx^\mu_\pm/ds_\pm, \tag{2.43}$$

$$^{(3)}\omega=u^\pm_\mu x^\mu_{\pm,i}dy^i=u_i dy^i,\quad {}^{(3)}\omega_{|\gamma}={}^{(3)}ds,\quad u^i=dy^i/{}^{(3)}ds. \tag{2.44}$$

Nongravitational interaction between particles of the dust is absent. Therefore we consider quantity d^2m to be unchanged when a flow line is varied.

First, consider variations $I_{\rm sh}$ with respect to the internal coordinates y^i. In this case $\int_\gamma\omega=\int_\gamma{}^{(3)}\omega_{|\gamma}=\int_\gamma{}^{(3)}ds$. Then the metric $h_{ik}(y^i)$ is given on $\Sigma^{(3)}_t$ and the variation of $I_{\rm sh}$ leads to the equations of three-dimensional geodesic on the hypersurface $\Sigma^{(3)}_t$,

$$u^i_{;k}u^k=0. \tag{2.45}$$

Here ''$_{;k}$'' denotes the covariant derivative with respect to the coordinate y^k calculated with the help of the metric h_{ik}.

The consideration of the variational principle $\delta I^{(g)}_{\rm sh}=0$ with respect to the exterior coordinates $x^\mu_\pm$ is more interesting treatment. In this case $\int_\gamma\omega=\int_\gamma\omega^\pm_{|\gamma}=\int^{(4)}_\gamma ds_\pm$. Then the metrics $g^\pm_{\mu\nu}(x^\rho)$ are given in a neighborhood of the shell. Since the normal variations of the shell are already used, it is possible to consider the variations of dynamical quantities, generated only by the tangential to $\Sigma^{(3)}_t$ variations of the coordinates x^μ. These variations of the values will be denoted by the sign $\tilde{\delta}$. Thus, omitting for simplicity signs ''$\pm$,'' we have

$$\tilde{\delta}x^\mu=\delta x^\mu+n^\mu n_\nu\delta x^\nu\equiv h^\mu_\nu\delta x^\nu\quad (n_\mu\tilde{\delta}x^\mu=0,\quad h^\mu_\nu=\delta^\mu_\nu+n^\mu n_\nu), \tag{2.46}$$

where δx^μ are arbitrary values. Then we find

$$\tilde{\delta}\omega_{|\gamma}=\tilde{\delta}\,{}^{(4)}ds=\tilde{\delta}\sqrt{g_{\mu\nu}dx^\mu dx^\nu}=-u_{\mu;\nu}u^\nu h^\mu_\rho\delta x^\rho\,{}^{(4)}ds+d(u_\mu\delta x^\mu). \tag{2.47}$$

Supposing that $\delta x^\mu=0$ on $\Sigma^{(3)}_t\cap\partial D^{(4)}$, from the requirement $\tilde{\delta}I^{(g)}_{\rm sh}=0$ we obtain the three-dimensional geodesic equations on $\Sigma^{(3)}_t$, but, here, in the four-dimensional form,

$$u_{\mu;\nu}u^\nu h^\mu_\rho=0. \tag{2.48}$$

This equation can be rewritten as

$$u_{\rho;\nu}u^\nu=-u_{\mu;\nu}u^\nu n^\mu n_\rho. \tag{2.49}$$

Hence, using the definition of $K_{\mu\nu}$ (2.15) one obtains

$$u_{\rho;\nu}u^{\nu}=n_{\rho}n_{\mu;\nu}u^{\mu}u^{\nu}=-n_{\rho}K_{\mu\nu}u^{\mu}u^{\nu}. \tag{2.50}$$

Here we again introduce signs ''$\pm$'' and use the relations $K_{\mu\nu|_{\pm}}=\overline{K}_{\mu\nu}\pm\frac{1}{2}[K_{\mu\nu}]$. Then, taking into account constraints (2.29) and (2.37), we come to the equations of motion for the shell's particles with respect to the exterior coordinates,

$$(u_{\mu;\nu}u^{\nu})_{|\pm}=\pm\frac{\chi}{4}\sigma n_{\mu}. \tag{2.51}$$

For completeness one should add the unused constraints,

$$[K_{\mu\nu}]u^{\mu}e_{i}^{\nu}=0, \quad [K_{\mu\nu}]e_{a}^{\mu}e_{b}^{\nu}=\frac{\chi\sigma}{2}h_{ab}, \tag{2.52}$$

where $e_{a}^{\mu}=\partial x^{\mu}/\partial y^{a}$.

From (2.51) it follows the well-known Israel equations,[1]

$$n^{\mu}\frac{Du_{\mu}}{ds}\bigg|_{+}+n^{\mu}\frac{Du_{\mu}}{ds}\bigg|_{-}=0, \quad e_{i}^{\mu}\frac{Du_{\mu}}{ds}\bigg|_{\pm}=0, \tag{2.53}$$

$$n^{\mu}\frac{Du_{\mu}}{ds}\bigg|_{+}-n^{\mu}\frac{Du_{\mu}}{ds}\bigg|_{-}=-\frac{\chi\sigma}{2}, \tag{2.54}$$

where $Du_{\mu}=u_{\mu;\nu}dx^{\nu}$ is the covariant differential.

The equations of motion of the dust shell (2.51) can immediately be found from the action I_{sh}. Indeed, acting in the same manner as when deducing the equations of motion (2.51), the variational formula (2.47) can be transformed to the form,

$$\tilde{\delta}^{(4)}ds_{|_{\pm}}=-u_{\mu;\nu}u^{\nu}\delta x^{\mu}_{|_{\pm}}{}^{(4)}ds_{|_{\pm}}\mp\tfrac{1}{2}[K_{\mu\nu}]u^{\mu}u^{\nu}n_{\rho}\delta x^{\rho}ds_{|_{\pm}}+d(u_{\mu}\delta x^{\mu})_{|_{\pm}} \tag{2.55}$$

or

$$\tilde{\delta}\omega_{|\gamma}^{\pm}=\tilde{\delta}^{(4)}ds_{|_{\pm}}=\left\{\left(-u_{\mu;\nu}u^{\nu}\pm\frac{\chi\sigma}{4}n_{\mu}\right)\delta x^{\mu}{}^{(4)}ds+d(u_{\mu}\delta x^{\mu})\right\}_{|\pm}. \tag{2.56}$$

From here, under the above conditions, the equations of motion follow.

The proposed variational deducing of the equations of motion makes the problem of construction of the effective action for the dust shell free from constrains (2.28) and (2.37). It turns out that it is possible for some special class of the configurations. To show it, we shall choose such interior coordinates y^{i}, which at $i=a=2,3$ are the Lagrange coordinates of particles on the shell $\Sigma_{t}^{(3)}$. In addition, we introduce the coordinates $x^{\mu}_{|\pm}$ in the regions $D_{\pm}^{(4)}$ so that, when $\mu=a=2,3$ the equalities $x_{+}^{a}|_{\Sigma_{t}^{(3)}}=x_{-}^{a}|_{\Sigma_{t}^{(3)}}=y^{a}$ are satisfied. These coordinates are arbitrary in any other respect. Then the formulas of embedding of $\Sigma_{t}^{(3)}$ into $D_{\pm}^{(4)}$ have the form $x_{\pm}^{n}=x_{\pm}^{n}(y^{0})$ $(n=0,1)$ or $f_{\pm}(x^{0},x^{1})=0$. Therefore we have $u_{\pm}^{\mu}=\{u_{\pm}^{0},u_{\pm}^{1},0,0\}$ and $n_{\mu}^{\pm}=\{n_{0}^{\pm},n_{1}^{\pm},0,0\}$. Using the conditions $(u_{\mu}u^{\mu})_{|\pm}=-(n_{\mu}n^{\mu})_{|\pm}=1$ and $(u_{\mu}n^{\mu})_{|\pm}=0$ one finds $n_{0}^{\pm}=u_{\pm}^{1}$, $n_{1}^{\pm}=-u_{\pm}^{0}$. Hence it follows

$$n_{\mu}\delta x^{\mu}ds_{|_{\pm}}=(u^{1}\delta x^{0}-u^{0}\delta x^{1})ds_{|_{\pm}}=(dx^{1}\delta x^{0}-dx^{0}\delta x^{1})_{|_{\pm}}. \tag{2.57}$$

Therefore the variational formula (2.56) has the form

$$\tilde{\delta}\omega^{\pm}_{|\gamma}=\tilde{\delta}^{(4)}ds_{|_{\pm}}=\left\{\delta^{(4)}ds\pm\tfrac{1}{4}\chi\sigma(dx^1\delta x^0-dx^0\delta x^1)+d(u_\mu\delta x^\mu)\right\}_{|\pm}. \tag{2.58}$$

Now we introduce the vector potential $U_n=U_n(x^0,x^1)$ by the relation

$$d\wedge(U_n dx^n)\equiv G_{01}dx^0\wedge dx^1=-\tfrac{1}{4}\chi\sigma dx^0\wedge dx^1, \tag{2.59}$$

where $G_{nm}\equiv U_{m,n}-U_{n,m}(n,m=0,1)$. Hence it follows that the configurations, being considered, admit such motions of matter for which $\sigma=\sigma(x^0,x^1)$.

Using the definition (2.59) and the relation

$$\delta(U_n dx^n)-d(U_n\delta x^n)=G_{10}(dx^0\delta x^1-dx^1\delta x^0), \tag{2.60}$$

the variational formula (2.58) can be rewritten in the following form:

$$\tilde{\delta}\omega^{\pm}_{|\gamma}=\tilde{\delta}^{(4)}ds_{|_{\pm}}=\{\delta(ds\mp U_n dx^n)+d[(u_n\pm U_n)\delta x^n+u_a\delta y^a]\}_{|\pm}. \tag{2.61}$$

Returning to action for the shell (2.40), we conclude, that in the case under consideration we have

$$\delta I_{\rm sh}=\delta I^{\pm}_{\rm sh}-\frac{c}{2}\int_{S^{(2)}_t}d^2m\{(u_n\pm U_n)x^n{}_{,0}\delta y^0+u_a\delta y^a\}_{\pm}|^B_A, \tag{2.62}$$

where

$$I^{\pm}_{\rm sh}=-\frac{c}{2}\int_{S^{(2)}_t}d^2m\int_\gamma(ds\mp U_n dx^n)_{|\pm}, \quad (n=0,1) \tag{2.63}$$

is the effective action for the shell written in terms of the exterior coordinates. Indices A and B indicate that the corresponding quantities are taken in initial and final positions of the shell. Since at fixed initial and final positions of particles $\delta y^i|_{A,B}=0$, then it follows $\delta I_{\rm sh}=\delta I^{\pm}_{\rm sh}$.

In such away, under the above conditions, the action of the shell (2.40) with the constraints (2.28), (2.37) and the action (2.62) without these constraints are equivalent. The actions $I^{+}_{\rm sh}$ and $I^{-}_{\rm sh}$ are equivalent in the same sense. Let us note, that in the considered above independent treatment of the interior and exterior faces of the shell there are new constraints following from isometry conditions of these faces.

III. EFFECTIVE ACTION FOR THE SPHERICAL DUST SHELL

Let us consider spherically-symmetric compound region $D^{(4)}=D^{(4)}_{-}\cup\Sigma^{(3)}_t\cup D^{(4)}_{+}\subset V^{(4)}$ into the spherically-symmetric space–time $V^{(4)}$, where $D^{(4)}_{\mp}$ are exterior and interior regions separated from each other by spherically-symmetric timelike hypersurface $\Sigma^{(3)}_t$. By using the curvature coordinates we can choose common in $D^{(4)}_{\pm}$, spatial, spherical coordinates $\{r,\theta,\alpha\}$, and individual time coordinates $t_{\pm}$ for $D^{(4)}_{\pm}$, respectively. Then the world sheet for the shell $\Sigma^{(3)}_t$, respectively, the interior and exterior coordinates is determined by the equations $r=R_{-}(t_{-})$ and $r=R_{+}(t_{+})$. Under appropriate choice of $t_{\pm}$ we have $R_{-}(t_{-})=R_{+}(t_{+})$. Thus, the interior and exterior regions are determined by the relations

$$D^{(4)}_{-}=\{t_{-},r,\theta,\alpha: r_0<r<R_{-}(t_{-})\},\quad D^{(4)}_{+}=\{t_{+},r,\theta,\alpha: R_{+}(t_{+})<r<\infty\}$$

for all $\{\theta,\alpha\}\in\{0\leqslant\theta\leqslant\pi, 0\leqslant\alpha<2\pi,\}$ and for all admissible $t_{\pm}$. The particles of the shell are described by one collective dynamical coordinate $R=R_{\pm}(t_{\pm})$ and by the two fixed individual (Lagrange) angular coordinates θ and α. The minimal value of r_0 is limited by the domain of definition of the curvature coordinates.

The gravitational fields into the regions $D^{(4)}_{\pm}$ are given by the metrics

$$^{(4)}ds_{\pm}^2 = f_{\pm}c^2dt_{\pm}^2 - f_{\pm}^{-1}dr^2 - r^2(d\theta^2 + \sin^2\theta d\alpha^2), \tag{3.1}$$

where

$$f_{\pm} = 1 - \frac{2\gamma M_{\pm}}{c^2 r}, \tag{3.2}$$

and $M_{\pm}$ are the Schwarzschild masses ($M_+ > M_-$).

Owing to the spherical symmetry $\sigma = \sigma(t_{\pm}, R)$. Therefore the conditions of applicability of the modified action (2.62) are satisfied. In this case we have

$$d^2m = \sigma d^2\Omega = \sigma R^2 \sin\theta d\theta d\alpha, \tag{3.3}$$

$$U_n dx^n = c\varphi(t_{\pm}, R)dt_{\pm} + U_R(t_{\pm}, R)dR. \tag{3.4}$$

Using the gauge condition $U_R(t_{\pm}, r) = 0$, the action (2.62) can be written in the form

$$I_{\rm sh}^{\pm} = -\frac{c}{2}\int_{S_t^{(2)}} \sigma R^2 \sin\theta d\theta d\alpha \int_{\gamma_{\pm}} (^{(2)}ds \mp c\varphi dt)_{|\pm}. \tag{3.5}$$

Since the particles move only radially ($\theta = \text{const}$, $\varphi = \text{const}$) we shall use the truncate interval

$$^{(2)}ds_{\pm}^2 = f_{\pm}c^2dt_{\pm}^2 - f_{\pm}^{-1}dR^2. \tag{3.6}$$

Further, from the formula (2.59) it follows

$$\frac{1}{4}\chi\sigma = \frac{\gamma m}{2c^2R^2} = \frac{\partial\varphi}{\partial R}, \tag{3.7}$$

where $m = 4\pi\sigma R^2$ is the rest mass of the shell. Hence, up to an additive constant, one finds

$$\varphi = -\frac{\gamma m}{2c^2 R}. \tag{3.8}$$

Finally, integrating in (3.5) over the angles θ and α and making use of (3.6) and (3.8), the effective action of the shell can be expressed in the form,

$$I_{\rm sh}^{\pm} = \frac{1}{2}\int_{\gamma_{\pm}} L_{\rm sh}^{\pm} dt_{|\pm} = -\frac{1}{2}\int_{\gamma_{\pm}} \left(mc^{(2)}ds \pm \frac{\gamma m^2}{2R}dt \right)_{|\pm}, \tag{3.9}$$

where

$$L_{\rm sh}^{\pm} = -mc^2\sqrt{f_{\pm} - f_{\pm}^{-1}R_{t\pm}^2/c^2} \pm U \tag{3.10}$$

are the Lagrangians of the dust shell with respect stationary observes into the regions $D_{\pm}^{(4)}$, ($R_{t\pm} = dR/dt_{\pm}$), and

$$U^{(G)} = -\frac{\gamma m^2}{2R} \tag{3.11}$$

is the effective potential energy of the gravitational self-action of the shell. It is important that the self-action (3.11) has the same form as that in the Newtonian theory [formula (C12) in Appendix C]. The Lagrangians (3.10) themselves can be obtained from the corresponding Newtonian analogs [see Appendix C, formulas (C13) and (C14)] by the formal replacement of the first and second terms describing the kinetic and potential energies of the shell into the external field by

their general relativistic analog, the geodesic Lagrangian $-mc^{(2)}ds_{\pm}/dt_{\pm}$. It is natural that the Lagrangians (C13), (C14), up to an additive constant, are the Newtonian limits of the relativistic Lagrangians (3.10).

It is easy to see that the actions (3.9) transform each into other under the discrete gauge transformation,

$$M_{\pm}\to M_{\mp}\quad (f_{\pm}\to f_{\mp}),\quad U^{(G)}\to -U^{(G)},\quad t_{\pm}\to t_{\mp}.$$

This transformation generalizes the corresponding transformation of the Newtonian theory of shells (see Appendix C) and reduce to the transformation from the interior observer to the exterior one and otherwise.

Note, that despite the equivalence of the actions $I^{\pm}_{\rm sh}$, similar to Newtonian case (C13), (C14), they can be considered quite independently. We also can consider the regions $D^{(4)}_{\pm}$ together with the corresponding gravitational fields (3.1) separately and independently, as manifolds with the edge $\Sigma^{(3)}_{t\pm}$. The edges $\Sigma^{(3)}_{t\pm}$ acquire the physical meaning of different faces of the shell with the world sheet $\Sigma^{(3)}_{t}$, provided the regions $D^{(4)}_{\pm}$ are joined along these edges $\Sigma^{(3)}_{t\pm}$. This can be performed only if the conditions of isometry of the edges $\Sigma^{(3)}_{t\pm}$ are satisfied

$$f_+c^2dt_+^2-f_+^{-1}dR^2=f_-c^2dt_-^2-f_-^{-1}dR^2=c^2d\tau^2, \tag{3.12}$$

where τ is the proper time of the shell. In addition we have $\Sigma^{(3)}_{t+}=\Sigma^{(3)}_{t-}=\Sigma^{(3)}_{t}$, $\gamma_+(t_+)=\gamma_-(t_-)=\gamma$.

Now we study some results following from the isometry conditions of the edges. First, we obtain the relations between the velocities,

$$c^2\frac{f_+}{R^2_{t+}}-\frac{1}{f_+}=c^2\frac{f_-}{R^2_{t-}}-\frac{1}{f_-}, \tag{3.13}$$

$$R^2_{\tau}\equiv\left(\frac{dR}{d\tau}\right)^2=\frac{c^2R^2_{t\pm}}{c^2f_{\pm}-f_{\pm}^{-1}R^2_{t\pm}},\quad R^2_{t\pm}\equiv\left(\frac{dR}{dt_{\pm}}\right)^2=\frac{c^2f^2_{\pm}R^2_{\tau}}{c^2f_{\pm}+R^2_{\tau}}. \tag{3.14}$$

Then from the Lagrangians $L^{\pm}_{\rm sh}$ (3.10) one finds the momenta and Hamiltonians of the shell,

$$P_{\pm}=\frac{\partial L^{\pm}_{\rm sh}}{\partial R_{t\pm}}=\frac{mR_{t\pm}}{f_{\pm}\sqrt{f_{\pm}-f_{\pm}^{-1}R^2_{t\pm}/c^2}}=\frac{m}{f_{\pm}}R_{\tau}, \tag{3.15}$$

$$H^{\pm}_{\rm sh}=\frac{mc^2f_{\pm}}{\sqrt{f_{\pm}-f_{\pm}^{-1}R^2_{t\pm}/c^2}}\mp U=mc^2f_{\pm}\frac{dt_{\pm}}{d\tau}\mp U \tag{3.16}$$

or

$$H^{\pm}_{\rm sh}=c\sqrt{f_{\pm}(m^2c^2+f_{\pm}P^2_{\pm})}\mp U=mc^2\sqrt{f_{\pm}+R^2_{\tau}/c^2}\mp U=E_{\pm}, \tag{3.17}$$

where $E_{\pm}$ are the energies of the shell which are conjugated to the time $t_{\pm}$, respectively, and conserve with respect to the corresponding interior or exterior stationary observers' point of view. After elimination of velocity R_{τ} from (3.15) and (3.17), the isometry conditions of the edges can be expressed in the form

$$f_+P_+=f_-P_-, \tag{3.18}$$

$$(E_--U)^2-m^2c^4f_-=(E_++U)^2-m^2c^4f_+. \tag{3.19}$$

Substituting U and $f_{\pm}$ from (3.2) and (3.11) for those in the last relation and equating the coefficients at the same power of R we obtain the relations between the Hamiltonian $H_{\rm sh}^{\pm}$ and the Schwarzschild masses $M_{\pm}$,

$$H_{\rm sh}^{+}=H_{\rm sh}^{-}=(M_{+}-M_{-})c^2=E. \tag{3.20}$$

Here $E=E_{\pm}$ is the full energy of the shell. This energy is conjugated to the coordinate time t_{+} and t_{-} as well, and does not depend on the position of the stationary observer (inside or outside the shell). We shall interpret the relations (3.18) and (3.20) following from the above independent consideration of the shell faces, as momentum and Hamiltonian constraints.

The Lagrangians $L_{\rm sh}^{\pm}$ (3.10), as well as the relations (3.13)–(3.20), are valid only in a limited domain, since the used curvature coordinates are valid outside the event horizon only. Therefore, $L_{\rm sh}^{-}$ can be used when $R>2\gamma M_{-}/c^2$, and $L_{\rm sh}^{+}$ when $R>2\gamma M_{+}/c^2 (M_{+}>M_{-})$.

As is known, the complete description of the shells can be performed in the Kruskal–Szekeres coordinates. With respect to these coordinates the full Schwarzschild geometry consists of the four regions R^{+}, T^{-}, R^{-}, T^{+}, detached by the event horizons. Our above consideration concerned with the R^{+} region only.

Supposing r to be a time coordinate, we can formally use the action in the form (3.9) under the horizon. However, here we encounter the ambiguity when choosing the sign before ${}^{(2)}ds$. It is usually ascribed to ambiguity of the radial component direction of the unit normal to $\Sigma_t^{(3)}$. The point is that in the curvature coordinates the regions T^{-} and T^{+} coincide. Hence the time singularity $r=0$ contains the two singularities: past singularity and future singularity. Therefore, for instance, the movement of a test particle with the energy $E=0$ consists of the two stages. At the first stage the particle begins to move into the expanding region T^{+} from the past singularity $r=0$ and reaches the horizon at a moment when r reaches $2\gamma M/c^2$. Then it goes over into the contracting T^{-} region and moves from the horizon to the future singularity $r=0$. In the coordinates $\{r,t\}$, where r is the time coordinate, the latter stage looks like the movement directed backwards in time.

Similarly, in the curvature coordinates the regions R^{-} and R^{+} of the Kruskal–Szekeres diagram coincide and ordinary movement of particles into the future of the R^{-}-region looks as the movement directed backwards in time which corresponds to the change $ds\to -ds$. It means that ordinary particles moving into the R^{-}-region are mapped into the R^{+}-region as antiparticles (remember the Feynman's interpretation of antiparticles as ordinary particles moving backwards in time). Such trajectories can be taken into account by the change of the sign before $mc\,{}^{(2)}ds_{\pm}$ in the expression for the action (3.9) of the shell.

In order to use simplicity and convenience of the curvature coordinates and, at the same time, to keep information about shells into the R^{-}-region we introduce an auxiliary discrete variable $\varepsilon=\pm 1$ and make a change ${}^{(2)}ds_{\pm}\to\varepsilon_{\pm}\,{}^{(2)}ds_{\pm}$ in $I_{sh}^{\pm}$ (3.9). Herewith $\varepsilon_{\pm}=1$ correspond to the shell into the R^{+}-region, and $\varepsilon_{\pm}=-1$ to the shell into the R^{-}-region. Then, we introduce the quantities $\mu_{\pm}=\varepsilon_{\pm}m$. As a result the extended action has the form

$$I_{\rm sh}^{\pm}(\mu_{\pm})=\frac{1}{2}\int_{\gamma_{\pm}} L_{\rm sh}^{\pm}(\mu_{\pm})dt_{|\pm}=-\frac{1}{2}\int_{\gamma_{\pm}}(\mu c\,{}^{(2)}ds\mp U^{G}dt)_{|\pm}, \tag{3.21}$$

where

$$L_{\rm sh}^{\pm}(\mu_{\pm})=-\mu_{\pm}c^2\sqrt{f_{\pm}-f_{\pm}^{-1}R_{t\pm}^2/c^2}\pm U \tag{3.22}$$

are the generalized Lagrangians describing the shell inside any of the $R^{\pm}$-regions with respect to the curvature coordinates of the interior $\{t_{-},R\}$ or exterior $\{t_{+},R\}$ regions. The event horizons $R_g=2\gamma M_{\pm}/c^2$ are, still, singular points of the dynamical systems (3.21) and must be excluded from consideration.

For the extended system (3.21) the Hamiltonian has the form

$$H^{\pm}_{\rm sh}(\mu_{\pm})=c\varepsilon_{\pm}\sqrt{f_{\pm}(m^2c^2+f_{\pm}P^2_{\pm})}\mp U=\mu_{\pm}c^2\sqrt{f_{\pm}+R^2_{\tau}/c^2}\mp U. \tag{3.23}$$

Hence, taking into account the Hamiltonian constraints (3.20) one finds the standard relations of the theory of dust spherical shells.[1] We shall rewrite them in terms of new designations,

$$\mu_{-}\sqrt{f_{-}+R^2_{\tau}/c^2}-\mu_{+}\sqrt{f_{+}+R^2_{\tau}/c^2}=\frac{\gamma\mu^2}{Rc^2}, \tag{3.24}$$

$$\mu_{-}\sqrt{f_{-}+R^2_{\tau}/c^2}+\mu_{+}\sqrt{f_{+}+R^2_{\tau}/c^2}=2(M_{+}-M_{-}). \tag{3.25}$$

In the end of the section we write out the Hamilton–Jacobi equations corresponding to the Hamiltonians (3.23) and to the constraints (3.18), (3.20) for truncated actions $S^{\pm}_0=S^{\pm}_0(R)$,

$$\frac{1}{f_{\pm}}\left(M_{+}-M_{-}\mp\frac{U}{c^2}\right)^2-\frac{f_{\pm}}{c^2}\left(\frac{dS^{\pm}_0}{dR}\right)^2=m^2, \tag{3.26}$$

$$f_{+}\,dS^{+}_0=f_{-}\,dS^{-}_0\,. \tag{3.27}$$

Then, the complete actions are determined by the formula $S^{\pm}=-c^2(M_{+}-M_{-})t_{\pm}+S^{\pm}_0$.

IV. PARTICULAR CASES OF SPHERICAL DUST CONFIGURATIONS

A. Self-gravitating dust shell

In this case $M_{-}=0$. Denote $M_{+}=M$ and consider the shell moving into the R_{+}-region. Then with respect to the exterior coordinates, the Lagrangian and the Hamiltonian of the shell have the form,

$$L^{+}_{\rm sh}=-mc^2\sqrt{1-\frac{2\gamma M}{c^2R}-\left(1-\frac{2\gamma M}{c^2R}\right)^{-1}\frac{R^2_{t+}}{c^2}}-\frac{\gamma m^2}{2R}, \tag{4.1}$$

$$H^{+}_{\rm sh}=c\sqrt{1-\frac{2\gamma M}{c^2R}}\sqrt{m^2c^2+\left(1-\frac{2\gamma M}{c^2R}\right)P^2_{+}}+\frac{\gamma m^2}{2R}. \tag{4.2}$$

The same shell with respect to the interior coordinates is described by the Lagrangian and the Hamiltonian,

$$L^{-}_{\rm sh}=-mc^2\sqrt{1-R^2_{t-}/c^2}+\frac{\gamma m^2}{2R}, \tag{4.3}$$

$$H^{-}_{\rm sh}=c\sqrt{m^2c^2+P^2_{-}}-\frac{\gamma m^2}{2R}. \tag{4.4}$$

This Hamiltonian was considered in the works.[8,9] The dynamical systems with $L^{\pm}_{\rm sh}$ obey momentum and Hamiltonian constraints $P_{-}=f_{+}P_{+}$, $H^{+}_{\rm sh}=H^{-}_{\rm sh}=Mc^2$ and they are canonically equivalent (see Appendix B).

B. The dust shell with vanishing full energy

Now we consider the shell for which the binding energy $E_b=(m+M_{-}-M_{+})c^2$ coincides with the rest energy mc^2. Denote $M_{+}=M_{-}\equiv M$, $f_{+}=f_{-}\equiv f=1-2\gamma M/c^2R$, $t_{+}=t_{-}\equiv t$. Then for the full energy we have $E=0$. This is possible, as it follows from (3.24), (3.25), only when $\mu_{+}=-\mu_{-}<0$, i.e., for the wormhole. Such a shell can be considered as a classical model for ''zeroth oscillations'' of dust matter with bare mass m under the gravitational field with $f=1-2\gamma M/c^2R$.

In terms $\{t, R\}$ the trajectories of ''zeroth oscillations'' are determined by the equation

$$\frac{dR}{dt}=\frac{2c^3}{\gamma m}\left(1-\frac{2\gamma M}{c^2R}\right)\sqrt{\frac{\gamma^2m^2}{4c^4}+\frac{2\gamma M}{c^2}R-R^2}. \tag{4.5}$$

Hence for the turning radius we have

$$R_m=\frac{\gamma}{c^2}\left(M+\sqrt{M+\frac{m^2}{4}}\right). \tag{4.6}$$

In the case of the flat space when $M=0$, from (4.5)and (4.6) we find

$$\frac{dR}{dt}=c\sqrt{1-\frac{R^2}{R_{m0}^2}},\quad R_{m0}=\frac{\gamma m}{2c^2}. \tag{4.7}$$

The equations of motion of such ''zeroth'' shells coincide with those for the oscillator,

$$\frac{d^2R}{dt^2}+\omega^2R=0. \tag{4.8}$$

Its oscillations $R(t)=R_{m0}\cos\omega(t-t_0)$ occur with the amplitude R_{m0} and frequency $\omega=c/R_{m0}=2c^3/\gamma m$. Hence we find the time of life of these shells into the flat space–time as a half-period of the oscillation,

$$T=\frac{\pi}{\omega}=\frac{\pi\gamma m}{2c^3}=\frac{\pi}{c}R_{m0}. \tag{4.9}$$

For the shell with mass equal to the mass of the Earth we have $R_g=2\gamma M/c^2\simeq 4cm$, $R_{m0}=R_g/4\simeq 1cm$, $T\simeq 10^{-10}c$. For the shells with Planck's mass $m=m_{\rm pl}=\sqrt{\hbar c/\gamma}$ the time of life equals $T=\pi T_{\rm pl}/2$, where $T_{\rm pl}=\sqrt{\hbar\gamma/c^5}$ is Planck's time. We underline, that the ''zero'' shells are characterized by that their gravitational binding energy completely compensate proper energy, leaving their total energy to be equal to zero. These shells can be thought of as a classical prototype of the Wheeler's space–time foam.[16]

C. The set of concentric dust shells

Now, consider briefly configurations consisting from the set of N concentric dust shells. Let R_a, m_a, τ_a be the radius, bare mass, and proper time of an ath shell, respectively ($a=1,2,\ldots,N$). For simplicity we suppose that $R_a>R_b$ if $a>b$. Then let M_a be the Schwarzschild mass determining the gravitational field $f_a=1-2\gamma M_a/c^2r$ on the right-hand side of an ath shell, into the region $R_a<r<R_{a+1}$. Suppose $f_a^-=1-2\gamma M_{a-1}/c^2R_a$ and $f_a^+=1-2\gamma M_a/c^2R_a$. Let $P_a^\pm=m_adR_a/f_a^\pm d\tau_a$ be the momenta of the ath shell, and $U_a^{(G)}=-\gamma m_a^2/2R_a$ be its potential energy of the self-action. Then,

$$H_a^\pm=c\varepsilon_a^\pm\sqrt{f_a^\pm(m_a^2c^2+f_a^\pm(P_a^\pm)^2)}\mp U_a \tag{4.10}$$

is the Hamiltonians of an ath shell. They, similarly to momenta $P_a^\pm$, are considered from the stationary observers' points of view, into the interior $R_{a-1}<r<R_a$ and exterior $R_a<r<R_{a+1}$, regions respectively. They satisfy the momentum and Hamiltonian constraints,

$$f_a^+P_a^+=f_a^-P_a^-,\quad H_a^+=H_a^-=(M_a-M_{a-1})c^2. \tag{4.11}$$

Now we are ready to determine the full Hamiltonian of this configuration,

$$H_N=\sum_{a=1}^{N} H_a^{\pm}. \tag{4.12}$$

For the self-gravitating configuration $M_0=0$. Then $H_1^{\pm}=M_1c^2$ and the full Hamiltonian of the configuration satisfies the constrain

$$H_N=Mc^2. \tag{4.13}$$

Here $M=M_N$ is the Schwarzschild mass of the configuration. The system admits the discrete gauge transformations,

$$M_a\leftrightarrow M_{a-1},\quad U_a\leftrightarrow -U_a,\quad t_a\leftrightarrow t_{a-1}\quad (a=1,2,\ldots,N),$$

where t_a is coordinate time determined on the right from an ath shell. The choice of sides (left or right) of the shells is not fixed beforehand and can be made by the reason of convenience.

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APPENDIX A: TRANSFORMATIONS OF THE SURFACE EQUATIONS

We show that the surface equations (2.26) reduce to the known equations for the jumps of the extrinsic curvature tensor on the shell.[1] First, we shall calculate $n_\mu[\omega^\mu]$.

We suppose that the following conditions are satisfied on the hypersurface $\Sigma_t^{(3)}$:

$$[n_\mu]=0,\quad [n_{\mu,\nu}]h_\sigma^\nu=0,\quad [n^\mu_{,\nu}]h_\sigma^\nu=0,\quad [g_{\mu\nu,\rho}]h_\sigma^\rho=0. \tag{A1}$$

Hence it follows

$$[\Gamma^\mu_{\rho\sigma}]h_\mu^\nu h_\beta^\rho h_\alpha^\sigma=0. \tag{A2}$$

Then from the definition (2.15) one finds

$$[\Gamma^\sigma_{\alpha\nu}]n_\sigma h_\beta^\nu=[K_{\alpha\beta}],\quad [\Gamma^\sigma_{\alpha\nu}]n_\sigma h^{\alpha\nu}=[K], \tag{A3}$$

$$[\Gamma^\sigma_{\alpha\nu}]n^\alpha h_\beta^\nu=-[K^\sigma_\beta]\quad ,[\Gamma^\sigma_{\alpha\nu}]n^\alpha h_\sigma^\nu=-[K], \tag{A4}$$

$$[\Gamma^\sigma_{\alpha\nu}]n_\sigma n^\alpha h_\beta^\nu=0. \tag{A5}$$

According to (2.12) we find

$$n_\mu\omega^\mu=n_\mu g^{\sigma\rho}\Gamma^\mu_{\sigma\rho}-n^\rho\Gamma^\sigma_{\rho\sigma}=n_\mu h^{\sigma\rho}\Gamma^\mu_{\rho\sigma}-n^\mu h^\sigma_\rho\Gamma^\rho_{\mu\sigma}.$$

Therefore, making use of Eqs. (A4) and (A5) we obtain the sought result (2.14).

Then, projecting the equation (2.26) into the hypersurface $\Sigma_t^{(3)}$ and into the normal n^ρ one finds

$$Q_{\sigma\rho}n^\rho-\tfrac{1}{2}Qn_\sigma=0, \tag{A6}$$

$$Q_{\sigma\rho}h^\sigma_\alpha h^\rho_\beta-\tfrac{1}{2}Qh_{\alpha\beta}=-\chi\sigma u_\alpha u_\beta. \tag{A7}$$

Using the definitions (2.27) and Eqs. (A2)–(A5) we obtain

$$Q=g_{\mu\nu}Q^{\mu\nu}=n_\mu[\omega^\mu]=2[K], \tag{A8}$$

$$
\begin{aligned}
Q_{\sigma\rho}n^{\rho} &= n_{\mu}n^{\rho}[\Gamma^{\mu}_{\rho\sigma}] - \tfrac{1}{2}n_{\sigma}n^{\rho}[\Gamma^{\mu}_{\rho\mu}] + \frac{1}{2}[\Gamma^{\mu}_{\sigma\mu}] \\
&= -n_{\sigma}(n_{\mu}[\Gamma^{\mu}_{\alpha\beta}]n^{\alpha}n^{\beta} + [\Gamma^{\mu}_{\mu\alpha}]n^{\alpha}) \\
&= -n_{\sigma}n^{\rho}[\Gamma^{\mu}_{\rho\nu}]h^{\nu}_{\mu} \\
&= [K]n_{\sigma}, \qquad \text{(A9)}
\end{aligned}
$$

$$
Q_{\sigma\rho}h^{\sigma}_{\alpha}h^{\rho}_{\beta} = n_{\mu}[\Gamma^{\mu}_{\sigma\rho}]h^{\sigma}_{\alpha}h^{\rho}_{\beta} = [K_{\alpha\beta}]. \qquad \text{(A10)}
$$

Thus Eqs. (A6) is satisfied identically, and Eq. (A7) yields the sought relations (2.28).

APPENDIX B: ON THE CANONICAL EQUIVALENCE OF THE ACTIONS $I^{\pm}_{\mathrm{sh}}$ FOR THE DUST SPHERICAL SHELL

In order to show the canonical equivalence of the actions $I^{\pm}_{\mathrm{sh}}$ in the extended phase space we write the variational principle (3.9) in the form

$$
\delta I^{\pm}_{\mathrm{sh}} = \delta \int (P_{\pm}dR - H_{\pm}dt_{\pm}) = 0, \qquad \text{(B1)}
$$

where

$$
P_{\pm} = \frac{1}{cf_{\pm}}\sqrt{(H_{\pm} \pm U)^2 - m^2c^4 f_{\pm}}\,. \qquad \text{(B2)}
$$

The dynamical systems with the actions $I^{\pm}_{\mathrm{sh}}$ are restricted by momentum and Hamiltonian constraints (3.18) and (3.20), which follow from the independent consideration of the faces of the shell.

The systems $I^{\pm}_{\mathrm{sh}}$ will be canonically equivalent in the extended phase space of variables $\{P_{\pm}, H_{\pm}, R, t_{\pm}\}$, if

$$
dI^{+}_{\mathrm{sh}} = dI^{-}_{\mathrm{sh}} + dF, \qquad \text{(B3)}
$$

or

$$
P_{+}dR - H_{+}dt_{+} = P_{-}dR - H_{-}dt_{-} + dF, \qquad \text{(B4)}
$$

where $F = F(R, t_{+}, t_{-})$ is the generating function of the canonical transformation $\{P_{+} = P_{+}(P_{-}, t_{-}, R),\ t_{+} = t_{+}(P_{-}, t_{-}, R)\}$. From (B4) we find

$$
H_{+} = -\frac{\partial F}{\partial t_{+}}, \quad H_{-} = \frac{\partial F}{\partial t_{-}}, \quad P_{+} = P_{-} - \frac{\partial F}{\partial R}. \qquad \text{(B5)}
$$

Using these relations the constraints (3.18) and (3.20) can be rewritten in the following way:

$$
-\frac{\partial F}{\partial t_{+}} = \frac{\partial F}{\partial t_{-}} = E\,, \quad \frac{\partial F}{\partial R} = P_{-}\left(1 - \frac{f_{-}}{f_{+}}\right). \qquad \text{(B6)}
$$

From here we find

$$
F = E(t_{-} - t_{+}) + \sigma(R, E), \qquad \text{(B7)}
$$

where

$$\sigma(R,E)=\frac{1}{c}\int\left(\frac{1}{f_-}-\frac{1}{f_+}\right)\sqrt{(E\pm U)^2-m^2c^4f_\pm}\,dR\,. \tag{B8}$$

The expression under the radical is invariant with respect to the replacement $f_\pm\to f_\mp$, $U\to -U$.

Then differentiating the expression (B7) over E one finds the relation between t_+ and t_-,

$$\frac{\partial F}{\partial E}=t_--t_++\frac{\partial\sigma}{\partial E}=\alpha, \tag{B9}$$

where the constant α cab be omitted. Thus, the transformations

$$\begin{cases} t_+=t_-+\dfrac{\partial\sigma(R,E)}{\partial E}, \\ P_+=P_-+\dfrac{\partial\sigma(R,E)}{\partial R}, \end{cases} \tag{B10}$$

are the sought canonical transformations of the extended phase space $\{P_\pm,H_\pm,R,t_\pm\}$ of the system. Herewith, the corresponding presymplectic form

$$dP_+\wedge dR-dE\wedge dt_+=dP_-\wedge dR-dE\wedge dt_- \tag{B11}$$

is invariant under these transformations.

The difference of the shell actions, which are considered from the point of view of the exterior and interior observers, up to an additive constant is $I^+_{\rm sh}(R,t_+)-I^-_{\rm sh}(R,t_-)=F(R,t_+,t_-)$, where $F=F(R,t_+,t_-)$ is the generating function, is calculated by the elimination of the energy E from the relations (B7) and (B9).

APPENDIX C: NONRELATIVISTIC DUST SHELL

Let us consider an infinitely thin dust layer in the Euclidean space $R^{(3)}$ in the form of the closed surface Σ_t moving in its own Newtonian gravitational field $\varphi=\varphi(\mathbf{r})$. The full action for this configuration has the form,

$$I^{(N)}_{\rm tot}=\int_{t_1}^{t_2}dt\left\{\int_{\Sigma_t}\left(\frac{1}{2}\sigma\mathbf{v}^2-\sigma\varphi\right)d^2f-\frac{1}{8\pi\gamma}\int_{D_-\cup D_+}(\nabla\varphi)^2\,dV\right\}. \tag{C1}$$

Here $\Sigma_t\,(t_1\leqslant t\leqslant t_2)$ is a one-parameter family of the closed surfaces, D_- and D_+ are interior and exterior regions of the shell Σ_t at a moment t, d^2f is the surface element on Σ_t, dV is the volume element in R^3, $\mathbf{v}$ is the velocity of particles of the shell, ∇ is the nabla operator, σ is surface mass density of dust on Σ_t. By virtue of the mass conservation law the value $dm\equiv\sigma d^2f$ conserves along the stream tube and in case of dust can be considered as a stationary value under arbitrary variations. Note also, that, we require that the potential φ be continuous, and, together with all its derivatives, vanish at infinity.

The requirement of extremity of the action $\delta I^{(N)}_{\rm tot}=0$ with respect to everywhere continuous variations $\delta\varphi$, vanishing on infinity, leads to the Laplace equation,

$$\Delta\varphi(\mathbf{r})=0,\quad \mathbf{r}\in D_-\cup D_+\,, \tag{C2}$$

with the boundary conditions for normal derivatives of φ on Σ_t. The latter, for completeness, will be written out together with the continuity conditions for φ on Σ_t,

$$[\varphi]\equiv\varphi_{|_+}-\varphi_{|_-}=0,\quad \left[\frac{\partial\varphi}{\partial\eta}\right]\equiv\left.\frac{\partial\varphi}{\partial\eta}\right|_+-\left.\frac{\partial\varphi}{\partial\eta}\right|_-=4\pi\gamma\sigma,\quad \mathbf{r}\in\Sigma_t\,(t=\text{const}). \tag{C3}$$

Here $\partial/\partial\eta=(\mathbf{n}\cdot\nabla)$ is the derivative with respect to the exterior normal $\mathbf{n}$ to Σ_t, vector $\mathbf{n}$ ($\mathbf{n}^2=1$) is directed from D_- to D_+. The solution of Eqs. (C2) and (C3) is the potential of a ''simple layer,''

$$\varphi_\sigma(\mathbf{r})=-\gamma\int_{\Sigma_t}\frac{\sigma(\mathbf{r}')d^2f'}{|\mathbf{r}-\mathbf{r}'|}. \tag{C4}$$

Now we can calculate $I^{(N)}_{\text{tot}}$ on the solutions of Eqs. (C2) and (C3). Thereby, the potential φ is excluded from the full action (C1). Note that owing to (C2) we have $(\nabla\varphi)^2=\nabla(\varphi\nabla\varphi)$. This allows to transform the volume integral of (C1) into the surface one on the boundaries of the regions $D_\pm$. Taking into account the boundary conditions (C3) and an asymptotic behavior of φ, we find the reduced action $I^{(N)}_{\text{tot}}$, as the value of the initial action on the solution (C4) of Eqs. (C2) and (C3),

$$I^{(N)}_{\text{tot}}|_{\{\text{solutions Eqs. (C2), (C3)}\}}=I^{(N)}_{\text{sh}}+I^{(N)}_0. \tag{C5}$$

Here $I^{(N)}_0$ contains the surface term, which is unessential for further consideration, and

$$I^{(N)}_{\text{sh}}=\int_{t_1}^{t_2}L^{(N)}_{\text{sh}}\,dt \tag{C6}$$

is the effective action for the shell with the Lagrangian,

$$L^{(N)}_{\text{sh}}=\frac{1}{2}\int_{\Sigma_t}\sigma\mathbf{v}^2df-U, \tag{C7}$$

where

$$U=\frac{1}{2}\int_{\Sigma_t}\sigma\varphi_\sigma\,df=-\frac{\gamma}{2}\int_{\Sigma_t}\int_{\Sigma_t}\frac{\sigma(\mathbf{r})\sigma(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}dfdf' \tag{C8}$$

is the functional of the potential energy of the gravitational self-action of the shell.

The Lagrangian of the shell in an external gravitational field $\varphi_0=\varphi_0(\mathbf{r})$ has the form,

$$L^{(N)}_{\text{sh}}=\int_{\Sigma_t}\left(\frac{1}{2}\sigma\mathbf{v}^2-\sigma\varphi_0\right)df-U. \tag{C9}$$

Now consider the spherical nonrelativistic dust shell. Let $R=R(t)$ be the radius of the spherical shell at a moment t. With respect to the spherical coordinates $\{r,\theta,\alpha\}$, we have $\sigma=\sigma(r)$, $d^2f=R(t)\sin\theta d\theta d\alpha$, $\mathbf{v}^2=\dot{R}^2=(dR/dt)^2$. The mass of the shell is $m=4\pi\sigma R^2=\text{const}$. The potential of the external field φ_0 on the shell has the value

$$\varphi_0\equiv\varphi_-=-\frac{\gamma m_-}{R(t)}, \tag{C10}$$

where m_- is the total mass of the interior source. The potential φ_σ and the self-action energy for the shell U prove to be equal

$$\varphi_\sigma(r)=\begin{cases}-\gamma m/r, & r\geqslant R(t)\\ -\gamma m/R(t), & r<R(t)\end{cases}, \tag{C11}$$

$$U=\frac{1}{2}m\varphi_\sigma=-\frac{\gamma m^2}{2R(t)}. \tag{C12}$$

Replacing the corresponding terms in (C9) by those of (C10)–(C12), we obtain the Lagrangian of the spherically-symmetric dust shell in Newtonian theory of gravity,

$$L^{(N)}_{\mathrm{sh}-}=\frac{1}{2}m\dot{R}^2+\frac{\gamma m m_-}{R}-U. \tag{C13}$$

A distinctive feature of spherical shell is that the two-valued description of the shell dynamic becomes possible with respect to the observer's position. From an interior observer's point of view, except for the force of self-action $-\partial U/\partial R$, the shell is effected by the external force $F_-=-md\varphi_-/dr$, which determines an interior gravitational field. This situation corresponds to the Lagrangian $L^{(N)}_{\mathrm{sh}-}$, therefore the latter can be interpreted as the Lagrangian describing the nonrelativistic shell from an interior observer's point of view.

An exterior observer $[r>R(t)]$ determines the field, judging by the force $F_+=-md\varphi_+/dr$ acting on the shell in the field $\varphi_+=\varphi_-+\varphi_\sigma=-\gamma m_+/R(t)$. This field is generated by the total mass of the system $m_+=m_-+m$. If, by making use of this relation, we eliminate m_- from $L^{(N)}_{\mathrm{sh}-}$ we obtain the following Lagrangian:

$$L^{(N)}_{\mathrm{sh}+}=\frac{1}{2}m\dot{R}^2+\frac{\gamma m m_+}{R}+U. \tag{C14}$$

It can be interpreted as the Lagrangian describing the Newtonian shell from an exterior observer's point of view.

In such a way, transformation from an exterior observer to an interior one stipulates the discrete transformation $m_\pm\to m_\mp=m_\pm\mp m$. Its can be interpreted as both the gravitational potential transformation $\varphi_\pm\to\varphi_\mp=\varphi_\pm\pm\gamma m/R$ and the change of sign of the self-action potential $U^{(N)}\to-U^{(N)}$. The above two-valued description of spherical shell in the Newtonian theory has a formal character. This ambiguity, arising when describing spherically-symmetric shell, is a matter of principle in General Relativity.

Note other feature of the shell, which has nontrivial meaning in General Relativity. The Lagrangians $L^{(N)}_{\mathrm{sh}\pm}$ completely and closely determine the motion of boundaries of regions $D_\pm$. That is why they can be thought of as independent systems with their momenta and Hamiltonians,

$$P_\pm=m\dot{R}_\pm,\quad H_\pm=\frac{P_\pm^2}{2m}-\frac{\gamma m m_\pm}{R_\pm}\mp U_\pm=E_\pm. \tag{C15}$$

Here $E_\pm$ are the total energies of these boundaries, $U^{(N)}_\pm=-\gamma m^2/2R_\pm$ are their potential energies of self-action, and $R_\pm=R_\pm(t)$ are the radiuses of the regions' boundary $D_\pm$. The systems (C15) describe the same shell provided the regions $D_\pm$ have a common boundary $R_+(t)=R_-(t)\equiv R(t)$ for all moments t. In this case, eliminating the momentum $P\equiv P_+=P_-$ from the equations $H_\pm=E_\pm$ one has

$$E_+-E_-=\frac{\gamma m}{R}(m_+-m-m_-). \tag{C16}$$

Hence it follows an ordinary equality of energies and the additivity of masses $E_+=E_-$, $m_+=m-m_-$. In General Relativity, a similar but not trivial procedure follows from the isometry conditions for the boundaries of the corresponding four-dimensional regions.

Finally we shall write the corresponding relations for a self-gravitating shell, when $m_-=0$,

$$L^{(N)}_{\mathrm{sh}-}=\frac{1}{2}m\dot{R}^2+\frac{\gamma m^2}{2R}, \tag{C17}$$

$$P = m\dot{R}, \quad H = \frac{P^2}{2m} - \frac{\gamma m^2}{2R} = E. \tag{C18}$$

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[15] In the four-dimensional case, for configurations with the dust density ρ, we have $\rho d^4\Omega = \omega \wedge d^3m$, where $d^3m = \rho\sqrt{-g}u^\mu d\Sigma_\mu$ is the 3-form of the element of the mass for some hypersurface. The requirement of the closure $d \wedge d^3m = 0$ gives a conservation law $(\sqrt{-g}\,\rho u^\mu)_{,\mu} = 0$. Therefore, in the Lagrange formulation of an perfect fluid, quantity $\sqrt{-g}\,\rho u^\mu$ does not vary when varying of the metric [see, S. W. Hawking and G. F. R. Ellis, *The Large Scale Structure of Space–Time* (Cambridge University Press, Cambridge, 1973)]. Therefore, the 3-form d^3m does not vary too. Similarly to this, in a three-dimensional case the 2-form d^2m is closed on $\Sigma_t^{(3)}$ and, by virtue of a conservation law, does not vary when varying the metric.
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The trace formula for Sturm–Liouville operator with operator coefficient

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We will obtain a formula for the trace of the Sturm–Liouville operator with operator coefficient. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1367866]

I. INTRODUCTION

Let H be a separable Hilbert space. Let us consider the operators L_0 and L in the space $H_1 = L_2(H;[0,\pi])$ which are formed by the following differential expression:

$$l_0(y) = -y''(x), \quad l(y) = -y''(x) + Q(x)y(x),$$

with the same boundary condition $y(0) = y(\pi) = 0$, respectively. Suppose that the operator function $Q(x)$ in the expression $l(y)$ satisfies the following conditions:

(1) For $\forall x \in [0,\pi]$, $Q(x)$: $H \to H$ is a self-adjoint kernel operator. Moreover, $Q(x)$ has continuous derivative of second order with respect to the norm in space $\sigma_1(H)$ in the interval $[0, \pi]$ and for $x \in [0,\pi]$, $Q^{(i)}(x)$: $H \to H$ are self-adjoint operators $(i = 1,2)$.

(2) $\mathrm{Sup}_{[0,\pi]} \|Q(x)\|_H < \frac{3}{2}$.

(3) There is an orthonormal basis $\{\varphi_n\}_{n=1}^{\infty}$ of the space H such that

$$\sum_{n=1}^{\infty} \|Q(x)\varphi_n\| < \infty.$$

Here $\sigma_1(H)$ is the space of kernel operators from H to H as in Ref. 1. Moreover $\|.\|_H$ and $\|.\|$ denote the norms in H and H_1, respectively, and $\mathrm{tr}\, A = \mathrm{trace}\, A$ denotes the sum of eigenvalues of a kernel operator A.

In Ref. 2, it is proved that the spectrum of the operator L is a subset of the union of the intervals $[m^2 - \frac{3}{2}, m^2 + \frac{3}{2}]$ $(m = 1,2,...)$ and that spectrum is a disjoint eigenvalue whose points, not belonging to the set $\{m^2\}_{m=1}^{\infty}$, have finite multiplicity. Again in Ref. 2, it is proved that m^2 $(m = 1,2,...)$ is a eigenvalue of L which has finite or infinite multiplicity and that

$$\lim_{n \to \infty} \lambda_{mn} = m^2$$

such that $\{\lambda_{mn}\}_{n=1}^{\infty}$ are eigenvalues which belong to the interval $[m^2 - \frac{3}{2}, m^2 + \frac{3}{2}]$. Moreover, the trace formula in the form

$$\sum_{m=1}^{\infty} \left[\sum_{n=1}^{\infty} (\lambda_{mn} - m^2) - \frac{1}{\pi} \int_0^{\pi} \mathrm{tr}\, Q(x)\, dx \right] = -\frac{\mathrm{tr}\, Q(0) + \mathrm{tr}\, Q(\pi)}{4} + \frac{1}{2\pi} \int_0^{\pi} \mathrm{tr}\, Q(x)\, dx$$

has been found for the self-adjoint operator L in Ref. 2.

In this work, we will find a formula for the sum of series

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$$\sum_{m=1}^{\infty}\left\{\sum_{n=1}^{\infty}(\lambda_{mn}^2-m^4)-\frac{2m^2}{\pi}\int_0^{\pi}\operatorname{tr}Q(x)\,dx-\frac{1}{2\pi}[\operatorname{tr}Q'(0)-\operatorname{tr}Q'(\pi)]\right.$$
$$\left.-\frac{1}{2\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)\,dx-\frac{1}{2\pi^2}\operatorname{tr}\left(\int_0^{\pi}Q(x)\,dx\right)^2\right\}.$$

The trace formulas for the scalar differential operators have been found by Gelfand and Levitan,[3] Dikiy,[4] Halberg and Kramer[5] and many other works. The list of the works on this subject is given in Levitan and Sargsyan[6] and Fulton and Pruess.[7] Note that we have only a few works on the trace of differential operators with operator coefficient. In Ref. 8, the trace of the Sturm–Liouville operator with unbounded operator coefficient has been investigated.

Let R_λ^0 and R_λ be the resolvents of the operators L_0 and L, respectively. The spectrum of the operator L_0 is the set $\{m^2\}_{m=1}^{\infty}$ and every point of this set is the eigenvalue of L_0 which has infinite multiplicity. The eigenvectors corresponding to eigenvalue m^2 are given by the form

$$\psi_{mn}=\sqrt{\frac{2}{\pi}}\operatorname{Sin}mx\cdot\varphi_n,\quad n=1,2,\ldots. \tag{1.1}$$

II. SOME FORMULAS ABOUT EIGENVALUES AND THE OPERATOR QR_λ^0

Since the operator Q satisfies the condition (3) and the system (1,1) of eigenvectors of operator L_0 is a orthonormal basis of the space H_1, it can be seen that QR_λ^0: $H_1\to H_1$ is a kernel operator for every $\lambda\notin\{m^2\}_{m=1}^{\infty}$. Then, from the relation

$$R_\lambda-R_\lambda^0=-R_\lambda QR_\lambda^0 \tag{2.1}$$

we see that $R_\lambda-R_\lambda^0\in\sigma_1(H)$ for each λ which belongs to the resolvent set of L. In this case, from Ref. 2, since

$$\operatorname{tr}(R_\lambda-R_\lambda^0)=\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\left(\frac{1}{\lambda_{mn}-\lambda}-\frac{1}{m^2-\lambda}\right)$$

we obtain

$$\frac{1}{2\pi i}\int_{|\lambda|=b_p}\lambda^2\operatorname{tr}(R_\lambda-R_\lambda^0)\,d\lambda=\sum_{m=1}^{p}\sum_{n=1}^{\infty}(m^4-\lambda_{mn}^2),$$

where $b_p=p^2+p$. From (2.1) and this last relation, we write

$$\sum_{m=1}^{p}\sum_{n=1}^{\infty}(\lambda_{mn}^2-m^4)=\sum_{j=1}^{N}M_{pj}+M_p^{(N)}. \tag{2.2}$$

Here N is a integer,

$$M_{pj}=\frac{(-1)^{j+1}}{2\pi i}\int_{|\lambda|=b_p}\lambda^2\operatorname{tr}[R_\lambda^0(QR_\lambda^0)^j]\,d\lambda$$

and

$$M_p^{(N)}=\frac{(-1)^N}{2\pi i}\int_{|\lambda|=b_p}\lambda^2\operatorname{tr}[R_\lambda(QR_\lambda^0)^{N+1}]d\lambda. \tag{2.3}$$

Since the operator function QR_λ^0 in the domain $\mathbb{C}\backslash\{m^2\}_{m=1}^{\infty}$ is analytic with respect to the norm in $\sigma_1(H_1)$, we can show that

$$M_{pj}=\frac{(-1)^j}{\pi i j}\int_{|\lambda|=b_p}\lambda\,\mathrm{tr}\,(QR_\lambda^0)^j\,d\lambda. \tag{2.4}$$

From relations (1.1) and (2.4), we write

$$\begin{aligned}M_{p1}&=-\frac{1}{\pi i}\int_{|\lambda|=b_p}\lambda\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(QR_\lambda^0\psi_{mn},\psi_{mn})\,d\lambda\\&=2\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}(Q\psi_{mn},\psi_{mn})\frac{1}{2\pi i}\int_{|\lambda|=b_p}\frac{\lambda}{\lambda-m^2}\,d\lambda\\&=2\sum_{m=1}^{p}\sum_{n=1}^{\infty}m^2(Q\psi_{mn},\psi_{mn})\\&=\frac{2}{\pi}\sum_{m=1}^{p}m^2\int_0^{\pi}\mathrm{tr}\,Q(x)\,dx-\frac{2}{\pi}\sum_{m=1}^{p}m^2\int_0^{\pi}\mathrm{tr}\,Q(x)\,\mathrm{Cos}\,2mx\,dx.\end{aligned}$$

On the other hand, since

$$\int_0^{\pi}\mathrm{tr}\,Q(x)\,\mathrm{Cos}\,2mx\,dx=\frac{\mathrm{tr}\,Q'(\pi)-\mathrm{tr}\,Q'(0)}{4m^2}-\frac{1}{4m^2}\int_0^{\pi}\mathrm{tr}\,Q''(x)\,\mathrm{Cos}\,2mx\,dx,$$

we have

$$M_{p1}=\frac{2}{\pi}\sum_{m=1}^{p}m^2\int_0^{\pi}\mathrm{tr}\,Q(x)\,dx+\frac{p}{2\pi}[\mathrm{tr}\,Q'(0)-\mathrm{tr}\,Q'(\pi)]+\frac{1}{2\pi}\sum_{m=1}^{p}\int_0^{\pi}\mathrm{tr}\,Q''(x)\,\mathrm{Cos}\,2mx\,dx. \tag{2.5}$$

Now, let us compute M_{p2}: From (2.4) we write

$$M_{p2}=\frac{1}{2\pi i}\int_{|\lambda|=b_p}\lambda\,\mathrm{tr}\,(QR_\lambda^0)^2\,d\lambda=\frac{1}{2\pi i}\int_{|\lambda|=b_p}\lambda\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}((QR_\lambda^0)^2\psi_{mn},\psi_{mn})\,d\lambda. \tag{2.6}$$

Moreover, we know that

$$QR_\lambda^0\psi_{mn}=\frac{Q\psi_{mn}}{m^2-\lambda}$$

and

$$\begin{aligned}(QR_\lambda^0)^2\psi_{mn}&=(m^2-\lambda)^{-1}QR_\lambda^0(Q\psi_{mn})\\&=(m^2-\lambda)^{-1}QR_\lambda^0\left\{\sum_{r=1}^{\infty}\sum_{q=1}^{\infty}(Q\psi_{mn},\psi_{rq})\psi_{rq}\right\}\\&=(m^2-\lambda)^{-1}\sum_{r=1}^{\infty}\sum_{q=1}^{\infty}(r^2-\lambda)^{-1}(Q\psi_{mn},\psi_{rq})Q\psi_{rq}.\end{aligned}$$

If we write this last expression, in (2.6), we find

$$M_{p2}=\frac{1}{2\pi i}\int_{|\lambda|=b_p}\lambda\left[\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\sum_{r=1}^{\infty}\sum_{q=1}^{\infty}\frac{(Q\psi_{mn},\psi_{rq})(Q\psi_{rq},\psi_{mn})}{(\lambda-m^2)(\lambda-r^2)}\right]d\lambda$$

$$=\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\sum_{r=1}^{\infty}\sum_{q=1}^{\infty}|(Q\psi_{mn},\psi_{rq})|^2\frac{1}{2\pi i}\int_{|\lambda|=b_p}\frac{\lambda}{(\lambda-m^2)(\lambda-r^2)}d\lambda$$

$$=\sum_{m=1}^{p}\sum_{n=1}^{\infty}\sum_{r=1}^{p}\sum_{q=1}^{\infty}|(Q\psi_{mn},\psi_{rq})|^2\frac{1}{2\pi i}\int_{|\lambda|=b_p}\frac{\lambda}{(\lambda-m^2)(\lambda-r^2)}d\lambda$$

$$+\sum_{m=1}^{p}\sum_{n=1}^{\infty}\sum_{r=p+1}^{\infty}\sum_{q=1}^{\infty}|(Q\psi_{mn},\psi_{rq})|^2\frac{1}{2\pi i}\int_{|\lambda|=b_p}\frac{\lambda}{(\lambda-m^2)(\lambda-r^2)}d\lambda$$

$$+\sum_{m=p+1}^{\infty}\sum_{n=1}^{\infty}\sum_{r=1}^{p}\sum_{q=1}^{\infty}|(Q\psi_{mn},\psi_{rq})|^2\frac{1}{2\pi i}\int_{|\lambda|=b_p}\frac{\lambda}{(\lambda-m^2)(\lambda-r^2)}d\lambda$$

$$+\sum_{m=p+1}^{\infty}\sum_{n=1}^{\infty}\sum_{r=p+1}^{\infty}\sum_{q=1}^{\infty}|(Q\psi_{mn},\psi_{rq})|^2\frac{1}{2\pi i}\int_{|\lambda|=b_p}\frac{\lambda}{(\lambda-m^2)(\lambda-r^2)}d\lambda$$

$$=\sum_{m=1}^{p}\sum_{n=1}^{\infty}\sum_{r=1}^{p}\sum_{q=1}^{\infty}|(Q\psi_{mn},\psi_{rq})|^2+2\sum_{m=1}^{p}\sum_{n=1}^{\infty}\sum_{r=p+1}^{\infty}\sum_{q=1}^{\infty}|(Q\psi_{mn},\psi_{rq})|^2\frac{m^2}{m^2-r^2}$$

$$=\sum_{m=1}^{p}\sum_{n=1}^{\infty}\sum_{r=1}^{\infty}\sum_{q=1}^{\infty}|(Q\psi_{mn},\psi_{rq})|^2-\sum_{m=1}^{p}\sum_{n=1}^{\infty}\sum_{r=p+1}^{\infty}\sum_{q=1}^{\infty}\left(1+\frac{2m^2}{r^2-m^2}\right)|(Q\psi_{mn},\psi_{rq})|^2$$

$$=\sum_{m=1}^{p}\sum_{n=1}^{\infty}\|Q\psi_{mn}\|^2-\sum_{m=1}^{p}\sum_{n=1}^{\infty}\sum_{r=p+1}^{\infty}\sum_{q=1}^{\infty}\frac{r^2+m^2}{r^2-m^2}|(Q\psi_{mn},\psi_{rq})|^2.$$

Here if we take

$$\alpha_p=\alpha_p(n,q)=\sum_{m=1}^{p}\sum_{r=p+1}^{\infty}\frac{r^2+m^2}{r^2-m^2}|(Q\psi_{mn},\psi_{rq})|^2,$$

then we write

$$M_{p2}=\sum_{m=1}^{p}\sum_{n=1}^{\infty}\|Q\psi_{mn}\|^2-\sum_{n=1}^{\infty}\sum_{q=1}^{\infty}\alpha_p. \tag{2.7}$$

From Eq. (1.1) we have

$$\alpha_p=\alpha_{p1}-\alpha_{p2}+\alpha_{p3}, \tag{2.8}$$

where

$$\alpha_{p1}=\pi^{-2}\sum_{m=1}^{p}\sum_{r=p+1}^{\infty}\frac{r^2+m^2}{r^2-m^2}\left|\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H\operatorname{Cos}(m-r)x\,dx\right|^2,$$

$$\alpha_{p2}=2\pi^{-2}\sum_{m=1}^{p}\sum_{r=p+1}^{\infty}\frac{r^2+m^2}{r^2-m^2}\operatorname{Re}\left[\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H\cdot\operatorname{Cos}(m-r)x\,dx\right.$$

$$\left.\times\int_0^{\pi}\overline{(Q(x)\varphi_n,\varphi_q)_H}\operatorname{Cos}(m+r)x\,dx\right], \tag{2.9}$$

$$\alpha_{p3}=\pi^{-2}\sum_{m=1}^{p}\sum_{r=p+1}^{\infty}\frac{r^2+m^2}{r^2-m^2}\left|\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H\operatorname{Cos}(m+r)x\,dx\right|^2. \tag{2.10}$$

For any integers p and i, we let

$$E=\{(r,m):r,m\in N;r-m=i;m\leqslant p;r>p\}.$$

Then, for the expression α_{p1}, we can write

$$\alpha_{p1}=\pi^{-2}\sum_{i=1}^{\infty}\left(\sum_{m,r\in E}\frac{r^2+m^2}{r^2-m^2}\right)\left|\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H\operatorname{Cos}(ix)\,dx\right|^2. \tag{2.11}$$

The equalities

$$\sum_{m,r\in E}\frac{r^2+m^2}{r^2-m^2}=p+\frac{1}{2}+i^2O(p^{-1})\quad\text{for}\quad i\leqslant p \tag{2.12}$$

and

$$\sum_{m,r\in E}\frac{r^2+m^2}{r^2-m^2}=O(p)\quad\text{for}\quad i\geqslant p \tag{2.13}$$

can be proved easily. Here $O(p^{-1})$ and $O(p)$ depend on p and i and they satisfy the inequalities

$$|O(p^{-1})|<\operatorname{const}p^{-1},\quad |O(p)|<\operatorname{const}p.$$

From (2.11)–(2.13), we obtain

$$\begin{aligned}\alpha_{p1}&=\pi^{-2}\left(p+\frac{1}{2}\right)\sum_{i=1}^{\infty}\left|\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H\operatorname{Cos}ix\,dx\right|^2\\&\quad+\sum_{i=1}^{\infty}i^2O(p^{-1})\left|\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H\operatorname{Cos}ix\,dx\right|^2\\&\quad+\sum_{i=p+1}^{\infty}O(p)\left|\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H\operatorname{Cos}ix\,dx\right|^2\\&=\alpha_{p1}^{(1)}+\alpha_{p1}^{(2)}+\alpha_{p1}^{(3)}.\end{aligned}$$

Here,

$$\begin{aligned}\alpha_{p1}^{(1)}&=\pi^{-2}\left(p+\frac{1}{2}\right)\sum_{i=1}^{\infty}\left|\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H\operatorname{Cos}ix\,dx\right|^2\\&=\frac{2p+1}{4\pi}\int_0^{\pi}|(Q(x)\varphi_n,\varphi_q)_H|^2dx-\frac{2p+1}{4\pi^2}\int_0^{\pi}|(Q(x)\varphi_n,\varphi_q)_H\,dx|^2,\end{aligned}$$

$$|\alpha_{p1}^{(2)}|=\left|\sum_{i=1}^{p}i^2O(p^{-1})\left|\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H\operatorname{Cos}ix\,dx\right|^2\right|\leqslant\operatorname{const}p^{-1}\int_0^{\pi}|(Q'(x)\varphi_n,\varphi_q)_H|^2\,dx,$$

and

$$|\alpha_{p1}^{(3)}|=\left|\sum_{i=p+1}^{\infty} O(p)\left|\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H \operatorname{Cos} ix\,dx\right|^2\right|\leqslant \text{const} p^{-1}\int_0^{\pi}|(Q'(x)\varphi_n,\varphi_q)_H|^2\,dx.$$

From (2.8) and these last relations, we find

$$\sum_{n=1}^{\infty}\sum_{q=1}^{\infty}\alpha_{p1}=\frac{2p+1}{4\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)\,dx-\frac{2p+1}{4\pi^2}\operatorname{tr}\left(\int_0^{\pi}Q(x)\,dx\right)^2+O(p^{-1}). \tag{2.14}$$

Since $Q(x)$ satisfies the condition (1), it can be shown that

$$\left|\sum_{n=1}^{\infty}\sum_{q=1}^{\infty}\alpha_{pj}\right|<\text{const}\,p^{-1}\quad (j=2,3). \tag{2.15}$$

By using (2.7), (2.8), (2.14) and (2.15), we find

$$M_{p2}=\sum_{m=1}^{p}\sum_{n=1}^{\infty}\|Q\psi_{mn}\|^2-\frac{2p+1}{4\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)\,dx+\frac{2p+1}{4\pi^2}\operatorname{tr}\left(\int_0^{\pi}Q^2(x)\,dx\right)^2+O(p^{-1}), \tag{2.16}$$

where $O(p^{-1})$ depends on p and satisfies the inequality

$$|O(p^{-1})|<\text{const}\,p^{-1}.$$

Now, let us compute the sum $\Sigma_{m=1}^{p}\Sigma_{n=1}^{\infty}\|Q\psi_{mn}\|^2$:

$$\begin{aligned}\sum_{m=1}^{p}\sum_{n=1}^{\infty}\|Q\psi_{mn}\|^2&=\frac{2}{\pi}\sum_{m=1}^{p}\sum_{n=1}^{\infty}\int_0^{\pi}\operatorname{Sin}^2 mx(Q^2(x)\varphi_n,\varphi_n)_H\,dx\\&=\frac{p}{\pi}\int_0^{\pi}\sum_{n=1}^{\infty}(Q^2(x)\varphi_n,\varphi_n)\,dx-\frac{1}{\pi}\sum_{m=1}^{p}\int_0^{\pi}\sum_{n=1}^{\infty}(Q^2(x)\varphi_n,\varphi_n)_H\operatorname{Cos}2mx\,dx\\&=\frac{p}{\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)\,dx-\frac{1}{\pi}\sum_{m=1}^{p}\int_0^{\pi}\operatorname{tr}Q^2(x)\operatorname{Cos}2mx\,dx.\end{aligned}$$

If we put this expression into (2.16), we have

$$\begin{aligned}M_{p2}=&\frac{2p-1}{4\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)+\frac{2p+1}{4\pi^2}\operatorname{tr}\left(\int_0^{\pi}Q(x)\,dx\right)^2\\&-\frac{1}{\pi}\sum_{m=1}^{p}\int_0^{\pi}\operatorname{tr}Q^2(x)\operatorname{Cos}2mx\,dx+O(p^{-1}).\end{aligned} \tag{2.17}$$

III. A FORMULA FOR THE TRACE OF THE OPERATOR *L*

In this section, we will find a formula for the sum

$$\sum_{m=1}^{\infty}\left[\sum_{n=1}^{\infty}(\lambda_{mn}^2-m^4)-\frac{2m^2}{\pi}\int_0^{\pi}\operatorname{tr}Q(x)\,dx-C\right],$$

where

$$C=\frac{1}{2\pi}[\operatorname{tr}Q'(0)-\operatorname{tr}Q'(\pi)]+\frac{1}{2\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)\,dx+\frac{1}{2\pi^2}\operatorname{tr}\left(\int_0^{\pi}Q(x)\,dx\right)^2.$$

For this, we will first show that the formulas

$$\lim_{p\to\infty} M_{pj}=0, \quad j\geqslant 3, \tag{3.1}$$

$$\lim_{p\to\infty} M_p^N=0, \quad N\geqslant 6, \tag{3.2}$$

are satisfied. It is not difficult to see that the inequalities

$$\|QR_\lambda^0\|_{\sigma_1(H_1)}<C_1 \quad (|\lambda|=b_p), \tag{3.3}$$

$$\|R_\lambda^0\|<C_1p^{-1} \quad \|R_\lambda\|<C_1p^{-1} \quad (|\lambda|=b_p), \tag{3.4}$$

are true. Here $C_1>0$ is a constant. From (2.4), (3.3), and (3.4) and since $Q(x)$ satisfies the condition (2), we have

$$\begin{aligned}
|M_{pj}| &= \frac{1}{\pi j}\left|\int_{|\lambda|=b_\rho} \lambda \operatorname{tr}(QR_\lambda^0)^j\, d\lambda\right| \\
&\leqslant \frac{b_p}{\pi j}\int_{|\lambda|=b_p} \|(QR_\lambda^0)^j\|_{\sigma_1(H_1)}|\, d\lambda| \\
&\leqslant \frac{b_p}{\pi j}\int_{|\lambda|=b_p} \|(QR_\lambda^0)\|_{\sigma_1(H_1)}\|(QR_\lambda^0)^{j-1}\||d\lambda| \\
&\leqslant \frac{C_1b_p}{\pi j}\int_{|\lambda|=b_p} \|Q\|^{j-1}\|R_\lambda^0\|^{j-1}|d\lambda| \\
&\leqslant \frac{C_1^jb_p}{\pi j}\int_{|\lambda|=b_p}\left(\frac{3}{2}\right)^{j-1} p^{1-j}|d\lambda| \\
&< C_2p^{5-j} \quad (C_2>0).
\end{aligned}$$

And so, we find

$$\lim_{p\to\infty} = M_{pj}=0 \quad (j\geqslant 6),$$

but we claim that this is true also for $j=3,4,5$. Let us try this for $j=3$. It can be seen that

$$M_{pj}=\frac{(-1)^j}{\pi ij}\sum_{m_1=1}^{\infty}\sum_{n_1=1}^{\infty}\cdots\sum_{m_j=1}^{\infty}\sum_{n_j=1}^{\infty}{}^{*}\left[\int_{|\lambda|=b_p}\lambda\prod_{l=1}^{j}(m_l^2-\lambda)^{-1}\,d\lambda\right]\cdot\prod_{l=1}^{j}(Q\psi_{m_ln_l},\psi_{m_{g(l)}n_{g(l)}}). \tag{3.5}$$

Here the symbol ''*'' denotes that there are numbers, between $m_1^4, m_2^4, \ldots, m_j^4$, less than or greater than b_p and

$$g(l)=\begin{cases} l+1, & l<j, \\ 1, & l=j. \end{cases}$$

For $j=3$, we write

$$M_{p3}=-\frac{1}{3\pi i}\sum_{m=1}^{\infty}\sum_{n=1}^{\infty}\sum_{r=1}^{\infty}\sum_{q=1}^{\infty}\sum_{R=1}^{\infty}\sum_{N=1}^{\infty}*\int_{|\lambda|=b_p}\frac{\lambda\,d\lambda}{(m^2-\lambda)(r^2-\lambda)(R^2-\lambda)}$$
$$\cdot(Q\psi_{mn},\psi_{rq})(Q\psi_{rq},\psi_{RN})(Q\psi_{RN},\psi_{mn}). \tag{3.6}$$

Let us take

$$F(m,r,R)=\sum_{n=1}^{\infty}\sum_{q=1}^{\infty}\sum_{N=1}^{\infty}(Q\psi_{mn},\psi_{rq})(Q\psi_{rq},\psi_{rN})(Q\psi_{rN},\psi_{mn}).$$

Since $F(m,r,R)=F(r,m,R)=F(R,m,r)=F(R,r,m)=F(m,R,r)=F(r,R,m)$ and from (3.6), we obtain

$$\begin{aligned}M_{p3}=&\frac{1}{\pi i}\sum_{m=1}^{p}\sum_{r=p+1}^{\infty}\sum_{R=p+1}^{\infty}\int_{|\lambda|=b_p}\frac{\lambda\,d\lambda}{(\lambda-m^2)(\lambda-r^2)(\lambda-R^2)}F(m,r,R)\\&+\frac{1}{\pi i}\sum_{m=1}^{p}\sum_{\substack{r=1\\m\neq r}}^{p}\sum_{R=p+1}^{\infty}\int_{|\lambda|=b_p}\frac{\lambda\,d\lambda}{(\lambda-m^2)(\lambda-r^2)(\lambda-R^2)}F(m,r,R)\\&+\frac{1}{\pi i}\sum_{m=1}^{p}\sum_{R=p+1}^{\infty}\int_{|\lambda|=b_p}\frac{\lambda\,d\lambda}{(\lambda-m^2)^2(\lambda-R^2)}F(m,m,R)\\=&2\sum_{m=1}^{p}\sum_{r=p+1}^{\infty}\sum_{R=p+1}^{\infty}\frac{m^2}{(r^2-m^2)(R^2-m^2)}F(m,r,R)\\&+4\sum_{m=1}^{p}\sum_{\substack{r=1\\m\neq r}}^{p}\sum_{R=p+1}^{\infty}\frac{m^2}{(m^2-r^2)(m^2-R^2)}F(m,r,R)\\&-2\sum_{m=1}^{p}\sum_{R=p+1}^{\infty}\frac{R^2}{(R^2-m^2)^2}(F(m,m,R)).\end{aligned}\tag{3.7}$$

Let

$$F_1(m,r,R)=\pi^{-3}\sum_{n=1}^{\infty}\sum_{q=1}^{\infty}\sum_{N=1}^{\infty}\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H\operatorname{Cos}(m-r)x\,dx\cdot\int_0^{\pi}(Q(x)\varphi_q,\varphi_N)_H$$
$$\times\operatorname{Cos}(r-R)x\,dx\int_0^{\pi}(Q(x)\varphi_N,\varphi_n)_H\operatorname{Cos}(R-m)x\,dx, \tag{3.8}$$

$$F_2(m,r,R)=F(m,r,R)-F_1(m,r,R),$$

$$A_{pi}=\sum_{m=1}^{p}\sum_{r=p+1}^{\infty}\sum_{R=p+1}^{\infty}\frac{m^2}{(r^2-m^2)(R^2-m^2)}F_i(m,r,R),$$

$$B_{pi}=\sum_{m=1}^{p}\sum_{\substack{r=1\\m\neq r}}^{p}\sum_{R=p+1}^{\infty}\frac{m^2}{(m^2-r^2)(m^2-R^2)}F_i(m,r,R),$$

$$C_{pi}=\sum_{m=1}^{p}\sum_{R=p+1}^{\infty}\frac{R^2}{(R^2-m^2)^2}F_i(m,m,R).$$

It can be shown that

$$A_{p1}=2\sum_{m=1}^{p}\sum_{\substack{r=p+1\\ r>R}}^{\infty}\sum_{R=p+1}^{\infty}\frac{m^2}{(r^2-m^2)(R^2-m^2)}F_1(m,r,R)+\sum_{m=1}^{p}\sum_{R=p+1}^{\infty}\frac{m^2}{(R^2-m^2)^2}F_1(m,m,R),$$

$$B_{p1}=-\sum_{m=1}^{p}\sum_{\substack{r=1\\ m<r}}^{p}\sum_{R=p+1}^{\infty}\frac{R^2}{(R^2-m^2)(R^2-r^2)}F_1(m,r,R). \tag{3.9}$$

Hence, we write M_{p3} as in the form

$$M_{p3}=4A_p^1-4B_p^1-2C_p^1+2A_{p2}+4B_{p2}-2C_{p2} \tag{3.10}$$

such that

$$A_p^1=\sum_{m=1}^{p}\sum_{\substack{r=p+1\\ r>R}}^{\infty}\sum_{R=p+1}^{\infty}\frac{m^2}{(r^2-m^2)(R^2-m^2)}F_1(m,r,R),$$

$$B_p^1=-B_{p1}, \tag{3.11}$$

$$C_p^1=\sum_{m=1}^{p}\sum_{R=p+1}^{\infty}\frac{1}{R^2-m^2}F_1(m,m,R).$$

Let $E_1=\{(m,r,R):m,r,R\in N;r-m=i;R-m=j;m\leqslant p;r,R>p\}$, where p, i and j are integers such that $p\geqslant j$, $i\geqslant j$ Then

$$\begin{aligned}A_p^1=&\sum_{m=1}^{p}\sum_{\substack{r=p+1\\ r>R,R-m\leqslant p}}^{\infty}\sum_{R=p+1}^{2p}\frac{m^2}{(r^2-m^2)(R^2-m^2)}F_1(m,r,R)\\&+\sum_{m=1}^{p}\sum_{\substack{r=p+1\\ r>R,R-m>p}}^{\infty}\sum_{R=p+1}^{\infty}\frac{m^2}{(r^2-m^2)(R^2-m^2)}F_1(m,r,R)\\&=\pi^{-3}\sum_{\substack{i=2\\ i>j}}^{\infty}\sum_{j=1}^{p}\left[\left(\sum_{m,r,R\in E_1}\frac{m^2}{(r^2-m^2)(R^2-m^2)}\right)\sum_{n=1}^{\infty}\sum_{q=1}^{\infty}\sum_{N=1}^{\infty}\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)\right]_H\\&\times\operatorname{Cos}ix\cdot\int_0^{\pi}(Q(x)\varphi_q,\varphi_N)_H\operatorname{Cos}(i-j)x\,dx\int_0^{\pi}(Q(x)\varphi_N,\varphi_n)_H\operatorname{Cos}ix\,dx\\&+\sum_{m=1}^{p}\sum_{\substack{r=p+1\\ r>R,R-m>p}}^{\infty}\sum_{R=p+1}^{\infty}\frac{m^2}{(r^2-m^2)(R^2-m^2)}F_1(m,r,R).\end{aligned} \tag{3.12}$$

If we let

$$\beta_{ij}=\pi^{-3}\sum_{n=1}^{\infty}\sum_{q=1}^{\infty}\sum_{N=1}^{\infty}\int_0^{\pi}(Q(x)\varphi_n,\varphi_q)_H\,\mathrm{Cos}\,ix\,dx\int_0^{\pi}(Q(x)\varphi_q,\varphi_N)_H$$

$$\times\mathrm{Cos}\,(i-j)x\,dx\cdot\int_0^{\pi}(Q(x)\varphi_N,\varphi_n)_H\,\mathrm{Cos}\,ix\,dx, \tag{3.13}$$

$$A_p^{11}=\sum_{\substack{i=2\\ i>j}}^{\infty}\sum_{j=1}^{p}\left[\left(\sum_{m,r,R\in E_1}\frac{m^2}{(r^2-m^2)(R^2-m^2)}\right)\beta_{ij}\right],$$

$$A_p^{12}=\sum_{\substack{m=1\\ r>R,R-m>p}}^{p}\sum_{r=p+1}^{\infty}\sum_{R=p+1}^{\infty}\frac{m^2}{(r^2-m^2)(R^2-m^2)}F_1(m,r,R),$$

then we write

$$A_p^1=A_p^{11}+A_p^{12}. \tag{3.14}$$

On the other hand, it can be shown that

$$\sum_{m,r,R\in E_1}\frac{m^2}{(r^2-m^2)(R^2-m^2)}=\frac{1}{4i}+\frac{j}{p}O(1),$$

where $O(1)$ satisfies the condition

$$|O(1)|<\mathrm{const}$$

and it depends on p, i and j. Moreover, if $Q(x)$ has a continuous derivative of second order at $[0,\ \pi]$ with respect to the norm in $\sigma_1(H)$, then we can show that

$$|\beta_{ij}|<\frac{\mathrm{const}}{i^2j^2}. \tag{3.15}$$

Hence, we have

$$A_p^{11}=\sum_{\substack{i=2\\ i>j}}^{\infty}\sum_{j=1}^{p}\left[\frac{\beta_{ij}}{4i}+\frac{O(1)}{pi^2j}\right]. \tag{3.16}$$

Since

$$\left|\sum_{i=2}^{\infty}\sum_{j=1}^{p}\frac{O(1)}{pi^2j}\right|\leqslant\mathrm{const}\left(\sum_{i=1}^{\infty}i^{-2}\right)\sum_{j=1}^{p}j^{-1}<\mathrm{const}\;p^{-1}\ln p,$$

we find

$$A_p^{11}=\sum_{\substack{i=2\\ i>j}}^{\infty}\sum_{j=1}^{p}\frac{\beta_{ij}}{4i}+o(1). \tag{3.17}$$

Here $o(1)$ is an expression which satisfies the condition

$$\lim_{p\to\infty} o(1)=0,$$

and it depends on p. From (3.14) and (3.17) we obtain

$$A_p^1=\sum_{i=2}^{\infty}\sum_{\substack{j=1\\ i>j}}^{p}\frac{\beta_{ij}}{4i}+A_p^{12}+o(1). \tag{3.18}$$

Now, let us find a formula for the B_p^1:

Let

$$B_p^{11}=\sum_{m=1}^{p}\sum_{\substack{r=1\\ m<r,R-m\leqslant p}}^{p}\sum_{R=p+1}^{2p}\frac{R^2}{(R^2-m^2)(R^2-r^2)}F_1(m,r,R)$$

and

$$B_p^{12}=\sum_{m=1}^{p}\sum_{\substack{r=1\\ m<r,R-m>p}}^{p}\sum_{R=p+1}^{\infty}\frac{R^2}{(R^2-m^2)(R^2-r^2)}F_1(m,r,R).$$

Then, from (3.9) and (3.11), we have

$$B_p^1=B_p^{11}+B_p^{12}. \tag{3.19}$$

By using (3.8) and (3.13), we write B_p^{11} as in the form

$$B_p^{11}=\sum_{j=2}^{p}\sum_{\substack{i=1\\ j>i}}^{p-1}\left(\sum_{m,r,R\in E_2}\frac{R^2}{(R^2-m^2)(R^2-r^2)}\right)\beta_{ij}, \tag{3.20}$$

where E_2 is a set defined by

$$E_2=\{(m,r,R):m,r,R\in N;r-m=i;R-m=j;m,r\leqslant p;R>p\}$$

such that $i<j\leqslant p$. Moreover, we can show that

$$\sum_{m,r,R\in E_2}\frac{R^2}{(R^2-m^2)(R^2-r^2)}=\frac{1}{4j}+\frac{i}{p}O(1). \tag{3.21}$$

From (3.15), (3.20) and (3.21) we obtain

$$B_p^{11}=\sum_{j=2}^{p}\sum_{\substack{i=1\\ j>i}}^{p-1}\left[\frac{\beta_{ij}}{4j}+\frac{O(1)}{pj^2i}\right]$$

and, since $\beta_{ij}=\beta_{ji}$, we write

$$B_p^{11}=\sum_{j=2}^{p}\sum_{\substack{i=1\\ i<j}}^{p-1}\frac{\beta_{ji}}{4j}+o(1).$$

By using (3.19) and this last equation, we find

$$B_p^1=\sum_{\substack{i=2\\ i>j}}^{p}\sum_{j=1}^{p-1}\frac{\beta_{ij}}{4i}+B_p^{12}+o(1).$$

On the other hand, by using (3.15), it can be shown that

$$\sum_{i=2}^{p}\sum_{j=1}^{p-1}\frac{\beta_{ij}}{i}=\sum_{\substack{i=2\\ i>j}}^{\infty}\sum_{j=1}^{p}\frac{\beta_{ij}}{4i}+o(1).$$

Thus, we have

$$B_p^1=\sum_{\substack{i=2\\ i>j}}^{\infty}\sum_{j=1}^{p}\frac{\beta_{ij}}{4i}+B_p^{12}+o(1). \tag{3.22}$$

From (3.10), (3.18) and (3.22) we obtain

$$M_{p3}=4A_p^{12}-4B_p^{12}-2C_p^1+2A_{p2}+4B_{p2}-2C_{p2}+o(1).$$

Here, it can be seen that

$$\lim_{p\to\infty}A_p^{12}=\lim_{p\to\infty}B_p^{12}=\lim_{p\to\infty}C_p^1=\lim_{p\to\infty}A_{p2}=\lim_{p\to\infty}B_{p2}=\lim_{p\to\infty}C_{p2}=0.$$

For this reason, it follows that

$$\lim_{p\to\infty}M_{p3}=0.$$

In a similar form, it is proved that

$$\lim_{p\to\infty}M_{p4}=\lim_{p\to\infty}M_{p5}=0.$$

Now let us prove the formula (3.2): By employing (2.3), (3.3) and (3.4), we obtain

$$\begin{aligned}
|M_p^{(N)}|&=\frac{1}{2\pi}\left|\int_{|\lambda|=b_p}\lambda^2\,\mathrm{tr}\,[R_\lambda(QR_\lambda^0)^{N+1}]\,d\lambda\right|\\
&\leqslant\frac{b_p^2}{2\pi}\int_{|\lambda|=b_p}\|R_\lambda(QR_\lambda^0)^{N+1}\|_{\sigma_1(H_1)}|d\lambda|\\
&\leqslant b_p^2\int_{|\lambda|=b_p}\|R_\lambda\|\|(QR_\lambda^0)^{N+1}\|_{\sigma_1(H_1)}|d\lambda|\\
&\leqslant C_1b_p^2p^{-1}\int_{|\lambda|=b_p}\|QR_\lambda^0\|^N\|QR_\lambda^0\|_{\sigma_1H_1}|d\lambda|\\
&\leqslant\mathrm{const}\,p^{5-N}.
\end{aligned}$$

This shows that

$$\lim_{p\to\infty} M_p^{(N)}=0; \quad N\geqslant 6.$$

The main result of this article is given by the following theorem.

Theorem 3.1: If the operator function $Q(x)$ satisfies the conditions (1)–(3), then

$$\sum_{m=1}^{\infty}\left[\sum_{n=1}^{\infty}(\lambda_{mn}^2-m^4)-\frac{2m^2}{\pi}\int_0^{\pi}\operatorname{tr}Q(x)\,dx-C\right]$$
$$=\frac{C}{2}+\frac{1}{8}[\operatorname{tr}Q''(0)+\operatorname{tr}Q''(\pi)]-\frac{1}{4}[\operatorname{tr}Q^2(0)+\operatorname{tr}Q^2(\pi)],$$

where

$$C=\frac{1}{2\pi}[\operatorname{tr}Q'(0)-\operatorname{tr}Q'(\pi)]+\frac{1}{2\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)\,dx+\frac{1}{2\pi^2}\operatorname{tr}\left(\int_0^{\pi}Q(x)\,dx\right)^2.$$

Proof: By using the relations (2.2), (2.5), (2.17), (3.1) and (3.2), we find

$$\sum_{m=1}^{p}\sum_{n=1}^{\infty}(\lambda_{mn}^2-m^4)=\frac{2}{\pi}\int_0^{\pi}\operatorname{tr}Q(x)\,dx\sum_{m=1}^{p}m^2+\frac{p}{2\pi}[\operatorname{tr}Q'(0)-\operatorname{tr}Q'(\pi)]$$
$$+\frac{1}{2\pi}\sum_{m=1}^{p}\int_0^{\pi}\operatorname{tr}Q''(x)\operatorname{Cos}2mx\,dx+\frac{2p-1}{4\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)\,dx$$
$$+\frac{2p+1}{4\pi^2}\operatorname{tr}\left(\int_0^{\pi}Q(x)\,dx\right)^2-\frac{1}{\pi}\sum_{m=1}^{p}\int_0^{\pi}\operatorname{tr}Q^2(x)\operatorname{Cos}2mx\,dx+o(1).$$

Or, by taking

$$g(x)=\operatorname{tr}Q''(x)-2\operatorname{tr}Q^2(x),$$

we get

$$\sum_{m=1}^{\infty}\left[\sum_{n=1}^{\infty}(\lambda_{mn}^2-m^4)-\frac{2m^2}{\pi}\int_0^{\pi}\operatorname{tr}Q(x)\,dx-C\right]$$
$$=\frac{1}{4\pi^2}\operatorname{tr}\left(\int_0^{\pi}Q(x)\,dx\right)^2-\frac{1}{4\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)\,dx+\frac{1}{2\pi}\sum_{m=1}^{\infty}\int_0^{\pi}g(x)\operatorname{Cos}2mx\,dx. \tag{3.23}$$

Here, we note that

$$\frac{1}{2\pi}\sum_{m=1}^{\infty}\int_0^{\pi}g(x)\operatorname{Cos}mx\,dx=\frac{1}{4\pi}\sum_{m=1}^{\infty}\left[\int_0^{\pi}g(x)\operatorname{Cos}mx\,dx+(-1)^m\int_0^{\pi}g(x)\operatorname{Cos}mx\,dx\right]$$
$$=\frac{1}{8}\left\{\sum_{m=1}^{\infty}\left[\frac{2}{\pi}\int_0^{\pi}g(x)\operatorname{Cos}mx\,dx\right]\operatorname{Cos}m0+\frac{1}{\pi}\int_0^{\pi}g(x)dx\operatorname{Cos}0\right\}$$
$$+\frac{1}{8}\left\{\sum_{m=1}^{\infty}\left[\frac{2}{\pi}\int_0^{\pi}g(x)\operatorname{Cos}mx\,dx\right]\operatorname{Cos}m\pi\right.$$
$$\left.+\frac{1}{\pi}\int_0^{\pi}g(x)\,dx\operatorname{Cos}0\pi\right\}-\frac{1}{4\pi}\int_0^{\pi}g(x)\,dx$$
$$=\frac{1}{8}[g(0)+g(\pi)]-\frac{1}{4\pi}\int_0^{\pi}g(x)\,dx.$$

By considering this in (3.23), we obtain

$$\sum_{m=1}^{\infty}\left[\sum_{n=1}^{\infty}(\lambda_{mn}^2-m^4)-\frac{2m^2}{\pi}\int_0^{\pi}\operatorname{tr}Q(x)\,dx-C\right]$$

$$=\frac{1}{4\pi^2}\operatorname{tr}\left(\int_0^{\pi}Q(x)dx\right)^2-\frac{1}{4\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)\,dx+\frac{1}{8}[\operatorname{tr}Q''(0)-2\operatorname{tr}Q^2(0)+\operatorname{tr}Q''(\pi)$$

$$-2\operatorname{tr}Q^2(\pi)]-\frac{1}{4\pi}\int_0^{\pi}\operatorname{tr}Q''(x)\,dx+\frac{1}{2\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)\,dx$$

$$=\frac{1}{4\pi^2}\operatorname{tr}\left(\int_0^{\pi}Q(x)\,dx\right)^2+\frac{1}{4\pi}\int_0^{\pi}\operatorname{tr}Q^2(x)\,dx+\frac{1}{4\pi}[\operatorname{tr}Q'(0)-\operatorname{tr}Q'(\pi)]$$

$$+\tfrac{1}{8}[\operatorname{tr}Q''(0)+\operatorname{tr}Q''(\pi)]-\tfrac{1}{4}[\operatorname{tr}Q^2(0)+\operatorname{tr}Q^2(\pi)]$$

or

$$\sum_{m=1}^{\infty}\left[\sum_{n=1}^{\infty}(\lambda_{mn}^2-m^4)-\frac{2m^2}{\pi}\int_0^{\pi}\operatorname{tr}Q(x)\,dx-C\right]$$

$$=\frac{C}{2}+\frac{1}{8}[\operatorname{tr}Q''(0)+\operatorname{tr}Q''(\pi)]-\frac{1}{4}[\operatorname{tr}Q^2(0)+\operatorname{tr}Q^2(\pi)].$$

This proves the theorem.

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An operator valued extension of the super Korteweg–de Vries equations

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An extension of the super Korteweg–de Vries (KdV) integrable system in terms of operator valued functions is obtained. Following the ideas of Gardner, a general algebraic approach for finding the infinitely many conserved quantities of integrable systems is presented. The approach is applied to the above described system and infinitely many conserved quantities are constructed. In a particular case they reduce to the corresponding conserved quantities of super KdV. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1368139]

I. INTRODUCTION

It was shown in Ref. 1 that among the one parameter supersymmetric extensions of the Korteweg–de Vries (KdV) equation there is a special system that has an infinite number of conservation laws. This system is equivalent to the super KdV equations obtained in Ref. 2 by reduction from the super-Kadomtsev–Petviashvili hierarchy. $N=2$ supersymmetric extension of the KdV equations have also been obtained in Refs. 3–5.

The supersymmetric extension of the KdV equation is a system of coupled equations for a commuting and an anticommuting field. The commuting field $u(x,t)$ takes values in the even part of a Grassmann algebra $\mathcal{G}$ while the anticommuting field $\xi(x,t)$ takes values on the odd part of $\mathcal{G}$. The explicit form of the supersymmetric extension with an infinite number of conservation laws is[1]

$$u_t = -u''' + 6uu' - 3\xi\xi'', \tag{1}$$

$$\xi_t = -\xi''' + 3(\xi u)'. \tag{2}$$

If we use, as a particular case, the four dimensional Grassman algebra with generators e_1 and e_2, and express

$$u(x,t) = u_0(x,t) + u_{12}(x,t)e_1e_2, \tag{3}$$

$$\xi(x,t) = \xi_1(x,t)e_1 + \xi_2(x,t)e_2, \tag{4}$$

the system (1) and (2) may be reformulated as a coupled system in terms of real or complex fields $u_0, u_{12}, \xi_1\xi_2$ in the following way:

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$$u_{0t} = -u_0''' + 6u_0u_0', \tag{5}$$

$$\xi_{1t} = -\xi_1''' + 3(\xi_1 u_0)', \tag{6}$$

$$\xi_{2t} = -\xi_2''' + 3(\xi_2 u_0)', \tag{7}$$

$$u_{12t} = -u_{12}''' + 6(u_0u_{12})' - 3(\xi_1\xi_2'' - \xi_2\xi_1''). \tag{8}$$

Equation (5) is exactly the KdV equation. Equations (6) and (7) are linear homogeneous in ξ_1 and ξ_2, respectively. Equation (8) is also linear in u_{12} but contains a source in terms of ξ_1 and ξ_2. The super KdV system (1) is not the only integrable extension of the KdV equation constructed using a single anticommuting field. Another such system is the one proposed in Ref. 6:

$$u_t = -u''' + 6uu' - 3\xi\xi'', \tag{9}$$

$$\xi_t = -4\xi''' + 6\xi' u + 3\xi u'. \tag{10}$$

This system also has an infinite number of conservation laws. Its expansion in the particular Grassmann algebra generated by e_1 and e_2 gives again for the u_0 the KdV equation. In the case of $N=2$ supersymmetric systems, the equation for u_0 is modified by nonlinear terms coming from the other even field of the $N=2$ superfield. But again, there is no contribution to this equation from the odd fields. In this work we present an extension of the super KdV system in terms of coupled system of partial differential equations which yields a nonlinear modification for the KdV equation with an interacting term constructed from complex spinors. Our formulation will be in terms of operator valued functions which for a particular case reduce to the supersymmetric algebra. The final form of the nonlinear system will be in terms of commuting real or complex functions in contrast with (1) and (2). There is also a physical motivation for our program. The classical formulation of supersymmetric field theory is always in terms of commuting and anticommuting fields which, after quantization, yield a field theory in terms of bosonic and fermionic operators. However, once we have the quantum field theory we may consider the mean values of the bosonic and fermionic operators. We then obtain real scalar or vector fields from the bosonic sector, while complex spinors come from the fermionic sector. That is, for many applications the quantum theory may be analyzed in terms of real fields and complex spinors, without introducing the commuting and anticommuting fields of the classical formulation. For example, all the analysis of the spontaneous breaking of supersymmetry is formulated in those terms. It is then natural to ask if there is an extension of the KdV equation in terms of a real field $u(x,t)$ and a complex spinor $\xi(x,t)$. One particular case of the general approach we will discuss is the following system:

$$\begin{aligned} u_t &= -u''' + 6uu' - 3(\varphi_1\varphi_2'' - \varphi_1''\varphi_2), \\ \varphi_{1t} &= -\varphi_1''' + 3(\varphi_1 u)', \\ \varphi_2 t &= -\varphi_2''' + 3(\varphi_2 u)', \end{aligned} \tag{11}$$

where we consider only one complex field $\Psi(x,t) = \varphi_1(x,t) + i\varphi_2(x,t)$. System (11) should be compared with (5)–(8) where the anticommuting fields in (1) and (2) have been explicitly expanded in terms of a basis of a Grassmann algebra with real or complex coefficients.

There is also another general, but maybe indirect, motivation to our program. It has been recently recognized in the formulation of M-theory as a matrix model (IKKT)[7] that the construction of the theory in terms of elements of a complex Lie algebra equipped with an invariant bilinear inner product is not only directly related to superstring theory but also contains Yang–Mills theory, for a suitable election of the Lie algebra. The relation between self-dual Yang–Mills equations and integrable systems is well known, in particular to the KdV hierarchy. It is then natural to ask for an integrable generalization of the self-dual Yang–Mills equations in terms of

operator valued geometrical objects related to the IKKT formulation of M-theory and its relation to KdV hierarchy. Our contribution in this article may be a first step in this construction.

In Sec. II we present, following the ideas of Gardner,[8] a general algebraic approach for obtaining the infinitely many conserved quantities of certain integrable systems. We consider as a particular case of our analysis the conserved quantities associated with the system (11). In Sec. IV we present a generalization of the super KdV system in terms of operator valued functions. We apply the general approach developed in Sec. III to prove the existence of the infinitely many operator valued, conserved quantities of the integrable system.

In Sec. V we discuss our conclusions.

II. AN ALGEBRAIC APPROACH TO NONLINEAR SYSTEMS AND THEIR CONSERVATION LAWS

In order to study nonlinear equations and their conservation laws, one can start by choosing a ring V of infinitely differentiable functions $\mathbb{R}\to\mathbb{R}$ which satisfies $(d/dx)V\subset V$. A system of equations gives a flow in the manifold $\mathcal{M}=V\times V\times\cdots\times V$, whose general element is written $u(x)=(u_1(x),u_2(x),\ldots,u_n(x))$. The general model for formulas involving sums of products of derivatives of the $u_p(x)$ is a polynomial

$$f(a_{10},a_{11},a_{20},\ldots)$$

in a finite number of the commuting symbols a_{pm} with $1\leqslant p\leqslant n$, $\leqslant 0\leqslant m<\infty$. Then, replacing a_{pm} by $(d/dx)^m(u_p(x)$, an element u of the manifold $\mathcal{M}$ is taken to

$$f(u)=f(u_1(x),x_1'(x),u_2(x),\ldots),$$

an element of V whose derivative is given by

$$\frac{d}{dx}f(u)=(Df)(u),$$

$$D=\sum_{p=1}^{n}\sum_{m=0}^{\infty}a_{p,m+1}\frac{\partial}{\partial a_{pm}}.$$

The commutative ring $\mathcal{A}$ consisting of all such polynomials f, together with the derivation $D:\mathcal{A}\to\mathcal{A}$, may be called the free derivation ring on n generators.

The algebra $Op\mathcal{A}$, on the other hand, consists of the linear operators $L:\mathcal{A}\to\mathcal{A}$ which have the form $L=\Sigma_{m=0}^{N}l_mD^m$ with $l_m\in\mathcal{A}$. The standard operator transpose anti-involution $Op\mathcal{A}\to Op\mathcal{A}$ sends L to L^*, where $L^*f=\Sigma_{m=0}^{N}(-l)^mD^m(l_mf)$. Then fLg and gL^*f differ by an element of $\mathcal{D}\mathcal{A}$ for all $f,g\in\mathcal{A}$.

Given $u\in\mathcal{M}$ and $L\in Op\mathcal{A}$, the function substitution operation replaces

$$L(a,D)=\sum l_m(a_{10},a_{11},a_{20},\ldots)D^m$$

by

$$L\left(u,\frac{d}{dx}\right)=\sum l_m(u_1(x),u_1'(x),u_2(x)\ldots)\left(\frac{d}{dx}\right)^m,$$

a variable coefficient differential operator

$$L\left(u,\frac{d}{dx}\right):V\to V.$$

In order to see how ordinary differential equation (ODE) systems are related by internal substitutions, the following constructions are performed in $\mathcal{A}$ and in $Op\mathcal{A}$.

(1) A ring homomorphism $S:\mathcal{A}\to\mathcal{A}$ which commutes with $D:\mathcal{A}\to\mathcal{A}$ is completely determined by its values on the generators a_{p0}, $1\leqslant p\leqslant n$. Conversely, if $b=(b_1,\ldots,b_n)$ is any n-tuple of elements of $\mathcal{A}$, there is a unique ring homomorphism $\mathcal{S}_b:\mathcal{A}\to\mathcal{A}$ which commutes with D and satisfies $\mathcal{S}_b(a_{p0})=b_p$, $1\leqslant p\leqslant n$. The effect of $\mathcal{S}_b$ on $f(a_{10},a_{11},a_{20},\ldots)$ is to replace a_{pm} by $(D^m b_p)(a_{10},a_{11},a_{20},\ldots)$.

The transformation $\mathcal{S}_b$ also sends $Op\mathcal{A}\to Op\mathcal{A}$. If $L=\Sigma l_m D^m$, then $\mathcal{S}_b L=\Sigma(\mathcal{S}_b l_m)D^m$. Again, as in $\mathcal{A}$, $\mathcal{S}_b$ preserves sums and products.

(2) In the special case $b_p=a_p+te_p(a_{10},a_{11},a_{20},\ldots)$ with $t\in\mathbb{R}$ and arbitrary $e_p\in\mathcal{A}$, one can take the derivative at $t=0$ of $\mathcal{S}_b f$. The result is

$$\sum_{p=1}^{n}\sum_{m=0}^{\infty}\frac{\partial f}{\partial a_{pm}}D^m e_p=\sum_{p=1}^{n}\partial_p f(a,D)e_p,$$

where, for $1\leqslant p\leqslant n$, the Fréchet derivative operator $\partial_p f\in\mathcal{O}p\mathcal{A}$ is defined to be

$$\partial_p f(a,D)=\sum_{m=0}^{\infty}\frac{\partial f}{\partial a_{pm}}D^m.$$

Taking the derivative of the equation $\mathcal{S}_b Df=D\mathcal{S}_b f$, one sees that the Fréchet derivative operators of Df are given by

$$\partial_p(Df)=D(\partial_p f).$$

When $\partial_p f$ is applied to $a_{p1}=Da_{p0}\in\mathcal{A}$, one gets

$$\sum_{p=1}^{n}(\partial_p f)a_{p1}=Df.$$

(3) Returning to the case of general b one can verify the chain rule

$$\partial_p S_b f=\sum_{q=1}^{n}(\mathcal{S}_b\partial_q f)(\partial_p b_q).$$

The first step is to apply the usual chain rule, obtaining

$$\frac{\partial}{\partial a_{pm}}\mathcal{S}_b f=\sum_{q=1}^{n}\sum_{r=0}^{\infty}\left(\frac{\partial f}{\partial a_{qr}}\bigg|^{a_{qr}=D^r b_q}\right)\frac{\partial}{\partial a_{pm}}(D^r b_q).$$

Multiplying on the right by D^m and summing over $0\leqslant m<\infty$ one gets

$$\partial_p\mathcal{S}_b f=\sum_{q=1}^{n}\sum_{r=0}^{\infty}\left(\frac{\partial f}{\partial a_{pr}}\bigg|^{a_{qr}=D^r b_q}\right)(\partial_p D^r b_q)=\sum_{q=1}^{n}(\mathcal{S}_b\partial_q f)(\partial_p b_p).$$

This completes the proof.

(4) Nonlinear ODE systems are given by n-tuples $g=(g_1,\ldots,g_n)$ of elements of $\mathcal{A}$. The unknown functions $v_p(x,t)$ are required to satisfy

$$\frac{\partial}{\partial t}v_p(x,t)=g_p\left(v_1(x,t),\frac{\partial}{\partial x}v_1(x,t),v_2(x,t),\ldots\right).$$

It then follows that

$$\frac{\partial}{\partial t}\left(\frac{\partial}{\partial x}\right)^m v_p(x,t)=(D^m g_p)(v_1(x,t),\ldots).$$

(5) Given $h\in\mathcal{A}$, the formula

$$H(v)=\int h(v)dx$$

defines a (nonlinear) functional $H:\mathcal{M}\to\mathbb{R}$ when, for example, v is the space of infinitely differentiable 2π-periodic functions and the integral is taken from 0 to 2π.

If $v(x,t)$ satisfies $(\partial/\partial t)v=g(v)$, then the derivative of H along the solution is given by

$$\frac{d}{dt}H=\int\sum_{p=1}^{\infty}\sum_{m=0}^{\infty}\frac{\partial h}{\partial a_{pm}}(v)\left(\frac{d}{dt}\left(\frac{\partial}{\partial x}\right)^m v_p(x,t)\right)dx=\int\sum_{p=1}^{m}\partial_p h\left(v,\frac{d}{dx}\right)g_p(v)dx.$$

For H to be a conservation law for $\dot v=g(v)$ it suffices that

$$\sum_{p=1}^{m}(\partial_p h)g_p\in\mathcal{DA}.$$

(6) Given $b=(b_1,\ldots,b_n)$, there arises the transformation $v=b(u)$ of $\mathcal{M}$ into itself, where

$$v_p(x)=b_p(u_1(x),u_1'(x),u_2(x),\ldots).$$

If $u=u(x,t)$ satisfies the ODE system $\dot u=f(u)$, then $v=b(u)$ satisfies

$$\frac{\partial}{\partial t}v_p(x,t)=\sum_{q=1}^{n}\sum_{m=0}^{\infty}\frac{\partial b_p}{\partial a_{qm}}(u)\left(\frac{\partial}{\partial t}\left(\frac{\partial}{\partial x}\right)^m u_q(x,t)\right)=\sum_{q=1}^{n}\partial_q b_p\left(u,\frac{\partial}{\partial x}\right)f_q(u).$$

On the other hand,

$$g_p(v)=g_p(b(u))=(\mathcal{S}_b g_p)(u).$$

Therefore, in order for $v=b(u)$ to be a ''Miura transformation'' taking solutions of $\dot u=f(u)$ to solutions of $\dot v=g(v)$, the equations

$$\sum_{q=1}^{n}(\partial_q b_p)f_q=\mathcal{S}_b g_p$$

should hold in $\mathcal{A}$.

(7) We should expect the pullback of a conserved quantity to be a conserved quantity. Suppose that $h\in\mathcal{A}$ gives a conserved quantity for $\dot v=g(v)$, and that $v=b(u)$ is a Miura transformation to $\dot v=g(v)$ from $\dot u=f(u)$.

Then the b-pullback of h, that is to say $\mathcal{S}_b h$, has Fréchet derivative operators given by

$$\partial_p\mathcal{S}_p h=\sum_{q=1}^{n}(\mathcal{S}_b\partial_q h)(\partial_p b_q).$$

After applying this equation to $f_p\in\mathcal{A}$ we get

$$\sum_p(\partial_p\mathcal{S}_b h)f_p=\sum_{p,q}(\mathcal{S}_b\partial_q h)(\partial_p b_q)f_p=\sum_q(\mathcal{S}_b\partial_q h)(\mathcal{S}_b g_q)$$

because $v=g(u)$ is a Miura transformation. Then, $\mathcal{S}_b$ being a ring homomorphism,

$$\sum_p (\partial_p \mathcal{S}_b h) f_p = \mathcal{S}_b \left(\sum_q (\partial_q h) g_q \right) = \mathcal{S}_b \mathcal{D} e$$

for some $e \in \mathcal{A}$, because h gives a conserved quantity for $\dot{v} = g(v)$. Since $\mathcal{S}_b$ commutes with $\mathcal{D}$, we may conclude that $\mathcal{S}_b h$ gives a conserved quantity for $\dot{u} = f(u)$.

III. CONSERVATION LAWS FOR A KdV SYSTEM

This theory will now be applied to a generalization of the KdV equation. The usual version corresponds to the element $-a_1''' + 6a_1 a_1'$ in the free derivation ring on one generator, where the double suffix notation is shortened to $a_p = a_{p0}$, $a_p' = a_{p1}$, $a_p'' = a_{p2}$, etc., for small values of m in a_{pm}.

For the extended KdV we go from $n=1$ to $n=3$ and set

$$g_1 = (-a_1'' + 3a_1^2 + 3[a_2, a_3])', \quad g_2 = (-a_2'' + 3a_1 a_2)', \quad g_3 = (-a_3'' + 3a_1 a_3)',$$

in which $[a_p, a_q] = a_p' a_q - a_p a_q'$ in general.

This system, to be called $\dot{v} = g(v)$, is subjected to the transformation $\mathcal{S}_b : \mathcal{A} \to \mathcal{A}$ where

$$\begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} + \varepsilon \begin{pmatrix} a_1' \\ a_2' \\ a_3' \end{pmatrix} + \varepsilon^2 \begin{pmatrix} a_1^2 + [a_2, a_3] \\ a_1 a_2 \\ a_1 a_3 \end{pmatrix}$$

and ε is any real number. When $\varepsilon = 0$, $\mathcal{S}_b$ reduces to the identity map. Since the g_p are quadratic one gets

$$\mathcal{S}_b g = \sum_{i=0}^{4} \varepsilon^i \mathcal{C}_i$$

in which g is the column vector $(g_1, g_2, g_3)^T$. Evidently $\mathcal{C}_0 = g$ and $\mathcal{C}_1 = \mathcal{D}_g$, the latter because $d/d\varepsilon|^{\varepsilon=0} \mathcal{S}_b f = \Sigma_p (\partial_p f) a_p' = \mathcal{D} f$ for any $f \in \mathcal{A}$.

The last two columns are

$$\mathcal{C}_3 = \begin{pmatrix} (2a_1^3 + 3a_1[a_2, a_3])' \\ 3a_1(a_1 a_2)' + 3a_2'[a_2, a_3] \\ 3a_1(a_1 a_3)' + 3a_3'^I[a_2, a_3] \end{pmatrix}'$$

and

$$\mathcal{C}_4 = \begin{pmatrix} 3a_1^4 + 9a_1^2[a_2, a_3] + 3[a_2, a_3]^2 \\ 3a_1^3 a_2 + 3a_1 a_2[a_2, a_3] \\ 3a_1^3 a_3 + 3a_1 a_3[a_2, a_3] \end{pmatrix}'.$$

Turning now to the Fréchet derivative operators of the three components of b, we find the 3×3 matrix of elements of $\mathcal{O}_p \mathcal{A}$ which is given by

$$\partial_q b_p = I + \varepsilon \mathcal{D} + \varepsilon^2 B_2$$

in which

$$B_2 = \begin{pmatrix} 2a_1 & [*, a_3] & [a_2, *] \\ a_2 & a_1 & 0 \\ a_3 & 0 & a_1 \end{pmatrix}.$$

In order for a system $\dot{u}=f(u)$ to be sent to $\dot{v}=g(v)$ by $v=b(u)$, the coefficients f_p must satisfy

$$\mathcal{S}_b g_p=\sum_{q=1}^{3}(\partial_q b_p)f_q.$$

The corresponding equation of column vectors, expanded in powers of ε, is

$$\sum_{i=0}^{4}\varepsilon^i\mathcal{C}_i=(I+\varepsilon\mathcal{D}+\varepsilon^2 B_2)\sum_{j=0}^{\infty}\varepsilon^j F_j.$$

All the column vectors F_j are determined recursively; in particular $F_0=\mathcal{C}_0=g$, $F_1=0$, and

$$F_2=\begin{pmatrix}(2a_1^3+3a_1[a_2,a_3])'\\ 3a_1(a_1a_2)'+3a_2'[a_2,a_3]\\ 3a_1(a_1a_3)'+3a_3'[a_2,a_3]\end{pmatrix}.$$

It now turns out that $F_j=0$ for $j\geqslant 3$, permitting the fourth degree polynomial $\mathcal{S}_b g_p$ to be written as the product of $(\partial_q b_p)$ by f_q with $f=(f_1,f_2,f_3)^T$, $f=g+\varepsilon^2 F_2$, that is, as a product of two quadratic polynomials in ε. This completes the construction of $\dot{u}=f(u)$, a system sent to $\dot{v}=g(v)$ by $v=b(u)$.

Conservation laws for $\dot{u}=f(u)$ are given by $h\in\mathcal{A}$ satisfying $\Sigma_{p=1}(\partial_p h)f_p\in\mathcal{D}\mathcal{A}$. Since $\partial_p a_q=\delta(p,q)$ in general, the choice $h=a_1$ gives just f_1, which by the construction of f is always in $\mathcal{D}\mathcal{A}$. Therefore $h=a_1$ is indeed a conserved quantity for $\dot{u}=f(u)$.

If the ring homomorphism $\mathcal{S}_b:\mathcal{A}\to\mathcal{A}$ could be inverted, the pullback of a_1 would give a conservation law for $\dot{v}=g(v)$, for all ε. But it can indeed be inverted if we embed $\mathcal{A}$ within $\mathcal{A}[[\varepsilon]]=B$, whose elements are the formal power series in ε with coefficients in $\mathcal{A}$. The given elements $b_p\in B$, $1\leqslant p\leqslant 3$, define a unique ring homomorphism $\mathcal{S}_b:\mathcal{A}\to B$ which sends a_{p0} to b_p and commutes with $\mathcal{D}$. Obviously it extends to $\mathcal{S}_b:B\to B$.

But when $\varepsilon=0$ the element $b_p\in B$ reduces to the element $a_p\in\mathcal{A}$. Therefore, for any $h(a_{10},a_{11},a_{20},\ldots)\in\mathcal{A}$, $\mathcal{S}_b h$ will have the form

$$\mathcal{S}_b h=h+\varepsilon h_1+\varepsilon^2 h_2+\cdots$$

for some $h_1,h_2,\ldots,\varepsilon\mathcal{A}$.

Within B one has the ideals $\mathcal{B}_k=\varepsilon^k\mathcal{B}$ and the filtration $B\supset B_1\supset B_2\supset\cdots$. The preceding observation shows that $\mathcal{S}_b$ sends each B_k into itself, and reduces to the identity map in each quotient space B_k/B_{k+1}. This shows that, given any $f_0,f_1,\ldots$ in $\mathcal{A}$, the equation

$$\mathcal{S}_b\left(\sum_{k=0}^{\infty}\varepsilon^k g_k\right)=\sum_{k=0}^{\infty}\varepsilon^k f_k$$

can be solved recursively for $g_0,g_1,\ldots,\varepsilon\mathcal{A}$. Therefore $\mathcal{S}_b:B\to B$ is an isomorphism.

In order to see the recursion algorithm more clearly we work in the space $\mathcal{A}\oplus\mathcal{A}\oplus\mathcal{A}$ of column vectors $e=(e_1,e_2,e_3)^T$. Then

$$b=a+\varepsilon a'+\varepsilon^2\langle a,a\rangle,$$

where in general

$$\langle f,g\rangle=(f_1g_1+[f_2,g_3],f_1g_2,f_1g_3)^T,$$

a bilinear map of $\mathcal{A}\oplus\mathcal{A}\oplus\mathcal{A}$ into itself. We ask that column vectors $\mathcal{C}_0,\mathcal{C}_1,\mathcal{C}_2,\ldots$ be determined in such a way that

$$\mathcal{C}=\mathcal{C}_0+\varepsilon\mathcal{C}_1+\varepsilon^2\mathcal{C}_2+\cdots$$

satisfies

$$a=\mathcal{C}+\varepsilon\mathcal{C}'+\varepsilon^2\langle\mathcal{C},\mathcal{C}\rangle.$$

That is, the ring homomorphism $\mathcal{S}_{\mathcal{C}}:B\to B$ should send b_p to a_p for $1\leqslant p\leqslant 3$.

After equating the coefficients of corresponding powers of ε one finds the recursion relation

$$0=\mathcal{C}_{m+2}+\mathcal{C}'_{m+1}+\langle\mathcal{C}_m,\mathcal{C}_0\rangle+\langle\mathcal{C}_{m-1},\mathcal{C}_1\rangle+\cdots+\langle\mathcal{C}_0,\mathcal{C}_m\rangle.$$

The values for $0\leqslant m\leqslant 4$ are

$$\mathcal{C}_0=a,$$

$$\mathcal{C}_1=-a',$$

$$\mathcal{C}_2=a''-\langle a,a\rangle,$$

$$\mathcal{C}_3=-a'''+2\langle a,a\rangle',$$

$$\mathcal{C}_4=a''''-2\langle a,a\rangle''+\langle a',a'\rangle+\langle\langle a,a\rangle,a\rangle+\langle a\langle a,a\rangle\rangle.$$

By construction, the transformation $\mathcal{S}_{\mathcal{C}}$ takes $\dot{v}=g(v)$ to $\dot{u}=f(u)$. The latter equation has a_1 as a conserved quantity. Its pullback is the top entry in the column $\mathcal{C}=\mathcal{C}(\varepsilon)$.

As this is true for all ε, we conclude that the top entries of all the columns $\mathcal{C}_m$ give conserved quantities for the extended KdV equation $\dot{v}=g(v)$.

Simplifying where possible by subtracting elements of $\mathcal{DA}$ or by changing signs, the first three nontrivial functionals $\mathcal{M}\to R$ are

$$H_m(v)=\int h_m(v_1(x),v_1'(x),v_2(x),\ldots)dx$$

with

$$h_0=a_1,$$

$$h_2=(a_1)^2+a_2'a_3-a_2a_3',$$

$$h_4=2(a_1)^3+(a_1')^2+a_2''a_3'-a_2'a_3''+4a_1(a_2'a_3-a_2a_3').$$

Evidently, the extended KdV equation has infinitely many conservation laws.

IV. EXTENSION OF THE KdV EQUATION TO OPERATOR-VALUED FUNCTIONS

This extension, which also has infinitely many conservation laws, includes the supersymmetric KdV as a special case, as well as the extension seen in the preceding section.

That extension is a system of equations in the three real-valued functions $v_p(x,t)$, $1\leqslant p\leqslant 3$. It is recast in operator form by writing

$$\mathcal{P}=v_1(x,t)I,$$

$$\mathcal{Q}=v_2(x,t)E_2+v_3(x,t)E_3,$$

where E_2 and E_3 are linear operators in some space which satisfy $[E_2,E_3]=E_2E_3-E_3E_2=I$. The quantity $v_2'v_3-v_2v_3'$, which was denoted before by $[v_2,v_3]$, will now appear as the coefficient of I in the usual commutator $[\mathcal{Q}',\mathcal{Q}]$. Thus we have the equivalent system of operator differential equations

$$\mathcal{P}_t = -\mathcal{P}''' + 6\mathcal{P}\mathcal{P}' + 3[\mathcal{Q}'', \mathcal{Q}],$$
$$\mathcal{Q}_t = -\mathcal{Q}''' + 3(\mathcal{P}\mathcal{Q})'. \tag{12}$$

Further, setting $p = u_1(x,t)I$ and $q = u_2(x,t)E_2 + u_3(x,t)E_3$, the Gardner transformation takes the form

$$\mathcal{P} = p + \epsilon p' + \epsilon^2(p^2 + [q', q]),$$
$$\mathcal{Q} = q + \epsilon q' + \epsilon^2 pq, \tag{13}$$

and the modified KdV equation $\dot{u} = f(u)$ takes the form

$$p_t = (-p'' + 3p^2 + 3[q', q])' + \epsilon^2(2p^3 + 3p[q', q])',$$
$$q_t = (-q'' + 3pq)' + \epsilon^2 3(p^2 q' + pp'q + q'[q', q]). \tag{14}$$

It was shown in the preceding section that the Gardner transformation takes a solution p,q of the latter system to a solution $\mathcal{P}$, $\mathcal{Q}$ of the former.

But more generally one can suppose that P and p have values in $\mathcal{P}$, a commutative algebra with unit, of operators acting in some vector space. Then, if $\mathcal{Q}$ is a linear space of operators satisfying

$$[\mathcal{Q}, \mathcal{P}] = 0,$$
$$\mathcal{Q}\mathcal{P} \subset \mathcal{Q}, \tag{15}$$
$$[\mathcal{Q}, \mathcal{Q}] \subset \mathcal{P},$$

then $\mathcal{Q}$ and q can take their values in $\mathcal{Q}$.

For the specific choice $\mathcal{P} = \{\alpha I\}$, $\mathcal{Q} = \{\beta_2 E_2 + \beta_3 E_3\}$ just considered, we have observed that the Gardner transformation (13) takes solutions of (14) to solutions of (12), this being no more than a restatement of the results of the preceding section.

However, upon reexamining the calculations in that section, one sees that they remain valid not just for the $\mathcal{P}$, $\mathcal{Q}$ just considered but for any $\mathcal{P}$ and $\mathcal{Q}$ satisfying (15).

Therefore the conservation laws of (12) and of (14) are interrelated by the Gardner transformation (13) and its inverse, just as before; in particular (12) has infinitely many conservation laws.

After simplifying by crossing out derivatives in x, the first four nontrivial conserved quantities for the operator-extended KdV system are

$$H_0 = \int \mathcal{P}\, dx,$$
$$H_2 = \int (\mathcal{P}^2 + [\mathcal{Q}', \mathcal{Q}])\, dx,$$
$$H_4 = \int (2\mathcal{P}^3 + (\mathcal{P}')^2 + 4\mathcal{P}[\mathcal{Q}', \mathcal{Q}] + [\mathcal{Q}'', \mathcal{Q}'])\, dx, \tag{16}$$
$$H_6 = \int (5\mathcal{P}^4 + 10\mathcal{P}(\mathcal{P}')^2 + (\mathcal{P}'')^2 + 15\mathcal{P}^2[\mathcal{Q}', \mathcal{Q}] - 2\mathcal{P}[\mathcal{Q}'', \mathcal{Q}']$$
$$-8\mathcal{P}[\mathcal{Q}''', \mathcal{Q}] + 3[\mathcal{Q}', \mathcal{Q}]^2 + [\mathcal{Q}''', \mathcal{Q}''])\, dx.$$

In each case, the conserved quantity has its values in the operator algebra $\mathcal{P}$.

The foregoing theory applies to any operator spaces $\mathcal{P}$, $\mathcal{Q}$ having the stipulated properties. For example, the $\mathcal{Q}$ seen before can be enlarged to $\mathcal{Q}=\{\Sigma_{k=1}^{m}(\mu_k E_k+\nu_k F_k)\}$ where $\mu_k,\nu_k \epsilon \mathbb{R}$ while $E_1,\ldots,E_m$, $F_1,\ldots,F_m$ are linearly independent operators in some vector space, satisfying $[E_k,F_k]=I$ but with all other commutator brackets zero. Then, with $\mathcal{P}=\{\alpha I\}$ as before, the operator-extended KdV system becomes a system of nonlinear differential equations for $2m+1$ functions $\alpha(x,t),\mu_k(x,t),\nu_k(x,t)$, specifically

$$\frac{\partial}{\partial t}\alpha=-\alpha'''+6\alpha\alpha'+3\sum_{k=1}^{m}(\mu_k''\nu_k-\mu_k\nu_k''),$$

$$\frac{d}{dt}\mu_k=-\mu_k'''+3(\alpha\mu_k)', \tag{17}$$

$$\frac{d}{dt}\nu_k=-\nu_k'''+3(\alpha\nu_k)'.$$

Another choice of $\mathcal{P}$ and $\mathcal{Q}$ leads to the supersymmetric extension of KdV. An exterior algebra Λ on a finite set of generators is the direct sum $\Lambda=\Lambda_0\oplus\Lambda_1$, where Λ_0 and Λ_1 consist of the linear combinations of even products, respectively odd products, of the generators. Then $\mathcal{P}$ and $\mathcal{Q}$ are, respectively, the operators of left multiplication in Λ by elements of Λ_0 and of Λ_1. In this example some of the equations in the general theory are to be simplified, for example $[\mathcal{Q}'',\mathcal{Q}]=2\mathcal{Q}''\mathcal{Q}$. The change of variables $\mathcal{P}=u$, $\mathcal{Q}=2^{-1/2}\xi$ converts the operator-extended KdV into

$$u_t=-u'''+6uu'-3\xi\xi'',$$

$$\xi_t=-\xi'''+3(\xi u)',$$

which is the supersymmetric extension of KdV given by Mathieu in Ref. 1. Moreover, the modified system (12) and the conserved quantity H_6 are simplified a bit by $q'[q',q]=0$ and $[\mathcal{Q}',\mathcal{Q}]^2=0$ in the supersymmetric case.

V. CONCLUSION

In this article an operator valued extension of the KdV equation was constructed. In a particular case the super KdV equations were recovered. A general algebraic method was developed and applied to show that there are infinitely many conserved quantities for certain integrable systems. When the method was applied to the operator extension of the KdV equation, the first few conserved quantities were computed explicitly. The conserved quantities H_0, H_2, and H_4 of the super KdV equation can be seen to correspond term by term with the corresponding quantities of the operator extension. However, the quantities $H_6,H_8,\ldots$ contain extra terms in the operator case which reduce to zero for the super KdV equation.

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Nonlinear Schrödinger-type equations from multiscale reduction of PDEs. II. Necessary conditions of integrability for real PDEs[a)]

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The multiscale method has been applied in J. Math. Phys. **41**, 6399 (2000) to evolution PDEs to obtain various nonlinear Schrödinger-type equations. Here these results are exploited to derive necessary conditions of integrability for nonlinear, real, evolution PDEs in $1+1$ dimensions. These conditions are given by explicit formulas, and several examples are detailed. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1366296]

I. INTRODUCTION

In the first paper of this series[1] we began a systematic exploration of results obtainable by applying ''multiscale expansions'' techniques to nonlinear evolution PDEs. In particular we exhibited a set of *universal nonlinear evolution equations of nonlinear Schrödinger type* obtained via such technique.[1] The qualifying adjective ''universal'' refers to the fact that, to each of these model equations, an entire *large* class of nonlinear evolution PDEs can be associated, via an appropriate *reduction* technique (involving a small parameter ϵ) which is asymptotically *exact* (in the $\epsilon \to 0$ limit).

An important by-product of this technique emerges from the observation[2] that the ''universal'' model equation obtainable from an entire class of nonlinear evolution PDEs via such an *asymptotically exact* technique cannot be ''less solvable'' than any one of the (many) equations contained in that class, since the solution of the model equation can indeed be obtained by making an appropriate asymptotic expansion of an appropriately chosen solution of any evolution equation in that class. The way is thereby opened to establish *necessary conditions of integrability* for nonlinear evolution PDEs: if a given nonlinear evolution PDE yields by reduction a *nonintegrable* model equation, then it cannot be itself *integrable*. This technique to obtain necessary conditions for the integrability of nonlinear PDEs was introduced by Wiktor Eckhaus and by one of us (F.C.) a dozen years ago[2,3] (for analogous approaches see Refs. 4 and 5); the present paper is devoted to a systematic presentation of such results, based on the findings reported in paper I. For simplicity we restrict attention in this paper to *real* nonlinear evolution PDEs of the kind treated in paper I, namely to real evolution PDEs featuring a *linear part* which is *dispersive* and a *nonlinear part* which is *analytic* but otherwise *largely arbitrary*. Hence the nonlinear evolution PDEs on which we hereafter focus read as follows:

$$Du = (\partial/\partial x)^h F, \tag{1.1}$$

where we have separated the linear part of the equation on the left-hand side from the nonlinear part on the right-hand side, according to the following specifications.

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The dependent variable $u \equiv u(x,t)$ is a *real* function of the two (real) independent variables x (''space'') and t (''time''). The (real) *linear* differential operator D,

$$D = \partial/\partial t + \sum_{m=0}^{M} (-1)^m \ a_{2m+1} \ (\partial/\partial x)^{2m+1}, \tag{1.2}$$

is characterized by the *real* coefficients a_{2m+1} (with M an arbitrary positive integer, $M \geqslant 1$, and of course $a_{2M+1} \neq 0$). The *nonlinear* function $F \equiv F(u,u_x,u_{xx},\ldots)$ is defined as follows:

$$F(u,u_x,u_{xx},\ldots) = \sum_{m=2}^{\infty} F^{(m)}(u,u_x,u_{xx},\ldots), \tag{1.3a}$$

where $F^{(m)}(u,u_x,u_{xx},\ldots)$ is a *homogeneous* polynomial of degree m in u and its x-derivatives $u_x,u_{xx},\ldots$:

$$F^{(m)}(u,u_x,u_{xx},\ldots) = \sum_{j_1=0}^{\infty} \sum_{j_2=j_1}^{\infty} \cdots \sum_{j_m=j_{m-1}}^{\infty} c^{(m)}_{j_1 j_2 \ldots j_m} u^{(j_1)} u^{(j_2)} \cdots u^{(j_m)}. \tag{1.3b}$$

Here and throughout $u^{(1)} \equiv u_x \equiv \partial u/\partial x$, $u^{(2)} \equiv u_{xx} \equiv \partial^2 u/\partial x^2$, and so on; and the (constant) coefficients $c^{(m)}_{j_1 j_2 \ldots j_m}$ are of course *real*. For instance, if the coefficients $c^{(2)}_{j_1 j_2}$ vanish for $j_2 > 2$,

$$F^{(2)} = c^{(2)}_{00} u^2 + c^{(2)}_{01} u u_x + c^{(2)}_{02} u u_{xx} + c^{(2)}_{11} u_x^2 + c^{(2)}_{12} u_x u_{xx} + c^{(2)}_{22} u_{xx}^2, \tag{1.4}$$

and likewise, if the coefficients $c^{(3)}_{j_1 j_2 j_3}$ vanish for $j_3 > 2$,

$$\begin{aligned} F^{(3)} = {} & c^{(3)}_{000} u^3 + c^{(3)}_{001} u^2 u_x + c^{(3)}_{002} u^2 u_{xx} + c^{(3)}_{011} u u_x^2 + c^{(3)}_{012} u u_x u_{xx} + c^{(3)}_{022} u u_{xx}^2 + c^{(3)}_{111} u_x^3 \\ & + c^{(3)}_{112} u_x^2 u_{xx} + c^{(3)}_{122} u_x u_{xx}^2 + c^{(3)}_{222} u_{xx}^3 . \end{aligned} \tag{1.5}$$

Finally, the derivative operator $(\partial/\partial x)^h$, with h a non-negative integer, is introduced in the right-hand side of (1.1) to take account of the possibility that the nonlinear part of the evolution equation under consideration be a perfect differential of order h, see (1.1). Such recognition is generally helpful to obtain more effective integrability conditions (see below), but it is of course not required for the validity of the results obtained below.

According to the notation we just detailed every nonlinear evolution PDE of the class under consideration in this paper is identified by assigning all the (nonvanishing) *real* coefficients a_{2m+1} and $c^{(m)}_{j_1 j_2 \ldots j_m}$, as well as the non-negative integer h; as for the latter, let us re-emphasize that any equation of type (1.1) with $h > 0$ can be equivalently rewritten with a smaller value of h, say by replacing h with $\tilde{h}$ where $0 \leqslant \tilde{h} < h$, and by correspondingly replacing, in an appropriate manner, the coefficients $c^{(m)}_{j_1 j_2 \ldots j_m}$ with $\tilde{c}^{(m)}_{j_1 j_2 \ldots j_m}$; this ambiguity does not affect the validity of the following findings; but it is generally advisable, to get more cogent results, to choose for h the largest non-negative integer value consistent with the nonlinear evolution equation under consideration. The user-friendly character of the results reported in this paper is evidenced by the possibility they provide to get information on the integrability of any equation of type (1.1)–(1.3), in the guise of conditions formulated directly in terms of these constants ($a_{2m+1}, c^{(m)}_{j_1 j_2 \ldots j_m}$ and h): conditions which, whenever they are *not* satisfied, guarantee that the nonlinear evolution PDE under consideration is *not integrable*.

In Sec. II we review some results of paper I, to the extent necessary and sufficient to render the present paper self-contained. In the subsequent Sec. III the notion of *integrability* is reviewed, with particular reference to certain model equations that provide the basic tools to derive those *necessary conditions of integrability* that constitute the core of this paper. These results, which are of course applicable to nonlinear evolution PDEs of type (1.1)–(1.3), are detailed in Sec. IV; readers more interested in using these findings than in understanding their origin are advised to

proceed immediately to that section, and as well to Sec. V, where some examples are exhibited which demonstrate the ease of applicability, and the efficacy, of these tools to test the possible integrability of nonlinear evolution PDE of type (1.1)–(1.3). Finally, let us emphasize that, while in this paper we have for simplicity restricted attention to *real scalar* nonlinear PDEs in *one* space variable only and only of *first-order* in time, clearly the approach used herein is applicable more generally.

II. REVIEW OF PREVIOUS RESULTS

In this section we review previous findings,[1] to the extent needed to derive, in Sec. 4, the main results of the present paper. Our presentation is notationally self-consistent, but of course for the justification of the assertions made herein the interested reader is referred to paper I.

Let k be a *real* and *nonvanishing* parameter, and define the following five (real) quantities in terms of this parameter and of the coefficients a_{2m+1} that characterize the linear differential operator (1.2):

$$A_0^{(1)}(k) = -\sum_{m=1}^{M} (2m+1)\, a_{2m+1}\, k^{2m}, \tag{2.1a}$$

$$A_1^{(2)}(k) = \sum_{m=1}^{M} m(2m+1)\, a_{2m+1}\, k^{2m-1}, \tag{2.1b}$$

$$A_2^{(0)}(k) = 2\sum_{m=1}^{M} (2^{2m}-1)\, a_{2m+1}\, k^{2m+1}, \tag{2.1c}$$

$$A_2^{(1)}(k) = \sum_{m=1}^{M} (2m+1)(2^{2m}-1)\, a_{2m+1}\, k^{2m}, \tag{2.1d}$$

$$A_2^{(2)}(k) = \frac{1}{2}\sum_{m=1}^{M} m(2m+1)\, 2^{2m}\, a_{2m+1}\, k^{2m-1}. \tag{2.1e}$$

Next define the following eight quantities in terms of the (real) parameter k and of the coefficients $c^{(m)}_{j_1 j_2 \cdots j_m}$ that characterize the nonlinear part of the evolution PDE (1.1) [see (1.3b)]:

$$g_{01}(k) = 2c_{00}^{(2)} + \sum_{j=1}^{\infty} (-1)^j k^{2j} c_{0,2j}^{(2)} + i\sum_{j=0}^{\infty} (-1)^j k^{2j+1} c_{0,2j+1}^{(2)}, \tag{2.2a}$$

$$g_{11}(k) = \sum_{j=0}^{\infty} (-1)^j k^{2j} \sum_{j'=0}^{j} c_{j',2j-j'}^{(2)} + i\sum_{j=0}^{\infty} (-1)^j k^{2j+1} \sum_{j'=0}^{j} c_{j',2j+1-j'}^{(2)}, \tag{2.2b}$$

$$g_{-1,1}(k) = 2\sum_{j=0}^{\infty} (-1)^j k^{2j} \sum_{j'=0}^{j} (-1)^{j'} c_{j',2j-j'}^{(2)}, \tag{2.2c}$$

$$\begin{aligned} g_{-1,2}(k) = {} & \sum_{j=0}^{\infty} (-1)^j k^{2j} \sum_{j'=0}^{j} (-1)^{j'} (2^{2j-j'} + 2^{j'})\, c_{j',2j-j'}^{(2)} \\ & + i\sum_{j=0}^{\infty} (-1)^j k^{2j+1} \sum_{j'=0}^{j} (-1)^{j'} (2^{2j+1-j'} - 2^{j'})\, c_{j',2j+1-j'}^{(2)}, \end{aligned} \tag{2.2d}$$

$$g_{-n,n,n}(k)=\sum_{l=0}^{\infty}(-1)^l(nk)^{2l}\sum_{j=0}^{[4l/3]}\sum_{j'=\mathrm{Max}[0,2j-2l]}^{[j/2]}[(-1)^{j'}+(-1)^j+(-1)^{j+j'}]$$
$$\times c^{(3)}_{j',j-j',2l-j}+i\sum_{l=0}^{\infty}(-1)^l(nk)^{2l+1}$$
$$\times\sum_{j=0}^{[4l+2/3]}\sum_{j'=\mathrm{Max}[0,2j-2l-1]}^{[j/2]}[(-1)^{j'}-(-1)^j+(-1)^{j+j'}]$$
$$\times c^{(3)}_{j',\,j-j',\,2l+1-j},\quad n=1,2, \tag{2.2e}$$

$$g_{-n,1,2}(k)=\sum_{0\leqslant j_1\leqslant j_2\leqslant j_3<\infty}(ik)^{j_1+j_2+j_3}[(-n)^{j_1}(2^{j_2}+2^{j_3})$$
$$+(-n)^{j_2}(2^{j_1}+2^{j_3})+(-n)^{j_3}(2^{j_1}+2^{j_2})]c^{(3)}_{j_1j_2j_3},\quad n=1,2. \tag{2.2 f}$$

The first four of these quantities, $g_{01}(k),g_{11}(k),g_{-1,1}(k),g_{-1,2}(k)$, are defined in terms of the coefficients $c^{(2)}_{j_1j_2}$ of the *quadratic* term $F^{(2)}$ [see (1.3)], on the right-hand side of (1.1); the last four of these quantities, $g_{-1,1,1}$, $g_{-2,2,2}$, $g_{-1,1,2}$, $g_{-2,1,2}$, are instead defined in terms of the coefficients $c^{(3)}_{j_1j_2j_3}$ of the *cubic* term, $F^{(3)}$ [see (1.3)], on the right-hand side of (1.1). Note that, of these eight quantities, only one, $g_{-1,1}(k)$ [see (2.2c)], is always real. The notation used here is closely analogous, if not identical, to the notation of Ref. 1 (note that the commas introduced occasionally to separate subscripts have no significance other than for typographical neatness).

Lemma 2.1. If $h\geqslant 1$ and

$$A^{(1)}_0(k)\neq 0,\quad A^{(2)}_1(k)\neq 0,\quad A^{(0)}_2(k)\neq 0, \tag{2.3}$$

an asymptotically exact reduction of (1.1)–(1.3) reads

$$i\psi_\tau+\alpha\psi_{\xi\xi}=\lambda|\psi|^2\psi, \tag{2.4a}$$

with $\psi\equiv\psi(\xi,\tau)$ and

$$\alpha\equiv\alpha(k)=A^{(2)}_1(k), \tag{2.4b}$$

$$\lambda\equiv\lambda(k)=-\delta_{h1}[A^{(1)}_0(k)]^{-1}kg_{01}(k)g_{-11}(k)+[A^{(0)}_2(k)]^{-1}(-2k^2)^hg_{-1,2}(k)g_{1,1}(k)$$
$$+i^{h+1}k^hg_{-1,1,1}(k). \tag{2.4c}$$

□

Remark 2.1. The model equation (2.4) is of course the standard NLS (nonlinear Schrödinger) equation. The validity of this *Lemma 2.1* is entailed by Eq. (C10) of paper I.

□

Lemma 2.2. If $h=0$ and

$$A^{(1)}_0(k)\neq 0,\quad A^{(2)}_1(k)\neq 0, \tag{2.5}$$

an asymptotically exact reduction of (1.1)–(1.3) reads

$$i\psi_\tau+\alpha\psi_{\xi\xi}=\lambda_1\varphi\psi, \tag{2.6a}$$

$$\varphi_\xi=\lambda_2|\psi|^2, \tag{2.6b}$$

with $\psi\equiv\psi(\xi,\tau)$, $\varphi\equiv\varphi(\xi,\tau)$, α given by (2.4b) and

$$\lambda_1 \equiv \lambda_1(k) = g_{01}(k), \tag{2.6c}$$

$$\lambda_2 \equiv \lambda_2(k) = [A_0^{(1)}(k)]^{-1} g_{-1,1}(k). \tag{2.6d}$$

□

Remark 2.2. Note that the model evolution equation takes now the form of a system of two coupled equations, see (2.6a) (2.6b). The validity of this *Lemma 2.2* is entailed by Eq. (C.11) of paper I.

□

Lemma 2.3. If, for some *real nonvanishing* value $k=\tilde{k}$, $A_2^{(0)}$ vanishes,

$$A_2^{(0)}(\tilde{k}) = 0, \tag{2.7}$$

and in addition there hold the relations

$$h \geqslant 1, \tag{2.8a}$$

$$A_1^{(2)}(\tilde{k}) \neq 0, \quad A_2^{(1)}(\tilde{k}) \neq 0, \tag{2.8b}$$

then an asymptotically exact reduction of (1.1)–(1.3) reads

$$i\psi_\tau + \alpha \psi_{\xi\xi} = \mu_1 \chi \psi^*, \tag{2.9a}$$

$$\chi_\xi = \mu_2 \psi^2 \tag{2.9b}$$

with $\psi \equiv \psi(\xi,\tau)$, $\chi \equiv \chi(\xi,\tau)$, and

$$\alpha = A_1^{(2)}(\tilde{k}), \tag{2.9c}$$

$$\mu_1 = i^{h+1} \tilde{k}^h g_{-1,2}(\tilde{k}), \tag{2.9d}$$

$$\mu_2 = (2i\tilde{k})^h [A_2^{(1)}(\tilde{k})]^{-1} g_{11}(\tilde{k}); \tag{2.9e}$$

while if (2.8a) does not hold, namely if

$$h = 0, \tag{2.10a}$$

but (2.7) continues to hold (for some real nonvanishing $\tilde{k}$) and (2.8b) is augmented to read

$$A_0^{(1)}(\tilde{k}) \neq 0, \quad A_1^{(2)}(\tilde{k}) \neq 0, \quad A_2^{(1)}(\tilde{k}) \neq 0, \tag{2.10b}$$

then an asymptotically exact reduction of (1.1)–(1.3) reads

$$i\psi_\tau + \alpha \psi_{\xi\xi} = i g_{0,1}(\tilde{k}) \varphi \psi + i g_{-1,2}(\tilde{k}) \chi \psi^*, \tag{2.11a}$$

$$\varphi_\xi = \nu_1 |\psi|^2, \tag{2.11b}$$

$$\chi_\xi = \nu_2 \psi^2, \tag{2.11c}$$

with $\psi \equiv \psi(\xi,\tau)$, $\varphi \equiv \varphi(\xi,\tau)$, $\chi \equiv \chi(\xi,\tau)$, α given by (2.9c), and

$$\nu_1 = [A_0^{(1)}(\tilde{k})]^{-1} g_{-1,1}(\tilde{k}), \tag{2.11d}$$

$$\nu_2 = [A_2^{(1)}(\tilde{k})]^{-1} g_{11}(\tilde{k}). \tag{2.11e}$$

□

Remark 2.3. This *Lemma 2.3*, in contrast to the previous two *Lemmata 2.1* and *2.2*, requires that k have a special value, see (2.7): note that this polynomial equation in k, (2.7) with (2.1c), has at most $2M$ *real nonvanishing* solutions (it might of course have none). Depending on the value of h, $h \geqslant 1$, respectively, $h=0$, the model equation is now a system of two, respectively, three coupled equations, see (2.9a) and (2.9b), respectively (2.11a), (2.11b), and (2.11c). The validity of *Lemma 2.3* is entailed by Eqs. (C.12) respectively (C.13) of paper I.

□

Lemma 2.4. If $h=1$ and for some *real nonvanishing* value $k=\tilde{k}$, $A_0^{(1)}$ vanishes and $A_1^{(2)}$ does not,

$$A_0^{(1)}(\tilde{k})=0, \tag{2.12a}$$

$$A_1^{(2)}(\tilde{k})\neq 0, \tag{2.12b}$$

then an asymptotically exact reduction of (1.1)–(1.3) reads

$$i\psi_\tau+\alpha\psi_{\xi\xi}=i\tilde{k}g_{01}(\tilde{k})\varphi\psi, \tag{2.13a}$$

$$\varphi_\tau=g_{-1,1}(\tilde{k})(|\psi|^2)_\xi, \tag{2.13b}$$

with α given by (2.9c).

□

Remark 2.4. In analogy to *Lemma 2.3*, and in contrast to *Lemmata 2.1* and *2.2*, this *Lemma 2.4* requires that k have a special value, see (2.12a): note that this polynomial equation in k, (2.12a) with (2.1a), has again at most $2M$ *real nonvanishing* solutions (it might of course have none). The model equation is now a system of two coupled equations, see (2.13a) and (2.13b). The validity of *Lemma 2.4* is entailed by Eq. (C15) of paper I.

□

The last result we report here is only applicable to evolution equations of type (1.1)–(1.3) which feature nonlinearities of *cubic*, or higher, degree. Hence we now assume

$$F^{(2)}(u,u_x,u_{xx},\ldots)=0 \tag{2.14}$$

[see (1.3)]. For the subclass of evolution PDEs of type (1.1)–(1.3) satisfying this restriction there then holds

Lemma 2.5. If, for some *real nonvanishing* value $k=\tilde{k}$, both $A_2^{(0)}$ and $A_2^{(1)}$ vanish,

$$A_2^{(0)}(\tilde{k})=A_2^{(1)}(\tilde{k})=0, \tag{2.15a}$$

and moreover

$$A_1^{(2)}(\tilde{k})\neq 0,\ A_2^{(2)}(\tilde{k})\neq 0, \tag{2.15b}$$

then an asymptotically exact reduction of (1.1)–(1.3) reads

$$i\psi_{1,\tau}+\alpha_1\psi_{1,\xi\xi}=(\lambda_{11}|\psi_1|^2+\lambda_{12}|\psi_2|^2)\psi_1, \tag{2.16a}$$

$$i\psi_{2,\tau}+\alpha_2\psi_{2,\xi\xi}=(\lambda_{21}|\psi_1|^2+\lambda_{22}|\psi_2|^2)\psi_2, \tag{2.16b}$$

with

$$\alpha_1 = A_1^{(2)}(\tilde{k}), \quad \alpha_2 = A_2^{(2)}(\tilde{k}), \tag{2.16c}$$

$$\begin{aligned} \lambda_{11} &= i^{h+1}\tilde{k}^h g_{-1,1,1}(\tilde{k}), \quad \lambda_{12} = i^{h+1}\tilde{k}^h g_{-2,1,2}(\tilde{k}), \\ \lambda_{21} &= i^{h+1}(2\tilde{k})^h g_{-1,1,2}(\tilde{k}), \quad \lambda_{22} = i^{h+1}(2\tilde{k})^h g_{-2,2,2}(\tilde{k}). \end{aligned} \tag{2.16d}$$

□

Remark 2.5. The applicability of this *Lemma 2.5* is restricted by the condition (2.14), and in addition by the requirement that *both equalities* (2.15a) hold [as well as the *inequalities* (2.15b)]: this generally entails that the coefficients a_{2m+1} satisfy one equation, see (2.15a) with (2.1c) and (2.1d). The model equation takes now the form of a coupled system of two NLS equations, see (2.16a) and (2.16b). The validity of this *Lemma 2.5* is entailed by Eq. (E3) of paper I.

□

This concludes our presentation of the results of paper I that are instrumental to derive useful necessary conditions for integrability. A crucial issue in this respect is the *integrable* (or rather the *nonintegrable*) character of the five model equations yielded by the five Lemmata we just reported. This is discussed in Sec. III.

III. INTEGRABILITY

In this section we discuss the all-important issue of *integrability*. As it is well known, although this notion is now well understood by practitioners, there does not yet exist a precise, universally accepted definition of integrability for (nonlinear evolution) PDEs. Hence we cannot formulate *necessary conditions for integrability* as *Theorems* backed by rigorous *Proofs*. Nevertheless we believe the results of this kind presented below are both cogent and useful.

The point of departure of our treatment is the following:

Axiom. Every nonlinear evolution PDE that yields via an *asymptotically exact* reduction process a nonlinear evolution PDE known *not* to be *integrable*, should itself be pronounced *nonintegrable*.

□

We use the term ''Axiom'' to denote this statement, because the lack of a precise, universally accepted definition of *integrability* precludes any hope to ''prove'' it. On the other hand, its validity is plain, being predicated, as we already noted, on the fact that the task of solving a model equation derived via an *asymptotically exact reduction* from a given equation, cannot be ''more difficult'' than that of solving the original equation; since the solution of the model equation can indeed be obtained by applying the asymptotic expansion process to an appropriately chosen solution of the original equation. Hence no model equation derived via an asymptotically exact reduction from a given equation can be ''less integrable'' than the original equation. Hence a nonlinear evolution PDE that yields via an asymptotically exact reduction process a model equation known *not* to be *integrable*, is necessarily itself *nonintegrable*.

This line of argumentation can be made more specific by introducing the heuristic (i.e., not quite precise but very useful) distinction[3] among *S-integrable* nonlinear evolution PDEs (i.e., those solvable via the spectral transform technique, or some variant of it; see, for instance, Ref. 6), and *C-integrable* nonlinear evolution PDEs (i.e., those solvable via some appropriate change of variables; see, for instance, Refs. 3 and 7). This *Axiom* is indeed equally applicable if the terms ''integrable'' respectively ''nonintegrable'' are systematically replaced by ''*C*-integrable'' respectively ''not *C*-integrable'' or, as the case may be, ''*S*-integrable'' respectively ''not *S*-integrable.'' In the following we use the terms ''integrable'' and ''integrability'' (as well as their negatives) whenever we do not wish to introduce the (fine!?) distinction among *S*-integrability and *C*-integrability; when we do instead specify the kind of integrability we refer to, it is useful that the reader be aware of the hierarchical character of this distinction, according to which *C-integrable* equations are ''more integrable'' than *S-integrable* ones: namely, every

C-integrable equation is automatically considered to also belong to the *S-integrable* class, while there are (many) examples of *S-integrable* equations which are *not C-integrable*.[3]

In the light of the results reported in the preceding section it is now clear that the next step of our treatment is to assess the integrable character of the five model equations detailed there. Before delving into this discussion we like to reiterate the word of caution already voiced above, related to the *lack* of a precise and universally accepted *definition of integrability* for nonlinear evolution PDEs. Thus our assertions in the remainder of this section must rely on what we consider *common knowledge*—or, equivalently, *universal lore*.

Statement 3.1. The NLS equation (2.4a), with α *real* and *nonvanishing*, is *not S-integrable* unless λ is real,

$$\mathrm{Im}(\lambda)=0, \tag{3.1a}$$

and it is *not C-integrable* unless λ vanishes,

$$\lambda=0. \tag{3.1b}$$

□

Statement 3.2. The model equation (2.6) with α *real* and *nonvanishing* is *not integrable* unless it effectively linearizes, namely unless at least one of the two constants λ_1,λ_2 vanishes, entailing

$$\lambda_1\lambda_2=0. \tag{3.2}$$

□

Statement 3.3. The model equation (2.9a) and (2.9b) with α *real* and *nonvanishing* is *not integrable* unless it effectively linearizes, namely unless at least one of the two constants μ_1,μ_2 vanishes, entailing

$$\mu_1\mu_2=0. \tag{3.3}$$

□

Statement 3.4. The model equation (2.11a), (2.11b), and (2.11c) with α *real* and *nonvanishing* is *not integrable* unless it effectively linearizes, namely unless at least one of the following four conditions holds:

$$g_{01}(\tilde{k})=\nu_2=0, \tag{3.4a}$$

or

$$g_{-1,2}(\tilde{k})=\nu_1=0, \tag{3.4b}$$

or

$$g_{01}(\tilde{k})=g_{-1,2}(\tilde{k})=0, \tag{3.4c}$$

or

$$\nu_1=\nu_2=0. \tag{3.4d}$$

□

Statement 3.5. The LW–SW (''long wave–short wave'') model equation (2.13a) and (2.13b) with α *real* and nonvanishing, is *not S-integrable* unless $g_{01}(\tilde{k})$ is *imaginary* and $g_{-1,1}(\tilde{k})$ is *real*,

$$\mathrm{Re}[g_{0,1}(\tilde{k})]=0, \quad \mathrm{Im}[g_{-1,1}(\tilde{k})]=0, \tag{3.5a}$$

and it is *not C-integrable* unless it effectively linearizes,

$$g_{0,1}(\tilde{k})\, g_{-1,1}(\tilde{k}) = 0. \tag{3.5b}$$

Statement 3.6. The system of two coupled NLS equations (2.16a) and (2.16b), is *not S-integrable* unless: either (i) it is *C-integrable*, see below; or (ii) the two *real nonvanishing quantities* α_1, α_2 are equal,

$$\alpha_1 = \alpha_2, \tag{3.6a}$$

and moreover the four quantities λ_{11}, λ_{12}, λ_{21}, λ_{22} are all *real* and are (appropriately) *pairwise equal*, namely

$$\mathrm{Im}(\lambda_{jk}) = 0, \quad j,k = 1,2, \tag{3.6b}$$

$$\lambda_{11} = \lambda_{21}, \quad \lambda_{12} = \lambda_{22}; \tag{3.6c}$$

and this system, (2.16a) and (2.16b), is *not C-integrable* unless it linearizes, namely unless the ''diagonal coupling constants'' $\lambda_{11}, \lambda_{22}$ both vanish,

$$\lambda_{11} = \lambda_{22} = 0, \tag{3.6d}$$

and moreover at least one of the two ''off-diagonal coupling constants'' λ_{12}, λ_{21} also vanishes, namely

$$\lambda_{12} = 0, \tag{3.6e}$$

or

$$\lambda_{21} = 0. \tag{3.6f}$$

□

Before ending this section, let us add a few more words to provide an appropriate context for the six statements proffered above.

Statement 3.1 is, we submit, so firmly embedded in universally accepted lore not to require any elaboration.

Statement 3.2 points out that the nonlinear evolution equation (2.6a) and (2.6b) is generally not integrable. It only becomes integrable if it effectively linearizes, due to the vanishing of λ_1 or λ_2: in the former case, the NLS-type equation (2.6a) becomes indeed linear, and once this has been solved, (2.6b) can be integrated by a quadrature; in the latter case, (2.6b) entails that φ is ξ independent, $\varphi(\xi,\tau) = \varphi(\tau)$, and under this condition (2.6a) becomes essentially the *linear* Schrödinger equation, indeed the term in the right-hand side can then be gotten rid of by introducing the new dependent variable $\tilde{\psi}(\xi,\tau) = \exp[i\lambda_1 \int^{\tau} d\tau'\, \varphi(\tau')]\psi(\xi,\tau)$. Arguments to support this *Statement 3.2* are given in paper I.

Analogous considerations apply to *Statement 3.3*, except for the impossibility, in the case $\mu_2 = 0$ entailing [see (2.9b)] $\chi(\xi,\tau) = \chi(\tau)$, to eliminate altogether the term on the right-hand side of (2.9a) via an appropriate change of dependent variable [but the essentially linear character, in this case, of (2.9a) remains]. Arguments to support this *Statement 3.3* are also given in paper I.

As for *Statement 3.4*, it can be seen as a combination of the two *Statements, 3.2* and *3.3*, that precede it; hence the elaborations given above with respect to those two *Statements, 3.2* and *3.3*, apply as well, to a large extent, to this *Statement 3.4*.

On the other hand, *Statement 3.5* is rather analogous to *Statement 3.1*: the *S-integrability* (provided the relevant coupling constants satisfy appropriate reality conditions) of the LW–SW (long wave–short wave) evolution equation (2.13) is a well-known fact [we believe, but we cannot prove, this was first noted in Ref. 8; see also Ref. 3, where it is shown how this nonlinear evolution equation, (2.13), can be obtained from the *S-integrable, second-order*, Boussinesq equation via a multiscale reduction process altogether analogous to that of paper I]. The fact that

S-integrability evaporates if the coupling constants *fail* to satisfy the relevant reality conditions is, as in the case of the NLS equation, universally accepted lore. Likewise for the *C-integrability* properties, as detailed in *Statement 3.5*.

Finally, some comments on *Statement 3.6*. For the *S-integrability* part we refer, as we did in paper I, to Ref. 9; and for the *C-integrability* part, to the universally accepted notion that, for coupled NLS equations, as indeed for a single NLS equation, *C-integrability* only holds if the equations become essentially *linear* [of course in this case—namely, when (3.6d) holds, as well as either (3.6e) or (3.6f)—the condition (3.6a) is no more necessary].

IV. NECESSARY CONDITIONS OF INTEGRABILITY

In this section we finally attain the core of our paper, namely the presentation of *necessary conditions of integrability* for nonlinear evolution PDEs of type (1.1)–(1.3). The strategy to obtain such results, and their import, have been adequately elaborated in the preceding sections. Hence here we proceed directly to their formulation. The user-friendly character of our presentation is augmented below by a step-by-step guide to the utilization of these findings in order to test whether any given nonlinear evolution PDE, belonging to the class (1.1)–(1.3), might be *integrable*: equations that do *not* pass the test are then guaranteed *not* to be *integrable* (and, more specifically, *not S-integrable* or *not C-integrable*, as the case may be).

But first let us formulate, and justify, these *necessary conditions for integrability*.

Proposition 4.1. *A necessary condition* for the *S-integrability*, respectively, for the *C-integrability*, of a nonlinear evolution PDE of type (1.1)–(1.3) with $h \geqslant 1$ is that, for *all* real values of k such that (2.3) hold, the quantity $\lambda(k)$, see (2.4c), be *real*, see (3.1a), respectively, that it *vanish*, see (3.1b).

□

This *Proposition 4.1* (which is not new[2,3]) follows from *Lemma 2.1* and *Statement 3.1*. The requirement (3.1b) that $\lambda(k)$ vanish for *all* values k entails a very stringent *necessary condition* for *C-integrability* (see examples and corollaries in the following section). The necessary condition (3.1a) for *S-integrability* involves both quantities related to the *linear* and *nonlinear* parts of the original equation (1.1)–(1.3), but in many cases [as can be easily checked; see (2.4c)] it amounts to the requirements that (i) the quantity $g_{01}(k)$ be *real* [note that $g_{-1,1}(k)$ is always *real*, see (2.2c)], if $h=1$; (ii) the quantities $g_{-1,2}(k)$ and $g_{11}(k)$ be *both real* or *both imaginary*; (iii) the quantity $g_{-1,11}(k)$ be *real* if h is *odd*, *imaginary* if h is *even*. Given the arbitrariness of k, the first of these three conditions clearly entails [see (2.2a)] the vanishing of all the coefficients $c^{(2)}_{0n}$ with n odd; the second, either it entails the vanishing of $c^{(2)}_{01}$ and $c^{(2)}_{03}$ (already implied by the first condition), of $c^{(2)}_{12}$, of $c^{(2)}_{14}$ and $c^{(2)}_{23}$ (if one assumes that $c^{(2)}_{05}$ vanishes, as entailed by the first condition) and many other relations for the coefficients $c^{(2)}_{nm}$ with $n+m$ odd, or it entails the vanishing of $c^{(2)}_{00}$, $c^{(2)}_{02}$, $c^{(2)}_{11}$ and many other relations for the coefficients $c^{(2)}_{nm}$ with $n+m$ even (see the Appendix); the third condition, either it entails the vanishing of $c^{(3)}_{001}$ and many other relations for the coefficients $c^{(3)}_{nml}$ with $n+m+l$ odd, or it entails the vanishing of $c^{(3)}_{000}$ and many other relations for the coefficients $c^{(3)}_{nml}$ with $n+m+l$ even. These are very stringent, and quite explicit, conditions on the nonlinear part of (1.1)–(1.3).

Proposition 4.2. *A necessary condition of integrability* for nonlinear evolution PDEs of type (1.1)–(1.3) with $h=0$ is the requirement that, for *all* real values of k such that (2.5) hold, at least one of the two quantities $g_{01}(k)$, $g_{-1,1}(k)$ [see (2.2a) and (2.2c)] vanish [see (3.2) with (2.6c) and (2.6d)].

□

This *Proposition 4.2* follows from *Lemma 2.2* and *Statement 3.2*. It complements the preceding *Proposition 4.1*, since that applies if $h \geqslant 1$, while this *Proposition 4.2* applies if $h=0$. The requirement that $g_{01}(k)$ or $g_{-1,1}(k)$ vanish for *all* (real) values of k entails, via (2.2a) and (2.2c), quite explicit restrictions (only) on the nonlinear part of (1.1)–(1.3). This is made explicit by the following:

Corollary 4.2.1. A *necessary* condition for the *integrability* of a nonlinear evolution PDE of type (1.1)–(1.3) with $h=0$ is that either

$$c_{0,n}^{(2)}=0, \quad n=0,1,2,\ldots, \tag{4.1}$$

or

$$\sum_{j=0}^{n}(-1)^j c_{j,2n-j}^{(2)}=0, \quad n=0,1,2,\ldots, \tag{4.2a}$$

namely

$$c_{0,0}^{(2)}=0, \tag{4.2b}$$

$$c_{0,2}^{(2)}-c_{1,1}^{(2)}=0, \tag{4.2c}$$

$$c_{0,4}^{(2)}-c_{1,3}^{(2)}+c_{2,2}^{(2)}=0, \tag{4.2d}$$

and so on.

□

Clearly the condition (4.1) comes from the requirement that $g_{01}(k)$ vanish, see (2.2a), while (4.2a) comes from the requirement that $g_{-1,1}(k)$ vanish, see (2.2c). Since they concur in the requirement that $c_{0,0}^{(2)}$ vanish, see (4.1) and (4.2b), we obtain the following remarkably neat result:

Corollary 4.2.2. Every nonlinear evolution PDE of type (1.1)–(1.3) (with $h=0$) featuring in its nonlinear part (right-hand side) a term $c_{00}^{(2)}u^2$ is *not integrable*.

□

Let us emphasize the remarkable nature of this finding, that holds irrespective of the specific form of the linear part of the nonlinear (real) PDE (1.1) [provided it is dispersive, see (1.2)] and, even more strikingly, quite independently of the specifics of the nonlinear part [provided it has the form (1.3), with the single requirement that $c_{00}^{(2)}$ not vanish, $c_{00}^{(2)}\neq 0$].

Proposition 4.3. A *necessary condition* for the *integrability* of a nonlinear evolution PDE of type (1.1)–(1.3) with $h\geqslant 1$ is that, for all the real values $\tilde{k}$ (if any) of the parameter k such that (2.7) and (2.8b) hold, at least one of the two quantitities $g_{-1,2}(\tilde{k})$, $g_{11}(\tilde{k})$ [namely, the values that the functions $g_{-1,2}(k)$, $g_{11}(k)$, see (2.2d) and (2.2b), take at $k=\tilde{k}$] vanish:

$$g_{-1,2}(\tilde{k})\,g_{11}(\tilde{k})=0. \tag{4.3}$$

□

This *Proposition 4.3* follows from the first part of *Lemma 2.3* and *Statement 3.3*. Its applicability and potency is of course somewhat reduced relative to *Proposition 4.1* (also applicable for $h\geqslant 1$), due to the requirement to restrict consideration to only those (real) values $\tilde{k}$ of k (if any) which satisfy the *equality* (2.7) [as well as the *inequalities* (2.8b)]. Yet there clearly is a large class of nonlinear evolution PDEs to which this *Proposition 4.3* is applicable (see examples in Sec. V).

Proposition 4.4. A *necessary condition* for the *integrability* of a nonlinear evolution PDE of type (1.1)–(1.3) with $h=0$ is that, for all the real values $\tilde{k}$ (if any) of the parameter k such that (2.7) and (2.10b) hold, at least one of the following four equalities holds [see (2.2a), (2.2b), (2.2d), (2.2c)]:

$$g_{01}(\tilde{k})=g_{11}(\tilde{k})=0, \tag{4.4a}$$

or

$$g_{-1,2}(\tilde{k})=g_{-1,1}(\tilde{k})=0, \tag{4.4b}$$

or

$$g_{01}(\tilde{k})=g_{-1,2}(\tilde{k})=0, \tag{4.4c}$$

or

$$g_{-1,1}(\tilde{k})=g_{11}(\tilde{k})=0. \tag{4.4d}$$

□

This *Proposition 4.4* follows from the second part of *Lemma 2.3* and *Statement 3.4*. It complements the preceding *Proposition 4.3*, since that applies if $h\geqslant 1$, while this *Proposition 4.4* applies if $h=0$. In this case, as well as in the preceding one, the applicability and potency of this *Proposition 4.4* is somewhat reduced relative to *Proposition 4.2* (also applicable for $h=0$), due to the requirement to restrict consideration to only those (real) values $\tilde{k}$ of k (if any) which satisfy the equality (2.7) [as well as the *inequalities* (2.10b)]. Yet in this case as well there is a large class of nonlinear evolution PDEs to which this *Proposition 4.4* is applicable (see examples in the next section).

Proposition 4.5. A necessary condition for the *S-integrability*, respectively, the *C-integrability*, of a nonlinear evolution PDE of type (1.1)–(1.3) with $h=1$ is that, for all the real values $\tilde{k}$ (if any) of the parameter k such that (2.12a) and (2.12b) hold, the quantity $g_{01}(\tilde{k})$ be *imaginary* (or vanish),

$$\mathrm{Re}[g_{01}(\tilde{k})]=0, \tag{4.5a}$$

respectively, at least one of the two quantities $g_{01}(\tilde{k}),g_{-1,1}(\tilde{k})$ vanish,

$$g_{0,1}(\tilde{k})g_{-1,1}(\tilde{k})=0. \tag{4.5b}$$

Here of course $g_{01}(\tilde{k})$, $g_{-1,1}(\tilde{k})$ are the values that $g_{01}(k)$, $g_{-1,1}(k)$ [see (2.2a) and (2.2c)] take at $k=\tilde{k}$.

□

This *Proposition 4.5* follows from *Lemma 2.4* and *Statement 3.5* [note that $g_{-1,1}(\tilde{k})$, as given by (2.2c), is always *real*]. Of course if the nonlinear evolution PDE under consideration passes the test to be *C-integrable* [namely if (4.5b) holds], it automatically also passes the test to be *S-integrable* [even if (4.5a) were not to hold]. This *Proposition 4.5* is analogous to *Propositions 4.3* and *4.4*, and different from *Propositions 4.1* and *4.2*, inasmuch as it requires focussing on special values $\tilde{k}$ of k, identified by the *equality* (2.12a); hence analogous remarks to those made in this respect after *Propositions 4.3* and *4.4* are relevant here (but they will not be repeated).

Proposition 4.6. A necessary condition for the *S-integrability*, respectively, the *C-integrability*, of a nonlinear evolution PDE of type (1.1)–(1.3) with only *cubic*, or higher, nonlinearities [see (2.14)] is that, for all the *real* values $\tilde{k}$ (if any) of the parameter k such that *both equalities* (2.15a), as well as the *inequalities* (2.15b), hold, the conditions (3.6a), (3.6b), and (3.6c) with (2.16c) and (2.16d) be satisfied, respectively the conditions (3.6d) with (2.16d), and at least one of the conditions (3.6e), (3.6f) with (2.16d), be satisfied. Of course the value(s) $\tilde{k}$ of k in the definitions (2.16d) [with (2.2)] must be the same one(s) (if any) that satisfy (2.15a) and (2.15b).

□

This *Proposition 4.6* follows from *Lemma 2.5* and *Statement 3.6*; it holds for *all* (non-negative integer) values of h [see (1.1)]. The applicability of this *Proposition 4.6* is however severely restricted by the requirement that the parameter k satisfy *both equalities* (2.15a); hence this necessary condition of integrability is only applicable to a subclass of nonlinear evolution PDEs of type (1.1)–(1.3), whose linear part, see (1.2), must satisfy a restriction that negates its genericity.

Let us now outline how these findings can be used, providing thereby a friendly guide for customers who are confronted with some given nonlinear evolution PDE of type (1.1)–(1.3) (possibly of applicative origin) and who are interested to find out whether *it might be integrable*. The first step is to write the nonlinear evolution PDE in question in the form (1.1), fixing thereby the value of the non-negative integer h. As noted in the Introduction, it is generally advisable to settle for the largest value of h compatible with the nonlinear evolution PDE under consideration; a clear advantage of this approach is to simplify the set of (nonvanishing) coefficients $c^{(m)}_{j_1 j_2 \cdots j_m}$ that characterize the nonlinear part of the equation, see (1.3). However, the possibility to get additional information by also considering other (smaller) values $\tilde{h}$ of h (with correspondingly redefined coefficients $\tilde{c}^{(m)}_{j_1 j_2 \cdots j_m}$) cannot be altogether excluded.

If $h=0$, the first *necessary condition of integrability* to be tested is provided by *Propositions 4.2* (but see also its two *Corollaries 4.2.1* and *4.2.2*), which can be synthesized by the formula

$$g_{01}(k)\, g_{-1,1}(k) = 0, \tag{4.6}$$

with $g_{01}(k)$, $g_{-1,1}(k)$ defined by (2.2a) and (2.2c) and where k is an *arbitrary (real)* parameter [only restricted by the *inequalities* (2.5) with (2.1a) (2.1b)]. If this test is passed, the next *necessary condition of integrability* comes from *Proposition 4.4*, and it consists of the requirement that (4.4a) or (4.4b) be satisfied, for those real values $\tilde{k}$ of k (if any) for which the *equality* (2.7) [with (2.1c)], as well as the *inequalities* (2.10b) [with (2.1a), (2.1b), (2.1d)] hold. Note that, in spite of the fact that the previous test, (4.6), is required to hold for *all* (real) values of k, this second test associated with *Proposition 4.4*, apparently much less potent because it is required to hold for only a finite set of values $\tilde{k}$ of k, is nevertheless not altogether redundant: there indeed are nonlinear evolution equations which pass the first test but fail the second (see examples in Sec. V).

Finally, if the nonlinear evolution PDE (with $h=0$) under scrutinity has passed both these tests, the last resort is to apply *Proposition 4.6*, which is however only applicable if (2.14) holds. An example in the following section shows that this third test is not redundant, although its applicability and potency are clearly quite limited.

Let us now outline the analogous procedure to test a nonlinear evolution PDE of type (1.1)–(1.3) with $h \geqslant 1$ (rather than $h=0$). In this case the first *necessary condition of integrability* to be tested is provided by *Proposition 4.1*; the second is provided by *Proposition 4.3*; the third (applicable however only if $h=1$) is provided by *Proposition 4.5*; and the fourth by *Proposition 4.6* [applicable only if (2.14) holds]. Note that in this case, $h \geqslant 1$, the possibility is provided from the very beginning to test separately for *S-integrability* and for *C-integrability* (see *Propositions 4.1*, *4.5* and *4.6*).

Two final obvious remarks conclude this section.

Remark 4.1. Let us reemphasize that, as soon as any given nonlinear evolution PDE *fails* to comply with a *necessary condition for integrability*, it can be pronounced *nonintegrable* (or, more specifically, *not S-integrable*, respectively, *not C-integrable*, as the case may be).

□

This information is often quite useful, for instance to terminate the search for integrability techniques applicable to the nonlinear evolution PDE under scrutinity. Of course, if a given nonlinear evolution PDE does comply with a *necessary condition of integrability*, no information is, strictly speaking, gained; although the hunch that it indeed be *integrable* becomes sometimes justified (see examples in Sec. V).

Remark 4.2. All the *necessary conditions of integrability* obtained in this paper only entail the *quadratic* and *cubic* nonlinear terms; in fact *Propositions 4.2, 4.3, 4.4*, and *4.5* refer only to the *quadratic* terms; but their applicability extends to nonlinear evolution PDEs featuring much more general nonlinearities, see (1.1) with (1.3).

□

V. EXAMPLES

In this section we display various examples; some of the results written below in fact qualify as *Corollaries* of the *Propositions* of the preceding section, although we do not denote them as such.

Example 5.1. Consider the class of nonlinear evolution PDEs (1.1)–(1.3) with $h=0$ and with $F^{(2)}$ given by (1.4) (no limitation on $F^{(m)}$ with $m>2$). Then *Proposition 4.2* (or, more directly, *Corollaries 4.2.2* and *4.2.1*) yield the following *necessary conditions of S-integrability*:

$$c_{00}^{(2)}=0, \tag{5.1a}$$

and in addition at least one of the following two couples of equalities:

$$c_{01}^{(2)}=0,\ c_{02}^{(2)}=0, \tag{5.1b}$$

or

$$c_{22}^{(2)}=0,\ \ c_{02}^{(2)}=c_{11}^{(2)}\,. \tag{5.1c}$$

If moreover $M=2$ [see (1.2)] and the two coefficients a_3 and a_5 do not vanish and have different signs,

$$a_3\,a_5<0, \tag{5.2}$$

Proposition 4.4, together with *Proposition 4.2*, yield the following (of course more stringent) *necessary conditions of integrability*:

$$c_{00}^{(2)}=0,\quad c_{01}^{(2)}=0,\quad c_{02}^{(2)}=0,\quad c_{12}^{(2)}=0, \tag{5.3a}$$

and in addition at least one of the following three equalities:

$$c_{11}^{(2)}=0,\ \ c_{22}^{(2)}=0, \tag{5.3b}$$

or

$$5a_5c_{11}^{(2)}+a_3c_{22}^{(2)}=0, \tag{5.3c}$$

or

$$5a_5c_{11}^{(2)}-2a_3c_{22}^{(2)}=0; \tag{5.3d}$$

or, in alternative to (5.3a),

$$c_{00}^{(2)}=0,\quad c_{02}^{(2)}=0,\quad c_{11}^{(2)}=0,\quad c_{22}^{(2)}=0, \tag{5.4a}$$

and in addition at least one of the following three equalities:

$$c_{01}^{(2)}=0,\quad c_{12}^{(2)}=0, \tag{5.4b}$$

or

$$5a_5c_{01}^{(2)}-2a_3c_{12}^{(2)}=0, \tag{5.4c}$$

or

$$5a_5c_{01}^{(2)}+a_3c_{12}^{(2)}=0. \tag{5.4d}$$

□

The derivation of these results [via (A11)] is straightforward if tedious; they illustrate the explicit potency of (some of) the *necessary conditions of integrability* given in Sec. IV.

Example 5.2. Consider the class of nonlinear evolution PDEs (1.1)–(1.3) with $M=1$ [and of course $a_3 \neq 0$, see (1.2)], $h=1$, $F^{(2)}$ given by (1.4), and $F^{(3)}=0$ (no limitation on $F^{(m)}$ with $m>3$). Then *Proposition 4.1* entails the following *necessary conditions of S-integrability*:

$$c_{01}^{(2)}=0, \quad c_{12}^{(2)}=0, \tag{5.5a}$$

or

$$c_{01}^{(2)}=0, \quad c_{22}^{(2)}=0, \quad c_{02}^{(2)}=2c_{11}^{(2)}, \tag{5.5b}$$

or

$$c_{00}^{(2)}=0, \quad c_{12}^{(2)}=0, \quad c_{22}^{(2)}=0, \quad c_{11}^{(2)}=4c_{02}^{(2)}, \tag{5.5c}$$

or

$$c_{00}^{(2)}=0, \quad c_{02}^{(2)}=0, \quad c_{11}^{(2)}=0, \quad c_{22}^{(2)}=0, \tag{5.5d}$$

as well as the following (of course more stringent) *necessary conditions of C-integrability*:

$$c_{00}^{(2)}=0, \quad c_{01}^{(2)}=0, \quad c_{12}^{(2)}=0, \tag{5.6a}$$

and in addition

$$c_{02}^{(2)}=0, \quad c_{11}^{(2)}=0, \tag{5.6b}$$

or

$$c_{22}^{(2)}=0, \quad 3[c_{02}^{(2)}]^2+3c_{02}^{(2)}c_{11}^{(2)}-4[c_{11}^{(2)}]^2=0. \tag{5.6c}$$

□

The derivation of these results via (A11) is again both straightforward and tedious: note that they only involve, in a quite simple and explicit manner, the coefficients $c_{j_1 j_2}^{(2)}$ of the *quadratic* term (1.4). This is a consequence of the, quite simple, assumed nature ($M=1$!) of the linear operator D, see (1.2). For this same reason the results of no *Proposition* of Sec. IV (other than *Proposition 4.1*) are applicable to this class of nonlinear evolution PDE.

Example 5.3. Consider the class of nonlinear evolution PDEs (1.1)–(1.3) with $h \geqslant 1$, $F^{(2)}=0, F^{(3)}$ given by (1.5) (no limitation on $F^{(m)}$ with $m>3$). Then *Proposition 4.1* yields the following *necessary conditions of S-integrability*: if h is *even*,

$$c_{000}^{(3)}=0, \quad c_{011}^{(3)}=3c_{002}^{(3)}, \quad c_{112}^{(3)}=3c_{022}^{(3)}; \tag{5.7a}$$

if h is *odd*,

$$c_{001}^{(3)}=0, \quad c_{012}^{(3)}=3c_{111}^{(3)}, \quad c_{122}^{(3)}=0. \tag{5.7b}$$

Likewise, the *necessary conditions of C-integrability* yielded by *Proposition 4.1* require the simultaneous validity of (5.7a) and (5.7b) (irrespective of the parity of h).

□

These results follow straightforwardly from (2.4c) via (A12). Let us again emphasize the simple and explicit nature of these conditions, (5.7a) and (5.7b), as well as their independence from the *linear part* of (1.1)–(1.3), see (1.2) (the assumption $M \geqslant 1$, with $a_{2M+1} \neq 0$, is of course essential). Note that the well-known *S-integrable* modified KdV equation (characterized by M

$=1, h=1, c^{(3)}_{000}\neq 0$ and all other coefficients $c^{m}_{j_1 j_2 \ldots j_m}$ vanishing) passes the test of *S-integrability* [see (5.7b)], but not that of *C-integrability* [see (5.7a)]; while the *C-integrable* nonlinear PDE[10]

$$u_t - u_{xxx} = 3u^2 u_{xx} + 9u u_x^2 + 3u^4 u_x, \tag{5.7c}$$

with $c^{(3)}_{002}=3, c^{(3)}_{011}=9$ and all other coefficients $c^{(3)}_{j_1 j_2 j_3}$ vanishing, does indeed pass the *C-integrability* test, namely it complies with *both* (5.7a) and (5.7b).

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APPENDIX

In this Appendix we discuss some points whose detailed treatment in the body of the paper would have been too distracting.

Let us first detail the implication of the condition that, for *all* real values of k, $g_{-1,2}(k)$ and $g_{11}(k)$ be (i) both real or (ii) both immaginary. In case (i) we get from (2.2d) and (2.2b) the conditions

$$\sum_{j=0}^{n} (-1)^j (2^{2n+1-j} - 2^j)\, c^{(2)}_{j,\,2n+1-j} = 0, \tag{A1a}$$

$$\sum_{j=0}^{n} c^{(2)}_{j,\,2n+1-j} = 0, \tag{A1b}$$

which are required to hold for all non-negative integer values of n. Hence by setting $n=0,1,2,\ldots$, we get

$$c^{(2)}_{0,1} = 0, \tag{A2a}$$

$$7c^{(2)}_{0,3} - 2c^{(2)}_{1,2} = c^{(2)}_{0,3} + c^{(2)}_{1,2} = 0, \tag{A2b}$$

$$31c^{(2)}_{0,5} - 14c^{(2)}_{1,4} + 4c^{(2)}_{2,3} = c^{(2)}_{0,5} + c^{(2)}_{1,4} + c^{(2)}_{2,3} = 0, \tag{A2c}$$

and so on. Clearly (A2b) entails

$$c^{(2)}_{0,3} = c^{(2)}_{1,2} = 0, \tag{A3}$$

and (A2c) entails

$$c^{(2)}_{1,4} = \tfrac{3}{2} c^{(2)}_{0,5}, \quad c^{(2)}_{2,3} = -\tfrac{5}{2} c^{(2)}_{0,5}. \tag{A4}$$

In case (ii) (2.2d) and (2.2b) yield the conditions

$$\sum_{j=0}^{n} (-1)^j (2^{2n-j} + 2^j) c^{(2)}_{j,2n-j} = 0, \tag{A5a}$$

$$\sum_{j=0}^{n} c^{(2)}_{j,2n-j}=0, \tag{A5b}$$

which are again required to hold for all non-negative integer values of n. Hence by setting $n=0,1,2,\ldots$, we get

$$c^{(2)}_{00}=0, \tag{A6a}$$

$$5c^{(2)}_{02}-4c^{(2)}_{11}=c^{(2)}_{02}+c^{(2)}_{11}=0, \tag{A6b}$$

$$17c^{(2)}_{04}-10c^{(2)}_{13}+8c^{(2)}_{22}=c^{(2)}_{04}+c^{(2)}_{13}+c^{(2)}_{22}=0, \tag{A6c}$$

and so on. Clearly (A6b) entail $c^{(2)}_{02}=c^{(2)}_{11}=0$.

Next let us detail the implication of the condition that $g_{-1,1,1}(k)$ be, for all (real) values of k, either *real* or *imaginary*. The first condition entails [see (2.2e)] the relations

$$\sum_{j=0}^{[(4n+2)/3]} \sum_{j'=\mathrm{Max}[0,2j-2n-1]}^{[j/2]} [(-1)^{j'}-(-1)^{j}+(-1)^{j+j'}]\, c^{(3)}_{j',j-j',2n+1-j}=0, \tag{A7}$$

which are again required to hold for all non-negative integer values of n. Hence

$$c^{(3)}_{001}=0, \tag{A8a}$$

$$c^{(3)}_{003}+c^{(3)}_{012}-3c^{(3)}_{111}=0, \tag{A8b}$$

and so on. Likewise the second condition entails [see (2.2e)]

$$\sum_{j=0}^{[4n/3]} \sum_{j'=0}^{[j/2]} [(-1)^{j'}+(-1)^{j}+(-1)^{j+j'}]\, c^{(3)}_{j',j-j',2n-j}=0, \tag{A9}$$

again for all non-negative integer values of n. Hence

$$c^{(3)}_{000}=0, \tag{A10a}$$

$$3c^{(3)}_{002}-c^{(3)}_{011}=0, \tag{A10b}$$

and so on.

We end this Appendix by displaying the explicit form taken by the four quantities $g_{01}(k)$, $g_{11}(k)$, $g_{-1,1}(k)$, $g_{-1,2}(k)$ if $c^{(2)}_{j_1j_2}$ vanishes for $j_2>2$, namely if $F^{(2)}$ has the form (1.4):

$$g_{01}(k)=2c^{(2)}_{00}-k^2c^{(2)}_{02}+ikc^{(2)}_{01}, \tag{A11a}$$

$$g_{11}(k)=c^{(2)}_{00}-k^2(c^{(2)}_{02}+c^{(2)}_{11})+k^4c^{(2)}_{22}+ik(c^{(2)}_{01}-k^2c^{(2)}_{12}), \tag{A11b}$$

$$g_{-1,1}(k)=2[c^{(2)}_{00}-k^2(c^{(2)}_{02}-c^{(2)}_{11})+k^4c^{(2)}_{22}], \tag{A11c}$$

$$g_{-1,2}(k)=2c^{(2)}_{00}-k^2(5c^{(2)}_{02}-4c^{(2)}_{11})+8k^4c^{(2)}_{22}+ik(c^{(2)}_{01}+2k^2c^{(2)}_{12}); \tag{A11d}$$

and the explicit form taken by the quantity $g_{-n,n,n}(k)$ if $c^{(3)}_{j_1j_2j_3}$ vanishes for $j_3>2$, namely if $F^{(3)}$ has the form (1.5):

$$\begin{aligned} g_{-n,n,n}(k)=&\,3c^{(3)}_{000}-(nk)^2(3c^{(3)}_{002}-c^{(3)}_{011})+(nk)^4(3c^{(3)}_{022}-c^{(3)}_{112}) \\ &+ink[c^{(3)}_{001}-(nk)^2(c^{(3)}_{012}-3c^{(3)}_{111})+(nk)^4c^{(3)}_{122}]. \end{aligned} \tag{A12}$$

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RTT relations, a modified braid equation and noncommutative planes

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With the known group relations for the elements (a,b,c,d) of a quantum matrix T as input a general solution of the RTT relations is sought without imposing the Yang–Baxter (YB) constraint for R or the braid equation for $\hat{R}=PR$. For three biparametric deformatios, $\mathrm{GL}_{(p,q)}(2)$, $\mathrm{GL}_{(g,h)}(2)$, and $\mathrm{GL}_{(q,h)}(1/1)$, the standard, the nonstandard, and the hybrid one, respectively, R or $\hat{R}$ is found to depend, apart from the two parameters defining the deformation in question, on an extra free parameter K, such that $\hat{R}_{(12)}\hat{R}_{(23)}\hat{R}_{(12)}-\hat{R}_{(23)}\hat{R}_{(12)}\hat{R}_{(23)}=[(K/K_1)-1][(K/K_2)-1](\hat{R}_{(23)}-\hat{R}_{(12)})$ with $(K_1,K_2)=(1,p/q),(1,1)$, and $(1,1/q)$, respectively. Only for $K=K_1$ or $K=K_2$ one has the braid equation. Arbitray K corresponds to a class (conserving the group relations independent of K) of the MQYBE or modified quantum YB equations studied by Gerstenhaber, Giaquinto, and Schack. Various properties of the triparametric $\hat{R}(K;p,q)$, $\hat{R}(K;g,h)$, and $\hat{R}(K;q,h)$ are studied. In the larger space of the modified braid equation (MBE) even $\hat{R}(K;p,q)$ can satisfy $\hat{R}^2=1$ outside the braid equation (BE) subspace. A generalized, K-dependent, Hecke condition is satisfied by each three-parameter $\hat{R}$. The role of K in noncommutative geometries of the $(K;p,q)$, $(K;g,h)$, and $(K;q,h)$ deformed planes is studied. K is found to introduce a ''soft symmetry breaking,'' preserving most interesting properties and leading to new interesting ones. Further aspects to be explored are indicated. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Our starting point will be the group relations of the elements of the quantum matrix

$$T=\begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{1.1}$$

Three known cases will be considered.

(1) The biparametric (p,q) or standard deformation of GL(2).
(2) The biparametric (g,h) or nonstandard deformation of Gl(2).
(3) The (q,h) or ''hybrid'' deformation of GL(1/1).

Each set will be presented explicitly below. These three have been studied in Ref. 1 where many original sources can be found. We start directly with the biparametric cases since the one-parameter deformations can then be systematically obtained through suitable constraints ($p=q^{-1}, g=h$ and so on).

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For the given group relations we construct for each case the matrix R satisfying

$$RT_1T_2=T_2T_1R, \tag{1.2}$$

where

$$T_1=T\otimes I_2, \quad T_2=I_2\otimes T.$$

To start with, we do not require R to satisfy the Yang–Baxter (YB) equation. It will be found that, apart from the parameters concerned $[(p,q),\ (g,h)$ or $(q,h)]$ the solution for R satisfying (2) contains a supplementary arbitrary parameter K. Two particular values of K (say K_1 and K_2) will give the two solutions of YB related through

$$((21)R(K_1))^{-1}=R(K_2) \tag{1.3}$$

both satisfying

$$R_{12}R_{13}R_{23}-R_{23}R_{13}R_{12}=0.$$

The existence of such a pair of solutions is assured by the fact that (1.2) can be written as

$$T_1T_2R^{-1}=R^{-1}T_2T_1.$$

The germ of our paper is in the question: what structure is obtained when K is not restricted to the values K_1 and K_2.

For arbitrary K the situation is best expressed in terms of

$$\hat{R}=PR,$$

where P is the permutation matrix and for our 4×4 case it permutes the second and third rows.

One obtains, for the normalizations we will choose,

$$\hat{R}_{(12)}\hat{R}_{(23)}\hat{R}_{(12)}-\hat{R}_{(23)}\hat{R}_{(12)}\hat{R}_{(23)}=\left(\frac{K}{K_1}-1\right)\left(\frac{K}{K_2}-1\right)(\hat{R}_{(23)}-\hat{R}_{(12)}). \tag{1.4}$$

This is our modified braid equation (MBE). (See Discussion for further comments.)

In terms of R one obtains

$$R_{12}R_{13}R_{23}-R_{23}R_{13}R_{12}=\left(\frac{K}{K_1}-1\right)\left(\frac{K}{K_2}-1\right)((123)R_{(12)}-(213)R_{(23)}), \tag{1.5}$$

where (123) and (213) denote corresponding permutations of the tensor factors of $V^{\otimes}3$ (R acting on $V\otimes V$). [Having pointed out the structure (1.5) we will use throughout (1.4) as our fundamental relation.]

Thus (1.2) by itself is seen to lead to a particular class of solutions of the ''modified quantum Yang–Baxter equations'' (MQYBE) introduced by Gerstenhaber *et al.*[2] Our (1.4) has the same structure as Eq. (2.4) of Ref. 3 for ''quantum transpositions'' $(\sigma_{12},\sigma_{23})$ defined by the authors, though we do not impose in general their ''unitarity'' leading to

$$\hat{R}^2=I.$$

An example of a solution of (1.2) with an arbitrary K can be found in Ref. 1.

We present below some particularly interesting explicit examples. Their properties will reveal that the existence of such a class of more general solutions of MBE is more than an accident and can play a significant role in various domains, such as noncommutative geometry.

II. EXPLICIT SOLUTIONS

A. Standard (p,q) deformation of GL(2)

The elements (a,b,c,d) of T satisfy

$$\begin{gathered} ab=qba, \quad pac=ca, \\ ad=da+(q-p)bc, \quad pqbc=cb, \\ pbd=db, \quad cd=qdc. \end{gathered} \tag{2.1}$$

Apart from a possible normalizing factor, the solution of (1.2) turns out to be (writing directly $\hat{R}=PR$ and assuming p to be nonzero)

$$\hat{R}(K;p,q)=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & (1-K) & \dfrac{K}{p} & 0 \\ 0 & Kq & \left(1-\dfrac{Kq}{p}\right) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2.2}$$

This is found to satisfy

$$\hat{R}_{(12)}\hat{R}_{(23)}\hat{R}_{(12)}-\hat{R}_{(23)}\hat{R}_{(12)}\hat{R}_{(23)}=(K-1)\left(\frac{Kq}{p}-1\right)(\hat{R}_{(23)}-\hat{R}_{(12)}) \tag{2.3}$$

with

$$K_1=1, \quad K_2=\frac{p}{q}.$$

B. Nonstandard (g,h) deformation of GL(2)

The group relations are

$$\begin{gathered} ca=ac-gc^2, \quad cb=bc-gdc-hac+ghc^2, \\ cd=dc-hc^2, \quad da=ad-gdc+hac, \\ db=bd+g(ad-bc+hac-d^2), \\ ba=ab-h(ad-bc+hac-a^2). \end{gathered} \tag{2.4}$$

From (1.2) one obtains

$$\hat{R}(K;g,h)=\begin{pmatrix} 1 & -hK & hK & ghK \\ 0 & (1-K) & K & gK \\ 0 & K & (1-K) & -gK \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2.5}$$

This is found to satisfy

$$\hat{R}_{(12)}\hat{R}_{(23)}\hat{R}_{(12)}-\hat{R}_{(23)}\hat{R}_{(12)}\hat{R}_{(23)}=(K-1)^2(\hat{R}_{(23)}-\hat{R}_{(12)}) \tag{2.6}$$

with, independently of (g,h),

$$K_1=K_2=1.$$

C. Hybrid (q,h) deformation of G(1/1)

The group relations are

$$\begin{gathered} ba=ab+hcd, \quad ac=qca, \quad bc=qcb, \\ dc+qcd=0, \quad ad-da+(1-q)cb=0, \\ bd+db=hca, \quad ha^2=hd^2+(q+1)b^2, \quad c^2=0. \end{gathered} \tag{2.7}$$

One obtains from (1.2)

$$\hat{R}(K;q,h)=\begin{pmatrix} 1 & 0 & O & Kh \\ 0 & (1-K) & Kq & 0 \\ 0 & K & (1-Kq) & 0 \\ 0 & 0 & 0 & (1-K(q+1)) \end{pmatrix}. \tag{2.8}$$

This satisfies

$$\hat{R}_{(12)}\hat{R}_{(23)}\hat{R}_{(12)}-\hat{R}_{(23)}\hat{R}_{(12)}\hat{R}_{(23)}=(K-1)(Kq-1)(\hat{R}_{(23)}-\hat{R}_{(12)}). \tag{2.9}$$

Here $K_1=1, K_2=q^{-1}$, both being independent of h.

III. PROPERTIES

A. K and triangularity

The matrix R is called ''triangular'' if

$$(21)R=R^{-1}$$

when

$$\hat{R}^2=(PR)^2=I.$$

In Ref. 2 the term ''unitary'' is used in this context. For an R matrix satisfying the Yang–Baxter constraint, the following features are well known.

(1) For standard [q or (p,q)] deformations the R satisfying YB is ''quasitriangular'' and

$$\hat{R}^2\neq I.$$

(2) For nonstandard [h or (g,h)] deformations for R satisfying YB one has ''triangularity'' or

$$\hat{R}^2=I.$$

(It is in this sense that we use the term triangular, without R being necessarily strictly upper or lower triangular.)

In the presence of an arbitrary K the modified braid equation (MBE) breaks this dichotomy. Specifically in the preceding three cases one has the following situation:

$$(21)R(K;p,q)=(R(K';p,q))^{-1}, \tag{3.1}$$

where

$$K'=K(K(1+qp^{-1})-1)^{-1},$$
$$(21)R(K;g,h)=(R(K';g,h))^{-1}, \tag{3.2}$$

where

$$K'=K(2K-1)^{-1},$$
$$(21)R(K;q,h)=(R(K';q,h))^{-1}, \tag{3.3}$$

where

$$K'=K(K(1+q)-1)^{-1}.$$

Thus in each case one obtains

$$K'=K\left(\frac{K}{K_1}+\frac{K}{K_2}-1\right)^{-1}. \tag{3.4}$$

In general none is triangular (or unitary). On the other hand, in each case one can have triangularity by choosing

$$K'=K$$

or

$$K=2K_1K_2(K_1+K_2)^{-1}. \tag{3.5}$$

For the three previous cases this gives, respectively,

$$K=2p(p+q)^{-1}, \quad 1, \quad 2(1+q)^{-1}. \tag{3.6}$$

Thus for the nonstandard case triangularity coincides with the YB property. In contrast, for the other two cases triangularity implies a nonzero right-hand side in (1.4). In particular for the (p,q) case one obtains (permuting the second and the third rows of $\hat{R}$) for

$$K=2p(p+q)^{-1},$$
$$R=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{2pq}{p+q} & \frac{p-q}{p+q} & 0 \\ 0 & \frac{q-p}{p+q} & \frac{2}{p+q} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.7}$$

Now one has

$$R(K;p,q)=((21)M)^{-1}M,$$

where one can set, choosing an upper triangular form,

$$M=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & (2pq/p+q)^{1/2} & \dfrac{p-q}{(2pq(p+q))^{1/2}} & 0 \\ 0 & 0 & (p+q/2pq)^{1/2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{3.8}$$

R is invariant under

$$M\rightarrow VM,$$

where

$$(21)V=V.$$

B. Projectors

For each case $((K;p,q),(K;g,h),(K;q,h))$ one obtains, I being the 4×4 unit matrix,

$$\hat{R}^2=X\hat{R}+(1-X)I, \quad X=2-\left(\frac{K}{K_1}+\frac{K}{K_2}\right). \tag{3.9}$$

Thus for the three cases $((p,q),(g,h),(q,h))$ one has, respectively,

$$X=2-K(1+qp^{-1}), \quad X=2(1-K), \quad X=2-K(1+q). \tag{3.10}$$

Two special cases are

$$X=0, \quad (\hat{R})^2=I$$

and

$$X=2, \quad (\hat{R}-I)^2=0.$$

For $X\neq 2$ one obtains for each deformation considered two projectors $(P^2=P)$ as follows:

$$P_1=\frac{(\hat{R}-I)}{(X-2)}, \tag{3.11}$$

$$P_2=\frac{(\hat{R}-(X-1)I)}{(2-X)}. \tag{3.12}$$

Finally one has

$$\hat{R}=(X-1)P_1+P_2 \tag{3.13}$$

with

$$P_1+P_2=I, \quad P_1P_2=0.$$

Note that one obtains a canonical formalism valid for all the deformations considered.

It follows from the preceding results that if C is a column vector (with 4 rows) a constraint (n being a constant)

$$C=n\hat{R}C$$

is only consistent for

$$n=1 \quad (P_1C=0,\ C=P_2C)$$

or

$$n=(X-1)^{-1} \quad (P_2C=0,\ C=P_1C).$$

This fact should be kept in mind for what follows.

IV. *K* AND NONCOMMUTATIVE PLANES

Detailed study of noncommutativity implemented via $\hat{R}$ in the plane and higher dimensional spaces can be found in Refs. 4, 5, and 6 where numerous sources are cited. Here we limit our considerations to the two dimensional plane. But we let our $\hat{R}$ be more general by letting it depend on an extra arbitrary parameter K permitted by our MBE. Our $\hat{R}$ will depend on three parameters. The biparametric nonstandard deformation with differential calculus was first presented (for $K=1, g=h, h=h'$) in Ref. 7. The original formalism is due to Wess and Zumino.[8]

We use the following notations:

$$x^i=(x^1,x^2)=(x,y),$$

$$dx^i=\xi^i=(\xi^1,\xi^2)=(\xi,\eta),$$

$$(\alpha,\beta)=(p,q),(g,h),(q,h).$$

We postulate

$$x^ix^j=(\hat{R}(K;\alpha,\beta))^{ij}_{i'j'}x^{i'}x^{j'}, \tag{4.1}$$

i.e.,

$$(P_1)^{(ij)}_{i'j'}x^{i'}x^{j'}=0,$$

$$\xi^i\xi^j=-\frac{1}{(1-X)}(\hat{R}(K;\alpha,\beta))^{(ij)}_{i',j'}\xi^{i'}\xi^{j'}, \tag{4.2}$$

i.e.,

$$(P_2)^{(ij)}_{i',j'}\xi^{i'}\xi^{j'}=0,$$

$$x^i\xi^j=\frac{1}{(1-X)}(\hat{R}(K;\alpha,\beta))^{(ij)}_{i',j'}\xi^{i'}x^{j'}, \tag{4.3}$$

where

$$(1-X)=\left(\frac{K}{K_1}+\frac{K}{K_2}-1\right).$$

The bilinear constraints (4.1), (4.2), (4.3), related through derivations, are required to satisfy suitable consistency relations. (See, for example, Sec. 4 of Ref. 4 and Ref. 7.) Following the usual procedure the required consistency for our case can be shown to be assured precisely by our generalized Hecke condition, namely,

$$(\hat{R}(K;\alpha,\beta)-I)\left(\frac{\hat{R}(K;\alpha,\beta)}{(1-X)}+I\right)=0 \tag{4.4}$$

or

$$P_1P_2=0.$$

This generalizes some well-known results. Thus, for example, setting

$$p=q^{-1},\quad K_1=1,\quad K=K_2=q^{-2}$$

and changing the normalization of R by a factor q one obtains the result (4.4.15) of Ref. 4. One obtains analogous generalizations for the other cases. Note that the consistency is obtained for our case by by implementing K nontrivially through the factor $(1-X)$ for the (ξ,η) constraints. But once this is done the final consequences of (4.1) and (4.2) turn out to be systematically independent of K. [Those of (4.3) do involve K but, as will be shown below, in a particularly simple fashion.] We recapitulate for completeness the first two sets of results which are the same as one would obtain with $K=(K_1,K_2)$.

One obtains for $(\alpha,\beta)=(p,q)$

$$pxy=yx, \tag{4.5}$$

$$\xi^2=0,\quad \eta^2=0,\quad \eta\xi+q\xi\eta=0. \tag{4.6}$$

For $(\alpha,\beta)=(g,h)$

$$xy-yx=gy^2, \tag{4.7}$$

$$\xi^2=h\xi\eta,\quad \eta^2=0,\quad \eta\xi+\xi\eta=0. \tag{4.8}$$

The results above are for GL(2). For GL(1/1), namely for

$$(\alpha,\beta)=(q,h)$$

one obtains

$$xy=qyx,\quad y^2=0, \tag{4.9}$$

$$(1+q)\xi^2+h\eta^2=0,\quad \eta\xi+\xi\eta=0. \tag{4.10}$$

For the deformed GL(1/1) y becomes fermionic. [After exhibiting as above how the three cases can be treated uniformly in our formalism, in what follows we will consider only the deformations $(K;p,q)$ and $(K;g,h)$ of GL(2). Those for GL(1/1) can easily be added.]

In contrast to the foregoing results, the consequences of (4.3) involve K nontrivially. For $\hat{R}(K;p,q)$ one obtains

$$x\xi=\frac{1}{(1-X)}\xi x,\quad x\eta=\frac{1}{(1-X)}\left(\xi y+\frac{K}{p}\Phi_1\right),$$

$$y\xi=\frac{1}{(1-X)}\left(\eta x-\frac{Kq}{p}\Phi_1\right),\quad y\eta=\frac{1}{(1-X)}\eta y \tag{4.11}$$

with

$$\Phi_1=(\eta x-p\xi y). \tag{4.12}$$

For $p=q^{-1}$, $K=q^{-2}$ and again suitably choosing the normalization of $\hat{R}$ these results reduce to (4.1.8) of Ref. 4. In order to compare with κ of (4.1.10) of Ref. 4 one can show by reordering terms

$$\Phi_1^2=\frac{1}{(1-X)}(-qp+Kqp+p^2-Kqp+pq-p^2)(\xi\eta xy)=0. \tag{4.13}$$

Note that K reappears on reordering but the coefficient of K in the numerator vanishes separately. Thus, apart from the overall factor, K appears as a factor of the nilpotent Φ_1. Moreover one can show that

$$\begin{gathered} px\Phi_1=\frac{1}{(1-X)}K\Phi_1 x, \quad y\Phi_1=\frac{1}{(1-X)}Kq\Phi_1 y, \\ \frac{1}{(1-X)}(p+q-Kq)\xi\Phi_1=-\Phi_1\xi, \quad \frac{1}{(1-X)}(p+q-Kq)\eta\Phi_1=-pq\Phi_1\eta. \end{gathered} \tag{4.14}$$

For the prescriptions indicated before ($K=q^{-2}$ and so on) one finds back the corresponding results of Sec. 4.1.13 and Sec. 4.1.17 of Ref. 4.

For $\hat{R}(K;g,h)$ one obtains [compare (3.1.6) of Ref. 5 where $K=1$ and $g=h$]

$$\begin{gathered} x\xi=\frac{1}{(1-X)}(\xi x+Kh\Phi_2), \quad x\eta=\frac{1}{(1-X)}(\xi y+K\Phi_2), \\ y\xi=\frac{1}{(1-X)}(\eta x-K\Phi_2), \quad y\eta=\frac{1}{(1-X)}\eta y \end{gathered} \tag{4.15}$$

with

$$\Phi_2=(\eta x-\xi y+g\eta y) \tag{4.16}$$

and

$$\Phi_2^2=0. \tag{4.17}$$

Moreover,

$$\begin{gathered} x\Phi_2=\frac{1}{(1-X)}(K\Phi_2 x+K(g-h)\Phi_2 y), \quad y\Phi_2=\frac{1}{(1-X)}Kq\Phi_2 y, \\ \frac{1}{(1-X)}(2-K)\xi\Phi_2=-(\Phi_2\xi+(h-g)\Phi_2\eta), \quad \frac{1}{(1-X)}(2-K)\eta\Phi_2=-\Phi_2\eta. \end{gathered} \tag{4.18}$$

The results for the (g,h) case can of course be obtained independently. But they are obtained more efficiently and with a deeper understanding by starting from the corresponding ones for (p,q) and using the ''contraction'' studied in the following section. It is instructive to see, in particular, how the $(g-h)$ factors in the results above arise (end of the next section). These terms are present even for the YB subspace ($K=1$) unless $g=h$. Finally, for $K=1$ and $g=h$ one obtains the simple results of Sec. 4.1.17 of Ref. 4.

V. $((K;p,q)\rightarrow(K;g,h))$: SINGULAR LIMIT OF A TRANSFORMATION

In Sec. 4 of Ref. 1 such a passage was presented for the case where $R(p,q)$ and $R(g,h)$ both satisfied YBE. Here we generalize it to include an arbitrary K. In fact the same transformation will

work again, leading to a well defined $R(K;g,h)$. We want to emphasize this fact. It underlines again the ''soft symmetry breaking'' role of K. Moreover we will display here how the corresponding features of the two noncommutative plains are related systematically through this ''contraction''procedure. The $(K;g,h)$-deformed plane emerges in full detail from the $(K;p,q)$ deformed one. Some previous sources are cited in Ref. 1, which in turn lead to some original ones.

Setting

$$G=\begin{pmatrix} 1 & \omega \\ 0 & 1 \end{pmatrix} \tag{5.1}$$

and with $R=P\hat{R}$ one obtains

$$(G^{-1}\otimes G^{-1})R(K;p,q)(G\otimes G)=\begin{pmatrix} 1 & -K(q-1)\omega & \frac{K}{p}(q-1)\omega & -\frac{K}{p}(p-1)(q-1)\omega^2 \\ 0 & Kq & \left(1-K\frac{q}{p}\right) & K\frac{q}{p}(p-1)\omega \\ 0 & (1-K) & \frac{K}{p} & \frac{K}{p}(p-1)\omega \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5.2}$$

Now, as in Ref. 1, let $p\to 1, q\to 1$ in such a way that $(p-1)(q-1)^{-1}$ remains constant. And ω_0 being a constant, define

$$\omega=\omega_0((p-1)(q-1))^{-1/2}.$$

Now one can define finite constants (g,h) such that as $p\to 1$ and $q\to 1$

$$((1-p)\omega)\to g, \quad ((q-1)\omega)\to h. \tag{5.3}$$

Now from (2.5) and (5.2) (with $R=P\hat{R}$), one obtains

$$(G^{-1}\otimes G^{-1})R(K;p,q)(G\otimes G)\to R(K;g,h). \tag{5.4}$$

The same procedure works for (a,b,c,d), (x,y), and (ξ,η). In this section, to distinguish the cases (p,q) and (g,h), we will use for the latter the notations

$$(\tilde{a},\tilde{b},\tilde{c},\tilde{d});(\tilde{x},\tilde{y});(\tilde{\xi},\tilde{\eta}).$$

Consistently with transformation of R one defines (with the previous definitions of G and T)

$$G^{-1}TG=\begin{pmatrix} \tilde{a} & \tilde{b} \\ \tilde{c} & \tilde{d} \end{pmatrix}, \quad G^{-1}\begin{pmatrix} x \\ y \end{pmatrix}=\begin{pmatrix} \tilde{x} \\ \tilde{y} \end{pmatrix}, \quad G^{-1}\begin{pmatrix} \xi \\ \eta \end{pmatrix}=\begin{pmatrix} \tilde{\xi} \\ \tilde{\eta} \end{pmatrix}.$$

Let us now consider some examples to appreciate how the technique works. From the preceding definitions one obtains

$$\tilde{a}=a-\omega c, \quad \tilde{b}=(b-\omega d)+\omega(a-\omega c), \quad \tilde{c}=c, \quad \tilde{d}=d+\omega c. \tag{5.5}$$

The inverse relations are easily obtained. Using them and the group relations for (a,b,c,d) one obtains

$$\tilde{c}\tilde{a}=c(a-\omega c)=pac-\omega c^2=p(\tilde{a}+\omega\tilde{c})\tilde{c}-\omega\tilde{c}^2=p\tilde{a}\tilde{c}-(1-p)\omega\tilde{c}^2.$$

Using the definition of g now one obtains, in the limit,

$$\tilde{c}\tilde{a}=\tilde{a}\tilde{c}-g\tilde{c}^2. \tag{5.6}$$

Again,

$$\begin{aligned}\tilde{c}\tilde{b}&=c(\omega a+b-\omega^2 c-\omega d)\\&=pqbc-\omega qdc+p\omega ac-\omega^2c^2\\&=pq\tilde{b}\tilde{c}+q(p-1)\omega\tilde{d}\tilde{c}-p(q-1)\omega\tilde{a}\tilde{c}+(1-p)(q-1)\omega^2\tilde{c}^2\end{aligned}$$

giving in the limit

$$\tilde{c}\tilde{b}=\tilde{b}\tilde{c}-g\tilde{d}\tilde{c}-h\tilde{a}\tilde{c}+gh\tilde{c}^2. \tag{5.7}$$

We have thus obtained the first two group relations (with tildes added to avoid confusion) for the nonstandard case (2.4). The others can be obtained analogously. Let us now look at the $(K;g,h)$-deformed plane. One obtains from the definitions introduced

$$\tilde{x}=x-\omega y,\quad \tilde{y}=y. \tag{5.8}$$

Hence, using the constraints for (x,y),

$$\tilde{x}\tilde{y}-\tilde{y}\tilde{x}=(x-\omega y)y-y(x-\omega y)=xy-yx=(1-p)xy=(1-p)(\tilde{x}\tilde{y}+\omega\tilde{y}^2).$$

Now taking limit and using the definition of g,

$$\tilde{x}\tilde{y}-\tilde{y}\tilde{x}=g\tilde{y}^2. \tag{5.9}$$

This is the nonstandard version (with tildes added).

Similarly starting with

$$\tilde{\xi}=\xi-\omega\eta,\quad \tilde{\eta}=\eta \tag{5.10}$$

and using

$$\xi^2=0,\quad \eta^2=0,\quad (\xi\eta+q\eta\xi)=0$$

one obtains in the limit the expected results

$$\tilde{\xi}^2=h\tilde{\xi}\tilde{\eta},\quad \tilde{\eta}^2=0,\quad (\tilde{\xi}\tilde{\eta}+\tilde{\eta}\tilde{\xi})=0.$$

These simple cases have been presented to give a feeling for the limiting process at work. But they have further usefulness. For the important nilpotent operators of the preceding section one easily obtains, taking our limits,

$$\Phi_1=(\eta x-p\xi y)\rightarrow(\tilde{\eta}\tilde{x}-\tilde{\xi}\tilde{y}+g\tilde{\eta}\tilde{y})=\Phi_2.$$

Hence avoiding a lengthy reordering process one obtains directly from

$$\Phi_1^2=0,$$

$$(\Phi_1^2)\rightarrow\Phi_2^2=0.$$

The commutators of Φ_2 can again be derived simply from those of Φ_1. The terms involving $(g-h)$ in the latter set can be seen to emerge as follows:

$$(p^{-1}-q)\omega=(p^{-1}(1-p)\omega-(q-1)\omega)\rightarrow(g-h),$$

$$(pq-1)\omega=(p(q-1)\omega-(1-p)\omega)\rightarrow(h-g).$$

VI. DISCUSSION

The following points are worth noting.

(1) If $\hat{R}(K;\alpha,\beta)$ depend linearly on K and satisfy the braid equation for $K=(K_1,K_2)$, then the right-hand side of (1.4) becomes almost evident as follows. One can set

$$\hat{R}_{(12)}\hat{R}_{(23)}\hat{R}_{(12)}-\hat{R}_{(23)}\hat{R}_{(12)}\hat{R}_{(23)}=\left(\frac{K}{K_1}-1\right)\left(\frac{K}{K_2}-1\right)Z. \tag{6.1}$$

The first two factors on the right-hand side assure the braid property for $K=(K_1,K_2)$. Next one notes the following points.

The left-hand side is trilinear in K. Hence Z, coming after the first two factors, should be linear in K.

The left-hand side is antisymmetric under the exchange

$$\hat{R}_{(12)}\leftrightarrow\hat{R}_{(23)}.$$

Hence Z should have the same property. Thus the evident ansatz is

$$Z=(\hat{R}_{(23)}-\hat{R}_{(12)}). \tag{6.2}$$

This is indeed found to be correct. A possible K-independent constant factor can be normalized to unity, as we have done.

(The following two properties have been pointed out to the author by Daniel Arnaudon.)

(2) For the (p,q) and the (q,h) cases one can write

$$\hat{R}(K;\alpha,\beta)=c_1\hat{R}(K_1;\alpha,\beta)+c_2\hat{R}(K_2;\alpha,\beta), \tag{6.3}$$

where

$$c_1+c_2=1, \quad c_1K_1+c_2K_2=K.$$

However, for the (g,h) case (since $K_1=K_2=1$) such a relation does not hold for $K\neq 1$.

(3) For

$$\hat{R}_{(12)}\hat{R}_{(23)}\hat{R}_{(12)}-\hat{R}_{(23)}\hat{R}_{(12)}\hat{R}_{(23)}=\lambda(\hat{R}_{(23)}-\hat{R}_{(12)}) \tag{6.4}$$

and

$$\hat{R}^2=X\hat{R}+(1-X)I \tag{6.5}$$

(λ and X not being necessarily restricted to the values considered previously) defining

$$\hat{S}=(\hat{R}-\mu I) \tag{6.6}$$

one can verify that

$$\hat{S}_{(12)}\hat{S}_{(23)}\hat{S}_{(12)}-\hat{S}_{(23)}\hat{S}_{(12)}\hat{S}_{(23)}=(\lambda+X\mu-\mu^2)(\hat{S}_{(23)}-\hat{S}_{(12)}). \tag{6.7}$$

This generalizes an analogous result of Ref. 2 since we do not restrict R to be ''unitary.'' One can choose μ so that $\hat{S}$ satisfies the braid equation. Directly connected with the last two equations is the following canonical relation valid for all the cases considered before,

$$\hat{R}(K;\alpha,\beta)=\left(\frac{K}{K_i}\right)\hat{R}(K_i;\alpha,\beta)-\left(\frac{K}{K_i}-1\right)I. \tag{6.8}$$

Here K_i denotes either one of the ''braid'' (or YB) values of K. This is of basic importance. The parameter $K/(K_i-K)$ can be shown to provide the prescription for Baxterization. In fact, (6.8) can be recognized to correspond to the usual ansatz for Baxterization.[9]

(4) The works of Gerstenhaber, Giaquinto, and Schak[2,3] assure that our MBE encodes deformations satisfying basic criteria but removing certain restrictive features of the standard (BE) (or (YB)). For our class the factor λ on the right-hand side in (6.4) is neither zero nor entirely arbitrary. It has the specific form given by (1.4) arising out of our basic condition: K-independence of the group relations. Our parametrization of of this factor carries information. The YB or the braid solutions are obtained effortlessly as byproducts. This leads also to agreeable properties designated here as ''soft symmetry breaking'' role of K in the noncommutative geometries studied. For all K (and all the cases studied) one obtains the crucial, canonical Hecke condition we have emphasized. It permits us to introduce consistently and uniformly the noncommutativity constraints. Let us recapitulate the remarkable consequences.

(a) The bilinear constraints for the coordinates and those for the differentials remain independent of K.

(b) In the constraints involving both coordinates and differentials K does appear, but in a ''minimal'' fashion. Apart from a simple overall factor, in the linear combinations on the right-hand side, K appears as a factor of a nilpotent combination (Φ_1 or Φ_2). Along with the commutation relations satisfied by these nilpotents, this has the consequence that reordering any higher order product one obtains, apart from an overall factor, finally linearity in K. The operator Φ, crucial for constructing covariant derivatives,[4] remains nilpotent for arbitrary K [see (4.13)]. The main point is that conserving the (x,y) and the (ξ,η) commutators and without violating the constraints imposed by the postulated actions of exterior derivations one can implement the parameter K in the mixed commutators [(x,ξ), etc.], even there conserving good properties.

(c) The ''contraction'' procedure leading from standard (p,q) to nonstandard (g,h) deformations is not perturbed by K. Even the titles of previous papers[10,11] give an idea of the scope of this approach. It is reassuring to note that one can continue to implement it in presence of K.

Having noted some interesting features of the results obtained let us now look at further developments they suggest. One naturally thinks of the following aspects.

(1) Extension of our results to higher dimensional MBE. First by going beyond the 4×4 cases for deformations of GL(2). Second by starting from group relations for deformed SL(N) and SO(N). Higher dimensional cases have already been studied in Refs. 2 and 3. Our aim would be to obtain explicit structures correponding to conserved group relations for such cases. Then one can see if our soft symmetry breaking still gets implemented and in what fashion.

(2) For $K=(K_1,K_2)$ the R matrix flips the tensor components of co-products. Having obtained more general modified R matrices it would be important to examine the consequences for co-products as K moves away from the YB values.

(3) A more complete study of the role of K in noncommutative geometries induced by three-parameter deformations $(K;\alpha,\beta)$. Even for the two-plane we have stopped at a certain point leaving much to be done. After constructing higher dimensional matrices $\hat{R}(K;\alpha,\beta)$ one can implement them in higher dimensional spaces.

(4) Study of twists in the context of ''modified'' R matrices. In particular, the fact that one can implement triangularity for all types of deformations by suitably choosing K suggests intriguing possibilities. Various aspects studied in Refs. 12, 13, and 14 can be re-examined in this broader context.

(5) Our MBE (or MYBQE of Gerstenhaber *et al.*) and Baxterization can be seen to be [see (6.8)] two facets of the same underlying construction, namely the general solution of the RTT relations. In the first case the parameter K is kept fixed in each term and the right-hand side of the braid equation is allowed to be nonzero. In the second one, the right-hand side is held fixed at zero and to permit this the parameter is suitably varied from term to term. The two procedures are complementary.

(6) What are the consequences for knot invariants associated to an $\hat{R}$ as K moves away from the ''braid values''? Can a conceptually consistent generalization (parametrized third Reidemeister move) be implemented fruitfully?

Presumably this list is not exhaustive. Some of these objectives should be directly accessible. Elsewhere one may encounter obstructions. We hope to explore different directions in future studies.

This work owes much to sustained and reassuring help from Daniel Arnaudon. It goes beyond results explicitly attributed to him. Our treatment of noncommutative planes took shape from succesive discussions with John Madore.

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Essential self-adjointness of *n*-dimensional Dirac operators with a variable mass term[a)]

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We give some results about the essential self-adjointness of the Dirac operator $H=\Sigma_{j=1}^{n}\alpha_j p_j+m(x)\,\alpha_{n+1}+V(x)\,I_N$ $(N=2^{[(n+1)/2]})$, on $[C_0^\infty(\mathbf{R}^n\backslash\{0\})]^N$, where the α_j $(j=1,2,\ldots,n)$ are Dirac matrices and $m(x)$ and $V(x)$ are real-valued functions. We are mainly interested in a singularity of $V(x)$ and $m(x)$ near the origin which preserves the essential self-adjointness of H. As a result, if $m=m(r)$ is spherically symmetric or $m(x)\equiv V(x)$, then we can permit a singularity of m and V which is stronger than that of the Coulomb potential. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1367331]

I. INTRODUCTION

In this article we consider the essential self-adjointness of the Dirac operator

$$H:=\sum_{j=1}^{n}\alpha_j p_j+m(x)\,\alpha_{n+1}+V(x)\,I_N$$

$$\left(x\in\mathbf{R}^n,\quad n\geqslant 2,\quad p_j=-i\frac{\partial}{\partial x_j},\quad N=N(n):=2^{[(n+1)/2]}\right)$$

in the Hilbert space $\mathbf{H}:=L^2(\mathbf{R}^n)^N$. Here I_N is the $N\times N$ unit matrix, and the α_j are $N\times N$ Dirac matrices, i.e., Hermitian matrices satisfying

$$\alpha_j\,\alpha_k+\alpha_k\,\alpha_j=2\,\delta_{jk}\,I_N\quad(j,k=1,2,\ldots,n+1);\tag{1}$$

$m(x)$ and $V(x)$ are real-valued functions.

In contrast to the Schrödinger case, the essential self-adjointness of H cannot be destroyed by the behavior of m and V at infinity (Ref. 1), but only by local singularities of these functions. For example, if m is constant and $V(r)=e/r$, H is essentially self-adjoint if and only if $|e|\leqslant\sqrt{3}/2$. Extending a seminal paper by Schmincke,[2] very general self-adjointness criteria were given by, e.g., Levitan and Otelbaev,[3] Arai,[4] Yamada,[5] Vogelsang[6] and Kalf[7] for the situation that m is a constant and V is a strongly singular potential that is not necessarily spherically symmetric.

The principal interest of Dirac operators with a variable mass term lies in the fact that they can have a purely discrete spectrum. That was why they were proposed in the 1960s as simple quark models. Brief historical remarks can be found in Vasconcelos[8] and Eich, Rein, and Rodenberg.[9] Vasconcelos[8] explicitly solves the bound-state problem $V(r)=e/r$, $m(r)=e'/r$; other specific cases were treated by Critchfield and Rein (see the references in Ref. 9).

In the article in hand we present three self-adjointness criteria for Dirac operators with a variable mass term, concentrating on the case that m and V have a singularity at the origin. We generalize the results given in Ref. 10 and show the complete proofs, which are not given in

[a)]Dedicated to Professor Joachim Weidmann on the occasion of his sixtieth birthday.

Ref. 10. Theorem 1 assumes that m is spherically symmetric and involves a pointwise bound on $V(x)$ and $m(r)$, $m'(r)$ which admits, in the presence of m, a singularity of V that is stronger than the Coulomb singularity. Theorem 1 reduces to Schmincke's result when $m=0$. In Theorem 2 an integral condition is imposed on V and m, neither of which necessarily rotationally symmetric. When $m=0$, this theorem reduces to the criterion of Levitan and Otelbaev.[3] Our last theorem concerns the special situation that $m\equiv V$. In this case it turns out that the condition which is necessary to define the canonical minimal operator is already sufficient to establish its essential self-adjointness. Since $(I_N\pm\alpha_{n+1})/2$ is a projection operator, it is possible to bring in the Laplace operator and use Kato's inequality.

In this article we employ the following abbreviations:

$$\alpha:=(\alpha_1,\alpha_2,\ldots,\alpha_n),\quad p:=(p_1,p_2,\ldots,p_n),\quad \alpha\cdot p:=\sum_{j=1}^{n}\alpha_j p_j,$$

$$\Omega:=\mathbf{R}^n\backslash\{0\},\quad \mathbf{R}_+:=(0,+\infty),\quad \mathbf{D}:=C_0^\infty(\Omega)^N.$$

Theorem 1: *Let $m=m(r)$ be spherically symmetric and absolutely continuous in $\mathbf{R}_+$ with the derivative $m'(r)\in L^2_{\mathrm{loc}}(\mathbf{R}_+)$. Assume that $\alpha\cdot p+m\,\alpha_{n+1}$ on $\mathbf{D}$ is essentially self-adjoint, and $V(x)\in L^2_{\mathrm{loc}}(\Omega)$ satisfies*

$$(1+\varepsilon)^2\left[V^2(x)+\frac{1}{4\,r^2}\right]+\left|m'(r)+\frac{m(r)}{r}\right|\leqslant m^2(r)+\left(\frac{n-1}{2r}\right)^2\quad(x\in\Omega)\tag{2}$$

for some $\varepsilon>0$. Then H is essentially self-adjoint. If $n\geqslant 3$ and $r\,m(r)$ is bounded, then the domain $D(\overline{H})$ of the closure $\overline{H}$ coincides with the Sobolev space $W^{1,2}(\mathbf{R}^n)^N$.

The next result does not require m to be spherically symmetric and extends a theorem of Levitan and Otelbaev.[3]

Theorem 2: *Let $n\geqslant 3$ and $m,V\in L^2_{\mathrm{loc}}(\Omega)$ be real-valued,*

$$q(r):=\sup_{|x|=r}\left[V^2(x)+m^2(x)+2\,|m(x)|\,\sqrt{V^2(x)+\frac{1}{4\,r^2}}\right]^{1/2}$$

and

$$a:=\sup_{r>0}\left(\frac{1}{r^{n-2}}\int_0^r t^{n-1}q^2(t)\,dt\right)^{1/2}<\sqrt{\frac{n}{2}}.\tag{3}$$

Then H is essentially self-adjoint with $D(\overline{H})=W^{1,2}(\mathbf{R}^n)^N$.

The Dirac operator is in general not essentially self-adjoint on $C_0^\infty(\mathbf{R}^n)^N$ if m, V are merely in $L^2_{\mathrm{loc}}(\mathbf{R}^n)$. By dint of a theorem of Kato[11] we do, however, have the following result.

Theorem 3: *Assume that $m(x)$ and $V(x)$ are $L^2_{\mathrm{loc}}(\mathbf{R}^n)$ functions satisfying $m(x)\equiv V(x)$ or $m(x)\equiv -V(x)$. Then $H=(\alpha\cdot p)+m\,\alpha_{n+1}+V$ on $C_0^\infty(\mathbf{R}^n)^N$ is essentially self-adjoint.*

II. PRELIMINARIES AND PROOF OF THEOREM 1

The existence of Dirac matrices satisfying (1) is well known. In the Appendix we sketch an inductive method of constructing Dirac matrices such that

$$\alpha_j:=\begin{pmatrix}\mathbf{0} & a_j\\ a_j^* & \mathbf{0}\end{pmatrix}\quad(j=1,2,\ldots,n),\quad \alpha_{n+1}:=\begin{pmatrix}I_{N/2} & \mathbf{0}\\ \mathbf{0} & -I_{N/2}\end{pmatrix},\tag{4}$$

where the a_j are $N/2\times N/2$ matrices (which are Hermitian if n is odd) with the property

$$a_j a_k^* + a_k a_j^* = 2\delta_{jk} I_{N/2}, \quad a_j^* a_k + a_k^* a_j = 2\delta_{jk} I_{N/2} \ \ (j,k=1,2,\ldots,n). \tag{5}$$

If $\{\alpha_1,\alpha_2,\ldots,\alpha_{n+1}\}$ and $\{\alpha_1',\alpha_2',\ldots,\alpha_{n+1}'\}$ are two sets of Dirac matrices, then there is a unitary matrix U such that $\alpha_j' = U\alpha_j U^{-1}$ $(j=1,2,\ldots,n+1)$ or $\alpha_j' = U[-\alpha_j]U^{-1}$ $(j=1,2,\ldots,n+1)$, and, if n is odd, we always have the former case (see, e.g., Ref. 12, p. 267). If n is even and $\alpha_j' = U[-\alpha_j]U^{-1}$ $(j=1,2,\ldots,n+1)$, we have

$$\begin{aligned} H' &:= \sum_{j=1}^{n} \alpha_j' p_j + m(x)\alpha_{n+1}' + V(x) I_N \\ &= (U\alpha_1\alpha_2\cdots\alpha_n)\left[\sum_{j=1}^{n} \alpha_j p_j - m(x)\alpha_{n+1} + V(x) I_N\right](U\alpha_1\alpha_2\cdots\alpha_n)^{-1}. \end{aligned}$$

Therefore, H' is unitarily equivalent to H or to

$$\sum_{j=1}^{n} \alpha_j p_j - m(x)\alpha_{n+1} + V(x) I_N .$$

It should be remarked that the condition (2) remains invariant under replacing $m(x)$ by $-m(x)$.

In order to explain the separation of variables of Dirac operators the spin-orbit coupling operator,

$$S := \frac{n-1}{2} - \sum_{1\leqslant j<k\leqslant n} i\alpha_j\alpha_k(x_j p_k - x_k p_j),$$

is needed, with the help of which we have

$$\alpha\cdot p = \alpha_r\left(p_r + \frac{i}{r}S\right),$$

where the α_j are given in (4) with (5) and

$$\alpha_r := \sum_{j=1}^{n} \frac{x_j}{r}\alpha_j, \quad p_r := -ir^{(1-n)/2}\frac{\partial}{\partial r}r^{(n-1)/2} = -i\left(\frac{\partial}{\partial r} + \frac{n-1}{2r}\right).$$

It is well known that the self-adjoint extension of S in $L^2(S^{n-1})^N$ has only discrete eigenvalues k with finite multiplicity such that

$$k \in -\left(\mathbf{N}_0 + \frac{n-1}{2}\right) \cup \left(\mathbf{N}_0 + \frac{n-1}{2}\right), \tag{6}$$

where $\mathbf{N}_0 := \{0,1,2,\cdots\}$ (see, e.g., Ref. 13, p. 161). Let

$$U := \begin{pmatrix} I_{N/2} & \mathbf{0} \\ \mathbf{0} & -ia_r^* \end{pmatrix}, \quad a_r := \sum_{j=1}^{n} \frac{x_j}{r} a_j ,$$

where

$$\alpha_j := \begin{pmatrix} \mathbf{0} & a_j \\ a_j^* & \mathbf{0} \end{pmatrix} \quad (j=1,2,\ldots,n), \quad \alpha_{n+1} := \begin{pmatrix} I_{N/2} & \mathbf{0} \\ \mathbf{0} & -I_{N/2} \end{pmatrix}.$$

Then U is a unitary matrix which commutes with α_{n+1} and satisfies

$$U^{-1}\alpha_r U=\begin{pmatrix} \mathbf{0} & -iI_{N/2} \\ iI_{N/2} & \mathbf{0} \end{pmatrix}.$$

Thus, if $V=V(r)$ and $m=m(r)$ are spherically symmetric, the Dirac operator on the eigenspace of S with respect to the eigenvalue k is unitarily equivalent to

$$\begin{pmatrix} \mathbf{0} & -I_{N/2} \\ I_{N/2} & \mathbf{0} \end{pmatrix}\frac{d}{dr}+\begin{pmatrix} [m(r)+V(r)]I_{N/2} & (-k/r)I_{N/2} \\ (-k/r)I_{N/2} & [-m(r)+V(r)]I_{N/2} \end{pmatrix}$$

in $L^2(\mathbf{R}_+)^N$. Therefore, the question if such Dirac operators are essentially self-adjoint reduces to the problem whether every one-dimensional Dirac operator in $L^2(\mathbf{R}_+)^2$,

$$L_k:=\begin{pmatrix} m(r)+V(r) & -(d/dr)+(k/r) \\ (d/dr)+(k/r) & -m(r)+V(r) \end{pmatrix},$$

is of limit point type at the origin for every k satisfying (6) (see, e.g., Ref. 14, Theorem 5.4).

We remark that, if $V(r)\equiv 0$, then any L_k is of limit point type at 0 for a relatively large class of $m(r)$. For example, the following proposition can be shown by Arnold, Kalf, and Schneider in Ref. 15, where more general theorems are given.

Proposition 2.1: Let $m=m(r)$ be a real-valued function and belong to $L^1_{\mathrm{loc}}(\mathbf{R}_+)$. Then the one-dimensional Dirac operator L_k with *$V=0$ is of limit point type at* 0, *if $m(r)$ satisfies one of the following conditions:*

(i) $\lim_{r\to 0} r\, m(r)$ *exists and is finite, or*
(ii) $\lim_{r\to 0} r\,|m(r)|=\infty$, *and* $\operatorname{sgn} m$ *is constant near the origin.*

The proof of Theorems 1 and 2 will rest upon the following well-known abstract result about the closure and bounded invertibility of the sum of two operators (for a proof see, e.g., Ref. 16, pp. 190 and 196).

Proposition 2.2: Let A, B be closable linear operators in a Hilbert space **H** *with $D(A)\subset D(B)$. Suppose that the closure $\overline{A}$ has a bounded inverse defined on* **H** *and that for some $\varepsilon>0$*

$$(1+\varepsilon)\|Bu\|\leqslant\|Au\| \quad [u\in D(A)].$$

Then $A+B$ is closable and $\overline{A+B}=\overline{A}+\overline{B}$ with domain $D(\overline{A})$. Moreover, $\overline{A+B}$ has a bounded inverse on **H**.

Let $W^{1,2}_{\mathrm{loc}}(\Omega)$ be the Sobolev space of all functions $u\in L^2_{\mathrm{loc}}(\Omega)$ with generalized first-order derivatives in $L^2_{\mathrm{loc}}(\Omega)$, and D_1 be the space of $u\in W^{1,2}_{\mathrm{loc}}(\Omega)^N$ with compact support in Ω. Note that $C_0^\infty(\Omega)^N\subset D_1$. If $g\in L^2_{\mathrm{loc}}(\Omega)$ has first-order derivatives in $L^2_{\mathrm{loc}}(\Omega)$, then we consider a multiplication operator

$$u\mapsto g\,u$$

for $u\in D_1$. It should be noted that $g\,v\in D_1$ for $v\in D_1$. The subsequent operator calculations will be valid on the domain D_1.

Lemma 2.3: Let s be a real number, $m(r)$ a real-valued function which is absolutely continuous in $\mathbf{R}_+$ with $m'\in L^2_{\mathrm{loc}}(\mathbf{R}_+)$ and

$$A_1:=\alpha\cdot p+m(r)\alpha_{n+1}+\frac{i}{2r}\alpha_r+is.$$

Then we have

$$A_1^* A_1 \geqslant m^2(r) + \left(\frac{n-1}{2r}\right)^2 - \left| m'(r) + \frac{m(r)}{r} \right|.$$

Proof: Since S anticommutes with α_r, a direct calculation gives us

$$A_1^* A_1 = p_r^2 + \frac{(n-1)(n-3)}{4r^2} + \frac{1}{r^2}\left[S^2 - \left(\frac{n-1}{2}\right)^2 \right] + \frac{2n-3}{4r^2} + s^2 + \frac{s}{r}\alpha_r + m^2 - i\alpha_r \alpha_{n+1}\left(m' + \frac{m}{r} \right)$$

$$\geqslant p_r^2 + \frac{(n-1)(n-3)}{4r^2} + \frac{1}{r^2}\left[S^2 - \left(\frac{n-1}{2}\right)^2 \right] + \frac{2n-3}{4r^2} + s^2 - \frac{|s|}{r} + m^2 - \left| m' + \frac{m}{r} \right|,$$

where the inequality stems from the observation that α_r and $i\alpha_r\alpha_{n+1}$ are Hermitian matrices with square I_N. The assertion now follows from the Hardy-type inequality

$$p_r^2 \geqslant \frac{1}{4r^2} + \frac{d}{r} - d^2 \quad (d \geqslant 0)$$

[see, e.g., Ref. 4, (3.15)] and

$$S^2 \geqslant \left(\frac{n-1}{2}\right)^2$$

[see (6)].

Proof of Theorem 1: Let

$$A_t := \alpha \cdot p + m(r)\alpha_{n+1} + \frac{it}{2r}\alpha_r + is \quad (0 \leqslant t \leqslant 1),$$

where $s = 1$ or -1 and

$$B := V(x) - \frac{i}{2r}\alpha_r .$$

Lemma 2.3 and assumption (2) imply

$$A_1^* A_1 \geqslant (1+\varepsilon)^2 \left(V^2 + \frac{1}{4r^2} \right) = (1+\varepsilon)^2 B^* B, \tag{7}$$

so that the range of $H \pm i = A_1 + B$ is dense in $\mathbf{H}$, once we know that $\overline{A_1}$ has a bounded inverse which is defined on the whole Hilbert space $\mathbf{H}$. For $0 \leqslant t \leqslant 1$ we conclude from (7)

$$\|A_t u\| = \left\| \left(A_1 - (1-t)\frac{i}{2r}\alpha_r \right) u \right\| \geqslant (\varepsilon + t) \left\| \frac{i}{2r}\alpha_r u \right\| \quad (u \in \mathbf{D}). \tag{8}$$

Since $\overline{A_0}^{-1}$ is bounded on $\mathbf{H}$ owing to our hypothesis, the same applies to the inverse of the closure of $A_0 + (it/2r)\alpha_r = A_t$ for $t < \varepsilon =: t_1$ by (8) and Propositon 2.2, and we are finished if $t_1 > 1$. Otherwise, this information, jointly with (8), shows that $\overline{A_t}^{-1}$ is bounded on $\mathbf{H}$ for $t < t_1 + \varepsilon + t_1 =: t_2$. For some $l \in \mathbf{N}$ we eventually arrive at some number $t_l = (2^l - 1)\varepsilon > 1$.

Finally we prove $D(\overline{H}) = W^{1,2}(\mathbf{R})^N$ if $rm(r)$ is bounded and $n \geqslant 3$. The inequality (7) implies that $D(\overline{H}) = D(\overline{A_1})$ is contained in $D(1/r)$. Let $u \in D(\overline{H})$. Since $V(x) = O(1/r)$ by means of (2), we conclude $(\alpha \cdot p)u \in \mathbf{H}$, which gives $u \in W^{1,2}(\mathbf{R})^N$. On the other hand, if we write $H_0 = \alpha \cdot p$ on $\mathbf{D}$, the inclusion

$$D(\overline{H_0}) = W^{1,2}(\mathbf{R}^n)^N \subset D(1/r)$$

is clear from Hardy's inequality

$$p^2 \geqslant \left(\frac{n-2}{2}\right)^2 \frac{1}{r^2}. \tag{9}$$

□

Remark: In Theorem 1 we can adopt a stronger singularity of m and V at the origin than the one of Coulomb potentials. For example, H is essentially self-adjoint if we assume

$$m(r) = \frac{C_1}{r^\mu}, \quad |V(x)| \leqslant \frac{C_2}{r^\mu}, \quad C_1 > C_2 > 0 \tag{10}$$

and $\mu > 1$, Indeed, if we set

$$\tilde{m} = \frac{C_1}{r^\mu} + C$$

for $C > 0$, then V and $\tilde{m}$ satisfy condition (2) if $\varepsilon > 0$ is sufficiently small and $C > 0$ is sufficiently large. Thus the essential self-adjointness is valid for $\alpha \cdot P + m\,\beta + VI_4 + C\,\beta$, and, therefore, for $\alpha \cdot D + m\,\beta + VI_4$.

In the special case $m(r) = C_1/r^\mu$ and $V(r) = C_2/r^\mu$ $(C_1 > C_2 > 0, \mu > 1)$ it follows from Theorem 3 in Ref. 15 that the equation $L_k v = 0$ has, for any $k \in \mathbf{Z}\backslash\{0\}$, a fundamental system of solutions $v_\pm$ with

$$|v_\pm(r)| = \exp\{[\pm\sqrt{C_1^2 - C_2^2}/(\mu-1) + o(1)]\, r^{1-\mu}\} \quad \text{as} \quad r \to 0.$$

This singularity of m therefore has the same effect on the solutions as an anomalous magnetic moment (Ref. 17).

If $\mu = 1$ in (9), then the condition (2) is satisfied provided $C_2^2 < C_1^2 + \frac{3}{4}$. This result corresponds to the case $b_1 = 0$ and $s = \frac{1}{2}$ in Theorem 3.1 by Arai.[4] In this case the essential self-adjointness still holds when $C_2^2 = C_1^2 + (\frac{3}{4})$, if we ignore the domain property of the closure (Ref. 5).

In the plane, $H = \sigma_1 P_1 + \sigma_2 P_2 + m\,\sigma_3 + VI_2$ with $m(r) = C_1/r$ and $V(r) = C_2/r$ is essentially self-adjoint if and only if $|C_2| \leqslant |C_1|$. Indeed, L_k $[k \in \mathbf{Z} + \frac{1}{2}$ if $n = 2]$ is of limit point type at 0 if and only if $C_2^2 - C_1^2 \leqslant k^2 - \frac{1}{4}$.

III. PROOF OF THEOREM 2

The proof is given along the line of Ref. 7.

Lemma 3.1: Let $q(r):(0,\infty) \to \mathbf{R}$ *satisfy*

$$\frac{1}{r^{n-2}} \int_0^r t^{n-1} q^2(t)\, dt \leqslant a^2$$

for some $a > 0$. *Then*

$$p_r^2 + \frac{(n-1)(n-3)}{4r^2} \geqslant \frac{n-2}{4a^2} q^2 + \frac{d}{r} - d^2$$

for any $d \geqslant 0$.

Proof: The Lemma is an n-dimensional version of (Ref. 7, Lemma 2). Let $b \geqslant 0$, $0 \leqslant c \leqslant (n-1)/2$ and

$$g(r):=\frac{b}{r^{n-1}}\int_0^r t^{n-1}q^2(t)dt-\frac{c}{r}+d.$$

Then we have

$$p_r^2+\frac{(n-1)(n-3)}{4r^2}\geqslant g'(r)-g^2+\frac{(n-1)(n-3)}{4r^2}\geqslant \phi(c)\frac{1}{r^2}-d^2+(c-a^2b)\frac{2d}{r}+bq^2,$$

where

$$\phi(c):=c(1-c+2a^2b)+\tfrac{1}{4}(n-1)(n-3)-(n-1)a^2b-a^4b^2.$$

This function has its maximum at $c=a^2b+\frac{1}{2}$, so that

$$\geqslant\left[\left(\frac{n-2}{2}\right)^2-(n-2)a^2b\right]\frac{1}{r^2}-d^2+\frac{d}{r}+bq^2.$$

Choose

$$b=\frac{n-2}{4a^2},\quad c=\frac{n}{4}\leqslant\frac{n-1}{2}$$

and we have the assertion. □

Proof of Theorem 2: Let $\varepsilon>0$, $s\in\mathbf{R}\backslash\{0\}$ and

$$f(r):=\frac{1-\varepsilon}{2\,a^2r^{n-1}}\int_0^r t^{n-1}\,q^2(t)\,dt+\frac{\varepsilon}{4\,r},\quad A:=\alpha\cdot p+i\,f(r)\,\alpha_r+is,$$

$$B:=m\,\alpha_{n+1}+V-i\,f(r)\,\alpha_r,\quad A_1:=\alpha\cdot p+is,\quad B_1:=-if(r)\alpha_r,$$

that is, $H=A+B$ and $A_1=A+B_1$. The definition of a in (3) gives

$$0\leqslant f(r)\leqslant\frac{1-\varepsilon}{2r}+\frac{\varepsilon}{4r}=\frac{1-(\varepsilon/2)}{2r}\leqslant\frac{1}{2r}.\tag{11}$$

It is well known that $\overline{A_1}$ has a bounded inverse defined on $\mathbf{H}$. In view of (11) and Hardy's inequality (9) we have

$$A_1^*A_1=p^2+s^2\geqslant\left(\frac{n-2}{2}\right)^2\frac{1}{r^2}\geqslant\left(\frac{n-2}{1-(\varepsilon/2)}\right)^2f^2=\left(\frac{n-2}{1-(\varepsilon/2)}\right)^2B_1^*B_1,$$

so that $\overline{A}^{-1}$ is bounded on $\mathbf{H}$ as well with $D(\overline{A})=D(\overline{A_1-B_1})=D(\overline{A_1})=W^{1,2}(\mathbf{R}^n)^N$.

Since $V\,\alpha_{n+1}+f\,(i\alpha_r\alpha_{n+1})$ is Hermitian with square V^2+f^2 we have

$$\begin{aligned}B^*\,B&=f^2+m^2+V^2+2\,m\,[V\,\alpha_{n+1}+f\,(i\alpha_r\alpha_{n+1})]\\&\leqslant f^2+m^2+V^2+2\,|m|\,\sqrt{V^2(x)+\frac{1}{4\,r^2}}=f^2+q^2.\end{aligned}\tag{12}$$

On the other hand,

$$
\begin{aligned}
A^*A &= p_r^2 + \frac{(n-1)(n-3)}{4r^2} + \frac{1}{r^2}\left[S^2 - S - \frac{(n-1)(n-3)}{4}\right] + \frac{2f}{r}\left(S - \frac{n-1}{2}\right) \\
&\quad + f' + \frac{n-1}{r}f + f^2 + s^2 + 2sf\alpha_r \\
&= p_r^2 + \frac{(n-1)(n-3)}{4r^2} + \left[S^2 - S - \frac{(n-1)(n-3)}{4}\right](1-2rf)\frac{1}{r^2} \\
&\quad + \left[S^2 - \left(\frac{n-1}{2}\right)^2\right]\frac{2f}{r} + f' + \frac{n-1}{r}f + f^2 + s^2 + 2sf\alpha_r \\
&\geqslant p_r^2 + \frac{(n-1)(n-3)}{4r^2} + f' + \frac{n-1}{r}f + f^2 + s^2 + 2sf\alpha_r
\end{aligned}
$$

on account of (6), (10) and

$$
S^2 - S - \frac{(n-1)(n-3)}{4} = \left(S - \frac{n-1}{2}\right)\left(S + \frac{n-3}{2}\right) \geqslant 0.
$$

Therefore, we have

$$
A^*A \geqslant p_r^2 + \frac{(n-1)(n-3)}{4r^2} + f' + \frac{n-1}{r}f + f^2 + s^2 - 2|s|f.
$$

Owing to Lemma 3.1 and

$$
f'(r) + \frac{n-1}{r}f = \frac{1-\varepsilon}{2a^2}q^2(r) + \frac{\varepsilon(n-2)}{4r^2}
$$

we find

$$
A^*A \geqslant \frac{n-2\varepsilon}{4a^2}q^2 + \frac{d}{r} - d^2 + \frac{\varepsilon(n-2)}{4r^2} + f^2 + s^2 - 2|s|f. \tag{13}
$$

Equations (12) and (13) imply

$$
\begin{aligned}
A^*A - (1+\varepsilon)B^*B &\geqslant \frac{n-2\varepsilon}{4a^2}q^2 + \frac{d}{r} - d^2 + \frac{\varepsilon(n-2)}{4r^2} + s^2 - 2|s|f - (1+\varepsilon)q^2 - \varepsilon f^2 \\
&\geqslant \left[\frac{n-2\varepsilon}{4a^2} - (1+\varepsilon)\right]q^2 + s^2 - d^2 + \left[d - \left(1 - \frac{\varepsilon}{2}\right)|s|\right]\frac{1}{r} \\
&\quad + \left[n - 2 - \left(1 - \frac{\varepsilon}{2}\right)^2\right]\frac{\varepsilon}{4r^2}.
\end{aligned}
$$

Since $n/4a^2 > 1$ in view of (3), an appropriate choice of $\varepsilon > 0$ yields

$$
A^*A - (1+\varepsilon)B^*B \geqslant 0.
$$

Since $\overline{A}$ has a bounded inverse on $\mathbf{H}$ with $D(\overline{A}) = W^{1,2}(\mathbf{R})^N$, H is essentially self-adjoint with $D(\overline{H}) = D(\overline{A+B}) = D(\overline{A}) = W^{1,2}(\mathbf{R})^N$. □

IV. PROOF OF THEOREM 3

We have only to see that the ranges of $(H\pm i)$ are dense in $\mathbf{H}$. We note that $u\in\mathbf{H}$ belongs to $D(H^*)$ if and only if $(\alpha\cdot p)\,u$ exists in the weak sense on $C_0^\infty(\mathbf{R}^n)^N$, and

$$(\alpha\cdot p)\,u+m\,\alpha_{n+1}\,u+V\,u\in\mathbf{H},$$

since $V\in L^2_{\mathrm{loc}}(\mathbf{R}^n)$. Let $u\in R(H+i)^\perp=\ker(H^*-i)$. Then we have

$$(\alpha\cdot p)\,u+m\,\alpha_{n+1}\,u+V\,u=iu.$$

As remarked at the beginning of Sec. II, every Dirac operator is unitarily equivalent to the Dirac operator defined by Dirac matrices in (4) with (5), replacing $m(x)$ by $-m(x)$ if necessary. Therefore, with suitable vectors

$$v:={}^t(v_1,v_2,\ldots,v_{N/2}),\quad w:={}^t(w_1,w_2,\ldots,w_{N/2})\in L^2(\mathbf{R}^n)^{N/2}$$

we have

$$u=\begin{pmatrix} v\\ w\end{pmatrix}$$

and

$$\sum_{j=1}^n a_j\,p_j\,w+(m+V)v=iv, \tag{14a}$$

$$\sum_{j=1}^n a_j^*\,p_j\,v+(-m+V)w=iw, \tag{14b}$$

or

$$\sum_{j=1}^n a_j\,p_j\,w+(-m+V)v=-iv,\quad \sum_{j=1}^n a_j^*\,p_j\,v+(m+V)w=-iw. \tag{15}$$

Let us consider the earlier case (14) and assume $m(x)\equiv V(x)$. By virtue of (14a) we can apply $\Sigma_{j=1}^n a_jp_j$ to (14b), and using (5) together with $Vv\in L^1_{\mathrm{loc}}(\mathbf{R}^n)^N$ we see that $\Delta v\in L^1_{\mathrm{loc}}(\mathbf{R}^n)^N$, and so

$$-\Delta\,v+2\,i\,V\,v=-v \tag{16}$$

in the weak sense. From (16) and Kato's inequality we have for $j=1,2,\ldots,N/2$,

$$(-\Delta+1)|v_j|\leqslant\mathrm{Re}[(\mathrm{sgn}\,\overline{v_j})(-\Delta+1)v_j]=0,$$

and so $v_j=0$ (see Ref. 11 or Ref. 18, p. 184). By (14b) we then have $w=0$, i.e., $u=0$. The proofs for (15), $m\equiv -V$, and $u\in R(H-i)^\perp$ are similarly obtained. □

APPENDIX

Finally we show that Dirac matrices of the special form (4) and (5) exist. $n+1$ $N(n)\times N(n)$ Dirac matrices with a simple block structure can be constructed inductively by starting with the Pauli matrices $(n=2)$

$$\alpha_1^{(2)}:=\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \alpha_2^{(2)}:=\sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \alpha_3^{(2)}:=\sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

If n is odd and we know the $N(n-1)\times N(n-1)$ matrices $\alpha_1^{(n-1)},\alpha_2^{(n-1)},\ldots,\alpha_n^{(n-1)}$, we define $N(n)\times N(n)$ matrices $[N(n)=2N(n-1)]$

$$\alpha_j^{(n)}:=\begin{pmatrix}\mathbf{0} & \alpha_j^{(n-1)}\\ \alpha_j^{(n-1)} & \mathbf{0}\end{pmatrix}\quad (j=1,2,\ldots,n),\quad \alpha_{n+1}^{(n)}:=\begin{pmatrix}I_{N(n-1)} & \mathbf{0}\\ \mathbf{0} & -I_{N(n-1)}\end{pmatrix}.$$

If n is even, we define $N(n)\times N(n)$ matrices $(N(n)=N(n-1)=2N(n-2))$

$$\alpha_1^{(n)}:=\begin{pmatrix}\mathbf{0} & I_{N(n-2)}\\ I_{N(n-2)} & \mathbf{0}\end{pmatrix},\quad \alpha_{j+1}^{(n)}:=\begin{pmatrix}\mathbf{0} & -i\alpha_j^{(n-2)}\\ i\alpha_j^{(n-2)} & \mathbf{0}\end{pmatrix}\quad (j=1,2,\ldots,n-1),$$

$$\alpha_{n+1}^{(n)}:=\begin{pmatrix}I_{N(n-2)} & \mathbf{0}\\ \mathbf{0} & -I_{N(n-2)}\end{pmatrix},$$

which are Hermitian matrices satisfying (1). Therefore, in any dimension n we can find $N\times N$ Dirac matrices $\alpha_1,\ldots,\alpha_{n+1}$ of the form

$$\alpha_j:=\begin{pmatrix}\mathbf{0} & a_j\\ a_j^* & \mathbf{0}\end{pmatrix}\quad (j=1,2,\ldots,n),\quad \alpha_{n+1}:=\begin{pmatrix}I_{N/2} & \mathbf{0}\\ \mathbf{0} & -I_{N/2}\end{pmatrix},$$

where the a_j are $N/2\times N/2$ matrices (which are Hermitian if n is odd) such that

$$a_j a_k^*+a_k a_j^*=2\delta_{jk}I_{N/2},\quad a_j^* a_k+a_k^* a_j=2\delta_{jk}I_{N/2}.$$

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Matrix theory compactification on noncommutative $\mathbb{T}^4/\mathbb{Z}_2$

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In this article, we construct gauge bundles on a noncommutative toroidal orbifold $\mathbb{T}^4_\theta/\mathbb{Z}_2$. First, we explicitly construct a bundle with constant curvature connections on a noncommutative $\mathbb{T}^4_\theta$ following Rieffel's method. Then, applying the appropriate quotient conditions for its $\mathbb{Z}_2$ orbifold, we find a Connes–Douglas–Schwarz type solution of matrix theory compactified on $\mathbb{T}^4_\theta/\mathbb{Z}_2$. When we consider two copies of a bundle on $\mathbb{T}^4_\theta$ invariant under the $\mathbb{Z}_2$ action, the resulting Higgs branch moduli space of equivariant constant curvature connections becomes an ordinary toroidal orbifold $\mathbb{T}^4/\mathbb{Z}_2$. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The pioneering work of Connes, Douglas, and Schwarz (CDS)[1] revealing the equivalence between noncommutative Yang–Mills theory living on the noncommutative torus and toroidally compactified IKKT (and also BFSS) M(atrix) theory[2,3] with the constant three-form background field has spurred various works[4] on noncommutative geometry and M/string theory since then. It has soon been known that the T-duality of M(atrix) theory can be understood in terms of Morita equivalence of the vector bundles over noncommutative tori.[5,6]

Many of these works have been related to the torus compactification and not much has been addressed to the noncommutative orbifold case. Recently, Konechny and Schwarz[7] worked out the compactification of M(atrix) theory on the $\mathbb{Z}_2$ orbifold of the noncommutative two-torus. However, physically more relevant compactification on the $\mathbb{Z}_2$ orbifold of noncommutative four-torus, a singular $K3$ surface, has not been worked out so far. In the commutative case, systems of D0-branes on the commutative orbifold $\mathbb{T}^4/\mathbb{Z}_2$ were studied in Refs. 8 and 9, and it is our main objective to extend the result of Ref. 8 to the noncommutative case.

We consider the compactification in the context of IKKT M(atrix) model[2] on the orbifold $\mathbb{T}^4/\mathbb{Z}_2$ where $\mathbb{Z}_2$ acts as a central symmetry $x \mapsto -x$. Thus, we need to find a Hilbert space $\mathcal{H}$ and unitary representations of $\mathbb{T}^4$ and $\mathbb{Z}_2$ on $\mathcal{H}$ and Hermitian operators X such that

$$U_i X_j U_i^{-1} = X_j + 2\pi\delta_i^j R_i, \quad i,j = 1, \ldots, 4, \tag{1}$$

$$U_i X_\nu U_i^{-1} = X_\nu, \tag{2}$$

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$$\Omega X_i \Omega = -X_i, \tag{3}$$

$$\Omega X_\nu \Omega = X_\nu, \quad \nu = 0,5,\ldots,9. \tag{4}$$

Following the description of Refs. 10 and 7 we can find operator relations compatible with the quotient conditions (1)–(4):

$$U_i U_j = e^{2\pi i \theta_{ij}} U_j U_i, \tag{5}$$

$$\Omega U_i \Omega = U_i^{-1}, \quad \Omega^2 = 1. \tag{6}$$

When $\theta = 0$, the relations (5) and (6) describe a $\mathbb{Z}_2$ equivariant vector bundle on the $\mathbb{Z}_2$ space $\mathbb{T}^4$ and X_i specify an equivariant connection on the bundle. Now the equivariant version of the Serre–Swan theorem indicates that there is a one-to-one correspondence between $\mathbb{Z}_2$ equivariant vector bundles on the $\mathbb{Z}_2$ space $\mathbb{T}^4$ and finitely generated projective modules over the crossed product C^*-algebra $C(\mathbb{T}^4) \rtimes_\alpha \mathbb{Z}_2$. As a noncommutative analog we see that the relations (5) and (6) imply that the Hilbert space $\mathcal{H}$ is simply a module over the crossed product algebra $C(\mathbb{T}^4_\theta) \rtimes_\alpha \mathbb{Z}_2$ or $\mathcal{A}_\theta \rtimes_\alpha \mathbb{Z}_2$, where α denotes the action of $\mathbb{Z}_2$ on $\mathcal{A}_\theta$ by involution. The crossed product $\mathcal{A}_\theta \rtimes_\alpha \mathbb{Z}_2$ is the C^*-completion of the linear space of $\mathcal{A}_\theta$-valued functions on $\mathbb{Z}_2$. Thus a general element of $\mathcal{A}_\theta \rtimes_\alpha \mathbb{Z}_2$ is a formal linear combination of elements of the form $\Pi_i U_i^{n_i} \Omega^{\epsilon_i}$, where $\epsilon_i \in \{0,1\}$. As noted in Ref. 7, an $\mathcal{A}_\theta$-module is a finitely generated projective module if and only if its corresponding module over $\mathcal{A}_\theta \rtimes_\alpha \mathbb{Z}_2$ is finitely generated projective. Thus, bundles on a noncommutative (NC) torus $\mathbb{T}^4_\theta$ are closely related with bundles on the noncommutative torodial orbifold $\mathbb{T}^4_\theta / \mathbb{Z}_2$.

In this article we find a projective module solution to the quotient conditions (1)–(4). First we calculate a CDS type solution of M(atrix) theory compactified on the noncommutative four-torus. There, we also show explicitly that the dual tori are actually related to each other through SO(4,4|$\mathbb{Z}$) transformations. From this solution we discuss that the moduli space of constant curvature connections can be identified with ordinary four-torus. Based on such an explicit CDS type solution on noncommutative $\mathbb{T}^4$, we find its $\mathbb{Z}_2$ orbifold solutions extending the result of Ref. 8 to the noncommutative torodial orbifold $\mathbb{T}^4_\theta / \mathbb{Z}_2$.

In Sec. II, we review the projective modules over noncommutative torus. In Sec. III, we construct a projective module on noncommutative four-torus *a la* Rieffel[11] explicitly, and find a CDS type solution of M(atrix) theory compactified on the noncommutative four-torus. It is also shown that the dual torus is actually related via SO(4,4|$\mathbb{Z}$) transformation. In Sec. IV, we find a solution for the noncommutative toroidal orbifold. From this solution we study the moduli space of equivariant constant curvature connections. We conclude in Sec. V.

II. NONCOMMUTATIVE VECTOR BUNDLES OVER NONCOMMUTATIVE TORUS

In this section we review noncommutative vector bundles over NC d-torus $\mathbb{T}^d_\theta$, following the lines of Refs. 12, 11, 5, and 6. Recall that $\mathbb{T}^d_\theta$ is the deformed algebra of the algebra of smooth functions on the torus $\mathbb{T}^d$ with the deformation parameter θ, which is a real $d \times d$ anti-symmetric matrix. This algebra is generated by operators $U_1, \ldots, U_d$ obeying the following relations:

$$U_i U_j = e^{2\pi i \theta_{ij}} U_j U_i \quad \text{and} \quad U_i^* U_i = U_i U_i^* = 1, \quad i,j = 1,\ldots,d.$$

The above relations define the presentation of the involutive algebra

$$\mathcal{A}^d_\theta = \left\{ \sum a_{i_1 \cdots i_d} U_1^{i_1} \cdots U_d^{i_d} \,\middle|\, a = (a_{i_1 \cdots i_d}) \in \mathcal{S}(\mathbb{Z}^d) \right\},$$

where $\mathcal{S}(\mathbb{Z}^d)$ is the Schwartz space of sequences with rapid decay. According to the dictionary in Ref. 13, the construction of a noncommutative vector bundle over $\mathbb{T}^d_\theta$ corresponds to the construc-

tion of finitely generated projective modules over $\mathcal{A}_\theta^d$. It was proved in Ref. 11 that when θ is not rational, every projective module over a smooth Algebra $\mathcal{A}_\theta^d$ can be represented by a direct sum of modules of the form $\mathcal{S}(\mathbb{R}^p\times\mathbb{Z}^q\times F)$, the linear space of Schwartz functions on $\mathbb{R}^p\times\mathbb{Z}^q\times F$, where $2p+q=d$ and F is a finite Abelian group. The module action is specified by operators on $\mathcal{S}(\mathbb{R}^p\times\mathbb{Z}^q\times F)$ and the commutation relation of these operators should be matched with that of elements in $\mathcal{A}_\theta^d$.

On such bundles or modules there are notions of connections and the Chern character.[1,5,6,14] Recall that there is the dual action of the torus group $\mathbb{T}^d$ on $\mathcal{A}_\theta^d$ which gives a Lie group homomorphism of $\mathbb{T}^d$ into the group of automorphisms of $\mathcal{A}_\theta^d$. Its infinitesimal form generates a homomorphism of Lie algebra L of $\mathbb{T}^d$ into Lie algebra of derivations of $\mathcal{A}_\theta^d$. Note that the Lie algebra L is Abelian and is isomorphic to $\mathbb{R}^d$. Let $\delta: L\to \mathrm{Der}(\mathcal{A}_\theta^d)$ be the homomorphism. For each $X\in L$, $\delta(X):=\delta_X$ is a derivation, i.e., for $u,v\in\mathcal{A}_\theta^d$,

$$\delta_X(uv)=\delta_X(u)v+u\,\delta_X(v).$$

Derivations corresponding to the generators $\{e_1,\ldots,e_d\}$ of L will be denoted by $\delta_1,\ldots,\delta_d$. For the generators U_i's of $\mathbb{T}_\theta^d$, it has the following property:

$$\delta_i(U_j)=2\pi i\,\delta_{ij}\cdot U_j.$$

If E is a projective $\mathcal{A}_\theta^d$-module, a connection ∇ on E is a linear map from E to $E\otimes L^*$ such that for all $X\in L$,

$$\nabla_X(\xi u)=(\nabla_X\xi)u+\xi\delta_X(u),\quad \xi\in E, u\in\mathcal{A}_\theta^d.$$

It is easy to see that

$$[\nabla_i,U_j]=2\pi i\,\delta_{ij}\cdot U_j.$$

Furthermore, for an $\mathcal{A}_\theta^d$-valued inner product $\langle\cdot,\cdot\rangle$ on E, if ∇ has the property that

$$\langle\nabla_X\xi,\eta\rangle+\langle\xi,\nabla_X\eta\rangle=\delta_X(\langle\xi,\eta\rangle),$$

then it is called a Hermitian connection. The curvature $\mathcal{F}_\nabla$ of a connection ∇ is a two-form on L with values in the algebra of endomorphisms of E. That is, for $X,Y\in L$,

$$\mathcal{F}_\nabla(X,Y):=[\nabla_X,\nabla_Y]-\nabla_{[X,Y]}.$$

Since L is Abelian, we simply have $\mathcal{F}_\nabla(X,Y)=[\nabla_X,\nabla_Y]$. Denote by $\mathcal{E}=\mathrm{End}_{\mathcal{A}_\theta}(E)$ the algebra of endomorphisms of E. Note that if ∇ and ∇' are two connections, then $\nabla_X-\nabla'_X$ belongs to the algebra $\mathcal{E}$. Thus once we have fixed a connection ∇, then every other connection is of the form $\nabla+A$ (here A is a linear map L into $\mathcal{E}$). Moreover, the space of Hermitian connections is an affine space with vector space consisting of the linear maps from L into the skew-adjoint part of $\mathcal{E}$ and also the algebra is related with a moduli space of a certain connections.

We now consider the endomorphisms algebra of a module over $\mathcal{A}_\theta^d$. Let Λ be a lattice in $H=M\times\hat{M}$, where $M=\mathbb{R}^p\times\mathbb{Z}^q\times F$ and $\hat{M}$ is its dual. Let T be the corresponding embedding map in the sense of Ref. 11. Thus Λ is the image of $\mathbb{Z}^d$ under the map T and this determines a projective module which will be denoted by E_Λ. Consider the lattice

$$\Lambda^\perp:=\{(m,\hat{s})\in M\times\hat{M}\,|\,\theta((m,\hat{s}),(n,\hat{t}))=\hat{t}(m)-\hat{s}(n)\in\mathbb{Z},\quad \text{for all}\quad (n,\hat{t})\in\Lambda\}.$$

From the definition, it is easy to see that every operator of the form

$$\mathcal{U}_{(m,\hat{s})}f(n)=e^{2\pi i\hat{s}(n)}f(n+m)$$

for $(m,\hat{s}) \in \Lambda^{\perp}$ commutes with all operators $\mathcal{U}_{(n,\hat{t})}$, $(n,\hat{t}) \in \Lambda$. In fact, one can show that the algebra of endomorphisms on E_{Λ}, denoted by $\mathrm{End}_{\mathcal{A}_\theta}(E_{\Lambda})$, is a C^*-algebra which is obtained by C^*-completion of the space spanned by operators $\mathcal{U}_{(m,\hat{s})}$, $(m,\hat{s}) \in \Lambda^{\perp}$. As shown in Ref. 11, the algebra $\mathrm{End}_{\mathcal{A}_\theta}(E_{\Lambda})$ can be identified with a noncommutative torus $\mathcal{A}_{\hat{\theta}}$ (here $\hat{\theta}$ is a bilinear form on $\Lambda^{\perp}$), i.e., $\mathcal{A}_{\hat{\theta}}$ is Morita equivalent to $\mathcal{A}_\theta$. Recall that a C^*-algebra A is said to be (strongly) Morita equivalent to A' if $A' \cong \mathrm{End}_A(E)$ for some finite projective module E. In general, as was proved in Ref. 6, a NC torus $\mathcal{A}_{\tilde{\theta}}$ is Morita equivalent to $\mathcal{A}_\theta$ if θ and $\tilde{\theta}$ are related by $\tilde{\theta} = (A\theta + B)(C\theta + D)^{-1}$, where $\left(\begin{smallmatrix} A & B \\ C & D \end{smallmatrix}\right) \in \mathrm{SO}(d,d|\mathbb{Z})$.

We shall now turn to the description of the Chern character. In general $K_0(\mathcal{A}_\theta^d)$ classifies projective modules over $\mathcal{A}_\theta^d$. In fact, the positive cone $K_0^+(\mathcal{A}_\theta^d)$ corresponds to genuine projective modules and, if θ is not rational, $K_0^+(\mathcal{A}_\theta^d)$ consists exactly of its elements of strictly positive trace. The Chern character of a gauge bundle, which corresponds to a projective module, on a noncommutative torus is an element in the Grassmann algebra $\wedge^{\cdot}(L^*)$, where L denotes the Lie algebra of $\mathbb{T}^d$ and L^* is the dual vector space of L. Since there is a lattice D in L, we see that there are elements of $\wedge^{\cdot} D^*$ which are integral. Now the Chern character is the map $\mathrm{Ch}: K_0(\mathcal{A}_\theta^d) \to \wedge^{\mathrm{ev}}(L^*)$ defined by

$$\mathrm{Ch}(E) := \hat{\tau}(e^{\mathcal{F}/2\pi i}) = \sum_{k=0} \frac{1}{(2\pi i)^k} \frac{\hat{\tau}(\mathcal{F}^k)}{k!},$$

where E is any gauge bundle and $\mathcal{F}$ is a curvature of an arbitrary connection on E and $\hat{\tau}$ is a trace on the algebra of endomorphisms. In general the Chern character is integral in the commutative case. This is no longer true for the noncommutative case. However, in the case of noncommutative torus, there is an integral element related to the Chern character by the formula

$$\mathrm{Ch}(E) = e^{i(\theta)} \mu(E). \tag{7}$$

Here $i(\theta)$ denotes the contraction with the deform parameter θ regarded as an element of $\wedge^2 L$. The formula (7) can be realized as a noncommutative generalization of Mukai vector.[15,16] In particular, $\mu(E) = e^{-i(\theta)}\mathrm{Ch}(E)$ is an integral element of $\wedge^{\cdot}(L^*)$ which is related with the Chern character on the classical torus. Also once we fix the deformation parameter, then the Chern character $\mathrm{Ch}(E)$ is completely determined by its integral part $\mu(E)$. Note that if, for θ not rational, the zeroth component of the Chern character or the trace is strictly positive, then the gauge bundle E belongs to the positive cone of $K_0(\mathcal{A}_\theta^d)$ and hence it can be written as a direct sum of the form $\mathcal{S}(\mathbb{R}^p \times \mathbb{Z}^q \times F)$.[11]

III. COMPACTIFICATION ON NONCOMMUTATIVE $\mathbb{T}^4$

In this section we study the compactification solutions on a noncommutative four-torus $\mathbb{T}_\theta^4$ for the case $e^{2\pi i \theta_{ij}} \neq 1$, following the guide line in Ref. 1. After we fix U_1, U_2, U_3 and U_4, or a projective module, the general solution has the form of $X_i = \overline{X_i} + A_i$, where $\overline{X_i}$ are particular solutions and A_i are operators commuting with U_i. Here we consider a projective module of the form $\mathcal{S}(\mathbb{R}^p \times \mathbb{Z}^q) \otimes \mathcal{S}(F)$, where $2p+q=4$. Thus there are three types of modules over $\mathcal{A}_\theta$ according to $p=0,1,2$. When $p=0$, it is a free module. The other two types are of the form $\mathcal{S}(\mathbb{R} \times \mathbb{Z}^2) \otimes \mathcal{S}(F)$ and $\mathcal{S}(\mathbb{R}^2) \otimes \mathcal{S}(F)$. As is discussed in Sec. II, a gauge bundle on $\mathbb{T}_\theta^4$ corresponds to an element of positive trace which is the zeroth component of the Chern character and the Chern character is determined by its integral part μ. Thus it is natural to start with the construction on $\mathcal{S}(F)$ to describe projective modules. Here we will only consider the case when $p=2$, which is related with (4220)-systems with a constant curvature considered in Ref. 17 and 18. Let $F = \mathbb{Z}_{M_1} \times \mathbb{Z}_{M_2}$, where $\mathbb{Z}_{M_i} = \mathbb{Z}/M_i\mathbb{Z}$, $(i=1,2)$ and consider the space $\mathbb{C}^{M_1} \otimes \mathbb{C}^{M_2}$ as the space of functions on $C(\mathbb{Z}_{M_1} \times \mathbb{Z}_{M_2})$. For all $M_i \in \mathbb{Z}$ and $N_i \in \mathbb{Z}/M_i\mathbb{Z}$ such that M_i and N_i are relatively prime, define operators W_i on $C(\mathbb{Z}_{M_1} \times \mathbb{Z}_{M_2})$ by

$$(W_1 f)(k_1,k_2)=f(k_1-N_1,k_2), \quad (W_2 f)(k_1,k_2)=\exp\left(-\frac{2\pi i k_1}{M_1}\right) f(k_1,k_2),$$

$$(W_3 f)(k_1,k_2)=f(k_1,k_2-N_2), \quad (W_4 f)(k_1,k_2)=\exp\left(-\frac{2\pi i k_2}{M_2}\right) f(k_1,k_2).$$

The operators satisfy the commutation relation

$$W_1 W_2=\exp\left(2\pi i \frac{N_1}{M_1}\right) W_2 W_1, \quad W_3 W_4=\exp\left(2\pi i \frac{N_2}{M_2}\right) W_4 W_3,$$

otherwise commuting. If we write $W_i W_j=\exp(2\pi i \psi_{ij}) W_j W_i$, then the antisymmetric 4×4 matrix $\psi=(\psi_{ij})$ is of the form

$$\psi=\begin{pmatrix} 0 & \frac{N_1}{M_1} & 0 & 0 \\ -\frac{N_1}{M_1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{N_2}{M_2} \\ 0 & 0 & -\frac{N_2}{M_2} & 0 \end{pmatrix}. \tag{8}$$

Let $T:\mathbb{Z}^4\to\mathbb{R}^2\times\mathbb{R}^{2*}$ be an embedding map. Thus its matrix representation $T=(x_{ij})$, $i,j=1,\ldots,4$, has nonzero determinant and satisfies $(\wedge^2 T^*)(\omega)=-\gamma$ where $\omega=e_3\wedge e_1+e_4\wedge e_2 \in\wedge^2(\mathbb{Z}^4)$ and e_i are standard basis for $\mathbb{Z}^4$. Equivalently, if we consider the Heisenberg representation of $\mathbb{Z}^4$ in a Hilbert space, the desired operators acting on the space of smooth functions on $\mathbb{R}^2$ are defined by the following form:

$$(V_i f)(s_1,s_2)=(V_{e_i} f)(s_1,s_2) := \exp(2\pi i(s_1 x_{3i}+s_2 x_{4i})) f(s_1+x_{1i},s_2+x_{2i}).$$

These operators obey the commutation relation

$$V_i V_j=e^{-2\pi i \gamma_{ij}} V_j V_i,$$

where

$$\gamma_{ij}=\begin{vmatrix} x_{1i} & x_{1j} \\ x_{3i} & x_{3j} \end{vmatrix}+\begin{vmatrix} x_{2i} & x_{2j} \\ x_{4i} & x_{4j} \end{vmatrix}.$$

Since γ is a real matrix, the operators V_i act on the Schwartz space $\mathcal{S}(\mathbb{R}^2)$. Now we define operators $U_i=V_i\otimes W_i$ acting on the space $E_T:=\mathcal{S}(\mathbb{R}^2)\otimes\mathbb{C}^{M_1}\otimes\mathbb{C}^{M_2}$ as follows:

$$(U_1 f)(s_1,s_2,k_1,k_2)=e^{2\pi i(s_1 x_{31}+s_2 x_{41})} f(s_1+x_{11},s_2+x_{21},k_1-N_1,k_2),$$

$$(U_2 f)(s_1,s_2,k_1,k_2)=e^{2\pi i(s_1 x_{32}+s_2 x_{42})}\cdot e^{-2\pi i k_1/M_1} f(s_1+x_{12},s_2+x_{22},k_1,k_2),$$

$$(U_3 f)(s_1,s_2,k_1,k_2)=e^{2\pi i(s_1 x_{33}+s_2 x_{43})} f(s_1+x_{13},s_2+x_{23},k_1,k_2-N_2),$$

$$(U_4 f)(s_1,s_2,k_1,k_2)=e^{2\pi i(s_1 x_{34}+s_2 x_{44})}\cdot e^{-2\pi i k_2/M_2} f(s_1+x_{14},s_2+x_{24},k_1,k_2).$$

Then it is easy to see that they satisfy

$$U_iU_j=\exp(-2\pi i\gamma_{ij}+2\pi i\psi_{ij})U_jU_i.$$

Thus we have solution of (5) if $\gamma=\psi-\theta$.

Consider operators $\overline{X_i}$ acting on $E_T=\mathcal{S}(\mathbb{R}^2)\otimes\mathbb{C}^{M_1}\otimes\mathbb{C}^{M_2}$ given by

$$(\overline{X_i}f)(s_1,s_2,k_1,k_2)=2\pi iA_i^1s_1f(s_1,s_2,k_1,k_2)+2\pi iA_i^2s_2f(s_1,s_2,k_1,k_2)$$
$$-A_i^3\frac{\partial f(s_1,s_2,k_1,k_2)}{\partial s_1}-A_i^4\frac{\partial f(s_1,s_2,k_1,k_2)}{\partial s_2}, \tag{9}$$

where A_i^k are any real numbers yet to be determined. From the definition of U_i and $\overline{X_i}$, it is easy to see that the operators W_i commute with $\overline{X_i}$. Suppose that the operators $\overline{X_i}$ satisfy the equation (1), i.e.,

$$U_i\overline{X_j}U_i^{-1}=\overline{X_j}+2\pi\delta_i^jR_i.$$

By a straightforward calculation, the constant matrix (A_i^j) in (9) can be obtained as in the following form:

$$(R_iA_i^j)T=-i\,\mathrm{Id}.$$

Since the inverse matrix of T can be written as

$$T^{-1}=\frac{1}{\det T}((-1)^{i+j}B_{ji}),$$

where B_{ij} is the (ij)-minor of the matrix T, we see that

$$A_i^k=(-1)^{i+k}\cdot\frac{R_i}{i}\cdot\frac{1}{\det T}\cdot B_{ki}, \tag{10}$$

and this gives a particular solution to the equations (2) and (3). It is easy to check that the commutator is of the form

$$[\overline{X_i},\overline{X_j}]=2\pi i\left(\begin{vmatrix}A_i^1 & A_i^3\\ A_j^1 & A_j^3\end{vmatrix}+\begin{vmatrix}A_i^2 & A_i^4\\ A_j^2 & A_j^4\end{vmatrix}\right).$$

By (10), we have

$$[\overline{X_i},\overline{X_j}]=-2\pi i\cdot\frac{R_iR_j}{(\det T)^2}\left\{(-1)^{i+1}(-1)^{j+1}\begin{vmatrix}B_{1i} & B_{3i}\\ B_{1j} & B_{3j}\end{vmatrix}+(-1)^i(-1)^j\begin{vmatrix}B_{2i} & B_{4i}\\ B_{2j} & B_{4j}\end{vmatrix}\right\}$$
$$=2\pi i(-1)^{i+j+1}\cdot\frac{R_iR_j}{(\det T)^2}\left\{\begin{vmatrix}B_{1i} & B_{3i}\\ B_{1j} & B_{3j}\end{vmatrix}+\begin{vmatrix}B_{2i} & B_{4i}\\ B_{2j} & B_{4j}\end{vmatrix}\right\}$$
$$=2\pi i(-1)^{i+j+1}\cdot\frac{R_iR_j}{\det T}\cdot*\gamma_{ij}.$$

Now we should find generators of the set of operators which commute with U_i's. To find such operators we need to describe an embedding map which corresponds to the dual lattice of the lattice defined by the embedding map T as discussed in Sec. II. For such a map, let

$$S=\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}\cdot (T^t)^{-1}=\frac{1}{\det T}\begin{pmatrix} B_{31} & -B_{32} & B_{33} & -B_{34} \\ -B_{41} & B_{42} & -B_{43} & B_{44} \\ -B_{11} & B_{12} & -B_{13} & B_{14} \\ B_{21} & -B_{22} & B_{23} & -B_{24} \end{pmatrix}. \tag{11}$$

Using the matrix (11), we define operators acting on E_T by

$$(Z_1 f)(s_1,s_2,k_1,k_2)=e^{2\pi i(-s_1B_{11}+s_2B_{21})/M_1|T|}\cdot e^{2\pi i b_1 k_1/M_1} f\left(s_1+\frac{B_{31}}{M_1|T|},s_2-\frac{B_{41}}{M_1|T|},k_1,k_2\right),$$

$$(Z_2 f)(s_1,s_2,k_1,k_2)=e^{2\pi i(s_1B_{12}-s_2B_{22})/M_1|T|} f\left(s_1-\frac{B_{32}}{M_1|T|},s_2+\frac{B_{42}}{M_1|T|},k_1-1,k_2\right),$$

$$(Z_3 f)(s_1,s_2,k_1,k_2)=e^{2\pi i(-s_1B_{13}+s_2B_{23})/M_2|T|}\cdot e^{2\pi i b_2 k_1/M_2} f\left(s_1+\frac{B_{33}}{M_2|T|},s_2-\frac{B_{43}}{M_2|T|},k_1,k_2\right),$$

$$(Z_4 f)(s_1,s_2,k_1,k_2)=e^{2\pi i(s_1B_{14}-s_2B_{24})/M_2|T|} f\left(s_1-\frac{B_{34}}{M_2|T|},s_2+\frac{B_{44}}{M_2|T|},k_1,k_2-1\right),$$

where $|T|=\mathrm{Pf}(\psi-\theta)$ denotes the determinant of T and b_1, b_2 are integers such that $a_iM_i+b_iN_i=1$, and a_i are also integers. To check the operators Z_i commute with all U_j's, let $Z_iU_j=e^{2\pi i\lambda_{ij}}U_jZ_i$. Then it is easy to see that

$$\lambda_{ij}=\frac{1}{M_k|T|}\left\{\begin{vmatrix} x_{1i} & x_{3i} \\ (-1)^{3+j}B_{3j} & (-1)^{1+j}B_{1j}\end{vmatrix}+\begin{vmatrix} x_{2i} & x_{4i} \\ (-1)^{4+j}B_{4j} & (-1)^{2+j}B_{2j}\end{vmatrix}\right\}-\delta_{ij}\frac{b_kN_k}{M_k}, \tag{12}$$

where $k=1,2$ depending on ij. From the relation (12),

$$\lambda_{ij}=0 \quad \text{when } i\neq j,$$

$$\lambda_{ii}=\frac{1}{M_k}-\frac{b_kN_k}{M_k}=\frac{-a_kM_k}{M_k}=-a_k\in\mathbb{Z}.$$

Thus Z_i commute with all U_j's.

Furthermore the operators satisfy

$$Z_iZ_j=e^{2\pi i\hat{\theta}}Z_jZ_i. \tag{13}$$

Now $\hat{\theta}$ can be calculated directly and it is given by

$$\hat{\theta}_{12}=\frac{a_1N_2+b_1N_2\theta_{12}+a_1M_2\theta_{34}-b_1M_2\mathrm{Pf}(\theta)}{M_1M_2\mathrm{Pf}(\psi-\theta)},\quad \hat{\theta}_{13}=\frac{\theta_{13}}{M_1M_2\mathrm{Pf}(\psi-\theta)},$$

$$\hat{\theta}_{14}=\frac{\theta_{14}}{M_1M_2\mathrm{Pf}(\psi-\theta)},\quad \hat{\theta}_{23}=\frac{\theta_{23}}{M_1M_2\mathrm{Pf}(\psi-\theta)},$$

$$\hat{\theta}_{24}=\frac{\theta_{24}}{M_1M_2\mathrm{Pf}(\psi-\theta)},\quad \hat{\theta}_{34}=\frac{a_2N_1+b_2N_1\theta_{34}+a_2M_1\theta_{12}-b_2M_1\mathrm{Pf}(\theta)}{M_1M_2\mathrm{Pf}(\psi-\theta)}.$$

Also we have

$$\hat{\theta}=(A\theta+B)(N-M\theta)^{-1}, \tag{14}$$

where

$$A=\begin{pmatrix} 0 & -a_1 & 0 & 0 \\ a_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -a_2 \\ 0 & 0 & a_2 & 0 \end{pmatrix}, \quad B=\begin{pmatrix} b_1 & 0 & 0 & 0 \\ 0 & b_1 & 0 & 0 \\ 0 & 0 & b_2 & 0 \\ 0 & 0 & 0 & b_2 \end{pmatrix}$$

and

$$N=\begin{pmatrix} N_1 & 0 & 0 & 0 \\ 0 & N_1 & 0 & 0 \\ 0 & 0 & N_2 & 0 \\ 0 & 0 & 0 & N_2 \end{pmatrix}, \quad M=\begin{pmatrix} 0 & M_1 & 0 & 0 \\ -M_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & M_2 \\ 0 & 0 & -M_2 & 0 \end{pmatrix}.$$

From the equation (14), we see that $-\theta$ and $\hat{\theta}$ are related by SO(4,4$|\mathbb{Z}$) transformation.

Note that U(n) theory on $\mathcal{A}_{-\theta}$ is equivalent to U(1) theory on $\mathcal{A}_{\hat{\theta}}$. For U(1) theory the generators Z_i can be identified with functions on the dual torus:

$$Z_j \to e^{i\sigma_j},$$

where σ_j are coordinates of the dual torus such that

$$[\sigma_i,\sigma_j]=-2\pi i\hat{\theta}_{ij}.$$

Now the general solution of the compactification is given by

$$X_i=\overline{X_i}+\sum_{i_1,\ldots,i_4\in\mathbb{Z}}\Psi_{i_1i_2i_3i_4}Z_1^{i_1}Z_2^{i_2}Z_3^{i_3}Z_4^{i_4},$$

where the coefficients $\Psi_{i_1i_2i_3i_4}$ are c-numbers.

Recall that a connection in a module E_T is determined by a set of operators $\nabla_1,\ldots,\nabla_4$ in E_T such that

$$[\nabla_i,U_j]=2\pi i\delta_{ij}U_j.$$

From the definition of $\overline{X_i}$ given in (9) we have

$$[\overline{X_i},U_j]=-2\pi\delta_{ij}R_jU_j.$$

Thus we see that the special solution $\overline{X_i}$ is related with connections by $\overline{X_i}=(R_i/i)\nabla_i$ and for such connection ∇, the constant curvature $\mathcal{F}=(\mathcal{F}_{ij})$ is given by

$$\mathcal{F}=\gamma^{-1}\cdot \mathrm{Id}_N, \quad \text{where } N=N_1N_2. \tag{15}$$

Now the general solution should be identified as

$$X_i=\frac{R_i}{i}\nabla_i+A_i(\sigma_1,\sigma_2,\sigma_3,\sigma_4), \tag{16}$$

where A_i are gauge fields defined on a noncommutative torus.

Note that from the curvature form (15), it corresponds to the $U(N)$ gauge theory with vanishing su(N) curvature. This type of solution has been studied in Ref. 19 for noncommutative $\mathbb{T}^2$ and in Ref. 20 for the higher torus case. This was generalized to a nonvanishing su(N) curvature case in Ref. 17 and it has been noted that the analysis for noncommutative tori is the same as that of Ref. 18 for commutative tori. In fact the above solution has been described by (4220) system with trivial SU(N) gauge fields in Ref. 18 and its moduli space can be identified with $\mathbb{T}^4$. So we may expect that the moduli space of constant curvature connections in noncommutative torus is of the same form as in the ordinary torus.

The operators

$$\tilde{\nabla}_j=\frac{i}{R_j}\overline{X}_j+\alpha_j, \quad j=1,\ldots,4, \tag{17}$$

where α_j is any real number, determine a Hermitian connection with constant curvature in E_T. Furthermore, connections of the form (16) define a representation on $L^2(\mathbb{R}^2,\mathbb{C}^{M_1}\otimes\mathbb{C}^{M_2})$ of the Heisenberg commutation relations and from this one can follow the same steps in Ref. 12 to show that connections of the form (17) can be found in each gauge orbit and two such connections $(i/R_j)\overline{X}_j+\alpha_j$ and $(i/R_j)\overline{X}_j+\mu_j$ are gauge equivalent if and only if $\alpha_j-\mu_j\in\mathbb{Z}$. Thus the moduli space of constant curvature connections can be identified with $(\mathbb{R}/\mathbb{Z})^4\cong(S^1)^4\cong\mathbb{T}^4$. In general, if we consider a projective module consisting of n copies of such modules, such as $E_{T_1}\oplus\cdots\oplus E_{T_n}$, where T_i is an embedding, then there is a constant curvature connection on each summand such that the overall curvature is given by $\mathcal{F}=\oplus\mathcal{F}_k$, where $\mathcal{F}_k$ is given as in (15) with the same γ. Thus for a constant curvature connection on E which breaks a projective module E into $\oplus_k E_{T_i}$, block diagonal construction gives the moduli space of the form $(\mathbb{T}^4)^n/S_n$, where S_n is the symmetric group.

IV. COMPACTIFICATION ON NONCOMMUTATIVE TOROIDAL ORBIFOLD $\mathbb{T}_\theta/\mathbb{Z}_2$

In this section we find solutions for the quotient conditions (1)–(4) along with the projective module actions (5) and (6) via the compactification solutions on a noncommutative torus $\mathbb{T}^4_\theta$ obtained in Sec. III. From this we find the moduli space of equivariant constant curvature connections on noncommutative toroidal orbifold $\mathbb{T}^4_\theta/\mathbb{Z}_2$.

Consider the module $E_T:=\mathcal{S}(\mathbb{R}^2)\otimes C(\mathbb{Z}_{M_1})\otimes C(\mathbb{Z}_{M_2})$ together with U_i's as operators acting on it. The general solution for the quotient conditions has been identified as

$$X_j=\frac{R_j}{i}\nabla_j+A_j(\sigma_1,\sigma_2,\sigma_3,\sigma_4), \quad 1\leqslant j\leqslant 4. \tag{18}$$

To find solutions for the quotient conditions on the compactified part we need to solve for Ω which satisfies $\Omega U_i\Omega=U_i^{-1}$ and $\Omega^2=1$. Consider an operator Ω_0 on E_T defined by

$$(\Omega_0 f)(s_1,s_2,k_1,k_2)=f(-s_1,-s_2,-k_1,-k_2).$$

It is easy to see that $\Omega_0U_i\Omega_0U_i=e^{2\pi i(x_{1i}x_{3i}+x_{2i}x_{4i})}$. By redefining $U_i\mapsto e^{-\pi i(x_{1i}x_{3i}+x_{2i}x_{4i})}U_i$, we get $\Omega_0U_i\Omega_0=U_i^{-1}$ and $\Omega_0^2=1$. Thus we have a solution for (6), i.e., Ω_0 together with U_i's define a projective module over $\mathcal{A}_\theta\rtimes\mathbb{Z}_2$. As was indicated in Ref. 7, there might be other $\mathbb{Z}_2$ actions on the module. To get other actions on the module, consider the operators Z_i defined in Sec. III. As for the U_i's, rescale Z_i by $e^{-\pi i(B_{1i}B_{3i}+B_{2i}B_{4i})}Z_i$ and we get the relation

$$\Omega_0Z_i\Omega_0=Z_i^{-1}. \tag{19}$$

Since Z_i commute with all U_j's, the operators $\Omega_{n_1\cdots n_4}=e^{i\phi}\Omega_0Z_1^{n_1}Z_2^{n_2}Z_3^{n_3}Z_4^{n_4}$ ($n_i\in\mathbb{Z}$) satisfy the equation (6), where ϕ is a phase which is chosen to get the relation $\Omega^2=1$ and it can be calculated explicitly by using the commutation relations given in (13). Now consider the general solution

(18) satisfying (1) and (2). Recall $\nabla_i=(i/R_i)\overline{X_i}$. For $\overline{X_i}$, which was defined in (9), it is easy to verify that $\Omega_0\overline{X_i}\Omega_0=-\overline{X_i}$. But since $\overline{X_i}$ do not commute with Z_i's, we see that Ω_0 is the unique solution for the equation $\Omega\overline{X_i}\Omega=-\overline{X_i}$. By definition of the functions A_i on the dual torus and by the relation (19), we have $\Omega_0 A_i(\sigma_1,\sigma_2,\sigma_3,\sigma_4)\Omega_0=A_i(-\sigma_1,-\sigma_2,-\sigma_3,-\sigma_4)$. Applying Ω_0 to the both sides of the equation (18) we see that

$$A_i(-\sigma_1,-\sigma_2,-\sigma_3,-\sigma_4)=-A_i(\sigma_1,\sigma_2,\sigma_3,\sigma_4), \tag{20}$$

which implies that the functions A_i are odd functions. If we consider a constant curvature connection ∇ on E_T, the functions A_i in (20) can be represented by a real constant and hence it vanishes. In other words the moduli space has no Higgs branch. Note that this type of solution has been studied in Ref. 8 for the ordinary torodial orbifold $\mathbb{T}^4/\mathbb{Z}_2$ under the name of Rep. II.

In the above representation, the moduli space of constant curvature connections on E_T over $\mathbb{T}^4_\theta$ is not preserved by the $\mathbb{Z}_2$ action on E_T. So it may be more natural to consider two copies of E_T which respect the $\mathbb{Z}_2$ action and this corresponds to Rep. I of Ref. 8. Consider the bundle of the form $E_T^2=E_T\oplus E_T$ and define operators acting on E_T^2 by

$$\Omega=\begin{pmatrix}\Omega_0 & 0\\ 0 & -\Omega_0\end{pmatrix} \quad \text{and} \quad \mathbf{U}_i=\begin{pmatrix}U_i & 0\\ 0 & U_i\end{pmatrix},$$

where Ω_0 and U_i's are operators on E_T given as above and in Sec. III. Then it is easy to check that

$$\begin{aligned}\mathbf{U}_i\mathbf{U}_j&=e^{2\pi i\theta_{ij}}\mathbf{U}_j\mathbf{U}_i,\\ \Omega\mathbf{U}_i\Omega&=\mathbf{U}_i^{-1} \quad \text{and} \quad \Omega^2=1.\end{aligned} \tag{21}$$

Thus the relations (21) defines a projective module over $\mathcal{A}_\theta\rtimes\mathbb{Z}_2$. Since $\overline{X_i}$ defines a particular solution, we may write the general solution on the torus as follows:

$$X_i=\overline{X_i}+\begin{pmatrix}A_i^{11} & A_i^{12}\\ A_i^{21} & A_i^{22}\end{pmatrix}.$$

Since the matrix $\left(\begin{smallmatrix}A_i^{11} & A_i^{12}\\ A_i^{21} & A_i^{22}\end{smallmatrix}\right)$ should commute with all the $\mathbf{U}_i$'s, each entry A_i^{jk} commutes with U_i's. In other words, the operators A_i^{jk} are generated by Z_i's. Thus they can be identified with functions on the dual torus. Now the general solutions should be identified as

$$X_i=\frac{R_i}{i}\nabla_i+\begin{pmatrix}A_i^{11}(\sigma_j) & A_i^{12}(\sigma_j)\\ A_i^{21}(\sigma_j) & A_i^{22}(\sigma_j)\end{pmatrix}. \tag{22}$$

By applying Ω we find

$$\begin{pmatrix}A_i^{11}(-\sigma_j) & A_i^{12}(-\sigma_j)\\ A_i^{21}(-\sigma_j) & A_i^{22}(-\sigma_j)\end{pmatrix}=\begin{pmatrix}-A_i^{11}(\sigma_j) & A_i^{12}(\sigma_j)\\ A_i^{21}(\sigma_j) & -A_i^{22}(\sigma_j)\end{pmatrix}.$$

Note that the diagonal entries of the matrix in (22) are odd functions on the dual torus, and this fact will be used in finding the moduli space below. Meanwhile, the off-diagonal entries are even fuctions of σ. Here, the gauge transformation should be invariant under Ω implementing the $\mathbb{Z}_2$ quotient condition. This implies that the gauge parameter in general should be given by $\Lambda=\left(\begin{smallmatrix}\lambda_{ev}^{11} & \lambda_{od}^{12}\\ \lambda_{od}^{21} & \lambda_{ev}^{22}\end{smallmatrix}\right)$, where the subscript ev or od indicates an even or odd function of σ. This indicates to us that not all the $U(2)$ group acts. We now consider the constant curvature connection ∇ on E_T considered in Sec. III. In this case, as discussed in Rep. II, we have constant gauge field in (22).

Thus the diagonal entries vanish and the bundle becomes singular at the fixed points. For the ordinary case this has been related to the existence of two-brane charge at the collapsing two-cycle of the blown-up space.[21–23]

Now the solutions of the constant curvature connection in this case are given by

$$X_i=\overline{X_i}+\begin{pmatrix} 0 & A_i^{12}(\sigma_j) \\ A_i^{12\dagger}(\sigma_j) & 0 \end{pmatrix}.$$

One of the A_i components can be gauged away by constant gauge transformation of the type $\left(\begin{smallmatrix}\lambda & 0\\ 0 & \lambda\end{smallmatrix}\right)$ which can be decomposed into two parts, one proportional to the identity and the other proportional to $\sigma_3=\left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$. Since we are only considering constant gauge transformations in dealing with the moduli space, the noncommutativity does not affect the result as in Sec. III. The remaining component of A_i has translational symmetry of the commutative four-torus. This fact together with a residual guage symmetry σ_3 now yields a Higgs branch moduli space of constant curvature connections to be an ordinary torodial orbifold $\mathbb{T}^4/\mathbb{Z}_2$.

For the uncompactified X_ν sector, the solution is the same as in the commutative case;[8] the moduli becomes $\mathbb{R}^5\times\mathbb{R}^5$ when $A_i=0$, and when $A_i\neq 0$ the transverse moduli becomes $\mathbb{R}^5$ for generic points in $\mathbb{T}^4/\mathbb{Z}_2$, and $\mathbb{R}^5\times\mathbb{R}^5$ at the fixed points in $\mathbb{T}^4/\mathbb{Z}_2$. Thus this can be viewed as a fibration over the Higgs branch of $\mathbb{T}^4/\mathbb{Z}_2$, with the fiber $\mathbb{R}^5$ at a generic point and with the fiber $\mathbb{R}^5\times\mathbb{R}^5$ at the orbifold fixed points as suggested in the commutative case.[8]

For the ordinary $\mathbb{T}^4$, the discussion above corresponds to the construction of the theory of zero branes on $\mathbb{T}^4/\mathbb{Z}_2$. We first considered a T-duality on the covering torus $\mathbb{T}^4$ to a dual torus $\hat{\mathbb{T}}^4$ and then project to $\hat{\mathbb{T}}^4/\mathbb{Z}_2$. So, for N identical D0-branes on $\mathbb{T}^4/\mathbb{Z}_2$ we need $2N$ zero branes on $\mathbb{T}^4$. This is described by $U(2N)$ gauge theory and the gauge group is broken down to $U(N)\times U(N)$. In Ref. 8, it has been shown that the moduli space of the flat connections is identified with $\mathbb{T}^4/\mathbb{Z}_2$. In fact our earlier analysis on the moduli space of constant curvature connections is exactly the same as the one in Ref. 8.

V. CONCLUSION AND PROSPECT

In this article, we construct a bundle on noncommutative toroidal orbifold $\mathbb{T}^4_\theta/\mathbb{Z}_2$. We start with the construction of a bundle on noncommutative $\mathbb{T}^4$ *a la* Rieffel[11] and find a CDS type solution of M(atrix) theory compactified on the noncommutative four-torus. There, we also show explicitly that the dual tori are actually related to each other through SO(4,4$|\mathbb{Z}$) transformations. Based on our explicit CDS type solution on noncommutative $\mathbb{T}^4$, we find its $\mathbb{Z}_2$ orbifold solutions, Rep. I and Rep. II, by looking into the systems of D0-branes on the covering space projected onto their invariant parts under the discrete symmetry group. From the solutions obtained, we study the moduli space of equivariant constant curvature connections. The Higgs branch moduli space has been identified with the ordinary toroidal orbifold in the Rep. I case where we consider two copies of a bundle over $\mathbb{T}_\theta$ which are invariant under the $\mathbb{Z}_2$ action on $\mathbb{T}_\theta$. In the Rep. II case, the moduli space has no Higgs branch. In conclusion, in the noncommutative $\mathbb{T}^4/\mathbb{Z}_2$ case the moduli space has the same form as its commutative counterpart.

In Ref. 18, the moduli space of D0-branes on commutative $\mathbb{T}^4$ with torons of $U(N)$ Yang–Mills theory was given as $(\mathbb{T}^4)^{p_1}/S_{p_1}\times(\mathbb{T}^4)^{p_2}/S_{p_2}$ where the $U(N)$ gauge group is broken down into $U(k_1)\times U(k_2)$ satisfying $k_1+k_2=N$, and $p_i=gcd(k_i,m_i)$, $i=1,2$ with fluxes m_i of $U(k_i)$. Its extension to the noncommutative case has been recently studied in Ref. 17 using 't Hooft's SU(N) solution of nontrivial twists,[24] and the resulting moduli space of connections turned out to be of the same form, $(\mathbb{T}^4)^{p_1}/S_{p_1}\times(\mathbb{T}^4)^{p_2}/S_{p_2}$. We expect that the same holds for the noncommutative toroidal $\mathbb{Z}_2$ orbifold case.

Note added: After completion of our article, a related paper[25] has appeared which has some overlap with our paper. Their methodology to get the relevant moduli spaces is to use the theory of representation of Heisenberg algebra defined by the commutation relations of a fixed connec-

tion. On the other hand, our approach is the usual one in that we construct a module on $\mathbb{T}^4_\theta$ with explicit computation, and then consider the $\mathbb{Z}_2$ orbifold condition on this module finding the moduli space in the specific cases.

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A class of integrable Davey–Stewartson type systems

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A new integrable Davey–Stewartson type class of systems of partial differential equations in $2+1$ dimensions is derived from a previously known integrable equation by means of an asymptotically exact nonlinear reduction method based on Fourier expansion and spatio–temporal rescaling. The integrability by the inverse scattering method is explicitly demonstrated, because the reduction technique is applied to the Lax pair of the starting equation and the corresponding Lax pair of the class of systems of equations is found. The particular characteristics of the reduction method imply that the new systems are likely to be of applicative relevance. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1370396]

I. INTRODUCTION

Many nonlinear evolution partial differential equations (PDEs), for instance the nonlinear Schrodinger and the Davey–Stewartson equations, are both of wide applicative relevance and integrable, i.e., characterized by a very simple mathematical structure and solvable or via the inverse scattering method (*S*-integrable) or via an appropriate change of variables (*C*-integrable).

A simple explanation of this fact is based on the observation that very large classes of nonlinear evolution PDEs in $1+1$ and $2+1$ dimensions with a dispersive linear part can be reduced, by a limiting procedure involving the wave modulation induced by weak nonlinear effects, to a very limited number of ''universal'' nonlinear evolution PDEs. Moreover, the same model equations obtained in this way appear in many applicative situations (for instance in plasma physics, nonlinear optics, hydrodynamics, etc.), where weakly nonlinear effects are important.[1–4]

The reduction method preserves integrability and then the model equations are likely to be integrable; it is sufficient that the very large class of equations from which they are obtainable contains just one integrable equation, provided the limiting procedure preserves integrability and then the property of integrability is inherited through this limiting technique. Obviously, the last statement about the integrability is based on heuristic considerations and could not be characterized as a rigorous theorem, because no precise definition of integrability is available for nonlinear evolution PDEs.

Thus this approach, besides explaining why certain model equations are integrable and applicable, provides a powerful tool to investigate the relation among different integrable equations, to test the integrability of nonlinear evolution PDEs, and, most importantly, to identify integrable evolution equations that are likely to be of applicative relevance.

In preceding papers, this method has been applied to certain integrable equations in $2+1$ dimensions. The most interesting results are that the Davey–Stewarston equation[5,6] is the typical model equation in $2+1$ dimensions, while new integrable nonlinear PDEs can be obtained together with their Lax pair.[7–10] Moreover, the reduction method has been used to derive two equations of applicative relevance in plasma physics.[11,12]

The basic idea of the reduction method is to consider a nonlinear evolution PDE whose linear part is dispersive; as it is well known that the linear evolution is most appropriately described in terms of Fourier modes and each Fourier mode evolves with constant amplitude and an associated group velocity, which represents the speed with which a wave packet peaked at that Fourier mode

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would move in configuration space. To evaluate the weak nonlinear effects it is convenient to consider a specific Fourier mode and follow it by going over to a frame of reference that moves with its group velocity. The weak nonlinear effects may involve a non-negligible contribution, because they give rise to a modulation of the amplitude of that Fourier mode (that would remain constant in the absence of nonlinear effects). The modulation is best described in terms of rescaled ''coarse grained'' and ''slow'' variables, which permit us to consider the weak nonlinear effects on larger space and time scales. Indeed, the first step of the reduction method is to use a moving frame of reference with the introduction of the slow variables

$$\xi=\varepsilon^p(x-V_1t),\ \eta=\varepsilon^p(y-V_2t),\ \tau=\varepsilon^q t,$$
$$p>0,q>0, \tag{1.1}$$

where $V_1=V_1(K_1,K_2), V_2=V_2(K_1,K_2)$ are the components of the group velocity $\mathbf{V}(\mathbf{K}) \equiv (V_1(K_1,K_2),V_2(K_1,K_2))$ of the linearized equation, i.e., of the equation obtained after neglecting all the nonlinear terms, and ε is the expansion parameter, supposed to be sufficiently small. Therefore it is demonstrated that the function which represents the amplitude modulation satisfies, in terms of the rescaled, slow variables, evolution equations having a universal character; since the coarse-grained nature of the new variables implies that only certain general features of the nonlinear interaction are important.

In this paper we expose an interesting extension of this approach. If the original nonlinear evolution PDE, which is the starting point for the reduction method, has a linear part characterized by the fact that two (or more) Fourier modes have the same group velocity, then we consider a solution that in the linear limit is a superposition (of course with constant coefficients) of these modes. As a consequence the nonlinear effects induce a modulation of the amplitudes of these modes, which also accounts for their interaction. In particular we consider the equation[13,14] integrable by means of the spectral transform.[15,16]

$$U_t-U_{xxxxx}-5U_{xxy}+5W_y-5U_xU_{xx}-5UU_{xxx}-5U^2U_x-5UU_y-5U_xW=0$$
$$W_x=U_y, \tag{1.2}$$

where $U=U(x,y,t)$, $W=W(x,y,t)$ and the subscripts denote partial differentiation. Applying the reduction method, a new class of integrable systems of nonlinear evolution PDEs depending on two real parameters (a,b) can be derived

$$i\Psi_\tau+L_1\Psi+\delta_1\alpha\Psi+\delta_2\beta\Psi+\delta_3|\Psi|^2\Psi+\delta_4|\Phi|^2\Psi=0, \tag{1.3a}$$

$$i\Phi_\tau+L_2\Phi+\delta_5\alpha\Phi+\delta_6\beta\Phi-\delta_3|\Phi|^2\Phi+\delta_7|\Psi|^2\Phi=0, \tag{1.3b}$$

$$\alpha_\xi+\alpha_\eta+\beta_\eta+(|\Psi|^2)_\xi-(|\Phi|^2)_\xi=0,\quad \beta_\xi=\delta_8\alpha_\eta, \tag{1.3c}$$

where the linear differential operators L_1 and L_2 are given by

$$L_1=\frac{(a+2b)^2(b^2-2a^2+ab)}{(a-b)^4}\frac{\partial^2}{\partial\xi^2}+\frac{2(a+2b)}{b-a}\frac{\partial^2}{\partial\xi\partial\eta}+\frac{\partial^2}{\partial\eta^2}, \tag{1.4a}$$

$$L_2=\frac{9bc(a+2b)^2}{(a-b)^3(4b-a)}\frac{\partial^2}{\partial\xi^2}+\frac{2a(a+2b)}{c(b-a)}\frac{\partial^2}{\partial\xi\partial\eta}+\frac{a}{c}\frac{\partial^2}{\partial\eta^2}, \tag{1.4b}$$

and

$$\delta_1=-10a,\quad \delta_2=\frac{10a(a+2b)}{(b-a)},\delta_3=\frac{10}{3}(b-a), \tag{1.4c}$$

$$\delta_4 = 10a + \frac{50(ab+2a^2+9bc)(4ab-a^2+ac+2bc)}{(a(61a-13a^2-305b)+b(161a^2-48b^2-504ab)+c(61a-305b-127ab-216b^2-61a^2))} + \frac{50a(ab+2a^2-9bc)(4ab-a^2-ac-2bc)}{(a(61a-13a^2-305b)+b(161a^2-48b^2-504ab)-c(61a-305b-127ab-216b^2-61a^2))}, \tag{1.4d}$$

$$\delta_5 = 10c, \quad \delta_6 = \frac{10c(a+2b)}{(b-a)}, \quad \delta_8 = -\frac{(a+2b)}{a(a-b)^2}, \tag{1.4e}$$

$$\delta_7 = 10c + \frac{50(2c^2+9ba+cb)(4ab-a^2+ac+2ba)}{(a(61a-305b-127ab-216b^2-61a^2)+b(161a^2-48b^2-504ab)+c(61a-13a^2-305b))} + \frac{50(2c^2+9ba-cb)(4ab-a^2-ac+2ba)}{(a(61a-305b-127ab-216b^2-61a^2)+b(161a^2-48b^2-504ab)-c(61a-13a^2-305b))}, \tag{1.4f}$$

where

$$c = \sqrt{\frac{a(4b-a)}{3}}. \tag{1.4g}$$

In the system of equations (1.3), $\Psi = \Psi(\xi,\eta,\tau)$ and $\Phi = \Phi(\xi,\eta,\tau)$ are complex, while $\alpha = \alpha(\xi,\eta,\tau)$ and $\beta = \beta(\xi,\eta,\tau)$ are real.

The paper is organized as follows. In Sec. II we apply the reduction method to the starting equation (1.2) and obtain the new system of equations (1.3). Reductions to known integrable equations are discussed. In Sec. III we discuss in some detail how the reduction method can be applied to the Lax pair of Eq. (1.2) and derive the Lax pair of the system of equations (1.3). Finally in Sec. IV we recapitulate the most important results and indicate some possible extensions.

II. A NEW INTEGRABLE SYSTEM IN 2+1 DIMENSIONS

In this section we derive a *S*-integrable system of nonlinear equations, by means of an extension of the reduction method, which is possible if the group velocity, relative to the linearized starting equation, is equal for two Fourier modes with different wave vector $\mathbf{K} = (K_1, K_2)$.

We can consider that particular solution which in the linear approximation is a superposition of these modes. The nonlinear term induces a modulation of their amplitudes, which is due to their interaction. The validity of the method is easily understood, because the variable transformation (1.1) operates in the same way upon the two Fourier modes which move with the same velocity and then can interfere.

The final system of nonlinear PDEs is relative to the modulation of the amplitudes of the two Fourier modes and inherits the integrability property of the starting equation, as it will be demonstrated in Sec. III, applying the reduction method to the Lax pair. The linear dispersive part of the starting equation (1.2) admits as a solution a Fourier mode, with a group velocity $\mathbf{V}(\mathbf{K}) = (V_1(K_1,K_2), V_2(K_1,K_2))$,

$$V_1(K_1,K_2) = -5\left(K_1^2 - \frac{K_2}{K_1}\right)^2, \quad V_2(K_1,K_2) = 5\left(K_1^2 + 2\frac{K_2}{K_1}\right), \tag{2.1}$$

where

$$\mathbf{V}(\mathbf{K}) = \frac{\partial \omega}{\partial \mathbf{K}} \tag{2.2}$$

and $\omega = \omega(K_1,K_2)$ is the dispersion relation.

Two Fourier modes $\mathbf{K}_A = (K_1,K_2)$, $\mathbf{K}_B = (K_3,K_4)$ possess equal group velocity, when

$$K_3=\sqrt{\frac{4K_2-K_1^3}{3K_1}},\quad K_4=\sqrt{\frac{(4K_2-K_1^3)}{3K_1}}\,\frac{K_2+2K_1^3}{3K_1}. \tag{2.3}$$

We can use the transformation (1.1) which is identical for the two Fourier modes and introduce the following formal asymptotic Fourier expansion:

$$U(x,y,t)=\sum_{n_1,n_2=-\infty}^{+\infty}\varepsilon^{\gamma_{n_1n_2}}\psi_{n_1n_2}(\xi,\eta,\tau;\varepsilon)\exp\{i(n_1z_1+n_2z_2)\}, \tag{2.4}$$

where $z_1=K_1x+K_2y-\omega t$, $z_2=K_3x+K_4y-\omega t$, $\gamma_{n_1n_2}=|n_1|+|n_2|$ for $n_1,n_2\neq 0$, $\gamma_{00}=r$, a nonnegative rational number which will be fixed afterward and $\psi_{n_1n_2}(\xi,\eta,\tau;\varepsilon)=\psi^*_{-n_1-n_2}(\xi,\eta,\tau;\varepsilon)$ (recall that $U(x,y,t)$ is real). The unknown functions $\psi_{n_1n_2}$s depend on ε and it is supposed that their limit for $\varepsilon\to 0$ exists and is finite. In the following this limit will be denoted by $\psi_{n_1n_2}(\xi,\eta,\tau)$. Moreover we suppose that they can be expanded in power series of ε, i.e.,

$$\psi_{n_1n_2}(\xi,\eta,\tau;\varepsilon)=\sum_{i=0}^{\infty}\varepsilon^i\psi^{(i)}_{n_1n_2}(\xi,\eta,\tau),\quad \psi_{n_1n_2}(\xi,\eta,\tau)=\psi^{(0)}_{n_1n_2}(\xi,\eta,\tau). \tag{2.5}$$

We now introduce an analog Fourier expansion

$$w(x,y,t)=\sum_{n_1,n_2=-\infty}^{+\infty}\varepsilon^{\tilde{\gamma}_{n_1n_2}}\varphi_{n_1n_2}(\xi,\eta,\tau;\varepsilon)\exp\{i(n_1z_1+n_2z_2)\} \tag{2.6}$$

and obtain

$$\varphi_{n_1n_2}=(n_1K_2+n_2K_4)(n_1K_1+n_2K_3)^{-1}\psi_{n_1n_2}+O(\varepsilon^{p_1},\varepsilon^{p_2}). \tag{2.7}$$

In the following for simplicity we use the abbreviations $\psi^{(0)}_{01}=\Psi$, $\psi^{(0)}_{01}=\Phi$, $\psi^{(0)}_{00}=\alpha$ (and $\phi^{(0)}_{n_1n_2}=\phi_{n_1n_2}$, $\phi^{(0)}_{00}=\beta$).

The final goal is to obtain the evolution equation for the modulation amplitudes $\Psi=\Psi(\xi,\eta,\tau)$ and $\Phi(\xi,\eta,\tau)$ and to understand how it is modified by choosing different wave numbers. We insert the expansions (2.4) and (2.6) into Eq. (1.3) and consider the different equations obtained considering the coefficients of the Fourier modes. From Eq. (1.3b) we get

$$\phi_{10}=\frac{K_2}{K_1}\Psi,\quad \phi^{(p)}_{10}=\frac{i}{K_1}\left(\frac{K_2}{K_1}\Psi_\xi-\Psi_\eta\right),\quad \phi^{(2p)}_{10}=\frac{1}{K_1^2}\left(\Psi_{\xi\eta}-\frac{K_2}{K_1}\Psi_{\xi\xi}\right), \tag{2.8a}$$

$$\phi_{01}=\frac{K_4}{K_3}\Phi,\quad \phi^{(p)}_{01}=\frac{i}{K_3}\left(\frac{K_4}{K_3}\Phi_\xi-\Phi_\eta\right),\quad \phi^{(2p)}_{01}=\frac{1}{K_3^2}\left(\Phi_{\xi\eta}-\frac{K_4}{K_3}\Phi_{\xi\xi}\right), \tag{2.8b}$$

$$\beta_\xi=\alpha_\eta. \tag{2.8c}$$

It is more convenient to separate the contributions of the linear and nonlinear parts

$$\varepsilon^{\gamma_{n_1n_2}}D_{n_1n_2}\psi_{n_1n_2}=\varepsilon^2F_{n_1n_2}, \tag{2.9}$$

where $D_{n_1n_2}$ is a linear differential operator acting on $\psi_{n_1n_2}(\xi,\eta,\tau)$ and $F_{n_1n_2}$ is the contribution of the nonlinear part. The operator $D_{n_1n_2}$ is

$$D_{n_1n_2}=(-in_1\omega-in_2\omega+\varepsilon^q\partial_\tau-V_1\varepsilon^p\partial_\xi-V_2\varepsilon^p\partial_\eta)-(in_1K_1+in_2K_3+\varepsilon^p\partial_\xi)^5$$
$$-5(in_1K_2+in_2K_4+\varepsilon^p\partial_\eta)(in_1K_1+in_2K_3+\varepsilon^p\partial_\xi)^2$$
$$+5\left(\frac{K_2}{K_1}-\frac{i}{K_1}\varepsilon^p\partial_\eta+\frac{iK_2}{K_1^2}\varepsilon^p\partial_\xi+\frac{1}{K_1^2}\varepsilon^{2p}\partial_{\xi\eta}-\frac{K_2}{K_1^3}\varepsilon^{2p}\partial_{\xi\xi}\right)+O(\varepsilon^{3p}). \tag{2.10}$$

$F_{n_1n_2}$ can be derived, evaluating the importance of the different terms, which originate from the interference of the Fourier amplitudes $\psi_{n_1n_2}(\xi,\eta,\tau)$ and $\varphi_{n_1n_2}(\xi,\eta,\tau)$:

$$F_{00}=10\left(\frac{K_2}{K_1}-K_1^2\right)(|\Psi|^2)_\xi\varepsilon^p-10\left(\frac{K_2}{K_1}-K_1^2\right)(|\Phi|^2)_\xi\varepsilon^p+O(\varepsilon^{p+2},\varepsilon^{p+2r}), \tag{2.11a}$$

$$F_{10}=(10iK_2-25iK_1^3)\psi_2\psi^*+(5iK_2-5iK_1^3)\psi\alpha+5iK_1\beta\psi+5iK_1|\psi|^2\psi$$
$$+5\left(K_2+K_4-K_1K_3^2+\frac{K_1K_4}{K_3}-K_1(K_1+K_3)^2-K_3\frac{K_2+K_4}{K_1+K_3}\right)\psi_{11}\psi^*$$
$$+5\left(K_2-K_4-K_1K_3^2+\frac{K_1K_4}{K_3}-K_1(K_1-K_3)^2+K_3\frac{K_2-K_4}{K_1-K_3}\right)\psi_{1-1}\psi^*+O(\varepsilon^{p+r-1},\varepsilon^{2p}) \tag{2.11b}$$

$$F_{20}=10(K_2-K_1^3)\Psi^2+O(\varepsilon^p), \tag{2.11c}$$

and so on.

After taking $q=2, p_1=p_2=1$, and $r=2$ for the proper balance of terms, the equations for the Fourier modes can be obtained at the lowest order for $n_1=0$, $n_2=0$, $n_1=1$, $n_2=\pm1$ and $n_1=2$, $n_2=0$, $n_1=0$, $n_2=2$ (with $\psi_{00}=\alpha$, $\varphi_{00}=\beta$, $\psi_{10}=\Psi$, $\psi_{01}=\Phi$),

$$V_1\alpha_\xi+V_2\alpha_\eta-5\beta_\eta+10\left(\frac{K_2}{K_1}-K_1^2\right)(|\Psi|^2)_\xi-10\left(\frac{K_2}{K_1}-K_1^2\right)(|\Phi|^2)_\xi=0, \tag{2.12a}$$

$$\psi_{1\pm1}=\frac{5\left[(K_2\pm K_4)-(K_1\pm K_3)(K_1^2+K_3^2)-\frac{K_1K_4}{K_3}\mp\frac{K_3K_2}{K_1}\right]}{(-\omega_1\pm\omega_2)-(K_1\pm K_3)^5+5(K_1\pm K_3)^2(K_2\pm K_4)+5\frac{(K_2\pm K_4)^2}{K_1\pm K_3}}\Psi\Phi_\pm, \tag{2.12b}$$

$$\psi_{20}=\frac{1}{3K_1^2}\Psi^2,\quad \psi_{02}=\frac{1}{3K_3^2}\Phi^2, \tag{2.12c}$$

where $\Phi_+=\Phi$, $\Phi_-=\Phi^*$, and for $n_1=1$, $n_2=0$, using (2.12c), we arrive at the nonlinear evolution equation

$$i\Psi_\tau+5\left(K_2-2K_1^3+\frac{K_2^2}{K_1^3}\right)\Psi_{\xi\xi}+10\left(K_1-\frac{K_2}{K_1^2}\right)\Psi_{\xi\eta}+\frac{5}{K_1}\Psi_{\eta\eta}+5(K_2-K_1^3)\alpha\Psi+5K_1\beta\Psi$$
$$+\frac{10}{3}\left(\frac{K_2}{K_1^2}-K_1\right)|\Psi|^2\Psi-5\left(K_2+K_4-K_1K_3^2+\frac{K_1K_4}{K_3}-K_1(K_1+K_3)^2-K_3\frac{K_2+K_4}{K_1+K_3}\right)\psi_{11}\Phi^*$$
$$-5\left(K_2-K_4-K_1K_3^2+\frac{K_1K_4}{K_3}-K_1(K_1-K_3)^2+K_3\frac{K_2-K_4}{K_1-K_3}\right)\psi_{1-1}\Phi=0. \tag{2.13}$$

In a similar way for $n_1=0$, $n_2=1$, we obtain

$$i\Psi_\tau+5\left(K_2-2K_1^3+\frac{K_2^2}{K_1^3}\right)\Psi_{\xi\xi}+10\left(K_1-\frac{K_2}{K_1^2}\right)\Psi_{\xi\eta}+\frac{5}{K_1}\Psi_{\eta\eta}+5(K_2-K_1^3)\alpha\Psi+5K_1\beta\Psi$$

$$+\frac{10}{3}\left(\frac{K_2}{K_1^2}-K_=\right)|\Psi|^2\Psi+10K|\Phi|^2\Psi-5\left(K_2+K_4-K_1K_3^2+\frac{K_1K_4}{K_3}-K_1(K_1+K_3)^2\right.$$

$$\left.-K_3\frac{K_2+K_4}{K_1+K_3}\right)\psi_{11}\Psi^*-5\left(K_4-K_2+K_1K_3^2-\frac{K_1K_4}{K_3}+K_1(K_1-K_3)^2-K_3\frac{K_2-K_4}{K_1-K_3}\right)\psi_{-11}\Psi=0. \tag{2.14}$$

This system must be integrable by the spectral transform, because it has been derived from an *S*-integrable equation, and that will be explicitly demonstrated in Sec. III.

If $K_2\neq K_1^3$, using (2.12b) and after the cosmetic rescaling

$$\xi'=\frac{V_2}{V_1}\sqrt{\frac{K_1}{5}}\,\xi,\quad \eta'=\sqrt{\frac{K_1}{5}}\,\eta, \tag{2.15a}$$

$$\chi'=\frac{V_1}{10\left(\frac{K_2}{K_1}-K_1^2\right)}\chi,\quad \Phi'=\frac{V_1}{2V_2\left(K_1^2-\frac{K_2}{K_1}\right)}\Phi, \tag{2.15b}$$

and with the introduction of two real parameters

$$a=K_1,\quad b=\frac{K_2}{K_1^2}, \tag{2.16a}$$

we arrive at the model equation of Davey–Stewartson type (1.3), where [see (2.3)]

$$c=K_3=\sqrt{\frac{a(4b-a)}{3}}. \tag{2.16b}$$

Integrable Davey–Stewartson type equations and system of equations have been extensively investigated by many authors.[17–21] A very detailed list of Davey–Stewartson systems and equations integrable by the inverse scattering method has been recently given.[22] The system of equations (1.3) does not appear in these papers. We expect that this new system be integrable by the inverse scattering method, because it has been obtained from an integrable equation and the property of integrability is supposed to keep through the application of the reduction method. The integrability of the system of equations (1.3) will be explicitly demonstrated in Sec. III.

Let us now consider the implications of these results in the context of the nonlinear evolution PDEs in $2+1$ dimensions. If we take $\Phi=0$, we obtain the equation

$$i\Psi_\tau+L_1\Psi+\delta_1\alpha\Psi+\delta_2\beta\Psi+\delta_3|\Psi|^2\Psi=0, \tag{2.17a}$$

$$\alpha_\xi+\alpha_\eta+\beta_\eta+(|\Psi|^2)_\xi=0,\quad \beta_\xi=\delta_8\alpha_\eta, \tag{2.17b}$$

where L_1, δ_1, δ_2, δ_3, δ_8 are given by (1.4a) and (1.4c). The nonlinear PDE (2.17), with trivial rescalings, coincides with the integrable equation found in a previous paper.[10]

III. THE LAX PAIR FOR THE INTEGRABLE SYSTEM OF EQUATIONS

We can also apply the reduction method to the Lax pair of the starting equation, to demonstrate explicitly the integrability by the spectral transform of the system (1.3), because in this way we identify the Lax pair that permits us to obtain a compatibility condition which reproduces the system of Eqs. (1.3).

We apply the reduction method to the Lax pair of Eq. (1.2). The Lax operators are

$$L=\frac{\partial}{\partial y}+\frac{\partial^3}{\partial x^3}+U(x,y,t)\frac{\partial}{\partial x},\quad L\phi(x,y,t)=0, \tag{3.1}$$

$$A=9\frac{\partial^5}{\partial x^5}+15U(x,y,t)\frac{\partial^3}{\partial x^3}+15U_x(x,y,t)\frac{\partial^2}{\partial x^2}$$
$$+5(2U_{xx}(x,y,t)+U^2(x,y,t)-W(x,y,t))\frac{\partial}{\partial x}, \tag{3.2}$$

with

$$\phi_t(x,y,t)+A\phi(x,y,t)=0. \tag{3.3}$$

It can be verified by direct substitution that the operator relation

$$L_T=i[L,A]=i(LA-AL) \tag{3.4}$$

reproduces Eq. (1.2).

The function $\phi(x,y,t)$ can be expanded in Fourier modes in the form

$$\phi(x,y,t)=\sum_{n_1,n_2=-\infty[n_1\text{odd},n_2\text{even}]}^{+\infty}\varepsilon^{\gamma_{n_1n_2}}\phi_{n_1n_2}(\xi,\eta,\tau;\varepsilon)\exp\left[i\left(\frac{n_1}{|n_1|}(\lambda_1x+\lambda_2y+\lambda_3t)+\frac{n_1}{2}z_1\right.\right.$$
$$\left.\left.+\frac{n_2}{2}z_2\right)\right]+\sum_{n_1,n_2=-\infty[n_1\text{even},n_2\text{odd}]}^{+\infty}\varepsilon^{\gamma_{n_1n_2}}\phi_{n_1n_2}(\xi,\eta,\tau;\varepsilon)\exp\left[i\left(\frac{n_2}{|n_2|}(\lambda_4x+\lambda_5y+\lambda_6t)\right.\right.$$
$$\left.\left.+\frac{n_1}{2}z_1+\frac{n_2}{2}z_2\right)\right], \tag{3.5}$$

with $z_1=K_1x+K_2y-\omega_1t$, $z_2=K_3x+K_4y-\omega_2t$, $\phi_{n_1n_2}(\xi,\eta,\tau;\varepsilon)$'s which parametrically depend on ε and remain finite when $\varepsilon\to0$, and finally $\gamma_{n_1n_2}$ non-negative rational numbers and $\lambda_j, j=1,...6$, real constants to be determined later on.

Inserting now the expression for $\phi(x,y,t)$ in (3.1), we derive a series of relations which are generated by the coefficients of the Fourier modes. Each relation must be valid for a given order of approximation in ε.

In particular, for the fundamental harmonics $n_1=\pm1,n_2=\pm1$, and $n_1=1,n_2=-2$, or $n_1=-2,n_2=1$, considering terms $O(\varepsilon^0)$ in (3.1) and (3.3), we obtain

$$\left(\pm\frac{iK_1}{2}\pm i\lambda_1\right)^3+\left(\pm\frac{iK_2}{2}\pm i\lambda_2\right)=0, \tag{3.6a}$$

$$\left(\mp\frac{i\omega}{2}\pm i\lambda_3\right)+9\left(\pm\frac{iK_1}{2}\pm i\lambda_1\right)^5=0, \tag{3.6b}$$

and then

$$\lambda_1=\frac{K_3}{2},\quad \lambda_2=\frac{K_4}{2},\quad \lambda_3=-\frac{K_3}{2}\left(K_1^4+\frac{K_2^2}{K_1^2}+7K_1K_2\right). \tag{3.7}$$

As a consequence, we understand that the harmonics

$$\phi_{10},\phi_{-10},\phi_{01},\phi_{0-1},\phi_{-21},\phi_{1-2} \tag{3.8}$$

are fundamental, i.e., for them $\gamma_{n_1n_2}$ assumes the smallest value, i.e., $\gamma_{n_1n_2}=0$. In particular the harmonics $\phi_{10},\phi_{-10},\phi_{1-2},\phi_{-12}$ are decoupled with respect to the other harmonics $\phi_{01},\phi_{0-1},\phi_{-21},\phi_{2-1}$ and we get two separate but identical spectral problems.

The successive order ε for Eq. (3.1) allow us to obtain the new spectral problem, because all the $\phi_{n_1n_2}$s may be expressed by means of the fundamental harmonics (3.8), which are connected through the relations

$$\frac{3}{4}(K_1+K_3)^2\phi_{\pm10,\xi}-\phi_{\pm10,\eta}\pm\frac{i}{2}(K_1+K_3)\Psi_\pm\phi_{\mp10}\mp\frac{i}{2}(K_1-K_3)\Phi_\pm\phi_{\pm1\mp2}=0, \tag{3.9}$$

$$\frac{3}{4}(K_1-K_3)^2\phi_{\pm1\mp2,\xi}-\phi_{\pm1\mp2,\eta}\mp\frac{i}{2}(K_1+K_3)\Phi_\mp\phi_{\pm10}=0. \tag{3.10}$$

By means of the variable rescaling (2.15), and introducing the 4×4 matrix operator L, we arrive at the final form

$$L\hat{\varphi}=0, \tag{3.11}$$

where

$$L=\begin{pmatrix}L_{11}&L_{12}\\L_{21}&L_{22}\end{pmatrix}, \tag{3.12a}$$

$$L_{11}=\begin{pmatrix}\partial_\eta+\dfrac{3(a+c)^2(a+2b)}{4a(a-b)^2}\partial_\xi & -i\sqrt{\dfrac{5}{a}}\dfrac{(a+c)}{2}\Psi\\ i\sqrt{\dfrac{5}{a}}\dfrac{(a+c)}{2}\Psi^* & \partial_\eta+\dfrac{3(a+c)^2(a+2b)}{4a(a-b)^2}\partial_\xi\end{pmatrix}, \tag{3.12b}$$

$$L_{12}=\begin{pmatrix}i\sqrt{\dfrac{5}{a}}\dfrac{(a-c)}{2}\Phi & 0\\ 0 & -i\sqrt{\dfrac{5}{a}}\dfrac{(a-c)}{2}\Phi^*\end{pmatrix}, \tag{3.12c}$$

$$L_{21}=\begin{pmatrix}i\sqrt{\dfrac{5}{a}}\dfrac{(a+c)}{2}\Phi^* & 0\\ 0 & -i\sqrt{\dfrac{5}{a}}\dfrac{(a-c)}{2}\Phi\end{pmatrix}, \tag{3.12d}$$

$$L_{22}=\begin{pmatrix}\partial_\eta+\dfrac{3(a-c)^2(a+2b)}{4a(a-b)^2}\partial_\xi & 0\\ 0 & \partial_\eta+\dfrac{3(a-c)^2(a+2b)}{4a(a-b)^2}\partial_\xi\end{pmatrix}, \tag{3.12e}$$

$$\hat{\varphi}=\begin{pmatrix}\varphi_{10}\\ \varphi_{-10}\\ \varphi_{1-2}\\ \varphi_{-1+2}\end{pmatrix}. \tag{3.12 f}$$

To calculate the temporal evolution, we must insert the expression (3.5) in (3.3) and consider the relation obtained for the different harmonics n_1, n_2 and for a given order of approximation in ε. If we consider the first order in ε, we newly obtain the spectral problem (3.11)–(3.12). Only if we take into account the next orders of approximation of Eq. (3.3), i.e., the order ε^2, can the temporal evolution be determined. However, new quantities, the corrections $\tilde{\phi}_{\pm 10}(\xi,\eta,\tau)$, $\tilde{\phi}_{\pm 1\mp 2}(\xi,\eta,\tau)$ of order ε, to the fundamental harmonics $\phi_{\pm 10}(\xi,\eta,\tau)$, $\phi_{\pm 1\mp 2}(\xi,\eta,\tau)$ appear. These unknown quantities can be eliminated in Eq. (3.3) taking advantage of the relation obtained from Eq. (3.1), considering terms of order ε^2. This elimination is possible only because Eqs. (3.1) and (3.3) are identical at the order ε. In particular, if we consider (3.1) calculated for the order ε^2 for $n_1=\pm 1, n_2=0$, $n_1=\pm 1, n_2=\mp 2$, we get

$$\begin{aligned}\tilde{\phi}_{\pm 10,\xi}&-\frac{4}{3(K_1+K_3)^2}\tilde{\phi}_{\pm 10,\eta}\pm\frac{2i}{3(K_1+K_3)}\Psi_{\pm}\tilde{\phi}_{\mp 10}\mp\frac{2i(K_1-K_3)}{3(K_1+K_3)^2}\Phi_{\pm}\tilde{\phi}_{\pm 1\mp 2}\\ &-\frac{4}{3(K_1+K_3)^2}\Big[\Psi_{\pm}\phi_{\mp 10,\xi}+\Phi_{\pm}\phi_{\pm 1\mp 2,\xi}\pm\frac{3i}{2}(K_1+K_3)\phi_{\pm 10,\xi\xi}\pm\frac{i}{2}(3K_1-K_3)\Psi_{\mp}\phi_{\pm 30}\\ &\pm\frac{i}{2}(K_1+K_3)\alpha\phi_{\pm 10}\pm\frac{i}{2}(K_1+3K_3)\Phi_{\mp}\phi_{\pm 1\pm 2}\mp\frac{i}{2}(3K_1+K_3)\Psi_{\pm 20}\phi_{\mp 30}\mp\frac{i}{2}(K_1\\ &-K_3)\psi_{\pm 1\mp 1}\phi_{\mp 1\pm 2}\Big]=0,\end{aligned} \tag{3.13a}$$

$$\begin{aligned}\tilde{\phi}_{\pm 1\mp 2,\xi}&-\frac{4}{3(K_1-K_3)^2}\tilde{\phi}_{\pm 1\mp 2,\eta}\mp\frac{2i(K_1+K_3)}{3(K_1-K_3)^2}\Phi_{\mp}\tilde{\phi}_{\pm 10}-\frac{4}{3(K_1-K_3)^2}\Big[\Phi_{\mp}\phi_{\pm 10,\xi}\pm\frac{3i}{2}(K_1\\ &-K_3)\phi_{\pm 1\mp 2,\xi\xi}\pm\frac{i}{2}(K_1-3K_3)\Phi_{\pm}\phi_{\pm 1\mp 4}\mp\frac{i}{2}(K_1+K_3)\Psi_{\pm}\phi_{\mp 1\mp 2}\pm\frac{i}{2}(3K_1\\ &-K_3)\Psi_{\mp}\phi_{\pm 3\mp 2}\pm\frac{i}{2}(K_1-K_3)\alpha\phi_{\pm 1\mp 2}\mp\frac{i}{2}(K_1+K_3)\psi_{\pm 1\mp 1}\phi_{\mp 10}\mp\frac{i}{2}(3K_1\\ &-K_3)\Psi_{\pm 20}\phi_{\mp 3\pm 2}\Big]=0.\end{aligned} \tag{3.13b}$$

To evaluate this expression we consider that $\phi_{\pm 30}, \phi_{\pm 1\pm 2}$ are connected with the fundamental harmonics [we must calculate (3.3) for $n_1=\pm 3, n_2=0$, $n_1=\pm 1, n_2=\pm 2$ at the lower order in ε]

$$\phi_{\pm 30}=\left(\frac{4(K_1+K_3)}{(3K_1+K_3)^3-4(3K_2+K_4)}\right)\Psi_{\pm}\phi_{\pm 10}, \tag{3.14a}$$

$$\phi_{\pm 1\pm 2}=\left(\frac{4(K_1+K_3)}{(K_1+3K_3)^2-4(K_2+3K_4)}\right)\Phi_{\pm}\phi_{\pm 10}. \tag{3.14b}$$

We now consider (3.3) at the order ε^2 for $n_1=\pm 1, n_2=0$, $n_1=\pm 1, n_2=\mp 2$, which furnishes the temporal evolution of the harmonics $\phi_{10}, \phi_{-10}, \phi_{1-2}$. Via the transformation (2.15) and after a lengthy calculation we arrive at the final form for the 4×4 matrix operator A which satisfies the equation

$$\hat{\phi}_t(x,y,t)+A\hat{\phi}(x,y,t)=0 \tag{3.15}$$

and is given by

$$A=\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \tag{3.16a}$$

where

$$A_{11}=\begin{pmatrix} a_{+1}\partial_\xi^2+a_{+4}|\Psi|^2+a_{+5}|\Phi|^2+a_{+6}\beta+a_{+7}\alpha & a_{+2}\Psi_\xi+a_{+3}\Psi_\eta+a_{+8}\Psi\partial_\xi \\ a_{-2}\Psi_\xi^*+a_{-3}\Psi_\eta^*+a_{-8}\Psi^*\partial_\xi & a_{-1}\partial_\xi^2+a_{-4}|\Psi|^2+a_{-5}|\Phi|^2+a_{-6}\beta+a_{-7}\alpha \end{pmatrix}, \tag{3.16b}$$

$$A_{12}=\begin{pmatrix} a_{+9}\Phi_\xi+a_{+10}\Phi\partial_\xi+a_{+11}\Phi_\eta & a_{+12}\Psi\Phi^* \\ a_{-12}\Psi^*\Phi & a_{-9}\Phi_\xi^*+a_{-10}\Phi^*\partial_\xi+a_{-11}\Phi_\eta^* \end{pmatrix}, \tag{3.16c}$$

$$A_{21}=\begin{pmatrix} b_{+2}\Phi^*\partial_\xi+b_{+3}\Phi_\xi^*+b_{+4}\Phi_\eta^* & b_{+9}\Psi\Phi^* \\ b_{-9}\Psi^*\Phi & b_{-2}\Phi\partial_\xi+b_{-3}\Phi_\xi+b_{-4}\Phi_\eta \end{pmatrix}, \tag{3.16d}$$

$$A_{22}=\begin{pmatrix} b_{+1}\partial_\xi^2+b_{+5}|\Psi|^2+b_{+6}|\Phi|^2+b_{+7}\beta+b_{+8}\alpha & 0 \\ 0 & b_{-1}\partial_\xi^2+b_{-5}|\Psi|^2+b_{-6}|\Phi|^2+b_{-7}\beta+b_{-8}\alpha \end{pmatrix}, \tag{3.16e}$$

and

$$a_{\pm1}=\pm\frac{3i(a+2b)^2(a+c)(a+2b+9c)}{4(a-b)^4}, \tag{3.17a}$$

$$a_{\pm2}=-\frac{\sqrt{5}(a+2b)(a+c)(3a+3c-8+2b)}{4\sqrt{a}(a-b)^2}, \quad a_{\pm3}=-\frac{\sqrt{5a}}{4}(a+c), \tag{3.17b}$$

$$a_{\pm4}=\mp\frac{5}{8}(a+c)^2, \quad a_{\pm5}=\frac{5(a-c)}{2c}, \quad a_{\pm6}=\mp5i(a+2b)(a+c), \tag{3.17c}$$

$$a_{\pm8}=\frac{(a+2b)}{\sqrt{5a}(a-b)^2}\left[\frac{20a^2(a-b)^2}{3(a+c)^2}-\frac{45}{4}(a+c)^2+15a(a+c)-10a^2-5ab\right], \tag{3.17d}$$

$$a_{\pm7}=\pm i\frac{15(a+c)c}{(a-b)}, \quad a_{\pm9}=\frac{\sqrt{5}(a+2b)(c-a)}{2\sqrt{a}(a-b)^2}\left[\frac{3(a-c)}{2}+4c-\frac{a(2a+b)}{3c}\right], \tag{3.17e}$$

$$a_{\pm10}=\frac{(a+2b)}{\sqrt{5a}(a-b)^2}\left[\frac{20a^2(a-b)^2}{3(a+c)^2}-\frac{45}{4}(a-c)^2-15c(a-c)+\frac{5a}{3}(7b-4a)\right], \tag{3.17f}$$

$$a_{\pm11}=\frac{\sqrt{5a}(a-c)}{2c}, \quad a_{\pm12}=\mp\frac{5}{4}(a+c)^2, \tag{3.17g}$$

and

$$b_{\pm1}=\mp i\frac{3(a+2b)^2(a-c)(a+2b+3c)}{2(a-b)^2}, \quad b_{\pm2}=\frac{5\sqrt{a}(a+2b)(4b-a+9c)}{2\sqrt{5}(a-b)^2}, \tag{3.18a}$$

$$b_{\pm 3}=\frac{\sqrt{5}(a+2b)(a+c)(5c-3a)}{3\sqrt{a(a-b)^2}}, \quad b_{\pm 4}=\pm i\frac{\sqrt{5a}}{c}, \tag{3.18b}$$

$$b_{\pm 5}=\frac{\sqrt{5}(a-2b)(a-c)(5c-3a)}{3\sqrt{a(a-b)^2}}, \quad b_{\pm 6}=\frac{\sqrt{5}(a+2b)(a+c)(5c+3a)}{3\sqrt{a(a-b)^2}}, \tag{3.18c}$$

$$b_{\pm 7}=\pm i\frac{5(a+2b)(a-c)}{(b-a)}, \quad b_{\pm 8}=\pm i\frac{15[(a-c)^3-4(a+c)^3]}{4a(a-b)}, \tag{3.18d}$$

$$b_{\pm 9}=\pm i\frac{5(a+2b)(a+c)}{(b-a)}. \tag{3.18e}$$

The determination of the Lax pair (3.12) and (3.16)–(3.18), which satisfies Eqs. (3.11) and (3.15), resolves the problem of S-integrability of the system (1.3).

IV. CONCLUSION

We have derived a new integrable and presumably of applicative interest nonlinear evolution Davey–Stewartson type system of equations from the integrable equation (1.2), by means of an extension of a reduction method based on Fourier expansion and space–time rescalings. It reduces to a known integrable equation in the single mode case. The application of this method is restricted to the case of same group velocities for different wave numbers. Moreover, we have applied the reduction method to the Lax pair (3.1)–(3.3) of the original equation and have demonstrated the integrability property of the new system of equations, by exhibiting the corresponding Lax pair (3.11)–(3.12) and (3.15)–(3.18).

We have outlined the approach that permits us to obtain such a system of equations and the next steps will be the explicit resolution of the spectral problem and the possible identification of localized or asymptotically finite solutions.

It is also convenient to push the approach beyond its ''leading order'' application by or considering different rescalings in the two spatial variables ($p_1 \neq p_2$) or looking at special cases when some key parameters vanish, on the analogy of the case of the model equations.[7,8]

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The Euler equations on Lie algebra so(4): An elementary approach to integrability condition

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We give a new derivation of the Manakov and the product case integrability conditions of the Euler equations on Lie algebra so(4). Fourth first integral functionally independent of the three already known integrals is obtained explicitly for *all values* of the parameters by an algorithmic approach. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1370550]

I. INTRODUCTION

Given a system of ordinary differential equations depending on parameters, the following question arises: How does one recognize the values of the parameters for which the equations have first integrals? Except for some simple cases, this problem is very hard and no satisfying methods to solve it are known. Up to now, the most successful approach has been offered by the so-called Painlevé analysis (see Refs. 1–4), the roots of which can be found in the seminal work of Kovalevskaya on the rigid body problem.[5,6] Unfortunately, this method of high practical value, is not based on a firmly established mathematical ground. The Painlevé analysis method puts emphasis on properties of solutions as functions of complex time.

Even for Hamiltonian systems with two degrees of freedom the problem of recognizing the values of parameters for which the equations are completely integrable is largely unsolved (see Ref. 7).

The same question is also relevant for the so-called *Euler equations on Lie algebras*.[8–26] For these equations also the problem is largely open.

In this paper we study one of the simplest examples of this kind—the Euler equations on Lie algebra so(4) corresponding to a ''diagonal quadratic Hamiltonian.'' Because these equations are used here exclusively as an interesting and nontrivial example of a multiparameter family of ordinary differential equations, we write them down without any explanations of their Lie algebraic origin, which can be found for example in Refs. 8, 11, 12, 18–25. We do not discuss their physical origin—relevant information can be found in the cited papers.

Let us take $\lambda := (\lambda_1, \ldots, \lambda_6) \in \mathbb{R}^6$, and let us consider the following system:

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$$\frac{dx_1}{dt}=(\lambda_3-\lambda_2)x_2x_3+(\lambda_6-\lambda_5)x_5x_6,$$

$$\frac{dx_2}{dt}=(\lambda_1-\lambda_3)x_1x_3+(\lambda_4-\lambda_6)x_4x_6,$$

$$\frac{dx_3}{dt}=(\lambda_2-\lambda_1)x_1x_2+(\lambda_5-\lambda_4)x_4x_5, \tag{I.1}$$

$$\frac{dx_4}{dt}=(\lambda_3-\lambda_5)x_3x_5+(\lambda_6-\lambda_2)x_2x_6,$$

$$\frac{dx_5}{dt}=(\lambda_4-\lambda_3)x_3x_4+(\lambda_1-\lambda_6)x_1x_6,$$

$$\frac{dx_6}{dt}=(\lambda_2-\lambda_4)x_2x_4+(\lambda_5-\lambda_1)x_1x_5.$$

The above-mentioned equations form the system of Euler equations on Lie algebra so(4) corresponding to the diagonal quadratic ''Hamiltonian'' $\frac{1}{2}\Sigma_{i=1}^{6}\lambda_i x_i^2$. It always has three first integrals:

$$H_1=x_1x_4+x_2x_5+x_3x_6, \quad H_2=\sum_{i=1}^{6}x_i^2, \quad H_3=\sum_{i=1}^{6}\lambda_i x_i^2. \tag{I.2}$$

Unless all the $(\lambda_i)_{1\leqslant i\leqslant 6}$ are equal, in which case system (I.1) is trivial, these three integrals are functionally independent. Thus from now on we assume that at least two $(\lambda_i)_{1\leqslant i\leqslant 6}$ are distinct.

The first integrals H_1 and H_2 are intimately related to the Lie algebra so(4). They represent its ''Casimir functions'' (see, e.g., Refs. 11 and 18).

To be integrable (Ref. 9, Sec. 28), system (I.1) needs a supplementary fourth first integral H_4, functionally independent of H_1, H_2, H_3, referred to here as a *fourth integral*. The only known cases when such fourth integral exists are the so-called *Manakov case*, defined by the *Manakov condition*

$$M\overset{\text{def}}{=}\lambda_1\lambda_4(\lambda_2+\lambda_5-\lambda_3-\lambda_6)+\lambda_2\lambda_5(\lambda_3+\lambda_6-\lambda_1-\lambda_4)+\lambda_3\lambda_6(\lambda_1+\lambda_4-\lambda_2-\lambda_5)=0, \tag{I.3}$$

and the *product case*, defined by the conditions

$$\lambda_4=\lambda_1, \quad \lambda_5=\lambda_2, \quad \lambda_6=\lambda_3. \tag{I.4}$$

We denote sets of λ satisfying the Manakov and the product case by $\mathcal{M}$ and $\mathcal{P}$, respectively.

One can prove that except for the above-mentioned two cases, system (I.1) is never algebraically completely integrable; see Refs. 8, 13, and 14, where also the precise definition of an algebraically completely integrable system can be found. Although we do not repeat this definition here, let us remark that it is based on the properties of the system when complex time is considered and goes back to Kovalevskaya's ideas.[5,6]

In the present paper we derive the Manakov and the product case conditions applying the following method. We search for the cases when the fourth integral does not depend on all variables. In fact, in the Manakov case, the existence of such fourth integral follows from the form of the fourth integral reported, e.g., in Refs. 8, 13, 14, and 22; in Ref. 10 one can find a fourth integral depending only on three variables (see also Ref. 22). In the product case, one can take as a fourth integral $H_4=\lambda_1x_1x_4+\lambda_2x_2x_5+\lambda_3x_3x_6$, which, when $(\lambda_1,\lambda_2,\lambda_3)\neq(c,c,c)$ for some c

$\in \mathbb{R}$, is always functionally independent of H_1, H_2, and H_3. Thus the fourth integral $\tilde{H}_4 = \lambda_1 H_1 - H_4 = (\lambda_1 - \lambda_2) x_2 x_5 + (\lambda_1 - \lambda_3) x_3 x_6$ does not depend on all variables.

Let us stress that we require only C^1 differentiability of the fourth integral. Moreover, all the considerations are *local*. We never use the fact that such fourth integral is globally defined.

The main tools used are the simplest facts from linear algebra and the following well-known fact. If F is a first integral common for two vector fields X and Y, then F is also a first integral of their Lie bracket $[X,Y]$. Indeed, if $X(F)=Y(F)=0$, then evidently $[X,Y](F)=X[Y(F)] - Y[X(F)]=0$. In Secs. V and VII we use the Frobenius integrability theorem. To study the functional independence of the first integrals we use the method from Ref. 27.

For the Euler equations (I.1) this program can be completely fulfilled and we arrive either at the Manakov (I.3) or the product case conditions (I.4). In this way we also obtain a nice expression for the fourth integral in the generic Manakov case, much more direct and simple than those reported in Refs. 8, 10–14, 22. In the Manakov case this leads also to a coherent, structured algorithmic approach and to an explicit description of the fourth integral for all values of $\lambda \in \mathcal{M}$ and not only for a generic one as in the above-cited papers.

In fact this method is not new. It was already applied in Ref. 28 to the successful study of integrable cases of the Euler–Poisson equations describing the motion of a heavy rigid body with a fixed point. The second author (S.I.P.) applied it in Refs. 29–31 to complete the results from Ref. 28.

Although to the best of our knowledge this method has not been applied to a system other than the one mentioned, its scope is undoubtedly substantially larger.

It is really astonishing that this method provides all known integrable cases of the Euler–Poisson system (for an overview of integrable cases see Ref. 16) as well as of the Euler equations on so(4).[8,13] We are convinced that this reflects a general fact, not yet understood.

To successfully complete this work, we used MAPLE. To avoid errors, all statements were verified using it.

The paper is sharply divided into two almost independent parts. The first one contains Secs. II and III. In Sec. II we study some symmetries of system (I.1) and their relation to the existence of first integrals. In Sec. III we arrive at the Manakov and the product case conditions assuming only the existence of a fourth integral which does not depend on all variables $(x_i)_{1\leqslant i\leqslant 6}$. In the second part we present an algorithm for finding a fourth integral for all $\lambda \in \mathcal{M}$. In Sec. IV we explain the choice of subsets of three variables among the variables $(x_i)_{1\leqslant i\leqslant 6}$, which are used later to find the fourth integral in the Manakov case. Sections V–VII are devoted to the explicit description of the fourth integral for all $\lambda \in \mathcal{M}$. After some preliminary considerations in Sec. V, the case of generic values of $\lambda \in \mathcal{M}$ is considered in Sec. VI. In Sec. VII the case of the remaining values of λ is considered. Our results are summarized in Table I at the end of Sec. VII.

A very preliminary account concerning this work was published in Ref. 32.

II. PERMUTATIONAL SYMMETRIES

The Euler equations (I.1) possess invariant property which we called *permutational symmetry*. The permutational symmetries can be described in a general framework as follows. Let $x = (x_1,\ldots,x_n) \in \mathbb{R}^n$, $\lambda = (\lambda_1,\ldots,\lambda_n) \in \mathbb{R}^n$, and let $V(x,\lambda) = (V_1(x,\lambda),\ldots,V_n(x,\lambda))$ depend smoothly on $(x,\lambda) \in \mathbb{R}^{2n}$. Let us consider the following system:

$$\frac{dx}{dt} = V(x,\lambda). \tag{II.1}$$

Let σ be an element of the symmetric group S_n, i.e., the group of all permutations of $\{1,\ldots,n\}$. For $a = (a_1,\ldots,a_n) \in \mathbb{R}^n$ we will note $\sigma(a) = (a_{\sigma(1)},\ldots,a_{\sigma(n)})$.

The permutation $\sigma \in \mathrm{S}_n$ will be called a *permutational symmetry* of system (II.1) if for all $(x,\lambda) \in \mathbb{R}^{2n}$, one has

$$V_k(\sigma(x),\sigma(\lambda)) = \varepsilon V_{\sigma(k)}(x,\lambda), \quad 1\leqslant k\leqslant n, \tag{II.2}$$

where $\varepsilon = \pm 1$ is a constant independent of k. It is obvious that all permutational symmetries of given equation form a group.

Before studying permutational symmetries of the Euler equations (I.1) let us prove the following.

Theorem II.1: *Let $F=F(x)$ be a first integral of system (II.1) and σ its permutational symmetry. Then function $G=F\circ\sigma^{-1}$,* i.e., *$G(x)=F(\sigma^{-1}(x))$ is a first integral of the system*

$$\frac{\mathrm{d}x}{\mathrm{d}t} = V(x,\sigma(\lambda)). \tag{II.3}$$

Proof: As F is a first integral of system (II.1), then

$$\sum_{k=1}^{n} V_k(x,\lambda)\left(\frac{\partial F}{\partial x_k}\right)(x)=0.$$

As σ is a permutation of $\{1,\ldots,n\}$, the last equality is equivalent to

$$\sum_{k=1}^{n} V_{\sigma(k)}(x,\lambda)\left(\frac{\partial F}{\partial x_{\sigma(k)}}\right)(x)=0.$$

Taking into account (II.2), we can write this as

$$\sum_{k=1}^{n} V_k(\sigma(x),\sigma(\lambda))\left(\frac{\partial F}{\partial x_{\sigma(k)}}\right)(x)=0.$$

The last equality is satisfied for every $x\in\mathbb{R}^n$. Then putting instead of x, $\sigma^{-1}(x)$ we obtain that for every $x\in\mathbb{R}^n$,

$$\sum_{k=1}^{n} V_k(x,\sigma(\lambda))\left(\frac{\partial F}{\partial x_{\sigma(k)}}\right)(\sigma^{-1}(x))=0.$$

On the other hand a function $G=G(x)$ is a first integral of system (II.3) if

$$\sum_{k=1}^{n} V_k(x,\sigma(\lambda))\left(\frac{\partial G}{\partial x_k}\right)(x)=0.$$

Thus to finish the proof it remains to prove that for $G=F\circ\sigma^{-1}$ and $1\leqslant k\leqslant n$ one has

$$\left(\frac{\partial F}{\partial x_{\sigma(k)}}\right)(\sigma^{-1}(x))=\left(\frac{\partial G}{\partial x_k}\right)(x),$$

but this is obvious. □

We denote by **P** the group of permutational symmetries of the Euler equations (I.1). The simplest permutational symmetry of (I.1) can be described as follows. Let σ_0 be a permutation of $\{1,2,3\}$. Let us extend σ_0 to the permutation σ of $\{1,2,3,4,5,6\}$ by the formula $\sigma(i)=\sigma_0(i-3)+3$, $4\leqslant i\leqslant 6$, then $\sigma\in\mathbf{P}$. The just described six permutations are the following:

$$\begin{aligned}
&\sigma_e:\ (1,2,3,4,5,6)\to(1,2,3,4,5,6),\\
&\sigma_1:\ (1,2,3,4,5,6)\to(2,1,3,5,4,6),\\
&\sigma_2:\ (1,2,3,4,5,6)\to(1,3,2,4,6,5),
\end{aligned} \tag{II.4}$$

$$\sigma_3:\ (1,2,3,4,5,6)\to(3,2,1,6,5,4),$$

$$\sigma_4:\ (1,2,3,4,5,6)\to(2,3,1,5,6,4),$$

$$\sigma_5:\ (1,2,3,4,5,6)\to(3,1,2,6,4,5).$$

They form a subgroup of **P**. We also consider the following three additional permutational symmetries of system (I.1):

$$\sigma_6:\ (1,2,3,4,5,6)\to(1,5,6,4,2,3),$$

$$\sigma_7:\ (1,2,3,4,5,6)\to(4,2,6,1,5,3), \tag{II.5}$$

$$\sigma_8:\ (1,2,3,4,5,6)\to(4,5,3,1,2,6).$$

Let us also consider the following products of permutations:

$$\sigma_{ij}=\sigma_i\circ\sigma_j,$$

where

$$i\in\{6,7,8\},\quad j\in\{1,2,3,4,5\}. \tag{II.6}$$

Then using MAPLE it is easy to check that among all $6!=720$ elements of group S_6, 24 permutations (II.4)–(II.6) exhaust group **P**.

It is interesting to observe that if $\lambda\in\mathcal{M}$ then for every permutation $\sigma\in\mathbf{P}$, $\sigma(\lambda)\in\mathcal{M}$. The same is true for the product case (I.4) too, i.e., if $\lambda\in\mathcal{P}$ then $\sigma(\lambda)\in\mathcal{P}$. In what concerns the Manakov case, this can be easily verified directly. In fact it suffices to verify that this is so only for permutations σ_i, $1\leqslant i\leqslant 8$. Another way to see it is to notice that the Manakov condition (I.3) can be also written in four equivalent different ways:

$$\begin{aligned}
M&=\lambda_{43}\lambda_{51}\lambda_{62}+\lambda_{16}\lambda_{24}\lambda_{35}=0,\\
M&=\lambda_{46}\lambda_{21}\lambda_{35}+\lambda_{13}\lambda_{54}\lambda_{62}=0,\\
M&=\lambda_{16}\lambda_{54}\lambda_{32}+\lambda_{43}\lambda_{21}\lambda_{65}=0,\\
M&=\lambda_{13}\lambda_{24}\lambda_{65}+\lambda_{46}\lambda_{51}\lambda_{32}=0,
\end{aligned} \tag{II.7}$$

where to simplify notation we will denote from now on $\lambda_{ij}=\lambda_i-\lambda_j$, $1\leqslant i,j\leqslant 6$. Now it is very easy to see that permutations σ_i, $1\leqslant i\leqslant 8$ always transform one of these four equivalent conditions to another. For the product case this verification is completely evident.

III. MANAKOV AND PRODUCT CASE CONDITIONS

In this section we come to the Manakov condition (I.3) and to the product case (I.4) by an approach which differs from already know derivations of these cases.[8,11–14,17]

In what follows we will always suppose that the considered first integrals are not constant on any open subset of their domain of definition.

Theorem III.1: *If system (I.1) admits, even only locally, a fourth integral which does not depend on all the variables, then* $\lambda\in\mathcal{M}\cup\mathcal{P}$.

Proof: The plan of the proof is as follows. First we show that our theorem is true if we assume that the fourth integral does not depend on x_6. Then, using permutational symmetries, we easily show that our theorem is valid in all remaining cases.

Thus let us suppose first that the function

$$F=F(x_1,x_2,x_3,x_4,x_5)$$

is such first integral of (I.1). This obviously means that

$$\frac{\mathrm{d}F}{\mathrm{d}t}=Y_\lambda(F)=(\lambda_{32}x_2x_3+\lambda_{65}x_5x_6)\partial_1F+(\lambda_{13}x_1x_3+\lambda_{46}x_4x_6)\partial_2F+(\lambda_{21}x_1x_2+\lambda_{54}x_4x_5)\partial_3F$$
$$+(\lambda_{35}x_3x_5+\lambda_{62}x_2x_6)\partial_4F+(\lambda_{43}x_3x_4+\lambda_{16}x_1x_6)\partial_5F=0,$$

or equivalently

$$\frac{\mathrm{d}F}{\mathrm{d}t}=Y_\lambda(F)=x_6Y_1(F)+Y_2(F)=0, \tag{III.1}$$

where Y_λ is the vector field defined by the Euler system (I.1) and Y_1 and Y_2 are the following vector fields defined in $\mathbb{R}^5=\mathbb{R}^5(x_1,x_2,x_3,x_4,x_5)$:

$$Y_1=\lambda_{65}x_5\partial_1+\lambda_{46}x_4\partial_2+\lambda_{62}x_2\partial_4+\lambda_{16}x_1\partial_5,$$

$$Y_2=\lambda_{32}x_2x_3\partial_1+\lambda_{13}x_1x_3\partial_2+(\lambda_{21}x_1x_2+\lambda_{54}x_4x_5)\partial_3+\lambda_{35}x_3x_5\partial_4+\lambda_{43}x_3x_4\partial_5.$$

Hereafter by ∂_i we denote the partial derivative with respect to x_i, for $1\leqslant i\leqslant 6$. Since (III.1) is an identity with respect to all the variables we have

$$Y_1(F)=Y_2(F)=0. \tag{III.2}$$

Let us compute the Lie brackets $Y_3=[Y_1,Y_2]$ and $Y_4=[Y_1,Y_3]$. We obtain

$$Y_3=x_3x_4(\lambda_{32}\lambda_{46}-\lambda_{43}\lambda_{65})\partial_1+x_3x_5(\lambda_{13}\lambda_{65}-\lambda_{35}\lambda_{46})\partial_2+[x_1x_4(\lambda_{16}\lambda_{54}+\lambda_{21}\lambda_{46})+x_2x_5(\lambda_{21}\lambda_{65}$$
$$+\lambda_{54}\lambda_{62})]\partial_3+x_1x_3(\lambda_{16}\lambda_{35}-\lambda_{13}\lambda_{62})\partial_4+x_2x_3(\lambda_{43}\lambda_{62}-\lambda_{16}\lambda_{32})\partial_5,$$

$$Y_4=x_2x_3(\lambda_{16}\lambda_{32}\lambda_{65}+\lambda_{32}\lambda_{46}\lambda_{62}-2\lambda_{43}\lambda_{62}\lambda_{65})\partial_1+x_1x_3(\lambda_{13}\lambda_{16}\lambda_{65}+\lambda_{13}\lambda_{46}\lambda_{62}-2\lambda_{16}\lambda_{35}\lambda_{46})\partial_2$$
$$+[x_1x_2(\lambda_{16}\lambda_{21}\lambda_{65}+\lambda_{21}\lambda_{46}\lambda_{62}+2\lambda_{16}\lambda_{54}\lambda_{62})+x_4x_5(\lambda_{16}\lambda_{54}\lambda_{65}+\lambda_{46}\lambda_{54}\lambda_{62}$$
$$+2\lambda_{21}\lambda_{46}\lambda_{65})]\partial_3+x_3x_5(\lambda_{16}\lambda_{35}\lambda_{65}+\lambda_{35}\lambda_{46}\lambda_{62}-2\lambda_{13}\lambda_{62}\lambda_{65})\partial_4+x_3x_4(\lambda_{16}\lambda_{43}\lambda_{65}$$
$$+\lambda_{43}\lambda_{46}\lambda_{62}-2\lambda_{16}\lambda_{32}\lambda_{46})\partial_5.$$

Equations (III.2) imply that

$$Y_3(F)=Y_4(F)=0. \tag{III.3}$$

Equations (III.2) and (III.3) can be considered as a system of four homogeneous linear algebraic equations with unknowns

$$F=(\partial_1F,\partial_2F,\partial_3F,\partial_4F,\partial_5F),$$

which do not vanish identically.

This system has a solution H with $H=H_3-\lambda_6H_2$. However, H is obviously dependent on the known first integrals. Thus, if a fourth integral F exists, system (III.2)–(III.3) has at least two linearly independent solutions. We will now try to *find the conditions under which system (III.2)–(III.3) has at least two linearly independent solutions*.

Let us consider the 4×5 matrix A of the coefficients of this system. It is clear that our problem has a solution if and only if

$$\operatorname{rank}A\leqslant 3. \tag{III.4}$$

Now we are going to study when (III.4) is fulfilled. For this purpose we calculate all possible determinants of order four which can be obtained from the matrix A. For $1\leqslant i\leqslant 5$, by D_i, we denote the determinant obtained from matrix A by scratching its ith column. We have

$$\begin{aligned} D_1&=-2\lambda_{16}x_1x_3^2MD,\\ D_2&=-2\lambda_{62}x_2x_3^2MD,\\ D_3&=-2\lambda_{36}x_3^3MD,\\ D_4&=2\lambda_{46}x_3^2x_4MD,\\ D_5&=2\lambda_{65}x_3^2x_5MD, \end{aligned} \tag{III.5}$$

where M is defined by (I.3), and

$$\begin{aligned} D=&x_1^3x_2\lambda_{16}(\lambda_{13}\lambda_{62}-\lambda_{16}\lambda_{35})+x_1^2x_4x_5\lambda_{16}(\lambda_{35}\lambda_{46}-\lambda_{13}\lambda_{65})+x_1x_2^3\lambda_{62}(\lambda_{43}\lambda_{62}-\lambda_{16}\lambda_{32})\\ &+x_1x_2x_4^2\lambda_{46}(\lambda_{16}\lambda_{32}-\lambda_{43}\lambda_{62})+x_1x_2x_5^2\lambda_{65}(\lambda_{16}\lambda_{35}-\lambda_{13}\lambda_{62})+x_2^2x_4x_5\lambda_{62}(\lambda_{32}\lambda_{46}-\lambda_{43}\lambda_{65})\\ &+x_4^3x_5\lambda_{46}(\lambda_{43}\lambda_{65}-\lambda_{32}\lambda_{46})+x_4x_5^3\lambda_{65}(\lambda_{13}\lambda_{65}-\lambda_{35}\lambda_{46}). \end{aligned}$$

Condition (III.4) is equivalent to five equations $D_i=0$ for $1\leqslant i\leqslant 5$. Now, let us assume that $\lambda\notin\mathcal{M}\cup\mathcal{P}$. Then, we have two cases when all the above-mentioned determinants vanish: either $D\neq 0$ or $D=0$.

In the first case when $D\neq 0$ and $M\neq 0$ (III.5) imply immediately that all components of λ are equal but it is in contradiction with our assumption that $M\neq 0$.

Now we prove that $D=0$ implies that $\lambda\in\mathcal{M}\cup\mathcal{P}$, i.e., it also implies a contradiction with our assumption. Indeed, let us write down the coefficients of D,

$$\lambda_{13}\lambda_{62}-\lambda_{16}\lambda_{35}=0, \tag{III.6}$$

$$\lambda_{32}\lambda_{46}-\lambda_{43}\lambda_{65}=0, \tag{III.7}$$

$$\lambda_{43}\lambda_{62}-\lambda_{16}\lambda_{32}=0, \tag{III.8}$$

$$\lambda_{35}\lambda_{46}-\lambda_{13}\lambda_{65}=0. \tag{III.9}$$

We can always suppose that all λ_{ij} which appear in the above-mentioned equations are different from zero. Let us prove this, e.g., for λ_{13}. If $\lambda_{13}=0$ then from (III.9) we have that either $\lambda_{35}=0$ or $\lambda_{46}=0$. But each of these possibilities leads to the Manakov case.

Consider now Eqs. (III.6) and (III.7). They represent a linear system in unknowns λ_2 and λ_5,

$$-\lambda_{13}\lambda_2+\lambda_{16}\lambda_5=\lambda_1\lambda_{36},\quad -\lambda_{46}\lambda_2+\lambda_{43}\lambda_5=-\lambda_4\lambda_{36}. \tag{III.10}$$

We denote by Δ_0 the determinant of (III.10) and consider two possible cases.

(1) $\Delta_0\neq 0$. Solving (III.10) we obtain

$$\lambda_2=\frac{\lambda_1\lambda_{43}+\lambda_4\lambda_{16}}{\lambda_{16}+\lambda_{43}},\quad \lambda_5=\frac{\lambda_1\lambda_{46}+\lambda_4\lambda_{13}}{\lambda_{16}+\lambda_{43}},$$

but, for these values of λ_2 and λ_5, we have $M=0$.

(2) $\Delta_0=0$. In this case, (III.10) have to be dependent because if not they have no solution. This is equivalent to requiring that all order two minors of the corresponding 2×3 matrix vanish, which means

$$\Delta_0=\lambda_{36}(\lambda_{13}+\lambda_{46})=0, \tag{III.11}$$

$$\Delta_1=\lambda_{36}(\lambda_1\lambda_{43}+\lambda_4\lambda_{16})=0, \tag{III.12}$$

$$\Delta_2=\lambda_{36}(\lambda_1\lambda_{46}+\lambda_4\lambda_{13})=0. \tag{III.13}$$

From (III.12) and (III.13) we have

$$\Delta_2-\Delta_1=\lambda_{36}^2\lambda_{14}=0.$$

The last equation shows that if $\lambda_{36}\neq 0$ then $\lambda_{14}=0$, and (III.11) leads to

$$\lambda_3=2\lambda_1-\lambda_6.$$

Now (III.8) and (III.9) write

$$2\lambda_{21}\lambda_{16}=0, \quad -2\lambda_{51}\lambda_{16}=0.$$

Since $\lambda_{16}\neq 0$ we have $\lambda_{51}=\lambda_{21}=0$, which together with $\lambda_{14}=0$ leads to $M=0$.

It remains only to study the possibility $\lambda_{36}=0$, i.e., $\lambda_3=\lambda_6$. From (III.6) and (III.8) we obtain

$$-\lambda_{13}\lambda_{25}=0, \quad \lambda_{32}\lambda_{14}=0.$$

But $\lambda_{13}\neq 0$ and $\lambda_{32}\neq 0$ and therefore

$$\lambda_5=\lambda_2, \quad \lambda_4=\lambda_1,$$

i.e., we come to the product case.

All the above considerations lead to the conclusion that the Euler equations (I.1) can admit a fourth integral which does not depend on the variable x_6 only when $\lambda\in\mathcal{M}\cup\mathcal{P}$.

Let us suppose now that the fourth integral does not depend on x_1. Let us consider the permutational symmetry σ_{63} [see (II.6)]. From Theorem II.1 we know that if for some $\lambda\in\mathbb{R}^6$, system (I.1), i.e., vector field Y_λ, admits a first integral F not depending on x_1, then function $F\circ\sigma_{63}^{-1}$ will be a first integral of $Y_{\sigma(\lambda)}$. But function $F\circ\sigma_{63}^{-1}$ does not depend of x_6. Thus, from what we proved previously it follows that $\sigma_{63}(\lambda)\in\mathcal{M}\cup\mathcal{P}$. However, as we have already noticed, both sets $\mathcal{M}$ and $\mathcal{P}$ are invariant with respect to the permutational symmetries. Thus $\lambda\in\mathcal{M}\cup\mathcal{P}$.

Exactly in the same way, using permutational symmetries σ_{62}, σ_6, σ_3, and σ_2, we prove the nonexistence of a fourth integral that does not depend on x_2, x_3, x_4, or x_5, respectively.□

Further we study only the Manakov case because in the product case we have already known the fourth integral. Thus, to the end of this paper we always assume that $\lambda\in\mathcal{M}$ although we do not write it explicitly all the time.

The main problem related to the present work that remains open is the following. Let us suppose that system (I.1) possesses a rational fourth integral G depending on all the variables $(x_i)_{1\leqslant i\leqslant 6}$. Deduce in this case the existence of a local C^1 smooth fourth integral that does not depend on all the variables. Taking into account Theorem III.1, this will imply that the rational fourth integral can exist only in the Manakov or product case. To the best of our knowledge, the last assertion has not yet been proved in its full generality.

IV. CHOICE OF GOOD VARIABLES

Our first aim is to find an explicit formula for the fourth integral which does not depend on all variables $(x_i)_{1\leqslant i\leqslant 6}$ for the *generic*, i.e., an open and dense subset of $\mathcal{M}$.

The purpose of this section is to select all triples of variables x_k, x_l, x_m, $1\leqslant k<l<m\leqslant 6$, such that the fourth integral depends only on these variables.

We say that a differentiable function $F=F(x_1,\ldots,x_n)$ depends *essentially* on variables $x_1,\ldots,x_n$ if partial derivatives $\partial_i F,\ 1\leqslant i\leqslant n$, do not vanish identically on any open subset of the domain of definition of F.

First let us note that the subset of parameters $\lambda\in\mathcal{M}$ for which there exists a first integral of the system (I.1) depending essentially only on one variable, is never generic. The same is true also for first integrals depending essentially only on two variables x_k and $x_l,\ 1\leqslant k<l\leqslant 6$. Indeed, let us suppose for example that a function $F=F(x_1,x_2)$ which depends essentially on variables x_1 and x_2 is a first integral of system (I.1). Then

$$\frac{\mathrm{d}F}{\mathrm{d}t}=(\lambda_{32}x_2x_3+\lambda_{65}x_5x_6)\partial_1F+(\lambda_{13}x_1x_3+\lambda_{46}x_4x_6)\partial_2F=0.$$

Thus $\lambda_{65}x_5x_6\partial_1F$ and $\lambda_{46}x_4x_6\partial_2F$ vanish identically. As ∂_1F and ∂_2F do not vanish identically on any open set, then $\lambda_{65}=\lambda_{46}=0$. But the subset of $\mathcal{M}$ defined by $\lambda_{65}=\lambda_{46}=0$ is not dense, and thus is not generic in $\mathcal{M}$. The same arguments cover also the case of first integral $F=F(x_1,x_4)$. Now using the permutational symmetries, like at the end of Sec. III we cover the remaining 13 cases of variables x_k and $x_l,\ 1\leqslant k<l\leqslant 6$.

Thus, to find fourth integrals corresponding to a generic subset of $\mathcal{M}$ we are obliged to consider the functions of at least three variables $x_k,\ x_l,\ x_m,\ 1\leqslant k<l<m\leqslant 6$. As we will prove, we can always find such fourth integrals depending on three properly chosen variables.

Let us consider now all possible 20 sets of three variables $x_k,\ x_l,\ x_m,\ 1\leqslant k<l<m\leqslant 6$. We will say that the set (x_k,x_l,x_m) is a *good set* of variables if there exists a generic set $\mathcal{G}_{k,l,m}\subset\mathcal{M}$ such that for any $\lambda\in\mathcal{G}_{k,l,m}$, the Euler equations (I.1) admit a fourth integral depending essentially only on variables $x_k,\ x_l$, and x_m.

Let us consider the four sets

$$(x_4,x_5,x_6), \tag{IV.1}$$

$$(x_2,x_3,x_4), \tag{IV.2}$$

$$(x_1,x_3,x_5), \tag{IV.3}$$

$$(x_1,x_2,x_6). \tag{IV.4}$$

Now we prove the following fact.

Theorem IV.1: *All 16 remaining cases of sets of variables* $(x_k,x_l,x_m),\ 1\leqslant k<l<m\leqslant 6$ *are never good.*

Proof: Let function F be a first integral of (I.1) functionally independent of integrals (I.2). First we prove that $(x_1,x_2,x_3)\notin\mathbf{G}$ (case 1) and $(x_1,x_2,x_4)\notin\mathbf{G}$ (case 2).

Case 1. To prove that $(x_1,x_2,x_3)\notin\mathbf{G}$ let us suppose that $(x_1,x_2,x_3)\in\mathbf{G}$ and let $F(x_1,x_2,x_3)$ be the corresponding first integral depending essentially on (x_1,x_2,x_3). Then

$$\frac{\mathrm{d}F}{\mathrm{d}t}=(\lambda_{32}x_2x_3+\lambda_{65}x_5x_6)\partial_1F+(\lambda_{13}x_1x_3+\lambda_{46}x_4x_6)\partial_2F+(\lambda_{21}x_1x_2+\lambda_{54}x_4x_5)\partial_3F=0. \tag{IV.5}$$

Equation (IV.5) is an identity with respect to all the variables $x_1,\ldots,x_6$. Since F depends essentially on (x_1,x_2,x_3), then from (IV.5) it follows that

$$\lambda_{65}=\lambda_{46}=\lambda_{54}=0.$$

So we are out of the generic case and consequently $(x_1,x_2,x_3)\notin\mathbf{G}$.

From this case and the permutational symmetry arguments like at the end of the proof of Theorem III.1 we also cover the three other cases:

(156)	(246)	(345)
σ_6	σ_7	σ_8

where we denote for brevity (klm) instead of (x_k, x_l, x_m).

Case 2. To prove that $(x_1, x_2, x_4) \notin \mathbf{G}$, let us suppose that $(x_1, x_2, x_4) \in \mathbf{G}$ and $F(x_1, x_2, x_4)$ is the corresponding first integral depending essentially on (x_1, x_2, x_4). Then

$$\frac{\mathrm{d}F}{\mathrm{d}t} = (\lambda_{32}x_2x_3 + \lambda_{65}x_5x_6)\partial_1 F + (\lambda_{13}x_1x_3 + \lambda_{46}x_4x_6)\partial_2 F + (\lambda_{35}x_3x_5 + \lambda_{62}x_2x_6)\partial_4 F = 0. \tag{IV.6}$$

Like in Case 1, one deduces from (IV.6) that $\lambda_{65} = \lambda_{35} = 0$ but this is not the generic case. Thus $(x_1, x_2, x_4) \notin \mathbf{G}$. By the permutational symmetry argument the same applies also to the remaining 11 cases:

(125)	(134)	(136)	(145)	(146)	(235)	(236)	(245)	(256)	(346)	(356)
σ_1	σ_2	σ_5	σ_6	σ_{62}	σ_4	σ_3	σ_{61}	σ_{64}	σ_{65}	σ_{63}

Thus in all 16 cases it turns out that $(x_k, x_l, x_m) \notin \mathbf{G}$. □

What concerns four cases (IV.1)–(IV.4), we have not proved yet that they belong to **G**. Let us note one characteristic feature of the four cases of (IV.1)–(IV.4). Looking at (I.1) one notices that the right-hand sides of equations corresponding to x_k, x_l, and x_m are linear homogeneous functions of the remaining variables. This is never the case for the 16 cases which do not belong to **G**.

In fact cases (IV.2)–(IV.4) are obtained from case (IV.1) by the permutational symmetry argument that can be seen from the table:

(234)	(135)	(126)
σ_6	σ_7	σ_8

In Secs. V and VI we investigate set (IV.1) and prove that it [and therefore (IV.2)–(IV.4) too] indeed belong to **G**.

V. TOWARD THE FIRST INTEGRALS

Let us consider case (IV.1) when the fourth integral of system (I.1) we look for has the form

$$F = F(x_4, x_5, x_6), \tag{V.1}$$

and depends essentially on x_4, x_5, and x_6. Thus we have

$$\begin{aligned}\frac{\mathrm{d}F}{\mathrm{d}t} &= x_1(\lambda_{16}x_6\partial_5 F + \lambda_{51}x_5\partial_6 F) + x_2(\lambda_{62}x_6\partial_4 F + \lambda_{24}x_4\partial_6 F) + x_3(\lambda_{35}x_5\partial_4 F + \lambda_{43}x_4\partial_5 F)\\ &= x_1\tilde{Y}_1(F) + x_2\tilde{Y}_2(F) + x_3\tilde{Y}_3(F) = 0,\end{aligned} \tag{V.2}$$

where the definition of vector fields $\tilde{Y}_i$ for $1 \leqslant i \leqslant 3$, is obvious. Since $\tilde{Y}_1(F)$, $\tilde{Y}_2(F)$, and $\tilde{Y}_3(F)$ do not depend on x_1, x_2, and x_3, and since (V.2) is an identity with respect to all the variables, then

$$\tilde{Y}_1(F) = \tilde{Y}_2(F) = \tilde{Y}_3(F) = 0. \tag{V.3}$$

Equations (V.3) give a system of three first-order linear homogeneous partial differential equations for determining the function F. This function depends essentially on x_4, x_5, and x_6. Therefore the determinant of linear system (V.3) with respect to the unknowns $\partial_i F$, $4 \leqslant i \leqslant 6$, has to vanish identically. We prove that it really vanishes. Indeed, we have

$$\det\begin{pmatrix} 0 & \lambda_{16}x_6 & \lambda_{51}x_5 \\ \lambda_{62}x_6 & 0 & \lambda_{24}x_4 \\ \lambda_{35}x_5 & \lambda_{43}x_4 & 0 \end{pmatrix} = (\lambda_{43}\lambda_{51}\lambda_{62}+\lambda_{16}\lambda_{24}\lambda_{35})x_4x_5x_6.$$

However

$$\lambda_{43}\lambda_{51}\lambda_{62}+\lambda_{16}\lambda_{24}\lambda_{35}=0,$$

because this coincides with the first form of the Manakov condition (II.7). Thus, in a way completely independent of Sec. III, we proved that the Manakov condition is necessary for the existence of a nontrivial first integral $F=F(x_4,x_5,x_6)$. Let us stress the great simplicity of this derivation.

In Sec. VI in an elementary way we prove that generically the Manakov condition is also sufficient for the existence of such fourth integral.

When the vector fields $\tilde{Y}_1$ and $\tilde{Y}_2$ are independent, equation $\tilde{Y}_3(F)=0$ follows from $\tilde{Y}_1(F)=\tilde{Y}_2(F)=0$ and it suffices to consider only these two equations, i.e.,

$$\begin{aligned} &\tilde{Y}_1(F)=\lambda_{16}x_6\partial_5F+\lambda_{51}x_5\partial_6F=0, \\ &\tilde{Y}_2(F)=\lambda_{62}x_6\partial_4F+\lambda_{24}x_4\partial_6F=0. \end{aligned} \tag{V.4}$$

As it is easy to see these two linear equations with unknowns ∂_4F, ∂_5F and ∂_6F are dependent if and only if the matrix of this system is of rank 0 or 1, or equivalently if at least one of the following conditions is satisfied:

$$\begin{aligned} &\text{case I:} \quad \lambda_{16}=\lambda_{62}=0, \\ &\text{case II:} \quad \lambda_{16}=\lambda_{51}=0, \\ &\text{case III:} \quad \lambda_{24}=\lambda_{62}=0. \end{aligned} \tag{V.5}$$

These singular cases will be investigated in Sec. VII.

We note here that the local solvability of system (V.4) around any point $(x_4,x_5,x_6) \neq (0,0,0)$ follows from the Frobenius integrability Theorem (see Ref. 33). Indeed, the Lie bracket $[\tilde{Y}_1,\tilde{Y}_2]$ of vector fields

$$\tilde{Y}_1=\lambda_{16}x_6\partial_5+\lambda_{51}x_5\partial_6=0, \quad \tilde{Y}_2=\lambda_{62}x_6\partial_4+\lambda_{24}x_4\partial_6=0,$$

is equal to

$$[\tilde{Y}_1,\tilde{Y}_2]=\lambda_{51}\lambda_{62}x_5\partial_4-\lambda_{16}\lambda_{24}x_4\partial_5.$$

The determinant formed by the coefficients of vector fields $\tilde{Y}_1$, $\tilde{Y}_2$ and $[\tilde{Y}_1,\tilde{Y}_2]$ is

$$\det\begin{pmatrix} 0 & \lambda_{16}x_6 & \lambda_{51}x_5 \\ \lambda_{62}x_6 & 0 & \lambda_{24}x_4 \\ \lambda_{51}\lambda_{62}x_5 & -\lambda_{16}\lambda_{24}x_4 & 0 \end{pmatrix} = 0.$$

Hence Eqs. (V.4) have, at least locally, a nontrivial solution. In fact one can find a global solution as shown in Sec. VI.

VI. FIRST INTEGRALS IN GENERIC CASE

We start this section with formulation of a useful criterion for the functional independence which we will use later in this section and Sec. VII.

Let $U\subset\mathbb{R}^n$ be an open set. Let us suppose that $F_1,\ldots,F_q\in C^1(U)$, $1\leqslant q<n$, are functionally independent functions at point $x\in U$, i.e.,

$$\operatorname{rank}\frac{\partial(F_1,\ldots,F_q)}{\partial(x_1,\ldots,x_n)}(x)=q. \tag{VI.1}$$

Let us define the following matrix:

$$S(x)=\begin{pmatrix} \partial_1F_1 & \ldots & \partial_1F_q & 0 & \ldots & 0 \\ \vdots & & & & & \\ \partial_qF_1 & \ldots & \partial_qF_q & 0 & \ldots & 0 \\ \partial_{q+1}F_1 & \ldots & \partial_{q+1}F_q & 1 & \ldots & 0 \\ \vdots & & & & \ddots & \\ \partial_nF_1 & \ldots & \partial_nF_q & 0 & \ldots & 1 \end{pmatrix},$$

and let

$$\Delta=\det\frac{\partial(F_1,\ldots,F_q)}{\partial(x_1,\ldots,x_q)}(x).$$

Matrix $S(x)$ is invertible if and only if $\Delta\neq 0$. Let $F\in C^1(U)$ be a function. When there exists $S(x)^{-1}$ we define vector $Z(x)=(Z_1(x),\ldots,Z_n(x))=S^{-1}(x)(\operatorname{grad}F)$.

Condition (VI.1) allows us to assume without any loss of generality that $\Delta\neq 0$ and we can now formulate a simple but very useful fact that goes back to Ref. 27.

Theorem VI.1: *Functions $F_1,\ldots,F_q$ and F are functionally independent at point x if and only if functions $Z_j(x)$, $q+1\leqslant j\leqslant n$, do not vanish simultaneously.*

The proof of this theorem is immediate if we note that $S^{-1}(x)(\operatorname{grad}F_k(x))$ is the kth vector of the standard basis of $\mathbb{R}^n$.

Now, we obtain first integral (V.1) in an explicit form. In order to find it we suppose that it is a homogeneous function of some degree $p\neq 0$. By the Euler theorem on homogeneous functions this is equivalent to

$$\sum_{i=4}^{6}x_i\partial_iF=pF. \tag{VI.2}$$

Let us note, that at least locally, as system (I.1) is homogeneous, then the existence of homogeneous of degree $p\neq 0$ first integrals follows from Ref. 34. We can suppose that $p=2$. This assumption is not restrictive because the power of a homogeneous function is homogeneous.

The searched first integral satisfies equations (V.4) and (VI.2). We solve this system of three equations with respect to the partial derivatives of F and obtain

$$\partial_4F=\frac{2\lambda_{16}\lambda_{24}x_4F}{\lambda_{16}\lambda_{24}x_4^2+\lambda_{51}\lambda_{62}x_5^2-\lambda_{16}\lambda_{62}x_6^2},$$

$$\partial_5 F = \frac{2\lambda_{62}\lambda_{51}x_5 F}{\lambda_{16}\lambda_{24}x_4^2+\lambda_{51}\lambda_{62}x_5^2-\lambda_{16}\lambda_{62}x_6^2},$$

$$\partial_6 F = \frac{-2\lambda_{16}\lambda_{62}x_6 F}{\lambda_{16}\lambda_{24}x_4^2+\lambda_{51}\lambda_{62}x_5^2-\lambda_{16}\lambda_{62}x_6^2}.$$

By inspection one immediately sees that

$$F=\lambda_{16}\lambda_{24}x_4^2+\lambda_{51}\lambda_{62}x_5^2-\lambda_{16}\lambda_{62}x_6^2 \tag{VI.3}$$

is a solution.

Let us notice that first integral F depends on first integrals (I.2) when $\lambda_{13}=\lambda_{32}=0$. Indeed in this case we can write F in the form

$$F=\lambda_{16}(\lambda_1 H_2 - H_3).$$

This is why we have to add to the three singular cases (V.5) another one

$$\text{case IV:} \quad \lambda_{13}=\lambda_{32}=0. \tag{VI.4}$$

Now we prove the following

Theorem VI.2: *For $\lambda \in \mathcal{M}$ first integrals H_1, H_2, H_3, and F are functionally independent except in cases* (V.5) *and* (VI.4).

Proof: We showed already that F depends on H_1, H_2, H_3 in case IV. Let us suppose now that we are out of case IV then, as it is easy to see, determinant

$$\Delta = \det\frac{\partial(H_1,H_2,H_3)}{\partial(x_1,x_2,x_3)} = 4(\lambda_{13}x_1x_3x_5+\lambda_{21}x_1x_2x_6+\lambda_{32}x_2x_3x_4), \tag{VI.5}$$

does not vanish. Thus matrix $S(x)$ is invertible and we can compute vector $Z(x)$. By virtue of Theorem VI.1 the first integral F of the Euler equations (I.1) is functionally independent of first integrals (I.2) if and only if the last three components of vector Z do not vanish simultaneously. Direct computations for the first integral F given by (VI.3) show that

$$Z_4=2\lambda_{16}\lambda_{24}x_4, \quad Z_5=2\lambda_{62}\lambda_{51}x_5, \quad Z_6=-2\lambda_{62}\lambda_{16}x_6.$$

One can easily see that $Z_4=Z_5=Z_6=0$ only in the following cases [see (V.5]:

- $\lambda_{16}=\lambda_{62}=0$ which coincides with case I,
- $\lambda_{16}=\lambda_{51}=0$ which coincides with case II,
- $\lambda_{24}=\lambda_{62}=0$ which coincides with case III. □

For our further considerations it is important to notice that determinant (VI.5) vanishes identically only when case IV is fulfilled.

VII. INVESTIGATION OF SINGULAR CASES

In this section we examine all values of parameters $(\lambda_i)_{1\leqslant i\leqslant 6}$ which satisfy one of conditions (V.5) or (VI.4). All these cases satisfy the Manakov condition.

First let us note that it suffices to examine only cases I and II. Indeed, by the permutational symmetry arguments we recover the fourth integral for case III [see (V.5) and case IV (see (VI.4)] from the fourth integral of case II by the permutations σ_1 and σ_6, respectively.

Let us consider case I when $\lambda_{16}=\lambda_{62}=0$. From (V.3) we have

$$\tilde{Y}_1(F)=\lambda_{56}x_5\partial_6 F=0, \quad \tilde{Y}_2(F)=\lambda_{64}x_4\partial_6 F=0,$$

$$\widetilde{Y}_3(F)=\lambda_{35}x_5\partial_4F+\lambda_{43}x_4\partial_5F=0.$$

We can immediately find a function satisfying these equations, i.e., a first integral of (I.1) depending only on variables x_4, x_5, and x_6. This is function $F=\lambda_{43}x_4^2-\lambda_{35}x_5^2$. However, instead of F, we prefer to use the first integral $G=x_3^2+x_4^2+x_5^2$ because, as we will see, in contrast to F, it remains functionally independent of first integrals (I.2) in some particular cases when F is functionally dependent. To verify the independence of integrals (I.2) and G we apply Theorem VI.1. Let us suppose that conditions $\lambda_{13}=\lambda_{32}=0$ are not fulfilled, i.e., we are in case I and out of case IV. Noticing that under this assumption $\lambda_{63}\neq 0$, let us compute the expressions Z_j, $4\leqslant j\leqslant 6$, for function G,

$$Z_4=\frac{2\lambda_{43}x_4}{\lambda_{63}},\quad Z_5=\frac{2\lambda_{53}x_5}{\lambda_{63}},\quad Z_6=0.$$

We have $Z_4=Z_5=Z_6=0$ only when $\lambda_{43}=\lambda_{53}=0$. However in this last case x_3, x_4, and x_5 are first integrals of (I.1). We compute

$$\det\frac{\partial(H_1,x_3,x_4,x_5)}{\partial(x_1,x_3,x_4,x_5)}=x_4,$$

so that H_1, x_3, x_4, and x_5 are functionally independent.

Now, let us assume that cases I and IV are fulfilled simultaneously. Function $G=x_3^2+x_4^2+x_5^2$ is still a first integral but instead of using Theorem VI.1 we can compute directly that

$$\det\frac{\partial(H_1,H_2,H_3,G)}{\partial(x_2,x_3,x_4,x_5)}=8x_2(\lambda_{65}x_1x_3x_5+\lambda_{54}x_4x_5x_6+\lambda_{46}x_2x_3x_4).$$

This expression vanishes identically only when $\lambda_{54}=\lambda_{64}=0$, and this, together with conditions of cases I and IV leads to the trivial case when all components of λ are equal. Hence the first integral G is functionally independent of (I.2) even when conditions of cases I and IV are fulfilled simultaneously and this does not happen when instead of G we take F.

In case II listed in (V.5) we have $\lambda_{16}=\lambda_{51}=0$. In this case from (V.3) we obtain that $\widetilde{Y}_1\equiv 0$. Now

$$\widetilde{Y}_2=\lambda_{62}x_6\partial_4+\lambda_{24}x_4\partial_6,\quad \widetilde{Y}_3=\lambda_{36}x_5\partial_4+\lambda_{43}x_4\partial_5.$$

We compute the Lie bracket $\widetilde{Y}_4=[\widetilde{Y}_2,\widetilde{Y}_3]$ and obtain

$$\widetilde{Y}_4=\lambda_{62}\lambda_{43}x_6\partial_5+\lambda_{24}\lambda_{63}x_5\partial_6.$$

One can easily see that $x_4\widetilde{Y}_4=\lambda_{63}x_5\widetilde{Y}_2+\lambda_{62}x_6\widetilde{Y}_3$. Thus, according to the Frobenius integrability theorem, the system $\widetilde{Y}_2(G)=0$, $\widetilde{Y}_3(G)=0$ admits at least locally a solution. To find it we apply the already used approach supposing that G is a homogeneous function of degree 2. Solving the system

$$\widetilde{Y}_2(G)=0,\quad \widetilde{Y}_3(G)=0,\quad x_4\partial_4G+x_5\partial_5G+x_6\partial_6G=2G,$$

with respect to the partial derivatives of G we obtain

$$\partial_4G=\frac{2\lambda_{24}\lambda_{43}x_4G}{\lambda_{24}\lambda_{43}x_4^2+\lambda_{24}\lambda_{63}x_5^2-\lambda_{43}\lambda_{62}x_6^2},$$

$$\partial_5 G = \frac{2\lambda_{63}\lambda_{24}x_5 G}{\lambda_{24}\lambda_{43}x_4^2+\lambda_{24}\lambda_{63}x_5^2-\lambda_{43}\lambda_{62}x_6^2},$$

$$\partial_6 G = \frac{-2\lambda_{43}\lambda_{62}x_6 F}{\lambda_{24}\lambda_{43}x_4^2+\lambda_{24}\lambda_{63}x_5^2-\lambda_{43}\lambda_{62}x_6^2}.$$

One can see that

$$G=\lambda_{24}\lambda_{43}x_4^2+\lambda_{24}\lambda_{63}x_5^2-\lambda_{43}\lambda_{62}x_6^2,$$

is a solution. Let us notice that in case IV this function is functionally dependent on first integrals (I.2).

Now, let us assume that we are out of case IV. Then determinant (VI.5) does not vanish identically and let us apply Theorem VI.1. We obtain

$$Z_4=2\lambda_{24}\lambda_{43}x_4, \quad Z_5=2\lambda_{24}\lambda_{63}x_5, \quad Z_6=-2\lambda_{43}\lambda_{62}x_6.$$

Thus $Z_4=Z_5=Z_6=0$ only in the following three subcases:

(1) $\lambda_{43}=\lambda_{63}=0$,
(2) $\lambda_{43}=\lambda_{24}=0$,
(3) $\lambda_{24}=\lambda_{62}=0$.

In subcase (1) x_5 is a first integral of (I.1). As we are still out of case IV determinant (VI.5) does not vanish and we can calculate Z_j for $4\leqslant j\leqslant 6$ for integrals (I.2) and x_5. We obtain $Z_5=1$ and therefore the first integrals (I.2) and x_5 are functionally independent. In subcase (2) again x_5 is a first integral and we again have $Z_5=1$. In subcase (3) x_6 is a first integral and we have $Z_6=1$.

Now let us assume that the conditions of cases II and IV are fulfilled simultaneously. Then, as it is easy to check, x_1 is a first integral and we have

$$\det\frac{\partial(H_1,H_2,H_3,x_1)}{\partial(x_1,x_2,x_3,x_4)}=4\lambda_{46}x_4(x_2x_6-x_3x_5),$$

i.e., if $\lambda_{46}\neq 0$ then x_1 is a functionally independent of (I.2) first integral. If $\lambda_{46}=0$ then we come to the trivial case when all components of λ are equal.

The results obtained in this and previous sections are summarized in Table I, which covers all the space of parameters $(\lambda_i)_{1\leqslant i\leqslant 6}$ satisfying the Manakov condition. In Table I all cases are explicitly written down, unless they can be deduced one from another by the permutational symmetry argument. The last column contains necessary and sufficient conditions for functional independence of the integrals. The generic case in Table I is defined explicitly by the conditions of functional independence of the first integrals H_1, H_2, H_3, and F given in the last column. For the last four rows the listed first integrals are functionally independent for $\lambda\in\mathcal{M}$ except for the trivial case when all components of λ are equal. The results given in Table I remain valid also when $\lambda\in\mathbb{C}^6$. Indeed, we can directly check that functions listed in the second column remain first integrals of (I.1) when $\lambda\in\mathbb{C}^6$. They are also functionally independent. This is so because our proof of independence also works in the complex case.

Let us note that if, for example, $\lambda_1\neq\lambda_6$ and $\lambda_1=\lambda_3=\lambda_4$ the fourth integral written in Refs. 8, 11, 13, 14, and 22 is not defined while our fourth integral (VI.3) remains valid.

Finally let us note that the starting point to produce Table I was the particular place that we attributed to integral F. If instead of it we chose the integrals coming from (IV.2), (IV.3), or (IV.4) the corresponding table would be different.

TABLE I. Functionally independent first integrals for the Manakov case.

Case	First integrals	Conditions
Generic	$H_1,\ H_2,\ H_3,$	$\lvert\lambda_{16}\rvert+\lvert\lambda_{62}\rvert>0$ and
	$F=\lambda_{16}\lambda_{24}x_4^2$	$\lvert\lambda_{16}\rvert+\lvert\lambda_{51}\rvert>0$ and
	$+\lambda_{51}\lambda_{62}x_5^2-\lambda_{16}\lambda_{62}x_6^2$	$\lvert\lambda_{24}\rvert+\lvert\lambda_{62}\rvert>0$ and
		$\lvert\lambda_{13}\rvert+\lvert\lambda_{32}\rvert>0$
$\lambda_{16}=\lambda_{62}=0$ (case I)	$H_1,\ H_2,\ H_3,$	$\lvert\lambda_{43}\rvert+\lvert\lambda_{53}\rvert>0$
	$G=x_3^2+x_4^2+x_5^2$	
$\lambda_{43}=\lambda_{53}=0$	$H_1,\ x_3,\ x_4,\ x_5$	No conditions
$\lambda_{16}=\lambda_{51}=0$ (case II)	$H_1,\ H_2,\ H_3,$	$\lvert\lambda_{43}\rvert+\lvert\lambda_{63}\rvert>0$ and
	$G=\lambda_{24}\lambda_{43}x_4^2$	$\lvert\lambda_{43}\rvert+\lvert\lambda_{24}\rvert>0$ and
	$+\lambda_{24}\lambda_{63}x_5^2-\lambda_{43}\lambda_{62}x_6^2$	$\lvert\lambda_{24}\rvert+\lvert\lambda_{62}\rvert>0$ and
		$\lvert\lambda_{13}\rvert+\lvert\lambda_{32}\rvert>0$
$\lambda_{43}=\lambda_{63}=0$	$H_1,\ H_2,\ H_3,\ x_5$	No conditions
$\lambda_{43}=\lambda_{24}=0$	$H_1,\ H_2,\ H_3,\ x_5$	No conditions
$\lambda_{24}=\lambda_{62}=0$	$H_1,\ H_2,\ H_3,\ x_6$	No conditions
$\lambda_{13}=\lambda_{32}=0$	$H_1,\ H_2,\ H_3,\ x_1$	No conditions

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Boson and differential realizations of polynomial angular momentum algebra

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The inhomogeneous multiboson and multivariable differential realizations of the polynomial angular momentum algebra of quadratic type, $\mathcal{L}_2$, which may be seen as the nonlinear extension of an ordinary angular momentum algebra su(2) or its noncompact form su(1,1), are obtained from Fock representations of $\mathcal{L}_2$, which are related to master representation of $\mathcal{L}_2$ on the space of its universal enveloping algebra $U(\mathcal{L}_2)$ or to induced representations on their respective quotient spaces $U(\mathcal{L}_2)/I_i$ with different left ideals I_i. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1369656]

I. INTRODUCTION

Lie groups and Lie algebras, associated tightly with symmetries, have played an important role in quantum physics. In recent years, many works[1–15] have been devoted to investigating various nonlinear Lie algebras, which correspondingly describe nonlinear symmetries, and their applications in some quantum problems. The nonlinear Lie algebra to be discussed in this article in fact is a so-called polynomial angular momentum algebra, denoted by $\mathcal{L}_n$ (the suffix n is referred to as the highest degree of polynomial).[12–15] Similar to an ordinary angular momentum algebra su(2) [or its noncompact form su(1,1)],[16,17] $\mathcal{L}_n$ is generated by three elements $\{J_3, J_+, J_-\}$, and however, they satisfy the following commutation relations:

$$[J_3, J_\pm] = \pm J_m, \quad [J_+, J_-] = P(J_3), \tag{1}$$

where $P(J_3)$ is a polynomial function of J_3 with a finite degree n, i.e., $P(J_3) = \Sigma_{i=0}^{n} C_i J_3^i$ (C_i are arbitrary real numbers). When $C_0 = 0, C_1 = 1$ (or -1), $C_j = 0$ ($j > 1$), the polynomial angular momentum algebra $\mathcal{L}_n$ defined by Eq. (1) goes back to the ordinary angular momentum algebra su(2) [or su(1,1)]. Therefore, $\mathcal{L}_n$ may be seen as nonlinear extension of su(2) [or su(1,1)]. More recently, Beckers *et al.*[14] studied the *single-variable* differential realizations of the polynomial angular momentum algebras of quadratic ($n = 2$) and cubic ($n = 3$) types, respectively, by suggesting the generators $\{J_3, J_+, J_-\}$ be functions of the real variable x and the corresponding differential operator d/dx, whose concrete forms are determined by Eq. (1).

In this paper, we shall discuss the various inhomogeneous boson realizations (IHBRs) and the corresponding inhomogeneous differential realizations (IHDRs) of $\mathcal{L}_n$ by a purely algebraic approach similar to one proposed by Gruber and his co-workers.[18,19] This approach is based upon the master representation[21,22] of $\mathcal{L}_n$ on its universal enveloping algebra $U(\mathcal{L}_n)$ or the induced repre-

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sentations on the quotient spaces $U(\mathcal{L}_n)/I_i$, where I_i are left ideals with respect to $U(\mathcal{L}_n)$. From these representations, we may define the corresponding Fock representations of $\mathcal{L}_n$ on the Fock spaces, and then obtain the IHBRs of $\mathcal{L}_n$. Moreover, by means of the corresponding relations between the boson creation and annihilation operators and the differential operators, we may obtain directly the IHDRs of $\mathcal{L}_n$. In the present paper, we restrict ourselves to the polynomial angular momentum algebra of quadratic type, $\mathcal{L}_2$.

This paper is arranged as follows: In Sec. II, the general approach of obtaining the IHBR and IHDR from the master representation or from the induced representation is reviewed, which is adapted to any Lie algebra or nonlinear Lie algebra. Then, in Sec. III, we will apply this approach to the polynomial angular momentum algebra $\mathcal{L}_2$, and discuss its various IHBRs and IHDRs in detail. A simple discussion is given in the final section.

The symbol $\mathcal{N}$ denotes the set of non-negative integers and the symbol $\mathcal{C}$ denotes the complex number field.

II. GENERAL APPROACH

Let the generators of (nonlinear) Lie algebra $\mathcal{G}$ be T_a $(a=1,2,...,M)$. In terms of the Poincaré–Birkhoff–Witt theorem,[17,21,22] a basis for its universal enveloping algebra $U(\mathcal{G})$ can be chosen as the following set of ordered elements:

$$\{X(i_1,i_2,\ldots,i_M)=T_1^{i_1}T_2^{i_2}\cdots T_M^{i_M}|i_1,i_2,\ldots,i_M\in\mathcal{N}\}. \tag{2}$$

Then, by acting with the generators of $\mathcal{G}$ from the left upon the basis (2), i.e.,

$$\rho(T_a)X(i_1,i_2,\ldots,i_M)=T_aT_1^{i_1}T_2^{i_2}\cdots T_M^{i_M}=\sum_{i_1',\ldots,i_M'}\rho(T_a)_{i_1,i_2,\ldots,i_M}^{i_1',i_2',\ldots,i_M'}X(i_1',i_2',\ldots,i_M'), \tag{3}$$

we can obtain a so-called master representation ρ of $\mathcal{G}$ on $U(\mathcal{G})$.[20,21] On the quotient space $U(\mathcal{G})/I$, where I is a left ideal of $U(\mathcal{G})$, ρ may induce a representation. The different choice of I enables us to obtain various representations of $\mathcal{G}$.

Now let us construct the IHBR of $\mathcal{G}$ from the master representation ρ on $U(\mathcal{G})$ or from the induced representation on $U(\mathcal{G})/I$. It is obvious from Eq. (3) that the matrix elements $\rho(T_a)_{i_1,i_2,\ldots,i_M}^{i_1',i_2',\ldots,i_M'}$, determined by the commutation relations of $\mathcal{G}$, are related to M independent parameters $i_1,i_2,\ldots,i_M$ (non-negative integers), so we need M sets of independent boson pairs $\{a_i^+,a_i\}$ $(i=1,2,...,M)$ to define a Fock space $\mathcal{F}$ in the following way:

$$\{|i_1,i_2,\ldots,i_M\rangle=(a_1^+)^{i_1}(a_2^+)^{i_2}\cdots(a_M^+)^{i_M}|0\rangle|i_1,i_2,\ldots,i_M\in\mathcal{N}\}, \tag{4}$$

where $|0\rangle$ stands for a ''vacuum state,'' and $a_i|0\rangle=0$. Then consider a mapping Φ: $U(\mathcal{G})\to\mathcal{F}$ defined by

$$\Phi(X(i_1,i_2,\ldots,i_M))=|i_1,i_2,\ldots,i_M\rangle, \tag{5}$$

which is automorphic to $U(\mathcal{G})$, and let

$$F(T_a)=\Phi\rho(T_a)\Phi^{-1}, \tag{6}$$

it follows from Eqs. (3), (5), and (6) that Eq. (6) defines a Fock representation of $\mathcal{G}$ on $\mathcal{F}$,

$$F(T_a)|i_1,i_2,\ldots,i_M\rangle=\sum_{i_i',\ldots,i_M'}\rho(T_a)_{i_1,i_2,\ldots,i_M}^{i_1',i_2',\ldots,i_M'}|i_1',i_2',\ldots,i_M'\rangle, \tag{7}$$

since $F(T_a)$ satisfies the same commutation relations as the generators T_a of $\mathcal{G}$, i.e.,

$$[F(T_a),F(T_b)]=F([T_a,T_b]). \tag{8}$$

Thus, by solving Eq. (7), we can obtain the IHBR of $\mathcal{G}$ provided that we know the explicit forms of $\rho(T_a)^{i_1',i_2',\ldots,i_M'}_{i_1,i_2,\ldots,i_M}$. In order to obtain the IHBRs for the various representations, the following formulas will be needed:

$$\begin{aligned}
&a_k^+|i_1,i_2,\ldots,i_M\rangle=|i_1,i_2,\ldots,i_k+1,\ldots,i_M\rangle,\\
&a_k|i_1,i_2,\ldots,i_M\rangle=i_k|i_1,i_2,\ldots,i_k-1,\ldots,i_M\rangle,\\
&a_k^+a_k|i_1,i_2,\ldots,i_M\rangle=i_k|i_1,i_2,\ldots,i_k,\ldots,i_M\rangle,\\
&e^{a_k}|i_1,i_2,\ldots,i_M\rangle=\sum_{j=0}^{i_k}\frac{i_k!}{j!(i_k-j)!}|i_1,i_2,\ldots,j,\ldots,i_M\rangle.
\end{aligned} \tag{9}$$

In this paper, the following corresponding relations between the boson creation and annihilation operators and the differential operators will be adopted for simplicity,

$$a_i^+\Leftrightarrow\xi_i,\quad a_i\Leftrightarrow\frac{\partial}{\partial\xi_i},\quad i=1,2,\ldots,M, \tag{10}$$

they satisfy, respectively,

$$\begin{aligned}
&[a_i,a_j^+]=\delta_{ij},\quad [a_i,a_j]=[a_i^+,a_j^+]=0;\\
&\left[\frac{\partial}{\partial\xi_i},\xi_j\right]=\delta_{ij},\quad \left[\frac{\partial}{\partial\xi_i},\frac{\partial}{\partial\xi_j}\right]=[\xi_i,\xi_j]=0.
\end{aligned} \tag{11}$$

Thus, by making use of Eq. (10), we can immediately obtain the IHDR of $\mathcal{G}$ from the IHBR of $\mathcal{G}$.

III. IHBRs AND IHDRs OF $\mathcal{L}_2$

According to the definition (1), the polynomial angular momentum algebra $\mathcal{L}_2$ is spanned by three elements $\{J_3,J_\pm\}$, which satisfy the commutation relations,

$$[J_3,J_\pm]=\pm J_\pm,\quad [J_+,J_-]=C_0+C_1J_3+C_2J_3^2, \tag{12}$$

where C_i $(i=0,1,2)$ are real numbers. The basis for its universal enveloping algebra $U(\mathcal{L}_2)$ can be written as

$$\{X(n,m,r)=J_+^nJ_-^mJ_3^r|n,m,r\in\mathcal{N}\}, \tag{13}$$

and $X(0,0,0)=1$ denotes the identity operator. It follows that we have

$$\begin{aligned}
\rho(J_3)X(n,m,r)&=X(n,m,r+1)+(n-m)X(n,m,r),\\
\rho(J_+)X(n,m,r)&=X(n+1,m,r),\\
\rho(J_-)X(n,m,r)&=X(n,m+1,r)-C_2nX(n-1,m,r+2)-[C_1n+C_2n(n-1-2m)]\\
&\quad\times X(n-1,m,r+1)-\{C_0n+\tfrac{1}{2}C_1n(n-1-2m)+\tfrac{1}{6}C_2n[(n-1)(2n-1)\\
&\quad-6m(n-1-m)]\}X(n-1,m,r).
\end{aligned} \tag{14}$$

Here we have used the following equations with respect to Eq. (12):

$$
\begin{aligned}
&[J_3, J_\pm^n] = \pm n J_\pm^n, \\
&[J_-, J_+^n] = -n J_+^{n-1}\{C_2 J_3^2 + [C_1 + C_2(n-1)]J_3 \\
&\qquad + [C_0 + \tfrac{1}{2}C_1(n-1) + \tfrac{1}{6}C_2(n-1)(2n-1)]\}.
\end{aligned} \tag{15}
$$

It is easy to prove that the map ρ forms a master representation of $\mathcal{L}_2$ on $U(\mathcal{L}_2)$, i.e., that

$$
[\rho(J_3), \rho(J_\pm)] = \pm \rho(J_\pm), \quad [\rho(J_+), \rho(J_-)] = C_0 + C_1\rho(J_3) + C_2\rho(J_3^2). \tag{16}
$$

The corresponding Fock representation may be obtained by the approach discussed in the preceding Sec. II as

$$
\begin{aligned}
&F(J_3)|n,m,r\rangle = |n,m,r+1\rangle + (n-m)|n,m,r\rangle, \\
&F(J_+)|n,m,r\rangle = |n+1,m,r\rangle, \\
&F(J_-)|n,m,r\rangle = |n,m+1,r\rangle - C_2 n|n-1,m,r+2\rangle - [C_1 n + C_2 n(n-1-2m)]|n-1,m,r+1\rangle \\
&\qquad - \{C_0 n + \tfrac{1}{2}C_1 n(n-1-2m) + \tfrac{1}{6}C_2 n[(n-1)(2n-1) \\
&\qquad - 6m(n-1-m)]\}|n-1,m,r\rangle.
\end{aligned} \tag{17}
$$

By making use of Eq. (9), we can immediately obtain from Eq. (17) the IHBR of $\mathcal{L}_2$,

$$
\begin{aligned}
&B(J_3) = a_3^+ + a_1^+ a_1 - a_2^+ a_2, \quad B(J_+) = a_1^+, \\
&B(J_-) = a_2^+ - (C_0 + C_1 a_3^+ + C_2 (a_3^+)^2)a_1 + (C_1 - C_2 + 2C_2 a_3^+)a_2^+ a_2 a_1 \\
&\qquad - \tfrac{1}{2}(C_1 + C_2 + 2C_2 a_3^+)a_1^+ a_1^2 - C_2 (a_2^+)^2 a_2^2 a_1 + C_2 a_2^+ a_1^+ a_2 a_1^2 - \tfrac{1}{3}C_2 (a_1^+)^2 a_1^3.
\end{aligned} \tag{18}
$$

The corresponding IHDR may be obtained directly in terms of the relation (10) as

$$
\begin{aligned}
&D(J_3) = \xi_3 + \xi_1 \frac{\partial}{\partial \xi_1} - \xi_2 \frac{\partial}{\partial \xi_2}, \quad D(J_+) = \xi_1, \\
&D(J_-) = \xi_2 - (C_0 + C_1 \xi_3 + C_2 \xi_3^2)\frac{\partial}{\partial \xi_1} + (C_1 - C_2 + 2C_2 \xi_3)\xi_2 \frac{\partial^2}{\partial \xi_1 \partial \xi_2} \\
&\qquad - \frac{1}{2}(C_1 + C_2 + 2C_2 \xi_3)\xi_1 \frac{\partial^2}{\partial \xi_1^2} - C_2 \xi_2^2 \frac{\partial^3}{\partial \xi_1 \partial \xi_2^2} + C_2 \xi_1 \xi_2 \frac{\partial^3}{\partial \xi_1^2 \partial \xi_2} - \frac{1}{3} C_2 \xi_1^2 \frac{\partial^3}{\partial \xi_1^3}.
\end{aligned} \tag{19}
$$

Equations (18) and (19) are the *three-boson* realization and the *three-variable* differential realization of $\mathcal{L}_2$, respectively. When $C_0 = 0$, $C_1 = 1$, and $C_2 = 0$, Eqs. (18) and (19) become the results of the ordinary angular momentum algebra su(2).[19,20]

In the following, we shall further consider several quotient spaces $U(\mathcal{L}_2)/I_i$, where I_i are the left ideals with respect to $U(\mathcal{L}_2)$, and discuss, by the same approach, the IHBRs and IHDRs of $\mathcal{L}_2$ from its induced representations on $U(\mathcal{L}_2)/I_i$.

(1) On the quotient space $U(\mathcal{L}_2)/I_1$, where the left ideal I_1 is generated by one element $J_3 - \Lambda 1 (\Lambda \in \mathcal{C})$, with the basis,

$$
\{X(n,m) \equiv X(n,m,0) \bmod I_1 | n,m \in \mathcal{N}\} \tag{20}
$$

the master representation ρ, given by Eq. (14), induces a representation

$$\rho_1(J_3)X(n,m)=(\Lambda+n-m)X(n,m),$$

$$\rho_1(J_+)X(n,m)=X(n+1,m), \tag{21}$$

$$\rho_1(J_-)X(n,m)=X(n,m+1)-\{C_2n\Lambda^2+[C_1n+C_2n(n-1-2m)]\Lambda+C_0n+\tfrac{1}{2}C_1n(n-1-2m)+\tfrac{1}{6}C_2n[(n-1)(2n-1)-6m(n-1-m)]\}X(n-1,m).$$

In the process of calculating Eq. (21), the property $\rho_1(J_3)1=\Lambda 1$ has been utilized. It is obvious that the operator $\rho_1(J_3)$ on $U(\mathcal{L}_2)/I_1$ has the eigenvector $X(n,m)$ corresponding to the eigenvalue $\Lambda+n-m$. Thus, by making use of Eq. (9), we may obtain from the Fock representation that corresponds to Eq. (21) the IHBR of $\mathcal{L}_2$,

$$B_1(J_3)=\Lambda+a_1^+a_1-a_2^+a_2,\quad B_1(J_+)=a_1^+,$$
$$B_1(J_-)=a_2^+-(C_0+C_1\Lambda+C_2\Lambda^2)a_1+(C_1-C_2+2C_2\Lambda)a_2^+a_2a_1-\tfrac{1}{2}(C_1+C_2+2C_2\Lambda)a_1^+a_1^2-C_2(a_2^+)^2a_2^2a_1+C_2a_2^+a_1^+a_2a_1^2-\tfrac{1}{3}C_2(a_1^+)^2a_1^3. \tag{22}$$

The corresponding IHDR reads

$$D_1(J_3)=\Lambda+\xi_1\frac{\partial}{\partial\xi_1}-\xi_2\frac{\partial}{\partial\xi_2},\quad D_1(J_+)=\xi_1,$$
$$D_1(J_-)=\xi_2-(C_0+C_1\Lambda+C_2\Lambda^2)\frac{\partial}{\partial\xi_1}+(C_1-C_2+2C_2\Lambda)\xi_2\frac{\partial}{\partial\xi_1\partial\xi_2}-\frac{1}{2}(C_1+C_2+2C_2\Lambda)\xi_1\frac{\partial^2}{\partial\xi_1^2}-C_2\xi_2^2\frac{\partial^3}{\partial\xi_1\partial\xi_2^2}+C_2\xi_1\xi_2\frac{\partial^3}{\partial\xi_1^2\partial\xi_2}-\frac{1}{3}C_2\xi_1^2\frac{\partial^3}{\partial\xi_1^3}. \tag{23}$$

Equations (22) and (23) are the *two-boson* realizations and the *two-variable* differential realizations of $\mathcal{L}_2$, respectively.

(2) Consider a left ideal I_2 generated by the one element $J_-\lambda 1(\lambda\in\mathcal{C})$. Then, on the quotient space $U(\mathcal{L}_2)/I_2$ with the basis

$$\{X(nr)\equiv X(n0r)\bmod I_2|n,r,\in\mathcal{N}\} \tag{24}$$

the master representation ρ, Eq. (14), induces a representation,

$$\rho_2(J_3)X(n,r)=X(n,r+1)+nX(n,r),$$

$$\rho_2(J_+)X(n,r)=X(n+1,r), \tag{25}$$

$$\rho_2(J_-)X(n,r)=\lambda\sum_{k=0}^{r}C_r^kX(n,k)-C_2nX(n-1,r+2)-[C_1n+C_2n(n-1)]X(n-1,r+1)-[C_0n+\tfrac{1}{2}C_1n(n-1)+\tfrac{1}{6}C_2n(n-1)(2n-1)]X(n-1,r),$$

where the symbol C_r^k is the usual binomial coefficient $C_r^k=r!/k!(r-k!,)$ and the property $\rho_2(J_-)1=\lambda 1$ has been used. From the Fock representation that corresponds to Eq. (25), we may obtain with the help of Eq. (9) the IHBR of $\mathcal{L}_2$,

$$B_2(J_3)=a_2^++a_1^+a_1,\quad B_2(J_+)=a_1^+,$$
$$B_2(J_-)=\lambda e^{a_2}-(C_0+C_1a_2^++C_2(a_2^+)^2)a_1-\tfrac{1}{2}(C_1+C_2+2C_2a_2^+)a_1^+a_1^2-\tfrac{1}{3}C_2(a_1^+)^2a_1^3. \tag{26}$$

The corresponding IHDR is obtained directly as

$$D_2(J_3)=\xi_2+\xi_1\frac{\partial}{\partial\xi_1},\quad D_2(J_+)=\xi_1,$$
$$D_2(J_-)=\lambda e^{\partial/\partial\xi_2}-(C_0+C_1\xi_2+C_2\xi_2^2)\frac{\partial}{\partial\xi_1}-\frac{1}{2}(C_1+C_2+2C_2\xi_2)\xi_1\frac{\partial^2}{\partial\xi_1^2}-\frac{1}{3}C_2\xi_1^2\frac{\partial^2}{\partial\xi_1^3}. \tag{27}$$

Compared to Eqs. (22) and (23), clearly, Eqs. (26) and (27) are another kind of *two-boson* realization and the *two-variable* differential realization of $\mathcal{L}_2$, respectively.

(3) On the quotient space $U(\mathcal{L}_2)/I_3$, where the left ideal I_3 is generated by two elements $\{J_-, J_3-\kappa 1\}(\kappa\in C)$, with the basis

$$\{X(n)\equiv X(n00)\bmod I_3 | n\in\mathcal{N}\}, \tag{28}$$

the master representation ρ, Eq. (14), induces a representation,

$$\rho_3(J_3)X(n)=(\kappa+n)X(n),$$
$$\rho_3(J_+)X(n)=X(n+1), \tag{29}$$
$$\rho_3(J_-)X(n)=-\{(C_0+C_1\kappa+C_2\kappa^2)n+(C_2\kappa+\tfrac{1}{2}C_1)n(n-1)+\tfrac{1}{6}C_2n(n-1)(2n-1)\}X(n-1),$$

by virtue of the property $\rho_3(J_3)1=\kappa 1$. The operator $\rho(J_3)$ on $U(\mathcal{L}_2)/I_3$ has the eigenvector $X(n)$ with $\kappa+n$ as the eigenvalue. From the Fock representation that corresponds to (29), we may obtain by making use of Eq. (9) the IHBR of $\mathcal{L}_2$,

$$B_3(J_3)=\kappa+a_1^+a_1,\quad B_3(J_+)=a_1^+, \tag{30}$$
$$B_3(J_-)=-(C_0+C_1\kappa+C_2\kappa^2)a_1-\tfrac{1}{2}(C_1+C_2+2C_2\kappa)a_1^+a_1^2-\tfrac{1}{3}C_2(a_1^+)^2a_1^3.$$

The corresponding IHDR reads

$$D_3(J_3)=\kappa+\xi_1\frac{d}{d\xi_1},\quad D_3(J_+)=\xi_1, \tag{31}$$
$$D_3(J_-)=-(C_0+C_1\kappa+C_2\kappa^2)\frac{d}{d\xi_1}-\frac{1}{2}(C_1+C_2+2C_2\kappa)\xi_1\frac{d^2}{d\xi_1^2}-\frac{1}{3}C_2\xi_1^2\frac{d^3}{d\xi_1^3}.$$

Equations (30) and (31) are the *single-boson* realization and the *single-variable* differential realization of $\mathcal{L}_2$, respectively. When $C_0=0$, $C_1=1$, and $C_2=0$, combined with $\kappa=-j$, Eq. (30) becomes the so-called Gel'fand–Dyson representation of the ordinary angular momentum algebra su(2).[23] The single-variable differential realization (31) is not any of the three kinds of single-variable differential realizations obtained by Beckers *et al.*[14]

IV. DISCUSSIONS

In this paper the single-, two-, and three-boson realizations and the corresponding single-, two-, and three-variable differential realizations of the polynomial angular momentum algebra of quadratic type, $\mathcal{L}_2$, are obtained, respectively, from the master representation of $\mathcal{L}_2$ on the space of its universal enveloping algebra and the induced representations on the quotient spaces. It is easy to check that all these realizations satisfy the commutation relations (12) of $\mathcal{L}_2$. It is worthy of noting that (a) these boson realizations, given by Eqs. (22), (26), and (30), are merely the basic forms since from them we may construct the more complex forms of boson realizations. For example, replacing the arbitrary constant numbers, Λ in Eq. (22), λ in Eq. (26), and κ in Eq. (30),

by $\Lambda a_3^+ a_3$, $\lambda a_3^+ a_3$, and $\kappa a_2^+ a_2$, respectively, will lead to the extended boson realizations of $\mathcal{L}_2$, which satisfy the commutation relations (12) of $\mathcal{L}_2$ as well. The similar property is held for the corresponding differential realizations. (b) For the universal enveloping algebra $U(\mathcal{L}_2)$, we can further choose the other bases by ordering three generators J_+, J_-, J_3 in different sequences such as $J_-^n J_+^m J_3^r$, $(n,m,r \in \mathcal{N})$, $J_3^n J_+^m J_-^r$ and so on, then the corresponding inhomogeneous boson and differential realizations of $\mathcal{L}_2$ may be obtained easily by the approach used above. In fact, the realizations based upon the base $\{J_-^n J_+^m J_3^r\}$ and upon the base $\{J_+^n J_-^m J_3^r\}$ adopted in this paper may be related by simple symmetry considerations. We see that the approach we employed is straightforward and simpler than the other methods, and may be applied to the polynomial angular momentum algebra of an higher degree, $\mathcal{L}_n (n>2)$, and the other nonlinear Lie (super)algebras associated with ordinary Lie (super)algebras.[24] This work is now underway.

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Classification of *R*-operators[a]

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We classified the *R*-operators which satisfy the quantum Yang–Baxter equation on a function space. In this study, we gave all the meromorphic solutions of the system of the functional equations which is a necessary and sufficient condition for the *R*-operator to satisfy the Yang–Baxter equation. Most of the solutions were expressed in terms of the elliptic, trigonometric and rational functions. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1367326]

I. INTRODUCTION

During the last 8 years, significant advances have been made in our understanding of the solutions of the (quantum) Yang–Baxter equation on a function space, which we call the *R*-operators.[1–3]

Definition 1 (R-operator[1]): For $x_1,x_2,\ldots,x_n\in\mathbb{C}$ and $r>0$, define the sets $C(x_1,r)$ and $C((x_1,x_2,\ldots,x_n),r)$ by $C(x_1,r)=\{x\in\mathbb{C};|x-x_1|<r\}$ and $C((x_1,x_2,\ldots,x_n),r)=C(x_1,r)\times C(x_2,r)\times\ldots\times C(x_n,r)$. Let functions $A(x)$ and $B(u,x)$ be meromorphic on $C(0,r)$ and $C((0,0),r)$, respectively. For a function f meromorphic on $C((0,0),r/2)$, we define the function $(R(u)f)(z_1,z_2)$ meromorphic on $C(0,r)\times C((0,0),r/2)(\ni(u,z_1,z_2))$ as

$$(R(u)f)(z_1,z_2)=A(z_1-z_2)f(z_1,z_2)-B(u,z_1-z_2)f(z_2,z_1).$$

We call this operator $R(u)$ the *R*-operator.

There are three kinds of the *R*-operators expressed in terms of the elliptic, trigonometric, and rational functions, respectively. The elliptic *R*-operator has been investigated in particular. We found it by taking the limit $n\to\infty$ of Belavin's *R*-matrix.[1] Belavin's *R*-matrix is conversely obtained through restricting the domain of a modified version of the elliptic *R*-operator to a suitable finite-dimensional subspace.[4] This suggests that the properties of Belavin's *R*-matrix are generalized to those of the elliptic *R*-operator. Actually the author constructed the incoming and outgoing intertwining vectors for the elliptic *R*-operator, and proved the vertex-IRF correspondence.[5] The boundary *K*-operators,[6,7] which satisfy the boundary Yang–Baxter equation for the elliptic *R*-operator, are also obtained. We essentially use the elliptic *R*-operator and boundary *K*-operators to construct the (generalized) Ruijsenaars operators,[8–10] the commuting difference operators. Therefore, it is very important to find out new solutions of the Yang–Baxter equation in order to investigate the integrable models. What remains a question is the classification of the *R*-operators.

The aim of this article is to classify the *R*-operators.

Proposition I.1: For any function f meromorphic on $C((0,0,0),r/2)$, a necessary and sufficient condition for the functions $R_{12}(u)R_{13}(u+v)R_{23}(v)f$ and $R_{23}(v)R_{13}(u+v)R_{12}(u)f$ meromorphic on $C((0,0,0,0,0),r/2)$ to satisfy the Yang–Baxter equation

$$R_{12}(u)R_{13}(u+v)R_{23}(v)f=R_{23}(v)R_{13}(u+v)R_{12}(u)f$$

is that the meromorphic functions A and B satisfy the following equations on $C((0,0,0,0),r/2)$:

[a]Dedicated to Professor Yoshiyuki Shimizu on the occasion of his sixtieth birthday.

$$B(u+v,x+y)(A(x)A(-x)-A(y)A(-y))$$
$$=B(v,y)B(u+v,x)B(u,y)-B(u,x)B(u+v,y)B(v,x), \tag{1}$$

$$A(y)B(u,x)B(v,x+y)=A(y)(B(u+v,x+y)B(u,-y)+B(v,y)B(u+v,x)). \tag{2}$$

Therefore, in order to classify the *R*-operators, we gave the complete classification of the meromorphic solutions A and B of the functional equations (1) and (2).

Theorem I.2: *The meromorphic solutions $A(x)$ and $B(u,x)$ of Eqs. (1) and (2) defined on the polydiscs $C(0,r)$ and $C((0,0),r)$, respectively, are one of the following*:
0. *Trivial case:*

$$A(x) \text{ is arbitrary}, \quad B(u,x)\equiv 0.$$

$$A(x)\equiv 0,$$

$$B(u,x)=\exp(F(x)u)G(u) \text{ on } C(0,r)\times C(0,r_1)$$

$$(0<r_1\leqslant r).$$

1. *Generic case:*
1-1. *Elliptic:*

$$A(x)=c\cdot h(x)\frac{\sigma(x+s;\tau_1,\tau_2)}{\sigma(x;\tau_1,\tau_2)\sigma(s;\tau_1,\tau_2)},$$

$$B(u,x)=c\exp(\rho u x)\frac{\sigma(x+au;\tau_1,\tau_2)}{\sigma(x;\tau_1,\tau_2)\sigma(au;\tau_1,\tau_2)}$$

$$(a,c,\tau_1,\tau_2\in\mathbb{C}\setminus\{0\},\operatorname{Im}\tau_2/\tau_1>0,s\in\mathbb{C}\setminus(\mathbb{Z}\tau_1+\mathbb{Z}\tau_2),\rho\in\mathbb{C}).$$

1-2. *Trigonometric:*

$$A(x)=\begin{cases} c\cdot h(x)\dfrac{\sinh(x+s)/\lambda}{\sinh(x/\lambda)\sinh(s/\lambda)}, \\ c\cdot h(x)\dfrac{1}{\sinh(x/\lambda)}, \end{cases}$$

$$B(u,x)=\begin{cases} c\exp(\rho u x)\dfrac{\sinh(x+au)/\lambda}{\sinh(x/\lambda)\sinh(au/\lambda)}, \\ c\exp(\rho u x)\dfrac{\exp(\pm x/\lambda)}{\sinh x/\lambda} \end{cases}$$

$$(a,c,\lambda\in\mathbb{C}\setminus\{0\},s\in\mathbb{C}\setminus\mathbb{Z}\pi\sqrt{-1}\lambda,\rho\in\mathbb{C}).$$

1-3. *Rational:*

$$A(x)=\begin{cases} c\cdot h(x)\dfrac{x+s}{xs}, \\ c\cdot h(x)\dfrac{1}{x}, \end{cases} \qquad B(u,x)=\begin{cases} c\exp(\rho u x)\dfrac{x+au}{axu}, \\ c\exp(\rho u x)\dfrac{1}{x} \end{cases}$$

$$(a,c,s\in\mathbb{C}\setminus\{0\},\rho\in\mathbb{C}).$$

2. *Singular case:*

$$A(x)=c_1h(x),\quad B(u,x)=c_2\exp(\rho ux)\frac{1}{u}$$

$$(c_1,\rho\in\mathbb{C},c_2\in\mathbb{C}\setminus\{0\}).$$

Here the function F is holomorphic on $C(0,r_1)$, the function $G(\not\equiv 0)$ is meromorphic on $C(0,r)$, the function h is meromorphic on $C(0,r)$ satisfying the relation $h(x)h(-x)=1$ and the function $\sigma(x)=\sigma(x;\tau_1,\tau_2)$ is the Weierstrass sigma function,

$$\sigma(x;\tau_1,\tau_2)=x\prod_{\omega=m_1\tau_1+m_2\tau_2}\left\{\left(1-\frac{x}{\omega}\right)\exp\left(\frac{x}{\omega}+\frac{1}{2}\left(\frac{x}{\omega}\right)^2\right)\right\},$$

where (m_1,m_2) in the product above runs over all the elements in $\mathbb{Z}^2$ except (0, 0).

We can show the following theorem easily.

Theorem I.3: *The functions A and B in Theorem I.2 satisfy Eqs. (1) and (2).*

Our strategy to solve the functional equations (1) and (2) is as follows. We reduced Eqs. (1) and (2) to the functional equation introduced by Braden and Buchstaber:[11]

$$\phi_1(x+y)(\phi_4(x)\phi_5(y)-\phi_4(y)\phi_5(x))=\phi_2(x)\phi_3(y)-\phi_2(y)\phi_3(x). \tag{3}$$

They have proved that the solutions of this functional equation above were characterized by those of the functional equation discussed by Bruschi and Calogero:[12,13]

$$\alpha(x+y)-\alpha(x)\alpha(y)=\varphi(x)\varphi(y)\psi(x+y). \tag{4}$$

Since Kawazumi and the author[14] have given the complete classification of the meromorphic solutions near the origin of Eq. (4), we obtained all the meromorphic solutions of Eqs. (1) and (2) near the origin.

Let us now explain how this article is organized. Section II gives a brief summary of the functional equations above. In Sec. III, we solve the functional equations (1) and (2) on the assumptions that $B\not\equiv 0$ and that $A(x)A(-x)$ is not identically constant. There are three kinds of meromorphic solutions of Eqs. (1) and (2) expressed in terms of the elliptic, trigonometric and rational functions. We discuss the elliptic case in Sec. IV, the trigonometric case in Sec. V and the rational case in Sec. VI, respectively. Section VII presents the classification of the meromorphic solutions of the functional equations (1) and (2) on the assumptions that $B\not\equiv 0$ and that $A(x)A(-x)(\not\equiv 0)$ is identically constant. In the final section, Sec. VIII, we classify the meromorphic solutions of the functional equations (1) and (2) with $A\equiv 0$ or $B\equiv 0$.

After finishing this article, the author found the thesis[15] in which Komori investigated the *R*-operators associated with root algebras. We note that the definition of the *R*-operators in his thesis was slightly different from that in this article.

II. REVIEWS OF CERTAIN FUNCTIONAL EQUATIONS OF ADDITION TYPE

In this section, we review the solutions of the functional equations (3) and (4) of addition type.

A. Solutions of Eq. (4)

Bruschi and Calogero have investigated the general analytic solution of Eq. (4).[12,13] They have obtained the elliptic solution in the most general case and some trigonometric and rational solutions by degenerating the periods of the elliptic functions.

Kawazumi and the author classified the meromorphic solutions near the origin of Eq. (4).

Theorem II.1 (Kawazumi-Shibukawa[14]): *Let α, φ and ψ be holomorphic functions defined on a punctured disk $\{x\in\mathbb{C};0<|x|<r'\}$ for some $r'>0$. If they satisfy the functional equation (4), then they are equal to one of the following functions.*

$$\text{(0-i)}\quad \alpha(x)=0 \ \ or \ \ \exp(\rho x)\ \ (\rho\in\mathbb{C}),$$

$$\varphi\equiv 0 \ \ and \ \ \psi\text{: arbitrary, } or \ \ \varphi\text{: arbitrary and } \psi\equiv 0.$$

$$\text{(0-ii)}\quad \alpha(x)=C\exp(\rho x),\quad \varphi(x)=C_1\exp(C_2x),$$

$$\psi(x)=C(1-C)C_1^{-2}\exp((\rho-C_2)x)$$

$$(C,\rho,C_1,C_2\in\mathbb{C}, C\neq 0,1, C_1\neq 0).$$

$$\text{(I)}\quad \alpha(x)=\exp(\rho x)\frac{\sigma(\nu;\tau_1,\tau_2)\sigma(x+\mu;\tau_1,\tau_2)}{\sigma(\mu;\tau_1,\tau_2)\sigma(x+\nu;\tau_1,\tau_2)},$$

$$\varphi(x)=\exp(C_1x+C_2)\frac{\sigma(x)}{\sigma(x+\nu)},$$

$$\psi(x)=\exp((\rho-C_1)x-2C_2)\frac{\sigma(\nu)\sigma(\mu-\nu)\sigma(x+\mu+\nu)}{\sigma^2(\mu)\sigma(x+\nu)},$$

$$(\rho,\mu,\nu,C_1,C_2\in\mathbb{C},\ \ \tau_1,\tau_2\in\mathbb{C}\setminus\{0\},\ \ \mathrm{Im}\,\tau_2/\tau_1>0\quad \mu,\nu\notin\mathbb{Z}\tau_1+\mathbb{Z}\tau_2,\quad \mu-\nu\notin\mathbb{Z}\tau_1+\mathbb{Z}\tau_2).$$

$$\text{(II)}\quad \alpha(x)=\exp(\rho x)\frac{a(\exp(2x/\lambda)-1)+b}{c(\exp(2x/\lambda)-1)+b},$$

$$\varphi(x)=\exp(C_1x+C_2)\frac{\exp(2x/\lambda)-1}{c(\exp(2x/\lambda)-1)+b},$$

$$\psi(x)=\exp(-C_1x-2C_2)\frac{(a-c)\{-ac(\exp(2x/\lambda)-1)+b^2-b(a+c)\}}{c(\exp(2x/\lambda)-1)+b}$$

$$(\lambda,\rho,a,b,c,C_1,C_2\in\mathbb{C},\ \ \lambda\neq 0,\ \ b(a-c)\neq 0).$$

$$\text{(III)}\quad \alpha(x)=\exp(\rho x)\frac{ax+b}{cx+b},\ \ \varphi(x)=\exp(C_1x+C_2)\frac{x}{cx+b},$$

$$\psi(x)=\exp((\rho-C_1)x-2C_2)\frac{(c-a)\{acx+b(a+c)\}}{cx+b}$$

$$(\rho,a,b,c,C_1,C_2\in\mathbb{C},\ \ b(a-c)\neq 0).$$

All the solutions except for the case (0-i) *extend themselves to meromorphic functions defined on the whole plane* $\mathbb{C}$.

Remark: In Theorem II.1 (I), we use τ_1, τ_2, μ and ν instead of τ_1/λ, τ_2/λ, μ/λ and ν/λ in Ref. 14. Moreover, we note that the condition $\mu-\nu\notin\mathbb{Z}\tau_1+\mathbb{Z}\tau_2$ in Theorem II.1 (I) was dropped in Ref. 14.

B. Solutions of Eq. (3)

Braden and Buchstaber[11] have investigated Eq. (3). They have shown that the solutions of Eq. (3) were characterized by the solutions of Eq. (4). We review their results briefly.

Let ϕ_1 be a holomorphic function on $C(2x_0,2r_0)$ and ϕ_2, ϕ_3, ϕ_4 and ϕ_5 be holomorphic functions on $C(x_0,r_0)$ for some $x_0\in\mathbb{C}$ and $r_0>0$. We assume that they satisfy the following conditions:

(a) Eq. (3) for all $x,y\in C(x_0,r_0)$,
(b) $\phi_2(x_0)\phi_3'(x_0)-\phi_2'(x_0)\phi_3(x_0)\neq 0$,
(c) $\phi_4(x_0)\phi_5'(x_0)-\phi_4'(x_0)\phi_5(x_0)\neq 0$.

Lemma II.2: We define the function $\tilde{\phi}_1$ *holomorphic on* $C(0,2r_0)$ *and the functions* $\tilde{\phi}_2,\ldots,\tilde{\phi}_5$ *holomorphic on* $C(0,r_0)$ *as follows*:

$$\tilde{\phi}_1(x)=c\,\phi_1(x+2x_0),$$

$$\begin{pmatrix}\tilde{\phi}_{2k}(x)\\ \tilde{\phi}_{2k+1}(x)\end{pmatrix}=\begin{pmatrix}\phi_{2k}'(x_0) & \phi_{2k}(x_0)\\ \phi_{2k+1}'(x_0) & \phi_{2k+1}(x_0)\end{pmatrix}^{-1}\begin{pmatrix}\phi_{2k}(x+x_0)\\ \phi_{2k+1}(x+x_0)\end{pmatrix}\quad(k=1,2),$$

where

$$c=\det\begin{pmatrix}\phi_4'(x_0) & \phi_4(x_0)\\ \phi_5'(x_0) & \phi_5(x_0)\end{pmatrix}\Big/\det\begin{pmatrix}\phi_2'(x_0) & \phi_2(x_0)\\ \phi_3'(x_0) & \phi_3(x_0)\end{pmatrix}.$$

Then they satisfy

$$\tilde{\phi}_1(x+y)(\tilde{\phi}_4(x)\tilde{\phi}_5(y)-\tilde{\phi}_4(y)\tilde{\phi}_5(x))=\tilde{\phi}_2(x)\tilde{\phi}_3(y)-\tilde{\phi}_2(y)\tilde{\phi}_3(x)$$

for all $x,\ y\in C(0,r_0)$.

By straightforward computation, we deduce $\tilde{\phi}_{2k}(0)=\tilde{\phi}_{2k+1}'(0)=0$ and $\tilde{\phi}_{2k}'(0)=\tilde{\phi}_{2k+1}(0)=1$ for $k=1,2$.

Lemma II.3: There exist $(0<)r_2\leqslant r_1$, *the functions* γ_k *and* ξ_k $(k=1,2)$ *holomorphic on* $C(0,r_2)$ *such that* $\gamma_k(x)\neq 0$ *for all* $x\in C(0,r_2)$,

$$\begin{pmatrix}\tilde{\phi}_{2k}(x)\\ \tilde{\phi}_{2k+1}(x)\end{pmatrix}=\frac{1}{\gamma_k(x)}\begin{pmatrix}\xi_k(x)\\ \xi_k'(x)\end{pmatrix}$$

for all $x\in C(0,r_2)$, $\xi_k(0)=0$, *and* $\xi_k'(0)=\gamma_k(0)=1$.

For $k=1,2$, define $\tilde{\xi}_k(x)=\exp(-\lambda_k x)\xi_k(x)$, where $\lambda_k=-\tilde{\phi}_{2k}''(0)/2$. Then the functions $\tilde{\xi}_k(x)$ are holomorphic on $C(0,r_2)$ and satisfy $\tilde{\xi}_k(0)=\tilde{\xi}_k''(0)=0$ and $\tilde{\xi}_k'(0)=1$. We define the functions $\tilde{\xi}_0$ on $x\in C(0,2r_2)$ and γ on $x\in C(0,r_2)$ by $\tilde{\xi}_0(x)=\exp((\lambda_1-\lambda_2)x)\tilde{\phi}_1(x)$ and $\gamma(x)=\exp(2(\lambda_1-\lambda_2)x)\gamma_2(x)/\gamma_1(x)$.

Lemma II.4: (1) *The function* $\tilde{\xi}_1(x)/\tilde{\xi}_2(x)$ *is holomorphic on* $C(0,r_2)$.
(2) *For all* $x,y\in C(0,r_2)$

$$\tilde{\xi}_0(x+y)(\tilde{\xi}_2(x)\tilde{\xi}_2'(y)-\tilde{\xi}_2(y)\tilde{\xi}_2'(x))=\gamma(x)\gamma(y)(\tilde{\xi}_1(x)\tilde{\xi}_1'(y)-\tilde{\xi}_1(y)\tilde{\xi}_1'(x)).$$

Since there exists $(0<)r_3\leqslant r_2$ such that $\tilde{\xi}_1(x)\neq 0$ and $\tilde{\xi}_2(x)\neq 0$ for all $x\in C(0,r_3)\backslash\{0\}$, we are led to the following.

Theorem II.5 (Braden–Buchstaber[11]):

(1) $\gamma(x)=(\tilde{\xi}_2(x)/\tilde{\xi}_1(x))^2$ *and* $\tilde{\xi}_0(x)=\tilde{\xi}_2(x)/\tilde{\xi}_1(x)$ *for all* $x\in C(0,r_3)$.
(2) *Define the functions* α *and* φ *holomorphic on* $C(0,r_3)$ *by* $\alpha(x)=\tilde{\xi}_2(x)/\tilde{\xi}_1(x)$ *and* $\varphi(x)=\tilde{\xi}_2(x)$. *Then they satisfy Eq. (4) for all* $x,\ y\in C(0,r_3/2)\backslash\{0\}$.

It is to be mentioned that the function ψ is determined by the functions α and φ. We can reconstruct the solutions $\phi_1,\ldots,\phi_5$ of Eq. (3) from the functions α and φ in the theorem above.

III. GENERIC CASE

In this section, we solve Eqs. (1) and (2) on the assumption below.

Assumption 1: (1) The meromorphic function $A(x)A(-x)$ is not identically constant on $C(0,r)$.

(2) The meromorphic function B is not identically zero on $C((0,0),r)$.

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

Theorem III.1: (1) *The function $A(x)A(-x)$ meromorphic on the disk $C(0,r)$ is one of the following:*

$$\textit{elliptic:}\quad A(x)A(-x)=\frac{a_1\wp(x;\tau_1,\tau_2)+a_2}{a_3\wp(x;\tau_1,\tau_2)+a_4}, \tag{5}$$

$$\textit{trigonometric:}\quad A(x)A(-x)=\frac{a_1\sinh^{-2}(x/\lambda)+a_2}{a_3\sinh^{-2}(x/\lambda)+a_4},$$

$$\textit{rational:}\quad A(x)A(-x)=\frac{a_1x^{-2}+a_2}{a_3x^{-2}+a_4},$$

where $\wp(x)=\wp(x;\tau_1,\tau_2)$ is the Weierstrass pe function

$$\wp(x;\tau_1,\tau_2)=-\frac{d}{dx}\left(\frac{\sigma'(x;\tau_1,\tau_2)}{\sigma(x;\tau_1,\tau_2)}\right),$$

and the constants $\tau_1,\ \tau_2,\ \lambda\in\mathbb{C}\backslash\{0\}$ and $a_1,\ a_2,\ a_3,\ a_4\in\mathbb{C}$ satisfy the relations $\mathrm{Im}\,\tau_2/\tau_1>0$ *and* $a_1a_4-a_2a_3\neq 0$.

(2) *There exists $C(u_1,r_1)\subset C(0,r/4)$ such that the function $B(u,x)$ is one of the following:*

$$\textit{elliptic:}\quad B(u,x)=\exp(\rho(u)x)b(u)\frac{\sigma(x+a(u);\tau_1,\tau_2)}{\sigma(x;\tau_1,\tau_2)}, \tag{6}$$

$$\forall(u,x)\in D_1\cap D^e\cap(C(u_1,r_1)\times C(0,r)),$$

$$\textit{trigonometric:}\quad B(u,x)=\exp(\tilde{\rho}(u)x)\tilde{b}(u)\times\frac{c(u)(\exp((x+2\tilde{a}(u))/\lambda)-\exp(-x/\lambda))+\exp(-x/\lambda)}{\sinh(x/\lambda)}, \tag{7}$$

$$\forall(u,x)\in D_1\cap D^t\cap(C(u_1,r_1)\times C(0,r)),$$

$$\textit{rational:}\quad B(u,x)=\exp(\rho(u)x)\frac{b(u)+a(u)x}{x},$$

$$\forall(u,x)\in D_1\cap D^r\cap(C(u_1,r_1)\times C(0,r)),$$

where $\rho(u),\ a(u),\ b(u)\in\mathbb{C}$ for all $u\in C(u_1,r_1)$. Here $D_1(\subset C((0,0),r))$ is the domain of the meromorphic function $B(u,x)$ and

$$D^e=C(0,r)\times(C(0,r)\backslash(\mathbb{Z}\tau_1+\mathbb{Z}\tau_2)),$$

$$D^t=C(0,r)\times(C(0,r)\backslash\mathbb{Z}\pi\sqrt{-1}\lambda),$$

$$D^r=C(0,r)\times(C(0,r)\backslash\{0\}).$$

Assumption 1 implies the following lemma. (For part (2), see Lemma 5 in Ref. 11.)

Lemma III.2: (1) *Equations (1) and (2) on* $C((0,0,0,0),r/2)$ *are equivalent to the following equations:*

$$A(x)A(-x)-A(y)A(-y)=B(u,x)B(u,-x)-B(u,y)B(u,-y), \tag{8}$$

$$B(u,x)B(v,x+y)=B(u+v,x+y)B(u,-y)+B(v,y)B(u+v,x) \tag{9}$$

on $C((0,0,0),r)$ *and* $C((0,0,0,0),r/2)$, *respectively.*

(2) *The meromorphic solutions* $A(x)$ *and* $B(u,x)$ *of the previous equations satisfy the equation*

$$\begin{aligned} &B(v,x+y)(A(x)A(-x)-A(y)A(-y)) \\ &\quad =B(u,-x)B(u+v,x)B(v,y)-B(u,-y)B(u+v,y)B(v,x) \end{aligned} \tag{10}$$

as meromorphic functions on $C((0,0,0,0),r/2)$.

Now we intend to apply Sec. II B to Eq. (10).

Lemma III.3: For any $C((u_0',x_0'),r_0')\subset C((0,0),r/2)$, *there exist* $(u_1,x_1)\in C((u_0',x_0'),r_0')$ *and* $r_1(>0)$ *such that*

(0) $C((u_1,x_1),r_1)\subset C((u_0',x_0'),r_0')$,

(1) $B(u,x)$ *is holomorphic on* $C((u_1,x_1),r_1)$, $C(u_1,r_1)\times C(2x_1,2r_1)$ *and* $C(2u_1,2r_1)\times C(x_1,r_1)$,

(2) $B(u,-x)$ *is holomorphic on* $C((u_1,x_1),r_1)$ *and* $C(u_1,r_1)\times C(2x_1,2r_1)$,

(3) $A(x)$ *is holomorphic on* $C(x_1,r_1)$ *and* $C(2x_1,2r_1)$,

(4) $A(-x)$ *is holomorphic on* $C(x_1,r_1)$ *and* $C(2x_1,2r_1)$,

(5) $B(u,x)\neq 0$ *for all* $(u,x)\in C((u_1,x_1),r_1)$.

By $C((u_0',x_0'),r_0')\coloneqq C((0,0),r/4)$ in Lemma III.3, there exist $(u_1,x_1)\in C((0,0),r/4)$ and r_1 (>0) satisfying the conditions in Lemma III.3.

Lemma III.4: (1) $(d/dx)(A(x)A(-x))\not\equiv 0$ *on* $C(x_1,r_1)$.

(2) *For all* u, $v\in C(u_1,r_1)$,

$$\begin{vmatrix} B(u,-x)B(u+v,x) & \dfrac{\partial}{\partial x}(B(u,-x)B(u+v,x)) \\ B(v,x) & \dfrac{\partial B}{\partial x}(v,x) \end{vmatrix} \not\equiv 0$$

on $C(x_1,r_1)$.

Proof: We prove part (2) only. The proof is by contradiction. Assume the assertion were false. Then there would exist u_0, $v_0\in C(u_1,r_1)$ such that

$$\begin{vmatrix} B(u_0,-x)B(u_0+v_0,x) & \dfrac{d}{dx}(B(u_0,-x)B(u_0+v_0,x)) \\ B(v_0,x) & \dfrac{\partial B}{\partial x}(v_0,x) \end{vmatrix} \equiv 0$$

on $C(x_1,r_1)$. Thus there exists $c\in\mathbb{C}$ such that

$$\frac{B(u_0,-x)B(u_0+v_0,x)}{B(v_0,x)}\equiv c \quad \text{on} \quad C(x_1,r_1).$$

By Eq. (10) and Assumption 1 (1), we have $B(v_0,x)\equiv 0$ on $C(2x_1,2r_1)$. From Lemma III.5, we get $B(v_0,x)\equiv 0$ on $C(0,r)$, which implies a contradiction of Assumption 1 (1) because of Eq. (8). □

Lemma III.5: Let $r_1,r_2>0$ and $F(u,x)$ be a function meromorphic on the polydisc $C(0,r_1)\times C(0,r_2)$. For any $v\in C(0,r_1)$ such that the function F is holomorphic at $(v,y)(y\in C(0,r_2))$, the function $F(v,x)$ is meromorphic on $C(0,r_2)$.

Proof: Because the polydisc $C(0,r_1)\times C(0,r_2)$ is Stein and $H^2(C(0,r_1)\times C(0,r_2),\mathbb{Z})=0$, the sharp form of the Poincaré theorem is valid on $C(0,r_1)\times C(0,r_2)$. (See, for example, Chap. V, Sec. 2 in Ref. 16 and Secs. I and K in Ref. 17.) Then there exist two functions g and h holomorphic on $C(0,r_1)\times C(0,r_2)$ such that h is not identically zero, $F(u,x)=g(u,x)/h(u,x)$, and the functions g and h are coprime locally. Since the function F is holomorphic at (v,y), we have $h(v,y)\neq 0$, which implies $h(v,x)\not\equiv 0$ on $C(0,r_2)$. Thus the function $g(v,x)/h(v,x)$ is meromorphic on $C(0,r_2)$. For any $x\in C(0,r_2)$ such that $h(v,x)\neq 0$, $F(v,x)=g(v,x)/h(v,x)$. This completes the proof of the lemma. □

Let $u_0,\ v_0\in C(u_1,r_1)$. Because of Lemmas III.3 (2) and III.4, we can apply the method introduced in Sec. II B to Eq. (10) for $u:=u_0$ and $v:=v_0$. That is to say, there exists $C(x_0,r_0)\subset C(x_1,r_1)$ such that $\phi_1(x):=B(v_0,x)$ defined on $C(2x_0,2r_0)$, $\phi_2(x):=B(u_0,-x)B(u_0+v_0,x)$, $\phi_3(x):=B(v_0,x)$, $\phi_4(x):=A(x)A(-x)$, and $\phi_5(x)\equiv 1$ defined on $C(x_0,r_0)$ satisfy the conditions (a)–(c) in Sec. II B.

From Theorems II.1 and II.5, the function $\alpha(x)=\tilde{\xi}_2(x)/\tilde{\xi}_1(x)$ defined near the origin is one of the following.

$$(0)\quad \alpha(x)=C\exp(\rho x),$$

$$(\mathrm{I})\quad \alpha(x)=\exp(\rho x)\frac{\sigma(\mu;\tau_1,\tau_2)\sigma(x+\nu;\tau_1,\tau_2)}{\sigma(\nu;\tau_1,\tau_2)\sigma(x+\mu;\tau_1,\tau_2)},$$

$$(\mathrm{II})\quad \alpha(x)=\exp(\rho x)\frac{a(e^{2x/\lambda}-1)+b}{c(e^{2x/\lambda}-1)+b},$$

$$(\mathrm{III})\quad \alpha(x)=\exp(\rho x)\frac{ax+b}{cx+b}.$$

Lemma III.6: $\alpha(x)\neq C\exp(\rho x)$.

Proof: The proof is by contradiction. Assume the assertion were false. With the aid of Theorem II.5, we get $\alpha(0)=1$, and, consequently, $B(v_0,x)=c^{-1}\exp((\rho-\lambda_1+\lambda_2)(x-2x_0))$ near $2x_0$. Here the constant c was defined in Lemma II.2. From Lemma III.5 and the identity theorem for the meromorphic functions, the above equation is also valid on $C(0,r)$, which implies a contradiction of Assumption 1 (1) by virtue of Eq. (8). □

From this lemma, the function φ is uniquely determined by the function α and so are the functions $\tilde{\xi}_1$ and $\tilde{\xi}_2$.

Proof of Theorem III.1 (1): We first note that Assumption 1 implies the condition $a_1a_4-a_2a_3\neq 0$.

By means of $\phi_5(x)\equiv 1$, we have $\tilde{\phi}_5(x)\equiv 1$ and $\gamma_2(x)=\xi_2'(x)$, and $\tilde{\phi}_4(x)=\xi_2(x)/\xi_2'(x)$ as a result. By the definition in Lemma II.2,

$$A(x)A(-x)$$
$$=\begin{cases}\phi_4(x_0)+\dfrac{\phi_4'(x_0)}{\zeta(x-x_0)-\zeta(x-x_0+\nu)+\lambda_2+\zeta(\nu)}, & \text{(I)}\\ \phi_4(x_0)\\ \quad+\dfrac{\phi_4'(x_0)\left(\exp\left(\dfrac{2(x-x_0)}{\lambda}\right)-1\right)\left\{c\left(\exp\left(\dfrac{2(x-x_0)}{\lambda}\right)-1\right)+1\right\}}{\left(\lambda_2+\dfrac{2c-1}{\lambda}\right)\left(\exp\left(\dfrac{2(x-x_0)}{\lambda}\right)-1\right)\left\{c\left(\exp\left(\dfrac{2(x-x_0)}{\lambda}\right)-1\right)+1\right\}+\dfrac{2}{\lambda}\exp\left(\dfrac{2(x-x_0)}{\lambda}\right)}, & \text{(II)}\\ \phi_4(x_0)+\dfrac{\phi_4'(x_0)(x-x_0)\{c(x-x_0)+1\}}{(\lambda_2+c)(x-x_0)\{c(x-x_0)+1\}+1}, & \text{(III)}\end{cases}$$

near x_0, where $\zeta(x)=\zeta(x;\tau_1,\tau_2)$ is the Weierstrass zeta function $\zeta(x;\tau_1,\tau_2)=\sigma'(x;\tau_1,\tau_2)/\sigma(x;\tau_1,\tau_2)$. With the aid of the identity theorem for the meromorphic functions, the equation above is valid on $C(0,r)$. Because $A(x)A(-x)$ is an even function on $C(0,r)$, we obtain the desired result. □

Now we prove Theorem III.1 (2).

Proposition III.7: Let $u_0\in C(u_1,r_1)$. For any $v_0\in C(u_1,r_1)$, there exist $x_0(v_0)\in C(x_1,r_1)$ and $r_2(v_0)(>0)$ such that the function $B(v_0,x)$ is one of the following: For all $x\in C(2x_0(v_0),r_2(v_0))$,

$$\textit{elliptic:}\quad B(v_0,x)=\exp(\rho(v_0)x)b(v_0)\frac{\sigma(x+a(v_0);\tau_1,\tau_2)}{\sigma(x;\tau_1,\tau_2)},$$

$$\textit{trigonometric:}\quad B(u,x)=\exp(\rho(u)x)\tilde{b}(u)\times\frac{c(u)(\exp((x+2\tilde{a}(u))/\lambda)-\exp(-x/\lambda))+\exp(-x/\lambda)}{\sinh(x/\lambda)},$$

$$\textit{rational:}\quad B(v_0,x)=\exp(\rho(v_0)x)\frac{b(v_0)+a(v_0)x}{x},$$

where $\rho(v_0)$, $a(v_0)$, $b(v_0)\in\mathbb{C}$.

Proof: For the sake of brevity, we only show the elliptic case. For any $v_0\in C(u_1,r_1)$, there exists $C(x_0(v_0),r_0(v_0))\subset C(x_1,r_1)\backslash(\mathbb{Z}\tau_1+\mathbb{Z}\tau_2)$ such that $\phi_1(x):=B(v_0,x)$ defined on $C(2x_0(v_0),\ 2r_0(v_0))$, $\phi_2(x):=B(u_0,-x)B(u_0+v_0,x)$, $\phi_3(x):=B(v_0,x)$, $\phi_4(x):=A(x)A(-x)$, and $\phi_5(x)\equiv 1$ defined on $C(x_0(v_0),r_0(v_0))$ satisfy the conditions (a)–(c) in Sec. II B by means of Lemma III.4. Thus we deduce

$$\tilde{\xi}_2(x)=\exp(\zeta(2x_0(v_0);\tau_1,\tau_2)x)\frac{\sigma(2x_0(v_0);\tau_1,\tau_2)\sigma(x;\tau_1,\tau_2)}{\sigma(x+2x_0(v_0);\tau_1,\tau_2)},\tag{11}$$

where τ_1 and τ_2 are in Theorem III.1 (1).

Lemma III.8: $\alpha(x)\neq 0$, $\exp(\rho x)$.

The proof is quite similar to that of Lemma III.6, so we omit it. Equation (11) tells us that the zeroes of the function $\tilde{\xi}_2$ are $\mathbb{Z}\tau_1+\mathbb{Z}\tau_2$. Hence the function α is an elliptic solution of Eq. (4) by means of Lemma III.8, and the periods of the Weierstrass sigma function σ in the function α are τ_1 and τ_2 as a consequence. (See Secs. 3 and 4 in Ref. 14.) Thus there exists $(0<)r_2<2r_1$ such that

$$\tilde{\xi}_1(x)=\exp(\zeta(\mu;\tau_1,\tau_2)x)\,\frac{\sigma(\mu;\tau_1,\tau_2)\sigma(x;\tau_1,\tau_2)}{\sigma(x+\mu;\tau_1,\tau_2)}$$

on $C(0,r_2)$. From Lemma II.2, Theorem II.5, Eq. (11) and $\phi_1(x)=B(v_0,x)$, we have proved the proposition. □

Proof of Theorem III.1 (2): For the sake of brevity, we only prove the elliptic case. For any $v_0\in C(u_1,r_1)$, the function $B(v_0,x)$ is meromorphic on $C(0,r)$ by Lemma III.5. On the other hand, by Proposition III.7,

$$B(v_0,x)=\exp(\rho(v_0)x)b(v_0)\,\frac{\sigma(x+a(v_0))}{\sigma(x)}$$

on some small disk in $C(0,r)$. Because the right hand side of the equation above is meromorphic on $C(0,r)$, we have proved the theorem. □

IV. ELLIPTIC CASE

This section presents the solutions A and B of Eqs. (8) and (9) in the elliptic case of Theorem III.1.

Lemma IV.1: For all $u\in C(u_1,r_1)$, $\sigma(a(u))\neq 0$ *and* $b(u)\neq 0$.

Proof: We only show that $\sigma(a(u))\neq 0$ for all $u\in C(u_1,r_1)$. The proof is by contradiction. Assume the assertion were false. Then there would exist $u\in C(u_1,r_1)$ such that $\sigma(a(u))=0$. By means of Eq. (6), there exist functions $\tilde{\rho}$ and $\tilde{b}$ such that $B(u,x)=\exp(\tilde{\rho}(u)x)\tilde{b}(u)$ for all $x\in C(x_1,r_1)\backslash(\mathbb{Z}\tau_1+\mathbb{Z}\tau_2)$, and this equation is also valid on $C(0,r)$ from Lemma III.5. By Eq. (8), this contradicts Assumption 1 (1). □

By virtue of Eqs. (5), (6), (8) and the lemma above, we conclude Lemma IV.2.

Lemma IV.2: We have $a_3=0$, *that is to say,* $A(x)A(-x)=\tilde{a}_1\wp(x)+\tilde{a}_2$ *on* $C(0,r)$, *where* $\tilde{a}_1=a_1/a_4$ *and* $\tilde{a}_2=a_2/a_4$.

We note that the relation $a_1a_4-a_2a_3\neq 0$ implies $\tilde{a}_1\neq 0$. It follows from the Lemma IV.2 and Eq. (8) that $b(u)^2\sigma^2(a(u))=-\tilde{a}_1$ for all $u\in C(u_1,r_1)$.

Lemma IV.3: There exist $c\in\mathbb{C}\backslash\{0\}$ *and* $C(u_2,r_2)\subset C(u_1,r_1)$ *such that* $b(u)\sigma(a(u))=c$ *for all* $u\in C(u_2,r_2)$, *and*

$$B(u,x)=c\,\exp(\rho(u)x)\,\frac{\sigma(x+a(u))}{\sigma(a(u))\sigma(x)}$$

for all $(u,x)\in D_1\cap D^e\cap(C(u_2,r_2)\times C(0,r))$ *as a consequence.*

For the proof, it suffices to show the following lemma.

Lemma IV.4: There exists $C((u_2,0),r_2)\subset C(u_1,r_1)\times C(0,r)$ *such that the function* $B(u,x)\sigma(x)$ *is holomorphic on* $C((u_2,0),r_2)$.

Proof: Since the sharp form of the Poincaré theorem is valid on $C((0,0),r)$, there exist two functions g and h holomorphic on $C((0,0),r)$ such that h is not identically zero, $B(u,x)\sigma(x)=g(u,x)/h(u,x)$, and the functions g and h are coprime locally. By Eq. (6), $g(u,x)=\exp(\rho(u)x)b(u)\sigma(x+a(u))h(u,x)$ for all $(u,x)\in D_1\cap D^e\cap(C(u_1,r_1)\times C(0,r))$.

We fix any $u\in C(u_1,r_1)$. Because the function $\exp(\rho(u)x)b(u)\sigma(x+a(u))$ is holomorphic on $C(0,r)$ and $g(u,x)=\exp(\rho(u)x)b(u)\sigma(x+a(u))h(u,x)$ for all $x\in C(x_1,r_1)\backslash(\mathbb{Z}\tau_1+\mathbb{Z}\tau_2)$, we have $g(u,x)=\exp(\rho(u)x)b(u)\sigma(x+a(u))h(u,x)$ for all $x\in C(0,r)$. Thus $g(u,0)=b(u)\sigma(a(u))h(u,0)$, which tells us that $(u,0)$ is not a pole of the function $B(u,x)\sigma(x)$ for all $u\in C(u_1',r_1')$. Since the set of points of indeterminacy of the meromorphic function of two variables is isolated, there exists a regular point $(u_2,0)\in C(u_1',r_1')\times C(0,r)$ of the function $B(u,x)\sigma(x)$. We have thus proved the lemma. □

Using Eq. (8), we are led to the following theorem.

Theorem IV.5: *The elliptic solution* $A(x)$ *defined on* $C(0,r)$ *is*

$$A(x)=c\cdot h(x)\frac{\sigma(x+s)}{\sigma(x)\sigma(s)},$$

where $h(x)$ *is a meromorphic function defined on* $C(0,r)$ *satisfying the relation* $h(x)h(-x)=1$ *and* s *is a complex constant such that* $\wp(s)=-\tilde{a}_2/\tilde{a}_1$.

In the sequel, we determine the function B.

Proposition IV.6: There exists $C(u_3',\delta')\subset C(u_2,r_2)$ *such that*

$$B(u,x)=\exp(\tilde{\rho}(u)x)\frac{\sigma(x+a_1(u))}{\sigma(a_1(u))\sigma(x)}$$

for all $(u,x)\in D_1\cap D^e\cap(C(u_3',\delta')\times C(0,r))$, *where the function* a_1 *is holomorphic on* $C(u_3',\delta')$.

We only give the proof in the case that there exists $v_1\in C(u_2,r_2)$ such that $\wp'(a(v_1))\neq 0$ because the proof is rather simple in the case that $\wp'(a(u))\equiv 0$ on $C(u_2,r_2)$. The function $\wp(x)$ is holomorphic at $x=a(v_1)$ by using Lemma IV.1, and the function $\wp$ has a holomorphic inverse g near $a(v_1)$ as a result. (See, for example, p. 215 of Ref. 18.) Then there exists $C(v_1,\delta)\subset C(u_2,r_2)$ such that $\wp(a(u))$ is in the domain of the function g for all $u\in C(v_1,\delta)$. Define a function $\tilde{a}$ holomorphic on $C(v_1,\delta)$ as $\tilde{a}(u)=g(\wp(a(u)))$. There exists a function $\epsilon(u)\in\{0,1\}$ such that $a(u)\equiv(-1)^{\epsilon(u)}\tilde{a}(u)\ (\mathrm{mod}\,\mathbb{Z}\tau_1+\mathbb{Z}\tau_2)$ for all $u\in C(v_1,\delta)$, and consequently

$$B(u,x)=\exp(\tilde{\rho}(u)x)(-1)^{\epsilon(u)}\frac{\sigma(x+(-1)^{\epsilon(u)}\tilde{a}(u))}{\sigma(\tilde{a}(u))\sigma(x)}$$

for all $(u,x)\in D_1\cap D^e\cap(C(v_1,\delta)\times C(0,r))$, where $\tilde{\rho}(u)\in\mathbb{C}$.

Proposition IV.6 now follows from the following lemma.

Lemma IV.7: There exist $C(v_1',\delta')\subset C(v_1,\delta)$ *such that* $a(u)\equiv\tilde{a}(u)(\mathrm{mod}\mathbb{Z}\tau_1+\mathbb{Z}\tau_2)$ *for all* $u\in C(v_1',\delta')$ *or* $a(u)\equiv-\tilde{a}(u)(\mathrm{mod}\,\mathbb{Z}\tau_1+\mathbb{Z}\tau_2)$ *for all* $u\in C(v_1',\delta')$.

To prove this lemma, it suffices to give the proof in the case that, for all $C(u,\delta_1)\subset C(v_1,\delta)$, there exist $v,w\in C(u,\delta_1)$ such that $\epsilon(v)\neq\epsilon(w)$. By the sharp form of the Poincaré theorem, there exist two functions g and h holomorphic on $C((0,0),r)$ such that h is not identically zero, $B(u,x)\sigma(x)=g(u,x)/h(u,x)$, and the functions g and h are coprime locally. We omit the proof of the lemma below because it is similar to that of Lemma IV.4.

Lemma IV.8: There exists $C(u_3',\delta')\subset C(v_1,\delta)$ *satisfying the following conditions.*

(1) *The function* $B(u,x)\sigma(x)$ *is holomorphic on* $C((u_3',0),\delta')$.
(2) *For all* $(u,x)\in C((u_3',0),\delta')$,

$$c\exp(\tilde{\rho}(u)x)(-1)^{\epsilon(u)}\frac{\sigma(x+(-1)^{\epsilon(u)}\tilde{a}(u))}{\sigma(\tilde{a}(u))}h(u,x)=g(u,x).$$

By means of Lemma IV.8,

$$\exp(\tilde{\rho}(u)x)(-1)^{\epsilon(u)}\sigma(x+(-1)^{\epsilon(u)}\tilde{a}(u))=c^{-1}B(u,x)\sigma(x)\sigma(\tilde{a}(u))$$

for all $(u,x)\in C((u_3',0),\delta')$. Since the function $\tilde{a}(u)$ is holomorphic on $C(u_3',\delta')$, the function $f(u,x):=c^{-1}B(u,x)\sigma(x)\sigma(\tilde{a}(u))$ is holomorphic on $C((u_3',0),\delta')$. The function $(\partial f/\partial x)(u,0)$ is consequently holomorphic on $C(u_3',\delta')$, and

$$\frac{\partial f}{\partial x}(u,0)=\tilde{\rho}(u)\sigma(\tilde{a}(u))+(-1)^{\epsilon(u)}\sigma'(\tilde{a}(u)) \tag{12}$$

for all $u\in C(u_3',\delta')$.

By $B\not\equiv 0$ and Lemma IV.1, we conclude the following.

Lemma IV.9: There exists $C((u_3'',x_3''),\delta'')\subset C((u_3',0),\delta')$ *satisfying the following conditions.*

(1) $C(x_3'',\delta'')\not\ni 0$.
(2) $f(u,x)\neq 0$ *for all* $(u,x)\in C((u_3'',x_3''),\delta'')$.
(3) $\sigma(x-\tilde{a}(u))\neq 0$ *for all* $(u,x)\in C((u_3'',x_3''),\delta'')$.
(4) $\sigma(x+\tilde{a}(u))\neq 0$ *for all* $(u,x)\in C((u_3'',x_3''),\delta'')$.

Lemma IV.7 follows from Lemma IV.10 immediately.

Lemma IV.10: For all $u\in C(u_3'',\delta'')$, $2\tilde{a}(u)\in\mathbb{Z}\tau_1+\mathbb{Z}\tau_2$.

Proof: To prove this lemma, we show

$$-\frac{\sigma(x_3+\tilde{a}(u_3))}{\sigma(x_3-\tilde{a}(u_3))}=\exp(2x_3\zeta(\tilde{a}(u_3)))$$

for all $(u_3,x_3)\in C((u_3'',x_3''),\delta'')$. From Lemma IV.9, the functions $-f(u,x)/\sigma(x-\tilde{a}(u))$ and $f(u,x)/\sigma(x+\tilde{a}(u))$ are holomorphic on $C((u_3'',x_3''),\delta'')$ and satisfy $-f(u,x)/\sigma(x-\tilde{a}(u))\neq 0$ and $f(u,x)/\sigma(x+\tilde{a}(u))\neq 0$ for all $(u,x)\in C((u_3'',x_3''),\delta'')$. For any $(u_3,x_3)\in C((u_3'',x_3''),\delta'')$, let $\mathrm{Log}^{(1)}(x)$ and $\mathrm{Log}^{(2)}(x)$ be branches of the logarithm defined on open connected sets $V_1,V_2\subset\mathbb{C}$ such that $\exp(\tilde{\rho}(u_3)x_3)\in V_1$ and $(-1)^{\epsilon(u_3)+1}f(u_3,x_3)/\sigma(x_3+(-1)^{\epsilon(u_3)+1}\tilde{a}(u_3))\in V_2$, respectively. Because the function $(-1)^{\epsilon(u_3)+1}f(u,x)/\sigma(x+(-1)^{\epsilon(u_3)+1}\tilde{a}(u))$ is continuous at $(u,x)=(u_3,x_3)$, there exist $\tilde{\epsilon}>0$ and $\tilde{\delta}>0$ satisfying the following conditions.

(1) $C((-1)^{\epsilon(u_3)+1}f(u_3,x_3)/\sigma(x_3+(-1)^{\epsilon(u_3)+1}\tilde{a}(u_3)),\tilde{\epsilon})\subset V_2$.
(2) $C((u_3,x_3),\tilde{\delta})\subset C((u_3'',x_3''),\delta'')$.
(3) For all $(u,x)\in C((u_3,x_3),\tilde{\delta})$

$$\frac{(-1)^{\epsilon(u_3)+1}f(u,x)}{\sigma(x+(-1)^{\epsilon(u_3)+1}\tilde{a}(u))}\in C\left(\frac{(-1)^{\epsilon(u_3)+1}f(u_3,x_3)}{\sigma(x_3+(-1)^{\epsilon(u_3)+1}\tilde{a}(u_3))},\tilde{\epsilon}\right).$$

Let $N\in\mathbb{N}$ such that $1/N<\tilde{\delta}$. For all $n\geqslant N$, there exists $\tilde{u}_n\in C(u_3,1/n)$ such that $\epsilon(\tilde{u}_n)\neq\epsilon(u_3)$. (This is the case which we now consider.) Then we have $\epsilon(\tilde{u}_n)\equiv\epsilon(u_3)+1\ (\mathrm{mod}\ 2)$, $\lim_{n\to\infty}\tilde{u}_n=u_3$, and $(-1)^{\epsilon(u_3)+1}f(\tilde{u}_n,x_3)/\sigma(x_3+(-1)^{\epsilon(u_3)+1}\tilde{a}(\tilde{u}_n))\in V_2$ for all $n\geqslant N$. By the conditions (1) and (2) above, $\exp(\tilde{\rho}(\tilde{u}_n)x_3)\in V_2$ for all $n\geqslant N$, and, consequently,

$$\tilde{\rho}(\tilde{u}_n)x_3=\mathrm{Log}^{(2)}\left(\frac{(-1)^{\epsilon(u_3)+1}f(\tilde{u}_n,x_3)}{\sigma(x_3+(-1)^{\epsilon(u_3)+1}\tilde{a}(\tilde{u}_n))}\right)$$

for all $n\geqslant N$. On account of Eq. (12),

$$\begin{aligned}\frac{\partial f}{\partial x}(u_3,0)&=\lim_{n\to\infty}\frac{\partial f}{\partial x}(\tilde{u}_n,0)\\&=\frac{1}{x_3}\mathrm{Log}^{(2)}\left(\frac{(-1)^{\epsilon(u_3)+1}f(u_3,x_3)}{\sigma(x_3+(-1)^{\epsilon(u_3)+1}\tilde{a}(u_3))}\right)\sigma(\tilde{a}(u_3))+(-1)^{\epsilon(u_3)+1}\sigma'(\tilde{a}(u_3)).\end{aligned}$$

Because of $\exp(\tilde{\rho}(u_3)x_3)\in V_1$,

$$\frac{\partial f}{\partial x}(u_3,0)=\frac{1}{x_3}\mathrm{Log}^{(1)}\left(\frac{(-1)^{\epsilon(u_3)}f(u_3,x_3)}{\sigma(x_3+(-1)^{\epsilon(u_3)}\tilde{a}(u_3))}\right)\sigma(\tilde{a}(u_3))+(-1)^{\epsilon(u_3)}\sigma'(\tilde{a}(u_3)).$$

By the straightforward calculation, we obtain the desired result, thereby completing the proof of Proposition IV.6. □

Proposition IV.11: There exists $C(u_3,r_3)\subset C(u_1,r_1)$ *such that*

$$B(u,x)=\exp(\rho_1(u)x)\,\frac{\sigma(x+a_1(u))}{\sigma(a_1(u))\sigma(x)} \tag{13}$$

as meromorphic functions on $C(u_3,r_3)\times C(0,r)$, *where the functions* ρ_1 and a_1 *are holomorphic on* $C(u_3,r_3)$.

Proof: It is enough to show that the function $\tilde{\rho}$ in Proposition IV.6 is holomorphic locally. Define $f_1(u,x):=e^{\tilde{\rho}(u)}\sigma(x+a_1(u))$. Since the function f_1 is expressed as $f_1(u,x)=c^{-1}B(u,x)\sigma(x)\sigma(a_1(u))$, there exists $C((u_3'',0),\delta'')\subset C((u_3',0),\delta')$ such that the function f_1 is holomorphic on $C((u_3'',0),\delta'')$ (see Lemma IV.4), and $(\partial f/\partial x)(u,0)=\tilde{\rho}(u)\sigma(a_1(u))+\sigma'(a_1(u))$ on $C(u_3'',\delta'')$ as a result. By Lemma IV.1, we are led to $\sigma(a_1(u))\neq 0$ on $C(u_3'',\delta'')$, thereby completing the proof. □

Proposition IV.12: We have $\rho_1(u)=\rho u+\rho_3$ *and* $a_1(u)=au+a_3$, *where* ρ, ρ_3, a, $a_3\in\mathbb{C}$. For the proof, we need the following.

Lemma IV.13: There exist $C(u_4,r_4)\subset C(u_3,r_3)$ *and a function* a_4 *holomorphic on* $C(u_4,r_4)$ *such that* $\sigma(a_4(u)+a_1(v))\neq 0$ *for all* $u,v\in C(u_4,r_4)$ *and* $\sigma(a_4(u))\neq 0$ *for all* $u\in C(u_4,r_4)$.

Proof: If $\sigma(2a_1(u))\not\equiv 0$ on $C(u_3,r_3)$, put $a_4:=a_1$. The proof in the case that $\sigma(2a_1(u))\equiv 0$ on $C(u_3,r_3)$ is simple, so we omit it. □

We take $C(\tilde{x}_1,\tilde{r}_1)\subset(C(x_1,r_1)\backslash(\mathbb{Z}\tau_1+\mathbb{Z}\tau_2))$ such that $C(2\tilde{x}_1,2\tilde{r}_1)\cap(\mathbb{Z}\tau_1+\mathbb{Z}\tau_2)=\emptyset$. From Theorem IV.5 and the three term identity of σ (see, for example, p. 377 of Ref. 19 and p. 461 of Ref. 20),

$$\begin{aligned}&\frac{B(v,x+y)(A(x)A(-x)-A(y)A(-y))}{B(v,x)B(v,y)}\\&\quad=\frac{c\sigma(a_1(v))}{\sigma(a_4(u))\sigma(a_4(u)+a_1(v))}\\&\qquad\times\left(\frac{\sigma(x+a_4(u)+a_1(v))\sigma(x-a_4(u))}{\sigma(x)\sigma(x+a_1(v))}-\frac{\sigma(y+a_4(u)+a_1(v))\sigma(y-a_4(u))}{\sigma(y)\sigma(y+a_1(v))}\right)\end{aligned}$$

for all $u,v\in C(u_4,r_4)$ and $x,y\in C(\tilde{x}_1,\tilde{r}_1)$. By virtue of Eq. (10), for all $u,v\in C(u_4,r_4)$, there exists a constant $\gamma(u,v)\in\mathbb{C}$ such that

$$\frac{B(u,-x)B(u+v,x)}{B(v,x)}=\frac{c\sigma(a_1(v))\sigma(x+a_4(u)+a_1(v))\sigma(x-a_4(u))}{\sigma(x)\sigma(x+a_1(v))\sigma(a_4(u))\sigma(a_4(u)+a_1(v))}+\gamma(u,v) \tag{14}$$

for all $x,y\in C(\tilde{x}_1,\tilde{r}_1)$.

From Lemma III.3 and $C((2u_4,2x_1),2r_4)\subset C((0,0),r/2)$, there exist $(u_1',x_1')\in C((2u_4,2x_1),2r_4)$ and $r_1'(>0)$ such that the conditions in Lemma III.3 hold. The proof of Lemma IV.14 is similar to that of Proposition IV.11, so we omit it.

Lemma IV.14: There exists $C(u_3',r_3')\subset C(u_1',r_1')$ *such that*

$$B(u,x)=\pm c\,\exp(\rho_2(u)x)\,\frac{\sigma(x+a_2(u))}{\sigma(x)\sigma(a_2(u))} \tag{15}$$

as meromorphic functions on $C(u_3',r_3')\times C(0,r)$ *with the functions* ρ_2 *and* a_2 *holomorphic on* $C(u_3',r_3')$.

Proof of Proposition IV.12: By Eqs. (13)–(15),

$$\pm\exp((\rho_2(u+v)-\rho_1(u)-\rho_1(v))x)\sigma(x-a_1(u))\sigma(x+a_2(u+v))$$
$$\times\sigma(a_1(v))\sigma(a_4(u))\sigma(a_4(u)+a_1(v))$$
$$=\sigma(a_1(v))\sigma(x+a_4(u)+a_1(v))\sigma(x-a_4(u))\sigma(a_1(u))\sigma(a_2(u+v))$$
$$+\gamma(u,v)\sigma(a_4(u))\sigma(x)\sigma(a_2(u+v))\sigma(x+a_1(v))\sigma(a_4(u)+a_1(v))$$

for any $x\in C(\tilde{x}_1,\tilde{r}_1)$ and $u,v\in C(u_3'/2,r_3'/2)$. We note that the equation above is valid on $\mathbb{C}$ $(\ni x)$ also by means of the identity theorem for the holomorphic functions. Since the both sides of the equation above are quasi-periodic with the periods τ_1 and $\tau_2, a_2(u+v)-a_1(u)-a_1(v)\in\mathbb{Z}\tau_1+\mathbb{Z}\tau_2$. Because the functions a_1 and a_2 are holomorphic and the set $\mathbb{Z}\tau_1+\mathbb{Z}\tau_2$ is discrete, the function $a_2(u+v)-a_1(u)-a_1(v)$ is constant on $C((u_3'/2,u_3'/2),r_3'/2)$ and so is the function $\rho_2(u+v)-\rho_1(u)-\rho_1(v)$. Hence we get the desired result. □

It is to be noted that $\rho_2(u)=\rho u+\rho_4$ and that $a_2(u)=au+a_4$, where $\rho_4,a_4\in\mathbb{C}$. By the straightforward computation, we deduce the following.

Theorem IV.15: *The elliptic solution $B(u,x)$ of Eqs. (8) and (9) defined on the polydisc $C((0,0),r)$ is*

$$B(u,x)=c\exp(\rho ux)\frac{\sigma(x+au)}{\sigma(x)\sigma(au)},$$

where $a\in\mathbb{C}\backslash\{0\}$ and $\rho\in\mathbb{C}$.

V. TRIGONOMETRIC CASE

In this section, we solve Eqs. (8) and (9) in the trigonometric case of Theorem III.1.

The proof of Lemma V.1 is the same as that of Lemmas IV.1 and IV.2, so we omit the proof.

Lemma V.1: (1) *For all $u\in C(u_1,r_1)$, $c(u)(\exp(2\tilde{a}(u)/\lambda)-1)+1\neq 0$ and $\tilde{b}(u)\neq 0$.*

(2) *We have $a_3=0$, that is to say, $A(x)A(-x)=\tilde{a}_1\sinh^{-2}(x/\lambda)+\tilde{a}_2$ on $C(0,r)$, where $\tilde{a}_1=a_1/a_4$ and $\tilde{a}_2=a_2/a_4$.*

From Eqs. (7), (8) and Lemma V.1 (2),

$$A(x)A(-x)-B(u,x)B(u,-x)=\tilde{a}_2+4\tilde{b}(u)^2\exp\left(\frac{2\tilde{a}(u)}{\lambda}\right)c(u)(1-c(u)) \tag{16}$$

for all $u\in C(u_1,r_1), x\in C(x_1,r_1)\backslash\mathbb{Z}\pi\sqrt{-1}\lambda$.

Lemma V.2: There exists $C(u_1',r_1')\subset C(u_1,r_1)$ such that

$$B(u,x)=\exp(\rho(u)x)b(u)\frac{\sinh(x+a(u))/\lambda}{\sinh(x/\lambda)},\quad \text{or}\quad B(u,x)=\exp(\rho(u)x)b(u)\frac{1}{\sinh(x/\lambda)}$$

for any $(u,x)\in D_1\cap D^t\cap(C(u_1',r_1')\times C(0,r))$.

If there exists $C(u_1',r_1')\subset C(u_1,r_1)$ such that $c(u)-c(u)^2\neq 0$ for all $u\in C(u_1',r_1')$, then there exists $a(u)\in\mathbb{C}$ such that $c(u)=\exp(a(u)/\lambda)/(2\sinh(a(u)/\lambda))$ for all $u\in C(u_1',r_1')$. For the proof of Lemma V.2, it suffices to show the following lemma.

Lemma V.3: If, for all $C(u,\tilde{r})\subset C(u_1,r_1)$, there exists $u_0\in C(u,\tilde{r})$ such that $c(u_0)-c(u_0)^2=0$, then $c(u)=0$ or 1 for all $u\in C(u_1,r_1)$.

Proof: The proof is by contradiction. Assume the assertion were false. Then there would exist $u_0'\in C(u_1,r_1)$ such that $c(u_0')\neq 0, 1$. We take $N\in\mathbb{N}$ such that $C(u_0',1/N)\subset C(u_1,r_1)$. For all $n\geqslant N$, there exists $u_n\in C(u_0',1/n)$ such that $c(u_n)-c(u_n)^2=0$ and, for all $n\geqslant N$,

$$\tilde{a}_2+4\tilde{b}(u_n)^2\exp\left(\frac{2\tilde{a}(u_n)}{\lambda}\right)c(u_n)(1-c(u_n))=\tilde{a}_2$$

as a result. The left hand side of Eq. (16) is holomorphic on $C(u_1,r_1)$ for a fixed $x \in C(x_1,r_1)\backslash\mathbb{Z}\pi\sqrt{-1}\lambda$, so it is continuous. Since $\lim_{n\to\infty} u_n = u_0'$,

$$\tilde{a}_2 + 4\tilde{b}(u_0')^2 \exp\left(\frac{2\tilde{a}(u_0')}{\lambda}\right) c(u_0')(1-c(u_0')) = \tilde{a}_2,$$

which is a contradiction of the choice of u_0' and Lemma V.1 (1). □

The proof of the theorem below is the same as that in Sec. IV, so we omit it.

Theorem V.4: (1) *The trigonometric solution $A(x)$ of Eqs. (8) and (9) defined on the polydisc $C(0,r)$ is*

$$A(x) = c\cdot h(x)\frac{\sinh(x+s)/\lambda}{\sinh(x/\lambda)\sinh(s/\lambda)} \quad or \quad c\cdot h(x)\frac{1}{\sinh(x/\lambda)},$$

where $c \in \mathbb{C}\backslash\{0\}$, $s \in \mathbb{C}\backslash\mathbb{Z}\pi\sqrt{-1}\lambda$ and $h(x)$ is a meromorphic function defined on $C(0,r)$ satisfying the relation $h(x)h(-x)=1$.

(2) *There exists $C(u_3,r_3)\subset C(u_1,r_1)$ such that the trigonometric solution $B(u,x)$ of Eqs. (8) and (9) is expressed as*

$$B(u,x) = c\exp(\rho_1(u)x)\frac{\sinh(x+a_1(u))/\lambda}{\sinh(a_1(u)/\lambda)\sinh(s/\lambda)}, \quad or \quad c\exp(\rho_1(u)x)\frac{1}{\sinh(x/\lambda)}$$

on $C(u_3,r_3)\times C(0,r)$. Here the functions ρ_1 and a_1 are holomorphic on $C(u_3,r_3)$.

(3) *There exist $C(u_4,r_4)\subset C(u_3,r_3)$ and a function a_4 holomorphic on $C(u_4,r_4)$ such that* $\sinh((a_4(u)+a_1(v))/\lambda)\neq 0$ *and* $\sinh(a_4(u)/\lambda)\neq 0$ *for all $u \in C(u_4,r_4)$.*

(4) *There exists $C(u_3',r_3')\subset C(2u_4,2r_4)$ such that the trigonometric solution $B(u,x)$ of Eqs. (8) and (9) is expressed as follows*:

$$B(u,x) = \pm c\exp(\rho_2(u)x)\frac{\sinh(x+a_2(u))/\lambda}{\sinh(a_2(u)/\lambda)\sinh(x/\lambda)} \quad or \quad \pm c\exp(\rho_2(u)x)\frac{1}{\sinh(x/\lambda)}$$

on $C(u_3',r_3')\times C(0,r)$. Here the functions ρ_2 and a_2 are holomorphic on $C(u_3',r_3')$.

We take $C(\tilde{x}_1,\tilde{r}_1)\subset(C(x_1,r_1)\backslash\mathbb{Z}\pi\sqrt{-1}\lambda)$ as $C(2\tilde{x}_1,2\tilde{r}_1)\cap\mathbb{Z}\pi\sqrt{-1}\lambda=\emptyset$, and fix any $u,v \in C(u_3'/2,r_3'/2)$. From Eq. (10) there exists $\gamma(u,v)\in\mathbb{C}$ such that

$$\frac{B(u,-x)B(u+v,x)}{B(v,x)} = \begin{cases} \dfrac{c\sinh(a_1(v)/\lambda)\sinh((x+a_4(u)+a_1(v))/\lambda)\sinh(x-a_4(u))/\lambda}{\sinh((a_4(u)+a_1(v))/\lambda)\sinh((a_4(u)/\lambda)\sinh(x/\lambda)\sinh((x+a_1(v))/\lambda)} + \gamma(u,v), \\ \dfrac{-c\exp(-x/\lambda)}{\sinh(x/\lambda)} + \gamma(u,v), \end{cases} \tag{17}$$

for all $x \in C(\tilde{x}_1,\tilde{r}_1)$, and, as a result, we are led to the four cases below:

$$\mp\exp((\rho_2(u+v)-\rho_1(u)-\rho_1(v))x)\times\frac{\sinh((x+a_2(u+v))/\lambda)\sinh((-x+a_1(u))/\lambda)\sinh(a_1(v)/\lambda)}{\sinh(a_2(u+v)/\lambda)\sinh(a_1(u)/\lambda)}$$
$$=\frac{c\sinh(a_1(v)/\lambda)\sinh((x+a_4(u)+a_1(v))/\lambda)\sinh((x-a_4(u))/\lambda)}{\sinh((a_4(u)+a_1(v))/\lambda)\sinh(a_4(u)/\lambda)}+\gamma(u,v)\sinh\frac{x}{\lambda}\sinh\frac{x+a_1(v)}{\lambda},\tag{18}$$

$$\mp\exp((\rho_2(u+v)-\rho_1(u)-\rho_1(v))x)\frac{\sinh((-x+a_1(u))/\lambda)\sinh(a_1(v)/\lambda)}{\sinh(a_1(u)/\lambda)}$$
$$=\frac{c\sinh(a_1(v)/\lambda)\sinh((x+a_4(u)+a_1(v))/\lambda)\sinh((x-a_4(u))/\lambda)}{\sinh((a_4(u)+a_1(v))/\lambda)\sinh(a_4(u)/\lambda)}+\gamma(u,v)\sinh\frac{x}{\lambda}\sinh\frac{x+a_1(v)}{\lambda},\tag{19}$$

$$\mp c\exp((\rho_2(u+v)-\rho_1(u)-\rho_1(v))x)\frac{\sinh((x+a_2(u+v))/\lambda)}{\sinh(a_2(u+v)/\lambda)}=-c\exp\left(-\frac{x}{\lambda}\right)+\gamma(u,v)\sinh\frac{x}{\lambda},\tag{20}$$

$$\mp c\exp((\rho_2(u+v)-\rho_1(u)-\rho_1(v))x)=-c\exp\left(-\frac{x}{\lambda}\right)+\gamma(u,v)\sinh\frac{x}{\lambda},\tag{21}$$

for any $x\in C(\tilde{x}_1,\tilde{r}_1)$. We note that the equations above are valid on $\mathbb{C}$. Substitution of 0 in x yields that all the signatures of Eqs. (18)–(21) are -1. From the periodicity of Eqs. (18)–(21),

$$\mp\exp((\rho_2(u+v)-\rho_1(u)-\rho_1(v))\pi\sqrt{-1}\lambda)=1,\tag{22}$$

and consequently, we have the following.

Lemma V.5: There exist $\rho,\rho_3,\rho_4\in\mathbb{C}$ *such that* $\rho_1(u)=\rho u+\rho_3$ *for all* $u\in C(u_3,r_3)$ *and* $\rho_2(u)=\rho u+\rho_4$ *for all* $u\in C(u_3',r_3')$.

In the case of (20), we can express the function B in two ways

$$B(u,x)=c\exp((\rho u+\rho_3)x)\frac{1}{\sinh(x/\lambda)},c\exp((\rho u+\rho_4)x)\frac{\sinh((x+a_2(u))/\lambda)}{\sinh(a_2(u)/\lambda)\sinh(x/\lambda)}.$$

This is a contradiction. In the case of (19), we deduce a contradiction in a similar fashion.

From Eq. (22) there exists $n\in\mathbb{Z}$ such that $\rho_4-2\rho_3=n/\lambda$, and one can regard Eqs. (18) and (21) as the polynomials of the variable $\exp(x/\lambda)$. Thus we deduce the following.

Proposition V.6: On $C((0,0),r)$

$$B(u,x)=\begin{cases}c\exp((\rho u+\rho_3)x)\dfrac{\sinh((x+au+a_3)/\lambda)}{\sinh(x/\lambda)\sinh((au+a_3)/\lambda)} & \text{for (18)},\\[2ex] c\exp((\rho u+\rho_4)x)\dfrac{1}{\sinh(x/\lambda)} & \text{for (21)},\end{cases}$$

where $a,a_3\in\mathbb{C}$.

From Eq. (17) we get $\rho_3=0$, $\rho_4=\pm 1/\lambda$ and $a_3\in\mathbb{Z}\pi\sqrt{-1}\lambda$, that is to say,

Theorem V.7: *The trigonometric solution $B(u,x)$ of Eqs. (8) and (9) defined on the polydisc $C((0,0),r)$ is*

$$B(u,x)=c\exp(\rho ux)\frac{\sinh(x+au)/\lambda}{\sinh(x/\lambda)\sinh(au/\lambda)},\quad \textit{or}\quad c\exp(\rho ux)\frac{\exp(\pm x/\lambda)}{\sinh(x/\lambda)},$$

where c is in Theorem V.4, *$a\in\mathbb{C}\backslash\{0\}$ and $\rho\in\mathbb{C}$.*

VI. RATIONAL CASE

In this section, we continue solving Eqs. (8) and (9) in the rational case of Theorem III.1.

The proof of Theorem VI.1 is the same as that in Sec. IV, so we omit it.

Theorem VI.1: (1) *The rational solution $A(x)$ of Eqs. (8) and (9) defined on the polydisc $C(0,r)$ is*

$$A(x)=c\cdot h(x)\frac{x+s}{xs},\quad \textit{or}\quad c\cdot h(x)\frac{1}{x},$$

where $c,s\in\mathbb{C}\backslash\{0\}$ and $h(x)$ is a meromorphic function defined on $C(0,r)$ satisfying the relation $h(x)h(-x)=1$.

(2) *There exist $C(u_3,r_3)\subset C(u_1,r_1)$ and $C(u_3',r_3')\subset C(2u_3,2r_3)$ such that the rational solution $B(u,x)$ of Eqs. (8) and (9) is expressed as follows:*

$$B(u,x)=\begin{cases}\exp(\rho_1(u)x)\dfrac{a_1(u)x+c}{x}, & \textit{on}\quad C(u_3,r_3)\times C(0,r),\\[2ex] \exp(\rho_2(u)x)\dfrac{a_2(u)x\pm c}{x}, & \textit{on}\quad C(u_3',r_3')\times C(0,r).\end{cases}$$

Here the functions ρ_1 and a_1 are holomorphic on $C(u_3,r_3)$ and the functions ρ_2 and a_2 are holomorphic on $C(u_3',r_3')$.

We fix any $u,v\in C(u_3'/2,r_3'/2)$. From Eq. (10), there exists $\gamma(u,v)\in\mathbb{C}$ such that

$$\frac{B(u,-x)B(u+v,x)}{B(v,x)}=-\frac{c^2}{x(a_1(v)x+c)}+\gamma(u,v)$$

for all $x\in C(x_1,r_1)\backslash\{0\}$, and consequently

$$\exp((\rho_2(u+v)-\rho_1(u)-\rho_1(v))x)=\frac{c^2}{(-a_1(u)x+c)(a_2(u+v)x\pm c)}-\frac{\gamma(u,v)x(a_1(v)x+c)}{(-a_1(u)x+c)(a_2(u+v)x\pm c)}\tag{23}$$

for all $x\in C(x_1,r_1)\backslash\{0\}$. Since the equation above is valid on $\mathbb{C}$, we obtain the following.

Lemma VI.2: There exist $\rho,\rho_3\in\mathbb{C}$ such that $\rho_1(u)=\rho u+\rho_3$ for all $u\in C(u_3,r_3)$ and $\rho_2(u)=\rho u+2\rho_3$ for all $u\in C(u_3',r_3')$.

From Eq. (23), $a_1(u)a_2(u+v)=(a_1(u)-a_2(u+v))a_1(v)$ for all $u,v\in C(u_3'/2,r_3'/2)$, which implies the following.

Lemma VI.3: The function $a_1(u)$ is identically zero on $C(u_3,r_3)$, or there exists $a,a_3\in\mathbb{C}$ such that

$$\frac{1}{a_1(u)}=\frac{au}{c}+\frac{a_3}{c},\quad \forall u\in C(u_3,r_3),$$

$$\frac{1}{a_2(u)}=\frac{au}{c}+\frac{2a_3}{c},\quad \forall u\in C(u_3',r_3').$$

By the straightforward computation, we deduce the following.

Theorem VI.4: *The rational solution $B(u,x)$ of Eqs. (8) and (9) defined on the polydisc $C((0,0),r)$ is*

$$B(u,x)=c\exp(\rho ux)\frac{x+au}{aux},\ \ \textit{or}\ \ c\exp(\rho ux)\frac{1}{x}.$$

Here c is in Theorem VI.1, *$a\in\mathbb{C}\{0\}$ and $\rho\in\mathbb{C}$.*

VII. SINGULAR CASE

This section describes the solutions A and B of Eqs. (1) and (2) on the assumption that $B\not\equiv 0$ and that $A(x)A(-x)(\not\equiv 0)$ is identically constant. It is to be mentioned that the assumption above and Eqs. (1) and (2) imply Eqs. (9) and

$$B(u,x)B(u,-x)=B(u,y)B(u,-y) \tag{24}$$

on $C((0,0),r)$. Let $D_1,D_2\subset C((0,0),r)$ be the domains of the meromorphic function $B(u,x)$ and $B(u,-x)$, respectively. From Eq. (24), for all $u\in C(0,r)$ such that $(u,x)\in D_1\cap D_2$, there exists $a(u)\in\mathbb{C}$ such that

$$B(u,x)B(u,-x)=a(u)\ \ \forall x\in C(0,r)\text{s.t.}(u,x)\in D_1\cap D_2. \tag{25}$$

It follows immediately that $a(u)$ is holomorphic at $u=u_0$ if $(u_0,y_0)\in D_1\cap D_2$.

Lemma VII.1: If $(u_0,y_0)\in D_1\cap D_2$, then $(u_0,0)$ is not a pole of the function $B(u,x)$.

Proof: The proof is by contradiction. Assume the assertion were false. For all $n\in\mathbb{N}$, there would exist $(u_n',x_n')\in C((0,0),r)$ such that $(u_n',x_n')\in C((u_0,0),1/n)\cap D_1$. Then there exists $r_n'>0$ such that $C((u_n',x_n'),r_n')\subset C((u_0,0),1/n)\cap D_1$. Hence there exists $(u_n,x_n)\in D_2$ such that $(u_n,x_n)\in C((u_n',x_n'),r_n')$. Because $(u_n,x_n)\in C((u_0,0),1/n)\cap D_1\cap D_2$, $\lim_{n\to\infty}u_n=u_0$ and $\lim_{n\to\infty}x_n=0$. Since $(u_0,0)$ is a pole of $B(u,x)$, $\lim_{n\to\infty}|B(u_n,x_n)|=\lim_{n\to\infty}|B(u_n,-x_n)|=\infty$, and $\lim_{n\to\infty}|B(u_n,x_n)B(u_n,-x_n)|=\infty$ as a consequence. As we mentioned earlier, we are led to $\lim_{n\to\infty}a(u_n)=a(u_0)$, which is a contradiction of Eq. (25). □

Thus the point $(u_0,0)$ in Lemma VII.1 is a regular point or a point of indeterminacy of $B(u,x)$.

Lemma VII.2. For any $(0<)r'\leqslant r$, there exists $u_0\in C(0,r')$ such that $(u_0,0)$ is a regular point of $B(u,x)$.

Proof: It suffices to consider the case that $(u_0,0)\in C((0,0),r')$ in Lemma VII.1 is a point of indeterminacy of the function $B(u,x)$.

Because the set of the points of the indeterminacy of the meromorphic function with two variables is isolated, there exists $r_0>0$ such that $B(u,x)$ has no points of indeterminacy in $C((u_0,0),r_0)\backslash\{(u_0,0)\}$ and $C((u_0,0),r_0)\subset C((0,0),r')$. That is to say, for any $u_1\in C(u_0,r_0)\backslash\{u_0\}$, $(u_1,0)$ is not a point of indeterminacy of $B(u,x)$, and there exists $s>0$ such that $C((u_1,0),s)\subset C((u_0,0),r_0)\backslash\{(u_0,0)\}$ as a result.

For $(u_3,y_3)\in D_1\cap D_2\cap(C(u_1,s)\times C(0,r'))$, $(u_3,0)$ is not a pole of $B(u,x)$ by means of Lemma VII.1. From $(u_3,0)\in C((u_1,0),s)$, $(u_3,0)$ is not a point of indeterminacy of $B(u,x)$. This point u_3 is the desired one. □

Proposition VII.3: There exist $r_0(>0)$ and $u_0\in C(0,r)$ satisfying the following conditions.

(1) $C((4u_0,0),4r_0)\subset C((0,0),r)$.
(2) $B(u,x)$ *is holomorphic on* $C((u_0,0),r_0)\cup C((2u_0,0),2r_0)\cup C((4u_0,0),4r_0)$.
(3) $B(u,x)\neq 0$ *for all* $(u,x)\in C((u_0,0),r_0)\cup C((2u_0,0),2r_0)\cup C((4u_0,0),4r_0)$.

Proposition VII.3 follows from Lemma VII.4 immediately.

Lemma VII.4: (1) *If there exists* $C((u_0,0),r_0)\subset C((0,0),r)$ *such that* $B(u,x)$ *is holomorphic on* $C((u_0,0),r_0)$ *and* $C((2u_0,0),2r_0)\subset C((0,0),r)$, *then there exists* $C((u_1,0),r_1)\subset C((u_0,0),r_0)$ *such that* $B(u,x)$ *is holomorphic on* $C((2u_1,0),2r_1)$.

(2) *If there exists* $C((u_0,0),r_0)\subset C((0,0),r)$ *such that* $B(u,x)$ *is holomorphic on* $C((u_0,0),r_0)$, *then there exists* $C((u_1,0),r_1)\subset C((u_0,0),r_0)$ *such that* $B(u,x)\neq 0$ *for all* $(u,x)\in C((u_1,0),r_1)$.

Proof: We prove (1) only. We take $C((u_2,y_2),r_2)\subset(C(2u_0,2r_0)\times C(0,r))\cap D_1\cap D_2$, and, for all $u\in C(u_2,r_2)$, there exists $y\in C(y_2,r_2)$ such that $(u,y)\in D_1\cap D_2$ as a result. By Lemma VII.1, $(u,0)$ is not a pole of $B(u,x)$ for all $u\in C(u_2,r_2)$. Because the set of the points of indeterminacy of the meromorphic function of two variables is isolated and $u/2\in C(u_0,r_0)$ for all $u\in C(u_2,r_2)$, there exists $u_1\in C(u_0,r_0)$ such that $(2u_1,0)\in D_1$. Thus there exists $r_1>0$ such that $C((u_1,0),r_1)\subset C((u_0,0),r_0)$ and $C((2u_1,0),2r_1)\subset D_1$. This completes the proof. □

By Eq. (9), there exists $\gamma(u,v)\in\mathbb{C}$ such that

$$\frac{B(u+v,x)}{B(u,x)B(v,x)}=\gamma(u,v) \tag{26}$$

for all $x\in C(0,r_0/2),u,v\in C(u_0,r_0/2)$, and, consequently, we have the following.

Proposition VII.5: We fix any $u,v\in C(u_0,r_0/2)$ *and put*

$$\alpha(x)=\frac{B(u+v,x)}{B(u,x)},\quad \varphi(x)=\frac{1}{B(u,x)},\quad \psi(x)=a(u)\gamma(u,v)B(u+v,x).$$

Then they satisfy Eq. (4) for all $x,y\in C(0,r_0/4)$.

With the aid of Proposition VII.3, the functions α, φ and ψ are all holomorphic on $C(0,r_0/2)$. Moreover, $\varphi(x)\neq 0$ and $\psi(x)\neq 0$ for all $x\in C(0,r_0/2)$. This tells us that the functions α, φ and ψ are the solutions of Eq. (4) with the conditions $\varphi(0)\neq 0$ and $\alpha(x+y)-\alpha(x)\alpha(y)\neq 0$ for all $x,y\in C(0,r_0/4)$. By virtue of Theorem II.1, we conclude the following.

Proposition VII.6: For $u\in C(u_0,r_0/2)$ *and* $x\in C(0,r_0/4)$,

$$B(u,x)=c_1(u)\exp(\rho_1(u)x),$$

where c_1 *and* ρ_1 *are holomorphic on* $C(u_0,r_0/2)$. *The function* c_1 *satisfies* $c_1(u)\neq 0$ *for all* $u\in C(u_0,r_0/2)$.

We obtain Proposition VII.7 in a similar fashion.

Proposition VII.7: For $u\in C(2u_0,r_0)$ *and* $x\in C(0,r_0/2)$,

$$B(u,x)=c_2(u)\exp(\rho_2(u)x),$$

where c_2 *and* p_2 *are holomorphic on* $C(2u_0,r_0)$. *The function* c_2 *satisfies* $c_2(u)\neq 0$ *for all* $u\in C(2u_0,r_0)$.

By virtue of Eqs. (9) and (26), we deduce Theorem VII.8.

Theorem VII.8: *The singular solutions* $A(x)$ *and* $B(u,x)$ *of Eqs. (1) and (2) defined on the polydiscs* $C(0,r)$ *and* $C((0,0),r)$, *respectively, are as follows*:

$$A(x)=c_1h(x),\quad B(u,x)=c_2\exp(\rho ux)\frac{1}{u}.$$

Here c_1, $c_2 \in \mathbb{C}\setminus\{0\}$, $\rho \in \mathbb{C}$ *and* $h(x)$ *is a meromorphic function defined on* $C(0,r)$ *satisfying the relation* $h(x)h(-x)=1$.

VIII. TRIVIAL CASE

In this section, we solve Eqs. (1) and (2) with $A \equiv 0$ or $B \equiv 0$.

Lemma VIII.1: If the function B is identically zero on $C((0,0),r)$, *then, for any function A meromorphic on* $C(0,r)$, *the functions A and* $B(\equiv 0)$ *satisfy Eqs. (1) and (2).*

In the sequel, we assume that $A \equiv 0$ and $B \not\equiv 0$. From the previous assumption, Eqs. (1) and (2) are equivalent to

$$\frac{B(u+v,x)}{B(u,x)B(v,x)} = \frac{B(u+v,y)}{B(u,y)B(v,y)}$$

on $C((0,0,0,0),r/2)$. By differentiating the equation above in the variable x, we get

$$\frac{(\partial B/\partial x)(u+v,x)}{B(u+v,x)} - \frac{(\partial B/\partial x)(u,x)}{B(u,x)} - \frac{(\partial B/\partial x)(v,x)}{B(v,x)} = 0$$

on $C((0,0,0),r/2)$ and, as a result, $(\partial^2 \tilde{B}/\partial u^2)(u,x)=0$ on $C((0,0),r)$, where $\tilde{B}(u,x)=(\partial B/\partial x)(u,x)/B(u,x)$.

Lemma VIII.2: There exists a function f meromorphic on $C(0,r)$ *such that* $\tilde{B}(u,x)=f(x)u$ *as meromorphic functions on* $C((0,0),r)$ *and the function f is holomorphic at* $x=0$.

Proof: We only show that the function f is holomorphic at $x=0$. Let D_1 be the domain of the meromorphic function B. By means of $B \not\equiv 0$, there exists $C((u_1,x_1),r_1) \subset D_1 \setminus (\{0\} \times C(0,r))$ such that $B(u,x) \neq 0$ for all $(u,x) \in C((u_1,x_1),r_1)$. Hence, for all $u \in C(u_1,r_1)$, $f(x)=(\partial B/\partial x)(u,x)/(uB(u,x))$ is meromorphic on $C(0,r)$. (See Lemma III.5) Laurent's expansions near $x=0$ of the functions f and $(\partial B/\partial x)(u,x)/(uB(u,x))$ are

$$f(x)=\sum_{k_1=l}^{\infty} a_{k_1}x^{k_1}, \quad \frac{(\partial B/\partial x)(u,x)}{uB(u,x)} = \frac{1}{u}\sum_{k_2=-1}^{\infty} b_{k_2}(u)x^{k_2} \quad (l, b_{-1}(u) \in \mathbb{Z}),$$

and we get $l=-1$ and $a_{-1}=b_{-1}(u)/u$ for all $u \in C(u_1,r_1)$ as a result. If $b_{-1}(u_1) \neq 0$, then, for all $u \in C(u_1,r_1)$, $u=(b_{-1}(u)/b_{-1}(u_1))u_1 \in \mathbb{Q}u_1$, which is a contradiction. Thus $b_{-1}(u_1)=0$, and consequently $a_{-1}=0$. We have completed the proof. □

Therefore we deduce the following theorem.

Theorem VIII.3: *There exist* $(0<)r_1(\leqslant r)$, *a function F holomorphic on* $C(0,r_1)$ *and a function G meromorphic on* $C(0,r)$ *such that the function G is not identically zero and* $B(u,x)=\exp(F(x)u)G(u)$ *as meromorphic functions on* $C(0,r)\times C(0,r_1)$.

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Erratum: ''Dynamics of axial channeling in quasicrystals: An averaging-theory approach'' [J. Math. Phys. 41, 5342 (2000)]

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(1) In line 5 after Eq. (3.4), ''$\varepsilon^* = 1/\sqrt{V(\xi)}$'' should read ''$\varepsilon^* = 1/\sqrt{2V(\xi)}$.''

(2) In lines 3 and 12 of paragraph 5, p. 5357, ''$W_\perp$'' should read ''$H_\perp(\zeta)$.''

(3) In Eq. (3.51), ''$\overline{W}$'' should read ''$\overline{H}(\xi,\eta)$.''

(4) In lines 2 and 3 after Eq. (3.52c), read ''... , where $\varepsilon^{**} = 1/\sqrt{\overline{V}(\xi_1,\xi_2)}$. Since...'' as ''... , where $\varepsilon^{**} = 1/\sqrt{2\overline{V}(\xi_1,\xi_2)}$. Since ... .''

(5) In lines 1 and 2 of the last paragraph of p. 5363, read ''...with $\|Z(t,\varepsilon) - \overline{Z}(t,\varepsilon)\|$ replaced by...'' as ''...with $\|Z(t,\varepsilon) - \overline{Z}(t,\overline{\varepsilon})\|$ replaced by... .''

The Hagedorn transition in noncommutative open string theory

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The Hagedorn transition in noncommutative open string theory (NCOS) is relatively simple because gravity decouples. For NCOS theories in no more than five space–time dimensions, the Hagedorn transition is second order, and the high temperature phase involves long, nearly straight fundamental strings separating from the D-brane on which the NCOS theory is defined. Above five spacetime dimensions interaction effects become important below the Hagedorn temperature. Although this complicates studies of the transition, we believe that the high temperature phase again involves long strings liberated from the bound state. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1372176]

I. INTRODUCTION

Just as noncommutative field theories (i.e., quantum field theories on noncommutative spaces) can be obtained as certain limits of D-branes with a background magnetic field,[1] noncommutative open string (NCOS) theories are defined as a special limit of Type II D-branes with a uniform electric field.[2,3] The bosonic part of the world volume action has the standard form

$$S=\int_\Sigma d^2\sigma\left[\frac{1}{4\pi\alpha'}((\partial_a X^0)^2-(\partial_a X^1)^2)-\frac{1}{4\pi\alpha'_t}\sum_{i=2}^{9}(\partial_a X^i)^2\right]+E\oint_{\partial\Sigma}X^0\frac{\partial}{\partial\sigma}X^1. \tag{1}$$

In the NCOS limit the electric field approaches its critical value, $E\to E_c=1/2\pi\alpha'$, and $\alpha'\to 0$ in such a way that the effective tension of an open string stretched along the direction of the electric field remains finite:

$$\alpha'_{\rm eff}=\alpha'\frac{E_c^2}{E_c^2-E^2}. \tag{2}$$

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There is a similar rescaling of the interaction strength:[4]

$$G_o^2 = g_{\rm str}\sqrt{\frac{E_c^2 - E^2}{E_c^2}}, \tag{3}$$

and the open string coupling G_o is held fixed in the NCOS limit. The inverse-tension parameter for the transverse directions, α_t', is finite from the start and independent of E (it is convenient to set $\alpha_t' = \alpha_{\rm eff}'$). A remarkable property of this limit is that, even though $g_{\rm str}\to\infty$, the closed strings decouple from the open strings.[2,3] Therefore, the NCOS is a nongravitational string theory.

This definition of NCOS theories leads naturally to a space–time where the space and time directions do not commute, i.e., $[X^0, X^i] = i\theta^{0i}$. Unlike the situation in noncommutative Yang–Mills theories, here the noncommutativity scale, $|\theta|$, is intrinsically tied to the string scale. This implies that in order to make sense of the notion of a noncommuting space/time manifold, we would have to first give precise meaning to the notion of Einsteinian spacetimes down at the string scale.

The relation (3) implies that $g_{\rm str}\to\infty$ in the NCOS limit. Therefore, *S*-duality may be used to map NCOS to D-brane systems at weak string coupling.[5,6] A particularly simple example of such duality is $1+1$-dimensional NCOS, which is found to be dual to maximally supersymmetric $U(N)$ gauge theory with one unit of electric flux. The open string coupling is $G_o^2 = 1/N$; it becomes weak in the large N limit. Therefore, the $1+1$-dimensional NCOS provides a new example of duality between large N gauge theory and strings. The fact that we find open strings rather than closed is related to the presence of the electric flux tube which binds the N D-strings. Massive open strings are dual to the excitations of this theory where locally $SU(N)$ is broken to $SU(N-1)\times U(1)$. The massless open strings are dual to the $U(1)$ part of the spectrum (the overall vibrations of the bound state), and the duality with the gauge theory predicts that the massless states decouple. In Ref. 6 this prediction was confirmed by explicit NCOS calculations. A further check on the duality performed in Ref. 6 involves the high-energy behavior of the massive amplitudes: it is found to exhibit the same power-law fall-off as expected from the gauge theory.

Another classic way of subjecting strings to extreme conditions is to heat them up to a high temperature. For conventional superstring theory this was extensively studied in the late 80's[7–9] and afterwards (see for instance Refs. 10, 11, 12). A complicating factor in these papers is that it is difficult to study the thermodynamics of gravitating systems. Nevertheless, a coherent picture has emerged suggesting a first-order phase transition happening well below the Hagedorn temperature.[9]

In this paper we study the thermodynamics of NCOS in various dimensions. Just like any other superstring theory, NCOS theory exhibits a Hagedorn density of states:

$$\rho(m) \sim m^{-9/2} e^{m/T_{\rm H}}, \tag{4}$$

with the scale for the Hagedorn temperature set by $\alpha_{\rm eff}'$:

$$T_{\rm H} = \frac{1}{\sqrt{8\pi^2\alpha_{\rm eff}'}}. \tag{5}$$

In particular, the partition function of NCOS theory appears to diverge above the temperature $T = T_{\rm H}$, where the Hagedorn transition is expected to take place. Our goal is to understand the physics of this transition and describe the thermodynamics of NCOS theory at $T > T_{\rm H}$. Since the NCOS theories are decoupled from gravity, we will not face the usual difficulties associated with gravitational thermodynamics. Furthermore, at least in $1+1$ dimensions the dual gauge theory provides an important guide to what happens at the transition. Here we find that the transition is

to a phase where some finite fraction of the strings are freed from the bound state, i.e., where the theory enters the Higgs branch $SU(N)\to SU(N-K)\times U(1)^K$. A calculation of the free energy below and above the transition shows that it is second order.

Guided by the intuition from the $1+1$-dimensional case we proceed to $p+1$ dimensions. For $p>1$, *S*-duality works differently, but on the NCOS side we may still think of some density of *F*-strings bound to a D*p*-brane. We will show that for all $p<5$ the Hagedorn transition is again second order and is associated with the liberation of strings from the bound state. For $p\geqslant 5$ the entropy of noninteracting open strings (and also the string length) diverges as T approaches $T_{\rm H}$ from below.[13] This suggests that string interaction effects become important already below $T_{\rm H}$. Nevertheless, we will argue that the high-temperature phase again contains a finite fraction of long strings liberated from the bound state. In all these cases the theory slightly above the transition appears to be effectively $1+1$-dimensional, with a preferred direction chosen by the electric field.

In previous work[3] it was suggested that there is a change in the behavior of zero-temperature NCOS at $p=7$, where non-planar amplitudes begin to diverge at $k^2=0$ (k is the momentum flowing in the closed string channel). We calculate a cross-section for graviton production and confirm that NCOS theories do not decouple from gravity for $p\geqslant 7$. Our work further shows that, at finite temperature, there is new physics appearing in the NCOS theory at a lower dimension, $p=5$: interaction effects become important already below $T_{\rm H}$. A special role of $p=5$ in open string thermodynamics was noted earlier in Ref. 13.

Other authors have recently studied phases of NCOS theories and Hagedorn behavior of string theories decoupled from gravity.[14–17] These works focused primarily on results derivable from supergravity. The current work takes the rather different approach of examining the free energy of bound states in a field theory approximation. The relevant temperatures for our analysis are so low that the near-extremal supergravity solutions are highly curved on the string scale and hence unreliable.

There is also an extensive literature on Hagedorn behavior in asymptotically free gauge theories. For important early contributions to the subject, see Refs. 18, 19, 20. In the current work we focus on perturbative string techniques rather than field theory. However, some information about strongly coupled gauge theories may be extracted from our results, particularly in the $1+1$-dimensional case.

II. NCOS THERMODYNAMICS FOR $T<T_{\rm H}$

In order to obtain a reliable picture of the thermodynamics of NCOS theory for $T<T_{\rm H}$ directly from the free string spectrum, two conditions must pertain. First, the open strings should interact weakly with one another. Second, the cubic coupling $\langle\phi\phi\sigma\rangle$ between an incipient thermal tachyon ϕ and the radius σ of the Euclidean time direction, which played a crucial role in the analysis of Ref. 9, is absent. This is because σ represents a closed string (gravitational mode), which decouples according to the arguments of Refs. 2, 3. This is the essential difference between the Hagedorn transition for NCOS theory and for critical string theory.[9] Whereas essentially gravitational effects drive the Hagedorn transition first order in critical string theory, we will see that in NCOS theory the transition remains second order.

The free string analysis proceeds in a similar way regardless of the spatial dimension p in which the open strings live. The calculation of free energy of noninteracting open strings on a D*p*-brane, which is not affected by the noncommutativity, was carried out in Ref. 13. We will largely rederive their results and adapt them for our purposes. The principal result is that the free energy is analytic in T for $T<T_{\rm H}$, and that the leading nonanalytic behavior in the expansion of F around $T=T_{\rm H}$ is

$$F\sim\begin{cases}(\text{analytic in } t)+t^{(7-p)/2}+\ldots, & \text{for } p \text{ even},\\ (\text{analytic in } t)+t^{(7-p)/2}\log t+\ldots, & \text{for } p \text{ odd},\end{cases}\tag{6}$$

where $t=(T_{\rm H}-T)/T_{\rm H}$. There are two equivalent means of obtaining this result. First, one may

directly evaluate the annulus diagram in the Matsubara formalism where the Euclidean time direction is compact with circumference $\beta = T^{-1}$. The one loop free energy for a Dp-brane with an electric field of strength E turned on is [21]

$$Z_{\text{single string}} = -c_1 \int_0^\infty \frac{dt}{(p+3)/2}\, \vartheta_2\left(0 \middle| \frac{i\beta^2}{2\pi^2 \alpha'_{\text{eff}} t}\right) \left[\frac{\vartheta_2(0|it)}{\vartheta_1'(0|it)}\right]^4$$
$$= -\frac{c_1}{(2\pi)^4} \int_0^\infty \frac{d\tau}{\tau^{9-p/2}}\, \vartheta_2\left(0 \middle| \frac{i\beta^2 \tau}{2\pi^2 \alpha'_{\text{eff}}}\right) \left[\frac{\vartheta_2(0|i\tau)}{\vartheta_1'(0|i\tau}\right]^4. \tag{7}$$

In the first line we have used t as the modular parameter of the cylinder. In the second line we substitute $\tau = 1/t$, which is the usual closed string modular parameter. The expressions in (7) are exact even away from the NCOS limit, provided we use the definition (2) and neglect coupling to closed strings. They are identical to the partition function of ordinary open superstrings on a Dp-brane, only with α' replaced by α'_{eff}. The constant c_1 is given as $V\beta\pi^4/2(2\pi)^5(2\pi\alpha'_{\text{eff}})^5$. The reduced Hagedorn temperature for the partition function was noted in Ref. 22.

The nonanalytic behavior arises from a divergence in the modular integral at large τ (the long cylinder limit). Near T_{H}, we can use the large τ asymptotics of the ϑ functions to obtain

$$F_{\text{NCOS}}(T \approx T_{\text{H}}) \sim -\int^\infty \frac{d\tau}{\tau^{(g-p)/2}}\, e^{(1/T_{\text{H}}^2 - 1/T^2)\tau}, \tag{8}$$

from which the claimed analyticity for $T < T_{\text{H}}$ and the leading nonanalyticity quoted in (6) are evident.

An equivalent, ''elementary'' approach to obtain the same result is to plug (4) into the standard formula for a partition function:

$$Z_{\text{single string}} = \sum_{\text{states}} e^{-E/T}$$
$$= \sum_{i \in \mathcal{H}_o^\perp} \int \frac{d^p k}{(2\pi)p}\, e^{-\sqrt{k^2 + m_i^2}/T}$$
$$\sim \int_0^\infty dm\, \rho(m)(mT)^{p/2} e^{-m/T} \sim \int^\infty dm\, m^{(p-9)/2} \exp\left[m\left(\frac{1}{T_{\text{H}}} - \frac{1}{T}\right)\right], \tag{9}$$

where in the third step we have made an approximation to the momentum integration which becomes exact in the limit of large masses m_i.[13] Evaluating the last integral leads again to (6).

Note that the free energy is finite at $T = T_{\text{H}}$ for $p < 7$ and diverges logarithmically for $p = 7$. The entropy, $S = -\partial F/\partial T$, remains finite only for $p < 5$, and diverges logarithmically for $p = 5$. For a single long string, the entropy is proportional to the length of the string. Hence when $t = (T_{\text{H}} - T)/T_{\text{H}}$ is small, the total entropy is proportional to the rms length of the excited open strings, l_{NCOS}, times the average number of these strings per unit volume, ρ_{NCOS}.[23] As $T \to T_{\text{H}}$ from below, we have the scalings

$$\rho_{\text{NCOS}} l_{\text{NCOS}} \sim \begin{cases} (\text{finite}), & \text{for } p < 5, \\ -\log t, & \text{for } p = 5, \\ 1/\sqrt{t}, & \text{for } p = 6, \end{cases} \tag{10}$$

and so on.

The quantity $\rho_{\text{NCOS}} l_{\text{NCOS}}$ is the average density of string at any given point. As long as this quantity remains finite, the effects of interactions may be suppressed by taking G_o sufficiently small. Thus for $p < 5$ one can ensure that string interactions are never significant, but for $p \geqslant 5$

they eventually will be. A figure of merit to measure the strength of string interactions is $\eta = G_o \rho_{\rm NCOS} l_{\rm NCOS}$. We work in units where $\alpha'_{\rm eff}=1$ to make η dimensionless. The free energy for $T<T_{\rm H}$, neglecting interactions, is order G_o^0. Interactions make a contribution of order η^2 to the free energy. Thus interactions become important when $\eta \gtrsim 1$, which is to say $\rho_{\rm NCOS} l_{\rm NCOS} \gtrsim 1/G_o$. One can now use (10) to make a rough estimate of the temperature at which string interactions matter. For $p=5$ this temperature is $t \sim e^{-{\rm const}/G_o}$, while for $p=6$ it is $t \sim G_o^2$.

In the next sections, we will propose that the physics above $T_{\rm H}$ involves the gradual emission of long strings. We will assume that the free string picture is valid up to $T=T_{\rm H}$: thus the discussion seems to be limited to $p<5$. Note however that for $p=5,6$ the entropy of the open string gas at the temperature where interactions become important is of order $1/G_o$. For weak string coupling, this is still much smaller than the entropy in the liberated string phase which, as we show in Sec. IV A, is of order $1/G_o^2$. So we speculate that long string liberation starts taking place near $T_{\rm H}$ for $p=5,6$ as well.

The calculations that we present for $p<5$ are clean because we can work in a limit where free string theory applies. The string liberation transition may still occur away from zero coupling, although it is possible that the transition becomes first order. The additional complication for $p=5,\ 6$ is that there is no limit in which free string theory applies uniformly.

III. TWO-DIMENSIONAL NCOS THEORY AT $T>T_{\rm H}$

In this section we focus on the specific example of the two-dimensional NCOS theory, $p=1$. In this case one can use Type IIB *S*-duality to describe a D1-brane with a near-critical electric field as a $(1,N)$ bound state[24,25] where the number, N, of D1-branes is related to the open string coupling constant, $G_o^2=1/N$. At low energies this system behaves as $SU(N)$ two-dimensional super-Yang–Mills theory with one unit of electric flux and coupling constant,

$$g_{\rm YM}^2 = \frac{N^2}{\alpha'_{\rm eff}}. \tag{11}$$

In this dual picture noncommutative open strings can be identified with excitations corresponding to the Higgsing $SU(N) \to SU(N-1)\times U(1)$. Indeed, to create an island (of size L) of the Higgs phase costs an energy [5,6] of

$$E = L\left(\frac{g_{\rm YM}^2}{4\pi(N-1)} - \frac{g_{\rm YM}^2}{4\pi N}\right) \approx \frac{L g_{\rm YM}^2}{4\pi N^2} = \frac{L}{4\pi\alpha'_{\rm eff}}. \tag{12}$$

In the last equality we used the relation (11) between the Yang–Mills coupling constant and the tension of open strings. In terms of the $(1,N)$ bound state, (12) represents the energy to have a D-string split off from the bound state and run parallel to it for a distance L before rejoining.

At finite temperature, there is a gain in entropy when a string splits off from the bound state, due to small fluctuations of the string. Since a long string in light-cone gauge is described by a free supermultiplet, this entropy is $S=4\pi LT$ [in the dual gauge theory it comes from the $U(1)$ part of the Higgsed gauge group $SU(N-1)\times U(1)$]. The corresponding free energy of these light modes is $F=-2\pi LT^2$. Therefore, the total free energy of a string liberated from the bound state,

$$F_{\text{liberated string}} = L\left(\frac{1}{4\pi\alpha'_{\rm eff}} - 2\pi T^2\right), \tag{13}$$

vanishes precisely at the Hagedorn temperature:

$$T_{\rm H} = \frac{1}{\sqrt{8\pi^2\alpha'_{\rm eff}}} = \frac{1}{\sqrt{8}\pi}\frac{g_{\rm YM}}{N}. \tag{14}$$

We would like to interpret the Hagedorn transition as the liberation of fundamental strings parallel to the electric field from the $(N,1)$ bound state. This interpretation is satisfying in that the Hagedorn transition is generally associated with the temperature at which it is favorable to create long closed strings (see for instance Refs. 10, 11). If we compactify in the direction of the electric field, then the liberated strings are precisely those long closed strings. What is special about the NCOS limit is that in the near-critical electric field, the closed strings are allowed to wind only in one direction. Furthermore, since their tension away from the bound state is α', they are nearly straight: the massless $U(1)$ degrees of freedom represent only slight fluctuations.

A crucial aspect of the analysis is that, once one string has been liberated, the Hagedorn temperature of the NCOS theory on the $(N-1,1)$ bound state is slightly higher: after freeing one string, we have

$$\alpha'^{\text{new}}_{\text{eff}}=\frac{(N-1)^2}{g^2_{\text{YM}}}, \quad T_{\text{H}}^{\text{new}}=\frac{g_{\text{YM}}}{\sqrt{8}\pi}\frac{1}{N-1}. \tag{15}$$

In order to free another fundamental string, we must increase T to $T_{\text{H}}^{\text{new}}$. The analysis in (12) and (13) carries over without change to this case, and the Hagedorn temperature of the bound state increases again. Thus we have good control over the physics above the original T_{H}: the liberated fundamental strings are only slightly fluctuating, and the NCOS strings attached to the bound state remain at or below their Hagedorn transition.

It is possible to summarize the analysis in a way that will generalize easily to other cases. Suppose k out of the N fundamental strings have been liberated, $k\gg 1$. The free energy per unit length of the total system, consisting of the $(N-k,1)$ bound state plus the k liberated strings, is

$$\begin{aligned}\frac{F_k}{L}&=\frac{1}{2\pi\alpha'}\sqrt{(N-k)^2+\frac{1}{g^2_{\text{str}}}}+\frac{k}{2\pi\alpha'}-2\pi kT^2+O(1)\\ &\approx\frac{N-k}{2\pi\alpha'}\left(1+\frac{1}{2g^2_{\text{str}}(N-k)^2}\right)+\frac{k}{2\pi\alpha'}-2\pi kT^2\\ &=\frac{N}{2\pi\alpha'}-2\pi NT^2+\frac{1}{4\pi\alpha' g^2_{\text{str}}(N-k)}+2\pi(N-k)T^2\\ &\geqslant\frac{N}{2\pi\alpha'}-2\pi NT^2+T\sqrt{\frac{2}{\alpha' g^2_{\text{str}}}}.\end{aligned} \tag{16}$$

In the first line of (16), we have summed up the total tension of the $(N-k,1)$ bound state, the total tension of the k liberated strings, the free energy of the fluctuations of those k strings, and the $O(1)$ free energy coming from fluctuating open strings attached to the bound state. [26] The symbol $O(1)$ means, more precisely, that this contribution to the free energy is a finite quantity of order 1 times LT^2. In the second line of (16) we have expanded the square root for $g_{\text{str}}(N-k)\gg 1$, and in the last line we have used the arithmetic–geometric mean inequality. Equality holds in the last line iff

$$N-k=\frac{1}{\sqrt{8\pi^2\alpha' g_{\text{str}}}T}. \tag{17}$$

Transforming to rescaled NCOS variables, we find that the fraction of liberated strings is

$$\nu=\frac{k}{N}=\frac{T-T_{\text{H}}}{T}, \tag{18}$$

where T_H is the original Hagedorn temperature defined in (14).

From (16) we immediately read off the total free energy for $T>T_H$:

$$\frac{F}{L}=\inf_k \frac{F_k}{L}=-2\pi N(T_H)^2+O(1). \tag{19}$$

Another way to arrive at this formula is to note that the entropy of the k liberated strings is

$$S=-\frac{dF}{dT}=4\pi kLT=4\pi NL(T-T_H). \tag{20}$$

Integrating this equation with the boundary condition that F/L is of order 1 at $T=T_H$ reproduces the result (19).

Actually, since k is a discrete variable, $F/L=-2\pi N(T-T_H)^2$ and $\nu=(T-T_H)/T$ only represent an approximation to a series of discrete transitions, from F_0 to F_1 to F_2 and so on. However, since we are operating at large N, the discrete transitions are very closely spaced, and can effectively be regarded as a single continuous transition. At some level, the approach we have taken is only meaningful in the large N limit: we have examined various competing minima of the free energy, corresponding to different numbers of liberated fundamental strings, at a completely classical level, ignoring the fact that in one spatial dimension strong infrared fluctuations smooth out any nonanalyticity in the free energy. What saves the day is large N: when a finite fraction of fundamental strings have been liberated, their fluctuations ''average out'' to an extent such that ν is a good order parameter for the transition. One should not take too seriously the literal picture of a single string peeling off the bound state at $T=T_H$, followed shortly thereafter by another, and then another; rather, the free energy starts as an $O(1)$ quantity for $T<T_H$ and rises to $O(N)$ through a transition in which fundamental strings are collectively liberated. There is *not*, after all, a series of closely spaced first-order transitions—this would be in violation of the general analyticity properties of the free energy in one spatial dimension—instead, the maximally smoothed free energy has the form (19), which indicates a discontinuity $\Delta C=2\pi N$ at $T=T_H$. This is essentially the classic picture of a second-order phase transition, only with integer critical exponents that just barely avoid the typical singularity in the specific heat.

Note that, since the equilibrium condition reads as

$$\frac{g_{YM}^2}{4\pi(N-k)^2}-2\pi T^2=0, \tag{21}$$

the open strings on the $(N-k,1)$ bound state are always at their effective Hagedorn temperature (which depends on k provided that g_{YM} is held fixed). Therefore, their contribution to F/L is aT^2, where a is a constant of order 1 which may be found by evaluating (7) directly at the Hagedorn temperature. It is quite possible that additional $O(1)$ contributions to F arise when one considers interactions of the liberated long strings. Also, the interactions could change the critical exponents by terms of order $G_o^2=1/N$. In principle, the effects of interactions can be studied starting from the maximally supersymmetric Yang–Mills description of the bound state. The liberated strings admit a matrix string description,[27–29] while the bound state represents a confining non-Abelian sector of the theory. As far as we can tell, the total problem is quite formidable, but some progress might be made via a lattice or DLCQ approach.

It is clear that as we increase the temperature, one unit of electric flux in the dual super-Yang–Mills theory becomes unimportant. Already when the temperature is a finite multiple of $T_H \sim g_{YM}/N$ (say $T=2T_H$), the free energy is dominated by the matrix string phase (recall that we are mainly interested in the large N limit). When $T\sim g_{YM}/\sqrt{N}$, the proper description of the system is no longer matrix string theory plus a D1-f1 bound state, but rather a single near-extremal black string solution in type IIB supergravity.[30,31] The considerations of Refs. 30, 31 were applied only to multiple, identical, (nearly) coincident branes, but their conclusions should carry over to

the current circumstance, because at $T=g_{\mathrm{YM}}/\sqrt{N}$, nearly all the D1-branes are in the matrix string phase: $\nu=1-O(N^{-1/2})$. The supergravity regime, then, is described by[30,31]

$$F\sim LN^{3/2}\frac{T^3}{g_{\mathrm{YM}}}, \quad \text{for } \frac{g_{\mathrm{YM}}}{\sqrt{N}}<T<g_{\mathrm{YM}}\sqrt{N}. \tag{22}$$

Finally, as we reach the 't Hooft scale $T\approx g_{\mathrm{YM}}\sqrt{N}$, we end up with a gas of free photons, N^2 in number. This crossover is in the general class of correspondence points studied by Horowitz and Polchinski.[32] At very high temperature the free energy looks like this:

$$F\sim LN^2T^2, \quad \text{for } g_{\mathrm{YM}}\sqrt{N}<T. \tag{23}$$

Historically, the Hagedorn transition was originally expected to be essentially a deconfinement transition. In the NCOS context, we see that there are actually two other phases, or regimes, in between the Hagedorn transition and the free gluon phase. In a superficial matching analysis, the transitions between the matrix string regime, the supergravity regime, and the free gluon regime appear to be first order. It could easily be, however, that there is only a second-order transition, or no sharp transition at all, between these phases. As yet, we know of no method of analysis powerful enough to distinguish among the possibilities. For the transition into the supergravity regime from below, one may hope that the perturbation of the matrix string CFT by the DVV twist operator[27] provides some hint of the formation of a horizon.

In summary, we find four different phases of $1+1$-dimensional NCOS theory. They are illustrated in Fig. 1. In more detail, we have the following.

(i) In the NCOS phase, F/LT^2 is an analytic function of order 1 (that is, no factors of N). String interactions are suppressed by $G_o^2=1/N$. Without an understanding of the gauge theory and the possibility of going to a Higgsed phase $SU(N-k)\times U(1)^k$, this is the only part of the phase diagram we would be able to understand.

(ii) Above $T=T_{\mathrm{H}}$, we gradually liberate more and more fundamental strings from the bound state, so that very soon the system becomes dominated by the matrix string phase. The open strings on the bound state stay at their effective Hagedorn temperature: this temperature adjusts as more strings are liberated. The continuous transition so described is the essential new physics of this paper.

(iii) At $T\approx g_{\mathrm{YM}}/\sqrt{N}$ significant departures from conformal invariance and nontrivial interactions drive us into the black string regime, where the thermodynamics is read off from a regular horizon.

(iv) Above $T\approx g_{\mathrm{YM}}\sqrt{N}$, the N^2 non-Abelian gluons (light D1-branes stretched between fundamental strings) are deconfined.

It is straightforward to extend our discussion to (N, M) bound states corresponding to $SU(N)$ theory with arbitrary number, M, of flux units. In that case, open string coupling constant is given by

$$G_o^2=\frac{M}{N},$$

and effective open string tension reads as

$$\frac{1}{\alpha'_{\mathrm{eff}}}=g_{\mathrm{YM}}^2\frac{M^2}{N^2}.$$

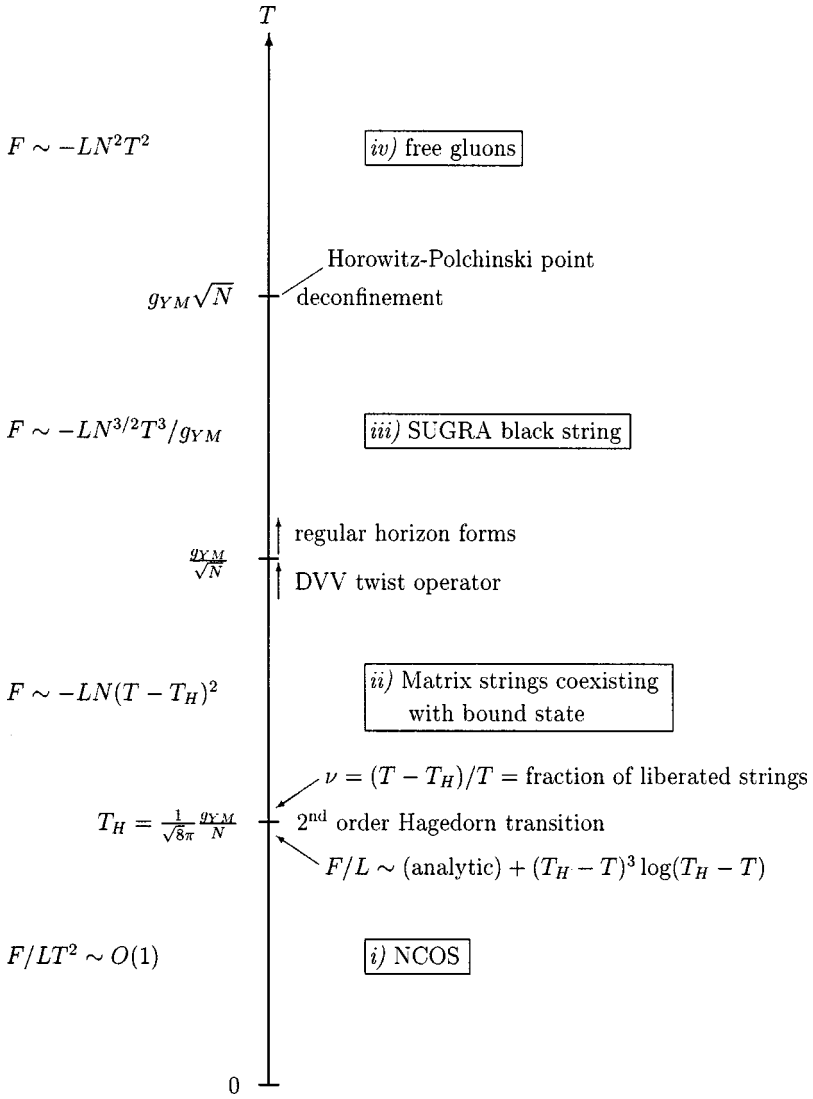

FIG. 1. The four phases of $1+1$-dimensional NCOS theory.

The phase diagram of this system is similar to that of the $(N,1)$ bound state: in particular, the same four phases appear. The only difference is that the phase transitions between phases (i)–(ii)–(iii) occur at different temperatures, greater by a factor of M. For instance, the Hagedorn temperature of such a theory is given by

$$T_{\mathrm{H}}=\frac{g_{\mathrm{YM}}M}{\sqrt{8}\,\pi^2 N}.$$

IV. HIGHER DIMENSIONAL EXAMPLES

Let us now elaborate on extensions of the ideas of the previous section to systems in which the strings are allowed to move in more than one spatial dimension (Sec. IV A), or where not strings but Dp-branes become light (Sec. IV B).

A. Thermodynamics of NCOS theories in higher dimensions

The Hagedorn transition in higher-dimensional NCOS theories (up to $4+1$ dimensions) may be understood in a manner similar to the situation in $1+1$ dimensions. The claim is that finitely above $T_{\rm H}$, a finite fraction of long strings are liberated from the bound state. This process is gradual as in the previous case, and the fraction of long strings that decouple may be computed in a similar fashion. To see this we need the formula for the number of fundamental strings per unit transverse volume bound to a Dp-brane with electric field E:

$$\frac{N}{V_t}\sim(\alpha_t')^{(1-p)/2}\frac{E}{g_{\rm str}\sqrt{E_c^2-E^2}}. \tag{24}$$

One way to get this formula is to consider the Dp-brane to be compactified on a circle of radius L in the direction of the electric field. Then the momentum conjugate to the gauge field is quantized: $P_1=NL$. Equating this to the momentum calculated from the Born–Infeld action, as in Ref. 4, gives (24).

Note that (24) implies

$$G_o^2\sim\frac{V_t(\alpha_t')^{(1-p)/2}}{N}.$$

To fix the precise factor in this expression, consider the BPS formula for the mass of the bound state of N fundamental strings and a Dp-brane wrapped over a transverse torus of volume V_t:

$$\frac{L}{2\pi\alpha'}\sqrt{N^2+\frac{V_t^2}{g_{\rm str}^2(2\pi)^{2p-2}(\alpha_t')^{p-1}}}=\frac{L}{2\pi\alpha'}N\left(1+\frac{V_t^2}{2N^2g_{\rm str}^2(2\pi)^{2p-2}(\alpha_t')^{p-1}}+\ldots\right). \tag{25}$$

Calculating the energy required to free one fundamental string, we get

$$\frac{LV_t^2}{4\pi\alpha' g_{\rm str}^2(2\pi)^{2p-2}(\alpha_t')^{p-1}}\left(\frac{1}{N-1}-\frac{1}{N}\right)\to\frac{LV_t^2}{4\pi\alpha'_{\rm eff}G_o^4N^2(2\pi)^{2p-2}(\alpha_t')^{p-1}}, \tag{26}$$

where we have used

$$\alpha' g_{\rm str}^2=\alpha'_{\rm eff}G_o^4. \tag{27}$$

(26) should be equated to the energy of a closed string wound around the direction of the electric field, which is $L/(4\pi\alpha'_{\rm eff})$.[6] Thus, we find

$$G_o^2=\frac{V_t(\alpha_t')^{(1-p)/2}}{(2\pi)^{p-1}N}. \tag{28}$$

This formula shows that for $p>1$, G_o^{-2} is not quantized, while for $p=1$ it is.

Suppose we start with a Dp-brane with a near-critical electric field E, which loses a fraction of its long strings above $T_{\rm H}$, such that the resulting system is a Dp-brane with a near-critical electric field E' and a bunch of free long strings. Assuming that the resulting brane configuration is right at its effective Hagedorn temperature as before, we find the ratio

$$\frac{T}{T_{\rm H}}=\frac{\sqrt{E_c^2-E'^2}}{\sqrt{E_c^2-E^2}}.$$

Using (24) and the fact that both E and E' are near-critical, we find the relation between temperature and the fraction of strings remaining in the bound state:

$$\frac{N'}{N}=\frac{T_{\mathrm{H}}}{T}. \tag{29}$$

This universal result is in accord with what we found in two-dimensional NCOS theory from its gauge theory dual; cf. (18).

Note that the transverse inverse-tension parameter, α_t', remains fixed for $T>T_{\mathrm{H}}$ because it does not depend on E. Thus, we may simply set $\alpha_t'=\alpha_{\mathrm{eff}}'$. However, the effective parameter governing the 0 and 1 directions starts decreasing as in the $1+1$-dimensional case. From (27) and (28) we find that

$$\alpha_{\mathrm{eff}}'^{\mathrm{new}}=\alpha_{\mathrm{eff}}'\left(\frac{N'}{N}\right)^2.$$

As in $1+1$ dimensions, the condition for equilibrium of long strings at temperature T is

$$\frac{1}{4\pi\alpha_{\mathrm{eff}}'^{\mathrm{new}}}-2\pi T^2=0,$$

from which the relation (29) follows.

One may be concerned that for $T>T_{\mathrm{H}}$ there are two different effective inverse-tension parameters: $\alpha_{\mathrm{eff}}'^{\mathrm{new}}$ for the 01 directions and α_{eff}' for the transverse directions. Which one sets the effective Hagedorn temperature? The answer is that it is $\alpha_{\mathrm{eff}}'^{\mathrm{new}}$, so that T is the effective Hagedorn temperature for $T>T_{\mathrm{H}}$. The dispersion relation for open strings is indeed asymmetric:

$$(k_0^2-k_1^2)-\frac{\alpha_{\mathrm{eff}}'}{\alpha_{\mathrm{eff}}'^{\mathrm{new}}}\sum_{i=2}^{p}k_i^2=\frac{\mathcal{N}}{\alpha_{\mathrm{eff}}'^{\mathrm{new}}},$$

where $\mathcal{N}$ is the excitation level. We see that $\alpha_{\mathrm{eff}}'^{\mathrm{new}}$ determines the mass spectrum. Then following, for instance, the approach in (9) we find that the effective Hagedorn temperature is $(8\pi^2\alpha_{\mathrm{eff}}'^{\mathrm{new}})^{-1/2}=T$. Therefore, the free energy of the gas of open strings on the bound state is a finite (for $p<7$) quantity of order 1, as far as the dependence on G_o is concerned.

For $T>T_{\mathrm{H}}$ the free energy is dominated by that of the $N-N'$ free long strings:

$$F=-2\pi NL(T-T_{\mathrm{H}})^2.$$

Using (28) we observe that this expression is extensive:

$$F=-LV_t(2\pi)^{2-p}(\alpha_{\mathrm{eff}}')^{(1-p)}G_o^{-2}(T-T_{\mathrm{H}})^2. \tag{30}$$

Just as for $p=1$, the free energy is of order G_o^{-2} for $T>T_{\mathrm{H}}$.

Now we are in a position to complete the phase diagram of the higher-dimensional NCOS theories. At very low temperatures, one has the open string phase of the NCOS. This description breaks down at the Hagedorn temperature (5), where one has a phase transition beyond which the tempertively two-dimensional although the free energy remains extensive. The details of the phase transition are dimension dependent. For all $p<5$ the Hagedorn transition is second order. In $p\geqslant 3$ the specific heat diverges as $T\to T_{\mathrm{H}}$ on the open string side.[13]

The free energy of noninteracting open strings becomes more singular with increasing p, and for $p\geqslant 5$ the entropy diverges at the transition. This implies that interaction effects become important already for $T<T_{\mathrm{H}}$. Nevertheless, it is likely that the high-temperature phase again involves liberated long strings. We may argue for this as follows. The free energy of noninteracting open strings is of order G_o^0, and interactions are unlikely to change this scaling. On the other hand, the free energy of liberated strings, (30), is of order G_o^{-2}. Therefore, for weak coupling and for T sufficiently above T_{H}, the system can lower its free energy by liberating long strings from

the bound state. It is not clear, however, whether the transition for $p>4$ is second order; it may be a first-order transition for all values of G_o. Additional ideas on the Hagedorn transition for 5-branes have appeared in Refs. 33, 14, 15.

In fact, one may suspect that for large enough p the Dp-brane does not decouple from gravity in the NCOS limit. In Ref. 3 the nonplanar one-loop amplitude was calculated for 4 open strings, and it was shown that for $p<7$ the amplitude is finite for $k^2=0$ (k is the momentum in the closed string channel). For $p\geqslant 7$ the amplitude blows up for $k^2=0$ which suggests that there is no decoupling from massless bulk modes. In order to check this, we have calculated the cross-section for two massless open strings of energy k_0 colliding along the electric field direction to produce an outgoing graviton. The term in the Born–Infeld action describing this process is

$$\frac{1}{2}\int d^{p+1}x(\partial_0\Phi^i\partial_0\Phi^j-\partial_1\Phi^i\partial_1\Phi^j)(\delta_{ij}+\sqrt{2}\kappa h_{ij}),$$

where we have rescaled the scalar fields so that they are canonically normalized. The cross-section we find,

$$\sigma\sim G_o^4(\alpha'_e)^4k_0^{9-p}(E_c^2-E^2)^{(7-p)/2},$$

vanishes for $p<7$, is finite for $p=7$, and diverges for $p>7$. This result is consistent with the annulus calculation in Ref. 3 and it indicates that nongravitational NCOS theories can exist only for $p<7$. It is interesting to note that $p=7$ is also special from the point of view of the thermodynamics: indeed here the free energy for the low energy phase, computed in Sec. II, diverges logarithmically at $T=T_{\mathrm{H}}$.

To summarize this section, we can draw the general conclusion that the physics of the Hagedorn transition is similar for all NCOS theories with $p<7$, in that above T_{H} the temperature dependence of F is effectively two-dimensional even though F is extensive in p dimensions. This is similar to the answer proposed in Ref. 9, although the justification there was different. In the NCOS case the two-dimensional behavior of the free energy above the Hagedorn temperature has to do with the presence of the electric field.

B. Extension to OD3 theory

In NCOS theory, a critical NS–NS 2-form field in presence of a Dp-brane leads to a decoupling limit in which fundamental strings are light. In certain variants of OM theory, a critical RR $(p+1)$-form field applied to an NS5-brane is associated with a decoupling limit in which Dp-branes become light.[5,16] No computational framework comparable to perturbative quantization of strings has emerged to study light Dp-branes for $p>1$. Indeed, one may wonder if it is logically consistent for higher-dimensional branes ever to be the ''fundamental'' degrees of freedom of a theory.[34] However, it appears from the decoupling arguments of Refs. 5, 16 that there are decoupling limits of string theory where the lightest excitations are indeed open Dp-branes with $p>1$.

It is tempting to adapt the reasoning used for NCOS theories to describe a possible phase transition for various OM-theories. In this section we will make an attempt in this direction, but our arguments will be much more heuristic than in previous sections. We will examine the relatively clean example of OD3-theory, which is the theory of open D3-branes on an NS5-brane in a decoupling limit with a critical 4-form potential turned on. Besides the obvious pitfall that the quantum states of fluctuating open D3-branes are hard to count, there is another interesting effect: fundamental strings living on the NS5-D3 bound state have a substantially reduced tension relative to their tension in flat space, and their Hagedorn behavior competes with the tendency to liberate D3-branes.

An NS5-brane with a near-critical RR 4-form potential can be described as a bound state of many D3-branes and a single NS5, such that the D3-branes make the dominant contribution to the tension. Let ρ be the number density of D3-branes in the two directions orthogonal to the D3-

branes but parallel to the NS5-brane. Then we require $\rho\tau_{\mathrm{D3}} \gg \tau_{\mathrm{NS5}}$. We will see below that this condition turns out to be trivially satisfied in the OD3 limit as defined in Ref. 5.

The tension of the NS5-D3 bound state is $\sqrt{\tau_{\mathrm{NS5}}^2+\rho^2\tau_{\mathrm{D3}}^2}$. The tension of an open D3-brane stuck to the NS5-brane is

$$\begin{aligned}\tau_{\mathrm{OD3}} &= \frac{d}{d(\delta\rho)}\left(\delta\rho\,\tau_{\mathrm{D3}}+\sqrt{\tau_{\mathrm{NS5}}^2+(\rho-\delta\rho)^2\tau_{\mathrm{D3}}^2}\right)\Big|_{\delta\rho=0} \\ &= \tau_{\mathrm{D3}}\left[1-\left(1+\left(\frac{\tau_{\mathrm{NS5}}}{\rho\tau_{\mathrm{D3}}}\right)^2\right)^{-1/2}\right] \approx \frac{1}{2}\left(\frac{\tau_{\mathrm{NS5}}}{\rho\tau_{\mathrm{D3}}}\right)^2\tau_{\mathrm{D3}},\end{aligned} \tag{31}$$

where in the last line we have used $\rho\tau_{\mathrm{D3}} \gg \tau_{\mathrm{NS5}}$. The near-critical scaling limit is described by two parameters:[5] a scale $\tilde{\alpha}'_{\mathrm{eff}}$ and a coupling $G^2_{o(3)}$, which happens to be precisely the closed string coupling g_{str} (this last fact is special to OD3-theory). The precise scaling of the parameters is given as $\tilde{\alpha}' = \sqrt{\epsilon}\tilde{\alpha}'_{\mathrm{eff}}$, the metric in directions transverse to the D3-branes scales as $g_{MN} = \epsilon\delta_{MN}$, and $g_s = G^2_{o(3)}$. The scaling of the metric implies that $\rho = \rho_0/\epsilon$, where ρ_0 is of order unity. This implies $\rho\tau_{\mathrm{D3}} \sim O(\epsilon^{-2})$, while $\tau_{\mathrm{NS5}} \sim O(\epsilon^{-3/2})$, thereby satisfying the aforementioned condition that $\rho\tau_{\mathrm{D3}} \gg \tau_{\mathrm{NS5}}$.

Just as we found in NCOS theory that it is thermodynamically favorable to liberate strings from the bound state at a temperature $T_{\mathrm{H}} \sim \sqrt{\tau_{\mathrm{eff}}}$, so we will find here that it is favorable to liberate D3-branes at a temperature $T_{c,\mathrm{D3}} \sim \tau_{\mathrm{OD3}}^{1/4}$. The argument proceeds along similar lines. First we note that a free $U(1)$ gauge multiplet in a flat-space theory in $p+1$ dimensions and sixteen supercharges has

$$\frac{F}{L^p T^{p+1}} = -c_{\mathrm{D}_p} \equiv -\frac{8\,\mathrm{Vol}\,S^{p-1}}{(2\pi)^p}\left(2-\frac{1}{2^p}\right)\Gamma(p)\zeta(p+1). \tag{32}$$

Here F is the free energy, L^p is the spatial world-volume, and T is the temperature. The low-energy dynamics of the bound state is noncommutative super-Yang–Mills theory in $5+1$ dimensions. Clearly, then, the free energy at low temperatures is order 1 in the sense that it does not grow with a power of the number density ρ. Let us assume that this remains the case up through the temperature where liberating D3-branes becomes thermodynamically favorable. Then the same manipulations that we went through in (16) are justified at large ρ: the free energy after a number density $\delta\rho$ of D3-branes have been liberated is

$$\begin{aligned}\frac{F_{\delta\rho}}{L^5} &= \sqrt{\tau_{\mathrm{NS5}}^2+(\rho-\delta\rho)^2\tau_{\mathrm{D3}}^2}+\delta\rho\,\tau_{\mathrm{D3}}-c_{\mathrm{D3}}\delta\rho T^4 \\ &\approx \rho\tau_{\mathrm{D3}}-c_{\mathrm{D3}}\rho T^4+\frac{\tau_{\mathrm{NS5}}^2}{2(\rho-\delta\rho)\tau_{\mathrm{D3}}}+c_{\mathrm{D3}}(\rho-\delta\rho)T^4 \\ &\geqslant \rho\tau_{\mathrm{D3}}+\tau_{\mathrm{NS5}}\sqrt{2c_{\mathrm{D3}}T^4/\tau_{\mathrm{D3}}}-c_{\mathrm{D3}}\rho T^4,\end{aligned} \tag{33}$$

where we neglect terms which are subleading in ρ. Equality pertains in the last line of (33) if and only if the last two terms in the second line are equal. One reads off the fraction of liberated D3-branes, the free energy, and the critical temperature $T_{c,\mathrm{D3}}$ as

$$\nu \equiv \frac{\delta\rho}{\rho} = \frac{T^2-T_{c,\mathrm{D3}}^2}{T^2},$$

$$\frac{F}{L^5} \approx \rho\tau_{\mathrm{D3}}-c_{\mathrm{D3}}\rho(T^2-T_{c,\mathrm{D3}}^2)^2, \tag{34}$$

$$T_{c,\mathrm{D3}}^2=\frac{\tau_{\mathrm{NS5}}}{\sqrt{2c_{\mathrm{D3}}\tau_{\mathrm{D3}}\rho}}=\sqrt{\tau_{\mathrm{OD3}}/c_{\mathrm{D3}}}=\frac{1}{(2\pi)^{7/2}}\frac{1}{\sqrt{2c_{\mathrm{D3}}}}\frac{1}{g_{\mathrm{str}}^{3/2}\tilde{\alpha}'^2\rho_0}.$$

[Formally, a similar analysis seems to be possible for many D5-branes bound to an NS5-brane. However, in this case, the absence of strong IR dynamics on N coincident D5-branes makes it likely that there are $O(N^2)$ massless degrees of freedom even at low energies. This would overwhelm the $O(N)$ effect due to liberated D5-branes, rendering the whole approach suspect.]

In the case of NCOS theory, it was essentially guaranteed that fundamental strings would start being liberated at the Hagedorn temperature of the noncommutative open strings, because the calculation of the free energy of liberated strings was equivalent to a computation in the light cone formalism of highly excited open strings. In OD3 theory, no analog of the latter computation exists as yet, so to be conservative we should regard $T_{c,\mathrm{D3}}$ as an upper bound on the temperature where some transition must take place. In fact, as we will now show, when $G_{o(3)}\ll 1$, there is a Hagedorn transition for closed fundamental strings living on the NS5-D3 system at a substantially lower temperature than $T_{c,\mathrm{D3}}$. These closed strings are excitations of the NS5-D3 bound state.

There is no net $f1$ charge in the NS5-D3 bound state that we wish to analyze; however, in order to extract the tension of the closed strings which live on the NS5-D3 system, it is convenient to first consider a BPS arrangement where an NS5-brane is oriented in the 012345 directions, ρ D3-branes per unit 45-volume are oriented in the 0123 directions, and ρ_4 fundamental strings per unit 2345-volume are oriented in the 01 directions. The total tension is

$$\tau=\sqrt{(\tau_{\mathrm{NS5}}+\rho_4\tau_{f1})^2+(\rho\tau_{\mathrm{D3}})^2}. \tag{35}$$

The effective tension of a fundamental string bound to the NS5-D3 system is

$$\tau_{f1,\mathrm{eff}}=\left.\frac{\partial\tau}{\partial\rho_4}\right|_{\rho 4=0}=\tau_{f1}\left.\frac{\tau_{\mathrm{NS5}}}{\tau}\right|_{\rho 4=0}\approx\tau_{f1}\frac{\tau_{\mathrm{NS5}}}{\rho\tau_{\mathrm{D3}}}\ll\tau_{f1}, \tag{36}$$

where in the last two steps we have used the fact that most of the mass of the bound state is carried by the D3-branes. Fundamental strings which are orthogonal to the D3-branes but contained in the NS5-branes are much heavier.

Another way to derive the effective tension $\tau_{f1,\mathrm{eff}}$ is to look at the supergravity solution for the NS5-D3 system. The string metric and dilaton are

$$ds_{\mathrm{str}}^2=\frac{1}{\sqrt{h_3}}(-dt^2+dx_1^3+dx_2^2+dx_3^2)+\sqrt{h_3}(dx_4^2+dx_5^2+h_5(dx_6^2+dx_7^2+dx_8^2+dx_9^2)),$$

$$e^{2(\phi-\phi_\infty)}=h_5,\quad h_3=1+\frac{q_3}{r^2},\quad h_5=1+\frac{q_5}{r^2}, \tag{37}$$

$$r^2=x_6^2+x_7^2+x_8^2+x_9^2.$$

In the limit where $\rho\tau_{\mathrm{D3}}\gg\tau_{\mathrm{NS5}}$, we have $q_5/q_3=\tau_{\mathrm{NS5}}/(\rho\tau_{\mathrm{D3}})$. The three-form field strengths need not concern us, except to note that $B_{\mu\nu}^{(NS)}$ may be chosen so that only B_{45} is nonzero. We are considering many D3-branes, but only a single NS5-brane, so the supergravity solution is trustworthy, in the sense that curvatures are sub-stringy, down to a radius $r_{\mathrm{match}}=\sqrt{q_5}$. Following the philosophy of Ref. 32, we assert that the tension and coupling of fundamental strings bound to the NS5-D3 system can be read off, up to factors of order unity, from the properties of a test string located at the matching radius r_{match}. The tension so derived agrees with (36). The advantage of this more heuristic approach is that we can extract the string coupling for the strings bound to the NS5-D3 system: up to a factor of 2 it is just $g_{\mathrm{str}}=G_{o(3)}^2$.

When $G_{o(3)} \ll 1$, we are entitled to use the free string spectrum to predict a Hagedorn temperature for the light fundamental strings whose orientation is within the D3-branes. It is

$$T_{c,f1} \sim \sqrt{\tau_{f1,\mathrm{eff}}} = \frac{1}{(2\pi)^{3/2}} \frac{1}{\sqrt{g_{\mathrm{str}} \tilde{\alpha}'^2 \rho_0}}. \tag{38}$$

From

$$\frac{T_{c,f1}}{T_{c,\mathrm{D3}}} \sim \frac{\sqrt{\tau_{f1,\mathrm{eff}}}}{\tau_{\mathrm{OD3}}^{1/4}} \sim g_{\mathrm{str}}^{1/4} = \sqrt{G_{o(3)}}, \tag{39}$$

we learn that the fundamental string Hagedorn transition happens at a lower temperature when $G_{o(3)} \ll 1$. This supports the view that the most relevant degrees of freedom in OD3-theory with $G_{o(3)} \ll 1$ may be little strings. Before one can ask whether the D3-brane liberation transitions occurs, one must understand what contribution the fundamental strings make to the free energy above $T_{c,f1}$.

When $G_{o(3)} \gg 1$, one can obtain a more natural description of the theory by *S*-dualizing. The scaling limit leading to OD3-theory *S*-dualizes into the zero slope limit used in Ref. 1 to obtain noncommutative Yang–Mills theory.[5] For $G_{o(3)} \gg 1$, this theory is weakly coupled in the sense that $g_{\mathrm{YM}} \ll \sqrt{\theta}$. However, the interacting theory is nonrenormalizable, so it might be inappropriate to regard the quanta of the gauge field as the fundamental degrees of freedom. It was suggested in Ref. 5 that OD3-theory provides an ultraviolet completion of $5+1$-dimensional noncommutative Yang–Mills theory. This is not a very effective description in the absence of a knowledge of how to quantize open D3-branes. It must be admitted that, for $G_{o(3)} \gtrsim 1$, there is neither a natural little string theory description of OD3-theory, nor a renormalizable interacting quantum field theory description. Despite all this uncertainty, the analysis following (33) may still be valid: it only depends on the free energy of the bound state being $O(\rho^0)$ in a $\rho \to \infty$ limit with $G_{o(3)}$ fixed.

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[34] It is unquestionable that p-branes on shrinking cycles play a role in gauge symmetry enhancement, as well as in elucidating singularities like the conifold. What seems less certain is whether some theory in noncompact spacetime exists which admits a fundamental description as a theory of fluctuating p-branes, $p>1$.

Noncommutative tachyons and K-theory

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We show that the relation between D-branes and noncommutative tachyons leads very naturally to the relation between D-branes and K-theory. We also discuss some relations between D-branes and K-homology, provide a noncommutative generalization of the ABS construction, and give a simple physical interpretation of Bott periodicity. In addition, a framework for constructing Neveu–Schwarz five-branes as noncommutative solitons is proposed. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1377270]

I. INTRODUCTION

D-branes can be incorporated into open string field theory as solitons of tachyon configurations[1–6] and carry charges which take values in K-theory.[7,2,3] It was recently pointed out[8,9] that the description of D-branes as solitons in the open string tachyon field theory simplifies dramatically when a B field is turned on, thus making the tachyon field theory into a noncommutative field theory with the D-branes appearing as noncommutative solitons.[10]

One point of the following paper is that this description provides another point of view on the relation between D-branes and K-theory. Indeed this point of view makes the relation between D-branes and K-theory manifest.

A second, more speculative point we would like to make is the following. In the discussion below we will encounter some simple C^*-algebras. It is natural to wonder if replacing string field algebras by C^*-algebras leads to some new and interesting string backgrounds, or whether the theory of C^*-algebras should play a more fundamental role in brane physics.

Some observations closely related to this paper have been independently made in Refs. 11, 12. Some of the points below were made in lectures at Strings 2000.[13] Other recent papers suggesting a role of K-homology in D-brane physics include Refs. 14–17.

II. NONCOMMUTATIVE TACHYONS ARE MAPS TO CLASSIFYING SPACES

We first consider noncommutative tachyons in the bosonic string. The basic setup in Ref. 9 is that we consider spacetime to be a product $X\times R^{2n}$, where X is a $26-2n$ manifold. (In Ref. 9, X was taken to be $R^{25-2n,1}$, but the generalization to arbitrary X is easy, and quite important for our point below.)

We now consider open bosonic string field theory with target $X\times R^{2n}$. The action depends on the on-shell background values of the closed string fields $g_{\mu\nu}, g_s, B_{\mu\nu}$, where g_s is the closed string coupling. We take g_s to be small, and assume that the natural generalization of the flat space formulas to curved $g_{\mu\nu}$ applies.

If the tachyon effective action at $B=0$ is

$$S=\frac{C}{g_s}\int_{X\times R^2} d^{26}x\,\sqrt{\det g}\left(\frac{1}{2}f(T)g^{\mu\nu}\,\partial_\mu T\,\partial_\nu T - V(T)+\cdots\right), \tag{2.1}$$

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where C is a constant and T is the tachyon field, then the generalization to $B\neq 0$ is given in terms of a noncommutative field theory:[18–20]

$$S=\frac{C}{G_s}\int_{X\times R^2} d^{26}x\sqrt{\det G}\left(\frac{1}{2}f(T)G^{\mu\nu}D_\mu T D_\nu T - V(T)+\cdots\right), \tag{2.2}$$

where G_s and $G_{\mu\nu}$ are the open string coupling and metric, given by standard formulas.[21,22,20] The effect of B is to transform $g_s\to G_s$, $g_{\mu\nu}\to G_{\mu\nu}$ and commutative products of fields to noncommutative products taken with the Moyal product. In addition, B induces a nonzero coupling of the tachyon to the noncommutative $U(1)$ gauge field.[23]

The tachyon potential is

$$V(T)=V_0-m^2 T*T+\lambda T*T*T+\cdots. \tag{2.3}$$

There are also higher derivative terms in (2.2) that we have ignored.

The construction in Refs. 8, 9 is heavily based on the noncommutative solitons of Ref. 10. According to Ref. 10 the most effective way to think about the tachyon dependence on the noncommutative directions is in terms of operators on Hilbert space. The coordinates x^{2i-1},x^{2i} on the transverse R^{2n} satisfy

$$[x^{2i-1},x^{2i}]:=x^{2i-1}*x^{2i}-x^{2i}*x^{2i-1}=-i\theta_i, \tag{2.4}$$

where the θ^i are the skew eigenvalues of the parameter θ^{ij} appearing in the Moyal product.

Letting x^a denote commutative coordinates along X, x^i, $i=1,...,2n$ denoting the noncommutative coordinates, the tachyon field $T(x^a,x^i)$ is now regarded as an operator valued function of the x^a. What kind of operator can T be? Since T is a real field. T should be a self-adjoint operator. Since we would like to speak of continuous tachyon fields, T should be a map of X into a C^* algebra, and since all such algebras are subalgebras of the algebra of bounded operators on Hilbert space we regard T as a continuous map:

$$T:X\to\mathcal{B}, \tag{2.5}$$

where $\mathcal{B}$ is the C^*-algebra of bounded operators on a Hilbert space $\mathcal{H}$ and we use the norm topology.

In fact, since we wish to have an action, T should have a derivative. (More precisely, T should have a Frechét derivative.) Moreover, the gauge fields should be introduced using unbounded operators $D_i=\theta_{ij}^{-1}\,\mathrm{ad}\,X_j+\mathrm{ad}\,A_i$ on $\mathcal{H}$.

After integrating out the massive string fields the effective action for the tachyon and gauge fields takes the form

$$\begin{aligned}S=\frac{C}{G_s}\int_X d^{26-2n}x\sqrt{\det G}\Bigg(\mathrm{Tr}\Bigg[&\frac{1}{2}f(T)G^{ab}D_aT D_bT+\frac{1}{2}f(T)G^{ij}[D_i,T][T,D_j^\dagger]\\&-V(T)-\frac{1}{4}h(T)G^{ik}G^{jl}F_{ij}F_{kl}-\frac{1}{4}h(T)G^{ac}G^{bd}F_{ab}F_{cd}\Bigg]+\cdots\Bigg).\end{aligned} \tag{2.6}$$

Here Tr is the trace of the operator on Hilbert space; x^a run over the commuting coordinate directions on X. Evidently, in addition to our other criteria, certain combinations of the map T in (2.5) must be trace class in order to have a finite action.

Let us now consider the limit of Ref. 9, $\alpha' B_{ij}\to\infty$, or equivalently, $\theta^{ij}/\alpha'\to 0$, and consider constant tachyon field configurations $\partial_a T=0$. Then by rescaling the coordinates to remove θ_i from the star product one sees that the action reduces to the potential term as $\alpha' B_{ij}\to\infty$ and hence T must satisfy $V'(T)=0$.

As noted by Ref. 10 this can be solved by

$$T=\sum_i \lambda_i P_i, \tag{2.7}$$

where P_i are orthogonal projection operators and λ_i are stationary points for $V(T)$.

In the bosonic string formulated in Witten's open string field theory with a $*$ product, the potential is purely cubic. If we assume that the basic shape of the potential remains unchanged after integrating out massive string fields (recent computations[24,25,6,26] have provided nontrivial evidence that this is correct), then there are two stationary points $\lambda=0$, $\lambda=t_*$. If we choose t_* to correspond to the perturbative open bosonic string vacuum, with $V(t_*)$ given by the tension of the D25-brane, then Sen's conjecture states that $V(0)=0$ represents the closed string vacuum. Therefore, the only nontrivial constant solution to (2.7) is $T=t_* P_n$ where P_n is a rank n projection operator.

Now, in the limit of Ref. 9 the action is proportional to $\mathrm{Tr}\, V(T)=nV(t_*)$ even if the projection operator P_n varies as we move in X. We immediately see the close connection to K-theory. Slowly varying tachyonic field configurations are given by maps from X into the space of rank n projection operators in Hilbert space. This space of projection operators is sometimes denoted $BU(n)$, so we have

$$T: X \to BU(n). \tag{2.8}$$

If we consider a rank $n<k$ projection operator in the finite dimensional Hilbert space C^k then the space of such projection operators is clearly $U(k)/(U(n)\times U(k-n))$. The space $BU(n)$ is defined as the inductive limit of this quotient space as $k\to\infty$.

The space $BU(n)$ is topologically intricate, and if X is topologically nontrivial then the set of homotopy classes of maps $[X,BU(n)]$ can be nontrivial. Indeed, $BU(n)$ is a model for a ''classifying space'' of vector bundles. This means there is an isomorphism,

$$\mathrm{Vect}_n(X)\cong[X,BU(n)], \tag{2.9}$$

where $\mathrm{Vect}_n(X)$ are the isomorphism classes of complex vector bundles on X of rank n. This is explained in detail in Refs. 27, 28. In this way we relate homotopy classes of tachyon field configurations directly to isomorphism classes of vector bundles, and therefore to K-theory classes.

In the bosonic string the physical interpretation of these K-theory classes is less clear than in type II theory since the branes carry no conserved charges and presumably are unstable, even if the K-theory class is nontrivial. Our hypothesis is that these K-theory classes label inequivalent unstable D-brane configurations or boundary states of the bosonic string.

It would be very interesting to extend this discussion to the case of finite θ and to include the effects of second derivatives. Such considerations lead to many new questions beyond the scope of this paper. Some of these considerations indicate the relevance of a nonlinear sigma model with target space $BU(n)$. (Such sigma models have been considered in a superficially different context by Losev, Nekrasov, and Shatashvili.[29])

III. WITTEN'S FACTORIZATION OF THE OPEN STRING * PRODUCT ALGEBRA

We now consider spacetime of the form $X\times R^2$ with X a 24-manifold. We also assume that the metric factorizes and denote the closed string metric on X by g_{ab} and the closed string metric on R^2 by g_{ij}. Witten has observed in Ref. 30 that in the limit of Ref. 9, where the closed string metric g_{ij} is fixed and $\alpha' B_{ij}\to\infty$ (so the open metric $G^{ij}\to 0$) the $*$ algebra of open string field theory factorizes as $\mathcal{A}\to\mathcal{A}_0\otimes\mathcal{A}_1$. Here $\mathcal{A}_0$ is the algebra of the vertex operators in the 26 dimensional open bosonic string with zero momentum in the noncommutative directions and $\mathcal{A}_1$ is the algebra of noncommutative functions on R^2.

We can trivially extend the analysis of Ref. 30 by considering the following two scaling limits. In the first we take $B_{ij}=tB^0_{ij}$ and $g_{ab}=t^2 g^0_{ab}$ and take $t\to\infty$, keeping B^0, g^0_{ab} and g_{ij} fixed.

In this limit the string algebra factorizes as above but with $\mathcal{A}_0$ the algebra of zero momentum vertex operators and $\mathcal{A}_1 = C(X) \otimes C_B(R^2)$ where the first term is the commutative algebra of functions on X and the second is the noncommutative algebra of functions on R^2 defined by the Moyal product. (There is an important question of whether the functions should be compactly supported, or not. We believe that rapid falloff, or compact support is appropriate.) The second scaling limit takes $B_{ij} = 0$ and scales both g_{ab} and g_{ij} as t^2. In this limit the string algebra factorizes with $\mathcal{A}_1 = C(X \times R^2) = C(X) \otimes C(R^2)$ being the algebra of commutative functions on $X \times R^2$.

It is natural to expect that the set of D-branes, or boundary states is somehow connected with a K-theory of the algebra $\mathcal{A}_0 \otimes \mathcal{A}_1$. However, since $\mathcal{A}_0$ is a vertex operator algebra, the meaning of its K-theory definitely requires some explanation. Without answering this question we can at least ask what we can say without knowing too much about $K(\mathcal{A}_0)$.

Our working hypothesis is that $\mathcal{A}_0, \mathcal{A}_1$ behave similar to C^* algebras. In C^*-algebra theory there is a Kunneth-type theorem which implies that, modulo torsion, we may identify $K(\mathcal{A}_0) \otimes K(\mathcal{A}_1)$ with $K(\mathcal{A}_0 \otimes \mathcal{A}_1)$. (See Ref. 31, Theorem 23.1.3.) Therefore, we will focus on the K-theory of the algebra $\mathcal{A}_1$ in the next section.

IV. BOTT PERIODICITY AND NONCOMMUTATIVE SOLITONS

The algebra of functions $\mathcal{A}_1$ is very different for $B = 0$ and for $B \neq 0$. Nevertheless we expect the K-theory classification of branes to be unmodified when we turn on B and scale the metric. We will interpret this statement as a manifestation of Bott periodicity. (See Ref. 32 for a related remark.)

Bott periodicity is usually formulated as

$$K(X) \cong K(X \times S^2) = K_{\mathrm{cpt}}(X \times R^2). \tag{4.1}$$

In Ref. 9, X is R^{23+1} with R^2 as the transverse 2 dimensions to the D23-brane constructed as a noncommutative soliton of the tachyon field theory. Equation (4.1) can be translated into the algebraic setting:

$$K(C(X)) \cong K(C(X) \otimes C_0(R^2)), \tag{4.2}$$

where $C(X)$ is the algebra of continuous functions on X, and $C_0(R^2)$ is the algebra of continuous functions going to zero at infinity.

K-theory is unchanged under ''Morita equivalence.'' Therefore

$$K(C(X)) = K(C(X) \otimes \mathrm{Mat}_N(C)). \tag{4.3}$$

Moreover, the norm-closure of the $N \to \infty$ limit of $\mathrm{Mat}_N(C)$ is the algebra of compact operators $\mathcal{K}$. Since K-theory behaves well under inductive limits,

$$K(C(X)) = K(C(X) \otimes \mathcal{K}). \tag{4.4}$$

If the transverse coordinates satisfy $[x^1, x^2] = -i\theta$ (θ is real) then the Stone–von Neuman theorem says there is a unique irreducible unitary representation $\mathcal{H}$, i.e. the Hilbert space of quantum mechanics. Moreover, to any $f \in \mathcal{S}(R^2)$, the Schwarz space of functions of rapid decrease, the Weyl ordered operators,

$$T(f) = \int dp_1\, dp_2\, \hat{f}(p_1, p_2) \exp[i(p_1 \hat{x}^1 + p_2 \hat{x}^2)], \tag{4.5}$$

where $\hat{f}(p_1,p_2)$ is the Fourier transform, generate the algebra $\mathcal{K}$ of compact operators.[33] If we suppose that the classification of D-branes is unchanged in the limit $B\to 0$ then it follows that $K(C(X)\otimes C_B(R^2))\equiv K(C(X)\otimes\mathcal{K})=K(C(X)\otimes C_0(R^2))$. Combining this with Morita equivalence we obtain the statement of Bott periodicity.

V. K-THEORETIC CLASSIFICATION OF D-BRANES FROM TACHYONS IN TYPE IIB STRINGS

Let us now turn to the tachyon field in the construction of type II D-branes via noncommutative solitons. We will focus on the case of BPS IIB branes. As shown in Ref. 30, the tachyon field must satisfy

$$T\overline{T}T=T, \tag{5.1}$$

where $\overline{T}$ is the Hermitian conjugate of T. Equation (5.1) is the defining equation of a ''partial isometry.'' Moreover, the net brane charge is given by the index of T. In an effective field theory approach the tachyon potential has the form

$$V(T,\overline{T})=U(\overline{T}T-1)+U(T\overline{T}-1). \tag{5.2}$$

(This result could presumably also be derived in string field theory.) To have a finite energy configuration the kernels of both T and $\overline{T}$ must be finite dimensional, thus T should be both a Fredholm operator and a partial isometry.

Once again, we split spacetime as $X\times R_B^{2n}$, where X has dimension $10-2n$ and might be topologically nontrivial. If we consider X-dependent configurations with a finite net number of branes then the tachyon field will give us a map

$$T:X\to\mathcal{F}, \tag{5.3}$$

where $\mathcal{F}$ are the Fredholm operators. But this is exactly one model for K-theory![28,34] Moreover, the map $[X,\mathcal{F}]\to K^0(X)\to 0$ is given by taking the index bundle whose fiber at $x\in X$ is just $\mathrm{Ind}(T)_x:=\mathrm{Ker}(T(x))-\mathrm{Cok}(T(x))$ and we identify this as the K-theory class of the Chan–Paton space of the D-brane. The argument that the map is onto, given in Appendix A of Ref. 28, shows that there is no loss of generality in supposing that the Fredholm operator is in fact a partial isometry. Thus, one recovers in a very straightforward way the classification of type II D-brane charge in terms of K-theory.

A closely related remark has been made (independently) by Witten in Ref. 11 in the type IIA context. Here Witten uses the Fredholm model identifying $K^1(X)$ with $[X,\mathcal{F}^{sa}]$ where $\mathcal{F}^{sa}$ are the self-adjoint Fredholm operators. This model is due to Atiyah and Singer.[35]

VI. TOEPLITZ OPERATORS AND THE ABS CONSTRUCTION

In the explicit solution for the D7-brane as a vortex in the noncommutative plane, explained in Refs. 9, 30, 36 the tachyon operator T is a special kind of partial isometry, namely, a shift operator $T=S$ where S is the shift operator,

$$S:|n\rangle\to|n+1\rangle,\quad n\geq 0, \tag{6.1}$$

in a ''harmonic oscillator'' basis $|n\rangle$, $n\geq 0$, for a separable Hilbert space. Note that $S^*S=1$, but SS^* is not 1, indeed, $SS^*=1-|0\rangle\langle 0|$. The C^* algebra generated by an operator such that $S^*S=1$, but $SS^*\neq 1$ is unique, and known as the ''Toeplitz algebra.'' This algebra can be realized in several ways, and the following is particularly apt for discussing generalizations of noncommutative tachyons.

We consider our Hilbert space to be the Hilbert space of square integrable functions on the circle, $L^2(S^1)$. The functions $1/\sqrt{2\pi}e^{in\theta}$ define a complete orthonormal basis $|n\rangle$ for $n\in\mathbb{Z}$. Given

a continuous function $f(\theta)$ we may associate an operator $M_f:\mathcal{H}\to\mathcal{H}$ simply by multiplying a wavefunction $\psi(\theta)$ by $f(\theta)$. This gives a representation of the commutative C^* algebra $C(S^1)$ on $\mathcal{H}$. Now consider the Dirac operator $D=-id/d\theta$ and split the Hilbert space into the negative and non-negative modes of D. Let P be the orthogonal projection onto the positive subspace H_+ of $L^2(S^1)$ spanned by $|n\rangle$ with $n\geqslant 0$. Equivalently, we could view P as the projection onto the subspace of $L^2(S^1)$ consisting of the boundary values of holomorphic functions. Then given a function $f(\theta)$ on S^1 we can define a Toeplitz operator which maps H_+ to H_+ by $T_f=PM_f$. Note that if f has negative Fourier modes then M_f does not preserve H_+, and hence the projector P acts nontrivially. For example, if $f_l=e^{il\theta}$, then T_{f_l} is just the shift operator S^l for $l>0$, but has a kernel for $l<0$. Quite generally, $(T_f)^\dagger=T_{f^*}$, so $f\to T_f$ preserves the adjoint $*$ action. However, the map f to T_f is not a homomorphism. Indeed, an easy computation shows that

$$T_1-T_{f_l}T_{f_l^*}=P_l \tag{6.2}$$

is the projection operator onto the first l levels in H_+. This is a compact operator, and in general it can be shown that, while $T_fT_g\neq T_{fg}$, the difference $T_fT_g-T_{fg}$ is a compact operator.

In what follows, this construction of Toeplitz operators will be generalized to L^2 functions on odd spheres in order to relate the index of Toeplitz operators to the winding number of ABS configurations.

A. Noncommutative ABS construction

Let us now generalize the construction of T in Refs. 9, 30 allowing for a $2p$-dimensional transverse noncommutative space. (The construction in Ref. 30 includes the possibility of a $2p$ dimensional transverse space for a single D9–anti D9 pair. Here we generalize this to 2^p pairs in order to explain the relation between the index of T and the winding number of the ABS configuration.)

First, we construct the noncommutative tachyon field. Let us skew-diagonalize θ^{ij} and take:

$$[x^{2i-1},x^{2i}]=-i\theta_i \quad \theta_i>0, \quad i=1,...p\,. \tag{6.3}$$

Moreover, we consider the irreducible Clifford representation γ_i for $\mathcal{C}l_{2p}$. These are $2^p\times 2^p$ dimensional complex Hermitian matrices of the form:

$$\gamma_i=\begin{pmatrix} 0 & \Gamma_i \\ \overline{\Gamma_i} & 0 \end{pmatrix}. \tag{6.4}$$

Now we take the noncommutative tachyon to be of the same form as the commutative ABS configuration:[37,2]

$$T=f(r)\Gamma_i x^i, \tag{6.5}$$

except that we now regard the tachyon as an operator,

$$T:\mathcal{H}\otimes S^-\to\mathcal{H}\otimes S^+, \tag{6.6}$$

where the Hilbert space $\mathcal{H}$ is realized as a representation of p oscillators and S^-, S^+ are negative and positive spin representations. To be specific, we will represent $\mathcal{H}$ as the Bargmann quantization,

$$\mathcal{H}_{\mathrm{B}}=\mathrm{Hol}\left(C^p,\exp\left[-2\sum\ \theta_i|z_i|^2\right]dv\right). \tag{6.7}$$

The wavefunctions are holomorphic functions of $z_i = x^{2i-1} + ix^{2i}$, normalizable with respect to the above measure and dv is the standard Euclidean volume element. An orthogonal basis for $\mathcal{H}_B$ is provided by the monomials $z^k := \Pi_i (z_i)^{k_i}$. We will let k stand for a multiindex $k \in (\mathbb{Z}_+)^p$.

We now show that T is a Fredholm operator, and also show how to determine $f(r)$ from the equations $T\overline{T}T = T$, $\overline{T}T\overline{T} = \overline{T}$. The key calculation is

$$\Gamma_i x^i \overline{\Gamma}_j x^j = \sum_{i=1}^{p} 2\theta_i \left(N_i + \frac{1}{2} \right) - i\Sigma_{ij}\theta^{ij},$$
$$\overline{\Gamma}_i x^i \Gamma_j x^j = \sum_{i=1}^{p} 2\theta_i \left(N_i + \frac{1}{2} \right) - i\overline{\Sigma}_{ij}\theta^{ij}. \tag{6.8}$$

Here $\Sigma_{ij} = 1/4(\Gamma_i \vec{\Gamma}_j - \Gamma_j \overline{\Gamma}_i)$, $\overline{\Sigma}_{ij} = 1/4(\overline{\Gamma}_i \Gamma_j - \overline{\Gamma}_j \Gamma_i)$ and $N_i = a_i^\dagger a_i$ is the ith occupation number. The second terms in (6.8) are diagonalized by the spinor weights to be $\Sigma_{i=1}^{p} \pm \theta_i$. Our convention is that in the second equation of (6.8) we have a spinor weight giving $-\Sigma \theta_i$. Therefore, the first operator has no kernel and the second operator has a one dimensional kernel, given by the oscillator ground state times the lowest weight spinor. Thus,

$$\overline{T} = \overline{\Gamma}_i x^i \frac{1}{\sqrt{\Gamma_i x^i \overline{\Gamma}_i x^i}} \tag{6.9}$$

satisfies the equation $T\overline{T}T = T$, has no kernel and is of index -1. We will refer to this as the ''noncommutative ABS construction.'' In order to explain the relation to the ABS construction we would like to make sense of restricting the tachyon field to a sphere in the noncommutative space. Classically, we restrict the field T to the solutions of the equation

$$\sum_i |z_i|^2 = R^2, \tag{6.10}$$

defining the sphere Σ of dimension $2p-1$ and radius R. At the nonzero B field the z_i become noncommuting, so the question arises as to what it means to restrict the operator to a noncommutative sphere. We will now propose one interpretation of what this might mean.

In quantum mechanics, restricting the wavefunctions in the Bargman space $\mathcal{H}_B$ to the sphere produces the Hardy space $\mathcal{H}_\Sigma$. This is the Hilbert subspace of $L^2(\Sigma; d\Omega)$ defined by the boundary values of holomorphic functions. Here $d\Omega$ is the standard round measure on the sphere such that $dv = R^{2p-1}\, dR\, d\Omega$. The projection operator from L^2 to $\mathcal{H}_\Sigma$ is given by

$$(Pf)(z) = \int_\Sigma K_\Sigma(z,w) f(w) d\Omega,$$
$$K_\Sigma(z,w) = (1 - z \cdot \overline{w})^{-p}. \tag{6.11}$$

An orthogonal basis for the Hardy space is again given by $\varphi_k = z^k$. Note that the norm of these states in the Hardy space is

$$(z^k, z^{k'}) = \delta_{k,k'} \frac{2\pi^p \Pi_i (k_i)!}{\Gamma(|k| + p)},$$

where $|k| = \Sigma k_i$ for a multi-index k.

Now let us consider the action of classical coordinates $z_i, \overline{z_i}$ on the Hardy space $\mathcal{H}_\Sigma$. To make sense of this we need to define Toeplitz operators. In general, if $f:\Sigma \to \mathbb{C}$ is any function we define $\mathcal{T}_f := PM_f$ where $M_f:\mathcal{H}_\Sigma \to L^2$ is the operator of multiplication by f. The operators $\mathcal{T}_{z_i}, \mathcal{T}_{\overline{z_i}}$ are easily computed:

$$\begin{aligned} \mathcal{T}_{z_i}\varphi_k &= \varphi_{k+e_i}, \\ \mathcal{T}_{\overline{z_i}}\varphi_k &= 0, \quad \text{if } k_i = 0, \\ &= 2\pi \frac{k_i}{|k|+p-1}\varphi_{k-e_i}, \quad \text{if } k_i > 0, \end{aligned} \tag{6.12}$$

where e_i is the ith unit vector in $(\mathbb{Z}_+)^p$.

By considering the Hilbert space $\mathcal{H}_\Sigma \otimes \mathbb{C}^N$, Toeplitz operators for functions are easily generalized to Toeplitz operators for matrix valued functions $f:\Sigma \to \mathrm{Mat}_N(C)$, and hence we can consider our tachyon operator (6.6) above as a Toeplitz operator:

$$T:\mathcal{H}_\Sigma \otimes S \to \mathcal{H}_\Sigma \otimes S, \tag{6.13}$$

where $S^+ \cong S^- \cong S$ is the irreducible spin representation in odd dimensions. The Toeplitz operator is the projection P_+ composed with matrix multiplication by $\beta:\Sigma \to GL(N,C)$ given, essentially by the ABS construction:

$$\beta(x) = \Gamma_i x^i \frac{1}{\sqrt{x^i x^i + \text{const}}}.$$

The operator T in (6.13) is bounded and Fredholm. Now, although the restriction map $\mathcal{H}_B \to \mathcal{H}_\Sigma$ is *not* unitary it is 1–1 and onto. Therefore, the *index* of T on $\mathcal{H}_B$ will be the same as the index of T on $\mathcal{H}_\Sigma$.

Now, we can invoke the index theorem of Boutet de Monvel,[38] according to which the index is

$$\mathrm{Index}(T|_{\mathcal{H}_\Sigma}) = \int_\Sigma \mathrm{ch}(\beta) Td(T\Sigma). \tag{6.14}$$

Here

$$\mathrm{ch}(\beta) = \beta^* \left(\sum_{j \geqslant 0} (-1)^{j-1} \frac{\omega_{2j-1}}{(j-1)!} \right),$$

and ω_i are standard generators of $H^i(GL(N,C),Q)$. Since $Td(T\Sigma) = 1$ in this case we have a direct connection between the index of the tachyon operator on $\mathcal{H}_B$, and the winding number of the classical ABS tachyon.

VII. REMARKS ON THE RELATION TO K-HOMOLOGY

The noncommutative ABS construction in the previous section leads rather naturally to a relation between D-branes and the work of Brown, Douglas, and Filmore (BDF) on the classification of algebras of essentially normal operators.[39] In this section we will give a brief review of that work, and then explain the relation to D-branes.

A. Brief review of BDF

An expository discussion of Ref. 39 can be found in Refs. 40, 31, 41, 42, 43. For the readers' convenience we give a brief summary here.

In Matrix theory,[44] spacetime emerges from an algebra of commuting operators. Here we will discuss algebras of ''almost commuting'' operators in the belief that these are related to D-branes. Recall that by Gelfand's theorem, C^*-algebras of commuting operators are naturally associated to Hausdorff topological spaces X by considering the algebra of continuous functions $C(X)$. [If X is noncompact, we add the condition that $f\to 0$ at infinity, and correspondingly $C(X)$ does not have a unit. For simplicity of discussion, we henceforth assume X is compact in this subsection.] Isomorphism classes of algebras are in 1–1 correspondence with homeomorphism classes of spaces. We will now consider noncommutative C^*-algebras $\mathcal{A}$ which fit into the short exact sequence:

$$0\to\mathcal{K}\to\mathcal{A}\overset{\beta}{\to}C(X)\to 0, \tag{7.1}$$

for some fixed space X. Note that if T_f denotes some operator in $\mathcal{A}$ mapping to the function f under β, then $T_{f_1}T_{f_2}-T_{f_1f_2}$ is in the kernel of β, and hence is a compact operator. It follows that $[T_{f_1},T_{f_2}]$ is compact and thus the algebra $\mathcal{A}$ is thus ''almost commuting'' in the sense that compact operators are considered to be ''small.'' An example of such an extension is given by the Toeplitz algebra generated by the shift operators, described at the beginning of Sec. VI: $S=T_z\to z$ defines a C^* morphism onto the continuous functions on $X=S^1$.

In Ref. 39, BDF investigated extensions of the form (7.1) for fixed X. To any such extension we can associate a C^*-algebra morphism (called the ''Busby invariant'') $\tau:C(X)\to Q(\mathcal{H})$ where Q is the ''Calkin algebra'' defined by $Q(\mathcal{H}):=B(\mathcal{H})/\mathcal{K}$ where $B(\mathcal{H})$ is the algebra of bounded operators on a separable Hilbert space. Indeed, for any $f\in C(X)$ we choose an operator $T_f\in\mathcal{A}$ projecting to it, and define τ by $\tau(f)=\pi(T_f)$ where $\pi:B(\mathcal{H})\to Q(\mathcal{H})$ is the projection. Since $T_{f_1}T_{f_2}-T_{f_1f_2}$ is a compact operator, τ is an algebra homomorphism. Conversely, given a C^*-algebra morphism $\tau:C(X)\to Q(\mathcal{H})$ one can form an extension (7.1), and, up to a natural notion of isomorphism, τ uniquely characterizes the extension. Full details can be found in Chap. 3 of Ref. 42. Suffice it to say here that, given $\tau:C(X)\to Q(\mathcal{H})$ we can form

$$0\to\mathcal{K}\to\mathcal{A}'\to C(X)\to 0 \tag{7.2}$$

by defining

$$\mathcal{A}':=\{(\mathcal{O},f):\pi(\mathcal{O})=\tau(f)\}\subset B(\mathcal{H})\oplus C(X), \tag{7.3}$$

and that (7.2) is equivalent to (7.1) in the sense that there is an isomorphism $\psi:\mathcal{A}\to\mathcal{A}'$ compatible with the two sequences.

One of the reasons the Busby invariant is useful is that it allows one to define a notion of direct sum of extensions. In order to do this we must first introduce ''unitary equivalence,'' also known as ''strong equivalence.'' Two extensions (7.1) are ''strongly equivalent'' if there is a unitary operator U on $\mathcal{H}$ such that the Busby invariants are related by $\tau_2(f)=\pi(U)\tau_1(f)\pi(U)^*$. Let $\mathbf{Ext}(C(X),\mathcal{K})$ denote the set of strong equivalence classes of extensions of $C(X)$ by $\mathcal{K}$. A direct sum operation on $\mathbf{Ext}(C(X),\mathcal{K})$ can then be defined by taking the extension corresponding to the Busby invariant,

$$\tau_1\oplus\tau_2:C(X)\to Q(\mathcal{H})\oplus Q(\mathcal{H})\to Q(\mathcal{H}\oplus\mathcal{H})\cong Q(\mathcal{H}). \tag{7.4}$$

It turns out that (7.4) defines a semigroup operation on $\mathbf{Ext}(C(X),\mathcal{K})$. Thus far, the theory could have been developed for general extensions $\mathbf{Ext}(A_1,A_2)$ of arbitrary C^*-algebras A_1 by A_2. However, specializing to $A_1=C(X)$ and $A_2=\mathcal{K}$, a number of nice things begin to happen. It turns out that there is a natural zero in the semigroup, corresponding to the ''trivial extensions.'' These are extensions for which the Busby invariant lifts to $B(\mathcal{H})$; equivalently, they are extensions such that the sequence (7.1) splits, and hence we can unambiguously write every operator in $\mathcal{A}$ in the form $T_f=N_f+k$ with $k\in\mathcal{K}$ and $N_{f_1}N_{f_2}=N_{f_1f_2}$. Let $\mathrm{Ext}(C(X),\mathcal{K})$ be the quotient of

Ext$(C(X),\mathcal{K})$ by the trivial extensions. In the above references it is shown that every extension has an inverse (up to the addition of a trivial extension) so that Ext$(C(X),\mathcal{K})$ in fact is an Abelian group. Moreover, Ext$(C(X),\mathcal{K})$ can even be used to define a homology theory on X! Indeed, if we define

$$\begin{aligned} K_1^a(X) &= \mathrm{Ext}(C(X),\mathcal{K}) \\ K_0^a(X) &= \mathrm{Ext}(C(X)\otimes C_0(\mathbb{R}),\mathcal{K}) \end{aligned} \tag{7.5}$$

(the superscript ''a'' is for ''analytic,'' K-homology, as opposed to ''topological'' K-homology), then it turns out that $K_*^a(X)$ is a mod 2 periodic homology theory, dual to K-theory.

One way to make the relation to a homology theory more evident is to introduce the noncommutative spheres $\mathcal{S}^0,\mathcal{S}^1$ with function spaces:

$$\begin{aligned} C(\mathcal{S}^1) &= \left\{ \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} : a_{ij}\in B(\mathcal{H}), a_{12}, a_{21}\in\mathcal{K} \right\}, \\ C(\mathcal{S}^0) &= \left\{ \begin{pmatrix} a_{11} & 0 \\ 0 & a_{22} \end{pmatrix} : a_{11}-a_{22}\in\mathcal{K} \right\}, \end{aligned} \tag{7.6}$$

and then define $K_i(X)$ to be homotopy classes of maps of X into $\mathcal{S}^i$, $K_i(X):=[\mathcal{S}^i,X]$. In the noncommutative setting this amounts to the homotopy classes of $*$-homomorphisms $C(X)\to C(\mathcal{S}^i)$. (The equivalence of this definition to what we described above is hardly obvious. The necessary technical details can be found in Ref. 31, Secs. 15.7 and 15.8.)

B. Algebra extensions associated to IIA-branes

We will now review a contruction from Ref. 41 which may be interpreted as saying that every IIA D-brane naturally provides a nontrivial extension of the algebra of functions on spacetime by compact operators.

Let W be an odd-dimensional Spin^c submanifold of a spacetime X. W is equipped with a complex vector bundle E with connection and inherits a metric from X. We think of W as the IIA-brane worldvolume and E as its Chan–Paton bundle. Using the above data we can form the Hilbert space $\mathcal{H}$ of L^2 spinors with values in $S\otimes E$, where $S\to W$ is the spin bundle. Denote the Dirac operator on $S\otimes E$ by $\not{D}_E$. Assuming the connection and metric are generic, $\not{D}_E$ will have no zero modes and we can decompose the Hilbert space into the positive and negative eigenspaces of $\not{D}_E$: $\mathcal{H}=\mathcal{H}_+\oplus\mathcal{H}_-$. The commutative algebra $C(W)$ is represented on $\mathcal{H}$ by multiplication operators M_f for $f\in C(W)$. In general, M_f does not preserve the subspace $\mathcal{H}_+$, but if we take the ''compression'' of M_f by composing with the projection operator $P_+:\mathcal{H}\to\mathcal{H}_+$ then we can define a Toeplitz operator $T_f=P_+M_f:\mathcal{H}_+\to\mathcal{H}_+$. As in the case $W=S^1$ described previously, it turns out that $T_{f_1}T_{f_2}-T_{f_1f_2}$ is a compact operator and we obtain an extension,

$$0\to\mathcal{K}\to\mathcal{A}\to C(W)\to 0, \tag{7.7}$$

where $\mathcal{A}$ is the C^* algebra generated by the T_f. By using pullback $\phi^*:C(X)\to C(W)$ we obtain an extension of the algebra of functions on all of spacetime. That is, if $\phi:W\to X$ is a continuous map then we can define a Busby invariant $\tau\phi^*:C(X)\to Q(\mathcal{H})$ from which we get an extension:

$$0\to\mathcal{K}\to\tilde{\mathcal{A}}\to C(X)\to 0 \tag{7.8}$$

It is shown in Ref. 41 that all classes in $K_1^a(X)=\mathrm{Ext}(C(X),\mathcal{K})$ can be obtained from the above construction using a suitable triplet (W,E,ϕ). Moreover, if a suitable equivalence relation is put on (W,E,ϕ) then classes in $K_1^a(X)$ are in 1–1 correspondence with classes $[(W,E,\phi)]$. The equivalence relations on (W,E,ϕ) make good physical sense: they include cobordism (i.e., con-

tinuous deformation of the worldvolume and Chan–Paton bundle) and a natural identification of direct sums of Chan–Paton bundles. In addition they include ''vector bundle modification,'' a mathematical construction reminiscent of the Myers dielectric effect.[45]

It is interesting to compare $K_1^q(X)$ with the group of D-brane charges, thought to be given by $K^1(X)$. If X is compact, even dimensional, and spin then, modulo torsion, $K_1(X)$ is isomorphic to $K^1(X)$ by Poincaré duality. However, when we include torsion a puzzling difference emerges. There is a universal coefficient theorem (Ref. 31, Theorem 16.3.3):

$$0 \to \mathrm{Ext}(K^0(X),\mathbb{Z}) \to \mathrm{Ext}(C(X),\mathcal{K}) \to \mathrm{Hom}(K^1(X),\mathbb{Z}) \to O. \tag{7.9}$$

Moreover, the sequence splits, so that the torsion can in principle differ from that of $K^1(X)$. This possible discrepancy in torsion charges deserves to be more thoroughly investigated.

C. The index theorem

We can now put the noncommutative ABS tachyon field of the previous section into its proper mathematical context: The equivalence of IIB D-brane charges in the commutative and noncommutative theory is simply the equality of the analytic and topological index, expressed in the framework of K-homology (as explained in Ref. 41).

In the language of Brown–Douglas–Filmore, the Toeplitz operators on the Hardy space defines an analytic K-homology class,

$$[(\mathcal{H}_\Sigma,\tau)] \in K_{1,a}(\Sigma^{2p-1}), \tag{7.10}$$

where τ is the Busby invariant. That is, the inverse image under $\pi: B(\mathcal{H}) \to Q(\mathcal{H})$ of $\tau(C(\Sigma^{2p-1}))$ in $B(\mathcal{H}_\Sigma)$ defines an algebra of operators $\mathcal{T}$ providing a nontrivial extension by compact operators:

$$0 \to \mathcal{K} \to \mathcal{T} \to C(\Sigma^{2p-1}) \to 0. \tag{7.11}$$

It is explained in Ref. 41 that the K-homology class (7.10) is the same as that determined by the Dirac operator $[\not{D}]$ on Σ using the construction of Sec. VI.2. In particular, the index theorem of Boutet de Monvel follows from the ordinary index theorem.

One usually associates IIB D-brane charge to $K^0(X)$, or for an infinitely extended D-brane with transverse space X_t, to $K^0_{\mathrm{cpt}}(X_t)$. The relation to (7.10) is explained as follows. We consider the exact sequence in K-homology for the pair (D^{2p},Σ^{2p-1}), where D^{2p} is the disk of dimension $2p$ with boundary Σ^{2p-1}. The connecting homomorphism gives an isomorphism,

$$\delta: K_0(D^{2p},\Sigma^{2p-1}) \cong K_1(\Sigma^{2p-1}). \tag{7.12}$$

In this way, the above construction associates an element of analytic K-homology $K_{0,a}$ to the noncommutative tachyon. By Poincare duality $K_0 \cong K^0$, (again, up to torsion) and we produce the same K-theory class we expected to associate to a IIB-brane.

D. Speculations on noncommutative D-branes

The above considerations lead to the idea that it might be fruitful to relax the equivalence relations we have put on the extensions (7.8). As we have discussed, any ''commutative D-brane'' defines a triple (W,E,ϕ) and hence a particular extension. Conversely, given an abstract extension (7.8) could one extract the data of a D-brane? We can easily answer one simple question about such generalized D-branes, namely: ''Where is the brane?'' as follows. The kernel of the Busby invariant $\tau: C(X) \to Q$ defines an ideal, and from the Gelfand corespondence therefore defines a subspace $W \subset X$. Concretely, the ideal is the subalgebra of functions vanishing on W. It would be natural to identify W with the worldvolume of a D-brane. Whether or not one can usefully recover other aspects of the structure of a D-brane, and in particular whether extensions (7.8) which do not come from triples (W,E,ϕ) can be usefully identified with ''noncommutative D-branes'' remains an interesting open question.

In any case, inspired by the result of BDF we would like to define an action whose solutions could be considered to be the set of possible IIA D-branes, generalized in the above sense. The action has some interesting similarities to the IKKT action. On the other hand, we caution the reader at the outset that it remains to be seen if the following action will play any useful role in the computation of any physical quantities.

The action is a function of pairs $(\mathcal{A}, \phi)$, where $\mathcal{A}$ is a C^*-algebra and ϕ is a C^*-algebra morphism $\phi: \mathcal{A} \to C(X) \to 0$, and is given by

$$S(A,\phi) := \sup_{f_1, f_2 \in C(X)} \inf_{\phi(a_i)=f_i} \mathrm{Tr}_{\mathrm{D}}([a_1,a_2][a_1,a_2]^\dagger). \tag{7.13}$$

Here we first take the infimum over all lifts T_f of a pair of functions f. Moreover, Tr_{D} is the Dixmier trace. Roughly speaking, Tr_{D} is defined as follows. Let $\mu_n(T)$ be the eigenvalues of $\sqrt{T^\dagger T}$ arranged in decreasing order. Define

$$\mathrm{Tr}_{\mathrm{D}}(T) := \lim_{N\to\infty} \frac{1}{\log N} \sum_{n=1}^{N} \mu_n(T). \tag{7.14}$$

For the real story, consult the book by Connes.[46]

The action (7.13) is positive semidefinite. So, in any reasonable ''space of $(\mathcal{A}, \phi)$'' the zeros of the action are automatically stationary points of minimal action. The action is identically zero only when, for all $f_1, f_2 \in C(X)$ there are lifts T_{f_1}, T_{f_2} such that the commutator $[T_{f_1}, T_{f_2}]$ has singular values falling off faster than $1/\sqrt{n}$. We may expect the relations (6.12) to give a good approximation to the general behavior of $[T_{f_1}, T_{f_2}]$ on spinors of large energy, and from this we expect that the extensions associated to (W,E,ϕ) described above will be zeros of the action. Conversely, any zero of the action can be used to define an extension of $C(X)$ by compact operators.

It is interesting to compare the action (7.13) with the IKKT model:

$$S = g_{IK} g_{JL} \mathrm{Tr}([X^I, X^J][X^K, X^L]), \tag{7.15}$$

where X^I are $N \times N$ Hermitian matrices and g_{IJ} is a nondegenerate constant metric on $\mathbb{R}^{10}$. If we consider the X^I as generators of the algebra of functions on $\mathbb{R}^9$ then there is a certain similarity between (7.13) and (7.15). However we note the following.

(1) The IKKT action does not generalize easily to curved spaces. Even on $\mathbb{R}^9$ if we attempt to include curved metrics g_{IJ} we run into ordering problems. (See Ref. 47 for the state of the art on this problem.)
(2) When producing D-branes from Matrix theory the solutions have infinite action. Of course, this is physically appropriate for infinitely extended planar branes. Nevertheless, it would be nice to work with finite action quantities when considering compact branes.

VIII. NONZERO H-FIELDS AND 5-BRANES

In this section we will focus on a description of Neveu–Schwarz fivebranes in the framework of Ref. 9. We should first discuss what we mean by an NS fivebrane in open string theory. In the original description[48] NS fivebranes are solutions to the closed string equations of motion with topology $M \times S^3 \times R$ with M the fivebrane worldvolume such that $\int_{S^3} H = Q_5$, H being the NS three-form field and Q_5 the quantized fivebrane charge. Since the tension scales like $1/g_s^2$ with g_s the closed string coupling, these are properly thought of as solitons in the closed string sector rather than the open string sector of the theory where soliton energies scale as $1/g_s$ (as for D-branes). In open string theory we cannot expect to see the detailed form of the closed string solution since closed string states only arise at the loop level in open string theory. We thus define a fivebrane to be a configuration in a ten dimensional spacetime X with $H \in H^3(X,Z)$ a nontrivial integer class.

Given the scaling of the fivebrane tension with g_s, the close connection between the framework of Ref. 9 and Matrix theory,[49] and the well-known difficulties in describing fivebranes in Matrix theory,[50,51] we can anticipate some problems here as well.

To explain the basic idea and the difficulty one expects, consider taking $X=W\times R_B^2$ to be the worldvolume of an unstable D9-brane in IIA with a large B-field on the R^2 component and take $W=R^5\times S^3$. W represents the commutative part of the D9-brane worldvolume. The effective action (2.6) contains gauge fields with gauge group $U(\mathcal{H})$ coupled to the tachyon field in the adjoint representation. Since the $U(1)$ component of $U(\mathcal{H})$ (with A_μ proportional to the identity operator) does not couple to T and has infinite action if its field strength is nonzero, it is more correct to say that the gauge group is $PU(\mathcal{H})\equiv U(\mathcal{H})/U(1)$. Defining more precisely what is meant by the $U(1)$ component when there is nontrivial topology is quite subtle as will be discussed below.

Since $U(\mathcal{H})$ is contractible,[52] $\pi_2(PU(\mathcal{H}))=\pi_1(U(1))=\mathbb{Z}$. Thus we can construct an ''instanton'' configuration of the $PU(\mathcal{H})$ gauge fields on S^3 by patching together gauge fields on the northern and southern hemispheres using a nontrivial element of $\pi_2(PU(\mathcal{H}))$ on the S^2 equator. Our proposal is that such a twisted $PU(\mathcal{H})$ bundle with the tachyon field $T=t_*$ represents a D9-brane in the presence of a NS fivebrane while condensing the tachyon field to $T=0$ removes the D9-brane and leaves an NS fivebrane. More generally, we can use nontrivial projection operators for the tachyon to study lower D-branes in the presence of NS fivebranes.

We can now see one difficulty we expect to encounter. Since the NS fivebrane world volume is six dimensional, it must span $R^5\in W$ and as well have one component in the noncommutative plane R_B^2. As a result, the trace in (2.6) is expected to diverge, i.e. the gauge field fieldstrength-squared for the twisted $PU(\mathcal{H})$ connection is not expected to be trace class. More precisely, we expect that if we cut off the trace by summing over a finite number of modes then the trace will diverge in the mode number cutoff. In fact, an evaluation of the gauge action $\int_W \mathrm{Tr}\, F\wedge *F$ for some examples of smooth nontrivial $PU(\mathcal{H})$ connections shows that the action is in indeed infinite. A proper interpretation of this infinity must be addressed in future work. Here we simply note that since the mode-number cutoff can be interpreted as an infrared cutoff in the noncommutative directions, there is room for an interpretation of the infinite gauge kinetic action as the volume divergence due to the extension of the 5-brane worldvolume in the noncommutative directions.

To see the connection to the fivebrane definition in terms of H, we note that a standard theorem states that principal $PU(\mathcal{H})$ bundles are classified by the Dixmier–Douady class $h\in H^3(W,Z)$. [A quick homotopy-theoretic proof is that $BPU(\mathcal{H})\sim K(\mathbb{Z},3)$ since $\Omega BPU(\mathcal{H})\sim PU(\mathcal{H})\sim K(\mathbb{Z},2)\sim\Omega K(\mathbb{Z},3)$.] This class has been interpreted in Refs. 53, 54, 11 as the cohomology class of the H-field of string theory. In addition to the arguments presented in these papers we would like to point out that the reasoning described by Kapustin in Ref. 55 for the case when h is torsion and in fact can be extended to the case of h nontorsion. This follows because a nontrivial $PU(\mathcal{H})$ bundle defines a nontrivial ''bundle gerbe with connection'' (where we are using the terminology explained in Refs. 56, 57). Then, using the equivalence to the formulation of Brylinski[58] one can argue that the ''holonomy of the $PU(\mathcal{H})$ connection in the fundamental representation'' can be given a concrete definition in terms of a covariantly constant section of a line bundle with connection over loop space LW. The line bundle with connection over LW is constructed using the bundle gerbe associated to the $PU(\mathcal{H})$ bundle with connection A in a way explained in Refs. 58, 56, 57.

In more physical terms, we wish to make sense of the expression

$$\exp\left[i\int_D B\right]\mathrm{Tr}_{\mathcal{H}} P\exp\int_\gamma A, \tag{8.1}$$

in the open string path integral, where D is the disk worldsheet with boundary $\gamma\subset W$, B is the background B-field, and A is a $PU(\mathcal{H})$ connection. In order to define this we must lift A to a compatible $U(\mathcal{H})$ connection $\tilde{A}$. In so doing the field strength acquires a ''$U(1)$ component''

which we denote by $\mathrm{Tr}\,F$, although since we are working with operators not necessarily of trace class this notation should be handled with great care. The essential physical point is that in infinite dimensions the commutator of two Hermitian operators can be proportional to the identity matrix, the standard example being a pair of operators representing the Heisenberg relations. Consequently the commutator term in $\tilde{F}=d\tilde{A}+\tilde{A}^2$ can in fact contribute to the $U(1)$ component of $\tilde{F}$ and in topologically interesting situations it must do so. This in turn means that the Bianchi identity for the $U(1)$ part of $\tilde{F}$ is *not* $d\,\mathrm{Tr}\,F=0$ but rather $d\,\mathrm{Tr}\,F=K$ where K is a globally well-defined 3-form on W. Moreover, by the general results of Ref. 58 it follows that the cohomology class of $K/(2\pi i)$ coincides with the Dixmier–Douady class h. Defining the holonomy of A as a covariantly constant section of a bundle over loopspace one can follow the strategy of Ref. 55 and conclude that the Dixmier–Douady class h must be identified with that of the physical H-field. It is not necessary to assume that h is a torsion class, although in infinite dimensions the trace Tr isolating the $U(1)$ part of the field strength requires an *ad-hoc* definition.[58]

One simple example of a nontrivial $PU(\mathcal{H})$ connection illustrating some of the above general remarks is the following. (This example is a paraphrase of Sec. 4.3 of Ref. 58.) We will take the base space to be the three-manifold $S^2\times S^1$, more appropriate to an H-monopole. A similar (but more elaborate) example applies directly to S^3 and can be extracted from Ref. 57.

We will construct a $PU(\mathcal{H})$ bundle over $S^2\times S^1$ by starting with a $U(1)\times\mathbb{Z}$ bundle over $S^2\times S^1$ and then embedding the $U(1)\times\mathbb{Z}$ transition functions into $PU(\mathcal{H})$. The $U(1)\times\mathbb{Z}$ bundle over $S^2\times S^1$ will simply be $S^3\times\mathbb{R}$ with a rightaction by $U(1)\times\mathbb{Z}$ given by

$$\begin{aligned}(u,x)&\sim(ue^{i\chi\sigma^3/2},x),\\(u,x)&\sim(u,x+1).\end{aligned}\tag{8.2}$$

Here $u\in S^3$ is identified with an $SU(2)$ matrix, the first line is the right $U(1)$ action and the second line is the $\mathbb{Z}$ action on $x\in\mathbb{R}$. Note that the S^3 is not to be thought of as embedded in spacetime. Rather, $W=\mathbb{R}^5\times S^2\times S^1$.

We now consider the Heisenberg algebra generated by operators $\hat{\theta}$, and $\hat{N}$ acting on functions in $L^2(S^1)$. This S^1 should be thought of as the fiber in the Hopf fibration $S^3\to S^2$. Let $\hat{\theta}$ be the position operator and $\hat{N}$ the integrally-quantized angular momentum, so that $[\hat{\theta},\hat{N}]=i$. Using these operators we can form a representation of $U(1)\times\mathbb{Z}$ in $PU(\mathcal{H})$ via

$$(e^{i\chi},n)\to e^{in\hat{\theta}}e^{i\chi\hat{N}}.\tag{8.3}$$

Note that $e^{in\hat{\theta}}$ and $e^{i\hat{\chi}\hat{N}}$ commute up to the phase $e^{in\chi}$ and hence (8.3) is indeed a representation of the commutative group $U(1)\times\mathbb{Z}$ in $PU(\mathcal{H})$. Using (8.3) we convert the transition functions of the $U(1)\times\mathbb{Z}$ bundle $S^3\times\mathbb{R}\to S^2\times S^1$ into $PU(\mathcal{H})$ transition functions. Of course, we can (by construction) lift the transition functions to $U(\mathcal{H})$ over contractible open sets in a good cover of $S^2\times S^1$, but then they will fail to satisfy the cocycle condition.

We now discuss how to isolate the $u(1)$ part. Technically, this is defined in Ref. 58 by the splitting of an exact sequence of bundles of the adjoint representation. Here the relevant Lie algebra of operators is generated by the invariant elements $(\hat{N}-x\mathbf{1})$ and $\mathbf{1}$. Note that $\mathbb{Z}$, being discrete, has no Lie algebra. Therefore, we do not need to include $\hat{\theta}$. Note too that we are forced to choose the combination $(\hat{N}-x\mathbf{1})$ so that $x\sim x+1$ is equivalent to conjugation by $e^{i\hat{\theta}}$. We define ''the $u(1)$ part'' to be the coefficient of $\mathbf{1}$ in this basis.

As an example of a nontrivial $PU(\mathcal{H})$ connection we choose standard Euler angle coordinates (ϕ,θ,ψ) for $u\in S^3$ and x on $\mathbb{R}$. Then we may define the connection using the globally defined Lie algebra valued form on $S^3\times\mathbb{R}$ given by

$$A_+(u,x)=i(d\psi_+ + \tfrac{1}{2}(1-\cos\theta)d\phi)(\hat{N}-x\mathbf{1}),$$
$$A_-(u,x)=i(d\psi_- - \tfrac{1}{2}(1+\cos\theta)d\phi)(\hat{N}-x\mathbf{1}), \tag{8.4}$$

where we have divided S^3 into two hemispheres labeled by $\pm$. One may easily check that $A(u,x+1)=e^{i\hat{\theta}}A(u,x)e^{-i\hat{\theta}}$ so this defines a connection on a bundle over $S^2\times S^1$. According to our definition of the $U(1)$ part of F we have $\mathrm{Tr}(F)=-i\,\mathrm{Ad}\,x$. This is globally defined on $S^3\times S^1$ but is not basic. It is also not closed, as promised, but $K=d\,\mathrm{Tr}(F)\wedge dx=(i/2)\sin\theta\,d\theta\,d\phi\,dx$ is a basic form, giving the globally defined ''gerbe curvature 3-form'' on $S^2\times S^1$ with $\int_{S^2\times S^1}K/(2\pi i)=1$.

In view of the above, we believe that by allowing for twisted $PU(\mathcal{H})$ bundles in the formalism of Ref. 9 we are able to include the effects of NS 5-branes in the picture of Ref. 9. Indeed, if $A\to W$ is a twisted bundle with fiber given by $\mathcal{K}$ and Dixmier–Douady class h then $\Gamma(A)$ is an algebra whose (Grothendieck group of) finitely generated projective modules define $K_{\mathrm{H}}(W)$. In the limit of large noncommutativity the tachyon field still defines a projection operator, hence a projective module for this algebra. In the context of type II strings it is important to note that since $PU(\mathcal{H})$ also acts on Fredholm operators, there is also a Fredholm model for $K_{\mathrm{H}}(W)$.

Obviously, many details need to be worked out in the above proposal. We hope to report on this elsewhere.

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Non-Abelian D-branes and noncommutative geometry

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We discuss the non-Abelian world-volume action which governs the dynamics of N coincident Dp-branes. In this theory, the branes' transverse displacements are described by matrix-valued scalar fields, and so this is a natural physical framework for the appearance of noncommutative geometry. One example is the dielectric effect by which Dp-branes may be polarized into a noncommutative geometry by external fields. Another example is the appearance of noncommutative geometries in the description of intersecting D-branes of differing dimensions, such as D-strings ending on a D3- or D5-brane. We also describe the related physics of giant gravitons. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The idea that noncommutative geometry should play a role in physical theories is an old one.[1,2] Suggestions have been made that such noncommutative structure may resolve the ultraviolet divergences of quantum field theories, or appear in the description of space–time geometry at the Planck scale. In the past few years, it has also become a topic of increasing interest to string theorists. From one point of view, the essential step in realizing a noncommutative geometry is replacing the space–time coordinates by noncommuting operators, $x^\mu \to \hat{x}^\mu$. In this replacement, however, there remains a great deal of freedom in defining the nontrivial commutation relations which the operators $\hat{x}^\mu$ must satisfy. Some explicit choices that have appeared in physical problems are as follows:
(i) Canonical commutation relations:

$$[\hat{x}^\mu, \hat{x}^\nu] = i\theta^{\mu\nu} \quad \theta^{\mu\nu} \in \mathbf{C}.$$

Such algebras have appeared in the Matrix theory description of planar D-branes[3]—for a review, see Ref. 4. This work also stimulated an ongoing investigation by string theorists of noncommutative field theories which arise in the low energy limit of a planar D-brane with a constant B-field flux, see, e.g., Refs. 5 6, 7.
(ii) Quantum space relations:

$$\hat{x}^\mu \hat{x}^\nu = q^{-1} R^{\mu\nu}{}_{\rho\tau} \hat{x}^\rho \hat{x}^\tau \quad R^{\mu\nu}{}_{\rho\tau} \in \mathbf{C}.$$

These algebras received some attention from physicists in the early 1990's, see, e.g., Refs. 8 and 9— and have appeared more recently in the geometry of the moduli space of $N=4$ super-Yang–Mills theory.[10]
(iii) Lie algebra relations:

$$[\hat{x}^\mu, \hat{x}^\nu] = i f^{\mu\nu}{}_\rho \hat{x}^\rho \quad f^{\mu\nu}{}_\rho \in \mathbf{C}.$$

Such algebras naturally arise in the description of fuzzy spheres as was discovered in early attempts to quantize the supermembrane.[11,12] These noncommutative geometries have also been

applied in Matrix theory to describe spherical D-branes.[13,14] In string theory, these noncommutative descriptions of spheres also arise in various contexts in the physics of D-branes, as will be discussed below.

For a system of N (nearly) coincident D-branes, the transverse displacements are described by a set of scalar fields, which are matrix-valued in the adjoint representation of U(N). Hence, noncommutative geometries with a Lie-algebra structure appear very naturally in the physics of D-branes. The appearance of a non-Abelian U(N) gauge symmetry in the world-volume theory of N coincident D-branes[15] is, of course, one of the most remarkable aspects of the D-brane story.[16,17] It lies at the heart of such recent developments as the entropy counting of near-BPS black holes[18] and the AdS/CFT correspondence.[19] Progress has recently been made on constructing the world-volume action that controls the dynamics of this non-Abelian theory.[20,21] In particular, one finds that this action includes a wide variety of new nonderivative terms for the world-volume scalars. Amongst these interactions are couplings by which the non-Abelian D-branes can interact with all of the Ramond–Ramond potentials of any form degree. Further, there is an interesting ''dielectric effect'' [20] in which the D-branes are polarized into a higher dimensional noncommutative geometry by nontrivial background fields.

An outline of this paper is as follows: We begin in Sec. II with a discussion of the non-Abelian D-brane action. Section III presents an outline of the dielectric effect for D-branes. Section IV describes the related physical effect by which branes carrying momentum expand in $AdS_m \times S^n$ backgrounds, producing giant gravitons. Finally, Sec. V gives a discussion of how noncommutative geometries can arise in the description of intersecting branes. Sections II and III are essentially a summary of the material appearing in Ref. 20. Section IV describes that in Ref. 22 and Sec. V describes that for Refs. 23 and 24. We direct the interested reader to these papers for a more detailed presentation of the associated works.

II. NON-ABELIAN D-BRANE ACTION

Within the framework of perturbative string theory, a Dp-brane is a $(p+1)$-dimensional extended surface in space–time which supports the end points of open strings.[16,17] The massless modes of this open string theory form a supersymmetric U(1) gauge theory with a vector A_a, $9-p$ real scalars Φ^i and their superpartner fermions—for the most part, the latter are ignored throughout the following discussion. At leading order, the low-energy action corresponds to the dimensional reduction of that for ten-dimensional U(1) super-Yang–Mills theory. However, as usual in string theory, there are higher order $\alpha' = l_s^2$ corrections—l_s is the string length scale. For constant field strengths, these stringy corrections can be resummed to all orders, and the resulting action takes the Born–Infeld form,[25]

$$S_{\rm BI} = -T_p \int d^{p+1}\sigma (e^{-\phi}\sqrt{-\det(P[G+B]_{ab}+\lambda F_{ab})}), \tag{1}$$

where T_p is the Dp-brane tension and λ denotes the inverse of the (fundamental) string tension, i.e., $\lambda = 2\pi l_s^2$. This Born–Infeld action describes the couplings of the Dp-brane to the massless Neveu-Schwarz fields of the bulk closed string theory, i.e., the metric, dilaton and Kalb–Ramond two-form. The interactions with the massless Ramond–Ramond (RR) fields are incorporated in a second part of the action, the Wess–Zumino term,[26–28]

$$S_{\rm WZ} = \mu_p \int P\left[\sum C^{(n)} e^B\right] e^{\lambda F}, \tag{2}$$

where $C^{(n)}$ denotes the n-form RR potentials. Equation (2) shows that a Dp-brane is naturally charged under the $(p+1)$-form RR potential with charge μ_p, and supersymmetry dictates that $\mu_p = \pm T_p$. If the Dp-brane carries a flux of $B+F$, it will also act as a charge source for RR potentials with a lower form degree.[26] Such configurations represent bound states of D-branes of different dimensions.[15]

In both of the expressions above, the symbol $P[\cdots]$ denotes the pullback of the bulk space–time tensors to the D-brane world-volume. Thus the Born–Infeld action (1) has a geometric interpretation, i.e., it is essentially the proper volume swept out by the Dp-brane, which is indicative of the fact that D-branes are actually dynamical objects. This dynamics becomes more evident with an explanation of the static gauge choice implicit in constructing the above action. To begin, we employ space–time diffeomorphisms to position the world-volume on a fiducial surface defined as $x^i=0$ with $i=p+1,\ldots,9$. With world-volume diffeomorphisms, we then match the world-volume coordinates with the remaining spacetime coordinates on this surface, $\sigma^a=x^a$ with $a=0,1,\ldots,p$. Now the world-volume scalars Φ^i play the role of describing the transverse displacements of the D-brane, through the identification

$$x^i(\sigma)=2\pi l_s^2\Phi^i(\sigma) \quad \text{with } i=p+1,\ldots,9. \tag{3}$$

With this identification the general formula for the pullback reduces to

$$P[E]_{ab}=E_{\mu\nu}\frac{\partial x^\mu}{\partial\sigma^a}\frac{\partial x^\nu}{\partial\sigma^b}=E_{ab}+\lambda\, E_{ai}\,\partial_b\Phi^i+\lambda\, E_{ib}\,\partial_a\Phi^i+\lambda^2 E_{ij}\partial_a\Phi^i\partial_b\Phi^j. \tag{4}$$

In this way, the expected kinetic terms for the scalars emerge to leading order in an expansion of the Born–Infeld action (1). Note that our conventions are such that both the gauge fields and world-volume scalars have the dimensions of length^{-1}—hence the appearance of the string scale in Eq. (3).

As N parallel D-branes approach each other, the ground state modes of strings stretching between the different D-branes become massless. These extra massless states carry the appropriate charges to fill out representations under a U(N) symmetry. Hence the $U(1)^N$ of the individual D-branes is enhanced to the non-Abelian group U(N) for the coincident D-branes.[15] The vector A_a becomes a non-Abelian gauge field,

$$A_a=A_a^{(n)}T_n, \quad F_{ab}=\partial_aA_b-\partial_bA_a+i[A_a,A_b], \tag{5}$$

where T_n are N^2 Hermitian generators with $\mathrm{Tr}(T_n\,T_m)=N\,\delta_{nm}$. The scalars Φ^i also transform in the adjoint of U(N) with covariant derivatives,

$$D_a\Phi^i=\partial_a\Phi^i+i[A_a,\Phi^i]. \tag{6}$$

Understanding how to accommodate this U(N) gauge symmetry in the world-volume action is an interesting puzzle. For example, the geometric meaning or even the validity of Eq. (3) seems uncertain when the scalars on the right-hand side are matrix-valued. In fact, this identification does remain roughly correct. Some intuition comes from the case where the scalars are commuting matrices and the gauge symmetry can be used to simultaneously diagonalize all of them. In this case, one interpretes the N eigenvalues of the diagonal Φ^i as representing the displacements of the N constituent D-branes, see, e.g., Ref. 4. Of course, to describe noncommutative geometries, we will be more interested in the case where the scalars do not commute and so cannot be simultaneously diagonalized.

References 20 and 21 recently made progress in constructing the world-volume action describing the dynamics of non-Abelian D-branes. The essential strategy in both of these papers was to construct an action which was consistent with the familiar string theory symmetry of T-duality.[29] Acting on D-branes, T-duality acts to change the dimension of the world-volume.[16,17] The two possibilities are: (i) if a coordinate transverse to the Dp-brane, e.g., $y=x^{p+1}$, is T-dualized, it becomes a D($p+1$)-brane, where y is now the extra world-volume direction; and (ii) if a world-volume coordinate on the Dp-brane, e.g., $y=x^p$, is T-dualized, it becomes a D($p-1$)-brane where y is now an extra transverse direction. Under these transformations, the role of the corresponding world-volume fields change as

$$\text{(i)}\ \ \Phi^{p+1}\to A_{p+1}, \quad \text{(ii)}\ \ A_p\to\Phi^p, \tag{7}$$

while the remaining components of A and scalars Φ are left unchanged. Hence in constructing the non-Abelian action, one can begin with the D9-brane theory, which contains no scalars since the world-volume fills the entire space–time. In this case, the non-Abelian extension of Eqs. (1) and (2) is given by simply introducing an overall trace over gauge indices of the non-Abelian field strengths appearing in the action.[30] Then applying T-duality transformations on $9-p$ directions yields the non-Abelian action for a Dp-brane. Of course, in this construction, one also T-dualizes the background supergravity fields according to the known transformation rules.[29,31–33] As in the Abelian theory, the result for non-Abelian action has two distinct pieces:[20,21] the Born–Infeld term,

$$S_{\rm BI}=-T_p\int d^{p+1}\sigma\, S\,\mathrm{Tr}\Big(e^{-\phi}\sqrt{\det(Q^i{}_j)}\sqrt{-\det(P[E_{ab}+E_{ai}(Q^{-1}-\delta)^{ij}E_{jb}]+\lambda F_{ab})}\Big), \tag{8}$$

with $E_{\mu\nu}=G_{\mu\nu}+B_{\mu\nu}$ $Q^i{}_j\equiv\delta^i{}_j+i\lambda[\Phi^i,\Phi^k]\,E_{kj}$; and the Wess–Zumino term,

$$S_{\rm WZ}=\mu_p\int S\,\mathrm{Tr}\Big(P\Big[e^{i\lambda\, i_\Phi i_\Phi}\Big(\sum C^{(n)}\,e^B\Big)\Big]e^{\lambda F}\Big). \tag{9}$$

Let us enumerate the non-Abelian features of this action.

(1) *Non-Abelian field strength:* The F_{ab} appearing explicitly in both terms is now non-Abelian, of course.

(2) *Non-Abelian Taylor expansion:* The bulk supergravity fields are in general functions of all of the space–time coordinates, and so in the action (8), (9), they are implicitly functionals of the non-Abelian scalars. For example, the metric functional appearing in the D-brane action would be given by a non-Abelian Taylor expansion,

$$\begin{aligned}G_{\mu\nu}&=\exp[\lambda\Phi^i\,\partial_{x^i}]G^0_{\mu\nu}(\sigma^a,x^i)\big|_{x^i=0}\\&=\sum_{n=0}^{\infty}\frac{\lambda^n}{n!}\Phi^{i_1}\cdots\Phi^{i_n}(\partial_{x^{i_1}}\cdots\partial_{x^{i_n}})G^0_{\mu\nu}(\sigma^a,x^i)\big|_{x^i=0}.\end{aligned} \tag{10}$$

(3) *Non-Abelian pullback:* As was noted in Refs. 34 and 35, the pullback of various space–time tensors to the world-volume must now involve covariant derivatives of the non-Abelian scalars in order to be consistent with the U(N) gauge symmetry. Hence Eq. (4) is replaced by

$$P[E]_{ab}=E_{ab}+\lambda E_{ai}D_b\Phi^i+\lambda E_{ib}D_a\Phi^i+\lambda^2E_{ij}D_a\Phi^iD_b\Phi^j. \tag{11}$$

(4) *Non-Abelian interior product:* In the Wess–Zumino term (9), i_Φ denotes the interior product with Φ^i regarded as a vector in the transverse space, e.g., acting on an n-form $C^{(n)}=1/n!\,C^{(n)}_{\mu_1\cdots\mu_n}dx^{\mu_1}\cdots dx^{\mu_n}$, we have

$$i_\Phi i_\Phi C^{(n)}=\frac{1}{2(n-2)!}[\Phi^i,\Phi^j]\,C^{(n)}_{ji\mu_3\cdots\mu_n}dx^{\mu_3}\cdots dx^{\mu_n}. \tag{12}$$

Note that acting on forms, the interior product is an anticommuting operator and hence for an ordinary vector (i.e., a vector v^i with values in $\mathbb{R}^{9-p}$): $i_vi_vC^{(n)}=0$. It is only because the scalars Φ are matrix-valued that Eq. (12) yields a nontrivial result.

(5) *Non-Abelian gauge trace:* As is evident above, both parts of the action are highly nonlinear functionals of the non-Abelian fields, and so Eqs. (8) and (9) would be incomplete without a precise definition for the ordering of these fields under the gauge trace. Above, $S\,\mathrm{Tr}$ denotes a maximally symmetric trace. To be precise, the trace includes a symmetric average over all orderings of F_{ab}, $D_a\Phi^i$, $[\Phi^i,\Phi^j]$, and the individual Φ^k appearing in the non-Abelian Taylor expan-

sions of the background fields. This choice matches that inferred from Matrix theory.[36] Finally, we should note that with this definition an expansion of the Born–Infeld term (1) does agree with the string theory to fourth order in F,[37,38] however, it does not seem to capture the full physics of the non-Abelian fields in the infrared limit.[39] Rather at sixth order, additional terms involving commutators of field strengths must be added to the action.[40]

Some other general comments on the non-Abelian action are as follows: In the Born–Infeld term (8), there are now two determinant factors as compared to one in the Abelian action (1). The second determinant in Eq. (8) is a slightly modified version of that in Eq. (1). One might think of this as the kinetic factor, since to leading order in the low energy expansion, it yields the familiar kinetic terms for the gauge field and scalars. In the same way, one can think of the new first factor as the potential factor, since to leading order in the low energy expansion, it reproduces the non-Abelian scalar potential expected for the super-Yang–Mills theory (see below). Further note that the first factor reduces to simply one when the scalar fields are commuting, even for general background fields.

As mentioned below Eq. (2), an individual Dp-brane couples not only to the RR potential with form degree $n=p+1$, but also to the RR potentials with $n=p-1,p-3,\ldots$ through the exponentials of B and F appearing in the Wess–Zumino action (2). Above in Eq. (9), $i_\Phi i_\Phi$ is an operator of form degree -2, and so world-volume interactions appear in the non-Abelian action (9) involving the higher RR forms. Hence in the non-Abelian theory, a Dp-brane can also couple to the RR potentials with $n=p+3,p+5,\ldots$ through the additional commutator interactions. To make these couplings more explicit, consider the D0-brane action (for which F vanishes),

$$S_{\mathrm{CS}}=\mu_0\int S\,\mathrm{Tr}\Bigg(P\Bigg[C^{(1)}+i\lambda\, i_\Phi i_\Phi(C^{(3)}+C^{(1)}B)-\frac{\lambda^2}{2}(i_\Phi i_\Phi)^2 \times\left(C^{(5)}+C^{(3)}B+\frac{1}{2}C^{(1)}B^2\right)-i\frac{\lambda^3}{6}(i_\Phi i_\Phi)^3\left(C^{(7)}+C^{(5)}B+\frac{1}{2}C^{(3)}B^2+\frac{1}{6}C^{(1)}B^3\right) +\frac{\lambda^4}{24}(i_\Phi i_\Phi)^4\left(C^{(9)}+C^{(7)}B+\frac{1}{2}C^{(5)}B^2+\frac{1}{6}C^{(3)}B^3+\frac{1}{24}C^{(1)}B^4\right)\Bigg]\Bigg). \tag{13}$$

Of course, these interactions are reminiscent of those appearing in Matrix theory.[3,41] For example, Eq. (13) includes a linear coupling to $C^{(3)}$, which is the potential corresponding to D2-brane charge,

$$i\lambda\,\mu_0\int \mathrm{Tr}\,P[i_\Phi i_\Phi C^{(3)}]=i\frac{\lambda}{2}\mu_0\int dt\,\mathrm{Tr}(C^{(3)}_{ijk}(\Phi,t)\,[\Phi^k,\Phi^j]+\lambda C^{(3)}_{ijk}(\Phi,t)\,D_t\Phi^k\,[\Phi^k,\Phi^j]), \tag{14}$$

where we assume that $\sigma^0=t$ in static gauge. Note that the first term on the right-hand side has the form of a source for D2-brane charge. This is essentially the interaction central to the construction of D2-branes in matrix theory with the large N limit.[3,41] Here, however, with finite N, this term would vanish upon taking the trace if $C^{(3)}_{ijk}$ was simply a function of the world-volume coordinate t (since $[\Phi^k,\Phi^j]\in\mathrm{SU}(N)$). However, in general these three-form components are functionals of Φ^i. Hence, while there would be no ''monopole'' coupling to D2-brane charge, nontrivial expectation values of the scalars can give rise to couplings to an infinite series of higher ''multipole'' moments.

Finally we add that by the direct examination of string scattering amplitudes using the methods of Refs. 42 and 43, one can verify at low orders the form of the non-Abelian interactions in Eqs. (8) and (9), including the appearance of the new commutator interactions in the non-Alelian Wess–Zumino action.[44]

III. DIELECTRIC BRANES

In this section, we wish to consider certain physical effects arising from the new non-Abelian interactions in the world-volume action, given by Eqs. (8) and (9). To begin, consider the scalar potential for Dp-branes in flat space, i.e., $G_{\mu\nu}=\eta_{\mu\nu}$ with all other fields vanishing. In this case, the entire scalar potential originates in the Born–Infeld term (8) as

$$V=T_p\,\mathrm{Tr}\sqrt{\det(Q^i{}_j)}=NT_p-\frac{T_p\lambda^2}{4}\mathrm{Tr}([\Phi^i,\Phi^j][\Phi^i,\Phi^j])+\cdots. \tag{15}$$

The commutator-squared term corresponds to the potential for ten-dimensional U(N) super-Yang–Mills theory reduced to $p+1$ dimensions. A nontrivial set of extrema of this potential is given by taking the $9-p$ scalars as constant commuting matrices, i.e.,

$$[\Phi^i,\Phi^j]=0 \tag{16}$$

for all i and j. Since they are commuting, the Φ^i may be simultaneously diagonalized and as discussed above, the eigenvalues are interpreted as the separated positions of N fundamental Dp-branes in the transverse space. This solution reflects the fact that a system of N parallel Dp-branes is supersymmetric, and so they can sit in static equilibrium with arbitrary separations in the transverse space.[16,17]

From the results described in the previous section, it is clear that in going from flat space to general background fields, the scalar potential is modified by new interactions and so one should reconsider the analysis of the extrema. It turns out that this yields an interesting physical effect that is a precise analog for D-branes of the dielectric effect in ordinary electromagnetism. That is when Dp-branes are placed in a nontrivial background field for which the Dp-branes would normally be regarded as neutral, e.g., nontrivial $F^{(n)}$ with $n>p+2$, new terms will be induced in the scalar potential, and generically one should expect that there will be new extrema beyond those found in flat space, i.e., Eq. (16). In particular, there can be nontrivial extrema with noncommuting expectation values of the Φ^i, e.g., with $\mathrm{Tr}\,\Phi^i=0$ but $\mathrm{Tr}(\Phi^i)^2\neq 0$. This would correspond to the external fields ''polarizing'' the Dp-branes to expand into a (higher dimensional) noncommutative world-volume geometry. This is the analog of the familiar electromagnetic process where an external field may induce a separation of charges in neutral materials. In this case, the polarized material will then carry an electric dipole (and possibly higher multipoles). The latter is also seen in the D-brane analog. When the world-volume theory is at a noncommutative extremum, the gauge traces of products of scalars will be nonvanishing in various interactions involving the supergravity fields. Hence at such an extremum, the Dp-branes act as sources for the latter bulk fields.

To make these ideas explicit, we will now illustrate the process with a simple example. We consider N D0-branes in a constant background RR field $F^{(4)}$, i.e., the field strength associated with D2-brane charge. We find that the D0-branes expand into a noncommutative two-sphere which represents a spherical bound state of a D2-brane and N D0-branes.

Consider a background where only RR four-form field strength is nonvanishing with

$$F^{(4)}_{tijk}=-2\,f\varepsilon_{ijk}\quad \text{for } i,j,k\in\{1,2,3\} \tag{17}$$

with f a constant (of dimensions length^{-1}). Since $F^{(4)}=dC^{(3)}$, we must consider the coupling of the D0-branes to the RR three-form potential, which is given above in Eq. (14). If one explicitly introduces the non-Abelian Taylor expansion (10), one finds the leading order interaction may be written as

$$\frac{i}{3}\lambda^2\mu_0\int dt\,\mathrm{Tr}(\Phi^i\Phi^j\Phi^k)F^{(4)}_{tijk}(t). \tag{18}$$

This final form might have been anticipated since one should expect that the world-volume potential can only depend on gauge invariant expressions of the background field. Given that we are considering a constant background $F^{(4)}$, the higher order terms implicit in Eq. (14) will vanish as they can only involve space–time derivatives of the four-form field strength. Combining Eq. (18) with the leading order Born–Infeld potential (15) yields the scalar potential of interest for the present problem,

$$V(\Phi)=NT_0-\frac{\lambda^2 T_0}{4}\mathrm{Tr}([\Phi^i,\Phi^j]^2)-\frac{i}{3}\lambda^2\mu_0\,\mathrm{Tr}(\Phi^i\Phi^j\Phi^k)F^{(4)}_{tijk}(t). \tag{19}$$

Substituting in the background field (17) and $\mu_0=T_0$, $\delta V(\Phi)/\delta\Phi^i=0$ yields

$$0=[[\Phi^i,\Phi^j],\Phi^j]+i\,f\varepsilon_{ijk}[\Phi^j,\Phi^k]. \tag{20}$$

Note that commuting matrices (16) describing separated D0-branes still solve this equation. The value of the potential for these solutions is simply $V_0=NT_0$, the mass of N D0-branes. Another interesting solution of Eq. (20) is

$$\Phi^i=\frac{f}{2}\alpha^i, \tag{21}$$

where α^i are any $N\times N$ matrix representation of the SU(2) algebra,

$$[\alpha^i,\alpha^j]=2i\,\varepsilon_{ijk}\,\alpha^k. \tag{22}$$

For the moment, let us focus on the irreducible representation for which one finds

$$\mathrm{Tr}[(\alpha^i_N)^2]=\frac{N}{3}(N^2-1)\quad\text{for } i=1,2,3. \tag{23}$$

Now evaluating the value of the potential (19) for this new solution yields

$$V_N=NT_0-\frac{T_0\lambda^2 f^2}{6}\sum_{i=1}^{3}\mathrm{Tr}[(\Phi^i)^2]=NT_0-\frac{\pi^2 l_s^3 f^4}{6g}N^3\left(1-\frac{1}{N^2}\right) \tag{24}$$

using $T_0=1/(gl_s)$. Hence the noncommutative solution (21) has lower energy than a solution of commuting matrices, and so the latter configuration of separated D0-branes is unstable towards condensing out into this noncommutative solution. One can also consider reducible representations of the SU(2) algebra (22), however, one finds that the corresponding energy is always larger than that in Eq. (24). Hence it seems that the irreducible representation describes the ground state of the system.

Geometrically, one can recognize the SU(2) algebra as that corresponding to the noncommutative or fuzzy two-sphere.[12,45] The physical size of the fuzzy two-sphere is given by

$$R=\lambda\left(\sum_{i=1}^{3}\mathrm{Tr}[(\Phi^i)^2]/N\right)^{1/2}=\pi l_s^2 fN\left(1-\frac{1}{N^2}\right)^{1/2} \tag{25}$$

in the ground state solution. From the matrix theory construction of Kabat and Taylor,[14] one can infer this ground state is not simply a spherical arrangement of D0-branes rather the noncommutative solution actually represents a spherical D2-brane with N D0-branes bound to it. In the present context, the latter can be verified by seeing that this configuration has a ''dipole'' coupling to the RR four-form. The precise form of this coupling is calculated by substituting the noncommutative scalar solution (21) into the world-volume interaction (18), which yields

$$-\frac{R^3}{3\pi g l_s^3}\left(1-\frac{1}{N^2}\right)^{-1/2}\int dt\, F^{(4)}_{t123} \tag{26}$$

for the ground state solution. Physically this $F^{(4)}$-dipole moment arises because antipodal surface elements on the sphere have the opposite orientation and so form small pairs of separated membranes and antimembranes. Of course, the spherical configuration carries no net D2-brane charge.

Given that the noncommutative ground state solution corresponds to a bound state of a spherical D2-brane and N D0-branes, one might attempt to match the above results using the dual formulation. That is, this system can be analyzed from the point of view of the (Abelian) worldvolume theory of a D2-brane. In this case, one would consider a spherical D2-brane carrying a flux of the U(1) gauge field strength representing the N bound D0-branes, and at the same time, sitting in the background of the constant RR four-form field strength (17). In fact, one does find stable static solutions, but what is more surprising is how well the results match those calculated in the framework of the D0-branes. The results for the energy, radius and dipole coupling are the same as in Eqs. (24), (25), and (26), respectively, except that the factors of $(1-1/N^2)$ are absent.[20] Hence for large N, the two calculations agree up to $1/N^2$ corrections.

One expects that the D2-brane calculations would be valid when $R \gg l_s$ while naively the D0-brane calculations would be valid when $R \ll l_s$. Hence it appears there is no common domain where the two pictures can both produce reliable results. However, a more careful consideration of range of validity of the D0-brane calculations only requires that $R \ll \sqrt{N} l_s$. This estimate is found by requiring that the scalar field commutators appearing in the full non-Abelian potential (15) are small so that the Taylor expansion of the square root converges rapidly. Hence for large N, there is a large domain of overlap where both of the dual pictures are reliable. Note the density of D0-branes on the two-sphere is $N/(4\pi R^2)$. However, even if R is macroscopic it is still bounded by $R \ll \sqrt{N} l_s$ and so this density must be large compared to the string scale, i.e., the density is much larger than $1/l_s^2$. With such large densities, one can imagine the discreteness of the fuzzy sphere is essentially lost and so there is good agreement with the continuum sphere of the D2-brane picture.

Finally note that the Born–Infeld action contains couplings to the Neveu–Schwarz two-form which are similar to that in Eq. (18). From the expansion of $\sqrt{\det(Q)}$, one finds a cubic interaction,

$$\frac{i}{3}\lambda^2 T_0 \int dt\, \mathrm{Tr}(\Phi^i \Phi^j \Phi^k) H_{ijk}(t). \tag{27}$$

Hence the noncommutative ground state, which has $\mathrm{Tr}(\Phi^i \Phi^j \Phi^k) \neq 0$, also acts as a source of the B field with

$$-\frac{R_0^3}{3\pi g l_s^3}\left(1-\frac{1}{N^2}\right)\int dt\, H_{123}. \tag{28}$$

This coupling is perhaps not so surprising given that the noncommutative ground state represents the bound state of a spherical D2-brane and N D0-branes. Explicit supergravity solutions describing D2–D0 bound states with a planar geometry have been found,[46,47] and are known to carry a long-range H field with the same profile as the RR field strength $F^{(4)}$. One can also derive this coupling from the dual D2-brane formulation. Furthermore, we observe that the presence of this coupling (27) means that we would find an analogous dielectric effect if the N D0-branes were placed in a constant background H field.

The example considered above must be considered simply a toy calculation demonstrating the essential features of the dielectric effect for D-branes. A more complete calculation would require analyzing the D0-branes in a consistent supergravity background. For example, the present case could be extended to consider the asymptotic supergravity fields of a D2-brane, where the RR four-form would be slowly varying but the metric and dilaton fields would also be nontrivial. Alternatively, one can find solutions with a constant background $F^{(4)}$ in M-theory, namely the

$AdS_4\times S^7$ and $AdS_7\times S^4$ backgrounds, see, e.g., Ref. 48. In lifting the D0-branes to M-theory, they become gravitons carrying momentum in the internal space. Hence the expanded D2–D0 system considered here correspond to the ''giant gravitons'' of Ref. 49. The analog of the D2–D0 bound state in a constant background $F^{(4)}$ corresponds to M2-branes with internal momentum expanding into AdS_4,[22,50] while that in a constant H field corresponds to the M2-branes expanding on S^4.[49] Alternatively, the dielectric effect has been found to play a role in other string theory contexts, for example, in the resolution of certain singularities in the AdS/CFT correspondence,[51] or in describing D-branes in the space–time background corresponding to a WZW model.[52,53] Further, one can consider more sophisticated background field configurations which through the dielectric effect generate more complicated noncommutative geometries.[54]

IV. GIANT GRAVITONS

From the above discussion, it seems that in the M-theory backgrounds of $AdS_4\times S^7$ or $AdS_7\times S^4$, one will find that an M2-brane carrying internal momentum will expand into a stable spherical configuration. While a matrix theory description of such states in terms of noncommutative geometry is not yet possible, one can instead analyze these configurations in terms of the Abelian world-volume theory of the M2-brane. In fact, the spherical M2-branes expanding into AdS_4 were actually discovered some time ago.[55] It turns out that M5-branes will expand in a similar way for these backgrounds, and further that expanded D3-branes arise in the type IIB supergravity background $AdS_5\times S^5$. A detailed analysis[22,49,50] shows that these expanded branes are BPS states with the quantum numbers of a graviton. In the following, we will discuss the details of the effect for the D3-branes. Most of the discussion applies equally well for the analogous M2- and M5-brane configurations.

The line element for $AdS_5\times S^5$ may be written as

$$ds^2=-\left(1+\frac{r^2}{L^2}\right)dt^2+\frac{dr^2}{1+\frac{r^2}{L^2}}+r^2d\Omega_3^2+L^2(d\theta^2+\cos^2\theta d\phi^2+\sin^2\theta d\tilde{\Omega}_3^2). \tag{29}$$

This background also involves a self-dual RR five-form field strength with terms proportional to the volume forms on the two five-dimensional subspaces, $F^{(5)}=(4/L)[\varepsilon(AdS_5)+\varepsilon(S^5)]$. With the coordinates chosen above, the four-form potential on the the AdS part of the space is

$$C^{(4)}_{\text{electric}}=-\frac{r^4}{L}dt\,\varepsilon(S^3), \tag{30}$$

where $\varepsilon(S^3)$ is the volume form for the three-sphere described by $d\Omega_3^2$. Similarly, the potential on the S^5 is

$$C^{(4)}_{\text{magnetic}}=L^4\sin^4\theta\,d\theta\,d\phi\,\varepsilon(\tilde{S}^3), \tag{31}$$

where $\varepsilon(\tilde{S}^3)$ is the volume form on $d\tilde{\Omega}_3^2$. For the D3-brane configurations of interest, the world-volume action in Eqs. (1) and (2) reduces to

$$S_3=-T_3\int d^4\sigma\sqrt{-\det(P[G])}+T_3\int P[C^{(4)}]. \tag{32}$$

Here, the world-volume gauge field has been set to zero, which will be consistent with the full equations of motion.

Following Ref. 49, one can find solutions where a D3-brane has expanded on the S^5 to a sphere of fixed θ while it orbits the S^5 in the ϕ direction. Our static gauge choice matches the spatial world-volume coordinates with the angular coordinates on $d\tilde{\Omega}_3^2$, and identifies $\sigma^0=t$. Now

we consider a trial solution of the form: $\theta=$constant, $r=0$ and $\phi=\phi(t)$. Substituting this ansatz into the world-volume action (32) and integrating over the angular coordinates, yields the following Lagrangian:

$$\mathcal{L}_3=\frac{N}{L}[-\sin^3\theta\sqrt{1-L^2\cos^2\theta\,\dot{\phi}^2}+L\sin^4\theta\,\dot{\phi}]. \tag{33}$$

Here we have introduced the (large positive) integer N which counts the five-form flux on S^5. This is also, of course, the rank of the U(N) gauge group in the dual super-Yang–Mills theory. Introducing the conjugate angular momentum $P_\phi=\delta\mathcal{L}_3/\delta\dot{\phi}$, we construct the Hamiltonian,

$$\mathcal{H}_3=P_\phi\dot{\phi}-\mathcal{L}_3=\frac{N}{L}\sqrt{p^2+\tan^2\theta\,(p-\sin^2\theta)^2}, \tag{34}$$

where $p=P_\phi/N$. Given that the Hamiltonian is independent of ϕ, the equations of motion will be solved with constant angular momentum (and hence constant $\dot{\phi}$). For fixed p, Eq. (34) can be regarded as the potential that determines the angle θ for equilibrium. Examining $\mathcal{H}_3$ in detail reveals degenerate minima at $\sin\theta=0$ and $\sin^2\theta=p$, and at any of these minima, the energy is $\mathcal{H}_3=P_\phi/L$. The expanded configurations are then the giant gravitons of Ref. 49. An important observation is that the minima at $\sin^2\theta=p$ only exist for $p\leqslant 1$. As p grows beyond $p=1$, the minima at $\theta\neq 0$ are lifted above that at $\sin\theta=0$ and then disappear completely if $p>9/8$.

The discussion above indicates that one can also consider the possibility of a brane expanding into the AdS part of the space–time.[22,50] That is we wish to find solutions where a D3-brane has expanded to a sphere of constant r while it still orbits in the ϕ direction on the S^5. Choosing static gauge, we again identify $\sigma^0=t$ but match the remaining world-volume coordinates with the angular coordinates on $d\Omega_3^2$. The trial solution is now $\theta=0$, $r=$constant, and $\phi=\phi(t)$. Beginning with the same world-volume action (32),[56] one calculates as before and arrives at the following Hamiltonian:

$$\mathcal{H}_3=\frac{N}{L}\left[\sqrt{\left(1+\frac{r^2}{L^2}\right)\left(p^2+\frac{r^6}{L^6}\right)}-\frac{r^4}{L^4}\right], \tag{35}$$

where as before $p=P_\phi/N$. Examining $\partial\mathcal{H}_3/\partial r=0$, one finds minima located at $r=0$ and $(r/L)^2=p$. The energy at each of the minima is $\mathcal{H}_3=P_\phi/L$. In Ref. 22, these expanded configurations were denoted as dual giant gravitons. An essential difference from the previous case, however, is that the minima corresponding to expanded branes persist for arbitrarily large p.

It is interesting to consider the motion of these expanded brane configurations. Evaluating $\dot{\phi}$ for any of the above solutions, remarkably one finds the same result: $\dot{\phi}=1/L$, independent of P_ϕ. Further the center of mass motion for any of the equilibrium configurations in the full ten-dimensional background is along a null trajectory. For example, for the D3-branes expanded on S^5,

$$ds^2=-(1-L^2\cos^2\theta\,\dot{\phi}^2)dt^2=0 \tag{36}$$

when evaluated for $\dot{\phi}=1/L$ and $\theta=0$(=the center of mass position). This is, of course, the expected result for a massless ''pointlike'' graviton, but it applies equally well for both of the expanded brane configurations. However, note that in the expanded configurations, the motion of each element of the sphere is along a timelike trajectory.

From the point of view of five-dimensional supergravity in the AdS space, the stable brane configurations correspond to massive states with $M=P_\phi/L$. Their angular momentum means that these states are also charged under a U(1) subgroup of the SO(6) gauge symmetry in the reduced supergravity theory. With the appropriate normalizations, the charge is $Q=P_\phi/L$, and hence one

finds that these configurations satisfy the appropriate BPS bound.[49] One can therefore anticipate that all of these configurations should be supersymmetric. The latter result has been verified by an explicit analysis of the residual supersymmetries.[22,50]

The $AdS_5 \times S^5$ background is a maximally supersymmetric solution of the type IIB supergravity equations with 32 residual supersymmetries. That is the background fields are invariant under supersymmetries parametrized by 32 independent Killing spinors. These Killing spinors are determined by setting

$$\delta\Psi_M = D_M \epsilon - \frac{i}{480} \Gamma_M^{PQRST} F^{(5)}_{PQRST} \epsilon = 0 \tag{37}$$

as the variations of all of the other type IIB supergravity fields vanish automatically. The solutions take the form $\epsilon = M(x^\mu)\epsilon_0$, where ϵ_0 is an arbitrary constant complex Weyl spinor.

A supersymmetric extension of the Abelian world-volume action has been constructed for D3-branes (and all other Dp-branes) in a General supergravity background.[57,58] This action can be viewed as a four-dimensional nonlinear sigma model with a curved superspace as the target space. Hence the theory is naturally invariant under the target-space supersymmetry. Further however, formulating the action with manifest ten-dimensional Lorentz invariance, requires an additional fermionic invariance on the world-volume called κ-symmetry. For a test brane configuration where both the target space and world-volume fermions vanish, residual supersymmetries may arise provided there are Killing spinors which satisfy a combined target-space supersymmetry and κ-symmetry transformation. The latter amounts to imposing a constraint $\Gamma\epsilon = \epsilon$, where

$$\Gamma = -\frac{i}{4!} \varepsilon^{i_1 \cdots i_4} \partial_{i_1} X^{M_1} \cdots \partial_{i_4} X^{M_4} \Gamma_{M_1 \cdots M_4}. \tag{38}$$

Of course, this constraint is only evaluated on the D3-brane world-volume. For all of the minima of the potentials in both Eqs. (34) or (35), this constraint reduces to imposing the same projection

$$(\Gamma^{t\phi} + 1)\epsilon_0 = 0. \tag{39}$$

Hence not only are the expanded branes and the pointlike states all BPS configurations, all of these configurations preserve precisely the same supersymmetries. Note that this projection is what one might have expected for a massless particle moving along the ϕ direction, e.g., one can compare to the supersymmetries gravitational waves propagating in flat space.[59]

Much of the interest in giant gravitons comes from an intriguing suggestion[49] that they may be related to the ''stringy exclusion principle.''[60–63] The latter arises in the AdS/CFT correspondence,[19] where it is easily understood in the conformal field theory. A family of chiral primary operators in the $N=4$ super-Yang–Mills theory terminates at some maximum weight because the U(N) gauge group has a finite rank. In terms of the dual AdS description, these operators are associated with single particle states carrying angular momentum on the internal five-sphere. So the appearance of an upper bound on the angular momentum seems mysterious from the point of view of the supergravity theory. The suggestion of McGreevy, Susskind, and Toumbas[49] is that if the dual single particle states are identified with the giant gravitons, the D3-branes expanded on the S^5, then the upper bound is produced by the fact that these BPS states only exist for $p \leqslant 1$. In fact, this exactly reproduces the desired upper bound on the angular momentum: $P_\phi \leqslant N$.

Unfortunately this interpretation is not entirely clear because rather than a unique candidate for the graviton state, there are *three* different ones, including the giant gravitons which expand on S^5, the dual giant gravitons which expand on AdS_5, and the pointlike states. All of these configurations have the same angular momentum and energy, and preserve precisely the same supersymmetries. Unfortunately the latter two of the candidates display no upper bound on the angular momentum, and so there is some uncertainty about the proposed mechanism for the stringy exclusion principle.

One tentative suggestion[22] is that the exclusion principle may be realized through the quantum mechanical mixing of these different states. One can find instanton configurations describing tunneling between the pointlike states and either of the expanded branes,[22,50] but not between the two expanded D3-brane solutions.[64] The suggestion is then that this mixing may spontaneously break supersymmetry in the regime $P_\phi > N$ where there are only two potential graviton states.

Reference 50 has done some interesting calculations in the context of the dual CFT. They seem to be able to identify certain classical field configurations with same properties as the dual giant gravitons. Further these calculations seem to indicate that the minimum corresponding to the pointlike graviton is lifted due to strong coupling effects. This then suggests a picture where the D3-branes expanded on AdS_5 are dual to coherent states in the $N=4$ super-Yang–Mills theory, and so do not directly correspond to the chiral primary operators considered in the stringy exclusion principle.

V. INTERSECTING BRANES

One interesting aspect of the (Abelian) Born–Infeld action (1) is that it supports solitonic configurations describing lower-dimensional branes protruding from the original D-brane.[65–67] For example, in the case of a D3-brane, one finds spike solutions, known as ''bions,'' corresponding to fundamental strings and/or D-strings extending out of the D3-brane. In these configurations, both the world-volume gauge fields and transverse scalar fields are excited. The gauge field corresponds to that of a point charge arising from the end point of the attached string, i.e., an electric charge for a fundamental string and a magnetic monopole charge for a D-string. The scalar field describes the deformation of the D3-brane geometry caused by attaching the strings. These solutions seem to have a surprisingly wide range of validity, even near the core of the spike where the fields are no longer slowly varying. In fact, one can show that the electric spike corresponding to a fundamental string is a solution of the full string theory equations of motion.[68] Further the dynamics of these solutions, as probed through small fluctuations, agrees with the expected string behavior.[69–72] In part, these remarkable agreements are probably related to the fact that these are supersymmetric configurations.

For the system of N D-strings ending on a D3-brane, there is also a dual description in terms of the non-Abelian world-volume theory of the N D-strings. There one finds solutions which have an interpretation, in terms of noncommutative geometry, as describing the D-strings expanding out in a funnel to become an orthogonal D3-brane. In fact, there is an extensive discussion of this system in the literature—see, e.g., Refs. 73–80—where the emphasis was on the close connection[73] of the D-string equations to the Nahm equations for BPS monopoles.[81] In Ref. 23, our emphasis was on the interpretation of these solutions in terms of noncommutative geometry and the remarkable agreement that one finds with the D3-brane spikes in the large N limit.

For N D-strings in flat space, the dynamics is determined completely by the Born–Infeld action (8) which reduces to[20,38]

$$S = -T_1 \int d^2\sigma\, S\, \mathrm{Tr}\sqrt{-\det(\eta_{ab} + \lambda^2 \partial_a \Phi^i Q^{-1}_{ij} \partial_b \Phi^j)\, \det(Q^{ij})}, \tag{40}$$

where

$$Q^{ij} = \delta^{ij} + i\lambda[\Phi^i, \Phi^j]. \tag{41}$$

Implicitly here, the world-volume gauge field has been set to zero, which will be a consistent truncation for the configurations considered below. With the usual choice of static gauge, we set the world-volume coordinates, $\tau = t = x^0$ and $\sigma = x^9$. For simplicity, one might consider the leading-order (in λ) equations of motion coming from this action,

$$\partial^a \partial_a \Phi^i = [\Phi^j, [\Phi^j, \Phi^i]]. \tag{42}$$

Of course, a simple solution of these equations are constant commuting matrices, as in Eq. (16). As discussed in the previous section, such a solution describes N separated parallel D-strings sitting in static equilibrium.

To find a dual description of the bion solutions of the D3-brane theory,[65,66] one needs a static solution which represents the D-strings expanding into a D3-brane. The corresponding geometry would be a long funnel where the cross section at fixed σ has the topology of a two-sphere. In this context, the latter cross section naturally arises as a fuzzy two-sphere[12,45] if the scalars have values in an $N\times N$ matrix representation of the SU(2) algebra (22). Hence one is lead to consider the ansatz,

$$\Phi^i=\frac{R(\sigma)}{\lambda\sqrt{N^2-1}}\alpha^i,\quad i=1,2,3, \tag{43}$$

where we will focus on case where the α^i are the irreducible $N\times N$ SU(2) matrices. Then with the normalization in Eq. (43), the function $|R(\sigma)|$ corresponds precisely to the radius of the fuzzy two-sphere,

$$R(\sigma)^2=\frac{\lambda^2}{N}\sum_{i=1}^{3}\mathrm{Tr}[\Phi^i(\sigma)^2]. \tag{44}$$

Substituting the ansatz (43) into the matrix equations of motion (42) yields a single scalar equation,

$$R''(\sigma)=\frac{8}{\lambda^2(N^2-1)}R(\sigma)^3, \tag{45}$$

for which one simple class of solutions is

$$R(\sigma)=\pm\frac{N\pi l_s^2}{\sigma-\sigma_\infty}\left(1-\frac{1}{N^2}\right)^{1/2}. \tag{46}$$

Given the above analysis, Eqs. (43) and (46) only represent a solution of the leading order equations of motion (42), and so naively one expects that it should only be valid for small radius. However, one can show by direct evaluation[23] that in fact these configurations solve the full equations of motion extremizing the non-Abelian action (40). The latter can also be inferred from an analysis of the world-volume supersymmetry of these configurations. Killing spinor solutions of the linearized supersymmetry conditions will exist provided that the scalars satisfy

$$D_\sigma\Phi^i=\pm\frac{i}{2}\varepsilon^{ijk}[\Phi^j,\Phi^k]. \tag{47}$$

The latter can be recognized as the Nahm equations.[73] Hence the duality between the D3-brane and D-string descriptions gives a physical realization of Nahm's transform of the moduli space of BPS magnetic monopoles. Now inserting the ansatz (43) into Eq. (47) yields

$$R'=\mp\frac{2}{\lambda\sqrt{N^2-1}}R^2, \tag{48}$$

which one easily verifies is satisfied by the configuration given in Eq. (46). Hence, one concludes that the solutions given by Eqs. (43) and (46) are in fact BPS solutions preserving 1/2 of the supersymmetry of the leading order D-string theory. Now in Ref. 82, it was shown that BPS solutions of the leading order theory are also BPS solutions of the full non-Abelian Born–Infeld action (40).

The geometry of the solution, Eqs. (43) and (46), certainly has the desired funnel shape. The fuzzy two-sphere shrinks to zero size as $\sigma \to \infty$ and opens up to fill the $x^{1,2,3}$ hypersurface at $\sigma = \sigma_\infty$. By examining the non-Abelian Wess–Zumino action (9), one can show that the noncommutative solution induces a coupling to the RR four-form potential $C^{(4)}_{t123}$. This calculation confirms then that, with the minus (plus) sign in Eq. (46), the D-strings expand into a(n anti-)D3-brane which fills the $x^{1,2,3}$ directions.[23] Given that the funnel solution of the D-string theory and the bion spike of the D3-brane theory are both BPS, one might expect that there will be a good agreement between these two dual descriptions. The formula for the height of D3-brane spike above the $x^{1,2,3}$ hyperplane is[65]

$$\sigma - \sigma_\infty = \frac{N \pi l_s^2}{R}. \tag{49}$$

Compared to Eq. (46), one finds that for large N the two descriptions are describing the same geometry up to $1/N^2$ corrections. One finds similar quantitative agreement for large N in calculating the energy, the RR couplings and the low energy dynamics in the two dual descriptions.[23] As in the discussion of the dielectric effect, one can argue that the D3-brane description is valid for $R \gg l_s$ while the D-string description is reliable for $R \ll \sqrt{N} l_s$.[23] Hence one can understand the good agreement between these dual approaches for large N since there is a large domain of overlap where both are reliable.

Note that in the configurations considered in this section, there are no nontrivial supergravity fields in the ambient space–time. Hence the appearance of the noncommutative geometry in these solutions is quite distinct from that in the dielectric effect, where the external fields drive the D-branes into a certain geometry in the ground state. In the funnel solutions, the noncommutative geometry was put into the ansatz (43) by hand. An interesting extension of these solutions is then to replace the SU(2) generators by those corresponding to some other noncommutative geometry, i.e., to replace Eq. (43) by

$$\Phi^i = \frac{R(\sigma)}{\lambda \sqrt{C}} G^i, \tag{50}$$

where the G^i are new $N \times N$ constant matrices satisfying $\mathrm{Tr} \Sigma (G^i)^2 = N C$. An interesting feature of such a construction is that near the core of the funnel, the leading order equations of motion will still be those given in Eq. (42). Thus for Eq. (50) to provide a solution, the new generators must satisfy $[G^j,[G^j,G^i]] = 2a^2 G^i$ for some constant a, and then the radius is determined by

$$R'' = \frac{2a^2}{\lambda^2 C} R^3, \tag{51}$$

which still has essentially the same form as Eq. (45) above. Further the funnel solution of this equation also has essentially the same form as Eq. (46) above, i.e.,

$$R = \pm \frac{\lambda \sqrt{C}}{a(\sigma - \sigma_\infty)}. \tag{52}$$

Hence the profile with $R \simeq \lambda/\sigma$ is universal for all funnels on the D-string, independent of the details of the noncommutative geometry that describes the cross-section of the funnel.

This universal behavior is curious. For example, one could consider using this framework to describe a D-string ending on an orthogonal Dp-brane with $p > 3$. However, from the dual Dp-brane formulation, one expects that for large R, solutions will essentially be harmonic functions behaving like $\sigma \propto R^{-(p-2)}$ or $R \propto \sigma^{-1/(p-2)}$. The resolution of this puzzle seems to be that the

two profiles apply in distinct regimes, the first for small R and the second for large R. Hence it must be that the nonlinearity of the full Born–Infeld action will generate solutions which display a transition from one kind of behavior to another.

One particular example that we have examined in detail[24] is the case where G^i in Eq. (50) are chosen to be generators describing a fuzzy four-sphere—these may be found in, e.g., Ref. 14. In this case, the funnel describes the D-strings expanding into a D5-brane. One does find the expected transition in the behavior of the geometry. That is, $\sigma \approx N^{2/3} l_s / R$ for small R in accord with Eq. (52), while at large R, higher order terms in the Born–Infeld action (40) become important yielding $\sigma \approx N^{2/3} l_s^4 / R^3$. The same kind of behavior is also found for the corresponding solutions in the dual D5-brane world-volume theory, although of course in that case the nonlinearities of the Born–Infeld action become important for small R. An interesting feature of the D5-brane spike is that it is also non-Abelian in character. Charge conservation arguments indicate that the D-string acts as a source of the second Chern class in the world-volume of the D5-brane.[83] More precisely, if N D-strings end on a D5-brane, then

$$\frac{1}{8\pi^2} \int_{S^4} \mathrm{Tr}(F \wedge F) = N, \tag{53}$$

for any four-sphere surrounding the D-string end point. Hence both of the dual descriptions have a noncommutative character. Again, we find that the dual constructions seem to agree at large N, however, the details of the solutions are more complex. In part, the latter must be due to the fact that the D5$\perp$D1 system is not supersymmetric.

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Superstrings and topological strings at large *N*

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We embed the large N Chern–Simons/topological string duality in ordinary superstrings. This corresponds to a large N duality between generalized gauge systems with $N=1$ supersymmetry in four dimensions and superstrings propagating on noncompact Calabi–Yau manifolds with certain fluxes turned on. We also show that in a particular limit of the $N=1$ gauge theory system, certain superpotential terms in the $N=1$ system (including deformations if spacetime is noncommutative) are captured to all orders in $1/N$ by the amplitudes of noncritical bosonic strings propagating on a circle with self-dual radius. We also consider D-brane/anti-D-brane system wrapped over vanishing cycles of compact Calabi–Yau manifolds and argue that at large N they induce a shift in the background to a topologically distinct Calabi–Yau, which we identify as the ground state system of the brane/anti-brane system. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The idea that large N gauge theories should have a phase described by perturbative strings, set forth by 't Hooft,[1] has been beautifully realized by various examples. The first example of this kind was found by Kontsevich,[2] which relates the bosonic string theory coupled to certain matter [(1, 2) minimal model, which is equivalent to pure topological gravity formulated by Witten[3]], to a matrix integral with cubic interaction (which can be viewed as a particular gauge theory in zero dimensions). (This is not the same as the old matrix model which discretizes the worldsheet—rather it is the target space description exactly in line with 't Hooft's conjecture.) Many more examples were also found in the context of noncritical bosonic strings. For example, it was found[4] that bosonic strings propagating on a circle with self-dual radius is equivalent to Penner matrix model.[5]

More recently it was recognized that 't Hooft's conjecture is also realized even for much more complicated and physically more interesting gauge theories.[6–8] In particular certain gauge theories at large N are equivalent to superstrings propagating on AdS backgrounds. Another example of a string/large N duality was discovered in Ref. 9, where it was shown that large N limit of Chern–Simons gauge theory on S^3 is equivalent to topological strings on a noncompact Calabi–Yau threefold which is a blow up of the conifold [given by $O(-1)+O(-1)$ bundle over $\mathbf{P}^1$]. This duality was tested to all orders in the $1/N$ expansion including checks at the level of Wilson loop observables of the Chern–Simons theory.[10,11] It is also known[12] that in some limit (large N, fixed Chern–Simons coupling k) this theory has the same partition function as bosonic strings at the self-dual radius.

This paper was motivated by trying to connect the duality discovered in Ref. 9 with the dualities discovered in the context of AdS/CFT correspondences. The basic idea is to consider type IIA superstring propagating in the conifold background (which is symplectically the same as T^*S^3) in the presence of N D6 branes wrapped around S^3 and filling the spacetime. It has been known[13] that the topological string amplitudes for the internal theory on the noncompact Calabi–Yau compute superpotential terms on the left-over R^4 world volume of the D6 brane. On the other hand, it is also known that the internal topological string theory with N D-branes wrapped on S^3 is equivalent to Chern–Simons gauge theory on S^3.[14] Thus the duality found in Ref. 9 suggests that type IIA string on the conifold with N D6 branes is equivalent to the blown up version of the

conifold with no branes left over. At first sight this seems strange, because having no D-branes left would naively suggest a theory with $N=2$ supersymmetry rather than $N=1$. Moreover Ramond fluxes should also be turned on in the blown up geometry corresponding to the flux generated by the D6 brane. The main question was why in the dual topological string theory discovered in Ref. 9 there is no mention of RR fluxes? Indeed it is an ordinary topological string (the A model) on the blown up conifold.

The resolution turns out to be that turning on the RR flux does not affect the topological string amplitudes, and the dual string theory *does* involve RR fluxes. Turning on RR flux, however, does generate an $N=1$ superpotential term,[15,16] which can be computed in terms of the topological string amplitudes. Thus the duality found in Ref. 9 can be viewed as an all order check in the $1/N$ expansion for the $N=1$ superpotential computations in the context of this type IIA superstring/gauge theory duality. One can also consider the mirror symmetry acting on all these statements, which as noted in Ref. 9 give rise to similar dualities. In the superstring realization, the mirror case (in a certain limit) would correspond to considering type IIB string on the blow up of the conifold with N D5 branes wrapped on $\mathbf{P}^1$ and we end up with type IIB on deformed conifold geometry T^*S^3 but with RR flux turned on.

One can also consider wrapped D-brane in the context of compact Calabi–Yau manifolds. However, in this case we also need to put anti-D-branes, in order to have no net D-branes. In this case we conjecture that the large N limit will correspond to having a new Calabi–Yau with fluxes, which can decay as discussed in Ref. 17 to a theory with no fluxes left over and with supersymmetry increased to $N=2$. The effect of the non-BPS states has been to shift the background to a new background. This is a novel way of deforming backgrounds, and as we will suggest later in the paper may have many interesting extensions.

The organization of this paper is as follows: In Sec. II we review aspects of topological string amplitudes and what they compute in the corresponding superstring theory. In Sec. III we revisit the duality of Ref. 9 and embed it in the context of type IIA superstrings. In Sec. IV we apply mirror symmetry to the statements in Sec. III and discuss the equivalent type IIB superstring theory. In Sec. V we discuss possible applications of $c=1$ noncritical bosonic strings to the question of generation of superpotential in the large N limit of $N=1$ supersymmetric gauge theory. In Sec. VI we discuss wrapped brane/anti-brane systems in the context of compact Calabi–Yau manifolds and use the above duality to make new predictions about the shift in the background. In Sec. VII we discuss some generalizations of this work.

While preparing this paper, three papers appeared which have overlaps with different aspects of our work. In particular, Refs. 18 and 19 have some overlap with our work in the context of large N duals of $N=1$ gauge theories in the context of type IIB strings, which we will briefly comment on in Sec. IV. Also the same configuration of wrapped D-branes/anti-D-branes considered in Sec. VI was also studied in Ref. 20 in a different context.

II. TOPOLOGICAL STRINGS AND SUPERSTRINGS

In this section we discuss aspects of topological strings and their relevance for superpotential computations in the corresponding superstring compactifications. We will divide our discussion to two parts: Closed string case (i.e., without D-branes) and open string case (i.e., including D-branes). We also point out the relevance of topological string amplitudes for $N=1$ superpotential computations when RR-fluxes are turned on.

A. Closed topological string and superstring amplitudes in 4D

Consider A model topological strings on a Calabi–Yau manifold K (similar remarks apply to the mirror B model). For simplicity of notation let us assume that the CY manifold has only one Kahler class, parametrized by the complexified Kahler parameter t. Then closed topological string amplitude on K is given by

$$F(t,\lambda_s)=\sum_g \lambda_s^{2g-2}F_g, \tag{2.1}$$

$$F_g = \sum_d F_{d,g} e^{-dt},$$

where, roughly speaking $F_{d,g}$ denote the ''numbers'' (Gromov–Witten invariants) of genus g curves in class d. The topological strings compute certain amplitudes in the corresponding type IIA superstring compactifications on the Calabi–Yau.[13,21,22] In particular they compute terms in the action of the form

$$\int d^4\theta \mathcal{W}^{2g} F_g(t) = g R^2 F^{2g-2} F_g(t) + \cdots,$$

where $\mathcal{W}_{\alpha\beta}$ denotes the graviphoton field strength multiplet, R^2 and F^{2g-2} denote certain contractions of the self-dual part of the Riemann tensor and of the gravi-photon field strength, and t denotes the vector superfield with the vev of the lowest component being the Kahler parameter t. One way to derive this formula is to note that with $2g-2$ insertions of the spin operator, needed to compute the amplitude involving the F^{2g-2}, the ordinary sigma model is topologically twisted. At genus 0 what one gets is

$$\int d^4\theta F_0(t) = \partial^2 F_0(t) F^t \wedge F^t + \cdots,$$

where F^t denotes the (self-dual part of the) U(1) field strength in the same multiplet as t. In the type IIA this arises from the 4-form field strength G by setting it to

$$G = F^t \wedge \omega_t,$$

where ω_t denotes the Kahler form associated to t.

It is natural to ask what changes in the closed topological string computations when we turn on some RR flux in the target space. The choices are the 2-form field strength in the internal space F, 4-form field strength G_{int} along the internal CY directions and the G along the spacetime directions G_4, which we equivalently study in terms of the dual 6-form field strength $G_6 = *G_4$. (We can also include the 0-form field strength dual to 10-form field strength in type IIA, but since we will not deal with it in this paper we will not discuss it. It will give rise to an $N=1$ superpotential of the form $\int G_0 \wedge k^3$.) It turns out that the topological string amplitudes in the presence of RR fields is not modified at all. This is particularly simple to show in the Berkovits formalism.[22–24] Instead of demonstrating it in this way we follow a related idea, which we will need later in this paper, by studying the generation of $N=1$ superpotential terms in the presence of RR fluxes, which we will discuss next.

B. Generation of superpotential due to internal field strength

RR fluxes have been studied in the context of CY compactifications.[25,26,15,16] In particular it has been shown in Refs. 15 and 16 that turning on internal field strength in the CY leads to generation of superpotential terms in 4D $N=1$ theory (see also similar situations considered in Refs. 27 and 28). In the context of type IIA theory with RR fluxes corresponding to F and G_{int} and G_6 discussed above, the superpotential is given by

$$\lambda_s W = \int F \wedge k \wedge k + i \int G \wedge k + \int G_6, \tag{2.2}$$

where k is the complexified Kahler class. To see this one considers the BPS charge in the presence of BPS domain walls which may be partially wrapped over the CY. For example, considering a D6-brane wrapped over 4-cycles of CY gives a domain wall with BPS tension $(1/\lambda_s)\int k \wedge k$ integrated over the internal part of the 6-brane. This in turn shifts the dual F by one unit. This BPS formula should be captured by a ΔW and we can see from the above form of (2.2) that the first

term above precisely captures this term. More precisely what we mean by the formula (2.2) is the *worldsheet quantum corrected* formula for the kahler forms (as is well known in the context of mirror symmetry the mass of the D-branes receives corrections by the worldsheet instantons). In particular if t denotes the complexified area of the basic 2-cycle, then the volumes of the 0-, 2-, 4- and 6-cycles are given by

$$1, t, \frac{\partial F_0}{\partial t}, 2F_0 - t\frac{\partial F_0}{\partial t},$$

where F_0 is the genus zero topological string amplitude. So in particular suppose we have N units of the F flux through the basic 2-cycle, where t denotes the complexified area of this 2-cycle. Then the first term in (2.2) is equivalent to

$$\int F \wedge k \wedge k = N\frac{\partial F_0}{\partial t}.$$

Similarly if we considered D4-branes wrapped over 2-cycles and D2-branes with no wrappings, we deduce the existence of the second and third term in (2.2). In particular if we denote the fluxes of F, G_{int}, G_6 by integers N,L,P relative to integral 2-, 4-, and 6-cycles, we have

$$\lambda_s W = N\frac{\partial F_0}{\partial t} + itL + P. \tag{2.3}$$

Note that Eq. (2.2) can also be written in the form

$$\lambda_s W = \int (F + i*G) \wedge k + \int G_6, \tag{2.4}$$

where again here by $*$ we mean the worldsheet quantum corrected $*$ operation.

Now we come to the discussion of why turning on RR fluxes should not modify the topological amplitudes. We will concentrate on genus 0 amplitudes (similar arguments can be advanced for the higher genus amplitudes as well). The vector superfield with bottom component t has an auxiliary field in the superspace of the form

$$t + \theta^2(F + *iG) + \cdots,$$

where F and G are the usual RR fluxes of the internal Calabi–Yau. (I have greatly benefited from discussions with Nathan Berkovits in connection with the auxiliary field structure of the superfields.) In the usual supersymmetric background they are set to zero. Now suppose we wish to turn them on. Suppose, for example, we wish to turn on N units of F. Consider the topological string amplitude $F_0(t)$. We claim that this already yields the correct structure for the generation of $N=1$ superpotential precisely if F_0 *is unmodified in the presence of* RR *flux*. To see this note that using the expansion of t in terms of the RR field strength auxiliary fields we have

$$\int d^4\theta F_0(t) = \int d^2\theta N\frac{\partial F_0}{\partial t}$$

which is exactly the expected answer if F_0 is unmodified. Similarly turning on the G_{int} flux and using (2.4) we see that the term in (2.2) involving G_{int} will also have the correct structure if F_0 is unmodified.

There is another auxiliary field in the vector multiplet which come from the $NS-NS$ sector which is relevant for us. This corresponds to the field strength associated with the lack of integrability of complex structure. In particular if we write $\bar{D} = \bar{\partial} + A\partial$, where A is an antiholomorphic one form taking values in the tangent bundle, then

$$\bar{D}^2=(\bar{\partial}A+[A,A])\partial=\mathcal{F}\partial,$$

where $\mathcal{F}$ is an antiholomorphic 2-form with values in the tangent bundle which is equivalent, by lowering the vector index by the three form, to a (2,2) form. If this is nonvanishing it also corresponds to making the (3,0) form in the CY not to be annihilated by $\bar{\partial}$. These turn out effectively to add to F and $G_{\rm int}$ complex pieces of the form iF^{NS}/λ_s and $iG^{NS}_{\rm int}/\lambda_s$. A similar NS auxiliary field gives rise effectively to the complex part of $*G_6$. (Turning these fields on is mirror to turning on H_{NS} on the mirror CY.) In other words, even with these fields turned on, the formula (2.3) remains correct but now N,L,P also include imaginary pieces of the form iN_I/λ_s, iL/λ_s, iP/λ_s. We will continue to denote the superpotential as (2.3) and keep in mind that N, L, and P can have complex pieces given by an integer over λ_s.

Turning these vevs on breaks the $N=2$ supersymmetry to $N=1$. The field t is now the bottom component of an $N=1$ chiral multiplet whose auxiliary field descends from another auxiliary field (which also comes from the NS sector) in the original $N=2$ multiplet which is not turned on.

Note also that the higher genus topological amplitudes also give rise to certain $N=1$ superpotential terms when the auxiliary field of the $N=2$ multiplet t takes a vev. In particular with N units of RR flux for F we get

$$\int d^4\theta \mathcal{W}^{2g}F_g(t)\to N\int d^2\theta \mathcal{W}^{2g}\frac{\partial F_g}{\partial t}, \tag{2.5}$$

where we continue to denote by $\mathcal{W}_{\alpha\beta}$ the reduction of the $N=2$ multiplet to an $N=1$ multiplet with the self-dual part of the gravi-photon field strength as its bottom component.

So in conclusion we have learned that the topological string amplitudes are not sensitive to turning on RR field strengths, but they are useful in determining the superpotential terms that will be generated once certain RR and NS fields take a vev. This is captured by Eq. (2.3).

C. Open topological strings and $N=1$ amplitudes in 4D

In the A-model, the open topological string corresponds to studying holomorphic maps from worldsheet with boundaries to the target space where the boundary lies on a three-dimensional Lagrangian subspace of the CY, i.e., the three-dimensional topological version of D-brane.[14] Moreover, it was shown that topological string field theory in this case is just the Chern–Simons gauge theory on the corresponding Lagrangian submanifold (possibly corrected with nontrivial worldsheet instantons). The implications of these theories for superstring amplitudes has been studied as well. In particular if we consider type IIA superstring in the presence of a CY with N D6-branes wrapping a Lagrangian 3-cycle of CY and filling the rest of the spacetime we get an $N=1$ gauge theory with SU(N) gauge group in 4D. Then it was shown in Ref. 13 that, for example, the genus 0 open topological string amplitudes compute corrections of the form

$$\lambda_s W=\sum_h \int d^2\theta F_{0,h}[NhS^{h-1}]+\alpha S+\beta, \tag{2.6}$$

where $F_{0,h}$ is the partition function of the topological string at genus 0 with h holes, and $S=\lambda_s \operatorname{Tr} W^2$ where W_α is the chiral superfield with gaugino as its bottom component. [The coefficient of Nh in front arises because, as discussed in Ref. 13, we have to choose $h-1$ holes to put the $\operatorname{tr} W^2$ fields and this can be done in h ways and also the trace over the hole without a field gives a factor of N. Note also that $\operatorname{Tr} W^2$ which is a fermion bilinear is nilpotent, in the sense that $(\operatorname{Tr} W^2)^k=0$ for $k>N^2$. It is relevant for us precisely because we are considering a large N limit. Thus in the large N limit the gaugino bilinear can even have a classical vev.] Here we have shown explicitly the contribution coming from $h=2$ in the form of αS. This term, coming from annulus, is typically divergent, signifying the RG flow of the coupling constant of the gauge theory and needs regularization. Also we have added a constant β to remind us that we cannot fix that from open topological string considerations. Here h is the number of holes on the sphere and $F_{0,h}$

denotes the topological amplitude on the sphere with h holes. If the target space has some Kahler moduli t they will correspond to chiral fields in the $N=1$ theory in four dimensions and $F_{0,h}$ will depend on t. The case of $h=1$ in the above formula was recently discussed in Refs. 29, 30, and 10. Some superstring implications of higher genus open topological strings, i.e., $F_{g,h}$ with arbitrary g, has also been noted in Ref. 10. In particular they compute terms of the form $\int d^2\theta F_{g,h}\mathcal{W}^{2g}[NhS^{h-1}]$.

Let us define the open topological string amplitude summed over all holes at a fixed genus by

$$F_g^{\text{open}}(r)=\sum_h F_{g,h}r^h.$$

Then, for example, the genus 0 open topological string amplitude computes the following correction to the superpotential:

$$\lambda_s W=N\int d^2\theta\frac{\partial F_0^{\text{open}}(S)}{\partial S}+\alpha S+\beta.$$

This is strikingly similar to the form obtained in (2.3) in the context of closed topological string amplitudes. Similarly the higher genus correction computes terms of the form

$$N\int d^2\theta\,\mathcal{W}^{2g}\frac{\partial F_g^{\text{open}}(S)}{\partial S}$$

which is also similar to the higher genus correction obtained in the closed string context in the presence of flux (2.5). The main difference being that S is an operator for the open string amplitudes but t is a parameter in the closed string setup. Nevertheless we will see in the next section why this is not an accidental similarity and provides the superstring interpretation of the duality found in Ref. 9, when S takes an expectation value equal to t.

III. EMBEDDING LARGE *N* TOPOLOGICAL STRING DUALITY IN SUPERSTRINGS

Consider type IIA strings in a noncompact CY three-fold geometry of the form of the conifold times the Minkowski space M^4: The internal geometry is given by

$$f=x_1^2+\cdots+x_4^2=\rho,$$

where each x_i parametrizes $\mathbf{C}$. The real subspace of the above geometry is S^3 (for real ρ) and the imaginary directions sweep the cotangent direction of S^3. The volume of S^3 in string units is given by ρ (here we are taking the canonical 3-form $\Omega=\Pi dx_i/df$, which scales as ρ to give the volume). Thus symplectically the conifold is T^*S^3. Consider N D6-branes wrapped over the S^3 of the conifold and filling the rest of the spacetime. On the uncompactified world volume of the D-brane we have an $N=1$ supersymmetric SU(N) gauge theory. Note that to leading order the action on the uncompactified world volume of the D-branes is given by the superpotential

$$\frac{1}{\lambda_s}\int d^2\theta\,SY, \tag{3.1}$$

where $S=\lambda_s\,\mathrm{Tr}\,W^2$ and where Y denotes the $N=1$ chiral superfield with its bottom component given by $iC+(\rho/\lambda_s)$, where C is the vev of the 3-form gauge field on IIA (normalized with periodicity 2π) and plays the role of the θ angle for the gauge theory and ρ denotes the volume of the S^3.

The choice of this type IIA geometry is based on the desire to utilize the topological open/closed string duality. In particular, as discussed in the preceding section the open topological string in this case computes corrections to the superpotential of the form

$$\frac{N}{\lambda_s}\int d^2\theta\, \partial_S F_0^{\text{open}}(S).$$

The topological A-model is insensitive to complex structure. In particular F^{open} is independent of ρ except for a linear terms in S (coming from the annulus) written in (3.1), which is related to the ambiguity of open topological string at the level of annulus. There is also a divergence of the annulus amplitude corresponding to the running of the gauge coupling constant, which, in the regularized form, can be viewed as addition of a linear term in S. The corrections above to the simple $YS=Y\,\mathrm{Tr}\,W^2$ involve higher dimension operators (more powers of S) and are captured by the open string amplitude which coincide with the large N expansion of the Chern–Simon amplitudes on S^3. Note also that the fact that they are independent of Y implies that they survive no matter what the size of the S^3 is.

Now we wish to consider the limit where we consider the $N\to\infty$ limit keeping $N\lambda_s$ fixed. In this limit, the analog of 't Hooft coupling for the gauge system is given by

$$\frac{1}{Ng_{\text{YM}}^2}\to\frac{Y}{N\lambda_s},$$

which remains fixed in this limit. We would like to consider the gravity dual of this gauge system. In the spirit of AdS/CFT correspondence we will have to consider the near horizon geometry. What the precise notion of ''near'' horizon geometry in this case should be is more subtle because the expectation value of Y undergoes an RG flow, as noted above, and it will depend at which scale we are probing it. In other words we have to readjust the size of Y depending on how close we are approaching the branes. The limit should be such that the S^3 has zero size when we probe it in the UV of the gravitational side but finite size in the IR. To avoid such subtleties we try to look for a consistent gravitational background which the branes create. In particular we should find an S^2 of finite size emerging, surrounding the S^3, with the D-branes completely disappeared and replaced by the corresponding fluxes. In the case at hand, since we have N D6-branes wrapping the S^3 in the geometry after transition we should get N units of the 2-form RR flux F through the dual S^2. We will now turn to studying this geometry.

A. Type IIA superstring on the blown up geometry

We thus seek the dual large N stringy description of the above gauge system, in the form of the type IIA background with the blown up conifold geometry, i.e., the geometry corresponding to $O(-1)+O(-1)$ bundle over $\mathbf{P}^1$, with N units of 2-form F flux through $\mathbf{P}^1$. However, we must also have internal 4-form and 6-form fluxes (in the form of *NS* and RR fields discussed before).

That there should be an *NS* 4-form flux corresponds to the fact that the size of the S^3 is changing (i.e., that Ω is no longer closed and $\rho=\int_{S^3}\Omega$ changes), inducing a running of the gauge coupling constant. Moreover to preserve $N=1$ supersymmetry for a finite value t of the complexified area of the blown up $\mathbf{P}^1$ we need both 4-form as well as 6-form fluxes. In fact, as discussed in the preceding section and summarized in Eq. (2.3) we have a superpotential of the form

$$W=N\partial_t F_0(t)+itL+P, \tag{3.2}$$

where for the geometry at hand $F_0(t)$ is, up to a cubic polynomial, the tri-logarithm function, given by

$$F_0(t)=\frac{1}{6}t^3-\sum_{n>0}\frac{e^{-nt}}{n^3}+P_2(t) \tag{3.3}$$

[where $P_2(t)$ is a polynomial of order 2 in t and is somewhat ambiguous]. Similarly for higher genus F_g we have

$$F_g(t)=\frac{B_{2g}}{2g(2g-2)!}\sum_{n>0} n^{2g-3}e^{-nt}+\frac{B_{2g}B_{2g-2}}{2g(2g-2)(2g-2)!},\quad g>1,$$

$$F_1(t)=\frac{t}{24}+\frac{1}{12}\log(1-e^{-t}),$$

where B_{2g} denotes the Bernoulli numbers. The terms involving e^{-nt} in the above formula reflects the corrections due to worldsheet instantons wrapping n times over the $\mathbf{P}^1$.

The content of the duality obtained in Ref. 9 is that

$$F_g^{\text{open}}(S)=F_g(t)$$

for all g if we set $S=t$. We now try to interpret this statement in the superstring context. For this we need to study solutions to the gravitational equations.

Typically in physics and mathematics when we try to solve some system of equations, there are topological obstructions that have to be shown to be absent. Once they are shown to be absent then a solution exists. For example, when we are trying to find Ricci-flat metrics on Kahler manifolds we need the first Chern class of the manifold to be zero. In fact this is also sufficient for being able to find a Calabi–Yau metric. Of course explicit solution for the metric has not been possible in almost all cases and in fact the Ricci-flat metric is only an approximate metric which gives rise to a conformal worldsheet theory. In a sense the topological condition, guaranteeing the existence of the solution is more fundamental than the solution itself.

Now we come to the case at hand. To preserve $N=1$ supersymmetry we need $W=dW=0$. Once these are satisfied, we expect physically that there must be a solution to the gravitational system. In fact a very similar example with the same number of supercharges (namely 4) was already studied from this point of view. Namely if we consider M-theory on Calabi–Yau fourfold with G-flux turned on, the gravitational equations have been studied in Ref. 31. The topological conditions they find for the existence of the gravitational solution has been shown to be identical to the condition that $W=dW=0$.[27]

Of course the low energy gravitational equation in the present case can also be studied similar to what was done in Ref. 31 and will involve warped geometries mixing the spacetime with the Calabi–Yau. Even though solving the gravity equations would be interesting, we have to remember that due to worldsheet instantons wrapping the $\mathbf{P}^1$ there are important corrections to the gravity equations, and so at best we can trust the low energy gravity description in the limit of large t. Nevertheless, as already noted above, the superpotential terms *including* the corrected string geometry, can be incorporated to all orders in the W which is computable by topological string amplitudes.

Before even solving the conditions $W=dW=0$ we can already interpret the duality of Ref. 9 in the superstring context. If we compare Eq. (3.2) with the superpotential given in the gauge theory side namely $W=N\partial_S F_0^{\text{open}}(S)+\alpha S+\beta$ we see that they are identical in form with an appropriate identification of α and β with L and P. Therefore, since the vacuum in the gauge theory side, as well as the moduli in the gravity side correspond to $W=dW=0$, and W has the same form for the gauge as well as the gravitational system, this will identify

$$\langle S\rangle=\langle \lambda_s \operatorname{Tr} W^2\rangle=t,\quad F_g^{\text{open}}(S)=F_g(t). \tag{3.4}$$

Thus the condition of vacuum configuration which sets $\langle S\rangle=t$ also translates the duality found in Ref. 9 to the match between amplitudes in the gravity side and the gauge theory side to all orders in $1/N$ at least as far as superpotential terms are concerned.

Note that the idea that $\langle S\rangle\neq 0$, i.e., that we have gaugino condensation, is very natural for the open string theory under discussion as it does have an $N=1$ Yang–Mills theory associated with it. Part of the above check involves, on the gauge theory side, the statement that gaugino condensation generates superpotential terms captured through topological open string amplitudes and in fact

this was already pointed out in Ref. 13. Of course here we have a more refined gauge theory than just the $N=1$ Yang–Mills theory and in particular we have in the open string system, also the higher dimension operators present, which are captured by the topological string amplitude. At any rate, the result of Ref. 9 strongly suggests not only the existence of a large N duality involving this $N=1$ brane system with this closed string background, but also that the gaugino condensation takes place.

We now come to finding solutions to the equations $W=dW=0$ on the gravity side, which should guarantee the existence of a solution. There are four parameters under control: the modulus t and the fluxes N,L,P. The two equations $W=dW=0$,

$$\partial_t W=0\rightarrow NF_0''+iL=0\rightarrow L=iNF_0'',$$

$$W=0\rightarrow P=-NF_0'+NtF_0''$$

imply that two of these four quantities are fixed in terms of the other two. The N is of course fixed for us by the number of D6-branes. As is clear from our description of the dual gauge system the choice of a shift in L is related to a shift in the bare coupling constant of the gauge system. In particular in order to agree with the bare coupling constant of the gauge theory $iL=\rho/\lambda_s$, where ρ is the volume of the S^3 where the D6-branes are wrapped around. Thus the value of t (and also of P) is fixed and from (3.3) and $\partial_t W=0$ the solution for t is given by

$$[c(e^t-1)]^N=\exp(-\rho/\lambda_s). \tag{3.5}$$

The constant c depends on the ambiguities hidden in the $P_2(t)$. As we will argue from the dual gauge theory description, it should be fixed in our case (by a suitable regularization of the one loop divergence of the gauge theory) to be $c\sim N\lambda_s$.

Next we turn to the question of how the dynamics of the gauge system is reflected in the W and the other superpotential terms. What do we expect for the dynamics of the $N=1$ supersymmetric theory living on the D6-brane? If we ignore the higher powers of S in the superspace integral, i.e., if we ignore the higher order operators, as already discussed, the leading term with the lowest number of derivatives, is given by the superpotential term

$$\frac{1}{\lambda_s}\int d^2\theta\, SY,$$

where $S=\lambda_s \operatorname{Tr} W^2$ and $Y=iC+(\rho/\lambda_s)$ where ρ denotes the size of the S^3 in the string frame. In the usual geometric engineering of standard $N=1$ gauge theories, and in particular the ones discussed in Ref. 32 one considers the limit where ρ is large, in which case the field Y gets demoted to a parameter in the Lagrangian (the corresponding D-term involving $Y\overline{Y}$ becomes very large). However, here we are not necessarily interested only in a regime where Y is very large. In other words we consider the field Y to be a dynamical field. Thus we have a nonstandard $N=1$ supersymmetric gauge theory with its coupling constant as a dynamical field. Even though it is somewhat unconventional, as we will now argue some of the basic features of this theory are similar to that of $N=1$ QCD, in the limit where we ignore the higher derivative terms of the form $\int d^2\theta[\operatorname{tr} W^2]^k$. In other words, if we consider the field space where $S=\operatorname{tr} W^2\ll 1$ (in string units) we have a theory which is more or less similar to $N=1$ supersymmetric Yang–Mills theory. Even though we do not have to restrict our attention only to this limit, and the duality with gravity holds regardless of which field configuration in S we consider, it is first instructive to consider the small S region to gain intuition for what this theory is.

In the dynamics of $N=1$ supersymmetric gauge theory, a prominent role is played by instantons. Here a similar effect exists: In particular if we consider Euclidean D2-brane instantons wrapping the S^3 the superpotential gets corrected. Moreover this can also be viewed as point-like instantons for the SU(N) gauge theory. To have the right number of fermionic zero modes to lead to a chiral superspace potential we need $1/N$-th of this instanton. Since the action for this instanton

is e^{-Y}, the term that can appear in the action is $e^{-Y/N}$. The coefficient in front of it should be of order N^2 (as argued in Ref. 33). So we must have the effective superpotential given by

$$W=\int d^2\theta\left(\frac{1}{\lambda_s}SY+iN^2\alpha e^{-Y/N}\right), \tag{3.6}$$

where the constant α, by a shift in $Y\to Y+Y_0$, can be identified with a shift in the bare coupling constant of S, i.e.,

$$\alpha=e^{-Y_0/N}. \tag{3.7}$$

(The choice of α is also related to how we regularize the one-loop divergence which corrects the action with a term $a\int d^2\theta S$.)

This effective superpotential has the same structure as that encountered in the proof of mirror symmetry in two dimensions.[34] This same superpotential structure was encountered in Ref. 10 in the context of $N=1$ domain walls in 4D, which we will also need in this paper, and we will discuss further below. Notice that here since Y is a dynamical field, we can integrate it out by setting

$$\partial_Y W=0\to\frac{1}{\lambda_s}S=iN\alpha e^{-Y/N}$$

which leads to

$$Y=\log\left(\frac{S}{iN\alpha\lambda_s}\right)^{-N}$$

plugging it back to the superpotential gives the effective superpotential for S:

$$W_{\text{eff}}(S)=\frac{1}{\lambda_s}\left[S\log\left(\frac{S}{iN\alpha\lambda_S}\right)^{-N}+NS\right].$$

This is the familiar effective superpotential expected for the gaugino bilinear S in the standard $N=1$ supersymmetric gauge theory. Indeed setting $\partial_S W=0$ leads to

$$\left[\frac{S}{iN\alpha\lambda_s}\right]^N=1\to S=iN\alpha\lambda_s e^{2\pi il/N}=iN\lambda_s e^{(-Y_0+2\pi il)/N}. \tag{3.8}$$

Note that we see the N vacua of SU(N) Yang–Mills, in the standard way.

Let us compare the vev we found for $S=\lambda_s\,\mathrm{Tr}\,W^2$ with the gaugino condensate for standard $N=1$ Yang–Mills, which is of the form

$$\mathrm{Tr}\,W^2=iN\Lambda^3 e^{[-1/Ng^2_{\mathrm{YM}}]+(2\pi il/N)}.$$

In comparison with what we have above, note that this is in perfect agreement with (3.8), where Λ corresponds to the string scale and $1/g^2_{\mathrm{YM}}\to Y_0$.

Note that the effective superpotential we have found for S, for small S, also follows from either the open topological string amplitudes in the limit $S\to 0$, or the dual closed topological string amplitude in the limit $S=t\to 0$ which is given by

$$F_0(t)\to-\tfrac{1}{2}t^2\log t+at^2+bt+c$$

and so

$$W(S)=\frac{1}{\lambda_s}[N\partial_S F_0(S)+\alpha S+\beta]=\frac{1}{\lambda_s}(S\log S^{-N}+N\,\text{const}\,S+N\,\text{const})$$

in perfect agreement with expectations based on the gauge theory analysis as well as with the contribution of the Euclidean D2-brane instantons in the string context. This comparison with gauge theory and recalling that $t\leftrightarrow\lambda_s\,\mathrm{Tr}\,W^2$, also fixes the value c in (3.5) to be $c\sim N\lambda_s$. Note that the choice of α, the linear terms in S, on the gravity side is controlled by the 4-form fluxes dual to the $\mathbf{P}^1$, as discussed before.

Having discussed the geometry of the vacua of $N=1$ theory, we now turn to another important feature of $N=1$ theories, namely the domain walls interpolating between various vacua.

B. Domain walls

$N=1$ Yang–Mills theory admits BPS domain walls interpolating between various vacua. As noted in Ref. 33 at large N they behave as D-branes for QCD string. In particular their tension is of the order of N. Since in the present context the QCD string is realized by the fundamental string, ordinary D-branes of string theory should play the role of domain walls. This is indeed the case: On the gravity side we have a blown up $\mathbf{P}^1$. If we consider D4-branes wrapped over $\mathbf{P}^1$ they correspond to domain walls. Their tension goes as

$$T\sim\frac{1}{\lambda_s}|t|=N\frac{|t|}{N\lambda_s}.$$

As discussed before $|N\lambda_s|\sim|t|$ so we obtain the expected behavior. For the QCD domain wall the phase of the S field should change as we go from one vacuum to another. In particular it should shift by $\exp(2\pi i/N)$ for domain walls interpolating adjacent vacua. Let us see how this is realized in the gravity setup. Since we have identified the domain wall with D4-brane wrapped over S^2 we should note that the value of the G flux shifts as we cross the domain wall. Consider in particular the imaginary part of the Y field introduced earlier, which was identified with

$$\mathrm{Im}\,Y=C_{S^3},$$

i.e., the vev of the C field along the S^3. We now discuss how this changes from the left-hand side of the domain wall to the right-hand side. Since the G flux should be equal to one for the $D4$-brane, it implies that $\mathrm{Im}\,Y$ should shift by 2π, i.e.,

$$Y\to Y+2\pi i$$

as we go across the domain wall. In fact we can find the geometry of the BPS domain walls by the usual technique of the LG theory in 2D with $N=2$ susy.[35] In fact for the case at hand similar BPS domain walls were considered in Ref. 36. These domain walls also featured in the discussion of $N=1$ generation of superpotential in Ref. 10. Note that since we have

$$S=\lambda_s N\exp(-(Y+Y_0)/N)$$

this implies that the phase of S changes by $\exp(-2\pi i/N)$ as expected. Of course this is suppressed at large N, in agreement with the fact that classically the wrapped D-brane does not change the value of t.

It is also easy to see from the form of the action (3.6) that the BPS tension, which is given by ΔW, is given by

$$\Delta W=\frac{1}{\lambda_s}S\Delta Y.$$

Since S is identified with t, this corresponds to

$$\Delta W = \frac{2\pi i}{\lambda_s} t$$

as expected for the tension of the BPS wrapped D4-brane.

C. Subleading corrections in the 1/N expansion

So far we have concentrated on the interpretation of the leading corrections in large N. In the context of topological strings also the subleading terms to all orders in $1/N$ were found to agree between the Chern–Simons gauge theory and the closed topological string expansion. What is the interpretation of these higher terms for the gauge theory system?

In the limit of small t the topological string amplitudes is given by

$$F(t) = \sum_g F_g \lambda_s^{2g-2} t^{2-2g},$$

where $F_g = [B_{2g}/2g(2g-2)]$ and B_{2g} are the Bernoulli numbers (F_g turns out to be equal to the Euler characteristic of the moduli space of genus g Riemann surfaces). In this limit the topological string partition function coincides with that of noncritical bosonic strings on a circle with self-dual radius (this connection is well understood and will be reviewed in Sec. V). The $N=2$ amplitude that this computes is given by

$$\int d^4\theta \mathcal{W}^{2g} F_g t^{2-2g} = g R^2 F^{2g-2} F_g t^{2-2g} + \cdots . \tag{3.9}$$

This correction has been physically understood by considering turning on constant gravi-photon field strength in the Minkowski space and computing the effect of wrapped D2-branes on $\mathbf{P}^1$ to the R^2 term.[37] In the present context the wrapped D2-branes correspond to the baryon vertex, as in the usual AdS/CFT correspondence.[38] The baryon fields are charged under the gravi-photon field with charge proportional to their BPS mass t. Thus turning on gravi-photon F effectively turns on a background field strength for F_v, i.e., the $U(1) \subset U(N)$ living on the D6-branes, which can be identified with a global U(1) symmetry (the baryon number symmetry). Let us try to see how this can come about from the gauge theory side.

On the world volume of the D6-branes we have terms of the form

$$\int_{R^4} [G_4 + F \wedge F_v] \left(\int_{S^3} [\mathrm{CS}(\omega) - \mathrm{CS}(A)] \right)$$

where ω denotes the spin connection on S^3 and A is the internal gauge field on S^3. This term arises (by integrating by parts) from the usual inducement of brane charge by gravitational and gauge curvature on the brane (see Ref. 39 and references therein). Thus shifting F effectively shifts F_v. (Note that if we change the G_4 flux this is equivalent to turning on an internal Chern–Simons action for the supersymmetric system on the brane. It should be possible to derive directly the relation between generation of superpotentials on the brane and the Chern–Simons theory on S^3 from this fact.)

There is another term that is also generated from (3.9) when we recall that t has some auxiliary field turned on. In particular this gives rise to the term

$$N \int d^2\theta \mathcal{W}^{2g} \partial_t F_g(t) = N \int d^2\theta F^{2g} \partial_t F_g(t) + \cdots .$$

Recalling that in the gauge theory setup t is replaced by S, the gaugino bilinear superfield, the above term corresponds to the superpotential term

$$\lambda_s W = N \int d^2\theta F^{2g} \partial_S F_g(S) = -N \int d^2\theta \frac{B_{2g}}{2g} F^{2g} S^{1-2g}.$$

So turning on the (self-dual) gravi-photon field strength in four dimensions deforms the superpotential. What is the gauge theory interpretation of this? As noted above turning on F has the effect of turning on the field strength F_v in the $U(1) \in U(N)$, which is also equivalent to turning on B field in spacetime. Thus this seems to be related to considering the noncommutative version of the above gauge system.[40] In particular considering a self-dual noncommutativity in spacetime presumably generates a superpotential, as is predicted from the above formula. Note that this is consistent with the fact that in the UV where S is smaller this modification of the superpotential is a more pronounced effect, and it disappears in the IR where S is larger. It would be interesting to derive this result directly in the context of the noncommutative $N=1$ Yang–Mills theory. Moreover the dependence of the genus g partition function on the noncommutativity parameter is identical (we thank R. Gopakumar for pointing this out to us) to that obtained in Ref. 41. Namely, in the large N expansion, there is no modification at the level of planar diagrams, i.e., at $g=0$. Moreover at genus g the amplitudes are expected (when we have a self-dual noncommutativity) to scale (in the leading order) as $(1/\theta^{4g}) \sim B^{4g}$ which in our case translates to an F^{4g} dependence. This is in agreement with the fact that $|\partial_S W|^2$ indeed scales as F^{4g}.

D. More general values of *S*

So far, in the context of gauge theory discussion we mainly considered the limit where $\langle S \rangle$ is small compared to the string scale. However, the duality we are proposing holds for arbitrary $\langle S \rangle$. If $\langle S \rangle$ is not small, on the gauge theory side we get modification to the form we have written above, which is computed by the Chern–Simons theory on S^3. What kind of gauge theory does this correspond to? The gravity side provides a hint: If we consider wrapped D4-brane domain walls, we have infinitely many species of domain walls. The reason for this is that we can consider the bound state of n D2-branes with the D4-brane manifested through turning on n units of U(1) flux through the S^2 part of the world volume of the D4-brane. This can also be viewed as the effect of changing the B-field on the $\mathbf{P}^1$ by $2\pi i n$. The effect of such domain walls is thus shifting $t = S \to S \exp(2\pi i/N) + 2\pi i n$. In other words we have the vev's of S, not only taking values around a circle about the origin, but also circles about $2\pi i n$ for any integer n. Moreover the BPS tension for such domain walls is given by

$$\Delta W = \frac{1}{\lambda_s}(S + 2\pi i n).$$

The geometry of these domain walls can be recovered from an enlarged field content:[10] We can introduce one variable Y_n for each n, capturing the corresponding domain wall by its shift in the argument, and consider the superpotential

$$W = \int d^2\theta \sum_n \left[(S + 2\pi i n) Y_n + i N^2 \alpha e^{-Y_n/N} \right] \tag{3.10}$$

the domain wall with 1 D4-brane wrapped over $\mathbf{P}^1$ bound to n D2-branes will now correspond to shifting $Y_n \to Y_n + 2\pi i$. Integrating the Y_n's out will give

$$W = \frac{1}{\lambda_s} \sum_n (S + 2\pi i n) \log(S + 2\pi i n)^{-N} + a(S + 2\pi i n) + b$$

which is indeed equal to

$$W = \int d^2\theta \frac{1}{\lambda_s} N \frac{\partial F_0(S)}{\partial S}.$$

The variables Y_n were introduced to incorporate the kinks, but their appearance on the original gauge theory side, except for Y_0 seems mysterious. It would be interesting to see if one can find a direct interpretation of all the Y_n's. We expect that to be related to the possibility of doing large SU(N) gauge transformations on the S^3 part of the world volume of D6-brane.

The higher genus corrections in the case of large S are also similar to the modification at the genus 0 case. In particular we get an infinite sum with S replaced by $S+2\pi in$. This in particular is related to the fact that we can have a new baryon vertex for each wrapped D2-brane with D0-brane turned on.[42]

E. Adding matter

In the context of geometric engineering of $N=1$ supersymmetric gauge theories realized as D6-branes wrapped around S^3 cycles of CY manifolds[32] matter can be realized as extra D6-branes wrapped around other S^3's intersecting the gauge theory S^3 along a circle (where the vev of the Wilson line around the circle on the probe brane plays the role of mass for the matter). How does our duality extend to this case? In fact in the topological string the duality does extend to this case.[10] In particular in computation of Wilson loop observable for the Chern–Simons theory one adds extra topological branes intersecting the original S^3 along a knot, and it was shown that the closed topological string amplitudes agrees with the expected result for knot invariants for Chern–Simons theory. More checks have been made in Ref. 11 for a large number of distinct knots. In the context of embedding the topological string dualities in the superstring what this means is that the dual gravitational system will not only have a blown up S^2 but will also have additional D6-branes (which for algebraic knots will intersect the S^2 along a circle). The fact that the topological computations agree on both sides translates to the statement that the superpotential computations on both sides agree and is further evidence for this duality in the superstring context. Note that for each knot we obtain a different ''matter'' system for this generalized gauge theory, which in the limit of large Y give rise to the same low energy physics, but are distinct theories in the context of generalized gauge theories we have been considering. The gauge theoretic interpretation of these results is currently under investigation.[43]

IV. THE MIRROR TYPE IIB DESCRIPTION

As is well known, type IIA on a CY is equivalent to type IIB on a mirror CY. This implies that everything we have said above in the context of type IIA has a type IIB counterpart.

For example, instead of D6-branes of type IIA wrapped around S^3 we consider D5-branes of type IIB wrapped around S^2. Also turning on even-form fluxes in type IIA is mirror to turning on 3-form H_{RR} and H_{NS} flux in the type IIB side and the superpotential that gets generated in this context is given by

$$W=\frac{1}{\lambda_s}\int \Omega\wedge[H_{RR}+\tau H_{NS}],$$

where τ is the complex coupling constant of type IIB, and Ω is the holomorphic 3-form of the CY. The above integral can be done and yields the formula in terms of the prepotential of the corresponding $N=2$ theory, as discussed in the type IIA case. Note however, that the type IIB system is simpler in that by mirror symmetry the worldsheet instantons that were relevant in the context of type IIA theory in computing the prepotential, are absent for the type IIB case, and classical geometry already captures these corrections. In particular the B-topological theory (known as the Kodaira–Spencer theory of gravity) simply involves aspects of complex geometry of Calabi–Yau.

So as far as writing a classical gravitational background, the type IIB description would be more useful because the worldsheet instanton effects are absent. However, as far as the conformal theory on the string worldsheet, i.e., the large N expansion description of the gauge system, the type IIA and type IIB theories are of course identical.

In the above context we would need to know the mirror of local CY:$O(-1)+O(-1)\rightarrow \mathbf{P}^1$. The mirror of this is known and it is essentially the conifold with one subtlety:[36] The conifold has only one compact 3-cycle, whereas $O(-1)+O(-1)\rightarrow \mathbf{P}^1$ has two compact even cycles, namely 0- and 2-cycle. As was noted in Ref. 36 in the limit where the Kahler class of $\mathbf{P}^1$ approaches zero, i.e., $t\rightarrow 0$, the mirror becomes effectively the conifold (the actual mirror differs from the conifold by having some variables being $\mathbf{C}^*$ variables rather than $\mathbf{C}$ variables). (The actual mirror is given by $x_1+x_2+x_1x_2e^{-t}+1-uv=0$ where x_1,x_2 are $\mathbf{C}^*$ variables and u,v are $\mathbf{C}$ variables.) Similar observations were made in Ref. 44. Even though in principle we can consider the full mirror geometry, since the complex geometry of the conifold is more familiar and better studied we restrict our attention to this case. [In this limit the internal topological theory corresponds to a G/G model on S^2 (coming from the holomorpohic Chern–Simons theory on S^2 (Refs. 14 and 45) which should also be equivalent, by mirror symmetry, to the large N fixed k limit of the Chern–Simons theory. This topological theory should also be equivalent to the Penner matrix model. It would be interesting to verify these equivalences among these topological gauge theories more directly.] This will correspond to a particular limit of our type IIA theory, where we consider only the small $\langle S\rangle$ region. Recall that this was the regime where the theory retained only the leading dimension operators in the action and led to a theory which was similar to the standard $N=1$ supersymmetric gauge theory.

We will be brief for this case, as most of the discussion can be literally borrowed from our discussion in the preceding section. We start with N D5-branes wrapped over the $\mathbf{P}^1$ in the $O(-1)+O(-1)\rightarrow \mathbf{P}^1$ geometry. The large N limit of this, in the limit of shrinking $\mathbf{P}^1$ corresponds to blowing up an S^3 with N units of H_{RR} flux through the S^3. Let us write the conifold geometry as

$$z_1z_2-z_3z_4=\mu.$$

Then the genus 0 prepotential is given as

$$F_0(\mu)=\frac{-1}{2}\mu^2\log\mu+P_2(\mu),$$

where $P_2(\mu)$ is an undetermined polynomial of degree 2 in μ. Now we consider turning on fluxes: The mirror of turning on *NS* 4-form flux corresponds here to turning on H_{NS} and in the cycle dual to S^3. Thus as far as the superpotential is concerned we have

$$W=\frac{1}{\lambda_s}[N\partial_\mu F_0(\mu)+M\mu]=\frac{1}{\lambda_s}[-N\mu\log\mu+a\mu+b],$$

where $M=M_1+\tau M_2$, and the discussion reduces to the small S limit of the discussion in the preceding section.

While this paper was being prepared, two papers[18,19] appeared which are related to this type IIB construction. In particular (among other things) they consider the gravitational background corresponding to $D5$-branes wrapped on 2-cycles of CY and their results are consistent with the superpotential analysis here.

V. $c=1$ NONCRITICAL BOSONIC STRING AND $N=1$ SUPERPOTENTIALS AT LARGE N

As discussed above the type IIA or type IIB near a conifold background with some fluxes turned on can be interpreted as large N limit of certain $N=1$ supersymmetric gauge theories. In particular the string expansion is equivalent to the large N expansion of a gauge theory. Moreover certain superpotential corrections of the gauge theory can be viewed as computations of the corresponding topological strings in the CY background. These are readily computed and thus carry a large amount of information to all orders in $1/N$, for the gauge theories in question. In particular here we will explain how the type IIA superstring near the small blow up of conifold, or

equivalently the type IIB superstrings in the conifold geometry relate the noncritical bosonic string amplitudes with that of the superpotential computations at the large N limit of the corresponding $N=1$ gauge systems.

It was shown in Ref. 46 that the conformal theory near the conifold is given by the same system found in Ref. 47 in connection with noncritical bosonic strings on a circle of self-dual radius. This conformal theory is that of a supersymmetric Kazama–Suzuki coset construction

$$\mathrm{SL}(2)/\mathrm{U}(1)$$

at level $k=3$, and the relation with noncritical bosonic strings is that the topological twisting of this system is equivalent to considering bosonic string propagating on a circle of self-dual radius with the fermions of the coset model playing the role of the ghosts in the bosonic string. This relation between bosonic string on a self-dual circle and the superconformal theory of a conifold is in agreement with the fact[48] that the ground ring of the bosonic string for this background is isomorphic to the holomorphic function on the conifold (which is generated by z_1,z_2,z_3,z_4 subject to the relation $z_1z_2-z_3z_4=\mu$) where the cosmological constant of the bosonic string is mapped to the deformation parameter of the conifold. Moreover, the observables of the $c=1$ theory are mapped to deformations of the conifold geometry:

$$\sum_n \epsilon_n(z_1,z_2,z_3,z_4)+z_1z_2-z_3z_4=\mu,$$

where ϵ_n is a polynomial of degree n is z_i. These deformation parameters get mapped to states of the bosonic string which are indexed by a representation of $\mathrm{SU}(2)_L\times\mathrm{SU}(2)_R$ of this system, viewing z_i as entries of a 2×2 matrix M with the conifold being defined as $\det M=\mu$ and where the $\mathrm{SU}(2)_L$ and $\mathrm{SU}(2)_R$ are realized by left and right multiplication of M with SU(2). In particular the degree n polynomial ϵ_n decomposes into representation of spin $(j_L,j_R)=(n/2,n/2)$ with $|m_L,m_R|\leqslant n/2$. Let us denote the totality of these parameters by μ_i (except for μ). The bosonic string amplitudes compute topological B-twisting of the deformed conifold. (Aspects of this relation has recently been verified and certain results of bosonic strings have been recovered directly using the Calabi–Yau picture and the Kodaira–Spencer theory.[49]) For various aspects of $c=1$ noncritical bosonic string see Ref. 50. As already discussed the genus g partition function will be a function $F_g(\mu,\mu_i)$ of these parameters deforming the conifold background. Recall that in the gauge theory context μ is identified with S and we will thus denote $F_g(S,\mu_i)$. The topological string computes, at genus g, the term in the effective action given by

$$\frac{N}{\lambda_s}\int d^2\theta[\mathcal{W}^2]^g\partial_S F_g(S,\mu_i)=\int d^2\theta F^{2g}\partial_S F_g(S,\mu_i)+\cdots.$$

What is the interpretation of this for the gauge theory? As in the usual AdS/CFT correspondences, we would expect that the μ_i will be related to operators on the gauge theory side, deforming the gauge theory action by terms $\mu_i\mathcal{O}_i$. In fact, in the context of 3-brane probes of the conifold[51] aspects of such deformations for the gravity side have been studied in Ref. 52 and a similar analysis should be extendable to the case at hand. Thus the topological strings compute the response of the system upon such deformations. In particular at genus 0, turning on the μ_i modifies the superpotential for the gaugino superfield. Also turning on F will give rise to $1/N$ correction to the superpotential. It would be extremely interesting to understand the source of these corrections on the gauge theory side.

It would also be interesting to find the conformal theory associated with the RR and NS fluxes turned on in the conifold geometry. This is very interesting in view of the fact that before turning fluxes on we have an exactly solvable conformal theory given by SL(2)/U(1) KS model. It would be very interesting to find the deformation of this theory. It is likely to involve ingredients similar to the ones encountered in Refs. 53 and 54.

VI. WRAPPED *D*-BRANES AND COMPACT CY

Consider type IIA superstrings compactified on a Calabi–Yau threefold. In the above, we considered a situation where we take a large number of D6–branes wrapped over an S^3 in the CY, and taking the analog of the near horizon geometry, to decouple the gravity, and then proposing a dual gravity description for the gauge system.

If we wish to repeat what we did in the preceding sections, by considering D6-branes wrapped on some S^3, which is part of a compact Calabi–Yau, and filling the rest of the spacetime, we immediately run into a problem. We cannot wrap a D6-brane over a 3-cycle as there would be nowhere for the flux to go for compact internal CY. However suppose we consider a CY manifold with some number of S^3's and we wrap D6-branes and anti-D6-branes over them, in such a way that the net D6-brane charge is zero. This is of course a non-supersymmetric situation. (We can also consider the type IIB mirror of this where we consider D5/anti-D5 branes wrapped around vanishing S^2's of the CY.) We expect that the branes will eventually annihilate each other leaving us with an $N=2$ background. If the S^3's are rigid then this annihilation process takes some time, because there is a potential barrier for the wrapped D6-branes to move in the CY (i.e., there is a potential for the scalar corresponding to moving them in the normal direction in the CY).

We now wish to apply the considerations of this paper and propose a large N dual in this context. For the considerations of the gauge theory to be applicable we have to consider the limit where S^3 has shrunk to zero size. This is the analog of $Y_0=0$ in the formula in Sec. III. What we will find is that taking the large N limit induces a transition to a topologically distinct CY, with some fluxes turned on. Moreover the fluxes can disappear as in Ref. 17 leaving us with an $N=2$ supersymmetric vacuum. Thus the effect of the brane annihilation at large N has been to shift the background.

Consider a Calabi–Yau with R vanishing S^3 cycles $[C_i]$ which span a $K<R$ dimensional subspace of H_3. In other words assume

$$\sum Q_{ji}[C_i]=0 \quad \text{for } j=1,...,R-K$$

for some integral matrix Q. Let us consider N_i D6-branes partially wrapped around C_i, where we allow some N_i to be negative, in which case we mean the number of the corresponding anti-branes. The condition that the net D6-brane flux is zero implies that

$$N_i=l_jQ_{ji}$$

for $R-K$ integers l_j. Now, let us consider the limit where the S^3's are vanishingly small. In this limit, applying the discussion of the near horizon geometry, we are naturally led to consider the S^2 blown up geometry where the blowup parameter for the ith sphere is given by

$$t_i=i\lambda_sN_i=i\lambda_sl_jQ_{ji}.$$

Notice that not all the t_i are independent. In particular there are only $R-K$ independent parameters l_j which determine them. This is exactly as it should be for the local geometry to have a blowup. [In fact this shift in the hodge numbers can be understood from the viewpoint of inverse process of Higgsing of $U(1)^{R-K}$ by R charged fields[55] where the charged fields can be viewed as wrapped $D2$-branes in the blown up geometry.] In other words the blowup geometry is a CY with K less dimension of $h^{2,1}$ but $R-K$ more dimensions of $h^{1,1}$. Moreover the condition on the various Kahler classes of the $\mathbf{P}^1$'s is exactly the same as that found above for the t_i. This gives further support for the conjecture that the large N limit of the wrapped brane–anti-brane geometry, when we have no net branes is equivalent to a blown up CY with the Kahler parameters for the blown up spheres given as above. However, here we will also have RR fluxes through the S^2's. In this case the supersymmetry is completely broken[25,26] by the RR fluxes. The fluxes can disappear as recently studied in Ref. 17.

It would be interesting to check this generalized conjecture in the topological string setup: Namely this suggests that the topological open string amplitudes in the context of compact CY manifolds when there is no net topological D-brane, and when the D-branes are wrapped over spheres is easily computable by a related closed string theory computation on the blown up CY with different Hodge numbers.

VII. GENERALIZATIONS

There are many natural generalizations of this work. In particular it is natural to consider transitions among topologically distinct manifolds, going through vanishing cycles, and find a large N-brane system/gravity duals, where the large N gauge system will lie on one side of the transition and the dual gravitational system will lie on the other side (this was in fact the philosophy advocated in Ref. 9). (If we consider a Morse function f on a manifold the critical points of it encode certain topological aspects of the manifold. Near a critical point with p positive and q negative eigenvalues for $\partial_i \partial_j f$, for $f \neq f_{\text{critical}}$ the manifold near the critical point has the geometry of a filled $S^{p-1} \times S^{q-1}$. For $f > f_{\text{critical}}$ the S^{q-1} is filled and for $f < f_{\text{critical}}$ the S^{p-1} is filled. This is the general kind of transition expected for large number of branes replaced by fluxes. If we consider two manifolds in the same cobordism class, and consider a Morse function on the interpolating manifold the above picture suggests that branes can induce the transition. So if the cobordism classes are trivial and we have suitable branes we can interpolate between any two manifolds in this way.) In other words the large N brane systems can be viewed as inducing transitions in the background geometry. For examples there are transitions in the CY which involve the vanishing of certain 3-cycles and blowing up 4 manifolds, such as Del-Pezzo manifolds. In this context it is natural to conjecture the existence of a duality involving a large N limit of wrapped D6-branes about the 3-cycles in the context of type IIA with the four manifold resolution of the singularity on the gravity side, with certain fluxes turned on. (In fact there is already evidence for some such cases based on quotienting the Chern–Simons duality on S^3 by finite groups on both sides.[56] For example Chern–Simons on S^3/Z_2 should be equivalent to $\mathbf{P}^1 \times \mathbf{P}^1$ blow up inside a Calabi–Yau. Some aspects of this predictions have already been checked.) Or in the context of M-theory on fourfolds it is natural to look for transitions involving shrinking S^3's and growing 4-cycles, where we consider a large number of $M5$-branes wrapped over the S^3's and filling the three-dimensional spacetime, which should be dual to the geometry involving the blowup of the 4-cycle with some G flux turned on (in fact in this context the gravity solutions are already worked out in Ref. 31).

It is also natural to extend our results for the case of SU(N) systems to SO and Sp groups by including orientifolds. In fact it has been shown in Ref. 57 that the large N duality of Chern–Simons theory for SU(N) groups extend to the SO and Sp case as well.

Finally, the idea that studying BPS/anti-BPS systems are important for a more fundamental understanding of basic degrees of freedom for string theory as advocated by Sen is in line with the example we have found: We can describe one string background in terms of the ground state of a different one in the presence of D-brane/anti-D-brane systems. In a sense, this idea, combined with the idea that various transitions among manifolds can be induced by large N limit of brane systems, suggests that if we start with any background in string theory, and consider complicated enough configurations of branes and anti-branes, we can effectively be discussing arbitrary backgrounds of string theory.

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D-branes, categories and $\mathcal{N}=1$ supersymmetry

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We show that boundary conditions in topological open string theory on Calabi–Yau (CY) manifolds are objects in the derived category of coherent sheaves, as foreseen in the homological mirror symmetry proposal of Kontsevich. Together with conformal field theory considerations, this leads to a precise criterion determining the supersymmetry preserving branes at any point in CY moduli space, completing the proposal of II-stability. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1374448]

I. INTRODUCTION

Over the last year, the basic elements of a picture of BPS D-branes in weakly coupled type II string theory on general Calabi–Yau (CY) backgrounds have been developed, following the lines described in Ref. 1. Such branes have world-volume theories with $\mathcal{N}=1$, $d=4$ supersymmetry or its equivalent and by analogy with the study of supersymmetric field theory, one might expect to be able to get a good understanding of the observables determined by holomorphic or ''protected'' quantities such as the superpotential and D-flatness conditions; these are the spectrum of BPS branes and their moduli spaces of supersymmetric vacua. By analogy with the study of $\mathcal{N}=2$ compactifications using mirror symmetry, one might even hope to get this understanding and determine the BPS spectrum everywhere in moduli space (i.e., for string scale CYs) from a suitable reinterpretation of large volume results.

In this work, we give a proposal for how to do this, building on the II-stability proposal of Ref. 2 and 3, by combining physical input, notably the theory of boundary conditions in (2,2) superconformal field theory (SCFT) and its topological twistings, with the wealth of relevant mathematics, especially Kontsevich's homological mirror symmetry proposal[4] and the formalism of the derived category.

A longer work with more introductory discussion is in preparation; here we try to give a relatively concise discussion of the ideas and results. In particular, we will not give very precise explanations of the fairly lengthy mathematical background (mostly homological algebra), instead focusing on its physical interpretation. This background can be found in the standard reference 5; we also recommend Ref. 6 for a nice introduction to the derived category.

A good way to identify observables which can be computed in the large volume limit is to consider the topologically twisted world-sheet theory. We will consider sigma models with CY target. These models have two twisted versions, the A twisted model whose observables depend only on (the stringy generalization of) the CY Kähler moduli, and the B twisted model whose observables depend only on the CY complex moduli. Stringy corrections are absent in the B model and thus these observables are computable at large volume; mirror symmetry can then be used to compute A model observables.

For the closed string, the basic ''topological'' observable is the prepotential of the $\mathcal{N}=2$ supergravity obtained by type II compactification on the CY. Equivalent information is the metric on moduli space, or the central charges of BPS states at a general point in moduli space. In the B model these central charges are the periods of the holomorphic three-form and are computable.

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For the open string, the basic topological observables are the set of allowed topological boundary conditions (which we could call ''topological D-branes''), and the spectrum of open strings between any pair of topological D-branes. Physically, these correspond to D-brane configurations which solve the F-flatness conditions, and the massless fermionic open strings between any pair of D-branes. Mathematically, this data can be thought of as defining a category of brane configurations, in which the objects are topological D-branes, and the morphisms are open strings.

In principle, this allows computing these observables in the B model at large volume, and extrapolating them to general points in Kähler moduli space. However, this is subtle—the naive extrapolation according to which B branes are holomorphic bundles or coherent sheaves at every point in Kähler moduli space is incorrect.[3]

The source of this contradiction is the following: if one makes a large variation of the Kähler moduli, in general a pair of branes, which has aligned BPS central charges (i.e., with the same phase, so preserving the same $\mathcal{N}=1$ supersymmetry), can vary into a pair with arbitrarily related and even antialigned central charges, as would be the case for a brane and an antibrane. Thus any candidate definition of ''topological D-brane'' which could make sense throughout Kähler moduli space must be able to describe branes and antibranes on the same footing, and thus include more objects than coherent sheaves.

Now there are already natural mathematical candidates for the category of topological D-branes—in the B model, the derived category of coherent sheaves, and in the A model the Fukaya category, as proposed some time ago by Kontsevich.[4] A lot of evidence has accumulated that this is correct, most notably in results of Seidel and Thomas[7] and Horja[8] which we discuss later. Physicists have also suggested various roles for this category.[9–13]

In the present work, we give physical arguments that this is correct. These follow the spirit of Witten's argument that the topological class of a D-brane on the space X is a K theory class on X:[14] we define objects to be bound states of D-branes modulo a relation which equates two configurations which differ by adding cancelling brane-antibrane pairs. However, we will keep track of far more information along the way—essentially, all of the morphisms between objects—and thus the result, the derived category, makes much finer distinctions than K theory. As an example, whereas the K theory class of a D0-brane does not depend on what point it sits at, in the derived category every point is a distinct object.

Technically, this begins with the discussion of topological open string theory as in Ref. 15, but we then generalize the BRST operator to carry additional ''homological'' information associated with the Chan–Paton factors. This will allow treating complexes of boundary states as objects; we will then physically motivate imposing equivalence relations under adding brane-antibrane pairs, under Q-exact variations of the additional data (homotopy equivalence), and under complex gauge transformations, and argue that the result is the derived category formed from the original category of boundary conditions.

Having some understanding of the topological D-branes, we will then discuss their relation to physical D-branes. The primary result in this direction is a flow of the gradings of objects and morphisms under variation of Kähler moduli, for which we give a simple CFT argument as well as explicit examples.

This result allows predicting the masses of bosons in chiral multiplets at arbitrary points in Kähler moduli space, and is thus the key to determining bound state formation and stability. In particular, there is an inconsistency in the CFT interpretation of morphisms of negative degree—they would correspond to operators of negative dimension—which forces certain topological D-branes to drop out of the physical spectrum. This gives a direct CFT argument for the Π-stability condition proposed in Ref. 2.

This agreement suggests that we look for a reformulation of Π-stability which does not require an Abelian category. The direct generalization of subobjects and exact sequences to the derived category is the ''distinguished triangle,'' and we discuss this notion and show how it unifies different versions of the bound state and decay processes involving branes and antibranes.

Combining this with the previous results leads to a proposal for a reformulated stability condition, which, although similar to Π-stability, does not require a preexisting notion of Abelian

category. This appears to be a good candidate for a mathematically precise definition of a BPS brane on a Calabi–Yau manifold, and is quite concrete in simple examples, predicting marginal stability lines and new BPS branes.

II. BPS D-BRANES, GRADING, AND IMAGES

Our starting point will be a (2,2) SCFT such as a sigma model on a Calabi–Yau threefold or a Gepner model, with integrally quantized $U(1)$ charges, so that it can be used to define a type II string compactification with $d=4$, $\mathcal{N}=2$ supersymmetry.

The most basic attributes of a BPS D-brane B (we take it to be a particle in four dimensions for this discussion) are its RR charge $Q(B)$ and its BPS central charge $Z(Q(B))$ or $Z(B)$. These are discussed in many references such as Ref. 16. We will consider B-type branes, for which $Q(B)$ is essentially the K theory class. $Z(B)$ depends on $Q(B)$ and on a point in the stringy Kähler moduli space $\mathcal{M}_k$ (best defined as the complex structure moduli space of the mirror CY).

A quantity which will be particularly important for us is the phase of the BPS central charge. As in Ref. 2, we define the *grade* φ or $\varphi(B)$ of a brane to be this phase normalized so that branes and antibranes have $\varphi(B)-\varphi(\overline{B})=1\,\mathrm{mod}\,2$:

$$\varphi(B)=\frac{1}{\pi}\,\mathrm{Im}\log Z(B). \tag{2.1}$$

We will need to extend this from the circle $[0, 2)$ to a real number; thus there is a $2Z$ ambiguity to be fixed for each brane. If we do this at some point in moduli space, the grades can be defined elsewhere by analytic continuation of Z; we will justify this shortly.

At large volume, BPS branes are either A branes (special Lagrangian manifolds carrying flat connections) or B branes (coherent sheaves carrying Hermitian Yang–Mills connections). The most basic observables in the classical theory are the massless fermion spectrum between a pair of branes. For B branes which fill the CY, these can be obtained by the standard arguments of Kaluza–Klein reduction: the oriented massless fermionic strings from branes carrying the bundle E to branes carrying the bundle F are elements of the complex cohomology group $H^{0,q}(M,E^*\otimes F)$. As we will review, these are the states of the B twisted topological open string theory, so this result does not obtain stringy corrections. The mirror A statement must involve stringy effects as is discussed in Refs. 15, 17 and 18; because of this we prefer the B picture.

A. BPS branes as boundary conditions

In world-sheet terms, a BPS brane corresponds to a boundary condition which preserves an $\mathcal{N}=2$ world-sheet supersymmetry, as discussed in Ref. 19.

For A boundary conditions we have (in the open string channel) $T_L=T_R$, $G_L^{\pm}=G_R^{\mp}$, $J_L=-J_R$, and

$$e^{i(Q_0/2)\phi_L}=e^{i\pi\varphi}e^{-i(Q_0/2)\phi_R}, \tag{2.2}$$

where $J_L=iQ_0\partial\phi_L$ and $J_R=iQ_0\overline{\partial}\phi_R$ define the bosonization of the $U(1)$ current in the (2,2) algebra, $Q_0=\sqrt{\hat{c}}$ and $\hat{c}=3$ for a CY sigma model is the complex dimension of the CY. B boundary conditions are similar to $J_R\to -J_R$ and $\phi_R=-\phi_R$.

The operators in (2.2) are the $\mathcal{N}=2$ spectral flow operators which directly enter the space–time supercharge and thus $e^{i\pi\varphi}$ directly specifies an unbroken $\mathcal{N}=1$ algebra. In sigma model compactification we have

$$e^{iQ_0\phi_L}=\Omega_{ijk}\psi^i\psi^j\psi^k$$

in terms of the world-sheet fermions and so for A boundary conditions φ is precisely as defined in (2.1). This is also true for B boundary conditions, of course. If the two boundary conditions have $\varphi_1-\varphi_2\in 2Z$, there is an overall unbroken $\mathcal{N}=1$ space–time supersymmetry; otherwise not.

From (2.2) we also see that A and B boundary conditions are Dirichlet and Neumann boundary conditions respectively on the boson ϕ, so φ is analogous to a ''position'' for A boundary conditions and a ''position on the T-dual circle'' for B boundary conditions. We will always use the Dirichlet language in which φ is a position and $U(1)$ charge is a ''winding number,'' even though we discuss B branes, just for pictorial convenience.

The massless Ramond sector can be obtained by spectral flow from $\mathcal{N}=2$ primary chiral states, whose $U(1)$ charge q is equal to the grading $H^{0,q}$ of cohomology in the large volume B brane discussion. In this limit the grade φ of all CY-filling branes is the same, and there is an $\mathcal{N}=1$ supersymmetry. Spectral flow can be used even when space–time supersymmetry is broken, but let us postpone discussion of this point.

B. Grading as a real number

We can now explain the extension of φ from a number defined modulo 2 to a real-valued number. The point is that this extension makes no difference for a single brane, but as soon as we consider pairs of branes a relative integer shift of φ in the boundary condition for one of them will modify the spectrum of strings stretched between them.

There is a familiar construction of D-brane world-volume theories on S^1 (or a torus) which is quite analogous.[20,21] Let us take the circumference to be 2 (like our variable φ); the idea is simply to define D-branes on $S^1 \cong \mathbb{R}/2Z$ as the theory of an infinite set of image D-branes in $\mathbb{R}$, located at lattice points $2n+\varphi$ for $n \in Z$, and quotient by a simultaneous shift in space–time and gauge transformation. As is well known, if we start with Dp-branes with world-volume $U(N)$ $p+1$-dimensional super Yang–Mills (SYM) theory, the resulting theory is equivalent to $p+2$-dimensional SYM theory on a circle with the T-dual radius.

In this context, it is clear that the integer part of φ is not a physical quantum number but rather is a gauge degree of freedom. However, open strings, and other quantities relating to a pair of branes, are labeled by an integer, the difference $m-n$ between the positions of the two images. On this point, the analogy with the grade is quite precise.

A difference between the two problems is that the periodicity in the string spectrum is different: for a single D-brane on S^1, the spectrum has the same periodicity as the images, while in $\mathcal{N}=2$ SCFT there is a more complicated correlation between the $U(1)$ sector and the rest of the theory, as discussed in Refs. 22 and 23. The open string partition function factorizes as a sum of products of partition functions in the two factors, say for strings between branes E and F,

$$Z^{(E,F)} = \sum_p \chi_p^{U(1)} \chi_p^{(E,F)_{\text{rest}}},$$

where the structure of the second factor determines the allowed winding numbers.

The spectrum is periodic under the action of the spectral flow operator. A periodicity between space–time bosons is obtained by acting with its square $e^{iQ_0\phi}$, which shifts the grade by $\hat{c}$. In the case at hand of $\hat{c}=3$, the true periodicity is $2\hat{c}$, as the GSO projection reverses sign under odd shifts.

All this does not invalidate the picture of a brane as having integer spaced images, but requires us to distinguish the images. This gives us a convenient way to picture the winding strings corresponding to higher morphisms, which will be reproduced later in the mathematics.

The antibrane of a brane is defined by reversing the open string GSO projection. This can be accomplished by shifting the fermion number by an odd integer, so these images should be interpreted as the antibrane and its images. We will make this precise by requiring the formalism to be invariant under a simultaneous shift of all gradings by 1 and reversal of all K theory classes, and interpreting this as a gauge symmetry.

C. Topologically twisted open string theory

A ''category'' of branes will be considered to be the set of branes themselves (the ''objects'' of the category) and the spectrum of massless fermionic strings between pairs of branes, or ''morphisms'' of the category. This data for BPS branes obeys the mathematical axioms of a category—in particular, the morphisms have an associative multiplication law which in CFT terms is essentially the multiplication law in the open string chiral ring.

By extension, one can consider all of the holomorphic data involving the branes—the space–time vector and chiral multiplets which contain these fermions, and the superpotential—to be part of the ''category'' as well. All of this data has been claimed to be independent of the Kähler class of the CY (for B branes), implicitly in work on topological open string theory and in Kontsevich's homological mirror symmetry proposal, and explicitly in Ref. 24. One can also give a simple space–time argument for this,[25] based on the fact that in type IIb string compactification (in which the branes can be taken to fill $3+1$ Minkowski dimensions) the Kähler moduli are paired under $\mathcal{N}=1$ supersymmetry with RR potentials, which do not have nonderivative couplings in perturbative string theory. (This answers the question of what determines the coordinates on moduli space for which decoupling holds.)

All this should allow determining the category from large volume considerations. To better understand this, we now consider the B twisted topological sigma model with CY target, following Ref. 15. We start with bosonic coordinates Z^i and $\overline{Z^i}$ and their fermionic partners. After twisting, the fermions split into left and right moving scalars $\eta^{\bar{i}}$ and θ_i, and one-forms ρ^i. The simplest boundary conditions are Neumann;[26] they set $\partial_n Z^i = \partial_n \overline{Z^i}$ and $\theta = (*\rho) = 0$. One can also couple to holomorphic bundles, adding a term $\mathrm{Tr} P \int Z^*(A) - i\rho^i F_{i\bar{J}} \eta^{\bar{J}}$ on the boundary.

States in a Hamiltonian quantization of this theory are determined by their dependence on the zero modes of Z and $\eta^{\bar{i}}$, and can thus be regarded as holomorphic p-forms. The BRST operator Q then satisfies $[Q,Z]=0$, $[Q,\overline{Z^i}] = -\eta^{\bar{i}}$ and $\{Q,\eta\}=0$, which means that it can be interpreted as a $\bar{\partial}$ operator coupled to $E^* \otimes F$. Thus, the topological open string Hilbert space with boundary conditions (E,F) is the Q-cohomology, which is $H^*(X, E^* \otimes F)$. The multiplication law is of course wedge product of forms.

In early studies of D-branes it was found that certain pointlike singularities are allowed and are nonsingular in string theory.[27] This motivates allowing more general coherent sheaves as boundary conditions.[28] The entire discussion can be generalized to this case at least formally by replacing $H^p(X, E^* \otimes F)$ with $\mathrm{Ext}^p(E,F)$, which for a pair of holomorphic bundles is equivalent. We will explain and justify this point later; for this reason we switch to use the Ext notation instead of cohomology. We also remind the reader that $\mathrm{Hom}(E,F) \equiv \mathrm{Ext}^0(E,F)$.

The basic topological correlation function is a disk amplitude, nonzero for a combination of states whose charge adds up to $\hat{c}=3$. This is determined by the algebra structure and the integral on $\mathrm{Ext}^3(E,E)$; this integral can also be regarded as a trace and this structure defines a ''Frobenius category.'' We can also use the integral to define Serre duality, which here identifies $\mathrm{Ext}^{3-i}(E,F) \cong \mathrm{Ext}^i(F,E)^*$.

It is known[4,29] that in general topological open string theory can correspond to an A_∞ category,[30] as appeared in Kontsevich's original proposal. An explicit construction of an A_∞ structure on the category of coherent sheaves appears in Refs. 31 and 32; the higher products are essentially correlation functions in holomorphic Chern–Simons theory (the third order product was already discussed in Ref. 15). They are related to the Massey products, which encode the obstruction theory or equivalently the physical superpotential. This structure is very useful in studying deformations, as we will discuss in subsequent work, but we will not need it for our present considerations. In particular, the A_∞ structure defined in Ref. 32 is a ''minimal model,'' i.e., an A_∞ category with $Q=m_1=0$, which satisfies conventional associativity.

III. TOPOLOGICAL D-BRANES AND THE DERIVED CATEGORY

As we discussed in the Introduction, a complete category of ''topological D-branes'' must contain both branes and antibranes. This might be naturally accomplished by introducing a Z_2

grading on the boundary conditions. However, the discussion of the previous section shows that this is contained in a Z grading of the boundary conditions, and that for $\hat{c}>1$ it is better to keep this, because it is related to the degree of morphisms. (One might instead keep a $Z_{2\hat{c}}$ grading, but there is no real advantage to doing this.)

Let us therefore introduce the notation E_n for a boundary condition located at $\varphi=n$, and the notation $E[n]$ for the shift of a boundary condition $(E[n])_m=E_{n+m}$ (the ''translation functor''). At the end of the discussion we will regard the simultaneous translation of all objects by $E \to E[1]$ combined with reversing all the K theory classes as a gauge symmetry, but until we get there, we will regard these as distinct objects.

As usual we can consider the direct sum of a set of boundary conditions to be a new boundary condition, distinguished by ''Chan–Paton factors.'' Let us generalize the preceding notation: if E is such a direct sum, let E_n be the component located at $\varphi=n$.

A map between two such direct sums E and F is a direct sum of components of definite $U(1)$ charge,

$$\mathrm{Ext}^p(E,F)=\oplus_{n,k}\mathrm{Ext}^{p-k}(E_n,F_{n+k}). \tag{3.1}$$

This formula includes a boundary contribution to $U(1)$ charge, by adding the ''distance'' between the images to the fermion number.

Since we now have $U(1)$ charge living on the boundary, we can make a further generalization to put a boundary component in the BRST operator, consistent with it having charge 1. Thus we write

$$Q_{(E,F)}=Q^{(0)}_{(E,F)}+d_E-d_F$$

with

$$d_E\in\oplus_{n,k}\mathrm{Ext}^{1-k}(E_n,E_{n+k})$$

and similarly for d_F. The operator $Q^{(0)}_{(E,F)}$ is the ''original'' BRST operator (not acting on the Chan–Paton factors) and, if we take all of our states to live in its cohomology, can be taken as zero (this could conceivably be generalized). In this case, the condition $Q^2=0$ will be satisfied if

$$\{d_E,d_F\}=0,$$

$$d_E^2=0,$$

$$d_F^2=0.$$

The first equation is conventional, while the other two tell us that (E,d_E) and (F,d_F) are ''complexes'' as defined in homological algebra. The Q-cohomology then consists of maps ϕ in (3.1) such that $d_F\phi=\phi d_E$ (chain maps) modulo the image of $d_F\epsilon-\epsilon d_E$ (homotopic equivalence).[33]

A. Adding brane-antibrane pairs

The main thing we gain from all of this formalism is the ability to describe branes and antibranes on an equal footing. This requires us to be able to identify an object E with an object F related by adding cancelling brane-antibrane pairs.

Now we want a finer equivalence relation than K theory: a pair $A\overline{B}$ will only be considered to cancel if A and B are isomorphic as holomorphic objects, in other words if there is an identity map 1 in $\mathrm{Hom}(A,B)$.[34] We furthermore require that adding the pair does not change the Q cohomology: for every object G, we have $\mathrm{Hom}(E,G)\cong\mathrm{Hom}(F,G)$.

This can be accomplished by adding a pair $B_n\oplus B_{n+1}$ with grades differing by 1, and taking the new BRST operator $Q_{F,G}$ to be the direct sum of the old BRST operator $Q_{E,G}$ with the identity map **1** on morphisms in $\mathrm{Hom}(B,G)$ involving the brane-antibrane pair:

$$Q_{F,G} = Q_{E,G} \oplus \mathbf{1}.$$

This identity map **1** is the composition $\mathrm{Hom}(B,B)\times\mathrm{Hom}(B,G)\to\mathrm{Hom}(B,G)$. If we had considered the (G,F) open string sector, it would act as $\mathrm{Hom}(G,B)\times\mathrm{Hom}(B,B)\to\mathrm{Hom}(G,B)$. This term in Q of course pairs each $\mathrm{Hom}(B_n,G)$ with a $\mathrm{Hom}(B_{n+1},G)$ and removes them from the topological Hilbert space.

By adding brane-antibrane pairs in various degrees to our original objects, we can get a large class of chain complexes. One can understand the main properties of this construction by thinking of the E_n as vector spaces of Chan–Paton factors and the summands of d as matrices. Although at first it looks like we will only get very special d (made up from identity matrices), of course change of basis (complex gauge transformation) and other operations will produce more general complexes.

We now define our category of topological D-branes as the result of identifying any pair of complexes which are related by the following types of morphisms: the morphism which adds brane-antibrane pairs discussed above, complex gauge transformations, morphisms homotopic to the identity (i.e., those of the form $1+Q\epsilon$ which are equivalent to the identity in Q-cohomology), and of course compositions of any of these. Furthermore, we identify two objects E and F if for each there is a morphism in this class mapping it to a third complex R, their ''common refinement.'' The additional identifications we postulated are unavoidable if we do not wish to distinguish objects related by an isomorphism. There is one subtlety in correctly making these identifications which we now explain. In identifying two configurations which differ by adding brane-antibrane pairs, it does not suffice to only identify configurations related by the direct sum we just discussed; a more general identification is required.

Physically, the point is that we want to identify E with $E+X+\overline{X}$ obtained by adding a cancelling brane-antibrane pair, even if E and X (or E and X) themselves were combined in a bound state, say F. To explain the mathematical point, we quote the incorrect argument from the original version, to see where it was wrong. The mathematical description of forming F as a bound state of the branes E and X is a non-split exact sequence:

$$O\to E \overset{f}{\to} F \overset{r}{\to} X\to 0.$$

By definition, the maps satisfy $r\cdot f=0$. A split exact sequence is one for which $F\cong E\oplus X$, in which case F is not physically a bound state. A bound state can be obtained by this by turning on an off-diagonal bosonic mode, breaking the gauge symmetry back to $U(1)$. Such a mode will again be associated to a partner fermionic open string between E and X, and (by general mathematical formalism we will come back to) to an element of $\mathrm{Ext}^1(X,E)$.

Now the point is that physics (crossing symmetry) requires that one can also make a partial annihilation $F+\overline{X}\to E$, and the same exact sequence must also describe this. This will be true if our identifications equate E with the complex $F\overset{r}{\to}X$. The physical identity of these configurations can also be checked in examples, say in large volume.

One can try to do this using a homotopy equivalence $1+Q\varepsilon$, and this is possible if a partial inverse ε to r can be found, satisfying $r\varepsilon=1|X$. However this is precisely the case in which $F=E\oplus X$ is not really a bound state; the open string mode is not turned on.

These considerations lead us to identify all complexes which are related by general quasi-isomorphisms. A quasi-isomorphism is an element of $\mathrm{Hom}(E^{\cdot}, F^{\cdot})$ the Q-cohomology in our previous language) which is an isomorphism when restricted to cohomology. This includes all the morphisms we discussed, but only transformations which add pairs or sequences of objects which cancel out of the cohomology, both of individual objects and of morphisms between objects.

A quasi-isomorphic pair is a pair of complexes each related by quasi-isomorphism to a common refinement; all such pairs are identified. The result of identifying all quasi-isomporphic pairs is the derived category $D(\mathcal{A})$ of the category $\mathcal{A}$ we started with—in our present discussion **Coh** X, the coherent sheaves on the CY X. As discussed in Ref. 5, this is usually done by

localization, i.e., one allows as morphisms formal inverses of all the quasi-isomorphisms, and then shows that one can write any product of morphisms in terms of a single morphism by commuting these inverses through other morphisms (or ''combining denominators''). The result is an associative category, though not abelian (kernels and cokernels need not make sense).

B. Resolutions and Ext

Resolutions are a key tool in homological algebra, and will turn out to give us a mathematical counterpart of the ''images'' we introduced in the previous section.

A free resolution of a complex E is a quasi-isomorphic complex R in which the terms are free. In the context of vector bundles on projective space $\mathbf{P}^n$ this means they are direct sums of line bundles. The point of this is that it means that there are no relations hidden in the definition of the terms; all the relations, and thus the homology, are explicit in the maps d_R.

Free objects or modules are too restrictive for most purposes and one usually discusses the more general concepts of injective and projective resolution. A projective object is a direct summand of a free object, while an injective object can be defined in terms of this by dualizing and reversing arrows. Considerations we mention shortly lead to a more useful criterion: a projective object P has $\mathrm{Ext}^i(P,X)=0\ \forall X$ and $i>0$, while an injective object I $\mathrm{Ext}^i(X,I)=0\ \forall X$ and $i>0$. An injective resolution of F is an exact sequence

$$0\to F\overset{f}{\to} I^0\overset{r_0}{\to} I^1\overset{r_1}{\to} I^2\to\ldots \tag{3.2}$$

where the I^n are injective, and one can similarly define projective resolutions

$$\cdots\to P^1\to P^0\to F\to 0$$

where the P^n are projective. It can be shown that every coherent sheaf on a space M has a resolution whose terms are locally free sheaves on M, i.e., sheaves which in any local region are equivalent to bundles, and thus the use of resolutions allows reducing general computations to those involving bundles. In particular, they can be used to define sheaf cohomology or better its generalization, the Ext groups. We can define $\mathrm{Ext}^k(E,F)$ as the cohomology H^k of the complex

$$0\to\mathrm{Hom}(E,I^0)\to\mathrm{Hom}(E,I^1)\to\mathrm{Hom}(E,I^2)\to\ldots \tag{3.3}$$

or equivalently as homotopy classes of chain maps from E into the resolution. Using the equivalence of F with its resolution in the derived category, this also tells us that

$$\mathrm{Ext}^p(E,F)\cong\mathrm{Hom}(E,F[p]).$$

In other words, an Ext^p is a degree zero map into the pth term of the resolution. This allows us to think of the successive terms in the resolution as providing a concrete picture for the ''images'' we introduced in the previous section.

We define the *length* of a complex to be the number of nonzero terms E_n minus one. For each object, there is a minimal length of the complex required for its free resolution. The maximal such length for a given category is the homological dimension *hd* of the category; for coherent sheaves on a complex manifold this will generally be the dimension of the manifold (it can be less). This is easy to see for bundles if we assume the relation $\mathrm{Ext}^k(E,F)\cong H^k(M,E^*\otimes F)$ and consider (3.3).

The relation between the length of the complex and the highest Ext group which can appear has another consequence, namely that one cannot get all sheaves on a d-fold by using resolutions of length less than d. In particular, the monad construction (which is closely related to this) with a complex of length two and with line bundles as constituents cannot describe all bundles on a generic Calabi–Yau three-fold. It would be interesting and probably quite useful if linear sigma models could be generalized to use longer complexes.

C. Properties of the derived category of coherent sheaves

As we mentioned in the Introduction, the derived category of coherent sheaves contains far more information than the K theory. An illustration of this is the reconstruction theorem of Bondal and Orlov:[35] in certain cases (with ample or anti-ample canonical bundle; this excludes Calabi–Yau), the variety X is determined by $D(\mathbf{Coh}\,X)$. The strategy is to first identify the set of objects corresponding to points; the morphism information can then be used to put a topology on this set and show that it is indeed the expected variety.

Although this result is not literally true for a Calabi–Yau, the reason that it fails is quite interesting and relevant for us. It is that there is not a unique definition of which objects are the points. Indeed, there are ''autoequivalences'' of the derived category—transformations which permute the objects but preserve the structure of the morphisms—which turn the points into other sheaves (or complexes).

These autoequivalences have been much studied in recent mathematical work and all of them can be obtained as Fourier–Mukai transformations (FMTs). A FMT from sheaves on a space X to sheaves on a space Y (possibly the same as X) is defined by specifying a sheaf $\mathcal{F}$ on $Y\times X$ satisfying certain properties; most notably, the restrictions to two points on X $\mathcal{F}_{x_1}$ and $\mathcal{F}_{x_2}$ must satisfy

$$\mathrm{Hom}(\mathcal{F}_{x_1},\mathcal{F}_{x_2})\cong\mathbb{C} \quad \text{if } x_1=x_2;$$

$$=0 \quad \text{if } x_1\neq x_2.$$

The transform of a sheaf E on X is then

$$\hat{E}=R\pi_{Y*}(\mathcal{F}\otimes^L\pi_X^*E). \tag{3.4}$$

The idea expressed by this formula is simple and well explained in Ref. 36: one pulls back E to the product space, tensors with $\mathcal{F}$, and then ''pushes forward'' in the sense that the resulting sheaf can have as local sections any of the local sections of the product sheaf (this construction is referred to as the ''direct image''), but with the dependence on X suppressed—this is the reason for the name ''Fourier,'' as taking all such sections is like integrating over X.

The detailed implementation of this idea requires resolving the sheaves which appear in intermediate steps (this is the meaning of the ''L'' and ''R'' symbols), and is greatly simplified by working with the derived category.

A particularly simple set of FMTs are the ''twist functors'' discussed in detail in Ref. 7. For every sheaf E on X there is a twist functor $\mathcal{T}_E$, which has all the right properties to correspond physically to a monodromy associated to a loop in Kähler moduli space around a point at which $Z(E)=0$, such as a conifold point. Assuming this is so, all of these monodromies preserve the derived category of topological branes and this is fairly strong evidence that any physical construction of a model associated to a CY with a specific complex structure will produce the same derived category of objects.

We will discuss this in more detail elsewhere; here we will motivate the theorem of Beilinson used in Ref. 3 using these ideas. This states that the derived category of sheaves on $\mathbb{P}^n$ is equivalent to the derived category of representations of the quiver-complex $QC(n+1,n+1)$ (to be defined in Sec. V), with $Y=0$.

This comes from a one-to-one correspondence between sheaves, implemented by a FMT in which $\mathcal{F}$ is a sheaf on $\mathbb{P}^n\times\mathbb{P}^n$ which is just the ''delta function'' (or structure sheaf) supported on the diagonal. Such an $\mathcal{F}$ will clearly produce the identity transformation on E.

The nontrivial content of this construction comes when we look at the resolution of this delta function sheaf. This is the ''Koszul resolution'' which is a complex with successive terms

$$\Lambda^n\Omega_Y(n)\times\mathcal{O}_X(-n)\to\ldots\to\Omega_Y(1)\times\mathcal{O}_X(-1)\to\mathcal{O}_Y\times\mathcal{O}_X\to\mathcal{F}.$$

The tensor product appearing in (3.4) is

$$\mathcal{F}\otimes E=\Lambda^n\Omega(n)\otimes E(-n)\rightarrow\ldots\rightarrow\Omega(1)\otimes E(-1)\rightarrow\mathcal{O}\otimes E$$

and, continuing in this vein, one finds that the FMT (which is equivalent to the original object in the derived category) is a complex of the sheaves $\Lambda^p\Omega_Y(p)$ tensored with the cohomologies of the original sheaf $H^m(E(-p))$. If these cohomologies are nonzero in a single degree m, they can be thought of as defining an object in $QC(n+1,n+1)$, providing the correspondence used in Ref. 3, while if they are nonzero in more than one degree, one gets an object in $D(QC(n+1,n+1))$.

IV. KÄHLER MODULI AND FLOW OF GRADING

Having understood the category of boundary conditions in the topological string theory (or-''topological D-branes''), we now can assert with confidence that every physical D-brane corresponds to a unique topological D-brane. We now want to understand why not every topological D-brane corresponds to a physical D-brane.

In particular, let us explore what happens if we start with a BPS configuration of two branes and then vary the Kähler moduli. In general, the grades of the two branes, φ_1 and φ_2, will no longer be equal.

Although open string sectors with $\varphi_1\neq\varphi_2$ bear some resemblance to twisted $\mathcal{N}=2$ sectors, they are not the same. Because a specific $\mathcal{N}=1$ world-sheet supersymmetry is gauged in the open superstring definition, this supersymmetry must still have conventional NS and R boundary conditions on the $\mathcal{N}=1$ supercurrents. Furthermore, it will still admit a GSO projection; two sectors related by a continuous deformation will share the same GSO projection. This is possible because both bosons and fermions in these sectors will have their moding changed; the fermions in a way determined by (2.2) and the bosons in a corresponding way to make NS and R supercurrents possible. A solvable example in which this can be seen is the theory of two three-branes oriented at angles.[37]

As discussed earlier, if we restrict ourselves to Kähler variations, the massless fermion sector will remain unchanged. Now even though these combinations of boundary conditions have broken supersymmetry, we can still identify bosonic partners of the massless fermions as the NS sectors accessible by varying the $U(1)$ charge (spectral flow). Another way to say this is that since the individual boundary CFT's correspond to BPS branes, they each have spectral flow operators, and we can use either of these to define the action of space–time supersymmetry. Depending on which one we use, we will get different results, but these will only differ by a phase. Thus we can still identify a unique NS state as the superpartner.

Let us discuss the various physical states in the CFT we obtain by this construction, and their space–time interpretation. We start with NS states in a sector with $\Delta\theta=0$ and the usual $\mathcal{N}=1$ supersymmetry. Let Q be the $U(1)$ charge in the $\mathcal{N}=2$ algebra; then $Q=q=0$ states are gauge bosons (the standard GSO projection will keep only states $\psi^\mu_{-1/2}|\rangle$ in the space–time CFT) while $Q=q=\pm1$ states are bosons in chiral multiplets ($q=-1$ will be the complex conjugates of the $q=+1$ states).

Varying the relative grading will shift the $U(1)$ charge of all of the states in this list, and preserve the GSO projection. Our conventions are such that the charge shift is equal to the shift in grading, $\Delta q=\Delta(\varphi_1-\varphi_2)$.

Let us write the Ramond vertex operator as a product of internal, bosonized $U(1)$ and space-time factors

$$O_\theta e^{i(q-3/2)\phi}V_{3+1}.$$

As previously discussed, varying φ by only varying the Kähler class keeps the Ramond state massless, and this means that the dimension of O_θ is determined by $h(O_\theta)+(q-3/2)^2/6=\frac{3}{8}$. We can then derive the dimension of the operators related to it by the usual $\mathcal{N}=2$ spectral flow and thus the mass squared of the partner NS states with $U(1)$ charge q. These will be

$$m^2=\frac{3}{8}+\frac{q^2}{6}-\frac{(q-3/2)^2}{6}-\frac{1}{2}$$

$$=\frac{1}{2}(q-1) \tag{4.1}$$

for chiral multiplets. A vector multiplet has $V_{3+1}=\psi^\mu$, so $m^2=q/2$.

The bosons in chiral multiplets come from $q=1$ states, and we see from this that $\Delta\varphi$ enters into their mass squared precisely as a Fayet–Ilipoulos term would. This is the CFT argument for the earlier description of BPS decay by D-term supersymmetry breaking[38,39,2] and indeed these masses can often be modelled by assigning the FI terms associated to the $U(N)$ space–time gauge groups of the two groups of branes the values $\zeta_1=\varphi_1$ and $\zeta_2=\varphi_2$. Starting from an Ext^1 (a massless chiral multiplet), this assignment reproduces (4.1). This explicit $\mathcal{N}=1$ field theory picture has its limitations, however, as seen in Ref. 40 and it is for this reason that, although the formalism and results are very similar to those in $\mathcal{N}=1$ supersymmetric field theory, we have not based our discussion on this similarity but instead on CFT.

We should also mention at this point that in our setup, the precise definition of a theory with tachyonic strings between a pair of branes is to take branes which do not fill Minkowski space (e.g., D0-branes) and separate them in these dimensions. This gives the tachyons large masses and makes the configuration with zero tachyon expectation value stable, while still allowing us to argue that such a configuration of coincident branes would be unstable.

Starting from $q=1$ and making such a flow, m^2 can decrease until we reach $q=0$. At this point, the operator O_θ has dimension zero. Because the world-sheet theory is a (correlated) product of a unitary theory with the bosonized $U(1)$, zero is the minimal possible dimension for O_θ. Thus, if we decrease q further, our assumptions must break down. One also knows from $\mathcal{N}=2$ representation theory that chiral operators must have $0\leqslant q\leqslant\hat{c}$ (for the same reason).

Now the boundary states we are discussing were unstable as soon as we had $q<1$ and a tachyonic open string; we interpret these arguments as showing that, nevertheless, we can treat them as sensible boundary states and use them to define a category of boundary states as discussed earlier, but only as long as $q\geqslant 0$. If $q<0$, the massless Ramond state no longer makes sense in unitary CFT, and must disappear from the theory. Note that it is not becoming massive (in general there is no state for it to pair with) but literally disappearing, which can only happen if one or both of the boundary states also disappear from the theory.

This is the essential subtlety in the relation between topologically twisted open string theory and the physical open string theory. From the point of view of topological theory, there is nothing wrong with these boundary states (since we varied only Kähler moduli, nothing changed). One can even keep track of the $U(1)$ charges in this situation: the same additive conservation laws will hold even though some $U(1)$ charges may be negative. However, any given physical CFT can only realize a subset of these boundary states, chosen so that morphisms of negative degree do not appear.

From our arguments, the choice of which boundary states are realized would be expected to depend on Kähler moduli. Starting from an Ext^1 between a pair of simultaneously BPS branes, one can reach $q=0$ if the relative phase difference reaches π, i.e., if the BPS central charges antialign. In this sense, the phenomenon under discussion has to do with branes turning into antibranes.

A. Special Lagrangian picture

Many of the statements we just made can also be seen from the geometry of the A brane picture.[41] The analog of a coherent sheaf in this picture is an isotopy class of Lagrangian manifolds, while a physical brane is a particular Lagrangian in this class satisfying the ''special'' condition for the chosen complex structure and holomorphic three-form. The morphisms are given by Floer cohomology.

The standard convention for the grading on Floer cohomology agrees with our notations Hom and Ext^1 for vector and chiral multiplets, respectively. To determine this grading, one looks at the

three relative angles $\Delta\theta_i$. There are basically two cases: where these all have the same sign (producing a Hom), or where one sign differs from the other two (producing an Ext). This rule agrees with the physical GSO projection in the branes at angles model of Ref. 37.

In these terms, our grading is $\mathrm{Hom}(A,B[n])$ or $\mathrm{Ext}^1(A,B[n])$ with $n=\Sigma_i\Delta\theta_i$. As one varies the complex structure, the $\Delta\theta_i$ will vary, leading to the flow we just described. In this picture, the reason the gradings cannot flow below zero (or above $\hat{c}$) is that given a pair of Lagrangians which intersect transversely they will continue to intersect transversely under any change of complex structure.

The conclusion is the same, that gradings will flow, but cannot flow below zero for physical objects.

B. Some convenient notation

As we motivated earlier (in terms of resolutions and the derived category), we will denote a morphism with $U(1)$ charge n, i.e., a fermionic string between the brane A and the nth image of the brane B, as an element of $\mathrm{Hom}(A,B[n])$. This group depends only on the difference between the grades: $\mathrm{Hom}(A,B[n])\cong\mathrm{Hom}(A[m],B[n+m])$.

In addition to its other mathematical advantages, this notation makes it simple to express the variation of the $U(1)$ charge of the morphism as we vary the Kähler moduli. It simply comes from varying the grades of the two branes: $\mathrm{Hom}(A,B[n])$ will flow to $\mathrm{Hom}(A[\Delta\varphi(A)],B[n+\Delta\varphi(B)])$.

We now introduce a notation which allows us to keep track of both our new grading and the ''original'' grading (that present in Floer cohomology), since both are needed in string theory. We distinguish the massless fermions leading to chiral and vector multiplets by writing a degree n morphism as $\mathrm{Hom}(A,B[n])$ for a gaugino and $\mathrm{Ext}^1(A,B[n-1])$ (or just Ext) for the fermion in a chiral multiplet. (One motivation for this notation is the observation that the partner boson has m^2 proportional to the quantity in brackets in both cases.)

The two groups Hom and Ext as we defined them are related by double spectral flow, which reverse the GSO projection. This tells us that $\mathrm{Hom}(A,B[n])\cong\mathrm{Ext}(A,B[n+\hat{c}-1])$ and thus Ext is not really independent.

We define the antibrane $\overline{A}$ to a brane A by reversing the GSO projection, so $\overline{A}\cong A[\hat{c}]$. Any simple brane A [with gauge group $U(1)$] will have $\mathrm{Hom}(A,A)\cong\mathbb{C}$, and we can infer the existence of the brane-antibrane tachyon $\mathrm{Ext}(A,\overline{A}[-1])$ from this. More generally one has $\mathrm{Hom}(A,B[n])\cong\mathrm{Ext}(A,\overline{B}[n-1])$.

In the large volume limit, we can use Serre duality to infer the existence of additional morphisms. In the CY theories of prime interest for us, this takes the form $\mathrm{Hom}(A,B[n])\cong\mathrm{Hom}(B,A[\hat{c}-n])^*$. This is a dual relation, not an identification, but can of course be used to relate the dimensions of these spaces. Its most fundamental role in this discussion is that it is the inner product of the topologically twisted open string theory [the shift $\hat{c}$ is the anomalous $U(1)$ charge of the disk].

In our application, this duality also reverses the GSO projection. This is because $\hat{c}$ is odd, so the Serre dual morphism will have opposite parity $U(1)$ charge, and we infer the GSO projection directly from this. This leaves us with the rule

$$\dim\ \mathrm{Hom}(A,B[n])=\dim\ \mathrm{Ext}^1(B,A[\hat{c}-n-1]). \tag{4.2}$$

These rules determine the gradings of morphisms at arbitrary points in Kähler moduli space given the gradings at one point. It is natural to start with the large volume limit as this point. One should note that gradings of morphisms between branes of different dimension (i.e., sheaves with support of different dimension) in our conventions do not agree with the usual grading of cohomology. We can get them either by carefully computing $U(1)$ charges, or masses of partner

bosons in CFT. The latter generally can be obtained from standard D-brane considerations;[42] in particular the lightest NS string between a Dp-brane and a Dq-brane has $m^2=|p-q|/8-\frac{1}{2}$ from the shift of the ground state energy due to ''DN bosons.''

This gives a morphism from a Dp-brane to a Dq-brane degree $n+(p-q)/4$ (one must be careful about orientations in identifying both objects as ''branes''). Taking this rule into account along with the large volume asymptotics for the periods, one finds that morphisms between simultaneously BPS branes (those whose grades differ by integers) will always have integer grading.

Another large volume subtlety we should mention is that one needs to be careful to define the grade in a way which depends smoothly on the Chern classes (the branch of the logarithm cannot jump). This in particular corrects an observation made in Ref. 3—by doing this, one can get the large volume limit of Π-stability to reproduce Gieseker stability in all cases (this comes from the dependence of subleading terms on the higher Chern classes). This is important as otherwise one finds many incorrect predictions—for example, ideal sheaves of points will destabilize the trivial line bundle unless one has Gieseker stability.

V. EXAMPLES OF FLOW OF GRADING

Two classes of examples have been studied in some detail: orbifolds $\mathbb{C}^3/Z_K$, and Gepner models or Landau–Ginzburg orbifolds, which in a certain sense are hypersurfaces in $\mathbb{C}^5/Z_K$ orbifolds. We will not review here the discussion of Refs. 24, 43, 3, and 40, which leads to the following identifications of boundary states and quiver theories, but only cite the results.

For the most recent work on Gepner models, see Refs. 44–46.

A. Quiver-complex theories

Besides defining the quiver theories which will appear in our examples, this subsection defines the quiver Ext groups, which will be compared with their large volume analogs, and illustrates how methods of homological algebra can be helpful in analyzing their moduli spaces of supersymmetric vacua.

Let us consider a theory with p gauge groups, $U(n_1)\times U(n_2)\times\cdots\times U(n_p)$, and a global $U(q)$ symmetry. The matter spectrum is bifundamentals X_i^a in the $(\overline{n_i},n_{i+1})$ for each $1\leqslant i\leqslant p-1$ and in the fundamental of $U(q)$, and bifundamentals $Y_i^{[ab]}$ in the $(\overline{n_{i+2}},n_i)$ for $1\leqslant i\leqslant p-2$ in the antisymmetric $[q-2]$ representation of $U(q)$. For $p>2$ there is a superpotential,

$$W=\sum_{i=1}^{p-2}\mathrm{tr}X_{i+1}^aX_i^bY_i^{[ab]}. \tag{5.1}$$

We will consider the category $QC(p,q)$ whose objects are (classical) solutions of the F-flatness constraints for all of these theories.

The simplest operation we can define for these objects is direct sum, and this allows us to define K theory in the usual way in terms of pairs of objects. Any ''topological'' definition of K theory class will not see the configuration (the X's and Y's can be continuously deformed to zero); thus the K theory class of an object is just the set of integers n_i.

It is also clear that the K theory class is only the most basic invariant of an object; in general the objects come in moduli spaces of finite dimension. For $p=2$, there is an obvious formula for the dimension of this moduli space, valid if the object is simple, i.e., breaks the complexified gauge group to $GL(1)$. It is

$$d=1+qn_1n_2-n_1^2-n_2^2, \tag{5.2}$$

obtained by counting matter fields modulo gauge symmetries. This formula generalizes in an obvious way to any quiver theory with no superpotential.

It turns out that there is no such universal formula which gives the dimension of moduli space just in terms of the K theory class for $p>2$. (There is a formula which works in almost all cases

for $p=3$ and $q\leqslant 3$, but not for higher p or q.) Well-known arguments that such a formula is not to be expected in general $\mathcal{N}=1$ theories are the possibility of lifting arbitrary pairs of chiral multiplets by changing the configuration, and the existence of cases in which the moduli space has several branches of different dimension.

One can, however, go further than these general statements by better understanding the problem. Given a superpotential, one might try to predict the dimension of the moduli space by subtracting the number of relations following from $W'=0$ from the prediction (5.2). Since there is one relation for each matter field, this always leads to a negative dimension and would predict that no solutions exist. In fact solutions can exist, but only when the relations are redundant; these redundancies will depend on the specific configuration.

The redundancies between relations in the quiver complex theory can be understood in homological terms. We start by considering only the configurations with $Y=0$; the relations are then

$$X^a_{i+1}X^b_i = X^b_{i+1}X^a_i\,,$$

which can be expressed (for $q\geqslant p$) as $d^2=0$ on a complex of vector spaces. This complex can be defined in terms of an exterior algebra ΛV where $V\cong\mathbb{C}^q$ has a basis e_a which we think of as anticommuting objects: $e_ae_b+e_be_a=0$. The operator d then acts on an element of $E_i\equiv\mathbb{C}^{n_i}\otimes\Lambda^{i-1}V$ to produce an element of E_{i+1} as multiplication by X^ae_a.

One then defines the ''morphism complex'' as follows. A ''chain map'' $\phi^{(n)}$ of degree n from E to F is a set of linear maps $\phi^{(n)}_i$ from E_i to F_{i+n} which can be written in terms of the e_a; i.e.,

$$\phi^{(n)}_i = \phi^{(n)}_{i,a_1\ldots a_n}e_{a_1}\cdots e_{a_n}.$$

One can then regard d_F-d_E as an operator acting on these chain maps; it squares to zero, so we can define a morphism of degree n as an element of its cohomology. The space of such morphisms will be denoted $\mathrm{Ext}^n(E,F)$ [or $\mathrm{Hom}(E,F)$ for $n=0$].

All of this is very parallel to the discussion we made in Sec. III and the reader may be wondering why we repeated it. The main reason is that while formally it is very parallel, physically its interpretation is rather different: in particular, we do not make the identifications we made in Sec. III, but instead interpret configurations just as we would in supersymmetric gauge theory (identifying only configurations related by complex gauge transformation). The result is (at least mathematically) an Abelian category to which one can then apply the construction of Sec. III, considering complexes of these complexes and forming the corresponding derived category. This is the type of derived category which, according to Beilinson's theorem, will be equivalent to derived categories of coherent sheaves.

Returning to concrete considerations, these definitions lead immediately to a formula for the relative Euler character:

$$\chi(M,N)\equiv\sum_{k=0}^{p}(-1)^k\dim\ \mathrm{Ext}^k(M,N)=\sum_{1\leqslant i\leqslant j\leqslant p}(-)^{i-j}\binom{q}{i-j}m_in_j\,. \tag{5.3}$$

This is proven by showing that $\chi(M,N)$ is ''topological'' (invariant under deformations of the X's), so that one can compute it for $X=0$.

Before going on to the generalization with $Y\neq 0$, let us discuss the physical meaning of this construction. It is not hard to see that elements of $\mathrm{Hom}(E,F)$ correspond to (complex) gauge symmetries which appear when we combine the theories E and F (the cohomology condition says that the matter configuration is preserved by this gauge transformation). Similarly, elements of $\mathrm{Ext}^1(E,F)$ correspond to massless matter multiplets (or linearized moduli): elements of cohomology correspond to deformations which are not lifted by the superpotential and are not pure gauge.

The higher Ext^n's do not admit such an obvious interpretation but clearly have to do with relations between the superpotential relations; when these exist, one cannot derive the dimension of moduli space, which is $\dim \mathrm{Ext}^1(E,E)$, just from the formula (5.3): one needs more information (such as the dimensions of the higher Ext groups).

In the case at hand, there is a second physical interpretation of $\mathrm{Ext}^2(E,F)$: it counts massless deformations of the Y multiplets. This can be seen by considering the ''physical'' inner product on $\mathrm{Ext}^n(E,F)\times\mathrm{Ext}^n(F,E)^*$ defined as

$$(\phi,\psi)=\sum_{i=1}^{p-n}\mathrm{tr}\,\phi^+_{i+n}\psi_i$$

and the adjoint to d defined by

$$(\phi^{(n)},d^*\psi^{(n+1)})=(d\phi^{(n)},\psi^{(n+1)}).$$

Now the F-flatness conditions on Y are linear, $X^aY_{[ab]}=Y_{[ab]}X^b=0$, and in fact are just $d^*Y=0$. The relation to Ext^2 then comes from the usual Hodge-style arguments that we can find a unique representative of each cohomology class satisfying $d^*Y=0$ and that all solutions of these equations arise in this way.

This result is very suggestive of the relation $\mathrm{Ext}^2(E,F)\cong\mathrm{Ext}^1(F,E)^*$ valid on a Calabi–Yau threefold, and indeed one expects such a relation to hold for any quiver theory which arises in this context. Morally speaking, the superpotential (5.1) is a finite dimensional analog of the holomorphic Chern–Simons functional.

Indeed, as explained in Refs. 3 and 40, the case $p=q=3$ is the $\mathbb{C}^3/Z_3$ quiver theory, while $p=q=5$ describes sheaves on the quintic CY, and the other CY theories which arose in Ref. 40 can be treated similarly. Unlike the analogous formula for sheaves on a CY_3, $\chi(E,E)$ can be nonzero; this is because one has separately described deformations which made sense on the ambient projective space (the X's) and those which appear on restriction (the Y's).[47] However, since $\dim \mathrm{Ext}^2$ enters into (5.3) with the wrong sign, one still needs more information than $\chi(E,E)$ to compute the dimension of the moduli space. [In special cases, the situation can be simpler; for example, in the $\mathbb{C}^3/Z_3$ quiver one can show that $\mathrm{Ext}^2(E,E)=0$ except for the D0-brane.]

This is made particularly clear by considering examples in which the moduli space has branches of different dimension; these branches will differ in $\dim \mathrm{Ext}^2$. A simple example of this type is the quiver with $n_1=1$, $n_2=2$ and $n_3=1$ in $QC(3,5)$ which appears as a rational boundary state $|11000\rangle$ in the quintic Gepner model;[24] this moduli space has branches of dimension 5, 7 and 11, distinguished by $\dim \mathrm{Ext}^2=0$, 1 and 3. The last of these must describe the rational boundary state.

These considerations define the morphisms in the quiver categories we are about to discuss; their gradings are always CFT $U(1)$ charges, which agree with the gradings we just defined for the $\mathbb{C}^3$ orbifold example (and in general if the fractional branes are simultaneously BPS), but must instead be taken from CFT in the Gepner model example (since the fractional branes are not simultaneously BPS).

We went into more detail than was required for this, to make the point that these are concrete examples which capture the complexities of categories of sheaves on Calabi–Yaus (and indeed are equivalent to them once one goes to the derived category) but for which computing the dimensions of homology groups (and thus of the local moduli space) is just a problem of linear algebra. Thus such problems, while not as easy as the cases with more supersymmetry, are by no means inaccessible.

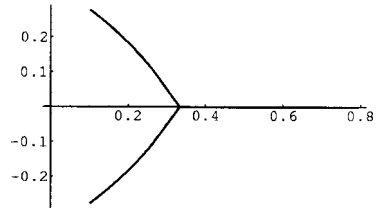

FIG. 1. The evolution of the central charges $Z(B_i)$ for fractional branes in $\mathbb{C}^3/Z_3$ from large volume, where they asymptote to $Q_4(B+iV)^2$, to the orbifold point where they are all equal.

B. The $\mathbb{C}^3/Z_3$ orbifold

This leads to a quiver-complex theory of type $QC(3,3)$. At large volume the orbifold is resolved to $\mathcal{O}_{\mathbb{P}^2}(-3)$ and the three elementary or fractional branes can be identified[43] with the bundles (always on $\mathbb{P}^2$) $B_1 \equiv \mathcal{O}(-1)$, $B_2 \equiv \overline{\Omega}(1)$ (the antibrane to the twisted cotangent bundle) and $B_3 \equiv \mathcal{O}$.

We first discuss the morphisms at the orbifold point. The quiver theory implicitly tells us what these are; since all nine chiral multiplets are massless we see that $\dim \mathrm{Ext}^1(B_i,B_j) = 3\delta_{j\equiv i+1(3)}$.

We next discuss the morphisms at large volume. We can use standard methods to compute morphisms from sheaves to sheaves, and then use the rules in Sec. IV B to infer the morphisms to ''antisheaves'' such as B_2. The elementary morphisms correspond to multiplication by the homogeneous coordinates: we have $\dim \mathrm{Hom}(B_1,B_3)=3$ and (using the Euler sequence) $\dim \mathrm{Hom}(B_1,\overline{B_2}) = \dim \mathrm{Hom}(\overline{B_2},B_3)=3$. Using the rule that $\mathrm{Hom}(A,B)\cong \mathrm{Ext}^1(A,\overline{B}[-1])$ we can also say that $\dim \mathrm{Ext}^1(B_1,B_2[-1]) = \dim \mathrm{Ext}^1(B_2,B_3[-1])=3$. These ''brane-antibrane'' pairs naturally come with tachyonic open strings. Finally, the morphisms $\mathrm{Hom}(B_1,B_3)$ have Serre duals, which according to our previous discussion are $\mathrm{Ext}^1(B_3,B_1[2])$'s.

We can now check that the two limits are related under the flow from large volume to orbifold point. Referring to Fig. 1, we see that $B_1 \to B_1[-1]$, $B_2 \to B_2$, and $B_3 \to B_3[1]$, and all of the morphisms we discussed work. We also see that the superpotential satisfies topological charge conservation, as the sum of the gradings ''around the triangle'' is always 3.

One wants to check that all the morphisms agree, not just these defining ones. This should follow from the equivalence of derived categories established in Ref. 47, which is between representations of the $\mathbb{C}^3/Z^3$ quiver and sheaves with compact support on the resolution $\mathcal{O}^2_{\mathbb{P}}(-3)$. The relation discussed in Ref. 3, between the quiver with some links set to zero and sheaves on $\mathbb{P}^2$, is a subset of this.

From a physical point of view, the difference between sheaves with compact support on $\mathbb{P}^2$ and on $\mathcal{O}^2_{\mathbb{P}}(-3)$ is that a D-brane wrapped on $\mathbb{P}^2$ in the second theory has an extra world-volume field corresponding to the coordinate transverse to $\mathbb{P}^2$, i.e., a chiral multiplet taking values in the line bundle $\mathcal{O}^2_{\mathbb{P}}(-3)$, and the corresponding additional morphisms. Thinking about the D-brane world-volume as a topologically twisted theory[48] shows that the fermion in this multiplet lives in $\mathrm{Ext}^1(E,F\otimes \mathcal{O}_{\mathbb{P}^2}(-3))$. Another way of deducing these morphisms is by using Serre duality twice, first on the total space and then on $\mathbb{P}^2$, which on a Hom amounts to tensoring with this one-form. Because of this, Serre duality on $\mathbb{P}^2$ also leads to relations on the morphisms.

As an example (coming from Ref. 3), we cite $\mathrm{Hom}(\mathcal{O},\mathcal{O}(-3))$ which is nonzero at the orbifold point. Flowing this back produces $\mathrm{Hom}(\mathcal{O}[-1],\mathcal{O}(-3)[1])$ in large volume which indeed agrees with $\dim H^2(\mathcal{O}(-3),\mathbb{P}^2)=1$. The Serre dual to this is the $\mathrm{Ext}^1\mathcal{O}^2_{\mathbb{P}},\mathcal{O}^2_{\mathbb{P}}(-3))$ we just discussed.

C. Gepner models

A product of five $\mathcal{N}=2$ minimal models A_{k_i} with $3=\Sigma_i 1-2/(k_i+2)$, so $\Sigma_i 1/(k_i+2)=1$. Let $K=\mathrm{lcm}(k_i+2)$ and $w_i=K/(k_i+2)$; this corresponds to a Fermat hypersurface in $WP(w_i)$ at a special point in Kähler moduli space with Z_K quantum symmetry.

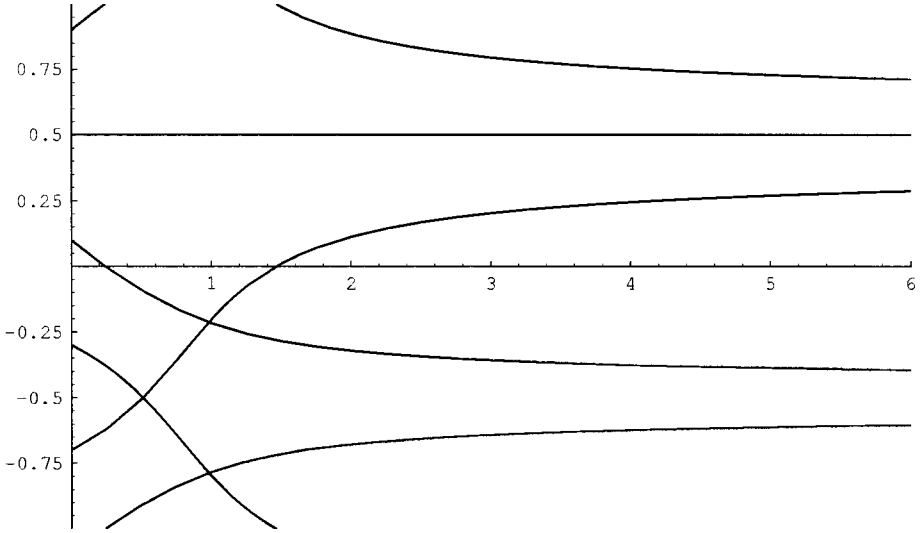

FIG. 2. The evolution of the grades for fractional branes on the quintic from the Gepner point [where $\varphi(B_k)=2k/5-\frac{7}{10}$] to large volume, where they asymptote to $\pm\frac{1}{2}$.

A useful subset of boundary states are the rational $L=0$ states with various M values. Their intersection form (counting massless Ramond strings) is

$$I=\prod_i (1-g^{w_j}). \tag{5.4}$$

The field corresponding to g^{w_j} in this expression (call it X^i) has an NS partner which is nontrivial only in the jth minimal model, where it is the chiral primary $\phi_{(k_i,k_i,0)}$. Thus it has $U(1)$ charge $1-2/(k_i+2)=1-2w_i/K$ and corresponds to a morphism of this degree. The field $Y_{[ij]}$ corresponding to $g^{w_i+w_j}$ is nontrivial in the other three minimal model factors, and has $U(1)$ charge $3-2\Sigma_{l\neq i,j}w_l/K$.

As argued in Ref. 40 the leading term in the superpotential is the cubic term (5.1). The constraints on the k_i guarantee that the degrees of $X^iX^jY_{[ij]}$ add up to 3 and thus this cubic term should correspond directly to the flow of a similar term computed at large volume. Perhaps more interestingly, a product of five fields including one of each X^i also has degree 3. These facts and the direct relation between the gradings of the morphisms and the $\Delta\varphi$ between pairs of branes go a long way towards guaranteeing that the flow will produce sensible large volume gradings; however, there is still something nontrivial to check, namely that the winding numbers of the gradings along the flow are as predicted.

We now consider the quintic with $w_i=1$. The five fractional branes are exterior products of a twisted cotangent bundle on $\mathbb{P}^4$, restricted to the quintic: $B_1=\mathcal{O}(-1)$, $B_2=\overline{\Omega}^3(3)$, $B_3=\Omega^2(2)$, $B_4=\overline{\Omega}(1)$, and $B_5=\mathcal{O}$. Their grades φ are plotted as a function of moduli along the C axis (in the conventions of Ref. 1) in Fig. 2.

The computation of the morphisms at large volume is straightforward as the restriction from $\mathbb{P}^4$ is trivial (it is given by tensoring with the exact sequence

$$0\to\mathcal{O}_{\mathbb{P}^4}(-5)\xrightarrow{f}\mathcal{O}_{\mathbb{P}^4}\to\mathcal{O}_X\to 0,$$

and for the maps we are considering, the first term gives zero). By considerations similar to the previous example, we find $\dim \mathrm{Ext}(B_i,B_{i+1}[-1])=5$ for $1\leqslant i\leqslant 4$, and $\dim \mathrm{Ext}(B_5,B_1[2])=5$.

We also have the composition of two successive Hom's which give $\dim \mathrm{Hom}(B_i, B_{i+2}) = 10$ and its Serre dual $\dim \mathrm{Ext}(B_{i+2}, B_i[2]) = 10$ for $1 \leqslant i \leqslant 3$, and three Hom's giving $\dim \mathrm{Ext}(B_i, B_{i+3}[-1]) = 10$ for $1 \leqslant i \leqslant 2$.

Going to the orbifold point, one has $\Delta(\varphi_{i+1} - \varphi_i) = \frac{3}{5}$ for the pairs $1 \leqslant i \leqslant 4$, leading to the first four degree $\frac{3}{5}$ morphisms X, while $\Delta(\varphi_1 - \varphi_5) = \frac{3}{5} - 3$ (since the sum is zero) leading to the fifth X. The Y morphisms work similarly (since the sum of degrees around each XXY triangle is 3).

VI. PHYSICAL BRANES AS A SUBCATEGORY OF TOPOLOGICAL BRANES

We now address the question of how to identify the physical branes at a specific point in Kähler moduli space $\mathcal{M}_k$.

One approach to this uses the close analogy between general lines of marginal stability, and the ''wall crossing'' associated with variation of μ-stability, which determines whether a holomorphic bundle admits a Hermitian Yang–Mills connection. This idea was developed in Ref. 2 into the proposal that BPS branes are the Π-stable objects. An object E is Π-stable if every subobject E' [i.e., one for which there is an injective $\mathrm{Hom}(E', E)$] satisfies $\varphi(E') < \varphi(E)$. Further discussion of this idea appears in Ref. 49.

Although well motivated, the difficulty in combining this proposal with the present considerations is that the derived category is not an Abelian category and does not have a notion of ''kernel'' or ''subobject.'' The basic reason for this is extremely simple: since we identify A with any combination $AB\overline{B}$ where $B\overline{B}$ is the trivial brane-antibrane bound state (a complex with the identity map), any brane B appears to be a subobject of A.

This point is not just academic, as one can check in examples (as we will do shortly) that the subobject relation is different at different points in $\mathcal{M}_k$.

To better understand this point, we will need to understand what universal structure underlies exact sequences and subobjects in the derived category, and how different Abelian categories can sit in the same derived category.

A. Triangulated categories and bound state formation

In the references, it is shown that derived categories are not Abelian; in particular there is no idea of exact sequence. Since every subobject relation $0 \to E' \to E$ can be completed to an exact sequence, this is the key point in making sense of Π-stability in this general context.

The closest analog to exact sequences are the ''distinguished triangles.'' Let us explain what these are in the context of the derived category $D(\mathcal{A})$ formed from the Abelian category $\mathcal{A}$. (One can axiomatize this structure and talk about triangulated categories which are not necessarily derived in this way, but we will not use that.)

First, for every morphism $A \xrightarrow{f} B$ one has a distinguished triangle

$$\cdots \to C_f[-1] \xrightarrow{\psi} A \xrightarrow{f} B \xrightarrow{\phi} C_f \to \cdots . \tag{6.1}$$

Here C_f is the ''cone'' of f, the quasi-isomorphism class of complexes with terms $A[1] \oplus B$ and differential $\left(\begin{smallmatrix} d_A & 0 \\ f & d_B \end{smallmatrix}\right)$. This is the basic construction we will try to use to represent the ''brane-antibrane bound state'' $\overline{A}B$ produced by condensing the tachyon f.[50] The sequence (6.1) repeats (with a shift of grading) indefinitely to the left and right and this is why it is better thought of as a triangle.

The expression (6.1) appears to single out one arrow as special, the morphism ψ with degree one. Actually this is only a choice of notation: for example we could define $D \equiv A[1]$ and find that the morphism f appeared to have degree one. If one consistently identifies shifted branes $B[2n+1]$ with antibranes $\overline{B}$, then the relation between the K theory classes of the objects is indepen-

dent of this choice. For example, in (6.1), we have $[A]+[C]=[B]$, while in terms of *BCD* we would have had $[B]+[D]=[C]$ which (since $[A]+[D]=0$) is the same. Similarly $[C[-1]]+[B]=[A]$.

The point now is that if we want to base our discussion on the derived category, we cannot talk about exact sequences *a priori* but must instead derive them from the distinguished triangles. If we know that our branes all live in some Abelian category within the derived category, there is a general result which allows us to do this:[51] if and only if three successive objects in the triangle all live in an Abelian subcategory $\mathcal{A}$, that subsequence is a short exact sequence in $\mathcal{A}$. The opposite of this is perhaps easier to see: the cases which do not correspond to exact sequences are those in which C_f has homology in both degrees, and thus is not a member of the Abelian category $\mathcal{A}$. This is interesting for our purposes as there will turn out to be more than one Abelian subcategory of $D(\mathbf{Coh}\,X)$.

Let us discuss this more physically. Suppose in bringing together two objects $\overline{A}$ and B we can form a bound state C, so that $[\overline{A}]+[B]=[C]$. (The choice of notation $\overline{A}$ rather than A is just to get the same K theory relation $[B]=[A]+[C]$ we discussed earlier. We are not assuming any specific relation between central charges yet.) This must start by condensing a tachyonic or massless open string between $\overline{A}$ and B. Let us denote the corresponding morphism (the ''Ext'') with a double arrow $\Rightarrow$, while single arrows denote Hom's (enhanced gauge symmetries).

From the point of view of BPS central charge, $Z_{\overline{A}}=-Z_A$ and Z_B might be aligned, antialigned or not aligned, and the process will look slightly different depending on this. If $Z_{\overline{A}}$ and Z_B are antialigned, there are two further possibilities $|Z_{\overline{A}}|>|Z_B|$ or $|Z_{\overline{A}}|<|Z_B|$, which determine whether the bound state Z_C aligns with $Z_{\overline{A}}$ or Z_B. We now explain how all of these possibilities are contained in the same distinguished triangle (6.1).

If $|Z_B|>|Z_{\overline{A}}|$, the appropriate description is an exact sequence

$$0\to A\overset{f}{\Rightarrow}B\overset{\phi}{\to}C\to 0 \tag{6.2}$$

with maps f and ϕ of degree 0. This is the special case in which C_f has homology only in degree 0, and every such exact sequence corresponds to a distinguished triangle (6.1).

If $|Z_{\overline{A}}|>|Z_B|$, we should use the exact sequence

$$0\to\overline{C}\overset{\psi}{\to}A\overset{f}{\Rightarrow}B\to 0, \tag{6.3}$$

appropriate if C_f has homology only in degree -1. Here we have identified $C[-1]$ with the antibrane $\overline{C}$.

Finally, if $Z_{\overline{A}}$ and Z_B are aligned, we have

$$0\to B\overset{\phi}{\to}C\overset{\psi}{\to}\overline{A}\to 0 \tag{6.4}$$

in which $\overline{A}\overset{f}{\Rightarrow}B[1]$ does not even appear in the exact sequence (it is the ''connecting map'' of the long exact sequence).

The point of all this is to show that the derived category can remain invariant under varying Kähler moduli, while describing somewhat different looking physical processes. The distinction between the processes comes when we identify a specific exact sequence in the triangle. In all three limiting cases (in which central charges align), the exact sequence is the subsequence of (6.1) containing the maps of degree 0, which is the subset of objects which can live in the same Abelian category.

There is some correspondence between our string-inspired notation and the usual mathematical notation and one might try to identify our double arrows $\Rightarrow$ with the special (degree one) morphisms of (6.1). Again, one must recognize that this is only a choice of notation: a single

distinguished triangle admits all three interpretations in which any of the links is a matter field (this could presumably be proven from crossing symmetry of the related BPS algebra).[28] More importantly, the ''special'' morphism in our notation need not have degree 1; this will change under flow.

B. Examples

Let us now look at some examples where we know the interpretations on both sides of a flow.

The simplest situation is illustrated by the brane-antibrane pairs which come out of the Beilinson and generalized McKay constructions. For example, in $\mathbb{C}^3/Z_3$, we have a tachyon $f \in \mathrm{Ext}^1(B_1, B_2[-1])$ at large volume [where $B_1=\mathcal{O}(-1)$ and $B_2=\overline{\Omega}(1)$], which flows to a massless field $f \in \mathrm{Ext}^1(B_1, B_2)$ at the orbifold point.

At large volume, the BPS central charge is dominated by the D4-brane charge (the rank of the bundle). Since $\Omega(1)$ is a rank 2 bundle while $\mathcal{O}(-1)$ has rank 1, at large volume there is a brane-antibrane bound state X, which is an antibrane (D4 charge -1) with these conventions. Its central charge aligns with that of B_2, so the bound state formation is described by the exact sequence

$$0 \to \overline{B}_1 \overset{f}{\Rightarrow} B_2 \overset{\phi}{\to} X \to 0 \tag{6.5}$$

with ϕ a degree zero Hom.

In moving to the orbifold limit, the grade of B_1 decreases by 1, which results in f of degree 1, ψ of degree 0 and ϕ of degree 0. The bound state is still X, but we now want to interpret it as a brane-brane bound state or extension

$$0 \to B_2 \overset{\phi}{\to} X \overset{\psi}{\to} B_1 \to 0 \tag{6.6}$$

with f the connecting map $B_1 \Rightarrow B_2[1]$.

Both come from the distinguished triangle

$$\cdots \to B_1[-1] \overset{f}{\Rightarrow} B_2 \overset{\phi}{\to} X \overset{\psi}{\to} B_1 \to \cdots$$

by specializing to the triple involving maps of degree zero or equivalently whose terms all have the same grade. Note that in the (6.5) interpretation, the object $\overline{B}_1$ has the same K theory class as $B_1[-1]$ (this does not change under flow) but grade zero instead of one.

In the language of Abelian categories, the difference is that at large volume $\overline{B}_1$ and B_2 are both in the Abelian category [justifying the use of (6.5)] while at the orbifold point B_1 and B_2 are in the Abelian category [justifying (6.6)].

We will now try to regard this as a valid description along the flow, where in general the maps will not have integral degree. Of course this is what we expect from the CFT discussion, but it means that we cannot *a priori* rely on the exact sequence interpretation of either (6.5) or (6.6). Nevertheless, physics tells us that we should regard this triangle as describing the formation of a bound state which exists all along the flow. Since the flow is continuous, the grade of X is everywhere determined—this is not something we could take for granted without the triangle, as there is no obvious canonical way to assign gradings to general complexes (they would have to depend on individual homologies, not the total K theory class). Since we have the triangle, we can assign X a grade, and one finds that the gradings of all three morphisms stay within the interval [0, 1] all along the flow. This is consistent with all three objects remaining stable along the flow (in principle they could still be destabilized by other objects).

We next discuss the two-brane, the structure sheaf $\mathcal{O}_\Sigma$ of a two-cycle Σ. There is a simple exact sequence which produces it from the B_i, namely

$$0 \to \mathcal{O}(-1) \overset{f}{\to} \mathcal{O} \overset{g}{\to} \mathcal{O}_\Sigma \to 0,$$

and the corresponding distinguished triangle is

$$\mathcal{O}(-1) \overset{f}{\to} \mathcal{O} \overset{g}{\to} \mathcal{O}_\Sigma \overset{h}{\to} \mathcal{O}(-1)[1] \to \cdots .$$

At large volume this is a perfectly good representation of the 2B; the definition (2.1) leads us (as discussed in Sec. IV) to assign it grade $\frac{1}{2}$ [in conventions where $\varphi(\mathcal{O})=0$] and thus the maps g and h have degree $\frac{1}{2}$. Thus at and near large volume, the 2B can be produced as a bound state of 4B's by condensing a tachyonic open string, as discussed in Ref. 10.

As we flow down, the grade of $\mathcal{O}(-1)$ decreases and the grade of $\mathcal{O}$ increases. Eventually these reach $-\frac{1}{2}$ and $\frac{1}{2}$, respectively, while the 2B remains at $\frac{1}{2}$. At this point, f has degree 1, and g and h have degree 0. If we pass this point, the degree of g goes negative and the 2B goes unstable, while the open string between 4B's becomes massive.

This conclusion basically agrees with that of Ref. 3, where it was justified in terms of Π-stability. However, there was an interesting subtlety noted there; the map g does not look injective when one follows the usual large volume definitions (a map from a sheaf to a sheaf with lower dimensional support could hardly be injective). In the present discussion, since both g and h have degree 0 at the transition, one wants to interpret them as forming an exact sequence at that point, in which case g would ''become'' an injective map. This type of argument can be tested against other known subobject relations at the orbifold point, and seems to work. It suggests a reformulation of Π-stability which we will make below.

By the time we reach the orbifold point, the map f has degree 2 and there is no obvious sign that the 2B ever existed. However, since we can determine that f existed from orbifold considerations (it was an Ext^2 in the quiver-complex formalism), we can run this backwards. From this point of view, we would define $\mathcal{O}_\Sigma$ as a cone C_f in (6.1). Coming back up, the degree of f eventually drops to 1, and it becomes consistent to postulate that this $\mathcal{O}_\Sigma$ becomes stable, with maps g and h of degree 0. Thus we could infer the existence of the 2B elsewhere in moduli space just from information obtained at the orbifold point.

A very similar discussion can be made for the ''mysterious'' bound state $|10000\rangle$ discussed in Refs. 1 and 52, which exists at the Gepner point in the quintic but not at large volume. This is a bound state of $\mathcal{O}(-1)$ and $\mathcal{O}$ and comes about because an $\mathrm{Ext}^3(\mathcal{O},\mathcal{O}(-1))$ at large volume eventually becomes tachyonic near the orbifold point. In this example, one can infer the existence of a bound state which is not a sheaf, just having information about sheaves and about the BPS central charges.

These results demonstrate how we can infer the existence of new BPS branes at distant points in $\mathcal{M}_k$. Given a set of BPS branes, we construct their derived category, including new objects which are candidate BPS branes elsewhere in moduli space. The K theory class of each such object is determined, and this determines the grade of the connecting maps up to an overall $2Z$ ambiguity. If this ambiguity can be fixed in a way that gives all the morphisms non-negative grade, then the object becomes stable.

C. t-structures

There is a mathematical formalism which makes it possible to identify Abelian categories within the derived category, the formalism of t-structures.[51,5] We will not actually use this in the proposal we are about to make, but it illustrates in a clear way how objects which look like complexes from one point of view can be individual objects (not complexes) in a different Abelian category.

A t-structure is defined by prescribing two subcategories $\mathcal{D}^{\geqslant 0}$ and $\mathcal{D}^{\leqslant 0}$ of the derived category $\mathcal{D}$. If $\mathcal{D}$ is derived from an Abelian category $\mathcal{A}$, these would be the categories of complexes

with cohomology only in degrees $n \geqslant 0$ and complexes with cohomology only in degrees $n \leqslant 0$, respectively. The original Abelian category would then be $\mathcal{A} = \mathcal{D}^{\geqslant 0} \cap \mathcal{D}^{\leqslant 0}$.

The nontrivial fact is now that there are a short list of axioms which $\mathcal{D}^{\geqslant 0}$ and $\mathcal{D}^{\leqslant 0}$ must satisfy in order to guarantee that their intersection is an Abelian category. This provides a general way to define new Abelian subcategories. In general, the intersection will contain objects which are complexes from the point of view of the original category; thus these complexes will be regarded as objects in the new category. In this sense, the distinction between ''object'' and ''complex'' is not invariant, and from this point of view it is quite natural to get complexes of coherent sheaves as stable BPS branes at other points in $\mathcal{M}_k$.

A simple way to get new t-structures on $D(\mathbf{Coh}\, X)$ for X Calabi–Yau is to use the Fourier–Mukai transforms discussed earlier. Taking the images of $\mathcal{D}^{\geqslant 0}$ and $\mathcal{D}^{\leqslant 0}$ under the FMT provides a new t-structure whose Abelian category, although isomorphic to the original (for an FMT implementing a monodromy), consists of different objects in $D(\mathbf{Coh}\, X)$. Since these monodromy groups are braid groups this presumably leads to infinitely many t-structures on $D(\mathbf{Coh}\, X)$.

This formalism might be directly usable to produce the Abelian categories which are needed by the original formulation of Π-stability. The basic way this could work would be to move objects between $\mathcal{D}^{\geqslant 0}$ and $\mathcal{D}^{\leqslant 0}$ when their gradings flow across zero.

Indeed, a very concrete example illustrating this idea can be found in work of Bridgeland.[53] In Ref. 53 it is proven that $D(\mathbf{Coh}\, X)$ is invariant under a flop transition, a previously known result,[54] but the interesting point is the way in which this is proven. This uses the theory of so-called perverse sheaves, which can be formulated using t-structures. The basic idea is to consider some submanifold (more generally a stratification of the manifold) and shift the grading of all objects supported on that submanifold in defining the t-structure. The corresponding Abelian category is referred to as a category of ''perverse sheaves.''

In Ref. 53, one considers perverse sheaves defined by shifting the grading of sheaves supported on an appropriate curve C in the CY by -1. Certain of these perverse sheaves can be identified as analogous to points, and it turns out that the moduli space of these ''perverse points'' is isomorphic to the CY X' which is the result of a flop transition on the curve C.

The point of contact with our present considerations is that in terms of periods and BPS central charges, a flop transition simply acts by taking the central charge $Z = B + iV$ of the 2B on the curve C from $V > 0$ to $V < 0$. This indeed shifts the grading of 2B's by ± 1 (the sign depends on the first Chern class) and, by arguments similar to Bridgeland's, might lead to the t-structure appropriate for the flopped CY.

It seems very likely to us that these ideas will be important in future work and more specifically that subcategories of $D(\mathbf{Coh}\, X)$ generated by the stable branes of a given grade on a CY with given moduli will provide a significant generalization of categories of ''perverse sheaves.'' However, we will leave the problem of making this more explicit to future work.

D. A proposal for a stability condition

The stability condition we will propose here builds more simply on the results we already presented and adds some plausible physical input. Unlike Π-stability, it does not provide a way to decide whether a brane is stable at a point in $\mathcal{M}_k$ by just considering that point, but only describes the variation in the set of stable branes as one moves in $\mathcal{M}_k$.

Many of the previous considerations can be summarized by defining a ''stable triangle.'' A distinguished triangle (6.1) involves three morphisms with grades $\alpha + \beta + \gamma = 1$. Let a stable triangle (at a given point in $\mathcal{M}_k$) be a distinguished triangle for which each of the three grades is in $[0, 1]$.

Since if two brane central charges are colinear, the third will be as well, the definitions lead to the constraint that the only stable triangles on the boundary of this region (or ''semistable'' triangles) are those with one grade 1 and the other two 0.

We cannot directly use this to say that a stable object only participates in stable triangles—there will always be lots of extra triangles involving negative morphisms. We only know that

every morphism between stable objects must have non-negative degree. Indeed, there is no physical argument that there should be a canonical definition of grade for unstable objects, and we will not assume that there is.

Let us now suppose that we know the stable objects at some point in $\mathcal{M}_k$, and we move a small distance in this space. The gradings of morphisms will flow: some triangles will become unstable and we must lose objects; others will become stable and we can gain objects.

When a triangle goes unstable, the brane which decays will always be the one sitting between the two morphisms of zero degree. This is because [in all three cases (6.2)–(6.4)] this will always be the heaviest of the three branes. This also means that one only need check lighter branes as possible destabilizing subobjects.

Conversely, when a triangle becomes stable, we will see it by a map f between stable objects having degree coming down through 1. Whenever this happens, we can try to add C_f with grade which gives the other maps degree 0. This uniquely determines the $2Z$ ambiguity in the grading of C_f. We should, however, only add C_f as a stable object if it is not also destabilized by a morphism of negative degree from some preexisting stable object. Once we do this, we might have further candidate bound states involving C_f, so the process must be iterated.

This more or less restates the phenomena we observed in our simple examples but now we must face the question of whether this procedure leads to an unambiguous modified list of stable objects or whether the result depends on the order in which we make these modifications.

One point where such dependence might enter is that we might find that A destabilizes B, but A also decays on the same line. The general result which prevents this type of ambiguity is that the subobject of A responsible for the decay will also be a subobject of B (by composing the Hom's), and typically would be a stable object which will destabilize B. In general it might decay, but this chain must terminate with some stable final product (assuming the spectrum of masses has a gap) which will also be a subobject.

Similarly, we cannot find that adding a new object C_f destabilizes preexisting objects, because there will be a subobject of C_f which already destabilized them before we added C_f.

These considerations suggest that the procedure as we stated it is unambiguous. The main physical assumption we needed was that the spectrum of BPS masses has a finite mass gap, so that we cannot have infinite chains of subobjects and decays.

VII. CONCLUSIONS

In this work, we gave a fundamental picture of BPS D-branes on Calabi–Yau manifolds, based on considerations in conformal field theory and the related topological string theory.

To summarize, we distinguished boundary conditions in topological open string theory or ''topological D-branes'' from BPS boundary conditions in CFT or ''physical D-branes,'' and argued that every physical D-brane had a topological analog but not vice versa. Topological D-branes (in the B model) are more general than holomorphic bundles or coherent sheaves; they can be arbitrary objects of the derived category. The grading of morphisms between topological D-branes depends on the Kähler moduli in a simple way and this is responsible for variation of the spectrum of physical D-branes and lines of marginal stability; branes involved in morphisms of negative degree cannot exist. This provides a CFT derivation of the Π-stability condition of Ref. 2. We went on to discuss the triangulated structure of the derived category, which allows us to dispense with the requirement of a preexisting Abelian category and subobject relation made in the original Π-stability proposal, instead deriving the subobject relations from the gradings and distinguished triangles. All of these points were illustrated in a number of examples; in simple cases these ideas lead directly to explicit predictions for marginal stability lines.

Many new phenomena are clearly possible and can now be studied systematically, such as the formation of branes away from the large volume limit which are not coherent sheaves but more general objects in the derived category.

All of these developments appear rather solid to us and provide a firm basis for further understanding of BPS branes on Calabi–Yau as well as a precise contact with the homological

mirror symmetry proposal of Kontsevich. The ''flow of gradings'' is a new structure in this problem which we believe will be quite important in future developments.

In the final subsection, we went further and stated a definite proposal for how to determine the spectrum of BPS branes at arbitrary points in Kähler moduli space. This proposal is somewhat harder to use than Π-stability in that it requires starting with the spectrum at a single point, say the large volume limit, and following its evolution to the point of interest. (It is not necessary to follow the entire spectrum in order to determine the existence of particular branes, however.) We did not prove that this procedure always leads to unambiguous results, though we did give suggestive arguments for this.

Clearly this proposal requires a great deal of testing and exploration at this point. There are numerous self-consistency checks that it must pass; for example it is not obvious that branes whose periods vanish at nonsingular points of Kähler moduli space will decay before reaching these points (as is required for physical consistency). We did not even prove that monodromies are symmetries of the physical spectrum.

Not having yet performed these basic checks, our main reason for believing in the proposal at present is that it seems to us to be the conceptually simplest proposal which could accomodate the known complexity of these problems as revealed in Ref. 3 and our further studies. Since it is the first such proposal, this point will have to be confirmed by further work as well. Hopefully there is a lot of scope for simplifying its application; ideally one would be able to derive a condition which can be applied at a single point in Kähler moduli space. One might well benefit from using more A model information as well.

We will not get into lengthy discussion of the likely applications of this work here, instead referring to the conclusions of Ref. 3. Perhaps the most direct application would be to provide a simpler invariant of $d=4$, $\mathcal{N}=2$ string compactifications than the explicit spectrum of BPS branes, namely the derived category obtained from this spectrum. The precise sense in which this is simpler is that it does not depend on the BPS central charges or the point in vector multiplet moduli space. Making interesting use of this idea in studying $\mathcal{N}=2$ duality probably requires generalizing the ideas to defining ''derived categories of quantum BPS branes,'' which would have some similarity to BPS algebras[28] but presumably would be independent of vector moduli.

As discussed in the conclusions to Ref. 3, we regard the more important goal of this line of work to be its eventual application to understanding $\mathcal{N}=1$ compactifications of string theory. Building on Ref. 2, in $\mathcal{N}=1$ language we have provided a rather complete discussion of the problem of solving the D-flatness conditions in a certain large class of theories. As will be discussed elsewhere, we believe it will turn out to be possible to get exact superpotentials in Gepner models and perhaps more general CYs as well.

A natural next question in this vein is whether a similar geometric understanding could be developed of non-BPS branes. One should distinguish two cases. The examples we know of are connected to BPS branes or combinations of BPS branes by varying CY moduli, and it seems very likely that these can be understood in the same way, with the non-BPS property arising from spontaneous breaking of space–time $\mathcal{N}=1$ supersymmetry, now involving a competition between D and F flatness conditions. There might be other non-BPS branes not connected to BPS branes by varying moduli; for these it is unclear whether such a picture would apply.

In any case, we believe our present results give further evidence that $\mathcal{N}=1$ string compactification can lead to problems which admit general solutions (not just case by case analysis) and a rich mathematical structure.

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Fundamental strings in open string theory at the tachyonic vacuum

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We show that the world-volume theory on a D-p-brane at the tachyonic vacuum has solitonic string solutions whose dynamics is governed by the Nambu–Goto action of a string moving in $(25+1)$ dimensional space–time. This provides strong evidence for the conjecture that at this vacuum the full $(25+1)$ dimensional Poincaré invariance is restored. We also use this result to argue that the open string field theory at the tachyonic vacuum must contain closed string excitations. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1377037]

I. INTRODUCTION AND SUMMARY

It has been conjectured that the tachyonic vacuum in open bosonic string theory on a D-brane describes the closed string vacuum without D-branes, and that various soliton solutions in this theory describe D-branes of lower dimension.[1] Similar conjectures have also been put forward for superstring theories.[2–4] Evidence for these conjectures come from both first[5,6] and second[7–10] quantized string theories.

Given that all D-branes can be regarded as solitons in the open string field theory,[11] one might wonder if the open string field theory could be used for a nonperturbative formulation of string theory.[12] For this one needs to show that not only the D-branes, but other known objects in string theory, namely the fundamental closed strings and the NS five-branes are also present in this open string field theory. Progress in identifying the fundamental string has been made in Refs. 13, 14, 8, 15, and 16. In particular, in Refs. 14, 8, 15, and 16 it was shown that the effective action[17] describing the dynamics of the D-brane around the tachyonic vacuum admits stringlike classical solution whose tension matches that of a fundamental string. It was also established that on a D-25-brane world-volume, the dynamics of these strings is described by that of a Nambu–Goto string moving in $(25+1)$ dimensions.

On the world-volume of a D-p-brane embedded in the $(25+1)$ dimensional space–time, the full $(25+1)$ dimensional Poincaré invariance is spontaneously broken to the product of $(p+1)$ dimensional Poincaré group, and the $(25-p)$ dimensional rotation group. However, if the tachyonic ground state really represents the vacuum without a D-brane, then we expect that in this vacuum the full $(25+1)$ dimensional Poincaré invariance should be restored. Thus the dynamics of the stringlike solutions should be described by a Nambu–Goto action with $(25+1)$ dimensional target space rather than a $(p+1)$ dimensional target space. This is what we shall demonstrate in this paper. (This question was partially addressed in Ref. 15 where it was shown that in the approximation where the contribution to the Hamiltonian is dominated by the electric flux on the D-brane world-volume, there is a symmetry that exchanges the velocity tangential to the D-brane with the velocity transverse to the D-brane.) Since the Nambu–Goto action in $(25+1)$ dimensional target space has full $(25+1)$ dimensional Poincaré invariance, this result provides strong support to the conjecture that at the tachyonic vacuum of the D-p brane the full $(25+1)$ dimensional Poincaré invariance is restored. Earlier string field theory analysis has provided evidence for

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the restoration of the translational invariance along directions transverse to the D-brane world-volume.[18,19]

Since the D-p-brane world-volume is $(p+1)$ dimensional, and the string solution lives on the D-p-brane, it may sound strange at first that this string actually moves in $(25+1)$ dimensions. The reason it can happen is that at the tachyonic vacuum the D-brane has vanishing tension, and hence it does not cost the D-brane any additional energy to adjust its world-volume to contain any given fundamental string world-sheet embedded in $(25+1)$ dimensional space–time. Thus the string world-sheet always lies inside the D-p-brane world-volume, as should be the case. The nontrivial fact here is that the dynamics of the string tangential to the D-brane world-volume, which is described by the gauge fields, and the dynamics transverse to the D-brane world-volume, which is described by the massless scalar fields associated with the transverse motion of the D-brane, are together described by the Nambu–Goto action in the full $(25+1)$ dimensional target space–time.

Although the dynamics of the string soliton constructed this way agrees with that of the fundamental string, there are some caveats. First of all the tension of the string is governed by the total amount of electric flux it carries, and only after properly taking into account the quantization rule for the electric flux one can show that the tension matches that of the fundamental string. Within the classical field theory which we shall be studying, there is no rationale for this quantization law. A related problem is as follows. Although the string solution constructed here has the correct degrees of freedom describing the dynamics of a fundamental string, it also has additional degrees of freedom corresponding to the energy density spreading out in the direction transverse to the original string solution instead of being confined in a thin tube along the string. We show that these problems can be avoided by making the solitonic string driven by an external open string. For this we consider the case where one of the directions transverse to the D-p-brane is compact, and we begin with a configuration of open strings starting on the D-brane, and ending on its image under translation along the compact direction. We then ask what happens when the tachyon on the D-brane rolls down to its ground state. We argue that at the tachyonic vacuum, the two ends of the original open string are connected by a flux line on the D-brane, with the total amount of flux fixed by the source (and the sink) of flux, namely the end points of the original open string on the brane. Furthermore, the condition for minimum energy prevents the flux from spreading, since the source and the sink of flux are pointlike objects on the D-p-brane world-volume. The net result is a single fundamental string winding along the compact direction. Using a T-duality transformation along the compact direction we can then argue that the T-dual D-$(p+1)$-brane at the tachyonic vacuum must contain closed string excitations carrying momentum along the compact direction.

Related earlier work in Ref. 20 analyzed the dynamics of tensionless D-branes in a different formalism and found that the D-brane world-volume is foliated by string world-sheet. It will be interesting to explore the precise relation between these results and the static gauge results of Refs. 14, 8, 15, 16 and the present paper.

The paper is organized as follows. In Sec. II we review the result for the effective action on the D-brane world-volume at the tachyonic vacuum[17] and its Hamiltonian formulation.[15] In Sec. III we show that given any solution of the equations of motion of a Nambu–Goto string moving in $(25+1)$ dimensional space–time, we can construct a solution of the equations of motion of the D-p-brane world-volume theory with energy density localized along the world-sheet of the corresponding Nambu–Goto string solution. This establishes that the D-p-brane world-volume theory admits stringlike soliton solutions whose dynamics is governed by the Nambu–Goto action in $(25+1)$ dimensions. In Sec. IV we use this result to argue that the open string field theory, describing the D-brane world-volume theory at the tachyonic vacuum, must contain closed string excitations.

II. LOW ENERGY EFFECTIVE FIELD THEORY ON THE D-BRANE AT THE TACHYONIC VACUUM

We shall analyze the dynamics of massless fields living on a D-p brane at the tachyonic vacuum in the static gauge. Let us denote by $x^\mu (0 \leqslant \mu \leqslant p)$ the world-volume coordinates on the

D-brane, by A_μ the U(1) gauge field living on the D-brane, and by Y^I $(p+1\leq I\leq 25)$ the massless scalars representing the transverse coordinates of the brane. The action is given by[17]

$$S=-V(T)\int d^{p+1}x\sqrt{-\det(\eta_{\mu\nu}+F_{\mu\nu}+\partial_\mu Y^I\partial_\nu Y^I)}, \tag{2.1}$$

where $V(T)$ is the tachyon potential which vanishes at the tachyonic vacuum $T=T_0$. We shall work in the gauge $A_0=0$, and denote by $\pi^i(x)$ and $p_I(x)$ the momenta conjugate to A_i and Y^I, respectively, for $1\leq i\leq p$. As was shown in Ref. 15, the dynamics of the brane at the tachyonic vacuum is best described in the Hamiltonian formalism, with the Hamiltonian

$$H=\int d^px\mathcal{H}, \tag{2.2}$$

with

$$\mathcal{H}=\sqrt{\pi^i\pi^i+p_Ip_I+(\pi^i\partial_iY^I)^2+b_ib_i}, \tag{2.3}$$

where

$$b_i\equiv F_{ij}\pi^j+\partial_iY^Ip_I. \tag{2.4}$$

$F_{ij}=\partial_iA_j-\partial_jA_i$ is the magnetic field strength. The π^i's satisfy a constraint:

$$\partial_i\pi^i=0. \tag{2.5}$$

In writing down the Hamiltonian (2.2), (2.3) we have taken the tachyon field T to be frozen at its minimum $T=T_0$. Proposals for the effective action including tachyon kinetic term have been put forward in Ref. 21.

Let us denote by $E_i=\partial_0A_i$ the electric field strength. Then the Bianchi identities and the equations of motion derived from the Hamiltonian given in (2.2), (2.3) are given by

$$\partial_{[i}F_{jk]}=0, \quad \partial_0F_{ij}=\partial_iE_j-\partial_jE_i, \tag{2.6}$$

$$E_i=\frac{1}{\mathcal{H}}(\pi^i+\partial_iY^I\pi^j\partial_jY^I-F_{ij}b_j), \tag{2.7}$$

$$\partial_0\pi^i+\partial_j\left(\frac{1}{\mathcal{H}}(\pi_jb_i-\pi_ib_j)\right)=0, \tag{2.8}$$

$$\partial_0Y^I=\frac{1}{\mathcal{H}}(p_I+\partial_iY^Ib_i), \tag{2.9}$$

$$\partial_0p^I=\partial_i\left(\frac{1}{\mathcal{H}}(\pi^i\pi^j\partial_jY^I+b_ip^I)\right). \tag{2.10}$$

For this system, there are conserved Noether currents $T_{\mu\nu}$ and $T_{\mu I}$ $(0\leq\mu,\nu\leq p,\ (p+1)\leq I\leq 25)$ associated with the translation along the spatial coordinates x^μ labeling the D-p-brane world-volume, as well as translation along the coordinates Y^I transverse to the world-volume. These are given by

$$T_{00}=\mathcal{H}, \quad T_{k0}=-b_k, \quad T_{0i}=-b_i, \quad T_{ki}=\frac{1}{\mathcal{H}}(\pi^k\pi^i-b_kb_i), \tag{2.11}$$

$$T_{0I}=p_I, \quad T_{kI}=\frac{1}{\mathcal{H}}(\pi^k\pi^j\partial_j Y^I+b_k p^I),$$

and satisfy

$$\eta^{\mu\nu}\partial_\mu T_{\nu\rho}=0, \quad \eta^{\mu\nu}\partial_\mu T_{\nu I}=0. \tag{2.12}$$

III. FUNDAMENTAL STRING SOLUTION

In this section we shall demonstrate that the equations of motion discussed in Sec. II admit fundamental string solutions whose dynamics is identical to that of a Nambu–Goto string moving in $(25+1)$ dimensional space–time. Using the results of Ref. 22, Ref. 15 showed that if we set the Y^I's to 0, then the dynamics of the solitonic string is described by the Nambu–Goto action in $(p+1)$ dimensional space–time. The new result is the incorporation of the Y^I's. Since the dynamics of a Nambu–Goto string in $(25+1)$ dimensional space–time has full $(25+1)$ dimensional Poincaré invariance, our result gives strong support to the conjecture that the tachyonic vacuum of the D-p-brane represents a configuration where the full $(25+1)$ dimensional Poincaré invariance is restored.

Our strategy will be as follows. We shall show that for every configuration of a Nambu–Goto string satisfying the string equations of motion we can construct a solution of the equations of motion (2.5)–(2.10), with energy density localized along the string. For this we start by writing down the action of the Nambu–Goto string in $(25+1)$ dimensional space–time:

$$S_{\rm NG}=-\int d\tau\, d\sigma \sqrt{-\det(\eta_{MN}\partial_\alpha Z^M\partial_\beta Z^N)}, \tag{3.1}$$

where ξ^α for $\alpha=0,1$ denote the world-volume coordinates of the string: $(\xi^0,\xi^1)\equiv(\tau,\sigma)$, Z^M $(0\leqslant M\leqslant 25)$ denote the space–time coordinates of the string, and η_{MN} is the Minkowski metric diag$(-1,1,1,\ldots,1)$. We shall choose the static gauge: $(Z^0=\tau, Z^1=\sigma)$ and go to the Hamiltonian formalism. If we denote by P_s the momenta conjugate to Z^s for $2\leqslant s\leqslant 25$, the Hamiltonian is given by

$$H_{\rm NG}\equiv\int d\sigma\,\mathcal{H}_{\rm NG}=\int d\sigma\,\sqrt{1+P_sP_s+\partial_\sigma Z^s\partial_\sigma Z^s+(P_s\partial_\sigma Z^s)^2}. \tag{3.2}$$

The equations of motion following from this Hamiltonian are given by

$$\partial_\tau Z^s=\frac{1}{\mathcal{H}_{\rm NG}}(P_s+\partial_\sigma Z^s P_t\partial_\sigma Z^t), \tag{3.3}$$

$$\partial_\tau P_s=\partial_\sigma\left(\frac{1}{\mathcal{H}_{\rm NG}}(\partial_\sigma Z^s+P_sP_t\partial_\sigma Z^t)\right). \tag{3.4}$$

In these equations s and t indices take values $2,3,\ldots,25$. For future use, we shall define

$$P_1=-\sum_{s=2}^{25}P_s\partial_\sigma Z^s, \quad Z^1(\tau,\sigma)=\sigma. \tag{3.5}$$

With these definitions, it is straightforward to verify that Eqs.(3.3) and (3.4) are satisfied also for $s=1$. (The sum over t in these equations still runs from 2 to 25).

Let $(Z^s(\tau,\sigma),P_s(\tau,\sigma))$ for $2\leqslant s\leqslant 25$ be a solution of Eqs. (3.3) and (3.4). Now consider the following field configuration on the D-p-brane:

$$\pi^i(x^0,\ldots,x^p)=\partial_\sigma Z^i(\tau,\sigma)f(x^0,\ldots,x^p)\big|_{(\tau,\sigma)=(x^0,x^1)}, \tag{3.6}$$

$$p_I(x^0,\ldots,x^p)=P_I(\tau,\sigma)f(x^0,\ldots,x^p)|_{(\tau,\sigma)=(x^0,x^1)},$$

where we have used the convention that the indices i,j,k run from 1 to p, the indices I,J,K run from $(p+1)$ to 25, and the indices s,t run from 2 to 25. $f(x^0,\ldots,x^p)$ is an arbitrary function of the variables $(x^m-Z^m(x^0,x^1))$ for $2\leqslant m\leqslant p$, and hence satisfies

$$\partial_\sigma Z^i\partial_i f|_{(\tau,\sigma)=(x^0,x^1)}=0, \quad (\partial_\tau Z^i\partial_i f+\partial_0 f)|_{(\tau,\sigma)=(x^0,x^1)}=0. \tag{3.7}$$

The fields $Y^I(x^0,\ldots,x^p)$ and $F_{ij}(x^0,\ldots,x^p)$ are subject to the following set of conditions:

$$(\partial_\sigma Z^j\partial_j Y^I-\partial_\sigma Z^I)|_{(\tau,\sigma)=(x^0,x^1)}=0, \tag{3.8}$$

and

$$(F_{ij}\partial_\sigma Z^j+\partial_i Y^I P_I+P_i)|_{(\tau,\sigma)=(x^0,x^1)}=0, \tag{3.9}$$

but are otherwise unspecified. Using Eqs. (3.6), (3.8), and (3.9) we can easily verify that for this background,

$$\begin{aligned}
&\mathcal{H}(x^0,\ldots,x^p)=H_{\rm NG}(\tau=x^0,\sigma=x^1)f(x^0,\ldots,x^p),\\
&b_i(x^0,\ldots,x^p)=-P_i(\tau=x^0,\sigma=x^1)f(x^0,\ldots,x^p),\\
&\pi^j\partial_j Y^I(x^0,\ldots,x^p)=\partial_\sigma Z^I(\tau=x^0,\sigma=x^1)f(x^0,\ldots,x^p).
\end{aligned} \tag{3.10}$$

Using Eqs. (3.3)–(3.7) and (3.10) we can now verify that Eqs. (2.5), (2.8), and (2.10) are satisfied by this background. Thus in order to construct a solution of the full set of equations of motion (2.5)–(2.10) we need to show that it is possible to find $F_{\mu\nu}$ and Y^I satisfying the constraints (2.6), (2.7), (2.9), (3.8), and (3.9).

First we shall establish the existence of Y^I's satisfying Eqs. (2.9) and (3.8). [Note that the Eq. (3.9) imposes a constraint on Y^I of the form $\partial_\sigma Z^i(\partial_i Y^I P_I+P_i)|_{(\tau,\sigma)=(x^0,x^1)}=0$, but due to Eq. (3.5), this is automatically satisfied once Eq. (3.8) is satisfied.] Using Eqs. (3.6) and (3.10), we shall now write Eqs. (2.9) and (3.8) as follows:

$$\begin{aligned}
&\partial_0 Y^I=\frac{1}{\mathcal{H}_{\rm NG}}(P_I-\partial_i Y^I P_i),\\
&\partial_1 Y^I=(-\partial_\sigma Z^m\partial_m Y^I+\partial_\sigma Z^I),
\end{aligned} \tag{3.11}$$

where the indices m,n,q run from 2 to p, and it will be understood from now on that τ and σ are to be identified with x^0 and x^1, respectively. We can now treat Eqs. (3.11) as the equations determining the x^0 and x^1 evolution of the functions Y^I. (We replace the $\partial_1 Y^I$ appearing on the right-hand side of the first equation by the right-hand side of the second equation.) Existence of a solution to these equations requires the integrability condition:

$$\partial_1\left(\frac{1}{\mathcal{H}_{\rm NG}}(P_I-\partial_m Y^I P_m+P_1(\partial_\sigma Z^m\partial_m Y^I-\partial_\sigma Z^I))\right)-\partial_0((-\partial_\sigma Z^m\partial_m Y^I+\partial_\sigma Z^I))=0. \tag{3.12}$$

It is a straightforward although tedious exercise to show that once Eqs. (3.3) and (3.4) are satisfied, Eq. (3.12) is satisfied.

Thus it remains to show the existence of a set of $F_{\mu\nu}$ satisfying Eqs. (2.6), (2.7), and (3.9). We begin with the F_{mn}'s $(2\leqslant m,n,q\leqslant p)$. We take them to satisfy the following identities:

$$\partial_{[m}F_{nq]}=0, \tag{3.13}$$

and

$$\partial_1 F_{mn} + \partial_1 Z^q[x^0,x^1]\partial_q F_{mn} = 0,$$
$$\partial_0 F_{mn} + \partial_0 Z^q[x^0,x^1]\partial_q F_{mn} = 0. \tag{3.14}$$

To see that it is possible to choose F_{mn}'s satisfying these conditions, we regard Eq. (3.14) as the evolution equation for F_{mn} in x^0 and x^1 from an initial configuration satisfying the Bianchi identities (3.13). It is easy to verify that the evolution equations (3.14) preserve the Bianchi identities at all values of x^0 and x^1. It is also easy to verify the integrability of Eq. (3.14):

$$\partial_0(\partial_1 Z^q[x^0,x^1]\partial_q F_{mn}) - \partial_1(\partial_0 Z^q[x^0,x^1]\partial_q F_{mn}) = 0. \tag{3.15}$$

Given F_{mn} satisfying (3.13) and (3.14), we can use (3.10) to write Eqs. (2.7) and (3.9) as follows:

$$F_{0i} = \frac{1}{\mathcal{H}_{\rm NG}}(\partial_\sigma Z^i + \partial_i Y^I \partial_\sigma Z^I + F_{ij}P_j), \tag{3.16}$$

and

$$F_{i1} = -F_{in}\partial_\sigma Z^n - \partial_i Y^I P_I - P_i\,. \tag{3.17}$$

If Eq. (3.17) is satisfied for $i=m$, then it is also automatically satisfied for $i=1$ with the help of Eqs. (3.5) and (3.11). Thus the independent equations in (3.17) are

$$F_{m1} = -F_{mn}\partial_\sigma Z^n - \partial_m Y^I P_I - P_m\,. \tag{3.18}$$

This gives F_{m1} in terms of F_{mn} and other known quantities. Replacing the F_{m1}'s appearing on the right-hand side of Eq. (3.16) by the right-hand side of Eq. (3.18), we can now regard Eq. (3.16) as expressions for F_{01} and F_{0m} in terms of F_{mn} and other known quantities.

We now need to check that F_{0i} and F_{m1} defined through Eqs. (3.16) and (3.18), satisfy the remaining Bianchi identities:

$$\partial_0 F_{mn} + \partial_m F_{n0} + \partial_n F_{0m} = 0,$$
$$\partial_1 F_{mn} + \partial_m F_{n1} + \partial_n F_{1m} = 0, \tag{3.19}$$
$$\partial_0 F_{m1} + \partial_m F_{10} + \partial_1 F_{0m} = 0.$$

It is straightforward to verify that all of these identities are consequences of Eqs. (3.3), (3.4), (3.11), (3.13), and (3.14). This completes the construction of a solution of the complete set of equations of motion (2.5)–(2.10) of the D-p-brane world-volume field theory.

We shall now make a special choice of the function f:

$$f(x^0,\ldots,x^p) = \prod_{m=2}^{p} \delta(x^m - Z^m(x^0,x^1)), \tag{3.20}$$

which satisfies Eq. (3.7). Furthermore we take

$$Y^I(x^0,x^1,x^m = Z^m(x^0,x^1)) = Z^I(x^0,x^1), \tag{3.21}$$

which can be seen to be compatible with Eq. (3.11). Indeed, Eqs. (3.11) and (3.14) can be interpreted as the requirement of vanishing of the derivatives of $(Y^I - Z^I)$ and F_{mn} along directions tangential to the string world-sheet. Thus we can solve these equations by taking $Y^I - Z^I$ and F_{mn} to be arbitrary functions g^I and g_{mn}, respectively, of $x^2 - Z^2(x^0,x^1),\ldots x^p - Z^p(x^0,x^1)$. Equation (3.21) can then be satisfied by requiring that $g^I(0,\ldots,0) = 0$. The Bianchi identities (3.13) are satisfied by requiring that the functions g_{mn} satisfy $\partial_{[q}g_{mn]} = 0$.

As can be seen from Eq. (3.10), for the choice of f given in Eq. (3.20), the energy density is localized along the surface $x^m = Z^m(x^0,x^1)$ for $2 \leqslant m \leqslant p$. Using Eq. (3.21) we see that in the full $(25+1)$ dimensional space–time, this describes the surface $x^s = Z^s(x^0,x^1)$ for $2 \leqslant s \leqslant 25$. This is precisely the world-sheet of the string described by the Nambu–Goto action (3.1). Thus our analysis shows that whenever the Nambu–Goto equation has a solution described by $Z^s(\sigma,\tau)$, there is a corresponding solution in the D-p-brane world-volume field theory with energy density localized along the world-sheet of the string. In other words, the D-p-brane world-volume theory contains a solution whose dynamics is exactly that of a Nambu–Goto string in $(25+1)$-dimensions.

Note, however, that the freedom of replacing the δ function by an arbitrary function of $x^m - Z^m(x^0,x^1)$ means that besides the usual degrees of freedom of the fundamental string, our solution has additional degrees of freedom which corresponds to the freedom of spreading out the electric flux in directions transverse to the string. Also the overall normalization on the right-hand side of Eq. (3.20), which fixes the tension/charge of the string, is arbitrary. We shall return to these questions in Sec. IV. There are also additional degrees of freedom stemming from the fact that Eqs. (3.11), (3.13), and (3.14) do not determine Y^I and F_{mn} completely for a given configuration of the Nambu–Goto string. This is analogous to the spurious degeneracy found in Ref. 23. It has been argued in Ref. 24 that this apparent degeneracy is due to the wrong choice of variables in describing the theory, and will disappear once we use the correct set of variables.

We shall end this section by writing down the expressions for the conserved Noether currents for the background described previously. This is a straightforward exercise, and the results are as follows:

$$
\begin{aligned}
&T_{00}(x^0,\ldots,x^p) = \mathcal{H}_{\rm NG}(\tau,\sigma) \prod_{m=2}^{p} \delta(x^m - Z^m(\tau,\sigma))\big|_{(\tau,\sigma)=(x^0,x^1)}, \\
&T_{0k}(x^0,\ldots,x^p) = T_{k0}(x^0,\ldots,x^p) = P_k(\tau,\sigma) \prod_{m=2}^{p} \delta(x^m - Z^m(\tau,\sigma))\big|_{(\tau,\sigma)=(x^0,x^1)}, \\
&T_{ki}(x^0,\ldots,x^p) = \frac{1}{\mathcal{H}_{\rm NG}}(\partial_\sigma Z^k \partial_\sigma Z^i - P_k P_i) \prod_{m=2}^{p} \delta(x^m - Z^m(\tau,\sigma))\big|_{(\tau,\sigma)=(x^0,x^1)}, \qquad (3.22) \\
&T_{0I}(x^0,\ldots,x^p) = P_I(\tau,\sigma) \prod_{m=2}^{p} \delta(x^m - Z^m(\tau,\sigma))\big|_{(\tau,\sigma)=(x^0,x^1)}, \\
&T_{kI}(x^0,\ldots,x^p) = \frac{1}{\mathcal{H}_{\rm NG}}(\partial_\sigma Z^k \partial_\sigma Z^I - P_k P_I) \prod_{m=2}^{p} \delta(x^m - Z^m(\tau,\sigma))\big|_{(\tau,\sigma)=(x^0,x^1)}.
\end{aligned}
$$

Verification of the conservation laws (2.12) for $T_{\mu\nu}$ and $T_{\mu I}$ is a straightforward application of Eqs. (3.3) and (3.4). It is also a simple exercise to verify that the corresponding conserved charges $\int d^p x\, T_{00}$, $\int d^p x T_{0i}$ and $\int d^p x\, T_{0I}$ agree with the Noether charges of the Nambu–Goto string associated with translation invariance along x^0, x^i, and x^I directions, respectively.

IV. CLOSED STRINGS IN THE D-BRANE WORLD-VOLUME THEORY

In this section we shall use the results of Sec. III to argue that at the tachyonic vacuum the D-brane world-volume theory must contain closed string excitations. Identification of closed strings as closed flux lines has been discussed earlier in Refs. 13, 14, 8, 15, and 16. The present construction is closely related, but differs in that here part of the closed string is formed by an external open string.

We begin with a thought experiment. Consider three well-separated D-branes A, B, and C, and a state on the world volume of this system consisting of a fundamental string stretched from

A to B, and another fundamental string stretched from B to C. Let us now ask: What happens to this state when the tachyon field on the brane B rolls down to its (local) minimum, but the branes A and C remain unchanged. The D-brane world-volume field theory analysis tells us that the ends of the AB and BC strings are source and sink of one unit of electric flux (measured in natural units) on the world-volume of the brane B. Thus the fate of the system is clear: The final configuration will consist of the AB string, the BC string, and an electric flux line (described by the solution given in Sec. III) on the B-brane world-volume connecting the end point of the AB string to the starting point of the BC string. Note that the condition for minimum energy will prevent the flux from spreading out as its source and sink are point objects. (Of course, one would still need to understand why local fluctuations on the string involving the spreading of the flux is absent. Some discussion on this can be found in Refs. 14 and 8.) Furthermore there is precisely one unit of electric flux and hence its tension is equal to that of a fundamental string.[14] Thus it is natural to interpret the flux line as a fundamental string stretched from the end point of the AB string to the starting point of the BC string. (This string, as well as the external AB and BC strings, can adjust their positions and orientations so as to minimize the energy of the configuration.) Thus the net result of this process is a single open string stretched between A and C. It is as if the tachyon condensation on the world-volume of the brane B joins the ends of the AB and BC strings by a fundamental string. Even before tachyon condensation on the brane B, the ends of AB and BC strings could join to produce an AC string. But there it was a perturbative quantum process, whereas the process described here is a nonperturbative classical process.

Now we consider a different system: Take a single D-brane and an open string with both ends on this D-brane. One can use the same argument to conclude that when the tachyon condenses to its ground state, the two ends of the open string will be connected by a flux line, and once we identify the flux line as the fundamental string, we get a closed string state! This argument can be made more concrete as follows. Take a D-brane with one of its transverse directions compact, and consider an open string stretched from the D-brane to its image under translation along the compact direction. Now let us ask what happens to this open string state when the tachyon on the D-brane condenses to its ground state. Since the original state carries fundamental string winding charge this state cannot disappear. To see what happens it is simplest to go to the infinite cover; in this case we have initially an infinite number of parallel D-branes at regular spacing, and between any two neighboring D-branes we have an open string suspended between the two. Thus on any of the D-branes we have an open string ending and another open string starting giving a source and a sink of electric flux. When the tachyon condenses to its ground state, each D-brane develops a flux line joining the source to the sink. If we identify this flux line as a fundamental string as before, the result is a single infinitely long string. After modding out by the discrete translation symmetry to compactify the direction, this is nothing but a closed string wrapped around the compact direction!

Thus we conclude that if we start with a D-brane with a transverse direction compact, then after tachyon condensation the open string field theory on the D-brane world-volume must contain excitations corresponding to closed string winding states along the compact direction. Let us now make a T-duality transformation along the compact direction. This converts the D-p brane to a D-$(p+1)$ brane, but is otherwise a symmetry of the open string field theory order by order in open string perturbation theory. On the other hand this transforms the closed string winding modes to closed string momentum modes. Thus if we start with a D-brane with one of its tangential directions compact, then after tachyon condensation the corresponding open string field theory will contain excitations corresponding to closed string states carrying momentum along the compact direction.

It will be interesting to see if we can study this phenomenon directly in open string field theory.

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Sigma model approach to string theory effective actions with tachyons

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Motivated by recent discussions of actions for tachyon and vector fields related to tachyon condensation in open string theory we review and clarify some aspects of their derivation within the sigma model approach. In particular, we demonstrate that the renormalized partition function $Z(T,A)$ of the boundary sigma model gives the effective action for massless vectors which is consistent with the string S-matrix and beta function, resolving an old problem with this suggestion in the bosonic string case at the level of the leading $F^2(dF)^2$ derivative corrections to Born–Infeld action. We give a manifestly gauge invariant definition of $Z(T,A)$ in non-Abelian NSR open string theory and check that its derivative reproduces the tachyon beta function in a particular scheme. We also discuss the derivation of similar actions for tachyon and massless modes in closed bosonic and NSR (type 0) string theories. In the bosonic case the tachyon potential has the structure $-T^2e^{-T}$, but it vanishes in the NSR string case. © *2001 American Institute of Physics.*
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I. INTRODUCTION

To try to address the question of the vacuum structure of string theory it is natural to look for a kind of field theory action which would interpolate between possible ground states, e.g., unstable perturbative some stable nonperturbative one. The original S-matrix based method[1] of reconstructing the string effective action order by order in powers of fields from on-shell scattering amplitudes does not in principle allow one to find such an action.

It was suggested in Ref. 2 that a natural framework for an off-shell approach should be a generalized two-dimensional (2-D) sigma model partition function representing a generating functional[3] for correlators of string vertex operators given by the Polyakov path integral.[4] The condensates of string fields are then sigma model couplings, and one may hope to determine the exact structure of the action without expanding in powers of them (e.g., expanding instead in derivatives of the fields). One advantage of this sigma model approach is that off-shell gauge symmetries of low-energy expansions become manifest.

The precise definition of the effective action (see Ref. 5 for a review) should be consistent with the string S-matrix near the perturbative vacuum and should also reproduce the conditions of Weyl invariance of the sigma model as its equations of motion.[6–10] (In critical string theory, where, by definition, one does not integrate over the conformal factor of the 2-D metric, the form of the off-shell action depends on a Weyl symmetry gauge, but that dependence should disappear at the stationary points described by 2-D conformal theories.)

While this sigma model partition function approach was successful for the massless string modes leading to covariant expressions to all orders in powers of gravitons and dilatons in the closed string case and the vector field strength in the open string case,[11] it produced unfamiliar expressions when applied to the tachyon field T. As was observed already in Ref. 2, the expression for the partition function $Z[T]$ computed by expanding in derivatives of T has the following

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structure in the critical bosonic string theory (both in the closed string case on the 2-sphere and the open string case on the disk): $Z=a_0\int d^Dx e^{-T}[1+a_1\alpha'\,\partial^2 T+O(\alpha'^2)]$. [For the closed string case this expression is given in Eqs. (39), (40) in Ref. 2. In the critical open string theory case one is to omit an additional integral over the length of the boundary in the expression following Eq. (54) in Ref. 2.] The constant a_1 was renormalization scheme dependent (logarithmically divergent before subtraction). Introducing $\Phi=e^{-T/2}$ and properly tuning a_1 one was able to reproduce the standard tachyon kinetic term. The meaning of that procedure was, however, unclear.

Indeed, to be able to make a connection with the standard tachyonic amplitudes it was obvious that one should expand in powers of T and not derivatives of T as the tachyon momentum should be close to its mass shell value. The corresponding tachyon beta-function then receives contributions which are nonperturbative in α'[6,12,13] and which are in agreement with the tachyonic terms in the effective action reconstructed directly from string amplitudes. The form of the ''tachyon potential,'' i.e., the zero-momentum part of such action is inherently ambiguous,[14,13] as one can always ''dress'' any factor of T by ∂^2 without changing on-shell amplitudes. Thus one needs some extra principle, not apparent at the level of the string S-matrix, to fix this ambiguity.

One could still hope that such extra input was, in fact, contained in the world-sheet sigma model approach. This was effectively vindicated by the recent derivations of the tachyon potential in the open string theory (which were motivated by the study of tachyon condensation on non-BPS D-branes):[15–18] (For some early studies of tachyon condensation see Ref. 19.) $e^{-T}(1+T)$ in the bosonic string case[20,21] and e^{-T^2} in the NSR string case.[22]

While the discussions in Refs. 20–22 were presented in the framework of Witten's background-independent open string field theory,[23,24] their results can be obtained directly in the context of the sigma model approach as we shall review below.

The idea is to return back to the original boundary sigma model[2] containing only the tachyon and massless vector couplings. This model is renormalizable within the standard derivative (α') expansion, i.e., its set of couplings is closed under perturbative RG flow. While one will certainly need to resum the α' expansion to be able to reproduce correct interaction terms at the standard tachyon vacuum point $T=0$, the low-energy expansion (approximate in ∂T but exact in T) may be useful in order to reveal the existence of a new stationary point invisible in perturbation theory near $T=0$.

As was argued in Refs. 10, 25 the tree level effective action $S[A]$ for the massless vector field should be given simply by the *renormalized* partition function of the boundary sigma model, as originally conjectured in Ref. 2. The renormalization of logarithmic infinities corresponds to subtraction of massless poles[10,6,26], while elimination of power divergences by a shift of the bare tachyon coupling accounts for a contribution of the tachyon poles in the massless amplitudes. When consistently implemented, this renormalization procedure resolves (as we shall explain in Sec. II B) an apparent contradiction between $S[A]=Z[A]$ ansatz and string S-matrix found at the level of the $F^2(\partial F)^2$ terms in Ref. 27.

In the presence of a nonzero (renormalized) tachyon background the $S=Z$ prescription requires a modification in the case of *bosonic* string theory. Indeed, $Z'=\partial Z/\partial T$ does not vanish at the standard vacuum point $T=0$, so one needs to make a subtraction of the derivative term $S[T]=Z[T]-T\cdot Z'[0]+\ldots$. A consistent modification of $S=Z$ satisfying $S[0]=0$ was suggested in the context of the Witten's approach.[23,24] $\hat{S}[T]=Z[T]+\beta^T\cdot Z'[T]$, where β^T is the tachyon β-function. This form of subtraction term is a natural one since it preserves the property of RG invariance of the action. This definition then leads to the expression $e^{-T}(1+T)$ for the open bosonic string tachyon potential.[20] We derive the corresponding low-energy effective action in Sec. II A and also generalize it to the presence of a constant F_{mn} background.

The complication of power divergences and associated shift of the tachyon coupling is absent in the case of world-sheet supersymmetric NSR string, where the $S[A]=Z[A]$ prescription is manifestly consistent[27] and, moreover, should apply also in the case of a nonvanishing tachyon background.[22] [In particular, while in the bosonic string the tachyon couples linearly to the fields of the massless sector, it decouples from them in the NSR case (interaction terms are quadratic in T).] We discuss the NSR case in detail in Sec. III, reproducing some of the results of Ref. 22. We

also give a manifestly gauge invariant definition of the partition function in the general non-abelian case and demonstrate that the second-derivative part of the action $S[T]=Z[T]$ taken in a special scheme has its variation over T proportional to the linear perturbative terms in the tachyon β-function. As in the bosonic case, we generalize this action to the presence of a constant F_{mn} background, when the potential term becomes $e^{-T^2}\sqrt{\det(I+F)}$.

One of the lessons of the application of the sigma model approach to open string theory is that the ''global'' covariant objects defined by the sigma model path integral—partition function or effective action—may contain more information than a set of β-functions (or, more precisely, Weyl anomaly coefficients) computed in a local coordinate patch in field (sigma model coupling) space. Indeed, the information on a metric[8] on the coupling space is effectively encoded in Z. The effective action then may have additional stationary points not seen from the β-functions computed in a ''standard'' coordinate patch. This may happen if the field space metric κ becomes degenerate at these points when described in terms of ''standard'' coordinates. For example, the field space may have a nontrivial topology, and thus may need to be represented by several coordinate patches.

It is natural to expect that the same should be true also in the *closed* string case. In Sec. IV we apply the sigma model approach to discuss the tachyon dependence of the effective actions in *closed* bosonic and NSR string theories. In the closed string theory the effective action for the massless modes is determined by the sigma model partition function on a 2-sphere in the following way:[28,29,5] $S[\lambda]=-(\partial Z/\partial \ln \epsilon)_{\epsilon=1}=\beta^i(\partial Z/\partial\lambda)$, so that $S=\int d^Dx\sqrt{G}e^{-2\phi}(\beta^\phi-1/4G^{mn}\beta^G_{mn})$ $=\int d^Dx\sqrt{G}e^{-2\phi}(D-26+\cdots)$. [The extra derivative over the logarithm of 2-D cutoff (compared to the original $S=Z$ conjecture of Ref. 2) accounts for the subtraction of the volume of the Möbius group which is lorathmically divergent in the 2-sphere case[28] (in both bosonic and fermionic string theories).] We shall suggest that like in the open string case, in the presence of a tachyon background this relation should again be modified by subtracting a term proportional to $\partial S/\partial T$ to satisfy the condition $\hat{S}[0]=0$. The resulting tachyon potential is then $-T^2e^{-T}$.

No such modification is necessary in the closed fermionic NSR (or type 0) string case, where we argue that (the NS–NS part of) the effective action depends on the tachyon field only through $(\partial T)^2$ and $\partial^2 T$, i.e., there appears to be *no* tachyon potential.

II. OPEN BOSONIC STRING

Let us first take a formal approach, forgetting about the possible connection to an on-shell string S-matrix and consider the partition function for the (Euclidean) boundary sigma model with two couplings, $I=\int d\varphi[(1/\epsilon)T(x)+iA_m(x)\dot{x}^m]$. This theory is power counting renormalizable if one expands in powers of derivatives of T and A_m, i.e., is closed under RG with all higher-derivative nonrenormalizable interactions (massive string modes) consistently decoupled. One can then ask which is the functional $S[T,A]$ (the boundary analog[30] of the c-function[8]) that reproduces the corresponding perturbative β-functions in the sense of $\partial S/\partial\lambda^i=\kappa_{ij}(\lambda)\beta^j$, $\lambda^i=(T,A_m)$. If we decouple the tachyon (solve for it in terms of A_m) the result should then be the effective action consistent with the S-matrix for the massless vector mode. More generally, such an ''effective action'' functional $S[T,A]$ may represent a natural off-shell extension, capturing non-trivial behavior of string theory far away from the standard tachyonic mass shell. Remarkably, this is indeed what happens to be true, as indicated by the discussions in Refs. 20 and 21.

It is useful to start by recalling the expression for the partition function (or the generating functional for tachyon and vector amplitudes in open string theory on the disk) in the general non-Abelian case[2,11]

$$Z[T,A,\epsilon]=\left\langle \operatorname{tr} P\exp\left(-\int d\varphi[\epsilon^{-1}T(x)+iA_m(x)\dot{x}^m]\right)\right\rangle, \tag{2.1}$$

where the averaging is done with the free string action in the bulk of the disk and $\varphi\in(0,2\pi)$ parametrizes its boundary. Here T and A_m are Hermitian matrices in the Chan–Paton algebra of

$U(N)$. (We consider the oriented string case relevant in the D-brane context and define the action so that continued to the Minkowski signature it becomes real.) $\epsilon = a/r \to 0$ is a dimensionless UV cutoff, i.e., the ratio of the short-distance cutoff and the radius of the disk. $\langle \cdots \rangle$ depends on ϵ through the propagator [see Eq. (2.5)]. One can make (2.1) more explicit by using the well-known representation[31] of path ordered exponent in terms of the path integral over 1-D anticommuting fields $\eta^a, \overline{\eta}_b$ in the fundamental and antifundamental representations of $U(N)$,

$$Z[T,A,\epsilon] = \left\langle \int [d\eta][d\overline{\eta}] \exp\left(- \int d\varphi [\, \overline{\eta}_a \dot{\eta}^a + \overline{\eta}_a (\epsilon^{-1} T^a_b(x) + i A^a_{bm}(x) \dot{x}^m) \eta^b] \right) \right\rangle. \quad (2.2)$$

The measure of integration is assumed to contain the factor $\overline{\eta}_c(0)\,\eta^c(2\pi)$. In the Abelian case (2.1) is simply

$$Z[T,A,\epsilon] = \langle e^{-\int d\varphi [\epsilon^{-1} T(x) + i A_m(x) \dot{x}^m]} \rangle. \quad (2.3)$$

The standard procedure[2,11,25] to compute Z is to first isolate the constant (''zero mode'') part of x^m and integrate over the internal points of the disk getting an effective 1-D path integral for the boundary theory

$$Z = a_0 \int d^D x\, \epsilon^{-W}, \quad e^{-W} = \langle e^{-I} \rangle = \int [d\xi] e^{-(1/4\pi\alpha') \int \xi G^{-1} \xi - I}, \quad (2.4)$$

$$G(\varphi_1, \varphi_2) = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{e^{-n\epsilon}}{n} \cos n\varphi_{12}, \quad \varphi_{12} = \varphi_1 - \varphi_2, \quad (2.5)$$

$$I = \int d\varphi \left[\epsilon^{-1} \left(T + \frac{1}{2} \xi^m \xi^k \partial_m \partial_k T + \frac{1}{6} \xi^m \xi^k \xi^l \partial_m \partial_k \partial_l T + \cdots \right) + i \left(\frac{1}{2} \xi^k F_{km} + \frac{1}{3} \xi^k \xi^l \partial_l F_{km} + \cdots \right) \dot{\xi}^m \right]. \quad (2.6)$$

We have shifted $x(\varphi) \to x + \xi(\varphi)$, $\int_0^{2\pi} d\varphi\, \xi(\varphi) = 0$ (so that W contains contributions of 1PI graphs only). In what follows we shall often set the inverse string tension $2\pi\alpha'$ to one, but the dependence on α' is easy to restore on dimensional grounds, $\partial^k T \to (\sqrt{2\pi\alpha'}\partial)^k T$, $\partial^k F_{mn} \to (\sqrt{2\pi\alpha'}\partial)^k (2\pi\alpha' F_{mn})$.

If one ignores all higher than second powers in ξ, i.e., assumes that $\partial_m \partial_n T$ and F_{mn} are constant, the resulting path integral becomes Gaussian and can be computed explicitly, as was done for $T=0$ in Ref. 11 (see also Ref. 32) and including $\partial_m \partial_n T$ in Ref. 33–36.

One may ''resum'' the perturbative expansion by including the $F\xi\xi$ term into the propagator;[37] regularizing the final expression one gets[25,27]

$$G^{mn}(\varphi_1, \varphi_2 | F) = \frac{1}{\pi} \sum_{n=1}^{\infty} \frac{e^{-\epsilon n}}{n} [\mathcal{G}^{mn}(F) \cos n\varphi_{12} - i \mathcal{H}^{mn}(F) \sin n\varphi_{12}], \quad (2.7)$$

$$\mathcal{G}^{mn}(F) \equiv [(I+F)^{-1}]^{(mn)} = [(I-F^2)^{-1}]^{mn} = \delta^{mn} + F^{mk} F^{kn} + \cdots, \quad (2.8)$$

$$\mathcal{H}^{mn} \equiv -[(I+F)^{-1}]^{[mn]} = [F(I-F^2)^{-1}]^{mn} = F^{mk} \mathcal{G}^{kn}.$$

It is then straightforward to compute the leading terms in the expansion of Z in derivatives of T and F but to all orders in F_{mn}.

The model (2.2), (2.3) is renormalizable in the derivative (α') expansion, so that T and A_m in (2.2) or (2.3) should be interpreted as ϵ-dependent bare couplings which cancel all the divergent terms, i.e.,[25]

$$Z[T(\epsilon), A(\epsilon), \epsilon] = Z_R[T_R, A_R], \quad (2.9)$$

where

$$T(\epsilon)=\frac{1}{2\pi}\epsilon[1+h_1(A_R)\ln\epsilon+h_2(A_R)\ln^2\epsilon+\cdots]T_R+[k_1(A_R)+k_2(A_R)\ln\epsilon+\cdots], \quad (2.10)$$

$$A(\epsilon)=A_R+f_1(A_R)\ln\epsilon+f_2(A_R)\ln^2\epsilon+\cdots. \quad (2.11)$$

Here the renormalized fields are defined at point $2\pi r$ and h_i contain differential operators acting on T_R. For example, it is easy to show that in the Abelian case and for the constant F_{mn} background,

$$h_1(A)T=\frac{1}{2\pi}\mathcal{G}^{mn}(F)\partial_m\partial_n T,\ \ [f_1(A)]_k=\frac{1}{2\pi}\mathcal{G}^{mn}(F)\partial_m F_{nk}. \quad (2.12)$$

f_1 represents the ''Born–Infeld'' β-function.[37,38] The inhomogeneous term in (2.10),[25]

$$k_1=-\frac{1}{4\pi}\ln\det(\delta_{mn}+F_{mn})=-\frac{1}{8\pi}F_{mn}^2+O(F^4), \quad (2.13)$$

corresponds to a shift of the bare tachyon needed to be done to absorb the F_{mn}-dependent linear divergence appearing in the computation of Z for $F_{mn}=\text{const}$ leading to the BI action,[11,25]

$$W=b_0\ln\det(\delta_{mn}+F_{mn}),\quad b_0=\sum_{n=1}^{\infty}e^{-2\epsilon n}=\frac{1}{2\epsilon}-\frac{1}{2}+O(\epsilon). \quad (2.14)$$

If one subtracts the term (2.13) from the beginning, it will not appear in the corresponding β^T-function. This is a scheme-dependent[39] property, as one can of course induce a similar term back by a field redefinition, $T\to T+f(F)$. (A similar inhomogeneous term does not appear in the tachyon β-function in the closed string case if one uses the natural scheme in which the general covariance of the theory is manifest.[13]) This scheme is fixed by the requirement that the corresponding effective action with $T=0$ and $F_{mn}=\text{const}$ is given simply by the BI action (which itself is related, via the D-brane action connection, to basic reparametrization symmetry of the underlying string theory). The subtraction of (2.13) to be done in the bare partition function will play an important role in Sec. II B.

The renormalized value of the partition function takes the form (here and in what follows we omit subscripts ''R'' on the renormalized value of Z and the fields)

$$Z=a_0\int d^Dx e^{-T}\sqrt{\det(\delta_{mn}+F_{mn})}[1+a_1\alpha'\mathcal{G}^{mn}(F)\partial_m\partial_n T + \mathcal{F}^{kmnacd}(F)\partial_k F_{mn}\partial_a F_{cd}+O(\partial^4 T,\partial^4 F^k)], \quad (2.15)$$

where $\mathcal{F}^{kmnacd}(F)\sim F^2+F^4+\cdots$[27] and $\alpha'=1/2\pi$ (i.e., $2\pi\alpha'=1$).

The coefficient a_1 is logarithmically divergent before renormalization $[\pi G(\varphi,\varphi)=\Sigma_{n=1}^{\infty}(1/n)e^{-\epsilon n}=-\ln\epsilon+O(\epsilon)]$ and thus is scheme dependent, i.e., its value can be changed by a field redefinition.[39,25]

A. Tachyon action

Let us first set $F_{mn}=0$ and consider the dependence of Z (2.15) on T,

$$Z=a_0\int d^Dx e^{-T}(1+a_1\alpha'\,\partial^2 T+\cdots)=a_0\int d^Dx e^{-T}[1+a_1\alpha'(\partial T)^2+\cdots], \quad (2.16)$$

i.e.,

$$Z = a_0 \int d^D x [\Phi^2 + 4 a_1 \alpha' (\partial \Phi)^2 + \cdots], \quad \Phi \equiv e^{-T/2}. \tag{2.17}$$

This expression which looks like an action for a massive field with $m^2 = (4 a_1 \alpha')^{-1}$ was first found in Ref. 2. However, its derivative does not vanish for $T=0$, i.e., does not reproduce the perturbative tachyon coupling β-function which is given, to all orders in the α' expansion, simply by

$$\beta^T = -T - \alpha' \partial^2 T. \tag{2.18}$$

This suggests that in the *bosonic* open string theory, the definition of the effective action as the renormalized sigma model partition function Z[2,25] needs a modification when the tachyon background is nonzero. The required refinement of the $S=Z$ relation was suggested in Refs. 23, 24: to define an action functional which will be stationary at conformal points one is to add an extra derivative term,

$$\hat{S} = S + \beta^T \cdot \frac{\delta}{\delta T} S = Z + \beta^T \cdot \frac{\delta}{\delta T} Z. \tag{2.19}$$

The second subtraction term is a natural one as it preserves the property of RG invariance of the action. Note that $\hat{S}$ and Z are equal at the stationary points of $\hat{S}$. Also,

$$\hat{S}[T] = S[T + \beta^T] + O((\beta^T)^2) = \epsilon^{\beta^T \cdot \delta / \delta T} Z[T] + O((\beta^T)^2), \tag{2.20}$$

i.e., changing from $S=Z$ to $\hat{S}$ may look like a field redefinition of T. This redefinition is, however, singular in the case of the tachyon coupling.

In general, if for a set of fields (sigma model couplings) λ^i which is closed under the RG one has[23,24]

$$\hat{S} = Z + \beta^i \partial_i Z, \quad \partial_i \hat{S} = \kappa_{ij} \beta^j; \tag{2.21}$$

then

$$\partial_i \hat{S} = \partial_i Z + \partial_i \beta^j \partial_j Z + \beta^j \partial_i \partial_j Z, \tag{2.22}$$

$$(\kappa_{ij} - \partial_i \partial_j Z) \beta^j = (\delta_i^j + \partial_i \beta^j) \partial_j Z, \tag{2.23}$$

so that $\partial_j Z = 0$ may not imply $\beta^j = 0$ if the ''shifted'' matrix of anomalous dimensions $\delta_i^j + \partial_i \beta^j$ is degenerate in some limit (e.g., at low momenta). This is precisely what happens in the tachyon field case [cf. (2.18)], so that the modification (2.19) is important here.

Using (2.16), (2.18) we find that (2.19) is given, to the leading order in derivatives of T, by (cf. Refs. 20, 21)

$$\hat{S} = a_0 \int d^D x e^{-T} [1 + T + (1 - a_1) \alpha' (\partial T)^2 + a_1 \alpha' T (\partial T)^2 + O(\partial^4 T)]. \tag{2.24}$$

Choosing a *special* scheme where

$$a_1 = \tfrac{1}{2}, \tag{2.25}$$

one finally gets

$$\hat{S} = a_0 \int d^D x e^{-T} \left[(1+T) \left(1 + \frac{1}{2} \alpha' \partial^m T \partial_m T \right) + O(\partial^4 T) \right]. \tag{2.26}$$

Then

$$\frac{\delta\hat{S}}{\delta T}=a_0 e^{-T}\Big[-T-\alpha'\,\partial^2 T-\alpha' T\,\partial^2 T+\frac{1}{2}\alpha' T(\partial T)^2+O(\alpha'^2\,\partial^4 T)\Big], \tag{2.27}$$

which is indeed proportional to the β^T-function (2.18) to the leading order in T.[20,21] Here e^{-T} should be interpreted as the field space metric $\kappa_{TT}(T)$ in (2.21) and the nonlinear terms in T should be redefinable away [within α' or derivative expansion (2.18) should be the exact expression for the β^T-function]. Equation (2.27) has two obvious zeros: $T=0$ and $T=\infty$ with the second one related to the tachyon condensation.[16,21] [Another solution $T(x)=a+ux^2$ with finite constants a, u[21] is an artifact of α' expansion (it does not correspond to a conformal 2-D theory).]

Including a $F_{mn}=$const background we get the following generalization of (2.15), (2.24):

$$\hat{S}=a_0\int d^D x e^{-T}\sqrt{\det(\delta_{mn}+F_{mn})}\Big[1+T+\frac{1}{2}\alpha'\mathcal{G}^{mn}(F)\partial_m\partial_n T+\cdots\Big], \tag{2.28}$$

or

$$\hat{S}=a_0\int d^D x e^{-T}\sqrt{\det(\delta_{mn}+2\pi\alpha' F_{mn})}\Big[(1+T)\Big[1+\frac{1}{2}\alpha'\mathcal{G}^{mn}(2\pi\alpha' F)\partial_m T\,\partial_n T\Big] + O(\alpha'^2\,\partial^4 T,\alpha'^2\,\partial^2 F)\Big], \tag{2.29}$$

where we restored the full dependence on α'. The variation of this action is proportional the β^T-function (2.18) with $\partial^2 T$ replaced by $\mathcal{G}^{mn}(F)\partial_m\,\partial_n T$ [in agreement with (2.12)], and which does not contain the inhomogeneous term (2.13).

One may raise the question of why the action (2.29) is consistent with the string S-matrix which contains a nonvanishing tachyon–vector–vector amplitude. The latter can be reproduced by the TF_{mn}^2 term in the effective action but such a term is not present in (2.29). However, the term $-\alpha' F_{mn}^2\,\partial^2 T$ (or $-2\alpha' T\,\partial_k F_{mn}\,\partial_k F_{mn}$) leads to the same on-shell 3-point amplitude since for the on-shell tachyon $\alpha'\,\partial^2 T=-T$. Such a higher derivative term is indeed present in (2.28) or (2.29). The corresponding $\partial_k F_{mn}\,\partial_k F_{mn}$ term in (2.27) or in the tachyon β-function is not visible in the α' expansion but can be reproduced if one expands in powers of the fields instead of powers of derivatives and sums all orders in α' (see Ref. 12). [This case is completely analogous to the RT vs $R_{mnkl}^2 T$ contribution (giving the same on-shell graviton–graviton–tachyon amplitude) in the closed string effective action discussed in Ref. 13].

B. Vector field action

Let us now set T to zero and consider the dependence of Z on the vector field A_m. In view of the arguments given in Refs. 10, 25, 27 the effective action $S[A]$ which reproduces the string S-matrix and is also consistent with the expression for the vector field β^A-function in the boundary sigma model should be given simply by the *renormalized* value of the sigma model partition function,

$$S[A_R]=Z_R[A_R,T_R=0]. \tag{2.30}$$

We shall again omit subscripts ''R'' below.

This relation passes a number of nontrivial tests. In the Abelian case, for $F_{mn}=$const one finds that Z is equal to the BI action[11] whose derivative over A_m is indeed to be proportional to the leading one-loop term $-\alpha'\mathcal{G}^{mn}(F)\partial_m F_{nk}$ in the β^A-function.[37] The F^4 term in the expansion of the BI action is also in agreement with the string 4-point amplitude.[10,40] In the non-Abelian case, the direct computation of $Z(A)$ defined by (2.3) gives, after a renormalization,[25]

$$Z=a_0\int d^Dx\,\mathrm{tr}\Big[1-(2\pi\alpha')^2\Big[\frac{1}{4}F_{mn}^2+\frac{2}{3}\alpha' F_{mn}F_{nk}F_{km}+d_1\alpha'(D_mF_{mn})^2\Big]+O(\alpha'^4)\Big], \tag{2.31}$$

where d_1 is scheme-dependent. This coincides with the non-Abelian F^2+F^3 terms in the action reconstructed from the bosonic string S-matrix.[1,10]

There was, however, a problem with $S=Z$ ansatz (2.30) in the *bosonic* string case pointed out in Ref. 27. The direct computation of the leading derivative ∂F-dependent terms in the Abelian partition function (2.3) gave the following expression $(2\pi\alpha'=1)$:[27]

$$Z=a_0\int d^Dx\Big[1+\frac{1}{4}F_{mn}^2-\frac{1}{8}\Big[(F_{mk}F_{kn})^2-\frac{1}{4}(F_{mn}^2)^2\Big]+b_1F_{kl}F_{kl}\,\partial_aF_{mn}\,\partial_aF_{mn}$$
$$+b_2F_{kl}F_{lm}\,\partial_aF_{mn}\,\partial_aF_{nk}+b_3F_{la}F_{lb}\,\partial_aF_{mn}\,\partial_bF_{mn}+O(\partial^2F^6)\Big], \tag{2.32}$$

where

$$b_1=\frac{1}{24\pi},\quad b_2=-\frac{1}{6\pi},\quad b_3=\frac{1}{12\pi}, \tag{2.33}$$

and we have ignored all terms which have scheme-dependent coefficients (i.e., vanish on $\partial_mF_{mn}=0$). At the same time, both the string 4-point amplitude[27] and the 2-loop sigma model β^A-function calculation[41] led to the action (2.32) with the coefficients

$$b_1=-\frac{1}{48\pi},\quad b_2=-\frac{1}{6\pi},\quad b_3=\frac{1}{12\pi}, \tag{2.34}$$

i.e., with the *same* b_2 and b_3 but with b_1 differing by factor $-1/2$. This apparent disagreement of the $S=Z$ ansatz with the S-matrix and the β^A-function was attributed in Ref. 27 to the presence of the tachyon in the bosonic string. The tachyon poles are formally expanded in momenta in the derivation of the massless field effective action from the string S-matrix, and it was suggested that the corresponding subtraction of power divergences in Z may be hard to implement unambiguously.

This problem has, in fact, a very simple resolution implied by the definition (2.30): a particular ''tachyon-related'' $F^2\,\partial F\,\partial F$ term was missed in Ref. 27 since the tachyon field there was set equal to zero *before* properly subtracting the linearly divergent F-dependent term (2.13). This subtraction effectively accounts for the contribution coming from the expansion of the tachyonic pole in the 4-vector amplitude which is included in the effective action if it is reconstructed from the S-matrix. Once this extra term is added, the agreement between $S[A]$ and $Z[A]$ is indeed restored!

As was stressed above, the effective action should be given by the *renormalized* value of $Z[A]$. The bare partition function has the same structure as (2.15) [with $T\equiv T_R\to(2\pi/\epsilon)T$] but in addition it contains the linearly divergent term in the exponent $e^{(2\pi/\epsilon)k_1}$ [see (2.14), (2.13)]. Shifting the bare tachyon (2.10) to absorb this linear divergence (and then setting $T_R=0$) introduces extra ∂F-dependent terms effectively originating from the ∂^2T term in (2.15). Explicitly, applying the *same* computational scheme [ϵ-regularization in (2.5) plus minimal subtraction] that was used in the original computation of (2.32), (2.33) in Ref. 27 one finds the following expression for $Z(T,A)$ in (2.4), (2.5) $(2\pi\alpha'=1)$, (In the form described below this computation was done by Andreev. It corrects the original version of this argument.)

$$Z=\int d^Dx\,e^{-(2\pi/\epsilon)T}[1+k_1(\epsilon)\partial^2T+k_2(\epsilon)F_{mn}^2+k_3(\epsilon)F_{mn}^2\,\partial^2T+k_4(\epsilon)F^{km}F^{kn}\partial_m\,\partial_nT+O(\partial^4)], \tag{2.35}$$

where

$$k_1=-\epsilon^{-1}I_1(\epsilon),\quad k_2=-\tfrac{1}{2}I_0(2\epsilon),\quad k_3=\tfrac{1}{2}\epsilon^{-1}I_0(2\epsilon)I_1(\epsilon),\quad k_4=\epsilon^{-1}I_1(3\epsilon),\quad (2.36)$$

and

$$I_0(\epsilon)\equiv\sum_{n=1}^{\infty} e^{-\epsilon n}=(e^{\epsilon}-1)^{-1}=\frac{1}{\epsilon}-\frac{1}{2}+\frac{\epsilon}{12}+O(\epsilon^2),\quad (2.37)$$

$$I_1(\epsilon)\equiv\sum_{n=1}^{\infty}\frac{1}{n}e^{-\epsilon n}=-\ln(1-e^{-\epsilon})=-\ln\epsilon+\frac{1}{2}\epsilon+O(\epsilon^2).\quad (2.38)$$

To cancel the leading power divergences in the F_{mn}^2 and $F_{mn}^2\,\partial^2 T$ terms one is to shift $T\to T-(1/8\pi)F_{mn}^2$ in the exponent. Using the *minimal* subtraction to absorb the singular logarithmic parts of the coefficients k_i into the bare couplings T and A_m one is left with the following values for their finite $(\epsilon\to 0)$ parts: $(k_2)_{\rm fin}=1/4$, $(k_3)_{\rm fin}=-1/8$, $(k_4)_{\rm fin}=3/2$. The additional $F^2\partial\partial F^2$ terms coming from (2.35) that should be added to (2.32) are then

$$\Delta Z=a_0\int d^Dx\left(\frac{1}{16\pi}\right)\left[\frac{1}{4}F_{kl}^2\partial^2(F_{mn}^2)-3F_{pq}^2\partial_m\partial_n(F_{mk}F_{nk})\right].\quad (2.39)$$

Using $\partial_{[k}F_{mn]}=0$ and dropping terms proportional to the equations of motion so that $\partial_nF_{mk}\,\partial_mF_{nk}=1/2\partial_kF_{mn}\,\partial_kF_{mn}+O(\partial_mF_{mn})$, we find

$$\Delta Z=a_0\int d^Dx\left(-\frac{1}{16\pi}\right)F_{pq}F_{pq}\,\partial_kF_{mn}\,\partial_kF_{mn}\,.\quad (2.40)$$

Thus this ''tachyonic'' correction contributes only to the coefficient of the first $F^2\,\partial F\,\partial F$ term in (2.32),

$$b_1\to b_1-\frac{1}{16\pi},\quad (2.41)$$

changing it precisely into the b_1 in (2.34). This implies the *equivalence* of the leading ∂F derivative terms in the effective actions obtained (i) from the partition function, (ii) from the string S-matrix, and (iii) from the β^A-function.

III. OPEN NSR STRING

Ignoring first the tachyon, the analog of the partition function (2.3), (2.4) which is the generating functional for massless vector scattering amplitudes is given by[10,42,27]

$$Z(A)=\left\langle \mathrm{tr}P\,\exp\left(-i\int d\varphi\left[\dot{x}^mA_m(x)-\frac{1}{2}\psi^m\psi^nF_{mn}(x)\right]\right)\right\rangle$$
$$=\int d^Dx\left\langle \mathrm{tr}P\,\exp\left(-i\int d\varphi\left[\dot{\xi}^mA_m(x+\xi)-\frac{1}{2}\psi^m\psi^nF_{mn}(x+\xi)\right]\right)\right\rangle,\quad (3.1)$$

where the averaging is done with the free string propagator restricted to the boundary of the disk, i.e., with the effective 1-D boundary action $I_0=(1/4\pi\alpha')\int(\xi G^{-1}\xi+\psi K^{-1}\psi)$ with periodic $\xi^m(\varphi)$ and antiperiodic $\psi^m(\varphi)$. The bosonic Green's function in (2.5) is now supplemented by the fermionic one,

$$G(\varphi_1,\varphi_2)=\frac{1}{\pi}\sum_{n=1}^{\infty}\frac{e^{-n\epsilon}}{n}\cos n\varphi_{12},\quad K(\varphi_1,\varphi_2)=\frac{1}{\pi}\sum_{r=1/2}^{\infty}e^{-r\epsilon}\sin r\varphi_{12}. \tag{3.2}$$

As discussed in Ref. 27, the $\epsilon\to+0$ regularization preserves underlying 1-D supersymmetry (which is spontaneously broken by the antiperiodic boundary condition on ψ^m, i.e., is an ''asymptotic'' symmetry).

P in (3.1) stands for the standard path ordering. The contact $[A_m,A_n]$ term in F_{mn} implying manifest non-Abelian gauge invariance of the resulting amplitudes can be derived[42,27] from the contact terms in the supersymmetric theta-functions in the manifestly 1-D supersymmetric definition of the path ordering (see also below).

To include the tachyon field, one may start with the standard NS[43] vertex operator $\int d\varphi\psi^m\partial_m T(x)$. This coupling cannot, however, be added directly into the exponent in (3.1) as ψ is Grassmann while T is not (integrating ψ^m out would leave no dependence on T). To get a nonzero answer for the correlators one is to properly order the interaction vertices. A simple way to do that, as suggested in Ref. 44 and elaborated on in Refs. 16, 22, is to introduce a nondynamical 1-D anticommuting, real, antiperiodic field $\zeta(\varphi)$, and to add to the action the following terms $\int d\varphi[\zeta\dot{\zeta}+i\zeta\psi^m\partial_m T(x)]$.

A. General non-Abelian case

More precisely, to automatically include the contact terms which will make the non-Abelian gauge invariance explicit, one is to insist on manifest world-sheet supersymmetry of the sigma model interaction terms.[45,42,27] As in Refs. 46, 27 here this is accomplished by replacing x^m by the 1-D scalar superfields $\hat{x}^m=x^m+\theta\psi^m$, and the $U(N)$ ''quarks'' η^a, $\overline{\eta}_\alpha$ in (2.2) and the new variable ζ by the ''spinor'' superfields $\hat{\eta}^a=\eta^a+\theta\chi^a$, $\hat{\overline{\eta}}_a=\overline{\eta}_a+\theta\overline{\chi}_a$ and $\hat{\zeta}=\zeta+\theta f$. This ensures the 1-D supersymmetry of the path ordering.[42,27] The resulting partition function is given by the path integral over $\hat{x}^m$, $\hat{\eta}$, $\hat{\overline{\eta}}$, $\hat{\zeta}$ similar to (2.2), with the interaction part of the action now being

$$I=-\int d\varphi\, d\theta(\hat{\overline{\eta}}D\hat{\eta}+\hat{\zeta}D\hat{\zeta}+i\hat{\overline{\eta}}[\hat{\zeta}\mathcal{T}(\hat{x})+A_m(\hat{x})D\hat{x}^m]\hat{\eta}), \tag{3.3}$$

where $D\equiv\theta\partial_\varphi-\partial_\theta$ and we suppressed the $U(N)$ indices on $\hat{\eta}^a$, $\hat{\overline{\eta}}_a$ and the fields $\mathcal{T}^a_b$, A^a_{bm}. Here $\mathcal{T}$ is the bare tachyon, i.e., $\mathcal{T}\sim(1/\sqrt{\epsilon})T$.

The component form of (3.3) is

$$\begin{aligned}I=\int d\varphi[&\overline{\eta}\dot{\eta}+\zeta\dot{\zeta}+f^2+\overline{\chi}\chi+i\overline{\eta}(\mathcal{T}\zeta+A_m\psi^m)\chi-i\overline{\chi}(\mathcal{T}\zeta-A_m\psi^m)\eta\\&+i\overline{\eta}[f\mathcal{T}-\zeta\psi^m\partial_m\mathcal{T}+(A_m\dot{x}^m-\psi^m\psi^n\partial_m A_n)]\eta].\end{aligned} \tag{3.4}$$

This action is manifestly 1-D supersymmetric, but its non-Abelian gauge invariance becomes apparent only after integrating over the auxiliary fields χ, $\overline{\chi}$,

$$I=\int d\varphi\left[\overline{\eta}\dot{\eta}+\zeta\dot{\zeta}+f^2+i\overline{\eta}\left[f\mathcal{T}-\zeta\psi^m\mathrm{D}_m\mathcal{T}+\left(A_m\dot{x}^m-\frac{1}{2}\psi^m\psi^nF_{mn}\right)\right]\eta\right], \tag{3.5}$$

where

$$\mathrm{D}_m\mathcal{T}=\partial_m\mathcal{T}+i[A_m,\mathcal{T}],\quad F_{mn}=\partial_mA_n-\partial_nA_m+i[A_m,A_n].$$

Integration over the auxiliary field f gives

$$I=\int d\varphi\left[\overline{\eta}\dot{\eta}+\zeta\dot{\zeta}+\frac{1}{4}(\overline{\eta}\mathcal{T}\eta)^2+i\overline{\eta}\left[-\zeta\psi^m\mathrm{D}_m\mathcal{T}+\left(A_m\dot{x}^m-\frac{1}{2}\psi^m\psi^nF_{mn}\right)\right]\eta\right]. \tag{3.6}$$

Finally, integrating over ζ we find

$$I=\int d\varphi\Big[\overline{\eta}\dot{\eta}+\frac{1}{4}(\overline{\eta}\mathcal{T}\eta)^2-\frac{1}{4}(\psi^m\overline{\eta}D_m\mathcal{T}\eta)\partial_\varphi^{-1}(\psi^n\overline{\eta}D_n\mathcal{T}\eta)+i\overline{\eta}\Big(A_m\dot{x}^m-\frac{1}{2}\psi^m\psi^nF_{mn}\Big)\eta\Big]. \tag{3.7}$$

Here [cf. (3.2)]

$$\partial_\varphi^{-1}(\varphi_1,\varphi_2)=\frac{1}{\pi}\sum_{r=1/2}^{\infty}\frac{1}{r}\sin r\varphi_{12}. \tag{3.8}$$

[Note that the δ-function defined on antiperiodic functions is $\delta^{(-)}(\varphi_1,\varphi_2)=(1/\pi)\Sigma_{r=1/2}^{\infty}\cos r\varphi_{12}$ so that (ignoring regularization; cf. Ref. 27) $K\cdot K=-\delta^{(-)}$ and $\partial_\varphi\cdot\partial_\varphi^{-1}=\delta^{(-)}$, $\partial_{\varphi_1}(\varphi_1,\varphi_2)\equiv\partial_{\varphi_1}\delta^{(-)}(\varphi_1,\varphi_2)=-(1/\pi)\Sigma_{r=1/2}^{\infty}r\sin r\varphi_{12}$. One could think of using the regularized expression $\partial_\varphi^{-1}(\varphi_1,\varphi_2)=(1/\pi)\Sigma_{r=1/2}^{\infty}(e^{-re}/r)\sin r\varphi_{12}$, but that leads to complicated expressions as it should be accompanied by a similar regularization in the f^2 term to preserve 1-D supersymmetry.] The resulting derivative expansion of Z is thus expressed in terms of $\mathcal{T}$, F_{mn} and their covariant derivatives.

In the Abelian $U(1)$ case the integral over η, $\overline{\eta}$ in (3.5) is trivial and the tachyonic part of (3.7) becomes equivalent to the terms originally derived in Refs. 16, 22 [cf. (2.3)]

$$I=\int d\varphi\Big(\frac{1}{4}\mathcal{T}^2(x)-\frac{1}{4}[\psi^m\partial_m\mathcal{T}(x)]\partial_\varphi^{-1}[\psi^n\partial_n\mathcal{T}(x)]+i\Big[A_m(x)\dot{x}^m-\frac{1}{2}\psi^m\psi^nF_{mn}(x)\Big]\Big). \tag{3.9}$$

It is easy to check directly that this action is invariant under 1-D supersymmetry $\delta x^m=\psi^m\epsilon$, $\delta\psi^m=\partial_\varphi x^m\,\epsilon$. Note that if $\mathcal{T}$ is a constant non-Abelian matrix then the path ordering [the integral over η in (3.5)] is not relevant, and integrating over f one gets the potential factor $\mathrm{tr}e^{-(\pi/2)\mathcal{T}}$.[22] In general, however, the non-Abelian generalization of (3.9) consistent with 1-D supersymmetry is obtained by using (3.7) [and not by adding trace with ordinary path ordering to (3.9)].

This 1-D supersymmetric theory defined by (3.2), (3.9),

$$Z[\mathcal{T},A]=\int d^Dx e^{-W},\quad e^{-W}=\langle e^{-I[x+\xi,\psi]}\rangle,$$
$$\langle\cdots\rangle=\int[d\xi][d\psi]e^{-(1/4\pi\alpha')\int(\xi G^{-1}\xi+\psi K^{-1}\psi)}, \tag{3.10}$$

has only logarithmic UV divergences, i.e., all power divergences cancel out.[47,27] This is true in the general non-Abelian case, and also in the presence of supersymmetric higher-derivative interactions, and is implied, e.g., by the nonlocal form of the 1-D supersymmetric lowest-dimension interaction in (3.7), (3.9).

In particular, there is no inhomogeneous F-dependent term (2.13) in the analog of (2.10). Indeed, the coefficient in the analog of (2.14) (i.e., in Z computed for $F_{mn}=\mathrm{const}$) now has both bosonic and fermionic contributions and is finite as a result:[47]

$$b_0=\sum_{n=1}^{\infty}e^{-2\epsilon n}-\sum_{r=1/2}^{\infty}e^{-2\epsilon r}=-\frac{1}{2}+O(\epsilon). \tag{3.11}$$

This cancellation of power divergences makes the NSR string partition function $Z[A,\mathcal{T},\ldots]$ much better defined than in the bosonic string case.

One consequence is that the tachyon field manifestly decouples from the massless vector sector. This follows of course from the conservation of G-parity ($\psi^m\to-\psi^m,\theta\to-\theta$) under

which the tachyonic vertex is odd, while the vector vertex is even. In the S-matrix language, there are no tachyonic poles in the massless NS vector amplitudes (so that the theory has of course consistent superstring truncation). Equivalently, this is obvious from (3.9) where $\mathcal{T}$ appears only quadratically.

As a result, the subtleties like the one discussed in Sec. II B do not appear in the NSR case, and the renormalized partition function $Z[A_R, \mathcal{T}_R=0]$ gives directly the vector field effective action consistent with the string S-matrix and β^A-function.[27] (Renormalization of logarithmic divergences corresponding to the subtraction of massless poles in the string amplitudes is still needed in order to define the effective action.) For example, it was demonstrated in Ref. 27 that the leading derivative correction to the BI term in the partition function Z (3.10), (3.9) which has the structure $F^2(\partial\partial F)^2$ is exactly the same as in the action reconstructed from the 4-point NSR string vector amplitude.

B. Tachyon action and correspondence with β-function

Let us compute the leading $\mathcal{T}$-dependent terms in the Abelian partition function (3.10) using a derivative expansion. Expanding in powers of the quantum fields ξ, ψ one finds

$$I=\frac{1}{4}\int d\varphi[\mathcal{T}^2(x+\xi)-[\psi^m\partial_m\mathcal{T}(x+\xi)]\partial_\varphi^{-1}[\psi^n\partial_n\mathcal{T}(x+\xi)]]$$

$$=\frac{1}{4}\int d\varphi[\mathcal{T}^2+(\mathcal{T}\partial_m\partial_n\mathcal{T}+\partial_m\mathcal{T}\,\partial_n\mathcal{T})\xi^m\xi^n-\psi^m\partial_m\mathcal{T}\,\partial_\varphi^{-1}\psi^n\partial_n\mathcal{T}+O(\xi^3,\psi^2\xi)]. \quad (3.12)$$

The leading one-loop contribution to (3.9) is thus ($2\pi\alpha'=1$)

$$W=\frac{\pi}{2}(\mathcal{T}^2+s_1\mathcal{T}\,\partial^2\mathcal{T}+s_2\partial_m\mathcal{T}\,\partial_m\mathcal{T})+O(\partial^4), \quad (3.13)$$

where

$$s_1=G(\varphi,\varphi)=\frac{1}{\pi}\sum_{n=1}^{\infty}\frac{e^{-\epsilon n}}{n}=-\frac{1}{\pi}\ln\epsilon+O(\epsilon), \quad (3.14)$$

$$s_2=(G+K\cdot\partial_\varphi^{-1})(\varphi,\varphi)=\frac{1}{\pi}\left(\sum_{n=1}^{\infty}\frac{e^{-\epsilon n}}{n}-\sum_{r=1/2}^{\infty}\frac{e^{-\epsilon r}}{r}\right)=-\frac{1}{\pi}\ln 4+O(\epsilon). \quad (3.15)$$

The exact expressions for the sums are[27] $\Sigma_{n=1}^{\infty}(e^{-\epsilon n}/n)=-\ln(1-e^{-\epsilon})$, $\Sigma_{r=1/2}^{\infty}(e^{-\epsilon r}/r)=-\ln[(1-e^{-\epsilon/2})/(1+e^{-\epsilon/2})]$. Thus while the coefficient of $\partial\mathcal{T}\,\partial\mathcal{T}$ term is finite[22] (it may probably depend on a regularization only if the latter break 1-D supersymmetry, cf. Ref. 36), the coefficient of $\mathcal{T}\,\partial^2\mathcal{T}$ term is logarithmically divergent. This divergence is to be renormalized by absorbing it into $\mathcal{T}$. Just as in the bosonic case, this logarithmic divergence determines the derivative term in the tachyon β-function. The coefficient of the logarithmic pole (i.e., the anomalous dimension of the tachyon vertex operator) is of course the same as in the bosonic case, but the dimension of the NS tachyon vertex is half the bosonic one ($\mathcal{T}\sim 1/\sqrt{\epsilon}$). Thus [cf. (2.18)]

$$\beta^{\mathcal{T}}=-\frac{1}{2}\mathcal{T}-\frac{1}{2\pi}\partial^2\mathcal{T}. \quad (3.16)$$

Introducing a constant F_{mn} background means replacing G by $G(F)$ in (2.7) and K in (3.2) by $K(F)$,[48,27]

$$K^{mn}(\varphi_1,\varphi_2|F)=\frac{1}{\pi}\sum_{r=1/2}^{\infty}e^{-\epsilon r}[\mathcal{G}^{mn}(F)\sin r\varphi_{12}+i\mathcal{H}^{mn}(F)\cos r\varphi_{12}]. \quad (3.17)$$

Then one finds again (3.13) but with the flat target space metric replaced by $\mathcal{G}^{mn}(F)$ in (2.8). In particular, then (3.16) takes the form (see also Ref. 36)

$$\beta^{\mathcal{T}}=-\frac{1}{2}\mathcal{T}-\frac{1}{2\pi}\mathcal{G}^{mn}(F)\partial_m\partial_n\mathcal{T}. \tag{3.18}$$

Ignoring first the F_{mn} background and expanding e^{-W} in derivatives of the tachyon field we obtain the renormalized value of the partition function in (3.10). To simplify the expression let us define the renormalized value of the tachyon T by rescaling $\mathcal{T}$ by $\sqrt{\pi/2}$. Then

$$Z[T]=c_0\int d^Dx e^{-T^2}[1-\overline{s_1}T\,\partial^2T-s_2(\partial T)^2+O(\partial^4T)], \tag{3.19}$$

where $\overline{s_1}$ stands for a renormalized value of s_1 in (3.14). The same expression, but without the $\overline{s_1}$ term was found in Ref. 22 where T was taken to be linear in x^m (i.e., ∂^2T was equal to zero).

It is natural to expect that in contrast to the bosonic string case where one needs to shift Z by a derivative term[23,24] to get the action (2.19) reproducing the tachyon beta function, in the NSR string case the (renormalized) partition function is itself the correct action, not only in the massless vector sector[27] but also in the tachyonic one.[22] To demonstrate that $S[T]=Z[T]$ (3.19) does indeed reproduce both terms in the perturbative β-function (3.16) it is crucial to include the $\overline{s_1}$ term in (3.19). The two derivative-dependent terms in (3.19) are closely related through integration by parts [cf. (2.24)]

$$S[T]=Z[T]=c_0\int d^Dx e^{-T^2}[1+c_1\alpha'(\partial T)^2+c_2\alpha' T^2(\partial T)^2+O(\partial^4T)], \tag{3.20}$$

$$c_1=2\pi(\overline{s_1}-s_2),\quad c_2=-4\pi\overline{s_1}. \tag{3.21}$$

Since s_1 was logarithmically divergent before renormalization, its renormalized value $\overline{s_1}$ is, in principle, ambiguous and, as in the bosonic case [see (2.24)–(2.27)] can be tuned to match the variation of $S[T]$ with the β^T-function in (3.16). Indeed, we find

$$\frac{\delta S}{\delta T}=2c_0e^{-T^2}[-T-c_1\alpha'\,\partial^2T-c_2\alpha' T^2\,\partial^2T+(c_1-c_2)\alpha' T(\partial T)^2 + c_2\alpha' T^3(\partial T)^2+O(\alpha'^2\,\partial^4T)]. \tag{3.22}$$

Thus the linear terms here are proportional to (3.16) if $\overline{s_1}=(1/\pi)(1-\ln 4)$, i.e., if

$$c_1=2. \tag{3.23}$$

Then $c_2=4(\ln 4-1)>0$ so that the kinetic term in (3.20) is positive for all T.

While it may seem nonsensical to try to reproduce the correct tachyonic mass plus kinetic terms in the action using the perturbative derivative expansion, the point is that the freedom of field redefinitions allows one to do that, both in the bosonic[20,49] and in the NSR cases. The resulting field space ''metric'' κ is then simplest in such a scheme.

The generalization of the action (3.20) to the presence of a $F_{mn}=$const background is straightforward [cf. (2.29)],

$$S=c_0\int d^Dx e^{-T^2}\sqrt{\det(\delta_{mn}+2\pi\alpha' F_{mn})}[1+c_1\alpha'\mathcal{G}^{mn}(2\pi\alpha' F)\partial_mT\,\partial_nT + c_2\alpha'\mathcal{G}^{mn}(2\pi\alpha' F)T^2\,\partial_mT\,\partial_nT+O(\alpha'^2\,\partial^4T,\alpha'^2\,\partial^2F)]. \tag{3.24}$$

where we restored the dependence on α'. [The partition function for $\partial_m T=\text{const}$, $F_{mn}=\text{const}$ background was computed in Ref. 36; its expansion in ∂T reproduces part of the c_1 term in the expression below which it corresponds to the s_2 term in (3.19).] This action is consistent with (3.18) for $c_1=2$.

The non-Abelian generalization of (3.24) may be obtained, in principle, from the gauge-invariant path integral defined by (3.7).

IV. CLOSED STRING THEORIES

In the bosonic closed string case we start with the sigma model,[2]

$$I=\int d^2z\sqrt{g}\left[\epsilon^{-2}T_0(x)+\frac{1}{4\pi\alpha'}\partial^\mu x^m\,\partial_\mu x^n\,G_{mn}(x)+\frac{1}{4\pi}R^{(2)}\phi(x)\right]. \tag{4.1}$$

(For simplicity, we shall ignore the Kalb–Ramond antisymmetric tensor coupling which is not essential for the present discussion and can be easily included.) This model is renormalizable within an α' expansion. The corresponding bare partition function on a 2-sphere has the form[2]

$$Z[T_0(\epsilon),G(\epsilon),\phi(\epsilon),\epsilon]=d_0\int d^Dx\sqrt{G}e^{-2\phi-\epsilon^{-2}AT_0}e^{-W}, \tag{4.2}$$

where we shifted $x(z)\to x+\xi(z)$ so that [as in (2.4)] W is given by the path integral over the nonconstant fluctuations ξ (see Refs. 2, 10, 29 for details). The coefficient A is the area of fiducial 2-D metric (it can be absorbed into the renormalized value of T_0). The leading logarithmically divergent terms in W are found to be[4,2]

$$\begin{gathered}W=\tfrac{1}{2}\gamma\ln\epsilon+O(\ln^2\epsilon)+\text{finite},\\ \gamma=c_0-\alpha'\mathcal{D}^2(\epsilon^{-2}AT_0)-2\alpha'\,\mathcal{D}^2\phi-\alpha' R+O(\alpha'^2),\quad c_0=\tfrac{1}{2}(D-26).\end{gathered} \tag{4.3}$$

For example, taking the derivative of Z over ϵ reproduces the standard perturbative closed string tachyon β-function,

$$\beta^T=-2T-\tfrac{1}{2}\alpha'\,\mathcal{D}^2T, \tag{4.4}$$

with the corresponding Weyl anomaly coefficient being $\overline{\beta^T}=\beta^T+\alpha'\,\partial^m\phi\,\partial_m T$.

To obtain the effective action for the massless fields $S[G,\phi]$ from the partition function Z one should, as in the open string case, renormalize the logarithmic infinities which corresponds to subtracting massless poles in the string amplitudes.[10] An additional subtlety of the closed string case is that the Möbius group volume has logarithmic divergence, and it should be subtracted, in the RG invariant way, by applying $\partial/\partial\ln\epsilon$ to the bare value of Z.[28] [To compare the formal generating functional Z to massless effective action reconstructed from string amplitudes one needs to subtract both Möbius infinities and massless poles (UV logarithms). While the former are power-like in the open string case, they are also logarithmic in the closed string case. That means that ''extra'' log should be subtracted from Z in the closed string case.] Expressed in terms of renormalized couplings, the effective action is then[28] [$\lambda^i=(T,G,\phi)$]

$$S=-\left(\frac{\partial Z}{\partial\ln\epsilon}\right)_{\epsilon=1}=\beta^i\cdot\frac{\delta Z}{\delta\lambda^i}, \tag{4.5}$$

or, explicitly,

$$S=\int d^Dx\sqrt{G}e^{-2\phi-T}\left(-2T+\frac{1}{2}\gamma\right)$$
$$=\int d^Dx\sqrt{G}e^{-2\phi-T}\left[\frac{1}{2}c_0-2T-\frac{1}{2}\alpha'\,\mathcal{D}^2T-\alpha'\,\mathcal{D}^2\phi-\frac{1}{2}\alpha' R+O(\alpha'^2)\right], \tag{4.6}$$

where T is a renormalized value of the tachyon rescaled by A. [Because of the diffeomorphism invariance; the expression for S can be written also as $S=\overline{\beta}^i\cdot\delta Z/\delta\lambda^i$, where $\overline{\beta}^i=\beta^i+(\delta\lambda^i)_{\alpha'\partial\phi}$ (i.e., $\overline{\beta}^\phi=\beta^\phi+\alpha'\partial^m\phi\,\partial_m\phi$, $\overline{\beta}^G_{mn}=\beta^G_{mn}+2\alpha'\mathcal{D}_m\mathcal{D}_n\phi$, etc.) are the Weyl anomaly coefficients, the vanishing of which should be equivalent to the conditions of stationarity of the action.] Equivalently,

$$S=\int d^Dx\sqrt{G}e^{-2\phi-T}\left(\beta^T+2\beta^\phi-\frac{1}{2}G^{mn}\beta^G_{mn}\right)$$
$$=\int d^Dx\sqrt{G}e^{-2\phi-T}\left(\overline{\beta}^T+2\overline{\beta}^\phi-\frac{1}{2}G^{mn}\overline{\beta}^G_{mn}\right), \tag{4.7}$$

i.e.,

$$S=-\left(\frac{d}{d\ln\epsilon}\mathcal{Z}\right)_{\epsilon=1},\quad \mathcal{Z}=\int d^Dx\sqrt{G}e^{-2\phi-T}. \tag{4.8}$$

Note that [in contrast to the open string case (2.15),(2.16)] the coefficients of derivative terms here are scheme-independent. Setting the tachyon to zero (and integrating by parts) we get the standard closed string effective action consistent with the S-matrix[1] and massless β-functions,[50,7]

$$S=-\frac{1}{2}\int d^Dx\sqrt{G}e^{-2\phi}[-c_0+4\alpha'(\partial\phi)^2+\alpha' R+O(\alpha'^2)]. \tag{4.9}$$

As discussed in Ref. 28, the definition (4.5) in general leads to S given by the space–time integral of the ''central charge'' coefficient.

The functional (4.6) is not, however, the right action for $T\neq 0$: it does not have the standard perturbative vacuum ($D=26$, $T=0$, $\phi=$const, $G_{mn}=\delta_{mn}$) as its stationary point [equivalently, the tachyon tadpole on a 2-sphere does not vanish even after taking the derivative in (4.5)]. Another indication of a problem in (4.6) is that one can almost completely absorb T into the dilaton: introducing $\tilde{\phi}=\phi+1/2T$ one is left with only a linear term in T. Furthermore, the kinetic term of T in (4.6) ($-1/2\alpha'\,\partial^mT\,\partial_mT$ after integration by parts) has apparently the ''wrong'' sign. [We use the Euclidean signature so the correct sign for a scalar kinetic term is plus. This is the sign of the dilaton kinetic term in (4.6) after redefining the metric to decouple the graviton from dilaton (i.e., after going to the Einstein frame). In general, T and ϕ and the graviton are mixed, so that their kinetic matrix is to be diagonalized before discussing the signs (see below).]

As in the open string case, to try to find a consistent action that reproduces $\overline{\beta}^i=0$ conditions for all the three fields one is thus to subtract the tachyon tadpole in an RG invariant way. By analogy with (2.19), let us define

$$\hat{S}=S+\frac{1}{2}\beta^i\cdot\frac{\delta S}{\delta\lambda^i}=\beta^i\cdot\frac{\delta}{\delta\lambda^i}Z+\frac{1}{2}\beta^j\cdot\frac{\delta}{\delta\lambda^j}\left(\beta^i\cdot\frac{\delta}{\delta\lambda^i}Z\right). \tag{4.10}$$

(The coefficient 1/2 accounts for the factor of two difference in dimensions of the open and closed strings tachyons; cf. (2.18), (4.4). Note that since S in (4.5) is RG invariant [$(d/d\ln\epsilon)Z=0\rightarrow(d/d\ln\epsilon)\,(\partial/\partial\ln\epsilon)Z=0$], the same applies to each of the two terms in $\hat{S}$.)

Expanding near the standard flat string vacuum ($D=26$, $G_{mn}=$const, $\phi=$const) one is to keep the dilaton and graviton perturbations in $\hat{S}$ and consistently decouple them from T by field redefi-

nitions. (We are grateful to Frolov for an important discussion of this point.) Observing that for small perturbations near the flat vacuum $\beta^{\phi}=-1/2\alpha'\,\partial^2\phi$, $\beta^G_{mn}=\alpha' R_{mn}$, one finds

$$\hat{S}=S+\frac{1}{2}\left(\beta^T\cdot\frac{\delta}{\delta T}+\beta^{\phi}\cdot\frac{\delta}{\delta\phi}+\beta^G_{mn}\cdot\frac{\delta}{\delta G_{mn}}\right)S$$
$$=\int d^Dx\sqrt{G}e^{-2\phi-T}\left[-2T^2+\frac{1}{2}\alpha'\,\mathcal{D}^2T-\alpha' T\,\mathcal{D}^2T-\frac{1}{2}\alpha'(1+2T)(R+2\,\mathcal{D}^2\phi)+O(\alpha'^2)\right]. \tag{4.11}$$

This action no longer has a tadpole T-term [cf. (4.6)], but to decouple the graviton from scalars we still need, as usual, to redefine the metric. Ignoring ''mixed'' (tachyon-massless) terms which are of higher than quadratic order in the fields we can approximately replace the $e^{-2\phi-T}(1+2T)$ factor in front of R by $\epsilon^{-2\varphi}$, $\varphi\equiv\phi-1/2T$ and set $G_{mn}=e^{4\varphi/(D-2)}g_{mn}$. Then $\int d^{\mathcal{D}}x\sqrt{G}e^{-2\phi-T}(1+2T)(R+2\,\mathcal{D}^2\phi)\to\int d^{\mathcal{D}}x\sqrt{g}[R(g)-[4/(D-2)](\partial\varphi)^2+2\,\partial^mT\,\partial_m\varphi]$. As a result, the action (4.11) takes the form

$$\hat{S}=\int d^Dx\sqrt{g}\left(e^{-2T}[-2T^2e^{4\varphi/(D-2)}+2\alpha'(1-T)(\partial T)^2]\right.$$
$$\left.-\frac{1}{2}\alpha'\left[R(g)-\frac{4}{D-2}(\partial\varphi)^2\right]+O(\alpha'^2)\right). \tag{4.12}$$

(If one does the exact redefinition $(1+2T)e^{-2\phi-T}=e^{-2\psi}$, i.e., $\psi=\phi+(1/2)T-(1/2)\ln(1+2T)$, and thus $G_{mn}=e^{4\psi/(D-2)}g_{mn}$, then one finds the following action:

$$\hat{S}=\int d^Dx\sqrt{g}\left(-\frac{2T^2}{1+2T}e^{4\psi/(D-2)}+\frac{2\alpha'}{(1+2T)^2}(\partial T)^2-\frac{1}{2}\alpha'\left[R(g)-\frac{4}{D-2}(\partial\psi)^2\right]+O(\alpha'^2)\right),$$

which is equivalent to the one above in the quadratic order in T. Introducing $\tilde{T}=(1/2)\ln(1+2T)$ (assuming $T>-1/2$) its tachyonic part becomes simply $\hat{S}=\int d^Dx[-2\sinh^2\tilde{T}+2\alpha'(\partial\tilde{T})^2]$.)

Ignoring the graviton and dilaton terms (decoupled to quadratic order in fluctuations) the tachyon part of the action is thus

$$\hat{S}=\int d^Dxe^{-2T}[-2T^2+2\alpha'(1-T)(\partial T)^2+O(\alpha'^2)]. \tag{4.13}$$

This action has a structure similar to (2.24), but the value of the coefficient of the second kinetic term, though now positive, is not the one needed to reproduce the β^T-function (4.4). It may be that the definition (4.10) still needs some further refinement.

The potential term in (4.13) $V=-2e^{-2T}T^2$ has a tachyonic maximum at $T=0$ and the stable minimum at $T=1$. However, that minimum is not reached as the kinetic term of T changes sign at $T=1$. In general, in discussing the vacuum structure one should take into account a nontrivial mixing of the tachyon with the dilaton and the metric. For example, for a linear dilaton and $D=2$ the tachyon should be massless (as follows from $\overline{\beta}^T=0$), and in this case one should expect to find no potential term. [The exponential potential in (4.13) may be suggesting (by analogy with the open string case) a possibility of T rolling to infinity along some directions, and such behavior should be accompanied by a nonconstant dilaton to preserve the central charge condition (see also Ref. 16 for related remarks).]

In the closed NSR string case the tachyon vertex has the following form (in the 0-ghost picture) $\int d^2z\,\psi^m\overline{\psi}^n\partial_m\partial_nT$. Its 2-D supersymmetric generalization is $\int d^2z\,d^2\theta\,T(\hat{x})$, where $\hat{x}^m=x^m+\theta\psi^m+\overline{\theta\psi}^m+\overline{\theta}\theta f^m$. Combined with the kinetic term $\int d^2z\,d^2\theta\,D\hat{x}^m\,\overline{D}\hat{x}^m$ it leads, after the

elimination of the auxiliary field f^m, to the following tachyon terms in the sigma model action [which are the familiar superpotential terms in $N=1$ supersymmetric scalar 2-D field theory; cf. also (3.9)],

$$\int d^2z[\partial^m T(x)\partial_m T(x)+\psi^m\bar{\psi}^n\partial_m\partial_n T(x)]. \tag{4.14}$$

As in the open NSR string case, the resulting partition function and thus the effective action (4.5) it generates are even in T. As a result, there is no need for an additional subtraction like (4.10). Since the sigma model depends on T only through its derivatives, there is no tachyon potential term in S.

The leading T-dependent logarithmic divergence in Z comes from the expansion of $\partial_m T\,\partial^m T$ term in (4.14) and corresponds to the β-function $(-1-(1/2)\alpha'\mathcal{D}^2)T$. The leading G_{mn} and ϕ-dependent terms in Z and S in the NSR case are the same as in the bosonic case[51] [with the obvious replacement of c_0 in (4.3) by $D-10$]. While the NS–NS part of the effective action generated by the sigma model appears to depend on T only through its derivatives, functions of T may still be present in the R-R sector (where one is to use the ghost -1 tachyon vertex[52]).

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Non-Abelian Born–Infeld and kappa-symmetry

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We define an iterative procedure to obtain a non-Abelian generalization of the Born–Infeld action. This construction is made possible by the use of the severe restrictions imposed by kappa-symmetry. In this paper we will present all bosonic terms in the action up to terms quartic in the Yang–Mills field strength and all fermion bilinear terms up to terms cubic in the field strength. Already at this order the fermionic terms do not satisfy the symmetric trace-prescription. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1374449]

I. INTRODUCTION

One of the most intriguing features of D-branes is their close connection with gauge theories. Indeed, the effective theory describing the worldvolume dynamics of a Dp-brane is a $p+1$-dimensional field theory with, in the static gauge, as bosonic degrees of freedom the transversal coordinates of the brane, appearing as $9-p$ scalar fields, and the massless states of the open strings ending on the brane which appear as a U(1) gauge field. When these fields vary slowly, the effective action governing their dynamics is known to all orders in α'. It is the ten-dimensional Born–Infeld action,[1] dimensionally reduced to $p+1$ dimensions.

Once several D-branes are present, the situation changes. The mass of the strings stretching between two branes is proportional to the shortest distance between the branes. Starting off with n well separated D-branes we end up with a $\mathrm{U}(1)^n$ theory, however, once the n branes coincide additional massless states appear which complete the gauge multiplet to a non-Abelian $\mathrm{U}(n)$-theory.[2] Contrary to the Abelian case, the effective action is not known to all orders in α'. The first term, quadratic in the field strength, is nothing but a dimensionally reduced $\mathrm{U}(n)$ Yang–Mills theory. The next order, which is quartic in the field strength, was obtained from the four-gluon scattering amplitude in open superstring theory[3] and from a three-loop β-function calculation.[4] Based upon these results and other considerations, an all order proposal was formulated for the effective action;[5] the non-Abelian Born–Infeld action assumes essentially the same form as the Abelian one, however, all Lie algebra valued objects have to be symmetrized first before taking the trace. Other trace prescriptions, involving commutators, have been given as well.[6] More recently, it was found that the symmetric trace prescription could not be correct as it did not reproduce the mass spectrum of certain D-brane configurations.[7,8] It was shown in Ref. 9 that by adding commutator terms to the action the problem might be cured. Indeed, as was pointed out in Ref. 1, the notion of an effective action for slowly varying fields is subtle in the non-Abelian case. In the effective action higher derivative terms are dropped. However because of

$$D_iD_jF_{kl}=\frac{1}{2}\{D_i,D_j\}F_{kl}-\frac{i}{2}[F_{ij},F_{kl}], \tag{1.1}$$

this is ambiguous. The analysis of the mass spectrum seems to indicate that the symmetrized product of derivatives acting on a field strength should be viewed as an acceleration term which can safely be neglected, while the anti-symmetrized products should be kept. A systematic study of the F^6 terms[10] showed that using the mass spectrum as a guideline, almost all terms at this order

could be determined. However due to the specific choices of backgrounds made in Ref. 10, certain terms do not contribute to the mass spectrum and as a result can not be fixed in this way. A direct calculation from a six-point open superstring amplitude or a five-loop β-function seems unfeasible, so another approach is called for.

Until now, we ignored the fermionic degrees of freedom in our discussion. The fully covariant worldvolume theory of a single D-brane in a type II theory can be formulated in terms of the following world volume fields: the embedding coordinates $X^\mu(\sigma)$ (of which only the transverse coordinates represent physical degrees of freedom), the Born–Infeld vector field $V_i(\sigma)$, and $N=2$ space–time fermionic fields $\theta(\sigma)$. In a curved background the D-brane can be coupled to the corresponding type II supergravity superfields, and $N=2$ supersymmetry is realized locally. In a flat background there is $N=2$ global supersymmetry. This world volume theory has a local κ-symmetry, which acts on the fermions as

$$\delta\overline{\theta}(\sigma)=\overline{\kappa}(\sigma)(1+\Gamma), \tag{1.2}$$

where Γ, which depends on world volume as well as background fields, satisfies

$$\Gamma^2=1. \tag{1.3}$$

The projection (1.2) makes it possible to gauge away half the fermionic degrees of freedom. The field content then corresponds in a static gauge to that of a supersymmetric Yang–Mills theory in $p+1$ dimensions. There is still $N=2$ supersymmetry, but half of this is realized nonlinearly. These covariant D-brane actions have been constructed in flat,[11] as well as in curved backgrounds.[12,13] This paper examines the suggestion in Ref. 8 that κ-symmetry might teach us something about the orderings appearing in the non-Abelian Born–Infeld action.

D-brane actions consist of the sum of a Born–Infeld term, coupling the world volume fields to the NS–NS sector of the background, and a Wess–Zumino term in which the couplings to the R–R fields occur. Each part is separately supersymmetric, but the two are related, in the Abelian case, by the κ-transformations. The Wess–Zumino term is of a topological nature, and can therefore be formulated in a metric-independent way. Its structure is severely restricted, also in the non-Abelian case. The Born–Infeld term is much more complicated, and consequently its generalization from the Abelian to the non-Abelian case is much more difficult. It is natural to assume that also in the non-Abelian case the Born–Infeld and Wess–Zumino term are related by a κ-symmetry. Our aim is to use the knowledge of the Wess–Zumino term and the properties of κ-symmetry to obtain information about the non-Abelian Born–Infeld term.

To construct this non-Abelian generalization we will use an iteration in the number of Yang–Mills field strengths $F(V)$. In this paper we will obtain all terms in the action up to and including the order F^2. As we discussed above, in the purely bosonic terms the conflict between string theoretic results and the symmetric trace prescription arises only at order F^6, so it is clear that in this paper we will not contribute to the discussion of these bosonic terms. However, we find that in the fermionic sector already at quadratic order some of the fermionic terms do not correspond to a symmetric trace.

This paper is organized as follows: We will discuss our choice of variables in Sec. II. In Sec. III we will define the iterative procedure and illustrate it for the Abelian case. In Secs. IV and V we derive and present our results for the non-Abelian case, and bring them to gauge fixed form in Sec. VI. In Sec. VII we give our conclusions, and point out a number of extensions and applications of this work.

We will end the Introduction by recalling briefly some related work on supersymmetric D-brane actions. In four dimensions the supersymmetrization of the Abelian Born–Infeld action in $N=1$ supersymmetry has been known for a long time.[14] More recently, this work has been extended to the non-Abelian Born–Infeld theory, and to $N=2$ supersymmetry.[15,16] In particular, in Ref. 15 it is remarked that $N=2$ supersymmetry in four dimensions is not sufficient to resolve the ordering ambiguities, several ordering prescriptions give rise to supersymmetric actions. So it

seems that it is indeed necessary (and hopefully sufficient) to consider $N=4$ in $D=4$, or, as in this paper, the ten-dimensional supersymmetric Born–Infeld action action. Several aspects of the ten-dimensional problem have been studied in Refs. 17 and 18. In particular, these authors investigate the dependence of the action on transverse scalars, where these scalars are generated by T-duality starting from the D9-brane action. However, this is in the context of the symmetric trace prescription.

II. WORLD VOLUME FIELDS AND TRANSFORMATIONS

The aim of this work is to obtain the effective action for n overlapping Dp-branes, with U(n) covariance on the world volume. Before embarking on the construction, one has to carefully choose the starting point of the calculation. For general Dp-branes the situation is complicated by the presence of the transverse scalar degrees of freedom, which are in the adjoint representation of the Yang–Mills group. Not only does one have to take commutators of these scalars into account, but also the background fields will depend on these scalars.[19] We avoid these complications by limiting ourselves to the case of n overlapping D9-branes, and by choosing a flat background. Through T-duality D-branes for other values of p can be obtained, the extension to curved backgrounds will be discussed in Sec. VII.

For n overlapping D9-branes the completely gauge fixed result should be the supersymmetric version of the non-Abelian Born–Infeld theory. Since the vector fields $V_i^A(\sigma)$, $A=1,...,n^2$, are in the adjoint representation of U(n), we have to make the same choice for the fermion fields θ. Therefore we start out with fields $\theta^A(\sigma)$, which form a doublet ($N=2$) of Majorana–Weyl spinors for each A, satisfying $\Gamma_{11}\theta^A=\theta^A$. After κ-gauge fixing only half of each doublet will remain, and we have the correct number of degrees of freedom for the supersymmetric Yang–Mills theory.

This requires, that there are as many κ-symmetries as θ's, so that the parameter of the κ transformations will have to be in the adjoint of U(n) as well. Thus the θ^A transform as follows under ordinary supersymmetry (ϵ), κ-symmetry (κ), Yang–Mills transformations (Λ^A), and world volume reparametrizations (ξ^i),

$$\delta\overline{\theta^A}(\sigma)=-\overline{\epsilon^A}+\overline{\kappa^B}(\sigma)(1\!\!1\delta^{BA}+\Gamma^{BA}(\sigma))+f^A{}_{BC}\Lambda^B(\sigma)\overline{\theta^C}(\sigma)+\xi^i(\sigma)\partial_i\overline{\theta^A}(\sigma). \tag{2.1}$$

Here ϵ^A are constant, Γ^{AB} depends on the world volume fields, and therefore on σ. It must satisfy

$$\Gamma^{AB}\Gamma^{BC}=\delta^{AC}1\!\!1. \tag{2.2}$$

We will usually write these transformations in terms of

$$\delta\overline{\theta^A}\equiv\overline{\eta^A}\equiv\overline{\kappa^B}(\sigma)(1\!\!1\delta^{BA}+\Gamma^{BA}(\sigma)). \tag{2.3}$$

Useful information is obtained by considering commutators of these transformations. Because ϵ^A is constant we find from the commutator of Yang–Mills and supersymmetry transformations that

$$f^A{}_{BC}\Lambda^B\epsilon^C=0\rightarrow f_{ABC}\epsilon^C=0. \tag{2.4}$$

Therefore $\epsilon=\epsilon^A T_A$, where T_A are the U(n) generators, must be proportional to the unit matrix, i.e., we can choose a basis in which there is only one nonvanishing ϵ parameter. So only a subset of the θ^A transform under supersymmetry, and there is only one independent supersymmetry parameter. The θ's which are presently inert under supersymmetry will obtain their supersymmetry transformations through κ-gauge fixing, as we shall see in Sec. VI. From the commutator of κ-symmetry and supersymmetry we find $\delta_\epsilon\eta^A=0$. This implies that

$$\delta_\epsilon\Gamma^{AB}=0. \tag{2.5}$$

The only scalars we have are the embedding coordinates $X^\mu(\sigma)$ for world volume directions. There are several options that one could consider for the X^μ:

(1) We could assume that we are in the static gauge, i.e.,
$$X^\mu(\sigma)=\delta^\mu_i\sigma^i, \tag{2.6}$$
from the beginning, so that the X^μ are absent. In this case there are no world volume reparametrizations, i.e., $\xi^i=0$ in (2.1);
(2) We could decide that the X^μ are in the singlet representation of the Yang–Mills group. The idea is that the n branes overlap, there is only one set of world volume coordinates, and the corresponding reparametrization group would be sufficient to gauge fix a singlet set of embedding coordinates;
(3) We could choose the X^μ in the adjoint representation of Yang–Mills in analogy with transverse coordinates for $p<9$. Here one thinks of starting with n separate branes where each has its own world volume and embedding coordinates. When the branes overlap the embedding coordinates ''fill up'' to form elements of the adjoint representation. Clearly this requires a different approach toward the worldvolume reparametrisation invariance, which must then correspond to a sufficiently large symmetry group to gauge fix all these embedding functions.

We have investigated the first two possibilities in the non-Abelian case, and we have found that only the first approach is consistent with the iterative procedure that we employ. In Sec. IV we will point out where the first two choices start to diverge, in Sec. VII we will briefly come back to the third possibility.

The transformation rules of the bosonic fields V_i^A, and, in case of the second choice above, of the X^μ, are determined iteratively by requiring invariance of the action.

A special case of a U(n) invariant non-Abelian D-brane action is of course the truncation to U(1)^n. In this case we know the answer: a κ-invariant action is given by the sum of n Abelian D-brane actions. This special case will be discussed again, since it plays a role in making a choice between the different possibilities for the variables X^μ discussed above.

Throughout this paper we will limit ourselves to terms in the action and transformation rules which are at most quadratic in the fermion fields.

III. THE ITERATIVE PROCEDURE AND THE ABELIAN EXAMPLE

In this section we will set up our iterative procedure and illustrate it for the Abelian case. To do this, we must first give some details of the effective D9-brane action in a flat background.[11] In this case we can use a covariant formulation with embedding coordinates X^μ, space–time fermions θ, and the Born–Infeld vector V_i. They transform under supersymmetry (ϵ), κ-symmetry, world volume reparametrizations (ξ^i), and Maxwell gauge transformations (Λ) as

$$\begin{aligned}
\delta X^\mu &= \tfrac{1}{2}\overline{\epsilon}\Gamma^\mu\theta+\tfrac{1}{2}\overline{\eta}\Gamma^\mu\theta+\xi^i\partial X^\mu,\\
\delta\overline{\theta} &= -\overline{\epsilon}+\overline{\eta}+\xi^i\partial_i\overline{\theta},\\
\delta V_i &= -\tfrac{1}{2}(\overline{\epsilon}+\overline{\eta})\gamma_i\theta+\xi^jF_{ji}+\partial_i(\Lambda+\xi^jV_j),
\end{aligned} \tag{3.1}$$

with

$$\overline{\eta}=\overline{\kappa}(1+\Gamma),\quad (\Gamma)^2=\mathbb{1}, \tag{3.2}$$

and

$$\gamma_i\equiv\Gamma^\mu\partial_iX^\mu. \tag{3.3}$$

The Born–Infeld contribution reads

$$\mathcal{L}_{BI} = -\sqrt{-\det(g+\mathcal{F})}$$
$$= -\sqrt{-\det g}\,(1+\tfrac{1}{4}\mathcal{F}_{ij}\mathcal{F}^{ij}+\cdots), \tag{3.4}$$

where in the second line we expand to second order in $\mathcal{F}$, which is given by

$$\mathcal{F}_{ij} = F_{ij}(V) - B_{ij}\,. \tag{3.5}$$

In a flat background and in the quadratic fermion approximation, B_{ij} is

$$B_{ij} = -\overline{\theta}\sigma_3\gamma_{[i}\partial_{j]}\theta. \tag{3.6}$$

The world volume metric reads

$$g_{ij} = \eta_{ij} + \overline{\theta}\gamma_{(i}\partial_{j)}\theta, \quad \eta_{ij} \equiv \partial_i X^\mu \partial_j X_\mu\,. \tag{3.7}$$

The metric g and $\mathcal{F}$ are invariant under supersymmetry and transform covariantly under κ-transformations. The most useful form for comparison with the non-Abelian case is the expansion of (3.4) to second order in fermions,

$$\mathcal{L}_{BI} = -\sqrt{-\det\eta}\,(1+\tfrac{1}{2}\overline{\theta}\gamma^i\partial_i\theta + \tfrac{1}{2}\overline{\theta}\sigma_3\gamma_{[i}\partial_{j]}\theta F^{ij} + \tfrac{1}{4}F^{ij}F_{ij} + \tfrac{1}{2}\overline{\theta}\gamma_i\partial_j\theta T^{ij} + \cdots), \tag{3.8}$$

where T^{ij} is the energymomentum tensor of the vector field,

$$T^{ij} = F^{ik}F^j_k + \tfrac{1}{4}\eta^{ij}F_{kl}F^{kl}. \tag{3.9}$$

The Wess–Zumino term takes on the following form:

$$\mathcal{L}_{WZ} = e^{i_1\cdots i_{10}} \times \sum_{k=0}^{4} \frac{(-1)^k}{2^{k+1}k!(9-2k)!}\,\overline{\theta}\mathcal{P}_{(k)}\gamma_{i_1\cdots i_{9-2k}}\partial_{i_{10-2k}}\theta(\mathcal{F}^k)_{i_{11-2k}\ldots i_{10}}, \tag{3.10}$$

where

$$\mathcal{P}_{(k)} = \sigma_1 \ \ (\text{for } \ k=0,2,4), \ \ \mathcal{P}_{(k)} = i\sigma_2 (\text{for } \ k=1,3). \tag{3.11}$$

Note that the sum in (3.10) runs only to $k=4$, since the RR-scalar field vanishes in the flat background.

It will be useful, also for the non-Abelian case, to discuss why we make this particular choice for the $\mathcal{P}_{(k)}$. The $\mathcal{P}_{(k)}$ are chosen such that the contributions to the Wess–Zumino term are not total derivatives. For odd k this fixes $\mathcal{P}_{(k)}$ to be $i\sigma_2$. For even k we could also have chosen 1 or σ_3. When we start looking at the iterative procedure later in this Section, we will find that we need

$$\{\mathcal{P}_{(0)}, \mathcal{P}_{(1)}\} = 0, \tag{3.12}$$

which excludes 1 for $k=0$. We have in principle the possibility to have either σ_1 or σ_3 (or both) for $k=0$, and taking σ_1 is a choice of basis for the $N=2$ fermions. Note that σ_3 in (3.6) is correlated with the choice for σ_1 in the Wess–Zumino term: had we chosen $\mathcal{P}_{(0)} = \sigma_3$ we would have found σ_1 in (3.6).

The structure of (3.10) guarantees that the WZ-action transforms into a total derivative under the global supersymmetry transformation $\delta\overline{\theta} = -\overline{\epsilon}$. Since we do not go beyond bilinear fermions we can use F instead of $\mathcal{F}$ in the Wess–Zumino term. The numerical coefficients in (3.10) are determined by κ-symmetry once the normalization of F and θ are fixed in the Born–Infeld term.

Let us now consider the iterative construction of κ-symmetry. The variation of the D-brane action takes on the form,

$$\delta\mathcal{L}=-\overline{\eta}(1-\Gamma)\mathcal{T}. \tag{3.13}$$

It indeed vanishes if η is given by (3.2). These variations have the following source:

$$\delta\mathcal{L}_{BI}=-\overline{\eta}\mathcal{T},\quad \delta\mathcal{L}_{WZ}=\overline{\eta}\Gamma\mathcal{T}. \tag{3.14}$$

The variation of the Wess–Zumino term, together with the information that $\Gamma^2=\mathbb{1}$, is sufficient to determine both Γ and $\mathcal{T}$ iteratively. Since $\mathcal{T}$ determines the variation of the Born–Infeld term this information is sufficient to obtain iteratively the Born–Infeld part of the action.

The iteration is obtained by expanding Γ and $\mathcal{T}$ in F,

$$\begin{aligned}\delta\mathcal{L}&=-\overline{\eta}(1-(\Gamma_0+\Gamma_1+\cdots))(\mathcal{T}_0+\mathcal{T}_1+\cdots)\\&=-\overline{\eta}(\mathcal{T}_0-\Gamma_0\mathcal{T}_0+\mathcal{T}_1-\Gamma_1\mathcal{T}_0-\Gamma_0\mathcal{T}_1+\cdots),\end{aligned} \tag{3.15}$$

where the indices indicate the order in F and the Γ_i satisfy various identities which follow from $\Gamma^2=\mathbb{1}$. Since it will be useful to have the Abelian results at hand for comparison with the non-Abelian calculation in Sec. IV, we will work out the beginning of this iteration in some detail.

Let us start with the order F^0. The contribution from (3.10) is

$$\mathcal{L}_{WZ0}=\frac{1}{2\cdot 9!}\epsilon^{i_1\cdots i_{10}}\overline{\theta}\sigma_1\gamma_{i_1\cdots i_9}\partial_{i_{10}}\theta. \tag{3.16}$$

For the κ-variation we only have to vary θ to obtain

$$\delta\mathcal{L}_{WZ0}=\frac{1}{9!}\epsilon^{i_1\cdots i_{10}}\overline{\eta}\sigma_1\gamma_{i_1\cdots i_9}\delta_{i_{10}}\theta=\sqrt{-\det\eta}\,\overline{\eta}\sigma_1\Gamma^{(0)}\gamma^i\partial_i\theta. \tag{3.17}$$

Here $\Gamma^{(0)}$ is given by

$$\Gamma^{(0)}=\frac{1}{10!\sqrt{-\det g}}\epsilon^{i_1\cdots i_{10}}\gamma_{i_1\cdots i_{10}}, \tag{3.18}$$

which satisfies

$$(\Gamma^{(0)})^2=\mathbb{1}. \tag{3.19}$$

In (3.17) we have used the property

$$\Gamma^{(0)}\gamma^{l_1\cdots l_k}=\frac{(-)^{k(k-1)/2}}{(10-k)!\sqrt{-\det g}}\epsilon^{i_1\cdots i_{10-k}l_1\cdots l_k}\gamma_{i_1\cdots i_{10-k}} \tag{3.20}$$

for $k=1$. From (3.17) we read off that

$$\Gamma_0=\Gamma^{(0)}\sigma_1,\quad \mathcal{T}_0=\gamma^i\partial_i\theta. \tag{3.21}$$

Obviously $\Gamma^2=\mathbb{1}$ to this order.

So the Born–Infeld term should vary into $\mathcal{T}$, which is indeed achieved by setting

$$\mathcal{L}_{BI0}=-\sqrt{-\det\eta}(1+\tfrac{1}{2}\overline{\theta}\gamma^i\partial_i\theta). \tag{3.22}$$

This gives

$$\delta\mathcal{L}_{BI0}=-\sqrt{-\det\eta}\,\overline{\eta}\gamma^i\partial_i\theta, \tag{3.23}$$

where we have used the variation of X^μ as given in (3.1).

A similar analysis can be done for the terms of higher order in F. At the linear level the variation of the Wess–Zumino term is

$$\delta\mathcal{L}_{WZ1}=\tfrac{1}{2}\sqrt{-\det\eta}\,\overline{\eta}(i\sigma_2)\Gamma^{(0)}(\gamma^{jk}F_{jk}\gamma^i\partial_i\theta-2\gamma_i\partial_j\theta F^{ij}). \tag{3.24}$$

The variation of the complete action should be

$$\delta\mathcal{L}_1=-\sqrt{-\det\eta}\,\overline{\eta}\{\mathcal{T}_1-(\Gamma_0\mathcal{T}_1+\Gamma_1\mathcal{T}_0)\}. \tag{3.25}$$

So we read off that

$$\Gamma_1=\Gamma^{(0)}(i\sigma_2)\tfrac{1}{2}\gamma^{kl}F_{kl},\quad \mathcal{T}_1=\sigma_3\gamma_i\partial_j\theta F^{ij}. \tag{3.26}$$

Note that $\Gamma^2=\mathbb{1}$ at this order in F because

$$\{\sigma_1,\Gamma_1\}=0. \tag{3.27}$$

This is a general feature: the condition that $\Gamma^2=\mathbb{1}$ only contains useful information at even orders in the expansion in F. At odd orders it is just a consequence of the properties of $\mathcal{P}_{(k)}$.

The variation under supersymmetry and κ-symmetry of the term linear in F in the Born–Infeld action (3.8) reads

$$\delta\mathcal{L}_{BI1}=-\sqrt{-\det\eta}\,\overline{\eta}\sigma_3\gamma_i\partial_j\theta F^{ij}-\tfrac{1}{2}(\overline{\epsilon}+\overline{\eta})\gamma_i\theta\partial_j\{\sqrt{-\det\eta}F^{ij}\}. \tag{3.28}$$

The first term is the required contribution of $\mathcal{T}_1$. The second term must be cancelled by the variation of V in the F^2 term. The F^2 term gives

$$-\delta V_i\partial_j\{\sqrt{-\det\eta}F^{ij}\}, \tag{3.29}$$

which implies the following variation of V_i:

$$\delta V_i=-\tfrac{1}{2}(\overline{\epsilon}+\overline{\eta})\sigma_3\gamma_i\theta. \tag{3.30}$$

Therefore the combination

$$\mathcal{F}_{ij}=F_{ij}+\overline{\theta}\sigma_3\gamma_{[i}\partial_{j]}\theta \tag{3.31}$$

is supersymmetric and transforms covariantly under κ-symmetry.

At the quadratic level we get

$$\delta\mathcal{L}_{WZ2}=\tfrac{1}{8}\sqrt{-\det\eta}\,\overline{\eta}\sigma_1\Gamma^{(0)}(\gamma_{ijkl}\gamma^m\partial_m\theta-4\gamma_{ijk}\partial_l\theta)F^{[ij}F^{kl]}. \tag{3.32}$$

The order 2 terms in the variation of the total action are

$$\delta\mathcal{L}_2=-\sqrt{-\det\eta}\,\overline{\eta}(-(\Gamma_2\gamma^i\partial_i\theta+\Gamma_1\mathcal{T}_1+\sigma_1\mathcal{T}_2)+\mathbb{1}\mathcal{T}_2), \tag{3.33}$$

where Γ_1 and $\mathcal{T}_1$ were determined at the linear level. On the other hand, from $\Gamma^2=\mathbb{1}$ we have

$$\sigma_1\Gamma_2+\Gamma_2\sigma_1+\Gamma_1\Gamma_1=0, \tag{3.34}$$

from which we obtain (using $\Gamma_2\sim\sigma_1$)

$$\Gamma_2=-\tfrac{1}{2}\sigma_1\Gamma_1\Gamma_1=\Gamma^{(0)}\sigma_1\{\tfrac{1}{8}\gamma_{ijkl}F^{ij}F^{kl}-\tfrac{1}{4}F^{kl}F_{kl}\}. \tag{3.35}$$

Substituting all this in (3.33), we find that

$$\mathcal{T}_2 = \gamma_i \partial_j \theta (F^{ik} F^j_k + \tfrac{1}{4} \eta^{ij} F^{kl} F_{kl}). \tag{3.36}$$

This indeed agrees with the variation of the Born–Infeld action.

There is a feature about the Abelian case which just starts being visible in the quadratic terms. It is obviously possible to write Γ at this order in the form

$$\Gamma = (1 - \tfrac{1}{4} F^{kl} F_{kl}) \Gamma^{(0)} ((\sigma_1 + \tfrac{1}{2}(i\sigma_2) \gamma^{kl} F_{kl} + \tfrac{1}{8} \sigma_1 \gamma_{ijkl} F^{ij} F^{kl}) \tag{3.37}$$

up to terms of higher order in F. In fact, this factorization is a general feature of the Abelian action which is also valid for the complete answer,

$$\Gamma = \frac{\sqrt{-\det g}}{\sqrt{-\det(g+\mathcal{F})}} \Gamma^{(0)} \sum_{k=0}^{5} \frac{1}{2^k k!} \mathcal{P}_{(k)} \gamma^{i_1 \cdots i_{2k}} \mathcal{F}^k_{i_1 \cdots i_{2k}}. \tag{3.38}$$

The iterative procedure will obviously confirm this factorization, as is shown by continuing to higher orders in F. However, in this construction it is not clear why the factorization should occur. This is an issue in the non-Abelian situation where the complete answer is not known. Note that the factor

$$\frac{\sqrt{-\det g}}{\sqrt{-\det(g+\mathcal{F})}} \tag{3.39}$$

in (3.38) contains the inverse of the Born–Infeld action. The idea that Γ provides the explicit form of the Born–Infeld action was part of our motivation to use κ-symmetry as a means of constructing the non-Abelian Born–Infeld action.

From (3.36) it is clear that $\mathcal{T}$, at least at the quadratic level, shows a similar factorization property as Γ. The full answer for $\mathcal{T}$ is of the form,

$$\mathcal{T} = \sqrt{-\det(g+\mathcal{F})} \sum_{k=0}^{\infty} (\sigma_3)^k \gamma_i \partial_j \theta (\mathcal{F}^k)^{ij}, \tag{3.40}$$

where

$$(\mathcal{F}^k)^{ij} = \mathcal{F}^{il_1} \mathcal{F}_{l_1 l_2} \cdots \mathcal{F}^{l_{k-1} j} \quad k > 0,$$

$$(\mathcal{F}^k)^{ij} = g^{ij} \quad k = 0. \tag{3.41}$$

We will see a similar feature in the non-Abelian case.

The Abelian case discussed above can easily be generalized to $\mathrm{U}(1)^n$. Then the κ-symmetric action is just the sum of n actions of the type discussed in this section. For n overlapping branes one would need only one set of embedding coordinates X^μ to describe this truncation of the non-Abelian situation. This would be similar to treating X^μ as a singlet of $\mathrm{U}(n)$ in the non-Abelian case. Note however that this sum of actions is very different from a single Born–Infeld action with world volume metric,

$$g_{ij} = \eta_{ij} + \overline{\theta^A} \gamma_{(i} \partial_{j)} \theta^A, \tag{3.42}$$

summed over the $n\mathrm{U}(n)$ branes. A metric (3.42) would be like taking the trace *inside* the root of the Born–Infeld term, while it is known from open string amplitude calculations that there should be a single trace (with some ordening prescription) which produces in the $\mathrm{U}(1)^n$ case a sum of separate Born–Infeld terms.

IV. THE NON-ABELIAN BORN–INFELD ACTION

For the non-Abelian case we start with the following Wess–Zumino term:

$$\mathcal{L}_{WZ}=\epsilon^{i_1\cdots i_{10}}\sum_{k=0}^{4}\frac{(-1)^k}{2^{k+1}k!(9-2k)!}\overline{\theta}^A\mathcal{P}_{(k)}^{ABC_1\cdots C_k}\gamma_{i_1\cdots i_{9-2k}}\mathcal{D}_{i_{10-2k}}\theta^B F^{C_1}_{i_{11-2k}i_{12-2k}}\cdots F^{C_k}_{i_9 i_{10}}. \tag{4.1}$$

The tensors $\mathcal{P}$ are symmetric in the indices C_i contracted with F. $\mathcal{P}$ also contains the Pauli matrices to specify the $N=2$ structure for the fermions. We have the following possibilites:

$$\begin{array}{lll} k \text{ even:} & 1_2,\sigma_1,\ \sigma_3 & \text{symmetry in } AB,\\ & i\sigma_2 & \text{antisymmetry in } AB,\\ k \text{ odd:} & 1_2,\ \sigma_1,\ \sigma_3 & \text{antisymmetry in } AB,\\ & i\sigma_2 & \text{symmetry in } AB. \end{array} \tag{4.2}$$

This requirement follows from the fact that the bilinear fermions in the action (4.1) should not be a total derivative. The Yang–Mills structure of $\mathcal{P}$ arises from the trace of $k+2$ generators in the fundamental representation of U(n), and will be built from the structure constant f_{ABC} (completely antisymmetric) and from the completely symmetric tensors d_{ABC}. In the Appendix we gather useful properties of these tensors.

The general form of (4.1) follows from the requirement that the Wess–Zumino term is of topological nature, i.e., independent of the metric. The coefficients have been chosen equal to those in the Abelian case, which amounts to a particular normalization of the $\mathcal{P}_{(k)}$. Note that we do not assume a particular ordening in the trace, i.e., there is no a priori symmetry imposed between the indices C_i on the one hand, and A, B on the other hand.

So at order 0 we start with

$$\mathcal{P}_{(0)}^{AB}=\sigma_1\,\mathrm{tr}\,T^AT^B=\sigma_1\delta^{AB}, \tag{4.3}$$

and the variation of the lowest order contribution in (4.1) is

$$\delta\mathcal{L}_{WZ0}=\sqrt{-\det\eta}\,\overline{\eta}^A\sigma_1\Gamma^{(0)}\gamma^i\mathcal{D}_i\theta^A. \tag{4.4}$$

We write the variation of the complete action at this order as

$$\delta\mathcal{L}_0=-\sqrt{-\det\eta}\,\overline{\eta}^A(\delta^{AB}-\Gamma_0^{AB})\mathcal{T}_0^B, \tag{4.5}$$

so that

$$\Gamma_0^{AB}=\Gamma^{(0)}\delta^{AB}\sigma_1,\quad \mathcal{T}_0^A=\gamma^i\mathcal{D}_i\theta^A. \tag{4.6}$$

Cleary $\Gamma^{AC}\Gamma^{CB}=\delta^{AB}$. In the above we considered X^μ to be a singlet under U(n) transformations. To go to the static gauge we would have to set $\det\eta\to-1$.

The Born–Infeld term must reproduce the first term in (4.5). The only choice is to have

$$\mathcal{L}_{BI}=-\sqrt{-\det\eta}(1+\tfrac{1}{2}\overline{\theta}^A\gamma^i\mathcal{D}_i\theta^A). \tag{4.7}$$

We indeed find the correct variation if we set

$$\delta X^\mu=\tfrac{1}{2}\overline{\epsilon}^A\Gamma^\mu\theta^A+\tfrac{1}{2}\overline{\eta}^A\Gamma^\mu\theta^A. \tag{4.8}$$

With this choice of δX the metric (3.42) becomes supersymmetric and covariant under κ-transformations. As we explained at the end of Sec. III this is not the natural metric for the non-Abelian [or for the U$(1)^n$] situation. So the different choices for X^μ start to diverge at this

point. At the linear level there is still no crucial difference between the choice of a singlet X^μ and the static gauge. At the quadratic level, however, the singlet choice will fail.

The variation of the linear contribution to the Wess–Zumino term gives

$$\delta\mathcal{L}_{WZ1}=\tfrac{1}{2}\sqrt{-\det\eta}\,\overline{\eta}^A\mathcal{P}^{ABC}_{(1)}\Gamma^{(0)}(\gamma_{ij}\gamma^k\mathcal{D}_k\theta^B-2\gamma_i\mathcal{D}_j\theta^B)F^{Cij}. \tag{4.9}$$

The first term must correspond to $\Gamma_1\mathcal{T}_0$, from which we read off that

$$\Gamma_1^{AB}=\Gamma^{(0)}\mathcal{P}^{ABC}_{(1)}\,\tfrac{1}{2}\gamma_{ij}F^{ijC}. \tag{4.10}$$

From $\Gamma^2=1$ at linear order we find

$$\{\sigma_1,\Gamma_1^{AB}\}=0, \tag{4.11}$$

so that $\mathcal{P}_{(1)}$ must have the following form:

$$\mathcal{P}^{ABC}_{(1)}=(i\sigma_2)d^{ABC}+c_1\sigma_3 f^{ABC}. \tag{4.12}$$

The coefficient of the *d*-term is chosen to agree with the Abelian case. The coefficient of the *f*-term is arbitrary, and with a field redefinition

$$\theta^A\to\theta^A-\tfrac{1}{4}c_1(i\sigma_2)f^{ABC}\gamma^{kl}\theta^B F^C_{kl}, \tag{4.13}$$

and a corresponding redefinition of the vector field, the *f*-term can be eliminated. This is the choice we will make, because then we stay as close as possible to the Abelian situation.

In fact, the whole term linear in F in the Wess–Zumino action can be transformed away by a field redefinition, also in the Abelian case. It is not surprising that these linear terms can be eliminated, since they are part of the supersymmetrization of the bosonic F^3 term, which we know to be absent. The reason we will keep the usual linear term is that in this form the answer in the Abelian case takes on a relatively simple form.[11]

We also find

$$\mathcal{T}_1^A=-\sigma_1\mathcal{P}^{ABC}_{(1)}\gamma_i\mathcal{D}_j\theta^B F^{ijC}, \tag{4.14}$$

so that in analogy with the Abelian case the Born–Infeld term must contain

$$\mathcal{L}_{BI1}=-\sqrt{-\det\eta}\,(-\tfrac{1}{2}\overline{\theta}^A\sigma_1\mathcal{P}^{ABC}_{(1)}\gamma_{[i}\mathcal{D}_{j]}\theta^B F^{ijC}+\tfrac{1}{4}F^{ijA}F^A_{ij}). \tag{4.15}$$

The variation of this term reproduces correctly the $\mathcal{T}_1$ contribution, and the remainder is cancelled by introducing a variation of V_i,

$$\delta V_i^C=+\tfrac{1}{2}(\overline{\epsilon}^A+\overline{\eta}^A)\sigma_{(1)}\mathcal{P}^{ABC}_{(1)}\gamma_i\theta^B. \tag{4.16}$$

We can then define a supersymmetric and κ-covariant $\mathcal{F}^C$ as

$$\mathcal{F}^C_{ij}=F^C_{ij}-\overline{\theta}^A\sigma_1\mathcal{P}^{ABC}_{(1)}\gamma_{[i}\mathcal{D}_{j]}\theta^B. \tag{4.17}$$

This defines the non-Abelian generalization of the NS–NS two-form field, to this order.

At the quadratic level things become more complicated. The variation of the Wess–Zumino term gives

$$\delta\mathcal{L}_{WZ2}=\sqrt{-\det\eta}\,\overline{\eta}^A\mathcal{P}^{ABCD}_{(2)}\Gamma^{(0)}\{\tfrac{1}{8}\gamma_{ijkl}\gamma^m\mathcal{D}_m\theta^B-\tfrac{1}{2}\gamma_{ijk}\mathcal{D}_l\theta^B\}F^{Cij}F^{Dkl}. \tag{4.18}$$

The variations quadratic in F will have to generate the following contributions:

$$\delta\mathcal{L}_2 = -\sqrt{-\det\eta}\,\overline{\eta}^A(-(\Gamma_2^{AB}\gamma^i\mathcal{D}_i\theta^B+\Gamma_1^{AB}\mathcal{T}_1^B+\Gamma_0^{AB}\mathcal{T}_2^B)+\mathbb{1}\mathcal{T}_2^A). \tag{4.19}$$

We can determine Γ_2 from the requirement that $\Gamma^2=\mathbb{1}$ at order 2,

$$\sigma_1\Gamma_2^{AB}+\Gamma_2^{AB}\sigma_1+\Gamma_1^{AC}\Gamma_1^{CB}=0. \tag{4.20}$$

This calculation assumes that $[\Gamma_2,\sigma_1]=0$, and requires the product of the $\mathcal{P}_{(1)}$-tensors. The result is

$$\Gamma_2^{AB}=-\Gamma^{(0)}\sigma_1(\mathcal{S}^{ABCD}(\tfrac{1}{8}\gamma_{ijkl}F^{ijC}F^{klD}-\tfrac{1}{4}F^C_{kl}F^{klD})+\mathcal{A}^{ABCD}\tfrac{1}{2}\gamma_{ij}F^{ikC}F_k^{jD}). \tag{4.21}$$

Here we have defined

$$\mathcal{S}^{ABCD}\equiv\mathcal{P}_{(1)}^{AE(C}\mathcal{P}_{(1)}^{BD)E}=-d^{AE(C}d^{BD)E}, \tag{4.22}$$

$$\mathcal{A}^{ABCD}\equiv\mathcal{P}_{(1)}^{AE[C}\mathcal{P}_{(1)}^{BD]E}=-d^{AE[C}d^{BD]E}, \tag{4.23}$$

where the (anti-)symmetrization is over the indices C and D only. Note that tensors $\mathcal{S}^{ABCD}$ and $\mathcal{A}^{ABCD}$ are then symmetric and antisymmetric, resp., in the index pairs AB and CD.

To solve the remainder of (4.19) we have to make the choice

$$\mathcal{P}_{(2)}^{ABCD}=-\sigma_1\mathcal{S}^{ABCD}. \tag{4.24}$$

We then find the following result for $\mathcal{T}_2$:

$$\mathcal{T}_2^A=-\mathcal{S}^{ABCD}\gamma_{(i}\mathcal{D}_{j)}\theta^B(F^{ikC}F_k^{jD}+\tfrac{1}{4}\eta^{ij}F^C_{kl}F^{klD})+\tfrac{1}{2}\mathcal{A}^{ABCD}\gamma_{ijk}\{\mathcal{D}^k\theta^BF^{ilC}F_l^{jD}-\mathcal{D}_l\theta^BF^{ijC}F^{klD}\}. \tag{4.25}$$

The result (4.25) agrees with the Abelian result (3.36) if we truncate from U(n) to U(1).

The Born–Infeld term now has to reproduce $\mathcal{T}_2$, while remaining contributions may be cancelled by introducing an additional variation of V_i^A. It is at this stage that the choice of X^μ as a Yang–Mills singlet runs into trouble. Contributions to this variation of the Born–Infeld term come from the F^2 term in the action, when the metric η_{ij}, depending on X^μ, is varied. Such variations contain a double sum over U(n) indices, i.e., they would be of the form [using (4.8)]

$$\partial_iX^\mu\partial_j(\eta^A\Gamma_\mu\theta^A)F^{Cik}F^{Cjk}. \tag{4.26}$$

Such terms would have the wrong U$(1)^n$ limit, and cannot be canceled by other contributions. Partial integration does not help, since it produces symmetric second derivatives on X^μ, which do not occur elsewhere. It is at this stage that we should say farewell to the embedding coordinates X^μ, and proceed in the static gauge.

Terms in the Born–Infeld action that might play a role in this analysis are

$$\begin{aligned}\mathcal{L}_{BI2}=-(&\tfrac{1}{4}F^{ijC}F^C_{ij}+\alpha F^{ikA}F_k^{jB}F^C_{ji}f^{ABC}-\tfrac{1}{2}\overline{\theta}^A\mathcal{S}^{ABCD}\gamma_{(i}\mathcal{D}_{j)}\theta^B\{F^{ikC}F_k^{jD}+\tfrac{1}{4}\eta^{ij}F^C_{kl}F^{klD}\}\\&+\tfrac{1}{4}\overline{\theta}^A\mathcal{A}^{ABCD}\gamma_{ijk}\{\mathcal{D}^k\theta^BF^{ilC}F_l^{jD}-\mathcal{D}_l\theta^BF^{ijC}F^{klD}\}).\end{aligned} \tag{4.27}$$

Note that an F^3 term is in principle not excluded in the non-Abelian case.

In the static gauge we know how to deal with these terms. Then we need not vary the F^2 term. In the F^3 term we have to vary F, which gives an F^2 variation with a single γ-matrix. Therefore it does not relate to the $\mathcal{A}$-terms, which have three γ-matrices, and we must choose α equal to zero. In the $\mathcal{S}$-and $\mathcal{A}$-terms we can perform partial integrations to get rid of the ϵ and $\partial\eta$ terms in the variation. These give equations of motion of V, and can be cancelled by new variations of V. The required identities are

$$\mathcal{D}_j(F^{ik(C}F_k^{jD)}+\tfrac{1}{4}\eta^{ij}F_{kl}^{(C}F^{klD)})=F^{ik(C}\mathcal{D}_jF_k^{jD)}, \tag{4.28}$$

$$\mathcal{D}_{[k}(F_i^{l[C}F_{ij]}^{D]})-\mathcal{D}_l(F_{[ij}^{[C}F_{k]}^{lD]})=-F_{[ij}^{[C}\mathcal{D}_lF_{k]}^{lD]}. \tag{4.29}$$

The remaining η terms in the variation give us precisely $\mathcal{T}_2$. This leads to the following new variations of V_i^A,

$$\delta V_i^A=+\tfrac{1}{2}(\bar{\epsilon}^B+\bar{\eta}^B)\mathcal{S}^{BCDA}\gamma_k\theta^CF^{kiD}+\tfrac{1}{4}(\bar{\epsilon}^B+\bar{\eta}^B)\mathcal{A}^{BCDA}\gamma_{ikl}\theta^CF^{klD}. \tag{4.30}$$

Note that the variation of V_i^A no longer agrees with the result given in (3.30). However, now we should compare with the Abelian result in static gauge. This gauge choice requires a compensating world volume coordinate transformation, which, when acting on V_i, produces the Abelian limit of the $\mathcal{S}$-contribution in (4.30). The $\mathcal{A}$-term in (4.30) vanishes in the Abelian limit.

V. SUMMARY

In this section we will summarize the results obtained in the non-Abelian case. The action is the sum of the Born–Infeld and Wess–Zumino terms. The Wess–Zumino term looks as follows:

$$\mathcal{L}_{WZ}=\epsilon^{i_1\cdots i_{10}}\Big\{\frac{1}{2\cdot 9!}\bar{\theta}^A\sigma_1\gamma_{i_1\cdots i_9}\mathcal{D}_{i_{10}}\theta^A-\frac{1}{4\cdot 7!}\bar{\theta}^A\mathcal{P}_{(1)}^{ABC}\gamma_{i_1\cdots i_7}\mathcal{D}_{i_8}\theta^BF_{i_9i_{10}}^C$$
$$+\frac{1}{16\cdot 5!}\bar{\theta}^A(-\sigma_1\mathcal{S}^{ABCD})\gamma_{i_1\cdots i_5}\mathcal{D}_{i_6}\theta^B(F^CF^D)_{i_7\cdots i_{10}}\Big\}. \tag{5.1}$$

The Born–Infeld action is

$$\mathcal{L}_{BI}=-\{1+\tfrac{1}{2}\bar{\theta}^A\gamma^i\mathcal{D}_i\theta^A-\tfrac{1}{2}\bar{\theta}^A\sigma_1\mathcal{P}_{(1)}^{ABC}\gamma_{[i}\mathcal{D}_{j]}\theta^BF^{ijC}+\tfrac{1}{4}F^{ijA}F_{ij}^A-\tfrac{1}{2}\bar{\theta}^A\mathcal{S}_{ABCD}\gamma_{(i}\mathcal{D}_{j)}\theta^B\{F^{ikC}F_k^{jD}$$
$$+\tfrac{1}{4}\eta^{ij}F_{kl}^CF^{klD}\}+\tfrac{1}{4}\bar{\theta}^A\mathcal{A}^{ABCD}\gamma_{ijk}\{\mathcal{D}^k\theta^BF^{ilC}F_l^{jD}-\mathcal{D}_l\theta^BF^{ijC}F^{klD}\}\}. \tag{5.2}$$

In the action we use the following Yang–Mills structures:

$$\mathcal{P}_{(1)}^{ABC}=(i\sigma_2)d^{ABC}, \tag{5.3}$$

$$\mathcal{S}^{ABCD}=\mathcal{P}_{(1)}^{AE(C}\mathcal{P}_{(1)}^{BD)E}=-d^{AE(C}d^{BD)E}, \tag{5.4}$$

$$\mathcal{A}^{ABCD}=\mathcal{P}_{(1)}^{AE[C}\mathcal{P}_{(1)}^{BD]E}=-d^{AE[C}d^{BD]E}. \tag{5.5}$$

The action is invariant under global supersymmetry transformations and local κ-transformations,

$$\delta\bar{\theta}^A=-\bar{\epsilon}^A+\bar{\eta}^A, \tag{5.6}$$

$$\delta V_i^A=\tfrac{1}{2}(\bar{\epsilon}^B+\bar{\eta}^B)\sigma_1\mathcal{P}_{(1)}^{BCA}\gamma_i\theta^C+\tfrac{1}{2}(\bar{\epsilon}^B+\bar{\eta}^B)\mathcal{S}^{BCDA}\gamma_k\theta^CF^{kiD}+\tfrac{1}{4}(\bar{\epsilon}^B+\bar{\eta}^B)\mathcal{A}^{BCDA}\gamma_{ikl}\theta^CF^{klD}, \tag{5.7}$$

where the parameters ϵ^A satisfy the condition,

$$f_{ABC}\epsilon^C=0. \tag{5.8}$$

As explained in the previous sections, the variation of the action under κ-symmetry can be expressed in terms of

$$\Gamma^{AB}=\Gamma^{(0)}\{\sigma_1\delta^{AB}+\mathcal{P}_{(1)}^{ABC}\tfrac{1}{2}\gamma^{kl}F_{kl}^C-\sigma_1\mathcal{S}^{ABCD}(\tfrac{1}{8}\gamma_{ijkl}F^{ijC}F^{klD}-\tfrac{1}{4}F_{kl}^CF^{klD})$$
$$-\sigma_1\mathcal{A}^{ABCD}\tfrac{1}{2}\gamma_{ij}F^{ikC}F_k^{jD}\}, \tag{5.9}$$

$$\mathcal{T}^A = \gamma^i \mathcal{D}_i \theta^A - \sigma_1 \mathcal{P}^{ABC}_{(1)} \gamma_i \mathcal{D}_j \theta^B F^{ijC} - \mathcal{S}^{ABCD} \gamma_{(i} \mathcal{D}_{j)} \theta^B (F^{ikC} F_k^{jD} + \tfrac{1}{4} \eta^{ij} F_{kl}^C F^{klD}) + \tfrac{1}{2} \mathcal{A}^{ABCD} \gamma_{ijk} \{ \mathcal{D}^k \theta^B F^{ilC} F_l^{jD} - \mathcal{D}_l \theta^B F^{ijC} F^{klD} \}. \tag{5.10}$$

VI. GAUGE FIXING

In the κ-symmetric system which we obtained in this paper, the ordinary supersymmetry is hidden in the local κ-symmetry, and to make it explicit, κ-symmetry should be gauge fixed. This analysis is very similar to the one done in the Abelian case in Ref. 11.

To do this analysis it is convenient to write out the $N=2$ doublets explicitly. We write

$$\Gamma = \begin{pmatrix} 0 & \gamma \\ \tilde{\gamma} & 0 \end{pmatrix}, \tag{6.1}$$

with

$$\Gamma^2 = \begin{pmatrix} \gamma\tilde{\gamma} & 0 \\ 0 & \tilde{\gamma}\gamma \end{pmatrix} = 1. \tag{6.2}$$

Here γ, $\tilde{\gamma}$ are 32×32 matrices, with in addition indices AB, where A, B run from 1 to n^2. Then, splitting also the fermions into separate $N=1$ fermions, we write variations as follows:

$$\delta\overline{\theta}_1^A = -\overline{\epsilon}_1^A + \overline{\eta}_1^A, \quad \delta\overline{\theta}_2^A = -\overline{\epsilon}_2^A + \overline{\eta}_2^A. \tag{6.3}$$

The parameters η can be expressed in terms of parameters κ,

$$\overline{\eta} = (\overline{\eta}_1 \quad \overline{\eta}_2) = (\overline{\kappa}_1 + \overline{\kappa}_2 \tilde{\gamma} \quad \overline{\kappa}_2 + \overline{\kappa}_1 \gamma). \tag{6.4}$$

Now we choose a κ-gauge by setting $\overline{\theta}_2 = 0$, which implies that the transformation parameters must satisfy

$$\overline{\kappa}_2 = \overline{\epsilon}_2 - \overline{\kappa}_1 \gamma. \tag{6.5}$$

So after κ-gauge fixing the remaining η is

$$\overline{\eta}_1 = \overline{\epsilon}_2 \tilde{\gamma}, \tag{6.6}$$

and the remaining fermions $\chi^A \equiv \theta_1^A$ transform as

$$\delta\overline{\chi}^A = -\overline{\epsilon}_1^A + \overline{\epsilon}_2^B \tilde{\gamma}^{BA}. \tag{6.7}$$

Let us now look at the gauge fixed action. The Wess–Zumino term vanishes after gauge fixing, since it was off-diagonal in the fermions θ_1 and θ_2. The Born–Infeld term gives

$$\mathcal{L}_{BI} = -\{1 + \tfrac{1}{2}\overline{\chi}^A \gamma^i \mathcal{D}_i \chi^A + \tfrac{1}{2} d_{ABC} \overline{\chi}^A \gamma_{[i} \mathcal{D}_{j]} \chi^B F^{ijC} + \tfrac{1}{4} F^{ijA} F_{ij}^A + \tfrac{1}{2} d^{AEC} d^{BDE} \overline{\chi}^A \gamma_{(i} \mathcal{D}_{j)} \chi^B \{ F^{ikC} F_k^{jD} + \tfrac{1}{4} \eta^{ij} F_{kl}^C F^{klD} \} - \tfrac{1}{4} d^{AE[C} d^{BD]E} \overline{\chi}^A \gamma_{ijk} \{ \mathcal{D}^k \chi^B F^{ilC} F_l^{jD} - \mathcal{D}_l \chi^B F^{ijC} F^{klD} \} \}. \tag{6.8}$$

Note that the terms of the form $\overline{\chi}\partial\chi F^2$ are not symmetric traces of $\mathrm{U}(n)$ generators. The symmetric trace is of the form,

$$\mathrm{tr}\, T_{(A} T_B T_C T_{D)} = \tfrac{1}{3}(d_{ABE} d_{CDE} + d_{CAE} d_{BDE} + d_{BCE} d_{ADE}). \tag{6.9}$$

The second line in (6.8) contains only two of the three contributions needed for the symmetric trace, the last line contains explicit antisymmetrizations and can be rewritten in terms of structure constants,

$$d_{AEC}d_{BDE}-d_{AED}d_{BCE}=f_{ABE}f_{CDE}\,. \tag{6.10}$$

Finally, the linear and nonlinear supersymmetry transformations which leave (6.8) invariant are of the form,

$$\delta\chi^A=-\bar{\epsilon}_1^A-\bar{\epsilon}_2^A+\bar{\epsilon}_2^B\{d^{BAC}\tfrac{1}{2}\gamma^{kl}F^C_{kl}+\mathcal{S}^{BACD}(\tfrac{1}{8}\gamma_{ijkl}F^{ijC}F^{klD}-\tfrac{1}{4}F^C_{kl}F^{klD})\},$$
$$\delta V_i^A=-\tfrac{1}{2}(\bar{\epsilon}_1^B-\bar{\epsilon}_2^B)d^{BCA}\gamma_i\chi^C-\tfrac{1}{4}\bar{\epsilon}_2^B d^{BED}d^{ECA}\gamma_{kl}\gamma_i\chi^C F^{klD}+\tfrac{1}{2}(\bar{\epsilon}_1^B-\bar{\epsilon}_2^B)\mathcal{S}^{BCDA}\gamma_k\chi^C F^{kiD}. \tag{6.11}$$

Note that contributions with $\mathcal{A}$, the antisymmetrized product of two d-tensors, do not appear because of (6.10) and the fact that ϵ must be in the U(1) direction.

VII. CONCLUSIONS

In this paper we have obtained the non-Abelian generalization of the Born–Infeld action up to terms quartic in the Yang–Mills field strength, and including all fermion bilinear terms up to terms cubic in the field strength. The terms of the form $\bar{\chi}\partial\chi F^2$ violate the symmetric trace conjecture.

The κ-symmetric construction of the Born–Infeld action involves the matrix Γ, satisfying $\Gamma^2=\mathbb{1}$, which is used to project away one of the components of the fermion doublet. In the Abelian case Γ factorizes in a part that is polynomial in F, and the inverse of the Born–Infeld action, which expands to an infinite series in F. In the non-Abelian case we are not yet at a stage that such a factorization could be recognized. We see however, that the result (5.9) is consistent with a factorization of the form,

$$\Gamma^{AB}=\Gamma^{(0)}\{\sigma_1\delta^{AC}+\mathcal{P}^{ACF}_{(1)}\tfrac{1}{2}\gamma^{kl}F^F_{kl}-\sigma_1\mathcal{S}^{ACFG}(\tfrac{1}{8}\gamma_{ijkl}F^{ijF}F^{klG})-\sigma_1\mathcal{A}^{ACFG}\tfrac{1}{2}\gamma_{ij}F^{ikF}F_k^{jG}\}$$
$$\times(\delta^{CB}+\mathcal{S}^{CBDE}\tfrac{1}{4}F^D_{mn}F^{mnE}). \tag{7.1}$$

Note that, as in the Abelian case, $\mathcal{T}$ (5.10) contains the inverse of the factor that we find in Γ. Clearly the second factor in the above expression is not a U(n) singlet, and therefore does not correspond to the inverse of the action. Further analysis, which we plan to do at the cubic and quartic level in F, should elucidate in which sense these factors are related to the Born–Infeld action.

It is intriguing that κ-symmetry and worldvolume reparametrization invariance appear to be incompatible. Although for applications such as the construction of non-Abelian BPS states this is not a drawback, issues of superspace and curved background remain unclear in the static gauge. One way to try to resolve the issue of embedding coordinates would be to look in more detail at the transformation rules of V_i^A. If a formulation with world volume reparametrization invariance exists, then our formulation should be its gauge fixed version, and we should recognize the corresponding compensating transformation in the transformation rule of V_i^A. To give an example, let us consider the possibility that the embedding coordinates are in the adjoint of U(n), and transform as

$$\delta X^{\mu A}=d^{ABC}\xi^{iB}\partial_i X^{\mu C}+\delta_\epsilon X^{\mu A}+\delta_\eta X^{\mu A}. \tag{7.2}$$

Let us now gauge fix this extended worldvolume symmetry, by setting $X^A=0$ for all $A\in\mathrm{SU}(n)$, and $X^{\mu 1}=\delta_i^\mu\sigma_i$ for $A=1\in\mathrm{U}(1)$. Then the compensating transformation which preserves this gauge is of the form,

$$\xi^{\mu A}=-\delta_\epsilon X^{\mu A}-\delta_\eta X^{\mu A}. \tag{7.3}$$

Here we have used that $d^{AB1}\sim\delta^{AB}$, in a basis where the U(1) component of U(n) is labeled by $A=1$. Then, if the variation of V_i^A under world volume coordinate transformations is of the form,

$$\delta V_i^A = d^{ABC}\xi^{kB}F_{ki}^C, \tag{7.4}$$

we see that the term proportional to $\mathcal{S}$ in (5.7) has almost the right form to be interpreted as a compensating transformation. However, the Yang–Mills structure in this expression is not quite correct, as the indices of V and F are not on the same d-tensor. We have found that if one chooses in (4.12) $c_1=1$, that then the structure comes out all right, and gives

$$\delta X^{\mu A} \sim d^{ABC}d^{BDE}(\bar{\epsilon}^D+\bar{\eta}^D)\gamma^k\theta^E\partial_k X^{\mu C}. \tag{7.5}$$

It would be interesting to see whether or not the construction of the generalized Born–Infeld action including the worldvolume structure indicated above is possible.

As mentioned above, the generalization to a curved background would be greatly facilitated by a better understanding of the superspace structure of the D-brane action. However, there is also another open issue to consider. Consider the expression (4.17), where we give the non-Abelian generalization of the relation $\mathcal{F}=F+B$ in a flat background. In going to a curved background we have to decide how and where to introduce the NS–NS fields. Should there be a non-Abelian generalization of the NS–NS field B, or do only the U(1) fields on the worldvolume couple effectively to the background fields? Similar questions can be raised about the RR-fields [see (4.1)], whose form in a flat background also suggests that a non-Abelian generalization should be required.

In a future publication,[20] we hope to extend this work to higher order in F, and to apply the results to the construction of non-Abelian BPS states. The simplest situation to think of is the relation between D-branes at angles[21] and overlapping branes through T-duality.[7] As was shown in Ref. 8 the BPS conditions between angles translate to conditions between magnetic fields F which include contributions cubic in F. Therefore we will have to go at least to order F^3 in the supersymmetry transformation rules to be able to compare our results with the predictions implied by Ref. 21. In the Abelian case the relation between κ-symmetric formulations and BPS states was formulated in Ref. 22. In particular, there it was shown that the knowledge of Γ is in fact sufficient to obtain BPS states. It would be interesting to generalize these results to the non-Abelian situation.

Finally, it would be instructive to apply other approaches than the one employed in this paper to find the complete answer. For instance, one could use the superembedding techniques developed in Refs. 23 and 24. Yet another approach could be to extend to the non-Abelian case the analysis of Ref. 25, where it was shown how the super world volume dynamics of superbranes can be obtained from nonlinear realizations.

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APPENDIX: PROPERTIES OF U(n) GENERATORS, ETC.

In these notes indices $A,B,\ldots$ run from 1,...,n^2. We freely raise and lower these indices.

We use the following conventions for Yang–Mills transformations of the non-Abelian Yang–Mills multiplet:

$$\delta\theta^A = f^A{}_{BC}\Lambda^B\theta^C, \tag{A1}$$

$$\delta V_i^A = -\mathcal{D}_i \Lambda^A, \tag{A2}$$

$$\mathcal{D}_i \theta^A = \partial_i \theta^A + f^A{}_{BC} V_i^B \theta^C, \tag{A3}$$

$$F_{ij}^A = \partial_i V_j^A - \partial_j V_i^A + f^A{}_{BC} V_i^B V_j^C, \tag{A4}$$

$$\mathcal{D}_{[i} \mathcal{D}_{j]} \theta^A = \tfrac{1}{2} f^A{}_{BC} F_{ij}^B \theta^C. \tag{A5}$$

The U(n) generators are Hermitian $n \times n$ matrices. Our normalization for the trace of two U(n)-generators is

$$\mathrm{tr}\, T_A T_B = \delta_{AB}. \tag{A6}$$

In general, we write for the product of two U(n) generators,

$$T_A T_B = +(d_{ABC} + i f_{ABC}) T_C, \tag{A7}$$

where d and f are symmetric and antisymmetric in AB, respectively. We recognize that

$$[T_A, T_B] = 2 i f_{ABC} T_C,$$

$$\{T_A, T_B\} = 2 d_{ABC} T_C. \tag{A8}$$

From this we conclude that

$$\mathrm{tr}[T_A, T_B] T_C = 2 i f_{ABC},$$

$$\mathrm{tr}\{T_A, T_B\} T_C = 2 d_{ABC}. \tag{A9}$$

This tells us that in fact f is completely antisymmetric, and d completely symmetric in ABC.

Then we have the Jacobi identity and its generalizations. These follow from

$$[[T_A, T_B], T_C] + [[T_B, T_C], T_A] + [[T_C, T_A], T_B] = 0,$$

$$[\{T_A, T_B\}, T_C] + [\{T_B, T_C\}, T_A] + [\{T_C, T_A\}, T_B] = 0,$$

$$[T_C, [T_A, T_B]] = \{T_B, \{T_C, T_A\}\} - \{T_A, \{T_B, T_C\}\}. \tag{A10}$$

From these we derive the following identities for the f and d tensors:

$$f_{ABE} f_{ECD} + f_{BCE} f_{EAD} + f_{CAE} f_{EBD} = 0, \tag{A11}$$

$$d_{ABE} f_{ECD} + d_{BCE} f_{EAD} + d_{CAE} f_{EBD} = 0, \tag{A12}$$

$$f_{ABE} f_{ECD} = d_{CAE} d_{BED} - d_{CBE} d_{AED}. \tag{A13}$$

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The future of string theory

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Prophesy is just for fun. The more useful purpose of the exercise is to identify important issues and to stimulate thought about where they stand and how they might be resolved. The subject areas that are fair game include all of particle physics and cosmology. © *2001 American Institute of Physics.*
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I. THIRTY YEARS OF PROGRESS

Since my topic is the future of string theory, I will discuss issues and problems that are currently unresolved and where there is still confusion, doubt, and uncertainty. However, if I were to do only that, it would give a distorted view of a subject that has undergone tremendous progress over the past thirty years. Therefore, to give a more balanced picture, I have decided to begin by presenting a brief chronology of some of the major developments that have taken place. I think we are entitled to look back on this with considerable pride and satisfaction.

- 1968–70: String theory developed to describe the strong interactions (hadron physics)
- 1971–73: Supersymmetry introduced in string theory and field theory
- 1974: String theory reinterpreted as a unified theory of gravity and other forces
- 1976–78: Supergravity; Montonen–Olive duality
- 1977–83: Superstring theory; path-integral formulation
- 1984: Anomaly cancellation; heterotic strings; Calabi–Yau compactification
- 1985–89: Conformal field theory; superstring perturbation theory; T duality; mirror symmetry; string field theory; matrix models
- 1990–94: S duality; p-branes; Seiberg–Witten theory
- 1995: Topology change; M theory; dualities relating all superstring theories and M theory; D-branes
- 1996: Black-hole entropy; F theory; matrix theory
- 1997–99: Brane configurations; AdS/CFT duality; noncommutative geometry; brane worlds

II. THE ISSUES

Let me now discuss where I think future progress will occur. There are two major fields that string theory ought to illuminate some day: particle physics and cosmology. (A third one is mathematics, but I will not discuss that.) Even though we think of particle physics as addressing the microscopic extreme and cosmology the macroscopic extreme, it is quite natural to consider them together when dealing with a theory that incorporates gravity, as string theory does. Relativists and particle theorists have both identified the important problem of reconciling quantum theory with general relativity. The prospect of achieving this attracts both of them to string theory. It is clear to many of us that string theory really does achieve this reconciliation, but it is also clear that there are important aspects of how this works that are not yet fully understood.

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One such issue concerns the status of quantum mechanics and information loss. In 1976, Hawking argued that the existence of black holes implies that a pure quantum state can evolve into a mixed state, in other words there is a loss of quantum coherence. Were this to happen, it would mean a breakdown of quantum mechanics. I think it is quite clear that string theory respects quantum mechanics, and it might even explain it. It gives unitary evolution without loss of coherence, and it can also describe black holes. Thus, it should be possible to study black holes in string theory and to explain precisely how Hawking's argument breaks down. Despite a great deal of effort, I don't think that this has yet been done in a clear and convincing way. However, I certainly believe that it should be possible.

Let me now turn to the most vexing and far-reaching of the unresolved issues: the cosmological constant.

A. The cosmological constant

The low energy effective theory of gravity contains the standard Einstein–Hilbert term:

$$S_{\mathrm{E}}=\frac{1}{16\pi G}\int \sqrt{-g}R\, d^4x.$$

Theoretically, it is natural to also include a vacuum energy, or cosmological, term,

$$S_{\Lambda}=\int \Lambda\sqrt{-g}\, d^4x.$$

Here, the parameter Λ—called the cosmological constant—can be interpreted as the energy density of the vacuum. Such a term is generically induced by radiative corrections even if it is zero in the classical theory. In particular, it receives contributions from the zero-point energies of all fields in the theory. You need a well-defined quantum theory of gravity, before the vacuum energy becomes something computable. String theory is the only such theory on the market. So it is only with the advent of string theory that proposals for understanding this parameter from a fundamental theoretical viewpoint can be analyzed.

Observationally, the bounds on Λ are exceedingly severe. As a first approximation, one can simply require that the energy in the form of vacuum energy is less than the amount that would give closure of the universe. Using this bound, one finds that Λ, expressed in Planck units, is less than 10^{-122}. This is the best measured approximation to zero of any physical parameter in nature. We do not yet have a convincing way to derive why Λ should be this small in the context of a realistic model. Even so, it seems much more likely that someday we will be able to derive the answer zero than an answer of order 10^{-122}.

In recent years, astrophysicists and cosmologists have settled on a fairly precise inventory of how mass and energy are distributed in the universe. Important constraints come from studies of the cosmic microwave background, large scale structure, and Type Ia supernovas, together with the rest of standard cosmology. Based on this, they have concluded the following: The total mass and energy in the universe give, to within about 10%, the critical closure density. This is the value required by inflation, which gives a flat open universe. It has been clear for some time that an appreciable fraction of the mass of the universe is in the form of *dark matter*, but now it appears that there is a second mysterious component, which could be called *dark energy*. The inventory of mass and energy is roughly as follows: 5% is baryonic matter, 25% is dark matter (mostly cold dark matter, but a small portion could be massive neutrinos), and 70% is dark energy. Cold dark matter is concentrated in the halos of galaxies, whereas dark energy is distributed uniformly throughout the universe.

Each component has an equation of state of the form $p=w\rho$, where p is pressure and ρ is density. Nonrelativistic matter has $w=0$ and radiation has $w=1/3$. To fit the data, the dark energy should have an equation of state with $-1.0\leqslant w<-0.5$. Future observations should determine this

parameter with greater accuracy. The most popular guess, which fits the data well, is that the dark energy is vacuum energy (i.e., a cosmological constant). This gives $w=-1$.

Components of the universe with different values of w evolve differently:

$$\rho \sim R^{-3(1+w)},$$

where R is the scale factor of the universe. Thus the universe was primarily comprised of matter (and radiation) in the distant past and will be more and more comprised of dark energy in the future. This means that the present epoch of the universe is rather special: it is the epoch in which the contributions of matter and dark energy are comparable. This is a surprising coincidence, but it seems to be a fact.

As we have already indicated, if the dark energy is vacuum energy, this corresponds to a value of the cosmological constant that is so small that it seems implausible that we will be able to derive it. Therefore it behooves us to ask whether there are any other candidates for the dark energy.

One alternative to a cosmological constant, which has been discussed quite a bit lately, goes by the name of *quintessence*—a word that originally referred to the human soul. In current usage it is the energy carried by a scalar field, which is not at the minimum of the potential, but is still rolling towards its minimum value. If it rolls sufficiently slowly, the phenomenology becomes very similar to that of a cosmological constant. (This kind of slow-roll mechanism is reminiscent of ''new inflation,'' though at a vastly lower energy scale than in the case of the big bang.) In such a scenario the fundamental value of Λ could be zero, if that is the minimum of the potential that is being approached asymptotically. In this way one avoids the need to explain an exceedingly small cosmological constant, but other equally challenging puzzles arise. For one thing, getting the field to roll slowly enough involves a fine-tuning of parameters that is just about as formidable as that for a tiny cosmological constant.

Such a slowly rolling scalar would correspond to a spin zero particle that is essentially massless, since the curvature of the potential would correspond to a Compton wavelength comparable to the size of the universe. Therefore this scalar could mediate long-range scalar forces. There are many ways in which massless scalar fields can arise in string theory, such as moduli associated with compactification and a dilaton. All of them typically have couplings to ordinary matter that is roughly of gravitational strength. The fact that gravity is observed to be a purely tensor force, to better that one percent accuracy, severely restricts the possibilities for massless scalars. So this seems to me to be a problem for accommodating the quintessence proposal in the context of string theory.

Another issue to be considered is that the values of scalar fields in string theory control observable parameters such as Newton's constant and the fine structure constant. A rolling scalar would therefore be expected to imply that these are changing with time. Observational bounds on such time variation are quite severe, so this is also a problem for the quintessence proposal.

If neither a cosmological constant nor quintessence is the right answer, what other possibilities are there? There has been some discussion of schemes in which the dark energy would be carried by topological defects. For example, domain walls that are solid (i.e., they resist shear) and have certain other special properties could give $w=-2/3$. As it stands, this does not look very convincing. However, neither do any of the alternatives.

So, to conclude this part of the discussion, even if we knew how to prove that the cosmological constant vanishes in string theory, there would still be a serious problem accounting for the cosmological observations. It will be interesting to see whether future high-precision determinations of the cosmological parameters confirm the present picture.

B. What is the role of supersymmetry?

Supersymmetry appears to be an essential feature in string theory and M-theory that is required to ensure mathematical consistency. Therefore it seems pretty clear that supersymmetry should be physically relevant at the fundamental scale, which is either the string scale or the

eleven-dimensional Planck scale. But a crucial question, whose answer is much less certain, is whether supersymmetry is also relevant to the description of physics at the electroweak scale. There are several unrelated arguments that suggest that a supersymmetry is broken near the electroweak scale. Even though none of them is conclusive, it is very impressive that they each lead to roughly the same scale for the typical mass of superpartners.

(1) Supersymmetry provides a solution to the gauge hierarchy problem. The ratio of the electroweak scale to the unification scale or the string scale is around 10^{-14}. In the context of the standard model this is puzzling, since quadratic divergences in the Higgs mass would renormalize the Higgs mass (and hence the electroweak scale) up to the cutoff. Supersymmetry builds in cancellations that softens these divergences to being only logarithmic, thereby protecting the hierarchy from being destroyed by radiative corrections. (This does not explain where the hierarchy comes from in the first place.) This reasoning requires that the energy scale that characterizes supersymmetry breaking should be comparable to the electroweak scale—i.e., around 100 GeV to 1 TeV. This argument is not a proof of supersymmetry, because there could be other solutions to the hierarchy problem. One is known, and there could be others.
(2) The unification of the three gauge couplings at a high energy scale works much better with supersymmetry than without it. In fact, studying the fits with a variable supersymmetry breaking scale one finds that unification of the couplings is achieved for a supersymmetry mass gap less than a few TeV. This is very impressive, but one could certainly imagine that other new physics at intermediate scales could also lead to successful unification.
(3) A neutralino LSP with a mass of about 50–500 GeV is an excellent candidate for cold dark matter. It is not possible to be much more precise than this, because we do not know yet the mixture of gauginos and Higgsinos that makes up the LSP, and that affects the relationship between the LSP mass and the cosmological mass fraction that it provides. If the LSP is the dominant component of cold dark matter, the universe could have five times as much mass in neutralinos as in baryons.
(4) In the context of supersymmetric grand unified models the renormalization group running of Higgs masses can give rise to electroweak symmetry breaking at roughly the right scale. In this way supersymmetry helps in establishing the hierarchy as well as in protecting it from radiative corrections.

Supersymmetry may be relevant to solving the cosmological constant problem. There are many known string theory solutions that give a flat Minkowski spacetime with unbroken supersymmetry. They are unrealistic, of course, since supersymmetry has to be broken. However, for these solutions, supersymmetry ensures that radiative corrections do not generate a cosmological constant. So, at least in the context of unrealistic solutions, there is a symmetry explanation of the vanishing of the cosmological constant. Unfortunately, it seems that this cancellation mechanism only works for solutions with unbroken supersymmetry. When supersymmetry is broken, one expects to get a cosmological constant with a size controlled by the supersymmetry mass gap. Assuming that scale is around 1 TeV, the resulting cosmological constant is still some 56 orders of magnitude too big. That's an improvement on 124 orders of magnitude, but it leaves a lot of room for further progress.

Therefore, I like to pose the problem of the cosmological constant as the following question: *Is there a supersymmetry breaking mechanism that does not generate a cosmological constant?* Such a mechanism is not known, but it seems to me that this is what we need. If one were discovered, that would be very exciting. Generic breaking of supersymmetry in the MSSM introduces over 100 new parameters, which is one of the reasons that it is so difficult to use it to make quantitative predictions. I would expect the ''right'' supersymmetry breaking mechanism to be highly constrained and therefore much more predictive.

Lest I leave you with the wrong impression, I should point out that this problem has received a lot of attention over the years. Ingenious proposals have been put forward by Moore, Witten, Kachru and Silverstein, and others. However, I suspect that the correct solution still remains to be

discovered. It might be that insights gained from AdS/CFT duality will provide a better framework for thinking about the cosmological constant. In any case, the importance of this problem cannot be overstated.

C. What is the theory?

What is the theory? What is the principle on which it is based? What is the best way to formulate it? It is rather striking that after 30 years of enormous progress and effort by many hundreds of the most talented physicists, string theory is not yet fully formulated.

Matrix theory and AdS/CFT duality can be viewed as providing exact nonperturbative definitions of string theory or M-theory for certain classes of solutions. This is a remarkable achievement, but we want more than a new recipe for each solution. We want a single formulation that applies to all possible solutions. When such a formulation is found, it is entirely possible that the name *string theory* will no longer be considered appropriate. I suspect that *M-theory* will not fill the bill either. But this is a secondary issue. Understanding the theory is much more important than naming it.

I do not know what form the theory will take when it is completed. It might, for example, be based on some abstract algebraic structure. The concepts of space and time are likely to emerge as properties of particular solutions rather than as smooth background geometries on which the theory is formulated in the first place. It is hard to begin to formulate a theory without reference to spacetime, since it is so radically different from anything we have dealt with before. The standard recipe would have us introduce quantum fields for particles or strings or whatever, and then formulate an action that describes their propagation in a given spacetime manifold. What we seem to need is a theory for which the particles or the strings, as well as the spacetime manifold, are properties of particular solutions rather than features of the underlying theory itself.

I expect that the optimal formulation of the theory will eventually be found, but I would not wish to attach a time frame to this prediction. One lesson I have learned during my career is that it is very hard to anticipate future developments. String theory has undergone several revolutions that have profoundly changed the way we think about the subject. Each one has caused us to ask new questions that we would not have even posed before. It is not at all clear to me how many more such revolutions are still required before we are in a position to formulate the theory properly. I would guess that the process is finite, and that we will eventually get there, but it is hard to assess how close we are at the present time. Once found, this theory will surely be a thing of great beauty, based on profound physical and mathematical principles. As I mentioned earlier, it will probably be sufficiently different from the present formulations to justify giving the subject a new name. However, I do not think there is yet a good reason to drop the name ''string theory.''

D. What is the right solution?

Formulating the theory is not the whole problem. What is likely to prove to be even harder is the determination of a realistic solution. While I am convinced that the theory should be completely unique, with no adjustable parameters, I suspect that the story for solutions is very different. Every indication is that the theory admits a large number of different solutions, most of which are completely unrealistic. Indeed, the ones that are known are supersymmetric, and therefore certainly unrealistic.

There are a number of obvious questions that need to be answered: Can one completely classify all solutions of the theory? Is there a realistic solution with a Lorentz invariant vacuum, that gives an accurate description of particle physics? Is there a cosmological solution that describes the evolving universe that we observe? Can these two questions be addressed separately or do we need to understand cosmology to give a proper description of particle physics?

For the reasons I discussed earlier, it would probably be better if there were no massless or rolling scalars. An added bonus of this is that it would mean that the quantum effective potential that describes the dynamics of all light scalar fields has an isolated minimum. If such a minimum

could be determined theoretically, the corresponding solution would have no continuously adjustable parameters, and all physical quantities would become computable in principle. This would be a very satisfying outcome.

E. Extra dimensions of space

Besides fermionic dimensions, string theory also requires extra spatial dimensions of a somewhat more conventional type. These have generally been assumed to form a compact space of six or seven dimensions with a size that is roughly comparable to the string scale, which might be some 10^{-32} cm. The details of the geometry of the compact space profoundly influence the physics that is observed in four large dimensions. Thus we can hope to infer the geometry indirectly, even though such small extra dimensions would not be directly accessible by foreseeable experiments.

Some physicists have recently suggested that the extra dimensions could be much larger than previously envisioned, maybe even so large as to be experimentally observable. There is now a rather large community actively exploring possible scenarios of this type. To be honest, I find the idea of large extra dimensions to be rather implausible, since it undermines some of the successful predictions of grand unification, such as unification of the couplings and suppression of proton decay. Nevertheless, I do feel that it is worthwhile to explore these ideas, and to improve the experimental bounds. Who knows what might turn up?

F. The role of experiment

I do not expect the right solution to be found by pure thought alone. Experimental guidance, and the more traditional back and forth between theory and experiment, will be important in this quest. One central issue that experimentalists will settle in the next ten or twenty years is what the new physics is that is responsible for electroweak symmetry breaking and mass generation.

The experiments will surely discover one or more Higgs particles. The bigger question, in my opinion, is whether they will find evidence for supersymmetry that is broken at the electroweak scale. If this is the case, then supersymmetry particles should be discovered experimentally at Fermilab or CERN in the early part of the century. This discovery would have profound theoretical and experimental consequences. It would provide evidence for a nontrivial extension of the known symmetries of space and time, an extension which could be described as the discovery of fermionic dimensions. Also, it would set the agenda for experimental particle physics for several decades. When I want to be sure to be quoted, I tell reporters that the discovery of supersymmetry would be more profound than life on Mars.

In addition to experiments at particle accelerators, there are also important nonaccelerator experiments being carried out. For example, dark matter searches are underway. Over the next few years they are expected to achieve the sensitivity required to cover most of the parameter space that is favored for axions or neutralinos. My guess is that a neutralino LSP will eventually turn up in these searches.

Such discoveries would make it clear that the abstract mathematical musings of the past thirty years can be connected to experimental science. Experimental facts about supersymmetry at the electroweak scale would provide crucial guidance in the quest to understand how to connect the underlying theory to the real world. Maybe it would even guide us to the discovery of a supersymmetry breaking mechanism that does not generate a cosmological constant.

G. The role of communication

The final decade of the old millennium saw the birth—from within particle physics—of a powerful new technology called the World Wide Web, which has been quietly revolutionizing education and bringing young people closer to physics than they could ever get when I was a boy in school. For example, on the Superstringtheory.com web site over Christmas break, the following message appeared posted by a teenager from Canada:

'This was a great site that agreed with many of my own theories of ''strings.'' For the first time in my life it seems that someone seems to know what the heck I ''know.'' (I am in grade 9 so when I bring up the topic of quantum mechanics I usually get a fuzzy stare.) Keep up the excellent work.'

So not only is the next generation of string theorists out there, we have a way to reach them, and they have a way to reach us, that has never existed before in history.

Therefore I would like to predict that the future could look very bright in that direction, if we take full advantage of this new technology.

III. CONCLUSION

In conclusion, string theory has developed into one of the most active areas of theoretical physics in recent years. The last third of the 20th century witnessed the construction of an amazing mathematical edifice, which we are struggling to understand. I expect to see equally striking progress achieved in the first third of the 21st century.

The theory is still not fully understood, but I am optimistic that a deeper formulation, which makes clear that it is a unique theory, will be found. I also think that there is a good chance that we will understand how to find solutions that are able to account for the observations of particle physics and cosmology.

The construction of the standard model arose as a collaborative effort in which theorists and experimentalists both made major contributions. In the case of string theory, the natural energy scale is much higher, and so it is more difficult to make contact with experiment. To date, the interactions with mathematicians have played a bigger role than the ones with experimentalists. In the future, I expect that both will be very important. The subject involves a lot of new and bizarre concepts, much as quantum mechanics did in the first half of the 20th century. Before we are through, it is likely that more of them will be identified. To get it right, we will need the help of our mathematical and experimental friends. It is only fitting that a theory that unifies particles and forces should also unify disciplines.

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An exact prediction of $\mathcal{N}=4$ supersymmetric Yang–Mills theory for string theory

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We propose that the expectation value of a circular BPS-Wilson loop in $\mathcal{N}=4$ supersymmetric Yang–Mills can be calculated exactly, to all orders in a $1/N$ expansion and to all orders in g^2N. Using the AdS/CFT duality, this result yields a prediction of the value of the string amplitude with a circular boundary to all orders in α' and to all orders in g_s. We then compare this result with string theory. We find that the gauge theory calculation, for large g^2N and to *all* orders in the $1/N^2$ expansion, does agree with the leading string theory calculation, to all orders in g_s and to lowest order in α'. We also find a relation between the expectation value of any closed smooth Wilson loop and the loop related to it by an inversion that takes a point along the loop to infinity, and compare this result, again successfully, with string theory. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1372177]

I. INTRODUCTION

There have been many tests of the conjectured duality of $\mathcal{N}=4$ supersymmetric Yang–Mills theory (SUSYM) with type IIB string theory in an $AdS_5\times S^5$ background. However, since the duality relates gauge theory with coupling g^2 and gauge group of rank N to type IIB string theory in an AdS background with radius $R^2=\sqrt{g^2N}\alpha'$ and string coupling $4\pi g_s=g^2$, the only precise tests have been of quantities so protected by supersymmetry that they receive no perturbative or nonperturbative corrections. It is easy to calculate quantities in the gauge theory for weak coupling—but these yield predictions for string theory in a very curved background, where there do not yet exist methods of computation. Conversely, it is easy to calculate quantities in the string theory for weak coupling (large N) and large curvature (or small α')—but these yield predictions for the gauge theory for large N and large g^2N, for which there are no reliable methods of computation. In neither case, so far, is there a prediction on either side that holds for all N and g^2.

We will suggest, in this paper, that the expectation value of a circular BPS-Wilson loop in $\mathcal{N}=4$ (SUSYM) can be calculated exactly, to all orders in a $1/N$ expansion and to all orders in g^2N. This then yields a prediction of the value of the string amplitude with a circular boundary to all orders in α' and to all orders in g_s. We then compare this result with string theory. We find that the gauge theory calculation, for large g^2N and to *all* orders in the $1/N^2$ expansion, does agree with the leading string theory calculation, to all orders in g_s and to lowest order in α'.

Our result is an extension of a beautiful paper,[1] in which Erickson, Semenoff and Zarembo calculated the contributions of rainbow graphs to the expectation value of a circular Wilson loop in $\mathcal{N}=4$ supersymmetric gauge theory. The result they found was that

$$\langle W\rangle_{\text{rainbow}}=\frac{2}{\sqrt{\lambda}}I_1(\sqrt{\lambda}), \tag{1.1}$$

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where $\lambda = g^2 N$ is the 't Hooft coupling and I_1 is a Bessel function. For large λ (1.1) behaves as

$$\langle W \rangle_{\text{rainbow}} \sim \sqrt{\frac{2}{\pi}} \frac{e^{\sqrt{\lambda}}}{\lambda^{3/4}}. \tag{1.2}$$

The expectation value of Wilson loops can also be calculated using the Maldacena conjecture,[2–4] and for the circular Wilson loop one finds, to leading order in large λ, that[5,6]

$$\langle W \rangle_{\text{circle}} = e^{\sqrt{\lambda}}, \tag{1.3}$$

in agreement with (1.2).

The authors of Ref. 1 conjectured that the rainbow graphs gave the exact large N behavior of the circular Wilson loop and gave some evidence (a 2 loop calculation) to this effect. We will outline a proof that the result (1.1) is indeed exact to all orders in $g^2 N$ for $N=\infty$. We will also generalize this result to all orders in the $1/N^2$ expansion.

How are we able to perform an exact calculation in strongly coupled gauge theory? The reason turns out to be that the circular Wilson loop is totally determined by an anomaly, a conformal anomaly. As in other cases one is able to calculate the anomaly exactly to all orders in the coupling.

To see this recall that the Wilson loop under discussion is the appropriate super-symmetric Wilson loop,

$$W = \frac{1}{N} \mathrm{Tr} \mathcal{P} \exp i \oint (A_\mu \dot{x}^\mu + i \Phi_i |\dot{x}| \theta^i) dt, \tag{1.4}$$

where A_μ and Φ_i are the gauge fields and the scalars that couple to $x^\mu(t)$, parametrizing the circle and to θ^i which is chosen to be some constant unit vector in R^6. This special Wilson loop is locally supersymmetric. If the contour $(x^\mu(t))$ is a straight line then the Wilson line is globally a BPS object whose expectation value is precisely one. A straight line and a circle are related by a conformal transformation. This fact was used by Ref. 5 to find the minimal surface ending along a circle. If the expectation value of a Wilson loop was truly invariant under all conformal transformations then the expectation value of a circular loop would also be one. However, this is not the case. We will show that there are quantum anomalies when one performs the type of global conformal transformations necessary to turn a straight line into a circle. These anomalies are responsible for the very nontrivial $g^2 N$ and $1/N$ behavior of the circular loop, and as often is the case with anomalies, can be calculated exactly.

Accepting for the moment the result of (1.1) (for $N=\infty$), we see that acting on a straight line with a special conformal transformation that changes it to a circle changes its expectation value by a factor of $2I_1(\sqrt{\lambda})/\sqrt{\lambda}$. Since this factor arises from an anomaly, we will be able to argue that this phenomenon is much more general—the same happens for a general Wilson loop. That is

$$\langle W \rangle_{N=\infty} = \frac{2}{\sqrt{\lambda}} I_1(\sqrt{\lambda}) \langle \tilde{W} \rangle, \tag{1.5}$$

where W is any closed smooth Wilson loop and $\tilde{W}$ is the loop related to it by a special conformal transformation that takes a point along W to infinity. Even more, we will generalize this result to all orders in the $1/N^2$ expansion.

The fact that the expectation value of circular Wilson loops and straight line Wilson loops (or more generally closed and open loops related by conformal transformations) are different should not be a surprise. Large conformal transformations, such as an inversion,

$$x^\mu \to \frac{x^\mu}{x^2}, \tag{1.6}$$

are not symmetries of R^4, since they exchange the point at infinity with a point at a finite distance. They are a symmetry of the theory on S^4, which includes the point at infinity. On the sphere there is no distinction between a circle and a line, and the expectation value of either is the same as for a circle on R^4.

There clearly could be a problem with the invariance under global conformal transformations. For example, a conformal transformation of a correlator of n local operators could take one of the points to infinity, and turn it into the correlator of $n-1$ operators. Here we are seeing an analogous statement for Wilson loops, by transforming the circle to the line, one point along the loop is taken to infinity. As such, one might guess that the difference between the line and the circle is the contribution of the fields at a single point. In fact the authors of Ref. 1 pointed out that (1.1) is equal to the Wilson loop of the large N Hermitian matrix model,

$$\frac{2}{\sqrt{\lambda}} I_1(\sqrt{\lambda}) = \left\langle \frac{1}{N} \mathrm{Tr} \exp(N) \right\rangle = \frac{1}{Z} \int \mathcal{D}M \frac{1}{N} \mathrm{Tr} \exp(M) \exp\left(-\frac{2}{g^2} \mathrm{Tr}\, M^2 \right), \tag{1.7}$$

and one could associate the field M with the fluctuations of the fields at the point at infinity.

We will demonstrate how Eq. (1.5), and its finite N generalization, can be proven in Sec. II. The idea for the proof is the following. Under a conformal transformation the gluon propagator is modified by a total derivative. This is analogous to a gauge transformation, and naively does not affect the gauge invariant loop. However the gauge transformation is singular at the point that is taken to infinity. While the perturbative expansion is naively invariant under gauge transformations, we find that this invariance breaks down at the singular point. By calculating the contribution from the singularities we are able to show that it is given by a matrix model. We did not complete the proof that the matrix model is quadratic, but there are many indications that it indeed is. Under that assumption we are able to evaluate the expectation value to all orders in perturbation theory. For large N we will recover (1.5), but our result yields an exact relation for any λ and any N. In the case of a circular loop we derive an exact expression for $\langle W \rangle$.

In Sec. III we compare our results with the dual string theory. We find that at the classical level the minimal area calculation shows the same universal behavior under a conformal transformation. In the case of the circular loop, where we are able to calculate in the gauge theory exactly, we argue that order by order in string perturbation theory, the leading contribution for small α' agrees with the gauge theory predictions. We also show that the agreement extends to large coupling where, after an S-duality transformation, it is given by a D1-brane.

In Sec. IV we generalize the calculation to more general observables in the matrix model. Those correspond to Wilson loops wound multiple times around the circle.

The Appendices contain the details of the explicit evaluation of the matrix model that yields the precise form of our results.

II. THE GAUGE THEORY CALCULATION

We shall explore the invariance of the Wilson loop under large conformal transformations order by order in perturbation theory.

We expand the expectation value of the Wilson loop around some contour C, as defined in (1.4),

$$\begin{gathered} \langle W_C \rangle = \sum_{n=0}^{\infty} A_n \lambda^n, \\ A_0 = 1, \\ A_1 = \frac{1}{2} \oint ds_1 \oint ds_2 \frac{1}{N} \mathrm{Tr}\left(-\dot{x}_1^\mu \dot{x}_2^\nu \langle A_\mu(x_1) A_\nu(x_2) \rangle + |\dot{x}_1| \theta_1^i |\dot{x}_2| \theta_2^j \langle \Phi_i(x_1) \Phi_j(x_2) \rangle \right), \\ A_2 = \cdots . \end{gathered} \tag{2.1}$$

We will work in R^4, where the propagators are translationally invariant and investigate the behavior of $\langle W_C \rangle$ under conformal transformations that take the closed contour C to $\tilde{C}$. We will compare $\langle W_C \rangle$ to

$$\langle \widetilde{W}_{\widetilde{C}} \rangle = \sum_{n=0}^{\infty} \widetilde{A}_n \lambda^n. \tag{2.2}$$

We could instead compare the gauge theory on R^4 to the theory on S^4. In the latter we would use propagators that transform covariantly under inversions. Those were studied in Ref. 7, and are related to the Feynman gauge propagator by a singular gauge transformation. The two computations turn out to be equivalent.

A. Quadratic term

Let us look at the first nontrivial term in the expansion of the Wilson loop and compare $\widetilde{A}_1$ to A_1. First consider the behavior of the propagators under a large conformal transformation. In particular we shall examine the behavior under an inversion about the origin,

$$x^\mu \to \frac{x^\mu}{x^2} = \tilde{x}^\mu. \tag{2.3}$$

All other large conformal transformations can be obtained by a combination of an inversion and small conformal transformations. Under inversion the scalar propagator,

$$G_{ij}^{ab}(x_1,x_2) = \langle \Phi_i^a(x_1)\Phi_j^b(x_2)\rangle = \frac{g^2}{4\pi^2}\frac{\delta_{ij}\delta^{ab}}{(x_1-x_2)^2}, \tag{2.4}$$

transforms to

$$\tilde{G}_{ij}^{ab}(\tilde{x}_1,\tilde{x}_2) = \frac{g^2}{4\pi^2} x_1^2 x_2^2 \frac{\delta_{ij}\delta^{ab}}{(x_1-x_2)^2}. \tag{2.5}$$

Taking into account the fact that under inversion $|\dot{x}| \to |\dot{x}|/x^2$, the one scalar exchange contribution,

$$|\dot{x}_1|\theta_1^i |\dot{x}_2|\theta_2^j \langle \Phi_i(x_1)\Phi_j(x_2)\rangle, \tag{2.6}$$

to the Wilson loop, is invariant under inversion. However, if this was the only term we would have to introduce an ultraviolet cutoff to render the integral finite, and this could spoil the conformal invariance. Indeed, the Wilson loop in a nonsupersymmetric theory exhibits a perimeter law in perturbation theory,

$$W \sim g^2 \frac{L}{\epsilon}, \tag{2.7}$$

which is definitely not invariant under conformal transformations. But the inclusion of both the scalars and the gluons in the Wilson loop exactly cancels this divergence.[6]

The story with the gauge fields is more complicated, since under inversion a vector field (of dimension one) transforms as

$$\widetilde{V}_\mu(\tilde{x}) = x^2 I_{\mu\nu}(x) V^\nu(x), \quad I_{\mu\nu}(x) = g_{\mu\nu} - 2\frac{x_\mu x_\nu}{x^2}. \tag{2.8}$$

This can easily be derived by noting that

$$\frac{\partial}{\partial \tilde{x}^\mu} = x^2 I_{\mu\nu}(x) \frac{\partial}{\partial x^\nu}, \tag{2.9}$$

so that if Φ is a dimensionless scalar field that transforms as $\Phi(\tilde{x})=\Phi(x)$, then the dimension one vector field, $\partial_\mu\Phi(x)$, will transform as above.

Thus the gluon propagator transforms as

$$\langle \tilde{A}^a_\mu(\tilde{x}_1)\tilde{A}^b_\nu(\tilde{x}_2)\rangle = x_1^2 x_2^2 I_{\mu\rho}(x_1) I_{\nu\sigma}(x_2)\langle A^a_\rho(x_1)A^b_\sigma(x_2)\rangle. \tag{2.10}$$

We shall work, for convenience in the Feynman gauge, $\langle A^a_\mu(x_1)A^b_\nu(x_2)\rangle=(g^2/4\pi^2)[g_{\mu\nu}\delta^{ab}/(x_1-x_2)^2]$. Then the transformed propagator is

$$\begin{aligned}\tilde{G}^{ab}_{\mu\nu}(\tilde{x}_1,\tilde{x}_2) &= \frac{g^2\delta^{ab}}{4\pi^2}\frac{x_1^2x_2^2}{(x_1-x_2)^2}\left(g_{\mu\nu}-2\frac{x_1^\mu x_1^\nu}{x_1^2}-2\frac{x_2^\mu x_2^\nu}{x_2^2}+4\frac{x_1\cdot x_2 x_1^\mu x_2^\nu}{x_1^2x_2^2}\right)\\ &= \frac{g^2\delta^{ab}}{4\pi^2}x_1^2x_2^2\left(\frac{g_{\mu\nu}}{(x_1-x_2)^2}+\frac{1}{2}\partial^1_\mu(\ln(x_1-x_2)^2\partial^2_\nu\ln x_2^2)\right.\\ &\quad\left.+\frac{1}{2}\partial^2_\nu(\ln(x_1-x_2)^2\partial^1_\mu\ln x_1^2)-\frac{1}{2}\partial^1_\mu\partial^2_\nu(\ln x_1^2\ln x_2^2)\right).\end{aligned} \tag{2.11}$$

Consequently, while we saw that the contribution of the scalars to the Wilson loop was invariant under inversion, the gluon contribution, $\dot{x}_1^\mu\dot{x}_2^\nu\langle A^a_\mu(x_1)A^b_\nu(x_2)\rangle$, is changed by a total derivative:

$$\begin{aligned}&\frac{g^2\delta^{ab}}{8\pi^2}\dot{x}_1^\mu\dot{x}_2^\nu[\partial^1_\mu(\ln(x_1-x_2)^2\partial^1_\nu\ln x_2^2)+\partial^2_\nu(\ln(x_1-x_2)^2\partial^1_\mu\ln x_1^2)-\partial^1_\mu\partial^2_\nu(\ln x_1^2\ln x_2^2)]\\ &\quad=\frac{g^2\delta^{ab}}{4\pi^2}\dot{x}_1^\mu\dot{x}_2^\nu\partial^1_\mu\left(\ln\frac{(x_1-x_2)^2}{|x_1|}\partial^2_\nu\ln x_2^2\right).\end{aligned} \tag{2.12}$$

Since the modification of the gluon contribution is a total derivative, which is equivalent to a gauge transformation, one might conclude that the inversion is a symmetry of the Wilson loop. This would be the case, except that the gauge transformation in (2.12) has potential singularities. We must therefore reexamine the proof of gauge invariance of the perturbative expansion and see whether it fails.

We are evaluating the integral

$$\tilde{A}_1-A_1=-\frac{1}{16\pi^2}\oint_C dx_1^\mu\oint_C dx_2^\nu\,\partial^1_\mu\left(\ln\frac{(x_1-x_2)^2}{|x_1|}\partial^2_\nu\ln x_2^2\right). \tag{2.13}$$

[Here we have included the contribution from the color indices that gives a factor of $(1/N)\mathrm{Tr}\,T^aT^a=N/2$.] There are two potential singularities that we encounter when doing the x_1 integral, at $x_1=x_2$, and at $x_1=0$. The second singularity only occurs if the point $x^\mu=0$ lies on the contour C. To examine the behavior at the singularities we introduce a cutoff ϵ.

First, consider the case where $x^\mu=0$ lies on the contour C. The contribution from $x_1=0$ is

$$-\frac{1}{16\pi^2}\oint_C dx_2^\nu\ln\frac{(x_2+\epsilon)^2}{(x_2-\epsilon)^2}\partial^2_\nu\ln x_2^2. \tag{2.14}$$

Here ϵ is an infinitesimal vector tangent to the loop at the origin. To perform the x_2 integral, we notice that for large x_2 the integrand is of order ϵ, the integrand can therefore be regarded as a delta function concentrated at $x_2=\pm\epsilon$. A similar term arises from regularizing the singularity at $x_1=x_2$, which is also zero for x_2 far from the origin. So the only contribution comes from the point $x_1=x_2=0$.

To find the contribution from the singular point one can use the expression

$$\int_{\epsilon}^{\infty} dx \frac{1}{x} \ln \frac{x-\epsilon}{x+\epsilon} = -\frac{\pi^2}{4}, \tag{2.15}$$

to find that

$$\tilde{A}_1 - A_1 = -\tfrac{1}{8}. \tag{2.16}$$

On the other hand if $x^\mu = 0$ does not lie on the contour C the integral is not singular enough and it vanishes. Thus in this case $\tilde{A}_1 - A_1 = 0$. Therefore we conclude that under inversion through the origin the quadratic contribution to the Wilson loop is invariant if the original loop does not pass through the origin. Such an inversion transforms a closed contour into another closed contour. On the other hand if C passes through the origin the transformed Wilson loop ($\tilde{C}$) is now extended to infinity, it is an open Wilson line that only meets at the point at infinity. In this case, to quadratic order,

$$\langle \tilde{W}_{\tilde{C}} \rangle - \langle W_C \rangle = -\lambda/8. \tag{2.17}$$

A safer route to the same result is to evaluate the modification to the propagator (2.11) directly, and not use integration by parts. That way one does not encounter any singularities. Let us do this for the two simplest examples. First we look at a circle passing through the origin,

$$x_1(s) = (1+\cos s, \quad \sin s) \quad x_2(t) = (1+\cos t, \sin t). \tag{2.18}$$

Under inversion this is mapped to the straight line: $x(s) = \frac{1}{2}(1, \tan(s/2))$. For this contour the modification of the gluon propagator contributes to $\tilde{W}$ the amount

$$\begin{aligned} &\frac{\lambda}{16\pi^2}\left[\dot{x}_1^\mu \dot{x}_2^\nu \partial_\mu^1 \left(\ln \frac{(x_1-x_2)^2}{|x_1|} \partial_\nu^2 \ln x_2^2 \right) + (x_1 \to x_2) \right] \\ &\quad = \frac{\lambda}{16\pi^2}\left[-\left(\frac{2\sin t}{4\sin^2 \frac{t}{2}} \right)\left(\frac{2\sin s}{4\sin^2 \frac{s}{2}} \right) + \frac{2\sin(s-t)}{4\sin^2\left(\frac{s-t}{2}\right)}\left(\frac{2\sin s}{4\sin^2 \frac{s}{2}} \right)\left(\frac{\sin t}{4\sin^2 \frac{t}{2}} \right) \right] = -\frac{\lambda}{32\pi^2}, \end{aligned} \tag{2.19}$$

which, when integrated over the circle, gives the result of (2.16).

It is even simpler to take a straight line that does not pass through the origin $x(s) = (1,s)$. Under the inversion it is mapped to a circle of radius 1/2 whose origin is at (1/2,0), and the point at infinity is mapped to the origin. Therefore we expect a contribution from the point at infinity that is exactly opposite to the previous calculation. Indeed

$$\begin{aligned} A_1 - \tilde{A}_1 &= -\frac{1}{16\pi^2} \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt \frac{1}{(s-t)^2}\left(-2\frac{s^2}{s^2+1} - 2\frac{t^2}{t^2+1} + 4\frac{st(st+1)}{(s^2+1)(t^2+1)} \right) \\ &= \frac{1}{8\pi^2} \int_{-\infty}^{\infty} ds \int_{-\infty}^{\infty} dt \frac{1}{(s^2+1)(t^2+1)} = \frac{1}{8}. \end{aligned} \tag{2.20}$$

Finally, we note that the calculation of the quadratic piece of the Wilson loop in the case of the circle and the straight line, which are related by an inversion through the origin, is easy to do directly. For the straight line we automatically get zero, since for a straight line,

$$\dot{x}_1 \cdot \dot{x}_2 - |\dot{x}_1||\dot{x}_2| = 0. \tag{2.21}$$

Thus for a straight line the sum of the gluon and scalar propagators vanishes. The reason for this triviality is the BPS nature of our Wilson loop, which for a straight line ensures that there are no contributions to any order in λ. In the case of the circle the propagators do not cancel, but their sum is a constant, since (for $|x| = |\dot{x}| = 1$)

$$(x_1 - x_2)^2 = -2(\dot{x}_1 \cdot \dot{x}_2 - |\dot{x}_1||\dot{x}_2|). \tag{2.22}$$

Explicitly, for the circle in (2.18),

$$\langle W \rangle = \int_0^{2\pi} ds\, dt \frac{\lambda}{16\pi^2} \frac{-\dot{x}(t)\cdot\dot{x}(s) + |\dot{x}(t)||\dot{x}(s)|}{(x(t)-x(s))^2} = \int_0^{2\pi} ds\, dt \frac{\lambda}{16\pi^2} \frac{1}{2} = \frac{\lambda}{8}. \tag{2.23}$$

So we have learned that to quadratic order the difference between the Wilson loop along an open line $\tilde{C}$ and along the closed contour C obtained by an inversion through the origin is

$$\langle \tilde{W}_{\tilde{C}} \rangle - \langle W_C \rangle = -\lambda/8. \tag{2.24}$$

In the case of the straight line $\langle \tilde{W}_{\tilde{C}} \rangle = 0$ and $\langle W_C \rangle = \lambda/8$. In the following we shall generalize the evaluation of the circle and the relationship (2.24) to all orders in λ.

B. The circle to all orders

It is simple to generalize the calculation of the circle to arbitrary order in perturbation theory. This is because the circle is related by an inversion to the straight line, and the straight line receives no corrections to any order (since it is BPS). So we start with a straight line contour C [say $x(s) = 1/2(1, \tan(s/2))$]. The Wilson loop along this contour is identically equal to one because of supersymmetry. We saw this explicitly to leading order, but the triviality holds to all orders. When we perform the inversion we will get the Wilson loop along the circle, expressed, diagram by diagram, in terms of the diagrams for the straight line loop with the gluon propagators modified according to (2.11). Of course, in addition to propagators and vertices involving the scalars and gluons we will also have to include ghosts—however these, like the scalars, transform covariantly under the inversion.

The modifications of the gluon propagators is of the form of a gauge transformation. Were it not for the fact that this gauge transformation is singular it would have no effect on any of the diagrams of a given order—the boundary terms that one would encounter upon integrating these total derivatives by parts would cancel order by order. This is the regular statement of gauge invariance of the perturbative expansion. Indeed in our case we do not even have to worry, in making these arguments, about the usual short distance singularities that in most theories require regularization and renormalization since the $\mathcal{N}=4$ SUSYM theory is finite when all the diagrams of a given order are included.

However, because of the singularities that occur in the modified propagator at the origin, the point about which the inversion is done, there is another boundary contribution, namely when and only when both ends of a single propagator hits the origin (or the point at infinity). As we saw above, by introducing a cutoff ϵ, when one end of the propagator hits the origin (or the point at infinity), the resulting modification to the propagator is of order ϵ unless the other end of the propagator also hit the origin. Thus it behaves like a one-dimensional delta-function that contributes a finite amount when the other end of the propagator is integrated over the loop. Therefore when both ends of a single propagator approach the origin (or the point at infinity) we get a constant factor of $-1/8$ (1/8).

One should worry about contributions when the other end of the propagator is on an internal vertex that approaches the origin. We think that at least for the $\mathcal{N}=4$ theory those graphs will not contribute, but we were unable to prove that. By using the same regularization as above, it is easy

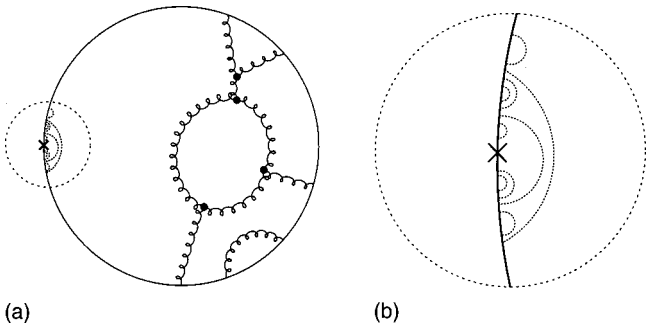

FIG. 1. (a) To go from a straight line to a circle one should include diagrams with some gluon propagators replaced by the total derivatives (dotted lines). Those give a boundary contribution only when all of them hit the point of inversion (marked by an x). (b) Regardless of the rest of the diagram, the anomaly is dependent only on the vicinity of the inversion point and since it lives at one point, is given by the matrix model expression.

to see that the contribution, if any, would come only when all the connected part of the diagram collapses to that point. This means that it can be described by an interaction term in the matrix model. An explicit calculation[1] shows that there is no term of order g^4. It would require a better regulator and a more careful calculation to show that the interaction terms vanish to all orders. The remarkable agreement between our results and the AdS calculation suggests that there are no interactions. In the remainder of the paper we will assume that indeed all the interaction terms vanish, and will provide evidence for that from the comparison to string theory in AdS.

So, ignoring interactions, if we integrate by parts all of the modified gluon propagators we will get nonvanishing contributions from single propagators that are not attached to other parts of the diagram when both ends of a single propagator approach the origin (or the point at infinity). These will yield constant factors times the rest of the diagram, as is illustrated (for a circle) in Fig. 1. But the sum of the rest of the diagrams (to any given order) vanishes in the case of the straight line. Therefore the calculation of the straight line Wilson loop, with modified gluon propagators, reduces to summing all graphs with just noninteracting modified gluon propagators. Each such modified propagator will give a factor as in (2.20). We simply have to add all these terms.

Alternatively we can argue that since the sum of the ordinary gluon and scalar propagators vanishes, we can add these as well. This then is inverted to the Wilson loop for a circle, where we should sum the Feynman diagrams of a noninteracting theory of scalars and vectors. This is a simple calculation to perform, since as we have seen—in the case of the circle—the sum of the gluon (in Feynman gauge) and scalar propagator contributions is a constant[see (2.23)]. Since each propagator just yields a constant, we can perform the sum and account for the factors of N by doing the calculation in a 0-dimension field theory, namely a matrix model. This leads to the expression

$$\langle W_{\text{circle}}\rangle = \left\langle \frac{1}{N}\operatorname{Tr}\exp(M)\right\rangle = \frac{1}{Z}\int \mathcal{D}M\,\frac{1}{N}\operatorname{Tr}\exp(M)\exp\left(-\frac{2N}{\lambda}\operatorname{Tr}\,M^2\right). \tag{2.25}$$

In the Appendix we shall show that this integral can be calculated exactly, in an expansion in powers of $1/N^2$. The result is [where L_n^m is the Laguerre polynomial $L_n^m(x)=1/n!\times\exp[x]x^{-m}(d/dx)^n(\exp[-x]x^{n+m})$]:

$$\begin{aligned}\langle W_{\text{circle}}\rangle &\equiv F(\lambda,N)\\ &= \frac{1}{N}L_{N-1}^1(-\lambda/4N)\exp[\lambda/8N]\\ &= \frac{2}{\sqrt{\lambda}}I_1(\sqrt{\lambda})+\frac{\lambda}{48N^2}I_2(\sqrt{\lambda})+\frac{\lambda^2}{1280N^4}I_4(\sqrt{\lambda})+\frac{\lambda^{5/2}}{9216N^4}I_5(\sqrt{\lambda})+\cdots.\end{aligned} \tag{2.26}$$

To leading order in $1/N$ we recover the result

$$\langle W_{\text{circle}}\rangle_{N=\infty}=\frac{2}{\sqrt{\lambda}}I_1(\sqrt{\lambda})=\sum_{n=0}^{\infty}\frac{(\lambda/4)^4}{n!(n+1)!}, \tag{2.27}$$

in agreement with Ref. 1, where the leading, noninteracting, rainbow graphs (the leading large N graphs) were summed.

Our result is based on a perturbative expansion, but we do not expect corrections due to instantons. We found that the only contributions are from diagrams collapsed to the point of inversion, and since instantons are smooth objects, the singular graphs have measure zero, and will not contribute.

C. Arbitrary loops

As was explained in the preceding section, the contribution to the circular Wilson loop can be localized near a single point. Going from the straight line to the circle, the contribution is from the point at infinity. Since the calculation can be pushed to one point, one would expect that it does not depend on the shape of the curve. Indeed we will see that for any smooth closed curve C and the open curve $\tilde{C}$ related to it by a conformal transformation the appropriate Wilson loops satisfy

$$\langle W_C\rangle=\left\langle\frac{1}{N}\operatorname{Tr}\exp(M)\right\rangle\langle\tilde{W}_{\tilde{C}}\rangle=F(\lambda,N)\langle\tilde{W}_{\tilde{C}}\rangle. \tag{2.28}$$

We will prove this equation below by comparing Feynman diagrams of the two Wilson loops.

First, we will explain one feature of (2.28), the fact that the left hand side has a single trace, while the right hand side has two traces—over $\exp(M)$ and over the open Wilson loop. The reason for this factorization is that the SUSYM fields and the matrix M are independent variables. In general, for two independent Hermitian matrices A and B with independent $U(N)$ invariant measures $\mu(A),\tilde{\mu}(B)$,

$$\begin{aligned}\left\langle\frac{1}{N}\operatorname{Tr}(f(A)g(B))\right\rangle&=\int\mathcal{D}A\mathcal{D}B\mu(A)\tilde{\mu}(B)\frac{1}{N}\operatorname{Tr}(f(A)g(B))\\&=\int\mathcal{D}A\mathcal{D}B\mu(A)\tilde{\mu}(B)\frac{1}{N}\operatorname{Tr}(U^{\dagger}f(A)UV^{\dagger}g(B)V),\end{aligned} \tag{2.29}$$

with arbitrary unitary U, V. Since they are independent, $W=UV^{\dagger}$ can take any value in $U(N)$, and we can integrate over it,

$$\int\mathcal{D}A\mathcal{D}B\frac{\mathcal{D}W}{\operatorname{Vol}[U(N)]}\mu(A)\tilde{\mu}(B)\frac{1}{N}\operatorname{Tr}(AWBW^{\dagger})=\int\mathcal{D}A\mathcal{D}B\mu(A)\tilde{\mu}(B)\frac{1}{N^2}\operatorname{Tr}A\operatorname{Tr}B. \tag{2.30}$$

Using this result,

$$\left\langle\frac{1}{N}\operatorname{Tr}\left[\exp(M)\mathcal{P}\exp i\int_{\tilde{C}}(A_{\mu}\dot{x}^{\mu}+i\Phi_i|\dot{x}|\theta^i)dt\right]\right\rangle=\left\langle\frac{1}{N}\operatorname{Tr}\exp(M)\right\rangle\langle\tilde{W}_{\tilde{C}}\rangle. \tag{2.31}$$

The proof for a general loop is again diagrammatic, order by order in perturbation theory. We write the loops again as

$$\langle W_C\rangle=\sum_{n=0}^{\infty}A_n\lambda^n,\quad\langle\tilde{W}_{\tilde{C}}\rangle=\sum_{n=0}^{\infty}\tilde{A}_n\lambda^n. \tag{2.32}$$

Let us look at a certain diagram Γ of W_C at order g^{2n} which contributes to A_n, and assume it has k vertices on the Wilson loop.

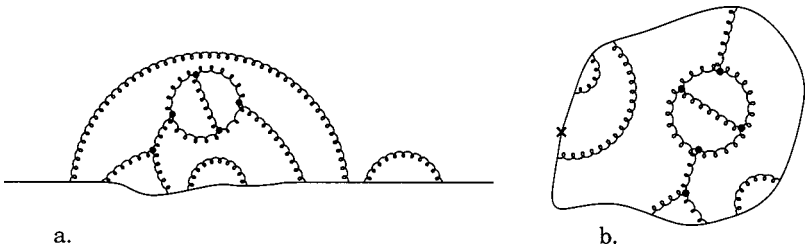

FIG. 2. Two graphs contributing (a) to the open Wilson loop $\langle \tilde{W}_{\tilde{C}} \rangle$ and (b) to the closed loop $\langle W_C \rangle$. The curves are related by a conformal transformation, and the two diagrams differ by total derivatives.

There is a similar diagram $\tilde{\Gamma}$ contributing to the coefficient $\tilde{A}_n$ of $\tilde{W}_{\tilde{C}}$. Those two diagrams are not equal to each other, rather Γ is equal to $\tilde{\Gamma}$ if we replace the gluon propagator by the modified propagator (2.11). Thus Γ is equal to $\tilde{\Gamma}$ plus total derivatives. See Fig. 2.

Exactly as in the case of the circle, the total derivatives terms will cancel unless they hit the origin. When one end hits this point the resulting expression is proportional to a one-dimensional delta-function, forcing the other end to the origin.

So considering $\tilde{\Gamma}$ with l boundary to boundary propagators replaced by the total derivatives will give a contribution from the singular point times the rest of the diagram $\tilde{\Gamma}'$, as in Fig. 3(c). We find the same sub diagram $\tilde{\Gamma}'$ by replacing propagators by total derivatives in other graphs, as illustrated in Fig. 3(d).

Summing all of them we see that the total derivative contribution is exactly the matrix model expression as before. From the example of the circle we know that l total derivatives give the same as the insertion of $[1/(2l)!\lambda^l]M^{2l}$. Since there is only one trace, this should be taken as a matrix multiplying the rest of the diagram. But by the argument above (2.30), the trace breaks in two. Therefore we see that A_n is equal to $\tilde{A}_n$ plus matrix model corrections,

$$A_n = \sum_{l=0}^{n} \left\langle \frac{1}{N(2l)!\lambda^l} \operatorname{Tr} M^{2l} \right\rangle \tilde{A}_{n-l}. \tag{2.33}$$

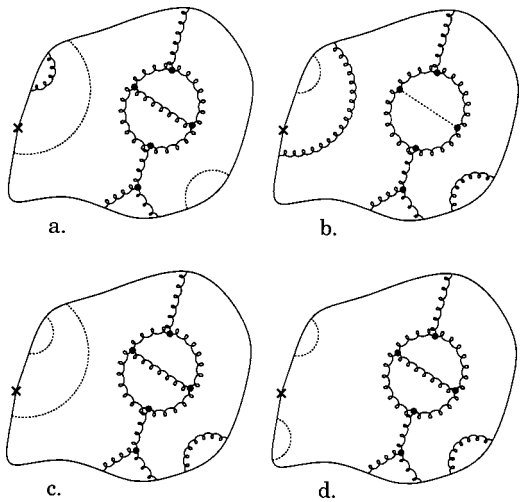

FIG. 3. We show here some diagrams one gets by replacing gluon propagators by total derivatives (dotted lines). Diagrams (a) and (b) will not contribute, since not all the total derivatives hit the inversion point. (c) Does contribute, since all the total derivatives can hit the origin. One gets diagram (d) by doing the same procedure to a sightly different graph. Summing (c), (d) and a few other such graphs gives the matrix model expression at order λ^2 times the rest of the diagram.

Therefore

$$\langle W_C\rangle=\sum_{n=0}^{\infty}A_n\lambda^n=\sum_{n=0}^{\infty}\sum_{l=0}^{n}\left\langle\frac{1}{N(2l)!}\mathrm{Tr}\,M^{2l}\right\rangle\tilde{A}_{n-l}\lambda^{n-1}=\left\langle\frac{1}{N}\mathrm{Tr}\exp(M)\right\rangle\langle\tilde{W}_{\tilde{C}}\rangle. \quad (2.34)$$

The crucial point in the proof is that the total derivative part of the graphs (the matrix model) totally decouple from the rest of the graph. The total derivatives live within an infinitesimal distance from the origin. It is a set of measure zero for any other part of the graph to be in that vicinity, and since the loop is smooth, and the theory is finite, this set of measure zero does not contribute.

The above argument is true for all N, not just planar graphs. Again, one has to note that if the matrix model part has genus p and the rest of the graph is at genus q, the total genus is $p+q$, since those two graphs are totally separated. Also, we assumed here that the matrix model is quadratic, but the statement would be correct regardless of that. Even if the interactions do not vanish, to get a contribution, the entire part of the diagram with interaction has to collapse to the singular point. It would still give a matrix model contribution times the rest of the graph.

III. THE COMPARISON WITH STRING THEORY

The AdS/CFT [2] correspondence allows one to calculate the expectation value of Wilson loops in $\mathcal{N}=4$ SUSYM for large λ from minimal surfaces in AdS space.[3,4] We will now compare our calculation of the ratio of Wilson loops that are related by inversion, as well as the exact expression for a circular Wilson loop, to string theory calculations.

We have shown that a Wilson loop, W_C, along a closed contour C passing through the origin, is related to a Wilson loop, $\tilde{W}_{\tilde{C}}$, along the open line, $\tilde{C}$, obtained by inverting the contour through the origin, by

$$\langle W_C\rangle=F(\lambda,N)\langle\tilde{W}_{\tilde{C}}\rangle. \quad (3.1)$$

We would like to prove the same statement from string theory. A complete proof is beyond our capabilities, since the calculational tools for string perturbation theory in AdS_5 are still undeveloped. However, we are able to give strong evidence from string theory for this relationship, to leading order in $1/\lambda=(l_s/R)^4$, and to all orders in the string coupling, $g_s=\lambda/(4\pi N)$, for arbitrary smooth loops!

A. Circular loops

For circular loops we can perform a precise test of the AdS/CFT correspondence, since we have derived an exact expression for the circular Wilson loop for all λ and N. In string theory, to a given order in $1/N^2$, we expect that the Wilson loop should be given by

$$\langle W_{\mathrm{circle}}\rangle_p=\frac{1}{N^{2p}}e^{-S_p}f_p(\lambda), \quad (3.2)$$

where S_p is the action for a minimal surface ending on the circle with p handles and $f(\lambda)$ would be calculated by evaluating the fluctuations about the minimal surface in powers of α' (or l_s/R, or equivalently $1/\lambda^{1/4}$).

The minimal area surface to leading order in $1/N^2$ can be constructed analytically and yields $S_0=-\sqrt{\lambda}$, it is a smooth, geodesic surface. To higher order in $1/N^2$ we need to find the minimal area surface with handles. It is intuitively obvious that the best we can do is to attach degenerate handles that have no area to the above surface. This is not a smooth surface, but it is the limit of smooth surfaces and has the minimal possible area. If this is the case then $S_p=S_0=-\sqrt{\lambda}$.

To do better than this one would need to evaluate the stringy fluctuations about the minimal surface, in an expansion in α'. This is beyond our capabilities. However, we can determine the overall power of the inverse coupling, $1/(l_s/R)$, that multiplies e^{-S}. We claim that

$$\langle W_{\text{circle}}\rangle_p^{\text{string}} \propto \frac{1}{N^{2p}} \frac{\lambda^{(6p-3)/4}}{p!} e^{\sqrt{\lambda}} \left[1 + O\left(\frac{1}{\sqrt{\lambda}} \right) \right]. \tag{3.3}$$

The factor of $1/p!$ arises since the handles are indistinguishable. We give two arguments for the power of λ in this expression. The string coupling is $g_s^2 \sim \lambda^2/N^2$, but in addition one has to be careful of the contribution of zero modes. The dimension of the moduli space of surfaces of genus p with one boundary is $6p-3$. Since the relevant surfaces are degenerate we have to impose two real constraints for each handle, in addition to the overall 3. Each constraint gives a power of $\lambda^{-1/4}$, from the correct normalization of the zero modes. This gives

$$\left(\frac{\lambda}{N} \right)^{2p} \to \frac{\lambda^{(6p-3)/4}}{N^{2p}}. \tag{3.4}$$

An equivalent calculation comes from the low energy effective supergravity, the degenerate handles are the same as the exchange of supergravity modes. In Ref. 5 the exchange of fields between two widely separated surfaces was calculated. One can redo their calculation for the case at hand, the self interaction of the surface ending on a circle. In their case the coupling of the Kaluza–Klein modes is proportional to $1/N^2$ and the integration over each of the surfaces gives a measure factor of λ.

Therefore the result for well separated surfaces was proportional to λ/N^2. For calculating the self interaction of a single surface we have to use the propagator at short distances, which, in 5 dimensions, has a cubic divergence. Integrating over the surface leaves a linear divergence, which should be cut off at the string scale, giving an extra factor of $R/l_s \sim \lambda^{1/4}$. In addition we should sum over all the KK modes, again imposing a cutoff—the angular momentum cannot exceed R/l_s. This gives the final result $\lambda^{3/2}/N^2$ for each handle.

This power of λ is also confirmed by the *S*-duality argument in the following section.

We can now compare this with the gauge theory result, $\langle W_{\text{circle}}\rangle = F(\lambda, N)$. In Appendix B we examine the large λ behavior of the $1/N^2$ expansion of $F(\lambda, N)$. We show that, order by order in the $1/N^2$ expansion, this function behaves, for large λ, as

$$\langle W_{\text{circle}}\rangle^{\text{gauge}} = F[\lambda, N] = \sum_p \frac{1}{N^{2p}} \frac{e\sqrt{\lambda}}{p!} \sqrt{\frac{2}{\pi}} \frac{\lambda^{(6p-3)/4}}{96^p} \left[1 - \frac{3(12p^2+8p+5)}{40\sqrt{\lambda}} + O\left(\frac{1}{\lambda} \right) \right]. \tag{3.5}$$

Thus we find precise agreement with the string theory calculation, order by order in $1/N^2$, to leading order in $1/\lambda$!

B. *S*-duality

Another very strong test of this expression comes from checking its region of validity. Clearly both the AdS expression (3.3) and the matrix model result (3.5) are valid for $\lambda \gg 1$. If we ignore the $1/\lambda$ correction the matrix model gives

$$\langle W_{\text{circle}}\rangle^{\text{gauge}} \sim \sqrt{\frac{2}{\pi}} \lambda^{-3/4} \exp\left(\sqrt{\lambda} + \frac{\lambda^{3/2}}{96N^2} \right). \tag{3.6}$$

Thus the approximation $\langle W_{\text{circle}}\rangle \sim \exp\sqrt{\lambda}$ is valid as long as $1 \ll \lambda \ll N^2$. The AdS expression is valid only for $\lambda \ll N$, or else string theory is strongly coupled. For $\lambda \gg N$ we should perform an *S*-duality transformation. Under *S*-duality the Wilson loop turns into a 't Hooft loop of the dual theory described by a D1-brane. The action for this configuration is given in terms of the dual couplings $\tilde{g}_s = 1/g_s$ and $\tilde{\lambda} = \lambda/g_s^2$,

$$\langle W_{\text{circle}}\rangle^{\text{dual string}} \sim \exp\frac{\sqrt{\tilde{\lambda}}}{\tilde{g}_s} = \exp\sqrt{\lambda}. \tag{3.7}$$

So the dual D1-brane has the same action as the original fundamental string. This dual description is valid as long as $\tilde{\lambda} \gg 1$, or $\lambda \ll N^2$. We see, therefore, that the range of validity of the two calculations is identical!

This can be regarded as another test of the matrix model expression, and in particular the power of λ accompanying the $1/N^2$ corrections. But it should also be considered a test of *S*-duality in $\mathcal{N}=4$ SUSYM. The matrix model is valid for all values of g, and with the replacement $g \to 4\pi/g$ it gives the value of the 't Hooft loop, which is confirmed by the AdS calculation.

C. Arbitrary loops

This story can be generalized, to some extent, to arbitrary loops. Indeed, a version of this statement for large λ and to lowest order in g_s was made in a footnote in Ref. 8. As shown in Ref. 6, the expectation value of the Wilson loop to leading order in the α' expansion, is

$$\langle W\rangle \propto e^{-S}, \tag{3.8}$$

where the action, *S*, is a Legendre transform of the area of the surface in AdS_5 whose boundary is the loop contour. The Legendre transform removes (for a smooth loop) the divergence in the area. For smooth loops the Legendre transform is equal (asymptotically) to the extrinsic curvature of the boundary κ. Then we can use the Gauss–Bonnet theorem to write the action for the minimal area as

$$S = \frac{\sqrt{\lambda}}{2\pi}\left[\int d^2\sigma\sqrt{g} - \int d\tau\sqrt{\gamma}\kappa\right] = \frac{\sqrt{\lambda}}{2\pi}\int d^2\sigma\sqrt{g}\left(1+\frac{1}{2}R^{(2)}\right) - \sqrt{\lambda}\chi, \tag{3.9}$$

where $R^{(2)}$ is the induced metric and χ the Euler number of the surface (given by this integral expression). It is easy to see that $R^{(2)}$ approaches -2 near the boundary of AdS, so the integral on the right hand side is manifestly convergent.

The action integral is invariant under isometries of AdS including conformal transformations. Since it is manifestly convergent, it is invariant also if the conformal transformation takes a point from finite distance to infinity, or vice versa. What does change in the latter case is the topology of the surface. The Euler number is one for the disk, the appropriate world sheet for a closed Wilson loop W_C. But for the open Wilson loop $\tilde{W}_{\tilde{C}}$ the world sheet is the half plane with Euler number zero. Therefore

$$\langle W_C\rangle = \exp(\sqrt{\lambda})\langle \tilde{W}_{\tilde{C}}\rangle. \tag{3.10}$$

In fact this statement can be generalized to any order in the string coupling, or the $1/N^2$, expansion. This is clearly the case if the minimal surface at higher genus is obtained by adding degenerate handles to the surface of lower genus—the handles do not change the action. But the proof does not require this assumption. To order $1/N^{2p}$ the relevant surface bounding the closed contour is topologically a disk with p handles, for which $\chi = 1-2p$, whereas the surface bounding the open contour is a half plane with p handles, for which $\chi = -2p$. Consequently, to any order in $1/N^2$ and for large λ, we expect from string theory that

$$\langle W_C\rangle = \exp(\sqrt{\lambda}(2p+1-2p))\langle \tilde{W}_{\tilde{C}}\rangle = \exp(\sqrt{\lambda})\langle \tilde{W}_{\tilde{C}}\rangle. \tag{3.11}$$

This is precisely what we find in the gauge theory from (3.1), using the result proved in Appendix B that, to any order in $1/N^2$,

$$F(\lambda,N)\sim e^{\sqrt{\lambda}}, \tag{3.12}$$

for large λ. Thus (3.1) is true to leading order in $1/\lambda$.

Understanding the $1/\lambda$ corrections are more difficult, since we cannot even calculate the expectation value of an arbitrary open loop. Still, the string theory argument leading to (3.3) is general and should apply to any closed curve (as long as there are no new smooth classical solutions at high genus). Therefore we might expect that

$$\langle W_C\rangle_p^{\text{string}}\propto \frac{1}{N^{2p}}\frac{\lambda^{3p/2-3/4}}{p!}e^{-s}\left[1+O\left(\frac{1}{\sqrt{\lambda}}\right)\right]. \tag{3.13}$$

This might look surprising, given that the corresponding open loop $\langle \tilde{W}_{\tilde{C}}\rangle$ is not one. The reason that it works is that the open loop asymptotes to a straight line, so it differs significantly from the BPS straight line only over a compact region. We can expect that the leading behavior of the asymptotically straight line and the true straight line would be the same. If a genus p surface is obtained by adding p degenerate handles, then there is a large probability that they will be attached within the asymptotically straight part of the world sheet, where they will not contribute because of supersymmetry. Therefore, for most of the volume of the moduli space, we will get no enhancement and we might conjecture that to order $1/N^{2p}$,

$$\langle \tilde{W}_{\tilde{C}}\rangle_p^{\text{string}}\propto \frac{1}{N^{2p}}e^{-S-\sqrt{\lambda}}\left[1+O\left(\frac{1}{\sqrt{\lambda}}\right)\right]. \tag{3.14}$$

Under these assumptions, the relation derived from the gauge theory (3.1) will agree with the string theory to all orders in $1/N^2$ for large λ, since

$$\langle W_C\rangle^{\text{string}}\propto\sum_p \frac{1}{N^{2p}}\frac{\lambda^{(6p-3)/4}}{p!}e^{-S}\sim\left[\sum_p \frac{e^{\lambda}}{N^{2p}}\frac{\lambda^{(6p-3)/4}}{p!}\right]\left[\sum_q \frac{1}{N^{2q}}e^{-S-\sqrt{\lambda}}\right]. \tag{3.15}$$

IV. MULTIPLY WOUND LOOPS

The above considerations can be extended to multiply wound Wilson lines or loops. Consider, for example, a Wilson loop consisting of two coincident circles. These can be tied together so that the loop winds twice around a circle, or traced independently. Under an inversion through a point on the circle they go into two coincident parallel straight lines, which are BPS and thus trivial. By the same arguments that we have presented above the evaluation of the multiply wound loops can be expressed in terms of the matrix model.

Consider first two circles on top of each other. If the untraced Wilson loop around the circle is denoted by $\mathcal{W}$, so that the ordinary Wilson loop traced around one circle is $W_1=1/N\langle \mathrm{Tr}\mathcal{W}\rangle$, then the two options for connecting the circles correspond to $W_2=1/N\langle \mathrm{Tr}\mathcal{W}^2\rangle$ and to $W_{1,1}=1/N^2\langle(\mathrm{Tr}\ \mathcal{W})^2\rangle$, respectively. In terms of the matrix model it is clear that

$$W^2=\frac{1}{N}\langle \mathrm{Tr}\exp(2M)\rangle,\quad W_{1,1}=\frac{1}{N^2}\langle[\mathrm{Tr}\exp(M)]^2\rangle. \tag{4.1}$$

The first case, that of a doubly wound loop, is very simple. Scaling $M\to M/2$, we see that the result is the same as the single circle with $\lambda\to 4\lambda$, thus

$$W_2(\lambda,N)=W_1(4\lambda,N)=\frac{1}{N}L_{N-1}^1(-\lambda/N)\exp[\lambda/2N]. \tag{4.2}$$

In the case of the squared singly wound loop we follow the same steps as in Appendix A:

$$W_{1,1}=\frac{1}{Z}\int \mathcal{D}M\left[\frac{1}{N}\mathrm{Tr}\ e^{M}\right]^2 e^{-(2N/\lambda)\mathrm{Tr}\ M^2}$$
$$=\frac{1}{Z}\int dm_i\,\Delta^2(m_i)\left[\frac{1}{N}\sum_i\ e^{m_i}\right]^2 e^{-(2N/\lambda)\Sigma m_i^2}$$
$$=\frac{1}{Z'}\int dm_i\,\Delta^2(m_i)e^{-\Sigma m_i^2}\left[\frac{1}{N}e^{2m_1\sqrt{\lambda/2N}}+\frac{N-1}{N}e^{(m_1+m_2)\sqrt{\lambda/2N}}\right]. \tag{4.3}$$

The first integral is, up to a factor of $1/N$, the same as W_2. The second can be evaluated by expressing, as in Appendix A, the Vandermonde determinant, $\Delta^2(m_i)$, in terms of Hermite polynomials, as

$$\frac{1}{N^2}\int dm\,dm'\sum_{i,j=0}^{N-1}[P_i^2(m)P_j^2(m')-P_i(m)P_j(m)P_i(m')P_j(m')]e^{-(m^2+m'^2)+\sqrt{\lambda/2N}(m+m')}. \tag{4.4}$$

The above integrals can then be done, with the final result being

$$W_{1,1}=\frac{1}{N}W_2+\left(1-\frac{1}{N}\right)(W_1)^2-\frac{2}{N^2}e^{\lambda/4N}\sum_{i=1}^{N-1}\sum_{j=0}^{i-1}\left[L_j^{i-j}\left(-\frac{\lambda}{4N}\right)\right]^2. \tag{4.5}$$

One of the sums in (4.5) can easily be done and the result compared with string theory for large λ. It is trivial to reproduce the correct semiclassical action and it would be interesting to try to account for the factors of λ as well. A similar analysis can be carried out, with increased complication, for loops wound any number of times around the circle. In fact, it does not have to be the exact same circle, one gets the same result from arbitrary loops that are tangent to each other at one point. Under an inversion around the common point they are mapped to a collection of parallel lines which is also a BPS configuration.

These Wilson loops correspond to the most general observables of the matrix model,

$$W_{i_1,i_2,\ldots i_n}\equiv\langle\mathrm{Tr}\exp(i_1M)\mathrm{Tr}\exp(i_2M)\cdots\mathrm{Tr}\exp(i_nM)\rangle, \tag{4.6}$$

and can be used, following the discussion in Refs. 11 and 12, to evaluate the expectation values of Wilson loops in definite representations of $U(N)$. We postpone this analysis for elsewhere.

V. CONCLUSIONS

In this paper we have extended, generalized and outlined a proof for the result of Erickson, Semenoff and Zarembo [1] on the value of the circular Wilson loop in $\mathcal{N}=4$ SUSYM. We showed that the expectation value of a circular BPS-Wilson loop in $\mathcal{N}=4$ SUSYM is determined by an anomaly in the conformal transformation that relates the circular and straight-line loops. As such it can be calculated exactly, to all orders in a $1/N^2$ expansion and to all orders in g^2N. A similar relation was derived between the expectation value of any closed smooth Wilson loop and the loop related to it by an inversion that takes a point along the loop to infinity. Using the AdS/CFT duality, this result yielded a prediction of the value of the string amplitude with a circular boundary to all orders in α' and to all orders in g_s. We then compared this result with string theory, and found that the gauge theory calculation, for large g^2N and to *all* orders in the $1/N^2$ expansion does agree with the leading string theory calculation, to all orders in g_s and to lowest order in α'.

We proved that the anomaly is given by a matrix model, but we leave for future work to complete the proof that all interactions vanish and the matrix model is indeed quadratic. The agreement with the AdS calculation is a very strong indication that the quadratic matrix model is correct, at least for the $\mathcal{N}=4$ theory. In principle the anomaly in other conformal field theories could be described by a more complicated matrix model.

This agreement is remarkable. It is a test of the AdS/CFT correspondence in the regime of strong gauge coupling (small α') and to all orders in $1/N^2$, the string coupling. The result even extends to the S-dual region where the fundamental string is replaced by a D1-brane. This gives strong evidence for the validity of the conjectured AdS/CFT correspondence.

All the calculations in this paper were done for gauge group $U(N)$, but the generalization to $SU(N)$ is trivial. We write the Hermitian matrix M as the sum of a traceless part and the trace times the unit matrix $M=M'+mI_N$. Then

$$\left\langle \frac{1}{N}\mathrm{Tr}\exp M\right\rangle_{U(N)} = \exp\left(\frac{\lambda}{8N^2}\right)\left\langle \frac{1}{N}\mathrm{Tr}\exp M'\right\rangle_{SU(N)}. \tag{5.1}$$

In string theory the difference between $SU(N)$ and $U(N)$ corresponds to the inclusion of some fields that do not have local dynamics, but can be gauged to infinity. In any case the difference is subleading in both N and λ, so it has no consequence on our discussion of the leading behavior for large λ, order by order in $1/N^2$.

It would be very interesting to try to understand the α' corrections to the minimal surface calculation in AdS, in order to compare our exact result with string theory. Consider the leading $N=\infty$ prediction for the circular Wilson loop. Using the asymptotic expansion of the Bessel function, we can write the expectation value of the circular loop as

$$\langle W_{\mathrm{circle}}\rangle^{\mathrm{gauge}} = \sqrt{\frac{2}{\pi}}\frac{e^{\sqrt{\lambda}}}{\lambda^{3/4}}\sum_{k=0}^{\infty}\left(\frac{-1}{2\sqrt{\lambda}}\right)^k\frac{\Gamma(\frac{3}{2}+k)}{k!\Gamma(\frac{3}{2}-k)} - i\sqrt{\frac{2}{\pi}}\frac{e^{-\sqrt{\lambda}}}{\lambda^{3/4}}\sum_{k=0}^{\infty}\left(\frac{1}{2\sqrt{\lambda}}\right)^k\frac{\Gamma(\frac{3}{2}+k)}{k!\Gamma(\frac{3}{2}-k)}. \tag{5.2}$$

The challenge is to reproduce, in an α' expansion, the asymptotic expansion given in (5.2). Note that this asymptotic expansion is not Borel summable. The terms behave as $(k/2\sqrt{\lambda})^k$, to order k. It would be interesting to understand this from the point of view of the world sheet theory. The non-Borel summability, as well as the second term in (5.2), might indicate that there is an instanton contribution to the world sheet amplitude.

Finally, it is interesting that the string theory with a circular boundary is described by the Hermitian matrix model. This model is related to noncritical string theory with $c=-2$.[9] Here it yields a particularly simple observable of the critical superstring theory in the AdS background. It is conceivable that one could derive the matrix model representation of the string amplitude directly, without having to use the duality to gauge theory.

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APPENDIX A: MATRIX MODEL CALCULATION

We wish to evaluate

$$\left\langle \frac{1}{N}\mathrm{Tr}\exp(M)\right\rangle = \frac{1}{Z}\int \mathcal{D}M\,\frac{1}{N}\mathrm{Tr}\exp(M)\exp\left(-\frac{2N}{\lambda}\mathrm{Tr}M^2\right). \tag{A1}$$

First, we do the angular integrations, to rewrite the integral in terms of the eigenvalues of M:

$$\left\langle \frac{1}{N}\mathrm{Tr}\exp(M)\right\rangle = \frac{1}{Z}\int \prod dm_i\,\Delta^2(m_i)\,\frac{1}{N}\sum e^{m_i}\exp\left[-\frac{2N}{\lambda}\sum m_i^2\right]$$
$$= \frac{1}{Z}\int \prod dm_i\,\Delta^2(m_i)\exp\left[\sqrt{\frac{\lambda}{2N}}m_1\right]\exp\left[-\sum m_i^2\right], \tag{A2}$$

where $\Delta(m_i)=\Pi_{i<j}(m_i-m_j)=\det[\{m_i^{j-1}\}]$ is the Vandermonde determinant, and we have rescaled the m_i absorbing the normalization into Z.

Now we use the standard trick, Ref. 10, of rewriting this determinant in terms of orthogonal polynomials. It is clear that, in evaluating the determinant of the matrix $\{m_i^{j-1}\}$, we can replace the row m_i^{j-1}, for a given i, by any polynomial in m_i of rank $j-1$, that starts with m_i^{j-1}. We can choose these polynomials to be orthonormal with respect to the measure $\int dm\exp[-m^2]$, thus rendering the resulting integrals easy. The appropriate polynomials are proportional to the Hermite polynomials,

$$H_n(x)=e^{x^2}\left(-\frac{d}{dx}\right)^n e^{-x^2},\quad \int_{-\infty}^{\infty}dx\,e^{-x^2}H_n(x)H_m(x)=\delta_{nm}2^n n!\sqrt{\pi}. \tag{A3}$$

So we choose the polynomials to be the orthonormalized Hermite polynomials [with respect to the measure $dx\exp(-x^2)$],

$$P_n(x)\equiv\frac{H_n(x)}{\sqrt{2^n n!\sqrt{\pi}}}, \tag{A4}$$

and write $\Delta(m_i)\propto\det[\{P_{j-1}(m_i)\}]$, again absorbing the normalization into Z. The integrals over m_i, $i=2\cdots N$, can easily be done leaving us with

$$\left\langle \frac{1}{N}\mathrm{Tr}\exp(m)\right\rangle = \frac{1}{N}\int_{-\infty}^{\infty}dm\sum_{j=0}^{N-1}P_j(m)^2\exp\left[-m^2+\sqrt{\frac{\lambda}{2N}}m\right]. \tag{A5}$$

Using the integral,

$$\int_{-\infty}^{\infty}dm\,P_j(m)^2\exp\left[-\left(m-\sqrt{\frac{\lambda}{8N}}\right)^2\right]=L_j(-\lambda/4N), \tag{A6}$$

where L_n^m is the Laguerre polynomial $L_n^m(x)=1/n!\,\exp[x]x^{-m}(d/dx)^n(\exp[-x]x^{n+m})$, $(L_n^0=L_n)$, we obtain

$$\left\langle \frac{1}{N}\mathrm{Tr}\exp(M)\right\rangle = \frac{1}{N}\sum_{j=0}^{N-1}L_j(-\lambda/4N)\exp[\lambda/8N]$$
$$= \frac{1}{N}L_{N-1}^1(-\lambda/4N)\exp[\lambda/8N]$$
$$= \frac{2e^{-\lambda/8N}}{N!\sqrt{\lambda/N}}\int_0^{\infty}dt\,e^{-t}t^{N-1/2}I_1(\sqrt{t\lambda/N}). \tag{A7}$$

In order to exhibit the $1/N$ expansion we write (A7) as a power series in λ,

$$\left\langle \frac{1}{N}\mathrm{Tr}\exp(M)\right\rangle = \exp[\lambda/8N]\sum_{k=0}^{N-1}\binom{N}{k+1}\frac{\lambda^k}{4^k N^{k+1}k!}$$

$$= \sum_{n=0}^{\infty}\frac{\lambda^n}{4^n n!(n+1)!}B(n,N), \tag{A8}$$

where

$$B(n,N)\equiv\sum_{k=0}^{n}\frac{n!(n+1)!2^{k-n}(N-1)!}{k!(k+1)!(n-k)!(N-1-k)!N^n}=\frac{(n+1)!}{(2N)^n}F(-n,1-N;2;2), \tag{A9}$$

and F is the hypergeometric function $[F(\alpha,\beta;\gamma;z)=1+(\alpha\beta/\gamma\cdot 1)z+\{[\alpha(\alpha+1)\beta(\beta+1)/[\gamma(\gamma+1)\cdot 2!]\}z^2+\cdots]$. $B(n,N)$ can easily be expanded in a power series in $1/N^2$ to yield

$$B(n,N)=1+\frac{n(n^2-1)}{12N^2}+\frac{(n+1)!}{(n-4)!}\frac{(5n-2)}{1440N^4}+\frac{(n+1)!}{(n-6)!}\frac{(35n^2-77n+12)}{2^7 3^4 5\cdot 7N^6}$$

$$+\frac{(n+1)!}{(n-8)!}\frac{(175n^3-945n^2+1094n-72)}{2^{11}3^5 5^2 7N^8}+\cdots\ . \tag{A10}$$

Using the definition of the Bessel function: $I_n(2x)=\Sigma_{k=0}^{\infty}[x^{n+2k}/k!(n+k)!]$, we can then use this expansion to derive the asymptotic expansion in powers of $1/N$,

$$\left\langle \frac{1}{N}\mathrm{Tr}\exp(M)\right\rangle = \frac{2}{\sqrt{\lambda}}I_1(\sqrt{\lambda})+\frac{\lambda}{48N^2}I_2(\sqrt{\lambda})+\frac{\lambda^2}{1280N^4}I_4(\sqrt{\lambda})+\frac{\lambda^{5/2}}{9216N^4}I_5(\sqrt{\lambda})+\cdots\ . \tag{A11}$$

APPENDIX B: EXPLICIT 1/*N* EXPANSION

We now present a systematic $1/N^2$ expansion of $F(\lambda,N)$. To this end we use the transformation formula, $F(\alpha,\beta;\gamma;z)=(1-z)^{-\alpha}F(\alpha,\gamma-\beta;\gamma;z/(z-1))$, to rewrite

$$B(n,N)=(-)^n\frac{(n+1)!}{(2N)^n}F(-n,N+1;2;2), \tag{B1}$$

and then we use the Gauss recursion relation,

$$(2\alpha-\gamma-\alpha z+\beta z)F(\alpha,\beta;\gamma;z)+(\gamma-\alpha)F(\alpha-1,\beta;\gamma;z)+\alpha(z-1)F(\alpha+1,\beta;\gamma;z)=0,$$

to derive the recursion relation:

$$B(n+1,N)=B(n,N)+[n(n+1)/4N^2]B(n-1,N). \tag{B2}$$

This recursion relation allows us to derive a systematic expansion of $B(n,N)$ in powers of $1/N^2$, starting with $B(0,N)=1$. It is easy to verify from (B2) that

$$B(n,N)=\sum_{k=0}^{\lfloor n/2\rfloor}\frac{b_k(n)}{N^{2k}},$$

where $b_k(n)$ is a polynomial in n of rank $3k$. It is also easy to see that $b_k(n)=0$ for $n=0,1,2,\ldots,2k-1$. We can therefore expand these polynomials in terms of the k polynomials, $(n+1)!/(n-3k+1+i)!$, that vanish for $n\leqslant 2k-1$:

$$b_k(n)=\sum_{i=0}^{k-1}\frac{(n+1)!}{(n-3k+1+i)!}X_k^i. \tag{B3}$$

To determine the X_k^i we use (B2) to derive

$$4X_k^i=\frac{3k-i-2}{3k-i}X_{k-1}^{i-1}+\frac{1}{3k-i}X_{k-1}^i, \tag{B4}$$

which, together with $X_1^0=1/12$, and $X_k^k=0$, can be used to evaluate the X_k^i's. In particular,

$$X_k^0=\frac{1}{12^k k!};\quad X_k^1=\frac{3}{20}\frac{1}{12^{k-1}(k-2)!}. \tag{B5}$$

The advantage of this expansion is that when we plug (B3) into the expression, (A.8), for $F(\lambda,N)$ the sum over n, order by order in $1/N^2$, can easily be performed to derive

$$F(\lambda,N)=\frac{2}{\sqrt{\lambda}}I_1(\sqrt{\lambda})+\sum_{k=1}^{\infty}\frac{1}{N^{2k}}\sum_{i=0}^{k-1}X_k^i\left(\frac{\lambda}{4}\right)^{(3k-i-1)/2}I_{3k-i-1}(\sqrt{\lambda}). \tag{B6}$$

This expression can then be used to determine the large λ behavior of F, order by order in $1/N^2$,

$$F(\lambda,N)=\sum_p\frac{1}{N^{2p}}e^{\sqrt{\lambda}}\sqrt{\frac{2}{\pi}}\frac{\lambda^{(6p-3)/4}}{96^p p!}\left[1-\frac{3(12p^2+8p+5)}{40\sqrt{\lambda}}+O\left(\frac{1}{\lambda}\right)\right]. \tag{B7}$$

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Finite *N* AdS/CFT correspondence for Abelian and non-Abelian orbifolds, and gauge coupling unification

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Although the AdS/CFT correspondence is rigorous only for an infinite $N\to\infty$ stack of D3-branes, it can be fruitfully studied for finite N as a source of gauge structures and choices for chiral fermions and complex scalars which solve the hierarchy problem by a conformal fixed point. We emphasize orbifolds $AdS_5\times S^5/\Gamma$ where the resulting GFT has $\mathcal{N}=0$ supersymmetry. The fact that the complex scalars are prescribed by the construction limits the possible spontaneous symmetry breaking. Both Abelian and non-Abelian Γ are illustrated by simple examples. An accurate $\sin^2\theta$ in electroweak unification can be obtained, suggesting that this approach merits further study. © *2001 American Institute of Physics.*
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I. INTRODUCTION

It has been a challenge over the last fifteen years to make a connection between superstring theory and the real world. The original attempts[1] to identify massless string modes with the familiar degrees of freedom (quarks, gluons, etc.) did not bear fruit so other ideas to make such identification merit exploration.

A very old idea which is basic to string theory is conformal invariance on the world sheet in two dimensions.[2–6] A more recent idea is that conformal invariance in four spacetime dimensions may guide the sought-for connection of superstring, and hence M theory, to observable physics.

Let us briefly outline the basis for AdS/CFT correspondence to set the scene (for a more complete review; see Ref. 7). Consider the type IIB superstring in flat ten-dimensional Minkowski space, and a number N of parallel D3 branes close to each other, filling a $(3+1)$ subspace of the $(9+1)$ spacetime. The system has two types of perturbative excitations: closed and open strings. Closed strings are the excitations in the bulk and open strings end on the D3-branes. At sufficiently low energies ($\ll l_{\text{string}}^{-1}$, the string scale), only massless states play a role. The massless closed string states form a type IIB supergravity multiplet: the massless open string states form an $\mathcal{N}=4$ vector supermultiplet in $(3+1)$ dimensions with interactions described by an $\mathcal{N}=4$ SU(N) supersymmetric gauge theory.

Next consider the same system but in the background of a D3-brane solution of supergravity:

$$ds^2=f^{-1/2}(-dt^2+dx_1^2+dx_2^2+dx_3^2)+f^{1/2}(dr^2+d\Omega_5), \tag{1}$$

with

$$f=1+(R/r)^4 \quad \text{and} \quad R=4\pi g_{\text{string}}(\alpha'_{\text{string}})^2N. \tag{2}$$

In this case, the energy of an object depends on r: if it is E_r at r then at $r=\infty$ it appears redshifted to $E_\infty=f^{-1/4}E_r$ because of the g_{tt} metric component in Eq. (1). Thus to an observer at infinity, the $r\to 0$ excitations in the ''throat'' appear of lowest energy. There are two types of

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massless excitations. In the bulk is the IIB supergravity multiplet interacting via supergravity: in the near-horizon region of the throat where $r \ll R$ and $f \sim (R/r)^4$ the geometry is that of $AdS_5 \times S^5$:

$$ds^2 = \left(\frac{r^2}{R^2}\right)(-dt^2 + dx_1^2 + dx_2^2 + dx_3^2) + \frac{R^2 dr^2}{r^2} + R^2\, d\Omega_5 . \tag{3}$$

In both backgrounds there are two decoupled theories in the low-energy limit. One theory in both cases is supergravity in flat space. It is natural to identify the other two theories: $\mathcal{N}=4$ SU(N) gauge theory in (3+1) spacetime corresponds to type IIB superstring theory on $AdS_5 \times S^5$.

Let us now step back from M theory and address the needs of a theory of the ''real world.''

In particle phenomenology, the impressive success of the standard theory based on SU(3) $\times$SU(2)$\times U(1)$ has naturally led to the question of how to extend the theory to higher energies. One is necessarily led by weaknesses and incompleteness in the standard theory. If one extrapolates the standard theory as it stands one finds (approximate) unification of the gauge couplings at $\sim 10^{16}$ GeV. But then there is the *hierarchy* problem of how to explain the occurrence of the tiny dimensionless ratio $\sim 10^{-14}$ of the weak scale to the unification scale. Inclusion of gravity leads to a *super-hierarchy* problem of the ratio of the weak scale to the Planck scale, $\sim 10^{18}$ GeV, an even tinier $\sim 10^{-16}$. Although this is obviously a very important problem about which conformality by itself is not informative, we shall discuss first the hierarchy rather than the super-hierarchy.

There are four well-defined approaches to the hierarchy problem:

- 1. Supersymmetry
- 2. Technicolor
- 3. Extra dimensions
- 4. Conformality

Supersymmetry has the advantage of rendering the hierarchy technically natural, that once the hierarchy is put into the Lagrangian it need not be retuned in perturbation theory. Supersymmetry predicts superpartners of all the known particles and these are predicted to be at or below a TeV scale if supersymmetry is related to the electroweak breaking. Inclusion of such hypothetical states improves the gauge coupling unification. On the negative side, supersymmetry does not explain the origin of the hierarchy.

Technicolor postulates that the Higgs boson is a fermion–antifermion composite bound by a new (technicolor) strong dynamics at or below the TeV scale. This obviates the hierarchy problem. On the minus side, no simple convincing model of technicolor has been found.

Extra dimensions can have a range as large as $1(\mathrm{TeV})^{-1}$ and the gauge coupling unification can happen quite differently than in only four spacetime dimensions. This replaces the hierarchy problem with a different fine-tuning question of why the extra dimension is restricted to a distance corresponding to the weak interaction scale. There is also a potentially serious problem with the proton lifetime.

Conformality is inspired by the AdS/CFT correspondence discussed above superstring duality and assumes that the particle spectrum of the standard model is enriched such that there is a conformal fixed point of the renormalization group at the TeV scale. Above this scale the coupling do not run so the hierarchy is nullified. Instead, the couplings $\alpha_1^{-1}, \alpha_2^{-1}, \alpha_3^{-1}$ run from low energy up to the TeV scale then combine to one energy-independent $\alpha_{\mathrm{conformal}}^{-1}$ (in most cases equal to α_3^{-1}). It is important to realize that the observed difference between α_1^{-1}, α_2^{-1} and $\alpha_3^{-1} = \alpha_{\mathrm{conformal}}^{-1}$ arise in this approach from the group theory associated with embedding SU(3)$\times$SU(2) $\times U(1)$ in a semi-simple unifying gauge group.

Conformality is the approach followed in this paper. We shall systematically analyze the compactification of the IIB superstring on $AdS_5 \times S^5/\Gamma$ where Γ is a discrete non-Abelian group designed to break all supersymmetries.

Until very recently, the possibility of testing string theory seemed remote, at best. The advent of the AdS/CFT correspondence suggests this point of view may be too pessimistic, since it could lead to ~TeV evidence for strings. With this thought in mind, we are encouraged to build AdS/CFT models with realistic fermionic structure, and reduce to the standard model below ~1 TeV.

Using AdS/CFT duality, one arrives at a class of gauge field theories of special recent interest. The simplest compactification of a ten-dimensional superstring on a product of an AdS space with a five-dimensional spherical manifold leads to an $\mathcal{N}=4$ SU(N) supersymmetric gauge theory, well known to be conformally invariant.[8] By replacing the manifold S^5 by an orbifold S^5/Γ one arrives at less supersymmetries corresponding to $\mathcal{N}=2$, 1 or 0 depending[9] on whether $\Gamma \subset \mathrm{SU}(2)$, SU(3), or $\not\subset \mathrm{SU}(3)$, respectively, where Γ is in all cases a subgroup of SU(4)~SO(6) the isometry of the S^5 manifold.

It was conjectured in Ref. 10 that such SU(N) gauge theories are conformal in the $N\to\infty$ limit. In Ref. 11 it was conjectured that at least a subset of the resultant nonsupersymmetric $\mathcal{N}=0$ theories are conformal even for finite N and that one of this subset provides the right extension of the standard model. Some first steps to check this idea were made in Ref. 12. Model-building based on Abelian Γ was studied further in Refs. 13, 14, arriving in Ref. 15 at an $\mathrm{SU}(3)^7$ model based on $\Gamma = Z_7$ which has three families of chiral fermions, a correct value for $\sin^2\theta$ and a conformal scale ~10 TeV.

II. ABELIAN ORBIFOLDS

Since, in the context of field-string duality, there has been a shift regarding the relationship of gravity to the standard model of strong and electroweak interactions we shall begin by characterizing how gravity fits in, then to suggest more specifically how the standard model fits in to the string framework.

The descriptions of gravity and of the standard model are contained in the string theory. In the string picture in ten spacetime dimensions, or upon compactification to four dimensions, there is a massless spin-two graviton but the standard model is not manifest in the way we shall consider it. In the conformal field theory extension of the standard model, gravity is strikingly absent. The field-string duality does not imply that the standard model already contains gravity and, in fact, it does not.

In the field theory description[11–14] used in this article, one will simply ignore the massless spin-two graviton. Indeed, since we are using the field theory description only below the conformal scale of ~1 TeV (or, as suggested later in this paper, 10 TeV) and forgoing any requirement of grand unification, the hierarchy between the weak scale and theory-generated scales like M_{GUT} or M_{PLANCK} is resolved. Moreover, seeking the graviton in the field theory description is possibly resolvable by going to a higher dimension and restricting the range of the higher dimension. Here we are looking only at the strong and weak interactions at accessible energies below, say, 10 TeV.

Of course, if we ask questions in a different regime, for example about the scattering of particles with center-of-mass energy of the order M_{PLANCK}, then the graviton will become crucial[16,17] and a string, rather than a field, description will be the viable one.

It is important to distinguish between the holographic description of the five-dimensional gravity in $(\mathrm{AdS})_5$ made by the four-dimensional CFT and the origin of the four-dimensional graviton. The latter could be described holographically only by a lower three-dimensional field theory which is not relevant to the real world. Therefore the graviton of our world can only arise by *compactification* of a higher-dimensional graviton. The introduction of gravity must break conformal invariance and it is an interesting question whether this breaking is related to the mass and symmetry-breaking scales in the low-energy theory. That is all I will say about gravity in the present paper; the remainder is on the standard model and its embedding in a CFT.

An alternative to conformality, grand unification with supersymmetry, leads to an impressively accurate gauge coupling unification.[18,19] In particular it predicts an electroweak mixing angle at the Z-pole, $\sin^2\theta = 0.231$. This result may, however, be fortuitous, but rather than abandon

gauge coupling unification, we can rederive $\sin^2\theta=0.231$ in a different way by embedding the electroweak $SU(2)\times U(1)$ in $SU(N)\times SU(N)\times SU(N)$ to find $\sin^2\theta=3/13\simeq 0.231$.[14] This will be a common feature of the models in this paper.

Actually, it may be premature to dismiss as accidental the success of grand unification with $\sin^2\theta$ since the principal topic here (AdS/CFT) teaches us that quite different theoretical descriptions can be ''dual'' and the same may eventually be understood for conformality and grand unification. For example, conformality is compatible with supersymmetry at low-energy.

The conformal theories will be finite without quadratic or logarithmic divergences. This requires appropriate equal numbers of fermions and bosons which can cancel in loops and which occur without the necessity of space–time supersymmetry. As we shall see in one example, it is possible to combine spacetime supersymmetry with conformality but the latter is the driving principle and the former is merely an option: additional fermions and scalars are predicted by conformality in the TeV range,[13,14] but in general these particles are different and distinguishable from supersymmetric partners. The boson–fermion cancellation is essential for the cancellation of infinities, and will play a central role in the calculation of the cosmological constant (not discussed here). In the field picture, the cosmological constant measures the vacuum energy density.

Here we shall focus on Abelian orbifolds characterized by the discrete group Z_p. Non-Abelian orbifolds will be discussed in the next section.

The steps in building a model for the abelian case (parallel steps hold for non-Abelian orbifolds) are the following:

- (1) Choose the discrete group Γ. Here we are considering only $\Gamma=Z_p$. We define $\alpha=\exp(2\pi i/p)$.
- (2) Choose the embedding of $\Gamma\subset SU(4)$ by assigning $\mathbf{4}=(\alpha^{A_1},\alpha^{A_2},\alpha^{A_3},\alpha^{A_4})$ such that $\Sigma_{q=1}^{q=4}A_q=0(\mathrm{mod}\,p)$. To break $\mathcal{N}=4$ supersymmetry to $\mathcal{N}=0$ (or $\mathcal{N}=1$) requires that none (or one) of the A_q is equal to zero (mod p).
- (3) For chiral fermions one requires that $\mathbf{4}\neq\mathbf{4}^*$ for the embedding of Γ in SU(4). The chiral fermions are in the bifundamental representations of $SU(N)^p$,

$$\sum_{i=1}^{i=p}\sum_{q=1}^{q=4}(N_i,\overline{N}_{i+A_q}). \tag{4}$$

  If $A_q=0$ we interpret $(N_i,\overline{N}_i)$ as a singlet plus an adjoint of $SU(N)_i$.
- (4) The **6** of SU(4) is real $\mathbf{6}=(a_1,a_2,a_3,-a_1,-a_2,-a_3)$ with $a_1=A_1+A_2$, $a_2=A_2+A_3$, $a_3=A_3+A_1$ (recall that all components are defined modulo p). The complex scalars are in the bifundamentals,

$$\sum_{i=1}^{i=p}\sum_{j=1}^{j=3}(N_i,\overline{N}_{i\pm a_j}). \tag{5}$$

  The condition in terms of a_j for $\mathcal{N}=0$ is $\Sigma_{j=1}^{j=3}(\pm a_j)\neq 0(\mathrm{mod}\,p)$.[11]
- (5) Choose the N of $\otimes_i SU(Nd_i)$ (where the d_i are the dimensions of the representations of Γ). For the Abelian case where $d_i\equiv 1$, it is natural to choose $N=3$ the largest $SU(N)$ of the standard model (SM) gauge group. For a non-Abelian Γ with $d_i\neq 1$ the choice $N=2$ would be indicated.
- (6) The p quiver nodes are identified as color (C), weak isospin (W), or a third SU(3) (H). This specifies the embedding of the gauge group $SU(3)_C\times SU(3)_W\times SU(3)_H\subset\otimes SU(N)^p$. This quiver node identification is guided by (7), (8) and (9) below.
- (7) The quiver node identification is required to give three chiral families under Eq. (4). It is sufficient to make three of the $(C+A_q)$ to be W and the fourth H, given that there is only one C quiver node, so that there are three $(3,\overline{3},1)$. Provided that $(\overline{3},3,1)$ is avoided by the $(C-A_q)$ being H, the remainder of the three family trinification will be automatic by chiral

anomaly cancellation. Actually, a sufficient condition for three families has been given; it is necessary only that the difference between the number of $(3+A_q)$ nodes and the number of $(3-A_q)$ nodes which are W be equal to three.

- (8) The complex scalars of Eq. (5) must be sufficient for their vacuum expectation values (VEVs) to spontaneously break $SU(3)^p \to SU(3)_C \times SU(3)_W \times SU(3)_H \to SU(3)_C \times SU(2)_W \times U(1)_Y \to SU(3)_C \times U(1)_Q$.
  Note that, unlike grand unified theories (GUTs) with or without supersymmetry, the Higgs scalars are here prescribed by the conformality condition. This is more satisfactory because it implies that the Higgs sector cannot be chosen arbitrarily.
- (9) Gauge coupling unification should apply at least to the electroweak mixing angle $\sin^2\theta = g_Y^2/(g_2^2+g_Y^2) \simeq 0.231$. For trinification $Y = 3^{-1/2}(-\lambda_{8W}+2\lambda_{8H})$ so that $(3/5)^{1/2}Y$ is correctly normalized. If we make $g_Y^2 = (3/5)g_1^2$ and $g_2^2 = 2g_1^2$ then $\sin^2\theta = 3/13 \simeq 0.231$ with sufficient accuracy.
  In the remainder of this section we answer all these steps for the choice $\Gamma = Z_p$ for successive $p = 2,3,\ldots,$ up to $p=7$, then add some concluding remarks.

- **p=2**
  In this case $\alpha = -1$ and therefore one cannot construct any complex **4** of SU(4) with **4**$\neq$**4***. Chiral fermions are therefore impossible.
- **p=3**
  The only possibilities are $A_q = (1,1,1,0)$ or $A_q = (1,1,-1,-1)$. The latter is real and leads to no chiral fermions. The former leaves $\mathcal{N}=1$ supersymmetry and is a simple three-family model[9] by the quiver node identification C-W-H. The scalars $a_j = (1,1,1)$ are sufficient to spontaneously break to the SM. Gauge coupling unification is, however, missing since $\sin^2\theta = 3/8$, in bad disagreement with experiment.
- **p=4**
  The only complex $\mathcal{N}=0$ choice is $A_q = (1,1,1,1)$. But then $a_j = (2,2,2)$ and any quiver node identification such as C-W-H-H has 4 families and the scalars are insufficient to break spontaneously the symmetry to the SM gauge group.
- **p=5**
  The two inequivalent complex choices are $A_q = (1,1,1,2)$ and $A_q = (1,3,3,3)$. By drawing the quiver, however, and using the rules for three chiral families given in (7) above, one finds that the node identification and the prescription of the scalars as $a_j = (2,2,2)$ and $a_j = (1,1,1)$, respectively, does not permit spontaneous breaking to the standard model.
- **p=6**
  Here we can discuss three inequivalent complex possibilities as follows:
  (6A) $A_q = (1,1,1,3)$ which implies $a_j = (2,2,2)$.
  Requiring three families means a node identification C-W-X-H-X-H where X is either W or H. But whatever we choose for the X the scalar representations are insufficient to break $SU(3)^6$ in the desired fashion down to the standard theory. This illustrates the difficulty of model building when the scalars are not in arbitrary representations.
  (6B) $A_q = (1,1,2,2)$ which implies $a_j = (2,3,3)$.
  Here the family number can be only zero, two or four as can be seen by inspection of the A_q and the related quiver diagram. So (6B) is of no phenomenological interest.
  (6C) $A_q = (1,3,4,4)$ which implies $a_j = (1,1,4)$.
  Requiring three families needs a quiver node identification which is of the form *either* C-W-H-H-W-H *or* C-H-H-W-W-H. The scalar representations implied by $a_j = (1,1,4)$ are, however, easily seen to be insufficient to do the required spontaneous symmetry breaking (S.S.B.) for both of these identifications.
- **p=7**
  Having been stymied mainly by the rigidity of the scalar representation for all $p \leqslant 6$, for

$p=7$ there are the first cases which work. Six inequivalent complex embeddings of $Z_7 \subset \mathrm{SU}(4)$ require consideration.
(7A) $A_q=(1,1,1,4) \Rightarrow a_j=(2,2,2)$
For the required nodes C-W-X-H-H-X-H the scalars are *insufficient* for S.S.B.
(7B) $A_q=(1,1,2,3) \Rightarrow a_j=(2,3,3)$
The node identification C-W-H-W-H-H-H leads to a *successful* model.
(7C) $A_q=(1,2,2,2) \Rightarrow a_j=(3,3,3)$
Choosing C-H-W-X-X-H-H to derive three families, the scalars *fail* in S.S.B.
(7D) $A_q=(1,3,5,5) \Rightarrow a_j=(1,1,3)$
The node choice C-W-H-H-H-W-H leads to a *successful* model. This is Model A of Ref. 14.
(7E) $A_q=(1,4,4,5) \Rightarrow a_j=(1,2,2)$
The nodes C-H-H-H-W-W-H are *successful*.
(7F) $A_q=(2,4,4,4) \Rightarrow a_j=(1,1,1)$
Scalars *insufficient* for S.S.B.

The three successful models (7B), (7D) and (7E) lead to an $\alpha_3(M) \simeq 0.07$. Since $\alpha_3(1\ \mathrm{TeV}) \geqslant 0.10$ this suggests a conformal scale $M \simeq 10\ \mathrm{TeV}$.[14] The above models have less generators than an $E(6)$ GUT and thus $\mathrm{SU}(3)^7$ merits further study. It is possible, and under investigation, that non-Abelian orbifolds will lead to a simpler model.

For such field theories it is important to establish the existence of a fixed manifold with respect to the renormalization group. It could be a fixed line but more likely, in the $\mathcal{N}=0$ case, a fixed point. It is known that in the $N \to \infty$ limit the theories become conformal, but although this 't Hooft limit[20] is where the field-string duality is derived we know that finiteness survives to finite N in the $\mathcal{N}=4$ case[8] and this makes it plausible that at least a conformal point occurs also for the $\mathcal{N}=0$ theories with $N=3$ derived above.

The conformal structure cannot by itself predict all the dimensionless ratios of the standard model such as mass ratios and mixing angles because these receive contributions, in general, from soft breaking of conformality. With a specific assumption about the pattern of conformal symmetry breaking, however, more work should lead to definite predictions for such quantities.

III. NON-ABELIAN ORBIFOLDS

Abelian orbifolds lead us to consider the finite N value $N=3$ guided by trinification $\mathrm{SU}(3)^3$ and the fact that all representations of Abelian groups Z_p are one dimensional.

A non-Abelian orbifold can allow the consideration of finite $N=2$ since for a Γ with doublet and singlet representations can lead to a generalization of a left–right structure of the type $\mathrm{SU}(4) \times \mathrm{SU}(2) \times \mathrm{SU}(2)$.

First we remind the reader of available non-Abelian Γ of low order $g \leqslant 31$.

Of the non-Abelian finite groups, the best known are perhaps the permutation groups S_N (with $N \geqslant 3$) of order $N!$ The smallest non-Abelian finite group is S_3 ($\equiv D_3$), the symmetry of an equilateral triangle with respect to all rotations in a three-dimensional sense. This group initiates two infinite series, the S_N and the D_N. Both have elementary geometrical significance since the symmetric permutation group S_N is the symmetry of the N-plex in N dimensions while the dihedral group D_N is the symmetry of the planar N-agon in 3 dimensions. As a family symmetry, the S_N series becomes uninteresting rapidly as the order and the dimensions of the represention increase. Only S_3 and S_4 are of any interest as symmetries associated with the particle spectrum;[21] also, the order (number of elements) of the S_N groups grow factorially with N. The order of the dihedral groups increases only linearly with N and their irreducible representations are all one- and two-dimensional. This is reminiscent of the representations of the electroweak $\mathrm{SU}(2)_L$ used in nature.

Each D_N is a subgroup of $O(3)$ and has a counterpart double dihedral group Q_{2N}, of order $4N$, which is a subgroup of the double covering $\mathrm{SU}(2)$ of $O(3)$.

With only the use of D_N, Q_{2N}, S_N and the tetrahedral group T (of order 12, the even permutations subgroup of S_4) we find 32 of the 45 non-Abelian groups up to order 31, either as simple groups or as products of simple non-Abelian groups with Abelian groups (Note that $D_6 \simeq Z_2 \times D_3, D_{10} \simeq Z_2 \times D_5$ and $D_{14} \simeq Z_2 \times D_7$):

g	
6	$D_3 \equiv S_3$
8	$D_4, Q = Q_4$
10	D_5
12	D_6, Q_6, T
14	D_7
16	$D_8, Q_8, Z_2 \times D_4, Z_2 \times Q$
18	$D_9, Z_3 \times D_3$
20	D_{10}, Q_{10}
22	D_{11}
24	$D_{12}, Q_{12}, Z_2 \times D_6, Z_2 \times Q_6, Z_2 \times T,$
	$Z_3 \times D_4, Z_3 \times Q, Z_4 \times D_3, S_4$
26	D_{13}
28	D_{14}, Q_{14}
30	$D_{15}, D_5 \times Z_3, D_3 \times Z_5$

There remain thirteen others formed by twisted products of Abelian factors. Only certain such twistings are permissable, namely the following (completing all $g \leqslant 31$).

g	
16	$Z_2 \tilde{\times} Z_8$ (two, excluding D_8), $Z_4 \tilde{\times} Z_4$, $Z_2 \tilde{\times} (Z_2 \times Z_4)$ (two)
18	$Z_2 \tilde{\times} (Z_3 \times Z_3)$
20	$Z_4 \tilde{\times} Z_5$
21	$Z_3 \tilde{\times} Z_7$
24	$Z_3 \tilde{\times} Q$, $Z_3 \tilde{\times} Z_8$, $Z_3 \tilde{\times} D_4$
27	$Z_9 \tilde{\times} Z_3$, $Z_3 \tilde{\times} (Z_3 \times Z_3)$

It can be shown that these thirteen exhaust the classification of *all* inequivalent finite groups up to order thirty-one.[22,23]

Of the 45 non-Abelian groups, the dihedrals (D_N) and double dihedrals (Q_{2N}), of order 2N and 4N, respectively, form the simplest sequences. In particular, they fall into subgroups of $O(3)$ and SU(2), respectively, the two simplest non-Abelian continuous groups.

For the D_N and Q_{2N}, the multiplication tables, as derivable from the character tables, are, in general, simple to express. D_N, for odd N, has two singlet representations $1,1'$ and $m=(N-1)/2$ doublets $2_{(j)}$ $(1 \leqslant j \leqslant m)$. The multiplication rules are

$$1' \times 1' = 1; \quad 1' \times 2_{(j)} = 2_{(j)}, \tag{6}$$

$$2_{(i)} \times 2_{(j)} = \delta_{ij}(1+1') + 2_{(\min[i+j, N-i-j])} + (1-\delta_{ij}) 2_{(|i-j|)}. \tag{7}$$

For even N, D_N has four singlets $1,1',1'',1'''$ and $(m-1)$ doublets $2_{(j)}$ $(1 \leqslant j \leqslant m-1)$ where $m=N/2$ with multiplication rules:

$$1' \times 1' = 1'' \times 1'' = 1''' \times 1''' = 1, \tag{8}$$

$$1' \times 1'' = 1'''; 1'' \times 1''' = 1'; 1''' \times 1' = 1'', \tag{9}$$

$$1' \times 2_{(j)} = 2_{(j)}, \tag{10}$$

$$1'' \times 2_{(j)} = 1''' \times 2_{(j)} = 2_{(m-j)}, \tag{11}$$

$$2_{(j)} \times 2_{(k)} = 2_{|j-k|} + 2_{(\min[j+k, N-j-k])} \tag{12}$$

[if $k \neq j, (m-j)$],

$$2_{(j)} \times 2_{(j)} = 2_{(\min[2j, N-2j])} + 1 + 1' \tag{13}$$

(if $j \neq m/2$),

$$2_{(j)} \times 2_{(m-j)} = 2_{|m-2j|} + 1'' + 1''' \tag{14}$$

(if $j \neq m/2$),

$$2_{m/2}\times 2_{m/2}=1+1'+1''+1'''. \tag{15}$$

This last case is possible only if m is even and hence if N is divisible by *four*.

For Q_{2N}, there are four singlets $1,1',1'',1'''$ and $(N-1)$ doublets $2_{(j)}$ $(1\leqslant j\leqslant(N-1))$.

The singlets have the multiplication rules:

$$1\times 1=1'\times 1'=1, \tag{16}$$

$$1''\times 1''=1'''\times 1'''=1', \tag{17}$$

$$1'\times 1''=1''';1'''\times 1'=1'', \tag{18}$$

for $N=(2k+1)$ but are identical to those for D_N when $N=2k$.

The products involving the $2_{(j)}$ are identical to those given for D_N (N even) above.

This completes the multiplication rules for 19 of the 45 groups. The complete multiplication tables for all the non-Abelian groups with order $g\leqslant 31$ are provided in Appendix A of Ref. 24.

Mathematical theorem: *A* pseudoreal 4 of SU(4) cannot yield chiral fermions

In Ref. 13 it was proved that if the embedding in SU(4) is such that the **4** is real, the resultant fermions are always nonchiral. It was implied there that the converse holds, that if **4** is complex, $\mathbf{4}=\mathbf{4}^*$, then the resulting fermions are necessarily chiral. Actually for $\Gamma\subset$SU(2) one encounters the intermediate possibility that the **4** is *pseudoreal*. In the present section we shall show that if **4** is pseudoreal then the resultant fermions are necessarily nonchiral. The converse now holds: if the **4** is neither real nor pseudoreal then the resultant fermions are chiral.

For $\Gamma\subset$SU(2) it is important that the embedding be consistent with the chain $\Gamma\subset$SU(2)$\subset$SU(4), otherwise the embedding is not a consistent one. One way to see the inconsistency is to check the reality of the $\mathbf{6}=(\mathbf{4}\otimes\mathbf{4})_{\text{antisymmetric}}$. If $\mathbf{6}\neq\mathbf{6}^*$ then the embedding is clearly improper. To avoid this inconsistency it is sufficient to include in the **4** of SU(4) only complete irreducible representations of SU(2).

An explicit example will best illustrate this propriety constraint on embeddings. Let us consider $\Gamma=Q_6$, the dicyclic group of order $g=12$. This group has six inequivalent irreducible representations: $1,1',1'',1''',2_1,2_2$. The 1, $1'$, 2_1 are real. The $1''$ and $1'''$ are a complex conjugate pair, The 2_2 is pseudoreal. To embed $\Gamma=Q_6\subset$SU(4) we must choose from the special combinations which are complete irreducible representations of SU(2) namely 1, $2=2_2$, $3=1'+2_1$ and $4=1''+1'''+2_2$. In this way the embedding either makes the **4** of SU(4) real, e.g., $4=1+1'+2_1$ and the theorem of Ref. 13 applies, and nonchirality results, or the **4** is pseudoreal, e.g., $4=2_2+2_2$. In this case one can check that the embedding is consistent because $(\mathbf{4}\otimes\mathbf{4})_{\text{antisymmetric}}$ is real. But it is equally easy to check that the product of this pseudoreal **4** with the complete set of irreducible representations of Q_6 is again real and that the resultant fermions are nonchiral.

The lesson is the following.

To obtain chiral fermions from compactification on $AdS_5\times S_5/\Gamma$, *the embedding of* Γ *in* SU(4) *must be such that the* 4 *of* SU(4) *is neither real nor pseudoreal.*

Now we are ready for a successful example.[23,24]

Group 24/7; also designated $D_4\times Z_3$

This has twelve singlets $1_1\alpha^i,1_2\alpha^i,1_3\alpha^i,1_4\alpha^i$ $(i=0-2)$ and three doublets $2\alpha^i$ $(i=0-2)$; here $\alpha=\exp(i\pi/3)$. The embedding $\mathbf{4}=(1_1\alpha,1_2,2\alpha)$ was studied in detail in a previous article[23] where it was shown how it can lead to precisely three chiral families in the standard model. For completeness we include the table[24] for the chiral fermions (it was presented in a different equivalent way in Ref. 23):

	1_1	1_2	1_3	1_4	2	$1_1\alpha$	$1_2\alpha$	$1_3\alpha$	$1_4\alpha$	2α	$1_1\alpha^2$	$1_2\alpha^2$	$1_3\alpha^2$	$1_4\alpha^2$	$2\alpha^2$
1_1		×				×				×					
1_2	×						×			×					
1_3				×				×		×					
1_4			×						×	×					
2					×	×	×	×	×	×					
$1_1\alpha$							×				×				×
$1_2\alpha$						×						×			×
$1_3\alpha$									×				×		×
$1_4\alpha$								×						×	×
2α										×	×	×	×	×	×
$1_1\alpha^2$	×				×							×			
$1_2\alpha^2$		×			×						×				
$1_3\alpha^2$			×		×									×	
$1_4\alpha^2$				×	×								×		
$2\alpha^2$	×	×	×	×	×										×

By identifying SU(4) with the diagonal subgroup of $SU(4)_{2,3}$, breaking $SU(4)_1$ to $SU(2)'_L \times SU(2)'_R$, then identifying $SU(2)_L$ with the diagonal subgroup of $SU(2)_{6,7,8}$ and $SU(2)'_L$ and $SU(2)_R$ with the diagonal subgroup of $SU(2)_{10,11,12}$ and $SU(2)'_R$ then leads to a three-family model.

This model is especially interesting because, uniquely among the large number of models examined in this study, the prescribed scalars are sufficient to break the gauge symmetry to that of the standard model with three chiral families.

IV. GAUGE COUPLING UNIFICATION

Most of the research beyond the standard model[25] is motivated by the hierarchy problem and uses the two assumptions of grand unification and low-energy (~TeV) supersymmetry. This is, in turn, driven largely by the successful prediction of one number, $\sin^2\theta$ of the electroweak mixing angle θ. It is proposed to replace the two assumptions of grand unification and low-energy supersymmetry by one assumption, conformality. It therefore is important to show that $\sin^2\theta$ can be derived from conformality alone; that is our principal objective in this section.

Before entering into conformality, let us briefly review the alternative. The experimental data give couplings at the Z pole of[26] $\alpha_3 = 0.118 \pm 0.003, \alpha_2 = 0.0338, \alpha_1 = \frac{5}{3}\alpha'_Y = 0.0169$ (where the

errors on $\alpha_{1,2}$ are less than 1%) and $\sin^2\theta=\alpha_Y'/(\alpha_2+\alpha_Y')=0.231$ with an error of less than 0.001. Note that α_2/α_1 is very nearly two; this will be used later. The RGEs for the supersymmetric grand unification[27,28] are

$$\frac{1}{\alpha_i(M_G)}=\frac{1}{\alpha_i(M_Z)}-\frac{b_i}{2\pi}\ln\left(\frac{M_G}{M_Z}\right). \tag{19}$$

Using the MSSM values $b_i=(6\frac{3}{5},1,-3)$ and substituting $\alpha_{2,3}$ at $M_Z=91.187\,\mathrm{GeV}$ gives $M_G=2.4\times10^{16}\,\mathrm{GeV}$ and $\alpha_{2,3}(M_G)^{-1}=24.305$. Using Eq. (19) with $i=1$ now predicts $\alpha_1(M_Z)=59.172$ and hence $\sin^2\theta=0.231$; this is impressive agreement with experiment and is sometimes presented as the accurate meeting of three straight lines on a $\alpha_i^{-1}(\mu)$ vs the $\ln\mu$ plot.[18,19]

As we have seen above, the relationship of the Type IIB superstring to conformal gauge theory in $d=4$ gives rise to an interesting class of gauge theories. Choosing the simplest compactification[10] on $\mathrm{AdS}_5\times S_5$ gives rise to an $\mathcal{N}=4$ SU(N) gauge theory which is known to be conformal due to the extended global supersymmetry and nonrenormalization theorems. All of the RGE β-functions for this $\mathcal{N}=4$ case are vanishing in perturbation theory. It is possible to break the $\mathcal{N}=4$ to $\mathcal{N}=2,1,0$ by replacing S_5 by an orbifold S_5/Γ where Γ is a discrete group with $\Gamma\subset\mathrm{SU}(2),\subset\mathrm{SU}(3),\not\subset\mathrm{SU}(3)$, respectively.

In building a conformal gauge theory model,[11–13] the steps are the following: (1) Choose the discrete group Γ; (2) embed $\Gamma\subset\mathrm{SU}(4)$; (3) choose the N of SU(N); and (4) embed the standard model $\mathrm{SU}(3)\times\mathrm{SU}(2)\times U(1)$ in the resultant gauge group $\otimes\mathrm{SU}(N)^p$ (quiver node identification). Here we shall look only at Abelian $\Gamma=Z_p$ and define $\alpha=\exp(2\pi i/p)$. It is expected from the string-field duality that the resultant field theory is conformal in the $N\to\infty$ limit, and will have a fixed manifold, or at least a fixed point, for N finite.

Before focusing on $\mathcal{N}=0$ nonsupersymmetric cases, let us first examine an $\mathcal{N}=1$ model first put forward in Ref. 9. The choice is $\Gamma=Z_3$ and the **4** of SU(4) is $\mathbf{4}=(1,\alpha,\alpha,\alpha^2)$. Choosing $N=3$, this leads to the three chiral families under $\mathrm{SU}(3)^3$ trinification,[29]

$$(3,\bar{3},1)+(1,3,\bar{3})+(\bar{3},1,3). \tag{20}$$

In this model it is interesting that the number of families arises as 4-1=3, the difference between the 4 of SU(4) and $\mathcal{N}=1$, the number of unbroken supersymmetries. However this model has no gauge coupling unification; also, keeping $\mathcal{N}=1$ supersymmetry is against the spirit of the conformality approach. We now present three examples, Models A, B and C, which accommodate three chiral families, break all supersymmetries ($\mathcal{N}=0$), and possess gauge coupling unification, including the correct value of the electroweak mixing angle.

Model A. Choose $\Gamma=Z_7$, embed the 4 of SU(4) as $(\alpha^2,\alpha^2,\alpha^{-3},\alpha^{-1})$ and choose $N=3$ to aim at a trinification $\mathrm{SU}(3)_C\times\mathrm{SU}(3)_W\times\mathrm{SU}(3)_H$.

The seven nodes of the quiver diagram will be identified as C-H-W-H-H-H-W.

The behavior of the 4 of SU(4) implies that the bifundamentals of chiral fermions are in the representations

$$\sum_{j=1}^{7}\left[2(N_j,\bar{N}_{j+2})+(N_j,\bar{N}_{j-3})+(N_j,\bar{N}_{j-1})\right]. \tag{21}$$

Embedding the C, W and H SU(3) gauge groups as indicated by the quiver mode identifications then gives the seven quartets of irreducible representations:

$$\begin{aligned}&[3(3,\bar{3},1)+(3,1,\bar{3})]_1+[3(1,1,1+8)+(\bar{3},1,3)]_2+[3(1,3,\bar{3})+(1,1+8,1)]_3\\&\quad+[(2(1,1,1+8)+(1,\bar{3},3)+(\bar{3},1,3)]_4+[2(1,1,1+8)+2(1,\bar{3},3)]_5\\&\quad+[2(\bar{3},1,3)+(1,1,1+8)+(1,\bar{3},3)]_6+[4(1,3,\bar{3})]_7.\end{aligned} \tag{22}$$

Combining terms gives, aside from (real) adjoints and overall singlets,

$$3(3,\overline{3},1)+4(\overline{3},1,3)+(3,1,\overline{3})+7(1,3,\overline{3})+4(1,\overline{3},3). \tag{23}$$

Cancelling the real parts (which acquire Dirac masses at the conformal symmetry breaking scale) leaves under trinification $\mathrm{SU}(3)_C\times\mathrm{SU}(3)_W\times\mathrm{SU}(3)_H$,

$$3[(3,\overline{3},1)+(1,3,\overline{3})+(\overline{3},1,3)], \tag{24}$$

which are the desired three chiral families.

Given the embedding of Γ in SU(4) it follows that the 6 of SU(4) transforms as $(\alpha^4,\alpha,\alpha,\alpha^{-1},\alpha^{-1},\alpha^{-4})$. The complex scalars therefore transform as

$$\sum_{j=1}^{7}[(N_j,\overline{N}_{j\pm4})+2(N_j,\overline{N}_{j\pm1})]. \tag{25}$$

These bifundamentals can by their VEVS break the symmetry $\mathrm{SU}(3)^7=\mathrm{SU}(3)_C\times\mathrm{SU}(3)_W^2\times\mathrm{SU}(3)_H^4$ down to the appropriate diagonal subgroup $\mathrm{SU}(3)_C\times\mathrm{SU}(3)_W\times\mathrm{SU}(3)_H$.

Now to the final aspect of Model A which is its motivation, the gauge coupling unification. The embedding in $\mathrm{SU}(3)^7$ *of* $\mathrm{SU}(3)_C\times\mathrm{SU}(3)_W^2\times\mathrm{SU}(3)_H^4$ *means that the couplings* $\alpha_1,\alpha_2,\alpha_3$ *are in the ratio* $\alpha_1/\alpha_2/\alpha_3=1/2/4$. *Using the phenomenological data given at the beginning, this implies that* $\sin^2\theta=0.231$.

On the other hand, the QCD coupling is $\alpha_3=0.0676$ which is too low unless the conformal scale is at least 10 TeV. We prefer a scale $\sim$1 TeV for conformal breaking where α_3 is nearer to 0.10. This motivates our Models B and C below which have larger α_3 but are otherwise more complicated.

Model B. Choose $\Gamma=Z_{10}$ and embed $Z_{10}\subset\mathrm{SU}(4)$ such that $4=(\alpha^4,\alpha^4,\alpha^{-3},\alpha^{-5})$. The chiral fermions are therefore

$$\sum_{j=1}^{10}[2(N_j,\overline{N}_{j+4})+(N_j,\overline{N}_{j-3})+(N_j,\overline{N}_{j-5})]. \tag{26}$$

To attain trinification we identify the quiver nodes as C-H-H-H-W-W-H-W-H-H and then the chiral fermions are in the ten quartets of irreducible representations.

$$\begin{aligned}&[4(3,\overline{3},1)]_1+[2(1,\overline{3},3)+(1,1,1+8)]_2+[2(1,1,1+8)+(1,\overline{3},3)]_3+[2(1,\overline{3},3)+(\overline{3},1,3)\\&\quad+(1,1,1+8)]_4+[4(1,3,\overline{3})]_5+[3(1,3,\overline{3})+(\overline{3},3,1)]_6+[2(\overline{3},1,3)+(1,1,1+8)]_7\\&\quad+[3(1,3,\overline{3})+(1,1+8,1)]_8+[3(1,1,1+8)+(1,\overline{3},3)]_9+[3(1,1,1+8)+(1,\overline{3},3)]_{10}.\end{aligned} \tag{27}$$

Removing the (real) octets and singlets leaves

$$4(3,\overline{3},1)+(\overline{3},3,1)+3(\overline{3},1,3)+10(1,3,\overline{3})+7(1,\overline{3},3), \tag{28}$$

so that the chiral (complex) part is again

$$3[(3,\overline{3},1)+(1,3,\overline{3})+(\overline{3},1,3)], \tag{29}$$

which are three chiral families.

The 6 of SU(4) transforms under $\Gamma=Z_{10}$ as $6=(\alpha^8,\alpha,\alpha,\alpha^{-1},\alpha^{-1},\alpha^{-8})$ and so the complex scalars are

$$\sum_{j=1}^{10} [(n_j, \overline{N}_{j\pm 8}) + 2(N_j, \overline{N}_{j\pm 1})]. \tag{30}$$

With the given quiver node identification VEVs for these scalars can break $SU(3)^{10} = SU(3)_C \times SU(3)_W^3 \times SU(3)_H^6$ to the diagonal subgroup $SU(3)_C \times SU(3)_W \times SU(3)_H$.

The couplings $\alpha_1, \alpha_2, \alpha_3$ are in the ratio $\alpha_1/\alpha_2/\alpha_3 = 1/2/6$ corresponding to $\sin^2\theta = 0.231$ and $\alpha_3 = 0.101$. This is within the range of a TeV conformal breaking scale. Nevertheless, it is numerically irresistible to notice that the Z-pole values satisfy $\alpha_1/\alpha_2/\alpha_3 = 1/2/7$ which leads naturally to Model C.

Model C. Choose $\Gamma = Z_{23}$ and embed in SU(4) by $4 = (\alpha^6, \alpha^6, \alpha^{-5}, \alpha^{-7})$. Given this embedding the quiver nodes can be chosen as C-C-X-X-X-H-H-W-H-X-X-X-X-X-X-W-H-H-W-X-X-X where the thirteen X's denote any distribution of four W's and nine H's that allows breaking by the complex scalars cited below. The quiver is arranged such that according to the rule of $(3_C - \overline{3}_W)$ minus $(3_W - \overline{3}_C)$ there are three chiral families. [The model in Ref. 13 did not follow this rule and has two families.] Note that because of anomaly cancellation and the occurrence of only bifundamentals the remainder of trinification is automatic and need not be checked in every case.

The chiral families are as in Models A and B.

The 6 of SU(4) transforms as $(\alpha^{12}, \alpha, \alpha, \alpha^{-1}, \alpha^{-1}, \alpha^{-12})$. This implies complex scalars whose VEVs can break $SU(3)^{23} = SU(3)_C^2 \times SU(3)_W^7 \times SU(3)_W^{14}$ to $SU(3)_C \times SU(3)_W \times SU(3)_H$ with a suitable distribution of W and H nodes on the quiver.

With this choice of diagonal subgroups the couplings are in the ratio $\alpha_1/\alpha_2/\alpha_3 = 1/2/7$ corresponding to $\sin^2\theta = 0.231$ and $\alpha_3 = 0.118$ which coincide with the Z-pole values.

In this section, we have given three examples of building conformal models from Abelian Γ with acceptable values of the couplings at the conformal scale, assuming that the SU(3) gauge couplings are all equal at the conformal scale. Model A is the simplest but its α_3 is too small unless the conformal scale is taken up to at least 10 TeV. Models B and C can accommodate a lower conformal scale but are more complicated.

There are two features of conformal models which bear repetition.

(1) Bifundamentals prohibit representations like (8,2) or (3,3) in the standard model consistent with nature.

(2) Charge quantization is incorporated since the Abelian $U(1)_Y$ group has a positive-definite β-function and cannot be conformal until it is embedded in a non-Abelian group.

There are three questions which merit further investigation.

(1) The first question bears on whether there is a fixed manifold (line, plane, ...) with respect to the renormalization group or only a fixed point which is, in any case, sufficient to apply our conformality constraints. In perturbation theory, do the β-functions vanish?

(2) Are the additional particles necessary to render the standard model conformal consistent with the stringent constraints imposed by the precision electroweak data?

(3) Coefficients of dimension-4 operators are prescribed by group theory and all dimensionless properties such as quark and lepton mass ratios and mixing angles are calculable. Do these work and, if not, can one refine the model-building to obtain a best fit?

V. DISCUSSION

String theory has existed for over thirty years and its connection with the real world (at least for ten-/eleven-dimensional versions) is unknown despite a multitude of attempts. The AdS/CFT correspondence offers, in our opinion, the most promising approach presently available to relate string theory to observable physics.

The use of the AdS/CFT correspondence involves the step of, in the first order, dropping the gravitational interaction. In any foreseeable high-energy experiment gravity will be negligible so the approximation is reasonable. On the other hand, if the particles predicted by the conformality

approach discussed in this article were to be discovered in the next (TeV) energy regime, it would provide support for the string approach, including as a theory of quantum gravity.

Whether or not string theory is the correct unifying theory with gravity, it does provide through the AdS/CFT correspondence very promising ideas of how to write conformal theories in four space-time dimensions with particular semi-simple gauge groups, chiral fermions and complex scalars and one of these theories could be the correct direction to proceed.

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Strings in AdS_3 and the SL(2,R) WZW model. I: The spectrum

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In this paper we study the spectrum of bosonic string theory on AdS_3. We study classical solutions of the SL(2,R) WZW model, including solutions for long strings with nonzero winding number. We show that the model has a symmetry relating string configurations with different winding numbers. We then study the Hilbert space of the WZW model, including all states related by the above symmetry. This leads to a precise description of long strings. We prove a no-ghost theorem for all the representations that are involved and discuss the scattering of the long string. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1377273]

I. INTRODUCTION

In this paper we study the spectrum of critical bosonic string theory on $AdS_3 \times \mathcal{M}$ with NS–NS backgrounds, where $\mathcal{M}$ is a compact space. Understanding string theory on AdS_3 is interesting from the point of view of the AdS/CFT correspondence since it enables us to study the correspondence beyond the gravity approximation. Another motivation is to understand string theory on a curved space–time, where the timelike component g_{00} of the metric is nontrivial.

This involves understanding the SL(2,R) WZW model. In this paper, we always consider the case when the target space is the universal cover of the SL(2,R) group manifold so that the timelike direction is noncompact. The states of the WZW model form representations of the current algebras $\widehat{\mathrm{SL}}(2,R)_L \times \widehat{\mathrm{SL}}(2,R)_R$. Once we know which representations of these algebras appear, we can find the physical states of a string in AdS_3 by imposing the Virasoro constraints on the representation spaces. The problem is to find the set of representations that one should consider. In WZW models for compact groups, the unitarity restricts the possible representations.[1] Representations of $\widehat{\mathrm{SL}}(2,R)$, on the other hand, are not unitary except for the trivial representation. Of course this is not a surprise; the physical requirement is that states should have non-negative norms only after we impose the Virasoro constraints. Previous work on the subject[2–10] typically considered representations with L_0 bounded below and concluded that the physical spectrum does not contain negative norm states if there is the restriction $0<j<k/2$ on the SL(2,R) spin j of the representation; the spin of the SL(2,R) is roughly the mass of the string state in AdS_3.

This restriction raises two puzzles. One is that it seems to imply an upper bound on the mass of the string states in AdS_3 so that the internal energy of the string could not be too high. For example, if the compact space $\mathcal{M}$ has a nontrivial 1-cycle, we find that there is an upper bound on the winding number on the cycle. This restriction, which is independent of the string coupling, looks very arbitrary and raises doubts about the consistency of the theory. The second puzzle is that, on physical grounds, we expect that the theory contains states corresponding to the long strings of Refs. 11 and 12. These are finite energy states where we have a long string stretched

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close to the boundary of AdS_3. These states are not found in any representation with L_0 bounded below. In this paper, we propose that the Hilbert space of the WZW model includes a new type of representations, and we show that this proposal resolves both the puzzles. In these new representations, L_0 is not bounded below. They are obtained by acting on the standard representations by elements of the loop group that are not continuously connected to the identity, through an operation called spectral flow. These representations in the SL(2,R) WZW model have also been considered, with some minor variations, in Refs. 13 and 14. The authors of these papers were motivated by finding a modular invariant partition function. They were, however, considering the case when the target space is SL(2,R) group manifold and not its universal cover.

Throughout this paper, we consider AdS_3 in global coordinates, which do not have a coordinate horizon. In these coordinates, the unitarity issue becomes clearer since strings cannot fall behind any horizon. The interested reader could refer to Refs. 15–17 for studies involving AdS_3 in Poincaré coordinates. From the point of view of the AdS/CFT correspondence, it is the spectrum of strings on AdS_3 in the global coordinates that determines the spectrum of conformal dimensions of operators in the boundary CFT, though in principle the same information could be extracted from the theory in Poincare coordinates.

In order to completely settle the question of consistency of the SL(2,R) WZW model, one needs to show that the OPE of two elements of the set of representations that we consider contains only elements of this set. We plan to discuss this issue in our future publication.

The organization of this paper is as follows: In Sec. II, we study classical solutions of the SL(2,R) WZW model and we show that the model has a spectral flow symmetry which relates various solutions. In Sec. III, we do a semiclassical analysis and have the first glimpse of what happens when we raise the internal excitation of the string beyond the upper bound implied by the restriction $j<k/2$. In Sec. IV, we study the full quantum problem and we propose a set of representations that gives a spectrum for the model with the correct semiclassical limits. In Sec. V, we briefly discuss scattering amplitudes involving the long strings. We conclude the paper with a summary of our results in Sec. VI. In Appendix A, we extend the proof of the no-ghost theorem for the representations we introduced in Sec. IV. In Appendix B, we study the one-loop partition function in AdS_3 with the Lorentzian signature metric and show how the sum over spectral flow reproduces the result[18] after taking an Euclidean signature metric, up to contact terms in the modular parameters of the worldsheet.

II. CLASSICAL SOLUTIONS

We start by choosing a parameterization of the SL(2,R) group element as

$$\begin{aligned} g &= e^{iu\sigma_2} e^{\rho\sigma_3} e^{iv\sigma_2} \\ &= \begin{pmatrix} \cos t \cosh\rho + \cos\phi \sinh\rho & \sin t \cosh\rho - \sin\phi \sinh\rho \\ -\sin t \cosh\rho - \sin\phi \sinh\rho & \cos t \cosh\rho - \cos\phi \sinh\rho \end{pmatrix}. \end{aligned} \tag{1}$$

Here $\sigma^i (i=1,2,3)$ are the Pauli matrices $[\sigma_1=\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$, $\sigma_2=\left(\begin{smallmatrix}0&-i\\i&0\end{smallmatrix}\right)$, and $\sigma_3=\left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)]$, and we set

$$u=\tfrac{1}{2}(t+\phi), \quad v=\tfrac{1}{2}(t-\phi). \tag{2}$$

Another useful parameterization of g is

$$g=\begin{pmatrix} X_{-1}+X_1 & X_0-X_2 \\ -X_0-X_2 & X_{-1}-X_1 \end{pmatrix}, \tag{3}$$

with

$$X_{-1}^2+X_0^2-X_1^2-X_2^2=1. \tag{4}$$

This parameterization shows that the SL(2,R) group manifold is a three-dimensional hyperboloid. The metric on AdS_3,

$$ds^2 = -dX_{-1}^2 - dX_0^2 + dX_1^2 + dX_2^2,$$

is expressed in the global coordinates (t, ϕ, ρ) as

$$ds^2 = -\cosh^2\rho dt^2 + d\rho^2 + \sinh^2\rho d\phi^2. \tag{5}$$

We will always work on the universal cover of the hyperboloid (4), and t is noncompact.

Our theory has the WZW action,

$$S = \frac{k}{8\pi\alpha'}\int d^2\sigma\,\mathrm{Tr}(g^{-1}\partial g g^{-1}\partial g) + k\Gamma_{\mathrm{WZ}}. \tag{6}$$

The level k is not quantized since H^3 vanishes for SL(2,R). The semiclassical limit corresponds to large k. We define the right and left moving coordinates on the worldsheet as,

$$x^{\pm} = \tau \pm \sigma, \tag{7}$$

where σ is periodic with the period 2π. This action has a set of conserved right and left moving currents

$$J_R^a(x^+) = k\,\mathrm{Tr}(T^a\partial_+ g g^{-1}),\quad J_L^a(x^-) = k\,\mathrm{Tr}(T^a * g^{-1}\partial_- g), \tag{8}$$

where T^a are a basis for the SL(2,R) Lie algebra. It is convenient to take them as

$$T^3 = -\frac{i}{2}\sigma^2,\quad T^{\pm} = \frac{1}{2}(\sigma^3 \pm i\sigma_1).$$

In terms of our parameterization, the currents are expressed as

$$\begin{aligned} J_R^3 &= k(\partial_+ u + \cosh 2\rho\,\partial_+ v),\\ J_R^{\pm} &= k(\partial_+\rho \pm i\sinh 2\rho\,\partial_+ v)e^{\mp i2u}, \end{aligned} \tag{9}$$

and

$$\begin{aligned} J_L^3 &= k(\partial_- v + \cosh 2\rho\,\partial_- u)\\ J_L^{\pm} &= k(\partial_-\rho \pm i\sinh 2\rho\,\partial_- u)e^{\mp i2v}. \end{aligned} \tag{10}$$

The zero modes of $J_{R,L}^3$ are related to the energy E and angular momentum l in AdS_3 as

$$\begin{aligned} J_0^3 &= \int_0^{2\pi}\frac{dx^+}{2\pi}J_R^3 = \frac{1}{2}(E+l),\\ \overline{J}_0^3 &= \int_0^{2\pi}\frac{dx^-}{2\pi}J_L^3 = \frac{1}{2}(E-l). \end{aligned} \tag{11}$$

The second Casimir of SL(2,R) is

$$c_2 = J^a J^a = \tfrac{1}{2}(J^+J^- + J^-J^+) - (J^3)^2. \tag{12}$$

The equations of motion derived from (6) is $\partial_-(\partial_+ g g^{-1})=0$, namely, that the currents, J_R and J_L, are purely right or left moving as indicated. A general solution of the equations of motion for SL(2,R) is the product of two group elements each of which depends only on x^+ or x^- as

$$g=g_+(x^+)g_-(x^-). \tag{13}$$

Comparing (13) with (1) we can find the embedding of the worldsheet in AdS_3. The requirement that the string is closed under $\sigma\to\sigma+2\pi$ imposes the constraint,

$$g_+(x^++2\pi)=g_+(x^+)M,\ \ g_-(x^--2\pi)=M^{-1}g_-(x^-), \tag{14}$$

with the same $M\in \mathrm{SL}(2,R)$ for both g_+ and g_-. The monodromy matrix M is only defined up to a conjugation by SL(2,R), and classical solutions of the WZW model are classified according to the conjugacy class of M.

For strings on $AdS_3\times\mathcal{M}$, we should impose the Virasoro constraints,

$$T^{\mathrm{total}}_{++}=T^{AdS}_{++}+T^{\mathrm{other}}_{++}=0, \tag{15}$$

and similarly $T^{\mathrm{total}}_{--}=0$, where

$$T^{Ads}_{++}=\frac{1}{k}J^a_R J^a_R$$

is the energy-momentum tensor for the AdS_3 part (In the quantum theory, we will have the same expression but with $k\to k-2$.) and T^{other}_{++} represents the energy-momentum tensor for the sigma-model on $\mathcal{M}$.

Let us analyze some simple classical solutions.

A. Geodesics in AdS_3

Consider a solution

$$g_+=Ue^{iv_+(x^+)\sigma_2},\ \ g_-=e^{iu_-(x^-)\sigma_2}V, \tag{16}$$

where U and V are constant elements of SL(2,R). The energy momentum tensor of this solution is

$$T^{AdS}_{++}=-k(\partial_+ v_+)^2,\ \ T^{AdS}_{--}=-k(\partial_- u_-)^2. \tag{17}$$

Suppose we have some string excitation in the compact part $\mathcal{M}$ of $AdS_3\times\mathcal{M}$, and set $T^{\mathrm{other}}_{\pm\pm}=h$ for some constant $h>0$. We may regard h as a conformal weight of the sigma-model on $\mathcal{M}$. The Virasoro constraints $T^{\mathrm{total}}_{\pm\pm}=0$ implies

$$(\partial_+ v_+)^2=(\partial_- u_-)^2=\frac{h}{k}.$$

Thus we can set $v_+=\alpha x^+/2$ and $u_-=\alpha x^-/2$ where $\alpha=\pm\sqrt{4h/k}$. Substituting this in (13), we obtain

$$g=U\begin{pmatrix}\cos(\alpha\tau) & \sin(\alpha\tau)\\ -\sin(\alpha\tau) & \cos(\alpha\tau)\end{pmatrix}V. \tag{18}$$

Since the solution depends only on τ and not on σ, we interpret that the string is collapsed to a point which flows along the trajectory in AdS_3 parameterized by τ (see Fig. 1). If $U=V=1$, the solution (18) represents a particle sitting at the center of AdS_3,

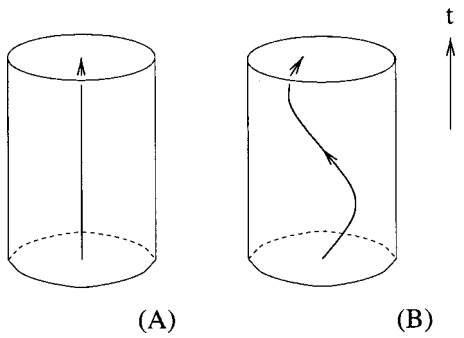

FIG. 1. Timelike geodesic; (A) a solution (18) with $U=V=1$, (B) a general geodesic is obtained by acting the SL(2,R) $\times$SL(2,R) isometry in (A).

$$t=\alpha\tau, \quad \rho=0. \tag{19}$$

A more general solution (18) is given by acting the SL(2,R)$\times$SL(2,R) isometry on (19), and therefore it is a timelike geodesic [In fact, any timelike geodesic can be expressed in the form (18)] in AdS_3. For this solution, the currents are given by

$$J_R^a T^a=\frac{k}{2}\alpha U T^3 U^{-1}, \tag{20}$$

and similarly for J_L. The monodromy matrix M defined by (14) is

$$M=\begin{pmatrix} \cos(\alpha\pi) & \sin(\alpha\pi) \\ -\sin(\alpha\pi) & \cos(\alpha\pi) \end{pmatrix}$$

and belongs to the elliptic conjugacy class SL(2,R).

A solution corresponding to a spacelike geodesic is

$$g=U\begin{pmatrix} e^{\alpha\tau} & 0 \\ 0 & e^{-\alpha\tau} \end{pmatrix}V, \tag{21}$$

with U, $V\in$ SL(2,R). The energy-momentum tensor has a sign opposite of (17)

$$T_{\pm\pm}^{AdS}=\tfrac{1}{4}k\alpha^2. \tag{22}$$

If we choose $U=V=1$, the solution is simply a straight line cutting the spacelike section $t=0$ of AdS_3 diagonally,

$$t=0, \quad \rho e^{i\phi}=\alpha\tau \tag{23}$$

[see Fig. 2(A)]. A general solution (21) is given from this by the action of the isometry, and therefore is a spacelike geodesic. The currents for this solution are

$$J_R^a T^a=\frac{k}{2}\alpha U T^1 U^{-1}, \tag{24}$$

and the monodromy matrix is

$$M=\begin{pmatrix} e^{\alpha\pi} & 0 \\ 0 & e^{-\alpha\pi} \end{pmatrix},$$

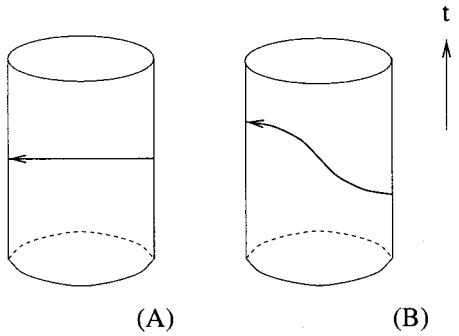

FIG. 2. Spacelike geodesic; (A) a solution (21) with $U=V=1$, (B) a general geodesic is obtained by acting the $SL(2,R)\times SL(2,R)$ isometry in (A).

which belongs to the hyperbolic conjugacy class of $SL(2,R)$.

There is one more class of solutions whose monodromy matrices are in the parabolic conjugacy class of $SL(2,R)$. They correspond to null geodesics in AdS_3.

B. Spectral flow and strings with winding numbers

Given one classical solution $g=\tilde{g}+\tilde{g}_-$, we can generate new solutions by the following operation:

$$g_+=e^{i(1/2)w_R x^+\sigma_2}\tilde{g}_+ \quad g_-=\tilde{g}_- e^{i(1/2)w_L x^-\sigma_2}. \tag{25}$$

Comparing this with the parameterization (1) of $g=g_+g_-$, we see that this operation amounts to

$$\begin{aligned} &t\to t+\tfrac{1}{2}(w_R+w_L)\tau+\tfrac{1}{2}(w_R-w_L)\sigma,\\ &\phi\to\phi+\tfrac{1}{2}(w_R+w_L)\sigma+\tfrac{1}{2}(w_R-w_L)\tau. \end{aligned} \tag{26}$$

The periodicity of the string worldsheet, under $\sigma\to\sigma+2\pi$, on the universal cover of $SL(2,R)$ requires [If the target space is the single cover of $SL(2,R)$, w_R and w_L can be different. In this case (w_R-w_L) gives the winding number along the closed timelike curve on $SL(2,R)$.] $w_R=w_L=w$ for some integer w.

One may regard (25) as an action by an element of the loop group $\widehat{SL}(2,R)\times\widehat{SL}(2,R)$ which is not continuously connected to the identity. [The loop group $\widehat{SL}(2,R)$ has such an element since $\pi_1(SL(2,R))=\mathbb{Z}$. Therefore, in the model whose the target space is the single cover of $SL(2,R)$, the full symmetry group of the model is the loop group of $SL(2,R)\times SL(2,R)$ and its connected components are parametrized by $\mathbb{Z}\times\mathbb{Z}$. In this paper, we are studying the model for the universal cover of $SL(2,R)$. In this case, some of these elements do not act properly on the field space, generating worldsheets which close only modulo time translation. However the ones parametrized by the diagonal $\mathbb{Z}$ are still symmetry of the model. The diagonal $\mathbb{Z}$ parameterizes the spectral flow operation performed simultaneously for both the left and right movers.] This particular symmetry of the theory will also be useful in our analysis of the Hilbert space. Here we see that it generates a new solution from an old solution. Furthermore, the currents (9) change in the following way:

$$J_R^3=\tilde{J}_R^3+\frac{k}{2}w, \quad J_R^\pm=\tilde{J}_R^\pm e^{\mp iwx^+} \tag{27}$$

and a similar expression for J_L^a. Or, in terms of the Fourier modes,

$$J_n^3=\tilde{J}_n^3+\frac{k}{2}w\,\delta_{n,0},\quad J_n^{\pm}=\tilde{J}_{n\mp w}^{\pm}. \tag{28}$$

This means that the stress tensor will change to

$$T_{++}^{AdS}=\tilde{T}_{++}^{AdS}-w\tilde{J}^3-\frac{k}{4}w^2. \tag{29}$$

In the CFT literature, this operation is known as the spectral flow.

Let us study what happens if we act with this symmetry on the solutions corresponding to geodesics, (18) and (21). These solutions depend only on the worldsheet time coordinate τ, and the spectral flow (26) with $w=w_R=w_L$ introduces σ dependence as

$$\begin{aligned} t&=t_0(\tau)+w\tau,\\ \rho&=\rho_0(\tau),\\ \phi&=\phi_0(\tau)+w\sigma. \end{aligned} \tag{30}$$

Here (t_0,ρ_0,ϕ_0) represents the original geodesic solution. So what the spectral flow does is to stretch the geodesic solution in the t-direction (by adding $w\tau$) and rotates it around w-times around the center $\rho=0$ of AdS_3 (by adding $w\sigma$). It is clear that the resulting solution describes a circular string, winding w-times around the center of AdS_3. Since the spectral flow changes the energy-momentum tensor, we need to impose the physical state condition $T_{\pm\pm}^{AdS}+T_{\pm\pm}^{\text{other}}=0$ with respect to the new energy-momentum tensor (29).

C. Short strings as the spectral flow of timelike geodesics

A timelike geodesic in AdS_3 makes a periodic trajectory as shown in Fig. 1, approaching the boundary of AdS_3, then coming back to the center and so on. In particular, when $V=U^{-1}$ in (18), the geodesic periodically passes through the center $\rho=0$ of AdS_3, with the period 2π in the t-coordinate. The spectral flow,

$$t\to t+w\tau,\quad \phi\to\phi+w\sigma,$$

stretches the geodesic in the time direction and rotate it around the center $\rho=0$; it is pictorially clear that the resulting solution describes a circular string which repeats expansion and contraction. This is shown in Fig. 3 in the case of $w=1$. Assuming $T_{\pm\pm}^{\text{other}}=h$ as in the case of geodesics, the Virasoro constraint for the solution is

$$T_{++}^{\text{total}}=\tilde{T}_{++}^{AdS}-w\tilde{J}^3-\frac{k}{4}w^2+T_{++}^{\text{other}}=0. \tag{31}$$

Since

$$\tilde{T}_{++}^{AdS}=-\frac{k}{4}\alpha^2$$

for the timelike geodesic, we find

$$J_0^3=\tilde{J}_0^3+\frac{k}{2}w=\frac{k}{4}w+\frac{1}{w}\left(-\frac{k}{4}\alpha^2+h\right). \tag{32}$$

The space–time energy E of the string is given by $E=2J_0^3$, and is bounded above as

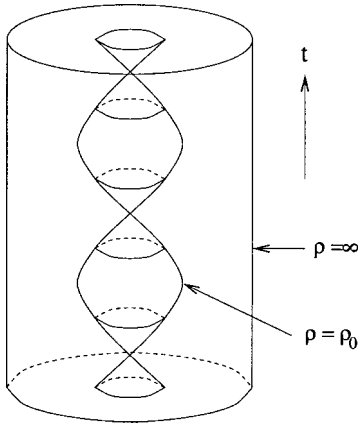

FIG. 3. A classical solution obtained by the spectral flow of a timelike geodesic. The solution repeats expansion and contraction. The maximum size of the string is $\rho=\rho_0$.

$$E=\frac{k}{2}w+\frac{1}{w}(-k\alpha^2+2h)<\frac{k}{2}w+\frac{2h}{w}. \tag{33}$$

It is not difficult to find an explicit form of the solution. When $V=U^{-1}$ in (18), without loss of generality, we can set (A different choice of $U=V^{-1}$ simply results in the shift of ϕ in the solution.) $U=V^{-1}=e^{(1/2)\rho_0\sigma_3}$. The solution (We have been informed that a similar classical solution has also been studied in Refs. 19 and 20.) obtained by the spectral flow of (18) is then

$$\begin{aligned} e^{i\phi}\sinh\rho &= ie^{iw\sigma}\sinh\rho_0\sin\alpha\tau, \\ \tan t &= \frac{\tan w\tau+\tan\alpha\tau/\cosh\rho_0}{1-\tan w\tau\tan\alpha\tau/\cosh\rho_0}. \end{aligned} \tag{34}$$

The currents of this solution are

$$\begin{aligned} J_R^3 &= \frac{k}{2}(\alpha\cosh\rho_0+w), \\ J_R^{\pm} &= \pm i\frac{k}{2}\alpha\sinh\rho_0 e^{\mp iwx^+}, \end{aligned} \tag{35}$$

and similarly for J_L. Comparing this with (32), we find

$$\alpha=\alpha_{\pm}=-w\cosh\rho_0\pm\sqrt{w^2\sinh^2\rho_0+\frac{4h}{k}}. \tag{36}$$

If we choose the branch $\alpha=\alpha_+$, the space–time energy E of the solution is positive and is given by

$$E=2J_0^3=2\bar{J}_0^3=k\left(\cosh\rho_0\sqrt{\frac{4h}{k}+w^2\sin^2\rho_0}-w\sinh^2\rho_0\right). \tag{37}$$

There are several interesting features of this formula for the energy E. Except for the case of $h=kw^2/4$, the energy is a monotonically increasing function of ρ_0, which approaches $E\to kw/2+2h/\omega$ as $\rho_0\to\infty$. One may view that the solution describe a bound state trapped inside of AdS_3.

At the exceptional value of $h=kw^2/4$, we have $\alpha_+=0$ and the energy of the solution becomes $E=kw$, completely independent of the size ρ_0 of the string. The solution in this case is

$$\rho=\rho_0, \quad t=w\tau, \quad \phi=w\sigma, \tag{38}$$

and represents a string staying at the fixed radius $\rho=\rho_0$, neither contracting nor expanding. The fact that we have such a solution at any radius ρ_0 means that the string becomes marginally unstable in AdS_3.

Now let us turn to the case when $U\neq V^{-1}$, or to be more precise, when UV does not commute with $T^3=-(i/2)\sigma^2$. (When UV commutes with T^3, one can shift the value of τ to set $U=V^{-1}$.) In this case, the geodesic does not necessarily pass through the center of AdS_3. Therefore the circular string obtained by its spectral flow does not collapse to a point. Since

$$\tilde{J}^a{}_L T^{*a}=\frac{k}{2}\alpha U T^3 U^{-1}, \quad \tilde{J}^\alpha{}_R T^a=\frac{k}{2}\alpha V^{-1} T^3 V, \tag{39}$$

$\tilde{J}^3_L\neq\tilde{J}^3_R$ unless UV commutes with $T^3=-(i/2)\sigma^2$, and the space–time angular momentum $l=J^3_R-J^3_L=\tilde{J}^3_R-\tilde{J}^3_L$ is nonzero. Thus one may view that the circular string is kept from completely collapsing by the centrifugal force. Since $T^{AdS}_{++}-T^{AdS}_{--}=-w(\tilde{J}^3_R-\tilde{J}^3_L)$, the Virasoro constraint $T^{\text{total}}_{\pm\pm}=0$ requires that the left and right conformal weights (h_L,h_R) of the internal part should be different and that $h_R-h_L=wl$.

D. Long strings as the spectral flow of spacelike geodesics

We have seen in (33) that the space–time energy E of the solution given by the spectral flow of the timelike geodesic is bounded above as $E<kw/2+2h/w$. What will happen if we raise the energy above this value? To understand this, let us look at the spectral flow of the spacelike geodesic. Since $\tilde{T}^{AdS}_{++}=+k\alpha^2/2$ for the spacelike geodesic, the Virasoro constraint (31) gives

$$J^3_0=\tilde{J}^3_0+\frac{k}{2}w=\frac{k}{4}w+\frac{1}{w}\left(\frac{k}{2}\sigma^2+h\right), \tag{40}$$

and the space–time energy is now bounded below,

$$E=2J^3_0>\frac{k}{2}w+\frac{2h}{w}. \tag{41}$$

As an example, let us consider the straight line cutting the spacelike section $t=0$ diagonally (23). The spectral flow with w of this solution is

$$t=w\tau, \quad \rho e^{i\phi}=\alpha\tau e^{iw\sigma}, \tag{42}$$

namely

$$\rho=\frac{\alpha}{w}|t|. \tag{43}$$

The solution starts in the infinite past $t=-\infty$ as a circular string of an infinite radius located at the boundary of AdS_3. The string then collapse, shrinks to a point at $t=0$, and expand away toward the boundary of AdS_3 as $t\to+\infty$. More generally, if we choose $U=V^{-1}=e^{(-1/2)\rho_0\sigma_1}$, the spectral flow of the geodesic (21) gives

$$e^{i\phi}\sinh\rho=e^{iw\sigma}\cosh\rho_0\sinh\alpha\tau, \tag{44}$$

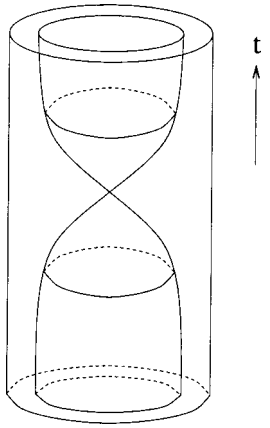

FIG. 4. A long string solution obtained by the spectral flow of a spacelike geodesic. The long string comes from the boundary of AdS_3, collapses to a point, and then expands away to the boundary of AdS_3 again.

$$\tan t = \frac{\tan w\tau + \tanh \alpha\tau \sinh \rho_0}{1 - \tan w\tau \tanh \alpha\tau \sinh \rho_0}.$$

This solution, which we call a long string, is depicted in Fig. 4.

The Virasoro constraint $T^{\text{total}}_{++}=0$ for the long string (44) is

$$T^{AdS}_{++} + T^{\text{other}}_{++} = \frac{k}{4}(\alpha^2 - 2\alpha w \sinh \rho_0 - w^2) + h = 0, \tag{45}$$

with the solutions

$$\alpha = \alpha_{\pm} = w \sinh \rho_0 \mp \sqrt{w^2 \cosh^2 \rho_0 - \frac{4h}{k}}. \tag{46}$$

The space–time energy E of these solutions are

$$E = 2J^2_0 = 2\bar{J}^3_0 = k\left(w \cosh^2 \rho_0 \mp \sinh \rho_0 \sqrt{w^2 \cosh^2 \rho_0 - \frac{4h}{k}} \right). \tag{47}$$

At the critical value $h = kw^2/4$, we have $\alpha_+ = 0$ and the energy for this solution becomes $E = kw$. At this point, the long string solution (44) coincides with (38). Thus we see that, as we increase the value of h to $h = kw^2/4$, the short string solution (34) can turn into the long string solution (44) and escape to infinity.

As explained in Refs. 11 and 12, a string that winds in AdS_3 close to the boundary has finite energy because there is a balance between two large forces. One is the string tension that wants to make the string contract and the other is the NS–NS B field which wants to make the string expand. These forces cancel almost precisely near the boundary and only a finite energy piece is left. The threshold energy for the long string computed in Refs. 11 and 12 is $kw/4$, in agreement with (41) when $h=0$. These strings can have some momentum in the radial direction and that is a degree of freedom α that we saw explicitly above. One may view the long string as a scattering state, while the previous solution (34) is like a bound state trapped inside of AdS_3.

In general, if UV commutes with $T^3 = -(i/2)\sigma^2$, the long string collapses to a point once in its lifetime. If UV does not commute with T^3, the angular momentum $l = J^3_R - J^3_L$ of the solution does not vanish and the centrifugal force keeps the string from collapsing completely. In this case, the Virasoro constraint $T^{\text{total}}_{\pm\pm}=0$ requires $h_R - h_L = wl$ for the conformal weights of the internal sector.

For the long strings, one can define a notion of the S-matrix. In the infinite past, the size of the long string is infinite but its energy is finite. Therefore the interactions between them are expected to be negligible, and one can define asymptotic states consisting of long strings. The strings then approach the center of AdS_3 and are scattered back to the boundary. In this process, the winding number could in principle change.

III. SEMICLASSICAL ANALYSIS

In studying the classical solutions, we were naively identifying the winding number w as associated to the cycle $\phi \to \phi + 2\pi$. But since this cycle is contractible in AdS_3, we should be careful about what we mean by the integer w. The winding number is well-defined when the string is close to the boundary, so we expect that long strings close to the boundary have definite winding numbers. On the other hand, when the string collapses to a point, as shown in Figs. 3 and 4, the winding number is not well-defined. Therefore, if we quantize the string, it is possible to have a process in which the winding number changes. There is however a sense in which string states are characterized by some integer w.

In order to clarify the meaning of w when the string can collapse, let us look at the Nambu action,

$$S = \int dt \frac{d\sigma}{2\pi} [\sqrt{\det g_{\rm ind}} - B_{t\phi}\partial_\sigma \phi], \tag{48}$$

where $g_{\rm ind}$ is the induced metric on the worldsheet, and $B_{t\phi}$ is the NS–NS B-field. We have chosen the static gauge in the time direction $t = \tau$. We assume that initially we have a state with $\rho = 0$, and we want to analyze small perturbations. Since the coordinate ϕ is not well-defined, it is more convenient to use

$$X^1 + iX^2 = \rho e^{i\phi}. \tag{49}$$

Let us compute the components of the induced metric $g_{\rm ind}$. To be specific, we consider the case when the target space $AdS_3 \times S^3 \times T^4$, and consider a string winding around a cycle on T^4. By expanding in the quadratic order in ρ, we find

$$\begin{aligned} g_{\rm ind,00} &= k[-(1+\rho^2) + \partial_0 X^a \partial_0 X^a] + \partial_0 Y^i \partial_0 Y^i, \\ g_{\rm ind,01} &= k\partial_0 X^a \partial_1 X^a + \partial_0 Y^i \partial_1 Y^i, \\ g_{\rm ind,11} &= k\partial_{11} X^a \partial_1 X^a + \partial_1 Y^i \partial_1 Y^i, \quad (a = 1,2), \end{aligned} \tag{50}$$

where Y^i's are coordinates on T^4. For simplicity, we consider purely winding modes on T^4, so that only $\partial_1 Y^i$ is nonzero. For these states, the conformal weight h is given by (One factor of 2 comes from the fact that this includes left and right movers and the other from the fact that the expression for the energy involves $1/2Y'^2$.)

$$4h \oint \frac{d\sigma}{2\pi} G_{ij} \partial_1 Y^i \partial_1 Y^j. \tag{51}$$

Substituting (50) and (51) into the action and expanding to the quadratic order in ρ, we find

$$\begin{aligned} S &= \sqrt{4kh} \int d\sigma^2 \left[1 - \frac{1}{2}(\partial_0 X^a)^2 + \frac{1}{2}\frac{k}{4h}\left(\partial_1 X^a + \epsilon_{ab}\sqrt{\frac{4h}{k}} X^b \right)^2 + \cdots \right] \\ &= \sqrt{4kh} \int d\sigma^2 \left[1 - \frac{1}{2}|\partial_0 \Phi|^2 + \frac{1}{2}\frac{k}{4h}\left| \left(\partial_1 - i\sqrt{\frac{4h}{k}} \right)\Phi \right|^2 + \cdots \right], \end{aligned} \tag{52}$$

where $\Phi = X^1 + iX^2$.

The action (52) is the one for a massless charged scalar field on $\mathbb{R}\times S^1$ coupled to a constant gauge field $A=\sqrt{4h/k}$ around S^1. As we vary A, we observe the well-know phenomenon of the spectral asymmetry. Let us first assume that A is not an integer. A general solution to the equation of motion derived from (52), requiring the periodicity in σ, is

$$\Phi \sim \sum_{n=-\infty}^{\infty} (a_n^\dagger e^{i(n-A)(\tilde{\tau}+\sigma)} + b_n e^{-i(n-A)(\tilde{\tau}-\sigma)}) \frac{e^{iA\sigma}}{n-A}, \tag{53}$$

where $A=\sqrt{4h/k}$ and $\tilde{\tau}=\tau/A$. Upon quantization, the commutation relations are given (modulo a positive constant factor) by

$$[a_n, a_m^\dagger] = (n-A)\delta_{n,m}, \quad [b_n, b_m^\dagger] = (n-A)\delta_{n,m}. \tag{54}$$

Notice that the sign in the right-hand side of (54) determines whether a_n or $a_n^\dagger$ should be regarded as the annihilation operator. Thus, assuming that the Hilbert space is positive definite, the vacuum state is defined by

$$\begin{aligned} a_n|0\rangle = b_n|0\rangle = 0, \quad (n>A), \\ a_n^\dagger|0\rangle = b_n^\dagger|0\rangle = 0, \quad (n<A). \end{aligned} \tag{55}$$

For $\Phi=\rho e^{i\phi}$ given by (53) and $t=A\tilde{\tau}$, we find

$$\begin{aligned} J_R^+ &= k(e^{-it}\partial_+\Phi^* - \Phi^*\partial_+ e^{-it}) \sim -ik\sum_n a_n e^{-in(\tilde{\tau}+\sigma)}, \\ J_R^- &= k(e^{it}\partial_+\Phi - \Phi\partial_+ e^{it}) \sim ik\sum_n a_n^\dagger e^{in(\tilde{\tau}+\sigma)}, \end{aligned} \tag{56}$$

and similarly for $J_L^\pm$. Therefore $J_n^+ = -ika_n$ and $J_n^- = ika_{-n}^\dagger$. The vacuum state $|0\rangle$ defined by (55) then obeys

$$J_n^+|0\rangle = 0 \quad (n>A), \quad J_n^-|0\rangle = 0 \quad (n>-A). \tag{57}$$

Thus the vacuum state $|0\rangle$ is not in a regular highest weight representation of the current algebra $\widehat{\mathrm{SL}}(2,R)$. If we set

$$J_n^\pm = \tilde{J}_{n\mp w}^\pm \tag{58}$$

with the integer w defined by

$$w<A<w+1, \tag{59}$$

then $|0\rangle$ obeys the regular highest weight condition with respect to $\tilde{J}_n^\pm$,

$$\tilde{J}_n^+|0\rangle = 0 \quad (n\geqslant 1), \quad \tilde{J}_n^-|0\rangle = 0 \quad (n\geqslant 0). \tag{60}$$

The change of the basis (58) is nothing but the spectral flow (28) discussed earlier, so we can identify w as the amount of spectral flow needed to transform the string state into a string state which obeys the regular conditions (60). We have found that, for a given value of h, there is a unique integer of w associated to the string state. As we vary the conformal weight h, $A=\sqrt{4h/k}$ will become an integer. At that point, one of the modes of the field Φ will have a vanishing potential. In fact we can check that classically this potential is completely flat. Giving an

expectation value to that mode, we find configurations as in (38). Corresponding to various values of its momentum in the radial direction, we have a continuum of states. So, at this value of h, we do not have a normalizable ground state; instead we have a continuum of states which are δ-function normalizable. If we continue to increase h, we find again normalizable states, but they are labeled by a new integer $(w+1)$. Notice that w is not directly related to the physical winding of the string. In fact by exciting a coherent state of the oscillators a_n or b_n we can find string states that look like expanding and collapsing strings with winding number n around the origin.

One of the puzzles we raised in the Introduction was what happens when we increase the internal conformal weight h of the string beyond the upper bound implied by the restriction $j < k/2$ on the SL(2,R) spin j due to the no-ghost theorem. In this section, we saw a semiclassical version of the puzzle and its resolution. When h reaches the bound, we find that the state can become a long string with no cost in energy. Above the bound, we should consider a Fock space with a different bose sea level. In the fully quantum description of the model given below, we will find a similar situation but with minor corrections.

IV. QUANTUM STRING IN AdS_3

The Hilbert space of the WZW model is a sum of products of representations of the left and the right-moving current algebras generated by

$$J_L^a = \sum_{n=-\infty}^{\infty} J_n^a e^{-inx^-}, \quad J_R^a = \sum_{n=-\infty}^{\infty} \overline{J}_n^a e^{-inx^+}, \tag{61}$$

with $a=3, \pm$, obeying the commutation relations

$$\begin{aligned} [J_n^3, J_m^3] &= -\frac{k}{2} n \delta_{n+m,0}, \\ [J_n^3, J_m^\pm] &= \pm J_{n+m}^\pm, \\ [J_n^+, J_m^-] &= -2J_{n+m}^3 + kn\delta_{n+m,0}, \end{aligned} \tag{62}$$

and the same for $\overline{J}_n^a$. We denote the current algebra by $\widehat{\mathrm{SL}}_k(2,R)$. The Virasoro generator L_n are defined by

$$\begin{aligned} L_0 &= \frac{1}{k-2}\left[\frac{1}{2}(J_0^+ J_0^- + J_0^- J_0^+) - (J_0^3)^2 + \sum_{m=1}^{\infty} (J_{-m}^+ J_m^- + J_{-m}^- J_m^+ - 2J_{-m}^3 J_m^3)\right], \\ L_{n\neq 0} &= \frac{1}{k-2}\sum_{m=1}^{\infty} (J_{n-m}^+ J_m^- + J_{n-m}^- J_m^+ - 2J_{n-m}^3 J_m^3), \end{aligned} \tag{63}$$

and obey the commutation relation,

$$[L_n, L_m] = (n-m)L_{n+m} + \frac{c}{12}(n^3 - n)\delta_{n+m,0}, \tag{64}$$

where the central charge c is given by

$$c = \frac{3k}{k-2}. \tag{65}$$

We will find that the Hilbert space of the WZW model consists of subsectors parameterized by integer w, labeling the amount of spectral flow in a sense to be made precise below. We then

formulate our proposal on how the complete Hilbert space of the WZW model is decomposed into representations of the current algebras and provide evidences for the proposal.

States in a representation of the current algebra are labeled by eigenvalues of L_0 and J_0^3. Since the kinetic term of the WZW model based on SL(2,R) has an indefinite signature, it is possible that the Hilbert space of the model contains states with negative eigenvalues of L_0 as well as states with negative norms, and indeed both types of states appear as we will see below. For the moment, we will consider a representation in which eigenvalues of L_0 is bounded below. We call them *positive energy representations*, or *unflowed* representations. Since the action of $J_n^{3,\pm}$ with $n \geqslant 1$ on a state lowers the eigenvalue of L_0 by n, there has to be a set of states which are annihilated by them. We will call such states the primary states of the positive energy representation. All other states in the representation are obtained by acting $J_{-n}^{3,\pm}(n \geqslant 1)$ on the primary states. The ground states make a representation of SL(2,R) generated by $J_0^{3,\pm}$. So let us review irreducible representations of SL(2,R).

A. Representations of the zero modes

We expect that physical states of a string in AdS_3 have positive norms. Since $J_0^{3,\pm}$ commute with the Virasoro constraints, physical spectrum of the string must be in unitary representations of SL(2,R). Most of the mathematical references on representation theory of SL(2,R) deal with the case with compact time; [For a review of representations of SL(2,R), see, for example, Ref. 21.] we are however interested in the case with noncompact time. A clear analysis from the algebraic point of view is presented in Ref. 22, which we now summarize with some minor changes is notation.

There are the following five types of unitary representations. All the representations are parameterized by j, which is related to the second Casimir $c_2 = \frac{1}{2}(J_0^+ J_0^- + J_0^- J_0^+) - (J_0^3)^2$ as $c_2 = -j(j-1)$.

(1) Principal discrete representations (lowest weight):

A representation of this type is realized in the Hilbert space

$$\mathcal{D}_j^+ = \{|j;m\rangle : m = j,\ j+1,\ j+2, ...\},$$

where $|j;j\rangle$ is annihilated by J_0^- and $|j;m\rangle$ is an eigenstate of J_0^3 with $J_0^3 = m$. The representation is unitarity if j is real and $j > 0$. For representations of the group SL(2,R), j is restricted to be a half-integer. Since we are considering the universal cover of SL(2,R), j can be any positive real number.

(2) Principal discrete representations (highest weight):

A charge conjugation of (1). A representation of this type is realized in the Hilbert space,

$$\mathcal{D}_j^- = \{|j;m\rangle : m = -j,\ -j-1,\ -j-2, ...\},$$

where $|j;j\rangle$ is annihilated by J_0^+ and $|j;m\rangle$ is an eigenstate of J_0^3 with $J_0^3 = m$. The representation is unitary if j is real and $j > 0$.

(3) Principal continuous representations:

A representation of this type is realized in the Hilbert space of

$$\mathcal{C}_j^\alpha = \{|j,\alpha;m\rangle : m = \alpha,\ \alpha \pm 1,\ \alpha \pm 2,\ \ldots\},$$

where $|j,\alpha;m\rangle$ is an eigenstate of J_0^3 with $J_0^3 = m$. Without loss of generality, we can restrict $0 \leqslant \alpha < 1$. The representation is unitary if $j = 1/2 + is$ and s is real. (Strictly speaking the representation with $j = 1/2$, $\alpha = 1/2$ is reducible as the sum of a highest weight and a lowest weight representation with $j = 1/2$.)

(4) Complementary representations:

A representation of this type is realized in the Hilbert space of

$$\mathcal{E}_j^\alpha = \{|j,\alpha;m\rangle : m = \alpha,\ \alpha \pm 1,\quad \alpha \pm 2, ...\},$$

where $|j,\alpha;m\rangle$ is an eigenstate of J_0^3 with $J_0^3 = m$. Without loss of generality, we can restrict $0 \leqslant \alpha < 1$. The representation is unitary if j is real, with $1/2 < j < 1$ and $j - 1/2 < |\alpha - 1/2|$.

(5) Identity representation:

This is the trivial representation with $j = 0$.

The analysis that led to the above representation was completely algebraic and in a particular physical system we can have only a subset of all possible representations. Which of these representations appear in the Hilbert space of the WZW model? As the first approximation, let us consider the $k \to \infty$ limit. If we expand around a short string solutions, i.e., oscillations near geodesics in AdS_3, the WZW model in this limit reduces to the quantum mechanics on AdS_3. The Hilbert space of the quantum mechanical model is the space of square-integrable (Since AdS_3 is noncompact, we consider square-integrability in the delta-function sense.) functions $\mathcal{L}^2(AdS_3)$ on AdS_3. The isometry of AdS_3 is SL(2,R)$\times$SL(2,R), and one can decompose $\mathcal{L}^2(AdS_3)$ into its unitary representations. It is convenient to choose the basis of the Hilbert space in the following way. For each representation $\mathcal{R}$, one can define a function on AdS_3 by $F_{m,\bar{m}}(g) = \langle m|g|\bar{m}\rangle$, where $g \in AdS_3$, i.e., universal cover of SL(2,R), and $|m\rangle$ is an eigenstate of J_0^3 with $J_0^3 = m$. Thus, for a given representation $\mathcal{H}$ of SL(2,R), the function $F_{m,\bar{m}}(g)$ on AdS_3 is in the tensor product of the representations $\mathcal{R}\times\mathcal{R}$ for the isometry group SL(2,R)$\times$SL(2,R).

For a discrete representation $\mathcal{D}_j^\pm$, the wave-function $f(\rho)$ behaves as $f(\rho) \sim e^{-2j\rho}$ for large ρ. Thus $\phi \in \mathcal{L}^2(AdS_3)$ if $j > 1/2$. Notice that in the range $0 < j < 1$ we have two representations with the same value of the Casimir but only one is in $\mathcal{L}^2(AdS_3)$, the one with $1/2 < j < 1$. As explained in Ref. 23, one could modify the norm so that the second solution with $0 < j < 1/2$ becomes normalizable. This modification of the norm is j-dependent. Similarly, supplementary series representations need a j-dependent modification to the norm to render them normalizable.[21] Therefore these representations would appear in nonstandard quantizations of geodesics, quantizations which do not use the $\mathcal{L}^2$ norm on AdS_3. In this paper, we will only consider the standard quantization using the $\mathcal{L}^2$ norm for the zero modes. [Notice however, that even if the primary states have $j > 1/2$, we could have states with smaller values of j_0 for the zero mode SL(2,R) among the descendents, for example, $J_{-1}^-|j\rangle$ with $1 < j < 3/2$, has $j_0 = j - 1 < 1/2$.] Wave-functions in $\mathcal{C}_{j=1/2+is}^\alpha$ are also delta-function normalizable with respect to the $\mathcal{L}^2$ norm. It is known that $\mathcal{C}_{j=1/2+is}^\alpha \times \mathcal{C}_{j=1/2+is}^\alpha$ and $\mathcal{D}_j^\pm \times \mathcal{D}_j^\pm$ with $j > 1/2$ form the complete basis of $\mathcal{L}^2(AdS_3)$.

For discrete lowest weight representations, the second Casimir is bounded above as $c_2 = -j(j-1) \leqslant 1/4$. This corresponds to the well-known Breitenlohner–Freedman bound $(\text{mass})^2 \geqslant -1/4$ for the Klein–Gordon equation. For the principal continuous representation $\mathcal{C}_j^\alpha$ with $j = 1/2 + is$, the second Casimir is $c_2 = 1/4 + s^2$. Therefore an existence of such a particle would violate the Breitenlohner–Freedman bound. In the bosonic string theory, the only physical state of this type is the tachyon. In a perturbatively stable string theory, such particle states should be excluded from its physical spectrum. On the other hand, the continuous representations appear in $\mathcal{L}^2(AdS_3)$ and they are expected to be part of the Hilbert space of the WZW model before the Virasoro constraint is imposed.

B. Representations of the current algebra and no-ghost theorem

Given a unitary representation $\mathcal{H}$ of SL(2,R), one can construct a representation of SL(2,R) by regarding $\mathcal{H}$ as its primary states annihilated by $J_{n\geqslant 1}^{3,\pm}$. The full representation space is generated by acting $J_{n\leqslant -1}^{3,\pm}$ on $\mathcal{H}$. Following the discussion in the previous subsection, we consider the cases when $\mathcal{H} = \mathcal{C}_{j=1/2+is}^\alpha$ and $\mathcal{D}_j^\pm$ with $j > 1/2$. We denote by $\hat{\mathcal{D}}_j^\pm$ and $\hat{\mathcal{C}}_j^\alpha$ the representations of the full current algebra built on the corresponding representations of the zero modes. In Fig. 5, we have shown the weight diagram of the positive energy representation $\hat{\mathcal{D}}_j^+$.

A representation of $\widehat{\text{SL}}_k(2,R)$ in general contains states with negative norms. In order for a string theory on AdS_3 to be consistent, one should be able to remove these negative norm states by imposing the Virasoro constraint,

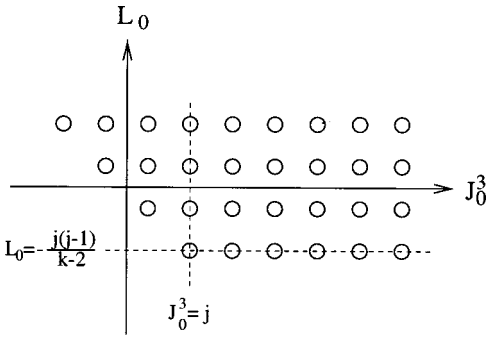

FIG. 5. Weight diagram the representation $\hat{\mathcal{D}}_j^+$, whose the primary states form a discrete lowest weight representation $\hat{\mathcal{D}}_j^+$.

$$(L_n+\mathcal{L}_n-\delta_{n,0})|\text{physical}\rangle=0,\ \ n\geqslant 0, \tag{66}$$

on the Hilbert space for a single string state, where L_n is the Virasoro generator of the SL(2,R)WZW model and $\mathcal{L}_n$ for the sigma-model on $\mathcal{M}$. It has been shown that this no-ghost theorem holds for states in $\hat{\mathcal{C}}^{\alpha}_{j=1/2+is}$ or $\hat{\mathcal{D}}^{\pm}_j$ with $0<j<k/2$.[2,3,6–9,22]

The no-ghost theorem is proven by first showing that all the solutions to the Virasoro constraint (66) can be expressed, modulo null states, as states in the coset SL(2,R)/U(1) obeying

$$J^3_n|\psi\rangle=0,\quad n\geqslant 1. \tag{67}$$

This statement is true for $\hat{\mathcal{C}}^{\alpha}_{1/2+is}$ and $\hat{\mathcal{D}}^{\pm}_j$ with $0<j<k/2$, if the total central charge of the Virasoro generator $L_n+\mathcal{L}_n$ is 26.[2–4,6–9] (We also assume $k>2$.) We review the proof of this statement in Appendix A.1. The second step is to show that the condition (67) removes all negative norm states. This was shown in Ref. 22 for the same class of representations.

The no-ghost theorem suggests that the spectrum of discrete representations has to be truncated for $j<k/2$. As we will see, this truncation is closely related to the existence of the long string states.

C. Spectral flow and the long string

The classical and semiclassical results discussed above indicate that, beyond positive energy representations that we have discussed so far, we have to include others related by spectral flow. To define a quantum version of the spectral flow, we note that, for any integer w, the transformation $J^{3,\pm}_n\to\tilde{J}^{3,\pm}_n$ given by

$$\tilde{J}^3_n=J^3_n-\frac{k}{2}w\,\delta_{n,0},\ \ \tilde{J}^+_n=J^+_{n+w},\ \ \tilde{J}^-_n=J^-_{n-w}, \tag{68}$$

preserves the commutation relations (62). The Virasoro generators $\tilde{L}_n$, which have the standard Sugawara form in terms of $\tilde{J}^a_n$, are different from L_n. They are given by

$$\tilde{L}_n=L_n+wJ^3_n-\frac{k}{4}w^2\delta_{n,0} \tag{69}$$

Of course, they obey the Virasoro algebra with the same central charge c. This is the same formula as saw in the classical counterpart (29) of the spectral flow.

The change of the basis (68) maps one representation into another, and this is called the spectral flow. In the case of a compact group such as SU(2), the spectral flow maps a positive

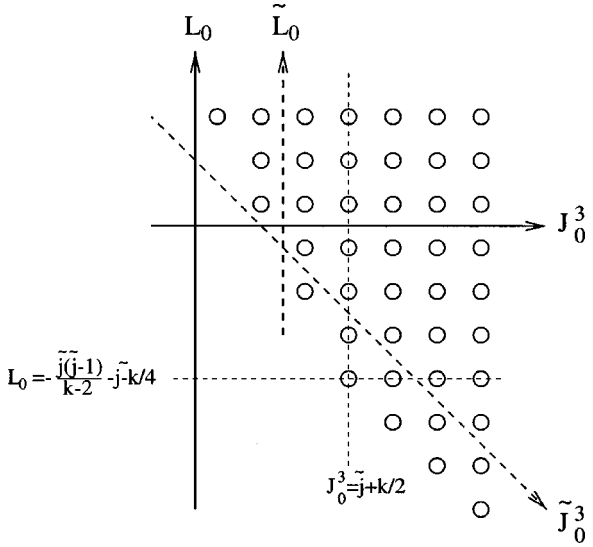

FIG. 6. Weight diagram of the representation $\hat{\mathcal{D}}_j^{+,w=1}$, which is the spectral flow of the diagram 5 with $w=1$. The worldsheet energy L_0 of this representation is not bounded below, but the space–time energy, J_0^3, is bounded below for states obeying the Virasoro constraint $L_0=1$.

energy representation of the current algebra into another positive energy representation. An analogous transformation in the case of the $N=2$ superconformal algebra in two dimensions has been used to construct the spacetime supercharges for superstring.

In the case of SL(2,R), the spectral flow generates a new class of representations. As shown in Fig. 6, the spectral flow with $w=1$ maps the lowest weight representation $\hat{\mathcal{D}}_{\tilde{j}}^{+}$ to a representation in which L_0 is not bounded below. The appearance of negative energy states is not too surprising since the kinetic term of the SL(2,R) model is not positive definite. In general, a spectral flow of $\hat{\mathcal{D}}_{\tilde{j}}^{+}$ with $w\geqslant 1$ or $w\leqslant -2$ gives a new representation in which L_0 is not bounded below. Similarly, the spectral flow of $\hat{\mathcal{C}}^{\alpha}_{j=1/2+is}$ with $w\neq 0$ gives a representation in which L_0 is not bounded below. We denote the resulting representations by $\hat{\mathcal{D}}_{\tilde{j}}^{\pm,w}$ and $\hat{\mathcal{C}}_{\tilde{j}}^{\alpha,w}$, where $\tilde{j}$ labels the SL(2,R) spin before the spectral flow (Fig. 7).

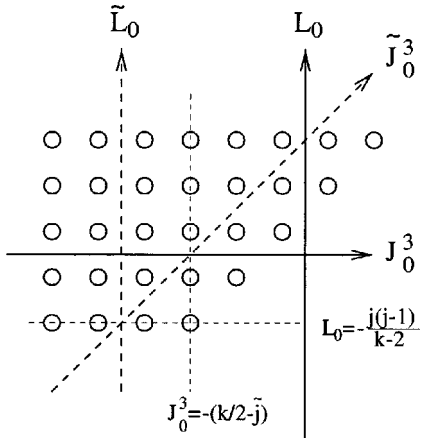

FIG. 7. The spectral flow of the diagram 5 with $w=-1$. $\hat{\mathcal{D}}_j^{+}$ is mapped to $\hat{\mathcal{D}}_j^{+,w=-1}=\hat{\mathcal{D}}_j^{-}$ with $j=k/2-\tilde{j}$. Since $\tilde{j}>1/2$, the resulting $\hat{\mathcal{D}}_j^{-}$ obeys $j<(k-1)/2$. In particular, the unitarity bound $j<k/2$ required by the no-ghost theorem is satisfied.

These representations obtained by the spectral flow also contain negative norm states. In Appendix A.2, we generalize the proof of the no-ghost theorem and show that the Virasoro constraints indeed remove all negative norm states in the representations $\hat{\mathcal{C}}^{\alpha,w}_{j=1/2+is}$ and $\hat{\mathcal{D}}^{\pm,w}_{\tilde{j}}$ with $\tilde{j}<k/2$, for any integer w.

The only case where we get a representation with L_0 bounded below by the spectral flow is $\hat{\mathcal{D}}^{\pm}_{j}$ with $w=\mp 1$. In this case, the representation is mapped to another positive energy representation $\hat{\mathcal{D}}^{\pm,w=\mp 1}_{\tilde{j}}=\hat{\mathcal{D}}^{\mp}_{k/2-\tilde{j}}$. Note that, if we start with the representation with $\tilde{j}>1/2$, the representation one gets after the spectral flow satisfies $j=k/2-\tilde{j}<(k-1)/2$. Conversely, if there were a representation $\hat{\mathcal{D}}^{\pm}_{j}$ with $j>(k-1)/2$ in the Hilbert space, the spectral flow would generate a representation $\hat{\mathcal{D}}^{\pm}_{j}$ with $j<1/2$ in contradiction with the standard harmonic analysis of the zero modes in Sec. IV A. Therefore, if we assume that the spectral flow is a symmetry of the WZW model, the discrete representations $\hat{\mathcal{D}}^{\pm}_{j}$ appearing in the Hilbert space are automatically restricted to be in $1/2<j<(k-1)/2$. In particular, the spectrum of j is truncated below the unitarity bound $j<k/2$ required by the no-ghost theorem. This further restriction on j was discussed in a related context by Ref. 24.

D. Physical spectrum

Let us consider first the spectrum for strings with $w=0$. This is fairly standard. We start from an arbitrary descendent at level N in the current algebra and some operator of the internal CFT with conformal weight h. The L_0 constraint reads

$$(L_0-1)|j,m,N,h\rangle=0\Rightarrow-\frac{j(j-1)}{k-2}+N+h-1=0. \tag{70}$$

If we demand that $1/2\leqslant j\leqslant(k-1)/2$, this equation will have a solution as long as $N+h$ is within the range

$$0\leqslant N+h-1+\frac{1}{4(k-2)}\leqslant\frac{(k-2)}{4}. \tag{71}$$

If we allow j to go all the way to $k/2$ we get $k/4$ on the right-hand side of (71).

To analyze physical states of strings with $w\neq 0$, we start with a positive energy representation $\hat{\mathcal{D}}^{+}_{\tilde{j}}$. After the spectral flow (68), a primary state $|\tilde{j},\tilde{m}\rangle$ of $\hat{\mathcal{D}}^{+}_{\tilde{j}}$, as a state of $\hat{\mathcal{D}}^{+,w}_{\tilde{j}}$, obeys

$$\begin{gathered}J^{+}_{n+w}|\tilde{j},\tilde{m}\rangle=0,\ \ J^{-}_{n-w}|\tilde{j},\tilde{m}\rangle=0,\ \ J^{3}_{n}|\tilde{j},\tilde{m}\rangle=0,\ \ n\geqslant 1,\\ J^{3}_{0}|\tilde{j},\tilde{m}\rangle=\left(\frac{k}{2}w+\tilde{m}\right)|\tilde{j},\tilde{m}\rangle.\end{gathered} \tag{72}$$

Let us look for physical states with respect to the Virasoro generator L_n. From (72), we find the Virasoro constraints are

$$\begin{gathered}(L_0-1)|\tilde{j},\tilde{m}\rangle=\left(-\frac{\tilde{j}(\tilde{j}-1)}{k-2}-w\tilde{m}-\frac{k}{4}w^2+\tilde{N}+h-1\right)|\tilde{j},\tilde{m},\tilde{N},h\rangle=0,\\ L_n|\tilde{j},\tilde{m}\rangle=(\tilde{L}_n-w\tilde{J}^3_n)|\tilde{j},\tilde{m}\rangle=0,\quad n\geqslant 1,\end{gathered} \tag{73}$$

where h is the contribution to the conformal weight from the internal CFT and $\tilde{N}$ is the level inside the current algebra before we take the spectral flow. The state obeys the physical state conditions provided

$$\tilde{m}=-\frac{k}{4}w+\frac{1}{w}\left(-\frac{\tilde{j}(\tilde{j}-1)}{(k-2)}+\tilde{N}+h-1\right). \tag{74}$$

The space–time energy of this state measured by J_0^3 is then

$$J_0^3=\tilde{m}+\frac{k}{2}w=\frac{k}{4}w+\frac{1}{w}\left(-\frac{\tilde{j}(\tilde{j}-1)}{(k-2)}+\tilde{N}+h-1\right). \tag{75}$$

This is the quantum version of the classical formula (32), with the replacement

$$\frac{k}{4}\alpha^2\to\frac{\tilde{j}(\tilde{j}-1)}{k-2}+1.$$

Notice that $\tilde{m}=\tilde{j}+q$ where q is some integer, which could be negative. ($\tilde{m}$ is the total $\tilde{J}^3$ eigenvalue of the state so it can be lowered by applying J^-_{-n} to the highest weight state. So we have the constraint $q\geqslant-\tilde{N}$.) Therefore the physical state condition becomes

$$\tilde{j}=\frac{1}{2}-\frac{k-2}{2}w+\sqrt{\frac{1}{4}+(k-2)\left(h-1+N_w-\frac{1}{2}w(w+1)\right)}. \tag{76}$$

Here

$$N_w=\tilde{N}-wq \tag{77}$$

is the level of the current algebra after the spectral flow by the amount w. Notice that the equation for $\tilde{j}$ is invariant under $\tilde{N}\to\tilde{N}\pm w$, $q\to q\pm1$. This is reflecting the fact that $J_0^{\pm}=\tilde{J}^{\pm}_{\mp w}$ commute with the Virasoro constraints and generate the space–time SL(2,R) multiplets. In particular, we see that the space–time SL(2,R) representations that we get are lowest energy representations, since repeated action of $J_0^-=\tilde{J}_w^-$ will eventually annihilate the state. In fact, it is shown in Appendix A.2 that the only physical state with zero spacetime energy, $J_0^3=0$, is the state $J_{-1}^-|j=1\rangle$, and its complex conjugate. This physical state corresponds to the dilaton field in AdS_3, which played an important role in the analysis of the spacetime Virasoro algebra in Ref. 25. All other states (except the tachyon with $w=0$) have nonzero energy, and form highest/lowest weight representations of SL(2,R) space–time algebra. The negative energy ones are the complex conjugates of the positive energy ones.

By solving the on-shell condition (76) for $\tilde{j}>0$ and substituting it into (75), one finds that the space–time energy of the string is given by

$$\frac{E+l}{2}=J_0^3=q+w+\frac{1}{2}+\sqrt{\frac{1}{4}+(k-2)\left(h-1+N_w-\frac{1}{2}w(w+1)\right)}. \tag{78}$$

Since both N_w and q are integers, the energy spectrum is discrete. This is reasonable since we are considering the string trapped inside of AdS_3. The constraint $1/2<\tilde{j}<(k-1)/2$ translates into the inequality

$$\frac{k}{4}w^2+\frac{w}{2}<N_w+h-1+\frac{1}{4(k-2)}<\frac{k}{4}(w+1)^2-\frac{w+1}{2}. \tag{79}$$

This is the quantum version of the semiclassical formula (59). In fact, if we take $k,h\gg\tilde{N},q,w$, (79) reduces to (59). As in the semiclassical discussion, w is not necessarily related to the physical winding number of the string. It is just an integer labeling the type of representation that the string state is in.

The analysis for the representations coming from the continuous representations for the zero modes is similar. If we do not spectral flow, the only state in the continuous representation is the tachyon. If we do spectral flow, we get Eq. (74), which can be conveniently rewritten as

$$J_0^3=\tilde{m}+\frac{wk}{2}=\frac{kw}{4}+\frac{1}{w}\left(\frac{\frac{1}{4}+s^2}{k-2}+\tilde{N}+h-1\right). \tag{80}$$

For continuous representations w is labeling the physical winding of the string when it approaches the boundary of *AdS*. In this case we do not get an equation like (76) since, for continuous representations, $\tilde{m}$ is not related to j. Comparing with the classical formula (40), we identify s as the momentum α/k of the long string along the radial direction of AdS_3. We clearly see that the energy of this state is above the threshold to produce an excitation that will approach the boundary as a w-times wound string.

We can see that, whenever the value of h is such that it saturates the range (79), we have a continuous representation with the same energy. This is clear for the lower bound in the case of $w=0$ since, for each state in the discrete representation with $j=1/2$, there is one in the continuous representation with the same values of L_0 and J_0^3. By the spectral flow, we see that the same is true for the lower bound in (79) for any w. Indeed we can check explicitly that a state in the discrete representation with parameters $(h,w,q,\tilde{N})$ saturating the lower bound in (79) has the same space–time energy as a state in the continuous representation with parameters $(h,w,s=0,\tilde{N})$. [The parameter α in the continuous representation is fixed by the value of J_0^3 in (80).] Similarly, if we have a state in a discrete representation saturating the upper bound in (79), it has the same spacetime energy as a state in the continuous representation with parameters $(h,w+1,\ s=0,\ \tilde{N}'=\tilde{N}+q)$. Note that, since $q\geqslant-\tilde{N}$ (see the footnote in the previous page), we have $\tilde{N}'\geqslant 0$. In this case, to show that the two states have the same energy, it is useful to identify the state in $\hat{\mathcal{D}}^{+,w}_{\tilde{j}=\tilde{j}}$ as a state in $\hat{\mathcal{D}}^{-,w+1}_{\tilde{j}=k/2-\tilde{j}}$. Since $\tilde{j}\to(k-1)/2$ corresponds to $\tilde{j}\to 1/2$ under this identification, we can apply the above argument for the lower bound to show that we will find a state in the continuous representation. The shift $\tilde{N}'=\tilde{N}+q$ comes from the fact that the identification $\hat{\mathcal{D}}^{+,w}_{\tilde{j}=\tilde{j}}=\hat{\mathcal{D}}^{-,w+1}_{\tilde{j}=k/2-\tilde{j}}$ involves spectral flow one more time.

The above paragraph explains what happens as we change $\tilde{j}$ in a discrete representation and we make it equal to the upper or lower bound: a continuous representation appears. Another question that one could ask is the following. Given a value of h, what is the state with the lowest value of J_0^3 that satisfies the physical state conditions? Let us first look for the lowest energy state in the discrete representations obeying the bound (79). Within this bound, one can show that $\partial J_0^3(h,w,q,\tilde{N})/\partial q\geqslant 0$ and $\partial J_0^3(h,w,q=-\tilde{N},\tilde{N})/\partial\tilde{N}\geqslant 0$. Therefore, if we can set $q=\tilde{N}=0$, it will give the lowest energy state in the discrete representations. This is possible if h is within the range,

$$\frac{k}{4}w^2+\frac{w}{2}<h-1+\frac{1}{4(k-2)}<\frac{k}{4}(w+1)^2-\frac{w+1}{2}. \tag{81}$$

With some more work, one can show that, for h in this range, there is not any state in a continuous representation whose energy is lower than that of the discrete representation state with $\tilde{N}=q=0$. As we saw in the above paragraph, at the upper or lower bound of (81), the energy of the discrete state $(q=0,\ \tilde{N}=0)$ coincides with that of the continuous state with $(s=0,\ \tilde{N}=0)$. Outside this range (81), it is not possible to set $\tilde{N}=q=0$, and the lowest energy state will be in a continuous representation. In our semi-classical discussion in the last section, we found that the discrete representation can decay into the continuous representation at $h=kw^2/4$. Now we see that, in the fully quantum description, the range over which a continuous representation has lower energy has expanded from the point $h=kw^2/4$ to a strip of width w,

$$\frac{k}{4}w^2-\frac{w}{2}<h-1+\frac{1}{4(k-2)}<\frac{k}{4}w^2+\frac{w}{2}. \tag{82}$$

So far we have restricted our attention to right-moving sectors of the Hilbert space. Let us now discuss how the left and right movers are combined together. For the classical solution of the long string, the worldsheet periodicity requires that the spectral flow has to be done simultaneously on both the left and right movers with the same amount. If AdS_3 were not the universal cover of SL(2,R) but its single cover, different amounts of the left and the right spectral flows would have been allowed since the resulting solution is periodic modulo the closed timelike curve of SL(2,R). It is straightforward to identify the corresponding constraint in the quantum theory. Suppose we perform the spectral flows by the amount w_L and w_R on the left and the right-movers. A state with conformal weights (h_L,h_R) and the J_0^3 charge $(\tilde{m}_L,\tilde{m}_R)$ is mapped by this transformation to a state with conformal weights $(h_L-w_L\tilde{m}_L-(k/4)w_L^2,\ h_R-w_R\tilde{m}_W-(k/4)w_R^2)$, according to (69). The worldsheet locality, which is the quantum counterpart of the periodicity of the classical solution, requires that the conformal weights h_L and h_R differ only by an integer. If this is the case before spectral flow, the same requirement after the flow implies

$$w_L\tilde{m}_L+\frac{k}{4}w_L^2=w_R\tilde{m}_R+\frac{k}{4}w_R^2 \ \ (\text{mod integer}). \tag{83}$$

For generic values of $(\tilde{m}_L,\tilde{m}_R)$, the only solution to this constraint is $w_L=w_R$. In this paper, we are considering only the universal cover of SL(2,R) as the target space of the model. In this case, the spectrum of $(\tilde{m}_L,\tilde{m}_R)$ is continuous, and only the left-right symmetric spectral flow $w_L=w_R$ is allowed.

Summary: We propose that the spectrum of the SL(2,R) WZW model [for the universal cover of SL(2,R)] contains the following two types of representations. First, the spectral flow of the continous representations, with the same amount of spectral flow on the left and right, $\hat{\mathcal{C}}^{\alpha,w}_{1/2+is,L}\times\hat{\mathcal{C}}^{\alpha,w}_{1/2+is,R}$. Then the discrete representations $\hat{\mathcal{D}}^{+,w}_{\tilde{j},L}\times\hat{\mathcal{D}}^{+,w}_{\tilde{j},R}$ with the same amount of spectral flow on the left and right and the same value of $\tilde{j}$, with $1/2<\tilde{j}<(k-1)/2$. In the string theory, these representations should be tensored with the states of the internal CFT, and the Virasoro constraints should be imposed.

V. SCATTERING OF THE LONG STRING

When a long string comes in from the boundary of AdS_3 to the center, it will scatter back to the boundary. In this process the winding number could in principle change. In order to study the S-matrix between incoming and outgoing long strings, it is convenient to perform the rotations to Euclidean signature spaces, both on the worldsheet and in space time. Following the standard procedure, we define the hermiticity as is natural in the Lorentzian theory. For this reason we still have the SL(2,R)$_L\times$SL(2,R)$_R$ currents in the Euclidean theory. The relevant conformal field theory, whose target space is the three-dimensional hyperbolic space $H_3=\mathrm{SL}(2,C)/\mathrm{SU}(2)$ has been studied in Refs. 18, 25–30.

A. Vertex operators

To compute the scattering amplitudes, we would like to find vertex operators for all representations considered above. Spectral flow is realized in the vertex operator for malism in the following standard fashion.[31] We bosonize the J^3 currents, introducing left and right moving chiral bosons [Reflecting the hermiticity of the SL(2,R) model, the scalar field ϕ is Hermitian, but with a wrong sign for the two-point function $\langle\phi(z)\phi(z')\rangle=\log(z-z')$.] through

$$J_R^3=-i\sqrt{\frac{k}{2}}\partial\phi(z),\quad J_L^3=-i\sqrt{\frac{k}{2}}\bar{\partial}\phi(\bar{z}). \tag{84}$$

A state with charge m under J_R^3 contains an exponential in $\phi(z)$ of the form $e^{im\sqrt{(2/k)}\phi(z)}$. The other two currents therefore can be expressed as

$$J_R^+ = \psi e^{i\sqrt{(2/k)}\phi(z)}, \quad J_R^- = \psi^\dagger e^{-i\sqrt{(2/k)}\phi(z)}, \tag{85}$$

and similarly for $J_L^\pm$. A primary field $\Phi_{jm\bar{m}}(z,\bar{z})$ of the current algebra can be expressed as

$$\Phi_{jm\bar{m}} = e^{im\sqrt{(2/k)}\phi(z)+i\bar{m}\sqrt{(2/k)}\phi(\bar{z})}\Psi_{jm\bar{m}}, \tag{86}$$

where $\Psi_{jm\bar{m}}$ carries no charges with respect to $J_{R,L}^3$. In the case of the SU(2) model, the field corresponding to Ψ is known as a parafermion. The parafermion for the SL(2,R) model was studied in Ref. 32. The conformal weights of the parafermion field $\Psi_{jm\bar{m}}$ is

$$\begin{aligned} h_{\Psi;jm\bar{m}} &= -\frac{j(j-1)}{k-2} + \frac{m^2}{k}, \\ \bar{h}_{\Psi;jm\bar{m}} &= -\frac{j(j-1)}{k-2} + \frac{\bar{m}^2}{k}. \end{aligned} \tag{87}$$

In the discrete lowest weight representation, $m,\bar{m} = j, j+1, j+2, \ldots$. In particular, when $j=k/2$, the field $\Psi_{j=k/2,m=\bar{m}=k/2}$ has conformal weights $h=\bar{h}=0$. Since the parafermion field lives in the unitary conformal field theory it is natural to assume that it is the identity operator. (Recently we have learned that a similar argument has appeared in unpublished notes by Zamolodchikov. We thank him for having his note available to us.[33]) Here we simply note that the operator,

$$e^{i\sqrt{(k/2)}(\phi(z)+\phi(\bar{z}))}$$

has the correct OPE for the primary field of spin $j=k/2$ with the SL(2,R) currents.

Using the parafermion notation, the operator obtained by the spectral flow by w units is expressed as

$$\Phi^w = e^{i(\tilde{m}+wk/2)\sqrt{(2/k)}\phi(z)+i(\tilde{\bar{m}}+wk/2)\sqrt{(2/k)}\phi(\bar{z})}\Psi_{j\tilde{m}\tilde{\bar{m}}}. \tag{88}$$

It is easy to see that the conformal weight is given by

$$L_0 = \frac{-j(j-1)}{k-2} - mw + kw^2/2. \tag{89}$$

B. Reflection coefficient

We will compute the amplitude, using the formulas obtained in Refs. 34, 35, 26, 33, in the case that the winding number does not change.

The long string states are in the spectral flow of the continuum representation. The corresponding vertex operators are

$$\begin{aligned} \Phi^j_{m\bar{m}} &= e^{m\phi(z)+\bar{m}\phi(\bar{z})}\Psi^j_{\tilde{m}\tilde{\bar{m}}}V_{h\bar{h}}(z,\bar{z}), \\ \tilde{m} = m - wk/2, &\quad \tilde{\bar{m}} = \bar{m} - wk/2, \quad j = \tfrac{1}{2} + is, \end{aligned} \tag{90}$$

where $V_{h\bar{h}}$ is an operator in the internal part with conformal weights $(h,\bar{h})$. The physical energy E and angular momentum l of a state in AdS_3 are given by

$$m = \tfrac{1}{2}(E+l), \quad \bar{m} = \tfrac{1}{2}(E-l). \tag{91}$$

The physical state constraint is (80) with $\tilde{N}=0$. This implies that

$$\tilde{m}=-wk/4+\frac{1}{w}\left[\frac{1/4+s^2}{k-2}+h-1\right]. \tag{92}$$

Now we can now consider the two point function[26,27,33]

$$\langle \Phi^{j}_{m\bar{m}}(z,\bar{z})\Phi^{j'}_{m',\bar{m}'}(z',\bar{z}')\rangle = \frac{\Gamma(1/2+is-\tilde{m})\Gamma(1/2+is+\tilde{m})\Gamma(-2is)\Gamma\left(\frac{2is}{k-2}\right)}{\Gamma(1/2-is-\tilde{m})\Gamma(1/2-is+\tilde{m})\Gamma(2is)\Gamma\left(\frac{-2is}{k-2}\right)} \times \delta(s-s')\,\delta_{N+N'}\,\delta(E+E'). \tag{93}$$

The z dependence is just $1/|z-z'|^4$ coming from the fact that the two operators have weight (1,1). This is the reflection amplitude and the values of $\tilde{m},\tilde{\bar{m}}$ are determined by (92) (notice that m is the physical energy, not $\tilde{m}$).

As explained in Ref. 28 in this context, in string theory we have to integrate over z and divide by the volume of SL(2,C). We can use SL(2,C) invariance to put $z=0$, $z'=\infty$ in the correlator. The volume of the rest of SL(2,C) then gives $\int(d^2z/|z|^2)$, which cancels one of the delta-functions in (93). Notice that $\delta(s-s')\,\delta(E+E')=\delta(s-s')\,\delta(0)$, the volume of SL(2,$C$) cancels the $\delta(0)$ piece.

Now if we study the poles of (93), we find that they are located at $1/2+is-\tilde{m}=-q$ with $q=0,1,2,\ldots$. They come from the first Gamma-function. Taking this condition together with (92) we find that

$$1/2+is+q=\tilde{m}=-wk/4+\frac{1}{w}\left[\frac{1/4+s^2}{k-2}+h-1\right] \tag{94}$$

and this equation is precisely the same as the usual mass shell equation for discrete states if we take $\tilde{j}=1/2+is$. There are similar poles from the second Gamma-function. There are no poles coming from the third factor since they cancel extra poles appearing in the other factors. Notice that the poles appearing in (94) satisfy precisely Eq. (76) for bound states in the representation $\hat{\mathcal{D}}^{+,w}_{\tilde{j}}$ (with $\tilde{N}=0$). There is however, an important difference. In (76) the value of $\tilde{j}$ obeyed the condition

$$\frac{1}{2}<\tilde{j}<\frac{k-1}{2}, \tag{95}$$

while we do not have such a condition in (94). It is interesting to note that if $\tilde{j}$ satisfies (95), then the residue at the pole has the proper sign to be interpreted as coming from a bound state. When $\tilde{j}=(k-1)/2$, i.e., at the upper bound of (95), we find that there is no pole. Moreover, immediately above that value, we have the wrong sign for the pole residue. This might make us worry that the amplitude is not having the right analytic structure. However, in order to have a one-to-one correspondence between poles of the scattering amplitude and bound states, the potential has to decrease sufficiently rapidly at the infinity,[36] a condition that is not met in our case. In such a situation, it is possible to have extra poles that do not correspond to physical states. We plan to analyze the poles and their implications for physical states in a future publication.

C. Relation to the scattering of the two-dimensional black hole

The coset of the SL(2,R) WZW by the U(1) generated by J^3 gives a sigma-model whose target space is the two-dimensional black hole with the Euclidean signature metric.[37] The geom-

etry of the black hole is like a semi-infinite cigar with an asymptotic region in the form of the cylinder $\mathbb{R}\times S^1$. The dilaton field grows as one approaches the center of the black hole, but it remains finite since the geometry is terminated at the tip of the cigar. The string theory on $\mathrm{SL}(2,R)/\mathrm{U}(1)\times(\text{time})\times\mathcal{M}$ is closely related to the string theory on $AdS_3\times\mathcal{M}$ since the physical state conditions for the latter implies $J^3_n|\text{physical}\rangle=0$ for $n\geqslant 1$, as we show in Appendix A. Similarly the superstring theory on $AdS_3\times\mathcal{M}$ is related to the Kazama–Suzuki coset $\mathrm{SL}(2,R)/\mathrm{U}(1)$.

There is however difference between the zero mode sectors of the theories on AdS_3 and on the two-dimensional black hole. In order to construct representations for SL(2)/U(1), we can start from the representations of $\widehat{\mathrm{SL}(2,R)}$ that we described above and impose the condition that $J^3_{n>0}$ annihilate the state and that the total AdS_3 energy vanishes, $J^3_{0,R}+J^3_{0,L}=m+\bar{m}=0$. In terms of the parafermion $\Psi_{j\tilde{m}\bar{\tilde{m}}}$ given in (86) and (88), the condition is $\tilde{m}+\bar{\tilde{m}}=wk$. The locality condition $m-\bar{m}=n$, where n is an integer implies that $\tilde{m}-\bar{\tilde{m}}=n$. These two quantization conditions are the ones in Ref. 38 [see Eq. (3.6) of that paper]. The SL(2)/U(1) theory has been studied recently in connection with ''little'' string theories in Refs. 24 and 39.

VI. CONCLUSION

In this paper, we studied the physical spectrum of bosonic string theory in AdS_3. We proposed that the complete Hilbert space of the $\mathrm{SL}(2,R)$ WZW model consists of the continuous representations and their spectral flow $\hat{\mathcal{C}}^{\alpha,w}_{j=1/2+is}\times\hat{\mathcal{C}}^{\alpha,w}_{j=1/2+is}$, and the discrete representations and their spectral flow $\hat{\mathcal{D}}^{\pm,w}_j\times\hat{\mathcal{D}}^{\pm,w}_j$ with the constraint $1/2<j<(k-1)/2$. The sum over the spectral flow is required if we assume that the Hilbert space realizes the full loop group of $\mathrm{SL}(2,R)$, including its topologically nontrivial elements. We found that this proposal leads to the physical spectrum of the string theory with the correct semiclassical limits.

In particular, we have solved the two puzzles which we mentioned in the Introduction. The no-ghost theorem for $\hat{\mathcal{D}}^{+}_j$ requires the constraint $0<j<k/2$. If we only had the unflowed sector (with $w=0$), it would imply the upper bound on allowed mass of string states, which appears artificial. This was one of the puzzles. We have resolved this puzzle by showing that the upper bound on the mass is removed if we include all the spectral flowed sectors in the Hilbert space. Moreover we showed that the consistency with the spectral flow and the standard harmonic analysis of the zero modes requires the constraint $1/2<j<(k-1)/2$, more stringent than the one required by the no-ghost theorem. The constraint $1/2<j<(k-1)/2$ is found to be consistent with the locations of the poles in the reflection coefficient (with the correct sign for the pole residues; see also Ref. 24 and the modular invariance of the partition function.

Another puzzle was to identify states in the Hilbert space corresponding to the long strings. We found that these states are in the spectral flow of the continuous representations, $\hat{\mathcal{C}}^{\alpha,w}_{j=1/2+is}\times\hat{\mathcal{C}}^{\alpha,w}_{j=1/2+is}$. The integer w, which parametrized the amount of the spectral flow, is identified with the winding number of the long string stretched closed the boundary of AdS_3. The physical spectrum of the long strings obtained from these representations agrees with the expectations from the semiclassical analysis in Refs. 11 and 12.

The resolutions of these puzzles removes the longstanding doubts about the consistency of the model. Moreover it appears that the $\mathrm{SL}(2,R)$ WZW model is exactly solvable, just as WZW models for compact groups, although its Hilbert space structure is significantly different from those of the compact cases. We hope that further study of the model will provide us more useful insights into the AdS/CFT correspondence and strings in curved spaces in general.

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APPENDIX A: NO-GHOST THEOREMS

In this Appendix we would like to extend the proof of the no-ghost theorem to all the representations considered above. We assume $k>2$. The proof of the no-ghost theorem for the standard lowest energy representations.[2–9,22] involves two parts. Part I consists of showing that a physical state can be chosen, up to a null state to be such that $J^3_n|\psi>=0$, for $n\geqslant 1$. This first part uses $0<j<k/2$ for the $\mathcal{D}^{\pm}_j$ representations as well as $c=26$ and the mass shell condition. This was shown in Refs. 2–9. Part II consists in showing that any state that is annihilated by $J^3_{n>0}$ has a non-negative norm. This step also uses $0<j<k/2$ for the $\mathcal{D}^{\pm}_j$ representations. This was done in Ref. 22. Here we will use the same strategy and prove Part I for the all our representations. The no-ghost theorem then follows from Part II.

We first review the proof of Part I for the representations with $w=0$ and then we do Part I for the $w\neq 0$ representations.

1. Proof of part I for unflowed representations

Here we follow the proof in Refs. 2, 3, 6, 7, 9. It has essentially three steps.

Step 1: The first step of the proof is to show that states of the form

$$\begin{gathered} L_{-n_1}L_{-n_2}\cdots L_{-n_N}J^3_{-m_1}J^3_{-m_2}\cdots J^3_{-m_M}|f\rangle, \\ n_1\geqslant n_2\geqslant\cdots\geqslant n_N, \quad m_1\geqslant m_2\geqslant\cdots\geqslant m_M, \\ \text{with } L_n|f\rangle=J^3_n|f\rangle=0 \text{ for } n\geqslant 1, \end{gathered} \tag{A1}$$

are linearly independent and that they form a complete basis of the Hilbert space.

The states $|f\rangle$ are constructed from states in the current algebra times some states in an internal conformal field theory. This internal piece is assumed to be unitary. This step involved separating the piece of L_n involving $L^{(3)}=:J^3J^3:$, defining $\hat{L}_n=L_n-L^{(3)}_n$. One can show that the states (A1) are in one to one correspondence with states of the form,

$$\begin{gathered} L_{-n_1}L_{-n_2}\cdots L_{-n_N}J^3_{-m_1}J^3_{-m_2}\cdots J^3_{-m_M}|f\rangle, \\ n_1\geqslant n_2\geqslant\cdots\geqslant n_N, \quad m_1\geqslant m_2\geqslant\cdots\geqslant m_M. \end{gathered} \tag{A2}$$

Notice that conditions (A1) on $|f\rangle$ are the same as $\hat{L}_{n>0}|f\rangle=J^3_{n>0}|f\rangle=0$. It is easier to show that (A2) is a basis since now we can think of the CFT as a product of a U(1) factor with the rest. The rest is a CFT with $c=25$ and therefore the fact that (A2) is a basis reduces to showing that there are no null states in the Virasoro descendents on a primary field. This will be true if the conformal weight of the rest is positive. This reduces to showing that $c_2/(k-2)+m^2/k+M>0$, where M is the grade in the SL(2,R) piece. For the continuous representations, this is obvious since $c_2>0$. For lowest weight representations, this inequality can be shown by rewriting it as

$$\frac{2j(k/2-j)}{k(k-2)}+\frac{2M}{k}\left(\frac{k}{2}-j\right)+\frac{2j}{k}(-j+m+M)+\frac{1}{k}(j-m)^2>0. \tag{A3}$$

We to use $0<j<k/2$ and also the fact that $m\geqslant j-M$, which is true in general. Notice that the m that appears here is the total J_0^3 value, after we applied $J_{-n}^{\pm}$ any number of times. Notice that in this step we did not use that the states were obeying the mass shell condition, but we used $0<j<k/2$ and that $c=26$.

Step 2: Here we show that a physical state can be chosen so that it involves no L_{-n} when written as (A1).

A physical state can be written as a state with no L_{-n} plus a spurious state. A spurious state is a state with at least one L_{-n}. Then we use the fact that, when $c=26$, $L_n(n\geqslant 1)$ acting on a spurious state which satisfies the $L_0=1$ condition leaves it as a spurious state.[40,41] If $L_{n>0}$ acts on a state of the form (A1) with no L_{-n} then it will not produce any L_{-n}. Together with the fact that (B1) is a basis this implies that the part of the state with no L_{-n} satisfies the physical state condition on its own, and therefore the rest is a null state (a spurious physical state).

Step 3: We show that if the physical state $|\psi\rangle$ involves no L_{-n} when written as in (A1) then $J_n^3|\psi\rangle=0$.

Since there are no L_{-n}'s in the physical state ψ this implies that $L_n^{(3)}\psi=0$ for $n\geqslant 1$. Then we try to show that the only states satisfying this will be states with $J_n^3\psi=0$ for $n\geqslant 1$. This would be true if there are no null states in the $L^{(3)}$ Virasoro descendents of the states $|f\rangle$ we considered above. If $m\neq 0$ then one can show that there is no null state in the Virasoro descendents in the $L^{(3)}$ Virasoro descendents. There are two states with $m=0$ one is in the continuous representation, but the mass shell condition automatically implies that $N=0$ (there are no J_{-n}^a in this state) and therefore the state has positive norm. The other is the state in the lowest weight representation

$$J_{-1}^-|j=1\rangle \tag{A4}$$

(and of course its complex conjugate in the highest weight representation). This state has positive norm. Note that m is the physical energy in AdS_3 of the state in question. Zero energy states, therefore imply that we have a normalizable zero mode. This is the state corresponding to the identity operator in the spacetime boundary conformal field theory, the state $\bar{J}J\Phi_1$ of Ref. 25 which played an important role in the computation of the spacetime Virasoro algebra.

One can show, using the mass shell condition, that all other states have $m\neq 0$. The mass shell condition is

$$-\frac{j(j-1)}{k-2}+N+h'-1=0, \tag{A5}$$

where N is the grade in the SL(2,R) part and h' is the conformal weight of the rest, $h'\geqslant 0$. If $0<j<1$ then m is nonzero because it can only change by an integer by the action of the $J_n^{\pm}$ currents. If $j=1$ with $N=1$ and $h'=0$ we find (A4) and states with positive m.

Consider now $j>1$. If we had $m=0$ then we also need $N\geqslant j, j\geqslant 2$ (since $m=0$ only if j is integer) and furthermore

$$-\frac{j(j-1)}{k-2}+N-1\geqslant\frac{(j-1)(k-2-j)}{k-2}>0 \tag{A6}$$

provided $j\leqslant k/2$. Since j has to be at least 2, then $k>4$ and therefore $k-2-k/2>0$. Thus we conclude that (A5) would not be obeyed if $m=0$.

2. Proof of Part I for flowed representations

Now we would like to generalize the above discussion to the spectral flowed representations that we called $\hat{\mathcal{C}}_{1/2+is}^{\alpha,w}$ and $\hat{\mathcal{D}}_{\tilde{j}}^{+,w}$. In the case of discrete representations we want to show that the no ghost theorem holds for $0<\tilde{j}<k/2$, where $\tilde{j}$ labels the representation before we perform the spectral flow operation, i.e., it labels a representation of the current algebra with $\tilde{L}_0$ bounded

below. So we consider the same representations we had above but we modify the physical state conditions. This is equivalent to imposing the usual conditions on the flowed representations. We would like to prove that, given any state built on a lowest weight or continuous representation with respect to $\tilde{J}_n$, the physical state condition $(L_n-\delta_{n,0})|\psi\rangle=0 \quad n\geqslant 0$ with respect to L_n removes non-negative norm states. We only consider spectral flow with $w>1$ on continuous or lowest weight representations $\hat{\mathcal{D}}_j^+$. These and their complex conjugates cover all the representations we needed to consider. We reproduce now the steps in Appendix A.1.

Step 1: In (A1) we need to show that they form a basis with $L_{-n}=\tilde{L}_{-n}-w\tilde{J}^3_{-n}$. We know that they would form a basis if we had an expression like (A1) with $L_{-n}\to\tilde{L}_{-n}$. Fortunately there is an invertible one to one map between these two sets of states, so that they form a basis.

Step 2: It is the same since only $c=26$ is used.

Step 3: If we write a physical state, $|\psi\rangle$, as a state with no L_{-n} then $L_n^{(3)}$ with $n\geqslant 1$ annihilates it. Again we will try to show that $m=\tilde{m}+kw/2$ is nonzero and that will imply that $J^3_{n>0}|\psi\rangle=0$. For this we need to use the new mass shell condition

$$\frac{\tilde{c}_2}{k-2}+\tilde{N}+h'-wm+\frac{kw^2}{4}=1, \tag{A7}$$

where $\tilde{N}$ is the level inside the current algebra before the spectral flow, $\tilde{c}_2$ is the second casimir in terms of $\tilde{j}$ and h' is the conformal weight of state in the internal conformal theory (the internal piece needs not be a primary state, and we only require that the whole combined state needs to be primary). We can assume with no loss of generality that $w\geqslant 1$. Let us start with the spectral flow of a continuous representation, (A7) implies that if $m=0$ then $\tilde{N}=0$ and there are no negative norm states. (The only solution with $m=0$ is in the case of $k=3$ and $\tilde{j}=1/2$.)

Let us turn to lowest weight representations. Thanks to the restriction $0<\tilde{j}<k/2$, we have $\tilde{c}_2/(k-2)>-k/4$. Therefore, if $m=0$, the left-hand side of (A7) is larger than $k/4(w^2-1)$. If $w\geqslant 2$, (A7) cannot be obeyed. If $w=1$, $m=0$ implies $\tilde{m}=-k/2$ and $\tilde{N}$ in (A7) has to be at least $\tilde{N}\geqslant\tilde{j}+k/2$. However, in this case we find $\tilde{c}_2/(k-2)+\tilde{N}+k/4\geqslant k/2+\tilde{j}>1$ (here we used $k>2$) and again (A7) is not satisfied.

So we conclude that all states can be mapped into states obeying $J^3_{n>0}|\psi\rangle=0$.

APPENDIX B: PARTITION FUNCTION

In this Appendix, we discuss the partition function of the SL(2,R) WZW model and its modular invariance.

1. Partition function of the SU(2) model

Before we begin discussing the modular invariance of the SL(2,R) theory, let us review the case of SU(2).

The characters $\chi_l^k(\tau,\theta)$ $(l=0,\frac{1}{2},1,\ldots,k/2)$ of the irreducible representations of the $SU(2)_k$ affine algebra transform under the modular transformation as

$$\chi_l^k(-1/\tau,-\theta/\tau)=\exp\left(2\pi i\frac{k}{4}\frac{\theta^2}{\tau}\right)\sum_{l'}S_{ll'}\chi_{l'}^k(\tau,\theta), \tag{B1}$$

where $S_{ll'}$ is some orthonormal $(k+1)\times(k+1)$ matrix. The diagonal (so-called A_k-type) modular invariant combination is therefore

$$e^{-2\pi(k/2)[(\mathrm{Im}\,\theta)^2/\mathrm{Im}\,\tau]}\sum_l|\chi_l(\tau,\theta)|^2. \tag{B2}$$

The exponential factor $e^{-2\pi(k/2)[(\mathrm{Im}\,\theta)^2/\mathrm{Im}\tau]}$ is there to cancel the exponential factor in (B1) as

$$\frac{[\mathrm{Im}(-\theta/\tau)]^2}{\mathrm{Im}(-1/\tau)}=\frac{(\mathrm{Im}\,\theta)^2}{\mathrm{Im}\,\tau}+i\frac{\theta^2}{2\tau}-i\frac{\bar{\theta}^2}{2\bar{\tau}}. \tag{B3}$$

It is known that the exponential factor in (B2) is a consequence of the chiral anomaly and therefore of the OPE singularity,

$$J^3(z)J^3(w)\sim\frac{k/2}{(z-w)^2}. \tag{B4}$$

2. Partition function of the SL(2,*C*)/SU(2) model

In string theory, one-loop computations are done after performing the Euclidean rotation on both the target space and the worldsheet (or stay in the Lorentzian signature space and use the $i\epsilon$ prescription). The modular invariance of the partition function is imposed on the Euclidean worldsheet. In our case, the Euclidean rotation of the target space means $\mathrm{SL}(2,R)\to H_3=\mathrm{SL}(2,C)/\mathrm{SU}(2)$. The partition function of the $\mathrm{SL}(2,C)/\mathrm{SU}(2)$ model has been evaluated in Ref. 18 as

$$Z_{\mathrm{SL}(2,C)/\mathrm{SU}(2)}\sim\frac{1}{\sqrt{\mathrm{Im}\,\tau}e^{[-2\pi(\mathrm{Im}\,\theta)^2/\mathrm{Im}\,\tau]}|\vartheta_1(\tau,\theta)|^2}. \tag{B5}$$

Note that our definition of the partition function differs from that in Ref. 18 by the factor $e^{2\pi(k/2)[(\mathrm{Im}\,\theta)^2/\mathrm{Im}\tau]}$. It appears that, without this factor, the partition function is not modular invariant. (The puzzle about the apparent lack of the modular invariance was recently resolved in Ref. 42.) One may expect that this partition function is related to the one for the $\mathrm{SL}(2,R)$ model by the Euclidean rotation. In the discussion below, we first evaluate the $\mathrm{SL}(2,R)$ partition function on the Lorentzian torus, and therefore take $\tau,\bar{\tau},\theta,\bar{\theta}$ to be independent real variables. We then analytically continue them to complex values so that (τ,θ) are complex conjugate of $(\bar{\tau},\bar{\theta})$. We will find that, by doing this analytic continuation, and ignoring contact terms, the $\mathrm{SL}(2,R)$ partition function turns into the $\mathrm{SL}(2,C)/\mathrm{SU}(2)$ partition function (B5), provided we impose the constraint $1/2<j<(k-1)/2$ on the discrete representations.

3. Discrete representations of SL(2,*R*)

The character of the discrete representation D_j^+ is

$$\begin{aligned}\chi_j^+(\tau,\theta)&=\mathrm{Tr}(e^{2\pi i\tau(L_0-[k/8(k-2)])}e^{2\pi i\theta J_0^3})\\&=\frac{\exp\left[2\pi i\tau\left(-\frac{j(j-1)}{k-2}-\frac{k}{8(k-2)}\right)+2\pi i\theta j\right]}{(1-e^{2\pi i\theta})\Pi_{n=1}^{\infty}(1-e^{2\pi in\tau})(1-e^{2\pi in\tau}e^{2\pi i\theta})(1-e^{2\pi in\tau}e^{-2\pi i\theta})}\\&=\frac{\exp\left[-\frac{2\pi i\tau}{k-2}\left(j-\frac{1}{2}\right)^2+2\pi i\theta\left(j-\frac{1}{2}\right)\right]}{i\vartheta_1(\tau,\theta)},\end{aligned} \tag{B6}$$

where $\vartheta_1(\tau,\theta)$ is the elliptic theta-function,

$$\vartheta_1(\tau,\theta)=-i\sum_{n=-\infty}^{\infty}(-1)^n\exp\left[\pi i\tau\left(n-\frac{1}{2}\right)^2+2\pi i\theta\left(n-\frac{1}{2}\right)\right]. \tag{B7}$$

The spectral flow,

$$\tilde{L}_0 = L_0 + wJ_0^3 - \frac{k}{4}w^2, \quad \tilde{J}_0^3 = J_0^3 - \frac{k}{2}w, \quad (w = 0, \pm 1, \pm 2, \ldots), \tag{B8}$$

transforms the character χ_j^+ as

$$\begin{aligned}
&\mathrm{Tr}\left(e^{2\pi i\tau(\tilde{L}_0 - [k/8(k-2)])} e^{2\pi i\theta \tilde{J}_0^3}\right) \\
&= \mathrm{Tr}\left(e^{2\pi i\tau(L_0 + wJ_0^3 - (k/4)w^2 - [k/B(k-2)])} e^{2\pi i\theta(J_0^3 - (k/2)w)}\right) \\
&= \frac{\exp\left[-2\pi i\tau\left(\frac{\left(j-\frac{1}{2}\right)^2}{k-2} - w\left(j-\frac{1}{2}\right) + \frac{k}{4}w^2\right) + 2\pi i\theta\left(j-\frac{1}{2}-\frac{k}{2}w\right)\right]}{i\vartheta_1(\tau, \theta + w\tau)} \\
&= (-1)^w \frac{\exp\left[-\frac{2\pi i\tau}{k-2}\left(j-\frac{1}{2}-\frac{k-2}{2}w\right)^2 + 2\pi i\theta\left(j-\frac{1}{2}-\frac{k-2}{2}w\right)\right]}{i\vartheta_1(\tau, \theta)},
\end{aligned} \tag{B9}$$

where we used

$$\vartheta_1(\tau, \theta + w\tau) = (-1)^w \exp(-\pi i\tau w^2 - 2\pi i\theta w)\,\vartheta_1(\tau, \theta). \tag{B10}$$

We have also performed an analytic continuation such as

$$\sum_{n=0}^{\infty} q^n = -\sum_{n=1}^{\infty} q^{-n},$$

ignoring terms like $\Sigma_{n=-\infty}^{\infty} q^n \sim \delta(\tau)$. From here on, we allow $(\tau,\ \theta)$ to take complex values and $(\overline{\tau}, \overline{\theta})$ to be their complex conjugates.

Let us sum over allowed representation. According to our proposal about the Hilbert space of the WZW model, all the representations in the allowed range $1/2 < j < (k-1)/2$ should appear. We also require that the spectrum to be invariant under the spectral flow (B8), so we need to sum over w. The part of the partition function made by discrete representations is then

$$\begin{aligned}
&e^{+2\pi(k/2)[(\mathrm{Im}\,\theta)^2/\mathrm{Im}\,\tau]} \sum_{w=-\infty}^{\infty} \int_{1/2}^{(k-1)/2} dj \\
&\quad \times \frac{\exp\left[\frac{4\pi\,\mathrm{Im}\,\tau}{k-2}\left(j-\frac{1}{2}-\frac{k-2}{2}w\right)^2 - 4\pi\,\mathrm{Im}\,\theta\left(j-\frac{1}{2}-\frac{k-2}{2}w\right)\right]}{|\vartheta_1(\tau, \theta)|^2} \\
&\quad = e^{+2\pi(k/2)[(\mathrm{Im}\,\theta)^2/\mathrm{Im}\,\tau]} \int_{-\infty}^{\infty} dt\, \frac{\exp\left[\frac{4\pi\,\mathrm{Im}\,\tau}{k-2}t^2 - 4\pi\,\mathrm{Im}\,\theta t\right]}{|\vartheta_1(\tau, \theta)|^2} \\
&\quad \sim \frac{1}{\sqrt{\mathrm{Im}\,\tau}\, e^{-2\pi[(\mathrm{Im}\,\theta)^2/\mathrm{Im}\,\tau]} |\vartheta_1(\tau, \theta)|^2}.
\end{aligned} \tag{B11}$$

It is interesting to note that the j-integral over the range $1/2 < j < (k-1)/2$ and the sum over w fit together to give the t-integral over $-\infty < t < \infty$. Since the spectral flow with $w = 1$ maps D_j^+ to $D_{k/2-j}^-$, we do not have to consider the orbit of D_j^- separately. The exponential factor

$e^{+2\pi(k/2)[(\mathrm{Im}\,\theta)^2/(\mathrm{Im}\,\tau)]}$ is due to the chiral anomaly, as in the SU(2) case. The sign in the exponent is opposite here since the sign of the OPE of J^3 is opposite in the SL(2,R) case.

The partition function computed in (B11) is manifestly modular invariant. In fact, it is identical to (B12) computed for the SL(2,C)/SU(2) model. This gives an additional support for our claim that the Hilbert space of the SL(2,R) model contains the discrete representations of $1/2 < j < (k-1)/2$ and their spectral flow.

The construction of the partition function here is closely related to the one given in Ref. 13. There, instead of the integral over j in (B11), the partition function was given by a sum over integral values of j. This is because they considered the string theory on the single cover of the SL(2,R) group manifold with the closed timelike curve. The resulting partition function, after analytic continuation, is also modular invariant and appears to be a correct one for such a model. It is, however, different from the partition function (B15) of the SL(2,C)/SU(2) model, as it should since the Euclidean rotation of the SL(2,C)/SU(2) model is naturally related to the model on the universal cover of SL(2,R) rather than on its single cover.

4. Continuous representations

It is curious that the sum over the discrete representations and their spectral flow alone reproduces the partition function of the SL(2,C)/SU(2) model. In fact, the sum over the continuous representations and their spectral flow, although formally modular invariant by itself, does not contribute to the partition function if we assume the analytic continuation in $\tau, \overline{\tau}, \theta, \overline{\theta}$ and ignore contact terms.

The character of the continuous representation is parametrized by a pair of real numbers (s,α) with $0 \leqslant \alpha < 1$ and s arbitrary. The character is given by

$$\chi_{j=1/2+is,\alpha} = \eta^{-3} e^{2\pi i[s^2/(k-2)]\tau} e^{i\alpha\theta} \sum_n e^{2\pi i n\theta}. \tag{B12}$$

As before, we regard the worldsheet metric to be of the Minkowski signature, and θ is real. So the sum Σ_n in the definition of $\chi_{j,\alpha}$ gives the periodic delta-function,

$$\sum_n e^{2\pi i n\theta} = 2\pi \sum_m \delta(\theta + m). \tag{B13}$$

After the spectral flow (B8), the character becomes

$$\chi_{j=1/2+is,\alpha;w} = \eta^{-3} e^{2\pi i([s^2/(k-2)]+(k/4)w^2)\tau} 2\pi \sum_m e^{2\pi i m(\alpha-(k/2)w)} \delta(\theta + w\tau + m). \tag{B14}$$

Now let us take $|\chi_{1/2+is,\alpha;w}|^2$ and integrate over s and α. The integral over α forces $m_L = m_R$ in the summation in (B14). The integral over s gives the factor $1/\sqrt{\mathrm{Im}\,\tau}$. So we have

$$\int_{-\infty}^{\infty} ds \int_0^1 d\alpha |\chi_{1/2+is,\alpha;w}|^2 = e^{-4\pi\,\mathrm{Im}\,\tau(k/4)w^2} \frac{1}{\sqrt{\mathrm{Im}\,\tau}|\eta|^6} \sum_m \delta^{(2)}(\theta + w\tau + m). \tag{B15}$$

Let us sum this over w. We get a nonzero result only when there is some integer w such that

$$w = -\frac{\mathrm{Im}\,\theta}{\mathrm{Im}\,\tau}. \tag{B16}$$

Therefore

$$e^{+2\pi(k/2)[(\mathrm{Im}\,\theta)^2/\mathrm{Im}\,\tau]}\sum_w \int_{-\infty}^{\infty} ds \int_0^1 d\alpha |\chi_{1/2+is,\alpha;w}|^2 = \frac{1}{\sqrt{\mathrm{Im}\,\tau}|\eta|^6}\sum_{w,m} \delta^{(2)}(\theta + w\tau + m). \tag{B17}$$

This expression is formally modular invariant since $\Sigma_{w,m}$ sums over the modular orbit of the delta-function and $1/|\eta|^4$ cancels its modular weight. If we assume the analytic continuation, terms of this form are all set equal to zero. So, in this sense, the continuous representation does not contribute to the partition function of the SL(2,C)/SU(2) theory after the Euclidean rotation.

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Strings in AdS_3 and the SL(2,R) WZW model. II: Euclidean black hole

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We consider the one-loop partition function for Euclidean BTZ black hole backgrounds or equivalently thermal AdS_3 backgrounds which are quotients of H_3 (Euclidean AdS_3). The one-loop partition function is modular invariant and we can read off the spectrum which is consistent to that found in hep-th/0001053. We see long strings and discrete states in agreement with the expectations. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1377039]

I. INTRODUCTION

In this paper we continue the investigation started in Ref. 1 of the SL(2,R) WZW model describing string theory on $AdS_3 \times \mathcal{M}$. For other work on this model, see Ref. 2. Our motivation is to understand string theories in curved spacetimes where the metric component g_{00} is nontrivial, of which AdS_3 is the simplest example. Moreover, it is possible to construct black hole solutions as quotients of AdS_3,[3] so understanding string theory on AdS_3 would lead to an understanding of strings moving near black hole horizons.

In Ref. 1 the spectrum of the SL(2,R) WZW model was studied, using spectral flow to generate new representations from the standard ones. These new representations include states corresponding to long strings,[5,6] with a continuous energy spectrum, as well as discrete states. The existence of spectral flow as a symmetry of the theory was argued on the basis of classical and semi-classical analysis. Further support was given by the fact that the seemingly arbitrary upper bound on the mass of string states in AdS_3 was removed, thus recovering the infinite tower of masses one expects from string theory. We would like to verify these results by an explicit calculation of the one-loop partition function. As shown in Ref. 4, the Euclidean black hole background is equivalent to the thermal AdS_3 background. So we will consider string theory on AdS_3 at a finite temperature, which is described by strings moving on a Euclidean AdS_3 background with the Euclidean time identified. The calculation of the partition function for this geometry is a minor variation on the calculation of Gawedzki in Ref. 7. From this we can read off the spectrum of the theory in Lorentzian signature by interpreting the result as the free energy of a gas of strings.

This paper is organized as follows. In Sec. II we review the spectrum found in Ref. 1. In Sec. III we compute the one-loop partition function on thermal AdS_3. In Sec. IV we read off the spectrum from the one-loop calculation. First we present a qualitative analysis, which is then followed by a precise calculation. We explain how the different parts of the spectrum arise from

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this calculation. We further show how the one-loop result contains information about the SL(2,R) and Liouville reflection amplitudes.

II. THE SPECTRUM

We begin by briefly summarizing the results of Ref. 1, where a concrete proposal for the spectrum of AdS_3 string theory was made. We consider a critical bosonic string theory on $AdS_3 \times \mathcal{M}$. The Hilbert space of the SL(2,R) WZW model is generated by the action of the left-moving and right-moving current algebra $\widehat{\mathrm{SL}(2,R)}_L \times \widehat{\mathrm{SL}(2,R)}_R$, and all the states form representations of this algebra. The simplest representations are built by first choosing representations for the zero modes, then regarding them as the primary states annihilated by $J^{3,\pm}_{n>0}$. The raising operators $J^{3,\pm}_{n<0}$ are then used to generate the representations of the current algebra. From harmonic analysis, i.e. quantum mechanical limit, it is known that the left–right symmetric combinations $\mathcal{C}^{\alpha}_{j=1/2+is} \times \mathcal{C}^{\alpha}_{j=1/2+is}$ and $\mathcal{D}^{\pm}_{j>1/2} \times \mathcal{D}^{\pm}_{j>1/2}$ form a complete basis in $\mathcal{L}^2(AdS_3)$, where $\mathcal{C}^{\alpha}_{j=1/2+is}$ is the principal continuous representation and $\mathcal{D}^{\pm}_{j>1/2}$ the principal discrete representation of SL(2,R). These representations are unitary, but the resulting current algebra representations $\hat{\mathcal{C}}^{\alpha}_{j=1/2+is} \times \hat{\mathcal{C}}^{\alpha}_{j=1/2+is}$ and $\hat{\mathcal{D}}^{\pm}_{j>1/2} \times \hat{\mathcal{D}}^{\pm}_{j>1/2}$, constructed as explained above, are not. This is not a surprise, for even in flat Minkowski space it is not until one imposes the Virasoro constraints,

$$(L_n + \mathcal{L}_n - \delta_{n,0})|\mathrm{physical}\rangle = 0, \quad n \geqslant 0, \tag{1}$$

that a unitary spectrum is obtained. Here $\mathcal{L}_n$ is the Virasoro generator for the internal conformal field theory corresponding to $\mathcal{M}$. The proposal of Ref. 1 is that one should consider not just these representations but also those obtained by the spectral flow

$$\begin{aligned} J^3_n &\to \tilde{J}^3_n = J^3_n - \frac{k}{2} w \delta_{n,0}, \\ J^+_n &\to \tilde{J}^+_n = J^+_{n+w}, \\ J^-_n &\to \tilde{J}^-_n = J^-_{n-w}. \end{aligned} \tag{2}$$

The Virasoro generators, given by the Sugawara form, then become $\tilde{L}_n = L_n + w J^3_n - k/4 w^2 \delta_{n,0}$. Imposing on $\hat{\mathcal{D}}^{\pm}_{j>1/2} \times \hat{\mathcal{D}}^{\pm}_{j>1/2}$ the condition (1) with $\tilde{L}_n$ one finds that these states have a discrete energy spectrum,

$$\begin{aligned} E &= J^3_0 + \overline{J}^3_0 = q + \overline{q} + kw + 2\tilde{j} \\ &= 1 + q + \overline{q} + 2w + \sqrt{1 + 4(k-2)(N_w + h - 1 - \tfrac{1}{2} w(w+1))}; \end{aligned} \tag{3}$$

here N_w is defined to be the level of the current algebra after spectral flow by the amount w, $N_w = \tilde{N} - wq$, and $\tilde{N}$ is the level before spectral flow. The state with energy (3) is obtained from a lowest weight state by acting with the SL(2,R) currents $\Pi \tilde{J}^{\pm}_{n \leqslant 0} |\tilde{j}, \tilde{j}\rangle$, with q the net number of $\pm$ signs in this expression. In other words, q is the number of spacetime energy raising operators J^+_a minus the number of spacetime energy lowering operators J^-_a that we have to apply to the lowest weight, lowest energy state $|\tilde{j}, m = \tilde{j}\rangle$ to get to the state whose spacetime energy is (3). $\overline{q}$ is the corresponding quantity for the generators $\overline{J^{\pm}_a}$. We also have a level matching condition of the form

$$N_w + h = \overline{N}_w + \overline{h}, \tag{4}$$

which implies that the angular momentum in AdS_3, $l=J_0^3-\overline{J}_0^3=q-\overline{q}$, is an integer. We argued in Ref. 1 that $\tilde{j}$ is further restricted to the range

$$\frac{1}{2}<\tilde{j}<\frac{k-1}{2}, \tag{5}$$

which implies

$$\frac{k}{4}w^2+\frac{1}{2}w<N_w+h-1+\frac{1}{4(k-2)}<\frac{k}{4}(w+1)^2-\frac{1}{2}(w+1). \tag{6}$$

A similar analysis on $\hat{\mathcal{C}}^{\alpha}_{j=1/2+is}\times\hat{\mathcal{C}}^{\alpha}_{j=1/2+is}$ yields a continuous spectrum,

$$E=\frac{k}{2}w+\frac{1}{w}\left(\frac{2s^2+\frac{1}{2}}{k-2}+\tilde{N}+h+\tilde{\bar{N}}+\overline{h}-2\right), \tag{7}$$

where s takes values over the real numbers and is interpreted as the momentum in the radial direction for the long strings. These states satisfy the level matching condition

$$\tilde{N}+h=\tilde{\bar{N}}+\overline{h}+w\times(\text{integer}). \tag{8}$$

In the rest of the paper we will do an independent calculation which will reproduce this single string spectrum.

III. ONE-LOOP PARTITION FUNCTION

In this section we compute the worldsheet one-loop partition function. First we explain the relation between various useful coordinate systems. Then we consider thermal $AdS_3=H_3/Z$ and show how the identification of Euclidean time in the global coordinates translates into particular boundary conditions for the target space fields. The partition function is then calculated by an explicit evaluation of the functional integral following Ref. 7.

A. Coordinates on H_3 and thermal AdS_3

The natural metric on H_3 is given by

$$ds^2=\frac{k}{y^2}(dy^2+dw\,d\overline{w}), \tag{9}$$

which is the Euclidean continuation of the Poincaré metric on AdS_3. By the coordinate transformation,

$$w=\tanh\rho e^{t+i\theta},\quad \overline{w}=\tanh\rho e^{t-i\theta},\quad y=\frac{e^t}{\cosh\rho}, \tag{10}$$

we obtain the cylindrical coordinates on Euclidean AdS_3,

$$\frac{ds^2}{k}=\cosh^2\rho\,dt^2+d\rho^2+\sinh^2\rho\,d\theta^2. \tag{11}$$

For the purpose of calculating the partition function, however, it is convenient to use coordinates in which the metric reads[7] as

$$\frac{ds^2}{k}=d\phi^2+(dv+v\,d\phi)(d\overline{v}+\overline{v}\,d\phi), \tag{12}$$

which corresponds to the parametrization of H_3 as

$$g=\begin{bmatrix} e^{\phi}(1+|v|^2) & v \\ \overline{v} & e^{-\phi} \end{bmatrix}. \tag{13}$$

The coordinate transformation from (11) to (12) is

$$\begin{aligned} v &= \sinh\rho e^{i\theta} \\ \overline{v} &= \sinh\rho e^{-i\theta} \\ \phi &= t-\log\cosh\rho. \end{aligned} \tag{14}$$

Thermal AdS_3 is given by the identification

$$t+i\theta\sim t+i\theta+\hat{\beta}, \tag{15}$$

where $\hat{\beta}$ represents the temperature T and the imaginary chemical potential $i\mu$ for the angular momentum,

$$\hat{\beta}=\beta+i\mu\beta=\frac{1}{T}+i\frac{\mu}{T}. \tag{16}$$

The corresponding identifications in the coordinates (12) are

$$\begin{aligned} v &\sim v e^{i\mu\beta} \\ \overline{v} &\sim \overline{v} e^{-i\mu\beta} \\ \phi &\sim \phi+\beta, \end{aligned} \tag{17}$$

which is a consistent symmetry of the WZW action,

$$S=\frac{k}{\pi}\int d^2z(\partial\phi\,\overline{\partial}\phi+(\partial\overline{v}+\partial\phi\,\overline{v})(\overline{\partial}v+\overline{\partial}\phi v)). \tag{18}$$

B. Computation of the partition function on thermal AdS_3

In this subsection we compute the partition function for string theory on thermal AdS_3. We consider a conformal field theory on a worldsheet torus with modular parameter τ ($z\sim z+2\pi\sim z+2\pi\tau$). The two-dimensional conformal field theory on the worldsheet is the sum of three parts: the conformal field theory on H_3, the internal conformal field theory on $\mathcal{M}$, and the (b, c) ghosts. First we start with the computation of the partition function for the conformal field theory describing the three dimensions of thermal AdS_3 and then we will multiply the result by the partition function of the ghosts and the internal conformal field theory.

Due to the identification (17), the string coordinates now satisfy the following boundary conditions:

$$\begin{aligned} &\phi(z+2\pi)=\phi(z)+\beta n, \quad \phi(z+2\pi\tau)=\phi(z)+\beta m, \\ &v(z+2\pi)=v(z)e^{in\mu\beta}, \quad v(z+2\pi\tau)=v(z)e^{im\mu\beta}. \end{aligned} \tag{19}$$

The thermal circle is noncontractible and therefore we get two integers (n,m) characterizing topologically nontrivial embeddings of the worldsheet in spacetime. In order to implement these boundary conditions it is convenient to define new fields $\hat{\phi},\hat{v}$ such that they are periodic:

$$\phi=\hat{\phi}+\beta f_{n,m}(z,\bar{z}),$$
$$v=\hat{v}\,\exp(i\mu\beta f_{n,m}(z,\bar{z})), \tag{20}$$

with

$$f_{n,m}(z,\bar{z})=\frac{i}{4\pi\tau_2}[z(n\bar{\tau}-m)-\bar{z}(n\tau-m)]. \tag{21}$$

When we substitute this into the action (18), we get

$$S=\frac{k\beta^2}{4\pi\tau_2}|n\tau-m|^2+\frac{k}{\pi}\int d^2z\left(|\partial\hat{\phi}|^2+\left|\left(\partial+\frac{1}{2\tau_2}U_{n,m}+\partial\hat{\phi}\right)\hat{\bar{v}}\right|^2\right), \tag{22}$$

where

$$U_{n,m}(\tau)=\frac{i}{2\pi}(\beta-i\mu\beta)(n\bar{\tau}-m). \tag{23}$$

We are interested in the functional integral

$$\mathcal{Z}(\beta,\mu;\tau)=\int \mathcal{D}\phi\,\mathcal{D}\bar{v}\,e^{-S}. \tag{24}$$

This integral is evaluated as explained in Ref. 7. We can first do the integral over $\hat{v},\hat{\bar{v}}$ which is quadratic, giving the determinant

$$\det\left|\partial+\frac{1}{2\tau_2}U_{n,m}+\partial\hat{\phi}\right|^{-2}. \tag{25}$$

We calculate the $\hat{\phi}$ dependence on the determinants by realizing that we can view (25) as an inverse of two fermion determinants. We can then remove $\hat{\phi}$ from the determinants by a chiral gauge transformation and using the formulas for chiral anomalies. The result is

$$\det\left|\partial+\frac{1}{2\tau^2}U_{n,m}+\partial\hat{\phi}\right|^{-2}=e^{2/\pi\int d^2z\,\partial\hat{\phi}\tilde{\partial}\hat{\phi}}\det\left|\partial+\frac{1}{2\tau^2}U_{n,m}\right|^{-2}. \tag{26}$$

The remaining integral over $\hat{\phi}$ gives the usual result for a free boson, except that $k\to k-2$ due to (26). The functional integral for the thermal AdS_3 partition function then gives

$$\begin{aligned}\mathcal{Z}(\beta,\mu;\tau)&=\frac{\beta(k-2)^{1/2}}{8\pi\sqrt{\tau_2}}\\&\quad\times\sum_{n,m}\frac{e^{-k\beta^2|m-n\tau|^2/4\pi\tau_2+2\pi(\mathrm{Im}\,U_{n,m})^2/\tau_2}}{|\sin(\pi U_{n,m})|^2|\Pi_{r=1}^{\infty}(1-e^{2\pi ir\tau})(1-e^{2\pi ir\tau}+2\pi iU_{n,m})(1-e^{2\pi ir\tau-2\pi iU_{n,m}})|^2}\\&=\frac{\beta(k-2)^{1/2}}{2\pi\sqrt{\tau_2}}(q\bar{q})^{-3/24}\sum_{n,m}\frac{e^{-k\beta^2|m-n\tau|^2/4\pi\tau_2+2\pi/(\mathrm{Im}\,U_{n,m})^2/r_2}}{|\vartheta_1(\tau,U_{n,m})|^2},\end{aligned} \tag{27}$$

where ϑ_1 is the elliptic theta function and $q=e^{2\pi i\tau}$. The factor $\beta(k-2)^{1/2}$ comes from the length of the circle in the ϕ direction. This partition function is explicitly modular invariant after summing over (n, m). [In our previous paper, there was a puzzle about the apparent lack of modular invariance of the SL(2,R) partition functions with J^3 insertions (see Appendix B of Ref. 1). Here

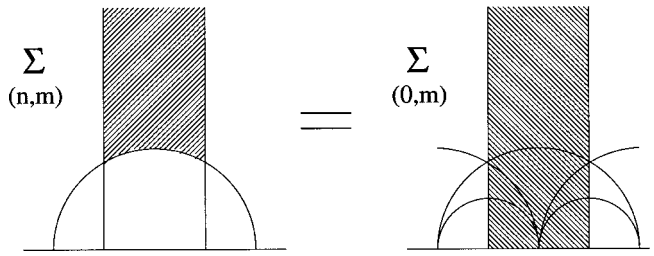

FIG. 1. The sum over n is traded for the sum over copies of the fundamental domain.

we have found that, if we introduce the twist by considering the physical set-up of thermal AdS_3, the result (27) turns out to be manifestly modular invariant. This resolves the puzzle raised in Ref. 1.]

We also need to include the contribution of the (b, c) ghosts and the internal CFT. A partition function of the latter will be of the form

$$\mathcal{Z}_{\mathcal{M}}=(q\bar{q})^{-c_{\rm int}/24}\sum_{h,\bar{h}} D(h,\bar{h})q^h\bar{q}^{\bar{h}}, \tag{28}$$

where $D(h,\bar{h})$ is the degeneracy at left-moving weight h and right-moving weight $\bar{h}$, and $c_{\rm int}$ is the central charge of the internal CFT. Modular invariance requires that $h-\bar{h}\in Z$, a fact which will be useful in the next section. Vanishing of the total conformal anomaly gives

$$c_{\mathrm{SL}(2,R)}+c_{\rm int}=26. \tag{29}$$

We can calculate now the total contribution to the ground state energy. We found a ground state energy of $-3/24$ in (27), the ghosts contribute with $2/24$ and the internal CFT with $-c_{\rm int}/24=(c_{\mathrm{SL}(2,R)}-26)/24$. Using $c_{\mathrm{SL}(2,R)}=3+6/(k-2)$, we find the overall factor,

$$(q\bar{q})^{-(1+c_{\rm int})/24}=e^{4\pi\tau_2(1-1/4(k-2))}. \tag{30}$$

[Note that $c_{\rm int}\geqslant 0$, $k>2$, and (29) imply that there will always be a tachyon in the theory.]

After multiplying (27) by the (b, c) ghosts and the internal CFT partition functions, we should integrate the resulting expression over the fundamental domain F_0 of the modular parameter τ. The computation is much facilitated by the trick invented in Ref. 8 to trade the sum over n in (27) for the sum over copies of the fundamental domain. See Fig. 1. This is possible since (n, m) transforms as a doublet under the modular group $\mathrm{SL}(2,Z)$. If $(n,m)\neq(0,0)$, it can be mapped by an $\mathrm{SL}(2,Z)$ transformation to $(0,m), m>0$. The $\mathrm{SL}(2,Z)$ transformation also maps the fundamental domain into the strip $\mathrm{Im}\,\tau\geqslant 0$, $|\mathrm{Re}\,\tau|\leqslant 1/2$. On the other hand, $(n,m)=(0,0)$ is invariant under the $\mathrm{SL}(2,Z)$ transformation, and the corresponding term still has to be integrated over the fundamental domain F_0. This term represents the zero temperature contribution to the cosmological constant, or the zero temperature vacuum energy. In addition to the usual tachyon divergence of bosonic string theory at large τ_2, it is also divergent due to the $\sin^{-1}$ factor in (27); this divergence can be interpreted as coming from the infinite volume of AdS_3. Since the temperature dependence of this term is trivial we will ignore it from now on. The final result then is that we fix $n=0$ in (27) and we integrate over the entire strip shown in Fig. 1. The one-loop partition function of bosonic string theory on $H_3/Z\times\mathcal{M}$ is then

$$Z(\beta,\mu)=\frac{\beta(k-2)^{1/2}}{8\pi}\int_0^\infty\frac{d\tau_2}{\tau_2^{3/2}}\int_{-1/2}^{1/2}d\tau_1\,e^{4\pi\tau_2(1-1/4(k-2))}\sum_{h,\bar{h}}D(h,\bar{h})q^h\bar{q}^{\bar{h}}$$
$$\times\sum_{m=1}^\infty\frac{e^{-(k-2)m^2\beta^2/4\pi\tau_2}}{|\sinh(m\hat{\beta}/2)|^2}\left|\prod_{n=1}^\infty\frac{1-e^{2\pi in\tau}}{(1-e^{m\hat{\beta}+2\pi in\tau}(1-e^{-m\hat{\beta}+2\pi in\tau})}\right|^2. \tag{31}$$

IV. READING OFF THE SPECTRUM

We will now extract the spectrum of Lorentzian string theory on AdS_3 by interpreting the one-loop partition function in the spacetime theory. The one-loop partition function is the single particle contribution to the spacetime thermal free energy, $Z(\beta,\mu)=-\beta F$. To this each string state makes a contribution $\beta^{-1}\log(1-e^{-\beta(E+i\mu l)})$, where E and l are the energy and the angular momentum of the state. The total free energy is the sum over all such factors:

$$F(\beta,\mu)=\frac{1}{\beta}\sum_{\text{string}\in\mathcal{H}}\log(1-e^{-\beta(E_{\text{string}}+i\mu l_{\text{string}})})=\sum_{m=1}^\infty f(m\beta,m\mu), \tag{32}$$

where

$$f(\beta,\mu)=\frac{1}{\beta}\sum_{\text{string}\in\mathcal{H}}e^{-\beta(E_{\text{string}}+i\mu l_{\text{string}})}. \tag{33}$$

Here $\mathcal{H}$ is the physical Hilbert space of single string states. In both (31) and (32), we have the sums over functions of $(m\beta,m\mu)$. It is therefore sufficient to compare the $m=1$ terms in these expressions. In other words, we want to verify that E_{string} and l_{string} extracted from the identification,

$$f(\beta,\mu)=\sum_{\text{string}\in\mathcal{H}}\frac{1}{\beta}e^{-\beta(E_{\text{string}}+i\mu l_{\text{string}})}$$
$$=\frac{(k-2)^{1/2}}{8\pi}\int_0^\infty\frac{d\rho_2}{\tau_2^{3/2}}\int_{-1/2}^{1/2}d\tau_1\,e^{4\pi\tau_2(1-1/4(k-2))}\sum_{h,\bar{h}}D(h,\bar{h})q^h\bar{q}^{\bar{h}}$$
$$\times\frac{e^{-(k-2)\beta^2/4\pi\tau_2}}{|\sinh(\hat{\beta}/2)|^2}\left|\prod_{n=1}^\infty\frac{1-e^{2\pi in\tau}}{(1-e^{\hat{\beta}+2\pi in\tau})(1-e^{-\hat{\beta}+2\pi in\tau})}\right|^2, \tag{34}$$

agree with the string spectrum found in our previous paper.[1] We will see that the sum over the Hilbert space breaks up into a sum over the discrete states and an integral over the continuous states, with the expressions for the energies that were reviewed in Sec. II. Since the one-loop calculation presented here is independent of the assumptions made in Ref. 1 about strings in Lorentzian AdS_3, we can regard this as a derivation of the spectrum starting from the well-defined Euclidean path integral.

A. Qualitative analysis

In this subsection we will analyze (34) in a qualitative way and explain where the different contributions to the spectrum come from. To keep the notation simple, we set $\mu=0$ in this subsection, leaving the exact computation for the next subsection.

As expected, in (34) there is an exponential divergence as $\tau_2\to\infty$, coming from the tachyon. This is just as in the flat space case, where $(\text{mass})^2<0$ of the tachyon causes its contribution to be weighted with a positive exponential. We will disregard this divergence. [A skeptical reader could think that we are really doing the superstring partition function (the fermions included in the internal CFT, etc.). Then the tachyon divergence will disappear but one would still find the

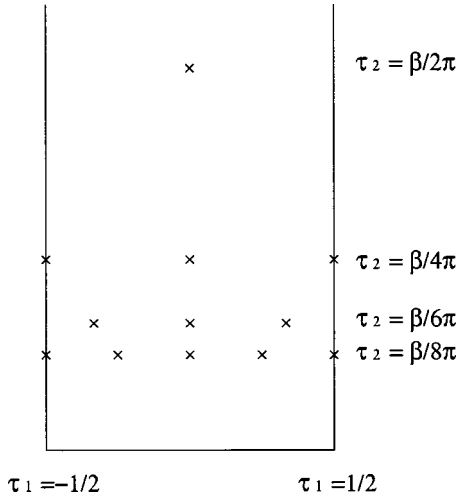

FIG. 2. Poles in the τ-plane, shown for $w=1$ to 4.

divergences that we discuss below. Of course, the one-loop partition function is nonvanishing even in the supersymmetric case since the thermal boundary conditions break supersymmetry.] However, rather unexpectedly, the expression above has additional divergences at finite values of τ. In string theory one might naively expect that divergences come only from the corners of the fundamental domain in the τ-plane, but in this case the divergence is coming from points in the interior of the fundamental domain. Overcoming the initial panic, one realizes that these divergences are related to the presence of long strings. In fact, as with any other string divergence, it can be interpreted as an IR effect. This divergence is due to the fact that long strings feel a flat potential as they go to infinity and therefore we get an infinite volume factor. To see this, note that near the pole (see Fig. 2),

$$\tau=\tau_{\text{pole}}+\epsilon, \tag{35}$$

where

$$\tau_{\text{pole}}=\frac{r}{w}+i\frac{\beta}{2\pi w}, \tag{36}$$

we can expand the partition function and replace τ in all terms by its value at the pole, except in the one term that has the pole. If we integrate (34) near the pole, i.e. in the region $\epsilon<|\tau-\tau_{\text{pole}}|\ll 1$, we find that it diverges as $\log\epsilon$ with the coefficient

$$\frac{1}{\sqrt{w\beta^3}}\exp\left[-\beta\left(\frac{k}{2}w+\frac{1}{w}\left(\tilde{N}+h+\tilde{\bar{N}}+\bar{h}-2+\frac{1}{2(k-2)}\right)\right)+\frac{2\pi i r}{w}(\tilde{N}+h-\tilde{\bar{N}}-\bar{h})\right]. \tag{37}$$

We now sum over r, with $|r/w|\leqslant 1/2$, since these are the ones corresponding to the poles in the strip. (If some poles are on the boundaries of the strip, $\tau_1=\pm 1/2$, then we only count them once.) This sum constrains $\tilde{N}+h-\tilde{\bar{N}}-\tilde{h}$ to be an integer multiple of w, as in (8), and it introduces an additional factor of w in (37). The log divergence in the τ-integral can therefore be expressed as

$$f(\beta,\mu)\sim\frac{1}{\beta}\log\epsilon\int_0^\infty ds\, e^{-\beta E(s)}+\cdots, \tag{38}$$

where $E(s)$ is the energy spectrum given by (7). Note that the s-integral and the sum over r we mentioned above give the factor $\sqrt{w/\beta}$ needed to match the prefactor in (37) to that in (38). This

reproduces the expected contribution from the long strings on the left hand side of (34). The logarithmic divergence should be interpreted as a volume factor due to the fact that the long string can be at any radial position. In the next subsections, we will see more precisely that it is indeed associated to the infinite volume in spacetime by relating ϵ to a long distance cutoff.

Now we would like to calculate the short string spectrum. Since the long string spectrum gives a divergent result, while the short string spectrum gives a finite one, it might appear at first that extracting the contributions due to the short strings from a divergent expression such as (34) will be problematic. Fortunately we can get around this difficulty since the temperature dependence of the long string free energy is different from that of the short string free energy. In the next subsection we will explain how to do this precisely and reproduce the short string spectrum which agrees with Ref. 1. One of the more puzzling aspects of the short string spectrum found there is that there is a cutoff $1/2<\tilde{j}<(k-1)/2$ in the value of the SL(2,R) spin $\tilde{j}$. In the remainder of this section we will explain in a qualitative way how this cutoff arises by doing the calculation for large k.

If we were to evaluate the right hand side of (34) naively (and incorrectly), we would expand the integrand in powers of $q=e^{2\pi i\tau}$ and then perform the τ-integral. If we did this, we would obtain the short string spectrum with $w=0$ and no upper bound on the value of $\tilde{j}$. However this expansion is not correct. How we can expand the integrand in (34) depends on the value of τ_2. When we cross the poles at $\tau_2=\beta/2\pi w$, a different expansion should be used for the denominator:

$$\frac{1}{1-e^{\beta+2\pi i w\tau}}=\sum_{q=0}^{\infty} e^{q(\beta+2\pi i w\tau)}\left(\tau_2>\frac{\beta}{2\pi w}\right),$$
$$=-\sum_{q=0}^{\infty} e^{-(q+1)(\beta+2\pi i w\rho)}\left(\tau_2<\frac{\beta}{2\pi w}\right). \tag{39}$$

When τ_2 is in the range

$$\frac{\beta}{2\pi(w+1)}<\tau_2<\frac{\beta}{2\pi w}, \tag{40}$$

the product over n in the first term in the denominator in (34) is broken up into two factors, a product in $1\leqslant n\leqslant w$ and a product in $w+1\leqslant n$. The first factor is expanded in powers of $e^{(-\beta+2\pi i n\tau)}$ and the second factor is expanded in powers of $e^{\beta+2\pi i n\tau}$. Combining them together with the terms coming from the expansion of the remaining products in (34), we get an exponent of the form[6]

$$-(\tfrac{1}{2}+q+w)\beta+2\pi i\tau(N_w-\tfrac{1}{2}w(w+1)), \tag{41}$$

for some integers q and N_w. [The first term $-\beta/2$ comes from expanding $1/\sinh(\beta/2)$ in (34).] There is a similar term for $\tau\to\bar{\tau}$. We are then to do the τ-integral of the form

$$\int \frac{d^2\tau}{\tau_2^{3/2}}$$
$$\times e^{4\pi\tau_2(1-1/4(k-2))-(k-2)(\beta^2/4\pi\tau_2)-\beta(1+q+\bar{q}+2w)+2\pi i\tau(N_w+h-(1/2)w(w+1))-2\pi i\bar{\tau}(\bar{N}_w+\bar{h}-(1/2)w(w+1))}, \tag{42}$$

over the region (40). The integral over τ_1 produces the level matching condition (4). Now we evaluate the integral over τ_2 using the saddle point approximation. We find that the saddle point is at

$$\tau_{\rm saddle}=\frac{(k-2)\beta}{2\pi\sqrt{1+4(k-2)(N_w+h-1-\frac{1}{2}w(w+1))}}, \tag{43}$$

and the integral gives

$$\frac{1}{\beta}\exp\left[-\beta\left(1+q+\bar{q}+2w+\sqrt{1+4(k-2)\left(N_w+h-1-\frac{1}{2}w(w+1)\right)}\right)\right]. \tag{44}$$

This is the correct form of the contributions due to the short strings on the left hand side of (34). Moreover we obtain the bound on $\tilde{j}$ precisely, because $\tau_{\rm saddle}$ has to be in the range (40) in order for the saddle point approximation to give a nonzero result. By (43), this condition is the same as the bound on the spectrum (6), which is equivalent to $1/2<\tilde{j}<(k-1)/2$. (It is a bit surprising that we get all factors precisely right from the saddle point approximation.) Notice then that the cutoff in $\tilde{j}$ is associated to the fact that we expand the integrand in (34) in different ways depending on the value of τ. The value of τ making the biggest contribution to the integral depends on the values of N and h of the string state.

B. A precise evaluation of the τ-integral

Now let us study the partition function (34) more systematically. In this subsection, we go back to the general case with $\mu\neq 0$. From what we saw in the previous subsection, we expect to find the discrete states from the integral over the range (40), and the continuous states from the poles after a suitable regularization.

In order to evaluate the τ-integral exactly, it is useful to introduce a new variable c by

$$e^{-(k-2)(\beta^2/4\pi\tau_2)}=-\frac{8\pi i}{\beta}\left(\frac{\tau_2}{k-2}\right)^{3/2}\int_{-\infty}^{\infty}dc\;\; ce^{-[4\pi\tau_2/(k-2)]c^2+2i\beta c}. \tag{45}$$

Now suppose τ_2 is in the range

$$\frac{\beta}{2\pi(w+1)}<\tau_2<\frac{\beta}{2\pi w}, \tag{46}$$

and expand the integrand in (34) as explained in the previous subsection. The right hand side of (34) becomes a sum of terms like

$$\frac{4}{\beta(k-2)i}\int_{-\infty}^{\infty}dc\;\; c\int_{\beta/2\pi(w+1)}^{\beta/2\pi w}d\tau_2\int_{-1/2}^{1/2}d\tau_1\exp\left[-\hat{\beta}\left(q+w+\frac{1}{2}\right)-\hat{\bar{\beta}}\left(\bar{q}+w+\frac{1}{2}\right)\right.$$
$$\left.+2\pi i\tau_1(N_w+h-\bar{N}_w-\bar{h})+2ic\beta-2\pi\tau_2\left(h+\bar{h}+N_w+\bar{N}_w+\frac{2c^2+\frac{1}{2}}{k-2}-w(w+1)-2\right)\right]. \tag{47}$$

The integral over τ_1 gives a delta function enforcing $N_w+h=\bar{N}_w+\bar{h}$, which is the level-matching condition (4). Integrating over τ_2 in the range (46) gives

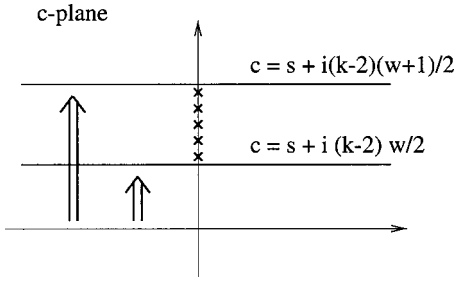

FIG. 3. Shifting the contour of integration picks up the pole residues corresponding to the short string spectrum.

$$\frac{1}{\beta\pi i}\int_{-\infty}^{\infty} dc\ \ c\,\frac{\exp[2ic\beta-\hat{\beta}(q+w+\frac{1}{2})-\hat{\bar{\beta}}(\bar{q}+w+\frac{1}{2})]}{c^2+\frac{1}{4}+(k-2)(N_w+h-1-\frac{1}{2}w(w+1))}$$
$$\times\left\{-\exp\left[-\frac{\beta}{w}\left(2N_w+2h-2+\frac{2c^2+\frac{1}{2}}{k-2}-w(w+1)\right)\right]\right.$$
$$\left.+\exp\left[-\frac{\beta}{w+1}\left(2N_w+2h-2+\frac{2c^2+\frac{1}{2}}{k-2}-w(w+1)\right)\right]\right\}, \tag{48}$$

where we used (4).

Let us first look at the first term (the second line) in (48). We note that the exponent can be expressed in the form of a complete square if we set $c=s+(i/2)(k-2)w$. As it will become clear shortly, it is natural to shift the contour of the c-integral from $\mathrm{Im}\,c=0$ to $\mathrm{Im}\,c=1/2(k-2)w$ so that s becomes real. During this process the contour crosses some poles in the integrand, picking up the residues of the poles in the range $0<\mathrm{Im}\,c<1/2(k-2)w$. See Fig. 3. The poles are located at

$$-\frac{c^2}{(k-2)}=N_w+h-\frac{1}{2}w(w+1)-1+\frac{1}{4(k-2)}<\frac{k-2}{4}w^2. \tag{49}$$

Similarly, for the second exponential term (the third line) in (48) we shift the contour to $c=s+(i/2)(k-2)(w+1)$ with s real. This picks up the poles at

$$-\frac{c^2}{(k-2)}=N_w+h-\frac{1}{2}w(w+1)-1+\frac{1}{4(k-2)}<\frac{k-2}{4}(w+1)^2. \tag{50}$$

It is important to note that the residues of these poles have a sign opposite to that of the residues of the poles obeying (49). So the result is that we are left with only those poles in the range

$$\frac{k-2}{2}w<\mathrm{Im}\,c<\frac{k-2}{2}(w+1), \tag{51}$$

with residues

$$\frac{1}{\beta}\exp[-\hat{\beta}q-\hat{\bar{\beta}}\bar{q}-\beta(1+2w+\sqrt{1+4(k-2)(N_w+h-1-\tfrac{1}{2}w(w+1))})]. \tag{52}$$

This is the expected contribution of the short strings to the right hand side of (34), and we see also that (51) translates into the correct bound on $\tilde{j}$ (5).

It remains to examine the resulting integral over s. Notice that the term coming from just above the pole at $\tau=\hat{\beta}/2\pi w$ has a very similar w dependence in the exponent as that coming from

just below the pole. In other words, we combine the first term of (48) with the second term of an expression similar to (48) but with $w\to w-1$ and we find, after shifting the contours as above,

$$\frac{1}{2\pi i\beta}\int_{-\infty}^{\infty}ds\left(\frac{2s}{w(k-2)}+i\right)\left(\frac{\exp\left[-\hat{\beta}q-\hat{\bar{\beta}}\bar{q}-\beta\left(\frac{k}{2}w+\frac{2}{w}\left(\frac{s^2+1/4}{k-2}+N_{w-1}+h-1\right)\right)\right]}{\frac{1}{2}+is-\frac{k}{4}w+\frac{1}{w}\left(N_{w-1}+h-1+\frac{s^2+1/4}{k-2}\right)}\right.$$
$$\left.-\frac{\exp\left[-\hat{\beta}q-\hat{\bar{\beta}}\bar{q}-\beta\left(\frac{k}{2}w+\frac{2}{w}\left(\frac{s^2+1/4}{k-2}+N_{w}+h-1\right)\right)\right]}{-\frac{1}{2}+is-\frac{k}{4}w+\frac{1}{w}\left(N_{w}+h-1+\frac{s^2+1/4}{k-2}\right)}\right). \tag{53}$$

Let us concentrate for now on the third line of (53). We first note that the sum of such terms over all states gives rise to the log divergence. To see this, it is useful to notice that the combinations

$$\tilde{N}=qw+N_w,\quad \tilde{\bar{N}}=\bar{q}w+\bar{N}_w, \tag{54}$$

that appear in the exponent of the third line of Eq. (53) are the levels before spectral flow. Thus, for a given state $|\psi\rangle$, states of the form $(\tilde{J}_0^+\tilde{\bar{J}}_0^+)^n|\psi\rangle$ all have the same value of $\tilde{N}$ and $\tilde{\bar{N}}$. Acting with $\tilde{J}_0^+\tilde{\bar{J}}_0^+$ on $|\psi\rangle$ does not change the exponent in (53), but it does change the denominator by one. This implies that when we sum over all the states of this type, we will find a divergent sum of the form

$$\sum_{n=0}^{\infty}\frac{1}{A-n}.$$

This divergence has the same origin as the divergence of the right hand side of (34) at the pole $\tau_{\rm pole}=\hat{\beta}/2\pi w$. In fact, if we regularize the τ-integral by removing a small region near the pole as $|\tau-\tau_{\rm pole}|>\epsilon$, we find an additional factor $e^{-n\epsilon}$ in the sum. In the next subsection, we will give the spacetime interpretation of this procedure. With this regularization, the sum behaves as $\log\epsilon$. More precisely we have

$$-\sum_{n=0}^{\infty}\frac{1}{A-n}e^{-n\epsilon}=\log\epsilon+\frac{d}{dA}\log\Gamma(-A)+\mathcal{O}(\epsilon), \tag{55}$$

where

$$A=-\frac{1}{2}+is-\frac{k}{4}w+\frac{1}{w}\left(\frac{s^2+\frac{1}{4}}{k-2}+\tilde{N}+h-1\right). \tag{56}$$

Here we have assumed that

$$\tilde{\bar{N}}+\bar{h}\leqslant\tilde{N}+h, \tag{57}$$

but it can be seen that the other case gives the same result.

Now we turn our attention to the second line of (53). In those terms we have one less unit of spectral flow, as compared to the third line in (53) that we analyzed above. In other words, now we will have that $(w-1)q+N_{w-1}=\tilde{N}'$. These states are in the spectral flow image of $\mathcal{D}_j^+$. Since we want to combine these states with the states coming from the third line in (53) it is convenient to do spectral flow one more time and think of these states as in the spectral flow image of $\mathcal{D}_j^-$ under w units of spectral flow. In this case we find that $q+\tilde{N}'=\tilde{N}$ where now $\tilde{N}$ is the level of the $\mathcal{D}_j^-$

representation before spectral flow. From now on the discussion is very similar to what we had above. The states with $(\tilde{J}_0^- \bar{\tilde{J}}_0^-)^n|\psi\rangle$ all have the same energies but they will contribute to the denominator of the second line in (53) with

$$\sum_{n=0}^{\infty} \frac{1}{B+n} e^{-ne} = \log \epsilon - \frac{d}{dB} \log \Gamma(B) + \mathcal{O}(\epsilon), \tag{58}$$

where

$$B = \frac{1}{2} + is - \frac{k}{4} w + \frac{1}{w} \left(\frac{s^2 + \frac{1}{4}}{k-2} + \bar{\tilde{N}} + \bar{h} - 1 \right). \tag{59}$$

again assuming (57).

After we perform these two sums, we find that (53) can be written in the form

$$\frac{2}{\beta} \int_0^{\infty} ds\, \rho(s) \exp\left[-\beta \left(E(s) + i \frac{\mu}{w} (\tilde{N} + h - \bar{\tilde{N}} - \bar{h}) \right) \right], \tag{60}$$

with $E(s)$ the energy of long strings (7) and $\rho(s)$ the density of states. We will later see that the physical momentum p of a long string in the ρ direction is equal to $p = 2s$. The angular momentum $l = (\tilde{N} + h - \bar{\tilde{N}} - \bar{h})/w$ is an integer since the states in (53) were obeying (4) and the definition (54) ensures that (8) is satisfied. The density of states $\rho(s)$ derived from this analysis is

$$\rho(s) = \frac{1}{2\pi} 2 \log \epsilon + \frac{1}{2\pi i} \frac{d}{2ds} \log \left(\frac{\Gamma(\frac{1}{2} - is + \tilde{m}) \Gamma(\frac{1}{2} - is - \bar{\tilde{m}})}{\Gamma(\frac{1}{2} + is + \tilde{m}) \Gamma(\frac{1}{2} + is - \bar{\tilde{m}})} \right), \tag{61}$$

where

$$\tilde{m} = -\frac{k}{4} w + \frac{1}{w} \left(\frac{s^2 + \frac{1}{4}}{k-2} + \tilde{N} + h - 1 \right), \quad \bar{\tilde{m}} = -\frac{k}{4} w + \frac{1}{w} \left(\frac{s^2 + \frac{1}{4}}{k-2} + \bar{\tilde{N}} + \bar{h} - 1 \right). \tag{62}$$

Note that, despite appearances to the contrary, (61) is actually symmetric under $\tilde{m} \leftrightarrow \bar{\tilde{m}}$ since $\tilde{m} - \bar{\tilde{m}} = l$ is an integer. In the next subsection we will show that this density of states (61) is what is expected from the spacetime meaning of the cutoff ϵ. In going from (53) to (60) we have states which could be interpreted as coming from the spectral flow of the discrete representations $\mathcal{D}_j^+$ and $\mathcal{D}_j^-$, with the zero modes essentially stripped off since they were explicitly summed over in (55) and (58). This implies that the states we have in the end belong to the continuous representation. Note also that the integral over s in (60) has only half the range in (53). We rewrote it in this way using the fact that the exponent is invariant under $s \to -s$, and that is the reason why we have four gamma functions in (61). In going from (53) to (60) we have also used that $d/dA = (1/d/dA(s)/ds)(d/ds)$ in (56) and similarly in (59).

Combining Eqs. (52) and (60), we have, finally,

$$f(\beta,\mu) = \frac{1}{\beta} \sum D(h,\bar{h},\tilde{N},\bar{\tilde{N}},w) \left[\sum_{q,q} e^{-\beta(E + i\mu l)} + \int_0^{\infty} ds \rho(s) e^{-\beta(E(s) + i\mu l)} \right] \tag{63}$$

which is the free energy due to the short strings and the long strings, respectively.

C. The density of long string states

What remains to be shown is the interpretation of $\rho(s)$ given by (61) as the density of long string states. Whenever we have a continuous spectrum the density of states may be calculated by

first introducing a long distance cutoff which will make the spectrum discrete, and then removing the cutoff. If the cutoff is related to the volume of the system then the density of states will have a divergent part, proportional to the volume and dependent only on the bulk physics, and a finite part which encodes information about the scattering phase shift and also has some dependence on the precise cutoff procedure. To see this, let us consider a one-dimensional quantum mechanical model on the half line, $\rho>0$, with a potential $V(\rho)$. We assume that $V(\rho)$ vanishes sufficiently fast for large ρ, and that there is continuous spectrum above a certain energy level. To define the density of states, it is convenient to introduce a long distance cutoff at large ρ so that the spectrum becomes discrete. Let us first consider a cutoff by an infinite wall at $\rho=L$. If L is sufficiently large, an energy eigenfunction $\psi(\rho)$ near the wall can be approximated by the plane wave,

$$\psi(\rho)\sim e^{-ip\rho}+e^{ip\rho+i\delta(p)}, \tag{64}$$

where $\delta(p)$ is the phase shift due to the original potential $V(\rho)$. Imposing Dirichlet boundary condition $\psi(L)=0$ at the wall, we have

$$2pL+\delta(p)=2\pi(n+\tfrac{1}{2}), \tag{65}$$

for some integer n. If L is sufficiently large, there is a unique solution $p=p(n)$ to this equation for a given n. As we remove the cutoff by sending $L\to\infty$, the spectrum of p becomes continuous. We then define the density of states $\rho(p)$ by

$$dn=\rho(p)dp. \tag{66}$$

From (65), we obtain

$$\rho(p)=\frac{1}{2\pi}\left(2L+\frac{d\delta}{dp}\right). \tag{67}$$

Thus the finite part of the density of states is given by the derivative of the phase shift.

Instead of the infinite wall at $\rho=L$, we may consider a more general potential $V_{\text{wall}}(\rho-L)$ which vanishes for $\rho<L$ but rises steeply for $L<\rho$ to confine the particle. Let us denote by $\delta_{\text{wall}}(p)$ the phase shift due to scattering from $V_{\text{wall}}(\rho)$. We then obtain the condition on the allowed values of momenta by matching these two wavefunctions and their derivatives at $\rho=L$ as

$$\psi(\rho)\sim e^{-ip\rho}+e^{ip\rho+i\delta(p)}\sim A[e^{-ip(\rho-L)}+e^{ip(\rho-L)+i\delta_{\text{wall}}(p)}] \quad (\rho\sim L). \tag{68}$$

It follows that

$$pL+\delta(p)=-pL+\delta_{\text{wall}}(p)+2\pi n. \tag{69}$$

In the limit $L\to\infty$, the density of states given by $dn=\rho(p)dp$ is then

$$\rho(p)=\frac{1}{2\pi}\left(2L+\frac{d\delta}{dp}-\frac{d\delta_{\text{wall}}}{dp}\right). \tag{70}$$

When we have the infinite wall, the phase shift due to the wall is independent of $p(\delta_{\text{wall}}=\pi)$, and (70) reduces to (67).

In order to apply this observation to our problem, it is useful to first identify the origin of the logarithmic divergence in the one-loop amplitude $Z(\beta,\mu)$ by examining the functional integral (24) near the boundary of AdS_3. In the cylindrical coordinates (11), the string worldsheet action (18) for large ρ takes the form

$$S\sim\frac{k}{\pi}\int d^2z\left(\partial\rho\,\bar{\partial}\rho+\frac{1}{4}e^{2\rho}|\bar{\partial}(\theta-it)|^2+\cdots\right). \tag{71}$$

Because of the factor $e^{2\rho}$, the functional integral for large ρ restricts (t,θ) to be a harmonic map from the worldsheet to the target space. Since (t,θ) are coordinates on the torus,

$$\theta - it \sim \theta - it + 2\pi n + i\hat{\beta} m \quad (n,m \quad \text{integers}), \tag{72}$$

the harmonic map from the torus to the torus is

$$\begin{aligned}\theta - it &= (2\pi w + i\hat{\beta} m)\sigma^t + (2\pi r + i\hat{\beta} n)\sigma^2 \\ &= [(2\pi w + i\hat{\beta} m)\tau - (2\pi r + i\hat{\beta} n)]\frac{\overline{z}}{2i\tau_2} \\ &\quad - [(2\pi w + i\hat{\beta} m)\overline{\tau} - (2\pi r + i\hat{\beta} n)]\frac{z}{2i\tau_2},\end{aligned} \tag{73}$$

where $z = \sigma^1 + \rho\sigma^2$ is the worldsheet coordinate and (r, w, n, m) are integers. In particular, the map $(\theta - it)$ with $(n,m) = (1,0)$ becomes w–to–1 and *holomorphic* when τ takes the special value

$$\tau_{\text{pole}} = \frac{r}{w} + i\frac{\hat{\beta}}{2\pi w}. \tag{74}$$

On the other hand, if τ is not at one of these points, $\overline{\partial}(\theta - it)$ cannot be set to zero. [For any τ, we also have a trivial holomorphic map $(t,\theta) = \text{const}$. The functional integral around such a map gives a result independent of β and we can neglect it in the following discussion.] This gives rise to an effective potential $e^{2\rho}$ for ρ, which keeps the worldsheet from growing towards the boundary. If τ is near τ_{pole},

$$\tau = \tau_{\text{pole}} + \epsilon, \tag{75}$$

the harmonic map (73) with $(n,m) = (1,0)$ gives

$$|\overline{\partial}(\theta - it)|^2 \sim \left(\frac{2\pi^2 w^2}{\beta}\right)^2 \epsilon^2. \tag{76}$$

Thus the action (71) generates the Liouville potential $\epsilon^2 e^{2\rho}$. When we computed the one-loop amplitude in Secs. IV A and IV B, we regularized the τ-integral by removing a small disk $|\tau - \tau_{\text{pole}}| < \epsilon$ around each of these special points. Near $\tau = \tau_{\text{pole}}$, this is equivalent to adding the infinitesimal Liouville potential $\epsilon^2 e^{2\rho}$ to the worldsheet action. For $|\tau - \tau_{\text{pole}}| \gg \epsilon$, the worldsheet can never grow large enough and the effect of the Liouville term is negligible. To be precise, the Gaussian functional integral of (t,θ) shifts $k \to (k-2)$ as in (26) and the effective action for ρ near $\tau = \tau_{\text{pole}}$ is

$$S_{\text{Liouville}} = \frac{k-2}{\pi}\int d^2z(\partial\rho\,\tilde{\partial}\rho + \epsilon^2 e^{2\rho}). \tag{77}$$

Therefore, we find that our choice of regularization in (55) and (58) amounts to introducing the Liouville wall which prevents the longs strings from going to very large values of ρ. By looking at the potential in (77), we see that the effective length of the interval is $L \sim \log\epsilon$. The central charge of this Liouville theory is such that the $e^{2\rho}$ term has conformal weight one,

$$c_{\text{Liouville}} = 1 + 6\left(b + \frac{1}{b}\right)^2, \quad b \equiv \frac{1}{\sqrt{k-2}}. \tag{78}$$

The finite part of the density of states will be given through (70) by $\delta(s)$, the phase shift in the SL(2,R) model, and $\delta_{\text{wall}}(s)$, the corresponding quantity in Liouville theory. The first one was calculated in Refs. 9 and 10,

$$i\,\delta(s)=\log\left(\frac{\Gamma\left(\frac{1}{2}+is-\tilde{m}\right)\Gamma\left(\frac{1}{2}+is+\tilde{m}\right)\Gamma(-2is)\Gamma\left(\frac{2is}{k-2}\right)}{\Gamma\left(\frac{1}{2}-is-\tilde{m}\right)\Gamma\left(\frac{1}{2}-is+\tilde{m}\right)(2is)\Gamma\left(\frac{-2is}{k-2}\right)}\right), \tag{79}$$

while the second one was obtained in Refs. 11 and 12,

$$i\,\delta_{\text{wall}}(s)=\log\left(\frac{\Gamma(-2is)\Gamma\left(\frac{2is}{k-2}\right)}{\Gamma(2is)\Gamma\left(\frac{-2is}{k-2}\right)}\right). \tag{80}$$

[In order to compare with the expressions in Refs. 11, 12, we use the value of b given in (78) and note that the relevant values of α are $\alpha=Q/2+$isb.] Using these two formulas we can check that indeed the density of states (61) is given by (70). We can view this as an independent calculation of (79) or as an overall consistency check. Notice that the physical momentum p of a long string along the ρ direction is $p=2s$. This can be seen by comparing the energy of a long string (7) with the energy expected from (77) with spacetime momentum p along the radial direction, $p=(k-2)w\dot{\rho}$. We have chosen the variable s since it is conventional to denote by $j=1/2+is$ the SL(2,R) spin of a continuous representation.

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Vertex operators for AdS3 with Ramond background

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This review gives results on vertex operators for the Type IIB superstring in an AdS3×S3 background with Ramond–Ramond flux, which were presented at Strings 2000. Constraint equations for these vertex operators are derived, and their components are shown to satisfy the supergravity linearized equations of motion for the six-dimensional (2, 0) theory of a supergravity and tensor multiplet expanded around AdS3×S3 space-time. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The conjectured duality between M-theory or Type IIB string theory on anti-de Sitter (AdS) space and the conformal field theory on the boundary of AdS space may be useful in giving a controlled systematic approximation for strongly coupled gauge theories. Examples with maximal supersymmetry correspond to a set of p-branes whose near horizon geometry looks like $\mathrm{AdS}_{p+2} \times S^{\mathcal{D}-p-2}$, where $\mathcal{D}=10$ or 11 for branes in string or M-theory, and $p=2,3,5$. The formulation of vertex operators and string theory tree amplitudes for the IIB superstring on $\mathrm{AdS}_5 \times S^5$ will allow access to the dual conformal SU(N) gauge field theory CFT_4 at large N, but *small* fixed 't Hooft coupling $x=g_{YM}^2 N$ in the dual picture, as $(g_{YM}^2 N)^{1/2}(4\pi)^{1/2}=R_{sph}^2/\alpha'$. Presently only the large N, and *large* fixed 't Hooft coupling x limit, is accessible in the *CFT*, since only the supergravity limit $(\alpha' \to 0)$ of the correlation functions of the AdS theory is known.

In this article we discuss a case with nonmaximal supersymmetry that is related to a system with a $D1$-brane and a $D5$-brane. Its quantizable worldsheet action[1] describes the IIB string on $\mathrm{AdS}_3 \times S^3 \times M$ with background Ramond–Ramond flux, where M is T^4 or $K3$. The vertex operators for this model can be computed explicitly in the bulk.[2] Correlation functions constructed from these vertex operators, restricted to the boundary of AdS_3, would be those for a two-dimensional space–time conformal field theory. We work to leading order in α', but because of the high degree of symmetry of the model, we expect our result for the vertex operators to be exact. Tree level n-point correlation functions for $n \geqslant 4$ presumably have α' corrections, since the worldsheet theory is not a free conformal field theory. But there may be sufficiently many symmetry currents to determine the tree level correlation functions exactly in α' as well.[3]

In terms of Berkovits–Vafa–Witten worldsheet variables, constraint equations for the vertex operators in the flat space $\mathcal{R}^6$ follow from the physical state conditions coming from an $N=4$ superconformal algebra. We generalize[2] these constraint equations to $\mathrm{AdS}_3 \times S^3$ for the vertex operators of the massless states that are independent of the compactification M. We then solve the constraints and identify the components of the vertex operators as supergravity fields that satisfy the $D=6$, $N=(2,0)$ theory[4] linearized around the $\mathrm{AdS}_3 \times S^3$ background.

Recent work[5,6] discusses covariant ten-dimensional worldsheet variables and extends our analysis to vertex operators on AdS_5 in a spinor formulation.

II. FORMULATING STRINGS ON AdS

In the Ramond–Neveu–Schwarz (RNS) formalism, the worldsheet action for strings on AdS space with background Ramond–Ramond flux involves 2-D spin fields. These violate supercon-

formal worldsheet symmetry, since the worldsheet supercurrents are not local with respect to the spin fields, and their presence makes the worldsheet theory difficult to understand.

For the Type IIB superstring on $AdS_3\times S^3$ case, a sigma model[1] with conventional local interactions (no spin fields in the action) was found using the supergroup PSU(2|2) as target, coupled to ghost fields ρ and σ. The space-time symmetry group is PSU(2|2)×PSU(2|2), acting by left and right multiplication on the group manifold, i.e., by $g\rightarrow agb^{-1}$ where g is a PSU(2|2)-valued field, and $a,b\in$ PSU(2|2) are the symmetry group's Lie algebra elements. The supergroup is generated by the super Lie algebra with 12 bosonic generators forming a subalgebra SO(4)×SO(4) together with 16 odd generators. Hence our model has nonmaximal supersymmetry with 16 supercharges.

The worldsheet field content generalizes the Berkovits–Vafa formalism which provides a manifest Lorentz covariant and supersymmetric quantization on R^6. Its six bosonic fields $x^p(z,\overline{z})$ contain both left- and right-moving modes. In addition there are left-moving fermi fields $\theta^a_L(z),p^a_L(z)$ of spins 0 and 1, together with ghosts $\sigma_L(z),\rho_L(z)$, and right-moving counterparts of all these left-moving fields. These variables allow Ramond–Ramond background fields to be incorporated without adding spin fields to the worldsheet action as follows: in the $AdS_3\times S^3$ case, i.e., after adding RR background fields to the worldsheet action, one can integrate out the p's, so that the model has ordinary conformal fields $x^p,\theta^a,\overline{\theta^a}$ (all now with both left- and right-moving components) as well as the ghosts. The PSU(2|2)-valued field g is given in terms of x, θ, and $\overline{\theta}$, which are identified as coordinates on the supergroup manifold. In addition, type IIB on $AdS_3\times S^3\times M$ has worldsheet variables describing the compactification on the four-dimensional space M. Their Virasoro currents have central charge $c=6$, and will be labeled with a subscript C.

III. $N=4$ SUPER VIRASORO GENERATORS

The holomorphic $N=4$ superconformal generators with $c=6$ are given for flat space by[1]

$$T=-\tfrac{1}{2}\partial x^m\partial x_m-p_a\partial\theta^a-\tfrac{1}{2}\partial\rho\partial\rho-\tfrac{1}{2}\partial\sigma\partial\sigma+\partial^2(\rho+i\sigma)+T_C,$$

$$G^+=-e^{-2\rho-i\sigma}(p)^4+\frac{i}{2}e^{-\rho}p_ap_b\partial x^{ab}$$
$$+e^{i\sigma}\big(-\tfrac{1}{2}\partial x^m\partial x_m-p_a\partial\theta^a-\tfrac{1}{2}\partial(\rho+i\sigma)\partial(\rho+i\sigma)+\tfrac{1}{2}\partial^2(\rho+i\sigma)\big)+G^+_C,$$

$$G^-=e^{-i\sigma}+G^-_C,\quad J=\partial(\rho+i\sigma)+J_C, \tag{1}$$

$$\tilde{G}^+=e^{iH_C}\Big[-e^{-3\rho-2i\sigma}(p)^4+\frac{i}{2}e^{-2\rho-i\sigma}p_ap_b\partial x^{ab}$$
$$+e^{-\rho}\Big(-\frac{1}{2}\partial x^m\partial x_m-p_a\partial\theta^a-\frac{1}{2}\partial(\rho+i\sigma)\partial(\rho+i\sigma)\Big)+\frac{1}{2}\partial^2(\rho+i\sigma)\Big]+e^{-\rho-i\sigma}\tilde{G}^-_C,$$

$$J^+=e^{\rho+i\sigma}J^+_C,\quad J^-=e^{-\rho-i\sigma}J^-_C.$$

These currents are given in terms of the left-moving bosons ∂x^m, ρ, σ, and the left-moving fermionic worldsheet fields p^a,θ^a, where $1\leqslant m\leqslant 6$, $1\leqslant a\leqslant 4$. There are corresponding anti-holomorphic expressions. Both sets of generators are used to implement the physical state conditions on the vertex operators, a procedure which results in a set of string constraint equations.

IV. STRING CONSTRAINT EQUATIONS FOR THE VERTEX OPERATORS

The expansion of the massless vertex operator in terms of the worldsheet fields is

$$V=\sum_{m,n=-\infty}^{\infty} e^{m(i\sigma+\rho)+n(i\bar{\sigma}+\bar{\rho})}V_{m,n}(x,\theta,\bar{\theta}). \tag{2}$$

In flat space, the constraints from the left- and right-moving worldsheet super Virasoro algebra are

$$\begin{gathered}(\nabla)^4V_{1,n}=\nabla_a\nabla_b\partial^{ab}V_{1,n}=0,\\ \tfrac{1}{6}\epsilon^{abcd}\nabla_b\nabla_c\nabla_dV_{1,n}=-i\nabla_b\partial^{ab}V_{0,n},\\ \nabla_a\nabla_bV_{0,n}-\frac{i}{2}\epsilon_{abcd}\partial^{cd}V_{-1,n}=0,\quad \nabla_aV_{-1,n}=0;\end{gathered} \tag{3}$$

$$\begin{gathered}\bar{\nabla}^4V_{n,1}=\bar{\nabla}_{\dot{a}}\bar{\nabla}_{\dot{b}}\bar{\partial}^{\dot{a}\dot{b}}V_{n,1}=0,\\ \tfrac{1}{6}\epsilon^{\dot{a}\dot{b}\dot{c}\dot{d}}\bar{\nabla}_{\dot{b}}\bar{\nabla}_{\dot{c}}\bar{\nabla}_{\dot{d}}V_{n,1}=-i\bar{\nabla}_{\dot{b}}\bar{\partial}^{\dot{a}\dot{b}}V_{n,0},\\ \bar{\nabla}_{\dot{a}}\bar{\nabla}_{\dot{b}}V_{n,0}-\frac{i}{2}\bar{\epsilon}_{\dot{a}\dot{b}\dot{c}\dot{d}}\bar{\partial}^{\dot{c}\dot{d}}V_{n,-1}=0,\quad \bar{\nabla}_{\dot{a}}V_{n,-1}=0;\end{gathered} \tag{4}$$

$$\partial^p\partial_pV_{m,n}=0; \tag{5}$$

for $-1\leqslant m,\ n\leqslant 1$, with the notation $\nabla_a=d/d\theta^a$, $\bar{\nabla}_{\dot{a}}=d/d\bar{\theta}^{\dot{a}}$, and $\partial^{ab}=-\sigma^{pab}\partial_p$. These equations were derived in flat space by requiring the vertex operators to satisfy the physical state conditions

$$\begin{gathered}G_0^-V=\tilde{G}_0^-V=\tilde{G}_0^-V=\bar{\tilde{G}}_0^-V=T_0V=\tilde{T}_0V=0,\\ J_0V=\bar{J}_0V=0,\quad G_0^+\tilde{G}_0^+V=\tilde{G}_0^+\bar{\tilde{G}}_0^+V=0,\end{gathered} \tag{6}$$

where T_n, $G_n^{\pm}$, $\tilde{G}_n^{\pm}$, J_n, $J_n^{\pm}$ and corresponding barred generators are the left and right $N=4$ worldsheet superconformal generators. These conditions further imply $V_{m,n}=0$ for $m>1$ or $n>1$ or $m<1$ or $n<1$, leaving nine nonzero components.

In $\mathrm{AdS}_3\times S^3$ space, we generalize these equations as follows:[2]

$$\begin{gathered}F^4V_{1,n}=F_aF_bK^{ab}V_{1,n}=0,\\ \tfrac{1}{6}\epsilon^{abcd}F_bF_cF_dV_{1,n}=-iF_bK^{ab}V_{0,n}+2iF^aV_{0,n}-E^aV_{-1,n},\\ F_aF_bV_{0,n}-\frac{i}{2}\epsilon_{abcd}K^{cd}V_{-1,n}=0,\quad F_aV_{-1,n}=0;\end{gathered} \tag{7}$$

$$\begin{gathered}\bar{F}^4V_{n,1}=\bar{F}_{\dot{a}}\bar{F}_{\dot{b}}\bar{K}^{\dot{a}\dot{b}}V_{n,1}=0\\ \tfrac{1}{6}\epsilon^{\dot{a}\dot{b}\dot{c}\dot{d}}\bar{F}_{\dot{b}}\bar{F}_{\dot{c}}\bar{F}_{\dot{d}}V_{n,1}=-i\bar{F}_{\dot{b}}\bar{K}^{\dot{a}\dot{b}}V_{n,0}+2i\bar{F}^{\dot{a}}V_{n,0}-\bar{E}^{\dot{a}}V_{n,-1}\\ \bar{F}_{\dot{a}}\bar{F}_{\dot{b}}V_{n,0}-\frac{i}{2}\bar{\epsilon}_{\dot{a}\dot{b}\dot{c}\dot{d}}\bar{K}^{\dot{c}\dot{d}}V_{n,-1}=0,\quad \bar{F}_{\dot{a}}V_{n,-1}=0.\end{gathered} \tag{8}$$

There is also a spin zero condition constructed from the Laplacian

$$(F_a E_a + \tfrac{1}{8}\epsilon_{abcd}K^{ab}K^{cd})V_{n,m} = (\bar{F}_{\bar{a}}\bar{E}_{\bar{a}} + \tfrac{1}{8}\bar{\epsilon}_{\bar{a}\bar{b}\bar{c}\bar{d}}\bar{K}^{\bar{a}\bar{b}}\bar{K}^{\bar{c}\bar{d}})V_{n,m} = 0. \tag{9}$$

We derived[2] the curved space equations (7)–(9) by deforming the equations for the flat case (3)–(5), by requiring invariance under the PSU(2|2) transformations (10) that replace the $D=6$ super Poincare transformations of flat space. The Lie algebra of the supergroup PSU(2|2) contains six even elements $K_{ab} \in \mathrm{SO}(4)$ and eight odd ones E_a, F_a. They generate the infinitesimal symmetry transformations of the constraint equations:

$$\begin{gathered}\Delta_a^- V_{m,n} = F_a V_{m,n}, \quad \Delta_{ab} V_{m,n} = K_{ab} V_{m,n}, \\ \Delta_a^+ V_{1,n} = E_a V_{1,n}, \quad \Delta_a^+ V_{0,n} = E_a V_{0,n} + iF_a V_{1,n}, \quad \Delta_a^+ V_{-1,n} = E_a V_{-1,n} - iF_a V_{0,n}.\end{gathered} \tag{10}$$

We write E_a, F_a, and K_{ab} for the operators that represent the left action of e_a, f_a, and t_{ab} on g. In the above coordinates,

$$\begin{gathered}F_a = \frac{d}{d\theta^a}, \quad K_{ab} = -\theta_a \frac{d}{d\theta^b} + \theta_b \frac{d}{d\theta^a} + t_{Lab}, \\ E_a = \frac{1}{2}\epsilon_{abcd}\theta^b \left(t_L^{cd} - \theta^c \frac{d}{d\theta_d} \right) + h_{a\bar{b}} \frac{d}{d\bar{\theta}_{\bar{b}}},\end{gathered} \tag{11}$$

where we have introduced an operator t_L that generates the left action of SU(2)×SU(2) on h alone, without acting on the θ's. Here

$$g = g(x,\theta,\bar{\theta}) = e^{\theta^a f_a} e^{(1/2)\sigma^{pcd} x_p t_{cd}} e^{\bar{\theta}^{\bar{a}} e_{\bar{a}}} = e^{\theta^a f_a} h(x) e^{\bar{\theta}^{\bar{a}} e_{\bar{a}}}, \tag{12}$$

$$t_{Lab} g = e^{\theta^a f_a}(-t_{ab}) h(x) e^{\bar{\theta}^{\bar{a}} e_{\bar{a}}}, \tag{13}$$

and we found (11) by requiring $F_a g = f_a g$, $E_a g = e_a g$, and $K_{ab} g = -t_{ab} g$. Similar expressions[2] hold for the right-acting generators $\bar{K}_{\bar{a}\bar{b}}$, $\bar{E}_{\bar{a}}$, and $\bar{F}_{\bar{a}}$.

V. SUPERSYMMETRY ALGEBRAS

In flat space, the $D=6$ supersymmetry algebra for the left-movers is given by

$$\begin{gathered}\{q_a^+, q_c^-\} = \tfrac{1}{2}\epsilon_{abcd}P^{cd}, \\ [P_{ab}, P_{cd}] = 0 = [P_{ab}, q_c^\pm] = \{q_a^+, q_b^+\} = \{q_a^-, q_b^-\},\end{gathered} \tag{14}$$

where $P_{ab} \equiv \delta_{ac}\delta_{bd}P^{cd}$ and

$$q_a^- = \oint F_a(z),$$

$$q_a^+ = \oint (e^{-\rho - i\sigma} F_a(z) + iE_a(z)), \tag{15}$$

$$P^{ab} = \oint \partial x_m(z) \sigma^{mab}. \tag{16}$$

In flat space we have $F_a(z) = p_a(z)$ and $E_a(z) = 1/2\epsilon_{abcd}\theta^b(z)\partial x_m(z)\sigma^{mcd}$. We distinguish between the currents and their zero moments E_a, F_a which together with P_{ab} also generate the flat space supersymmetry algebra

$$[P_{ab},P_{cd}]=0=[P_{ab},F_c]=[P_{ab},E_c],$$
$$\{E_a,F_b\}=\tfrac{1}{2}\epsilon_{abcd}P^{cd},\quad \{E_a,E_b\}=\{F_a,F_b\}=0. \tag{17}$$

On $AdS_3\times S^3$, the Poincare supersymmetry algebra (17) is replaced by the PSU(2|2) superalgebra

$$[K_{ab},K_{cd}]=\delta_{ac}K_{bd}-\delta_{ad}K_{bc}-\delta_{bc}K_{ad}+\delta_{bd}K_{ac},$$
$$[K_{ab},E_c]=\delta_{ac}E_b-\delta_{bc}E_a,\quad [K_{ab},F_c]=\alpha_{ac}F_b-\delta_{bc}F_a, \tag{18}$$
$$\{E_a,F_b\}=\tfrac{1}{2}\epsilon_{abcd}K^{cd},\quad \{E_a,E_b\}=0=\{F_a,F_b\}.$$

The generators $q_a^{\pm}$, which generate the AdS transformations (10), still have a form similar to (15) but $E_a(z,\overline{z})$, $F_a(z,\overline{z})$, and $K_{ab}(z,\overline{z})$ are no longer holomorphic and their zero moments with respect to z satisfy (18).

VI. STRING EQUATIONS FOR THE AdS VERTEX OPERATOR COMPONENTS

The AdS supersymmetric constraints (7)–(9) imply[2]

$$F_aF_bK^{ab}V_{1,1}=0,\quad \overline{F}_{\dot a}\overline{F}_{\dot b}\overline{K}^{\dot a\dot b}V_{1,1}i \tag{19}$$

$$\left(F_aE_a+\tfrac{1}{8}\epsilon_{abcd}K^{ab}K^{cd}\right)V_{1,1}=\left(\overline{F}_{\dot a}\overline{E}_{\dot a}+\tfrac{1}{8}\overline{\epsilon}_{\dot a\dot b\dot c\dot d}\overline{K}^{\dot a\dot b}\overline{K}^{\dot c\dot d}\right)V_{1,1}=0. \tag{20}$$

The vertex operators $V_{-1,1},V_{1,-1},V_{0,-1},V_{-1,0},V_{-1,-1}$ can be gauge fixed to zero, and therefore do not correspond to propagating degrees of freedom. Furthermore, this gauge symmetry can be used both to set to zero the components of $V_{1,1}$ with no θ's or no $\overline{\theta}$'s, and to gauge fix all components of $V_{0,1},V_{1,0},V_{0,0}$ that are independent of those of $V_{1,1}$. The physical degrees of freedom of the massless compactification independent vertex operators are thus described by a superfield

$$\begin{aligned}V_{1,1}=&\theta^a\overline{\theta^{\dot a}}V_{a\dot a}^{--}+\theta^a\theta^b\overline{\theta^{\dot a}}\sigma^m_{ab}\overline{\xi}^-_{m\dot a}+\theta^a\overline{\theta^{\dot a}}\overline{\theta^{\dot b}}\sigma^m_{\dot a\dot b}\xi^-_{ma}+\theta^a\theta^b\overline{\theta^{\dot a}}\overline{\theta^{\dot b}}\sigma^m_{ab}\sigma^n_{\dot a\dot b}(g_{mn}+b_{mn}+\overline{g}_{mn}\phi)\\&+\theta^a(\overline{\theta^3})_{\dot a}A_a^{-+\dot a}+(\theta^3)_a\overline{\theta^{\dot a}}A_{\dot a}^{+-a}+\theta^a\theta^b(\overline{\theta^3})_{\dot a}\sigma^m_{ab}\overline{\chi}_m^{+\dot a}\\&+(\theta^3)^a\overline{\theta^{\dot a}}\overline{\theta^{\dot b}}\sigma^m_{\dot a\dot b}\chi_m^{+a}+(\theta^3)_a(\overline{\theta^3})_{\dot a}F^{++a\dot a}.\end{aligned} \tag{21}$$

This has the field content of $D=6$, $N=(2,0)$ supergravity with one supergravity and one tensor multiplet. Further massless multiplets correspond to the compactification degrees of freedom. In flat space, the surviving constraint equations imply that the component fields Φ are all on shell massless fields, that is $\Sigma_{m=1}^6\partial^m\partial_m\Phi=0$ as in (5), and in addition

$$\partial^m g_{mn}=-\partial_n\phi,\quad \partial^m b_{mn}=0,\quad \partial^m\chi_m^{\pm b}=\partial^m\overline{\chi}_m^{\pm\dot b}=0,$$
$$\partial_{ab}\chi_m^{\pm b}=\partial_{\dot a\dot b}\overline{\chi}_m^{\pm\dot b}=0,\quad \partial_{cb}F^{\pm\pm b\dot a}=\partial_{\dot c\dot b}F^{\pm\pm\dot b\dot a}=0, \tag{22}$$

where

$$F^{+-a\dot a}=\partial^{\dot a\dot b}A_{\dot b}^{+-a},\quad F^{-+a\dot a}=\partial^{ab}A_b^{-+\dot a},\quad F^{--a\dot a}=\partial^{ab}\partial^{\dot a\dot b}V_{b\dot b}^{--},$$
$$\chi_m^{-a}=\partial^{ab}\xi^-_{mb},\quad \overline{\chi}_m^{-\dot a}=\partial^{\dot a\dot b}\overline{\xi}^-_{m\dot b}. \tag{23}$$

The equations of motion for the flat space vertex operator component fields describe $D=6$, $N=(2,0)$ supergravity[4] expanded around the six-dimensional Minkowski metric.

In $AdS_3\times S^3$ space corresponding gauge transformations reduce the number of degrees of freedom in a similar fashion, but the Laplacian must be replaced by the AdS Laplacian, and the constraints are likewise deformed. We focus on the vertex operator V_{11} that carries the physical degrees of freedom. We show the string constraint equations are equivalent to the $D=6$, $N=(2,0)$ linearized supergravity equations expanded around the $AdS_3\times S^3$ metric.

For the bosonic field components of the vertex operator the AdS constraint equations result in

$$\Box h_a^g V_{ag}^{--}=-4\sigma_{ab}^m\sigma_{gh}^n\delta^{bh}h_a^g G_{mn}, \tag{24}$$

$$\Box h_a^g h_b^h\sigma_{ab}^m\sigma_{gh}^n G_{mn}=\tfrac{1}{4}\epsilon_{abce}\epsilon_{fghk}\delta^{ch}h_a^f h_b^g F^{++ek}, \tag{25}$$

$$\Box h_g^{\bar a}F^{++ag}=0,\quad \Box h_g^{\bar a}A_a^{-+g}=0,\quad \Box h_a^g A_g^{+-a}=0, \tag{26}$$

$$\epsilon_{eacd}t_L^{cd}h_{\bar a}^b A_b^{+-a}=0,\quad \epsilon_{\bar e\bar a\bar b\bar c\bar d}t_R^{\bar c\bar d}h_{\bar a}^{\bar a}A_{\bar a}^{-+\bar b}=0, \tag{27}$$

$$\epsilon_{eacd}t_L^{cd}h_{\bar b}^{\bar a}F^{++ab}=0,\quad \epsilon_{\bar e\bar b\bar c\bar d}t_R^{\bar c\bar d}h_{\bar a}^{a}F^{++\bar a\bar b}=0, \tag{28}$$

$$t_L^{ab}h_a^g h_b^h\sigma_{ab}^m\sigma_{gh}^n G_{mn}=0,\quad t_R^{\bar a\bar b}h_{\bar a}^{\bar g}h_{\bar b}^{\bar h}\sigma_{\bar g\bar h}^{m}\sigma_{\bar a\bar b}^{n}G_{mn}=0. \tag{29}$$

We have expanded $G_{mn}=g_{mn}+b_{mn}+\bar g_{mn}\phi$. The SO(4) Laplacian is $\Box\equiv 1/8\epsilon_{abcd}t_L^{ab}t_L^{cd}=1/8\epsilon_{\bar a\bar b\bar c\bar d}t_R^{\bar a\bar b}t_R^{\bar c\bar d}$. In order to compare this with supergravity, we need to reexpress the above formulas containing the right- and left-invariant vielbeins t_L^{ab}, $t_R^{\bar a\bar b}$ in terms of covariant derivatives D_p on the group manifold. So we write

$$\mathcal{T}_L^{cd}\equiv-\sigma^{pcd}D_p,\quad \mathcal{T}_R^{\bar c\bar d}\equiv\sigma^{p\bar c\bar d}D_p. \tag{30}$$

Acting on a scalar, $\mathcal{T}_L=t_L$ and $\mathcal{T}_R=t_R$, since both just act geometrically. But they differ in acting on fields that carry spinor or vector indices. For example, on spinor indices,

$$t_L^{ab}V_e=\mathcal{T}_L^{ab}V_e+\tfrac{1}{2}\delta_e^a\delta^{bc}V_c-\tfrac{1}{2}\delta_e^b\delta^{ac}V_c. \tag{31}$$

For $AdS_3\times S^3$ we can write the Riemann tensor and the metric tensor as

$$\bar R_{mnp\tau}=\tfrac{1}{4}(\bar g_{m\tau}\bar R_{np}+\bar g_{np}\bar R_{m\tau}-\bar g_{n\tau}\bar R_{mp}-\bar g_{mp}-\bar R_{n\tau}),\quad \bar g_{mn}=\tfrac{1}{2}\sigma_m^{ab}\sigma_{nab}. \tag{32}$$

The sigma matrices σ^{mab} satisfy the algebra $\sigma^{mab}\sigma_{ac}^n+\sigma^{nab}\sigma_{ac}^m=\eta^{mn}\delta_c^b$ in flat space, where η^{mn} is the six-dimensional Minkowski metric. Sigma matrices with lowered indices are defined by $\sigma_{ab}^m=1/2\epsilon_{abcd}\sigma^{mcd}$, although for other quantities indices are raised and lowered with δ^{ab}, so we distinguish σ_{ab}^m from $\delta_{ac}\delta_{bd}\sigma^{mcd}$. In curved space, η_{mn} is replaced by the $AdS_3\times S^3$ metric $\bar g_{mn}$.

We then find from the string constraints that the six-dimensional metric field g_{rs}, the dilaton ϕ, and the two-form b_{rs} satisfy

$$\begin{aligned}\tfrac{1}{2}D^pD_pb_{rs}=&-\tfrac{1}{2}(\sigma_r\sigma^p\sigma^q)_{ab}\delta^{ab}D_p[g_{qs}+\bar g_{qs}\phi]+\tfrac{1}{2}(\sigma_s\sigma^p\sigma^q)_{ab}\delta^{ab}D_p[g_{qr}+\bar g_{qr}\phi]\\&-R_{\tau rs\lambda}b^{\tau\lambda}-\tfrac{1}{2}\bar R_r^{\tau}b_{\tau s}-\tfrac{1}{2}\bar R_s^{\tau}b_{r\tau}+\tfrac{1}{4}F_{asy}^{++gh}\sigma_r^{ab}\sigma_s^{ef}\delta_{ah}\delta_{be}\delta_{gf},\end{aligned} \tag{33}$$

$$\tfrac{1}{2}D^pD_p(g_{rs}+\overline{g}_{rs}\phi)=-\tfrac{1}{2}(\sigma_r\sigma^p\sigma^q)_{ab}\delta^{ab}D_pb_{qs}+\tfrac{1}{2}(\sigma_s\sigma^p\sigma^q)_{ab}\delta^{ab}D_pb_{rq}-\overline{R}_{\tau rs\lambda}(g^{\tau\lambda}+\overline{g}^{\tau\lambda}\phi)$$
$$-\tfrac{1}{2}\overline{R}^{\tau}_{r}(g_{\tau s}+\overline{g}_{\tau s}\phi)-\tfrac{1}{2}\overline{R}^{\tau}_{s}(g_{r\tau}+\overline{g}_{r\tau}\phi)+\tfrac{1}{4}F^{++gh}_{\rm sym}\sigma_{rga}\sigma_{shb}\delta^{ab}. \tag{34}$$

This is the curved space version of the flat space zero Laplacian condition $\partial^p\partial_pb_{rs}=\partial^p\partial_pg_{rs}=\partial^p\partial_p\phi=0$.

Four self-dual tensor and scalar pairs come from the string bispinor fields F^{++ab}, V^{--}_{ab}, A^{+-a}_{b}, A^{-+b}_{a}. From the string constraint equations they satisfy

$$\sigma^p_{da}D_pF^{++ab}_{\rm asy}=0, \tag{35}$$

$$\tfrac{1}{4}[\,\delta^{Ba}\sigma^r_{ga}D_rF^{++gH}_{\rm sym}-\delta^{Ha}\sigma^r_{ga}D_rF^{++gB}_{\rm sym}]=-\tfrac{1}{4}\epsilon^{BH}{}_{cd}F^{++cd}_{\rm asy}. \tag{36}$$

We also find

$$\tfrac{1}{2}D^pD_pV^{--}_{cd}-\tfrac{1}{2}\delta^{gh}\sigma^p_{ch}D_pV^{--}_{gd}+\tfrac{1}{2}\delta^{gh}\sigma^p_{dh}D_pV^{--}_{cg}+\tfrac{1}{4}\epsilon^{gh}_{cd}V^{--}_{gh}=-4\sigma^m_{ce}\sigma^n_{df}\delta^{ef}G_{mn}. \tag{37}$$

The last constraints can be written as

$$\begin{aligned}
&\epsilon_{eacd}t^{cd}_Lh^{\bar b}_{\bar b}F^{+-ab}=0,\quad \epsilon_{\bar e\bar b\bar c\bar d}t^{\bar c\bar d}_Rh^{\bar a}_{\bar a}F^{+-\bar a\bar b}=0,\\
&\epsilon_{eacd}t^{cd}_Lh^{\bar b}_{\bar b}F^{-+ab}=0,\quad \epsilon_{\bar e\bar b\bar c\bar d}t^{\bar c\bar d}_Rh^{\bar a}_{\bar a}F^{-+\bar a\bar b}=0,
\end{aligned} \tag{38}$$

where

$$F^{+-a\bar a}\equiv\delta^{\bar a\bar b}A^{+-a}_{\bar b}+t^{\bar a\bar b}_RA^{+-a}_{\bar b},\quad F^{-+a\bar a}\equiv\delta^{ab}A^{-+\bar a}_{b}+t^{ab}_LA^{-+\bar a}_{b}, \tag{39}$$

so F^{+-ab} and F^{-+ab} satisfy equations similar to those for F^{++ab}.

Independent conditions on the fermion fields are

$$\begin{aligned}
&\Box h^{\bar g}_{\bar a}\sigma^m_{\bar a\bar b}\bar\xi^-_{mg}=-\sigma^m_{\bar g\bar h}\epsilon_{\bar e\bar d\bar a\bar b}h^{\bar h}_{\bar a}\delta^{\bar g\bar d}\overline{\chi}^{+\bar e}_m,\quad \Box h^{g}_{a}\sigma^m_{ab}\bar\xi^-_{mg}=-\sigma^m_{gh}\epsilon_{edab}h^{h}_{a}\delta^{gd}\chi^{+e}_m,\\
&t^{ab}_Lh^{g}_{a}\sigma^m_{ab}\bar\xi^-_{mg}=0,\quad t^{\bar a\bar b}_Rh^{\bar g}_{\bar a}\sigma^m_{\bar a\bar b}\bar\xi^-_{mg}=0,\\
&t^{ab}_L\sigma^m_{ab}h^{\bar a}_{\bar g}\overline{\chi}^{+g}_m=0,\quad t^{\bar a\bar b}_R\sigma^m_{\bar a\bar b}h^{a}_{\bar g}\chi^{+\bar g}_m=0,\\
&\epsilon_{deab}t^{ab}_Lh^{g}_{a}h^{h}_{b}\sigma^m_{gh}\chi^{+e}_m=0,\quad \epsilon_{\bar d\bar e\bar a\bar b}t^{\bar a\bar b}_Rh^{\bar g}_{\bar a}h^{\bar h}_{\bar b}\sigma^m_{\bar g\bar h}\overline{\chi}^{+\bar e}_m=0.
\end{aligned} \tag{40}$$

VII. COMPARISON WITH LINEARIZED AdS SUPERGRAVITY EQUATIONS

We now show that the $AdS_3\times S^3$ supersymmetric vertex operator constraint equations are equivalent to the linearized supergravity equations for the supergravity multiplet and one tensor multiplet of $D=6$, $N=(2,0)$ supergravity[4] expanded around the $AdS_3\times S^3$ metric and a self-dual three-form. We give the identification of the string vertex operator components in terms of the supergravity fields.

We will see that the two-form b_{mn} is a linear combination of *all* the oscillations corresponding to the five self-dual tensor fields and the anti-self-dual tensor field, *including the oscillation with nonvanishing background*. In flat space, b_{mn} corresponds to a state in the Neveu–Schwarz sector. In our curved space case, the string model describes vertex operators for AdS_3 background with Ramond–Ramond flux. When matching the vertex operator component fields with the supergrav-

ity oscillations, we find that not only the bispinor V^{--}_{ab} (which is a Ramond–Ramond field in the flat space case), but also the tensor b_{mn} include supergravity oscillations with nonvanishing self-dual background.

The linearized supergravity equations are given by

$$D^p D_p \phi^i = \tfrac{2}{3} \overline{H}^i_{prs} g^{6prs}, \tag{41}$$

$$\begin{aligned} &\tfrac{1}{2} D^p D_p h_{rs} - \overline{R}_{\tau rs\lambda} h^{\tau\lambda} + \tfrac{1}{2} \overline{R}^{\tau}_{r} h_{\tau s} + \tfrac{1}{2} \overline{R}^{\tau}_{s} h_{\tau r} - \tfrac{1}{2} D_s D^p h_{pr} - \tfrac{1}{2} D_s D^p h_{pr} + \tfrac{1}{2} D_r D_s h^p_p \\ &\quad = -\overline{H}^i_{r\ pq} g^i_{spq} - \overline{H}^i_{s\ pq} g^i_{rpq} + 2 h^{pt} \overline{H}^i_{rp\ q} \overline{H}^i_{stq}, \end{aligned} \tag{42}$$

$$D^p H_{prs} = -2 \overline{H}^i_{prs} D^p \phi^i + B^i [-\overline{H}^i_{r\ pq} D_p h_{qs} + \overline{H}^i_{s\ pq} D_p h_{qr} + \overline{H}^i_{rs\ q} D^p h_{pq} - \tfrac{1}{2} \overline{H}^i_{rs\ q} D_q h^p{}_p], \tag{43}$$

where we have defined $H_{prs} \equiv g^6_{prs} + B^i g^i_{prs}$ as a combination of the supergravity exact forms $g^6 \equiv db^6$, $g^i \equiv db^i$, since we will equate this with the string field strength $H = db$. We will choose $B^1 = 2$. In zeroth order, the equations are $\overline{R}_{rs} = -\overline{H}^i_{rpq} \overline{H}^i_{s\ pq}$.

We define the vertex operator components in terms of the supergravity fields g^i_{prs}, g^6_{prs}, h_{rs}, ϕ^i, $1 \leqslant i \leqslant 5$ (and $2 \leqslant I \leqslant 5$) as

$$\begin{gathered} H_{prs} \equiv g^6_{prs} + 2 g^1_{prs} + B^I g^I_{prs}, \\ g_{rs} \equiv h_{rs} - \tfrac{1}{6} \overline{g}_{rs} h^\lambda_\lambda, \quad \phi = -\tfrac{1}{3} h^\lambda_\lambda, \\ F^{++ab}_{\text{sym}} = \tfrac{2}{3} (\sigma_p \sigma_r \sigma_s)^{ab} B^I g^I_{prs} + \delta^{ab} \phi^{++}, \\ F^{++ab}_{\text{asy}} = \sigma^{pab} D_p \phi^{++}, \quad \phi^{++} = 4 C^I \phi^I, \end{gathered} \tag{44}$$

which follows from choosing the graviton trace h^λ_λ to satisfy $\phi^1 - h^\lambda_\lambda \equiv -2 C^I \phi^I$, and we have used $H_{prs} \equiv \partial_p b_{rs} + \partial_r b_{sp} + \partial_s b_{pr}$.

The combinations $C^I \phi^I$ and $B^I g^I_{prs}$ reflect the $\mathrm{SO}(4)_{\mathrm{R}}$ symmetry of the $D = 6$, $N = (2,0)$ theory on $\mathrm{AdS}_3 \times S^3$. We relabel $C^I = C^I_{++}$ and $B^I = B^I_{++}$. To define the remaining string components in terms of supergravity fields, we consider linearly independent quantities $C^I_{\mathrm{l}} \phi^I$, $B^I_{\mathrm{l}} g^I_{prs}$, $\mathrm{l} = ++, +-, -+, --$.

$$\begin{gathered} F^{+-ab}_{\text{sym}} = \tfrac{2}{3} (\sigma_p \sigma_r \sigma_s)^{ab} B^I_{+-} g^I_{prs} + \delta^{ab} \phi^{+-}, \\ F^{+-ab}_{\text{asy}} = \sigma^{pab} D_p \phi^{+-}, \quad \phi^{+-} = 4 C^I_{+-} \phi^I, \\ F^{-+ab}_{\text{sym}} = \tfrac{2}{3} (\sigma_p \sigma_r \sigma_s)^{ab} B^I_{-+} g^I_{prs} + \delta^{ab} \phi^{-+}, \\ F^{-+ab}_{\text{asy}} = \sigma^{pab} D_p \phi^{-+}, \quad \phi^{-+} = 4 C^I_{-+} \phi^I. \end{gathered} \tag{45}$$

Here V^{--}_{ab} is given in terms of the fourth tensor/scalar pair $C^I_{--} \phi^I, B^I_{--} g^I_{mnp}$ through

$$D^p D_p V^{--}_{cd} - \delta^{gh} \sigma^p_{ch} D_p V^{--}_{gd} + \delta^{gh} \sigma^p_{dh} D_p V^{--}_{cg} + \tfrac{1}{2} \epsilon^{gh}_{cd} V^{--}_{gh} = -8 \sigma^m_{ce} \sigma^n_{df} \delta^{ef} G_{mn}. \tag{46}$$

These field definitions allow us to identify the string constraint equations for the AdS_3 vertex operators as precisely those which require the vertex operator field components to satisfy the linearized supergravity equations reviewed in this section.

Likewise, the fermion constraints imply the linearized AdS supergravity equations for the gravitinos and spinors, due to the above correspondence for the bosons and the supersymmetry of the two theories.

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Superparticle and superstring in $AdS_3 \times S^3$ Ramond–Ramond background in the light-cone gauge

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We discuss superparticle and superstring dynamics in $AdS_3 \times S^3$ supported by R–R 3-form background using light-cone gauge approach. Starting with the superalgebra $\mathrm{psu}(1,1|2) \oplus \widetilde{\mathrm{psu}}(1,1|2)$ representing the basic symmetry of this background we find the light-cone superparticle Hamiltonian. We determine the harmonic decomposition of light-cone superfield describing fluctuations of type IIB supergravity fields expanded near $AdS_3 \times S^3$ background and thus the corresponding Kaluza–Klein spectrum. We fix the fermionic and bosonic light-cone gauges in the covariant Green–Schwarz $AdS_3 \times S^3$ superstring action and find the corresponding light-cone string Hamiltonian. We also obtain a realization of the generators of $\mathrm{psu}(1,1|2) \oplus \widetilde{\mathrm{psu}}(1,1|2)$ in terms of the superstring 2-d fields in the light-cone gauge. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1377274]

I. INTRODUCTION

Understanding how to quantize superstrings in Ramond–Ramond backgrounds is of topical interest, in particular, in connection with string theory—gauge theory duality.[1,2] The basic example of type IIB Green–Schwarz string in $AdS_5 \times S^5$ with R–R 5-form background[2] was studied, e.g., in. Refs. 3–10. One may hope that a progress towards understanding the spectrum of this theory may be achieved by using a light-cone gauge approach recently developed in Refs. 11, 12 (for an alternative covariant approach, see Ref. 13). To get a better understanding of this light-cone approach it may be useful to consider first a similar but somewhat simpler string model.

An obvious candidate for such simpler model is type IIB string in $AdS_3 \times S^3 \times T^4$ with R–R 3-form background. In what follows we shall ignore the trivial T^4 factor. The $AdS_3 \times S^3 \times T^4$ with NS–NS 3-form background represents the near-horizon limit of NS 5-brane—fundamental string configuration[14] and a fundamental superstring probe in it may be described by the standard $\mathrm{SL}(2,R) \times \mathrm{SU}(2)$ WZW model in the NSR formulation. However, the superstring propagation in S-dual R–R background which is the near-horizon limit of D5–D1 system[15] cannot be studied directly in the usual NSR formalism. The explicit form of the covariant GS string action in this R–R background was found in Refs. 16–18 by applying the same supercoset method which was used in the $AdS_5 \times S^5$ string case in Ref. 3. An alternative ''hybrid'' approach to quantization of superstring in $AdS_3 \times S^3$ R–R background was developed in Ref. 19 (see also Ref. 20).

In this paper we shall discuss several aspects of superstring dynamics in the $AdS_3 \times S^3$ R–R background in the light-cone approach developed for the $AdS_5 \times S^5$ case in Refs. 11, 12. Since the simplest limiting case of superstring is superparticle, we also consider in some detail the light-cone superparticle theory in $AdS_3 \times S^3$, following closely the treatment of the $AdS_5 \times S^5$ case in Ref. 21. First quantization of superparticle determines the spectrum of fluctuations of type IIB supergravity in $AdS_3 \times S^3 \times T^4$ (found directly in component form in Ref. 22) and thus also the ''ground state'' spectrum of the corresponding string theory. In the treatment of the superstring theory our starting point will be the covariant GS action (see Refs. 16–18) where we shall fix the

light-cone-type fermionic (κ-symmetry) and bosonic (2-d diffeomorphism) gauges and derive the light-cone Hamiltonian along the lines of the phase space approach of Ref. 12.

The paper is organized as follows: In Sec. II we review the structure of the underlying symmetry superalgebra of the type IIB superstring theory in $AdS_3\times S^3$ R–R background—$\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ (Ref. 23) and present its (anti)commutation relations in a light-cone basis.

In Sec. III we consider superparticle dynamics in $AdS_3\times S^3$. We find the light-cone superparticle Hamiltonian and a realization of the generators of $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ on phase space of (first-quantized) superparticle.

In Sec. IV we develop a manifestly supersymmetric light-cone gauge formulation of type IIB supergravity on $AdS_3\times S^3$ background. The quadratic term in the action for fluctuation fields is written in terms of a single unconstrained scalar light-cone superfield, allowing us to treat all the component fields on an equal footing. We also present a superfield version of S^3 harmonic decomposition and find the corresponding K–K spectra of the supergravity modes propagating in AdS_3.

In Sec. V we find the κ-symmetry light-cone gauge fixed form of the superstring action in $AdS_3\times S^3$. We give the superstring Lagrangian both in the ''Wess–Zumino'' and ''Killing'' parametrizations of the basic coset superspace $[\mathrm{PSU}(1,1|2)\times\widetilde{\mathrm{PSU}}(1,1|2)]/[\mathrm{SO}(2,1)\times\mathrm{SO}(3)]$ on which the superstring is propagating. We also discuss a reformulation of the resulting superstring action in terms of 2-d Dirac world-sheet fermions.

Section VI is devoted to the light-cone phase space approach to superstring theory. We fix the analog of the GGRT bosonic light-cone gauge and derive the phase space analog of the superstring Lagrangian of Sec. V and the corresponding light-cone gauge Hamiltonian.

In Sec. VII we obtain a realization of the generators of the symmetry superalgebra $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ as Noether charges expressed in terms of the 2-d fields which are the coordinates of the $AdS_3\times S^3$ superstring in the light cone gauge.

Some technical details are collected in five Appendices. In Appendix A we summarize our notation and definitions used in this paper and give some relations relevant for a coset description of S^3. In Appendix B we describe correspondence between the ''covariant'' and ''light-cone'' forms of the $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ superalgebra. In Appendix C we explain the construction of Poincaré supercharges in the case of superparticle. In Appendix D we give some details of computation of the spectrum of type IIB supergravity fluctuations in $AdS_3\times S^3$. In Appendix E we present the expressions for the supercoset Cartan 1-forms which are the basic elements in the construction of the GS superstring action, and describe our procedure of fixing the fermionic light-cone gauge in the string action.

II. $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ SUPERALGEBRA

The symmetry algebra of the $AdS_3\times S^3$ with R–R 3-form background may be represented as a direct sum of two copies of $\mathrm{psu}(1,1|2)$ superalgebra, i.e., as $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ superalgebra.[23] The even part of this superalgebra consists of the bosonic subalgebras su(1,1), su(2) and $\widetilde{\mathrm{su}}(1,1)$, $\widetilde{\mathrm{su}}(2)$ respectively. su(1,1) and $\widetilde{\mathrm{su}}(1,1)$ combine into so(2,2) algebra while su(2) and $\widetilde{\mathrm{su}}(2)$ form the so(4) algebra. These so(2,2) and so(4) algebras are the isometry algebras of the AdS_3 and S^3 factors, respectively. The odd part of the superalgebra consists of 16 supercharges which correspond to the 16 Killing spinors of $AdS_3\times S^3$ geometry.

The superalgebra $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ will play the central role in our constructions. Let us review its commutation relations in the two forms (''covariant'' and ''light-cone'') we are going to use. In $\mathrm{su}(1,1)\oplus\mathrm{su}(2)$ covariant basis the $\mathrm{psu}(1,1|2)$ superalgebra has the following generators: $m^{\alpha}{}_{\beta}$ and $m^{i}{}_{j}$ which are generators of su(1,1) and su(2) and 8 supercharges q_i^{α}, q^{i}_{α} ($\alpha,\beta=1,2$; $i,j=1,2$). Their (anti)commutation relations have the following well known form,

$$[m^{\alpha}{}_{\beta},m^{\gamma}{}_{\delta}]=\delta^{\gamma}_{\beta}m^{\alpha}{}_{\delta}-\delta^{\alpha}_{\delta}m^{\gamma}{}_{\beta},\quad [m^{i}{}_{j},m^{k}{}_{n}]=\delta^{k}_{j}m^{i}{}_{n}-\delta^{i}_{n}m^{k}{}_{j}, \tag{2.1}$$

$$[m^{\alpha}{}_{\beta},q^{k}_{\gamma}]=-\delta^{\alpha}_{\gamma}q^{k}_{\beta}+\tfrac{1}{2}\delta^{\alpha}_{\beta}q^{k}_{\gamma},\quad [m^{i}{}_{j},q^{k}_{\alpha}]=\delta^{k}_{j}q^{i}_{\alpha}-\tfrac{1}{2}\delta^{i}_{j}q^{k}_{\alpha}, \tag{2.2}$$

$$[m^i{}_j,q_k^\alpha]=-\delta_k^i q_j^\alpha+\tfrac{1}{2}\delta_j^i q_k^\alpha,\quad [m^\alpha{}_\beta,q_k^\gamma]=\delta_\beta^\gamma q_k^\alpha-\tfrac{1}{2}\delta_\beta^\alpha q_k^\gamma, \tag{2.3}$$

$$\{q_\alpha^i,q_j^\beta\}=a(\delta_j^i m^\beta{}_\alpha+\delta_\alpha^\beta m^i{}_j),\quad a^2=-1. \tag{2.4}$$

We assume the following Hermitian conjugation rules:

$$(m^\alpha{}_\beta)^\dagger=-m^\alpha{}_\beta,\quad (m^i{}_j)^\dagger=m^j{}_i,\quad (q_i^\alpha)^\dagger=\epsilon^{\alpha\beta}q_\beta^i,\quad (q_\alpha^i)^\dagger=q_i^\beta\epsilon_{\beta\alpha}, \tag{2.5}$$

where $\epsilon^{\alpha\beta}$ is the Levi-Civita tensor, $\epsilon_{12}=\epsilon^{12}=1$. The $\widetilde{\mathrm{psu}}(1,1|2)$ superalgebra has the same commutation relations but with the constant a in (2.4) replaced by $\tilde{a}(\tilde{a}^2=-1)$ such that its sign is opposite to that of a, i.e., $a\tilde{a}=1$.

It will be useful to decompose the generators according to their light-cone SO(1,1) group transformation properties (we shall call this ''light-cone basis''). In the light-cone basis the generators of $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ include translations $P^\pm$, conformal boosts $K^\pm$, Lorentz rotation J^{+-}, dilatation D, R-symmetry generators of su(2) and $\widetilde{\mathrm{su}}(2)$ $J^i{}_j$ and $\tilde{J}^i{}_j$, Poincaré algebra supercharges $Q^{\pm i}$, and conformal algebra supercharges $S^{\pm i}$. To simplify the notation here we use the same type of indices for su(2) and $\widetilde{\mathrm{su}}(2)$. The Hermitian conjugation rules are

$$(P^\pm)^\dagger=P^\pm,\quad (K^\pm)^\dagger=K^\pm,\quad (Q^{\pm i})^\dagger=Q_i^\pm,\quad (S^{\pm i})^\dagger=S_i^\pm, \tag{2.6}$$

$$(J^{+-})^\dagger=-J^{+-},\quad D^\dagger=-D,\quad J^{i\dagger}{}_j=J^j{}_i,\quad \tilde{J}^{i\dagger}{}_j=\tilde{J}^j{}_i. \tag{2.7}$$

The anti(commutation) relations then include (their derivation from the above relations is explained in Appendix B)

$$[P^\pm,K^\mp]=D\mp J^{+-}, \tag{2.8}$$

$$[D,P^\pm]=-P^\pm,\quad [D,K^\pm]=K^\pm,\quad [J^{+-},P^\pm]=\pm P^\pm,\quad [J^{+-},K^\pm]=\pm K^\pm, \tag{2.9}$$

$$[D,Q_i^\pm]=-\tfrac{1}{2}Q_i^\pm,\quad [D,S_i^\pm]=\tfrac{1}{2}S_i^\pm,\quad [J^{+-},Q_i^\pm]=\pm\tfrac{1}{2}Q_i^\pm,\quad [J^{+-},S_i^\pm]=\pm\tfrac{1}{2}S_i^\pm, \tag{2.10}$$

$$[S_i^\mp,P^\pm]=Q_i^\pm,\quad [Q^{\mp i},K^\pm]=S^{\pm i},\quad \{Q^{\pm i},Q_j^\pm\}=\pm P^\pm\delta_j^i,\quad \{S^{\pm i},S_j^\pm\}=\pm K^\pm\delta_j^i, \tag{2.11}$$

$$\{Q^{+i},S_j^-\}=\tfrac{1}{2}(J^{+-}-D)\delta_j^i-\tilde{J}^i{}_j,\quad \{Q^{-i},S_j^+\}=\tfrac{1}{2}(J^{+-}+D)\delta_j^i+J^i{}_j, \tag{2.12}$$

plus Hermitian conjugations of the above ones. The remaining relations can be summarized as follows. The supercharges Q_i^-, Q^{-i}, S^{+i}, S_i^+ transform in the (anti)fundamental representations of su(2)—they are rotated only by $J^i{}_j$, i.e.,

$$[J^i{}_j,Q^{-k}]=\delta_j^k Q^{-i}-\tfrac{1}{2}\delta_j^i Q^{-k},\quad [J^i{}_j,Q_k^-]=-\delta_k^i Q_j^-+\tfrac{1}{2}\delta_j^i Q_k^-, \tag{2.13}$$

and the same for S_i^+, S^{+i}. The remaining supercharges Q^{+i}, Q_i^+, S^{-i}, S_i^- transform in the (anti)fundamental representations of $\widetilde{\mathrm{su}}(2)$—they are rotated only by $\tilde{J}^i{}_j$, i.e.,

$$[\tilde{J}^i{}_j,Q^{+k}]=\delta_j^k Q^{+i}-\tfrac{1}{2}\delta_j^i Q^{+k},\quad [\tilde{J}^i{}_j,Q_k^+]=-\delta_k^i Q_j^++\tfrac{1}{2}\delta_j^i Q_k^+, \tag{2.14}$$

and the same for S^{-i}, S_i^-. The generators $J^i{}_j$, $\tilde{J}^i{}_j$ satisfy the standard relations

$$[J^i{}_j,J^k{}_n]=\delta_j^k J^i{}_n-\delta_n^i J^k{}_j,\quad [\tilde{J}^i{}_j,\tilde{J}^k{}_n]=\delta_j^k\tilde{J}^i{}_n-\delta_n^i\tilde{J}^k{}_j. \tag{2.15}$$

III. SUPERPARTICLE DYNAMICS IN $AdS_3\times S^3$ BACKRGOUND

Before discussing the superstring it is instructive to consider first a superparticle propagating in $AdS_3\times S^3$ space. The covariant Brink–Schwarz κ-symmetric action for a superparticle in $AdS_3\times S^3$ can be obtained, e.g., from the superstring action of Refs. 16–18 by taking the zero slope limit $\alpha'\to 0$. By applying the light-cone gauge fixing procedure (see Ref. 12 and below) one could then obtain the superparticle light-cone gauge fixed action. On the other hand, there is a method[24] which reduces the problem of constructing a new (light-cone gauge) dynamical system to the problem of finding a new solution of the commutation relations of the defining symmetry algebra [in our case $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$]. This method of Dirac was applied to the case of superparticle in $AdS_5\times S^5$ in Ref. 21 (see also Ref. 25) and here we would like to demonstrate how it works for the superparticle in $AdS_3\times S^3$. Quantization of superparticle determines the quadratic part of the action of type IIB supergravity expanded near $AdS_3\times S^3$ background.

In the light-cone formalism the generators of the $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ superalgebra can be split into the two groups:

$$P^+, K^+, Q^{+i}, Q_i^+, S^{+i}, S_i^+, D, J^{+-}, J^i{}_j, \tilde{J}^i{}_j, \tag{3.1}$$

which we shall refer to as kinematical generators, and

$$P^-, K^-, Q^{-i}, Q_i^-, S^{-i}, S_i^-, \tag{3.2}$$

which we shall refer to as dynamical generators. The kinematical generators have positive or zero J^{+-} (Lorentz) charges, while the dynamical generators have negative J^{+-} charges. It turns out that in the superfield realization the kinematical generators taken at $x^+=0$ are quadratic in the physical fields, while the dynamical generators receive higher-order interaction-dependent corrections. In general, the kinematical generators have the structure $G=G_1+x^+G_2+(x^+)^2G_3$, where G_1 is quadratic but G_2, G_3 contain higher order terms in second-quantized fields. The first step is to find a free (quadratic) superfield representation for the generators of $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$. The generators we obtain below will be used for the description of Sec. II B supergravity in $AdS_3\times S^3$ background.

Let us explain step by step how the method of Ref. 24 works in the present case: First, we introduce a light-cone superspace on which we are going to realize the generators of our superalgebra. The superspace coordinates include the position coordinates $x^\pm$, z of AdS_3, a unit vector u^M representing S^3, and the Grassmann coordinates θ^i, η^i. In this parametrization the metric of $AdS_3\times S^3$ is ($M=1,2,3,4$),

$$ds^2=\frac{1}{z^2}(2dx^+dx^-+dz^2)+du^Mdu^M,\quad u^Mu^M=1. \tag{3.3}$$

In formulating our results we shall trade the bosonic coordinate x^- and the Grassmann coordinates θ^i, η^i for the bosonic momentum p^+ and the Grassmann momenta λ_i, ϑ_i.

Let us start with the kinematical generators and consider them on the surface of the initial data $x^+=0$. The kinematical generators which have positive J^{+-}-charge are fixed to be

$$P^+=p^+,\quad K^+=\tfrac{1}{2}z^2p^+, \tag{3.4}$$

$$Q_i^+=\lambda_i,\quad Q^{+i}=p^+\theta^i\quad S_i^+=\frac{1}{\sqrt{2}}z\vartheta_i,\quad S^{+i}=\frac{1}{\sqrt{2}}zp^+\eta^i, \tag{3.5}$$

where the coordinates θ^i, η^i and their momenta λ_i, ϑ_i satisfy the canonical anticommutation relations

$$\{\lambda_i,\theta^j\}=\delta_i^j,\quad \{\vartheta_i,\eta^j\}=\delta_i^j. \tag{3.6}$$

Let us note that in the language of an action based on a supercoset construction the above parametrization of the kinematical generators corresponds to special choices of (i) coset representative and (ii) light-cone gauges for 1-d diffeomorphism symmetry and κ-symmetry. In fact, these choices may be motivated by a simple form of the resulting generators.

Once the above generators are chosen, the remaining kinematical generators which have zero J^{+-}-charge are fixed by the commutation relations of the superalgebra,

$$J^{+-}=\partial_{p^+}p^+-\tfrac{1}{2}\theta\lambda-\tfrac{1}{2}\eta\vartheta+1,\quad D=-\partial_{p^+}p^++z\partial_z+\tfrac{1}{2}\theta\lambda+\tfrac{1}{2}\eta\vartheta-\tfrac{1}{2}, \tag{3.7}$$

$$J^i{}_j=l^i{}_j+\eta^i\vartheta_j-\tfrac{1}{2}\delta^i_j\eta\vartheta,\quad \tilde{J}^i{}_j=\tilde{l}^i{}_j+\theta^i\lambda_j-\tfrac{1}{2}\delta^i_j\theta\lambda, \tag{3.8}$$

where $\partial_{p^+}\equiv\partial/\partial p^+$, $\partial_z\equiv\partial/\partial z$. The orbital parts $l^i{}_j$ and $\tilde{l}^i{}_j$ of the angular momenta $J^i{}_j$ and $\tilde{J}^i{}_j$ are given by

$$l^i{}_j=\tfrac{1}{4}(\sigma^{MN})^i{}_j l^{MN},\quad \tilde{l}^i{}_j=\tfrac{1}{4}(\bar{\sigma}^{MN})^i{}_j l^{MN}, \tag{3.9}$$

where the so(4) orbital momentum l^{MN} can be chosen as

$$l^{MN}=u^M\hat{\partial}^N-u^N\hat{\partial}^M. \tag{3.10}$$

Here $\hat{\partial}^M$ is covariant tangent derivative on S^3 which is fixed by the constraint $u^M\hat{\partial}^M=0$ and by the commutation relations,

$$[\hat{\partial}^M,u^N]=v^{MN},\quad [\hat{\partial}^M,\hat{\partial}^N]=u^M\hat{\partial}^N-u^N\hat{\partial}^N,\quad v^{MN}\equiv\delta^{MN}-u^Mu^N. \tag{3.11}$$

Note that the concrete parametrization of the S^3 part is not very important to us as in the case of the superparticle all the generators are expressed in terms of the orbital part of the angular momentum. The operator $l^i{}_j$ satisfies the following basic relation:

$$l^i{}_k l^k{}_j=\tfrac{1}{2}l^2\delta^i_j+l^i{}_j, \tag{3.12}$$

where $l^2\equiv l^i{}_j l^j{}_i$. The same relation is true for $\tilde{l}^i{}_j$. The Hermitian conjugation rules are

$$\lambda_i^\dagger=p^+\theta^i,\quad \theta^{i\dagger}=\frac{\lambda_i}{p^+},\quad \vartheta_i^\dagger=p^+\eta^i,\quad \eta^{i\dagger}=\frac{\vartheta_i}{p^+},\quad (\partial_{p^+}p^+)^\dagger=-\partial_{p^+}p^++\theta\lambda+\eta\vartheta-2. \tag{3.13}$$

Once the all the kinematical generators are fixed, the dynamical generators are found from the commutation relations of the basic superalgebra (for details see Appendix C)

$$P^-=\frac{1}{2p^+}\left(\partial_z^2-\frac{1}{z^2}A\right), \tag{3.14}$$

$$Q_i^-=\frac{1}{\sqrt{2}p^+}\left(-\vartheta_i\partial_z-\frac{1}{z}(\eta\vartheta)\vartheta_i+\frac{1}{2z}\vartheta_i+\frac{2}{z}(\vartheta l)_i\right), \tag{3.15}$$

$$Q^{-i}=\frac{1}{\sqrt{2}}\left(\eta^i\partial_z-\frac{1}{z}\eta^i(\eta\vartheta)+\frac{1}{2z}\eta^i+\frac{2}{z}(l\eta)^i\right), \tag{3.16}$$

$$K^-=-\bar{S}\frac{1}{p^+}S-\frac{1}{2p^+}(\tilde{l}^2+2\lambda\tilde{l}\theta), \tag{3.17}$$

$$S^{-i}=\theta^i S-(\tilde{l}\,\theta)^i,\quad S_i^-=\lambda_i\bar{S}\frac{1}{p^+}-\frac{1}{p^+}(\lambda\tilde{l})_i, \tag{3.18}$$

where the operators A, S, and $\bar{S}$ are defined by

$$A\equiv X-\tfrac{1}{4},\quad X\equiv 2l^2+4\,\vartheta l\,\eta+(\eta\vartheta-1)^2, \tag{3.19}$$

$$S\equiv-\partial_{p^+}p^+ +\tfrac{1}{2}z\partial_z+\theta\lambda+\tfrac{1}{2}\,\eta\vartheta-\tfrac{3}{4},\quad \bar{S}\equiv\partial_{p^+}p^+ -\tfrac{1}{2}z\partial_z-\tfrac{1}{2}\,\eta\vartheta+\tfrac{3}{4}, \tag{3.20}$$

and we used the notation

$$(\vartheta l)_i\equiv\vartheta_j l^j{}_i,\quad (l\,\eta)^i\equiv l^i{}_j\eta^j,\quad (\lambda\tilde{l})_i\equiv\lambda_j\tilde{l}^j{}_i,\quad (\tilde{l}\,\theta)^i\equiv\tilde{l}^i{}_j\eta^j,\quad (\vartheta l\,\eta)\equiv\vartheta_i l^i{}_j\eta^j, \tag{3.21}$$

$$l^2\equiv l^i{}_j l^j{}_i,\quad \tilde{l}^2\equiv\tilde{l}^i{}_j\tilde{l}^j{}_i,\quad \eta\vartheta\equiv\eta^i\vartheta_i,\quad \theta\lambda\equiv\theta^i\lambda_i. \tag{3.22}$$

In the light-cone approach the operator P^- plays the role of the (minus) Hamiltonian of the superparticle. The expressions for the supercharges can be rewritten as follows:

$$Q_i^-=-\frac{1}{\sqrt{2}p^+}\left(\vartheta_i\partial_z+\frac{1}{2z}[\vartheta_i,A]\right),\quad Q^{-i}=\frac{1}{\sqrt{2}}\left(\eta^i\partial_z+\frac{1}{2z}[\eta^i,A]\right). \tag{3.23}$$

As in Ref. 26 and 27 we shall call A in (3.19) the AdS mass operator. This operator satisfies the following basic relation

$$\{[\eta^i,A],[\vartheta_j,A]\}+2[\eta^i,A]\vartheta_j+2[\vartheta_j,A]\eta^i=-4A\delta^i_j, \tag{3.24}$$

which is useful in checking that $\{Q_i^-,Q^{-j}\}=-\delta_i^j P^-$. Let us note that A is equal to zero only for massless representations which can be realized as irreducible representations of the conformal algebra,[28,27] i.e., of so(3,2) in the case of AdS_3. The values of this operator for various fields are discussed in Ref. 29. Below in Sec. IV B we shall demonstrate that A is not equal to zero for the whole spectrum of the S^3 compactification of type IIB supergravity to AdS_3.

The generators given above were defined on the initial data surface $x^+=0$. In general, they have the structure $G=G(x^+,\mathcal{X}(x^+))$, where $\mathcal{X}$ stands for all of the dynamical variables. Let us use the notation,

$$G|_{x^+=0}\equiv G(0,\mathcal{X}(x^+)). \tag{3.25}$$

The generators $G|_{x^+=0}$ can be obtained from the above expressions by expressing the dynamical variables $\mathcal{X}$ in terms of light-cone time variable x^+ using the Hamiltonian equations of motion which are postulated in our approach. The form of the generators for arbitrary x^+, i.e., $G(x^+,\mathcal{X}(x^+))$, is then found from the conservation laws for the charges,

$$J^{+-}=J^+|_{x^+=0}+x^+P^-,\quad D=D^+|_{x^+=0}+x^+P^-, \tag{3.26}$$

$$K^+=K^+|_{x^+=0}+x^+(D|_{x^+=0}+J^{+-}|_{x^+=0})+x^{+2}P^-, \tag{3.27}$$

$$S_i^+=S_i^+|_{x^+=0}-\mathrm{i}x^+Q_i^-,\quad S^{+i}=S^{+i}|_{x^+=0}+\mathrm{i}x^+Q^{-i}. \tag{3.28}$$

The remaining generators do not have explicit dependence on x^+, i.e., they have the structure $G(x^+,\mathcal{X}(x^+))=G(0,\mathcal{X}(x^+))$.

IV. LIGHT-CONE GAUGE SUPERFIELD FORMULATION OF TYPE IIB SUPERGRAVITY ON $AdS_3\times S^3$

In this section we shall present the light-cone gauge superfield description of type IIB supergravity on $AdS_3\times S^3$ background, implied by the quantization of the superparticle described in the previous section. Linearized equations of motion for fluctuations of supergravity fields in $AdS_3\times S^3\times K3$ background and the corresponding spectrum were found in component form.[22] We shall use instead the light-cone superfield approach.

This analysis can be viewed as a step towards understanding the spectrum of string theory in $AdS_3\times S^3$. As is well known in the case of (super)strings in flat space, reproducing the correct spectrum of the massless modes plays an important role in determining a consistent quantization scheme. The $AdS_3\times S^3$ spectrum we shall find below should be a useful guiding principle in quantising superstrings in this space. In particular, the operator ordering and renormalization scheme should be chosen so that the ground state of the superstring theory in $AdS_3\times S^3$ (with R–R 3-form background) will have the spectrum described below. Note that the selection of R–R as opposed to NS–NS background is predetermined by our choice of the basic superalgebra in Sec. II.

Finding even the quadratic part of the action for fluctuations of the supergravity fields in a curved background is a complicated problem. There are two ways of determining spectra of compactifications of the type II supergravity. The first one uses oscillator construction.[30] The second one is based on the analysis of equations of motion.[22,31] In our construction of the spectrum we shall follow the second approach. A new element which substantially simplifies the analysis is the use of the light-cone superfield formulation.

A. Quadratic light-cone superfield action

We could in principle use the covariant superfield description of type IIB supergavity,[32] starting with linearized expansion of superfileds, imposing light-cone gauge on fluctuations and then solving the constraints to eliminate non-physical degrees of freedom in terms of physical ones. That would be quite tedious. The light-cone gauge method provides a self-contained approach which does not rely upon existence of a covariant description and which gives a much shorter way to arrive to final results. The key idea is that, as in flat space,[33] the superparticle supercharges found in the previous section provide realization of the generators of the basic $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ superalgebra in terms of the differential operators acting on the scalar supergravity superfield $\Phi(x^{\pm},z,u,\theta,\eta)$. It is convenient to Fourier transform to the momentum space for all of the coordinates except the radial AdS_3 coordinate z and S^3 directions u^M. This means using p^+, λ_i, ϑ_i instead of x^-, θ^i, η^i [λ_i and ϑ_i are in the fundamental representations of $\widetilde{\mathrm{su}}(2)$ and $\mathrm{su}(2)$]. Thus our basic superfield will be $\Phi(x^+,p^+,z,u,\lambda,\vartheta)$ with the following expansion in powers of the Grassmann momenta λ_i and ϑ_i:

$$\Phi(x^+,p^+,z,u,\lambda,\vartheta)=p^+\phi+\lambda_i\psi_1^i+\vartheta_i\psi_2^i+(\epsilon\lambda^2)\phi_1+\lambda_i\vartheta_j\phi_2^{ij}+(\epsilon\vartheta^2)\phi_1^*+\frac{1}{p^+}((\epsilon\lambda)^i(\epsilon\vartheta^2)\psi_1^{i*}+(\epsilon\vartheta)^i(\epsilon\lambda^2)\psi_2^{i*})-\frac{1}{p^+}(\epsilon\lambda^2)(\epsilon\vartheta^2)\phi^*, \tag{4.1}$$

where the coefficients $\phi,\phi_1,\phi_2,\psi_1,\psi_2$ are functions of x^+, the momentum p^+, and the bosonic coordinates z,u^M. We used the notation,

$$(\epsilon\lambda^2)\equiv\tfrac{1}{2}\epsilon^{ij}\lambda_i\lambda_j,\quad (\epsilon\lambda)^i\equiv\epsilon^{ij}\lambda_j, \tag{4.2}$$

and the same for ϑ. The only constraint which this superfield is to satisfy is the reality constraint

$$\Phi(-p^+,z,u,\lambda,\vartheta)=(p^+)^2\int d^2\lambda^\dagger d^2\vartheta^\dagger e^{(\lambda_i\lambda_i^\dagger+\vartheta_i\vartheta_i^\dagger)/p^+}(\Phi(p^+,z,u,\lambda,\vartheta))^\dagger, \tag{4.3}$$

where we assume the convention $(\lambda_1\lambda_2)^\dagger=\lambda_2^\dagger\lambda_1^\dagger$. This reality constraint implies that the component fields ϕ,ϕ_n are related to ϕ^*,ϕ_n^* by the Hermitian conjugation rule for the Fourier components, i.e. $(\phi^*(-p^+))^*=\phi(p^+),(\phi_n^*(-p^+))^*=\phi_n(p^+)$. Equation (4.3) leads also to the following self-duality condition:

$$\phi_2^{ij}(p^+)=-\epsilon^{ik}\epsilon^{jl}\phi_2^{kl*}(-p^+). \tag{4.4}$$

The light-cone action has the following ''noncovariant form:''

$$S=\int dx^+dzdp^+d^3ud^2\lambda d^2\vartheta\,\Phi(-p^+,z,u,-\lambda,-\vartheta)[p^+(i\partial_{x^+}+P^-)]\Phi(p^+,z,u,\lambda,\vartheta), \tag{4.5}$$

where the Hamiltonian density $(-P^-)$ is given by (3.14) and d^3u stands for the S^3 volume element, i.e., $d^4u\,\delta(u^Mu^M-1)$.

Transforming back to the position coordinate x^- this action can be cast into the ''relativistic-invariant'' form,

$$S=\frac{1}{2}\int d^3xd^3ud^2\lambda d^2\vartheta\,\Phi(x,u,-\lambda,-\vartheta)\left(\Box-\frac{1}{z^2}A\right)\Phi(x,u,\lambda,\vartheta), \tag{4.6}$$

where $\Box$ is the flat D'Alembertian $\Box=2\partial_{x^-}\partial_{x^+}+\partial_z^2$, and $d^3x\equiv dx^+dx^-dz$.

As was already mentioned above, the superparticle charges found in Sec. III give the representation of $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ in terms of differential operators acting on the supergravity superfield Φ. We can thus write down the ''superfield-theory'' (or ''second-quantized'') realization of $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ generators,

$$\hat{G}=\int dp^+dzd^3ud^2\lambda d^2\vartheta\,p^+\Phi(-p^+,z,u,-\lambda,-\vartheta)G\Phi(p^+,z,u,\lambda,\vartheta), \tag{4.7}$$

where G indicates representation of $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ superalgebra in terms of differential operators given in previous section.

B. Harmonic decomposition of the light-cone superfield and the spectrum

The light-cone description given above provides a convenient way to analyze the harmonic decomposition of basic component fields and thus the corresponding spectra of fluctuation modes. A nice feature of this approach is that this can be done at the level of superfields, i.e., in a manifestly supersymmetric way. The action (4.6) gives the following equation of motion for the basic superfield Φ:

$$\left(\Box-\frac{1}{z^2}A\right)\Phi=0. \tag{4.8}$$

To find the spectrum we are thus to decompose Φ into the eigenvectors of the AdS mass operator A defined in (3.19). Let us first make the standard harmonic decomposition (we absorb the coefficients of the expansion in the ''basic'' vectors),

$$\Phi=\sum_{k=0}^{\infty}\Phi_k, \tag{4.9}$$

where Φ_k are the so(4) harmonic superfields, satisfying, by definition,

$$2l^2\Phi_k=k(k+2)\Phi_k. \tag{4.10}$$

In this subsection the index k is used to indicate the Kaluza–Klein modes. We can further expand each Φ_k in power series with respect to the Grassmann momentum ϑ writing

$$\Phi_k=\sum_{\sigma=0}^{2}\Phi_{k,\sigma}, \tag{4.11}$$

where $\Phi_{k,\sigma}$ satisfies

$$2l^2\Phi_{k,\sigma}=k(k+2)\Phi_{k,\sigma}, \quad \eta\vartheta\Phi_{k,\sigma}=(2-\sigma)\Phi_{k,\sigma}. \tag{4.12}$$

These equations tell us that the harmonic superfield $\Phi_{k,\sigma}$ is a polynomial of degree σ in the Grassmann momentum ϑ. From the expression for the operator X (3.19) it is then clear the superfields $\Phi_{k,0}$ are its eigenvectors,

$$X\Phi_{k,0}=(k+1)^2\Phi_{k,0}. \tag{4.13}$$

It is easy to demonstrate that $\Phi_{k,2}$ are also the eigenvectors of X with the same eigenvalues, i.e., $X\Phi_{k,2}=(k+1)^2\Phi_{k,2}$. This gives the following equations of motion determining the part of the mass spectrum corresponding to $\Phi_{k,0},\Phi_{k,2}$:

$$\left(\Box-\frac{(2k+1)(2k+3)}{4z^2}\right)\Phi_{k,0}=0, \quad \left(\Box-\frac{(2k+1)(2k+3)}{4z^2}\right)\Phi_{k,2}=0. \tag{4.14}$$

It turns out that the remaining superfields $\Phi_{k,1}$ are not eigenvectors of X. They can be decomposed, however, into the eigenvectors of this operator as follows (for details see Appendix B)

$$\Phi_{k,1}=\Phi_{k,1}^{(1)}+\Phi_{k,1}^{(2)}, \tag{4.15}$$

where

$$\Phi_{k,1}^{(1)}=\left(\vartheta_i-\frac{2}{k+2}(\vartheta l)_i\right)\Phi_{k,1}^i, \quad k\geqslant 0; \tag{4.16}$$

$$\Phi_{k,1}^{(2)}=\left(\vartheta_i-\frac{2}{k}(\vartheta l)_i\right)\Phi_{k,1}^i, \quad k>0. \tag{4.17}$$

Here $\Phi_{k,1}^i$ does not depend on the Grassmann momentum ϑ but still depend on Grassmann momentum λ. Then,

$$X\Phi_{k,1}^{(1)}=k^2\Phi_{k,1}^{(1)}, \quad X\Phi_{k,1}^{(2)}=(k+2)^2\Phi_{k,1}^{(2)}, \tag{4.18}$$

and this gives the following equations of motion:

$$\left(\Box-\frac{(2k-1)(2k+1)}{4z^2}\right)\Phi_{k,1}^{(1)}=0, \quad \left(\Box-\frac{(2k+3)(2k+5)}{4z^2}\right)\Phi_{k,1}^{(2)}=0, \tag{4.19}$$

determining the spectra of these superfields.

Note that the operator A is equal to zero (i.e., $X=\frac{1}{4}$) only for massless representations which can be realized as irreducible representations of the conformal algebra[27,28] [so(3,2) in the case of AdS_3]. From the above spectra one can see that the mass terms, i.e., the eigenvalues of the operator A, are never equal to zero. That means, in particular, that the fluctuation modes for the compactification of Sec. II B supergravity on S^3 do not satisfy the conformally invariant equations of motion in AdS space.

V. LIGHT CONE SUPERSTRING ACTION IN $AdS_3\times S^3$ R–R BACKGROUND

In this section we shall find the form of the type IIB superstring action in $AdS_3\times S^3$ background with R–R 3-form flux in the light-cone gauge. The Green–Schwarz action for a superstring background was constructed in Refs. 16–18 following a similar construction for the $AdS_5\times S^5$ case in Ref. 3. Our discussion of light-cone gauge fixing will also repeat closely the same steps as in Refs. 11 and 12, where the $AdS_5\times S^5$ case was treated.

In flat space superstring light-cone gauge fixing procedure in flat space consists of the two stages:

(I) fermionic light-cone gauge choice, i.e., fixing the κ-symmetry by $\Gamma^+\theta^I=0$;

(II) bosonic light-cone gauge choice, i.e., using the conformal gauge $\sqrt{g}g^{\mu\nu}=\eta^{\mu\nu}$ and fixing the residual conformal diffeomorphism symmetry by $x^+(\tau,\sigma)=p^+\tau$. Note that we use Minkowski signature 2-d world sheet metric $g_{\mu\nu}$ with $g\equiv-\det g_{\mu\nu}$.

Our fermionic κ-symmetry light-cone gauge will be different from the naive $\Gamma^+\theta^I=0$ but will be related to it in the flat space limit. It will reduce the 16 fermionic coordinates θ^I_α to 8 physical Grassmann variables: ''linear'' θ^i and ''nonlinear'' η^i and their Hermitian conjugates θ_i and η_i. As in the case of the superparticle the 2-d fields θ^i, θ_i, and η^i, η_i transform according to the fundamental representations of $\widetilde{\mathrm{SU}}(2)$ and SU(2), respectively. The superconformal algebra $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ dictates that these variables should be related to the Poincaré and conformal supersymmetry in the light-cone gauge description of the boundary theory. As in the case of superparticle the superstring action and symmetry generators will have simple (quadratic) dependence on θ^i, but complicated (quartic) dependence on η^i. Note that it is these fermionic coordinates that are most suitable for light-cone gauge fixing of kappa symmetry in AdS space, both in the superparticle and superstring cases. These coordinates were introduced in Ref. 21 in the study of light-cone gauge dynamics of superparticle in $AdS_5\times S^5$. Light-cone gauge superstring action in $AdS_5\times S^5$ written in terms of these coordinates was found in Ref. 11. The light-cone gauge action can be found in two related forms. One of them corresponds to the choice of the Wess–Zumino-type gauge in superspace while another is based on the Killing gauge. These ''gauges'' or ''parametrizations'' do not reduce the number of fermionic degrees of freedom but only specialize a choice of fermionic coordinates.

A. Fermionic light-cone gauge action in WZ parametrization

Let us consider first fixing fermionic light-cone gauge in the action written in the WZ parametrization. This action turns out to be more convenient for reformulation of superstring action in terms of 2-*d* Dirac spinors (see next section). Using the parametrization of the basic supercoset $[\mathrm{PSU}(1,1|2)\times\widetilde{\mathrm{PSU}}(1,1|2)]/[\mathrm{SO}(2,1)\times\mathrm{SO}(3)]$ described in Appendix E and fixing a light-cone gauge the $AdS_3\times S^3$ superstring Lagrangian can be written as the sum of the bosonic term, term quadratic in fermions and quartic fermionic term,

$$\mathcal{L}=\mathcal{L}_B+\mathcal{L}_F^{(2)}+\mathcal{L}_F^{(4)}. \tag{5.1}$$

Here,

$$\mathcal{L}_B=-\sqrt{g}g^{\mu\nu}[e^{2\phi}\partial_\mu x^+\partial_\nu x^-+\tfrac{1}{2}\partial_\mu\phi\partial_\nu\phi+\tfrac{1}{2}e^{A'}_\mu e^{A'}_\nu], \tag{5.2}$$

where $e^{A'}_\mu$ is the projection of the vielbein of S^3 which in the special parametrization we will be using is given by

$$e^{A'}_\mu=-\frac{\mathrm{i}}{2}\mathrm{Tr}(\sigma^{A'}\partial_\mu UU^{-1})+\frac{\mathrm{i}}{2}\mathrm{Tr}(\sigma^{A'}\partial_\mu\tilde{U}\tilde{U}^{-1}), \tag{5.3}$$

$$U^i{}_j\equiv(e^y)^i{}_j,\quad \tilde{U}^i{}_j\equiv(e^{-y})^i{}_j,\quad U^\dagger U=I,\quad \tilde{U}^\dagger\tilde{U}=I, \tag{5.4}$$

where the trace is over $i,j=1,2$. The matrices $U\in \mathrm{SU}(2)$, $\tilde{U}\in \widetilde{\mathrm{SU}}(2)$ depends on 3 independent coordinates $y^{A'}$,

$$y^i{}_j \equiv \frac{\mathrm{i}}{2} y^{A'} (\sigma^{A'})^i{}_j, \quad (y^i{}_j)^* = -y^j{}_i, \quad y^i{}_i = 0, \tag{5.5}$$

where $\sigma^{A'}$ are 3 Pauli matrices. The quadratic part of the fermionic action is

$$\mathcal{L}_F^{(2)} = e^{2\phi}\partial_\mu x^+ \left[\frac{\mathrm{i}}{2}\sqrt{g} g^{\mu\nu} (-\theta_i \tilde{\mathcal{D}}_\nu \theta^i - \eta_i \mathcal{D}_\nu \eta^i + \mathrm{i}\eta_i e^i_{\nu j}\eta^j) + \epsilon^{\mu\nu}\eta^i C'_{ij}\tilde{\mathcal{D}}_\nu \theta^j \right] + \text{h.c.} \tag{5.6}$$

The $\epsilon^{\mu\nu}$ dependent (P-odd) term in (5.6) came from the WZ term in the covariant GS action on the supercoset. We used the following notation:

$$\mathcal{D}\eta^i = d\eta^i - \Omega^i{}_j \eta^j, \quad \mathcal{D}\eta_i = d\eta_i + \eta_j \Omega^j{}_i, \quad \tilde{\mathcal{D}}\theta^i = d\theta^i - \tilde{\Omega}^i{}_j \theta^j, \quad \tilde{\mathcal{D}}\theta_i = d\theta_i + \theta_j \tilde{\Omega}^j{}_i, \tag{5.7}$$

$$e^i{}_j \equiv (\sigma^{A'})^i{}_j e^{A'}, \tag{5.8}$$

and $\mathcal{D} = d\sigma^\mu \mathcal{D}_\mu$, $e^i{}_j = d\sigma^\mu e^i_{\mu j}$, where $\sigma^\mu = (\tau,\sigma)$ are 2-d coordinates. $\mathcal{D}$, $\tilde{\mathcal{D}}$ are the generalized spinor derivatives on S^3. They have the structure $\mathcal{D} = d + \Omega^i{}_j J^j{}_i$, $\tilde{\mathcal{D}} = d + \tilde{\Omega}^i{}_j \tilde{J}^j{}_i$ and satisfy the relation $\mathcal{D}^2 = 0$, $\tilde{\mathcal{D}}^2 = 0$. The connections $\Omega^i{}_j$, $\tilde{\Omega}^i{}_j$ are given by

$$\Omega = dUU^{-1}, \quad \tilde{\Omega} = d\tilde{U}\tilde{U}^{-1}, \quad d\Omega - \Omega\wedge\Omega = 0, \quad d\tilde{\Omega} - \tilde{\Omega}\wedge\tilde{\Omega} = 0, \tag{5.9}$$

and can be written in terms of the S^3 spin connection $\omega^{A'B'}$ and the 3-bein $e^{A'}$ as follows:

$$\Omega^i{}_j = -\frac{1}{4}(\sigma^{A'B'})^i{}_j \omega^{A'B'} + \frac{\mathrm{i}}{2}(\sigma^{A'})^i{}_j e^{A'}, \quad \tilde{\Omega}^i{}_j = -\frac{1}{4}(\sigma^{A'B'})^i{}_j \omega^{A'B'} - \frac{\mathrm{i}}{2}(\sigma^A)^i{}_j e^{A'}. \tag{5.10}$$

C'_{ij} is the constant charge conjugation matrix of the SO(3) Dirac matrix algebra (see Appendix A). The Hermitian conjugation rules are $\theta_i^\dagger = \theta^i$, $\eta_i^\dagger = \eta^i$.

The quartic fermionic term in (5.1) depends only on half of the Grassmann variables—on η but not on θ,

$$\mathcal{L}_F^{(4)} = 2\sqrt{g} g^{\mu\nu} e^{4\phi} \partial_\mu x^+ \partial_\nu x^+ (\eta^i \eta_i)^2. \tag{5.11}$$

B. "2-d spinor" form of the action

Like in the flat space case[34] and in the "long string" cases in $AdS_5\times S^5$ (Ref. 9) the resulting action can then be put into the "2-d spinor" form, where the $4+4$ fermionic degrees of freedom are organized into 2 Dirac 2-d spinors, defined in *curved* 2-d geometry (we shall follow similar discussion in $AdS_5\times S^5$ case in Ref. 11). Such action may be useful to establishing a relation to NSR formulation.

In order to do that one needs to impose, addition to fermionic light-cone gauge, the bosonic light-cone gauge. Using the following light-cone gauge:[35]

$$x^+ = \tau, \quad \sqrt{g} g^{\mu\nu} = \mathrm{diag}(-e^{-2\phi}, e^{2\phi}), \tag{5.12}$$

we can write the kinetic term (5.6) as

$$\mathcal{L}_F^{(2)} = \frac{\mathrm{i}}{2}(\theta_i \tilde{\mathcal{D}}_0 \theta^i + \eta_i \tilde{\mathcal{D}}_0 \eta^i - 2\mathrm{i}\eta_i e^i_{0j}\eta^j) + e^{2\phi}\eta^i C'_{ij}\tilde{\mathcal{D}}_1 \theta^j + \text{h.c.}, \tag{5.13}$$

where we used the relation $\mathcal{D}\eta^i=\tilde{\mathcal{D}}\eta^i-\mathrm{i}e^i{}_j\eta^j$ [see (5.10)]. Introducing a 2-d zweibein corresponding to the metric in (5.12),

$$e^m_\mu=\mathrm{diag}(e^{2\phi},1), \quad g_{\mu\nu}=-e^0_\mu e^0_\nu+e^1_\mu e^1_\nu, \tag{5.14}$$

we can put (5.13) in the 2-d form as follows:

$$e^{-1}\mathcal{L}^{(2)}_F=-\frac{\mathrm{i}}{2}\bar{\psi}\varrho^m e^\mu_m\tilde{\mathcal{D}}_\mu\psi+\frac{\mathrm{i}}{2}\bar{\psi}\psi\partial_1\phi-\sqrt{2}\bar{\psi}_i e^i_{0j}\varrho^-\psi^j+\mathrm{h.c.}, \tag{5.15}$$

where ϱ^m are 2-d Dirac matrices,

$$\varrho^0=\mathrm{i}\sigma_2, \quad \varrho^1=\sigma_1, \quad \varrho^3=\varrho^0\varrho^1=\sigma_3, \quad \varrho^\pm\equiv\frac{1}{\sqrt{2}}(\varrho^3\pm\varrho^0), \tag{5.16}$$

$\bar{\psi}_i=(\psi^i)^\dagger\varrho^0$, $\bar{\psi}\psi$ stands for $\bar{\psi}_i\psi^i$, ψ^T denotes the transposition of 2-d spinor and ψ's are related to the original (2-d scalar) fermionic variables θ's and η's by

$$\psi^i=\begin{pmatrix}\psi^i_1\\ \psi^i_2\end{pmatrix}, \quad \psi^i_1=\frac{1}{\sqrt{2}}[\theta^i-\mathrm{i}(C'^{-1})^{ij}\eta_j], \quad \psi^i_2=\frac{1}{\sqrt{2}}[\theta^i+\mathrm{i}(C'^{-1})^{ij}\eta_j]. \tag{5.17}$$

In our notation $\mathrm{i}\bar{\psi}\varrho^m\nabla_m\psi=-\mathrm{i}\psi^\dagger_1(\nabla_0-\nabla_1)\psi_1-\mathrm{i}\psi^\dagger_2(\nabla_0+\nabla_1)\psi_2$, $\nabla_m=e^\mu_m\partial_\mu$. The quartic interaction term (5.11) then takes the following form:

$$e^{-1}\mathcal{L}^{(4)}_F=-(\bar{\psi}_i\varrho^-\psi^i)^2. \tag{5.18}$$

The total action is thus a kind of G/H bosonic sigma model coupled to a Thirring-type 2-d fermionic model in curved 2-d geometry (5.14) (determined by the profile of the radial function of the AdS space), and coupled to some 2-d vector fields. The interactions are such that they ensure the quantum 2-d conformal invariance of the total model.[3]

The mass term $\bar{\psi}\psi\partial_1\phi$ in (5.15) is similar to the one in Ref. 9 (where the background string configuration was non-constant only in the radial ϕ direction) and has its origin in the $\epsilon^{\mu\nu}e^{2\phi}\partial_\mu x^+\partial_\nu\phi\,\eta^iC'_{ij}\theta^j$ term appearing after $\eta\leftrightarrow\theta$ symmetrization of the $\epsilon^{\mu\nu}$ term in (5.6) (its ''noncovariance'' is thus a consequence of the choice $x^+=\tau$). The action is symmetric under shifting $\psi^i\to\psi^i+\varrho^-\epsilon^i$, where ϵ^i is the 2-d Killing spinor. This symmetry reflects the fact that our original action is symmetric under shifting θ^i by a Killing spinor on S^3.

Note also that the 2-d Lorentz invariance is preserved by the fermionic light-cone gauge (original GS fermions θ are 2-d scalars) but is broken by our special choice of the bosonic gauge (5.12) The special form of $g_{\mu\nu}$ in (5.12) implies ''noncovariant'' dependence on ϕ in the bosonic part of the action: the action (5.2) for the field ϕ and the 3-sphere coordinates $y^{A'}$ has the form,

$$\mathcal{L}_B=\tfrac{1}{2}e^{-2\phi}\dot{\phi}^2-\tfrac{1}{2}e^{2\phi}\acute{\phi}^2+\tfrac{1}{2}G_{\mathcal{AB}}(e^{-2\phi}\dot{y}^{\mathcal{A}}\dot{y}^{\mathcal{B}}-e^{2\phi}\acute{y}^{\mathcal{A}}\acute{y}^{\mathcal{B}}), \tag{5.19}$$

where $G_{\mathcal{AB}}$ is the metric of 5-sphere ($y^{\mathcal{A}}$ are coordinates of S^3). A consequence of the unusual $g_{\mu\nu}$ gauge choice in (5.12) compared to the standard conformal gauge is that now the S^3 part of the action is no longer decoupled from the radial AdS_3 direction ϕ.

C. Fermionic light-cone gauge action in the Killing parametrization

Now let us consider the string action in the Killing parametrization. The action is again formulated in terms of 6 bosonic coordinates $(x^\pm,\phi,y^{\mathcal{A}})$ ($\mathcal{A}$ label 3 independent coordinates of S^3) in terms of which the metric of $AdS_3\times S^3$ is

$$ds^2=2e^{2\phi}dx^+dx^-+d\phi^2+G_{\mathcal{AB}}(y)dy^{\mathcal{A}}dy^{\mathcal{B}}, \tag{5.20}$$

and 8 fermionic coordinates (θ^i,θ_i), (η^i,η_i) in the fundamental representations of $\widetilde{\mathrm{SU}}(2)$ and SU(2), respectively. In contrast to the WZ parametrization, the fermions in the Killing parametrization transform in the linear representations of SU(2) and $\widetilde{\mathrm{SU}}(2)$, and thus the covariant derivatives in WZ case (5.7) here will become ordinary derivatives. The Lagrangian is given by the sum of the ''kinetic'' and ''Wess–Zumino'' terms (see Appendices A and B for notation),

$$\mathcal{L}=\mathcal{L}_{\mathrm{kin}}+\mathcal{L}_{\mathrm{WZ}},$$

$$\mathcal{L}_{\mathrm{kin}}=-\sqrt{g}g^{\mu\nu}[e^{2\phi}\partial_\mu x^+\partial_\nu x^-+\tfrac{1}{2}\partial_\mu\phi\partial_\nu\phi+\tfrac{1}{2}G_{\mathcal{AB}}(y)D_\mu y^{\mathcal{A}}D_\nu y^{\mathcal{B}}]-\frac{\mathrm{i}}{2}\sqrt{g}g^{\mu\nu}e^{2\phi}\partial_\mu x^+[\theta^i\partial_\nu\theta_i$$
$$+\theta_i\partial_\nu\theta^i+\eta^i\partial_\nu\eta_i+\eta_i\partial_\nu\eta^i+\mathrm{i}e^{2\phi}\partial_\nu x^+(\eta^2)^2], \tag{5.21}$$

$$\mathcal{L}_{WZ}=\epsilon^{\mu\nu}e^{2\phi}\partial_\mu x^+\,\eta^iC^U_{ij}\partial_\nu\theta^j+\mathrm{h.c.}, \tag{5.22}$$

where

$$D_\mu y^{\mathcal{A}}=\partial_\mu y^{\mathcal{A}}-2\mathrm{i}\,\eta_i(V^{\mathcal{A}})^i{}_j\eta^je^{2\phi}\partial_\mu x^+,\quad C^U_{ij}\equiv U^k{}_iC'_{kl}\tilde{U}^l{}_j. \tag{5.23}$$

Here $G_{\mathcal{AB}}$ and $(V^{\mathcal{A}})^i{}_j$ are the metric tensor and the Killing vectors of S^3, respectively (see Appendix A). This form of the superstring action (which we shall call ''intermediate'') is most convenient for deriving other forms which differ in the way one chooses the bosonic coordinates that parametrize $AdS_3\times S^3$. For example, a useful form of the action is found by introducing a unit 4-vector u^M defined

$$u^{A'}=n^{A'}\sin|y|,\quad u^4=-\cos|y|, \tag{5.24}$$

in terms of which the $AdS_3\times S^3$ metric is

$$ds^2=e^{2\phi}dx^adx^a+d\phi^2+du^Mdu^M,\quad u^Mu^M=1. \tag{5.25}$$

Then the string action takes the form,

$$\mathcal{L}_{\mathrm{kin}}=-\sqrt{g}g^{\mu\nu}\left[e^{2\phi}\partial_\mu x^+\partial_\nu x^-+\frac{1}{2}\partial_\mu\phi\partial_\nu\phi+\frac{1}{2}D_\mu u^MD_\nu u^M\right]-\frac{\mathrm{i}}{2}\sqrt{g}g^{\mu\nu}e^{2\phi}\partial_\mu x^+[\theta^i\partial_\nu\theta_i+\theta_i\partial_\nu\theta^i$$
$$+\eta^i\partial_\nu\eta_i+\eta_i\partial_\nu\eta^i+\mathrm{i}e^{2\phi}\partial_\nu x^+(\eta^2)^2], \tag{5.26}$$

$$\mathcal{L}_{\mathrm{WZ}}=\epsilon^{\mu\nu}e^{2\phi}\partial_\mu x^+(\eta^iy_{ij}\partial_\nu\theta^j+\eta_iy^{ij}\partial_\nu\theta_j), \tag{5.27}$$

where we used the relation $C^U_{ij}=-\mathrm{i}C'_{ik}u^k{}_j$, made the rescalings $\eta^i\to\mathrm{i}\eta^i$, $\eta_i\to-\mathrm{i}\eta_i$ and introduced the following notation:

$$u^i{}_j\equiv(\sigma^M)^i{}_ju^M,\quad y_{ij}\equiv C'_{ik}u^k{}_j,\quad y^{ij}\equiv-u^i{}_k(C'^{-1})^{kj}, \tag{5.28}$$

$$D_\mu u^M=\partial_\mu u^M-2\mathrm{i}\,\eta_i(R^M)^i{}_j\eta^je^{2\phi}\partial_\mu x^+,\quad (R^M)^i{}_j=-\tfrac{1}{2}(\sigma^{MN})^i{}_ju^N, \tag{5.29}$$

with σ^{MN} defined in (A4). Note that $u^i{}_j$, y_{ij}, y^{ij} transform in the fundamental representation of SU(2) with respect to the index i and in fundamental representation of $\widetilde{\mathrm{SU}}(2)$ with respect to the index j. They satisfy

$$y^*_{ij}=-y^{ij},\quad u^i{}^*_j=\bar{u}^j{}_i,\quad \bar{u}^\dagger{}_j\equiv(\bar{\sigma}^M)^i{}_ju^M,\quad \bar{u}^\dagger{}_k(C'^{-1})^{kj}=u^j{}_k(C'^{-1})^{ki}. \tag{5.30}$$

The parametrization based on u^M is the most convenient one for the discussion of the superparticle in $AdS_3\times S^3$ and of the harmonic decomposition of the light-cone superfield of type IIB supergravity into the Kaluza–Klein modes (see Secs. III and IV). We shall use this parametrization in the study of the light-cone superstring Hamiltonian in Sec. VI.

The superstring Lagrangian (5.21), (5.22) taken in any of its forms mentioned above can be represented in the following way:

$$\mathcal{L}=\mathcal{L}_1+\mathcal{L}_2, \tag{5.31}$$

$$\mathcal{L}_1=-h^{\mu\nu}\partial_\mu x^+\partial_\nu x^- +\partial_\mu x^+ A^\mu+\tfrac{1}{2}h^{\mu\nu}\partial_\mu x^+\partial_\nu x^+ B-\tfrac{1}{2}h^{\mu\nu}g_{\mathcal{AB}}D_\mu y^{\mathcal{A}}D_\nu y^{\mathcal{B}}, \tag{5.32}$$

$$\mathcal{L}_2=-\tfrac{1}{2}h^{\mu\nu}e^{-2\phi}\partial_\mu\phi\partial_\nu\phi+T, \tag{5.33}$$

where

$$g_{\mathcal{AB}}\equiv e^{-2\phi}G_{\mathcal{AB}},\quad D_\mu y^{\mathcal{A}}\equiv\partial_\mu y^{\mathcal{A}}+F^{\mathcal{A}}\partial_\mu x^+, \tag{5.34}$$

and $h^{\mu\nu}$ is defined by

$$h^{\mu\nu}\equiv\sqrt{g}g^{\mu\nu}e^{2\phi},\quad h^{00}h^{11}-(h^{01})^2=-e^{4\phi}. \tag{5.35}$$

The decomposition (5.31) is made so that the functions A^μ, B, $F^{\mathcal{A}}$ depend (i) on the anticommuting coordinates and their derivatives with respect to both τ and σ, and (ii) on the bosonic coordinates and their derivatives with respect to the world sheet spatial coordinate σ only. The reason for this decomposition is that below we shall use the phase space description with respect to the bosonic coordinates only, i.e., we shall not make the Legendre transformation with respect to the fermionic coordinates.

In the case of the ''intermediate'' form of the action (5.21),(5.22) these functions are

$$A^\mu=-\frac{\mathrm{i}}{2}h^{\mu\nu}(\theta^i\partial_\nu\theta_i+\eta^i\partial_\nu\eta_i)+\epsilon^{\mu 1}e^{2\phi}\eta^i C^U_{ij}\acute{\theta}^j+\text{h.c.}, \tag{5.36}$$

$$B=e^{2\phi}(\eta^2)^2,\quad F^{\mathcal{A}}=-2\mathrm{i}e^{2\phi}\eta_i(V^{\mathcal{A}})^i{}_j\eta^j,\quad T=-e^{2\phi}\acute{x}^+\eta^i C^U_{ij}\dot{\theta}^j+\text{h.c.} \tag{5.37}$$

VI. LIGHT CONE HAMILTONIAN APPROACH TO THE SUPERSTRING IN $AdS_3\times S^3$

Our next task is to fix the bosonic part of the light-cone gauge. We shall use the generalization of the phase space GGRT approach[36] to a curved AdS-type space described in Ref. 12, fixing the diffeomorphisms in $AdS_3\times S^3$ cases by the *same* gauge condition as in flat space. Most of the discussion below will follow closely to Ref. 12.

A. Phase space lagrangian

Computing the canonical momenta for the bosonic coordinates,

$$\mathcal{P}_a=\frac{\partial\mathcal{L}}{\partial\dot{x}^a},\quad \Pi=\frac{\partial\mathcal{L}}{\partial\dot{\phi}},\quad \mathcal{P}_{\mathcal{A}}=\frac{\partial\mathcal{L}}{\partial\dot{y}^{\mathcal{A}}}, \tag{6.1}$$

we get from (5.31),

$$\Pi=-h^{00}e^{-2\phi}\dot{\phi}^+-h^{01}e^{-2\phi}\acute{\phi}^+, \tag{6.2}$$

$$\mathcal{P}^+=-h^{00}\dot{x}^+-h^{01}\acute{x}^+, \tag{6.3}$$

$$\mathcal{P}^{\mathcal{A}}=-h^{00}\dot{y}^{\mathcal{A}}-h^{01}\acute{y}^{\mathcal{A}}+F^{\mathcal{A}}\mathcal{P}^+, \tag{6.4}$$

$$\mathcal{P}^- = -h^{00}\dot{x}^- - h^{01}\acute{x}^- + A^0 - B\mathcal{P}^+ + \mathcal{P}_{\mathcal{A}}F^{\mathcal{A}}, \tag{6.5}$$

where $\mathcal{P}^{\pm}\equiv\mathcal{P}_{\mp}$, $\mathcal{P}^{\mathcal{A}}\equiv g^{\mathcal{A}\mathcal{B}}\mathcal{P}_{\mathcal{B}}$. By applying the same procedure as in the bosonic case we find then the following phase space Lagrangian $\mathcal{L}=\mathcal{L}_1+\mathcal{L}_2$ (see. Ref. 12):

$$\begin{aligned}\mathcal{L}_1 &= \mathcal{P}^+\dot{x}^- + \mathcal{P}^-\dot{x}^+ + \mathcal{P}_{\mathcal{A}}\dot{y}^{\mathcal{A}} + \frac{1}{2h^{00}}[2\mathcal{P}^+\mathcal{P}^- + 2e^{4\phi}\acute{x}^+\acute{x}^- + g^{\mathcal{A}\mathcal{B}}\mathcal{P}_{\mathcal{A}}\mathcal{P}_{\mathcal{B}} + e^{4\phi}g_{\mathcal{A}\mathcal{B}}D_1y^{\mathcal{A}}D_1y^{\mathcal{B}}\\ &\quad + (\mathcal{P}^{+2} - e^{4\phi}\acute{x}^{+2})B - 2F^{\mathcal{A}}\mathcal{P}_{\mathcal{A}}\mathcal{P}^+] + \frac{h^{01}}{h^{00}}(\mathcal{P}^+\acute{x}^- + \mathcal{P}^-\acute{x}^+ + \mathcal{P}_{\mathcal{A}}\acute{y}^{\mathcal{A}})\\ &\quad - \frac{1}{h^{00}}(\mathcal{P}^+ + h^{01}\acute{x}^+)A^0 + \acute{x}^+A^1,\end{aligned} \tag{6.6}$$

$$\mathcal{L}_2 = \Pi\dot{\phi} + \frac{1}{2h^{00}}e^{2\phi}(\Pi^2 + \acute{\phi}^2) + \frac{h^{01}}{h^{00}}\Pi\acute{\phi} + T. \tag{6.7}$$

Next, we impose the light-cone gauge,

$$x^+ = \tau, \qquad \mathcal{P}^+ = p^+. \tag{6.8}$$

Using these gauge conditions in the action and integrating over $\mathcal{P}^-$ we get the expression for h^{00},

$$h^{00} = -p^+. \tag{6.9}$$

Inserting this into (6.6), (6.7) we get the following general form of the phase space light-cone Lagrangian:

$$\mathcal{L}_1 = \mathcal{P}_{\mathcal{A}}\dot{y}^{\mathcal{A}} - \frac{1}{2p^+}(g^{\mathcal{A}\mathcal{B}}\mathcal{P}_{\mathcal{A}}\mathcal{P}_{\mathcal{B}} + e^{4\phi}g_{\mathcal{A}\mathcal{B}}\acute{y}^{\mathcal{A}}\acute{y}^{\mathcal{B}} + p^{+2}B - 2p^+F^{\mathcal{A}}\mathcal{P}_{\mathcal{A}}) - \frac{h^{01}}{p^+}(p^+\acute{x}^- + \mathcal{P}_{\mathcal{A}}\acute{y}^{\mathcal{A}}) + A^0, \tag{6.10}$$

$$\mathcal{L}_2 = \Pi\dot{\phi} - \frac{1}{2p^+}e^{2\phi}(\Pi^2 + \acute{\phi}^2) - \frac{h^{01}}{p^+}\Pi\acute{\phi}. \tag{6.11}$$

Note that the function T in (5.37) is equal to zero in the light-cone gauge (6.8) This general form of the phase space Lagrangian can be specialized to different choices of bosonic coordinates by using the corresponding functions A^0, B, and $F^{\mathcal{A}}$. For the ''intermediate'' case (5.21),(5.22) these functions are given by (5.36),(5.37) so that we get

$$\begin{aligned}\mathcal{L} &= \mathcal{L}_1 + \mathcal{L}_2\\ &= \Pi\dot{\phi} + \mathcal{P}_{\mathcal{A}}\dot{y}^{\mathcal{A}} + \frac{\mathrm{i}}{2}p^+(\theta^i\dot{\theta}_i + \eta^i\dot{\eta}_i + \theta_i\dot{\theta}^i + \eta_i\dot{\eta}^i) - \frac{e^{2\phi}}{2p^+}[\Pi^2 + \acute{\phi}^2 + 2l^2 + G_{\mathcal{A}\mathcal{B}}\acute{y}^{\mathcal{A}}\acute{y}^{\mathcal{B}}\\ &\quad + p^{+2}(\eta^2)^2 + 4p^+\eta_i l^i{}_j\eta^j] + e^{2\phi}(\eta^iC^U_{ij}\acute{\theta}^j + \eta_iC^{ij}_U\acute{\theta}_j) - \frac{h^{01}}{p^+}\Big[p^+\acute{x}^- + \Pi\acute{\phi} + \mathcal{P}_{\mathcal{A}}\acute{y}^{\mathcal{A}}\\ &\quad + \frac{\mathrm{i}}{2}p^+(\theta^i\acute{\theta}_i + \eta^i\acute{\eta}_i + \theta_i\acute{\theta}^i + \eta_i\acute{\eta}^i)\Big].\end{aligned} \tag{6.12}$$

Here $C^{ij}_U = -(C^U_{ij})^*$, and we used the relation

$$G^{\mathcal{A}\mathcal{B}}\mathcal{P}_{\mathcal{A}}\mathcal{P}_{\mathcal{B}} = 2l^2, \quad l^i{}_j \equiv \mathrm{i}(V^{\mathcal{A}})^i{}_j\mathcal{P}_{\mathcal{A}}, \quad l^2 \equiv l^i{}_jl^j{}_i. \tag{6.13}$$

By applying a coordinate transformation one gets the phase space Lagrangian corresponding to the case (5.26),(5.27) in which the S^3 part is parametrized by the unit 4-vector u^M,

$$\mathcal{L}=\Pi\dot{\phi}+\mathcal{P}_M\dot{u}^M+\frac{\mathrm{i}}{2}p^+(\theta^i\dot{\theta}_i+\eta^i\dot{\eta}_i+\theta_i\dot{\theta}^i+\eta_i\dot{\eta}^i)$$
$$-\frac{e^{2\phi}}{2p^+}[\Pi^2+\acute{\phi}^2+2l^2+\acute{u}^M\acute{u}^M+p^{+2}(\eta^2)^2+4p^+\eta_i l^i{}_j\eta^j]+e^{2\phi}(\eta^i y_{ij}\acute{\theta}^j+\eta_i y^{ij}\acute{\theta}_j)$$
$$-\frac{h^{01}}{p^+}\left[p^+\acute{x}^-+\Pi\acute{\phi}+\mathcal{P}_M\acute{u}^M+\frac{\mathrm{i}}{2}p^+(\theta^i\acute{\theta}_i+\eta^i\acute{\eta}_i+\theta_i\acute{\theta}^i+\eta_i\acute{\eta}^i)\right], \tag{6.14}$$

where $\mathcal{P}_M$ is the canonical momentum for u^M and $l^i{}_j$ in (6.13) has the following explicit form:

$$l^i{}_j=\frac{\mathrm{i}}{2}(\sigma^{MN})^i{}_j u^M\mathcal{P}^N. \tag{6.15}$$

Here and below $l^i{}_j$ is for the classical orbital momentum [note that going to the superparticle limit, after the quantization we get $\mathcal{P}^M=-\mathrm{i}\hat{\partial}^M$ and then the classical orbital momentum $l^i{}_j$ (6.15) becomes the quantum momentum $l^i{}_j$ in (3.9)]. Taking into account the constraint $u^M\mathcal{P}^M=0$ [see (6.32)] we get

$$l^i{}_k l^k{}_j=\tfrac{1}{4}\mathcal{P}^M\mathcal{P}^M\delta^i{}_j, \quad l^2=\tfrac{1}{2}\mathcal{P}^M\mathcal{P}^M. \tag{6.16}$$

The above Lagrangian leads to the following (minus) Hamiltonian:

$$P^-=\int_0^1 d\sigma\mathcal{P}^-, \tag{6.17}$$

where the Hamiltonian density $-\mathcal{P}^-$ is given by

$$\mathcal{P}^-=-\frac{e^{2\phi}}{2p^+}[\Pi^2+\acute{\phi}^2+2l^2+\acute{u}^M\acute{u}^M+p^{+2}(\eta^2)^2+4p^+\eta_i l^i{}_j\eta^j]+e^{2\phi}(\eta^i y_{ij}\acute{\theta}^j+\eta_i y^{ij}\acute{\theta}_j). \tag{6.18}$$

It should be supplemented by the constraint,

$$p^+\acute{x}^-+\Pi\acute{\phi}+\mathcal{P}_M\acute{u}^M+\frac{\mathrm{i}}{2}p^+(\theta^i\acute{\theta}_i+\eta^i\acute{\eta}_i+\theta_i\acute{\theta}^i+\eta_i\acute{\eta}^i)=0. \tag{6.19}$$

As usual, this constraint allows one to express the nonzero modes of the bosonic coordinate x^- in terms of the transverse physical ones.

It is easy to see that in the particle theory limit the superstring Hamiltonian (6.18) reduces to the superparticle one which was found in Sec. III by applying the direct method of constructing relativistic dynamics[24] based on the symmetry algebra. Indeed, the (quantum, operator-ordered) superparticle light-cone Hamiltonian in (3.14),(3.19) can be rewritten as follows:

$$\mathcal{P}^-=-\frac{1}{2p^+}[e^{\phi}\Pi e^{\phi}\Pi+e^{2\phi}(2l^2+(p^+\eta^2-1)^2+4p^+\eta_i l^i{}_j\eta^j)]. \tag{6.20}$$

The string Hamiltonian (6.18) reduces to (6.20) modulo terms ''quantum'' terms proportional to η^2 and a constant (in string Hamiltonian we ignore operator ordering). The derivation of the light-cone string action from the covariant one given above thus provides, in the particle limit, also a self-contained Lagrangian derivation of the light-cone gauge superparticle Hamiltonian (3.14)

(obtained indirectly from the symmetry algebra in Sec. III) from a covariant action. This represents a consistency check on the two different methods used in Sec. III and in the present section.

B. Equations of motion

The equations of motion corresponding to the phase space superstring Lagrangian (6.14) are

$$\dot{\phi}=\frac{e^{2\phi}}{p^+}\Pi, \quad \dot{\Pi}=\frac{1}{p^+}\partial_\sigma(e^{2\phi}\acute{\phi})+2\mathcal{P}^-, \tag{6.21}$$

$$\dot{u}^M=\frac{e^{2\phi}}{p^+}\mathcal{P}^M-\mathrm{i}e^{2\phi}\eta_i(\sigma^{MN})^i{}_j\eta^j u^N, \tag{6.22}$$

$$\dot{\mathcal{P}}^M=-\frac{e^{2\phi}}{p^+}u^M\mathcal{P}^N\mathcal{P}^N+\frac{1}{p^+}v^{MN}\partial_\sigma(e^{2\phi}\acute{u}^N)-\mathrm{i}e^{2\phi}\eta_i(\sigma^{MN})^i{}_j\eta^j\mathcal{P}^N \tag{6.23}$$

$$+e^{2\phi}v^{MN}\eta^i\rho^N_{ij}\acute{\theta}^j+e^{2\phi}v^{MN}\eta_i(\rho^N)^{ij}\acute{\theta}_j, \tag{6.24}$$

$$\dot{\theta}^i=\frac{\mathrm{i}}{p^+}\partial_\sigma(e^{2\phi}\eta_j y^{ji}), \quad \dot{\theta}_i=\frac{\mathrm{i}}{p^+}\partial_\sigma(e^{2\phi}\eta^j y_{ji}), \tag{6.25}$$

$$\dot{\eta}^i=e^{2\phi}\left[\mathrm{i}\eta^2\eta^i-\frac{2\mathrm{i}}{p^+}(l\eta)^i+\frac{\mathrm{i}}{p^+}y^{ij}\acute{\theta}_j\right], \quad \dot{\eta}_i=e^{2\phi}\left[-\mathrm{i}\eta^2\eta_i+\frac{2\mathrm{i}}{p^+}(\eta l)_i+\frac{\mathrm{i}}{p^+}y_{ij}\acute{\theta}^j\right], \tag{6.26}$$

where v^{MN} is given by (3.11) and, as previously, do not distinguish between the upper and lower "S^3" indices M,N, i.e., use the convention $\mathcal{P}_M=\mathcal{P}^M$. These equations can be written in the Hamiltonian form. Introducing the notation $\mathcal{X}$ for the phase space variables $(\Pi,\phi,\mathcal{P}^M,u^M,\theta^i,\theta_i,\eta^i,\eta_i)$, the Hamiltonian equations are

$$\dot{\mathcal{X}}=[\mathcal{X},\mathcal{P}^-], \tag{6.27}$$

where the phase space variables satisfy the (classical) Poisson–Dirac brackets,

$$[\Pi(\sigma),\phi(\sigma')]=\delta(\sigma,\sigma'), \tag{6.28}$$

$$[\mathcal{P}^M(\sigma),u^N(\sigma')]=v^{MN}\delta(\sigma,\sigma'), \quad [\mathcal{P}^M(\sigma),\mathcal{P}^N(\sigma')]=(u^M\mathcal{P}^N-u^N\mathcal{P}^M)\delta(\sigma,\sigma'), \tag{6.29}$$

$$\{\theta_i(\sigma),\theta^j(\sigma')\}=\frac{\mathrm{i}}{p^+}\delta^j_i\delta(\sigma,\sigma'), \quad \{\eta_i(\sigma),\eta^j(\sigma')\}=\frac{\mathrm{i}}{p^+}\delta^j_i\delta(\sigma,\sigma'), \tag{6.30}$$

$$[x_0^-,\theta^i]=\frac{1}{2p^+}\theta^i, \quad [x_0^-,\theta_i]=\frac{1}{2p^+}\theta_i, \quad [x_0^-,\eta^i]=\frac{1}{2p^+}\eta^i, \quad [x_0^-,\eta_i]=\frac{1}{2p^+}\eta_i. \tag{6.31}$$

x_0^- is the zero mode of x^- so that $[p^+,x_0^-]=1$. All the remaining brackets are equal to zero. The structure of (6.29) reflects the fact that in the Hamiltonian formulation the condition $u^Mu^M=1$ should be supplemented by the constraint,

$$u^M\mathcal{P}^M=0. \tag{6.32}$$

These are second class constraints, and the Dirac procedure leads then to the classical Poisson–Dirac brackets (6.29). To derive (6.30) and (6.31) one is to take into account that the Lagrangian (6.14) has the following second class constraints:

$$p_{\theta^i}+\frac{\mathrm{i}}{2}p^+\theta_i=0, \quad p_{\theta_i}+\frac{\mathrm{i}}{2}p^+\theta^i=0, \tag{6.33}$$

where p_{θ^i}, p_{θ_i} are the canonical momenta of fermionic coordinates. The same constraints are found for the fermionic coordinates η^i, η_i. Starting with the Poisson brackets

$$\{p_{\theta^i},\theta^j\}_{\mathrm{P.B.}}=\delta_i^j, \quad \{p_{\theta_i},\theta_j\}_{\mathrm{P.B.}}=\delta_j^i, \quad [p^+,x_0^-]_{\mathrm{P.B.}}=1, \tag{6.34}$$

one gets then the Poisson–Dirac brackets given in (6.30) and (6.31).

VII. NOETHER CHARGES AS GENERATORS OF THE SUPERALGEBRA psu(1,1|2) $\oplus\widetilde{\mathrm{psu}}$(1,1|2)

The Noether charges play an important role in the analysis of the symmetries of dynamical systems. The choice of the light-cone gauge spoils manifest global symmetries, and in order to demonstrate that these global invariances are still present one needs to find the Noether charges which generate them. In what follows ''currents'' and ''charges'' will mean both bosonic and fermionic ones, i.e., will include supercurrents and supercharges. These charges determine the structure of superstring field theory in the light-cone gauge.[37] The first step in the construction of superstring field theory is to find a free (quadratic) superfield representation of the generators of the $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ superalgebra. The charges we obtain below can be used to obtain (after quantization) these free superstring field charges.

The Noether charges for a superparticle in $AdS_3\times S^3$ were found in Sec. III. These charges are helpful in establishing a correspondence between the bulk fields of type IIB supergravity and the chiral primary operators of the boundary theory in a manifestly supersymmetric way. Superstring Noether charges should thus be important for the study of the AdS/CFT correspondence at the full string-theory level. Our discussion below will be an adaptation to the $AdS_3\times S^3$ case of the results for the currents in the $AdS_5\times S^5$ case given in Ref. 12.

A. Currents for κ-symmetry light-cone gauge fixed superstring action

As usual, symmetry generating charges can be obtained from conserved currents. Since currents themselves may be helpful in some applications, we shall first derive them starting with the κ-symmetry gauge fixed Lagrangian in the form given in (5.26),(5.27) and using the standard Noether method based on the localization of the parameters of the associated global transformations. Let ϵ be a parameter of some global transformation which leaves the action invariant. Replacing it by a function of worldsheet coordinates τ,σ, the variation of the action takes the form,

$$\delta S=\int d^2\sigma\mathcal{G}^\mu\partial_\mu\epsilon, \tag{7.1}$$

where $\mathcal{G}^\mu$ is the corresponding current. Making use of this formula, we shall find below those currents which are related to symmetries that do not involve compensating κ-symmetry transformation. The remaining currents will be found in the next subsection starting from the action (6.14) where both the κ-symmetry and the bosonic light-cone gauges are fixed.

Let us start with the translation invariance $\delta x^a=\epsilon^a$. Applying (7.1) to the Lagrangian (5.26),(5.27) gives the translation currents,

$$\mathcal{P}^{+\mu}=-\sqrt{g}g^{\mu\nu}e^{2\phi}\partial_\nu x^+, \tag{7.2}$$

$$\mathcal{P}^{-\mu}=-\sqrt{g}g^{\mu\nu}(e^{2\phi}\partial_\nu x^-+F^MD_\nu u^M)-\frac{\mathrm{i}}{2}\sqrt{g}g^{\mu\nu}e^{2\phi}(\theta^i\partial_\nu\theta_i+\theta_i\partial_\nu\theta^i+\eta^i\partial_\nu\eta_i+\eta^i\partial_\nu\eta^i$$
$$+2\mathrm{i}e^{2\phi}\partial_\nu x^+(\eta^2)^2)+\epsilon^{\mu\nu}e^{2\phi}(\eta^iy_{ij}\partial_\nu\theta^j+\eta_iy^{ij}\partial_\nu\theta_j), \quad F^M\equiv\mathrm{i}\eta_i(\sigma^{MN})^i{}_j\eta^je^{2\phi}u^N. \tag{7.3}$$

Some of the remaining bosonic currents can be expressed in terms of supercurrents. The invariance with respect to the supertransformations,

$$\delta\theta^i=\epsilon^i,\quad \delta\theta_i=\epsilon_i,\quad \delta x^-=-\frac{\mathrm{i}}{2}\epsilon^i\theta_i-\frac{\mathrm{i}}{2}\epsilon_i\theta^i, \tag{7.4}$$

gives the supercurrents

$$\mathcal{Q}^{+i\mu}=-\sqrt{g}g^{\mu\nu}e^{2\phi}\theta^i\partial_\nu x^+ +\mathrm{i}\epsilon^{\mu\nu}e^{2\phi}\eta_j y^{ji}\partial_\nu x^+, \tag{7.5}$$

$$\mathcal{Q}^{+\mu}_i=-\sqrt{g}g^{\mu\nu}e^{2\phi}\theta_i\partial_\nu x^+ +\mathrm{i}\epsilon^{\mu\nu}e^{2\phi}\eta^j y_{ji}\partial_\nu x^+. \tag{7.6}$$

The invariance of the action (5.26),(5.27) with respect to the rotation of (super) coordinates in the (x^+,x^-) plane,

$$\delta x^\pm=e^{\pm\epsilon}x^\pm,\quad \delta(\theta^i,\theta_i,\eta^i,\eta_i)=e^{-\epsilon/2}(\theta^i,\theta_i,\eta^i,\eta_i), \tag{7.7}$$

leads to

$$\mathcal{J}^{+-\mu}=x^+\mathcal{P}^{-\mu}-x^-\mathcal{P}^{+\mu}+\frac{\mathrm{i}}{2}\theta^i\mathcal{Q}^{+\mu}_i+\frac{\mathrm{i}}{2}\theta_i\mathcal{Q}^{+i\mu}, \tag{7.8}$$

while the invariance with respect to the dilatations,

$$\delta x^a=e^\epsilon x^a,\quad \delta\phi=-\epsilon,\quad \delta(\theta^i,\theta_i,\eta^i,\eta_i)=e^{\epsilon/2}(\theta^i,\theta_i,\eta^i,\eta_i), \tag{7.9}$$

implies conservation of the dilatation current,

$$\mathcal{D}^\mu=x^a\mathcal{P}^{a\mu}+\sqrt{g}g^{\mu\nu}\partial_\nu\phi-\frac{\mathrm{i}}{2}\theta^i\mathcal{Q}^{+\mu}_i-\frac{\mathrm{i}}{2}\theta_i\mathcal{Q}^{+i\mu}. \tag{7.10}$$

The invariances with respect to the SU(2) ($\epsilon^i{}_i=0$) and $\widetilde{\mathrm{SU}}(2)$ rotations ($\tilde\epsilon^i{}_i=0$),

$$\delta y^{ij}=\epsilon^i{}_l y^{lj},\quad \text{i.e.,}\quad \delta u^M=-\tfrac{1}{2}\epsilon^i{}_j(\sigma^{MN})^j{}_i u^N,\quad \delta\eta^i=\epsilon^i{}_j\eta^j,\quad \delta\eta_i=-\eta_j\epsilon^j{}_i, \tag{7.11}$$

$$\delta y^{ij}=\tilde\epsilon^j{}_l y^{il},\quad \text{i.e.,}\quad \delta u^M=-\tfrac{1}{2}\tilde\epsilon^i{}_j(\bar\sigma^{MN})^j{}_i u^N,\quad \delta\theta^i=\tilde\epsilon^i{}_j\theta^j,\quad \delta\theta_i=-\theta_j\tilde\epsilon^j{}_i, \tag{7.12}$$

give the following SU(2) and $\widetilde{\mathrm{SU}}(2)$ currents, respectively:

$$\mathcal{J}^{i\mu}_j=-\mathrm{i}\sqrt{g}g^{\mu\nu}\tfrac{1}{2}(\sigma^{MN})^i{}_j u^M D_\nu u^N+(\eta^i\eta_j-\tfrac{1}{2}\delta^i_j\eta^2)\mathcal{P}^{+\mu}. \tag{7.13}$$

$$\begin{aligned}\tilde{\mathcal{J}}^{i\mu}_j=&-\mathrm{i}\sqrt{g}g^{\mu\nu}\tfrac{1}{2}(\bar\sigma^{MN})^i{}_j u^M D_\nu u^N+(\theta^i\theta_j-\tfrac{1}{2}\delta^i_j\theta^2)\mathcal{P}^{+\mu}-\mathrm{i}\epsilon^{\mu\nu}e^{2\phi}\partial_\nu x^+\\ &\times(\eta^l y_{lj}\theta^i-\tfrac{1}{2}\delta^i_j\eta^k y_{kl}\theta^l)+\mathrm{i}\epsilon^{\mu\nu}e^{2\phi}\partial_\nu x^+(\eta_l y^{li}\theta_j-\tfrac{1}{2}\delta^i_j\eta_k y^{kl}\theta_l).\end{aligned} \tag{7.14}$$

B. Charges for bosonic and κ-symmetry light-cone gauge fixed superstring action

In the previous section we have listed the (super)currents starting with the κ-symmetry light-cone gauge fixed action given in (5.26),(5.27). They can be used to find currents for the action where both the fermionic κ-symmetry and the bosonic reparametrization symmetry are fixed by the light-cone type gauges (6.14). To find the components of currents ($\mathcal{G}^0$) in the world-sheet time direction one needs to use the relations (6.2)–(6.5) for the canonical momenta and to insert the light-cone gauge conditions (6.8) and (6.9) into the expressions for the currents. The charges are then $G=\int d\sigma\mathcal{G}^0$.

Let us start with the kinematical generators (charges) (3.1). The results for the currents imply the following representations:

$$P^+ = p^+, \quad Q^{+i} = \int p^+ \theta^i, \quad Q_i^+ = \int p^+ \theta_i . \tag{7.15}$$

Note that these charges depend only on the zero modes of string coordinates (the integrands are $\mathcal{G}^0$ parts of the corresponding currents in world-sheet time direction: $\mathcal{Q}^{+i0}$, $\mathcal{Q}_i^{+0}$ and $\mathcal{P}^{+0}=p^+$). The remaining kinematical charges depend on nonzero string modes,

$$J^{+-} = \int x^+ \mathcal{P}^- - x^- p^+, \quad D = \int x^+ \mathcal{P}^- + x^- p^+ - \Pi, \tag{7.16}$$

$$J^i{}_j = \int l^i{}_j + p^+ \eta^i \eta_j - \frac{1}{2}\delta^i_j p^+ \eta^2, \quad \tilde{J}^i{}_j = \int \tilde{l}^i{}_j + p^+ \theta^i \theta_j - \frac{1}{2}\delta^i_j p^+ \theta^2, \tag{7.17}$$

where $l^i{}_j$ is given by (6.15) and $\tilde{l}^i{}_j = (\mathrm{i}/2)\,(\bar{\sigma}^{MN})^i{}_j u^M \mathcal{P}^N$. The derivation of the remaining charges follows the procedure described in Appendix D of Ref. 12. The conformal (super)charges are given by (3.27), (3.28), where

$$S_i^+|_{x^+=0} = \int \frac{1}{\sqrt{2}} e^{-\phi} p^+ \eta_i, \quad S^{+i}|_{x^+=0} = \int \frac{1}{\sqrt{2}} e^{-\phi} p^+ \eta^i, \tag{7.18}$$

$$K^+|_{x^+=0} = \int -\frac{1}{2} e^{-2\phi} p^+ . \tag{7.19}$$

The dynamical Poincaré charges Q^{-i}, Q_i^- and the conformal charges S^{-i}, S_i^- are

$$Q_i^- = \int \frac{e^{\phi}}{\sqrt{2}} (\mathrm{i}\eta_i \Pi - p^+ \eta^2 \eta_i + 2\eta_j l^j{}_i + y_{ij}\acute{\theta}^j), \tag{7.20}$$

$$Q^{-i} = \int \frac{e^{\phi}}{\sqrt{2}} (-\mathrm{i}\eta^i \Pi - p^+ \eta^2 \eta^i + 2 l^i{}_j \eta^j - y^{ij}\acute{\theta}_j), \tag{7.21}$$

$$S^{-i} = \int \theta^i S - \tilde{l}^i{}_j \theta^j + \frac{1}{2} e^{-\phi} \partial_\sigma (e^{\phi}\eta_j) y^{ji}, \tag{7.22}$$

$$S_i^- = \int \theta_i \bar{S} - \theta_j \tilde{l}^j{}_i - \frac{1}{2} e^{-\phi} \partial_\sigma (e^{\phi}\eta^j) y_{ji}, \tag{7.23}$$

$$S = \mathrm{i}x^- p^+ - \frac{\mathrm{i}}{2}\Pi + \frac{1}{2} p^+ \theta^2, \qquad \bar{S} = -\mathrm{i}x^- p^+ + \frac{\mathrm{i}}{2}\Pi + \frac{1}{2} p^+ \theta^2 . \tag{7.24}$$

Note that the $G|_{x^+=0}$ parts of the kinematical charges (3.1) can be obtained from the superparticle ones simply by replacing the particle coordinates by the string ones. The remaining dynamical generator K^- can be found by using the expressions found above and applying the commutation relations of $\mathrm{psu}(1,1|2) \oplus \widetilde{\mathrm{psu}}(1,1|2)$ superalgebra.

Our classical charges are normalized so that after the quantization, i.e., the replacement of the classical Poisson–Dirac brackets (6.28)–(6.31) by quantum (anti)commutators

$$[,]_{\mathrm{P.B.}} \to \mathrm{i}[,], \quad \{,\}_{\mathrm{P.B.}} \to \mathrm{i}\{,\}, \tag{7.25}$$

redefinitions $J^{+-}\to -iJ^{+-}$, $D\to -iD$, $K^{\pm}\to -K^{\pm}$, and appropriate operator ordering the charges satisfy the commutation relations of psu(1,1|2) $\oplus$ $\widetilde{\text{psu}}(1,1|2)$ superalgebra given in (2.8)–(2.15).

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APPENDIX A: NOTATION AND BASIC DEFINITIONS

In the main part of the paper we use the following conventions for the indices:

$$a,b=0,1 \quad \text{boundary Minkowski space indices,}$$

$$\mathcal{A},\mathcal{B},\mathcal{C}=1,2,3 \quad S^3 \text{ coordinate space indices,}$$

$$A',B',C'=1,2,3 \quad \text{so}(3) \text{ vector indices } (S^3 \text{ tangent space indices),}$$

$$M,N,K,L=1,\ldots,4 \quad \text{so}(4) \text{ vector indices,}$$

$$i,j,k,n=1,2 \quad \text{su}(2) \text{ and } \widetilde{\text{su}}(2) \text{ vector indices,}$$

$$\mu,\nu=0,1 \quad \text{world-sheet coordinate indices.}$$

We decompose x^a into the light-cone coordinates $x^a=(x^+,x^-)$, where $x^{\pm}\equiv(1/\sqrt{2})(x^1\pm x^0)$. We suppress the flat space metric tensor $\eta_{ab}=(-,+)$ in scalar products, i.e., $A^aB^a\equiv\eta_{ab}A^aB^b$. The SO(1,1) vector A^a is decomposed as $A^a=(A^+,A^-)$ so that the scalar product is $A^aB^a=A^+B^-+A^-B^+$. The derivatives with respect to the world-sheet coordinates (τ,σ) are

$$\dot{x}\equiv\partial_\tau x, \quad \acute{x}\equiv\partial_\sigma x. \tag{A1}$$

The world-sheet Levi-Civita $\epsilon^{\mu\nu}$ is defined with $\epsilon^{01}=1$.

The four matrices $(\sigma^M)^i{}_j$, $(\bar{\sigma}^M)^i{}_j$ are off-diagonal blocks of the SO(4) Dirac matrices γ^M in the chiral (Weyl) representation, i.e.,

$$\gamma^M=\begin{pmatrix} 0 & \sigma^M \\ \bar{\sigma}^M & 0 \end{pmatrix}, \quad (\sigma^M)^i{}_k(\bar{\sigma}^N)^k{}_j+(\sigma^N)^i{}_k(\bar{\sigma}^M)^k{}_j=2\,\delta^{MN}\delta^i_j, \tag{A2}$$

$$C'_{ik}(\sigma^M)^k{}_j=C'_{jk}(\bar{\sigma}^M)^k{}_i, \quad (\sigma^M)^i{}_j^*\equiv(\bar{\sigma}^M)^j{}_i, \tag{A3}$$

where C' is a charge conjugation matrix. σ^{MN}, $\bar{\sigma}^{MN}$ are defined by

$$(\sigma^{MN})^i{}_j\equiv\tfrac{1}{2}(\sigma^M)^i{}_k(\bar{\sigma}^N)^k{}_j-(M\leftrightarrow N), \quad (\bar{\sigma}^{MN})^i{}_j\equiv\tfrac{1}{2}(\bar{\sigma}^M)^i{}_k(\sigma^N)^k{}_j-(M\leftrightarrow N). \tag{A4}$$

We use the following explicit form of σ^M, $\bar{\sigma}^M$, and C'_{ij}:

$$\sigma^M=(\sigma^{A'},-iI), \quad \bar{\sigma}^M=(\sigma^{A'},iI), \quad C'_{ij}=c\,\epsilon_{ij}, \quad |c|=1. \tag{A5}$$

We also use the matrices ρ^M defined by

$$\rho^M_{ij}\equiv C'_{ik}(\sigma^M)^k{}_j, \quad (\rho^M)^{ij}\equiv-(\sigma^M)^i{}_k(C'^{-1})^{kj}, \quad (\rho^M_{ij})^*=-(\rho^M)^{ij}. \tag{A6}$$

We assume the following Hermitian conjugation rule for the fermionic coordinates and the notation for their squares,

$$\theta_i^\dagger=\theta^i, \quad \eta_i^\dagger=\eta^i, \quad \theta^2\equiv\theta^i\theta_i, \quad \eta^2\equiv\eta^i\eta_i. \tag{A7}$$

The generators of the su(2) and $\widetilde{\mathrm{su}}(2)$ subalgebras of so(4),

$$[J^{MN},J^{KL}]=\delta^{NK}J^{ML}+3 \text{ terms} \tag{A8}$$

are defined by

$$J^i{}_j=\tfrac{1}{4}(\sigma^{MN})^i{}_jJ^{MN}, \quad \tilde{J}^i{}_j=\tfrac{1}{4}(\bar{\sigma}^{MN})^i{}_jJ^{MN}. \tag{A9}$$

The translation operator $J^{4A'}$ on S^3 is

$$J^{4A'}=\frac{\mathrm{i}}{2}(\sigma^{A'})^j{}_i(J^i{}_j-\tilde{J}^i{}_j). \tag{A10}$$

The coset representative of S^3 defined by $g_y\equiv\exp(y^{A'}J^{4A'})$ takes then the form given in (E6) below. In terms of these coordinates, the 3-sphere interval, metric tensor and vielbein are given by

$$ds^2_{S^3}=d|y|^2+\sin^2|y|ds^2_{S^2}, \quad ds^2_{S^2}=dn^{\mathcal{A}}dn^{\mathcal{A}}, \quad n^{\mathcal{A}}n^{\mathcal{A}}=1, \tag{A11}$$

$$G_{\mathcal{AB}}=e^{\mathcal{A}}_{\mathcal{A}'}e^{\mathcal{A}'}_{\mathcal{B}}, \quad e^{\mathcal{A}'}_{\mathcal{A}}=\frac{\sin|y|}{|y|}(\delta^{\mathcal{A}'}_{\mathcal{A}}-n_{\mathcal{A}}n^{\mathcal{A}'})+n_{\mathcal{A}}n^{\mathcal{A}'}, \tag{A12}$$

$$G_{\mathcal{AB}}=\frac{\sin^2|y|}{|y|^2}(\delta_{\mathcal{AB}}-n_{\mathcal{A}}n_{\mathcal{B}})+n_{\mathcal{A}}n_{\mathcal{B}}, \quad n^{\mathcal{A}}\equiv\frac{y^{\mathcal{A}}}{|y|}, \quad |y|=\sqrt{y^{A'}y^{A'}}. \tag{A13}$$

We use the convention $y^{\mathcal{A}}=\delta^{\mathcal{A}}_{A'}y^{A'}$ and the same for $n^{A'}$. The S^3 Killing vectors $V^{A'}$ and $V^{A'\mathrm{B}'}$ corresponding to the 3 translations and 3 SO(3) rotations are

$$V^{A'}=[|y|\cot|y|(\delta^{A'\mathcal{A}}-n^{A'}n^{\mathcal{A}})+n^{A'}n^{\mathcal{A}}]\partial_{y^{\mathcal{A}}}, \quad V^{A'\mathrm{B}'}=y^{A'}\partial_{y^{\mathrm{B}'}}-y^{\mathrm{B}'}\partial_{y^{A'}}. \tag{A14}$$

They can be collected into the SU(2) combination,

$$(V^{\mathcal{A}})^i{}_j\partial_{y^{\mathcal{A}}}=\frac{1}{4}(\sigma^{A'\mathrm{B}'})^i{}_jV^{A'\mathrm{B}'}+\frac{\mathrm{i}}{2}(\sigma^{A'})^i{}_jV^{A'}. \tag{A15}$$

These relations and (5.24) imply the following relations:

$$G_{\mathcal{AB}}(\eta V^{\mathcal{A}}\eta)(\eta V^{\mathcal{B}}\eta)=(\eta R^M\eta)^2, \qquad G_{\mathcal{AB}}(\eta V^{\mathcal{A}}\eta)dy^{\mathcal{B}}=(\eta R^M\eta)du^M, \tag{A16}$$

where R^M is defined by (5.29), which have been used to transform (5.21)–(5.26).

APPENDIX B: LIGHT-CONE BASIS OF psu(1,1|2)⊕$\widetilde{\mathrm{psu}}$(1,1|2)

Here we explain the relation between the su(1,1)⊕su(2) covariant and light-cone bases of the psu(1,1|2) algebra and define the light-cone basis of psu(1,1|2)⊕$\widetilde{\mathrm{psu}}$(1,1|2). We find it convenient to introduce intermediate basis defined by

$$m^{+-}\equiv-m^1{}_1, \quad m^{+1}\equiv\frac{1}{\sqrt{2}}m^2{}_1, \quad m^{-1}\equiv-\frac{1}{\sqrt{2}}m^1{}_2, \tag{B1}$$

$$q^{+i}\equiv -q_1^i, \quad q^{-i}\equiv q_2^i, \quad q_i^+\equiv q_i^2, \quad q_i^-\equiv q_i^1. \tag{B2}$$

In this basis the Hermitian rules for supercharges take conventional form $(q^{+i})^\dagger = q_i^+$, $(q^{-i})^\dagger = q_i^-$, and for the (anti)commutators one has

$$[m^{+-},m^{\pm 1}]=\pm m^{\pm 1}, \quad [m^{+1},m^{-1}]=-m^{+-}, \quad [m^{+-},q_i^\pm]=\pm\tfrac{1}{2}q_i^\pm, \tag{B3}$$

$$\{q^{\pm i},q_j^\pm\}=-a\sqrt{2}\,\delta_j^i m^{\pm 1}, \quad \{q^{\pm i},q_j^\mp\}=a(\delta_j^i m^{+-}\mp m^i{}_j), \tag{B4}$$

$$[q^{-i},m^{+1}]=-\frac{1}{\sqrt{2}}q^{+i}, \quad [q^{+i},m^{-1}]=\frac{1}{\sqrt{2}}q^{-i}. \tag{B5}$$

The light-cone basis of $\mathrm{psu}(1,1|2)\oplus\widetilde{\mathrm{psu}}(1,1|2)$ superalgebra is defined by

$$P^+=\sqrt{2}\tilde{m}^{+1}, \quad P^-=\sqrt{2}m^{-1}, \quad K^+=\sqrt{2}m^{+1}, \quad K^-=\sqrt{2}\tilde{m}^{-1}, \tag{B6}$$

$$J^{+-}=m^{+-}+\tilde{m}^{+-}, \quad D=m^{+-}-\tilde{m}^{+-}, \quad J^i{}_j=m^i{}_j, \quad \tilde{J}^i{}_j=\tilde{m}^i{}_j, \tag{B7}$$

$$Q^{+i}=\tilde{q}^{+i}, \quad Q_i^+=\tilde{q}_i^+, \quad Q^{-i}=q^{-i}, \quad Q_i^-=q_i^-, \tag{B8}$$

$$S^{-i}=\tilde{a}\tilde{q}^{-i}, \quad S_i^-=\tilde{a}^*\tilde{q}_i^-, \quad S^{+i}=aq^{+i}, \quad S_i^+=a^*q_i^+. \tag{B9}$$

The constants $a,\tilde{a}$ are chosen to be $a=-\mathrm{i}$, $\tilde{a}=\mathrm{i}$. Then the commutation relations are

$$\begin{gathered}
[P^\pm,K^\mp]=D\mp J^{+-},\\
[D,P^\pm]=-P^\pm, \quad [D,K^\pm]=K^\pm, \quad [J^{+-},P^\pm]=\pm P^\pm, \quad [J^{+-},K^\pm]=\pm K^\pm,\\
[D,Q_i^\pm]=-\tfrac{1}{2}Q_i^\pm, \quad [D,S_i^\pm]=\tfrac{1}{2}S_i^\pm, \quad [J^{+-},Q_i^\pm]=\pm\tfrac{1}{2}Q_i^\pm, \quad [J^{+-},S_i^\pm]=\pm\tfrac{1}{2}S_i^\pm,\\
[S_i^\pm,P^\mp]=\mathrm{i}Q_i^\mp, \quad [Q^{\pm i},K^\mp]=-\mathrm{i}S^{\mp i}, \quad \{Q^{\pm i},Q_j^\pm\}=\mp\mathrm{i}P^\pm\delta_j^i,\\
\{S^{\pm i},S_j^\pm\}=\pm\mathrm{i}K^\pm\delta_j^i \quad \{Q^{+i},S_j^-\}=\tfrac{1}{2}(J^{+-}-D)\delta_j^i-\tilde{J}^i{}_j,\\
\{Q^{-i},S_j^+\}=\tfrac{1}{2}(J^{+-}+D)\delta_j^i+J^i{}_j.
\end{gathered} \tag{B10}$$

The supercharges Q_i^-, Q^{-i}, S^{+i}, S_i^+ transform in the fundamental representation of su(2) i.e., they are rotated only by $J^i{}_j$ and satisfy (2.13). The remaining supercharges Q^{+i}, Q_i^+, S^{-i}, S_i^- transform in fundamental representation of $\widetilde{\mathrm{su}}(2)$, i.e., they are rotated only by $\tilde{J}^i{}_j$ and satisfy (2.14). All the generators except K^a and P^a satisfy the Hermitian conjugation rules in (2.6), while K^a and P^a are taken to be anti-Hermitian: $(P^\pm)^\dagger=-P^\pm$, $(K^\pm)^\dagger=-K^\pm$. The light-cone basis for generators described above is used in the calculation of the Cartan forms in Appendix E. Making the substitutions $P^\pm\to\mathrm{i}P^\pm$, $K^\pm\to-\mathrm{i}K^\pm$ we obtain the basis used in Secs. II–IV.

APPENDIX C: DERIVATION OF SUPERCHARGES

Here we would like to demonstrate how the knowledge of kinematical charges and commutation relations of superalgebra allows one to get dynamical charges systematically. Consider, for example, the dynamical supercharges Q^{-i} whose most general form is

$$Q^{-i}=Q^{-i}(p^+,\partial_{p^+},z,\partial_z,\theta,\lambda,\eta,\vartheta), \tag{C1}$$

where a dependence on S^3 is not shown explicitly. From $[P^+,Q^{-i}]=0$ we get

$$Q^{-i}={}^{(1)}Q^{-i}(p^+,z,\partial_z,\theta,\lambda,\eta,\vartheta), \tag{C2}$$

i.e., we learn that Q^{-i} does not depend on ∂_{p^+}. From $\{Q^{-i},Q^{+j}\}=0$ we get

$$^{(1)}Q^{-i}(p^+,z,\partial_z,\theta,\lambda,\eta,\vartheta)=^{(2)}Q^{-i}(p^+,z,\partial_z,\theta,\eta,\vartheta), \tag{C3}$$

i.e., Q^{-i} does not depend on λ. The anticommutator $\{Q^{-i},Q_j^+\}=0$ tell us that Q^{-i} does not depend on θ, i.e.,

$$^{(2)}Q^{-i}(p^+,z,\partial_z,\theta,\eta,\vartheta)=^{(3)}Q^{-i}(p^+,z,\partial_z,\eta,\vartheta). \tag{C4}$$

From $[Q^{-i},K^+]=S^{+i}$ we get

$$^{(3)}Q^{-i}=\frac{1}{\sqrt{2}}\eta^i\partial_z+^{(4)}Q^{-i}(p^+,z,\eta,\vartheta), \tag{C5}$$

i.e.,

$$Q^{-i}=\frac{1}{\sqrt{2}}\eta^i\partial_z+^{(4)}Q^{-i}(p^+,z,\eta,\vartheta), \tag{C6}$$

and from $\{Q^{-i},S^{+j}\}=0$ we get

$$^{(4)}Q^{-i}=-\frac{1}{\sqrt{2}z}\eta^i(\eta\vartheta)+^{(5)}Q^{-i}(p^+,z,\eta), \tag{C7}$$

i.e.,

$$Q^{-i}=\frac{1}{\sqrt{2}}\eta^i\partial_z-\frac{1}{\sqrt{2}z}\eta^i(\eta\vartheta)+^{(5)}Q^{-i}(p^+,z,\eta). \tag{C8}$$

The second anticommutator in (2.12) gives

$$^{(5)}Q^{-i}(p^+,z,\eta)=\frac{1}{2\sqrt{2}z}\eta^i+\frac{2}{\sqrt{2}z}(l\eta)^i+^{(6)}Q^{-i}(p^+,z), \tag{C9}$$

and the su(2) covariance implies $^{(6)}Q^{-i}(p^+,z)=0$. Taking this into account and plugging (C9) into (C8) we get Q_i^- given by (3.16). Using the Hermitian conjugation rule $(Q^{-i})^\dagger=Q_i^-$ we get the expression for Q_i^- in (3.15). The anticommutator $\{Q_i^-,Q^{-j}\}=-P^-\delta_i^j$ determines P^-, i.e., the Hamiltonian. The remaining dynamical generators K^-, S^{-i}, S_i^- can be obtained in a similar way.

APPENDIX D: EIGENVECTORS OF THE *AdS* MASS OPERATOR

Here we would like to explain the procedure of finding the eigenvectors of the AdS mass operator A or the operator X in (3.19) in Sec. IV A. Since the superfield $\Phi_{k,\sigma}$ in (4.11) diagonalizes the operators l^2 and $\eta\vartheta$ we have to diagonalize the operator $\vartheta l\eta\equiv\vartheta_i l^i{}_j\eta^j$, i.e., to find the solution to equation

$$\vartheta l\eta\Phi_{k,1}=m\Phi_{k,1}, \tag{D1}$$

where m is an eigenvalue. We look for the following most general solution:

$$\Phi_{k,1}=(\vartheta_i+c(\vartheta l)_i)\Phi_{k,1}^i, \tag{D2}$$

where Φ^i does not depend on ϑ and c should be determined. Making use of

$$\{(\vartheta l)_j,(l\eta)^i\}=\tfrac{1}{2}(l^2+2\vartheta l\eta)\delta^i_j+(\eta\vartheta-1)l^i{}_j \tag{D3}$$

and $\eta^j\Phi^i_{k,1}=0$ we get

$$(\vartheta l\eta)\Phi_{k,1}=\left((1+c)(\vartheta l)_i+\frac{k(k+2)}{4}c\,\vartheta_i\right)\Phi^i_{k,1}. \tag{D4}$$

From (D1) we then find the equations

$$\frac{k(k+2)}{4}c=m,\quad (1+c)=mc, \tag{D5}$$

which are solved by

$$m^{(1)}=-\frac{k}{2},\quad c^{(1)}=-\frac{2}{k+2};\quad m^{(2)}=\frac{k+2}{2},\quad c^{(2)}=-\frac{2}{k}. \tag{D6}$$

Thus we have the two solution and the two eigenvectors,

$$\Phi^{(1)}_{k,1}=\left(\vartheta_i-\frac{2}{k+2}(\vartheta l)_i\right)\Phi^i_{k,1},\quad \Phi^{(2)}_{k,1}=\left(\vartheta_i-\frac{2}{k}(\vartheta l)_i\right)\Phi^i_{k,1}. \tag{D7}$$

Taking into account the relation

$$2l^2\Phi^{(1,2)}_{k,1}=k(k+2)\Phi^{(1,2)}_{k,1},\quad (\eta\vartheta-1)\Phi^{(1,2)}_{k,1}=0, \tag{D8}$$

and the eigenvalues $m^{(1)}$ and $m^{(2)}$ of $\vartheta l\eta$ given in (D6) we get the following eigenvalues of the operator X:

$$X\Phi^{(1)}_{k,1}=k^2\Phi^{(1)}_{k,1},\quad X\Phi^{(2)}_{k,1}=(k+2)^2\Phi^{(2)}_{k,1}. \tag{D9}$$

APPENDIX E: SUPERSTRING ACTION

The standard kinetic term of superstring action in $AdS_3\times S^3$,[16–18]

$$\mathcal{L}_{\rm kin}=-\tfrac{1}{2}\sqrt{g}g^{\mu\nu}(\hat{L}^A_\mu\hat{L}^A_\nu+L^{A'}_\mu L^{A'}_\nu), \tag{E1}$$

can be rewritten in conformal algebra notation as[11]

$$\mathcal{L}_{\rm kin}=-\tfrac{1}{2}\sqrt{g}g^{\mu\nu}(\hat{L}^a_\mu\hat{L}^a_\nu+L_{D\mu}L_{D\nu}+L^{A'}_\mu L^{A'}_\nu), \tag{E2}$$

where the Cartan 1-forms,

$$\hat{L}^a\equiv L^a_P-\frac{1}{2}L^a_K,\quad L^{A'}\equiv-\frac{\mathrm{i}}{2}(\sigma^{A'})^i{}_jL^j{}_i+\frac{\mathrm{i}}{2}(\sigma^{A'})^i{}_j\tilde{L}^j{}_i, \tag{E3}$$

in the light-cone basis are defined by

$$\begin{aligned}G^{-1}dG=&L^a_PP^a+L^a_KK^a+L_DD+L^{-+}J^{+-}+L^i{}_jJ^j{}_i+\tilde{L}^i{}_j\tilde{J}^j{}_i+L^{-i}_QQ^+_i+L^-_{Q\,i}Q^{+i}+L^{+i}_QQ^-_i\\&+L^+_{Q\,i}Q^{-i}+L^{-i}_SS^+_i+L^-_{S\,i}S^{+i}+L^{+i}_SS^-_i+L^+_{S\,i}S^{-i},\end{aligned} \tag{E4}$$

where the generators are taken in the basis described in Appendix B. To represent the Cartan 1-forms in terms of the even and odd coordinate fields we shall start with the following supercoset representative,

$$G=\exp(x^aP^a+\theta^{-i}Q_i^+ +\theta_i^-Q^{+i}+\theta^{+i}Q_i^- +\theta_i^+Q^{-i})\exp$$
$$\times(\eta^{-i}S_i^+ +\eta_i^-S^{+i}+\eta^{+i}S_i^- +\eta_i^+S^{-i})\, g_y g_\phi , \tag{E5}$$

where g_ϕ and g_y depend on the radial AdS_3 coordinate ϕ and S^3 coordinates $y^{A'}$, respectively,

$$g_\phi \equiv \exp(\phi D), \quad g_y \equiv \exp(y^i{}_j(J^j{}_i-\tilde{J}^j{}_i)), \quad y^i{}_j \equiv \frac{\mathrm{i}}{2}(\sigma^A)^i{}_j y^{A'}. \tag{E6}$$

Choosing the parametrization of the coset representative in the form (E5) corresponds to what is usually referred to as ''Killing gauge'' in superspace. Equation (E4) provides the definition of the Cartan forms in the light-cone basis. Let us further specify them by setting to zero some of the fermionic coordinates which corresponds to fixing a particular κ-symmetry gauge. Namely, we shall fix the κ-symmetry by putting to zero all the Grassmann coordinates which carry positive J^{+-} charge: $\theta^{+i}=\theta_i^+=\eta^{+i}=\eta_i^+=0$. To simplify the notation in what follows we shall set $\theta^i \equiv \theta^{-i}$, $\theta_i \equiv \theta_i^-$, $\eta^i \equiv \eta^{-i}$, $\eta_i \equiv \eta_i^-$. Note that since S^{+i} and Q^{+i} transform in the fundamental representations of su(2) and $\widetilde{\mathrm{su}}(2)$ the corresponding fermionic coordinates η's and θ's also transform in the fundamental representation of su(2) and $\widetilde{\mathrm{su}}(2)$. As a result, the κ-symmetry fixed form of the coset representative (E5) is

$$G_{\mathrm{g.f.}}=\exp(x^aP^a+\theta^iQ_i^+ +\theta_iQ^{+i})\exp(\eta^iS_i^+ +\eta_iS^{+i})g_y g_\phi . \tag{E7}$$

Plugging $G_{\mathrm{g.f.}}$ into (E4) we get the κ-symmetry gauge fixed expressions for the Cartan 1-forms,

$$L_P^+ = e^\phi dx^+, \quad L_P^- = e^\phi\left(dx^- -\frac{\mathrm{i}}{2}\tilde{\theta}^i\tilde{d}\theta_i -\frac{\mathrm{i}}{2}\tilde{\theta}_i\tilde{d}\theta^i\right), \tag{E8}$$

$$L_K^- = e^{-\phi}\left[\frac{1}{4}(\tilde{\eta}^2)^2dx^+ +\frac{\mathrm{i}}{2}\tilde{\eta}^i\tilde{d}\eta_i +\frac{\mathrm{i}}{2}\tilde{\eta}_i\tilde{d}\eta^i\right], \quad L_D=d\phi, \tag{E9}$$

$$L^i{}_j=(dUU^{-1})^i{}_j+\mathrm{i}(\tilde{\eta}^i\tilde{\eta}_j-\tfrac{1}{2}\tilde{\eta}^2\delta^i_j)dx^+, \quad \tilde{L}^i{}_j=(d\tilde{U}\tilde{U}^{-1})^i{}_j, \tag{E10}$$

$$L_Q^{-i}=e^{\phi/2}\tilde{d}\theta^i, \quad ,L_{Qi}^-=e^{\phi/2}\tilde{d}\theta_i, \quad L_Q^{+i}=-\mathrm{i}e^{\phi/2}\tilde{\eta}^idx^+, \quad L_{Qi}^+=\mathrm{i}e^{\phi/2}\tilde{\eta}_idx^+, \tag{E11}$$

$$L_S^{-i}=e^{-\phi/2}\left(\tilde{d}\eta^i+\frac{\mathrm{i}}{2}\tilde{\eta}^2\tilde{\eta}^idx^+\right), \quad L_{Si}^-=e^{-\phi/2}\left(\tilde{d}\eta_i-\frac{\mathrm{i}}{2}\tilde{\eta}^2\tilde{\eta}_idx^+\right), \tag{E12}$$

with all the remaining forms equal to zero. We have introduced the notation

$$\tilde{\eta}^i\equiv U^i{}_j\eta^j, \quad \tilde{\eta}_i\equiv\eta_j(U^{-1})^j{}_i, \quad \tilde{\theta}^i\equiv\tilde{U}^i{}_j\theta^j, \quad \tilde{\theta}_i\equiv\theta_j(\tilde{U}^{-1})^j{}_i, \tag{E13}$$

$$\widetilde{d\eta^i}\equiv U^i{}_jd\eta^j, \quad \widetilde{d\eta_i}\equiv d\eta_j(U^{-1})^j{}_i, \quad \widetilde{d\theta^i}\equiv\tilde{U}^i{}_jd\theta^j, \quad \widetilde{d\theta_i}\equiv d\theta_j(\tilde{U}^{-1})^j{}_i. \tag{E14}$$

The fact that θ^i and η^i are rotated by $\widetilde{\mathrm{SU}}(2)$ and SU(2) is related to the presence of the matrices $\tilde{U}\in\widetilde{\mathrm{SU}}(2)$ and $U\in\mathrm{SU}(2)$ in the definition of $\tilde{\theta}^i$ and $\tilde{\eta}^i$. These matrices defined by (5.4) can be written explicitly as

$$U=\cos\frac{|y|}{2}+\mathrm{i}\sigma^{A'}n^{A'}\sin\frac{|y|}{2}, \quad \tilde{U}=\cos\frac{|y|}{2}-\mathrm{i}\sigma^{A'}n^{A'}\sin\frac{|y|}{2}, \tag{E15}$$

where $|y|$ and $n^{A'}$ are given by (A13).

The S^3 components $L^{A'}$ of the Cartan forms defined by (E3) can be written in the following equivalent ways:

$$L^{A'}=e^{A'}-\tfrac{1}{2}\tilde{\eta}_i(\sigma^{A'})^i{}_j\tilde{\eta}^j dx^+, \quad L^{A'}=e^{A'}_{\mathcal{A}}(dy^{\mathcal{A}}+\mathrm{i}\eta_i(V^{\mathcal{A}})^i{}_j\eta^j dx^+), \tag{E16}$$

where $e^{A'}_{\mathcal{A}}$ and $(V^{\mathcal{A}})^i{}_j$ are defined by (A12) and (A15) and we used the relation,

$$e^{A'}_A(U^\dagger\sigma^{A'}U)^i{}_j=-2\mathrm{i}(V^{\mathcal{A}})^i{}_j, \quad e^{\mathcal{A}\ B'}_{A'\ \mathcal{A}}=\delta^{B'}_{A'}. \tag{E17}$$

Plugging the Cartan 1-forms into the kinetic part of the string Lagrangian (E2) we get

$$\begin{aligned}\mathcal{L}_{\mathrm{kin}}=&-\sqrt{g}g^{\mu\nu}[e^{2\phi}\partial_\mu x^+\partial_\nu x^-+\tfrac{1}{2}\partial_\mu\phi\partial_\nu\phi+\tfrac{1}{2}L^{A'}_\mu L^{A'}_\nu]+\sqrt{g}g^{\mu\nu}\partial_\mu x^+\\&\times\left[\left(e^{2\phi}\left(\frac{\mathrm{i}}{2}\theta^i\partial_\nu\theta_i+\frac{\mathrm{i}}{2}\theta_i\partial_\nu\theta^i\right)+\frac{\mathrm{i}}{4}\eta^i\partial_\nu\eta_i+\frac{\mathrm{i}}{4}\eta_i\partial_\nu\eta^i+\frac{1}{8}(\eta^2)^2\partial_\nu x^+\right)\right].\end{aligned} \tag{E18}$$

In order to get the action in the Killing parametrization one needs to use $L^{A'}$ given by the second expression in (E16) and then make the rescalings,

$$\eta^i\to\sqrt{2}e^{\phi}\eta^i, \quad \eta_i\to\sqrt{2}e^{\phi}\eta_i, \quad x^a\to-x^a. \tag{E19}$$

The action in the WZ parametrization is found by using $L^{A'}$ given by the first expression in (E16) and after the transformation

$$\theta^i\to(\tilde{U}^{-1})^i{}_j\theta^i, \quad \theta_i\to\theta_j\tilde{U}^j{}_i, \quad \eta^i\to\sqrt{2}e^{\phi}(U^{-1})^i{}_j\eta^j, \quad \eta_i\to\sqrt{2}e^{\phi}\eta_j U^j{}_i, \quad x^a\to-x^a, \tag{E20}$$

and use of the Fierz rearrangement rule $(\eta_i(\sigma^{A'})^i{}_j\eta^j)^2=-3(\eta^2)^2$.

The P-odd WZ part of the covariant string Lagrangian $\mathcal{L}_{\mathrm{WZ}}$ (see, e.g., (Refs. 16–18) takes the following form in the light-cone gauge:

$$\mathcal{L}_{\mathrm{WZ}}=-\frac{\mathrm{i}}{\sqrt{2}}\epsilon^{\mu\nu}L^{+i}_{Q\mu}C'_{ij}L^{-j}_{Q\nu}+\mathrm{h.c.} \tag{E21}$$

Plugging in the expressions for the Cartan 1-forms and making the rescalings given above we get $\mathcal{L}_{\mathrm{WZ}}$ in the Killing parametrization (5.22) [see also (5.27)] and in the WZ parametrization [see the $\epsilon^{\mu\nu}$ term in (5.6)].

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Representations of superconformal algebras in the $AdS_{7/4}/CFT_{6/3}$ correspondence

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We perform a general analysis of representations of the superconformal algebras OSp(8/4, $\mathbb{R}$) and OSp($8^*/2N$) in harmonic superspace. We present a construction of their highest-weight UIR's by multiplication of the different types of massless conformal superfields (''supersingletons''). In particular, all ''short multiplets'' are classified. Representations undergoing shortening have ''protected dimension'' and may correspond to BPS states in the dual supergravity theory in anti-de Sitter space. These results are relevant for the classification of multitrace operators in boundary conformally invariant theories as well as for the classification of AdS black holes preserving different fractions of supersymmetry. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1374451]

I. INTRODUCTION

Superconformal algebras and their representations play a crucial rôle in the AdS/CFT correspondence because of their dual role of describing the gauge symmetries of the AdS bulk supergravity theory and the global symmetries of the boundary conformal field theory.[1–3]

A special class of configurations which are particularly relevant are the so-called BPS states, i.e., dynamical objects corresponding to representations which undergo ''shortening.''

These representations can only occur when the conformal dimension of a (super)primary operator is ''quantized'' in terms of the R symmetry quantum numbers and they are at the basis of the so-called ''nonrenormalization'' theorems of supersymmetric quantum theories.[4]

There exist different methods of classifying the UIR's of superconformal algebras. One is the so-called oscillator construction of the Hilbert space in which a given UIR acts.[5] Another one, more appropriate to describe field theories, is the realization of such representations on superfields defined in superspaces.[6,7] The latter are ''supermanifolds'' which can be regarded as the quotient of the conformal supergroup by some of its subgroups.

In the case of ordinary superspace the subgroup in question is the supergroup obtained by exponentiating a nonsemisimple superalgebra which is the semidirect product of a super-Poincaré graded Lie algebra with dilatation [SO(1,1)] and the R symmetry algebra. This is the superspace appropriate for non-BPS states. Such states correspond to bulk massive states which can have a ''continuous spectrum'' of the AdS mass (or, equivalently, of the conformal dimension of the primary fields).

BPS states are naturally associated to superspaces with a lower number of ''odd'' coordinates and, in most cases, with some internal coordinates of a coset space G/H. Here G is the R symmetry group of the superconformal algebra, i.e., the subalgebra of the even part which com-

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mutes with the conformal algebra of space–time and H is some subgroup of G having the same rank as G.

Such superspaces are called ''harmonic'' [8] and they are characterized by having a subset of the initial odd coordinates θ. The complementary number of odd variables determines the fraction of supersymmetry preserved by the BPS state. If a BPS state preserves K supersymmetries then the θ's of the associated harmonic superspace will transform under some UIR of H_K.

For 1/2 BPS states, i.e., states with maximal supersymmetry, the superspace involves the minimal number of odd coordinates (half of the original one) and H_K is then a maximal subgroup of G. On the other hand, for states with the minimal fraction of supersymmetry H_K reduces to the ''maximal torus'' whose Lie algebra is the Cartan subalgebra of G.

It is our aim in the present paper to give a comprehensive treatment of BPS states related to ''short representations'' of superconformal algebras for the cases which are most relevant in the context of the AdS/CFT correspondence, i.e., the $d=3$ $(N=8)$ and $d=6$ $[N=(2,0)]$. The underlying conformal field theories correspond to world-volume theories of N_c copies of M_2, M_5 and D_3 branes in the large N_c limit[9–13] which are ''dual'' to AdS supergravities describing the horizon geometry of the branes.[14]

The present contribution summarizes the results which have already appeared elsewhere.[15–17] We first carry out an abstract analysis of the conditions for Grassmann (G-)analyticity[18] (the generalization of the familiar concept of chirality[7]) in a superconformal context. We find the constraints on the conformal dimension and R symmetry quantum numbers of a superfield following from the requirement that it does not depend on one or more Grassmann variables. Introducing G-analyticity in a traditional superspace cannot be done without breaking the R symmetry. The latter can be restored by extending the superspace by harmonic variables[19,8,20–24] parametrizing the coset G/H_K. We also consider the massless UIR's (''supersingleton'' multiplets),[25,26] first as constrained superfields in ordinary superspace[27–29] and then, for a part of them, as G-analytic harmonic superfields.[8,24,29] Next we use supersingleton multiplication to construct UIR's of OSp($8^*/2N$) and OSp(8/4, $\mathbb{R}$). We show that in this way one can reproduce the complete classification of UIR's of Ref. 30. We also discuss different kinds of shortening which certain superfields (not of the BPS type) may undergo. We conclude the paper by listing the various BPS states in the physically relevant cases of M_2 and M_5 branes horizon geometry where only one type of supersingleton appears.

Massive towers corresponding to 1/2 BPS states are the K–K modes coming from compactification of M-theory on $AdS_{7/4}\times S_{4/7}$.[31,9] Short representations of superconformal algebras also play a special rôle in determining N-point functions from OPE.[32,33]

Another area of interest is the classification of AdS black holes,[34–37] according to the fraction of supersymmetry preserved by the black hole background.

In a parallel analysis with black holes in an asymptotically flat background,[38] the AdS/CFT correspondence predicts that such BPS states should be dual to superconformal states undergoing ''shortening'' of the type discussed here.

II. THE SIX-DIMENSIONAL CASE

In this section we describe highest-weight UIR's of the superconformal algebras OSp($8^*/2N$) in six dimensions. Although the physical applications refer to $N=1$ and $N=2$, it is worthwhile to carry out the analysis for general N, along the same lines as in the four-dimensional case.[39,40] We first examine the consequences of G-analyticity and conformal supersymmetry and find out the relation to BPS states. Then we will construct UIR's of OSp($8^*/2N$) by multiplying supersingletons. The results exactly match the general classification of UIR's of OSp($8^*/2N$) of Ref. 30.

A. The conformal superalgebra OSp($8^*/2N$) and Grassmann analyticity

The standard realization of the conformal superalgebra OSp($8^*/2N$) makes use of the superspace,

$$\mathbb{R}^{6/8N}=\frac{\mathrm{OSp}(8^*/2N)}{\{K,S,M,D,T\}}=(x^\mu,\theta^{\alpha\ i}), \tag{2.1}$$

where $\theta^{\alpha i}$ is a left-handed spinor carrying an index $i=1,2,...,2N$ of the fundamental representation of the R symmetry group $\mathrm{USp}(2N)$. Unlike the four-dimensional case, here chirality is not an option but is already built in. The only way to obtain smaller superspaces is through Grassmann analyticity. We begin by imposing a single condition of G-analyticity on the superfield defined in (2.1):

$$q^1_\alpha\Phi(x,\theta)=0, \tag{2.2}$$

which amounts to considering the coset

$$\mathbb{A}^{6/4(2N-1)}=\frac{\mathrm{OSp}(8^*/2N)}{\{K,S,M,D,T,Q^1\}}=(x^\mu,\theta^{\alpha\ 1,2,...,2N-1}). \tag{2.3}$$

From the algebra of $\mathrm{OSp}(8^*/2N)$ we obtain

$$m_{\mu\nu}=0, \tag{2.4}$$

$$t^{11}=t^{12}=\cdots=t^{1\ 2N-1}=0, \tag{2.5}$$

$$4t^{1\ 2N}+l=0. \tag{2.6}$$

Equation (2.4) implies that the superfield Φ must be a Lorentz scalar. In order to interpret Eqs. (2.5) and (2.6), we need to split the generators of $\mathrm{OSp}(2N)$ into raising operators (corresponding to the positive roots), $T^{k\ 2N-1}$, $k=1,...,N$, $l=k,\ldots,2N-k$ (simple if $l=k$), $[\mathrm{U}(1)]^N$ charges $H_k=-2T^{k\ 2N-k+1}$, $k=1,...,N$ and lowering operators. The Dynkin labels a_k of a $\mathrm{OSp}(2N)$ irrep are defined as follows:

$$a_k=H_k-H_{k+1},\ \ k=1,...,N-1,\ \ a_N=H_N, \tag{2.7}$$

so that, for instance, the generator Q^1 is the HWS of the fundamental irrep (1, 0, ..., 0).

Now it becomes clear that (2.5) is part of the $\mathrm{USp}(2N)$ irreducibility conditions whereas (2.6) relates the conformal dimension to the sum of the Dynkin labels:

$$l=2\sum_{k=1}^{N}a_k. \tag{2.8}$$

Let us denote the highest-weight UIR's of the $\mathrm{OSp}(8^*/2N)$ algebra by

$$\mathcal{D}(l;J_1,J_2,J_3;a_1,\ldots,a_N),$$

where l is the conformal dimension, J_1, J_2, J_3 are the SU*(4) Dynkin labels and a_k are the $\mathrm{OSp}(2N)$ Dynkin labels of the first component. Then the G-analytic superfields defined above are of the type

$$\Phi(\theta^{1,2,...,2N-1})\Leftrightarrow\mathcal{D}\left(2\sum_{k=1}^{N}a_k;0,0,0;a_1,\ldots,a_N\right). \tag{2.9}$$

From the superconformal algebra it is clear that we can go on in the same manner until we remove half of the θ's, namely $\theta^{N+1},\ldots,\theta^{2N}$. Each time we have to set a new Dynkin label to zero. We can summarize by saying that the superconformal algebra $\mathrm{OSp}(8^*/2N)$ admits the following short UIR's corresponding to BPS states:

$$\frac{p}{2N}\text{BPS:}\quad \mathcal{D}\left(2\sum_{k=p}^{N} a_k;0,0,0;0,...,0,a_p,\ldots,a_N\right),\quad p=1,...,N. \tag{2.10}$$

B. Supersingletons

There exist three types of massless multiplets in six dimensions corresponding to ultrashort UIR's (supersingletons) of OSp(8*/2N) (see, e.g., Ref. 41 for the case $N=2$). All of them can be formulated in terms of constrained superfields as follows.

(i) The first type is described by a superfield $W^{\{i_1\cdots i_n\}}(x,\theta)$, $1\leqslant n\leqslant N$, which is antisymmetric and traceless in the external USp($2N$) indices (for even n one can impose a reality condition). It satisfies the constraint (see Refs. 27 and 42)

$$D_\alpha^{(k_W\{i_1)i_2\ldots i_n\}}=0\Rightarrow\mathcal{D}(2;0,0,0;0,...,0,\ a_n=1,0,...,0). \tag{2.11}$$

The components of this superfield are massless fields. In the case $N=n=1$ this is the on-shell (1, 0) hypermultiplet and for $N=n=2$ it is the on-shell (2, 0) tensor multiplet.[27,28]

(ii) The second type is described by a (real) superfield without external indices, $w(x,\theta)$ obeying the constraint

$$D_{[\alpha}^{(i}D_{\beta]}^{j)}w=0\Rightarrow\mathcal{D}(2;0,0,0;0,...,0). \tag{2.12}$$

(iii) Finally, there exists an infinite series of multiplets described by superfields with n totally symmetrized external Lorentz spinor indices, $w_{(\alpha_1\cdots\alpha_n)}(x,\theta)$ (they can be made real in the case of even n) obeying the constraint

$$D_{[\beta}^{i}w_{(\alpha_1]\ldots\alpha_n)}=0\Rightarrow\mathcal{D}(2+n/2;n,0,0;0,...,0). \tag{2.13}$$

As shown in Ref. 16, the six-dimensional massless conformal fields only carry reps $(J_1,0)$ of the little group SU(2)×SU(2) of a light-like particle momentum. This result is related to the analysis of conformal fields in d dimensions.[43,44] This fact implies that massless superconformal multiplets are classified by a single SU(2) and USp($2N$) R symmetry and are therefore identical to massless super-Poincaré multiplets in five dimensions. Some physical implication of the above circumstance have recently been discussed in Ref. 45 where it was suggested that certain strongly coupled $d=5$ theories effectively become six-dimensional.

C. Harmonic superspace

The massless multiplets (i), (ii) admit an alternative formulation in harmonic superspace (see Refs. 46, 47, 29 for $N=1,2$). The advantage of this formulation is that the constraints (2.11) become conditions for G-analyticity. We introduce harmonic variables describing the coset USp($2N$)/$[\mathrm{U}(1)]^N$:

$$u\in\mathrm{USp}(2N):\ \ u_i^I u_J^i=\delta_J^I,\ \ u_i^I\Omega^{ij}u_j^J=\Omega^{IJ},\ \ u_i^I=(u_I^i)^*. \tag{2.14}$$

Here the indices i, j belong to the fundamental representation of USp($2N$) and I, J are labels corresponding to the $[\mathrm{U}(1)]^N$ projections. The harmonic derivatives,

$$D^{IJ}=\Omega^{K(I}u_i^{J)}\frac{\partial}{\partial u_i^K}, \tag{2.15}$$

form the algebra of USp$(2N)_R$ realized on the indices I, J of the harmonics.

Let us now project the defining constraint (2.11) with the harmonics $u_k^K u_{i_1}^1\cdots u_{i_n}^n$, $K=1,...,n$:

$$D^1_\alpha W^{12\cdots n} = D^2_\alpha W^{12\cdots n} = \ldots = D^n_\alpha W^{12\cdots n} = 0, \tag{2.16}$$

where $D^K_\alpha = D^i_\alpha u^K_i$ and $W^{12\cdots n} = W^{\{i_1\cdots i_n\}} u^1_{i_1} \ldots u^n_{i_n}$. Indeed, the constraint (2.11) now takes the form of a G-analyticity condition. In the appropriate basis in superspace the solution to (2.16) is a short superfield depending on part of the odd coordinates:

$$W^{12\cdots n}(x_A, \theta^1, \theta^2, \ldots, \theta^{2N-n}, u). \tag{2.17}$$

In addition to (2.16), the projected superfield $W^{12\cdots n}$ automatically satisfies the USp($2N$) harmonic irreducibility conditions,

$$D^{K\ 2N-K} W^{12} = 0, \quad K = 1,...,N \tag{2.18}$$

[only the simple roots of USp($2N$) are shown]. The equivalence between the two forms of the constraint follows from the obvious properties of the harmonic products $u^K_{[k} u^K_{i]} = 0$ and $\Omega^{ij} u^K_i u^L_j = 0$ for $1 \leqslant K < L \leqslant n$. The harmonic constraints (2.18) make the superfield ultrashort.

Finally, in case (ii), projecting the constraint (2.12) with $u^I_i u^I_j$ where $I = 1,...,N$ (no summation), we obtain the condition

$$D^I_\alpha D^I_\beta w = 0. \tag{2.19}$$

It implies that the superfield w is *linear* in each projection $\theta^{\alpha I}$.

D. Series of UIR's of OSp(8*/2*N*) and shortening

It is now clear that we can realize the BPS series of UIR's (2.10) as products of the different G-analytic superfields (supersingletons) (2.16).[48] BPS shortening is obtained by setting the first $p-1$ USp($2N$) Dynkin labels to zero:

$$\frac{p}{2N}\text{BPS:}\quad W^{[0,\ldots,0,a_p,\ldots,a_N]}(\theta^1, \theta^2, \ldots, \theta^{2N-p}) = (W^{1\cdots p})^{a_p} \cdots (W^{1\cdots N})^{a_N} \tag{2.20}$$

(note that even if $a_1 \neq 0$ we still have $1/2N$ shortening).

We remark that our harmonic coset USp($2N$)/$[\mathrm{U}(1)]^N$ is effectively reduced to

$$\frac{\mathrm{USp}(2N)}{\mathrm{U}(p) \times [\mathrm{U}(1)]^{N-p}}, \tag{2.21}$$

in the case of $p/2N$ BPS shortening (just as it happened in four dimensions). Such a smaller harmonic space was used in Ref. 29 to formulate the (2, 0) tensor multiplet.

A study of the most general UIR's of OSp(8*/$2N$) [similar to the one of Ref. 50 for the case of SU(2,2/N)] is presented in Ref. 30. We can construct these UIR's by multiplying the three types of supersingletons above:

$$w_{\alpha_1 \ldots \alpha_{m_1}} w_{\beta_1 \ldots \beta_{m_2}} w_{\gamma_1 \ldots \gamma_{m_3}} w^k W^{[a_1,\ldots,a_N]}, \tag{2.22}$$

where $m_1 \geqslant m_2 \geqslant m_3$ and the spinor indices are arranged so that they form an SU*(4) UIR with Young tableau (m_1, m_2, m_3) or Dynkin labels $J_1 = m_1 - m_2$, $J_2 = m_2 - m_3$, $J_3 = m_3$. Thus we obtain four distinct series:

$$\text{(A)}\quad l \geqslant 6 + \frac{1}{2}(J_1 + 2J_2 + 3J_3) + 2\sum_{k=1}^{N} a_k;$$

$$\text{(B)}\quad J_3=0,\qquad l\geqslant 4+\frac{1}{2}(J_1+2J_2)+2\sum_{k=1}^{N}a_k;$$

$$\text{(C)}\quad J_2=J_3=0,\qquad l\geqslant 2+\frac{1}{2}J_1+2\sum_{k=1}^{N}a_k; \tag{2.23}$$

$$\text{(D)}\quad J_1=J_2=J_3=0,\qquad l=2\sum_{k=1}^{N}a_k.$$

The superconformal bound is saturated when $k=0$ in (2.22). Note that the values of the conformal dimension we can obtain are ''quantized'' since the factor w^k has $l=2k$ and k must be a non-negative integer to ensure unitarity. With this restriction Eq. (2.23) reproduces the results of Ref. 30. However, we cannot comment on the existence of a ''window'' of dimensions $2+1/2J_1+2\Sigma_{k=1}^{N}a_k\leqslant l\leqslant 4+1/2J_1+2\Sigma_{k=1}^{N}a_k$ conjectured in Ref. 30 (see also Ref. 49).

In the generic case the multiplet (2.22) is ''long,'' but for certain special values of the dimension some shortening can take place.[30]

III. THE THREE-DIMENSIONAL CASE

In this section we carry out the analysis of the $d=3$ $N=8$ superconformal algebra OSp(8/4, $\mathbb{R}$) in a way similar to the above. Some of the results have already been presented in Ref. 15. As in the previous cases, our results could easily be extended to OSp(N/4,$\mathbb{R}$) superalgebras with arbitrary N. The $N=2$ and $N=3$ cases were considered in Ref. 52.

A. The conformal superalgebra OSp(8/4, $\mathbb{R}$) and Grassmann analyticity

The standard realization of the conformal superalgebra OSp(8/4, $\mathbb{R}$) makes use of the superspace

$$\mathbb{R}^{3/16}=\frac{\mathrm{OSp}(8/4,\mathbb{R})}{\{K,S,M,D,T\}}=(x^{\mu},\theta^{\alpha\ i}). \tag{3.1}$$

In order to study G-analyticity we need to decompose the generators Q_{α}^{i} under $[\mathrm{U}(1)]^4\subset\mathrm{SO}(8)$. Besides the vector representation 8_v of SO(8) we are also going to use the spinor ones, 8_s and 8_c. In this context we find it convenient to introduce the four subgroups U(1) by successive reductions: $\mathrm{SO}(8)\to\mathrm{SO}(2)\times\mathrm{SO}(6)\sim\mathrm{U}(1)\times\mathrm{SU}(4)\to[\mathrm{SO}(2)]^2\times\mathrm{SO}(4)\sim[\mathrm{U}(1)]^2\times\mathrm{SU}(2)\times\mathrm{SU}(2)\to[\mathrm{SO}(2)]^4\sim[\mathrm{U}(1)]^4$. Denoting the four U(1) charges by $\pm$, $(\pm)$, $[\pm]$ and $\{\pm\}$, we decompose the three 8-dimensional representations as follows:

$$8_v:\ \ Q^{i}\to Q^{\pm\pm},Q^{(\pm\pm)},Q^{[\pm]\{\pm\}}, \tag{3.2}$$

$$8_s:\ \ \phi^{a}\to\phi^{+(+)\{\pm\}},\phi^{-(-)[\pm]},\phi^{+(-)\{\pm\}},\phi^{-(+)\{\pm\}}, \tag{3.3}$$

$$8_c:\ \ \sigma^{\dot{a}}\to\sigma^{+(+)\{\pm\}},\sigma^{-(-)\{\pm\}},\sigma^{+(-)\{\pm\}},\sigma^{-(+)\{\pm\}}. \tag{3.4}$$

Let us denote a quasi primary superconformal field of the OSp(8/4, $\mathbb{R}$) algebra by the quantum numbers of its HWS:

$$\mathcal{D}(l;J;a_1,a_2,a_3,a_4), \tag{3.5}$$

where l is the conformal dimension, J is the Lorentz spin and a_i are the Dynkin labels (see, e.g., Ref. 53) of the SO(8) R symmetry.

In order to build G-analytic superspaces we have to add one or more projections of Q_{α}^{i} to the coset denominator. In choosing the subset of projections we have to make sure that (i) they anticommute among themselves; (ii) the subset is closed under the action of the raising operators

of SO(8). Then we have to examine the consistency of the vanishing of the chosen projections with the conformal superalgebra. Thus we find the following sequence of G-analytic superspaces corresponding to BPS states:

$$\frac{1}{8}\text{BPS:}\quad \begin{cases} q_\alpha^{++}\Phi=0\rightarrow \\ \Phi(\theta^{++},\theta^{(\pm\pm)},\theta^{[\pm]\{\pm\}}) \\ \mathcal{D}(a_1+a_2+\frac{1}{2}(a_3+a_4);0;a_1,a_2,a_3,a_4) \end{cases} \tag{3.6}$$

$$\frac{1}{4}\text{BPS:}\quad \begin{cases} q_\alpha^{++}\Phi=q_\alpha^{(++)}\Phi=0\rightarrow \\ \Phi(\theta^{++},\theta^{(++)},\theta^{[\pm]\{\pm\}}) \\ \mathcal{D}(a_2+\frac{1}{2}(a_3+a_4);0;0,a_2,a_3,a_4) \end{cases} \tag{3.7}$$

$$\frac{3}{8}\text{BPS:}\quad \begin{cases} q_\alpha^{++}\Phi=q_\alpha^{(++)}\Phi=q_\alpha^{[+]\{+\}}\Phi=0\rightarrow \\ \Phi(\theta^{++},\theta^{(++)},\theta^{[\pm]\{\pm\}},\theta^{[-]\{+\}}) \\ \mathcal{D}(\frac{1}{2}(a_3+a_4);0;0,0,a_3,a_4) \end{cases} \tag{3.8}$$

$$\frac{1}{2}\text{BPS(type I):}\quad \begin{cases} q_\alpha^{++}\Phi=q_\alpha^{(++)}\Phi=q_\alpha^{[+]\{\pm\}}\Phi=0\rightarrow \\ \Phi(\theta^{++},\theta^{(++)},\theta^{[+]\{\pm\}}) \\ \mathcal{D}(\frac{1}{2}(a_3;0;0,0,a_3,0) \end{cases} \tag{3.9}$$

$$\frac{1}{4}\text{BPS(type II):}\quad \begin{cases} q_\alpha^{++}\Phi=q_\alpha^{(++)}\Phi=q_\alpha^{[\pm]\{+\}}\Phi=0\rightarrow \\ \Phi(\theta^{++},\theta^{(++)},\theta^{[\pm]\{+\}}) \\ \mathcal{D}(\frac{1}{2}(a_4;0;0,0,0,a_4) \end{cases} . \tag{3.10}$$

Note the existence of two types of 1/2 BPS states due to the two possible subsets of projections of q^i closed under the raising operators of SO(8).

B. Supersingletons and harmonic superspace

The supersingletons are the simplest OSp(8/4, $\mathbb{R}$) representations of the type (3.9) or (3.10) and correspond to $\mathcal{D}(1/2;\,0;\,0,\,0,\,1,\,0)$ or $\mathcal{D}(1/2;\,0;\,0,\,0,\,0,\,1)$. The existence of two distinct types of $d=3$ $N=8$ supersingletons has first been noted in Ref. 54. Each of them is just a collection of eight Dirac supermultiplets[26] made out of ''Di'' and ''Rac'' singletons.[25]

In order to realize the supersingletons in superspace we note that the HWS in the two supermultiplets above has spin 0 and the Dynkin labels of the 8_s or 8_c of SO(8), correspondingly. Therefore we take a scalar superfield $\Phi_\alpha(x^\mu,\theta_i^\alpha)$ [or $\Sigma_{\dot a}(x^\mu,\theta_i^\alpha)$] carrying an external 8_s index a (or an 8_c index $\dot a$). These superfields are subject to the following on-shell constraints:[55]

$$\text{type I:}\quad D_\alpha^i\Phi_a=\tfrac{1}{8}\gamma^i_{ab}\overline{\gamma}^j_{bc}D_\alpha^j\Phi_c\,; \tag{3.11}$$

$$\text{type II:}\quad D_\alpha^i\sum_{\dot a}=\frac{1}{8}\tilde\gamma^i_{\dot a b}\gamma^j_{b\dot c}D_\alpha^j\sum_{\dot c}\,. \tag{3.12}$$

The two multiplets consist of a massless scalar in the $8_s(8_c)$ and spinor in the $8_c(8_s)$.

The harmonic superspace description of these supersingletons can be realized by taking the harmonic coset,[56]

$$\frac{\mathrm{SO}(8)}{[\mathrm{SO}(2)]^4}\sim\frac{\mathrm{Spin}(8)}{[\mathrm{U}(1)]^4}. \tag{3.13}$$

Since SO(8)~Spin(8) has three inequivalent fundamental representations, $8_s,8_c,8_v$, following Ref. 57 we introduce three sets of harmonic variables:

$$u_a^A, w_{\dot a}^{\dot A}, v_i^I, \tag{3.14}$$

where A, $\dot A$ and I denote the decompositions of an 8_s, 8_c and 8_v index, correspondingly, into sets of four U(1) charges [see (3.2)–(3.4)]. Each of the 8×8 real matrices (3.14) belongs to the corresponding representation of SO(8)~Spin(8). This implies that they are orthogonal matrices [this is a peculiarity of SO(8) due to triality]:

$$u_a^A u_a^B=\delta^{AB}, \qquad w_{\dot a}^{\dot A} w_{\dot a}^{\dot B}=\delta^{\dot A\dot B}, \quad v_i^I v_i^J=\delta^{IJ}. \tag{3.15}$$

Further, we introduce harmonic derivatives [the covariant derivatives on the coset (3.13)]:

$$D^{IJ}=u_a^A(\gamma^{IJ})^{AB}\frac{\partial}{\partial u_a^B}+w_{\dot a}^{\dot A}(\gamma^{IJ})^{\dot A\dot B}\frac{\partial}{\partial w_{\dot a}^{\dot B}}+v_i^{[I}\frac{\partial}{\partial v_i^{J]}}. \tag{3.16}$$

They respect the algebraic relations (3.15) among the harmonic variables and form the algebra of SO(8) realized on the indices $A,\dot A,I$ of the harmonics.

We now use the harmonic variables for projecting the supersingleton defining constraints (3.11), (3.12). It is easy to show that the projections $\Phi^{+(+)[+]}$ and $\Sigma^{+(+)\{+\}}$ satisfy the following G-analyticity constraints:

$$D^{++}\Phi^{+(+)[+]}=D^{(++)}\Phi^{+(+)[+]}=D^{[+]\{\pm\}}\Phi^{+(+)[\pm]}=0, \tag{3.17}$$

$$D^{++}\Sigma^{+(+)\{+\}}=D^{(++)}\Sigma^{+(+)\{+\}}=D^{[+]}\Sigma^{+(+)\{+\}}=0, \tag{3.18}$$

where $D_\alpha^I=v_i^I D_\alpha^i$, $\Phi^A=u_a^A\Phi_a$ and $\Sigma^{\dot A}=w_{\dot a}^{\dot A}\Sigma_{\dot a}$. This is the superspace realization of the 1/2 BPS shortening conditions (3.9), (3.10). In the appropriate basis in superspace $\Phi^{+(+)[+]}$ and $\Sigma^{+(+)\{+\}}$ depend on different halves of the odd variables as well as on the harmonic variables:

$$\text{type I:}\quad \Phi^{+(+)[+]}(x_A,\theta^{++},\theta^{(++)},\theta^{[+]\{+\}},u,w), \tag{3.19}$$

$$\text{type II:}\quad \Sigma^{+(+)\{+\}}(x_A,\theta^{++},\theta(++),\theta^{[\pm]\{+\}},u,w). \tag{3.20}$$

In addition to the G-analyticity constraints (3.17), (3.18), the on-shell superfields $\Phi^{+(+)[+]},\Sigma^{+(+)\{+\}}$ are subject to the SO(8) irreducibility harmonic conditions obtained by replacing the SO(8) raising operators by the corresponding harmonic derivatives. The combination of the latter with Eq. (3.17) is equivalent to the original constraint (3.11).

C. OSp(8/4, $\mathbb{R}$) supersingleton composites

One way to obtain short multiplets of OSp(8/4, $\mathbb{R}$) is to multiply different analytic superfields describing the type I supersingleton. The point is that above we chose a particular projection of, e.g., the defining constraint (3.11) which lead to the analytic superfield $\Phi^{+(+)[+]}$. In fact, we could have done this in a variety of ways, each time obtaining superfields depending on different halves of the total number of odd variables. Leaving out the 8_v lowest weight θ^{--}, we can have four distinct but equivalent analytic descriptions of the type I supersingleton:

$$\begin{aligned}
&\Phi^{+(+)[+]}(\theta^{++},\theta^{(++)},\theta^{[+]\{+\}},\theta^{[+]\{-\}}),\\
&\Phi^{+(+)[-]}(\theta^{++},\theta^{(++)},\theta^{[-]\{+\}},\theta^{[-]\{-\}}),\\
&\Phi^{+(-)\{+\}}(\theta^{++},\theta^{(--)},\theta^{[+]\{+\}},\theta^{[-]\{+\}}),\\
&\Phi^{+(-)\{-\}}(\theta^{++},\theta^{(--)},\theta^{[+]\{-\}},\theta^{[-]\{-\}}).
\end{aligned} \tag{3.21}$$

Then we can multiply them in the following way:

$$(\Phi^{+(+)[+]})^{p+q+r+s}(\Phi^{+(+)[-]})^{q+r+s}(\Phi^{+(-)\{+\}})^{r+s}(\Phi^{+(-)\{-\}})^{s}, \tag{3.22}$$

thus obtaining three series of OSp(8/4, $\mathbb{R}$) UIR's exhibiting 1/8, 1/4 or 1/2 BPS shortening:

$$\begin{aligned}
&\tfrac{1}{8}\text{BPS:}\quad \mathcal{D}(a_1 a_2+\tfrac{1}{2}(a_3+a_4),0;a_1,a_2,a_3,a_4),\quad a_1-a_4=2s\geqslant 0;\\
&\tfrac{1}{4}\text{BPS:}\quad \mathcal{D}(a_2+\tfrac{1}{2}a_3,0;0,a_2,a_3,0);\\
&\tfrac{1}{2}\text{BPS:}\quad \mathcal{D}(\tfrac{1}{2}a_3,0;0,0,a_3,0),
\end{aligned} \tag{3.23}$$

where

$$a_1=r+2s,\quad a_2=q,\quad a_3=p,\quad a_4=r. \tag{3.24}$$

We see that multiplying only one type of supersingletons cannot reproduce the general result of Sec. III B for all possible short multiplets. Most notably, in (3.23) there is no 3/8 series. The latter can be obtained by mixing the two types of supersingletons:

$$[\Phi^{+(+)[+]}(\theta^{++},\theta^{(++)},\theta^{[+]\{\pm\}})]^{a_3}[\Sigma^{+(+)\{+\}}(\theta^{++},\theta^{(++)},\theta[\pm]\{+\})]^{a_4} \tag{3.25}$$

(or the same with Φ and Σ exchanged). Counting the charges and the dimension, we find exact matching with the series (3.8):

$$\tfrac{3}{8}\text{BPS:}\quad \mathcal{D}(\tfrac{1}{2}(a_3+a_4);0;0,0,a_3,a_4). \tag{3.26}$$

Further, mixing two realizations of type I and one of type II supersingletons, we can construct the 1/4 series,

$$[\Phi^{+(+)[+]}]^{a_2+a_3}[\Phi^{+(+)[-]}]^{a_2}[\Sigma^{+(+)\{+\}}]^{a_4}, \tag{3.27}$$

which corresponds to (3.7):

$$\tfrac{1}{4}\text{BPS:}\quad \mathcal{D}(a_2+\tfrac{1}{2}(a_3+a_4);0;0,a_2,a_3,a_4). \tag{3.28}$$

Finally, the full 1/8 series (3.6) [i.e., without the restriction $a_1-a_4=2s\geqslant 0$ in (3.23)] can be obtained in a variety of ways.

D. BPS states of OSp(8/4, $\mathbb{R}$)

Here we give a summary of all possible OSp(8/4, $\mathbb{R}$) BPS multiplets. Denoting the UIR's by

$$\mathcal{D}(l;J;a_1,a_2,a_3,a_4), \tag{3.29}$$

where l is the conformal dimension, J is the spin and a_1,a_2,a_3,a_4 are the SO(8) Dynkin labels, we find four BPS conditions:

3.4.1.

$$\tfrac{1}{8}\text{BPS}: \quad q_\alpha^{++}=0. \tag{3.30}$$

The corresponding UIR's are

$$\mathcal{D}(a_1+a_2+\tfrac{1}{2}(a_3+a_4);0;a_1,a_2,a_3,a_4) \tag{3.31}$$

and the harmonic coset is

$$\frac{\text{Spin}(8)}{[U(1)]^4}. \tag{3.32}$$

If $a_2=a_3=a_4=0$ this coset becomes Spin(8)/U(4).
3.4.2.

$$\tfrac{1}{4}\text{BPS}: \quad q_\alpha^{++}=q_\alpha^{(++)}=0. \tag{3.33}$$

The corresponding UIR's are

$$\mathcal{D}(a_2+\tfrac{1}{2}(a_3+a_4);0;0,a_2,a_3,a_4), \tag{3.34}$$

and the harmonic coset is

$$\frac{\text{Spin}(8)}{[\text{U}(1)]^2\times\text{U}(2)}. \tag{3.35}$$

If $a_3=a_4=0$ this coset becomes Spin(8)/U(1)$\times$[SU(2)]^3.
3.4.3.

$$\tfrac{3}{8}\text{BPS}: \quad q_\alpha^{++}=q_\alpha^{(++)}=q_\alpha^{[+]\{+\}}=0. \tag{3.36}$$

The corresponding UIR's are

$$\mathcal{D}(\tfrac{1}{2}(a_3+a_4);0;0,0,a_3a_4), \tag{3.37}$$

and the harmonic coset is

$$\frac{\text{Spin}(8)}{U(1)\times U(3)}. \tag{3.38}$$

3.4.4.

$$\tfrac{1}{2}\text{BPS(type I)}: \quad q_\alpha^{++}=q_\alpha^{(++)}=q_\alpha^{[+]\{+\}}q_\alpha^{[+]\{\pm\}}=0; \tag{3.39}$$

$$\tfrac{1}{2}\text{BPS(type II)}: \quad q_\alpha^{++}=q_\alpha^{(++)}=q_\alpha^{[+]\{+\}}=q_\alpha^{[\pm]\{+\}}=0. \tag{3.40}$$

The corresponding UIR's are

$$\tfrac{1}{2}\text{BPS(type I)}: \quad \mathcal{D}(\tfrac{1}{2}a_3;0;0,0,a_3,0); \tag{3.41}$$

$$\tfrac{1}{2}\text{BPS(type II)}: \quad \mathcal{D}(\tfrac{1}{2}a_4;0;0,0,0,a_4), \tag{3.42}$$

and the harmonic coset is

$$\frac{\text{Spin}(8)}{U(4)}. \tag{3.43}$$

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A supersymmetric type IIB Randall–Sundrum realization

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We show that an earlier domain wall solution of type IIB supergravity provides a supersymmetric realization of the Randall–Sundrum brane-world, and give its ten-dimensional interpretation in terms of IIB 3-branes. We also explain how previous no-go theorems are circumvented. In particular, whereas $D=5$ supergravity scalars have AdS_5 energy $E_0 \leqslant 4$ and are unable to support a $D=5$ positive tension brane, our scalar has $E_0=8$, and is the breathing mode of the S^5 compactification. Another essential element of the construction is the implementation of a Z_2 symmetry by patching together compactifications with opposite signs for their 5-form field strengths. This is thus a IIB analog of a previous $D=5$ 3-brane realization of the Hořava–Witten orbifold. A mode-locking phenomenon avoids the appearance of negative energy zero-modes in spite of the necessity of a $D=10$ negative tension brane-source. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1372698]

I. INTRODUCTION

Our purpose in this paper is first to show that the type IIB domain wall solution of Bremer *et al.*[1] provides a supersymmetric realization of the Randall–Sundrum brane-world[2,3] and second to give its ten-dimensional interpretation in terms of IIB 3-branes.

The idea that our universe may be a 3-brane in a higher-dimensional spacetime has a history going back nearly two decades.[4–9] More recently, another viewpoint on this basic idea has grown out of the Hořava–Witten[10,11] model for M-theory/heterotic string duality, based upon an S^1/Z_2 orbifold in $D=11$ spacetime. This orbifold construction was later realized in a $D=5$ compactification by a concrete solution to semiclassical M-theory, i.e., $D=11$ supergravity.[12,13] A key point in this construction was the introduction of flux for the M-theory 4-form field strength $G_{[4]}$ wound around the compact dimensions, which were taken to be a Calabi–Yau 3-fold. The resulting reduced theory is a specific version of matter-coupled $D=5$, $N=2$ supergravity. This dimensionally-reduced theory has a scalar potential arising from the $G_{[4]}$ flux, which rules out flat space or indeed any maximally symmetric space as a solution to the equations of motion. But this $D=5$ reduced theory readily admits domain wall, i.e., 3-brane, solutions. A natural configuration is a pair of two 3-branes in a Z_2 symmetric configuration; projecting the fields of this theory into the subspace of Z_2 invariant configurations then reproduces the Hořava–Witten orbifold. As in the original $D=11/D=10$ discussion, the massless brane-wave excitations of this scenario are not easily deduced by direct analysis of the solution, but one may obtain information about the zero-modes by anomaly inflow arguments. These may either be carried out in $D=10$, leading to the original Hořava–Witten prediction of a $D=10$, $N=1$ super Yang–Mills E_8 gauge multiplet residing on each of the two fixed planes of the orbifold, with the resulting structure subsequently reduced to $D=5$, or one may carry out the anomaly analysis directly in $D=5$, yielding more general possibilities for gauge structure.[14]

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Another theory in which similar constructions can be made is $D=10$ type IIB supergravity. This has a self-dual 5-form field strength that supports the D3-brane, which is the basis for much recent discussion of the Maldacena conjecture, linking string theory in the near-horizon region of the D3-brane to a Yang–Mills theory quantized on the boundary of the associated asymptotic anti de Sitter space, which is the near-horizon limiting spacetime. In the pure supergravity context, relations between p-branes in higher dimensions and domain walls arising after dimensional reduction on spheres was developed in Ref. 1, including the case of the D3-brane of type IIB theory.

Meanwhile, another development was brewing. Randall and Sundrum[2] proposed a simple model of physics on 3-branes embedded in $D=5$ anti de Sitter space, first in a model with two 3-branes, one of positive and one of negative tension. This model was criticized for the apparent danger of nonphysical modes from the negative tension brane, and also because the modulus related to the distance between the two branes gave another parameter needing fixing in any phenomenological analysis. Subsequently, a revision of this scenario was put forward,[3] in which there was only one 3-brane, of positive tension, essentially obtained from the first scenario by sending the negative tension brane to the Cauchy horizon of anti de Sitter space. The striking result found in this second scenario is that, although the fifth dimension of spacetime is now infinite, the effective gravity theory on the single remaining 3-brane nonetheless has $D=4$ and not $D=5$ leading behavior. The gravitational potential for static sources starts out with a Newtonian $1/r$, corrected by terms of order Λ^{-1}/r^3, where Λ is the $D=5$ cosmological constant. This ''binding of gravity'' to the 3-brane happens when a $D=5$ spacetime has a warped product structure, with the warp factor, i.e., the factor multiplying the $D=4$ submetric, decreasing as one recedes on either side from the single Randall–Sundrum 3-brane. This corresponds in general terms to the 3-brane acting as a positive-tension source on the right-hand side of the Einstein equations. It was not clear, however, whether this scenario could arise from an explicit solution to a supergravity theory.

Links between the Randall–Sundrum model and supergravity were made in Refs. 15–20. In Refs. 17, 18, the $D=5$ 3-brane solutions to the type II theory presented in Ref. 1 were used to make an analogy to the Randall–Sundrum model. The explicit relation between this construction and the specific Randall–Sundrum model was not fully pinned down, however. This perspective was further elaborated in Refs. 19, 20. Despite the existence of these works, there still seems to be some confusion in the literature as to whether the Randall–Sundrum model can in fact be obtained from an explicit supergravity solution. (Note, however, that the equivalence of the graviton propagator calculated from closed loops of the $N=4$ SCFT in the Maldacena picture and that calculated from tree graphs in the Randall–Sundrum picture was already strongly indicative of a supersymmetric Randall–Sundrum brane-world.[21])

Moreover, there are powerful general arguments[22–24] as to why smooth supersymmetric solutions obtained from $D=5$ gauged supergravity coupled to various combinations of $D=5$ matter cannot reproduce a Randall–Sundrum scenario with binding of gravity to the 3-brane. A key word here is ''smooth.'' Although one might well like to replace the Randall–Sundrum scenario, with its delta-function source, by a smooth solution, experience with domain walls in supergravity (i.e., codimension-one brane solutions) shows them always to be based upon a linear harmonic function in the $d=1$ codimension. In order for such a solution to have a localized energy concentration, i.e., a ''brane,'' some kind of ''kink'' must be introduced into the linear harmonic function so as to give a location to the domain wall. Thus, the search for a smooth codimension-one solution looks rather unlikely to be successful. (Some rigorous results along these lines have recently been spelled out in Ref. 25. See also Ref. 26.) Moreover, the remainder of the argument of Refs. 22, 23 concerns the general behavior of renormalization group flows between critical points of coupled supergravity-matter potentials. This gives the impression that even if one were to relax the requirement of smoothness, there would be no solution leading to the binding of gravity to the 3-brane.

In this paper, we shall first explicitly obtain the original (kinked) Randall–Sundrum geometry from type IIB supergravity. This follows from the work of Refs. 1, 17, 20. This construction

makes essential use[17] of the ''breathing mode'' of the S^5 dimensional reduction of type IIB supergravity of Ref. 1. We shall show why this massive mode escapes the constraints on supersymmetric flows by reason of its transforming in a representation with AdS lowest energy $E_0 = 8 > 4$, thus falling outside the scope of the analysis of Refs. 22, 23. The breathing-mode solutions, although Kaluza–Klein consistent in a purely bosonic context containing just the breathing mode and gravity, do not really correspond to a pure $D=5$ supergravity theory. The construction retains an essential memory of its $D=10$ type IIB origin. This is particularly so when one considers the superpartners of the breathing mode, which include massive spin two modes that cannot be retained in a consistent truncation to a finite number of $D=5$ fields.

Another memory of $D=10$ supergravity in the supersymmetric realization of the Randall–Sundrum geometry resides in the Z_2 symmetry of this geometry. This geometry is very similar to the Z_2 symmetric configuration of two M-theory 3-branes in $D=5$ that explicitly realizes the Hořava–Witten construction as an M-theory brane solution.[12,13] In the M-theory solution, the Z_2 symmetry is central to the appearance of the orbifold, and it also plays a critical role in the preservation of unbroken $D=4$ supersymmetry on the brane world-volumes.[13] The same is true in the double 3-brane type IIB solution that we present as the supergravity realization of the Randall–Sundrum geometry: continuity of the unbroken supersymmetry Killing spinor depends on the way the Z_2 symmetry is implemented. In particular, in the M-theory case[13] as well as in the type IIB construction,[27] the constant parameter determining the flux of the relevant underlying form field is Z_2 odd, and so flips sign upon crossing either of the 3-branes; this flip is crucial for the continuity of the unbroken supersymmetry parameter. Accordingly, in the type IIB case as in the M-theory case, the $D=5$ theory is really obtained from a dimensional reduction on a *pair* of Kaluza–Klein ansätze, one on each side of the Z_2 symmetric spacetime. Although this construction requires the presence of brane sources for the form-field flux, it is natural in the context of the higher-dimensional M- or type IIB theory. This split ansatz, however, means that it is much less natural to view the geometry as arising in a single $D=5$ theory.

Having shown how to obtain the Randall–Sundrum model from type IIB supergravity, we next set out to study the brane-wave oscillations of the solution. This analysis is quite natural in the type IIB analog of the M-theory Z_2 symmetric double 3-brane construction.[12,13] Although, as in Ref. 2, this configuration involves both a positive and a negative tension brane, thus leading to concerns about negative energies, we show that there is a ''mode-locking'' phenomenon that reduces the zero-modes to just one (positive energy) $D=4$, $N=4$ Maxwell multiplet in the case of one singly charged brane. This happens because the Z_2-odd modes turn out to be nonzero modes constrained to be related to Kaluza–Klein massive modes by the Bianchi identities for the type IIB 5-form field strength $H_{[5]}$ and for the gravitational curvature. Thus, one does not have to make an explicit projection by hand into a Z_2-invariant subspace of fields: this projection happens spontaneously, by normal Kaluza–Klein dynamical mechanisms freezing out massive Kaluza–Klein modes. The type IIB models considered here have the great advantage that one can carry out more of the Kaluza–Klein analysis explicitly than in the analogous discussion of M-theory reduced on Calabi–Yau spaces.[12,13] But it is to be expected that an analogous mode-locking mechanism will operate there as well. And in that case, the mode-locking can be expected to lead to a spontaneous appearance of $D=4$ chirality, thus generalizing the appearance of chirality by explicit Z_2 projection.

II. SUPERSYMMETRIC DOMAIN WALLS AND RENORMALIZATION GROUP FLOWS

While there are many ways of representing a metric on anti de Sitter space, perhaps the most natural form of the metric from a domain wall point of view is given in terms of Poincaré coordinates,

$$ds^2 = e^{-2gy}\eta_{\mu\nu}dx^\mu dx^\nu + dy^2. \tag{2.1}$$

Written in this manner, the Minkowski signature boundary of AdS is reached when $y \to -\infty$, while the point $y \to \infty$ is instead a null surface, the AdS Killing horizon. In the AdS/CFT corre-

spondence, this metric is viewed as the near-horizon geometry of N coincident D3-branes, which is described by $\mathcal{N}=4$ super Yang–Mills living on the boundary. Furthermore, the distance to the boundary is regarded as an energy; from the bulk point of view $y\to-\infty$ is a flow to the UV, while $y\to\infty$ is a flow to the IR.

The Randall–Sundrum brane-world is obtained by taking two Poincaré patches of AdS, both given by (2.1), and joining them at the brane location $y=0$. The resulting Randall–Sundrum metric has the form

$$ds^2=e^{-2g|y|}\eta_{\mu\nu}\,dx^\mu\,dx^\nu+dy^2, \tag{2.2}$$

and its geometry gives rise to a localized graviton on the ''Planck'' brane. Presented as ''an alternative to compactification,'' much has been made of the fact that this scenario binds gravity even though the y direction has an infinite extent. Nevertheless, it is apparent from the form of (2.2) that the Planck brane only lives in a tiny portion of AdS, and that movement away from the brane flows towards the Killing horizon and not towards the Minkowski boundary of AdS. Had one instead chosen to join together the $y<0$ regions of (2.1), the resulting geometry would preserve the vast majority of the original space, including the entire portion of AdS near the boundary. This then would yield a divergent ''localization'' volume and give rise to a brane of opposite character to the Randall–Sundrum brane, namely one that does not bind gravity.

In fact, the above observation motivated the authors of Ref. 28 to view the Randall–Sundrum geometry as a warped compactification of F-theory on a Calabi–Yau four-fold. In this picture, the warped geometry arises from the presence of D3-branes situated on the elliptically fibered Calabi–Yau manifold. The five-dimensional Randall–Sundrum universe then corresponds to the noncompact four-dimensional spacetime with the addition of a single y coordinate which provides a preferred slicing of the internal space along flows between separated stacks of D3-branes. One thus sees that the Randall–Sundrum brane itself is not identified with any one of the D3-branes, but is instead viewed as an effective geometry that arises in interpolating between the near-horizon locations of the D3-branes. In terms of the parametrization in (2.2), the D3-branes are located at the horizons, $y=\pm\infty$, and the apparent infinite extent of the y coordinate is simply a result of the warping of the compact space by the D3-branes themselves. The localization of gravity is then explained by the compactness of the underlying F-theory construction. Heterotic and M-theory realizations based on warped Calabi–Yau compactifications have been examined in Ref. 29.

Returning to a five-dimensional picture, there have been many attempts to explain the Randall–Sundrum scenario from a supersymmetric domain-wall point of view. The advantage of this approach is that one can generally ignore the added complications of the compactification of the underlying IIB theory, and instead focus only on brane constructions in the resulting $D=5$ gauged supergravity theory. However, as we emphasize below, it is important to realize that there is no reason (other than simplicity) to expect that the relevant degrees of freedom lie only in the massless supergravity sector. In fact, as emphasized in Refs. 22, 23, massless gauged supergravity precludes the localization of gravity on a brane. Thus massive fields are a necessity.

For the Randall–Sundrum picture to be realistic, where the Planck brane is a dynamical object, it would have to be supported by bulk scalar fields. Thus, in the language of bulk renormalization group flow, we seek a brane solution with stable flows to AdS critical points in the IR on both sides of it. This approach has been studied extensively in both the AdS/CFT[30,31] and brane-world[22,23,32,33] pictures, with considerable overlap. Nevertheless, the distinction between flows of massless and massive scalars has not always been made clear, so we wish to do so below.

Since we demand that the flow away from the brane is towards an AdS background, the scalars must reach some fixed values corresponding to a critical point in the potential. Then, independent of any specific model, at that point, we may expand the scalars about their fixed values. However before doing so, it is worth realizing that representations in AdS differ from those in a flat background.

Recall that, for AdS_5, general representations of $SU(2,2)$ may be labeled by $D(E_0,j_1,j_2)$ where E_0 is the lowest energy (which may be given in terms of the natural mass scale of the AdS

background). For scalars, $D(E_0,0,0)$, unitarity requires $E_0 \geqslant 1$ with $E_0=1$ corresponding to the singleton representation. General unitarity bounds for $SU(2,2)$ as well as for the $SU(2,2|N/2)$ superalgebras have been obtained in Refs. 34–39 (see also Ref. 40). For a scalar field in AdS_5, the mass is given in terms of E_0 by $m^2=E_0(E_0-4)$, so that ''massless'' scalars in fact correspond to $E_0=4$. Of course, negative mass squared is not to be feared in an AdS background, provided the Breitenlohner–Freedman bound[41] is satisfied. For this case it corresponds to $m^2 \geqslant -4$, which is saturated for $E_0=2$.

To be specific, we now consider the case of a brane supported by a single scalar coupled to gravity, where the Lagrangian takes the form

$$e^{-1}\mathcal{L}=R-\tfrac{1}{2}\partial\phi^2-V(\phi). \tag{2.3}$$

While one may generalize by including more scalars, this single scalar example is sufficient to bring out our conclusion. The resulting equations of motion have the form

$$R_{MN}=\tfrac{1}{2}\partial_M\phi\,\partial_N\phi+\tfrac{1}{3}g_{MN}V(\phi), \quad \nabla^2\phi=\partial_\phi V(\phi). \tag{2.4}$$

Note that we do not insist that (2.3) necessarily originates from a supersymmetric theory. However, in many cases we are of course interested in supersymmetry. This suggests the identification of a putative ''superpotential'' $W(\phi)$ with

$$V=(\partial_\phi W)^2-\tfrac{2}{3}W^2, \tag{2.5}$$

and the putative ''transformations,''

$$\delta\psi_\mu=\left[\nabla_\mu-\frac{1}{6\sqrt{2}}W\gamma_\mu\right]\epsilon, \quad \delta\lambda=\frac{1}{2}[\gamma\cdot\partial\phi+\sqrt{2}\partial_\phi W]\epsilon. \tag{2.6}$$

Identification of the above transformations with those of an actual supergravity theory requires some care.[42] In particular, from an $N=2$ (i.e., minimal supersymmetry in $D=5$) point of view, the field ϕ may reside in either a vector, tensor or hypermatter multiplet, with possibly different forms of coupling to the fermions. In all cases, the fields $(g_{\mu\nu},\psi_\mu)$ and (ϕ,λ) would be part of a (not necessarily consistent) truncation of the actual supergravity theory.

As emphasized previously in discussions of holographic renormalization group flows, the equations of motion following from a domain-wall ansatz take on a simple form. Starting with the metric

$$ds^2=e^{2A(y)}\eta_{\mu\nu}\,dx^\mu\,dx^\nu+e^{2B(y)}\,dy^2, \tag{2.7}$$

one obtains the following equations:

$$A'^2=\tfrac{1}{24}\phi'^2-\tfrac{1}{12}e^{2B}V, \quad A''-A'B'=-\tfrac{1}{6}\phi'^2, \tag{2.8}$$

$$\phi''+(4A'-B')\phi'=e^{2B}\partial_\phi V,$$

where primes denote y derivatives. The first two equations were obtained by combining components of the Einstein equation. Note that the three equations are not all independent, and we find it convenient to focus only on the first two.

In codimension-one, the second metric factor e^{2B} is redundant, and may be removed by defining a new coordinate $\tilde{y}=\int e^B\,dy$ (keeping in mind that explicit domain wall solutions often have a simpler form when presented in terms of a metric with the e^{2B} factor). We proceed by setting $B=0$, so the equations resulting from (2.8) take the form

$$A''=-\tfrac{1}{6}\phi'^2,\quad A'^2=\tfrac{1}{24}\phi'^2-\tfrac{1}{12}V,\quad \phi''+4A'\phi'=\partial_\phi V. \tag{2.9}$$

As emphasized in Refs. 31, 30, the first of these equations indicates that $A''\leqslant 0$, with saturation of the inequality corresponding to sitting in the pure AdS vacuum. For the present case, this has the consequence that the function $A(y)$ must be concave-down, which is in fact exactly what is needed to support a ''kink-down'' (i.e., positive tension) Randall–Sundrum brane of the form (2.2) with a continuous metric function.

To study the behavior of the flow to the IR fixed point, we may expand about the fixed value, ϕ_*, of the scalar. To quadratic order, the potential then has the form

$$V=-12g^2+\tfrac{1}{2}m^2(\phi-\phi_*)^2+\cdots, \tag{2.10}$$

where the constant factor is chosen to give the conventional normalization of the AdS curvature,

$$R_{MNPQ}=-g^2(g_{MP}g_{NQ}-g_{MQ}g_{NP}). \tag{2.11}$$

While in some cases g may coincide with the coupling constant of gauged supergravity, we only take it to parametrize the AdS background at the specific fixed point in which we are interested.

We now insert (2.10) into the second equation of (2.9) to find that $A(y)\approx\pm gy$, at least up to linear order in ϕ. Thus we recover the expected linear behavior giving rise to an AdS background. Continuing with the ϕ equation of motion, and again working to linear order in ϕ (which amounts to making the substitution $A'\approx\pm g$), we find

$$\phi''\pm 4g\phi'-m^2\phi\approx 0, \tag{2.12}$$

which has in general two solutions:

$$\phi\approx\phi_*+ce^{-E_0A(y)},\quad \text{and}\quad \phi\approx\phi_*+ce^{-(4-E_0)A(y)}, \tag{2.13}$$

where $E_0=2+\sqrt{(m/g)^2+4}\geqslant 2$ is given exactly by the mass/E_0 relation for a scalar field in AdS space. Additionally, for either flow, the metric function behaves like

$$A\approx\pm gy-\tfrac{1}{24}(\phi-\phi_*)^2. \tag{2.14}$$

Finally, this allows us to examine the IR flow, corresponding to the behavior in the direction $A\to-\infty$. We see that IR stability is ensured for $E_0>4$ by taking the second solution of (2.13), while the flow is always unstable for $2\leqslant E_0<4$, and the massless case, $E_0=4$, is marginal.

As a result, the above analysis indicates that $E_0>4$ is a necessary condition for IR stability, and hence for the construction of a Randall–Sundrum brane. Note, furthermore, that this result was derived without having to appeal to supersymmetry. Thus it holds in general for both BPS and non-BPS flows. However, as we see below, BPS flows impose a further condition on the relative signs of the terms in the superpotential. This powerful and completely general result was in fact present, although hidden in the discussion of Refs. 22, 23. However, in Refs. 22, 23, only scalars residing in massless vector multiplets of $N=2$ gauged supergravity (i.e., the $\mathcal{D}(2,0,0,0)$ representation, where the last value denotes the $U(1)_r$ charge) were considered. In particular, the authors of Ref. 22 relied on the relation $(\partial_i\partial_j W)_{\rm cr}=1/3\,g_{ij}W_{\rm cr}$ (in our normalization) arising from very special geometry. Such scalars always have $E_0=2$, yielding the negative reported result. Curiously, while it may not have been appreciated that scalars in the decomposition of an $N=8$ gauged supergravity multiplet reside in $N=2$ tensor and hypermatter multiplets as well as vector multiplets, such $N=8$ scalars all have $E_0=2$, 3 or 4 so that they also do not lead to IR stable branes.

Turning now to the case of a supersymmetric flow, it is straightforward to see from (2.6) that the Killing spinor conditions yield the first order equations,

$$A' = \pm \frac{1}{3\sqrt{2}} e^B W, \quad \phi' = \mp \sqrt{2} e^B \partial_\phi W, \tag{2.15}$$

for a domain wall preserving exactly half of the supersymmetries. This result may in fact also be derived without using the transformations (2.6), but instead by a traditional BPS argument for finding static minimum energy configurations.[30,33] Combining both equations gives rise to a holographic renormalization group flow,

$$\frac{d\phi}{dA} = -6 \frac{\partial_\phi W}{W}, \tag{2.16}$$

consistent with the second order equations (2.8). In this case, we expand the superpotential as

$$W = \pm 3\sqrt{2} g (1 + \tfrac{1}{12} \lambda (\phi - \phi_*)^2 + \cdots), \tag{2.17}$$

corresponding to the potential (2.10), provided λ is identified with either E_0 or $4 - E_0$. Note that this introduces a two-fold ambiguity. However this is in fact somewhat artificial, since knowledge of the actual supersymmetric theory would fully determine the superpotential (but see, e.g., Ref. 43 for a discussion on the relation between V and W without supersymmetry). In contrast to (2.13), the supersymmetric flow condition, (2.16), gives only a single approach to the fixed point,

$$\phi \approx \phi_* + c e^{-\lambda A(y)}. \tag{2.18}$$

As a result, for a BPS flow, not only do we require $E_0 > 4$, but also we learn from the above analysis that $\lambda = 4 - E_0$ must be negative in the superpotential (2.17). The requirement of $\lambda < 0$ was previously noted in Ref. 22.

This connection between E_0 and the behavior of a scalar field in AdS was initially made in investigations of the Maldacena conjecture,[44,45] where E_0 was related to the conformal dimension of appropriate operators on the CFT side of the AdS/CFT conjecture. In this case, (2.12) taken with exact equality is simply the massive scalar equation in the reference AdS background (2.1). This in itself highlights the similarity between the brane-world scenario and the AdS/CFT conjecture. In some sense, the Randall–Sundrum brane, being inserted at some fixed location in AdS, cuts off the flow to the UV and hence may be described by a Maldacena CFT cut off at some energy scale related to the location of the brane.

III. BREATHING MODE DOMAIN WALLS AND THE BRANE-WORLD

Based on the preceding analysis, it is clear that consideration of the massless sector of ($N = 2$, 4 or 8) gauged supergravities alone does not lead to realistic brane-world configurations. However, for a five-dimensional model originating from IIB theory, many other degrees of freedom may come into play. While round S^5 compactifications of IIB supergravity yield $N = 8$ gauged supergravity at the massless level, this is also accompanied by a Kaluza–Klein tower of massive states. In general, consistent truncations of sphere reductions are a delicate matter.[46,47] However it is consistent to include the breathing mode φ in the truncation: although it lives in a massive supermultiplet, it is nevertheless a gauge singlet. Domain walls supported by the breathing mode have been investigated in Refs. 1, 17, 20, and have recently been suggested as possible realizations of the brane-world scenario. Note that we use φ to denote the breathing mode rather than ϕ, in order to emphasize that it is distinct from the $D = 10$ dilaton of the type IIB theory.

To make a connection with the Randall–Sundrum model, we examine type IIB string theory compactified on S^5. This sphere reduction, with the inclusion of a single squashing mode along with the breathing mode, was investigated in Ref. 1. Focusing only on the scalar modes, the resulting five-dimensional Lagrangian is

$$e^{-1} \mathcal{L}_5 = R - \tfrac{1}{2} \partial \tilde{\varphi}^2 - \tfrac{1}{2} \partial \tilde{f}^2 - V(\tilde{\varphi}, \tilde{f}). \tag{3.1}$$

The scalar potential has the form

$$V(\tilde{\varphi},\tilde{f})=8m^2e^{(10/\sqrt{15})\tilde{\varphi}}+e^{(4/\sqrt{15})\tilde{\varphi}}(\mu^2e^{(6/\sqrt{10})\tilde{f}}-R_4e^{(1/\sqrt{10})\tilde{f}}), \tag{3.2}$$

where the constants (m,μ,R_4) are parameters of the compactification.[1]

While this potential may now be expanded in the form of Eq. (2.10), it is perhaps more enlightening to first express it in the form of a ''superpotential'' according to (2.5). We find

$$W=2\sqrt{2}me^{(5/\sqrt{15})\tilde{\varphi}}-e^{(2/\sqrt{15})\tilde{\varphi}}\left(\sqrt{2}\mu e^{(3/\sqrt{10})\tilde{f}}+\frac{R_4}{2\sqrt{2}\mu}e^{-(2/\sqrt{10})\tilde{f}}\right). \tag{3.3}$$

Note that there is a slight sign ambiguity in inverting (2.5); here we have chosen the signs so that W has a critical point at

$$e^{(3/\sqrt{15})\tilde{\varphi}_*}=\frac{\mu}{2m}\left(\frac{R_4}{6\mu^2}\right)^{3/5},\quad e^{(5/\sqrt{10})\tilde{f}_*}=\frac{R_4}{6\mu^2}, \tag{3.4}$$

corresponding to that of V as well. Expansion of W then gives

$$W=-3\sqrt{2}m\left(\frac{\mu}{2m}\right)^{5/3}\left(\frac{R_4}{6\mu^2}\right)\left[1-\frac{1}{3}(\tilde{\varphi}-\tilde{\varphi}_*)^2+\frac{1}{2}(\tilde{f}-\tilde{f}_*)^2+\cdots\right]. \tag{3.5}$$

A comparison with (2.17) then demonstrates explicitly that the breathing mode $\tilde{\varphi}$ has $E_0=8$ while the squashing mode $\tilde{f}$ has $E_0=6$. Curiously, the two modes enter with opposite signs in W. While this $N=8$ symmetric critical point is indeed a minimum of the potential, it is only a saddle point of W.

The consequences for the resulting supersymmetric flow were investigated in the previous section. For supersymmetric flows, this critical point is IR stable for the breathing mode, while it is unstable for the squashing mode. This indicates explicitly that simply having a domain wall supported by a scalar with $E_0>4$ may be insufficient to ensure the stability of a supersymmetric Randall–Sundrum configuration. Nevertheless, we have now seen why use of the massive breathing mode of sphere reductions has been successful in constructing brane-world domain walls,[17,20] avoiding the limitations on supersymmetric flows presented in Refs. 22, 23.

To proceed, we now truncate out the squashing mode by setting $\tilde{f}=0$ and $R_4=6\mu^2=(6/5)R_5$. After dropping tildes, the resulting potential for the breathing mode is simply

$$V(\varphi)=8m^2e^{(10/\sqrt{15})\,\varphi}-R_5e^{(4/\sqrt{15})\,\varphi}, \tag{3.6}$$

and has an AdS minimum at

$$e^{(6/\sqrt{15})\,\varphi_*}=\frac{R_5}{20m^2}. \tag{3.7}$$

Here R_5 is the curvature scalar of the round S^5, arising from the type IIB Kaluza–Klein ansatz,[1]

$$ds_{10}^2=e^{2\alpha\varphi}\,ds_5^2+e^{2\beta\varphi}\,ds^2(S^5),\quad H_{[5]}=4me^{8\alpha\varphi}\epsilon_{[5]}+4m\epsilon_{[5]}(S^5), \tag{3.8}$$

where

$$\alpha=\tfrac{1}{4}\sqrt{\tfrac{5}{2}},\quad \beta=-\tfrac{3}{5}\alpha. \tag{3.9}$$

This also indicates that m is essentially the 5-form flux of the Freund–Rubin compactification. Thus the two parameters m and R_5 of the five-dimensional potential, (3.6), have their origin in the Kaluza–Klein compactification from ten dimensions. Note that the Kaluza–Klein ansatz (3.8) for

the $H_{[5]}$ field strength implies that the Freund–Rubin parameter m must be odd under transformations $y \to -y$. In order for this to be realized as a symmetry of the type IIB theory, this ''lower'' $D=5$ transformation must be accompanied by an orientation-reversing transformation of S^5, so that the self-dual structure of $H_{[5]}$ is preserved, but with $m \to -m$. By the ''skew-whiffing theorem,'' [46] both orientations have the same (maximal) supersymmetry in the case of S^5. For any other compactifying 5-manifold the supersymmetries would not match.

For a complete truncation of the sphere compactification down to $D=5$, in which all Kaluza–Klein modes except for the breathing mode are discarded, the two parameters m and R_5 satisfy trivial Bianchi identities, and hence must be constant. In this case only a single combination of the two is actually physical. The constant parameter R_5 may then be viewed as a necessary dimensionful parameter for measuring coordinate distances on the five sphere (much as one would have to introduce a length scale L for toroidal compactification, where periodic coordinates are identified as $y=y+2\pi L$). The actual invariant (physical) size of the five sphere is then set by the expectation of the breathing mode φ. To see formally how R_5 may be scaled away, consider a shift of φ along with a scaling of m,

$$\varphi \to \varphi + \sqrt{\tfrac{15}{4}} \log \lambda, \quad m \to m\lambda^{-5/4}. \tag{3.10}$$

This transformation has the effect of multiplying R_5 by λ in the potential (3.6), so that an appropriate choice of λ may be used to scale R_5 to any desired value. A particularly natural choice would be to set $R_5=20m^2$, so that the AdS critical point is reached at $\varphi_*=0$. From a ten-dimensional point of view, the transformation (3.10) results in

$$\begin{aligned} ds_{10}^2 &= \lambda^{5/8}[e^{2\alpha\varphi}\, ds_5^2 + e^{2\beta\varphi}\lambda^{-1}\, ds^2(S^5)], \\ H_{[5]} &= \lambda^{5/2}[4me^{8\alpha\varphi}\epsilon_{[5]} + 4m\lambda^{-5/2}\epsilon_{[5]}(S^5)], \end{aligned} \tag{3.11}$$

which is thus a rescaling of S^5 combined with a $D=5$ ''trombone'' symmetry.

However, as we will discuss in the following section, if one no longer truncates out the additional Kaluza–Klein modes, then both m and R_5 no longer need to be taken as constant. In this case, attempts to scale away $R_5(x)$ would result in a dynamical scaling by $\lambda(x)$. In this sense one simply trades one parameter for another, and cannot fully eliminate R_5. With this in mind, we maintain both parameters m and R_5 in the solution below.

Breathing-mode domain wall solutions follow by making the standard ansatz (2.7) and by solving the resulting equations (2.8). As mentioned above, keeping two independent factors in the ansatz, $A(y)$ and $B(y)$, is redundant. For $B=0$, the solution was presented in Ref. 17, while it was originally presented in Ref. 1 with a different choice of coordinates. The advantage of the original choice is its highlighting of a linear harmonic function as a natural feature of codimension-one p-brane solutions. This solution has the basic form[1]

$$e^{-(7/\sqrt{15})\varphi} = H, \quad e^{4A} = e^{-B} = \tilde{b}_1 H^{2/7} + \tilde{b}_2 H^{5/7}, \quad H = e^{-(7/\sqrt{15})\varphi_0} + ky, \tag{3.12}$$

where

$$\tilde{b}_1 = \eta_1 \frac{28m}{3|k|}, \quad \tilde{b}_2 = \eta_2 \frac{14\sqrt{5R_5}}{15|k|}. \tag{3.13}$$

Here $\eta_{1,2}=\pm 1$ are in general independent choices of signs for the solution. For our purposes they are fixed by requiring an appropriate AdS limit for $\varphi \to \varphi_*$. This gives $\eta_2 = -\eta_1$ and η_1 chosen so that $e^{4A}>0$ in order for the metric to be real at a given initial value of y.

The linear harmonic function H is restricted to be nonnegative. Examination of the solution indicates that the AdS horizon is located at $H=H_* \equiv e^{-7\varphi_*/\sqrt{15}}$, where e^{4A} vanishes. For initial $H>H_*$ the five-dimensional space asymptotically flattens out as $H \to \infty$, with a corresponding limit for the scalar field $\varphi \to -\infty$, yielding an asymptotically vanishing scalar potential. This case

is the second branch of Ref. 17, where it was referred to as a hybrid type II and dilatonic domain wall. On the other hand, for initial $H<H_*$, the solution soon runs into a singularity at $H=0$. Note, however, that if one starts with a solution with $H>H_*$ initially and signs $\eta_{1,2}$ chosen so as to make $e^{4A}>0$ initially, but then follows the evolution of H within the spacetime through the $H=H_*$ horizon, the metric in the region with $H<H_*$ becomes complex, so one should really treat the region below the horizon using different, appropriately chosen coordinates. Both the $H>H_*$ and $H<H_*$ cases have a natural interpretation in the lifting of (3.12) to ten dimensions. In the IIB theory, (3.12) lifts directly to the geometry of N coincident D3-branes with total charge $\tilde{k}=m(20/R_5)^{5/2}$.[1] The two regions $H\gtrless H_*$ then correspond to the regions either ''outside'' or ''inside'' the D3-brane horizon. This furthermore demonstrates that the first, $H>H_*$, case is nothing but the conventional near-horizon limit occurring prominently in the Maldacena conjecture. The second, $H<H_*$, case is unphysical as it stands, however, as it sees a different region of the D3-brane geometry containing a singularity.

Neither case by itself provides a suitable framework for a Randall–Sundrum configuration. While in one direction one may reach an AdS horizon, in the other direction one will either run into a singularity or on out into unbounded flat space. One obvious possibility for obtaining an asymptotically AdS space on both sides of a domain wall is to reflect the solution at $y=0$, imposing thus a $y\to -y$ Z_2 symmetry. The resulting two-sided domain wall, supported by an absolute value kink in the linear harmonic function,

$$H=e^{-(7/\sqrt{15})\varphi_0}+k|y|, \tag{3.14}$$

was in fact how the solution was originally presented in Ref. 1. The presence of such a kink is rather natural for a codimension-one object. Supergravity p-brane solutions are generally supported by δ-function sources at the locations of the branes themselves, and this remains true for domain walls. Passing through a domain wall, one jumps through a sheet of charge, and this jump in charge manifests itself in a change in the slope of the linear harmonic function. *A priori*, the slope could take any values on the two sides of the domain wall, but clearly the Z_2 symmetric jump from k to $-k$ is a natural configuration. We shall see that this configuration is distinguished also by preserving unbroken supersymmetry.

For either the plain unkinked (3.12) or the kinked (3.14) solution, the slope k may be scaled away by taking $y\to y/|k|$ and $x^\mu\to x^\mu|k|^{1/4}$. This explains why the apparent domain wall charge k is not directly related to lifted quantities such as the D3-brane charge $\tilde{k}$. However, note that this scaling does not eliminate the sign of k, thus leaving a distinction between the slope-up and slope-down possibilities. For discussions of multiple domain wall configurations or brane fluctuations, it is more convenient to retain k.

If one chooses to restrict the coordinate y in (3.14) to range only over the interval $-y_0\leqslant y\leqslant y_0$, identifying the points y_0 and $-y_0$, then one obtains a Z_2 symmetric solution that can serve as the background for a Z_2 orbifold construction. This orbifold construction is analogous to the treatment of M-theory 3-branes given in Refs. 12, 13 as a brane realization of the Hořava–Witten S^1/Z_2 orbifold, and has also been proposed in the Randall–Sundrum context in Ref. 20. The identification of y_0 and $-y_0$ essentially reproduces the original Randall–Sundrum model[2] with both an attractive and a repulsive brane (if one chooses $k<0$, then the attractive brane is the one located at $y=0$). From the five-dimensional point of view, the $y\to -y$ Z_2 map is a parity flip. As we have mentioned above, however, this alone is not a good symmetry of the underlying type IIB theory. In order for this transformation to be compatible with the round-sphere compactification of the IIB theory, this Z_2 transformation must combine the flip in y with an orientation-reversing transformation[27] of the S^5. For example, an allowable transformation flips all six of the coordinates transverse to the underlying $D=10$ D3-brane. The net effect is to send $m\to -m$ as well as $y\to -y$.

This orientation reversal has important consequences for the supersymmetry transformations (2.6), since the superpotential W also flips, $W\to -W$, under these transformations. Actually, this is what one wants, because if the superpotential were to not to flip in this way, then all supersym-

metries would be broken by the domain wall, and it would then no longer be BPS. To see this, consider for example the $\delta\lambda$ transformation for the solution (3.12) with the linear harmonic function (3.14). By truncating out the squashing mode from (3.3), one arrives at the breathing-mode superpotential:

$$W=\sqrt{2}m\left[2e^{(5/\sqrt{15})\,\varphi}-5\sqrt{\frac{R_5}{20m^2}}\,e^{(2/\sqrt{15})\,\varphi}\right]. \tag{3.15}$$

Written as above, this clearly changes sign as $m\to -m$. On the other hand, If one were to assume instead that W remains invariant, one would find

$$\begin{aligned}\partial_\varphi W&=\frac{2}{3}\sqrt{30}m\left[e^{(5/\sqrt{15})\,\varphi}-\sqrt{\frac{R_5}{20m^2}}\,e^{(2/\sqrt{15})\,\varphi}\right]\\&=\frac{\sqrt{30}}{14}|k|H^{-1}(|\tilde{b}_1|H^{2/7}-|\tilde{b}_2|H^{5/7})\\&=-\frac{1}{\sqrt{2}}|\varphi'|e^{-B},\end{aligned} \tag{3.16}$$

where the signs $\eta_{1,2}$ have been chosen to obtain the outside (i.e., $H>H_*$) AdS solution. Inserting this into (2.6) we would find

$$\delta\lambda=\tfrac{1}{2}e^{-B}(\gamma^{\bar{y}}\varphi'-|\varphi'|)\epsilon, \tag{3.17}$$

where $\bar{y}$ denotes a local Lorentz index. Because of the absolute value in the linear harmonic function (3.14), φ' changes sign on opposite sides of $y=0$. Therefore the assumption of an invariant W would leave no possibility of obtaining a Killing spinor that is consistently defined on both sides of $y=0$. If one were to attempt to patch together separate Killing spinors on both sides of $y=0$, in the case of an invariant W, the $y\gtrless 0$ projections on the supersymmetry parameter would be into mutually orthogonal components, $(1+\gamma^y)\epsilon_+=0$ vs $(1-\gamma^y)\epsilon_-=0$. However, since the superpotential *does* change sign under the Z_2, the absolute value in (3.17) is in fact not present, and we accordingly find global Killing spinors of the form $\epsilon=e^{A/2}(1+\gamma^{\bar{y}})\epsilon_0$. Similar considerations apply at the location of the second kink in the Z_2 invariant background. If one expands the theory in modes about this Z_2 invariant background, keeping only the Z_2 invariant modes, the resulting theory is equivalent to one defined on an S^1/Z_2 orbifold.

As we have just demonstrated, the domain wall solution is always one half supersymmetric, with or without the absolute value kink. In particular, the Z_2 orbifolding has not destroyed any further supersymmetry beyond the original half-BPS solution. On the other hand, there is no restoration of supersymmetry either in the presence of a kink. Consider taking a simultaneous limit $k\to 0$ and $\varphi_0\to\varphi_*$. Without the kink, this limit would yield pure AdS, i.e., the D3-brane near-horizon limit in which full supersymmetry is restored. But with the kink, one obtains instead a Z_2 symmetric patching of AdS, with a Randall–Sundrum brane located, say, at $y=0$. The presence of the orbifold fixed point prevents the full supersymmetry from being restored. However, this is fully expected when a domain wall is present. Although the Z_2 symmetrization introduces an absolute value into functions, the Killing spinor equations are of first order, and so do not see any δ-function singularities. As long as the conditions (2.15) are satisfied, the solution remains supersymmetric.

Of course the second order equations of motion will see the δ-function brane source. For the solution (3.14), we find that the extra source terms at $y=0$ are

$$T^{\text{brane}}_{MN}=\frac{3k}{14}(2\tilde{b}_1^2 e^{(3/\sqrt{15})\,\varphi_0}+5\tilde{b}_2^2 e^{-(3/\sqrt{15})\,\varphi_0}-7|\tilde{b}_1\tilde{b}_2|)\,\delta(y)\,\delta^\mu_M\delta^\nu_N g_{\mu\nu},$$
$$Q^{\text{brane}}=-4\sqrt{\frac{5}{3}}\frac{3k}{14}(\tilde{b}_1^2 e^{(3/\sqrt{15})\,\varphi_0}+\tilde{b}_2^2 e^{-(3/\sqrt{15})\,\varphi_0}-2|\tilde{b}_1\tilde{b}_2|)\,\delta(y), \tag{3.18}$$

assuming $\tilde{b}_1\tilde{b}_2<0$ as indicated above. These ''brane sources'' enter in the equations of motion as

$$R_{MN}-\tfrac{1}{2}g_{MN}R=T^{\varphi}_{MN}+T^{\text{brane}}_{MN},\quad \nabla^2\varphi=\partial_\varphi V(\varphi)+Q^{\text{brane}}, \tag{3.19}$$

where

$$T_{MN}=\tfrac{1}{2}(\partial_M\varphi\partial_N\varphi-\tfrac{1}{2}g_{MN}\partial\varphi^2)-\tfrac{1}{2}g_{MN}V(\varphi). \tag{3.20}$$

Depending on the sign of k, the branes have either positive or negative energy density. However, in both cases the relation between charge and tension is the same, so the branes may be stacked up in BPS configurations.

We have thus seen that the kinks at the brane locations have different consequences for supersymmetry and for the equations of motion. Since the supersymmetry variations and Killing spinor conditions are of first order, the kinks give rise to possibly discontinuous quantities, but no δ-function singularities. On the other hand, the equations of motion will be sensitive to the additional δ-function sources. Although one may view the equations of motion as a composition of two supersymmetries, there is no contradiction in the presence and absence of the δ-function terms since the Killing spinor equations only give rise to a subset of the full equations of motion. To see this consider again for simplicity the $\delta\lambda$ transformation (2.6),

$$\delta\lambda=\tfrac{1}{2}[\,\gamma\cdot\partial_\phi+\sqrt{2}\partial_\varphi W]\epsilon=\tfrac{1}{2}e^{-B}[\,\varphi'\,\bar{\gamma^y}+\sqrt{2}e^B\,\partial_\varphi W]\epsilon. \tag{3.21}$$

Partial breaking of supersymmetry then demands the BPS condition $\varphi'=-\sqrt{2}e^B\,\partial_\varphi W$, relating the scalar to its potential. One may of course choose the other sign if so desired. However this is a global choice, and must be consistent in all patches of space. Similarly, vanishing of the gravitino relates the metric to the scalar potential, $A'=e^B W/3\sqrt{2}$, as given in (2.15). Now consider deriving the second order A'' equation of motion by taking a derivative of $e^{-B}A'$,

$$e^{-B}(A''-A'B')=\frac{1}{3\sqrt{2}}W'. \tag{3.22}$$

For a continuous W, one simply uses the chain rule, $W'=\partial_\varphi W\,\phi'$, and substitutes in the φ' equation to arrive at the A'' equation of motion given in (2.8). However, the assumption of a continuous W is actually too strong. For the Z_2 invariant case, where W changes sign at the brane (say at $y=0$), one would also pick up a source term upon differentiating, resulting in

$$A''-A'B'=-\frac{1}{6}\varphi'^2+\frac{\sqrt{2}}{3}e^B W\delta(y). \tag{3.23}$$

Thus, while supersymmetry implies most of the equations of motion, it does not in fact determine all of them. In fact, for higher codimension branes, there is even more slack between the BPS conditions and the equations of motion. The harmonic function condition, of primary importance in brane constructions, is generally a consequence of the equations of motion, and *not* supersymmetry.[48,49]

IV. D3-BRANES AND THE WORLD IN TEN DIMENSIONS

Until now we have focused almost exclusively on the five-dimensional viewpoint of the Randall–Sundrum scenario. Since the breathing-mode domain wall has its origins in the S^5 compactification of IIB theory, it has a natural interpretation in terms of IIB D3-branes.[1] Following this connection from the brane-world geometry to breathing-mode branes and then to D3-branes, one is led to a realization of the Randall–Sundrum scenario in terms of IIB theory in an appropriate D3-brane background.

While the lifting of the breathing mode brane to patches of the D3 geometry is straightforward, the resulting configuration has unusual features. Following Ref. 1, lifting of the solution given in (3.12) proceeds by identifying a ten-dimensional Schwarzschild coordinate,

$$\rho = \sqrt{\frac{20}{R_5}} H^{3/28}. \tag{4.1}$$

Using the charge relation $\tilde{k} = m(20/R_5)^{5/21}$ and the Kaluza–Klein ansatz (3.8), one finds the resulting ten-dimensional metric,

$$ds_{10}^2 = \tilde{b}_2^{1/2} \left(1 - \frac{\tilde{k}}{\rho^4}\right)^{1/2} dx_\mu^2 + \left(1 - \frac{\tilde{k}}{\rho^4}\right)^{-2} d\rho^2 + \rho^2 \, d\Omega_5^2, \tag{4.2}$$

which is that of N D3-branes of total charge $\tilde{k}$.[8,9] A further change of coordinates, $r^4 = \rho^4 - \tilde{k}$, may be performed to transform this into standard isotropic form,

$$ds_{10}^2 = \sqrt{\tilde{b}_2} H_{D3}^{-1/2} \, dx_\mu^2 + H_{D3}^{1/2} (dr^2 + r^2 \, d\Omega_5^2), \tag{4.3}$$

with a harmonic function $H_{D3} = 1 + \tilde{k}/r^4$. Note that the constant $\tilde{b}_2$ may easily be scaled out of the longitudinal coordinates.

For the Z_2 symmetric configuration, obtained by kinking the linear harmonic function, (3.14), we see that H is a double valued function of y. This has the consequence that the lifting relation (4.1) is similarly double valued; opposite sides of the breathing-mode brane lift to identical ρ values. While the orbifold picture corresponds to a single slice of the D3-brane geometry, $\rho \in [\rho_-, \rho_+]$, the full circle compactification instead corresponds to two copies of the D3-brane geometry patched together at ρ_- and ρ_+. Note that the AdS horizon, located at H_*, lifts to the D3-brane horizon, located at $\rho_* = \tilde{k}^{1/4}$. Thus taking the Randall–Sundrum configuration (kink-down with $H > H_*$) and pushing the second brane off to the Cauchy horizon corresponds in ten dimensions to taking two copies of the near-horizon geometry of N D3-branes, and gluing them together at a value ρ_0 of the Schwarzschild coordinate corresponding to the initial value H_0 of the linear harmonic function.

For this Randall–Sundrum configuration, it is instructive to ''unfold'' the doubled metric (4.3) by defining a new radial coordinate $\xi \in [-r_0, r_0]$ such that $r = r_0 - |\xi|$. After scaling out $\tilde{b}_2$ from (4.3), the lifted Randall–Sundrum metric has the form

$$ds_{10}^2 = \left(1 + \frac{\tilde{k}}{(r_0 - |\xi|)^4}\right)^{-1/2} dx_\mu^2 + \left(1 + \frac{\tilde{k}}{(r_0 - |\xi|)^4}\right)^{1/2} (d\xi^2 + (r_0 - |\xi|)^2 \, d\Omega_5^2). \tag{4.4}$$

The positive tension brane is located at $\xi = 0$, while the negative tension brane is pushed off to the AdS horizon at $\xi = \pm r_0$ (the two values are identified under the Z_2 orbifolding). As seen explicitly here, this act of patching together two stacks of D3-branes essentially compactifies the six-dimensional space transverse to the branes, and also introduces a curvature discontinuity at $\xi = 0$, the location of the patching. Furthermore, this compactification introduces a charge conservation condition, implying that the net D3 charge must vanish. Thus the resulting kink at $\xi = 0$

must include a stack of $2N$ negative tension D3-branes, with $-2N$ units of charge soaking up the $N+N$ units of charge from the two stacks of positive tension D3-branes.

The question arises, however, whether placing this stack of $2N$ negative tension D3-branes at $\xi=0$ is sufficient for generating the kinked Randall–Sundrum geometry. Furthermore, the reduction of D3-brane tension from $D=10$ to $D=5$ yields the simple result $T_{D=5}=T_{D=10}$. In addition to giving rise to the tension discrepancy pointed out in Ref. 27, it also leaves unexplained how positive $D=5$ tension arises from negative $D=10$ tension. As it turns out, the resolution to both issues is the realization that the Z_2 orbifolding, or the doubling of spacetime, itself gives rise to a positive tension contribution at $\xi=0$, the location of the kink. Of course, it is easy to see that the net tension has to be positive, as that is what is required to ''fold up'' or compactify the space transverse to the branes. The resulting picture is one of negative tension D3-branes trapped on a positive tension Z_2 orbifold plane giving rise to a composite description of the Randall–Sundrum configuration.[50]

By starting with a brane-world scenario on a circle, one obviously obtains a compact Kaluza–Klein geometry, corresponding to expanding IIB theory about a $\mathcal{M}^{1,3}\times S_1\times S^5$. The S_1 coordinate y lifts to the radial coordinate ρ, living in a restricted annular range between the two D3 source shells in a double D3-brane background. Of course there is no surprise in starting with a compact geometry and lifting it to another compact scenario. However, by taking the limit of placing the second brane at the Cauchy horizon of AdS, one effectively decompactifies the original Randall–Sundrum geometry of Ref. 2 into the picture of Ref. 3. Nevertheless, from a ten-dimensional point of view, this corresponds to simply extending the range of ρ a finite distance so as to reach the doubled D3-brane horizon: the internal space remains compact (at least if the inside-horizon brane cores are disregarded). By smoothing out the patching of the double D3-brane configuration, one presumably obtains a warped compactification with an internal six-manifold in the spirit of Ref. 28.

To complete this D3-brane picture of the brane-world, we present the limit in which the Z_2 symmetric supergravity solution literally reproduces the Randall–Sundrum configuration of a single positive-tension ''kink-down'' brane between two patches of anti de Sitter space.[3] Starting from the $D=5$ 3-brane metric (3.12) with $\tilde{b}_2>0$, $\tilde{b}_1<0$, $k<0$, we want to take a limit as $k\to 0_-$. However, the inverse power of k in $\tilde{b}_1$ and $\tilde{b}_2$ (3.13) makes this appear singular. The cure for this is to take a coordinated limit as $k\to 0_-$ and $\varphi\to\varphi_*$. We implement this explicitly by taking

$$e^{-(7/\sqrt{15})\,\varphi_0}=\left(\frac{20m^2}{R_5}\right)^{7/6}+\beta|k|,\quad \beta>0. \tag{4.5}$$

Note that for $\beta>0$, one has $e^{-(7/\sqrt{15})\,\varphi_0}>e^{-(7/\sqrt{15})\,\varphi_*}$, i.e., $H_0>H_*$. Accordingly, for finite $k<0$, the harmonic function H decreases from its value H_0, reaching the Cauchy horizon value H_* at $y=y_h$. This is the natural point at which to make an identification $y_h\leftrightarrow -y_h$, putting the second (negative tension) 3-brane at the horizon. For finite k, one thus has a ''semi-interpolating soliton'' in the sense that one of the asymptotic limits of the solution, but not both, corresponds to a vacuum solution of the theory, in this case the AdS space with asymptotic scalar φ_*. At the Randall–Sundrum brane, however, there is no horizon.

Taking the joint limit defined by (4.5) as $k\to 0_-$, the difference between the two harmonic functions in e^{2A} partially cancels, giving an expression proportional to k, which cancels the k in the denominators of $\tilde{b}_1$ and $\tilde{b}_2$. The resulting metric function is then given by

$$e^{4A}=4m\left(\frac{R_5}{20m^2}\right)^{5/6}(\beta-|y|)=\frac{4}{L}(\beta-|y|), \tag{4.6}$$

where $L=m^{-1}(20m^2/R_5)^{5/6}$ and the y coordinate remains restricted to a compact range, $|y|<\beta$. This corresponds to the line element

$$ds^2=\frac{2}{\sqrt{L}}(\beta-|y|)^{1/2}\eta_{\mu\nu}\,dx^\mu\,dx^\nu+\frac{L^2}{16}\frac{dy^2}{(\beta-|y|)^2}. \tag{4.7}$$

The apparent infinite range of the fifth dimension[51] is obtained by making a change of variables,

$$\beta-|y|=\beta e^{-4|\tilde{y}|/L},\quad x^\mu=\left(\frac{L}{4\beta}\right)^{1/4}\tilde{x}^\mu, \tag{4.8}$$

resulting in the five-dimensional metric,

$$ds^2=e^{-2|\tilde{y}|/L}\eta_{\mu\nu}\,d\tilde{x}^\mu\,d\tilde{x}^\nu+d\tilde{y}^2, \tag{4.9}$$

which is literally the Randall–Sundrum solution.[2,3] This sign of the kink ($k<0$) thus corresponds to a binding of gravity to the 3-brane at $y=0$, with a metric corresponding to segments of pure anti de Sitter space everywhere off this brane surface.

In taking the above Randall–Sundrum limit $k\to 0_-$, $\varphi_0\to\varphi_*$, the ten-dimensional coordinate ρ is restricted to a progressively limited range near $\tilde{k}$, or, equivalently, r is progressively restricted to a range near $r=0$. Thus, from a $D=10$ perspective, the ''infinite'' Randall–Sundrum scenario[3] corresponds to shrinking the outer (RS) brane source tightly around the inner horizon brane. Clearly, what is infinite and what is infinitesimal in this subject is frame-dependent.

It is instructive to see in addition the scaling of the ''brane sources'' (3.18) in the Randall–Sundrum limit. Taking $k\to 0_-$, we find

$$T^{\text{brane}}_{MN}=-\frac{24}{L^2}\delta(y/\beta)\,\delta^\mu_M\delta^\nu_N g_{\mu\nu}=2V_*\delta(y/\beta)\,\delta^\mu_M\delta^\nu_N g_{\mu\nu}, \tag{4.10}$$

while $Q^{\text{brane}}=0$. This vanishing of the scalar charge is in fact forced on us since φ decouples from the solution in this limit. This brings up a key observation that it is not so much the breathing mode φ that supports the brane, but rather $H_{[5]}$ flux corresponding to D3 charge. In addition, it is also the behavior of $H_{[5]}$ flux that saves the BPS condition with $Q^{\text{brane}}=0$; the variation $\delta\lambda$ becomes trivial (as it must for a decoupling scalar), while the gravitino transformation becomes that of pure AdS but with a sign flip $W_*\to -W_*$ at $y=0$ (corresponding to a Freund–Rubin compactification with opposite S^5 orientations). This preservation of supersymmetry further supports the D3-brane origin of the Randall–Sundrum brane-world, *via* the double 3-brane configuration that we have presented.

The above successful reproduction of the Randall–Sundrum scenario with a ''kink-down'' (i.e., positive tension) domain wall embedded into $D=5$ anti de Sitter space depends crucially upon use of the breathing mode φ, which we have shown to transform in a necessary $E_0>4$ anti de Sitter representation. Noted as a possibility for a Randall–Sundrum scenario in Refs. 17, 20, this mode escapes the analysis of Refs. 22, 23 because it belongs to a massive spin-two multiplet, and thus does not belong to an intrinsically $D=5$ supergravity theory. This is because the full multiplet of the breathing mode's superpartners cannot be retained in a ''consistent'' Kaluza–Klein reduction, since it involves a massive spin two mode, which never can be kept in a consistent reduction on spheres.[52] With respect to the $D=5$, $N=8$ supersymmetry, the breathing mode belongs to a multiplet containing 20 copies of the following sets of fields: 1 spin 2, 4 spin 3/2, 26 spin 1, 20 spin 1/2, 15 spin 0. With respect to a $D=5$, $N=2$ decomposition, it belongs to a long massive vector supermultiplet[53] which is another way of explaining why it escaped the analysis of Refs. 22, 23. Since the breathing mode is an $SO(6)$ singlet, only the inclusion of the breathing mode's nonsinglet superpartners leads to difficulties with Kaluza–Klein consistency; truncation to the purely bosonic theory involving just $D=5$ gravity and the breathing mode is fully consistent.

V. MODE LOCKING AND SPONTANEOUS REDUCTION TO AN ORBIFOLD

The Z_2 symmetric scenario presented above, with two branes of opposite tension and opposite magnetic charge, corresponding to (3.14), is clearly similar to the brane constructions of Hořava–Witten orbifolds in M-theory given in Refs. 12, 13. The analogous type IIB situation has the great advantage that one can work out explicitly many features of the dynamics, whereas the analogous discussions in M-theory reduced on Calabi–Yau 3-folds must necessarily remain rather implicit. Here, we wish to explore further the properties of this Z_2 symmetric solution, and see to which extent it naturally corresponds to an orbifold compactification.

The orbifold compactification may be viewed as a compactification on a circle with an additional projection of all the fluctuations into Z_2 even states only. In a Kaluza–Klein spirit, however, one can investigate the possibility of removing the enforced Z_2 projection, in order to see what the theory does purely of its own accord when compactified about the double 3-brane background. Thus, we start without making any Z_2 projections, but still shall take the y direction to be a circle. As explained above, from a ten-dimensional point of view, the D3-branes now have no noncompact transverse directions. Thus there is an added cohomology constraint, which demands that there cannot be any nonzero net magnetic charge in the compact transverse space. Unlike general warped compactifications, which allow for additional fields and nontrivial topology, we shall maintain our focus on the round S^5 and the breathing mode of the compactification. Then, the simplest allowed configuration on the circle is to have a simple pair of 3-branes with opposite magnetic charges. Placing the branes at opposite points on the circle gives rise to a Z_2 symmetric configuration. However, without imposing the Z_2 orbifold symmetry, it would appear that the branes are free to move independently. But we shall now demonstrate that this is not the case; instead, there is a mode-locking phenomenon that links the fluctuations of the two 3-branes into a Z_2 invariant combination.

Consider the y coordinate to be periodic with length $2l$, making the identification at $y=\rho_1 \leftrightarrow -\rho_2$. For bosonic fields on this circle, one must impose continuity conditions at both the locations of the 3-branes. Demanding continuity of the scalar field φ and the metric component e^{2A} at $y=0$ and also at $y=\rho_1 \leftrightarrow y=-\rho_2$, one has four continuity conditions to satisfy. In this discussion we shall take the overall periodicity length $2l$ to be fixed, so $\rho_1+\rho_2=2l$. From continuity of the scalar field φ, one simply obtains at $y=0$ that the value φ_0 must be a common limit of φ as one approaches the $y=0$ RS brane either from the left or from the right. Continuity at $y=\rho_1 \leftrightarrow -\rho_2$ implies continuity of the harmonic function H, so one obtains $|k_1|\rho_2=|k_2|\rho_2$, or, using $\rho_1+\rho_2=2l$, that $|k_1/k_2|=2l/\rho_1-1$. Imposing as well the periodicity conditions on the metric function e^{2A} at $y=0$ and $y=\rho_1 \leftrightarrow -\rho_2$, one obtains the continuity conditions

$$\left|\frac{k_2}{k_1}\right| = \frac{|m_2| - \sqrt{\frac{R_{5(2)}}{20}}\, e^{(-3/\sqrt{15})\,\varphi_0}}{|m_1| - \sqrt{\frac{R_{5(1)}}{20}}\, e^{(-3/\sqrt{15})\,\varphi_0}} = \frac{|m_2| - \sqrt{\frac{R_{5(2)}}{20}}\,(e^{(-3/\sqrt{15})\,\varphi_0} + |k_2|\rho_2)}{|m_1| - \sqrt{\frac{R_{5(1)}}{20}}\,(e^{(-3/\sqrt{15})\,\varphi_0} + |k_1|\rho_1)}. \tag{5.1}$$

These conditions are solved by matching relations for m and R_5 between the two regions:

$$m_2 = \left(\frac{2l}{\rho_1} - 1\right)^{-1} m_1, \quad \sqrt{R_{5(2)}} = \left(\frac{2l}{\rho_1} - 1\right)^{-1} \sqrt{R_{5(1)}}. \tag{5.2}$$

Accordingly, if one now makes a standard soliton-physics ansatz by letting the Z_2-odd modulus ρ_1 become dependent upon the $D=4$ coordinates x^μ, then upon substitution back into the field equations, one obtains the effective equation for $\rho_1(x^\mu)$. Because the oscillations of this coordinate are linked by (5.2) to the Kaluza–Klein ansatz parameters m and R_5, however, this specific

modulus has special restrictions on its oscillations. Both m and R_5 are curvature components, and are thus subject to Bianchi identities. To see this for m, consider the Kaluza–Klein ansatz (3.8), together with the Bianchi identity

$$dH_{[5]} + \tfrac{1}{2}\epsilon_{ij}F^i_{[3]}F^j_{[3]} \equiv 0. \tag{5.3}$$

Letting $m \to m(x)$ and substituting the original ansatz (3.8), one obtains directly a suppression of m fluctuations, $\partial_\mu m(x) = 0$. For this reason, parameters entering into generalized Kaluza–Klein ansätze like (3.8) have been sometimes been called ''nonzero modes.'' [13] In order to see the dynamics of such modes in more detail, one should restore the massive Kaluza–Klein modes that are normally set to zero in a compactification. In the case of m, this means replacing the ansatz (3.8) by

$$H_{[5]} = 4m(x)e^{8\alpha\varphi}\epsilon_{[5]} + 4m(x)\epsilon_{[5]}(S^5) + h_{[5]}, \tag{5.4}$$

where $h_{[5]}$ represents the fluctuating massive Kaluza–Klein modes. Re-performing the analysis of the Bianchi identity (5.3) for this generalized ansatz, one now shows that a nonvanishing $\partial_\mu m$ must be proportional to $\epsilon^{z_1 z_2 z_3 z_4 z_5}\partial_{[z_1}h_{|\mu|z_2 z_3 z_4 z_5]}$, where $h_{\mu z_2 z_3 z_4 z_5}$ is a Kaluza–Klein massive mode, with mass determined as usual by the inverse radius of the S^5 internal sphere, i.e., corresponding to the length scale of the $D=5$ anti de Sitter space. Thus, $m(x)$, and hence $\rho_1(x)$ are in fact Kaluza–Klein massive modes, and become ''frozen out'' at energies lower than the AdS scale. Similar considerations apply to the nonzero mode R_5, which is the Ricci scalar of the internal S^5 sphere, upon use of the gravitational curvature Bianchi identity. Specifically, in the simple case with Kaluza–Klein massive modes set to zero, if one sets to zero the $D=5$ Bianchi identity $\nabla^M(R_{MN} - 1/2\, g_{MN}R) = 0$ and uses the dimensionally reduced field equations, one finds, for $R_5 \to R_5(x^\mu)$, the constraint $\partial_\nu R_5 \exp(1/2\sqrt{5/3}\varphi) - m\,\partial_\nu m = 0$, thus locking out the low energy $R_5(x^\mu)$ fluctuations as well.

Given that the Z_2 odd modes are linked *via* Bianchi identities to massive Kaluza–Klein modes, one expects the theory to settle down into a low energy effective theory that is Z_2 symmetric. Strictly speaking, all that has been demonstrated above so far is that the $D=4$ derivatives $\partial_\mu m$, $\partial_\mu R_5$ are locked out at low energies. In order to show that the theory settles down into a Z_2 symmetric lowest energy configuration, one would need either to analyze in detail the energy functional for the compactified theory, or to study in more detail the equations of motion of the massive modes. It is likely that the analysis of Z_2 odd modes can only be done fully consistently if one keeps the entire Kaluza–Klein towers of massive states.

However, one can get an idea of the situation that is obtained with non-Z_2-symmetric configurations if one considers in a little more detail the question of supersymmetry preservation in a patched background with the matching conditions (5.1), (5.2). Locally, in a patch, there is no difficulty in finding a Killing spinor. However, once one declares that the overall compact part of the spacetime is $S^5 \times S^1$, one is required to impose continuity and periodicity conditions both for bosons and for fermions.

In the Z_2 symmetric configuration of the two 3-branes, we have already demonstrated while discussing the unbroken supersymmetry transformation of Sec. III,

$$\delta\lambda = \tfrac{1}{2}e^{-B}(\gamma^{\bar{y}}\varphi' - \varphi')\epsilon, \tag{5.5}$$

that there is a consistently defined and continuous unbroken supersymmetry transformation with a Z_2 even global Killing spinor $\epsilon = e^{A/2}(1+\gamma^{\bar{y}})\epsilon_0$. Now consider the form of the *broken* supersymmetry transformations in the double 3-brane background. As one can see from the supersymmetry algebra the anticommutator $\{Q_{\text{broken}}, Q_{\text{preserved}}\}$ involves a translation in the fifth coordinate y, which is clearly Z_2 odd. Indeed, the broken supersymmetry parameters will have Z_2 odd projection conditions. This Z_2 odd character is canceled, however, in expressions for Goldstone spinor zero modes like (5.5), by the Z_2 odd character of φ'. Combining the Goldstino expression for

$y>0$ with the Z_2 map for $y<0$ amounts to inserting an absolute value sign around φ' in (5.5), taking a broken supersymmetry parameter for ϵ. Thus, overall, the Goldstino zero mode is Z_2 even, as it must be in a consistent truncation. Note that the ''kink'' in the Goldstino expression resulting from (5.5) with the replacement $\varphi' \to |\varphi'|$ corresponds to the sign flip of the superpotential W. That W flips without necessarily passing through zero is what allows the Goldstino mode to be normalizable in the present case, thus circumventing the normalizability problems for Goldstinos described in Ref. 54. Overall, the zero modes of the double 3-brane geometry form a single $D=4$, $N=4$ super Maxwell multiplet.

Now consider what happens if one tries to expand around a non-Z_2-symmetric configuration of 3-branes. For the Killing spinor itself, one may observe that $\epsilon = e^{A/2}(1+\gamma^{\bar{y}})\epsilon_0$ is in fact still continuous and well-behaved in the nonsymmetric case, since the metric function e^{2A} is by construction matched at the branes. However the situation is different for the candidate Goldstinos. For a non-Z_2-symmetric configuration the derivative φ' differs by more than a sign as one crosses a 3-brane: in this case one has $|k_2| \neq |k_1|$, so there is a nonunimodular factor present as well. This prevents one from having continuity both of the unbroken supersymmetry parameter and of the Goldstinos. Thus, although things look locally like one has a BPS configuration with unbroken supersymmetry for a non-Z_2-symmetric configuration, analysis of the putative zero-mode supermultiplets finds them to be inconsistent with the available matching conditions. So, one is led to conclude that only the Z_2 symmetric configuration has a proper unbroken supersymmetry and zero-mode multiplets transforming correctly with respect to it.

The configuration with globally unbroken supersymmetry should be the proper ''vacuum'' in this double 3-brane sector of type IIB theory compactified on S^5. A fuller analysis of this spontaneous reduction to a Z_2 invariant effective theory on the basis of energy functionals and the equations of motion for the Kaluza–Klein massive modes would be desirable. But it is already clear that this double 3-brane model displays a remarkable spontaneous appearance of an orbifold structure. This happens not by insistent projection into a Z_2 invariant sector of the theory, but naturally by virtue of the Kaluza–Klein dynamics of the theory.

Our discussion has indicated that the original Randall–Sundrum model[2] arises naturally when the fifth dimension y direction is taken to be compact, and one may view the model as a system of two D3-branes transverse to the internal $S_1 \times S^5$. From the $D=5$ point of view, there are two branes: one with positive and one with negative tension, constrained by Kaluza–Klein dynamics to live at diametrically opposed points on the circle. While the presence of a negative tension brane might appear troublesome, we have shown that it does not contribute to the naïvely anticipated negative energy modes; these are nonzero modes and mix with higher Kaluza–Klein massive modes. The negative tension 3-brane has the effect of protecting the spacetime from curvature singularities in the geometry that might reside behind the Cauchy horizon. Of the *a priori* two independent types of motion of the 3-branes along the S^1 direction, only the Z_2 even modes, corresponding to an overall ''rotation'' of both branes along the circle, localized in the $D=4$ coordinates x^μ, correspond to genuine zero modes.

VI. CONCLUSIONS

We have found that an appropriately constructed D3-brane configuration provides a supersymmetric and dynamically stable Randall–Sundrum scenario. This is achieved in a solution to the $D=10$ type IIB supergravity equations which can be given a $D=5$ interpretation, but is not fully a $D=5$ solution, for it employs an intrinsically massive Kaluza–Klein mode, the S^5 breathing mode. This mode has AdS energy $E_0=8$, satisfying the bound $E_0>4$ that is required for an asymptotic approach to AdS space from a downwards-facing warp-factor kink in a Randall–Sundrum scenario. There is also a Z_2 flip in the sign of the Freund–Rubin parameter m. This is natural enough in a $D=10$ context where m is a field-strength value, but it is less natural from a $D=5$ viewpoint, where m normally would appear as a parameter. We have found, moreover, that although one can decide to exclude the Z_2 odd modes when expanding the theory around the presented Z_2 invariant background, and thus reproduce an S^1/Z_2 orbifold reduction, it is not

actually necessary to make this projection by hand. Bianchi identities for the curvature values entering in the solution relate the Z_2 odd modes to Kaluza–Klein massive states of the theory, and so they decouple naturally at low energy. Although charge conservation on the circle requires branes to come in oppositely charged pairs, we have seen that one can recover a single brane Randall–Sundrum model by pushing the second brane off to the Cauchy horizon (i.e., by taking $\varphi_1=\varphi_*$ for the second brane). From the $D=10$ point of view, however, this corresponds to shrinking an outer RS shell of D3 brane tightly around an inner ''horizon'' D3 brane of opposite charge and tension. Clearly, an important problem is whether this geometry can be realized in a string theory context.

Note added in proof. As this paper was in the final stages of preparation, a very interesting paper appeared[55] that sheds light on the relationship between constructions such as those of Refs. 12, 13 or the present paper and the supersymmetry scheme of Ref. 56, which was otherwise puzzling. In Ref. 55 supersymmetry in orbifolds, and in particular the $D=5$ case of interest here is discussed. In order to obtain a continuous Killing spinor at orbifold singularities (necessary for the Killing equation to be realized everywhere, including at the singular points), Ref. 55 introduces a 5-form ''theory of nothing'' field strength, which has just a constant as a solution, but allows for this variable to be only piecewise constant. This allows for a Z_2 sign flip in the prepotential that is critical for having a preserved supersymmetry allowing coupling to supermatter. This sign flip was not made in the discussion of Ref. 56, leading to problems with matter coupling. This difficulty of Ref. 56, and the resolution of Ref. 55 was also investigated in Refs. 57, 58 and independently worked out by Ref. 59. We anticipate that a fuller Kaluza–Klein treatment of the type IIB theory, including all fermions and making a careful reduction of the type IIB supersymmetry transformations, will show that the $D=5$ supersymmetry realization adopted in Ref. 55 can also be viewed as the natural dimensional reduction of the type IIB theory using a Z_2 symmetrized ansatz of the type employed in Refs. 12, 13 and the present paper. In particular, we expect that the 5-form ''theory of nothing'' field introduced in Refs. 58, 55 can be identified with the $D=5$ residue of the type IIB self-dual 5-form field strength.

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Brane-world Kaluza–Klein reductions and branes on the brane

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We present a systematic study of a new type of consistent ''brane-world Kaluza–Klein reduction,'' which describes fully nonlinear deformations of codimension one objects that arise as solutions of a large class of gauged supergravity theories in diverse dimensions, and whose world-volume theories are described by ungauged supergravities with-one half of the original supersymmetry. In addition, we provide oxidations of these ansätz which are in general related to sphere compactified higher dimensional string theory or M-theory. Within each class we also provide explicit solutions of brane configurations localized on the world-brane. We show that at the Cauchy horizon (in the transverse dimension of the consistently Kaluza–Klein reduced world-brane) there is a curvature singularity for any configuration with a non-null Riemann curvature or a nonvanishing Ricci scalar that lives in the world-brane. Since the massive Kaluza–Klein modes can be consistently decoupled, they cannot participate in regulating these singularities. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1377272]

I. INTRODUCTION

The conventional way of extracting an effective lower-dimensional theory from a higher-dimensional one is by performing a Kaluza–Klein reduction in which the extra dimensions are wrapped up into a compact space such as a torus or a sphere. Provided that the scale size of these internal dimensions is sufficiently small in relation to the energy scale of excitations in the lower dimension, then the mass gap separating the massless modes from the massive ones will be sufficient to ensure that the internal dimensions are essentially unobservable, and the world will appear to be effectively lower dimensional.

If an extra dimension were noncompact then seen from the lower-dimensional viewpoint there would usually be a continuum of modes, with masses extending down to zero. One would normally expect that this would mean that the observable world would be the higher-dimensional one, and that one could not usefully describe it in terms of a lower-dimensional viewpoint. (We cannot usefully view our four-dimensional space–time as being effectively three-dimensional simply by shutting our eyes to the existence of the z axis!) However, it has been shown that under suitable circumstances it may be that the continuous mass eigenvalues for the massive lower-dimensional metric perturbations are distributed in such a way that the effects of the nearly-massless modes is suppressed, implying that the world does in fact appear to be lower-dimensional, with only small modifications to the gravitational forced law appropriate to the lower dimension.[1] In its original form this Randall–Sundrum II scenario is realised by starting from pure gravity with a negative

cosmological constant in five dimensions, and patching together two segments of AdS_5. In horospherical coordinates one has

$$d\hat{s}_5^2 = e^{-2k|z|}\,\eta_{\mu\nu}\,dx^\mu\,dx^\nu + dz^2, \tag{1}$$

where the 3-brane is located at $z=0$. (For a review on the global and local space–time structure of the codimension one objects, see Ref. 2.) It was found that gravity is effectively localized on the 3-brane corresponding to the join between the two segments of AdS_5.[1] Specifically, it was shown that the metric fluctuations around the flat Minkowski space–time of the 3-brane are localized near the brane.

More generally, if the flat Minkowski metric on the 3-brane is replaced by any Ricci-flat 4-metric the five-dimensional metric will still, in the bulk, satisfy the Einstein equations with a negative cosmological constant. In other words, one can view

$$d\hat{s}_5^2 = e^{-2k|z|}\,ds_4^2 + dz^2 \tag{2}$$

as a Kaluza–Klein reduction ansatz that gives a consistent embedding of four-dimensional pure Einstein gravity in five-dimensional Einstein gravity with a negative cosmological constant. In fact the construction could be extended to give an embedding of four-dimensional $N=1$ ungauged supergravity in five dimensions, by starting from $N=2$ (i.e., minimal) gauged supergravity in $D=5$. Note, however, that the bosonic sector in $D=4$ would still only comprise the metric, and there would be no Maxwell field that could support charged Reissner–Nordström black holes. In particular, it should be noted that one cannot get a Maxwell field as a standard type of Kaluza–Klein vector by writing $d\hat{s}_5^2 = e^{-2k|z|}\,ds_4^2 + (dz + \mathcal{A}_{(1)})^2$, since $\partial/\partial z$ is not a Killing vector.

In a recent paper, it was shown that if one instead starts with $N=4$ gauged supergravity in five dimensions, then it is possible to construct a consistent Kaluza–Klein reduction ansatz that gives an embedding of four-dimensional ungauged $N=2$ supergravity on the 3-brane.[3] This is a new kind of dimensional reduction, which we shall refer to as ''brane-world Kaluza–Klein reduction.'' It should be emphasized that it is nontrivial that a *consistent* Kaluza–Klein reduction of this sort is possible, (A consistent reduction is one where all the higher-dimensional equations of motion are satisfied provided that the lower-dimensional fields satisfy their equations of motion.) and there is no obvious group-theoretic explanation for why it should work. Two further examples of consistent brane-world Kaluza–Klein reductions were obtained in Ref. 3, describing the embedding of six-dimensional ungauged chiral $N=(1,0)$ supergravity in seven-dimensional SU(2)-gauged $N=2$ supergravity, and the other describing the embedding of five-dimensional ungauged $N=2$ supergravity in six-dimensional SU(2)-gauged $N=2$ supergravity. More generally, it was conjectured that it should be possible to find a consistent brane-world Kaluza–Klein reduction from any gauged supergravity in D dimensions to an ungauged supergravity with half the supersymmetry in $(D-1)$ dimensions.[3]

The purpose of this paper is to provide a systematic construction of consistent brane-world Kaluza–Klein reductions for gauged supergravity theories (with maximal supersymmetry) in diverse dimensions, thus in general leading to the ungauged supergravities with one-half of the original (maximal) gauged supersymmetry. In addition, the studied examples provide compactifications on both AdS and dilatonic codimension one objects. In the first of these examples, in Sec. II, we show that five-dimensional maximal $(N=8)$ SO(6)-gauged supergravity admits a consistent brane-world reduction to four-dimensional ungauged $N=4$ supergravity. Next, in Sec. III, we show that massive type IIA supergravity admits a consistent brane-world reduction to nine-dimensional ungauged $N=1$ supergravity. Next, in Sec. IV we show that eight-dimensional maximal SU(2)-gauged supergravity admits a consistent brane-world reduction to seven-dimensional ungauged $N=2$ supergravity. Then, in Sec. V, we show that seven-dimensional maximal SO(5)-gauged supergravity admits a consistent brane-world reduction to seven-dimensional ungauged $N=(2,0)$ chiral supergravity.

All the brane-world reductions that were constructed in Ref. 3, and the brane-world reductions of five-dimensional maximal SO(6)-gauged supergravity and seven-dimensional maximal SO(5)-

TABLE I. The ungauged supergravities in $(D-1)$ dimensions obtained by brane-world Kaluza–Klein reductions.

D	D-dimensional theory	$(D-1)$-dimensional theory from brane-world reduction
10	Massive IIA	$D=9,\ N=1$
8	SU(2)-gauged $N=2$	$D=7,\ N=2$
7	SO(5)-gauged $N=4$	$D=6,\ N=(2,0)$
6	SU(2)-gauged $N=2$	$D=5,\ N=2$
5	SO(6) gauged $N=8$	$D=4,\ N=4$

gauged supergravity in this paper, are examples where the higher-dimensional theory admits an anti-de Sitter vacuum solution. By contrast, massive type IIA supergravity and the eight-dimensional SU(2)-gauged supergravity that we also consider in this paper do not admit anti-de Sitter solutions, but instead they have dilatonic domain walls as their most symmetric ''vacuum'' solutions. In all the cases, the brane-world Kaluza–Klein reductions can be thought of as fully nonlinear descriptions of deformations around the anti-de Sitter or domain-wall background, in which the $(D-1)$-dimensional Minkowski metric on the $(D-2)$-brane in the D-dimensional AdS or domain-wall vacuum is allowed to become arbitrary, along with the other necessary fields that complete the $(D-1)$-dimensional ungauged supergravity multiplet. (We should emphasize that as with any fully nonlinear Kaluza–Klein ansatz, the reduction is not pinned to any specific solution. Although it may sometimes be convenient to think of the AdS or domain-wall solution as playing a preferred role, it is really just one out of an infinity of solutions of the reduced theory.)

A brane-world type of Kaluza–Klein reduction can also be performed in those cases where the p-brane cannot trap gravity. A classification of domain walls that can and cannot trap gravity was given in Refs. 4 and 5. In these cases, gravity can arise by placing the p-brane on orbifold points[6] à la Hořava–Witten.[7]

At the level of the supergravity theory, the requirement of the consistency of the brane-world Kaluza–Klein reduction does not discriminate between whether or not the brane is capable of trapping gravity. This is analogous to the situation for a standard Kaluza–Klein reduction on S^1; at the level of the massless modes, which are the only ones retained in the consistent truncation, one cannot distinguish between an extra dimension that is a circle or an infinite real line. In particular, we shall usually write the brane-world reduction ansatz, as in (2), with an absolute-value sign for the coordinate z, i.e., insisting on a Z_2 symmetric codimension one ansatz for the transverse dimension. Thus, there is an actual delta function source needed at $z=0$, whose origin lies outside the supergravity Lagrangian description. However, from the mathematical point of view we could perfectly well write the ansatz without the absolute-value sign, thus describing the bulk solution only, which would still correspond to a consistent reduction. In fact now the ansatz will satisfy the equations everywhere, without the need for any external delta-function sources. [However, one would now lose the brane-world interpretation (at $z=0$) of the reduced theory.]

We conclude this Introduction with Table I that summarizes the principal results that we obtain in this paper, and those of Ref. 3.

In addition, we shall consider S^1 reductions of the $D=8$ and $D=7$ gauged supergravities. The former provides a brane-world reduction from $D=7$ that gives the nonchiral $N=(1,1)$ ungauged supergravity in $D=6$, while the latter provides a brane-world reduction from $D=6$ that gives the $N=4$ ungauged theory in $D=5$. The brane-world reduction of the $D=6$ SU(2)-gauged supergravity was obtained in Ref. 3, as were the brane-world reductions of the SU(2)-gauged $N=2$ seven-dimensional supergravity, and the $\mathrm{SU}(2)\times\mathrm{U}(1)$ gauged $N=4$ five-dimensional supergravity. These two cases are contained within reductions with larger supersymmetries that we consider here. It should be noted that an intrinsic feature of brane-world Kaluza–Klein reductions is that the reduced theory never has more than half the maximal supersymmetry that is allowed in that dimension. This is associated with the fact that there is always a halving of supersymmetry on the brane solution of the higher-dimensional gauged or massive supergravity.

II. FOUR-DIMENSIONAL $N=4$ SUPERGRAVITY FROM MAXIMAL FIVE-DIMENSIONAL GAUGED SUPERGRAVITY

A. Direct reduction from type IIB supergravity

In Sec. II B, we shall obtain the brane-world embedding of four-dimensional ungauged $N=4$ supergravity in five-dimensional maximal gauged supergravity, thus providing the brane-world Kaluza–Klein compactification in $D=4$ with the maximal allowed ungauged supersymmetry. However, since this five-dimensional theory is rather complicated, we shall begin in the current section by constructing the brane-world embedding of the four-dimensional $N=4$ theory directly in ten-dimensional type IIB supergravity. This exploits the fact that the five-dimensional gauged theory can itself be obtained via an S^5 reduction from $D=10$. Having done this, we shall then be in a position to re-express our results in terms of a brane-world reduction from $D=5$ to $D=4$. From the five-dimensional viewpoint the fields that we use are the metric, the dilaton and axion [which are singlets under the SO(6) gauge group], and the two sets of six 2-form potentials. Thus in $D=5$ the 15 Yang–Mills gauge fields and the $10+\overline{10}+20'$ of scalars are set to zero.

The bosonic equations of motion of type IIB supergravity can be derived from the Lagrangian,

$$\mathcal{L}_{10}^{\mathrm{IIB}}=\hat{R}\hat{*}\mathbb{1}-\tfrac{1}{2}\hat{*}d\hat{\phi}\wedge d\hat{\phi}-\tfrac{1}{2}e^{2\hat{\phi}}\hat{*}d\hat{\chi}\wedge d\hat{\chi}-\tfrac{1}{4}\hat{*}\hat{F}_{(5)}\wedge\hat{F}_{(5)}-\tfrac{1}{2}e^{-\hat{\phi}}\hat{*}\hat{F}^2_{(3)}\wedge\hat{F}^2_{(3)}-\tfrac{1}{2}e^{\hat{\phi}}\hat{*}\hat{F}^1_{(3)}\wedge\hat{F}^1_{(3)}$$
$$-\tfrac{1}{2}\hat{A}_{(4)}\wedge d\hat{A}^1_{(2)}\wedge d\hat{A}^2_{(2)}, \tag{3}$$

where $\hat{F}^2_{(3)}=d\hat{A}^2_{(2)}$, $\hat{F}^1_{(3)}=d\hat{A}^1_{(2)}-\hat{\chi}\,d\hat{A}^2_{(2)}$, $\hat{F}_{(5)}=d\hat{A}_{(4)}-\frac{1}{2}\hat{A}^1_{(2)}\wedge d\hat{A}^2_{(2)}+\frac{1}{2}\hat{A}^2_{(2)}\wedge d\hat{A}^1_{(2)}$, and we use carets to denote ten-dimensional fields and the ten-dimensional Hodge dual $\hat{*}$. The equations of motion following from the Lagrangian, together with the self-duality condition, are

$$\hat{R}_{MN}=\tfrac{1}{2}\partial_M\hat{\phi}\,\partial_N\hat{\phi}+\tfrac{1}{2}e^{2\hat{\phi}}\partial_M\hat{\chi}\,\partial_N\hat{\chi}+\tfrac{1}{96}\hat{F}^2_{MN}+\tfrac{1}{4}e^{\hat{\phi}}((\hat{F}^1_{(3)})^2_{MN}$$
$$-\tfrac{1}{12}(\hat{F}^1_{(3)})^2\hat{g}_{MN})+\tfrac{1}{4}e^{-\hat{\phi}}((\hat{F}^2_{(3)})^2_{MN}-\tfrac{1}{12}(\hat{F}^2_{(3)})^2\hat{g}_{MN}),$$

$$d\hat{*}d\hat{\phi}=-e^{2\hat{\phi}}\hat{*}d\hat{\chi}\wedge d\hat{\chi}-\tfrac{1}{2}e^{\hat{\phi}}\hat{*}\hat{F}^1_{(3)}\wedge\hat{F}^1_{(3)}+\tfrac{1}{2}e^{-\hat{\phi}}\hat{*}\hat{F}^2_{(3)}\wedge\hat{F}^2_{(3)},$$

$$d(e^{2\hat{\phi}}\hat{*}d\hat{\chi})=e^{\hat{\phi}}\hat{*}\hat{F}^1_{(3)}\wedge\hat{F}^2_{(3)},$$

$$d(e^{\hat{\phi}}\hat{*}\hat{F}^1_{(3)})=\hat{F}_{(5)}\wedge\hat{F}^2_{(3)},\quad d(e^{-\hat{\phi}}\hat{*}\hat{F}^2_{(3)}-\hat{\chi}\,e^{\hat{\phi}}\hat{*}\hat{F}^1_{(3)})=-\hat{F}_{(5)}\wedge(\hat{F}^1_{(3)}+\hat{\chi}\,\hat{F}^2_{(3)}),$$

$$d(\hat{*}\hat{F}_{(5)})=-\hat{F}^1_{(3)}\wedge\hat{F}^2_{(3)},\quad \hat{F}_{(5)}=\hat{*}\hat{F}_{(5)}. \tag{4}$$

The ungauged four-dimensional $N=4$ supergravity that we are seeking to embed in type IIB supergravity is described by the following Lagrangian (Actually this Lagrangian corresponds to a special truncation of toroidally compactified heterotic string theory where the gauge fields of the original heterotic string are turned off and the momentum and winding modes of the NS–NS sector are identified, thus freezing the internal metric and antisymmetric two-form fields of the six-torus):

$$\mathcal{L}_4=R*\mathbb{1}-\tfrac{1}{2}*d\phi\wedge d\phi-\tfrac{1}{2}e^{2\phi}*d\chi\wedge d\chi-\tfrac{1}{2}e^{-\phi}*F^i_{(2)}\wedge F^i_{(2)}-\tfrac{1}{2}\chi\,F^i_{(2)}\wedge F^i_{(2)}, \tag{5}$$

where $1\leqslant i\leqslant 6$, and $F^i_{(2)}=dA^i_{(1)}$.

We find that the following is a consistent reduction ansatz that gives the embedding of the four-dimensional $N=4$ theory in type IIB supergravity,

$$d\hat{s}^2_{10} = e^{-2k|z|}\, ds^2_4 + dz^2 + g^{-2}\, d\Omega^2_5,$$

$$\hat{F}_{(5)} = 4g^{-4}\,\Omega_{(5)} + 4g\, e^{-4k|z|}\,\epsilon_{(4)} \wedge dz,$$

$$\hat{A}^1_{(2)} = \frac{1}{\sqrt{2}} g^{-1}\, e^{-k|z|}\,\mu_i\,(e^{-\phi} * F^i_{(2)} + \chi\, F^i_{(2)}), \tag{6}$$

$$\hat{A}^2_{(2)} = \frac{1}{\sqrt{2}} g^{-1}\, e^{-k|z|}\,\mu_i\, F^i_{(2)},$$

$$\hat{\phi} = \phi, \quad \hat{\chi} = \chi,$$

where $d\Omega^2_5$ is the metric on the unit 5-sphere, which we can write in terms of six coordinates μ_i that are subject to the constraint $\mu_i\,\mu_i = 1$, as $d\Omega^2_5 = d\mu_i\, d\mu_i$. The 5-form $\Omega_{(5)}$ is the volume form of the metric $d\Omega^2_5$, and $\epsilon_{(4)}$ is the volume form of the metric ds^2_4. Note that $\Omega_{(5)}$ can be written as

$$\Omega_{(5)} = \frac{1}{5!}\,\epsilon_{ij_1\cdots j_5}\,\mu_i\, d\mu_{j_1} \wedge \cdots \wedge d\mu_{j_5}. \tag{7}$$

The constant k (which we take to be positive) is related to the gauge-coupling constant g of the five-dimensional theory by $k^2 = g^2$. In fact, to be precise, we must have

$$g = \begin{cases} k, & z > 0, \\ -k, & z < 0. \end{cases} \tag{8}$$

Substituting the ansatz (6) into the equations of motion of type IIB supergravity (4), we find that they are all exactly satisfied if and only if the four-dimensional fields ds^2_4, ϕ, χ, and $F^i_{(2)}$ satisfy the equations of motion of ungauged $N=4$ supergravity, which can be derived from (5). Note in particular that the six abelian gauge fields $F^i_{(2)}$ satisfy the equations of motion,

$$d(e^{-\phi} * F^i_{(2)} + \chi\, F^i_{(2)}) = 0. \tag{9}$$

The following results are useful for verifying the consistency of the reduction ansatz. First, we have from (6) that

$$\hat{F}^1_{(3)} = \frac{1}{\sqrt{2}} g^{-1}\, e^{-k|z|}\, e^{-\phi} * F^i_{(2)} \wedge (d\mu_i - g\,\mu_i\, dz),$$

$$\hat{F}^2_{(3)} = \frac{1}{\sqrt{2}} g^{-1}\, e^{-k|z|}\, F^i_{(2)} \wedge (d\mu_i - g\,\mu_i\, dz). \tag{10}$$

[Here, we have for convenience of presentation already made use of the fact that the $F^i_{(2)}$ satisfy the Bianchi identities $dF^i_{(2)} = 0$ and the field equations (9); they can, of course, be *derived* by substituting the ansatz into the ten-dimensional equations of motion.] Next, we can write the ten-dimensional Hodge duals of these field strengths as follows:

$$
\begin{aligned}
*\hat{F}^1_{(3)} &= \frac{1}{\sqrt{2}} g^{-5} e^{-k|z|} e^{-\phi} F^i_{(2)} \wedge (\mu_i \Omega_{(5)} - g Z_i \wedge dz), \\
*\hat{F}^2_{(3)} &= -\frac{1}{\sqrt{2}} g^{-5} e^{-k|z|} *F^i_{(2)} \wedge (\mu_i \Omega_{(5)} - g Z_i \wedge dz),
\end{aligned}
\tag{11}
$$

where the 4-form Z_i is defined by

$$
Z_i \equiv \frac{1}{4!} \epsilon_{ijk_1\cdots k4} \mu_j d\mu_{k_1} \wedge \cdots \wedge d\mu_{k_4}. \tag{12}
$$

This 4-form is the Hodge dual of $d\mu_i$ in the unit 5-sphere metric, $*_5 d\mu_i = -Z_i$. Note that Z_i has the following properties:

$$
d\mu_i \wedge Z_j = -(\delta_{ij} - \mu_i \mu_j) \Omega_{(5)}, \quad dZ_i = 5 \mu_i \Omega_{(5)}. \tag{13}
$$

It is now straightforward to verify that all the type IIB ten-dimensional equations of motion consistently yield the equations of motion of four-dimensional ungauged $N=4$ supergravity; in particular, all the dependence on the coordinates z and μ_i consistently matches in all the equations.

It is worth noting that the $N=4$ gauged supergravity in the four-dimensional world-volume of the D3-brane has an SL(2,$\mathbb{Z}$) electric/magnetic S-duality, with the two scalars (ϕ,χ) parameterizing the SL(2,$\mathbb{R}$)/O(2) coset. It is easy to see from the reduction ansatz (6) that this SL(2,$\mathbb{Z}$) symmetry of the theory in the world-volume of the D3-brane originates from the SL(2,$\mathbb{Z}$) of the original type IIB theory in $D=10$, which is not an electric/magnetic duality.

It is of interest to see how the brane-world embedding of the four-dimensional $N=4$ supergravity that we have derived here reduces to the $N=2$ supergravity embedding that was constructed in Ref. 3. In the $N=2$ theory there is just one 2-form field strength $F_{(2)}$, and the dilaton ϕ and axion χ are absent. It is easy to see that the equations of motion for ϕ and χ in (5) imply that in order to set $\phi=\chi=0$, we must have

$$
*F^i_{(2)} \wedge F^i_{(2)} = 0, \quad F^i_{(2)} \wedge F^i_{(2)} = 0. \tag{14}
$$

The minimal nontrivial way to satisfy these conditions is by taking all but two of the six field strengths to vanish, and for the remaining ones, say $F^1_{(2)}$ and $F^2_{(2)}$, to be related by $F^2_{(2)} = *F^1_{(2)}$. If we define $F^2_{(2)} = *F^1_{(2)} = -F_{(2)}/\sqrt{2}$, and at the same time we parameterize the six coordinates μ_i that define the 5-sphere as

$$
\mu_1 = \sin\xi \cos\tau, \quad \mu_2 = -\sin\xi \sin\tau, \quad \mu_\alpha = \nu_\alpha \cos\xi, \quad (\alpha = 3,4,5,6), \tag{15}
$$

where $\nu_\alpha \nu_\alpha = 1$, defining a unit 3-sphere, the ansatz for $d\hat{s}^2_{10}$, $\hat{A}^1_{(2)}$, and $\hat{A}^2_{(2)}$ in (6) become

$$
\begin{aligned}
d\hat{s}^2_{10} &= e^{-2k|z|} ds^2_4 + dz^2 + d\xi^2 + \sin^2\xi \, d\tau^2 + \cos^2\xi \, d\Omega^2_3, \\
\hat{A}^1_{(2)} + i\hat{A}^2_{(2)} &= -\tfrac{1}{2} g^{-1} e^{-k|z|} \sin\xi \, e^{-i\tau} (F_{(2)} - i *F_{(2)}).
\end{aligned}
\tag{16}
$$

This is precisely the form of the ansatz found in Ref. 3 for the consistent brane-world embedding of four-dimensional $N=2$ supergravity.

B. Ungauged $D=4$, $N=4$ from gauged $D=5$, $N=8$

In the previous subsection, we considered the reduction from type IIB to the ungauged $N=4$ theory in $D=4$ directly, omitting the intermediate description as a brane-world KK reduction of five-dimensional $N=8$ gauged supergravity on account of the complexity of the five-

dimensional theory. We can now in fact reinterpret our results as a reduction of the maximal five-dimensional gauged theory. However, in order to avoid the full complexity of this theory, we shall work with a truncation of the full set of five-dimensional fields in which just the metric, the dilaton ϕ and axion χ, and the $6+6$ of 2-form potentials are retained. In other words, we set the 15 Yang–Mills SO(6) gauge fields and the $10+\overline{10}+20'$ of scalars to zero. It should be emphasized that this is in general an *inconsistent* truncation of the five-dimensional theory. However, we can still work with it provided that we impose the necessary algebraic constraints on the $6+6$ of 2-form potentials. Of course these constraints are precisely the ones that *are* satisfied by the brane-world KK reduction ansatz, now expressed simply as a reduction from $D=5$ to $D=4$.

We find that the above truncated five-dimensional theory is obtained from $D=10$ by making the following ansatz for the type IIB fields:

$$d\hat{s}^2_{10}=ds^2_5+g^{-2}\,d\Omega^2_5,$$

$$\hat{F}_{(5)}=4g^{-4}\,\Omega_{(5)}+4g\,\epsilon_{(5)},$$

$$\hat{A}^{\alpha}_{(2)}=\mu_i\,A^{i\alpha}_2,$$

$$\hat{\phi}=\phi,\quad \hat{\chi}=\chi, \tag{17}$$

where $\alpha=1,2$. We immediately find from the Bianchi identity for $\hat{F}_{(5)}$ that the following equations must be satisfied:

$$A^{i\alpha}_{(2)}\wedge A^{j\beta}_{(2)}\,\epsilon_{\alpha\beta}=0,\quad dA^{i\alpha}_{(2)}\wedge A^{j\beta}_{(2)}\,\epsilon_{\alpha\beta}=0. \tag{18}$$

These are the algebraic constraints alluded to above. We must impose them because we have set other fields of the maximal five-dimensional theory to zero, which is in general in conflict with the equations of motion of those fields.

Substituting the ansatz (17) into the remaining equations of motion of type IIB supergravity, and making use of the constraints (18), we find that they consistently imply the following five-dimensional equations:

$$dA^{i1}_{(2)}-\chi\,dA^{i2}_{(2)}=-g\,e^{-\phi}*A^{i2}_{(2)},$$

$$dA^{i2}_{(2)}=g\,e^{\phi}*(A^{i1}_{(2)}-\chi\,A^{i2}_{(2)}),$$

$$d(e^{2\phi}*d\chi)=-g^2\,e^{\phi}*(A^{i1}_{(2)}-\chi\,A^{i2}_{(2)})\wedge A^{i2}_{(2)},$$

$$d*d\phi=e^{2\phi}*d\chi\wedge d\chi+\tfrac{1}{2}g^2\,e^{\phi}*(A^{i1}_{(2)}-\chi\,A^{i2}_{(2)})\wedge(A^{i1}_{(2)}-\chi\,A^{i2}_{(2)})-\tfrac{1}{2}g^2\,e^{-\phi}*A^{i2}_{(2)}\wedge A^{i2}_{(2)},$$

$$R_{\mu\nu}=\tfrac{1}{2}\partial_\mu\phi\,\partial_\nu\phi+\tfrac{1}{2}e^{2\phi}\,\partial_\mu\chi\,\partial_\nu\chi+\tfrac{1}{2}g^2\,[e^{\phi}\,(A^{i1}_{\mu\rho}-\chi\,A^{i2}_{\mu\rho})\,(A^{i1\,\rho}_{\nu}-\chi\,A^{i2\,\rho}_{\nu})+e^{-\phi}\,A^{i2}_{\mu\rho}A^{i2\,\rho}_{\nu}]. \tag{19}$$

[$A^{i1}_{(2)}$ and $A^{i2}_{(2)}$ denote $A^{i\alpha}_{(2)}$ with $\alpha=1$ and $\alpha=2$, respectively.] These equations, together with the constraints (18), are precisely equivalent to those of maximal five-dimensional gauged supergravity, after setting the Yang–Mills fields and the $10+\overline{10}+20'$ of scalars to zero. The $6+6$ of 2-form fields $A^{i\alpha}_{(2)}$ satisfy first-order equations of motion, known as ''odd-dimensional self-duality equations.'' These, together with the constraint equations (18), imply that the trace of the 2-form contributions in the energy-momentum tensor vanishes; $e^{\phi}(A^{i1}_{\mu\nu}-\chi\,A^{i2}_{\mu\nu})(A^{i1\,\mu\nu}-\chi\,A^{i2\,\mu\nu})+e^{-\phi}A^{i2}_{\mu\nu}A^{i2\,\mu\nu}=0$. Note that the imposition of the constraints (18) is sufficient to ensure that *all* the type IIB equations of motion are consistently satisfied by the ansatz (17), including the internal and mixed components of the Einstein equations.

It is useful to observe that the equations of motion (19) can be derived from the Lagrangian,

$$\mathcal{L}_5 = R*\mathbb{1} - \tfrac{1}{2}*d\phi\wedge d\phi - \tfrac{1}{2}e^{2\phi}*d\chi\wedge d\chi - \tfrac{1}{2}g^2\,e^{\phi}*(A^{i1}_{(2)}-\chi A^{i2}_{(2)})\wedge(A^{i1}_{(2)}-\chi A^{i2}_{(2)})$$
$$-\tfrac{1}{2}g^2\,e^{-\phi}*A^{i2}_{(2)}\wedge A^{i2}_{(2)} - g\,dA^{i1}_{(2)}\wedge A^{i2}_{(2)} + 12g^2*\mathbb{1}. \tag{20}$$

Finally, we note that the brane-world Kaluza–Klein reduction of the previous subsection, now expressed as a reduction from $D=5$ to $D=4$, is given by

$$ds_5^2 = e^{-2k|z|}\,ds_4^2 + dz^2,$$

$$A^{i1}_{(2)} = \frac{1}{\sqrt{2}}g^{-1}\,e^{-k|z|}\,(e^{-\phi}*F^i_{(2)} + \chi F^i_{(2)}), \tag{21}$$

$$A^{i2}_{(2)} = \frac{1}{\sqrt{2}}g^{-1}\,e^{-k|z|}\,F^i_{(2)},$$

with ϕ and χ just reducing directly. One can easily verify that this reduction ansatz is indeed compatible with the constraints (18).

C. Branes on the D3-brane

One can construct electric and magnetic black holes, strings and instantons in $D=4$, $N=4$ supergravity. They become branes on the D3-brane (in the near-horizon region) when they are lifted back to $D=10$. We analyze these solutions in this section.

Case 1: SL(2,$\mathbb{Z}$) *dyonic black holes on the D3-brane:* We can use one of the six 2-form field strengths to construct an electric or magnetic black hole. As a concrete example, let us consider an electric black hole supported by the field strength $F^1_{(2)}$. Once the solution is lifted back to $D=10$, it becomes

$$d\hat{s}_{10}^2 = e^{-2k|z|}[-H^{-1}\,dt^2 + H(dr^2 + r^2 d\Omega_2^2)] + dz^2 + g^{-2}d\Omega_5^2,$$

$$\hat{F}_{(5)} = 4g^{-4}\Omega_5 + 4g\,e^{-4k|z|}\,r^2 H\,dt\wedge dr\wedge\Omega_2,$$

$$\hat{A}^1_{(2)} = \frac{Q}{\sqrt{2}}g^{-1}\,e^{-k|z|}\,\mu_1\,\Omega_2, \tag{22}$$

$$\hat{A}^2_{(2)} = \frac{1}{\sqrt{2}}g^{-1}\,e^{-k|z|}\,\mu_1\,dt\wedge dH^{-1},$$

$$e^{\phi} = H, \quad H = 1 + \frac{Q}{r},$$

where μ_1 is one of the coordinates μ_i for S^5 appearing in the ansatz (17), corresponding to our choice to consider a black hole supported by $F^1_{(2)}$. Starting with the electric black hole, we can then apply the SL(2,$\mathbb{R}$) symmetry to get a multiplet of dyonic black holes, where the electric and magnetic charges are carried by the same 2-form field strength. The metric of this dyonic solution remains unchanged, but the charge configuration alters.

Case 2: Threshold dyonic black holes on the D3-brane: In $D=4$, $N=4$ supergravity, one can also construct a multicharge black hole solution, where the electric charge is carried by one 2-form field strength, say $F^1_{(2)}$, and the magnetic charge is carried by another, say $F^2_{(2)}$.[8] [Note that the generating technique, as employed, for example, for the four-charge solution[9] of toroidally compactified heterotic string, may allow for a construction of more general dyonic black holes with all the U(1) charges turned on.] Lifting this solution back to $D=10$, it becomes

$$d\hat{s}_{10}^2 = e^{-2k|z|}[-(H_1H_2)^{-1}\,dt^2 + H_1H_2\,(dr^2 + r^2 d\Omega_2^2)] + dz^2 + g^{-2}\,d\Omega_5^2,$$

$$\hat{F}_{(5)} = 4g^{-4}\,\Omega_5 + 4g\,e^{-4k|z|}\,r^2(H_1H_2)\,dt\wedge dr\wedge d\Omega_2,$$

$$\hat{A}^1_{(2)} = \frac{1}{\sqrt{2}}\,g^{-1}\,e^{-k|z|}\,(Q_e\,\mu_1\,\Omega_2 + \mu_2\,dt\wedge dH_2^{-1}),$$

$$\hat{A}^2_{(2)} = \frac{1}{\sqrt{2}}\,g^{-1}\,e^{-k|z|}\,(\mu_1\,dt\wedge dH_1^{-1} + \mu_2\,Q_m\,\Omega_2),$$

$$e^{\phi} = \frac{H_1}{H_2}, \quad H_1 = 1 + \frac{Q_e}{r}, \quad H_2 = 1 + \frac{Q_m}{r}. \tag{23}$$

Case 3: String on the D3-brane: A magnetic string (four-dimensional domain wall), supported by the axion, exists in the four-dimensional supergravity theory. Lifting this solution back to $D = 10$, we have a string living on the D3-brane,

$$d\hat{s}_{10}^2 = e^{-2k|z|}[-dt^2 + dx^2 + H(dr^2 + r^2 d\theta^2)] + dz^2 + g^{-2}d\Omega_5^2,$$

$$\hat{F}_{(5)} = 4g^{-4}\,\Omega_{(5)} + 4g\,e^{-4k|z|}\,rH\,dt\wedge dx\wedge dr\wedge d\theta,$$

$$e^{\hat{\phi}} = H^{-1}, \quad \chi = Q\,\theta,$$

$$H = 1 + Q\log r. \tag{24}$$

This solution is a non-standard intersection of a D3-brane and D7-brane, where there is no overall transverse space. It should be distinguished from the solution describing a D3-brane in the D7-brane, which has a two-dimensional overall transverse space.

Case 4: Instanton on the D3-brane: The axion in the $D=4$ theory also supports a BPS instanton solution when the theory is Euclideanized. The axion χ becomes imaginary under this procedure, the metric ds_4^2 becomes purely flat Euclidean space, and $\hat{F}_{(5)}$ becomes complex, since in ten Euclidean dimensions a real 5-form cannot be self-dual.

III. $N=1$ SUPERGRAVITY IN $D=9$ FROM MASSIVE TYPE IIA

A. D8-brane in massive type IIA theory

The highest dimensional D-brane that can be found in any supergravity theory is the D8-brane in massive type IIA supergravity. This theory was constructed in Ref. 10, but in a formulation where there is not a straightforward massless limit to ordinary type IIA supergravity. However, it is simply a matter of performing a field redefinition to resolve this problem.[11] The Lagrangian for the bosonic sector of the massive type IIA supergravity can then be written as the following differential form:[12]

$$\mathcal{L}_{10} = \hat{R}\,\hat{*}\mathbb{1} - \tfrac{1}{2}\hat{*}d\hat{\phi}\wedge d\hat{\phi} - \tfrac{1}{2}e^{3/2\hat{\phi}}\,\hat{*}\hat{F}_{(2)}\wedge\hat{F}_{(2)} - \tfrac{1}{2}e^{-\hat{\phi}}\,\hat{*}\hat{F}_{(3)}\wedge\hat{F}_{(3)} - \tfrac{1}{2}e^{1/2\hat{\phi}}\,\hat{*}\hat{F}_{(4)}\wedge\hat{F}_{(4)}$$
$$- \tfrac{1}{2}d\hat{A}_{(3)}\wedge d\hat{A}_{(3)}\wedge\hat{A}_{(2)} - \tfrac{1}{6}m\,d\hat{A}_{(3)}\wedge(\hat{A}_{(2)})^3 - \tfrac{1}{40}m^2\,(\hat{A}_{(2)})^5 - \tfrac{1}{2}m^2\,e^{5/2\hat{\phi}}\,\hat{*}\mathbb{1}, \tag{25}$$

where the field strengths are given in terms of potentials by

$$\hat{F}_{(2)} = d\hat{A}_{(1)} + m\,\hat{A}_{(2)}, \quad \hat{F}_{(3)} = d\hat{A}_{(2)},$$

$$\hat{F}_{(4)} = d\hat{A}_{(3)} + \hat{A}_{(1)}\wedge d\hat{A}_{(2)} + \tfrac{1}{2}m\,\hat{A}_{(2)}\wedge\hat{A}_{(2)}. \tag{26}$$

The Bianchi identities for the field strengths are therefore

$$d\hat{F}_{(2)}=m\,\hat{F}_{(3)},\quad d\hat{F}_{(3)}=0,\quad d\hat{F}_{(4)}=\hat{F}_{(2)}\wedge\hat{F}_{(3)}, \tag{27}$$

and the field equations are

$$\begin{aligned} d\hat{F}_{(6)}&=-\hat{F}_{(3)}\wedge\hat{F}_{(4)},\quad d\hat{F}_{(8)}=-\hat{F}_{(3)}\wedge\hat{F}_{(6)},\\ d\hat{F}_{(7)}&=-\tfrac{1}{2}\hat{F}_{(4)}\wedge\hat{F}_{(4)}-m\,\hat{F}_{(8)}-\hat{F}_{(2)}\wedge\hat{F}_{(6)},\\ d\hat{*}d\hat{\phi}&=-\tfrac{1}{4}\hat{F}_{(4)}\wedge\hat{F}_{(6)}-\tfrac{3}{4}\hat{F}_{(2)}\wedge\hat{F}_{(8)}-\tfrac{1}{2}\hat{F}_{(3)}\wedge\hat{F}_{(7)}+\tfrac{5}{4}m^2\,e^{5/2\hat{\phi}}\hat{*}1, \end{aligned} \tag{28}$$

where we have defined the dual field strengths

$$\hat{F}_{(6)}\equiv e^{1/2\hat{\phi}}\hat{*}\hat{F}_{(4)},\quad \hat{F}_{(8)}\equiv e^{3/2\hat{\phi}}\hat{*}\hat{F}_{(2)},\quad \hat{F}_{(7)}\equiv e^{-\hat{\phi}}\hat{*}\hat{F}_{(3)}. \tag{29}$$

This massive type IIA theory supports a ''vacuum'' solution, namely, the D8-brane,

$$d\hat{s}_{10}^2=W^{2/25}\,dx^\mu dx_\mu+dz^2,\quad e^{\hat{\phi}}=W^{-(4/5)}, \tag{30}$$

where the one-dimensional harmonic function is given by

$$W=1+k|z|,\quad k^2=\frac{625}{256}m^2. \tag{31}$$

In fact the sign of m must be opposite on opposite sides of the domain wall,

$$g=\begin{cases} \frac{16}{25}k, & z>0,\\ -\frac{16}{25}k, & z<0, \end{cases} \tag{32}$$

where k is assumed to be positive. This means that one cannot strictly speaking view the domain wall as a solution within the massive type IIA theory as formulated in Ref. 10, since there m is a fixed parameter in the Lagrangian. However, the theory can be re-expressed in a formulation where m is replaced by a 10-form field, with the mass parameter now arising as a constant of integration. It now makes sense for the parameter to be only piecewise constant. In what follows, we shall implicitly assume that we are working with this reformulation of the theory, which allows (32) to hold.

Note that the nine-dimensional flat Minkowskian spacetime $dx^\mu dx_\mu$ of the solution (30) can be replaced by any Ricci-flat Minkowski-signatured space–time.[13] On the other hand, it was observed that domain walls associated with Dp-branes with $p\geqslant 6$ cannot trap gravity. Nevertheless, one can still obtain gravity on the world-volume in such a case by locating the branes at orbifold points, so that the space–time is compact.[6] In this case, we would expect that the resulting theory on the world-volume of the D8-brane would be the ungauged $N=1$, $D=9$ supergravity. We shall prove in the next subsection that this can indeed be obtained from the massive type IIA theory via a consistent brane-world Kaluza–Klein reduction.

B. $N=1$ supergravity in $D=9$ from massive type IIA

We find that the following Kaluza–Klein ansatz for the ten-dimensional massive type IIA fields yields a consistent reduction to nine dimensions,

$$d\hat{s}_{10}^2 = e^{-(5/16)\sqrt{(2/7)}\phi} W^{(2/25)} ds_9^2 + e^{(35/16)\sqrt{(2/7)}\phi} dz^2,$$

$$\hat{A}_{(1)} = 0, \quad \hat{A}_{(2)} = \frac{1}{2m} W^{16/25} F_{(2)}, \quad \hat{A}_{(3)} = \frac{1}{4m} W^{32/25} F_{(3)}, \tag{33}$$

$$e^{\hat{\phi}} = W^{-(4/5)} e^{-(7/8)\sqrt{(2/7)}\phi},$$

where W is given by (31) and g is related to k by (32). Substituting this ansatz into the massive type IIA equations of motion, we find that they are all satisfied provided that the nine-dimensional fields ds_9^2, φ, $F_{(2)} = dA_{(1)}$ and $F_{(3)} = dA_{(2)} - \frac{1}{2} A_{(1)} \wedge F_{(2)}$ satisfy the equations of motion of nine-dimensional ungauged simple supergravity. These equations can be derived from the Lagrangian,

$$\mathcal{L}_9 = R * \mathbb{1} - \tfrac{1}{2} * d\phi \wedge d\phi - \tfrac{1}{2} e^{-\sqrt{(8/7)}\phi} * F_{(3)} \wedge F_{(3)} - \tfrac{1}{2} e^{-\sqrt{(2/7)}\phi} * F_{(2)} \wedge F_{(2)}. \tag{34}$$

C. Branes on the D8-brane

Having consistently embedded the ungauged $N=1$, $D=9$ supergravity in massive type IIA supergravity, we can lift all the solutions of this nine-dimensional theory back to $D=10$. The nine-dimensional theory supports BPS p-branes such as the string, 4-brane, black hole and 5-brane. These solutions are straightforward and well known. When they are lifted back to massive type IIA supergravity using the ansatz (33), they can be viewed as branes living on the D8-brane.

Case 1: String on the D8-brane: The solution of the $D=9$ string lifted back to $D=10$ becomes

$$d\hat{s}_{10}^2 = W^{(2/25)}[H^{-(5/8)}(-dt^2 + dx^2) + H^{3/8}(dr^2 + r^2 d\Omega_6^2)] + H^{-(5/8)} dz^2,$$

$$\hat{A}_{(3)} = \frac{1}{4m} W^{32/25}\, dt \wedge dx \wedge dH^{-1}, \tag{35}$$

$$e^{\hat{\phi}} = W^{-(4/5)} H^{1/4}, \quad H = 1 + \frac{Q}{r^5}.$$

This solution can be viewed as a D2-brane ending on the D8-brane, with the end points forming a string. To see this, it is helpful to introduce a new coordinate y in place of z, defined by $dy = \frac{24}{25} W^{-(1/25)} dz$, and hence

$$W = (1 + k\,|y|)^{25/24}. \tag{36}$$

Using this variable, the y-dependence of the metric is extracted as an overall conformal factor, and we have

$$d\hat{s}_{10}^2 = (1 + k|y|)^{1/12}[H^{-(5/8)}(-dt^2 + dx^2 + dy^2) + H^{3/8}(dr^2 + r^2 d\Omega_6^2)]. \tag{37}$$

Case 2: 4-brane on the D8-brane: The $D=9$ 4-brane solution (the magnetic dual of the string solution), lifted back to $D=10$, becomes

$$d\hat{s}_{10}^2 = W^{2/25}[H^{-(3/8)}\, dx^\mu dx_\mu + H^{5/8}(dr^2 + r^2 d\Omega_3^2)] + H^{5/8} dz^2,$$

$$\hat{A}_{(3)} = \frac{Q}{4m} W^{32/25}\, \Omega_3, \tag{38}$$

$$e^{\hat{\phi}} = W^{-(4/5)} H^{-(1/4)}, \quad H = 1 + \frac{Q}{r^2}.$$

Using the same coordinate transformation (36), the metric can be re-expressed as

$$d\hat{s}_{10}^2=(1+k|y|)^{1/12}[H^{-(3/8)}\,dx^\mu dx_\mu+H^{5/8}(dy^2+dr^2+r^2d\Omega_3^2)]. \tag{39}$$

Thus the solution can be viewed as a D4-brane intersecting with a D8-brane, with the D4-brane uniformly delocalized on the one-dimensional transverse space of the D8-brane.

In Case 1 above, the intersection of the D2-brane and the D8-brane is such that the overall world-volume is a string, and the solution describes a D2-brane ending on the D8-brane. In Case 2, the intersection of the D4-brane and D8-brane is such that the overall world-volume is the entire 4-brane, and so the solution describes a D4-brane living in the D8-brane.

Case 3: Black hole on the D8-brane: The black hole solution of the $D=9$ theory can be lifted to $D=10$, where it becomes

$$d\hat{s}_{10}^2=W^{(2/25)}[-H^{-(13/8)}\,dt^2+H^{3/8}(dr^2+r^2d\Omega_7^2)]+H^{-(5/8)}\,dz^2,$$

$$\hat{A}_{(2)}=\frac{1}{2m}W^{(16/25)}\,dt\wedge dH^{-1},$$

$$e^{\hat{\phi}}=W^{-(4/5)}H^{1/4},\quad H=1+\frac{Q}{r^6}. \tag{40}$$

Using (36), the metric can be cast into the form,

$$d\hat{s}_{10}^2=(1+k|y|)^{1/12}[-H^{-(13/8)}\,dt^2+H^{-(5/8)}\,dy^2+H^{3/8}(dr^2+r^2d\Omega_7^2)]. \tag{41}$$

The solution can be viewed as the intersection of an NS–NS string and a D0-brane with the D8-brane. In particular, the string NS–NS string ends on the D8-brane whilst the D0-brane lives in the D8-brane. To see this, we note that a standard solution for the intersection of a string and a D0-brane would be

$$ds_{10}^2=-H_0^{-(7/8)}H_1^{-(3/4)}\,dt^2+H_0^{1/8}H_1^{-(3/4)}\,du^2+H_0^{1/8}H_1^{1/4}\,d\mathbf{y}^2, \tag{42}$$

where H_0 and H_1 are independent harmonic functions on the eight-dimensional common transverse space of the $\mathbf{y}$ coordinates. If these two harmonic functions are set equal, $H_0=H_1=H$, then we obtain the structure found in (41).

Case 4: 5-brane on the D8-brane: The 5-brane solution (the magnetic dual of the black hole) can be lifted to $D=10$, where it becomes

$$d\hat{s}_{10}^2=W^{2/25}[H^{-(3/8)}\,dx^\mu dx_\mu+H^{13/8}(dr^2+r^2d\Omega_2)]+H^{5/8}\,dz^2,$$

$$\hat{A}_{(2)}=\frac{Q}{2m}W^{16/25}\,\Omega_2, \tag{43}$$

$$e^{\hat{\phi}}=W^{-(4/5)}H^{-(1/4)},\quad H=1+\frac{Q}{r}.$$

Using the redefinition (36), the metric can be cast into the form

$$d\hat{s}_{10}^2=(1+k|y|)^{1/12}(-H^{-(3/8)}\,dx^\mu dx_\mu+H^{5/8}\,dy^2+H^{13/8}(dr^2+r^2d\Omega_2^2)). \tag{44}$$

The solution can be viewed as an intersection of a NS–NS 5-brane and a D6-brane with the D8-brane. In particular, the NS–NS 5-brane lives in the D8-brane, whilst the D6-brane ends on the D8-brane. (The standard solution for the intersection of a 5-brane and a 6-brane would be of the form,

$$ds_{10}^2=H_5^{-(1/4)}H_6^{-(1/8)}\,dx^\mu\,dx_\mu+H_5^{3/4}H_6^{-(1/8)}\,du^2+H_5^{3/4}H_6^{7/8}\,d\mathbf{y}^3, \tag{45}$$

where H_5 and H_6 are independent harmonic functions on the common transverse 3-space of the **y** coordinates. In our case, the two harmonic functions are equal, $H_5=H_6=H$.)

Note that it is straightforward also to construct pp-wave and Taub-NUT solutions on the world-volume of the D8-brane.

IV. REDUCTIONS OF SU(2)-GAUGED $D=8$ SUPERGRAVITY

A. Brane-world reduction to $D=7$

Although there is no gauged supergravity in eight dimensions that admits a maximally-symmetric AdS_8 solution, there *is* a gauged theory that arises from the dimensional reduction of eleven-dimensional supergravity on S^3.[14] Since only the gauge bosons of the left-acting SU(2) of the $SO(4)\sim SU(2)\times SU(2)$ are retained in the truncation, the consistency of this reduction to $D=8$ is guaranteed by the standard group-theoretic arguments of Ref. 15. The theory can also be obtained from the S^2 reduction of type IIA theory, and the SU(2) is the isometry group of the 2-sphere. The eleventh coordinate is the fibre coordinate of the S^3, which can be viewed as a U(1) bundle over S^2.[16] The eight-dimensional theory admits a dilatonic 6-brane domain-wall solution, and this provides a starting-point for the construction of a brane-world Kaluza–Klein reduction to $D=7$.

The bosonic sector of the eight-dimensional theory contains the metric, a dilatonic scalar φ, five further scalars that can be parameterized by a unimodular 3×3 symmetric matrix T_{ij}, the SU(2) Yang–Mills potentials $A^i_{(1)}$, three 2-form potentials $B^i_{(2)}$, and a 3-form potential $A_{(3)}$. The description of the theory is a little involved, but the majority of the complications come from the scalars T_{ij} and the Yang–Mills potentials $A^i_{(1)}$ that will in fact be set to zero in our brane-world Kaluza–Klein reduction to $D=7$. It is not in general consistent in $D=8$ to set $T_{ij}=\delta_{ij}$ and $A^i_{(1)}=0$ while keeping all the other fields nonvanishing, since the retained fields will act as sources for those that are set to zero. However, since in our brane-world reduction to $D=7$ the ansatz for the remaining nonvanishing eight-dimensional fields will be such that these source terms vanish, it is sufficient for our purposes to present the truncated eight-dimensional theory, together with constraints that will be identically satisfied by the brane-world reduction ansatz. These constraints are precisely the conditions that the sources that would have excited the truncated fields should be zero.

It is in fact easy to obtain this truncation of the eight-dimensional gauged theory as an S^3 reduction from $D=11$. The ansatz is given by

$$\begin{aligned} d\hat{s}^2_{11} &= e^{-(1/3)\varphi} ds^2_8 + e^{2/3\varphi} g^{-2} d\Omega^2_3, \\ \hat{A}_{(3)} &= A_3 + \tfrac{1}{2} g^{-1} B^i_{(2)} \wedge \sigma_i . \end{aligned} \tag{46}$$

The quantities σ_i are the three left-invariant 1-forms on the group manifold SU(2), satisfying $d\sigma_i = -\frac{1}{2}\epsilon_{ijk}\sigma_j\wedge\sigma_k$. In terms of these, the unit metric on S^3 can be written as $d\Omega^2_3=\frac{1}{4}\sigma_i\sigma_i$. Substituting the ansatz into the bosonic equations of motion of eleven-dimensional supergravity,

$$d\hat{F}_{(4)} = \tfrac{1}{2}\hat{F}_{(4)}\wedge\hat{F}_{(4)}, \quad \hat{R}_{MN} = \tfrac{1}{12}(\hat{F}^2_{MN} - \tfrac{1}{12}\hat{F}^2_{(4)}\hat{g}_{MN}), \tag{47}$$

we find that the field equation for $\hat{F}_{(4)}$ implies

$$\begin{aligned} d(e^{\varphi} * F_{(4)}) &= -2g\, B^i_{(2)}\wedge G^i_{(3)}, \\ d*G^i_{(3)} &= -4g^2 e^{-\varphi} * B^i_{(2)} - 2g\, F_{(4)}\wedge B^i_{(2)} - g\,\epsilon_{ijk}\, G^j_{(3)}\wedge G^g_{(3)}, \\ F_{(4)}\wedge F_{(4)} &= 0, \end{aligned} \tag{48}$$

where $F_{(4)} \equiv dA_{(3)}$ and $G^i_{(3)} \equiv dB^i_{(2)}$. Note that the last equation in (48) is one of the constraints that results from our having truncated out the T_{ij} and $A^i_{(1)}$ fields. From the Einstein equation in (47), we obtain the following eight-dimensional equations of motion:

$$R_{\mu\nu} = \tfrac{1}{2}\partial_\mu\varphi\,\partial_\nu\varphi - \tfrac{1}{6}\Box\varphi\, g_{\mu\nu} + \tfrac{1}{12}e^{\varphi}[F_{\mu\rho\sigma\lambda}F_{\nu}{}^{\rho\sigma\lambda} - \tfrac{1}{12}F^2_{(4)}\, g_{\mu\nu}]$$
$$+ \tfrac{1}{4}[G^i_{\mu\rho\sigma}G^{i\,\rho\sigma}_{\nu} - \tfrac{1}{9}(G^i_{(3)})^2\, g_{\mu\nu}] + 2g^2 e^{-\varphi}[B^i_{\mu\rho}B^{i\,\rho}_{\nu} - \tfrac{1}{6}(B^i_{(2)})^2\, g_{\mu\nu}],$$

$$\Box\varphi = 6g^2 e^{-\varphi} + \tfrac{1}{48}e^{\varphi}F^2_{(4)} - g^2 e^{-\varphi}(B^i_{(2)})^2, \tag{49}$$

together with the further constraints

$$e^{\varphi}F_{\mu\nu\rho\sigma}G^{i\,\nu\rho\sigma} + 6g\,\epsilon_{ijk}G^j_{\mu\rho\sigma}B^{k\,\rho\sigma} = 0,$$

$$e^{\varphi}G^i_{\mu\nu\rho}G^{j\,\mu\nu\rho} - 12g^2 B^i_{\mu\nu}B^{j\,\mu\nu} = 0. \tag{50}$$

These come from the mixed and the purely internal components of the eleven-dimensional Einstein equation, respectively.

The eight-dimensional equations of motion admit a domain-wall ''ground-state'' solution, where all fields except ds^2_8 and φ are set to zero, and

$$ds^2_8 = W^{2/3}dx\cdot dx + dz^2, \quad e^{\varphi} = W^2, \tag{51}$$

where

$$W = 1 + k|z|, \quad k^2 = \tfrac{9}{4}g^2. \tag{52}$$

Specifically,

$$g = \begin{cases} \tfrac{2}{3}k, & z > 0, \\ -\tfrac{2}{3}k, & z < 0. \end{cases} \tag{53}$$

(As usual, g is allowed to have the necessary sign-change across the domain-wall provided that one thinks of obtaining the eight-dimensional gauged theory as an S^3 reduction from $D=11$, since then g arises as a constant of integration, rather than as a fixed parameter in the eight-dimensional Lagrangian.)

This motivates the construction of the following brane-world reduction ansatz, to give ungauged seven-dimensional $N=2$ supergravity from the gauged eight-dimensional theory,

$$d\hat{s}^2_8 = e^{-(1/2\sqrt{5})\,\phi}W^{2/3}ds^2_7 + e^{(\sqrt{5}/2)\phi}dz^2,$$

$$\hat{B}^i_{(2)} = \frac{1}{2\sqrt{2}}g^{-1}W^{4/3}F^i_{(2)}, \tag{54}$$

$$\hat{A}_{(3)} = A_{(3)}, \quad e^{\hat{\varphi}} = W^2 e^{(\sqrt{5}/2)\phi},$$

where we have now placed hats on all the eight-dimensional fields.

Substituting this ansatz into the equations of motion for the eight-dimensional gauged theory given above, we find that they are satisfied provided that the seven-dimensional fields satisfy the equations of motion of ungauged seven-dimensional $N=2$ supergravity. Specifically, these can be derived from the Lagrangian,

$$\mathcal{L}_7 = R*\mathbb{1} - \tfrac{1}{2}*d\phi\wedge d\phi - \tfrac{1}{2}e^{\sqrt{(8/5)}\phi}*F_{(4)}\wedge F_{(4)} - \tfrac{1}{2}e^{-\sqrt{(2/5)}\phi}*F^i_{(2)}\wedge F^i_{(2)} - \frac{1}{2}F^i_{(2)}\wedge F^i_{(2)}\wedge A_{(3)}\,. \tag{55}$$

It should be noted also that the ansatz (54) identically satisfies the constraint equations in (48) and (50), and so indeed our assumption that these would eventually be satisfied in the brane-world reduction is justified. Note that the theory naturally arises with a 4-form field strength rather than the 3-form field strength that would naturally come from the T^3 reduction of the heterotic theory. This suggests that the former and the latter can be related by a strong/weak duality.

Having obtained the brane-world reduction from eight-dimensional gauged supergravity, we may now lift it back to $D=11$, by using the S^3 reduction ansatz (46). Thus we find that the eleven-dimensional fields are given in terms of seven-dimensional fields by

$$d\hat{s}^2_{11} = e^{-\sqrt{(8/45)}\phi}\,ds^2_7 + e^{\sqrt{(5/18)}\phi}[\,W^{-(2/3)}\,dz^2 + g^{-2}\,W^{4/3}\,d\Omega^2_3], \tag{56}$$

$$\hat{A}_{(3)} = A_{(3)} + \frac{1}{4\sqrt{2}}g^{-2}\,W^{4/3}\,F^i_{(2)}\wedge\sigma_i\,.$$

It is interesting to note that if we perform a coordinate transformation from z to r, defined by $W^{-(1/3)}\,dz = dr$, and hence

$$W = (g\,r)^{3/2}, \tag{57}$$

then this ansatz for the reduction from $D=11$ to $D=7$ becomes

$$\begin{aligned} d\hat{s}^2_{11} &= e^{-\sqrt{8/45}\phi}\,ds^2_7 + e^{\sqrt{5/18}\phi}\,(dr^2 + r^2\,d\Omega^2_3), \\ \hat{A}_{(3)} &= A_{(3)} + \frac{1}{4\sqrt{2}}r^2\,F^i_{(2)}\wedge\sigma_i\,. \end{aligned} \tag{58}$$

This is recognizable as a standard type of Kaluza–Klein reduction on T^4, in which a truncation to the fields of $N=2$ supergravity in $D=7$ has been performed.

B. Brane-world reduction to $D=7$, from type IIA supergravity

Taking the results of the previous subsection, we can perform an additional S^1 Kaluza–Klein reduction on the Hopf fibers of the compactifying 3-sphere that was used in the reduction from $D=11$ to $D=8$, thereby allowing us to obtain a brane-world reduction to $D=7$ that can be viewed as coming from type IIA supergravity compactified first on S^2.

To implement this procedure, we first specialize some results for the Hopf reduction of S^3 that were obtained in Ref. 17. In terms of Euler angles (θ,φ,ψ), the three left-invariant 1-forms of SU(2) can be written as

$$\begin{aligned} \sigma_1 &= \cos\psi\,d\theta + \sin\psi\sin\theta\,d\varphi, \\ \sigma_2 &= -\sin\psi\,d\theta + \cos\psi\sin\theta\,d\varphi, \\ \sigma_3 &= d\psi + \cos\theta\,d\varphi. \end{aligned} \tag{59}$$

Clearly $\partial/\partial\varphi$ is a Killing vector for the 3-sphere metric $d\Omega^2_3 = \frac{1}{4}\sigma_i\,\sigma_i$, and it also leaves the 3-form ansatz in (56) invariant. Let μ_i be three coordinates on $\mathbb{R}^3$ subject to the constraint $\mu_i\,\mu_i = 1$, given in terms of θ and ψ by

$$\mu_1 = \sin\theta\sin\psi, \quad \mu_2 = \sin\theta\cos\psi, \quad \mu_3 = \cos\theta. \tag{60}$$

It is easily seen that in terms of these we can write the left-invariant 1-forms as

$$\sigma_i = -\epsilon_{ijk}\,\mu_j\,d\mu_k + \mu_i\,(d\varphi + \cos\theta\,d\psi). \tag{61}$$

We can now perform a Kaluza–Klein S^1 reduction of the eleven-dimensional expressions (56) on the Hopf fiber coordinate φ, using the standard ansatz,

$$d\hat{s}_{11}^2 = e^{-(1/6)\Phi}\,d\bar{s}_{10}^2 + e^{(4/3)\Phi}\,(d\varphi + \overline{\mathcal{A}}_{(1)})^2,$$

$$\hat{A}_{(3)} = \overline{A}_{(3)} + \overline{A}_{(2)} \wedge (d\varphi + \overline{\mathcal{A}}_{(1)}), \tag{62}$$

where Φ is the type IIA dilaton. Using (61), we therefore obtain the following reduction ansatz for the fields of type IIA supergravity:

$$d\bar{s}_{10}^2 = W^{(1/6)}\,[e^{-(9/8\sqrt{10})\,\phi}\,ds_7^2 + W^{-(2/3)}\,e^{(15/8\sqrt{10})\,\phi}\,dz^2 + \tfrac{1}{4}g^{-2}\,W^{4/3}\,e^{(15/8\sqrt{10})\,\phi}\,d\Omega_2^2],$$

$$\overline{A}_{(3)} = A_{(3)} + \frac{1}{4\sqrt{2}}\,g^{-2}\,W^{4/3}\,\epsilon_{ijk}\,\mu_i\,F_{(2)}^j \wedge d\mu_k,$$

$$\overline{A}_{(2)} = \frac{1}{2\sqrt{2}}\,g^{-1}\,W^{4/3}\,\mu_i\,F_{(2)}^i, \tag{63}$$

$$\overline{\mathcal{A}}_{(1)} = \tfrac{1}{2}g^{-1}\cos\theta\,d\psi,$$

$$e^{\Phi} = W\,e^{(5/4\sqrt{10})\,\phi},$$

where the unit 2-sphere metric $d\Omega_2^2$ is given by

$$d\Omega_2^2 = d\mu_i\,d\mu_i = d\theta^2 + \sin^2\theta\,d\psi^2. \tag{64}$$

The ''vacuum'' solution, corresponding to the metric (63) with $\phi = 0$, can be viewed as the near-horizon limit of a D6-brane.

C. Branes on the D6-brane

The $D=7$, $N=2$ supergravity admits membrane and string solutions supported by electric or magnetic charges for $F_{(4)}$. When lifted back to $D=11$, the membrane becomes an M2-brane delocalised on a 4-hyperplane, whilst the string can be viewed as an M5-brane wrapped on the 4-hyperplane. The seven-dimensional theory also admits black hole and 3-brane solutions, which can be viewed as intersections of two M2-branes, and intersections of two M5-branes, respectively. From the type IIA point of view, they can be viewed as membranes, strings, black holes or 3-branes living in a D6-brane.

V. REDUCTIONS OF GAUGED MAXIMAL $D=7$ SUPERGRAVITY

A. Gauged maximal seven-dimensional supergravity

The bosonic Lagrangian for maximal SO(5)-gauged supergravity in $D=7$ can be written as

$$\mathcal{L}_7 = \hat{R}\,\hat{*}\mathbb{1} - \tfrac{1}{4}T_{ij}^{-1} * DT_{jk} \wedge T_{kl}^{-1}\,DT_{li} - \tfrac{1}{4}T_{ik}^{-1}\,T_{jl}^{-1}\,\hat{*}\hat{F}_{(2)}^{ij} \wedge \hat{F}_{(2)}^{kl} - \tfrac{1}{2}T_{ij}\,\hat{*}\hat{S}_{(3)}^i \wedge \hat{S}_{(3)}^j$$

$$+ \frac{1}{2g}\,\hat{S}_{(3)}^i \wedge \hat{H}_{(4)}^i - \frac{1}{8g}\,\epsilon_{ij_1\cdots j_4}\,\hat{S}_{(3)}^i \wedge \hat{F}_{(2)}^{j_1 j_2} \wedge \hat{F}_{(2)}^{j_3 j_4} + \frac{1}{g}\,\Omega_{(7)} - V\,\hat{*}\mathbb{1}, \tag{65}$$

where

$$\hat{H}^i_{(4)} \equiv D\hat{S}^i_{(3)} = d\hat{S}^i_{(3)} + g\,\hat{A}^{ij}_{(1)} \wedge \hat{S}^j_{(3)}\,. \tag{66}$$

The potential V is given by

$$V = \tfrac{1}{2} g^2 (2T_{ij}\,T_{ij} - (T_{ii})^2), \tag{67}$$

and $\Omega_{(7)}$ is a Chern–Simons-type of term built from the Yang–Mills fields, which has the property that its variation with respect to $\hat{A}^{ij}_{(1)}$ gives

$$\delta\Omega_{(7)} = \tfrac{3}{4}\,\delta^{j_1 j_2 j_3 j_4}_{i_1 i_2 k l}\,\hat{F}^{i_1 i_2}_{(2)} \wedge \hat{F}^{j_1 j_2}_{(2)} \wedge \hat{F}^{j_3 j_4}_{(2)} \wedge \delta\hat{A}^{kl}_{(1)}\,. \tag{68}$$

An explicit expression for $\Omega_{(7)}$ can be found in Ref. 18 Note that the $S^i_{(3)}$ are viewed as fundamental fields in the Lagrangian. The symmetric unimodular SO(5)-valued tensor T_{ij} describes the 14 scalar fields.

Let us now set the SO(5) Yang–Mills potentials $A^{ij}_{(1)}$ to zero, and take the scalars to be trivial also, $T_{ij} = \delta_{ij}$. This is not in general a consistent truncation, since the remaining fields $\hat{S}^i_{(3)}$ would act as sources for the Yang–Mills and scalar fields that have been set to zero. If we impose that these source terms vanish, i.e.,

$$\hat{S}^i_{(3)} \wedge \hat{S}^j_{(3)} = 0, \quad \hat{*}\hat{S}^i_{(3)} \wedge \hat{S}^j_{(3)} = 0, \tag{69}$$

then the truncation will be consistent. (As we shall see below, these sources terms will indeed vanish in the brane-world reduction that we shall be considering.) The remaining equations of motion following from (65) are then

$$\begin{gathered} d\hat{*}\hat{S}^i_{(3)} = 0, \quad d\hat{S}^i_{(3)} = g\,\hat{*}\hat{S}^i_{(3)}\,, \\ \hat{R}_{AB} = \tfrac{1}{4}(\hat{S}^i_{ACD}\,\hat{S}^{i\,CD}_B - \tfrac{2}{15}(S^i_{(3)})^2\,\hat{g}_{AB}) - \tfrac{3}{2} g^2\,\hat{g}_{AB}\,. \end{gathered} \tag{70}$$

B. Chiral $N=(2,0)$ supergravity from $D=7$

We find that the following Kaluza–Klein ansatz for the seven-dimensional fields yields a consistent reduction to six dimensions,

$$\begin{gathered} d\hat{s}^2_7 = e^{-2k|z|}\,ds^2_6 + dz^2, \\ \hat{S}^i_{(3)} = e^{-2k|z|}\,F^i_{(3)}\,, \\ \hat{A}^{ij}_{(1)} = 0, \quad T_{ij} = \delta_{ij}\,, \end{gathered} \tag{71}$$

where the constant k is related to the gauge coupling constant g by

$$g = \begin{cases} -2k, & z > 0\,, \\ +2k, & z < 0. \end{cases} \tag{72}$$

Substituting this ansatz into the field equations of seven-dimensional SO(5)-gauged supergravity, we find that all the equations are consistently satisfied provided that the six-dimensional fields ds^2_6 and $F^i_{(3)}$ satisfy the equations of motion of six-dimensional ungauged $N=(2,0)$ chiral supergravity, namely,

$$F^i_{(3)} = *F^i_3\,, \quad dF^i_{(3)} = 0, \quad R_{\mu\nu} = \tfrac{1}{4} F^i_{\mu\rho\sigma} F^{i\,\rho\sigma}_{\nu}\,. \tag{73}$$

Note that the self-duality of the 3-forms ensures that the constraints (69) are indeed satisfied, since $F^i_{(3)} \wedge F^j_{(3)} = 0$ for any pair of self-dual 3-forms. Of course the self-duality of the $F^i_{(3)}$ fields also implies one cannot write a covariant Lagrangian for this theory.

Since we know the exact embedding of seven-dimensional maximal SO(5)-gauged supergravity in $D=11$, via the S^4 reduction, we can lift the above ansatz to an embedding in eleven-dimensional supergravity. Using the S^4 reduction ansatz, we therefore obtain

$$\begin{aligned} d\hat{s}^2_{11} &= e^{-2k|z|} ds^2_6 + dz^2 + g^{-2} d\mu_i d\mu_i, \\ \hat{F}_{(4)} &= \frac{1}{8g^3} \epsilon_{i_1 \cdots i_5} \mu_{i_1} d\mu_{i_2} \wedge \cdots \wedge d\mu_{i_5} - g^{-1} d(\mu_i e^{-2k|z|} F^i_{(3)}), \end{aligned} \tag{74}$$

where μ_i are coordinates on $\mathbb{R}^5$, subject to the constraint

$$\mu_i \mu_i = 1, \tag{75}$$

which defines the unit 4-sphere.

C. Five-dimensional $N=4$ ungauged supergravity from SO(5)-gauged $D=6$ supergravity

By dimensionally reducing the embedding (74) of six-dimensional chiral $N=(2,0)$ supergravity on a circle in the six-dimensional space–time, we can obtain an embedding of five-dimensional $N=4$ supergravity in type IIA supergravity. Thus we begin by performing a standard S^1 Kaluza–Klein reduction of the six-dimensional fields,

$$\begin{aligned} ds^2_6 &= e^{-2\alpha\phi} d\tilde{s}^2_5 + e^{6\alpha\phi} (dx_5 + \mathcal{A}_{(1)})^2, \\ F^i_{(3)} &= e^{-4\alpha\phi} * \tilde{F}^i_{(2)} + \tilde{F}^i_{(2)} \wedge (dx_5 + \mathcal{A}_{(1)}), \end{aligned} \tag{76}$$

where $\alpha = 1/(2\sqrt{6})$ and $\tilde{F}^i_{(2)} = d\tilde{A}^i_{(1)}$. (Note that the form of the reduction ansatz for the six-dimensional fields $F^i_{(3)}$ is dictated by the fact that they are self-dual.) The theory that results from this dimensional reduction is ungauged $N=4$ supergravity in $D=5$. It is straightforward to show that the equations of motion in $D=5$ that follow from substituting (76) into (73) are derivable from the Lagrangian,

$$\mathcal{L}_5 = \tilde{R} * \mathbb{1} - \tfrac{1}{2} * d\phi \wedge d\phi - \tfrac{1}{2} e^{-4\alpha\phi} * \tilde{F}^i_{(2)} \wedge \tilde{F}^i_{(2)} - \tfrac{1}{2} e^{8\alpha\phi} * \mathcal{F}_{(2)} \wedge \mathcal{F}_{(2)} - \tfrac{1}{2} \tilde{F}^i_{(2)} \wedge \tilde{F}^i_{(2)} \wedge \mathcal{A}_{(1)}, \tag{77}$$

where $\mathcal{F}_{(2)} = d\mathcal{A}_{(1)}$.

We now substitute (76) into (74), and compare it with a standard Kaluza–Klein S^1 reduction from $D=11$ to $D=10$,

$$\begin{aligned} d\hat{s}^2_{11} &= e^{-(1/6)\Phi} ds^2_{10} + e^{(4/3)\Phi} (dx_5 + A_{(1)})^2, \\ \hat{F}_{(4)} &= F_{(4)} + F_{(3)} \wedge (dx_5 + A_{(1)}). \end{aligned} \tag{78}$$

By doing this, we arrive at the ansatz for the embedding of the five-dimensional ungauged $N=4$ supergravity in type IIA supergravity,

$$ds_{10}^2 = e^{-(9/4)\,k|z| - (5/4)\,\alpha\phi}\, d\tilde{s}_5^2 + e^{-(1/4)\,k|z| + (3/4)\,\alpha\phi}\, dz^2 + g^{-2}\, e^{-(1/4)k|z| + (3/4)\,\alpha\phi}\, d\mu_i\, d\mu_i\,,$$

$$F_{(4)} = \frac{1}{8g^3}\,\epsilon_{i_1\cdots i_5}\,\mu_{i_1}\, d\mu_{i_2}\wedge\cdots\wedge d\mu_{i_5} - g^{-1}\, e^{-4\alpha\phi}\, d(\mu_i\, e^{-2k|z|} \hat{*} \widetilde{F}^i_{(2)}),$$

$$F_{(3)} = -g^{-1}\, d(\mu_i\, e^{-2k|z|}\, \widetilde{F}^i_{(2)}), \tag{79}$$

$$F_2 = \mathcal{F}_{(2)}, \quad e^{\Phi} = e^{-(3/4)\,k|z|}\, e^{(9/2)\,\alpha\phi}.$$

D. Chiral $N=(2,0)$ supergravity from type IIA NS5-brane

We showed in Sec. V B that the chiral (2,0) six-dimensional supergravity can be obtained as a brane-world Kaluza–Klein reduction from maximal gauged supergravity in $D=7$, and in turn, this can be obtained as an S^4 reduction from $D=11$. It was shown recently that one can take a singular limit of the S^4 reduction of eleven-dimensional supergravity, in which the 4-sphere degenerates to $S^3\times\mathbb{R}$.[19] The reduction can then be reinterpreted as an S^3 reduction of type IIA supergravity, yielding a maximal SO(4)-gauged supergravity in $D=7$ that admits a domain-wall, but not AdS_7, as a solution. One may refer to this theory as a ''domain-wall'' supergravity.

By applying this limiting procedure in the context of the brane-world reduction to the (2,0) supergravity in $D=6$ that we constructed in Secs. V A and V B, we can now obtain a brane-world reduction of the $D=7$ domain-wall supergravity to the (2,0) theory in $D=6$. Furthermore, we can lift this back, via its S^3 embedding, to an ansatz for type IIA supergravity. Rather than repeating the details of how the singular limit is taken here, we shall simply quote and make use of the general results already obtained in Ref. 19.

We begin by considering the brane-world reduction of the maximal seven-dimensional SO(4)-gauged domain-wall supergravity. As in our previous examples, many of the fields are set to zero in the brane-world reduction, and so rather than presenting the full seven-dimensional theory obtained in Ref. 19, we shall instead give it in an already-truncated form, where all but the participating fields have already been set to zero. As usual, we should add the cautionary remark that one cannot in general consistently set these fields to zero while allowing the remaining fields to take generic configurations. But in anticipation of the fact that the brane-world reduction *will* be consistent, we can make the truncation provided that we take note also of the consequent required constraints, which will be satisfied by the brane-world reduction ansatz.

In this spirit, we therefore set to zero all the fields of the seven-dimensional SO(4)-gauged domain-wall supergravity constructed in Ref. 19 except for the metric, the dilatonic scalar field ϕ, and the 3-forms $S^0_{(3)}$ and $S^\alpha_{(3)}$. Note that $S^0_{(3)}$ is viewed as a 3-form field strength that is derived from a 2-form potential, whilst the four 3-forms $S^\alpha_{(3)}$ are viewed as independent fields in their own right, which satisfy first-order equations of motion. Defining $\gamma=\sqrt{2/5}$, we read off from Ref. 19 that the equations of motion for these remaining fields will be

$$d\hat{*}d\phi = -\gamma\, e^{-2\gamma\phi}\,\hat{*}S^0_{(3)}\wedge S^0_{(3)} + \tfrac{1}{4}\gamma\, e^{(1/2)\,\gamma\phi}\,\hat{*}S^\alpha_{(3)}\wedge S^\alpha_{(3)} - 4\gamma g^2\, e^{\gamma\phi}\,\hat{*}\mathbb{1},$$

$$d(e^{-2\gamma\phi}\,\hat{*}S_{(3)}) = 0, \quad dS^0_{(3)} = 0,$$

$$dS^\alpha_{(3)} = g\, e^{1/2\,\gamma\phi}\,\hat{*}S^\alpha_{(3)}\,, \tag{80}$$

$$\hat{R}_{MN} = \tfrac{1}{2}\partial_M\phi\,\partial_N\phi + \tfrac{1}{4}e^{-2\gamma\phi}[S^0_{MPQ}\,S^{0\,PQ}_N - \tfrac{2}{15}(S^0_{(3)})^2\,\hat{g}_{MN}]$$
$$+ \tfrac{1}{4}e^{(1/2)\,\gamma\phi}[S^\alpha_{MPQ}\,S^{\alpha\,PQ}_N - \tfrac{2}{15}(S^\alpha_{(3)})^2\,\hat{g}_{MN}] - \tfrac{4}{5}g^2\, e^{\gamma\phi}\,\hat{g}_{MN}\,.$$

(Note that we have placed hats on all quantities associated with the seven-dimensional metric, in anticipation of the upcoming brane-world reduction to $D=6$.)

We may first note that these equations of motion admit a domain-wall solution given by $d\hat{s}_7^2 = W^2\, dx\cdot dx + dz^2$, $e^{-\gamma\phi} = W^2$, where $W = 1 + k|z|$ and $k^2 = 4g^2/25$. This provides the basis for the brane-world reduction ansatz to $D=6$. Specifically, we find that all the equations given in (80) are satisfied if we make the following ansatz:

$$d\hat{s}_7^2 = W^2\, ds_6^2 + dz^2\,, \quad e^{-\gamma\phi} = W^2,$$
$$S^0_{(3)} = F^0_{(3)}, \quad S^\alpha_{(3)} = W^{5/2} F^\alpha_{(3)}\,, \tag{81}$$

where the fields ds_7^2 and $F^i_{(3)}$ satisfy the equations of motion of ungauged six-dimensional (2,0) supergravity, as given in (73). Note that here, the index i on $F^i_{(3)}$ runs over the five values $i = (0,\alpha)$.

We can also use the results in Ref. 19 to lift the seven-dimensional fields to those of ten-dimensional type IIA supergravity. For the truncated system that we are considering here, we find that the embedding is simply given by

$$d\bar{s}_{10}^2 = e^{(3/8)\gamma\phi}\, ds_7^2 + g^{-2} e^{-(5/8)\gamma\phi}\, d\Omega_3^2,$$
$$e^{\Phi} = e^{(5/4)\gamma\phi}, \quad \bar{A}_{(1)} = 0,$$
$$\bar{F}_{(4)} = -e^{(1/2)\gamma\phi}\, \mu_\alpha S^\alpha_{(3)} + g^{-1} S^\alpha_{(3)} \wedge d\mu_\alpha\,, \tag{82}$$
$$\bar{F}_{(3)} = 2g^{-3}\,\Omega_{(3)} + g^{-1} S^0_{(3)},$$

where μ_α denote Cartesian coordinates on $\mathbb{R}^4$ subject to the constraint $\mu_\alpha \mu_\alpha = 1$ that defines the unit 3-sphere with metric $d\Omega_3^2$ and volume form $\Omega_{(3)}$. The barred fields are those of type IIA supergravity, with Φ being the type IIA dilaton.

Substituting our brane-world reduction ansatz (81) into this, we obtain the following brane-world embedding of six-dimensional (2,0) supergravity in type IIA supergravity:

$$d\bar{s}_{10}^2 = W^{(5/4)}\,(ds_6^2 + W^{-2}\, dz^2 + g^{-2}\, d\Omega^2_{(3)}),$$
$$e^{\Phi} = W^{-(5/2)}, \quad \bar{A}_{(1)} = 0,$$
$$\bar{F}_{(4)} = -W^{3/2}\, \mu_\alpha F^\alpha_{(3)} + g^{-1} W^{5/2} F^\alpha_{(3)} \wedge d\mu_\alpha\,, \tag{83}$$
$$\bar{F}_{(3)} = 2g^{-3}\,\Omega_{(3)} + g^{-1} F^0_{(3)}.$$

E. Chiral $N=(1,0)$ supergravity from heterotic 5-brane

It was shown in Refs. 20, 21, 19 that one can obtain the chiral $N=(1,0)$ theory from the $N=2$ SU(2)-gauged supergravity in $D=7$ that admits an AdS_7 vacuum solution, via a brane-world Kaluza–Klein reduction. There is also an SU(2)-gauged supergravity in $D=7$ that admits a domain wall instead of AdS_7 as a vacuum solution. This theory can be obtained from the S^3 reduction of $N=1$ supergravity in $D=10$, and its domain-wall solution is therefore the S^3 reduction of the heterotic 5-brane. Clearly it can also obtained from the truncation of the $N=4$ SO(4)-gauged maximal supergravity discussed in the previous subsection. It is straightforward to reduce the seven-dimensional theory or the heterotic theory in $D=10$ on the world-volume of the 5-brane and obtain the chiral $N=(1,0)$ supergravity. The reduction ansatz is identical to that of Sec. V D, but with all the fields that carry the index α set to zero.

Both the (2,0) and (1,0) theories admit a self-dual string solution in $D=6$. This solution can be lifted to $D=11$, where it becomes a self-dual string living in the world-volume of M5-brane,

which can also be viewed as an open membrane ending on the M5-brane.[3] When lifted back to $D=10$ instead, it can be viewed as a self-dual string living in the NS5-brane or the heterotic 5-brane.

F. $N=(1,1)$ supergravity from $D=7$ gauged supergravity

So far, we obtained the chiral ungauged supergravity in $D=6$ from gauged supergravity in $D=7$, which itself can be obtained from S^4 reduction of M-theory, or the S^3 reduction of the type IIA or heterotic theories. There also exist gauged supergravities in $D=7$ that give rise instead to the $N=(1,1)$ nonchiral theory in six dimensions, through a brane-world Kaluza–Klein reduction. One example is the SU(2)-gauged supergravity that is the S^1 reduction of eight-dimensional SU(2)-gauged supergravity, which itself can be obtained from the S^3 reduction of eleven-dimensional supergravity,[14] as we discussed in Sec. IV. This is because the brane-world reduction of the eight-dimensional gauged supergravity gives rise to $N=2$ supergravity in $D=7$. If we perform a further S^1 reduction on a brane-world direction, the bulk gauged-supergravity in $D=8$ becomes a gauged $N=4$ supergravity in $D=7$, whilst the world-volume seven-dimensional ungauged theory becomes the $N=(1,1)$ ungauged theory in $D=6$.

There should also be an SO(4)-gauged supergravity in $D=7$ that gives rise to the $N=(1,1)$ theory in $D=6$. This can be obtained from the S^3 reduction of the type IIB theory. The bulk T-duality of the type IIA and type IIB theories then translates into a T-duality between the $N=(1,1)$ and $N=(2,0)$ theories in the 5-brane world-volume.

VI. CONCLUSION

In this paper, we have constructed several new examples of brane-world Kaluza–Klein reductions. Our focus was to construct the reductions with larger supersymmetry and in diverse dimensions that in general involve consistent Kaluza–Klein reductions with dilatonic codimension one objects, thus extending the results obtained in Ref. 3 in several ways. Specifically, we have shown that it is possible to construct consistent brane-world reductions of five-dimensional $N=8$ SO(6)-gauged supergravity to ungauged $N=4$ supergravity in $D=4$; of massive type IIA supergravity to ungauged $N=1$ supergravity in $D=9$; of eight-dimensional $N=2$ SU(2)-gauged supergravity to ungauged $N=2$ supergravity in $D=7$; and of seven-dimensional $N=4$ SO(5)-gauged supergravity to ungauged $N=2$ supergravity in $D=6$. In all these cases, just as in the original examples constructed in Ref. 3, the degree of ungauged supersymmetry in the lower dimension is one-half of the gauged one in the higher dimension, and in this paper we have focused mainly on the supergravity multiplets.

A simple calculation shows that for any brane-world (codimension one) reduction ansatz of the form

$$d\hat{s}^2 = e^{-2k|z|}\, ds^2 + dz^2, \tag{84}$$

the Riemann tensor $\hat{R}_{ABCD}$ of the D-dimensional metric $d\hat{s}^2$ satisfies

$$\hat{R}_{ABCD}\hat{R}^{ABCD} = e^{4k|z|} R_{abcd} R^{abcd} - 4k^2 e^{2k|z|} R + 2D(D-1)k^4 \tag{85}$$

in the bulk, where R_{abcd} and R are the Riemann tensor and Ricci scalar of the reduced metric ds^2. This implies that any curvature of the lower-dimensional metric for which $R_{abcd}R^{abcd}$ or R is nonzero, no matter how small, will lead to curvature singularities in the higher-dimensional metric on the Cauchy horizons at $z=\pm\infty$. These singularities were discussed in detail for a Schwarzschild black hole on the brane in Ref. 22. In Ref. 23, it was argued that such curvature singularities on the horizons arise as an artifact of considering only the zero-mode of the metric tensor, and that if the massive Kaluza–Klein modes are taken into account they could actually become dominant near the horizons, and may lead to a finite curvature there. The results of Ref. 3 and this paper suggest that the phenomenon of diverging curvature on the Cauchy horizons for the AdS domain wall reductions (or null horizons for the dilatonic domain wall reductions) may be more severe.

Specifically these results show that the brane-world reductions correspond to exact fully nonlinear consistent embeddings in which the massive Kaluza–Klein modes can be consistently decoupled. This implies that there certainly exist exact solutions on the brane-world where Kaluza–Klein modes do not enter the picture, even at the nonlinear level. For these solutions, the curvature will inevitably diverge at the horizons. It becomes necessary, therefore, either to live with these (null) singularities or else to find a principle, perhaps based on the imposition of appropriate boundary conditions, for rejecting the solutions of this type. (Let us also remark that a deviation of the dilatonic domain wall solutions from the flat (BPS)-limit generically introduces naked singularities,[24] again pointing towards difficulties with the interpretation of such solutions within a more realistic set-up.) It should be emphasized, however, that regardless of the physical questions that are prompted by these results, the brane-world Kaluza–Klein reductions remain valid mathematical constructs in their own right. In fact as relatively simple examples of consistent reductions that have no obvious group-theoretic explanation, they can be viewed as precursors of the remarkable examples of consistent reductions on spheres.

Finally, we again emphasize that the absolute-value sign in Eq. (84) for the brane-world metrics in the AdS codimension one brane (as well as dilatonic examples as discussed in the text) actually requires an explicit delta function source to support such a Z_2-symmetric codimension one object that in turn allows for the trapping of gravity on the world-volume of the brane (at $z=0$). The understanding of such delta-function sources in the lower dimension may require a subtle interpretation in terms of fundamental sources, such as D-brane sources of the higher dimensional theory.[25] Nevertheless, the consistency of the Kaluza–Klein reduction in the bulk (for $z\neq 0$) is valid quite independently of the origin of the domain wall sources.

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Excision of singularities by stringy domain walls

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We study supersymmetric domain walls on $S_1/\mathbf{Z}_2$ orbifolds. The supergravity solutions in the bulk are given by the attractor equation associated with Calabi–Yau (CY) spaces and have a naked space–time singularity at some $|y_s|$. We are looking for possibilities to cut off this singularity with the second wall by a stringy mechanism. We use the collapse of the CY cycle at $|y_c|$ which happens before and at a finite distance from the space–time singularity. In our example with three Kähler moduli the second wall is at the end of the moduli space at $|y_c|$ where also the enhancement of SU(2) gauge symmetry takes place so that $|y_e|=|y_c|<|y_s|$. The physics of the excision of a naked singularity via the enhançon in the context of domain wall has an interpretation on the heterotic side related to $R\to 1/R$ duality. The position of the enhançon is given by the equation $R(|y_e|)=1$. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1373424]

The supersymmetric domain wall solutions of $D=5$, $N=2$, U(1) gauged supergravity[1] with brane sources on $S^1/\mathbf{Z}_2$ orbifolds have been described recently in Ref. 2. It has been observed there that in the context of Calabi–Yau (CY) compactifications the collapse of CY cycles may put some restrictions on the distance between the walls.[3,4] In this article we will study this type of domain wall both for $D=5$, $N=2$, U(1) gauged supergravity[1] (GST model) and for Calabi–Yau compactifications of 11-D supergravity with fluxes turned on. The latter is the five-dimensional heterotic M-theory[5,6] obtained by a reduction on a CY threefold of Horava–Witten M-theory[7] on $S^1/\mathbf{Z}_2$ (HW model). The explicit form of the solution with general dependence on the vector multiplets is obtained for both models by solving the generalized attractor equation.[8–11] Since the domain wall solutions[2,6] of the two models behave very similarly, we will discuss them in parallel.

The purpose of this article is to find a possibility to remove the space–time singularity of the domain wall solution via some particular property of the CY space. Specifically we would like to find a situation when the collapse of the CY cycle at $|y_c|$ happens closer to the first wall which is at $y=0$ and at a finite distance from the space–time singularity $|y_s|$, so that

$$|y_c|<|y_s|. \tag{1}$$

In the case of excision of repulson singularities by the enhançon mechanism,[12] the distance between the repulson and enhançon is finite. The hope, therefore, is that also for some domain walls the analogous situation may be possible, particularly if enhancement of gauge symmetry is somehow involved. The finite distance between the naked singularity of the supergravity solution and the position of the collapse of the CY cycle may allow us to use the physics of string theory already at the end of the moduli space which in this case excludes the singularity of the general relativity as unphysical. The generic interest in such a mechanism is supported by some interesting

recent investigations of the brane world scenarios[13] where the naked singularities may be present in solutions of the Einstein equations and need to be removed by a natural stringy-type mechanism.

Our walls are supersymmetric everywhere, including the position of the branes,[2] therefore they do not directly address the problems of the models in Ref. 13. But due to supersymmetry in our model the matching conditions for the solutions are satisfied automatically on both walls. We have more control over the situation and may clearly indicate conditions when a natural mechanism of stringy excision of singularities is available.

We have found that in most cases the singularities of the CY space tend to coincide with the space–time singularity of the domain wall solutions, i.e.,

$$|y_c| = |y_s|. \tag{2}$$

Only in some special cases we will find the singularities in space–time and CY space at some finite distance in the y direction from each other as in Eq. (1). Within the classification of the possible behavior of the CY manifold at the boundary of the Kähler cone[9,14] we consider the special case when a complex divisor D is collapsing to a curve E of A_1 singularities, so that there is an SU(2) enhancement of gauge symmetry at the boundary. The position $|y_c|$ where the cycle collapses therefore corresponds to the position $|y_e|$ of the enhançon. We will find examples where

$$|y_c| = |y_e| < |y_s|. \tag{3}$$

Domain wall solutions of the two models have a metric of the form[15]

$$ds^2 = a^2(y) dx^\mu dx^\nu \eta_{\mu\nu} + a^{2\gamma}(y) dy^2, \tag{4}$$

where $\gamma = -2$ is the GST model and $\gamma = 4$ is the HW model.[16] In both cases the function $a(y)$ and the scalar fields are determined in terms of harmonic functions through generalized attractor equations[9,10] which require that the rescaled variables $\tilde{h}^I \equiv a(y) h^I$ have to satisfy

$$C_{IJK} \tilde{h}^J \tilde{h}^k = H_I(y), \tag{5}$$

where $H_I(y)$ are harmonic functions. Then the physical scalars are given by either solving the hypersurface constraint or by using the the ratios $\tilde{h}^x/\tilde{h}^0$ and the metric is determined by

$$a^3(y) = C_{IJK} \tilde{h}^I \tilde{h}^J \tilde{h}^K = \tilde{h}^I H_I. \tag{6}$$

In the HW model one additional scalar enters nontrivially into the solution. This scalar is the overall volume V, or ''breathing mode'' of the Calabi–Yau space. Since there is no solution with constant V, there are no anti-de Sitter (AdS) vacua in the HW case in contrast to domain walls in 5-D supergravity.[2] For our purpose it is important that V is uniquely determined by the vector multiplet scalars. In fact, V is just some power of a, and therefore a rational function of the harmonic functions:

$$V = a^6 = (C_{IJK} \tilde{h}^I \tilde{h}^J \tilde{h}^K)^2. \tag{7}$$

As a consequence the flow through moduli space is the same as in the GST model. The two models differ in the precise form of the space–time metric and by the fact that a^6 in the HW case is the volume of the internal space.

Following Ref. 2 we consider a setup where the fifth direction is a $S^1/\mathbf{Z}_2$ orbifold with three-branes at the fixed points $y = 0$ and $y = \tilde{y}$, which act as sources for the harmonic functions:

$$\partial_y^2 H_I = -2g q_I [\delta(y) - \delta(y - \tilde{y})], \quad H_I = c_I - 2g q_I |y|. \tag{8}$$

Concerning space–time singularities both models behave very similarly. Components of curvature tensors become singular if either $a=0$ or if its derivatives diverge. The corresponding Ricci scalar is

$$\mathcal{R}=-4a^{-2-2\gamma}((3-2\gamma)(a')^2+2aa''). \tag{9}$$

To find explicit domain wall solutions we consider some CY spaces with three Kähler moduli[17,18] for which the relevant prepotential was identified in 5-D supergravity and the attractor equations have been solved. Many of such solutions are displayed and analyzed in Refs. 9 and 11 for the extended Kähler cone of a CY which is an elliptic fibration over the Hirzebruch surface $\mathcal{F}_1$. The extended Kähler cone consists of two Kähler cones related by a flop transition.[19] We will refer to the two CY compactifications as model III and model II, respectively. Model I forms a particular boundary of the moduli space of the model II. The moduli space of model III has a boundary where SU(2) enhancement occurs in the way described above. Moreover, the metric on the moduli space is finite at this boundary. As explained in Refs. 17 and 18, the region III CY is related to two other CY spaces by deformation of the base of the elliptic fibration into the Hirzebruch surfaces $\mathcal{F}_0$ and $\mathcal{F}_2$, respectively. These models likewise have a boundary with SU(2) enhancement, and the physics close to the boundary is completely isomorphic to the one of the region III $\mathcal{F}_1$ model. Though we will discuss the region III model for definiteness, our results will be automatically valid for these models as well. The M-theory compactifications on the elliptically fibered CY spaces with bases $\mathcal{F}_0$, $\mathcal{F}_1$, $\mathcal{F}_2$ have a dual description by compactifications of the $E_8\times E_8$ heterotic string on $K3\times S^1$ with instanton numbers (12, 12), (13, 11), (14, 10), respectively. To be precise this duality is known to be valid in the absence of G-flux inside the M-theory CY. We will later use the heterotic picture to describe the SU(2) enhancement in a simple way, assuming that the duality is still valid in presence of G-flux. Since switching on G-flux does not interfere with the mechanism underlying gauge symmetry enhancement this is a reasonable assumption.

Let us return to the M-theory compactification on the CY with base $\mathcal{F}_1$. The boundaries of the extended Kähler cone are defined by the collapse of some cycles to zero volume. The whole picture is shown in Fig. 2 of Ref. 9. Some of the boundaries have a vanishing metric of the moduli space, some have an infinite metric. Equations of motion relate the space–time curvature $\mathcal{R}$ with expressions which depend on moduli space metric, $g_{xy}(\phi^x)'(\phi^y)'a^{-2\gamma}$, as well as with expressions depending on the inverse moduli space metric, $W_{,x}g^{xy}W_{,y}$. This indicates that it is likely that the space–time curvature is infinite if the moduli space metric g_{xy} or its inverse g^{xy} are infinite.[20] We have studied several cases explicitly and found that they indeed have coinciding singularities of the space–time and the moduli space.

We proceed therefore directly with the domain walls of the model III, which has a boundary with finite metric. The classical prepotential for this model was derived in Ref. 18. In terms of the variables adapted to the Kähler cone, the prepotential is

$$\mathcal{V}=\tfrac{4}{3}(h^1)^3+\tfrac{3}{2}(h^1)^2h^2+\tfrac{1}{2}h^1(h^2)^2+(h^1)^2h^3+h^1h^2h^3=1, \tag{10}$$

and the Kähler cone is simply $h^I>0$. In the new variables

$$h^1=U,\quad h^2=T-\tfrac{1}{2}U-W,\quad h^3=W-U, \tag{11}$$

the prepotential becomes

$$\mathcal{V}=\tfrac{5}{24}U^3+\tfrac{1}{2}UT^2-\tfrac{1}{2}UW^2+\tfrac{1}{2}U^2W=1. \tag{12}$$

The Kähler cone is $W>U>0$ and $T>W+1/2U$. There are three boundaries when either of h^I vanishes: (*i*) $U=0\Leftrightarrow h^1=0$: here the metric of moduli space becomes singular, (*ii*) $T=W+U/2\Leftrightarrow h^2=0$: the metric of moduli space is regular and one has non-Abelian gauge symmetry enhancement; and (*iii*) $W=U\Leftrightarrow h^3=0$: there is a flop transition, and again the metric is regular. We can solve (12) for T: $T=\sqrt{(2/U)(1-5U^3/24-U^2W/2+UW^2/2)}$ and keep as independent

scalars $\phi^x=(U,W)$. By looking at the resulting moduli space metric g_{xy} with determinant $\det g_{xy}\simeq 12(3-4U^3)/(24U-5U^4-12U^3W+12U^2W^2)$ we recover the picture given in Fig. 2 in Ref. 9: U varies within a finite interval, whereas W varies from 0 to ∞ at $U=0$ and is cutoff by the curves $U=W$ and $T-W-1/2U$ for positive W:

$$0<U<\left(\frac{3}{4}\right)^{1/3}, \quad U<W<\frac{3-U^3}{3U^2}. \tag{13}$$

The stabilization equations (5) are a system of quadratic equations for the rescaled scalars $\tilde{h}^I=a(y)h^I\coloneqq\tilde{U},\tilde{T},\tilde{W}$. For our model they are solved following Ref. 9 by [21]

$$\tilde{U}=\sqrt{\alpha-\sqrt{\alpha^2-\beta}}, \quad \tilde{T}=\frac{H_T}{\tilde{U}}, \quad \tilde{W}=\frac{1}{2}\tilde{U}-\frac{H_W}{2\tilde{U}}, \tag{14}$$

where

$$\alpha=\tfrac{1}{4}(H_U+\tfrac{1}{2}H_W), \quad \beta=\tfrac{1}{8}(H_T^2-H_W^2). \tag{15}$$

One needs to impose that the scalars are real and inside the Kähler cone. Therefore the harmonic functions are subject to the inequalities

$$\tfrac{2}{3}H_U\geqslant H_T\geqslant -H_W\geqslant \tfrac{2}{9}(H_U-\sqrt{H_U^2-\tfrac{9}{4}H_T^2}), \tag{16}$$

which are mutually consistent. The boundary $T=W+U/2$ corresponds to $2H_U=3H_T$, whereas the boundary $W=U$ corresponds to $-H_W=2/9(H_U-\sqrt{H_U^2-9/4H_T^2})$ and the boundary $U=0$ corresponds to $H_T=-H_W$. We would like to mention that the second branch of the attractor equations found in Ref. 11 does not describe a solution inside the Kähler cone, as can be verified by a full analysis of the constraints.

Let us show that for generic values of the parameters of the harmonic functions the collapse of the modulus h^2 is taking place at the point $|y_c|$ which is at a finite distance from the space–time singularity.

First of all we have to find out under which conditions space–time curvature can diverge. Looking at the formula (9) for the Ricci scalar we find that this happens if either $a=0$ or one of its derivatives diverges.[22] The same is true for the components of the Ricci tensor and of the Riemann tensor, which we did not display explicitly. The only point within the extended Kähler cone where a vanishes is $U=W=0$, $T=\infty$. At this point the moduli space metric is infinite. Divergences in the derivatives of a occur when either $\alpha=\sqrt{\alpha^2-\beta}$ or $\alpha^2=\beta$. The first case corresponds to $U=0$, which is a boundary of the Kähler cone on which the moduli space metric diverges. This includes the point where $a=0$ as a subcase. Thus on the boundary $U=0$ one finds the expected coincidence of space–time singularities with moduli space singularities. The only kind of space–time singularities which need to concern us here are the ones related to $\alpha^2=\beta$.

The equation $\alpha^2=\beta$ has no solutions if $9H_T^2<4H_U^2$ which corresponds to $T>W+1/2U$. Therefore no space–time singularity can occur as long as the moduli are inside the Kähler cone. If $9H_T^2>4H_U^2$, then $\alpha^2=\beta$ has two solutions, $H_W=-2/9(H_U\pm\sqrt{8}\sqrt{9/4H_T^2-H_U^2})$. Thus the generic situation is that one *first* crosses the enhancement boundary $T=W+1/2U$ and *then* runs into a space–time singularity at a finite distance. If $9H_T^2=4H_U^2$, which is precisely true on the enhancement boundary, then $\alpha^2=\beta$ has one solution given by $2H_U+9H_W=0$. Thus the only possibility for the space–time singularity to coincide with the boundary of moduli space is when the parameters are fine tuned such that $2H_U(y_c)=3H_T(y_c)=-9H_W(y_c)$. The corresponding point in moduli space is the intersection point of the enhancement boundary $T=W+1/2U$ with the flop boundary $U=W$. At this point the metric on moduli space is degenerate, which nicely fits with our observation that a singularity in moduli space generically induces a singularity in space–time.

The coordinates W, T, U cover both regions of model III and II and allow us to analyze the flop transition in the framework of special geometry, as shown in Ref. 9. It is also interesting to use the description of the region III in STU parametrization. In this parametrization we can also show that the singularities of the space–time and CY space are at finite distance and we will give a numerical example. Moreover, the interpretation of the enhançon-type physics in terms of T-duality is manifest.

After the substitution $W=S'-1/2(T'-U')$, $T=S'+1/2T'$, and $U=U'$, the region III prepotential takes the form

$$\mathcal{V}=S'T'U'+\tfrac{1}{3}U'^3. \tag{17}$$

The original CY Kähler moduli are now related to the heterotic string variables as follows:

$$h^1=U', \quad h^2=T'-U', \quad h^3=S'-\tfrac{1}{2}(T'+U'). \tag{18}$$

The solution in these variables is[23]

$$\tilde{U}'=\frac{1}{2}\sqrt{H'_U-\sqrt{(H'_U)^2-4H'_SH'_T}}, \quad \tilde{T}'=\frac{H'_S}{2\tilde{U}'}, \quad \tilde{S}'=\frac{H'_T}{2U'}. \tag{19}$$

Note that the harmonic functions are now associated with the primed variables. The boundaries of region III are

$$\begin{gathered} U>0\Leftrightarrow U'>0, \\ W>U\Leftrightarrow S'>\tfrac{1}{2}(T'+U'), \\ T>W+\frac{U}{2}\Leftrightarrow T'>U'. \end{gathered} \tag{20}$$

For convenience we drop the primes on moduli and harmonic functions in the rest of the article, denoting moduli simply by S, T, U. One should keep in mind that the T-variables in both parametrizations are different!

Let us look at the moduli space metric. We solve the hypersurface equation $\mathcal{V}=STU+1/3U^3=1$ for $S{:}S=(3-U^3)/3TU$. The determinant of the vector kinetic matrix is $\det G_{IJ}\simeq 1-4/3U^3$. Thus $0\leqslant U\leqslant(3/4)^{1/3}$ as expected, because the U variable is the same in the TUW and STU parametrization. The determinant of the scalar kinetic term is

$$\det g_{xy}\simeq\frac{3-4U^3}{T^2U^2}, \tag{21}$$

implying $0<U<(3/4)^{1/3}$ and $T\neq 0$. Since T is positive for our CY moduli space, the moduli space metric is regular for

$$0<U<(\tfrac{3}{4})^{1/3} \quad \text{and} \quad 0<T. \tag{22}$$

In particular, it becomes singular on $U=0$, which is a boundary from the CY point of view (tensionless strings). On the boundary $U=T$ (symmetry enhancement) it is regular, as long as U takes allowed values. The third boundary (flop) is given by

$$S(T,U)=\tfrac{1}{2}(T+U), \tag{23}$$

which can be solved for T as $T(U)=-1/2U+(\sqrt{3}/6U)\sqrt{24U-5U^4}$. Note that $T(U)$ is positive for all $0<U<(3/4)^{1/3}$. Therefore the moduli space metric is regular along the flop line. The reality of the ''inner'' and ''outer'' roots in (19) imposes

$$H_U^2>4H_SH_T>0. \tag{24}$$

A further look at (19) and (20) tells us that the harmonic functions H_S, H_T, H_U have to be positive. When combining this with (24) then all expressions are real and $U>0$. The other boundaries are $T\geqslant U$ and $S\geqslant 1/2(T+U)$. The condition $T\geqslant U$ takes a very simple form,

$$H_U\geqslant H_S+H_T, \tag{25}$$

which is compatible with (24). We are interested in the limit $H_U\to H_S+H_T$. We still have to implement the constraint that h^3 is positive, which in these variables is $S>1/2(T+U)$. We will impose the stronger constraint $S>T$ which yields a simpler constraint on the harmonic functions and has the additional advantage to guarantee that our solution is also inside the Kähler cones of the related $\mathcal{F}_0$ and $\mathcal{F}_2$ models. For these models the prepotential likewise can be brought to the form (17). However, the boundaries of the Kähler cones are different. For the $\mathcal{F}_2$ model the Kähler cone is defined by $S>T>U>0$, whereas for the $\mathcal{F}_0$ model one has $S,T>U>0$. Note that all models share the $U=T$ boundary, though the other boundaries are different. Moreover, when imposing the strongest constraint $S>T>U>0$ we can discuss the limit $T-U\to 0$ for all three models simultaneously. Now $S>T$ simply implies

$$H_T>H_S. \tag{26}$$

The constraints we found are compatible: evaluating (24), when (26) is saturated, gives $(H_T-H_S)^2\geqslant 0$. Thus the boundary $U=T$ requires that $H_U=H_S+H_T$. This defines its position as

$$|y_c|=\frac{c_U-c_T-c_S}{d_U-d_T-d_S}. \tag{27}$$

A closer inspection of the analytic form of the Ricci scalar $\mathcal{R}$ and of the function a and its space–time derivatives shows that curvature singularity precisely occurs when $H_U^2=4H_SH_T$. Given the inequalities (24)–(26) we see that this can never happen inside the Kähler cone. Moreover, the generic situation is that the space–time singularity is encountered after crossing the $T=U$ boundary. The only possibility to have the space–time singularity coincide with the boundary of moduli space is to fine tune the parameters such that $H_T(y_c)=H_S(y_c)$ coincides with $H_U^2(y_s)=4H_T(y_s)H_U(y_s)$ at $y=y_s=y_c$. At such a point one has $S=T=U$ or $H_U^2(y_c)=4H_S^2(y_c)=4H_T^2(y_c)$. In terms of the parameters in the harmonic function this means that one must arrange $(c_U-c_T-c_S)/(d_U-d_T-d_S)=(c_T-c_S)/(d_T-d_S)\Leftrightarrow|y_c|=|y_s|$. Generically this condition is not satisfied and therefore $|y_c|<|y_s|$.

Now we can set up an example of a solution running into the enhancement boundary. We take care of the constraint $H_T>H_S$ by setting $H_T=2H_S$. It will turn out that this will lead to relatively simple analytic expressions. Note that this choice implies that at the enhancement boundary $U=T$ one has $S=2U$ or in terms of h^I: at $h^2=0$ one has $h^1=h^3$, (see Fig. 2).

The harmonic functions take the form $H_I=c_I-d_I|y|$ dictated by the presence of two space–time boundaries. The constants c_I define the initial condition on the first space–time boundary whereas the slopes d_I determine how the solution flows through moduli space. The c_I are undetermined integration constants, which are only restricted by the fact that all scalars should be inside the Kähler cone at $y=0$ and by the conventional normalization $a=1$ that we impose on the metric at $y=0$. On the other hand, the d_I are, in the context of a Calabi–Yau compactification with flux, determined by the sources of flux put on the boundaries.[4,15] We will choose some values for d_I to simplify the calculations and not try to connect these values to particular sources of fluxes,

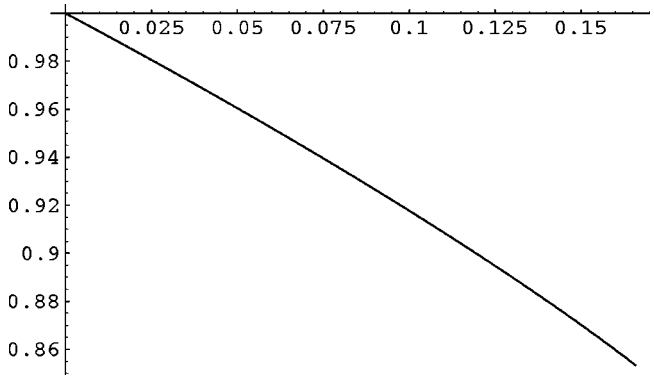

FIG. 1. The function $a(y)$ for $0 \leqslant y \leqslant 0.17$.

since we have shown that the picture is generic. It will not change when taking different slopes, as long as the solution runs into the enhancement boundary without reaching any other boundary of moduli space first.

Now we choose initial data. We have $c_T = 2c_S$ and have to impose $c_U > c_T + c_S = 3c_S$. For definiteness we take $c_U = 4c_S$. Then c_S is fixed by the normalization condition $a(0) = 1$. This can be solved exactly with the result

$$c_S = \left(\frac{45}{49} + \frac{9}{49\sqrt{2}} \right)^{1/3}. \tag{28}$$

Now we have to set the slope. We already decided to take $d_T = 2d_S$. Then the boundary $T = U$ is reached once the inequality

$$|y| \leqslant |y_e| = \frac{C_U - c_T - c_S}{d_U - d_T - d_S} = \frac{c_S}{d_U - 3d_S} \tag{29}$$

is saturated. We are free to choose $d_U > 3d_S$. For definiteness we take $d_U = 10$ and $d_S = 1$. The analytical value of $|y_e|$ is

$$|y_e| = \frac{1}{7} \left(\frac{45}{49} + \frac{9}{49\sqrt{2}} \right)^{1/3} \simeq 0.145\,118. \tag{30}$$

Then $a(|y|)$ is well behaved for $0 \leqslant |y| \leqslant |y_e|$. However, a^3 becomes complex and the scalar curvature $\mathcal{R}$ becomes infinite for some $|y_s| > |y_e|$. Looking at the explicit analytic expressions for a and $\mathcal{R}$ one sees that this happens, independently of our concrete choice of parameters, because $\sqrt{H_U^2 - 4H_S H_T}$ vanishes and then becomes complex.

In our concrete numerical example the equation $H_U^2 - 4H_S H_T = 0$ has two roots, the relevant being

$$|y_s| = \frac{1}{23} \left(8 \left(\frac{45}{49} + \frac{9}{49\sqrt{2}} \right) \right)^{1/3} - 3\sqrt{2} \left(\frac{45}{49} + \frac{9}{49\sqrt{2}} \right)^{1/3} \simeq 0.165\,949, \tag{31}$$

such that indeed $|y_s| > |y_e|$. As we explained earlier, this holds generically for solutions running into the direction of the enhancement boundary. *Whenever the solution runs into the specific boundary of moduli space, where gauge symmetry is enhanced, then it reaches this boundary before the space–time curvature becomes infinite. This is an example where a moduli space boundary shields a space–time singularity.*

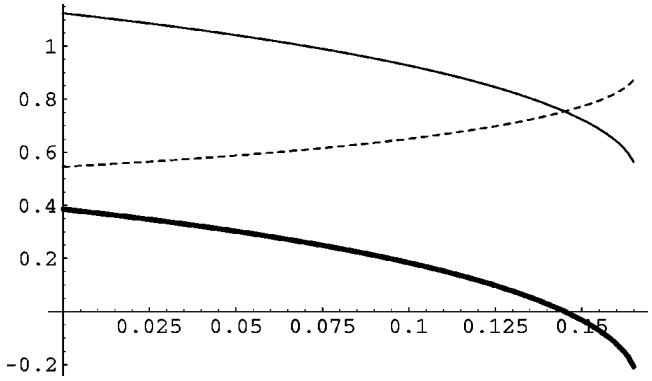

FIG. 2. The Kähler moduli $h^1(y)$ (dashed line), $h^2(y)$ (thick line), and $h^3(y)$ (thin line) for $0 \leqslant y \leqslant 0.17$. At $y=y_c \cong 0.145\,118$ the four-cycle associated to h^2 has collapsed. Note that this happens before the space–time singularity occurs at $y=y_s \cong 0.165\,949$.

The analytical values of a, $\mathcal{R}$ at $|y_e|$ in the example are

$$a(|\tilde{y}|)=\left(\frac{3}{7}\left(\frac{45}{49}+\frac{9}{49\sqrt{2}}\right)\right)^{1/6} \quad \text{and} \quad \mathcal{R}(|\tilde{y}|)=\frac{7}{3}\left(\frac{7}{3}\right)^{1/3}. \tag{32}$$

The analytical expressions of a, $\mathcal{R}$ at $|y_s|$ for our example are complicated and therefore we do not display them. It is, however, instructive to plot various quantities for our specific set of parameters.

We display the metric a in Fig. 1, the moduli h^1, h^2, h^3 which solve the generalized attractor equation in Fig. 2, and the space–time curvature $\mathcal{R}$ in Fig. 3 for $0 \leqslant y \leqslant 0.17$. Clearly, the cycle h^2 collapses at $|y_c|=|y_e| \simeq 0.145\,118...$. At this point the space–time is perfectly regular! Further down at $|y_s| \simeq 0.165\,949...$, where the cycle $h^2 \simeq -0.2527...$ is already negative, i.e., unphysical, the space–time has a naked singularity. *All this follows from the solution of the Einstein equation in the bulk under the condition that we have not yet put the second wall at some* $|\tilde{y}|$.

Note that the GST and HW models show the same qualitative behavior. This is as expected because the singular behavior is due to singularities in the function a and its derivatives.

From the point of view of supergravity nothing special happens along the line $T=U$ in the scalar manifold. A negative value of the scalar field $h^2=T-U$ is as good as a positive one since the metric on the moduli space at $h^2=0$ is regular and there is no reason to consider $T=U$ as a boundary. According to supergravity one can continue the solution to negative $T-U$ and finally

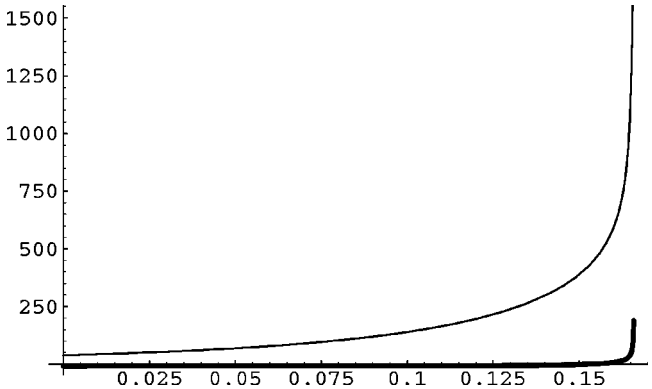

FIG. 3. The Ricci scalar $R(y)$ for $0 \leqslant y \leqslant 0.17$. The thick line refers to the GST model, the thin line to the HW model. In both cases the Ricci scalar diverges at $y=y_s \cong 0.165\,949$.

one encounters a space–time singularity at $|y|=|y_s|$. In order to avoid the singularity one has to put the second brane at some place $|\tilde{y}|<|y_s|$, but there is no distinguished choice of such $|\tilde{y}|$, nor a physical mechanism which excises the singularity. Since our solution is supersymmetric, it has zero energy, as shown in Ref. 2, independently of the position of the second brane.

This is different in M/string theory. In M-theory compactified on CY three-folds h^2 must be positive as a volume of the cycle. $T=U$ is a line of SU(2) gauge symmetry enhancement and $T-U$ is the associated Higgs field. Therefore the moduli space ends at $T=U$, and negative values of $T-U$ are related to positive values by the action of the generator of the Weyl group of SU(2), which is isomorphic to $\mathbf{Z}_2$. This takes a particularly familiar form when using the dual heterotic description, where $R:=\sqrt{T/U}$ is the radius of the sixth dimension. Therefore the Weyl twist acts as T-duality $R\to 1/R$ and SU(2) gauge symmetry enhancement occurs at the self-dual radius, $R=1$.[24,25] Since the gauge symmetry enhancement happens at $y_e<y_s$ it does not make sense to naively continue to $y>y_e$ and in this way the singularity is excised. Moreover, it may be natural to put the second brane precisely at the enhançon point $y=y_e$, defined by the equation

$$R(y_e)=1, \quad R^2(y)\equiv\frac{T(y)}{U(y)}=\frac{h^1+h^2}{h^1}. \tag{33}$$

In this case the $\mathbf{Z}_2$ orbifold symmetry is acting on y and the Weyl twist/T-duality transformation is acting on the moduli coincide. By putting the second wall at the enhançon point $y=y_e$ we enforce the physics to depend on $|T-U|$. When putting the second wall at a different place we would break T-duality spontaneously.

So far we have worked with the prepotential $STU+1/3U^3$ valid inside the Kähler cone. We found that both the resulting theory and the domain wall solutions were regular at $T=U$. However, we had to stop there because we reached a boundary and new physics occurred. One way to capture this new physics is to use the $T\leftrightarrow U$ symmetric form of the prepotential that was found in Ref. 26 in the context of heterotic string theory on $K3\times S^1$:

$$\mathcal{V}=STU+\tfrac{1}{3}U^3\theta(T-U)+\tfrac{1}{3}T^3\theta(U-T). \tag{34}$$

This is now valid for both positive and negative $T-U$. The build-in $T\leftrightarrow U$ symmetry reflects that negative $T-U$ is related to positive $T-U$ by a large gauge transformation. The resulting discontinuities are consequences of the SU(2) gauge symmetry enhancement and reflect the presence of extra massless states at $T=U$. They are analogs of the logarithmic branch cuts one encounters in four dimensions.[26,27]

Earlier we mentioned that it may be natural to put the second wall at the enhançon locus so that $|\tilde{y}|=|y_e|$. We can use the heterotic prepotential (34) to give an additional argument for this. Namely, the presence of the discontinuities in the prepotential automatically causes a δ-function singularity in the space–time geometry of a domain wall which tries to cross the boundary $T=U$. Therefore the enhançon itself acts like a source. Note that this kink singularity is different from the naked singularities of the supergravity solution that we want to excise.

To see this explicitly we first recall that singularities of the Ricci scalar come from singularities of a'', where $'$ is the derivative with respect to y and $a(y)=(\mathcal{V}(\tilde{h}(y)))^{1/3}$. Singularities in a'' can therefore descend from the θ-functions which are present in (34) through application of the chain rule. To work this out we need to be more precise about how $\mathcal{V}$ behaves as a function of $\tilde{T}-\tilde{U}$. Despite the presence of the θ-functions, $\mathcal{V}$ itself is actually continuous, but its derivative with respect to $\tilde{T}-\tilde{U}$ has a finite jump at $\tilde{T}=\tilde{U}$. Consequently the second derivative gives a δ-function: $\partial^2\mathcal{V}/\partial(\tilde{T}-\tilde{U})\partial(\tilde{T}-\tilde{U})=-((\tilde{T}+\tilde{U})/2)^2\delta(\tilde{T}-\tilde{U})+\text{finite}$. This contributes to $a'':a''=1/3\mathcal{V}(\tilde{h})^{-2/3}\mathcal{V}''+\text{finite}\simeq[\partial^2\mathcal{V}/\partial(\tilde{T}-\tilde{U})\partial(\tilde{T}-\tilde{U})][(\tilde{T}-\tilde{U})']^2+\text{finite}$, where we dropped terms, both additive and multiplicative, that stay finite for $\tilde{T}=\tilde{U}$. Since $\tilde{T}-\tilde{U}$ has $y=y_e$ as its only zero we find

$$a'' \sim -\left(\frac{\tilde{T}+\tilde{U}}{2}\right)^2 (\tilde{T}-\tilde{U})' \delta(y-y_e). \tag{35}$$

This would justify our assertion that it is natural to put the second wall at the enhancement point so that $|\tilde{y}|=|y_e|$. Any other position will break the T-duality symmetry.

By five-dimensional heterotic–M-theory duality we expect that the physics of SU(2) enhancement can be equivalently described in the M-theory language. In the context of Calabi–Yau compactifications SU(2) gauge symmetry enhancement (with $g \geqslant 0$ additional hypermultiplets) occurs when a divisor collapses into a (genus g) curve of A_1 singularities. In our case we know from the heterotic analysis that this curve must have genus 0. The Weyl group $\mathbf{Z}_2$ is encoded in the geometry through the local form of the A_1 singularity, $\mathbf{C}^2/\mathbf{Z}_2$. It seems that the Weyl reflections relating positive to negative $T-U$ in the heterotic language correspond to the ''elementary transformations'' discussed in Ref. 28. The extension of the range of moduli as done in (34) presumably corresponds to the procedure of gluing in a reflected Kähler cone at the enhancement boundary, which is described in Ref. 28.

In this article we have shown that there is a stringy mechanism which in certain cases excises space–time singularities which plague supergravity solutions. The mechanism is based on the fact that the stringy moduli space has a boundary on which the moduli space metric is finite. Whereas this boundary does not have a particular meaning in supergravity, so that solutions can be continued beyond until a space-time singularity occurs, one encounters new physics at the boundary in string theory, which makes the space–time singularity unphysical.

This observation leads to a variety of new issues which have to be addressed in the future. Most importantly one would like to understand in detail how the new M/string theory physics modifies space–time geometry and excises the singularity. Since SU(2) gauge symmetry enhancement occurs at the boundary, the situation resembles the enhançon geometry[12] and it would be interesting to explore how far this parallel goes. There are some further facts which might be relevant. In particular at the boundary the tensionless magnetic strings are present in addition to charged massless gauge bosons: it was shown in Ref. 9 that the magnetic string states with charges $\pm(1,-2,1)$ have a vanishing tension. Also one should take into account that the five-dimensional prepotential is purely cubic for five noncompact dimensions. However, in our domain wall setup the fifth dimension is compact and subject to an orbifold projection which reduces the number of unbroken supersymmetries. Thus the new stringy physics at the boundary might be more complex and more interesting than naively expected.

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Effective theories and black hole production in warped compactifications

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We investigate aspects of the four-dimensional (4D) effective description of brane world scenarios based on warped compactification on anti-de Sitter space. The low-energy dynamics is described by visible matter gravitationally coupled to a ''dark'' conformal field theory. We give the linearized description of the 4D stress tensor corresponding to an arbitrary 5D matter distribution. In particular a 5D falling particle corresponds to a 4D expanding shell, giving a 4D interpretation of a trajectory that misses a black hole only by moving in the fifth dimension. Breakdown of the effective description occurs when either five-dimensional physics or strong gravity becomes important. In scenarios with a TeV brane, the latter can happen through the production of black holes near the TeV scale. This could provide an interesting experimental window on quantum black hole dynamics.
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I. INTRODUCTION

It is an old idea that, as an alternative to compactification, the observed Universe instead lives on a brane in a higher-dimensional space. Such ''branification'' scenarios had however until recently been hard to realize, largely because of the difficulty of recovering four-dimensional gravitational dynamics. Two new approaches have changed this and at the same time suggested new views of the origin of the hierarchy of scales in physics. The first, pursued by Ref. 1, is a hybrid of branification and compactification, in which matter is confined to a brane and then large-radius compactification of the extra dimensions yields four-dimensional gravity at long distances.

A more recent approach utilizes warped compactifications to achieve effectively four-dimensional gravitational dynamics. An outline of such a picture has been provided by the RSII model.[2] This utilizes a ''Planck brane'' that serves as the boundary of five-dimensional anti-de Sitter space, and the curvature of anti-de Sitter space effectively ''localizes'' low-energy gravity to the brane. Related models are the RSI model[3] in which AdS is terminated above the horizon by a ''negative tension brane,'' and the model of Lykken and Randall[4] in which visible sector matter lives on a probe brane. None of these are fundamental pictures as they do not provide a microscopic dynamics for the Planck, ''negative-tension,'' and probe branes, but recent work in string theory has begun to provide descriptions of such objects. In particular Ref. 5 has given a geometrical realization of an object akin to a Planck brane, and Refs. 6, 7 have provided geometrical realizations of objects similar to ''negative-tension'' branes. At the same time, these models have been connected to renormalization group flows in four-dimensional gauge theories through the AdS/CFT correspondence.

In providing a new view of the hierarchy problem, either through large radius or other geo-

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metrical mechanisms, these scenarios suggest the exciting possibility that quantum gravity effects could be observed at scales far below the usual Planck scale, and perhaps even near the TeV scale. They also suggest the possibility of interesting new gravitational phenomena, particularly in scenarios with infinite extra dimensions (e.g., RSII) and with nontrivial curvature and horizon structure of the resulting spacetime.

Some aspects of this gravitational dynamics has been studied in Refs. 8–11. In particular, in Ref. 11 linearized gravity in the RSII scenario was studied, and both prescriptions for computing propagators and a general picture of the structure of black holes bound to the Planck brane were given. The latter were found to be pancake-like objects, whose transverse sizes are logarithmically smaller than their four-dimensional Schwarzschild radii. Cosmology of these scenarios has also been extensively studied (see, e.g., Refs. 12–15) with suggestions that they offer new approaches to the cosmological constant problem.[16–25]

Many open questions remain, however, in the RSII scenario and its variants. One set of questions centers on the four-dimensional representation of the five-dimensional dynamics. In particular, localization of gravity is not complete and in the RSII scenario there is a gapless spectrum of analogs to Kaluza–Klein modes that are weakly coupled to excitations on the brane. Therefore a four-dimensional low-energy effective field theory does not follow from the usual Kaluza–Klein reasoning, and so one challenge has been to deduce what this effective theory is. It has previously been argued[5,26,27,11,28] that the bulk dynamics can be replaced via the AdS/CFT correspondence by a conformal field theory on the brane, and this suggests an answer, namely that the effective field theory is provided by conformal field theory coupled to the visible sector solely through gravity. In this paper we amplify on this statement, clarify the role of the cutoff, which in RSII is expected to be at the AdS radius scale, and provide one entry in the map between the five-and four-dimensional descriptions by computing a linearized approximation to the four-dimensional stress tensor corresponding to an arbitrary five-dimensional matter distribution. This stress tensor is both conserved and traceless. Corresponding statements should hold for other warped compactification scenarios, using realizations of the AdS/CFT correspondence in more general warped compactifications.

Given the novelties of the gravitational dynamics, for example the above picture of black holes, one is also prodded to investigate whether this field theory has unusual properties. For example, consider the following question:[11] suppose that a particle is launched towards a black hole on the brane with zero four-dimensional impact parameter, but such that it follows a trajectory that misses the black hole through the fifth-dimension. Does this correspond in the four-dimensional perspective to matter that enters a black hole and exists the opposite side? (This question was asked by L. Susskind.) This would surely be a radical departure from usual four-dimensional effective theory!

However, standard AdS/CFT reasoning suggests a more mundane answer. In the UV/IR correspondence outlined in Ref. 29, a state deep in AdS corresponds to a state in the far infrared of the corresponding field theory. This suggests that a falling particle corresponds to a state that spreads. Indeed, using our results for the stress tensor we find that in the four-dimensional description, the falling particle corresponds to an expanding shell of CFT matter. The condition that the five-dimensional trajectory misses the black hole becomes the four-dimensional statement that the shell misses by expanding to a size larger than the black hole.

It is important to emphasize that the CFT description is an effective description, and another interesting set of questions therefore regards breakdown of the effective field theory and the question of whether strong gravitational dynamics—for example black hole formation—is observable at scales far below the four-dimensional Planck scale. We investigate the scales at which scattering experiments would be expected to encounter dynamics beyond the four-dimensional description in the three scenarios outlined, RSII, the probe brane scenario, and terminated AdS. In particular, in the latter scenario with a certain set of assumptions it appears possible to create black holes that decay into observable matter in scattering experiments in the vicinity of the TeV scale. This exciting possibility deserves more theoretical investigation; in particular through construction of concrete models with the required properties.

In an outline, in Sec. II of this paper we discuss conformal field theory as the 4D low-energy effective theory of RSII. In Sec. III we computes the linearized effective stress tensor of bulk matter, as well as solving a corresponding simpler problem of the 4D scalar profile of a five-dimensional scalar source. We also elaborate on the black hole flyby scenario mentioned above. In Sec. IV we then discuss questions of the scale of breakdown for the 4D effective theories, and of the possibility of low-energy black hole production. In Sec. V we close with conclusions.

We have been informed that in related work in progress[30] issues of black hole production and corrections to the effective theory in TeV brane scenarios are also addressed.

II. THE EFFECTIVE THEORY OF RSII

We begin with a quick review of the RSII scenario, and of its transcription into conformal field theory via the AdS/CFT correspondence[26,27,11] in which we will offer some refinements. The upshot of this discussion is that the low-energy effective field theory for the RSII scenario consists of visible 4D matter gravitationally coupled to dark matter described by a cutoff CFT. In subsequent sections we will explore consequences and extensions of this picture.

The RSII scenario is of course just an example of a much broader class of warped compactifications, which have recently been widely studied both in the context of model building, and in the context of string theory and the correspondence between renormalization group flows and supergravity geometries. While many of our comments will be made within the framework of this greatly simplified example (for which the only known microscopic construction is Ref. 5), corresponding arguments should apply to other models including those with stringy realizations. In particular in later sections we will also comment on other variants of the RSII scenario (those with a terminated AdS space or with a probe or ''TeV'' brane) and their possible stringy realizations.

We therefore begin by considering the geometry with a single ''Planck'' brane. Although our central interest is dimension $d=4$, most of the relevant formulas easily generalize and will be given in an arbitrary dimension. We assume that matter fields, denoted by ψ, live only on this Planck brane. The action is

$$S=\int d^{d+1}X\sqrt{-G}(M^{d-1}\mathcal{R}-\Lambda)+\int d^{d}x\sqrt{-\gamma}[\mathcal{L}(\gamma,\psi)-\tau] \tag{2.1}$$

where G, M, $\mathcal{R}$, and Λ are the $d+1$-dimensional metric, Planck mass, curvature scalar, and cosmological constant, respectively, γ is the induced metric on the Planck brane, $\mathcal{L}$ is the action of matter on the brane, and τ is the brane tension. The bulk AdS metric is

$$ds^2=\frac{R^2}{z^2}(dz^2+dx_d^2), \tag{2.2}$$

in $d+1$-dimensional coordinates $X=(x,z)$; here dx_d^2 is the d-dimensional Minkowski metric and the AdS radius R is given by

$$R=\sqrt{\frac{-d(d-1)M^{d-1}}{\Lambda}}. \tag{2.3}$$

The brane tension is fine tuned to the value

$$\tau=\frac{4(d-1)M^{d-1}}{R}, \tag{2.4}$$

in order to maintain a Poincaré invariant Planck brane. We may take the Planck brane to reside at an arbitrary elevation $z=\rho$.

As argued in Refs. 3, 2, 11, at a long distances compared to R, the gravitational dynamics appears d-dimensional. However, there is also a gapless spectrum of weakly-coupled bulk modes.

An obvious question is what serves as a d-dimensional low-energy effective field theory describing the dynamics. Within string theory, an answer to this is provided by the conjectured AdS/CFT correspondence.[26,27,11]

To see this, recall that the AdS/CFT correspondence equates the $d+1$-dimensional bulk gravity (or more precisely, string theory) functional integral to a generating function in the CFT. A regulator is provided by excluding the AdS volume outside $z=\rho$. Suppose that we put the fluctuating metric in a gauge such that near this boundary,

$$ds^2=\frac{R^2}{z^2}[dz^2+g_{\mu\nu}(z,x)dx^\mu dx^\nu]. \tag{2.5}$$

The induced metric γ on the boundary $z=\rho$ is thus

$$ds_d^2=\frac{R^2}{\rho^2}g_{\mu\nu}(\rho,x)dx^\mu dx^\nu\equiv\gamma_{\mu\nu}dx^\mu dx^\nu. \tag{2.6}$$

Define the functional integral over bulk metrics G for fixed boundary metric γ as

$$Z[\gamma,\rho]=\int_\gamma \mathcal{D}G e^{i\int d^{d+1}X\sqrt{-G}(M^{d-1}\mathcal{R}-\Lambda)+2iM^{d-1}\int d^dx\sqrt{-\gamma}K}, \tag{2.7}$$

where K is the extrinsic curvature of the boundary. The AdS/CFT correspondence then states that for small fluctuations about the flat boundary geometry, $g_{\mu\nu}=\eta_{\mu\nu}+h_{\mu\nu}$,

$$\lim_{\rho\to 0} e^{-iS_{\rm grav}[\gamma]}Z[\gamma,\rho]=\langle e^{i\int h_{\mu\nu}T^{\mu\nu}}\rangle_{\rm CFT}. \tag{2.8}$$

Here $S_{\rm grav}$ is a counterterm action formed purely from the induced metric γ,[31,32] in the case $d=4$

$$S_{\rm grav}=\int d^4x\sqrt{-\gamma}\left[\frac{6M^3}{R}+\frac{RM^3}{2}\mathcal{R}(\gamma)-2M^3R^3\log(\rho)\mathcal{R}_2(\gamma)\right], \tag{2.9}$$

where

$$\mathcal{R}_2=-\tfrac{1}{8}\mathcal{R}_{\mu\nu}\mathcal{R}^{\mu\nu}+\tfrac{1}{24}\mathcal{R}^2. \tag{2.10}$$

While the AdS/CFT correspondence was originally stated in terms of small fluctuations, a natural assumption is that it extends to more general boundary geometries. We therefore assume that the CFT generating functional can be written as a functional integral over the CFT degrees of freedom, which we collectively denote χ, in the background metric $g_{\mu\nu}$, and that the correspondence thus becomes

$$\lim_{\rho\to 0} e^{-iS_{\rm grav}[\gamma]}Z[\gamma,\rho]=\int \mathcal{D}\chi\, e^{i\int d^dx\sqrt{-g}\mathcal{L}_{\rm CFT}(g_{\mu\nu},\chi)}. \tag{2.11}$$

Following the ideas of the UV/IR correspondence,[29] we connect this with the RS scenario by extending the conjecture to a statement with a finite cutoff, and assume that

$$e^{-iS_{\rm grav}[\gamma]}Z[\gamma,\rho]=\int [\mathcal{D}\chi]_\rho e^{i\int d^dx\sqrt{-g}\mathcal{L}_{\rm CFT}(g_{\mu\nu},\chi)}, \tag{2.12}$$

where on the RHS ρ provides the cutoff scale for the CFT. While a precise description of this cutoff in the language of the CFT is not known, for the sake of intuition one may imagine that it is for example given by only considering fluctuations on scales Δx such that

$$g_{\mu\nu}\Delta x^\mu \Delta x^\nu > \rho^2. \tag{2.13}$$

In particular, notice that since the only dependence of the CFT on the scale of the metric is through the cutoff, this implies

$$\int [\mathcal{D}\chi]_\rho e^{i\int d^d x\sqrt{-g}\mathcal{L}_{\rm CFT}(g_{\mu\nu},\chi)} = \int [\mathcal{D}\chi]_R e^{i\int d^d x\sqrt{-\gamma}\mathcal{L}_{\rm CFT}(\gamma_{\mu\nu},\chi)}, \tag{2.14}$$

where on the RHS the cutoff is thought of as restricting to fluctuations with

$$\gamma_{\mu\nu}\Delta x^\mu \Delta x^\nu > R^2. \tag{2.15}$$

From (2.12) and (2.14) we therefore see that the integral over the bulk modes can be replaced by a correlator in the CFT, as originally proposed in Refs. 26, 27, 11, with a cutoff given by R. Specifically, d-dimensional dynamics is summarized by a functional integral of the form

$$\int [\mathcal{D}\gamma\,\mathcal{D}\psi\,\mathcal{D}\chi]_R e^{i\int d^d x\sqrt{-\gamma}[(1/2)\mathcal{L}(\gamma,\psi)+\mathcal{L}_{\rm CFT}(\gamma,\chi)+\mathcal{L}_{\rm grav}(\gamma)-\tau]}(\cdots). \tag{2.16}$$

For consistency with the cutoff (2.15) the other modes also presumably should have a corresponding cutoff, as indicated. One consistency check on this approach is cancellation of the brane tension τ by the corresponding term in $S_{\rm grav}$, using (2.4). This indicates that the low-energy effective field theory for the system, up to the scale determined by R, is the theory of brane-matter gravitationally coupled to ''dark'' matter described by the CFT. The d-dimensional Planck mass follows from the d-dimensional version of (2.9), and is given by

$$M_d^{d-2} = \frac{RM^{d-1}}{d-2}. \tag{2.17}$$

III. EFFECTIVE STRESS TENSOR OF BULK MATTER

We now investigate some of the consequences of the above identification of the CFT as the low-energy effective field theory for the RSII scenario. In particular, we start by giving an entry in the bulk to boundary dictionary, by computing a linearized approximation to the CFT stress tensor corresponding to a perturbation in the bulk. We then investigate the particular case of a particle freely falling into the bulk.

Using this calculation, we discuss a test of the AdS/CFT correspondence and of our effective description of RSII: suppose that we shoot a particle towards a black hole with a zero 4D impact parameter, but such that it will miss the black hole through the z direction. How does a 4D observer understand the failure of the black hole to absorb the particle?

A. General results

In this subsection we turn to the problem of deriving the d-dimensional brane stress tensor that corresponds to a general $d+1$-dimensional bulk matter distribution. In general this is a difficult problem, requiring a solution of the bulk Einstein equations, so we will only give a linear treatment.

The basic strategy is as follows. Reference 11 computes the linearized bulk gravitational field of a general matter perturbation. This in particular gives the linearized metric and therefore Einstein tensor induced on the brane. We can then read off the matter stress tensor from the right hand side of the d-dimensional Einstein equations along the brane.

Although the resulting stress tensor has a number of special properties, we have not yet found a particularly illuminating expression for it. However, in the next subsection we specialize to the case of a particle falling into the bulk; in the long distance approximation the corresponding stress tensor simplifies substantially.

In studying gravitational perturbations it proves convenient to introduce the proper ''height'' coordinate y, given by

$$z = \mathrm{Re}^{y/R}, \tag{3.1}$$

in terms of which the linearized metric takes the form

$$ds^2 = dy^2 + e^{-2y/R}(\eta_{\mu\nu} + h_{\mu\nu})dx^\mu dx^\nu. \tag{3.2}$$

Equations (3.20), (3.24), and (3.26) of Ref. 11 then give the linearized bulk Einstein equations in terms of the metric perturbation $\overline{h}_{\mu\nu} = h_{\mu\nu} - \frac{1}{2}h\eta_{\mu\nu}$ as

$$\partial_y(e^{-2y/R}\partial y h) = \frac{1}{(d-1)M^{d-1}}[T^\mu_\mu - (d-2)e^{-2y/R}T^y_y], \tag{3.3}$$

$$\partial_y \partial^\nu h_{\mu\nu} = \partial_y \partial_\mu h + \frac{T^y_\mu}{M^{d-1}}, \tag{3.4}$$

and

$$\Box\overline{h}_{\mu\nu} = \frac{\eta_{\mu\nu}}{2}e^{yd/R}\partial_y(e^{-yd/R}\partial_y h) + e^{2y/R}(-\eta_{\mu\nu}\partial^\lambda\partial^\sigma\overline{h}_{\lambda\sigma} + \partial^\lambda\partial_\mu\overline{h}_{\nu\lambda} + \partial^\lambda\partial_\nu\overline{h}_{\mu\lambda}) - \frac{e^{2y/R}}{M^{d-1}}T_{\mu\nu}. \tag{3.5}$$

The right hand side of (3.5) is determined by the stress tensor and the solutions of Eqs. (3.3), (3.4). This equation can then be solved for $h_{\mu\nu}$ using the scalar Neumann Green function Δ_{d+1}, satisfying

$$\Box\Delta_{d+1}(X,X') = \frac{\delta^{d+1}(X-X')}{\sqrt{-G}},$$

$$\partial_y\Delta_{d+1}(X,X')|_{y=0} = 0, \tag{3.6}$$

and which was derived in Ref. 11. In the present situation we need the retarded propagator rather than the Feynman propagator; the relation between these and approximate expressions for them are given in the Appendix. The resulting expression for the metric has three terms arising from the three lines of (3.5). However, the second term is inessential as a short calculation shows it to be pure gauge on the brane. Therefore its contribution drops when we compute the Einstein tensor on the brane.

One must also specify boundary conditions at the brane; in the case of a surface stress tensor,

$$T^{\mathrm{brane}}_{\mu\nu} = S_{\mu\nu}(x)\delta(y), \quad T^{\mathrm{brane}}_{yy} = T^{\mathrm{brane}}_{y\mu} = 0, \tag{3.7}$$

these become

$$\partial_y(h_{\mu\nu} - \eta_{\mu\nu}h)_{|y=0} = -\frac{S_{\mu\nu}(x)}{2M^{d-1}}. \tag{3.8}$$

In order to simplify the resulting expression for the metric, it is useful to rewrite the scalar Green's function in terms of a new function F as

$$\Delta_{d+1}(y,x;y',x')=e^{(d-2)y'/R}\partial_{y'}[e^{-(d-2)y'/R}F_{y'}(y;x-x')]. \tag{3.9}$$

One nice property of the redefinition is immediate: one readily checks that

$$\int_0^\infty dy'\, e^{(2-d)y'/R}\Delta_{d+1}(X,X')=-F_0(y;x-x') \tag{3.10}$$

satisfies the equation for the d-dimensional Green's function, and so

$$F_0(y;x-x')=-\Delta_d(x,x'). \tag{3.11}$$

Using this and integrating by parts gives the contribution to $\overline{h}_{\mu\nu}$ from the first line in (3.5) as

$$\overline{h}^{(1)}_{\mu\nu}(x,y)=\frac{\eta_{\mu\nu}}{2(d-1)M^{d-1}}\int dV'\,\partial_{y'}F_{y'}(y;x-x')[e^{2y/R}T^\mu_\mu(X')-(d-2)T^y_y(X')]. \tag{3.12}$$

Equation (3.12) combines with the terms induced by the stress tensor and the surface stress (3.7) to give a complete expression of the form

$$\begin{aligned}\overline{h}_{\mu\nu}=&-\frac{1}{M^{d-1}}\int dV'\,e^{dy'/R}\partial_{y'}[e^{-(d-2)y'/R}F_{y'}(y;x-x')]T_{\mu\nu}(X')\\&+\frac{\eta_{\mu\nu}}{2(d-1)M^{d-1}}\int dV'\,\partial_{y'}F_{y'}(y;x-x')[e^{2y/R}T^\mu_\mu(X')-(d-2)T^y_y(X')]+\overline{h}^S_{\mu\nu}+\overline{h}^{\text{gauge}}_{\mu\nu}.\end{aligned} \tag{3.13}$$

Here $\overline{h}^{\text{gauge}}_{\mu\nu}$ is the piece that is pure gauge on the brane, mentioned above, and $\overline{h}^S_{\mu\nu}$ is the contribution due to the surface stress (we will see an example of this shortly).

For simplicity consider a purely bulk distribution ($S_{\mu\nu}=0$). The four-dimensional effective stress tensor is readily computed from (3.13) via Einstein's equations,

$$T^{\text{eff}}_{\mu\nu}=2M_d^{d-2(d)}\mathcal{G}^\mu_\nu=-\frac{RM^{d-1}}{d-2}(\partial^2\overline{h}_{\mu\nu}+\eta_{\mu\nu}\partial^\alpha\partial^\beta\overline{h}_{\alpha\beta}-\partial_\mu\partial^\alpha\overline{h}_{\alpha\nu}-\partial_\nu\partial^\alpha\overline{h}_{\alpha\mu})\big|_{y=0}, \tag{3.14}$$

with $\overline{h}_{\mu\nu}$ given by (3.13). The contribution of $\overline{h}^{\text{gauge}}_{\mu\nu}$ drops out.

One may expand out the expression (3.14) to write it explicitly in terms of the bulk stress tensor $T_{\mu\nu}$:

$$\begin{aligned}T^{\text{eff}}_{\mu\nu}=\frac{R}{d-2}\int dV'\Big\{&e^{dy'/R}\partial_{y'}[e^{-(d-2)y'/R}F_{y'}(0;x-x')](\partial^2T_{\mu\nu}+\eta_{\mu\nu}\partial^\alpha\partial^\beta T_{\alpha\beta}-\partial^\alpha\partial_\mu T_{\alpha\nu}\\&-\partial^\alpha\partial_\nu T_{\alpha\mu})+\frac{1}{d-1}\partial_{y'}F_{y'}(0;x-x')(\partial_\mu\partial_\nu-\eta_{\mu\nu}\partial^2)[e^{2'/R}T^\mu_\mu-(d-2)T^y_y]\Big\}.\end{aligned} \tag{3.15}$$

Note that $T^{\text{eff}}_{\mu\nu}$ satisfies two important properties. First, from its construction and the Bianchi identities, it is conserved:

$$\partial^\mu T^{\text{eff}}_{\mu\nu}=0. \tag{3.16}$$

Second, one may readily verify that it is traceless,

$$\eta^{\mu\nu}T^{\rm eff}_{\mu\nu}=0, \tag{3.17}$$

which accords nicely with its interpretation as arising from a conformal field theory on the brane. Indeed, this easily follows from the (yy) Einstein equation, which states (cf. Ref. 11, Eq. (3.14)]

$${}^{(d)}\mathcal{R}+\frac{(d-1)}{R}\partial_y h\,\epsilon(y)=-\frac{T^y_y}{M^{d-1}}, \tag{3.18}$$

where $\epsilon(y)$ is a step function. On the brane $\partial_y h$ and T^y_y vanish [the former by (3.8)], implying ${}^{(d)}\mathcal{R}(y=0)=0$, and thus $T^{\rm eff}=0$.

Note that in the above discussion we have said nothing about bending of the brane, which was described in Refs. 10, 11. The reason for this is that we are interested in the metric on the brane, and for this it is best to work in a gauge where the brane is straight. In Ref. 11 the resulting metric was computed by first working in the bent gauge, and then transforming back, but an equivalent result is found by working directly in the straight gauge. (For purposes of measurements on the brane, the apparent breakdown of the linearized approximation at $y\to\infty$ may be ignored; for another treatment of these matters see Ref. 33.)

B. Matter on the brane

In order to illustrate this equivalence—and because the result will be used in the next subsection—we will compute the linearized metric and effective stress tensor due to matter on the brane in this approach. Specifically, suppose that there is a surface stress of the form (3.7), but that otherwise $T_{IJ}=0$. The field equations (3.3)–(3.5) should then be solved subject to the boundary conditions (3.8). By tracing the latter can be rewritten in terms of $\overline{h}$, and take the form

$$\partial_y\overline{h}_{\mu\nu}|_{y=0}=-\frac{1}{2M^{d-1}}\left[S_{\mu\nu}-\frac{\eta_{\mu\nu}}{2(d-1)}S\right]. \tag{3.19}$$

By Green's theorem these give a contribution

$$\overline{h}^S_{\mu\nu}(X)=-\frac{1}{2M^{d-1}}\int d^dx'\,\Delta_{d+1}(X;0,x')\left[S_{\mu\nu}(x')-\frac{\eta_{\mu\nu}}{2(d-1)}S(x')\right] \tag{3.20}$$

to the metric. As above, the second term on the RHS of (3.5) is pure gauge, and the third term vanishes, so the remaining contribution comes from the first term. The trace equation (3.3) and the boundary condition (3.8) imply

$$\partial_y h=\frac{e^{2y/R}}{2(d-1)M^{d-1}}S, \tag{3.21}$$

which gives a contribution

$$\overline{h}^{(1)}_{\mu\nu}=\frac{\eta_{\mu\nu}(2-d)}{4(d-1)RM^{d-1}}\int d^dx'\,S(x')\int dy'\,e^{(2-d)y/R}\Delta_{d+1}(X,X'). \tag{3.22}$$

The integral over y' is eliminated by using the identities (3.10) and (3.11), and the combined expressions (3.20) and (3.22) yield

$$\overline{h}_{\mu\nu}(x)=-\frac{1}{2M^{d-1}}\int d^dx'\left\{\Delta_{d+1}(x,0;x',0)S_{\mu\nu}(x')-\eta_{\mu\nu}\left[\Delta_{d+1}(x,0;x',0)-\frac{(d-2)}{R}\Delta_d(x,x')\right]\frac{S^\lambda_\lambda(x')}{2(d-1)}\right\}, \tag{3.23}$$

in agreement with Ref. 11. In particular, this expression may be evaluated for a stress tensor corresponding to a point mass at rest on the brane at $\mathbf{x}=0$,

$$T_{tt}=2m\,\delta^{d-1}(x)\,\delta(y). \tag{3.24}$$

[The extra factor of two is present because of the orbifold boundary conditions, and compensates the 1/2 in (2.16).] Using the long-distance expansion of the propagator,[11]

$$\Delta_{d+1}(x,0;x',0)=\frac{d-2}{R}\,\Delta_d(x,x')\left[1+\left(\frac{R^{d-2}}{r^{d-2}}\right)\right], \tag{3.25}$$

this gives the $d=4$ expression

$$\overline{h}_{tt}=\frac{m}{2\pi RM^3 r}\left[1+\mathcal{O}\left(\frac{R^2}{r^2}\right)\right],\quad \overline{h}_{ij}=\mathcal{O}\left(\frac{mR}{M^3r^3}\right). \tag{3.26}$$

C. The falling particle

The above expression (3.15) for the stress tensor appears rather complicated, but simplifies significantly in the long-distance limit. To illustrate this, we compute the effective stress tensor of a particle falling into the bulk. (The corresponding approximate metric has also been computed by Gregory, Rubakov, and Sibiryakov in Ref. 34.) This case will also apply to our later discussion of black hole flybys; by performing a boost along the brane we get a trajectory that can sail behind a black hole through the extra dimension.

Concretely, consider a particle of mass m that is stuck to the brane at $\mathbf{x}=0$ until time $t=0$ and then released and allowed to freely fall into the bulk. The trajectory for $t>0$ is easily seen to be given by the equation

$$z^2-t^2=R^2. \tag{3.27}$$

For $t<0$ the only nonzero component of the stress tensor is given by (3.24). For $t>0$ the stress tensor is given by the general formula

$$T_{IJ}=m\,\frac{dX_I}{d\tau}\,\frac{dX_J}{dt}\,\frac{\delta^{d-1}(x-x(t))\,\delta(y-y(t))}{\sqrt{-G}}, \tag{3.28}$$

which in the present case gives nonvanishing components,

$$T_{tt}=me^{(d-2)y/R}\,\delta^{d-1}(\mathbf{x})\,\delta(y-y(t)), \tag{3.29}$$

$$T_{yy}=m\,\frac{t^2}{R^2}\,e^{(d-2)y/R}\,\delta^{d-1}(\mathbf{x})\,\delta(y-y(t)), \tag{3.30}$$

and

$$T_{ty}=-m\,\frac{t}{R}\,e^{(d-2)y/R}\,\delta^{d-1}(\mathbf{x})\,\delta(y-y(t)). \tag{3.31}$$

Therefore the contribution to the metric from the trajectory for $t<0$ is a special case of the general surface-stress result of the preceding subsection, (3.23), with

$$S_{tt}=2m\,\delta^{d-1}(x)\,\theta(-t),\quad S_{\mu i}=0. \tag{3.32}$$

The contribution to the metric from the second half of the trajectory is given by our formula (3.13). Specifically, rewriting the $t>0$ stress tensor as

$$T_{IJ}=\mathcal{S}_{IJ}(t,y)\,\delta(y-y(t)), \tag{3.33}$$

we find

$$\overline{h^{>}_{\mu\nu}}(x)=-\frac{1}{M^{d-1}}\int_{t'>0}d^dx'\left\{\partial_y[e^{-(d-2)y/R}F_y(0;x-x')]\mathcal{S}_{\mu\nu}(x',y)\right.$$
$$\left.-\frac{\eta_{\mu\nu}}{2(d-1)}e^{-(d-2)y/R}\partial_yF[\mathcal{S}^\mu_\mu-(d-2)e^{-2y/R}\mathcal{S}^y_y]\right\}\Bigg|_{y=y(t)}+\overline{h}^{\text{gauge}}_{\mu\nu}. \tag{3.34}$$

The expression for the effective stress tensor follows directly from computing the Einstein tensor (3.14) from these expressions for the linearized metric. In order to gain some intuition for this expression, consider the approximation of distances and times much greater than the AdS scale R, which we've seen is the cutoff for the effective theory:

$$x^2-t^2\gg R^2, \tag{3.35}$$

In this limit the Green's function simplifies dramatically (see the Appendix),

$$F_y(0;x-x')\simeq\frac{1}{2\pi}\,\delta(z^2+(x-x')^2)\,\theta(t-t'), \tag{3.36}$$

and the trajectory (3.27) becomes

$$z=\mathrm{Re}^{y/R}\simeq t. \tag{3.37}$$

Defining $r=|x|$, in $d=4$ the approximate metric is then

$$\overline{h}_{\mu\nu}\simeq\frac{m}{2\pi M^3Rr}\,\delta^t_\mu\delta^t_\nu, \tag{3.38}$$

for $r>t$, and

$$\overline{h}_{\mu\nu}\simeq\frac{m}{2\pi M^3R}\left[\left(\frac{3}{2t}-\frac{\mathbf{x}^2}{2t^3}\right)\delta^t_\mu\delta^t_\nu+\frac{t^2-\mathbf{x}^2}{4t^3}\,\eta_{\mu\nu}\right], \tag{3.39}$$

for $r<t$, as in Ref. 34. A straightforward computation shows that the Einstein tensor of both of these metrics vanishes! Thus the effective stress tensor is concentrated on the surface where they match, $r=t$. This stress tensor is

$$T^{\text{eff}}_{\mu\nu}\simeq\frac{m}{4\pi t^2}\,\delta(t-r)u^\mu u^\nu, \tag{3.40}$$

where $u^\mu=x^\mu/t$.

The effective stress tensor of the conformal field theory configuration describing a falling particle is thus concentrated on a thin shell of radius r which expands outward with time, $r=t$. We can estimate the thickness of the shell by investigating the size of the leading corrections in the limit (3.35). One readily sees that the metric is corrected at order $R^2/t^2,R^2/r^2$, both due to corrections to the trajectory and to the Green's function. This suggests that the thickness of the shell of CFT matter is the expected $\mathcal{O}(R)$, the cutoff length scale.

This spreading behavior appears to be quite generic, as one might expect from the IR/UV duality of the AdS/CFT correspondence. Another example of this behavior is provided by a falling charged particle coupled to a bulk gauge field, as investigated in Ref. 35. Indeed, an even simpler example is provided by a falling particle coupled to a bulk scalar field. Specifically, consider a Lagrangian,

$$S=-\int dV\frac{1}{2}(\nabla\phi)^2-q\int d\tau\,\phi(X(\tau)), \tag{3.41}$$

with a coupling of a bulk scalar field ϕ to a particle of scalar charge q falling along a trajectory $X(\tau)$. This determines the scalar field,

$$\phi(X)=q\int d\tau\,\Delta_{d+1}(X,X(\tau)). \tag{3.42}$$

If we assume that the particle again follows the trajectory (3.27) and works at large distances as compared to R and with $d=4$, then the field at $y=0$ takes the approximate form

$$\phi(x,t)\simeq-\frac{q}{2\pi R}\left[\frac{1}{r}\,\theta(r-t)+\frac{4R^2t}{(r^2-t^2)^2}\,\theta(t-r)\right]\left[1+\mathcal{O}\left(\frac{R}{r}\right)^2\right]. \tag{3.43}$$

If we compute the effective source, $J=\Box_4\phi$, we find it vanishes except at $r=t$. Again, subleading $\mathcal{O}(R)$ corrections appear to smooth this into a shell of thickness R.

Note that similar behavior was found by Horowitz and Itzhaki,[36] who investigated the CFT stress tensor corresponding to a particle moving geodesically in the full, infinite AdS. This work also found a shell expanding outward at the speed of light. Indeed, the two calculations are directly related in the infrared limit, as discussed in Appendix B.

This behavior can also be understood directly in terms of the CFT using an argument of Coleman and Smarr,[37] which shows that a stress tensor that is conserved, traceless, and has positive energy density will be localized on the light cone. The basic idea for the proof is to show that the average squared energy radius.

$$\overline{r}(t)^2=\frac{\int d^3x\,r^2T_{00}}{\int d^3x\,T_{00}}, \tag{3.44}$$

satisfies

$$\frac{d^2\overline{r^2}}{dt^2}=2, \tag{3.45}$$

from which it immediately follows that a configuration initially localized at a point will expand on the light cone. Reference 36 argues that the argument extends even to the quantum case, where the energy density may be negative, as long as the total energy is positive.

These results neglect the backreaction of gravity on the outgoing shell. It would be interesting to understand what dynamics results when strong self gravitation of the shell is included.

Vanishing of the Einstein tensor for the metric (3.39) at first sight leads to another puzzle. Specifically, suppose we consider a ''bounce'' trajectory, where the particle follows the trajectory (3.27) for all time. The calculation of the metric above is modified by extending to the trajectory for $t<0$, but still yields a stress tensor that vanishes everywhere. This contradicts our expectation of a shell that collapses and then reexpands. However, note that this computation is not complete. The z coordinates only cover the region outside the AdS horizon, and thus this calculation would miss the contribution of the piece of the trajectory behind the past horizon. If this is not included, energy-momentum conservation is violated at the horizon, and consequently gravity cannot be consistently coupled. A correct calculation includes this piece, but also requires more information about the structure of the Green's function. Specifically, one needs to know what boundary conditions it obeys in the far past. In order to make predictions in the RSII scenario, one needs to understand the physics determining the boundary conditions at the past horizon. Correspondingly, in CFT language on needs to know in what state the CFT sector began.

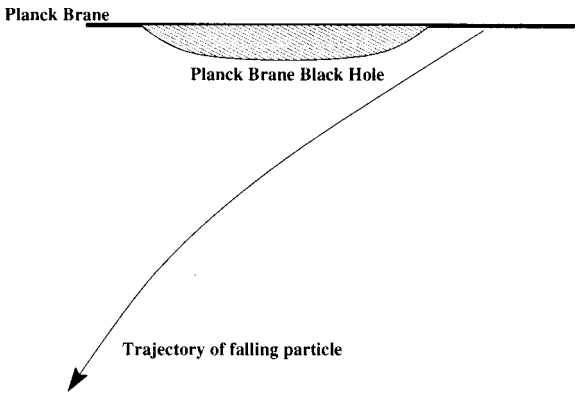

FIG. 1. A particle trajectory that misses a black hole on the brane because of its motion in the extra dimension.

D. Black hole flybys

We now have the necessary tools to discuss particles flying past black holes through the bulk; for simplicity we discuss the four-dimensional case. Specifically, suppose that there is a black hole of mass m located at $\mathbf{x}=0$ and that a particle is shot at it with zero four-dimensional impact parameter, but is allowed to fall in z long enough that it misses the black hole by passing it in the z direction (see Fig. 1). How does a four-dimensional observer describe such an experiment, and in particular does one see radical departures from usual gravitational dynamics, such as matter entering and then escaping a 4D event horizon?

The answer to the latter question is, of course, no. Indeed, a black hole with mass and 4D Schwarzschild radius m has a horizon extending to $z_h \sim m$ in the bulk picture. In order for the particle to miss the black hole, the particle must have $z \gg m$ when $\mathbf{x}=0$. As we have seen above, in the CFT description the particle corresponds to a shell of CFT matter. If it has reached $z \gg m$ by the time it reaches the black hole at $\mathbf{x}=0$, then the shell has expanded to size $r \gg m$ by the time it has reached the black hole, and is continuing to expand outward. No novel physics need be invoked to explain why the shell is not absorbed by the black hole. (Note, however, that a small piece of the shell may be absorbed by the black hole; a quantum treatment of the bulk should yield a corresponding result.) The process has a perfectly adequate four-dimensional effective description in terms of the matter conformal field theory coupled to four-dimensional gravity.

IV. BREAKDOWN OF EFT; CUTOFFS, STRONG GRAVITY, AND BLACK HOLE PRODUCTION

In Sec. II we argued that at low energies the RS scenario is equivalent to coupling ordinary matter to a hidden CFT. In Sec. III we provided illustrations of this statement. An obvious question regards the limitations of this description. At what scale does it fail? Is there any practical advantage or consequence of the five-dimensional description? And what conclusions can one draw about strong gravitational phenomena, such as the production of black holes in high-energy scattering?

In this section we will first consider the scenario with a single Planck brane, and then comment on extensions of the discussion to scenarios with an added probe or ''TeV'' brane or with AdS terminated by a brane-like object are large z (like the ''negative tension'' brane proposal of Ref. 3).

A. Scattering on the Planck brane

The four-dimensional effective action for the scenario with a single Planck brane is given in (2.16). Recall that the fundamental parameters determine the 4D Planck mass by the relation (2.17). We would like to understand what this scenario predicts for high-energy scattering.

The simplest assumption (if one is not trying to solve the hierarchy problem) is that the five-dimensional Planck scale and inverse AdS radius, and hence the four-dimensional Planck scale, are all comparable:

$$M \sim 1/R \approx M_4 . \tag{4.1}$$

In that case all new physics is clearly at the Planck scale. How much can this statement be relaxed? One would expect observable deviations in microgravity experiments—as in the scenario of Ref. 1—for $R \sim 1$ nm. This puts a lower bound of $M \gtrsim 10^8$ GeV on the five-dimensional Planck scale.

Consider now high-energy scattering of particles confined to the brane. From the bulk perspective, we see that at distances $\ll R$ the dynamics is effectively five-dimensional. This is mirrored in the four-dimensional description of (2.16); energies above $1/R$ are past the cutoff and the cutoff CFT description is incomplete.

Does this mean that we can see what a 4D observer would interpret as strong gravitational phenomena at energies just above $1/R$? Clearly not, except when the parameters satisfy $1/R \sim M$, in which case we are at Planckian 4D energies anyway. Consider for example black hole production. There are two types of black holes that one might produce. The first type is the AdS/Schwarzschild black hole, which moves freely in the bulk, and in general will fall towards the AdS horizon once produced. The threshold for producing such black holes is the 5D Planck energy $M \gtrsim 10^8$ GeV. The second type of black hole is bound to the brane, as described in Refs. 38, 11. The horizon radius of such a black hole is $r_h \sim m/M_4^2$; this should be larger than the 5D Planck length which implies $m > RM^2$. Since $RM \gtrsim 1$, the threshold is again at M or above.

From this discussion we see that scattering pushes beyond the cutoff scale at the threshold $1/R$ and in the bulk perspective begins to explore the extra dimension. While this may have visible consequences through the production of the Kaluza–Klein modes, strong gravitational dynamics such as black hole production has a much higher threshold of M, which in the most ''optimistic'' scenario of $M \sim 10^8$ GeV is still a long ways off.

B. Scattering on a probe brane

The preceding Planck-brane scenario is not favored from the viewpoint of low-energy phenomenology in any case, given the expected relation (4.1) between scales. Scenarios which try to generate the hierarchy via the exponential warp factor show more promise. Consider first the probe brane scenario of Ref. 4. Here 4D matter is taken to reside on a ''TeV'' brane at an elevation $z = \rho_T$; the Planck brane is again at $z = \rho$. This brane must be stabilized by a mechanism such as in Refs. 39, 40. The 4D Planck mass is again given by (2.17), but matter on the TeV brane has its energy redshifted by ρ/ρ_T relative to the Planck brane. If $\rho/\rho_T \sim \text{TeV}/M_4$, this gives a mechanism to generate TeV scale effective masses from particles with fundamentally Planckian masses.

To elaborate on these comments, note that in giving a four-dimensional description of the physics it is necessary to specify a reference frame at a definite value of z in terms of which four-dimensional energies are measured. The natural frame to use is that of the Planck brane, as this is where the 4D graviton bound state is supported. Then if we consider an energy E_{prop} as measured by an observer at another value of z, it will be redshifted so that the energy in the frame of the Planck brane is $E = \rho E_{\text{prop}}/z$. In particular, a particle of mass m at rest in the frame at z will have an energy $m\rho/z$ relative to the Planck brane, and that will be interpreted as its four-dimensional mass.

The Lagrangian in this scenario is expected to take the form

$$S = \int d^{d+1}X \sqrt{-G}(M^{d-1}\mathcal{R} - \Lambda + \mathcal{L}_{\text{stab}}) + \int d^d x [\sqrt{-\gamma(x,\rho_T)}\mathcal{L}(\gamma(x,\rho_T),\psi) - \sqrt{-\gamma(x,\rho)}\tau]. \tag{4.2}$$

Here we denote by $\mathcal{L}_{\rm stab}$ the Lagrangian of the stabilizing fields; we assume that beyond stabilizing the brane they do not qualitatively affect our conclusions.

What is the CFT description of this scenario? Here we encounter subtleties beyond the derivation of (2.16). Specifically, the action depends on the metric at $z=\rho_T$. In attempting to relate the bulk functional integral to the boundary CFT we have to confront the nontrivial z-dependence of γ, and in particular give a CFT prescription for computing the metric in the bulk. We have not yet found a convincing prescription to derive such off-shell information from the AdS/CFT correspondence.

In the absence of such a prescription we will consider two approaches to this problem. The first is to work with long-wavelength excitations of the theory such that the simple scaling approximation,

$$\gamma(x,\rho)\simeq\frac{\rho_T^2}{\rho^2}\,\gamma(x,\rho_T), \tag{4.3}$$

holds. We use this equation to replace $\gamma(x,\rho_T)$ by $\gamma(x,\rho)$ in the Lagrangian for matter on the TeV brane. This effectively rescales parameters of dimension δ in that Lagrangian by a factor $(\rho/\rho_T)^\delta$ (cf. Ref. 4). Rewriting the functional integral as in Sec. II produces a 4D effective action analogous to (2.16) in the Planck brane scenario,

$$S_{\rm TeV}=\int d^4x\sqrt{-\gamma}[\mathcal{L}(\gamma,\psi,m\rho/\rho_T)+\mathcal{L}_{\rm CFT}(\gamma,\chi)+\mathcal{L}_{\rm grav}(\gamma)-\tau]. \tag{4.4}$$

Here we have explicitly indicated the rescaling of a typical mass parameter in the matter Lagrangian. Again $\mathcal{L}_{\rm CFT}(\chi)$ represents the Lagrangian of ''dark'' CFT matter, and $\mathcal{L}_{\rm grav}$, given by (2.9), is the gravitational action.

The simple approximation (4.3) fails at short wavelengths, where the z-dependence becomes nontrivial. This effect can be estimated from the long-distance expansion of the propagator,[11]

$$\Delta(x,z;x',z')\sim\frac{1}{Rr^{d-2}}\left[1+\frac{R^{d-2}}{r^{d-2}}+\frac{z^d}{r^d}+\frac{z^{2d}}{r^{2d}}\frac{r^{d-2}}{R^{d-2}}\right]\left[1+\mathcal{O}\left(\frac{z^2}{r^2},\frac{R^2}{r^2}\right)\right]. \tag{4.5}$$

In $d=4$, the correction due to the last term becomes large at distances,

$$r\sim\left(\frac{\rho_T}{\rho}\right)^{4/3}R, \tag{4.6}$$

or at about 10 Fermi for $\rho/\rho_T\sim{\rm TeV}/M$.

In order to understand the origin of corrections at this scale, first let us recall a similar phenomenon in the large scale compactification scenario of Ref. 1. If one for example considers such a compactification with two extra dimensions of size $\mathcal{O}(mm)$, gravitational experiments performed at shorter scales reveal the six-dimensional nature of spacetime: the part of the four-dimensional effective Lagrangian describing the gravitational sector breaks down. One way of understanding this is to note that sources with shorter wavelengths than a millimeter will generically have coupling to the Kaluza–Klein modes that is comparable to the coupling to the gravitational zero mode; summing over these modes produces the six-dimensional gravitational field. While the gravitational part of the 4D effective action breaks down, nonetheless the gauge part of the effective action remains four-dimensional up to scales of order a TeV where gravity itself becomes strongly coupled.

A similar phenomena occurs here. At scales given by (4.6), the couplings of the TeV brane matter to the continuum analogs of the Kaluza–Klein states become comparable to the coupling to the four-dimensional graviton. This means that in the gravitational sector the 4D effective theory

fails, but of course the gauge part of the theory remains four-dimensional up to the TeV scale. The stress tensor of the TeV brane matter acts as the source for these couplings to the Kaluza–Klein modes.

Corresponding statements can be made in the CFT, and will tell us the form of the corrections to the action (4.4) that are responsible for its failure as a 4D effective description. In particular, we expect that corresponding to the couplings to the KK modes, a term is induced in (4.4) in which there is a direct coupling of the stress tensor of the TeV brane matter to the stress tensor of the CFT, and by scaling the coefficient of this should include a factor of $(\rho_T/\rho)^4$. Such terms are responsible for the breakdown of the gravitational part of the 4D effective theory.

A second approach would be to use the holographic renormalization group[41] to evolve the Lagrangian from the Planck brane to the TeV brane. We would expect this to produce similar results, namely a gravitationally coupled CFT with a cutoff scale $\sim$10 MeV. We expect the $T_\chi T_\psi$ terms described above to be present in the Lagrangian at the Planck scale, and then to be rescaled by the renormalization group flow. A better understanding along these lines of the relationship between operators at different z would also clearly be illuminating for our fundamental understanding of holography in the AdS/CFT correspondence.

As in the scenario of Ref. 1, there is a distinction between the scale at which the 5D nature of gravity becomes important and the scale at which gravity becomes strongly coupled. A particularly interesting question is when do we expect to be able to manufacture configurations which would manifest signatures for black holes that we as four-dimensional observers could see?

Within the context of the TeV brane scenario, there are again two kinds of black hole solutions known. The first is the AdS-Schwarzschild black hole. The minimum energy to create these should be $\mathcal{O}(M)$. A collision of TeV brane matter with a proper energy of this magnitude is a collision at the TeV energy scale as measured with respect to the four-dimensional observer. However, it appears that such black holes are not bound to the brane. In the probe-brane limit, where the gravitational backreaction is neglected, this is manifest, but even taking into account the small energy density of the probe brane it seems likely that the binding of the black hole to the brane will be overcome by the gravitational pull of the black hole towards the AdS horizon. (There may be interesting transitory effects—such as stretching and then recoil of the probe brane—that we leave for future investigation.) While a complete analysis of this requires a detailed investigation of stabilized probe brane scenarios, it appears that such a black hole will therefore generically fall towards the AdS horizon, and that the 4D observer will therefore not perceive it as a black hole. In the CFT picture, such black holes will be perceived as complex excitations of the CFT which spread out over time, and it is very unlikely that their signature can be experimentally disentangled from other excitations of the CFT.

The second type of solution is the black hole on the Planck brane. These are truly perceived as 4D black holes. However, given the relation (4.1) between scales, the minimum energy to create such a black hole is again of the order of the Planck energy. The TeV brane scenario does not seem to allow access to what a 4D observer would perceive as strongly coupled gravitational dynamics at lower scales.

In fact, notice the following novelty. A small black hole bound to the Planck brane will not intersect the TeV brane, until its horizon reaches the TeV^{-1} size. Therefore matter moving on the TeV brane may bypass such a black hole, in a close analogy to the black hole flybys discussed in Sec. III B. (See Fig. 2.) In other words, 4D observers made of TeV brane matter have difficulty resolving sub-TeV size black holes. How is this interpreted in four-dimensional language?

To really study this question requires a detailed model of the stabilization and the TeV brane matter. However, a plausible answer to this also comes directly from our earlier discussion. Matter passing a black hole by moving on the TeV brane should be interpreted in the 4D perspective as matter smeared out on the TeV scale. Such matter has a small probability of probing a black hole with a radius much less than 1/TeV.

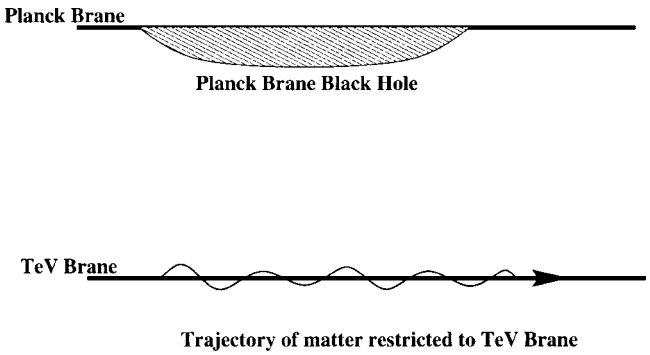

FIG. 2. A particle moving on a probe brane can bypass a small black hole localized on the Planck brane.

C. Terminated AdS scenario

Another interesting possibility is that AdS is terminated at both ends in z. The outlines of such a picture was suggested in Ref. 3 with a idealized lower brane taken to have a finely-tuned negative tension.

Recent developments in string theory have suggested a concrete means to construct geometries with similar properties. Specifically Refs. 6, 7 describe geometries that terminate at a definite value of z. These geometries do not arise from negative tension objects, or even singular branes, but rather are rounded off at the maximal z in a smooth geometry that uses the extra dimensions of string theory in a nontrivial way.

References 6, 7 do not have a simultaneous microscopic construction of the analog of a Planck brane. However, one can envision building such a model by using Verlinde's geometric realization[5] of the Planck brane as a piece of a compactification manifold on the ultraviolet end, and then realize the IR brane as in Refs. 6, 7 or in a variant of these scenarios producing other low-energy dynamics. There may of course be other inequivalent stringy constructions of such doubly-terminated AdS spaces. Constructing detailed models of this kind is an interesting problem for the future.

The models of Refs. 6, 7 have explicit gauge theory duals. If one constructs a model with a geometric ''Planck brane,'' one would expect these to be modified at the UV end and depend on the internal structure of the compactification manifold. Nonetheless, these gauge theories should serve as good effective theories at lower scales, in parallel with our earlier discussion.

Such a scenario—or others with a microscopic realization of an IR brane—may have very interesting consequences for the observability of strong gravitational phenomena. Assume that in such a construction there is a gauge theory sector that we may think of as being truly localized in the vicinity of the maximal z which we take to be $z \simeq \rho_T$. This would then realize what was referred to as matter living on the ''negative tension brane'' of Ref. 3. As explained above, energies at $z \simeq \rho_T$ are redshifted relative to those at the Planck brane, and so if a suitable way is found of stabilizing the separation between the branes, TeV scale scattering corresponds to a proper energy comparable to M, the five-dimensional Planck scale, if the scattering takes place at $z \simeq \rho_T$. Thus scattering at this scale should begin to make black holes. These should be similar to AdS-Schwarzschild solutions, or to the analogous solutions in the new geometry of Refs. 6, 7. (For an explicit formula for the smooth metric in question, see Sec. 5.1 of Ref. 6.)

In the probe-brane picture, these black holes were expected to fall off the brane and into the horizon at $z=\infty$. Now this is not possible since the geometry terminates at $z \simeq \rho_T$. One expects such a black hole to undergo approximately geodesic motion in this vicinity, and ultimately to evaporate.

Note that one may achieve a clean separation of scales in situations where the AdS radius R is larger than the 5D Planck length M^{-1}. In this situation [which can be achieved by taking large 't Hooft parameter g^2M—here only M is the dimension of $SU(M)$—in Ref. 6], there exist black

holes larger than the Planck size but smaller than the AdS radius. These would have an approximately (five-dimensional) Schwarzschild description.

In the probe brane picture, the evaporation of 5D black holes was expected to be nearly exclusively into bulk modes, since the black hole becomes well separated from the TeV brane and so will not couple to its excitations. However, in the present picture, the black hole remains in the vicinity of the analog of the IR brane and this suggests that there is no reason for it to decouple from the matter modes in this vicinity. Indeed, in the idealized ''negative tension brane'' picture, gauge modes on the brane will directly see the black hole metric. Therefore, with this assumption, on general grounds one expects the black hole to Hawking radiate into all available modes, including the visible matter sector modes. As explained in Ref. 42, the radiation in the visible sector is generically expected to be important.

This suggests an interesting scenario in which a black hole could be created at an accelerator operating in the vicinity of the TeV scale. Assuming the black hole is sufficiently coupled to the visible modes, these would provide a channel for the Hawking decay and provide an observational window on this process. One would observe such an object by looking for the characteristic approximately thermal spectrum—with increasing temperature—of the Hawking process.

The basic assumptions that could lead to this possibility being realized are (1) that one has a geometry effectively terminated at a maximal z corresponding to the TeV scale, (2) that one has a description of visible-sector matter localized to the vicinity of this maximal z, and (3) that black holes near the maximal z couple to the visible sector. Whether these assumptions will hold in models based on the ideas of Refs. 6, 7 remains to be seen, but they plausibly do, and there may also be other models with these properties, for which the creation and visible-sector decay of TeV-scale black holes seems a generic prediction.

V. CONCLUSIONS

In this paper we have investigated the interplay between the four- and five-dimensional descriptions of the physics of warped compactifications. In the simplified example of the RSII scenario, at distances long as compared to the AdS radius R there is a four-dimensional effective description of the dynamics given by observable brane matter coupled gravitationally to a sector described by a conformal field theory. At shorter distances the derivation of this description fails. One expects similar 4D effective descriptions for other warped compactification scenarios.

One element of the correspondence between the 4D and 5D descriptions is supplied by the computation of the 4D stress tensor corresponding to a 5D matter distribution. At the linear level we have given a formula for this stress tensor. We have also investigated an amusing scenario that illustrates the interplay between the 4D and 5D descriptions, that of a particle passing a black hole through the fifth dimension, with a corresponding 4D description in terms of a matter distribution expanding into a shell larger than the black hole.

Finally, we have explored situations in which strong gravitational dynamics may give important modifications to the 4D description. In particular, in scenarios where the hierarchy is addressed by visible matter being effectively localized to a large z in AdS space, one potentially has access to strong gravitational dynamics such as black hole formation at TeV energy scales. In probe brane scenarios this may not lead to observable effects since the resulting black hole seems to rapidly decouple from the visible sector by falling off the brane, but scenarios with AdS terminated at this maximal z show much more promise as such a black hole should stay localized in the vicinity of the maximal z. This leads to the possibility of the creation and observable Hawking decay of a black hole in the vicinity of the TeV scale. It would be particularly interesting to find extensions of the work of Ref. 5 and Refs. 6, 7 which give explicit string theory realizations of such terminated AdS scenarios.

Note added in proof. String solutions have now been constructed that realize terminated AdS scenarios.[43]

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APPENDIX A: THE RETARDED GREEN'S FUNCTION

In this appendix we describe some properties of the scalar Green's function for the RSII geometry. This was given in Ref. 11 and takes the form

$$\Delta_{d+1}(x,z;x',z') = \frac{i\pi}{2R^{d-1}}(zz')^{d/2}\int \frac{d^d p}{(2\pi)^d} e^{ip(x-x')} \times\left[\frac{J_{d/2-1}(qR)}{H^{(1)}_{d/2-1}(qR)} H^{(1)}_{d/2}(qz)H^{(1)}_{d/2}(qz') - J_{d/2}(qz_<)H^{(1)}_{d/2}(qz_>)\right]. \tag{A1}$$

For the following discussion it is most convenient to use the z coordinate, related to y by (3.1).

The scalar propagator with $d=4$ and one point on the boundary is given by[11]

$$\Delta_{4+1}(x,z;x',R) = \left(\frac{z}{R}\right)^2 \int \frac{d^4 p}{(2\pi)^4} e^{ip(x-x')} \frac{1}{q}\frac{H^{(1)}_2(qz)}{H^{(1)}_1(qR)}, \tag{A2}$$

where $q^2 = -p^2$. As in Eq. (3.9), let us define a function F,

$$\Delta_{4+1}(R,x;z',x') = \frac{z'^3}{R}\partial_{z'}\left[\frac{F_{z'}(R;x-x')}{z'^2}\right]. \tag{A3}$$

Hence, F is given as Fourier transform of Hankel functions,

$$F_{z'}(R;x-x') = -\frac{z'}{R}\int \frac{d^4 p}{(2\pi)^4} e^{ip(x-x')} \frac{1}{q^2}\frac{H^{(1)}_1(qz')}{H^{(1)}_1(qR)}. \tag{A4}$$

In our conventions [given by (3.6)] the Feynman propagator is

$$\Delta_{\mathrm{F}}(X,X') = -i[\,\theta(t-t')\Delta^+(X,X') + \theta(t'-t)\Delta^-(X,X')], \tag{A5}$$

where Δ^+ is the Wightman function $\langle\phi(X)\phi(X')\rangle$ and Δ^- is its Hermitian conjugate. The retarded Green's function is defined as

$$\Delta_R(X,X') = -i\,\theta(t-t')[\Delta^+(X,X') - \Delta^-(X,X')]; \tag{A6}$$

this manifestly vanishes for $t<t'$ and can easily be shown to obey (3.6). We therefore find that

$$\Delta_R(X,X') = 2\,\mathrm{Re}\,\Delta_{\mathrm{F}}(X,X')\,\theta(t-t'). \tag{A7}$$

In order to compute the asymptotic retarded Green's function, note that in the long-distance approximation $(qR\ll 1)$, F reduces to the following form:

$$F_{z'}(R;x-x') \approx -\frac{\pi i z'}{2}\int \frac{d^4 p}{(2\pi)^4} e^{ip(x-x')}\frac{1}{q}H^{(1)}_1(qz'). \tag{A8}$$

We then perform a Euclidean rotation on the above integral, giving

$$F_{z'}(R;x-x') \approx \frac{\pi i z'}{2} \int \frac{d^4p}{(2\pi)^4} e^{ip(x-x')} \frac{1}{p} H_1^{(1)}(ipz')$$

$$\approx \frac{i}{4\pi^2} \frac{1}{(x-x')^2+z^2}. \tag{A9}$$

The Feynman prescription is then to replace $(x-x')^2$ with $(x-x')^2+i\epsilon$. Making this replacement and taking the real part gives

$$F_{z'}^{\mathrm{Ret}}(R;x-x') \approx \frac{1}{2\pi} \delta((x-x')^2+z'^2)\theta(t-t'), \tag{A10}$$

which finally yields the retarded scalar propagator,

$$\Delta_{4+1}(R,x;z',x') \approx \frac{1}{\pi R}[z'^2\delta'((x-x')^2+z'^2) - \delta((x-x')^2+z'^2)]\theta(t-t'). \tag{A11}$$

APPENDIX B: THE INFRARED LIMIT

As we saw in the text, our calculation of the effective source on the boundary produces an expanding shell in the infrared limit. This is true for scalar vector, and graviton fields. This is also the result that Horowitz and Itzhaki found in Ref. 36, using the boundary conditions appropriate for infinite AdS rather than the brane boundary conditions (3.8). In this appendix we sketch the relation between the calculations. For simplicity we only treat the scalar case although the derivation extends to the other cases.

In our calculation with brane boundary conditions, we solve the bulk equation

$$\Box_{d+1}\phi = T, \tag{B1}$$

with the Neumann condition

$$\partial_n \phi|_{z=\rho} = 0. \tag{B2}$$

Here T is the scalar source, in the text given by the falling particle, and ∂_n denotes the normal derivative. The effective boundary source is found by restricting this solution to the boundary and computing its Laplacian:

$$J = \Box_d \phi|_\partial. \tag{B3}$$

Another way to get the same solution is to solve (B1) subject to the Dirichlet boundary condition,

$$\phi|_\partial = \varphi. \tag{B4}$$

The solution is given in terms of the Dirichlet Green's function as

$$\phi(X) = \int dV'\, \Delta_{d+1}^D(X,x')T(X') + \oint_\partial dn'\, \partial_{n'}\Delta_{d+1}^D(X,X')\varphi(x'). \tag{B5}$$

The effective boundary action for φ is computed by evaluating the $d+1$-dimensional action of this solution, which using the bulk equation of motion becomes

$$S[\varphi] = -\frac{1}{2} \oint_\partial dn'\, \varphi\, \partial_{n'}\phi. \tag{B6}$$

The boundary equation of motion for φ then states

$$\partial_n \phi|_\partial = 0. \tag{B7}$$

Thus a solution of the Dirichlet boundary problem such that the boundary field satisfies the boundary equations of motion corresponds to a solution of the Neumann boundary problem.

In the latter approach the effective boundary source can be read off from the boundary equation of motion. Inserting the second term of (B5) into (B7) gives the kinetic operator acting on φ, which becomes $\Box_d$ in the long-distance limit. Thus in this limit (B7) states that

$$J = \Box_d \varphi \sim \partial_z \phi_{\rm D}|_\partial, \tag{B8}$$

where $\phi_{\rm D}$, the first term in (B5), is the solution to (B1) with Dirichlet boundary conditions, $\phi_{\rm D}|_\partial = 0$. In the limit as the cutoff is removed, $\rho \to 0$, this corresponds to the desired solution in infinite AdS. And aside from a rescaling, $\partial_z \phi_{\rm D}$ corresponds to the source on the boundary, which if we had been discussing the metric would be the boundary stress tensor of Ref. 36.

It is also possible to check the relationship to Ref. 36 directly, by acting with $\Box_d$ on (3.42), using Eq. (3.6) to eliminate the d-dimensional Laplacian in favor of y derivatives, and then using the fact that in the infrared limit (A1) is the standard bulk propagator plus a y-independent piece which therefore does not contribute.

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$D=4$ chiral string compactifications from intersecting branes

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Intersecting Dp-branes often give rise to chiral fermions living on their intersections. We study the construction of four-dimensional chiral gauge theories by considering configurations of type II D$(3+n)$-branes wrapped on nontrivial n-cycles on $\mathbf{T^{2n}}\times(\mathbf{R^{2(3-n)}}/\mathbf{Z_N})$, for $n=1,2,3$. The gauge theories on the four noncompact dimensions of the brane world-volume are generically chiral and nonsupersymmetric. We analyze consistency conditions (RR tadpole cancellation) for these models, and their relation to four-dimensional anomaly cancellation. Cancellation of $U(1)$ gauge anomalies involves a Green–Schwarz mechanism mediated by RR partners of untwisted and/or twisted moduli. This class of models is of potential phenomenological interest, and we construct explicit examples of $SU(3)\times SU(2)\times U(1)$ three-generation models. The models are nonsupersymmetric, but the string scale may be lowered close to the weak scale so that the standard hierarchy problem is avoided. We also comment on the presence of scalar tachyons and possible ways to avoid the associated instabilities. We discuss the existence of (meta)stable configurations of D-branes on 3-cycles in $(\mathbf{T^2})^3$, free of tachyons for certain ranges of the six-torus moduli. © *2001 American Institute of Physics.*
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I. INTRODUCTION

D-branes have turned out to be a key ingredient in our present understanding of the structure of string theory. Interestingly, the fact that D-branes contain gauge fields localized on their world-volume has also suggested new scenarios for string phenomenology and phenomenology beyond the standard model in general (see, e.g., Refs. 1–5). From this point of view, it is important to explore different configurations of branes which can lead to interesting features for phenomenological model building.

An important observation[6] is that intersecting D-branes in flat space may give rise to chiral fermions propagating on the intersection of their world-volumes, arising from open strings stretching between the D-branes. Hence, it is natural to consider the construction of four-dimensional chiral models by compactifications including intersecting D-branes. In this framework, the compactification space can be essentially flat, like a six-torus, since chirality arises from fermions at the intersection of D-brane world-volumes, and does not depend so much on the holonomy group

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of the ambient space. This is in contrast with more familiar compactifications with D-branes, like type IIB orientifolds[7–9] or heterotic string compactifications,[10,11] where chirality arises due to the ambient space being Calabi–Yau threefold.

In this paper we perform a systematic exploration of configurations of $D(3+n)$-branes wrapped on n-cycles in an $2n$-dimensional torus $\mathbf{T^{2n}}$, and sitting at a point in a transverse $6-2n$-dimensional space $\mathbf{B}$. We are interested in configurations leading to chiral four-dimensional gauge theories after reduction on the torus. Chirality is automatically achieved for D6-branes on 3-cycles on $\mathbf{T^6}$. However, for models with D4- or D5-branes, if the point in $\mathbf{B}$ at which the D-branes sit is smooth, the resulting intersection lead to vector-like matter. Chiral matter at the intersections can be obtained by considering branes sitting at singular points in $\mathbf{B}$. We will center on Abelian orbifold singularities, whose local geometry can be modeled as $\mathbf{R^{6-2n}/Z_N}$.

Hence we consider configurations of stacks of $D(3+n)$-branes wrapped on n-cycles in $\mathbf{T^{2n}\times R^{6-2n}/Z_N}$. Each stack of D-branes gives rise to gauge factors, while open strings stretched between them give rise to chiral fermions propagating on the intersections. The resulting four-dimensional gauge theories are of potential phenomenological interest. When the singularity is embedded in a globally compact $(6-2n)$-dimensional variety, one obtains a full-fledged compactification, where gravity is also four-dimensional.

Notice that the case of $n=0$ corresponds to configurations of D3-branes at $\mathbf{R^6/Z_N}$ singularities, which were employed in Ref. 5 to build realistic gauge theories (see Ref. 12 for more formal applications of these systems). Full-fledged compactifications were subsequently obtained by embedding the singularities in global compact geometries. Our approach here is similar in spirit to the bottom-up approach introduced in Ref. 5, although we mainly center on local features in the present paper. The models also present a number of interesting new properties.

The opposite extreme case, $n=3$, corresponds to D6-branes wrapped on 3-cycles in $\mathbf{T^6}$. Configurations of this type have appeared in Ref. 13, but in the presence of an additional orientifold projection. (Other models with branes at angles and orientifold and orbifold projections have appeared in Ref. 14.) This projection is not a necessary ingredient, and it does not improve the phenomenological or theoretical features of the model, hence we choose not to include it. In particular, this allows us to get around the orientifold symmetry constraints in Ref. 13, which prevented the appearance of three-generation models. Without orientifold action, three-family models are easy to build, and we present a specific example.

In this paper we perform a detailed analysis of the configurations for $n=1,2,3$, their construction with explicit examples, and the main features of the resulting four-dimensional theories. We determine the tadpole cancellation conditions, their geometrical interpretation, and their interplay with the cancellation of chiral four-dimensional anomalies. Interestingly, we find that the theories contain several anomalous $U(1)$'s, and that their anomalies are cancelled by a generalized Green–Schwarz mechanism. The fields that mediate this mechanism correspond, for D6-branes wrapped on 3-cycles on $\mathbf{T^6}$, to *untwisted* closed string modes, in contrast with the situation in other string constructions. For $n=1,2$ the exchanged fields correspond to the reduction on $\mathbf{T^{2n}}$ of fields in twisted sectors of $\mathbf{R^{6-2n}/Z_N}$.

The models are generically nonsupersymmetric, even if the orbifold twist is chosen to preserve some bulk supersymmetry. This leads to two important issues. First, although the discussion of more phenomenological aspects in these constructions will appear elsewhere,[15] we would like to mention here the question of scales. Even though models are nonsupersymmetric, it is possible to avoid a hierarchy problem in any realistic application, by lowering the string scale down to a TeV. This is possible, i.e., consistent with a large four-dimensional Planck mass, for models with D4- or D5-branes, in the usual way, by simply taking the transverse $(6-2n)$-dimensional space $\mathbf{B}$ large enough. Notice that the $2n$-torus should remain small (with compactification scale $\approx$ TeV) to avoid too light KK resonances of gauge bosons. Hence, as observed in Ref. 13, for models with D6-branes solving the hierarchy problem by large volume compactification is not possible. It is interesting to consider them, however, in case another mechanism is eventually devised. On the other hand, let us emphasize again that a low string scale is consistent with low-energy physics in models with D4- or D5-branes, with a large transverse volume.

The second comment concerns the generic presence of tachyons at brane intersections, which signal an instability against recombining intersecting branes into a single smooth one. Interestingly, for the case of D6-branes on 3-cycles, there exist brane orientations such that the brane recombination process is not energetically favored, since it implies an increase of the wrapped volume. The corresponding intersection hence does not lead to tachyonic states. Hence it is in principle possible to construct compact models of D6-branes on $\mathbf{T^6}$ where all intersections have this property, and the resulting model is (meta)stable, as we discuss in some detail. In models with D4- or D5-branes, it is possible to construct models where most of the tachyons at intersections are projected out by the $\mathbf{Z_N}$ orbifold twist in the quotient singularity.

In any event, we think it is also interesting to consider models with a small set of tachyons. Recent developments (see Ref. 16 for a review) have suggested that much can be learned by considering unstable configurations in string theory and their decay. On the speculative side, a possible phenomenological application of these ideas would be to interpret the tachyon condensation process as a Higgs mechanism, in which the two gauge factors associated to the intersecting branes break to a smaller subgroup carried by the recombined brane. In fact, it is possible to construct explicit semirealistic models of D4-branes, where the only tachyons have the quantum numbers of Standard Model Higgs multiplets. It is tempting to speculate that the effect of the instability is Higgs breaking of electroweak symmetry (see Ref. 15 for further details).

The paper is organized as follows. In Sec. II we discuss generalities about the configuration of intersecting branes, and the spectrum arising on their world-volume and on their intersections. In Sec. III we discuss the construction of models of D6-branes wrapped on 3-cycles in $\mathbf{T^6}$. We analyze their spectrum, the tadpole cancellation conditions and their interpretation, and cancellation of non-Abelian and mixed $U(1)$ anomalies. We also present several explicit examples, e.g., leading to three-generation Standard Model gauge sectors. We also comment on the possibility of understanding tachyon condensation as symmetry breaking by a Higgs mechanism. A similar analysis is carried out for configurations of D4-branes in Sec. IV, and of D5-branes in Sec. V. Section VI contains our final remarks.

II. INTERSECTING Dp-BRANES

Let us start by considering some generic properties of the spectrum for branes at angles. We start considering D-branes wrapped on d-cycles $\mathbf{T^{2d}}$. We choose a factorizable $\mathbf{T^{2d}}$, product of d two-dimensional rectangular tori $\mathbf{T_I^2}$ parametrized by compact coordinates X_1^I, X_2^I, with radii R_1^I, R_2^I, with $I=1,\ldots,d$. We introduce K different sets of N_a coincident Dp_a-branes, labeled by an index a, $a=1,\ldots,K$. Each set wraps around a 1-cycle Π_a^I, of type (n_a^I, m_a^I), on each of the d two-tori. Namely, it wraps n_a^I times around the X_1^I direction and m_a^I times around the X_2^I direction. The angle of these branes with the X_1^I axis is hence given by

$$\tan \vartheta_a^I = \frac{m_a^I R_2^I}{n_a^I R_1^I}, \tag{2.1}$$

with an obvious modification for skewed two-tori.

The compactification preserves all 32 supersymmetries of type II theory in the closed string sector. The sector of open strings stretching between Dp_a-branes within the same set, preserves 16 supersymmetries, hence giving rise to the corresponding gauge supermultiplet with gauge group $U(N_a)$. [If the wrapping numbers (n,m) are not coprime, $r=\gcd(n,m)\neq 1$, the D-brane is multiwrapped r times over the cycle $(n/r,m/r)$. This state can be equivalently described as r D-branes on $(n/r,m/r)$ with an order r permutation Wilson line turned on. For N such multiwrapped branes, the world-volume gauge group is $U(N)^r$. We thank R. Blumenhagen, B. Körs, and D. Lüst for a discussion on multiwrapped branes.] This piece of the spectrum is non-chiral, so the only source of chiral fields is the sector of open strings stretched between different sets of branes.

The spectrum of such sectors has been studied in Ref. 6. World-sheet bosonic fields for open strings stretching between Dp_a- and Dp_b-branes, at a relative angle $\vartheta^I_{ba}=(\vartheta^I_b-\vartheta^I_a)/\pi$ (given in ''units of π'' for convenience), in the Ith two-torus, satisfy the boundary conditions

$$\begin{aligned}\sin\vartheta^I_a\,\partial_\sigma X^I_1-\cos\vartheta^I_a\partial_\sigma X^I_2=0,\\ \sin\vartheta^I_a\,\partial_t X^I_2-\cos\vartheta^I_a\,\partial_t X^I_1=0,\end{aligned}\tag{2.2}$$

at $\sigma=0$, and a similar equation for $\sigma=\pi$ with $a\to b$. Corresponding equations are satisfied by fermionic coordinates. Such boundary conditions lead to *twisted* mode expansions, with twist given by the relative angle ϑ^I_{ba} between branes. For instance, one obtains world-sheet fermionic modes $\psi^I_{r_-}$, $\psi^I_{r_+}$, with modes $r_\pm=n\pm\vartheta^I_{ba}+\nu$, where n is an integer and $\nu=0,1/2$ for R and NS boundary conditions, respectively. No windings or KK momenta are allowed for nontrivial angles. Antiparticles of states in the ab sector appear in the ba sector.

We are mainly interested in four-dimensional intersections, hence we consider the cases of D$(3+n)$-branes wrapped on n-cycles on $\mathbf{T^{2n}}$, for $n=1,2,3$. As mentioned in the Introduction, configurations $n<3$ would lead to nonchiral intersections, hence we will eventually turn to configurations with singular transverse spaces, namely D$(3+n)$-branes on n-cycles in $\mathbf{T^{2n}\times R^{6-2n}/Z_N}$. Before that, it is convenient to discuss the simpler case of $\mathbf{T^{2n}\times R^{6-2n}}$ in this section, namely D6-branes on $\mathbf{T^6}$, D5-branes on $\mathbf{T^4\times C}$, D4-branes on $\mathbf{T^2\times C^2}$.

The mass operator for strings stretching between branes in the ath and bth set, which make an angle $\vartheta^I\equiv\vartheta^I_{ab}$ on the Ith two-torus is[17,6]

$$\alpha' M^2_{ab}=\frac{Y^2}{4\pi^2\alpha'}\sum_{I=1}^{d}\left[N(\vartheta^I)+\vartheta^I_{ab}\right]-\nu,\tag{2.3}$$

where Y^2 measures the length of the stretched string (minimal distance between branes for minimum winding states), and N_ν is the number operator given by

$$\begin{aligned}N(\vartheta^I)&=\sum_{n>0}\alpha_{-n}\cdot\alpha_n+\sum_{n>0}\alpha^I_{-n_+}\cdot\alpha^I_{n_+}+\sum_{n>0}\alpha^I_{-n_-}\cdot\alpha^I_{n_-}+\alpha^I_{-\vartheta^I}\alpha^I_{\vartheta^I}\\&=+\sum_{n>0}r\psi_{-r}\psi_r+\sum_{n>0}r_+\psi^I_{-r_+}\cdot\psi^I_{r_+}+\sum_{n>0}r_-\psi^I_{-r_-}\cdot\psi^I_{r_-}\\&\quad+\frac{1}{2}\left[(\vartheta^I+\nu)\psi^I_{-(\vartheta^I+\nu)}\cdot\psi^I_{\vartheta^I+\nu}+(-\vartheta^I+\nu)\psi^I_{(\vartheta^I-\nu)}\cdot\psi^I_{-\vartheta^I+\nu}\right].\end{aligned}\tag{2.4}$$

Some comments are in order for the correct use of this expression. We have assumed in its derivation that $0\leqslant\vartheta^I_{ab}\leqslant\frac{1}{2}$, so oscillators modes as above are correctly normal ordered. For negative angles one should replace $\vartheta_I\to|\vartheta_I|$. The ϑ^I_{ab} in the mass equation (2.3) arises from normal ordering of twisted modes.

The spectrum can be described in bosonic language as follows. We introduce a four-dimensional twist vector v_ϑ, whose Ith entry is given by ϑ^I_{ab}. The GSO projected states are labeled by a four-dimensional vector $r+v_\vartheta$, where $r_I\in\mathbf{Z},\mathbf{Z}+\frac{1}{2}$ for NS, R sectors, respectively, and $\Sigma_I r_I=$ odd. The last entry provides four-dimensional Lorentz quantum numbers. The mass of the states is then given by

$$\alpha' M^2=\frac{Y^2}{4\pi^2\alpha'}+N_{\rm bos}(\vartheta)+\frac{(r+v)^2}{2}-\frac{1}{2}+E_{ab},\tag{2.5}$$

with

$$E_{ab}=\sum_I \frac{1}{2}|\vartheta_I|(1-|\vartheta_I|), \tag{2.6}$$

and $N_{\rm bos}(\vartheta)$ is a contribution from bosonic oscillators.

Let us discuss the computation of lowest lying states in the different models. As mentioned above, models for $n<3$ have a nonchiral spectrum, as is easily seen from the fact that all massless states can be made massive in a continuous way by increasing the separation Y^2 in transverse space.

We first consider the case of D4-branes on $\mathbf{T^2\times C^2}$. In the NS sector, the lowest mass state allowed by GSO projection[6] corresponds to $\psi^I_{(\vartheta^1-1/2)}|0>_{\rm NS}$, or $r+v=(-1+\vartheta^1,0,0,0)$ in bosonic language. Its mass is given by

$$\alpha' M_1^2=\frac{Y}{4\pi^2\alpha'}-\frac{1}{2}|\vartheta^1|. \tag{2.7}$$

Thus, a tachyon is generated when D4-branes come closer than the critical distance $Y^2=2\pi^2\alpha'|\vartheta^1|$. The tachyon signals an instability against joining the intersecting branes into a single one, which then wraps a one-cycle in the homology class $[\Pi_a]+[\Pi_b]$, namely a (n_a+n_b,m_a+m_b) cycle on $\mathbf{T^2}$. In Sec. IV we discuss how to use a $\mathbf{Z_N}$ orbifold twist to project out some of these tachyons.

The R groundstate contains four fermions that become massless at zero transverse distance. They are given by

$$\begin{aligned}&(-\tfrac{1}{2}+\vartheta^1,-\tfrac{1}{2},-\tfrac{1}{2},+\tfrac{1}{2});\quad (-\tfrac{1}{2}+\vartheta^1,-\tfrac{1}{2},+\tfrac{1}{2},-\tfrac{1}{2}),\\ &(-\tfrac{1}{2}+\vartheta^1,+\tfrac{1}{2},-\tfrac{1}{2},-\tfrac{1}{2});\quad (-\tfrac{1}{2}+\vartheta^1,+\tfrac{1}{2},+\tfrac{1}{2},+\tfrac{1}{2}).\end{aligned} \tag{2.8}$$

There are two pairs of opposite chirality spinors, so the spectrum is nonchiral. A possibility to obtain a chiral spectrum is to project out some of the above fermions, for instance by locating the D4-branes at $\mathbf{C^2/Z_N}$ singularities in transverse space; see Sec. IV.

In the case of configurations of D5-branes on $\mathbf{T^2\times T^2\times C}$, open strings at intersections have a twist vector $(\vartheta_1,\vartheta_2,0,0)$. In the NS sector, assuming $0<\vartheta_I<1$ the lowest mass NS states correspond to $\psi_{-1/2+\vartheta_1}|0>$, $\psi_{-1/2+\vartheta_2}|0>$, or in bosonic language $(-1+\vartheta_1,0,0,0)$, $(0,-1+\vartheta_2,0,0)$. Their masses are $M_1^2=\frac{1}{2}(\vartheta_2-\vartheta_1)$ and $M_2^2=-\frac{1}{2}(\vartheta_2-\vartheta_1)=-M_1^2$, respectively. Thus, unless $|\vartheta_2|=|\vartheta_1|$, in which case the intersection preserves some supersymmetry, there is always a tachyonic state. The R spectrum contains a set of nonchiral massless fermions, corresponding to the states $(-\frac{1}{2}+\vartheta^1,-\frac{1}{2}+\vartheta^2,-\frac{1}{2},\frac{1}{2})$ and $(-\frac{1}{2}+\vartheta^1,-\frac{1}{2}+\vartheta^2,\frac{1}{2},-\frac{1}{2})$. Again, tachyon elimination and chirality may be obtained by imposing an orbifold projection, namely by considering D5-branes wrapped on $\mathbf{T^4}$ and located at the origin of a $\mathbf{C/Z_N}$ singularity, as we do in Sec. V.

As mentioned, a chiral spectrum is obtained for D6-brane intersections on $\mathbf{T^6}$. The twist vector is now given by $(\vartheta_1,\vartheta_2,\vartheta_3,0)$. In the NS sector, the lowest lying states, for $0\leqslant\vartheta^I\leqslant 1$, are given by $(-1+\vartheta^1,\vartheta^2,\vartheta^3,0)$, $(\vartheta^1,-1+\vartheta^2,\vartheta^3,0)$, $(\vartheta^1,\vartheta^2,-1+\vartheta^3,0)$, and $(-1+\vartheta^1,-1+\vartheta^2,-1+\vartheta^3,0)$. As discussed in more detail in Sec. III, some of them may be tachyonic, but not necessarily. In the R sector, we obtain a single chiral fermion, given by $(-\frac{1}{2}+\vartheta^1,-\frac{1}{2}+\vartheta_2,-\frac{1}{2}+\vartheta_3,+\frac{1}{2})$.

We conclude by emphasizing an important point. Branes wrapped on cycles generically intersect at multiple points, hence the above states in mixed ab sectors appear in several copies, this multiplicity being given by the intersection number of the corresponding wrapped cycles. [If, e.g.,

one of the branes, say the bth, has noncoprime (n,m), the multiplets in the ab sector transform as $\Sigma_{l=1}^{r}\tilde{I}_{ab}(N_a,N_{b,r})$ under the gauge group $U(N_a)\times U(N_b)^r$, and $\tilde{I}_{ab}=I_{ab}/r$.]

III. D6-BRANES WRAPPING AT ANGLES ON $(T^2)^3$

A. Construction

In this section we consider type IIA theory compactified on a factorizable $\mathbf{T^6}$. We consider a configuration containing K stacks of N_a D6-branes, $a=1,\ldots,K$, wrapped on three-cycles Π_a obtained as the product of one-cycles (n_a^I,m_a^I) on each of the three two-tori $I=1,2,3$. [This type of configuration is a particular case of configurations of D6-branes wrapped on special Lagrangian cycles in a Calabi–Yau threefold (see Ref. 18 for recent discussions).] In Ref. 13 these kinds of D6-brane configurations were considered in the presence of an orientifold projection. Since the projection is not required for consistency, we prefer not to impose this restriction and keep our analysis general.

The models admit a T-dual description[6,13] in terms of type IIB compactified on a T-dual torus $\tilde{\mathbf{T}}^6$ (with the Kahler and complex structure on each two-tori exchanged with respect to the original one), with a set of D9-branes (and anti-D9-branes), with wrapping numbers n_a^I and world-volume magnetic flux with charge m_a^I along the Ith two-torus. (Models with such fluxes and orbifold and orientifold projections have appeared in Ref. 19.) Even though we phrase our discussion in D6-brane language, we will find it useful to occasionally turn to this T-dual picture.

The configuration can be described by a free world-sheet CFT, and the consistency conditions (tadpole cancellation conditions) can be analyzed by the usual factorization of one-loop amplitudes. They read as

$$\begin{aligned}
&\sum_a N_a n_a^1 n_a^2 n_a^3=0, \quad \sum_a N_a n_a^1 m_a^2 m_a^3=0,\\
&\sum_a N_a m_a^1 n_a^2 n_a^3=0, \quad \sum_a N_a m_a^1 n_a^2 m_a^3=0,\\
&\sum_a N_a n_a^1 m_a^2 n_a^3=0, \quad \sum_a N_a m_a^1 m_a^2 n_a^3=0,\\
&\sum_a N_a n_a^1 n_a^2 m_a^3=0, \quad \sum_a N_a m_a^1 m_a^2 m_a^3=0.
\end{aligned} \tag{3.1}$$

In the D6-brane picture, they are equivalent to the condition that the homology classes $[\Pi_a]$ of the cycles Π_a wrapped by the D6-branes, counted with multiplicity N_a, add up to zero. Denoting by $[a_I]$, $[b_I]$ the homology classes of the (1,0) and (0,1) basis cycles in the Ith two-torus, we have

$$[\Pi_a]=(n_a^1[a_1]+m_a^1[b_1])\otimes(n_a^2[a_2]+m_a^2[b_2])\otimes(n_a^3[a_3]+m_a^3[b_3]), \tag{3.2}$$

and (3.1) can be recast as

$$\sum_a N_a[\Pi_a]=0. \tag{3.3}$$

The vanishing of the total homology class is required by consistency with the equations of motion for the RR 7-form, under which the D6-branes are electrically charged,

$$d*H_8=\sum_a N_a\delta(\Pi_a), \tag{3.4}$$

where H_8 is the field strength of the 7-form, and $\delta(\Pi_a)$ is a three-form supported at the location of the D6$_a$-branes, the Poincare dual of $[\Pi_a]$. Since $d*H_8$ is exact, the above equation in homology becomes (3.3).

In the language of D9-branes with fluxes, conditions (3.1) receive the following interpretation. In the presence of background magnetic fluxes, D9-branes carry charges under RR forms of all even degrees, due to the WZ world-volume couplings.[20] The above tadpole conditions amount to the cancellation of overall D9-, D7$_I$-, D5$_I$- and D3-brane charges, (where D5$_I$- and D7$_I$-branes, are wrapped on, or transverse to, the Ith two-torus, respectively). This is required for consistency of the equations of motion of the corresponding RR forms, i.e., the T-dual statement to our argument in the D6-brane picture.

From our discussion in Sec. II, the four-dimensional field theory arising after compactification of the D6-branes on the torus contains chiral fermions arising from brane intersections, hence *a priori* have phenomenological interest. They are also nonsupersymmetric, but in principle the existence of a tachyon-free stable configuration is not excluded; see Sec. III D.

Let us obtain the massless (and tachyonic) four-dimensional spectrum. The 6_a6_a sector has unbroken $\mathcal{N}=4$ supersymmetry, and leads, in component fields, to $U(N_a)$ gauge bosons, six real scalars in the adjoint representation and four Majorana fermions in the adjoint as well. In the mixed 6_a6_b and 6_b6_a sectors, the field content appears in general in several replicas, due to the multiple intersection number I_{ab} of the cycles Π_a and Π_b, given by

$$I_{ab}=[\Pi_a]\cdot[\Pi_b]=\prod_i (n_a^i m_b^i - m_a^i n_b^i). \tag{3.5}$$

(In the T-dual picture in terms of D9-branes with magnetic fluxes, the multiplicities arise from the Landau level multiplicities.) In the R sector, we obtain I_{ab} chiral left-handed fermions in the bifundamental representation $(N_a,\overline{N_b})$, with the understanding that a negative multiplicity corresponds to a positive multiplicity of right-handed fermions. In the NS sector, we obtain a set of I_{ab} bifundamental scalars, whose masses are controlled by the angles ϑ_I between the $D6_a$- and the $D6_b$-branes, which depend on the six-torus moduli. Their masses are given by (assuming $0\leqslant\vartheta_i\leqslant 1$)

State	Mass
$(-1+\vartheta_1,\vartheta_2,\vartheta_3,0)$	$\alpha' M^2=\frac{1}{2}(-\vartheta_1+\vartheta_2+\vartheta_3)$,
$(\vartheta_1,-1+\vartheta_2,\vartheta_3,0)$	$\alpha' M^2=\frac{1}{2}(\vartheta_1-\vartheta_2+\vartheta_3)$,
$(\vartheta_1,\vartheta_2,-1+\vartheta_3,0)$	$\alpha' M^2=\frac{1}{2}(\vartheta_1+\vartheta_2-\vartheta_3)$,
$(-1+\vartheta_1,-1+\vartheta_2,-1+\vartheta_3,0)$	$\alpha' M^2=1-\frac{1}{2}(\vartheta_1+\vartheta_2+\vartheta_3)$.

(3.6)

Hence certain intersections may lead to the appearance of tachyons. If present, they signal an instability against joining the intersecting branes into a single smooth one. As observed in Ref. 21, tachyon modes arise precisely in the range of ϑ_I's for which the joining process is energetically favored, namely decreases the 3-cycle volume. In Sec. III D we discuss the construction of models which, for a range of six-torus moduli, do not contain tachyons at brane intersections. Hence the corresponding configurations are protected against recombination by a energy barrier.

In the next section we center robust aspects of the theory, such us the chiral fermion content, and potential gauge anomalies. Hence recall that the gauge group and chiral fermions in the models are

$$\prod_{a=1}^{K} U(N_a), \quad \sum_{a<b} I_{ab}(N_a, \bar{N}_b). \tag{3.7}$$

[In fact, the chiral piece of the spectrum of a set of D6-branes wrapped on 3-cycles in a threefold (not necessarily Calabi–Yau) has this form, and our arguments about the cancellation of four-dimensional anomalies are valid (with some obvious modifications) in this general case.] The spectrum is generically chiral, leading to an interesting set of four-dimensional field theories.

B. Anomaly cancellation

1. Non-Abelian anomalies

Following, Refs. 6, 22, the gauge anomaly induced by the chiral fermions living on each intersection is cancelled by an anomaly inflow mechanism associated to the intersecting branes (see Ref. 23 for string computations of the relevant couplings). Namely, the violation of charge induced by the anomaly is compensated by a charge inflow from the bulk of the intersecting branes. This explanation is sufficient in situations where the branes are infinitely extended. In the compact context, however, within a single brane the charge ''inflowing'' into an intersection must be compensated by charge ''outflowing'' from other intersections. (This anomaly flow picture is analogous to that in Ref. 24.) Consistency of anomaly inflow in a compact manifold imposes global constraints on the configuration.

From the point of view of the compactified four-dimensional effective field theory, which does not resolve the localization of the different chiral fermions, these global constraints correspond to cancellation of triangle gauge anomalies in the usual sense. In fact, the cancellation of cubic non-Abelian anomalies for the gauge factor $SU(N_a)$ in (3.7) reads as

$$\sum_{b=1}^{K} I_{ab} N_b = 0. \tag{3.8}$$

From the ten-dimensional viewpoint, (3.8) expresses the cancellation of inflows from different intersections in the $D6_a$-branes.

By replacing (3.5) in (3.8), one can see that tadpole cancellation conditions imply the cancellation of cubic non-Abelian anomalies. Thus, as usual, string theory consistency conditions imply consistency of the low-energy effective theory. However, tadpole cancellation conditions are in general much stronger than anomaly cancellation conditions (see also Ref. 25), a feature also found in the context of standard type IIB orientifolds[26] (see also Refs. 27, 25).

2. Mixed $U(1)$ anomaly cancellation

Let us turn to mixed $U(1)$ anomalies. Again, anomalies at each intersection are cancelled by the inflow mechanism.[6,22] However, the global consistency of the inflow, or equivalently, cancellation of anomalies from the perspective of the compactified four-dimensional theory, is in this case more intricate, and involves a Green–Schwarz mechanism. (The interplay between the inflow and Green–Schwarz anomaly cancellation mechanisms has been studied in Ref. 28 in a different context.) Using the fermion spectrum in (3.7), the mixed $U(1)_a - SU(N_b)$ triangle anomaly reads as

$$\mathcal{A}_{ab} = \tfrac{1}{2}\delta_{ab} \sum_c N_c I_{bc} + \tfrac{1}{2} N_b I_{ab}. \tag{3.9}$$

The first piece is proportional to the non-Abelian anomaly, and vanishes, while the last piece is generically nonvanishing even after imposing tadpole conditions.

We now show that the residual anomaly is cancelled by a generalized Green–Schwarz mechanism mediated by RR partners of closed string *untwisted* geometric moduli. This situation contrasts with that in type IIB orientifolds, where $U(1)$ anomalies are cancelled through exchange of

closed string *twisted* moduli[29] (see Ref. 30 for the six-dimensional case, and, e.g., Refs. 31, 32 for subsequent work). It also differs from that in heterotic compactifications, in not involving the dilaton multiplet, and in allowing the existence of several anomalous $U(1)$'s.

Let us consider a $D6_a$-brane wrapped on a 3-cycle $[\Pi_a]$. It has several relevant world-volume couplings[20] to the RR 3-form C_3 and its ten-dimensional Hodge dual, the 5-form C_5,

$$\int_{D6_a} C_3 \wedge F_a \wedge F_a ; \quad \int_{D6_a} C_5 \wedge F_a . \tag{3.10}$$

In order to obtain the couplings after a Kaluza–Klein reduction to four dimensions, it is convenient to introduce two basis of homology 3-cycles, $\{[\Sigma_i]\}$, $\{[\Lambda_i]\}$, dual to each other, namely $[\Lambda_i]\cdot[\Sigma_j]=\delta_{ij}$. On these two basis, the $D6_a$-brane 3-cycle $[\Pi_a]$ has the expansions

$$[\Pi_a]=\sum_i r_{ai}[\Sigma_i]; \quad M[\Pi_a]=\sum_i p_{ai}[\Lambda_i]. \tag{3.11}$$

Defining the untwisted RR fields $\Phi_i=\int_{[\Lambda_i]} C_3$; $B_2^i=\int_{[\Sigma_i]} C_5$, which are Hodge duals in the four-dimensional sense, the couplings (3.10) read as

$$\sum_i p_{ai}\int_{M_4}\Phi_i F_a \wedge F_a ; \quad MN_a\sum_i r_{ai}\int_{M_4} B_2^i \wedge F_a , \tag{3.12}$$

where the prefactor N_a arises from normalization of the $U(1)$ generator, as in Ref. 29. These couplings can be combined in a GS diagram where $U(1)_a$ couples to the ith untwisted field, which then couples to F_b^2. The coefficient of this amplitude is (modulo an a, b independent numerical factor)

$$N_a\sum_i r_{ai}p_{bi}=N_a\sum_{i,j} r_{ai}p_{bj}[\Sigma_i]\cdot[\Lambda_j]=N_a[\Pi_a]\cdot[\Pi_b]=N_a I_{ab}, \tag{3.13}$$

precisely of the form required to cancel the residual $U(1)_a-SU(N_b)^2$ anomaly in (3.9).

The same mechanism may be described in the T-dual picture of D9-branes with magnetic fluxes. The couplings on the world-volume of D9-branes to bulk RR fields (the role of these couplings in anomaly cancellation in a different class of models has been suggested in Ref. 19) are of the form (wedge products implied)

$$\begin{gathered}\int_{D9_a} C_0 F_a^5; \quad \int_{D9_a} C_2 F_a^4; \quad \int_{D9_a} C_4 F_a^3, \\ \int_{D9_a} C_6 F_a^2; \quad \int_{D9_a} C_8 F_a ; \quad \int_{D9_a} C_{10}.\end{gathered} \tag{3.14}$$

In order to obtain the four-dimensional version of these couplings, we define

$$C_2^I=\int_{(\mathbf{T^2})_\mathbf{I}} C_4; \quad C_0^I=\int_{(\mathbf{T^2})_\mathbf{I}} C_2,$$

$$B_2^I=\int_{(\mathbf{T^2})_\mathbf{J}\times(\mathbf{T^2})_\mathbf{K}} C_6; \quad B_0^I=\int_{(\mathbf{T^2})_\mathbf{J}\times(\mathbf{T^2})_\mathbf{K}} C_4,$$

$$B_2=\int_{(\mathbf{T^2})_\mathbf{1}\times(\mathbf{T^2})_\mathbf{2}\times(\mathbf{T^2})_\mathbf{2}} C_8; \quad B_0=\int_{(\mathbf{T^2})_\mathbf{1}\times(\mathbf{T^2})_\mathbf{2}\times(\mathbf{T^2})_\mathbf{3}} C_6,$$

where $I\neq J\neq K\neq I$ in the second row. The fields C_2 and C_6, and also C_0 and C_8 are Hodge duals, while C_4 is self-dual. In four dimensions, the duality relations are

$$dC_0=*dB_2;\quad dB_0^I=*dC_2^I,$$

$$dC_0^I=-*dB_2^I;\quad dB_0=-*dC_2.$$

In the dimensional reduction, one should take into account that the integration of F_a along the Ith two-torus yields a factor m_a^I. Also, integrating the pullback of the RR forms on the (multiply wrapped) $D9_a$-brane over the Ith two-torus yields a factor n_a^I. We obtain the couplings

$$N_a\, m_a^1\, m_a^2\, m_a^3\int_{M_4} C_2\wedge F_a;\quad n_b^1\, n_b^2\, n_b^3\int_{M_4} B_0\wedge F_b\wedge F_b,$$

$$N_a\, n_a^I\, m_a^J\, m_a^K\int_{M_4} C_2^I\wedge F_a;\quad n_b^J\, n_b^K\, m_b^I\int_{M_4} B_0^I\wedge F_b\wedge F_b,$$

$$N_a\, n_a^J\, n_a^K\, m_a^I\int_{M_4} B_2^I\wedge F_a;\quad n_b^I\, m_b^J\, m_b^K\int_{M_4} C_0^I\wedge F_b\wedge F_b,$$

$$N_a\, n_a^1\, n_a^2\, n_a^3\int_{M_4} B_2\wedge F_a;\quad m_b^1\, m_b^2\, m_b^3\int_{M_4} C_0\wedge F_b\wedge F_b.$$

As usual, the N_a prefactors arise from $U(1)_a$ normalization.

The GS amplitude where $U(1)_a$ couples to one untwisted field which propagates and couples to two $SU(N_b)$ gauge bosons is proportional to

$$-N_a\, m_a^1 m_a^2 m_a^3 n_b^1 n_b^2 n_b^3+N_a\sum_I\ n_a^I m_a^J m_a^K n_b^J n_b^K m_b^I-N_a\sum_I\ n_a^I n_a^J m_a^K n_b^K m_b^I m_b^J+N_a\, n_a^1 n_a^2 m_a^3 m_b^1 m_b^2 m_b^3$$

$$=N_a\prod_I\ (n_a^I m_b^I-m_a^I n_b^I)=N_a I_{ab}, \tag{3.15}$$

as required to cancel the residual mixed $U(1)$ anomaly in (3.9).

Finally, it is straightforward to check that these theories do not produce mixed $U(1)$ gravitational anomalies.

Due to the linear couplings between the $U(1)$'s and the closed string moduli, anomalous $U(1)$'s become massive with a mass of the order of the string scale. Therefore it is important, for any (phenomenological or not) application of these models, to determine the precise linear combinations becoming massive and those staying massless.

One can advance that since there are eight fields mediating the anomaly cancellation, at most eight $U(1)$ linear combinations can gain mass. Denoting Q_a the generator of the ath $U(1)$, and writing a general linear combination as

$$Q=\sum_{a=1}^{K}\frac{c_a}{N_a}Q_a, \tag{3.16}$$

nonanomalous $U(1)$'s correspond to zero modes of the intersection matrix $\Sigma_a c_a I_{ab}=0$.

We conclude with a brief discussion of Fayet–Iliopoulos terms for the anomalous $U(1)$'s. An important observation is that the standard low-energy field theory arguments relating a GS mechanism with FI terms in Ref. 33 are based on supersymmetry, hence do not directly apply to our models. Notice however that the string theory diagram giving rise to linear couplings between anomalous $U(1)$ and closed string modes is a disk, with boundary on the relevant D6-brane and

a closed string mode insertion. This diagram does not notice the breaking of supersymmetries by other branes, hence yields superpartner interactions, and in particular a FI term, proportional to the NS–NS part of untwisted moduli. As opposed to supersymmetric cases, where the FI terms are not renormalized, in the present nonsupersymmetric situations higher loop contributions are expected.

C. Explicit models

Here we construct an example with a Standard Model gauge group and three quark-lepton families, in order to illustrate how our more general starting point overcomes the difficulty found in Ref. 13 to obtain three generations. Notice that the model, just like the examples in Ref. 13, contains tachyons, but we prefer not to list them since they are moduli dependent (and might even disappear for certain regions in parameter space).

We consider six stacks of D6-branes, $K=6$, with multiplicities and wrapping numbers given by

$$\begin{array}{cccc} \mathbf{N_a} & (\mathbf{n_a^1},\mathbf{m_a^1}) & (\mathbf{n_a^2},\mathbf{m_a^2}) & (\mathbf{n_a^3},\mathbf{m_a^3}) \\ N_1=3 & (1,2) & (1,-1) & (1,-2) \\ N_2=2 & (1,1) & (1,-2) & (-1,5) \\ N_3=1 & (1,1) & (1,0) & (-1,5) \\ N_4=1 & (1,2) & (-1,1) & (1,1) \\ N_5=1 & (1,2) & (-1,1) & (2,-7) \\ N_6=1 & (1,1) & (3,-4) & (1,-5) \end{array} \tag{3.17}$$

This choice satisfies the tadpole conditions. The intersection numbers are

$$\begin{gathered} I_{12}=3,\ I_{13}=-3,\ I_{14}=0,\ I_{15}=0,\ I_{16}=-3, \\ I_{23}=0,\ I_{24}=6,\ I_{25}=3,\ I_{26}=0,\ I_{34}=-6, \\ I_{35}=-3,\ I_{36}=0,\ I_{45}=0,\ I_{46}=6,\ I_{56}=3. \end{gathered} \tag{3.18}$$

The spectrum under $U(3)\times U(2)\times U(1)^4$ is

$$\begin{aligned} &3(3,2)_{[1,-1,0,0,0,0]}+3(\overline{3},1)_{[-1,0,1,0,0,0]}+3(\overline{3},1)_{[-1,0,0,0,0,1]}+6(1,2)_{[0,1,0,-1,0,0]}+3(1,2)_{[0,1,0,0,-1,0]} \\ &+6(1,1)_{[0,0,-1,1,0,0]}+3(1,1)_{[0,0,-1,0,1,0]}+6(1,1)_{[0,0,0,1,0,-1]}+3(1,1)_{[0,0,0,0,1,-1]}, \end{aligned} \tag{3.19}$$

where subindices give $U(1)$ charges. Out the six $U(1)$'s the diagonal linear combination decouples, and two of the remaining are anomalous. A basis of nonanomalous linear combinations (3.16) is provided by the coefficient vectors,

$$\vec{c}=(1,0,0,0,1,0);\quad \vec{c}=(0,1,1,0,0,0);\quad \vec{c}=(0,1,0,0,0,1). \tag{3.20}$$

One can check that the nonanomalous linear combination,

$$Q_Y=-\tfrac{1}{3}Q_1-\tfrac{1}{2}Q_2-Q_3-Q_5, \tag{3.21}$$

can play the role of hypercharge. Indeed, the spectrum, showing only charges under this $U(1)$, is

$$\begin{aligned} &SU(3)\times SU(2)\times U(1)_Y\times 3(3,2)_{1/6}+3(\overline{3},1)_{-2/3}+3(\overline{3},1)_{1/3}+6(1,2)_{-1/2} \\ &+3(1,2)_{1/2}+6(1,1)_1+3(1,1)_0+6(1,1)_0+3(1,1)_{-1}, \end{aligned} \tag{3.22}$$

giving the chiral fermion content of a three-generation standard model [up to charges under additional $U(1)$ symmetries].

This example illustrates that it is relatively easy to do model building in this framework. Unfortunately, as explained in the Introduction, these models suffer a hierarchy problem, since they are not supersymmetric, and it is not possible to lower the string scale by making the six-torus volume large, since this would give rise to too light KK resonances for gauge bosons. However, we cannot exclude that further modifications of the setup improve this aspect. It is conceivable to consider spaces with a small volume region similar to $\mathbf{T^6}$, where D6-branes wrap leading to heavy KK excitation, while the volume of the complete space is much larger. A simple example can be obtained by surgery, taking a small $\mathbf{T^6}$, removing a ball in a region away from the branes, and gluing a throat connecting it to a large volume manifold. Of course, a concrete realization of this would require a much more careful analysis, and our comment is just intended for illustration. In any event, the problem in lowering the string scale is not present in the models of D4- and D5-branes, to be studied in the next sections.

D. Stability and tachyons

The lowest lying states in the NS sector of an open string stretched between intersecting D6-branes are given in (3.6), along with their masses. These can be tachyonic or not, depending on the angles between the D-branes. For instance, for $\vartheta_1 \leqslant \vartheta_2+\vartheta_3$, $\vartheta_2 \leqslant \vartheta_3+\vartheta_1$, $\vartheta_3 \leqslant \vartheta_1+\vartheta_2$, $\vartheta_1+\vartheta_2+\vartheta_3 \leqslant 2$, all states at the intersections have a non-negative mass square. In fact, these are the conditions for the two intersecting 3-cycles to be stable against recombination into a single smooth 3-cycle.[21]

In principle there seems to be no obstruction to the existence of compactifications on $\mathbf{T^6}$ with D6-branes wrapped on 3-cycles, such that every intersection fulfills the above conditions, yielding a four-dimensional nonsupersymmetric chiral theory free of tachyons. Such configurations would be stable against small perturbations, but, carrying no net charges may decay to the vacuum by tunneling through a potential barrier. Such metastable (rather than absolutely stable) non-BPS configurations could however lead to perfectly sensible phenomenological models if their lifetime, exponentially suppressed by the barrier height, is long enough for cosmological standards.

E. Explicit examples of tachyon elimination

In this section we construct specific models where all intersections are tachyon-free for certain regions in the six-torus parameter space, namely the complex structure of the two-tori.

It turns out that it is easier to build such models if the construction includes an orientifold projection ΩR (where $R: z_i \to \overline{z_i}$) as in Ref. 13. The only differences with respect to our configurations above is that the angle between the tori axis is projected out, the $D6_a$-branes wrapped on cycles (n_a^I, m_a^I) must have ΩR orientifold images (denoted $D6a'$-branes) wrapped on cycles (n_a^I, m_a^I), and the first tadpole condition in (3.1) becomes $\Sigma_a N_a\, n_a^1\, n_a^2\, n_a^3 = 16$ (not counting images). The potential tachyon masses are however obtained as above.

The model under consideration is one of the four-dimensional constructions presented in Ref. 13. The sets of D6-branes are given by

N_a	$(\mathbf{n_a^1},\mathbf{m_a^1})$	$(\mathbf{n_a^2},\mathbf{m_a^2})$	$(\mathbf{n_a^3},\mathbf{m_a^3})$
$N_1=3$	(1,0)	(1,0)	(1,1)
$N_2=3$	(1,2)	(1,1)	(1,0)
$N_3=1$	(1,2)	(1,−2)	(1,0)
$N_4=1$	(1,0)	(1,0)	(10,1)

(3.23)

plus their ΩR images. The main advantage in searching tachyon-free models by using constructions with an ΩR orientifold projection, is that, as can be appreciated in (3.23), it allows all

integers n_a^I to be positive. This simplifies the search for tachyon-free regions, since it ensures that taking large ratios R_1/R_2 all angles between branes become small, and states become less tachyonic. For instance, choosing

$$R_2^1/R_1^1=1; \quad R_2^2/R_1^2=3/2; \quad R_2^3/R_1^3=2, \tag{3.24}$$

the masses for the scalars (3.6) at the different intersections are

Intersection	$\alpha'\mathbf{m}_1^2$	$\alpha'\mathbf{m}_2^2$	$\alpha'\mathbf{m}_3^2$	$\alpha'\mathbf{m}_4^2$
$12, 12', 21', 1'2'$	0.16	0.20	0.16	0.49
$13, 13', 31', 1'3'$	0.20	0.15	0.20	0.45
$24, 24', 42', 2'4'$	0.01	0.05	0.30	0.64
$34, 34', 43', 3'4'$	0.05	0.01	0.34	0.59

(3.25)

We can see that they are all positive, hence the intersections are free of tachyons, and the system is stable against recombination of the corresponding cycles.

Pairs of branes with zero intersection number are parallel in some two-torus. In this model, in the nongeneric case that the branes overlap in this two-torus, open strings stretched between them would lead to additional tachyons,

Intersection	$\alpha'\mathbf{m}_1^2$	$\alpha'\mathbf{m}_2^2$	$\alpha'\mathbf{m}_3^2$	$\alpha'\mathbf{m}_4^2$
$11'$	0.35	0.35	-0.35	0.65
$22'$	-0.04	0.04	0.67	0.33
$33'$	0.05	-0.05	0.75	0.25
$44'$	0.06	0.06	-0.06	0.94
$14, 1'4'$	0.14	0.14	-0.14	0.86
$14', 41'$	0.21	0.21	-0.21	0.79
$23, 2'3'$	0.36	-0.36	0.36	0.64
$23', 32'$	-0.31	0.31	0.39	0.61

(3.26)

However, these states are not tachyonic if the branes are separated beyond a critical distance in the corresponding two-torus. It is possible that higher effects, due to brane interactions (one loop in the open string channel), induce a nonzero attractive force between such nonintersecting branes, pushing them to the tachyonic region. In any event, this would be a higher order effect which might be avoided in more complicated models. Our point here is that tachyons and intersections, which appear at tree level and are therefore more dangerous, can be eliminated in some models by a suitable choice of background geometry.

In principle it is possible that this kind of tachyon-free configurations exist in models without the orientifold projection, even though a systematic exploration of parameter space is more difficult. We would like to conclude by pointing out that, since the main difficulty arising from satisfying the tadpole conditions, the above ideas may have a much simpler implementation in other contexts, where such conditions are not relevant. For instance, one may construct a large class of (meta)stable non-BPS states in type IIB theory on $\mathbf{T}^6$, by considering D3-branes wrapped on 3-cycles with tachyon-free intersections.

F. Tachyons and Higgs mechanism

Even if tachyons are present, we would like to point out a quite different perspective on them, which is actually applicable to more general examples (among others, those of D4- and D5-branes in the coming sections). As in the more familiar example of brane–antibrane systems (see, e.g.,

Refs. 16, 34), the condensation of open string tachyons may in certain situations be interpreted as a Higgs mechanism. In our present context, the tachyon is charged under the gauge groups on the intersecting branes, and its condensation reduces the gauge symmetry to that of the recombined brane. From the spacetime viewpoint, it is physically clear that the tachyon has a potential with a minimum, at which the energy of the condensate compensates the difference of tensions between the final and initial states, and at which the tachyon vev breaks the initial gauge symmetry. Adapting Sen's ideas,[16] the intersecting branes with the tachyon condensed to its minimum is *exactly* the final configuration of the recombined brane (stretched along a minimum volume cycle in its homology class). (This is particularly clear in the T-dual picture of D9-branes with magnetic fluxes, where the above process often amounts to annihilation of topological defects on the D9-brane world-volume. Some remarks on tachyon condensation as a Higgs mechanism in this picture have appeared in Ref. 35.)

This idea has an important and interesting caveat, in the interpretation of the inverse process as un-Higgsing. Basically, the final state does not keep track of what initial state it came from. Hence if the system is given energy, it will nucleate not only the W bosons corresponding to the original initial state, but also W bosons of enhanced symmetries associated to all other possible initial states in the same energy range. However, there may be situations where one possible initial state is substantially lighter than the rest. In this situation, a low-energy observer, with a limited range of available energies, would systematically find a single pattern of gauge symmetry enhancement. This situation is close enough to a standard Higgs mechanism, so that tachyons may be interpreted as standard Higgs fields (at least for processes in the appropriate range of energies), even for electroweak symmetry breaking. A more detailed understanding of the tachyon potential and dynamics[34] would help in determining if such a scenario is indeed viable for electroweak or other phenomenological Higgs mechanisms. For the moment, we just point out the tantalizing existence of tachyon fields with the quantum numbers of standard model Higgs fields in some of the models we have explored (see Sec. IV C and Ref. 15 for further details).

IV. D4-BRANES WRAPPING AT ANGLES ON $\mathbf{T^2\times C^2/Z_N}$

A. Construction

As discussed in Sec. II, configurations of D4-branes wrapped on 1-cycles in $\mathbf{T^2\times C^2}$ lead necessarily to nonchiral spectra. In this section we study a simple modification of this basic framework, which leads to generically chiral four-dimensional gauge field theories on the D-brane world-volume.

We consider configurations of D4-branes on $\mathbf{T^2\times(C^2/Z_N)}$, where the D4-branes are distributed in stacks of multiplicity N_a, wrapped along one-cycles Π_a defined by wrapping numbers (n_a,m_a), on $\mathbf{T^2}$ and sitting at the origin in $\mathbf{C^2/Z_N}$. The models admit a T-dual description in terms of type IIB D5-branes on $\mathbf{T^2\times(C^2/Z_N)}$, with nontrivial wrapping numbers and fluxes on $\mathbf{T^2}$. We usually phrase our results in the D4-brane picture, but translation to the D5-brane picture is straightforward, as in the models in Sec. III.

The twist $\mathbf{Z_N}$ is generated by a geometric action θ with a twist vector given by $v=(1/N)(b_1,b_2,0,0)$, where $b_1=b_2$ mod 2 for the variety to be spin. The supersymmetric case is recovered when $b_2=-b_1$ mod N, hence with twist $v=(1/N)(b_1,-b_1,0,0)$. In this case, since b_1 and N must be coprime for a $\mathbf{Z_N}$ action, the orbifold group can be equivalently generated by the twist θ^k, with $kb_1=1$ mod N, which has the more familiar twist vector $v=(1/N)(1,-1,0,0)$.

We would like to emphasize that we imagine this framework as a local description of the configuration near the location of the branes. Globally, the local configuration above may be embedded in a spacetime of the form $\mathbf{T^2\times B}$, where $\mathbf{B}$ is a four-dimensional space (not necessarily Calabi–Yau) with a $\mathbf{C^2/Z_N}$ singularity at which the D-branes sit. More generally, the complete space may not be globally a product, but rather a torus bundle over $\mathbf{B}$, or even a torus fibration, as long as singular fibers are away from the D-brane location. Our configuration is a good local description in these cases, and completely controls the structure of the D-brane world-volume gauge theory.

Let us briefly mention another interesting aspect. These configurations admit a seemingly simple lift to M-theory, as a set of M-theory fivebranes sitting at a $\mathbf{C^2/Z_N}$ singularity, and wrapped on a two-cycle in $\mathbf{T^2\times S^1}$. Obviously, a detailed description of the model in M-theory will involve a number of interesting subtleties, on which our analysis may shed some light. Note that the existence of this six-dimensional parent theory, which reduces to the four-dimensional field theory after compactification, is not in contradiction with chirality in the latter. The higher-dimensional theory is not a conventional field theory, and in fact four-dimensional chiral states arise from membranes stretched between M5-branes and wrapped on $\mathbf{S^1}$, i.e., they do not descend by KK reduction from any six-dimensional field.

Let us describe the computation of the spectrum in our configuration. The closed string sector is computed using standard orbifold techniques. In the supersymmetric case, it gives rise to an $D=4$ $\mathcal{N}=4$ $U(1)^{N-1}$ gauge multiplet. In the nonsupersymmetric case, the main feature is that it leads to tachyons in the NS–NS sector. Their interpretation is, as usual with closed string tachyons, not understood, and we will have nothing new to say about them. Nevertheless, we choose to study these models and in particular their open string spectrum even for nonsupersymmetric singularities.

The $\mathbf{Z_N}$ action may be embedded in the $U(N_a)$ gauge degrees of freedom of the ath stack of D4-branes, through a unitary matrix of the form

$$\gamma_{\theta,a}=\mathrm{diag}(\mathbf{1}_{N_a^0},e^{2\pi i\,(1/N)}\mathbf{1}_{N_a^1},\ldots,e^{2\pi i\,[(N-1)/N]}\mathbf{1}_{N_a^{N-1}}), \tag{4.1}$$

with $\Sigma_i N_a^i=N_a$.

Let us compute the spectrum in the open string sector. In the 4_a4_a sector, the massless states surviving the GSO projection, along with their behavior under the $\mathbf{Z_N}$ twist, are

NS State	$\mathbf{Z_N}$ phase	R State	$\mathbf{Z_N}$ phase
$(\pm 1,0,0,0)$	$e^{\pm 2\pi i\,(b_1/N)}$	$\pm\frac{1}{2}(-,+,+,+)$	$e^{\mp\pi i\,[(b_1-b_2)/N]}$
$(0,\pm 1,0,0)$	$e^{\mp 2\pi i\,(b_2/N)}$	$\pm\frac{1}{2}(+,-,+,+)$	$e^{\pm\pi i\,[(b_1-b_2)/N]}$
$(0,0,\pm 1,0)$	1	$\pm\frac{1}{2}(+,+,-,+)$	$e^{\pm\pi i\,[(b_1+b_2)/N]}$
$(0,0,0,\pm 1)$	1	$\pm\frac{1}{2}(+,+,+,-)$	$e^{\pm\pi i\,[(b_1+b_2)/N]}$

(4.2)

The open string spectrum is obtained by keeping states invariant under the combined geometric plus Chan–Paton $\mathbf{Z_N}$ action.[36] After the $\mathbf{Z_N}$ projections, the resulting gauge group and matter fields are

$$\begin{aligned}
&\text{Gauge bosons} \quad \prod_{a=1}^{K}\prod_{i=1}^{N} U(N_a^i),\\
&\text{Cmplx. scalars} \quad \sum_{a=1}^{K}\sum_{i=1}^{N}\left[\,(N_a^i,\overline{N_a^{i+b_1}})+(N_a^i,\overline{N_a^{i+b_2}})\right],\\
&\text{Left fermion} \quad \sum_{a=1}^{K}\sum_{i=1}^{N}\left[(N_a^i,\overline{N_a^{i+(b_1-b_2)/2}})+(N_a^i,\overline{N_a^{i-(b_1-b_2)/2}}),\right.\\
&\text{Right fermion} \quad \sum_{a=1}^{K}\sum_{i=1}^{N}\left[(N_a^i,\overline{N_a^{i+(b_1+b_2)/2}})+(N_a^i,\overline{N_a^{i-(b_1+b_2)/2}}).\right.
\end{aligned} \tag{4.3}$$

Notice that this piece of the spectrum is generically nonsupersymmetric, and always nonchiral. In the supersymmetric case, $v=(1,-1,0,0)/N$, this sector preserves $\mathcal{N}=2$ supersymmetry in the four-dimensional field theory. The above fields form the multiplets,

$$\mathcal{N}=2 \quad \text{vector} \quad \prod_{a=1}^{K}\prod_{i=1}^{N} U(N_a^i),$$
$$\mathcal{N}=2 \quad \text{hyper} \quad \sum_{a=1}^{K}\sum_{i=1}^{N} (N_a^i,\overline{N}_a^{i+1}). \tag{4.4}$$

In the 4_a4_b sector, open strings are twisted by the angle formed by the branes, denoted ϑ, resulting in a sector twisted by the shift $(\vartheta,0,0,0)$. Assuming $0\leqslant\vartheta\leqslant 1$, tachyonic and massless states, along with their $\mathbf{Z_N}$ phases, are

Sector	State	$\mathbf{Z_N}$ phase
NS	$(-1+\vartheta,0,0,0)$	1
R	$(-\frac{1}{2}+\vartheta,-\frac{1}{2},-\frac{1}{2},+\frac{1}{2})$	$e^{-2\pi i[(b_1+b_2)/2N]}$
	$(-\frac{1}{2}+\vartheta,-\frac{1}{2},+\frac{1}{2},-\frac{1}{2})$	$e^{-2\pi i[(b_1-b_2)/2N]}$
	$(-\frac{1}{2}+\vartheta,+\frac{1}{2},-\frac{1}{2},-\frac{1}{2})$	$e^{2\pi i[(b_1-b_2)/2N]}$
	$(-\frac{1}{2}+\vartheta,+\frac{1}{2},+\frac{1}{2},+\frac{1}{2})$	$e^{2\pi i[(b_1+b_2)/2N]}$

(4.5)

This piece of the spectrum is nonsupersymmetric, even for supersymmetric $\mathbf{Z_N}$ twists. The NS states are tachyonic, with $\alpha' M^2$ equal to $-\frac{1}{2}|\vartheta|$, and signal an instability against recombining intersecting D4-branes with the same Chan–Paton eigenvalue. Hence, they may be avoided by suitable choices of the $\mathbf{Z_N}$ actions $\gamma_{\theta,4_a}$. A different possibility is to interpret these tachyons as triggering breaking of gauge symmetries by a Higgs mechanism, as mentioned in Sec. III D. The R states are massless, and provide a set of chiral fermions in the model. Notice that the antiparticles of these states appear in the 4_b4_a sector, which is twisted by $(-\vartheta,0,0,0)$.

In these sectors the spectrum generically appears in several replicas, whose number is given by the intersection number I_{ab} of the one-cycles Π_a and Π_b in $\mathbf{T^2}$,

$$I_{ab}=n_am_b-m_an_b\,. \tag{4.6}$$

The spectrum after the Chan–Paton projections is given by

$$\text{Cmplx. tachyons} \quad \sum_{a<b}\sum_{i=1}^{N} I_{ab}\times(N_a^i,\overline{N}_b^i),$$
$$\text{Left fermion} \quad \sum_{a<b}\sum_{i=1}^{N} I_{ab}\times[(N_a^i,\overline{N}_b^{i+(b_1+b_2)/2}+(N_a^i,\overline{N}_b^{i-(b_1+b_2)/2}], \tag{4.7}$$
$$\text{Right fermion} \quad \sum_{a<b}\sum_{i=1}^{N} I_{ab}\times[(N_a^i,\overline{N}_b^{i+(b_1-b_2)/2}+(N_a^i,\overline{N}_b^{i-(b_1-b_2)/2}],$$

which is nonsupersymmetric and generically chiral. Therefore the resulting field theories may lead to phenomenologically interesting models. In fact, in Sec. IV C we construct an explicit example with a Standard Model group and three quark lepton generations.

B. Tadpoles and anomalies

1. Tadpole cancellation conditions

The consistency conditions (RR tadpole cancellation conditions) for these configurations are easily computed, and read as

$$\prod_{r=1,2} \sin(\pi k b_r/N) \sum_{a=1}^{K} n_a \mathrm{Tr}\gamma_{\theta^k,4_a} = 0,$$

$$\prod_{r=1,2} \sin(\pi k b_r/N) \sum_{a=1}^{K} m_a \mathrm{Tr}\gamma_{\theta^k,4_a} = 0,$$

for $k=1,\ldots,N-1$.

There is no constraint associated to $k=0$, since the untwisted tadpole is associated to a flux that can escape along the noncompact dimensions of $\mathbf{C}^2/\mathbf{Z}_\mathbf{N}$.

These conditions can be interpreted geometrically, at least for supersymmetric singularities, by regarding the fractional[37] $D4_a^s$-branes (i.e., the set of $D4_a$ branes associated to the phase $e^{2\pi i (s/N)}$ in $\gamma_{\theta,4_a}$) as D6-branes wrapped on the 1-cycle $[\Pi_a]=n_a[a]+m_a[b]$ in $\mathbf{T}^2$ times the sth collapsed two-cycle $[\Sigma_s]$ in the singularity. The conditions above amount to the vanishing of the total homology class,

$$\sum_{a=1}^{K} \sum_{s=0}^{N-1} N_a^s [\Pi_a] \otimes [\Sigma_s] = 0. \tag{4.8}$$

Since $\Sigma_{s=0}^{N-1}[\Sigma_s]=0$, one can increase the N_a^s by an s-independent (but possibly a-dependent) amount and still satisfy the homological condition. Hence, the Chan–Paton matrices for $k=0$ are unconstrained. Note that regarding branes at singularities as branes wrapped on collapsed cycles, our models of D4-branes become a degenerate version of D6-branes wrapped on 3-cycles in a curved ambient space, and our results here are reminiscent of those in Sec. III B.

2. Anomaly cancellation

The spectrum of the model is generically chiral, and has potential gauge anomalies. In analogy with the case of D6-branes on $\mathbf{T}^6$, cancellation of the anomalies due to chiral fermions at each intersection would be achieved by an inflow mechanism. Since the intersections sit at the singularity in transverse space, this inflow mechanism would be more involved and interesting, but still tractable. Leaving aside its study, we prefer to center on the compactified effective four-dimensional description of anomaly cancellation.

The cancellation of cubic non-Abelian anomalies for $SU(N_a^i)$ gives the conditions

$$\sum_{b=1}^{K} I_{ab}(-N_b^{i+(b_1+b_2)/2} - N_b^{i-(b_1+b_2)/2} + N_b^{i+(b_1-b_2)/2} + N_b^{i-(b_1-b_2)/2}) = 0. \tag{4.9}$$

These conditions should follow from the tadpole cancellation conditions. In fact, using (4.1) we can rewrite

$$N_b^i = \frac{1}{N} \sum_{k=0}^{N-1} e^{-2\pi i (ki/N)} \mathrm{Tr}\gamma_{\theta^k,4_b}, \tag{4.10}$$

as in Ref. 38, and the anomaly cancellation conditions read as

$$\prod_{r=1,2} \sin(\pi k b_r/N) \sum_{b=1}^{K} I_{ab} \mathrm{Tr}\gamma_{\theta^k,4_b} = 0. \tag{4.11}$$

These conditions are indeed guaranteed by the tadpole conditions (4.8), but, as usual, are much milder than the latter.

Let us consider cancellation of mixed $U(1)$ anomalies, which involves a generalized Green–Schwarz mechanism, mediated by $2(N-1)$ fields, corresponding to the integration of $N-1$ twisted RR-fields along the two independent 1-cycles in the $\mathbf{T}^2$.

In fact, one can compute the mixed anomaly between the $U(1)_{ai}$ and $SU(N_b^j)$ using the chiral piece of the spectrum (4.7). After removing a vanishing piece proportional to the non-Abelian anomaly, there remains

$$\mathcal{A}_{ai,bj}=\tfrac{1}{2}N_a^i I_{ab}(\delta_{j,i+(b_1+b_2)/2}+\delta_{j,i-(b_1+b_2)/2}-\delta_{j,i+(b_1-b_2)/2}-\delta_{j,i-(b_1-b_2)/2}). \tag{4.12}$$

Substituting the discrete Fourier transform representation of the Kronecker deltas, as in Ref. 29, the anomaly acquires the nice factorized form

$$A_{ai,bj}=iN_a^i I_{ab}\frac{1}{N}\sum_{k=1}^{N-1}4\prod_{r=1,2}\sin(\pi k b_r/N)e^{2\pi i(ki/N)}e^{-2\pi i(kj/N)}. \tag{4.13}$$

The anomaly may therefore be cancelled by exchange of the four-dimensional fields obtained by integrating over the two one-cycles in $\mathbf{T^2}$ the RR twisted forms, which give the four-dimensional couplings:

$$c_k N_a^i n_a\int_{M_4}\mathrm{Tr}(\gamma_{\theta^k,4_a}\lambda_i)\,C_2^{(k)}\wedge\mathrm{tr}F_{a,i};\quad c_k m_b\int_{M_4}\mathrm{Tr}(\gamma_{\theta^k,4_b}\lambda_j^2)\,C_0^{(k)}\wedge\mathrm{Tr}F_{b,j}^2,$$

$$-c_k N_a^i m_a\int_{M_4}\mathrm{Tr}(\gamma_{\theta^k,4_a}\lambda_i)\,B_2^{(k)}\wedge\mathrm{tr}F_{a,i};\quad c_k n_b\int_{M_4}\mathrm{Tr}(\gamma_{\theta^k,4_b}\lambda_j^2)\,B_0^{(k)}\wedge\mathrm{Tr}F_{b,j}^2,$$

where λ denotes the CP wavefunction of the gauge boson state. The prefactors $c_k=[\Pi_r\sin(\pi k b_r/N)]^{1/2}$ can be thought of as arising from $\hat{A}^{1/2}$ in D-brane couplings,[20] and have been explicitly computed in string theory in, e.g., Refs. 31, 32. Since B_2 and B_0, and C_2 and C_0 are Hodge dual in four dimensions, the sum over GS diagrams has the structure (4.13). The GS mechanism is analogous to that for D6-branes on $\mathbf{T^6}$, as is manifest from the appearance of the intersection number, the main difference being that the exchanged fields belong to twisted sectors of the $\mathbf{C^2/Z_N}$ factor.

The above results can be interpreted geometrically by regarding the fractional $D4_a$-branes as D6-branes wrapped on collapsed cycles Σ_s of the singularity and the one-cycle Π_a in $\mathbf{T^2}$. This is simplest in the more familiar supersymmetric case where the anomaly is given by

$$A_{ai,bj}=\tfrac{1}{2}N_b^j I_{ab}(2\delta_{j,i}-\delta_{j,i+1}-\delta_{j,i-1}). \tag{4.14}$$

The collapsed two-cycles have intersections given by (minus) the Cartan matrix of the (affine) $\hat{A}_{N-1}$ algebra, $C_{ij}=[\Sigma_i]\cdot[\Sigma_j]=-2\delta_{ji}+\delta_{j,i+1}+\delta_{j,i-1}$. Hence, the intersection number of D6-branes wrapped on cycles $[\Pi_a]\otimes[\Sigma_i]$ and $[\Pi_b]\otimes[\Sigma_j]$ is $I_{ab}C_{ij}$. Introducing a composite index I grouping together indices a and i, we can express the mixed anomaly (4.14) as

$$A_{IJ}=\tfrac{1}{2}N_I\mathcal{I}_{IJ}, \tag{4.15}$$

where $\mathcal{I}_{IJ}$ denotes the 3-cycle intersection form. The situation is hence analogous to that in Sec. III B. As suggested, the GS cancellation mechanism in Sec. III B can be directly translated, with the obvious modifications, reproducing the cancellation of anomalies in the present context. Since here the wrapped 3-cycles are exceptional divisors of the singularity, the forms mediating the GS mechanism arise as twisted states in string theory. The above geometric interpretation follows also for nonsupersymmetric $\mathbf{Z_N}$ twist, by using the corresponding intersection matrix, obtained from (4.12).

As in Sec. III B, anomalous $U(1)$'s get a mass of the order of the string scale. To find nonanomalous $U(1)$'s, we consider linear combinations,

$$Q=\sum_{a=1}^{K}\sum_{j=0}^{N-1}\frac{c_{a,j}}{N_a^j}Q_{a,j} \tag{4.16}$$

(we choose $c_{b,i}=0$ if the corresponding group is not present, namely if $N_a^i=0$). Nonanomalous $U(1)$'s can again be found as zero modes of the (generalized) intersection matrix. In fact, we can be slightly more explicit. Taking the supersymmetric singularity case for concreteness, and using the expression (4.13), anomaly-free linear combinations satisfy

$$\frac{1}{N}\sum_{k=1}^{N-1}e^{-2\pi i\,(kj/N)}\sin^2(\pi k/N)\sum_{a=1}^{K}I_{ab}\sum_{i=0}^{N-1}e^{2\pi i\,(ki/N)}c_{a,i}=0, \tag{4.17}$$

for each $b=1,\ldots,K$ and $j=0,\ldots,N-1$. A useful trick is to perform the change of coordinates[5] $r_{a,k}=\Sigma_{i=0}^{N-1}e^{2\pi i\,(ki/N)}c_{a,i}$, and obtain the conditions

$$\sin^2(\pi k/N)\sum_{a=1}^{K}I_{ab}\,r_{a,k}=0. \tag{4.18}$$

A set of solutions is given by choosing, for a fixed a, $r_{a,k}=\delta_{k,0}$, and $r_{b,k}=0$ for $b\neq a$. The resulting generator is

$$Q_a=\sum_{i=0}^{N-1}\frac{Q_{a,i}}{N_a^i}. \tag{4.19}$$

Another combination is obtained by choosing $c_{a,i}=N_a^i$, or equivalently by $r_{a,k}=\mathrm{Tr}\,\gamma_{\theta^k,4_a}$, namely

$$Q=\sum_{a=1}^{K}\sum_{i=0}^{N-1}Q_{a,i}. \tag{4.20}$$

Depending on the details of the orbifold group, there may be additional nonanomalous $U(1)$'s. These are most easily determined by directly computing the zero modes of the anomaly matrix in each case.

C. Explicit models

In the present context it is not possible to get rid of all the tachyons while maintaining a chiral fermion spectrum. A general argument goes as follows. Since tachyons arise in $4_a4_b+4_b4_a$ sectors from strings stretching between D4-branes with the same Chan–Paton phase, to avoid tachyons we must consider models where any two intersecting branes have no common Chan–Paton eigenvalues. Consider models with N stacks of $\mathrm{D4}_a$-branes, hence $K=N$, at a $\mathbf{C^2/Z_N}$ singularity, with twist, e.g., $v=(1,-1)/N$, and wrapped on arbitrary 1-cycles Π_a on $\mathbf{T^2}$, and choose the Chan–Paton embeddings,

$$\gamma_{\theta,4_a}=e^{2\pi i\,(a/N)}\mathbf{1}_{N_a}, \tag{4.21}$$

hence $N_a^i=N_a\delta_{a\,i}$ (more general choices can be treated analogously). The spectrum one naively obtains seems chiral, but the tadpole conditions,

$$\sum_{a=1}^{N}e^{2\pi i\,(ka/N)}N_a[\Pi_a]=0,\quad \text{for } k=1,\ldots,N-1, \tag{4.22}$$

turn out to be very constraining. By discrete Fourier transforming, they imply that all $[\Pi_a]$ are actually identical, so all D4-branes are parallel, leading to nonchiral spectra.

Allowing a nonsupersymmetric singularity may relax the tadpole conditions, but introduces (closed string) tadpoles. Also, the case $K<N$ reduces to the above with some $N_a=0$, while additional branes ($K>N$) necessarily repeat eigenvalues and must be nonintersecting, i.e., parallel, to the existing ones to avoid tachyons.

Allowing for some tachyons in the model, however, one can obtain large classes of models with a chiral spectrum, which moreover can be quite close to realistic models. Let us discuss a simple explicit model, which illustrates a possible model building strategy.

Since $\mathbf{Z_2}$ leads to vector-like models, let us consider sets of D4-branes at $\mathbf{T^2\times C^2/Z_3}$, with twist $v=(1,-1,0,0)/3$. A typical tachyon-free and hence nonchiral model would have three stacks of D4-branes, with $\gamma_{\theta,4_a}=e^{2\pi i\, a/3}\mathbf{1}$, and parallel cycles. Consider, e.g., the stack with $\gamma_\theta=\mathbf{1}$ with multiplicity 3 and cycle (1,0), and the remaining two with multiplicity 1 and cycle (3,0), yielding a gauge group $U(3)\times U(1)\times U(1)$ with vector-like matter. To get chirality, we must allow one of these sets to split into several intersecting stacks, a process which also implies the appearance of tachyons (which would trigger the recombination to the original configuration). Let us build this enlarged model with a Standard Model gauge group, namely including a stack with group $U(2)$, and with triplicated intersections. A possible choice is to split the brane with $\gamma_\theta=e^{2\pi i/3}$ wrapped on (3,0), into two branes wrapped on (1,3), one brane on $(0,-3)$ and one brane on $(1,-3)$. Hence we end up with

Multiplicity	Cycle	CP phase
$N_1=3$	(1,0)	1
$N_2=2$	(1,3)	$e^{2\pi i/3}$
$N_3=1$	$(0,-3)$	$e^{2\pi i/3}$
$N_4=1$	$(1,-3)$	$e^{2\pi i/3}$
$N_5=1$	(3,0)	$e^{2\pi i\, 2/3}$

(4.23)

The chiral spectrum contains left-handed fermions transforming under $U(3)\times U(2)\times U(1)_3^3\times U(1)_4\times U(1)_5^3$ as

$$\begin{aligned}&3(3,2)_{[1,-1,(0^3),0,(0^3)]}+(\overline{3},1)_{[-1,0,\underline{1,0,0},0,(0^3)]}+3(\overline{3},1)_{[-1,0,(0^3),1,(0^3)]}\\&\quad+2(1,2)_{[0,1,\underline{-1,0,0},0,(0^3)]}+12(1,2)_{[0,1,(0^3),-1,(0^3)]}+3(1,2)_{[0,-1,(0^3),0,\underline{1,0,0}]}\\&\quad+2(1,1)_{[0,0,\underline{-1,0,0},1,(0^3)]}+(1,1)_{[0,0,\underline{1,0,0},0,\underline{-1,0,0}]}+3(1,1)_{[0,0,(0^3),1,\underline{-1,0,0}]},\end{aligned}\tag{4.24}$$

where underlining means permutation. Besides the diagonal combination, which decouples, there are six nonanomalous $U(1)$ linear combinations. One of them, given by

$$Q_Y=-\tfrac{1}{3}Q_1-\tfrac{1}{2}Q_2-Q_4-(Q_5^{(1)}+Q_5^{(2)}+Q_5^{(3)}),\tag{4.25}$$

provides the correct hypercharge assignments for the above theory, which therefore has the chiral content of a three-generation standard model. Indeed, highlighting the charges under this $U(1)$, the fermion spectrum is

$$3(3,2)_{1/6}+3(\overline{3},1)_{1/3}+3(\overline{3},1)_{-2/3}+15(1,2)_{-1/2}+12(1,2)_{1/2}+6(1,1)_{-1}+9(1,1)_1+9(1,1)_0.\tag{4.26}$$

Further properties of these models will be discussed in Ref. 15. Here let us simply point out that, in models constructed using the above strategy, the tachyons trigger the recombination of branes involving the $U(2)$ factor, and therefore have the gauge quantum numbers of standard

model Higgs fields. These models therefore illustrate that tachyonic modes may be phenomenologically interesting (to trigger electroweak or other extended symmetry breakings), and that in this class of models they are linked to the existence of chiral fermions.

As mentioned in the Introduction, even though the models are nonsupersymmetric, the hierarchy problem is avoided by considering a low string scale and a compactification with large volume for the space transverse to the two-torus.

V. D5-BRANES WRAPPING AT ANGLES ON $(T^2)^2 \times C/Z_N$

A. Construction

For completeness, in this section we center on a last type of configuration, similar to those in the preceding section, and also leading to four-dimensional chiral theories. We consider configurations of D5-branes in $\mathbf{T^4}\times(\mathbf{C}/\mathbf{Z_N})$, where the D5-branes sit at the origin in $\mathbf{C}/\mathbf{Z_N}$, and are grouped in stacks of multiplicity N_a wrapped on 2-cycles defined by (n_a^I, m_a^I), with $I=1,2$, in a factorizable $\mathbf{T^4}$.

The $\mathbf{Z_N}$ action on the third dimension is encoded in the twist vector of the form $v = (1/N)\,(0,0,2,0)$ for the variety to be spin. The closed string sector necessarily contains tachyons in its twisted sector, whose interpretation is unclear. Nevertheless, we proceed studying these models. The Chan–Paton twist matrices have the general form

$$\gamma_{\theta,a} = \mathrm{diag}(\mathbf{1}_{N_a^0}, e^{2\pi i\,(1/N)}\mathbf{1}_{N_a^1}, \ldots, e^{2\pi i\,[(N-1)/N]}\mathbf{1}_{N_a^{N-1}}), \tag{5.1}$$

with $\Sigma_i N_a^i = N_a$. The lowest lying states in the 5_a5_a open string NS and R sectors, along with their $\mathbf{Z_N}$ phases, are

NS state	$\mathbf{Z_N}$ phase;	R State	$\mathbf{Z_N}$ phase
$(\pm 1,0,0,0)$	1	$\pm\frac{1}{2}(-,+,+,+)$	$e^{\pm 2\pi i\,(1/N)}$
$(0,\pm 1,0,0)$	1	$\frac{1}{2}(+,-,+,+)$	$e^{\pm 2\pi i\,(1/N)}$
$(0,0,\pm 1,0)$	$e^{\pm 4\pi i\,(1/N)}$	$\pm\frac{1}{2}(+,+,-,+)$	$e^{\mp 2\pi i\,(1/N)}$
$(0,0,0,\pm 1)$	1	$\pm\frac{1}{2}(+,+,+,-)$	$e^{\pm 2\pi i\,(1/N)}$

(5.2)

The spectrum is nonsupersymmetric. The fourth NS state leads to $\Pi_{a=1}^K \Pi_{i=1}^N U(N_a^i)$ gauge bosons, while the remaining give a set of scalars in bifundamental or adjoint representations. In the R sector, no state is invariant under $\mathbf{Z_N}$, and the model contains no gauginos. On the other hand, it contain a nonchiral set of fermions in diverse bifundamental representations. Summarizing, the spectrum contains the following fields:

$$\begin{aligned}
&\text{Gauge bosons} \quad \prod_{a=1}^{K}\prod_{i=1}^{N} U(N_a^i),\\
&\text{Real scalars} \quad \sum_{a=1}^{K}\sum_{i=1}^{N} [(N_a^i, \overline{N}_a^{i+2}) + 2\times \mathrm{Adj}_{a,i}],\\
&\text{Right fermion} \quad \sum_{a=1}^{K}\sum_{i=1}^{N} (N_a^i, \overline{N}_a^{i+1}),\\
&\text{Left fermion} \quad \sum_{a=1}^{K}\sum_{i=1}^{N} (\overline{N}_a^{i+1}, N_a^i).
\end{aligned} \tag{5.3}$$

In the 5_a5_b sector, open strings are twisted by the angle formed by the branes in the two-tori, encoded in a twist vector $(\vartheta_1,\vartheta_2,0,0)$. The lowest lying states, along with their behavior under $\mathbf{Z_N}$, are (assuming $0\leqslant\vartheta_I\leqslant 1$)

Sector	State	$\mathbf{Z_N}$ phase
NS	$(-1+\vartheta_1,0,0,0)$	1
	$(0,-1+\vartheta_2,0,0)$	1
R	$(-\frac{1}{2}+\vartheta_1,-\frac{1}{2}+\vartheta_2,+\frac{1}{2},-\frac{1}{2})$	$e^{2\pi i\,1/N}$
	$(-\frac{1}{2}+\vartheta_1,-\frac{1}{2}+\vartheta_2,-\frac{1}{2},+\frac{1}{2})$	$e^{-2\pi i\,(1/N)}$

Recall that at most one of the two NS states is tachyonic (both are massless for $|\vartheta_1|=|\vartheta_2|$), while fermions are massless.

The spectrum of tachyonic and massless states, after the Chan–Paton projections, and taking into account the multiplicity due to the intersection numbers,

$$I_{ab}=I^1_{ab}I^2_{ab}=(n^1_am^1_b-m^1_an^2_b)(n^2_am^2_b-m^2_an^2_b), \tag{5.4}$$

is given by

$$\begin{aligned}
&\text{Cmplx. Tachyons} \quad \sum_{a<b}\sum_{i=1}^{N} I_{ab}\times(N^i_a,\overline{N^i_b}),\\
&\text{Left fermion} \quad \sum_{a<b}\sum_{i=1}^{N} I_{ab}\times(N^i_a,\overline{N^{i+1}_b}),\\
&\text{Right fermion} \quad \sum_{a<b}\sum_{i=1}^{N} I_{ab}\times(N^i_a,\overline{N^{i-1}_b}).
\end{aligned} \tag{5.5}$$

In the case $|\vartheta_2|=|\vartheta_1|$ we would have two bosonic massless states instead of the above tachyon.

B. Tadpoles and anomalies

The analysis of tadpole and anomaly cancellation is similar to that for configurations in Sec. IV B, hence our discussion is more sketchy.

Tadpole cancellation conditions read as

$$\begin{aligned}
&\sin(4\pi k/N)\,n^1_a\,n^2_a\,\mathrm{Tr}\,\gamma_{\theta^k,4_b}=0; \quad \sin(4\pi k/N)\,m^1_a\,n^2_a\,\mathrm{Tr}\,\gamma_{\theta^k,4_b}=0,\\
&\sin(4\pi k/N)\,n^1_a\,m^2_a\,\mathrm{Tr}\,\gamma_{\theta^k,4_b}=0; \quad \sin(4\pi k/N)\,m^1_a\,ma^2\,\mathrm{Tr}\,\gamma_{\theta^k,4_b}=0,
\end{aligned} \tag{5.6}$$

and clearly have the interpretation of the cancellation of charges analogous to that for Eqs. (4.8).

These conditions must ensure the consistency of the low-energy four-dimensional field theory on the D-brane world-volume. In particular, the cancellation of cubic non-Abelian chiral anomalies for $SU(N^i_a)$ reads as

$$\sum_{b=1}^{K} I_{ab}(N^{i+1}_b-N^{i-1}_b)=0, \tag{5.7}$$

or, equivalently, by performing the discrete Fourier transform (4.10),

$$\sin(4\pi k/N)I_{ab}\mathrm{Tr}\,\gamma_{\theta^k,5_b}=0. \tag{5.8}$$

By substituting (5.4) in this equation, we see that it is implied by the tadpole constraints.

Using the spectrum (5.3) it is easy to compute the mixed anomalies between $U(1)_{ai}$ and $SU(N_{bj})$. We obtain

$$A_{ai,bj}=\frac{1}{2}N_a^j I_{ab}(\delta_{j,i+1}-\delta_{j,i-1})=i\,N_a^i I_{ab}\frac{1}{N}\sum_{k=1}^{N-1}\sin(2\pi k/N)\,e^{2\pi i\,(ki/N)}\,e^{-2\pi i\,(kj/N)}, \quad (5.9)$$

where, again, the second equality shows the residual anomaly has a factorized structure, which can be cancelled by a GS mechanism mediated by four-dimensional fields obtained by integrating twisted RR fields on diverse two-cycles in $\mathbf{T^4}$.

The existence and form of nonanomalous (and therefore massless) $U(1)$ linear combinations can be carried out in complete analogy with that in Sec. IV B 2.

VI. FINAL COMMENTS AND OUTLOOK

In this paper we have studied the construction of four-dimensional chiral string compactifications with a gauge sector localized on D-branes wrapped on nontrivial cycles in the internal space. Specifically, we have studied configurations of D$(3+n)$-branes wrapped on n-cycles in $\mathbf{T^{2n}\times C^{3-n}/Z_N}$, where the last factor should be understood as a local model of a singularity within a compact $(6-2n)$-dimensional variety, so that correct four-dimensional gravity is recovered. Several properties (like the anomaly cancellation mechanisms) however hold in more general setups.

The configurations allow a bottom-up approach to embedding realistic gauge sectors in string theory models, in the sense explained in Ref. 5. In fact, the configurations are a natural extension of the work on D3-branes at threefold singularities (e.g., $\mathbf{C^3/Z_N}$) in Ref. 5. However, we have found a number of interesting differences, and original features in the configurations considered in this paper.

Our results in this paper extend the early results in Ref. 6 on intersecting branes to the context of compact models, leading to a large class of nonsupersymmetric chiral four-dimensional models. We have provided a simple set of rules to construct explicit models, and there studied general features. One amusing feature is that, as observed in Ref. 13, compact models of intersecting branes lead naturally to replication of the chiral fermion content, due to the multiple intersections between different wrapped branes. In fact, we have used this property to construct explicit three-generation models with realistic gauge groups.

In analogy with other string compactifications, we have found a rich structure of mixed $U(1)$ anomalies. We have shown that they are cancelled by a generalized GS mechanism mediated by untwisted or twisted RR fields. While the GS mediation by the latter is familiar from type IIB orientifolds,[30,29] the former (valid for D6-brane models) is rather unusual and interesting. We expect it to have relevant phenomenological applications.

Finally, we have discussed that although the models are nonsupersymmetric, they can be used for phenomenological purposes without a hierarchy problem, by simply lowering the string scale, and enlarging the volume transverse to the D-branes. A lack of supersymmetry also induces the appearance of tachyons, for which we have suggested an elimination mechanism, and a tantalizing phenomenological application in certain regimes.

Leaving further phenomenological properties of these configurations for a discussion in Ref. 15, we conclude hoping these results are helpful in the construction of new open string vacua, and in their phenomenological application in the brane-world scenario.

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Nonrelativistic closed string theory

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We construct a Galilean invariant nongravitational closed string theory whose excitations satisfy a nonrelativistic dispersion relation. This theory can be obtained by taking a consistent low energy limit of any of the conventional string theories, including the heterotic string. We give a finite first order worldsheet Hamiltonian for this theory and show that this string theory has a sensible perturbative expansion, interesting high energy behavior of scattering amplitudes and a Hagedorn transition of the thermal ensemble. The strong coupling duals of the Galilean superstring theories are considered and are shown to be described by an eleven-dimensional Galilean invariant theory of light membrane fluctuations. A new class of Galilean invariant nongravitational theories of light-brane excitations are obtained. We exhibit dual formulations of the strong coupling limits of these Galilean invariant theories and show that they exhibit many of the conventional dualities of M theory in a nonrelativistic setting. © *2001 American Institute of Physics.*
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I. INTRODUCTION

One of the legacies of the second superstring revolution is the realization that the different superstring theories describe very special corners of the space of vacua of a single hypothetical structure dubbed M Theory. Another important lesson that has emerged is that there are regions of the space of vacua describable by a theory without gravity. Two beautiful examples of such theories are Matrix Theory[1] and Maldacena's conjecture.[2] The realization that there are consistent limits of M Theory without gravity has led to a geometrical understanding of some field theory dualities and to new, hitherto unknown, field theories in higher dimensions.

The nongravitational limits studied thus far involve considering certain low energy limits of M Theory in the presence of branes. Typically, these limits lead to a theory where the appropriate effective description is given in terms of the massless degrees of freedom propagating on the branes. Such low energy limits lead, for example, to gauge theories in various dimensions. In such examples, the massive open string states on the branes and the entire closed string spectrum decouple from the low energy physics and the truncation to the theory of the massless fluctuations is consistent. These low energy theories are described by field theories.

Recently, very interesting generalizations have been found in which closed strings decouple but the massive open string excitations on the branes need to be taken into account for physical processes.[3,4] These theories appear in low energy limits of branes in near critical electric field backgrounds and are not conventional field theories due to the presence of a tower of massive excitations. Since massive states cannot be neglected, the field theory truncation is not unitary.[5–7] These nongravitational theories describe all the fluctuations on the branes. For example, one can obtain a consistent open string theory without any closed string states. Such theories arise from studying D-branes in a background electric field (NCOS),[3,4] M5-branes in a three-form background (OM)[8] and Neveu–Schwarz five-branes in various constant Ramond–Ramond *p*-form backgrounds (OD).[8–10]

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In this paper we find that there are corners of the moduli space of vacua of M Theory without branes that are described by nongravitational theories whose excitations live in space–time. These massive excitations satisfy a nonrelativistic dispersion relation and the theory that describes their dynamics is unitary and has a sensible perturbative description (whenever one is available). Since background branes are not required to define these nonrelativistic theories, they can be obtained by taking certain low energy limits of all five superstring theories, including the heterotic string. We will call these theories nonrelativistic closed string theories (NRCS).

The simplest limit leading to NRCS is obtained by considering string theory in the presence of a near critical NS–NS two-form field without any D-brane (when the NS–NS two-form exceeds the critical value, the space–time energy of a closed string becomes unbounded below and can become indefinitely negative as we increase the winding number). In the context of $(1+1)$-dimensional NCOS, Klebanov and Maldacena[11] observed that when the spatial direction is compactified on a circle, that there are finite energy winding closed string states that do not decouple from the open strings. An example of NRCS can be obtained by considering precisely the NCOS limit without any D-brane. Naively, one might think that, in the absence of D-branes, that a constant NS–NS two-form can be gauged away and that one ends up getting a conventional relativistic closed string theory. This is obviously true in noncompact space. However, in the presence of a circle, the background NS–NS field modifies the spectrum, which remains relativistic. Once the NCOS limit is taken, there is a truncation of the low energy spectrum and one obtains a new theory with a Galilean invariant Hamiltonian. Perhaps surprisingly, the closed string theory in the NCOS limit without any D-brane has a well-behaved perturbative expansion, described by the Lagrangian in Sec. III. It is also interesting to study the worldsheet theory we propose when the worldsheet has a boundary. Then, our formalism reproduces the relativistic open string spectrum of NCOS and its interactions.

In Sec. III, we give a worldsheet Lagrangian for NRCS, which has Galilean invariance and from which we derive the nonrelativistic spectrum of closed strings and their interactions. The Lagrangian we propose can be derived from the conventional Polyakov path integral quantization of the relativistic string by rewriting it in variables that are conducive to taking the low energy limit that defines NRCS (see Sec. III for details of the limit). We explicitly solve the Virasoro constraints, thus yielding the spectrum, show that the theory is unitary and that it has a sensible perturbative expansion. The string spectrum, being nonrelativistic, does not contain a massless graviton and it is thus nongravitational in nature. However, there is an instantaneous Newtonian potential between the massive strings. This string theory exhibits interesting properties such as an unusual high energy behavior of scattering amplitudes and a Hagedorn transition of the thermal ensemble.

NRCS depends on two parameters, the effective string scale α'_{eff} and the effective string coupling constant g. One may ask what is the strong coupling dual of these theories. For the superstrings, this can be reliably answered. We find that the strong coupling limits of supersymmetric NRCS are given by a Galilean invariant eleven-dimensional theory of light membranes which we call GM (Galilean membrane theory). This eleven-dimensional theory has a unique dimensionful parameter l_{eff} which is the effective Planck length. The relation between the NRCS superstrings and GM is reminiscent to the relation between the conventional superstrings and M theory. For example, Type IIA NRCS with coupling g and string scale α'_{eff} is equivalent to GM on a circle of radius R such that $R=g\sqrt{\alpha'_{\text{eff}}}$ and $l_{\text{eff}}=g^{1/3}\sqrt{\alpha'_{\text{eff}}}$. The conventional dualities and relations with M theory still hold, such that, for example. Type IIB NRCS has an $SL(2,Z)$ symmetry. We discuss these relations in Sec. VII. It is interesting that duality symmetries in string theories do not rely on relativistic invariance nor the presence of gravity.

There are many interesting generalizations that can be made that lead to nonrelativistic, nongravitational theories. The construction of such theories is quite general. The basic idea is to study the low energy limit of M Theory vacua in the presence of any of the many possible gauge fields available. Then, one can take a low energy, near critical limit such that all states of M Theory become infinitely massive, and thus decouple, except for those states that couple to the constant near critical background gauge field. Tuning to the critical value, defined such that that

energy coming from the background field precisely cancels the rest energy of the states in question, ensures that even though we are taking a low energy limit, that there are states that survive and satisfy a nonrelativistic dispersion relation. For example, if we tune the background NS–NS B field to its critical value, then one obtains finite energy nonrelativistic fluctuations of strings winding around the circle. Clearly, such NRCS can be defined in Type II, Type I and heterotic theories. Moreover, if one considers, for example, a near critical R–R gauge field C_{p+1} and takes a low energy limit, then there are light Dp-branes (in order for the constant background C_{p+1} field to affect the energy of a Dp-brane, the brane has to be wrapped on a p-cycle, otherwise the gauge field can be gauged away without changing the energetics) which are nonrelativistic that decouple from all the rest of the modes and lead to decoupled Galilean invariant theories which we will call GDp (Galilean Dp-brane theories). The myriad of gauge fields that exist in M Theory vacua can be used to define new nongravitational Galilean invariant theories. We study such theories in Sec. VII. The dualities of the underlying relativistic M Theory, lead to interesting webs of dualities for these nonrelativistic theories. These nonrelativistic theories may be a promising ground in which to address some of the important questions of M Theory without the complication of gravity.

The rest of the paper is organized as follows.

In Sec. II a very general low energy limit is presented which yields a finite nonrelativistic dispersion relation from the spectrum of a charged relativistic brane. The limit, when applied to the fundamental closed string, yields the spectrum of NRCS. Generalizations to other relativistic objects in M Theory are briefly described.

In Sec. III we find the worldsheet theory of NRCS. We quantize the Galilean invariant, first order Hamiltonian and find under what conditions there is a physical closed string spectrum. We then reproduce the NRCS spectrum in Sec. II within our Hamiltonian formalism. We compute the BRST cohomology of the string and show that there are no ghosts in the spectrum. The possibility of adding a boundary to the worldsheet is considered. The formalism of Sec. III results in the spectrum and worldsheet correlation functions of NCOS. Using this formalism, it is straightforward to prove the decoupling of the massless open string states on worldsheets with any number of handles and holes when the longitudinal direction is noncompact. This extends the result of Ref. 11 to all orders in the perturbative expansion.

Section IV is devoted to performing tree level computations in NRCS. We show that scattering amplitudes have the correct pole structure required by unitarity and have a peculiar behavior of high energy fixed angle scattering amplitudes in NRCS. Despite the absence of gravity in this theory, we exhibit a Newtonian potential among the nonrelativistic strings.

In Sec. V we compute loop amplitudes and show that NRCS is a sensible theory in perturbation theory. We evaluate the Helmholtz free energy at one loop and reproduce from it the spectrum of NRCS found in Sec. II. We find that NRCS behaves similarly to the long string near the boundary of AdS_3.[12] We exhibit the existence of a Hagedorn temperature in NRCS and sketch higher loop computations. We also study in some detail N-point loop amplitudes and show that the amplitudes are finite.

In Sec. VI we elucidate the relation between NRCS and the discrete light-cone quantization (DLCQ) of closed string theory. NRCS is related by T-duality to the discrete light-cone quantization (DLCQ) of closed string theory. Therefore, the formalism developed in this paper provides a useful description of DLCQ string theories as well.

In Sec. VII we study Galilean invariant theories of light branes and some of their dualities. In eleven dimensions we study the Galilean invariant theory of membrane fluctuations (GM) and five-brane fluctuations (GF). In ten dimensions we discuss the theory of nonrelativistic light Dp-branes (GDp) and light Neveu–Schwarz five-branes (GNS). These theories lie in the same moduli space and exhibit the same dualities that the underlying relativistic M theory possesses. In particular we show that the strong coupling limits of some NRCS have an eleven-dimensional description in terms of light-brane excitations.

II. NONRELATIVISTIC LIMIT

In this section we show that by taking a low energy limit of the theory of a relativistic p-brane and by tuning the $p+1$ gauge field that couples to it, that one can obtain an exact nonrelativistic dispersion relation. The idea is to study the low energy spectrum in a scaling limit in which the background gauge field cancels the rest energy of the brane and such that the nonrelativistic approximation becomes exact. In this limit, all the states of the theory decouple, except the light p-brane excitations. We present the truncation to a nonrelativistic theory in a very simple toy model which captures the essence of the limit which defines NRCS and the other generalizations we describe in this paper.

For simplicity, consider a relativistic charged point particle of mass m and charge e coupled to a gauge field A_μ propagating in a geometry with metric components $g_{00}=-1$ and g_{ij} arbitrary with $i, j \neq 0$. The Lagrangian which describes its motion is given by

$$L=-m\sqrt{-\dot{x}^2}+eA_\mu \dot{x}^\mu. \tag{2.1}$$

Worldline reparametrization invariance implies Einstein's dispersion relation,

$$p_0=\sqrt{m^2+g^{ij}(p_i-eA_i)(p_j-eA_j)}+eA_0. \tag{2.2}$$

Consider the following low energy limit:

$$g_{ij}=\frac{m_{\text{eff}}}{m}\delta_{ij}, \quad eA_0=-m+e\hat{A}_0, \tag{2.3}$$

as $m\to\infty$. In this limit, Einstein's relation (2.2) reduces to the following nonrelativistic dispersion law:

$$p_0=\frac{1}{2m_{\text{eff}}}(p_i-eA_i)^2+e\hat{A}_0. \tag{2.4}$$

Although a constant gauge field can be locally gauged away and does not affect the equations of motion, it changes the energy spectrum in the sector of the theory carrying electric charge. In fact, the shift in the energy due to the gauge field precisely cancels the rest mass of the particle and ensures that the energy remains finite in the limit (2.3). Turning on a background field and tuning it to the critical value is an efficient way of rearranging the spectrum of the theory such that only states charged under the gauge field have finite energy, the neutral states acquire infinite proper energy.

The charged point particle model can also be used to show that the there are finite energy, nonrelativistic winding closed string states in the NCOS limit whenever the near critical NS–NS B_{01}-field is along a compact spatial direction. The mass of a closed string winding w-times around a circle of radius R is

$$m^2=\left(\frac{wR}{\alpha'}\right)^2+\frac{2(N+\tilde{N})}{\alpha'}, \tag{2.5}$$

where N and $\overline{N}$ are the amounts of stringy excitations in the left and the right mover oscillators of the string. Moreover, the winding string states are charged under the $U(1)$ gauge field obtained by reducing the NS–NS B-field along the circle. The charge is given by

$$eA_0=-2\pi R w B_{01}. \tag{2.6}$$

We now take the NCOS limit[3,4] in the point particle analogy (2.4),

$$g_{ij}=\frac{\alpha'}{\alpha'_{\rm eff}}\delta_{ij}, \quad eA_0=-\frac{wR}{\alpha'}\left(1-\frac{\alpha'}{2\alpha'_{\rm eff}}\right). \tag{2.7}$$

Taking $\alpha'\to 0$ results in the following nonrelativistic spectrum:

$$p_0=\frac{wR}{2\alpha'_{\rm eff}}+\frac{\alpha'_{\rm eff}k^2}{2wR}+\frac{N+\tilde{N}}{wR}. \tag{2.8}$$

Thus the NCOS limit can be thought of an example of the nonrelativistic limit (2.3). Note that demanding positive energy states selects strings winding only in a particular direction. Indeed, the closed string spectrum (2.8) coincides with the one found by Maldacena and Klebanov in Ref. 11. In the next section we give a Galilean invariant, finite first order Hamiltonian that describes these closed strings and verify that there is a consistent perturbative expansion.

The nonrelativistic limit we found in (2.3) can also be generalized to any state of M Theory which is charged under a gauge field. If one considers winding fundamental closed strings in the near critical NS–NS B_{0i} background of any of the known string theories, one obtains NRCS theories. But we could have considered any of the branes of M Theory. One could, for example, consider a wrapped membrane of M Theory on any two-cycle (say on a two-torus or a two-cycle of a Calabi–Yau) in a critical three-form background. Then, the membrane is charged under a gauge field A_0 obtained by reducing the three-form on the two-cycle. In the limit (2.3) one obtains a nonrelativistic theory without gravity. Likewise, for any other brane. Just like in NCOS, positivity of the energy selects only those states which are wrapped in a particular direction, states of opposite orientation are unphysical. In Sec. VII we will find low energy limits leading to Galilean theories of branes and study their strong coupling duals.

III. LAGRANGIAN AND QUANTIZATION

In this section we construct the worldsheet theory of NRCS and analyze its spectrum and interactions. We consider a certain low energy limit of string theory in a near critical NS–NS B-field. The bosonic worldsheet action which describes this background is given by (here the worldsheet and target space metric are taken to be of Lorentzian signature)

$$S_0=-\frac{1}{4\pi\alpha'}\int d^2\sigma(g_{MN}\,\partial_a X^M\,\partial^a X^N-2\pi\alpha' B_{MN}\epsilon^{ab}\,\partial_a X^M\,\partial_b X^N), \tag{3.1}$$

where $M, N=0,...,9$ and $a, b=0,1$. NRCS is obtained by choosing the B-field with a time-like and a space-like component. Without loss of generality we consider a $B_{01}\equiv B$ background. NRCS is obtained by taking the following zero slope, near critical field limit (this is precisely the NCOS limit of Refs. 3, 4 but without any D-brane),

$$2\pi\alpha' B_{01}=1-\frac{\alpha'}{2\alpha'_{\rm eff}}, \quad g_{\mu\nu}=\eta_{\mu\nu}, \quad g_{ij}\frac{\alpha'}{\alpha'_{\rm eff}}\delta_{ij}, \quad g_s=g\sqrt{\frac{\alpha'_{\rm eff}}{\alpha'}}, \tag{3.2}$$

as $\alpha'\to 0$ where $\mu, \nu=0,1$ and $i,j=2,...9$, and $\alpha'_{\rm eff}$ is the finite effective string scale of NRCS and g its effective coupling constant.

Using

$$\gamma=X^0+X^1, \quad \overline{\gamma}=-X^0+X^1, \tag{3.3}$$

for the target space coordinates,

$$z=e^{i(\sigma^0+\sigma^1)}, \quad \overline{z}=e^{i(\sigma^0-\sigma^1)}, \tag{3.4}$$

for the worldsheet coordinates, and the background given in (3.2), the action (3.1) can be written for finite α' as

$$S_0 = -\frac{1}{4\pi\alpha'}\int d^2z(\partial\gamma\bar{\partial}\bar{\gamma}+\partial\bar{\gamma}\bar{\partial}\gamma-2\pi\alpha' B(\partial\gamma\bar{\partial}\bar{\gamma}-\partial\bar{\gamma}\bar{\partial}\gamma)+2g_{ij}\partial X^i\bar{\partial}X^j). \tag{3.5}$$

We now perform a Euclidean rotation in both the worldsheet and target space such that the Euclidean action is

$$S_0 = \frac{1}{4\pi\alpha'}\int d^2z(\partial\lambda\,\bar{\partial}\bar{\gamma}+\partial\bar{\gamma}\bar{\partial}\gamma-2\pi\alpha' B(\partial\gamma\bar{\partial}\bar{\gamma}-\partial\bar{\gamma}\bar{\partial}\gamma)+2g_{ij}\partial X^i\bar{\partial}X^j). \tag{3.6}$$

Note that, unlike the case of a *B*-field with only space-like components, there is no factor of *i* in the term in the Euclidean action depending on *B*.

In order to obtain a finite worldsheet description in the NRCS limit, it is convenient to introduce Lagrange multipliers β and $\bar{\beta}$. In these variables the worldsheet theory (3.6) is given by

$$S_1 = \int\frac{d^2z}{2\pi}\left(\beta\bar{\partial}\gamma+\bar{\beta}\bar{\partial}\bar{\gamma}-\frac{2\alpha'}{1+2\pi\alpha' B}\beta\bar{\beta}+\frac{1+2\pi\alpha' B}{2\alpha'}\partial\gamma\bar{\partial}\bar{\gamma}+\frac{1}{\alpha'}g_{ij}\partial X^i\bar{\partial}X^j\right), \tag{3.7}$$

where (3.6) is reproduced by integrating out β and $\bar{\beta}$. Therefore, in the strict decoupling limit (3.2), one has the following Lagrangian description of NRCS:

$$S_1 = \int\frac{d^2z}{2\pi}\left(\beta\bar{\partial}\gamma+\bar{\beta}\bar{\partial}\bar{\gamma}+\frac{1}{4\alpha'_{\rm eff}}\partial\gamma\bar{\partial}\bar{\gamma}+\frac{1}{\alpha'_{\rm eff}}\partial X^i\bar{\partial}X_i\right). \tag{3.8}$$

We note that the worldsheet theory of NRCS is defined in terms of more variables than a conventional critical string theory since we have extra β and $\bar{\beta}$ variables. However, the CFT defined by (3.8) has the correct Virasoro central charge to define a consistent string action (see the next subsection for more details). It is interesting to note that the Lagrangian (3.8) is invariant under the Galilean group in the transverse coordinates. This is consistent with the nonrelativistic spectrum that we will find for NRCS. It is crucial, for this symmetry to be realized, that the description has the extra variables β and $\bar{\beta}$.

We will concentrate on the conformal field theory of β, $\bar{\beta}$ and γ, $\bar{\gamma}$ since the transverse coordinates lead to familiar contributions. The equations of motion force β and γ to be holomorphic and $\bar{\beta}$ and $\bar{\gamma}$ to be antiholomorphic. The Lagrange multiplier β forces γ to be a holomorphic map from the worldsheet to the $(1+1)$-dimensional part of the target space parameterized by coordinates X^0 and X^1. Therefore, it describes a worldsheet instanton and the third term in the Lagrangian (3.8) $(1/8\pi\alpha'_{\rm eff})\partial\gamma\bar{\partial}\bar{\gamma}$ is the instanton action. We will show in the rest of this section that this Lagrangian reproduces the spectrum in (2.8). Moreover, we will see that if the string worldsheet has a boundary that (3.8) reproduces the open string spectrum of NCOS and string interactions. In our formalism, one can show that the decoupling of the massless open string modes exhibited by Ref. 11 at the disk level can be extended to all orders in perturbation theory. Thus, (3.8) can be used to perform manifestly finite worldsheet computations for NCOS theories. In the later sections, we will use this Lagrangian to describe amplitudes involving closed strings and higher loops.

A. Closed string spectrum

Here we consider a worldsheet without boundaries. The equations of motion of (3.8) imply that $\beta(z)$ and $\gamma(z)$ are holomorphic and that $\bar{\beta}(\bar{z})$ and $\bar{\gamma}(\bar{z})$ are antiholomorphic. Their OPE's are given by

$$\beta(z)\gamma(w)\sim\frac{-1}{z-w},\quad \overline{\beta}(\overline{z})\overline{\gamma}(\overline{w})\sim\frac{-1}{\overline{z}-\overline{w}},$$

$$\gamma(z)\beta(w)\sim\frac{1}{z-w},\quad \overline{\gamma}(\overline{z})\overline{\beta}(\overline{w})\sim\frac{1}{\overline{z}-\overline{w}},\tag{3.9}$$

$$\gamma(z)\overline{\gamma}(\overline{w})\sim\text{regular},\quad \beta(z)\overline{\beta}(w)\sim\frac{-\pi}{2\alpha'_{\text{eff}}}\delta^{(2)}(z-w).$$

The variables β and γ behave analogously to the bosonic ghost system, except for the contact term in $\beta(z)\overline{\beta}(\overline{w})$. The conformal dimension of γ is (0, 0) while the conformal dimension of β is (1, 0). Moreover, their contribution to the Virasoro central charge takes the required value $c=2$. Note that although it seems that we have added more degrees of freedom to the description, the worldsheet degrees of freedom are identical to those of two worldsheet scalars. A similar story holds for the $\overline{\beta}$ and $\overline{\gamma}$ system.

We will first consider the case when the x^1 coordinate is noncompact. Then we can expand the operators as

$$\gamma(z)=\sum_{n=-\infty}^{\infty}\gamma_n z^{-n},\quad \beta(z)=\sum_{n=-\infty}^{\infty}\beta_n z^{-n-1}.\tag{3.10}$$

Since γ is holomorphic and x^1 is noncompact the standard space–time momentum term in γ is not allowed. Otherwise, γ would be multi-valued function of σ, which is only possible if the string is winding. The oscillator modes satisfy the following commutation relation:

$$[\gamma_n,\beta_m]=\delta_{n+m,0}.\tag{3.11}$$

We now study the Virasoro constraints for NRCS. The energy momentum tensor is given by

$$T(z)=-\beta\,\partial\gamma,\tag{3.12}$$

and the Virasoro generators are

$$L_n=\sum_m m\beta_{n-m}\gamma_m.\tag{3.13}$$

In particular, L_0 is the excitation level of the (β, γ) system, whose spectrum is positive definite. Therefore the Virasoro constraint $L_0+\tilde{L}_0=1$ has no solutions (except for the tachyon, which is projected out in supersymmetric theories), where $\tilde{L}_0$ is the Virasoro generator for the rest of the system, which we assume to be positive definite. Thus, the closed string has no physical states. This can be easily understood. If all coordinates are noncompact the background NS–NS B-field can be gauged away without changing the Hamiltonian of the theory and the closed string spectrum is the usual one. Therefore, in the NRCS limit (3.2), all the closed strings acquire infinite proper energy and thus are unphysical.

When the x^1 direction is compactified on a circle of radius R, there is a nonzero winding sector in $\gamma(z)$. The mode expansion now reads as

$$\gamma(z)=iwR\log z+\sum_{n=-\infty}^{\infty}\gamma_n z^{-n},\tag{3.14}$$

and the Virasoro generator is then given by

$$L_n = -i\beta_n wR + \sum_m m\beta_{n-m}\gamma_m . \tag{3.15}$$

Now the Virasoro constraint $L_0+\tilde{L}_0=1$ has a solution. As we will show later, all physical states are in the vacuum of the (β, γ)-system. Thus the solution to the Virasoro constraint is of the form

$$i\beta_0 = \frac{N}{wR} + \frac{\alpha'_{\rm eff}k^2}{4wR}, \tag{3.16}$$

where N is the conformal weight of the rest of the system (N includes -1 for the bosonic string and $-1/2$ for the NS sector of superstring) and k is the transverse momentum of the string. According to the Lagrangian (3.8), the canonical momentum P conjugate to γ is not equal to β, but in the winding sector it is shifted by an amount proportional to $\bar{\partial}\bar{\gamma}$ as in

$$\frac{1}{2}(P_0+P_1) = \frac{\beta}{2\pi} - \frac{1}{8\pi\alpha'_{\rm eff}}\bar{\partial}\bar{\gamma}, \quad \frac{1}{2}(P_0-P_1) = \frac{\bar{\beta}}{2\pi} - \frac{1}{8\pi\alpha'_{\rm eff}}\partial\gamma. \tag{3.17}$$

Taking the zero mode parts of these equations, one finds that the total energy p_0 and momentum p_1 of the closed string are given by

$$\frac{1}{2}(p_0+p_1) = i\beta_0 + \frac{1}{4\alpha'_{\rm eff}}wR, \quad \frac{1}{2}(p_0-p_1) = i\bar{\beta}_0 + \frac{1}{4\alpha'_{\rm eff}}wR. \tag{3.18}$$

Since x^1 is periodic, its conjugate momentum is quantized as

$$p_1 = \frac{n}{R}. \tag{3.19}$$

Thus we find

$$p_0 = \frac{wR}{2\alpha'_{\rm eff}} + \frac{\alpha'_{\rm eff}k^2}{2wR} + \frac{N+\bar{N}}{wR}, \tag{3.20}$$

with the level matching condition $N-\bar{N}=wn$. In this way, we have recovered the nonrelativistic spectrum in (2.8).

It is straightforward to prove the no-ghost theorem in this case. We introduce the (b, c) ghost and write the BRST operator $Q_{\rm BRST}$ as

$$Q_{\rm BRST} = Q_{-1} + Q_0, \tag{3.21}$$

where

$$Q_{-1} = wR\sum_n \beta_{-n}c_n, \tag{3.22}$$

and Q_0 is defined as the remainder. They obey

$$Q_{-1}^2 = Q_0^2 = \{Q_{-1}, Q_0\} = 0. \tag{3.23}$$

Following the use of the BRST operator in Ref. 13 (see also Sec. 4.4 of Ref. 14), one can show that the cohomology of $Q_{\rm BRST}$ is isomorphic to that of Q_{-1}. The cohomology of the quadratic

operator Q_{-1} is easy to evaluate[15] and it is spanned by the vacuum state $|0\rangle_{\beta\gamma}\otimes|0\rangle_{bc}$ of (β, γ) and (b, c), times any states in the rest of the system. Assuming that the rest of the system is unitary, this proves the no-ghost theorem of NRCS.

B. Open string spectrum

It is possible to consider D-branes in NRCS, and what one gets is of course NCOS. Here we show that the open string spectrum of NCOS is reproduced in this way. Suppose the worldsheet is the upper half plane with the boundary located at $\sigma^1=0$. In the bulk, γ and β are still holomorphic. The equation of motion at the boundary gives

$$\delta\gamma\left(\beta+\frac{1}{4\alpha'_{\rm eff}}\bar{\partial}\bar{\gamma}\right)=0, \quad \delta\bar{\gamma}\left(\bar{\beta}+\frac{1}{4\alpha'_{\rm eff}}\partial\gamma\right)=0. \tag{3.24}$$

For a Dp-brane with $p\geqslant 1$, the boundary values of $(\gamma,\bar{\gamma})$ are not fixed. Therefore

$$\beta=-\frac{1}{4\alpha'_{\rm eff}}\bar{\partial}\bar{\gamma}, \quad \bar{\beta}=-\frac{1}{4\alpha'_{\rm eff}}\partial\gamma, \tag{3.25}$$

at the boundary. This suggests that we analytically continue (γ,β) to $\sigma^1<0$ and use (3.25) to identify (γ, β) on $\sigma^1\geqslant 0$ to $(\bar{\gamma},\bar{\beta})$ in $\sigma^1\leqslant 0$. Since

$$\beta(z)\gamma(w)\sim-\frac{1}{z-w}, \quad \bar{\beta}(\bar{z})\bar{\gamma}(\bar{w})\sim-\frac{1}{\bar{z}-\bar{w}}, \tag{3.26}$$

we find

$$\gamma(z)\bar{\gamma}(\bar{w})\sim 4\alpha'_{\rm eff}\log(z-\bar{w}). \tag{3.27}$$

For points on the real axis this reproduces the correct propagator for open strings in NCOS.

To compute the open string spectrum, we consider a worldsheet that is a strip $-\pi\leqslant\sigma^1\leqslant\pi$, we identify (γ, β) on $0\leqslant\sigma^1\leqslant\pi$ to $(\bar{\gamma},\bar{\beta})$ on $-\pi\leqslant\sigma^1\leqslant 0$ according to (3.25). Thus we have the expansion of these fields as

$$\begin{aligned}
&\beta=\frac{1}{2\sqrt{\alpha'_{\rm eff}}}\sum_n \bar{\alpha}_n\bar{z}^{-n-1}, \quad \gamma=x+4ip\alpha'_{\rm eff}\log z+2\sqrt{\alpha'_{\rm eff}}\sum_{n\neq 0}\frac{\alpha_n}{n}z^{-n},\\
&\bar{\beta}=\frac{1}{2\sqrt{\alpha'_{\rm eff}}}\sum_n \alpha_n z^{-n-1}, \quad \bar{\gamma}=\bar{x}+4i\bar{p}\alpha'_{\rm eff}\log\bar{z}+2\sqrt{\alpha'_{\rm eff}}\sum_{n\neq 0}\frac{\bar{\alpha}_n}{n}\bar{z}^{-n},
\end{aligned} \tag{3.28}$$

and nonzero commutators are

$$[\alpha_n,\bar{\alpha}_m]=n\delta_{n+m,0}, \quad [x,\bar{p}]=[\bar{x},p]=i. \tag{3.29}$$

Note that, unlike the case of closed string, the space–time momentum term $4ip\,\alpha'_{\rm eff}\log z$ is allowed in γ even when x^1 is noncompact. This is because we can choose the branch cut of $\log z$ to be away from the worldsheet. The Virasoro generators are then

$$L_n=\sum_m \bar{\alpha}_{n-m}\alpha_m. \tag{3.30}$$

Thus we reproduce the standard open string spectrum.

C. Free the $U(1)$ to all order

In Ref. 11, it was shown that any tree level amplitude containing a massless open string state in $NCOS_2$ vanishes when the longitudinal direction is noncompact. This is what is expected from the point of view of the S-dual theory, where the massless open strings correspond to the free $U(1)$ gauge fields and their superpartners in the $(1+1)$-dimensional $U(N)$ gauge theory. Using the formalism developed here, it is straightforward to generalize this result to all orders in perturbation theory. The open string amplitude on a worldsheet with h holes and g handles is computed by considering a closed Riemann surface of genus $2g$ with a complex conjugate involution such that the fixed point set of the involution gives the boundaries of the open string worldsheet. Since there is no vertex operator inserted away from the boundary (when the longitudinal direction is noncompact there is no closed string physical state), $\gamma(z)$ is holomorphic everywhere except at the boundaries. Moreover, the vertex operator for a massless open string state is also holomorphic (vertex operators for massive states are not holomorphic; they also depend on $\overline{\gamma}$). Since the sum of the boundaries of the h holes obtained as the fixed point set of the involution is homologically trivial on the genus $2g$ surface, the contour integral of the vertex operator can be deformed away through the middle of the Riemann surface. This proves the decoupling of the massless open string states to all order in the perturbation theory.

IV. TREE AMPLITUDES

In this section we will compute the scattering amplitude of four physical closed string states and show that it factorizes properly into nonrelativistic closed string poles. Moreover, we will see that the truncated closed string scattering amplitudes have a different high energy behavior than in conventional string theory.

For simplicity, we will compute the 4-tachyon amplitude. Since all the physical states are in the vacuum of the (β, γ)-system as we saw in the last section, the essential novelty of NRCS is captured by the tachyon amplitude. The vertex operator for a closed string tachyon is given by (we will not include the cocycles which only change relative signs between amplitudes; the factor $\sqrt{w}$ is included for later convenience)

$$V(v,\overline{v},k;z,\overline{z}) = g\sqrt{w}:e^{i\overline{v}\gamma(z)+iwR\int^z\beta+iv\overline{\gamma(z)}+iwR\int^{\overline{z}}\overline{\beta}+ik\cdot X(z,\overline{z})}:. \tag{4.1}$$

Since

$$\begin{aligned} \gamma(z)V(z') &\sim iwR\log(z-z')V(z'), \\ \beta(z)V(z') &\sim \frac{-i\overline{v}}{z-z'}V(z'), \end{aligned} \tag{4.2}$$

the vertex operator carries $(\beta_0,\overline{\beta}_0)$ eigenvalues of $(-i\overline{v},-iv)$ and winding number w. Thus, according to (3.18), the energy ϵ and the longitudinal momentum n/R of the tachyon state are given by

$$\epsilon = v+\overline{v}+\frac{1}{2\alpha'_{\text{eff}}}wR, \quad \frac{n}{R}=\overline{v}-v. \tag{4.3}$$

Let us evaluate the 4-point amplitude on the sphere, $\langle V_1(z_1)V_2(z_2)V_3(z_3)V_4(z_4)\rangle$, by performing the functional integral with the Lagrangian (3.8). The extremum of the functional integral is given by

$$\gamma(z) = i\sum_{a=1}^{4} w_a R\log(z-z_a), \quad \beta(z) = -i\sum_{a=1}^{4}\frac{\overline{v}_a}{z-z_a}. \tag{4.4}$$

For closed string amplitudes, the winding number has to be conserved (the winding number is not conserved when one considers worldsheet with boundaries), such that $\Sigma_a w_a = 0$. Since the action is free, we can evaluate the amplitude by substituting (4.4) back into the integrand [as is always the case with the Gaussian integral; the same result is obtained by substituting the extremal value (4.4) into the product of the vertex operators $V_1V_2V_3V_4$ alone and by taking its square root]. The amplitude is given by

$$\begin{aligned}
&\langle V_1(z_1)V_2(z_2)V_3(z_3)V_4(z_4)\rangle \\
&\quad = \sqrt{w_1\cdots w_4}\prod_{a\neq b}(z_a-z_b)^{-\bar{v}_a w_b R}(\bar{z}_a-\bar{z}_b)^{-v_a w_b R}|z_a-z_b|^{(\alpha'_{\rm eff}/2)k_a k_b} \\
&\quad = \sqrt{w_1\cdots w_4}\prod_{a<b}|z_a-z_b|^{-(\epsilon_a+\epsilon_b)(w_a+w_b)R+(R^2/2\alpha'_{\rm eff})(w_a+w_b)^2+(\alpha'_{\rm eff}/2)(k_a+k_b)^2-4}. \quad (4.5)
\end{aligned}$$

Here we used the on-shell condition for the tachyon,

$$\begin{aligned}
\epsilon_a &= \frac{w_a R}{2\alpha'_{\rm eff}} + \frac{\alpha'_{\rm eff}k_a^2}{2w_a R} - \frac{2}{w_a R}, \\
v_a &= \bar{v}_a \quad (a=1,\ldots,4).
\end{aligned} \tag{4.6}$$

It is a good test of our formalism to compute the same correlation function using the standard closed string theory and then take the NCOS limit (3.2). One can verify that (4.5) is reproduced in the limit. The tachyon scattering amplitude is then given by

$$\mathcal{A} = ig^4 C_{\rm sphere}\int d^2z\langle V_1(0)V_2(z)V_3(1)V_4(\infty)\rangle. \tag{4.7}$$

Here g is the closed string coupling constant and $C_{\rm sphere}$ is the normalization constant that normalizes the path integral of the string when the topology of the worldsheet is the sphere. The normalization constant can be found by unitarity. Namely, the amplitude in (4.7) has poles associated with intermediate closed string states and a straightforward application of the optical theorem determines it. Therefore, by repeating the analysis in, for example, Sec. 6.6 of Ref. 14, we find

$$C_{\rm sphere} = \frac{2\pi}{g^2 R}. \tag{4.8}$$

This means that even though the theory is defined in the $g_s\to\infty$ limit, that the closed string theory has a sensible perturbation expansion in powers of g. This is consistent with the observation made in Ref. 4 regarding closed string loop diagrams in NCOS.

The amplitude given by (4.5) and (4.7) is very similar to the familiar Virasoro–Shapiro amplitude. It has poles in the energies in the intermediate channels, and they are located at

$$\epsilon_a+\epsilon_b = \frac{(w_a+w_b)R}{2\alpha'_{\rm eff}} + \frac{\alpha'_{\rm eff}(k_a+k_b)^2}{2(w_a+w_b)R} + \frac{2n-2}{(w_a+w_b)R} \quad (n=0,1,2,\ldots). \tag{4.9}$$

This is precisely the closed string spectrum of NRCS, as required by unitarity. From (4.7) we can also see that NRCS exhibits a different behavior of high energy, fixed-angle scattering amplitudes. Since the mass-shell condition of the strings is nonrelativistic, the dependence of the amplitude on energy E is $\mathcal{A}\sim e^{-E}$, as opposed to the conventional dependence $\mathcal{A}\sim e^{-E^2}$.

Although there are no physical states in the sector with 0-winding number and in particular no graviton in the spectrum, there is an instantaneous Newtonian potential between winding strings.

To see this, let us consider the process in which the winding number is not exchanged among strings, i.e., $w_1+w_3=0$ and $w_2+w_4=0$. In this case, the correlation function (4.5) becomes

$$\begin{aligned}
&\langle V_1(z_1)V_2(z_2)V_3(z_3)V_4(z_4)\rangle \\
&\quad = w_1 w_2 (|z_1-z_3||z_2-z_4|)^{\alpha'_{\rm eff}(k_1+k_3)^2-4} \\
&\qquad \times (|z_1-z_2||z_3-z_4|)^{-(\epsilon_1+\epsilon_2)(w_1+w_2)R+(R^2/2\alpha'_{\rm eff})(w_1+w_2)^2+(\alpha'_{\rm eff}/2)(k_1+k_2)^2-4} \\
&\qquad \times (|z_1-z_4||z_2-z_3|)^{-(\epsilon_1+\epsilon_4)(w_1-w_2)R+(R^2/2\alpha'_{\rm eff})(w_1-w_2)^2+(\alpha'_{\rm eff}/2)(k_1+k_4)^2-4}. \qquad (4.10)
\end{aligned}$$

Since the winding number along the (k_1+k_3)-channel is 0, no physical states are propagating in this channel. Nevertheless, after doing the z-integral in (4.7), one finds that there are contributions from the exchange of off-shell states in the 0-winding number sector. In particular, the leading long-range contribution to the 4-point amplitude contains $\sim(k_1+k_3)^{-2}$, corresponding to the Newtonian potential. Thus, even though the theory contains no gravitons, there is an instantaneous gravitational force between winding strings.

V. LOOP AMPLITUDES

In this section, we will compute the one-loop free energy at finite temperature and one-loop corrections to N-point functions of winding states. We will also examine the general structure of higher loop amplitudes and demonstrate that there is a sensible perturbative expansion of NRCS.

On a genus-g surface, the β-field [the (1, 0)-form we introduced in Sec. III as a Lagrangian multiplier] has g zero modes. If we were quantizing the bosonic ghost system, we would introduce delta-functions in the path integral to absorb these zero modes. However, one can show that the rules of the NRCS perturbation theory deduced from the factorization conditions do not call for these delta-functions. Thus one may naively think that zero mode integrals are divergent in NRCS. This would be similar to the problem in DLCQ of field theory,[16,17] where integrals over states carrying zero longitudinal momentum pose difficulties in evaluating loop amplitudes.[18]

It turns out that, whenever we evaluate physical observables such as the temperature dependent part of the free energy and scattering amplitudes of closed strings with nonzero winding numbers, the amplitudes contain terms of *stringy nature* which depend on all the g zero modes of β, so that the zero-mode integrals are convergent. It is easy to understand where these terms come from; they appear because β is a Lagrange multiplier which constrains γ to be a holomorphic map from the worldsheet to the $(1+1)$-dimensional part of the target space. If vertex operators for winding states are inserted on the worldsheet, a holomorphic map γ, if it exists, has to be a nontrivial one since the image of the worldsheet has to wind around each of the vertex operators. As we will show below, a nontrivial holomorphic map from the worldsheet to the $(1+1)$-dimensional part of the target space, which is a cylinder, exists only in a subspace of codimension g of the moduli space of a genus-g Rieman surface. The integral over the g zero modes of β gives a delta-function which exactly picks up the subspace where the holomorphic maps exist.

On the other hand, if we consider amplitudes which do not contain winding strings, such as the vacuum amplitude at zero temperature, then the zero-mode integral gives a divergence. In this case, γ can be a *trivial* map which maps the worldsheet to a point in the target space. Such a map exists everywhere on the moduli space of the worldsheet, and therefore the worldsheet amplitude is independent of the g zero modes of β. The integral over these zero modes is then flatly divergent. If one traces through the NCOS limit in Sec. III, one finds that it is exactly the type of divergence that was pointed out in Ref. 18. Fortunately all the physical states in NRCS have a nonzero winding number, and these divergent amplitudes have no physical meaning and can be safely ignored.

We will demonstrate these points by computing one-loop amplitudes and show how they are generalized to higher loops.

A. Free energy

The one-loop free energy at temperature T is evaluated by performing a Euclidean rotation of the target space–time coordinate and periodically identifying $X^0 \sim X^0 + T^{-1}$. The path integral then involves a sum over maps $(\gamma, \overline{\gamma})$ from the worldsheet torus of modulus τ to the target space torus of periods $(T^{-1}, 2\pi R)$.

The zero-mode dependence of the free energy can be computed by performing the path integral over the maps from the worldsheet to space–time. Thus we write

$$\gamma = \left(2\pi n R + i\frac{m}{T}\right)\frac{\sigma^0}{2\pi} + \left(2\pi w R + i\frac{s}{T}\right)\frac{\sigma^1}{2\pi} + (\text{periodic}), \tag{5.1}$$

where $0 \leqslant \sigma^0$, $\sigma^1 < 2\pi$ and (n, m, w, s) are integers labeling the different winding sectors. For this γ,

$$\overline{\partial}\gamma = \frac{i}{4\pi\,\mathrm{Im}\,\tau}\left[2\pi n R + i\frac{m}{T} - \tau\left(2\pi w R + i\frac{s}{T}\right)\right] + \overline{\partial}(\text{periodic}). \tag{5.2}$$

On the other hand, β can be written as $\beta = \beta_0 + \partial(\text{periodic})$, where β_0 is the zero mode. The worldsheet action depends on β_0 as

$$S = i\beta_0\left[2\pi n R + i\frac{m}{T} - \tau\left(2\pi w R + i\frac{s}{T}\right)\right] + \cdots. \tag{5.3}$$

Thus the integral over β_0 gives a delta-function which fixes the worldsheet modulus τ at

$$\tau = \frac{2\pi n R + i m\dfrac{1}{T}}{2\pi w R + i s\dfrac{1}{T}}. \tag{5.4}$$

Thus the τ-integral becomes a sum over these special points on the worldsheet moduli space. These are the points at which there are holomorphic maps from the worldsheet to the target space.

The one-loop free energy is obtained by a sum over the integers (n, m, w, s) such that τ is in the fundamental domain of the moduli space. To do the summation, it is convenient to use the trick invented in Ref. 19 to trade the sum over s for the sum over copies of the fundamental domain. If $(m,s) \neq (0,0)$, there is an $SL(2,Z)$ transformation which sends (m, s) to $(m, 0)$ with $m > 0$, and it also maps the fundamental domain of τ into the strip, $|\mathrm{Re}\,\tau| \leqslant 1/2$, in the upper half-plane $\mathrm{Im}\,\tau \geqslant 0$. The sum over s covers the strip exactly once by copies of the fundamental domain. On the other hand, the $(m,s) = (0,0)$ term is independent of the temperature T and corresponds to the zero temperature vacuum energy. We will ignore this contribution since it has no physical meanings in NRCS and it vanishes in supersymmetric theories anyway. Thus we have

$$\tau = \frac{2\pi n R + i m\dfrac{1}{T}}{2\pi w R}, \tag{5.5}$$

and we sum over integers (n, m, w). Since $m > 0$ and τ must be in the strip in the upper half-plane, we require $w > 0$ and $|n| \leqslant w/2$ (n at the boundary $n = \pm w/2$ is counted with a factor 1/2).

We can now evaluate the path integral over γ and $\overline{\gamma}$. The zero mode piece is obtained by evaluating the instanton action. Therefore, substituting (5.1) (with $s = 0$) into the action (3.8) and evaluating it at the points (5.5) of the moduli space, we find that the zero mode part of the action is

$$S=\int d^2z\left(\frac{1}{8\pi\alpha'_{\rm eff}}\partial\gamma\bar{\partial}\bar{\gamma}+\cdots\right)=\frac{mwR}{2\alpha'_{\rm eff}T}+\cdots. \tag{5.6}$$

As usual, the contribution from the nonzero modes of (β,γ) is canceled by the determinant of the (b,c) ghost system. Therefore, the one-loop contribution to the free energy takes the form

$$F(T)=-\sum_{n,m,w}\frac{T}{wm}\sum_{h,\bar{h}}D(h,\bar{h})\exp\left[-\frac{m}{T}\left(\frac{wR}{2\alpha'_{\rm eff}}+\frac{h+\bar{h}}{wR}\right)+2\pi i\frac{n}{w}(h-\bar{h})\right]. \tag{5.7}$$

This is obtained by evaluating the partition function of the worldsheet theory at the special points (5.5) on the moduli space. Here $(h,\bar{h})$ are the conformal weights coming from the transverse excitations of the string and $D(h,\bar{h})$ is their multiplicity. To simplify the expression in (5.7), we have included in h the contribution from the transverse momenta k. Thus, in comparison with the notion in Sec. III, h and $\bar{h}$ are defined as

$$h=\frac{\alpha'_{\rm eff}}{4}k^2+N,\quad \bar{h}=\frac{\alpha'_{\rm eff}}{4}k^2+\bar{N}. \tag{5.8}$$

The factor $-T/wm$ in (5.7) is determined as follows. The β_0 integral with the action (5.3) gives a factor $(2\pi wR)^{-2}$ times the delta-function for τ [we set $s=0$ in (5.3)]. The measure for the τ-integral contains the factor

$$\frac{1}{{\rm Im}\,\tau}=\frac{2\pi wRT}{m}. \tag{5.9}$$

The zero-mode integral of γ gives the volume $2\pi R/T$ of the target space. Finally, the definition of the one-loop free energy is $F=-TZ(T)$, where $Z(T)$ is the one-loop vacuum amplitude at temperature T. Combining these factors together, we obtain

$$\frac{1}{(2\pi wR)^2}\frac{2\pi wRT}{m}\frac{2\pi R}{T}(-T)=-\frac{T}{wm}, \tag{5.10}$$

as in (5.7).

The sum over n in $|n|\leqslant w/2$ gives the constraint $h-\bar{h}\equiv 0 \pmod{w}$, which we recognize as the level matching condition. After summing over m, the free energy given by (5.7) becomes

$$F(T)=T\sum_{w=1}^{\infty}\sum_{h,\bar{h}}D(h,\bar{h})\log(1-e^{E(w,h,\bar{h})/T}). \tag{5.11}$$

This is the conventional expression for the one-loop free energy of quantum field theory. Here

$$E(w,h,\bar{h})=\frac{wR}{2\alpha'_{\rm eff}}+\frac{h+\bar{h}}{wR}=\frac{wR}{2\alpha'_{\rm eff}}+\frac{\alpha'_{\rm eff}k^2}{2wR}+\frac{N+\bar{N}}{wR}. \tag{5.12}$$

With the level matching condition for $(h,\bar{h})$, the expression for $E(w,h,\bar{h})$ precisely agrees the energy spectrum of closed strings in NRCS computed in Sec. III, with the correct multiplicity factor.

The computation of the free energy described here is similar to the one for string in AdS_3 discussed in Ref. 12. In that case, the one-loop amplitude has poles exactly at the special points in (5.4), and they are due to the presence of long strings winding near the boundary of AdS_3. Here we have delta-functions at these points and they correspond to the closed strings winding in the x^1 direction.

We now study the high temperature behavior of the free energy. It is clear that, for a fixed winding number w, that the free energy is convergent for any temperature T. However, there might be a divergence when one performs the sum over winding modes. To see whether the sum over w gives a divergence, we use the Cardy's formula,

$$\sum_{h,\bar{h}} D(h,\bar{h})\exp(2\pi i\tau h - 2\pi i\bar{\tau}\bar{h}) \sim \exp\left[\frac{2\pi i c}{24}\left(\frac{1}{\tau}\,\frac{1}{\bar{\tau}}\right)\right], \tag{5.13}$$

for Im $\tau\to 0$. Here c is the central charge of the rest of the system, and $c=12$ for a Type II superstring. Therefore, the high temperature behavior of NRCS is given by

$$\sum_{|n|\leqslant w/2}\sum_{h\bar{h}} D(h,\bar{h})\exp\left[-\frac{m}{T}\left(\frac{wR}{2\alpha'_{\rm eff}}+\frac{h+\bar{h}}{wR}\right)+2\pi i\,\frac{n}{w}(h-\bar{h})\right] \sim \exp\left[2\pi wR\left(\frac{\pi cT}{6m}-\frac{m}{4\pi\alpha'_{\rm eff}T}\right)\right], \tag{5.14}$$

for large w. Therefore, the sum over winding states will be divergent whenever $T\geqslant T_{\rm H}$, where

$$T_{\rm H}=\frac{1}{2\pi}\sqrt{\frac{6}{\alpha'_{\rm eff}c}}. \tag{5.15}$$

This gives the Hagedorn temperature of NRCS. For Type II NRCS we find that $T_{\rm H}=1/2\pi\sqrt{2\alpha'_{\rm eff}}$. It coincides with the location of the Hagedorn transition of NCOS studied in Refs. 11, 20. Just like in conventional string theory, the Hagedorn temperature $T_{\rm H}$ is the temperature at which the tachyonic mode which appears in the spectrum (5.12) due to the finite temperature GSO projection becomes massless. It would be interesting to study the behavior of the closed strings of NRCS above the Hagedorn temperature. In NRCS, the breakdown of the thermal ensemble may not occur unlike for relativistic closed string theories since there is no graviton and the Hamiltonian is positive definite. However, there can be a Jeans instability.

We have demonstrated explicitly that the β zero-mode integral is convergent when one computes the one-loop free energy. As a result of the β zero-mode integral, the integral over τ is localized to a sum over the special points in the moduli space of the worldsheet torus where there is a holomorphic map from the worldsheet to the target space torus. It is straightforward to generalize this observation to higher loops. A simple computation shows that a map from a genus g worldsheet to the target space torus exists only on a $(2g-3)$-dimensional subspace. Such a holomorphic map exists whenever the following condition on the worldsheet period matrix Ω_{ij} $(i,j=1,\ldots,g)$ is satisfied:

$$G_i(\Omega)=\sum_{j=1}^{g}\Omega_{ij}\left(2\pi w^j R+i\,\frac{s^j}{T}\right)+2\pi n_i R+i\,\frac{m_i}{T}=0, \tag{5.16}$$

for some integers (n_i,m_i,w^i,s^i). This generalizes (5.4) for $g=1$. On a genus-g surface, β has g linearly independent zero modes, and their integrals give delta-functions imposing the constraints $G_i=0$ $(i=1,\ldots,g)$.

B. *N*-point amplitudes

Here we analyze the effects of the β zero-mode integrals on the scattering amplitudes. We will discuss the N-point tachyon amplitudes for simplicity, but a generalization to amplitudes involving arbitrary external states is straightforward. As in the case of the tree amplitudes discussed in the last section, the computation of $\langle \pi_{i=1}^{n} e^{i\bar{v}_a\gamma(u_a)+v_a\overline{\gamma(x_a)}}\rangle$ requires finding (β,γ) which are holomorphic away from u_a's and behave near $z=u_a$ as

$$\gamma(z)\sim iw_aR\log(z-u_a),$$
$$\beta(z)\sim\frac{-i\bar{v}_a}{z-u_a}\quad(z\to u_a), \tag{5.17}$$

where w_a is the winding number for the i-th external state. The functional integral is nonzero only when such β and γ exist. As for $\beta(z)$, there is always a meromophic one-form given by

$$\beta(z)=-i\sum_{a=1}^{N}\bar{v}_a\partial_z\log\vartheta_1(z-u_a)+\text{const}, \tag{5.18}$$

where $\vartheta_1(z)$ is the elliptic theta function. This β is single-valued on the worldsheet torus as far as momentum is conserved, $\Sigma_a v_a=0$. On the other hand, $\gamma(z)$ obeying (5.17) does not always exist. To see this, let us try

$$\gamma(z)=i\sum_{a=1}^{N}w_aR\log\vartheta_1(z-u_a)+cz, \tag{5.19}$$

for some constant c. Due to the quasi-periodicity of the elliptic function, we find

$$\gamma(z+2\pi)=\gamma(z)+2\pi c,$$
$$\gamma(z+2\pi r)=\gamma(z)+2\pi\left(-R\sum_{a=1}^{N}w_au_a+c\tau\right), \tag{5.20}$$

where we assumed that the winding number is conserved, $\Sigma_a w_a=0$. By requiring that $\gamma(z)$ is periodic modulo the target space periodicity $\gamma\sim\gamma+2\pi R$, we find that c must be of the form $c=mR$ for some integer m and

$$\sum_{a=1}^{N}w_au_a=n+m\tau, \tag{5.21}$$

for some integer n. This gives a condition on the locations of the N points. Thus we find that, rather than being divergent, the integral over the zero mode of β imposes the condition (5.21) on the locations of the vertex operators on the worldsheet.

High loops

It is straightforward to generalize this result to higher loops. On a genus-g worldsheet, the holomorphic map $\gamma(z)$ winding w_a-times at $z=u_a$ should be of the form

$$\gamma(z)=i\sum_{a=1}^{N}w_aR\log E(z,u_a)+\sum_{i=1}^{g}c^i\int^z\omega_i, \tag{5.22}$$

for some constants c_i, where ω_i are holomorphic one-forms, and $E(z,w)$ is the prime form, a $(-1/2)$-differential with respect to z and w that vanishes linearly on the diagonal $z=w$ only (see, for example, Sec. IIIb.1 of Ref. 21). The periodicity of γ in the α-cycles of the worldsheet requires that c^i must be of the form $c^i=2\pi m^iR$ for some integers m^i, and the periodicity around the β-cycles requires

$$G_i=\sum_{a=1}^{N}w_a\int^{u_a}\omega_i-\left(n_i+\sum_{j=1}^{g}\Omega_{ij}m^j\right)=0, \tag{5.23}$$

for some integers n_i. This imposes g conditions on the $(3g-3+N)$-dimensional moduli space of the genus-g worldsheet with N points. To verify that the g conditions $G_i=0$ are independent of

each other and pick up a codimension g subspace, we need to compute their partial derivatives with respect to the worldsheet moduli y_I $(I=1,\ldots,3g-3)$ and the vertex operator locations u_a. They are given by

$$\frac{\partial G_i}{\partial u_a}=\omega^i(u_a)w_a,$$
$$\frac{\partial G_i}{\partial y_I}=\int d^2z\,\omega_i(z)\,\eta^I(z,\overline{z})\left(\sum_{a=1}^{N} w_a\partial_z \log E(z,u_a)-2\pi i\sum_{j=1}^{g} m^j\omega_j(z)\right), \tag{5.24}$$

where η^I are the Beltrami differentials associated to the moduli y_I. Note that the partial derivatives of G_i are all of the form, $\int d^2z\,\omega_i(z)\,\nu(z,\overline{z})$ for some differential ν. Since

$$\det_{i,j=1,\cdots g}(\omega_i(z_j))\neq 0, \tag{5.25}$$

for generic g points z_i, it is clear that the rank of the $(3g-3+N)\times g$ matrix $(\partial_{u_a}G_i,\partial_{y_I}G_i)$ is generically g. Thus the integral over the g zero modes of β exactly pick up the subspace of the moduli space where the holomorphic map $\gamma(z)$ exists.

VI. RELATION TO DLCQ

In this section we show that the NRCS limit we have studied is related by T-duality to the DLCQ limit of string theory. This follows by performing T-duality along the circle of radius R where the B-field lies. After T-duality, we get string theory without any background B-field, with a metric

$$g_{\mu\nu}=\begin{pmatrix} -1+(2\pi\alpha' B)^2 & 2\pi\alpha' B \\ 2\pi\alpha' B & 1 \end{pmatrix}, \tag{6.1}$$

and where the radius of the circle is α'/R. In the NRCS limit the metric is given by

$$ds^2=-\frac{\alpha'}{\alpha'_{\rm eff}}(dx^0)^2+2\,dx^0\,dx^1+(dx^1)^2. \tag{6.2}$$

We now rescale coordinates such that $x^1\to(\alpha'/\alpha'_{\rm eff})x^1$. In the NRCS $(\alpha'\to 0)$ limit the metric in these coordinates is

$$\frac{1}{\alpha'}ds^2=\frac{1}{\alpha'_{\rm eff}}[-(dx^0)^2+2\,dx^0\,dx^1], \tag{6.3}$$

and the periodicity of the compact direction is given by

$$x^1\sim x^1+2\pi\frac{\alpha'_{\rm eff}}{R}. \tag{6.4}$$

Since in this limit the x^1 coordinate is light-like, we see that DLCQ of closed string theory with string scale $\alpha'_{\rm eff}$ and null radius $\alpha'_{\rm eff}/R$ is T-dual to NRCS.

Because of the relation between NRCS and DLCQ, the formalism developed in this paper gives a useful description of DLCQ closed string theory also. In Refs. 22, 23, loop amplitudes of DLCQ closed string theory were studied to address the issue of divergence due to the longitudinal zero modes.[16–18] In particular, it was found in Ref. 22 that one-loop scattering amplitudes, when external strings carry nonzero longitudinal momenta, have finite DLCQ limits and that the positions of the vertex operators are constrained in the limit. These constraints can be viewed as the T-dual of (5.21) in NRCS. The description of NRCS developed here does not involve the process

of taking the NCOS limit, and thus loop amplitudes are manifestly finite. In fact, the one-loop observation in Ref. 22 has a straightforward generalization to higher loops, as we saw in (5.23). Evidently, unlike in ordinary field theories, the longitudinal zero modes do not cause a problem in DLCQ closed string theory. In the case of Type IIA string theory, this is related, via the hypothetical 11-dimensional Lorentz invariance of M theory, to the existence of the smooth DLCQ limit of M Theory described by the finite N Matrix Theory.[24–26]

For closed strings, the relation between NRCS and DLCQ provides another way to understand the origin of the nonrelativistic dispersion relation. The nonrelativistic limit described in Sec. II, however, is much broader and includes cases that are not related to DLCQ, as we will see in the next section.

VII. GALILEAN THEORIES

In this section we find new theories whose excitations satisfy a nonrelativistic dispersion relation. The light degrees of freedom that survive the low energy limit are light-branes (these theories do not have background branes, unlike the theories discussed in Ref. 8). Depending on which background gauge field one tunes to its critical value, different brane states are light while the rest of the states in M Theory decouple.

We will first consider M Theory limits where the light degrees of freedom are membranes and five-branes. We will call these theories GM (Galilean membrane) and GF (Galilean five-brane), respectively. The first one is obtained by tuning to the critical value the background three-form and the second one by turning on the background six-form of M Theory. The low energy limit is taken such that the terms in the world volume action depending on the transverse coordinates to the background remain finite in the limit. Just as for NRCS, the spectrum is modified if the brane directions are compactified, otherwise there are no finite energy physical excitations surviving the limit.

Therefore, the low energy limit leading to GM is given by (throughout the rest of the paper we will have in mind compactification on tori; it is straightforward to generalize the decoupling limits when branes wrap curved geometries)

$$\begin{aligned} g_{\mu\nu} &= \eta_{\mu\nu} \quad \mu,\nu = 0,1,2, \\ g_{ij} &= \frac{l_p^3}{l_{\text{eff}}^3}\delta_{ij} \quad i,j = 3,\ldots,10, \\ C_{012} &= T_{\text{M2}} - T_{\text{eff}}, \end{aligned} \tag{7.1}$$

with the eleven-dimensional Planck scale $l_p \to 0$ while the effective length scale l_{eff} is kept finite. Here $T_{\text{M2}} = 1/4\pi^2 l_p^3$ is the membrane tension and $T_{\text{eff}} = 1/4\pi^2 l_{\text{eff}}^3$ is the finite effective tension of the light membranes that survive the limit. Note that GM has no coupling constant and it contains a unique dimensionful parameter l_{eff}. This is reminiscent of some of the properties of eleven-dimensional M Theory.

The decoupling limit giving rise to GF is given by

$$\begin{aligned} g_{\mu\nu} &= \eta_{\mu\nu}, \quad \mu,\nu = 0,1,\ldots,5, \\ g_{ij} &= \frac{l_p^6}{l_{\text{eff}}^6}\delta_{ij}, \quad i,j = 6,\ldots,10, \\ C_{012345} &= T_{\text{M5}} - T_{\text{eff}}, \end{aligned} \tag{7.2}$$

with $l_p \to 0$ while the effective length scale l_{eff} is kept finite. Here T_{eff} denotes the effective tension of the light five-brane excitations. Just as GM, GF has no coupling constant and l_{eff} is the unique dimensionless parameter of the theory.

Similar theories can be obtained from light Dp-branes, which we will call GDp (Galilean D-p-branes). As we will now see, these theories are connected by dualities which are reminiscent of the dualities of the fully relativistic theories from which we obtain these Galilean theories. We first discuss the relation between supersymmetric Type IIA NRCS and the eleven-dimensional theory GM.

Here we will show that in fact the strong coupling dual to Type IIA NRCS is described by eleven-dimensional GM such that the parameters of the two theories are related to each other in a similar fashion to the usual relation in the relativistic setting.

Consider GM theory (7.1) compactified on a circle of proper radius R. The background critical three-form potential reduces to a NS–NS two-form potential,

$$B_{01}=2\pi R C_{012}. \tag{7.3}$$

Using the usual relation of parameters between M theory and Type IIA superstring theory,

$$R=g_s\sqrt{\alpha'}, \quad l_p=g_s^{1/3}\sqrt{\alpha'}, \tag{7.4}$$

we can write R and l_p in the limit (3.2) which defines NRCS, so that

$$R=g\sqrt{\alpha'_{\rm eff}}, \quad l_p=g^{1/3}\alpha'^{1/6}_{\rm eff}\alpha'^{1/3}, \tag{7.5}$$

as $\alpha'\to 0$.

Substituting the eleven-dimensional limit (7.1) in (7.3) we see that the background NS–NS two-form potential is given by

$$2\pi\alpha' B_{01}=1-\frac{l_p^3}{l_{\rm eff}^3}. \tag{7.6}$$

Using (7.5) and comparing with the limit defining NRCS in (3.2), we see that NRCS with coupling constant g and effective string scale $\alpha'_{\rm eff}$ is equivalent to GM theory on a circle of radius R and effective Planck scale $l_{\rm eff}$. The parameters are related by

$$R=g\sqrt{\alpha'_{\rm eff}}, \quad l_{\rm eff}=g^{1/3}\sqrt{\alpha'_{\rm eff}}. \tag{7.7}$$

A. GDp and GNSF theories

In this subsection we present some generalizations to the construction we made for perturbative closed strings in a near critical NS–NS B-field to Dp-branes in a near critical Ramond–Ramond $p+1$-form background. In order for the background to affect the Hamiltonian, the spatial directions of the brane have to be compactified on an orientable p-cycle of space–time. In this case, the winding number plays the role of electric charge in the discussion in (2.4) and again positivity of the energy allows only wrapping in one orientation.

The nonrelativistic limit that needs to be taken requires keeping finite the terms in the world volume action depending on the transverse coordinates to the brane and tuning the background field to the tension of the D-brane (this is the analog of the NRCS limit. There, we scaled α' and the metric in the transverse directions to the B-field such that terms of the string worldsheet action depending on the transverse coordinates are kept finite). The limit is given by

$$\begin{aligned} g_{\mu\nu}&=\eta_{\mu\nu}, \quad \mu,\nu=0,1,\ldots,p,\\ g_{ij}&=\left(\frac{\alpha'}{\alpha'_{\rm eff}}\right)^2\delta_{ij}, \quad i,j=p+1,\ldots,9,\\ g_s&=\left(\frac{\alpha'}{\alpha'_{\rm eff}}\right)^{(3-p)/2} g_p, \end{aligned} \tag{7.8}$$

$$C_{01\cdots p}=T_p-T_p^{\rm eff},$$

as $\alpha'\to 0$. Here T_p is the tension of the D-brane (which is infinite in the limit),

$$T_p=\frac{1}{(2\pi)^p g_s \alpha'^{(p+1)/2}}. \tag{7.9}$$

$T_p^{\rm eff}$ is the finite scale of the nonrelativistic theory and g_p the coupling of the theory. The effective tension is given by

$$T_p^{\rm eff}=\frac{1}{(2\pi)^p g_p \alpha_{\rm eff}^{(\prime p+1)/2}}. \tag{7.10}$$

In the limit (7.8) all states of string theory decouple except the light Dp-branes that have finite proper energy excitations. In particular, open and closed strings decouple from the low energy spectrum.

There is a very simple explanation for the limit we take in (7.8). Except for the presence of the background gauge field $C_{01\cdots p}$, (7.8) is the conventional low energy limit that results in a gauge theory on a Dp-brane.[27] This can be easily recognized by noting that the Yang–Mills coupling constant is given by $g_{\rm YM}^2\sim g_p\alpha_{\rm eff}'^{(p-3)/2}$ and that the limit (7.8) keeps the coupling finite. Moreover, the metric for the transverse coordinates X^i to the brane is given as in (7.8) whenever we express them in terms of the Higgs field Φ^i of the gauge theory as $X^i=\alpha'\Phi^i$ and require that the metric for Φ^i remains finite. The low energy limit is supplemented by turning a near critical background gauge field which results in light Dp-brane fluctuations.

There is one more theory we can define by tuning a massless gauge field of string theory, namely the one where the light excitations are NS five-branes. We will call these theories GNSF (Galilean Neveu–Schwarz five-brane). Just like NRCS, these theories can be obtained as a low energy limit of the different superstring theories. This low energy limit can also be motivated by considering the low energy limit on NS five-branes which yields the little string theories.[28] The nonrelativistic limit is given by

$$\begin{aligned} &g_{\mu\nu}=\eta_{\mu\nu}, \quad \mu,\nu=0,1,...,5,\\ &g_{ij}=\left(\frac{g_s}{G}\right)^2\delta_{ij}, \quad i,j=6,...,9,\\ &B_{012345}=T_5-T_5^{\rm eff}, \end{aligned} \tag{7.11}$$

as $g_s\to 0$ while keeping the string scale α' finite in the limit. Now the effective tension of the light NS five-branes is given by

$$T_5^{\rm eff}=\frac{1}{(2\pi)^5 G^2 \alpha_{\rm eff}'^3}. \tag{7.12}$$

Thus, (7.11) defines a nonrelativistic theory GNSF of light fluctuations of NS five-branes.

We will now briefly describe the theory one obtains for different values of p.

1. Zero-branes

For GD0, one may lift the description to M Theory (for a lift to eleven dimensions of a similar limit see Ref. 8). After a suitable rescaling of energy scales in M Theory, the M Theory circle goes from a space-like circle to a light-like circle of finite radius $R=g_0\sqrt{\alpha'_{\rm eff}}$. Then, if we consider the limit (7.8) for N D0-branes one obtains a DLCQ description of M Theory with eleven-dimensional Planck length $l_p=g_0^{1/3}\sqrt{\alpha'_{\rm eff}}$ in a sector with N units of longitudinal momentum.

2. One-branes

For $p=1$, the light states are D1-branes. The strong coupling dual of the theory of light D1-branes can be found by using Type IIB S-duality. S-duality maps the critical R–R background C_{01} to a critical NS–NS background B_{01}. The parameters $\tilde{g}_s$ and $\tilde{\alpha}'$ of the S-dual theory are given by

$$\tilde{g}_s=\frac{1}{g_s}, \quad \tilde{\alpha}'=\alpha' g_s. \tag{7.13}$$

Writing the limit (7.8) for $p=1$ in terms of the S-dual variables and comparing with (3.2) shows that the S-dual of GD1 is given precisely by NRCS if the parameters of the two theories are related by

$$g=\frac{1}{\tilde{g}}, \quad \alpha'_{\text{eff}}=\tilde{g}\tilde{\alpha}'_{\text{eff}}. \tag{7.14}$$

Thus Type IIB NRCS is related to GD1 by a strong–weak coupling duality which takes the same form as the conventional Type IIB S-duality. At the end of this section we will realize S-duality of Type IIB NRCS by studying GM theory compactified on a two-torus.[29,30]

3. Two-branes

GD2 can also be lifted to an eleven-dimensional picture. The D2-branes lift to M2-branes and the parameters (the eleventh-dimensional proper radius R and the Planck length l_p) of M Theory are related to those of GD2 by

$$R=\frac{\alpha'}{\sqrt{\alpha'_{\text{eff}}}}g_2, \quad l_p=g_2^{1/3}\frac{\alpha'^{2/3}}{\alpha'^{1/6}_{\text{eff}}}. \tag{7.15}$$

Moreover, the near critical R–R background lifts to a near critical background for the three-form of eleven-dimensional supergravity. Therefore, GD2 can be identified with GM on a transverse circle. Using the parameters in (7.1) we see that GM with an effective Planck scale l_{eff} on a transverse circle of coordinate size L is GD2 with coupling g_2 and effective string scale α'_{eff}. The parameters are related by

$$L=g_2\sqrt{\alpha'_{\text{eff}}}, \quad l_{\text{eff}}=g_2^{1/3}\sqrt{\alpha'_{\text{eff}}}. \tag{7.16}$$

Thus, the relation between GD2 and GM is reminiscent of the conventional duality between Type IIA and M Theory.

4. Three-branes

In order to get light D3-branes one must turn on a critical RR four-form. We can analyze the strong coupling dual of GD3. In fact, GD3 is self-dual, since S-duality of the underlying string theory maps the limit (7.8) to an analogous limit but with a different coupling constant and effective string scale. Therefore, GD3 with parameters g_3 and α'_{eff} is dual to GD3 with parameters $\tilde{g}_3$ and $\tilde{\alpha}'_{\text{eff}}$. The parameters are related by

$$\tilde{g}_3=\frac{1}{g_3}, \quad \tilde{\alpha}'_{\text{eff}}=g_3\alpha'_{\text{eff}}. \tag{7.17}$$

At the end of this section we realize the S-duality of CD3 from an eleven-dimensional perspective.

5. Four-branes

The GD4 limit can also be lifted to M Theory. The main difference here is that $g_s \to \infty$ in the limit. Therefore, it is required to analyze the configuration in eleven dimensions. The D4-branes lift to M5-branes wrapped on the M Theory circle. The proper size of the circle and the corresponding eleven-dimensional Planck length are given by

$$R = g_4 \sqrt{\alpha'_{\rm eff}}, \quad l_p = g_4^{1/3} \alpha'^{1/3} \alpha'^{1/6}_{\rm eff}. \tag{7.18}$$

Since the background RR five-form lifts to a near critical six-form of eleven-dimensional supergravity, one sees that the strong coupling dual to GD4 is given by GF. Comparing the parameters in (7.18) with those that define GF (7.2) one finds that the parameters of the two theories are related by

$$R = g_4 \sqrt{\alpha'_{\rm eff}}, \quad l_{\rm eff} = g_4^{1/3} \sqrt{\alpha'_{\rm eff}}. \tag{7.19}$$

6. Five-branes

We now consider the OD5 theory. For $p=5$, one also has to perform S-duality since in the decoupling limit $g_s \to \infty$. S-duality maps the D5-branes to NS five-branes. Moreover, the critical RR field gets mapped to a critical NS–NS electric field for the NS five-branes. Thus we are led to studying NS five-branes in a critical field. Type IIB S-duality maps the limit (7.8) for $p=5$ to a theory with string scale and string coupling given by

$$\tilde{\alpha}' = g_s \alpha' = g_5 \alpha'_{\rm eff}, \quad \tilde{g}_s = \frac{1}{g_s} = \frac{\alpha'}{\alpha'_{\rm eff}} \frac{1}{g_5}. \tag{7.20}$$

Note that the string scale of the S-dual theory is finite while the string coupling vanishes. This is precisely the limit that defines Type IIB GNSF (7.11). The parameters of GD5 $(g_5, \alpha'_{\rm eff})$ are related to those of GNSF $(G, \tilde{\alpha}')$ by

$$\alpha'_{\rm eff} = G \tilde{\alpha}', \quad G = \frac{1}{g_5}. \tag{7.21}$$

In the limit that defines GD5, apart from having low energy D5-brane excitations, there are also finite energy D1-string excitations. These are identified in the Type IIB GNSF theory with strings of tension $\tilde{\alpha}'^{-1}$ fluctuating inside the five-branes.

7. Type IIA Neveu–Schwarz five-branes

Type IIA GNSF has an interesting strong coupling dual. The limit in (7.11) can be realized by considering the decoupled theory of light fluctuating five-branes of M Theory on a transverse circle of proper size R. The near critical six-form background of eleven-dimensional supergravity becomes a near critical RR six-form of Type IIA string theory and the M5-brane becomes a NS five-brane on a transverse circle of proper radius R. The parameters of the two theories are related by

$$R = g_s \sqrt{\alpha'}, \quad l_p = g_s^{1/3} \sqrt{\alpha'}. \tag{7.22}$$

By comparing the scaling limit (7.2) with (7.11) and using (7.22) one finds the following relation between the effective length scales of the two theories,

$$l_{\rm eff} = G^{1/3} \sqrt{\alpha'_{\rm eff}}. \tag{7.23}$$

Moreover, the NS five-branes now sit at a point in the transverse circle, whose coordinate length is given by

$$L = G\sqrt{\alpha'}. \tag{7.24}$$

We see that the Galilean theories we have found sit on the same moduli space and satisfy many of the properties of the parent theories from which we define them by taking a low energy limit. The reduced number of degrees of freedom that these theories have can be an interesting avenue in which to study in a simplified setting M Theory dualities.

8. S-duality of Type IIB NRCS from GM

We first notice that Type IIB NRCS can be obtained by considering eleven-dimensional GM theory compactified on a two-torus, where one circle is along the membrane and the other is transverse to it, and then shrinking the torus.

Let us consider GM theory compactified on a rectangular torus of coordinate size radii R_1 and R_2. We will take the circle of radius R_1 to be along the background three-form of supergravity and the circle of radius R_2 to be transverse to it. If we reduce GM on R_1 one gets Type IIA NRCS. The string coupling is given by

$$g_s = \frac{R_1}{\sqrt{\alpha'}}. \tag{7.25}$$

We now perform T-duality along the circle of radius R_2. This maps the limit to a Type IIB set-up. T-duality inverts the proper size of the circle one T-duals along and changes the dilaton in the conventional fashion. The new string coupling is given by

$$g_s' = \frac{R_1}{R_2}\sqrt{\frac{\alpha'_{\text{eff}}}{\alpha'}}. \tag{7.26}$$

Therefore, comparing with (3.2) we see that this compactification of GM leads to Type IIB NRCS with coupling constant

$$g = \frac{R_1}{R_2}, \tag{7.27}$$

compactified on a transverse circle of coordinate size α'_{eff}/R_2. Therefore, one gets Type IIB NRCS from GM in the limit that the coordinate area of the torus vanishes at fixed ratio R_1/R_2.

However, one could have chosen to reduce GM on the circle of coordinate radius R_2. As we showed, this leads to CD2 theory on a parallel circle of coordinate size R_1. The Type IIA coupling is given by

$$\tilde{g}_s = \frac{\sqrt{\tilde{\alpha}'}}{\tilde{\alpha}'_{\text{eff}}} R_2. \tag{7.28}$$

One can perform a T-duality transformation along the circle of radius R_1 such that we get a low energy limit in the Type IIB superstring where the string coupling is given by

$$\tilde{g}_s' = \frac{\tilde{\alpha}'}{\tilde{\alpha}'_{\text{eff}}}\frac{R_2}{R_1} \tag{7.29}$$

and the circle is of coordinate size $\tilde{\alpha}'_{\text{eff}}/R_1$. Thus, by looking at (7.8) for $p=1$ we see that one gets CD1 theory with coupling,

$$\tilde{g}_1 = \frac{R_2}{R_1}. \tag{7.30}$$

Therefore, S-duality of Type IIB NRCS can be understood from an eleven-dimensional perspective as the symmetry that exchanges the two circles when one considers GM theory compactified on a two-torus.[29,30]

9. S-duality of GDS from GF

Consider a single M5 brane compactified on a rectangular two-torus of radii R_1 and R_2 along the background directions in the decoupling limit (7.2). If we treat the circle of radius R_1 to be the one that results in GD4, then the parameters of GD4 are given by

$$R_1 = g_4 \sqrt{\alpha'_{\text{eff}}}, \quad l_{\text{eff}} = g_4^{1/3} \sqrt{\alpha'_{\text{eff}}}. \tag{7.31}$$

One may perform T-duality along the circle of radius R_2. Then, we obtain the Galilean theory of light D3-branes. The string coupling after T-duality is given by

$$g'_s = g_s \frac{\sqrt{\alpha'}}{R_2} = g_4 \sqrt{\frac{\alpha'_{\text{eff}}}{R_2}}. \tag{7.32}$$

Comparing (7.32) with (7.8) for $p=3$ and using (7.31) one finds that the effective coupling of the theory of light D3-branes is

$$g_3 = \frac{R_1}{R_2}, \tag{7.33}$$

which is reminiscent of the relation between M Theory on a two-torus and Type IIB string theory.

If one reduces first on the circle of radius of R_2 and then performs T-duality along the circle of radius R_1 one again obtains GD3 but with the inverse coupling. Therefore, S-duality of GD3 follows from the interchange of the two circles of the two-torus in the GF realization of GD3.

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Bosonic M theory

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We conjecture that there exists a strong coupling limit of bosonic string theory which is related to the 26 dimensional theory in the same way that 11 dimensional M theory is related to superstring theory. More precisely, we believe that bosonic string theory is the compactification on a line interval of a 27 dimensional theory whose low-energy limit contains gravity and a three-form potential. The line interval becomes infinite in the strong coupling limit, and this may provide a stable ground state of the theory. We discuss some of the consequences of this conjecture.
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I. INTRODUCTION

There is growing evidence that all the known perturbative ten-dimensional superstring theories are limits of an eleven dimensional theory called M theory.[1–3] In particular, the ubiquitous dilaton which controls the string coupling is simply related to the size of the extra dimension. The 26 dimensional bosonic string has not been included in these developments mostly due to the widespread belief that the existence of the tachyon indicates that the theory is ill defined. (The strong coupling limits of the ten-dimensional bosonic Type 0 theories have been discussed in Ref. 4, and other nonsupersymmetric theories have been considered in Ref. 5.) However, during the past year the significance of the open string tachyon has been understood. Rather than indicating that the theory is sick, it just shows that the usual vacuum is unstable. As Sen first proposed,[6] this vacuum can be viewed as a closed string vacuum together with an unstable D 25-brane. There is increasing evidence that there is a stable minimum of the open string tachyon potential at a value equal to minus the tension of a D 25-brane, and about this minimum there are no open string excitations. This raises the possibility that the closed string tachyon can similarly be removed by appropriately shifting to a new ground state. However, there are good arguments that the closed string tachyon cannot be removed by direct analogy to the open string case. There is probably no stable minimum of the closed string tachyon potential.[7] Something more dramatic is needed.

In this paper we study the strong coupling limit of bosonic string theory and argue that the tachyon instability may be removed in this limit. Unfortunately we have very little firm ground to stand on when trying to determine the strong coupling limit of a theory without supersymmetry. In this paper we make a guess based on the assumption that bosonic string theory is not wholly dissimilar to IIA and heterotic string theory.

The main clue motivating our guess comes from the existence of the dilaton and its connection to the coupling constant. The action for the massless sector of bosonic string theory is

$$S=\int d^{26}x\sqrt{-g}e^{-2\phi}\left[R+4\nabla_\mu\phi\nabla^\mu\phi-\frac{1}{12}H_{\mu\nu\rho}H^{\mu\nu\rho}\right]. \tag{1.1}$$

Evidently, as in IIA string theory, the dilaton enters the action just as it would if it represented the compactification scale of a Kaluza–Klein theory. We propose to take this seriously and try to interpret bosonic string theory as a compactification of a 27 dimensional theory. We will refer to

this theory as bosonic M theory. (The possibility that the bosonic string has a 27 dimensional origin was also briefly discussed in Ref. 8, in the context of a proposed matrix string formulation.)

In the case of IIA string theory there was a second clue that led to its interpretation as a Kaluza–Klein compactification of an 11 dimensional theory; the existence of a vector boson in the string spectrum. Closed bosonic string theory does not have a massless vector. This means it cannot be a compactification on an S^1. In this respect the situation is more analogous to that of heterotic string theory. The solution to the strong coupling problem in that case is a compactification of M theory on a line interval, or more exactly on the orbifold S^1/Z_2.[9] The absence of a $U(1)$ symmetry means that there is no massless gauge boson. Accordingly, we propose that closed bosonic string theory is a compactification of 27 dimensional bosonic M theory on S^1/Z_2. In the supersymmetric case, to cancel anomalies one had to add E_8 gauge fields at each end of the line interval. In the bosonic case, since there are no fermions or chiral bosons, there are no anomalies to cancel. So there are no extra degrees of freedom living at the fixed points.

As in the case of the M theory–heterotic connection, the weakly coupled string theory is the limit in which the compactification length scale becomes much smaller than the 27 dimensional Planck length and the strong coupling limit is the decompactification limit. The 27 dimensional theory should contain membranes but no strings, and would not have a dilaton or variable coupling strength. The usual bosonic string corresponds to a membrane stretched across the compactification interval.

Some support for bosonic M theory comes from the following simple observation. The left moving modes of the heterotic string are precisely those of the 26 dimensional bosonic string. It has been argued[10] that at least perturbatively, the right moving modes of the bosonic string can be embedded in the right moving modes of the heterotic string. So the entire bosonic string is contained in the heterotic string. Since we now know that nonperturbatively the heterotic string grows an extra dimension, it is plausible that the bosonic string will similarly gain an extra dimension at strong coupling.

II. THE LOW-ENERGY THEORY

In this section we study the low-energy limit of bosonic M theory which is a gravity theory in 27 dimensions. Without the powerful tool of supersymmetry it is difficult to give rigorous arguments. Nevertheless there are some plausible guesses that we can make about the form of the low-energy action, using the fact that it must reduce to the usual bosonic string theory in the weak coupling limit. After deriving the low-energy action, we show how the tachyon instability may be removed in the strong coupling limit, and then study branes in this theory.

A. Motivation from weak coupling limit

In order to reproduce the known spectrum of weakly coupled bosonic string theory, bosonic M theory will have to contain an additional field besides the 27 dimensional gravitational field, namely a three-form potential $C_{\mu\nu\rho}$. Let us consider the various massless fields that would survive in the weak coupling limit. First of all, there would be the 26 dimensional graviton. As usual, general covariance in 26 dimensions would insure that it remains massless. The component of the 27 dimensional gravitational field $g_{27,27}$ is a scalar in the 26 dimensional theory. It is of course the dilaton. No symmetry protects the mass of the dilaton. In fact we know that at the one loop level a dilaton potential is generated that lifts the dilatonic flat direction. Why the mass vanishes in the weak coupling limit is not clear.

Massless vectors have no reason to exist since there is no translation symmetry of the compactification space. This is obvious if we think of this space as a line interval. If we think of it as S^1/Z_2 then the two fixed points of the orbifold break the symmetry.

The three-form gauge field $C_{\mu\nu\sigma}$ gives some massless fields. If one of the indices of the three-form is in the compact 27th direction, the resulting 26 dimensional field is the two-form $B_{\mu\nu}$ which is well known in bosonic string theory. It remains massless due to its gauge invariance. The components of $C_{\mu\nu\sigma}$ in which all three components are in the 26 dimensional subspace give a three-form which is absent in the usual bosonic string spectrum. Once again we take a hint from

heterotic string theory. In that case the the three-form that would be inherited from the 11 dimensional origin of heterotic string theory is projected away by the Z_2 identification. This is because M theory includes a Chern–Simons term which implies that the action is invariant under Z_2 only if C is odd under this identification. In the present case we will also assume that C is odd under the Z_2. [If y is the coordinate along the S^1, the fact that the basis vector $\partial/\partial y$ points away from the fixed point $y=0$, means that it also must change sign under the Z_2. This means that the components C_{yij} are even under $y\to -y$, while C_{ijk} are odd (where i,j,k denote all directions other than y)]. Given our limited knowledge of the theory, we do not know if this is required by a symmetry of the action or not.

We are thus led to the following low-energy action for bosonic M theory:

$$S=\int d^{27}x\sqrt{-\hat{g}}\left[R(\hat{g})-\frac{1}{48}F_{\mu\nu\rho\sigma}F^{\mu\nu\rho\sigma}\right], \tag{2.1}$$

where $F=dC$. To see the relation to (1.1), we set

$$\hat{ds}^2=e^{2\sigma}dy^2+e^{-\sigma}g_{\mu\nu}dx^\mu dx^\nu, \tag{2.2}$$

where σ and $g_{\mu\nu}$ are functions of x^μ but independent of y, and set

$$H_{\mu\nu\rho}=F_{y\mu\nu\rho}. \tag{2.3}$$

The coordinate y takes values $-1\leqslant y\leqslant 1$ and we identify y with $-y$. This prevents a term like $A_\mu dy dx^\mu$ from appearing in (2.2). Substituting into the action and integrating by parts yields

$$S=\int d^{26}x\sqrt{-g}e^{-11\sigma}[R(g)+125\nabla_\mu\sigma\nabla^\mu\sigma-\tfrac{1}{12}H_{\mu\nu\rho}H^{\mu\nu\rho}]. \tag{2.4}$$

There is no four-form in 26 dimensions since, as we have just explained, it is projected out by the identification on y. If we now define $2\phi\equiv 11\sigma$, this becomes the standard action for bosonic string theory (1.1) except that the coefficient of the $(\nabla\phi)^2$ is off by a factor of 125/121. So we recover the right fields and interactions, but one numerical coefficient is slightly off. This is not a contradiction since the action (2.1) is only valid on scales larger than the 27 dimensional Planck length, and to recover (1.1) we need to take a limit where one direction becomes much smaller than this. Without supersymmetry to protect coefficients, they can change as the coupling increases. In this respect, the factor of 125/121 may be analogous to the factor of 3/4 which arises in comparing the entropy of weakly coupled $3+1$ Yang–Mills with the near extremal three-brane.[11]

The relation between the 27 dimensional Planck length l_p and the 26 dimensional string length l_s and coupling $g=e^\phi$, follows from the relation between σ and ϕ. Since $g^2 l_s^{24}=G_{26}=G_{27}/e^\sigma l_p$ we get

$$g^{1/11}l_s=l_p. \tag{2.5}$$

Since $g=e^{11\sigma/2}$, weak coupling corresponds to a small distance in the extra dimension, as expected.

There is a possibility of adding a cosmological constant to the action (2.1). Indeed, in the absence of supersymmetry, it would appear inevitable that one is generated. We will discuss this in Sec. IV, but for now, we will assume the cosmological constant is zero.

B. Tachyon

We now consider the fate of the closed string tachyon at strong coupling. The trivial solution to (2.1) consisting of $F=0$ and flat spacetime compactified on S^1/Z_2 has a nonperturbative instability. This is analogous to the instability of the Kaluza–Klein vacuum found by Witten,[12] and

very similar to its application to heterotic–M theory in Ref. 13. The process that destabilizes the space is mediated by an instanton in which the two ends of the world (ends of the compactification interval) come together and produce a ''hole'' in space. In Minkowski space the hole rapidly grows and eats the entire space.

The appropriate instanton is (a projection of) the 27 dimensional euclidean Schwarzschild metric.

$$ds^2=\left[1-\left(\frac{r_0}{r}\right)^{24}\right]dy^2+\left[1-\left(\frac{r_0}{r}\right)^{24}\right]^{-1}dr^2+r^2(d\theta^2+\sin^2\theta d\Omega_{24}). \tag{2.6}$$

The coordinate y is periodic with period $P=\pi r_0/6$. To apply it to our case, we identify y and $-y$. So the size of the extra dimension at infinity is $\pi r_0/12$. To obtain the Lorentzian evolution, one analytically continues $\theta\to(\pi/2)+it$. To picture this evolution, consider the surfaces at the ends of the interval, $y=0,\pi r_0/12$. The separation between these surfaces goes to zero smoothly at $r=r_0$, so the two surfaces are really one surface with the shape of a wormhole. At the initial time, $t=0$, the proper size of the wormhole is r_0, but as time evolves, it grows exponentially.

This instanton description is only valid for $r_0\gg l_p$. However similar instabilities occur in various nonsupersymmetric D–brane systems. A typical example is a D–brane anti D–brane system. If the distance between the branes is larger than the string scale, an instanton process bridging the two branes can again lead to a runaway hole eating the branes.[14] When the branes are closer than the string scale the same process can take place by a perturbative mechanism. At a critical point the lightest string connecting the branes becomes massless and then tachyonic.[15,16] This pattern is seen in several examples and leads to the following conjecture:

When the two ends of the world are closer than the 27 dimensional Planck length a tachyon appears in the spectrum. This is just the closed string tachyon found in string perturbation theory.

The action for the instanton (2.6) is proportional to $(r_0/l_p)^{25}$. So in the limit of strong string coupling, $r_0\to\infty$, this nonperturbative instability is suppressed. Uncompactified 27 dimensional flat space may be a stable ground state of bosonic M theory.

C. Branes

In the absence of supersymmetry, there are no BPS states. Nevertheless, there are stable brane configurations. In terms of the low energy action (2.1) they arise as the extremal limit of black brane solutions. Since the charge must be carried by a four-form, there are 2-branes which are electrically charged and 21-branes which are magnetically charged. It is natural to assume that there are fundamental 2-branes and 21-branes with Planck tension, and these black brane solutions describe the gravitational field of a stack of parallel branes. A nontrivial check of this idea is to compute the tension of a fundamental 2-brane stretched across the extra dimension. It is given by $T=e^{\sigma}/l_p^2$. Using (2.5), and the relation between σ and ϕ we get $T=1/l_s^2$ which is the right answer for a fundamental string. Similarly, the tension of a 21-brane which is not oriented along the extra dimension is $T_{21}=1/l_p^{22}=1/(g^2 l_s^{22})$ which again is the right answer for a solitonic 21-brane in string theory.

The black brane solutions can be read off from the general discussion of nondilatonic black branes in Ref. 17. The black 2-brane is given by

$$\begin{aligned}ds^2=&-\left[1-\left(\frac{r_+}{r}\right)^{22}\right]\left[1-\left(\frac{r_-}{r}\right)^{22}\right]^{-1/3}dt^2+\left[1-\left(\frac{r_-}{r}\right)^{22}\right]^{2/3}dx_i dx^i\\&+\left[1-\left(\frac{r_+}{r}\right)^{22}\right]^{-1}\left[1-\left(\frac{r_-}{r}\right)^{22}\right]^{-1}dr^2+r^2d\Omega_{23},\end{aligned} \tag{2.7}$$

with four-form

$$*F=Nl_p^{22}\epsilon_{23}, \tag{2.8}$$

where ϵ_{23} is the volume form on a unit S^{23}. The charge N is the number of fundamental two branes, and is related to the two free parameters $r_\pm$ via

$$N^2=\frac{1100}{3}\left(\frac{r_+r_-}{l_p^2}\right)^{22}. \tag{2.9}$$

There is an event horizon at $r=r_+$ and a curvature singularity at $r=r_-$. The Hawking temperature of this black 2-brane is

$$T=\frac{11}{2\pi r_+}\left[1-\left(\frac{r_-}{r_+}\right)^{22}\right]^{1/3}. \tag{2.10}$$

If we compactify the two directions along the brane on a torus with side L, then the horizon area is

$$A=r_+^{23}\Omega_{23}L^2\left[1-\left(\frac{r_-}{r_+}\right)^{22}\right]^{2/3}, \tag{2.11}$$

where Ω_{23} is the area of a unit S^{23}. In the extremal limit, $r_+=r_-$, (2.7) takes a simpler form by setting $\rho^{22}=r^{22}-r_-^{22}$

$$ds^2=f(\rho)^{-2/3}[-dt^2+dx_i dx^i]+f(\rho)^{1/11}[d\rho^2+\rho^2 d\Omega_{23}], \tag{2.12}$$

where

$$f(\rho)=1+\left(\frac{r_-}{\rho}\right)^{22}. \tag{2.13}$$

This extremal brane has zero Hawking temperature and is quantum mechanically stable. The surface $\rho=0$ is a smooth horizon. There is no force between two parallel extremal branes. Static, multibrane solutions can be obtained by replacing f with a more general solution of Laplace's equation.

We now turn to the black 21-brane. The metric is

$$\begin{aligned}ds^2=&-\left[1-\left(\frac{r_+}{r}\right)^3\right]\left[1-\left(\frac{r_-}{r}\right)^3\right]^{-10/11}dt^2+\left[1-\left(\frac{r_-}{r}\right)^3\right]^{1/11}dx_i dx^i\\&+\left[1-\left(\frac{r_+}{r}\right)^3\right]^{-1}\left[1-\left(\frac{r_-}{r}\right)^3\right]^{-1}dr^2+r^2d\Omega_4,\end{aligned} \tag{2.14}$$

and the four-form is $F=Nl_p^3\epsilon_4$, where

$$N^2=\frac{75}{11}\left(\frac{r_+r_-}{l_p^2}\right)^3. \tag{2.15}$$

The Hawking temperature is

$$T=\frac{3}{4\pi r_+}\left[1-\left(\frac{r_-}{r_+}\right)^3\right]^{1/22}, \tag{2.16}$$

and the horizon area is

$$A=r_+^4\Omega_4L^{21}\left[1-\left(\frac{r_-}{r_+}\right)^3\right]^{21/22}, \tag{2.17}$$

where we have again compactified the directions along the brane to have size L. Setting $\rho^3 = r^3 - r_-^3$, the extremal limit is

$$ds^2 = f(\rho)^{-1/11}[-dt^2 + dx_i dx^i] + f(\rho)^{2/3}[d\rho^2 + \rho^2 d\Omega_4], \tag{2.18}$$

where now

$$f(\rho) = 1 + \left(\frac{r_-}{\rho}\right)^3. \tag{2.19}$$

Like the 5-brane of M theory, this 21-brane is completely nonsingular. The space–time behind the horizon $\rho = 0$ is identical to the space–time in front.

We now suppose that one direction of spacetime is compactified on S^1/Z_2, and the four-form F is odd under the Z_2 identification. The situation is similar to the usual heterotic string construction.[18] Recall that, if y is the coordinate in the compact direction, the components F_{yijk} must be even under $y \to -y$, while F_{ijkl} are odd (where i,j,k,l denote all directions other than y). Thus, if y is one of the two directions along the 2-brane, the identification can be done trivially since the solution is invariant. As we have already noted, this corresponds to N bosonic strings in 26 dimensions. If the 2-brane is perpendicular to y, a static solution can still be constructed by putting the 2-brane half way between the two fixed points and adding an anti-2-brane at its image point under the Z_2. (This solution is not known explicitly and will be unstable.) It results in an unstable D2-brane in 26 dimensions. If the 21-brane is perpendicular to y, an invariant solution is obtained by adding another 21-brane (not anti-brane) at its image point under the Z_2. This corresponds to a 21-brane in string theory which is magnetically charged with respect to the three-form H. If y is one of the directions along the 21-brane, then no invariant solution can be constructed, since $F_{ijkl} \neq 0$ at $y = 0$.

As an aside, we note that there is also a brane solution of 26 dimensional bosonic string theory which has both electric and magnetic charge associated with the three-form H. It is a 21-brane with fundamental strings lying in it and smeared over the remaining 20 directions. Dimensionally reducing to six dimensions by compactifying on a small T^{20}, one recovers the usual self dual black string in six dimensions.

III. HOLOGRAPHIC DUALS

In this section we go beyond the low-energy limit, and try to say something about exact bosonic M theory. Since it contains gravity it should be holographic. There are two types of holographic duals that we have become familiar with. The first is Matrix theory which is based on the existence of stable D0-branes in type IIA theory and the existence of a DLCQ quantization of M theory. However, in the present case in which the compactification is on a line interval rather than a circle this type of construction is questionable (but see Ref. 8).

The other type of holographic dual is through AdS/CFT duality.[19] Following the arguments used for the superstring, we consider the near horizon limit of the extreme black brane solutions. As usual, the near horizon limit corresponds to dropping the one in f in the solutions (2.12) and (2.18). Starting with the 2-brane, the resulting space is $AdS_4 \times S^{23}$. From (2.9), the radius of each is proportional to $N^{1/11}$. The CFT dual would be a $2+1$ dimensional conformal field theory with a global SO(24) symmetry. The natural candidate would be the dimensional reduction of 26 dimensional Yang–Mills theory which has 23 scalars in the adjoint representation. This theory has manifest SO(23) symmetry. The mechanism for enhancing the symmetry would have to be similar to the enhancement of SO(7) to SO(8) in the supersymmetric case. However, in the present situation we have no superconformal symmetry to ensure the enhanced symmetry. A strong test of the existence of bosonic M theory is the existence of a conformal fixed point with SO(24) symmetry at least in the $N \to \infty$ limit. In other words, if there does not exist a $2+1$ CFT with SO(24) global symmetry, bosonic M theory would be disproven.

As in the usual AdS/CFT correspondence, thermodynamics of the CFT should be related to the near extremal 2-brane. From (2.9) to (2.11), the entropy of near extremal 2-branes can be expressed

$$S \propto N^{25/22}(LT)^2. \tag{3.1}$$

This looks like the entropy of a $2+1$ field theory. The N dependence is analogous to the $N^{3/2}$ which appears in the usual M 2-brane, and can similarly be viewed as a prediction for the density of states of the theory at strong coupling.

Since there are also solutions of the form $AdS_4 \times K$ where K is any 23 dimensional Einstein space, there may also exist holographic duals of the theory with these boundary conditions. They would be $2+1$ conformal field theories with less symmetry.

Starting with the extreme 21-brane (2.18), the near horizon limit is $AdS_{23} \times S^4$, where the radii of each is proportional to $N^{2/3}$. If the theory exists, its holographic dual will be a 22 dimensional conformal field theory with a global SO(5) symmetry. It follows from (2.15) to (2.17) that in the near extremal limit, the entropy of the black 21-brane can be expressed

$$S \propto N^{25/3}(LT)^{21}. \tag{3.2}$$

Once again, this is consistent with a 22 dimensional field theory with a large number of degrees of freedom.

IV. DISCUSSION

We have proposed that a bosonic version of M theory exists, which is a 27 dimensional theory with 2-branes and 21-branes. One recovers the usual bosonic string by compactifying on S^1/Z_2 and shrinking its size to zero. In particular, a Planck tension 2-brane stretched along the compact direction has the right tension to be a fundamental string. This picture offers a plausible explanation of the tachyon instability and suggests that uncompactified 27 dimensional flat space may be stable. A definite prediction of this theory is the existence of a $2+1$ CFT with SO(24) global symmetry, which should be its holographic dual for $AdS_4 \times S^{23}$ boundary conditions.

The conjecture that bosonic M theory exists raises a number of questions which we now address:

(1) What kind of theory do we get if we compactify bosonic M theory on a circle instead of a line interval? Do we get a weakly coupled string theory in the limit that the circle shrinks to zero? This seems problematic since, whatever the resulting theory is, it should have a massless vector and three-form potential. Of course the open string has a massless vector, but as far as we know, there is no 26 dimensional bosonic string theory with a three-form potential. Instead we believe the limit of bosonic M theory compactified on a circle as the radius $R \to 0$ is the same as the limit $R \to \infty$, i.e., the uncompactified 27 dimensional theory. If we compactify bosonic M theory on $S^1 \times (S^1/Z_2)$, and take the second factor very small, this is a consequence of the usual T-duality of the bosonic string. More generally, it appears to be the only possibility with the right massless spectrum;

(2) must bosonic M theory have a vanishing cosmological constant? If not, what is the sign of the cosmological constant? If it is negative then there should be a 27 dimensional AdS solution. The holographic representation of this theory should be an isolated 26 dimensional conformal field theory. Since it is likely that the cosmological constant would be of order one in Planck units we would not expect classical Einstein gravity to be an accurate description. The best description would be the CFT. If the cosmological constant is positive, how do we make sense out of the theory in de Sitter space? This would be the first example of a de Sitter solution emerging out of string theory.

Even with a cosmological constant Λ, there are solutions of the form $AdS_4 \times S^{23}$. The only difference is that the curvature on the two spaces need not be comparable, and are related to different combinations of the four-form charge N and Λ. If $\Lambda > 0$, there is a particularly

interesting special case in which the solution is a sphere cross four dimensional Minkowski spacetime. This may have phenomenological applications. It is worth emphasizing that this solution exists for any (positive) cosmological constant, as long as F can be chosen appropriately. It would certainly be interesting to find a dynamical mechanism which would require F to cancel Λ in this way. (For a recent discussion of a possible mechanism, see Ref. 20.) In any event, we find it intriguing that four-dimensional space–times arise naturally in this theory;

(3) bosonic string theory contains unstable Dp-branes for all p. What are the analog of these in bosonic M theory? It appears that most of these do not survive the strong coupling limit and do not exist as new degrees of freedom in 27 dimensions. This is not surprising since Type II superstring also has unstable Dp-branes which do not appear to have an analog in M theory. However, some Dp-branes may remain. We already saw a construction of an unstable D2-brane in Sec. II. D0-branes can be identified with modes in the 27th direction. In the theory compactified on S^1/Z_2, these modes are unstable since they bounce off the fixed points, interact with themselves and decay into radiation in the other directions. In the uncompactified limit, they should become stable;

(4) even if 27 dimensional flat space, M_{27}, is a stable vacuum, one might ask what is the ''ground state'' of the theory at finite string coupling, or finite compactification size? Tachyon condensation is not likely to lead back to M_{27}, and there is probably no stable minimum of the tachyon potential in 26 dimensions.[7] Instead, we believe tachyon condensation may lead to an exotic state with zero metric $g_{\mu\nu}=0$. It is an old idea that quantum gravity may have an essentially topological phase with no metric. We have argued that the tachyon instability is related to nucleation of ''bubbles of nothing'' which is certainly reminiscent of zero metric. Further support for this idea comes from some old results on the closed string tachyon. Using modular invariance of the one loop vacuum amplitude, one can relate the existence of a tachyon to the asymptotic density of states. It was shown that the tachyon is absent only if, at high energies, the theory has at most a finite number of fields propagating in two spacetime dimensions.[21] Similar results were found by studying the theory near the Hagadorn transition.[22] If the theory starts in 26 (or 27) dimensions, the only way to get down to two dimensions is to have a highly degenerate metric. The most symmetric state would then be $g_{\mu\nu}=0$, and two dimensional subspaces might arise as excitations.

This raises an interesting question in string field theory. Witten's open bosonic string field theory[23] takes the form

$$S=\int A*QA+\frac{2g}{3}A*A*A, \tag{4.1}$$

where Q is the BRST operator and $*$ is a noncommutative product. Formally, $\int$ and $*$ are independent of the metric and other closed string backgrounds but Q is not. Since an interacting theory of open strings must include closed strings, it is awkward having this explicit background dependence in the action. It was shown in Ref. 24 that (4.1) could be derived from the purely cubic action

$$S=\int \Phi*\Phi*\Phi. \tag{4.2}$$

There is a solution Φ_0 to the equation of motion $\Phi*\Phi=0$ such that expanding about this solution, $\Phi=\Phi_0+g^{1/3}A$, one recovers Witten's action. The natural ground state of the purely cubic action is $\Phi=0$. Since this corresponds to zero BRST operator, it has been interpreted as a state of zero metric. But the purely cubic action can be viewed as the strong coupling limit $g\to\infty$ of (4.1) (we thank S. Shenker for pointing this out). If this is similar to the strong coupling limit of purely closed bosonic string theory, the natural ground state should be M_{27}. Could it be that $\Phi=0$ really

corresponds to M_{27} and the fact that $Q=0$ is just the statement that there are no open string excitations? If so, how can one recover the metric and three-form excitations?

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Extended objects from warped compactifications of M theory

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We study the massive spectrum of fully wrapped branes in warped M-theory compactifications, including regimes where these states are parametrically lighter than the Planck scale or string scale. We show that many such states behave classically as extended objects in the noncompact directions in the sense that their mass grows with their size as measured along the Poincare slices making up the noncompact dimensions. On the other hand, these states can be quantized in a nontrivial regime: in particular, their spectrum of excitations in a limited regime can be obtained by a warped Kaluza–Klein reduction from ten dimensions. We briefly discuss scattering processes and loop effects involving these states, and also note the possibility of an exponential growth in the number of bound states of these objects as a function of energy. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1373422]

I. INTRODUCTION

One of the features of the web of M-theory duals is the presence of various limits in which a distinctive spectrum of states emerges as the lightest excitation above the (super-) gravity modes. For example, in some limits strings dominate, in others particles including those coming from wrapped branes.

Compactifications of M theory down to d Poincare-invariant dimensions are generically warped products, with d-dimensional Minkowski space varying over a compact $11-d$-manifold K. That is, the metric is of the form

$$ds^2 = a(y)dx_{\|}^2 + H_{ij}(y)dy^i dy^j, \tag{1.1}$$

where $x_{\|}^{\mu}$, $\mu = 0,...,d-1$ are coordinates along the Poincare slices and y_i, $i = d,\ldots,10$ are coordinates along the internal manifold. In this article we will study basic aspects of the massive spectrum in such compactifications (focusing on two concrete examples: Horava–Witten theory compactified on $K3$,[1] and type I′ theory as studied by Polchinski and Witten[2] compactified on a five-torus).

We will find objects which behave in the noncompact $x_{\|}$ directions in a way that is in some sense intermediate between particles and higher branes. These come from ordinary particles or fully wrapped branes in the 10 or 11-dimensional description of the physics, but ones for which the mass and effective size as measured along the Poincare slices vary over the compactification in such a way that the energy grows as some positive power of the thickness $\delta x_{\|}$. We will refer to such objects as elastic states. By size of the object we will mean its thickness or the size of the short-distance cutoff scale, measured with respect to the $x_{\|}$ coordinates, as probed in appropriate scattering experiments. As we will discuss, in some regimes this is greater than or equal to the Compton wavelength of our excitations so that in these cases this is a classically intuitive accounting of the size scale.

In a general warped geometry of the form (1.1), the size R of an object as measured in the $x_{\|}$ coordinates ($R \equiv \delta x_{\|}$) depends on its characteristic proper size $r_0(y)$ and on the warp factor $a(y)$, via the relation

$$R = \frac{1}{\sqrt{a(y)}} r_0(y). \tag{1.2}$$

The energy of an object depends on $a(y)$ and the metric $H_{ij}(y)$ of the internal space (as well as the profiles of any additional fields with nontrivial VEVs in a given background). As we move the object around K to different values of y_i, its effective size changes and its energy changes. For ordinary point-particle quantum field theory the energy is inversely related to the size at high energies. [In anti-de Sitter (AdS) realizations of quantum field theory one sees membrane-shaped objects when a particle falls toward the horizon in AdS,[3–5] with their energy decreasing as their size increases as opposed to the cases we will focus on here.] We will see in our examples that the size instead grows as some positive power of the energy for certain massive states in warped compactifications. This variation in the size of the object results from a combination of its intrinsic thickness in $11d$ M theory and the warping of the metric involved in measuring its size in the $x_\parallel$ coordinates.

The phenomenon of growth of the size of states with energy is generic at high energies due to the presence of black holes, and is seen in other contexts in many corners of M theory (see Ref. 6 for a recent example and references to earlier ones). One result of our analysis is that warped compactifications provide another place where this intriguing effect emerges. Our analysis uses the basic relations arising from the gravitational redshift in geometries of the form (1.1) that also comes into the UV/IR correspondence developed for AdS space in studying the AdS/CFT correspondence;[7] our work involves in some ways a generalization of those studies to other warped geometries where there is no (evident) field theory dual, but where the energy/size relation can be studied directly in the gravity theory. The wrapped branes we study are in some sense generalizations of the baryon states studied in backgrounds with quantum field theory duals.[8]

Although the elastic states have a growth in size with energy reminiscent of branes, their spectrum and interactions at long distances can be calculated via ordinary Kaluza–Klein reduction in the warped geometry (1.1). This spectrum of states, while growing in number faster with energy than for ordinary unwarped Kaluza–Klein states on a circle, exhibits fewer degrees of freedom than a real brane. In this sense our elastic states are intermediate between particles and branes (and perhaps analogous to elastic solids, hence our nomenclature). However, if we consider the set of potential bound states of any number N of elastic states, we obtain a spectrum with enough degrees of freedom to describe modes of a continuous medium, and we discuss at the end a speculation for using these ideas to construct and quantize real branes using warped compactifications.

Direct couplings of objects of different size in this type of system are suppressed due to their separation in the internal dimensions, much like in similar systems studied in the context of the AdS/CFT correspondence. The size of these objects, however, does manifest itself in the cross sections for scattering processes mediated by electromagnetism and gravity.

One limitation of this approach is that these objects in the regime we study here are heavier than certain Kaluza–Klein (KK) modes of massless 11-D supergravity fields. So in the d-dimensional description, we see one or more extra dimensions before we see the elastic states. As we will see, the elastic states can be made very nearly stable in this same limit, and therefore at least do not decay into the lighter KK modes. (In some circumstances it may transpire that there is an AdS/CFT-like duality between a d-dimensional QFT and the supergravity modes, coupled to the rest of the system including the elastic states. Then the elastic states could be studied consistently in a completely d-dimensional description of the system.)

Another limitation is in our ability to calculate detailed physical quantities at the length scale corresponding to the size of the objects here. In the Horava–Witten (HW) example, the size is determined by the intrinsic thickness of the M2-brane, whose proper size is of order l_{11}. We can ameliorate this problem by considering the classical physics of a large-N collection of such objects, as we discuss in Secs. II and III. To discuss the quantum behavior of systems of this sort,

it might be useful to find an example in which the basic object is a (possibly wrapped) fundamental string, in a perturbative regime.

The article is organized as follows. In Sec. II we will introduce the Horava–Witten example and compute the energy/size relations that arise there (explaining in particular how the size is defined and determined). We will work out the scale of masses and sizes arising from Kaluza–Klein reduction. In Sec. III we work out (in less detail) the same procedure for type I′ theory. In Sec. IV we will provide a preliminary discussion of several interesting aspects and applications of these results. In Sec. IV A we will comment on the similarities and differences with branes, and discuss a possibility for an exponentially growing spectrum of bound states. In Sec. IV B we discuss scattering amplitudes and loop effects in these models. In Sec. IV C we conclude with a discussion of other issues and future directions.

II. HORAVA–WITTEN EXAMPLE

A. Mass-size relation in HW theory

M theory compactified on $S^1/\mathbb{Z}_2\times K3$ has a warped metric[1]

$$ds^2=y^{-1/3}dx_\parallel^2+y^{2/3}\left(dK^2+\frac{V_0^2}{l_{11}^6}dy^2\right), \tag{2.1}$$

where l_{11} is the 11-dimensional Planck length, and $y=c+2\sqrt{2}w$ with

$$w=\frac{\pi\rho_0-x^{11}}{V_0}6\pi\sqrt{2}l_{11}^3(k-12), \tag{2.2}$$

where x^{11} is a coordinate along the $S^1/\mathbb{Z}_2$ direction and k is the number of five-branes at the $x^{11}=0$ end of the interval. In these formulas, $\pi\rho_0$ is the size of the $S^1/\mathbb{Z}_2$ as measured with the coordinate x^{11} and V_0 is the volume of the K3 as measured in the K3 metric dK^2. These along with c are three of the moduli of the solution (the others being the other moduli of the K3 metric dK^2). The result (2.2) is valid in the regime $V_0\gg l_{11}^4$ and $\rho_0\gg V_0^{1/4}$.

Consider an M2-brane held at a point y in the interval, and wrapped on a cycle of the K3 with area $A(y)=A_0y^{2/3}$. Because the interval is very large ($\rho_0\gg l_{11}$), the 11-dimensional three-form gauge potential C_{MNP} has a Kaluza–Klein excitation with a tunably small mass. This means that our wrapped M2-brane can be made stable to a good approximation by taking the interval large enough.

Its energy, taking into account the warping, is

$$E=\sqrt{g_{00}}\,m_0=y^{-1/6}\left(y^{2/3}\frac{A_0}{l_{11}^3}\right)=y^{1/2}\frac{A_0}{l_{11}^3}, \tag{2.3}$$

where $m_0=y^{2/3}A_0/l_{11}^3$ is the proper energy of the wrapped M2-brane.

The extent of this wrapped brane along the $x_\parallel$ directions is, on the other hand, given by (1.2),

$$R=\frac{1}{\sqrt{a(y)}}r_0(y), \tag{2.4}$$

in terms of a characteristic proper size r_0. We will presently argue that this characteristic size is in fact l_{11}. Taking this value, we obtain from (2.4)

$$R=l_{11}y^{1/6}. \tag{2.5}$$

Combining (2.3) and (2.5), we obtain an energy-size relation

$$E=TR^3, \tag{2.6}$$

where the effective tension T is

$$T=\frac{A_0}{l_{11}^6}. \tag{2.7}$$

It is tempting to infer a mass scale for excitations from this relation of the order $\tilde{\mu}\sim T^{1/4}$. However, the scale of the tension is *a priori* not the only one in this problem; the kinetic energy of the elastic state will in general depend on further parameters. Therefore we will have to wait for the KK analysis of Sec. II B to obtain a determination of the scale of excitations of this system.

Now let us fix r_0 for this example. We can do so in two different regimes that will be of interest. First, consider the case where $A(y)\gg l_{11}^2$ for all y relevant to a given process. In this regime the supergravity solution for a wrapped membrane has a profile of characteristic size l_{11},[9] plus small corrections down by powers of l_{11}^2/A. At the scale l_{11}, the supergravity/general relativity approximation breaks down and we expect new structure at this scale. We therefore expect this scale to be seen by appropriate $11d$ supergravity modes in scattering processes, and we take it as a natural choice of the intrinsic proper thickness r_0 of the object.

Let us also consider the case of a regime of the K3 moduli space where dk^2 describes a K3 near an ALE singularity, so that there are two-cycles in the K3 with area $A_0\ll l_{11}^2$, and moreover consider a range of y for which $A(y)\ll l_{11}^2$. [We still take $V_0\gg l_{11}^4$ to be able to continue to use the results (2.1) and (2.2).] Strictly speaking the supergravity analysis[1] does not apply if there are sub-Planckian defects in the manifold, but the warping is caused by excess five-branes on one side of the interval scaling up the volume of the K3, which will presumably still happen in a regime where the K3 has localized ALE singularities. The analogous question has been studied in the Calabi–Yau threefold case in Ref. 10.) The UV cutoff of the gauge theory obtained near an ALE singularity (where the wrapped M2-branes emerge as Higgsed gauge bosons of an ADE gauge theory) is $1/l_{11}$. Therefore l_{11} is the short-distance cutoff of the theory, plus possibly small corrections going like powers of A/l_{11}^2. This is also the scale of the gauge coupling of the nonrenormalizable gauge theory obtained at the ALE singularity. The Coulomb forces between the Higgsed gauge bosons will go like $1/r^4$ for separations r much greater than the cutoff l_{11}. The form factor for scattering of these states will then have a characteristic size of order l_{11}. So in this case also, we will take l_{11} as the proper size r_0 of our M2-brane states.

Finally, for a collection of N M2-branes, we will take r_0 to be $l_{11}N^{1/6}$, which is the characteristic scale appearing in the supergravity solution. In Sec. II C we will study these regimes in more detail given the behavior of the KK wavefunctions we determine in the next subsection.

B. HW Kaluza–Klein analysis

We will now compute the spectrum of Kaluza–Klein modes of the wrapped M2-branes in the geometry (2.1). Let us consider for simplicity here the case of an M2-brane wrapped on a genus zero cycle of K3. For these the normal bundle is the line bundle $\mathcal{O}(-2)$ (which has no sections), so the M2-brane cannot move on the K3 without cost in energy. Here we will focus on the motion of the wrapped branes in the y direction, which dominates over the motion in the K3 in appropriate regimes of moduli. Let us for simplicity also consider the scalar components of the wrapped M2-branes.

In order to calculate the spectrum of excitations of these wrapped M2-branes, we can use a Kaluza–Klein reduction of the action

$$S_{\mathrm{HW}}=\int d^6x_{\|}dy\sqrt{G}[-G^{MN}\partial_M\phi\partial_N\phi-m_0^2(y)\phi^2]. \tag{2.8}$$

Here the indices M, N run over the seven dimensions of the warped interval, and G_{MN} is given by the corresponding components of (2.1), so that $G_{\mu\nu}=\eta_{\mu\nu}y^{-1/3}$ and $G_{yy}=y^{2/3}V_0^2/l_{11}^6$. There no explicit dependence in the action on the y-dependent K3 volume $V(y)=V_0y^{4/3}$ since the curve is isolated; there is dependence on the cycle area $A(y)=A_0y^{2/3}$ through the mass term in (2.8).

The modes are given by solutions of the equation of motion

$$\partial_M(\sqrt{G}G^{MN}\partial_N\phi)=\sqrt{G}m_0^2(y)\phi. \tag{2.9}$$

This becomes, upon plugging in our background,

$$y^{-1/3}\partial_{x_\parallel}^2\phi+\frac{l_{11}^6}{V_0^2}\partial_y(y^{-4/3}\partial_y\phi)=y^{2/3}\frac{A_0^2}{l_{11}^6}\phi. \tag{2.10}$$

Letting $\phi=e^{ik_\parallel x_\parallel}\tilde{\phi}$ we have that $\partial_{x_\parallel}^2\phi=-k_\parallel^2\phi=\mu^2\phi$, where μ is the mass of the excitation in six dimensions.

Defining $\eta=y^{-2/3}\phi$, this becomes

$$\eta''-\left[\frac{10}{9y^2}+ay^2-by\right]\eta=0, \tag{2.11}$$

where

$$a=\frac{A_0^2V_0^2}{l_{11}^{12}},\quad b=\frac{\mu^2V_0^2}{l_{11}^6}. \tag{2.12}$$

This is related to a nonrelativistic quantum mechanics problem with effective potential

$$V(z)=ay^2-by+\frac{10}{9y^2}. \tag{2.13}$$

We are interested in the discrete set of values of μ^2 [which comes into the parameter b (2.12)] for which this quantum mechanics problem has a state with zero energy eigenvalue.

For simplicity let us work in a regime where the last term in (2.13) can be dropped. The problem then reduces to a harmonic oscillator potential. We will be interested in determining the mass scale μ and the locations y_c where the solutions η are peaked. We will then check for self-consistency of this approximation.

In this regime, (2.11) can be rewritten

$$-\eta''+a\left(y-\frac{b}{2a}\right)^2\eta=\frac{b^2}{4a}\eta. \tag{2.14}$$

The energy eigenvalues in the corresponding harmonic oscillator problem are given by

$$E_n=\frac{b_n^2}{4a}=\sqrt{a}\left(n+\frac{1}{2}\right). \tag{2.15}$$

Using this and (2.12) we find a tower of masses

$$\mu_n^2=\frac{2A_0^{3/2}}{V_0^{1/2}l_{11}^3}\sqrt{\left(n+\frac{1}{2}\right)}=\frac{1}{\lambda_C^2}, \tag{2.16}$$

where we have indicated the Compton wavelength determined by this mass scale in the last step.

The nontrivial locations of the peaks of the wavefunction are at the length scale

$$y_n=\frac{b}{a}=\frac{2l_{11}^3\sqrt{n+\frac{1}{2}}}{A_0^{1/2}V_0^{1/2}}. \tag{2.17}$$

The values (2.17) are consistent with our assumption that the $1/y^2$ term in (2.13) could be ignored relative to the linear and quadratic terms for large enough μ^2.

From (2.17) and (2.5), we can determine the effective size of these excitations:

$$R_n \approx y_n^{1/6} l_{11} = \mu_n^{1/3} \frac{l_{11}^2}{A_0^{1/3}}. \tag{2.18}$$

They satisfy a mass-size relation

$$\mu_n \sim T R_n^3 \tag{2.19}$$

with a tension T agreeing with that found in our analysis in Sec. II A.

Since these excitations have a nontrivial size R_n, the point-particle Kaluza–Klein analysis we have done breaks down at this scale, which is to say that the mode solutions of (2.9) apply only for momentum $k_\parallel$ along the Poincare slices which is smaller than the scale $1/R_n$.

Note that these states grow (in number) faster than, for example, Kaluza–Klein modes on a circle. Of course the states of a single elastic state grow much more slowly than those of, say, a perturbative string. In Sec. IV A we will discuss briefly possible bound states of these objects, whose density of states does appear to grow exponentially with some power of the energy.

C. Size scales and regimes of moduli

In order for (2.2) to be reliable, we need $V_0 \gg l_{11}^4$. We can then consider different regimes of area $A(y)$ and M2-brane number N. Our arguments at the beginning of this section fixing $r_0 = l_{11}$ involved assuming $A(y)$ to be either very large or very small relative to l_{11}^2 for the range of y's of interest. Let us check here that that can be arranged for our KK excitations (2.16) and (2.17). At the typical y-values y_n, we have

$$A(y_n) = \frac{2 A_0^{2/3} l_{11}^2 \left(n + \frac{1}{2}\right)^{1/3}}{V_0^{1/3}}. \tag{2.20}$$

Suppose we wish to arrange for $A(y) \gg l_{11}^2$. From (2.20) this requires

$$A_0^{2/3} (n + \tfrac{1}{2})^{1/3} \gg V_0^{1/3}. \tag{2.21}$$

In this regime, the membrane is wrapped on a very large two-cycle, and is therefore heavy and behaves classically. Indeed, the condition (2.21) is the same as the condition that the Compton wavelength be much smaller than the object: $\lambda_C \ll R_n$. When (2.21) is satisfied for all n, the K3 is rather skew in shape, since in particular $(A_0/l_{11}^2) \gg (V_0/l_{11}^4)^{1/2}$. In this regime the elastic states behave classically.

On the other hand, suppose we wish to consider the case where $A(y) \ll l_{11}^2$. Then we need

$$A_0^{2/3} (n + \tfrac{1}{2})^{1/3} \ll V_0^{1/3}. \tag{2.22}$$

For this regime, the Compton wavelength is large compared to the size scale R_n, and the objects behave very quantum mechanically. When the K3 is near an ALE singularity, we argued at the beginning of this section that the cutoff scale and gauge coupling scale l_{11} determines the size of the object in this regime as well.

In both regimes we have studied here, for a small number N of branes the size R we have been discussing is determined by the warping from a fundamental proper size $r_0 = l_{11}$. Although we expect structure at this scale as discussed above, this being the scale of the profile of the supergravity solutions for M-branes for example, we do not have direct control over the details of processes at this scale. [Perhaps a more tractable generalization would be a case involving a (possibly wrapped) perturbative string. In such a case one could calculate reliably scattering

processes at the relevant size scale (l_s).] To study the elastic states' physics in a classical regime where we do have control, we can introduce a large number N of wrapped M2-branes. Then as discussed above, $r_0 \sim N^{1/6} l_{11}$. As in studies of black hole systems (Ref. 11, etc.) the branes then become amenable to a classical analysis in certain regions of the solution.[12]

Of course in adding branes to increase N, we increase both the mass and the size of the object as a function of N. Our point here is that in addition to that well-known effect, at fixed N there is the effect we have identified here: the stretching of the object along $x_\parallel$ due to the warping as one increases its energy. Considering a fixed large N allows us to study the classical physics of the elastic state effect in a regime where the physics at the scale of the object is under control.

We have thus obtained a consistent description of the wrapped M2-branes in the HW geometry which shows that they grow in size as a function of their energy. In this sense they behave like extended objects. We will begin a study in Sec. IV of the question of the extent to which these objects and their bound states might behave as familiar extended objects such as branes.

III. THE TYPE I′ CASE

In this section we will do a similar analysis of NS5-branes in the type I′ geometry derived in Ref. 2. We will work this case out a little more schematically than the last one, since the procedure is hopefully clear, but it is worth exhibiting a second example of the basic effect under consideration.

By some rescalings of the moduli and coordinates defined in Ref. 2 we can write the string-frame metric and dilaton schematically in the form

$$ds^2_{\text{string}} = \frac{\gamma^{5/3}}{(\beta + w)^{1/3}} (dx_\parallel^2 + l_s^2 dw^2), \tag{3.1}$$

$$e^{\phi} = \frac{1}{[\gamma(\beta + w)]^{5/6}}, \tag{3.2}$$

where β and γ are some combinations of the dilaton and radial modulus of the type I′ theory. Here $x_\parallel$ denotes the coordinates along the $9d$ Poincare slices in this geometry.

Let us compactify five of the spatial $x_\parallel$ dimensions on a T^5. For simplicity let us take the simple square shape

$$x_\parallel^{5,\ldots,9} \cong x_\parallel^{5,\ldots,9} + R_0. \tag{3.3}$$

The thickness of N NS5-branes in the remaining $x_\parallel$ directions can be determined in a large N limit from the supergravity solution. This gives[13]

$$r_0 \sim l_s N^{1/2}. \tag{3.4}$$

We can determine the energy-size relation from the warped metric and dilaton as follows. Let us work in terms of a coordinate $y \equiv w + \beta$. Taking into account the variation of the volume of the T^5 and the variation of the dilaton as a function of y, the energy is

$$E = \sqrt{g_{00}} m_0 = \frac{R_0^5}{l_s^6} \gamma^{20/3} y^{2/3}. \tag{3.5}$$

The size is

$$R = \frac{y^{1/6}}{\gamma^{5/6}} l_s N^{1/2}. \tag{3.6}$$

Putting these together leads to a growth in size with energy:

$$E = TR^4, \tag{3.7}$$

with effective tension

$$T = \frac{R_0^5 \gamma^{10}}{l_s^{10} N^2}. \tag{3.8}$$

The Kaluza–Klein analysis in this case can be done similarly to that for the Horava–Witten case.

IV. DISCUSSION: BOUND STATES, SCATTERING, AND OTHER ISSUES

A. Remarks on bound states and branes

Though our elastic states have a growth in size with energy somewhat reminiscent of branes, they each individually only have a Kaluza–Klein theory's worth of states. However, bound states of elastic states might exist (establishing or ruling out this possibility would require a careful analysis such as was done for D0-branes[14]). If so, these could have a much faster (exponential) growth in number with energy.

In the HW case, the wrapped M2-branes experience gravitational attraction and gauge (C_{MNP}) repulsion. Because the $S^1/\mathbb{Z}_2$ direction is compact, the relevant modes of C_{MNP} are slightly massive, as discussed in Sec. II. Therefore at very long distances the different elastic states attract each other. This suggests bound states might be possible, though an analysis of the short-distance structure is required to establish (or rule out) this possibility.

Consider a bound collection of bound states of N_n elastic states at level n in the spectrum (2.16) derived in Sec. II. An upper bound on the energy of such a state (in that it does not take into account the binding energy) is

$$\mu_{\rm tot} \sim \sum_n N_n \mu_n = \sum_n N_n \left(n + \frac{1}{2} \right)^{1/4} \frac{\sqrt{2} A_0^{3/4}}{V_0^{1/4} l_{11}^{3/2}}. \tag{4.1}$$

This spectrum grows exponentially.

If bound states do exist here, it is tempting to speculate that a large number of elastic states could mock up an effective brane (perhaps in a somewhat analogous way to the way D0-branes mock up higher branes in matrix theory[15]). It is further tempting to speculate that this approach can then provide a new way to quantize effective branes and study their interactions in some nontrivial regime.

B. Remarks on scattering amplitudes

Given the growth in size with energy of the objects we have been studying, it is interesting to consider where this effect would arise in scattering amplitudes. Contact interactions between large and small elastic states (which are particles at different points y_1, y_2 in the interval) are suppressed by the separation between y_1 and y_2. As in the case of objects going by each other in the AdS bulk,[16] in the d-dimensional description our objects appear to pass right through each other. (One possibility is that the large objects form a ring instead of a filled-in ball in the $x_\parallel$ dimensions as in some states in AdS.[3,5])

However if we consider the electromagnetic and gravitational interactions of our objects, their size is evident at tree level. In particular, the thickness of the object leads to a form factor with characteristic scale R in gauge and gravity-mediated scattering processes.

It will be interesting to study the effects of elastic states and bound states of elastic states in loops. For example, it will be interesting to calculate the contribution these objects and their bound states make to the vacuum energy. For this we need to know the spectrum of bound states as well

as a controlled prescription for describing their interactions. It may be very useful to consider an analogous case where the elastic states originate as strings (with a warping which amplifies their l_s-scale size).

C. Discussion

There are many issues to explore further with these states (and their many cousins in other warped compactifications). Generalizations which could be important for a potential brane picture include cases where the wrapped branes oscillate in more than one direction of a warped compactification. As discussed above, a case which would give more tractable calculations would be one in which the basic object is a perturbative string whose mass and size get warped by the compactification so as to give an energy-size relation of the kind we have studied here.

One question involves the relevance of AdS/CFT ideas and results to more generic warped compactifications. In some ways the elastic states we have discussed here are a generalization of the baryon states identified in AdS/CFT duals and their generalizations.[8] The growth in size of states with energy is characteristic of gravity in various high-energy regimes, but can also occur for some collective excitations in ordinary quantum field theory (and exponential growth of the density of states can also occur there in certain regimes[17]). It would be interesting to classify the behavior of states at high energy in QFT versus gravity in this regard, and in particular to understand if the class of states studied here is characteristic of gravity or could occur in a theory with a completely quantum field-theoretic dual.

Another interesting application of warped geometries is potentially to cosmology (obtained in appropriate cases by viewing the direction along which the warping appears as time t). In such a situation, the wrapped branes can become zero-action instantons at a singularity occuring at $t=0$ in the cosmology. It would be interesting to understand whether the corresponding instanton sum accounts for (and is related to a resolution of) the initial singularity in this sort of setup.

Particularly in the context of gravity, the effects of nonlocality are potentially important for many problems (see, e.g., Ref. 18 for a recent application). It would be interesting to understand what role, if any, these extended states play in the nonlocality of gravity in warped compactifications.

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Dynamical topology change in M theory

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We study the topology change in M theory compactifications on Calabi–Yau threefolds in the presence of G flux (the four form field strength). In particular, we discuss vacuum solutions in strongly coupled heterotic string theory in which the topology change is *inevitable* within a single space–time background. For rather generic choices of initial conditions, the field equations drive the Kähler moduli outside the classical moduli space of a Calabi–Yau manifold. Consistency of the solution suggests that degenerate flop curves—just as wrapped M theory fivebranes—carry magnetic charges under the four form field strength. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1377038]

I. INTRODUCTION

Over the years, several works[1,2] have established definitively that there are physically smooth processes in string theory which result in a change in the topology of space–time. In these studies, as well as studies of topology change in M theory,[3] one considers a one parameter family of vacuum solutions—a one parameter family of space–times—that passes from one Calabi–Yau manifold to another which is topologically distinct. The referenced works succeeded in showing that there is no obstruction to such a topology change, but no dynamics was ascribed to motion through the family. In the present work, we study a variation on this theme of topology change in which dynamics does drive the evolution from one topology to another. Specifically, (a) the topology change occurs within a single (not a family of) space–time background and (b) for generic choices of initial conditions, the dynamics (i.e., the field equations) drive us through a topology change.

To be concrete, we focus our studies on Calabi–Yau compactifications of M theory to five dimensions in the presence of G flux (the four form field strength). As discussed in Refs. 4–7, the effective five-dimensional theory does not admit a flat space vacuum solution. Rather, the space–time metric is warped and the solution is of the domain wall type with one of the five dimensions singled out as the transverse direction. In addition to the effective five-dimensional space–time metric, the moduli of the Calabi–Yau will generically vary along the transverse direction. In this paper, we show that there exist Calabi–Yau compactifications in which the field equations force the Kähler moduli to pass from one Kähler cone into an adjacent cone, while the overall volume of the Calabi–Yau manifold remains large. This implies that the Calabi–Yau manifold undergoes

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a flop transition and continues on to a topologically distinct Calabi–Yau manifold as we move along the transverse dimension.

One may think of our work as being complementary to that of Refs. 8–10 in which it was shown that in the presence of certain dyonic black holes, a Calabi–Yau with particular moduli at spatial infinity can be driven by the attractor equations through a flop transition on the way to the black hole's horizon. Here we find vacuum solutions whose structure requires topology change.

One feature of these topology changing solutions is that flop curves appear to be magnetic sources for the G flux. This becomes apparent from the Bianchi identity for the four-form G in the context of strongly coupled heterotic string theory (which we shall henceforth refer to as Horava–Witten theory), i.e., M theory on $S_1/\mathbb{Z}_2$. In this set-up, the orbifold planes provide magnetic sources for the four form G and this requires a modification of the Bianchi identity by a topological source term.[11] As we will see, consistency of the topology changing solutions suggests that the zero-size flop curve provides an additional magnetic source for G.

While we will not pursue it in this paper, the results of the present work may have implications for the ''brane world'' scenario.[11,5,12–15,13] Strongly coupled heterotic string theory is a rich context for the brane-world scenario in which fairly realistic low energy models can be constructed.[5] The class of models of interest, however, is substantially enlarged, as we allow the topology, and not just the metric, of the Calabi–Yau to change from one end of the world to another.

This paper is organized as follows. In Sec. II, we summarize the essential results of M theory and Horava–Witten theory compactified on Calabi–Yau three-folds in the presence of G flux. In Sec. III, we give an explicit example in which the solution to the field equations inevitably drives us through a flop transition. In Sec. IV, we discuss general features of topology changing solutions in Horava–Witten theory, and examine properties of G flux and the Bianchi identity in such geometric backgrounds. We end with some discussion in Sec. V.

After the presentation of these results by one of us,[16] M. Wijnholt and S. Zhukov notified us that they had also observed that the Bianchi identity requires modification in the presence of a flop transition.

II. KALUZA–KLEIN REDUCTION OF M THEORY ON A CALABI–YAU THREE-FOLD

Let us briefly summarize the results of the Kaluza–Klein reduction of eleven dimensional supergravity on a manifold with boundaries, that is, strongly coupled heterotic theory on a Calabi–Yau three-fold $\mathcal{M}$. (Many details can be found in the papers,[5,6,17,18] we differ in approach by using a first order formalism for the field strengths; see also Ref. 19. The appropriate Bianchi identities are imposed as an additional field equation.) We concentrate here only on the fields which are relevant to our subsequent discussion. Since we seek solutions with a nontrivial variation of the Kähler moduli, we keep the hypermultiplet scalar V (the Calabi–Yau breathing mode) which couples to the bulk potential terms, the vector multiplet scalars b^i (the Kähler moduli) as well as the axionic field strengths a_i and their dual potentials $\tilde{\lambda}^i$. The 5-dimensional action can be consistently truncated to this reduced field content leading to[5]

$$S_5 = -\frac{L^6}{2l^9}\Bigg[\int_{M_5}\sqrt{-g}\Big(R + G_{ij}(b)\partial_M b^i\,\partial^M b^j + \frac{1}{2}V^{-2}\,\partial_M V\,\partial^M V + \lambda(\mathcal{K}-1)\Big) + \frac{1}{4}V^{-2}G^{ij}(b)a_i\wedge\star a_j + d\tilde{\lambda}^i\wedge a_i\Bigg] - \sum_{n=0}^{N+1}\alpha_i^{(n)}\int_{M_4^{(n)}}\Big(\tilde{\lambda}^i + \frac{b^i}{V}\sqrt{f^*g}\Big). \tag{1}$$

Here λ is a Lagrange multiplier, the a_i arise from the Kaluza–Klein reduction of G with respect to a basis of $H^4(\mathcal{M})$, G_{ij} is the metric on the Kähler moduli space (not the 5-dimensional metric which is denoted by g_{MN}; f^*g is its pullback to the three-brane world-volume) and $\mathcal{K}$ its prepotential;

$$G_{ij}=-\frac{1}{2}\frac{\partial^2}{\partial b_i\,\partial b_j}\ln\mathcal{K},\quad \mathcal{K}\equiv\frac{1}{3!}d_{ijk}b^ib^jb^k, \tag{2}$$

where d_{ijk} are the intersection numbers of the (1,1) forms on $\mathcal{M}$. The gravitational coupling l is that of the original eleven-dimensional theory, and L the length scale of the Calabi–Yau.

The boundary terms include the relevant contributions from N five-branes at *a priori* arbitrary locations, with charges $\alpha_i^{(1)},\ldots,\alpha_i^{(N)}$. In units of the five-brane tension/charge these correspond to the multiplicity or equivalently the winding number of five-branes around the various two-cycles. The first order action includes the Bianchi identity, modified in the presence of five-branes, as the field equation for the dual potential $\tilde{\lambda}^i$,

$$da_i\equiv J_i^{(5)}\Rightarrow\begin{cases}\partial_{11}a_i=\dfrac{2l^9}{L^6}\displaystyle\sum_{k=0}^{N+1}\alpha_i^{(k)}\delta(x^{11}-x_k^{11}),\\ \partial_\mu a_i=0,\end{cases} \tag{3}$$

with the solution[5,6]

$$a_i=\frac{2l^9}{L^6}\left(\sum_k\alpha_i^{(k)}\epsilon(x^{11}-x_k^{11})+c_i\right). \tag{4}$$

The constants $\alpha_i^{(0)}$, $\alpha_i^{(N+1)}$ are the effective M5-brane charges carried by the end-of-the-universe 9-plane domain-walls. On each end-of-the-universe plane, the effective five-brane charge has two constituents, similar to the effective Dp',$(p'<p)$ charge carried by Dp-branes in non-trivial backgrounds. One constituent is the E_8 instanton number, which may be interpreted as M5-branes immersed in the 9-brane;[4,20] the second is the induced five-brane charge due to the nonvanishing curvature of the Calabi–Yau and proportional to $c_2(\mathcal{M})$,[4,5]

$$\alpha_i^{(k)}=\frac{T_5L^2}{8\pi^2}\int_{D_i}\left(\operatorname{tr}F^{(k)}\wedge F^{(k)}-\frac{1}{2}\operatorname{tr}R\wedge R\right),\quad k=0,N+1. \tag{5}$$

Here D_i is a 4-cycle of the Calabi–Yau, and the elementary five-brane charge T_5 equals

$$T_5=\frac{2\pi}{(4\pi)^{2/3}l^6}. \tag{6}$$

In the remainder we set all scales to unity.

The total five-brane charge must vanish on the orbifold interval $S_1/\mathbb{Z}_2$;

$$\sum_{k=1}^{N}\alpha_i^{(k)}+\sum_{j=0,N+1}\int_{D_i}\operatorname{tr}F^{(j)}\wedge F^{(j)}=\int_{D_i}c_2. \tag{7}$$

This is the Kaluza–Klein reduction of the invariant eleven-dimensional statement that the modified Bianchi identity,[11]

$$\begin{aligned}dG=\Bigg(&\left[\operatorname{tr}F_{(1)}\wedge F_{(1)}-\frac{1}{2}\operatorname{tr}R\wedge R\right]\delta(y)\\&+\left[\operatorname{tr}F_{(2)}\wedge F_{(2)}-\frac{1}{2}\operatorname{tr}R\wedge R\right]\delta(y-\pi R_{11})+\sum_i n_5^i\delta_{C^i}\delta(y-y_i)\Bigg)\wedge dy,\end{aligned} \tag{8}$$

due to the presence of boundaries and five-branes is integrable, i.e.,

$$\int_{S_1/\mathbb{Z}_2\times D_i} dG = 0 \quad \forall \quad D_i \in H_4(\mathcal{M}). \tag{9}$$

In (8) $\{C^i\}$ is a basis of $H_2(\mathcal{M})$ dual to the basis $\{D_i\}$ of $H_4(\mathcal{M})$ and δ_{C^i} is the four-form Poincaré dual to the 2-cycle C^i with delta-function support on C^i. Preservation of supersymmetry allows only configurations of instantons and five-branes (or anti-instantons and anti-branes).

If one chooses the standard embedding of the spin connection in the first E_8 gauge group such that

$$\operatorname{tr} F^{(1)} \wedge F^{(1)} = \operatorname{tr} R \wedge R, \tag{10}$$

then $\alpha_i^{(1)} = -\alpha_i^{(2)}$, no additional five-branes are needed and the effective five-brane charge on the Horava–Witten-plane with an unbroken gauge group at $y = \pi R_{11}$ is just the topologically induced charge $\alpha_i^{(2)} = -\frac{1}{2}\int_{D_i} c_2$.

In this formulation the fields a_i appear algebraically and may be integrated out, yielding the 4-dimensional domain-wall action with electric 5-form field-strengths $\mathcal{F}^i = d\tilde{\lambda}^i$;

$$S_5 = -\int_{M_5} \sqrt{-g}\left(R + G_{ij}\partial_M b^i \partial^M b^j + \frac{1}{2} V^{-2} \partial_M V \partial^M V + \lambda(\mathcal{K}-1) \right)$$
$$- V^2 G_{ij}(b) \mathcal{F}^i \wedge * \mathcal{F}^j] - \sum_{n=0}^{N+1} \alpha_i^{(n)} \int_{M_4^{(n)}} \left(\tilde{\lambda}^i + \frac{b^i}{V}\sqrt{f^* g} \right). \tag{11}$$

The supersymmetric domain-wall or three-brane solution to the field equations is given by[5]

$$ds_5^2 = e^{2A} dx_4^2 + e^{8A} dy^2$$

$$V = e^{6A},$$

$$e^{3A} = \left(\frac{1}{3!} d_{ijk} f^i f^j f^k \right),$$

$$b^i = e^{-A} f^i,$$

$$\mathcal{F}^i_{11,\mu\nu\rho\sigma} = \epsilon_{\mu\nu\rho\sigma} e^{-10A}(-\partial_{11} b^i + 2 b^i \partial_{11} A), \tag{12}$$

where the f^i's are defined in terms of one-dimensional harmonic functions,

$$d_{ijk} f^j f^k = H_i, \quad H_i = \sum_n \alpha_i^{(n)} |y - y_n| + c_i \tag{13}$$

$$= \sum_{n=0}^{k} 2\alpha_i^{(n)} y + k_i, y_k < y < y_{k+1}, \tag{14}$$

and the k_i are arbitrary constants of integration.

The solution can be obtained from the supersymmetry variations by searching for a global Killing spinor,[5,18,19]

$$\delta\psi_\mu^A = \gamma_\mu \left((\partial A)\gamma_{11}\epsilon^A - \frac{e^{4A} b^i a_i}{6V} (\tau_3)_B^A \epsilon^B \right),$$

$$\delta\psi_{11}^A = \partial\epsilon^A - \frac{e^{4A} b^i a_i}{12} (\tau_3)_B^A \gamma_{11} \epsilon^B, \tag{15}$$

$$\delta\zeta^A=(\partial \ln V)\,\gamma_{11}\epsilon^A-\frac{e^{4A}b^i a_i}{V}(\tau_3)^A_B\epsilon^B,$$

$$\delta\lambda^{iA}=(\partial b^i)\,\gamma_{11}\epsilon^A+\frac{e^{4A}}{2V}\left(a^i-\frac{2}{3}b^j a_j b^i\right)(\tau_3)^A_B\epsilon^B. \tag{15}$$

The Killing spinor,

$$\epsilon^A=e^A(\delta^A_B+\gamma_{11}(\tau_3)^A_B)\epsilon^B_0, \tag{16}$$

is preserved, provided the following conditions are satisfied:

$$\begin{aligned}\partial A-\frac{e^{-2A}}{6}b^i a_i&=0,\\ \partial b^i+\frac{e^{-2A}}{2}\left(a^i-\frac{2}{3}(b\cdot a)b^i\right)&=0.\end{aligned} \tag{17}$$

These are direct analogs of the attractor equations describing spherically symmetric BPS black-holes in four- and five-dimensional supergravities with eight supercharges.[21–23] By contracting the second equation in (17) with $\partial b^j G_{ji}(b)$, the third term vanishes whereas the first term yields the length (in the moduli space) of the vector tangent to the path the solution follows. Defining a central charge $Z=b^i a_i$, and using the fact that the $a_i=\alpha_i^{(n)}\epsilon(y-y_n)$ are (piecewise) constant, the resulting equation exhibits the monotonic flow of Z,

$$\partial Z=-2e^{2A}\,\partial b^i\,G_{ij}\,\partial b^j\leqslant 0. \tag{18}$$

Alternatively one can define the dimensionful central charge $\tilde{Z}=u^i\alpha_i$ where $u^i=e^{-2A}b^i$. The attractor equation can be written in the form

$$\partial\tilde{Z}=-\tfrac{1}{2}\partial_i\tilde{Z}\,G^{ij}(u)\partial_j\tilde{Z}\leqslant 0, \tag{19}$$

which relates the flow in the target space with the flow in the moduli space. Here,

$$\partial_i\tilde{Z}=\frac{\partial\tilde{Z}}{\partial u^i}. \tag{20}$$

Notice that as in Ref. 5, we are holding the hypermultiplets (which control the complex structure) fixed, and we shall continue to do so throughout this paper. It would be interesting to relax this assumption as one would need to do to study, for example, conifold transitions.

III. AN EXAMPLE

An essential aspect of (12) is that the moduli of the Calabi–Yau manifold will generically vary along the transverse direction y. This raises the question of whether one can find solutions in which the Kähler moduli vary through a Kähler wall in the moduli space; i.e., the Calabi–Yau manifold undergoes a flop transition as we move along y.

Suppose we are able to find such a solution; this will have consequences for the analysis of the action and the field equations in the previous section. Specifically, notice that the equations (12) and (13) depend upon the second Chern numbers through $\alpha_i^{(0)}$ and $\alpha_i^{(N+1)}$, and the intersection numbers d_{ijk} of the Calabi–Yau. These numbers jump when a Calabi–Yau manifold undergoes a flop. Hence, to exhibit an example where topology change occurs, we must search for solutions that (a) pass through a wall of the Kähler moduli space and (b) are a solution to the field equations of the form (12) for values of the topological numbers d_{ijk} and c_2 appropriate to the Calabi–Yau

on *each* side of the wall. Furthermore, in order to trust the supergravity approximation in which we work, we must also ensure that the overall Calabi–Yau volume V stays large.

In this section, through an explicit example involving some fairly tedious algebra, we will show that such topology changing solutions can indeed be found. In this example we will choose the standard embedding for the gauge bundles as this will facilitate our discussion of the Bianchi identity and flop-curves as sources of G-flux, in the next section.

A simple example of a pair of Calabi–Yau manifolds connected by a flop transition are the well studied $(h^{1,1},h^{2,1})=(3,243)$ Calabi–Yau manifolds considered in Refs. 24–26, 8, 9, 21. To investigate whether a flop can occur dynamically, we will attempt to match the solutions to the field equations for each of the Calabi–Yau manifolds across the singular point. We will find that, though the values of the fields can be matched continuously, their first derivatives are discontinuous at the flop. The jumps in the first derivatives of the Kähler moduli imply that there is an additional source of magnetic under the G-flux charge where the solutions are matched together (the flop point), and the Kähler moduli are sensitive to this magnetic source. In the next section, we will discuss the generality of this class of solutions.

Before we proceed, let us collect the essential data of the Calabi–Yau and its flopped cousin.[25] Details can be found in the aforementioned papers. In these works the manifold we denote with $\mathcal{M}$ is known as model III and $\tilde{\mathcal{M}}$ as model II. Both are elliptic fibrations over Hirzebruch surfaces.

(i) *Calabi–Yau manifold* $\mathcal{M}$. The intersection numbers are summarized in the classical prepotential $\mathcal{K}_{\mathcal{M}}=(1/3!)\,d_{ijk}t^it^jt^k$. For $\mathcal{M}$ the prepotential equals

$$\mathcal{K}_{\mathcal{M}}=\frac{1}{3!}(8(t^1)^3+9(t^1)^2t^2+3t^1(t^2)^2+6(t^1)^2t^3+6t^1t^2t^3). \tag{21}$$

The t^i are the components of the Kähler form expanded in a natural basis (a basis in which the Kähler cone is defined by $t^i>0$) of 2-forms ω_i for $H^2(\mathcal{M},\mathbb{Z})$,

$$J=t^i\omega_i\,. \tag{22}$$

Integrating J over an arbitrary 2-cycle C^i shows that the corresponding t^i measures its size.

The moduli t^i are related to the dimensionless fields b^i defined in the previous section by $b^i=V^{-1/3}t^i$. Therefore, the dependence of t^i on the transverse direction y is governed by the one-dimensional harmonic functions $H_i(y)$. The slopes of these harmonic functions are in turn determined by the effective five-brane charges. For the end of the world branes with standard embedding, the slopes are proportional to the periods of the second Chern class; in terms of the divisors $D_i\epsilon H_4(\mathcal{M})$ dual to ω_i, they are

$$c_2(D_1)=92,\quad c_2(D_2)=36,\quad c_2(D_3)=24. \tag{23}$$

(ii) *Flopped Calabi–Yau manifold* $\tilde{\mathcal{M}}$. The intersection numbers of this Calabi–Yau may be determined from its cousin $\mathcal{M}$ with the help of the relation (see, e.g., Ref. 1)

$$(D_{i_1}\cap D_{i_2}\cap D_{i_3})_{\tilde{\mathcal{M}}}=(D_{i_1}\cap D_{i_2}\cap D_{i_3})_{\mathcal{M}}-\sum_{\beta}\prod_{k}(D_{i_k}\cap C^{\beta}). \tag{24}$$

The C^{β} represent the curves that are flopped and the D_i on $\tilde{\mathcal{M}}$ are the proper transforms of the D_i on $\mathcal{M}$. In the present case there is only one such curve, and its intersection with the D_i is $D_i\cap C=\delta_{i3}$. Hence, the only intersection number which changes is d_{333}. It is shifted by -1. Thus, if we choose the D_i and their proper transforms as bases on $\mathcal{M}$ and $\tilde{\mathcal{M}}$ we find that the prepotential of $\tilde{\mathcal{M}}$ is equal to

$$\mathcal{K}_{\tilde{\mathcal{M}}}=\mathcal{K}_{\mathcal{M}}-\frac{(t^3)^3}{6}. \tag{25}$$

The Chern coefficients $\tilde{c}_2(D_i)$ of the flopped Calabi–Yau $\tilde{\mathcal{M}}$ can be calculated from the Tian–Yau theorem in Eq. (60) or using the relation

$$\int_{D_i} c_2 + 2(D_i \cap D_i \cap D_i) = 12\chi(D_i), \tag{26}$$

and noting that the holomorphic Euler characteristic $\chi(D_i)$ is invariant under flops. Hence,

$$\tilde{c}_2(D_1) = 92, \quad \tilde{c}_2(D_2) = 36, \quad \tilde{c}_2(D_3) = 26. \tag{27}$$

(iii) *Solutions to the field equations*. To find the explicit dependence of the moduli $f^i = V^{-1/6} t^i$ on the transverse direction we need to invert the nonlinear relations for $\mathcal{M}$ and $\tilde{\mathcal{M}}$ between f^i and H_i. As mentioned, we consider the case of standard embedding, i.e., $\mathrm{tr}\, F \wedge F = \mathrm{tr}\, R \wedge R$ at $y = 0$ and $\mathrm{tr}\, F \wedge F = 0$ at $y = \pi R_{11}$. In that case the slopes α_i of the harmonic functions H_i are solely proportional to periods of the second Chern class:

$$\alpha_i = \frac{1}{16\pi^2} \int_{D_i} \mathrm{tr}\, R \wedge R = \frac{1}{2} \int_{CY} \omega_i \wedge c_2(CY). \tag{28}$$

First we choose a more convenient basis,[25,8]

$$\begin{aligned} t^1 &= U, \\ t^2 &= T - \tfrac{1}{2} U - W, \\ t^3 &= W - U. \end{aligned} \tag{29}$$

In this basis the respective Kähler cones of $\mathcal{M}$ and $\tilde{\mathcal{M}}$ are defined by the regions

$$\begin{aligned} \mathcal{M}&: W > U > 0, T > \tfrac{1}{2} U + W, \\ \tilde{\mathcal{M}}&: U > W > 0, T > \tfrac{3}{2} U \end{aligned} \tag{30}$$

and the area of the flop curve equals $W - U$.

The relation between the moduli and the harmonic functions can now be straightforwardly inverted.[9] For $\mathcal{M}$ one finds

$$\begin{aligned} T &= \frac{1}{2} \frac{H_T}{U}, \\ U &= \frac{1}{2} \sqrt{\left(H_U + \frac{1}{2} H_W \right)} \pm \sqrt{\left(H_U + \frac{1}{2} H_W \right)^2 + 2H_W^2 - 2H_T^2}, \\ W &= -\frac{1}{2} \frac{H_W}{U} + \frac{1}{2} U, \end{aligned} \tag{31}$$

with

$$\begin{aligned} H_T &= 18|y| + k_T, \\ H_U &= 25|y| + k_U, \\ H_W &= -6|y| + k_W, \end{aligned} \tag{32}$$

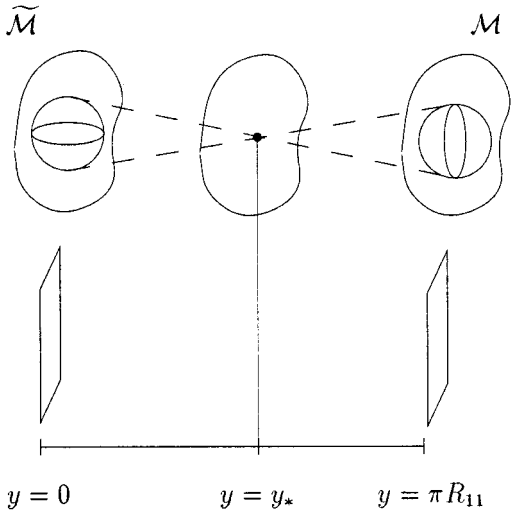

FIG. 1. Calabi–Yau configuration in heterotic M theory which undergoes a flop.

and for $\widetilde{\mathcal{M}}$,

$$T=\sqrt{\frac{1}{2}\tilde{H}_u\pm\frac{1}{2}\sqrt{\tilde{H}_u^2-\frac{9}{4}\tilde{H}_T^2}},$$

$$U=\frac{2}{3}\sqrt{\frac{1}{2}\tilde{H}_u\mp\frac{1}{2}\sqrt{\tilde{H}_u^2-\frac{9}{4}\tilde{H}_T^2}}, \tag{33}$$

$$W=\sqrt{-\tilde{H}_W},$$

with

$$\tilde{H}_T=18|y|+\tilde{k}_T,$$

$$\tilde{H}_U=24|y|+\tilde{k}_U, \tag{34}$$

$$\tilde{H}_W=-5|y|+\tilde{k}_W.$$

Requiring that we are in the correct Kähler cone for $\widetilde{\mathcal{M}}$ selects the positive and negative sign in the expressions for $T_{\tilde{\mathcal{M}}}$ and $U_{\tilde{\mathcal{M}}}$, respectively.

A. Matching the solutions

1. Location of the flop

If the field equations (whose behavior within the framework on each of the Calabi–Yau's we have already deduced) allow for a topology changing transition, it must be possible to match the solutions across the point where the flop-curve $t^3=W-U$ degenerates. As the relation between one of the moduli, W, of the Calabi–Yau $\widetilde{\mathcal{M}}$ and the harmonic functions is rather simple, we will first consider the flop solution from its point of view (see Fig. 1).

From the data in (33) and (34) we see that at the flop point the following quantity must vanish:[9]

$$9\tilde{H}_W^2+4\tilde{H}_U\tilde{H}_W+\tilde{H}_T^2=0. \tag{35}$$

Substituting the harmonic functions we find a quadratic equation for y. This equation has a solution if the discriminant is positive. The latter is a quadratic expression in the three integration constants $\tilde{k}_i$ and vanishes at the two roots:

$$25\tilde{k}_U=\left(45\pm\frac{5\sqrt{69}}{2}\right)\tilde{k}_T+(42\pm 9\sqrt{69})\tilde{k}_W. \tag{36}$$

A brief inspection shows that large $|\tilde{k}_U|$ corresponds to a positive discriminant and for a flop to occur we must therefore tune our integration constants such that

$$25\tilde{k}_U>\left(45\pm\frac{5\sqrt{69}}{2}\right)\tilde{k}_T+(42\pm 9\sqrt{69})\tilde{k}_W, \tag{37}$$

or

$$25\tilde{k}_U<\left(45\pm\frac{5\sqrt{69}}{2}\right)\tilde{k}_T+(42\pm 9\sqrt{69})\tilde{k}_W. \tag{38}$$

Regardless of the flop a necessary condition is that at the location of the brane at $y=0$, we are using the correct Calabi–Yau data. One condition, $2T>3U$, is guaranteed by the choice of solution in (33). The second one, $W>0$, is obeyed by requiring $\tilde{k}_W<0$. The last constraint, $W<U$, yields a lower bound on $\tilde{k}_U$ in terms of $\tilde{k}_T$ and $\tilde{k}_W$

$$\tilde{k}_U<-\frac{9\tilde{k}_W^2+\tilde{k}_T^2}{4\tilde{k}_W}. \tag{39}$$

Third, by requiring that (33) has solutions, we see that $\tilde{H}_U^2>9\tilde{H}_T^2/4$ or $2|\tilde{k}_U|>3|\tilde{k}_T|$. Fourth, in order that the solution to (35) truly corresponds to a point where $U=W$, the lower bound,

$$\tilde{k}_U>\frac{\tilde{k}_W}{2}, \tag{40}$$

must be satisfied. Finally, in order that all divisors also have positive area at $y=0$ one finds an additional constraint $\tilde{k}_T>0$.

The parameter space that obeys all these conditions consists of two regions, and it is quite generic that a flop occurs for some choice of intitial conditions. The two regions correspond to two possible flop scenarios: (a) both roots, y_+ and y_-, of (35) are larger than zero or (b) both roots are less than zero. *A priori*, there is the third possibility that $y_+>0>y_-$. However, this is not allowed because the quadratic (35) is convex and were we to find $y_+>0>y_-$, W would be larger than U at the location of the brane at $y=0$. Hence we would be in the wrong Kähler cone.

Given the explicit values of the roots,

$$y_\pm=\tfrac{1}{69}(10\tilde{k}_U-18\tilde{k}_T-3\tilde{k}_W\pm\sqrt{\mathcal{D}}),$$

$$\mathcal{D}=-612\tilde{k}_W^2-336\tilde{k}_U\tilde{k}_W+108\tilde{k}_T\tilde{k}_W+100\tilde{k}_U^2-360\tilde{k}_U\tilde{k}_T+255\tilde{k}_T^2, \tag{41}$$

the location of the minimum of (35) is

$$y_{\min}=\tfrac{1}{69}(10\tilde{k}_U-18\tilde{k}_T-3\tilde{k}_W). \tag{42}$$

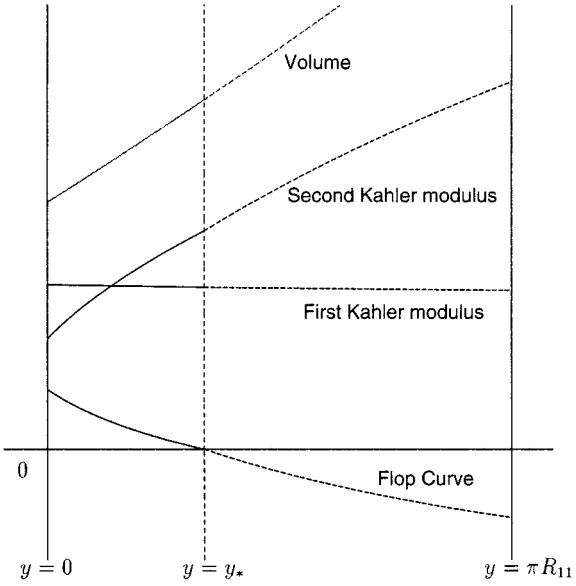

FIG. 2. Profile of the areas of the two cycles and the Calabi–Yau volume along y in a basis appropriate for Calabi–Yau $\tilde{\mathcal{M}}$. Solid lines belong to the validity region $y<y_*$ of the Calabi–Yau $\tilde{\mathcal{M}}$. Dashed lines belong to the Calabi–Yau $\mathcal{M}$ and hold for $y>y_*$.

We will consider the region of parameter space such that $y_{\min}$ is positive. [As it turns out, the field equations do not allow topology changing solutions with standard embedding in scenario (b).] It is easy to see that $y_{\min}>0$ for large $\tilde{k}_U$ provided that the other $\tilde{k}_i$ obey the above constraints (for example, $k_U=100, k_T=30$ and $k_W=1$). This region thus corresponds to scenario (a); the Calabi–Yau manifold at $y=0$ is model II with an $SU(3)$ gauge bundle and that at $y=\pi R$ is model III with no gauge bundle.

2. Continuity

We demand that the solution for the 2-cycles $b^i=V^{-1/6}f^i$ can be matched across the flop at the flop location $y_*\equiv y_-$. This implicitly requires that the harmonic functions match as well; $H_i(y_*)=\tilde{H}_i(y_*)$. As $c_2(D_T)=\tilde{c}_2(D_T)$ this implies that $\tilde{H}_T(y)=H_T(y)$ for all y. Similarly $H_U(y)+H_W(y)=\tilde{H}_U(y)+\tilde{H}_W(y)$. Combining this with the final requirement that $H_U(y_*)-H_W(y_*)=\tilde{H}_U(y_*)-\tilde{H}_W(y_*)$ yields

$$k_T=\tilde{k}_T,$$

$$k_U+k_W=\tilde{k}_U+\tilde{k}_W, \tag{43}$$

$$k_U-k_W=\tilde{k}_U-\tilde{k}_W-\tfrac{1}{2}y_*((c_2(U)-\tilde{c}_2(U))-(c_2(W)-\tilde{c}_2(W))).$$

In order that $U_{\mathcal{M}}(y_*)-W_{\mathcal{M}}(y_*)$ indeed vanishes at the flop point on Calabi–Yau $\mathcal{M}$ with the above values of k_i, we need to choose the negative sign in front of the square root in (31).

It is now straightforward to plot the solutions on both sides of the flop for a particular choice of constants k_i in region (a) and establish the occurrence of a flop transition; see Fig. 2.

3. Discontinuity in the first derivatives

We have seen that the function values of the moduli in the Calabi–Yau manifold $\mathcal{M}$ can be continuously connected to that in the flopped Calabi–Yau $\tilde{\mathcal{M}}$ at the location of the flop. We now check whether the first derivatives are continuous.

In a universal, basis independent, notation the derivatives of the 2-cycles f^i are related to those of the harmonic functions as

$$M_{ij}\,\partial f^j = \partial H_i\,. \tag{44}$$

Here M is the symmetric matrix $M_{ij}=2d_{ijk}f^j$. This equation is nothing but the condition for the existence of a global Killing spinor (17) and therefore a component version of the attractor equation (19). Indeed $M_{ij}\,\partial f^j \sim G_{ij}\,\partial b^j$.

In a natural orthogonal basis such as the t^i where exactly one of the t^i shrinks to zero, one sees immediately that at the flop point M is continuous. The potential source of discontinuity, the jump in the intersection numbers, always multiplies the very cycle which goes to zero. Recalling that the derivative of the harmonic function is just the slope,

$$\partial f^j = (M^{-1})^{ji}\alpha_i\,, \tag{45}$$

continuity of the first derivative of the cycles rests solely on the continuity of the slopes. Here, knowing its relation to the moduli space metric, we assume that the matrix M is invertible. The slopes, of course, are the five-brane charges at each end of the universe. And these jump due to the flop transition:

$$\begin{aligned}\partial f^j(y_*) - \partial \tilde{f}^j(y_*) &= (M^{-1}(y_*))^{ji}\alpha_i - (\tilde{M}(y_*)^{-1})^{ji}\tilde{\alpha}_i \\ &= (M^{-1}(y_*))^{ji}(\alpha_i - \tilde{\alpha}_i).\end{aligned} \tag{46}$$

Since M is generically not (block-)diagonal, the first derivatives of *all* cycles are discontinuous, as is evident in Fig. 2. The reason for the jump is the mismatch in $\int_{D_i} c_2(R)$ on different sides of the flop.

Let us also briefly check the behavior of the volume V of the Calabi–Yau,

$$V = \left(\frac{1}{3!}d_{ijk}f^i f^j f^k\right)^2 = \frac{1}{36}(f^i H_i)^2. \tag{47}$$

It is obviously continuous for the same reason that M is continuous. As for its derivative, it equals

$$\partial V = \frac{\sqrt{V}}{3}(\partial f^i\, H_i + f^i\,\partial H_i). \tag{48}$$

Using the above result for ∂f^i and the implicit relation $f^i = \frac{1}{2}M^{-1}(f(H))H$, this yields

$$6\,\partial\sqrt{V} = (\partial H \cdot M^{-1}\cdot H + \tfrac{1}{2}H\cdot M^{-1}\cdot \partial H) \tag{49}$$

and one recognizes the first Killing spinor equation in (17). Again the expression is simplified at the flop; and one would guess that the volume is discontinuous as well, as $H_i(y)$ and $M^{-1}(y)$ are continuous, but the slopes $\partial H_i(y)$ are not,

$$\partial\sqrt{V} - \partial\sqrt{\tilde{V}} = \tfrac{1}{4}((\alpha - \tilde{\alpha})\cdot M^{-1}\cdot H). \tag{50}$$

However, using the implicit relation, $f^i = \frac{1}{2}M^{-1}H$, once more, this is seen to be equal to

$$\partial\sqrt{V} - \partial\sqrt{\tilde{V}} = \tfrac{1}{2}((\alpha - \tilde{\alpha})\cdot f). \tag{51}$$

The only elements of the charge vector which jump are exactly those parallel to the flopping curve f^i_{flop}, which shrinks to zero. The potential source of discontinuity is therefore absent and ∂V is in fact continuous. This also means that the second derivative of V has no delta-function singularity.

B. Physical properties of the flop point

1. Charge of the flop

In comparing the solutions of the two topologically distinct Calabi–Yau manifolds at the flop, we find that the first derivatives of the Kähler moduli, $\partial_{11} b^i \sim \partial f^i$, are discontinuous.

By virtue of our gluing together solutions whose (piecewise) constant G-fluxes differ in magnitude, there is a jump in G-flux on crossing the flop point, and such a jump will cause a discontinuity in the fields. As we will discuss in more detail in the next section, this is part of why we will associate a magnetic G-charge with the flop point. More generally, though, for the G-flux to be globally defined, we require that

$$\int dG = 0, \tag{52}$$

which implies that the sum of magnetic charges under the four-form G must vanish. If the topology of the Calabi–Yau does not change, this condition is manifest for the standard embedding configuration; the geometrical five-brane charge induced from $\text{tr} R \wedge R$ is cancelled by that of the instanton configuration. However, as the topology of the Calabi–Yau on one ''end of the world'' changes, the global charge conservation constraint is no longer satisfied.

Denoting the induced magnetic charges, $\int_{D_i} G$, associated with the divisors D_i of the Calabi–Yau manifolds by (q_1, q_2, q_3), the brane at $y=0$ reduced over the flopped Calabi–Yau $\tilde{\mathcal{M}}$ has induced geometric charge $\alpha^{y=0}_{\text{geom}} = -\frac{1}{2}\tilde{c}_2(D_1, D_2, D_3) = (-46, -18, -13)$ compensated by the instantons with charge $\alpha^{y=0}_{\text{inst}} \equiv \tilde{c}_2(D_i) = (92, 36, 26)$. The brane at $y = \pi R_{11}$ only has induced geometric charges which equal $\alpha^{y=\pi}_{\text{geom}} = -\frac{1}{2} c_2(D_i) = (-46, -18, -12)$. Adding all contributions we see that we have an excess of $q_{\text{total}} = (0,0,1)$ units of charge.

The question is: what accounts for the missing (0,0,-1) units of magnetic charge? As indicated, a natural candidate is the flop curve which degenerates to zero volume at the flop point. This situation is not completely unfamiliar. There are examples where geometric singularities are magnetic sources (e.g., orbifold singularities in Ref. 27). The singular object in the present setting is the degenerate flop curve. It is therefore natural to conjecture that the flop must in some way be accompanied by $(0,0,-1)$ units of charge to ensure global charge conservation. If this is so, the discontinuities in the solution to the field equations is just a consequence of the fact that the flop carries magnetic charges, thereby inducing a jump in the G-flux.

We will examine in more detail the nature of the charge at the flop point in the next section.

2. Tension of the flop

If the flop point is a charge source, it is natural to inquire as to its possibly being a stress–energy source as well. The tension may be deduced from the curvature singularity. For a metric of the form (12), the nonvanishing components of the Einstein tensor are

$$\begin{aligned} G_{\mu\nu} &= -3e^{-6A}(A'' - 2(A')^2)\eta_{\mu\nu}, \\ G_{11,11} &= -6A'^2. \end{aligned} \tag{53}$$

The delta function singularities of the Einstein tensor, indicating a source of tension, can only come from the term A'', where $e^A = V^{1/6}$. In the previous subsection we showed that the second derivative of V is at most discontinuous. Hence, the tension of the flop point is zero. We note that this is in accord with the tension one would have from a five-brane wrapped around the flopping curve at the flop point.

3. Supersymmetry

Finally, we should check whether the charge of the flop is consistent with supersymmetry. In order that the supersymmetries which are preserved all have the same chirality, the inner products $f^i\alpha_i^{(n)}$ for all charged objects with charges $\alpha_i^{(n)}$ must have the same sign [from the Killing spinor equations, Eqs. (15)]

$$f^i\alpha_i^{(n)} \geqslant 0. \tag{54}$$

This inner product is equivalent to $\int_{\mathrm{CY}} J\wedge c_2(V)$ for vector bundles and $\int_{C^{(n)}} J$ for five-branes wrapping a curve $C^{(n)}$. This gives the well known condition that in order to preserve supersymmetry the bundles must be holomorphic and stable, and that five-branes must wrap around holomorphic curves. See also Ref. 19 for an in depth analysis of the supersymmetry structure.

What about the proposed charge located at the flop curve? As the volume of a flopped curve $\int_C J$ vanishes at a flop point it preserves the global Killing spinor.

Note that since f^i changes sign for the curve which flops, we see from Eq. (54) that a supersymmetric five-brane wrapping around the flopping holomorphic curve on either side of the flop will have *opposite* charge α_i. (Naively, one might think that it is possible to introduce as many 5-branes wrapping around the flopping curve C as possible, provided that we introduce an equal number of 5-branes wrapping around the curve $\tilde{C}$ on the other side of the flop. However, one has to check that the resulting configuration still has a consistent topology changing solution to the field equations.) This can be understood by noting that for a fixed set of divisors D_j, if the flopping holomorphic curve C meets, say, D_i transversely with $C\cap D_i=+1$ in Calabi–Yau manifold $\mathcal{M}$, then the corresponding holomorphic curve $\tilde{C}$ on the flopped Calabi–Yau manifold $\tilde{\mathcal{M}}$ lies inside D_i, with $\tilde{C}\cap D_i=-1$.

IV. TOPOLOGY CHANGING SOLUTIONS

In the above example, we have seen that consistency of the solution suggests that the zero-size flop curve is a source of magnetic charge. The effect of a magnetic charge at the flop is to modify the Horava–Witten Bianchi identity so that G is globally defined. In this section, we discuss this idea in more detail.

Let us begin by considering the global charge constraint anew. For simplicity, let us temporarily ignore the possibility of additional five-branes wrapped on other, nondegenerating, two-cycles in the bulk. In the eleven-dimensional theory on $S_1/\mathbb{Z}_2$, the Bianchi identity for G is modified by boundary sources.[11] We have

$$dG=([\operatorname{tr}F_{(1)}\wedge F_{(1)}-\tfrac{1}{2}\operatorname{tr}R_{(1)}\wedge R_{(1)}]\delta(y)+[\operatorname{tr}F_{(2)}\wedge F_{(2)}-\tfrac{1}{2}\operatorname{tr}R_{(2)}\wedge R_{(2)}]\delta(y-\pi R_{11}))\wedge dy, \tag{55}$$

where we are now taking care to distinguish the curvatures of the different Calabi–Yau spaces at each end of the interval. In the usual case, where $\operatorname{tr}R_{(1)}\wedge R_{(1)}=\operatorname{tr}R_{(2)}\wedge R_{(2)}$, we have the familiar standard embedding solution,

$$\operatorname{tr}F_{(1)}\wedge F_{(1)}=\operatorname{tr}R\wedge R,\quad \operatorname{tr}F_{(2)}\wedge F_{(2)}=0, \tag{56}$$

to the global consistency constraint that

$$\int_{S_1/\mathbb{Z}_2\times D} dG=\int_{S_1/\mathbb{Z}_2\times D} dy\left(\frac{1}{2}\operatorname{tr}R\wedge R\,\delta(y)-\frac{1}{2}\operatorname{tr}R\wedge R\,\delta(y-\pi R_{11})\right)=0. \tag{57}$$

But if $\operatorname{tr}R_{(1)}\wedge R_{(1)}\neq\operatorname{tr}R_{(2)}\wedge R_{(2)}$ (cohomologically) then the mismatch implies that solely embedding either spin connection into the gauge group is no longer a solution.

A natural suggestion, then, is to seek out different holomorphic stable bundles to place at $y=0$ and $y=\pi R_{11}$ with different second Chern classes, so as to find new consistent solutions to the

Bianchi identity. Indeed, one may be able to find appropriate bundles to restore anomaly freedom. However, for a number of reasons, we propose a more general and universal solution. Namely, when $\mathrm{tr}R_{(1)}\wedge R_{(1)}\neq \mathrm{tr}R_{(2)}\wedge R_{(2)}$ because the Calabi–Yau has flopped somewhere along y, there is a new contribution to the Bianchi identity associated with the collapsed flop curves.

To motivate our proposal, notice that given a potential flop solution to (12), *specifically* with standard embedding, we can vary the location in y at which the flop occurs, by varying the integration constants k_i—as we have seen explicitly in the previous section. Imagine now that we have such a solution where a cycle shrinks to zero size but we choose the k_i such that the flop does not occur in the physical range $0\leqslant y\leqslant \pi R_{11}$; rather, it happens formally at $y=\pi R_{11}+\epsilon$. This is just the usual situation in which the topologies of the Calabi–Yau manifolds at $y=0$ and $y=\pi R_{11}$ are identical. Therefore, as expected, the choice of a standard embedding of the spin connection into the gauge group is consistent.

Let's now adjust the k_i so that the flop occurs at $\pi R_{11}-\epsilon$, in the physical range so that the pure standard embedding, with no other charge sources, no longer provides a consistent solution. Where can the necessary other charge sources be? Four natural possibilities are the following: (1) Additional gauge structure at $y=0$; (2) new gauge structure at $y=\pi R_{11}$; (3) new wrapped 5-branes; or (4) magnetic charge associated with the geometrical singularity at y_*. By locality we do not expect to fix the Bianchi identity by adjusting the gauge bundle at $y=0$, as that lies at ''the other end of the universe'' from where the flop occurs, making possibility (1) seem unlikely. Nor do we expect to excite the new nontrivial gauge structure by changing the geometry/topology of the Calabi–Yau at $y=\pi R_{11}$ (where the initial gauge bundle was chosen to be trivial). In fact, as we will see in a moment, possibility (2) seems to be ruled out because the sign of the new magnetic source required to fix the Bianchi identity conflicts with the requirement that the new gauge bundle at $y=\pi R_{11}$ is stable. Possibility (3) immediately raises the following question: where along y_{11} should the purported new 5-brane wrapping C be located? From the discussion of the preceeding section, to contribute the correct charge, it must be located at a point y with $y\leqslant y_*$. Locality, and consistency with the solutions we have constructed in Sec. III in which the flux jumps at the flop point, pick out $y=y_*$. We will come back to this in a moment.

To understand possibility (4) we note that since a flop causes the geometrical G-source contribution $\mathrm{tr}\,R\wedge R$ to change, it is natural to suggest that a compensating magnetic source is provided by the geometrical singularity at the location of the flop itself. Strictly speaking, we are considering M theory compactified on a 7-manifold with boundaries, as the Calabi–Yau moduli are varying over the $S^1/\mathbb{Z}_2$. At the location of the flop, the 7-manifold is also singular—with the singularity of the form of a cone over CP^3 (see, e.g., Ref. 28). (We thank Edward Witten and Chien-Hao Liu for discussions on this point.) Geometrical singularities are known to carry magnetic charges (e.g., orbifold singularities in Ref. 27, and orientifolds). The singular objects in the present setting are the flop curves when they attain zero quantum volume.

To complete the proposal, we need to specify the strength of the charge carried by the flop. A theorem of Tian and Yau, which we will discuss directly below, suggests that, if a flop occurs at $y=y_*$, the gravitational contribution to the Bianchi identity is modified to

$$dG_{\mathrm{grav}}=\left(-\frac{1}{2}\mathrm{tr}\,R_{(1)}\wedge R_{(1)}\delta(y)-\frac{1}{2}\mathrm{tr}\,R_{(2)}\wedge R_{(2)}\delta(y-\pi R_{11})+\sum_{\beta}\delta_{C^\beta}\delta(y-y_*)\right)\wedge dy, \tag{58}$$

where β sums over all the holomorphic curves $\{C^\beta\}$ that flop at $y=y_*$.

This additional gravitional contribution has a close analogy with bulk five-brane sources wrapped on nonsingular curves.[27] The gauge bundle contribution to dG can be augmented by having five-branes wrapped on two-cycles $C^i\subset\mathcal{M}$ at locations $y=y_i$. This causes the matter part of the Bianchi identity to take the form[5] [see Eq. (8)]

$$dG_{\mathrm{matter}}=\left(\mathrm{tr}\,F_{(1)}\wedge F_{(1)}\delta(y)+\mathrm{tr}\,F_{(2)}\wedge F_{(2)}\delta(y-\pi R_{11})+\sum_{i}\delta_{C^i}\delta(y-y_i)\right)\wedge dy, \tag{59}$$

in the case of singly wrapped five-branes on holomorphic curves.

There is, however, an important subtlety in the above expression (58). In the presence of a flop, one has to define precisely what one means by the curves C^β. With respect to a chosen basis of divisors D_i, which (via invoking the proper transform map) can be made universal on both sides of the flop, flopping curves differ in orientation from one side to the other. To be concrete, suppose that the flopping curve C^β and the set of divisors D_i meet transversely on a Calabi–Yau manifold $\mathcal{M}$ with $C^\beta \cap D_i = 1$. In the flopped Calabi–Yau manifold $\tilde{\mathcal{M}}$, as we mentioned earlier, the flopping curve $\tilde{C}^\beta$ is no longer transverse to D_i, but instead lies inside D_i, with $\tilde{C}^\beta \cap D_i = -1$. Therefore, one has to specify in Eq. (58) on which Calabi–Yau manifold the holomorphic curve C^β is collapsing in order that the geometrical data is complete. In fact, this subtlety in assigning magnetic charges when a curve collapses is not intrinsic to the flop point, and is already present when one considers a five-brane wrapped around a collapsing curve. We have discussed this subtlety in the analysis of supersymmetry in the previous section. In the same manner, one has to specify on which Calabi–Yau manifold the curve C_i (that the five-brane wraps) is collapsing. The reason is that with respect to a fixed divisor D_i (and its proper transform), the charge of the five-brane differs by a sign depending on whether one approaches the flop point from one Calabi–Yau or from its flopped cousin.

Let us examine more closely which holomorphic curve C^β one should use in Eq. (58). Recall that our topology changing solution can be obtained, starting from a standard solution in which the topology of the Calabi–Yau does not change in the physical regime $0 \leqslant y \leqslant \pi R_{11}$ (which we call the ''parent'' solution). Subsequently by varying the initial conditions of the two-cycles (the integration constants k_i), while keeping the gauge bundle fixed, we can bring the flop point to $y = \pi R_{11} - \epsilon$. This causes a jump in $\mathrm{tr}\, R \wedge R$, which must be compensated by the flop charge. The question, then, is the following: What is the jump in $\mathrm{tr}\, R \wedge R$ under a flop? A theorem of Tian and Yau[29] states that starting from a Calabi–Yau manifold $\tilde{\mathcal{M}}$ and a collection of holomorphic curves $\{C^\beta\}$ on $\tilde{\mathcal{M}}$, the second Chern numbers of $\tilde{M}$ and its flopped cousin M are related by

$$c_2(\mathcal{M}) = c_2(\tilde{\mathcal{M}}) + 2\sum_\beta \int_D [C^\beta], \tag{60}$$

with D an arbitrary divisor and $[C^\beta] \in H^4(\tilde{\mathcal{M}})$, the Poincare dual of C^β. We therefore see that

$$-\frac{1}{2}\mathrm{tr}_{\mathcal{M}}\, R_{(2)} \wedge R_{(2)} + \sum_\beta \delta_{C^\beta_{(1)}} = -\frac{1}{2}\mathrm{tr}_{\tilde{\mathcal{M}}}\, R_{(1)} \wedge R_{(1)}\,. \tag{61}$$

Hence, the C^β in (58) are holomorphic curves on the Calabi–Yau manifold $\tilde{\mathcal{M}}$ of the ''parent'' solution. The total G-charge, including that carried by the flop, still equals $\mathrm{tr}\, R_{(1)} \wedge R_{(1)}$, which is exactly cancelled by the standard embedding on the brane wrapping $\tilde{\mathcal{M}}$; the charge conservation constraint is satisfied.

Notice that the flop contribution to the Bianchi identity is the same as that of a five-brane wrapping the flopping curve on the Calabi–Yau of the ''parent'' solution (which lies at $y = 0$ in our setup). However due to the fact that supersymmetric five-branes wrapping the ''flopping'' curve on the other ''flopped'' Calabi–Yau, must carry the opposite charge, the missing charge required to satisfy the Bianchi identity *cannot* be carried by a five-brane on the other side of the flop. Nevertheless, this means that the magnetic source contributed by a wrapped 5-brane over the appropriate degeneration of the flop curve is identical to the magnetic source of the singularity at y_* to which we are led by the result of Tian and Yau. Hence, at our level of analysis possibility (3)—realized at y_*— and possibility (4) are indistinguishable. [An argument for possibility (3) is, perhaps, that the above calculation indicates that the form of the local singularity does not uniquely determine the sign of the charge it is required to carry. Namely, as we have phrased the calculation, the additional data of which Calabi–Yau is used in the ''parent'' theory is needed. Equivalently, the sign of the charge depends upon the details of the background G-flux.]

We can now also complete the promised argument that seems to rule out possibility (2). The missing magnetic source for dG in the presence of a single flopped curve is $\delta_C = -\delta_{C'}$ where C lies on the Calabi–Yau to the left of y_* and C' lies on the Calabi–Yau to the right of y_*. The question then is whether there is a stable holomorphic vector bundle V on the Calabi–Yau at $y = \pi R_{11}$ such that

$$c_2(V) = \tfrac{1}{2}(c_2(T_2) - c_2(T_1)) = -\delta_{C'}. \tag{62}$$

But if there were such a bundle, then

$$\int c_2(V) \wedge J = -\int_{C'} J < 0, \tag{63}$$

violating the stability condition on V. Hence, a gauge instanton at $y = \pi R_{11}$ alone cannot account either for the missing charge required to satisfy the Bianchi identity.

We note that the inability of G-charge considerations to distinguish between a five-brane of the ''parent'' solution wrapping the zero-size flop curve and a purely geometrical singularity raises the interesting question whether flop transitions aside from new sources of five-brane charge are also accompanied by the introduction of new low-energy degrees of freedom. (We note that preliminary analysis indicates that we can deform the solutions of Sec. III so that the jump in the G-flux occurs to the left of the flop point, with all quantitites then being smooth across the flop point itself. This would naturally be interpreted as the required G-charge being carried by a 5-brane wrapped on the ''would-be'' flop curve, to the left of the flop point. A further analysis of these solutions would likely help clarify this issue.)

We propose therefore, that in strongly coupled heterotic string theory, the general Bianchi identity for arbitrary gauge bundles at $y = 0$ and $y = \pi R_{11}$, in a space–time background in which the Calabi–Yau undergoes a flop transition at $y = y_*$, together with an arbitrary assortment of 5-branes wrapping two-cycles other than those involved in the flop transition itself, is

$$dG = \Bigg(\left[\operatorname{tr} F_{(1)} \wedge F_{(1)} - \frac{1}{2} \operatorname{tr} R_{(1)} \wedge R_{(1)} \right] \delta(y) + \left[\operatorname{tr} F_{(2)} \wedge F_{(2)} - \frac{1}{2} \operatorname{tr} R_{(2)} \wedge R_{(2)} \right] \times \delta(y - \pi R_{11}) + \sum_i n_5^i \delta_{C^i} \delta(y - y_i) + \delta(y - y_*) \sum_\beta \delta_{C^\beta} \Bigg) \wedge dy, \tag{64}$$

with C^i being holomorphic curves in the Calabi–Yau that the corresponding five-brane wraps, and C^β being the flop curve on the appropriate Calabi–Yau as described above. Of course, the last two contributions can be grouped together, as long as the contribution associated with any degenerating curves is calculated according to the limiting procedure from the correct side of the flop point.

V. CONCLUSION

In this paper, we have studied topology changing solutions in M theory compactifications on Calabi–Yau three-folds with nonzero G-flux. In the presence of G-flux, the field equations do not admit five-dimensional Minkowski space as a vacuum solution. The space–time metric is warped, with the solution of the domain-wall type so that one of the five dimensions is singled out as the transverse direction. In addition to the space–time metric, other moduli of the Calabi–Yau manifold also vary along the transverse directions. We have studied an example in strongly coupled heterotic string theory—the supersymmetric domain wall solution—in which the field equations force us to go through a flop transition as we move from one end of the world to the other. Consistency of the solution suggests that a flop curve—like an ordinary (wrapped) M theory five-brane—carries a single unit of magnetic charge under the G-flux.

We have focused our attention on flop transitions. As in Ref. 5 we have assumed that the hypermultiplets can be consistently decoupled in the five-dimensional effective theory. Especially

in nontrivial geometric situations as presented here, it would be interesting to revisit this issue of decoupling. Moreover, this would allow the study of a more drastic change of topology, such as conifold transitions, in which the hypermultiplets necessarily play a role. As the number of moduli of the Calabi–Yau changes across a conifold transition, it is perhaps more appropriate to treat the compact manifold as a G_2 7-manifold with boundaries which are Calabi–Yau's. The low energy degrees of freedom in the effective four-dimensional theory then correspond to Ricci flat deformations of metric of the 7-manifold. We will leave this investigation for future work. From a phenomenological point of view, it might be interesting to look for more general solutions in which the topology changes also with time. This may have implications for cosmology as well as other physics of the brane world scenario.

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The metric and strong coupling limit of the M5-brane

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We find the analog of the Boillat metric of Born–Infeld theory for the M5-brane. We show that it provides the propagation cone of *all* 5-brane degrees. In an arbitrary background field, this cone never lies outside the Einstein cone. An energy momentum tensor for the three-form is defined and shown to satisfy the Dominant Energy Condition. The theory is shown to be well defined for all values of the magnetic field but there is a limiting electric field strength. We consider the strong coupling limit of the M5-brane and show that the corresponding theory is conformally invariant and admits infinitely many conservation laws. On reduction to the Born–Infeld case this agrees with the work of Białynicki-Birula. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1376158]

I. INTRODUCTION

The behavior of the low energy states of the super-string theories in ten dimensions are described by supergravity theories which are uniquely specified by their type of supersymmetry. These theories satisfy a form of the the Equivalence Principle: the characteristics and hence the limiting propagation speeds of all the fields, be they the graviton, the gravitini, p-form fields, scalars and spinors are given universally by the light-cone of the Einstein metric g_{mn}. The characteristics cones determine the paths of null geodesics which are associated with massless particles. Violations of the Weak Equivalence Principal, that is that all freely falling particles, massive or massless, follow geodesics of the Einstein metric, are known to occur for massive particles in string theory, because the former can couple to a background dilaton field Φ. This may be seen by noting that the unique effective actions, that is the maximal supergravity theories in ten dimensions,[1,2] contain different powers of e^{Φ} in front of the field strengths associated with the Neveu–Schwarz⊗Neveu–Schwarz and Ramond⊗Ramond sectors. It is also known that string theory induces higher derivative corrections which may affect the characteristics[3] in a nontrivial background.

The behavior of the states of open string theories are described by Dirac–Born–Infeld type actions provided one discards derivatives acting on field strengths. In a recent paper[4] it was argued that in a nontrivial background these open string states obey a modified form of the Equivalence Principle: the characteristics are universally given by a metric first introduced in nonlinear electrodynamics by Boillat and which is conformal to what is usually referred to as the open string metric.[5]

It was found that the Boillat cone never lies outside the Einstein cone and in general touches it along the two principal null directions of the two-form $\mathcal{F}_{\mu\nu}=F_{\mu\nu}+B_{\mu\nu}$, where $F_{\mu\nu}$ is the Born–Infeld gauge field strength and $B_{\mu\nu}$ is the Kalb–Ramond 2-form gauge field. In the limit of large field strength or equivalently large α', propagation perpendicular to the principal null directions is suppressed.

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In this paper we shall consider the analog of the Boillat metric for the M-5-brane equations of motion.[6] We shall call this metric C_{mn} Note that the characteristics may be read off from the co-metric C^{mn}. The speed of the rays are read off from its inverse $(C^{-1})_{mn}$ which is traditionally called a metric. If more than one metric is involved one must distinguish carefully between metrics and their inverses, i.e., between metrics and co-metrics. In the context of lattices and elsewhere, the prefix ''co-'' is frequently replaced by the adjective ''reciprocal.'' We prefer ''co-'' because it is shorter. Note that there is no analog of the Boillat co-metric for the M-2-brane because the world volume theory has no gauge fields. We shall find that indeed a modified form of the Equivalence Principal holds for the M-5-brane: the characteristics of fluctuations are given universally by an analog of the Boillat cone which never lies outside the Einstein cone. We will show that if one dimensionally reduces the theory to Born–Infeld theory then the fivebrane metric becomes the Boillat metric of the D4-brane. We shall define an energy momentum tensor for the fivebrane. It satisfies the striking identity,

$$T^{mn}=g^{mn}-C^{mn}, \tag{1}$$

and we show that it obeys the dominant energy condition.

One may show that the fivebrane has a limiting electric field strength beyond which the theory breaks down. By contrast, there is no limiting magnetic field strength. Finally we consider a high energy, or zero tension, limit of the fivebrane which is Weyl invariant and admits infinitely many conservation laws.

The plan of the paper is as follows. In Sec. II we introduce the 5-brane metric and 5-brane Clifford algebra. We show that the 5-brane metric gives the characteristics of the propagating fields whose speeds can never exceed that of light. In Sec. III we show that the two lightcones touch along a circle of null directions. In Sec. IV we introduce the covariantly conserved energy momentum tensor for the three-form and show that it satisfies an identity analogous to Hooke's law in classical elasticity theory. We show that in general its trace is nonvanishing and hence the three-form equations of motion are not invariant under a Weyl rescaling of the Einstein metric. In Sec. V we develop the idea that there is a 5-brane Equivalence Principal. In Sec. VI we show how our metric agrees with the Boillat metric of Born–Infeld theory. In Sec. VIII we show that plane wave solutions of the linear theory are exact solutions of the full nonlinear theory. In Sec. IX we discuss the limiting electric field strength and the behavior the theory near it. In Sec. X we consider this strong coupling limit in detail. We show that the theory is Weyl-invariant in this limit and that it admits infinitely many conserved quantities.

II. THE 5-BRANE METRIC

The equations of motion of the scalars X^N, closed three-form, H_{lmn} and spinors Θ,[6]

$$G^{mn}\nabla_m\nabla_n X^N=0, \tag{2}$$

$$G^{mn}\nabla_m H_{nrs}=0, \tag{3}$$

$$\nabla_m\Theta(1-\Gamma)\Gamma^n m_{mn}=0, \tag{4}$$

where ∇_m is the Levi-Civita covariant derivative with respect to the Einstein metric g_{mn}. To begin with, we consider their characteristics which require only the leading derivative terms. A short calculation shows that the characteristics of the X^N and H_{lmn} fields given by the co-metric G^{mn} which is defined by

$$G^{mn}=m^{mr}g_{rs}m^{sn}=\left(1+\tfrac{2}{3}k^2\right)g^{mn}-4k^{mn}, \tag{5}$$

where G_{mn} which will be defined to be $(G^{-1})_{mn}$, with $G^{mn}=(G)^{mn}$. All indices are raised and lowered using the Einstein metric g_{ab}, which is taken to have signature $-1,+1,+1,+1,+1$,

$+1$, *with the exception of* G_{mn} which will be defined to be $(G^{-1})_{mn}$, with $G^{mn}=(G)^{mn}$. In fact it seems to be possible to avoid explicit use of the covariant form of the metric in all of the equations of motion. Only the contra-variant form is required:

$$m^{mn}=g^{mn}-2k^{mn}, \tag{6}$$

$$k^{mn}=h^{n}{}_{ab}h^{mab}, \tag{7}$$

where h_{abc} is a self-dual three-form,

$$h_{abc}=\tfrac{1}{6}\epsilon_{abcdef}h^{def}, \tag{8}$$

and

$$k^2=k_{ab}k^{ab}. \tag{9}$$

In what follows shall repeatedly use the identities[7,6]

$$g_{ab}k^{ab}=0, \tag{10}$$

and

$$k^{ab}g_{bc}k^{cd}=\tfrac{1}{6}g^{ad}k^2=\tfrac{1}{6}g^{ad}k_{ef}k^{ef}. \tag{11}$$

Thus, for example,

$$C^{mn}=m_a^m m^{an}=2Q^{-1}m^{mn}-g^{mn}. \tag{12}$$

The self-dual field h_{abc} obeys the relations[7]

$$h_{abe}h^{cde}=\delta^{[c}_{[a}k^{d]}_{b]}, \tag{13}$$

and

$$k_a{}^c k_c{}^b=\tfrac{1}{6}\delta^b_a k^2. \tag{14}$$

For later use we define

$$Q=1-\tfrac{2}{3}k^2. \tag{15}$$

The closed three-form H_{abc} is related to the self-dual field h_{abc} by $h_{abc}=m_a{}^e H_{ebc}$, or equivalently by $H_{abc}=(m^{-1})_a{}^e h_{ebc}$ where $m^{-1}=Q^{-1}(1+2k)$. It will be proven useful in what follows to translate the self-duality condition on h_{abc} to one expressed entirely in terms of H_{abc}. This was carried out in Ref. 7 and refined in Ref. 8. Since $k_a{}^e h_{ebc}$ is anti-self-dual we can express

$$H^{+}_{abc}\equiv\frac{1}{2}\left(H_{abc}+\frac{1}{3!}\epsilon_{abcdef}H^{def}\right)=Q^{-1}h_{abc} \tag{16}$$

and

$$H^{-}_{abc}\equiv\frac{1}{2}\left(H_{abc}-\frac{1}{3!}\epsilon_{abcdef}H^{def}\right)=2Q^{-1}k_a{}^e h_{ebc}. \tag{17}$$

Taking the sum and difference we find that

$$H_{abc}=Q^{-1}(1+2k)_a{}^e h_{ebc},\ *H_{abc}=Q^{-1}(1-2k)_a{}^e h_{ebc}. \tag{18}$$

Multipying the second equation by the matrix $(1+2k)^2$ and using the first equation we conclude that

$$*H^a{}_{bc}=Q^{-1}G^{ae}H_{ebc}. \tag{19}$$

Substituting the relation $h_{abc}=m_a{}^eH_{ebc}$ into Eq. (13) we find that

$$H_{abe}H^{cde}=\tfrac{1}{2}\delta^c_{[a}\delta^d_{b]}Q^{-1}(Q^{-1}-1)+2Q^{-2}k^c_{[a}k^d_{b]}+Q^{-2}(2-Q)\,\delta^{[c}_{[a}k^{d]}_{b]}. \tag{20}$$

Taking the trace of this equation we find that

$$k_a{}^c=\frac{Q^2}{(2-Q)}\left((H^2)_a{}^c-\frac{1}{6}\,\delta_a{}^cH^2\right), \tag{21}$$

and tracing again

$$H^2=6Q^{-1}(Q^{-1}-1), \tag{22}$$

where $(H^2)_a{}^c=H_{aef}H^{cef}$.

We may express the last equation as

$$Q=-\frac{3}{H^2}\left(1-\sqrt{1+\frac{2}{3}H^2}\right). \tag{23}$$

It is now straightforward to express the matrix m^2 as

$$(m^2)^{ac}=G^{ac}=\frac{Q^2}{(2-Q)}\left(\eta^{ac}\left(1+\frac{4}{3}H^2\right)-4(H^2)^{ac}\right) \tag{24}$$

and

$$(m^{-2})_{ac}=G_{ac}=\frac{1}{(2-Q)}(\eta_{ac}+4(H^2)_{ac}). \tag{25}$$

Finally, we may express the self-duality of h_{abc} in terms of H_{mnp} by using Eqs. (19) and (20) and find that

$$*H_{abc}=\frac{1}{\sqrt{1+\frac{2}{3}H^2}}\left(\left(1+\frac{4}{3}H^2\right)\delta_a{}^e-4(H^2)_a{}^e\right)H_{ebc}. \tag{26}$$

We now turn briefly to the fermion sector. The projector in the spinor equation of motion is defined by

$$\Gamma=-\tfrac{1}{6}\,\eta^g_{lmnpqr}\Gamma^{lmnpqr}+\tfrac{1}{3}h_{lmn}\Gamma^{lmn}, \tag{27}$$

where η^g_{lmnpqr} is the alternating tensor (not density) constructed from the Einstein metric.

In the case that the scalar and spinors vanish, the covariant equations of motion, when expressed in terms of 5-dimensional language, agree with a particular case of the equations of Ref. 9. The particular case is the one that upon reduction gives Born–Infeld theory. One advantage of the covariant formulation used here is that, not only does it cover the more general case of nonvanishing scalars and spinors, but also the derivation of the characteristics is especially transparent.

The characteristics determine a metric only up to a conformal factor. It turns out that it is more convenient to Weyl rescale the co-metric G^{mn} and we therefore adopt as our definition of the M5-brane metric C^{mn},

$$C^{mn}=Q^{-1}G^{mn}=Q^{-1}m^{mp}g_{pq}m^{qn}. \tag{28}$$

We recall that in the Born Infeld theory the characteristics are given by the Boillat metric[4] up to a conformal factor. The Boillat metric which is proportional to the open string metric has the advantage that it is invariant under electric magnetic duality rotations rather than merely being invariant up to a conformal factor as is the open string metric. In a two recent papers[10] an analog for the fivebrane of the open string metric was proposed. Specifically, it was suggested that the analogous metric should be given by

$$\phi(H_{lpq}H^{lpq})(g_{mn}+4H_{mpq}H_n^{pq}), \tag{29}$$

where the function ϕ should behave like $(H_{lpq}H^{lpq})^{-2/3}$ for large $H_{lpq}H^{lpq}$ in order that, upon reduction, it agrees with the open string metric of string theory in the relevant limit.

The two proposals are both conformally related to the metric in the fivebrane equations. We will see that with our choice of conformal factor we obtain the Boillat metric of the D4-brane upon reduction. Our choice has the additional advantage that in terms of it the equations of motion can be rewritten in a natural way.

We now turn to the characteristics associated with the Dirac equation (4). While the gamma matrices Γ^m give a Dirac square root of the restriction of the bulk Einstein co-metric to the brane,

$$\Gamma^m\Gamma^n+\Gamma^n\Gamma^m=2g^{mn}, \tag{30}$$

the spinor equation of motion contains the 5-brane Gamma matrices $\tilde{\Gamma}^m=n^m{}_n\Gamma^n$, where $n^m{}_n=Q^{-1/2}m^m{}_n$ which give a Dirac square root of the 5-brane co-metric C^{mn},

$$\tilde{\Gamma}^m\tilde{\Gamma}^n+\tilde{\Gamma}^n\tilde{\Gamma}^m=2C^{mn}. \tag{31}$$

One may view the $n^m{}_n$ as a sort of sechbein for the 5-brane metric C_{mn} since

$$C^{mn}=n^m{}_p n^n{}_q g^{pq}. \tag{32}$$

Note that $n_{nm}=g_{ml}n^l{}_m$ is symmetric.

Writing out the Dirac equation in terms of the gamma matrices $\tilde{\Gamma}^m$ reveals that the spinor characteristics are also given by C^{mn}.

In the absence of a background H_{lmn} field, C^{mn} and g^{mn} coincide. Note that there is a *single* G^{mn} and thus a single characteristic cone. That is just as in Born–Infeld theory; there is no bi-refringence: all polarization states travel with the same speed. Since any nonlinear electrodynamic theory, including ones exhibiting bi-refringence can be made $N=1$ supersymmetric, its absence cannot be attributed to just one supersymmetry. However one might imagine that this property is a consequence of maximal superymmetry. In the case of Born–Infeld theory, the absence of bi-refringence, and the exceptional property that the system exhibits no shocks, characterizes the theory uniquely (see Ref. 4 for references). It is an attractive conjecture that the same uniqueness property holds for the M-5-brane equations of motion.

We now establish that the 5-brane co-cone $C_G^\star\in T^\star M$ lies outside or on the Einstein co-cone $T^\star M\supset C_G^\star\supseteq C_g^\star$. The notation here is as follows. $C_g^\star$ consists of timelike co-vectors $p_m\in T^\star M$ such that $g^{mn}p_m p_n\leqslant 0$ and its boundary consists of the lightlike co-vectors l_m for which $g^{mn}l_m l_n=0$. Since passing to the dual space TM reverses inclusions we have that the 5-brane cone lies inside or on the Einstein cone, $TM\supset C_g\supseteq C_G$. In plain language this means that 5-brane

excitations travel with speeds no greater than that of light. Note that the cone $C_G^\star$ depends only on the conformal equivalence class of co-metrics of which G^{mn} is one representative and C^{mn} another.

To establish our basic causality result we consider a co-vector l_a lying on the boundary of $C_g^\star$, i.e., for which

$$g^{mn}l_m l_n = 0. \tag{33}$$

Using (12) we find that

$$C^{mn}l_m l_n = -4Q s_{mn}s^{mn}, \tag{34}$$

where $s_{mn} = -s_{nmb} = h_{mnl}l^l$. Thus

$$s_{mn}l^m = 0. \tag{35}$$

By choice of frame $l^m = (1,0,0,0,0,1)$ and thus $s_{05} = 0$ and $s_{0i} + s_{5i} = 0$, where $i = 1,2,3,4$ are spatial indices. One thus has

$$s_{ab}s^{ab} = s_{ij}s^{ij} \geqslant 0. \tag{36}$$

Thus

$$C^{mn}l_m l_n \leqslant 0. \tag{37}$$

It follows that the boundary of $C_g^\star$ lies inside or on $C_G^\star$ and we are done.

III. PRINCIPAL NULL DIRECTIONS

In the case of Born–Infeld theory in four spacetime dimensions, generically the Boillat and Einstein cones touch along two principal null directions of the electromagnetic two-form $F_{\mu\nu}$.[4] In fact this result holds in all dimensions. The common null direction $l^m = (1,n_i)$ with $n_i n_i = 1$ must satisfy

$$l^n F_{na}F_{mb}g^{ab}l^m = 0. \tag{38}$$

For a generic two-form one may find a frame in which the only nonvanishing components are $F_{01} = -F_{10}, F_{23} = -F_{32}, F_{45} = -F_{54}\cdots$. The touching condition becomes

$$F_{01}^2(1-n_1^2) + F_{23}^2(n_2^2+n_3^2) + F_{45}^2(n_4^2+n_5^2)\cdots = 0. \tag{39}$$

There are only two solutions; $l^m = (1,\pm 1,0,\ldots,0)$.

One may ask what is the analog of this result for the fivebrane with its self-dual three-form h_{lmn} in six spacetime dimensions? In order to answer this question we need to put k_{ab} rather than F_{ab} in standard form by diagonalizing with respect to to g_{ab}. Using (10) and (11) one easily sees that generically k_{ab} takes the form, up to permutations of the spatial axes,

$$k_{ab} = \sqrt{\frac{k^2}{6}}\,\mathrm{diag}(1,1,1,1,-1,-1). \tag{40}$$

The common null directions must be common solutions of

$$-1 + n_1^2 + n_2^2 + n_3^2 + n_4^2 + n_5^2 = 0, \tag{41}$$

and

$$1 + n_1^2 + n_2^2 + n_3^2 - n_4^2 - n_5^2 = 0. \tag{42}$$

There is in general a circle of such directions,

$$l^m=(1,0,0,0,\cos\alpha,\sin\alpha), \tag{43}$$

along which the Einstein and Boillat cones coincide. In all other directions the Boillat cone lies inside the Einstein cone.

IV. THE ENERGY MOMENTUM TENSOR AND HOOKE'S LAW

Following the discussion of the energy momentum tensor in Ref. 11, we shall in this paper define the energy momentum tensor as

$$T^{mn}=g^{mn}-\frac{G^{mn}}{Q}. \tag{44}$$

The main difference from the energy momentum tensor defined in Ref. 11, also used in Ref. 8, is that we have added the metric tensor g_{mn} to the tensor defined there so as to make the energy momentum tensor vanish for zero three-form field $h_{abc}=0$. In fact it is (44) which enters directly into the superysymmetry algebra and hence the Bogomol'nyi bound of the theory.[12] The energy momentum tensor so defined has some important positivity properties which we will explore shortly.

In terms of C^{mn} we have the strikingly simple formula

$$T^{mn}=g^{mn}-C^{mn}. \tag{45}$$

This formula has an interesting interpretation which appears to be closely related to Hooke's law in the classical theory of nonlinear elasticity theory. This is formulated in terms of diffeomorphisms ϕ from the manifold Σ of the elastic body into flat three-dimensional Euclidean space $\mathbb{E}^3$ with metric δ. The relaxed or unstretched state of least energy corresponds to a diffeomorphism ϕ_0. One defines the strain tensor tensor σ_{ij} of a general stretched state corresponding to a diffeomorphism ϕ by

$$\sigma_{ij}=\delta_{\star ij}-\delta_{0ij}, \tag{46}$$

where $\delta_\star$ is the pull-back of the flat Euclidean metric δ under the diffeomorphism ϕ and δ_{0ij} is the pull-back of the flat metric under ϕ_0. For an isotropic medium Hooke's law states that the strain σ_{ij} is proportional to the applied stress T_{ij}. Our formula (1) is similar but not identical because the tensors are contra-variant not co-variant. Thus our case for the analog of $\delta_{\star ij}$ is the pull-back of the bulk closed string co-metric to the M-5-brane world volume. The analog of the unstretched metric δ_{0ij} is the 5-brane co-metric C^{mn}. We believe that it would be worthwhile exploring this analogy further.

Another formula which is similar to one occurring in the Born–Infeld case[4] is the remarkable identity

$$\det C^{mn}=\det g^{mn}. \tag{47}$$

To check conformal invariance we compute the trace of the energy momentum tensor. It is given by

$$T^m_m=-\frac{8k^2}{(1-\frac{2}{3}k^2)}. \tag{48}$$

Thus, the theory is Weyl-invariant in the weak field limit in which the equations of motion become linear. However it is not Weyl-invariant for finite values of the fields. We see shall see later that Weyl invariance is restored in the strong coupling limit.

Later we shall make use of some other identities involving the energy momentum tensor which we derive here. Because the energy momentum tensor is conserved with respect to the Levi-Civita connection,

$$\nabla_m T^{mn}=0, \tag{49}$$

we have, from Hooke's Law, the following identities:

$$\nabla_n C^{mn}=0. \tag{50}$$

These will be used in the next section to establish the M-5-brane Equivalence Principal. Some additional useful identities may be obtained as follows. One defines

$$n^{mn}=Q^{-1/2}m^{mn}=Q^{-1/2}(g^{mn}-2k^{mn}). \tag{51}$$

Thus

$$n^{-1}_{mn}=Q^{-1/2}(g_{mn}+2k_{mn}). \tag{52}$$

We thus have

$$C^{mn}=n^{ma}g_{ab}n^{bn}, \tag{53}$$

and of course,

$$\tilde{\Gamma}^n=n^{na}g_{ab}\Gamma^b. \tag{54}$$

Now one easily finds

$$g_{mn}C^{mn}=\frac{1+\frac{2}{3}k^2}{1-\frac{2}{3}k^2}=g^{mn}C_{mn}. \tag{55}$$

In Ref. 11 an energy momentum tensor was introduced that treated the scalars and three-form in a more symmetric fashion. This tensor is given by

$$S^{mn}=T^{mn}-g^{mn} \tag{56}$$

and is covariantly conserved. Reference 11 also found a tensor density,

$$\mathfrak{G}^{mn}=\sqrt{-g}(T^{mn}-g^{mn}), \tag{57}$$

that was conserved in the sense

$$\partial_m \mathfrak{G}^{mn}=0. \tag{58}$$

In the case that the three-form vanishes, we have $T^{mn}=0$, but $S^{mn}\neq 0$, and so the quantity $\sqrt{-g}g^{mn}$ is a measure of the energy–momentum of the scalars. In fact it is the canonical stress tensor with respect to the flat metric δ_{mn}. It may be obtained from the Lagrangian for the scalars written down in ''static,'' or more accurately ''Monge,'' gauge.

V. THE M5-BRANE EQUIVALENCE PRINCIPLE

It is striking fact that the co-metric C^{mn} rather than the Einstein co-metric g^{mn} enters in the equations of motion of all the 5-brane fields in such a way that it is impossible to determine the Einstein metric by means of observations using 5-brane fields alone. In this respect the situation

resembles attempts to reinterpret General Relativity as a flat space theory by introducing a flat metric $\eta_{\mu\nu}$ into spacetime. The problem is that by the Equivalence Principal no physical measurement can detect the flat metric.

Our aim in this section is to explore further this enhanced version of the Equivalence Principle for the fivebrane. Our claim is that there exists a preferred set of variables to describe the theory that are related in a direct way to the physical observables. In particular, in Sec. II we showed that the characteristics of the fivebrane were given by the metric C_{mn}. This means that the metric can be determined up to a conformal factor by observing the motion of small fluctuations. Another physically relevant variable is the gauge invariant field strength H_{lmn}. This satisfies the Bianchi identity and hence can be written in terms of a two-form potential that couples directly to a twobrane probe. Hence using a twobrane probes allows one to measure the H_{lmn} field.

To illustrate this point we now show how to write the fivebrane equations of motion entirely in terms of the variables C_{mn} and H_{lmn} and X^N. In particular, we will find that the equations of motion for the scalar and the three-form can be written using the Levi-Civita covariant derivative with respect to the metric C_{mn}. The situation is analogous to how the usual Equivalence Principal works in General Relativity. Because all physical equations are writen in terms of the metric C_{mn} the metric g_{mn} is not directly observable.

We begin with the scalar equation of motion. Because G^{mn} is proportional to C^{mn}, this equation can be written as

$$C^{mn}\nabla_m\nabla_n X^N = 0. \tag{59}$$

Following Ref. 11 and using (50) we may re-write this as

$$\nabla_m(C^{mn}\,\partial_n X^N) = \frac{1}{\sqrt{-g}}\partial_m(\sqrt{-g}C^{mn}\,\partial_n X^N) = 0. \tag{60}$$

Now using (47) we have

$$\frac{1}{\sqrt{-C}}\partial_m(\sqrt{-C}C^{mn}\,\partial_n X^N) = \Delta_m(C^{mn}\,\Delta_n X^N) = 0, \tag{61}$$

where Δ_m is the Levi-Civita covariant derivative with respect to the 5-brane metric C_{mn} which is defined by

$$\Delta_m C^{ab} = 0. \tag{62}$$

We see that (61) is just the covariant wave equation with respect to the 5-brane metric C_{mn}.

The closure condition for the three-form H_{lmn},

$$\partial_{[p}H_{qrst]} = 0, \tag{63}$$

clearly requires no metric. The equation of motion of the three-form may be written as

$$C^{mn}\nabla_m(H_{nab}) = 0. \tag{64}$$

Using (50) and the fact that $\nabla_m g^{ab} = 0$, we re-write (64) as

$$\nabla_m(P^{mab}) = 0, \tag{65}$$

where

$$P^{mab} = C^{mn}g^{ac}g^{bd}H_{ncd}. \tag{66}$$

Now the contravariant tensor P^{mab} is totally antisymmetric and satisfies [Ref. 11, Eq. (17)]

$$P^{lmn} = \star_g H^{lmn}, \tag{67}$$

and therefore we may rewrite (64) as

$$\frac{1}{\sqrt{-g}} \partial_m (\sqrt{-g} P^{mab}) = 0. \tag{68}$$

Now using (47) we get

$$\frac{1}{\sqrt{-C}} \partial_m (\sqrt{-C} P^{mab}) = 0. \tag{69}$$

This may now be put in the fivebrane metric covariant form,

$$\Delta_m (\star_C H^{mnp}) = 0. \tag{70}$$

The Hodge operations $\star_g$ and $\star_C$ are taken with respect to the Einstein and 5-brane metric, respectively. However they are related because if η_C^{mabncd} is the contravariant alternating tensor which is covariantly constant with respect to the Levi-Civita connection of the 5-brane metric C_{mn}, we have

$$\sqrt{-C}\, \eta_C^{mabncd} = \sqrt{-g}\, \eta_g^{mabncd}, \tag{71}$$

where η_g^{mabncd} is the contravariant alternating tensor which is covariantly constant with respect to the Levi-Civita connection of the Einstein metric g_{mn}.

Finally we consider the Dirac equation. Following Ref. 11, Eq. (13), this may be written as

$$\nabla_m (\Psi' (1 - \Gamma) \tilde{\Gamma}^m) = 0, \tag{72}$$

where

$$\Psi' = Q^{-1/2} \Theta. \tag{73}$$

Now we must rewrite the projector Γ in terms of the 5-brane gamma-matrices $\tilde{\Gamma}^m$. We have the formula

$$\Gamma = -\tfrac{1}{6} \eta_{C_{lmnrst}} \tilde{\Gamma}^l \tilde{\Gamma}^m \tilde{\Gamma}^n \tilde{\Gamma}^r \tilde{\Gamma}^s \tilde{\Gamma}^t + \tfrac{1}{2} H_{lmn} \tilde{\Gamma}^l \tilde{\Gamma}^m \tilde{\Gamma}^n. \tag{74}$$

The covariant derivative ∇_m is the spinor derivative with respect to the Einstein metric. We expect that one may be able to rewrite this in terms of the spinor covariant derivative Δ_m. This is likely to require a more elaborate redefinition of the spinor than in (73), along the lines of that discussed in Ref. 12.

VI. DIMENSIONAL REDUCTION AND THE RELATION TO THE OPEN STRING METRIC

It is known[7,6] that under double dimensional reduction to five-dimensions the equations of motion of the fivebrane reduce to those of Dirac–Born–Infeld theory. We shall now investigate the relation between the fivebrane metric and the Boillat metric of the D4-brane in this case. We assume that the fields h_{lmn} are independent of the fifth spatial dimension and that

$$H_{mn5} = F_{mn}. \tag{75}$$

Using the results of Ref. 6, Eq. (136)[6] we have (after rescaling F to be consistent with the standard normalization) we find the reduction of fivebrane metric to be given by

$$C^{mn}=Z(1-F^2)^{-1}, \tag{76}$$

where

$$Z=\sqrt{1+2x-y^2}=\sqrt{-\det(g_{mn}-F_{mn})}. \tag{77}$$

The Boillat co-metric is given by

$$C^{mn}_{\text{Boillat}}=Z((1-F^2)^{-1})^{mn}. \tag{78}$$

In other words the two metric coincide.

We now extend the work of Ref. 4 to give an enhanced Equivalence Principle similar to that discussed for the fivebrane earlier. The Born–Infeld equations may be written as

$$\partial_{[l}F_{mn]}=0, \tag{79}$$

and

$$\nabla_m P^{mn}=\frac{1}{\sqrt{-g}}\partial_m(\sqrt{-g}P^{mn})=0. \tag{80}$$

Clearly (79) requires no metric and (80) may be re-written [using (47)] in terms of the Boillat metric as

$$\Delta_m P^{mn}=\frac{1}{\sqrt{-C}}\partial_m(\sqrt{-C}P^{mn})=0. \tag{81}$$

One may check, just as for the 5-brane, that the scalar equations of motion may be written as

$$\Delta_m \Delta^m X^N=0. \tag{82}$$

VII. DOMINANT ENERGY CONDITION

Almost all physically well behaved classical energy momentum tensors satisfy the Dominant Energy Condition. This states that for every pair of future directed casual vectors $p^m, q^m \in C_g^+$ one has

$$T_{mn}p^m q^n \geqslant 0. \tag{83}$$

Note that, if the Dominant Energy Condition holds with respect to the Einstein metric, it necessarily holds with respect to the fivebrane metric, since the lightcone of the former includes that of the latter.

The importance of the Dominant Energy Condition is that it guarantees the classical fields whose energy momentum tensors satisfy the condition propagate causally. It is also an essential ingredient in the Positive Energy Theorems of General Relativity. A theorem of Hawking implies that if the Dominant Energy Condition holds then matter cannot escape from, or enter, a bounded spatial region at a speed faster than light.[13] In particular it guarantees some sort of stability since matter obeying the condition cannot just simply disappear.[13]

Let us evaluate the left hand side of (83) for the fivebrane. Using Eqs. (12), (1) we find that

$$Q^{-1}\left(2k_{mn}p^m q^n+\frac{2}{3}k^2 p\cdot q\right), \tag{84}$$

where

$$p \cdot q = -g_{mn} p^m q^n \geqslant 0. \tag{85}$$

We will now show that the left hand side of the above equation is indeed positive since the quantities k^2 and $k_{mn}p^m q^n$ and are non-negative.

To see that k^2 is positive we introduce an electric two-form in five dimensions by

$$e_{ij} = h_{oij}\,. \tag{86}$$

Self-duality of h_{lmn} implies that

$$e_{ij} = b_{ij} = -\tfrac{1}{6}\epsilon_{ijkrs} h^{krs}. \tag{87}$$

A calculation reveals that

$$k_{ij} = \delta_{ij} e^{pq} e_{pq} - 4 e_{ir} e_j{}^r. \tag{88}$$

From (10) we deduce that

$$k_{00} = e_{rs} e^{rs}, \tag{89}$$

and using (11) we obtain

$$\tfrac{2}{3} k^2 = 16 e_{ij} e^{jk} e_{ks} e^{si} - 4 (e_{ij} e^{ij})^2. \tag{90}$$

Now using $SO(5)$ transformations we can skew-diagonalize the two-form e_{ij}, that is choose a basis in which the only nonvanishing components are $e_{12} = -e_{21} = e_1$ and $e_{34} = -e_{43} = e_2$. In this basis, one finds that

$$k^2 = 24 (e_1^2 - e_2^2)^2. \tag{91}$$

The quantity $k_{mn}p^m q^n$ may be dealt with in a similar way. If p^n is timelike we can choose a six-dimensional Lorentz frame in which $p^m = (p^0,0,0,0,0,0)$. This choice allows us to use the $SO(5)$ freedom to skew diagonalize e_{ij} as above. A short calculation then gives

$$k_{mn} p^p q^n = 2 p^0 q^0 \left(e_1^2 + e_2^2 - 2 \frac{q^5}{q^0} e_1 e_2 \right). \tag{92}$$

Since q^n is causal, $|q^5/q^0| \leqslant 1$ and $e_1^2 + e_2^2 \geqslant 2 e_1 e_2$, we find the desired result, namely $k_{mn} p^m q^n \geqslant 0$.

Interestingly, k^2 vanishes if and only if e_{ij} determines a self- or anti self-dual two-form in the four space orthogonal to its kernel. We also see that $T_{mn} p^m p^n$ is strictly positive for timelike p^n and hence taking the choice $p^n = (p^0,0,0,0,0,0)$ we conclude that T_{00} is strictly positive.

VIII. EXACT PLANE WAVE SOLUTIONS

In this section we shall establish that plane wave solutions of the linearized theory are in fact *exact* solutions of the full nonlinear equations of motion, a property which also holds in Born–Infeld theory (compare Ref. 4) and classical general relativity. We shall suppose that the metric g_{mn} is flat, $g_{mn} = \eta_{mn}$, although one might consider more general cases. We make the ansatz

$$H_{lmn} = H^0{}_{lmn} f(l_n x^n), \tag{93}$$

where H^0_{lmn} is a constant three-form, $f(u)$ is an arbitrary function of its argument and the constant vector l^n is null,

$$\eta_{mn} l^m l^n = 0. \tag{94}$$

The closure condition becomes

$$l_{[l}H^0_{mno]}=0. \tag{95}$$

Thus

$$\epsilon^{pqrstu}l_r H^0_{stu}=0. \tag{96}$$

If we assume that $l_m=(1,1,0,0,0,0)$ and let Greek indices run from 2 to 5, we find that

$$H^0_{\alpha\beta\gamma}=0, \quad H^0_{0\gamma\delta}=H^0_{1\gamma\delta}. \tag{97}$$

This may be written covariantly as

$$H^0_{mnp}=l_{[m}A^0_{np]}, \tag{98}$$

where A^0_{np} is a constant polarization two-form. It is determined only up to

$$A^0_{np}\rightarrow A^0_{np}+l_{[n}A^0_{p]}, \tag{99}$$

where A^0_p is a constant one-form.

We now make the further assumption that

$$l^m H_{mnp}=0. \tag{100}$$

The reason we have to assume (100) is that quantities $H^0_{01\alpha}$ are not constrained by Eq. (96). In order to eliminate this freedom we are in effect assuming that

$$H^0_{01\alpha}=0. \tag{101}$$

Having made this ansatz, i.e., assuming (98), (100), it follows that

$$H_{lmn}H^{lmn}=0. \tag{102}$$

Thus $Q=1$ and hence $C^{mn}=G^{mn}$.

It remains to solve the self-duality condition. Now using (24) we see that the fivebrane metric is of the so-called Kerr–Schild form:

$$G^{mn}=\eta^{mn}-\text{constant}\, f^2 l^m l^n. \tag{103}$$

The constant is positive. To evaluate it we could introduce a (nonunique) null vector n^m, normalized so that

$$\eta_{mn}n^m l^n=-1. \tag{104}$$

One then has

$$\text{constant}=(H^{0^2})_{mn}n^m n^n. \tag{105}$$

Because l^m is null [i.e., from (94)] it follows that

$$G_m{}^q H_{npq}=H_{npm}. \tag{106}$$

Thus the self-duality condition (26) becomes

$$\star H_{lmn}=H_{lmn}, \tag{107}$$

which is the same as the condition for the linear theory.

Using Hooke's Law (1) we deduce that the energy momentum tensor is given by

$$T^{mn} = \text{constant}\, f^2 l^m l^n. \tag{108}$$

Equation (108) is the energy momentum tensor of a fluid of energy density constant moving at the speed of light in the direction l^m. This is often referred to as a null fluid. We shall encounter null fluids again later when we examine the energy momentum tensor in the strong coupling limit.

IX. THE $SO(5)$ COVARIANT FORMALISM AND THE LIMITING FIELD STRENGTH

Born–Infeld theory has a built in upper-bound for the electric field strength. The string theoretic interpretation is that when electric fields approach the limiting field strength, copious pair production of open string states occurs.[14,15] One may ask whether a similar phenomenon takes place in M-Theory.[10]

In Born–Infeld theory one must take care to express the upper-bound in terms of the correct variables. The Lagrangian density is

$$L = 1 - \sqrt{1 - \mathbf{E}^2 + \mathbf{B}^2 - (\mathbf{E}\cdot\mathbf{B})^2}, \tag{109}$$

which shows that the electric field **E** cannot be too big for fixed **B** since then the Lagrangian density becomes complex. However the Hamiltonian density[16] is

$$\mathcal{H} = \sqrt{1 + \mathbf{B}^2 + \mathbf{D}^2 + (\mathbf{B}\times\mathbf{D})^2} - 1. \tag{110}$$

This shows that there is no limit on either the magnetic induction **B** or electric inductions **D**. However the dual Lagrangian[16] is

$$\hat{L} = \sqrt{1 - \mathbf{H}^2 + \mathbf{D}^2 - (\mathbf{D}\cdot\mathbf{H})^2} - 1, \tag{111}$$

which indicates that there is an upper-bound on the magnetic intensity **H**, as there has to be, by electric–magnetic duality invariance. This point is re-enforced by considering the dual Hamiltonian,[16]

$$\hat{H} = 1 - \sqrt{1 - \mathbf{H}^2 - \mathbf{E}^2 + (\mathbf{H}\times\mathbf{E})^2}. \tag{112}$$

In the case of the M5-brane we have a similar range of possible choices of field variables. The fivebrane has a self-duality condition which means that if we define

$$B_{ij} = -\frac{1}{6}\epsilon_{ijklm}H^{klm}, \quad E_{ij} = H_{0ij}, \tag{113}$$

where $i,j,k,.. = 1,2,\ldots,5$, then we can express E_{ij} in terms of B_{ij} and *vice versa*. Thus the energy density $T_{00} = \mathcal{H}$ can be expressed in terms of either variable. To achieve this we will have in effect to solve the self-duality constraint. The self-duality condition on H_{mnp} can be expressed as

$$H^{+}_{mnp} = Q^{-1}h_{mnp}, \quad H^{-}_{mnp} = 2Q^{-1}k_m{}^r h_{rnp}, \tag{114}$$

where $H^{\pm}_{mnp} = \frac{1}{2}(H_{mnp} \pm (1/3!)\,\epsilon_{mnprst}H^{rst})$. In the special frame used above one then finds that

$$B_1 = \frac{e_1}{1 - 4(e_1^2 - e_2^2)}, \quad B_2 = \frac{e_2}{1 + 4(e_1^2 - e_2^2)}, \tag{115}$$

$$E_1 = \frac{e_1}{1 + 4(e_1^2 - e_2^2)}, \quad E_2 = \frac{e_2}{1 - 4(e_1^2 - e_2^2)}. \tag{116}$$

Inverting these equations leads to

$$8e_1=\frac{B_1}{B_2^2-B_1^2}\sqrt{1+16B_2^2}[\sqrt{1+16B_2^2}-\sqrt{1+16B_1^2}], \tag{117}$$

and

$$8e_2=\frac{B_2}{B_1^2-B_2^2}\sqrt{1+16B_1^2}[\sqrt{1+16B_1^2}-\sqrt{1+16B_2^2}]. \tag{118}$$

Note that

$$E_1E_2=B_1B_2. \tag{119}$$

The required solutions of the self-duality constraint are therefore

$$E_1=B_1\sqrt{\frac{1+16B_2^2}{1+16B_1^2}},\quad E_2=B_2\sqrt{\frac{1+16B_1^2}{1+16B_2^2}}, \tag{120}$$

or inversely,

$$B_1=E_1\sqrt{\frac{1-16E_2^2}{1-16E_1^2}},\quad B_2=E_2\sqrt{\frac{1-16E_1^2}{1-16E_2^2}}. \tag{121}$$

Expressing the energy momentum tensor in terms of h_{mnp} and using the relations of section four we find that

$$T_{00}=\frac{1+16(e_1^2-e_2^2)+8(e_1^2+e_2^2)}{1-16(e_2^2-e_1^2)^2}-1. \tag{122}$$

Using the above equations we conclude that

$$T_{00}=\sqrt{(1+16B_1^2)(1+16B_2^2)}-1. \tag{123}$$

The expression for the energy density (123) may be cast in the $SO(5)$ covariant form,

$$\mathcal{H}=\sqrt{\det(\delta_{ij}+4B_{ij})}-1=(\det(\delta_{ij}+16B_{ik}B_{jk}))^{1/4}-1. \tag{124}$$

A Hamiltonian density was derived from the action formulation of the five-brane in Ref. 17 Our $\mathcal{H}$ coincides with that Hamiltonian density.

From (116) and (123) we have

$$E_1=\frac{1}{16}\frac{\partial\mathcal{H}}{\partial B_1},\quad E_2=\frac{1}{16}\frac{\partial\mathcal{H}}{\partial B_2}, \tag{125}$$

which may be cast in the manifestly $SO(5)$-covariant form:

$$E_{ij}=\frac{1}{16}\frac{\partial\mathcal{H}}{\partial B_{ij}}=\frac{(1-8\ \mathrm{Tr}\,B^2)B_{ij}+16B_{ij}^3}{\sqrt{1-8\ \mathrm{Tr}\,B^2+(16)^2W_i^2}}, \tag{126}$$

where

$$W_i=\tfrac{1}{8}\epsilon_{ijrst}B^{jr}B^{st}. \tag{127}$$

Now the Legendre transform of the Hamiltonian density is

$$\hat{\mathcal{H}}=1-\sqrt{(1-16E_1^2)(1-16E_1^2)}=1-\sqrt{\det(\delta_{ij}+4\sqrt{-1}E_{ij})}, \tag{128}$$

so that

$$\hat{\mathcal{H}}+\mathcal{H}=\tfrac{1}{2}E_{ij}B^{ij} \tag{129}$$

and

$$B_{ij}=\frac{1}{16}\frac{\partial\hat{\mathcal{H}}}{\partial E_{ij}}=\frac{(1+8\ \mathrm{Tr}\,E^2)E_{ij}+16E_{ij}^3}{\sqrt{1+8\ \mathrm{Tr}\,E^2+(16)^2U_i^2}}, \tag{130}$$

where

$$U_i=\tfrac{1}{8}\epsilon_{ijrst}E^{jr}E^{st}. \tag{131}$$

In our special frame this equation reduces to (121). For a helpful review of the various formulations of the 5-brane equations of motion which covers some of this material the reader is referred to Ref. 18.

The Hamiltonian density $\mathcal{H}$ is a well defined convex function for all finite values of the magnetic induction B_{ij}. The Legendre transform maps all of B_{ij} space in a one–one fashion onto the open region of E_{ij} space for which the dual Hamiltonian density $\hat{\mathcal{H}}$ is a well defined convex function. That is for which the matrix $\delta_{jk}-16E_{ji}E_{ki}$, which occurs in the dual Hamiltonian, is positive definite. In our special frame, the allowed region is just $4|E_1|<1$ and $4E_2<1$.

The Bianchi identities read as

$$\partial_i B_{ij}=0, \quad \frac{\partial B_{ij}}{\partial t}+\frac{1}{2}\epsilon_{ijkrs}\partial_k E_{rs}=0. \tag{132}$$

Taking the solution (126) for the self-duality condition implies the equations of motion.

X. STRONG COUPLING LIMIT

We are now going to discuss the strong coupling limit of the theory. This is equivalent to taking the tension of the fivebrane to zero and may be thought of as a high energy limit. We shall find that the situation is similar to that of the strong coupling limit of Born–Infeld theory in four spacetime dimensions which has been thoroughly investigated by Białynicki-Birula and called by him UBI theory.[16,19] In that case, the Lagrangian vanishes, but there is a well defined Hamiltonian. Moreover the theory is Lorentz invariant and has the energy momentum tensor of a null fluid. As a consequence there are infinitely many conserved currents in flat spacetime. Because the invariants $F_{\mu\nu}F^{\mu\nu}$ and $F_{\mu\nu}\star F_{\mu\nu}$ both vanish on shell one might speculate that the theory is quantum mechanically finite. As we shall see, there is just as much evidence to warrant a similar speculation about the M-Theory version.

The limit we are considering differs from that discussed in Refs. 10, 20

To proceed we introduce into the Hamiltonian a parameter T with the dimensions of mass cubed. We then take the limit $T\downarrow 0$. The Hamiltonian density is

$$\mathcal{H}=T^2\sqrt{\det\left(1+\frac{4B_{ij}}{T}\right)}-T^2. \tag{133}$$

Letting $T\downarrow 0$, we get the well defined limit

$$\mathcal{H}=16|B_1B_2|. \tag{134}$$

We now evaluate the energy momentum tensor in the strong coupling limit in terms of the variable B_{ij}. In this process we will find quantities that are nonvanishing only when one takes a next to leading contribution in T. One finds that in the limit of small T,

$$e_1\rightarrow \frac{2}{T}\frac{B_1B_2}{B_1+B_2}-\frac{T}{16}\frac{1}{B_1}\frac{B_1-B_2}{B_1+B_2}, \tag{135}$$

$$e_2\rightarrow \frac{2}{T}\frac{B_1B_2}{B_1+B_2}+\frac{T}{16}\frac{1}{B_1}\frac{B_1-B_2}{B_1+B_2}. \tag{136}$$

It follows that

$$e_1^2-e_2^2\rightarrow \frac{1}{4}\frac{B_1-B_2}{B_1+B_2}. \tag{137}$$

Reinstating the coupling constant T, the energy momentum tensor is given by

$$T_{mn}=-T^2\frac{m_{mn}^2}{Q}+T^2g_{mn}. \tag{138}$$

In the small T limit the only nonvanishing components are

$$T_{00}=16|B_1B_2|, \tag{139}$$

$$T_{55}=16|B_1B_2|, \tag{140}$$

$$T_{05}=-16B_1B_2. \tag{141}$$

Thus

$$T_{mm}=\mathcal{H}l_ml_n, \tag{142}$$

with

$$l^m=(1,0,0,0,0,1), \tag{143}$$

and

$$l^ml^ng_{mn}=0. \tag{144}$$

We have been working in a local frame. However, Eqs. (142) and (144) are manifestly covariant and hence hold in a general frame. In particular we have in general, that the null vector l^m is given by

$$l^m=(1,n^i), \tag{145}$$

where n^i is a unit vector in the direction of the Poynting vector T^{0i} and therefore

$$T^{om}=\mathcal{H}l^m. \tag{146}$$

From (142) we see that the trace of the energy momentum tensor vanishes,

$$T_m^m=0. \tag{147}$$

Thus we have shown that the theory is Weyl-invariant in the strong coupling limit. The energy momentum tensor (142) is the same form as the energy momentum tensor of the strong coupling limit of Born–Infeld theory, UBI theory.

Because the energy momentum tensor has the form of a null fluid (see Refs. 16, 19) one may easily check that one has infinitely many conservation laws. The conservation of energy equation $\partial_t T^{00}+\partial_i T^{0i}=0$ may be written covariantly as

$$\nabla_m(\mathcal{H}l^m)=0. \tag{148}$$

The remaining conservation law implies that

$$l^n\nabla_n l^l=0. \tag{149}$$

From (149) it follows that the integral curves tangent to l^m, that is the solutions of

$$\frac{dx^m}{d\lambda}=l^m, \tag{150}$$

are null geodesics with affine parameter λ. In fluid dynamic language (148) corresponds to the conservation of entropy, sometimes thought of as the ''photon'' number. The integral curves are thought of as the world lines of the fluid. In the case of UBI theory[16,19] it turns out[21] (cf. Ref. 22) that the fluid may be thought of as a gas of massless Schild strings.[23] In fluid dynamic language the world-sheets of the strings are the histories of magnetic field lines which are swept out with velocity l^m. We shall turn later to the possible fluid interpretation in the M5-brane case.

It follows from (148) and (149) that the tensors,

$$T^{m_1m_2\cdots m_k}=\mathcal{H}l^{m_1}l^{m_2}\cdots l^{m_k}, \tag{151}$$

satisfy

$$\nabla_m T^{mm_2\cdots m_k}=0, \tag{152}$$

for any positive integer k.

In flat spacetime the divergence identities (152) may be integrated over space to give rise to infinitely many conservation laws.

In order to cast the limiting equations of motion in a manifestly $SO(5)$ covariant form, we recall from (126) and (132) that

$$\frac{\partial B^{ij}}{\partial t}+\frac{1}{2}\epsilon^{ijrst}\partial_r\left\{\frac{(B-8(\mathrm{Tr}\,B^2)B+16B^3)_{st}}{\sqrt{1-8\,\mathrm{Tr}\,B^2+16^2W_i^2}}\right\}=0. \tag{153}$$

One may now re-instate T and then take the limit $T\downarrow 0$ in (153) to obtain

$$\frac{\partial B^{ij}}{\partial t}+\frac{1}{2}\epsilon^{ijrst}\partial_r\left\{\frac{(-\frac{1}{2}(\mathrm{Tr}\,B^2)B+B^3)_{st}}{\sqrt{W_i^2}}\right\}=0. \tag{154}$$

Using the identity

$$(-\mathrm{Tr}\,B^2B+2B^3)^{ij}=\epsilon^{ijklm}W_kB_{lm}, \tag{155}$$

we may show that in the limit, the electric field becomes

$$E^{ij}=\frac{1}{2}\epsilon^{ijrst}\frac{W_r}{\sqrt{W_k^2}}B_{st}, \tag{156}$$

and the field equation becomes

$$\frac{\partial B_{ij}}{\partial t}+\frac{1}{4}\epsilon_{ij}{}^{klm}\partial_k\epsilon_{lmrst}\frac{W^rB^{st}}{\sqrt{W_p^2}}. \tag{157}$$

This is very similar in form to the Born–Infeld case.[16,19] One may also give an $SO(5,1)$ covariant formulation of the 5-brane in the $T\downarrow 0$ limit. It is sufficient to derive the self-duality conditions in this limit as they, together with the Bianchi Identity, imply the field equations.

By multiplying through by m^{-1}, the self-duality condition $*H_{abc}=Q^{-1}(m^2)_a{}^eH_{ebc}$ can be reexpressed as

$$(m^{-1})_a{}^e*H_{ebc}=Q^{-1}(m)_a{}^eH_{ebc} \tag{158}$$

or

$$(1+2k)_a{}^e*H_{ebc}=Q^{-1}(1-2k)_a{}^eH_{ebc}\,. \tag{159}$$

Taking the limit and using the equation for k in terms of H^2 we find that the self-duality condition can be expressed covariantly as

$$(H^2)_a{}^e*H_{ebc}=\left(\tfrac{1}{3}H^2\delta_a^e-(H^2)_a{}^e\right)H_{ebc}\,. \tag{160}$$

In view of the interpretation of the strong coupling limits of Born–Infeld theory as string fluids,[22] it is of interest to consider the detailed structure of the three-form H. Point-wise, i.e. locally, it may be expressed in the general case as

$$H=E_1\,dt\wedge dx^1\wedge dx^2+E_2\,dt\wedge dx^3\wedge dx^4-B_2\,dx^5\wedge dx^1\wedge dx^2-B_1\,dx^5\wedge dx^3\wedge dx^4, \tag{161}$$

$$\star H=E_1\,dx^3\wedge dx^4\wedge dx^5+E_2x^1\wedge dx^2\wedge dx^5+B_2\,dt\wedge dx^3\wedge dx^4+B_1\,dt\wedge dx^1\wedge dx^2. \tag{162}$$

In the strong coupling limit we get the well defined limits,

$$H=(dt-dx^5)\wedge(B_2\,dx^1\wedge dx^2+B_1\,dx^4\wedge dx^5), \tag{163}$$

$$*H=(dt-dx^5)\wedge(B_2\,dx^2\wedge dx^3+B_1\,dx^1\wedge dx^2). \tag{164}$$

By contrast since

$$h=e_1(dt\wedge dx^1\wedge dx^2-dx^5\wedge dx^3\wedge dx^4)+e_2(dt\wedge dx^3\wedge dx^4-dx^5\wedge dx^1\wedge dx^2), \tag{165}$$

the three-form h_{lmn} diverges in the limit of small T,

$$h\rightarrow\frac{2}{T}\frac{B_1B_2}{B_1+B_2}(dt-dx^5)(dx^1\wedge dx^2+dx^3\wedge dx^5). \tag{166}$$

We see that in the limit H and $\star H$ contain a one-dimensional null factor $dt-dx^5=-l_m\,dx^m$, with

$$H_{lmn}l^n=0,\quad \star H_{lmn}l^n=0. \tag{167}$$

It is tempting to give the stress tensor an interpretation in terms of a fluid of p-branes. The null vector l^m clearly provides us with the velocity of the putative fluid and since it is null, we should expect a null fluid analogous to the gas of null or Schild strings[23] considered in Ref. 24 and elaborated in Refs. 25, 26 in four dimensions. In the case of UBI theory[16,19] one has the condition

$$\sqrt{\det(F_{\mu\nu})}=\tfrac{1}{4}F_{\mu\nu}\star F^{\mu\nu}=\mathbf{E}\cdot\mathbf{B}=0. \tag{168}$$

This is equivalent to the simplicity condition

$$F \wedge F = 0, \tag{169}$$

which implies the existence of one-forms a_μ and b_μ such that

$$F_{\mu\nu} = a_\mu b_\nu - a_\nu b_\mu . \tag{170}$$

The co-vectors a_μ and b_μ are not unique; one may choose them such that $a_\mu b^\mu = 0$. Thus, in the tangent space at each point of spacetime, the two-form $F_{\mu\nu}$ is tangent to the two-plane spanned by a_μ and b_μ. The equations of motion imply the integrability condition that these two-planes mesh together to provide a foliation of spacetime by two-surfaces. If

$$F_{\mu\nu} F^{\mu\nu} = 0, \tag{171}$$

then the two-plane is null, and one of the co-vectors, call it a_μ, is null and the other spacelike. Therefore

$$F_{\mu\nu} = l_\mu b_\nu - l_\nu b_\mu . \tag{172}$$

The null vector l_μ satisfies

$$F_{\mu\nu} l^\nu = 0. \tag{173}$$

If (171) then the principal null directions of the two-form $F_{\mu\nu}$ coincide and may be identified with l^μ. One may regard b_μ as the (un-normalized) tangent vector to the magnetic field lines and obtain in this way a picture of the solutions of classical Born–Infeld field theory, subject to the simplicity constraint (168) or (169), as a fluid of strings. This viewpoint is similar to that originally envisaged by Nielsen and Olesen.[27]

In the case of the M5-brane, we have a three-form and one might have thought that some sort of null membrane is involved. However although the three-forms H and and $\star H$ both have a null factor neither quotient two-form, that is neither

$$B_2\, dx^1 \wedge dx^2 + B_1\, dx^4 \wedge dx^5 \quad \text{nor} \quad B_2\, dx^2 \wedge dx^3 + B_1\, dx^1 \wedge dx^2 \tag{174}$$

is simple. Therefore no obvious membrane world volume is picked out.

We observe that this limiting theory admits an infinite number of conserved charges that carry Lorentz indices. Presumably (cf. Ref. 28) the scattering of particlelike excitations is trivial in this limit. It is not obvious whether this is true for 2-branes and 5-branes since they have internal degrees of freedom associated to their world volumes.

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An M-theory flop as a large *N* duality

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We show how a recently proposed large N duality in the context of type IIA strings with $\mathcal{N}=1$ supersymmetry in 4 dimensions can be derived from purely geometric considerations by embedding type IIA strings in M-theory. The phase structure of M-theory on G_2 holonomy manifolds and an S^3 flop are the key ingredients in this derivation. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1376159]

I. INTRODUCTION

String propagation in the presence of branes has been studied from many different angles, and has been the intersection point of many fruitful ideas in the context of dualities. A beautiful example of it is in the context of the AdS/CFT correspondence.[1] This idea is a refinement of the statement that if we consider strings in the presence of branes, in certain regime of parameters the system is better described by strings propagating on the gravitational back reaction of light string modes to the presence of branes. This is an example of duality in the sense that two different theories are continuously connected by a change in parameters. On the one end one has a geometry involving branes and on the other extreme the geometry has been deformed and the branes have disappeared.

A recent example of a large N duality in type IIA superstring, was proposed in Ref. 2 based on embedding the large N Chern–Simons/topological gravity duality of Ref. 3 in type IIA superstrings. The duality states that if we consider N D6-branes wrapped on an S^3 in the deformed conifold geometry T^*S^3, then the same system is equivalent to a type IIA geometry where the D-branes have disappeared but where an S^2 has blown up so that the CY geometry is the $O(-1)+O(-1)$ bundle over $\mathbf{P}^1$. [Mathematicians use the terminology ''quadric'' for the deformed conifold and ''quadric cone'' for a singular quadric. The small resolution of conifold is called the small resolution (blow up) of the quadric cone.] In other words, the topology is that of the so called ''small resolution'' of the conifold, where the S^2 has finite size. Moreover there are N units of 2-form field strength flux through $\mathbf{P}^1$, and the complexified Kahler parameter t of $\mathbf{P}^1$ is related to the volume V of the S^3 and the string coupling constant g_s by

$$(e^t-1)^N=a\exp(-V/g_s). \tag{1.1}$$

Note that for large V and when $Ng_{\mathrm{YM}}^2=Ng_s/V\ll 1$, the wrapped D-brane description is good and the blown up description is bad as $t\to 0$, and when $t\gg 0$ where the blown up $\mathbf{P}^1$ description is good the $V\to-\infty$ and the original wrapped D-brane description is bad. In this sense we only really have at most one good description in each regime of parameters and the parameters being related by (1.1). This situation is similar to other cases one encounters in the context of large N string

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dualities. For example with N D3 branes in R^{10} if $Ng_{\rm YM}^2 = Ng_s \ll 1$ the D-brane description ignoring the gravitational backreaction is fine; when $Ng_s \gg 1$ the gravitationally deformed background description without the D-brane is the right description.

Our main aim in this paper is to embed this type IIA duality in M-theory. We find that the statement of this duality in the context of M-theory translates to a simple geometric duality. Turning it around, we can derive the type IIA string duality of Ref. 2 from its relation with M-theory.

The organization of this paper is as follows. In Sec. II we review a perturbative string theory duality which is a good exercise for the M-theory duality of interest. In Sec. III we discuss M-theory in a 7 dimensional background with G_2 holonomy and a simple geometric duality. In Sec. IV we reinterpret the M-theory duality in the context of type IIA strings and obtain the duality of Ref. 2. In the Appendix we discuss some aspects of the G_2 holonomy metric.

The derivation of the large N duality in this case reinforces the philosophy advocated in Refs. 3 and 2 that large N dualities in general correspond to transitions in geometry. It would be interesting to try to understand other large N dualities in the same spirit.

While we were completing this paper we received Ref. 4 which has some overlap with this paper.

II. A STRING THEORY DUALITY

Consider type IIA superstrings propagating on a noncompact CY background given by a $O(-1)+O(-1)$ bundle over $\mathbf{P}^1$. A powerful worldsheet description of this sigma model is in terms of linear sigma model[5] where one considers a (2,2) supersymmetric $U(1)$ gauge theory with four fields $(\Phi_1,\Phi_2,\Phi_3,\Phi_4)$ with charges $(+1,+1,-1,-1)$, with an FI term given by r and a $U(1)\,\theta$ angle. The low energy vacuum of this theory is characterized by

$$\mathcal{V}: |\Phi_1|^2+|\Phi_2|^2-|\Phi_3|^2-|\Phi_4|^2=r. \tag{2.1}$$

The actual vacuum of this theory is given by the gauge inequivalent solutions to (2.1), i.e., one considers $\mathcal{V}/U(1)$. This can be naturally identified with a $O(-1)+O(-1)$ bundle over $\mathbf{P}^1$. If we take $r>0$ the $\mathbf{P}^1$ is identified as the locus $\Phi_3=\Phi_4=0$, and the normal directions are identified with Φ_3 and Φ_4. This space is also called the ''small resolution'' of the conifold, where the S^2 has a finite size.

An important aspect of this theory is its phase structure and in particular what happens as $r \to 0$. In fact the natural phase structure for this theory is parameterized by the *complex* parameter,

$$t = r + i\,\theta.$$

It turns out that both positive and negative r make sense and in fact are smoothly connected if we vary the θ because the only singularity in the moduli space of this theory is at the origin $t=0$. From the equation (2.1) one may naively have thought that there should be some singularity at $r=0$ for all θ, but this is lifted by worldsheet instanton corrections. Of course there is a simple reason why this had to happen. The structure of (2,2) supersymmetry leads to a naturally complex moduli space and it does not allow any real locus singularity in moduli space.

A. A perturbative string duality

From the above description we notice a symmetry: If we replace $t \to -t$ we obtain the same geometry with the role of the $(\Phi_1,\Phi_2) \leftrightarrow (\Phi_3,\Phi_4)$ exchanged. Geometrically this is called a flop. Even though in the geometric setup there is a discontinuity at $r=0$, and one just considers either $r>0$ or $r<0$, the situation in string theory is different because of the θ angle. Both regions are smoothly connected. In particular if we start with $r \gg 0$ and do some computations as a function of t, then an analytic continuation of these quantities by $t \to -t$ should yield the answers for the other side. This in fact was directly checked at the level of instanton computations on both sides.[5,6] In particular the worldsheet instantons at genus 0 (with three points fixed on S^2) have a partition function,

$$\partial_t^3 F_0 = C + \frac{q}{1-q},$$

where $q = e^{-t}$ (the constant term C is somewhat ambiguous and is related to the classical triple intersection of the 4-cycle dual to $\mathbf{P}^1$). This makes sense as an instanton expansion when $r \gg 0$. However if we analytically continue this quantity to $t \to -t$ we obtain in terms of $\tilde{q} = 1/q$,

$$-\partial_t^3 F_0 = 1 - C + \frac{\tilde{q}}{1-\tilde{q}},$$

which is the statement of the symmetry under $t \to -t$. The shift in the constant term is reflecting the geometric fact that under flop the classical triple intersection shifts by one.

Suppose however we consider a modified theory where we mod out the Φ_i's by some discrete group G which does not necessarily act symmetrically under the exchange $(\Phi_1, \Phi_2) \leftrightarrow (\Phi_3, \Phi_4)$. Let us call the resulting theory $Q_G[t]$, exhibiting explicitly the dependence of the theory Q on the choice of the group G as well as the (complexified) size of $\mathbf{P}^1$ given by t. Now we ask what happens when we consider $t \to -t$. In this case in general we do not come back to the same theory because of the asymmetric action of G. We obtain

$$Q_G[-t] = Q_{G'}[t], \tag{2.2}$$

where G' is related to G by conjugation with the element exchanging the pairs,

$$U: (\Phi_1, \Phi_2) \leftrightarrow (\Phi_3, \Phi_4),$$

$$G' = UGU^{-1}.$$

To better appreciate the content of this duality statement let us consider a simple example. Consider the case where G is generated by the element

$$(\Phi_1, \Phi_2, \Phi_3, \Phi_4) \to (\omega \Phi_1, \omega^{-1} \Phi_2, \Phi_3, \Phi_4),$$

where ω is an n-th root of unity (this can also be viewed as introducing an additional Z_n gauge group). Geometrically this corresponds to considering the following action on $O(-1) + O(-1)$ over $\mathbf{P}^1$:

$$(\zeta_1, \zeta_2, z) \to (\omega \zeta_1, \omega \zeta_2, \omega^{-2} z),$$

where z denotes the coordinate of $\mathbf{P}^1$ (say near the north pole) and ζ_i denote the coordinates of the bundle $O(-1) + O(-1)$ over it. Note in particular that modding by this group leads to two orbifold singularities, namely the north and south poles at the origin of the ζ_i. The group G' on the other hand is obtained by conjugating G with U and is generated by

$$(\zeta_1, \zeta_2, z) \to (\omega \zeta_1, \omega^{-1} \zeta_2, z).$$

This is a very different group action from G and in particular it leads to an A_{n-1} singularity over $\mathbf{P}^1$. Thus changing $t \to -t$ has led to a totally new but nevertheless ''dual'' theory. Note that this duality is a perturbative string duality (i.e., can be understood genus by genus in worldsheet expansion).

III. AN M-THEORY DUALITY

We will be interested in compactifications of M-theory on G_2 holonomy manifolds (see Ref. 7 for the construction of some compact 7-manifolds with G_2 holonomy). This leads to $\mathcal{N} = 1$ supersymmetry in $d = 4$. In the compact case, the number of moduli of the Ricci-flat metric is given by the dimension of the third homology of the manifold, i.e. b_3. The point on the moduli

space of Ricci-flat metrics can be characterized by the volume of some basis for 3-cycles. (In the noncompact case there could be additional deformations which change the asymptotic behavior of the metric at infinity.) Physically we know that these should correspond to lowest components of chiral fields in $\mathcal{N}=1$ supersymmetry multiplets. Thus one again expects a complexification of the volumes. In fact this happens because there is a 3-form gauge field C in M-theory and its vev about each 3-cycle leads to the complexification of the volume elements. Moreover the moduli space of M-theory compactifications are given by analytic expressions and thus singularities occur in *complex* codimension 1 and higher. Thus there are in particular no boundary walls in moduli space of M-theory.

Let us now come to the concrete example that we will be interested in. Consider the noncompact 7-manifold given by the spin bundle over S^3. This has the topology of $R^4\times S^3$ and admits a G_2 holonomy metric. We will present the metric later in this section. The topology of the manifold can be viewed as

$$(u_1^2+u_2^2+u_3^2+u_4^2)-(v_1^2+v_2^2+v_3^2+v_4^2)=V,$$

where u_i, v_i are real parameters. For $V>0$ the S^3 is identified as the locus $v_i=0$, and v_i correspond to the R^4 normal directions over S^3. Note that if we consider $V<0$ then the role of the u's and v's have been interchanged and another S^3 blows up, corresponding to $u_i=0$. We can also write this in complex notation by

$$(|z_1|^2+|z_2|^2)-(|z_3|^2+|z_4|^2)=V,$$

where z_i are complex variables. It should be emphasized that the G_2 holonomy manifold does not admit a complex structure (it is odd dimensional) and so there is no intrinsic meaning to writing the equation in terms of complex coordinates, other than for simpler book keeping. We can also use a quaternionic notation and write it as

$$|q_1|^2-|q_2|^2=V.$$

We can view the quaternion as $q_1=\Sigma_i u_i\sigma_i$ and $q_2=\Sigma_i v_i\sigma_i$, where σ_i denotes the realization of quaternionic generators as 2×2 matrices. This way of writing it suggests that one can have $SU(2)^{1,2}_{L,R}$ symmetries, which act on each quaternion, as left and right multiplication by $SU(2)_{L,R}$. This is the same, as the *Spin*(4) action on the u's or on the v's.

A G_2 holonomy metric can be defined on this manifold.[8,9] It is given as

$$ds^2=\alpha^2\,dr^2+\gamma^2(\tilde{w}^a)^2+\beta^2\left(w^a-\tfrac{1}{2}\tilde{w}^a\right)^2, \tag{3.1}$$

with

$$\alpha^{-2}=1-\frac{a^3}{r^3},\quad \beta^2=\frac{r^2}{9}\left(1-\frac{a^3}{r^3}\right),\quad \gamma^2=r^2/12, \tag{3.2}$$

where $\tilde{w}^a$ and w^a are the left invariant one-forms on S^3 and S^3, respectively. The two S^3's are associated to each of the two quaternions at a fixed norm, and the r variable fills one of the S^3's depending on the sign of V. In the form shown above $r\geqslant a$ and it fills the S^3 associated with the left invariant one-forms w^a, while $\tilde{w}^a$ are associated with $\tilde{S}^3$ which is topologically nontrivial. Note that the volume of the $\tilde{S}^3$ is proportional to a^3. This G_2 holonomy metric has an $[SU(2)]^3$ isometry group,

$$SU(2)^1_L\times SU(2)^2_L\times[SU(2)^1_R\times SU(2)^2_R]_D,$$

where $SU(2)^i_{L,R}$ denotes the L, R multiplication of q_i by the $SU(2)$ group and D denotes the diagonal subgroup. This is almost obvious from the above presentation of the metric, where $SU(2)^i_L$ do not act on the left invariant forms and so do not modify the metric. The left invariant

1-forms transform in the adjoint representation of the corresponding $SU(2)_R$. The diagonal combination of $SU(2)_R^i$ leaves the metric invariant [the last term in the metric is what requires choosing the diagonal $SU(2)_R$ as the symmetry group]. To fix notation let us associate $SU(2)^1$ with the $\tilde{S}^3$ sphere and $SU(2)^2$ with the contractible S^3. The space (3.1) is asymptotic to a cone whose base has $\tilde{S}^3 \times S^3$ topology,

$$ds^2 \sim dr^2 + \frac{r^2}{9}[(\tilde{w}^a)^2 + (w^a)^2 - \tilde{w}^a w^a].$$

As we will note later, when we discuss the connection to type IIA string theory we expect a one parameter family of G_2 holonomy metric deformations which breaks the $SU(2)_L^i$ to $U(1)$, for either $i=1$ or $i=2$.

As noted above, in the context of M-theory propagating in this background the moduli space of the theory is parametrized in addition to the volume V of the S^3 by the flux of the C-field through it. Let us denote this complex combination by $V_M = V + iC$. Just as in the case of string propagation on the $O(-1)+O(-1)$ bundle over $\mathbf{P}^1$, the phase structure of M-theory as a function of V_M is expected to have a singularity at most only at the origin and that turning on the C-field should smooth out the singularity where $V=0$ in moduli space. This follows from the number of supersymmetries we are preserving in 4 dimensions and the fact that V_M is the lowest component of a chiral field. A similar situation (with twice as many supersymmetries) in the context of M-theory and type IIA strings on Calabi–Yau threefolds containing an S^3 was analyzed in Ref. 10 where it was shown that Euclidean M2-brane instantons modify the moduli space and in fact remove the singularity at $V=0$. Here also we expect the same to be true, though we do not know how to rigorously argue this. At any rate we can argue, based on supersymmetry alone, that a singularity at most will happen at isolated points in moduli space, and for the theory at hand this means potentially only at $V_M=0$ (in particular $V=0$ and $C\neq 0$ is not a singular point). This observation implies that we can continuously go from regions where the real part of V_M is large and positive to regions where it is large and negative without encountering any singularity. (For a discussion of topology change in the context of G_2 holonomy manifolds see the recent work.[11]) Moreover it is clear that $V_M \to -V_M$ is a flop, and otherwise gives rise to an equivalent ''dual'' M-theory background. Let us denote M-theory in the presence of this background by $Q[V_M]$. Then we have

$$Q[V_M] = Q[-V_M].$$

Notice that for positive V_M, S^3 is contractible in the full geometry and $\tilde{S}^3$ is topologically nontrivial while the opposite is true of negative V_M.

Parallel to our discussion of the string duality in the previous section, we can consider modding out by some group actions which are isometries of the G_2 holonomy manifold. As discussed in the Appendix this leads to manifolds (possibly with singularities) which continue to have G_2 holonomy. In this way we obtain a statement of duality where

$$Q_G[-V_M] = Q_{G'}[V_M],$$

where $G = UG'U^{-1}$ and U is the Z_2 outer automorphism exchanging the u's and the v's, and acts on the $SU(2)$'s as

$$U[SU(2)_{L,R}^{1,2}]U^{-1} = SU(2)_{L,R}^{2,1}.$$

The special case we will be interested in is when G is generated by a Z_N subgroup of $SU(2)_L^2$. In complex coordinates we can view this transformation as

$$g\colon\ (z_1, z_2, z_3, z_4) \to (z_1, z_2, \omega z_3, \omega z_4).$$

Then G' is generated by

$$g':\ (z_1,z_2,z_3,z_4)\to(\omega z_1,\omega z_2,z_3,z_4),$$

and we have an M-theory duality,

$$Q_G[-V_M]=Q_{G'}[V_M]. \tag{3.3}$$

Let us consider $Q_G[V_M]$ when $V\gg 0$. In this case the element g acts with a fixed point: The $\tilde{S}^3$ defined by $z_3=z_4=0$. Moreover the singularity is of the type of A_{N-1} singularity as the normal direction is R^4/Z_N in the usual action of Z_N on R^4. As is well known, this singularity in M-theory gives rise to an $SU(N)$ gauge symmetry on the singular locus. In the present case, taking the number of supersymmetries into account, we have an $\mathcal{N}=1$ supersymmetric $SU(N)$ Yang–Mills gauge theory living on $\tilde{S}^3$ times the Minkowski space. On the other hand when we consider $Q_{G'}[V_M]$ for $V\gg 0$, the g' corresponds to the Z_N action with no fixed points (the would be fixed point locus $z_1=z_2=0$ is not on the manifold for $V\gg 0$).

A. Gauge theoretic interpretation of the duality

From (3.3) we see that M-theory in one background is continuously connected with another one. In particular $Q_G[V_M]$ when $V\gg 0$ contains as light excitations an $\mathcal{N}=1$ Yang–Mills sector in 4 dimensions with the Yang–Mills coupling given by

$$\frac{1}{g^2_{\mathrm{YM}}}+i\theta=V_M,$$

where g^2_{YM} should be viewed as the gauge coupling at the Planck scale. As we know the coupling will start to run. More precisely, the effective coupling constant depends on the scale we probe. Through the above relation we see that V_M itself should run and its value will depend on which scale we measure it at. In particular $V_M(\mu)$ should decrease logarithmically at infrared as

$$V_M(\mu)=V_M+\text{const}\log\frac{\mu}{M_{pl}}.$$

This running should be induced by quantum effects in the presence of the Z_N singularity in measuring the volume of S^3, which is at the singular locus. For small μ, we expect V_M to become small. In fact if we trust the above formula we seem to get a *negative* volume V_M. Even though this is not allowed in the usual gauge theory (negative $1/g^2_{\mathrm{YM}}$ naively does not make sense), here we can make sense of negative V_M as a flop. In fact we are thus led to view the infrared behavior of the same theory at negative and large values of $V\ll 0$. However this theory for negative V is best viewed as the dual theory $Q_G[-V_M]=Q_{G'}[V_M]$, in terms of which there is no singularity in geometry and we obtain an $\mathcal{N}=1$ theory in four dimensions with no sign of $SU(N)$ gauge symmetry. This is exactly what one expects for a confining gauge theory. Moreover we should see N vacua. This is also present here; the G' group corresponds to modding out the S^3 by a Z_N. So the volume of the final S^3 is smaller by a factor of $V\to V/N$. However we also have to decide about the choice of the theta angle. If we change the theta angle by $2\pi k$ on S^3, which in the original $Q_G[V_M]$ corresponds to not changing the theory at all, as we go to negative V_M, it does give rise to a change. Namely quotienting the S^3 by a Z_N gives rise to a fractional change in the C-flux of the quotient theory by $2\pi k/N$. Thus we obtain N choices for the phase of the theory in the infrared. These are the N vacua of $\mathcal{N}=1$ supersymmetric $SU(N)$ Yang–Mills, and we have thus found a purely geometric interpretation of them. One can also identify the domain wall of the $\mathcal{N}=1$ system with the $M5$-brane wrapped over S^3/Z_N.

IV. RE-INTERPRETATION OF THE M-THEORY DUALITY IN TYPE IIA STRING

We now view the same geometry from the type IIA perspective. In order to do this we need to choose the ''11-th'' circle. There are many ways to do this. In order to connect this to the duality of Ref. 2 we identify the 11-th direction with the fibers of the $U(1)$ sitting in $SU(2)_L^2$, where the Z_N that we modded out in the previous section, is a subgroup of it. In other words $Z_N \subset U(1) \subset SU(2)(2)_L^2$. We start with $Q_G[V_M]$ with $V \gg 0$. Kaluza Klein reducing along this circle produces an R^3 fibration over $\tilde{S}^3$ with a singularity at the origin. The singularity at the origin has the interpretation of a $D6$-brane, before modding out by Z_N, or N units of $D6$-branes after modding out. Thus we expect this to correspond to type IIA string theory on the conifold background T^*S^3 with N D6-branes wrapped around S^3. A more precise statement is the following. Suppose we start with the deformed conifold before we put any branes on it. In M-theory we add an extra circle of constant radius so that we have a seven dimensional geometry which is the deformed conifold times a circle. Now we add N D6-branes on $\tilde{S}^3$. At large distances from the D6-branes, the presence of the branes is signaled in IIA theory by the presence of a two-form field strength on the surrounding S^2. When we lift this up to M-theory this means that the eleventh circle S^1 is nontrivially fibered over the S^2. In fact the total topology of this S^1 fibration over S^2 ends up being that of S^3/Z_N. (Notice that for $N=1$ we just have S^3.) For very large r we expect that the dilation will be constant, so that the size of the S^1 fiber is constant, while the size of $S^2 \times \tilde{S}^3$ should grow. For small r, on the other hand, we enter the near horizon region of the six branes. The dilation decreases as we approach the ''core'' of a six-brane. In fact, the near horizon region of N six-branes in flat space lifts up in M-theory to an A_{N-1} singularity and the M-theory circle is just one of the angles on the three-sphere. So when we wrap this on $\tilde{S}^3$ we expect a geometry which is that of the region $r \sim a$ of (3.1). The asymptotics of (3.1) is not what we expect in the IIA situation since the radius of the M-theory circle continues to grow as $r \to \infty$. In fact the geometry (3.1) looks more like the infinite coupling limit of the IIA geometry, where we take the limit in such a way as to keep V_M finite. In principle we expect to find a gravity solution in M-theory that describes more precisely the situation we expect in IIA theory for a finite string coupling constant. That should be a deformation of the above G_2 holonomy metric where the $SU(2)_L^2$ symmetry of (3.1) is broken to $U(1)_L$ so that the circle can have a constant asymptotic size as $r \to \infty$. This deformation should exist for both signs of V_M which means, in terms of (3.1), that we should also find a second deformation where $SU(2)_L^1$ is broken to $U(1)$. This would describe the situation after the transition where, in IIA theory, we have the small resolution of the conifold with N units of F_2 flux. Again, we expect a solution where the string coupling asymptotes to a constant. Assuming this deformation of the metric exists, it is natural to expect that under the flop $V_M \to -V_M$ we get from one kind of deformation to the other. In other words the considerations of Sec. III should also apply to this deformed metric. With this assumption we now rederive the large N type IIA duality, including the identification of parameters on both sides in the geometric regime.

Let us denote the volume of the $\tilde{S}^3$ in the type IIA setup by V_A, and consider N D6-branes wrapped over it. Then from the map between M-theory parameters and type IIA parameters one deduces that

$$V_M = V_A / g_s , \tag{4.1}$$

where g_s is the type IIA coupling constant. Now let us consider the limit where $V_M \ll 0$. In this case the theory is better described by another M-theory background with group modding out by G', and where the volume of the S^3 is $-V_M$. Again we use the same 11-th direction for the circle fibration, which means that we choose G' to be a subgroup of the corresponding $U(1)$. Now the fibration we get gives a geometry which has an S^2 and the M-theory S^3 over it is a quotient of Hopf fibration by Z_N. This means, in the type IIA terminology that we have N units of RR 2-form field strength through S^2. Moreover the volume of the (minimal) S^2 is given, changing the parameters from M-theory to type IIA, as

$$t = -V_M/N. \tag{4.2}$$

This relation is trustable for large t where the supergravity description of M-theory would be adequate. Thus we see that we have a duality which in the type IIA description corresponds to N units of D6-branes wrapping the S^3 of volume V_A and on the other side an S^2 with N units of RR flux through it, with Kahler class t and with the relation [combining (4.1) and (4.2)]

$$t = \frac{-V_A}{Ng_s}. \tag{4.3}$$

This agrees, in the limit of large t, with the result obtained in Ref. 2:

$$(e^t - 1)^N = a \exp(-V_A/g_s). \tag{4.4}$$

The modified relation (4.4) includes the contribution of worldsheet instantons, which is neglected in the identification at the large volume limit given in (4.3). Note that in Ref. 2 the parameter t was identified as the lowest component of the gaugino chiral field $t = g_s \operatorname{Tr} W^2 = S$. Note that in the limit of large V, which corresponds to small t if we include the instanton correction, we deduce a gaugino condensation exactly as one would expect for the $\mathcal{N}=1$ Yang–Mills theory, namely in the form $S^N = \exp(-1/g_{\mathrm{YM}}^2)$ (where the g_{YM} is the Yang–Mills coupling constant at the string scale).

From the relation to M-theory it is natural that the worldsheet instantons know about gaugino condensation. This is similar to the worldsheet instantons for the flopped geometry in the $O(-1)+O(-1)$ over $\mathbf{P}^1$. Thus the worldsheet instantons of the $O(-1)+O(-1)$ theory over $\mathbf{P}^1$ with N units of flux, which in M-theory correspond to superpotential corrections due to Euclidean $M2$-brane instantons, know, by analytic continuation, about the Euclidean $M2$-brane instantons of the flopped geometry, which correspond to the usual gauge theory instantons.

Note that regardless of whether we find the new deformed G_2 holonomy solutions or not, we do not expect to find a geometry that truly decouples from the bulk and which can be interpreted as a decoupled field theory. There is a limit where we expect a decoupled field theory, the large V_M limit, and the region very close to the singularity, but it is not a limit where we expect a weakly coupled geometrical description. This corresponds as we saw above to $t \sim 0$. Though a weakly coupled *string* description is expected for large N. The field theory we have been considering, therefore, has more degrees of freedom than pure $\mathcal{N}=1$ Yang–Mills. In particular, it has the parameter V_M which is not a parameter in $\mathcal{N}=1$ SYM.

It is important to remark that when we talk about the resolved conifold of IIA theory with some units of flux, we are characterizing the space in terms of its topology, but we do not have a complex manifold. So in what sense is the consideration of topological strings as used in Ref. 2 relevant? The answer turns out to be that if we consider the BPS charge measured by the $M2$-brane, when we integrate over the 11-th circle, it leads to a BPS charge seen by the fundamental string, which corresponds to a symplectic form on the quotient geometry, which topologically is $R^4 \times S^2$. The symplectic structure induced from this reduction agrees with the symplectic structure of $O(-1)+O(-1)$ bundle over $\mathbf{P}^1$, as is shown in the Appendix (the corresponding symplectic two form k is obtained by integrating the G2 invariant three form Ω_3 over the 11-th circle, $k = \int_{S^1} \Omega_3$). This implies that we expect to obtain the same results in consideration of topological strings for this reduction of the 7-manifold.

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APPENDIX: ASPECTS OF G_2 HOLONOMY METRIC

A G_2 holonomy manifold is a seven dimensional manifold whose holonomy group is the simple group G_2. It can be proven that in such manifolds there is a special harmonic three form Ω, $d\Omega = d^*\Omega = 0$, which is such that it locally determines the reduction of the holonomy group from Spin(7) to G_2. More precisely, at each point the subgroup of GL(7) that leaves Ω invariant is G_2.

It was shown in[9,8] that the following metric (on $R^4 \times S^3$) has G_2 holonomy:

$$ds^2 = \alpha^2\, dr^2 + \gamma^2 (\tilde{w}^a)^2 + \beta^2 \left(w^a - \tfrac{1}{2}\tilde{w}^a \right)^2, \tag{A1}$$

with

$$\alpha^{-2} = 1 - \frac{a^3}{r^3}, \quad \beta^2 = \frac{r^2}{9}\left(1 - \frac{a^2}{r^3}\right), \quad \gamma^2 = r^2/12, \tag{A2}$$

where $\tilde{w}^a$ and w^a are left invariant one-forms on two three-spheres, which we denote as $\tilde{S}^3$ and S^3. We think of S^3 as the $SU(2)$ group manifold. We can use the following formulas:

$$\begin{gathered}
g = e^{i\psi/2\sigma^3} e^{i\theta/2\sigma^1} e^{i\phi/2\sigma^3}, \\
\frac{i}{2} w_R^a \sigma^a = dg\, g^{-1}, \quad \frac{i}{2} w_L^a \sigma^a = g^{-1}\, dg, \\
(w_R^1 + i w_R^2) = e^{-i\psi}(d\theta + i \sin\theta\, d\phi), \quad w_R^3 = d\psi + \cos\theta\, d\phi, \\
(w_L^1 + i w_L^2) = e^{+i\phi}(d\theta - i \sin\theta\, d\psi), \quad w_L^3 = d\phi + \cos\theta\, d\psi, \\
dw_R^a = \tfrac{1}{2}\epsilon^{abc} w_R^b w_R^c, \\
dw_L^a = \tfrac{1}{2}\epsilon^{abc} w_L^b w_L^c .
\end{gathered} \tag{A3}$$

We can see from these definitions that the forms w_L^a are invariant under left multiplications of g, $g \to h_L g$ while they transform in the adjoint representation of $SU(2)$ under right multiplication $g \to g h_R$. We can write the metric of the unit three-sphere as

$$ds^2 = \frac{1}{4}\sum_a (w_L^a)^2 = \frac{1}{4}\sum_a (w_R^a)^2. \tag{A4}$$

We can easily check that the metric (A1) has $SU(2)^3$ isometry. Two $SU(2)$'s arise from left multiplication in each of the $S^3 s$ while the third $SU(2)$ arises from right multiplication on both three-spheres by the same group element. This last fact we can check by noticing that the index a, which transforms in the adjoint of $SU(2)$ is contracted in an $SU(2)$ invariant fashion.

Finally we can write the explicit form of the three-form,

$$\begin{aligned}
\Omega &= \frac{a^3}{12}\frac{1}{6}\epsilon_{abc}\tilde{w}^a\tilde{w}^b\tilde{w}^c - \frac{1}{18}(r^3 - a^3)\epsilon_{abc}(\tilde{w}^a w^b w^c - \tilde{w}^a \tilde{w}^b w^c) + \frac{r^2}{3} dr\, \tilde{w}^a w^a \\
&= \frac{a^3}{12}\frac{1}{6}\epsilon_{abc}\tilde{w}^a\tilde{w}^b\tilde{w}^c + d\left(\frac{r^3 - a^3}{9}\tilde{w}^a w^a\right).
\end{aligned} \tag{A5}$$

From this expression we see that the $SU(2)^3$ isometry group of the metric also leaves the three form invariant. In other words, these symmetries leave the G_2 structure invariant.

The metric (A.1) is asymptotic at large r to

$$ds^2 \sim dr^2 + r^2 \tfrac{1}{9}[(\tilde{w}^a)^2 + (w^a)^2 - w^a \tilde{w}^a]. \tag{A6}$$

The manifold on the right hand side of (A6) is a cone whose base is topologically $\tilde{S}^3 \times S^3$. This cone has a singularity at $r=0$. This singularity is eliminated in (A1) by giving a finite volume to one of the three-spheres, $\tilde{S}^3$. We could similarly consider a situation where we give a finite volume to the other sphere S^3. In that case the manifold we obtain is just given by (A1) with $w^a \leftrightarrow \tilde{w}^a$. These two manifolds are related by a flop. We see from the explicit expression of Ω that we can continuously go from one to the other, passing through a singular manifold at the point where both spheres have zero volume.

If we quotient this manifold by any subgroup of the isometry group described above we will obtain again a G_2 manifold, since the isometry group leaves the three form invariant. We will consider two different quotients.

1. Singular quotient

In this quotient we mod out by $Z_N \subset U(1) \subset SU(2)_L^2$ which acts on the coordinates of S^3. After modding out the metric (A1) by Z_N as above we get a singular space. We get an A_{N-1} singularity wrapped over $\tilde{S}^3$. If we KK reduce over the circle associated to this $U(1)$ and we go to type IIA theory, the singularity looks like the singularity we have in the near horizon region of N sixbranes wrapped on $\tilde{S}^3$. The normal bundle of this S^3 in IIA theory is the same as what we have when we wrap branes on the S^3 of a deformed conifold. In more mathematical notation, it is $T^*\tilde{S}^3$. Notice that in this IIA description, there is a singularity at the position of the branes even for $\mathcal{N}=1$. [Mathematically the point is that when we quotient $R^4=C^2$ by the circle (acting as complex scalars) the resulting space can be naturally identified with R^3 topologically but not differentiably—the identification being singular at the origin. This singularity in type IIA is interpreted as a D6-brane.] As usual, in the near horizon region of six-branes in IIA theory, the dilation is varying and it is approaching zero at the core of the six-branes.[12] The string metric in the directions along the six-brane is also shrinking as we approach the core, but it does so in such a way that $V_M = V_A / g_s$ is constant and equal to the volume of $\tilde{S}^3$ in M-theory. The above remarks about the near horizon region of a six-brane apply close to the singularity at $r=a$, for the region $r-a \ll a$. For large N there is a large region where the IIA description is valid.[12] As we go farther away from the singularity the geometry becomes more and more strongly coupled and the 11 dimensional description becomes better. For large r the dilation goes to infinity. In principle there should be another solution where the dilation goes to a constant.

2. Nonsingular quotient

If we choose $Z_N \subset U(1) \subset SU(2)^1$. This group acts as left multiplication on $\tilde{S}^3$. Since the volume of this three-sphere is nowhere vanishing we conclude that the quotient is nonsingular. We can further Kaluza Klein reduce the metric along this circle. This produces a nonsingular IIA metric on a space which has the topology of the small resolution of the conifold and with N units of two-form flux on S^2. If N is very large, then this IIA geometry is weakly coupled at the origin. When we start moving out in the radial direction the string coupling starts increasing and it becomes infinite asymptotically. In principle there should be another solution where the string coupling does not diverge. If we integrate the three-form (A5) on this S^1 we find the symplectic form on the small resolution of the conifold. It should be noted that, though we get the same two form as the Kahler form of the local CY, the IIA geometry with the flux is not Kahler.

Let us see this more explicitly. The circle in question is parametrized by $\tilde{\psi}$. In order to do the KK reduction it is convenient to define the new one-forms $\hat{w}^a$ and the vector n^a as follows:

$$\tilde{w}_L^a = \tilde{w}^a + n^a \, d\tilde{\psi}. \tag{A7}$$

Notice that $n^a n^a = 1$. We have extracted the dependence on $\tilde{\psi}$ in order to KK reduce. This splitting preserves $SU(2)_R^1$ but breaks $SU(2)_L^1$ to $U(1)_L$.

The IIA dilation, metric and one-form RR potential are

$$e^{4\phi/3} = \frac{1}{N^2}\left[\gamma^2 + \frac{\beta^2}{4}\right],$$

$$ds^2_{\rm str} = e^{2\phi/3}\left[dx_4^2 + \alpha^2\, dr^2 - e^{4\phi/3}A_1^2 + \gamma^2(\hat{w}^a)^2 + \beta^2\left(w^a - \tfrac{1}{2}\hat{w}^a\right)^2\right], \tag{A8}$$

$$A_1 = N\left[\hat{w}^a n^a - \frac{\beta^2}{2(\gamma^2+\beta^2/4)}\, w^a n^a\right],$$

where A_1 is the RR one-form potential.

Similarly we can integrate the three-form over S^1 and we obtain

$$J = \frac{a^3}{12}\frac{1}{2}\epsilon_{abc} n^a \hat{w}^b \hat{w}^c - \left(\frac{r^3}{18} - \frac{a^3}{18}\right)\epsilon_{abc}(n^a w^b w^c - 2 n^a w^b \hat{w}^c) - \frac{r^2}{3} dr\, n^a w^a, \tag{A9}$$

which is closed since Ω was closed.

We can further simplify these expressions by doing a coordinate transformation that amounts to switching from the left invariant one-forms to the right invariant one-forms in $\tilde{S}^3$. This translates into the following replacements:

$$\hat{w}^a \to \check{w}^a_R, \quad n^a \to \check{n}^a_R, \quad w^a \to w^a + \check{w}^a_R, \tag{A10}$$

where now $\check{w}^a_R, \check{n}^a_R$ are defined through,

$$\tilde{w}^a_R|_{\tilde{\psi}=0} = \check{w}^a_R + \check{n}^a_R\, d\tilde{\psi}.$$

In these variables,

$$\check{n}^a_R = \delta^a_3, \quad ,\check{w}^1 = \tilde{\theta}, \quad \check{w}^2 = \sin\tilde{\theta}\, d\tilde{\phi}, \quad \check{w}^3 = \cos\tilde{\theta}\, d\tilde{\phi}.$$

In these variables the two-form (A9) becomes

$$J = \frac{a^3}{12}\sin\tilde{\theta}\, d\tilde{\theta}\, d\tilde{\phi} - d\left(\frac{r^3 - a^3}{9}(w^3 + \cos\tilde{\theta}\, d\tilde{\phi})\right). \tag{A11}$$

This agrees with the two-form of the small resolution of the conifold which is

$$k = t\sin\tilde{\theta}\, d\tilde{\theta}\, d\tilde{\phi} - d(h(\rho)(w^3 + \cos\tilde{\theta} d\tilde{\phi})), \tag{A12}$$

where $h(\rho)$ is some function of the radial coordinate. These two expressions coincide if we identify $h(\rho) = (r^3 - a^3)/9$ which just amounts to a reparametrization of the radial coordinate.

We can also write the IIA metric (A8) and the RR 1-form potential in a more explicit form,

$$ds^2_{\rm str} = e^{2\phi/3}\left[dx_4^2 + \alpha^2\, dr^2 + \gamma^2(d\tilde{\theta}^2 + \sin^2\tilde{\theta}\, d\tilde{\phi}^2) + \beta^2\left[\left(w^1 + \frac{1}{2}d\tilde{\theta}\right)^2 + \left(w^2 + \frac{1}{2}\sin\tilde{\theta}\, d\tilde{\phi}\right)^2 + (w^3 + \cos\tilde{\theta}\, d\tilde{\phi})^2\right] - \frac{\beta^4}{4(\gamma^2+\beta^2/4)}(w^2 + \cos\tilde{\theta}\, d\tilde{\phi})^2\right]$$

$$A_1 = N\left[\cos\tilde{\theta}\, d\tilde{\phi} - \frac{\beta^2}{2(\gamma^2+\beta^2/4)}(w^3 + \cos\tilde{\theta}\, d\tilde{\phi})\right] \tag{A13}$$

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Continuous-time histories: Observables, probabilities, phase space structure and the classical limit

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The continuous-time histories program stems from the consistent histories approach to quantum theory and aims to provide a fully covariant formalism for quantum mechanics. In this paper we examine some structural points of the formalism. We demonstrate a general construction of history Hilbert spaces and identify a large class of time-averaged observables. We pay particular attention to the construction of the decoherence functional (the object that encodes probability information) in the continuous-time limit and its relation to the temporal structure of the theory. Phase space observables are introduced, through the study of general representations of the history group, which is the analog of the canonical group in the formalism. We can also define a closed-time-path (CTP) generating functional for each observable, which encodes the information of its correlation functions. The phase space version of the CTP generating functional leads to the implementation of Wigner–Weyl transforms, that gives a description of quantum theory solely in terms of phase space histories. These results allow the identification of an algorithm for going to the classical (stochastic) limit for a generic quantum system. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1383975]

I. INTRODUCTION

A. Canonical vs covariant

Physical systems can be described in two different ways, depending on one's attitude towards time evolution. The first description can be called ''canonical:'' it focuses on properties of a system at a single moment of time and studies how these properties change. It, therefore, provides an evolutionary picture of physical phenomena. The other type is best described as ''covariant:'' its main objects are histories of the physical system. Its main aim is to find criteria that determine which of them are realizable. As such, this description provides a timeless and (in a sense) teleological picture of physical processes.

In classical mechanics the ''canonical'' description is Hamilton's formalism. States of the system correspond to points of the phase space, which is a symplectic manifold. Time evolution is implemented by the action of a one-parameter group of symplectic transformations. Alternatively, one can start from the action principle, which provides the covariant description of classical mechanics. Histories are paths, and the physically realized are the ones that minimize the action subject to fixed boundary conditions.

These two approaches also appear in classical probability theory. A physical system at a moment of time is described by a probability distribution on a space Ω of elementary alternatives. We then study how this distribution evolves in time: the evolution law is a linear partial differential equation, like the Fokker–Planck equation. The ''covariant'' description of probability theory is provided by the theory of stochastic processes. Here, histories are paths on Ω and the physical information is encoded in a probability measure $d\mu$ in the space of all histories; it incorporates information about both initial conditions and dynamics.

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Quantum theory was developed in the ''canonical'' framework. The probabilistic information about a system is encoded in a Hilbert space vector, or more generally a density matrix. Its time evolution is given by a one-parameter group of unitary transformations: this is equivalent to Schrödinger's equation. The general structure is very similar to classical probability theory, except for the fact that the observables do not form a commutative algebra.

B. Quantum mechanical histories

When one tries to construct a ''covariant'' description of quantum theory, a problem immediately arises: *the natural probability measure for histories is not additive*. This is due to the fact, that quantum theory is based on amplitudes. When one constructs probabilities out of these amplitudes, interference between histories appears.

In general, a history corresponds to properties of the physical system at successive instants of time. Since in quantum theory a property (or a proposition about it) is represented by a projection operator, a discrete-time history α will correspond to a string $\hat{\alpha}_{t_1},\hat{\alpha}_{t_2},\ldots,\hat{\alpha}_{t_n}$ of projectors, each labeled by an instant of time. From them, one can construct the class operator

$$\hat{C}_\alpha=\hat{U}^\dagger(t_1)\hat{\alpha}_{t_1}\hat{U}(t_1)\cdots\hat{U}^\dagger(t_n)\hat{\alpha}_{t_n}\hat{U}(t_n), \tag{1.1}$$

where $\hat{U}(s)=e^{-i\hat{H}s}$ is the time-evolution operator. The probability for the realization of this history is

$$p(\alpha)=\mathrm{Tr}(\hat{C}_\alpha^\dagger\hat{\rho}_0\hat{C}_\alpha), \tag{1.2}$$

where $\hat{\rho}_0$ is the density matrix describing the system at time $t=0$.

This expression does not define a probability measure in the space of all histories, because the Kolmogorov additivity condition cannot be satisfied: if α and β are exclusive histories and $\alpha\vee\beta$ denotes their conjunction as propositions, then it is not true that

$$p(\alpha\vee\beta)=p(\alpha)+p(\beta). \tag{1.3}$$

The histories formulation of quantum theory does not, therefore, enjoy the status of a genuine probability theory.

1. The consistent histories interpretation

The formalism sketched above was developed as a part of the consistent histories approach to quantum theory, by Griffiths, Omnés, Gell-Mann, and Hartle.[1–4] In this approach, the problem of the nonadditivity of the probability measure is addressed by the remark that an additive probability measure *is* definable, when we restrict to particular sets of histories. These are called *consistent sets*. They are more conveniently defined through the introduction of a new object: the decoherence functional. This is a complex-valued function of a pair of histories given by

$$d(\alpha,\beta)=\mathrm{Tr}(\hat{C}_\alpha^\dagger\hat{\rho}_0\hat{C}_\beta). \tag{1.4}$$

A set of exclusive and exhaustive alternatives is called consistent, if for all pairs of different histories α and β in the set, we have

$$d(\alpha,\beta)=0. \tag{1.5}$$

In that case one can use Eq. (1.2) to assign a probability measure to this set. The consistent histories interpretation then proceeds by postulating that any prediction or retrodiction, we can make based on probabilities *must always make reference to a given consistent set*. This leads to counterintuitive and arguably unphysical situations of getting mutually incompatible predictions, when reasoning within different consistent sets.[5,6] The predictions of this theory are therefore contextual: but in any case, this is a general feature of all realist interpretations of quantum theory.

Even if the formalism of quantum mechanical histories was originally introduced as part of the consistent histories approach, it is conceptually distinct. The same formalism can be viewed in the light of any other interpretational scheme. The Copenhagen interpretation, for instance, would view the nonadditivity of the probability measure in a neutral light. The expression (1.2) describes the statistics of an ensemble of time-ordered sequences of measurements. There would be no *a priori* theoretical reason for the statistics to correspond to a genuine probability measure.

In this paper, we shall focus on the formal aspect of quantum mechanical histories. We do not find it necessary to commit to any particular interpretation: we only assume that all physical information about probabilities and interference of histories is encoded in the decoherence functional, something very explicitly shown by Gell-Mann and Hartle. It is not our aim to insist on how this information can be extracted: both the logic of consistent sets and the Copenhagen stance provide ways of doing this. Perhaps these ways do not exhaust the physical content of the theory—we have argued this in Ref. 7, but each of them is separately adequate to account for all minimal predictions of standard quantum theory.

We view the histories formalism simply as the covariant version of quantum theory. As such, it incorporates features of the covariant formulation of both classical mechanics and probability theory. But interference of probabilities highlights its quantum nature, and for this reason we shall pay particular attention to the structure of the decoherence functional.

2. Temporal logic histories

We shall work in the context of temporal logic histories. This is a scheme initiated by Isham:[8,9] its main point is that the quantum logic is preserved in the histories theory if we represent a history proposition $(\alpha_{t_1},\ldots,\alpha_{t_n})$ by a projection operator on a tensor product of the Hilbert spaces of the canonical theory $\mathcal{V}=\otimes_i H_{t_i}$. This history proposition will then be written as $\alpha=\alpha_{t_1}\otimes\cdots\otimes\alpha_{t_n}$. This construction is completely analogous to the construction of the space of classical histories as a *Cartesian product* of single-time sample spaces.

In this formulation a self-adjoint operator on $\mathcal{V}$ represents a history observable for the physical system. As in any covariant theory, more general observables can be defined. They correspond to time averages and include, for instance, an *action operator*.

One of the great strengths of this formalism is found in its temporal structure. It was shown by Savvidou,[10,11] that one can mathematically distinguish between two qualities of time: its partial ordering properties (the notion of before and after) and its status as a dynamical parameter in the equations of motion.

To see this, examine Eq. (1.1) for the class operator $\hat{C}_\alpha$ entering the expression for the decoherence functional. There, time appears in two places: as an index of the projectors $\hat{\alpha}_t$ and as the argument of the unitary operators $\hat{U}(t)$. In its former status, it is purely a kinematical parameter labelling the moment upon which a proposition is asserted. Its function is to determine the order upon which propositions are asserted, in the sense that if $t_1\leqslant t_2$ the projection operator $\hat{\alpha}_{t_1}$ will appear on the left of the operator $\hat{\alpha}_{t_2}$ in Eq. (1.1) for $\hat{C}_\alpha$. In its latter status as the argument of the unitary operators, time is the parameter of the Heisenberg-type evolution. It, thereby, implements the dynamics of the system.

These two roles of the time parameter are completely disentangled, when we view histories in the tensor product Hilbert space $\mathcal{V}=\otimes_t H_t$. This is an intriguing property, since it allows us to *mathematically distinguish* between the two conceptually distinct roles by which time appears in physical theories: in the form of a causal structure, that determines the order of events and in the form of the parameter by which change is effected in a physical system.

Indeed in the histories formalism there appear two mathematically distinct laws of time transformation. The partial ordering aspect of time is manifested in translations of the form $H_t \rightarrow H_{t+a}$, by which a property asserted at time t is translated to the same property at time $t+a$. At the continuum limit these transformations are generated by the kinematical part of an action operator. Dynamical time transformations are equivalent to a separate unitary transformation for each single-time Hilbert space H_t. They correspond to the Hamiltonian part of the action.

This distinguishing presence of two laws of time transformation is an important physical principle, that will provide a guideline for the construction of history theories, in the case where the canonical formalism does not provide sufficient insight. In retrospect, one can see that this distinction is present in *all* physical theories that are formulated in a covariant (histories) fashion.[11]

C. This paper

Since our aim is to show how histories provide a covariant formulation of quantum theory, we need to go beyond the discrete-time description that is usually effected: time, in physics, is a continuum. Continuous-time histories have been introduced in Ref. 12 and further studied in Refs. 10 and 13–15. This work relied on the use of a Fock space for the history Hilbert space, which is only justified if the Hamiltonian is quadratic.

The first aim of this paper is to explore the nature of continuous time in this framework. In particular, we highlight the structures that arise in the probability assignment. The analogy with stochastic processes is quite helpful in this regard, both at a conceptual and at a technical level.

In Sec. II we explain how a continuous-time Hilbert space with physically interesting observables can be constructed. We then analyze the decoherence functional: we show that it can be decomposed in a way that respects the two laws of time transformation. In fact, its components reflect the distinction between the geometric and the dynamical phase of canonical quantum theory.[16] Finally, we discuss the time-reversal transformations, which are substantially different from the ones of standard quantum theory.

In Sec. III we study the phase space structure of histories. This is incorporated in the quantum theory through the use of the history group, the history analog of the canonical group. The history Hilbert space carries one of its representations. This allows the identification of self-adjoint operators in this Hilbert space with objects that have a classical phase space analog. We explain, how one can construct such representations from the knowledge of the canonical theory.

The analogy with classical probability suggests that one should treat the decoherence functional as the quantum analog of a classical probability measure. In this sense its ''Fourier transform'' yields the analog of the generating function of classical probability: this is the closed-time-path (CTP) generating functional, first introduced by Schwinger.[17] We show how to construct this object for phase space histories. This construction suggests that the Wigner transform is of relevance: it enables us to write the decoherence functional as a complex-valued measure on the space of phase space paths and provides a picture of quantum theory that makes reference only to classical objects. One of the merits of this construction is that it provides an algorithmic procedure for passing into the classical limit of generic quantum theories.

In the final section we review our results. We argue that the formalism is flexible enough to accommodate a large number of applications in different fields. In particular, we stress the importance of our results as part of the developing continuous-time histories program.

Overall, our attitude is to highlight similarities of structures between the histories formalism and more familiar physical formalisms, such as stochastic processes or canonical quantum theory.

1. Notation

In the following, our expressions will make reference to two different types of Hilbert space: canonical ones and history ones. We adopt the following conventions: we will use the braket notation to denote vectors of both types of Hilbert space. But we will insert a subscript in the ket denoting a *canonical* Hilbert space. Hence, for instance, $|\psi_t\rangle_{H_t}$ will denote a vector on the canonical Hilbert space H_t, while $|\psi\rangle$ will denote a vector on a history Hilbert space $\mathcal{V}$.

Also, operators on canonical Hilbert spaces will carry a hat, while the history ones will be unhatted.

As already seen in the introduction, we use the same symbol (small greek letters) to denote both a proposition and the projector that represents it. We let the meaning be determined by the context.

The notation in Sec. III is more complicated, because of the many spaces involved. Points of the (linear) phase space Γ will be denoted as (q,p). But there is also the space $\tilde{\Gamma}$, which is the

vector space dual of Γ and (if Γ is a Hilbert space) isomorphic to it. Points on this space will be denoted as (χ,ξ): they correspond to elements of the canonical group or labels of coherent state vectors. The latter will often be denoted as $|z\rangle$. The inner product in these spaces, will be denoted by a dot: we will write invariably $q\cdot p$ or $q\cdot\xi$, without reference to whether the arguments are elements of Γ or $\tilde{\Gamma}$. In fact, we shall mostly ignore their distinction.

Paths on Γ will be denoted as $(q,p)(\cdot)$, or $t\to(q_t,p_t)$, or simply γ. Paths on $\tilde{\Gamma}$, corresponding to coherent state histories by $(\chi,\xi)(\cdot)$, or $t\to(\chi_t,\xi_t)$, or simply $z(\cdot)$. We will write $(q,\xi)=\int d\mu(t)q_t\xi(t)$. When we want to emphasize that ξ also acts as a smearing function on q_t we will denote the same object as q_ξ.

II. CONTINUOUS-TIME HISTORIES

A. The basic structure

The temporal logic histories scheme is based on ideas from quantum logic. It seeks to represent the set of all history propositions about a physical system with elements of a lattice, that contains the information about the temporal structure.[8]

Let us denote by T the set of all instants of time (this can be either discrete, or the real line $\mathbf{R}$ or a subset of $\mathbf{R}$). Standard quantum theory is recovered, when we consider that history propositions correspond to projection operators on a Hilbert space $\mathcal{V}$, given by the tensor product $\otimes_{t\in T}H_t$. Here H_t is a *copy* of the Hilbert space of the canonical theory indexed by t.

Self-adjoint operators on this Hilbert space correspond to history observables.

As an example, let us consider the case where T is a finite set. Let $\hat{A}$ be a bounded operator on the Hilbert space H of the canonical theory, and let us denote by $\hat{A}_t$ its copy on a Hilbert space H_t. Then we can define the *product operator* $\otimes_{t\in T}\hat{A}_t$ on $\mathcal{V}$.

If $\hat{A}_t$ is unit everywhere, but a single point $t\in T$, then we shall denote the product operator on $\mathcal{V}$ as A_t. If $f:T\to\mathbf{R}$ then we can define the *time-averaged* operator A_f as

$$A_f=\sum_{t\in T}f(t)A_t. \tag{2.1}$$

It corresponds to the average in time of the family $t\to\hat{A}_t$, with a weight given by the function f. We can easily verify the following identity. If $\hat{A}$ is a self-adjoint operator on H, then its time-averaged counterpart on $\mathcal{V}$ satisfies

$$e^{iA_fs}=\otimes_{t\in T}e^{i\hat{A}f(t)s}. \tag{2.2}$$

We shall use this identity to *define* time-averaged operators in the continuous-time case.

Note also that for the case of projection operators, a map $\hat{\alpha}\to\alpha_t$ provides a continuous embedding of the lattice of propositions at a single moment of time to the lattice of history propositions.

The probabilistic content of the theory is contained in the decoherence functional. This is assumed to satisfy the following conditions:

$$\begin{gathered} d(1,1)=1,\\ d(\alpha,\beta)=d^*(\beta,\alpha),\\ d(0,\alpha)=0,\\ d(\alpha+\beta,\alpha')=d(\alpha,\alpha')+d(\beta,\alpha'),\\ d(\alpha,\alpha)\geqslant 0. \end{gathered} \tag{2.3}$$

In general, there exists a class of operators X on $\mathcal{V}\otimes\mathcal{V}$, such that a decoherence functional can be written as[18,19]

$$d(\alpha,\beta)=\mathrm{Tr}_{\mathcal{V}\otimes\mathcal{V}}(X\alpha\otimes\beta). \tag{2.4}$$

When the space T is finite, the construction of the tensor product Hilbert space is straightforward and Eq. (1.4) can be used to construct the decoherence functional. The question arises then, how one deals with continuous time. This is the case when T is a closed subset of the real line. For particular systems the construction of such Hilbert spaces has been carried in Ref. 12. For more general cases, we believe it is instructive to look at the analogous situation in the classical setting.

B. Classical stochastic processes

Let us assume we have a classical system that at a moment of time is described by a sample space Ω. Let us also consider the space T of time instants to be a closed subset of the real line, say $[0,a]$. The space of histories Π is then some suitable subset of the set Ω^T of all measurable maps $\gamma: T\to\Omega$. If Ω is a vector space one can define a norm on Ω^T, and take as Π the subspace of Ω^T, that contains paths with a finite norm.

A function f on Ω defines a family of functions F_t on Π by

$$F_t(\gamma)=f(\gamma(t)). \tag{2.5}$$

As a stochastic process, we usually define a triplet consisting of the space Π, a family F_t, and a measure $d\mu$ on Π. The issue is how to construct physically interesting measures on Π, which is an infinite dimensional function space.

This is effected as follows: Let dx be for brevity a natural integration measure on Ω (say a Lebesque measure). Let $T=[t_0,t_f]$ be an interval and let us also consider a discretization $I=\{t_0,t_1,\ldots,t_n=t_f\}$ of T. Then define the space of discrete time histories $\Omega^I=\times_{t_j\in I}\Omega_{t_j}$, which is a finite dimensional manifold. This admits the measure $\Pi_{t_j\in I}\,dx_{t_j}$. Any probability distribution $p_I(x_{t_1},\ldots,x_{t_n})$ on Ω^I defines a measure $d\mu(x)=p_I(x_{t_1},\ldots,x_{t_n})\Pi_{t_j\in I}\,dx_{t_j}$.

As we consider all possible discretizations I of T, we can encode a choice of probability measure for each discretization in a hierarchy of positive functions

$$\begin{gathered} p_1(x,t),\\ p_2(x_1,t_1;x_2,t_2),\\ \cdots,\\ p_n(x_1,t_1;\ldots;x_n,t_n),\\ \cdots. \end{gathered} \tag{2.6}$$

These have to be symmetric with respect to interchange of their (x,t) arguments.

Now, the fundamental theorem of Kolmogorov asserts the following: If a hierarchy of functions as above, satisfies the *additivity condition*:

$$\int dx_n\, p_n(x_1,t_1;\ldots;x_{n-1},t_{n-1};x_n,t_n)=p_{n-1}(x_1,t_1;\ldots;x_{n-1},t_{n-1}) \tag{2.7}$$

then there exists an essentially unique probability measure $d\mu(\cdot)$ on Ω^T such that it gives the correct discrete time probability measures, i.e., for each partition I, $j_I^*\,d\mu=d\mu_I$, where j_I is the natural injection map $j_I: I\to T$.

Kolmogorov's proof is standard textbook material and is one instance of a general categorical construction of taking the inductive limit. The essential point in the proof is the fact that j_I is a measurable map (with respect to the Borel sets of T) and as such it respects the measurable structure in the definition of $d\mu$.

Hence a probability measure is defined for continuous time, while making reference only to discrete time expressions. This is the theorem that we will try to employ, in order to construct the decoherence functional for continuous-time histories.

C. The continuum limit

1. The Hilbert space

The first objective would be to define a suitable version of the Hilbert space $\mathcal{V}=\otimes_{t\in T}H_t$. This expression cannot be taken literally, for a continuous tensor product of Hilbert spaces leads to a nonseparable Hilbert space. What we will do is a generalization of an idea that has been applied to ''continuous tensor products'' of Fock spaces.[12]

Consider the space $B(T,H)$ of continuous maps $|\psi(\cdot)\rangle$ from T to H. In fact, we can start our construction considering only measurable maps. But since we will later want to define Stieljes integrals, we should impose the restriction that the maps are of *bounded variation*, i.e., they satisfy the following property.

For any finite discretization of T. $\{t_0\leqslant t_1,\leqslant\cdots\leqslant t_i\leqslant\cdots\leqslant t_n\}$, the sum $\Sigma_{i=1}^{n}\|\psi_{t_i}-\psi_{t_{i-1}}\|_H$ is finite.

Assume that T has a measure $d\mu(t)$, which in the standard case should be taken as dt/τ. Here τ is a time parameter that makes the measure dimensionless. If T is compact it can be used to normalize the measure $\mu(T)=1$.

Then define the inner product

$$\langle\psi(\cdot)|\phi(\cdot)\rangle=\prod_{d\mu(t)}\langle\psi_t|\phi_t\rangle:=\exp\left(\int d\mu(t)\log[\langle\psi_t|\phi_t\rangle_{H_t}]\right), \tag{2.8}$$

where it is understood that the inner product vanishes if $\langle\psi_t|\phi_t\rangle_{H_t}=0$ in a subset of T that is not of measure zero, and that the logarithm takes values on the principal branch.

This space then has a norm $\|\psi(\cdot)\|=(\langle\psi(\cdot)|\psi(\cdot)\rangle)^{1/2}$. We identify two elements $\psi_1(\cdot),\psi_2(\cdot)$ of $B(T,H)$, if $\|\psi_1(\cdot)-\psi_2(\cdot)\|=0$. *This identification makes the resulting Hilbert space separable*.

Let us, suggestively, denote the vector space we obtained after identification, as $\times_{t\in T}H_t$. To construct $\otimes_{t\in T}H_t$ we consider the space of all formal linear combinations $\Sigma_i c_i|\psi_i(\cdot)\rangle$. Here i runs over a finite set, $c_i\in\mathbf{C}$, and $\{|\psi_i(\cdot)\rangle\}$ is a finite set of vectors of $\times_{t\in T}H_t$. On the space of these formal linear combinations we define the inner product as

$$\sum_i \overline{c'}_i c_i\langle\psi_i'(\cdot)|\psi_i(\cdot)\rangle \tag{2.9}$$

and close this space with respect to the norm. We have thus defined a Hilbert space $\otimes_{t\in T}H_t$. Note that the time parameter τ enters explicitly into the definition.

The vectors $|\psi(\cdot)\rangle$ form a total set of $\otimes_{t\in T}H_t$. As such, we can define operators on the history Hilbert space by their action on these vectors.

Some properties of this construction are easy to see. For instance,

$$\otimes_t e^{\lambda_t}|\psi_t\rangle_{H_t}=e^{\int d\mu(t)\lambda(t)}|\psi(\cdot)\rangle. \tag{2.10}$$

Also, if T_1 and T_2 are two disjoint subsets of $\mathbf{R}$ with nonzero measure, then

$$\otimes_{t\in T_1\cup T_2}H_t=(\otimes_{t\in T_1}H_t)\otimes(\otimes_{t\in T_2}H_t). \tag{2.11}$$

2. Time-averaged observables

Let $\hat{A}_t$ be a continuous family of bounded operators on H indexed by t. Then one can define the product operator $\otimes_{t\in T}\hat{A}_t$ by its action on $|\psi(\cdot)\rangle$,

$$(\otimes_{t\in T}\hat{A}_t)|\psi(\cdot)\rangle=\otimes_{t\in T}(\hat{A}_t|\psi_t\rangle_{H_t}). \tag{2.12}$$

This definition is extended by linearity to the whole Hilbert space. However, one has to restrict the families $t\to\hat{A}_t$. We have

$$\begin{aligned}\|(\otimes_{t\in T}\hat{A}_t)|\psi(\cdot)\rangle\|^2&=\exp\left(\int d\mu(t)\log(\langle\psi_t|\hat{A}_t^2|\psi_t\rangle_{H_t})\right)\\&\leqslant\exp\left(\int d\mu(t)\log(\|A_t\|^2\langle\psi_t|\psi_t\rangle_{H_t})\right)\\&=e^{\int d\mu(t)\log(\|\hat{A}_t\|^2)}\langle\psi(\cdot)|\psi(\cdot)\rangle,\end{aligned} \tag{2.13}$$

hence one has to demand that $\int d\mu(t)\log(\|\hat{A}_t\|^2)\leqslant\infty$. If T is a compact subset of $\mathbf{R}$, this holds automatically provided the map $t\to\|\hat{A}_t\|$ is measurable. If T is noncompact, e.g., the whole of $\mathbf{R}$, the right-hand side is not finite and one has to additionally demand that $\hat{A}_t=1$ outside some compact subset of $\mathbf{R}$, or that $\|\hat{A}_t-\hat{1}\|_H$ falls to zero sufficiently rapidly.

It is easy to see that

$$\mathrm{Tr}_{\mathcal{V}}(\otimes_{t\in T}\hat{A}_t)=\prod_{t\in T}(\mathrm{Tr}_{H_t}\hat{A}_t)=\exp\left(\int d\mu(t)\log\mathrm{Tr}_{H_t}\hat{A}_t\right). \tag{2.14}$$

Having defined the product operators we can define time-averaged observables, by exploiting Eq. (2.2). Let $\hat{A}$ be a bounded self-adjoint operator on H. We can write the family $t\to\hat{U}_t(s)=e^{i\hat{A}f(t)s}$ of unitary operators and construct the product operator $U_f(s)=\otimes_{t\in T}\hat{U}_t(s)$. This is well-defined if $f(t)\neq 0$ only within a compact subset of $\mathbf{R}$ and corresponds to a one-parameter group of unitary operators on $\mathcal{V}$. By Stone's theorem, if the matrix elements of this operator are continuous functions of s at $s=0$, there exists a self-adjoint operator A_f such that $U_f(s)=e^{iA_fs}$.

It is easy to check that

$$\langle\phi(\cdot)|U_f(s)|\psi(\cdot)\rangle=\exp\left(\int d\mu(t)\log(\langle\phi_t|e^{i\hat{A}f(t)s}|\psi_t\rangle)\right) \tag{2.15}$$

is a continuous function of s at $s=0$, when the operator $\hat{A}$ is bounded. Thus, given suitable functions f, a self-adjoint operator representing the time average of $\hat{A}$ is well defined on $\mathcal{V}$.

3. Unbounded operators

The construction of time-averaged counterparts to unbounded operators on H is more complicated. From Eq. (2.15) we see that even if the matrix elements $\langle\psi_t|e^{i\hat{A}f(t)s}|\phi_t\rangle_{H_t}$ are continuous functions of s, there is no guarantee that so will be the integral.

Also if $\hat{A}$ is unbounded, there exist vectors $|\psi_t\rangle$, for which the action of $\hat{A}_t$ is not defined, hence one cannot write $|\langle\phi_t|e^{i\hat{A}f(t)s}-1|\psi_t\rangle\leqslant c|s|$, which would be sufficient to prove continuity. There is *no guarantee* that the time average of an unbounded operator is definable.

This is unfortunate, because in physical situations we are interested in operators like position, or momentum, or the Hamiltonian, that are typically unbounded. This failure is due to the fact that the Hilbert space $\otimes_{t\in T}H_t$ is still very large. In concrete physical situations one should identify the histories Hilbert space $\mathcal{V}$ with a closed linear subspace of $\otimes_{t\in T}H_t$.

One has to choose this closed linear subspace, in such a way that the tensor product structure is preserved. The simplest way is to restrict the set of vectors that can be used to construct the "paths" $|\psi(\cdot)\rangle$ to a subset $\mathcal{L}$ of H. This set $\mathcal{L}$ has to be sufficiently large to be able to capture all physical information from H (it cannot be a subspace of H), but small enough to allow interesting operators to be definable on the history Hilbert space. A good choice for $\mathcal{L}$ is an overcomplete and continuous family of vectors, like the coherent states.

Having chosen $\mathcal{L}$, the construction proceeds as before, only we substitute $B(T,H)$ with $B(T,\mathcal{L})$: the space of all continuous maps from T to $\mathcal{L}$. It is easy to check that the resulting Hilbert space is a closed linear subspace of $\otimes_{t\in T}H_t$.

If we demand that a particular unbounded operator A exists (time averaged) in our Hilbert space, it would be necessary to take $\mathcal{L}$ consisting of vectors in the domain of A. In that case the matrix elements (2.15) would be a continuous function of s and (by Stone's theorem) A_f would exist. We shall see how this construction works in more detail, in Sec. III. In this section, we shall work with the larger Hilbert space $\otimes_{t\in T}H_t$. All results we obtain will be valid for any of its physically relevant subspaces.

4. The decoherence functional

If T is compact, one can choose $A_t=A$ for all t and therefore interpret A_f as the time average of the quantity associated to A. But, if we try to define an operator on $\mathcal{V}$, that corresponds to an observable at a *sharp* moment of time, we run into problems. Since a point in the real axis is of measure zero, an observable defined at a sharp moment of time can exist only if we can take f to be a delta function. This is unacceptable in our construction. We conclude that one *cannot embed continuously the lattice of single-time propositions into the lattice of history propositions*, in the case of continuous time.

Let us now examine the possibility of defining a decoherence functional for continuous-time histories as a continuous limit of the discrete-time expression (1.4). Let us assume a partition $I=\{t_1,\ldots,t_n\}$ of an interval T of the real line and a proposition $\alpha=\alpha_{t_1}\otimes\ldots\otimes\alpha_{t_n}$ that is a projector operator on $H^I=\otimes_{t_i\in I}H_{t_i}$. Then one can construct the class operator $\hat{C}_\alpha$ defined on one copy of H as in Eq. (1.1). The value of decoherence functional $d_{I,I'}$ between a history on H^I and another on some other discrete-time Hilbert space $H^{I'}$ is given by Eq. (1.4).

The aim is to generalize Kolmogorov's theorem in this histories setting. We want to construct a bilinear, Hermitian, additive map on the space $P(\mathcal{V})\times P(\mathcal{V})$ [by $P(H)$ we mean the lattice of projectors on the Hilbert space H]. If we consider then a pair of discretizations I and I' of T, we can costruct the Hilbert spaces H^I and $H^{I'}$. The point is whether there exist an injection map $j_{I,I'}: H^I\times H^{I'}\to\mathcal{V}\times\mathcal{V}$; if this exists and preserves the lattice structures then Kolmogorov's proof goes through and the decoherence functional d on H^T exists as an inductive limit of the decoherence functional defined on $H^I\times H^{I'}$ for all choices of I and I'. We would also have $d_{I,I'}=j^*_{I,I'}d_T$.

For the map to be lattice preserving it would have to be continuous. But, we showed earlier, that this cannot be true for a single moment of time. The map $j_{I,I'}$ might be continuous in the weak topology, but this is insufficient to define an order preserving map. Recall that the continuity of the Hilbert space enters in a decisive point in the definition of the lattice of propositions: a projection operator corresponds to a *closed* linear subspace. Hence Kolmogorov's theorem does not go through in this case.

But if we restrict to an Abelian sublattice (for instance, to propositions about position) the map $j_{I,I'}$ does not need to be a continuous, linear map, but simply a measurable map from the spectra of the corresponding operators $\mathbf{R}^I\times\mathbf{R}^{I'}$ to $\mathbf{R}^T\times\mathbf{R}^T$. This clearly exists; it is the same as in the case of classical probability theory.

We therefore conclude that *one cannot write the decoherence functional for continuous time, as a limit of discrete-time ones*, unless one restricts to Abelian subalgebras. We might have a continuous-time decoherence functional for each subalgebra, but not one defined on the whole of

$P(\mathcal{V})$. We shall return to this issue again and propose two different ways, by which the decoherence functional can be defined.

D. The structure of the decoherence functional

The presence of two laws of time transformation is an important structural feature of history theories. In this section, we shall show how they are manifested in the probability assignment. We shall see that the decoherence functional for discrete time can be written in such a way, that these two notions of time are distinctly represented. This is a feature, that in the canonical theory is reflected in the distinction between the geometric and dynamical phase.[16] We shall attempt to generalize this feature in the continuous-time case.

For simplicity we shall consider a special class of decoherence functionals. They are of the type (1.4), but with $\hat{\rho}_0$ corresponding to a pure state. This means that we can absorb the projector into the initial state as part of the definition of each history and as such write the decoherence functional in the form

$$d(\alpha,\beta)=\mathrm{Tr}_H(\hat{C}_\alpha^\dagger \hat{C}_\beta). \tag{2.16}$$

Clearly one of the single-time projectors has to be trace-class if the above expression is to be finite. Equation (2.16) can be written as[18]

$$d(\alpha,\beta)=\mathrm{Tr}_{H\otimes H}(Z\hat{C}_\alpha^\dagger\otimes \hat{C}_\beta), \tag{2.17}$$

where Z is an operator on $H\otimes H$ given by

$$Z(|i\rangle\otimes|j\rangle)=|j\rangle\otimes|i\rangle. \tag{2.18}$$

One can write $Z=\Sigma_{rs}\hat{A}^{rs}\otimes\hat{A}^{\dagger rs}$ in terms of a basis on H, where $\hat{A}^{rs}$ is an operator on H with matrix elements

$$\langle k|\hat{A}^{rs}|i\rangle=\delta_{ks}\delta_{ri}. \tag{2.19}$$

Let us now assume that both histories are defined in the same instants of time $t_0,t_1,\ldots,t_n$. Let us for simplicity take $t_0=0$. The corresponding history Hilbert space is then $\mathcal{V}=\otimes_i H_{t_i}$.

Let us also write the *boundary Hilbert space* $\partial\mathcal{V}=H_{t_0}\otimes H_{t_n}$. The indices rs of the operators $\hat{A}^{rs}$ are then indices corresponding to $\partial\mathcal{V}$. It is easy to verify that the expression (2.17) can be written as a trace over the boundary Hilbert space[14]

$$d(\alpha,\beta)=\mathrm{Tr}_{\partial\mathcal{V}}(c(\alpha)c^\dagger(\beta)), \tag{2.20}$$

where $c(\alpha)$ is an operator on $\partial\mathcal{V}$ defined by

$$c(\alpha)=\mathrm{Tr}_H\hat{A}\hat{C}_\alpha^\dagger. \tag{2.21}$$

$\hat{A}$ denotes here a map from H to $\mathcal{V}$. It is easy now to write $c(\alpha)$ as a trace over the history Hilbert space, through the introduction of the *unitary* operator $\mathcal{S}$ on $\mathcal{V}$,

$$\mathcal{S}|v_{t_0}\rangle|v_{t_2}\rangle\cdots|v_{t_n}\rangle=|v_{t_n}\rangle|v_{t_0}\rangle\cdots|v_{t_{n-1}}\rangle. \tag{2.22}$$

Indeed, since $\alpha=\hat{\alpha}_{t_0}\otimes\hat{\alpha}_{t_1}\otimes\cdots\otimes\hat{\alpha}_{t_n}$, we can write

$$c(\alpha)=\mathrm{Tr}_{\mathcal{V}}(\mathcal{A}\mathcal{S}\mathcal{U}^\dagger\alpha\mathcal{U}), \tag{2.23}$$

where

$$\mathcal{U}=\hat{U}(t_0)\otimes\hat{U}(t_1)\cdots\otimes\hat{U}(t_n), \tag{2.24}$$

$$\mathcal{A}=\hat{A}\otimes 1\otimes\cdots\otimes 1. \tag{2.25}$$

This accomplishes the task of writing the decoherence functional in such a way as the two different notions of time are made manifest. The operator $\mathcal{U}$ clearly contains the dynamics. The operator $\mathcal{S}$ induces a transformation that takes from a single-time Hilbert space to the next one. Finally, the operators A incorporate the information about the beginning and the end of the interval. Had we kept the initial density matrix, $\hat{A}$ would explicitly depend upon it. In that case the analog of Eq. (2.19) would be

$$\langle k|\hat{A}^{rs}|i\rangle=\delta_{ks}(\rho_0^{1/2})_{ri}\,. \tag{2.26}$$

E. The continuum limit

Let us now examine whether one can construct these operators in the continuous-time Hilbert space $\otimes_{t\in T}H_t$, which we defined earlier.

The operator $\mathcal{U}$ is relatively easy to define. It would act on a vector $|\psi(\cdot)\rangle$ as

$$\mathcal{U}|\psi(\cdot)\rangle=\otimes_{t\in T}(e^{-i\hat{H}t}|\psi_t\rangle_{H_t}). \tag{2.27}$$

This would have as matrix elements

$$\langle\phi(\cdot)|\mathcal{U}|\psi(\cdot)\rangle=\exp\left(\int d\mu(t)\log\langle\phi_t|e^{-i\hat{H}t}|\psi_t\rangle\right). \tag{2.28}$$

According to our previous analysis this is a genuine unitary operator on $\mathcal{V}$.

1. The geometric phase

The operator $\mathcal{S}$ has an important geometric significance. It incorporates information about the geometric phase[20,21] that is associated to a history. To see this, one has first to recall that a Hilbert space H is a line bundle over the projective Hilbert space PH, i.e., the equivalence class of all vectors that differ by a multiplication with a complex number. We shall denote an element of PH as $[\psi]$. The inner product on H inherits two important geometric structures on PH: a metric

$$ds^2=\|d|\psi\rangle\|^2-|\langle\psi|d|\psi\rangle|^2, \tag{2.29}$$

and a $U(1)$ connection

$$A=-i\langle\psi|d|\psi\rangle. \tag{2.30}$$

When a point of PH evolves along a loop γ, its total phase change consists of a piece that depends upon the dynamics and a piece that is essentially the holonomy of the connection A.[22,23] This is known as the Berry phase and equals

$$e^{i\theta_g[\gamma]}=e^{i\int_\gamma A}=\exp\left(\int\langle\psi|d|\psi\rangle\right). \tag{2.31}$$

The geometric phase can also be defined for open paths. The trick is that any path on the projective Hilbert space can be closed by joining its endpoints with a geodesic, with respect to the natural metric. The geometric phase of the loop thus constructed is then *defined* to equal the geometric phase associated to the open path. Hence if $\gamma=[\psi(\cdot)]$ is a path on PH its associated geometric phase can be found[24]

$$e^{i\theta_g[\gamma]} = \exp\left(\int_{t_i}^{t_f} dt \langle \psi(t) | \dot{\psi}(t) \rangle \right) \langle \psi_i | \psi_f \rangle. \tag{2.32}$$

This expression is defined only if the endpoints are not orthogonal.

Now let us consider a discretized approximation to an element $|\psi(\cdot)\rangle$ of $\mathcal{V}$. Let us write therefore,

$$\alpha = \otimes_{t_j} |\psi_{t_j}\rangle\langle\psi_{s_j}|, \tag{2.33}$$

where $|\psi_{t_j}\rangle$ are normalized vectors on H_{t_j}.

We then calculate

$$\mathrm{Tr}(\mathcal{S}\alpha) = \langle \psi_{t_0} | \psi_{t_n} \rangle \langle \psi_{t_1} | \psi_{t_0} \rangle \langle \psi_{t_2} | \psi_{t_1} \rangle \cdots \langle \psi_{t_n} | \psi_{t_{n-1}} \rangle. \tag{2.34}$$

Let us then assume that $\max|t_j - t_{j-1}| = \delta t$, and we choose the number of time steps n very large, so that $\delta t \sim O(n^{-1})$. Then $|\psi_{t_j}\rangle$ approximates a path $[\psi(t)]$ on PH. Writing formally $\alpha_{\psi(\cdot)}$ for the projector we get

$$\begin{aligned} \log \mathrm{Tr}(\mathcal{S}\alpha_{\psi(\cdot)}) &= \log\langle \psi_{t_0} | \psi_{t_n} \rangle + \sum_{i=1}^{n} \log\langle \psi_{t_i} | \psi_{t_{i-1}} \rangle \\ &= \log\langle \psi_{t_0} | \psi_{t_n} \rangle + \sum_{i=1}^{n} \log(1 - \langle \psi_{t_i} | \psi_{t_i} - \psi_{t_{i-1}} \rangle), \end{aligned} \tag{2.35}$$

which in the limit of large n yields

$$\log \mathrm{Tr}(\mathcal{S}\alpha_{\psi(\cdot)}) = \log\langle \psi_{t_0} | \psi_{t_n} \rangle - \sum_{i=1}^{n} \langle \psi_{t_i} | \psi_{t_i} - \psi_{t_{i-1}} \rangle + O((\delta t)^2). \tag{2.36}$$

As $\delta t \to 0$ the sum in the right-hand side converges to a Stieljes integral $-\int_{t_i}^{t_f} dt \langle \psi(t) | \dot{\psi}(t) \rangle$ and hence

$$\mathrm{Tr}(\mathcal{S}\alpha_{\psi(\cdot)}) = e^{i\theta_g[\psi(\cdot)]}. \tag{2.37}$$

This is the Berry phase associated to the path $\psi(\cdot)$. This implies that $\mathcal{S}$ exists as an operator on $\mathcal{V}$. Its matrix elements can be defined as

$$\langle \phi(\cdot) | \mathcal{S} | \psi(\cdot) \rangle = \langle \phi(t_0) | \psi(t_f) \rangle \exp\left(\int \langle \psi(t) | d | \psi(t) \rangle \right), \tag{2.38}$$

where the integral in the exponential is of the Stieljes type (rather than of the Lebesque, that was used in the definition of $\otimes_{t \in T} H_t$). The Stieljes integral is defined for all measurable functions of bounded variation. Hence the matrix elements of $\mathcal{S}$ are finite. This implies, it is a well-defined bounded operator and it is easy to check that it remains unitary even in the continuous limit.

2. Another attempt to construct the decoherence functional

We have shown that the main operators that form the decoherence functional exist in the continuous limit. Could we then proceed and define a continuous-time decoherence functional from Eq. (2.20)? The answer is no, at least not straightforwardly. The problem is that the analog of the maps $\mathcal{A}$ does not exist in the continuous limit. The reason is the same as before: an embedding of single-time Hilbert spaces to the history Hilbert space fails to be continuous.

Therefore, one has two options. First, it should be noted that an initial and final moment of time is necessary in the decoherence functional, because they incorporate information about the

preparation of the system. From an operational viewpoint, one could then say that the specification of an initial state cannot be sharp in time and as such they should be incorporated in the decoherence functional by an object that is extended in time. This would imply a generalization of expression (2.23), where the map $\mathcal{A}$ is defined from $\mathcal{V}$ not to $\partial\mathcal{V}$, but to some other Hilbert space, which is associated with a finite time subinterval of T. The introduction of such an operator could provide a construction of a continuous decoherence functional in this case. This would be mathematically well defined and operationally meaningful, but would diverge from the standard canonical quantum theory. For this reason, we shall not pursue this further in this paper.

An alternative would be to abandon the effort to define a continuous decoherence functional and assume at most weak continuity.

If we assume two one-dimensional projectors $\alpha_{\psi(\cdot)}$ and $\alpha_{\psi(\cdot)}$ we get an expression for the decoherence functional with zero Hamiltonian

$$d(\alpha_{\psi(\cdot)},\alpha_{\psi(\cdot)}) = \langle\psi(t_i)|\hat{\rho}_0|\psi(t_i)\rangle\langle\psi(t_f)|\psi(t_f)\rangle \times \exp\left(\int_{t_i}^{t_f} dt\langle\psi(t)|\dot{\psi}(t)\rangle - \int_{t_i}^{t_f} dt\langle\dot{\psi}(t)|\psi(t)\rangle\right). \tag{2.39}$$

In the special case where $\hat{\rho}_0 = |\psi(t_i)\rangle\langle\psi(t_i)| = |\psi(t_i)\rangle\langle\psi(t_i)|$ and $|\psi(t_f)\rangle\langle\psi(t_f)| = |\psi(t_f)\rangle\langle\psi(t_f)|$ its value is equal to

$$d(\alpha_{\psi(\cdot)},\alpha_{\psi(\cdot)}) = e^{i\theta_g[\psi(\cdot),\psi(\cdot)]}, \tag{2.40}$$

the Berry phase for the *loop* formed from $\psi(\cdot)$ and $\psi(\cdot)$, since now they have the same endpoints.

More interestingly, when the Hamiltonian is included the decoherence functional becomes

$$d(\alpha_{\psi(\cdot)},\alpha_{\psi(\cdot)}) = \langle\psi(t_i)|\hat{\rho}_0|\psi(t_i)\rangle\langle\psi(t_f)|\hat{\rho}_f|\psi(t_f)\rangle e^{iS[\psi(\cdot)]-iS^*[\psi(\cdot)]}, \tag{2.41}$$

where the action is given by the familiar expression (its variation gives the Schrödinger equation)

$$S[\psi(\cdot)] = \int_{t_i}^{t_f} dt\langle\psi(t)|i\frac{d}{dt} - H|\psi(t)\rangle. \tag{2.42}$$

One might then give Eq. (2.41) as a *definition* of a decoherence functional for pairs of one-dimensional projectors and then extend this definition by finite addition to projectors with finite trace. But there is no *a priori* guarantee that one would thus construct an object taking finite values to a general projector on $\otimes_{t\in T}H_t$. Nonetheless, Eq. (2.41) *highlights the importance of the action as the object relating kinematics, dynamics and the probabilistic structure of quantum theory*.

We shall return to the issue of the definition of a continuous-time decoherence functional in Sec. III E 3.

F. Time reversal

A symmetry on a history Hilbert space is represented either by a unitary or an antiunitary operator. This has been established by Schreckenberg.[25]

Of particular interest are the time-reversal transformations. In discrete time they are defined by[12]

$$\mathcal{T}|v_{t_1}\rangle|v_{t_2}\rangle\cdots|v_{t_n}\rangle = |v_{t_n}\rangle|v_{t_{n-1}}\rangle\cdots|v_{t_1}\rangle. \tag{2.43}$$

Clearly

$$\mathcal{T}\mathcal{T}^\dagger = 1, \tag{2.44}$$

$$\mathcal{T}\mathcal{S}\mathcal{T}^{\dagger}=\mathcal{S}^{\dagger}. \tag{2.45}$$

Also for the operator $\mathcal{U}$ defined by (2.24) we have

$$\mathcal{T}\mathcal{U}\mathcal{T}^{\dagger}=e^{-i\hat{H}t_n}\otimes\cdots\otimes e^{-i\hat{H}t_1} \tag{2.46}$$

and when time runs in the full real line

$$\mathcal{T}\mathcal{U}\mathcal{T}^{\dagger}=\mathcal{U}^{\dagger}. \tag{2.47}$$

Finally for the time-inverted projection operators $\alpha^T=\mathcal{T}\alpha\mathcal{T}^{\dagger}$ (corresponding to homogeneous histories) we have

$$d(\alpha^T,\beta^T)=\mathrm{Tr}(\hat{C}_{\alpha}^{T\dagger}\rho_0\hat{C}_{\beta}^{T}\rho_f), \tag{2.48}$$

where $\hat{C}_{\alpha}^{T}=\hat{\alpha}_{t_1}(t_n)\cdots\hat{\alpha}_{t_n}(t_1)$. In the discrete case this form is not transparent, but when time takes values in all $\mathbf{R}$ the Heisenberg picture operators transform as $\alpha_t(t)\rightarrow\alpha_t(-t)$ and therefore

$$d(\alpha^T,\beta^T)=d(\beta,\alpha)=[d(\alpha,\beta)]^*. \tag{2.49}$$

Of course this later equation does not hold if the Hamiltonian is time dependent and the system is not time homogeneous.

The operator $\mathcal{T}$ is naturally defined also on $\otimes_{t\in\mathbf{R}}H_t$,

$$\mathcal{T}\,|\psi(\cdot)\rangle=\mathcal{T}\,|\psi(-\cdot)\rangle. \tag{2.50}$$

It is important to note that the time-reversal operator is linear rather than antilinear as in canonical quantum mechanics. This has again to do with the presence of two laws of time transformations in history theories; here time reversal implemented by $\mathcal{T}$ corresponds to the causal, kinematical properties of time. The time inversion operator of canonical quantum mechanics is obtained by the study of the Schrödinger equation and as such is clearly associated to the dynamical aspect of time.

Of course we can always define an antilinear time-reversal operator in complete analogy with the canonical case; a complex conjugation on H naturally defines a complex conjugation on $\mathcal{V}$. It would act on the Heisenberg picture operators as $\alpha_t(t)\rightarrow\alpha_t(-t)$.

G. Summary

Let us summarize here the results of this section. We showed how a Hilbert space $\otimes_{t\in T}H_t$ for continuous time histories can be constructed and how time-averaged observables can be defined as operators acting on it. Then we argued that in general we will have to restrict to a particular subset of $\otimes_{t\in T}H_t$. We then showed that the decoherence functional cannot be defined as a limiting case of its discrete-time form.

We then analyzed the structure of the decoherence functional. We identified the pieces out of which it is constructed, in light of the two laws of time transformation of history theories, and showed their relation to the dynamical and geometric phase of canonical quantum theory. We discussed a possible way to construct the continuous-time decoherence functional and finally saw how *unitary* time-reversal transformations are implemented in this scheme.

III. PHASE SPACE HISTORIES

In the preceding section we examined the general structure of continuous-time histories, without making any reference to a particular physical system, or class of systems. In order to do so, we necessarily have to make reference to a corresponding classical system and seeks to

identify operators on the Hilbert space with observables that have a classical analog. This is, in effect, the *quantization* procedure. In this section, we will study how the classical phase space structure is manifested in the histories formalism.

We refer the reader to Sec. I C 1 for explanation of the notations we will use in this section.

A. The canonical group

1. The Weyl group

In quantum theory the information about the corresponding classical theory can be encoded in the *canonical group*. This is classically identified as a group that acts transitively by canonical transformations on the classical phase space Γ.[26] When $\Gamma=\mathbf{R}^{2n}$ the canonical group is the $(2n+1)$-dimensional Weyl group. This is defined whenever the phase space has a vector space structure. It can therefore be infinite dimensional, as in a field theory. For its definition an inner product on Γ has to be assumed, so we usually consider Γ to be a real Hilbert space.

The Weyl group is generated by $q_i, p_i, 1$ and has basic Lie algebra relations

$$\{q_i, q_j\}=0, \tag{3.1}$$

$$\{p_i, p_j\}=0, \tag{3.2}$$

$$\{q_i, p_j\}=\delta_{ij}. \tag{3.3}$$

A generator of the Weyl group reads $\chi\cdot p+\xi\cdot q+c$, in terms of the inner product in Γ, and is labeled by (χ_i,ξ_i,c). The corresponding group element will be denoted as (χ,ξ,c). The group multiplication law is

$$(\chi_1,\xi_1,c_1)\cdot(\chi_2,\xi_2,c_2)=(\chi_1+\chi_2,\xi_1+\xi_2,c_1+c_2+\tfrac{1}{2}(\xi_1\cdot\chi_2-\xi_2\cdot\chi_1)). \tag{3.4}$$

When the canonical group has been identified, the Hilbert space of the theory is constructed through the selection of one of its unitary *irreducible* representations. The criterion for this selection is the existence of self-adjoint operators that correspond to the generators of classical symmetries (e.g., the Hamiltonian, the Lorentz group, etc.).

2. Coherent states

Suppose we have a representation of the canonical group by unitary operators $\hat{U}(g)$ on a Hilbert space. Furthermore, let $\hat{h}$ denote the Hamiltonian of this system and by $|0\rangle_H$ the vacuum, i.e., the Hamiltonian's lowest eigenstate. Then we define the coherent states as the vectors

$$|g\rangle=\hat{U}(g)|0\rangle. \tag{3.5}$$

Now consider the equivalence relation on the canonical group defined as $g\sim g'$ if $|g\rangle$ and $|g'\rangle$ correspond to the same ray. The phase space Γ is identified as the quotient space $G/\sim$ and we can label a coherent state by points $z\in\Gamma$.

Hence the canonical group defines a map $i:\Gamma\to PH$ as $z\to|z\rangle$. As we explained PH has a natural metric and a $U(1)$ bundle structure with a connection. These structures can be pullbacked to Γ with i^*. We have then on Γ a $U(1)$ bundle with a connection A given by

$$A=-i\langle z|d|z\rangle \tag{3.6}$$

and a metric

$$ds^2=\|d|z\rangle\|^2-|\langle z|d|z\rangle|^2, \tag{3.7}$$

where d is the exterior derivative on Γ. The fundamental property of coherent states is that they are an overcomplete basis; i.e., any vector $|\Psi\rangle$ can be written as

$$|\Psi\rangle = \int d\mu(z) f(z) |z\rangle, \tag{3.8}$$

in terms of some complex-valued function f on Γ. Here $d\mu$ denotes some natural measure on Γ. In n dimensions it equals $d^n\overline{z}\,dz/(2\pi)^n$. There is also a decomposition of the unity

$$\int d\mu(z) |z\rangle\langle z| = \hat{1}. \tag{3.9}$$

If the phase space Γ has a vector space structure the canonical group is the Weyl group. Its most usual representation is on $e^{\Gamma_C} = \oplus_{n=1}^{\infty} (\otimes_n H)_S$, the symmetric Fock space generated by the complex vector space Γ_C, a complexification of Γ.[27,28] On the Fock space there exist the unnormalized coherent states $|\exp z\rangle$ that to each $z \in \Gamma_C$ they assign the vector $|\exp z\rangle = \oplus_{n=0}^{\infty} \otimes_n z$. The inner product of such states is given by

$$\langle \exp z' | \exp z \rangle = e^{(z', z)_C}, \tag{3.10}$$

where $(\,,\,)_C$ denotes an inner product on Γ_C (its choice depends upon the way Γ is complexified). The corresponding normalized states are denoted simply as $|z\rangle$, or $|\chi, \xi\rangle$.

3. The overlap kernel

For the finite-dimensional Weyl group, the Stone–von Neumann theorem asserts that all irreducible representations are unitarily equivalent to the Fock one. This is not true in infinite dimensions. In this case, the information about the representation is encoded in the coherent states overlap $\langle \chi' \xi' | \chi \xi \rangle$.

This is determined by the expectation functional $K(\chi, \xi) = \langle 0 | \chi, \xi \rangle$ as a consequence of the group combination law

$$\langle \chi' \xi' | \chi \xi \rangle = e^{i/2(\chi \cdot \xi' - \xi \cdot \chi')} K(\chi - \chi', \xi - \xi'). \tag{3.11}$$

The expectation functional suffices to describe the connection and metric structure on phase space. If we write $K = e^W$, we find

$$A = \xi_i d\chi^i, \tag{3.12}$$

$$ds^2 = -\mathrm{Re}\left(\frac{\partial^2 W}{\partial \chi^i \partial \chi^j} d\chi^i\, d\chi^j + \frac{\partial^2 W}{\partial \xi^i \partial \xi^j} d\xi^i\, d\xi^j + \left(\frac{\partial^2 W}{\partial \chi^i \partial \xi^j} + \frac{\partial^2 W}{\partial \chi^j \partial \xi^i} \right) d\chi^i\, d\xi^j \right). \tag{3.13}$$

In the case of an harmonic oscillator with frequency ω, the functional W reads

$$W(\chi, \xi) = -\tfrac{1}{2}[\omega \chi^2 + \omega^{-1} \xi^2]. \tag{3.14}$$

The knowledge of the overlap suffices to construct the Hilbert space and the representation.[29]

A vector of the Hilbert space can be constructed as a function on phase space of the form $\Psi(\chi, \xi) = \Sigma_l c_l \langle \chi \xi | \chi_l \xi_l \rangle$ for a finite number of complex numbers c_l and χ_l, ξ_l. The inner product between two vectors characterized by c_l, χ_l, ξ_l and c_l', χ_l', ξ_l' is

$$\sum_l c_l'^{*} c_l \langle \chi_l' \xi_l' | \chi_l \xi_l \rangle. \tag{3.15}$$

The Weyl group is then represented by the operators $\hat{U}(\chi, \xi)$, which are defined as

$$(\hat{U}(\chi', \xi')\Psi)(\chi, \xi) = e^{(i/2)(\chi' \cdot \xi - \xi' \cdot \chi)} \Psi(\chi - \chi', \xi - \xi'). \tag{3.16}$$

The above equation is written for the finite-dimensional Weyl group, but with little modification is also valid for the infinite-dimensional case. The only difference is that in finite dimensions the Stone–von Neumann theorem holds: *all irreducible, strongly continuous, unitary representations of the Weyl group, are unitarily equivalent.*

In the infinite-dimensional case the vector space out of which the Weyl group is constructed is a functional space. For field theories in Minkowski spacetime this is a subspace of the space of square integrable functions on $\mathbf{R}^3$. In this case, the group of spatial translations is also represented unitarily on the Hilbert space. If the vacuum is the *unique translationary invariant state* in the representing Hilbert space, then it can be proven that *all unitarily equivalent representations share the same expectation functional*, and conversely, if two representations differ in their expectation functionals, they are unitarily inequivalent.[30] We shall refer to this as the *uniqueness theorem* for the expectation functional.

B. Classical histories

In order to study the phase space structure of quantum mechanical histories, we need to describe histories in classical mechanics in a way that is amenable to a direct comparison. We shall, therefore, reproduce here the main points of this description, referring the reader to Refs. 11 and 15 for details.

Consider the space of classical histories Π viewed as the set of continuous paths on the classical phase space Γ. An element of Π is a path $\gamma: T\to\Gamma$.

For any function f on Γ one can define a family of functions F_t on Π as

$$F_t(\gamma)=f(\gamma(t)). \tag{3.17}$$

Taking for simplicity $\Gamma=\mathbf{R}\times\mathbf{R}=\{(q,p)\}$, we can define q_t and p_t as elements of $C^\infty(\Pi)$ through

$$q_t(\gamma)=q(\gamma(t)), \tag{3.18}$$

$$p_t(\gamma)=p(\gamma(t)). \tag{3.19}$$

Two other functions on Π can be identified

$$V(\gamma)=\int_T dt\, p_t\dot{q}_t(\gamma), \tag{3.20}$$

$$H(\gamma)=\int_T dt\, h(p_t,q_t), \tag{3.21}$$

with h denoting the standard canonical Hamiltonian. If we furthermore equip Π with a symplectic form

$$\omega=\int dt\, dp_t\wedge dq_t, \tag{3.22}$$

corresponding to the Poisson bracket

$$\{q_t,p_{t'}\}=\delta(t,t'), \tag{3.23}$$

we can examine the canonical transformations generated by the functions V and H. These are the generators of the two distinct laws of time transformation that characterize history theories.

The transformations generated by V perform translations of the t argument in a path, that is $\gamma\to\gamma'$ with $\gamma'(t)=\gamma(t+s)$ (s is the affine parameter of the corresponding one-parameter group) or in its induced action on the functions

$$F_t \to F_{t+s}. \tag{3.24}$$

H respects the time labelling of the points of the path. It acts on each point of the path by transforming it (while keeping t fixed) according to Hamilton's equations. This means its action on $C^\infty(\Pi)$ is

$$(q_t, p_t) \to (q_t(s), p_t(s)), \tag{3.25}$$

where $q_t(s)$ is the function that to each path γ assigns the q coordinate of the point obtained by integrating the Hamilton equations from initial point with coordinates (q_t, p_t) to time s; similarly for $p_t(s)$.

In the classical setting this distinction of two laws of time transformation, is nicely related to the least action principle. A path γ is a solution to the classical equations of motions iff it is a fixed point of the canonical transformation generated by the action $S=V-H$. This implies the condition

$$\{q_t, S\}(\gamma) = \{p_t, S\}(\gamma) = 0. \tag{3.26}$$

Hence for the solutions to the equations of motion the laws of time evolution generated by V and H coincide.

C. The history group

The construction of the history Hilbert space through the tensor product of single-time Hilbert spaces suggests a natural generalization; the history Hilbert space has to carry the representation of the history group, the history analog of the canonical group.[12] This is a group that acts by symplectic transformations on the space of phase space histories. For linear phase spaces this is

$$[q^i_t, p^j_{t'}] = i\,\delta^{ij}\delta(t,t'). \tag{3.27}$$

It is clearly an infinite-dimensional Weyl group. Its proper definition involves a choice of smearing functions: we define $q_\xi = \int d\mu(t)\xi_i(t)q^i_t$ and p_χ similarly, and write the commutator as

$$[q_\xi, p_\chi] = i\int d\mu(t)\chi(t)\cdot\xi(t). \tag{3.28}$$

The precise choice of a test-function space depends on the physics of the system, but it definitely has to consist of square-integrable functions, if the right-hand side of (3.28) is to be defined. Here $d\mu$ stands for any measure on the real line, but what is mainly used is the measure employed in the construction of $\otimes_t H_t$, i.e., $d\mu(t) = dt/\tau$.

This history group is an infinite-dimensional Weyl group and admits many unitarily inequivalent representations.

The analysis of the classical histories suggests the criterion for selecting a representation. *There should exist self-adjoint operators in the Hilbert space, that correspond to the functions V and H of the classical theory*. For quadratic Hamiltonians, a Fock representation (that has the structure of a continuous tensor product) can be constructed,[13] in which both the Hamiltonian H_κ and an operator corresponding to V (the Liouville operator) exist. An important feature of this construction is the existence of a Hilbert space vector $|0\rangle$, which is the lowest eigenstate of the Hamiltonian and is left invariant under the action of e^{isV}.[13,10] The projector $|0\rangle\langle 0|$ corresponds to the proposition that at all times the systems is to be found in the ground state.

Another important feature of this construction is the fact that *the continuous tensor product of coherent states of the harmonic oscillator exists as a coherent state in the Fock–Hilbert space*. This is a feature that can be generalized for systems with nonquadratic Hamiltonian. Indeed, it will form the basis of our construction.

1. General representations

Representations cannot be explicitly constructed for nonquadratic Hamiltonians (it is the same situation with the one in canonical quantum field theory). Nonetheless, if we have some information about the canonical theory, we can exploit this to construct representations for the history group.

As we explained in Sec. II C, unbounded operators can be defined on a history Hilbert space, if we start our construction from a subset $\mathcal{L}$ of the Hilbert space. Since we want a Hilbert space that carries a representation of the history group, the natural choice for $\mathcal{L}$ would be the coherent states of the corresponding canonical group. If H carries a representation of the canonical group $\hat{U}(\chi,\xi)$ and $\hat{h}$ is the Hamiltonian with a unique ground state $|0\rangle_H$, we define the canonical coherent states $|z\rangle=|\chi\xi\rangle=\hat{U}(\chi,\xi)|0\rangle_H$. Then the history Hilbert space $\mathcal{V}$ is generated by all vectors

$$|z(\cdot)\rangle=|\chi(\cdot)\xi(\cdot)\rangle:=\otimes_{t\in T}|\chi_t\xi_t\rangle_{H_t}. \tag{3.29}$$

Furthermore, we demand that the vectors $|z(\cdot)\rangle$ on $\mathcal{V}$ are the coherent states associated with the corresponding history group. In this case we shall have a history overlap kernel

$$\langle\chi'(\cdot)\xi'(\cdot)|\chi(\cdot)\xi(\cdot)\rangle=\exp\left(\int d\mu(t)\log(\langle\chi'_t\xi'_t|\chi_t\xi_t\rangle_{H_t})\right). \tag{3.30}$$

The corresponding expectation functional $K_h[\chi(\cdot),\xi(\cdot)]=e^{W_h[\chi(\cdot),\xi(\cdot)]}$ will read in terms of the canonical expectation functional $K(\chi,\xi)=e^{W[\chi,\xi]}$,

$$W_h[\chi(\cdot),\xi(\cdot)]=\int d\mu(t)W[\chi_t,\xi_t]. \tag{3.31}$$

Clearly certain conditions have to be imposed on the admissible paths $(\chi,\xi)(\cdot)$ if the integral is to be finite. (We shall take $T=\mathbf{R}$ without any loss of generality in this section.)

Now, there exists a norm $|\cdot|_\Gamma$ on the phase space [it can be constructed from the metric (3.7) or from the inner product]. This induces a norm in the space of paths $t\to z_t$, which is given by

$$|z(\cdot)|_\Pi=\int d\mu(t)|z_t|_\Gamma. \tag{3.32}$$

Our first restriction, will be to consider only continuous paths with a finite value for the norm. For simplicity we shall assume that the maps $z(\cdot)$ take values (0,0) except within compact subsets of $\mathbf{R}$. But we expect that our results would still be valid, if the paths $x(\cdot)$ converge to (0,0) sufficiently fast (exponentially) outside compact sets.

We shall also assume that the canonical coherent states, viewed as maps from the phase space to H are smooth functions of their arguments. This implies that $W[\chi,\xi]$ is a smooth function of its variables. Since by definition $W[0,0]=0$, the above conditions are sufficient for the integral (3.31) to be finite.

We shall also impose the restriction that the maps $z(\cdot)$ are everywhere *Lifschitz*: in any compact subset U of $\mathbf{R}$, there exists $C>0$, such that for all $t_1,t_2\in U$, $|z_{t_1}-z_{t_2}|_\Gamma<C|t_1-t_2|$. This is a stronger assumption than continuity, but weaker than differentiability and it is necessary for proving existence of the Liouville operator.

If $|\chi(\cdot)\xi(\cdot)\rangle$ are to correspond to coherent states, *they have to be continuous functions of their arguments*. This is proven as follows.

Let us assume that $|z_1(\cdot)-z_2(\cdot)|_\Pi=\delta>0$. Then

$$\||z_1(\cdot)\rangle-|z_2(\cdot)\rangle\|^2_{\mathcal{V}}=2\left(1-\cosh\int d\mu(t)\log\langle z_{1t}|z_{2t}\rangle\right). \tag{3.33}$$

Let us write $|f_t\rangle = |z_{2t}\rangle - |z_{1t}\rangle$. Then we have

$$\| |z_1(\cdot)\rangle - |z_2(\cdot)\rangle \|_{\mathcal{V}}^2 = 2 - 2\cosh \int d\mu(t) \log(1 + \langle z_t | f_t \rangle). \tag{3.34}$$

The finiteness of $|z_1(\cdot) - z_2(\cdot)|_{\Pi}$, implies that except for a set of measure zero, there exists $c \geqslant 0$, such that $|\langle z_t | f_t \rangle| \leqslant \sqrt{\langle f_t | f_t \rangle} < c\delta$. Now, there exist complex numbers c_t, such that $\log(1 + \langle z_t | f_t \rangle) = c_t \langle z_t | f_t \rangle$. By our previous result (except perhaps in a set of measure zero) these c_t satisfy $|c_t| < C$, for $C > 0$. Using this result, we get

$$\| |z_1(\cdot)\rangle - |z_2(\cdot)\rangle \|_{\mathcal{V}}^2 = 2 - 2\cosh\left(\int d\mu(t) c_t \langle z_t | f_t \rangle \right). \tag{3.35}$$

The integral is bounded $|\int d\mu(t) c_t \langle z_t | f_t \rangle| \leqslant C\delta$, so for sufficiently small δ, there exists a constant $C' > 0$ such that

$$\| |z_1(\cdot)\rangle - |z_2(\cdot)\rangle \|_{\mathcal{V}}^2 \leqslant C' \delta^2, \tag{3.36}$$

showing that $|z(\cdot)\rangle$ is a continuous function of $z(\cdot)$.

This implies that W is also a continuous function of $\chi(\cdot), \xi(\cdot)$; so as explained in Sec. III A 3, we define a representation of the history group using Eq. (3.16).

But the representation can also be defined straightforwardly. Indeed, we can write a unitary operator $U(\chi(\cdot), \xi(\cdot))$ as $\otimes_{t \in \mathbf{R}} U(\chi_t, \xi_t)$, i.e., by its action on the coherent state vectors

$$U(\chi(\cdot), \xi(\cdot)) |\chi'(\cdot) \xi'(\cdot)\rangle = e^{(i/2) \int d\mu(t) (\chi_t' \cdot \xi_t - \chi_t \cdot \xi_t')} |\chi(\cdot) + \chi'(\cdot), \xi(\cdot) + \xi'(\cdot)\rangle. \tag{3.37}$$

Therefore time averaged operators for position $q_\xi = \int d\mu(t) q_t \cdot \xi(t)$ and momentum $p_\chi = \int d\mu(t) p_t \chi(t)$ *do exist* on $\mathcal{V}$.

2. Operators

Let us first see how we can define the analog of the Hamiltonian $H_\kappa = \int d\mu(t) h(q_t, p_t)$ in this Hilbert space.

Let $\hat{h}$ be the Hamiltonian on the canonical Hilbert space. We assume that the representation of the Weyl group can be chosen, so that all coherent state vectors lie in the domain of $\hat{h}$. This suffices to show that there exist complex numbers $A(s)$, such that

$$\langle \chi' \xi' | e^{-i\hat{h}s} | \chi \xi \rangle = \langle \chi' \xi' | \chi \xi \rangle (1 - iA(s) h(\chi, \xi; \chi', \xi') s), \tag{3.38}$$

where $h(\chi, \xi; \chi', \xi') = \langle \chi' \xi' | \hat{h} | \chi \xi \rangle / \langle \chi' \xi' | \chi \xi \rangle$, and for each neighborhood of $s = 0$ there exists $C > 0$ such that $|A(s)| \leqslant C$. Let us try to define a version of the operator $U_\kappa(s) = e^{-iH_\kappa s}$ as $\otimes_t e^{-i\hat{h}\kappa(t)s}$. It is easy to show, as in Sec. II C 3, that it is well defined; the issue is to show it is continuous at $s = 0$, for then by Stone's theorem H_κ exists. We have

$$\begin{aligned} |\langle \chi'(\cdot) \xi'(\cdot) | U(s) - 1 | \chi(\cdot) \xi(\cdot) \rangle| &= \left| \exp\left(\int d\mu(t) \log(\langle \chi_t' \xi_t' | e^{-i\hat{h}\kappa(t)s} | \chi_t \xi_t \rangle_{H_t}) \right) - 1 \right| \\ &= \left| \exp\left(\int d\mu(t) \log(1 - iA(s) s \kappa(t) h(\chi_t, \xi_t; \chi_t', \xi_t')) \right) - 1 \right| \\ &\leqslant C \left| \int d\mu(t) \kappa(t) h(\chi_t, \xi_t : \chi_t', \xi_t') \right| |s|. \end{aligned} \tag{3.39}$$

Here C is a real positive number. Therefore $U(s)$ has matrix elements continuous with respect to s if $\int d\mu(t) \kappa(t) h(\chi_t, \xi_t; \chi_t', \xi_t')$ exists. We can take $\kappa(t)$ to be a measurable function that

grows at most polynomially. We have adjusted $\hat{h}$ so that $\hat{h}|0\rangle_H=0$, then it suffices that $h(\chi_t,\xi_t;\chi_t',\xi_t')$ is continuous. We have demanded that $(\chi_t,\xi_t)\to 0$ exponentially fast outside some compact set, hence $h(\chi_t,\xi_t;\chi_t',\xi_t')\to 0$ outside this compact set.

The operator H_κ *can be therefore defined*.

A Liouville operator corresponding to the classical function $\int dt\, p_t\dot{q}_t$ is also defined by its action on coherent states

$$e^{isV}|\chi(\cdot)\xi(\cdot)\rangle\to=|\chi'(\cdot)\xi'(\cdot)\rangle, \tag{3.40}$$

where $(\chi'(t),\xi'(t))=(\chi(t+s),\xi(t+s))$. We need to check that it is continuous at $s=0$. We have

$$\langle\chi(\cdot)\xi(\cdot)|e^{isV}|\chi(\cdot)\xi(\cdot)\rangle=\exp\left(\int d\mu(t)\log\langle\chi_t\xi_t|\chi_{t+s}\xi_{t+s}\rangle_{H_t}\right). \tag{3.41}$$

Since the coherent states are continuous functions of their arguments and the paths $(\chi,\xi)(\cdot)$ have been assumed Lifschitz, there exists a vector $|f_t,s\rangle_{H_t}$ on H such that

$$|\chi_{t+s}\xi_{t+s}\rangle_{H_t}=|\chi_t\xi_t\rangle_{H_t}+s|f_t,s\rangle_{H_t}, \tag{3.42}$$

and $\langle f_t,s|f_t,s\rangle<C_t$ for some constants $C_t>0$. Therefore

$$|\langle\chi(\cdot)\xi(\cdot)|e^{isV}-1|\chi(\cdot)\xi(\cdot)\rangle|=\left|\exp\left(\int d\mu(t)\log(1+s\langle\chi_t\xi_t|f_t,s\rangle)_{H_t}\right)-1\right|\leqslant A|s|\int d\mu(t)C_t, \tag{3.43}$$

for some constant $A>0$. Now, since we assume $(\chi_t,\xi_t)\to(0,0)$ outside compact intervals, C_t can always be chosen to be constant in this compact interval and vanish outside this, thus rendering the integral finite. We therefore establish continuity of the matrix elements of e^{isV} around $s=0$.

The operator V, therefore, exists.

The existence of V and H_κ also implies the existence of an action operator $S_\kappa=V-H_\kappa$.

To summarize, assuming that

(1) the canonical coherent states are smooth functions of their arguments,
(2) they lie in the domain of $\hat{h}$,
(3) $\hat{h}$ has a unique ground state $|0\rangle_H$, in which $\hat{h}|0\rangle_H=0$,
(4) we consider paths $t\to z_t$, that satisfy the Lifschitz condition,

we can define a representation of the history group in a Hilbert space $\mathcal{V}$ in the fashion described, such that the two generators of time transformation are self-adjoint operators on $\mathcal{V}$.

An issue that can be raised at this point is that the choice of paths is restricted to ones that $(\chi_t,\xi_t)\to 0$ as time goes to infinity. These are not sufficient to describe all conceivable phase space motions, as for instance oscillators that oscillate eternally. However, one can consider such properties in an arbitrarily large, but finite, time interval. This restriction is a consequence of the way we have chosen to define the smearing functions for the generators of the history group. A possibility that might lift this difficulty in a natural manner is briefly presented in Sec. IV A.

3. Uniqueness of the representation

As $(\chi_t,\xi_t)\to(0,0)$ for large t, the only vector that is left invariant under the time translations generated by the Liouville operator is the ''vacuum'' vector $|0\rangle=\otimes_{t\in\mathbf{R}}|0\rangle_{H_t}$. (It corresponds to the proposition that the system is on the ground state at all times.) Since the history Weyl group is isomorphic to the Weyl group of a field theory, we can use the uniqueness theorem for the expectation functional, to establish that any two of the representations, we have constructed are unitarily inequivalent, if they have *different expectation functionals*.

This has different implications according to whether the *canonical* Weyl group is finite or infinite dimensional. If it is infinite dimensional and corresponds to a well-behaved quantum field theory (i.e., with a unique translationally invariant vacuum), then the expectation functional of the canonical theory is independent of the representation and unique. Hence, the expectation functional for the history theory, constructed by Eq. (3.30) is also unique. This means for a given representation of the canonical group, we can obtain a representation of the history group, in such a way, that unitarily equivalent representations of the canonical group yield unitarily equivalent representations of the history group. This is, indeed, very satisfactory.

However, for finite-dimensional canonical Weyl group, all representations are unitarily equivalent. Hence different expectation functionals correspond to unitarily equivalent theories. But different expectation functionals canonically, lead to different expectation functionals for the history group. And these give rise to unitarily inequivalent representations. We are then in the unpleasant situation of having many inequivalent history theories corresponding to one canonical theory. There is no remedy for this. But, we should remark that the conditions developed throughout this section, constrain severely the choice of the representation of the canonical group we are allowed to use. The canonical coherent states have to lie in the domain of all operators that we want to also define in the histories theory. Even if this does not guarantee uniqueness, at least it gives a guideline for which type of representations are interesting to use.

4. The decoherence functional

We saw that we have to restrict to paths (χ_t,ξ_t) that fall to zero rapidly at large t. This means that the single-time Hilbert space at $t=\pm\infty$ is essentially one dimensional, consisting only of the vector $|0\rangle$.

We saw that in the construction of the decoherence functional, the main problem came from the operators defined at the boundary Hilbert space. In this construction, when time is taken in the whole of the real line, the boundary Hilbert space is one dimensional and the boundary operator $\mathcal{A}$ is just multiplicative. Hence the decoherence functional splits in the product of two phases:

$$d(\alpha,\beta)=\mathrm{Tr}_{\mathcal{V}}(\mathcal{S}\mathcal{U}^{\dagger}\alpha\mathcal{U})\,\mathrm{Tr}_{\mathcal{V}}(\mathcal{S}^{\dagger}\mathcal{U}^{\dagger}\beta\mathcal{U}). \tag{3.44}$$

The operator $\mathcal{U}$ is easily identified as e^{-iH_κ} for $\kappa(t)=t$.

The construction of the operator $\mathcal{S}$ is more intricate. Complex analyticity of the coherent states makes consideration of the diagonal matrix elements sufficient.

From the basic operation of the Weyl group we get that

$$\langle\chi'\xi'|\chi\xi\rangle=\exp(i/2(\xi\cdot\chi'-\chi\cdot\xi')+W[\chi-\chi',\xi-\xi']). \tag{3.45}$$

Assuming a discetization $t_0,t_1,\ldots,t_n=t_f$ of the interval $[t_i,t_f]$ the definition (2.22) yields

$$\begin{aligned}
&\langle\chi_{t_0},\xi_{t_0};\ldots;\chi_{t_n},\xi_{t_n}|\mathcal{S}|\chi_{t_0},\xi_{t_0};\ldots;\chi_{t_n},\xi_{t_n}\rangle\\
&\quad=\langle\chi_{t_0}\xi_{t_0}|\chi_{t_n}\xi_{t_n}\rangle\prod_i\langle\chi_{t_i}\xi_{t_i}|\chi_{t_{i-1}}\xi_{t_{i-1}}\rangle\\
&\quad=e^{(i/2)(\xi_{t_n}\cdot\chi_{t_0}-\chi_{t_n}\cdot\xi_{t_0})+W[\chi_{t_n}-\chi_{t_0},\xi_{t_n}-\xi_{t_0}]}\\
&\qquad\times\exp\left(\sum_i\frac{i}{2}(\xi_{t_{i-1}}\cdot\chi_{t_i}-\xi_{t_i}\cdot\chi_{t_{i-1}})+W[\chi_{t_{i-1}}-\chi_{t_i},\xi_{t_{i-1}}-\xi_{t_i}]\right)\\
&\quad=e^{(i/2)(\xi_{t_n}\cdot\chi_{t_0}-\chi_{t_n}\cdot\xi_{t_0})+W[\chi_{t_n}-\chi_{t_0},\xi_{t_n}-\xi_{t_0}]}\\
&\qquad\times\exp\left(\sum_i\frac{i}{2}[\xi_{t_i}\cdot(\chi_{t_i}-\chi_{t_{i-1}})-\chi_{t_i}\cdot(\xi_{t_i}-\xi_{t_{i-1}})]\right.\\
&\qquad\left.-\frac{\partial W}{\partial\xi}[\chi_{t_i},\xi_{t_i}](\xi_{t_i}-\xi_{t_{i-1}})-\frac{\partial W}{\partial\chi}[\chi_{t_i},\xi_{t_i}](\chi_{t_i}-\chi_{t_{i-1}})\right).
\end{aligned}\tag{3.46}$$

Hence at the continuous limit we get

$$\begin{aligned}\langle\chi(\cdot)\xi(\cdot)|\mathcal{S}|\chi(\cdot)\xi(\cdot)\rangle &= e^{(i/2)(\xi(t_f)\cdot\chi(t_0)-x(t_f)\cdot\xi(t_0))+W[\chi(t_f)-\chi(t_0),\xi(t_f)-\xi(t_0)]}\\ &\quad\times\exp\left(\int_{t_0}^{t_f}dt\,\frac{i}{2}(\xi\cdot\dot{\chi}-\chi\cdot\dot{\xi})-\int_{W_{t_0}}^{W_{t_f}}dW\right)\\ &=\exp\left(\frac{i}{2}(\xi(t_f)\cdot\chi(t_0)-\chi(t_f)\cdot\xi(t_0))+W[\chi(t_f)-\chi(t_0),\xi(t_f)-\xi(t_0)]\right.\\ &\quad\left.-W[\chi(t_f),\xi(t_f)]+W[\chi(t_0),\xi(t_0)]\right)\\ &\quad\times\exp\left(\frac{i}{2}\int_{t_0}^{t_f}dt(\xi\cdot\dot{\chi}-\chi\cdot\dot{\xi})\right).\end{aligned}\tag{3.47}$$

Clearly as $[t_0,t_f]\to(-\infty,\infty)$ we get

$$\langle\chi(\cdot)\xi(\cdot)|\mathcal{S}|\chi(\cdot)\xi(\cdot)\rangle=\exp\left(i\int_{-\infty}^{\infty}\xi\cdot\dot{\chi}\right).\tag{3.48}$$

In particular, for a pair of coherent-state histories the decoherence functional reads

$$d((\xi,\chi)(\cdot),(\xi',\chi')(\cdot))=e^{iS[\xi(\cdot),\chi(\cdot)]-iS^*[\xi'(\cdot),\chi'(\cdot)]},\tag{3.49}$$

where

$$iS[\xi,\chi]=\langle\xi,\chi|\left(\frac{d}{dt}-iH\right)|\xi,\chi\rangle\tag{3.50}$$

is the classical phase space action.

D. The generating functional

1. N-point functions

A probability theory does not only give probabilities to possible scenaria, it also provides expectation values for observables. In fact, a probability measure can be fully reconstructed from the knowledge of a sufficiently large number of expectation values: these are known as the moments of the distribution or in physics as the N-point functions. We shall write the relevant formulas in the context of stochastic processes, rather than single-time probability theory, for it is the analog of these expressions that we shall attempt to generalize in the quantum context.

Let us denote by x a vector that corresponds to a point of a sample space Ω and Ω^T the space of histories with elements the paths $x(\cdot)$. Let also $d\mu(x(\cdot))$ denote the probability measure in the space of paths. One then defines the N-point functions

$$G^{(n)}(a_1,t_1;\ldots;a_n,t_n)=\int d\mu(x(\cdot))X^{a_1}_{t_1}\cdots X^{a_n}_{t_n},\tag{3.51}$$

where $X^a_t(x(\cdot))=x^a(t)$ is a function on Ω^T.

The information of the N-point functions is encoded in the generating functional

$$Z[J]=\sum_{n=0}^{\infty}\frac{(i)^n}{n!}\int dt_1\cdots dt_n\sum_{a_1\cdots a_n}G^{(n)}(a_1,t_1;\cdots;a_n,t_n)J_{a_1}(t_1)\cdots J_{a_n}(t_n).\tag{3.52}$$

The generating functional is just the Fourier transform of the stochastic measure

$$Z[J(\cdot)]=\int d\mu(x(\cdot))\exp\left(i\int dt\, X_t^a J_a(t)\right). \tag{3.53}$$

The N-point functions (3.51) fully exhaust the physical content of the theory; hence the generating functional (3.53) provides a complete specification of the probability measure. In general, one can define generating functionals containing less complete information, e.g., ones that refer to one single observable. For instance given a function f on Ω we can define

$$Z_f[J(\cdot)]=\int d\mu(x(\cdot))e^{i\int dt\, F_t J(t)} \tag{3.54}$$

which generates the correlation functions of f. Or more generally, one can define generating functionals of time-averaged quantities F (functions on Ω^T) as

$$Z_F(j)=\int d\mu(x(\cdot))e^{iF(x(\cdot))j}, \tag{3.55}$$

for some real number j.

2. The CTP generating functional

Since the decoherence functional is defined through bounded operators on $\mathcal{V}$, its definition can be extended to a bilinear functional over all bounded operators on $\mathcal{V}$: $d: B(\mathcal{V})\times B(\mathcal{V})\to\mathbf{C}$.

We shall first examine the discrete-time case. Let us consider an operator $\hat{A}$ on H. Then if A_t denotes the corresponding single-time operator on $\mathcal{V}$ (see Sec. II A), we can see that

$$d(A_{t_1}\otimes A_{t_2},1)=\Theta(t_1-t_2)\mathrm{Tr}(\hat{\rho}_0\hat{A}(t_1)\hat{A}(t_2))+\Theta(t_2-t_1)\mathrm{Tr}(\hat{\rho}_0\hat{A}(t_2)\hat{A}(t_1)), \tag{3.56}$$

$$d(1,A_{t_1}\otimes A_{t_2})=\Theta(t_2-t_1)\mathrm{Tr}(\hat{\rho}\hat{A}(t_1)\hat{A}(t_2))+\Theta(t_1-t_2)\mathrm{Tr}(\hat{\rho}\hat{A}(t_2)\hat{A}(t_1)), \tag{3.57}$$

where $\hat{A}(t)$ is the Heisenberg picture operator on H: $e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t}$. The right-hand side of (3.56) and (3.57) are the time-ordered and anti-time-ordered two-point function for this observable. Similarly we can construct higher time-ordered and anti-time-ordered functions, respectively, as well as mixed ones, e.g., $d(A_{t_1},A_{t_2}\otimes A_{t_3})$. They are usually denoted by (r,s) correlation functions r denoting the number of time-ordered and s of anti-time-ordered appearances of A in the expectation value. Such N-point functions have been first used in the classic study of quantum Brownian motion by Schwinger.[17] They are obtained by an object known as the closed-time-path (CTP) generating functional.[17,31]

If we want to construct an object that encodes the information about the N-point functions at all times, we need to go to the continuum limit.

Let us by A_f denote the time averaged version of an operator $\hat{A}$ on H, defined in the way we explained in Sec. II C. Then we define the closed-time-path generating functional associated to the operator $\hat{A}$ as a function of a pair of smearing functions J_+ and J_- through

$$Z_{\hat{A}}[J_+(\cdot),J_-(\cdot)]=d(e^{iA_{J_+}},e^{-iA_{J_-}}). \tag{3.58}$$

The signs $+$ and $-$ correspond, respectively, to the part that generates time-ordered, vs anti-time-ordered correlation functions. In general the (r,s) mixed correlation function for A will be given by

$$G_A^{(r,s)}(t_1,\ldots,t_r;t_1',\ldots,t_s')=(-i)^r i^s\frac{\delta^r}{\delta J_+(t_1)\cdots\delta J_+(t_r)}\frac{\delta^s}{\delta J_-(t_1)\cdots\delta J_-(t_s)}Z[J_+,J_-]|_{J_+=J_-=0}. \tag{3.59}$$

When the Hilbert space carries a representation $U(\chi,\xi)=e^{-iq_\xi - ip_\chi}$ of the history Weyl group, there exist time-averaged versions of the position and momentum operators. We can then construct the configuration space CTP generating functional as

$$Z_q[\xi_+,\xi_-]=d(e^{i(q,\xi_+)},e^{-i(q,\xi_-)}). \tag{3.60}$$

This generating functional has been widely used, mainly because it has a convenient path-integral expression. One can construct a corresponding effective action through a Legendre transform of $W=-i\log Z$ (known as the CTP effective action).[32]

But we can also write a generating functional that contains all *phase space* correlation functions. This is simply defined[14] as

$$Z[\xi_+,\chi_+;\xi_-,\chi_-]=d(U(\chi_+,\xi_+),U^\dagger(\chi_-,\xi_-)). \tag{3.61}$$

Since our representation of the history group is irreducible, all physical information about the physical system is contained in the CTP generating functional (3.61). Indeed, it is the quantum analog of the generating functional (3.53) of a general stochastic process.

E. The Wigner–Weyl transform

1. The canonical case

In quantum mechanics a representation $\hat{U}(\chi,\xi)$ of the canonical group enables one to construct a *linear* map that takes a large class of Hilbert space operators to phase space functions. This is known as the Wigner–Weyl transform. It is implemented as follows: If $\hat{A}$ is a trace-class operator on H then, we define the function $F_{\hat{A}}(q,p)$ on phase space as

$$F_{\hat{A}}(q,p)=\int d\chi\, d\xi\, e^{-i\xi\cdot q-i\chi\cdot p}\,\mathrm{Tr}(\hat{U}(\xi,\chi)\hat{A}):=\mathrm{Tr}(\hat{\Delta}(q,p)\hat{A}), \tag{3.62}$$

where $\hat{\Delta}(q,p)=\int d\chi\, d\xi\, e^{-i\xi\cdot q-i\chi\cdot p}\hat{U}(\chi,\xi)$. This operator satisfies

$$\int dq\, dp\, \hat{\Delta}(q,p)=\hat{1}, \tag{3.63}$$

and its matrix elements in a coherent state basis are given by

$$\langle\chi'\xi'|\Delta(q,p)|\chi\xi\rangle=e^{i\xi\cdot(\chi-\chi')+iq\cdot(p-p')+i(\chi\cdot\xi-\chi'\cdot\xi')}\times\tilde{K}\left[p+\frac{\xi+\xi'}{2},q-\frac{\chi+\chi'}{2}\right], \tag{3.64}$$

in terms of the Fourier transform of the expectation functional

$$\tilde{K}[p,q]=\int d\mu(\chi,\xi)e^{-i\chi\cdot p-i\xi\cdot q}K[\chi,\xi]. \tag{3.65}$$

Note that by $dq\,dp$ we denote the standard Lebesque measure on $\Gamma=\mathbf{R}^{2n}$, normalized by a factor of $(2\pi)^{-n}$.

This definition can be extended to bounded operators (at least when the Weyl group is finite dimensional) and to a large class of unbounded ones. The Wigner–Weyl transform of a density matrix is known as the *Wigner function*. There are two important properties of the Wigner transform

$$\int dq\, dp\, F_{\hat{A}}(q,p)=\mathrm{Tr}_H\hat{A}, \tag{3.66}$$

$$\int dq\, dp\, F_{\hat{A}}(q,p)F_{\hat{B}}(q,p)=\mathrm{Tr}_H(\hat{A}\hat{B}). \tag{3.67}$$

The operator commutator induces on the phase the Moyal bracket $\{\,,\}_M$. For a pair of operators $\hat{A}$ and $\hat{B}$ their commutator $\hat{C}=[\hat{A},\hat{B}]$ is associated with the symbol

$$\frac{1}{i}F_{\hat{C}}=\{F_{\hat{A}},F_{\hat{B}}\}_M:=2F_{\hat{A}}\sin\left(\frac{1}{2}\{\,,\}\right)F_{\hat{B}} \tag{3.68}$$

here $\{\,,\}$ is the Poisson bracket on phase space, written as a bilinear operator: $f\{\,,\}g=\{f,g\}$. The sinus in this expression refers to its Taylor series viewed as a function of this bilinear operator.

2. The histories analog

We can proceed similarly in the histories case and to each trace-class operator A on $\mathcal{V}$ associate a function F_A on Π, the space of classical histories as

$$F_A[\gamma]=F_A[q(\cdot),\xi(\cdot)]=\int D\xi(\cdot)D\chi(\cdot)e^{-i(q,\xi)(\gamma)-i(p,\chi)(\gamma)}\,\mathrm{Tr}(U(\xi,\chi)A). \tag{3.69}$$

This expression is only formal, since the measures $D\chi(\cdot)$, etc., do not exist. What is implied is $F_A(\gamma)=\mathrm{Tr}_{\mathcal{V}}(A\Delta(q(\cdot),p(\cdot)))$. By $\Delta(q(\cdot),p(\cdot))$ we denote a linear map that is given by

$$\Delta(q(\cdot),p(\cdot))=\otimes_t\hat{\Delta}(q_t,p_t). \tag{3.70}$$

If the operator A is a product operator $\otimes_t\hat{A}_t$, then using Eq. (2.14) we see that

$$F_{A_f}[q(\cdot),p(\cdot)]=\exp\left(\int d\mu(t)\log F_{\hat{A}_t}(q_t,p_t)\right). \tag{3.71}$$

It is also easy to calculate the symbol for a time averaged operator A_f by constructing the Weyl transform for e^{iA_fs} and expanding around $s=0$. The result is

$$F_{A_f}[q(\cdot),p(\cdot)]=\int d\mu(t)f(t)F_{\hat{A}}(q_t,p_t). \tag{3.72}$$

Such is for instance the case of position, momentum operators, and the Hamiltonian, so that

$$q_f\rightarrow F_{q_f}=\int d\mu(t)q_tf(t), \tag{3.73}$$

$$p_f\rightarrow F_{p_f}=\int d\mu(t)p_tf(t), \tag{3.74}$$

$$H_\kappa\rightarrow F_{H_\kappa}=\int d\mu(t)\kappa(t)h(q_t,p_t), \tag{3.75}$$

where $h(q,p)=F_{\hat{h}}(q,p)$ is the Wigner transform of the canonical Hamiltonian.

For more general operators on $\mathcal{V}$, the Weyl transform is effected by constructing first a suitable discrete-time expression in $\otimes_i H_{t_i}$ and then going to the continuum limit. It is more convenient to employ the decomposition of the unity for the canonical coherent states in order to compute the trace:

$$\mathrm{Tr}_{\mathcal{V}}A=\int\prod_i d\mu(\chi_{t_i},\xi_{t_i})\langle\chi_{t_1}\xi_{t_1};\chi_{t_2}\xi_{t_2}\cdots\chi_{t_n}\xi_{t_n}|A|\chi_{t_1}\xi_{t_1};\chi_{t_2}\xi_{t_2}\cdots\chi_{t_n}\xi_{t_n}\rangle. \tag{3.76}$$

For operators that map coherent states into coherent states, the calculations are easier to perform. Such is, for instance, the operator e^{isV}. We can compute

$$e^{isV}\rightarrow F_{e^{isV}}=\int \prod_t d\mu(\chi_t,p_t)\langle\chi_t\xi_t|\hat{\Delta}(q_t,p_t)|\chi_{t+s}\xi_{t+s}\rangle_{H_t}. \tag{3.77}$$

If we expand this around $s=0$ we find that

$$V\rightarrow F_V=\int dt\, p_t\dot{q}_t, \tag{3.78}$$

where the integral is of a Stieljes type.

Note that Eqs. (3.69) and (3.76) are, as yet, defined for a discretization of the time interval. In order to compute any traces we will always need to check the finiteness of the expressions at the continuum limit. We will return to this later in Sec. III E 3.

3. The decoherence functional

In an analogous manner, one can assign to the decoherence functional a ''function'' on $\Pi\times\Pi$ as

$$\begin{aligned} &W[q(\cdot),p(\cdot)|q'(\cdot),p'(\cdot)]\\ &\quad=W[\gamma|\gamma']\\ &\quad=\int D\xi_+(\cdot)D\chi_+(\cdot)D\xi_-(\cdot)D\chi_-(\cdot)e^{-i(q,\xi_+)-i(p,\chi_+)+i(q',\xi_-)+i(p',\chi_-)}\\ &\qquad\times Z[\xi_+,\chi_+;\xi_-,\chi_-]. \end{aligned} \tag{3.79}$$

Given then some operators (these might be projectors that correspond to a history proposition) A and B on $\mathcal{V}$ we have

$$d(A,B)=\int D\mu(\gamma)D\mu(\gamma')W[\gamma|\gamma']F_A(\gamma)F_B(\gamma'), \tag{3.80}$$

where $D\mu(\gamma)$ is a shorthand for $D\chi(\cdot)D\xi(\cdot)$.

In spite of the general nondefinability of the integration measure, there is a very good sense in which the $W[\gamma|\gamma']$ exists: as the inductive limit of its discrete-time expressions, in complete analogy with the Kolmogorov's construction of the stochastic probability measure. This proceeds as follows.

In standard quantum mechanics one can define objects that correspond to classical multitime probabilities using the Wigner transform.[33] They are of the form

$$W(q_1,p_1,t_1;\ldots;q_n,p_n,t_n)=\mathrm{Tr}(\hat{\rho}_0e^{i\hat{H}t_1}\hat{\Delta}(q_1,p_1)e^{-i\hat{H}t_1}\cdots e^{i\hat{H}t_n}\hat{\Delta}(q_n,p_n)e^{-i\hat{H}t_n}). \tag{3.81}$$

These distributions do not define a probability measure: they are complex and do not satisfy the Kolmogorov additivity condition. Rather they are the building blocks of the decoherence functional. In analogy with the stochastic case if we consider two discretizations $I=\{t_1,\ldots,t_n\}$ and $I'=\{t'_1,\ldots,t'_m\}$ of an interval T, we can define the objects as

$$W_{n,m}[q_1,p_1,t_1;\ldots;q_n,p_n,t_n|q'_1,p'_1,t'_1;\ldots;q'_m,p'_m,t'_m]=\mathrm{Tr}(\hat{C}_n^{\dagger}\hat{\rho}_0\hat{C'}_m), \tag{3.82}$$

where

$$\hat{C}_m=e^{i\hat{H}t_1}\hat{\Delta}(q_1,p_1)e^{-i\hat{H}t_1}\cdots e^{i\hat{H}t_m}\hat{\Delta}(q_m,p_m)e^{-i\hat{H}t_m} \tag{3.83}$$

and similarly for $\hat{C}'_m$.

Let us write Ω^I and $\Omega^{I'}$ as the spaces of discrete-time phase space histories. They can be equipped with the standard Lebesque measure $\Pi_t dq_t\, dp_t$, so that $W_{n,m}$ can be used to define genuine decoherence functionals $d_{I,I'}$ that satisfy properties (2.3). If we denote by Ω^T the space of phase space histories we can consider the injection map $i_{I,I'}: \Omega^n \times \Omega^m \to \Omega^T \times \Omega^T$. These maps are *measurable*. It is easy to check that the hierarchy of functions $W_{n,m}$ satisfies an additivity condition

$$\int dq_{t_1}\, dq_{t_2}\, W_{n,m}[q_1,p_1,t_1;\ldots;q_n,p_n,t_n|q'_1,p'_1,t'_1;\ldots;q'_m,p'_m,t'_m] = W_{n-1,m}[q_2,p_2,t_2;\ldots;q_n,p_n,t_n|q'_1,p'_1,t'_1;\ldots;q'_m,p'_m,t'_m]. \tag{3.84}$$

In complete analogy to Kolmogorov's theorem, the above properties are sufficient to prove the existence of an additive, complex-valued, Hermitian measure on $\Pi \times \Pi$, i.e., a decoherence functional d_Π, such that

$$d_{I,I'} = i^*_{I,I'} d_\Pi. \tag{3.85}$$

It is important to remark that the definition of the decoherence functional on phase space took place with respect to the *measurable subsets* of Π, which define a Boolean algebra. This is clearly distinct from the logic of projectors on the Hilbert space $\mathcal{V}$. This is what enabled us to sidestep the nondefinability of a decoherence functional from the discrete-time expressions.

This construction does not highlight the general structure of the decoherence functional. To see this, it is necessary to compute the Wigner transformations of the operators $\mathcal{S}$ and $\mathcal{U}$.

When the Hamiltonian is quadratic, the coherent states are Gaussians and the calculation of traces reduces to Gaussian integrals. In this case the functional relations of operators is preserved by the Weyl–Wigner transform. For the harmonic oscillator, we get

$$\mathcal{U} \to F_{\mathcal{U}} = e^{-iH\kappa}, \quad \kappa(t) = t, \tag{3.86}$$

$$\mathcal{S} \to F_{\mathcal{S}} = \exp(-\tfrac{1}{2}[\omega(q_{t_f} - q_{t_0})^2 + \omega^{-1}(p_{t_f} - p_{t_0})^2 + i(p_{t_f} \cdot q_{t_0} - q_{t_f} \cdot p_{t_0})]) \times e^{i/2\int_{t_i}^{t_f} dt (p_t \cdot \dot{q}_t - q_t \cdot \dot{p}_t)}. \tag{3.87}$$

In the case of more general Hamiltonians the calculations are more difficult to perform. But if we assume that the interval upon which histories are defined is the whole real line, the boundary condition forces that

$$F_{\mathcal{S}} = e^{i\int dt\, p_t \dot{q}_t}. \tag{3.88}$$

The operator $\mathcal{U}$ is unitary, hence a transformation $A \to \mathcal{U} A \mathcal{U}^\dagger$ preserves the trace. The trace is also preserved by the Weyl–Wigner transform, hence phase space $\mathcal{U}$ corresponds to a trace-preserving automorphism $\mathbf{T}$ of the algebra of functions on the space Π of phase space paths. Explicitly this would be the continuum limit of

$$\mathbf{T} = T_{t_1} \otimes \cdots \otimes T_{t_n}, \tag{3.89}$$

where T_t corresponds to the automorphism of the algebra of single-time functions $A \to T_t[A]$ given by the Moyal bracket version of the Heisenberg equations of motion

$$\frac{\partial}{\partial_t} T_t[A] = \{H, T_t[A]\}_M \tag{3.90}$$

with $T_0[A] = A$.

In general the decoherence functional for phase space paths in a time interval $[t_i,t_f]$ will read

$$d(A,B)=\int_{\Gamma_{t_i}\times\Gamma_{t_f}} dx\,\lambda_x^*(F_A)\lambda_x(F_B), \tag{3.91}$$

where by x we denote points on the boundaries $\Gamma_{t_i}\times\Gamma_{t_f}$. It is then a collective index for $(q_{t_i},p_{t_i},q_{t_f},p_{t_f})$. It is obtained by the Weyl–Wigner transform of the boundary operator with respect to the rs indices in Eq. (2.19). $dx=dq_{t_0}\,dp_{t_0}\,dq_{t_f}\,dp_{t_f}$ is the standard measure on $\Gamma_{t_0}\times\Gamma_{t_f}$. $\lambda_x(\cdot)$ is a family of complex valued measures on the space of paths that have a functional dependence on boundary points x which incorporates the actual initial state of the system. If by $\mathbf{T}$ we denote the automorphism generated by $\mathcal{U}$ then

$$\lambda_x(A)=\int d\mu(\gamma)F_{\mathcal{A}^x\mathcal{S}}(\gamma)\mathbf{T}(A)(\gamma). \tag{3.92}$$

In this equation $F_{\mathcal{A}^x\mathcal{S}}$ is the Weyl symbol associated with the operator $\mathcal{A}^x\mathcal{S}$ of Eq. (2.23). The collective variable x again corresponds to the Weyl–Wigner transform of the indices (r,s) of Eq. (2.19).

In this expression it is very clear that phases appear in the probability assignment solely because of the geometric phase encoded in the operator $\mathcal{S}$. This has been argued in Ref. 16, but in the present context it is clearer, since the automorphism $\mathbf{T}$ makes no reference to complex numbers in its definition. The presence of complex numbers in the decoherence functional is purely due to the presence of a $U(1)$ connection on phase space, as encoded in the function $F_{\mathcal{S}}$.

F. The stochastic limit

Rather than considering the decoherence condition (1.5) as a law of nature, that has to be exactly satisfied (as the consistent histories interpretation does), we can view it as a condition for the approximation of the physical system by a classical probabilistic theory. We remarked how the unequal time pseudoprobability distributions $W_{n,m}$ do not satisfy the Kolmogorov additivity conditions. Perhaps a smeared version would (approximately) satisfy them so that one would get decoherence. So one can try to define smeared pseudoprobability distributions like

$$\begin{aligned}\overline{W}_{n,0}(\overline{q}_1,\overline{p}_1,t_1;\ldots;\overline{q}_n,\overline{p}_n,t_n)\\ =\int dq_1\,dp_1\cdots dq_n\,dp_n\,\chi_{\overline{q}_1\overline{p}_1}(q_1,p_1)\cdots\chi_{\overline{q}_n\overline{p}_n}(q_n,p_n)W_{n,0}(q_1,p_1,t_1;\ldots;q_n,p_n,t_n),\end{aligned} \tag{3.93}$$

Here $\chi_{\overline{\chi}\overline{\xi}}$ denotes a smeared characteristic function of a cell centered around $\overline{\chi}\overline{\xi}$. This will depend on some parameters V which will determine the volume of the cell, within which smearing is effected.

The objects $\overline{W}_{n,0}$ are expectation values. They can be properly normalized if we divide them with the smearing volume. In that case they can be taken as the discrete-time probability densities that might correspond to a measure. If these smeared densities satisfy the Kolmogorov criterion (which is to be expected in many systems given sufficient smearing) they would define a classical probability measure, that would give an effective stochastic description for the quantum system.

1. General operators

The above description is valid for general observables and not only the generators of the canonical group. Indeed if $\hat{A}$ is a self-adjoint operator with continuous spectrum Σ, one defines its

corresponding generating functional $Z_{\hat{A}}[f_+,f_-]$ as in Eq. (3.58). Now if $x\in\mathbf{R}$ denote points of the spectrum of A, we can construct a decoherence functional in the space of histories $x(\cdot):T\rightarrow\Sigma$ by an analogous expression to (3.78),

$$W[x(\cdot)|x'(\cdot)]=\int Df_+(\cdot)Df_-(\cdot)e^{-i(x,f_+)+i(x',f_-)}Z_{\hat{A}}[f_+,f_-]. \tag{3.94}$$

For any two functions F and G on the space of paths, we will have

$$d(F,G)=\int Dx(\cdot)Dx'(\cdot)F[x(\cdot)]G[x'(\cdot)]W[x(\cdot)|x'(\cdot)]. \tag{3.95}$$

The distribution W can again be defined as the inductive limit of the discrete-time distributions $W_{n,m}(x_1,t_1;\ldots;x_n,t_n|x_1',t_1';\ldots;x_n',t_n')$ as in Eq. (3.81), but with the operators

$$\hat{\Delta}(x)=\int dJ\,e^{-ixJ}e^{i\hat{A}J} \tag{3.96}$$

substituting $\hat{\Delta}(p,q)$.

Again one can look for the classical limit by constructing smeared characteristic functions $\chi_{\overline{x}}(x)$ for subsets of Σ. It is convenient to use a Gaussian function for $\chi_{\overline{x}}$. For instance,

$$\chi_{\overline{x}}(x)=\exp\left(-\frac{1}{2\sqrt{V}}(x-\overline{x})^2\right). \tag{3.97}$$

2. Smearing

Let us give a description of how the above prescription for finding the classical limit. We may start with discrete time histories with n time steps, which we shall simply call t and consider the smearing functions $\chi_{\overline{x}}$:

$$\chi_{\overline{x}(\cdot)}=\prod_t \chi_{\overline{x}_t}=\exp\left(-\frac{1}{2\sqrt{V}}\sum_t (x_t-\overline{x}_t)^2\right). \tag{3.98}$$

Then we evaluate the decoherence functional at a pair of χ's (actually their corresponding positive operators) to be

$$\begin{aligned} &d(\chi_{\overline{x}(\cdot)},\chi_{\overline{x}'(\cdot)})\\ &\quad=\int DJ_+\,DJ_-\,Z_{\hat{A}}[J_+,J_-]\left(\int Dx\,Dx'\,\chi_{\overline{x}(\cdot)}[x(\cdot)]\chi_{\overline{x}'(\cdot)}[x'(\cdot)]e^{-i(J_+,x)+i(J_-,x')}\right)\\ &\quad=V^n\int DJ_+\,DJ_-\,Z_{\hat{A}}[J_+/\sqrt{V},J_-/\sqrt{V}]\\ &\qquad\times\exp(-\tfrac{1}{4}(J_+,J_+)-\tfrac{1}{4}(J_-,J_-)-i(\overline{x},J_+)+i(\overline{x}',J_-)). \end{aligned} \tag{3.99}$$

By (J,J') we imply here a discrete sum $\Sigma_t J_t J_t'$. When, we go to the continuous limit it will imply $\int d\mu(t)J_tJ_t'$.

3. The probability measure

Assume now that with sufficient coarse graining we can get approximate satisfaction of the decoherence condition for disjoint $\chi_{\overline{x}(\cdot)}$ and $\chi_{\overline{x}'(\cdot)}$. The next step is to assume that the probabilities $p(\chi_{\overline{x}})=d(\chi_{\overline{x}},\chi_{\overline{x}})$ can be used to define a probability measure

$$p[\overline{x}(\cdot)]=\frac{1}{V^n}d(\chi_{\overline{x}},\chi_{\overline{x}}). \tag{3.100}$$

This is standard practice. It corresponds to the mathematical operation of extending a classical probability measure that is defined in only a part of the lattice of propositions (in this case a semilattice), to the whole of the lattice. This gives then a generating functional (note that $p[\overline{x}(\cdot)]$ has no multiplicative dependence on V^n hence it is safe to go to the continuous limit)

$$\begin{aligned} Z_A[J]&=\int D\overline{x}\,p[\overline{x}(\cdot)]e^{i(\overline{x},J)}\\ &=\int DJ_+\exp(-\tfrac{1}{2}(J_+,J_+)-\tfrac{1}{2}|J-J_+|^2)\times Z[(J_+)/\sqrt{V},(J-J_+)/\sqrt{V}]. \end{aligned} \tag{3.101}$$

This is the generating functional of a stochastic process for a classical observable A, that is obtained as the classical limit of a general quantum mechanical operator $\hat{A}$.

The above construction can be repeated for phase space observables with no modifications. In this case, the representation of the canonical group, provides a *natural metric on phase space*, which can be used in order to construct smearing functions. In this case, a parameter analogous to V plays the role of the volume of the phase space cell (with respect to this metric), within which one smears.

Details on how to obtain the classical stochastic limit of quantum systems with this method, together with a number of examples, are found in Ref. 34.

G. Summary

After giving a brief review of the canonical group construction and the histories version of classical mechanics, we showed how to construct a large class of representations of the history group, using coherent state techniques. A particular nice result was, that for well-behaved quantum field theories the representation of the canonical group uniquely determines one for the history group.

We then showed how to encode the correlation functions for generic observables of the theory into a CTP generating functional. The Wigner–Weyl transform offered a way of representing quantum mechanical objects on the phase space and define a continuous-time decoherence functional as the continuous limit of discrete-time ones.

Finally, we developed a general procedure for taking the classical probability limit of quantum mechanical histories.

IV. DISCUSSION

We shall now discuss a number of topics that explain or put into context the results of the previous two sections.

A. Time averaging

First, we need to address a rather important issue, that we left uncommented. What is the role of the parameter τ that enters the definition of the time integral? It appeared there originally in order to render the measure dimensionless, so that operators A_f would be dimensionally the same with their canonical counterparts $\hat{A}$.

In the case where T is compact, we remarked that τ can be chosen as to normalize the measure to unity. But in the more general case, that $T=\mathbf{R}$, this cannot be done and one would have to accept τ as an additional parameter entering the histories quantum theory. On one hand, it would not appear into the physical predictions of the theory: the values of the decoherence functional are independent of τ. Nonetheless, it would be present in the definition of the time averaged operators and perhaps in the physical correspondence with classical observables.

One possible idea is to substitute all integrals over $d\mu(t)$ with the limit as $\tau\to\infty$ of $(1/\tau)\int_{-\tau/2}^{\tau/2}dt$. Classical quantities of the form

$$q_f=\lim_{\tau\to\infty}\frac{1}{\tau}\int_{-\tau/2}^{\tau/2}dt\, q_t f(t) \tag{4.1}$$

are more naturally interpreted as time-averaged values of the observable q. This implies that we can enlarge the space of possible test functions. It would suffice to demand, that the smearing functions f are *constant* outside a compact set (rather than zero), in order for the integral to be defined.

This could have as immediate consequence, that the boundary Hilbert spaces at infinities would not be one dimensional, as is the case of when f is of compact support.

But this would severely weaken our uniqueness theorem. We need to have a unique translationary invariant ''vacuum'' vector, in order for the uniqueness theorem to hold. This is not any more true, if f is not a function of compact support: any vector $|z(\cdot)\rangle$ with constant values of $z(t)$ would be translationary invariant.

The representation theory for this history group would therefore be very different; in fact, the history group itself is different. Intuitively, one expects that the representation we would obtain from such a construction would be a reducible one: a direct integral of representations like the ones we constructed, each labeled by different boundary conditions for the coherent states as $t\to\pm\infty$.

These considerations will be taken further in another paper.

B. The decoherence functional

We tried various different ways to define a continuous-time decoherence functional. The straightforward analogy with Kolmogorov's construction failed, because we cannot continuously embed the lattice of single-time propositions to the lattice of history ones. We were then left with two choices: one is to incorporate the information about the initial condition in an object that is extended in time, rather than a density matrix as is the case in the canonical approach. This might be operationally meaningful (after all the initial state corresponds to a preparation that takes place in a time interval), but it contradicts our intuition that information about the system can be encoded at a single moment of time, without any need of knowing anything about its past history. (In a sense, such a construction might be considered as the violation of the analog of the Markov condition for stochastic processes.)

The other alternative, is to define the decoherence functional with respect to the structure of propositions about phase space histories. This involves abandoning continuity, but in phase space the natural condition is measurability and using this we can construct a mathematically sensible continuous-time decoherence functional. Operationally it is a very satisfactory construction: phase space measurements exhaust the physical content of quantum theories. But one might raise the objection that we sacrificed the quantum logic structure of history propositions in order to achieve this.

This objection is valid, assuming one considers quantum logic to be a fundamental part of quantum theory. This is however an interpretational attitude towards quantum theory, which we do not feel obliged to adopt. But even should we concede this point, we could still argue, that the true quantum logic is the one corresponding to time-averaged history propositions, and the standard single-time one just an approximation.

It is nonetheless true, that our construction would be conceptually more complete, and aesthetically more satisfying, if we were able to provide a reconstruction theorem: that the knowledge of the decoherence functional on phase space, allows us to uniquely construct the Hilbert space of the theory, the decoherence functional defined as a bilinear functional on the histories Hilbert space and perhaps get some correspondence between phase space symmetries and quantum mechanical unitary operators. This would be an analog of Wightman's reconstruction theorem in

quantum field theory:[35] constructing the Hilbert space, the vacuum and the representations of the history group from the correlation functions. The analogy is very accurate, because the decoherence functional on phase space is equivalent to the CTP generating functional and thus incorporates information about all correlation functions.

So far, we have not been able to find a direct way to prove such a theorem. Of course, one could always proceed indirectly: define the Wightman functions from the CTP generating functional, from them the canonical Hilbert space, the vacuum and the Hamiltonian, and then repeat the construction of Sec. III to construct the history Hilbert space and the representation of the history group. Even though this lends plausibility in the existence of a reconstruction theorem, it does not provide any physical or mathematical insight on the structure of history theories.

C. The classical limit

The identification of the history Hilbert space was based on the representations of the history group. When we have a representation of a group, we inherit all structures associated to it: coherent states, their symbols and the Weyl–Wigner transform. The phase space, then, appears as the most fundamental ingredient of the quantum theory.

Indeed, through the Weyl–Wigner transform we can cast quantum mechanical histories in a language that makes only indirect references to a Hilbert space and is completely based on classical phase space objects. This is important, because on phase space we know how to implement coarse grainings, that are of interest for a wide class of physical systems.

For instance, in many particle systems, one could study coarse grainings of the Boltzmann type (focusing on a description in terms of densities on a single-particle phase space) and derive their stochastic behavior, by the method described in (3.6). This might provide a way to proceed towards a declared aim of the consistent histories scheme: to find how hydrodynamic variables and their quasideterministic evolution laws arise from quantum theory.[3,36–39] In fact, all types of coarse graining of classical statistical mechanics can be implemented for phase space histories.

Another area, where our results are relevant is in the study of back-reaction of quantum fields on geometry. The semiclassical treatment assumes that we can couple the Einstein tensor to the expectation value of a quantum stress-energy tensor.

For quantum fields in curved spacetime, the stress-energy tensor is not defined as an operator or even an operator-valued distribution on the Hilbert space of the theory. This is why it has to be renormalized,[28] but, even so, one cannot remove the divergences from its correlation functions. Our construction suggests that one could first take the stochastic limit for the field in a histories version of the theory, and then construct a *classical* stress-energy tensor from the classicalized field. This would give a fully consistent scheme for dealing with the back-reaction of the matter to geometry, without the dangerous assumptions involved in computing expectation values of stress-energy tensors. This idea has been tentatively developed in Ref. 34.

D. Perturbation theory

In practice, we cannot explicitly construct the Hilbert space of the theory and the basic objects for most interesting physical systems. That is, why we rely on approximation methods, like perturbation theory. In analogy to quantum field theory, we could perhaps develop a perturbation expansion for the decoherence functional, together with a renormalization scheme, in order to adequately treat nonlinear systems

The first problem we would face, is the generic inadequacy of perturbation theory to deal with real-time evolution. In this case we have to expand the operator $e^{-i\hat{H}t}$ in powers of the coupling constant, something that becomes increasingly inaccurate with large values of t. In standard quantum theory, this problem is addressed by performing the perturbation expansion, not to the evolution operator, but to its resolvent $(E-\hat{H})^{-1}$, which is essentially its Fourier transform.

The CTP generating functional plays the same role, since it is a ''Fourier transform'' of the decoherence functional. In the CTP formalism, the perturbation theory is well defined, for instance, in the path integral representation, and its accuracy does not depend on the time t. This

leads to a perturbative evaluation of the decoherence functional, that does not suffer from the problems of real-time perturbation theory. As such, it provides a valuable tool for the construction of powerful approximation schemes in the histories program.

E. The histories quantization program

The main motivation of this paper is to be found in the histories quantization program. This aims to exploit the covariant nature and the richer content of the histories approach, in order to study quantum theories of systems with nontrivial temporal structure. The eventual aim is a theory of quantum gravity.

So far the program has dealt with quantum fields in curved spacetime[14,40] (where, unlike the canonical case, we can construct a theory accepting an instantaneous Hamiltonian) and with constrained systems. The two laws of time transformation have enabled a treatment of parametrized systems[15] (prototypes of general relativity), in which the problem of time does not appear. More recent results involve the more elaborate presence of Poincaré groups in quantum field theory[41] and the appearance of a representation of the spacetime diffeomorphism group in the histories version of general relativity.[42]

The main obstacle to further generalization has been the restriction to Fock representations for the history group, and hence only to quadratic systems. In this paper, we have constructed a larger class of representations and therefore enlarged the domain of applicability of the program. We have also indicated, how a perturbative construction of history theories could be implemented.

This will provide tools for continuation of the program: it will be possible to rigorously construct covariant quantum theories for a large class of systems, at least with the same level of rigor as the canonical approach.

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Effective action for QED_4 through ζ function regularization

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We obtain, through ζ function methods, the one-loop effective action for massive Dirac fields in the presence of a uniform, but otherwise general, electromagnetic background. After discussing renormalization, we compare our ζ function result with Schwinger's proper-time approach. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In QED, the effective one-loop Lagrangian describes the effective nonlinear interaction of the electromagnetic fields due to a single fermion loop. In two dimensions, its general form has been obtained both through proper time and ζ function regularizations.[1,2] In four dimensions, on the other hand, only particular field configurations have been studied.

The $3+1$ dimensional problem of constant electromagnetic fields was first studied by Euler and Heisenberg[3] and independently by Weisskopf.[4] These authors obtained an integral expression for the one-loop effective Lagrangian in the framework of the electron-hole theory. Later on, Schwinger rederived this integral representation in a field-theoretical scenario, by making use of proper time techniques.[5] In all these references, explicit results were derived in some limits, the most famous being the weak-field one. This and other particular field configurations were subsequently studied through the proper-time regularization by a number of authors (see, for example, Refs. 6–10).

More recently, the interest in the subject was renewed, and the Euclidean effective action for constant electromagnetic background configurations was studied through ζ function techniques:[11,12] In Ref. 13 analytic expressions were found for the case of purely magnetic fields in any number of dimensions. In this same reference, the case of equal electric and magnetic fields in four Euclidean dimensions was also studied. A step towards more general field configurations was given in Ref. 14, where the authors obtained the effective Lagrangian as a power series in B/E.

It is the aim of this article to obtain, through ζ function methods, an explicit nonperturbative expression for the full one-loop effective action of quantum electrodynamics in four dimensions in the case of constant, but otherwise arbitrary, electromagnetic fields. To this end, we will work in Euclidean space–time, and define the determinant of the relevant Dirac operator $\not{D}$ through the derivative of the ζ function of $\not{D}^\dagger \not{D}$.

The organization of the article is as follows:

After summarizing some well-known generalities in Sec. II, we devote Sec. III to analytically extending the relevant ζ function to the region $\Re s > -2$. (The main point here is the analytic extension of a Barnes ζ function.) Its value at $s=0$ is also given in this section.

In Sec. IV, a complete analytical expression for the effective action in terms of special functions is given, and the renormalization issue is discussed.

Section V contains a comparison between ζ and proper-time regularizations.

The Appendices A and B contain the derivation of some particular limits for the relevant zeta

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and for the effective action, thus allowing for the comparison with previous work on less general field configurations.

II. GENERALITIES

We study the effective action for massive Dirac particles in the presence of uniform, but otherwise arbitrary, electromagnetic background fields. We work in four-dimensional Euclidean space. Then, the effective action in the one-loop approximation is given by

$$S[A_\mu]=S_{\rm cl}[A_\mu]-\log\mathrm{Det}(\not{D}[A_\mu]), \tag{1}$$

where $S_{\rm cl}[A_\mu]$ is the classical Euclidean action and $\not{D}[A_\mu]=\gamma_\mu(\partial_\mu-ieA_\mu)+im$ is the Euclidean Dirac operator, m being the fermion mass.

Note that, even though $\not{D}$ is not self-adjoint, it is normal; so, the functional determinant appearing in the one-loop correction to the action can be defined through ζ function regularization,[11,12] which leads to

$$S_{\rm eff}[A_\mu]=S_{\rm cl}[A_\mu]+S^{(1)}[A_\mu]=S_{\rm cl}[A_\mu]+\frac{1}{2}\frac{\partial}{\partial s}\zeta(s;\not{D}^\dagger\not{D})\big]_{s=0}. \tag{2}$$

In order to evaluate the one-loop correction $S^{(1)}$ in the previous expression, it is necessary to obtain the spectrum of the operator $\not{D}^\dagger\not{D}$, which is well known in the case of uniform fields.[15] In this particular situation, one can always choose a reference frame such that $F_{03}=-F_{30}=E$ and $F_{12}=-F_{21}=B$, while the remaining components of the field tensor vanish. When doing so, the required zeta function turns out to be

$$\begin{aligned}\zeta(s;\not{D}^\dagger\not{D})=\mu^4\Omega\frac{ab}{4\pi^2}\Bigg[&2\sum_{n_a=1}^{\infty}(2n_a a+c)^{-s}+2\sum_{n_b=1}^{\infty}(2n_b b+c)^{-s}\\&+4\sum_{n_a=1}^{\infty}\sum_{n_b=1}^{\infty}(2n_a a+2n_b b+c)^{-s}+c^{-s}\Bigg].\end{aligned} \tag{3}$$

Here, Ω is the volume of the four-dimensional Euclidean space, $a=e|E|/\mu^2$, $b=e|B|/\mu^2$, $c=m^2/\mu^2$, and μ is a parameter with mass dimension, introduced to render the ζ function dimensionless. Note that the series in Eq. (3) are all convergent for $\Re s>2$, where they define an analytic function of s.

III. ANALYTIC EXTENSION OF THE ζ FUNCTION

In this section, we will perform the analytic extension of the relevant ζ function to a region containing $s=0$. In particular, we will show it to be finite at $s=0$ and give its value at this point.

The first two terms in Eq. (3) can be rewritten in terms of Hurwitz' zeta functions, which are well known to be meromorphic functions with a unique simple pole at $s=1$. On the other hand, the third term is a zeta function of the Barnes' type[16,17] (see also Refs. 18 and 19 and references therein). In order to analytically extend this term, we write it in integral form. After doing so, we get

$$\begin{aligned}\zeta(s;\not{D}^\dagger\not{D})=\mu^4\Omega\frac{ab}{4\pi^2}\Bigg\{&\frac{2}{(2a)^s}\zeta\left(s,\frac{c}{2a}+1\right)+\frac{2}{(2b)^s}\zeta\left(s,\frac{c}{2b}+1\right)\\&+\frac{1}{\Gamma(s)}\int_0^\infty dt\,t^{s-1}\frac{4e^{-2at}e^{-2bt}e^{-ct}}{(1-e^{-2at})(1-e^{-2bt})}+c^{-s}\Bigg\}\\=&\,\mathrm{A}(s)+\mathrm{B}(s)+\mathrm{C}(s)+\mathrm{D}(s),\end{aligned} \tag{4}$$

where $\zeta(s,v)$ is Hurwitz' zeta function. This expression (invariant under $a\leftrightarrow b$) is, in principle, well defined for $\Re s>2$. Since the analytic structure of $A(s)$ and $B(s)$ is well known, we will concentrate on the Barnes term $C(s)$, which will be extended to $\Re s>-2$.

To this end, we will use the expansion[20]

$$\frac{1}{e^{at}-e^{-at}}=\frac{1}{2at}+at\sum_{k=1}^{\infty}(-1)^k\frac{1}{(at)^2+(k\pi)^2}, \tag{5}$$

thus obtaining

$$\begin{aligned}C(s)&=2\mu^4\Omega\frac{ab}{4\pi^2}\frac{1}{\Gamma(s)}\left\{\frac{1}{2a}\int_0^\infty dt\,t^{s-2}\frac{e^{-(a+b+c)t}}{e^{bt}-e^{-bt}}\right.\\&\quad\left.+a\int_0^\infty dt\,t^s\frac{e^{-(a+b+c)t}}{e^{bt}-e^{-bt}}\sum_{k=1}^{\infty}(-1)^k\frac{1}{(at)^2+(k\pi)^2}\right\}+a\leftrightarrow b\\&=C_1(s)+C_2(s).\end{aligned} \tag{6}$$

The first term, $C_1(s)$, can be easily seen to be

$$C_1(s)=2\mu^4\Omega\frac{ab}{4\pi^2}\frac{1}{2a}\frac{1}{(s-1)(2b)^{s-1}}\zeta\left(s-1,\frac{a+2b+c}{2b}\right)+a\leftrightarrow b. \tag{7}$$

As all the terms we have analytically extended up to this point, $C_2(s)$ in Eq. (6) involves an integral which diverges at $s=0$. In order to isolate this singularity, we will rewrite this term as

$$\begin{aligned}C_2(s)&=2\mu^4\Omega\frac{ab}{4\pi^2}\frac{1}{\Gamma(s)}a\int_0^\infty dt\,t^s\frac{e^{-(a+b+c)t}}{(e^{bt}-e^{-bt})}\left\{\sum_{k=1}^{\infty}(-1)^k\left[\frac{1}{(at)^2+(k\pi)^2}-\frac{1}{(k\pi)^2}\right]\right.\\&\quad\left.+\sum_{k=1}^{\infty}(-1)^k\frac{1}{(k\pi)^2}\right\}+a\leftrightarrow b\\&=CF_2(s)+CD_2(s).\end{aligned} \tag{8}$$

The integral appearing in $CD_2(s)$ is divergent at $s=0$ but, after performing the sum, this term is easily seen to be

$$CD_2(s)=-\mu^4\Omega\frac{ab}{4\pi^2}\frac{a}{6}\frac{s}{(2b)^{s+1}}\zeta\left(s+1,1+\frac{a+c}{2b}\right)+a\leftrightarrow b. \tag{9}$$

Now, once the difference between brackets is performed, $CF_2(s)$ can be rewritten as

$$CF_2(s)=-2\mu^4\Omega\frac{ab}{4\pi^2}\frac{1}{\Gamma(s)}a^3\sum_{k=1}^{\infty}\frac{(-1)^k}{(k\pi)^2}\int_0^\infty dt\,t^{s+2}\frac{e^{-(a+2b+c)t}}{(1-e^{-2bt})}\frac{1}{(at)^2+(k\pi)^2}+a\leftrightarrow b. \tag{10}$$

As is easily seen, this integral converges for $\Re s>-2$. We have thus obtained an analytic extension for the ζ of the operator as a meromorphic function with only simple poles. Such extension is valid for $\Re s>-2$.

Now, the factor $1/[(at)^2+(k\pi)^2]$ can be written as an integral. In fact,

$$\frac{1}{(at)^2+(k\pi)^2}=\frac{-1}{2ik\pi}\left[\frac{1}{at+ik\pi}-\frac{1}{at-ik\pi}\right]=\frac{1}{k\pi}\int_0^\infty du\, e^{-atu}\sin(k\pi u).$$

When replaced in Eq. (10), this gives

$$\mathrm{CF}_2(s)=-2\mu^4\Omega\frac{ab}{4\pi^2}\frac{1}{\Gamma(s)}a^3\sum_{k=1}^{\infty}\frac{(-1)^k}{(k\pi)^3}\int_0^\infty dt\, t^{s+2}\frac{e^{-(a+2b+c)t}}{(1-e^{-2bt})}\int_0^\infty du\, e^{-atu}\sin(k\pi u)+a\leftrightarrow b$$

or, after interchanging the integrals

$$\mathrm{CF}_2(s)=-2\mu^4\Omega\frac{ab}{4\pi^2}\frac{a^3}{\Gamma(s)}\sum_{k=1}^{\infty}\frac{(-1)^k}{(k\pi)^3}\int_0^\infty du\,\sin(k\pi u)\frac{\Gamma(s+3)}{(2b)^{s+3}}\zeta\left(s+3,\frac{a+2b+c+au}{2b}\right)$$
$$+a\leftrightarrow b.$$

When the ζ function is written in terms of its series development (which is valid for $\Re s>-2$) one has (after interchanging this series and the integral)

$$\mathrm{CF}_2(s)=-2\mu^4\Omega\frac{ab}{4\pi^2}\frac{a^3}{\Gamma(s)}\frac{\Gamma(s+3)}{(2b)^{s+3}}\sum_{k=1}^{\infty}\frac{(-1)^k}{(k\pi)^3}\sum_{l=1}^{\infty}\int_0^\infty du\,\sin(k\pi u)\left(l+\frac{a+c+au}{2b}\right)^{-(s+3)}$$
$$+a\leftrightarrow b.$$

Finally, after performing the remaining integral and making use of the functional relations between incomplete gamma functions,[21] one gets

$$\mathrm{CF}_2(s)=i\mu^4\Omega\frac{ab}{4\pi^2}\frac{\Gamma(s+3)}{\Gamma(s)}a^{-s}\frac{1}{s+2}\sum_{k=1}^{\infty}\frac{(-1)^k}{(k\pi)^{1-s}}\sum_{l=1}^{\infty}\left[i^{s+2}e^{i(k\pi/a)(2bl+a+c)}\Gamma\left(-s\right.\right.$$
$$\left.\left.-1,i\frac{k\pi}{a}(2bl+a+c)\right)-(-i)^{s+2}e^{-i(k\pi/a)(2bl+a+c)}\Gamma\left(-s-1,-i\frac{k\pi}{a}(2bl+a+c)\right)\right]$$
$$+a\leftrightarrow b. \tag{11}$$

The replacement of Eqs. (7), (9) and (11) into Eq. (4) completes the analytic extension of the relevant ζ function. Its value at $s=0$ can be easily computed, which gives

$$\zeta(0;\mathbb{D}^\dagger\mathbb{D})=\frac{\mu^4\Omega}{4\pi^2}\left\{\frac{1}{2}c^2+\frac{a^2+b^2}{3}\right\}. \tag{12}$$

The agreement with the known results for null and equal fields is shown in Appendix A.

IV. THE EFFECTIVE ACTION AND ITS RENORMALIZATION

This section contains the main result in this article, i.e., the one-loop correction to the Euclidean effective action. According to Eq. (2), to obtain such result, one must perform the derivatives at $s=0$ of the various terms in Eq. (4).

We start from $\mathrm{A}(s)$, which contributes with

$$\frac{1}{2}\frac{\partial}{\partial s}\mathrm{A}(s)\Big|_{s=0}=\mu^4\Omega\frac{ab}{4\pi^2}\left\{\log(2a)\left(\frac{1}{2}+\frac{c}{2a}\right)+\log\Gamma\left(\frac{c}{2a}+1\right)-\frac{1}{2}\log(2\pi)\right\}. \tag{13}$$

In a completely analogous way, one has

$$\frac{1}{2}\frac{\partial}{\partial s}\mathrm{B}(s)\Big|_{s=0}=\mu^4\Omega\,\frac{ab}{4\pi^2}\left\{\log(2b)\left(\frac{1}{2}+\frac{c}{2b}\right)+\log\Gamma\left(\frac{c}{2b}+1\right)-\frac{1}{2}\log(2\pi)\right\}. \tag{14}$$

It is also through a direct calculation that one gets

$$\frac{1}{2}\frac{\partial}{\partial s}\mathrm{C}_1(s)\Big|_{s=0}=\mu^4\Omega\,\frac{ab}{4\pi^2}\,\frac{1}{2a}\left\{2b(-1+\log(2b))\zeta\left(-1,1+\frac{a+c}{2b}\right)\right.$$
$$\left.-2b\,\frac{\partial}{\partial s}\Big|_{s=0}\zeta\left(s-1,1+\frac{a+c}{2b}\right)\right\}+a\leftrightarrow b. \tag{15}$$

$$\frac{1}{2}\frac{\partial}{\partial s}\mathrm{CD}_2(s)\Big|_{s=0}=\mu^4\Omega\,\frac{ab}{4\pi^2}\,\frac{a}{24b}\left\{\log(2b)+\Psi\left(1+\frac{a+c}{2b}\right)\right\}+a\leftrightarrow b. \tag{16}$$

As regards $\mathrm{CF}_2(s)$, due to the presence of $\Gamma(s)$ in the denominator, the required derivative reduces to the product $\Gamma(s)\,\mathrm{CF}_2(s)$ at $s=0$, i.e.,

$$\frac{1}{2}\frac{\partial}{\partial s}\mathrm{CF}_2(s)\Big|_{s=0}=-\frac{i}{2}\mu^4\Omega\,\frac{ab}{4\pi^2}\sum_{k=1}^{\infty}\frac{(-1)^k}{k\pi}\sum_{l=1}^{\infty}\left[e^{i(k\pi/a)(2bl+a+c)}\Gamma\left(-1,\frac{ik\pi}{a}(2bl+a+c)\right)\right.$$
$$\left.-e^{-i(k\pi/a)(2bl+a+c)}\Gamma\left(-1,-\frac{ik\pi}{a}(2bl+a+c)\right)\right]+a\leftrightarrow b. \tag{17}$$

Summarizing, the Euclidean effective action is given by the sum of the partial contributions in Eqs. (13)–(17), plus

$$\frac{1}{2}\frac{\partial}{\partial s}\mathrm{D}(s)\Big|_{s=0}=-\mu^4\Omega\,\frac{ab}{8\pi^2}\log(c). \tag{18}$$

Notice that even though the result is finite, it depends on the arbitrary parameter μ. However, this effective action still admits a finite renormalization. We will perform it by adopting the criterium (used, for instance, in Ref. 22), that a very massive field does not fluctuate. Thus, we will subtract the one loop correction to the effective action in the limit $m\to\infty$. From Eq. (B6) in Appendix B, the effective action in this limit can be seen to be

$$\mu^4\Omega\,\frac{1}{4\pi^2}\left\{\left[\frac{3}{8}-\frac{1}{4}\log(c)\right]c^2-\frac{1}{6}(b^2+a^2)\log(c)\right\}. \tag{19}$$

After doing this subtraction, all dependence on the parameter μ disappears, and the Euclidean effective action is given by

$$S_{\mathrm{eff}}^{\mathrm{Ren}}[A_\mu]=\frac{\Omega\mu^4}{2e^2}(a^2+b^2)+\mu^4\Omega\,\frac{ab}{4\pi^2}\left\{\frac{1}{8}\log\left(\frac{4ab}{c^2}\right)-\frac{1}{24}\,\frac{(a^2+b^2)}{ab}\log\left(\frac{4ab}{c^2}\right)+\frac{c}{4a}\log\left(\frac{a}{b}\right)\right.$$
$$-\frac{c^2}{16ab}\log\left(\frac{4ab}{c^2}\right)+\log\left(\frac{\Gamma(c/2a+1)}{\sqrt{2\pi}}\right)-\frac{b}{a}\zeta\left(-1,1+\frac{a+c}{2b}\right)-\frac{b}{a}\,\frac{\partial}{\partial s}\Big|_{s=0}\zeta\left(s-1,1\right.$$
$$\left.\left.+\frac{a+c}{2b}\right)-\frac{i}{2}\sum_{k=1}^{\infty}\frac{(-1)^k}{k\pi}\sum_{l=1}^{\infty}\left[e^{i(k\pi/a)(2bl+a+c)}\Gamma\left(-1,\frac{ik\pi}{a}(2bl+a+c)\right)\right.\right.$$

$$-e^{-i(k\pi/a)(2bl+a+c)}\Gamma\left(-1,\frac{-ik\pi}{a}(2bl+a+c)\right)\Bigg]$$

$$+\frac{a}{24b}\Psi\left(1+\frac{a+c}{2b}\right)-\frac{3}{16}\frac{c^2}{ab}+a\leftrightarrow b\Bigg\}. \tag{20}$$

The renormalization performed amounts to subtracting the zero field effective action (thus redefining the cosmological constant), and renormalizing the classical action. As a result, one gets the following running charge relationship:

$$\frac{1}{e^2}=\frac{1}{e_0^2}+\frac{1}{12\pi^2}\log\frac{\mu^2}{m^2}. \tag{21}$$

Equivalently, for the fine structure constant one has

$$\alpha=\frac{\alpha_0}{1+(\alpha_0/3\pi)\log\mu^2/m^2}. \tag{22}$$

Note that this expression reduces, in the perturbative limit, to the well known result (see, for example, Ref. 23)

$$\alpha=\alpha_0\left(1-\frac{\alpha_0}{3\pi}\log\frac{\mu^2}{m^2}\right). \tag{23}$$

V. COMPARISON WITH THE PROPER TIME RESULT

In Appendix B we show that, in the weak field limit, our result for the ζ regularized effective action coincides, once renormalized, with the Euclidean version of the well known Schwinger's proper time one.

In this section, we will show that this is also the case for arbitrary field strengths. In fact, Schwinger's integral expression for the one loop correction to the effective action is given, after subtracting the divergent terms, by

$$S_{PT}^{(1)}=\mu^4\Omega\Bigg\{\frac{ab}{8\pi^2}\int_0^\infty dt\,t^{s-1}e^{-ct}\coth(bt)\coth(at)-\frac{1}{8\pi^2}\int_0^\infty dt\,t^{s-3}e^{-ct}$$

$$-\frac{a^2+b^2}{24\pi^2}\int_0^\infty dt\,t^{s-1}e^{-ct}\Bigg\}\Bigg|_{s=0}. \tag{24}$$

Now, performing the integrals in the last two terms and comparing with Eq. (4) (with the Hurwitz's zetas written in integral form), the previous expression can be rewritten as

$$S_{PT}^{(1)}=\frac{1}{2}\left\{\Gamma(s)\zeta(s;\mathcal{D}^\dagger\mathcal{D})-\frac{\mu^4\Omega}{4\pi^2}\left(c^{2-s}\Gamma(s-2)+\frac{a^2+b^2}{3}c^{-s}\Gamma(s)\right)\right\}\Bigg|_{s=0}. \tag{25}$$

After developing around $s=0$, it is easy to see that

$$S_{PT}^{(1)}=S_\zeta^{(1)}-\frac{\mu^4\Omega}{4\pi^2}\left[\frac{3}{8}c^2-\left(\frac{c^2}{4}+\frac{a^2+b^2}{6}\right)\log c\right], \tag{26}$$

where $S_\zeta^{(1)}$ is the ζ-regularized one loop correction to the effective action, as defined in Eq. (2), and the remaining terms are precisely the ones we have subtracted through renormalization. So, the exact agreement between both renormalized effective actions is apparent.

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APPENDIX A: THE LIMITS OF NULL AND EQUAL FIELDS

In this section, we will show the agreement of our general ζ function with the results obtained by other authors for some particular cases, i.e., the case of a null electric or magnetic field[13,14] and that of equal electric and magnetic fields.[13]

We will start with the $B\to 0$ limit. It is easy to see that $\lim_{b\to 0}\mathrm{A}(s)=0$. As regards $\lim_{b\to 0}\mathrm{B}(s)$, it can be studied by making use of the asymptotic expansion for Hurwitz' ζ function (see, for example, Ref. 24),

$$\zeta(s,v)=\frac{1}{\Gamma(s)}\left\{v^{1-s}\Gamma(s-1)+\frac{1}{2}v^{-s}\Gamma(s)+\sum_{n=1}^{N}B_{2n}\frac{\Gamma(s+2n-1)}{(2n)!}v^{1-s-2n}\right\}+O(v^{-2N-s-1}), \tag{A1}$$

$$\lim_{b\to 0}\mathrm{B}(s)=\lim_{b\to 0}\left\{\mu^4\Omega\,\frac{ab}{4\pi^2}\,\frac{2}{(2b)^s}\,\frac{\Gamma(s-1)}{\Gamma(s)}\left(\frac{c}{2b}+1\right)^{1-s}\right\}=\frac{\mu^4\Omega}{4\pi^2}\,\frac{a}{s-1}c^{1-s}. \tag{A2}$$

The only contribution to $\mathrm{C}(s)$ in this limit comes from $\mathrm{C}_1(s)$, which gives

$$\lim_{b\to 0}\mathrm{C}(s)=\frac{\mu^4\Omega}{4\pi^2}\,\frac{(2a)^{2-s}}{s-1}\left\{\zeta\left(s-1,\frac{c}{2a}\right)-\left(\frac{c}{2a}\right)^{1-s}\right\}. \tag{A3}$$

Finally, $\mathrm{D}(s)$ vanishes for $b=0$. Then, replacing all these partial results into Eq. (4), one obtains

$$\zeta(s,\mathbb{D}^\dagger\mathbb{D})\rfloor_{b=0}=\frac{\mu^4\Omega}{4\pi^2}\,\frac{(2)^{1-s}}{s-1}a^{2-s}\left\{2\zeta\left(s-1,\frac{c}{2a}\right)-\left(\frac{c}{2a}\right)^{1-s}\right\}, \tag{A4}$$

which is in complete agreement with previous results.[13,14]

Of course, the $E\to 0$ limit gives an analogous expression, which can be obtained by changing $a\to b$ in Eq. (A4).

We will now study the equal fields limit. In this situation, taking $a=b$ in the different terms appearing in the ζ function (4), we have

$$\begin{aligned}\zeta(s;\mathbb{D}^\dagger\mathbb{D})\rfloor_{a=b}=\mu^4\Omega\,\frac{a^2}{4\pi^2}\Bigg\{&\frac{4}{(2a)^s}\zeta\left(s,\frac{c}{2a}+1\right)+c^{-s}+\frac{2^{2-s}a^{-s}}{s-1}\zeta\left(s-1,\frac{3}{2}+\frac{c}{2a}\right)\\&-\frac{1}{6}(2a)^{-s}\,\zeta\left(s+1,\frac{3}{2}+\frac{c}{2a}\right)-i\,2\,a^{-s}(s+1)s\\&\times\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{(k\pi)^{1-s}}\sum_{l=1}^{\infty}\left[i^{s+2}e^{ik\pi(2l+1+c/a)}\Gamma\left(-s-1,ik\pi\left(2l+1+\frac{c}{a}\right)\right)\right.\end{aligned}$$

$$-(-i)^{s+2}e^{-ik\pi(2l+1+c/a)}\Gamma\left(-s-1,-ik\pi\left(2l+1+\frac{c}{a}\right)\right)\Bigg]\Bigg\}. \tag{A5}$$

In order to compare this expression with the result in Ref. 13, we use the functional relations between incomplete gamma functions once more, thus getting

$$\begin{aligned}\zeta(s;\mathbb{D}^{\dagger}\mathbb{D})\rfloor_{a=b}=\mu^4\Omega\frac{a^2}{4\pi^2}\Bigg\{&\frac{4}{(2a)^s}\zeta\left(s,\frac{c}{2a}+1\right)+c^{-s}+\frac{2^{2-s}a^{-s}}{s-1}\zeta\left(s-1,\frac{3}{2}+\frac{c}{2a}\right)\\&-i\,2\,a^{-s}s\sum_{k=1}^{\infty}\frac{(-1)^k}{(k\pi)^{1-s}}\sum_{l=1}^{\infty}\Bigg[i^{s+2}e^{ik\pi(2l+1+c/a)}\Gamma\left(-s,ik\pi\left(2l+1+\frac{c}{a}\right)\right)\\&-(-i)^{s+2}e^{-ik\pi(2l+1+\frac{c}{a})}\Gamma(-s,-ik\pi(2l+1+c/a))\Bigg]\Bigg\}.\end{aligned} \tag{A6}$$

We now use the integral representation for the incomplete gamma function

$$\Gamma(\alpha,x)=\int_x^{\infty}dt\,e^{-t}t^{\alpha-1}.$$

When doing so, and after interchanging the integral and the sum over l, the last term in Eq.(A6) can be written as

$$\begin{aligned}&(2a)^{-s}s\sum_{k=1}^{\infty}\frac{(-1)^k}{(k\pi)^2}\int_0^{\infty}du\,e^{-u}\left[\zeta\left(s+1,\frac{3}{2}+\frac{c}{2a}-\frac{iu}{2k\pi}\right)+\zeta\left(s+1,\frac{3}{2}+\frac{c}{2a}+\frac{iu}{2k\pi}\right)\right]\\&=2(2a)^{-s}\frac{1}{\Gamma(s)}\sum_{k=1}^{\infty}(-1)^k\int_0^{\infty}dt\,t^s\frac{e^{-(3/2+c/2a)t}}{1-e^{-t}}\frac{1}{(k\pi)^2+(t/2)^2}\end{aligned}$$

where we have used the integral form for the Hurwitz's zeta functions, interchanged the integrals and performed the interior one.

Interchanging now the integral with the sum, and using Eq. (5), we obtain

$$\begin{aligned}&2^{2-s}a^{-s}\frac{1}{\Gamma(s)}\int_0^{\infty}dt\,t^{s-1}\frac{e^{-(3/2+c/2a)t}}{1-e^{-t}}\left[\frac{e^{-t/2}}{1-e^{-t}}-\frac{1}{t}\right]\\&=2^{2-s}a^{-s}\left[\zeta\left(s-1,\frac{c}{2a}+1\right)-\left(\frac{c}{2a}+1\right)\zeta\left(s,\frac{c}{2a}+1\right)-\frac{1}{s-1}\zeta\left(s-1,\frac{3}{2}+\frac{c}{2a}\right)\right].\end{aligned}$$

When replaced in (A6), the final result is

$$\begin{aligned}\zeta(s;\mathbb{D}^{\dagger}\mathbb{D})\rfloor_{a=b}&=\mu^4\Omega\frac{a^2}{4\pi^2}\left\{c^{-s}+2^{2-s}a^{-s}\left[\zeta\left(s-1,\frac{c}{2a}+1\right)-\frac{c}{2a}\zeta\left(s,\frac{c}{2a}+1\right)\right]\right\}\\&=\mu^4\Omega\frac{a^2}{4\pi^2}\left\{c^{-s}+4(2a)^{-s}\left(\zeta\left(s-1,\frac{c}{2a}\right)-\frac{c}{2a}\zeta\left(s,\frac{c}{2a}\right)\right)\right\}.\end{aligned} \tag{A7}$$

This expression coincides with the result obtained in Ref. 13 [see Eqs. (5.2.6) and (5.2.4) in that reference].

APPENDIX B: THE WEAK-FIELD LIMIT

An unavoidable test our effective action must resist is its coincidence with the well known result for weak fields.[3,5] In order to check this is the case, we will develop the different contributions to the effective action [Eqs. (13)–(18)] in powers of the fields over the squared mass. In the cases of Eqs. (13)–(16), such development can be obtained by making use of the well known asymptotic expansions[24] for $\log\Gamma(x)$, $\psi(x)$, and $\zeta(s,x)$ [see also our Eq. (A1)]. When doing so, and retaining terms up to the order of squared fields over mass to the fourth, one gets, after a straightforward though tedious calculation,

$$\frac{1}{2}\frac{\partial}{\partial s}\mathrm{A}(s)\Big|_{s=0} \simeq \mu^4\Omega\,\frac{ab}{4\pi^2}\left\{\frac{1}{6}ac^{-1}+\frac{1}{2}\log(c)+\frac{1}{2a}(\log(c)-1)c\right\}, \tag{B1}$$

$$\frac{1}{2}\frac{\partial}{\partial s}\mathrm{B}(s)\Big|_{s=0} \simeq \mu^4\Omega\,\frac{ab}{4\pi^2}\left\{\frac{1}{6}bc^{-1}+\frac{1}{2}\log(c)+\frac{1}{2b}(\log(c)-1)c\right\}, \tag{B2}$$

$$\begin{aligned}\frac{1}{2}\frac{\partial}{\partial s}\mathrm{C}_1(s)\Big|_{s=0} \simeq{}& \mu^4\Omega\,\frac{ab}{4\pi^2}\frac{1}{ab}\left\{\left(\frac{1}{4}-\frac{1}{4}\log c+\frac{1}{8}\right)c^2+\left(\frac{1}{2}(a+b)-\frac{1}{2}(a+b)\log c\right)c-\frac{5}{24}(a^2\right.\\ &+b^2)\\ &-\frac{1}{2}ab\log c-\frac{1}{24}(5ba^2+5ab^2+a^3+b^3)c^{-1}\\ &\left.+\left(\frac{1}{24}b^3a+\frac{1}{24}a^3b+\frac{1}{12}b^2a^2+\frac{7}{1440}a^4+\frac{7}{1440}b^4\right)c^{-2}\right\},\end{aligned} \tag{B3}$$

$$\begin{aligned}\frac{1}{2}\frac{\partial}{\partial s}\mathrm{CD}_2(s)\Big|_{s=0} \simeq{}& \mu^4\Omega\,\frac{ab}{4\pi^2}\frac{1}{24}\left\{\left(\frac{a}{b}+\frac{b}{a}\right)\log c+\left(a+b+\frac{a^2}{b}+\frac{b^2}{a}\right)c^{-1}\right.\\ &\left.-\frac{1}{2}\left(2a^2+2b^2+\frac{a^3}{b}+\frac{b^3}{a}+\frac{4}{3}ba\right)c^{-2}\right\}.\end{aligned} \tag{B4}$$

As regards $\frac{1}{2}(\partial/\partial s)\mathrm{CF}_2(s)\rfloor_{s=0}$, one has to use the asymptotic expansions for the incomplete Γ function and for the Hurwitz' zeta functions [Eq. (A1)]. After doing so, one obtains

$$\frac{1}{2}\frac{\partial}{\partial s}\mathrm{CF}_2(s)\Big|_{s=0} \simeq \mu^4\Omega\,\frac{ab}{4\pi^2}\,\frac{7}{1440}\left(\frac{a^3}{b}+\frac{b^3}{a}\right)c^{-2}. \tag{B5}$$

By summing up the contributions in Eqs. (B1)–(B5), plus the one coming from $\frac{1}{2}(\partial/\partial s)\mathrm{D}(s)\rfloor_{s=0}$, the one-loop correction to the effective action is seen to reduce, in this weak-field limit, to

$$S^{(1)}=\mu^4\Omega\,\frac{1}{4\pi^2}\left\{\left[\frac{3}{8}-\frac{1}{4}\log(c)\right]c^2-\frac{1}{6}(b^2+a^2)\log(c)+\left[\frac{7}{90}(ab)^2-\frac{1}{90}(a^2+b^2)^2\right]c^{-2}\right\}. \tag{B6}$$

Now, renormalizing according to the criterium discussed in Sec. IV, one is left with

$$S_{\mathrm{eff}}=\frac{\Omega}{2}(B^2+E^2)+\frac{\Omega e^4}{8\pi^2m^4}\left[\frac{7}{45}(EB)^2-\frac{1}{45}(E^2+B^2)^2\right], \tag{B7}$$

where the definitions of a, b and c given in the paragraph following Eq. (3) were used.

The expression in (B7) is precisely the Euclidean version of the Euler–Heisenberg effective action for weak fields.[3,5]

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Monopoles and dyons in SO(3) gauged Skyrme models

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Three-dimensional SO(3) gauged Skyrme models characterized by specific potentials imposing special asymptotic values on the chiral field are considered. These models are shown to support finite energy solutions with nonvanishing magnetic and electrix flux, whose energies are bounded from below by two distinct charges—the magnetic (monopole) charge and a noninteger version of the Baryon charge. Unit magnetic charge solutions are constructed numerically and their properties characterized by the chosen asymptotics and the Skyrme coupling are studied. For a particular value of the chosen asymptotics, charge-2 axially symmetric solutions are also constructed and the attractive nature of the like-monopoles of this system are exhibited. As an indication toward the possible existence of large clumps of monopoles, some consideration is given to axially symmetric monopoles of charges 2,3,4. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In the O(4), or usual, Skyrme[1] model in three dimensions, the finite energy conditions uniquely specify the asymptotic value at large distances of the chiral field. Depending on the parametrization, either the SU(2) valued field U or the S^3 valued field ϕ^a, subject to $|\phi^a|^2$, with $a=1,2,3,4$, this asymptotic value is

$$\lim_{r\to\infty} U=\mathbb{1} \qquad \text{or} \qquad \lim_{r\to\infty}\phi^4=1. \tag{1}$$

The fields U and ϕ^a are related through

$$U=\phi^a\sigma^a, \quad U^\dagger=\phi^a\tilde{\sigma}^a, \tag{2}$$

where in terms of the Pauli matrices $\vec{\tau}$, $\sigma^a=(i\tau^i,\mathbb{1})$ and $\tilde{\sigma}^a=(-i\tau^i,\mathbb{1})$.

Often, the static Hamiltonian of the Skyrme system is augmented with a ''pion-mass'' potential

$$V_\pi(\phi^a)=m_\pi(1-\phi^4), \tag{3}$$

consistent with the asymptotics (1). The only practical effect that the inclusion of this potential (3) has is that it renders the asymptotic behavior of the chiral function exponential, where in its absence this would have been a power decay.

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The situation is very different when the Skyrme model is gauged in one[2] or other[3] gauging prescription, as a result of which the asymptotic value of the chiral field is not fixed uniquely by finite energy conditions. This feature of three-dimensional gauged Skyrme models was considered and highlighted in Ref. 4.

In the present work, we augment the three-dimensional SO(3) gauged Skyrme model studied in Refs. 5 and 3 with the following potential:

$$V=\lambda(\cos\omega-\phi^4)^2, \quad \pi\geqslant\omega\geqslant 0, \tag{4}$$

whose effect is to specify the asymptotic values of the chiral field uniquely, consistent with finiteness of the energy. Like (3), this potential is also chosen such that it results in the exponential behavior of ϕ^4 asymptotically. The new asymptotics are

$$\lim_{r\to 0}\phi^4=-1, \quad \lim_{r\to\infty}\phi^4=\cos\omega. \tag{5}$$

It is clear from (5) that the volume integral of the density that maps the field space to the configuration space is not going to be an integer except in the case where $\omega=0$. Thus the lower bounds labeled by this charge cannot be identified with the degree of the map, or the topological baryon charge, except when $\omega=0$. Such a noninteger charge, however, does supply a legitimate lower bound on the energy integral. For want of a better name, we shall persist in calling such charges $Q_B(\omega)$, with the understanding that only $Q_B(0)$ is really the baryon charge.

In the generic case $\pi\geqslant\omega\geqslant 0$, there will be an independent lower bound in addition to $Q_B(\omega)$, namely the magnetic monopole flux $\mu(\omega)$, which also depends on ω. These lower bounds will be stated explicitly in the following. The main feature of the dynamics characterized by the potential (4), with $\omega\neq 0$, is that the SO(3) is broken down to U(1), with the residual Maxwell field described by the corresponding 't Hooft-tensor supporting a magnetic flux. Like the charge $Q_B(\omega)$, this magnetic flux $\mu(\omega)$ is integer also only modulo a continuous factor depending on ω, and takes an integer value only when $\omega=\pi/2$. The solutions we have found turn out, as expected, to respect both lower bounds $\mu(\omega)$ and $Q_B(\omega)$.

We have confirmed the existence of finite energy solutions bounded by the charges $\mu(\omega)$ and $Q_B(\omega)$ by numerical construction. An interesting result is that when $\omega\neq 0$, the solution persists even when the Skyrme coupling constant vanishes, i.e., $\kappa_2=0$ in (7) and (8). This is not surprising since the presence of the Yang–Mills term satisfies the (Derrick) scaling requirement independent of the Skyrme term, and in this case, the soliton is bounded from below only by the magnetic flux μ. This will be explained in more detail in Sec. II, where the model is defined and the two said lower bounds will be stated. Then in Sec. III, we study the spherically symmetric solutions for various ω and κ, and find the ranges of these two parameters for which solutions exist by numerical construction. In Sec. IV, we study the axially symmetric magnetic charge-2 solution for the particular value of the parameter $\omega=\pi/2$, with a view to learning whether two like monopoles of that system can be in an attractive or a repulsive phase. We encounter the rather surprising result that even for $\kappa_2=0$ this is *attractive*, and then as expected it becomes even more attractive with increasing $\kappa_2>0$. Section V is devoted to summarizing and discussing our results.

II. THE MODEL AND LOWER BOUNDS

The model is specified by the gauging prescription and is the three-dimensional model used in Refs. 5 and 3, augmented by the potential (4). Usually, we will treat this potential as a *gedanken* entity and will not exploit it save as an agency justifying the asymptotics (5). In terms of the S^3 valued field $\phi^a=(\phi^\alpha,\phi^4)$, $\alpha=1,2,3$, and the SO(3) gauge connection A^α_μ with curvature $F^\alpha_{\mu\nu}$, the covariant derivative is defined by the prescription

$$D_\mu\phi^\alpha=\partial_\mu\phi^\alpha+\varepsilon^{\alpha\beta\gamma}A^\beta_\mu\phi^\gamma, \qquad D_\mu\phi^4=\partial_\mu\phi^4. \tag{6}$$

Since much of the analysis will be almost identical to that in (the relevant) Sec. III of Ref. 3, we will use the same notation here. This will enable us to present some of the new results without the necessity of repeating the detailed analyses leading to them. The model is described by the Lagrangian

$$\mathcal{L}=-\kappa_0^4|F_{\mu\nu}^{\alpha}|^2+\tfrac{1}{2}\kappa_1^2|D_\mu\phi^a|^2-\tfrac{1}{2}\kappa_2^4|D_{[\mu}\phi^a D_{\nu]}\phi^b|^2-V(\phi^4), \tag{7}$$

which in the temporal gauge $A_0^{\alpha}=0$ yields the static Hamiltonian

$$\mathcal{H}=\kappa_0^4|F_{ij}^{\alpha}|^2+\tfrac{1}{2}\kappa_1^2|D_i\phi^a|^2+\tfrac{1}{2}\kappa_2^4|D_{[i}\phi^a D_{j]}\phi^b|^2+V(\phi^4). \tag{8}$$

The potential $V(\phi^4)$ in both (7) and (8) is that given by (4). In our study of the ''monopole,'' we will be mainly concerned with the energy density functional (8), but we give the corresponding Lagrangian (7) too in anticipation of our discussion of the corresponding ''dyon'' solution.

We proceed to state the two distinct lower bounds on the energy, namely the volume integral of (8). Both bounds, the ''magnetic monopole'' charge and the noninteger ''baryon charge,'' pertain to the generic asymptotics (5) with $\omega\neq 0$, dictated by (4).

The first of these follows from the classic Bogomol'nyi inequality

$$\kappa_0^4|F_{ij}^{\alpha}|^2+\tfrac{1}{2}\kappa_1^2|D_i\phi^{\alpha}|^2\geqslant\kappa_0^2\kappa_1\varepsilon_{ijk}\partial_k(\phi^{\alpha}F_{ij}^{\alpha}). \tag{9}$$

It is obvious that the left-hand side of (9) can be replaced by $\mathcal{H}$ of (8), by adding suitable positive definite terms to it, resulting in

$$\mathcal{H}\geqslant\kappa_0^2\kappa_1\varepsilon_{ijk}\partial_k(\phi^{\alpha}F_{ij}^{\alpha}), \tag{10}$$

on the right-hand side of which we recognize the U(1) 't Hooft-tensor, $\phi^{\alpha}F_{ij}^{\alpha}$, of the residual gauge field responsible for the magnetic flux provided that $\omega\neq 0$, so that $|\phi^{\alpha}|\to\sin\omega\neq 0$ asymptotically.

To state the corresponding inequality for the other lower bound, we define the ''baryon charge'' density and its covariantized version, respectively,

$$\varrho_0=\frac{1}{12\pi^2}\varepsilon_{ijk}\varepsilon^{abcd}\partial_i\phi^a\partial_j\phi^b\partial_k\phi^c\phi^d, \tag{11}$$

$$\varrho_G=\frac{1}{12\pi^2}\varepsilon_{ijk}\varepsilon^{abcd}D_i\phi^a D_j\phi^b D_k\phi^c\phi^d. \tag{12}$$

The volume integral of (11) is the noninteger ''baryon charge''

$$\int \mathrm{d}^3x\,\varrho_0=(\pi-\omega)N, \tag{13}$$

except when $\omega=0$, when it is simply the integer N, the degree of the map or the usual baryon charge. The actual gauge invariant charge density which enters the relevant inequality is defined in terms of ϱ_G in (12) by[5,3]

$$\varrho=\varrho_G+3\varepsilon_{ijk}\phi^{\alpha}F_{ij}^{\alpha}D_k\phi^4, \tag{14}$$

whose volume integral turns out to be equal to the ''baryon charge'' (13).

As shown in Ref. 3, it follows that

$$\mathcal{H} \geqslant \frac{\kappa_1 \kappa_2^2}{\sqrt{1+9\left(\frac{\kappa_2}{\kappa_0}\right)^4}} \varrho . \tag{15}$$

We can now conclude from (9) and (15) the two distinct lower bounds on the energy $E = \int \mathrm{d}^3 x \mathcal{H}$, namely the ''magnetic'' and ''baryonic'' lower bounds, following from the asymptotics (5)

$$E \geqslant 4\pi \kappa_0^2 \kappa_1 \sin \omega, \tag{16}$$

$$E \geqslant \frac{12\pi \kappa_1 \kappa_2^2}{\sqrt{1+9\left(\frac{\kappa_2}{\kappa_0}\right)^4}} (\pi - \omega). \tag{17}$$

The two inequalities (16) and (17) signal the possibility of finding finite energy solutions bounded from below, provided that the (Derrick) scaling requirement is satisfied, which for (8) in three dimensions, it is. For the limiting case of $\omega = 0$ considered in Ref. 3, inequality (16) trivializes and (17) then coincides with the lower bound used in Ref. 3. In the other limit when $\omega = \pi$, both (16) and (17) trivialize so we would expect to find no nontrivial solutions in this case. This will be confirmed by our numerical results to be given in the following. For generic values of ω between these two limiting values, both lower bounds are valid independently, and any nontrivial finite energy solution must respect these. This will also be confirmed by our numerical results.

It should perhaps be pointed out that neither of the bounds (10) or (15) can be saturated. As we shall see in Sec. III, for $\omega \neq 0$ finite energy solutions persist also for $\kappa_2 = 0$. But even in that case, the inequality (10) cannot be saturated. Thus in the $\kappa_2 = 0$ model, we have a system which does not saturate a Bogomol'nyi bound and whose stress-energy tensor therefore never vanishes. It follows that the charge-2 monopole of this model is *either* attractive *or* repulsive, a property which it shares with the usual (ungauged) Skyrme model,[1] in the latter case as is well known it being attractive.[6] We shall find in Sec. IV that the model with $\kappa_2 = 0$ supports solutions describing mutually attracting like monopoles. Then as expected, when the Skyrme coupling constant κ_2 is switched on this binding energy will grow further, as is usual with other theories[7] involving Skyrme-like kinetic terms.

III. SPHERICALLY SYMMETRIC SOLUTIONS

In Sec. III A we present the reduced one-dimensional subsystems of (7) and (8), while in Sec. III B we present our numerical results.

A. One-dimensional subsystems

As in Ref. 3, we impose the spherical symmetry thus

$$A_0^\alpha = \kappa_1^{-1} g(r)\, \hat{x}^\alpha, \quad A_i^\alpha = \frac{a(r)-1}{r} \varepsilon_{i\alpha\beta} \hat{x}^\beta, \tag{18}$$

$$\phi^\alpha = \sin f(r) \hat{x}^\alpha, \quad \phi^4 = \cos f(r). \tag{19}$$

The ensuing reduced one-dimensional Lagrange and (static) Hamiltonian, subject to a suitable rescaling $r \to x$ such that all constants but the Skyrme coupling $\kappa_2^4 \equiv \kappa$ are suppressed, are, respectively,

$$L=-2\left(2a'^2+\frac{(a^2-1)^2}{x^2}\right)-\frac{1}{2}(x^2f'^2+2a^2\sin^2 f)$$
$$-2\kappa a^2\sin^2 f\left(2f'^2+\frac{a^2\sin^2 f}{x^2}\right)+x^2g'^2+2a^2g^2, \tag{20}$$

$$H=2\left(2a'^2+\frac{(a^2-1)^2}{x^2}\right)+\frac{1}{2}(x^2f'^2+2a^2\sin^2 f)+2\kappa a^2\sin^2 f\left(2f'^2+\frac{a^2\sin^2 f}{x^2}\right). \tag{21}$$

Note that we have suppressed the potential terms arising from (4) in (20) and (21), since as will be explained in the following, nearly all of numerical constructions will be carried out in the $\lambda=0$ limit.

While (21) is positive definite, (20) is not. The latter will be relevant only in some remarks that follow concerning the dyon solution of this system.

Let us first consider the case of primary interest, namely the monopole solutions of the equations following from the static energy density functional (21). The finite energy conditions require the following asymptotic values:

$$\lim_{x\to 0} f(x)=\pi, \quad \lim_{x\to\infty} f(x)=\omega, \tag{22}$$

$$\lim_{x\to 0} a(x)=1, \quad \lim_{x\to\infty} a(x)=0, \tag{23}$$

as long as $\omega\neq 0$. This is the case of interest in the present work. (The $\omega=0$, which is only a limiting case here, was studied in detail in Ref. 3.)

The behaviors of the functions $f(x)$ and $a(x)$ in the $x\ll 1$ region are independent of the value of λ in (4), and they are

$$f(x)=\pi+F_1x+o(x^3) \quad (x\ll 1), \tag{24}$$

$$a(x)=1+A_1x^2+o(x^4) \quad (x\ll 1). \tag{25}$$

In the $x\gg 1$ region, the asymptotic behavior of the function $a(x)$ is again independent of the value of λ and is

$$a(x)=A\,e^{(-1/2)\,x\sin\omega}, \quad A=\text{const}, \tag{26}$$

while that of the function $f(x)$ does depend on λ. In the limit of vanishing λ and finite λ, these are, respectively, the power and exponential decays,

$$f(x)=\omega-\frac{F}{x}+o\left(\frac{1}{x^2}\right), \tag{27}$$

$$f(x)=\omega-\tilde{F}\frac{e^{-\sqrt{2\lambda}x}}{x}, \tag{28}$$

where F and $\tilde{F}$ are constants which can be evaluated by the numerical process.

Thus, like with the usual (ungauged) Skyrme model, the addition of this potential results in the exponential localization of the chiral function $f(r)$. In the numerical work presented in the following we have used $\lambda=0$ throughout, since the qualitative properties of the solutions are unchanged when $\lambda>0$. This was verified in many typical cases and thereafter the potential (4)

played a *gedanken* role, rather like for the Prasad–Sommerfield limit of the Georgi–Glashow model, except that here the $\lambda=0$ limit is not particularly interesting since it does not lead to the saturation of any Bogomol'nyi bound.

Dyon solution. Before proceeding to describe our numerical results concerning the monopole solutions of this model, we briefly allude to the corresponding dyon solutions. Following Julia and Zee[8] we vary the energy density (20) with respect to the functions $a(r)$, $g(r)$, and $f(r)$. Since (20) is not positive definite, the radial ansatz (18) and (19) is not guaranteed to be consistent with the full Euler–Lagrange equations of this system. It has, however, been verified in Ref. 9 that (18) and (19) are indeed consistent.

The crucial equation that signals the existence of a dyon solution is the $r\gg 1$ asymptotic equation arising from the variation of the function $a(x)$,

$$a''=a\left(\frac{a^2-1}{x^2}-g^2+\sin^2 f+\ldots\right), \tag{29}$$

which in the $x\to\infty$ limit reduces to

$$a''=(\sin^2\omega-g^2)a,$$

which yields acceptable exponentially decaying solutions only when the asymptotic value of $q=\lim_{x\to\infty} g(x)$ satisfies the condition

$$0\leqslant q\leqslant \sin\omega, \tag{30}$$

and otherwise leading to unacceptable oscillatory behavior for the function $a(r)$ asymptotically.

With the asymptotic condition (30), one has the behavior

$$g(x)=q-\frac{c}{x}+o(x^{-2}), \tag{31}$$

in which the constant c is evaluated by the numerical integrations and parametrizes the electric flux of the dyon. We do not repeat here the detailed results of the numerical process as this is identical to that for the dyon[8] of the Georgi–Glashow model, as presented in Ref. 9. The relevant analysis in Sec. V of Ref. 9 can be adapted to the present model, by substituting the condition $0\leqslant q\leqslant 1$ there, by (30).

The only qualitative difference between the dyon of the Georgi–Glashow model and the dyon of the present model is, that unlike in the former case there is no Prasad–Sommerfield limit here.

B. Numerical results

Solving the spherically symmetric equations for numerous values of the parameters $\kappa\in]0,\infty[$ and $\omega\in]0,\pi[$, strongly indicates that they admit at least one regular, finite-energy solution for each choice of these parameters.

The behavior of the solution in the limit $\omega\to 0$ is different according to the value of κ and is strongly influenced by the pattern of solutions occurring in the case $\omega=0$. We briefly recall (see Refs. 3 and 9 for further details) that for $\omega=0$, solutions with $a(\infty)=0$ exist only for $\kappa>\kappa_{\rm cr}$, $\kappa_{\rm cr}\approx 0.697$. For $\kappa\in]0.0,0.697[$ the relevant solution has $a(\infty)=1$.

Let us now describe how the solutions look like for fixed κ, with ω varying. We have found it convenient to characterize the solutions by the value of the asymptotic coefficient F defined in Eq. (27). The evolution of this parameter is reported in Fig. 1 for several values of κ. For $\kappa>\kappa_{\rm cr}$ the solutions are such that the function $f(x)$ [respectively $a(x)$] decreases monotonically from π (respectively, 1) for $x=0$ to ω (respectively, 0) for $x\to\infty$. The parameter F is positive as seen in Fig. 1 for $\kappa=1.0$. The classical energy decreases monotonically when ω increases. In the limit $\omega\to 0$ the classical solutions of Ref. 3 are smoothly approached.

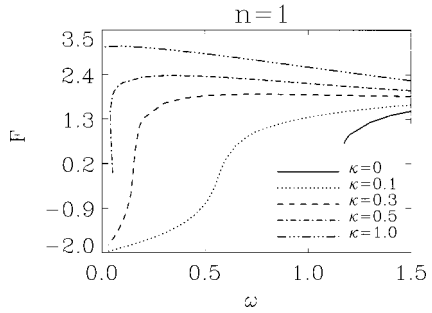

FIG. 1. The quantity F that determines the asymptotic behavior of the Skyrme field function f with $f(x\gg 1)=\omega-F/x+o(1/x^2)$ is shown as a function of ω for $n=1$ and different values of κ.

The behavior of the solutions is more elaborate when $\kappa<\kappa_{\mathrm{cr}}$; this is illustrated in Figs. 1 and 2 for $\kappa=0.1$. One new feature is that the parameter F undergoes a change of sign when ω varies from 0 to π. For large enough values of ω (say, $\omega>\omega_{\max}$, $\omega_{\max}\approx 0.5$ in the case $\kappa=0.1$), the profiles of $f(x)$ and of $a(x)$ monotonically decrease as functions of x and the classical energy decreases for ω increasing. For $\omega<\omega_{\max}$ the function $f(x)$ develops a local minimum at an intermediate value of x and the parameter F defined in Eq. (27) becomes negative. Moreover, the function $a(x)$ develops a local minimum and a local maximum at finite values (say x_m, x_M) of the radial variable. In this region of ω the classical energy increases with ω. When the limit $\omega\to 0$ is considered our numerical analysis indicates that x_m stays finite, x_M increases, and the value $a(x_M)$ approaches $a=1$ in such a way that the corresponding profile of the $\omega=0$ solution is approached on $[0,x_M]$. The corresponding value of the classical energy is also reproduced. These different features are illustrated in Figs. 1 and 2.

Considered as a function of ω, we also observed (see Fig. 2) that the classical energy is maximal at an intermediate value of ω. Our numerical analysis indicates that the maximum is attained precisely for $\omega=\omega_{\max}$, i.e., at the value where the change of sign of the parameter F occurs. The κ dependence of $\omega_{\max}$ is reported in Fig. 3.

As further suggested by Fig. 1, in the region $\kappa\approx 0.5$, $\omega\approx 0.05$ the pattern of the solutions becomes very complicated. We obtained strong numerical evidence that several branches of solutions exist in this region. That is to say, e.g., that we find more than one solution for $\kappa=0.5$, $\omega=0.05$. However these new branches seem to exist on a very small domain of the parameter ω, the numerical analysis is therefore rather difficult in this region. Since the study of such details is not the aim of the present paper, we refrained from further pursuing our numerical analysis in this region.

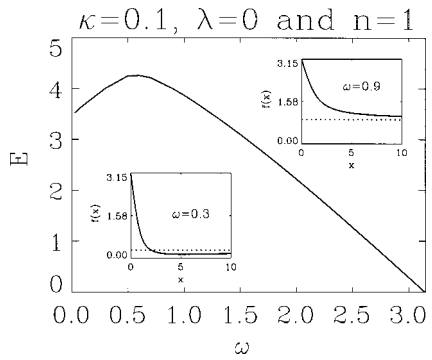

FIG. 2. The energy E of the $n=1$ solution is shown as a function of ω for $\kappa=0.1$ and $\lambda=0$. The two inlets show the Skyrme field function $f(x)$ as function of the radial coordinate x for (a) $\omega=0.3<\omega_{\max}$ and (b) $\omega=0.9>\omega_{\max}$.

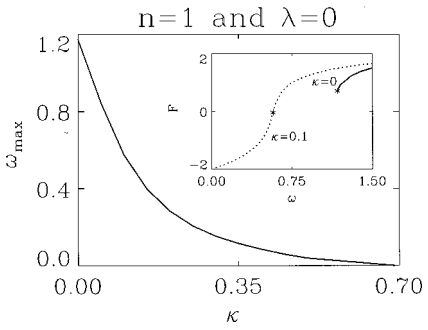

FIG. 3. $\omega_{\max}$, the value of ω at which the energy has its maximum, is shown as a function of κ. The inlet shows the quantity F (see Fig. 1) over ω for $\kappa=0$ and 0.1. The asterisks mark $\omega_{\max}(\kappa)$.

To finish this section, we mention that, choosing $\kappa=0$, we were able to construct numerical solutions for $\omega>1.1729$. The analysis of the solutions in the limit $\kappa\to 0$ (with fixed $\omega<1.1729$), seems to lead to a discontinuity of the function $f(x)$.

IV. AXIALLY SYMMETRIC SOLUTIONS

In Sec. IV A the axially symmetric ansatz and the boundary conditions of the axially symmetric solutions are stated. In Sec. IV B, the numerical results are given.

Our objective in this section is to construct higher magnetic charge solutions, and in the first instance charge-2 axially symmetric solutions, with the aim of discovering whether like monopoles of this model are in an attractive or a repulsive phase. In this framework, we will restrict our analysis to monopole rather than dyon solutions, in the temporal gauge $A_0=0$.

The analysis carried out in this section is less general than that given in Sec. III for the spherically symmetric solutions. There, we studied the detailed dependence of the solutions on the parameter ω specifying the dynamics. Having exposed these properties satisfactorily, we proceed to study the most natural subset of models here, namely those specified by $\omega=\pi/2$, supporting monopoles of *integer* magnetic charges.

Within this $\omega=\pi/2$ subset of models, we consider the models specified by the Skyrme coupling κ_2, or the effective parameter κ for the range $\kappa\geqslant 0$ which includes interestingly the point $\kappa=0$.

A. Ansatz and boundary conditions

With magnetic charge, or azimuthal winding, $n=1,2,3,...$, the axially symmetric ansatz[10] for the gauge field is

$$A_\mu\,\mathrm{d}x^\mu=\frac{1}{2r}[\,\tau_\phi^n(H_1\,\mathrm{d}r+(1-H_2)r\,\mathrm{d}\theta)-n(\tau_r^n H_3+\tau_\theta^n(1-H_4))r\sin\theta\,\mathrm{d}\phi], \tag{32}$$

and for the Skyrme field it is

$$U=\tfrac{1}{2}(\cos f\mathbb{1}+\sin f[(\sin g\sin\theta+\cos g\cos\theta)\tau_r^n+(\sin g\cos\theta-\cos g\sin\theta)\tau_\theta^n]), \tag{33}$$

where H_1,H_2,H_3,H_4,f, and g are functions of the coordinates r and θ. The symbols τ_r^n, τ_θ^n, and τ_ϕ^n denote the dot products of the Cartesian vector of Pauli matrices, $\vec{\tau}=(\tau_x,\tau_y,\tau_z)$, with the spatial unit vectors

$$\vec{e}_r^{\,n}=(\sin\theta\cos n\phi,\sin\theta\sin n\phi,\cos\theta),$$

$$\vec{e}_\theta^{\,n}=(\cos\theta\cos n\phi,\cos\theta\sin n\phi,-\sin\theta), \tag{34}$$

$$\vec{e}_{\phi}^{\,n}=(-\sin n\phi,\cos n\phi,0),$$

respectively.

For $n=1$, $H_1=H_3=0$, $H_2=H_4=a(r)$, $f=f(r)$, and $g=\theta$ the spherically symmetric ansatz of (18) and (19) is recovered.

The residual U(1) gauge degree of freedom[10] is fixed by the condition $r\partial_r H_1-\partial_\theta H_2=0$, which is just the Coulomb gauge in the two-dimensional residual U(1) subsystem resulting from the imposition of radial symmetry in the $x-y$ plane, i.e., with radius $\rho=\sqrt{x^2+y^2}$.

At the origin the boundary conditions for the gauge field functions read

$$H_2|_{r=0}=H_4|_{r=0}=1,\quad H_1|_{r=0}=H_3|_{r=0}=0, \tag{35}$$

and for the Skyrme functions

$$f|_{r=0}=\pi,\quad \partial_r g|_{r=0}=0. \tag{36}$$

For the gauge field to approach the asymptotic configuration of a monopole we choose

$$H_2|_{r=\infty}=H_4|_{r=\infty}=0,\quad H_1|_{r=\infty}=H_3|_{r=\infty}=0, \tag{37}$$

and for the Skyrme field functions

$$f|_{r=\infty}=\omega,\quad g|_{r=\infty}=\theta. \tag{38}$$

The boundary conditions along the ρ and z axes are determined by the symmetries. For the gauge field functions symmetry considerations lead to the boundary conditions

$$\begin{aligned} &H_1|_{\theta=0}=H_3|_{\theta=0}=0,\quad \partial_\theta H_2|_{\theta=0}=\partial_\theta H_4|_{\theta=0}=0,\\ &H_1|_{\theta=\pi/2}=H_3|_{\theta=\pi/2}=0,\quad \partial_\theta H_2|_{\theta=\pi/2}=\partial_\theta H_4|_{\theta=\pi/2}=0 \end{aligned} \tag{39}$$

along the axes, as well as the condition

$$H_2|_{\theta=0}=H_4|_{\theta=0}. \tag{40}$$

Along these axes the Skyrme field functions satisfy the following boundary conditions:

$$\begin{aligned} &\partial_\theta f|_{\theta=0}=0,\quad \partial_\theta g|_{\theta=0}=1,\\ &\partial_\theta f|_{\theta=\pi/2}=0,\quad \partial_\theta g|_{\theta=\pi/2}=1. \end{aligned} \tag{41}$$

B. Numerical results

Solving the set of partial differential equations numerically for the model characterized by $\omega=\pi/2$, and for different values of κ, we find that even for $\kappa=0$ there is only an attractive phase. As shown in Fig. 4, the difference δE of the energy per winding number n between the $n=1$ and $n=2$ increases with increasing κ. This is an indication that in this model two monopole bound states can exist. However, a definitive demonstration of this is well beyond the scope of the present work. (That would involve finding the dependence of the interaction energy on the separation of the two monopoles.)

Moreover, we calculated the energy $E_n(\kappa)$ for different values of κ and n. The values are given in the tables below. Unfortunately the numerical process becomes less reliable with increasing monopole charge n. As a result we restrict our numerical constructions to $n\leqslant 4$ only. For $\kappa=0$, $\kappa=3$, and $\kappa=5$ we find

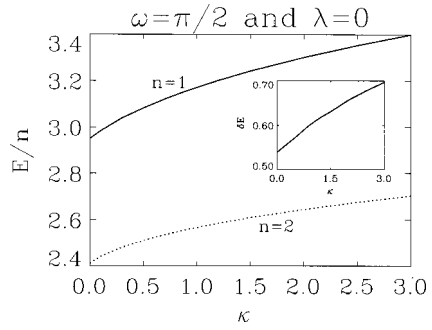

FIG. 4. The energy per winding number E/n is shown as a function of κ for $n=1$ and $n=2$, $\omega=\pi/2$, and $\lambda=0$. The inlet shows the difference of the energy per winding number $\delta E=E(n=1)-E(n=2)/2$ between the $n=1$ and the $n=2$ solution.

n	1	2	3	4
$E_n(0)$	2.95	4.82	6.63	7.56

n	1	2	3	4
$E_n(3)$	3.40	5.40	7.30	8.80

n	1	2	3	4
$E_n(5)$	3.48	5.60	7.50	9.31

From this data we can deduce some quantitative information on the interaction energies of the monopoles leading to the possible formation of lumps of charges $n\leqslant 4$. To this end we define the following ''binding energy'' corresponding to the energy needed to dissociate a charge-n lump into a charge-$n-1$ and a charge-1 lump, divided by the energy of the charge-n lump.

$$\Delta E_n^{\{n-1,1\}}(\kappa)=\frac{[E_{n-1}(\kappa)+E_1(\kappa)]-E_n(\kappa)}{E_n(\kappa)}. \tag{42}$$

The values for different κ and n are given as follows:

n	$\Delta E_n^{\{n-1,1\}}(0)$	$\Delta E_n^{\{n-1,1\}}(3)$	$\Delta E_n^{\{n-1,1\}}(5)$
2	0.22	0.26	0.24
3	0.17	0.21	0.21
4	0.27	0.22	0.18

This table shows that for all three values of κ, $\Delta E_n^{\{n-1,1\}}(\kappa)$ remains positive, which is an indication of the existence of monopole lumps of charges up to $n=4$.

It is hard to extract any reliable conclusion from such meagre data, but the fact that the binding energies do not seem to decrease with increasing n is encouraging from the point of view

of the possibility of finding very large monopole clumps. This question will be investigated elsewhere, using different numerical techniques.

V. SUMMARY AND DISCUSSION

We have studied a particular variant of the Skyrme model gauged according to the prescription (6), equivalent to the commutator gauging with respect to the SU(2) gauge connection $A_i = -(i/2)\vec{A}_i \cdot \vec{\tau}$,

$$D_i U = \partial_i U + [A_i, U], \tag{43}$$

which is augmented by the potential (4). The function of this potential is to fix the boundary value of the Skyrme field at large distances which, unlike in the usual (ungauged) Skyrme model, is not fixed by the requirement of finite energy.[11] Thus we have considered a set of the gauged Skyrme models characterized by the parameter ω appearing in the potential (4). In the usual Skyrme model $\omega = 0$.

The qualitative properties of the solitons, depending on the parameters ω and κ characterizing the models, are studied in the spherically symmetric case.

The main effect of the boundary condition $\omega \neq 0$ is the breaking of the SO(3) gauge symmetry of the solution down to SO(2), asymptotically. This is related to the nonvanishing VEV of the Skyrme field ϕ^α. This can be seen clearly from the second member of (5). In addition to this magnetic charge, a noninteger version of the baryon number given by (13) is also associated with this solution. We have verified the existence of finite energy solutions bounded from below by both these charges for the allowed ranges of ω. The latter (ranges) depend also on the (effective) Skyrme coupling κ of the model. These ranges have been illustrated in Fig. 1.

A surprising if not unexpected property of these models is that the model characterized by $\kappa = 0$ does support a soliton. This could have been expected since in the presence of the Yang–Mills term it is not necessary to have a Skyrme term to satisfy the (Derrick) scaling requirement. We found that the solitons of the $\kappa = 0$ models are generally quite similar to those of the models with $\kappa \neq 0$, with one noticeable qualitative difference. This concerns the restricted range of allowed ω for the $\kappa = 0$ model as seen in Fig. 1 (and in Fig. 3), which in addition to this qualitative feature also illustrates the fact that for small enough κ the profile of the chiral function $f(r)$ sinks below its asymptote ω and approaches it from below.

By contrast when $\omega = 0$, the model with $\kappa = 0$ cannot support a soliton because in that case the lower bound (10) disappears, leaving only the lower bound (13) in place, and the latter trivializes in the $\kappa = 0$ limit. This is also borne out by the graphs in Fig. 1.

After exposing the qualitative features of the solitons in the spherically symmetric case, we studied axially symmetric solutions of the model. Our aim here was to discover if like monopoles of the $\omega \neq 0$ models are in attractive or repulsive phases. For this purpose we restricted ourselves to the $\omega = \pi/2$ model, which has the nice feature of having integer magnetic charge. We did however consider varying values of the (effective) Skyrme parameter κ, including the distinguished case of $\kappa = 0$.

The main interest in the model specified by $\kappa = 0$ in this respect is that, like the usual (ungauged) Skyrme model, it exhibits no free coupling constants that can parametrize the crossover from an attractive to a repulsive phase. Like the latter it also lacks a neutral, or Bogomol'nyi saturated phase, where the (static Euclidean) stress-energy tensor would have vanished leading to noninteracting solitons. Thus the unique phase in which the solitons are supported is of special interest, especially if it were attractive because then the switching on of κ would most likely not result in a crossover to a repulsive phase. We have verified that this is precisely what happens, as illustrated in Fig. 4 for the magnetic charge-2 soliton. An outstanding problem in this context is the calculation of the (attractive) interaction energy of two one-monopoles as a function of their separation. This would demonstrate the existence of bound states definitively.

In addition to verifying that these models support mutually attracting like monopoles, we sought some indications as to whether there is the possibility of forming bound states of monopole

charge greater than 2. (Apart from its intrinsic interest, the formation of very large monopole clumps may be relevant in cosmology.) To this end, axially symmetric solutions with monopole charges $n=2,3,4$, for the $\kappa=0$, $\kappa=3$, and the $\kappa=5$ models were constructed. It was seen that all these solitons remained in attractive phases. While it is expected that these axially symmetric solitons with $n>2$ are not the lowest energy solutions, the latter probably exhibiting (solid) Platonic symmetries[12,13] as in the usual Skyrme model, it is nonetheless true that they give a reliable indication toward the existence of such bound states. To this end we list the binding energies against the dissociation of an axially symmetric charge-n monopole into a charge-$n-1$ and a charge-1 monopole in the last table of Sec. IV. We see that this binding energy stays positive and does not change too much as n increases, at least for $n\leqslant 4$. Unfortunately the numerical process was not reliable much beyond $n=4$.

While in the present work our primary aim has been the qualitative study of the solitons of the gauged Skyrme model characterized by $\omega\neq 0$, and the resulting property of the interaction of like monopoles in these theories, it may be in order to emphasize some physically attractive features of these models. These models combine some attractive features of (a) Higgs models, in this case the Georgi–Glashow model in that they support monopoles, and features of (b) Skyrme models, in this case the usual Skyrme model[1] in that the like-charged solitons are in an attractive phase. Indeed it appears that the attraction properties of these models are considerably more pronounced than those of the Skyrme model.[1]

Apart from the practical consideration of the possibility of supporting large monopole clumps, there are two theoretical properties of the models that deserve mention. One is the physically desirable property of the symmetry breaking from SU(2) to U(1), and the other one is the fact that the $\kappa=0$ model supports solitons with much the same qualitative properties as the generic models. The considerable advantage of this is that we avail of the Skyrme THEORTIC feature of mutually attracting solitons without having to pay the price of featuring a (quartic kinetic) Skyrme term in the Lagrangian, thus avoiding the attendant severe problems of quantization.

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Generalized Goldstone theorem: Automatic imposition of the Higgs mechanism and application to scale and conformal symmetry breaking

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Standard discussions of Goldstone's theorem based on a symmetry of the action assume constant fields and global transformations, i.e., transformations which are independent of spacetime coordinates. By allowing for arbitrary field distributions in a general representation of the symmetry we derive a generalization of the standard Goldstone's theorem. When applied to gauge bosons coupled to scalars with a spontaneously broken symmetry the generalized theorem automatically imposes the Higgs mechanism, i.e., if the expectation value of the scalar field is nonzero then the gauge bosons must be massive. The other aspect of the Higgs mechanism, the disappearance of the ''would be'' Goldstone boson, follows directly from the generalized symmetry condition itself. We also use our generalized Goldstone's theorem to analyze the case of a system in which scale and conformal symmetries are both spontaneously broken. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Symmetry, symmetry breaking, Goldstone bosons and the Higgs mechanism play a very important role in modern physics. (See, for example, Refs. 1–5.) Here we present a more general approach to these ideas which explores the consequences of Goldstone's theorem for spacetime and gauge symmetries and shows that the Higgs mechanism is not as ''mysterious'' or ''miraculous'' as it is sometimes presented to be. We also resolve some old questions regarding the breaking of scale and conformal symmetry.

We consider the physical consequences of actions which have a symmetry or a set of symmetries. Precisely what we mean by this is discussed in detail below. For concreteness we work out the details for the classical action of a set of fields Φ_a, which we denote by $S[\Phi]$. To treat the quantum theory one computes the functional integral over all field configurations (in a given function space) of $\exp(iS[\Phi]+iJ\cdot\Phi)$ to obtain the generating functional $Z[J]$. Here the dot indicates the appropriate inner product over spacetime position, spacetime indices and internal indices. The effective action $\Gamma[\Phi]$,[1–4] defined via a Legendre transformation of $\ln(Z[J])$, is the analog of $S[\Phi]$ but includes all quantum effects. That is, whereas $\delta S/\delta\Phi(x)=0$ is the equation of motion for the classical field configuration $\Phi_C(x)$, $\delta\Gamma/\delta\Phi(x)=0$ is the equation of motion for the vacuum expectation value of the field $\langle\Phi(x)\rangle$. Indeed the nth functional derivative of $\Gamma[\Phi]$ is the n-point quantum Green's function. Generally, but certainly not always, $\Gamma[\Phi]$ will have the same symmetry properties as $S[\Phi]$. To lowest or ''tree'' order the two actions coincide and in a sense $\Gamma[\Phi]$ can be thought of as just a more complicated functional of Φ than $S[\Phi]$. Hence our approach applies to both $S[\Phi]$ and to $\Gamma[\Phi]$ for any given symmetry that holds for either functional. We will generally assume that Φ is classically a commuting field or quantum mechanically

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a bosonic field, but the same approach can be applied to classical Grassmann fields or to quantum Fermionic fields yielding similar results with, of course, the requisite care in factor ordering.

II. GENERAL SYMMETRY CONDITION

Consider a Lagrangian density $\mathcal{L}(\Phi(x),\partial\Phi(x))$ which depends on a set of fields Φ_a and their first derivatives, $\partial_\mu\Phi_a$. Here a can be an internal index, a spacetime index or a combination of the two. The action is defined by

$$S[\Phi]=\int d^Dx\,\mathcal{L}(\Phi(x),\partial\Phi(x)), \tag{1}$$

and is taken to be invariant, i.e., $S[\Phi]=S[\Phi']$, under a continuous set of transformations of the fields given by

$$\Phi_a(x)\to\Phi'_a(x)=F(\Phi(x),\partial\Phi(x),\ldots,x)=\Phi_a(x)+\Delta_a(\Phi(x),\partial\Phi(x),\ldots,x)+\cdots, \tag{2}$$

where the last expression is the infinitesimal form of the transformation. In terms of the Lagrangian this symmetry has the form

$$\begin{aligned}\int d^Dx\,\mathcal{L}(\Phi(x),\partial\Phi(x))&=\int d^Dx\,\mathcal{L}(\Phi'(x),\partial\Phi'(x))\\&=\int d^Dx\,\mathcal{L}(F(\Phi(x),\partial\Phi(x),\ldots,x),\partial F(\Phi(x),\partial\Phi(x),\ldots,x)).\end{aligned} \tag{3}$$

We have assumed the change in Φ_a may depend locally on Φ_a and possibly explicitly on x as well. For ease of notation we will abbreviate the Φ dependence of $\mathcal{L}$, F and Δ as

$$\begin{aligned}\mathcal{L}(\Phi(x),\partial\Phi(x))&\equiv\mathcal{L}[\Phi(x)],\\F_a(\Phi(x),\partial\Phi(x),\ldots,x)&\equiv F_a[\Phi(x),x],\\\Delta_a(\Phi(x),\partial\Phi(x),\ldots,x)&\equiv\Delta_a[\Phi(x),x].\end{aligned} \tag{4}$$

Infinitesimally a symmetry is simply the statement that the gradient of the action at any point in function space is perpendicular to the direction defined by Δ_a, i.e.,

$$\int d^Dx\,\frac{\delta S[\Phi]}{\delta\Phi_a(x)}\Delta_a[\Phi(x),x]=0. \tag{5}$$

The symmetry condition expressed in (5) is not an equation for Φ and in fact must hold for all values of Φ. Thus all the functional derivatives of (5) with repect to Φ must vanish. This condition effectively assumes the equivalent of analyticity of $S[\Phi]$ in function space. If the same idea is applied to $\Gamma[\Phi]$, the effective action computed by evaluating a functional integral, then the vanishing of the various functional derivatives yields the generalized Ward–Takahashi identities.

Taking one functional derivative of the symmetry condition (5) and evaluating it at the equation of motion yields, as shown below, what can be seen as a generalized Goldstone theorem:

$$\int d^Dx'\left(\frac{\delta^2S}{\delta\Phi_a(x)\,\delta\Phi_b(x')}\Delta_a[\Phi(x'),x']\right)_{\Phi_C}=0. \tag{6}$$

Substituting (1) and assuming locality of Δ_a as expressed in (4) yields the following after some simple manipulations:

$$\left[-\partial_\alpha\left(\frac{\partial^2\mathcal{L}}{\partial(\partial_\alpha\Phi_a)\partial(\partial_\mu\Phi_b)}\partial_\mu\Delta_b\right)-\partial_\alpha\left(\frac{\partial^2\mathcal{L}}{\partial(\partial_\alpha\Phi_a)\partial\Phi_b}\Delta_b\right)+\frac{\partial^2\mathcal{L}}{\partial\Phi_a\,\partial(\partial_\mu\Phi_b)}\partial_\mu\Delta_b+\frac{\partial^2\mathcal{L}}{\partial\Phi_a\,\partial\Phi_b}\Delta_b\right]_{\Phi_C}$$
$$=0. \tag{7}$$

In the remainder of the paper we explore some of the consequences of this equation.

III. GOLDSTONE'S THEOREM

There are nominally two consequences of Goldstone's theorem. The primary one is the requirement for the existence of some number of massless bosons, called Goldstone bosons, in the theory if the symmetry is spontaneously broken. The secondary condition is that the Goldstone bosons decouple from the other degrees of freedom in the limit of zero momentum.

Symmetry breaking is based on the additive nature of (2) which indicates that a given field configuration is not invariant under the symmetry transformation. In particular it is often the case that $\Delta_a\equiv 0$ if and only if $\Phi_a=0$ and so for any nonzero field configuration the transformation in (2) is inhomogeneous and the symmetry is spontaneously broken, i.e., a nonzero field configuration is not invariant under the symmetry transformation whereas the zero field configuration is invariant. This is discussed very clearly in Ref. 5.

We begin by reviewing the standard approach to Goldstone's theorem as given for example in the book by Peskin and Schroeder.[1] This form of the derivation proceeds by considering constant fields and field transformations for Lagrangians of the form

$$\mathcal{L}=T(\partial\Phi)-V(\Phi). \tag{8}$$

Specializing to constant fields the equations of motion reduce to

$$\left.\frac{\partial V}{\partial\Phi_a}\right|_{\Phi_C}=0, \tag{9}$$

which shows that the constant field Φ_C is an extremum, commonly a minimum, of V. Expanding V about this miminum yields

$$V(\Phi)=V(\Phi_C)+\frac{1}{2}(\Phi-\Phi_C)_a(\Phi-\Phi_C)_b\left(\frac{\partial^2 V}{\partial\Phi_a\,\partial\Phi_b}\right)_{\Phi_C}+\ldots. \tag{10}$$

The coefficient of the quadratic term is a symmetric matrix, known as the mass matrix, whose eigenvalues are the square of the masses of the various fields obtained from $(\Phi-\Phi_C)_a$ after applying the linear transformation which diagonalizes the matrix. Since the symmetry condition is taken to hold for arbitrary field configurations it holds as well for constant fields in which case the potential V itself is invariant, i.e.,

$$V(\Phi)=V(\Phi+\Delta), \tag{11}$$

which implies

$$\frac{\partial V}{\partial\Phi_a}\Delta_a(\Phi)=0. \tag{12}$$

Now differentiate with respect to Φ_b and evaluate the result at Φ_C to obtain

$$\left(\frac{\partial^2 V}{\partial\Phi_b\,\partial\Phi_a}\right)_{\Phi_C}\Delta_a(\Phi_C)=0. \tag{13}$$

This shows that the mass matrix has a zero eigenvalue for each linearly independent symmetry vector $\Delta(\Phi_C)$ satisfying the above equation. The number of linearly independent nonzero vectors $\Delta(\Phi_C)$ is referred to as the number of broken generators, N_B, and hence there is one Goldstone boson for each broken generator. Our more general result (6) or equivalently (7) yields this same condition as well if we assume Lagrangians of the form given in (8) and set Φ_C to a constant field in Eq. (6) or (7) which can now clearly be seen as a generalization of the above equation.

The decoupling follows from considering a change of variables which diagonalizes the mass matrix. This can be done by writing

$$\Phi_a = \Phi_a(\xi_i, \rho_j), \tag{14}$$

where $i=1,\ldots,N_B$ and $j=1,\ldots,N-N_B$ with ξ_i and ρ_j defined implicitly by choosing $\Phi_a(\xi_i,\rho_j)$ so that

$$\begin{aligned}\begin{pmatrix} \dfrac{\partial^2 V(\Phi(\xi,\rho))}{\partial\xi_i\,\partial\xi_{i'}} & \dfrac{\partial^2 V(\Phi(\xi,\rho))}{\partial\xi_i\partial\rho_{j'}} \\ \dfrac{\partial^2 V(\Phi(\xi,\rho))}{\partial\rho_j\,\partial\xi_{i'}} & \dfrac{\partial^2 V(\Phi(\xi,\rho))}{\partial\rho_j\,\partial\rho_{j'}} \end{pmatrix}_{\Phi_C} &= \begin{pmatrix} \dfrac{\partial\Phi_a}{\partial\xi_i}\dfrac{\partial^2 V}{\partial\Phi_a\,\partial\Phi_b}\dfrac{\partial\Phi_b}{\partial\xi_{i'}} & \dfrac{\partial\Phi_a}{\partial\xi_i}\dfrac{\partial^2 V}{\partial\Phi_a\,\partial\Phi_b}\dfrac{\partial\Phi_b}{\partial\rho_{j'}} \\ \dfrac{\partial\Phi_a}{\partial\rho_j}\dfrac{\partial^2 V}{\partial\Phi_a\,\partial\Phi_b}\dfrac{\partial\Phi_b}{\partial\xi_{i'}} & \dfrac{\partial\Phi_a}{\partial\rho_j}\dfrac{\partial^2 V}{\partial\Phi_a\,\partial\Phi_b}\dfrac{\partial\Phi_b}{\partial\rho_{j'}} \end{pmatrix}_{\Phi_C} \\ &= \begin{pmatrix} 0 & 0 \\ 0 & -(m_j(\Phi_C))^2\delta_{jj'} \end{pmatrix},\end{aligned} \tag{15}$$

where there is no sum on j in the last matrix. The ξ_i are the Goldstone bosons (the $\xi\xi$ sector of the mass matrix vanishes by definition) and the ρ_i are the remaining bosons, i.e., at any given value of Φ_C the ξ_i are tangent to the symmetry directions at that point in function space whereas the ρ_j are perpendicular to these directions. The symmetry transformation (5) becomes $\xi_i \to \xi_i + \delta\xi_i$, $\rho_j \to \rho_j$ for $\Phi_a \to \Phi_a + \Delta_a(\Phi)$ or equivalently,

$$\Delta_a(\Phi) = \frac{\partial\Phi_a}{\partial\xi_i}\delta\xi_i\,. \tag{16}$$

Note that $\delta\xi_i$ must be constant for $\Delta(\Phi)$ constant. The symmetry condition (5) in terms of the new variables yields

$$\begin{aligned} 0 &= \frac{\delta\mathcal{L}[\Phi(\xi,\rho)]}{\delta\xi_i}\delta\xi_i \\ &= \frac{\partial\mathcal{L}[\Phi(\xi,\rho)]}{\partial\xi_i}\delta\xi_i \\ &= \frac{\partial\mathcal{L}'(\xi,\rho)}{\partial\xi_i}\delta\xi_i\,, \end{aligned} \tag{17}$$

where the $\partial_\mu\delta\xi_i$ term vanishes since $\delta\xi_i$ must be constant for the symmetry to hold. Hence $\partial\mathcal{L}'/\partial\xi_i = 0$ and $\mathcal{L}'$ can depend only on $\partial_\mu\xi_i$. Since $\partial_\mu\xi_i$ vanishes in the limit of zero momentum the Goldstone bosons vanish or decouple in this limit.

IV. AUTOMATIC HIGGS

Consider a $U(1)$ gauge model in which a complex scalar field $\phi = \phi_1 + i\phi_2$ with ϕ_i real, $i=1,2$, is coupled in a locally gauge invariant way to a $U(1)$ gauge field, A_μ. In this case,

$$\Phi_a \to (A_\mu, \phi_i), \tag{18}$$

$$\Delta_a \to (\partial_\mu \theta, \varepsilon_{ij}\phi_j \theta),$$

with θ an arbitrary infinitesimal scalar function of position. Note we are working in units with the electric charge $e=1$. Take the Lagrangian to have the form

$$\begin{aligned}\mathcal{L} &= \mathcal{L}_A(\partial_\mu A_\nu) + \mathcal{L}_\phi(\partial_\mu \phi_i, \phi_i) + \mathcal{L}_{A\phi}(A_\mu, \partial_\mu \phi_i, \phi_i) \\ &= -\tfrac{1}{4} F_{\mu\nu}F^{\mu\nu} + \partial_\mu \phi_i\, \partial^\mu \phi_i - V(\phi_i \phi_i) + \mathcal{L}_{A\phi}(A_\mu, \partial_\mu \phi_i, \phi_i),\end{aligned} \tag{19}$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ so that $\mathcal{L}_A$ is invariant under gauge transformations and $\mathcal{L}_\phi$ is invariant under $\phi \to e^{i\theta}\phi$ for θ constant. The extra term $\mathcal{L}_{A\phi}$ is explicitly included to "boost" the symmetry from a global one to a local one. It allows for terms of the form $A\phi\,\partial\phi$ and $AA\phi\phi$ which are the lowest order terms with saturated indices. That is for arbitrary, i.e., not necessarily infinitesimal θ the full Lagrangian is required to be symmetric under

$$\begin{aligned}A_\mu &\to A_\mu + \partial_\mu \theta, \\ \phi &\to e^{i\theta}\phi.\end{aligned} \tag{20}$$

We explicitly assume the only $\partial\phi\,\partial\phi$ term in $\mathcal{L}$ is the standard kinetic energy term from $\mathcal{L}_\phi$.

For arbitrary infinitesimal functions θ local gauge invariance yields the following symmetry condition for the action:

$$0 = \int d^D x \frac{\delta S}{\delta A_\beta}\partial_\beta \theta + \int d^D x \frac{\delta S}{\delta \phi_j}\varepsilon_{jk}\phi_k \theta. \tag{21}$$

Note that $\mathcal{L}$ is locally gauge invariant and not just S thus the remaining $\int d^D x$ integration in the above equation can be dropped. The generalized symmetry equation yields two distinct equations since we can take derivatives with respect to A and ϕ:

$$\begin{aligned}0 &= \left(\int d^D x \frac{\delta^2 S}{\delta A_\alpha\, \delta A_\beta}\partial_\beta \theta + \int d^D x \frac{\delta^2 S}{\delta A_\alpha\, \delta \phi_j}\varepsilon_{jk}\phi_k \theta \right)_{\Phi_C} \\ &= -\partial_\nu\left(\frac{\partial^2 \mathcal{L}}{\partial(\partial_\nu A_\alpha)\partial(\partial_\mu A_\beta)}\partial_\mu \partial_\beta \theta \right) + \frac{\partial^2 \mathcal{L}}{\partial A_\alpha \partial(\partial_\mu A_\beta)}\partial_\mu \partial_\beta \theta - \partial_\nu\left(\frac{\partial^2 \mathcal{L}}{\partial(\partial_\nu A_\alpha)\partial A_\beta}\partial_\beta \theta \right) \\ &\quad + \frac{\partial^2 \mathcal{L}}{\partial A_\alpha\, \partial A_\beta}\partial_\beta \theta - \partial_\nu\left(\frac{\partial^2 \mathcal{L}}{\partial(\partial_\nu A_\alpha)\partial(\partial_\mu \phi_j)}\partial_\mu \varepsilon_{jk}\,\phi_k \theta \right) + \frac{\partial^2 \mathcal{L}}{\partial A_\alpha \partial(\partial_\mu \phi_j)}\partial_\mu \varepsilon_{jk}\,\phi_k \theta \\ &\quad - \partial_\nu\left(\frac{\partial^2 \mathcal{L}}{\partial(\partial_\nu A_\alpha)\partial \phi_j}\varepsilon_{jk}\phi_k \theta \right) + \frac{\partial^2 \mathcal{L}}{\partial A_\alpha\, \partial \phi_j}\varepsilon_{jk}\phi_k \theta\end{aligned} \tag{22}$$

and

$$\begin{aligned}0 &= \left(\int d^D x \frac{\delta^2 S}{\delta \phi_i\, \delta A_\beta}\partial_\beta \theta + \int d^D x \frac{\delta^2 S}{\delta \phi_i\, \delta \phi_j}\varepsilon_{jk}\phi_k \theta \right)_{\Phi_C} \\ &= -\partial_\nu\left(\frac{\partial^2 \mathcal{L}}{\partial(\partial_\nu \phi_i)\partial(\partial_\mu A_\beta)}\partial_\mu \partial_\beta \theta \right) + \frac{\partial^2 \mathcal{L}}{\partial \phi_i \partial(\partial_\mu A_\beta)}\partial_\mu \partial_\beta \theta - \partial_\nu\left(\frac{\partial^2 \mathcal{L}}{\partial(\partial_\nu \phi_i)\partial A_\beta}\partial_\beta \theta \right) \\ &\quad + \frac{\partial^2 \mathcal{L}}{\partial \phi_i\, \partial A_\beta}\partial_\beta \theta - \partial_\nu\left(\frac{\partial^2 \mathcal{L}}{\partial(\partial_\nu \phi_i)\partial(\partial_\mu \phi_j)}\varepsilon_{jk}\partial_\mu(\phi_k \theta) \right) + \frac{\partial^2 \mathcal{L}}{\partial \phi_i \partial(\partial_\beta \phi_j)}\varepsilon_{jk}\partial_\beta(\phi_k \theta) \\ &\quad - \partial_\nu\left(\frac{\partial^2 \mathcal{L}}{\partial(\partial_\nu \phi_i)\partial \phi_j}\varepsilon_{jk}\phi_k \theta \right) + \frac{\partial^2 \mathcal{L}}{\partial \phi_i\, \partial \phi_j}\varepsilon_{jk}\phi_k \theta.\end{aligned} \tag{23}$$

To simplify notation in both equations we have implicitly assumed that the results have been evaluated at a solution to the equations of motion.

In (22) the first term vanishes identically, the second and third terms vanish because we have not allowed for any derivative coupling of the gauge fields. The fifth term and seventh terms vanish since there are no $\phi\,\partial A$ or $\partial A\,\partial\phi$ terms. In (23) the first and second terms vanish. Using the fact that $\partial_\mu\phi_i\,\partial^\mu\phi_i = g^{\mu\nu}\delta_{ij}\,\partial_\mu\phi_i\,\partial_\nu\phi_j$ is the only term quadratic in the derivatives of ϕ and expanding out all the derivatives of product terms we obtain

$$0=\left(\frac{\partial^2\mathcal{L}}{\partial A_\alpha\,\partial A_\beta}+\frac{\partial^2\mathcal{L}}{\partial A_\alpha\partial(\partial_\beta\phi_j)}\varepsilon_{jk}\phi_k\right)\partial_\beta\theta+\left(\frac{\partial^2\mathcal{L}}{\partial A_\alpha\,\partial\phi_j}\varepsilon_{jk}\phi_k+\frac{\partial^2\mathcal{L}}{\partial A_\alpha\partial(\partial_\beta\phi_j)}\varepsilon_{jk}\,\partial_\beta\phi_k\right)\theta \tag{24}$$

and

$$\begin{aligned}0=&-\left(\frac{\partial^2\mathcal{L}}{\partial(\partial_\nu\phi_i)\partial A_\beta}+2g^{\nu\beta}\varepsilon_{ik}\phi_k\right)\partial_\nu\partial_\beta\theta+\left(\begin{array}{c}\dfrac{\partial^2\mathcal{L}}{\partial\phi_i\,\partial A_\beta}-\partial_\nu\left(\dfrac{\partial^2\mathcal{L}}{\partial(\partial_\nu\phi_i)\partial A_\beta}\right)-4\varepsilon_{ik}\,\partial^\beta\phi_k\\ +\left(\dfrac{\partial^2\mathcal{L}}{\partial\phi_i\partial(\partial_\beta\phi_j)}-\dfrac{\partial^2\mathcal{L}}{\partial(\partial_\beta\phi_i)\partial\phi_j}\right)\varepsilon_{jk}\phi_k\end{array}\right)\partial_\beta\theta\\ &+\left(\begin{array}{c}-2\varepsilon_{ik}\,\partial^2\phi_k+\left(\dfrac{\partial^2\mathcal{L}}{\partial\phi_i\partial(\partial_\beta\phi_j)}-\dfrac{\partial^2\mathcal{L}}{\partial(\partial_\beta\phi_i)\partial\phi_j}\right)\varepsilon_{jk}\,\partial_\beta\phi_k\\ +\left(\dfrac{\partial^2\mathcal{L}}{\partial\phi_i\,\partial\phi_j}-\partial_\nu\left(\dfrac{\partial^2\mathcal{L}}{\partial(\partial_\nu\phi_i)\partial\phi_j}\right)\right)\varepsilon_{jk}\phi_k\end{array}\right)\theta.\end{aligned} \tag{25}$$

Since θ is an arbitrary function the coefficients of $\theta,\partial\theta$ and $\partial\partial\theta$ must vanish independently which yields the following:

$$0=\frac{\partial^2\mathcal{L}}{\partial A_\alpha\,\partial A_\beta}+\frac{\partial^2\mathcal{L}}{\partial A_\alpha\partial(\partial_\beta\phi_j)}\varepsilon_{jk}\phi_k, \tag{26}$$

$$0=\frac{\partial^2\mathcal{L}}{\partial A_\alpha\,\partial\phi_j}\varepsilon_{jk}\phi_k+\frac{\partial^2\mathcal{L}}{\partial A_\alpha\partial(\partial_\beta\phi_j)}\varepsilon_{jk}\,\partial_\beta\phi_k, \tag{27}$$

$$0=\frac{\partial^2\mathcal{L}}{\partial(\partial_\nu\phi_i)\partial A_\beta}+2g^{\nu\beta}\varepsilon_{ik}\phi_k, \tag{28}$$

$$0=\frac{\partial^2\mathcal{L}}{\partial\phi_i\,\partial A_\beta}-\partial_\nu\left(\frac{\partial^2\mathcal{L}}{\partial(\partial_\nu\phi_i)\partial A_\beta}\right)-4\varepsilon_{ik}\,\partial_\beta\phi_k+\left(\frac{\partial^2\mathcal{L}}{\partial\phi_i\partial(\partial_\beta\phi_j)}-\frac{\partial^2\mathcal{L}}{\partial(\partial_\beta\phi_i)\partial\phi_j}\right)\varepsilon_{jk}\phi_k-2\varepsilon_{ik}\partial^2\phi_k, \tag{29}$$

$$0=+\left(\frac{\partial^2\mathcal{L}}{\partial\phi_i\partial(\partial_\beta\phi_j)}-\frac{\partial^2\mathcal{L}}{\partial(\partial_\beta\phi_i)\partial\phi_j}\right)\varepsilon_{jk}\,\partial_\beta\phi_k+\left(\frac{\partial^2\mathcal{L}}{\partial\phi_i\,\partial\phi_j}-\partial_\nu\left(\frac{\partial^2\mathcal{L}}{\partial(\partial_\nu\phi_i)\partial\phi_j}\right)\right)\varepsilon_{jk}\phi_k. \tag{30}$$

For a constant solution to the ϕ equations of motion, i.e., $\phi=\text{const}$ but A_μ unspecified, these equations reduce to

$$0=\frac{\partial^2\mathcal{L}}{\partial A_\alpha\,\partial A_\beta}+\frac{\partial^2\mathcal{L}}{\partial A_\alpha\partial(\partial_\beta\phi_j)}\varepsilon_{jk}\phi_k, \tag{31}$$

$$0=\frac{\partial^2\mathcal{L}}{\partial A_\alpha\,\partial\phi_j}\varepsilon_{jk}\phi_k, \tag{32}$$

$$0=\frac{\partial^2\mathcal{L}}{\partial(\partial_\nu\phi_i)\partial A_\beta}+2g^{\nu\beta}\varepsilon_{ik}\phi_k, \tag{33}$$

$$0=\frac{\partial^2\mathcal{L}}{\partial\phi_i\,\partial A_\beta}-\partial_\nu\left(\frac{\partial^2\mathcal{L}}{\partial(\partial_\nu\phi_i)\partial A_\beta}\right)+\left(\frac{\partial^2\mathcal{L}}{\partial\phi_i\partial(\partial_\beta\phi_j)}-\frac{\partial^2\mathcal{L}}{\partial(\partial_\beta\phi_i)\partial\phi_j}\right)\varepsilon_{jk}\phi_k, \tag{34}$$

$$0=\left(\frac{\partial^2\mathcal{L}}{\partial\phi_i\,\partial\phi_j}-\partial_\nu\left(\frac{\partial^2\mathcal{L}}{\partial(\partial_\nu\phi_i)\partial\phi_j}\right)\right)\varepsilon_{jk}\phi_k. \tag{35}$$

Substituting (33) into (31) yields

$$\frac{\partial^2\mathcal{L}}{\partial A_\alpha\,\partial A_\beta}=2g^{\alpha\beta}\phi_i\phi_i,$$

and so for constant nonzero ϕ_i solutions to the equation, the gauge bosons must have a nonzero mass equal to $\sqrt{2\phi_i\phi_i}$. The sign of the gauge boson mass is correct since the Lagrangian for massive vector bosons, the Proca Lagrangian, has the form $-\frac{1}{4}F^2+\frac{1}{2}M^2A^2$. Hence the first part of the Higgs mechanism, the gauge bosons acquire a mass, is automatic and can be seen to be simply a direct requirement of the generalized Goldstone's theorem, Eq. (6) or equivalently (7).

Applying $\varepsilon_{il}\phi_l$ to Eq. (34) and using (32) yields

$$\partial_\nu\left(\frac{\partial^2\mathcal{L}}{\partial(\partial_\nu\phi_i)\partial A_\beta}\right)\varepsilon_{il}\phi_l=0, \tag{36}$$

and applying $\varepsilon_{il}\phi_l$ to (35) yields

$$\varepsilon_{il}\phi_l\frac{\partial^2\mathcal{L}}{\partial\phi_i\,\partial\phi_j}\varepsilon_{jk}\phi_k=\varepsilon_{il}\phi_l\partial_\nu\left(\frac{\partial^2\mathcal{L}}{\partial(\partial_\nu\phi_i)\partial\phi_j}\right)\varepsilon_{jk}\phi_k. \tag{37}$$

These two equations along with (32) are automatically satisfied by taking

$$\mathcal{L}_{A\phi}=2A_\mu\varepsilon_{ij}\phi_i\,\partial^\mu\phi_j+\phi_i\phi_iA_\mu A^\mu, \tag{38}$$

which is the standard form.

The second part of the Higgs mechanism, the disappearance of the ''would-be'' Goldstone boson, follows from the symmetry condition (21) itself which after changing variables to ξ and ρ using $\phi=\rho e^{i\xi}$ reads as

$$0=\frac{\partial\mathcal{L}}{\partial(\partial_\mu A_\nu)}\partial_\mu\partial_\nu\theta+\left(\frac{\partial\mathcal{L}}{\partial A_\nu}+\frac{\partial\mathcal{L}}{\partial(\partial_\nu\xi)}\right)\partial_\nu\theta+\left(\frac{\partial\mathcal{L}}{\partial\xi}\right)\theta. \tag{39}$$

Again, since θ is an arbitrary function, each term must vanish separately. The first term vanishes due to the gauge invariance $\mathcal{L}_A$ since $\partial\mathcal{L}/\partial(\partial_\mu A_\nu)=\partial\mathcal{L}_A/\partial(\partial_\mu A_\nu)$. The last term demands $\partial\mathcal{L}/\partial\xi=0$ and so $\mathcal{L}$ may depend only on derivatives of ξ, i.e., $\mathcal{L}(A,\rho,\partial\rho,\xi,\partial\xi)\rightarrow\mathcal{L}(A,\rho,\partial\rho,\partial\xi)$. If we make the change of variables $A_\mu\rightarrow B_\mu=A_\mu-\partial_\mu\xi$, the first and third terms still vanish. The first automatically since for $\mathcal{L}_A$ alone this is just a gauge tranformation and the last still yields the condition $\partial\mathcal{L}/\partial\xi=0$. But now the middle term can be written as

$$0=\left(\frac{\partial\mathcal{L}(B,\rho,\partial\rho,\partial\xi)}{\partial B_\nu}\right)\frac{\partial B_\nu}{\partial A_\mu}+\left(\frac{\partial\mathcal{L}(B,\rho,\partial\rho,\partial\xi)}{\partial B_\nu}\right)\frac{\partial B_\nu}{\partial(\partial_\mu\xi)}+\left(\frac{\partial\mathcal{L}(B,\rho,\partial\rho,\partial\xi)}{\partial(\partial_\nu\xi)}\right)$$

$$=\left(\frac{\partial\mathcal{L}(B,\rho,\partial\rho,\partial\xi)}{\partial B_\nu}\right)\delta^\mu_\nu+\left(\frac{\partial\mathcal{L}(B,\rho,\partial\rho,\partial\xi)}{\partial B_\nu}\right)(-\delta^\mu_\nu)+\left(\frac{\partial\mathcal{L}(B,\rho,\partial\rho,\partial\xi)}{\partial(\partial_\nu\xi)}\right)$$

$$=\frac{\partial\mathcal{L}(B,\rho,\partial\rho,\partial\xi)}{\partial(\partial_\nu\xi)}, \tag{40}$$

and hence $\mathcal{L}$ does not depend on $\partial\xi$ and so the "would-be" Goldstone boson ξ has completely vanished from the model. Effectively it has become the longitudinal component of a now massive gauge boson.

V. SCALE AND CONFORMAL SYMMETRY BREAKING

It has been noted in the literature,[4] see also Ref. 6, that in theories with a spontaneously broken scale and conformal invariance, although five symmetries are broken, only one Goldstone boson appears. A similar thing occurs for broken Lorentz invariance in a class of three dimensional gauge theories as discussed in Ref. 7. In this section we use our more general treatment of Goldstone's theorem to study this question. In particular, we see that our equation predicts only one Goldstone mode, but also imposes four other conditions, not having to do with particle masses, that represent the extra information contained in the spontaneous breakdown of conformal symmetry.

We have in mind a model of the kind considered by Coleman, which contains a scalar and a fermion field, and another scalar, the dilaton, whose role is to implement the broken symmetry. Since we do not consider fermions in this paper, we shall omit them here. Also, we note that the extension of the following discussion to include more than one scalar (but still only one dilaton) is straightforward, but to keep our notation simple we do not put them in explicitly.

Here ϕ_i will be a doublet: $\phi_i=\left[\begin{smallmatrix}\phi\\ \sigma\end{smallmatrix}\right]$, where ϕ is the ordinary scalar field and σ is the dilaton. Under dilations, they transform as

$$\delta\phi=\phi+x^\mu\,\partial_\mu\phi \tag{41}$$

and

$$\delta\sigma=\frac{1}{f}+x^\mu\,\partial_\mu\sigma, \tag{42}$$

where f is a scale characterizing the symmetry breaking. Under special conformal transformations, we have

$$\begin{aligned}\delta^\lambda\phi&=(2x^\lambda x^\rho-g^{\lambda\rho}x^2)\partial_\rho\phi+2x^\lambda\phi,\\ \delta^\lambda\sigma&=(2x^\lambda x^\rho-g^{\lambda\rho}x^2)\partial_\rho\sigma+\frac{2x^\lambda}{f}.\end{aligned} \tag{43}$$

In what follows, we shall assume that translation invariance is not broken. Hence ϕ and σ must be constants. However, one sees that the Δ's will not be constants. We have, in fact,

$$\delta\phi=\phi,\quad \delta\sigma=\frac{1}{f}\quad(\text{dilations}), \tag{44}$$

but

$$\delta^\lambda \phi = 2x^\lambda \phi, \quad \delta^\lambda \sigma = \frac{2x^\lambda}{f} \quad \text{(conformal transfs.)}. \tag{45}$$

Noting further that the spacetime derivatives of the Lagrangian density $\mathcal{L}$ or of its derivatives with respect to the fields will vanish, we obtain from (7),

$$\begin{bmatrix} \frac{\partial^2 \mathcal{L}}{\partial \phi^2} & \frac{\partial^2 \mathcal{L}}{\partial \phi\, \partial \sigma} \\ \frac{\partial^2 \mathcal{L}}{\partial \sigma\, \partial \phi} & \frac{\partial^2 \mathcal{L}}{\partial \sigma^2} \end{bmatrix} \begin{bmatrix} \phi \\ 1/f \end{bmatrix} = 0 \quad \text{(dilations)} \tag{46}$$

and

$$\left(x^\lambda \begin{bmatrix} \frac{\partial^2 \mathcal{L}}{\partial \phi^2} & \frac{\partial^2 \mathcal{L}}{\partial \phi \partial \sigma} \\ \frac{\partial^2 \mathcal{L}}{\partial \sigma\, \partial \phi} & \frac{\partial^2 \mathcal{L}}{\partial \sigma^2} \end{bmatrix} + \begin{bmatrix} 0 & \frac{\partial^2 \mathcal{L}}{\partial \phi \partial(\partial_\lambda \sigma)} - \frac{\partial^2 \mathcal{L}}{\partial \sigma \partial(\partial_\lambda \phi)} \\ \frac{\partial^2 \mathcal{L}}{\partial \sigma \partial(\partial_\lambda \phi)} - \frac{\partial^2 \mathcal{L}}{\partial \phi \partial(\partial_\lambda \sigma)} & 0 \end{bmatrix} \right) \begin{bmatrix} \phi \\ 1/f \end{bmatrix}$$
$$= 0 \quad \text{(conformal transfs.)}. \tag{47}$$

In the second equation, the two terms must separately vanish, because the first is proportional to the variable x^λ and the second is not. But the first term encodes exactly the same information as does Eq. (46). This is the origin of the fact that dilations and special conformal transformations give rise to the same Goldstone boson. There is, however, the second term in (47), which provides an additional set of four constraints:

$$\frac{\partial^2 \mathcal{L}}{\partial \sigma \partial(\partial_\lambda \phi)} = \frac{\partial^2 \mathcal{L}}{\partial \phi \partial(\partial_\lambda \sigma)}. \tag{48}$$

This is, in principle, the ''extra'' information about the Lagrangian (or the effective action, when quantum corrections are considered) that follows from spontaneously broken conformal symmetry.

Let us see how this works at tree level in the specific model considered by Coleman. The Lagrange density is

$$\mathcal{L} = \frac{1}{2} \partial_\mu \phi\, \partial^\mu \phi + \frac{1}{2f^2} \partial_\mu (e^{f\sigma}) \partial^\mu (e^{f\sigma}) - \frac{\mu^2}{2} \phi^2 e^{2f\sigma} - \frac{\lambda}{4!} \phi^4. \tag{49}$$

The equations (46) and (47) imply

$$\begin{bmatrix} 1 + \frac{\lambda}{2\mu^2} \phi^2 e^{-2f\sigma} & 2f\phi \\ 2f\phi & 2f^2\phi^2 \end{bmatrix} \begin{bmatrix} \phi \\ 1/f \end{bmatrix} = 0, \tag{50}$$

which requires $\phi = 0$ and identifies $\left[\begin{smallmatrix} 0 \\ 1/f \end{smallmatrix}\right]$ (i.e., the σ particle) as the Goldstone mode. The extra information furnished in Eq. (47) is trivial in this case, since the relevant terms were set to zero from the beginning.

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False vacuum decay: Effective one-loop action for pair creation of domain walls

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An effective one-loop action built from the soliton field itself for the two-dimensional (2D) problem of soliton pair creation is proposed. The action consists of the usual mass term and a kinetic term in which the simple derivative of the soliton field is replaced by a covariant derivative. In this effective action the soliton charge is treated no longer as a topological charge but as a Noether charge. Using this effective one-loop action, the soliton–antisoliton pair production rate $\Gamma/L = A\ \exp[-S_0]$ is calculated and one recovers Stone's exponential factor S_0 and the prefactor A of Kiselev, Selivanov, and Voloshin. The results are also valid straightforwardly to the problem of pair creation rate of domain walls in dimensions $D \geqslant 3$. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1380442]

I. INTRODUCTION

Stone[1] has studied the problem of a scalar field theory in (1+1)D with a metastable vacuum, i.e., with a scalar potential that has a false vacuum, ϕ_+, and a true vacuum, ϕ_-, separated by an energy density difference, ϵ. Stone has noticed that the decay process can be interpreted as the false vacuum decaying into the true vacuum plus a creation of a soliton–antisoliton pair: $\phi_+ \to \phi_- + s + \bar{s}$. The energy necessary for the materialization of the pair comes from the energy density difference between the two vacua. The soliton–antisoliton pair production rate per unit time and length, Γ/L, can then be identified with the decay rate of the false vacuum and is given by ($\hbar = c = 1$):[1]

$$\Gamma/L = A\ e^{-S_0} = Ae^{-\pi m^2/\epsilon}, \tag{1}$$

where m is the soliton mass and prefactor A is a functional determinant whose value was first calculated by Kiselev and Selivanov[2,3] and later by Voloshin.[4] Extensions to this decay problem, such as induced false vacuum decay, have been studied by several authors (for a review and references see, e.g., Refs. 5 and 6).

The method used in Refs. 1–4 is based one the instanton method introduced by Langer in his work about decay of metastable thermodynamical states.[7] This powerful method has been applied to several different studies, namely: Coleman and Callan[8,9] have computed the bubble production rate that accompanies the cosmological phase transitions in a (3+1)D scalar theory (this was indeed previously calculated by other methods by Voloshin, Kobzarev, and Okun[10]); Affleck and Manton[11] have studied monopole pair production in a weak external magnetic field and Affleck, Alvarez, and Manton,[12] have studied e^+e^- boson pair production in a weak external electric field. Recent developments studying pair production of boson and spinorial particles in external Maxwell fields have been performed by several authors using different methods[13–15] and similar results in the Euler–Heisenberg theory, a modified Maxwell theory, have been also obtained.[16] The decay of false vacuum in a condensed matter system providing soliton tunneling has been studied in Refs. 17 and 18.

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In this paper we propose an effective one-loop action built from the soliton field itself to study the problem of Stone,[1] Kiselev and Selivanov,[2,3] and Voloshin.[4] The action consists of the usual mass term and a kinetic term in which the simple derivative of the soliton field is replaced by a kind of covariant derivative. In this effective action the soliton charge is treated no longer as a topological charge but as a Noether charge. This procedure of working with an effective action for the soliton field itself has been introduced by Coleman[19] where the equivalence between the Sine–Gordon model and the Thirring model was shown, and by Montonen and Olive[20] who have proposed an equivalent dual field theory for the Prasad–Sommerfield monopole soliton. More connected to our problem, Manton[21] has proposed an effective action built from the soliton field itself which reproduces the soliton physical properties of (1+1)D nonlinear scalar field theories having symmetric potentials with degenerate minima. In this paper we deal instead with a potential with nondegenerate minima in a (1+1)D scalar field theory. Thus, our effective action is new since Manton was not dealing with the soliton pair production process.

Using the effective one-loop action and the method presented in Ref. 12, we calculate the soliton–antisoliton pair production rate, (1). One recovers Stone's exponential factor S_0 (Ref. 1) and the prefactor A of Kiselev and Selivanov[2,3] and Voloshin.[4]

II. EFFECTIVE ONE-LOOP ACTION

In order to present some useful soliton properties let us consider a scalar field theory in a (1+1)D spacetime, whose dynamics is governed by the action (see, e.g., Ref. 22),

$$S[\phi(x,t)]=\int d^2x\left[\frac{1}{2}\partial_\mu\phi\partial^\mu\phi-U(\phi)\right], \tag{2}$$

where U is a generic potential. A particular important case is when U is a symmetric potential, $U=U_s(\phi)$, with two or more degenerate minima. In the ϕ^4 theory the potential is $U_s(\phi)=\frac{1}{4}\lambda(\phi^2-\mu^2/\lambda)^2$, with $\mu\geqslant 0$ and $\lambda\geqslant 0$. Stationarizing the action one obtains the solutions of the theory which have finite and localized energy. The solutions are the soliton

$$\psi\equiv\phi_{\rm sol}=+\frac{\mu}{\sqrt{\lambda}}\tanh\left[\frac{\mu}{\sqrt{2}}\frac{(x-x_0)-vt}{\sqrt{1-v^2}}\right], \tag{3}$$

and the antisoliton $-\psi$. From the Hamiltonian density, $\mathcal{H}=\frac{1}{2}(\partial_x\phi)^2+U_s(\phi)$, one can calculate the mass of the soliton and antisoliton

$$m=\int_{-\infty}^{+\infty}dx\,\mathcal{H}(x)=\frac{2\sqrt{2}}{3}\frac{\mu^3}{\lambda}. \tag{4}$$

One can also define the topological charge, $Q=\frac{1}{2}[\psi(x=+\infty)-\psi(x=-\infty)]$, (conserved in time) which has the positive value $Q_s=+\mu/\sqrt{\lambda}$ in the case of the soliton and the negative value $Q_s^-=-\mu/\sqrt{\lambda}$ in the case of the antisoliton. To this charge one associates the topological current $k^\mu=\frac{1}{2}\varepsilon^{\mu\nu}\partial_\nu\psi$ which is conserved, $\partial_\mu k^\mu=0$, and such that $Q=\int_{-\infty}^{+\infty}dx\,k^0$.

Now, let us consider a nondegenerate potential U in action (2) by adding to U_s a small term that breaks its symmetry:[1,9] $U(\phi)=U_s(\phi)+(\epsilon\sqrt{\lambda}/2\mu)(\phi-\mu/\sqrt{\lambda})$, where ϵ is the energy density (per unit length) difference between the true ($\phi_-=-\mu/\sqrt{\lambda}$) and false ($\phi_+=+\mu/\sqrt{\lambda}$) vacua. As noticed in Refs. 1–3, ϵ is responsible for both the decay of false vacuum and soliton–antisoliton pair creation.

We want to find an effective one-loop action built from the soliton field itself and that describes the above pair creation process. The soliton field should be a charged field since the system admits two charges, Q_s and Q_s^-. Therefore, the action should contain the mass term $m^2\psi\psi^*$, where m is the soliton mass given in Eq. (4), and the kinetic term $(\partial_\mu\psi)(\partial^\mu\psi^*)$. Thus, the free field effective action is $\int d^2x[(\partial_\mu\psi)(\partial^\mu\psi^*)-m^2\psi\psi^*]$. However, if one demands local gauge invariance one has to introduce an "electromagnetic" 2-vector potential A_μ which trans-

forms the common derivative $\partial_\mu\psi$ into a covariant derivative $(\partial_\mu+iQ_sA_\mu)\psi$. As is well known, the field A_μ itself should contribute to the action. This contribution must be gauge invariant since the covariant kinetic term plus the mass term are already gauge invariant. This is achieved by defining the invariant 2-form field, $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$. In two dimensions, an antisymmetric field can only be of the form $F_{\mu\nu}=\sigma(t,x)\varepsilon_{\mu\nu}$, where $\varepsilon_{\mu\nu}$ is the Levi-Cevita tensor and $\sigma(t,x)$ is a function. Therefore the effective one-loop action should be $S^{\rm eff}=\int d^2x[(\partial_\nu\psi+iQ_sA_\nu\psi)(\partial^\nu\psi^*-iQ_sA^\nu\psi^*)-m^2\psi\psi^*-\frac{1}{4}F_{\mu\nu}F^{\mu\nu}]$.

Note now that the charged soliton acts also as a source, thus modifying the surrounding field. As a first approximation we shall neglect this effect and assume A_μ fixed by external conditions. This allows us to drop the contribution of the term $F_{\mu\nu}F^{\mu\nu}$ in the effective action. Moreover, the external field responsible for the pair creation is essentially represented by the energy density difference ϵ so we postulate that $F^{\rm ext}_{\mu\nu}=(\epsilon\sqrt{\lambda}/\mu)\,\varepsilon_{\mu\nu}$. Therefore, $A^{\rm ext}_\mu$ is given by $A^{\rm ext}_\mu=\frac{1}{2}(\epsilon\sqrt{\lambda}/\mu)\,\varepsilon_{\mu\nu}x^\nu$.

Finally, if the system is analytically continued to Euclidean spacetime ($t_{\rm min}\to -it_{\rm Euc}$; $A_0\to iA_2$) one obtains the Euclidean effective one-loop action for the soliton pair creation problem

$$S^{\rm eff}_{\rm Euc}=\int d^2x\left[\left|\left(\partial_\mu-\frac{1}{2}\epsilon\,\varepsilon_{\mu\nu}x_\nu\right)\psi\right|^2+m^2|\psi|^2\right]. \tag{5}$$

In the next section this Euclidean effective one-loop action is going to be used to calculate the soliton-antisoliton pair production rate (1). Although the calculations are now similar to those found in Affleck, Alvarez, and Manton pair creation problem,[12] we present some important steps and results since in two dimensions they are slightly different.

III. PAIR PRODUCTION RATE

The soliton–antisoliton pair production rate per unit time is equal to the false vacuum decay rate per unit time

$$\Gamma=-2\ {\rm Im}\,E_0, \tag{6}$$

where the vacuum energy, E_0, is given by the Euclidean functional integral

$$e^{-E_0T}=\lim_{T\to\infty}\int[\mathcal{D}\psi][\mathcal{D}\psi^*]e^{-S^{\rm eff}_{\rm Euc}(\psi;\psi^*)}\ . \tag{7}$$

As it will be verified, E_0 will receive a small imaginary contribution from the negative-mode associated to the quantum fluctuations about the instanton (which stationarizies the action) and this fact is responsible for the decay. Combining (6) and (7) one has

$$\Gamma=\lim_{T\to\infty}\frac{2}{T}{\rm Im}\ln\int[\mathcal{D}\psi][\mathcal{D}\psi^*]e^{-S^{\rm eff}_{\rm Euc}(\psi;\psi^*)}, \tag{8}$$

where $S^{\rm eff}_{\rm Euc}$ is given by (5). Integrating out ψ and ψ^* in (8) one obtains

$$\Gamma=-\lim_{T\to\infty}\frac{2}{T}{\rm Im\,tr}\ln\left[\left(\partial_\mu-\frac{1}{2}\epsilon\,\varepsilon_{\mu\nu}x_\nu\right)^2+m^2\right]. \tag{9}$$

The logarithm in (9) can be written as a "Schwinger proper time integral," $\ln u=-\int_0^\infty(d\mathcal{T}/\mathcal{T})\exp(-\frac{1}{2}u\mathcal{T})$. Taking $u=[(\partial_\mu-\frac{1}{2}\epsilon\,\varepsilon_{\mu\nu}x_\nu)^2+m^2]$, yields

$$\Gamma=\lim_{T\to\infty}\frac{2}{T}{\rm Im}\int_0^\infty\frac{d\mathcal{T}}{\mathcal{T}}e^{-m^2\mathcal{T}/2}\,{\rm tr}\exp\left[-\frac{1}{2}\left(P_\mu-\frac{1}{2}\epsilon\,\varepsilon_{\mu\nu}x_\nu\right)^2\mathcal{T}\right]. \tag{10}$$

Notice that now the trace is of the form $\mathrm{tr}\, e^{-H\mathcal{T}}$, with $H=\frac{1}{2}[P_\mu-\frac{1}{2}\epsilon\ \varepsilon_{\mu\nu}x_\nu]^2$ being the Hamiltonian for a particle subjected to the interaction with the external scalar field in a (2+1)D spacetime, and the proper time playing the role of a time coordinate. One has started with a scalar field theory in a Euclidean 2D spacetime and now one has found an effective theory for particles in a 3D spacetime. It is in this new context that the pair production rate is going to be calculated. The gain in having the trace in the given form is that it can be written as a path integral $\mathrm{tr}\, e^{-H\mathcal{T}}=\int[dx]\exp[-\int d\mathcal{T}L]$, where $L=\frac{1}{2}\dot{x}_\mu\dot{x}_\mu+\frac{1}{2}\epsilon\ \varepsilon_{\mu\nu}x_\nu\dot{x}_\mu$ is the Lagrangian associated with our Hamiltonian. Thus,

$$\Gamma=\lim_{T\to\infty}\frac{2}{T}\,\mathrm{Im}\int_0^\infty\frac{d\mathcal{T}}{\mathcal{T}}e^{-m^2\mathcal{T}/2}\int[dx]\exp\left[-\int_0^{\mathcal{T}}d\mathcal{T}\left(\frac{1}{2}\dot{x}_\mu\dot{x}_\mu+\frac{1}{2}\epsilon\ \varepsilon_{\mu\nu}x_\nu\dot{x}_\mu\right)\right]. \tag{11}$$

Rescaling the proper time variable, $d\mathcal{T}\to d\tau/\mathcal{T}$, and noticing that the path integral is over all the paths, $x_\mu(\tau)$, such that $x_\mu(1)=x_\mu(0)$, one has

$$\Gamma=\lim_{T\to\infty}\frac{2}{T}\,\mathrm{Im}\int[dx]e^{-(\epsilon/2)\oint\varepsilon_{\mu\nu}x_\nu\,dx_\mu}\int_0^\infty\frac{d\mathcal{T}}{\mathcal{T}}\exp\left[-\left(\frac{1}{2}m^2\mathcal{T}+\frac{1}{2\mathcal{T}}\int_0^1 d\tau\,\dot{x}_\mu\dot{x}_\mu\right)\right]. \tag{12}$$

The $\mathcal{T}$ integral can be calculated expanding the function about the stationary point $\mathcal{T}_0^2=\int_0^1 d\tau\,\dot{x}^2/m^2$:

$$\int\frac{d\mathcal{T}}{\mathcal{T}}e^{-f(\mathcal{T})}\sim e^{-f(\mathcal{T}_0)}\frac{1}{\mathcal{T}_0}\sqrt{\frac{\pi}{\frac{1}{2}f''(\mathcal{T}_0)}}\sim e^{-m\sqrt{\int_0^1 d\tau\,\dot{x}^2}}\frac{1}{m}\sqrt{2\pi}\,. \tag{13}$$

Then (12) can be written as

$$\Gamma=\lim_{T\to\infty}\frac{1}{T}\frac{2}{m}\sqrt{2\pi}\,\mathrm{Im}\int[dx]e^{-S_{\mathrm{Euc}}[x_\mu(\tau)]}, \tag{14}$$

where $S_{\mathrm{Euc}}=m\sqrt{\int_0^1 d\tau\dot{x}_\mu\dot{x}_\mu}+\frac{1}{2}\epsilon\oint\varepsilon_{\mu\nu}x_\nu\,dx_\mu$. This integral can be solved using the instanton method. Stationarizing the action, one gets the equation of motion in the (2+1)D spacetime

$$\frac{m\ddot{x}_\mu(\tau')}{\sqrt{\int_0^1 d\tau\dot{x}^2}}=-\epsilon\varepsilon_{\mu\nu}\dot{x}_\nu(\tau')\quad\text{with}\ \ \mu=1,2\ \ \text{and}\ \ \dot{x}_\mu=\frac{dx_\mu}{d\tau}. \tag{15}$$

The instanton, $x_\mu^{\mathrm{cl}}(\tau)$, i.e., the solution of the Euclidean equation of motion that obeys the boundary conditions $x_\mu(\tau=1)=x_\mu(\tau=0)$ is

$$x_\mu^{\mathrm{cl}}(\tau)=R(\cos 2\pi\tau,\sin 2\pi\tau)\quad\text{with}\ \ R=\frac{m}{\epsilon}. \tag{16}$$

The instanton represents a particle describing a loop of radius R in the plane defined by the time x_2 and by the direction x_1. The loop is a thin wall that separates the true vacuum located inside the loop from the false vacuum outside.

The Euclidean action of the instanton is given by $S_0=S_{\mathrm{Euc}}[x_\mu^{\mathrm{cl}}(\tau)]=m2\pi R-\epsilon\pi R^2$. The first term is the rest energy of the particle times the orbital length and the second term represents the interaction of the particle with the external scalar field. The loop radius, $R=m/\epsilon$, stationarizies the instanton action. The action is then $S_0=\pi m^2/\epsilon$.

The second order variation operator is given by

$$M_{\mu\nu}\equiv \left.\frac{\delta^2 S}{\delta x_\nu(\tau')\,\delta x_\mu(\tau)}\right|_{x^{\rm cl}} = \left[-\left(\frac{m\,\delta_{\mu\nu}}{\sqrt{\int_0^1 d\tau \dot{x}^2}}\frac{d^2}{d\tau^2} + \epsilon\ \varepsilon_{\mu\nu}\frac{d}{d\tau}\right)\delta(\tau-\tau') - \frac{m\ddot{x}_\mu(\tau)\ddot{x}_\nu(\tau')}{[\int_0^1 d\tau \dot{x}^2]^{3/2}}\right]_{x^{\rm cl}}$$

$$= -\left[\frac{\epsilon}{2\pi}\delta_{\mu\nu}\frac{d^2}{d\tau^2} + \epsilon\varepsilon_{\mu\nu}\frac{d}{d\tau}\right]\delta(\tau-\tau') - \frac{2\pi\epsilon x_\mu^{\rm cl}(\tau)x_\nu^{\rm cl}(\tau')}{R^2}. \tag{17}$$

The eigenvectors η_μ^n, and the eigenvalues λ_n, associated with the operator $M_{\mu\nu}$ are such that

$$M_{\mu\nu}\ \eta_\nu^n(\tau') = \lambda_n\ \eta_\mu^n(\tau')\ \delta(\tau-\tau'). \tag{18}$$

From this one concludes:

(i) the positive eigenmodes are $(\cos 2n\pi\tau, \sin 2n\pi\tau)$ and $(\sin 2n\pi\tau, -\cos 2n\pi\tau)$ with $\lambda_n = 2\pi\epsilon(n^2-n)$, $n=2,3,4,...$; $(\sin 2n\pi\tau, \cos 2n\pi\tau)$ and $(\cos 2n\pi\tau, -\sin 2n\pi\tau)$ with $\lambda_n = 2\pi\epsilon(n^2+n)$, $n=1,2,3,...$;

(ii) there are two zero-modes associated with the translation of the loop along the x_1 and x_2 directions: $(1,0)$ and $(0,1)$ with $\lambda=0$;

(iii) there is a zero-mode associated with the translation along the proper time, τ: $(\sin 2\pi\tau, -\cos 2\pi\tau) = -\dot{x}_\mu^{\rm cl}/(2\pi R)$ with $\lambda=0$;

(iv) there is a single negative mode associated to the change of the loop radius R: $(\cos 2\pi\tau, \sin 2\pi\tau) = x_\mu^{\rm cl}/R$ with $\lambda_- = -2\pi\epsilon$.

Now, we consider small fluctuations about the instanton, i.e., we do $x_\mu(\tau) = x_\mu^{\rm cl}(\tau) + \eta_\mu(\tau)$. The Euclidean action is expanded to second order so that the path integral (14) can be approximated by

$$\Gamma \simeq \lim_{T\to\infty}\frac{1}{T}\frac{2}{m}\sqrt{\frac{2\pi}{\mathcal{T}_0}}e^{-S_0}\,{\rm Im}\int [d\eta(\tau)]\exp\left[-\frac{1}{2}\int d\tau\, d\tau'\ \eta_\mu(\tau)M_{\mu\nu}\ \eta_\nu(\tau')\right]. \tag{19}$$

The path integral in Eq. (19) is the one-loop factor and is given by $\mathcal{N}(\det M)^{-1/2} = \mathcal{N}\Pi\,(\lambda_n)^{-1/2}$, where λ_n are the eigenvalues of $M_{\mu\nu}$ and $\mathcal{N}$ is a normalization factor that will not be needed. To overcome the problem that arises from having an infinite product of eigenvalues, one compares our system with the free particle system

$$\int [d\eta]\exp\left[-\frac{1}{2}\int d\tau\, d\tau'\ \eta_\mu(\tau)\ M_{\mu\nu}\ \eta_\nu(\tau')\right]$$

$$= \int [d\eta]\exp\left[-\frac{1}{2}\int d\tau\, d\tau'\ \eta_\mu(\tau)\ M^0_{\mu\nu}\ \eta_\nu(\tau')\right]\frac{\Pi\ (\lambda_n)^{-1/2}}{\Pi\ (\lambda_n')^{-1/2}}, \tag{20}$$

where $M^0_{\mu\nu} = -(1/\mathcal{T}_0)\,\delta_{\mu\nu}(d^2/d\tau^2)\,\delta(\tau-\tau')$ is the second variation operator of the free system with eigenvalues $\lambda_n' = 2\pi\epsilon n^2$, $n=0,1,2,3,...$ (each with multiplicity 4). In Eq. (20) the first factor is the path integral of a free particle in a $(2+1)$D Euclidean spacetime

$$\int [d\eta]\exp\left[-\frac{1}{2}\int d\tau\, d\tau'\ \eta_\mu\ M^0_{\mu\nu}\ \eta_\nu\right] = \int [d\eta]\exp\left[-\frac{1}{2\mathcal{T}_0}\int d\tau\ \dot{\eta}_\mu\dot{\eta}_\mu\right] = \frac{1}{2\pi\mathcal{T}_0}. \tag{21}$$

In the productory, one omits the zero eigenvalues, but one has to introduce the normalization factor $(||dx_\mu^{\rm cl}/d\tau||/||\eta_\mu^0||)\sqrt{1/2\pi}=\sqrt{2\pi}R$ which is associated with the proper time eigenvalue. In addition, associated with the negative eigenvalue one has to introduce a factor of 1/2 which accounts for the loops that do expand. The other half contracts (representing the annihilation of recently created pairs) and so does not contribute to the creation rate. So, the one-loop factor becomes

$$\frac{1}{2\pi\mathcal{T}_0}\frac{\Pi\ (\lambda_n)^{-1/2}}{\Pi\ (\lambda_n')^{-1/2}}=\frac{1}{2\pi\mathcal{T}_0}\frac{1}{2}\frac{i}{\sqrt{2\pi\epsilon}}\sqrt{2\pi}R\frac{\Pi_{\lambda>0}\ (\lambda_n)^{-1/2}}{\Pi_{\lambda'>0}\ (\lambda_n')^{-1/2}}=i\frac{1}{2\pi\mathcal{T}_0}\frac{1}{2}\sqrt{2\pi\epsilon}\ \sqrt{2\pi}R\ . \tag{22}$$

Written like this, the one-loop factor accounts only for the contribution of the instanton centered in $(x_1,x_2)=(0,0)$. The translational invariance in the x_1 and x_2 directions requires that one multiplies (22) by the spacetime volume factor $\int dx_2\int dx_1=TL$, which represents the spacetime region where the instanton might be localized. So, the correct one-loop factor is given by

$$\int\ [d\eta(\tau)]\exp\left[-\frac{1}{2}\int d\tau\, d\tau'\ \eta_\mu(\tau)\ M_{\mu\nu}\ \eta_\nu(\tau')\right]=i\frac{LT}{2\pi\mathcal{T}_0}\frac{1}{2}\sqrt{2\pi\epsilon}\ \sqrt{2\pi}R\ . \tag{23}$$

Putting (23) into (19), using $\mathcal{T}_0^2=\int d\tau\,\dot{x}^2/m^2=(2\pi R)^2/m^2$, $R=m/\epsilon$, and $S_0=\pi m^2/\epsilon$, one finally has that the soliton–antisoliton pair production rate per unit time and length is given by

$$\Gamma/L=\frac{\epsilon}{2\pi}e^{-(\pi m^2/\epsilon)}. \tag{24}$$

We have recovered Stone's exponential factor $e^{-\pi m^2/\epsilon}$ (Ref. 1) as well as the prefactor $A=\epsilon/2\pi$ of Kiselev and Selivanov[2,3] and Voloshin.[4]

Note the difference to the 4D problem of Affleck *et al.*[12] and Schwinger,[23] who have found for the factor A the value $(eE)^2/(2\pi)^3$ which is quadratic in eE and not linear, as in our case. This difference has to do with the dimensionality of the problems.

It is well known that a one-particle system in 2D can be transformed straightforwardly to a thin line in 3D and a thin wall in 4D, where now the mass m of the soliton should be interpreted as a line density and surface density, respectively. In fact, a particle in (1+1)D, as well as an infinite line in (2+1)D, can be considered as walls as seen from within the intrinsic space dimension, justifying the use of the name wall for any dimension. Our calculations apply directly to the domain wall pair creation problem in any dimension.

IV. CONCLUSIONS

The equation for the loop of radius R in 2D Euclidean spacetime is given by $x^2+t_E^2=R^2$, where we have put $x=x_1$ and $t_E=x_2$. One can make an analytical continuation of the Euclidean time (t_E) to the Minkowskian time $(t_E=it)$ and obtain the solution in 2D Minkowski spacetime

$$x^2-t^2=R^2. \tag{25}$$

At $t_E=t=0$ the system makes a quantum jump and a soliton–antisoliton pair materializes at $x=\pm R=\pm m/\epsilon$. After the materialization, the soliton and antisoliton are accelerated, driving away from each other, as (25) shows. To check these statements note first that the energy necessary for the materialization of the pair at rest is $E=2m$, where m is the soliton mass. This energy comes from the conversion of false vacuum into true vacuum. Since ϵ is the energy difference per unit length between the two vacua, we conclude that an energy of value $E=2R\epsilon$ is released when this

conversion occurs in the region $(2R)$ within the pair. So, the pair materialization should occur only when R is such that the energy released is equal to the rest energy: $2R\epsilon=2m\Rightarrow R=m/\epsilon$. This value agrees with the one that has been determined in Sec. III.

After the materialization the pair is accelerated so that its energy is now $E=2m/\sqrt{1-v^2}$. Differentiating (25), we get the velocity $v=\sqrt{1-R^2/x^2}$. The energy of the pair is then given by $E=2(m/R)\,|x|=\epsilon\,2|x|$. Notice now that $\epsilon\,2|x|$ is the energy released in the conversion of false vacuum into true vacuum. So, after pair creation, all the energy released in the conversion between the two vacua is used to accelerate the soliton–antisoliton pair.

This discussion agrees with the interpretation of the process as being the false vacuum decaying to the true vacuum plus a creation of a soliton–antisoliton pair. It also justifies the presence of the interaction term $\epsilon\varepsilon_{\mu\nu}x_\nu\psi$ present in the covariant derivative of the proposed effective one-loop action (5), since ϵx is the energy released in the decay and responsible for the creation and acceleration of the pair.

With the proposed effective one-loop action (5) we have recovered Stone's exponential factor S_0 (Ref. 1) of the pair creation rate in (1), and the prefactor A of Kiselev and Selivanov[2,3] and Voloshin.[4] In the proposed effective one-loop action the soliton charge is treated no longer as a topological charge but as a Noether charge. Such an interchange between the topological and the Noether charges was already present in Refs. 19 and 20.

The problem of false vacuum decay coupled to gravity has been introduced in Ref. 24 and recently there has been a renewed interest in it (see, e.g., Refs. 25 and 26). With the proposed effective one-loop action (5) we pretend to further analyze this problem.

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Cliffordons

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At higher energies the present complex quantum theory with its unitary group might expand into a real quantum theory with an orthogonal group, broken by an approximate i operator at lower energies. Implementing this possibility requires a real quantum double-valued statistics. A Clifford statistics, representing a swap (12) by a difference $\gamma_1-\gamma_2$ of Clifford units, is uniquely appropriate. Unlike the Maxwell–Boltzmann, Fermi–Dirac, Bose–Einstein, and para-statistics, which are tensorial and single-valued, and unlike anyons, which are confined to two dimensions, Clifford statistics are multivalued and work for any dimensionality. Nayak and Wilczek such Clifford statistics for the fractional quantum Hall effect. We apply them to toy quanta here. A complex-Clifford example has the energy spectrum of a system of spin-1/2 particles in an external magnetic field. This supports the proposal that the double-valued rotations—spin—seen at current energies might arise from double-valued permutations—swap—to be seen at higher energies. Another toy with real Clifford statistics illustrates how an effective imaginary unit i can arise naturally within a real quantum theory. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379314]

I. INTRODUCTION: QUANTIFICATION PROCEDURES

Nayak and Wilczek[1] have proposed a startling new statistics for fractional quantum Hall effect carriers. It has great potential for even more fundamental applications to sub-particle structure.[2] To learn its properties we apply it here to some toy models.

The common statistics—Fermi–Dirac (FD), Bose-Einstein (BE), and Maxwell–Boltzmann (MB)—may be regarded as differing prescriptions for constructing the algebra of an ensemble of many individuals from the vector space of one individual. These procedures take qualitative yes-or-no questions about an individual into quantitative how-many questions about an ensemble of similar individuals. Such procedures were termed *quantification*. Now they are sometimes called ''second quantization,'' somewhat misleadingly.

We use a well-known operational formulation of quantum theory. The main point of quantum theory is that mathematical objects may be completely describable, since we make them up, but physical quanta are not. An electron, a physical entity, is not a spinor wave function, a linear operator, or any other mathematical object. But it seems that mathematical objects can usefully represent what we do to an electron. Kets represent input modes (preparation), bras represent outtake modes (registration), operators represent intermediate operations on quantum.[3]

Each of the usual statistics is defined by an associated linear mapping $Q^\dagger$ that maps any one-body initial mode ψ into a many-body creation operator:

$$Q^\dagger: V_I \to \mathcal{A}_S, \quad \psi \mapsto Q^\dagger \psi =: \hat{\psi}. \tag{1}$$

Here V_I is the initial-mode vector space of the individual I and $\mathcal{A}_S = \text{End } V_S$ is the operator (or endomorphism) algebra of the quantified system S. The † in $Q^\dagger$ reminds us that $Q^\dagger$ is contragredient to the initial modes ψ. We write the mapping $Q^\dagger$ to the left of its argument ψ to respect the conventional Dirac order of cogredient and contragredient vectors in a contraction.

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Dually, the final modes $\psi^\dagger$ of the dual space $V_I^\dagger$ are mapped to annihilators in $\mathcal{A}_S$ by the linear operator Q

$$Q: V_I^\dagger \to \mathcal{A}_S, \quad \psi^\dagger \mapsto \psi^\dagger Q =: \hat{\psi}^\dagger. \tag{2}$$

We call the transformation Q the *quantifier* for the statistics. Q and $Q^\dagger$ are tensors of the type

$$Q = (Q^{aB}{}_C), \quad Q^\dagger = (Q^{\dagger C}_{\ \ a\ B}), \tag{3}$$

where a indexes a basis in the one-body space V_I and B,C index a basis in the many-body space V_S.

The basic creators and annihilators associated with an arbitrary basis $\{e_a | a = 1, \ldots, N\} \subset V_I$ and its reciprocal basis $\{e^a |\ a = 1, \ldots, N\} \subset V_I^\dagger$ are then

$$Q^\dagger e_a := \hat{e}_a =: Q^\dagger{}_a \tag{4}$$

and

$$e^a Q := \hat{e}^a =: Q^a. \tag{5}$$

The creator and annihilator for a general initial mode ψ are

$$\begin{aligned} Q^\dagger(e_a \psi^a) &= Q^\dagger{}_a \psi^a, \\ (\phi^\dagger{}_a e^a) Q &= \phi^\dagger{}_a Q^a, \end{aligned} \tag{6}$$

respectively.

We require that quantification respects the adjpoint †. This relates the two tensors Q and $Q^\dagger$

$$\psi^\dagger Q = (Q^\dagger \psi)^\dagger. \tag{7}$$

The rightmost † is the adjoint operation for the quantified system. Therefore,

$$\hat{e}_a^\dagger = M_{ab} \hat{e}^b, \tag{8}$$

with M_{ab} being the metric, the matrix of the adjoint operation, for the individual system.

We now generalize from the common statistics. A *linear statistics* shall be defined by a linear correspondence $Q^\dagger$ called the quantifier

$$Q^\dagger: V_I \to \mathcal{A}_S, \quad \psi \mapsto Q^\dagger \psi =: \hat{\psi}, \tag{9}$$

[compare (1)] from one-body modes to many-body operators, †-algebraically generating the algebra $\mathcal{A}_S := \text{End } V_S$ of the many-body theory. We further require that the quantifier $Q^\dagger$ induce an isomorphism from the one-body unitary group U_I into the many-body unitary group U_S, as described in Sec. IV. This is the *representation principle* for quantifiers.

The representation principle implies bilinear algebraic commutation relations discussed below.

In general $Q^\dagger$ does not produce a creator and Q does not produce an annihilator, as they do in the common statistics.

We construct the quantified algebra $\mathcal{A}_S$ from the individual space V_I in three easy steps:

(1) We form the quantum algebra $\mathcal{A}(V_I)$, defined as the free † algebra generated by (the vectors of) V_I. Its elements are all possible iterated sums and products and †-adjoints of the vectors of V_I. We require that the operations $(+, \times, \dagger)$ of $\mathcal{A}(V_I)$ agree with those of V_I where both are meaningful;
(2) we construct the ideal $\mathcal{R} \subset \mathcal{A}$ of all elements of $\mathcal{A}(V_I)$ that vanish in virtue of the statistics. It is convenient and customary to define $\mathcal{R}$ by a set of expressions **R**, such that the commutation

relations between elements of $\mathcal{A}(V_I)$' have the form $r=0$ with $r\in\mathbf{R}$. Then $\mathcal{R}$ consists of all elements of $\mathcal{A}(V_I)$ that vanish in virtue of the commutation relations and the postulates of a †-algebra.

Let $\mathbf{R}$ be closed under †. Let $\mathcal{R}_0$ be the set of all evaluations of all the expressions in $\mathbf{R}$ when the variable vectors ψ in these expressions assume any values $\psi\in V_I$. Then $\mathcal{R}=\mathcal{A}(V_I)\mathcal{R}_0\,\mathcal{A}(V_I)$;

(3) we form the quotient algebra (actually, a residue algebra)

$$\mathcal{A}_S=\mathcal{A}(V_I)/\mathcal{R}, \tag{10}$$

by identifying elements of $\mathcal{A}(V_I)$ whose differences belong to $\mathcal{R}$.

Then $Q^\dagger$ maps each vector $\psi\in V_I$ into its residue class $\psi+\mathcal{R}$.

Historically, physicists carried out one special quantification first. Since classically one multiplies phase spaces when quantifying, they assumed that quantally one multiplies Hilbert spaces, forming the tensor product

$$V_S=\bigotimes_{p=0}^{N} V_I=V_I^N \tag{11}$$

of N individual spaces V_I. Then in order to improve agreement with experiment they removed degrees of freedom in the tensor product connected with permutations, reducing V_I^N to a subspace PV_I^N invariant under all permutations of individuals. Here P is a projection operator characterizing the statistics. The many-body algebra was then taken to be the algebra of linear operators on the reduced space: $\mathcal{A}_S=\mathrm{End}\ PV_I^N$.

We call a statistics built in that way on a subspace of the tensor algebra over the one-body initial mode space, a *tensorial* statistics. Tensorial statistics represents permutations in a single-valued way. The common statistics are tensorial.

Linear statistics is more general than tensorial statistics, in that the quotient algebra $\mathcal{A}_S=\mathcal{A}-\mathcal{R}$ defining a linear statistics need not be the operator algebra of any subspace of the tensor space $\mathrm{Ten}\,V_I$ and need not be single-valued. Commutation relations permit more general statistics than projection operators do. For example, anyon statistics is linear but not tensorial.

For another example, $\mathcal{A}_S$ may be the endomorphism algebra of a spinor space constructed from the quadratic space V_I. Such a statistics we call a *spinorial statistics*. Clifford statistics, the main topic of this paper, is a spinorial statistics. Linear statistics includes both spinorial and tensorial statistics.

The FD, BE, and MB statistics are readily presented as tensorial statistics. We give their quantifiers next.[3] We then generalize to spinorial, nontensorial, statistics.

II. STANDARD STATISTICS

A. Maxwell–Boltzmann statistics

Classical an MB aggregate is a sequence (up to isomorphism) and $Q=\mathrm{Seq}$, the *sequence*-forming quantifier. The quantum individual I has a Hilbert space $V=V_I$ over the field $\mathbb{C}$. The vector space for the q sequence is the (contravariant) tensor algebra $V_S=\mathrm{Ten}\,V_I$, whose product is the tensor product $\otimes$

$$V_S=\mathrm{Ten}\,V_I, \tag{12}$$

with the natural induced †. The kinematic algebra $\mathcal{A}_S$ of the sequence is the †-algebra of endomorphisms of $\mathrm{Ten}\,V_I$, and is generated by $\psi\in V_I$ subject to the generating relations

$$\hat{\psi}^\dagger\hat{\phi}=\psi^\dagger\phi. \tag{13}$$

The left-hand side is an operator product, and the right-hand side is the contraction of the dual vector $\psi^\dagger$ with the vector ϕ, with an implicit unit element $1 \in \mathcal{A}_S$ as a factor.

B. Fermi–Dirac statistics

Here $Q = \text{Set}$, the *set*-forming quantifier. The kinematic algebra for the quantum set has defining relations

$$\begin{aligned} \hat{\psi}\hat{\phi} + \hat{\phi}\hat{\psi} &= 0, \\ \hat{\psi}^\dagger\hat{\phi} + \hat{\phi}\hat{\psi}^\dagger &= \psi^\dagger\phi. \end{aligned} \tag{14}$$

for all $\psi, \phi \in V_I$.

C. Bose–Einstein statistics

Here $Q = \text{Sib}$, the *sib*-forming quantifier. The sib-generating relations are

$$\begin{aligned} \hat{\psi}\hat{\phi} - \hat{\phi}\hat{\psi} &= 0, \\ \hat{\psi}^\dagger\hat{\phi} - \hat{\phi}\hat{\psi}^\dagger &= \psi^\dagger\phi, \end{aligned} \tag{15}$$

for all $\psi, \phi \in V_I$.

The individuals in each of the discussed quantifications, by construction, have the same (isomorphic) initial spaces. We call such individuals *isomorphic*.

III. RELATION TO THE PERMUTATION GROUP

A statistics is *abelian* if it represents the permutation group S_N on its N individuals by an abelian group of operators in the N-body mode space.

The FD or BE representations are not only abelian but scalar. They represent each permutation by a number, a projective representation of the identity operator. One calls entities with scalar statistics *indistinguishable*. Bosons and fermions are indistinguishable.

Non-abelian statistics describe distinguishable entities.

Nayak and Wilczek[1,4] give a spinorial statistics based on the work on nonabelions of Read and Moore.[5,6] Read and Moore use a subspace corresponding to the degenerate ground mode of some realistic Hamiltonian as the representation space for a nonabelian representation of the permutation group S_{2n} acting on the composite of $2n$ quasiholes in the fractional quantum Hall effect. This statistics, Wilczek showed, represents the permutation group on a spinor space, and permutations by noncommuting spin operators. The quasiholes of Read and Moore and of Wilczek and Nayak are distinguishable, but their permutations leave the ground subspace invariant.

Our own interest in the statistics of distinguishable entitities arises from a study of quantum space–time structure.[2] The dynamical process of any system is composite, it is generally believed, composed of isomorphic elementary actions going on all over, all the time. The first question that has to be answered in setting up an algebraic quantum theory of this composite process is: What statistics do the elementary actions have?

The elementary processes have ordinarily, though implicitly, been assumed to be distinguishable, being addressed by space–time coordinates, and to obey Maxwell–Boltzmann statistics. This repeats the history of particle statistics on the greater field of process statistics.

The Clifford statistics studied below is proposed primarily for the elementary processes of nature. We apply it here to toy models of particles in ordinary space–time to familiarize ourselves with its properties. In our construction, the representation space of the permutation group is the whole (spinor) space of the composite. The permutation group is not assumed to be a symmetry of the Hamiltonian or of its ground subspace any longer. It is used as a dynamical group, not a symmetry group.

IV. NO QUANTIFICATION WITHOUT REPRESENTATION

If we have defined how, for example, one translates individuals, this should define a way to translate the ensemble. We shall require of a quantification that any unitary transformation on an individual quantum entity induces a unitary transformation on the quantified system, defined by the quantifier.

This does not imply that, for example, the actual time-translation of an ensemble is carried out by translating the individuals. This would imply that the Hamiltonians combine additively, without interaction. There is still room for arbitrary interaction. The representation principle means only that there is a well-defined time-translation without interaction. This gives a physical meaning to interaction: it is the difference between the induced time translation generator and the actual one.

Thus we posit that an arbitrary (†-)unitary transformation $U:V_I\to V_I, \psi\mapsto U\psi$ of the individual ket-space V_I, also act naturally on the quantified mode space V_S through an operator $\hat{U}:V_S\to V_S$, defining a representation of the individual unitary group. This is the *representation principle*.

Then U also acts on the algebra $\mathcal{A}_S$ according to

$$\hat{U}:\mathcal{A}_S\to\mathcal{A}_S,\quad \hat{\psi}\mapsto\widehat{U\psi}=\hat{U}\hat{\psi}\hat{U}^{-1}. \tag{16}$$

Every unitary transformation $U:V_I\to V_I$ infinitesimally different from the identity is defined by a *generator* G

$$U=1+G\,\delta\theta, \tag{17}$$

where $G=-G^{\dagger}:V_I\to V_I$ is anti-Hermitian and $\delta\theta$ is an infinitesimal parameter. The infinitesimal anti-Hermitian generators G make up the Lie algebra dU_I of the unitary group U_I of the one-body theory.

By the representation principle, each individual generator G induces a *quantified generator* $\hat{G}\in\mathcal{A}_S$ of the quantified system, defined (up to an added constant) by its adjoint action on $\mathcal{A}_S$

$$\hat{G}:\hat{\psi}\mapsto\widehat{G\psi}=[\hat{G},\hat{\psi}], \tag{18}$$

and (18) and (20) define a representation (Lie homomorphism) $R_Q:dU_I\to dU_S$ of the individual Lie algebra dU_I in the quantified Lie algebra dU_S.

Since

$$G=\sum_{a,b} e_a G^a{}_b e^b, \tag{19}$$

holds by the completeness of the basis e_a and the reciprocal basis e^a, we can express the quantified generator $\hat{G}$ by

$$\hat{G}:=Q^{\dagger}GQ=\sum_{a,b} Q^{\dagger}{}_a G^a{}_b Q^b\equiv\sum_{a,b}\hat{e}_a G^a{}_b\hat{e}^b. \tag{20}$$

The representation principle holds for the usual statistics (MB, FD, BE) and for the Clifford statistics discussed below.

Proposition: If Q is a quantifier for a linear statistics then

$$[\hat{G},Q^{\dagger}\psi]=GQ^{\dagger}\psi, \tag{21}$$

hold for all anti-Hermitian generators G.

Proof: We have

$$
\begin{aligned}
[\hat{G}, Q^\dagger \psi] &= G^a{}_b\,(\hat{e}_a\,\hat{e}^b\,Q^\dagger\psi - Q^\dagger\psi\,\hat{e}_a\,\hat{e}^b) \\
&= G^a{}_b\,(\hat{e}_a\,(e^b\psi + (-1)^\kappa\,Q^\dagger\psi\,\hat{e}^b) - Q^\dagger\psi\,\hat{e}_a\,\hat{e}^b) \\
&= G^a{}_b\,\hat{e}_a\,e^b\psi = G^a{}_b\,\hat{e}_a\,\psi^b = G\,Q^\dagger\psi. \qquad (22)
\end{aligned}
$$

Here $\kappa = 1$ for Fermi statistics and 0 for Bose.

If $\mathcal{A}$ is any algebra, by the *commutator algebra* $\Delta\mathcal{A}$ of $\mathcal{A}$ we mean the Lie algebra on the elements of $\mathcal{A}$ whose product is the commutator $[a,b] = ab - ba$ in $\mathcal{A}$. By the commutator algebra of a quantum system I we mean that of its operator algebra $\mathcal{A}_I$.

In the usual cases of Bose and Fermi statistics, and not in the cases of complex and real Clifford statistics discussed below, the quantification rule (20) defines a Lie isomorphism, $\Delta\mathcal{A}_I \to \Delta\mathcal{A}_S$, from the commutator algebra of the individual to that of the quantified system. Namely, if H and P are two (arbitrary) operators acting on the one-body ket-space, then

$$
\widehat{[H, P]} = [\hat{H}, \hat{P}]. \qquad (23)
$$

Explicitly

$$
\begin{aligned}
[\hat{H}, \hat{P}] &= \hat{H}\hat{P} - \hat{P}\hat{H} \\
&= \hat{e}_r H^r{}_s \hat{e}^s \hat{e}_t P^t{}_u \hat{e}^u - \hat{e}_t P^t{}_u \hat{e}^u \hat{e}_r H^r{}_s \hat{e}^s \\
&= H^r{}_s P^t{}_u (\hat{e}_r \hat{e}^s \hat{e}_t \hat{e}^u - \hat{e}_t \hat{e}^u \hat{e}_r \hat{e}^s) \\
&= H^r{}_s P^t{}_u (\hat{e}_r (\delta^s_t \pm \hat{e}_t \hat{e}^s) \hat{e}^u - \hat{e}_t \hat{e}^u \hat{e}_r \hat{e}^s) \\
&= H^r{}_s P^t{}_u (\hat{e}_r \delta^s_t \hat{e}^u \pm \hat{e}_r \hat{e}_t \hat{e}^s \hat{e}^u - \hat{e}_t \hat{e}^u \hat{e}_r \hat{e}^s) \\
&= H^r{}_s P^t{}_u (\hat{e}_r \delta^s_t \hat{e}^u \pm \hat{e}_t \hat{e}_r \hat{e}^u \hat{e}^s - \hat{e}_t \hat{e}^u \hat{e}_r \hat{e}^s) \\
&= H^r{}_s P^t{}_u (\hat{e}_r \delta^s_t \hat{e}^u \pm \hat{e}_t (\mp \delta^u_r \pm \hat{e}^u \hat{e}_r) \hat{e}^s - \hat{e}_t \hat{e}^u \hat{e}_r \hat{e}^s) \\
&= H^r{}_s P^t{}_u (\hat{e}_r \delta^s_t \hat{e}^u - \hat{e}_t \delta^u_r \hat{e}^s) \\
&= \hat{e}_r (H^r{}_t P^t{}_u - P^r{}_t H^t{}_u) \hat{e}^u \\
&= \widehat{[H, P]}. \qquad (24)
\end{aligned}
$$

This implies that for BE and FD statistics, the quantification rule (20) can be extended from the unitary operators and their anti-Hermitian generators to the whole operator algebra of the quantified system.

V. CLIFFORD QUANTIFICATION

Now let the one-body mode space $V_I = \mathbb{R}^{N_+,N_-} = N_+\mathbb{R} \oplus N_-\mathbb{R}$ be a real quadratic space of dimension $N = N_+ + N_-$ and signature $N_+ - N_-$. Denote the symmetric metric form of V_I by $g = (g_{ab}) := (e_a^\dagger e_b)$. We do not assume that g is positive-definite.

We define *Clifford quantification* (9) by:

(1) the Clifford-like generating relations

$$
\hat{\psi}\hat{\phi} + \hat{\phi}\hat{\psi} = \frac{\zeta}{2}\,\psi^\dagger\phi, \qquad (25)
$$

for all $\phi, \psi \in V_I$, where ζ is a $\pm$ sign that can have either value;

(2) the Hermiticity condition (7)

$$
\hat{e}_a^\dagger = g_{ab}\hat{e}^b, \qquad (26)
$$

(3) a rule for raising and lowering indices

$$
\hat{e}_a := \zeta'\,g_{ab}\hat{e}^b, \qquad (27)
$$

where ζ' is another $\pm$ sign, and

(4) the definition (20) to quantify one-body generators.

Here $\zeta=\pm 1$ covers the two different conventions used in the literature. In Sec. VI we will see that $\zeta=\zeta'$, and that $\zeta=\zeta'=+1$ and $\zeta=\zeta'=-1$ are both allowed physically at the present theoretical stage of development. They lead to two different real quantifications, with either Hermitian or anti-Hermitian Clifford units.

For the quantified basis elements of V_I (25) leads to

$$\hat{e}_a\hat{e}_b+\hat{e}_b\hat{e}_a=\frac{\zeta}{2}g_{ab}\,. \tag{28}$$

The ψ's, which are assigned grade 1 and taken to be either Hermitian or anti-Hermitian, generate a graded †-algebra that we call the *free Clifford †-algebra* associated with $\mathbb{R}^{N_+,N_-}$ and write as $\mathrm{Cliff}(N_+,N_-)\equiv\mathrm{Cliff}(N_\pm)$. $\mathrm{Cliff}(N_\pm)$ contains a double-valued (or projective) representation of the permutation group S_N.

We call quanta obeying Clifford statistics *cliffordons*. Clifford statistics assembles cliffordons individually described by vectors into a composite described by spinors, which we call a *squadron*. We intend the -on suffix to remind us that unlike the common statistics the Clifford statistics has no classical correspondent.

A cliffordon is a hypothetical quantum-physical entity, like an electron, not to be confused with a mathematical object like a spinor or an operator. We cannot describe a cliffordon completely, but we represent our actions on a squadron of cliffordons adequately by operators in a Clifford algebra of operators. One encounters cliffordons only in permuting them, never in creating or annihilating them as individuals.

In assuming a real vector space of quantum modes instead of a complex one, we give up i-invariance but retain quantum superposition $a\psi+b\phi$ with real coefficients. Our theory is nonlinear from the complex point of view. Others considered nonlinear quantum theories, but gave up real superposition as well as i-invariance.[7,8] We are not *that* nonlinear.

VI. QUANTIFYING OBSERVABLES

In the usual statistics, the quantifier Q can be usefully extended from the Lie algebra of the individual to the commutator algebra of the individual; that is, from anti-Hermitian operators to all operators. This is not the case for Clifford quantification. There the quantification of any symmetric operator is a scalar, in virtue of Clifford's law, and so the commutator of any two operators is just the commutator of their antisymmetric parts. A straightforward calculation shows that

$$[\hat{H},\hat{P}]=\hat{H}\hat{P}-\hat{P}\hat{H}=\zeta\,\zeta'(\tfrac{1}{2}[\widehat{H,P}]+\tfrac{1}{4}([\widehat{P,H^\dagger}]+[\widehat{P^\dagger,H}])). \tag{29}$$

The three simplest cases are:

(1) $H=H^\dagger,\ H'=H'^\dagger\Rightarrow[\hat{H},\hat{H}']=0$;
(2) $H=H^\dagger,\ G_1=-G_1^\dagger\Rightarrow[\hat{H},\hat{G}_1]=0$;
(3) $G=-G^\dagger,\ G'=-G'^\dagger\Rightarrow[\hat{G},\hat{G}']=\zeta\,\zeta'\,[\widehat{G,G'}]$.

Thus Clifford quantification respects the commutation relations for anti-Hermitian generators if and only if $\zeta=\zeta'=+1$ or $\zeta=\zeta'=-1$; but not for Hermitian observables, contrary to the Bose and Fermi quantifications, which respect both.

VII. NAYAK–WILCZEK STATISTICS

The *complex* graded algebra generated by the ψ's with the relations (25) is called the *complex Clifford algebra* $\mathrm{Cliff}_{\mathbb{C}}(N)$ over $\mathbb{R}^{N_+,N_-}$. It is isomorphic to the full complex matrix algebra $\mathbb{C}(2^n)\otimes\mathbb{C}(2^n)$ for even $N=2n$, and to the direct sum $\mathbb{C}(2^n)\otimes\mathbb{C}(2^n)\oplus\mathbb{C}(2^n)\otimes\mathbb{C}(2^n)$ for odd $N=2n+1$. We regard $\mathrm{Cliff}_{\mathbb{C}}(N)$ as the kinematic algebra of the complex Clifford composite. As a vector space, it has dimension 2^N.

Schur[9] used complex spinors and complex Clifford algebra to represent permutations some years before Cartan used them to represent rotations. There is a fairly widespread view that spinors may be more fundamental than vectors, since vectors may be expressed as bilinear combinations of spinors. One of us took this direction in much of his work. Clifford statistics support the opposite view. There a vector describes an individual, a spinor an aggregate. Wilczek and Zee[10] seem to have been the first to recognize that spinors represent composites in a physical context, although this is implicit in the Chevalley construction of spinors within a Grassmann algebra.

For dimension $N=3$ spinors have as many parameters as vectors, but for higher N the number of components of the spinors associated with Cliff$(N_\pm)$ grows exponentially with N. The physical relevance of this irreducible double-valued (or projective) representation of the permutation group S_N was recognized by Nayak and Wilczek[1,4] in a theory of the fractional quantum Hall effect. We call the complex statistics based on Cliff$_{\mathbb{C}}(N)$ the *Nayak–Wilczek* or NW statistics.

Clifford statistics, unlike the more familiar particle statistics,[11–13] provides no creators or annihilators. With each individual mode e_a of the quantified system they associate a Clifford unit $\gamma_a = 2Q^\dagger{}_a$.

We may represent any swap (transposition of two cliffordons, say 1 and 2) by the difference of the corresponding Clifford units

$$t_{12} := \frac{1}{\sqrt{2}}(\gamma_1 - \gamma_2), \tag{30}$$

and represent an arbitrary permutation, which is a product of elementary swaps, by the product of their representations. That is, as direct computation shows, this defines a projective homomorphism from S_N into the Clifford algebra generated by the γ_k.

By definition, the number N of cliffordons in a squadron is the dimensionality of the individual initial mode space V_I. N is conserved rather trivially, commuting with every Clifford element. We can change this number only by varying the dimensionality of the one-body space. In one use of the theory, we can do this, for example, by changing the space–time four-volume of the corresponding experimental region. Because our theory does not use creation and annihilation operators, an initial action on the squadron represented by a spinor ξ should be viewed as some kind of spontaneous transition condensation into a coherent mode, analogous to the transition from the superconducting to the many-vertex mode in a type-II superconductor. The initial mode of a set or sib of (FD or BE) quanta can be regarded as a result of possibly entangled creation operations. That of a squadron of cliffordons cannot.

As with (22), let us verify that definition (20) is consistent in the Clifford case:

$$[\hat{G}, Q^\dagger\psi] = G^a{}_b(\hat{e}_a \hat{e}^b Q^\dagger\psi - Q^\dagger\psi \hat{e}_a \hat{e}^b) = \tfrac{1}{2} G^a{}_b(\hat{e}_a \psi^b + \psi_a \hat{e}^b) = G\, Q^\dagger\psi. \tag{31}$$

This shows that $Q^\dagger\psi$ transforms correctly under the infinitesimal unitary transformation of $\mathbb{R}^{N_+,N_-}$ (cf. Ref. 14).

VIII. BREAKING *i* INVARIANCE

Thus we cannot construct useful Hermitian variables of a squadron by applying the quantifier to the Hermitian variables of the individual cliffordon.

This is closely related to fact that the real initial mode space $\mathbb{R}^{N_\pm}$ of a cliffordon has no special operator to replace the imaginary unit i of the standard complex quantum theory. The fundamental task of the imaginary element i in the algebra of complex quantum physics is precisely to relate conserved Hermitian observables H and anti-Hermitian generators G by

$$H = -i\hbar G. \tag{32}$$

To perform this function exactly, the operator i must commute exactly with all observables.

The central operators x and p of classical mechanics are contractions of noncentral operators $\check{x}$ and $\check{p}=-i\hbar\partial/\partial\check{x}$.[2] In the limit of large numbers of individuals organized coherently into suitable condensate modes, the expanded operators of the quantum theory contract into the central operators of the classical theory. Condensations produce nearly commutative variables.

Likewise we expect the central operator i to be a contraction of a noncentral operator $\check{\imath}$ similarly resulting from a condensation in a limit of large numbers. In the simpler expanded theory, $\check{\imath}$, the correspondent of i, is not central.

One clue to the nature of $\check{\imath}$ and the locus of its condensation is how the operator i behaves when we combine separate systems. Since infinitesimal generators $G,G',\ldots$ combine by addition, the imaginaries $i,i',\ldots$ of different individuals must combine by identification

$$i=i'=\cdots, \tag{33}$$

for (32) to hold exactly, and nearly so for (32) to hold nearly. The only other variables in present physics that combine by identification in this way are the time t of clasical mechanics and the space–time coordinates x^μ of field theories. All systems in an ensemble must have about the same i, just as all particles have about the same t in the usual instant-based formulation, and all fields have about the same space–time variables x^μ in field theory. We identify the variables t and x^μ for different systems because they are set by the experimenter, not the system. This suggests that the experimenter, or more generally the environment of the system, mainly defines the operator i. The central operators x,p characterize a small system that results from the condensation of many particles. The central operator i must result from a condensation in the environment; we take this to be the same condensation that forms the vacuum and the spatiotemporal structure represented by the variables x^μ of the standard model.

The existence of this contracted i ensures that at least approximately, every Lie commutation relation between dimensionless anti-Hermitian generators A,B,C of the standard complex quantum theory

$$[A,B]=C, \tag{34}$$

corresponds to a commutation relation between Hermitian variables $-i\hbar A,\ -i\hbar B,\ -i\hbar C$

$$[-i\hbar A,-i\hbar B]=-i\hbar(-i\hbar C). \tag{35}$$

It also tells us that this correspondence is not exact in nature.

Stückelberg[15] reformulated complex quantum mechanics in the real Hilbert space $\mathbb{R}^{2N}$ of twice as many dimensions by assuming a special real antisymmetric operator $J:\mathbb{R}^{2N}\to\mathbb{R}^{2N}$ commuting with all of the variables of the system.

A real † or Hilbert space has no such operator. For example, in $\mathbb{R}^2$ the operator

$$E:=\begin{bmatrix}\varepsilon_1 & 0\\ 0 & \varepsilon_2\end{bmatrix}, \tag{36}$$

is a symmetric operator with an obvious spectral decomposition representing, according to the usual interpretation, two selection operations performed on the system, and cannot be written in the form $G=-(J/\hbar)E$ relating it to some antisymmetric generator G for any real antisymmetric J commuting with E.

On the other hand, if we restrict ourselves to observable operators of the form

$$E':=\begin{bmatrix}\varepsilon & 0\\ 0 & \varepsilon\end{bmatrix}, \tag{37}$$

we can use the operator J

$$J := \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \tag{38}$$

to restore the usual connection between symmetry transformations and corresponding observables. This restriction can be generalized to any even number of dimensions.[15]

IX. BREAKDOWN OF THE EXPECTATION VALUE FORMULA

For a system described in terms of a general real Hilbert space there is no simple relation of the form $G=(i/\hbar)H$ between the symmetry generators and the observables: the usual notions of Hamiltonian and momentum are meaningless in that case. This amplifies our earlier observation that Clifford quantification $A\rightarrow\hat{A}$ respects the Lie commutation relations among anti-Hermitian generators, not Hermitian observables.

Operationally, this means that selective acts of individual and quantified cliffordons use essentially different sets of filters. This is not the case for complex quantum mechanics and the usual statistics. There some important filters for the composite are simply assemblies of filters for the individuals.

Again, in the complex case the expectation value formula for an assembly

$$Av\,X = \psi^\dagger X \psi / \psi^\dagger \psi, \tag{39}$$

is a consequence of the eigenvalue principle for individuals, rather than an independent assumption.[3,16] The argument presented in Refs. 3 and 16 assumes that the individuals over which the average is taken combine with Maxwell–Boltzmann statistics. For highly excited systems this is a good approximation even if the individuals have FD or BE or other tensorial statistics. It is not necessarily a good approximation for cliffordons, which have spinorial, not tensorial, statistics.

X. SPIN-1/2 COMPLEX CLIFFORD MODEL

In this section we present a simplest possible model of a complex Clifford composite. The resulting many-body energy spectrum is isomorphic to that of a sequence of spin-1/2 particles in an external magnetic field.

Recall that in the usual complex quantum theory the Hamiltonian is related to the infinitesimal time-translation generator $G=-G^\dagger$ by $G=iH$. Quantifying H gives the many-body Hamiltonian. In the framework of spinorial statistics, as discussed above, this does not work, and quantification in principle applies to the anti-Hermitian time-translation generator G, not to the Hermitian operator H. Our task now is to choose a particular generator and to study its quantified properties.

We assume an even-dimensional real initial-mode space $V_I=\mathbb{R}^{2n}$ for the quantum individual, and consider the dynamics with the simplest non-trivial time-translation generator

$$G := \varepsilon \begin{bmatrix} \mathbf{0}_n & \mathbf{1}_n \\ -\mathbf{1}_n & \mathbf{0}_n \end{bmatrix}, \tag{40}$$

where ε is a constant energy coefficient.

The quantified time-translation generator $\hat{G}$ then has the form

$$\begin{aligned} \hat{G} &:= \sum_{l,j}^{N} \hat{e}_l G^l{}_j \hat{e}^j = -\varepsilon \sum_{k=1}^{n} (\hat{e}_{k+n}\hat{e}^k - \hat{e}_k \hat{e}^{k+n}) \\ &= +\varepsilon \sum_{k=1}^{n} (\hat{e}_{k+n}\hat{e}_k - \hat{e}_k \hat{e}_{k+n}) \\ &= 2\varepsilon \sum_{k=1}^{n} \hat{e}_{k+n}\hat{e}_k \\ &\equiv \frac{1}{2}\varepsilon \sum_{k=1}^{n} \gamma_{k+n}\gamma_k . \end{aligned} \tag{41}$$

By Stone's theorem, the generator $\hat{G}$ of time translation in the spinor space of the complex Clifford composite of $N=2n$ individuals can be factored into a Hermitian $H^{(N)}$ and an imaginary unit i that commutes strongly with $H^{(N)}$

$$\hat{G}=iH^{(N)}. \tag{42}$$

We suppose that $H^{(N)}$ corresponds to the Hamiltonian and seek its spectrum.

We note that by (41), $\hat{G}$ is a sum of n commuting anti-Hermitian algebraically independent operators $\gamma_{k+n}\gamma_k, k=1,2,\ldots,n$, $(\gamma_{k+n}\gamma_k)^\dagger=-\gamma_{k+n}\gamma_k$, $(\gamma_{k+n}\gamma_k)^2=-1^{(N)}$.

We use the well-known $2^n\times 2^n$ complex matrix representation of the γ-matrices of the complex universal Clifford algebra associated with the real quadratic space $\mathbb{R}^{2n}$ (Brauer and Weyl[17]):

$$\begin{aligned}\gamma_{2j-1}&=\sigma_3\otimes\cdots\otimes\sigma_3\otimes\sigma_1\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1},\\ \gamma_{2j}&=\sigma_3\otimes\cdots\otimes\sigma_3\otimes\sigma_2\otimes\mathbf{1}\otimes\cdots\otimes\mathbf{1},\\ j&=1,2,3,\ldots,n,\end{aligned} \tag{43}$$

where σ_1, σ_2 occur in the jth position, the product involves n factors, and σ_1, σ_2, σ_3 are the Pauli matrices. The representation of the corresponding permutation group S_{2n} is reducible. We can simultaneously diagonalize the $2^n\times 2^n$ matrices representing the commuting operators $\gamma_{k+n}\gamma_k$, and use their eigenvalues, $\pm i$, to find the spectrum λ of $\hat{G}$, and consequently of $H^{(N)}$.

A simple calculation shows that the spectrum of $\hat{G}$ consists of the eigenvalues

$$\lambda_k=\tfrac{1}{2}\varepsilon(n-2k)i, \quad k=0,1,2,\ldots,n, \tag{44}$$

with multiplicity

$$\mu_k=C_k^n:=\frac{n!}{k!(n-k)!}. \tag{45}$$

The spectrum of eigenvalues of the Hamiltonian $H^{(N)}$ then consists of $n+1$ energy levels

$$E_k=\tfrac{1}{2}(n-2k)\varepsilon, \tag{46}$$

with degeneracy μ_k. Thus E_k ranges over the interval

$$-\tfrac{1}{4}N\varepsilon<E<\tfrac{1}{4}N\varepsilon, \tag{47}$$

in steps of ε, with the given degeneracies.

Thus the spectrum of the structureless N-body complex Clifford composite is the same as that of a system of N spin-1/2 Maxwell–Boltzmann particles of magnetic moment μ in a magnetic field $\mathbf{H}$, with the identification

$$\tfrac{1}{4}\varepsilon=\mu H. \tag{48}$$

Even though we started with such a simple one-body time-translation generator as (40), the spectrum of the resulting many-body Hamiltonian possesses some complexity, reflecting the fact that the units in the composite are distinguishable, and their swaps generate the dynamical variables of the system.

This spin-1/2 model does not tell us how to swap two Clifford units experimentally. Like the phonon model of the harmonic oscillator, the statistics of the individual quanta enters the picture only through the commutation relations among the fundamental operators of the theory.

XI. REAL CLIFFORD STATISTICS

Real Clifford quantification establishes a morphism (20) from the Lie algebra of the individual into that of the composite. The proof for real Clifford statistics parallels that for the complex Clifford case closely.

According to the Periodic Table of the Spinors,[18,19–21] the free (or universal) Clifford algebra $\mathrm{Cliff}_{\mathbb{R}}(N_+,N_-)$ is algebra-isomorphic to the endomorphism algebra of a module $\Sigma(N_+,N_-)$ over a ring $\mathcal{R}(N_+,N_-)$. We give the table to simplify reference to it (here $\zeta=-1$):

N_+ \ N_-	0	1	2	3	4	5	6	7	...
0	$\mathbb{R}$	$\mathbb{R}_2$	$2\mathbb{R}$	$2\mathbb{C}$	$2\mathbb{H}$	$2\mathbb{H}_2$	$4\mathbb{H}$	$8\mathbb{C}$	...
1	$\mathbb{C}$	$2\mathbb{R}$	$2\mathbb{R}_2$	$4\mathbb{R}$	$4\mathbb{C}$	$4\mathbb{H}$	$4\mathbb{H}_2$	$8\mathbb{H}$	...
2	$\mathbb{H}$	$\mathbb{C}_2$	$4\mathbb{R}$	$4\mathbb{R}_2$	$8\mathbb{R}$	$8\mathbb{C}$	$8\mathbb{H}$	$8\mathbb{H}_2$	...
3	$\mathbb{H}_2$	$2\mathbb{H}$	$4\mathbb{C}$	$8\mathbb{R}$	$8\mathbb{R}_2$	$16\mathbb{R}$	$16\mathbb{C}$	$16\mathbb{H}$	...
4	$2\mathbb{H}$	$2\mathbb{H}_2$	$4\mathbb{H}$	$8\mathbb{C}$	$16\mathbb{R}$	$16\mathbb{R}_2$	$32\mathbb{R}$	$32\mathbb{C}$	...
5	$4\mathbb{C}$	$4\mathbb{H}$	$4\mathbb{H}_2$	$8\mathbb{H}$	$16\mathbb{C}$	$32\mathbb{R}$	$32\mathbb{R}_2$	$64\mathbb{R}$	...
6	$8\mathbb{R}$	$8\mathbb{C}$	$8\mathbb{H}$	$8\mathbb{H}_2$	$16\mathbb{H}$	$32\mathbb{C}$	$64\mathbb{R}$	$64\mathbb{R}_2$	...
7	$8\mathbb{R}_2$	$16\mathbb{R}$	$16\mathbb{C}$	$16\mathbb{H}$	$16\mathbb{H}_2$	$32\mathbb{H}$	$64\mathbb{C}$	$128\mathbb{R}$	...
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	

(49)

It shows that the ring of coefficients $\mathcal{R}(N_+,N_-)$ varies periodically with period 8 in each of the dimensionalities N_+ and N_- of V_I, and is a function of signature N_+-N_- alone. In the first cycle, $N_+-N_-=0,1,\ldots,7$, and $\mathcal{R}=\mathbb{R},\mathbb{C},\mathbb{H},\mathbb{H}\oplus\mathbb{H},\mathbb{H},\mathbb{C},\mathbb{R},\mathbb{R}\oplus\mathbb{R}$, respectively. Then the cycle repeats ad infinitum.

In our application the module $\Sigma(N_+,N_-)$, the spinor space supporting $\mathrm{Cliff}_{\mathbb{R}}(N_+,N_-)$, serves as the initial mode space of a squadron of N real cliffordons. $\mathcal{R}(N_\pm)$ we call the *spinor coefficient ring* for $\mathrm{Cliff}_{\mathbb{R}}(N_+,N_-)$.

XII. PERMUTATIONS

In the standard statistics there is a natural way to represent permutations of individuals in the N-body composite. Each N-body ket is constructed by successive action of N creation operators on the special vacuum mode. Any permutation of individuals can be achieved by permuting these creation operators in the product. The identity and alternative representations of the permutation group S_N in the BE and FD cases then follow from the defining relations of Sec. II.

In the case of Clifford statistics, some things are different. There is still an operator associated with each cliffordon; now it is a Clifford unit. Permutations of cliffordons are still represented by operators on a many-body † space. But the mode space on which these operators act is now a spinor space, and its basis vectors are not constructed by creation operators acting on a special ''vacuum'' ket.

The Clifford representation of the permutation group that we have employed is reducible into two irreducible Schur representations. It is a bit easier to write than Schur's because our individual operators γ_i anticommute exactly, corresponding to exactly orthogonal directions in the one-body mode space, like the generators of Dirac's Clifford algebra. In Schur's irreducible representation (slightly simplified) these operators are replaced by their projections normal to the principle diagonal direction $n:=\Sigma\gamma_i/\sqrt{N}$, which is invariant under all permutations. The corresponding angles are those subtended by the edges of a regular simplex of N vertices in $N-1$ dimensions as seen from the center. These angles are all determined by

$$\cos^2\theta = \frac{1}{N-1}. \tag{50}$$

They differ from $\pi/2$ by an angle that vanishes for large N like $1/N$.

XIII. EMERGENCE OF A QUANTUM *i*

The Periodic Table of the Spinors (Sec. XI) suggests another origin for the complex i of quantum theory, and one that is not approximately central but exactly central. Some Clifford algebras $\mathrm{Cliff}_{\mathbb{R}}(N_+,N_-)$ have the spinor coefficient ring $\mathbb{C}$, containing an element i. Multiplication by this i then represents an operator in the center of the Clifford algebra, which we designate also by i. We may use i-multiplication to represent the top element $\gamma^{\uparrow}$ whenever $\gamma^{\uparrow}$ is central and has square -1. This $i \in \mathrm{Cliff}_{\mathbb{R}}(N_{\pm})$ corresponds to the i of complex quantum theory.

$\mathrm{Cliff}_{\mathbb{R}}(1,0)$ contains such an i but is commutative. According to the Periodic Table (with the choice of $\zeta=-1$), the smallest noncommmutative Clifford algebras of Euclidean signature with complex spinor coefficients are $\mathrm{Cliff}_{\mathbb{R}}(0,3)$ with negative Euclidean signature, and $\mathrm{Cliff}_{\mathbb{R}}(5,0)$ with positive Euclidean signature. Triads or pentads of such cliffordons could underlie the physical ''elementary'' particles, giving rise to complex quantum mechanics within the real. We consider these two cases in turn.

$\mathrm{Cliff}_{\mathbb{R}}(0,3)=\mathbb{C}(2)$ has the familiar Pauli representation $\gamma_1 := i\sigma_1$, $\gamma_2 := i\sigma_2$, $\gamma_3 := i\sigma_3$ with $\zeta=-1$. We choose a particular one-cliffordon dynamics of the form

$$G := \begin{bmatrix} 0 & V & 0 \\ -V & 0 & \varepsilon \\ 0 & -\varepsilon & 0 \end{bmatrix}. \tag{51}$$

Quantification (20) of G gives

$$\hat{G} = iH^{(-3)} \tag{52}$$

with the Hamiltonian

$$H^{(-3)} = \frac{1}{2}\begin{bmatrix} V & \varepsilon \\ \varepsilon & -V \end{bmatrix}. \tag{53}$$

This is also the Hamiltonian for a generic two-level quantum-mechanical system (with the energy separation ε) in an external potential field V, like the ammonia molecule in a static electric field discussed in Ref. 22.

$\mathrm{Cliff}_{\mathbb{R}}(5,0)=\mathbb{C}(4)$ has the matrix representation $\gamma_1 := i\sigma_1\otimes\mathbf{1}$, $\gamma_2 := i\sigma_2\otimes\mathbf{1}$, $\gamma_3 := i\sigma_3\otimes\sigma_1$, $\gamma_4 := i\sigma_3\otimes\sigma_2$, $\gamma_5 := i\sigma_3\otimes\sigma_3$, again with $\zeta=-1$. Its top Clifford unit is $\gamma^{\uparrow} := \Pi_k\gamma_k = \gamma^{\uparrow\dagger} = \gamma^{\uparrow -1}$ with eigenvalues ± 1. We choose a specimen dynamics (for the individual cliffordon) in the form

$$G := \begin{bmatrix} 0 & V & 0 & 0 & 0 \\ -V & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{54}$$

Quantification (20) of G gives

$$\hat{G} = iH^{(5)}, \tag{55}$$

with the Hamiltonian

$$H^{(5)}=\frac{1}{2}V\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix}. \tag{56}$$

The two examples considered above show how a squadron of several real cliffordons can obey a truly complex quantum theory.

XIV. FERMI AND CLIFFORD STATISTICS

The FD algebra of creators and annihilators is a special case of a Clifford algebra over a quadratic space with neutral quadratic form, called the quantum algebra by Saller[23] and the mother algebra by Doran *et al.*[24] Is FD statistics ever a special case of Clifford statistics? Specifically, are their †-algebras ever isomorphic?

From the N annihilators a_k of the complex FD statistics we can form a sequence of anticommuting hermitian square roots of unity

$$i_k=a_k+a_k^\dagger, \quad i_{k+N}=\frac{a_k-a_k^\dagger}{i}. \tag{57}$$

Moreover, the complex †-algebra that these generate is a Clifford †-algebra Cliff$(2N,0)$. The transformation from the FD generators to the Clifford is invertible. Therefore complex FD statistics and complex Clifford statistics have isomorphic †-algebras.

The graded †-algebras are obviously not isomorphic. The two grade operators do not even commute.

The question is more complicated for the real Fermi and Clifford quantifications. We follow Doran *et al.*,[24] among others.

In the real FD formulation we begin with a real one-fermion n-dimensional space $F\cong n\mathbb{R}$ with no metric or adjoint. The FD quantified algebra $\mathcal{A}$ has the bilinear associative product defined by the FD relations

$$\begin{aligned} f_if_j+f_jf_i&=0,\\ f_if^j+f^jf_i&=\delta_i^j, \end{aligned} \tag{58}$$

and the adjoint defined by

$$f_i^\dagger:=f^i. \tag{59}$$

The f_i are creation and f^j are annihilation operators.

To present $\mathcal{A}$ as a Clifford algebra we form the direct sum

$$W=F\oplus F^\dagger. \tag{60}$$

In a basis $\{f_i, f^i\}_{i=1}^n$ adapted to this direct sum, we define the following GL(V)-invariant metric for W

$$g\sim\begin{bmatrix}0&1/2\\1/2&0\end{bmatrix}, \tag{61}$$

corresponding to

$$f_i \cdot f_j = 0, \quad f^i \cdot f^j = 0, \quad f^i \cdot f_j = \tfrac{1}{2}\delta^i_j . \tag{62}$$

Since F supports a quantum theory it too has a quadratic form $*: F \otimes F \to \mathbb{R}$, which we assume to be Euclidean. We did not use $*$ in the construction of $\mathcal{A}$ and g.

We quantify this fermion by a mapping $Q^\dagger: W \to \mathcal{A}$ into the †-algebra of the composite. For brevity we write f_i for $Q^\dagger f_i$ as is also customary.

The quantification Q has the representation property. In the FD case this means that Q represents the orthogonal group $\mathrm{SO}(F,*)$ in $\mathcal{A}$; in fact it represents the larger group $\mathrm{GL}(F)$, for $*$ has not entered into the definition of Q.

The basis $\{\gamma_i, \tilde{\gamma}_i\}_{i=1}^n$ defined by

$$\gamma_i := f_i + f^i, \quad \tilde{\gamma}_i := f_i - f^i, \tag{63}$$

gives the metric g of W the diagonal form

$$g \sim \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{64}$$

corresponding to

$$\gamma_i \cdot \gamma_j = 1, \quad \tilde{\gamma}_i \cdot \tilde{\gamma}_j = -1, \quad \tilde{\gamma}_i \cdot \gamma_j = 0. \tag{65}$$

That is, $W = E \oplus \tilde{E}$ is a neutral quadratic space, with Eucidean subspace E and anti-Euclidean subspace $\tilde{E}$.

The γ's obey

$$\begin{gathered} \gamma_i \gamma_j + \gamma_j \gamma_i = +2\delta_{ij}, \\ \tilde{\gamma}_i \tilde{\gamma}_j + \tilde{\gamma}_j \tilde{\gamma}_i = -2\delta_{ij}, \\ \tilde{\gamma}_i \gamma_j + \gamma_j \tilde{\gamma}_i = 0. \end{gathered} \tag{66}$$

Therefore the FD algebra (58) is isomorphic to a real Clifford algebra $\mathrm{Cliff}(W,\dagger) = \mathrm{Cliff}(E \oplus \tilde{E})$.

Are the Clifford and FD †-algebras also isomorphic?

With respect to the Fermi adjoint †, half of the Clifford generators (the γ_i) are Hermitian and the other half (the $\tilde{\gamma}_i$) are anti-Hermitian. In a Clifford † algebra, however, all the generators are anti-Hermitian or Hermitian together. Therefore the Clifford-algebra generators $\{\gamma_i, \tilde{\gamma}_i\}_{i=1}^n$ are not Clifford †-algebra generators.

In some cases we construct suitable generators using the top element $\tilde{\gamma}^\uparrow$ of $\tilde{E}$:

If the dimension n of E (and F) is a multiple of 4, then $\overline{\gamma_i} := \tilde{\gamma}^\uparrow \tilde{\gamma}_i$ anticommutes with the γ_j, and is Hermitian like the γ_j. Then the elements $\{\gamma_i, \overline{\gamma_i}\}_{i=1}^n$ generate a Clifford †-algebra with [cf. (66)]

$$\begin{gathered} \gamma_i \gamma_j + \gamma_j \gamma_i = +2\delta_{ij}, \\ \overline{\gamma_i}\,\overline{\gamma_j} + \overline{\gamma_j}\,\overline{\gamma_i} = +2\delta_{ij}, \\ \overline{\gamma_i} \gamma_j + \gamma_j \overline{\gamma_i} = 0, \end{gathered} \tag{67}$$

which is isomorphic to the FD algebra of F. Then the Clifford-quantified †-algebra (the case $\zeta = \zeta' = +1$) is isomorphic to a Fermi-quantified one when $n = 4m$, and the adjoint of the one-cliffordon space is positive definite. The two quantified theories then predict the same transition amplitudes and spectra.

Analogously, when $\zeta=\zeta'=-1$ and all the Clifford generators are anti-Hermitian, and $n=4m$, the FD and Clifford statistics again give isomrphic † algebras.

They still differ in their grades. The FD quantified system has a grade G_F with spectrum $-N,\ldots,0,\ldots,N$, corresponding to the creation and annihilation fermions. The Clifford quantified system has a positive grade operator G_C with spectrum $0,1,\ldots 2N$. The operators G_C and G_F do not even commute. The FD and Clifford graded-algebras are not isomorphic.

This is merely a difference in language. The operators that are said to create and annihilate things in FD statistics are said to permute things in Clifford statistics. In Clifford statistics nothing is created or destroyed.

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Becchi–Rouet–Stora–Tyutin formalism and zero locus reduction

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In the Becchi–Rouet–Stora–Tyutin (BRST) quantization of gauge theories, the zero locus $\mathcal{Z}_{\mathbf{Q}}$ of the BRST differential $\mathbf{Q}$ carries an (anti)bracket whose parity is opposite to that of the fundamental bracket. Observables of the BRST theory are in a 1:1 correspondence with Casimir functions of the bracket on $\mathcal{Z}_{\mathbf{Q}}$. For any constrained dynamical system with the phase space $\mathcal{N}_0$ and the constraint surface Σ, we prove its equivalence to the constrained system on the BFV-extended phase space with the constraint surface given by $\mathcal{Z}_{\mathbf{Q}}$. Reduction to the zero locus of the differential gives rise to relations between bracket operations and differentials arising in different complexes (the Gerstenhaber, Schouten, Berezin–Kirillov, and Sklyanin brackets); the equation ensuring the existence of a nilpotent vector field on the reduced manifold can be the classical Yang–Baxter equation. We also generalize our constructions to the bi-*QP* manifolds which from the BRST theory viewpoint correspond to the BRST–anti-BRST-symmetric quantization. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1367867]

I. INTRODUCTION

The Becchi–Rouet–Stora–Tyutin (BRST) quantization of general gauge theories in the Hamiltonian and Lagrangian formalisms includes the Batalin–Fradkin–Vilkovisky (BFV)[1] and Batalin–Vilkovisky (BV)[2] formalisms. From a geometric standpoint, these quantization formalisms deal with an even or odd *QP* manifold $\mathcal{N}$,[3,4] i.e., a symplectic or antisymplectic manifold equipped with a compatible odd vector field $\mathbf{Q}$ such that $\mathbf{Q}^2=0$. This condition is ensured by imposing the *master equation* on the Hamiltonian function of the vector field $\mathbf{Q}$. In the standard physicists' notation, the respective equations are

$$\{\Omega,\Omega\}=0 \quad \text{and} \quad (S,S)=0, \tag{1.1}$$

where Ω (by a widespread abuse of terminology) is the ''BRST generator'' in the Hamiltonian quantization and S is the master action in the Lagrangian quantization.

Under appropriate regularity conditions, the zero locus $\mathcal{Z}_{\mathbf{Q}}\subset\mathcal{N}$ of $\mathbf{Q}=\{\Omega,\cdot\}$ [of $\mathbf{Q}=(S,\cdot)$] is an odd Poisson manifold (respectively, a Poisson manifold),[4,5] whose geometry captures crucial information about the theory on $\mathcal{N}$. In this paper, we mainly concentrate on *even QP* manifolds (which correspond to the BFV quantization and were implicit in Ref. 7) because they have not been considered before; however, we formulate the general facts about the zero-locus reduction such that they apply to both even and odd *QP* manifolds. On an even *QP* manifold, $\mathcal{Z}_{\mathbf{Q}}$ carries an *anti*bracket; we then show that the equivalence classes of observables (the cohomology of $\mathbf{Q}$) are in a 1:1 correspondence with characteristic (Casimir) functions of the antibracket on $\mathcal{Z}_{\mathbf{Q}}$ and gauge symmetries in the BFV theory on $\mathcal{N}$ are Hamiltonian vector fields on $\mathcal{Z}_{\mathbf{Q}}$.

Moreover, the zero locus $\mathcal{Z}_{\mathbf{Q}}$ of the BFV differential on the extended phase space is a proper counterpart of the constraint surface in the following sense. In geometric terms, a first-class constrained system can be specified by its phase space (a symplectic manifold $\mathcal{N}_0$) and the

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constraint surface Σ. On the extended phase space $\mathcal{N}$ constructed in the BFV quantization, we can consider the dynamical system whose constraint surface, by definition, is $\mathcal{Z}_{\mathbf{Q}}$ (in local coordinates on $\mathcal{N}$, the constraints can be chosen as the components of $\mathbf{Q}$). Then the constrained systems $(\mathcal{N}_0,\Sigma)$ and $(\mathcal{N},\mathcal{Z}_{\mathbf{Q}})$ *are equivalent*: the respective algebras of the equivalence classes of observables are naturally isomorphic as Poisson algebras.

Beyond the BRST context, algebras of functions on *QP* manifolds, which are differential Poisson algebras (associative supercommutative algebras endowed with a bracket operation and a differential that is a derivation of the bracket) can arise from complexes endowed with a supercommutative associative multiplication and a Gerstenhaber-like multiplication (''*bracket*''); the differential is then interpreted as the $\mathbf{Q}$ structure, and the bracket becomes the P structure [the Poisson or the BV bracket on the dual (super)manifold]. The basic examples are the cohomology complexes of a Lie algebra $\mathfrak{a}$ with coefficients in $\bigwedge\mathfrak{a}$ or $\mathrm{S}\mathfrak{a}$ (the exterior and symmetric tensor algebras); the general case involves L_∞ algebras.[8]

In this algebraic context, reduction to the zero locus can yield relations between different complexes. In certain cases, the zero-locus reduction can be applied *repeatedly*; the equation ensuring the existence of a nilpotent vector field on the reduced manifold at the second step of the reduction can be the classical Yang–Baxter equation (CYBE), in which case the reduction leads to the well-known Sklyanin and Berezin–Kirillov brackets.

In addition to the usual *QP* manifolds, one can consider *bi-QP* manifolds, which are the geometric counterparts of bicomplexes, and in physical terms, originate in the BRST–anti-BRST [Sp(2)-symmetric/triplectic] quantization.[9–12] With two BRST operators represented by two commuting (odd and nilpotent) vector fields, bi-*QP* manifolds might be called *QQP* manifolds; interestingly enough, the corresponding zero-locus reduction (to the submanifold on which both vector fields vanish) results in a ''*PP*'' manifold, i.e., gives rise to a *bi-Hamiltonian* structure. A typical example is obtained by starting with a Lie algebra $\mathfrak{a}$ and deriving the second differential from a *co*algebra structure. Compatibility between two differentials then implies that $(\mathfrak{a},\mathfrak{a}^*,\mathfrak{a}\oplus\mathfrak{a}^*)$ is a Manin triple.[13] There also exists an alternative construction of a bi-*QP* manifold from a *single* Lie algebra structure, which results in non-Abelian triplectic antibrackets[14] on the space of common zeroes of the differentials (and thus, the zero locus reduction leads to a nontrivial relation to the bicomplex used in the extended BRST symmetry).

This paper is organized as follows. In Sec. 2.2, we recall the main points of the zero locus reduction on (odd or even) *QP* manifolds. Symmetries of *QP* manifolds are reviewed in Sec. 2.3. In Sec. 3, we turn to a more detailed analysis of even *QP* manifolds corresponding to the BFV quantization. In Secs. 3.1–3.2, we recall several facts about the BFV formalism in the form that is suitable for what follows. The results given in 3.4 state the relation between objects in the bulk of the phase space and on the zero locus submanifold. We briefly discuss in Sec. 3.5 how these results can be restated for the BV formalism. In Sec. 4, we consider specific brackets resulting from the zero-locus reduction. In Sec. 5, we study *bi-QP* manifolds.

II. GEOMETRY OF *QP* MANIFOLDS AND ZERO LOCUS REDUCTION

Geometric objects underlying the BRST quantization are the *QP* manifolds.

2.1. Definition (Refs. 3 and 4): A QP manifold is a supermanifold $\mathcal{N}$ equipped with a bracket $\{\cdot,\cdot\}$ such that

$$\{F,G\}=-(-1)^{(\mathrm{p}(F)+\kappa)(\mathrm{p}(G)+\kappa)}\{G,F\},$$

$$\{F,GH\}=\{F,G\}H+(-1)^{(\mathrm{p}(F)+\kappa)\mathrm{p}(G)}G\{F,H\}, \tag{2.1}$$

$$\{F,\{G,H\}\}=\{\{F,G\},H\}+\{G,\{F,H\}\}(-1)^{(\mathrm{p}(F)+\kappa)(\mathrm{p}(G)+\kappa)},$$

for F, G, $H\in\mathcal{F}_{\mathcal{N}}$ (smooth functions on $\mathcal{N}$), and with an odd nilpotent vector field $\mathbf{Q}$, $\mathbf{Q}^2=0$, such that

$$\mathbf{Q}\{F,G\}-\{\mathbf{Q}F,G\}-(-1)^{\mathrm{p}(F)+\kappa}\{F,\mathbf{Q}G\}=0, \quad F,G\in\mathcal{F}_{\mathcal{N}} \tag{2.2}$$

[where $p(()\cdot)$ is the Grassmann parity]. QP manifolds with a Poisson bracket ($\kappa=0$) *are called even, and those with an* antibracket ($\kappa=1$), *odd.*

Odd *QP* manifolds arise in the BV quantization, and even ones in the BFV quantization. Odd *QP* manifolds were introduced in Ref. 3 and were studied in Refs. 4 and 5. In most of our definitions, *QP* manifolds can be either even or odd; in Sec. 3, however, we concentrate on even *QP* manifolds, which have not been given enough attention previously.

2.2. The zero locus of $\mathbf{Q}$. In what follows, $\mathcal{Z}_{\mathbf{Q}}$ denotes the zero locus of the odd vector field $\mathbf{Q}$ on a *QP* manifold $\mathcal{N}$. We assume $\mathcal{Z}_{\mathbf{Q}}$ to be a nonempty smooth submanifold and denote by $\mathcal{J}_{\mathcal{Z}_{\mathbf{Q}}}\subset\mathcal{F}_{\mathcal{N}}$ *the ideal of smooth functions vanishing on* $\mathcal{Z}_{\mathbf{Q}}$.

The odd vector field $\mathbf{Q}$ is called *regular* if each function $f\in\mathcal{J}_{\mathcal{Z}_{\mathbf{Q}}}$ can be represented as

$$f=\sum_{\alpha} f_{\alpha}\mathbf{Q}\Gamma^{\alpha}, \tag{2.3}$$

with some f_{α}, $\Gamma^{\alpha}\in\mathcal{F}_{\mathcal{N}}$ (i.e., if the components of $\mathbf{Q}$ generate $\mathcal{J}_{\mathcal{Z}_{\mathbf{Q}}}$). We say that a submanifold $\mathcal{L}\subset\mathcal{N}$ is *coisotropic* if

$$\{\mathcal{J}_{\mathcal{L}},\mathcal{J}_{\mathcal{L}}\}\subset\mathcal{J}_{\mathcal{L}}. \tag{2.4}$$

2.2.1. Lemma: If $\mathbf{Q}$ *is regular,* $\mathcal{Z}_{\mathbf{Q}}$ *is a coisotropic submanifold of the QP manifold* $\mathcal{N}$.

Proof: Let $f, g\in\mathcal{F}_{\mathcal{N}}$ vanish on $\mathcal{Z}_{\mathbf{Q}}$. Using representation (2.3), the Leibnitz rule, Eq. (2.2), and nilpotency of $\mathbf{Q}$, we see that $\{f_{\alpha}(\mathbf{Q}\Gamma^{\alpha}),(\mathbf{Q}\Gamma^{\beta})g_{\beta}\}|_{\mathcal{Z}_{\mathbf{Q}}}=(f_{\alpha}\{\mathbf{Q}\Gamma^{\alpha},\mathbf{Q}\Gamma^{\beta}\}g_{\beta})|_{\mathcal{Z}_{\mathbf{Q}}}=0$. □

In what follows, we assume $\mathcal{Z}_{\mathbf{Q}}$ to be coisotropic even in those cases where $\mathbf{Q}$ is not regular. The algebra $\mathcal{F}_{\mathcal{Z}_{\mathbf{Q}}}$ of smooth functions on $\mathcal{Z}_{\mathbf{Q}}$ is the quotient $\mathcal{F}_{\mathcal{N}}/\mathcal{J}_{\mathcal{Z}_{\mathbf{Q}}}$. We then have

2.2.2. Lemma: There is a well-defined binary operation given by $\{,\}_{\mathbf{Q}}:\mathcal{F}_{\mathcal{Z}_{\mathbf{Q}}}\times\mathcal{F}_{\mathcal{Z}_{\mathbf{Q}}}\to\mathcal{F}_{\mathcal{Z}_{\mathbf{Q}}}$

$$\{f,g\}_{\mathbf{Q}}=\{F,\mathbf{Q}G\}|_{\mathcal{Z}_{\mathbf{Q}}}, \quad f,g\in\mathcal{F}_{\mathcal{Z}_{\mathbf{Q}}}, \quad F,G\in\mathcal{F}_{\mathcal{N}}, \quad F|_{\mathcal{Z}_{\mathbf{Q}}}=f, \quad G|_{\mathcal{Z}_{\mathbf{Q}}}=g, \tag{2.5}$$

where F *and* $G\in\mathcal{F}_{\mathcal{N}}$ *are viewed as representatives of functions on* $\mathcal{Z}_{\mathbf{Q}}$. *It makes* $\mathcal{Z}_{\mathbf{Q}}$ *into a Poisson manifold.*

The proof is a straightforward generalization of a proof given in Ref. 5. It is obvious that the parity of the induced bracket on $\mathcal{Z}_{\mathbf{Q}}$ is opposite to the parity of the $\{,\}$ bracket on $\mathcal{N}$. An important characteristic of the differential $\mathbf{Q}$ is the homology of the linear operators $\mathbf{Q}_p:T_p\mathcal{N}\to T_p\mathcal{N}$, $p\in\mathcal{Z}_{\mathbf{Q}}$, defined as follows. We consider the tangent space $T_p\mathcal{N}$ as the quotient of the vector fields $\mathrm{Vect}_{\mathcal{N}}$ modulo those that vanish at p. Then

$$\mathbf{Q}_p(x)=([\mathbf{Q},X])|_p, \quad X\in\mathrm{Vect}_{\mathcal{N}}, \quad x=X_p\in T_p\mathcal{N}. \tag{2.6}$$

This operation is well-defined once $\mathbf{Q}$ vanishes at p.

2.2.3. Definition: A QP manifold $\mathcal{N}$ *is called* proper *if the homology of the linear operator* $\mathbf{Q}_p:T_p\mathcal{N}\to T_p\mathcal{N}$ *is trivial at each point* $p\in\mathcal{Z}_{\mathbf{Q}}$.

This definition is equivalent to the one given in Ref. 4 (and Ref. 5), but uses only invariant notions [in local coordinates Γ^A, we would have $(\mathbf{Q}_p x)^A=(-1)^{p(x)+1}x^B(\partial\mathbf{Q}^A/\partial\Gamma^B)$]. We now have the following proposition.

2.2.4. Proposition (Refs. 4 and 5): Let $\mathcal{N}$ *be a proper QP manifold with a nondegenerate bracket. Then* $\mathcal{Z}_{\mathbf{Q}}$ *is (anti)symplectic with respect to the induced bracket* (2.5).

One can replace $\mathcal{Z}_{\mathbf{Q}}$ with a submanifold that still is coisotropic. As a straightforward generalization of 2.2.2, we have

2.2.5. Theorem: *Let* $\mathcal{N}$ *be a QP manifold and* $\mathcal{L}\subset\mathcal{Z}_{\mathbf{Q}}\subset\mathcal{N}$ *a coisotropic submanifold of* $\mathcal{N}$. *Then* $\mathcal{L}$ *is a Poisson manifold with the Poisson structure given by (by Poisson manifolds, we mean those with either an even Poisson bracket or an antibracket):*

$$\{f,g\}_{\mathbf{Q}}=\{F,\mathbf{Q}G\}|_{\mathcal{L}},\quad f,g\in\mathcal{F}_{\mathcal{L}},\quad F,G\in\mathcal{F}_{\mathcal{N}},\quad F|_{\mathcal{L}}=f,\quad G|_{\mathcal{L}}=g. \tag{2.7}$$

Proof: It is easy to see that (2.7) does not depend on the choice of representatives $F,G\in\mathcal{F}_{\mathcal{N}}$ of $f,g\in\mathcal{F}_{\mathcal{L}}$. The Jacobi identity and the Leibnitz rule follow in the same way as for the bracket in Eq. (2.5), see Ref. 5. □

2.3. Symmetries of QP manifolds (Ref. 5). We now recall several basic facts about symmetries of *QP* structures on a manifold.

2.3.1. Definition: A vector field X on a QP manifold $\mathcal{N}$ is called a symmetry of $\mathcal{N}$ if it commutes with $\mathbf{Q}$ *and is a Poisson vector field, i.e.,*

$$X\{F,G\}-\{XF,G\}-(-1)^{(\mathrm{p}(F)+\kappa)\mathrm{p}(X)}\{F,XG\}=0,\quad F,G\in\mathcal{F}_{\mathcal{N}}. \tag{2.8}$$

Symmetries of the form $X=\{\mathbf{Q}F,\cdot\}$ *(with* $F\in\mathcal{F}_{\mathcal{N}}$*) are called* trivial.

The Lie algebras of symmetries and trivial symmetries behave in a very regular manner under the restriction to $\mathcal{Z}_{\mathbf{Q}}$.

2.3.2. Proposition: Let X be a symmetry of $\mathcal{N}$. Then X restricts to $\mathcal{Z}_{\mathbf{Q}}$ and its restriction x is a Poisson vector field on $\mathcal{Z}_{\mathbf{Q}}$ with respect to the bracket (2.7) on $\mathcal{Z}_{\mathbf{Q}}$, namely

$$x\{F,G\}_{\mathbf{Q}}-\{xF,G\}_{\mathbf{Q}}-(-1)^{(\mathrm{p}(F)+\kappa+1)\mathrm{p}(X)}\{F,xG\}_{\mathbf{Q}}=0,\quad F,G\in\mathcal{F}_{\mathcal{Z}_{\mathbf{Q}}}. \tag{2.9}$$

If in addition $X=\{\mathbf{Q}H,\cdot\}$ *is a trivial symmetry, x is a Hamiltonian vector field with respect to the* $\{,\}_{\mathbf{Q}}$ *bracket.*

Proof: Any symmetry X restricts to $\mathcal{Z}_{\mathbf{Q}}$ because $XF|_{\mathcal{Z}_{\mathbf{Q}}}=0$ for any F vanishing on $\mathcal{Z}_{\mathbf{Q}}$. Indeed, every such function can be represented as $F=F_\alpha\cdot\mathbf{Q}\Gamma^\alpha$ with some functions F_α and Γ^α, provided $\mathbf{Q}$ is regular. Because $[X,\mathbf{Q}]=0$, we have $XF|_{\mathcal{Z}_{\mathbf{Q}}}=((XF_\alpha)(\mathbf{Q}\Gamma^\alpha))|_{\mathcal{Z}_{\mathbf{Q}}}+(-1)^{p(X)(p(F_\alpha)+1)F_\alpha}(\mathbf{Q}X\Gamma^\alpha)|_{\mathcal{Z}_{\mathbf{Q}}}=0$. Equation (2.9) immediately follows from the definition of the zero locus bracket and the definition of symmetries. If in addition $X=\{\mathbf{Q}H,\cdot\}$ is a trivial symmetry, for any function $f\in\mathcal{F}_{\mathcal{Z}_{\mathbf{Q}}}$ we have

$$xf=X|_{\mathcal{Z}_{\mathbf{Q}}}f=\{\mathbf{Q}H,F\}|_{\mathcal{Z}_{\mathbf{Q}}}=(-1)^{p(H)+\kappa+1}\{H|_{\mathcal{Z}_{\mathbf{Q}}},f\}_{\mathbf{Q}}, \tag{2.10}$$

where $F\subset\mathcal{F}_{\mathcal{N}}$ is a lift of f (i.e., $f=F|_{\mathcal{Z}_{\mathbf{Q}}}$) and κ is the parity of the $\{,\}$ bracket. Thus, $x=X|_{\mathcal{Z}_{\mathbf{Q}}}$ is a Hamiltonian vector field with respect to the bracket $\{,\}_{\mathbf{Q}}$. □

III. OBSERVABLES, GAUGE SYMMETRIES, AND ZERO LOCUS REDUCTION IN BFV AND BV QUANTIZATIONS

We now consider the embedding of a constrained system into the BFV extended theory with the BRST charge Ω and study the ''on-shell'' gauge symmetries in the two descriptions of the same theory. In the Dirac (''nonextended'') formalism, the on-shell gauge symmetries are those nonvanishing on the constraint surface, and in the BFV extended formalism, these are symmetries nonvanishing on the zero locus $\mathcal{Z}_{\mathbf{Q}}$. We show that the former are mapped into the latter such that the equivalence classes of observables in the original theory are mapped into equivalence classes of observables in the BFV theory (the latter can be considered as gauge invariant functions on $\mathcal{Z}_{\mathbf{Q}}$). In this sense, *the zero locus* $\mathcal{Z}_{\mathbf{Q}}$ *plays the role of a constraint surface in the BFV theory*. We concentrate on the BFV case, where we assume the phase space to be finite-dimensional; reformulation of our results for the BV quantization, although straightforward at the formal level, requires some care because the BV configuration space of any realistic model is infinite-dimensional (see 3.5).

3.1. A reminder on constrained dynamics. We begin with recalling several basic facts about constrained dynamics in the form that will be suitable in what follows.

3.1.1. Basics of the Dirac constrained dynamics. We consider a first-class constrained Hamiltonian system, defined on a phase space (symplectic manifold) $\mathcal{N}_0$ with the *constraints* T_α (functions on $\mathcal{N}_0$) such that

$$\{T_\alpha, T_\beta\} = U^\gamma_{\alpha\beta} T_\gamma, \tag{3.1}$$

where $\{,\}$ is the Poisson bracket on $\mathcal{N}_0$. For simplicity, we assume the first-class constraints T_α to be irreducible. Let Σ denote the *constraint surface* $T_\alpha = 0$. A geometrically invariant way to specify a first-class constrained system is to fix the pair $(\mathcal{N}_0, \Sigma)$ (a symplectic manifold and a coisotropic submanifold). Different choices for T_α then give different generators of the ideal of functions vanishing on Σ.

By definition, an *observable* is a function on $\mathcal{N}_0$ satisfying $\{A, T_\alpha\}|_\Sigma = 0$. Under the standard regularity conditions, each function vanishing on Σ is proportional to the constraints, and therefore,

$$\{A, T_\alpha\} = A^\beta_\alpha T_\beta \tag{3.2}$$

for some functions A^α_β. Observables vanishing on Σ are called *trivial*. Two observables are called *equivalent* if they differ by a trivial observable. The space of equivalence classes of observables is a Poisson algebra, i.e., is closed under multiplication and under the Poisson bracket (these operations are well defined on the equivalence classes via representatives). This algebra can be conveniently thought of as a subalgebra in the algebra of functions on Σ.

Infinitesimal gauge transformations, or gauge symmetries, are the Hamiltonian vector fields $X_0 = \{\phi_0, \cdot\}$, where $\phi_0 = \phi_0^\alpha T_\alpha$ is a trivial observable. Gauge symmetries form a Lie algebra with respect to the commutator. For any observable A and a gauge symmetry $X_0 = \{\phi_0, \cdot\}$, we have

$$X_0 A = \{\phi_0, A\} = \{\phi_0^\alpha T_\alpha, A\} = \phi_0^\alpha \{T_\alpha, A\} + T_\alpha \{\phi_0^\alpha, A\}, \tag{3.3}$$

which vanishes on Σ because A is an observable. Therefore, gauge symmetries preserve equivalence classes of observables.

By the *on-shell gauge symmetries*, we mean the equivalence classes of gauge symmetries modulo those vanishing on the constraint surface Σ. On-shell gauge symmetries can also be viewed as a subalgebra in the algebra of vector fields on Σ. Equivalence classes of observables (viewed as functions on Σ) are then represented by functions annihilated by on-shell gauge symmetries.

3.1.2. Basics of the BFV/BRST approach. In the BFV quantization, the extended phase space $\mathcal{N}$ is an even *QP* manifold whose $\mathbf{Q}$-structure is given by $\mathbf{Q} = \{\Omega, \cdot\}$, where Ω is a function on $\mathcal{N}$ (called the BRST charge) satisfying $\{\Omega, \Omega\} = 0$. In applications, the BFV extended phase space is usually equipped with an additional structure, the ghost charge $G \in \mathcal{F}_\mathcal{N}$. Functions with a definite ghost number are eigenfunctions of the ghost number operator

$$g = \{G, \cdot\}, \tag{3.4}$$

corresponding to integer eigenvalues. The BRST charge is required to have the ghost number 1,

$$\{G, \Omega\} = \Omega. \tag{3.5}$$

We now consider a *QP* manifold $\mathcal{N}$ that is not necessarily constructed via the BFV prescription; however, we refer to the objects on $\mathcal{N}$ as BFV ones because the applications in what follows will be to the case where $\mathcal{N}$ does result from the BFV construction. This also helps to distinguish between observables and symmetries on the *QP* manifold and those in the initial theory (Sec. 3.1.1), with 'BFV' used to refer to the former.

A BFV observable A is a function on the *QP* manifold $\mathcal{N}$ satisfying

$$\mathbf{Q}A = \{\Omega, A\} = 0, \quad \mathrm{gh}(A) = 0. \tag{3.6}$$

TABLE I.

	Dirac (Sec. 3.1.1)	BFV (Sec. 3.1.2)
Observables	$A_0, \{A_0, T_\alpha\} = A_\alpha^\beta T_\beta$	$\mathbf{Q}A = \{\Omega, A\} = 0$, $\mathrm{gh}(A) = 0$
Trivial observables	$(A_0)\vert_\Sigma = 0$	$A = \mathbf{Q}B$
Equivalent observables	$A_0 \sim A_0 + a^\alpha T_\alpha$	$A \sim A + \mathbf{Q}B$
Gauge symmetries	$X_0 = \{\phi_0^\alpha T_\alpha, \cdot\}$	$X = \{\mathbf{Q}H, \cdot\}$, $\mathrm{gh}(X) = 0$

The **Q**-exact BFV observables are called *trivial*. Two BFV observables A and $\tilde{A}$ are equivalent if $A - \tilde{A} = \mathbf{Q}B$ for some function B; the equivalence classes of observables are then the cohomology of **Q** in the ghost number zero. The algebra of BFV observables is a Poisson algebra (multiplication and the Poisson bracket can be defined via representatives).

A vector field X is called a *BFV gauge symmetry* if $X = \{\mathbf{Q}H, \cdot\}$ for some function H with $\mathrm{gh}(X) = \mathrm{gh}(\mathbf{Q}H) = 0$ [these are trivial symmetries (see 2.3.1) of the corresponding *QP* manifold]. In other words, BFV gauge symmetries are the Hamiltonian vector fields generated by trivial BFV observables. If A is an observable and $X = \{\mathbf{Q}H, \cdot\}$ a BFV gauge symmetry, we see that $XA = \{\mathbf{Q}H, A\} = \mathbf{Q}\{H, A\}$ is a trivial observable, i.e., BFV gauge symmetries preserve the equivalence classes of BFV observables.

3.2. From Dirac to the BFV formulation of a constrained system. Formal similarities between the Dirac and BFV formalisms are summarized in Table I. We now make contact between 3.1.1 and 3.1.2 by taking the extended phase space $\mathcal{N}$ and the BRST charge Ω to be those arising in the BFV formalism from a given first-class constrained system $(\mathcal{N}_0, \Sigma)$. As before, the constraints $T_\alpha \in \mathcal{F}_{\mathcal{N}_0}$ are taken to be irreducible; to construct the BFV formalism, one then introduces ghosts c^α, with $\mathrm{gh}(c^\alpha) = 1$, $\mathsf{p}(c^\alpha) = \mathsf{p}(T_\alpha) + 1$ and their conjugate momenta $\mathcal{P}_\alpha$,

$$\{c^\alpha, \mathcal{P}_\beta\} = \delta_\beta^\alpha, \tag{3.7}$$

with $\mathrm{gh}(\mathcal{P}_\alpha) = -1$, $\mathsf{p}(\mathcal{P}_\alpha) = \mathsf{p}(T_\alpha) + 1$. The extended phase space $\mathcal{N}$ is the direct product of $\mathcal{N}_0$ with the superspace spanned by c^α and $\mathcal{P}_\alpha$. The Poisson bracket on $\mathcal{N}$ is the product Poisson bracket of that on $\mathcal{N}_0$ and (3.7). Note that when the constraints are defined *locally*, the extended phase space is a vector bundle over the original phase space, as, for example, in Ref. 16.

One introduces the ghost charge (where we assume the constraints to be bosonic to avoid extra sign factors)

$$G = c^\alpha \mathcal{P}_\alpha, \quad \{G, c^\alpha\} = c^\alpha, \quad \{G, \mathcal{P}_\alpha\} = -\mathcal{P}_\alpha. \tag{3.8}$$

The BRST charge Ω is an odd function defined by the condition that it has the ghost number 1 and satisfies

$$\{\Omega, \Omega\} = 0 \tag{3.9}$$

with the boundary condition

$$\Omega = c^\alpha T_\alpha + \cdots, \tag{3.10}$$

where $\cdots$ means higher-order terms in the ghost momenta. It is well known[1,15,9,17] that under standard assumptions, the BRST charge Ω exists for any constrained system. Up to the first order in $\mathcal{P}_\alpha$, one has

$$\Omega = c^\alpha T_\alpha - \tfrac{1}{2} \mathcal{P}_\gamma U_{\alpha\beta}^\gamma c^\alpha c^\beta + \cdots, \tag{3.11}$$

where the structure functions are those from (3.1).

As regards observables, the following statement is well known[1,15] (see also Ref. 17).

3.2.1. Proposition: The algebra of the equivalence classes of observables on $\mathcal{N}_0$ and the algebra of the equivalence classes of BFV observables (the cohomology of $\mathbf{Q}$ *in the ghost number zero) on the extended phase space $\mathcal{N}$ are isomorphic as Poisson algebras.*

This means that if $A_0 \in \mathcal{F}_{\mathcal{N}_0}$ is an observable of the constrained system on $\mathcal{N}_0$, there exists a BFV observable $A \in \mathcal{F}_{\mathcal{N}}$ with $\mathrm{gh}(A)=0$ such that

$$A|_{\mathcal{N}_0}=A_0. \tag{3.12}$$

Moreover, two BFV observables corresponding to the same observable A_0 differ by a trivial BFV observable. If in addition A_0 is a trivial observable, it follows that $A=\{\Omega,B\}$. The Poisson bracket on $\mathcal{N}$ induces a bracket on the cohomology of $\mathbf{Q}$, and one has

$$\{A,B\}|_{\mathcal{N}_0}=\{A_0,B_0\}. \tag{3.13}$$

The isomorphism between the BRST cohomology in the ghost number zero and the algebra of equivalence classes of observables of the constrained system on $\mathcal{N}_0$ is given by the restriction of representatives to the initial constrained surface $\Sigma \subset \mathcal{N}_0 \subset \mathcal{N}$ (recall that equivalence classes of observables are gauge invariant functions on Σ).

It also follows from 3.2.1 that because gauge symmetries of the initial system $(\mathcal{N}_0,\Sigma)$ are generated by trivial observables, each gauge symmetry can be lifted to a BFV gauge symmetry.

3.3. Zero locus $\mathcal{Z}_{\mathbf{Q}}$ in the BFV theory, the general case. We now consider an even *QP*-manifold $\mathcal{N}$ that is not necessarily constructed by the BFV procedure for a constrained system. We assume $\mathcal{N}$ to be symplectic, and the odd nilpotent vector field $\mathbf{Q}$ to be regular in the sense of 2.3. The zero locus $\mathcal{Z}_{\mathbf{Q}}$ is thus a coisotropic submanifold of $\mathcal{N}$. Because each trivial BFV observable $A=\mathbf{Q}B$ vanishes on $\mathcal{Z}_{\mathbf{Q}}$, each cohomology class uniquely determines a function on $\mathcal{Z}_{\mathbf{Q}}$. Thus, there is a mapping

$$H^0_{\mathbf{Q}} \to \mathcal{F}_{\mathcal{Z}_{\mathbf{Q}}} \tag{3.14}$$

from the space of inequivalent observables to functions on $\mathcal{Z}_{\mathbf{Q}}$.

In what follows, we say that a statement holds locally if it is true in every sufficiently small neighborhood. Mapping (3.14) is locally an embedding in view of the following proposition.

3.3.1. Proposition: Let $\mathbf{Q}=\{\Omega,\cdot\}$ *be regular in the sense of 2.2. Locally, each BFV observable vanishing on $\mathcal{Z}_{\mathbf{Q}}$ is a trivial BFV observable.*

Proof: Let A be an observable vanishing on $\mathcal{Z}_{\mathbf{Q}}$ i.e., $\mathbf{Q}A=0$, $A|_{\mathcal{Z}_{\mathbf{Q}}}=0$. We must show that $A=\mathbf{Q}X$ in a sufficiently small neighborhood U of any point $p \in \mathcal{Z}_{\mathbf{Q}}$. It is well known that locally there exists a coordinate system $p_i,q^j,p_\alpha,q^\beta,c^\alpha,\mathcal{P}_\beta$ on $\mathcal{N}$ such that

$$\Omega=p_i c^i,$$

$$\{q^i,p_j\}=\delta^i_j, \quad \{q^\alpha,p_\beta\}=\delta^\alpha_\beta, \quad \{c^\alpha,\mathcal{P}_\beta\}=\delta^\alpha_\beta. \tag{3.15}$$

Since the function A vanishes on $\mathcal{Z}_{\mathbf{Q}}$, it can be represented as

$$A=A^\alpha p_\alpha + A_\alpha c^\alpha. \tag{3.16}$$

Now the odd vector field $\mathbf{Q}$ becomes

$$\mathbf{Q}=-c^\alpha \frac{\partial}{\partial q^\alpha}+p_\alpha \frac{\partial}{\partial \mathcal{P}_\alpha}, \tag{3.17}$$

and can be considered as the exterior differential under the identification $c^\alpha=-dq^\alpha$, $p_\alpha=d\mathcal{P}_\alpha$, while A becomes a 1-form. The assertion immediately follows from the super analog of the Poincaré lemma in U. □

3.3.2. Embedding $H^0_{\mathbf{Q}}$ into functions on $\mathcal{Z}_{\mathbf{Q}}$. As before, $\mathcal{Z}_{\mathbf{Q}}$ is the zero locus submanifold of $\mathbf{Q}=\{\Omega,\cdot\}$ We recall from 2.3.2 that each BFV gauge symmetry X can be restricted to $\mathcal{Z}_{\mathbf{Q}}$ and the restriction $x=X|_{\mathcal{Z}_{\mathbf{Q}}}$ is a $\{,\}_{\mathbf{Q}}$-Hamiltonian vector field on $\mathcal{Z}_{\mathbf{Q}}$. The image of BFV gauge symmetries under the restriction to $\mathcal{Z}_{\mathbf{Q}}$ is called the algebra of the *on-shell BFV symmetries*. The functions on $\mathcal{Z}_{\mathbf{Q}}$ that are annihilated by the on-shell BFV symmetries are then the characteristic functions of the $\{,\}_{\mathbf{Q}}$ antibracket on $\mathcal{Z}_{\mathbf{Q}}$. We recall that a function f on the (odd) Poisson manifold $\mathcal{N}$ is said to be a characteristic (Casimir) function of an (odd) Poisson bracket $\{,\}$ if $\{f,h\}=0$ for any function h.

Because BFV observables are annihilated by BFV gauge symmetries, the restriction to $\mathcal{Z}_{\mathbf{Q}}$ maps BFV observables into characteristic functions of $\{,\}_{\mathbf{Q}}$. For the equivalence classes of BFV observables (the cohomology of $\mathbf{Q}$), this mapping is certainly an embedding locally. It is also an isomorphism in the important case of a BFV *QP* manifold considered in 3.4. Locally, we choose flat coordinates in some neighborhood U of a point $p\in\mathcal{Z}_{\mathbf{Q}}$ and use explicit form (3.15) of the BRST charge Ω and the Poisson bracket to arrive at

3.3.3. Theorem: *Locally, the equivalence classes of BFV observables (the cohomology of* $\mathbf{Q}$*) are in a 1:1 correspondence with characteristic functions of the* $\{,\}_{\mathbf{Q}}$ *antibracket on* $\mathcal{Z}_{\mathbf{Q}}$.

We note that in one direction, this statement holds in general (i.e., not only locally) because for any observable A, we have

$$\{f,A|_{\mathcal{Z}_{\mathbf{Q}}}\}_{\mathbf{Q}}=\{F,\mathbf{Q}A\}|_{\mathcal{Z}_{\mathbf{Q}}}=0, \tag{3.18}$$

where $F\in\mathcal{F}_{\mathcal{N}}$ is the lift of a function $f\in\mathcal{F}_{\mathcal{Z}_{\mathbf{Q}}}$ and $A|_{\mathcal{Z}_{\mathbf{Q}}}$ is the image of A under (3.14). Thus, $A|_{\mathcal{Z}_{\mathbf{Q}}}$ is a characteristic function of the antibracket $\{,\}_{\mathbf{Q}}$ on $\mathcal{Z}_{\mathbf{Q}}$.

The "$\mathcal{Z}_{\mathbf{Q}}$-based" view on the BFV formalism developed here can be expressed as follows. *Any even QP manifold* $\mathcal{N}$ *gives rise to the constrained system* $(\mathcal{N},\mathcal{Z}_{\mathbf{Q}})$*, i.e., a constrained system whose phase space is* $\mathcal{N}$ *and the constrained surface is* $\mathcal{Z}_{\mathbf{Q}}$. We recall from 3.1.1 that gauge transformations and the algebra of observables can be reconstructed if a first-class constrained system is specified in geometric terms, via its phase space (a symplectic manifold) and the constraint surface (a coisotropic submanifold). We now take this pair to be $(\mathcal{N},\mathcal{Z}_{\mathbf{Q}})$ (with $\mathcal{Z}_{\mathbf{Q}}$ being coisotropic in view of 2.2.1). In local coordinates, the constraints are the components of $\mathbf{Q}$; in a neighborhood $U\subset\mathcal{N}$, the following statement is obvious in the special coordinates in which Ω and $\{,\}_{\mathbf{Q}}$ are given by (3.15).

3.3.4. Theorem: *On a QP manifold* $\mathcal{N}$*, the constrained system* $(\mathcal{N},\mathcal{Z}_{\mathbf{Q}})$ *is locally equivalent to the BFV theory on the extended phase space* $\mathcal{N}$ *with the BRST charge* Ω *(i.e., the respective algebras of equivalence classes of observables are isomorphic as Poisson algebras).*

In a more physical language, the equivalence can be reformulated by saying that the two constrained dynamics are equivalent.

The above considerations show that BFV observables are related to $\mathcal{Z}_{\mathbf{Q}}$ in the same way as observables in the initial theory (Sec. 3.1.1) are related to the constraint surface Σ. This allows us to interpret $\mathcal{Z}_{\mathbf{Q}}$ as the extended constraint surface. In the general case, this correspondence takes place at the local level only.

3.4. Zero locus $\mathcal{Z}_{\mathbf{Q}}$ *in the BFV formulation of a constrained system.* We now concentrate on the important case where the *QP* manifold under consideration is a BFV extended phase space obtained by the BFV procedure from a given constrained system $(\mathcal{N}_0,\Sigma)$.

3.4.1. Proposition: The initial constraint surface $\Sigma\subset\mathcal{N}_0$ *is a submanifold of the zero locus* $\mathcal{Z}_{\mathbf{Q}}\subset\mathcal{N}$ *of the BRST differential* $\mathbf{Q}=\{\Omega,\cdot\}$.

Proof: We restrict ourselves to an irreducible theory with constraints T_α (although the statement is also true for reducible constraints); the structure of the BRST charge is then given by (3.10). Considered as a submanifold in $\mathcal{N}$, the initial phase space $\mathcal{N}_0$ is determined by the equations $c^\alpha=0$ and $\mathcal{P}_\alpha=0$. It follows from (3.10) and from $\mathrm{gh}(\Omega)=1$ that the zero locus $\mathcal{Z}_{\mathbf{Q}}$ is determined by the equations

$$T_\alpha+\cdots=0,\quad \cdots=0, \tag{3.19}$$

where $\cdots$ denotes terms vanishing on $\mathcal{N}_0$. Then the intersection $\mathcal{Z}_\mathbf{Q}\cap\mathcal{N}_0$ (considered as a submanifold in $\mathcal{N}_0$) is determined by the equations $T_\alpha=0$, and therefore, coincides with the initial constraint surface Σ. Thus, Σ is a submanifold in $\mathcal{Z}_\mathbf{Q}$. □

The zero locus can be described somewhat more explicitly if we recall that in the BFV formalism, functions on the extended phase space are formal power series in the ghost variables c^α and $\mathcal{P}_\alpha$. This means that $\mathcal{Z}_\mathbf{Q}$ is actually determined by the equations

$$T_\alpha=0, \quad c^\alpha=0. \tag{3.20}$$

This, in its turn, gives an explicit construction of the antibracket $\{,\}_\mathbf{Q}$ on $\mathcal{Z}_\mathbf{Q}$. Let y^i be local coordinates on Σ. Then y^i and $\mathcal{P}_\alpha$ can be considered as local coordinates on $\mathcal{Z}_\mathbf{Q}$. Evaluating (2.5), we now obtain

$$\{y^i,y^j\}_\mathbf{Q}=0, \quad \{\mathcal{P}_\alpha,y^i\}_\mathbf{Q}=R^i_\alpha(y), \quad \{\mathcal{P}_\alpha,\mathcal{P}_\beta\}_\mathbf{Q}=U^\gamma_{\alpha\beta}(y)\mathcal{P}_\gamma, \tag{3.21}$$

where $R^i_\alpha(y)=\{T_\alpha,y^i\}|_\Sigma$ and $U^\gamma_{\alpha\beta}(y)=U^\gamma_{\alpha\beta}|_\Sigma$ with $U^\gamma_{\alpha\beta}$ from (3.11).

Using the explicit form (3.21) of the antibracket on $\mathcal{Z}_\mathbf{Q}$, it is easy to describe its characteristic functions in terms of the initial constraint surface Σ. The following statement is obvious for irreducible constraints T_α and can be easily generalized to reducible constraints.

3.4.2. Proposition: Characteristic functions of the antibracket $\{,\}_\mathbf{Q}$ *are in a* 1:1 *correspondence with gauge invariant functions on* Σ.

On a *QP* manifold constructed in accordance with the BFV prescription, the relation between the BRST cohomology and the geometry of the extended constrained surface $\mathcal{Z}_\mathbf{Q}$ can be made more precise than in the preceding section. In particular, the respective counterparts of statements 3.3.1, 3.3.3, and 3.3.4 *hold globally*. We first see that (3.14) is an embedding.

3.4.3. Proposition: On a QP manifold $\mathcal{N}$ *constructed in the BFV formalism, each BFV observable that vanishes on* $\mathcal{Z}_\mathbf{Q}\subset\mathcal{N}$ *is a trivial BFV observable.*

Proof: Let A be a BFV observable and $A|_{\mathcal{Z}_\mathbf{Q}}=0$. According to 3.4.1, $\Sigma\subset\mathcal{Z}_\mathbf{Q}$. Then $A|_{\mathcal{Z}_\mathbf{Q}}=0$ implies $A|_\Sigma=0$ (a trivial observable). By 3.2.1, A is a trivial BFV observable. □

We now consider the *QP* manifold constructed in the BFV formalism. Combining 3.4.3 with the argument given after 3.3.3 proves the next theorem in one direction; the other direction follows because each characteristic function on $\mathcal{Z}_\mathbf{Q}$ can be lifted to a BFV observable on $\mathcal{N}$, see 3.2.1 and 3.4.2.

3.4.4. Theorem: *Equivalence classes of BFV observables (the cohomology of* $\mathbf{Q}$ *with the ghost number zero) on the BFV QP manifold are in a 1:1 correspondence with characteristic functions of the zero locus antibracket on* $\mathcal{Z}_\mathbf{Q}$.

As in 3.3.3, we now consider the extended phase space of the BFV formulation as the phase space of a ''new'' constrained system determined by the constraint surface $\mathcal{Z}_\mathbf{Q}$. With $\mathcal{N}$ in its turn obtained from a constrained dynamical system $(\mathcal{N}_0,\Sigma)$ in accordance with the BFV formalism, we have a *global* version of 3.3.4.

3.4.5. Theorem: *Let* $\mathcal{N}$ *be a QP manifold constructed in the BFV formalism. The constrained system determined by the pair* $(\mathcal{N},\mathcal{Z}_\mathbf{Q})$ *is equivalent to the BFV theory on* $\mathcal{N}$ *(i.e., the respective algebras of equivalence classes of observables are isomorphic as Poisson algebras).*

Combining this with 3.2.1, we obtain a remarkable relation between the constrained systems specified by the respective pairs $(\mathcal{N}_0,\Sigma)$ and $(\mathcal{N},\mathcal{Z}_\mathbf{Q})$:

3.4.6. Corollary: The constrained systems $(\mathcal{N}_0,\Sigma)$ *and* $(\mathcal{N},\mathcal{Z}_\mathbf{Q})$ *are equivalent (the respective algebras of inequivalent observables are isomorphic as Poisson algebras).*

We also note a difference between the initial and the extended constraint surfaces Σ and $\mathcal{Z}_\mathbf{Q}$ in that Σ carries an action of the gauge generators $\{T_i,\cdot\}$, while $\mathcal{Z}_\mathbf{Q}$ is equipped with the zero locus antibracket. This is not unnatural, because the on-shell gauge symmetries are Hamiltonian vector fields with respect to the zero-locus antibracket, while inequivalent observables are (identified with) the characteristic functions of the zero-locus antibracket.

The consideration above applies at the classical level. The notion of the initial and the extended constraint surfaces is essentially classical and has no obvious counterparts at the quantum level. At the quantum level, restrictions to the constraint surface should be understood as restriction to some quotient of the full Hilbert space of the quantum system. We do not discuss this very interesting subject here, and refer instead to Ref. 18, where a related problem [19] was considered.

Finally, we note that there is a slightly different point of view on the interpretation of BFV observables in terms of the geometry of $\mathcal{Z}_{\mathbf{Q}}$. Namely, to each (odd) Poisson structure, one can associate the coboundary operator (differential) acting on antisymmetric tensor fields, with the action being the adjoint action of the Poisson bivector with respect to the Schouten–Nijenhuis bracket. Inequivalent observables are then the *zero-degree cohomology* of this differential on $\mathcal{Z}_{\mathbf{Q}}$ (tensors of zero degree are functions).

3.5. Observables, gauge symmetries, and zero-locus reduction in the BV quantization. The above can be reformulated for odd *QP* manifolds/BV quantization. In the BV formulation, the zero locus of $\mathbf{Q}=(S,\cdot)$, where S is the master action, is the stationary surface of S [provided the BV antibracket (,) is nondegenerate]. The BV observables are the cohomology of $\mathbf{Q}$ in the ghost number zero. The BV gauge symmetries are the vector fields of the form

$$X=(QB,\cdot), \tag{3.22}$$

and, thus, are Hamiltonian vector fields generated by trivial observables. Whenever the master action S is constructed via the BV prescription starting from a given initial action S_0, the zero locus of $\mathbf{Q}=(S,\cdot)$ is a certain extension of the stationary surface of the initial action S_0.

At the formal level, all the statements considered in the BFV scheme have their counterparts in the BV formalism. We do not restate here the contents of 3.1–3.4 for the odd case and refer instead to Refs. 5 and 6. We only point out one important difference. Unlike the Hamiltonian picture, the Lagrangian one can be considered in the scope of a finite dimensional analog only formally. The finite dimensional configuration space (the space of field histories) does not correspond to any physically relevant system. Thus all the BV counterparts of the statements of the preceding section should be considered with some care. In particular, the BV quantization prescription requires the master action S to be a proper solution to the master equation. The condition imposed on the master action to be proper has no counterpart in the Hamiltonian picture. It implies that the corresponding configuration space is a proper *QP* manifold (which in general is not the case for the BFV phase space). In the finite dimensional case, this in turn implies that all the observables (the cohomology of $\mathbf{Q}$) are trivial (except those of a topological nature). The $\mathbf{Q}$ cohomology becomes nontrivial only when evaluated on space-time local functionals.[20,21]

IV. TOWERS OF BRACKETS

In this section, we study the possibility of a ''second'' zero-locus reduction, i.e., the reduction on a *QP* manifold which itself is the result of a zero-locus reduction. This leads to several well-known structures, including the classical Yang–Baxter equation.

4.1. A "second" zero-locus reduction. On a *QP* manifold $\mathcal{N}$ (which can be either even or odd), a coisotropic submanifold $\mathcal{L}\subset\mathcal{Z}_{\mathbf{Q}}$ (for example, a Lagrangian submanifold in $\mathcal{N}$) is a P manifold, i.e., is equipped with an (even or odd) Poisson structure (see 2.2.5). One can try to equip $\mathcal{L}$ with a compatible $\mathbf{Q}$ structure, thereby making it into a *QP* manifold. On a general *QP* manifold $\mathcal{N}$, there is no canonical structure inducing a $\mathbf{Q}$ operator on $\mathcal{L}$. Instead, we can look for a $\mathbf{Q}$ operator on $\mathcal{L}$ in the form $\mathbf{Q}_{\mathcal{L}}=\{H,\cdot\}_{\mathbf{Q}}$ where $\{,\}_{\mathbf{Q}}$ is the bracket given by (2.7) and H is a solution of the equation

$$\{H,H\}_{\mathbf{Q}}=0, \quad H\in\mathcal{F}_{\mathcal{L}}, \quad \mathrm{p}(H)=\mathrm{p}(\{,\}_{\mathbf{Q}})+1. \tag{4.1}$$

Whenever such an H is found, $\mathcal{L}$ becomes a *QP* manifold. With this $\mathbf{Q}$ structure, we can repeat the procedure, thereby producing a sequence of *QP* manifolds.

This construction can be restated in terms of differential Poisson algebras (the algebras of functions on *QP* manifolds). Even "more algebraically," we consider the case where a differential Poisson algebra arises from a *complex* endowed with a super-commutative associative multiplication and a Gerstenhaber-like multiplication (see the Appendix). To these differential Poisson algebras, we can then apply one or more zero-locus reduction steps, resulting in relations between different complexes.

4.2. Examples of the zero-locus reduction on an even QP manifold. Let $\mathcal{M}$ be a cotangent bundle $\mathcal{M}=T^*\mathcal{X}$. We then write (q^a,p_a) for local coordinates on $\mathcal{M}$ (which we take to be bosonic to avoid extra sign factors); the Poisson bracket then is $\{q^a,p_b\}=\delta^a_b$. We assume a Hamiltonian action of a Lie algebra $\mathfrak{a}$ on $\mathcal{M}$. For simplicity, we consider the Hamiltonian action that is the lift of an action on $\mathcal{X}$ via the vector fields $X_i=X_i^a(\partial/\partial q^a)$, with $[X_i,X_j]=C_{ij}^kX_k$. The generators of the Hamiltonian action on $\mathcal{M}$ are then given by $T_i=-p_aX_i^a(q)$. Applying the BFV scheme to the constraints T_i gives the BRST generator

$$\Omega=-p_aX_i^a(q)\,\theta^i-\tfrac{1}{2}C_{ij}^k\xi_k\theta^i\theta^j. \tag{4.2}$$

We now take the submanifold $\mathcal{L}\subset\mathcal{Z}_{\mathbf{Q}}$ (which is Lagrangian in $\mathcal{M}$) determined by $\theta^i=0$ and $p_a=0$ and view q^a and ξ_i as local coordinates on $\mathcal{L}$. The antibracket $(,)\equiv\{,\}_{\mathbf{Q}}$ from 2.2.5 is then given by

$$(\xi_i,\xi_j)=C_{ij}^k\xi_k,\quad (q^a,\xi_i)=-X_i^a. \tag{4.3}$$

Using this antibracket structure on $\mathcal{L}$, we consider the equation

$$(H,H)=0 \tag{4.4}$$

for an even function $H\in\mathcal{F}_{\mathcal{L}}$. Given a solution H, we can construct the odd nilpotent vector field $\mathbf{Q}=(H,\cdot)$ that makes $\mathcal{L}$ into a *QP* manifold.

We consider solutions to (4.4) of the form

$$H_{\mathrm{YB}}=-\tfrac{1}{2}r^{ij}\xi_i\xi_j, \tag{4.5}$$

where r is a skew-symmetric matrix with entries from $\mathcal{F}_{\mathcal{X}}$. Explicitly, Eq. (4.4) is the following generalization of the CYBE:

$$r^{l[i}C_{lm}^kr^{j]m}+X_l^ar^{l[i}\frac{\partial}{\partial q^a}r^{jk]}=0. \tag{4.6}$$

We now proceed with the next stage of the zero-locus reduction. The zero locus of the "Yang–Baxter differential" $\mathbf{Q}_{\mathrm{YB}}=(H_{\mathrm{YB}},\cdot)$ is determined by $r^{ij}\xi_j=0$. We choose a smaller submanifold $\mathcal{X}\subset\mathcal{Z}_{\mathbf{Q}_{\mathrm{YB}}}$ determined by $\xi_i=0$. Whenever (4.4) is satisfied, $\{\cdot,\cdot\}=(\cdot,\mathbf{Q}_{\mathrm{YB}}\cdot)$ is a Poisson bracket on $\mathcal{X}$. Explicitly, the Poisson brackets are given by

$$\{q^a,q^b\}=X_i^ar^{ij}X_j^b. \tag{4.7}$$

4.2.1. The classical Yang–Baxter equation. Antibracket (4.3) considered on q-independent functions coincides with the Schouten bracket on $\wedge\mathfrak{a}$ viewed as the Grassmann algebra generated by ξ_i. In the case where r^{ij} is a constant matrix, (4.6) becomes the CYBE,

$$r^{j[i}C_{jl}^kr^{m]l}=0. \tag{4.8}$$

For each r^{ij} satisfying (4.8), the corresponding differential $\mathbf{Q}_{\mathrm{YB}}$ (considered on $\wedge\mathfrak{a}$) is nothing but the cohomology differential of the Lie algebra complex with trivial coefficients (see Appendix A), for the Lie algebra defined on $\mathfrak{a}^*$ by the structure constants $F_k^{ij}=r^{il}C_{lk}^j-r^{jl}C_{lk}^i$.

4.2.2. The Sklyanin bracket. With $\mathcal{X}$ taken to be the Lie group corresponding to the Lie algebra $\mathfrak{a}$, we have two natural ways to define the action of $\mathfrak{a}$ on $\mathcal{X}$, by the left- and right-invariant vector fields L_i and R_i. Proceeding along the steps described in the previous paragraphs with X_i^a taken to be L_i^a or R_i^a, we arrive at two Poisson brackets on $\mathcal{X}$,

$$\{q^a,a^b\}_{\text{right}}=L_i^a r^{ij} L_j^b \quad \text{and} \quad \{q^a,q^b\}_{\text{left}}=R_i^a r^{ij} R_j^b, \tag{4.9}$$

which are compatible in view of $[R_i,L_j]=0$. The Poisson bracket

$$\{q^a,q^b\}_{\text{Sklyanin}}=\{q^a,q^b\}_{\text{right}}-\{q^a,q^b\}_{\text{left}} \tag{4.10}$$

makes the Lie group $\mathcal{X}$ into a Poisson–Lie group.

4.3. Zero-locus reduction on an odd QP manifold. To reformulate the above for an odd *QP* manifold, we construct the BV scheme starting with a manifold $\mathcal{X}$ with an $\mathfrak{a}$ action. The ξ_i variables are then even, and because of the symmetry properties, the ''tower of reductions'' is shorter than for odd ξ_i. We then introduce antifields q_a^*, ghosts θ^i, and their antifields ξ_i, with $(\theta^i,\xi_j)=\delta_j^i$ (where restored the traditional notation for the antibracket). The differential

$$\mathbf{Q}=(S,\cdot), \quad S=q_a^* X_i^a \theta^i - \tfrac{1}{2}\xi_k C_{ij}^k \theta^i \theta^j \tag{4.11}$$

corresponds to the quantization of a theory with the vanishing classical action.

We choose a Lagrangian subspace $\mathcal{L}\subset\mathcal{Z}_{\mathbf{Q}}$ determined by $\theta^i=0$ and $q_a^*=0$. In accordance with Sec. 2, the zero locus reduction induces a Poisson bracket $\{,\}_{\mathbf{Q}}$ on $\mathcal{L}$ with the nonvanishing components

$$\{\xi_i,\xi_j\}_{\mathbf{Q}}=C_{ij}^k\xi_k, \quad \{q^a,\xi_i\}_{\mathbf{Q}}=X_i^a. \tag{4.12}$$

Unless $\mathcal{X}$ is a *super*manifold, $\mathcal{L}$ is a purely even manifold, and therefore, the new generating equation with respect to the $\{,\}_{\mathbf{Q}}$-bracket has only the trivial solution. The tower of brackets is thus terminated.

We now recall that the *even* variables ξ_i generate the algebra of functions on $\mathfrak{a}^*$. Restricting ourselves to functions that are independent of the coordinates on $\mathcal{X}$, we see that (4.12) becomes the Berezin–Kirillov bracket on $\mathfrak{a}^*$,

$$\{f,g\}=f\frac{\overleftarrow{\partial}}{\partial\xi_i}\xi_k C_{ij}^k \frac{\partial}{\partial\xi_j}g. \tag{4.13}$$

4.3.1. Linear and nonlinear brackets. The bracket in (4.13) is ''linear'' in the sense of its explicit dependence on ξ_i. For a Lie algebra $\mathfrak{a}$, one can construct ''nonlinear'' brackets $(\overleftarrow{\partial}/\partial\xi_i)\Omega_{ij}(\partial/\partial\xi_j)$ on $\mathfrak{a}^*$, where the expansion of Ω_{ij} in ξ_i starts with $\xi_k C_{ij}^k$. For a given bracket of this form, a natural problem is whether it can be transformed into the Berezin–Kirillov bracket by a change of coordinates. With the help of the zero-locus reduction, this is solved as follows. The Poisson bracket is represented as the zero-locus reduction of the *canonical* antibracket on a *QP* manifold with $\mathbf{Q}$ determined by the Hamiltonian $H=\Omega_{ij}(\xi)\theta^i\theta^j$. The Jacobi identity for the Poisson bracket is rewritten as the master equation for H, and moreover, the terms containing higher powers of ξ_i are closed with respect to the differential $\mathbf{Q}_0=\{H_0,\cdot\}$, where $H_0=\xi_k C_{ij}^k\theta^i\theta^j$ is the ''linear'' part of the Hamiltonian. We thus have proved the fact known from other considerations (and in a more powerful analytic version).[22]

4.3.2. Corollary. *Let* $\Omega_{ij}(\xi)=\xi_k C_{ij}^k+\xi_k\xi_l C_{ij}^{kl}+\cdots$ *be the matrix of a Poisson bracket on* $\mathfrak{a}^*$, *where* C_{ij}^k *are the structure constants of a Lie algebra* $\mathfrak{a}$. *Then* $\Omega_{ij}(\xi)$ *can be reduced to the form* $\xi_k C_{ij}^k$ *by a change of variables* $\xi_i\mapsto f_i(\xi)$ *if the second cohomology group* $H^2(\mathfrak{a},\mathrm{S}\mathfrak{a})$ *of* $\mathfrak{a}$ *with coefficients in* $\mathrm{S}\mathfrak{a}$ *is trivial*.

Similar considerations in the BFV case lead to similar statements for the nonlinear antibracket.

V. Bi-*QP* MANIFOLDS

Up to now, we have studied *QP* manifolds whose differential corresponds to a *single* solution of the corresponding "master" equation. We now consider bi-*QP* manifolds.

5.1. A BFV-like formulation of the bialgebra complex. In the preceding section, we associated an even *QP* manifold with a vector space $\mathfrak{a}$ and a smooth manifold $\mathcal{M}=T^*\mathcal{X}$. Namely, a Lie algebra structure on $\mathfrak{a}$ and the vector fields X_i (giving an $\mathfrak{a}$-module structure on $\mathcal{F}_\mathcal{X}$) can be read off from a solution of the generating equation

$$\{\Omega,\Omega\}=0 \tag{5.1}$$

with the ansatz (4.2). The algebra of functions on the thus constructed *QP* manifold is $\mathfrak{A}=\mathrm{Hom}(\wedge\mathfrak{a},\wedge\mathfrak{a})\otimes\mathcal{F}_{T^*\mathcal{X}}$; we interpret $\mathrm{Hom}(\wedge\mathfrak{a},\wedge\mathfrak{a})$ as the algebra generated by the odd variables θ^i and ξ_j. The basic Poisson bracket relations are

$$\{\theta^i,\xi_j\}=\delta^i_j,\quad \{q^a,p_b\}=\delta^a_b, \tag{5.2}$$

where q, p are the standard local coordinates on the cotangent bundle $\mathcal{M}=T^*\mathcal{X}$. We have the solution

$$C=-p_aX^a_i(q)\,\theta^i-\tfrac{1}{2}\,\xi_kC^k_{ij}\theta^i\theta^j. \tag{5.3}$$

At the same time, every solution of (5.1) of the form

$$F=-p_aX^{ia}\xi_i-\tfrac{1}{2}\theta^kF^{ij}_k\xi_i\xi_j \tag{5.4}$$

determines a coalgebra structure on the vector space $\mathfrak{a}$, or equivalently, a Lie algebra structure on $\mathfrak{a}^*$, and makes $\mathcal{F}_\mathcal{X}$ into an $\mathfrak{a}^*$-module, with the vector fields $X^i=R^{ia}(\partial/\partial q^a)\in\mathrm{Vect}_\mathcal{X}$ representing the action of the basis elements of $\mathfrak{a}^*$. Then $\mathfrak{A}$ is equipped with Poisson bracket (5.2) and the differentials

$$\begin{aligned}
d_C&=\{C,\cdot\}\\
&=-\frac{1}{2}C^k_{ij}\theta^i\theta^j\frac{\partial}{\partial\theta^k}-\xi_kC^k_{ij}\theta^i\frac{\partial}{\partial\xi_j}-p_aX^a_i\frac{\partial}{\partial\xi_i}+\theta^iX^a_i\frac{\partial}{\partial q^a}-\theta^ip_aX^a_{i,b}\frac{\partial}{\partial p_b},\\
d_F&=\{F,\cdot\}\\
&=-\frac{1}{2}F^{ij}_k\xi_i\xi_j\frac{\partial}{\partial\xi_k}-\theta^kF^{ij}_k\xi_i\frac{\partial}{\partial\theta^j}-p_aX^{ia}\frac{\partial}{\partial\theta^i}+\xi_iX^{ia}\frac{\partial}{\partial q^a}-\xi_ip_aX^{ia}_{,b}\frac{\partial}{\partial p_b}.
\end{aligned} \tag{5.5}$$

We next impose the condition that the differentials be compatible, i.e.,

$$[d_C,d_F]=0\Leftrightarrow\{C,F\}=0. \tag{5.6}$$

5.1.1. Proposition: Condition (5.6) *implies that* ($\mathfrak{a}$, $\mathfrak{a}^*$, $\mathfrak{a}\oplus\mathfrak{a}^*$) *is a Manin triple,*[13] *with the Lie bracket on* $\mathfrak{a}\oplus\mathfrak{a}^*$ *given by*

$$[e_i,e_j]=C^k_{ij}e_k\quad [e^i,e^j]=F^{ij}_ke^k,\quad [e_i,e^j]=C^j_{ik}e^k+F^{jk}_ie_k. \tag{5.7}$$

where e_i *and* e^i *are dual bases in* $\mathfrak{a}$ *and* $\mathfrak{a}^*$ *respectively. Equivalently,* $\mathfrak{a}$ *is a Lie bialgebra. Moreover,* $\mathcal{F}_\mathcal{X}$ *is a module over the Lie algebra* $\mathfrak{a}\oplus\mathfrak{a}^*$.

The proof is straightforward.

That $\mathcal{F}_\mathcal{X}$ is a module over $\mathfrak{a}\oplus\mathfrak{a}^*$ means that under the mapping $e_i\mapsto X_i$, $e^i\mapsto X^i$, the following commutation relations between vector fields are satisfied:

$$[X_i,X_j]=C_{ij}^k X_k,\quad [X^i,X^j]=F_k^{ij}X^k,\quad [X_iX^j]=C_{ik}^j X^k+F_i^{jk}X_k. \tag{5.8}$$

It also follows from (5.6) that

$$X^{ia}X_i^b+X^{ib}X_i^a=0. \tag{5.9}$$

5.1.2. Zero locus reduction on a bi-*QP manifold*. We next consider the submanifolds of the zero loci, $\mathcal{L}_C\subset\mathcal{Z}_C$ and $\mathcal{L}_F\subset\mathcal{Z}_F$ defined by $(\theta^i=0,\ p_a=0)$ and $(\xi_i=0,\ p_a=0)$, respectively. Since $\mathcal{L}_C$ and $\mathcal{L}_F$ are coisotropic, we can apply Theorem 2.2.5. We thus have the respective antibrackets

$$\begin{aligned}&\{\xi_i,\xi_j\}_C=C_{ij}^k\xi_k,\quad \{\xi_i,q^q\}_C=Z_i^a,\\ &\{\theta^i,\theta^j\}_F=F_k^{ij}\theta^k,\quad \{\theta^i,q^a\}_F=X^{ia},\end{aligned} \tag{5.10}$$

on $\mathcal{L}_C$ and $\mathcal{L}_F$.

5.1.3. Proposition: The differential d_C induces a well-defined operator (vector field) $\overline{d}_C=d_C|_{\mathcal{L}_F}:\mathcal{F}_{\mathcal{L}_F}\to\mathcal{F}_{\mathcal{L}_F}$ and the differential d_F induces an operator $\overline{d}_F=d_F|_{\mathcal{L}_C}:\mathcal{F}_{\mathcal{L}_C}\to\mathcal{F}_{\mathcal{L}_C}$. Thus, $\mathcal{F}_{\mathcal{L}_F}(\mathcal{F}_{\mathcal{L}_C})$ is an odd differential Poisson algebra and $\mathcal{L}_F$ (respectively, $\mathcal{L}_C$) is an odd QP manifold.

Thus, the manifolds $\mathcal{L}_C$ and $\mathcal{L}_F$ are equipped with **Q** structures. We now proceed to the next step of the zero-locus reduction.

Recall that the submanifold $\mathcal{X}=\mathcal{L}_C\cap\mathcal{L}_F$ is determined by the equations $p_a=\xi_i=\theta^j=0$. It is easy to see that $\mathcal{X}$ is a coisotropic submanifold of $\mathcal{L}_C$ and also a coisotropic submanifold of $\mathcal{L}_F$. On $\mathcal{X}$, we then have the Poisson bracket

$$\{\cdot,\cdot\}_{\mathcal{X}}=\{\cdot,\overline{d}_F\cdot\}_C=\{\cdot,\overline{d}_C\cdot\}_F \tag{5.11}$$

or in the coordinate form

$$\{q^a,q^b\}_{\mathcal{X}}=X_i^aX^{ib}. \tag{5.12}$$

It follows from (5.9) that bracket (5.12) is skew-symmetric; the Jacobi identity follows from the compatibility of d_C and d_F.

5.1.4. Coboundary bialgebras. Up to this point, the situation was symmetric with respect to $\theta^i\leftrightarrow\xi_i$, but now we try to solve Eq. (5.6) for F. Namely, suppose that F is a coboundary

$$F=d_Cr=\{C,r\}, \tag{5.13}$$

where $r=r^{ij}\xi_i\xi_j$ and r^{ij} is taken to be a constant matrix. Then the condition $d_F^2=0$ yields

$$\{C,\{r,\{C,r\}\}\}=d_C\{r,d_Cr\}=0. \tag{5.14}$$

This is the generalized CYBE. An even stronger condition

$$\{r,d_Cr\}=\{r,r\}_C=0 \tag{5.15}$$

leads to the CYBE [see (4.4)].

5.2. Two differentials from a Lie algebra action. We now look at the bicomplex setting from a somewhat different point of view. Rather than associating a second differential with a coalgebra structure, we construct a pair of differentials for a single Lie algebra. This subject attracts one's attention because of its possibly deep relation to the extended BRST symmetry.[9,10] We now show that the bicomplex generalization of the zero locus reduction method induces the so-called non-Abelian triplectic antibrackets on the space of common zeroes of the differentials. The non-

Abelian triplectic antibrackets were introduced in Ref. 14, see also Ref. 23, as the structure underlying a possible generalization of the well-known Lagrangian version of the extended BRST quantization.

5.2.1. Left and right $\mathfrak{a}$ *actions*. We consider the left and the right actions of $\mathfrak{a}$ on $\mathcal{X}$. To illustrate the idea, we restrict ourselves to the case where $\mathcal{X}=\mathcal{G}$ is the Lie group corresponding to the Lie algebra $\mathfrak{a}$. Let the basis elements e_i of $\mathfrak{a}$ act on $\mathcal{G}$ via the left invariant vector fields L_i (which correspond to the right action) and via the right invariant vector fields R_i (which correspond to the left action). Obviously, $[L_i,R_j]=0$. Let q^a and p_a be the standard coordinates on $T^*\mathcal{G}$. Unlike in the case considered above, we introduce the doubled set of variables ξ_i^1, ξ_j^2, θ_1^k, and θ_2^l, $i, j, k, l=1,...,\dim \mathfrak{a}$, with the basic Poisson brackets

$$\{q^a,p_b\}=\delta_b^a, \quad \{\theta_1^i,\xi_j^1\}=\delta_j^i, \quad \{\theta_2^i,\xi_j^2\}=\delta_j^i. \tag{5.16}$$

The functions

$$\begin{aligned}\Omega^1&=-p_aR_i^a\theta_1^i-\tfrac{1}{2}\xi_k^1C_{ij}^k\theta_1^i\theta_1^j,\\ \Omega^2&=-p_aL_i^a\theta_2^i-\tfrac{1}{2}\xi_k^2C_{ij}^k\theta_2^i\theta_2^j,\end{aligned} \tag{5.17}$$

satisfy $\{\Omega^\alpha,\Omega^\beta\}=0$ for $\alpha,\beta=1,2$, as follows immediately from the commutativity of the left- and right-invariant vector fields. These generating functions give rise to the anticommuting differentials $\mathbf{Q}^a=\{\Omega^a,\cdot\}$, thereby providing $\mathcal{F}_{\text{ext}}$ with a bicomplex structure.

5.2.2. Zero-locus reduction in $\mathcal{F}_{\text{ext}}$ *and non-Abelian triplectic antibrackets*. We now apply the zero locus reduction along the lines of Sec. 2. We identify the zero-locus $\mathcal{Z}_{\mathbf{Q}^1}$ (respectively, $\mathcal{Z}_{\mathbf{Q}^2}$) of the differential $\mathbf{Q}^1$ (of $\mathbf{Q}^2$) determined by the equations $\theta_1^i=0$ and $p_a=0$ (respectively, $\theta_2^i=0$ and $p_a=0$). The intersection $\mathcal{L}=\mathcal{Z}_{\mathbf{Q}^1}\cap\mathcal{Z}_{\mathbf{Q}^2}$ is then endowed with a pair of compatible antibrackets. Identifying $\mathcal{F}_{\mathcal{L}}$ (functions on the intersection) with functions of q^a, ξ_i^1, and ξ_j^2, we have

$$\begin{aligned}\{\xi_i^1,q^a\}_{\mathbf{Q}^1}&=R_i^a, \quad \{\xi_i^1,\xi_j^1\}_{\mathbf{Q}^1}=C_{ij}^k\xi_k^1,\\ \{\xi_i^2,q^a\}_{\mathbf{Q}^2}&=L_i^a, \quad \{\xi_i^2,\xi_j^2\}_{\mathbf{Q}^2}=C_{ij}^k\xi_k^2,\end{aligned} \tag{5.18}$$

with all the other brackets vanishing. These are precisely the non-Abelian triplectic antibrackets from Ref. 14.

VI. CONCLUSIONS

Our results give a geometric interpretation to a number of structures involved in the BFV/BV formalism; the interpretation of the BRST cohomology in terms of the constraint surface geometry[24] can thus be extended in terms of geometry of a ''more invariant'' object—the zero locus $\mathcal{Z}_{\mathbf{Q}}$ that plays the role of the *extended constraint surface*. Although this is presently limited to the ghost number zero, it would be interesting to extend this interpretation to other ghost numbers. Another interesting application of the zero locus reduction consists in interpreting $\mathcal{Z}_{\mathbf{Q}}$ with the induced Poisson bracket in the BV formulation of a pure-gauge model as an extended phase space and the extended Poisson bracket in the BFV formulation of the same model.[25] As noted above, the zero-locus reduction applies to finite-dimensional models; it would be interesting to extend it to local field theory, for example, in the jet language formulation of the BRST formalism.[26]

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APPENDIX: LIE ALGEBRA COHOMOLOGY AND THE (ANTI)BRACKET

Let $\mathfrak{a}$ denote a Lie algebra of dimension N and $\mathfrak{M}$ denote an $\mathfrak{a}$-module. We denote by

$$\wedge a = \bigoplus_{n=0}^{N} \wedge^n \mathfrak{a} \tag{A1}$$

the exterior algebra of the vector space $\mathfrak{a}$ and by $\mathsf{S}\mathfrak{a}$ the symmetric tensor algebra.

The cohomology complex of $\mathfrak{a}$ with coefficients in the module $\mathfrak{M}$ is

$$\mathsf{C}^*(\mathfrak{a},\mathfrak{M}) = \{\mathsf{Hom}(\wedge\mathfrak{a},\mathfrak{M}), d\}. \tag{A2}$$

Decomposition (A1) induces the grading $\mathsf{C}^*(\mathfrak{a},\mathfrak{M}) = \oplus_{n=0}^{N} C^n(\mathfrak{a},\mathfrak{M})$, where $C^n(\mathfrak{a},\mathfrak{M}) = \mathsf{Hom}(\wedge^n\mathfrak{a},\mathfrak{M})$. The differential d has the degree 1 and acts as $d: C^n(\mathfrak{a},\mathfrak{M}) \to C^{n+1}(\mathfrak{a},\mathfrak{M})$ via

$$(da)(g_1,\ldots,g_{n+1}) = \sum_{1\leqslant i<j\leqslant n+1} (-1)^{i+j-1} a([g_i,g_j],g_1,\ldots,\hat{g}_i,\ldots,\hat{g}_j,\ldots,g_{n+1})$$

$$+ \sum_{1\leqslant iLZn+1} (-1)^i g_i a(_1,\ldots,\hat{g}_i,\ldots,g_{n+1}), \quad a \in C^n(\mathfrak{a},\mathfrak{M}). \tag{A3}$$

In what follows we use the simplified notation $C^n = C^n(\mathfrak{a},\mathfrak{M})$.

Assume that $\mathfrak{a}$ is finite dimensional or graded, $\mathfrak{a} = \oplus_i \mathfrak{a}_i$, with finite dimensional homogeneous spaces $\mathfrak{a}_i$, and $\mathfrak{a}^*$ is by definition $\mathfrak{a}^* = \oplus_i \mathfrak{a}_i^*$, where $\mathfrak{a}_i^*$ are finite dimensional spaces dual to $\mathfrak{a}_i$. We then can identify the cohomology complex $\mathsf{C}^*(\mathfrak{a},\mathfrak{M})$ with $\wedge\mathfrak{a}^* \otimes \mathfrak{M}$ as follows. Let e_i be a basis in $\mathfrak{a}$, with $[e_i,e_j] = C_{ij}^k e_k$. Let also θ^i be the basis of $\mathfrak{a}^*$ dual to e_i. The Grassmann algebra generated by θ^i is then identified with $\wedge\mathfrak{a}^*$. To every cochain $x \in \mathsf{Hom}(\wedge^n\mathfrak{a},\mathfrak{M})$, we associate the element (with the summations implied)

$$\overline{x} = \frac{1}{n!} x(e_{i_1},\ldots,e_{i_n})\,\theta^{i_1}\cdots\theta^{i_n} \in \wedge\mathfrak{a}^* \otimes \mathfrak{M}. \tag{A4}$$

The differential d then acts on $\wedge\mathfrak{a}^* \otimes \mathfrak{M}$ as the differential operator

$$d = \frac{1}{2} C_{ij}^k \theta^i \theta^j \frac{\partial}{\partial \theta^k} - \theta^i X_i, \tag{A5}$$

where $X_i : \mathfrak{M} \to \mathfrak{M}$ is the action of $e_i \in \mathfrak{a}$ on $\mathfrak{M}$.

We next specialize to the coefficients in $\mathfrak{a}$ (viewed as the adjoint representation $\mathfrak{a}$-module). The complex is then endowed with the Gerstenhaber bracket[27] (see Ref. 28, and references therein),

$$\{\cdot,\cdot\}: C^n \otimes C^m \to C^{n+m-1}$$

given by

$$\{x,y\} = x\circ y - (-1)^{(m+1)(n+1)} y\circ x, \quad x \in C^n, \quad y \in C^m, \tag{A6}$$

where

$$(x\circ y)(a_1,\ldots,a_{n+m-1})$$

$$=\frac{1}{m!(n-1)!}\sum_{\sigma\in P_{n+m-1}}(-1)^{\sigma}x(a_{\sigma(1)},\ldots,a_{\sigma(n-1)},y(a_{\sigma(n)},\ldots,a_{\sigma(n+m-1)})). \tag{A7}$$

This makes $\mathrm{Hom}(\wedge\mathfrak{a},\mathfrak{a})$ into a graded differential Lie algebra.

Let ξ_i denote the basis of $\mathfrak{a}$ viewed as an $\mathfrak{a}$-module (equivalently, *coordinates* on $\mathfrak{a}^*$). For each cochain $x\in C^n$, we then expand $\overline{x}$ from (A4) as

$$\overline{x}=\frac{1}{n!}\xi_j x^j(e_{i_1},\ldots,e_{i_n})\,\theta^{i_1}\cdots\theta^{i_n} \tag{A8}$$

and rewrite the Gerstenhaber bracket as

$$\{\overline{x},\overline{y}\}=\overline{x\circ y}-(-1)^{(k+1)(l+1)}\overline{y\circ x},\quad \overline{x}\,\overline{y}=\overline{x}\frac{\overleftarrow{\partial}}{\partial\theta^i}\frac{\partial}{\partial\xi_i}\overline{y},\quad x\in C^k,\quad y\in C^l, \tag{A9}$$

where $\overleftarrow{\partial}/\partial\theta^i$ is the (right) derivative in the Grassmann algebra and the $\partial/\partial\xi_i$ operation is defined on the elements of form (A8) as the contraction with the element ξ_i^* of the dual basis in $\mathfrak{a}^*$. The differential then becomes

$$d=\left\{-\frac{1}{2}C_{ij}^k\xi_k\theta^i\theta^j,\cdot\right\}=\frac{1}{2}C_{ij}^k\theta^i\theta^j\frac{\partial}{\partial\theta^k}-\xi_k\theta^iC_{ij}^k\frac{\partial}{\partial\xi_j}. \tag{A10}$$

On the elements $\underline{a}$ as in (A8), the second term represents the adjoint action (in accordance with the above choice $\mathfrak{M}=\mathfrak{a}$). Equation (A9) suggests the interpretation of a Poisson/Batalin–Vilkovisky bracket. As it stands, however, (A9) can be neither of these, since no associative supercommutative multiplication has been defined on the cochains.

Superficially, the bracket in (A9) has the grade -1 since it maps as $C^m\times C^n\to C^{m+n-1}$, however the gradings of all the terms in the complex can be shifted by 1, after which the bracket becomes a grade-0 operation. On the other hand, an associative graded commutative multiplication defined on the complex would fix the grading, and (A9) would become either the Batalin–Vilkovisky or the Poisson bracket. Thus there are two remarkable possibilities to embed $\mathrm{C}^*(\mathfrak{a},\mathfrak{M})=\mathrm{C}^*(\mathfrak{a},\mathfrak{a})$ into a complex endowed with a multiplication: the complex

$$\mathrm{C}^*(\mathfrak{a},\mathrm{S}\mathfrak{a})=\wedge\mathfrak{a}^*\otimes\mathrm{S}\mathfrak{a} \tag{A11}$$

corresponding to the BV quantization, or the complex

$$\mathrm{C}^*(\mathfrak{a},\wedge\mathfrak{a})=\wedge\mathfrak{a}^*\otimes\wedge\mathfrak{a} \tag{A12}$$

corresponding to the BFV quantization. Geometrically, these two possibilities correspond to even and odd *QP* manifolds (see Definition 2.1).

Choosing $\mathfrak{M}=\mathrm{S}\mathfrak{a}$, we have the complex $\oplus_{m,n}\mathrm{Hom}(\wedge^m\mathfrak{a},\mathrm{S}^n\mathfrak{a})$, which can be viewed as the associative supercommutative algebra generated by the variables θ^i and ξ_j satisfying $\xi_i\xi_j-\xi_j\xi_i=0$, $\theta^i\theta^j+\theta^j\theta^i=0$, and $\theta^i\xi_j-\xi_j\theta^i=0$.[29] It then follows that (A9) can be extended to an odd bracket on this complex. The differential extends to $\mathrm{Hom}(\wedge\mathfrak{a},\mathrm{S}\mathfrak{a})$ by the same formula $d=\{C_0,\cdot\}$, $C_0=-\frac{1}{2}C_{ij}^k\xi_k\theta^i\theta^j$. The complex is endowed with the grading known as the *ghost number* in the BV quantization or as the Weyl complex grading in homology theory: for a cochain $x\in\mathrm{Hom}(\wedge^m\mathfrak{a},\mathrm{S}^n\mathfrak{a})$, one has $\mathrm{gh}(x)=m-2n$.

On the other hand, taking the coefficients to be the *exterior* algebra $\wedge\mathfrak{a}$, we can extend (A9) to an even bracket. With $\wedge\mathfrak{a}$ identified with the algebra generated by ξ_i viewed as *anticommuting variables* (with obvious modifications in the case where $\mathfrak{a}$ is a Lie *super*algebra, see Ref. 29, the bracket becomes the Poisson bracket on the space $\wedge\mathfrak{a}^*\otimes\wedge\mathfrak{a}$ (which is identified with functions of

θ^i and ξ_j; we also assume that $\xi_i\theta^j+\theta^j\xi_i=0$ in addition to $\xi_i\xi_j+\xi_j\xi_i=0$). The ghost number grading on this complex taken from the BFV quantization is $\mathrm{gh}(x)=m-n$ for an element $x \in \mathsf{Hom}(\wedge^m\mathfrak{a},\wedge^n\mathfrak{a})$.

The coefficients can be further extended (cf. Ref. 28) by $\mathfrak{M}=\mathcal{F}_{\mathcal{M}}$, the algebra of smooth functions on a manifold $\mathcal{M}$ such that $\mathfrak{a}$ acts on $\mathcal{F}_{\mathcal{M}}$ *by derivations* (vector fields on $\mathcal{M}$). We write X_i for the image of the basis elements of $\mathfrak{a}$ in $\mathrm{Vect}_{\mathcal{M}}$. In accordance with the BRST paradigm, one wishes the vector fields representing the action of $\mathfrak{a}$ on $\mathcal{M}$ to be Hamiltonian with respect to a bracket structure. For *even* ξ_i, this can be achieved by replacing $\mathcal{M}$ with the odd cotangent bundle $\Pi T^*\mathcal{M}$ and, thus, the algebra $\mathcal{F}_{\mathcal{M}}$ with the algebra $\mathcal{F}_{\Pi T^*\mathcal{M}}$ of smooth functions on the odd cotangent bundle. Then each vector field $V=V^a(\partial/\partial q^a)$ on $\mathcal{M}$ is generated by the canonical antibracket structure on $\Pi T^*\mathcal{M}$; the action of the basis elements $X_i=X_i^a(\partial/\partial q^a)$ on functions is given by the antibracket

$$X_iF=-\{X_i^aq_a^*,F\},\quad F\in\mathcal{F}_{\mathcal{M}}, \tag{A13}$$

with q_a^* being the standard coordinates on the fibers of $\Pi T^*\mathcal{M}$ (and the standard antibracket given by $\{q^a,q_b^*\}=\delta_b^a$).

For odd ξ_i, similarly, we can consider the functions $\mathcal{F}_{T^*\mathcal{M}}$ on the cotangent bundle, which allows the action of $\mathfrak{a}$ to be implemented by the bracket on $\mathcal{F}_{T^*\mathcal{M}}$ [the same formula (A13) for the bracket, where now q_a^* are the canonical coordinates on the fibers of $T^*\mathcal{M}$].

We note, however, that the differential

$$d=\{-\tfrac{1}{2}C_{ij}^k\xi_k\theta^i\theta^j,\cdot\}+\theta^i\{X_i^aq_a^*,\cdot\} \tag{A14}$$

in either of the complexes

$$\mathsf{C}^*_{\mathrm{odd}}(\mathfrak{a},\mathcal{M})=\mathsf{C}^*(\mathfrak{a},\mathsf{S}\mathfrak{a})\otimes\mathcal{F}_{\Pi T^*\mathcal{M}}, \tag{A15}$$

$$\mathsf{C}^*_{\mathrm{even}}(\mathfrak{a},\mathcal{M})=\mathsf{C}^*(\mathfrak{a},\wedge\mathfrak{a})\otimes\mathcal{F}_{T^*\mathcal{M}}, \tag{A16}$$

is *not* compatible with the bracket. Remarkably, the compatibility can be achieved by changing the differentials such that (A15) and (A16) become the well-known BV and BFV complexes used in the Lagrangian and Hamiltonian quantization of gauge theories. The term to be added to the differential is the Koszul differential involving precisely the same ''auxiliary'' variables ξ_i that were originally introduced to rewrite the Gerstenhaber bracket in the ''geometric'' form.

To conclude, we note that we have given a homological interpretation of the structures appearing in the BRST quantization in the example of a Lie algebra structure (i.e., in the case where the constraints or gauge generators form a Lie algebra). In the most general setting, the BRST charge and the master action in the BFV and BV cases, respectively, can be considered as the generating functions for the L_∞ algebras[8] (see also Ref. 4). From this general standpoint, the Lie algebra structure appears as a particular case.

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Ground state of a spin-1/2 charged particle in a two-dimensional magnetic field

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It is investigated that the structure of the kernel of the Dirac–Weyl operator **D** of a charged particle in the magnetic-field $B=B_0+B_1$, given by the sum of a strongly singular magnetic field $B_0(\cdot)=\Sigma_\nu \gamma^\nu \delta(\cdot-\mathbf{a}_\nu)$ with some singular points $\mathbf{a}_\nu$ and a magnetic-field B_1 with a bounded support. Here the magnetic field B_1 may have some singular points with the order of the singularity less than 2. At a glance, it seems that, following ''Aharonov–Casher Theorem'' [Phys. Rev. A **19**, 2461 (1979)], the dimension of the kernel of **D**, dim ker **D**, is a function of one variable of the total magnetic flux $(=\Sigma_\nu \gamma_\nu+\int_{\mathbf{R}^2} B_1 dxdy)$ of B. However, since the influence of the strongly singular points works, dim ker **D** indeed is a function of several variables of the total magnetic flux and each of γ_ν's. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379312]

I. INTRODUCTION

In 1979, Y. Aharonov and A. Casher[1] investigated the dimension of the kernel of the Dirac–Weyl operator **D** for a spin-1/2 charged particle in a two-dimensional magnetic field. And after that, many authors[2–10] (and references therein) studied it with various situations.

Aharonov and Casher[1] treated the case when the magnetic-field B is a smooth function on $\mathbf{R}^2$. In this case, **D** is essentially selfadjoint operator on $C_0^\infty(\mathbf{R}^2)$, the space of smooth functions with compact supports, and dim ker **D** is equal to the largest natural number which is less than $|q\Phi|/2\pi-1$, where q is the charge of the particle and the quantity Φ is the total magnetic flux of B defined by $\Phi=\int_{\mathbf{R}^2} B dxdy$. This result is well known as ''Aharonov–Casher Theorem.''

In 1993, A. Arai[2] treated another case than theirs. His is the case when B is strongly singular, more precisely, B is equal to 0 except on some finite points $\mathbf{a}_\nu \in \mathbf{R}^2 (\nu=1,...,n)$ and can be written as the sum of delta functions with coefficients $\gamma_\nu (\nu=1,...,n)$ and their derivatives [see, Eq. (1)]. The total magnetic flux Φ of B is equal to $\Sigma_{\nu=1}^n \gamma_\nu$. He have proved that, for this situation, **D** is not essentially selfadjoint on $C_0^\infty(M)$ with $M=\mathbf{R}^2\backslash\{\mathbf{a}_1,\ldots,\mathbf{a}_n\}$, and that each dimension of the kernels of two selfadjoint extensions of **D** depends on not only Φ but also each of γ_ν's. (He also has given an explicit formula.[2]) This means that, if B is strongly singular, ''Aharonov–Casher Theorem'' is not valid for this case.

In our article, we argue the case when magnetic field is a mixture of the Aharonov–Casher type and the Arai type, i.e., the case when the configuration space has both smooth and singular magnetic fields. No one has treated this situation yet. The following question arises: which theorem determines dim ker **D**, Aharonov–Casher's theorem or Arai's? Roughly speaking, we prove that dim ker **D** can be expressed by a formula similar to Arai's one [see Theorem 11].

We imagine the following physical situations: (1) Consider observation of a quantized magnetic field[11] penetrating a type II superconducting film by an electron microscope, such as in Refs. 12–14. To get such a quantized magnetic field, one applies a magnetic field **H** to the type II

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superconducting film first, and strengthens **H** next within the mixed state, so-called Schubnikov phase, between the lower critical field $\mathbf{H}_{c1}$ and upper one $\mathbf{H}_{c2}$. Then, following Abrikosov's theory and some experiments, the magnetic fluxes start to enter cores (normal regions on the inside of vortexes) on the type II superconducting film, and the entered magnetic field has the form of the bundle of fluxons (flux quanta). Following Tonomura's explanation about the experiments,[14] when one raise temperature up to the neighborhood of the critical temperature T_c with fixed **H** within the Schubnikov phase, the roots of the lines of magnetic fluxes become thick and the fluxons suddenly start to move. And, at the temperature over T_c the film fills with the normal cores, and the superconducting state is broken, namely the state changes to normal state from superconducting state. To observe the quantized magnetic field, for instance, in the experiment[12] the electron incident from the emitter of the electron microscope skims low over the surface of the type II superconductor. We are interested in the magnetic field on the normal cores in the critical phase near T_c. Our simple setup tries to represent mathematically the fired electron for the observation of the magnetic field on the normal cores in the critical phase though, of course, the representation cannot describe perfectly the physical realistic situation. (2) When we observe the quantized magnetic fluxes of a superconductor with the electron fired from an electron microscope, the fired electron needs to keep straight on. The electron, however, sometimes meets another magnetic field caused by, for instance, another electron microscope. This magnetic field from another electron microscope may, indeed, give no influence on the object because of the Meissner effect, but the magnetic field, as a noise, hinders the electron in its keeping straight on. In spite of such a situation, experimenters have to observe the object, the quantized magnetic fluxes. Thus, we have to investigate theoretically how the noise of another magnetic field influences the electron for the observation of the quantized magnetic fluxes. We try that as a first simplified case in our article (see Remark 3).

The plan of this article is as follows: In Sec. II, we define **D** and prove some lemmas. In Sec. III, we prove ''Vanishing Theorem.'' In Sec. IV, we prove our main theorem, which states the dimension of the kernel of **D**.

II. PRELIMINARY

Our aim is to investigate the structure of the kernel of the Dirac–Weyl operator **D** of a charged spin-1/2 particle in the magnetic field $B=B_0+B_1$, the sum of a strongly singular magnetic field B_0 [see, Eq. (1) and Ref. 2] and a magnetic-field B_1 with a bounded support. As mentioned above, the magnetic-field B_1 may have some singular points with the order of the singularity less than 2.

In this article, we denote the charge of the particle by $q \in \mathbf{R}\backslash\{0\}$. We assume that B_0 and B_1 may be singular at the finite isolated points $\mathbf{a}_\nu=(a_{\nu_1},a_{\nu_2}) \in \mathbf{R}^2$, $\nu=1,...,n$, and we put

$$M=\mathbf{R}^2\backslash\{\mathbf{a}_1,\ldots,\mathbf{a}_n\}.$$

In the case when B_1 is equal to 0, our model is the same one as in Ref. 2.

A. Strongly singular part B_0 of B

We denote by B_0 the strongly singular part of the given magnetic field B. Let

$$B_0(\mathbf{z})=\sum_{\nu=1}^{n}\sum_{0\leqslant\alpha+\beta\leqslant m} C_{\alpha\beta}^{(\nu)} D_x^\alpha D_y^\beta \delta(\mathbf{z}-\mathbf{a}_\nu), \quad \mathbf{z}=(x,y)\in\mathbf{R}^2, \tag{1}$$

with a nonnegative integer m and real constants $C_{\alpha,\beta}^{(\nu)}$, where D_x and D_y are the distributional partial differential operators in x and y, respectively, and $\delta(\mathbf{z})$ is the Dirac delta distribution on $\mathbf{R}^2$. A gauge potential $\mathbf{A}_0(\mathbf{z})$ of B_0 is defined by an $\mathbf{R}^2$-valued function $\mathbf{A}_0=(A_{01},A_{02})$ on M so that

$$B_0(x,y)=D_xA_{02}(x,y)-D_yA_{01}(x,y),$$

in the sense of distribution on $\mathbf{R}^2$.

Let

$$\phi_0(\mathbf{z})=\sum_{\nu=1}^{n}\sum_{0\leqslant\alpha+\beta\leqslant m}\frac{C_{\alpha,\beta}^{(\nu)}}{2\pi}D_x^{\alpha}D_y^{\beta}\log|\mathbf{z}-\mathbf{a}_\nu|,$$

which satisfies

$$\Delta\phi_0(\mathbf{z})=B_0(\mathbf{z}),$$

in the sense of distribution on $\mathbf{R}^2$. Thus, we can choose

$$\mathbf{A}_0=(A_{01},A_{02})=(-D_y\phi_0,D_x\phi_0),$$

as a gauge potential of B_0. We use later some of the same symbols as in Ref. 2. Put

$$C_k^{(\nu)}=(-1)^k k!\sum_{\alpha=0}^{k}C_{\alpha,k-\alpha}^{(\nu)}i^{k-\alpha},\quad \gamma_\nu=C_{0,0}^{(\nu)}=C_0^{(\nu)}\ \text{ and }\ \Phi_0=\sum_{\nu=1}^{n}\gamma_\nu. \tag{2}$$

B. Remainder B_1 of B

Through this article, we suppose that the remainder B_1 of B satisfies that

$$B_1\in C_0^{\infty}(M)=\{f\in C^{\infty}(M);\ \text{supp}\ \ f\ \ \text{is bounded}\} \tag{3}$$

and that for arbitrary $\nu=1,...,n$, there exist constants $d_\nu>0$ and $\epsilon_\nu<2$ such that

$$|B_1(\mathbf{z})|\leqslant\frac{d_\nu}{|\mathbf{z}-\mathbf{a}_\nu|^{\epsilon_\nu}}\ \text{ near }\ \mathbf{z}=\mathbf{a}_\nu. \tag{4}$$

Let

$$\phi_1(\mathbf{z})=\frac{1}{2\pi}\int_{\mathbf{R}^2}B_1(\mathbf{z}')\log|\mathbf{z}-\mathbf{z}'|d\mathbf{z}'\ \text{ for }\ \mathbf{z}=(x,y)\in\mathbf{R}^2.$$

Then we have that $B_1(\mathbf{z})=\Delta\phi_1(\mathbf{z})$ on M. Since $B_1\in L^{\epsilon}(\mathbf{R}^2)$ with $1<\epsilon<2$, using Young's inequality, we can prove the following lemma.

Lemma 1: Let $B_1\in C_0^{\infty}(M)$ and suppose Eq. (4). Then $\phi_1\in C(\mathbf{R}^2)$.

We shall need the local boundedness of ϕ_1 on $\mathbf{R}^2$ as a conclusion of this lemma.

Let

$$\Phi_1=\int_{\mathbf{R}^2}B_1(\mathbf{z})d\mathbf{z}.$$

Since $B_1\in C_0^{\infty}(M)$ and Eq. (4), we have $B_1\in L^1(\mathbf{R}^2)$. Thus, Φ_1 has a finite value. Considering the boundedness of the support of B_1, we can prove the following lemma with calculating a little.

Lemma 2: Suppose $B_1\in C_0^{\infty}(M)$. Then

$$e^{\phi_1(\mathbf{z})}\sim|\mathbf{z}|^{\Phi_1}\ \ as\ \ \mathbf{z}\to\infty.$$

Remark: We write that $f(\mathbf{z})\sim g(\mathbf{z})$ as $\mathbf{z}\to\infty$ if and only if there exist positive constants, c and d, such that for all $|\mathbf{z}|$ large enough, $cf(\mathbf{z})\leqslant g(\mathbf{z})\leqslant df(\mathbf{z})$ holds.

Define an $\mathbf{R}^2$-valued function $\mathbf{A}_1=(A_{11},A_{12})$ on M by

$$\mathbf{A}(\mathbf{z})=(A_{11}(\mathbf{z}),A_{22}(\mathbf{z}))=(-\partial_y\phi_1(\mathbf{z}),\partial_x\phi_1(\mathbf{z})).$$

Here, $\partial_x=\partial/\partial x$ and $\partial_y=\partial/\partial y$. Then $\mathbf{A}_1$ is a gauge potential of B_1, i.e.,

$$B_1(x,y)=D_xA_{12}(x,y)-D_yA_{11}(x,y)$$

in the sense of distribution on $\mathbf{R}^2$.

Remark 3: For the sake of simplicity, we assume Eq. (3). P. Exner and the authors[10] *have proven that under the assumptions,* $B_1(x)=\mathcal{O}(|x|^{-2-\delta})$ *for some* $\delta>0$ *and* $B_1\in L^{1+\epsilon}_{\mathrm{loc}}(\mathbf{R}^2)$ *for some* $\epsilon>0$*, there exists a positive R such that*

$$|\phi_1(x)-\Phi_1\ln|x||<\epsilon|\ln x|,$$

for all $|x|>R$ *and* ϕ_1 *is continuous.* (*See, Prop. 2.2 and Prop. 2.5 in* Ref. 10.) *Since we do not need the compactness of the support of* B_1*, we can remove this restriction.*

C. The total magnetic-field *B*

From now on, using the notations in the previous subsections, we rewrite the given (total) magnetic field B as

$$B(\mathbf{z})=B_0(\mathbf{z})+B_1(\mathbf{z}),$$

and take

$$\mathbf{A}(\mathbf{z})=\mathbf{A}_0(\mathbf{z})+\mathbf{A}_1(\mathbf{z}),$$

as a gauge potential of B. We denote by Φ the total magnetic flux:

$$\Phi=\Phi_0+\Phi_1.$$

Let

$$\phi(\mathbf{z})=\phi_0(\mathbf{z})+\phi_1(\mathbf{z}).$$

Then we have

$$\mathbf{A}(\mathbf{z})=(-D_y\phi(\mathbf{z}),D_x\phi(\mathbf{z})).$$

D. Dirac–Weyl operators

In this subsection, we define the Dirac–Weyl operators with B_0 and B acting in $\mathbf{C}^2\otimes L^2(\mathbf{R}^2)$. Let σ_j, $j=1,2,3$, be the Pauli matrices:

$$\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

We denote the domain of an operator T by *Dom(T).*

Let

$$p_1=-iD_x,\quad p_2=-iD_y,$$

be distributional differential operators acting in $L^2(\mathbf{R}^2)$. The velocity operator $\mathbf{P}_0=(P_{01},P_{02})$ with the gauge potential $\mathbf{A}_0$ is given by

$$P_{0j}=p_j-qA_{0j}\ \text{ with }\ \mathrm{Dom}(P_{0j})=C_0^\infty(M).$$

Define the Dirac–Weyl operator $Q_{\min}$ with the strongly singular magnetic-field B_0 by

$$Q_{\min}=\sigma_1P_{01}+\sigma_2P_{02}\ \text{ with }\ \mathrm{Dom}(Q_{\min})=\mathbf{C}^2\otimes C_0^\infty(M).$$

As the above equation, we often omit the tensorial sign, $\otimes$, between two operators. The velocity operator $\mathbf{P}=(P_1,P_2)$ with the gauge potential $\mathbf{A}$ is given by

$$P_j=p_j-q(A_{0j}+A_{1j}) \quad \text{with} \quad \mathrm{Dom}(P_j)=C_0^\infty(M).$$

Define the Dirac–Weyl operator $D_{\min}$ with the total magnetic field B by

$$D_{\min}=\sigma_1P_1+\sigma_2P_2 \quad \text{with} \quad \mathrm{Dom}(D_{\min})=\mathbf{C}^2\otimes C_0^\infty(M).$$

Note that $Q_{\min}$ is written in the form of

$$Q_{\min}=\begin{pmatrix} 0 & Q_- \\ Q_+ & 0 \end{pmatrix},$$

where

$$Q_\pm=P_{01}\pm iP_{02} \quad \text{with} \quad \mathrm{Dom}(Q_\pm)=C_0^\infty(M),$$

and $D_{\min}$ is written in the form of

$$D_{\min}=\begin{pmatrix} 0 & D_- \\ D_+ & 0 \end{pmatrix},$$

where

$$D_\pm=P_1\pm iP_2 \quad \text{with} \quad \mathrm{Dom}(D_\pm)=C_0^\infty(M).$$

The operators $Q_{\min}$ and $D_{\min}$ are symmetric, and thus, $Q_{\min}$ and $D_{\min}$ are closable. We denote by $\overline{Q}_{\min}$ and $\overline{D}_{\min}$ the closures of $Q_{\min}$ and $D_{\min}$, respectively.

Let

$$\mathbf{D}_1=\begin{pmatrix} 0 & D_+^* \\ \overline{D}_+ & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{D}_2=\begin{pmatrix} 0 & \overline{D}_- \\ D_-^* & 0 \end{pmatrix},$$

be Dirac–Weyl operators with B acting in $\mathbf{C}^2\otimes L^2(\mathbf{R}^2)$. These are selfadjoint extensions of $D_{\min}$. In Sec. IV, it is proven that these do not coincide under some conditions.

Remark: In Ref. 2, for the two self-adjoint extensions $Q_{\min}^{(1)}$ and $Q_{\min}^{(2)}$ of the symmetric operator $Q_{\min}$ have been constructed in the same fashion as above. Under some conditions, these selfadjoint extensions are not coincided with each other.

E. Generalized kernel

In this subsection, we preliminary examine the generalized kernel (the space of generalized eigenvectors with eigenvalue 0) of $D_{\min}$ to identify the kernels of $\mathbf{D}_1$ and $\mathbf{D}_2$. We use the following natural identification of $\mathbf{R}^2$ and $\mathbf{C}$: Each $\mathbf{z}=(x,y)\in\mathbf{R}^2$ corresponds to $z=x+iy\in\mathbf{C}$ with the imaginary unit i. We set $\partial=(\partial/\partial x-i\partial/\partial y)/2$, $\overline{\partial}=(\partial/\partial x+i\partial/\partial y)/2$, and $a_\nu=a_{\nu_1}+ia_{\nu_2}$ for $\mathbf{a}_\nu=(a_{\nu_1},a_{\nu_2})$.

The following proposition shall be needed later.

Proposition 4: *The following identity as differential operators holds on* $C^\infty(M)$*:*

$$D_\pm=e^{\mp q\phi_1}Q_\pm e^{\pm q\phi_1}.$$

Proof: By direct computations, we have

$$Q_+=-2ie^{-q\phi_0}\overline{\partial}e^{+q\phi_0},$$

$$Q_- = -2ie^{+q\phi_0}\partial e^{-q\phi_0},$$

$$D_+ = -2ie^{-q\phi}\overline{\partial} e^{+q\phi},$$

$$D_- = -2ie^{+q\phi}\partial e^{-q\phi}$$

on $C^\infty(M)$. Thus, we obtain the desired result.

Let $\mathcal{D}(M)=C_0^\infty(M)$ and $\mathcal{D}'(M)$ be the space of distributions on M. We say that $f\in\mathcal{D}'(M)$ is a generalized eigenvector with eigenvalue 0 of an operator T on $C_0^\infty(M)$ if

$$\langle f,(Tg)^*\rangle = 0 \quad \text{for all } g\in C_0^\infty(M),$$

where $\langle\cdot,\cdot\rangle$ denotes the canonical bilinear form on $\mathcal{D}'(M)\times C_0^\infty(M)$. We denote by $S(T)$ the space of all the generalized eigenvectors with eigenvalue 0 of T. Note that $\ker \overline{D}_\pm \subset S(D_\pm)$.

For a function ψ on M, let

$$H_\psi(M)=\{e^{-q\psi}f;\ f \text{ is holomorphic on } M\},$$

$$H_\psi^q(M)=\{e^{q\psi}g;\ g \text{ is antiholomorphic on } M\}$$

The following lemma is Lemma 4.4 in Ref. 2.

Lemma 5: We have

$$S(Q_+)=H_{\phi 0}(M) \quad \text{and} \quad S(Q_-)=H_{\phi 0}^q(M).$$

The following lemma can be proven in the same way as in the proof of Lemma 4.4 in Ref. 2.

Lemma 6: We have

$$S(D_+)=H_\phi(M) \quad \text{and} \quad S(D_-)=H_\phi^q(M).$$

Note that $S(Q_{\min})=S(Q_+)\oplus S(Q_-)$ and $S(D_{\min})=S(D_+)\oplus S(D_-)$.

III. VANISHING THEOREM

In this section, we examine the vanishing theorem for Dirac–Weyl operators $\mathbf{D}_1$ and $\mathbf{D}_2$. Suppose that $B_1\in C_0^\infty(M)$ and that Eq. (4) holds. We need the following lemma proved by Arai.

Lemma 7 (Arai, Lemma 4.3 in Ref. 2): We have $\ker \overline{Q}_\pm=\{0\}$, i.e., $\ker \overline{Q}_{\min}=\{0\}$.

The following is the main theorem in this section.

Theorem 8 (Vanishing Theorem): Suppose that the multiplication operator $e^{q\phi_1}$ (*resp.* $e^{-q\phi_1}$) *acting in* $L^2(\mathbf{R}^2)$ *is bounded. Then*

$$\ker \overline{D}_+=\{0\}. \quad (\text{resp. } \ker \overline{D}_-=\{0\}.)$$

Remark: For ϵ in Remark 3, (i) if $q\Phi_1\leqslant -|q|\epsilon$, then $e^{q\phi_1}$ is bounded; (ii) if $e^{q\phi_1}$ is bounded, then $q\Phi_1\leqslant|q|\epsilon$.

Proof: Consider the case when $e^{q\phi_1}$ is bounded. By Proposition 4, we have

$$e^{q\phi_1}S(D_+)=S(Q_+). \tag{5}$$

Let $\Psi\in\ker \overline{D}_+$. Then there exists a sequence $\{\Psi_n;n\in\mathbf{N}\}\subset C_0^\infty(M)$ such that $\Psi_n\to\Psi$ and $D_+\Psi_n\to 0$ in $L^2(\mathbf{R}^2)$ as $n\to\infty$. Since $\Psi\in S(D_+)$, by Eq. (5) and the assumption

$$e^{q\phi_1}\Psi\in S(Q_+)\cap L^2(\mathbf{R}^2).$$

We have $e^{q\phi_1}\Psi_n\in C_0^\infty(M)$ for all $n\in\mathbf{N}$ and, since $e^{q\phi_1}$ is bounded, we have

$$e^{q\phi_1}\Psi_n \to e^{q\phi_1}\Psi \quad \text{in} \quad L^2(\mathbf{R}^2),$$

as $n\to\infty$. Moreover

$$\|Q_+ e^{q\phi_1}\Psi_n\| \leqslant \|e^{q\phi_1}\|\|e^{-q\phi_1}Q_+ e^{q\phi_1}\Psi_n\| = \|e^{q\phi_1}\|\|D_+\Psi_n\| \to 0,$$

as $n\to\infty$. Thus, $e^{q\phi_1}\Psi \in \mathrm{Dom}(\overline{Q}_+)$ and $\overline{Q}_+ e^{q\phi_1}\Psi = 0$. Therefore, by Lemma 7, $e^{q\phi_1}\Psi = 0$. Thus, we have $\Psi = 0$, which means $\ker \overline{D}_+ = \{0\}$. In the case when $e^{-q\phi_1}$ is bounded, we can obtain the desired result in the same way as above.

IV. KERNEL OF DIRAC–WEYL OPERATOR

In the previous section, in the case when $e^{q\phi_1}$ (resp. $e^{-q\phi_1}$) is bounded, we proved that $\ker \overline{D}_+ = \{0\}$ (resp. $\ker \overline{D}_- = \{0\}$). In this section, we examine $\ker \overline{D}_-$ and $\ker \overline{D}_+$, and we identify the kernels of the two selfadjoint extensions $\mathbf{D}_1$ and $\mathbf{D}_2$ in restricted cases, respectively.

Let $\mathbf{Z}_+$ be the set of nonnegative integers. We introduce the set

$$W_\pm(\Phi) = \left\{ (p,k_1,\ldots,k_n) \in \mathbf{Z}_+ \times \mathbf{Z}^n; p + \sum_{\nu=1}^{n} k_\nu < \pm\frac{q\Phi}{2\pi} - 1, \ \pm\ \frac{q\gamma_\nu}{2\pi} - 1 < k_\nu, \nu = 1,\ldots,n \right\},$$

and put

$$N_\pm(\Phi;n;q) = \#W_\pm(\Phi),$$

the number of the elements of $W_\pm(\Phi)$. Note that $N_-(\Phi;n;q) = N_+(\Phi;n;-q)$. Let

$$F(z) = -\frac{1}{2\pi}\sum_{\nu=1}^{n}\sum_{k=1}^{m}\frac{C_k^{(\nu)}}{k(z-a_\nu)^k}.$$

Here, the constants $C_k^{(\nu)}$ were defined by Eq. (2). For $(p_\pm,k_1,\ldots,k_n) \in \mathbf{Z}_+ \times \mathbf{Z}^n$, define functions on M by

$$\Omega^{+}_{p_+,k_1,\ldots,k_n}(\mathbf{z}) = \left(\prod_{\nu=1}^{n} |\mathbf{z}-\mathbf{a}_\nu|^{-q\gamma_\nu/2\pi}(z-a_\nu)^{k_\nu} \right) P_+(z)^{iq\Im F(z)},$$

$$\Omega^{-}_{p_-,k_1,\ldots,k_n}(\mathbf{z}) = \left(\prod_{\nu=1}^{n} |\mathbf{z}-\mathbf{a}_\nu|^{q\gamma_\nu/2\pi}(\overline{z}-\overline{a}_\nu)^{k_\nu} \right) P_-(\overline{z})^{-iq\Im\overline{F}(z)},$$

where $P_\pm$ is a polynomial of order $p_\pm$ such that $P_+(a_\nu) \neq 0$, $P_-(\overline{a}_\nu) \neq 0$, $\nu = 1,\ldots,n$.

Remark: The sets $W_\pm(\Phi_0)$ and the numbers $N_\pm(\Phi_0;n;q)$ are equal to $W_\pm$ and $N_\pm(n;q)$ given in Ref. 2, respectively, and these functions $\Omega^{\pm}_{p_\pm,k_1,\ldots,k_n}$ are the same ones given in Ref. 2.

First of all, we solve the differential equations $D_\pm\Omega = 0$ on M and examine when it is solutions Ω are in $L^2(M)$.

Lemma 9: (i) The functions $e^{\mp q\phi_1}\Omega^{\pm}_{p_\pm,k_1,\ldots,k_n}$ satisfy the partial differential equations

$$D_\pm e^{\mp q\phi_1}\Omega^{\pm}_{p_\pm,k_1,\ldots,k_n} = 0 \quad \text{on} \quad M,$$

respectively.

(ii) The functions $e^{\mp q\phi_1}\Omega^{\pm}_{p_\pm,k_1,\ldots,k_n}$ are in $L^2(\mathbf{R}^2)$ if and only if $(p_\pm,k_1,\ldots,k_n) \in W_\pm(\Phi)$, respectively.

Proof: By Lemma 4.6 (i) in Ref. 2, we have

$$Q_\pm\Omega^{\pm}_{p_\pm,k_1,\ldots,k_n} = 0 \quad \text{on} \quad M.$$

Thus, with Proposition 4, we obtain part (i). We prove part (ii). We have

$$|e^{-q\phi_1}\Omega^+_{p_+,k_1,\ldots,k_n}(\mathbf{z})| \sim \text{const}|\mathbf{z}|^{-(q\Phi/2\pi)+p_+ +\Sigma_{\nu=1}^n k_\nu},$$

as $|\mathbf{z}|\to\infty$, and

$$|e^{-q\phi_1}\Omega^+_{p_+,k_1,\ldots,k_n}(\mathbf{z})| \sim \text{const}|\mathbf{z}-\mathbf{a}_\nu|^{-(q\gamma_\nu/2\pi)+p_+},$$

as $\mathbf{z}\to\mathbf{a}_\nu$. Therefore, the desired assertion on $e^{-q\phi_1}\Omega^+_{p_+,k_1,\ldots,k_n}$ follows. Similarly we can prove the assertion on $e^{q\phi_1}\Omega^-_{p_-,k_1,\ldots,k_n}$.

Using this lemma, we can identify the kernels of $D^*_\pm$.

Theorem 10: *We have*

$$\ker D^*_- = \{e^{-q\phi_1}\Omega^+_{p,k_1,\ldots,k_n}; (p,k_1,\ldots,k_n)\in W_+(\Phi)\}, \tag{6}$$

where $\ker D^*_- = \{0\}$ *if* $W_+(\Phi)=\varnothing$, *and*

$$\ker D^*_+ = \{e^{q\phi_1}\Omega^-_{p,k_1,\ldots,k_n}; (p,k_1,\ldots,k_n)\in W_-(\Phi)\}, \tag{7}$$

where $\ker D^*_+ = \{0\}$ *if* $W_-(\Phi)=\varnothing$.

Proof: By Lemma 9, the sets on the right-hand side (rhs) of Eqs. (6) and (7) are included in $\ker D^*_-$ and $\ker D^*_+$, respectively. To prove the converse inclusion relations, let

$$\Omega=(\Omega_+,\Omega_-)\in \ker D^*_-\oplus\ker D^*_+.$$

Note that

$$\ker D^*_-\oplus\ker D^*_+ = \ker D^*_{\min} = \mathbf{C}^2\otimes L^2(\mathbf{R}^2)\cap S(D_{\min}).$$

Hence $\Omega\in S(D)$ and $\Omega_\pm\in L^2(\mathbf{R}^2)$. Therefore, by Lemma 6, there exists a holomorphic function f and an anti-holomorphic function g on M such that

$$\Omega_+ = e^{-q(\phi_1+\phi_0)}f, \quad \Omega_- = e^{q(\phi_1+\phi_0)}g.$$

We note that

$$\phi_0(\mathbf{z}) = \Re F(z) + \sum_{\nu=1}^n \frac{\gamma_\nu}{2\pi}\log|\mathbf{z}-\mathbf{a}_\nu|,$$

and $\phi_1\in C(\mathbf{R}^2)$. Thus, using the condition of that $\Omega_+\in L^2(\mathbf{R}^2)$, we see that f must be of the form

$$f(z) = e^{qF(z)}h(z),$$

with a meromorphic function h on $\mathbf{C}\cup\{\infty\}$ with possible poles at $z=a_\nu$, $\nu=1,\ldots,n$. Thus, Ω_+ has to take the form

$$\Omega_+ = e^{-q\phi_1}\Omega^+_{p,k_1,\ldots,k_n},$$

with some $(p,k_1,\ldots,k_n)\in\mathbf{Z}_+\times\mathbf{Z}^n$. By Lemma 9 (ii), $(p,k_1,\ldots,k_n)$ must be in $W_+(\Phi)$. Thus, Ω_+ is in the set on the rhs of Eq. (6). In the same way, we can prove that Ω_- is in the set on the rhs of Eq. (7).

Consequently, we obtain our main theorem.

Theorem 11: *(i) If* $e^{q\phi_1}$ *is bounded, we have*

$$\ker \mathbf{D}_1 = \left\{ \begin{pmatrix} 0 \\ e^{q\phi_1}\Omega^-_{p,k_1,\ldots,k_n} \end{pmatrix};\ (p,k_1,\ldots,k_n) \in W_-(\Phi) \right\}, \tag{8}$$

where $\ker \mathbf{D}_1 = \{0\}$ *if* $W_-(\Phi) = \varnothing$. *In particular,*

$$\dim\ \ker \mathbf{D}_1 = N_-(\Phi;n;q). \tag{9}$$

(ii) If $e^{-q\phi_1}$ *is bounded, we have*

$$\ker \mathbf{D}_2 = \left\{ \begin{pmatrix} e^{-q\phi_1}\Omega^+_{p,k_1,\ldots,k_n} \\ 0 \end{pmatrix};\ (p,k_1,\ldots,k_n) \in W_+(\Phi) \right\}, \tag{10}$$

where $\ker \mathbf{D}_2 = \{0\}$ *if* $W_+(\Phi) = \varnothing$. *In particular,*

$$\dim\ \ker \mathbf{D}_2 = N_+(\Phi;n;q). \tag{11}$$

Proof: Consider the part (i). By Theorem 8, we have

$$\ker \mathbf{D}_1 = \left\{ \begin{pmatrix} 0 \\ \Omega \end{pmatrix}; \Omega \in \ker \mathbf{D}_+^* \right\}.$$

Hence it follows from Lemma 9 that the set on the rhs of Eq. (8) is included in $\ker \mathbf{D}_1$. By Theorem 10, we obtain the converse inclusion relation. Therefore, we obtain Eq. (8). In the same way, we can obtain Eq. (10). We write as $(p,k_1,\ldots,k_n) = (p,\mathbf{k})$. Thus, $\{e^{\mp q\phi_1}\Omega^{\pm}_{p_j,\mathbf{k}_j}\}_{j=1}^{l}$ are linearly independent if and only if $(p_j,\mathbf{k}_j) \neq (p_i,\mathbf{k}_i)$, $i \neq j$, $i,j = 1,\ldots,l$. Thus, Eq. (9) and Eq. (11) follow.

Remark: In Theorem 4.7 (ii) in Ref. 2, both $W_\pm(\Phi)$ is empty for $n=1$. On the other hand, in our case, $W_\pm(\Phi)$ is not always empty. For instance, we can rewrite $W_\pm(\Phi)$ as

$$W_\pm(\Phi) = \left\{ (p,k_1) \in \mathbf{Z}_+ \times \mathbf{Z}; p + k_1 < \pm\frac{q}{2\pi}(\Phi_0 + \gamma_1) - 1 < \pm\frac{q}{2\pi}\Phi_0 - k_1 \right\},$$

for $n=1$, since $\Phi = \Phi_0 + \gamma_1$. Thus, if $k_1 > q\gamma_1/2\pi - 1$ and $q\Phi_0/2\pi \geqslant 1$, then $W_+(\Phi)$ is not empty and $W_-(\Phi) = \varnothing$. This is the difference caused by the effect of B_1. We remark that B_1 prevents the magnetic flux from locally quantization defined by Arai in Ref. 2.

As a corollary of Theorem 11, we have the following.

Corollary 12: Let $n \geqslant 2$ *and suppose that* $N_+(\Phi;n;q) + N_-(\Phi;n;q) \geqslant 1$. *Then* $D_{\min}$ *is not essentially selfadjoint.*

Proof: In this case, the two self-adjoint extensions $\mathbf{D}_1$ and $\mathbf{D}_2$ are not coincided with each other. Thus, $D_{\min}$ is not essentially selfadjoint.

Remark: In the same way as in the proof of Proposition 4.9 in Ref. 2, we can prove under some conditions that $N_\pm(\Phi_1;n;q) \geqslant 1$ and, thus, $D_{\min}$ is not essentially self-adjoint.

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Intertwined isospectral potentials in an arbitrary dimension

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The method of intertwining with n-dimensional (nD) linear intertwining operator $\mathcal{L}$ is used to construct nD isospectral, stationary potentials. It has been proven that the differential part of $\mathcal{L}$ is a series in Euclidean algebra generators. Integrability conditions of the consistency equations are investigated and the general form of a class of potentials respecting all these conditions have been specified for each $n=2, 3, 4, 5$. The most general forms of 2D and 3D isospectral potentials are considered in detail and construction of their hierarchies is exhibited. The followed approach provides coordinate systems which make it possible to perform separation of variables and to apply the known methods of supersymmetric quantum mechanics for 1D systems. It has been shown that in choice of coordinates and $\mathcal{L}$ there are a number of alternatives increasing with n that enlarge the set of available potentials. Some salient features of higher dimensional extension as well as some applications of the results are presented. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The method of intertwining provides a unified approach to constructing exactly solvable linear and nonlinear problems and their hierarchies in various fields of physics and mathematics.[1–5] This is closely connected with the supersymmetric (SUSY) methods such as Darboux's transformation, Schrödinger's factorization, and shape invariant potential concept which deal with pairs of Hamiltonians having the same energy spectra but different eigenstates.[6,7] In general, the object of the intertwining is to construct the so-called intertwining operator $\mathcal{L}$ which performs an intertwining between two given operators of the same type (differential, integral, matrix, or, operator-valued matrix operator, etc.). In the context of quantum mechanics $\mathcal{L}$ is taken to be a linear differential operator which intertwines two Hamiltonian operators H_0 and H_1 such that

$$\mathcal{L}H_0 = H_1\mathcal{L}. \tag{1}$$

Two simple and important facts that are at the heart of the usefulness of this method can be stated as follows: (i) If ψ^0 is an eigenfunction of H_0 with eigenvalue of E^0, then $\psi^1=\mathcal{L}\psi^0$ is an (unnormalized) eigenfunction of H_1 with the same eigenvalue E^0. Hence $\mathcal{L}$ transforms one solvable problem into another. (ii) When H_0 and H_1 are Hermitian (on some common function space) $\mathcal{L}^\dagger$ intertwines in the other direction $H_0\mathcal{L}^\dagger=\mathcal{L}^\dagger H_1$ and this in turn implies that $[H_0,\mathcal{L}^\dagger\mathcal{L}]=0=[\mathcal{L}\mathcal{L}^\dagger,H_1]$, where † and $[,]$ stand for Hermitian conjugation and commutator. Therefore , two hidden dynamical symmetry operators of H_0 and H_1 are immediately constructed in terms of $\mathcal{L}$.[5] These are dimension and form independent general properties of this method.[2] Despite this fact, like the above mentioned SUSY methods, the intertwining method is mostly studied in the context of one-dimensional (1D) systems where $\mathcal{L}$ is taken to be the first order differential operator and

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Hamiltonians are in the standard potential forms. Two additional properties that arise in that case are that;[8] (i) Every eigenfunction of H_0 (without regard to boundary conditions or normalizability) can be used to generate a transformation to a new solvable problem [see Eq. (20) below]. (ii) A direct connection to a SUSY algebra can be established by constructing a diagonal matrix Hamiltonian $H=\mathrm{diag}(H_0,H_1)$ and two nilpotent supercharges $Q^+=(Q^-)^\dagger$ such that the only nonvanishing element of Q^+ matrix is $Q^+_{21}=\mathcal{L}$. These obey the defining relations of the simplest SUSY algebra,

$$\{Q^+,Q^-\}=H, \quad (Q^+)^2=(Q^-)^2=0,$$

which imply $[H,Q^\pm]=0$ and emphasize in a compact algebraic form of the spectral equivalence of two 1D systems. In the nomenclature of the SUSY quantum mechanics $\mathcal{L}$ is known as the supercharge operator and its zeroth-order (in derivatives) term as the superpotential.

There are important studies in the literature which aim to generalize the SUSY methods beyond 1D problems. These can be classified as (i) curved-space approach[1,2,9] (for recent studies, see Ref. 10), and (ii) Matrix-Hamiltonian approach.[5,11–13] Both are based on the intertwining method and they mostly concentrate on extension to two dimensions.

The application of the first approach to quantum mechanics was motivated by Ref. 1 which deals with free particle propagation on a Lie group manifold (see also Ref. 14). Later on, this has been advanced to find the propagator of a free particle moving on an nD sphere[9] as well as to solve both ordinary and partial differential equations with applications to symmetric spaces.[2] These approaches are expected to produce solvable 1D n-particle problems from an nD free motion via some projection methods like that used in Refs. 15 and 16. The second approach, appeared for the first time in Ref. 11, performs the extension by preserving the connection with a SUSY algebra.[12,13] This inevitably restricts the consideration to two matrix Hamiltonian such that one of them has off-diagonal entries. Accordingly, a matrix with elements having higher order derivative terms participates as the intertwining operator. This approach establishes the equivalence of two matrix systems but does not establish spectral equivalence between two scalar Hamiltonians. To improve it in this regard, an algorithm called the polynomial SUSY in which $\{Q^+,Q^-\}$ is a polynomial of the H-matrix was introduced.[13]

The classification given above is by no means exhaustive; for instance one may find a nice method based on integral intertwining operator in Ref. 3 (Sec. II 8) to generate a hierarchy of 2D problems. We should also note that recently the intertwining method has been used for the nonstationary Schrödinger operator.[5,17,18]

The main purpose of this paper is to extend the intertwining method to an arbitrary dimension by applying it to a pair of nD systems characterized by Hamiltonian operators of potential form,

$$H_i=-\nabla^2+V_i, \quad i=0,1, \tag{2}$$

where the potentials V_i and eigenvalues of H_i are expressed in terms of $2m/\hbar^2$ and $\nabla^2=\Sigma_{j=1}^n\partial_j^2$ is the Laplace's operator of R^n. We shall use the Cartesian coordinates $\{x_k;k=1,\ldots,n\}$, the convention $\partial_k\equiv\partial/\partial x_k$, and the abbreviation $V_i\equiv V_i(x_1,\ldots,x_n)$ throughout the paper. We purpose the ansatz that $\mathcal{L}$ is the most general first-order linear operator,

$$\mathcal{L}=L_0+L_d=L_0+\sum_{k=1}^n L_k\partial_k, \tag{3}$$

where L_0,L_k are some functions of $\{x_k;k=1,\ldots,n\}$ which together with V_i are to be determined from consistency equations of Eq. (1). In terms of the vector field $\mathbf{L}=(L_1,\ldots,L_n)$ and nD gradient operator ∇ the operator $L_d=\Sigma_{k=1}^n L_k\partial_k$ will be usually written as $L_d=\mathbf{L}\cdot\nabla$, where "$\cdot$" denotes the usual Euclidean inner product.

In the next section by solving the first $n(n+1)/2$ consistency equations we will show that the operator L_d is a series in generators of the Euclidean algebra in n-dimension. There remain $n+1$ consistency equations which consist of n linear and 1 nonlinear partial differential equations.

Some particular solutions of these equations for an arbitrary n are presented in Sec. III. In Sec. IV we take up the integrability conditions of the remaining n linear equations in the context of the Frobenius integrability theory.[19] General forms of the potentials respecting all integrability conditions for $n=2,3,4,5$ are obtained in Sec. V. A detailed investigation of 2D and 3D isospectral potentials are given in Secs. VI, VII, VIII, where we also exhibit how to generate hierarchies of potentials.

II. INTERTWINING IN *N* DIMENSION: EUCLIDEAN ALGEBRA

In view of (2) and (3) the intertwining relation (1) can be written as

$$[\nabla^2, L_d] = -[\nabla^2, L_0] + [V_0, L_d] + P\mathcal{L}, \tag{4}$$

where $P = V_1 - V_0$. At a glimpse of the right-hand side of Eq. (4) and

$$[\nabla^2, L_d] = \sum_{j,k} (\partial_j^2 L_k)\partial_k + 2\sum_j (\partial_j L_j)\partial_j^2 + 2\sum_{j<k} (\partial_j L_k + \partial_k L_j)\partial_j\partial_k, \tag{5}$$

$$[\nabla^2, L_0] = (\nabla^2 L_0) + 2\sum_j (\partial_j L_0)\partial_j, \tag{6}$$

$$[V_0, L_d] = -(L_d V_0) = -\sum_j L_j(\partial_j V_0), \tag{7}$$

we see that the second order derivatives in Eq. (4) come, together with some first order derivatives, only from $[\nabla^2, L_d]$. Therefore by setting their coefficients to zero we obtain two sets of consistency equations,

$$\partial_j L_j = 0, \quad j = 1, \ldots, n; \quad \partial_j L_k + \partial_k L_j = 0, \quad j < k = 2, \ldots, n. \tag{8}$$

The first set gives $L_j = a_j + f_j(x)$, where a_j's are constants and $f_j(x)$ depends on all of x_k's except x_j. The second set determines f_j as $f_j = \Sigma_k c_{jk} x_k$, where c_{jk}'s are all constants and antisymmetric in j and k: $c_{jk} + c_{kj} = 0$. Hence,

$$L_j = a_j + \sum_k c_{jk} x_k. \tag{9}$$

These solutions make the first order derivative terms at the right-hand side of (5) vanish so that $[\nabla^2, L_d] = 0$. As a result of this the intertwining relation (4) simplifies to

$$[\nabla^2, L_0] = [V_0, L_d] + P(L_0 + L_d). \tag{10}$$

From (6), (7), and (10) we get, by equating the coefficients of the first and zeroth powers of derivatives,

$$2\partial_j L_0 = P L_j; \quad j = 1,2,\ldots,n, \tag{11}$$

$$(-\nabla^2 + P)L_0 = (L_d V_0). \tag{12}$$

These $n+1$ equations constitute a reduced form of the consistency conditions for three unknown functions L_0, V_0, and V_1. While Eq. (12) is nonlinear, Eqs. (11) are linear since all components of L_d have been found.

Equation (12) can be considered in the following way. By virtue of

$$\partial_j L_k = c_{kj}, \tag{13}$$

Eqs. (11) imply that

$$\nabla^2 L_0 = \tfrac{1}{2}(L_d P). \tag{14}$$

Combining this with (12) we arrive at

$$L_0 P = \tfrac{1}{2} L_d (V_1 + V_0), \tag{15}$$

which can be used instead of Eq. (12).

By defining

$$T_j = \partial_j, \quad L_{jk} = x_k \partial_j - x_j \partial_k, \tag{16}$$

and using (9), L_d can be written as

$$L_d = \sum_j a_j T_j + \sum_{j<k} c_{jk} L_{jk}. \tag{17}$$

The generators T_j's and L_{jk}'s obey the following commutation relations:

$$[T_j, T_k] = 0,$$

$$[T_j, L_{km}] = \delta_{jm} T_k - \delta_{jk} T_m, \tag{18}$$

$$[L_{jk}, L_{lm}] = \delta_{jm} L_{lk} - \delta_{jl} L_{mk} + \delta_{kl} L_{mj} - \delta_{km} L_{lj}.$$

These are the defining relations of $n(n+1)/2$ dimensional Euclidean algebra $e(n)$, also known as the algebra of rigid motion denoted by iso(n).[14,20] n translational generators T_j's form the invariant Abelian subalgebra $t(n)$ and $n(n-1)/2$ rotational generators L_{jk}'s form the semisimple subalgebra so(n). As is well known $e(n)$ is semidirect sum of $t(n)$ and so(n) and $\Sigma T_j^2 = \nabla^2$ is a Casimir operator of $e(n)$.

Now, we shall show that the above analysis includes and naturally generalizes the well known 1D case. It is evident that for $n=1$ we have $\mathcal{L} = L_0 + \partial_x$ and $P = 2L_0'(x)$, where we take $x \equiv x_1, a_1 = 1$ and we use the prime(s) to denote differentiation(s) with respect to the argument (when there is no risk of confusion the argument will be suppressed). In that case Eq. (15) yields $\partial_x(V_0 + L_0' - L_0^2) = 0$ from which we recover the well-known forms of the 1D partner potentials:

$$V_0 = L_0^2 - L_0' + b, \quad V_1 = L_0^2 + L_0' + b. \tag{19}$$

It is a standard procedure of 1D SUSY quantum mechanics to take the constant b and L_0 as $b = \lambda_1$ and $L_0(x) = -\partial_x[\ln \phi_1(x)]$. When these are substituted into the first equation of (19) we obtain $-\phi_1''(x) + V_0 \phi_1(x) = \lambda_1 \phi_1(x)$, that is, $\phi_1(x)$ is the eigenfunction of the Schrödinger's equation $-\phi''(x) + V_0 \phi(x) = \lambda \phi(x)$ corresponding to the eigenvalue $\lambda = \lambda_1$. Therefore the Schrödinger's equation remains covariant under the Darboux's transformations,

$$(\phi, V_0) \to (L\phi = \phi' - [\ln \phi_1]' \phi, \quad V_1 = V_0 - 2[\ln \phi_1]''). \tag{20}$$

Obviously, instead of ϕ_1, any other fixed eigenfunction can be used to generate a transformation to another new potential V_1. It is this fact which allows us to apply the Darboux's transformations successively and to construct a hierarchy of potentials for a given V_0.

We conclude this section by saying that for $n \geqslant 1$ the differential part of the intertwining operator is a series in generators of $e(n)$. In saying that we have identified the algebra generated by ∂_x with $e(1)$. A related result is that intertwined potentials have symmetry generators differential part of which are quadratic in the generator of $e(n)$, that is, they belong to universal enveloping algebra of $e(n)$. From now on we assume that a_j's and c_{jk}'s are real constants.

III. APPLICATIONS

Before proceeding further we consider some particular cases of Eqs. (11) and (12).

When $P=0$, Eqs. (11) and (15) give $L_0=$constant and $(L_d V_0)=0$. In view of Eq. (1) these imply, as an expected result, that $\mathcal{L}$ is a symmetry generator of $H_0=H_1$:$[H_0,\mathcal{L}]=0$.

Next we take P to be a constant such that $P=p_0\neq 0$. In that case the integrability conditions $\partial_j\partial_k L_0=\partial_k\partial_j L_0$ of Eqs. (11) require that $c_{jk}=0$ for all j,k which lead to $2L_0=p_0\mathbf{a}\cdot\mathbf{r}+2b$, where $\mathbf{r}=(x_1,\ldots,x_n)$ is the position vector and $\mathbf{a}$ represents the constant vector $\mathbf{a}=(a_1,\ldots,a_n)$. Taking the constant b as $b=\mathbf{a}\cdot\mathbf{b}$ we get from (15),

$$\mathbf{a}\cdot(p_0^2\mathbf{r}+2p_0\mathbf{b}-2\nabla V_0)=0,$$

which is solved by

$$V_0=\tfrac{1}{4}p_0^2r^2+p_0\mathbf{b}\cdot\mathbf{r}+g(x), \tag{21}$$

where $\mathbf{b}$ is a constant vector, $r^2=\Sigma_j x_j^2$, and $g(x)\equiv g(x_1,\ldots,x_n)$ is any differentiable function subjected to the constraint $\mathbf{a}\cdot\nabla g(x)=0$. One may take

$$g(x)=g(\mathbf{b}_{(1)}\cdot\mathbf{r},\ldots,\mathbf{b}_{(n-1)}\cdot\mathbf{r}), \tag{22}$$

such that $\mathbf{b}_{(j)}$'s are linearly independent vectors perpendicular to $\mathbf{a}$. Different choices of g define different systems which accept

$$\mathcal{L}^\dagger\mathcal{L}=-(\mathbf{a}\cdot\nabla)^2+[\mathbf{a}\cdot(\tfrac{1}{2}p_0\mathbf{r}+\mathbf{b})]^2-\tfrac{1}{2}p_0a^2, \tag{23}$$

as a common symmetry generator. Accordingly,

$$\mathcal{L}\mathcal{L}^\dagger=-(\mathbf{a}\cdot\nabla)^2+[\mathbf{a}\cdot(\tfrac{1}{2}p_0\mathbf{r}+\mathbf{b})]^2+\tfrac{1}{2}p_0a^2, \tag{24}$$

is a common symmetry generator for $V_1=V_0+p_0$. These also imply that $\mathcal{L}/a$ and $\mathcal{L}^\dagger/a$ are a pair of ladder operators for H_0,

$$[H_0,\mathcal{L}]=-p_0\mathcal{L},\quad [H_0,\mathcal{L}^\dagger]=p_0\mathcal{L}^\dagger,\quad [\mathcal{L},\mathcal{L}^\dagger]=p_0a^2.$$

As a result of these we recover the existence of harmonic oscillator like spectrum in the spectrum of a class of nD systems described by H_0 which contains many parameters and an arbitrary function.

Now we set all of c_{jk}'s to zero. From (11) and (15) we get $L_0=f(\zeta)$ and $P=f'(\zeta)$ where f is an arbitrary differentiable function of $\zeta=\mathbf{a}\cdot\mathbf{r}/2$. Defining

$$V_\pm=\frac{1}{a^2}f^2(\zeta)\pm\frac{1}{2}f'(\zeta), \tag{25}$$

we obtain, by virtue of (11) and (15),

$$V_0=\tfrac{1}{2}g(x)+V_-;\quad V_1=\tfrac{1}{2}g(x)+V_+, \tag{26}$$

where $g(x)$ may be taken as in (22). Observing that $V_\pm$ are form equivalent to (19) we can say that all the known techniques of 1D SUSY quantum mechanics can equally well be used in this case. For this application the intertwining operator is $\mathcal{L}=f(\zeta)+\mathbf{a}\cdot\nabla$ and the symmetry generators are

$$\mathcal{L}\mathcal{L}^\dagger=a^2V_+-(\mathbf{a}\cdot\nabla)^2,\quad \mathcal{L}^\dagger\mathcal{L}=a^2V_--(\mathbf{a}\cdot\nabla)^2. \tag{27}$$

IV. INTEGRABILITY CONDITIONS

In this section we concentrate on the integrability conditions of n linear equations given by (11). It turns out that once these conditions are well understood all the consistency equations can be tackled more easily.

By considering L_0 as the $(n+1)$th coordinate $x_{n+1}\equiv L_0$ of R^{n+1} and P as a function defined on it we introduce the 1-form,

$$\Omega = dL_0 - \tfrac{1}{2} P\Gamma, \tag{28}$$

on R^{n+1}. Here d stands for the exterior derivative and Γ denotes the 1-form,

$$\Gamma = \sum_{j=1}^{n} L_j dx_j, \tag{29}$$

on R^n. Now n linear equations given by (11) can be expressed as a single Pfaffian equation $\Omega = 0$. In the Frobenius theory, integrability of this Pfaffian equation amounts to being able to find a positive valued integrating factor f and a function g such that $\Omega = f dg$.[19] If this is possible, then $\Omega = 0$ and $dg = 0$ are equivalent Pfaffian equations and the solution (integral surface) of $\Omega = 0$ is the hypersurface $g =$ constant. According to the Frobenius theorem a necessary and sufficient condition for the existence of functions g and f is the fulfillment of the so-called Frobenius condition,

$$\Omega \wedge d\Omega = 0, \tag{30}$$

where $\wedge$ denotes the usual exterior product.

From (28) and (29) we have

$$d\Omega = -\frac{1}{2}\left[(\partial_{n+1} P) dL_0 \wedge d(P\Gamma) + \sum_{j=1}^{n} (\partial_j P) dx_j \wedge \Gamma + P d\Gamma \right],$$

and therefore

$$\Omega \wedge d\Omega = -\tfrac{1}{2}[dL_0 \wedge d(P\Gamma) - \tfrac{1}{2} P^2 \Gamma \wedge d\Gamma], \tag{31}$$

where d in $d(P\Gamma)$ and $d\Gamma$ stands for the exterior derivative of R^n. The Frobenius conditions (30) is therefore equivalent to the following two conditions:

$$d(P\Gamma) = 0, \tag{32}$$

$$\Gamma \wedge d\Gamma = 0, \tag{33}$$

provided that $P \neq 0$. Since both of these conditions are valid in R^n, P is defined on R^n.

The condition (32) gives $n(n-1)/2$ equations,

$$K_{jk} P = -2 c_{jk} P, \tag{34}$$

where

$$K_{jk} = L_j \partial_k - L_k \partial_j. \tag{35}$$

Observe that Eq. (34) can also be obtained from $\partial_j \partial_k L_0 = \partial_k \partial_j L_0$ and in deriving it we have used Eq. (13). The condition (33) could also be inferred from Eq. (32) upon exterior multiplication of $dP \wedge \Gamma + P d\Gamma = 0$ by Γ. It leads to $n(n-1)(n-2)/6$ equations,

$$L_{[j} c_{kl]} = 0, \tag{36}$$

where $j<k<l\leqslant n$ and the square bracket [ ] enclosing the subindexes means antisymmetrization. Equation (36) shows that any three of L_j's are linearly dependent, that is

$$L_j c_{kl}+L_k c_{lj}+L_l c_{jk}=0. \tag{37}$$

Making use of (9) this can be written as

$$a_{[j}c_{kl]}=\sum_m x_m c_{m[j}c_{kl]}. \tag{38}$$

This gives nothing in the case of $n=2$ because $\Gamma\wedge d\Gamma$ is a 3-form and therefore identically vanishes on R^2.

By a simple reasoning making use of the antisymmetry of c_{jk}'s we see that for $n=3$ the right-hand side of Eq. (38) vanishes identically and a single condition

$$\mathbf{L}\cdot\mathbf{c}=\mathbf{a}\cdot\mathbf{c}=0 \tag{39}$$

results. Here we have made use of the fact that in the case of $n=3$ we have

$$\mathbf{L}=\mathbf{a}+\mathbf{r}\times\mathbf{c}, \tag{40}$$

where $\mathbf{c}=(c_1,c_2,c_3)=(c_{23},c_{31},c_{12})$ and "$\times$" stands for the usual cross product of R^3. For $n\geqslant 4$ more care is needed. It is not hard to check that $c_{m[m}c_{kl]}=0$ for any n and hence for $n=4$ the terms $c_{1[j}c_{kl]},\ldots,c_{4[j}c_{kl]}$are equal to each other up to a sign "$-$". These imply that in the case of $n=4$, Eq. (38) restricts all the coordinates to some constant values. But, as is evident from Eq. (38), at the expense of constraining the form of L we can get rid of all these coordinate restrictions by imposing the conditions,

$$a_{[j}c_{kl]}=0; \quad j<k<l, \tag{41}$$

$$c_{m[j}c_{kl]}=0; \quad m=1,\ldots,n. \tag{42}$$

As is mentioned above in the case of $n=4$, Eqs. (42) give only one condition

$$c_{12}c_{34}+c_{13}c_{42}+c_{14}c_{23}=0,$$

and Eqs. (41) give conditions which reduce the total number of parameters. To see this more concretely we define the following four vectors:

$$\mathbf{c}_{(1)}=(0,c_{34},-c_{24},c_{23}), \quad \mathbf{c}_{(2)}=(c_{34},0,c_{41},-c_{31}),$$

$$\mathbf{c}_{(3)}=(c_{24},c_{41},0,c_{12}), \quad \mathbf{c}_{(4)}=(c_{23},c_{31},c_{12},0).$$

Now Eqs. (41) can be rewritten as $\mathbf{a}\cdot\mathbf{c}_{(j)}=0, j=1,2,3,4$. It is easy to check that, in view of Eq. (42), the determinant of the matrix formed by the components of the vectors $\mathbf{c}_{(j)}$'s has rank two. Therefore Eqs. (41) provide two of a_j's as free parameters, or, for a given $\mathbf{a}$ two constraints for c_{jk}'s. By taking into account also (42) we get seven free parameters: five c_{jk}'s and two a_j's, or, three c_{jk}'s and four a_j's. These can be chosen in many different ways. Moreover, one can also choose a lesser number of parameters without destroying the integrability conditions.

For the number of conditions implied by (41)–(42) exceeds the number of parameters the investigation is getting harder and harder for $n\geqslant 5$. But, in the case of $n=5$ one can keep again 5 of c_{jk}'s as free parameters by setting all a_j's to zero. In that case Eqs. (41) disappear and Eqs. (42) give 5 constraints which reduce the number of c_{jk}'s from 10 to 5. Note also that, as has been done in Sec. III, for $n\geqslant 2$ one can always set all c_{jk}'s to zero and keep n a_j's as parameters. In such a case condition (36) completely disappears.

TABLE I. In 3-dimension the special choices of parameters and corresponding coordinates. Note that in each case further choices are possible. For example, in the first three cases c_j which does not appear in the first column can be set to zero and instead of η, one can also use η_2, or η_3. As a completely different case in which all c_{jk}'s are zero has been presented in Sec. III for any $n>1$.

	β	$2\gamma=a^2-L^2$	η	$p(\eta)$
$a_1=0;a_2c_2+a_3c_3=0$	$\mathbf{r}\cdot\mathbf{c}$	$2\mathbf{r}\cdot(\mathbf{a}\times\mathbf{c})+(\mathbf{r}\cdot\mathbf{c})^2-c^2r^2$	$\frac{c_3y-c_2z}{a_2-c_3x+c_1z}$	$p(\eta)$
$a_2=0;a_1c_1+a_3c_3=0$	$\mathbf{r}\cdot\mathbf{c}$	$2\mathbf{r}\cdot(\mathbf{a}\times\mathbf{c})+(\mathbf{r}\cdot\mathbf{c})^2-c^2r^2$	$\frac{a_1+c_3y-c_2z}{-c_3x+c_1z}$	$p(\eta)$
$a_3=0;a_1c_1+a_2c_2=0$	$\mathbf{r}\cdot\mathbf{c}$	$2\mathbf{r}\cdot(\mathbf{a}\times\mathbf{c})+(\mathbf{r}\cdot\mathbf{c})^2-c^2r^2$	$\frac{a_1+c_3y-c_2z}{a_2-c_3x+c_1z}$	$p(\eta)$
$a_1=0=a_2;c_3=0$	c_1x+c_2y	$2a_3(c_1y-c_2x)+(c_1x+c_2y)^2-(c_1^2+c_2^2)r^2$	$\frac{-c_2z}{a_3+c_2x-c_1y}$	$p_2(\eta_2)$
$a_1=0=a_3;c_2=0$	c_1x+c_3z	$2a_2(c_3x-c_1z)+(c_1x+c_3z)^2-(c_1^2+c_3^2)r^2$	$\frac{c_3y}{a_2-c_3x+c_1z}$	$p(\eta)$
$a_2=0=a_3;c_1=0$	c_2y+c_3z	$2a_1(c_2z-c_3y)+(c_2y+c_3z)^2-(c_2^2+c_3^2)r^2$	$\frac{a_1+c_3y-c_2z}{-c_3x}$	$p(\eta)$
$a_1=0;c_2=0=c_3$	c_1x	$2c_1(a_2y-a_3z)-c_1^2(y^2+z^2)$	$\frac{a_2+c_1z}{a_3-c_1y}$	$p_3(\eta_3)$
$a_2=0;c_1=0=c_3$	c_2y	$2c_2(-a_3x+a_1z)-c_2^2(x^2+z^2)$	$\frac{a_1-c_2z}{a_3+c_2x}$	$p_2(\eta_2)$
$a_3=0;c_1=0=c_2$	c_3z	$2c_3(a_2x-a_1y)-c_3^2(x^2+y^2)$	$\frac{a_1+c_3y}{a_2-c_3x}$	$p(\eta)$
$a_1=a_2=a_3=0$	$\mathbf{r}\cdot\mathbf{c}$	$(\mathbf{r}\cdot\mathbf{c})^2-c^2r^2$	$\frac{c_3y-c_2z}{-c_3x+c_1z}$	$p(\eta)$

These remarks imply an important property of the intertwining method in higher dimensions; due to integrability conditions there are a number of choices in specifying $\mathcal{L}$. Evidently this fact enriches the set of intertwined potentials (see Table I in the case of $n=3$). In the next section by taking $c_{jk}\neq 0$ for at least a pair of j,k, we carry out an investigation which will enable us to find out the general forms of a class of potentials for $n=2,3,4,5$ endowed with mentioned richness for $n\geqslant 3$.

V. GENERAL FORM OF POTENTIALS

By making use of Eqs. (13), (35), and (37) one can easily verify the following relations:

$$\partial_m\left(\frac{L_i}{L_j}\right)=\frac{c_{ij}}{L_j^2}L_m, \tag{43}$$

$$K_{mn}\left(\frac{L_i}{L_j}\right)=0, \tag{44}$$

$$K_{mn}\left(\frac{1}{L_j^k}\right)=-k\frac{c_{mn}}{L_j^k}, \tag{45}$$

$$\mathbf{L}\cdot\nabla\left(\frac{L_i}{L_j}\right)=c_{ij}\frac{L^2}{L_j^2}, \tag{46}$$

$$\mathbf{L}\cdot\nabla g(L^2)=\left(2\sum_{ij} L_iL_jc_{ij}\right)g'(L^2)=0. \tag{47}$$

In Eq. (47), g is an arbitrary function of $L^2=\Sigma_jL_j^2$. Comparing Eqs. (43) and (11) we see that the general form of L_0 is

$$L_0=f\left(\frac{L_i}{L_j}\right), \tag{48}$$

provided that $c_{ij}\neq 0$. Then from any of Eqs. (11), P is found to be

$$P=\frac{2c_{ij}}{L_j^2}f'(\eta), \tag{49}$$

where $\eta=L_i/L_j$. Fortunately, Eqs. (44) and (45) imply that solution (49) respects all the integrability conditions given by (34).

The only equation that remained unsolved is Eq. (15) which is now as follows:

$$\mathbf{L}\cdot\nabla(V_1+V_0)=\frac{2c_{ij}}{L_j^2}\partial_\eta[f^2(\eta)]. \tag{50}$$

From (46) and (47) it is evident that the general solution of this equation is of the form,

$$V_1+V_0=h+2\frac{f^2(\eta)}{L^2}, \tag{51}$$

where $2f^2(\eta)/L^2$ accounts for the right-hand side of (50) and h is the general solution of the homogeneous equation,

$$\mathbf{L}\cdot\nabla h=0. \tag{52}$$

Hence, the general forms of V_0 and V_1 are, by combining (49) and (51),

$$V_0=\frac{1}{2}h+\frac{V_-}{L^2}, \tag{53}$$

$$V_1=\frac{1}{2}h+\frac{V_+}{L^2}, \tag{54}$$

where

$$V_\pm=f^2(\eta)\pm c_{ij}\frac{L^2}{L_j^2}f'(\eta). \tag{55}$$

As a result, the number of consistency equations has been reduced from $(n+1)(n+2)/2$ [the sum of the number of Eqs. (8), (11), and (12)] to 1, i.e., to Eq. (52). Geometrically, Eq. (52) means that at each point of the surface $h=$constant, $\mathbf{L}$ always lies on the local tangent space. Equivalently, $\mathbf{L}$ is always perpendicular to the (classical) force field determined by ∇h. On the other

hand, from group theoretical point of view Eq. (52) means that the common part of the intertwined potentials is invariant under the action of the Euclidean group $E(n)$, i.e., $e^{L_d}h=h$. For all these statements and the integrability conditions are dimension-dependent h must be determined in each case separately. The rest of the paper is devoted to a detailed investigation of $n=2$ and $n=3$ cases.

As our investigation for an arbitrary dimension is completed two remarks are in order. (i) The above analysis enables us to write down a class of nD isospectral potentials provided that at least one of c_{jk}'s is different from zero. For instance, if only $c_{jk}\neq 0$, then Eq. (37) implies that $L_m=0$ for $m\neq j,k$ and Eqs. (11) require L_0 to depend only on x_j and x_k. In such a case, after defining $\eta=L_j/L_k$ it remains to solve Eq. (52) to find suitable $n-1$ coordinate functions. (ii) When the number of nonzero c_{jk}'s is greater than one there are a number of choices [at most $n(n-1)/2$] for η. But, from Eq. (37) we see that these are all functionally dependent to each other. For example, in the case of $n=3$ we have three choices $\eta=L_1/L_2, \eta_2=L_1/L_3, \eta_3=L_2/L_3$ which obey the following relations:

$$\eta_3=\eta_2/\eta, \quad \eta_2 c_{23}+\eta_3 c_{31}=-c_{12}.$$

Instead of η_i one may choose one of the variables $\alpha_i=L_i/\mathbf{r}\cdot\mathbf{L}=L_i/\mathbf{r}\cdot\mathbf{a}$, or for $n=3,\sigma_i=L_i/(\mathbf{c}\times\mathbf{L})_i$. It is easy to verify that each of these satisfies relations similar to Eqs. (43)–(44) and (46) and enables us to express $L_0,P,V_\pm$ in terms of them. This freedom in the choice of coordinates once again manifests the largeness of the set of intertwined potentials. But, we should emphasize that these are all functionally dependent since the differential of any variable obeying (43) is proportional to $\Gamma=\mathbf{L}\cdot d\mathbf{r}$ and therefore $d\eta_i\wedge d\alpha_i=0$, etc. This also proves that as long as first order intertwining is concerned $V_\pm$ depend only on one variable.

VI. 2D ISOSPECTRAL POTENTIALS

In two dimensions we have $L_1=(a_1+cy)$ and $L_2=(a_2-cx)$, where $c=c_{12},x=x_1,y=x_2$. From Eq. (47) we see that, in terms of

$$\kappa=[L_1^2+L_2^2]^{1/2}=[(a_1+cy)^2+(a_2-cx)^2]^{1/2}, \tag{56}$$

the general solution of Eq. (52) is $h=h(\kappa)$, where h is an arbitrary differentiable function. Taking $\eta=L_1/L_2$ and noting that $L^2/L_2^2=1+\eta^2$, by Eqs. (53)–(55) the general forms of the 2D isospectral potentials are found to be

$$V_0=\frac{1}{2}h(\kappa)+\frac{V_-}{\kappa^2}, \quad V_1=\frac{1}{2}h(\kappa)+\frac{V_+}{\kappa^2}, \tag{57}$$

where

$$V_\pm=f^2(\eta)\pm c(1+\eta^2)f'(\eta). \tag{58}$$

In that case the intertwining operator is

$$\mathcal{L}=f(\eta)+(a_1+cy)\partial_x+(a_2-cx)\partial_y=f(\eta)+c(1+\eta^2)\partial_\eta. \tag{59}$$

As is well known, for a 2D stationary system the existence of a symmetry generator means that the system is completely integrable in the Liouville sense. Recalling that $\mathcal{L}^\dagger\mathcal{L}$ and $\mathcal{L}\mathcal{L}^\dagger$ are symmetry generators of H_0 and H_1, the potentials given by (57) are the most general forms of 2D integrable potentials which can be intertwined by a first order operator.

We shall now present some examples in which for some simple forms of V_- we consider the Riccati's equation (58) for dependent variable f and by solving it we construct the corresponding

potentials. As the simplest case we take $V_0=0$. This may happen in two different cases: (i) $h=0, V_-=0$, and (ii) $h=-2b/\kappa^2, V_-=b$, where b is a constant. In these cases (58) is a separable equation of the form,

$$f^2-c(1+\eta^2)f'=b, \tag{60}$$

which has the general solution,

$$f=(-b)^{1/2}\tan\left[\frac{(-b)^{1/2}}{c}(\tan^{-1}\eta-b_1)\right] \tag{61}$$

for $b<0$. This should be read as $f=b^{1/2}\tanh[(b^{1/2}/c)(b_1-\tan^{-1}\eta)]$ for $b>0$ and as $f=c(b_1-\tan^{-1}\eta)^{-1}$ for $b=0$, where b_1 is an integration constant. From (58) we have

$$V_1=2c^2[\kappa(b_1-\tan^{-1}\eta)]^{-2}, \tag{62}$$

for the case (i) and

$$V_1=-2b\left\{\kappa\cos\left[\frac{(-b)^{1/2}}{c}(\tan^{-1}\eta-b_1)\right]\right\}^{-2};$$

$$V_1=-2b\left\{\kappa\cosh\left[\frac{b^{1/2}}{c}(\tan^{-1}\eta-b_1)\right]\right\}^{-2}, \tag{63}$$

for the case (ii) corresponding to $b<0$ and $b>0$, respectively. As a result we have found a two parameter family of 2D potentials that are intertwined to 2D free motion. Note that for $b=-c^2, b_1=0$ we have $f=c\eta$ and

$$V_1=2c^2\frac{\eta^2+1}{\kappa^2}=\frac{2c^2}{(a_2-cx)^2}. \tag{64}$$

As another example, taking $V_-=b=-c^2$ and $h=(2c^2/\kappa^2)+2g(\kappa)$ in (57) leads us to the partner potentials,

$$V_0=g(\kappa), \quad V_1=g(\kappa)+2c^2\frac{1+\eta^2}{\kappa^2} \tag{65}$$

for $f=c\eta$. In particular, for $g(\kappa)=\kappa^2$, H_0 represents a 2D isotropic displaced harmonic oscillator and H_1 a 2D Calogero's type system for which

$$V_1=\frac{2c^2}{(a_2-cx)^2}+(a_2-cx)^2+(a_1+cy)^2. \tag{66}$$

In that case for any choice of $g(\kappa)$ we have $\mathcal{L}=c[\eta+(\eta^2+1)\partial_\eta]$. This explicitly shows that two different families of potentials, such as that given by (65) can be intertwined by the same $\mathcal{L}$. This is an important property that we do not have in one dimension. It is evident that this arises from the separability of the problem that we shall analyze in the next section. It is also worth mentioning that after a simple affine transformation of the coordinates and a restriction on c^2 one can easily recognize (66) as one of the four superintegrable the Smorodinsky–Winternitz 2D potentials.[21] The above particular example shows that this potential is intertwined to the harmonic oscillator and one of its symmetry generators is immediately obtained as $\mathcal{L}\mathcal{L}^\dagger$.

VII. SEPARATION OF VARIABLES AND HIERARCHY OF 2D POTENTIALS

The above analysis suggests the variables (κ,η) as a new coordinate system. This is a kind of the orthogonal polar coordinate system with displaced center in which we have

$$\nabla^2=\frac{c^2}{\kappa^2}\{\kappa\partial_\kappa(\kappa\partial_\kappa)+(1+\eta^2)\partial_\eta[(1+\eta^2)\partial_\eta]\}. \tag{67}$$

This implies that the eigenvalue equations of H_i accept the separation of variables in terms of (κ,η). In fact, this can be carried out in an easier way by introducing the coordinates

$$\rho=\frac{1}{c}\ln\kappa, \quad \xi=\frac{1}{c}\tan^{-1}\eta. \tag{68}$$

From (59) and (67) we get

$$\mathcal{L}=f(\xi)+\partial_\xi, \tag{69}$$

and $\nabla^2=e^{-2c\rho}(\partial_\rho^2+\partial_\xi^2)$. By defining

$$H_\rho=-\partial_\rho^2+\tfrac{1}{2}e^{2c\rho}h(\rho), \quad H_\pm=-\partial_\xi^2+V_\pm(\xi),$$

and

$$V_\pm=f^2(\xi)\pm f'(\xi), \tag{70}$$

the Hamiltonians can be written as

$$H_0=e^{-2c\rho}(H_\rho+H_-), \quad H_1=e^{-2c\rho}(H_\rho+H_+). \tag{71}$$

If we take $\psi^0(\rho,\xi)=R(\rho)U^0(\xi)$ the eigenvalue equation $H_0\psi^0(\rho,\xi)=E^0\psi^0(\rho,\xi)$ separates as follows:

$$H_-U^0(\xi)=MU^0(\xi), \tag{72}$$

$$(H_\rho-E^0e^{2c\rho})R(\rho)=-MR(\rho), \tag{73}$$

where M is the separation constant. For given E^0 ρ-equation for H_1 is the same as Eq. (73), but ξ-equation is $H_-U^1(\xi)=MU^1(\xi)$. $\mathcal{L}$ given by (69) intertwines only solutions of H_- to that of H_+ by $U^1(\xi)=\mathcal{L}U^0(\xi)$.

We shall now briefly describe how to generate a hierarchy of 2D isospectral potentials.

Taking $f(\xi)=-\phi'(\xi)/\phi(\xi)$ in Eq. (70) yields $V_-(\xi)=\phi''(\xi)/\phi(\xi)$. This is the same as Eq. (72) for $M=0$. Therefore, each solution of (72) with $M=0$ can be used to generate a transformation to a new problem with potential V_1. In fact, by keeping analogy with 1D SUSY methods we can do more than that. For this purpose let us take

$$V_-(\xi)=\mathcal{V}(\xi)-\mathcal{E}_n, \quad f(\xi)=-\frac{\phi_n'(\xi)}{\phi_n(\xi)}, \tag{74}$$

in Eq. (70) and suppose that the resulting stationary Schrödinger's equation,

$$[-\partial_\xi^2+\mathcal{V}(\xi)]\phi_n(\xi)=\mathcal{E}_n\phi_n(\xi) \tag{75}$$

is exactly solvable, where n is a quantum number labeling the eigenvalues and eigenfunctions. If together with (74) we take

$$h(\rho)=2e^{-2c\rho}[\mathcal{H}(\rho)+\mathcal{E}_n], \tag{76}$$

then from Eq. (57) V_i are found to be

$$V_0=e^{-2c\rho}[\mathcal{V}(\xi)+\mathcal{H}(\rho)],$$

$$V_1=e^{-2c\rho}\left[2\left(\frac{\phi_n'(\xi)}{\phi_n(\xi)}\right)^2+2\mathcal{E}_n-\mathcal{V}(\xi)+\mathcal{H}(\rho)\right].$$

In that case the separated equations of H_0 are

$$[-\partial_\xi^2+\mathcal{V}(\xi)]U_n^0(\xi)=(\mathcal{E}_n+M)U_n^0(\xi), \tag{77}$$

$$[-\partial_\rho^2+\mathcal{H}(\rho)-e^{2c\rho}E^0]R_n(\rho)=-(\mathcal{E}_n+M)R_n(\rho). \tag{78}$$

Let us choose M such that

$$\mathcal{E}_{n_\pm}=\mathcal{E}_n\pm M. \tag{79}$$

This amounts to the fact that ξ-equation of H_0 is the same as Eq. (75). Therefore, $U_n^0(\xi)=\phi_{n_+}(\xi)$ and $E^0,R_n(\rho)$ must be labeled by n_+. Accordingly Eq. (78) must be rewritten as

$$[-\partial_\rho^2+\mathcal{H}(\rho)-e^{2c\rho}E_{n_+}^0]R_{n_+}(\rho)=-\mathcal{E}_{n_+}R_{n_+}(\rho). \tag{80}$$

The eigenvalue equation of H_1 corresponding to the same $E_{n_+}^0$ can be separated such that the ρ-equation is the same as Eq. (80) and ξ-equation reads

$$\left[-\partial_\xi^2+2\left(\frac{\phi_n'(\xi)}{\phi_n(\xi)}\right)^2-\mathcal{V}(\xi)\right]U_{n_+}^1(\xi)=-\mathcal{E}_{n_-}U_{n_+}^1(\xi), \tag{81}$$

where

$$U_{n_+}^1(\xi)=\mathcal{L}U_{n_+}^0(\xi)=\left[-\frac{\phi_n'(\xi)}{\phi_n(\xi)}+\partial_\xi\right]\phi_{n_+}(\xi). \tag{82}$$

The function $\phi_n(\xi)$ that generates the transformation is annihilated by the action of $\mathcal{L}$, i.e., $\mathcal{L}\phi_n(\xi)=\{[\phi_n'(\xi)/\phi_n(\xi)]-\partial_\xi\}\phi_n(\xi)=0$. Hence, in the case of $M=0$ the function $U_n^1(\xi)$ corresponding to $\phi_n(\xi)$ can not be found in this way. But, by referring to a well-known theorem of the theory of ordinary differential equations U_n^1 can be constructed. This theorem says that if $y_0(x)$ is a particular nontrivial solution of the equation $a_0(x)y''+a_1(x)y'+a_2(x)y=0$, then the second solution y_1 linearly independent from y_0 is given by

$$y_1=y_0\int\frac{\exp[-\int(a_1(x)/a_0(x))\,dx]}{y_0^2}dx. \tag{83}$$

Adopting this theorem to Eq. (75), where $a_0=-1$ and $a_1=0$ the second solution linearly independent from $\phi_n(\xi)$ is found to be $Y(\xi)=\phi_n(\xi)\int d\xi/\phi_n^2(\xi)$. $\mathcal{L}$ generated by $\phi_n(\xi)$ applied to $Y(\xi)$ gives $Y_0(\xi)=\mathcal{L}Y(\xi)=-1/\phi_n(\xi)$. Inserting this (as y_0) into (83) yields the desired eigenfunction corresponding to $\phi_n(\xi)$,

$$U_n^1(\xi)=-\frac{1}{\phi_n(\xi)}\int\phi_n^2(\xi)d\xi.$$

As a result, changing the eigenfunction of Eq. (75) used to generate the transformation will lead us to a new eigenvalue problem given by Eq. (81). In that way a hierarchy of 2D isospectral potentials can be constructed.

VIII. 3D ISOSPECTRAL POTENTIALS

In order to find the general solution of Eq. (52) for $n=3$ we first recall the integrability condition (39) and the relation (40). Secondly we observe that the set $\{\mathbf{L},\mathbf{c},\mathbf{L}\times\mathbf{c}\}$ forms a right-handed (unnormalized) orthogonal moving frame which "moves" about fixed direction of $\mathbf{c}=(c_1,c_2,c_3)=(c_{23},c_{31},c_{12})$. By using $x=x_1, y=x_2, z=x_3$ we now introduce the variables,

$$\beta=\mathbf{r}\cdot\mathbf{c},$$

$$\gamma=\tfrac{1}{2}\mathbf{r}\cdot[(\mathbf{a}+\mathbf{L})\times\mathbf{c}]=\mathbf{r}\cdot(\mathbf{a}\times\mathbf{c})+\tfrac{1}{2}[(\mathbf{r}\cdot\mathbf{c})^2-c^2r^2], \tag{84}$$

$$\eta=\frac{L_1}{L_2}=\frac{a_1+c_3y-c_2z}{a_2-c_3x+c_1z}.$$

These obey the following relations:

$$(\mathbf{L}\cdot\nabla)\beta=\mathbf{L}\cdot\mathbf{c}=0, \tag{85}$$

$$(\mathbf{L}\cdot\nabla)\gamma=\mathbf{L}\cdot(\mathbf{L}\times\mathbf{c})=0, \tag{86}$$

$$(\mathbf{L}\cdot\nabla)\eta=p(\eta), \tag{87}$$

where $p(\eta)$ is a quadratic polynomial in η,

$$p(\eta)=c_3\frac{L^2}{L_2^2}=\frac{1}{c_3}[(c^2-c_2^2)\eta^2+2c_1c_2\eta+(c^2-c_1^2)], \tag{88}$$

and $c^2=c_1^2+c_2^2+c_3^2$. In deriving this we assumed $c_3\neq 0$ and made use of Eq. (37).

It is now easy to see that, in view of (85) and (86), the general solution of (52) is $h=h(\beta,\gamma)$ where $h:R^2\to R$ is an arbitrary differentiable function. On the other hand, from (53)–(55) the general forms of the potentials are

$$V_0=\frac{1}{2}h(\beta,\gamma)+\frac{V_-}{L^2},\quad V_1=\frac{1}{2}h(\beta,\gamma)+\frac{V_+}{L^2}, \tag{89}$$

where

$$V_\pm=f^2(\eta)\pm p(\eta)f'(\eta), \tag{90}$$

$$L^2=a^2-2\gamma. \tag{91}$$

Making use of Eqs. (84)–(87), $\mathcal{L}$ is found to be

$$\mathcal{L}=f(\eta)+(\mathbf{a}+\mathbf{r}\times\mathbf{c})\cdot\nabla=f(\eta)+p(\eta)\partial_\eta.$$

If instead of $\eta=L_1/L_2$ had we taken one of the variables

$$\eta_2=\frac{L_1}{L_3}=\frac{a_1+c_3y-c_2z}{a_3+c_2x-c_1y},\quad \eta_3=\frac{L_2}{L_3}=\frac{a_2-c_3x+c_1z}{a_3+c_2x-c_1y},$$

we would have obtained $(\mathbf{L}\cdot\nabla)\eta_j=p_j(\eta_j), j=2,3$ and $V_\pm=f_j^2(\eta_j)\pm p_j(\eta_j)f_j'(\eta_j)$, where

$$p_2(\eta_2)=-c_2\frac{L^2}{L_3^2}=-\frac{1}{c_2}[(c^2-c_3^2)\eta_2^2+2c_1c_3\eta_2+(c^2-c_1^2)],$$

$$p_3(\eta_3)=c_1\frac{L^2}{L_3^2}=\frac{1}{c_1}[(c^2-c_3^2)\eta_3^2+2c_2c_3\eta_3+(c^2-c_2^2)].$$

Without any change in the β,γ dependence merely $\mathcal{L}$ would have been changed as $\mathcal{L}=f_j(\eta_j)+p_j(\eta_j)\partial_{\eta_j}$.

As an application we again consider the simplest case $V_0=0$. Following an analysis similar to that made in Sec. VI one can easily verify that the following three different potentials:

$$V_1^{(1)}=\frac{2f_1^2}{L^2},$$

$$V_1^{(2)}=\frac{2}{L^2}\left[c^2+\frac{1}{4}p'^2(\eta)\right],$$

$$V_1^{(3)}=\frac{2}{L^2}\left\{c^2+\left[\frac{1}{2}p'(\eta)+\frac{p(\eta)}{b_1-\eta}\right]^2\right\},$$

are intertwined to 3D free motion, respectively, by

$$\mathcal{L}^{(1)}=f_1+p(\eta)\partial\eta,\quad \mathcal{L}^{(2)}=\tfrac{1}{2}p'(\eta)+p(\eta)\partial\eta,$$

$$\mathcal{L}^{(3)}=\left[\frac{1}{2}p'(\eta)+\frac{p(\eta)}{b_1-\eta}\right]+p(\eta)\partial\eta,$$

where $f_1=[b_1-(cc_3^2)^{-1}\tan^{-1}(p'(\eta)/2c)]^{-1}$ and b_1 is an integration constant. More generally, a two parameter family of potentials can be constructed by means of $f=(-b)^{1/2}\tan[(-b)^{1/2}(b_1+\int d\eta/p(\eta))]$.

We shall now show that in terms of (β,γ,η) the eigenvalue equations of H_i's accept separation of variables. Starting with

$$d\beta=\mathbf{c}\cdot d\mathbf{r},\quad d\gamma=(\mathbf{L}\times\mathbf{c})\cdot d\mathbf{r},\quad d\eta=\frac{c_3}{L_2^2}\mathbf{L}\cdot d\mathbf{r}, \tag{92}$$

one can easily write the differentials dx,dy,dz in terms of $d\beta,d\gamma,d\eta$. These are as follows:

$$d\mathbf{r}=\frac{1}{c^2}\mathbf{c}d\beta+\frac{1}{c^2L^2}(\mathbf{L}\times\mathbf{c})d\gamma+\frac{L_2^2}{c_3L^2}\mathbf{L}d\eta. \tag{93}$$

With the help of these relations the volume form $dV=dx\wedge dy\wedge dz$, the metric $ds^2=d\mathbf{r}\cdot d\mathbf{r}$, and ∇^2 are found to be

$$dV=\frac{1}{c^2p(\eta)}d\beta\wedge d\gamma\wedge d\eta, \tag{94}$$

$$ds^2=\frac{1}{c^2}(d\beta)^2+\frac{1}{c^2L^2}(d\gamma)^2+\frac{L_2^4}{c_3^2L^2}(d\eta)^2, \tag{95}$$

$$\nabla^2 = c^2[\partial_\beta^2 + \partial_\gamma(L^2\partial_\gamma)] + \frac{p(\eta)}{L^2}\partial_\eta[p(\eta)\partial_\eta]. \tag{96}$$

From Eq. (94) we infer that the Jacobian determinant of the transformation $(x,y,z)\to(\beta,\gamma,\eta)$ is $1/c^2p(\eta)$. On the other hand, Eq. (95) manifestly shows that the coordinate system (β,γ,η) is orthogonal. In virtue of (96) the eigenvalue equation $H_0\psi^0(\beta,\gamma,\eta)=E^0\psi^0(\beta,\gamma,\eta)$ separates, by taking $\psi^0(\beta,\gamma,\eta)=U^0(\beta,\gamma)R^0(\eta)$, as

$$H_{\beta\gamma}U^0(\beta,\gamma)=MU^0(\beta,\gamma), \quad H_\eta R^0(\eta)=-MR^0(\eta), \tag{97}$$

where M is a separation constant and

$$H_{\beta\gamma}=-c^2L^2[\partial_\beta^2+\partial_\gamma(L^2\partial_\gamma)]+L^2[\tfrac{1}{2}h(\beta,\gamma)-E^0], \tag{98}$$

$$H_\eta=-p(\eta)\partial_\eta[p(\eta)\partial_\eta]+f^2(\eta)-p(\eta)f'(\eta). \tag{99}$$

At this point we will be content with saying that by following the similar steps as for Sec. VII, one can construct a hierarchy of 3D isospectral potentials.

Finally we would like to emphasize that the 3D potentials we have found depend on six parameters such that a large number of potentials can be generated by setting some of them to zero, or, to some particular values. Possible choices of parameters are represented in Table I. The corresponding potentials can be read off from the expressions in the main text.

IX. CONCLUDING REMARKS

The main results of this study can be summarized as follows. We have studied a pair of nD Hamiltonians of potential forms that intertwine by first order operator $\mathcal{L}$ and proved that the differential part of $\mathcal{L}$ is an element of the Euclidean algebra $e(n)$. These imply that so-intertwined systems have symmetry operators whose differential parts belong to the enveloping algebra of $e(n)$. The integrability conditions of consistency equations are dimension dependent and therefore have been considered for each case separately. The general form of potentials have been specified for $n=2,3,4,5$, where only one linear partial differential equation which determines the common part of the potential remains unsolved. We have found the general solution of this equation in cases of $n=2$ and $n=3$.

Three distinctive features of the higher dimensional extension of the intertwining method are that: (i) The method suggests coordinate systems which allows us to do the separation of variables and to utilize, in one of the variable, all the methods of the 1D SUSY quantum mechanics. (ii) In the choice of this variable and $\mathcal{L}$ itself one has a number of alternatives increasing with n. This fact enlarges the set of available potentials for each $n\geqslant 3$. (iii) There exists families of potentials accepting the same intertwining operator.

2D and 3D isospectral potentials we have obtained involve two arbitrary functions. The former constitute the most general integrable potentials which admit first order intertwining. Particular forms of these potentials may be of special interest for various purposes. Having in mind the projection techniques which produce exactly solvable lower dimensional problems from the higher dimensional one-particle problems[15,16] our analysis in Secs. VI–VIII must be continued also for $n=4$ and $n=5$. As is implied by the last example of Sec. VI, it seems to be possible to investigate connections among the superintegrable potentials[21] as well as to construct related potentials by repeated Darboux's transformations in the context of the intertwining method. Velocity dependent, stationary, and nonstationary problems[22,23] can also be considered within our approach. Work on 2D and 3D isospectral potentials which are at the same time superintegrable is in progress.

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Functional differentiation, line integration, and departures from homogeneity of the single-particle kinetic energy functional for one-dimensional systems of *N* fermions

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The differential virial theorem of March and Young for N fermions moving in a common one-dimensional potential energy $V(x)$ is here combined with the Euler equation of density functional theory expressing the constancy of the chemical potential throughout the entire inhomogeneous particle density. The functional derivative of the single-particle kinetic energy is thereby expressed directly in terms of the kinetic energy density; a line integral being involved in establishing the connection. This result is then used to establish a formula measuring departures from simple homogeneity of the kinetic energy functional: a matter of current interest in density functional theory. Finally, the general theory of the functional derivative of the single-particle kinetic energy with respect to the particle density is exemplified for the case of harmonic confinement of fermions in one dimension. [DOI: 10.1063/1.1379069]

I. BACKGROUND AND OUTLINE

Density functional theory is of considerable current interest in connection with atomic, molecular, and condensed matter physics.[1–3] The origins of the theory go back to Thomas[4] and Fermi,[5] whose work was formally completed by the theorem of Hohenberg and Kohn,[6] which states that the ground-state energy E of a many-fermion assembly of N interacting particles is a unique functional of the corresponding particle density n. Unfortunately, to date this functional remains unknown.

As background to the present study of the (single-particle) kinetic energy functional $T_s[n]$ of N fermions moving independently in a one-dimensional common potential $V(x)$, let us write immediately the Thomas–Fermi (TF) approximation to the ground-state energy $E_{\mathrm{TF}}[n]$, namely[7] (atomic units are used throughout)

$$E_{\mathrm{TF}}[n]=\frac{\pi^2}{6}\int_{-\infty}^{\infty} n^3(x)\,\mathrm{d}x+\int_{-\infty}^{\infty} n(x)\,V(x)\,\mathrm{d}x. \tag{1}$$

The variational principle underlying the density functional theory may be expressed as

$$\delta(E-N\mu)=0, \tag{2}$$

where δ represents variation with respect to the particle density $n(x)$ while μ is a Lagrange multiplier taking care of the normalization condition

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$$\int_{-\infty}^{\infty} n(x)\,dx = N. \tag{3}$$

The physical significance of μ, as Hulthén[8] pointed out, is that it represents the chemical potential, which is constant throughout the entire inhomogeneous fermion particle density $n(x)$. Applying the general result (2) to the approximate Thomas–Fermi functional in Eq. (1) yields the well-known result

$$\mu = \frac{\pi^2}{2} n^2(x) + V(x), \tag{4}$$

which involves semiclassical approximations and therefore comes into its own when the microscopic system under consideration has many states with large quantum numbers occupied. Bohr's correspondence principle then assures us that in such a limit the predictions of a fully quantal theory will be usefully represented by semiclassical theory.

Generalizing Eq. (4) to such a formally exact quantal theory, one writes[9]

$$\mu = \frac{\delta T_s[n]}{\delta n(x)} + V(x). \tag{5}$$

Here $T_s[n]$ is the so-called single-particle kinetic energy functional of density functional theory, and though a much simpler (one-body) problem than that of $E[n]$ cited previously, it also remains an unknown functional to date. Obviously, by comparing Eqs. (4) and (5), we see that the functional derivative of the Thomas–Fermi kinetic energy in Eq. (1) (a ''local'' density approximation) is $(\pi^2/2)\, n^2(x)$.

It was von Weizsäcker[10] (W) who first recognized the need to correct the Thomas–Fermi kinetic energy function(al) in Eq. (1) by introducing a kinetic energy term dependent on the density gradient. His so-called inhomogeneity kinetic energy, T_W say, will be written in the following in terms of a kinetic energy density $t_W(x)$, as

$$T_W = \int_{-\infty}^{\infty} t_W(x)\,dx, \quad t_W(x) = \frac{1}{8}\frac{(n'(x))^2}{n(x)}. \tag{6}$$

In an early attempt to synthesize density matrix theory with what is now called density functional theory, March and Young[11] derived an approximate form of $T_s[n]$ which was the linear combination of $T_W[n]$ and $T_{\mathrm{TF}}[n]$ given by $T_W[n] + \gamma(N)\, T_{\mathrm{TF}}[n]$, where $\gamma(1) = 0$, since the von Weizsäcker form (6) is the exact single-particle kinetic energy functional for one level only occupied. Baltin[12,13] subsequently made generalizations of such results relating to the single-particle kinetic energy functional $T_s[n]$. Searches for improved approximations to $T_s[n]$ are continuing,[14–16] in order to use so-called ''orbital-free'' density functional theory, thereby bypassing the need to solve one-electron (Slater–Kohn–Sham) Schrödinger equations.[17,18] But even for formal properties of $T_s[n]$, such as its homogeneity or otherwise,[19] current interest remains, this area having been one of some controversy.[20] One of the purposes of this investigation is to settle the matter of (departures from simple) homogeneity of $T_s[n]$ for N fermions in one dimension.[21]

The outline of the present study is then as follows. In Sec. II the Euler Eq. (5) of density functional theory is combined with the differential virial theorem of March and Young[22] to allow by a single integration the functional derivative $\delta T_s[n]/\delta n(x)$ to be written in terms of the corresponding kinetic energy plus properties of the particle density $n(x)$. Section III is then concerned with using this result to discuss the homogeneity departures of the (formally exact) $T_s[n]$ in one dimension for an arbitrary number of fermions. Section IV is devoted to exemplifying the formally exact results of Secs. II and III particularly for the (exactly soluble) case of harmonic confinement.[23,24] Section V constitutes a summary, and includes some proposals for possible further studies in the general area of the nonlocal kinetic energy functional $T_s[n]$. In the

Appendix, the ''box'' model of finite length L is considered for N fermions. The thermodynamic limit of this model, the so-called semi-infinite gas, has been discussed earlier by one of us in this Journal[25] and has in fact been treated in d dimensions. For $d=1$, the Appendix contains a generalization of the differential equation for a spherical Bessel function, which incorporates all inhomogeneities in $n(x)$ due to the finite length L of the box.

II. FORMALLY EXACT FUNCTIONAL DERIVATIVE OF SINGLE-PARTICLE KINETIC ENERGY IN TERMS OF KINETIC ENERGY AND PARTICLE DENSITIES

The March–Young[22] differential virial theorem reads, for kinetic energy density $t_G(x)$ defined from the positive $(\text{grad}\,\psi)^2$ wave function form:

$$t_G'(x) = -\frac{1}{2}\; n(x)\,\frac{\mathrm{d}V(x)}{\mathrm{d}x} + \frac{n'''(x)}{8}. \tag{7}$$

This exact result was derived from the equation of motion for the first-order density matrix, which was then solved by expansion around the diagonal element, which is just the particle density $n(x)$. The near-diagonal behavior of the density matrix is precisely determined by the kinetic energy density $t_G(x)$ plus $n(x)$. An immediate check of Eq. (7) is to multiply both sides by x, and then to integrate over all x from $-\infty$ to ∞. The left-hand side, after integration by parts, then gives the total kinetic energy, while the first term on the right-hand side is in magnitude half the virial of the force $(-\mathrm{d}V/\mathrm{d}x)$. Since the $n'''(x)$ term in Eq. (7) makes no contribution, Eq. (7) contains correctly the (integral) quantum-mechanical virial theorem.

Following the force-balance equation approach used by Holas and March[26] in their derivation of the force $-\nabla V_{\mathrm{xc}}$ associated with the exchange–correlation potential $V_{\mathrm{xc}}(\mathbf{r})$ in terms of low-order density matrices, we rewrite Eq. (7) for the force $(-\mathrm{d}V/\mathrm{d}x)$ acting on the N fermions occupying singly the levels generated by the common potential $V(x)$. Then

$$n(x) = \sum_{m=1}^{N} \psi_m^*(x)\,\psi_m(x), \tag{8}$$

where the normalized wave functions $\psi_m(x)$ are, of course, generated by $V(x)$. One finds from Eq. (7) after multiplying by $2/n(x)$, the so-called force-balance equation

$$-\frac{\mathrm{d}V(x)}{\mathrm{d}x} = \frac{2\,t_G'(x)}{n(x)} - \frac{n'''(x)}{4n(x)}. \tag{9}$$

Next we appeal to the Euler equation of density functional theory,[9] which is a statement of the constancy of the chemical potential μ throughout the entire fermion particle density $n(x)$, however inhomogeneous this may be. With

$$T_s[n] = \int_{-\infty}^{\infty} t_G(x)\,\mathrm{d}x \tag{10}$$

one has for the functional derivative of the single-particle kinetic energy $T_s[n]$ the result quoted already in Eq. (5). Differentiating Eq. (5) with respect to x to exploit the constancy of μ, one can evidently rewrite Eq. (9) as

$$\left(\frac{\delta T_s[n]}{\delta n(x)}\right)' = \frac{2\,t_G'(x)}{n(x)} - \frac{n'''(x)}{4n(x)}. \tag{11}$$

We now proceed to integrate this Eq. (11) to obtain the desired expression for the functional derivative $\delta T_s/\delta n(x)$. The result, as is readily verified, can be expressed in the form

$$\frac{\delta T_s[n]}{\delta n(x)} = 2\frac{t_G(x)}{n(x)} - \frac{n'^2(x)}{8n^2(x)} - \frac{n''(x)}{4n(x)} + 2\int^x \frac{n'(s)}{n(s)}\left[\frac{t_G(s)-t_W(s)}{n(s)}\right]\mathrm{d}s \tag{12}$$

by repeated integration by parts. In Eq. (12) we have introduced the von Weizsäcker inhomogeneity kinetic energy density $t_W(x)$ defined in Eq. (6). From there, the following functional derivative is readily calculated as

$$\frac{\delta T_W}{\delta n(x)} = \frac{1}{8}\left[\frac{n'(x)}{n(x)}\right]^2 - \frac{n''(x)}{4n(x)}. \tag{13}$$

Using Eqs. (6) and (13) in Eq. (12) one reaches the general one-dimensional form of the functional derivative of $T_s[n]$ as

$$\frac{\delta\{T_s[n]-T_W[n]\}}{\delta n(x)} = 2\left[\frac{t_G(x)-t_W(x)}{n(x)}\right] + 2\int^x \frac{n'(s)}{n(s)}\left[\frac{t_G(s)-t_W(s)}{n(s)}\right]\mathrm{d}s, \tag{14}$$

which, for arbitrary N, is defined to within an N-dependent constant.

One immediate check of Eq. (14) is the case $N=1$, where $T_s=T_W$ and $t_G(x)=t_W(x)$. Evidently Eq. (14) is trivially satisfied, with no arbitrary constant left for this special case [compare Eq. (13)].

Of course, for a general potential $V(x)$, the kinetic energy $t_G(x)$ is not known solely in terms of the density $n(x)$. However, for the case of harmonic confinement, we shall return to Eq. (14) in Sec. IV.

III. DEPARTURES FROM HOMOGENEITY OF THE SINGLE-PARTICLE KINETIC ENERGY FUNCTIONAL $T_s[n]$ FOR N FERMIONS IN ONE DIMENSION

Having obtained $\delta T_s/\delta n(x)$ in Eq. (14), let us now consider the departures from homogeneity of the single-particle kinetic energy functional $T_s[n]$. Since the work of Liu and Parr,[20] this has been an area of considerable interest (see, e.g., Ref. 19) and also some degree of controversy.[21]

Let us start from the customary definition of homogeneity. A functional $F[n]$ is homogeneous of order α in $n(x)$ if

$$F[\lambda\, n] = \lambda^{\alpha} F[n]. \tag{15}$$

Let us immediately use the examples cited above of (a) Thomas–Fermi and (b) von Weizsäcker kinetic energies to explore the validity (or otherwise) of Eq. (15) when F becomes the single-particle kinetic energy functional $T_s[n]$.

A. Thomas–Fermi and von Weizsäcker functionals, $T_{\mathrm{TF}}[n]$ and $T_W[n]$

Using Eq. (1),

$$T_{\mathrm{TF}}[n] = \frac{\pi^2}{6}\int_{-\infty}^{\infty} n^3(x)\,\mathrm{d}x$$

and hence $T_{\mathrm{TF}}[\lambda\, n]=\lambda^3\, T_{\mathrm{TF}}[n]$. Therefore we see immediately that the functional $T_{\mathrm{TF}}[n]$ is homogeneous of order three.

Next let us consider again the von Weizsäcker functional already given in Eq. (6),

$$T_W[n] = \frac{1}{8}\int_{-\infty}^{\infty} \frac{(n'(x))^2}{n(x)}\,\mathrm{d}x.$$

It follows immediately that $T_W[\lambda n]=\lambda T_W[n]$ and hence $T_W[n]$ is homogeneous of order one, as already emphasized by Liu and Parr.[20] This means, since T_W is the exact functional for $N=1$, that for all confining potentials $V(x)$ the single-particle kinetic energy $T_s[n]$ has this exact homogeneity property in this special case.

B. Example of harmonic confinement of an arbitrary number of fermions

March, Senet, and Van Doren[24] have constructed the fully nonlocal single-particle kinetic energy $T_s[n]$ for harmonic confinement of N fermions. We quote their functional here:

$$T_s[n]=T_W[n]+\int_{-\infty}^{\infty} dx\, \xi(x)\, t_{\mathrm{TF}}(x), \tag{16}$$

where

$$t_{\mathrm{TF}}(x)=\frac{\pi^2}{6}\ n^3(x). \tag{17}$$

In Eq. (16), the function $\xi(x)$ is explicitly given in Ref. 24 as

$$\xi(x)=\xi(0)+\frac{3}{\pi^2}\int_0^x ds\ \frac{(n'(s))^3}{n^5(x)}. \tag{18}$$

Thus, introducing the kinetic energy term on the right-hand side of Eq. (1), it follows by inserting Eq. (18) into Eq. (16) that

$$T_s[n]=T_W[n]+\xi(0)\, T_{\mathrm{TF}}[n]+\frac{3}{\pi^2}\int_{-\infty}^{\infty} dx\, t_{\mathrm{TF}}(x)\int_0^x ds\ \frac{(n'(s))^3}{n^5(x)}. \tag{19}$$

But we have already discussed the order of homogeneity of T_{TF} and T_W in Sec. III A above, the orders being, respectively, three and one. The quantity $\xi(0)$ is itself a weak function of N, tending rapidly to a constant as N becomes large. The order of the final term in Eq. (19) is unity, and hence it is clear that $T_s[n]$ is not homogeneous. Thus it follows that while

$$\int_{-\infty}^{\infty} n(x)\ \frac{\delta T_s}{\delta n(x)}\,dx=T_s[n] \tag{20}$$

is true for $N=1$ (when $T_s\equiv T_W$), for N arbitrary there are departures from homogeneity until $N\to\infty$, when $T_s\to T_{\mathrm{TF}}$ and the order of homogeneity tends to three (see Sec. III A).

Thus, having demonstrated departures from homogeneity for a specific potential energy $V(x)=x^2/2$ representing harmonic confinement, it follows naturally that the general result (14) must reflect such departures, being true for arbitrary one-dimensional confining potentials $V(x)$.

IV. ILLUSTRATIONS OF GENERAL EQUATION (14)

In this section, we shall illustrate the functional derivative in Eq. (14) by reference to some specific cases. As a first example, let us take the two-level system, i.e., $N=2$, for an arbitrary confining potential $V(x)$.

A. Two-level system with arbitrary confining potential $V(x)$

Here we work out explicitly the example for a given potential $V(x)$ for two levels only occupied. We invoke the so-called Dawson–March[27] transformation in which the wave functions $\psi_1(x)$ and $\psi_2(x)$ associated with the two levels are written in terms of density ''amplitude'' $\sqrt{n(x)}$ and phase $\theta(x)$ as

$$\psi_1(x)=\sqrt{n(x)}\ \cos\theta(x), \quad \psi_2(x)=\sqrt{n(x)}\ \sin\theta(x), \tag{21}$$

leading, of course, to $n(x)=\psi_1^2(x)+\psi_2^2(x)$. It is then readily shown that the kinetic energy density $t_G(x)$ is given by

$$t_G(x)=t_W(x)+\frac{1}{2}n(x)\left(\frac{\mathrm{d}\theta(x)}{\mathrm{d}x}\right)^2. \tag{22}$$

The phase $\theta(x)$ is related to the particle density $n(x)$ by the nonlinear pendulumlike equation, with eigenvalue ϵ:

$$\theta''(x)+\frac{n'(x)}{n(x)}\theta'(x)+\epsilon\sin 2\theta(x)=0. \tag{23}$$

Introducing Eq. (22) into Eq. (14) yields almost immediately

$$\frac{\delta(T_s-T_W)}{\delta n(x)}=(\theta'(x))^2+\int^x\frac{n'(s)}{n(s)}(\theta'(s))^2\,\mathrm{ds}. \tag{24}$$

But multiplying Eq. (23) by $\theta'(x)$ and using the result for $n'(\theta')^2/n$ in Eq. (24) one can readily evaluate the integral to find, to within a constant of integration

$$\frac{\delta(T_s-T_W)}{\delta n(x)}=\frac{1}{2}(\theta'(x))^2+\frac{\epsilon}{2}\cos 2\theta(x). \tag{25}$$

This result Eq. (25) is now to be compared with Eq. (B10) of Holas *et al.*,[28] namely

$$\frac{\delta(T_s-T_W)}{\delta n(x)}=\frac{1}{2}(\theta'(x))^2+\frac{1}{2}\left(\theta''(x)+\frac{n'(x)}{n(x)}\theta'(x)\right)\tan\theta(x). \tag{26}$$

Again using Eq. (23) in the last term of this equation, it is readily verified that it agrees with our result Eq. (25) to within an additive constant. This completes the demonstration that Eq. (14) holds for all two-level systems with an arbitrary confining potential.

B. Large *N* limit with arbitrary confining potential *V*(*x*)

Here, from the studies, for example, of Lieb,[29] we know that the Thomas–Fermi method is asymptotically correct in the limit $N\to\infty$. Then, one can drop $n''(x)$ in the difference between t_G and t, this being expressed precisely in

$$t_G(x)=t(x)+\frac{n''(x)}{4}, \tag{27}$$

and can neglect the von Weizsäcker contribution relative to the Thomas–Fermi kinetic energy. Equation (14) then simplifies to read

$$\frac{\delta T_{\mathrm{TF}}}{\delta n(x)}=2\frac{t_{\mathrm{TF}}}{n(x)}+2\int^x\frac{n'(s)}{n(s)}\frac{t_{\mathrm{TF}}(s)}{n(s)}\mathrm{ds}+(\text{constant}). \tag{28}$$

But from Eq. (1), $t_{\mathrm{TF}}=(\pi^2/6)n^3(x)$, and hence Eq. (28) becomes

$$\frac{\delta T_{\mathrm{TF}}}{\delta n(x)}=2\frac{t_{\mathrm{TF}}}{n(x)}+\frac{\pi^2}{3}\int^x n'(s)\,n(s)\,\mathrm{ds}=3\frac{t_{\mathrm{TF}}(x)}{n(x)}+(\text{constant}), \tag{29}$$

which can be confirmed by direct appeal to Eqs. (1) and (4). Thus, for arbitrary potential $V(x)$, Eq. (14) is now confirmed asymptotically as $N\to\infty$.

C. Harmonic confinement: Arbitrary number *N* of fermions

The above-mentioned Thomas–Fermi example, applicable asymptotically in the limit of large N, has encouraged us to consider the harmonic confinement case treated in earlier work as a further example. Let us use the form of March, Senet, and Van Doren[24] for the kinetic energy density $t(x)$, namely [their Eq. (27)]:

$$t(x)=t_W(x)+\xi(x)t_{\mathrm{TF}}(x). \tag{30}$$

Here $\xi(x)$ is given by (18). Thus, it follows that

$$\xi'(x)=\frac{3}{\pi^2}\frac{(n'(x))^3}{n^5(x)}. \tag{31}$$

But differentiating Eq. (30) and substituting Eq. (31) for $\xi'(x)$ and Eq. (17) yields

$$3\xi(x)\,t_{\mathrm{TF}}(x)=\frac{n(x)}{n'(x)}[t'(x)-t'_W(x)]-\frac{1}{2}\frac{(n'(x))^2}{n(x)}. \tag{32}$$

Inserting this equation into Eq. (30) for $t(x)$ and using Eq. (6), one finds

$$3t(x)+t_W(x)=\frac{n(x)}{n'(x)}[t'(x)-t'_W(x)]. \tag{33}$$

But from Eq. (16) of Ref. 24

$$\frac{t'(x)}{n'(x)}=N-\frac{x^2}{2} \tag{34}$$

and therefore

$$3t(x)+t_W(x)=n(x)\left[N-\frac{x^2}{2}\right]-\frac{n(x)}{n'(x)}t'_W(x). \tag{35}$$

From here, and using Eq. (6)

$$t(x)+\frac{n(x)}{6}(x^2-2N)=-\frac{n''(x)}{12\,n(x)}, \tag{36}$$

or from Eq. (5)

$$\frac{3t(x)}{n(x)}+\frac{t_W(x)}{n(x)}+\frac{t'_W(x)}{n'(x)}=\frac{\delta T_s}{\delta n(x)}+K(N), \tag{37}$$

where $K(N)$ is a constant depending on the number of fermions.

Now again using Eq. (6)

$$\frac{t'_W(x)}{n'(x)}=\frac{1}{4}\frac{n''(x)}{n(x)}-\frac{1}{8}\left(\frac{n'(x)}{n(x)}\right)^2=-\frac{\delta T_W}{\delta n(x)}. \tag{38}$$

Thus Eq. (37) becomes

$$\frac{\delta T_s}{\delta n(x)} = -K(N) + \frac{3t(x)}{n(x)} + \frac{1}{4}\frac{n''(x)}{n(x)}, \tag{39}$$

which agrees with Eq. (35) of March, Senet, and Van Doren.[24] Thus

$$\left[\frac{\delta T_s}{\delta n(x)}\right]' = 3\frac{n(x)t'(x) - n'(x)t(x)}{n^2(x)} + \frac{1}{4}\frac{n(x)n'''(x) - n'(x)n''(x)}{n^2(x)} \tag{40}$$

and at this point we shall compare with the general Eq. (14) which yields by differentiation

$$\left[\frac{\delta T_s}{\delta n(x)}\right]' = 2\ \frac{t_G'(x) - t_W'(x)}{n(x)} + \left[\frac{\delta T_W}{\delta n(x)}\right]'. \tag{41}$$

Using the two equalities in Eq. (38) the last term in Eq. (41) becomes

$$\left[\frac{\delta T_W}{\delta n(x)}\right]' = \frac{2}{n(x)}\left[t_W'(x) - \frac{n'''(x)}{8}\right]. \tag{42}$$

Returning to the harmonic oscillator, using Eq. (27) in Eq. (40) yields

$$\left[\frac{\delta T_s}{\delta n(x)}\right]' = \frac{2}{n}(t_G' - t_W') + \frac{2}{n}t_W' - \frac{n'''}{4n} + \left[\frac{t'}{n} - \frac{3t\,n'}{n^2} - \frac{n'\,n''}{4n^2}\right]. \tag{43}$$

But the last term in brackets is readily seen to be zero using Eqs. (34) and (36). Therefore, Eq. (43) agrees completely with Eqs. (41) and (42), confirming once more the validity of the general Eq. (14).

V. SUMMARY AND POSSIBLE FUTURE DIRECTIONS

What has been demonstrated here is that the combination of the differential virial theorem (7) of March and Young with the Euler equation (5) of density functional theory allows the explicit expression (14) to be obtained for the functional derivative $\delta T_s/\delta n(x)$ of the single-particle kinetic energy $T_s[n]$. This Eq. (14) has, therefore, by measuring $T_s[n]$, and its kinetic energy density $t_G(x)$, from the von Weizsäcker counterparts $T_W[n]$ and $t_W(x)$, respectively, bypassed the process of functional differentiation by recourse to a line integration. This allows, in principle, a much more straightforward route to the functional derivative of $T_s[n]$. Of course, the general form of $[t_G(x) - t_W(x)]/n(x)$ is still lacking and therefore the illustrations of the validity of Eq. (14), set out in Sec. IV, have been either for models (e.g., harmonic confinement) or asymptotic for large particle number N but for arbitrary confining potential $V(x)$.

As to future directions, it would naturally be important to find other soluble models to add to the harmonic confinement example invoked extensively in Sec. IV. But in the case of a quite general potential $V(x)$ and an arbitrary number of fermions, Eq. (14) may perhaps afford an approximate route to the functional derivative, and hence to the desired differential equation for the ground-state density $n(x)$, given $V(x)$. It is presently only for such models as harmonic confinement that such a differential equation exists [see also the Appendix, especially Eqs. (A10) and (A11)], as derived by Lawes and March[23] in this case. The fact that one has a line integration in the final term of Eq. (14) makes it tempting to contemplate inserting an approximation for $[t_G(x) - t_W(x)]/n(x)$ in this term, possibly modeled on the harmonic confinement example already fully solved.

The final comments concern what has been until recently the vexed question of homogeneity of $T_s[n]$. The present argument, set out explicitly in Sec. III, and most precisely in Eq. (19) for admittedly the special case of harmonic confinement, can leave no possible doubt that $T_s[n]$ in one-dimensional N fermion problems is a linear combination of terms with different scaling properties as the density $n(x)$ goes to $\lambda\, n(x)$. Of course, in the case $N=1$, the von Weizsäcker

functional is the exact form of $T_s[n]$ and from well-known arguments $T_W[n]$ has homogeneity of order one. Again, in the asymptotic limit $N\to\infty$, the Thomas–Fermi kinetic energy functional in Eq. (1) is again homogeneous, but now of order three. For intermediate N, one must expect therefore departures from homogeneity, as clearly evidenced in the harmonic example set out in Eq. (19) where each of the three terms on the right-hand side has its own specific scaling properties with the parameter λ.

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APPENDIX: KINETIC ENERGY AND PARTICLE DENSITY FOR FREE MOTION IN A BOX OF LENGTH *L*

In this Appendix we will calculate $t_G(x)$ and $n(x)$ for N fermions occupying singly the free particle levels for confinement in a box of length L, with normalized eigenfunctions $\psi_m(x)=\sqrt{2/L}\,\sin(m\pi x/L)$. In this case the particle density $n(x)$ is given by[30]

$$\begin{aligned} n(x) &= \frac{2}{L}\sum_{m=1}^{N}\sin^2\left[\frac{m\pi x}{L}\right] \\ &= \frac{1}{L}\left[N-\frac{\cos\left[\dfrac{(N+1)\pi x}{L}\right]\sin\left[\dfrac{N\pi x}{L}\right]}{\sin\left[\dfrac{\pi x}{L}\right]}\right] \\ &= \frac{1}{L}\left\{N+\sin^2\left[\frac{N\pi x}{L}\right]-\cot\left[\frac{\pi x}{L}\right]\sin\left[\frac{N\pi x}{L}\right]\cos\left[\frac{N\pi x}{L}\right]\right\}. \end{aligned} \tag{A1}$$

As N and L both tend to infinity in such a way that N/L tends to a finite value, $n_0\equiv k_f/\pi$ say, Eq. (A1) becomes

$$n(x)=n_0\left[1-\frac{\sin(2k_fx)}{2k_fx}\right]=n_0[1-j_0(2k_fx)], \tag{A2}$$

k_f being the wave number of the Fermi gas in this limit and $j_\ell(z)$ the spherical Bessel function of order ℓ. This result (A2) is the special case corresponding to one dimension ($d=1$) of the d-dimensional semi-infinite electron gas treated earlier by one of us in this Journal.[25]

The kinetic energy density corresponding to Eq. (A2) was also given in this earlier work in the ''thermodynamic'' limit discussed previously as

$$t(x)=t_0+\frac{k_f^2}{2}\,[n(x)-n_0]+\frac{k_f^3}{\pi}\,\frac{j_1(2k_fx)}{2k_fx}. \tag{A3}$$

The generalization of Eq. (A3) before passing to the thermodynamic limit, in the $(\mathrm{grad}\,\psi)^2$ wave function form of the kinetic energy $t_G(x)$ is evidently

$$t_G(x)=\frac{1}{2}\sum_{m=1}^{N}(\psi_m'(x))^2. \tag{A4}$$

Hence we find

$$t_G(x)=\frac{\pi^2}{L^3}\sum_{m=1}^{N} m^2\cos^2\left(\frac{m\pi x}{L}\right)$$

$$=\frac{\pi^2}{24L^3}\left\{\frac{6}{\sin\left[\frac{\pi x}{L}\right]}\left(N+N^2\sin^2\left[\frac{\pi x}{L}\right]\right)\cos\left[\frac{2N\pi x}{L}\right]\right.$$

$$\left.-3\,\frac{\cos\left[\frac{\pi x}{L}\right]}{\sin^3\left[\frac{\pi x}{L}\right]}\left(1-2N^2\sin^2\left[\frac{\pi x}{L}\right]\right)\sin\left[\frac{2N\pi x}{L}\right]+2N(N+1)(2N+1)\right\}. \tag{A5}$$

Except at the box "edges" $x=0$ and L,

$$t_G'(x)=\frac{n'''(x)}{8}, \tag{A6}$$

from the March-Young virial result. Using Eq. (A5) explicitly one finds the integral of Eq. (A6) as

$$t_G(x)=\frac{\pi^2}{12L^3}\;N(N+1)(2N+1)+\frac{n''(x)}{8}. \tag{A7}$$

Connection with the semi-infinite electron gas result[25] is readily established using the second-order differential equation for the spherical Bessel function.

This has stimulated us to construct a generalized differential equation for the exact density $n(x)$ without invoking the thermodynamic limit. The argument goes as follows. Using the definition from Eq. (A1) that

$$S(x)=n(x)-\frac{N}{L}-\frac{1}{2L}, \tag{A8}$$

where the last term is introduced to have a homogeneous equation [see Eq. (A10)] for $S(x)$, we have

$$\sin\left[\frac{\pi x}{L}\right]\;S(x)=-\frac{1}{2L}\;\sin\left[\frac{(2N+1)\pi x}{L}\right]. \tag{A9}$$

From here it is very easy to prove that the function $S(x)$ satisfies the following second-order linear differential equation

$$S''(x)+\left[\frac{2\pi/L}{\tan\left[\frac{\pi x}{L}\right]}\right]S'(x)+\left[\frac{4N(N+1)\pi^2}{L^2}\right]S(x)=0, \tag{A10}$$

which we will term a generalized spherical Bessel equation. If we consider now the thermodynamic limit in Eq. (A10) and we call $S_0(x)$ the resulting function from $S(x)$, one can immediately prove that $S_0(x)$ satisfies the following spherical Bessel equation:

$$S_0''(x)+\frac{2}{x}\;S_0'(x)+(2k_f)^2\;S_0(x)=0, \tag{A11}$$

the solution of which is essentially given by (A2). It seems to us somewhat remarkable that the major ''size effects'' due to the finite length L of the box enter Eq. (A10) through the factor $(2\pi/L)/\tan[\pi x/L]$ multiplying the first derivative of $S(x)$, the change in the coefficient $S(x)$ for finite N being minor in comparison. As $L\to\infty$ and $N\to\infty$, such that N/L tends to a finite limit n_0, the tangent factor with $0<x<L$ has a node at $L/2$ for finite box length which moves out to infinity, and the factor $2/x$ multiplying $S_0'(x)$ in the spherical Bessel equation (A11) is recovered.

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Variational Sturmian approximation: A nonperturbative method of solving time-independent Schrödinger equation

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A variationally improved Sturmian approximation for solving time-independent Schrödinger equation is developed. This approximation is used to obtain the energy levels of a quartic anharmonic oscillator, a quartic potential, and a Gaussian potential. The results are compared with those of the perturbation theory, the WKB approximation, and the accurate numerical values. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1385374]

I. INTRODUCTION

Since the early days of quantum mechanics, the main technical tools for solving the time-independent Schrödinger equation have been the time-independent perturbation theory, the semiclassical or WKB approximation, and the variational method.[1,2] Starting form the late 1950s, physical chemists and nuclear physicists have explored the use of what is called the *Sturmian basis functions* in solving this equation for a variety of potentials arising in molecular and atomic physics.[3,4] Recently, Antonsen[5] and Szmytkowski and Zywicka-Mozeiko[6] have studied the harmonic oscillator Sturmian functions. The purpose of the present paper is to outline a general variationally improved Sturmian approximation scheme that provides a nonperturbative method of solving time-independent Schrödinger equation.

The organization of the paper is as follows. In Sec. II, we give the definition of the Sturmian basis vectors, derive their general properties, and discuss the conventional Sturmian approximation. In Sec. III we present an improved Sturmian approximation which makes use of the variational method. In Sec. IV we study the harmonic oscillator Sturmians and use them for the solution of time-independent Schrödinger equation in one dimension. In Sec. V we apply our general results to some concrete problems, and compare our results with those obtained using perturbation theory, the WKB approximation, and the highly accurate numerical investigations. In particular, we obtain the energy levels of a quartic anharmonic oscillator, a quartic potential, and a Gaussian potential. Finally, in Sec. VI we summarize our results and present our conclusions.

II. CONVENTIONAL STURMIAN APPROXIMATION

Consider the time-independent Schrödinger equation:

$$H|E,a\rangle = E|E,a\rangle, \tag{1}$$

where H is a self-adjoint Hamiltonian operator and a is a degeneracy label.

The method of Sturmian approximation is based on an expansion of the eigenvectors $|E,a\rangle$ in terms of solutions $|\phi_\nu,\alpha\rangle$ of the equation

$$(H_0+\beta_\nu V_0)|\phi_\nu,\alpha\rangle = \mathcal{E}|\phi_\nu,\alpha\rangle, \tag{2}$$

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where H_0 and V_0 are self-adjoint operators, β_ν and $\mathcal{E}$ are real scalar parameters, and α is a degeneracy label. Note that in order to obtain $|\phi_\nu,\alpha\rangle$, one must fix $\mathcal{E}$ and solve Eq. (2) for $|\phi_\nu,\alpha\rangle$. Clearly, every solution $|\phi_\nu,\alpha\rangle$ would correspond to a choice for the value of the coupling constant β_ν.

Suppose that $H_0=\vec{p}^2/(2m)$ is the Hamiltonian for a free particle moving in the configuration space $\mathbb{R}^d$, $V_0=V_0(\vec{x})$ is a real interaction potential, and H is a standard Hamiltonian of the form

$$H=\frac{\vec{p}^2}{2m}+V(\vec{x}), \tag{3}$$

where $\vec{p}$ and $\vec{x}$ are momentum and position operators, respectively. If $V_0(\vec{x})$ tends to infinity as $|\vec{x}|\to\infty$, all the eigenstates of V_0 are bound states.[7] In this case, only for a discrete set of positive values of β_ν, can we find square-integrable solutions $|\phi_\nu,\alpha\rangle$ of Eq. (2). In this case, the label ν will take values in a discrete set which we shall choose to be $\{0,1,2,...\}$.

The only difference between Eq. (2) and the eigenvalue equation for the potential $\beta_\nu V_0(\vec{x})$ is that in the former $\mathcal{E}$ is a fixed parameter which can be arbitrarily chosen. Therefore, a solution of Eq. (2) corresponds to a pair $(\beta_\nu,|\phi_\nu,\alpha\rangle)$.

The vectors $|\phi_\nu,\alpha\rangle$ are called the *Sturmian basis vectors* or simply the *Sturmians*.[3] They satisfy certain orthonormality conditions which we shall derive below. We should, however, note that the square-integrable Sturmians do not generally constitute a complete set of basis vectors of the Hilbert space.[6] There are certain potentials V_0, such as the Coulomb potential, that lead to a complete set of square-integrable Sturmians.[8]

Let us first note that the defining equation (2) does not determine $|\phi_\nu,\alpha\rangle$ uniquely. This is reflected in the presence of the degeneracy label α. What is uniquely determined by Eq. (2) is the degeneracy subspace $\mathcal{H}_\nu$ spanned by $\{|\phi_\nu,1\rangle,|\phi_\nu,2\rangle,\ldots,|\phi_\nu,l_\nu\rangle\}$, where l_ν is the degree of degeneracy, i.e., the number of linearly independent solutions of Eq. (2) associated with a given (admissible) value of β_ν. Clearly, we can construct an orthonormal basis of $\mathcal{H}_\nu$ and choose the Sturmian vectors $|\phi_\nu,\alpha\rangle$ to be the basis vectors. In other words, without loss of generality, we can choose to work with the Sturmians $|\phi_\nu,\alpha\rangle$ satisfying

$$\langle\phi_\nu,\alpha|\phi_\nu,\gamma\rangle=\delta_{\alpha\gamma}, \tag{4}$$

where $\delta_{\alpha\gamma}$ denotes the Kronecker delta function. Clearly, any unitary transformation of $\mathcal{H}_\nu$ would lead to a new set of Sturmians satisfying (4). Therefore, the condition (4) reduces the freedom in the choice of the Sturmians $|\phi_\nu,\alpha\rangle$, but does not eliminate it.

Next, we evaluate the Hermitian adjoint of both sides of Eq. (2), change (ν,α) to (μ,γ), and take the inner product of both sides of the resulting equation with $|\phi_\nu,\alpha\rangle$. This yields

$$\beta_\mu\langle\phi_\mu,\gamma|V_0|\phi_\nu,\alpha\rangle=\langle\phi_\mu,\gamma|(\mathcal{E}-H_0)|\phi_\nu,\alpha\rangle. \tag{5}$$

We can compute the right-hand side of this equation using Eq. (2). Substituting the result in (5), we find

$$(\beta_\mu-\beta_\nu)\langle\phi_\mu,\gamma|V_0|\phi_\nu,\alpha\rangle=0. \tag{6}$$

If we define

$$N_\nu^{\gamma\alpha}:=\langle\phi_\nu,\gamma|V_0|\phi_\nu,\alpha\rangle, \tag{7}$$

then we can write Eq. (6) in the form

$$\langle\phi_\mu,\gamma|V_0|\phi_\nu,\alpha\rangle=N_\nu^{\gamma\alpha}\delta_{\mu\nu}. \tag{8}$$

Equation (8) is the desired orthogonality property of the Sturmians. We can further simplify Eq. (8), by noting that the $l_\nu \times l_\nu$ matrix N_ν formed by $N_\nu^{\gamma\alpha}$ is a Hermitian matrix. This means that we can choose $|\phi_\nu,\alpha\rangle$ in such a way that N_ν is a diagonal matrix. Making this choice, we have

$$N_\nu^{\alpha\gamma}=N_\nu^\alpha\delta_{\alpha\gamma}, \tag{9}$$

$$\langle\phi_\mu,\gamma|V_0(\vec{x})|\phi_\nu,\alpha\rangle=N_\nu^\alpha\delta_{\mu\nu}\delta_{\alpha\gamma}, \tag{10}$$

where N_α^ν, with $\alpha\in\{1,2,\ldots,l_\nu\}$, are eigenvalues of the matrix N_ν. Since N_ν is Hermitian, N_ν^α are real.

In summary, we can choose a set of Sturmian vectors $|\phi_\nu,\alpha\rangle$ which are eigenvectors of the matrices N_ν. Therefore, for each value of ν, $\{|\phi_\nu,1\rangle,\ldots,|\phi_\nu,l_\nu\rangle\}$ forms an orthonormal eigenbasis of N_ν in the degeneracy subspace $\mathcal{H}_\nu$. However, $|\phi_\nu,\alpha\rangle$ with different values of ν are not orthogonal. Instead, they satisfy a modified orthogonality condition, namely (10).

Now, let us expand a solution $|E,a\rangle$ of the Schrödinger equation (1), in a Sturmian basis corresponding to a solvable potential V_0, i.e., seek solutions of the form

$$|E,a\rangle=\sum_{\nu=0}^{\infty}\sum_{\alpha=1}^{l_\nu}C_\nu^\alpha|\phi_\nu,\alpha\rangle, \tag{11}$$

where C_ν^α are complex coefficients and ν is supposed to take discrete values 0,1,2,... . Note that if the Sturmians $|\phi_\nu,\alpha\rangle$ do not form a complete basis, then Eq. (11) yields the eigenvectors that belong to the span of $|\phi_\nu,\alpha\rangle$.

The *Sturmian approximation of order N* is the approximation in which one neglects all the coefficients C_ν^α in Eq. (11) but those with ν belonging to a subset $\mathcal{S}_{N+1}$ of non-negative integers of order $N+1$. Alternatively, in considering the Sturmian approximation of order N, one confines the range of the indices (of type) ν to a fixed finite set $\mathcal{S}_{N+1}$. In this way, the infinite sum $\Sigma_{\nu=0}^{\infty}\cdots$ in Eq. (11) is replaced by the finite sum $\Sigma_{\nu\in\mathcal{S}_{N+1}}\cdots$. We shall abbreviate the latter by Σ_ν. The set $\mathcal{S}_{N+1}$ may, in principle, be chosen arbitrarily. We will comment on this choice in Sec. III.

Substituting (11) in the Schrödinger equation (1) and making use of Eqs. (2) and (3), we find

$$\sum_\nu\sum_{\alpha=1}^{l_\nu}C_\nu^\alpha(E-\mathcal{E}-V+\beta_\nu V_0)|\phi_\nu,\alpha\rangle=0. \tag{12}$$

Now, evaluating the inner product of both sides of this equation with $|\phi_\mu,\gamma\rangle$ and using the orthogonality relation (10), we obtain

$$\sum_\nu\sum_{\alpha=1}^{l_\nu}[(E-\mathcal{E})T_{\mu\nu}^{\gamma\alpha}-(W_{\mu\nu}^{\gamma\alpha}-\beta_\nu N_\nu^\alpha\delta_{\mu\nu}\delta_{\gamma\alpha})]C_\nu^\alpha=0. \tag{13}$$

Here we have introduced

$$T_{\mu\nu}^{\gamma\alpha}:=\langle\phi_\mu,\gamma|\phi_\nu,\alpha\rangle, \tag{14}$$

$$W_{\mu\nu}^{\gamma\alpha}:=\langle\phi_\mu,\gamma|V|\phi_\nu,\alpha\rangle. \tag{15}$$

We can express Eq. (13) in a more compact form, if we use a single label for the pair (ν,α). Introducing $\mathcal{N}:=(\nu,\alpha)$ and $\mathcal{M}:=(\mu,\gamma)$, we write Eq. (13) in the form

$$\sum_{\mathcal{N}}[(E-\mathcal{E})T_{\mathcal{M}\mathcal{N}}-S_{\mathcal{M}\mathcal{N}}]C_{\mathcal{N}}=0, \tag{16}$$

where

$$T_{\mathcal{MN}}=T^{\gamma\alpha}_{\mu\nu},\quad S_{\mathcal{MN}}=W_{\mathcal{MN}}-\beta_\nu N_{\mathcal{N}}\delta_{\mathcal{MN}},\tag{17}$$

$$W_{\mathcal{MN}}=W^{\gamma\alpha}_{\mu\nu},\quad N_{\mathcal{N}}=N^{\alpha}_{\nu}.\tag{18}$$

Equations (16) form a linear system of homogeneous first order algebraic equations for $C_{\mathcal{N}}$. This system has a nontrivial solution provided that the determinant of the matrix of coefficients vanishes, i.e.,

$$\det[(E-\mathcal{E})T-S]=0.\tag{19}$$

Here T and S are matrices with entries $T_{\mathcal{MN}}$ and $S_{\mathcal{MN}}$, respectively.

Solving Eq. (19), we can express E in terms of $\mathcal{E}$, β_ν, and the Sturmians $|\phi_\nu,\alpha\rangle$. Now, we recall that for a fixed choice of V_0, the coupling constants β_ν and the corresponding Sturmians $|\phi_\nu,\alpha\rangle$ depend on the parameter $\mathcal{E}$. Therefore, Eq. (19) yields E as a function of $\mathcal{E}$. Furthermore, substituting the value of $E=E(\mathcal{E})$ obtained by solving (19) in (16) and solving for the coefficients $C_{\mathcal{N}}$, we obtain an expression for the eigenvector $|E,a\rangle$ that involves $\mathcal{E}$. As we discuss in the following section, the fact that the Sturmian approximation yields the eigenvalues and the eigenvectors of the Hamiltonian as functions of a free parameter seems to have been overlooked. This is mainly because there is a choice for the parameter $\mathcal{E}$ that simplifies the calculations.

It should also be emphasized that Eq. (19) is an algebraic equation of order $N+1$. Therefore, in general, it has $N+1$ solutions. This can be understood by noting that in the Sturmian approximation one actually approximates the Hilbert space by a finite-dimensional vector space. Consequently, the Hamiltonian is replaced with a matrix with a finite number of eigenvalues.

III. VARIATIONAL STURMIAN APPROXIMATION

In general, the accuracy of the Sturmian approximation depends on the following factors.
(1) *Choice of* V_0*:* In practice, V_0 must be one of the exactly solvable potentials. Therefore, the available choices for V_0 are few in number. For the potentials V with bound states, we can choose V_0 to be a harmonic oscillator potential. For example, for the quartic anharmonic oscillator

$$V(x)=\frac{k}{2}x^2+\epsilon x^4,\tag{20}$$

we shall take

$$V_0(x)=\frac{k}{2}x^2.\tag{21}$$

Similarly, for the Gaussian potential

$$V(x)=-\lambda e^{-\epsilon x^2/2},\tag{22}$$

we shall take

$$V_0(x)=\tfrac{1}{2}\lambda\epsilon x^2-\lambda.\tag{23}$$

This will enable us to compare the results of the Sturmian approximation with those of the perturbation theory, for in the limit $\epsilon\to 0$, $V(r)\to V_0(r)$. Note that multiplying V_0 by a positive real number does not change the results of the Sturmian approximation. This is simply because we can always absorb such a number in the definition of β_ν.
(2) *Choice of the Sturmians included in the sum (16):* This is also directly related to the choice of the potential V_0. If V_0 is obtained from V by a limiting process as in the case of the potentials (20)

and (22), then a natural choice for the computation of the nth energy eigenvalue E_n and the corresponding eigenvectors $|E_n,\alpha\rangle$ is to include the $|\phi_\nu,\alpha\rangle$ with ν equal or close to n. In particular, in the Sturmian approximation of order zero, we have

$$|E_n,a\rangle=\sum_{\alpha=1}^{l_n} C_n^\alpha|\phi_n,\alpha\rangle. \tag{24}$$

(3) *Choice of the parameter $\mathcal{E}$:* The conventional choice[4,5] for the parameter $\mathcal{E}$ is $\mathcal{E}=E$. This simplifies Eq. (19) considerably. The basic idea pursued in this paper is the fact that this simplification does not necessarily justify the conventional choice for $\mathcal{E}$.

It is well known[2] that the eigenvalue equation (1) is equivalent to the variational equation

$$\frac{\delta}{\delta\langle\psi|}\left(\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}\right)=0. \tag{25}$$

In other words, the eigenvalues E are the minima of the expectation value

$$\langle H\rangle:=\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle},$$

and the eigenvectors are the vectors $|E\rangle=|E,a\rangle$ that minimize $\langle H\rangle$. This observation suggests that the most efficient choice for the parameter $\mathcal{E}$ appearing in the Sturmian approximation is the one that minimizes $E=E(\mathcal{E})$. Therefore, the most reliable Sturmian approximation is obtained by choosing $\mathcal{E}$ to be a solution of

$$\frac{dE}{d\mathcal{E}}=0. \tag{26}$$

If this equation does not have a solution, then one must either make another choice for the set $\mathcal{S}_{N+1}$ or proceed with a higher order Sturmian approximation.

IV. VARIATIONAL STURMIAN APPROXIMATION USING HARMONIC OSCILLATOR STURMIANS

Consider a quantum system with the configuration space $\mathbb{R}$, a standard Hamiltonian (3), and a real-valued potential $V=V(x)$. Suppose that the system has an infinite number of bound states with nondegenerate energy eigenvalues E_n. Here $n\in\{0,1,2,\ldots\}$ and E_0 stands for the ground state.

Now, consider the Sturmian basis vectors associated with a harmonic oscillator[5,6]

$$V_0=V_0(x)=\frac{k}{2}x^2. \tag{27}$$

In order to solve Eq. (2) for this choice of V_0, we introduce

$$\omega_\nu:=\left(\frac{\beta_\nu k}{m}\right)^{1/2}, \tag{28}$$

$$\alpha_\nu:=\frac{m\omega_\nu}{\hbar}, \tag{29}$$

$$a_\nu:=\left(\frac{\alpha_\nu}{2}\right)^{1/2}\left(x+\frac{ip}{\hbar\alpha_\nu}\right). \tag{30}$$

$$|l\rangle_\nu := \frac{1}{\sqrt{l!}} a_\nu^{\dagger l} |0\rangle_\nu, \tag{31}$$

where $|0\rangle_\nu$ is the normalized real ground state vector for a harmonic oscillator with mass m and frequency ω_ν. That is

$$\langle x|0\rangle_\nu := \left(\frac{\alpha_\nu}{\pi}\right)^{1/4} e^{-\alpha_\nu x^2/2}. \tag{32}$$

In view of the similarity of Eq. (2) with the eigenvalue equation for the potential $\beta_\nu V_0$, we can easily deduce that

$$\mathcal{E} = \hbar\omega_\nu(\nu + \tfrac{1}{2}), \tag{33}$$

$$|\phi_\nu\rangle = |\nu\rangle_\nu \tag{34}$$

where $\nu \in \{0,1,2,\ldots\}$.

We can invert Eqs. (33) and (28) to express ω_ν and β_ν in terms of $\mathcal{E}$. This yields

$$\omega_\nu = \frac{2\mathcal{E}}{\hbar(2\nu+1)}, \tag{35}$$

$$\beta_\nu = \frac{4m\mathcal{E}^2}{\hbar^2 k(2\nu+1)^2}. \tag{36}$$

Substituting Eq. (35) in (29), we have

$$\alpha_\nu = \frac{2m\mathcal{E}}{\hbar^2(2\nu+1)} = \frac{\alpha_0}{2\nu+1}. \tag{37}$$

Next, we compute the term $\beta_\nu N_\nu = \beta_\nu \langle \phi_\nu | V_0 | \phi_\nu \rangle$. We can use the properties of the annihilation operator a_ν, namely

$$a_\nu|l\rangle_\nu = \sqrt{l}\,|l-1\rangle_\nu, \quad a_\nu^\dagger|l\rangle_\nu = \sqrt{l+1}\,|l+1\rangle_\nu, \quad x = (2\alpha_\nu)^{-1/2}(a_\nu + a_\nu^\dagger), \tag{38}$$

and the orthonormality of $|l\rangle_\nu$ to compute

$${}_\nu\langle l|x^2|\nu\rangle_\nu = (2\alpha_\nu)^{-1}[(2\nu+1)\delta_{l,\nu} + \sqrt{(\nu+1)(\nu+2)}\,\delta_{l,\nu+2} + \sqrt{\nu(\nu-1)}\,\delta_{l,\nu-2}]. \tag{39}$$

In view of Eqs. (27) and (39), we obtain, after some remarkable simplifications,

$$\beta_\nu N_\nu = \frac{\mathcal{E}}{2}. \tag{40}$$

A. Variational Sturmian approximation of order zero

For the variational Sturmian approximation of order zero, $\nu = n$, and Eq. (19) takes the form

$$(E_n - \mathcal{E})T - S = 0, \tag{41}$$

where

$$T = \langle \phi_n | \phi_n \rangle = 1, \quad S = W - \beta_n N_n, \quad W = \langle \phi_n | V | \phi_n \rangle. \tag{42}$$

According to Eqs. (41), (42), and (40), the energy eigenvalues E_n are given by

$$E_n = W + \frac{\mathcal{E}}{2}. \tag{43}$$

Next, we fix the parameter $\mathcal{E}$ using Eq. (26). This requires the computation of $dW/d\mathcal{E}$. We first evaluate the variation of W,

$$\delta W = (\delta\langle\phi_n|)V|\phi_n\rangle + \langle\phi_n|V(\delta|\phi_n\rangle) = 2\langle\phi_n|V(\delta|\phi_n\rangle) = 2\sum_{l=0}^{\infty} {}_n\langle n|V|l\rangle_n\, {}_n\langle l|(\delta|n\rangle_n). \tag{44}$$

Here we have made use of Eq. (34), the fact that the Sturmians and the potential V are real and $|l\rangle_n$ form a complete set of basis vectors.

We can compute ${}_n\langle l|(\delta|n\rangle_n)$ using the eigenvalue equation

$$(H_0 + \beta_n V_0)|j\rangle_n = \mathcal{E}_j|j\rangle_n, \tag{45}$$

where $\mathcal{E}_j = \hbar\omega_n(j+1/2)$. Taking the variation of both sides of this equation and computing the inner product with $|l\rangle_n$, we find

$${}_n\langle l|\delta|j\rangle_n = \frac{{}_n\langle l|V_0|j\rangle_n(\delta\beta_n)}{\mathcal{E}_j - \mathcal{E}_l} \quad \text{for } l \neq j. \tag{46}$$

Furthermore, using the fact that the eigenfunctions $\langle x|l\rangle_n$ are real, we can easily show that

$${}_n\langle l|(\delta|l\rangle_n) = 0. \tag{47}$$

Equations (44), (46) and (47) reduce the computation of δW to that of

$${}_n\langle l|V_0|n\rangle_n = \frac{k}{2}\,{}_n\langle l|x^2|n\rangle_n. \tag{48}$$

We have already computed ${}_n\langle l|x^2|n\rangle_n$ in Eq. (39). Substituting this equation in Eq. (48) and using Eqs. (46) and (44), we find, after some remarkable cancellations,

$$\delta W = \left(\frac{\delta\mathcal{E}}{2\mathcal{E}}\right)[\sqrt{n(n-1)}\,{}_n\langle n|V|n-2\rangle_n - \sqrt{(n+1)(n+2)}\,{}_n\langle n|V|n+2\rangle_n]. \tag{49}$$

Now, in view of Eqs. (43) and (49),

$$\frac{dE_n}{d\mathcal{E}} = \left(\frac{1}{2\mathcal{E}}\right)[\sqrt{n(n-1)}\,{}_n\langle n|V|n-2\rangle_n - \sqrt{(n+1)(n+2)}\,{}_n\langle n|V|n+2\rangle_n] + \frac{1}{2}.$$

Substituting this equation in Eq. (26) yields

$$\mathcal{E} = \sqrt{(n+1)(n+2)}\,{}_n\langle n|V|n+2\rangle_n - \sqrt{n(n-1)}\,{}_n\langle n|V|n-2\rangle_n. \tag{50}$$

Note that the right-hand side of this equation also involves $\mathcal{E}$. This is because $|l\rangle_n$ depend on $\mathcal{E}$.

Using Eqs. (50) and (43) we can express the energy eigenvalue E_n in terms of V. This yields

$$E_n = {}_n\langle n|V|n\rangle_n + \tfrac{1}{2}[\sqrt{(n+1)(n+2)}\,{}_n\langle n|V|n+2\rangle_n - \sqrt{n(n-1)}\,{}_n\langle n|V|n-2\rangle_n]. \tag{51}$$

For the ground state $n=0$ and Eq. (51) reduces to

$$E_0 = {}_0\langle 0|V|0\rangle_0 + \frac{1}{\sqrt{2}}\,{}_0\langle 0|V|2\rangle_0. \tag{52}$$

Note that the vectors $|l\rangle_n$ appearing in Eqs. (51) and (52) are those of Eq. (31) with $\mathcal{E}$ being a solution of Eq. (50).

Equations (51) and (52) are of limited importance. In practice, one obtains the energy eigenvalue E_n by substituting the solution of Eq. (50) in Eq. (43).

The variational Sturmian approximation of order zero, as outlined above, is a valid approximation scheme, if Eq. (50) has a unique positive solution $\mathcal{E}$. If such a solution does not exist, one may attempt to construct higher order variational Sturmian approximations. As we shall see in Sec. V, for all the potentials that we have considered, Eq. (50) has a unique positive solution. This is very remarkable, for this equation turns out to be an algebraic equation of order three for the quartic anharmonic oscillator and the quartic potential, and of order four for the Gaussian potential.

B. Variational Sturmian approximation of order one

In the variational sturmian approximation of order one, the number of Sturmians contributing to the eigenvector $|E\rangle$ is two. We shall denote them by $|\phi_n\rangle$ and $|\phi_m\rangle$.

The matrices T and W are Hermitian 2×2 matrices. They can be written in the form

$$T=\begin{pmatrix} 1 & t^* \\ t & 1 \end{pmatrix}, \quad W=\begin{pmatrix} v_n & w^* \\ w & v_m \end{pmatrix}, \tag{53}$$

where we have used the fact that the Sturmians are normalized and introduced

$$t:=\langle \phi_m|\phi_n\rangle, \quad v_\nu:=\langle \phi_\nu|V|\phi_\nu\rangle, \quad w:=\langle \phi_m|V|\phi_n\rangle. \tag{54}$$

Next, we construct the matrix S. In view of Eqs. (17) and (53),

$$S=\begin{pmatrix} v_n-\beta_n N_n & w^* \\ w & v_m-\beta_m N_m \end{pmatrix}. \tag{55}$$

Note that because the Sturmians for the harmonic oscillator are real-valued, t and w are real-valued functions of the parameter $\mathcal{E}$. In particular, the matrices T, W, and S are real and symmetric.

Substituting Eqs. (53) and (55) in the Eq. (19), making use of Eq. (40), and simplifying the resulting expression, we find

$$A\left(E-\frac{\mathcal{E}}{2}\right)^2+B\left(E-\frac{\mathcal{E}}{2}\right)+C=0, \tag{56}$$

where

$$A:=1-t^2, \quad B:=t(t\mathcal{E}+2w)-(v_n+v_m), \quad C:=v_n v_m-\left(\frac{t\mathcal{E}}{2}+w\right)^2. \tag{57}$$

Note that the coefficients A, B, and C are functions of $\mathcal{E}$. Equation (56) can be easily solved to express E in terms of $\mathcal{E}$. The result is

$$E=E_\pm:=\frac{\mathcal{E}}{2}+\frac{-B\pm\sqrt{B^2-4AC}}{2A}. \tag{58}$$

The next step is to determine $\mathcal{E}$ using the variational principle, i.e., setting $dE/d\mathcal{E}=0$. The resulting formulas are complicated and we shall not include them here.

We conclude this section with the following remarks.

(1) As seen from Eq. (58), the first order Sturmian approximation leads to a pair of energy eigenvalues. For the potentials which are related to V_0 via a limiting process, one expects these two eigenvalues to be those labeled by m and n. That is, for $n<m$,

$$E_n=E_-, \quad E_m=E_+. \tag{59}$$

(2) In the variational Sturmian approximation of order one, there are two variational equations $dE_\pm/d\mathcal{E}=0$. It is not clear whether these equations lead to a unique minimum for $E_\pm(\mathcal{E})$ with a positive value for $\mathcal{E}$. As we shall show in the following sections, for all the specific examples that we have considered each of these equations lead to a unique minimum with a positive value for $\mathcal{E}$. Lack of such a solution may be interpreted as the failure of the variational Sturmian approximation of order one.

C. Variational Sturmian approximation of order two

In the variational Sturmian approximation of order two, one uses three Sturmians to expand the energy eigenvectors $|E\rangle$. We shall denote these by $|\phi_{n_l}\rangle$ where $n_l\in\mathcal{S}_3:=\{n_1,n_2,n_3\}$.

The matrices T, W, and S are given by

$$T=\begin{pmatrix} 1 & t_1^* & t_2^* \\ t_1 & 1 & t_3^* \\ t_2 & t_3 & 1 \end{pmatrix}, \quad W=\begin{pmatrix} v_3 & w_1^* & w_2^* \\ w_1 & v_2 & w_3^* \\ w_2 & w_3 & v_1 \end{pmatrix}, \tag{60}$$

$$S=\begin{pmatrix} v_3-\beta_{n_3}N_{n_3} & w_1^* & w_2^* \\ w_1 & v_2-\beta_{n_2}N_{n_2} & w_3^* \\ w_2 & w_3 & v_1-\beta_{n_1}N_{n_1} \end{pmatrix}, \tag{61}$$

where we have used the fact that $|\phi_{n_l}\rangle$ are normalized and introduced

$$t_1:=\langle\phi_{n_2}|\phi_{n_3}\rangle, \quad t_2:=\langle\phi_{n_1}|\phi_{n_3}\rangle, \quad t_3:=\langle\phi_{n_1}|\phi_{n_2}\rangle, \quad v_l:=\langle\phi_{n_l}|V|\phi_{n_l}\rangle, \tag{62}$$

$$w_1:=\langle\phi_{n_2}|V|\phi_{n_3}\rangle, \quad w_2:=\langle\phi_{n_1}|V|\phi_{n_3}\rangle, \quad w_3:=\langle\phi_{n_1}|V|\phi_{n_2}\rangle. \tag{63}$$

Because the harmonic oscillator Sturmian functions are real-valued, t_l, v_l, and w_l are real, and T, W, and S are real symmetric matrices.

In view of Eq. (40), we can write the secular equation (19) in the form

$$A\left(E-\frac{\mathcal{E}}{2}\right)^3+B\left(E-\frac{\mathcal{E}}{2}\right)^2+C\left(E-\frac{\mathcal{E}}{2}\right)+D=0, \tag{64}$$

where

$$A:=1-\sum_{l=1}^{3} t_l^2+2t_1t_2t_3, \tag{65}$$

$$B:=\sum_{l=1}^{3}\left[(t_l^2-1)v_l+2t_l\xi_l\right]-2(t_1t_2\xi_3+t_3t_1\xi_2+t_2t_3\xi_1), \tag{66}$$

$$C:=v_1v_2+v_2v_3+v_3v_1+2(t_1\xi_2\xi_3+t_3\xi_1\xi_2+t_2\xi_3\xi_1)-\sum_{l=1}^{3}(\xi_l^2+2t_lv_l\xi_l), \tag{67}$$

$$D := \sum_{l=1}^{3} v_l \xi_l^2 - 2\xi_1\xi_2\xi_3 - v_1 v_2 V_3, \tag{68}$$

$$\xi_l := \tfrac{1}{2} t_l \mathcal{E} + w_l. \tag{69}$$

Equation (64) has, in general, three solutions. The desired eigenvalues are the minima of these solutions corresponding to positive values of $\mathcal{E}$. Again for the cases where V is related to V_0 by a limiting process the minima of the solutions of Eq. (64) correspond to E_{n_1}, E_{n_2}, and E_{n_3}.

V. APPLICATIONS

In this section, we apply our general results to compute the energy eigenvalues of a quartic anharmonic oscillator, a quartic potential, and a Gaussian potential.

A. The quartic anharmonic oscillator

Consider the potential

$$V(x) = \frac{k}{2}x^2 + \epsilon x^4. \tag{70}$$

In order to obtain the energy levels of this potential using variational Sturmian approximation of order zero, we need to calculate ${}_n\langle n|V|l\rangle_n$. We first use Eqs. (38) to compute

$$\begin{aligned} {}_n\langle n|x^4|l\rangle_n = (2\alpha_n)^{-2}[&3(2n^2+2n+1)\delta_{l,n} + 4(n+1)\sqrt{(n+1)(n+2)}\,\delta_{l,n+2} \\ &+ 2(2n-1)\sqrt{n(n-1)}\,\delta_{l,n-2} + \sqrt{(n+1)(n+2)(n+3)(n+4)}\,\delta_{l,n+4} \\ &+ \sqrt{(n-3)(n-2)(n-1)n}\,\delta_{l,n-4}]. \end{aligned} \tag{71}$$

In view of this equation and Eqs. (39) and (70),

$$W = {}_n\langle n|V|n\rangle_n = \frac{(2n+1)k}{4\alpha_n} + \frac{3(2n^2+2n+1)\epsilon}{4\alpha_n^2}, \tag{72}$$

$${}_n\langle n|V|n+2\rangle_n = \sqrt{(n+1)(n+2)}\left(\frac{k}{4\alpha_n} + \frac{(n+1)\epsilon}{\alpha_n^2}\right), \tag{73}$$

$${}_n\langle n|V|n-2\rangle_n = \sqrt{n(n-1)}\left(\frac{k}{4\alpha_n} + \frac{(2n-1)\epsilon}{2\alpha_n^2}\right), \tag{74}$$

Next, we substitute Eqs. (73) and (74) in Eq. (50). Using Eq. (37), we then obtain

$$\mathcal{E}^3 - p_n\mathcal{E} - q_n = 0, \tag{75}$$

where

$$p_n := \left(\frac{\hbar^2 k}{m}\right)\left(n+\frac{1}{2}\right)^2, \quad q_n := \left(\frac{\hbar^4\epsilon}{2m^2}\right)\left(n+\frac{1}{2}\right)^2(11n^2+9n+4). \tag{76}$$

It is not difficult to show that Eq. (75) has a single positive solution [this is true for any positive p_n and q_n] given by[9]

$$\mathcal{E} = \left(\frac{q_n}{2}\right)^{1/3}(1+\sqrt{1-r_n})^{1/3} + \left(\frac{p_n}{3}\right)\left(\frac{2}{q_n}\right)^{1/3}(1+\sqrt{1-r_n})^{-1/3}, \tag{77}$$

TABLE I. First 10 energy levels of the Hamiltonian $H=p^2+x^2+(x^4/10)$ in units where $\hbar=1$. $E_n^{\#}$ are the highly accurate numerical values of Ref. 10. E_n are the values obtained using the zero order variational Sturmian approximation. $E_n^{\rm CSA}$ are the values obtained by the zero order conventional Sturmian approximation in Ref. 5. $E_n^{(0)}$ and $E_n^{(1)}$ are the energy eigenvalues obtained using the zero and first order perturbation theory, respectively.

n	$E_n^{\#}$	E_n	$\frac{\lvert E_n-E_n^{\#}\rvert}{E_n^{\#}}$	$E_n^{\rm CSA}$	$\frac{\lvert E_n^{\rm CSA}-E_n^{\#}\rvert}{E_n^{\#}}$	$E_n^{(0)}$	$\frac{\lvert E_n^{(0)}-E_n^{\#}\rvert}{E_n^{\#}}$	$E_n^{(1)}$	$\frac{\lvert E_n^{(1)}-E_n^{\#}\rvert}{E_n^{\#}}$
0	1.065 286	1.066 92	1.5×10^{-3}	1.07500	9.1×10^{-3}	1.000	0.061	1.075	9.1×10^{-3}
1	3.306 872	3.311 82	1.5×10^{-3}	3.37500	0.021	3.000	0.032	3.450	0.043
2	5.747 959	5.750 52	4.5×10^{-4}	5.97500	0.040	5.000	0.13	5.975	0.039
3	8.352 678	8.349 85	3.4×10^{-4}	8.87500	0.063	7.000	0.16	8.875	0.063
4	11.098 60	11.0881	9.5×10^{-4}	12.0750	0.088	9.000	0.19	12.08	0.088
5	13.969 93	13.9499	1.4×10^{-3}			11.00	0.21	15.58	0.11
6	16.954 79	16.9235	1.8×10^{-3}			13.00	0.23	19.38	0.14
7	20.043 86	19.9998	2.2×10^{-3}			15.00	0.25	23.48	0.17
8	23.229 55	23.1715	2.5×10^{-3}			17.00	0.27	27.88	0.20
9	26.505 55	26.4322	2.8×10^{-3}			19.00	0.28	32.58	0.23

where

$$r_n:=\frac{4p_n^3}{27q_n^2}=\left(\frac{8n+4}{11n^2+9n+4}\right)^2 r_0,\quad r_0:=\frac{mk^3}{108\hbar^2\epsilon^2}. \tag{78}$$

The right-hand side of Eq. (77) is manifestly real and positive for $r_n\leqslant 1$. It is not difficult to check that it is also real and positive for $r_n>1$. In fact, we can express $\mathcal{E}$ in the form

$$\mathcal{E}=2\sqrt{\frac{p_n}{3}}\cos\left(\frac{\phi_n}{3}\right)=\sqrt{\frac{k}{3m}}(2n+1)\cos\left(\frac{\phi_n}{3}\right), \tag{79}$$

where

$$\phi_n:=\tan^{-1}(\sqrt{r_n-1}). \tag{80}$$

Note that for $r_n<1$, ϕ_n is imaginary, but $\cos(\phi_n/3)$ is still real and positive.

Having fixed the parameter $\mathcal{E}$, we can determine the energy eigenvalues E_n using Eqs. (43) and (72). We first use Eqs. (37) and (79) to compute

$$\alpha_n=\left(\frac{2}{\hbar}\right)\sqrt{\frac{mk}{3}}\cos\left(\frac{\phi_n}{3}\right). \tag{81}$$

Then substituting this equation in Eq. (72) and using Eq. (43), we find

$$E_n=\left(\frac{\hbar}{24}\right)\sqrt{\frac{3k}{m}}(2n+1)\left[7+3\tan^2\left(\frac{\phi_n}{3}\right)\right]\cos\left(\frac{\phi_n}{3}\right)+\left(\frac{9\hbar^2\epsilon}{16mk}\right)(2n^2+2n+1)\left[1+\tan^2\left(\frac{\phi_n}{3}\right)\right]. \tag{82}$$

In particular, the ground state energy is given by

$$E_0=\left(\frac{\hbar}{24}\right)\sqrt{\frac{3k}{m}}\left[7+3\tan^2\left(\frac{\phi_0}{3}\right)\right]\cos\left(\frac{\phi_0}{3}\right)+\left(\frac{9\hbar^2\epsilon}{16mk}\right)\left[1+\tan^2\left(\frac{\phi_0}{3}\right)\right]. \tag{83}$$

In Table I, we list the numerical values obtained using Eq. (82) for the first 10 energy levels of a quartic anharmonic oscillator with $m=1/2$, $k=2$, $\epsilon=1/10$ in units where $\hbar=1$. This table also

TABLE II. Energy levels of the Hamiltonian $H=p^2+x^2+x^4/10$ obtained using the first order variational Sturmian approximation. δE_n stands for $|E_n-E_n^{\#}|/E_n^{\#}$.

$\mathcal{S}_2$	E_0	δE_0	E_1	δE_1	E_2	δE_2	E_3	δE_3	E_4	δE_4
{0,2}	1.066 14	8.0×10^{-4}			5.761 17	2.3×10^{-3}				
{1,3}			3.309 22	7.1×10^{-4}			8.372 84	2.4×10^{-3}		
{2,4}					5.745 58	4.1×10^{-4}			9.663 70	0.13
{0,4}	1.066 20	8.6×10^{-4}							9.645 02	0.13

includes the accurate numerical values of Ref. 10, the values obtained using the conventional Sturmian approximation and the zero and first order perturbation theory. [The zero and first order perturbation theory yield

$$E_n^{(0)}=\hbar(k/m)^{1/2}(n+1/2),\quad E_n^{(1)}=E_n^{(0)}+3\hbar^2\epsilon^2(2n^2+2n+1)/(4mk), \tag{84}$$

respectively.] The relative difference between the results of the variational Sturmian approximation of order zero with the highly accurate numerical results ($E_n^{\#}$) of Ref. 10, i.e., the quantity $|E_n-E_n^{\#}|/E_n^{\#}$, varies between 3.38×10^{-4} and 2.77×10^{-3}. For the ground state, this number is 1.53×10^{-3}. Even for the lowest lying energy levels where perturbation theory yields reliable results, the zero order variational Sturmian approximation produces more accurate values than both the zero and first order perturbation theory. As seen from Table I, the variational Sturmian approximation is better than the conventional Sturmian approximation.

In the remainder of this section we present the results obtained using the first and second order variational Sturmian approximation. The numerical results are respectively presented in Tables II and III.

As we explained in Sec. IV, in the variational Sturmian approximation of order one one chooses an indexing set $\mathcal{S}_2$ consisting of two Sturmians to be included in the expansion of the eigenvector $|E\rangle$. One then solves the corresponding secular equation (19), expresses the solutions $E_\pm$ in terms of the parameter $\mathcal{E}$, and finds the minima of $E_\pm(\mathcal{E})$. In general, $E_\pm$ are complicated functions of $\mathcal{E}$. However, it turns out that for all the cases that we considered $E_\pm$ has a unique minimum corresponding to a positive value of $\mathcal{E}$.

In order to choose the indexing set $\mathcal{S}_2$, we first note that the Sturmian functions $\langle x|\phi_n\rangle$ with even (respectively, odd) n are even (respectively odd) functions of x. We expect the energy eigenfunctions of the anharmonic oscillator (70) to have the same parity structure as the Sturmian functions. This, in particular, suggests that in the calculation of E_0 we should take $\mathcal{S}_2=\{0,2\}$.

For a quartic anharmonic oscillator with $m=1/2$, $k=2$, $\epsilon=1/10$, the first order variational Sturmian approximation corresponding to $\mathcal{S}_2=\{0,2\}$ yields $E_0=E_-=1.066\,14$ and $E_2=E_+=5.761\,17$. The value obtained for E_0 differs from the accurate numerical value by one part in 10^4. It is one order of magnitude better than the value obtained using the zero order variational Sturmian approximation. The value for E_2 is however less accurate. One may argue that the choice made for $\mathcal{S}_2$ is appropriate only for the ground state. In order to compute E_2 using the first order

TABLE III. Energy levels of the Hamiltonian $H=p^2+x^2+x^4/10$ obtained using the second order variational Sturmian approximation with the choice {0,2,4} for the indexing set $\mathcal{S}_3$. $E_n^{\#}$ are the highly accurate numerical values of Ref. 10.

n	$E_n^{\#}$	E_n	$\frac{\lvert E_n-E_n^{\#}\rvert}{E_n^{\#}}$
0	1.065 286	1.066 13	7.9×10^{-4}
2	5.750 52	5.752 75	8.3×10^{-4}
4	11.098 60	9.684 83	0.127

variational Sturmian approximation, one may alternatively choose $\mathcal{S}_2=\{2,4\}$. This choice yields $E_2=E_-=5.745\,58$ and $E_4=E_+=9.6637$. Again this value for E_2 is an order of magnitude better than the value obtained using the zero order variational Sturmian approximation, whereas the value for E_4 is less accurate. One can also try $\mathcal{S}_2=\{0,4\}$. As expected, this choice yields a less accurate value than the choices $\mathcal{S}_2=\{0,2\}$ and $\mathcal{S}_2=\{2,4\}$ for both E_0 and E_4.

For the calculation of the first excited state we choose $\mathcal{S}_2=\{1,3\}$. Then we find $E_1=E_-=3.309\,22$ and $E_3=E_+=8.372\,84$. Once again the first order variational Sturmian approximation of order one with the choice $\mathcal{S}_2=\{1,3\}$ yields a more accurate result for E_1 and a less accurate result for E_3.

In general, in the calculation of the energy levels E_n with $n\geqslant 2$, there are two alternative choices for the indexing set $\mathcal{S}_2$. In view of the parity properties of the eigenvectors, these are $\{n,n+2\}$ and $\{n-2,n\}$. The fact that there is no physical reason to distinguish between these two choices suggests that for these levels one should consider the second order variational Sturmian approximation with the choice $\mathcal{S}_3=\{n-2,n,n+2\}$.

Table III includes the results of the second order variational Sturmian approximation corresponding to the indexing set $\mathcal{S}_3=\{0,2,4\}$. This approximation yields more accurate values for E_0 than the zero and first order variational Sturmian approximations. However, contrary to our expectation the value obtained for E_2 is less accurate than the one given by the zero order approximation and the first order approximation with $\mathcal{S}_2=\{2,4\}$.

B. The quartic potential

Consider the quartic potential

$$V(x)=\epsilon x^4. \tag{85}$$

We can easily obtain the energy levels of this potential using the zero order variational Sturmian approximation by simply setting $k=0$ in our formulas for the quartic anharmonic oscillator. Substituting $k=0$ in (76), we can write Eq. (75) in the form

$$\mathcal{E}=q_n^{1/3}=\hbar\left(\frac{\hbar\epsilon}{2m^2}\right)^{1/3}\left[\left(n+\frac{1}{2}\right)^2(11n^2+9n+4)\right]^{1/3}. \tag{86}$$

In view of Eqs. (37), (43), (72), (86), and $k=0$, we have

$$\alpha_n=\hbar^{-1}(m\hbar\epsilon)^{1/3}\left(\frac{11n^2+9n+4}{2n+1}\right)^{1/3}, \tag{87}$$

$$E_n=\left(\frac{8n+4}{11n^2+9n+4}\right)^{2/3}\left(\frac{17}{7}n^2+\frac{15}{7}n+1\right)E_0, \tag{88}$$

$$E_0:=\frac{7\hbar}{8}\left(\frac{\hbar\epsilon}{2m^2}\right)^{1/3}. \tag{89}$$

In Table IV, we present the values obtained using Eq. (88) for the energy levels of a quartic potential with $m=1/2$ and $\epsilon=1$ in units where $\hbar=1$. This table also includes accurate numerical results $E_n^{\#}$ and the results of the zero and first order WKB approximation given in Refs. 11 and 12. The relative difference $|E_n-E_n^{\#}|/E_n^{\#}$ is about 0.04 for the ground state and ranges between 6.4×10^{-4} and 8.7×10^{-3} for the energy levels E_2,E_4,E_6,E_8,E_{10}, and E_{16}.

Table V includes the results of the first and second order variational Sturmian approximation for E_0,E_2, and E_4.

TABLE IV. Energy levels of the Hamiltonian $H=p^2+x^4$ in units where $\hbar=1$. $E_n^{\#}$ are the highly accurate numerical values of Refs. 11 and 12. E_n are the values obtained using the zero order variational Sturmian approximation. $E_n^{\mathrm{WKB}(0)}$ and $E_n^{\mathrm{WKB}(1)}$ are the values obtained using the zero and first order WKB approximation (Ref. 11), respectively.

n	$E_n^{\#}$	E_n	$\frac{\lvert E_n-E_n^{\#}\rvert}{E_n^{\#}}$	$E_n^{(0)}$	$\frac{\lvert E_n^{\mathrm{WKB}(0)}-E_n^{\#}\rvert}{E_n^{\#}}$	$E_n^{(1)}$	$\frac{\lvert E_n^{\mathrm{WKB}(1)}-E_n^{\#}\rvert}{E_n^{\#}}$
0	1.060 362	1.102 43	0.040	0.87	0.17	0.98	0.076
1		3.869 29					
2	7.455 697	7.460 48	6.4×10^{-4}	7.4140	5.6×10^{-3}	7.4558	1.4×10^{-5}
3		11.6007					
4	16.261 826	16.1691	5.7×10^{-3}	16.233 615	1.7×10^{-3}	16.261 937	6.8×10^{-6}
6	26.528 471	26.3349	7.3×10^{-3}	26.506 336	8.3×10^{-4}	26.528 513	1.9×10^{-5}
8	37.923 001	37.6218	7.9×10^{-3}	37.904 472	4.9×10^{-4}	37.923 021	5.3×10^{-7}
10	50.256 255	49.8404	8.3×10^{-3}	50.240 152	3.1×10^{-4}	50.256 266	2.2×10^{-7}
16	91.798 06	91.0012	8.7×10^{-3}				

C. The Gaussian potential

Consider the Gaussian potential

$$V(x)=-\lambda e^{-\epsilon x^2/2}. \tag{90}$$

In order to apply the results of Sec. IV to this potential, we write $V(x)=\tilde{V}(x)-\lambda$ where

$$\tilde{V}(x)=\lambda(1-e^{-\epsilon x^2/2}). \tag{91}$$

Then as ϵ tends to zero, $\tilde{V}(x)$ approaches to the harmonic oscillator potential (27) with $k=\lambda\epsilon$.

Clearly, the energy eigenvalues associated with V and $\tilde{V}$ are related by

$$E_n=\tilde{E}_n-\lambda. \tag{92}$$

In the following we use the zero order variational Sturmian approximation to obtain the ground state energy of the potential $\tilde{V}$. The excited energy levels can be obtained similarly.

We first note that for the ground state $n=0$, and Eq. (50) for the potential $\tilde{V}$ takes the form

$$\mathcal{E}=\sqrt{2}\,{}_0\langle 0|\tilde{V}|2\rangle_0=\sqrt{2}{}_0\langle 0|V|2\rangle_0=-\sqrt{2}\lambda\,{}_0\langle 0|e^{-\epsilon x^2/2}|2\rangle_0=-\sqrt{2}\lambda\int_{-\infty}^{\infty}{}_0\langle 0|x\rangle e^{-\epsilon x^2/2}\langle x|2\rangle_0\,dx. \tag{93}$$

We can evaluate the right-hand side of (93) using the well-known expression for the eigenfunctions of the harmonic oscillator, namely (32) and

$$\langle x|2\rangle_0=\left(\frac{\alpha_0}{4\pi}\right)^{1/4}(2\alpha_0x^2-1)e^{-\alpha_0x^2/2}. \tag{94}$$

TABLE V. Energy levels of the Hamiltonian $H=p^2+x^4$ obtained using the first and second order variational Sturmian approximation. N is the order of the approximation. $E_n^{\#}$ are the accurate numerical results reported in Ref. 11.

N	$\mathcal{S}_N$	E_0	$\frac{\lvert E_0-E_0^{\#}\rvert}{E_0^{\#}}$	E_2	$\frac{\lvert E_2-E_2^{\#}\rvert}{E_2^{\#}}$	E_4	$\frac{\lvert E_4-E_4^{\#}\rvert}{E_4^{\#}}$
2	{0,2}	1.081 10	0.0196	7.608 84	0.0205		
2	{2,4}			7.426 69	3.89×10^{-3}	16.4461	0.0113
2	{0,4}	1.081 66	0.0200			16.4114	9.12×10^{-3}
3	{0,2,4}	1.080 10	0.0195	7.565 28	0.0147	16.5670	0.0188

Substituting Eqs. (32) and (94) in Eq. (93) and performing the necessary calculations, we find

$$\mathcal{E}(\mathcal{E}+p)^3=\lambda^2p^2, \tag{95}$$

where

$$p:=\frac{\hbar^2\epsilon}{4m}. \tag{96}$$

Introducing

$$\eta:=1+\frac{\mathcal{E}}{p}, \tag{97}$$

we can write Eq. (95) in the form

$$f(\eta):=\eta^4-\eta^3-r=0, \tag{98}$$

where

$$r:=\frac{\lambda^2}{p^2}=\frac{16\lambda^2m^2}{\hbar^4\epsilon^2}. \tag{99}$$

It is not difficult to show that for all $r>0$, $f(\eta)$ has a single minimum at $\eta=3/4$. The minimum is $f(3/4)=-(27/256+r)<0$. Furthermore, $f(0)=f(1)=-r<0$ and $\lim_{\eta\to\infty}f(\eta)=\infty$. Therefore, $f(\eta)$ has a single positive root that is greater than 1. This root is given by

$$\eta_\star=\tfrac{1}{4}(1+2\xi+\sqrt{3-4\xi^2+\xi^{-1}}), \tag{100}$$

where

$$\xi:=\tfrac{1}{2}\sqrt{1-a+b},\quad a:=\tfrac{3}{2}\zeta(1+\sqrt{1+\zeta^3})^{1/3},$$

$$b:=\tfrac{3}{2}\zeta(-1+\sqrt{1+\zeta^3})^{1/3},\quad \zeta:=\frac{4}{3}(4r)^{1/3}.$$

In view of Eq. (97) and the fact that $\eta_0>1$, Eq. (95) has a single positive solution, namely

$$\mathcal{E}=p(\eta_\star-1). \tag{101}$$

Having obtained the parameter $\mathcal{E}$, we next compute

$$W={}_0\langle 0|\tilde{V}|0\rangle_0=\lambda(1-\sqrt{1-\eta_\star^{-1}}). \tag{102}$$

Here we have made use of Eqs. (32), (37), (91), (96), and (101). Substituting this equation and Eq. (101) in Eq. (43) and using Eqs. (92) and (99), we find the ground state energy of the Gaussian potential (90) to be

$$E_0=\tilde{E}_0-\lambda=-\lambda\left[\sqrt{1-\eta_\star^{-1}}+\frac{1-\eta_\star}{2\sqrt{r}}\right]. \tag{103}$$

In order to reveal the asymptotic behavior of E_0, we investigate the power series expansion of the right-hand side of Eq. (103).

For $r\gg 1$, i.e., $(\epsilon/\lambda)\to 0$,

$$E_0 = -\lambda[1 - r^{-1/4} + \tfrac{3}{8}r^{-1/2} - \tfrac{1}{32}r^{-3/4} - \tfrac{1}{128}r^{-1} + \mathcal{O}(r^{-5/4})]. \tag{104}$$

For $r \ll 1$, i.e., $(\epsilon/\lambda) \to \infty$,

$$E_0 = -\left(\frac{\lambda\sqrt{r}}{2}\right)[1 - r + 3r^2 - 13r^3 + 68r^4 + \mathcal{O}(r^5)]. \tag{105}$$

Therefore, for fixed λ,

$$\lim_{\epsilon \to 0^+} E_0 = -\lambda, \tag{106}$$

$$\lim_{\epsilon \to \infty} E_0 = \lim_{\epsilon \to \infty}\left[-\frac{4m^2\lambda^2}{\hbar^2\epsilon}\right] = 0^-, \tag{107}$$

and for fixed ϵ,

$$\lim_{\lambda \to 0^+} E_0 = \lim_{\lambda \to 0}\left[-\frac{4m^2\lambda^2}{\hbar^2\epsilon}\right] = 0^-, \tag{108}$$

$$\lim_{\lambda \to \infty} E_0 = -\infty. \tag{109}$$

Clearly, the asymptotic behavior of E_0, as given by Eqs. (106)–(109), agrees with the qualitative analysis of the eigenvalue problem for the Gaussian potential.

It is not difficult to see that in the limit $\epsilon \to 0$ perturbation theory provides reliable results. Writing the Gaussian potential (90) in the form

$$V = V_0 + \delta V, \tag{110}$$

with V_0 given by Eq. (23) and performing the standard calculations,[1] we find that the zero and first order perturbation theory yield, respectively,

$$E_0^{(0)} = -\lambda(1 - r^{-1/4}), \tag{111}$$

$$E_0^{(1)} = -\lambda(1 + r^{-1/4})^{-1/2} = -\lambda[1 - \tfrac{1}{2}r^{-1/4} + \tfrac{3}{8}r^{-1/2} - \tfrac{5}{16}r^{-3/4} + \mathcal{O}(r^{-1})]. \tag{112}$$

Here $E_0^{(l)}$ is the ground state energy for the Gaussian potential (90) obtained using the lth order perturbation theory.

Comparing Eq. (104) with Eqs. (111) and (112), one finds that in the pertubative region where $r \gg 1$, the variational Sturmian approximation of order zero agrees with the results of the perturbation theory. In fact, since by construction E_0 is the expectation value of the energy of the Sturmian $|\phi_0\rangle$, the fact that $E_0 < E_0^{(0)}$ shows that even in the pertubative region the variational Sturmian approximation of order zero is a better approximation than the zero order perturbation theory. By the same reasoning, because $E_0 > E_0^{(1)}$, the first order perturbation theory yields a better result. Note however that the wave function obtained in the first order perturbation theory is an infinite sum whereas the wave function in the zero order Sturmian approximation is given explicitly.

Another interesting limit is the delta function limit of the potential V where $\lambda = a\sqrt{\epsilon/(2\pi)}$, $\epsilon \to \infty$, and $V(x) \to -a\,\delta(x)$. Here a is a fixed coupling constant. In this limit $r \to 0$ and the ground state energy is given by Eq. (105) according to

$$E_0 = -\frac{ma^2}{\pi\hbar^2}. \tag{113}$$

This result has the same order of magnitude as the exact result:

$$E_0 = -\frac{ma^2}{2\hbar^2}. \tag{114}$$

VI. DISCUSSION AND CONCLUSION

We have outlined a variationally improved Sturmian approximation and applied our results to the harmonic oscillator Sturmians. For these Sturmians we could solve the associated variational problem in the zero order Sturmian approximation exactly. We have used our variational Sturmian approximation in the calculation of the energy levels of various potentials. We have shown that using a few harmonic oscillator Sturmians, one obtains quite reliable results. In general, the variational Sturmian approximation is a better approximation than the conventional Sturmian approximation.

Because the harmonic oscillator potential is a confining potential, we expect that the method is more suitable for the confining potentials such as the quartic anharmonic oscillator and the quartic potential. We can base this argument on a more quantitative reasoning by addressing the problem of classifying the potentials for which the Sturmian approximation is exact. It is not difficult to show that these potentials satisfy

$$V(\vec{x}) = E - \mathcal{E} + \left(\frac{\Sigma_{\nu=0}^{N} \Sigma_{\alpha} C_{\nu}^{\alpha} \beta_{\nu} \phi_{\nu,\alpha}(\vec{x})}{\Sigma_{\nu=0}^{N} C_{\nu}^{\alpha} \phi_{\nu,\alpha}(\vec{x})} \right) V_0(\vec{x}), \tag{115}$$

where E, $\mathcal{E}$, and C_{ν}^{α} are constants and $\phi_{\nu,\alpha}(\vec{x}) := \langle \vec{x} | \phi_{\nu}, \alpha \rangle$. Equation (115) follows from Eqs. (1), (2), (3), and (11).

For example, the potentials for which the first order harmonic oscillator Sturmian approximation with $\mathcal{S}_2 = \{0,2\}$ yields an exact eigenfunction are of the form

$$V(x) = E - \frac{\hbar^2 \alpha_0}{2m} + \left(\frac{\hbar^2 \alpha_0^2}{2m} \right) \left[\frac{e^{-2\alpha_0 x^2/5} + \left(\frac{\zeta}{5} \right)(2\alpha_0 x^2 - 5)}{e^{-2\alpha_0 x^2/5} + 5\zeta(2\alpha_0 x^2 - 5)} \right] x^2, \tag{116}$$

where α_0 is a real parameter with the dimension of (length)$^{-2}$ and ζ is a dimensionless real parameter. As seen from Eq. (116), these potentials tend to the harmonic oscillator potential for $|x| \to \infty$. In particular, as $|x| \to \infty$, $V \to \infty$. This asymptotic behavior is also valid for higher order harmonic oscillator Sturmian approximations. This observation shows that the harmonic oscillator Sturmian approximation is more reliable for confining potentials.

We conclude this paper with a couple of remarks.

(1) The variational principle used in the variational Sturmian approximation leads to an algebraic (nondifferential) equation for the parameter $\mathcal{E}$. The acceptable solutions for this equation are those which are real and positive. The fact that for all the cases we consider there is a unique real positive solution corresponding to each eigenvalue E_n is quite remarkable. This observation may be viewed as a consistency check for the Sturmian approximation.

(2) In our selection of the Sturmians in the first and higher order Sturmian approximation, we used the information about the parity properties of the Sturmians and the energy eigenfunctions. For example we ruled out the first order variational Sturmian approximation with $\mathcal{S}_2 = \{0,1\}$. If we perform the necessary calculations, we find that for this choice the functions t and w vanish identically and the matrices T and S are diagonal. Therefore, the secular equation (19) yields the same results as the zero order Sturmian approximation. This can also be seen from the results of Ref. 5.

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Hartree approximation I: The fixed point approach

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We consider the Hartree approximation at finite temperature. We give a justification of this approximation by using the methods of functional integration. For finite temperatures, a fixed point approach to solving the Hartree problem is proposed. For a class of two-body interactions and background potentials that includes the Coulomb interaction, we prove that the Hartree equation has a unique solution provided the coupling constant is small. We also prove a similar result for local density theory. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379747]

I. INTRODUCTION

For an interacting fermionic system, we consider the approximation that, diagrammatically, can be written as in Fig. 1. In solid state physics, this approximation is also called the Hartree approximation. This approximation is different from the classical Hartree approximation,[1–3] which neglects the Fermi–Dirac statistics for particles. In the following, we will refer to diagram 1 (including the Fermi–Dirac statistics) as the Hartree approximation. The equations for this approximation [see Eqs. (16) and (18)] are formally the same as the equations for the restricted classical Hartree approximation. Consider for example zero temperature. Then, in both cases, the equations are $(H_0+n*v)\,\eta_i=\lambda_i\eta_i$, where $n=\Sigma_i|\eta_i|^2$ is the density of particles and v is the two-body interaction. In the restricted classical Hartree approximation, the only constraint imposed on $\{\eta_i\}_i$ is that they are normalized.[4] These functions can be the same, for example. Thus, this constraint does not prevent particles from collapsing into a single state. This problem has been considered in Ref. 5 and classified as an open question. In a recent paper,[6] it was proven that indeed, for the restricted classical Hartree problem, particles do collapse into a single state under special conditions and the approximation reduces to a purely local density approximation. For what we here call the Hartree approximation, this collapse will not happen because of the Pauli exclusion principle, which only allows one particle in each state. We also mention that the classical Hartree approximation cannot be extended at finite temperatures. For this, one has to assume a statistics on the particles.

One can see that the Hartree approximation follows from the Hartree–Fock approximation if one omits the exchange diagram (Fig. 2). Let us mention a few reasons why the Hartree approximation is of interest. One reason for considering this approximation rather than the Hartree–Fock approximation is that the later one may give up to 100% error when applied to homogeneous electron gas.[7] Another reason is that analyzing diagram 1 is the first step towards a rigorous analysis of the solutions of the local density approximation. Also, we found that the Hartree approximation is equivalent to the Gaussian approximation.[8] Given the importance of the Gaussian approximation in the study of the bosonic quantum fields, this equivalence is another strong reason for considering the Hartree approximation. Finally, this approximation may be interesting because the symmetry breaking phenomenon is present. We found that, at low temperatures and in the absence of any background potential, the stable solution of the Hartree equation corresponds to a nonuniform, periodic density of particles.

We decided to divide our results in three parts, where three important aspects of this model are analyzed. Our analysis covers only the small limit of the coupling constants. In the first part, we

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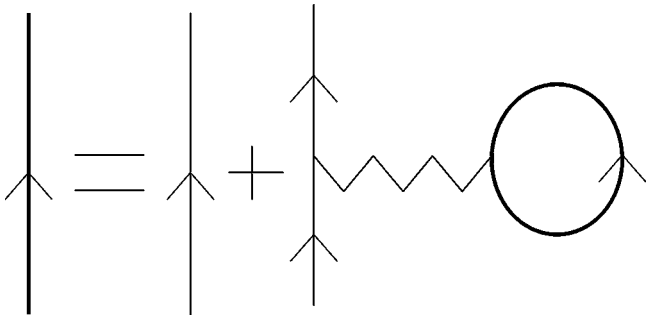

FIG. 1. The Hartree equation: the thick lines represents the exact propagator.

investigate the Hartree approximation for finite systems (i.e., finite volumes and finite number of particles). In the second part, we investigate the thermodynamic limit and in the third part we present the proof of a symmetry breaking within this model. This paper includes the first part. The main result is that, at finite temperatures, the Hartree equation can be formulated as a fixed point problem. The fixed point approach is used then to prove that there is a unique solution to the Hartree equations, provided the coupling constant is small enough. A similar result is proven for the local density theory. The fixed point approach has been advocated by some pedagogical text books[9] as a standard method for solving the Hartree or Hartree–Fock equations. Various iterative schemes have been proposed for finding this fixed point. In practice, all these iterative schemes may have convergence problems,[10–12] and there are only a few rigorous results about their convergency.[11–14] The fact that these schemes converge does not necessarily mean that the absolute minimum of the energy has been achieved. All one can say, in general, is that the absolute minimum exists.[4,5] The uniqueness is still an open problem.[15] To our knowledge, our result is the first step in this direction. Unfortunately, the result is valid only in the small limit of the coupling constants. Still, as we shall see, this limit is not trivial at all.

II. HARTREE APPROXIMATION FROM A FUNCTIONAL INTEGRAL POINT OF VIEW

We consider in this paper only spin independent interactions. Therefore, we will not take into account the spin degree of freedom. Let us consider a two-body interaction:

$$L_I=\frac{1}{2}\int \psi^\dagger(\vec{x})\psi^\dagger(\vec{y})v(\vec{x}-\vec{y})\psi(\vec{y})\psi(\vec{x})d\vec{x}\,d\vec{y}. \tag{1}$$

Suppose that the one particle system is described by a Hamiltonian $H_0:\mathcal{D}(H_0)\subset\mathcal{H}\to\mathcal{H}$, where $\mathcal{H}$ is a Hilbert space. In the Euclidean region (i.e., imaginary time), the system is described by the interacting measure:[16]

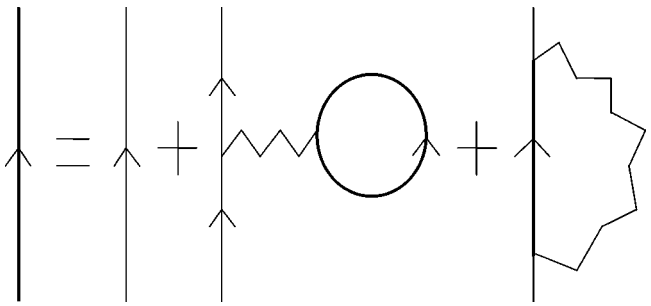

FIG. 2. The Hartree–Fock equation: the thick line represents the exact propagator.

$$d\mu = e^{-\mathcal{A}(\psi^\dagger,\psi)} d\mu_C \Big/ \int e^{-\mathcal{A}(\psi^\dagger,\psi)} d\mu_C, \tag{2}$$

where the action is given by

$$\mathcal{A}(\psi^\dagger,\psi) = \frac{1}{2}\int \psi^\dagger(\vec{x},\tau)\psi^\dagger(\vec{y},\tau')v(\vec{x}-\vec{y})\delta(\tau-\tau')\psi(\vec{y},\tau')\psi(\vec{x},\tau)d\vec{x}\,d\tau\,d\vec{y}\,\tau'. \tag{3}$$

The Grassmann Gaussian measure, μ_C, corresponds to covariance:

$$C = (\partial_\tau + H_0 - \mu)^{-1}. \tag{4}$$

The variable τ takes values in $I=[-\beta/2,\beta/2]$ and anti-periodic boundary conditions are imposed at $\pm\beta/2$. By using the anti-commutation relations (in the Euclidean region, ψ and $\psi^\dagger$ anti-commutes), the action can be written in the analogous form

$$\mathcal{A}(\psi^\dagger,\psi) = \frac{1}{2}\int [\hat{n}(\vec{x},\tau)-n(\vec{x})]v(\vec{x}-\vec{y})\delta(\tau-\tau')[\hat{n}(\vec{y},\tau')-n(\vec{y})]d\vec{x}\,d\tau\,d\vec{y}\,\tau'$$
$$+\int V_n(\vec{x})\hat{n}(\vec{x},\tau)d\vec{x}\,d\tau - E_n, \tag{5}$$

where $\hat{n}(\vec{x},\tau)=\psi^\dagger(\vec{x},\tau)\psi(\vec{x},\tau)$ is the density of particles operator, V_n and E_n are given by

$$V_n(\vec{x}) = \int v(\vec{x}-\vec{y})n(\vec{y})d\vec{y}, \tag{6}$$

$$E_n = \beta/2\int n(\vec{x})v(\vec{x}-\vec{y})n(\vec{y})d\vec{x}\,d\vec{y}, \tag{7}$$

and $n(\vec{x})$ is yet an unknown function. The way to the Hartree approximation is similar to the way to the Gaussian approximation for boson fields.[8] Our goal is to cancel the quadratic term of the action by a change of covariance and by normal ordering.

Proposition 1: Let C' be defined by

$$C' = (\partial_\tau + H_0 + V_n - \mu)^{-1}.$$

Then

$$d\mu = e^{-\mathcal{A}'(\psi^\dagger,\psi)} d\mu_{C'} \Big/ \int e^{-\mathcal{A}'(\psi^\dagger,\psi)} d\mu_{C'},$$

where

$$\mathcal{A}'(\psi^\dagger,\psi) = \frac{1}{2}\int (\hat{n}(x)-n(\vec{x}))v(x-y)(\hat{n}(y)-n(\vec{y}))dx\,dy,$$

and $v(x-y)\equiv v(\vec{x}-\vec{y})\delta(\tau-\tau')$. We denoted $x\equiv(\tau,\vec{x})$.

Proof: Let us consider an orthonormal basis $\{e_j\}_{j\in\mathbf{N}}$. For $f\in\mathcal{H}$, we use the notation

$$\psi(f) \equiv \int dx f(x)\psi(x). \tag{8}$$

The quadratic term can be expressed as

$$\int V_n(\vec{x})\hat{n}(x)dx=\Sigma_{i,j}\langle e_i, V_n(\vec{x})e_j\rangle \psi^\dagger(e_i)\psi(e_j). \tag{9}$$

We notice that this operator commutes with the field operator. Then we have successively

$$\begin{aligned} e^{-\int V_n(\vec{x})\hat{n}(x)dx}\, d\mu_C &= e^{-\Sigma_{i,j}\langle e_i, V_n e_j\rangle \psi^\dagger(e_i)\psi(e_j)}\frac{1}{\det C^{-1}}\, e^{-\Sigma_{i,j}\langle e_i, C^{-1}e_j\rangle \psi^\dagger(e_i)\psi(e_j)}\prod_{i,j} d\psi^\dagger(e_i)d\psi(e_j) \\ &= \frac{1}{\det C^{-1}}\, e^{-\Sigma_{i,j}\langle e_i(C^{-1}+V_n)e_j\rangle \psi^\dagger(e_i)\psi(e_j)}\prod_{i,j} d\psi^\dagger(e_i)d\psi(e_j) \\ &= \frac{\det[1+V_nC]}{\det C'^{-1}}\, e^{-\Sigma_{i,j}\langle e_i, C'^{-1}e_j\rangle \psi^\dagger(e_i)\psi(e_j)}\prod_{i,j} d\psi^\dagger(e_i)d\psi(e_j) \\ &= \det[1+V_nC]d\mu_{C'}. \end{aligned} \tag{10}$$

This is in fact the Gaussian identity for fermions. With this expression, the proposition follows immediately. ■

The next step is to observe that if

$$\langle \hat{n}(x)\rangle_{\mu_{C'}} \equiv \int \hat{n}(x)d\mu_{C'} = n(\vec{x}), \tag{11}$$

then

$$\hat{n}(x)-n(\vec{x})=:\psi^\dagger(x)\psi(x):_{\mu_{C'}}, \tag{12}$$

the normal ordering with respect to the measure $\mu_{C'}$. Condition (11) is a self-consistent equation for n and, as we shall see, it coincides with the Hartree equation. Let us summarize. We proved that, if (11) has a solution, the original interacting measure is equal to

$$d\mu = e^{-\mathcal{A}'(\psi^\dagger,\psi)}d\mu_{C_{\mathrm{H}}} \Big/ \int e^{-\mathcal{A}'(\psi^\dagger,\psi)}d\mu_{C_{\mathrm{H}}}, \tag{13}$$

where

$$\mathcal{A}'(\psi^\dagger,\psi)=\frac{1}{2}\int :\psi^\dagger(x)\psi(x):_{\mu_{C_{\mathrm{H}}}} v(x-y):\psi^\dagger(y)\psi(y):_{\mu_{C_{\mathrm{H}}}} dx\, dy. \tag{14}$$

The covariance C_{H} is constructed from the solution to the Hartree equations through Eq. (17). Indeed, a simple calculus shows

$$\langle \hat{n}(x)\rangle_{\mu_{C'}} = -C'(\vec{x},\tau;\vec{x},\tau+0). \tag{15}$$

If $\{\eta_i,\varepsilon_i\}_i$ is the set of eigenvectors and the corresponding eigenvalues of H_0+V_n:

$$\left(H_0+\int v(\vec{x}-\vec{y})n(\vec{y})d\vec{y}\right)\eta_i=\varepsilon_i\eta_i; \tag{16}$$

then

$$C'(\vec{x},\tau;\vec{x}',\tau')=\Sigma_i \eta_i(\vec{x})\,\eta_i(\vec{x}')^* e^{-\xi_i(\tau-\tau')}\begin{cases} 1-f_\beta(\xi_i), & \text{for } \tau\geqslant\tau', \\ -f_\beta(\xi_i), & \text{for } \tau<\tau', \end{cases} \tag{17}$$

where $\xi_i=\varepsilon_i-\mu$ and $f_\beta(x)=(1+e^{\beta x})^{-1}$ is the Fermi–Dirac distribution. Then Eq. (11) reduces to

$$n(\vec{x})=\Sigma_i f_\beta(\xi_i)|\eta_i(\vec{x})|^2. \tag{18}$$

One can recognize in (16) and (18) the usual Hartree equations. Thus, from the functional integral point of view, the Hartree approximation is just a convenient (probably the best) starting point for future expansions. This is because, due to the normal ordering in $\mathcal{A}'(\psi^\dagger,\psi)$, the tadpole diagrams are no longer present in any diagrammatic analysis beyond the Hartree approximation: they have been absorbed in the covariance C_{H}. We end this section by noticing that already condition (11) suggests a fixed point approach for this problem. This is developed in the next section.

III. THE FIXED POINT APPROACH

From now on, H_0 will be the sum of $-\frac{1}{2}\Delta_{\mathrm{D}}$ and a background potential U, defined over a finite box $\mathrm{vol}=[-a,a]^d\in R^d$, $d\geqslant 1$. We denoted by Δ_{D} the Laplace operator with Dirichlet boundary conditions (other boundary conditions can be also considered). Later calculations (Sec. IV) force us to define H_0 through the Kato–Relich theorem. More precisely, we need the same type of estimates as in the Kato–Relich theorem. Thus it is natural to define the Hamiltonian in this way. In the variational approach, is natural to define the Hamiltonian through the KLM theorem,[17] based on estimates on the symmetric quadratic forms which are needed anyway in this approach. The class of potentials included in the later case is larger than the class of potentials we can include in our approach. We start with the following result.

Proposition 2: Let $V\in L^p(\mathrm{vol})$, $p\geqslant\max\{2,(d+1)/2\}$. *Let* Λ *denote the lattice* $[(\pi/2a)Z_+]^d$, *where* Z_+ *is the set of strictly positive integers and let* $\Delta^d\vec{k}=(\pi/2a)^d$ *be the volume of its unit cell. Then, for* $f\in D(-\frac{1}{2}\Delta_{\mathrm{D}})$ *and* $z\notin R_+$ *:*

$$\|Vf\|_{L^2(\mathrm{vol})}\leqslant k_{p,z}\|V\|_{L^p(\mathrm{pol})}\|(-\tfrac{1}{2}\Delta_{\mathrm{D}}-z)f\|_{L^2(\mathrm{vol})}.$$

The constant is given by

$$k_{p,z}=[(\pi/2)^d\Sigma_{\vec{k}\in\Lambda}|\tfrac{1}{2}\vec{k}^2-z|^{-p}\Delta^d\vec{k}]^{1/p}.$$

Proof: This will be an extension of the estimates presented in Ref. 17 (p. 171) to the case when the boundary conditions are present. The eigenvalues and eigenstates of $-\frac{1}{2}\Delta_{\mathrm{D}}$ are labeled by a point of the lattice Λ:

$$\vec{k}=\left(\frac{\pi}{2a}n_1,\ldots,\frac{\pi}{2a}n_d\right). \tag{19}$$

They are given by

$$E_{\vec{k}}=\frac{1}{2}\vec{k}^2,\quad \phi_{\vec{k}}(x)=a^{-d/2}\prod_{i=1}^{d}\varphi_{n_i}(x_i/a), \tag{20}$$

where

$$\varphi_n(x)=\begin{cases}\sin(n\pi x/2), & \text{for } n=1,3,5,\ldots,\\ \cos(n\pi x/2), & \text{for } n=2,4,6,\ldots.\end{cases} \tag{21}$$

We denote by l^p the Banach space of p-summable infinite sequences. For $f\in L^2(\mathrm{vol})$, we denote by $\Sigma_{\vec{k}\in\Lambda}f_{\vec{k}}\phi_{\vec{k}}(x)$ its decomposition in the basis $\{\phi_{\vec{k}}\}_{\vec{k}\in\Lambda}$. We need to prove first a Hausdorf–Young type inequality, namely,

$$\|f\|_{L^q(\mathrm{vol})} \leqslant a^{-(d/2)(1/p-1/q)} \|\{f_{\vec{k}}\}_{\vec{k}\in\Lambda}\|_{l^p}, \quad \frac{1}{q}+\frac{1}{p}=1, q\geqslant 2. \tag{22}$$

This inequality follows from

$$\|f\|_{L^\infty(\mathrm{vol})} \leqslant a^{-d/2} \|\{f_{\vec{k}}\}_{\vec{k}\in\Lambda}\|_{l^1} \text{ and } \|f\|_{L^2(\mathrm{vol})} = \|\{f_{\vec{k}}\}_{\vec{k}\in\Lambda}\|_{l^2}, \tag{23}$$

which can be interpolated using the Riesz–Thorin theorem to get (22). Then, for an arbitrary $f \in D(-\frac{1}{2}\Delta_{\mathrm{D}})$ and $1/p+1/r=1/2$:

$$\begin{aligned} \|Vf\|_{L^2(\mathrm{vol})} &\leqslant \|V\|_{L^p(\mathrm{vol})} \|f\|_{L^r(\mathrm{vol})} \\ &\leqslant a^{-(d/2)(1/q-1/r)} \|V\|_{L^p(\mathrm{vol})} \|\{f_{\vec{k}}\}_{\vec{k}\in\Lambda}\|_{l^q}, \end{aligned} \tag{24}$$

with $1/r+1/q=1$. Moreover,

$$\begin{aligned} \|\{f_{\vec{k}}\}_{k\in\Lambda}\|_{l^q} &= \|\{(\tfrac{1}{2}\vec{k}^2-z)^{-1}(\tfrac{1}{2}\vec{k}^2-z) f_{\vec{k}}\}_{\vec{k}\in\Lambda}\|_{l^q} \\ &\leqslant \|\{(\tfrac{1}{2}\vec{k}^2-z)^{-1}\}_{\vec{k}\in\Lambda}\|_{l^s} \|\{(\tfrac{1}{2}\vec{k}^2-z) f_{\vec{k}}\}_{\vec{k}\in\Lambda}\|_{l^2} \\ &= \|\{(\tfrac{1}{2}\vec{k}^2-z)^{-1}\|_{\vec{k}\in\Lambda}\|_{l^s} \|(-\tfrac{1}{2}\Delta_{\mathrm{D}}-z) f\|_{L^2(\mathrm{vol})}, \end{aligned} \tag{25}$$

where $1/q=1/s+1/2$. In fact this constraint imposes $s=p$. We can conclude that

$$\|Vf\|_{L^2(\mathrm{vol})} \leqslant a^{-d/p} \|\{(\tfrac{1}{2}\vec{k}^2-z)^{-1}\}_{\vec{k}\in\Lambda}\|_{l^p} \|(-\tfrac{1}{2}\Delta_{\mathrm{D}}-z) f\|_{L^2(\mathrm{vol})}. \tag{26}$$

In the above relation, p must be greater than $(d+1)/2$ in order to have a finite right hand side. The starting constraint $1/p+1/r=1/2$ imposes $p\geqslant 2$ and this finishes the proof. ■

Proposition 3: Suppose the two-body interaction, v, belongs to $L^p(R^d)$. Then so it does V_n as long as $n \in L^1(\mathrm{vol})$.

Proof: Because the two-body interaction is given, in general, over R^d, we can extend $V_n = v*n$ over the entire R^d. Then, from the Young inequality,

$$\begin{aligned} \|V_n\|_{L^p(\mathrm{vol})} &\leqslant \|V_n\|_{L^p(R^d)} \\ &\leqslant \|v\|_{L^p(R^d)} \|\chi_{\mathrm{vol}} n\|_{L^1(R^d)} = \|v\|_{L^p(R^d)} \|n\|_{L^1(\mathrm{vol})}. \end{aligned} \tag{27}$$

■

From the above estimates, it seems that a natural class of potentials and two-body interactions will be L^p with $p\geqslant \max\{2,(d+1)/2\}$. For a given potential, we have, in general, to take care of its singularities and the way it decreases to infinity. We can separate them by dividing the potential in two: one part includes the singularities and the other part includes the behavior at infinity. Thus a more natural class of potentials will be L^p+L^q, where p must be small to include the singularities and q large to include different decays at infinity. In fact, based on our previous estimates, the optimal class will be L^m+L^∞, where $m=\max\{2,(d+1)/2\}$. We do not know if our estimates are optimal. However, for $d=3$, it follows from Ref. 17 [problem (14)] that L^2+L^∞ is indeed the maximal class of potentials for which the Kato–Relich theorem applies. Thus we will consider from now on that $U\in L^m(\mathrm{vol})+L^\infty(\mathrm{vol})$ and $v\in L^m(R^d)+L^\infty(R^d)$. This potential can be as singular as $|x|^{-(d-1)/2-\varepsilon}$ with $\varepsilon<1/2$. For $d=3$, this includes the Coulomb interaction. Along this paper, $\|\cdot\|$ will denote the operatorial norm on $L^2(\mathrm{vol})$.

Theorem 4: *Suppose the background and the two-body interaction satisfies the above conditions and let $U=U^{(1)}+U^{(2)}$ and $v=v^{(1)}+v^{(2)}$ be a decomposition in L^m+L^∞. Then we have the following.*

(i) $H_0=-\frac{1}{2}\Delta_{\mathrm{D}}+U$ and $H_n=H_0+V_n$ are self-adjoint on $D(-1/2\Delta_{\mathrm{D}})$.

(ii) H_0 and H_n have only pure punctual spectrum.

(iii) $\exp(-H_0)$ *is of trace class.*
(iv) For $z \notin \sigma_{H_0} \cup R_+$ *:*

$$\|V_n(H_0-z)^{-1}\| \leqslant K_1(z)\|n\|_{L^1(\mathrm{vol})},$$

where the constant is given by:

$$K_1(z)=k_{m,z}(1+\|U(H_0-z)^{-1}\|)\|v^{(1)}\|_{L^m(R^d)}+d(z,\sigma_{H_0})^{-1}\|v^{(2)}\|_{L^\infty(R^d)},$$

and

$$\|U(H_0-z)^{-1}\| \leqslant (1-k_{m,z}\|U^{(1)}\|_{L^m(\mathrm{vol})})^{-1}\{k_{m,z}\|U^{(1)}\|_{L^m(\mathrm{vol})}+d(z,\sigma_{H_0})^{-1}\|U^{(2)}\|_{L^\infty(\mathrm{vol})}\}.$$

Proof: (i) The affirmation follows from the Kato–Relich theorem.
(ii) Both operators have compact resolvents which can be easily seen from resolvent identity.
(iii) Using a technique that will be extensively used later, the affirmation follows from the fact that $\exp(\frac{1}{2}\Delta_D)$ is trace class operator.[18]
(iv) It easily follows from Propositions 1 and 2. ■

We are ready now to define the fixed point approach. If the total number of particles, N, is conserved, then we must impose the following constraint: $\|n\|_{L^1}=N$.

Proposition 5: In the above conditions, for $\beta<\infty$*, we have the following.*

(i) The map:

$$T: L^1(\mathrm{vol}) \to L^1(\mathrm{vol}),$$

$$L^1(\mathrm{vol}) \ni n \to T[n](\vec{x})=(1+e^{\beta(H_0+V_n-\mu_n)})^{-1}(\vec{x},\vec{x}),$$

is well defined. Here, μ_n *is the unique solution of*

$$N=\mathrm{Tr}(1+e^{\beta(H_0+V_n-\mu)})^{-1}.$$

(ii) The fixed points of T are solutions for the Hartree equation.

Proof: (*i*) The proof is based on the following classic result.[19]

Proposition 6: For A a trace class, self-adjoint operator and ϕ *a convex function on* $\sigma(A)$*, the following is true:*

$$\mathrm{Tr}\phi(A) \geqslant \sum_m \phi((\eta_m, A\eta_m)),$$

where $\{\eta_m\}_m$ *is any complete orthonormal set.*

We use $\|\cdot\|_1$ to denote the trace norm. Also, let us denote $\phi_{\mu,\beta}(t)\equiv(1+e^{\beta(t-\mu)})^{-1}$. For a large, positive α, let

$$\gamma_\alpha=\|V_n(H_0+\alpha)^{-1}\|, \tag{28}$$

which is a decreasing function of α. Consider $\{\eta_m,\varepsilon_m\}_m$, the eigenvectors and the corresponding eigenvalues of H_0+V_n. Then, if $\phi'_{\mu,\beta}(t)\equiv e^{-\beta(t-\mu)}$ and α is large enough:

$$
\begin{aligned}
\mathrm{Tr}\phi'_{\mu,\beta}(H_0) &= \mathrm{Tr}\phi'_{\mu+\alpha,\beta}(H_0+\alpha) \\
&\geqslant \sum_m \phi'_{\mu+\alpha,\beta}((\eta_m,(H_0+\alpha)\eta_m)) \\
&= \sum_m \phi'_{\mu+\alpha,\beta}[(\varepsilon_m+\alpha)\langle \eta_m,(H_0+\alpha)(H_0+\alpha+V_n)^{-1}\eta_m\rangle] \\
&= \sum_m \phi'_{\mu+\alpha,\beta}[(\varepsilon_m+\alpha)\langle \eta_m,(1+V_n(H_0+\alpha)^{-1})^{-1}\eta_m\rangle] \\
&\geqslant \sum_m \phi'_{\mu+\alpha,\beta}[(\varepsilon_m+\alpha)/(1-\gamma_\alpha)] \\
&\geqslant \sum_m \phi_{\mu+\alpha,\beta}[(\varepsilon_m+\alpha)/(1-\gamma_\alpha)] \\
&= \sum_m \phi_{(1-\gamma_\alpha)\mu-\alpha\gamma_\alpha,\beta/(1-\gamma_\alpha)}[\varepsilon_m] \\
&= \mathrm{Tr}\phi_{(1-\gamma_\alpha)\mu-\alpha\gamma_\alpha,\beta/(1-\gamma_\alpha)}[H_0+V_n]. \qquad (29)
\end{aligned}
$$

Taking

$$
\mu' = (\mu+\alpha\gamma_\alpha)/(1-\gamma_\alpha) \quad \text{and} \quad \beta' = (1-\gamma_\alpha)\beta, \qquad (30)
$$

we conclude that

$$
\|(1+e^{\beta(H_0+V_n-\mu)})^{-1}\|_1 < e^{\beta'\mu'}\,\mathrm{Tr}\exp(-\beta' H_0) < \infty. \qquad (31)
$$

Thus the equation (in μ)

$$
N = \mathrm{Tr}(1+e^{\beta(H_0+V_n-\mu)})^{-1}, \qquad (32)
$$

makes sense. One can check that the right hand side is a continuous, strict monotone increasing function of μ. Moreover, the right hand side goes to ∞ and 0 as μ goes to $\pm\infty$ respectively. Thus, Eq. (32) has a unique solution. Because $(1+e^{\beta(H_0+V_n-\mu_n)})^{-1}$ is a positive defined self-adjoint operator:

$$
\int (1+e^{\beta(H_0+V_n-\mu_n)})^{-1}(\vec{x},\vec{x})\,d\vec{x} = \|(1+e^{\beta(H_0+V_n-\mu_n)})^{-1}\|_1 < \infty, \qquad (33)
$$

from (31). This proves that $(1+e^{\beta(H_0+V_n-\mu_n)})^{-1}(\vec{x},\vec{x})$ exists as a $L^1(\mathrm{vol})$ function.

(*ii*) From spectral decomposition:

$$
T[n](\vec{x}) = \sum_m f\beta(\varepsilon_m-\mu_n)|\eta_m(\vec{x})|^2. \qquad (34)
$$

Thus the Hartree equation can be written as $n(\vec{x}) = T[n](\vec{x})$. ■

The condition $\beta<\infty$ is essential here. If H_0+V_n has degenerate eigenvalues, then it is not possible all the time to match the number of eigenvalues below the Fermi energy with N, whatever value the Fermi energy has. This is why, at zero temperature, one has to assume that H_0+V_n has only nondegenerate eigenvalues, which is not necessarily at finite temperatures. The fixed point approach for a classical Hartree approximation also encounters a similar problem.[5]

IV. THE SOLUTION OF THE HARTREE EQUATION

We investigate in this section the solutions of the Hartree equations. In many cases, a background charge, n_0, is present to assure the neutrality of the system: $\int n_0(\vec{x})d\vec{x}=N$. In this case, V_n is replaced by

$$V_n(\vec{x})\to V_{n-n_0}(\vec{x})=\lambda\int v(\vec{x}-\vec{y})(n(\vec{y})-n_0(\vec{y}))d\vec{y}, \tag{35}$$

where we inserted a scaling parameter λ. As we mentioned in the Introduction, a common way of solving the Hartree problem consists of the following. The density of particles in the absence of the two-body interaction (denoted here by n_1) is chosen as the starting point for Hartree iteration. Then one tests if the sequence $\{T^{\circ k}n_1\}_k$ converges. In our approach, the convergence must be in $L^1(\mathrm{vol})$.

Theorem 7: *If the two-body interaction satisfies the conditions enunciated at the beginning of the previous section, then, for* λ *small enough, the sequence* $\{T^{\circ k}n_1\}_k$ *converges to the unique solution of the Hartree equation.*

Remark: According to our estimates, the maximum value of the coupling constant depends on the number of particles and temperature. Only if one assumes special conditions like periodicity of the background potential, then one can prove (second part of this work) that this value does not depend on the number of particles. The dependency on temperature it is not due to our imperfect estimates. We will prove in third part that there is a symmetry breaking at zero temperature. Thus, the maximum value of the coupling constant for which the Hartree problem has a unique solution does go to zero at low temperatures, unless some special conditions are imposed (like nondegenerate eigenvalues, band gaps, etc.). The proof of the theorem is based on several propositions.

Proposition 8: Let n_1, $n_2\in L^1(\mathrm{vol})$ *and let us use the shortening:* $H_{n_{1,2}}=H_0+V_{n_{1,2}-n_0}$. *Then*

$$\|T[n_1]-T[n_2]\|_{L^1}\leqslant 2\|(1+e^{\beta(H_{n_1}-\mu_M)})^{-1/2}-(1+e^{\beta(H_{n_2}-\mu_M)})^{-1/2}\|(\|(1+e^{\beta(H_{n_1}-\mu_M)})^{-1/2}\|_1 + \|(1+e^{\beta(H_{n_2}-\mu_M)})^{-1/2}\|_1),$$

where $\mu_M=\max\{\mu_{n_1},\mu_{n_2}\}$.

Proof: Suppose $\mu_{n_2}\geqslant\mu_{n_1}$. We have, successively,

$$\begin{aligned}\|T[n_1]-T[n_2]\|_{L^1}&\leqslant\|(1+e^{\beta(H_{n_1}-\mu_{n_1})})^{-1}-(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1}\|_1\\&\leqslant\|(1+e^{\beta(H_{n_1}-\mu_{n_1})})^{-1}-(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}\|_1\\&\quad+\|(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}-(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1}\|_1.\end{aligned} \tag{36}$$

From

$$N=\mathrm{Tr}(1+e^{\beta(H_{n_1}-\mu_{n_1})})^{-1}=\mathrm{Tr}(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1}, \tag{37}$$

it follows that

$$\begin{aligned}&\|(1+e^{\beta(H_{n_1}-\mu_{n_1})})^{-1}-(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}\|_1\\&\quad=\mathrm{Tr}\{(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}-(1+e^{\beta(H_{n_1}-\mu_{n_1})})^{-1}\}\\&\quad=\mathrm{Tr}\{(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}-(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1}\}\\&\quad\leqslant\|(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}-(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1}\|_1.\end{aligned} \tag{38}$$

At this step we can conclude that

$$\|T[n_1]-T[n_2]\|_{L^1}\leqslant 2\|(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}-(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1}\|_1. \tag{39}$$

Then the proposition follows from the identity

$$\begin{aligned}(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}&-(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1}\\ &=(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1/2}\{(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1/2}-(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1/2}\}\\ &\quad+\{(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1/2}-(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1/2}\}(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1/2},\end{aligned} \tag{40}$$

and the basic inequality $\|AB\|_1\leqslant\|A\|_1\|B\|_{L^2}$ or $\|A\|_{L^2}\|B\|_1$ for A trace class and B bounded, or *vice versa*. ■

We continue with the evaluation of the two terms that appear in the above proposition. Let us denote $\phi_{\mu,\beta}(t)=(1+e^{\beta(t-\mu)})^{-1/2}$. Because this function is convex for $t\geqslant\mu+\beta^{-1}\ln 2$, one can define a family of convex functions, $\overline{\phi}_{\mu,\beta}$, such that $\overline{\phi}_{\mu,\beta}(t)\geqslant\phi_{\mu,\beta}(t)$ for any μ, $t\in R$ and $\beta\in R_+$, with equality for t larger than some $t_c(\mu,\beta)>\mu+\beta^{-1}\ln 2$. Also, $\overline{\phi}_{\mu,\beta}(t)$ can be chosen continuous in the parameters μ and β, increasing with respect to μ and decreasing with respect to β.

Proposition 9: With the above notations, for α negative and $|\alpha|$ large enough,

$$\|(1+e^{(\beta H_0+\lambda V_{n-n_0}-\mu)})^{-1/2}\|_1\leqslant\mathrm{Tr}\overline{\phi}_{\mu',\beta'}(H_0),$$

where

$$\mu'=(\mu-\alpha K_1(\alpha)\xi)/(1-K_1(\alpha)\xi)$$

and

$$\beta'=(1-K_1(\alpha)\xi)\beta.$$

We used the notation $\xi\equiv\lambda\|n-n_0\|_{L^1(\mathrm{vol})}$.

Proof: Let $\{\eta_m,\varepsilon_m\}_m$ be the eigenvectors and the corresponding eigenvalues of $H_0+\lambda V_{n-n_0}$. Then we have successively,

$$\begin{aligned}\mathrm{Tr}\overline{\phi}_{\mu,\beta}(H_0)&=\mathrm{Tr}\overline{\phi}_{\mu-\alpha,\beta}(H_0-\alpha)\\ &\geqslant\sum_m\overline{\phi}_{\mu-\alpha,\beta}[\langle\eta_m,(H_0-\alpha)\eta_m\rangle]\\ &=\sum_m\overline{\phi}_{\mu-\alpha,\beta}[(\varepsilon_m-\alpha)\langle\eta_m,(H_0-\alpha)(H_0+\lambda V_{n-n_0}-\alpha)^{-1}\eta_m\rangle]\\ &=\sum_m\overline{\phi}_{\mu-\alpha,\beta}[(\varepsilon_m-\alpha)\langle\eta_m,(1+\lambda V_{n-n_0}(H_0-\alpha)^{-1})^{-1}\eta_m\rangle]\\ &\geqslant\sum_m\overline{\phi}_{\mu-\alpha,\beta}[(\varepsilon_m-\alpha)/(1-\lambda\|V_{n-n_0}(H_0-\alpha)^{-1}\|)]\\ &\geqslant\sum_m\overline{\phi}_{\mu-\alpha,\beta}[(\varepsilon_m-\alpha)/(1-\lambda K_1(\alpha)\|n-n_0\|_{L^1})]\\ &\geqslant\sum_m\phi_{\mu-\alpha,+gb}[(\varepsilon_m-\alpha)/(1-K_1(\alpha)\xi)]\\ &=\mathrm{Tr}\phi_{\mu-\alpha,\beta}[(H_n-\alpha)/(1-K_1(\alpha)\xi)].\end{aligned} \tag{41}$$

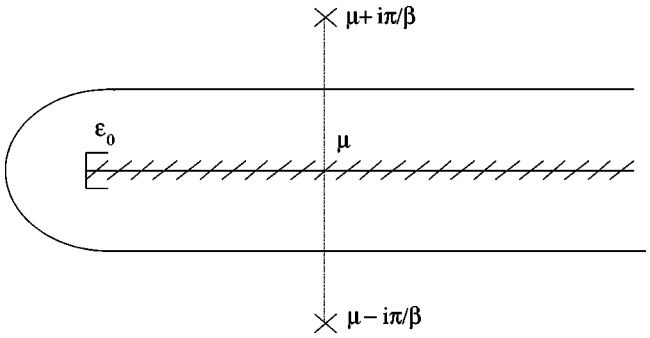

FIG. 3. Contour $\mathcal{C}$, used in Proposition 10. The poles of $(1+e^{\beta(z-\mu)})^{-1}$ at $\mu \pm i\pi/\beta$ are marked.

Replacing μ and β by μ' and β', the proposition follows. ■

An important remark is that the bound found in the above proposition is a continuous, increasing function of ξ and μ.

Proposition 10: For n_1, $n_2 \in L^1(\mathrm{vol})$ *the following is true:*

$$\|(1+e^{\beta(H_{n_1}-\mu)})^{-1/2}-(1+e^{\beta(H_{n_2}-\mu)})^{-1/2}\|_{L^2} \leqslant K_2(\mu,\beta,\xi)\lambda\|n_1-n_2\|_{L^1(\mathrm{vol})},$$

where ξ *denotes now* $\max\{\lambda\|n_1-n_0\|_{L^1},\lambda\|n_2-n_0\|_{L^1}\}$.

Proof: From

$$\begin{aligned}(1+e^{\beta(H_{n_1}-\mu)})^{-1/2}&-(1+e^{\beta(H_{n_2}-\mu)})^{-1/2}\\ &=\frac{\lambda}{2\pi i}\int_{\mathcal{C}}(1e^{\beta(z-\mu)})^{-1/2}(z-H_{n_1})^{-1}\\ &\quad\times(V_{n_1-n_0}-V_{n_2-n_0})(z-H_{n_2})^{-1}dz,\end{aligned} \tag{42}$$

where $\mathcal{C}$ is a curve in the complex plane that surrounds the spectrum of $H_{n_{1,2}}$ and $\phi_{\mu,\beta}$ is analytic inside of $\mathcal{C}$. Then

$$\begin{aligned}&\|(1+e^{\beta(H_{n_1}-\mu)})^{-1/2}-(1+e^{\beta(H_{n_2}-\mu)})^{-1/2}\|\\ &\quad\leqslant\frac{\lambda}{2\pi}\int_{\mathcal{C}}|dz||1+e^{\beta(z-\mu)}|^{-1/2}d(z,\sigma)^{-1}\|V_{n_1-n_2}(z-H_{n_2})^{-1}\|,\end{aligned} \tag{43}$$

where σ is the semi-axis starting from ε_0, the bottom of $\sigma_{H_{n_1}}\cup\sigma_{H_{n_2}}$. Choosing $\mathcal{C}$ as in Fig. 3, $d(z,\sigma)=\pi/(2\beta)$:

$$\begin{aligned}&\|(1+e^{\beta(H_{n_1}-\mu)})^{-1/2}-(1+e^{\beta(H_{n_2}-\mu)})^{-1/2}\|\\ &\quad\leqslant\frac{\lambda\beta}{\pi^2}\int_{\mathcal{C}}|dz||1+e^{\beta(z-\mu)}|^{-1/2}\|V_{n_1-n_2}(z-H_{n_2})^{-1}\|.\end{aligned} \tag{44}$$

Because Theorem 4 gives an estimate of $\|V_{n_1-n_2}(z-H_0)^{-1}\|$, one can try

$$\begin{aligned}&\|V_{n_1-n_2}(z-H_{n_2})^{-1}\|\\ &\quad=\|V_{n_1-n_2}(z-H_0)^{-1}(1-\lambda V_{n_2-n_0}(z-H_0)^{-1})^{-1}\|\\ &\quad\leqslant\|V_{n_1-n_2}(z-H_0)^{-1}\|/(1-\lambda\|V_{n_2-n_0}(z-H_0)^{-1}\|).\end{aligned} \tag{45}$$

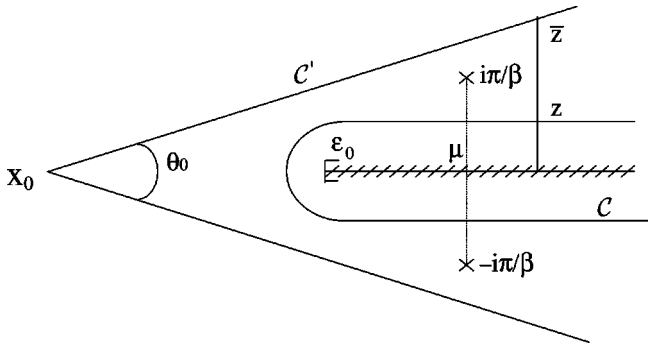

FIG. 4. Contour $\mathcal{C}'$ used in Proposition 10. It is shown, graphically, how $\overline{z}$ is chosen.

However, this will not work for two reasons. The first reason is that, for $d=3$, $k_{m,z}$ (defined in Proposition 2) diverges as $\mathrm{Re}\, z$ goes to infinity and $\mathrm{Im}\, z$ is kept finite, so it will diverge at the ends of $\mathcal{C}$. This can be seen for large volumes, when $k_{m,z}$ can be approximated by

$$k_{m,z}=\left[(2\pi)^{-d}\int_{R^d}|k^2/2-z|^{-2}d^dk\right]^{1/2}=\sqrt{\frac{S_{d-1}}{2^{2+d/2}\pi^{d-1}\rho^{2-d/2}\sin\theta/2}}, \tag{46}$$

where $z=\rho e^{i\theta}$ and S_d is the surface of the d dimensional sphere. The second reason is that, as the temperature decreases, we are forced to take the curve $\mathcal{C}$ closer and closer to the real axis to avoid the poles of $(1+e^{\beta(z-\mu)})^{-1}$ and to stay in the domain of analyticity of $(1+e^{\beta(z-\mu)})^{-1/2}$. In either case, $\lambda\|V_{n_2-n_0}(z-H_0)^{-1}\|$ becomes greater than one, for any finite value of λ. However, the following procedure solves the problem. Consider the curve $\mathcal{C}'$ as in Fig. 4. For $z\in\mathcal{C}$ we consider the line that passes through z and the closest point of σ to the z. Then, we associate to every $z\in\mathcal{C}$ a point $\overline{z}\in\mathcal{C}'$ defined by the intersection of this line with $\mathcal{C}'$. With the notations from Fig. 4, it is clear that $k_{\overline{z}}(\overline{z}\in\mathcal{C}')$ can be made smaller than any positive number by properly choosing x_0 and θ_0. This means that $K_1(\overline{z})$ (defined in Theorem 4) can be made as small as we want. Moreover, the following is true:

$$\begin{aligned}
&\|V_{n_1-n_2}(z-H_{n_2})^{-1}\|\\
&\quad=\|V_{n_1-n_2}(\overline{z}-H_{n_2})^{-1}(\overline{z}-H_{n_2})(z-H_{n_2})^{-1}\|\\
&\quad\leqslant\|V_{n_1-n_2}(\overline{z}-H_{n_2})^{-1}\|\sup_{x\in[\varepsilon_0,\infty)}(\overline{z}-x)/(z-x)\\
&\quad=\|V_{n_1-n_2}(\overline{z}-H_{n_2})^{-1}\|d(\overline{z},\sigma)/d(z,\sigma).
\end{aligned}\tag{47}$$

With the above remark, one can continue:

$$\begin{aligned}
\|V_{n_1-n_2}(z-H_{n_2})^{-1}\|&\leqslant\|V_{n_1-n_2}(\overline{z}-H_0)^{-1}\|\frac{d(\overline{z},\sigma)/d(z,\sigma)}{1-\|V_{n_2-n_0}(\overline{z}-H_0)^{-1}\|}\\
&\leqslant\frac{d(\overline{z},\sigma)}{d(z,\sigma)}\frac{K_1(\overline{z})}{1-K_1(\overline{z})\xi}\lambda\|n_1-n_2\|_{L^1(\mathrm{vol})}.
\end{aligned}\tag{48}$$

Thus we can conclude that

$$\begin{aligned}
&\|(1+e^{\beta(H_{n_1}-\mu)})^{-1/2}-(1+e^{\beta(H_{n_2}-\mu)})^{-1/2}\|\\
&\quad\leqslant K_2(\mu,\beta,\xi)\lambda\|n_1-n_2\|_{L^1(\mathrm{vol})},
\end{aligned}\tag{49}$$

where

$$K_2(\mu,\beta,\xi)=\frac{2\beta^2}{\pi^3}\int_{\mathcal{C}}|dz||1+e^{\beta(z-\mu)}|^{-1/2}\frac{d(\overline{z},\sigma)K_1(\overline{z})}{1-K_1(\overline{z})\xi}. \tag{50}$$

The divergence of $d(\overline{z},\sigma)$ as $\mathrm{Re}\,z\to\infty$ is canceled by the exponential decay of $|1+e^{\beta(z-\mu)}|^{-1/2}$. One can easily check that $K_2(\mu,\beta,\xi)$ is increasing with respect to μ and ξ. ■

The last estimate we need is a bound on μ_n. For this, we define a convex function, $\phi_{\mu,\beta}$ that goes below $(1+e^{\beta(t-\mu)})^{-1}$:

$$\phi_{\mu,\beta}(t)\leqslant(1+e^{\beta(t-\mu)})^{-1},\quad \text{for any } t,\mu\in R \quad\text{and}\quad \beta\in R_+. \tag{51}$$

This function needs to be convex only for $t\geqslant\varepsilon_0$, the bottom of $\sigma_{H_0+V_n}$. To be more explicit, let $g(t)$ be the linear function that, for $t\in[\varepsilon_0,\infty)$, goes below the Fermi–Dirac distribution, $\phi_{\mu,\beta}(t)=(1+e^{\beta(t-\mu)})^{-1}$, and it is as close as it is possible to $(1+e^{\beta(t-\mu)})^{-1}$. In this case, $g(t)$ is tangent to $(1+e^{\beta(t-\mu)})^{-1}$ in some point, t_c, and $g(\varepsilon_0)=\phi_{\mu,\beta}(\varepsilon_0)$. Then $\phi_{\mu,\beta}(t)$ can be chosen as $g(t)$ for $t\in[\varepsilon_0,t_c]$ and as $\phi_{\mu,\beta}(t)$ for $t>t_c$.

Proposition 11: The constraint $N=\mathrm{Tr}\phi_{\mu_n}(H_0+V_{n-n_0})$ imposes an upper limit on μ_n. An estimate of this limit can be found from the following implicit relation:

$$N\geqslant\mathrm{Tr}\phi_{\mu_n,\beta}((1+K_1(\alpha)\xi)H_0-\alpha K_1(\alpha)\xi),$$

where α is a negative number and $\xi=\lambda\|n-n_0\|_{L^1(\mathrm{vol})}$.

Proof: Let $\{\eta_m^0,\lambda_m\}_m$ be the set of eigenvectors and the corresponding eigenvalues of H_0. Then, for α negative and $|\alpha|$ large enough,

$$\begin{aligned}
N&=\mathrm{Tr}\phi_{\mu_n,\beta}[H_0+\lambda V_{n-n_0}]\\
&\geqslant\mathrm{Tr}\phi_{\mu_n}[H_0+\lambda V_{n-n_0}]\\
&\geqslant\sum_m\ \phi_{\mu_n,\beta}[\langle\eta_m^0,(H_0+\lambda V_{n-n_0})\eta_m^0\rangle]\\
&=\sum_m\ \phi_{\mu_n,\beta}[\langle\eta_m^0,(H_0+\lambda V_{n-n_0}-\alpha)\eta_m^0\rangle+\alpha]\\
&=\sum_m\ \phi_{\mu_n,\beta}[\langle\eta_m^0,(1+\lambda V_{n-n_0}(H_0-\alpha)^{-1})\eta_m^0\rangle(\lambda_m-\alpha)+\alpha]\\
&\geqslant\sum_m\ \phi_{\mu_n,\beta}[(1+\lambda K_1(\alpha)\|n-n_0\|_{L^1})(\lambda_m-\alpha)+\alpha]\\
&=\mathrm{Tr}\phi_{\mu_n,\beta}[(1+\lambda K_1(\alpha)\|n-n_0\|_{L^1})H_0-\alpha\lambda K_1(\alpha)\|n-n_0\|_{L^1}].
\end{aligned}\tag{52}$$

An important property of $\phi_{\mu,\beta}$ is that

$$\phi_{\mu,\beta}(t)>\phi_{\mu',\beta}(t),\quad \text{for } \mu>\mu'. \tag{53}$$

Also, $\phi_\mu(t)\to1$ as $\mu\to\infty$. This means that

$$\mathrm{Tr}\phi_{\mu_n,\beta}((1+K_1(\alpha)\xi)H_0-\alpha K_1(\alpha)\xi)\xrightarrow[\mu\to\infty]{}\infty, \tag{54}$$

monotonically, so that

$$N \geqslant \mathrm{Tr}\phi_{\mu_n,\beta}[(1+K_1(\alpha)\xi)H_0 - \alpha K_1(\alpha)\xi], \tag{55}$$

does impose an upper limit on μ_n. ■

Proof of Theorem 7: Let us consider an ε-ball around n_1:

$$n \in B_\varepsilon(n_1) \Leftrightarrow \|n-n_1\|_{L^1} \leqslant \varepsilon. \tag{56}$$

Let $\delta = \|n_0 - n_1\|_{L^1}$ and let us note that $B_\varepsilon(n_1) \subset B_{\varepsilon+\delta}(n_0)$. We are interested first to find those conditions in which $T[B_\varepsilon(n_1)] \subset B_\varepsilon(n_1)$. We denote $\xi \equiv \lambda(\varepsilon+\delta)$. From Proposition 11, it follows that, for $n \in B_{\varepsilon+\delta}(n_0)$,

$$\mathrm{Tr}\phi_{\mu_n,\beta}((1+K_1(\alpha)\xi)H_0 - \alpha K_1(\alpha)\xi) \leqslant N, \tag{57}$$

where α is a negative number. This shows that μ_n is bounded by some μ_M which is a function only of ξ. Moreover, $\mu_M(\xi)$ is an increasing function of ξ. Because $\overline{\phi}_{\mu,\beta}$ in Proposition 9 is increasing with respect to μ and decreasing with respect to β and $K_2(\mu,\beta,\xi)$ in Proposition 10 is increasing with respect to μ and ξ, it follows that, for any $n, n' \in B_{\varepsilon+\delta}(n_0)$,

$$\|T[n]-T[n']\|_{L^1} \leqslant 4\,\mathrm{Tr}\overline{\phi}_{\mu'_M(\xi),\beta'(\xi)}(H_0)K_2(\mu_M(\xi),\beta,\xi)\lambda\|n-n'\|_{L^1}, \tag{58}$$

where

$$\mu'_M(\xi) = (\mu_M(\xi) - \alpha K_1(\alpha)\xi)/(1-K_1(\alpha)\xi), \tag{59}$$

$$\beta'(\xi) = (1-K_1(\alpha)\xi)\beta. \tag{60}$$

Then, for $n \in B_\varepsilon(n_1)$,

$$\begin{aligned}\|T[n]-n_1\|_{L^1} &= \|T[n]-T[n_0]\|_{L^1} \\ &\leqslant 4\,\mathrm{Tr}\overline{\phi}_{\mu'_M(\xi),\beta'(\xi)}(H_0)K_2(\mu_M(\xi),\beta,\xi)\xi.\end{aligned} \tag{61}$$

If

$$4\,\mathrm{Tr}\overline{\phi}_{\mu'_M(\xi),\beta'(\xi)}(H_0)K_2(\mu_M(\xi),\beta,\xi)\xi \leqslant \varepsilon, \tag{62}$$

then $T[B_\varepsilon(n_1)] \subset B_\varepsilon(n_1)$. Moreover, if (62) is fulfilled, then T is a contraction on $B_\varepsilon(n_1)$. Indeed, for any $n, n' \in B_\varepsilon(n_1)$,

$$\begin{aligned}\|T[n]-T[n']\|_{L^1} &\leqslant 4\,\mathrm{Tr}\overline{\phi}_{\mu'_M(\xi),\beta'(\xi)}(H_0)K_2(\mu_M(\xi),\beta,\xi)\lambda\|n-n'\|_{L^1} \\ &\leqslant \frac{\varepsilon}{\varepsilon+\delta}\|n-n'\|_{L^1}.\end{aligned} \tag{63}$$

Because the left hand side of (62) is a continuous function of ξ which goes to zero as ξ goes to zero, it follows that, for any $\varepsilon > 0$, the condition (62) is fulfilled provided λ is small enough. In consequence, we proved that, for λ small enough, $B_\varepsilon(n_1)$ is invariant for T and T is a contraction on $B_\varepsilon(n_1)$. In consequence, T has a single fixed point in $B_\varepsilon(n_1)$. In particular, $\{T^{\circ k}n_1\}_k$ is convergent. Because any fixed point of T satisfies $\|n\|_{L^1} = N$, they belongs to $B_{2N}(n_1)$. Taking $\varepsilon = 2N$, the uniqueness on $L^1(\mathrm{vol})$ follows. ■

At the end, we consider the extension of the above result to the local density approximation.[20] Without going into detail, we want to prove the following proposition.

Proposition 12: Consider the conditions enunciated at the beginning of Sec. III. Then Theorem 7 is true if V_n is replaced with

$$V_n(\vec{x}) \to V_n^{\mathrm{tot}}(\vec{x}) = \lambda \left[\int v(\vec{x}-\vec{y}) n(\vec{y}) d\vec{y} + v_{\mathrm{xc}}(n(\vec{x})) \right],$$

where v_{xc} is a continuous, differentiable on R_+ less a finite number of points. Also, we ask that dv_{xc}/dn is uniformly bounded.

For $n>0$, the conditions we impose on v_{xc} are satisfied by most of the expressions used in local density functional calculations. For example, the potential proposed in Ref. 21 is continuous and differentiable on intervals. The new expression provided in Ref. 22 is differentiable on the entire $(0, \infty)$. Moreover, dv_{xc}/dn is uniformly bounded for large n. At small concentrations, v_{xc} behaves as $n^{1/3}$ which makes dv_{xc}/dn to diverge as $n \to 0$. Thus, one has to modify only the very low density behavior of v_{xc} in order to be in our conditions.

Sketch of proof: We prove first that $v_{\mathrm{xc}}(n)(H_0-z)^{-1}$ is a bounded operator for $n \in L^1(\mathrm{vol})$ and $z \notin \sigma_{H_0} \cup R_+$. Indeed, for $f \in \mathcal{D}(-\frac{1}{2}\Delta_B)$:

$$\| v_{\mathrm{xc}}(n) f \|_{L^2(\mathrm{vol})} \leqslant k_{p,z} \| v_{\mathrm{xc}}(n) \|_{L^p(\mathrm{vol})} \| (-\tfrac{1}{2}\Delta - z) f \|_{L^2(\mathrm{vol})}, \tag{64}$$

and

$$\begin{aligned} \| v_{\mathrm{xc}}(n) \|_{L^p(\mathrm{vol})} &= \left[\int_{\mathrm{vol}} \frac{v_{\mathrm{xc}}(n(\vec{x}))^p}{n(\vec{x})} n(\vec{x}) d\vec{x} \right]^{1/p} \\ &\leqslant \sup_{t \in R_+} \left\{ \frac{v_{\mathrm{xc}}(t)^p}{t} \right\} \| n \|_{L^1(\mathrm{vol})}^{1/p}. \end{aligned} \tag{65}$$

Choosing different values for p, $v_{\mathrm{xc}}(t)^p/t$ can be made uniformly bounded. In the case of homogeneous electron gas, p must be chosen 3. We notice that in this case, the estimate (65) remains true even if we do not modify the low density behavior of the exchange-correlation potential. Then, one can find a bound for $\| (1+e^{\beta(H_n-\mu)})^{-1/2} \|_1$ and μ_n exactly as in Propositions 9 and 11, respectively. A result similar to that of Proposition 10 can be proven by starting from

$$\begin{aligned} \langle f, [v_{\mathrm{xc}}(n) - v_{\mathrm{xc}}(n')] g \rangle &\leqslant \| v_{\mathrm{xc}}(n) - v_{\mathrm{xc}}(n') \|_{L^1} \| f \|_{L^\infty} \| g \|_{L^\infty}, \\ &\leqslant k_{m,z}^2 \| v_{\mathrm{xc}}(n) - v_{\mathrm{xc}}(n') \|_{L^1} \| (H_0 - z^*) f \|_{L^2} \| (H_0 - z) g \|_{L^2}, \end{aligned} \tag{66}$$

for any $f, g \in \mathcal{D}(H_0)$. We ignored the background potential for simplicity and notation. Thus,

$$\begin{aligned} &\langle (H_0 - z^*)^{-1} f, [v_{\mathrm{xc}}(n) - v_{\mathrm{xc}}(n')] (H_0 - z)^{-1} g \rangle \\ &\quad \leqslant k_{m,z}^2 \| v_{\mathrm{xc}}(n) - v_{\mathrm{xc}}(n') \|_{L^1} \| f \|_{L^2} \| g \|_{L^2}, \end{aligned} \tag{67}$$

for any $f, g \in L^2(\mathrm{vol})$, which shows that

$$\begin{aligned} &\| (H_0 - z)^{-1} [v_{\mathrm{xc}}(n) - v_{\mathrm{xc}}(n')] (H_0 - z)^{-1} \| \\ &\quad \leqslant k_{m,z}^2 \| v_{\mathrm{xc}}(n) - v_{\mathrm{xc}}(n') \|_{L^1} \\ &\quad = k_{m,z}^2 \int_{\mathrm{vol}} \left| \int_{n'(\vec{x})}^{n(\vec{x})} \frac{dv_{\mathrm{xc}}(t)}{dt} dt \right| d\vec{x} \\ &\quad \leqslant k_{m,z}^2 \sup_{t \in R_+} \left| \frac{dv_{\mathrm{xc}}(t)}{dt} \right| \| n - n' \|_{L^1}. \end{aligned} \tag{68}$$

If v_{xc} is not differentiable on a set of points, then the integral $\int_{n'(\vec{x})}^{n(\vec{x})} dt$ must be broken on the intervals. The result is the same with the only difference that the supremum is taken over R_+ less the points where the derivative is not defined. Then

$$
\begin{aligned}
&(1+e^{\beta(H_{n_1}-\mu)})^{-1/2}-(1+e^{\beta(H_{n_2}-\mu)})^{-1/2}\\
&\quad=\frac{\lambda}{2\pi i}\int_{\mathcal{C}}(1+e^{\beta(z-\mu)})^{-1/2}(z-H_{n_1})^{-1}V_{n_1-n_2}(z-H_{n_2})^{-1}dz\\
&\quad+\frac{\lambda}{2\pi i}\int_{\mathcal{C}}(1+e^{\beta(z-\mu)})^{-1/2}(z-H_{n_1})^{-1}\\
&\qquad\times[v_{\mathrm{xc}}(n_1)-v_{\mathrm{xc}}(n_2)](z-H_{n_2})^{-1}dz. \qquad (69)
\end{aligned}
$$

The first term can be bounded as before while the second one,

$$
\begin{aligned}
&\left\|\frac{\lambda}{2\pi i}\int_{\mathcal{C}}(1+e^{\beta(z-\mu)})^{-1/2}(z-H_{n_1})^{-1}[v_{\mathrm{xc}}(n_1)-v_{\mathrm{xc}}(n_2)](z-H_{n_2})^{-1}dz\right\|\\
&\quad\leqslant\frac{\lambda}{2\pi}\int_{\mathcal{C}}|dz|\,|1+e^{\beta(z-\mu)}|^{-1/2}\|(z-H_{n_1})^{-1}[v_{\mathrm{xc}}(n_1)-v_{\mathrm{xc}}(n_2)](z-H_{n_2})^{-1}\|\\
&\quad\leqslant\frac{\lambda}{2\pi}\int_{\mathcal{C}}|dz|\,|1+e^{\beta(z-\mu)}|^{-1/2}\frac{d(\bar{z},\sigma)^2/d(z,\sigma)^2}{(1-\|V_{n_1}^{\mathrm{tot}}(\bar{z}-H_0)^{-1}\|)(1-\|V_{n_2}^{\mathrm{tot}}(\bar{z}-H_0)^{-1}\|)}\\
&\qquad\times\|(\bar{z}-H_0)^{-1}[v_{\mathrm{xc}}(n_1)-v_{\mathrm{xc}}(n_2)](\bar{z}-H_0)^{-1}\|\\
&\quad\leqslant k_{m,z}^2\frac{\sup_{t\in R_+}dv_{\mathrm{xc}}(t)/dt}{2\pi}\int_{\mathcal{C}}|dz|\,|1+e^{\beta(z-\mu)}|^{-1/2}\\
&\qquad\times\frac{d(\bar{z},\sigma)^2/d(z,\sigma)^2}{(1-\|V_{n_1}^{\mathrm{tot}}(\bar{z}-H_0)^{-1}\|)(1-\|V_{n_2}^{\mathrm{tot}}(\bar{z}-H_0)^{-1}\|)}\|n_1-n_2\|_{L^1}, \qquad (70)
\end{aligned}
$$

where we use the same notation as in Proposition 10 and H_n represents $H_0+V_n^{\mathrm{tot}}$. Thus, Propositions 9 to 11 remain true when the exchange-correlation potential is considered and one can repeat the proof of Theorem 7. ■

The problem at low density comes from the fact that we were not able to find a suitable norm in which $n^{1/3}-n'^{1/3}$ is bounded by $\|n-n'\|_{L^1(\mathrm{vol})}$ as it is needed in the fixed point theorem. If one tries an L^p norm in (68) instead of the L^1 norm, then the best one can get is a bound proportional to $\|n-n'\|_{L^1(\mathrm{vol})}^{1/p}$ which is not enough. However, our result can be relevant for the general case, if one can prove that, after each iteration, $\|n\|_{L^\infty(\mathrm{vol})}$ is greater than the value from where the exchange-correlation potential has been artificially modified.

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Hartree approximation II: The thermodynamic limit

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We investigate the thermodynamic limit of the Hartree approximation for periodic background potentials and short range two-body interactions. We prove that, for any finite volume, the Hartree problem has a unique solution among the periodic densities of particles provided the coupling constant is smaller than a certain value. This value is independent of volume. We also prove that these solutions converge as the thermodynamic limit is considered. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379748]

I. INTRODUCTION

We continue our investigation[1] of the Hartree approximation at finite temperatures. As in Ref. 1, we neglect the spin degrees of freedom. In this paper, we analyze the thermodynamic limit of this model. Only the three dimensional case will be considered. Let us consider a periodic background potential: $u(\vec{x}+\vec{R})=u(\vec{x})$, for any $\vec{R}$ belonging to the infinite lattice:

$$\Gamma=\{\vec{y}\in R^3|\vec{y}=\Sigma_{i=1}^3 n^i\vec{\delta}_i,\ \ n_i\in\mathbf{Z}\},\tag{1}$$

where $\vec{\delta}_i$, $i=\overline{1,3}$, are three independent vectors. Let us consider a finite crystal, confined in

$$V=\{\vec{y}\in R^3|\vec{y}=\Sigma_{i=1}^3 x^i\vec{\delta}_i,\ \ x^i\leqslant K,\ \ i=\overline{1,3}\},\tag{2}$$

where K is a positive integer number. We denote its unit cell by

$$\text{cell}=\{\vec{y}\in R^3|\vec{y}=\Sigma_{i=1}^3 x^i\vec{\delta}_i,\ \ x^i\leqslant 1,\ \ i=\overline{1,3}\}.\tag{3}$$

The crystal is formed from K^3 cells. Let the independent particles be described by the Hamiltonian: $H_0=-\frac{1}{2}\Delta_p+u$, where Δ_p denotes the periodic Laplace operator on V. Suppose a two-body interaction, v, is given. The Hartree problem consists in finding the fixed points of the map:[1]

$$T:L^1(V)\to L^1(V),\ \ T[n](\vec{x})=(1+e^{\beta(H_n-\mu_n)})^{-1}(\vec{x},\vec{x}),\tag{4}$$

where

$$H_n=H_0+\lambda\int_V v(\vec{x}-\vec{y})n(\vec{y})d\vec{y}.\tag{5}$$

In (4), μ_n represents the unique solution of the equation (in μ): $N=\mathrm{Tr}(1+e^{\beta(H_n-\mu)})^{-1}$, N being the number of particles. Because the background potential is periodic, it seems natural to search for the fixed points of T among the periodic functions. However, the space of periodic functions is not invariant for T. This is because the potential,

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$$V_n(\vec{x}) = \int_V v(\vec{x}-\vec{y})n(\vec{y})d\vec{y}, \tag{6}$$

is not periodic even if the density n is. It will be periodic if the opposite faces of the crystal are identified. This is why we will consider that the particles are trapped on the torus: $\mathcal{T}=S_1\times S_2\times S_3$, where S_i are circles of length: $K\delta_i$. We denote the Laplace operator on $\mathcal{T}$ by the same Δ_p. The two-body interaction has to be modified because, on the torus, particles on different faces of the crystal will be closer to each other. Supposing that the two-body interactions is invariant under the spatial reflections, we can write the interaction between two particles, situated in two points, $\vec{x}$, $\vec{y}\in\mathcal{T}$, as

$$\tilde{v}(\vec{x},\vec{y}) = v(d_1(x_1-y_1),d_2(x_2-y_2),d_3(x_3-y_3)), \tag{7}$$

where $d_i(\cdot,\cdot)$ represents the distance on the circle S_i. We will replace this expression in (6). Our conditions are

- restricted to the unit cell, $u\in L^2(\text{cell})+L^\infty(\text{cell})$.
- the two-body interaction belongs to $L^2(R^3)+L^\infty(R^3)$.
- the two-body interaction is of short range: $|v(\vec{x})|<|\vec{x}|^{-3+\epsilon}$ for large $|\vec{x}|$, where $\epsilon>0$.

Thus, our class of background potential includes the Coulomb force, while the class of the two-body interactions includes only the screened Coulomb force. Assume now that N particles are trapped on the torus $\mathcal{T}$. We denote by N_0 the number of particles per unit cell: $N_0=N/K^3$. Our goal in this paper is to study the Hartree model in the limit $N\to\infty$, $K\to\infty$, when $N_0=N/K^3$ remains constant. Specifically, we prove that the conditions of the fixed point theorem are uniformly satisfied on the invariant set of periodic densities of particles as the thermodynamic limit is considered. The case of nonperiodic densities cannot be treated by the method presented here. For this periodic solution, we prove that the chemical potential, energy per unit volume and the density of particles have a well defined thermodynamic limit. We mention that, very recently, a similar analysis has been carried out for the classical Hartree approximation by Catto, Le Bris and Lions.[2]

II. PRELIMINARY RESULTS

Let us introduce first a few notations: $L^1_{\text{per}}(\mathcal{T})$ will denote the set of L^1 integrable functions over $\mathcal{T}$ with $f(\vec{x}+\vec{R})=f(\vec{x})$ for $\vec{R}\in\Gamma$. Also, let $\mathcal{C}=\{\Sigma_{i=1}^3 q^i\vec{\delta}_i, \mathbf{q}\in\Lambda\}$, where $\Lambda\equiv\{0,1,...,K-1\}$.[3] We also introduce a new scalar product. For two vectors: $v_{1,2}=\Sigma_{i=1}^3 v^i_{1,2}\vec{\delta}_i$, $\vec{v}_1\vec{v}_2$ will be by definition, $\Sigma_{i=1}^3 v^i_1 v^i_2$. Also, the norm of vectors will be calculated using this scalar product. The scalar product defined above will simplify the notation and will not play any other special role. To any point $\vec{x}\in R^3$, one can associate a point on the torus by considering the point in V with the coordinates: $\tilde{x}^i=x^i \bmod K\delta_i$, $i=\overline{1,3}$. In the following, all points in R^3 are considered modulo V.

As we already mentioned, if $n\in L^1_{\text{per}}(\mathcal{T})$, then $V_n(\vec{x}+\vec{R})=V_n(\vec{x})$ for any $\vec{R}\in\Gamma$. In this case, there exists a unitary transformation:

$$U: L^2(\mathcal{T})\to\oplus_{\mathbf{q}\in\Lambda}L^2(\text{cell}), \tag{8}$$

such that

$$U(-\tfrac{1}{2}\Delta_p+u+\lambda V_n)U^{-1}=\oplus_{\mathbf{q}\in\Lambda}[-\tfrac{1}{2}\Delta_{\mathbf{q}}+u+\lambda V_n]. \tag{9}$$

Here, $\Delta_{\mathbf{q}}$ denotes the Laplace operator over the unit cell, with the boundary conditions

$$f(\vec{x}+\vec{\delta}_j)=e^{i2\pi q^j/K}f(\vec{x}) \quad\text{and}\quad f'(\vec{x}+\vec{\delta}_j)=e^{i2\pi q^j/K}f'(\vec{x}), \tag{10}$$

for $\vec{x}$ and $\vec{x}+\vec{\delta}_j$ on the faces of the unit cell. The unitary transformation is given by

$$L^2(\mathcal{T}) \ni f \to (Uf)_{\mathbf{q}}(\vec{x}) = K^{-3} \sum_{\vec{R} \in \mathcal{C}} e^{-i\vec{R}\vec{\theta}_{\mathbf{q}}} f(\vec{x}+\vec{R}), \tag{11}$$

where $\vec{\theta}_{\mathbf{q}} = 2\pi K^{-1} \Sigma_{i=1}^{3} q^i \vec{\delta}_i$ for any $\mathbf{q} \in \Lambda$. We start now the analysis of $H_n^{(\mathbf{q})} = -1/2\Delta_{\mathbf{q}} + u + \lambda V_n$. In this section, if not specified, all the L^p norms are over the unit cell and $\|\cdot\|$ denotes the operatorial norm over L^2(cell).

Proposition 1: For $f \in \mathcal{D}(-\frac{1}{2}\Delta_{\mathbf{q}})$ *and* $a > 0$:

$$\|f\|_{L^\infty} \leqslant k_a \|(-\tfrac{1}{2}\Delta_{\mathbf{q}} + a) f\|_{L^2},$$

where k_a *is given by*

$$k_a = 1/(2\sqrt{2a}\,\pi) \sum_{\vec{R} \in \Gamma} e^{-\sqrt{2a}|\vec{R}|}.$$

It is only this place where $|\cdot|$ denotes the usual norm on R^3. Because the explicit expression of k_a will not play a special role in the following, we hope that the notation is not confusing.

Proof: Let $f \in \mathcal{D}(-\frac{1}{2}\Delta_{\mathbf{q}})$ and let us denote $g = (-\frac{1}{2}\Delta_{\mathbf{q}} + a) f$ and by $G_{\mathbf{q}}(\vec{x},\vec{y};a)$ the kernel of $(-\frac{1}{2}\Delta_{\mathbf{q}} + a)^{-1}$. Then

$$f(\vec{x}) = \left(\left(-\frac{1}{2}\Delta_{\mathbf{q}} + a \right)^{-1} g \right)(\vec{x}) = \int_{\text{cell}} G_{\mathbf{q}}(\vec{x},\vec{y};a) g(\vec{y})\, d\vec{y}, \tag{12}$$

which leads to

$$|f(\vec{x})| \leqslant \sup_{x \in \text{cell}} \int_{\text{cell}} |G_{\mathbf{q}}(\vec{x},\vec{y};a)|^2\, d\vec{y} \|g\|_{L^2}. \tag{13}$$

The kernel of $(-\frac{1}{2}\Delta_{\mathbf{q}} + a)^{-1}$ is given by

$$G_{\mathbf{q}}(\vec{x},\vec{y};a) = \sum_{\vec{R} \in \Gamma} e^{-i\vec{R}\vec{\theta}_{\mathbf{q}}} G(\vec{x}-\vec{y}+\vec{R};a), \tag{14}$$

where G is the kernel of $(-\frac{1}{2}\Delta + a)^{-1}$, Δ being the Laplace operator over R^3. Because G is a real, positive function,

$$\left| \sum_{\vec{R} \in \Gamma} e^{-i\vec{R}\vec{\theta}_{\mathbf{q}}} G(\vec{x}-\vec{y}+\vec{R};a) \right| \leqslant \sum_{\vec{R} \in \Gamma} G(\vec{x}-\vec{y}+\vec{R};a) = G_{\mathbf{0}}(\vec{x},\vec{y};a), \tag{15}$$

thus

$$\|f\|_{L^\infty} \leqslant \sup_{x \in \text{cell}} \int_{\text{cell}} |G_{\mathbf{0}}(\vec{x},\vec{y};a)|^2 d\vec{y} \left\| \left(-\frac{1}{2}\Delta_{\mathbf{q}} + a \right) f \right\|_{L^2}. \tag{16}$$

One can recognize

$$\int_{\text{cell}} |G_0(\vec{x},\vec{y};a)|^2 dy = \left(-\frac{1}{2}\Delta_{\mathbf{0}} + a \right)^{-2} (\vec{x},\vec{x}) \equiv C_{\mathbf{0}}(\vec{x},\vec{x};a). \tag{17}$$

If $C(\vec{x}-\vec{y};a)$, is the kernel of $(-\frac{1}{2}\Delta + a)^{-2}$, then

$$C_{\mathbf{0}}(\vec{x},\vec{y};a)=\sum_{\vec{R}\in\Gamma} C(\vec{x}-\vec{y}+\vec{R};a). \tag{18}$$

A simple calculus shows $C(\vec{x};a)=1/(2\sqrt{2a}\pi)e^{-\sqrt{2a}|\vec{x}|}$, which leads to

$$\|f\|_{L^\infty}\leqslant 1/(2\sqrt{2a}\pi)\sum_{\vec{R}\in\Gamma} e^{-\sqrt{2a}|\vec{R}|}\left\|\left(-\frac{1}{2}\Delta_{\mathbf{q}}+a\right)f\right\|_{L^2}. \tag{19}$$

■

Proposition 2: If $u\in L^\infty(\text{cell})+L^2(\text{cell})$, *then, for* $a>0$,

$$\|u(-\tfrac{1}{2}\Delta_{\mathbf{q}}+a)^{-1}\|<K_1(a),$$

where $K_1(a)$ *is a decreasing function.*

Proof: From previous theorem, for any $f\in\mathcal{D}(-\frac{1}{2}\Delta_{\mathbf{q}})$,

$$\|uf\|_{L^2}\leqslant\|u^{(1)}\|_{L^\infty}\|f\|_{L^2}+1/(2\sqrt{2a}\pi)\sum_{\vec{R}\in\Gamma} e^{-\sqrt{2a}|\vec{R}|}\|u^{(2)}\|_{L^2}\left\|\left(-\frac{1}{2}\Delta_{\mathbf{q}}+a\right)f\right\|_{L^2}, \tag{20}$$

which leads to

$$\begin{aligned}\left\|u\left(-\frac{1}{2}\Delta_{\mathbf{q}}+a\right)^{-1}f\right\|_{L^2}&\leqslant\|u^{(1)}\|_{L^\infty}\left\|\left(-\frac{1}{2}\Delta_{\mathbf{q}}+a\right)^{-1}f\right\|_{L^2}+1/(2\sqrt{2a}\pi)\sum_{\vec{R}\in\Gamma} e^{-\sqrt{2a}|\vec{R}|}\|u^{(2)}\|_{L^2}\|f\|_{L^2}\\&\leqslant\left\{a^{-1}\|u^{(1)}\|_{L^\infty}+1/(2\sqrt{2a}\pi)\sum_{\vec{R}\in\Gamma} e^{-\sqrt{2a}|\vec{R}|}\|u^{(2)}\|_{L^2}\right\}\|f\|_{L^2}.\end{aligned} \tag{21}$$

■

In the following, we denote the trace norm by $\|\cdot\|_1$.

Proposition 3: Let $n,n'\in L^1_{\text{per}}(\mathcal{T})$ *and* $\|n\|_{L^1(\mathcal{T})}=N$. *Then*

(i) $\|V_n(-\frac{1}{2}\Delta_{\mathbf{q}}+a)^{-1}\|\leqslant N_0K_2(a)$;

(ii) $\|(-\frac{1}{2}\Delta_{\mathbf{q}}+a)^{-1}V_{n'}(-\frac{1}{2}\Delta_{\mathbf{q}}+a)^{-1}\|_1\leqslant k_aK^{-3}\|v\|_{L^1(R^3)}\|n'\|_{L'(\mathcal{T})}$.

where K_2 *is independent of N and it is a decreasing function of a.*

Proof: (i) Let us denote by $\mathcal{N}$ the number of cells around the unit cell that have at least one point infinitely close to the unit cell. We divide the torus in $\text{vol}^{(1)}+\text{vol}^{(2)}$, where $\text{vol}^{(1)}$ comprises all these $\mathcal{N}$ cells plus the unit cell. Then

$$V_n(\vec{x})=\int_{\text{vol}^{(1)}}\tilde{v}(\vec{x},\vec{y})n(\vec{y})d\vec{y}+\int_{\text{vol}^{(2)}}\tilde{v}(\vec{x},\vec{y})n(\vec{y})d\vec{y}, \tag{22}$$

and let us analyze first the second term:

$$\int_{\text{vol}^{(2)}}\tilde{v}(\vec{x},\vec{y})n(\vec{y})d\vec{y}=\sum_{\vec{k}}\int_{\text{cell}(\vec{k})}\tilde{v}(\vec{x},\vec{y})n(\vec{y})d\vec{y}, \tag{23}$$

where the sum goes over all crystal cells in $\text{vol}^{(2)}$. Let us denote

$$\alpha_{\vec{k}}=\sup_{\substack{x\in\text{cell}\\ y\in\text{cell}(\vec{k})}}\tilde{v}(\vec{x},\vec{y}). \tag{24}$$

Then

$$\left| \int_{\mathrm{vol}^{(2)}} \tilde{v}(\vec{x},\vec{y}) n(\vec{y}) d\vec{y} \right| \leqslant \sum_{\vec{k}} \alpha_{\vec{k}} \int_{\mathrm{vol}(\vec{k})} |n(\vec{y})| d\vec{y} = N_0 \sum_{\vec{k}} \alpha_{\vec{k}}, \tag{25}$$

where we use the periodicity of n. For short range potentials considered in this paper,

$$\sum_{\vec{k}} \alpha_{\vec{k}} \leqslant \lim_{K\to\infty} \sum_{\vec{k}} \alpha_{\vec{k}} < \infty, \tag{26}$$

which means that the second term in (22) is a bounded operator:

$$\left\| \int_{\mathrm{vol}^{(2)}} \tilde{v}(\vec{x},\vec{y}) n(\vec{y}) d\vec{y} \right\| \leqslant N_0 A, \tag{27}$$

where A is independent of K. Let $v = v^{(1)} + v^{(2)}$ be the decomposition of v in $L^\infty(R^3) + L^2(R^3)$ and let

$$V_n^{(i)} = \int_{\mathrm{vol}^{(1)}} \tilde{v}^{(i)}(\vec{x},\vec{y}) n(\vec{y}) d\vec{y} = \int_{\mathrm{vol}^{(1)}} v^{(i)}(\vec{x}-\vec{y}) n(\vec{y}) d\vec{y}, \quad i = 1,2. \tag{28}$$

The second equality is true if we assume K sufficiently large. Then

$$\|V_n f\|_{L^2} \leqslant N_0 A \|f\|_{L^2} + \|V_n^{(1)}\|_{L^\infty} \|f\|_{L^2} + \|V_n^{(2)}\|_{L^2} \|f\|_{L^\infty}. \tag{29}$$

Denoting by χ_Ω the characteristic function for some $\Omega \in R^3$, it follows that

$$\begin{aligned} \|V_n^{(1)}\|_{L^\infty} \leqslant \|V_n^{(1)}\|_{L^\infty(R^3)} &= \|v^{(1)} * (n\chi_{\mathrm{vol}^{(1)}})\|_{L^\infty(R^3)} \\ &\leqslant \|v^{(1)}\|_{L^\infty(R^3)} \|n\chi_{\mathrm{vol}^{(1)}}\|_{L^1(R^3)} \\ &= (1+\mathcal{N}) N_0 \|v^{(1)}\|_{L^\infty(R^3)}, \end{aligned} \tag{30}$$

and

$$\begin{aligned} \|V_n^{(2)}\|_{L^2} \leqslant \|V_n^{(2)}\|_{L^2(R^3)} &= \|v^{(2)} * (n\chi_{\mathrm{vol}^{(1)}})\|_{L^2(R^3)} \\ &\leqslant \|v^{(2)}\|_{L^2(R^3)} \|n\chi_{\mathrm{vol}^{(1)}}\|_{L^1(R^3)} \\ &= (1+\mathcal{N}) N_0 \|v^{(2)}\|_{L^2(R^3)}. \end{aligned} \tag{31}$$

From (29) and Proposition 1,

$$\|V_n f\|_{L^2} \leqslant N_0 (A + (1+\mathcal{N}) \|v^{(1)}\|_{L^\infty(R^3)}) \|f\|_{L^2} + (1+\mathcal{N}) N_0 \|v^{(2)}\|_{L^2(R^3)} k_a \| (-\tfrac{1}{2}\Delta_{\mathbf{q}} + a) f\|_{L^2}, \tag{32}$$

which leads to

$$\|V_n (-\tfrac{1}{2}\Delta_{\mathbf{q}} + a)^{-1}\| \leqslant N_0 \{ (A + (1+\mathcal{N}) (\|v^{(1)}\|_{L^\infty(R^3)})/a + k_a \|v^{(2)}\|_{L^2(R^3)}) \}. \tag{33}$$

(ii) Using the polar decomposition, $V_n = S|V_n|$, it follows that

$$\begin{aligned} &\|(-\tfrac{1}{2}\Delta_{\mathbf{q}} + a)^{-1} V_n (-\tfrac{1}{2}\Delta_{\mathbf{q}} + a)^{-1}\|_1 \\ &\quad = \|V_n (-\tfrac{1}{2}\Delta_{\mathbf{q}} + a)^{-2}\|_1 = \|S|V_n| (-\tfrac{1}{2}\Delta_{\mathbf{q}} + a)^{-2}\|_1 \\ &\quad \leqslant \| |V_n| (-\tfrac{1}{2}\Delta_{\mathbf{q}} + a)^{-2}\|_1 = \| |V_n|^{1/2} (-\tfrac{1}{2}\Delta_{\mathbf{q}} + a)^{-2} |V_n|^{1/2}\|_1. \end{aligned}$$

Because $|V_n|^{1/2} (-\frac{1}{2}\Delta_{\mathbf{q}} + a)^{-2} |V_n|^{1/2}$ is a positive defined, self-adjoint operator:

$$
\begin{aligned}
&\| |V_n|^{1/2}(-\tfrac{1}{2}\Delta_{\mathbf{q}}+a)^{-2}|V_n|^{1/2}\|_1 \\
&\quad=\int_{\text{cell}} |V_n(\vec{x})^{1/2} C_{\mathbf{q}}(\vec{x},\vec{x};a)|V_n(\vec{x})|^{1/2}\,d\vec{x} \\
&\quad\leqslant \int_{\text{cell}} |V_n(\vec{x})| C_{\mathbf{0}}(\vec{x},\vec{x};a)\,d\vec{x} \\
&\quad= k_a \|V_n\|_{L^1} \\
&\quad= k_a K^{-3} \|V_n\|_{L^1(\mathcal{T})} \\
&\quad= k_a K^{-3} \int_{\mathcal{T}} d\vec{x} \left| \int_{\mathcal{T}} \tilde{v}(\vec{x},\vec{y}) n(\vec{y})\,dy \right| \\
&\quad\leqslant k_a K^{-3} \int_{\mathcal{T}} d\vec{y} |n(\vec{y})| \int_{\mathcal{T}} d\vec{x} |\tilde{v}(\vec{x},\vec{y})| \\
&\quad= k_a K^{-3} \int d\vec{x} |\tilde{v}(\vec{x},\vec{y})| \|n\|_{L^1(\mathcal{T})}, \qquad (34)
\end{aligned}
$$

because $\int d\vec{x}|\tilde{v}(\vec{x},\vec{y})|$ does not depend on $\vec{y}$. Finally, using: $\int_{\mathcal{T}} d\vec{x}|\tilde{v}(\vec{x},\vec{y})| \leqslant \|v\|_{L^1(R^3)} < \infty$, the affirmation follows. ■

From the above propositions, one can give an estimate of the bottom of σ_{H_n}, the spectrum of H_n. For $n \in L^1_{\text{per}}(\mathcal{T})$, $\|n\|_{L^1(\mathcal{T})} = N$, $H_n^{(\mathbf{q})} + a$ is invertible as soon as $K_1(a) + \lambda N_0 K_2(a) < 1$. Because we study the range of small coupling constants, we assume $\lambda < 1$. If ϵ_0 is the solution of $K_1(-\epsilon_0) + N_0 K_2(-\epsilon_0) = 1$, then $\inf\sigma(H_n) = \min \inf\sigma(H_n^{(\mathbf{q})}) \geqslant \epsilon_0$. What is important here is that this lower limit depends only on N_0, thus it is valid, uniformly, as the thermodynamic limit is considered. In next section, we will also need the following bound:

$$
\|(u + \lambda V_n)(-\tfrac{1}{2}\Delta_{\mathbf{q}} + a)^{-1}\| < K_1(a) + N_0 K_2(a) \equiv K_3(a), \qquad (35)
$$

if one considers $\lambda < 1$.

III. UNIFORM ESTIMATES

We start now to investigate if the conditions of the fixed point theorem are uniformly satisfied as the thermodynamic limit is considered. We start with upper and lower estimates on μ_n.

Proposition 4: For any $n \in L^1_{\text{per}}(\mathcal{T})$ with $\|n\|_{L^1(\mathcal{T})} = N$, there is an upper and a lower limit for μ_n that depend only on N_0.

Proof: Let us denote by $\phi_{\mu,\beta}$ the Fermi–Dirac distribution: $\phi_{\mu,\beta}(t) = (1 + e^{\beta(\tau-\mu)})^{-1}$. We consider a decreasing, convex function on $[\epsilon_0, \infty)$, $\underline{\phi}_{\mu,\beta}$, such that $\underline{\phi}_{\mu,\beta}(t) \leqslant (1 + e^{\beta(t-\mu)})^{-1}$ for all $\beta > 0$ and $\mu \in R$. The best choice of $\underline{\phi}_{\mu,\beta}$ was presented in Ref. 1. We add here that ϵ_0 depends only on N_0, so the definition of $\underline{\phi}_{\mu,\beta}$ depends only on N_0. If $(\eta_m^{\mathbf{q}}, \lambda_m^{\mathbf{q}})$ are the eigenvectors and the corresponding eigenvalues of $-\frac{1}{2}\Delta_{\mathbf{q}}$, then, for large, positive a,

$$
\begin{aligned}
N = \operatorname{Tr} \phi_{\mu_n,\beta}(H_n) &= \sum_{\mathbf{q}\in\Lambda} \operatorname{Tr} \phi_{\mu_n,\beta}(H_n^{(\mathbf{q})}) \\
&\geqslant \sum_{\mathbf{q}\in\Lambda} \operatorname{Tr} \underline{\phi}_{\mu_n,\beta}(H_n^{(\mathbf{q})}) \\
&\geqslant \sum_{\mathbf{q}\in\Lambda} \sum_m \underline{\phi}_{\mu_n,\beta}(\langle \eta_m^{\mathbf{q}}, H_n^{(\mathbf{q})} \eta_m^{\mathbf{q}} \rangle)
\end{aligned}
$$

$$\geqslant \sum_{\mathbf{q}\in\Lambda}\sum_{m} \underline{\phi}_{\mu_n,\beta}(\langle \eta_m^{\mathbf{q}}, (H_n^{(\mathbf{q})}+a)\,\eta_n^{\mathbf{q}}\rangle - a)$$

$$= \sum_{\mathbf{q}\in\Lambda}\sum_{m} \underline{\phi}_{\mu_n,\beta}\left((\lambda_m^{\mathbf{q}}+a)\left\langle \eta_m^{\mathbf{q}}, \left[1+(u+\lambda V_n)\left(-\frac{1}{2}\Delta_{\mathbf{q}}+a\right)^{-1}\right]\eta_m^{\mathbf{q}}\right\rangle - a\right)$$

$$\geqslant \sum_{\mathbf{q}\in\Lambda}\sum_{m} \underline{\phi}_{\mu_n,\beta}((\lambda_m^{\mathbf{q}}+a)(1+K_3(a)) - a)$$

$$\geqslant K^3 \inf_{q\in\Lambda} \mathrm{Tr}\,\underline{\phi}_{\mu_n,\beta}\left(\left(-\frac{1}{2}\Delta_{\mathbf{q}+a}\right)(1+K_3(a)) - a\right), \tag{36}$$

for $\lambda \leqslant 1$. In conclusion,

$$N_0 \geqslant \inf_{\vec{\theta}\in[0,2\pi)^3} \mathrm{Tr}\,\underline{\phi}_{\mu_n,\beta}((1+K_3(a))(-\tfrac{1}{2}\Delta_{\vec{\theta}}+a) - a). \tag{37}$$

Because $\underline{\phi}_{\mu,\beta}$ goes pointwise to 1 as μ goes to infinity, the above inequality imposes an upper limit on μ_n, that depends only on N_0. We consider now a decreasing convex function, $\overline{\phi}_{\mu,\beta}(t)$, such that $\overline{\phi}_{\mu,\beta}(t) \geqslant \phi_{\mu,\beta}(t)$ for any $\mu \in R$ and $\beta \in R_+$. If $(\chi_m^{\mathbf{q}}, \epsilon_m^{\mathbf{q}})$ are the eigenvectors and the corresponding eigenvalues of $H_n^{(\mathbf{q})}$, then

$$\mathrm{Tr}\,\overline{\phi}_{\mu,\beta}\left(-\frac{1}{2}\Delta_p\right) = \sum_{\mathbf{q}\in\Lambda} \mathrm{Tr}\,\overline{\phi}_{\mu,\beta}\left(-\frac{1}{2}\Delta_{\mathbf{q}}\right)$$

$$\geqslant \sum_{\mathbf{q}\in\Lambda}\sum_{m} \overline{\phi}_{\mu,\beta}(\langle \chi_m^{\mathbf{q}}, H_0^{(\mathbf{q})}\chi_m^{\mathbf{q}})\rangle$$

$$= \sum_{\mathbf{q}\in\Lambda}\sum_{m} \overline{\phi}_{\mu,\beta}(\langle \chi_m^{\mathbf{q}}, (H_n^{(\mathbf{q})} - u - \lambda V_n + a)\chi_m^{\mathbf{q}}\rangle - a)$$

$$= \sum_{\mathbf{q}\in\Lambda}\sum_{m} \overline{\phi}_{\mu,\beta}((\epsilon_m^{\mathbf{q}}+a)\langle \chi_m^{\mathbf{q}}, [1-(u+\lambda V_n)(H_n^{(\mathbf{q})}+a)^{-1}]\chi_m^{\mathbf{q}}\rangle - a)$$

$$\geqslant \sum_{\mathbf{q}\in\Lambda}\sum_{m} \overline{\phi}_{\mu,\beta}((\epsilon_m^{\mathbf{q}}+a)(1+K_3(a)(1-K_3(a))^{-1}) - a)$$

$$= \sum_{\mathbf{q}\in\Lambda}\sum_{m} \overline{\phi}_{\mu,\beta}((\epsilon_m^{\mathbf{q}}+a)(1-K_3(a))^{-1} - a)$$

$$= \sum_{\mathbf{q}\in\Lambda}\sum_{m} \overline{\phi}_{\mu,\beta}((\epsilon_m^{\mathbf{q}}+aK_3(a))/(1-K_3(a)))$$

$$\geqslant \sum_{\mathbf{q}\in\Lambda}\sum_{m} \phi_{\mu,\beta}((\epsilon_m^{\mathbf{q}}+aK_3(a))/(1-K_3(a)))$$

$$= \mathrm{Tr}\,\phi_{\mu,\beta}((H_n+aK_3(a))/(1-K_3(a))) = \mathrm{Tr}\,\phi_{\mu'',\beta''}(H_n), \tag{38}$$

where

$$\mu'' = \mu - aK_3(a) \quad \text{and} \quad \beta'' = \beta/(1-K_3(a)). \tag{39}$$

Replacing μ and β with

$$\mu' = \mu_n + aK_3(a) \quad \text{and} \quad \beta' = (1-K_3(a))\beta, \tag{40}$$

it follows that

$$\mathrm{Tr}\,\phi_{\mu',\beta'}(-\tfrac{1}{2}\Delta_p)\geqslant \mathrm{Tr}\,\phi_{\mu_n,\beta}(H_n)=N, \tag{41}$$

or

$$\sup_{\vec{\theta}\in[0,2\pi)^3}\mathrm{Tr}\,\overline{\phi}_{\mu',\beta'}(-\tfrac{1}{2}\Delta_{\vec{\theta}})\geqslant N_0, \tag{42}$$

which implies that $\mu'=\mu_n+aK_3(a)$ is greater than a certain finite value, which depends only on N_0. ■

We will denote the upper/lower limit of μ_n by μ_M/μ_m, respectively.

Theorem 5: *At finite temperature, there exists a constant* $\lambda_{\max}>0$, *independent of K, such that the map T is a contraction over the set* $\mathcal{S}=\{n\in L^1_{\mathrm{per}}(\mathcal{T}),\|n\|_{L^1(\mathrm{cell})}=N_0\}$, *for any K and* $\lambda<\lambda_{\max}$.

Proof: Supposing $\mu_{n_2}=\max\{\mu_{n_1},\mu_{n_2}\}$:

$$\begin{aligned}\|T[n_1]-T[n_2]\|_{L^1(T)}&\leqslant\|\hat{T}[n_1]-\hat{T}[n_2]\|_1\\&\leqslant 2\|(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}-(1+e^{\beta(H_{n_2}-\mu_{n_2})}\|_1\\&=2\sum_{\mathbf{q}\in\Lambda}\|(1+e^{\beta(H_n^{(\mathbf{q})}-\mu_{n_2})})^{-1}-(1+e^{\beta(H_n^{(\mathbf{q})}-\mu_{n_2})})^{-1}\|_1,\end{aligned} \tag{43}$$

where the first inequality can be proven as in Ref. 1. If $\mathcal{C}$ is a contour in the complex plane that surrounds $[\epsilon_0,\infty)$ and avoids the poles of $(1+e^{\beta(z-\mu_{n_2})})^{-1}$, then

$$\begin{aligned}&(1+e^{\beta(H_{n_1}^{(\mathbf{q})}-\mu_{n_2})})^{-1}-(1+e^{\beta(H_{n_2}^{(\mathbf{q})}-\mu_{n_2})})^{-1}\\&\quad=\frac{\lambda}{2\pi i}\int_{\mathcal{C}}dz(1+e^{\beta(z-\mu_{n_2})})^{-1}(z-H_{n_1}^{(\mathbf{q})})^{-1}V_{n_1-n_2}(z-H_{n_2}^{(\mathbf{q})})^{-1}\\&\quad=\frac{\lambda}{2\pi i}\int_{\mathcal{C}}dz(1+e^{\beta(z-\mu_{n_2})})^{-1}(H_{n_1}^{(\mathbf{q})}-z)^{-1}(H_{n_1}^{(q)}+a)\\&\qquad\times(H_{n_1}^{(\mathbf{q})}+a)^{-1}V_{n_1-n_2}(H_{n_2}^{(\mathbf{q})}+a)^{-1}(H_{n_2}^{(\mathbf{q})}+a)(z-H_{n_2}^{(\mathbf{q})})^{-1}.\end{aligned} \tag{44}$$

The contour $\mathcal{C}$ can be chosen independent of μ_{n_2}. Denoting

$$g_a(z)=\sup_{x\in[\epsilon_0,\infty)}|(x+a)/(x-z)|, \tag{45}$$

it follows that

$$\begin{aligned}&\|(1+e^{\beta(H_{n_1}^{(\mathbf{q})}-\mu_{n_2})})^{-1}-(1+e^{\beta(H_{n_2}^{(\mathbf{q})}-\mu_{n_2})})^{-1}\|_1\\&\quad\leqslant\frac{\lambda}{2\pi}\int_{\mathcal{C}}|dz||(1+e^{\beta(z-\mu_{n_2})})^{-1}|[g_a(z)/(1-K_3(a))]^2\\&\qquad\times\left\|\left(-\frac{1}{2}\Delta_{\mathbf{q}}+a\right)^{-1}V_{n_1-n_2}\left(-\frac{1}{2}\Delta_{\mathbf{q}}+a\right)^{-1}\right\|_1\\&\quad\leqslant\frac{\lambda k_a\|v\|_{L^1(R^3)}}{2\pi K^3(1-K_3(a))^2}\int_{\mathcal{C}}|dz||(1+e^{\beta(z-\mu_M)})^{-1}|g_a(z)^2\|n_1-n_2\|_{L^1(T)}.\end{aligned} \tag{46}$$

This, together with (43), leads to

$$\|T[n_1]-T[n_2]\|_{L^1(T)}\leqslant \lambda\gamma\|n_1-n_2\|_{L^1(T)}, \tag{47}$$

where

$$\gamma=\frac{k_a\|v\|_{L^1(R^3)}}{\pi(1-K_3(a))^2}\int_{\mathcal{C}}|dz||(1+e^{\beta(z-\mu_M)})^{-1}|g_a(z)^2, \tag{48}$$

in independent of K. ■

Because $\mathcal{S}$ is a closed, invariant set for T, the above result proves that, for $\lambda<\lambda_{\max}$, T has a unique fixed point in $\mathcal{S}$ for any K. In other words, the Hartree equation has a unique periodic solution for any finite volume. The result is valid only at finite temperatures, because γ diverges as the poles of $(1+e^{\beta(z-\mu_M)})^{-1}$ come closer and closer to the real axis (zero temperature limit). Of course, the zero temperature limit is well defined if $\mu_{m,M}$ are in a gap. We prove in the following that the chemical potential, $\{\mu_{T^{(om)}[n]}\}_m$, also converge to a well defined limit.

Lemma 6: For $\mu_{1,2}\in[\mu_m,\mu_M]$ *and* $n\in L^1_{\text{per}}(\mathcal{T})$, $\|n\|_{L^1(\mathcal{T})}=K^3N_0$, *the following are true:*
(i) $|\mu_1-\mu_2|\leqslant C^{-1}K^{-3}|\mathrm{Tr}(1+e^{\beta(H_n-\mu_1)})^{-1}-\mathrm{Tr}(1+e^{\beta(H_n-\mu_2)})^{-1}|$,
(ii) $K^{-3}|\mathrm{Tr}(1+e^{\beta(H_n-\mu_1)})^{-1}-\mathrm{Tr}(1+e^{\beta(H_n-\mu_2)})^{-1}\leqslant C'|\mu_1-\mu_2|$,
(iii) $K^{-3}|\mathrm{Tr}\,H_n(1+e^{\beta(H_n-\mu_1)})^{-1}-\mathrm{Tr}\,H_n(1+e^{\beta(H_n-\mu_2)})^{-1}|\leqslant C''|\mu_1-\mu_2|$,
where C *is a strictly positive constant and* C', $C''<\infty$. *All three constants do not depend on* K.

Proof: (i) Let us denote

$$F(\mu)=K^{-3}\,\mathrm{Tr}(1+e^{\beta(H_n-\mu)})^{-1}. \tag{49}$$

Then

$$\begin{aligned}\partial F/\partial\mu&=K^{-3}\beta e^{-\beta\mu}\,\mathrm{Tr}(1+e^{\beta(H_n-\mu)})^{-2}\\&\geqslant K^{-3}\beta e^{-\beta\mu_M}\,\mathrm{Tr}(1+e^{\beta(H_n-\mu_m)})^{-2}\\&=K^{-3}\beta e^{-\beta\mu_M}\sum_{\mathbf{q}\in\Lambda}\mathrm{Tr}(1+e^{\beta(H_n^{(\mathbf{q})}-\mu_m)})^{-2}.\end{aligned} \tag{50}$$

Considering a decreasing, convex function on $[\epsilon_0,\infty)$, $\underline{\phi}'_{\mu,\beta}(t)$, with the property

$$\underline{\phi}'_{\mu,\beta}(t)\leqslant(1+e^{\beta(t-\mu)})^{-2}\quad\text{for}\quad\beta\in R_+\quad\text{and}\quad\mu\in R, \tag{51}$$

it follows that

$$\begin{aligned}\partial F/\partial\mu&\geqslant K^{-3}\beta e^{-\beta\mu_M}\sum_{\mathbf{q}\in\Lambda}\mathrm{Tr}\,\underline{\phi}'_{\mu_m,\beta}(H_n^{(\mathbf{q})})\\&\geqslant K^{-3}\beta e^{-\beta\mu_M}\sum_{\mathbf{q}\in\Lambda}\sum_m\mathrm{Tr}\,\underline{\phi}'_{\mu_m,\beta}\left(\left\langle\eta_m^{\mathbf{q}},\left(-\frac{1}{2}\Delta_q+u+\lambda V_n\right)\eta_m^q\right\rangle\right)\\&\geqslant K^{-3}\beta e^{-\beta\mu_M}\sum_{\mathbf{q}\in\Lambda}\sum_m\mathrm{Tr}\,\underline{\phi}'_{\mu_m,\beta}((\lambda_m^{\mathbf{q}}+a)(1+K_3(a))-a)\\&\geqslant\beta e^{-\beta\mu_M}\inf_{\vec{\theta}\in[0,2\pi)^3}\mathrm{Tr}\,\underline{\phi}'_{\mu_m,\beta}\left(\left(-\frac{1}{2}\Delta_{\vec{\theta}}+a\right)(1+K_3(a))-a\right).\end{aligned} \tag{52}$$

The function $\underline{\phi}'_{\mu,\beta}$ can be chosen equal to $(1+e^{\beta(t-\mu)})^{-2}$ for t much larger than μ, in which case, (52) shows that $\partial F/\partial\mu\geqslant C>0$. Then

$$|F(n,\mu_1)-F(n,\mu_2)|=\int_{\min\{\mu_1,\mu_2\}}^{\max\{\mu_1,\mu_2\}}(\partial F/\partial\mu)d\mu>C|\mu_1-\mu_2|, \tag{53}$$

which proves the first affirmation.

(ii) One has

$$\partial F/\partial\mu = K^{-3}\beta e^{-\beta\mu}\sum_{\mathbf{q}\in\Lambda}\mathrm{Tr}(1+e^{\beta(H_n^{(\mathbf{q})}-\mu)})^{-2}. \tag{54}$$

If one considers a convex function on $[\epsilon_0,\infty)$ with the properties

$$\begin{aligned}\overline{\phi}'_{\mu,\beta}(t)&\geqslant(1+e^{\beta(t-\mu)})^{-2},\ \text{ for }\ \beta\in R_+\ \text{ and }\ \mu\in R,\\ \overline{\phi}'_{\mu,\beta}(t)&=(1+e^{\beta(t-\mu)})^{-2},\ \text{ for }\ t\gg\mu,\end{aligned} \tag{55}$$

one can evaluate the right hand side of (54) by following the same steps as in Proposition 4.

(iii) Consider

$$F'(\mu)=K^{-3}\,\mathrm{Tr}\,H_n(1+e^{\beta(H_n-\mu)})^{-1}, \tag{56}$$

with

$$\begin{aligned}\partial F'/\partial\mu &= K^{-3}\beta e^{-\beta\mu}\,\mathrm{Tr}\,H_n(1+e^{\beta(H_n-\mu)})^{-2}=K^{-3}\beta\mu e^{-\beta\mu}\,\mathrm{Tr}(1+e^{\beta(H_n-\mu)})^{-2}\\ &\quad+K^{-3}\beta e^{-\beta\mu}\,\mathrm{Tr}(H_n-\mu)(1+e^{\beta(H_n-\mu)})^{-2}.\end{aligned} \tag{57}$$

The first term has been estimated above. Because $\beta(t-\mu)(1+e^{\beta(t-\mu)})^{-2}$ is a convex function for $t\gg\mu$, we can find, again, a decreasing, convex function on $[\epsilon_0,\infty)$ such that

$$\begin{aligned}\overline{\phi}''_{\mu,\beta}(t)&\geqslant\beta(t-\mu)(1+e^{\beta(t-\mu)})^{-2},\quad \text{for }\ \beta\in R_+\ \text{ and }\ \mu\in R,\\ \overline{\phi}''_{\mu,\beta}(t)&=\beta(t-\mu)(1+e^{\beta(t-\mu)})^{-2},\quad \text{for }\ t\gg\mu.\end{aligned} \tag{58}$$

Then $|\partial F'/\partial\mu|$ can be bounded as in Proposition 4. ■

Theorem 7: *For any $n\in L^1_{\mathrm{per}}(\mathcal{T})$, $\|n\|_{L^1(\mathcal{T})}=K^3N_0$, the sequence $\{\mu_{\mathcal{T}^{\circ m}[n]}\}_m$ converges to a unique limit as m goes to infinity, provided $\lambda<\lambda_{\max}$. In other words, the chemical potential is well defined in the Hartree model, for any finite volume.*

Proof: For $n_{1,2}\in L^1_{\mathrm{per}}(T)$, $\|n_{1,2}\|=K^3N_0$:

$$\begin{aligned}|\mu_{n_1}-\mu_{n_2}|&\leqslant C^{-1}K^{-3}|\mathrm{Tr}(1+e^{\beta(H_{n_1}-\mu_{n_1})})^{-1}-\mathrm{Tr}(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}|\\ &=C^{-1}K^{-3}|\mathrm{Tr}(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1}-\mathrm{Tr}(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}|\\ &\leqslant C^{-1}K^{-3}\|(1+e^{\beta(H_{n_2}-\mu_{n_2})})^{-1}-(1+e^{\beta(H_{n_1}-\mu_{n_2})})^{-1}\|_1\\ &<\frac{\lambda\gamma}{2C}\|n_1-n_2\|_{L^1(\mathrm{cell})}.\end{aligned} \tag{59}$$

This shows that

$$\lim_{m\to\infty}|\mu_{T^{\circ(m+p)}[n]}-\mu_{T^{\circ m}[n]}|\to 0, \tag{60}$$

for any positive p, so the sequence is convergent. Also, (59) shows that the limit does not depend on n. ■

A similar result can be proven for the energy. However, we will not present them here, because we will return in the next section to this problem. The following result will be useful for proving the thermodynamic limit.

Proposition 8: For any $K \in \mathbf{N}$, let E_K be the energy of the system in the Hartree approximation. Then there exists E_M, independent of K, such that $|E_K/K^3| < E_M < \infty$.

The affirmation can be proven by following the same steps as in Lemma 6.

IV. THE THERMODYNAMIC LIMIT

For a given K, we denote by n_K, μ_K, E_K the density of particles, chemical potential and the energy of the system in the Hartree approximation. We proved in the last section that these objects exist for any $K \in \mathbf{N}$ provided the coupling constant smaller than some $\lambda_{\max}$, independent of K. We will use the notation Λ_K, $\mathcal{T}_K$, T_K, $H_n^{(K)}$ to indicate that these objects correspond to some $K \in \mathbf{N}$. The estimates we use in this section are based on the following technical proposition which will be proven at the end of this section.

Proposition 9: For $n \in L^1_{\text{per}}(T)$, $\|n\|_{L^1(\text{cell})} = N_0$ and $\mu \in [\mu_m, \mu_M]$, let us consider

$$f_{1,2}:[0,2\pi)^3 \to \mathcal{L}_1, \begin{cases} f_1(\vec{\theta}) = (1 + e^{\beta(-1/2\Delta_{\vec{\theta}} + u + \lambda V_n - \mu)})^{-1} \\ f_2(\vec{\theta}) = (-\frac{1}{2}\Delta_{\vec{\theta}} + u + \lambda V_n) f_1(\vec{\theta}) \end{cases},$$

where $\mathcal{L}_1$ denotes the trace class operators defined over the unit cell. Then $f_{1,2}$ are continuous:

$$\|f_i(\vec{\theta}) - f_i(\vec{\theta}')\|_1 < ct.|\vec{\theta} - \vec{\theta}'|^{\epsilon}, \quad i = 1,2,$$

where ϵ is a strictly positive constant which depends only on N_0.

The thermodynamic limit of the physical parameters will follow from the lemma below.

Lemma 10: With the above notations:

$$\|n_{K+1} - n_K\|_{L^1(\text{cell})} \to 0, \quad \text{as } K \to \infty.$$

Proof: There is a unique extension of n_K over $\mathcal{T}_{K+1}$ such that n_K remains periodic. This extension will be denoted by the same n_K:

$$\begin{aligned} \|n_{K+1} - n_K\|_{L^1(\text{cell})} &= \|\sum_{m=1}^{\infty} (T_{K+1}^{\circ m}[n_K] - T_{K+1}^{\circ(m-1)}[n_K])\|_{L^1(\text{cell})} \\ &\leqslant \sum_{m=1}^{\infty} \|(T_{K+1}^{\circ m}[n_K] - T_{K+1}^{\circ(m-1)}[n_K])\|_{L^1(\text{cell})} \\ &\leqslant (1 - \lambda\gamma)^{-1} \|T_{K+1}[n_K] - n_K\|_{L^1(\text{cell})}. \end{aligned} \tag{61}$$

Let μ_{n_K} be the chemical potential corresponding to n_K, i.e.,

$$(K+1)^3 N_0 = \text{Tr}(1 + e^{\beta(H_{n_K}^{(K+1)} - \mu_{n_K})})^{-1}. \tag{62}$$

We prove first that

$$\delta_K = |\mu_K - \mu_{n_K}| \to 0, \quad \text{as } K \to \infty. \tag{63}$$

From Lemma 6:

$$\begin{aligned} |\mu_K - \mu_{n_K}| &\leqslant C^{-1}(K+1)^{-3} |\text{Tr}(1 + e^{\beta(H_{n_K}^{(K+1)} - \mu_K)})^{-1} - \text{Tr}(1 + E^{\beta(H_{n_K}^{(K+1)} - \mu_{n_K})})^{-1}| \\ &= C^{-1} |(K+1)^{-3} \text{Tr}(1 + e^{\beta(H_{n_K}^{(K+1)} - \mu_K)})^{-1} - N_0| \\ &= C^{-1} |(K+1)^{-3} \text{Tr}(1 + e^{\beta(H_{n_K}^{(K+1)} - \mu_K)})^{-1} - K^{-3} \text{Tr}(1 + e^{\beta(H_{n_K}^{(K)} - \mu_K)})^{-1}| \\ &\leqslant C^{-1}[(K+1)^3/K^3 - 1] N_0 + C^{-1}(K+1)^{-3} \end{aligned}$$

$$\times\Big|\sum_{\mathbf{q}\in\Lambda_{K+1}}\mathrm{Tr}(1+e^{\beta(H^{(K+1,\mathbf{q})}_{n_K}-\mu_K)})^{-1}-\sum_{\mathbf{q}\in\Lambda_K}\mathrm{Tr}(1+e^{\beta(H^{(K,\mathbf{q})}_{n_K}-\mu_K)})^{-1}\Big|$$

$$\leq C^{-1}[(K+1)^3/K^3-1]N_0+C^{-1}(K+1)^{-3}\sum_{q\in\partial\Lambda_{K+1}}\mathrm{Tr}(1+e^{\beta(H^{(K+1,\mathbf{q})}_{n_K}-\mu_K)})^{-1}$$

$$+C^{-1}(K+1)^{-3}\sum_{\mathbf{q}\in\Lambda_K}\big|\mathrm{Tr}(1+e^{\beta(H^{(K+1,\mathbf{q})}_{n_K}-\mu_K)})^{-1}-\mathrm{Tr}(1+e^{\beta(H^{(K,\mathbf{q})}_{n_K}-\mu_K)})^{-1}\big|$$

$$\leq C^{-1}N_0[(K+1)^3/K^3-1]+ct.(K+1)^{-1}$$

$$+C^{-1}(K+1)^{-3}\sum_{\mathbf{q}\in\Lambda_K}|f_1(2\pi\mathbf{q}/(K+1))-f_1(2\pi\mathbf{q}/K)|$$

$$\leq C^{-1}N_0[(K+1)^3/K^3-1]+ct.(K+1)^{-1}$$

$$+ct.C^{-1}(K+1)^{-3}\sum_{\mathbf{q}\in\Lambda_K}\left|\frac{2\pi\mathbf{q}}{K+1}-\frac{2\pi\mathbf{q}}{K}\right|^{\epsilon}$$

$$\leq C^{-1}N_0[(K+1)^3/K^3-1]+ct.(K+1)^{-1}+ct.C^{-1}(K+1)^{-\epsilon}, \tag{64}$$

which proves (63). Now

$$\begin{aligned}\|T_{K+1}[n_K]-n_K\|_{L^1(\mathrm{cell})}&=\|(1+e^{\beta(H^{(K+1)}_{n_K}-\mu_{n_K})})^{-1}(\vec{x},\vec{x})-(1+e^{\beta(H^{(K)}_{n_K}-\mu_K)})^{-1}(\vec{x},\vec{x})\|_{L^1(\mathrm{cell})}\\&\leq\|(1+e^{\beta(H^{(K)}_{n_K}-\mu_{n_K})})^{-1}(\vec{x},\vec{x})-(1+e^{\beta(H^{(K)}_{n_K}-\mu_K)})^{-1}(\vec{x},\vec{x})\|_{L^1(\mathrm{cell})}\\&\quad+\|(1+e^{\beta(H^{(K+1)}_{n_K}-\mu_{n_K})})^{-1}(\vec{x},\vec{x})-(1+e^{\beta(H^{(K)}_{n_K}-\mu_{n_K})})^{-1}(\vec{x},\vec{x})\|_{L^1(\mathrm{cell})}\\&\leq K^{-3}\|(1+e^{\beta(H^{(K)}_{n_K}-\mu_{n_K})})^{-1}-(1+e^{\beta(H^{(K)}_{n_K}-\mu_K)})^{-1}\|_1\\&\quad+\|(K+1)^{-3}\sum_{\mathbf{q}\in\Lambda_{K+1}}(1+e^{\beta(H^{(K+1,\mathbf{q})}_{n_K}-\mu_{n_K})})^{-1}(\vec{x},\vec{x})\\&\quad-K^{-3}\sum_{\mathbf{q}\in\Lambda_K}(1+e^{\beta(H^{(K,\mathbf{q})}_{n_K}-\mu_{n_K})})^{-1}(\vec{x},\vec{x})\|_{L^1,(\mathrm{cell})}.\end{aligned}\tag{65}$$

The first term, above, have been evaluated in Lemma 6, so we can continue:

$$\begin{aligned}\|T_{K+1}[n_K]-n_K\|_{L^1(\mathrm{cell})}&\leq C'|\mu_{n_K}-\mu_K|+|(K+1)^{-3}\\&\quad-K^{-3}\Big|\Big\|\sum_{\mathbf{q}\in\Lambda_{K+1}}(1+e^{\beta(H^{(K+1,\mathbf{q})}_{n_K}-\mu_{n_K})})^{-1}(\vec{x},\vec{x})\Big\|_{L^1(\mathrm{cell})}\\&\quad+K^{-3}\Big\|\sum_{\mathbf{q}\in\Lambda_{K+1}}(1+e^{\beta(H^{(K+1,\mathbf{q})}_{n_K}-\mu_{n_K})})^{-1}(\vec{x},\vec{x})\\&\quad-\sum_{\mathbf{q}\in\Lambda_K}(1+e^{\beta(H^{(K,\mathbf{q})}_{n_K}-\mu_{n_K})})^{-1}(\vec{x},\vec{x})\Big\|_{L^1(\mathrm{cell})}\\&\leq C'\delta_K+|1-K^{-3}/(K+1)^3|N_0+K^{-3}\sum_{\mathbf{q}\in\partial\Lambda_{K+1}}\|(1+e^{\beta(H^{(K+1,\mathbf{q})}_{n_K}-\mu_{n_K})})^{-1}\|_1\\&\quad+K^{-3}\sum_{\mathbf{q}\in\Lambda_K}\|(1+e^{\beta(H^{(K+1,\mathbf{q})}_{n_K}-\mu_{n_K})})^{-1}-(1+e^{\beta(H^{(K,\mathbf{q})}_{n_K}-\mu_{n_K})})^{-1}\|_1\end{aligned}$$

$$\leqslant C'\,\delta_K+\left|1-K^{-3}/(K+1)^3\right|N_0+ct.(K+1)^2/K^3$$
$$+K^{-3}\sum_{\mathbf{q}\in\Lambda_K}\left\|f_1\left(\frac{2\pi\mathbf{q}}{K+1}\right)-f_1\left(\frac{2\pi\mathbf{q}}{K}\right)\right\|_1$$
$$\leqslant C'\,\delta_K+\left|1-K^{-3}/(K+1)^3\right|N_0+ct.(K+1)^2/K^3$$
$$+ct.K^{-3}\sum_{\mathbf{q}\in\Lambda_K}K^{-\epsilon}(K+1)^{-\epsilon}|\mathbf{q}|^{\epsilon}$$
$$\leqslant C'\,\delta_K+\left|1-K^{-3}/(K+1)^3\right|N_0+ct.(K+1)^2/K^3+ct.(K+1)^{-\epsilon}, \quad (66)$$

which finishes the proof. ■

Theorem 11: *If n_K is viewed as a linear functional over L^∞(cell):*

$$\hat{n}_K(g)=\int_{\text{cell}} n_K(\vec{x})g(\vec{x})d\vec{x}, \quad g\in L^\infty(\text{cell}),$$

then we have the following.

(i) $\{\hat{n}_K\}_K$ converges weakly in L^∞(cell), i.e., $\{\hat{n}_K(g)\}_K$ converges for any $g\in L^\infty$(cell)*

(ii) The chemical potential converges in the thermodynamic limit.

(iii) The energy per unit volume converges in the thermodynamic limit.

Unfortunately, exactly for $p=1$ it occurs that $(L^p)^*\neq L^q$, where q is the Holder conjugate of p.[3] This means that we need additional information in order to prove that the thermodynamic limit of particle density is in L^1.

Proof: (i) One knows from the Banach–Alaoglu theorem[3] that the closed balls in L^∞(cell)* are compact in the weak topology. Because $\|\hat{n}_K\|=\|n_K\|_{L^1(\text{cell})}=N_0$, it follows that $\{\hat{n}_K\}_K$ must have at least one accumulation point. Due to the fact that

$$\|\hat{n}_{K+1}(g)-\hat{n}_K(g)\|\leqslant\|n_{K+1}-n_K\|_{L^1(\text{cell})}\|g\|_{L^\infty(\text{cell})}, \quad (67)$$

for any $g\in L^\infty$(cell), it follows from Lemma 10 that there must be one and only one accumulation point.

(ii) Because $\{\mu_K\}_K$ is confined in a compact set (see Proposition 4), this sequence has at least one point of accumulation. Using the results of Theorem 7 and Lemma 10, one has successively,

$$|\mu_{K+1}-\mu_K|\leqslant|\mu_{K+1}-\mu_{n_K}|+|\mu_{n_K}-\mu_K|\leqslant\gamma/(2C)|n_K-n_{K+1}|+\delta_K. \quad (68)$$

Then, from a previous theorem, we can conclude that $|\mu_{K+1}-\mu_K|\to 0$ as $K\to\infty$, which shows that there is one and only one accumulation point for $\{\mu_K\}_K$.

(iii) The energy per unit volume is also confined in a compact set (Proposition 8), $|E_K/K^3|<E_M$. Also,

$$\left|(K+1)^{-3}E_{K+1}-K^{-3}E_K\right|$$
$$=\left|((K+1)^{-3}-K^{-3})E_{K+1}+K^{-3}\,\mathrm{Tr}\,H^{(K+1)}_{n_{K+1}}(1+e^{\beta(H^{(K+1)}_{n_{K+1}}-\mu_{K+1})})^{-1}\right.$$
$$\left.-K^{-3}\,\mathrm{Tr}\,H^{(K)}_{n_K}(1+e^{\beta(H^{(K)}_{n_K}-\mu_K)})^{-1}\right|$$
$$\leqslant((K+1)^3/K^3-1)E_M+K^{-3}\Big|$$
$$\times\sum_{\mathbf{q}\in\Lambda_{K+1}}\mathrm{Tr}\,H^{(K+1,\mathbf{q})}_{n_{K+1}}(1+e^{\beta(H^{(K+1,\mathbf{q})}_{n_{K+1}}-\mu_{K+1})})^{-1}$$

$$
\begin{aligned}
&- \sum_{\mathbf{q}\in\Lambda_K} \mathrm{Tr}\, H_{n_K}^{(K,\mathbf{q})}(1+e^{\beta(H_{n_K}^{(K,\mathbf{q})}-\mu_K)})^{-1}\big| \\
\leqslant &((K+1)^3/K^3-1)E_M+K^{-3} \\
&\times \sum_{\mathbf{q}\in\partial\Lambda_{K+1}} \big|\mathrm{Tr}\, H_{n_{K+1}}^{(K+1,\mathbf{q})}(1+e^{\beta(H_{n_{K+1}}^{(K+1,\mathbf{q})}-\mu_{K+1})})^{-1}\big| \\
&+K^{-3}\sum_{\mathbf{q}\in\Lambda_K} \big\|H_{n_{K+1}}^{(K+1,\mathbf{q})}(1+e^{\beta(H_{n_{K+1}}^{(K+1,\mathbf{q})}-\mu_{K+1})})^{-1}-H_{n_K}^{(K,\mathbf{q})}(1+e^{\beta(H_{n_K}^{(K,\mathbf{q})}-\mu_K)})^{-1}\big\|_1 \\
\leqslant &((K+1)^3/K^3-1)E_M+6K^{-3}(K+1)^2E_M \\
&+K^{-3}\sum_{\mathbf{q}\in\Lambda_K} \big\|H_{n_{K+1}}^{(K+1,\mathbf{q})}(1+e^{\beta(H_{n_{K+1}}^{(K+1,\mathbf{q})}-\mu_{K+1})})^{-1}-H_{n_K}^{(K+1,\mathbf{q})}(1+e^{\beta(H_{n_K}^{(K+1,\mathbf{q})}-\mu_{K+1})})^{-1}\big\|_1 \\
&+K^{-3}\sum_{\mathbf{q}\in\Lambda_K} \big\|H_{n_K}^{(K+1,\mathbf{q})}(1+e^{\beta(H_{n_K}^{(K+1,\mathbf{q})}-\mu_{K+1})})^{-1} \\
&-H_{n_K}^{(K,\mathbf{q})}(1+e^{\beta(H_{n_K}^{(K,\mathbf{q})}-\mu_{K+1})})^{-1}\big\|_1 \\
&+K^{-3}\sum_{\mathbf{q}\in\Lambda_K} \big\|H_{n_K}^{(K,\mathbf{q})}(1+e^{\beta(H_{n_K}^{(K,\mathbf{q})}-\mu_{K+1})})^{-1}-H_{n_K}^{(K,\mathbf{q})}(1+e^{\beta(H_{n_K}^{(K,\mathbf{q})}-\mu_K)})^{-1}\big\|_1 \\
= &((K+1)^3/K^3-1)E_M+6K^{-3}(K+1)^2E_M+K^{-3}\sum_{\mathbf{q}\in\Lambda_K} \|H_{n_{K+1}}^{(K+1,\mathbf{q})}(1+e^{\beta(H_{n_{K+1}}^{(K+1,\mathbf{q})}-\mu_{K+1})})^{-1} \\
&-H_{n_K}^{(K+1,\mathbf{q})}(1+e^{\beta(H_{n_K}^{(K+1,\mathbf{q})}-\mu_{K+1})})^{-1}\|_1+K^{-3}\sum_{\mathbf{q}\in\Lambda_K}\left\| f_2\left(\frac{2\pi\mathbf{q}}{K+1}\right) \quad -f_2\left(\frac{2\pi\mathbf{q}}{K}\right)\right\|_1 \\
&+K^{-3}\sum_{\mathbf{q}\in\Lambda_K} \big\|H_{n_K}^{(K,\mathbf{q})}(1+e^{\beta(H_{n_K}^{(K,\mathbf{q})}-\mu_{K+1})})^{-1}-H_{n_K}^{(K,\mathbf{q})}(1+e^{\beta(H_{n_K}^{(K,\mathbf{q})}-\mu_K)})^{-1}\big\|_1 . \qquad (69)
\end{aligned}
$$

The third term, above, can be shown to be smaller than $\gamma'\|n_{K+1}-n_K\|_{L^1(\mathrm{cell})}$. To evaluate this term, we have to replace in Eq. (46) $(1+e^{\beta(z-\mu)})^{-1}$ by $z(1+e^{\beta(z-\mu)})^{-1}$. This will not affect the next equations, so the conclusion will be the same. The fourth term can be evaluated using the continuity of f_2 (Lemma 9) and the fifth term has been evaluated in Lemma 6. It follows that

$$
\big|(K+1)^{-3}E_{K+1}-K^{-3}E_K\big|\to 0, \quad \text{as } K\to\infty, \qquad (70)
$$

which implies that the sequence $\{E_K/K^3\}_K$ has one and only one accumulation point. ■

Proof of Lemma 9: Let us denote $H_{\vec{\theta}}=-1/2\Delta_{\vec{\theta}}+u+\lambda V_n$. By simple manipulations,

$$
\begin{aligned}
f_1(\vec{\theta})-f_1(\vec{\theta}') = &[e^{-\beta(H_{\vec{\theta}}-\mu)}-e^{-\beta(H_{\vec{\theta}'}-\mu)}]\mathrm{ch}^{-1}\,\beta/2(H_{\vec{\theta}}-\mu) \\
&+e^{-\beta(H_{\vec{\theta}'}-\mu)}[\mathrm{ch}^{-1}\,\beta/2(H_{\vec{\theta}}-\mu)-\mathrm{ch}^{-1}\,\beta/2(H_{\vec{\theta}'}-\mu)], \qquad (71)
\end{aligned}
$$

and

$$
\begin{aligned}
f_2(\vec{\theta})-f_2(\vec{\theta}') = &[H_{\vec{\theta}}e^{-\beta(H_{\vec{\theta}}-\mu)}-H_{\vec{\theta}'}e^{-\beta(H_{\vec{\theta}'}-\mu)}]\mathrm{ch}^{-1}\,\beta/2(H_{\vec{\theta}}-\mu)+H_{\vec{\theta}'}e^{-\beta(H_{\vec{\theta}'}-\mu)} \\
&\times[\mathrm{ch}^{-1}\,\beta/2(H_{\vec{\theta}}-\mu)-\mathrm{ch}^{-1}\,\beta/2(H_{\vec{\theta}'}-\mu)]. \qquad (72)
\end{aligned}
$$

Because $e^{-\beta(H_{\vec{\theta}}-\mu)}$, $H_{\vec{\theta}}e^{-\beta(H_{\vec{\theta}}-\mu)}$ and $\mathrm{ch}^{-1}\,\beta/2(H_{\vec{\theta}}-\mu)$ are bounded in $\mathcal{L}_1$, with a bound independent of $\vec{\theta}$, n and μ, the lemma follows if we prove the L^2 norm continuity of $g(H_{\vec{\theta}})$ with respect to $\vec{\theta}$, for $g(z)$ equal to $e^{-\beta(z-\mu)}$, $ze^{-\beta(z-\mu)}$ or $\mathrm{ch}^{-1}\,\beta/2(z-\mu)$. In all cases,

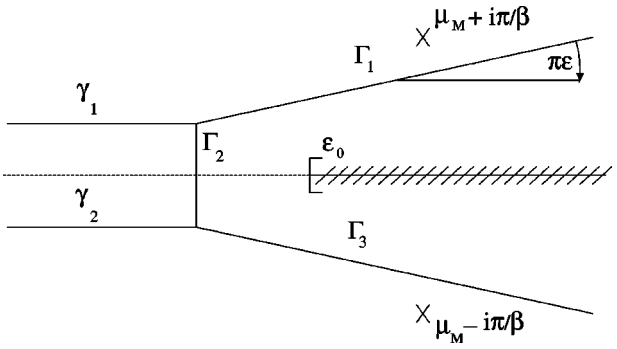

FIG. 1. The contour used in Lemma 9: $\Gamma=\Gamma_1\cup\Gamma_2\cup\Gamma_3$. The contour $\gamma=\gamma_1\cup\Gamma_2\cup\gamma_3$ is also used in Proposition 12. The poles of $\mathrm{ch}^{-1}\beta/2(z-\mu)$ at $\mu\pm i\pi/\beta$ limit the value of ϵ. The lowest limit of ϵ is obtained when $\mu=\mu_M$.

$$g(H_{\vec{\theta}})-g(H_{\vec{\theta}'})=\frac{1}{2\pi i}\int_{\Gamma}dz g(z)[(z-H_{\vec{\theta}})^{-1}-(z-H_{\vec{\theta}'})^{-1}], \tag{73}$$

where Γ is shown in Fig. 1.

Proposition 12: Let Γ be the contour shown in Fig. 1. In the conditions of Lemma 9, $(-\frac{1}{2}\Delta_{\vec{\theta}}+u+\lambda V_n-z)^{-1}$ is uniformly continuous with respect to $\vec{\theta}\in[0,2\pi)^3$, more exactly:

$$\|(-\tfrac{1}{2}\Delta_{\vec{\theta}}+u+\lambda V_n-z)^{-1}-(-\tfrac{1}{2}\Delta_{\vec{\theta}'}+u+\lambda V_n-z)^{-1}\|\leqslant ct.|\vec{\theta}-\vec{\theta}'|^{\epsilon},$$

for any $z\in\Gamma$, where $\epsilon>0$ and the ct. depends only on N_0.
We can conclude that

$$\|g(H_{\vec{\theta}})-g(H_{\vec{\theta}'})\|\leqslant ct.|\vec{\theta}-\vec{\theta}'|^{\epsilon}\frac{1}{2\pi}\int_{\Gamma}|dz||g(z)|, \tag{74}$$

and the lemma follows. ■

Proof of Proposition 12: Let us denote $u+\lambda V_n=U$. We prove first that

$$\|(-\tfrac{1}{2}\Delta_{\vec{\theta}}+U-z)^{-1}-(-\tfrac{1}{2}\Delta_{\vec{\theta}'}+U-z)^{-1}\|<ct.|\vec{\theta}-\vec{\theta}'|, \tag{75}$$

for any $z\in\gamma_1\cup\Gamma_2\cup\gamma_3$ (see Fig. 1). Because

$$\begin{aligned}(-\tfrac{1}{2}\Delta_{\vec{\theta}}+U-z)^{-1}-(-\tfrac{1}{2}\Delta_{\vec{\theta}'}+U-z)^{-1}=&(1+(-\tfrac{1}{2}\Delta_{\vec{\theta}}-z)^{-1}U)^{-1}[(-\tfrac{1}{2}\Delta_{\vec{\theta}}-z)^{-1}\\&-(-\tfrac{1}{2}\Delta_{\vec{\theta}'}-z)^{-1}](1+U(-\tfrac{1}{2}\Delta_{\vec{\theta}}-z)^{-1})^{-1},\end{aligned} \tag{76}$$

and the operators $(1+U(-\frac{1}{2}\Delta_{\vec{\theta}}-z)^{-1})^{-1}$ and $(1+(-\frac{1}{2}\Delta_{\vec{\theta}}-z)^{-1}U)^{-1}$ are uniformly bounded for $z\in\gamma_1\cup\Gamma_2\cup\gamma_3$ and the bound is independent of n (see Proposition 3), it is sufficient to prove that

$$\|(-\tfrac{1}{2}\Delta_{\vec{\theta}}-z)^{-1}-(-\tfrac{1}{2}\Delta_{\vec{\theta}'}-z)^{-1}\|<ct.|\vec{\theta}-\vec{\theta}'|. \tag{77}$$

If $G(\vec{x}-\vec{y};z)$ is the kernel of $(-\frac{1}{2}\Delta-z)^{-1}$, then

$$\left[\left(-\frac{1}{2}\Delta_{\vec{\theta}}+U-z\right)^{-1}-\left(-\frac{1}{2}\Delta_{\vec{\theta}'}+U-z\right)^{-1}\right](\vec{x},\vec{y})=\sum_{\vec{R}\in\Gamma}e^{-i\vec{R}\vec{\theta}'}(e^{-i\vec{R}(\vec{\theta}-\vec{\theta}')}-1)G(\vec{x}-\vec{y}+\vec{R};z). \tag{78}$$

Denoting by $\hat{A}_{\vec{R}}(z)$ the bounded operator on $L^2(\text{cell})$ corresponding to the kernel $G(\vec{x}-\vec{y}+\vec{R};z)$, then, for f and $g \in L^2(\text{cell})$, the following estimates are true:

$$\langle g,\hat{A}_{\vec{R}}(z)f\rangle=\langle \chi_{\text{cell}}g,(-\tfrac{1}{2}\Delta-z)^{-1}f_{\vec{R}}\rangle \leqslant |z|^{-1}\|g\|_{L^2(\text{cell})}\|f_{\vec{R}}\|_{L^2(R^3)}, \tag{79}$$

where $f_{\vec{R}}(\vec{x})=f(\vec{x}+\vec{R})$ for $\vec{x}+\vec{R}\in\text{cell}$ and zero otherwise. It is obvious that $\|f_{\vec{R}}\|_{L^2(R^3)}=\|f\|_{L^2(\text{cell})}$, which leads to $\|\hat{A}_{\vec{R}}(z)\|\leqslant|z|^{-1}$ which is a useful estimate for small $|\vec{R}|$. For large $|\vec{R}|$,

$$\begin{aligned}(\hat{A}_{\vec{R}}(z)f)(\vec{x})&=\int G(\vec{x}-\vec{y}+\vec{R};z)f(\vec{y})d\vec{y}\\ &\leqslant\sqrt{\int |G(\vec{x}-\vec{y}+\vec{R};z)|^2\,d\vec{y}}\,\|f\|_{L^2(\text{cell})}\leqslant\beta_{\vec{R}}(z)\sqrt{V_{\text{cell}}}\|f\|_{L^2(\text{cell})},\end{aligned} \tag{80}$$

where

$$\beta_{\vec{R}}(z)=\inf_{\vec{x},\vec{y}\in\text{cell}}|G(\vec{x}-\vec{y}+\vec{R};z)|. \tag{81}$$

This parameter exponentially decays as $|\vec{R}|\to\infty$, and it decreases as $\text{Re}\,z\to-\infty$. Thus

$$\|\hat{A}_{\vec{R}}(z)f\|_{L^2\text{cell}}\leqslant V_{\text{cell}}\sup_{z\in\gamma_1\cup\Gamma_2\cup\gamma_3}\beta_{\vec{R}}(z)\|f\|_{L^2(\text{cell})}. \tag{82}$$

From (77),

$$\left\|\left(-\frac{1}{2}\Delta_{\vec{\theta}}+U-z\right)^{-1}-\left(-\frac{1}{2}\Delta_{\vec{\theta}'}+U-z\right)^{-1}\right\|\leqslant|\vec{\theta}-\vec{\theta}'|\sum_{\vec{R}\in\Gamma}|\vec{R}|\|\hat{A}_{\vec{R}}(z)\|, \tag{83}$$

and the sum is convergent, because, for $\vec{R}$ large, one can use (82) while for the rest one can use (79). The sum converges due to exponential decay of $\beta_{\vec{R}}$. We turn now to investigate the case when $z\in\Gamma_1\cup\Gamma_3$. Because

$$\begin{aligned}&\|(-\tfrac{1}{2}\Delta_{\vec{\theta}'}+U-z)^{-1}-(-\tfrac{1}{2}\Delta_{\vec{\theta}'}+U-z)^{-1}\|\\ &\quad=\sup_{\|f\|,\|g\|=1}|\langle f,[(-\tfrac{1}{2}\Delta_{\vec{\theta}'}+U-z)^{-1}-(-\tfrac{1}{2}\Delta_{\vec{\theta}'}+U-z)^{-1}]g\rangle|,\end{aligned}$$

it will be sufficient to prove that

$$F(\vec{\theta},\vec{\theta}';z)\equiv\langle f,[(-\tfrac{1}{2}\Delta_{\vec{\theta}}+U-z)^{-1}-(-\tfrac{1}{2}\Delta_{\vec{\theta}'}+U-z)^{-1}]g\rangle, \tag{84}$$

satisfies

$$|F(\vec{\theta},\vec{\theta}';z)|<ct|\vec{\theta}-\vec{\theta}'|^{\epsilon},$$

for any $f, g\in L^2$ (cell), two unitary vectors. Now F is analytic on $\mathbf{C}\backslash[\epsilon_0,\infty)$ with respect to z and we just proved that $|F(z)|<ct.|\vec{\theta}-\vec{\theta}'|$, for $z\in\gamma_1$ and *ct.* independent of f and g. Then, from the two-constants theorem,[4] it follows that $|F(z)|<ct.|\vec{\theta}-\vec{\theta}'|^{\epsilon}$ for any $z\in\Gamma_1$, where $\pi\epsilon$ is the angle shown in Fig. 1. As is shown in Fig. 1, this angle depends only on the values of ϵ_0 and μ_M which, in turn, depend only on N_0. The same arguments apply for $z\in\Gamma_3$. ■

ACKNOWLEDGMENTS

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Hartree approximation III: Symmetry breaking

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We consider a one dimensional fermionic gas confined on a circle of finite length. At finite temperatures, in the absence of any background potential, one can show that a constant density of particles is a solution to the Hartree equation, regardless of the type of interparticle interaction. Moreover, at finite temperatures and small coupling constants, our previous analysis shows that this is the only solution of the Hartree equations. We show in this paper that, at zero temperature, there is another solution, which has an asymptotic expansion: $n(x)=n_0(1+ct.\cos 2k_F x)+o(\lambda)$, where λ is the coupling constant. Moreover, this solution is stable while the trivial solution become unstable at zero temperature. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379749]

I. INTRODUCTION

Let us consider a spinless, one dimensional fermionic gas confined on a circle, $\mathcal{T}_L$, of length L. Let us initially neglect the interaction between particles. In the absence of any background potential, the ground state of the system is nondegenerate, while the excited states are all double degenerate. Suppose there are $2N$ particles trapped on $\mathcal{T}_L$, where N is an integer number. At zero temperature, these particles occupy the energetic levels in order, starting with the lowest energy. Then there is only one particle that occupies the last energetic level (Fig. 1). In other words, the Fermi energy coincides with a degenerate energy level. In this case, the density of particles is not defined, because the state of the particle on the last occupied energy level is not known. Let us analyze this in a little more detail. The energy levels of the noninteracting system are given by $E_m=1/2(2\pi m/L)^2$. Let E_K $(K=N)$ be the last occupied energy level. In this case, the Fermi energy is given by

$$\varepsilon_F=\tfrac{1}{2}k_F^2=\tfrac{1}{2}(2\pi K/L)^2\Rightarrow L/(\lambda_F/2)=2K, \tag{1}$$

or, in other words, the half of the Fermi wavelength divides the length of the crystal in an even number. Things become clearer if we look at H_0 as a periodic Hamiltonian, with period $\delta=\lambda_F/2=\pi/k_F$. We consider the usual unitary transformation:

$$U:L^2(\mathcal{T}_L)\rightarrow\bigoplus_{q=0}^{2K-1}L^2[0,\delta],$$

$$L^2(\mathcal{T}_L)\ni f\rightarrow(Uf)_q(x)=\frac{1}{\sqrt{2K}}\sum_{m=0}^{2K-1}e^{-i\theta_q m}f(x+m\delta), \tag{2}$$

where $\theta_q=2\pi(q/2K)$. In this case,

$$UH_0U^{-1}=\bigoplus_{q=0}^{2K-1}-\frac{1}{2}\left(\frac{d^2}{dx^2}\right)_{\theta_q}\equiv\bigoplus_{q=0}^{2K-1}H_0^{(q)}, \tag{3}$$

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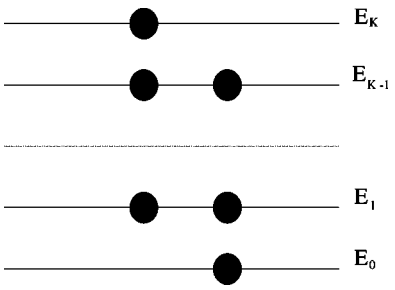

FIG. 1. The $2N$ particles occupy the lowest energetic levels. The last particle occupies a double degenerate level.

where $(d^2/dx^2)_{\theta_q}$ is the Laplace operator over $[0,\ \delta]$ with the boundary conditions:

$$f(\delta)=e^{i\theta_q}f(0) \quad \text{and} \quad f'(\delta)=e^{i\theta_q}f'(0). \tag{4}$$

Their eigenvalues and the corresponding eigenvectors are given by

$$\varepsilon_m^{(q,0)}=\tfrac{1}{2}(\omega_m+\theta_q/\delta)^2;\ \ \varphi_m^{(q,0)}(x)=\delta^{-1/2}e^{i(\omega_n+\theta_q/\delta)x}, \quad m\in\mathbf{Z}, \tag{5}$$

where $\omega_m=2\pi m/\delta$. We mention a few important properties of H_0^q.

(1) $H_0^{(q)}$ and $H_0^{(2K-q)}$ are anti-unitarily equivalent for $q=1,2,...,2K-1$, relative to the complex conjugation. This means that H_0^q and H_0^{2K-q} have the same eigenvalues and the corresponding eigenvectors are complex conjugate.

(2) For $q<K$, the ground state is defined by $m=0$. The ground state is given by

$$\varepsilon_0^{(q,0)}=\tfrac{1}{2}(\theta_q/\delta)^2;\ \ \varphi_0^{(q,0)}(x)=\delta^{-1/2}e^{i(\theta_q/\delta)x}. \tag{6}$$

The first excited state is $\varepsilon_{-1}^{(q,0)}$.

(3) For $q=K$, the ground state is degenerate:

$$\varepsilon_0^{(q=K,0)}=\varepsilon_{-1}^{(q=K,0)}=\tfrac{1}{2}(\pi/\delta)^2,$$
$$\varphi_0^{(q=K,0)}(x)=\delta^{-1/2}e^{i(\pi/\delta)x},\ \ \varphi_{-1}^{(q=K,0)}(x)=\varphi_0^{(q=K,0)}(x)^*. \tag{7}$$

(4) For $q>K$, the ground state is again nondegenerate:

$$\varepsilon_{-1}^{(q,0)}=\tfrac{1}{2}(-2\pi/\delta-\theta_q/\delta)^2;\ \ \varphi_{-1}^{(q,0)}(x)=\delta^{-1/2}e^{i(-2\pi/\delta+\theta_q/\delta)x}. \tag{8}$$

The first excited state is $\varepsilon_0^{(q,0)}$.

Then there is an alternative way of looking on the problem. As in Fig. 2, one can think that $2N-1$ particles occupy the nondegenerate ground states of $H_0^{(q\neq K,0)}$, while the last particle sits on the double degenerate ground state of $H_0^{(K,0)}$. Suppose, now, that a periodic potential is added:

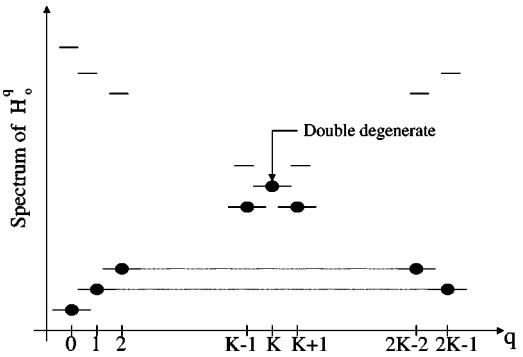

FIG. 2. The spectrum of $H_0^{(q)}$. The last particle occupies the double degenerate ground state of $H_0^{(K)}$.

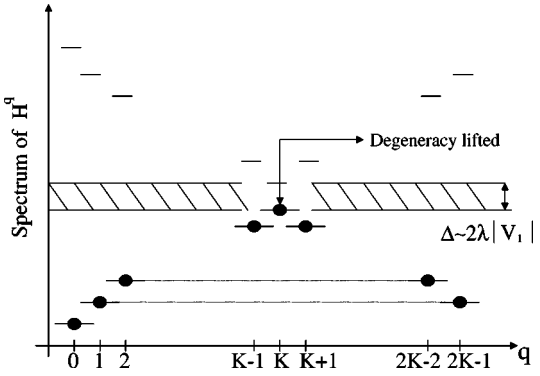

FIG. 3. The spectrum of $H_n^{(q)}$. The gap is opened due to the periodic potential.

$V(x+\delta)=V(x)$. If $V_1=\int_0^\delta e^{-i(2\pi/\delta)x}V(x)dx\neq 0$, perturbation theory shows that the degeneracy of the ground state of $H_0^{(K,0)}$ is lifted, or, in other words, a gap will open exactly at the Fermi energy. In this case, $H=H_0+V$ will be unitarily equivalent, through the same unitary transformation (1), to

$$UHU^{-1}=\bigoplus_{q=0}^{2K-1}\left[-\frac{1}{2}\left(\frac{d^2}{dx^2}\right)_{\theta_q}+V\right]\equiv\bigoplus_{q=0}^{2K-1}H^{(q)}. \tag{9}$$

In the limit of small coupling constants, the spectrum of these Hamiltonians can be pictured as in Fig. 3. Because the last occupied energy level is nondegenerate, the density of particles will be well defined at zero temperature. If $P^{(q)}$ is the projector onto the ground state of $H^{(q)}$, then the density of particles is given by

$$n(x)=\sum_{q=0}^{2K-1}(U^{-1}P^{(q)}U)(x,x)\Leftrightarrow n(x+m\delta)=\frac{1}{2K}\sum_{q=0}^{2K-1}P^{(q)}(x,x), \tag{10}$$

for $x\in[0,\delta]$ and any integer m. In the Hartree approximation, this periodic potential may come from a modulation of the particles density. Indeed, denoting by $|x,y|$ the distance between two points of the circle $\mathcal{T}$ and if v denotes the two-body interaction, then

$$H_n=H_0+\lambda\int_{\mathcal{T}}v(|x,y|)[n(y)-n_0]dy \tag{11}$$

is a periodic Hamiltonian. This happens because, if $n(x+\delta)=n(x)$,

$$\begin{aligned}V_n(x+\delta)&=\int_{\mathcal{T}}v(|x+\delta,y|)[n(y)-n_0]dy\\&=\int_{\mathcal{T}}v(|x,y-\delta|)[n(y)-n_0]dy\\&=\int_{\mathcal{T}}v(|x,y|)[n(y+\delta)-n_0]dy=V_n(x).\end{aligned} \tag{12}$$

Here we used $|x+t,y|=|x,y-t|$. We will consider in this paper that the real axis is winded around $\mathcal{T}$, thus, any point of the real axis may be considered also a point of the circle. In (11), a

background charge has been considered. Its effect is a constant added to the Hamiltonian. However, this will be useful because it cancels the zero-th Fourier coefficient of V_n. We use the following notations:

$$UH_nU=\bigoplus_{q=0}^{2K-1}\left[-\frac{1}{2}\left(\frac{d^2}{dx^2}\right)_{\theta_q}+\lambda V_n\right]\equiv\bigoplus_{q=0}^{2K-1}H_n^{(q)}. \tag{13}$$

The eigenvalues of $H_n^{(q)}$ will be denoted by $\varepsilon_m^{(q,n)}$ and the corresponding projectors by $P_m^{(q,n)}$. Also we will use in the next section $P_{0-1}^{(q,n)}$ to denote the projector for $\varepsilon_0^{(q,n)}$ and $\varepsilon_{-1}^{(q,n)}$. The notation implies that $\varepsilon_m^{(q,n)}$ are perturbations of $\varepsilon_m^{(q,n_0)}$. This is unambiguous for $q\neq K$. For $q=K$, there is an ambiguity about $\varepsilon_{0,-1}^{(K,n)}$ because the unperturbed eigenvalues are equal. Our convention will be that $\varepsilon_0^{(K,n)}$ denotes the lowest energy level of $H_n^{(K)}$. With the remarks above, it follows that the Hartree problem is well defined on the set:

$$\mathcal{S}_\epsilon=\left\{n\in L^1_{\rm per}(\mathcal{T}_L)\,\middle|\,\|n\|_{L^1(\mathcal{T})}=2N,\left|\frac{1}{\delta}\int_0^\delta e^{-i(2\pi/\delta)x}n(x)dx\right|>\epsilon\right\}, \tag{14}$$

for some $\epsilon>0$, because, for $n\in\mathcal{S}_\epsilon$, the first Fourier coefficient of V_n is nonzero, which means the gap is opened in the spectrum (at least in the range of small coupling constants) exactly at the Fermi energy, so the projector on the spectrum below Fermi energy is well defined. This means we can define the map

$$T:\mathcal{S}_\epsilon\to L^1_{\rm per}(\mathcal{T});\quad T[n](x)=P_{(-\infty,\epsilon_F)}(H_n)(x,x)=\sum_{q=0}^{2K-1}(U^{-1}P^{(q,n)}U)(x,x). \tag{15}$$

The value of ϵ is fixed, such that $\epsilon\ll 1/(4\delta K)$ for reasons that will be explained in the next section. The Hartree problem consists[1] of solving $n=T[n]$, which, as we shall see in the next sections, has a solution for λ small.

II. THE $\lambda\to 0^+$ LIMIT

We start by computing the asymptotic expansion of the map T. We will see that the perturbation of the degenerate ground state of $H_0^{(K)}$ has a nontrivial effect.

Proposition 1: The asymptotic expansion of T around $\lambda=0$ *is given by*

$$T[n](x+m\delta)=\frac{1}{\delta}+\frac{\lambda v_1}{2K\delta(\varepsilon_0^{(K,n)}-\varepsilon_{-1}^{(K,n)})}(n_1e^{i2\pi x/\delta}+n_{-1}e^{-i2\pi x/\delta})+o(\lambda),$$

for $x\in[0,\delta]$ *and any integer m. The Fourier coefficients are given by*

$$n_m=\frac{1}{\delta}\int_0^\delta e^{-i\omega_m x}n(x)dx\quad\text{and}\quad v_m=\int_{\mathcal{T}}e^{-i\omega_m(x-y)}v(|x,y|)dx.$$

Before proving this proposition, we need to compute the perturbed eigenvalues. In the classical perturbation theory,[2] one needs to calculate the projectors in order to find the corresponding perturbed eigenvalues. There is a direct way of finding the perturbed eigenvalues, without involving the projectors.

Proposition 2: If $v\in L^{(2)}(R)+L^\infty(R)$, *then the eigenvalues of* $H_n^{(K)}$ *are the solutions of the following equation (in E)*:

$$E-\varepsilon_0^{(K,n)}=\lambda M_{00}(E)\pm|\lambda M_{0,-1}(E)|,$$

where

$$M_{ij}(E)=\langle \varphi_i^{(K,n_0)},[1-\lambda V_n G_0^{(K,n_0)}(E)]^{-1}V_n\varphi_j^{(K,n_0)}\rangle$$

and $G_0^{(K,n_0)}(E)$ *is the bounded operator for* E *in a vicinity of* $\varepsilon_0^{(K,n_0)}=\varepsilon_{-1}^{(K,n_0)}$, *given by*

$$G_{0,-1}^{(K,n_0)}(E)=(E-H_0^{(K)})^{-1}-(E-\varepsilon_0^{(K,n_0)})^{-1}P_{0,-1}^{(K,n_0)}.$$

Proof: For $E\neq\varepsilon_0^{(K,n_0)}$ one has successively,

$$\begin{aligned}(E-H_0^{(K)}-\lambda V_n)&=[1-\lambda V_n(E-H_0^{(K)})^{-1}](E-H_0^{(K)})\\&=[1-\lambda V_n(E-\varepsilon_0^{(K,n_0)})^{-1}P_{0,-1}^{(K,n_0)}-\lambda V_n G_{0,-1}^{(K,n_0)}](E-H_0^{(K)})\\&=(1-\lambda V_n G_{0,-1}^{(K,n_0)})\\&\quad\times[1-\lambda(E-\varepsilon_0^{(K,n_0)})^{-1}(1-\lambda V_n G_{0,-1}^{(K,n_0)})^{-1}V_n P_{0,-1}^{(K,n_0)}](E-H_0^{(K)}).\end{aligned}\tag{16}$$

We used that $V_n G_{0,-1}^{(K,n_0)}$ is a bounded operator for E in a vicinity of $\varepsilon_0^{(K,n_0)}$, which easily follows from Ref. 3. Assuming that the perturbed eigenvalues are different from the unperturbed ones, we can conclude that $E-H_0^{(K)}-\lambda V_n$ is not invertible if and only if

$$\det[1-\lambda(E-\varepsilon_0^{(K,n_0)})^{-1}(1-\lambda V_n G_{0,-1}^{(K,n_0)})^{-1}V_n P_{0,-1}^{(K,n_0)}]=0.\tag{17}$$

For two trace class operators, $\det(1+AB)=\det(1+BA)$, which allows us to write

$$\det[1-\lambda(E-\varepsilon_0^{(K,n_0)})^{-1}P_{0,-1}^{(K,n_0)}(1-\lambda V_n G_{0,-1}^{(K,n_0)})^{-1}V_n P_{0,-1}^{(K,n_0)}]=0,\tag{18}$$

which is equivalent to

$$\det[P_{0,-1}^{(K,n_0)}-\lambda(E-\varepsilon_0^{(K,n_0)})^{-1}P_{0,-1}^{(K,n_0)}(1-\lambda V_n G_{0,-1}^{(K,n_0)})^{-1}V_n P_{0,-1}^{(K,n_0)}]=0.\tag{19}$$

This is just an ordinary determinant:

$$\det\begin{pmatrix}1-\lambda(E-\varepsilon_0^{(K,n_0)})^{-1}M_{00}(E) & -\lambda(E-\varepsilon_0^{(K,n_0)})^{-1}M_{01}(E)\\ -\lambda(E-\varepsilon_0^{(K,n_0)})^{-1}M_{01}(E)^* & 1-\lambda(E-\varepsilon_0^{(K,n_0)})^{-1}M_{-1-1}(E)\end{pmatrix}=0,\tag{20}$$

where we use the fact that $(1-\lambda V_n G_{0,-1}^{(K,n_0)})^{-1}V_n$ is self-adjoint ($\Rightarrow M_{-10}(E)=M_{0-1}(E)^*$). This can be seen by expanding this operator. Thus

$$E-\varepsilon_0^{(K,n_0)}=\lambda\frac{M_{00}(E)+M_{-1-1}(E)}{2}\pm\frac{|\lambda|}{2}\sqrt{(M_{00}(E)-M_{-1-1}(E))^2+4|M_{0-1}|^2}.\tag{21}$$

Because the kernel of the operator $(E-H_0^{(K)})^{-1}$ has no imaginary part for $E\in R$,[4] $(1-\lambda V_n G_{0,-1}^{(K,n_0)})^{-1}V_n$ commutes with the complex conjugation, C^*. Then $M_{00}(E)=M_{-1-1}(E)$. Indeed,

$$\begin{aligned}&\langle\varphi_0^{(K,n_0)},[1-\lambda V_n G_0^{(K,n_0)}(E)]^{-1}V_n\varphi_0^{(K,n_0)}\rangle\\&\quad=\langle C^*\varphi_{-1}^{(K,n_0)},[1-\lambda V_n G_0^{(K,n_0)}(E)]^{-1}V_n C^*\varphi_{-1}^{(K,n_0)}\rangle\\&\quad=\langle C^*\varphi_{-1}^{(K,n_0)},C^*[1-\lambda V_n G_0^{(K,n_0)}(E)]^{-1}V_n\varphi_{-1}^{(K,n_0)}\rangle\\&\quad=\langle[1-\lambda V_n G_0^{(K,n_0)}(E)]^{-1}V_n\varphi_{-1}^{(K,n_0)},\varphi_{-1}^{(K,n_0)}\rangle\end{aligned}$$

$$= \langle \varphi_{-1}^{(K,n_0)}, [1-\lambda V_n G_0^{(K,n_0)}(E)]^{-1} V_n \varphi_{-1}^{(K,n_0)} \rangle. \tag{22}$$

In the same way, it follows that $M_{0-1}(E)$ is a real number. In consequence, the equation for the perturbed eigenvalues is

$$E - \varepsilon_0^{(K,n_0)} = \lambda M_{00}(E) \pm |\lambda M_{0,-1}(E)|. \tag{23}$$

It is useful to give the asymptotic expansion of the eigenvalues. A simple calculus shows

$$M_{00}(E) = \langle \varphi_0^{(K,n_0)}, V_n \varphi_0^{(K,n_0)} \rangle + \lambda \langle \varphi_0^{(K,n_0)}, V_n G_0^{(K,n_0)}(E) V_n \varphi_0^{(K,n_0)} \rangle = o(\lambda), \tag{24}$$

because the background charge cancels the zero-th Fourier coefficient of V_n:

$$\begin{aligned} M_{0-1}(E) &= \langle \varphi_0^{(K,n_0)}, V_n \varphi_{-1}^{(K,n_0)} \rangle + o(\lambda) \\ &= \frac{1}{\delta} \int_0^{\delta} e^{-i\omega_1 x} V_n(x) dx + o(\lambda) \\ &= \frac{1}{\delta} \frac{1}{2K} \int_{\mathcal{T}} dx \int_{\mathcal{T}} dy e^{-i\omega_1 x} v(|x,y|)(n(y)-n_0) + o(\lambda) \\ &= \int_{\mathcal{T}} dx\, e^{-i\omega_1 (x-y)} v(|x,y|) \frac{1}{\delta} \int_0^{\delta} e^{-i\omega_1 y} n(y) = v_1 n_1 + o(\lambda). \end{aligned} \tag{25}$$

Finally,

$$\begin{aligned} \varepsilon_0^{(K,n)} &= \varepsilon_0^{(K,n_0)} - |\lambda v_1 n_1| + o(\lambda^2), \\ \varepsilon_{-1}^{(K,n)} &= \varepsilon_0^{(K,n_0)} + |\lambda v_1 n_1| + o(\lambda^2), \end{aligned} \tag{26}$$

Due to our notation, these eigenvalues are not analytic at $\lambda = 0$, because here they switch places such that $\varepsilon_0^{(K,n)}$ is always the lowest eigenvalue, as our notation requires. Equation (26) also shows that the perturbed eigenvalues are different by $\varepsilon_0^{(K,n_0)}$ for small λ, which means the assumption we made is true. ■

Proof of Proposition 1: Using resolvent calculus, it follows that

$$P^{(q,n)} = P_0^{(q,n_0)} + \lambda R^{(q,n)} \quad \text{for} \quad q < K, \tag{27}$$

where $R^{(q,n)}$ is a finite rank operator, uniformly bounded for λ in a vicinity of 0 and $n \in \mathcal{S}_\epsilon$. For $q = K$ we can write only

$$P_0^{(K,n)} + P_{-1}^{(q,n)} = P_0^{(K,n_0)} + P_{-1}^{(K,n_0)} + \lambda Q^{(K,n)}, \tag{28}$$

where, again, $Q^{(K,n)}$ is a finite rank operator, uniformly bounded for λ in a vicinity of 0 and $n \in \mathcal{S}_\epsilon$. If the eigenvalues of $H_n^{(K)}$ are known, then

$$(\varepsilon_0^{(K,n)} - \varepsilon_{-1}^{(K,n)}) P_0^{(K,n)} = P_{0,-1}^{(K,n)} (H_n^{(K)} - \varepsilon_{-1}^{(K,n)}) P_{0,-1}^{(K,n)}, \tag{29}$$

can be used to calculate the projector. Indeed, if one plugs in the right-hand side of (29) the expression (28),

$$\begin{aligned} (\varepsilon_0^{(K,n)} - \varepsilon_{-1}^{(K,n)}) P_0^{(K,n)} &= P_{0,-1}^{(K,n_0)} (H_n^{(K)} - \varepsilon_{-1}^{(K,n)}) P_{0,-1}^{(K,n_0)} + \lambda (\varepsilon_0^{(K,n)} - \varepsilon_{-1}^{(K,n)}) P_0^{(K,n)} Q^{(q,n)} \\ &\quad + \lambda Q^{(q,n)} (H_n^{(K)} - \varepsilon_{-1}^{(K,n)}) P_{0,-1}^{(K,n_0)}. \end{aligned} \tag{30}$$

We simplify the notation by

$$\hat{K}_0 \equiv (\varepsilon_0^{(K,n)} - \varepsilon_{-1}^{(K,n)})^{-1} P_{0,-1}^{(K,n_0)} (H_n^{(K)} - \varepsilon_{-1}^{(K,n)}) P_{0,-1}^{(K,n_0)}. \tag{31}$$

Then

$$P_0^{(K,n)}(1-\lambda Q^{(K,n)}) = \hat{K}_0 + \lambda (\varepsilon_0^{(K,n)} - \varepsilon_{-1}^{(K,n)})^{-1} Q^{(q,n)} (H_n^{(K)} - \varepsilon_{-1}^{(K,n)}) P_{0,-1}^{(K,n_0)}. \tag{32}$$

Using the identity

$$(1-\lambda Q^{(K,n)})^{-1} = 1 + \lambda Q^{(K,n)} (1-\lambda Q^{(K,n)})^{-1}, \tag{33}$$

we can finally give the asymptotic expansion of $P_0^{(K,n)}$:

$$P_0^{(K,n)} = \hat{K}_0 + \lambda R^{(K,n)}, \tag{34}$$

where

$$R^{(K,n)} = \left[\hat{K}_0 Q^{(K,n)} + Q^{(K,n)} \hat{K}_0 + \frac{\lambda}{\varepsilon_0^{(K,n)} - \varepsilon_{-1}^{(K,n)}} Q^{(K,n)} (P_{0,-1}^{(K,n_0)})^{\perp} V_n P_{0,-1}^{(K,n_0)} \right] \times (1-\lambda Q^{(K,n)})^{-1}, \tag{35}$$

is uniformly bounded for small λ and $n \in \mathcal{S}_\epsilon$. We can write now the asymptotic expansion of the map T:

$$T[n](x+m\delta) = \frac{1}{2K} \left[P_0^{(0,n_0)}(x,x) + 2 \sum_{q=1}^{K-1} P_0^{(q,n_0)}(x,x) + \hat{K}_0(x,x) + \lambda R'[n](x,x) \right]. \tag{36}$$

Because the operators $R^{(q,n)}$, $q = \overline{0,K}$, are of finite rank and uniformly bounded, it follows that $\lambda R'[n](x,x)$ actually goes to zero in $L^1(\mathcal{T})$ as λ goes to zero. Using the expressions for the projectors,

$$T[n](x+m\delta) = \frac{1}{\delta} + \frac{\lambda v_1}{2K(\varepsilon_0^{(K,n)} - \varepsilon_{-1}^{(K,n)})\delta} (n_1 e^{i2\pi x/\delta} + n_{-1} e^{-i2\pi x/\delta}) + \frac{2\varepsilon_0^{(K,n_0)} - \varepsilon_0^{(K,n)} - \varepsilon_{-1}^{(K,n)}}{2K(\varepsilon_0^{(K,n)} - \varepsilon_{-1}^{(K,n)})\delta} + \lambda R'[n](x,x), \tag{37}$$

where we also used $v_1 = v_{-1}$. The leading term is given by

$$\frac{1}{\delta} + \frac{\lambda v_1}{2K(\varepsilon_0^{(K,n)} - \varepsilon_{-1}^{(K,n)})\delta} (n_1 e^{i2\pi x/\delta} + n_{-1} e^{-i2\pi x/\delta}), \tag{38}$$

because the third term is of order λ, as it follows from Proposition 2. ■

We formulate now the principal result of this section.

Proposition 3: If the Hartree equation $n = T[n]$ has a solution for λ small, then this solution has a well defined limit as λ goes to zero, given by

$$\lim_{\lambda \to 0^+} n(x) = \frac{1}{\delta} \left[1 + \frac{1}{2K} \cos(2k_F x + \phi) \right],$$

provided $v_1 < 0$. The limit is in $L^1(\mathcal{T})$.

Proof: Because $R^{(q,n)}$, $q=0,1,...,K$, are of finite rank, uniformly bounded for $n\in\mathcal{S}_\epsilon$ and small λ, we have

$$\lim_{\lambda\to 0^+} n_\lambda(x)=\lim_{\lambda\to 0^+} T[n_\lambda](x)=\frac{1}{\delta}-\frac{1}{2K\delta}\frac{v_1}{2|v_1 n_1|}(n_1 e^{i2\pi x/\delta}+n_{-1}e^{-i2\pi x/\delta}), \tag{39}$$

where the limit is true in $L^1(\mathcal{T}_L)$. Writing $n_{\pm 1}=|n_1|e^{\pm i\phi}$:

$$\lim_{\lambda\to 0^+} n_\lambda(x)=\frac{1}{\delta}-\frac{1}{2K\delta}\frac{v_1}{|v_1|}\cos[2\pi x/\delta+\phi]. \tag{40}$$

On the other hand,

$$n(x)=n_0+2|n_1|\cos[2\pi x/\delta+\phi]+\sum_{|m|>1} n_m e^{i2\pi m x/\delta}, \tag{41}$$

which leads to $|n_1|=-v_1/(4K\delta|v_1|)$. This is the reason we chose $\epsilon<1/(4K\delta)$. Then there is a solution if and only if $v_1<0$. For example, an attractive, short range interaction will satisfy this condition. Assuming $v_1<0$,

$$\lim_{\lambda\to 0^+} n(x)=\frac{1}{\delta}\left[1+\frac{1}{2K}\cos(2k_F x+\phi)\right]. \tag{42}$$

■

The parameter ϕ is free, and it comes, basically, from the symmetry of the problem relative to the rotation of the circle $\mathcal{T}$. Specifically, if n is a solution of the Hartree equation so it is $n_\phi(x)=n(x+\phi)$.

III. THE $\lambda>0$ CASE

There is another symmetry that we will exploit in this section. Because the interparticle interaction depends only on the distance between particles, it follows that $V_n(-x)=V_n(x)$ whenever $n(-x)=n(x)$. Because the kinetic energy is symmetric relative to $x\to -x$ transformation, it follows that $T[n](-x)=T[n](x)$ whenever $n(-x)=n(x)$. In other words, the space of densities with this property is invariant under T. In this section, we restrict T to the intersection of $\mathcal{S}_\epsilon$ with the space of densities with this property. The new set is denoted by the same symbol $\mathcal{S}_\epsilon$. We mention that, for $n\in\mathcal{S}_\epsilon$, the Fourier coefficients of n are real numbers, which is a major advantage as we will see in the following. Let us analyze first the leading term of T.

Proposition 4: For small λ, *the leading term of the map T,*

$$T_0[n]=\frac{1}{\delta}+\frac{1}{2K\delta}\frac{\lambda v_1}{\varepsilon_0^{(K,n)}-\varepsilon_{-1}^{(K,n)}}(n_1 e^{i\omega_1 x}+n_{-1}e^{-i\omega_1 x}),$$

has a fixed point in $\mathcal{S}_\varepsilon$.

Proof: Restricted to $\mathcal{S}_\varepsilon$, T_0 becomes

$$T_0[n]=\frac{1}{\delta}+\frac{1}{2K\delta}\frac{\lambda v_1}{\varepsilon_0^{(K,n)}-\varepsilon_{-1}^{(K,n)}}2n_1\cos\omega_1 x. \tag{43}$$

Of course, the fixed point must be of the form $1/\delta+2n_1\cos\omega_1 x$, which leads to

$$\frac{1}{2K\delta}\lambda v_1/(\varepsilon_0^{(K,n)}-\varepsilon_{-1}^{(K,n)})=1. \tag{44}$$

We use the implicit function theorem to prove that, for small, positive λ, this equation has a solution, i.e., there is a $n_1(\lambda)$ such that (44) is satisfied. First we remember that, with our notation, $\varepsilon_{0,-1}^{(K,n)}$ are not analytic at $\lambda=0$. The eigenvalues were the solutions of the equations

$$E-\varepsilon_0^{(K,n_0)}=\lambda M_{00}(E)\pm|\lambda M_{0,-1}(E)|. \tag{45}$$

We will replace $\varepsilon_{0,-1}^{(K,n)}$ by $\varepsilon_{\pm}^{(K,n)}$ given by the solutions of the equations:

$$E-\varepsilon_0^{(K,n_0)}=\lambda(M_{00}(E)\pm M_{0-1}(E)). \tag{46}$$

The asymptotic expansion of $M_{0,-1}(E)$ was given in Proposition 2:

$$M_{0-1}(E)=v_1n_1+o(\lambda)<0, \tag{47}$$

for small λ and n_1 in a vicinity of the solution found last section, $\underline{n}_1=1/(4K\delta)$. This means $\varepsilon_{\pm}^{(K,n)}=\varepsilon_{0,-1}^{(K,n)}$ for $\lambda>0$ and $\varepsilon_{\mp}^{(K,n)}=\varepsilon_{0,-1}^{(K,n_0)}$ for $\lambda<0$. We consider the function

$$F(\lambda,n_1)=\frac{1}{2K\delta}\lambda v_1/(\varepsilon_+^{(K,n)}(\lambda)-\varepsilon_-^{(K,n)}(\lambda)). \tag{48}$$

For this particular expression of n, $V_n=2v_1n_1\cos\omega_1x$. If we denote by $\varepsilon_{\pm}(\xi)$ the eigenvalues of $H_0^{(K)}+2\xi v_1\cos\omega_1x$, then $\varepsilon_{\pm}^{(K,n)}(\lambda)=\varepsilon_{\pm}(\xi=\lambda v_1)$. Thus, if we define

$$\tilde{F}(\xi)=\frac{1}{2K\delta}\xi v_1/(\varepsilon_+(\xi)-\varepsilon_-(\xi)), \tag{49}$$

we can write $F(\lambda,n_1)=\tilde{F}(\lambda n_1)/n_1$. Now, $\tilde{F}$ is analytic for $\xi\neq0$, with a well defined limit as $\xi\to0$. This means that $\tilde{F}$ is analytic in a vicinity of 0 which implies that $F(\lambda,n_1)$ is analytic in both arguments, for λ in a vicinity of 0 and n_1 in a vicinity of $\underline{n}_1$. Moreover,

$$\frac{\partial F(\lambda,n_1)}{\partial n_1}=-\frac{1}{n_1^2}\tilde{F}(\lambda n_1)+\frac{\lambda}{n_1}\frac{d\tilde{F}}{d\xi}(\lambda n_1), \tag{50}$$

which leads to $\partial F(\lambda,n_1)/\partial n_1|_{\lambda=0,n_1=\underline{n}_1}=-1/\underline{n}_1\neq0$. Collecting all these results,

$$\begin{aligned}&F(\lambda,n_1),\text{analytic around } (0,\underline{n}_1);\\ &\left.\frac{\partial F(\lambda,n_1)}{\partial n_1}\right|_{(0,\underline{n}_1)}\neq0;\quad F(0,\underline{n}_1)=1,\end{aligned} \tag{51}$$

so the conditions of the analytic implicit function theorem are satisfied. This means there is an analytic solution $n_1(\lambda)$ such that $F(\lambda,n_1(\lambda))=1$, for small λ. Of course, for small λ, $n_1(\lambda)>\varepsilon$. Then the proposition follows from the fact that, for $\lambda>0$,

$$F(\lambda,n_1)=\frac{1}{2K\delta}\lambda v_1/(\varepsilon_0^{(K,n)}-\varepsilon_{-1}^{(K,n)}). \tag{52}$$

Let us denote by n_λ the fixed point of T_0. Next we prove that T_0 is a contraction in a vicinity of n_λ. We will make use of the following result.

Proposition 5: Let X, Y two Banach spaces. Let f: $X\to Y$ be a function such that

$$\lim_{t\to0}\|f(x+t(x-x'))-f(x)\|/t<\chi,$$

for any x, x′ with $\|x-x'\|=1$, and $x\in B_{2\varepsilon}(x_0)$. Then, for x, $x'\in B_\varepsilon(x_0)$,

$$\|f(x')-f(x)\|<\chi\|x-x'\|.$$

Proof: For $x, x' \in B_\varepsilon(x_0)$,

$$\begin{aligned}
&\|f(x')-f(x)\| \\
&\quad=\left\|\sum_{m=0}^{N-1}\left[f\left(x+\frac{(m+1)\|x-x'\|}{N}\frac{(x-x')}{\|x-x'\|}\right)-f\left(x+\frac{m\|x-x'\|}{N}\frac{(x-x')}{\|x-x'\|}\right)\right]\right\| \\
&\quad\leqslant\frac{\|x-x'\|}{N}\sum_{m=0}^{N-1}\left\|f\left(x_m+t_N\frac{(x-x')}{\|x-x'\|}\right)-f(x_m)\right\|/t_N,
\end{aligned} \tag{53}$$

where $t_N=\|x-x'\|/N$ and $x_m=x+m/N(x-x')$ belongs to $B_{2\varepsilon}(x_0)$. Taking the limit $N\to\infty$ and using the property given in the proposition, the affirmation follows easily. ■

Proposition 6: Let $\varepsilon>0$ such that $L^1_{\mathrm{per}}(\mathcal{T})\cap B_{2\varepsilon}(n_\lambda)\subset\mathcal{S}_\varepsilon$. Then, for $n, n'\in\mathcal{S}_\varepsilon\cap B_\varepsilon(n_\lambda)$:

$$\|T_0[n]-T_0[n']\|_{L^1}\leqslant\chi\|n-n'\|_{L^1},\quad \chi=o(\lambda).$$

Proof: We take X and Y in the last proposition as $L^1_{\mathrm{per}}(\mathcal{T})$. We want to calculate

$$\lim_{t\to0}\|(T_0[n+t(n'-n)]-T_0[n])/t\|_{L^1(\mathcal{T})}, \tag{54}$$

for $n\in L^1_{\mathrm{per}}(\mathcal{T}_L)\cap B_{2\varepsilon}(n_\lambda)$ and $n'\in L^1_{\mathrm{per}}(\mathcal{T}_L)$, with $\|n-n'\|=1$. The limit (54) makes sense because, for small t, $n+t(n'-n)\subset\mathcal{S}_\varepsilon$. Because

$$T_0[n+t(n'-n)](x)=\frac{1}{\delta}+\frac{v_1}{2K\delta}\frac{\lambda n_1+\lambda t(n_1'-n_1)}{\varepsilon_0^{(K)}(n+t(n'-n))-\varepsilon_{-1}^{(K)}(n+t(n'-n))}2\cos\omega_1 x, \tag{55}$$

it is natural to consider the Hamiltonian:

$$H(\lambda,\xi)=H_n^{(K)}+\xi\int_{\mathcal{T}}v(|x,y|)(n(y)-n'(y))dy, \tag{56}$$

which is an analytic perturbation of $H_n^{(K)}$ for ξ in a vicinity of 0. Let us denote its eigenvalues by $\varepsilon_\pm(\lambda,\xi)$. Considering

$$f(\lambda,\xi)\equiv[\lambda n_1+\xi(n_1'-n_1)]/[\varepsilon_+(\lambda,\xi)-\varepsilon_-(\lambda,\xi)], \tag{57}$$

the limit (54) can be expressed as

$$\lim_{t\to0}(T_0[n+t(n'-n)]-T_0[n])/t=\lambda\frac{v_1}{K\delta}\frac{\partial f}{\partial\xi}(\lambda,0)\cos\omega_1 x. \tag{58}$$

But

$$\partial_\xi f(\lambda,0)=[(n_1'-n_1)\Delta\varepsilon(\lambda,0)-\lambda n_1\,\partial_\xi\Delta\varepsilon(\lambda,0)]/\Delta\varepsilon(\lambda,0)^2, \tag{59}$$

where we denoted $\Delta\varepsilon(\lambda,\xi)=\varepsilon_+(\lambda,\xi)-\varepsilon_-(\lambda,\xi)$. From the asymptotic expansion of the eigenvalues given in Proposition 2,

$$\Delta\varepsilon(\lambda,\xi)=-2v_1[\lambda n_1+\xi(n_1'-n_1)]+o(\lambda^2,\lambda\xi,\xi^2), \tag{60}$$

which leads to

$$\partial_\xi f(\lambda,0)=\frac{(n_1'-n_1)(-2v_1\lambda n_1+o(\lambda^2))-\lambda n_1(-2v_1(n_1'-n_1)+o(\lambda))}{[-2v_1\lambda n_1+o(\lambda^2)]^2},$$

$$=\frac{o(\lambda^2)}{[-2v_1\lambda n_1+o(\lambda^2)]^2}. \tag{61}$$

For $n\in L^1_{\mathrm{per}}(\mathcal{T}_L)\cap B_{2\varepsilon}(n_\lambda)$, $n_1>\varepsilon$, in which case $\partial_\xi f(\lambda,0)$ has a finite limit as λ goes to zero. We can conclude that $\partial_\xi f(\lambda,0)$ is analytic for λ in the vicinity of zero. The proposition follows from (58). ■

The last result we need is the following proposition.

Proposition 7: For n, $n'\in\mathcal{S}_\varepsilon\cap B_\varepsilon(n_\lambda)$ and λ small,

$$\|R[n]-R[n']\|_{L^1(\mathcal{T})}\leqslant ct.\|n-n'\|_{L^1(\mathcal{T})},\quad ct.<\infty.$$

Proof: From Proposition 1,

$$R[n](x)=\frac{2\varepsilon_0^{(K,n_0)}-\varepsilon_0^{(K,n)}-\varepsilon_{-1}^{(K,n)}}{2K\lambda(\varepsilon_0^{(K,n)}-\varepsilon_{-1}^{(K,n)})}+(U^{-1}R^{(0,n)}U)(x,x)$$
$$+2\sum_{q=1}^{K-1}(U^{-1}R^{(q,n)}U)(x,x)+U^{-1}R^{(K,n)}U(x,x). \tag{62}$$

Let us analyze the first term denoted by $F[n]$ in the following. With the notations of the last proposition, we define

$$g(\lambda,\xi)=\frac{2\varepsilon_0^{(K,n_0)}-\varepsilon_+(\lambda,\xi)-\varepsilon_-(\lambda,\xi)}{2K\lambda(\varepsilon_+(\lambda,\xi)-\varepsilon_-(\lambda,\xi))}. \tag{63}$$

Then

$$\lim_{t\to 0}\|(F[n+t(n'-n)]-F[n])/t\|_{L^1(\mathcal{T})}=\lambda\,\partial_\xi g(\lambda,0)L, \tag{64}$$

and

$$\partial_\xi g(\lambda,0)=\frac{1}{2K\lambda}\,\frac{\Delta\varepsilon(\lambda,0)\partial_\xi\Delta'\varepsilon(\lambda,0)-\Delta'\varepsilon(\lambda,0)\partial_\xi\Delta\varepsilon(\lambda,0)}{\Delta\varepsilon(\lambda,0)^2}, \tag{65}$$

where $\Delta'\varepsilon(\lambda,\xi)=2\varepsilon_0^{(K,n_0)}-\varepsilon_+(\lambda,\xi)-\varepsilon_-(\lambda,\xi)$. From Proposition 2,

$$\Delta'\varepsilon(\lambda,\xi)=o(\lambda^2,\lambda\xi,\xi^2)\Rightarrow\partial_\xi\Delta'\varepsilon(\lambda,0)=o(\lambda). \tag{66}$$

We can conclude that

$$\lambda\,\partial_\xi g(\lambda,0)=\frac{1}{2K}\,\frac{o(\lambda^2)}{[-2v_1\lambda n_1+o(\lambda^2)]^2}, \tag{67}$$

which shows that $\lambda\,\partial_\xi g(\lambda,0)$ is analytic in a vicinity of 0. Then (64) together with Proposition 5 allows us to say

$$\|F[n']-F[n]\|_{L^1(\mathcal{T})}<ct.\|n'-n\|_{L^1(\mathcal{T})}. \tag{68}$$

Because $R^{(q,n)}$, $q=0,1,\ldots,K$, are self-adjoint operators:

$$\begin{aligned}\|(U^{-1}R^{(q,n)}U)(x,x)-(U^{-1}R^{(q,n')}U)(x,x)\|_{L^1(\mathcal{T})}&\leqslant\|(U^{-1}[R^{(q,n)}-R^{(q,n')}]U\|_1\\&=\|R^{(q,n)}-R^{(q,n')}\|_1.\end{aligned}\tag{69}$$

For $q<K$,

$$\begin{aligned}R^{(q,n)}-R^{(q,n')}=P_0^{(q,n')}(V_n-V_{n'})\sum_{m\neq 0}\frac{P_m^{(q,n)}}{\varepsilon_0^{(q,n')}-\varepsilon_m^{(q,n)}}\\+\sum_{m\neq 0}\frac{P_m^{(q,n')}}{\varepsilon_0^{(q,n)}-\varepsilon_m^{(q,n')}}(V_{n'}-V_n)P_0^{(q,n)},\end{aligned}\tag{70}$$

and we can write

$$\begin{aligned}\|R^{(q,n)}-R^{(q,n')}\|_1&\leqslant\left\|P_0^{(q,n')}(V_n-V_{n'})\sum_{m\neq 0}\frac{P_m^{(q,n)}}{\varepsilon_0^{(q,n')}-\varepsilon_m^{(q,n)}}\right\|_{L^2}\\&\quad+\left\|\sum_{m\neq 0}\frac{P_m^{(q,n')}}{\varepsilon_0^{(q,n)}-\varepsilon_m^{(q,n')}}(V_{n'}-V_n)P_0^{(q,n)}\right\|_{L^2}\\&=\left\|P_0^{(q,n')}(V_n-V_{n'})(H_n^{(q)}+a)^{-1}\sum_{m\neq 0}\frac{\varepsilon_m^{(q,n)}+a}{\varepsilon_0^{(q,n')}-\varepsilon_m^{(q,n)}}P_m^{(q,n)}\right\|_{L^2}\\&\quad+\left\|\sum_{m\neq 0}\frac{P_m^{(q,n')}}{\varepsilon_0^{(q,n)}-\varepsilon_m^{(q,n')}}(V_{n'}-V_n)(H_n^{(q)}+a)^{-1}(\varepsilon_0^{(q,n)}+a)P_0^{(q,n)}\right\|_{L^2}.\end{aligned}\tag{71}$$

From Ref. 3, we already know that

$$\|(V_{n'}-V_n)(H_n^{(q)}+a)^{-1}\|\leqslant K(a)\|n-n'\|_{L^1(\mathcal{T})},\tag{72}$$

which leads to

$$\|R^{(q,n)}-R^{(q,n')}\|_1\leqslant K(a)\left[\frac{\varepsilon_{-1}^{(q,n)}+a}{\varepsilon_{-1}^{(q,n)}-\varepsilon_0^{(q,n')}}+\frac{\varepsilon_0^{(q,n)}+a}{\varepsilon_{-1}^{(q,n')}-\varepsilon_0^{(q,n)}}\right]\|n-n'\|_{L^1(\mathcal{T})}.\tag{73}$$

Because $\varepsilon_m^{(q,n)}$ are analytic in λ, it follows that

$$\varepsilon_{-1}^{(q,n)}-\varepsilon_0^{(q,n')}=\varepsilon_{-1}^{(q,n_0)}-\varepsilon_0^{(q,n_0)}+o(\lambda)>0,\tag{74}$$

and

$$\varepsilon_{-1}^{(q,n')}-\varepsilon_0^{(q,n)}=\varepsilon_{-1}^{(q,n_0)}-\varepsilon_0^{(q,n_0)}+o(\lambda)>0,\tag{75}$$

for λ small and $q<K$. In this case, we can conclude from (73),

$$\|R^{(q,n)}-R^{(q,n')}\|_1\leqslant ct.\|n-n'\|_{L^1(\mathcal{T})},\quad ct<\infty.\tag{76}$$

The last operator in (62) has a relatively complicated expression:

$$R^{(K,n)}=\left[\hat{K}_0 Q^{(K,n)}+Q^{(K,n)}\hat{K}_0+\frac{\lambda}{\varepsilon_0^{(K,n)}-\varepsilon_{-1}^{(K,n)}}Q^{(K,n)}\right)(P_{0,-1}^{(K,n_0)})^{\perp}V_n P_{0,-1}^{(K,n_0)}]$$
$$\times(1-\lambda Q^{(K,n)})^{-1}, \tag{77}$$

where $\hat{K}_0=\hat{K}_0[n]$ is given by

$$\hat{K}_0[n]=\frac{\varepsilon_0^{(K,n_0)}-\varepsilon_{-1}^{(K,n)}}{\varepsilon_0^{(K,n)}-\varepsilon_{-1}^{(K,n)}}P_0^{(K,n_0)}+\frac{\varepsilon_{-1}^{(K,n_0)}-\varepsilon_{-1}^{(K,n)}}{\varepsilon_0^{(K,n)}-\varepsilon_{-1}^{(K,n)}}P_{-1}^{(K,n_0)} \tag{78}$$

However, when the difference $R^{(K,n)}-R^{(K,n')}$ is considered, we can form terms like $K_0[n]-K_0[n']$, $Q^{(K,n)}-Q^{(K,n')}$, $(V_n-V_{n'})P_{0,-1}^{(K,n_0)}$ and

$$\lambda/(\varepsilon_0^{(K,n)}-\varepsilon_{-1}^{(K,n)})-\lambda/(\varepsilon_0^{(K,n')}-\varepsilon_{-1}^{(K,n')}). \tag{79}$$

Moreover, because $K_0[n]=P_{0,-1}^{(K,n_0)}\hat{K}_0[n]P_{0,-1}^{(K,n_0)}$ we have to evaluate the L^2 norm instead of the trace class norm. The terms involved in K_0 have been already evaluated in Proposition 6 and above. Also, $Q^{(K,n)}-Q^{(K,n')}$ can be evaluated as we did above for $q<K$ and the third term can be evaluated using (72). The last term was evaluated in Proposition (6). ■

We are ready now to formulate the main result of this paper.

Theorem 8: *The Hartree equation has a solution in* $\mathcal{S}_\varepsilon\cap B_\varepsilon(n_\lambda)$.

Proof: We show first that $\mathcal{S}_\varepsilon\cap B_\varepsilon(n_\lambda)$ is invariant for T. For $n\in\mathcal{S}_\varepsilon\cap B_\varepsilon(n_\lambda)$,

$$\begin{aligned}\|T[n]-n_\lambda\|_{L^1(T)}&=\|T_0[n]-T_0[n_\lambda]+\lambda R[n]\|_{L^1(T)}\\&\leqslant\|T_0[n]-T_0[n_\lambda]\|_{L^1(T)}+\lambda\|R[n]\|_{L^1(T)}\\&\leqslant o(\lambda)\varepsilon+\lambda\|R[n]\|_{L^1(T)}\leqslant\varepsilon,\end{aligned} \tag{80}$$

if λ is small enough. We mention that, because n_λ is analytic and

$$n_\lambda\to\frac{1}{\delta}\left[1+\frac{1}{2K}\cos 2k_F x\right],\quad \text{as}\ \ \lambda\to 0, \tag{81}$$

we can choose ε independent of λ. We can prove also that T is a contraction on $\mathcal{S}_\varepsilon\cap B_\varepsilon(n_\lambda)$ for small λ. Indeed, for n, $n'\in B_\varepsilon(n_\lambda)$,

$$\begin{aligned}\|T[n]-T[n']\|_{L^1(T)}&\leqslant\|T_0[n]-T_0[n']\|_{L^1(T)}+\lambda\|R[n]-R[n']\|_{L^1(T)}\\&\leqslant o(\lambda)\|n-n'\|_{L^1(T)}+\lambda ct.\|n-n'\|_{L^1(T)}.\end{aligned} \tag{82}$$

The proposition follows from the fixed point theorem. ■

We remember that ε was defined such that for all $n\in B_{2\varepsilon}(n_\lambda)$, $n_1>\varepsilon$. The above result implies that the solution of the Hartree equation we proved to exist, is not uniform, i.e., the symmetry is broken. Moreover, as $\lambda\to 0$, we can take ε smaller and smaller which shows that the limit of this solution is well defined as λ goes to zero which is another way of proving the assertion of Theorem 3.

IV. THE THERMODYNAMIC LIMIT

We are not able yet to prove that the previous results are true in the thermodynamic limit. To see the difficulties that appear, let us analyze the $\lambda\to 0$ limit. As $K\to\infty$, $\varepsilon_0^{(K-q,n_0)}-\varepsilon_{-1}^{(K-q,n_0)}$ becomes smaller and smaller, for a fixed q. This means that these eigenvalues must be treated together in the perturbation theory. One can repeat the steps of Proposition 1 to show

$$P_0^{(K-q,n)}=(\varepsilon_0^{(K-q,n)}-\varepsilon_{-1}^{(K\text{-}q,n)})^{-1}P_{0,-1}^{(K-q,n_0)}(H_n^{(K-q)}-\varepsilon_{-1}^{(K-q,n)})P_{0,-1}^{(K-q,n_0)}+o(\lambda), \tag{83}$$

where the rest is bounded in the limit $K\to\infty$. We will use this expression for all $K/2<q<3K/2$. Then

$$T[n](x+m\delta)=1/\delta-\frac{1}{K}\sum_{q=0}^{q<K/2}\frac{\lambda v_1}{\varepsilon_{-1}^{(K-q,n)}-\varepsilon_0^{(K-q,n)}}2n_1\cos\omega_1 x+o(\lambda), \tag{84}$$

for $x\in[0,\delta]$ and an m integer. We can also apply Proposition 2 to compute $\varepsilon_{-1}^{(K-q,n}-\varepsilon_0^{(K-q,n)}$. Keeping the notation, but replacing

$$G_{0,-1}^{(K,n_0)}(E)\to G_{0,-1}^{(q,n_0)}=(E-H_0^{(q)})^{-1}-(E-\varepsilon_0^{(q,n_0)})P_0^{(q,n_0)}-(E-\varepsilon_{-1}^{(q,n_0)})P_{-1}^{(q,n_0)}, \tag{85}$$

it follows that

$$\varepsilon_{-1}^{(K-q,n)}-\varepsilon_0^{(K-q,n)}=2\sqrt{(\lambda M_{00}-\lambda M_{-1-1}-\Delta\varepsilon^{(K-q)})^2+4|M_{0-1}|^2}, \tag{86}$$

where

$$\Delta\varepsilon^{(K-q)}=\varepsilon_{-1}^{(K-q,n_0)}-\varepsilon_0^{(K-q,n_0)}=\frac{4\pi^2}{\delta^2}\frac{q}{K}. \tag{87}$$

Asymptotically,

$$\varepsilon_{-1}^{(K-q,n)}-\varepsilon_0^{(K-q,n)}=2\sqrt{\left(\frac{4\pi^2}{\delta^2}\frac{q}{K}\right)^2+4\lambda^2|n_1v_1|^2+o(\lambda^3)}. \tag{88}$$

In the limit $K\to\infty$, the leading therm of T is given by

$$\begin{aligned}T_0[n](x+m\delta)&=1/\delta-\lambda v_1\int_0^{1/2}\frac{dt}{2\sqrt{(4\pi^2/\delta^2t)^2+4\lambda^2|n_1v_1|^2}}2n_1\cos\omega_1x\\&=1/\delta-\frac{\lambda v_1\delta^2}{8\pi^2}\operatorname{arcosh}\left(\frac{\pi^2}{\lambda\delta^2|n_1v_1|}\right)2n_1\cos\omega_1x.\end{aligned} \tag{89}$$

The self-consistent equation leads to

$$n_1=\pi^2/\{\lambda|v_1|\delta^2\,\mathrm{sh}[-8\pi^2/(\lambda v_1\delta^2)]\}. \tag{90}$$

This means the band gap will be proportional to

$$\Delta\propto\mathrm{sh}[-8\pi^2/(\lambda v_1\delta^2)]^{-1}\approx 2\exp[-8\pi^2/(\lambda v_1\delta^2)], \tag{91}$$

a BCS like expression. This slow opening of the gap request sharper estimates in order to prove that T is a contraction.

V. CONCLUSIONS

It is easy to check that the map T becomes infinitely unstable as n_1 goes to zero. This means that the solution n constant is unstable. The key element for a successful expansion beyond the Hartree approximation (which we proved that it is equivalent to the Gaussian approximation) will be the stability of the solution. Also, the perturbed eigenvalues are smaller than the unperturbed ones. We have already proved this for $H_n^{(K)}$. For $q<K$, one can use:

$$\varepsilon_0^{(q,n)}\leqslant\langle\varphi_0^{(q,n_0)},H_n^{(q)}\varphi_0^{(q,n_0)}\rangle=\varepsilon_0^{(q,n_0)}, \tag{92}$$

where we used that the zero-th Fourier coefficient of V_n is zero. Then it follows that the total energy is smaller for the broken phase than for the unbroken one. Condition $v_1<0$ seems to rule out the phase transition for repulsive interactions. However, one expects that the phase transition to be there for these cases too. One can convince oneself that, in any local theory, the effective potential must be low where the density of particles is high for modulations of the particles density to occur. For repulsive interactions, the exchange-correlation potential is attractive. We proved in Ref. 3 that the fixed point approach works also for local density approximation provided the very low density behavior of the exchange-correlation potential, v_{xc}, is modified. Supposing that one can extend the analysis of this paper to the local density approximation, we can predict the following. Because $v_{\mathrm{xc}}(n)$ behaves as $n^{1/3}$ at low densities, the attractive term will dominate the repulsive Hartree term at low densities. This means that, for repulsive interactions and at low densities, the symmetry breaking will also be present.

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Homotopy arguments for quantized Hall conductivity

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Using the strong localization bounds obtained by the Aizenman–Molcanov method for a particle in a magnetic field and a disordered potential, we show that the zero-temperature Hall conductivity of a gas of such particles is quantized and constant as long as both Fermi energy and disorder coupling parameter vary in a region of strong localization of the corresponding two-dimensional phase diagram.
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I. INTRODUCTION

In quantum Hall effect experiments,[1] one measures the Hall resistance of an effectively two-dimensional electron gas. For a wide range of the experimental parameters (such as the magnetic field and the particle density), the Hall resistance is an integer multiple of the fundamental constant e^2/h (here e is the charge of an electron and h is Planck's constant). The two most remarkable facts of this so-called integer quantum Hall effect, namely, (1) the appearence of an integer number and (2) its stability with respect to changes of the parameters, can both be explained within a one-particle framework.[1,2] The integers are known to be of topological origin, whereas their stability is due to Anderson localization in the sample. Here we focus on this second issue and study a one-particle Hamiltonian $H^\lambda = H_0 + \lambda V$, $\lambda \in \mathbf{R}$, given by the sum of a free magnetic operator H_0 of the Harper type and a disordered potential V. We prove that in a region of the (λ,μ)-plane of coupling constant λ and Fermi level μ in which localization estimates hold, the Hall conductivity is constant and equal to an integer multiple of e^2/h.

II. MODELS AND RESULTS

A. Covariant operators

Let $(\Omega, T, \mathbf{Z}^2, \mathbf{P})$ be a dynamical system given by a compact probability space Ω endowed with a probability measure $\mathbf{P}$ which is invariant and ergodic with respect to the action T of the group $\mathbf{Z}^2$. A family $A = (A_\omega)_{\omega \in \Omega}$ of bounded operators on $l^2(\mathbf{Z}^2)$ is called covariant with respect to the action if it is weakly continuous (in ω) and it satisfies the covariance relation

$$U^n A_\omega U^{*n} = A_{T^n \omega}, \quad n \in \mathbf{Z}^2.$$

Here the magnetic translation operators U^n, $n = (n_x, n_y)$, acting on $l^2(\mathbf{Z}^2)$ are defined by

$$U^n \psi(m) = \exp\left(\frac{\imath}{2} \theta \, n \wedge m \right) \psi(m-n), \quad m = (m_x, m_y) \in \mathbf{Z}^2, \quad \psi \in l^2(\mathbf{Z}^2),$$

where $a \wedge n = a_x n_y - a_y n_x$ and θ is the magnetic flux per unit cell. Given a covariant operator family $A = (A_\omega)_{\omega \in \Omega}$, Birkhoff's ergodic theorem implies that its trace per unit volume

$$\mathcal{T}(A) = \lim_{\Lambda \to \mathbf{Z}^2} \frac{1}{|\Lambda|} \mathrm{Tr}_\Lambda (A_\omega) = \lim_{\Lambda \to \mathbf{Z}^2} \frac{1}{|\Lambda|} \sum_{n \in \Lambda} \langle 0 | A_{T^n \omega} | 0 \rangle,$$

is **P**-almost surely independent of $\omega \in \Omega$ and is equal to $\int d\mathbf{P}(\omega)\, \langle 0|A_\omega|0\rangle$. If X and Y denote the components of the position operator on $l^2(\mathbf{Z}^2)$, new covariant operator families $\nabla_x A$ and $\nabla_y A$ are defined by

$$(\nabla_x A)_\omega = \imath[X, A_\omega], \quad (\nabla_y A)_\omega = \imath[Y, A_\omega],$$

whenever the right-hand-sides are bounded operators. Let now $P=(P_\omega)_{\omega\in\Omega}$ be a covariant family of projection operators (i.e., $P_\omega^2 = P_\omega^* = P_\omega$). Its Chern number is defined by

$$\mathrm{Ch}(P) = 2\pi\imath\, \mathcal{T}(P[\nabla_x P, \nabla_y P]). \tag{1}$$

The Chern number is a topological invariant of the equivalence class of covariant projections defined by P. For further details and a more algebraic formulation of these notions, please consult.[2]

B. Hamiltonian and physical quantities

We consider disordered two-dimensional magnetic operators in the tight-binding appoximation on the rectangular lattice Hilbert space $l^2(\mathbf{Z}^2)$ which are of the form,

$$H_\omega^\lambda = H_0 + \lambda V_\omega, \quad V_\omega = \sum_{n\in\mathbf{Z}^2} \omega_n |n\rangle\langle n|. \tag{2}$$

Here $H_0 = H_0^*$ is a polynomial in the magnetic translations. The most simple nontrivial example is given by the Harper Hamiltonian $H_{\mathrm{Har}} = U^{(1,0)} + U^{(-1,0)} + U^{(0,1)} + U^{(0,-1)}$. Furthermore, $\omega = (\omega_n)_{n\in\mathbf{Z}^2}$ is a point in the space of disorder configurations given by the topological product $\Omega = [-1,1]^{\otimes \mathbf{Z}^2}$. We suppose that the ω_n's are independent and identically distributed random variables with a probability distribution ρ. The product measure $\mathbf{P} = \rho^{\otimes \mathbf{Z}^2}$ then defines a probability on Ω which is invariant and ergodic with respect to the shift action T of $\mathbf{Z}^2$ on Ω. Hence we dispose of a dynamical system $(\Omega, T, \mathbf{Z}^2, \mathbf{P})$ as in Sec. II A.

The family $H=(H_\omega^\lambda)_{\omega\in\Omega}$ and any function $f(H)$ of it (f measurable) are covariant. Given a Fermi level $\mu \in \mathbf{R}$, we consider the associated Fermi projection $P^{\lambda,\mu} = \chi_{(-\infty,\mu]}(H^\lambda)$, where $\chi_{(-\infty,\mu]}$ is the characteristic function of the interval $(-\infty,\mu]$. Whenever well-defined, its Chern number is linked to the bulk Hall conductivity $\sigma_\perp(\lambda,\mu)$ via the Kubo–Chern formula,[2]

$$\sigma_\perp(\lambda,\mu) = \frac{e^2}{h}\,\mathrm{Ch}(P^{\lambda,\mu}).$$

Furthermore we consider the density of states of H^λ, notably the probability measure $\mathcal{N}^\lambda$ defined by

$$\int d\mathcal{N}^\lambda(E)\, f(E) = \mathcal{T}(f(H^\lambda)), \quad f \in C_0(\mathbf{R}).$$

C. Localization regime

Here we shall study the quantities $\sigma_\perp(\lambda,\mu)$ and $\mathcal{N}^\lambda$ in the

Aizenman–Molcanov Localization Regime (AMLR): A spectral interval $\Delta \subset \mathbf{R}$ is in the AMLR for the covariant Hamiltonian $H=(H_\omega)_{\omega\in\Omega}$ if for any $s\in(0,1)$ there exist positive constants Λ and $c_{s,\epsilon}$ such that

$$\int d\mathbf{P}(\omega) |\langle n|(E+\imath\epsilon - H_\omega)^{-1}|m\rangle|^s \leq c_{s,\epsilon} e^{-\Lambda|n-m|} \tag{3}$$

for all $E\in\Delta$ and $\epsilon \neq 0$.

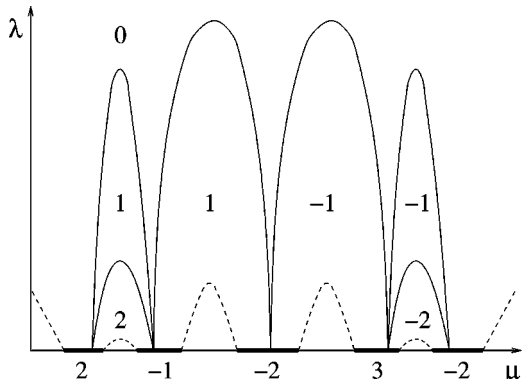

FIG. 1. Phase diagram for the Hall conductivity in a disordered Harper model with rational flux $\theta = 2\pi \cdot 3/5$ (following Ref. 7) The fat lines are the Bloch bands of the free Harper operator, each with its Chern number given below. These numbers can easily be calculated using the diophantine equation in Ref. 10. The solid lines show the critical energies separating the regions of the phase diagram with constant Chern number; this number is written inside each region. The dashed lines show the boundaries of the spectrum.

Under appropriate regularity conditions on the probability measure ρ (absolute continuity is sufficient), the AMLR is known to hold in the strong disorder regime (large λ) (Refs. 3, 4) as well as at the band edges in the weak disorder regime.[5,6] Furthermore note that the AMLR holds for a (**P**-almost sure) gap of the spectrum of H^λ by a standard Combes–Thomas argument. However, it is not known rigorously (as suggest, for example, the numerical calculations of Tan[7] discussed below) that the AMLR holds for all but a set of critical energies for the 2D magnetic models defined by Eq. (2).

D. Main result and phase diagram

Theorem 1: *Let* $\mathcal{R} \subset \{(\mu,\lambda) \in \mathbf{R}^2\}$ *be a connected set such that for every* λ *the set* $\Delta(\lambda) = \{\mu | (\mu,\lambda) \in \mathcal{R}\}$ *is an interval for which the* AMLR *holds for* H^λ. *Then:*

(i) The map $(\mu,\lambda) \in \mathcal{R} \mapsto \mathcal{N}^\lambda((-\infty,\mu])$ *is Hölder continuous for any exponent less than* 1/2;

(ii) $(\mu,\lambda) \in \mathcal{R} \mapsto \sigma_\perp(\lambda,\mu)$ *is constant and equal to an integer multiple of* q^2/h.

The fact that $\mu \mapsto \sigma_\perp(\lambda,\mu)$ is constant as long as μ varies in an interval for which the AMLR holds was already proven in Ref. 2 (see also Ref. 4). Hence the new result concerns constancy in λ. Concerning (i), the continuity of the DOS for fixed λ is well known (by Wegner estimate even absolute continuity[8]), so that again the main issue is continuity in λ. Even though $\lambda \mapsto H^\lambda$ is norm continuous, this is nontrivial because $\mathcal{N}^\lambda((-\infty,\mu])$ is expressed in terms of a discontinuous function of H^λ.

Theorem 1 (ii) combined with a recent work by Avron and Sadun[9] allows us to clarify the (μ,λ)-phase diagram (Fig. 1) which was obtained numerically by Tan[7] for the family of disordered Harper Hamiltonians $H_{\mathrm{Har}} + \lambda V_\omega$, where ρ is the uniform distribution on $[-1,1]$. There are regions where the Hall conductivity is constant. These regions correspond to a localization region, whereas the lines indicate critical lines where the Hall conductivity jumps. Generically, such jumps are by unity,[9] which is actually satisfied except on the line $\lambda = 0$ where the integrable character of Harper's equation leads to singularities in this respect.

Let us further note that at large disorder the whole spectrum belongs to the phase with vanishing Chern number and hence zero Hall conductance. This is compatible with the proof of AMLR for large disorder.[3] There is a corresponding result of Nakamura and Bellissard[11] for the continuous case showing that for fixed Fermi energy, there is a value of the disorder coupling constant λ_c such that for $\lambda > \lambda_c$ the Hall conductivity vanishes. In this situation, the current carrying lines do not annihilate as in Fig. 1, but bend towards higher energies.[12]

An interesting open problem is to show that the edge Hall conductivity as defined in Ref. 13 is well-defined and also remains constant in the regions of the above phase-diagram.

III. PROOFS

Let us denote the disorder average w.r.t. **P** by **E**. For technical reasons, we consider a covariant family $H^{(\nu)}=(H_\omega^{(\nu)})_{\omega\in\Omega}$ given by

$$H_\omega^{(\nu)}=H_\omega^{\lambda}+\nu\, W_\omega,$$

where $W=(W_\omega)_{\omega\in\Omega}$ is a family of uniformly bounded covariant operators which is diagonal in the basis $(|n\rangle)_{n\in\mathbf{Z}^2}$. If $W=V$, then $H^{(\nu)}=H^{\lambda+\nu}$, but we will also be interested in the case $W=1$ to study continuity in the energy. The following result also holds for a (magnetic) Anderson model in arbitrary dimension.

Lemma 1: Let f be a real, piecewise continuous and bounded function such that the discontinuities of f are within AMLR of $H^{(\nu)}$ for all $\nu\in[\nu_1,\nu_2]$. Then for any $s<1/2$,

$$\mathbf{E}(|\langle n|f(H_\omega^{(\nu_1)})|m\rangle-\langle n|f(H_\omega^{(\nu_2)})|m\rangle|)\leqslant c\,|\nu_1-\nu_2|^s\, e^{-\Lambda|n-m|}. \tag{4}$$

Proof: First let us recall the resolvent identity,

$$(z-H_\omega^{(\nu_1)})^{-1}-(z-H_\omega^{(\nu_2)})^{-1}=(\nu_1-\nu_2)\,(z-H_\omega^{(\nu_1)})^{-1}W_\omega(z-H_\omega^{(\nu_2)})^{-1}.$$

Now using the convexity inequality $|\Sigma_j x_j|^s\leqslant\Sigma_j|x_j|^s$ and the fact that W is diagonal and $|W_\omega(k)|\leqslant c$, one obtains therefore

$$\begin{aligned}&|\langle n|(z-H_\omega^{(\nu_1)})^{-1}|m\rangle-\langle n|(z-H_\omega^{(\nu_2)})^{-1}|m\rangle|^s\\&\quad\leqslant c|\nu_1-\nu_2|^s\sum_{k\in\mathbf{Z}^2}|\langle n|(z-H_\omega^{(\nu_1)})^{-1}|k\rangle|^s|\langle k|(z-H_\omega^{(\nu_2)})^{-1}|m\rangle|^s.\end{aligned}$$

This gives

$$\begin{aligned}&|\langle n|(z-H_\omega^{(\nu_1)})^{-1}|m\rangle-\langle n|(z-H_\omega^{(\nu_2)})^{-1}|m\rangle|\\&\quad\leqslant c|\nu_1-\nu_2|^s\sum_{k\in\mathbf{Z}^2}|\langle n|(z-H_\omega^{(\nu_1)})^{-1}|k\rangle|^s|\langle k|(z-H_\omega^{(\nu_2)})^{-1}|m\rangle|^s\\&\qquad\cdot(|\langle n|(z-H_\omega^{(\nu_1)})^{-1}|m\rangle|^{1-s}+|\langle n|(z-H_\omega^{(\nu_2)})^{-1}|m\rangle|^{1-s}).\end{aligned}$$

Now we use the bound $|\langle n|(z-H_\omega^{(\nu_{1,2})})^{-1}|m\rangle|\leqslant|\Im m(z)|^{-1}$, then take the disorder average and apply the Cauchy–Schwarz inequality in order to get

$$\begin{aligned}&\mathbf{E}(|\langle n|(z-H_\omega^{(\nu_1)})^{-1}|m\rangle-\langle n|(z-H_\omega^{(\nu_2)})^{-1}|m\rangle|)\\&\quad\leqslant c|\nu_1-\nu_2|^s|\Im m(z)|^{s-1}\cdot\sum_{k\in\mathbf{Z}^2}(\mathbf{E}(|\langle n|(z-H_\omega^{(\nu_1)})^{-1}|k\rangle|^{2s}))^{1/2}\\&\qquad\times(\mathbf{E}(|\langle k|(z-H_\omega^{(\nu_2)})^{-1}|m\rangle|^{2s}))^{1/2},\end{aligned}$$

so that replacing the AMLR bound we finally obtain by using for example the Young inequality,

$$\mathbf{E}(|\langle n|(z-H_\omega^{(\nu_1)})^{-1}|m\rangle-\langle n|(z-H_\omega^{(\nu_2)})^{-1}|m\rangle|)\leqslant c|\nu_1-\nu_2|^s|\Im m(z)|^{s-1}e^{-\Lambda|m-n|} \tag{5}$$

for $s<1/2$.

Now let f be an analytic function on an interval $\Delta=[E_l,E_r]$ the end points of which fall into the AMLR. Then we use holomorphic functional calculus in the following way:

$$f(H_\omega^{(\nu)}) = Q_f(H_\omega^{(\nu)} - E_r) - R_f(H_\omega^{(\nu)}) - Q_f(H_\omega^{(\nu)} - E_l) + R_f(H_\omega^{(\nu)})^*, \tag{6}$$

where

$$Q_f(z) = \int_{-1}^{1} \frac{dt}{2\pi} \frac{f(\imath t)}{\imath t - z}, \quad R_f(z) = \int_{E_l}^{E_r} \frac{dt}{2\pi} \frac{f(t)}{t - \imath - z}.$$

Because we are in the AMLR, the spectrum is pure-point and it is then well-known that E_l and E_r are almost surely not in the spectrum of $H_\omega^{(\nu)}$. Hence the intergrals in (6) are almost surely well-defined (a similar argument was already used in Ref. 4). Now we can estimate the differences for different coupling parameters ν,

$$\begin{aligned}
&\mathbf{E}(|\langle n|Q_f(H_\omega^{(\nu_1)} - E_r)|m\rangle - \langle n|Q_f(H_\omega^{(\nu_2)} - E_r)|m\rangle|) \\
&\quad \leqslant \left(\sup_{t' \in [-1,1]} |f(\imath t')| \right) \int_{-1}^{1} \frac{dt}{2\pi} \mathbf{E}(|\langle n|(z - H_\omega^{(\nu_1)})^{-1}|m\rangle - \langle n|(z - H_\omega^{(\nu_2)})^{-1}|m\rangle|) \\
&\quad \leqslant c\,|\nu_1 - \nu_2|^s \int_{-1}^{1} \frac{dt}{|t|^{1-s}} e^{-\Lambda|m-n|} \leqslant c'\,|\nu_1 - \nu_2|^s\, e^{-\Lambda|m-n|}.
\end{aligned} \tag{7}$$

Of course, the terms with E_l instead of E_r can be treated in the same way. Concerning the R_f-contributions in (6), let us first remark that a bound like (3) but with $s=1$ actually holds for all complex energies off the real axis (by a Combes–Thomas argument, cf. Ref. 4). Using this fact, one can either proceed as above or more directly use the resovent identity. We skip the details.

Combining these estimates, we see that (4) holds for an analytic function f on Δ. Because the above estimate is continuous w.r.t. the maximum norm on the space of continuous functions [cf. the bound (7), for example], a standard Stone–Weierstrass approximation argument allows us to obtain the same bound also for every continuous function f. Finally, for a piecewise continuous function we can treat each continuous part separately provided the points of discontinuity of f are within the AMLR. □

Proof of Theorem 1 (i): Because the indicator function χ_μ on the interval $(-\infty, \mu]$ is piecewise continuous and the discontinuity varies within the AMLR according to hypothesis, we can apply the above lemma with $W=V$ and $W=1$, respectively. With the notation $\mathcal{N}^\lambda(\mu) = \mathcal{N}^\lambda((-\infty,\mu])$, we therefore obtain

$$\begin{aligned}
|\mathcal{N}^{\lambda_1}(\mu_1) - \mathcal{N}^{\lambda_2}(\mu_2)| &\leqslant |\mathcal{N}^{\lambda_1}(\mu_1) - \mathcal{N}^{\lambda_2}(\mu_1)| + |\mathcal{N}^{\lambda_2}(\mu_1) - \mathcal{N}^{\lambda_2}(\mu_2)| \\
&\leqslant \mathbf{E}(|\langle 0|\chi_{\mu_1}(H^{\lambda_1})|0\rangle - \langle 0|\chi_{\mu_1}(H^{\lambda_2})|0\rangle|) \\
&\quad + \mathbf{E}(|\langle 0|\chi_{\mu_1}(H^{\lambda_2})|0\rangle - \langle 0|\chi_{\mu_1}(H^{\lambda_2} + \mu_2 - \mu_1)|0\rangle|) \\
&\leqslant c\,|\lambda_1 - \lambda_2|^s + c\,|\nu_1 - \nu_2|^s \quad (s < 1/2).
\end{aligned}$$

This gives the desired Hölder continuity. □

Proof of Theorem 1 (ii): As in Ref. 2, let us introduce a noncommutative Sobolov space as the set of all weakly continuous covariant operator families $A = (A_\omega)_{\omega \in \Omega}$ for which the norm

$$\|A\|_{\mathcal{S}}^2 = \mathcal{T}(|A|^2) + \mathcal{T}(|\nabla A|^2) \tag{8}$$

is finite (here $|\nabla A|^2 = |\nabla_x A|^2 + |\nabla_y A|^2$). Note that the Chern number (1) is continuous w.r.t. this norm. An important result of Ref. 2 is the following: if $t \mapsto P(t) \in \mathcal{S}$ is a one-parameter family of covariant projection operators which is continuous w.r.t. to the Sobolev norm $\|.\|_{\mathcal{S}}$, then $t \mapsto \mathrm{Ch}(P(t))$ is constant and equal to an integer. Hence it is sufficient to show that the map $(\mu, \lambda) \in \mathcal{R} \mapsto \|P^{\lambda,\mu}\|_{\mathcal{S}}$ is Hölder continuous. According to part (i) proven above, this actually holds for the $\mathcal{T}(|\,.\,|^2)$-part of the norm. For the second part, we begin with

$$|\mathcal{T}(|\nabla P^{\mu_1,\lambda_1}|^2)-\mathcal{T}(|\nabla P^{\mu_2,\lambda_2}|^2)|\leqslant \sum_{m\in\mathbf{Z}^2}|m|^2\,\mathbf{E}(||\langle 0|\chi_{\mu_1}(H^{\lambda_1})|m\rangle|^2-|\langle 0|\chi_{\mu_2}(H^{\lambda_2})|m\rangle|^2|). \tag{9}$$

Now the bound $|\langle 0|\chi_\mu(H^\lambda)|m\rangle|\leqslant 1$ implies that

$$||\langle 0|\chi_{\mu_1}(H^{\lambda_1})|m\rangle|^2-|\langle 0|\chi_{\mu_2}(H^{\lambda_2})|m\rangle|^2|\leqslant 2\,|\langle 0|\chi_{\mu_1}(H^{\lambda_1})|m\rangle-\langle 0|\chi_{\mu_2}(H^{\lambda_2})|m\rangle|,$$

so that an argument similar to that in the proof of (i) shows that

$$\mathbf{E}(||\langle 0|\chi_{\mu_1}(H^{\lambda_1})|m\rangle|^2-|\langle 0|\chi_{\mu_2}(H^{\lambda_2})|m\rangle|^2|)\leqslant c(|\lambda_1-\lambda_2|^s+|\mu_1-\mu_2|^s)\,e^{-\Lambda|m|}.$$

Inserting this into (9) allows us to conclude. □

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Quantum Chern–Simons vortices on a sphere

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The quantization of the reduced first-order dynamics of the nonrelativistic model for Chern–Simons vortices introduced by Manton is studied on a sphere of given radius. We perform geometric quantization on the moduli space of static solutions, using a Kähler polarization, to construct the quantum Hilbert space. Its dimension is related to the volume of the moduli space in the usual classical limit. The angular momenta associated with the rotational SO(3) symmetry of the model are determined for both the classical and the quantum systems. The results obtained are consistent with the interpretation of the solitons in the model as interacting bosonic particles. © *2001 American Institute of Physics*. [DOI: 10.1063/1.1379315]

I. INTRODUCTION

Over the past decade, much attention has been given to $(1+2)$-dimensional field theories including a Chern–Simons term. The pure Chern–Simons gauge theory, although still interesting both from the mathematical and the physical points of view, has no dynamics by itself. However, many interesting models for field dynamics can be obtained by adding to the Chern–Simons action Maxwell or Yang–Mills terms and/or interactions with other fields.[1] Some of these models have been shown to admit classical solitonic solutions (vortices), at least for critical or ''self-dual'' values of the parameters in the Lagrangian. These objects can be regarded as smeared-out particles which retain a characteristic size and superpose nonlinearly; unlike some types of solitons, they can also be assigned a pointlike core individually. In specific models, vortices often turn out to possess rather exotic properties, which may be relevant in applications. For example, models with abelian vortices have been important in attempts to explain phenomena in condensed matter theory such as superconductivity and the fractional quantum Hall effect.

In Ref. 2, Manton constructed a nonrelativistic Lagrangian for a U(1) gauge field minimally coupled to a complex scalar on the plane which describes vortex dynamics. The action for the gauge field includes a Chern–Simons term and the purely spatial part of the Maxwell action. The equations of motion for the field theory are first-order in time, and they admit the well-known Bogomol'nyĭ vortices[3] of the Ginzburg–Landau theory as static solutions, for special values of the parameters. Mathematically, Bogomol'nyĭ vortices are rather well understood, even though on general surfaces they cannot be constructed analytically. Their space of gauge equivalence classes splits into disjoint sectors $\mathcal{M}_N$ labeled by an integer vortex number $N \in \mathbb{Z}$, each $\mathcal{M}_N$ (the moduli space of N vortices) being a smooth $2|N|$-dimensional manifold. In his paper, Manton explored the dynamics of time-dependent fields by explicitly reducing the field theory Lagrangian to an effective (finite-dimensional) mechanical system on the moduli space $\mathcal{M}_N$. The Lagrangian equations of motion for the reduced system are again first-order in time, and so the moduli space is to be regarded as the phase space where a noncanonical Hamiltonian dynamics takes place. The symplectic form defining the dynamics, determined by the kinetic term, contains nontrivial information about the system; of course, it may still be written in canonical form locally, but not in a natural way. Time evolution is determined by the potential energy alone, which is supposed to be small so that the field configurations are still approximately Bogomol'nyĭ vortices. In the case of

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two vortices, the reduced system describes namely a rigid uniform rotation of the two vortex cores about their midpoint, with an angular velocity which is maximal when the distance between the two is roughly a vortex diameter.

If we place the vortices on a compact surface Σ, with a Riemannian metric and an orientation, rather than on the plane, the moduli spaces $\mathcal{M}_N$ also become compact. The metric on Σ fixes a complex structure, which in turn induces a complex structure on $\mathcal{M}_N$. This complex structure can be shown to be compatible with the symplectic form relevant for the dynamics, and so each $\mathcal{M}_N$ becomes a Kähler manifold. Compact Kähler phase spaces are optimal stages for geometric quantization.[4,5] The complex geometry supplies a natural (Kähler) polarization, for which the corresponding quantum Hilbert space turns out to be finite-dimensional. This approach to the quantization of the vortex system is to be included in a more general framework, pioneered by Gibbons and Manton in the context of BPS monopoles.[6] The idea is to probe the quantum behavior of solitons through geometric quantization of the reduced dynamics on the moduli space of static solutions, when such a space is available. In the more familiar situation of the Abelian Higgs model,[7] where the reduced system is of second order, there is a canonical Hamiltonian description of the classical dynamics and the quantization can be carried out using the vertical polarization of $T^*\mathcal{M}_N$, which leads to a truncated Schrödinger representation of the quantum system. The accuracy of the approximation involved is very difficult to assess, and the study of an example where the Schrödinger representation is not available, as is the case here, is of considerable interest. From the point of view of geometric quantization itself, it is fortunate that Manton's system seems to provide us with a nontrivial example where it may be put to work rather directly.

The main aim of the present work is to discuss the geometric quantization of Manton's reduced system of periodic vortex dynamics, when space is taken to be a sphere of a given radius R. In particular, we shall determine the dimension of the Hilbert space and construct the quantum operators corresponding to the conserved angular momenta determined by the natural action of SO(3).

Let us summarize how this paper is organized. In Sec. II, we describe the generalization of Manton's model to the case where the spatial surface is compact. In Sec. III, we gather some results concerning the moduli space of Bogomol'nyĭ vortices on a sphere and its use in the study of the field theory dynamics. The effective Lagrangian on the moduli space is constructed in Sec. IV. In Sec. V, we obtain conservation laws for both the field theory and the reduced dynamical system, and show that they are consistent. In Sec. VI, the setup for the geometric quantization of the reduced dynamics on the moduli space of static solutions is presented. The dimension of the Hilbert space of wavefunctions is computed in Sec. VII, and we show how to construct the quantum angular momentum operators in Sec. VIII. Finally, we discuss the results obtained and address some outstanding issues.

II. FIRST-ORDER CHERN–SIMONS VORTICES

We start by discussing the generalization of the model introduced by Manton[2] to the situation where space is compact. We shall consider time-periodic boundary conditions in the formulation of the variational principle, and accordingly we fix space–time to be of the form $S^1\times\Sigma$, where Σ is a compact and oriented two-dimensional riemannian manifold. In the remaining sections of this paper we will assume that Σ is a sphere, but for now this restriction is unnecessary. Since in two dimensions any metric is conformally flat, we can introduce a complex coordinate z locally on Σ and write

$$ds^2=dt^2-\Omega^2(z,\overline{z})dzd\overline{z}, \tag{1}$$

where t parametrises time.

Naively, the Lagrangian we would like to consider is

$$\mathcal{L}[A,\phi]=\gamma\left(\frac{i}{2}(\overline{\phi}D_t\phi-\phi\overline{D_t\phi})-A_t\right)\Omega^2+\mu(BA_t+2i(E_zA_{\bar{z}}-E_{\bar{z}}A_z))$$
$$-\left(\frac{1}{2}B^2\Omega^{-2}+(|D_z\phi|^2+|D_{\bar{z}}\phi|^2)+\frac{\lambda}{8}(1-|\phi|^2)^2\Omega^2\right). \tag{2}$$

This reduces to Manton's Lagrangian[2] without transport current if we take Σ to be the plane and set $\Omega^2=1$. Here, $A=A_tdt+A_zdz+A_{\bar{z}}d\bar{z}$ is the real-valued $U(1)$ gauge field, with curvature $F_A=dA=(E_zdz+E_{\bar{z}}d\bar{z})\wedge dt+(i/2)Bdz\wedge d\bar{z}$, and ϕ the Higgs scalar field. The covariant derivatives are $D_\nu\phi=\partial_\nu\phi-iA_\nu\phi$, where $\nu=t$, z or $\bar{z}$. Of course, $(i/2)\mathcal{L}$ is to be thought of as the coefficient of a three-form on some open subset of $S^1\times\Sigma$ where local expressions for the fields can be given, and the factors of Ω introduced in (2) are imposed by the natural interpretation given to the different terms.

To set up the classical field theory, we must give as global data a principal U(1) bundle P over $S^1\times\Sigma$. With respect to local trivializations, the gauge field is interpreted as a connection on this bundle, the Higgs field as a section of the complex line bundle associated to P by the defining representation, and $\overline{\phi}$ is a section of the bundle dual to this one. It is natural to restrict to the situation where P is the pull-back to $S^1\times\Sigma$ of a U(1) bundle on Σ; in particular, the transition functions will be time-independent. Topologically, U(1) bundles on a compact surface are classified by their first Chern class $N\in\mathbb{Z}$, which can be interpreted as the net number of units of quantized magnetic flux through space at any time,

$$\frac{i}{2}\oint_\Sigma Bdz\wedge d\bar{z}=2\pi N. \tag{3}$$

We may assume without loss of generality that the bundle we are considering over Σ can be trivialized on an open disc $U_1\subset\Sigma$ and on an open neighborhood U_2 of its complement, with $U_1\cap U_2$ being a very narrow annulus which for most purposes can be identified with its retraction ∂U_1. More precisely, we may have to consider sub-patches of U_2 to make sense of local data such as the relevant coordinate z, but this will not affect the discussion of the aspects related to the nontriviality of P which will be our main concern, because $P|_{U_2}$ is trivial. Thus we shall consider P to be defined by the homotopy class of a single transition function $f_{12}:\partial U_1\to U(1)$ whose degree is N, and we refrain from introducing partitions of unity to keep the discussion as simple as possible.

The term with coefficient μ is the Chern–Simons density $\mu A\wedge dA$. On the overlap of the two trivializing patches U_1, U_2,

$$A^{(1)}\wedge dA^{(1)}=A^{(2)}\wedge dA^{(2)}-if_{12}^{-1}df_{12}\wedge dA^{(2)},$$

where $A^{(j)}$ denotes the connection one-form on U_j, and so its values on the trivializing patches do not agree on the overlap $U_1\cap U_2$. So in general we cannot define an action by just using partitions of unity to patch together pieces of the Lagrangian given by (2), as we can do for gauge-invariant Lagrangians. Notice that the term proportional to A_t, although gauge-dependent, is unambiguously defined globally since we are assuming that the transition functions are time-independent. The most elegant way to define the Chern–Simons action is as the integral of the gauge-invariant second Chern form $\mu dA\wedge dA$, on any four-dimensional manifold M with boundary $\partial M=S^1\times\Sigma$. Here, A is a connection on a principal U(1) bundle on M which restricts to our bundle P on $S^1\times\Sigma$. There is no obstruction to the existence of such an extension of $P\to S^1\times\Sigma$, since in our case it would lie in the group $H_3(\mathbb{CP}^\infty;\mathbb{Z})$, which is trivial.[8] The action should be independent (mod 2π) of the choice of the manifold M and the bundle over it, and this imposes the constraint

$$\mu\in\frac{1}{4\pi}\mathbb{Z} \tag{4}$$

on the Chern–Simons coefficient. We shall write $\kappa := 4\pi\mu$.

The group of gauge transformations $\mathcal{G}$ consists of smooth maps from $S^1\times\Sigma$ to U(1). The connected component of the identity $\mathcal{G}^0$ is the subgroup of maps homotopic to the identity (the small gauge transformations), and the connected components of $\mathcal{G}$ are labeled by two-homology classes of space-time, dual to the one-cycles around which the gauge transformations have non-trivial winding:

$$\mathcal{G}/\mathcal{G}^0 \cong H_2(S^1\times\Sigma;\mathbb{Z}) \cong \mathbb{Z}\oplus\mathbb{Z}^{\oplus 2\mathsf{g}}. \tag{5}$$

Here, g is the genus of Σ, and we can choose for the generator σ of the first $\mathbb{Z}$ factor the class of a positively oriented copy of Σ at a particular instant. It can be shown[9] that a gauge transformation in the connected component of $\mathcal{G}$ labeled by a class whose first component in the above decomposition is $k\sigma$ has the effect of adding the term $2\pi\kappa k N$ to the Chern–Simons action, so that this action is gauge-invariant (mod 2π) if and only if the condition (4) holds.

It is possible to express the Chern–Simons action entirely in terms of the three-dimensional data by treating carefully the boundary terms of the four-dimensional Chern action introduced above.[9] The result is that we should add a correction to the sum of the integrals of the Chern–Simons bulk term appearing in (2) over U_1 and U_2. The correction term is the double integral

$$\mu i \oint_{S^1\times\partial U_1} f_{12}^{-1} df_{12} \wedge A^{(1)}. \tag{6}$$

We still have to ensure that the term proportional to A_t in the action is gauge-invariant (mod 2π). Under a gauge transformation g, A_t changes as

$$A_t \mapsto A_t - ig^{-1}\partial_t g.$$

If the class of g in the first factor of $\mathcal{G}/\mathcal{G}^0$ in (5) is $k\sigma$, then everywhere on Σ

$$i \oint_{S^1} g^{-1}\partial_t g\, dt = k,$$

and the change in the action is

$$-\frac{i}{2}\gamma k \oint_{\Sigma} \Omega^2 dz\wedge d\bar{z} = -\gamma k \,\mathrm{Vol}(\Sigma).$$

This will be in $2\pi\mathbb{Z}$ for all $k\in\mathbb{Z}$ if and only if we impose the constraint

$$\gamma\,\mathrm{Vol}(\Sigma) \in \mathbb{Z}. \tag{7}$$

The action for Manton's model on Σ can then be written as

$$S[A,\phi] = \sum_{j=1}^{2} \int_{S^1\times U_j} \mathcal{L}[A^{(j)},\phi^{(j)}]\, d^3x + \mu i \oint_{S^1\times\partial U_1} f_{12}^{-1} df_{12}\wedge A^{(1)}, \tag{8}$$

where we impose the constraints (4) and (7) to the classical parameters to ensure that e^{iS} is well defined and gauge invariant. To implement the variational principle, we consider variations δA, $\delta\phi$ and $\delta\overline{\phi}$ of the fields which are a one-form and sections of the bundles associated to P by the fundamental representation and its dual, respectively. As usual, the variation of the first (bulk) term in (8) yields after integration by parts

$$\delta S = \sum_{\psi}\sum_{j=1}^{2}\left\{\int_{S^1\times U_j}\left[\frac{\delta\mathcal{L}}{\delta\psi} - \partial_\nu\left(\frac{\delta\mathcal{L}}{\delta\partial_\nu\psi}\right)\right]\delta\psi\, d^3x + \int_{S^1\times U_j}\partial_\nu\left(\frac{\delta\mathcal{L}}{\delta\partial_\nu\psi}\,\delta\psi\right) d^3x\right\}. \tag{9}$$

Here, ψ is any of A_ν, ϕ, or $\overline{\phi}$, and the (j) subscripts have been suppressed. If we define on each U_j the one-form

$$\Psi := \Omega^{-2}\left(\frac{\delta\mathcal{L}}{\delta\partial_t\psi}\right)dt - \left(\frac{\delta\mathcal{L}}{\delta\partial_{\overline{z}}\psi}\right)dz - \left(\frac{\delta\mathcal{L}}{\delta\partial_z\psi}\right)d\overline{z},$$

and denote the Hodge star of (1) by $*$, then the last integral in the expression (9) can be written as

$$\int_{S^1\times U_j}\partial_\nu\left(\frac{\delta\mathcal{L}}{\delta\partial_\nu\psi}\,\delta\psi\right)d^3x = \oint_{S^1\times\partial U_j} *\Psi\ \delta\psi. \tag{10}$$

It is easy to verify by direct computation that, for the terms in $\mathcal{L}$ which are locally gauge-invariant, the contributions to the components of the two-form $*\Psi\,\delta\psi$ are just functions on each trivializing patch. Therefore, their corresponding $j=1,2$ contributions in (10) cancel as they should, since the boundaries ∂U_1 and ∂U_2 are very close but carry opposite orientations. For the term proportional to A_t, the values of the contributions on the $j=1,2$ patches also cancel because of our assumption of the time-independence of f_{12}. However, the Chern–Simons term has a nonvanishing contribution. Indeed,

$$\delta(A\wedge dA) = 2\,dA\wedge\delta A - d(A\wedge\delta A),$$

and so the sum of the $j=1,2$ contributions to (10) is

$$\mu\oint_{S^1\times\partial U_1}(A^{(1)}\wedge\delta A - A^{(2)}\wedge\delta A) = -\mu i\oint_{S^1\times\partial U_1} f_{12}^{-1}df_{12}\wedge\delta A,$$

which exactly cancels the variation of the correction (6) to the Chern–Simons bulk term. So we conclude that the stationarity of the action (8) is exactly expressed by the Euler–Lagrange equations for the naive Lagrangian (2) in each trivializing coordinate patch. They read

$$\gamma i D_0\phi = -(D_z D_{\overline{z}}\phi + D_{\overline{z}}D_z\phi)\Omega^{-2} - \frac{\lambda}{4}(1-|\phi|^2)\phi, \tag{11}$$

$$\partial_z(B\Omega^{-2}) = -iJ_z + 2\mu E_z, \tag{12}$$

$$2\mu B = \gamma(1-|\phi|^2)\Omega^2, \tag{13}$$

where the gauge-invariant supercurrent J_z is defined by

$$J_z := -\frac{i}{2}(\overline{\phi}D_z\phi - \phi\overline{D_{\overline{z}}\phi}). \tag{14}$$

We are making the assumption that these equations admit nonstatic time-periodic solutions which can be patched together on Σ. Notice that no higher than first-order time derivatives of the fields appear in (11)–(13). Equation (11) is a gauge-invariant nonlinear Schrödinger equation for ϕ, while (12) is a version of Ampère's law and (13) can be interpreted as a magnetic Gauss' law.

III. STATIC VORTICES ON A SPHERE

Static configurations are time-independent solutions of the field equations of motion with vanishing A_t. For them, our Lagrangian reduces to the Ginzburg–Landau energy functional $\mathcal{E}$, given by the last bracket in (2). Notice that this is also the functional relevant to the discussion of static solutions in the Abelian Higgs model. If $\lambda=1$, one can show that all the critical points of $\mathcal{E}$ satisfy the two-dimensional Bogomol'nyĭ equations[10] on Σ. For configurations with $N>0$, these read

$$D_{\bar{z}}\phi = 0, \tag{15}$$

$$2B = (1-|\phi|^2)\Omega^2, \tag{16}$$

and their solutions are known as vortices. If $N<0$, they are called antivortices and satisfy similar equations, with $D_{\bar{z}}$ replaced by D_z in (15), whereas a minus sign is introduced in (16). Solutions (A,ϕ) to the Bogomol'nyĭ equations for which (3) holds have energy $\mathcal{E}=|N|\pi$. Henceforth, we shall be interested in the $N>0$ case only. Write $\phi = e^{h/2+i\chi}$; the function h is gauge-invariant while χ (defined only modulo 2π) is not, and both are real. Equation (15) can be used to obtain A_z in terms of h and χ, and substitution in (16) yields

$$4\partial_z\partial_{\bar{z}}h - (e^h-1)\Omega^2 = 4\pi\sum_{r=1}^{N}\delta^{(2)}(z-z_r). \tag{17}$$

The solution to this equation provides all the information needed to reconstruct the fields on Σ; χ has to give the required winding properties of ϕ in each patch, but the gauge freedom leaves it otherwise undetermined.

The Bogomol'nyĭ equations were first studied on a compact Riemann surface Σ by Bradlow[11] (cf. also Ref. 12 and references therein). He showed existence and uniqueness of a solution satisfying (3) with the Higgs field having exactly N zeros (counted with well-defined multiplicities) in any configuration, provided

$$\mathrm{Vol}(\Sigma) > 4\pi N. \tag{18}$$

Thus, given the topological constraint (3), and if the bound (18) is satisfied, the moduli space of solutions to the Bogomol'nyĭ equations can be described as the symmetric product $\mathcal{M}_N = S^N\Sigma = \Sigma^N/\mathfrak{S}_N$, a smooth $2N$-manifold. These solutions can be interpreted as nonlinear superpositions of N indistinguishable vortices located at the zeros of the Higgs field (the vortex cores), which play the rôle of moduli.

For the rest of this paper, we shall restrict to the situation where Σ is a two-sphere of radius R, which for later convenience we assume to be centered at the origin of $\mathbb{R}^3$. We choose the open subsets U_1 and U_2 introduced in Sec. II to be discs around the North and South poles, respectively, where stereographic coordinates can be used. In the next Section, we will argue that actually we can shrink U_2 to a point, and focus entirely on a U_1 which covers all of Σ except the South pole. So we can parametrize the position of the vortices in the open dense U_1 by a coordinate z with inverse

$$z \mapsto R\left(\frac{z+\bar{z}}{1+|z|^2}, -i\frac{z-\bar{z}}{1+|z|^2}, \frac{1-|z|^2}{1+|z|^2}\right). \tag{19}$$

As usual, we write $z=\infty$ to refer to the South pole. In terms of this coordinate, the conformal factor in (1) is just

$$\Omega^2(z,\bar{z}) = \frac{4R^2}{(1+|z|^2)^2}. \tag{20}$$

The positions $z_1,\ldots,z_N$ of N vortices define coordinates almost everywhere on the moduli space. They are regular only in the subset of configurations for which all the zeros of ϕ are simple and none of them occur at the South pole. To parametrize the whole subset $V_0 \subset \mathcal{M}_N$ of static configurations with no zeros of the Higgs field at $z=\infty$, we can introduce instead the elementary symmetric polynomials in the N variables z_r

$$s_k := s_k^{[N]}(z_1,\ldots,z_N) = \sum_{1\leqslant j_1<\cdots<j_k\leqslant N} z_{j_1}\cdots z_{j_k}, \quad 1\leqslant k\leqslant N. \tag{21}$$

More generally, let $V_j \subset \mathcal{M}_N$ denote the subset of configurations with exactly j vortices at $z=\infty$; it is parametrized by the symmetric polynomials $s_k^{[N-j]}$ of the coordinates of the $N-j$ remaining vortices. Clearly, $\mathcal{M}_N = \amalg_{j=0}^N V_j$ gives a decomposition of $\mathcal{M}_N$ into $N+1$ disjoint $2(N-j)$-cells $V_j \cong \mathbb{C}^{N-j}$, and it is easy to verify that they are glued together so as to give $\mathcal{M}_N = \mathbb{CP}^N$.

Later on, it will be useful to consider the standard decomposition of the moduli space as union of affine pieces $\mathcal{M}_N = \cup_{j=0}^N W_j$, where the W_j are defined in terms of homogeneous coordinates as usual

$$W_j := \{(Y_0 : Y_1 : \cdots : Y_N) \mid Y_j \neq 0\} \cong \mathbb{C}^N.$$

We may set $W_0 = V_0$ say, and identify the s_k in (21) with the inhomogeneous coordinates of W_0,

$$s_k = y_k^{(0)} := \frac{Y_k}{Y_0}, \quad 1 \leqslant k \leqslant N.$$

Letting $s_0 := 1$, we can relate the inhomogeneous coordinates in the other W_j to the s_k by

$$y_k^{(j)} := \frac{Y_k}{Y_j} = \frac{s_k}{s_j}, \quad 0 \leqslant k \leqslant N, \quad k \neq j.$$

It is not hard to see that V_j is being identified with the $(N-j)$-plane $y_0^{(j)} = \cdots = y_{j-1}^{(j)} = 0$ in W_j.

We still need to introduce a further piece of notation. Near the position $z = z_r$ of an isolated vortex, $h = \log|\phi|^2$ can be expanded as[7,13]

$$h(z; z_1, \ldots, z_N) = \log|z - z_r|^2 + a_r + \frac{b_r}{2}(z - z_r) + \frac{\overline{b_r}}{2}(\overline{z} - \overline{z_r}) + O(|z - z_r|^2). \tag{22}$$

Here, a_r and b_r are functions of the positions $z_1, \ldots, z_N$ of all the N vortices. If $N=1$, spherical symmetry can be used to show that[14]

$$b_1 = -\frac{2\overline{z_1}}{1 + |z_1|^2}.$$

This function describes how the level curves of $|\phi|^2$, which consist of circles centered around the core of the vortex on the sphere, are distorted by the stereographic projection onto the z-plane. An analogous situation arises when we consider more generally the subvariety $\mathcal{M}_N^{\mathrm{co}} \subset \mathcal{M}_N$ of configurations of N coincident vortices. It is parametrized by the position $z = Z$ of the only zero of the Higgs field, whose modulus squared has a logarithm with an expansion identical to (22) around Z, but with a coefficient N before the logarithmic term; the coefficient of $\frac{1}{2}(z - Z)$ is then

$$b = -\frac{2N\overline{Z}}{1 + |Z|^2}. \tag{23}$$

When the positions of the N vortices do not coincide, there is an additional distortion to the $|\phi|^2$ contours caused by the mutual interactions, and this leads to nontrivial b_r coefficients in (22). It turns out that the functions b_r contain all the information about the interactions relevant for the kinetic term of the reduced mechanical system. This was also the case in Samols' analysis of the Abelian Higgs model.[7]

It will be useful later to relate the functions b_r to their pullbacks

$$T^* b_r(z_1, \ldots, z_N) := b_r(T(z_1), \ldots, T(z_N)),$$

under an isometry T of the sphere. This relationship is easy to obtain directly from the expansion (22) by requiring that h be invariant:

$$T^* b_r = \frac{b_r}{T'(z_r)} - \frac{T''(z_r)}{(T'(z_r))^2}. \tag{24}$$

If we interpret T as a (passive) change of coordinates, this equation can be regarded as the formula for the transformation of Christoffel symbols for an affine connection, as pointed out in Ref. 15. In fact, we shall define a natural unitary connection on a line bundle over the moduli space of static vortices. In the next Section, we show that this connection is the essential ingredient of the reduced Lagrangian for Manton's model. The functions b_r are part of the coefficients of the connection one-form, and they incorporate the interactions among the vortices at zero potential energy into the reduced dynamics.

IV. THE EFFECTIVE MECHANICAL SYSTEM

Ultimately, we are interested in understanding the dynamics of the field configurations, and this is a much harder problem than the study of static solutions. However, it is natural to expect that, for λ close to 1, slow-varying solutions of the field theory should be well approximated by static solutions evolving along the directions defined by the linearized Bogomol'nyĭ equations. This idea was introduced by Manton in the context of Yang–Mills–Higgs monopoles[16] and has proven very fruitful in many situations. For the Abelian Higgs model, a careful analysis by Stuart[17] showed that this so-called adiabatic approximation is exponentially accurate in the limit of small velocities, and that it holds even when the coupling differs slightly from the self-dual value $\lambda = 1$. The field dynamics of N vortices is reduced to an effective mechanical system on the moduli space $\mathcal{M}_N$. The relevant Lagrangian can be obtained by evaluating the Lagrangian for the field theory at static solutions with time-dependent moduli and then integrating out the space dependence. Samols[7] showed that the reduced dynamics at self-dual coupling corresponds to geodesic motion on the moduli space, with respect to a Kähler metric that encodes information about the local behavior of the Higgs field at its zeros; we shall explain this more precisely at the end of this Section. For general values of $\lambda \simeq 1$, the geodesic motion is distorted by conservative forces, which are absent at self-dual coupling.

In what follows, we shall study Manton's model within the adiabatic approximation, in the regime $\lambda \simeq 1$ and $\gamma = \mu$. The latter assumption enables one to obtain a neat expression for the reduced kinetic-energy term, as will be shown below. Notice that, when $\gamma = \mu$, Eq. (13) reduces to (16), and this raises our hope that the adiabatic picture is a good approximation to the field theory in this model, as Manton pointed out.[2] Another check is provided by the existence of consistent conservation laws, which we shall explore in Sec. V.

We shall follow the analysis in Ref. 2 to obtain the Lagrangian for the reduced mechanical system on the moduli space. When γ and μ are set to be equal, consistency of the conditions (4) and (7) is expressed by

$$\frac{\kappa}{4\pi}\mathrm{Vol}(\Sigma) = \kappa R^2 \in \mathbb{Z}. \tag{25}$$

The kinetic energy consists of the terms in (8) which contain time derivatives and A_t. After using (16), it can be written in the form

$$T = \frac{i\gamma}{2}\sum_{j=1}^{2} \int_{U_j} \mathrm{Im}(4A_{\bar{z}}\dot{A}_z - \bar{\phi}\dot{\phi}\Omega^2)\, dz \wedge d\bar{z},$$

where the overdots denote time derivatives and z is the relevant stereographic coordinate on each of the discs U_j. Notice that the correction to the naive Chern–Simons action has now been canceled by a boundary term coming from the bulk. In terms of the functions h and χ introduced in Sec. III, we can write

$$T=\frac{i\gamma}{2}\sum_{j=1}^{2}\int_{U_j}(2i(\partial_{\bar z}\zeta_z-\partial_z\zeta_{\bar z})+\partial_t(\partial_z h\partial_{\bar z}\chi+\partial_{\bar z}h\partial_z\chi)-\dot\chi\Omega^2)dz\wedge d\bar z, \tag{26}$$

where ζ_z, $\zeta_{\bar z}$ are the components of the one-form

$$\zeta=\dot\chi(d\chi+\star dh)+\tfrac{1}{4}\dot h\, dh$$

in each trivializing coordinate patch; here, $\star$ is the Hodge star of the metric on Σ. To evaluate (26), we cut discs of small radius ϵ around each vortex position (where the integrand is singular) and apply Stokes' theorem, letting $\epsilon\to 0$ at the end.

The only contributions to the integrals around ∂U_j come from the first term in (26), yielding

$$i\gamma\oint_{\partial U_1}\dot\chi f_{12}^{-1}df_{12},$$

where χ denotes the argument of $\phi^{(1)}$. If we choose U_2 small enough so that it does not overlap with any of the trajectories of the vortices, χ is globally defined on U_2. So this term is a total time derivative and can be discarded from the kinetic energy. No other contribution coming from the nontriviality of the bundle P arises, and hence we may safely shrink U_2 to the South pole, while $U_1\cong\mathbb{C}$ becomes dense in Σ. Henceforth, z shall always denote the coordinate in (19).

To describe the contributions coming from the neighborhood of the vortices, we write[2] near vortex r

$$\chi=\theta_r+\psi_r, \tag{27}$$

where θ_r is the polar angle in the z-plane with respect to z_r, and ψ_r is a function of the position of the vortices only. Of course, Eq. (27) assumes that the gauge freedom has been reduced in the neighborhood of the vortices. The analysis in Ref. 2 goes through unchanged to conclude that the contributions from the first two terms in (26) add up to

$$\pi\gamma\sum_{r=1}^{N}(2\dot\psi_r+ib_r\dot z_r-i\bar b_r\dot{\bar z}_r). \tag{28}$$

It follows from the expansion (22) that the coefficient b_r has a singularity when vortex r approaches another vortex $s\neq r$,

$$b_r(z_1,\ldots,z_N)=2\sum_{s\neq r}\frac{1}{z_r-z_s}+\tilde b_r(z_1,\ldots,z_N), \tag{29}$$

where $\tilde b_r$ is a smooth function. However, a gauge can be chosen for which each ψ_r is given by

$$\psi_r(z_1,\ldots,z_N)=\arg\prod_{s\neq r}^{N}(z_r-z_s)\pmod{2\pi},$$

and then

$$\sum_{r=1}^{N}\dot\psi_r=-i\sum_{r=1}^{N}\sum_{s\neq r}\left(\frac{\dot z_r}{z_r-z_s}-\frac{\dot{\bar z}_r}{\bar z_r-\bar z_s}\right)$$

exactly cancels the singularity from the b_r coefficients.

The last term in (26) yields again a contribution from the metric on Σ. Its time integral gives $-2\pi\gamma$ times the signed area enclosed by the trajectories of the vortices $z_r(t)$. In our local coordinate z, the area form can be expressed as

$$\omega_\Sigma = 2iR^2 \frac{dz\wedge d\overline{z}}{(1+|z|^2)^2} = iR^2 d\left(\frac{z d\overline{z} - \overline{z} dz}{1+|z|^2}\right) =: d\vartheta.$$

Therefore, we may write

$$-2\pi\gamma \oint_{S^1}\left(\int_\Sigma \dot{\chi}\omega_\Sigma\right)dt = -2\pi\gamma \oint_{S^1}\sum_{r=1}^N z_r^*\vartheta = 2i\pi\gamma R^2 \oint_{S^1}\sum_{r=1}^N \frac{\overline{z}_r\dot{z}_r - z_r\dot{\overline{z}}_r}{1+|z_r|^2}dt \tag{30}$$

and interpret the integrand in the last expression above as the relevant contribution to T.

Putting (28) and (30) together, we conclude that the kinetic-energy term in the effective Lagrangian is given by

$$T^{\mathrm{red}} = \pi i\gamma \sum_{r=1}^N \left[\left(2R^2\frac{\overline{z}_r}{1+|z_r|^2} + \tilde{b}_r\right)\dot{z}_r - \left(2R^2\frac{z_r}{1+|z_r|^2} + \overline{\tilde{b}_r}\right)\dot{\overline{z}}_r\right]. \tag{31}$$

Unfortunately, the potential energy is harder to deal with. It can be written as

$$\begin{aligned} V^{\mathrm{red}} &= N\pi + \frac{i}{16}(\lambda-1)\int_\Sigma (1-e^h)^2\Omega^2 dz\wedge d\overline{z} \\ &= N\pi\lambda - \frac{\pi}{2}(\lambda-1)R^2 + \frac{i}{16}(\lambda-1)\int_\Sigma e^{2h}\Omega^2 dz\wedge d\overline{z}. \end{aligned}$$

It does not seem possible to simplify the integral involving e^{2h} to a local expression in the moduli. Stuart has shown[18] that, for $N=2$, V^{red} can be approximated by a rational function of the distance between the two vortices, in the limit where Bradlow's bound (18) comes close to the equality.

The reduced Lagrangian $L^{\mathrm{red}} = T^{\mathrm{red}} - V^{\mathrm{red}}$ is first-order in the time derivatives, just as the field theory Lagrangian. So, as mentioned in the Introduction, the equations of motion already arise in Hamiltonian form and the moduli space is to be interpreted as a phase space. The potential energy V^{red} is the only contribution to the Hamiltonian, while the kinetic term determines a symplectic potential $\mathcal{A}$ in our coordinate patch W_0 for a noncanonical symplectic form on $\mathcal{M}_N$. Indeed, $T^{\mathrm{red}} = \mathcal{A}(d/dt)$ with d/dt the vector field determining time evolution, and $\mathcal{A}$ the real one-form

$$\mathcal{A} = \pi i\gamma \sum_{r=1}^N \left[\left(2R^2\frac{\overline{z}_r}{1+|z_r|^2} + \tilde{b}_r\right)dz_r - \left(2R^2\frac{z_r}{1+|z_r|^2} + \overline{\tilde{b}_r}\right)d\overline{z}_r\right]. \tag{32}$$

This one-form is regular throughout W_0. The equations of motion can be cast as

$$\iota_{\frac{d}{dt}}\omega = -dV^{\mathrm{red}},$$

where the (global) symplectic form $\omega = d\mathcal{A}$ is given on W_0 by

$$-\frac{4i}{\kappa}\omega = d\sum_{r=1}^{N}\left[\left(2R^2\frac{\overline{z_r}}{1+|z_r|^2}+\tilde{b}_r\right)dz_r-\left(2R^2\frac{z_r}{1+|z_r|^2}+\overline{\tilde{b}_r}\right)d\overline{z_r}\right]$$

$$=\sum_{r=1}^{N}\sum_{s\neq r}\left(\frac{\partial\tilde{b}_s}{\partial z_r}dz_r\wedge dz_s-\frac{\partial\overline{\tilde{b}_s}}{\partial\overline{z_r}}d\overline{z_r}\wedge d\overline{z_s}\right)$$

$$-\sum_{r,s=1}^{N}\left(\frac{\partial b_r}{\partial\overline{z_s}}+\frac{\partial\overline{b_s}}{\partial z_r}+\frac{4R^2\delta_{rs}}{(1+|z_r|^2)^2}\right)dz_r\wedge d\overline{z_s}.$$

Notice that we are allowed to replace b_r by $\tilde{b}_r$ in expressions like $\partial b_r/\partial\overline{z_s}$, since it is know from (29) that $b_r-\tilde{b}_r$ is holomorphic. Either of the two arguments given in Ref. 7 shows that locally

$$\tilde{b}_r=\frac{\partial\mathcal{B}}{\partial z_r}, \tag{33}$$

for a real function $\mathcal{B}$. Hence

$$\omega=-\frac{i\kappa}{2}\sum_{r,s=1}^{N}\left(\frac{2R^2\delta_{rs}}{(1+|z_r|^2)^2}+\frac{\partial\overline{b_s}}{\partial z_r}\right)dz_r\wedge d\overline{z_s}. \tag{34}$$

It is easily verified that Eq. (33) is equivalent to ω being a Kähler form on W_0 with respect to the complex structure on the moduli space induced by the one on Σ. Moreover, we conclude from (34) that it is proportional to the Kähler form ω_{Sam} of Samols' metric[7]

$$\omega=-\frac{\kappa}{2}\omega_{\mathrm{Sam}}. \tag{35}$$

It is a global (1,1)-form on $\mathcal{M}_N$ with respect to the complex structure defined by our coordinates. It becomes apparent that ω_{Sam} (or ω) is a central object in the reduced dynamics of both the Abelian Higgs model and Manton's model; but we should emphasize that it plays completely different rôles in the two contexts. In the Abelian Higgs model, ω_{Sam} is the (1,1)-form corresponding to a Kähler metric on the configuration space $\mathcal{M}_N$. In the Hamiltonian picture, the dynamics takes place on the cotangent bundle $T^*\mathcal{M}_N$ with its canonical (tautological) symplectic form, and time evolution is determined by the laplacian of Samols' metric, possibly with an extra potential term if we allow $\lambda\neq 1$. On the other hand, in Manton's system ω is the symplectic form of a Hamiltonian system on $\mathcal{M}_N$ itself, which has no time evolution unless the potential V^{red} is switched on. We can also interpret ω as the curvature of the one-form $\mathcal{A}$ in (32), which represents a unitary connection on a Hermitian line bundle over $\mathcal{M}_N$ in a local orthonormal frame. This point of view leads directly to the geometric quantization of Manton's system using the natural Kähler polarization, as we shall see in Sec. VI.

V. SYMMETRIES AND CONSERVED QUANTITIES

In this section, we analyze the symmetries of Manton's model on the sphere, following the similar analysis for the plane.[19] More precisely, we will study the isometries of the metric (1). We shall make standard use of Noether's theorem to obtain the corresponding conserved quantities in the Lagrangian formulations of both the field theory and the reduced mechanical system. The conserved quantities reduced to static solutions are interesting observables of the effective classical system of vortices, and later we will be concerned with their quantization.

A. Symmetries in the field theory

Here, we shall be concerned with the Lagrangian (2). When computing the Lie derivatives of the different terms along a vector field ξ, one obtains gauge-dependent quantities in general.

However, we can supplement the field variations under the flow of ξ by a gauge transformation by $e^{-i\alpha A(\xi)}$, where α is the flow parameter, so as to obtain gauge-invariant variations.[19] The whole operation can be interpreted as a covariant Lie derivative, in the spirit of the discussion in the Appendix of Ref. 18.

The simplest symmetry of the model is time translation, generated by ∂_t. The $\mathrm{O}(\alpha)$ variation of the Lagrangian is

$$\alpha\,\delta\mathcal{L}=\alpha[\,\partial_t(\mathcal{L}+\gamma A_t\Omega^2-\mu BA_t)+2\mu i(\partial_{\bar z}(A_tE_z)-\partial_z(A_tE_{\bar z}))\,],$$

where we included a gauge transformation by $e^{-i\alpha A_t}$ in the fields. Noether's theorem then gives the conserved density

$$\begin{aligned} j^t&=\sum_{\psi}\frac{\delta\mathcal{L}}{\delta\partial_t\psi}\,\delta\psi-\partial_t(\mathcal{L}+\gamma A_t\Omega^2-\mu BA_t)\\ &=\frac{1}{2}B^2\Omega^{-2}+(|D_z\phi|^2+|D_{\bar z}\phi|^2)+\frac{\lambda}{8}(1-|\phi|^2)^2\Omega^2. \end{aligned}$$

This is the density of potential energy, so we learn that V is a constant of motion. This result does not depend on the particular form (20) for the conformal factor of the metric, and so it is also valid for more general Σ.

The SO(3) action on the sphere Σ by rotations about axes through the origin of $\mathbb{R}^3$ provides conservation laws for angular momentum. In our coordinate z, this action is described by elliptic Möbius transformations with antipodal fixed points,

$$z\mapsto\frac{(e^{i\alpha}+|a|^2)z+a(1-e^{i\alpha})}{\bar a(1-e^{i\alpha})z+(1+|a|^2e^{i\alpha})}, \tag{36}$$

where $a\in\mathbb{C}$ and $\alpha\in\mathbb{R}$. We shall consider the effect of rotations $R^{(j)}_\alpha$ $(j=1,2,3)$ by an angle α about the three Cartesian axes, which correspond to taking $a=1,i,0$.

The variation of the Lagrangian under the rotation $R^{(1)}_\alpha$, to be supplemented by the gauge transformation $e^{-\frac{\alpha}{2}((1-z^2)A_z-(1-\bar z^2)A_{\bar z})}$, is given up to $\mathrm{O}(\alpha)$ by

$$\begin{aligned} \alpha\,\delta_{(1)}\mathcal{L}=\frac{\alpha}{2}i[\,&\partial_t[(\mu B-\gamma\Omega^2)((1-z^2)A_z-(1-\bar z^2)A_{\bar z})]\\ &-\partial_z[(1-z^2)\mathcal{L}+2\mu i((1-z^2)A_zE_{\bar z}-(1-\bar z^2)A_{\bar z}E_{\bar z})]\\ &+\partial_{\bar z}[(1-z^2)\mathcal{L}+2\mu i((1-\bar z^2)A_{\bar z}E_z-(1-z^2)A_zE_z)]\,], \end{aligned}$$

and the variations $\delta_{(2)}\mathcal{L}$, $\delta_{(3)}\mathcal{L}$ are given by similar expressions. The densities of the conserved quantities can then be shown to be

$$j^t_{(1)}=\frac{\gamma i}{2}((1-z^2)(J_z+A_z)-(1-\bar z^2)(J_{\bar z}+A_{\bar z}))\Omega^2,$$

$$j^t_{(2)}=-\frac{\gamma}{2}((1+z^2)(J_z+A_z)+(1+\bar z^2)(J_{\bar z}+A_{\bar z}))\Omega^2,$$

$$j^t_{(3)}=-\gamma i(z(J_z+A_z)-\bar z(J_{\bar z}+A_{\bar z}))\Omega^2,$$

where J_z is the supercurrent defined in (14). These densities are still not gauge invariant. As in Ref. 19, we can remedy this by adding to the vector field $X_{(k)}$ in $\delta_{(k)}\mathcal{L}=:\partial_\nu X^\nu_{(k)}$ a divergenceless vector field. So we substitute $X^\nu_{(k)}$ by $\widetilde X^\nu_{(k)}$ given by

$$\tilde{X}^t_{(k)} = X^t_{(k)} - \partial_z(\Lambda_{(k)}A_{\bar{z}}) + \partial_{\bar{z}}(\Lambda_{(k)}A_z),$$

$$\tilde{X}^z_{(k)} = X^z_{(k)} + \partial_t(\Lambda_{(k)}A_{\bar{z}}) - \partial_{\bar{z}}(\Lambda_{(k)}A_t),$$

$$\tilde{X}^{\bar{z}}_{(k)} = X^{\bar{z}}_{(k)} - \partial_t(\Lambda_{(k)}A_z) + \partial_z(\Lambda_{(k)}A_t),$$

using

$$(\Lambda_{(1)},\Lambda_{(2)},\Lambda_{(3)}) = -2i\gamma R^2\left(\frac{z+\bar{z}}{1+|z|^2}, -i\frac{z-\bar{z}}{1+|z|^2}, \frac{1-|z|^2}{1+|z|^2}\right).$$

The new densities $\tilde{j}^t_{(k)}$ are now gauge invariant, and their space integrals are the conserved quantities

$$M_1 = -\frac{\gamma}{4}\int_{\mathbb{C}}\left[((1-z^2)J_z - (1-\bar{z}^2)J_{\bar{z}})\Omega^2 + 2iR^2\frac{z+\bar{z}}{1+|z|^2}B\right]dz\wedge d\bar{z},$$

$$M_2 = \frac{\gamma i}{4}\int_{\mathbb{C}}\left[((1+z^2)J_z + (1+\bar{z}^2)J_{\bar{z}})\Omega^2 - 2iR^2\frac{z-\bar{z}}{1+|z|^2}B\right]dz\wedge d\bar{z},$$

$$M_3 = \frac{\gamma i}{2}\int_{\mathbb{C}}\left[i(zJ_z - \bar{z}J_{\bar{z}})\Omega^2 + 2R^2\frac{1-|z|^2}{1+|z|^2}B\right]dz\wedge d\bar{z},$$

which can be interpreted as angular momenta around the three independent axes. Although Noether's theorem determines the conserved quantities corresponding to a given symmetry generator only up to an additive constant, the requirement that M_k be the components of a Hamiltonian moment of SO(3) removes this ambiguity.

Just as on the plane,[19] the quantities M_k can be neatly written as moments of the vorticity of the system. This is defined to be the gauge-invariant real quantity

$$\mathcal{V} = 2i(\partial_{\bar{z}}J_z - \partial_z J_{\bar{z}}) + B,$$

which is well-defined and smooth everywhere on Σ. Typically, it approaches zero away from the vortex cores, where both the magnetic field and the supercurrent (and its derivatives) become negligible. We obtain

$$M_1 = \frac{i\gamma}{2}R^2\int_{\mathbb{C}}\frac{z+\bar{z}}{1+|z|^2}\mathcal{V}\,dz\wedge d\bar{z}, \tag{37}$$

$$M_2 = \frac{i\gamma}{2}R^2\int_{\mathbb{C}}\frac{(-i)(z-\bar{z})}{1+|z|^2}\mathcal{V}\,dz\wedge d\bar{z}, \tag{38}$$

$$M_3 = \frac{i\gamma}{2}R^2\int_{\mathbb{C}}\frac{1-|z|^2}{1+|z|^2}\mathcal{V}\,dz\wedge d\bar{z}. \tag{39}$$

The expressions in the integrands should be compared with the Cartesian coordinates on the sphere as given by Eq. (19). We can anticipate that $\mathbf{M}=(M_1,M_2,M_3)$ is a vector in $\mathbb{R}^3$ which contains information about a center of mass of the vortex configurations. In particular, when N vortices become coincident, we expect $\mathbf{M}$ to point in the direction of the core, given the circular symmetry of the fields.

B. Symmetries in the effective mechanical system

There is an action of SO(3) on $\mathbb{CP}^N$ by simultaneous rotation of the vortex positions z_r as in (36). It is generated by the vector fields

$$\xi_{(1)}=-\frac{i}{2}\sum_{r=1}^{N}\left((1-z_r^2)\frac{\partial}{\partial z_r}-(1-\overline{z}_r^2)\frac{\partial}{\partial\overline{z}_r}\right), \tag{40}$$

$$\xi_{(2)}=\frac{1}{2}\sum_{r=1}^{N}\left((1+z_r^2)\frac{\partial}{\partial z_r}+(1+\overline{z}_r^2)\frac{\partial}{\partial\overline{z}_r}\right), \tag{41}$$

$$\xi_{(3)}=i\sum_{r=1}^{N}\left(z_r\frac{\partial}{\partial z_r}-\overline{z}_r\frac{\partial}{\partial\overline{z}_r}\right), \tag{42}$$

which can be seen to extend smoothly to $\mathbb{CP}^N$ after changing coordinates from the z_r to the s_k defined in (21). The rotational symmetry yields three independent relations among the functions b_r, which we shall now derive. Notice that the fluxes of the vector fields $\xi_{(j)}$ are given by acting on each z_r by the rotations $R_\alpha^{(j)}$ introduced in Sec. V.A. The Lie derivatives of the b_r can be computed by making use of (24),

$$\pounds_{\xi_{(j)}}b_r=\lim_{\alpha\to 0}\frac{R_\alpha^{(j)*}b_r-b_r}{\alpha}.$$

We then find the following relations:

$$-\frac{i}{2}\sum_{s=1}^{N}\left((1-z_s^2)\frac{\partial b_r}{\partial z_s}-(1-\overline{z}_s^2)\frac{\partial b_r}{\partial\overline{z}_r}\right)=\pounds_{\xi_{(1)}}b_r=-i(1+z_rb_r), \tag{43}$$

$$\frac{1}{2}\sum_{s=1}^{N}\left((1+z_s^2)\frac{\partial b_r}{\partial z_s}+(1+\overline{z}_s^2)\frac{\partial b_r}{\partial\overline{z}_s}\right)=\pounds_{\xi_{(2)}}b_r=-(1+z_rb_r), \tag{44}$$

$$i\sum_{s=1}^{N}\left(z_s\frac{\partial b_r}{\partial z_s}-\overline{z}_s\frac{\partial b_r}{\partial\overline{z}_s}\right)=\pounds_{\xi_{(3)}}b_r=-ib_r. \tag{45}$$

Using (33), Eqs. (43) and (44) can be written as

$$\sum_{s=1}^{N}\left((1\mp z_s^2)\frac{\partial b_s}{\partial z_r}\mp(1\mp\overline{z}_s^2)\frac{\partial\overline{b}_s}{\partial z_r}\right)\mp 2(1+z_rb_r)=0,$$

which together imply that the quantity $\Sigma_{s=1}^{N}(2z_s+z_s^2b_s+\overline{b}_s)$ is constant for all vortex configurations. To find what this constant is, we remark that all the singular parts in (29) cancel in pairs in the sum over s, and that in the limit of coincidence of the vortices the functions $\tilde{b}_r$ in (29) tend to b in (23). In particular, when all the vortices are at $Z=0$

$$\sum_{r=1}^{N}b_r(0,\ldots,0)=0. \tag{46}$$

So we conclude that

$$\sum_{s=1}^{N}(2z_s+z_s^2b_s+\overline{b}_s)=0. \tag{47}$$

Similarly, Eq. (45) and its conjugate imply that the quantity $\Sigma_{r=1}^{N}(z_s b_s - \overline{z_s}\overline{b_s})$ is independent of the vortex positions. Using the explicit formula (23) for N coincident vortices, we then deduce that this constant has to be zero, obtaining

$$\sum_{s=1}^{N} z_s b_s \in \mathbb{R}. \tag{48}$$

We remark that Eqs. (47) and (48) are analogues of the statement that the sum of the b_r vanishes for any vortex configuration on the plane, as found by Samols[7] as a consequence of translational symmetry. In fact, this statement follows from (47) in the limit where all vortices approach the origin, and (46) may be regarded as a special case of it. Equation (48) is also valid for vortices on the plane, and is a consequence of the SO(2) symmetry, but it has not been noted before in the literature.

The SO(3) action on $\mathbb{CP}^N$ leaves the symplectic form (34) invariant, i.e.,

$$\pounds_{\xi}\omega = d\iota_{\xi}\omega = 0, \tag{49}$$

for all ξ generating a rotation. To establish this, we make use of the relations (47) and (48). For example, $\xi_{(3)}$ satisfies (49) if and only if

$$\frac{\partial}{\partial \overline{z_q}}\left[\sum_{s=1}^{N}\left(\overline{z_s}\frac{\partial \overline{b_s}}{\partial z_r} - z_s\frac{\partial b_s}{\partial z_r}\right) - b_r\right] = 0,$$

for all q and r, and this follows from (48) or the weaker statement (45). Since $H^1(\mathbb{CP}^N;\mathbb{R})$ is trivial, (49) implies that there exist globally defined functions M_j^{red} satisfying

$$\iota_{\xi_{(j)}}\omega = -dM_j^{\mathrm{red}}. \tag{50}$$

The functions M_j^{red} are determined from (50) only up to a constant, and the $\xi_{(j)}$ are their corresponding Hamiltonian vector fields. We can fix this constant by requiring that the M_j^{red} are the components of a moment map, i.e., that the SO(3) action is Hamiltonian[20]

$$\{M_i^{\mathrm{red}}, M_j^{\mathrm{red}}\} := \omega(\xi_{(i)}, \xi_{(j)}) = -\sum_{k=1}^{3}\epsilon_{ijk}M_k^{\mathrm{red}}. \tag{51}$$

The M_j^{red} turn out to be the conserved quantities corresponding to the rotational symmetry in the reduced mechanical system. Recall that the connection one-form $\mathcal{A}$ in (32) is a symplectic potential for ω, and thus Eq. (50) is equivalent to

$$\pounds_{\xi_{(j)}}\mathcal{A} = dW_j, \tag{52}$$

with

$$W_j = \mathcal{A}(\xi_{(j)}) - M_j^{\mathrm{red}}. \tag{53}$$

Equation (52) is the statement of rotational invariance of the U(1) connection represented by $\mathcal{A}$ (see Ref. 21 for a discussion in the more general situation of connections on bundles with nonabelian structure group). The reduced Lagrangian L^{red} has a kinetic term (31) of the form

$$T^{\mathrm{red}} = \sum_{r=1}^{N}\mathcal{A}_r\dot{z}_r + \text{c.c.},$$

and a rotationally invariant potential. Using (52), we can establish that

$$\pounds_{\xi_{(j)}} L^{\mathrm{red}} = \partial_t W_j \,, \tag{54}$$

and so Noether's theorem implies that M_j^{red} as given by (53) is a conserved quantity. Notice that W_j depends on the choice of symplectic potential for ω, whereas M_j^{red} does not—cf. Eqs. (52) and (50). We can determine M_j^{red} by integrating (50), or alternatively from (54) and (53). We shall follow the latter route, which provides a direct proof of the spherical symmetry of the reduced system. Using Eqs. (43)–(45), we find that

$$\pounds_{\xi_{(1)}} L^{\mathrm{red}} = -\pi\gamma(R^2 - N)\partial_t \sum_{r=1}^{N} (z_r - \overline{z_r}),$$

$$\pounds_{\xi_{(2)}} L^{\mathrm{red}} = \pi i \gamma(R^2 - N)\partial_t \sum_{r=1}^{N} (z_r + \overline{z_r}),$$

$$\pounds_{\xi_{(3)}} L^{\mathrm{red}} = 0 = -2\pi\gamma\partial_t(N(R^2 - N)).$$

The constant term after the time derivative in the last equation was chosen so that the conserved quantities M_j^{red} obey (51). Making use of the relations (47) and (48) for the functions b_r, they can be written as

$$M_1^{\mathrm{red}} = \frac{\kappa}{4} \sum_{r=1}^{N} \left(2R^2 \frac{z_r + \overline{z_r}}{1 + |z_r|^2} + b_r + \overline{b_r} \right), \tag{55}$$

$$M_2^{\mathrm{red}} = \frac{i\kappa}{4} \sum_{r=1}^{N} \left(-2R^2 \frac{z_r - \overline{z_r}}{1 + |z_r|^2} + b_r - \overline{b_r} \right), \tag{56}$$

$$M_3^{\mathrm{red}} = \frac{\kappa}{2} \sum_{r=1}^{N} \left(R^2 \frac{1 - |z_r|^2}{1 + |z_r|^2} - (z_r b_r + 1) \right). \tag{57}$$

A consistency check of the reduction procedure can be made by comparing the conserved angular momenta in the two pictures. To do this, we shall write the quantities M_k in Sec. V A for static solutions in terms of the moduli. This is most easily done from Eqs. (37)–(39), expressing the fields in terms of the function h and making use of Eqs. (17) and (22) to reduce each M_k to the moduli space, similarly to what we did for the Lagrangian in Sec. IV. For example, to obtain the expression for M_1 we start by writing

$$\begin{aligned} \frac{z + \overline{z}}{1 + |z|^2} \mathcal{V} &= \frac{2}{R^2} \frac{z + \overline{z}}{1 + |z|^2} \partial_z \left(\frac{\partial_{\overline{z}} h \, \partial_z \partial_{\overline{z}} h}{1 + |z|^2} \right) \\ &= \frac{4}{R^2} \partial_z \left((z + \overline{z}) \partial_z \left(\frac{(\partial_{\overline{z}} h)^2}{1 + |z|^2} \right) - \frac{(\partial_{\overline{z}} h)^2}{1 + |z|^2} \right) + \text{c.c.} \end{aligned}$$

and use Stokes' theorem to evaluate (37) as a sum of contour integrals along small discs C_r of radius ϵ around the vortex positions:

$$M_1 = \frac{\gamma i}{4} \sum_{r=1}^{N} \oint_{C_r} ((z + \overline{z})(\overline{z}(\partial_{\overline{z}} h)^2 + (1 + |z|^2)\partial_{\overline{z}} h \partial_z \partial_{\overline{z}} h) - (1 + |z|^2)(\partial_{\overline{z}} h)^2) d\overline{z} + \text{c.c.}\,.$$

Assuming that the vortices are isolated, we may write on C_r

$$\partial_z \partial_{\bar{z}} h = -\frac{R^2}{(1+|z_r|^2)^2} + \mathrm{O}(\epsilon^2),$$

$$\partial_{\bar{z}} h = \frac{e^{i\theta_r}}{\epsilon} + \frac{\overline{b_r}}{2} + \mathrm{O}(\epsilon),$$

and then obtain in the limit $\epsilon \to 0$

$$M_1 = \frac{\pi\gamma}{2} \sum_{r=1}^{N} \left(4R^2 \frac{z_r + \overline{z_r}}{1+|z_r|^2} + (1-z_r^2) b_r + (1-\overline{z_r}^2)\overline{b_r} - 2(z_r + \overline{z_r}) \right)$$
$$= \frac{\kappa}{4} \sum_{r=1}^{N} \left(2R^2 \frac{z_r + \overline{z_r}}{1+|z_r|^2} + b_r + \overline{b_r} \right),$$

where we made use of (47). Similarly, we find

$$M_2 = \frac{\pi\gamma i}{2} \sum_{r=1}^{N} \left(-4R^2 \frac{z_r - \overline{z_r}}{1+|z_r|^2} + (1+z_r^2) b_r - (1+\overline{z_r}^2)\overline{b_r} + 2(z_r - \overline{z_r}) \right)$$
$$= \frac{\kappa i}{4} \sum_{r=1}^{N} \left(-2R^2 \frac{z_r - \overline{z_r}}{1+|z_r|^2} + b_r - \overline{b_r} \right)$$

and

$$M_3 = \pi\gamma \sum_{r=1}^{N} \left(2R^2 \frac{1-|z_r|^2}{1+|z_r|^2} - (z_r b_r + \overline{z_r}\overline{b_r}) - 2 \right)$$
$$= \frac{\kappa}{2} \sum_{r=1}^{N} \left(R^2 \frac{1-|z_r|^2}{1+|z_r|^2} - (z_r b_r + 1) \right).$$

So each M_j agrees with M_j^{red}.

It is instructive to compare the conserved quantities that we have found for the sphere with the ones obtained for the plane.[19] On the plane, space isometries are described by the Euclidean group $E(2)$. Convenient generators are the translations along the x_1 and x_2 axes and the rotation about the origin, and their conserved quantities in the reduced picture were determined to be

$$P_1 = -\pi\gamma i \sum_{r=1}^{N} (Z_r - \overline{Z_r}), \tag{58}$$

$$P_2 = \pi\gamma \sum_{r=1}^{N} (Z_r + \overline{Z_r}), \tag{59}$$

$$M = 2\pi\gamma \sum_{r=1}^{N} \left(\frac{1}{2}|Z_r|^2 + B_r Z_r + \overline{B_r}\overline{Z_r} + 1 \right), \tag{60}$$

where Z_r denote the positions of the vortex cores, B_r the coefficients in an expansion equivalent to (22), and we removed the "red" superscripts. In the limit where the radius R is large and the vortices are close together, say in a small neighborhood of the North pole, one should expect that our M_k should be well approximated by quantities directly related to the ones in (58)–(60). Indeed, identifying $2Rz_r = Z_r$ we obtain from (55) to (57)

$$M_1 = -RP_2 + \pi\gamma R \sum_{r=1}^{N} (B_r + \overline{B}_r) + \mathrm{O}(|z_s|), \tag{61}$$

$$M_2 = RP_1 + \pi\gamma i R \sum_{r=1}^{N} (B_r - \overline{B}_r) + \mathrm{O}(|z_s|), \tag{62}$$

$$M_3 = 2\pi\gamma N R^2 - M + \mathrm{O}(|z_s|). \tag{63}$$

Since it is known[7] that $\Sigma_{r=1}^{N} B_r = 0$ [cf. Eq. (46)], we see that M_1, M_2 and P_1, P_2 are related as expected, but Eq. (63) for M_3 is rather surprising. It means that, as $R \to \infty$, M_3 becomes infinite, and we should subtract from it the quantity $2\pi\gamma N R^2$, itself infinite in the limit, to be able to compare it with the angular momentum in the plane, M. Notice that when (61)–(63) are inserted in (51), we obtain

$$\{P_1, P_2\} = 2\pi\gamma N - \frac{1}{R^2} M + \mathrm{O}(|z_s|).$$

Thus when $R \to \infty$ we recover the nonvanishing classical Poisson brackets for the linear momenta in the plane as calculated by Hassaïne *et al.*[22]

For N coincident vortices, we can make use of (23) to obtain the angular momentum vector in closed form:

$$\mathbf{M}^{[N]} = 2\pi\gamma N(R^2 - N)\left(\frac{Z + \overline{Z}}{1 + |Z|^2}, -i\frac{Z - \overline{Z}}{1 + |Z|^2}, \frac{1 - |Z|^2}{1 + |Z|^2} \right). \tag{64}$$

As before, Z denotes the position of the common core. If we take $N = 1$, (64) implies that a single vortex on Σ should be assigned a nonzero $\mathbf{M}$ vector. Its direction gives just the vortex position, and its conservation implies that the single vortex does not move (even if $\lambda \neq 1$), as expected. The length of $\mathbf{M}^{[1]}$ can be interpreted as a nonzero intrinsic angular momentum of the single vortex at rest. This was also a feature of the model in the plane, where a single vortex was found to have an intrinsic momentum $-2\pi\gamma$. This agrees with our result, provided that we subtract the "tail" momentum $2\pi\gamma N R^2$ as discussed above. It should be noted that on the sphere this intrinsic momentum is quantized, from the considerations in Sec. II—it is a half integer in units of $\hbar = 1$. On the plane, this feature is not apparent, since γ could take any value. More generally, a configuration of N coincident vortices has angular momentum $-2\pi\gamma N^2$ after subtraction of $2\pi\gamma N R^2$, and this is consistent with the results of Ref. 19.

VI. INGREDIENTS FOR GEOMETRIC QUANTIZATION

We would like to investigate the quantum version of the reduced mechanics in the framework of geometric quantization. We shall follow the conventions in Ref. 5 and refer to Ref. 23 for background on complex geometry. To construct the quantum system, we need to supplement the classical theory (specified by the phase space $\mathcal{M}_N = \mathbb{CP}^N$, endowed with the symplectic form ω) with a Hermitian line bundle L over $\mathcal{M}_N$. The wave functions in the quantum Hilbert space are particular sections of L.

To start with, we should verify whether our phase space is quantizable at all. This is equivalent to the integrality of the class represented by the closed form $\omega/(2\pi)$ in de Rham cohomology,

$$\frac{1}{2\pi}[\omega] \in H^2(\mathcal{M}_N; \mathbb{Z}) \subset H^2(\mathcal{M}_N; \mathbb{R}). \tag{65}$$

In general, this requirement leads to nontrivial constraints on the parameters of the classical theory—the Weil (pre)quantization conditions. If they are satisfied, we may regard $[\omega]/(2\pi)$ as the first Chern class of a smooth complex line bundle over $\mathcal{M}_N$, which is what we call the prequantum line bundle L.

Recall that $H^2(\mathbb{CP}^N;\mathbb{R})$ is cyclic and we can take as generator the first Chern class $\eta \in H^2(\mathbb{CP}^N;\mathbb{Z})$ of the hyperplane bundle of $\mathbb{CP}^N$. Then $[\omega]=2\pi\ell\eta$ for suitable $\ell\in\mathbb{R}$. To determine ℓ, we can refer to Eq. (35) and use the formula for the cohomology class of ω_{Sam} obtained by Manton.[14] (This formula has been generalized[15] for Σ of arbitrary genus.) For the benefit of the reader, we reproduce Manton's argument here. Let $\mathcal{M}_N^{\mathrm{co}}\subset\mathcal{M}_N$ be the subvariety of configurations of N coincident vortices. This is a projective line parametrized by the position Z of the zero of the Higgs field. Equation (23) implies that ω restricts to it as

$$\omega|_{\mathcal{M}_N^{\mathrm{co}}}=-i\kappa\frac{N(R^2-N)}{(1+|Z|^2)^2}dZ\wedge d\overline{Z}. \tag{66}$$

It is readily seen that $\mathcal{M}_N^{\mathrm{co}}$ is embedded as a projective curve of degree N in $\mathcal{M}_N$, and is thus homologous to $\pm N[\mathbb{CP}^1]$. Here, we denote by $[\mathbb{CP}^1]$ the homology class of a projective line inside $\mathcal{M}_N$, which is dual to η and a generator of $H_2(\mathcal{M}_N;\mathbb{Z})$. The integral of (66) over $\mathcal{M}_N^{\mathrm{co}}$ is just $-2\pi\kappa N(R^2-N)$, and so we conclude that $\ell=-\kappa(R^2-N)$,

$$\frac{1}{2\pi}[\omega]=\ell\eta=-\kappa(R^2-N)\eta. \tag{67}$$

Equation (65) is equivalent to ℓ being an integer,

$$\kappa(R^2-N)\in\mathbb{Z},$$

and this is weaker than the conditions $\kappa,\kappa R^2\in\mathbb{Z}$ that we already had to impose in (4) and (25) from considerations of gauge invariance (mod 2π) of the classical field theory action. We conclude that no further constraints arise from prequantization.

In geometric quantization, the prequantum line bundle L is to be equipped with a Hermitian metric and a unitary connection. The fact that $\mathbb{CP}^N$ is simply-connected implies that in our case L is uniquely determined as a smooth bundle by the symplectic structure, and so is the Hermitian metric and the connection $\mathcal{D}$. The basic idea in the standard construction of L is to interpret (real) symplectic potentials of ω as local expressions for the connection, and then use parallel transport to define local sections and construct the bundle.[5] A given symplectic potential determines a unique local section σ of L up to a phase of modulus one. The Hermitian metric is introduced by requiring that each σ is a local orthonormal frame

$$\langle\sigma,\sigma\rangle=1. \tag{68}$$

This is unambiguous since two symplectic potentials must differ by the exterior derivative of a real function u, and then the corresponding local sections are related by the factor e^{-iu}.

The wave functions in geometric quantization are defined as the L^2 polarized sections of L. By L^2 we mean square-integrable with respect to the Hermitian product (68) on the fibres and the symplectic measure $\omega^N/N!$ on the base $\mathcal{M}_N$. Roughly speaking, polarized means that they only depend on half of the real coordinates of the phase space, just as the wave functions in the Schrödinger representation of quantum mechanics only depend on the position and not on the momentum. More precisely, a polarization $\mathcal{P}$ is defined as a Lagrangian (i.e., maximally isotropic) integrable subbundle of the complexification $T_{\mathbb{C}}\mathcal{M}_N$ of the tangent bundle of the phase space, and the condition

$$\mathcal{D}_{\overline{X}}\psi=0,\quad \forall X\in\Gamma(\mathcal{M}_N,\mathcal{P}) \tag{69}$$

defines what is meant for a section ψ to be $\mathcal{P}$-polarized. When the classical dynamics takes place in a Kähler phase space, as is our case, there is a natural choice of polarization $\mathcal{P}$—namely, the one determined by the i-eigenspaces of the compatible complex structure. It is generated by the holomorphic vector fields in the local complex coordinates. The introduction of a Kähler polarization can be interpreted naturally in terms of complex geometry as follows. A connection on the prequantum line bundle defines a holomorphic structure for L: By definition, the holomorphic sections are the ones which are annihilated by the part of $\mathcal{D}$ that takes values in $\Omega^{(0,1)}(\mathcal{M}_N,L)$, which is defined from the complex structure in the base. But such sections are precisely the ones satisfying the condition (69) for the Kähler polarization. Thus, polarized sections of L are nothing but holomorphic sections with respect to the holomorphic structure on L induced by the unitary connection $\mathcal{D}$.

VII. THE QUANTUM HILBERT SPACE

The Picard variety of $\mathbb{CP}^N$ is trivial, and this implies that L is uniquely determined as a holomorphic line bundle by its first Chern class, which can be read off from (67). A classical result[24] on the sheaf cohomology of $\mathbb{CP}^N$ establishes that L admits nontrivial global holomorphic sections if and only if $\ell > 0$ (i.e., $\kappa < 0$), and then they form the vector space

$$H^0(\mathbb{CP}^N,\mathcal{O}(L)) \cong \mathbb{C}[Y_0,\ldots,Y_N]_\ell, \tag{70}$$

where the right-hand side denotes the homogeneous polynomials of degree ℓ in the $N+1$ variables Y_j. This gives a concrete way to realize L and its sections (up to multiplication by a constant in $\mathbb{C}^\times$). Recall that the local symplectic potential $\mathcal{A}$ in (32) for the connection $\mathcal{D}$ determines a nonvanishing local section $\sigma: W_0 \to L$. It is not holomorphic though, as $\mathcal{A}$ has a nonzero component in $\Omega^{(0,1)}(W_0)$. But we can obtain a holomorphic local section from it by using a nonunitary gauge transformation: Since

$$\mathcal{A} = 2\pi\gamma i \sum_{r=1}^{N} \left(2R^2 \frac{\overline{z_r}}{1+|z_r|^2} + \tilde{b}_r \right) dz_r - 2\pi\gamma i d\left(\frac{1}{2}\mathcal{B} + R^2 \sum_{r=1}^{N} \log(1+|z_r|^2) \right), \tag{71}$$

where $\mathcal{B}$ is defined up to an additive real constant by (33), we can define on W_0

$$\sigma^{(0)}(z_1\ldots,z_N) := \sigma(z_1\ldots,z_N) e^{-2\pi\gamma(\frac{1}{2}\mathcal{B} + R^2 \sum_{r=1}^{N} \log(1+|z_r|^2))}; \tag{72}$$

this is a holomorphic section of L on W_0. It is uniquely determined from σ up to a positive real constant, and thus from $\mathcal{A}$ up to a constant in $\mathbb{C}^\times$. It extends to a global section of L, vanishing in the complement of W_0; we identify it with the homogeneous polynomial Y_0^ℓ in (70). From it, we can define the sections

$$\sigma^{(j)} := \left(\frac{Y_j}{Y_0} \right)^\ell \sigma^{(0)} = (y_j^{(0)})^\ell \sigma^{(0)},$$

which trivialize L on each W_j, and determine the line bundle through the transition functions

$$\varphi_{ij} : W_i \cap W_j \to \mathbb{C}^\times$$

$$(y_1^{(i)},\ldots,y_N^{(i)}) \mapsto (y_j^{(i)})^\ell = \left(\frac{s_j}{s_i} \right)^{-\kappa(R^2-N)}.$$

On each W_j, global holomorphic sections of L are given by multiplying $\sigma^{(j)}$ by polynomials in the $y_k^{(j)}$ of degree less than or equal to ℓ.

The quantum Hilbert space $\mathcal{H}_{\mathcal{P}}$ is the space of holomorphic sections of L which are normalizable with respect to the inner product defined by the symplectic measure of $\mathcal{M}_N$ and the product on the fibres given by (68), as we said in Sec. VI. This inner product can be easily written down as an integral over the open dense W_0, where L is trivialized by $\sigma^{(0)}$, by making use of (34), (68) and (72). Since we are dealing with a compact phase space, all the holomorphic sections have finite norm, so the Hilbert space $\mathcal{H}_{\mathcal{P}}$ is $H^0(\mathbb{CP}^N,\mathcal{O}(L))$ itself, with dimension

$$\dim\mathcal{H}_{\mathcal{P}}=\binom{N+\ell}{\ell}. \tag{73}$$

All these quantum states belong to a single degenerate energy level when $\lambda=1$. Recall that in this situation the Hamiltonian vanishes and no motion occurs at the classical level.

We may interpret the expression (73) as giving the number of states in a quantum system of N interacting bosons. By interacting, we mean that the area available for the dynamics on the sphere is affected by the space which the vortices themselves occupy. Recall that Bradlow's bound (18) establishes that N vortices can only live on a sphere which has an area exceeding $4\pi N$. Heuristically, we can say that a single vortex occupies 4π units of area. So we can regard (73) as the formula for the number of states for a system of N bosons which can be assigned to any of the $(|\kappa|/4\pi)\cdot 4\pi(R^2-N)$ states corresponding to the room available on the sphere, after the total area of the vortices has been discounted. (For $\kappa=-1$, there is a similiar interpretation for (73) as the number of states of a system of N noninteracting fermions, but it breaks down for $\kappa\neq -1$.)

From the formula (67), it is immediate to compute the volume of the moduli space determined by the Kähler form ω:

$$\mathrm{Vol}_{\omega}(\mathcal{M}_N)=\frac{(2\pi|\kappa|(R^2-N))^N}{N!}=\frac{(2\pi\ell)^N}{N!}.$$

It is of course proportional to the volume determined by Samols' metric, as first computed by Manton.[14,15] This volume has been used to deduce the thermodynamics of an ideal gas of Abelian Higgs vortices at $\lambda=1$ in the framework of Gibbs' classical statistical mechanics. In Manton's model at $\lambda=1$, there is only a ground state as we noted above, and its degeneracy, in Gibbs' approximation, is given by

$$d_{\mathrm{Gibbs}}=\frac{1}{(2\pi\hbar)^N}\mathrm{Vol}(\mathcal{M}_N)=\frac{\ell^N}{N!}. \tag{74}$$

Notice that Planck's constant is $2\pi\hbar=2\pi$ in our units. Gibbs' partition function is simply $Z_{\mathrm{Gibbs}}=d_{\mathrm{Gibbs}}e^{-\beta N\pi}$. At $\lambda\neq 1$, the degeneracy is lifted but the formula above is still to be interpreted as the total number of states of the system. It is of interest to study the quotient

$$Q:=\frac{\dim\mathcal{H}_{\mathcal{P}}}{d_{\mathrm{Gibbs}}},$$

which gives information about how appropriate Gibbs' estimate for the number of states of the quantum system is. From (73) and (74), we find

$$Q=\frac{(N+\ell)!}{\ell^N\ell!}.$$

Using Stirling's formula for the gamma function, we obtain

$$Q=\left(1+\frac{N+1}{\ell}\right)^N\left(1+\frac{N}{\ell+1}\right)^{-\frac{1}{2}}\left[\left(1+\frac{N}{\ell+1}\right)^{\ell+1}e^{-N}\right]e^{J(N+\ell+1)-J(\ell+1)}, \tag{75}$$

where J is the asymptotic series

$$J(z)=\sum_{n=1}^{\infty}\frac{B_n}{(2n-1)2n}\frac{1}{z^{2n-1}}.$$

In the context of Chern–Simons theories, the classical approximation is described as the limit $|\kappa|\to\infty$; this is equivalent to keeping the coupling μ as constant and letting $\hbar\to 0$. So we keep N fixed and let $\ell\to\infty$ in the expression (75), and this gives indeed $Q\to 1$. We might also try to obtain a classical regime in a thermodynamical limit, where both N and the area of the sphere become very large, but keeping a finite (possibly small) density, which we might want to define as

$$\nu:=\frac{|\kappa|N}{\ell}=\frac{\dfrac{N}{R^2}}{\left(1-\dfrac{N}{R^2}\right)}.$$

But it follows from (75) that in this limit Q is infinite, however small ν is taken to be.

VIII. QUANTUM ANGULAR MOMENTA

From the prequantization data, it is possible to construct prequantum operators $\mathcal{P}(f)$ for any classical observable $f\in C^{\infty}(\mathcal{M}_N)$ as

$$\mathcal{P}(f):=-i\mathcal{D}_{\xi_f}+f. \tag{76}$$

Here, ξ_f is the Hamiltonian vector field of f with respect to ω, defined by

$$d\iota_{\xi_f}\omega=-df. \tag{77}$$

Equation (50) is of course a special case of (77), with $\xi_{M_j^{\mathrm{red}}}=\xi_{(j)}$. In general, the linear operator $\mathcal{P}(f)$ does not map polarized sections of L to polarized sections. It is easy to show that it does if and only if ξ_f preserves the polarization:

$$[\xi_f,\Gamma(\mathcal{M}_N,\mathcal{P})]\subset\Gamma(\mathcal{M}_N,\mathcal{P}). \tag{78}$$

Then we may interpret $\mathcal{P}(f)$ as the quantum operator corresponding to the observable f. In the Kähler case, (78) can be seen to be equivalent to ξ_f being the real part of a holomorphic vector field. This condition is true for the Hamiltonian vector fields (40)–(42) of the angular momenta in (55)–(57).

We can determine explicitly the action of the quantum operators on the wave functions Ψ in the quantum Hilbert space $\mathcal{H}_{\mathcal{P}}=H^0(\mathcal{M}_N,\mathcal{O}(L))$. In the holomorphic frame on W_0 provided by $\sigma^{(0)}$, one can write $\Psi=\Psi^{(0)}\sigma^{(0)}$ with

$$\Psi^{(0)}(z_1,\ldots,z_N)=\sum_{j_1+\cdots+j_N=0}^{\ell}\alpha_{j_1\cdots j_N}\prod_{k=1}^{N}s_k^{[N]}(z_1,\ldots,z_N)^{j_k}, \tag{79}$$

with $\alpha_{j_1\cdots j_N}\in\mathbb{C}$. The one-form representing $\mathcal{D}$ with respect to this frame can be read off from (71) to be

$$\mathcal{A}^{(0)}=2\pi\gamma i\sum_{r=1}^{N}\left(2R^2\frac{\overline{z_r}}{1+|z_r|^2}+\tilde{b}_r\right)dz_r.$$

Substitution in (76) now gives the local representatives of the quantum operators in the local frame $\sigma^{(0)}$. For example, for M_3 we obtain

$$\begin{aligned}\mathcal{P}(M_3) &= -i(\iota_{\xi_{(3)}} d - i\mathcal{A}^{(0)}(\xi_{(3)})) + M_3 \\ &= -i\iota_{\xi_{(3)}} d + \frac{\kappa}{2} N(R^2-1) - \kappa \sum_{r=1}^{N} \sum_{s\neq r}^{N} \frac{z_r}{z_r - z_s} \\ &= -i\iota_{\xi_{(3)}} d - \frac{N\ell}{2}.\end{aligned}$$

Acting on Ψ as in (79), this yields

$$\mathcal{P}(M_3)\Psi^{(0)} = \sum_{j_1+\cdots+j_N=0}^{\ell} \left(j_1 + 2j_2 + \cdots + Nj_N - \frac{N\ell}{2} \right) \alpha_{j_1\cdots j_N} \prod_{k=1}^{N} s_k^{[N]}(z_1,\ldots,z_N)^{j_k}. \quad (80)$$

From this expression, it is easy to read off the eigenvalues of $\mathcal{P}(M_3)$ as

$$-\frac{N\ell}{2}, -\frac{N\ell}{2}+1, \ldots, \frac{N\ell}{2},$$

together with their multiplicities. The same spectrum is obtained for $\mathcal{P}(M_1)$ and $\mathcal{P}(M_2)$.

For $N=1$ and a given negative $\kappa \in \mathbb{Z}$, we see that the Hilbert space $\mathcal{H}_{\mathcal{P}}$ yields the irreducible (projective) $(\ell+1)$-dimensional representation of SO(3) through the action of the generators M_j^{red}. The situation here is exactly equivalent to the geometric quantization of the spin degrees of freedom of a particle of spin $\ell/2$, which are described classically by a two-sphere of half-integer radius $\ell/2$ and the standard Fubini–Study symplectic form. More generally, for any N, it follows from (80) that the representation of SO(3) carried by $\mathcal{H}_{\mathcal{P}}$ is the Nth symmetric power $\text{Sym}^N(\ell + \mathbf{1})$; notice that ℓ itself depends on N. This indicates once again that the vortices in our model can be regarded as interacting bosons, as we have put forward in Sec. VII. It is worthwhile to emphasize how our approach differs from the usual treatment of a system of indistinguishable bosons in quantum mechanics. In the latter context, the N-particle sector of the Fock space is constructed as the Nth symmetric power of the Hilbert space of a single particle. In our situation, the N-particle sector is constructed directly from the quantization of a classical N-particle phase space.

IX. DISCUSSION

In this paper, we have investigated an effective quantization of Manton's model of first-order Chern–Simons vortices on a sphere Σ of radius R. We have seen that the nontrivial topology of the space manifold leads to the integer constraints (4) and (7) on the parameters γ and μ in the Lagrangian. The periodic motion in the classical field theory was reduced to a Hamiltonian system on the moduli space of N vortices imposing the condition $\gamma = \mu$. At the self-duality point $\lambda = 1$, the effective dynamics is frozen, whereas for $\lambda \simeq 1$ the vortices move slowly, preserving their energy and angular momenta. The energy is purely potential and depends on the relative position of the vortices only.

The angular momenta along the three Cartesian axes have been computed in Sec. V, both for the field theory and the reduced dynamics, and the two results were shown to be consistent. In the latter context, the expressions for the angular momenta can be simplified using the relations (47) and (48) for the functions b_r, which we derived from rotational symmetry. The angular momenta along the three independent directions fit together to form a moment map $\mathbf{M}^{\text{red}}$ which we can regard as taking values in an $\text{so}(3)^* \cong \mathbb{R}^3$ where the sphere Σ is embedded. The direction of the vector $\mathbf{M}^{\text{red}}$ gives a point on the sphere that can be interpreted as the center of mass of the configuration of N vortices. Notice that there is no natural notion of centroid for a configuration of N points on a sphere (unless they lie on the same great circle and are not equidistant). We might be tempted to define it for generic configurations as the direction of the sum of the points, regarded as vectors in an $\mathbb{R}^3$ containing the sphere. (This definition is better behaved if we replace the target

sphere by the elliptic plane by identifying antipodal points.) For a configuration of vortices, this centroid does not coincide with the direction of the angular momentum, as can be seen from our formula for $\mathbf{M}^{\mathrm{red}}$ in (55)–(57). We believe that, for configurations where the vortices are not symmetrically distributed, the areas of the sphere where vortices are most close together give a contribution to the angular momentum which is smaller than the one corresponding to taking the sum of the vortex positions; this is based on the fact that the total angular momentum of N coincident vortices is proportional to $N(R^2-N)$ rather than to N, as was shown at the end of Sec. V B. On the plane,[19] the total linear momentum in Manton's model is proportional to the ordinary centroid in $\mathbb{R}^2$ of the positions of the vortices.

A rather unexpected feature of the analysis in Sec. V is that the angular momentum of a given number of vortices grows with the square of the radius R of the sphere. In the limit where the vortices are kept close together and $R\to\infty$, the modulus of the angular momentum blows up, and it was found necessary to subtract the constant $2\pi\gamma NR^2$, which becomes infinite in the limit, in order to compare it with the angular momentum of the system of vortices on the plane. This constant was seen to be related to the central charge for the linear momentum Poisson algebra for Manton's model on the plane.

The geometric quantization of the reduced model is rather straightforward to set up. The prequantum line bundle is uniquely determined by the Kähler structure on the moduli space defined by the kinetic energy term. To construct it, we made use of an argument of Manton[14] to obtain the cohomology class of Samols' Kähler two-form on the moduli space of Bogomol'nyĭ vortices, which appears in the study of the Abelian Higgs model. It is presumed that the quantum system we have obtained approximates a finite truncation of the quantum field theory, in which most of the excitations are kept in the ground state. However, it is not clear how one should assess the validity of this approximation. For $\lambda=1$, the quantization of the reduced system yields a single degenerate energy level; this degeneracy is lifted when the potential becomes nontrivial, and in principle its spectrum can be determined using degenerate perturbation theory. In Sec. VII, we have computed the dimension of the quantum Hilbert space and it was shown that it approaches Gibbs' estimate for the number of quantum states, as determined by the volume of the moduli space, in the classical limit of large Chern–Simons coefficient. Another result which comes from the analysis of the quantized effective system is that the solitons in the model should be interpreted as interacting bosons with the characteristic size 4π, as explained in Sec. VII. The bosonic character of the vortices is also apparent from the analysis of the representations of $\mathrm{SO}(3)$ arising in the algebra of the quantum angular momentum operators. In Sec. VIII, we found that for N vortices the Hilbert space is the N-fold symmetric product of an irreducible representation of $\mathrm{SO}(3)$. This irreducible representation is the same as the one obtained from quantizing a single vortex on a sphere whose area is the one of the original sphere minus the total area occupied by N vortices.

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Semiclassical Coulomb differential excitation function: Asymptotic expansions

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We have obtained asymptotic expansions of the electric dipole ($E1$) *differential* excitation function for large values of the adiabaticity parameter ξ and for all values of the eccentricity (ε) of the projectile orbit. To accomplish this, we have developed a new asymptotic power series of exponential integrals related to the Airy integrals, introduced originally in a paper by Brussaard *et al.* [Ann. Phys. (N.Y.) **7**, 47 (1962)], in which asymptotic expansions of the *total* excitation function were derived. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379067]

I. INTRODUCTION

In the semiclassical treatment of the Coulomb excitation of positive ions[1,2] by nuclei, the incoming particle is assumed to follow a classical positive energy (Rutherford) orbit, while the excitation of the ion is handled using the techniques of first-order, time-dependent perturbation theory on the resulting time-varying Coulomb field. Expanding the interaction in multipoles and neglecting the penetration of the projectile into the target results, for each multipole order λ, in a problem which factors into two parts—a factor solely dependent on the properties of the target in question, which controls the strength of the interaction, and a differential excitation function $\mathrm{d}f_{E\lambda}(\varepsilon,\xi)/d\Omega$, which determines the angular distribution of the scattered projectile.

In the electric dipole ($E1$) case, the semiclassical Coulomb *differential* excitation function is expressible in the closed form,[3]

$$\frac{\mathrm{d}f_{E1}(\varepsilon,\xi)}{d\Omega}=\frac{\pi}{18}\varepsilon^4\{I^2_{1,-1}(\varepsilon,\xi)+I^2_{1,1}(\varepsilon,\xi)\}$$

$$=\frac{4\pi}{9}\xi^2\varepsilon^2\exp(\pm\pi|\xi|)\{(\varepsilon^2-1)K^2_{\mathrm{i}\xi}(|\xi|\varepsilon)+\varepsilon^2K'^2_{\mathrm{i}\xi}(|\xi|\varepsilon)\}, \tag{1.1}$$

for ξ finite. The Coulomb integrals are given by[4]

$$I_{1,\pm1}(\varepsilon,\xi)=-2\xi\exp(\pm\tfrac{1}{2}\pi|\xi|)[K'_{\mathrm{i}\xi}(|\xi|\varepsilon)\pm(1-\varepsilon^{-2})^{1/2}K_{\mathrm{i}\xi}(|\xi|\varepsilon)], \tag{1.2}$$

where the $(\pm)$ sign in the exponential correspond to attractive and repulsive potentials, respectively, $K_\nu(z)$ is the modified Bessel function and $K'_\nu(z)$ is its derivative with respect to its argument. The eccentricity ε of the hyperbolic orbit is related to the deflection angle θ of the projectile by $\varepsilon=\sin(\theta/2)^{-1}$. The nondimensional adiabaticity parameter ξ is defined by

$$\xi=Z_1Z_2\sqrt{\frac{M}{(E_i/Ry)}}[(E_i/E_f)^{1/2}-1], \tag{1.3}$$

where the indices *i* and *f* refer to the initial and the final states, respectively, E_i is the initial kinetic energy of relative motion, with Ry standing for rydberg (about 13.8 eV), Z_1 and Z_2 are the charge numbers of the projectile and the atomic system, M is the reduced mass of the system in electron mass units.

For heavy ions and $E_f \to 0$ (threshold energy), $\xi \to \infty$. The complexity of the way in which both the argument ($|\xi|\varepsilon$) and the order ($i\xi$) go to infinity simultaneously, without one being significantly larger than the other, results in a paucity of asymptotic expressions, valid over all angles. Only for ε very large ($\theta \approx 0$), or $\varepsilon \approx 1 (\theta \approx \pi)$, can an asymptotic expression from Ref. 5 be adequately applied.

In Ref. 6, the authors make use of a modification of the saddle-point method to obtain a large-ξ asymptotic expansion for the semiclassical Coulomb integrals, which is used to derive an asymptotic expression for the *total* excitation functions $f_{E\lambda}(\xi)$. Their method, however, can not be directly applied to the case of *differential* excitation functions $df_{E\lambda}(\varepsilon,\xi)/d\Omega$, since they make use of the stretched variable $\xi^{-1/3}\sqrt{\varepsilon^2-1}$, which limits the possibilities for evaluation of the final result to angles very near the backwards-scattering direction. In this section, we modify their result, sacrificing uniform validity of the resulting expansion, to obtain an asymptotic form for the semiclassical differential excitation function useful for large ξ in the $E1$ case, provided θ is not near π. We then apply the method of Ref. 6 more directly to obtain expressions when $\theta = \pi$ and $\theta \to \pi$.

Note that, because of our extensive use of results from Ref. 6, we use the convention of these authors in our definition of the semiclassical Coulomb integrals.

We used the symbolic computation program MAPLE VI (Ref. 7) to help us with the algebraic manipulations in this work.

II. METHOD OF STEEPEST DESCENTS

For the sake of clarity, we go over the details and principles involved in the method of steepest descents,[8] sketched briefly in Ref. 6. The semiclassical Coulomb integrals in the form applied in Ref. 6 are

$$I_{\lambda,\mu}(\varepsilon,\xi) = \int_{-\infty}^{\infty} e^{-i\xi(\varepsilon \sinh w + w)} \frac{[\cosh w + \varepsilon - i\sqrt{\varepsilon^2-1}\sinh w]^{\mu}}{[\varepsilon \cosh w + 1]^{\lambda+\mu}} dw, \tag{2.1}$$

where λ and μ are the quantum numbers describing the multipole transition.

In the $E1$ case, this expression simplifies to

$$I_{1,\pm 1}(\varepsilon,\xi) = \int_{-\infty}^{\infty} e^{-i\xi(\varepsilon \sinh w + w)} \frac{1}{\cosh w + \varepsilon \pm i\sqrt{\varepsilon^2-1}\sinh w} dw, \tag{2.2}$$

where we have used the identity,

$$(\varepsilon \cosh w + 1)^2 = (\varepsilon + \cosh w + i\sqrt{\varepsilon^2-1}\sinh w)(\varepsilon + \cosh w - i\sqrt{\varepsilon^2-1}\sinh w), \tag{2.3}$$

to simplify the result.

In the method of steepest descents, we divide the integrand up into an exponential function $\exp[\xi f(w)]$ and a slowly varying part $h_{\lambda,\mu}(w)$. Let $f(w) = -i(\varepsilon \sinh w + w)$ and $h_{\lambda,\mu}(w) = (\cosh w + \varepsilon \pm i\sqrt{\varepsilon^2-1}\sinh w)^{-1}$, which puts (2.1) in the standard form

$$I_{\lambda,\mu}(\varepsilon,\xi) = \int_{-\infty}^{\infty} e^{\xi f(w)} h_{\lambda,\mu}(w) dw. \tag{2.4}$$

The principle to be applied here is that, for large ξ, the most important part of the integral comes from a region of the integrand around the point where $\mathrm{Re}\, f(w)$ is at a maximum. For large ξ, the exponential factor will cause this region of the integrand to become larger than any other part.

Working against this effect, however, are the effects of the imaginary part of $f(w)$. As ξ becomes large, $\mathrm{Im}\, f(w)$ results in rapid oscillations, which integrate to zero. The result is that regions where $\mathrm{Im}\, f(w)$ changes most slowly are preferentially represented in the integral. Failure

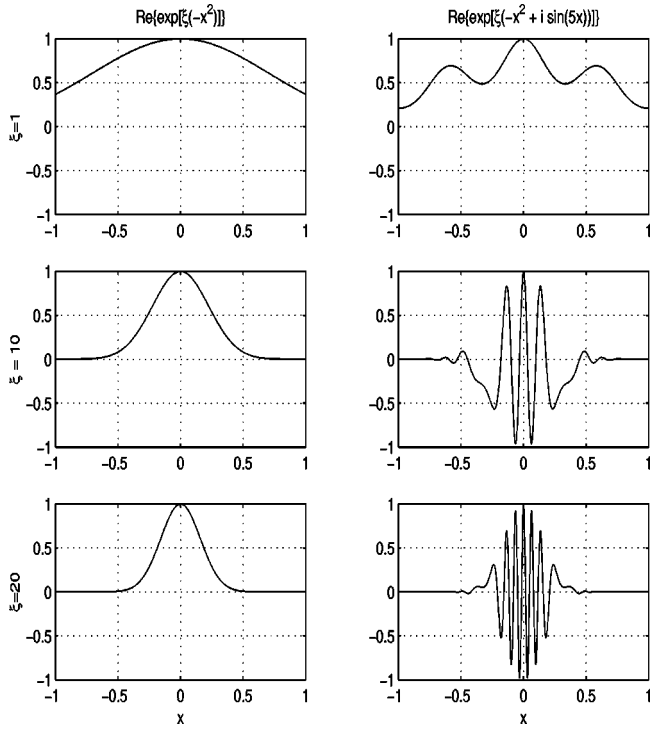

FIG. 1. Principle to be applied in the method of steepest descent. If the exponentiated function is purely real, the region around a maximum of this function becomes the most important part of the integral as $\xi\to\infty$. If it has an imaginary part, however, rapid oscillations eat into the peak as $\xi\to\infty$ and it is no longer obvious where the most important part of the integral is.

to resolve these two, possibly conflicting, influences can result in the difficulties shown in Fig. 1. To maximize the effect of Re $f(w)$, and minimize the effect of the oscillations caused by Im $f(w)$, we analytically extend $f(w)$ into the complex plane and make use of Cauchy's theorem to distort the path of integration through a stationary point of $f(w)$. Since $f(w)$ is analytic, the Cauchy–Riemann equations guarantee that both the real and imaginary parts of $f(w)$ are harmonic, and thus, must have a saddle point at this point.

We pick the path through the saddle point where Im $f(w)$ is constant and Re $f(w)$ decreases most rapidly on moving away from the saddle point. This choice, if it is possible to make it, amplifies the maximizing effect associated with Re $f(w)$, while minimizing the effect of the rapid oscillations resulting from Im $f(w)$.

In the case at hand, the stationary points are where $f'(w)=0$, or

$$\cosh w_0 = -\frac{1}{\varepsilon}. \tag{2.5}$$

We use the Eqs. (4.6.9), (4.6.12), and (4.5.8) of Ref. 9, and the triangle (see Fig. 2) to obtain

$$w_0 = \pm \mathrm{i}\arccos\left(\frac{1}{\varepsilon}\right) + (2k\mp 1)\pi\mathrm{i} = \pm \mathrm{i}\arctan(s) + (2k\mp 1)\pi\mathrm{i}, \tag{2.6}$$

where $s=\sqrt{\varepsilon^2-1}$. If we choose the plus sign and $k=0$, we obtain the saddle point we will use in this expansion. We will see that this choice allows us to avoid the complications associated with distorting the path of integration through a pole of the integrand. We want to verify that the saddle point we have selected, viz.,

$$w_0 = -\pi\mathrm{i} + \mathrm{i}\arctan(s), \tag{2.7}$$

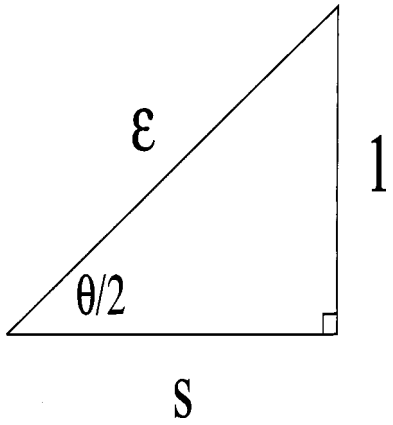

FIG. 2. Triangle used to deduce $\arccos(1/\varepsilon)=\arctan(s)$.

admits a path of steepest descent into which the real axis may be deformed. We notice that $\mathrm{Im}(f(w_0))=0$, so our path of integration must satisfy, for all $w=x+iy$,

$$0=\mathrm{Im}(f(w))=-\varepsilon\,\mathrm{Re}(\sinh w)-\mathrm{Re}(w)=-\varepsilon\,\sinh(x)\cos(y)-x, \tag{2.8}$$

whose solution is $x\equiv 0$, or

$$\cos(y)=\frac{-x}{\varepsilon\,\sinh(x)},$$

$$\begin{aligned} y&=\pm\arccos\left(-\frac{x}{\varepsilon\,\sinh(x)}\right)+2k\pi \\ &=\pm\arccos\left(\frac{x}{\varepsilon\,\sinh(x)}\right)+(2k\mp 1)\pi. \end{aligned} \tag{2.9}$$

Note that the imaginary part of $f(w)$, being zero along this path, means that we have not only reduced, but have in fact eliminated, the effect of oscillations for large ξ.

Along this path,

$$\lim_{x\to 0} y=\pm\arccos\left(\frac{1}{\varepsilon}\right)+(2k\mp 1)\pi, \tag{2.10}$$

which gives our w_0, if we select the positive sign and $k=0$,

$$y=\arccos\left(\frac{x}{\varepsilon\,\sinh(x)}\right)-\pi. \tag{2.11}$$

For this path, we have that $\lim_{x\to-\infty} y=-(\pi/2)$ for all ε. Because of this, along the path

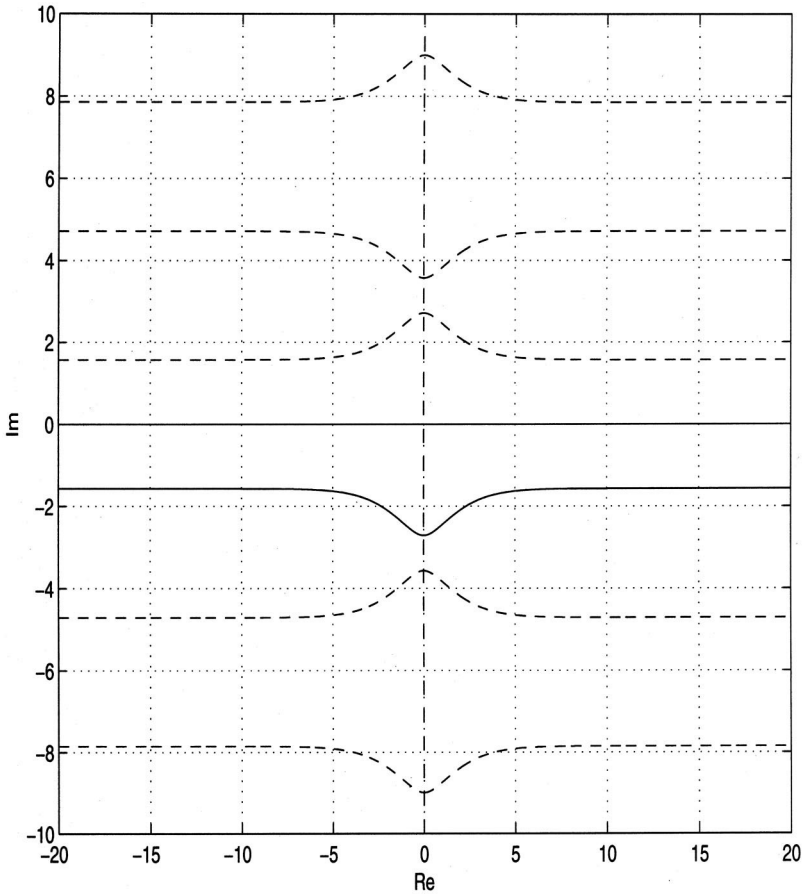

FIG. 3. Paths of steepest descent/ascent. The path that we use is plotted as a solid line, as is the real axis, while all others are plotted as dashed lines. $\varepsilon = 1.1$ in this figure.

$$\mathrm{Re}(f(w)) = \varepsilon \cosh(x)\sin(y) + y \to -\varepsilon \cosh(x) - \frac{\pi}{2} \to -\infty, \tag{2.12}$$

as $x \to \infty$. This confirms that the path we have chosen is a path of steepest descent (rather than one of steepest *ascent*), and also that the tails of the integrand (for a well-enough behaved $h_{\lambda,\mu}$) will decay exponentially, guaranteeing convergence of the integral in that regard.

This path is illustrated in Fig. 3.

We are now justified in expanding the integrand around this point. Letting $w = w_0 + \omega$,

$$\begin{aligned} f(w) &= -\mathrm{i}\varepsilon \sinh(w_0+\omega) - \mathrm{i}(w_0+\omega) \\ &= -\mathrm{i}\varepsilon[\sinh(w_0)\cosh(\omega) + \cosh(w_0)\sinh(\omega)] - \mathrm{i}(w_0+\omega) \\ &= -\mathrm{i}w_0 - \mathrm{i}\omega - s\cosh(\omega) + \mathrm{i}\sinh(\omega) \\ &= -\pi - [s - \arctan(s)] + \left[\mathrm{i}\left(\frac{\omega^3}{3!} + \frac{\omega^5}{5!} + \cdots\right) - s\left(\frac{\omega^2}{2!} + \frac{\omega^4}{4!} + \cdots\right)\right]. \end{aligned} \tag{2.13}$$

Similarly, we expand the parts of the slowly-varying part of the integrand,

$$\cosh w+\varepsilon+\mathrm{i}s\sinh w=\frac{1}{\varepsilon}\left\{2s^2+(-1+s^2)\left(\frac{\omega^2}{2!}+\frac{\omega^4}{4!}+\cdots\right)-2\mathrm{i}s\left(\omega+\frac{\omega^3}{3!}+\cdots\right)\right\}, \quad (2.14)$$

$$\cosh w+\varepsilon-\mathrm{i}s\sinh w=-\varepsilon\left\{\frac{\omega^2}{2!}+\frac{\omega^4}{4!}+\cdots\right\}, \quad (2.15)$$

$$\varepsilon\cosh w+1=-\left\{\frac{\omega^2}{2!}+\frac{\omega^4}{4!}+\cdots\right\}-\mathrm{i}s\left\{\omega+\frac{\omega^3}{3!}+\cdots\right\}. \quad (2.16)$$

The normal procedure of evaluating integrals of the form,

$$\int_c e^{-\xi f(x)}g(z)\mathrm{d}z, \quad (2.17)$$

by introducing a variable of integration along the new path of integration, fails here due to the presence of poles in the slowly-varying part of the integrand at the saddle point. The procedure used in Ref. 6 allows us to circumvent this problem.

After the distortion of the path of integration and the expansion about w_0 the integral becomes

$$I_{\lambda,\mu}(s,\xi)=e^{-\pi\xi}\exp[-\xi(s-\arctan s)]\int_{-\infty}^{\infty}\exp\left[\xi\left(-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}-\cdots\right)\right]h_{\lambda,\mu}(s,\omega)\mathrm{d}\omega. \quad (2.18)$$

The exponential term inside the integral gives an exponentially decaying factor ($\exp[-\xi s\omega^2/2]$) and an oscillatory factor ($\exp[\mathrm{i}\xi\omega^3/6]$). In order to have a Gaussian form for the integrand, we need the decaying factor to decay almost to zero, before the first root of the real part of the oscillatory factor (we do not worry about the imaginary part, since it is odd in ω and disappears upon integration anyway). Since the first such root is of order $\xi^{-(1/3)}$, when, s, which controls the rate of decay, becomes smaller than or comparable to $\xi^{-(1/3)}$, the integrand is no longer nearly Gaussian and has significant side lobes, as seen in Fig. 4.

The most significant part of the integral comes from the central lobe of the integrand, a neighborhood of $\omega=0$ with width of order $\xi^{-(1/3)}$. To stretch this region to a uniform width for all ξ, and to help isolate the powers of ξ to be used in the expansion, we perform the scale transformation $s\to s\xi^{-(1/3)}, \omega\to\omega\xi^{-(1/3)}$. Retaining the first two terms in the exponential and expanding the remainder gives

$$I_{\lambda,\mu}(s\xi^{-(1/3)},\xi)=e^{-\pi\xi}\exp[-\xi(s\xi^{-(1/3)}-\arctan(s\xi^{(-1/3)}))]\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\exp\left[\xi^{-(2/3)}\left(-s\frac{\omega^4}{4!}+\mathrm{i}\frac{\omega^5}{5!}\right)+\cdots\right]h_{\lambda,\mu}(s\xi^{-(1/3)},\omega\xi^{-(1/3)})\xi^{-(1/3)}\mathrm{d}\omega. \quad (2.19)$$

Note that, unlike Ref. 6, we do not expand the arctangent in the exponential outside the integral, although we notice that the argument of this exponential stays finite, but nonzero, as $\xi\to\infty$, due to the cancellation of the first term in the Maclaurin series for the arctangent.

As was pointed out in Ref. 6, this transformation shows, that the appropriate expansion parameter is $u=\xi^{-(2/3)}$.

With the scale transformation in place, the components of the slowly-varying part transform as

$$\cosh w+\varepsilon+\mathrm{i}s\sinh w\to-\frac{u}{\varepsilon}\left[\frac{1}{2}(\omega^2+4\mathrm{i}s\omega-4s^2)\right]$$

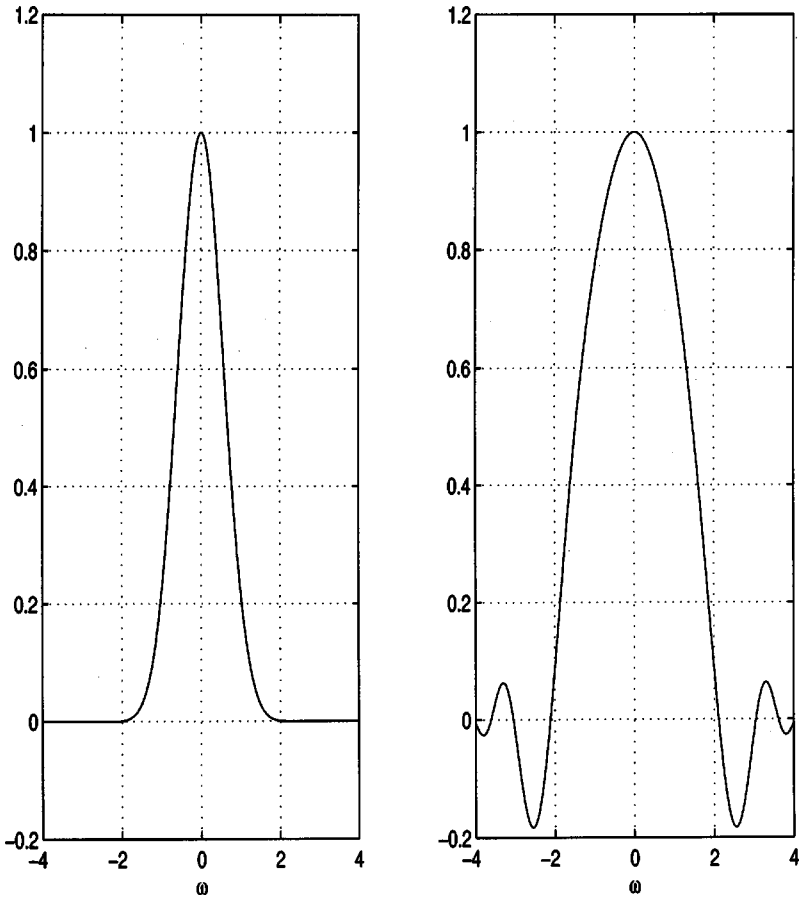

FIG. 4. Exponential factor in the integrand of Eq. (2.18). In the plot on the left ($\xi=1$, $s=3$) the decaying factor decays almost to zero before the oscillatory part has its first root resulting in a nearly Gaussian curve. In the plot on the right ($\xi=1$, $s=0.5$) the oscillatory part has several oscillations before the decaying part decays significantly resulting in several significant side lobes.

$$-\frac{u}{\varepsilon}\sum_{n=2}^{\infty}\frac{\omega^{2n-2}}{(2n)!}[\omega^2+4n\mathrm{i}s\omega-2n(2n-1)s^2]u^{n-1}, \tag{2.20}$$

$$\cosh w+\varepsilon-\mathrm{i}s\sinh w\rightarrow-u\varepsilon\sum_{n=1}^{\infty}\frac{\omega^{2n}}{(2n)!}u^{n-1}. \tag{2.21}$$

We have not expressed ε explicitly in terms of s, since at the end we will reverse the scale change anyway. However, it is important to realize that the scale change has affected ε, via its dependence on s through the relation $\varepsilon=\sqrt{s^2+1}\rightarrow\sqrt{s^2\xi^{-(2/3)}+1}$.

These transformed relations indicate that u is definitely the correct expansion parameter and that the integrands will consist of integral powers of ω and $\omega+2\mathrm{i}s$ modulated by the exponential factor $\exp[-s\omega^2/2-\mathrm{i}\omega^3/6]$. Brussaard *et al.*[6] introduced the following integral expressions:

$$Q_{k,m}(s)=\mathrm{i}^{-k-m}\int_{-\infty}^{\infty}\exp\left(-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right)\omega^k(\omega+2\mathrm{i}s)^m\mathrm{d}\omega, \tag{2.22}$$

which appear in the coefficients of the asymptotic expressions. It is necessary to derive some properties of these functions to aid in their evaluation. An extensive analysis of the properties and

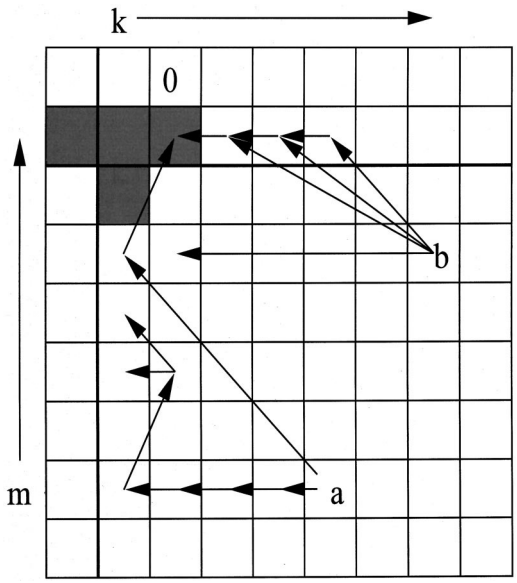

FIG. 5. Use of the recurrence relations to reduce the $Q_{k,-m}$ for $k,m>0$. If $k\leqslant m$ (a) we apply (A13) to express it in terms of $Q_{k,-m}$s with smaller k and then use (A4) to increase $-m$. If $k>m$ (b) we use the division algorithm on the integrand to express it in terms of the previous case and several $Q_{k,m}$ with $m=0$ which are handled easily using (A9)–(A11).

power series expansions of the $Q_{k,m}(s)$ are given in the Appendix. Notice that, in addition to the ascending power series provided by Ref. 6, which gives a good approximation for small values of s, in order to obtain an expression for the *differential* excitation function, we need asymptotic expressions valid for large s as well. Using a slight modification of an extension to Watson's lemma provided in Ref. 10 (p. 24ff) allows us to obtain an asymptotic power series for the four basic integrals $Q_{1,0}(s)$, $Q_{0,0}(s)$, $Q_{-1,0}(s)$, and $Q_{0,-1}(s)$.

III. SEMICLASSICAL COULOMB INTEGRALS

While the $Q_{k,m}(s)$ expressions, obtained using the stretched variable $s\xi^{-(1/3)}$ in Ref. 6, are useful for obtaining *total* excitation functions in the large-ξ limit (the dependence on the stretched variable is integrated out), reversing the scale change to obtain $I_{1,\pm1}(s,\xi)$ from $I_{1,\pm1}(s\xi^{-(1/3)},\xi)$, in order to obtain an expression for the differential excitation functions, proves to be much more difficult.

For very large ξ, we find that we must substitute a large value of s (i.e., make the inverse transformation $s\rightarrow s\xi^{1/3}$) in order to obtain a result for a moderate scattering angle. For this reason, we must consider s to be an asymptotically large variable, growing like $\xi^{1/3}$. Unfortunately, performing the expansion in *ascending* powers of s results in expansion coefficients that contain positive powers of s, in addition to the negative powers of ξ. As a result, we no longer have a guarantee, as we did for moderate s, that the terms decrease in size as $\xi\rightarrow\infty$. That is, we do not know, after truncating to two terms, that some higher term will not become more significant, as $\xi\rightarrow\infty$, due to a large power of s in the coefficient.

Instead, we will perform the expansion in negative powers of s, ensuring that the terms will be decreasing in size, as both ξ and s increase.

A. Orbital integrals $I_{1,+1}(s,\xi)$

We begin with the more complicated $\lambda=1$, $\mu=+1$ integral. Applying the inversion formula (Ref. 11, Sec. 20),

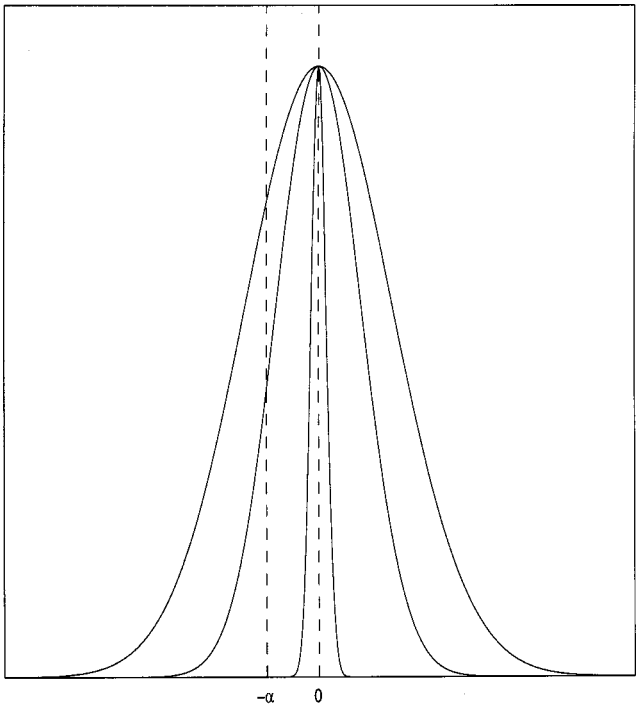

FIG. 6. Modulation factor of the integral (A34), e^{-xt^2}. If we select $-\alpha$ as our lower bound, no matter how small α is, for large enough x most of the integral is included. If we select 0 as our lower bound, only half of the integral is included no matter how large x is.

$$\left[\sum_{n=1}^{\infty} a_n u^{n-1}\right]^{-1} = \frac{1}{a_1} - \frac{a_2}{a_1^2}u + \left(\frac{a_2^2 - a_1 a_3}{a_1^3}\right)u^2 + \cdots, \tag{3.1}$$

to Eq. (2.20), gives the coefficients,

$$\frac{1}{a_1} = \frac{2}{(\omega + 2\mathrm{i}s)^2}\left(-\frac{\varepsilon}{u}\right), \tag{3.2}$$

$$-\frac{a_2}{a_1^2} = -\frac{2}{(\omega+2\mathrm{i}s)^2}\left[\frac{2}{4!}\frac{\omega^2(\omega+2\mathrm{i}s)(\omega+6\mathrm{i}s)}{(\omega+2\mathrm{i}s)^2}\right]\left(-\frac{\varepsilon}{u}\right)$$

$$= -\frac{1}{2}\frac{\omega^2}{(\omega+2\mathrm{i}s)^2}\left[1 + \frac{1}{3}\mathrm{i}\omega\frac{1}{s} - \frac{1}{6}\omega^2\frac{1}{s^2} - \cdots\right]\left(-\frac{\varepsilon}{u}\right), \tag{3.3}$$

$$\frac{a_2^2 - a_1 a_3}{a_1^3} = \frac{2}{(\omega+2\mathrm{i}s)^2}\left[\frac{\frac{1}{240}\omega^8 + \frac{1}{15}\mathrm{i}\omega^7 s - \frac{23}{60}\omega^6 s^2 - \frac{13}{15}\mathrm{i}\omega^5 s^3 + \frac{1}{6}\omega^4 s^4}{(\omega+2\mathrm{i}s)^4}\right]\left(-\frac{\varepsilon}{u}\right)$$

$$= \frac{1}{12}\frac{\omega^4}{(\omega+2\mathrm{i}s)^2}\left[1 + \frac{7}{10}\mathrm{i}\omega\frac{1}{s} - \frac{19}{40}\omega^2\frac{1}{s^2} + \cdots\right]\left(-\frac{\varepsilon}{u}\right). \tag{3.4}$$

This gives the following expansion for the slowly varying part of the integrand in negative powers of ξ (positive powers of u) and s:

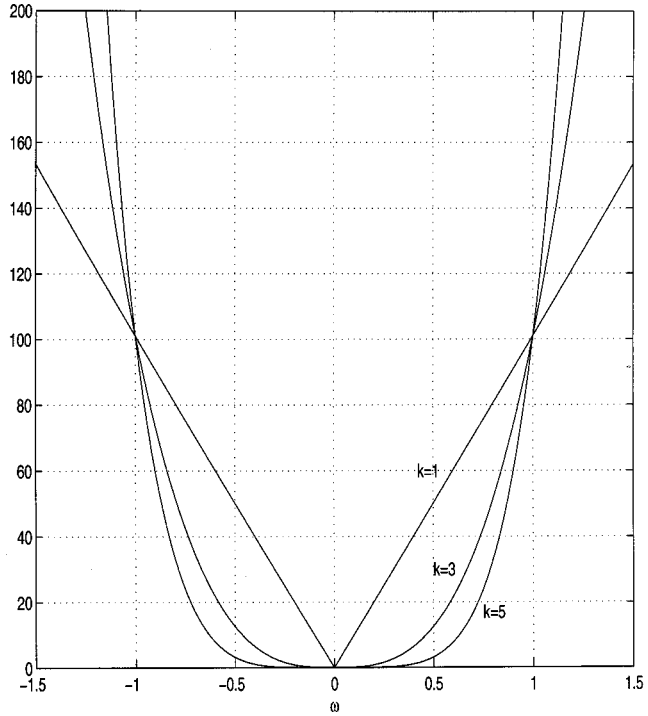

FIG. 7. Magnitude of the slowly-varying part of the integrand of Eq. (A48), $|\omega^k(\omega+2\mathrm{i}s)^m|$. As k gets larger, the slowly-varying part of the integrand is pushed out of the central part of the integral—all-important for large s—by the factor of ω^k. In this figure, $s=5$ and $m=2$.

$$h_{1,+1}(s\xi^{-(1/3)},\omega\xi^{-(1/3)})\sim-\frac{\varepsilon}{u}\left\{\frac{2}{(\omega+2\mathrm{i}s)^2}-\frac{1}{2}\frac{\omega^2}{(\omega+2\mathrm{i}s)^2}\left[1+\frac{1}{3}\mathrm{i}\omega\frac{1}{s}-\frac{1}{6}\omega^2\frac{1}{s^2}+\cdots\right]u\right.$$
$$\left.+\frac{1}{12}\frac{\omega^4}{(\omega+2\mathrm{i}s)^2}\left[1+\frac{7}{10}\mathrm{i}\omega\frac{1}{s}-\frac{19}{40}\omega^2\frac{1}{s^2}+\cdots\right]u^2\right\}. \tag{3.5}$$

We must now expand the exponential factor in the integral. Unlike the slowly-varying part, there is no convenient way to expand this factor as a descending power series in s, so we must settle for an ascending series. As we shall see, this compromise is an added complication, but not a fatal flaw in the technique,

$$\exp\left[\sum_{n=1}^{\infty}\left(-s\frac{\omega^{2n+2}}{(2n+2)!}+\mathrm{i}\frac{\omega^{2n+3}}{(2n+3)!}\right)u^n\right]$$
$$=\exp\left[\left(-s\frac{\omega^4}{4!}+\mathrm{i}\frac{\omega^5}{5!}\right)u+\left(-s\frac{\omega^6}{6!}+\mathrm{i}\frac{\omega^7}{7!}\right)u^2+\cdots\right]$$
$$\sim1+u\omega^4\left(-\frac{1}{24}s+\frac{1}{120}\mathrm{i}\omega\right)+u^2\omega^6\left[\left(\frac{\mathrm{i}\omega}{5040}-\frac{\omega^4}{28800}\right)\right.$$
$$\left.+\left(-\frac{1}{720}-\frac{\mathrm{i}\omega^3}{2880}\right)s+\frac{\omega^2}{1152}s^2\right]. \tag{3.6}$$

An important thing to realize about this expansion is that each term contains only powers of

s less than or equal to the corresponding power of u. When the scattering angle is held fixed, s grows like $\xi^{1/3}$. Since u decays like $\xi^{-(2/3)}$, this fact ensures that every positive power of s is cancelled asymptotically.

Now, forming the product of these terms, we obtain

$$\begin{aligned}
&\exp\left[\sum_{n=1}^{\infty}\left(-s\frac{\omega^{2n+2}}{(2n+2)!}+\mathrm{i}\frac{\omega^{2n+3}}{(2n+3)!}\right)u^n\right]h_{1,+1}(s\xi^{-(1/3)},\omega\xi^{-(1/3)})\\
&\quad\sim\frac{-\varepsilon}{u}\left\{\frac{2}{(\omega+2\mathrm{i}s)^2}+u\left[-\frac{1}{2}\frac{\omega^2}{(\omega+2\mathrm{i}s)^2}\left(1+\frac{1}{3}\mathrm{i}\omega\frac{1}{s}-\frac{1}{6}\omega^2\frac{1}{s^2}+\cdots\right)\right.\right.\\
&\qquad\left.+2\frac{\omega^4}{(\omega+2\mathrm{i}s)^2}\left(-\frac{1}{24}s+\frac{1}{120}\mathrm{i}\omega\right)\right]+u^2\left[\frac{1}{12}\frac{\omega^4}{(\omega+2\mathrm{i}s)^2}\left(1+\frac{7}{10}\mathrm{i}\omega\frac{1}{s}-\frac{19}{40}\omega^2\frac{1}{s^2}+\cdots\right)\right.\\
&\qquad+\frac{2\omega^6}{(\omega+2\mathrm{i}s)^2}\left(\left(\frac{\mathrm{i}\omega}{5040}-\frac{\omega^4}{28800}\right)+\left(-\frac{1}{720}-\frac{\mathrm{i}\omega^3}{2880}\right)s+\frac{\omega^2}{1152}s^2\right)\\
&\qquad\left.\left.-\frac{1}{2}\frac{\omega^6}{(\omega+2\mathrm{i}s)^2}\left(1+\frac{1}{3}\mathrm{i}\omega\frac{1}{s}-\frac{1}{6}\omega^2\frac{1}{s^2}+\cdots\right)\left(-\frac{1}{24}s+\frac{1}{120}\mathrm{i}\omega\right)\right]\right\}. \qquad (3.7)
\end{aligned}$$

After multiplying by the common exponential factor, and integrating with respect to ω, we find

$$\begin{aligned}
&\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\exp\left[\sum_{n=1}^{\infty}\left(-s\frac{\omega^{2n+2}}{(2n+2)!}+\mathrm{i}\frac{\omega^{2n+3}}{(2n+3)!}\right)u^n\right]\\
&\quad\times h_{1,+1}(s\xi^{-(1/3)},\omega\xi^{-(1/3)})\xi^{-(1/3)}d\omega\\
&\quad\sim\frac{\varepsilon}{u}\xi^{-(1/3)}\left\{2Q_{0,-2}(s)+u\left[-\frac{s}{12}Q_{4,-2}(s)-\frac{1}{60}Q_{5,-2}(s)+\frac{1}{2}Q_{2,-2}(s)-\frac{1}{6s}Q_{3,-2}(s)\right.\right.\\
&\qquad\left.\left.+\frac{1}{12s^2}Q_{4,-2}(s)+\cdots\right]+u^2\left[\frac{s^2}{576}Q_{8,-2}(s)+\cdots\right]\right\}, \qquad (3.8)
\end{aligned}$$

where terms of low order in s are omitted.

It is not yet, however, a foregone conclusion that the first term in the expansion is asymptotically the largest, since in addition to the complication added by the positive powers of s, each of the $Q_{k,m}(s)$ decays at a different rate. Analysis is still required to determine the correct method of truncating this expansion.

Firstly, we realize that the relationship between the powers of u and s, noted in the expansion of the exponential factor, namely, that the highest power of s in the coefficient of u^n is equal to n, carries over to this expansion as well, which means that we can place asymptotic bounds on the contribution of later terms.

We note that, for large s and small u, the asymptotic order of the nth term [ignoring the asymptotic properties of the $Q_{k,m}(s)$] is $s^n u^n$. After performing the inverse scale change, $s \to s\xi^{1/3}$, and noting that $u=\xi^{-(2/3)}$, this order becomes $s^n\xi^{-(n/3)}$, for large ξ. So this factor, at least, decreases in size as n becomes larger.

Since, for all of the $Q_{k,m}(s)$ present in the expansion, $k>0$ and $m=-2$, by (A51) and (A52), we know that they all decay to zero as $s\to\infty$ at rate at least $s^{-(5/2)}\to s^{-(5/2)}\xi^{-(5/6)}$, so they cannot increase the asymptotic order of a term as $\xi\to\infty$.

This indicates that the contribution of the terms does, in fact, decrease as the series progresses. That is, for example, once the u^3 term is included, we know that we have the complete contribution of order ξ^{-1} and that no later term can give an asymptotic contribution larger than this.

This knowledge is sufficient to allow us to use the series (3.8) directly, without any further consideration, knowing that eventually, at least, the terms become asymptotically small. However, in the interests of efficiency, and since the coefficients are themselves infinite sums, we would like to isolate specifically the contribution from each power of ξ. We start by considering the constant term in Eq. (3.8) [see also Eq. (A41)],

$$2Q_{0,-2}(s)=Q_{1,0}(s)\sim\frac{\sqrt{2\pi}}{2}s^{-5/2}\quad\text{as}\quad s\to\infty,$$

$$2Q_{0,-2}(s\xi^{1/3})\sim\frac{\sqrt{2\pi}}{2}s^{-5/2}\xi^{-(5/6)}\quad\text{as}\quad\xi\to\infty. \tag{3.9}$$

This leading-order term attains the minimum possible decay rate as $s\to\infty$. Any contribution from the u^1 term must decay faster than this, since it also has to include the contribution from s and u, which must decay at least like $\xi^{-1/3}$.

To obtain a first-order correction to this result, we examine the higher-order asymptotic terms from the u^0 coefficient,

$$2Q_{0,-2}(s\xi^{1/3})\sim\sqrt{2\pi}\left[\frac{1}{2}s^{-5/2}\xi^{-(5/6)}-\frac{35}{48}s^{-11/2}\xi^{-(11/6)}\right]\quad\text{as}\quad\xi\to\infty. \tag{3.10}$$

To be part of the next-highest-order term, terms from the u^1 coefficient need to be of order $\xi^{-11/6}$ or higher. We examine each individually [see Eqs. (A51) and (A52)],

$$(s\xi^{1/3})uQ_{4,-2}(s\xi^{1/3})\sim\tfrac{3}{4}\sqrt{2\pi}s^{-7/2}\xi^{-11/6}\quad\text{as}\quad\xi\to\infty, \tag{3.11}$$

$$uQ_{5,-2}(s\xi^{1/3})\sim\tfrac{15}{4}\sqrt{2\pi}s^{-11/2}\xi^{-5/2}\quad\text{as}\quad\xi\to\infty, \tag{3.12}$$

$$uQ_{2,-2}(s\xi^{1/3})\sim-\tfrac{1}{4}\sqrt{2\pi}s^{-7/2}\xi^{-11/6}\quad\text{as}\quad\xi\to\infty, \tag{3.13}$$

$$\frac{u}{s\xi^{1/3}}Q_{3,-2}(s\xi^{1/3})\sim-\tfrac{3}{4}\sqrt{2\pi}s^{-11/2}\xi^{-5/2}\quad\text{as}\quad\xi\to\infty. \tag{3.14}$$

The terms from (3.11) and (3.13) contribute to the first-order correction.

The remaining terms from the u^1 coefficient we know do not contribute to the $\xi^{-11/6}$ term, since both the power of s they are divided by and the value of k increase from this point on in the series.

In the coefficient of the second-order term, the highest power of s is s^2, while all of the $Q_{k,m}$ have $k\geqslant 4$. Therefore, all of the terms must be asymptotically smaller than

$$u^2s^2Q_{4,-2}(s\xi^{1/3})\sim\tfrac{3}{4}\sqrt{2\pi}s^{-5/2}\xi^{-13/6}\quad\text{as}\quad\xi\to\infty, \tag{3.15}$$

meaning that none of these terms can contribute to the $\xi^{-11/6}$ term. Through similar reasoning, we see that higher-order terms in u can not contribute either.

Combining these terms, leads to the asymptotic expression [see also Eqs. (2.19) and (3.8)],

$$I_{1,+1}(s\xi^{-1/3},\xi)\sim\sqrt{2\pi}\xi^{1/3}e^{-\pi\xi}(1+s^2\xi^{-2/3})^{1/2}\exp[-\xi(s\xi^{-1/3}-\arctan(s\xi^{-1/3}))]$$
$$\times[\tfrac{1}{2}s^{-5/2}-\tfrac{35}{48}s^{-11/2}-\tfrac{3}{16}s^{-7/2}\xi^{-2/3}]\quad\text{as}\quad s\to\infty, \tag{3.16}$$

$$I_{1,+1}(s,\xi)\sim\sqrt{\frac{\pi}{2}}\,\xi^{-1/2}e^{-\pi\xi}s^{-5/2}(1+s^2)^{1/2}\exp[-\xi(s-\arctan(s))]$$
$$\times\left[1-\left(\frac{3}{8}+\frac{35}{24}s^{-2}\right)s^{-1}\xi^{-1}\right]\quad\text{as}\quad\xi\to\infty,\tag{3.17}$$

for the $\lambda=1$, $\mu=+1$ semiclassical Coulomb integral.

B. Orbital integrals $I_{1,-1}(s,\xi)$

Similar analysis of the $\mu=-1$ case is significantly easier, since the coefficients in the expansion of the slowly-varying part do not contain s.

Proceeding as before from

$$\cosh w+\varepsilon-\mathrm{i}s\sinh w\to-u\varepsilon\sum_{n=1}^{\infty}\frac{\omega^{2n}}{(2n)!}u^{n-1},\tag{3.18}$$

and applying the inversion formula (3.1) gives the coefficients

$$\frac{1}{a_1}=\frac{2}{\omega^2}\left(-\frac{1}{\varepsilon u}\right),\tag{3.19}$$

$$-\frac{a_2}{a_1^2}=-\frac{1}{6}\left(-\frac{1}{\varepsilon u}\right),\tag{3.20}$$

$$\frac{a_2^2-a_1a_3}{a_1^3}=\frac{1}{120}\omega^2\left(-\frac{1}{\varepsilon u}\right).\tag{3.21}$$

The absence of s in the coefficients simplifies the task greatly, since we no longer need to concern ourselves with expanding the coefficients in negative powers of s. This gives the asymptotic expression,

$$h_{1,-1}(s\xi^{-(1/3)},\omega\xi^{-(1/3)})\sim-\frac{1}{\varepsilon u}\left[\frac{2}{\omega^2}-\frac{1}{6}u+\frac{1}{120}\omega^2u^2\right].\tag{3.22}$$

Using again (3.6) gives

$$\exp\left[\sum_{n=1}^{\infty}\left(-s\frac{\omega^{2n+2}}{(2n+2)!}+\mathrm{i}\frac{\omega^{2n+3}}{(2n+3)!}\right)u^n\right]h_{1,-1}(s\xi^{-(1/3)},\omega\xi^{-(1/3)})$$
$$\sim-\frac{1}{\varepsilon u}\left\{\frac{2}{\omega^2}+u\left[\left(-\frac{1}{6}+\frac{\mathrm{i}\omega^3}{60}\right)-\frac{\omega^2}{12}s\right]\right.$$
$$\left.+u^2\left[\left(\frac{\omega^2}{120}-\frac{\mathrm{i}\omega^5}{1008}-\frac{\omega^8}{14400}\right)+\left(\frac{\omega^4}{240}-\frac{\mathrm{i}\omega^7}{1440}\right)s+\frac{\omega^6}{570}s^2\right]\right\}.\tag{3.23}$$

After multiplying the previous expression by $\exp(-s\omega^2/2+\mathrm{i}\omega^3/6)$ and integrating with respect to ω the result is

$$\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\exp\left[\sum_{n=1}^{\infty}\left(-s\frac{\omega^{2n+2}}{(2n+2)!}+\mathrm{i}\frac{\omega^{2n+3}}{(2n+3)!}\right)u^n\right]$$
$$\times h_{1,-1}(s\xi^{-(1/3)},\omega\xi^{-(1/3)})\xi^{-(1/3)}d\omega$$

$$\sim \frac{\xi^{-1/3}}{\varepsilon u}\left\{2Q_{-2,0}(s)+\left[\frac{1}{6}Q_{0,0}(s)-\frac{1}{60}Q_{3,0}(s)-\frac{s}{12}Q_{2,0}(s)\right]u+\left[\frac{1}{120}Q_{2,0}(s)+\cdots\right]u^2\right\}. \tag{3.24}$$

The $\cdots$ in the last term includes only terms with $Q_{k,m}(s)$ with $k\geqslant 4$ and power of s at most s^2.

Again, we have a bound on the maximum possible order in ξ that allows us to use this expansion directly. For efficiency, we again want to isolate those terms of same order in ξ.

To obtain a leading order approximation, we make use of the recurrence relations (A11) and Eqs. (A41) and (A42),

$$Q_{-2,0}(s)=sQ_{0,0}(s)+\tfrac{1}{2}Q_{1,0}(s)\sim\sqrt{2\pi}s^{1/2}\quad \text{as}\ \ s\to\infty,$$

$$Q_{-2,0}(s\xi^{1/3})\sim\sqrt{2\pi}s^{1/2}\xi^{1/6}\quad \text{as}\ \ \xi\to\infty. \tag{3.25}$$

The higher-order terms all go to zero as $\xi\to\infty$, so they can not make a contribution exceeding this term.

We can now look for a first-order correction term. Expanding the previous result a little further gives

$$Q_{-2,0}(s\xi^{1/3})\sim\sqrt{2\pi}[s^{1/2}\xi^{1/6}+\tfrac{1}{24}s^{-5/2}\xi^{-5/6}]\quad \text{as}\ \ \xi\to\infty, \tag{3.26}$$

which leads us to believe that the next term in the series will have order $\xi^{-5/6}$. We look for terms of that order or lower in the u^1 term,

$$uQ_{0,0}(s\xi^{1/3})\sim\sqrt{2\pi}s^{-1/2}\xi^{-5/6}\quad \text{as}\ \ \xi\to\infty, \tag{3.27}$$

$$uQ_{3,0}(s\xi^{1/3})\sim-\tfrac{5}{2}\sqrt{2\pi}s^{-7/2}\xi^{-11/6}\quad \text{as}\ \ \xi\to\infty, \tag{3.28}$$

$$(s\xi^{1/3})uQ_{2,0}(s\xi^{1/3})\sim-\sqrt{2\pi}s^{-1/2}\xi^{-5/6}\quad \text{as}\ \ \xi\to\infty. \tag{3.29}$$

The terms from (3.27) and (3.29) contribute at this order.

We can see that no terms from the u^2 term contribute at this order, by noting that the terms consist of:

(a) $u^2Q_{2,0}(s\xi^{1/3})$ which decays like $s^{-3/2}\xi^{-11/6}$ as $\xi\to\infty$;

(b) Terms containing $Q_{k,m}$, where $k\geqslant 4$ and power of s at most 2. These all decay faster than

$$(s\xi^{1/3})^2u^2Q_{4,0}(s\xi^{1/3})\sim-3\sqrt{2\pi}s^{-1/2}\xi^{-3/2},\quad \xi\to\infty. \tag{3.30}$$

None of these can contribute to the $\xi^{-5/6}$ term.

Moreover, the u^3 or higher terms cannot contribute, since each contains a $u^3=\xi^{-2}$ factor and a power of s no greater than $s^3\to s^3\xi$. Since all of the $Q_{k,m}(s\xi^{-1/3})$ in this term decay as $\xi\to\infty$, this means that each term can contribute at no higher than the ξ^{-1} order.

So, finally [see also Eqs. (2.19) and (3.24)], as an expansion in the $\mu=-1$ case we have

$$I_{1,-1}(s\xi^{-1/3},\xi)\sim\sqrt{2\pi}\xi^{1/3}e^{-\pi\xi}(1+s^2\xi^{-2/3})^{-1/2}\exp[-\xi(s\xi^{-1/3}-\arctan(s\xi^{-1/3}))]$$
$$\times[2s^{1/2}+\tfrac{1}{12}s^{-5/2}+\tfrac{1}{4}s^{-1/2}\xi^{-2/3}],\quad \text{as}\ \ s\to\infty, \tag{3.31}$$

$$I_{1,-1}(s,\xi)\sim 2\sqrt{2\pi}\xi^{1/2}e^{-\pi\xi}s^{1/2}(1+s^2)^{-1/2}\exp[-\xi(s-\arctan(s))]$$
$$\times[1+(\tfrac{1}{8}+\tfrac{1}{24}s^{-2})s^{-1}\xi^{-1}],\quad \text{as}\ \ \xi\to\infty. \tag{3.32}$$

We notice that the leading order of the expansion for $\mu=-1$ is a full power of ξ larger than that for the $\mu=+1$ term, which means that we need to consider only the $\mu=-1$ term in the expansion for the differential excitation function, at least to leading order.

We also note that, while the leading-order term of the $\mu=-1$ expansion is well-behaved, the correction terms are singular at $s=0$, corresponding to the backscatter direction, as are *all* of the terms in the expansion for $\mu=+1$. Even using only the nonsingular leading order term of $I_{1,-1}$ gives the result of $df_{E1}(\theta=\pi)/d\Omega=0$, which we know to be wrong, so this case must be handled separately.

IV. DIFFERENTIAL EXCITATION FUNCTION

A. Parameter s bounded away from zero (θ bounded away from π)

Dismissing the $I_{1,+1}$ term as asymptotically much smaller than the $I_{1,-1}$ term, we obtain the following expression for the semiclassical excitation function for large ξ (repulsive potential),

$$\frac{df_{E1}}{d\Omega}(s,\xi)\sim\frac{4}{9}\pi^2\xi e^{-2\pi\xi}s(1+s^2)\exp[-2\xi(s-\arctan(s))]\times\{1+(\tfrac{1}{4}+\tfrac{1}{12}s^{-2})s^{-1}\xi^{-1}\},\quad \text{as}\ \ \xi\to\infty. \tag{4.1}$$

The behavior of the leading order of this expression is qualitatively similar to the semiclassical result, with the exception that it goes to 0 in the backscattering direction $\theta=\pi(s=0)$, while the semiclassical result remains a small positive number.

B. Parameter $s=0$ ($\theta=\pi$)

While the previous expansions are useful for s large (θ bounded away from π), the leading-order term for $df_{E1}(\theta=\pi)/d\Omega$ is 0 in this approximation, while all of the correction terms are singular for that direction. This situation arises, due to our use of large-s asymptotic expressions for the $Q_{k,m}(s)$, when, in the present case of $\theta=\pi$, we should be considering small values for the argument of these functions.

To obtain information about $\theta=\pi$, we need to follow the method of Ref. 6 and expand in ascending powers of s. As in the large-s case, however, we will not expand $\exp[-\xi(s-\arctan(s))]$ or ε in powers of ξ.

Our situation is simplified by the fact that, for the backscatter direction, the integral for $\mu=+1$ and the integral for $\mu=-1$ are exactly the same. Since the $\mu=-1$ case presents the simpler expansion, we shall use it, rather than bothering with the more complicated $\mu=+1$ expansion. In fact, we can derive it directly from the results of the previous section [Eq. (3.24)] and Eq. (2.19),

$$I_{1,-1}(s\xi^{-1/3},\xi)\sim\xi^{1/3}e^{-\pi\xi}(1+s^2\xi^{-2/3})^{-1/2}\exp[-\xi(s\xi^{-1/3}-\arctan(s\xi^{-1/3}))]\times\left\{2Q_{-2,0}(s)+u\left[\frac{1}{6}Q_{0,0}(s)-\frac{1}{60}Q_{3,0}(s)-\frac{s}{12}Q_{2,0}(s)\right]\right\},\quad \text{as}\ \ s\to0. \tag{4.2}$$

In taking the limit as $\xi\to\infty$, we see that there is some degeneracy in the expansion we get, since any constant value of s will give a result for backscatter at $\xi=\infty$. However, since we are seeking approximations for large, but finite ξ, it is best to pick $s=0$ to obtain the backscatter direction for all ξ.

We do not encounter, as we did in the $s\neq0$ case, the problem with differing asymptotic behavior of the $Q_{k,m}$, since, in this case, we are merely evaluating each of them at $s=0$.

We see that, in the leading order of Eq. (4.2) [see also Eqs. (A21), (A22), (A25)],

$$2Q_{-2,0}(0)=Q_{1,0}(0)=2^{2/3}3^{1/6}\Gamma(2/3), \tag{4.3}$$

and, in the first-order correction of Eq. (4.2),

$$Q_{0,0}(0)=2^{1/3}3^{1/6}\Gamma(1/3), \tag{4.4}$$

$$Q_{3,0}(0)=-2Q_{0,0}(0)=-2^{4/3}3^{-1/6}\Gamma(1/3), \tag{4.5}$$

which results in the expansion,

$$I_{1,-1}(0,\xi)\sim\xi^{1/3}e^{-\pi\xi}2^{2/3}3^{1/6}\Gamma(2/3)\left[1+\frac{1}{5}6^{-1/3}\frac{\Gamma(1/3)}{\Gamma(2/3)}\xi^{-2/3}\right], \quad \text{for } \xi^{2/3}\gg 1, \tag{4.6}$$

Using the equality of $I_{1,+1}(0,\xi)$ and $I_{1,-1}(0,\xi)$, gives the following expression for the $E1$ differential excitation function:

$$\begin{aligned}\frac{df_{E1}}{d\Omega}(0,\xi)&=\frac{1}{9}\pi I_{1,-1}^2(0,\xi)\\ &\sim\frac{2}{9}\pi 6^{1/3}\Gamma^2(2/3)\xi^{2/3}e^{-2\pi\xi}\left[1+\frac{2}{5}6^{-1/3}\frac{\Gamma(1/3)}{\Gamma(2/3)}\xi^{-2/3}\right], \quad \text{for } \xi^{2/3}\gg 1,\end{aligned} \tag{4.7}$$

and repulsive potentials.

The same result is obtained using Watson's asymptotic expansion of the Bessel functions $K_\nu(z)=\frac{1}{2}\pi\mathrm{i}\exp(\frac{1}{2}\nu\pi\mathrm{i})H_\nu^{(1)}(ze^{1/2\pi\mathrm{i}})$ in Eq. (1.1), whose order and argument are nearly equal (Sec. 8.42 of Ref. 5).

An interesting result is that, upon conversion to the attractive case through multiplication by $\exp(2\pi|\xi|)$ of Eqs. (4.1) and (4.7), we see that Eq. (4.1) still decays to 0, albeit at a slower rate, while Eq. (4.7) tends to infinity as $\xi\to\infty$. This is explained by the fact that, as $E_f\to 0$, those classical orbits, which come closer to the target, are more strongly emphasized. Those same orbits result in scattering angles near the backscatter direction. This effect is not seen in the repulsive case, since the classical orbits do not come arbitrarily close to the ion, making it increasingly unlikely for a transition to occur when $E_f\to 0$.

C. Parameter $s\to 0$ (i.e., $\theta\to\pi$)

The approach in the previous section can be extended to handle the case $\xi^{2/3}\gg 1$ and $s\xi^{1/3}\ll 1$ by using the small-argument expansions (A28)–(A33) for the $Q_{k,m}$ in Eq. (4.2) and in the equation

$$\begin{aligned}I_{1,1}(s\xi^{-1/3},\xi)\sim{}&\xi^{1/3}e^{-\pi\xi}(1+s^2\xi^{-2/3})^{1/2}\exp[-\xi(s\xi^{-1/3}-\arctan(s\xi^{-1/3}))]\\ &\times\left\{2Q_{0,-2}(s)+u\left[\frac{1}{6}Q_{2,-2}(s)-\frac{2}{3}sQ_{2,-3}(s)-\frac{s}{12}Q_{4,-2}(s)-\frac{1}{60}Q_{5,-2}(s)\right]\right\}.\end{aligned} \tag{4.8}$$

The results obtained are, for the relevant Coulomb integral,

$$I_{1,-1}(s,\xi)\sim\xi^{1/3}e^{-\pi\xi}2^{2/3}3^{1/6}\Gamma(2/3)\left\{1+\frac{1}{5}6^{-1/3}\frac{\Gamma(1/3)}{\Gamma(2/3)}\xi^{-2/3}+6^{-1/3}\frac{\Gamma(1/3)}{\Gamma(2/3)}(s\xi^{1/3})\right\} \tag{4.9}$$

and

$$I_{1,1}(s,\xi)\sim\xi^{1/3}e^{-\pi\xi}2^{2/3}3^{1/6}\Gamma(2/3)\left\{1+\frac{1}{5}6^{-1/3}\frac{\Gamma(1/3)}{\Gamma(2/3)}\xi^{-2/3}-6^{-1/3}\frac{\Gamma(1/3)}{\Gamma(2/3)}(s\xi^{1/3})\right\}, \tag{4.10}$$

and hence, for the repulsive potential excitation function,

$$\frac{df_{E1}}{d\Omega}(s,\xi)\sim\frac{2}{9}\pi 6^{1/3}\Gamma^2(2/3)\xi^{2/3}e^{-2\pi\xi}\left\{1+\frac{2}{5}6^{-1/3}\frac{\Gamma(1/3)}{\Gamma(2/3)}\xi^{-2/3}\right\}, \tag{4.11}$$

for $\xi^{2/3}\gg 1$ and $s\xi^{1/3}\ll 1$. The match between the exact semiclassical $E1$ differential excitation function [Eq. (1.1)] and the asymptotic expansions derived in this paper is shown in Fig. 8.

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APPENDIX: PROPERTIES OF THE $Q_{K,M}(S)$

While, in general, the integral in (2.22) cannot be solved in closed form, there is one important case where a closed-form integral exists,

$$Q_{1,1}(s)=\left[2\mathrm{i}\exp\left(-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right)\right]_{\omega=-\infty}^{\infty}\equiv 0, \tag{A1}$$

for $s>0$. The principal-value prescription assigns a value of 0 at $s=0$ as well. The explicit knowledge of this case will help us to eliminate pathological cases in the recurrence relations we will derive presently.

For brevity, we will in general not write the explicit dependence of the $Q_{k,m}$ on its argument from this point on, unless it is absolutely necessary.

1. Recurrence relations for $Q_{k,m}$

Integration by parts provides several recurrence relations among these integrals that may be used to reduce the problem of evaluating any of the $Q_{k,m}$ to that of evaluating four basic integrals, $Q_{1,0}$, $Q_{0,0}$, $Q_{-1,0}$, and $Q_{0,-1}$.

Using integration by parts on the definition (2.22), assuming $m\neq -1$,

$$\begin{aligned}Q_{k,m}&=\mathrm{i}^{-k-m}\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\omega^k(\omega+2\mathrm{i}s)^m\mathrm{d}\omega\\&=-\frac{\mathrm{i}^{-k-m}}{m+1}\left\{k\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\omega^{k-1}(\omega+2\mathrm{i}s)^{m+1}\mathrm{d}\omega\right.\\&\quad\left.-\frac{\mathrm{i}}{2}\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\omega^{k+1}(\omega+2\mathrm{i}s)^{m+2}\mathrm{d}\omega\right\}\\&=\frac{-k}{m+1}Q_{k-1,m+1}-\frac{1}{2(m+1)}Q_{k+1,m+2}.\end{aligned} \tag{A2}$$

Selecting other factors for the integration by parts, and now assuming $k\neq -1$, gives

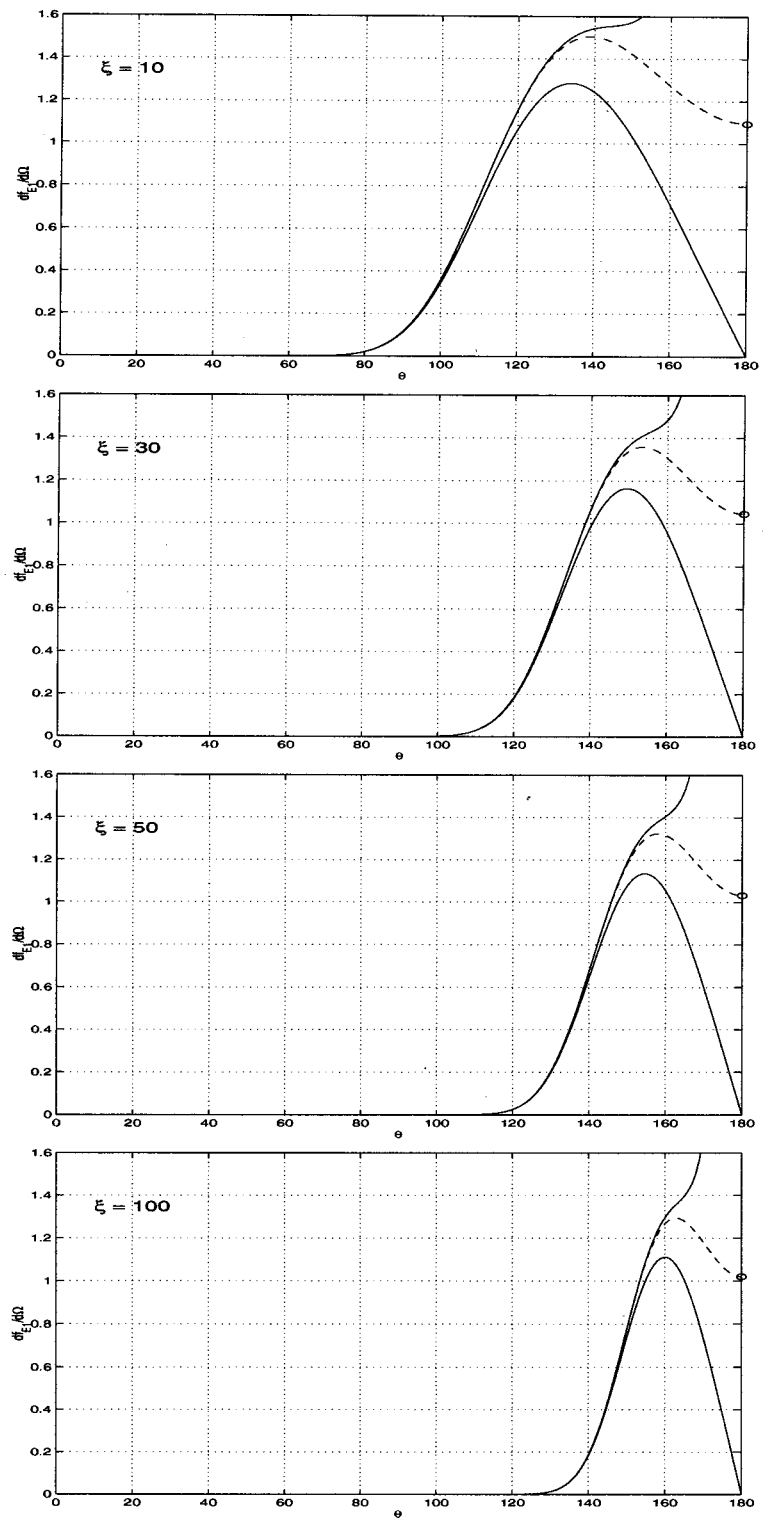

FIG. 8. Semiclassical approximation for large ξ. The function $(9/2\pi)\Gamma^{-2}(2/3)\exp(2\pi\xi)\mathrm{d}f_{E1}/\mathrm{d}\Omega$ is plotted as a function of θ for different values of the parameter ξ. Under this normalization, the plots for the attractive and repulsive cases are equivalent. The semiclassical expression (1.1) for $\lambda=1$ is shown as a dashed line while the one- and two-term asymptotic expression (4.1) is shown as solid lines. The two-terms asymptotic expression (4.7) for $\theta=\pi$ is shown as a circle.

$$
\begin{aligned}
Q_{k,m} &= \mathrm{i}^{-k-m}\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\omega^k(\omega+2\mathrm{i}s)^m\mathrm{d}\omega \\
&= -\frac{\mathrm{i}}{k+1}\left\{m\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\omega^{k+1}(\omega+2\mathrm{i}s)^{m-1}\mathrm{d}\omega\right. \\
&\quad \left.-\frac{\mathrm{i}}{2}\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\omega^{k+2}(\omega+2\mathrm{i}s)^{m+1}\mathrm{d}\omega\right\} \\
&= -\frac{m}{k+1}Q_{k+1,m-1}-\frac{1}{2(k+1)}Q_{k+2,m+1}. \qquad \text{(A3)}
\end{aligned}
$$

While (A2) is valid only for $m\neq -1$ and (A3) is good only for $k\neq -1$, upon multiplying the former by $(m+1)$ and the latter by $(k+1)$, we find that we can transform one into the other by permuting indices, meaning both are valid for $(k,m)\neq(-1,-1)$. Knowing that $Q_{1,1}=0$, allows us to remove even this restriction, resulting in three recurrence relations for the $Q_{k,m}$ of general applicability (the two above, plus a third from permuting indices),

$$(m+1)Q_{k,m}=-kQ_{k-1,m+1}-\tfrac{1}{2}Q_{k+1,m+2}, \qquad \text{(A4)}$$

$$(k+1)Q_{k,m}=-mQ_{k+1,m-1}-\tfrac{1}{2}Q_{k+1,m+1}, \qquad \text{(A5)}$$

$$\tfrac{1}{2}Q_{k,m}=-(k-1)Q_{k-2,m-1}-(m-1)Q_{k-1,m-2}. \qquad \text{(A6)}$$

If $m=0$, we can derive other recurrence relations. If $k\neq -1$,

$$
\begin{aligned}
Q_{k,0} &= \mathrm{i}^{-k}\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\omega^k\mathrm{d}\omega \\
&= -\frac{\mathrm{i}^{-k}}{k+1}\int_{-\infty}^{\infty}\left(-s\omega+\mathrm{i}\frac{\omega^2}{2}\right)\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\omega^{k+1}\mathrm{d}\omega \\
&= -\frac{s}{k+1}Q_{k+2,0}-\frac{1}{2(k+1)}Q_{k+3,0}. \qquad \text{(A7)}
\end{aligned}
$$

Similarly, if we multiply by $k+1$, we can extend to general applicability by noting that

$$
\begin{aligned}
-sQ_{1,0}-\frac{1}{2}Q_{2,0} &= \int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\omega\left(\mathrm{i}s+\frac{\omega}{2}\right)\mathrm{d}\omega \\
&= -\tfrac{1}{2}Q_{1,1}=0. \qquad \text{(A8)}
\end{aligned}
$$

Again, permuting indices gives three versions of this recurrence relation,

$$(k+1)Q_{k,0}=-sQ_{k+2,0}-\tfrac{1}{2}Q_{k+3,0}, \qquad \text{(A9)}$$

$$Q_{k,0}=-2sQ_{k-1,0}-2(k-2)Q_{k-3,0}, \qquad \text{(A10)}$$

$$sQ_{k,0}=-(k-1)Q_{k-2,0}-\tfrac{1}{2}Q_{k+1,0}. \qquad \text{(A11)}$$

While the three recurrence relations for $m=0$, (A9)–(A11) are quite readily applicable, the three more general relations, (A4)–(A6) are much more difficult to apply to obtain a combination of only the basic four $Q_{k,m}$. Another recurrence relation, derived from partial fractions aids us here, especially in the frequently-encountered case, when k is positive and m is negative.

From the binomial theorem,

$$(\omega+2\mathrm{i}s)^k=\sum_{j=0}^{k}\binom{k}{j}\omega^{k-j}(2\mathrm{i}s)^j$$

$$=\omega^k+\sum_{j=1}^{k}\binom{k}{j}\omega^{k-j}(2\mathrm{i}s)^j, \tag{A12}$$

so

$$Q_{k,-m}=\mathrm{i}^{-k+m}\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\frac{\omega^k}{(\omega+2\mathrm{i}s)^m}\,\mathrm{d}\omega,$$

$$Q_{k,-m}=\mathrm{i}^{-k+m}\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\frac{1}{(\omega+2\mathrm{i}s)^m}\left[(\omega+2\mathrm{i}s)^k-\sum_{j=1}^{k}\binom{k}{j}\omega^{k-j}(2\mathrm{i}s)^j\right]\mathrm{d}\omega,$$

$$=Q_{0,k-m}-\sum_{j=1}^{k}\binom{k}{j}(2s)^jQ_{k-j,-m}. \tag{A13}$$

This relation expresses a $Q_{k,-m}$ in terms of an integral with $k=0$ and several with the same value of m, but lower values of k. If $k\leqslant m$, this can be used repeatedly to obtain a result in terms of only the $Q_{k,-m}$ with $k=0$ and $m\geqslant 0$. In this situation, Eq. (A4) takes a simple form (one term drops out), which can be used to increase $-m$. Repeated application of (A13) and (A4) is guaranteed to be able to express any $Q_{k,m}$ with positive k and negative m in terms of $Q_{1,0}$, $Q_{0,0}$, and $Q_{0,-1}$.

If $k>m$, we use the division algorithm on the integrand to express it in terms of $Q_{k,-m}$ with $k<m$ and those with $m=0$, which are handled easily by (A9)–(A11).

The use of these recurrence relations is shown in Fig. 5.

2. Ascending power series for $Q_{k,m}$

Since we have reduced the problem of computing the general $Q_{k,m}$ to that of computing the four basic integrals $Q_{1,0}$, $Q_{0,0}$, $Q_{-1,0}$, and $Q_{0,-1}$, we now set ourselves to obtaining power series for these four integrals. We begin by expressing each of these in real form,

$$Q_{1,0}=2\int_0^{\infty}\exp\left(-s\frac{\omega^2}{2}\right)\omega\sin\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega, \tag{A14}$$

$$Q_{0,0}=2\int_0^{\infty}\exp\left(-s\frac{\omega^2}{2}\right)\cos\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega, \tag{A15}$$

$$Q_{-1,0}=\pi-2\int_0^{\infty}\exp\left(-s\frac{\omega^2}{2}\right)\frac{1}{\omega}\sin\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega, \tag{A16}$$

$$Q_{0,-1}=4\int_0^{\infty}\exp\left(-s\frac{\omega^2}{2}\right)\frac{s}{\omega^2+4s^2}\cos\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega-2\int_0^{\infty}\exp\left(-s\frac{\omega^2}{2}\right)\frac{\omega}{\omega^2+4s^2}\sin\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega. \tag{A17}$$

The π-term in the expression for $Q_{-1,0}$ comes from distorting the path of integration around the pole in the integrand at $\omega=0$, while the remainder is the principal value of the the integral.

As a preliminary to deriving power series for the four principal $Q_{k,m}$, we evaluate every integral of the form $Q_{k,0}$ at $s=0$. We note that

$$Q_{1,0}(0)=2\int_0^\infty \omega \sin\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega. \tag{A18}$$

Making the substitution $v=\omega^{1/3}$ gives

$$Q_{1,0}(0)=\frac{2}{3}\int_0^\infty v^{-(1/3)}\sin\left(\frac{v}{3}\right)\mathrm{d}v. \tag{A19}$$

This is an example of a representation of the Gamma function [Ref. 12, Eq. 6.312(8)]

$$\Gamma(z)=\frac{b^z}{\mathrm{trig}\left(\frac{\pi}{2}z\right)}\int_0^\infty t^{z-1}\,\mathrm{trig}(bt)\mathrm{d}t, \tag{A20}$$

where trig(x) stands for either sin(x) or cos(x), for $b>0$, $0<\mathrm{Re}(z)<1$, which gives the integral in terms of the Gamma function,

$$Q_{1,0}(0)=2^{2/3}3^{1/6}\Gamma\left(\frac{2}{3}\right). \tag{A21}$$

Similarly,

$$\begin{aligned}Q_{0,0}(0)&=2\int_0^\infty \cos\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega\\&=2^{(1/3)}3^{-(1/6)}\Gamma\left(\frac{1}{3}\right).\end{aligned} \tag{A22}$$

In contrast, $Q_{-1,0}$ is expressible in closed form without invoking a special function (although an intermediate step makes use of the sine integral function),

$$\begin{aligned}Q_{-1,0}(0)&=\pi-2\int_0^\infty \frac{1}{\omega}\sin\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega\\&=\pi-\frac{2}{3}\int_0^\infty \frac{1}{v}\sin\left(\frac{v}{6}\right)\mathrm{d}v\\&=\pi-\frac{2}{3}\lim_{v\to\infty}\mathrm{Si}(v)=\frac{2\pi}{3}.\end{aligned} \tag{A23}$$

While not immediately useful, for completeness, we note that

$$Q_{0,-1}(0)=\mathrm{i}\int_{-\infty}^\infty \exp\left(\mathrm{i}\frac{\omega^3}{6}\right)\frac{1}{\omega}\mathrm{d}\omega=Q_{-1,0}(0)=\frac{2\pi}{3}. \tag{A24}$$

Using these known quantities and Eq. (A9) we obtain for positive k,

$$\begin{aligned}Q_{3n-1,0}(0)&=0 \quad n=1,2,3,4,...,\\Q_{3n,0}(0)&=(3n-1)!!!(-2)^nQ_{0,0}(0) \quad n=0,1,2,3,...,\\Q_{3n+1,0}(0)&=(3n-1)!!!(-2)^nQ_{1,0}(0) \quad n=0,1,2,3,...,\end{aligned} \tag{A25}$$

and, for negative k,

$$Q_{1-3n,0}(0)=\frac{1}{2^n(3n-2)!!!}Q_{1,0}(0) \quad n=0,1,2,3,...,$$

$$Q_{-3n,0}(0)=\frac{1}{2^n(3n-1)!!!}Q_{0,0}(0) \quad n=0,1,2,3,..., \tag{A26}$$

$$Q_{-1-3n,0}(0)=\frac{1}{2^n(3n-1)!!!}\frac{2\pi}{3} \quad n=0,1,2,3,...,$$

where the triple factorial is defined by

$$A!!!=A(A-3)(A-6)\cdots\left\{\begin{matrix}3\\2\\1\end{matrix}\right\}, \quad 0!!!=1. \tag{A27}$$

To obtain ascending power series for these four integrals, we write $\sin(\omega^3/6)$ and $\cos(\omega^3/6)$ in terms of $\exp(\pm i\omega^3/6)$ and we expand the part of the exponential in the integrand which contains s, namely,

$$\begin{aligned}
Q_{1,0}(s)&=-i\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+i\frac{\omega^3}{6}\right]\omega d\omega,\\
&=-i\int_{-\infty}^{\infty}\sum_{n=0}^{\infty}(-)^n\frac{s^n}{2^n n!}\exp\left(i\frac{\omega^3}{6}\right)\omega^{2n+1}d\omega\\
&=\sum_{n=0}^{\infty}\frac{s^n}{2^n n!}Q_{2n+1,0}(0)\\
&=Q_{1,0}(0)-sQ_{0,0}(0)+\sum_{n=1}^{\infty}\left\{Q_{1,0}(0)\frac{(6n-1)!!!}{(3n)!2^n}s^{3n}-Q_{0,0}(0)\frac{(6n+1)!!!}{(3n+1)!2^n}s^{3n+1}\right\}.
\end{aligned} \tag{A28}$$

Similarly,

$$\begin{aligned}
Q_{0,0}(s)&=\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+i\frac{\omega^3}{6}\right]d\omega\\
&=\sum_{n=0}^{\infty}\frac{s^n}{2^n n!}Q_{2n,0}(0)\\
&=Q_{0,0}(0)+\sum_{n=1}^{\infty}\left\{-Q_{1,0}(0)\frac{(6n-4)!!!}{(3n-1)!2^n}s^{3n-1}+Q_{0,0}(0)\frac{(6n-1)!!!}{(3n)!2^n}s^{3n}\right\},
\end{aligned} \tag{A29}$$

and

$$
\begin{aligned}
Q_{-1,0}(s) &= \mathrm{i}\int_{-\infty}^{\infty} \exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\frac{1}{\omega}\,\mathrm{d}\omega \\
&= \sum_{n=0}^{\infty}\frac{s^n}{2^n n!}Q_{2n-1,0}(0) \\
&= \frac{2\pi}{3}+\frac{1}{2}sQ_{1,0}(0)-\frac{1}{4}s^2Q_{0,0}(0) \\
&\quad +\sum_{n=1}^{\infty}\left\{Q_{1,0}(0)\frac{(6n-1)!!!}{(3n+1)!2^{n+1}}s^{3n+1}-Q_{0,0}(0)\frac{(6n+1)!!!}{(3n+2)!2^{n+1}}s^{3n+2}\right\}. \qquad \text{(A30)}
\end{aligned}
$$

To apply the same procedure to $Q_{0,-1}$, we make use of the result

$$
\begin{aligned}
\exp\left(-s\frac{\omega^2}{2}\right)\frac{1}{\omega+2\mathrm{i}s} &= \sum_{m=0}^{\infty}\sum_{k=0}^{\infty}\left((-)^m\frac{s^m\omega^{2m}}{2^m m!}\right)\left(\frac{1}{\omega^{k+1}}(-2\mathrm{i}s)^k\right) \\
&= \sum_{m=0}^{\infty}\sum_{k=0}^{\infty}(-)^{m+k}\frac{\mathrm{i}^k}{2^{m-k}m!}s^{m+k}\omega^{2m-k-1}. \qquad \text{(A31)}
\end{aligned}
$$

We can change the order of summation to make one of the sums finite. Let $n=m+k$,

$$
\exp\left(-s\frac{\omega^2}{2}\right)\frac{1}{\omega+2\mathrm{i}s} = \sum_{n=0}^{\infty}\sum_{m=0}^{n}\frac{(-)^n\mathrm{i}^{n-m}}{2^{2m-n}m!}s^n\omega^{3m-n-1}, \qquad \text{(A32)}
$$

i.e., we have

$$
\begin{aligned}
Q_{0,-1}(s) &= \mathrm{i}\int_{-\infty}^{\infty}\exp\left[-s\frac{\omega^2}{2}+\mathrm{i}\frac{\omega^3}{6}\right]\frac{1}{\omega+2\mathrm{i}s}\,\mathrm{d}\omega \\
&= \int_{-\infty}^{\infty}\sum_{n=0}^{\infty}\sum_{l=0}^{n}\frac{(-)^n\mathrm{i}^{n-l+1}}{2^{2l+n}l!}s^n\omega^{3l-n-1}\mathrm{d}\omega \\
&= \sum_{n=0}^{\infty}\sum_{l=0}^{n}\frac{(-)^{l+n}}{2^{2l-n}l!}s^nQ_{3l-n-1,0}(0). \qquad \text{(A33)}
\end{aligned}
$$

Using the known forms for the $Q_{k,0}(0)$, (A25) and (A26), gives the result cited in Ref. 6. The first 30 coefficients of each of these power series are tabulated in Ref. 6.

3. Descending power series for $Q_{k,m}$

In addition to the ascending power series provided by Ref. 6, which give a good approximation for small values of s, to obtain an expression for the *differential* excitation function, we need asymptotic expressions valid for large s as well. Using a slight modification of an extension to Watson's lemma provided in Ref. 10 (pp. 24ff) allows us to obtain asymptotic power series for the four basic integrals.

Consider the function

$$
f(x)=\int_0^{\sqrt{T}}e^{-xt^2}\varphi(t)\,\mathrm{d}t \qquad \text{(A34)}
$$

(contrast this with the theorem in Ref. 10, where the integration starts at a small negative number).

Making the substitution $t=\tau^{1/2}$ yields

$$f(x)=\frac{1}{2}\int_0^T e^{-x\tau}\varphi(\tau^{1/2})\tau^{-(1/2)}\mathrm{d}\tau. \tag{A35}$$

Suppose that φ admits a Maclaurin series, $\sum_{n=0}^{\infty} a_n t^n$ for $t\in\mathcal{R}$, then

$$f(x)=\frac{1}{2}\int_0^T e^{-x\tau}\tau^{-(1/2)}(a_0+a_1\tau^{1/2}+a_2\tau+a_3\tau^{3/2}+\cdots)\mathrm{d}\tau. \tag{A36}$$

Interchanging the order of integration and summation, we can provide asymptotic forms for all of the terms in the series. We note here that, unlike in Ref. 10, we can not assume that the odd powered terms disappear,

$$\begin{aligned}\int_0^t e^{-x\tau}\tau^{-(1/2)}\mathrm{d}\tau&=\int_0^\infty e^{-x\tau}\tau^{-(1/2)}\mathrm{d}\tau-\int_T^\infty e^{-x\tau}\tau^{-(1/2)}\mathrm{d}\tau\\&=\frac{1}{\sqrt{x}}\int_0^\infty e^{-s}s^{-(1/2)}\mathrm{d}s+\mathcal{O}\left(\frac{e^{-xT}}{x}\right)\\&=\sqrt{\frac{\pi}{x}}+\mathcal{O}\left(\frac{e^{-xT}}{x}\right)\quad\text{as}\quad x\to\infty,\end{aligned} \tag{A37}$$

$$\int_0^T e^{-x\tau}\mathrm{d}\tau=\frac{1}{x}+\mathcal{O}\left(\frac{e^{-xT}}{x}\right), \tag{A38}$$

$$\begin{aligned}\int_0^T x^n e^{-x\tau}\mathrm{d}\tau&=\frac{1}{x^{n+1}}\int_0^\infty s^n e^{-s}\mathrm{d}s+\mathcal{O}\left(\frac{e^{-xT}}{x}\right)\\&=\frac{\Gamma(n+1)}{x^{n+1}}+\mathcal{O}\left(\frac{e^{-xT}}{x}\right);\quad n>0,\end{aligned} \tag{A39}$$

which gives the asymptotic form,

$$\begin{aligned}f(x)&\sim\frac{1}{2}a_0\int_0^T e^{-x\tau}\tau^{-(1/2)}\mathrm{d}\tau+\frac{1}{2}a_1\int_0^T e^{-x\tau}\tau\mathrm{d}\tau+\frac{1}{2}\sum_{n=2}^{\infty}a_n\int_0^T e^{-x\tau}\tau^{(n-1)/2}\mathrm{d}\tau\\&\sim\frac{a_0}{2}\sqrt{\frac{\pi}{x}}+\frac{a_1}{2}\frac{1}{x}+\sum_{n=2}^{\infty}\frac{a_n}{2}\frac{\Gamma\left(\frac{n+1}{2}\right)}{x^{(n+1)/2}}.\end{aligned} \tag{A40}$$

The remainder term of each integral being of higher asymptotic order than all of the other terms.

There are two main differences between this formula and that given in Ref. 10: (1) as it was already noted, the odd-powered terms do not disappear in this derivation, and (2) a factor of $\frac{1}{2}$ has been introduced. Both of these effects can be seen to be a result of replacing the negative lower bound, $-\alpha$ used in Ref. 10 with 0 used here.

As is seen in Fig. 6, since the modulation factor requires that parts of the integral near zero become more and more important as x becomes large, even if the lower bound on the integral is a very small negative number, for large enough x, the region from $-\infty$ to $-\alpha$ becomes insignificant and ''most'' of the integral is included. Since odd-powered terms are odd functions, they

integrate to 0. Taking the lower bound as 0 integrates only half the integrand, no matter how large x is, resulting in odd-powered terms that do not vanish and even-powered terms of half the magnitude given in Ref. 10.

We can now use this theorem to find asymptotic expressions for the four principal integrals $(x=s/2)$,

$$Q_{1,0}=2\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\omega\sin\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega,$$

$$\varphi(\omega)=\omega\sin\left(\frac{\omega^3}{6}\right)=\frac{1}{6}\omega^4-\frac{1}{1296}\omega^{10}+\frac{1}{933120}\omega^{16}+\cdots,$$

$$Q_{1,0}\sim\frac{1}{6}\frac{\Gamma(\frac{5}{2})}{x^{5/2}}-\frac{1}{1296}\frac{\Gamma(\frac{11}{2})}{x^{11/2}}+\frac{1}{933120}\frac{\Gamma(\frac{17}{2})}{x^{17/2}}$$

$$=\sqrt{2\pi}\left[\frac{1}{2}s^{-(5/2)}-\frac{35}{48}s^{-(11/2)}+\frac{5005}{2304}s^{-(17/2)}\right], \tag{A41}$$

$$Q_{0,0}=2\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\cos\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega,$$

$$\varphi(\omega)=\cos\left(\frac{\omega^3}{6}\right)=1-\frac{1}{72}\omega^6+\frac{1}{31104}\omega^{12}\cdots,$$

$$Q_{0,0}\sim\sqrt{2\pi}[s^{-(1/2)}-\tfrac{5}{24}s^{-(7/2)}+\tfrac{385}{1152}s^{-(13/2)}], \tag{A42}$$

$$Q_{-1,0}=\pi-2\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\frac{1}{\omega}\sin\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega,$$

$$\varphi(\omega)=\frac{1}{\omega}\sin\left(\frac{\omega^3}{6}\right)=\frac{1}{6}\omega^2-\frac{1}{1296}\omega^8+\frac{1}{933120}\omega^{14}+\cdots,$$

$$Q_{-1,0}\sim\pi+\sqrt{2\pi}\left[-\frac{1}{6}s^{-(3/2)}+\frac{70}{843}s^{-(9/2)}-\frac{1001}{6912}s^{-(15/2)}\right]. \tag{A43}$$

Handling $Q_{0,-1}$ [Eq. (A17)] is a little more complicated, since there are two integrals involved, and both integrands depend on s in a more complicated way than simply through the exponential factor. We accommodate this by first expanding the s-dependent factor $(\omega^2+4s^2)^{-1}$ as a descending power series in s using

$$\frac{1}{\omega^2+4s^2}=\frac{1}{4s^2}-\frac{\omega^2}{16s^4}+\frac{\omega^4}{64s^6}+\cdots, \tag{A44}$$

and the expressions

$$
\begin{aligned}
I_1 &= 4\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\frac{s}{\omega^2+4s^2}\cos\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega \\
&= \frac{1}{s}\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\cos\left(\frac{\omega^3}{6}\right)d\omega - \frac{1}{4s^3}\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\omega^2\cos\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega \\
&\quad + \frac{1}{16s^5}\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\omega^4\cos\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega + \cdots \\
&= \frac{1}{s}\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\left(1-\frac{1}{72}\omega^6+\frac{1}{31104}\omega^{12}+\cdots\right)\mathrm{d}\omega \\
&\quad - \frac{1}{4s^3}\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\left(\omega^2-\frac{1}{72}\omega^8+\frac{1}{31104}\omega^{14}+\cdots\right)\mathrm{d}\omega + \frac{1}{16s^5} \\
&\quad \times \int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\left(\omega^4-\frac{1}{72}\omega^{10}+\frac{1}{31104}\omega^{16}+\cdots\right)\mathrm{d}\omega + \cdots \\
&\sim \sqrt{2\pi}\left[\tfrac{1}{2}s^{-(3/2)} - \tfrac{11}{48}s^{-(9/2)} + \tfrac{1021}{2304}s^{-(15/2)}\right],
\end{aligned}
\tag{A45}
$$

$$
\begin{aligned}
I_2 &= -2\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\frac{\omega}{\omega^2+4s^2}\sin\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega \\
&= -\frac{1}{2s^2}\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\omega\sin\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega + \frac{1}{8s^4}\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\omega^3\sin\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega \\
&\quad + \frac{1}{32s^6}\int_0^\infty \exp\left(-\frac{s}{2}\omega^2\right)\omega^5\sin\left(\frac{\omega^3}{6}\right)\mathrm{d}\omega \\
&\sim \sqrt{2\pi}\left[-\tfrac{1}{8}s^{-(9/2)} + \tfrac{65}{192}s^{-(15/2)} - \tfrac{12145}{9216}s^{-(21/2)}\right].
\end{aligned}
\tag{A46}
$$

Therefore,

$$
Q_{0,-1} = I_1 + I_2 \sim \sqrt{2\pi}\left[\tfrac{1}{2}s^{-(3/2)} - \tfrac{17}{48}s^{-(9/2)} + \tfrac{1801}{2304}s^{-(15/2)}\right]. \tag{A47}
$$

All four of these asymptotic expansions enjoy a very rapid increase in the order of the terms, as each exponent is 3 less than the previous. The condition for these to be a good approximation is therefore not merely that s be large, but the much less restrictive $s^3 \gg 1$.

In principle, these asymptotic expansions may be used to obtain asymptotic expansions for any $Q_{k,m}$, since any $Q_{k,m}$ may be represented as a finite combination of these four basic functions. In practice, however, low-order terms frequently cancel and higher-order terms must be derived to get a useful expansion for these integrals. For this reason, we derive from first principles a leading-order asymptotic expression for these integrals in the more general case of $k \geqslant 0$. In this case, we can apply Murray's extension to Watson's lemma directly to the definition of $Q_{k,m}$,

$$
Q_{k,m} = \mathrm{i}^{-k-m}\int_{-\infty}^\infty \exp\left(-\frac{s}{2}\omega^2\right)\exp\left(\mathrm{i}\frac{\omega^3}{6}\right)\omega^k(\omega+2\mathrm{i}s)^m\mathrm{d}\omega. \tag{A48}
$$

When $k \geqslant 0$, the portion of the integrand outside the first exponential admits a Maclaurin series. While we cannot, in general, immediately apply Murray's extension, due to the dependence on s outside the exponential, we may expand $(\omega+2\mathrm{i}s)^m$ in a descending power series in s prefixed by a power of s,

$$(\omega+2\mathrm{i}s)^m=(2\mathrm{i}s)^m\left(1+\frac{\omega}{2\mathrm{i}s}\right)^m=(2\mathrm{i}s)^m\left(1+\frac{m\omega}{2\mathrm{i}s}+\cdots\right). \tag{A49}$$

Using this, we can expand the integral in terms of integrals suitable for applying Murray's extension,

$$\begin{aligned}Q_{k,m}&=\mathrm{i}^{-k-m}(2\mathrm{i}s)^m\int_{-\infty}^{\infty}\exp\left(-\frac{s}{2}\omega^2\right)\exp\left(\mathrm{i}\frac{\omega^3}{6}\right)\omega^k\left(1+\frac{m\omega}{2\mathrm{i}s}+\cdots\right)\mathrm{d}\omega\\&=\mathrm{i}^{-k-m}(2\mathrm{i}s)^m\int_{-\infty}^{\infty}\exp\left(-\frac{s}{2}\omega^2\right)\exp\left(\mathrm{i}\frac{\omega^3}{6}\right)\omega^k\mathrm{d}\omega+\mathrm{i}^{-k-m}m(2\mathrm{i}s)^{m-1}\\&\quad\times\int_{-\infty}^{\infty}\exp\left(-\frac{s}{2}\omega^2\right)\exp\left(\mathrm{i}\frac{\omega^3}{6}\right)\omega^{k+1}\mathrm{d}\omega+\cdots.\end{aligned} \tag{A50}$$

The later integrals (in the $\cdots$) do not contribute in the leading order, since they have both a higher leading-order power of ω in the integrand and a higher power of s in the denominator of the coefficient, both of which lower the leading order of the integral in s.

Since the leading order of $\exp(\mathrm{i}\omega^3/6)$ is 1, and only even-powered terms contribute asymptotically, only one of the integrals in (A50) contributes in the leading order, the first if k is even, and the second if k is odd.

If k is even, we have the asymptotic form,

$$Q_{k,m}\sim(-)^{k/2}\sqrt{2\pi}2^m[1\times3\times\cdots\times(k-1)]s^{-(k/2)+m-(1/2)}, \tag{A51}$$

and if k is odd

$$Q_{k,m}\sim(-)^{(k+1)/2}\sqrt{2\pi}m2^{m-1}[1\times3\times\cdots\times k]s^{-[(k+1)/2]+m-(1/2)}. \tag{A52}$$

There are several important things that we can learn from this expansion. First, if k is even and $m>(k/2)+(1/2)$, or if k is odd and $m>(k/2)+1$ the integrals actually increase without bound as $s\to\infty$. Secondly, as k becomes larger, the integral decays at a faster rate. This is to be expected, since, for large k, the factor of ω^k "forces" the slowly-varying part of the integrand away from 0—the most important part of the integral asymptotically (see Fig. 7). We will use this fact later to prove that higher-order terms in the expansion for the semiclassical Coulomb integrals are actually insignificant.

Armed with these facts, we are ready to tackle the $E1$ semiclassical Coulomb integrals.

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Singular and nonsingular eigenvectors for the Gaudin model

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We present a method to construct a basis of singular and nonsingular common eigenvectors for Gaudin Hamiltonians in a tensor product module of the Lie algebra $SL(2)$. The subset of singular vectors is completely described by analogy with covariant differential operators. The relation between singular eigenvectors and the Bethe Ansatz is discussed. In each weight subspace the set of singular eigenvectors is completed to a basis, by a family of nonsingular eigenvectors. We discuss also the generalization of this method to the case of an arbitrary Lie algebra. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379750]

I. INTRODUCTION

The Gaudin model[1] is an example of an integrable system in statistical quantum mechanics, associated to N spin particles with magnetic interaction, based on N independent and commuting Hamiltonians. As originally formulated, this model is related to the Lie algebra $SL(2)$. In this simplest case, the problem of the diagonalization of the Hamiltonians was partially solved. Using a constructive method, known as Bethe Ansatz, Gaudin[2] constructed a family of common eigenvectors for all Hamiltonians.

More generally, integrable systems can be associated to any semi-simple complex Lie algebra. For such systems, generalizations of the set of Gaudin Hamiltonians have been constructed.[3] The methods proposed for diagonalization of these Hamiltonians revealed remarkable connections between integrable models and two dimensional conformal field theories.

In Ref. 3, the structure of the Bethe vectors for the Gaudin model is related to the representation theory of affine Lie algebras. The diagonalization of Gaudin Hamiltonians is based on a concept of invariant functionals (correlation functions) on tensor products of representations of an affine Lie algebra at the critical level.

Another approach for the problem of diagonalization,[4,5] is related to the connection between eigenvectors of the Gaudin Hamiltonians and the solutions[6] of the Knizhnik–Zamolodchikov equations.[7] In this approach, the common eigenvectors are constructed inductively and each eigenvector leads to an integral solution of the KZ equations. Conversely, in Ref. 8 it was proved that in the quasi-classical limit, the first term of the asymptotic solutions of KZ equation leads to a common eigenvector of the Hamiltonians. In this case the Bethe equations for the Gaudin model appear as conditions of critical points.

In Sec. II we review some aspects concerning the Gaudin model, originally formulated for the Lie algebra $SL(2)$. We recall the expression of the N Hamiltonians, introduced by Gaudin. The space Ω of physical states is defined as a tensor product of N finite-dimensional highest weight representations of the Lie algebra $SL(2)$. It is decomposed as a direct sum of weight subspaces, i.e., $\Omega = \oplus \mathcal{V}_m$. We explain how the Bethe Ansatz works to construct common eigenvectors for Gaudin Hamiltonians in each eigenspace $\mathcal{V}_m$. However, this method cannot give all the common eigenvectors of Gaudin Hamiltonians. Therefore, supplementary common eigenvectors have to be determined.

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In Sec. III we give a general, recursive method to construct a basis of common eigenvectors in each invariant subspace $\mathcal{V}_m$. Knowing a basis of $\mathcal{V}_{m-1}$, we construct a family of linear independent common eigenvectors in $\mathcal{V}_m$, which are nonsingular. This family is completed to a basis of $\mathcal{V}_m$, by a basis of the subspace of singular vectors of $\mathcal{V}_m$. Using an analog of the Gordan operator,[9] we give a basis of $\mathrm{Sing}\,\mathcal{V}_m$. Finally, we show that the Bethe Ansatz gives a family of singular common eigenvectors for Gaudin Hamiltonians, but in some particular cases, this family could not be complete.

Section IV is devoted to a discussion of the generalized model associated to an arbitrary simple Lie algebra. We recall the generalization of the Gaudin Hamiltonians and explain how the Bethe Ansatz was generalized to construct common eigenvectors for these Hamiltonians. We show that Bethe equations, which appear as conditions that Bethe type vectors be common eigenvectors, are also conditions of singularity for them. This constructive method does not ensure the completeness of the system of eigenvectors.

II. GAUDIN MODEL AND THE $SL(2)$ LIE ALGEBRA

The Gaudin spin model is related to the Lie algebra $SL(2)$, with generators E, F and H satisfying the commutation relations:

$$[E,F]=H; \quad [H,E]=2E; \quad [H,F]=-2F.$$

For this Lie algebra we consider N finite-dimensional highest weight modules: $V_{\lambda_1},\ldots,V_{\lambda_N}$ with highest weights $\lambda_1,\ldots,\lambda_N$ and highest weight vectors $v_{\lambda_1},\ldots,v_{\lambda_N}$. The tensor product of these N modules constitutes the space of physical states for a system of N spin particles:

$$\Omega = V_{\lambda_1}\otimes\cdots\otimes V_{\lambda_N}.$$

The Lie algebra action on each vector $v=v_1\otimes\cdots\otimes v_N$ of this tensor module is defined as

$$\mathbf{X}\,v=\sum_{i=1}^{N} X^{(i)}v, \quad \forall X\in SL(2), \tag{1}$$

where $X^{(i)}$ denotes the operator on Ω which acts as X on the ith module and as the identity operator on all other factors:

$$X^{(i)}v_1\otimes\cdots\otimes v_N=v_1\otimes\cdots\otimes Xv_i\otimes\cdots\otimes v_N, \quad \forall v_1\otimes\cdots\otimes v_N\in\Omega. \tag{2}$$

For such a system of N spin particles, Gaudin proposed a set of N Hamiltonians defined on Ω, depending on N distinct, complex parameters $z_1,\ldots,z_N$:

$$\mathcal{H}_i(z_1,\ldots,z_N)=\sum_{j=1,j\neq i}^{N}\frac{1}{z_i-z_j}\left[\frac{1}{2}H^{(i)}H^{(j)}+E^{(i)}F^{(j)}+F^{(i)}E^{(j)}\right], \quad \forall i=1,\ldots,N. \tag{3}$$

All these operators commute:

$$[\mathcal{H}_i,\mathcal{H}_j]=0, \quad \forall i,j=1,\ldots,N,$$

but they are not independent, because $\Sigma_{i=1}^{N}\mathcal{H}_i=0$. It can easily be verified that among the N Gaudin Hamiltonians there are exactly $N-1$ which are independent. To integrate a system of N spin particles, with N degrees of freedom, the family of commuting operators is completed by the Cartan generator (also called the total spin operator), of which action on the tensor module is

$$\mathbf{H}\,v=\sum_{i=1}^{N} H^{(i)}v, \quad \forall v\in\Omega,$$

and which commutes with all Gaudin Hamiltonians.

For this family of N independent Hamiltonians which commute there is a complete system of common eigenvectors in Ω. Our goal is to construct a basis in Ω, of common eigenvectors of Gaudin Hamiltonians.

A. The structure of the space Ω

In order to analyze the structure of Ω it is useful to recall some elements of the theory of highest weight representations of the Lie algebra $SL(2)$. Such a representation is completely determined by a highest weight vector v_λ, on which the action of the algebra is given by

$$Hv_\lambda=\lambda v_\lambda, \quad Ev_\lambda=0,$$

and the representation space is generated by vectors:

$$\{v_n=F^n v_\lambda\}_{n\in\mathbb{N}}.$$

The action of the Lie algebra on these vectors is

$$Hv_n=(\lambda-2n)v_n, \tag{4}$$

$$Ev_n=n(\lambda-n+1)v_{n-1}, \tag{5}$$

$$Fv_n=v_{n+1}. \tag{6}$$

If the highest weight λ is not a positive integer, the representation is infinite dimensional and irreducible. If $\lambda\in\mathbb{N}$, then in $\{v_n=F^n v_\lambda\}_{n\in\mathbb{N}}$ there is an invariant subspace, generated by $\{v_{\lambda+1}, v_{\lambda+2}, \dots\}$ and the quotient representation is irreducible and finite dimensional, of dimension $\lambda+1$, generated by vectors $\{v_n=F^n v_\lambda\}_{n=0,\dots,\lambda}$. We denote V_λ this quotient representation, for which we have $F^n v_\lambda=0$ for all $n\geqslant\lambda+1$.

We will consider the space Ω as a tensor product of finite-dimensional representations V_λ, which is completely determined by the vector $v_0=v_{\lambda_1}\otimes\cdots\otimes v_{\lambda_N}$, called vacuum vector and is generated by vectors $\{F^{n_1}v_{\lambda_1}\otimes F^{n_2}v_{\lambda_2}\cdots\otimes F^{n_N}v_{\lambda_N}\}_{n_i=0,\dots,\lambda_i;i=1,\dots,N}$, with n_i operators F applied on the ith component. Such a vector can be written as a product of $m=n_1+n_2+\cdots+n_N$ operators of type (2), denoted

$$v_m^{(k_1,\dots,k_m)}=F^{(k_1)}F^{(k_2)}\cdots F^{(k_m)}v_0,$$

with $1\leqslant k_1\leqslant\cdots\leqslant k_m\leqslant N$. Note that for finite-dimensional representations, m can vary between 0 and a maximal value $m_{\max}=\Sigma_{i=1}^N\lambda_i$.

Note also the particular action of the Hamiltonians on the vacuum vector:

$$\mathbf{H}v_0=\left(\sum_{k=1}^N\lambda_k\right)v_0, \quad \mathcal{H}_i v_0=\left(\frac{1}{2}\sum_{j=1,j\neq i}^N\frac{\lambda_i\lambda_j}{z_i-z_j}\right)v_0. \tag{7}$$

The Cartan operator $\mathbf{H}$ has a privileged place in the family of commuting Hamiltonians. According to (4), it gives a gradation of the representation spaces V_{λ_i}, which induces a gradation of the tensor product module, on $\mathbf{H}$-invariant subspaces:

$$\Omega=\oplus_{m=0}^{m_{\max}}\mathcal{V}_m,$$

where $\mathcal{V}_m$ is a weight subspace, of weight $\Sigma_{i=1}^N\lambda_i-2m$, also called space of spin deviation m. It is generated by $\mathbf{H}$-eigenvectors:

$$\{v_m^{(k_1,\ldots,k_m)}=F^{(k_1)}\cdots F^{(k_m)}v_0\}_{1\leqslant k_1\leqslant\cdots\leqslant k_m\leqslant N}, \tag{8}$$

which we call states of spin deviation m:

$$\mathbf{H}F^{(k_1)}F^{(k_2)}\cdots F^{(k_m)}v_0=\left(\sum_{i=1}^{N}\lambda_i-2m\right)F^{(k_1)}F^{(k_2)}\cdots F^{(k_m)}v_0.$$

Note that for spin deviations $m\leqslant\min\{\lambda_1,\ldots,\lambda_N\}$, a subspace $\mathcal{V}_m$ has the dimension

$$\dim\mathcal{V}_m=\sum_{1\leqslant k_1\leqslant\cdots\leqslant k_m\leqslant N}1=\sum_{1\leqslant j_1<\cdots<j_m\leqslant N+m-1}1=C_{N+m-1}^{m}. \tag{9}$$

From the explicit form of the Gaudin Hamiltonians (3) and from the action (4)–(6) of the $SL(2)$ Lie algebra on the spaces V_{λ_i}, it follows that the weight subspaces $\mathcal{V}_m$ are invariant under the action of any $\mathcal{H}_i$. Therefore, in each subspace $\mathcal{V}_m$, we can construct a basis of common eigenvectors of $\mathcal{H}_i$.

B. The construction of common eigenvectors by Bethe Ansatz

Bethe Ansatz is a method to construct a family of common eigenvectors for Gaudin Hamiltonians in each invariant subspace $\mathcal{V}_m$, but this family is not a basis of $\mathcal{V}_m$.

Since $\mathcal{V}_m$ is generated by (8), any common eigenvector in $\mathcal{V}_m$ has the form

$$\psi_m=\sum_{k_1=1}^{N}\cdots\sum_{k_m=1}^{N}c_{k_1\cdots k_m}F^{(k_1)}\cdots F^{(k_m)}v_0.$$

The central idea of the Bethe method is to consider the coefficients $c_{k_1\cdots k_m}$ as rational complex functions:

$$c_{k_1\cdots k_m}=\frac{1}{w_1-z_{k_1}}\cdots\frac{1}{w_m-z_{k_m}},$$

depending on some unknown, distinct, complex parameters: $w_1,\ldots,w_m$. We call such a vector a Bethe vector. Hereafter we shortly present this method.

1. Bethe vectors of spin deviation m=1

The eigenspace $\mathcal{V}_1$ is generated by vectors $\{F^{(k)}v_0\}_{k=1,\ldots,N}$. A Bethe vector of spin deviation $m=1$ is defined as an expansion on this basis, with rational coefficients depending on one complex parameter w:

$$\psi_1(w)=\mathcal{F}(w)v_0,$$

where we denoted by $\mathcal{F}(w)$ the operator on Ω:

$$\mathcal{F}(w)=\sum_{k=1}^{N}\frac{1}{w-z_k}F^{(k)}. \tag{10}$$

Straightforward calculations give the commutator

$$[\mathcal{H}_i,\mathcal{F}(w)]=\mathcal{F}(w)\frac{H^{(i)}}{(w-z_i)}-\frac{F^{(i)}}{(w-z_i)}\sum_{k=1}^{N}\frac{H^{(k)}}{w-z_k}. \tag{11}$$

Applying this operator on v_0 and using (7) we obtain the action of a Gaudin Hamiltonian $\mathcal{H}_i$ on $\psi_1(w)$:

$$\mathcal{H}_i\,\psi_1(w)=\left(\frac{1}{2}\sum_{j=1;j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}+\frac{\lambda_i}{w-z_i}\right)\psi_1(w)-\left(\sum_{k=1}^{N}\frac{\lambda_k}{w-z_k}\right)\frac{F^{(i)}}{w-z_i}v_0,$$

and we have the following lemma.

Lemma 1: Given N distinct complex numbers $\{z_i\}_{i=1,\ldots,N}$ *and fixed, positive, integer highest weights* $\{\lambda_i\}_{i=1,\ldots,N}$, *the Bethe vector* $\psi_1(w)$ *of spin deviation* $m=1$ *is an eigenvector for all Gaudin Hamiltonians:*

$$\mathcal{H}_i\,\psi_1(w)=s_i^1\,\psi_1(w),\quad \forall i=1,\ldots,N,$$

if the complex parameter w satisfies the condition

$$\sum_{k=1}^{N}\frac{\lambda_k}{w-z_k}=0, \tag{12}$$

called Bethe equation associated to $\mathcal{V}_1$. *The eigenvalue* s_i^1 *of* $\mathcal{H}_i$, *depends on the solution w of this equation:*

$$s_i^1(w)=\frac{1}{2}\sum_{j=1;j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}+\frac{\lambda_i}{w-z_i}.$$

2. Bethe vectors of spin deviation m=2

The eigenspace $\mathcal{V}_2$ is generated by vectors $\{F^{(k_1)}F^{(k_2)}v_0\}_{1\leqslant k_1\leqslant k_2\leqslant N}$. A Bethe vector of spin deviation $m=2$ is defined as an expansion on this basis, with rational coefficients depending on two complex parameters w_1, w_2:

$$\psi_2(w_1,w_2)=\mathcal{F}(w_1)\mathcal{F}(w_2)v_0.$$

Remark that the order of the two operators $\mathcal{F}$ is not significant because they commute.

In order to compute the action of a Hamiltonian on this state, we have to commute $\mathcal{H}_i$ successively with the two operators $\mathcal{F}$. Using (11) we obtain the commutator formula:

$$[[\mathcal{H}_i,\mathcal{F}(w_1)],\mathcal{F}(w_2)]=\frac{2}{w_1-w_2}\left(\frac{F^{(i)}}{w_1-z_i}\mathcal{F}(w_2)-\frac{F^{(i)}}{w_2-z_i}\mathcal{F}(w_1)\right). \tag{13}$$

From (11) and (13) the action of a Gaudin Hamiltonian $\mathcal{H}_i$ on the state ψ_2 is

$$\begin{aligned}\mathcal{H}_i\,\psi_2(w_1,w_2)=&\left(\frac{1}{2}\sum_{j=1;j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}+\frac{\lambda_i}{w_1-z_i}+\frac{\lambda_i}{w_2-z_i}\right)\psi_2(w_1,w_2)-\left(\sum_{k=1}^{N}\frac{\lambda_k}{w_1-z_k}+\frac{2}{w_2-w_1}\right)\\&\times\frac{F^{(i)}}{w_1-z_i}\psi_1(w_2)-\left(\sum_{k=1}^{N}\frac{\lambda_k}{w_2-z_k}+\frac{2}{w_1-w_2}\right)\frac{F^{(i)}}{w_2-z_i}\psi_1(w_1),\end{aligned}$$

and we have the following lemma.

Lemma 2: The Bethe vector $\psi_2(w_1,w_2)$ *of spin deviation* $m=2$ *is an eigenvector for all Gaudin Hamiltonians:*

$$\mathcal{H}_i\,\psi_2(w_1,w_2)=s_i^2\,\psi_2(w_1,w_2),\quad \forall i=1,\ldots,N,$$

if the complex parameters w_1, w_2 *satisfy the Bethe equations associated to* $\mathcal{V}_2$:

$$\sum_{k=1}^{N}\frac{\lambda_k}{w_1-z_k}+\frac{2}{w_2-w_1}=0,\quad \sum_{k=1}^{N}\frac{\lambda_k}{w_2-z_k}+\frac{2}{w_1-w_2}=0. \tag{14}$$

The eigenvalues s_i^2 *depend on the solutions* w_1, w_2 *of these equations:*

$$s_i^2(w_1,w_2)=\frac{1}{2}\sum_{j=1;j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}+\frac{\lambda_i}{w_1-z_i}+\frac{\lambda_i}{w_2-z_i}.$$

3. Bethe vectors of spin deviation m

In the subspace $\mathcal{V}_m$, generated by vectors $\{F^{(k_1)}\cdots F^{(k_m)}v_0\}_{1\leqslant k_1\leqslant\cdots\leqslant k_m\leqslant N}$, a Bethe vector of spin deviation m is defined as an expansion with coefficients depending on m complex parameters $w_1,\ldots,w_m$:

$$\psi_m(w_1,\ldots,w_m)v_0=\mathcal{F}(w_1)\cdots\mathcal{F}(w_m)v_0. \tag{15}$$

The action of a Gaudin Hamiltonian $\mathcal{H}_i$ on this state is calculated by induction on m:

$$\begin{aligned}\mathcal{H}_i\,\psi_m(w_1,\ldots,w_m)v_0&=\mathcal{H}_i\,\mathcal{F}(w_m)\psi_{m-1}(w_1,\ldots,w_{m-1})v_0\\&=\mathcal{F}(w_m)\mathcal{H}_i\psi_{m-1}(w_1,\ldots,w_{m-1})v_0+\psi_{m-1}(w_1,\ldots,w_{m-1})\\&\quad\times[\mathcal{H}_i,\mathcal{F}(w_m)]v_0+[[\mathcal{H}_i,\mathcal{F}(w_m)],\psi_{m-1}(w_1,\ldots,w_{m-1})]v_0.\end{aligned}$$

The first term is computed from the induction hypothesis, the second from (11) and the last term from relation (13). Putting all together it follows that

$$\begin{aligned}\mathcal{H}_i\,\psi_m(w_1,\ldots,w_m)v_0=&\left(\frac{1}{2}\sum_{j=1;j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}+\sum_{k=1}^{m}\frac{\lambda_i}{w_k-z_i}\right)\psi_m(w_1,\ldots,w_m)v_0\\&-\sum_{k=1}^{m}\left(\sum_{j=1}^{N}\frac{\lambda_j}{w_k-z_j}+\sum_{l=1;l\neq k}^{m}\frac{2}{w_l-w_k}\right)\frac{F^{(i)}}{w_k-z_i}\psi_{m-1}(\ldots,\hat{w}_k,\ldots)v_0,\end{aligned} \tag{16}$$

where $\psi_{m-1}(\ldots,\hat{w}_k,\ldots)$ denotes $\psi_{m-1}(w_1,\ldots,w_{k-1},w_{k+1},\ldots,w_m)$. Hence, we obtain the following theorem.

Theorem 3: *The Bethe vector* $\psi_m(w_1,\ldots,w_m)v_0$ *of spin deviation* m *is a common eigenvector for all Gaudin Hamiltonians:*

$$\mathcal{H}_i\,\psi_m(w_1,\ldots,w_m)v_0=s_i^m\,\psi_m(w_1,\ldots,w_m)v_0,\quad\forall i=1,\ldots,N,$$

if the complex parameters $w_1,\ldots,w_m$ *satisfy the Bethe equations associated to* $\mathcal{V}_m$:

$$\sum_{j=1}^{N}\frac{\lambda_j}{w_k-z_j}+\sum_{l=1;l\neq k}^{m}\frac{2}{w_l-w_k}=0,\quad\forall\,k=1,\ldots,m. \tag{17}$$

The eigenvalues s_i^m *depend on the solution of these equations:*

$$s_i^m(w_1,\ldots,w_m)=\frac{1}{2}\sum_{j=1;j\neq i}^{N}\frac{\lambda_i\lambda_j}{z_i-z_j}+\sum_{k=1}^{m}\frac{\lambda_i}{w_k-z_i}.$$

As observed in Ref. 10, the Bethe Ansatz does not give all the common eigenvectors of Gaudin Hamiltonians. Therefore, supplementary common eigenvectors have to be determined, which will be done in the following section.

III. A CONSTRUCTION OF A BASIS OF COMMON EIGENVECTORS FOR GAUDIN HAMILTONIANS

In this section we give a general method to construct a basis of common eigenvectors in each invariant subspace $\mathcal{V}_m$. This is a recursive method, which will be applied for subspaces $\mathcal{V}_m$, with $m \leqslant \min\{\lambda_1, \ldots, \lambda_N\}$. Knowing a basis of $\mathcal{V}_{m-1}$, we construct a family of linear independent common eigenvectors in $\mathcal{V}_m$, which are nonsingular. This family is completed to a basis of $\mathcal{V}_m$ by a basis of the subspace of singular vectors of $\mathcal{V}_m$.

There are two important properties of Gaudin Hamiltonians which are useful in this section, namely they commute with the operators **E** and **F**, on the tensor product module:

$$[\mathcal{H}_i, \mathbf{E}] = 0, \tag{18}$$

$$[\mathcal{H}_i, \mathbf{F}] = 0, \tag{19}$$

where **E** and **F** are defined by (1) as

$$\mathbf{E} = \sum_{i=1}^{N} E^{(i)}, \quad \mathbf{F} = \sum_{i=1}^{N} F^{(i)}.$$

Definition 4: We call $v^s \in \Omega$ a singular vector of Ω if the generator **E** *acts trivially on v^s,*

$$\mathbf{E}\, v^s = 0.$$

We denote Sing *V the subspace of singular vectors in V.*

It was shown in Ref. 11 that the dimension of the subspace $\mathrm{Sing}\,\mathcal{V}_m$ is

$$\dim(\mathrm{Sing}\,\mathcal{V}_m) = C^m_{m+N-2}. \tag{20}$$

Since according to (9), for $m \leqslant \min\{\lambda_1, \ldots, \lambda_N\}$ the dimension of the space $\mathcal{V}_m$ is C^m_{m+N-1}, it follows that a basis of $\mathrm{Sing}\,\mathcal{V}_m$ can be completed to a basis of $\mathcal{V}_m$, by a family of C^{m-1}_{m+N-2} nonsingular linear independent vectors. The space spanned by this family of nonsingular vectors is denoted $\mathrm{NonSing}\,\mathcal{V}_m$. Hence,

$$\mathcal{V}_m = \mathrm{Sing}\,\mathcal{V}_m \oplus \mathrm{NonSing}\,\mathcal{V}_m.$$

From the property (18) we obtain the following.

Lemma 5: $\mathrm{Sing}\,\mathcal{V}_m$ *is a C^m_{m+N-2}-dimensional vector subspace of $\mathcal{V}_m$ and it is $\mathcal{H}_i$-invariant:*

$$\mathcal{H}_i(\mathrm{Sing}\,\mathcal{V}_m) \subseteq \mathrm{Sing}\,\mathcal{V}_m, \quad \forall\, i = 1, \ldots, N.$$

Then $\mathrm{Sing}\,\mathcal{V}_m$ admits a basis formed by singular common eigenvectors of Gaudin Hamiltonians $\mathcal{H}_i$. Denote $\mathcal{B}^s_m$ this basis.

From the property (19) of the Gaudin Hamiltonians we can construct recursively a basis of common eigenvectors in $\mathrm{NonSing}\,\mathcal{V}_m$:

Proposition 6: The basis of common eigenvectors in $\mathrm{NonSing}\,\mathcal{V}_m$ *is obtained by the application of the operator* **F** *on all common eigenvectors (singular and nonsingular) which form the basis of the invariant subspace $\mathcal{V}_{m-1}$. Denote $\mathcal{B}^{ns}_m$ this basis:*

$$\mathcal{B}^{ns}_m = \mathbf{F}(\mathcal{B}_{m-1}),$$

where $\mathcal{B}_{m-1}$ is a basis of common eigenvectors of $\mathcal{V}_{m-1}$.

Proof: (1) The vectors of $\mathcal{B}^{ns}_m$ are linear independent. Indeed, for $m \leqslant \min\{\lambda_1, \ldots, \lambda_N\}$ the operator $\mathbf{F}: \mathcal{V}_{m-1} \to \mathcal{V}_m$ is injective, since $\mathrm{Ker}\,\mathbf{F} = \{0\}$. Moreover, the injectivity of **F** implies that the number of elements of the family $\mathcal{B}^{ns}_m$ is equal to the dimension of $\mathcal{V}_{m-1}$, namely C^{m-1}_{m+N-2}.

(2) The vectors of $\mathcal{B}_m^{ns}$ are common eigenvectors of $\mathcal{H}_i$. If $v_{m-1} \in \mathcal{B}_{m-1}$ is a common eigenvector:

$$\mathcal{H}_i v_{m-1} = a_{m-1}^i v_{m-1},$$

then, from the property (19) it follows that the vector $v_m = \mathbf{F} v_{m-1} \in \mathcal{B}_m^{ns}$ is also an eigenvector, with the same eigenvalue a_{m-1}^i.

(3) The vectors of $\mathcal{B}_m^{ns}$ are nonsingular.

Note first that in $\mathcal{V}_0$ there is only one vector, the vacuum vector v_0. Thus, there is one common eigenvector $v_1 = \mathbf{F} v_0$ in the family $\mathcal{B}_1^{ns}$, which is indeed nonsingular:

$$\mathbf{E} v_1 = \mathbf{E}\mathbf{F} v_0 = \mathbf{H} v_0 = \left(\sum_{i=1}^{N} \lambda_i \right) v_0 \neq 0.$$

Now suppose by induction that for all $k \leqslant m-1$, with $m \leqslant \min\{\lambda_1, \ldots, \lambda_N\}$, we have constructed a basis of $\mathcal{V}_k$ of the form $\mathcal{B}_k^s \cup \mathcal{B}_k^{ns}$, where $\mathcal{B}_k^{ns}$ is obtained by application of the operator $\mathbf{F}$ on vectors of the basis $\mathcal{B}_{k-1}$ of $\mathcal{V}_{k-1}$. Then for a vector v_m^{ns} of $\mathcal{B}_m^{ns}$ we have

$$\mathbf{E} v_m^{ns} = \mathbf{E}\mathbf{F} v_{m-1} = \mathbf{H} v_{m-1} + \mathbf{F}\mathbf{E} v_{m-1} = \left(\sum_{i=1}^{N} \lambda_i - 2(m-1) \right) v_{m-1} + \mathbf{F}\mathbf{E} v_{m-1}. \tag{21}$$

If v_{m-1} is singular, then the last term of (21) vanishes and v_m^{ns} is nonsingular, since

$$\sum_{i=1}^{N} \lambda_i - 2(m-1) \geqslant Nm - 2(m-1) > 0, \quad \forall\, N \geqslant 2.$$

If v_{m-1} is nonsingular, then by the induction hypothesis, there is a $k \in \{1, \ldots, m-1\}$ such that $v_{m-1} = \mathbf{F}^k v_{m-1-k}^s$ with v_{m-1-k}^s a common singular eigenvector of $\mathcal{B}_{m-1-k}^s$. Then relation (21) becomes

$$\mathbf{E} v_m^{ns} = (k+1) \left(\sum_{i=1}^{N} \lambda_i - 2(m-1) + k \right) v_{m-1} \neq 0, \quad \forall\, N \geqslant 2. \tag{22}$$

(4) The vectors of $\mathcal{B}_m^{ns}$ are linear independent of the singular vectors of the basis $\mathcal{B}_m^s$. Consider a null linear combination of the vectors $v_m^{ns}(i) \in \mathcal{B}_m^{ns}$ and $v_m^s(j) \in \mathcal{B}_m^s$:

$$\sum_i a(i)\, v_m^{ns}(i) + \sum_j b(j)\, v_m^s(j) = 0.$$

Applying the operator $\mathbf{E}$, the second sum (of singular vectors) vanishes. Hence,

$$\sum_i a(i)\, \mathbf{E} v_m^{ns}(i) = 0.$$

It follows from (22) that each vector $\mathbf{E} v_m^{ns}(i)$ is colinear with the vector $v_{m-1}(i)$, which form the basis of $\mathcal{V}_{m-1}$. Then, the coefficients $a(i)$ are all zero. Since $v_m^s(j)$ form also a basis, in $\mathrm{Sing}\, \mathcal{V}_m$, the coefficients $b(j)$ vanish too.

Properties (1)–(4) from above show that $\mathcal{B}_m^{ns} = \mathbf{F}(\mathcal{B}_{m-1})$ is a basis of $\mathrm{NonSing}\, \mathcal{V}_m$ and then $\mathcal{B}_m^{ns} \cup \mathcal{B}_m^s$ is a basis of common eigenvectors in $\mathcal{V}_m$. In this basis, the sub-family $\mathcal{B}_m^{ns}$ is completely determined by Proposition 6, whereas for the subset of singular vectors $\mathcal{B}_m^s$ we have only the existence Lemma 5 and not the structure. In the next section we will characterize the singular vectors of a tensor product module of $SL(2)$.

A. Singular vectors of the $SL(2)$ tensor modules

For a finite-dimensional highest weight module V_λ of the Lie algebra $SL(2)$ there is only one singular vector: the highest weight vector v_λ. Nevertheless, for tensor product modules $\Omega=\otimes_{i=1}^{N} V_{\lambda_i}$ the vacuum vector $v_0=\otimes_{i=1}^{N} v_{\lambda_i}$ is not the only singular vector. There exist singular vectors in every subspace $\mathcal{V}_m$.

1. The case N=2

Consider first $N=2$ and $\Omega=V_{\lambda_1}\otimes V_{\lambda_2}$ with the decomposition on invariant subspaces $\Omega=\oplus_{m=0}^{m_{\max}}\mathcal{V}_m$. In this case an invariant subspace $\mathcal{V}_m$ is generated by vectors:

$$\{F^k v_{\lambda_1}\otimes F^{m-k} v_{\lambda_2}\}_{k=0,m},$$

and the singular vectors of such a subspace are characterized by the following proposition.

Proposition 7: Let $\mathcal{V}_m$ be an invariant subspace of $\Omega=V_{\lambda_1}\otimes V_{\lambda_2}$, with $m\leqslant\min\{\lambda_1,\lambda_2\}$. Then a vector $v_m^s\in\mathcal{V}_m$,

$$v_m^s=\sum_{k=0}^{m} c_k F^k v_{\lambda_1}\otimes F^{m-k} v_{\lambda_2},$$

is singular if and only if the coefficients c_k satisfy the conditions

$$c_{k+1}(k+1)(k-\lambda_1)+c_k(m-k)(m-k-1-\lambda_2)=0,\quad \forall k=0,\ldots,m-1. \tag{23}$$

The proof is based on straightforward calculation using relation (5):

$$\begin{aligned}\mathbf{E}\, v_m^s &= E^{(1)} v_m^s + E^{(2)} v_m^s \\ &= \sum_{k=0}^{m-1}\{c_{k+1}(k+1)(\lambda_1-k)+c_k(m-k)(\lambda_2+k+1-m)\}F^k v_{\lambda_1}\otimes F^{m-k-1} v_{\lambda_2}.\end{aligned}$$

Remark that the conditions (23), satisfied by the coefficients c_k, coincide with the conditions determined in Ref. 12, satisfied by the coefficients of a bilinear differential operator which is projective covariant. The system (23) was solved in this article and for $m\leqslant\min\{\lambda_1,\lambda_2\}$ it admits a unique solution (up to a constant factor):

$$c_k=(-1)^k C_m^k\frac{(m-k-\lambda_2)_k}{(-\lambda_1)_k},\quad \forall\, k=0,\ldots,m,$$

with C_m^k the binomial coefficient and $(x)_i$ the Pochhammer symbol:

$$(x)_i=x(x+1)\cdots(x+i-1),\quad \forall\, i\in\mathbb{N}^*,\quad (x)_0=1.$$

By analogy with covariant differential operators, we introduce the bilinear operator P_m defined on the subspace $\mathcal{V}_m$ of $\Omega=V_{\lambda_1}\otimes V_{\lambda_2}$ by

$$P_m(v_1\otimes v_2)=\sum_{k=0}^{m}(-1)^k C_m^k\frac{(m-k-\lambda_2)_k}{(-\lambda_1)_k}F^k v_1\otimes F^{m-k} v_2, \tag{24}$$

which is analogous to the Gordan operator.

Conclusion: In the case of $N=2$ in every invariant subspace $\mathcal{V}_m$ with $m\leqslant\min\{\lambda_1,\lambda_2\}$ there is a unique singular vector (up to a constant factor) which is

$$v_m^s = P_m(v_{\lambda_1} \otimes v_{\lambda_2}) = \sum_{k=0}^{m} (-1)^k C_m^k \frac{(m-k-\lambda_2)_k}{(-\lambda_1)_k} F^k v_{\lambda_1} \otimes F^{m-k} v_{\lambda_2}.$$

2. The case N=3

Consider now $N=3$ and $\Omega = V_{\lambda_1} \otimes V_{\lambda_2} \otimes V_{\lambda_3}$ with its decomposition on invariant subspaces. In this case, a subspace $\mathcal{V}_m$ is generated by vectors:

$$\{F^{k_1} v_{\lambda_1} \otimes F^{k_2} v_{\lambda_2} \otimes F^{m-k_1-k_2} v_{\lambda_3}\}_{\substack{k_1=0,\ldots,m \\ k_2=0,\ldots,m-k_1}},$$

and the singular vectors of this subspace are characterized by the following result.

Proposition 8: Let $\mathcal{V}_m$ be an invariant subspace of $\Omega = V_{\lambda_1} \otimes V_{\lambda_2} \otimes V_{\lambda_3}$, with $m \leqslant \min\{\lambda_1, \lambda_2, \lambda_3\}$. Then a vector v_m^s of $\mathcal{V}_m$,

$$v_m^s = \sum_{k_1=0}^{m} \sum_{k_2=0}^{m-k_1} c_{k_1 k_2} F^{k_1} v_{\lambda_1} \otimes F^{k_2} v_{\lambda_2} \otimes F^{m-k_1-k_2} v_{\lambda_3}, \tag{25}$$

is singular if and only if the coefficients $c_{k_1 k_2}$ satisfy the conditions:

$$c_{k_1+1,k_2}(k_1+1)(k_1-\lambda_1) + c_{k_1,k_2+1}(k_2+1)(k_2-\lambda_2) + c_{k_1,k_2}(m-k_1-k_2)(m-k_1-k_2-1-\lambda_3) = 0, \tag{26}$$

$\forall\, k_1 = 0,\ldots,m-1, \quad \forall\, k_2 = 0,\ldots,m-1-k_1.$

The proof is analogous to that of $N=2$. As in the case $N=2$, we note that the system (26), which has to be satisfied by the coefficients of the development (25) in order that v_m^s be singular, coincides with the conditions given in Ref. 12 for the coefficients of a trilinear differential operator which is projective covariant. The system (26) was also solved in Ref. 12 and for $m \leqslant \min\{\lambda_1, \lambda_2, \lambda_3\}$ it admits $m+1$ linear independent solutions. In addition, it was shown that the space of covariant trilinear operators is generated only by successive applications of covariant bilinear operators.

Conclusion: In the case of $N=3$ in every subspace $\mathcal{V}_m$ with $m \leqslant \min\{\lambda_1, \lambda_2, \lambda_3\}$ there are $m+1$ linear independent singular vectors:

$$\dim(\mathrm{Sing}\, \mathcal{V}_m) = m+1.$$

Moreover, using the operator on Ω introduced in (27) we can construct a basis of $\mathrm{Sing}\, \mathcal{V}_m$, given by the vectors

$$\{v_m^s = \mathbf{P}_{3,k}(\mathbf{P}_{2,m-k}(v_{\lambda_1} \otimes v_{\lambda_2}) \otimes v_{\lambda_3})\}_{k=0,\ldots,m}.$$

3. General case

The results obtained for $N=2$ and $N=3$ can be generalized for an arbitrary N. For each $N \geqslant 2$, consider the space $\Omega = \Omega^N = \Omega^{N-1} \otimes \mathcal{V}_{\lambda_N}$, where $\Omega^{N-1} = \otimes_{i=1}^{N-1} \mathcal{V}_{\lambda_i}$ and define on Ω^N the operator

$$\mathbf{P}_{N,m}(v_1 \otimes v_2) = \sum_{k=0}^{m} (-1)^k C_m^k \frac{(m-k-\lambda_2)_k}{(-\lambda_1)_k} \mathbf{F}^k v_1 \otimes F^{m-k} v_2, \quad \forall\, v_1 \in \Omega^{N-1},\, v_2 \in \mathcal{V}_{\lambda_N}, \tag{27}$$

where $\mathbf{F} = \Sigma_{i=1}^{N-1} F^{(i)}$ is defined by (1) on Ω^{N-1}. Then we have the following.

Proposition 9: Let $\mathcal{V}_m$ be an invariant subspace of Ω^N with $m \leqslant \min\{\lambda_1,\ldots,\lambda_N\}$. Then in $\mathcal{V}_m$ there is a family of C^m_{m+N-2} linear independent singular vectors, given by the formula

$$v^s_m = \mathbf{P}_{N,k}(v^s_{m-k} \otimes v_{\lambda_N}), \quad k=0,\ldots,m, \tag{28}$$

where v^s_{m-k} is a singular vector of weight $\Sigma_{i=1}^{N-1}\lambda_i - 2(m-k)$ in the basis of the subspace Sing $\mathcal{V}_{m-k}$ *of* Ω^{N-1}.

The singularity of these vectors arises from straightforward calculation analogous to the case $N=2$.

These vectors are linear independent because v^s_{m-k} are the elements of the basis of the subspace Sing $\mathcal{V}_{m-k}$ of Ω^{N-1} and for different k the maximal number of operators F applied on the last component v_{λ_N} is different.

The fact that by this construction we obtain exactly C^m_{m+N-2} linear independent singular vectors, can be demonstrated by induction with respect to N: For $N=2$ and $N=3$ this number of singular vectors was already obtained. Suppose now that for an arbitrary N the number of linear independent singular vectors v^s_{m-k} in $\mathcal{V}_{m-k}$ is $C^{m-k}_{m-k+N-2}$. Then for $N+1$, the number of linear independent singular vectors obtained by the construction (28) is

$$\sum_{k=0}^{m} C^{m-k}_{m-k+N-2} = \sum_{j=0}^{m} C^j_{j+N-2} = C^m_{m+N-1}.$$

Proposition 9 allows to construct inductively a basis in Sing $\mathcal{V}_m$ which has the form

$$\{\mathbf{P}_{N,k_{N-1}}(\ldots \mathbf{P}_{3,k_2}(\mathbf{P}_{2,k_1}(v_{\lambda_1}\otimes v_{\lambda_2})\otimes v_{\lambda_3})\cdots \otimes v_{\lambda_N})\}_{\substack{k_i=0,\ldots,m \\ k_1+k_2+\cdots+k_{N-1}=m}}. \tag{29}$$

4. Remark

We point out that in this section we have considered invariant subspaces $\mathcal{V}_m$ of Ω with spin deviation m which does not exceed any of the N weights $\lambda_i \in \mathbb{N}$:

$$m \leqslant \min\{\lambda_1,\ldots,\lambda_N\}.$$

If m is greater than at least one of the weights λ_i, then in the set

$$\{F^{n_1}v_{\lambda_1}\otimes\cdots\otimes F^{n_N}v_{\lambda_N}\}_{n_1+\cdots+n_N=m},$$

there are elements for which the number of operators F acting on v_{λ_i} is greater then λ_i. These vectors are zero because for finite-dimensional irreducible representations of $SL(2)$ we have $F^n v_\lambda = 0$, $\forall\, n \geqslant \lambda+1$. Therefore in this case the dimension of the space $\mathcal{V}_m$ is less than C^m_{m+N-1} and depends on the weights λ which are less than m.

Moreover, if m exceeds one or more of the weights λ, the dimension of the space Sing $\mathcal{V}_m$ is also less than C^m_{m+N-2}. For example, in the case $N=2$, it was shown in Ref. 12 that for $m \leqslant m_{\max}=\lambda_1+\lambda_2$, but $m>\lambda_1$ and $m>\lambda_2$ there are two independent bilinear covariant differential operators, to which correspond singular vectors of the type

$$P_{m-(1+\lambda_1)}(F^{1+\lambda_1}v_{\lambda_1}\otimes v_{\lambda_2}) \quad \text{and} \quad P_{m-(1+\lambda_2)}(v_{\lambda_1}\otimes F^{1+\lambda_2}v_{\lambda_2}),$$

which are zero in the considered finite-dimensional irreducible representations of $SL(2)$. For an arbitrary N we claim that relation (29) still gives the basis of Sing $\mathcal{V}_m$ but some of the elements of the form (29) vanish. This fact implies the decreasing of the dimension of Sing $\mathcal{V}_m$.

B. Singular common eigenvectors and Bethe Ansatz

The basis (29) of $\mathrm{Sing}\,\mathcal{V}_m$ constructed in the previous section is not a basis of common eigenvectors. In this section we show that the Bethe eigenvectors constructed in Sec. II using the Bethe Ansatz are singular, but their number could be less than the dimension of $\mathrm{Sing}\,\mathcal{V}_m$. More precisely, the Bethe equations (17), which appear in the Bethe Ansatz as conditions that Bethe type vectors (15) be common eigenvectors of $\mathcal{H}_i$ are also conditions that Bethe type vectors be singular.

Proposition 10: If the distinct parameters $w_1,\ldots,w_m$ are solutions of the Bethe system:

$$\sum_{j=1}^{N}\frac{\lambda_j}{w_k-z_j}+\sum_{l=1;l\neq k}^{m}\frac{2}{w_l-w_k}=0,\quad \forall\, k=1,\ldots,m, \tag{30}$$

then the corresponding Bethe type vector $\psi_m(w_1,\ldots,w_m)\,v_0=\mathcal{F}(w_1)\cdots\mathcal{F}(w_m)v_0$ of $\mathcal{V}_m$ is a singular vector of the tensor product module Ω.

Proof: Using the commutators,

$$[\mathbf{E},\mathcal{F}(w)]=h(w)\quad \text{and}\quad [h(w_1),\mathcal{F}(w_2)]=\frac{2}{w_1-w_2}(\mathcal{F}(w_1)-\mathcal{F}(w_2)),$$

with $h(w)=\Sigma_{k=1}^{N}[1/(w-z_k)]\,H^{(k)}$, we obtain

$$\mathbf{E}\,\psi_m(w_1,\ldots,w_m)\,v_0=\sum_{i=1}^{m}\left(\sum_{k=1}^{m}\frac{\lambda_k}{w_i-z_k}+\sum_{\substack{k=1\\k\neq i}}^{N}\frac{2}{w_k-w_i}\right)\times\psi_{m-1}(w_1,\ldots,w_{i-1},w_{i+1},\ldots,w_m)\,v_0.$$

Therefore if the parameters $w_1,\ldots,w_m$ are solutions of the system (30), then $\psi_m(w_1,\ldots,w_m)$ is a singular vector.

The number of common Bethe eigenvectors is equal to the number of distinct solutions of the Bethe system (30). If they are C_{m+N-2}^{m} then they form a basis of $\mathrm{Sing}\,\mathcal{V}_m$. For $m=1$ and $m=2$ we can easily show that the number of complex solutions of the Bethe system is $N-1$ and $N(N-1)/2$, respectively, but we cannot say how many of them are distinct. For example, in the case $m=1$, $N=3$, the Bethe equation is equivalent to a second order equation. For some particular values of the parameters λ_i and z_i, $i=1,2,3$, this equation could have a double solution.

For arbitrary m and N, the number of solutions of the Bethe system seems to be C_{m+N-2}^{m} but to our knowledge there is no estimate of the number of distinct solutions. In any case, the Bethe Ansatz gives a family of singular common eigenvectors which could be completed, if necessary, to a basis of $\mathrm{Sing}\,\mathcal{V}_m$ with common eigenvectors constructed using the basis (29).

IV. THE GAUDIN MODEL FOR AN ARBITRARY SIMPLE LIE ALGEBRA *G*

Consider a simple Lie algebra G, of dimension d and rank r. Denote Δ the root system of G, Δ_+ the system of positive roots and Δ_0 the system of simple roots. The Cartan basis of G is formed by the Cartan generators $\{H_i\}_{i=1,\ldots,r}$, the generators of positive roots $\{E_\alpha\}_{\alpha\in\Delta_+}$ and the generators of negative roots $\{F_\alpha=E_{-\alpha}\}_{\alpha\in\Delta_+}$. The commutation relations are

$$[E_\alpha,F_\alpha]=\frac{2}{\langle\alpha,\alpha\rangle}H_\alpha;\quad [H,E_\alpha]=\alpha(H)E_\alpha;\quad [H,F_\alpha]=-\alpha(H)F_\alpha;$$

$$[E_\alpha,E_\beta]=N_{\alpha,\beta}E_{\alpha+\beta},\quad \forall\,\alpha,\beta\in\Delta\ \text{ such that }\ \alpha+\beta\in\Delta.$$

The Killing form of G defines a symmetrical, G-invariant, bilinear form $\langle,\rangle$ on G, which allows us to identify the Cartan sub-algebra $\mathcal{K}$ of G with its dual, by the isomorphism $\alpha(H)=\langle H_\alpha,H\rangle$, for all $H\in\mathcal{K}$. The scalar product on $\mathcal{K}$ induces a scalar product on its dual, which is nondegenerate,

$$\langle\alpha,\beta\rangle=\langle H_\alpha,H_\beta\rangle,$$

normalized such that $\langle\alpha_l,\alpha_l\rangle=2$ for a long root α_l.

All generators of G are orthogonal with respect to the bilinear form $\langle,\rangle$ except

$$\langle H_i,H_i\rangle=\tfrac{1}{2}\chi,\quad \forall i=1,\ldots,r,$$

$$\langle E_\alpha,F_\alpha\rangle=\frac{2}{\langle\alpha,\alpha\rangle},\quad \forall\alpha\in\Delta_+,$$

where $\chi=\Sigma_{i=1}^r\alpha_l^2(H_i)$ is the square of the length of a long root. Then, for the Cartan basis we can define the dual basis with respect to this bilinear form:

$$\tilde{H}_i=\frac{2}{\chi}H_i;\quad \tilde{E}_\alpha=\frac{\langle\alpha,\alpha\rangle}{2}F_\alpha;\quad \tilde{F}_\alpha=\frac{\langle\alpha,\alpha\rangle}{2}E_\alpha,$$

such that $\langle H_i,\tilde{H}_j\rangle=\delta_{ij}$ and $\langle E_\alpha,\tilde{E}_\beta\rangle=\langle F_\alpha,\tilde{F}_\beta\rangle=\delta_{\alpha\beta}$.

For this algebra, consider N finite-dimensional highest weight G-modules, $V_{\lambda_1},\ldots,V_{\lambda_N}$, with dominant integral highest weights $\lambda_1,\ldots,\lambda_N$ and highest weight vectors $v_{\lambda_1},\ldots,v_{\lambda_N}$. The tensor product module of these N G-modules is the space of physical states:

$$\Omega=V_{\lambda_1}\otimes\cdots\otimes V_{\lambda_N}.$$

Recall that the Lie algebra action on this tensor module is defined by (1).

The fundamental building blocks of the generalized Gaudin Hamiltonians are the quadratic generalized Casimir operators, defined on Ω as

$$\omega^{(ij)}=\sum_{a=1}^{d}I_a^{(i)}\tilde{I}_a^{(j)},\quad \forall\, i,j=1,\ldots,N, \tag{31}$$

where $\{I_a\}_{a=1,d}$ is a basis of G and $\{\tilde{I}_a\}_{a=1,d}$ its dual with respect to the scalar product, $\langle I_a,\tilde{I}_b\rangle=\delta_{ba}$. We recall two fundamental properties of these operators, which will be useful in this section.

(1) $\omega^{(ij)}$ are independent of the choice of the basis in G. In particular, in the Cartan basis they take the form

$$\omega^{(ij)}=\frac{2}{\chi}\sum_{l=1}^{r}H_l^{(i)}H_l^{(j)}+\sum_{\alpha\in\Delta_+}\frac{\langle\alpha,\alpha\rangle}{2}(E_\alpha^{(i)}F_\alpha^{(j)}+F_\alpha^{(i)}E_\alpha^{(j)});$$

(2) $\omega^{(ij)}$ commute with the action of the algebra on the tensor module:

$$[\omega^{(ij)},\mathbf{X}]=0,\quad \forall X\in G.$$

The operators $\omega^{(ij)}$ do not commute between themselves, but we can construct N linear combinations which commute.

Lemma 11: The operators $\omega_i:\Omega\to\Omega$, $i=1,\ldots,N$,

$$\omega_i=\sum_{j=1,j\neq i}^{N}c_{ij}\,\omega^{(ij)},$$

commute: $[\omega_i,\omega_j]=0$, $\forall i,j=1,\ldots,N$ *if and only if the coefficients* c_{ij} *satisfy the equations*

$$c_{ik}c_{jk}-c_{ik}c_{ji}-c_{jk}c_{ij}=0, \quad \forall\, i\neq j\neq k\neq i,\ \ i,j,k=1,\ldots,N. \tag{32}$$

In particular, if $z_1,\ldots,z_N$ are distinct complex parameters, the coefficients $c_{ij}=1/(z_i-z_j)$ fulfill the conditions (32). With these coefficients we can construct the following N operators on Ω:

$$\mathcal{H}_i=\sum_{i=1,i\neq j}^{N}\frac{1}{z_i-z_j}\omega^{(ij)}, \tag{33}$$

which are the generalized Gaudin Hamiltonians. They preserve the properties (1) and (2) of the operators $\omega^{(ij)}$. More precisely, if we consider the Cartan basis in G, we have

$$[\mathcal{H}_i,\mathbf{H}_\alpha]=0, \tag{34}$$

$$[\mathcal{H}_i,\mathbf{E}_\alpha]=0, \tag{35}$$

$$[\mathcal{H}_i,\mathbf{F}_\alpha]=0, \tag{36}$$

$\forall\, i=1,\ldots,N$; $\forall\,\alpha\in\Delta_+$, where $\mathbf{H}_\alpha=\Sigma_{i=1}^{N}H_\alpha^{(i)}$, $\mathbf{E}_\alpha=\Sigma_{i=1}^{N}E_\alpha^{(i)}$, $\mathbf{F}_\alpha=\Sigma_{i=1}^{N}F_\alpha^{(i)}$ are operators on the tensor product module, defined by (1). The generalized Gaudin Hamiltonians commute between themselves, but only $N-1$ of them are independent. Due to the property (34) we can complete this system by other r operators, the generators $\mathbf{H}_\alpha$ of the Cartan sub-algebra, which commute with all $\mathcal{H}_i$. For this family of independent and commuting Hamiltonians there is a complete system of common eigenvectors in Ω.

A. The structure of Ω

Since the space Ω is a tensor product of N highest weight representations V_λ of G, it is useful to recall some basic results concerning the theory of highest weight representations of Lie algebras.

Such a representation is completely determined by a highest weight vector v_λ, on which the action of the algebra is given by

$$H_\alpha v_\lambda=\langle\alpha,\lambda\rangle v_\lambda, \quad E_\alpha v_\lambda=0.$$

As in the $SL(2)$ case, the representation space V_λ is linearly generated only by monomials in generators of negative roots:

$$\{v^{n_1\cdots n_l}_{\alpha_1\cdots\alpha_l}=F^{n_1}_{\alpha_1}\cdots F^{n_l}_{\alpha_l}v_\lambda\}_{\alpha_i\in\Delta_+,n_i\in\mathbb{N}}, \tag{37}$$

but in this case, the monomials are ordered with respect to the roots, as showed by the Poincaré–Birkhoff–Witt theorem.[13] These vectors are eigenvectors for the Cartan generators:

$$H_\alpha v^{n_1\cdots n_l}_{\alpha_1\cdots\alpha_l}=\left(\langle\alpha,\lambda\rangle-\sum_{\beta\in\Delta_+}n_\beta\langle\alpha,\beta\rangle\right)v^{n_1\cdots n_l}_{\alpha_1\cdots\alpha_l}, \tag{38}$$

and the action of a positive root generator on monomials $v_\alpha^{n_\alpha}$ is

$$E_\alpha v_\alpha^{n_\alpha}=n_\alpha\left(2\frac{\langle\lambda,\alpha\rangle}{\langle\alpha,\alpha\rangle}-n_\alpha+1\right)v_\alpha^{n_\alpha-1}. \tag{39}$$

Concerning the dimension of a highest weight representation of G, recall that a weight λ is a dominant integral if

$$r_\alpha = 2\frac{\langle \lambda, \alpha\rangle}{\langle \alpha, \alpha\rangle} \in \mathbb{N}, \quad \forall\, \alpha \in \Delta_0 .$$

If the highest weight λ is not dominant integral, then the representation is infinite dimensional and irreducible. If the highest weight λ is dominant integral then there is an invariant subspace, generated by vectors $v^{n_1 \dots n_l}_{\alpha_1 \dots \alpha_l}$, with $n_\alpha \geqslant r_\alpha + 1$.[13] The quotient representation, denoted V_λ is an irreducible, finite-dimensional representation of G, generated by ordered monomials:

$$\{v^{n_1 \dots n_l}_{\alpha_1 \dots \alpha_l} = F^{n_1}_{\alpha_1} \dots F^{n_l}_{\alpha_l} v_\lambda\}_{\alpha_j \in \Delta_+, n_j = 0, \dots, r_{\alpha_j}}.$$

As in the $SL(2)$ case, the space Ω is a finite-dimensional tensor product module of G, completely determined by the vacuum vector $v_0 = v_{\lambda_1} \otimes \cdots \otimes v_{\lambda_N}$ and generated by ordered monomials:

$$F^{(k_1)}_{\alpha_1} F^{(k_2)}_{\alpha_2} \cdots F^{(k_m)}_{\alpha_m} v_0 ,$$

with $1 \leqslant k_i \leqslant N$. Note that for finite-dimensional representations, m can vary between 0 and a maximal value $m_{\max} = \Sigma_{i=1}^N \Sigma_{\alpha \in \Delta_+} r^i_\alpha$. Note also that the action of the Hamiltonians on the vacuum vector is

$$\mathbf{H}_\alpha v_0 = \left(\sum_{k=1}^N \langle \lambda_k, \alpha\rangle \right) v_0 , \quad \alpha \in \Delta_0 ,$$

$$\mathcal{H}_i v_0 = \left(\sum_{j=1, j\neq i}^N \frac{\langle \lambda_i, \lambda_j\rangle}{z_i - z_j} \right) v_0 , \quad i = 1, \dots, N.$$

As in the case of the Lie algebra $SL(2)$, the Cartan operators $\mathbf{H}_\beta$ have the particular role to give a gradation of the tensor product module:

$$\Omega = \oplus \mathcal{V}_\mu ,$$

on weight subspaces $\mathcal{V}_\mu$, of weight $\mu = \Sigma_{i=1}^N \lambda_i - \Sigma_{j=1}^m \gamma_j$, generated by $\mathbf{H}_\beta$ eigenvectors:

$$\mathbf{H}_\beta F^{(k_1)}_{\gamma_1} \cdots F^{(k_m)}_{\gamma_m} v_0 = \left(\sum_{i=1}^N \langle \lambda_i, \beta\rangle - \sum_{j=1}^m \langle \gamma_j, \beta\rangle \right) F^{(k_1)}_{\gamma_1} \cdots F^{(k_m)}_{\gamma_m} v_0 ,$$

with $\gamma_1, \dots, \gamma_m \in \Delta_+$ and $1 \leqslant k_i \leqslant N$. Since a positive root can be written as a sum of simple roots, with positive integer coefficients, in a unique way, the weight subspaces will be labeled by a family of simple roots: $\mathcal{V}_\mu = \mathcal{V}_{\alpha_1 \dots \alpha_s}$, with $\alpha_1 \dots \alpha_s \in \Delta_0$, not necessarily distinct and satisfying $\Sigma_{j=1}^m \gamma_j = \Sigma_{k=1}^s \alpha_k$. Hence

$$\Omega = \oplus \mathcal{V}_{\alpha_1 \dots \alpha_s}.$$

From the explicit form of the generalized Gaudin Hamiltonians (33) and from the action (37)–(39) of the Lie algebra on each module V_{λ_i}, it follows that the weight subspaces $\mathcal{V}_{\alpha_1 \dots \alpha_s}$ are invariant under the action of any $\mathcal{H}_i$. Therefore, in each subspace $\mathcal{V}_{\alpha_1 \dots \alpha_s}$, we can construct a basis of common eigenvectors of $\mathcal{H}_i$.

Unlike the case of the Lie algebra $SL(2)$, there is no result concerning the dimension of the invariant subspaces $\mathcal{V}_{\alpha_1 \dots \alpha_s}$ and neither for Sing $\mathcal{V}_{\alpha_1 \dots \alpha_s}$. However, using the properties (35) and (36), the recursive procedure presented in Sec. III can be generalized to construct in each subspace $\mathcal{V}_{\alpha_1 \dots \alpha_s}$ a family of common nonsingular eigenvectors, by applying operators $\mathbf{F}_{\alpha_i}$ on vectors of the sub-spaces $\mathcal{V}_{\alpha_1 \dots \alpha_{i-1} \alpha_{i+1} \dots \alpha_s}$. Concerning the subspace of singular vectors in

$\mathcal{V}_{\alpha_1 \ldots \alpha_s}$ we do not have a generalization of the result presented in Sec. III A, for the construction of a basis of singular vectors. The only result[4] concerning this problem is a generalization of the Bethe Ansatz, which we discuss hereafter.

B. Common eigenvectors in $\mathcal{V}_\alpha$

Consider a simple root α. The subspace $\mathcal{V}_\alpha$ of weight $\Sigma_{i=1}^N \lambda_i - \alpha$ is generated by vectors $\{F_\alpha^{(k)} v_0\}_{k=1,\ldots,N}$. A Bethe vector in this subspace is defined as an expansion on the basis, with rational coefficients depending on one complex parameter w:

$$\psi_1(w,\alpha)v_0 = \sum_{i=1}^N \frac{F_\alpha^{(i)}}{w-z_i} v_0 = \mathcal{F}(w,\alpha)v_0. \tag{40}$$

To give the action of a Hamiltonian $\mathcal{H}_i$ on this vector it is useful to calculate the commutator:

$$[\mathcal{H}_i, \mathcal{F}(w,\alpha)] = \mathcal{F}(w,\alpha)\frac{H_\alpha^{(i)}}{w-z_i} - \frac{F_\alpha^{(i)}}{w-z_i}\left(\sum_{j=1}^N \frac{H_\alpha^{(j)}}{w-z_j}\right) + \sum_{\beta\in\Delta_+,\beta>\alpha} \frac{\langle\beta,\beta\rangle}{2} N_{\beta,-\alpha}\left\{\mathcal{F}(w,\beta)\frac{E_{\beta-\alpha}^{(i)}}{w-z_i} - \frac{F_\beta^{(i)}}{w-z_i}\sum_{j=1}^N \frac{E_{\beta-\alpha}^{(j)}}{w-z_j}\right\}. \tag{41}$$

Applied on the vacuum vector all the terms of the last sum vanish and the action of a Gaudin Hamiltonian $\mathcal{H}_i$ on the vector (40) is

$$\mathcal{H}_i\psi_1(w,\alpha)v_0 = \left(\sum_{j=1;j\neq i}^N \frac{\langle\lambda_i,\lambda_j\rangle}{z_i-z_j} + \frac{\langle\alpha,\lambda_i\rangle}{w-z_i}\right)\psi_1(w,\alpha)v_0 - \left(\sum_{k=1}^N \frac{\langle\alpha,\lambda_k\rangle}{w-z_k}\right)\frac{F_\alpha^{(i)}}{w-z_i}v_0. \tag{42}$$

Hence we have the following.

Lemma 12: Given N complex numbers $\{z_i\}_{i=1,\ldots,N}$ *and dominant integral highest weights* $\{\lambda_i\}_{i=1,\ldots,N}$, *the Bethe vector* $\psi_1(w,\alpha)v_0$ *is an eigenvector for all Gaudin Hamiltonians:*

$$\mathcal{H}_i\,\psi_1(w,\alpha)v_0 = s_i^1(w,\alpha)\,\psi_1(w,\alpha)v_0, \quad \forall i=1,\ldots,N,$$

if the complex parameter w satisfies the Bethe equation:

$$\sum_{k=1}^N \frac{\langle\alpha,\lambda_k\rangle}{w-z_k} = 0. \tag{43}$$

The eigenvalue $s_i^1(w,\alpha)$ *of the Hamiltonian* $\mathcal{H}_i$ *depends on the solution of this equation:*

$$s_i^1(w,\alpha) = \sum_{j=1;j\neq i}^N \frac{\langle\lambda_i,\lambda_j\rangle}{z_i-z_j} + \frac{\langle\alpha,\lambda_i\rangle}{w-z_i}, \quad i=1,\ldots,N.$$

C. Common eigenvectors in $\mathcal{V}_{\alpha_1,\alpha_2}$

Consider two simple roots α_1 and α_2, which are not necessarily distinct. The subspace $\mathcal{V}_{\alpha_1,\alpha_2}$, of weight $\Sigma_{i=1}^N \lambda_i - \alpha_1 - \alpha_2$ is generated by vectors $\{F_{\alpha_1}^{(k_1)} F_{\alpha_2}^{(k_2)} v_0\}_{k_1,k_2=1,\ldots,N;\ k_1\neq k_2}$, with two generators of negative roots applied on two distinct components of v_0, but also by vectors $\{(F_{\alpha_1}F_{\alpha_2})^{(k)}v_0\}_{k=1,\ldots,N}$ and $\{(F_{\alpha_2}F_{\alpha_1})^{(k)}v_0\}_{k=1,\ldots,N}$ with two generators of negative roots applied on the same component of v_0. A Bethe vector in $\mathcal{V}_{\alpha_1,\alpha_2}$ is defined as an expansion on all these vectors, with some particular coefficients depending on two complex parameters w_1, w_2:

$$\psi_2(w_1,\alpha_1;w_2,\alpha_2)v_0=\sum_{k_1=1}^{N}\sum_{k_2\neq k_1}^{N}\frac{F_{\alpha_1}^{(k_1)}F_{\alpha_2}^{(k_2)}}{(w_1-z_{k_1})(w_2-z_{k_2})}v_0+\frac{1}{w_1-w_2}\sum_{k=1}^{N}\frac{(F_{\alpha_1}F_{\alpha_2})^{(k)}}{w_2-z_k}v_0$$
$$+\frac{1}{w_2-w_1}\sum_{k=1}^{N}\frac{(F_{\alpha_2}F_{\alpha_1})^{(k)}}{w_1-z_k}v_0.$$

As element of the representation space V_{λ_k}, one of the two last terms is not a good ordered monomial and we must write, for instance, $(F_{\alpha_2}F_{\alpha_1})^{(k)}=(F_{\alpha_1}F_{\alpha_2})^{(k)}+[F_{\alpha_2},F_{\alpha_1}]^{(k)}$. Then this vector can be also written in the following form, using the operators $\mathcal{F}$:

$$\psi_2(w_1,\alpha_1;w_2,\alpha_2)v_0=\mathcal{F}(w_1,\alpha_1)\mathcal{F}(w_2,\alpha_2)v_0+\frac{1}{w_1-w_2}\mathcal{F}(w_1,[F_{\alpha_1},F_{\alpha_2}])v_0. \tag{44}$$

In order to compute the action of a Hamiltonian $\mathcal{H}_i$ on the vector ψ_2, we use the result (41) and (42) to obtain

$$\mathcal{H}_i\,\psi_2(w_1,\alpha_1;w_2,\alpha_2)v_0=s_i^2(w_1,w_2)\psi_2(w_1,\alpha_1;w_2,\alpha_2)v_0$$
$$-f_1\left(\frac{F_{\alpha_1}^{(i)}}{w_1-z_i}\mathcal{F}(w_2,\alpha_2)+\frac{1}{w_1-w_2}\frac{[F_{\alpha_1}^{(i)},F_{\alpha_2}^{(i)}]}{w_1-z_i}\right)v_0$$
$$-f_2\left(\mathcal{F}(w_1,\alpha_1)\frac{F_{\alpha_2}^{(i)}}{w_2-z_i}+\frac{1}{w_1-w_2}\frac{[F_{\alpha_1}^{(i)},F_{\alpha_2}^{(i)}]}{w_1-z_i}\right)v_0,$$

where

$$s_i^2=\sum_{j=1;j\neq i}^{N}\frac{\langle\lambda_i,\lambda_j\rangle}{z_i-z_j}+\frac{\langle\alpha_1,\lambda_i\rangle}{w_1-z_i}+\frac{\langle\alpha_2,\lambda_i\rangle}{w_2-z_i},$$

$$f_1=\sum_{k=1}^{N}\frac{\langle\alpha_1,\lambda_k\rangle}{w_1-z_k}+\frac{\langle\alpha_1,\alpha_2\rangle}{w_2-w_1}\quad\text{and}\quad f_2=\sum_{k=1}^{N}\frac{\langle\alpha_2,\lambda_k\rangle}{w_2-z_k}+\frac{\langle\alpha_1,\alpha_2\rangle}{w_1-w_2}.$$

Note that the action of $\mathcal{H}_i$ on the second term of the vector (44) must be calculated separately, because (42) does not hold for the positive root $\alpha_1+\alpha_2$ which is no more simple. It follows from these considerations the following lemma.

Lemma 13: The Bethe vector $\psi_2(w_1,\alpha_1;w_2,\alpha_2)v_0$ is an eigenvector for all Gaudin Hamiltonians,

$$\mathcal{H}_i\,\psi_2(w_1,w_2)v_0=s_i^2\,\psi_2(w_1,\alpha_1;w_2,\alpha_2)v_0,$$

if the parameters w_1, w_2 satisfy the Bethe equations:

$$f_1=\sum_{k=1}^{N}\frac{\langle\alpha_1,\lambda_k\rangle}{w_1-z_k}+\frac{\langle\alpha_1,\alpha_2\rangle}{w_2-w_1}=0,\quad f_2=\sum_{k=1}^{N}\frac{\langle\alpha_2,\lambda_k\rangle}{w_2-z_k}+\frac{\langle\alpha_1,\alpha_2\rangle}{w_1-w_2}=0. \tag{45}$$

D. Common eigenvectors in $\mathcal{V}_{\alpha_1,\ldots,\alpha_m}$

For m simple roots $\alpha_1,\ldots,\alpha_m$, not necessarily distinct, the subspace $\mathcal{V}_{\alpha_1,\ldots,\alpha_m}$ of weight $\Sigma_{i=1}^{N}\lambda_i-\Sigma_{k=1}^{m}\alpha_k$ is generated by ordered monomials $F_{\gamma_1}^{(k_1)}\ldots F_{\gamma_n}^{(k_n)}v_0$ with $k_1,\ldots,k_n$

$=1,\ldots,N$ and $\gamma_1,\ldots,\gamma_n$ positive roots with $\Sigma_{i=1}^{n}\gamma_i=\Sigma_{k=1}^{m}\alpha_k$. In this general case it is difficult to define an appropriate Bethe type vector, with rational coefficients on the basis of $\mathcal{V}_{\alpha_1,\ldots,\alpha_m}$. In Ref. 4. a recursive procedure was proposed to define such a vector:

$$\psi_m(w_1,\alpha_1;\ldots;w_m,\alpha_m)v_0=\psi_{m-1}(w_1,\alpha_1;\ldots;w_{m-1},\alpha_{m-1})\mathcal{F}(w_m,\alpha_m)v_0+\sum_{j=1}^{m-1}\frac{1}{w_j-w_m}$$
$$\times\psi_{m-1}(w_1,\alpha_1;\ldots;w_j,[F_{\alpha_j},F_{\alpha_m}];\ldots;w_{m-1},\alpha_{m-1})v_0, \quad (46)$$

with $\psi_1(w,\alpha)=\mathcal{F}(w,\alpha)$. However, to our knowledge there is no proof that the action of a Hamiltonian $\mathcal{H}_i$ on the vector $\psi_m v_0$ is

$$\mathcal{H}_i\,\psi_m(w_1,\alpha_1;\ldots;w_m,\alpha_m)v_0=s_i^m\psi_m(w_1,\alpha_1;\ldots;w_m,\alpha_m)v_0-\sum_{k=1}^{m}f_k^m\overline{\psi}_m^k v_0, \quad (47)$$

with $\overline{\psi}_m^k$ some vectors in $\mathcal{V}_{\alpha_1,\ldots,\alpha_m}$ and

$$s_i^m=\sum_{j=1;j\neq i}^{N}\frac{\langle\lambda_i,\lambda_j\rangle}{z_i-z_j}+\sum_{k=1}^{m}\frac{\langle\alpha_k,\lambda_i\rangle}{w_k-z_i},\quad f_k^m=\sum_{j=1}^{N}\frac{\langle\alpha_k,\lambda_j\rangle}{w_k-z_j}+\sum_{l=1,l\neq k}^{m}\frac{\langle\alpha_k,\alpha_l\rangle}{w_l-w_k}.$$

Such a recursive construction of generalized Bethe vectors seems to be appropriate for inductive calculations, but for the action (47) of Hamiltonians on these vectors such a calculation raises some problems, as explained in Ref. 10. Similar problems occur if we intend to prove inductively that all Bethe eigenvectors are singular. For a small number of roots this can be done by direct calculation.

We call $v^s\in\Omega$ a singular vector of Ω if all the generators of simple roots $\mathbf{E}_\alpha$ act trivially on v^s:

$$\mathbf{E}_\alpha v^s=0.$$

Note first that $[E_\beta,F_\alpha]=\delta_{\alpha\beta}(2/\langle\alpha,\alpha\rangle)\forall\, i=1,\ldots,N;\ \forall\,\alpha\in\Delta_{+H_\alpha}$ for any simple roots α and β.

Consider now the weight subspace $\mathcal{V}_\alpha$. If β is a simple root we have

$$[E_\beta,\psi_1(w,\alpha)]=\delta_{\alpha\beta}\frac{2}{\langle\alpha,\alpha\rangle}\sum_{i=1}^{N}\frac{H_\alpha^{(i)}}{w-z_i}. \quad (48)$$

Hence,

$$E_\beta\psi_1(w,\alpha)v_0=\delta_{\alpha\beta}\frac{2}{\langle\alpha,\alpha\rangle}\left(\sum_{i=1}^{N}\frac{\langle\alpha,\lambda_i\rangle}{w-z_i}\right)v_0,\quad\forall\,\beta\in\Delta_0.$$

Therefore, if w is a solution of the Bethe equation (43), then $\psi_1(w,\alpha)\,v_0$ is a singular vector of $\mathcal{V}_\alpha$.

In order to calculate the action of a generator E_β of simple root on a generalized Bethe vector (44) of $\mathcal{V}_{\alpha_1,\alpha_2}$, we use (48) but also

$$[E_\beta,\psi_1(w,[F_{\alpha_1},F_{\alpha_2}])]=2\frac{\langle\alpha_1,\alpha_2\rangle}{\langle\beta,\beta\rangle}\{\delta_{\beta\alpha_2}\mathcal{F}(w,\alpha_1)-\delta_{\beta\alpha_1}\mathcal{F}(w,\alpha_2)\},$$

to obtain

$$E_\beta\psi_2(w_1,\alpha_1;w_2,\alpha_2)v_0=\delta_{\beta\alpha_1}\frac{2}{\langle\alpha_1,\alpha_1\rangle}\left\{\sum_{i=1}^{N}\frac{\langle\lambda_i,\alpha_1\rangle}{w_1-z_i}+\frac{\langle\alpha_1,\alpha_2\rangle}{w_2-w_1}\right\}\mathcal{F}(w_2,\alpha_2)v_0$$
$$+\delta_{\beta\alpha_2}\frac{2}{\langle\alpha_2,\alpha_2\rangle}\left\{\sum_{i=1}^{N}\frac{\langle\lambda_i,\alpha_2\rangle}{w_2-z_i}+\frac{\langle\alpha_1,\alpha_2\rangle}{w_1-w_2}\right\}\mathcal{F}(w_1,\alpha_1)v_0.$$

Therefore, if (w_1,w_2) is a solution of the Bethe equations (45), then $\psi_2(w_1,\alpha_1;w_2,\alpha_2)\,v_0$ is a singular vector of $\mathcal{V}_{\alpha_1,\alpha_2}$.

For Bethe vectors (46) depending on more than 3 simple roots we claim that the commutator of E_β with ψ_m is given by

$$[E_\beta,\psi_m(w_1,\alpha_1;\dots w_m,\alpha_m)]=\sum_{i=1}^{m}\delta_{\beta\alpha_i}\frac{2}{\langle\alpha_i,\alpha_i\rangle}\left\{\psi_{m-1}(\dots\widehat{w_i,\alpha_i};\dots)\sum_{j=1}^{N}\frac{H^{(j)}_{\alpha_i}}{w_i-z_j}\right.$$
$$\left.-\left(\sum_{j=1,j\neq i}^{m}\frac{\langle\alpha_i,\alpha_j\rangle}{w_i-w_j}\right)\psi_{m-1}(\dots\widehat{w_i,\alpha_i}\dots)\right\},$$

where $\psi_{m-1}(\dots\widehat{w_i,\alpha_i}\dots)$ denotes $\psi_{m-1}(\dots w_{i-1},\alpha_{i-1};w_{i+1},\alpha_{i+1}\dots)$. As for the action (47) of the Hamiltonians, there is no inductive proof of this relation. The action of E_β on the Bethe vector is then

$$E_\beta\psi_m(w_1,\alpha_1;\dots w_m,\alpha_m)v_0=\frac{2\,\delta_{\beta\alpha_i}}{\langle\beta,\beta\rangle}\left\{\sum_{j=1}^{N}\frac{\langle\alpha_i,\lambda_j\rangle}{w_i-z_j}-\sum_{\substack{k=1\\k\neq i}}^{m}\frac{\langle\alpha_i,\alpha_k\rangle}{w_i-w_k}\right\}\psi_{m-1}(\dots\widehat{w_i,\alpha_i}\dots)v_0.$$

Hence, the Bethe vector is singular if the parameters w satisfy the Bethe equations $f_k^m=0$, $\forall k=1,\dots,m$.

V. CONCLUSIONS

In this article we recall the Gaudin model associated to the Lie algebra $SL(2)$ and its partial diagonalization by the Bethe Ansatz.

We give a general recursive method to construct a basis of common eigenvectors in each invariant subspace $\mathcal{V}_m$. Knowing a basis of $\mathcal{V}_{m-1}$, we construct a family of nonsingular independent common eigenvectors in $\mathcal{V}_m$. This family is completed to a basis of $\mathcal{V}_m$, by a basis of the subspace of singular vectors of $\mathcal{V}_m$.

In order to describe the subspace $\mathrm{Sing}\,\mathcal{V}_m$, we establish a relation between singular vectors and covariant differential operators. This allows us to construct a basis of $\mathrm{Sing}\,\mathcal{V}_m$ using an analog of the Gordan operator. On the other hand we show that the Bethe Ansatz gives a family of singular common eigenvectors. If Bethe equations have a maximal number of distinct solutions, then Bethe eigenvectors form a basis of common eigenvectors in $\mathrm{Sing}\,\mathcal{V}_m$.

We discuss also the generalization of this method to the case of an arbitrary Lie algebra. We recall the generalization of the Gaudin Hamiltonians and of the Bethe Ansatz. The generalized Bethe vectors are defined recursively, but this definition allows neither to calculate the action of the Hamiltonians, nor to prove that Bethe eigenvectors are singular. For a small number of simple roots we prove by direct calculation that the Bethe equations are conditions that Bethe type vectors be singular and common eigenvectors. The recursive method to construct nonsingular common eigenvectors could also be generalized to the case of an arbitrary Lie algebra.

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The Painlevé analysis for $N=2$ super Korteweg–de Vries equations

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The Painlevé analysis of a generic multiparameter $N=2$ extension of the Korteweg–de Vries (KdV) equation is presented. Unusual aspects of the analysis, pertaining to the presence of two fermionic fields, are emphasized. For the general class of models considered, we find that the only ones which manifestly pass the test are precisely the four known integrable supersymmetric KdV equations, including the SKdV_1 case. © *2001 American Institute of Physics.*
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I. MOTIVATION AND SUMMARY OF THE RESULTS

Even in its simplest form, the Painlevé analysis,[1] as applied to a multiparameter class of equations, is a powerful tool for identifying those special values of the parameters for which the equations are potentially integrable.

However, for fermionic—and in particular, supersymmetric—extensions of known integrable systems, the application of the test is made a little tricky by the presence of fermionic fields[2,3] and actually very few systems have been fully studied so far (see also Ref. 4). For a single fermionic extension (with a fermionic field of degree 3/2 in the normalization where the degree of ∂_x is 1) of the Korteweg–de Vries (KdV) equation, which contains 3 free parameters, the test has selected the very two integrable nontrivial extensions of the KdV equation, namely, the Kuper–KdV (Ref. 5) (which is not invariant under supersymmetry) and the supersymmetric KdV (sKdV-the small s refers to $N=1$) equation[6,7,8]—the latter being called here the sKdV_3 equation for reasons explained below. There is an additional integrable supersymmetric system[6,9] which will be referred to, in the following, as the sKdV_0 equation. Although the latter is somewhat trivial in that the fermionic fields do not appear in the bosonic evolution equations (and for this reason it was excluded from the generic family considered in Ref. 2), this will not be an issue here.[10] That the integrability of these models had already been established by other means supports the validity of the application of the test, or more precisely, its reliability as an integrability indicator, in the presence of fermionic fields.

No similar studies have been performed for the extension of the KdV equation with two fermions and an additional bosonic field. Six such systems are known to be integrable: the three usual $N=2$ supersymmetric KdV (SKdV, the capital S is used for $N=2$) equations, i.e., the SKdV_a equation (where a is a free parameter in a second Hamiltonian formulation) for $a=-2$, 1, 4, [11,12,13] the $\mathrm{SKdV}_{\mathcal{O}}$ (where the subscript stands for ''odd'') equation,[14] which has an *odd* Poisson bracket formulation, the SKdV-B equation[15] and the osp(2, 2) KdV equation, the direct extension of the Kuper-KdV equation (which is thus not invariant under $N=2$ supersymmetry).[11,16] (See note added in proof.)

The details of the Painlevé analysis of these systems has never been presented in the literature. Actually, it has been claimed that for the SKdV_1 equation, the test is failed (see in particular the concluding remarks in Ref. 13). The particular interest for this case, at the time, was due to its conjectural integrability status for some years before the discovery of its Lax formulation in Ref. 13. But given that this system is now known to be integrable,[17] that it does not have the Painlevé

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property sounds as an extremely surprising statement. Clearly, the failure of the Painlevé test is not by itself a clear indication of nonintegrability. For instance, the equation might have to be somewhat transformed in order to successfully pass the test. However, in a multiparameter deformation of an equation, we definitely expect that if the test is satisfied for some values of the parameters (corresponding to a known integrable system), it should be equally satisfied for all other values of the parameters for which the equations are known to be integrable. But to rule on the $SKdV_1$ equation, we need to perform the test for the other cases too in order to see if, in the presence of two fermionic fields, it is again a reliable integrability indicator.

The natural expectation is that all six extended KdV equations known to be integrable should have the Painlevé property. However, precisely because there are two fermions, the test displays unusual features. This point in itself is certainly not surprising given some of the odd technical aspects of the test as applied to a single fermionic extension of the KdV equation.[2,3] Clearing up the status of the Painlevé property for the $SKdV_1$ equation was our first motivation for this work.

We present here the result of a ''complete'' Painlevé analysis for four supersymmetric integrable systems [excluding the SKdV-B equation by requiring an $O(2)$ invariance, see below]. More precisely, we perform a simplified analysis, in which, in addition to verifying the plain properties of a genuine pole behavior of the leading singularities and the integrality of the resonance positions, we only check the compatibility conditions at the non-negative resonances. The qualitative ''complete'' refers to the fact that we consider the full set of four evolution equations in each case. In addition to be rather complicated, even though the analysis is done with the simplified Kruskal ansatz,[18] it reveals an unusual feature: in two cases out of four (and this includes the $SKdV_1$ equation), in order to verify the last resonance conditions—whenever this resonance is bosonic—say, at level n, we need to solve the set of recursion equations at level $n+1$. In other words, at first sight the compatibility conditions are *not* satisfied. However, they involved some field components that get determined only at the next recursion level. But when this is done and the solutions are substituted back into the level n resonance relations, the compatibility conditions are found to be satisfied. We thus conclude that, in this context, the Painlevé test is still in par with the other integrability indicators.

A second motivation for this work was to initiate the search for new integrable $N=2$ extensions of the KdV equations by using the Painlevé property as a probing tool to test generic deformations of the known SKdV equations. In the present work we treat the most general deformation (which contains 4 free parameters) compatible with a natural $O(2)$ invariance.

Instead of starting with a brute force analysis of this four-parameter equation, we use a simple observation in order to constrain these parameters, which is that the reduction (by which we mean setting some fields equal to zero) of an integrable system has to be integrable. For instance, a clear signal of this integrability persistence is that, after the reduction of an integrable system, there remains an infinite number of conservation laws. In particular, the $N=1$ reduction of an integrable SKdV equation has to be either the $sKdV_3$ or $sKdV_0$ equations. This fixes two parameters and selects two classes of two-parameter equations. Another simplifying feature of the above observation is that the bosonic core of the full set of equations (obtained by setting the two fermionic fields equal to zero) must also be integrable. The analysis of such bosonic systems (here a system of two coupled evolution equations) is much easier and puts severe constraints on the remaining parameters. In fact, the bosonic core of the test is satisfied (modulo a technical restriction discussed below) for only four cases, which are precisely *the four known integrable supersymmetric systems*.

Our search for new systems is thus unsuccessful. The results suggest in particular, that (most probably) there are no integrable deformations of the $SKdV_{\mathcal{O}}$ equation.

The analysis of the complete fermionic systems is then performed case by case and the Painlevé property is verified in all four cases, as already mentioned.

We should point out a technical limitation of the present analysis, which is restricted to the study of the so-called *principal family*—in the terminology of Ref. 19. That means that we only look for non-negative resonances, in addition to the resonance at level $n=-1$. For a complete analysis, solutions with negative resonances must also be considered. The perturbative Painlevé

test[19] provides a method for investigating such solutions. However, there is no finite algorithm ensuring the absence of movable logarithms (only for the principal families one can guarantee that the system has the Painlevé property). As a result, the computations are much more involved. We intend to return to this question elsewhere. Here we only indicate the cases where the negative resonances occur but without further analysis. Our statements concerning the nonexistence of new integrable systems must thereby be tinged by this technical restriction.

The article is organized as follows: In Sec. II, we present the general class of $N=2$ supersymmetric equations to be studied and discuss the constraints resulting from integrability under truncation to $N=1$ supersymmetric equations. The general structure of the recursion relations is displayed in Sec. III. The delicate question of fixing the dominant resonance of the fermionic fields is discussed in full detail in Appendix B. In the following section, we present the essential results of the bosonic-core analysis, relegating the details to Appendix A. This analysis turns out to be rather involved, necessitating the consideration of a large number of special cases. Finally, Sec. V presents a brief discussion of the study of the equations incorporating the fermionic fields. Here we only present the salient features of the SKdV_1 case and briefly comment on the differences that occur in the other cases. Our conclusions are reported in Sec. VI.

II. THE GENERAL EQUATIONS AND THE $N=1$ CONSTRAINTS

The $N=1$ supersymmetrization of the KdV equation,

$$u_t=-u_{xxx}+6uu_x \tag{2.1}$$

is obtained by extending the u field to a fermionic superfield as

$$u(x)\to\phi(x,\theta)=\theta u(x)+\xi(x). \tag{2.2}$$

Here θ is a Grassmannian variable ($\theta^2=0$) and ξ is a fermionic field, $\xi(x)\xi(x')=-\xi(x')\xi(x)$. The direct supersymmetrization reads[6,20]

$$\phi_t=-\phi_{xxx}+c(\phi D\phi)_x+(6-2c)\phi_x(D\phi), \tag{2.3}$$

where c is a free parameter and D is the superderivative; $D=\theta\partial_x+\partial_\theta$ so that $D^2=\partial_x$. It turns out that this equation is integrable only if $c=0$ or 3.[6] We call the resulting equation the sKdV_c equation. Its component version reads

$$\begin{aligned} u_t&=-u_{xxx}+6uu_x-c\xi\xi_{xx},\\ \xi_t&=-\xi_{xxx}+(6-c)u\xi_x+cu_x\xi. \end{aligned} \tag{2.4}$$

For $c=0$ we see that ξ decouples from the first equation.[21]

The $N=2$ superextension is obtained by lifting u to a bosonic superfield defined as follows (with the time dependence being implicit):

$$\Phi(x,\theta_1,\theta_2)=\theta_2\theta_1u(x)+\theta_1\xi^{(2)}(x)+\theta_2\xi^{(1)}(x)+w(x). \tag{2.5}$$

$\xi^{(1)}$ and $\xi^{(2)}$ are two fermionic fields and w is a new bosonic field. Using the superderivatives,

$$D_i=\theta_i\partial_x+\partial_{\theta_i}\Rightarrow D_i^2=\partial_x\quad(i=1,2)\quad D_1D_2=-D_2D_1, \tag{2.6}$$

the most general version (subject to some restrictions to be specified shortly) of the $N=2$ extension of the KdV equation reads

$$\Phi_t=-\Phi_{xxx}+\alpha_1\Phi D_1D_2\Phi_x+\alpha_2\Phi_xD_1D_2\Phi+\frac{\alpha_3}{2}(D_1D_2\Phi^2)_x+\frac{\alpha_4}{3}(\Phi^3)_x. \tag{2.7}$$

This equation contains all possible terms that are compatible with an homogeneity requirement under a gradation defined by $\deg \Phi = 1$, $\deg D_i = 1/2$, and the $O(2)$ invariance, that is, invariance under the transformation $\Phi \to -\Phi$ and $D_1 \leftrightarrow D_2$. {For instance, terms like $[D_1(\Phi_x D_2 \Phi) - D_2(\Phi_x D_1 \Phi)]$ or $[D_1(\Phi D_2 \Phi_x) - D_2(\Phi D_1 \Phi_x)]$ or even $[(D_1\Phi)(D_2\Phi_x) - (D_2\Phi)(D_1\Phi_x)]$ are not independent, i.e., they are linear combinations of those already given.}

The $N=1$ reduction is obtained by setting

$$\Phi(x, \theta_1, \theta_2) = \theta_2 \phi(x, \theta_1) + \mathcal{F}(x, \theta_1) \tag{2.8}$$

and keeping only the linear terms in θ_2 with $\mathcal{F}=0$. All *integrable* versions of this four-parameter equation *must reduce* to the sKdV_c equation for either $c=0$ or 3. This fixes two parameters,

$$\alpha_1 = c, \quad \alpha_2 = 6 - c. \tag{2.9}$$

The other two are redefined as follows:

$$\alpha_3 = \alpha - 1, \quad \alpha_4 = \beta, \tag{2.10}$$

and we are left with two distinct two-parameter equations,

$$\Phi_t = -\Phi_{xxx} + c\Phi D_1 D_2 \Phi_x + (6-c)\Phi_x D_1 D_2 \Phi + \frac{\alpha - 1}{2}(D_1 D_2 \Phi^2)_x + \beta \Phi^2 \Phi_x \tag{2.11}$$

$(c = 0,3)$. In terms of component fields, it leads to four coupled equations,

$$\begin{aligned} u_t &= -u_{xxx} + 6uu_x - c\xi^{(i)}\xi^{(i)}_{xx} - cww_{xxx} - (6-c)w_x w_{xx} \\ &\quad - \frac{\alpha - 1}{2}(w^2)_{xxx} + \beta(uw^2)_x + 2\beta(\xi^{(2)}\xi^{(1)}w)_x, \\ \xi^{(i)}_t &= -\xi^{(i)}_{xxx} + cu_x\xi^{(i)} + (6-c)u\xi^{(i)}_x - c\epsilon_{ij}\xi^{(j)}_{xx}w - (6-c)\epsilon_{ij}\xi^{(j)}_x w_x \\ &\quad - (\alpha - 1)\epsilon_{ij}(\xi^{(j)}w)_{xx} + \beta(\xi^{(i)}w^2)_x, \\ w_t &= -w_{xxx} + cu_x w + (6-c)uw_x + (\alpha - 1)(uw + \xi^{(2)}\xi^{(1)})_x + \beta w^2 w_x \end{aligned} \tag{2.12}$$

with $i,j = 1, 2$ and $\epsilon_{12} = -\epsilon_{21} = 1$.

III. THE PAINLEVÉ ANALYSIS: RECURSION RELATIONS

We next proceed with the Painlevé analysis by solving the recursion equations in order to find those values of the parameters α and β for which the test is satisfied. In the present work, we content ourself with a minimal version of the test, which consists in verifying:

(1) That the leading singularity is an integer (i.e., polelike);
(2) The resonances occur at integer levels;
(3) The compatibility conditions are satisfied at the non-negative resonances.

We will further give all possible solutions with integer resonances but without further analysis of these last cases.

The expansion of the component fields about a movable singular manifold $\varphi(x,t)$ reads

$$u = \sum_{n=0}^{\infty} u_n \varphi^{n-p}, \quad \xi^{(i)} = \sum_{n=0}^{\infty} \xi^{(i)}_n \varphi^{n-r}, \quad w = \sum_{n=0}^{\infty} w_n \varphi^{n-q} \tag{3.1}$$

($i=1,2$). By symmetry, the value of the leading singularity must be the same for the two fermionic fields. To simplify the analysis, we will use the Kruskal's ansatz,

$$\varphi(x,t)=x-f(t),\ \ u_n=u_n(t),\ \ \xi_n^{(i)}=\xi_n^{(i)}(t),\ \ w_n=w_n(t). \tag{3.2}$$

The first step amounts to fix the leading singularity; we easily find that $p=2$, $q=1$. Note that this is a consequence of the SKdV degree-homogeneity already mentioned: setting $\deg(\partial_x)=1$, it follows that $\deg(u)=2$ and $\deg(w)=1$. Now since $\deg(\varphi)=\deg(x)=-1$ and u_0 and w_0 are constants, hence of degree zero, we thus conclude that $\deg(u)=2$ and $\deg(w)=1$ only if $p=2$ and $q=1$.

The determination of the leading singularity for the fermionic fields is a bit tricky (see for instance Ref. 3); it is shown in appendix B that $r=2$ is a solution and all other possible solutions do not pertain to a principal family. However, for the rest of this section, we leave r unspecified since the recursion relations themselves are needed to fix it, cf. Appendix B. Moreover, the precise value found for r depends explicitly on the first bosonic terms and these are fixed from the bosonic-core analysis.

A direct substitution of (3.1), (3.2) with $p=2$, $q=1$ into (2.12) leads to the general recursion formulas

$$\begin{aligned}
u_{n-3,t}+(n-4)u_{n-2}\varphi_t=&-(n-2)(n-3)(n-4)u_n+3(n-4)\\
&\times\sum_{m=0}^{n}u_{n-m}u_m-(\alpha-1+c)\sum_{m=0}^{n}(m-1)(m-2)(m-3)w_{n-m}w_m\\
&-\frac{1}{2}(3\alpha+3-c)(n-4)\sum_{m=0}^{n}(n-m-1)(m-1)w_{n-m}w_m+\beta(n-4)\\
&\times\sum_{m=0}^{n}\sum_{l=0}^{m}u_{u-m}w_{m-l}w_l+\frac{1}{2}c(n-4)\\
&\times\sum_{m=0}^{n+2r-3}(n+2r-3-2m)\xi^{(i)}_{n+2r-3-m}\xi^{(i)}_m+2\beta(n-4)\\
&\times\sum_{m=0}^{n+2r-3}\sum_{l=0}^{m}\xi^{(2)}_{n+2r-3-m}\xi^{(1)}_{m-l}w_l
\end{aligned}$$

$$\begin{aligned}
\xi^{(i)}_{n-3,t}+(n-r-2)\xi^{(i)}_{n-2}\varphi_t=&-(n-r)(n-r-1)(n-r-2)\xi^{(i)}_n\\
&+c\sum_{m=0}^{n}(n-m-2)u_{n-m}\xi^{(i)}_m+(6-c)\\
&\times\sum_{m=0}^{n}(m-r)u_{n-m}\xi^{(i)}_m+\beta(n-r-2)\\
&\times\sum_{m=0}^{n}\sum_{l=0}^{m}\xi^{(i)}_{n-m}w_{m-l}w_l-c\sum_{m=0}^{n}(n-m-r)(n-m-r-1)\\
&\times\epsilon_{ij}\xi^{(j)}_{n-m}w_m-(6-c)\sum_{m=0}^{n}(n-m-r)(m-1)\epsilon_{ij}\xi^{(j)}_{n-m}w_m\\
&-(\alpha-1)(n-r-1)(n-r-2)\sum_{m=0}^{n}\epsilon_{ij}\xi^{(j)}_{n-m}w_m
\end{aligned} \tag{3.3}$$

$$w_{n-3,t}+(n-3)w_{n-2}\varphi_t=-(n-1)(n-2)(n-3)w_n+c\sum_{m=0}^{n}(n-m-2)u_{n-m}w_m+(6-c)$$
$$\times\sum_{m=0}^{n}(m-1)u_{u-m}w_m+(\alpha-1)(n-3)\sum_{m=0}^{n}u_{n-m}w_m+\frac{1}{3}\beta(n-3)$$
$$\times\sum_{m=0}^{n}\sum_{l=0}^{m}w_{n-m}w_{m-l}w_l+(\alpha-1)(n-3)\sum_{m=0}^{n+2r-3}\xi^{(2)}_{n+2r-3-m}\xi^{(1)}_m.$$

Here n takes any integer value from $\min(3-2r,0)$ to ∞ (sticking to the principal family). It is understood that every field-component with a negative index is zero. For the system of equations to be integrable, the solution needs to contain a sufficient number of arbitrary functions. For the case under study, the system being composed of four coupled third order equations, there should be twelve arbitrary functions, six bosonic and six fermionic. With the leading singularities fixed, we need to determine those (recursion) levels n—the resonances—in (3.3) for which there are arbitrary functions. That clearly requires n to be an integer. At each such level, the equation must vanish identically without enforcing any constraints on the lower-order arbitrary functions. These are the compatibility conditions at the resonances. We then proceed in two steps. We first find all the possible values of the free parameters for which the bosonic-core system has the Painlevé property. Then, for those special parameters, we complete the analysis for the full system with the fermionic fields reintroduced.

IV. THE PAINLEVÉ ANALYSIS OF THE BOSONIC CORE

The bosonic-core analysis is the most important and also the most involved part of this work. It amounts to consider one-by-one a long sequence of special cases. Although the analysis is straightforward for most of them, there is a number of cases (that include cases in which the test is satisfied) for which this is not so. For this reason, a somewhat detailed presentation of all the possibilities is required. It is reported in Appendix A. For the ease of reading, we collect in this section the final results of this Appendix.

The only cases for which the Painlevé property of the bosonic core is fully satisfied are listed below. Note that the ''body'' (i.e., without the nilpotent part) values of u_0 and w_0 represent an important part of the data since it is necessary to fix uniquely the leading singularity of the fermionic fields. Here, $k=\pm i$,

(I) SKdV_{-2}

$c=3,\ \alpha=-2,\ \beta=-6,\ u_0=-1,\ w_0=k;$

(II) SKdV_1

$c=3,\ \alpha=1,\ \beta=3,\ u_0=1,\ w_0=k;$

(III) SKdV_4

$c=3,\ \alpha=4,\ \beta=12,\ u_0=\frac{1}{2},\ w_0=\frac{1}{2}k;$

(IV) $\mathrm{SKdV}_{\mathcal{O}}$

$c=0,\ \alpha=1,\ \beta=0,\ u_0=1,\ w_0=k;$

(V) SKdV_{-2} (''degenerate'' case)

$c=3,\ \alpha=-2,\ \beta=-6,\ u_0=2,\ w_0=0.$

Cases (I)–(V) are those with nonnegative resonances. For completeness, we also present all other possible solutions that are not in principal families. These are listed below. It is always understood that j_1, k_1, and k_2 are integers,

(VI) $c=3,\ \alpha=\frac{1}{2}j_1(j_1-3)-1,\ \beta=\frac{3}{2}j_1(j_1-3)-1,$

$$u_0=2, \qquad w_0=0$$

$$(j_1\geqslant 4);$$

(VII) $$c=3,\ \alpha=\frac{6k_1}{k_1(3-k_2)+k_2(k_2+1)-6}-2,$$

$$\beta=108\frac{k_1-2}{(k_1(3-k_2)+k_2(k_2+1)-6)^2},$$

$$u_0=\tfrac{1}{6}(k_1(3-k_2)+k_2(k_2+1)-6),$$

$$w_0=ku_0$$

$$(k_1\geqslant\max(5,2k_2+1),\ k_2\geqslant -1);$$

(VIII) $$c=3,\ \alpha=\frac{6k_1}{k_1(3-k_2)+k_2(k_2+1)-6}-2,$$

$$\beta=108\frac{k_1-2}{(k_1(3-k_2)+k_2(k_2+1)-6)^2},$$

$$u_0=\tfrac{1}{6}(k_1(3-k_2)+k_2(k_2+1)-6),$$

$$w_0=ku_0$$

$$(k_1\geqslant 5,\ k_2\leqslant -4);$$

(IX) $$c=3,\ \alpha=2\frac{7-k_1^2}{2+k_1^2},\quad \beta=\frac{108}{(2+k_1^2)^2},$$

$$u_0=\tfrac{1}{6}(2+k_1^2),\ w_0=ku_0$$

$$(k_1\geqslant 5);$$

(X) $$c=3,\ \alpha=-4\frac{k_1}{5k_1+6},\ \beta=108\frac{k_1}{(5k_1+6)^2},$$

$$u_0=\tfrac{5}{6}k_1+1, \qquad w_0=ku_0$$

$$(k_1\leqslant -7);$$

(XI) $$c=3,\ \alpha=-4\frac{k_1}{5k_1+6},\ \beta=108\frac{k_1}{(5k_1+6)^2},$$

$$u_0=\tfrac{5}{6}k_1+1, \qquad w_0=ku_0$$

$$(k_1\geqslant 3);$$

(XII) $c=0,\ \alpha=7,\ u_0=2,\ w_0=0;$

(XIII) $c=0,\ \alpha=1,\ u_0=2,\ w_0=0;$

(XIV) $c=0,\ \alpha=-\frac{7}{31},\ \beta=-\frac{78}{961},\ u_0=-31,\ w_0=ku_0;$

(XV) $c=0,\ \alpha=-\frac{5}{21},\ \beta=-\frac{6}{49},\ u_0=-21,\ w_0=ku_0;$

(XVI) $c=0,\ \alpha=-\frac{1}{7},\ \beta=\frac{15}{98},\ u_0=14,\ w_0=ku_0;$

(XVII) $c=0,\ \alpha=-\frac{7}{5},\ \beta=0,\ u_0=-5,\ w_0=ku_0.$

V. THE PAINLEVÉ ANALYSIS OF THE FULL FERMIONIC SYSTEMS OF THE FOUR INTEGRABLE $N=2$ SUPERSYMMETRIC SYSTEMS

In a second step, the Painlevé analysis is completed for the fermionic extension of the successful bosonic systems. We omit the details of the $\mathrm{SKdV}_{-2,4,\mathcal{O}}$ analysis and sketch some aspects of the analysis of the SKdV_1 equation.

A. Analysis of the SKdV_1 equation

In Appendix B, it is shown that the leading singularity of fermionic fields must be $r=2$ and that the following condition must hold:

$$\xi_0^{(2)}=k_0\xi_0^{(1)}, \tag{5.1}$$

where $k_0^2=-1$.[22] With this condition, (3.3) for $n=-1$, which reads

$$-30\alpha\xi_0^{(1)}\xi_0^{(2)}w_0=0,\ \ -4(\alpha-1)\xi_0^{(1)}\xi_0^{(2)}=0, \tag{5.2}$$

is automatically satisfied.

From the resonance equations obtained in Appendices A and B, the bosonic resonances must occurs at the roots of

$$(n+1)(n-1)(n-2)(n-3)(n-4)(n-6)=0 \tag{5.3}$$

corresponding to the arbitrariness of φ, w_1, w_2, w_3, u_4, and w_6, whereas the fermionic ones are determined by the roots of

$$n(n-2)^2(n-4)^2(n-6)=0 \tag{5.4}$$

corresponding to the arbitrariness of $\xi_0^{(1)}$, $\xi_2^{(1)}$, $\xi_2^{(2)}$, $\xi_4^{(1)}$, $\xi_4^{(2)}$, and $\xi_6^{(1)}$.

The introduction of the fermionic fields brings a little complexity right at the beginning of the analysis in that it is necessary to use both the $n=0$ and $n=1$ conditions in order to fix u_0, $\xi_0^{(i)}$, and w_0 unambiguously. Once this is settled, the remaining part of the analysis is straightforward, apart from the plain fact that the equations are rather complicated.

The most general solution to the recursion formulas at level $n=0$, for which the bosonic part reduces to the one found in the bosonic-core analysis (with constant k appearing in w_0 fixed to $k=-k_0$, as shown in Appendix B), is

$$u_0=1-\tfrac{2}{3}\lambda_0\xi_0^{(1)},\ \ \xi_0^{(2)}=k_0\xi_0^{(1)},$$

$$w_0=-k_0+\lambda_0\xi_0^{(2)},\ \ \xi_1^{(2)}=k_0\xi_1^{(1)}+\tfrac{4}{3}k_0\lambda_0+k_1\xi_0^{(2)}, \tag{5.5}$$

where $k_0^2=-1$, k_1 is a (even) constant, λ_0 is a fermionic constant, and $\xi_0^{(1)}$ is an arbitrary fermionic function.

In order to fix uniquely u_0 and w_0, we need to consider the equations for $n=1$. At this level, a substitution of (5.5) into the recursion equations leads to ($k_0^2=-1$)

$$u_0=1,\ \xi_0^{(1)}\text{arbitrary},\ \xi_0^{(2)}=k_0\xi_0^{(1)},\ w_0=-k_0,$$

$$u_1=0,\ \xi_1^{(1)}=0,\ \xi_1^{(2)}=0,\ w_1=0. \tag{5.6}$$

Pursuing the analysis of (3.3), one can verify that all the compatibility conditions at the various resonances are satisfied. Since the resulting equations are very long, this part of the analysis will be omitted. Notice that since the equation for w_6 depends upon the value of $\xi_7^{(i)}$ ($i=1,2$), we have to go up to level $n=7$ to fix completely the different nonarbitrary functions needed to verify this particular compatibility condition. The analysis for levels $n=5$ to $n=7$ is actually very complicated; the computations have been made with Maple (with the package Grassmann).

B. Comments on the other three cases

The analysis for the other three cases singled out by the bosonic-core analysis has also been performed successfully.

For the SKdV$_{-2}$ equation, only one of the two possible cases identified by the bosonic-core analysis is found to have the Painlevé property; this is case (I). The analysis for this case is not too difficult since the last resonance is fermionic, occurring at level $n=5$, so that we only have to push the analysis up to this level. The arbitrary functions are φ, $\xi_0^{(1)}$, u_1, $\xi_2^{(1)}$, u_3, $\xi_3^{(1)}$, w_3, u_4, $\xi_4^{(1)}$, $\xi_4^{(2)}$, w_4, and $\xi_5^{(1)}$.

For the so-called ''degenerate'' SKdV$_{-2}$ case (V), the Painlevé test immediately fails at the first level since both $\xi_0^{(1)}$ and $\xi_0^{(2)}$ need to be arbitrary and, at the same time, satisfy $\xi_0^{(1)}\xi_0^{(2)}=0$ [cf. (5.2)]. This condition is completely independent of the value of r.

For the SKdV$_4$ equation, the compatibility conditions are all verified and φ, $\xi_0^{(1)}$, w_1, $\xi_2^{(1)}$, u_3, $\xi_3^{(1)}$, w_3, u_4, $\xi_4^{(1)}$, $\xi_4^{(2)}$, u_5, and $\xi_5^{(1)}$ are found to be arbitrary. Notice that there are two resonances at level $n=5$, one of which being bosonic; the analysis must then be extended up to level $n=6$.

For the SKdV$_{\mathcal{O}}$ equation, the bosonic evolution equations decouple from the fermionic ones; this eliminates the necessity of extending the analysis to a higher level in order to check the compatibility condition at the highest resonance. With $r=2$ we find that φ, $\xi_0^{(1)}$, w_1, $\xi_2^{(1)}$, $\xi_2^{(2)}$, w_2, $\xi_3^{(1)}$, w_3, u_4, $\xi_4^{(1)}$, u_6, and $\xi_7^{(1)}$ are arbitrary hence it is not necessary to perform the test for other values of r (since we already know that the system SKdV$_{\mathcal{O}}$ has the Painlevé property).

VI. CONCLUSION

In this work, we have presented the Painlevé analysis (at least, a reduced form of it) for the complete set of bosonic and fermionic evolution equations pertaining to a general multiparameter family of $N=2$ supersymmetric equations. Such an analysis is interesting for a number of reasons. First, very few fermionic extensions of integrable systems have been analyzed from that point of view. The detailed analysis of specific examples is of a clear interest in view of confirming (or limiting or even, in principle, invalidating) the direct extension of the test to fermionic systems. The successful analysis presented here for four $N=2$ supersymmetric extensions of the KdV equation, known to be integrable from other methods, indeed confirms the validity of the naive extension of the test. This, in turn, gives credit to the test when viewed as an exploratory tool in the search for new integrable systems among a multiparameter class of equations. In that respect, the present results have not signaled the existence of a single new integrable equation (although new integrable systems could still in principle be revealed by an analysis that goes beyond the principal families).

Manifestly, that only a rather limited number of examples have been studied so far is partly due to the intrinsic complications of such computations (involving here four coupled nonlinear

equations); however, it is also due to the special complications brought by the fermionic fields themselves. In particular, even the determination of the leading singularity is somewhat problematic (and a simple degree-homogeneity requirement cannot be put forward). This particular question has been treated in great detail here. Another aspect of the present analysis is to have put in light unusual features of the verification of the compatibility conditions for systems involving fermions, unusual in that these conditions can be satisfied in some case only if higher-order recursion relations are solved.

For completeness, we have also checked the Painlevé property for the osp(2, 2) KdV equation, which is $O(2)$ symmetric but not supersymmetric, and found that it successfully passes the test. The equations take the form,

$$u_t=\partial_x[-u_{xx}+3u^2-12\xi^{(i)}\xi_x^{(i)}+24\xi^{(2)}\xi^{(1)}w+2(w_x)^2+2ww_{xx}-6uw^2+3w^4],$$

$$\begin{aligned}\xi_t^{(i)}=&-4\xi_{xxx}^{(i)}+3u_x\xi^{(i)}+6u\xi_x^{(i)}+6w^2\xi_x^{(i)}+6ww_x\xi^{(i)}-12\epsilon_{ij}\xi_{xx}^{(j)}w\\&-12\epsilon_{ij}\xi_x^{(j)}w_x-4\epsilon_{ij}\xi^{(j)}w_{xx}+6u\epsilon_{ij}\xi^{(j)}w-2\epsilon_{ij}\xi^{(j)}w^3\end{aligned}\tag{6.1}$$

with $w_t=0$. Since the w-evolution equation is trivial this field has no singularity; however, relying on the degree-homogeneity property, we have set $w=\Sigma_{n=0}^{\infty}w_n\varphi^{n-1}$ and $w_0=0$. Moreover, the fermionic fields are also singularity-free at the leading order; therefore, u is the only field having a leading singularity, which in itself is a rather uncommon feature.

We stress finally that the analysis has been presented here in terms of the component fields. Hence, we have not taken advantage of the economical superfield formalism. In fact, the Painlevé test has never been formulated in superspace. That would be a definite progress since it is only in such a case that we could face a more refined analysis that does not rely upon the simplified Kruskal ansatz. The benefit of such a generalization is the ability to make contact, in the early steps of the analysis, with Backlünd transformations and Lax pairs (see e.g., Ref. 23). We hope to report elsewhere on this topic.

Note added in proof. Apart from the cases mentioned in the third paragraph of Sec. I, there are two further integrable extensions of the KdV equation with an extra boson and two fermions also defined via the 'second' Hamiltonian structure equivalent to the classical superconformal algebra (see e.g., Eqs. (4.14)–(4.17) and (4.23)–(4.24) of F. Delduc, L. Gallot, E. Ivanov, Phys. Lett. B **396**, 122 (1997), hep-th/9611033). The first has $N=1$ supersymmetry and $O(2)$ invariance, while the second has no supersymmetry but it is $O(2)$ invariant (and it differs from the $osp(2,2)$ extension of the Kuper-KdV equation). We thank E. Ivanov for drawing our attention to this point.

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APPENDIX A: ANALYSIS OF THE BOSONIC CORE

In this Appendix, we analyze the bosonic core of the generic supersymmetric KdV equations. This boils down to the study of the recursion formulas (3.3) in which we set all fermionic fields equal to zero: $\xi_n^{(i)}=0$ for $i=1,2$. Further references to (3.3) in this appendix are to be understood with this restriction, which transforms this system into a set of two coupled bosonic equations.

Before considering the general recursion equations and determining its resonances, we first analyze the recursion formulas at levels $n=0,1$ for the cases $c=0,3$, in order to impose as much constraints as possible in the very early steps of the analysis. For every solution found at those levels, we need to write the resonance equation in order to identify those cases that are potentially Painlevé admissible. Note however that a single solution to the $n=0,1$ relations can lead to more than one resonance equation; the different possibilities must then be analyzed one by one. The cases $c=0,3$ are studied separately.

1. The $c=3$ case

The recursion formulas (3.3), with $c=3$, can be written under the form,

$$A_1^1 u_n + A_2^1 w_n = F_n^1,$$

$$A_1^2 u_n + A_2^2 w_n = F_n^2, \tag{A1}$$

where

$$A_1^1(n) = [-(n-2)(n-3) + 6u_0 + \beta w_0^2](n-4),$$

$$A_2^1(n) = [-(\alpha+2)n^2 + (5\alpha+4)n - 6(\alpha+1) + 2\beta u_0](n-4)w_0,$$

$$A_1^2(n) = (\alpha+2)(n-3)w_0,$$

$$A_2^2(n) = [-(n-1)(n-2) + (\alpha+2)u_0 + \beta w_0^2](n-3), \tag{A2}$$

and F_n^1 and F_n^2 are functions of $u_0, u_1, \ldots, u_{n-1}$ and $w_0, w_1, \ldots, w_{n-1}$. There is a resonance when this system is not defined, that is, when

$$A(n) = \det|A_j^i(n)| = 0 \quad (i,j = 1,2). \tag{A3}$$

The substitution of α, β, u_0, and w_0 (whenever they are known) for each case identified will then yield the values of the resonance levels n. It should be stressed that we are particularly interested in cases in which there is a resonance at level $n=-1$ (corresponding to the arbitrariness of the singular manifold φ) with the other ones being integers $\geqslant 1$, unless either u_0 or w_0 is arbitrary, in which case we also need a resonance at level zero. The cases for which negative resonances appear will be given, but the search for movable logarithms will be omitted.

Here are the solutions of the recursion equations for levels $n=0,1$, the results of the resonance analysis and their compatibility conditions. When the test is not satisfied, we simply indicate the reason (and avoid repeating: therefore the test is not satisfied).

(i) $$u_0 = 0, \qquad u_1 = 0,$$

$$w_0 = 0, \quad w_1 \text{ arbitrary.}$$

This case can readily be eliminated given the absence of singularities. Similarly, cases (ii) and (iii) below could have been eliminated from the start since there are no singularities for the field w; however, being interested in a supersymmetric extension for the field u— which is thus the ''leading'' field—this restriction will not be imposed.

(ii) $$u_0 = 2, \quad u_1 = 0,$$

$$w_0 = 0, \quad w_1 = 0,$$

$$A(n) = (n+1)(n-3)(n-4)(n-6)(n^2 - 3n - 2(\alpha+1)).$$

Given that the two roots of the second order polynomial are j_1 and j_2, we thus have

$$j_2 = 3 - j_1, \quad \alpha = \tfrac{1}{2} j_1(j_1 - 3) - 1, \tag{A4}$$

and we can choose $j_1 \geqslant j_2$. Now since the coefficients at level 0 and 1 are fixed, a resonance at one of those levels would signal the presence of a movable logarithm. In consequence, there is no

solution in a principal family (with both j_1 and $j_2 \geqslant 0$) free from movable logarithms. The only other cases left are those for which $j_1 \geqslant 4$. For those cases, the compatibility conditions at level 6 are satisfied only for $\beta = 3\alpha$.

(iii) $\alpha = -2$,

$$u_0 = 2, \quad u_1 = 0,$$

$$w_0 = 0, \quad w_1 \text{ arbitrary},$$

$$A(n) = (n+1)(n-1)(n-2)(n-3)(n-4)(n-6).$$

The resonances correspond to the arbitrariness of $\varphi, w_1, w_2, w_3, u_4, u_6$. All compatibility conditions are verified without constraints on the parameters, except the one at level 6 which forces $\beta = 3\alpha = -6$. This will turn out to correspond to a nonintegrable solution of the recursion relations associated to the $\mathrm{SKdV}_{\alpha=-2}$ equation.

(iv) $\alpha = -1$,

$$u_0 \text{ not fixed yet or arbitrary}, \quad u_1 = 0,$$

$$w_0 = k\sqrt{\frac{3}{\beta}(u_0 - 2)}, \quad w_1 = 0,$$

$$A(n) = (n+1)n(n-3)(n-4)(n^2 - 9n - (u_0 - 20) - (3/\beta)(u_0 - 2)),$$

where (here and below) $k^2 = -1$. The resonance at level 0 would signal a movable logarithm if u_0 would have to be fixed. Moreover, $A(n)$ would need to be independent of u_0 for this coefficient to be arbitrary. This leads to $\beta = -3$ and

$$A(n) = (n+1)n(n-3)^2(n-4)(n-6). \tag{A5}$$

However, the compatibility conditions at level 3 are not satisfied.

(v) $\alpha = -1, \quad \beta = 3\left[\frac{u_0 - 2}{P}\right]$,

$$u_0 \text{ fixed by value of } \beta, \quad u_1 = 0,$$

$$w_0 = k\sqrt{P}, \quad w_1 = 0,$$

$$A(n) = (n+1)n(n-3)(n-4)[(n-1)(n-8) - 3u_0(u_0 - 2)],$$

with $P = 3(u_0)^2 - 7u_0 + 12$. The resonance at level 0 signals the presence of a movable logarithm.

(vi) $\alpha = -1, \quad \beta = -\frac{8}{3}$,

$$u_0 = -\tfrac{4}{3}, \quad u_1 = 0,$$

$$w_0 = \tfrac{1}{2}k\sqrt{15}, \quad w_1 = 0,$$

$$A(n) = (n+1)n(n-3)(n-4)\left[n^2 - 9n + \frac{211}{12}\right].$$

$A(n)$ has noninteger roots.

(vii) $\beta=3\left[\dfrac{(\alpha+2)u_0-2}{u_0^2}\right]$,

$$u_0 \text{ fixed by the value of } \beta, \quad u_1=0,$$

$$w_0=ku_0, \quad w_1=0,$$

$$A(n)=(n+1)(n-3)(n-4)(n-m)[n^2+(m-9)n+6(4-u_0-m)],$$

where $m=4-(\alpha+2)u_0$. Writing the two roots of the second order polynomial as j_1 and j_2, the general solution can be written (with k_1 and k_2 integers)

$$m=4-k_1, \ j_1=3+k_2, \ j_2=2+k_1-k_2, \ k_1\geqslant 2k_2+1 \tag{A6}$$

with

$$u_0=\tfrac{1}{6}(k_1(3-k_2)+k_2(k_2+1)-6),$$

$$\alpha=\frac{6k_1}{k_1(3-k_2)+k_2(k_2+1)-6}-2,$$

$$\beta=108\frac{k_1-2}{(k_1(3-k_2)+k_2(k_2+1)-6)^2}. \tag{A7}$$

The principal families are characterized by

$$-1\leqslant k_2\leqslant 2k_2+1\leqslant k_1\leqslant 2 \tag{A8}$$

for which the possible solutions are

	m	j_1	j_2	α	β	u_0
vii.a	2	2	5	4	0	$\frac{1}{3}$
vii/b	2	3	4	$\sim\frac{1}{u_0}$	$\sim\frac{1}{u_0^2}$	0
vii.c	3	2	4	-5	-27	$-\frac{1}{3}$
vii.d	3	3	3	-4	-12	$-\frac{1}{2}$
vii.e	4	2	3	-2	-6	-1
vii.f	5	2	2	$-\frac{7}{5}$	$-\frac{81}{25}$	$-\frac{5}{3}$

Case vii.b can be eliminated since there are no singularities (and moreover $\alpha, \beta\to\infty$). For cases vii.a, c, d and f, the compatibility conditions at level $n=2,3,3,2$, respectively, are not satisfied. For vii.e all the conditions are satisfied so that this system passes the test (φ, u_1, u_3, w_3, u_4, and w_4 are all arbitrary functions). It corresponds to the bosonic core of the $\mathrm{SKdV}_{\alpha=-2}$ equation.
The only other solutions of interest (with negative resonances) are given by

vii.g	$k_1\geqslant\max(5,2k_2+1)$	$k_2\geqslant -1$
vii.h	$k_1\geqslant 5$	$k_2\leqslant -4$

(viii) $\beta=\frac{1}{3}(\alpha+2)^2$,

$$u_0=\frac{3}{\alpha+2}, \quad u_1=0,$$

$$w_0=ku_0, \quad w_1 \text{ arbitrary},$$

$$A(n)=(n+1)(n-1)(n-3)(n-4)(n^2-8n-6(u_0-3)).$$

We write the two roots of the quadratic term as

$$j_1=4-k_1, \ j_2=4+k_1, \ k_1\geqslant 1, \tag{A9}$$

with k_1 an integer and

$$u_0=\tfrac{1}{6}(2+k_1^2), \ \alpha=2\,\frac{7-k_1^2}{2+k_1^2}. \tag{A10}$$

The principal families (free from movable logarithms) are characterized by $k_1=1,2$ so that we have

	j_1	j_2	α	β	u_0
viii.a	2	6	1	3	1
viii.b	3	5	4	12	$\frac{1}{2}$

For viii.a and b, all the compatibility conditions are satisfied. Those systems describe the bosonic core of the $\mathrm{SKdV}_{\alpha=1}$ (with φ, w_1, w_2, w_3, u_4, and w_6 arbitrary) and $\mathrm{SKdV}_{\alpha=4}$ (with φ, w_1, u_3, w_3, u_4, and u_5 arbitrary) equations, respectively.
The other possible cases are those for which $k_1\geqslant 5$,

(ix) $\beta=-\frac{9}{8}\alpha(5\alpha+4)$,

$$u_0=\frac{4}{5\alpha+4}, \quad u_1=\frac{1}{2}\left(\frac{11\alpha+4}{\alpha+2}\right)kw_1,$$

$$w_0=ku_0, \quad w_1 \text{ arbitrary}.$$

Note however that in the singular case where $\alpha=-2$, $w_1=0$, and u_1 is arbitrary.

$$A(n)=(n+1)(n-1)(n-3)(n-4)(n+\tfrac{6}{5}u_0-\tfrac{16}{5})(n-\tfrac{6}{5}u_0-\tfrac{24}{5}).$$

We can write the two roots of the last two factors as

$$j_1=2-k_1, \quad j_2=6+k_1, \tag{A11}$$

with

$$u_0=\frac{5}{6}k_1+1, \quad \alpha=-4\,\frac{k_1}{5k_1+6}. \tag{A12}$$

The principal families (with $-4\leqslant k_1\leqslant 0$) are thus

	j_1	j_2	α	β	u_0
ix.a	2	6	0	0	1
ix.b	3	5	4	-108	$\frac{1}{6}$
ix.c	4	4	-2	$-\frac{27}{2}$	$-\frac{2}{3}$
ix.d	5	3	$-\frac{4}{3}$	-4	$-\frac{3}{2}$
ix.e	6	2	$-\frac{8}{7}$	$-\frac{108}{49}$	$-\frac{7}{3}$

The resonance conditions are not met at level $n=2,3,4,3,2$, respectively. The other solutions are

ix.f	$k_1 \leqslant -7$
ix.g	$k_1 \geqslant 3.$

When $c=3$, there are thus only 4 cases in principal families for which the Painlevé test is satisfied for the bosonic core of our multiparameter version of the SKdV equation. Those cases correspond to (I), (II), (III), and (V) in the list of Sec. IV. There is also some other cases with negative resonances. Those cases will be classified as (VI), (VII), (VIII), (IX), (X), and (XI).

2. The $c=0$ case

The recursion formulas (3.3) with $c=0$ take the form (A1) with

$$A_1^1(n)=[-(n-2)(n-3)+6u_0+\beta w_0^2](n-4),$$

$$A_2^1(n)=[-(\alpha-1)n(n+1)+6\alpha(n-1)+2\beta u_0](n-4)w_0,$$

$$A_1^2(n)=[(\alpha-1)(n-3)-6]w_0,$$

$$A_2^2(n)=-(n-1)(n-2)(n-3)+(\alpha-1)(n-3)u_0+6(n-1)u_0+\beta(n-3)w_0^2. \quad \text{(A13)}$$

The possible solutions of the resonance conditions are now listed in turn.

(i) $u_0=0, \quad u_1=0,$

$$w_0=0, \quad w_1 \text{ arbitrary.}$$

Again, this case is eliminated due to the absence of singularity but, as before, we will keep the cases (ii) and (iii) below even if w is not singular.

(ii) $u_0=2, \quad u_1=0,$

$$w_0=0, \quad w_1=0,$$

$$A(n)=(n+1)(n-4)(n-6)(n^3-6n^2+n-2\alpha(n-3)).$$

Writing the last factor under the form $(n-j_1)(n-j_2)(n-j_3)$, the constants j_1,j_2,j_3 must satisfy

$$j_1+j_2+j_3=6, \quad j_1j_2+(j_1+j_2)j_3=1-2\alpha, \quad j_1j_2j_3=-6\alpha, \quad \text{(A14)}$$

and we can choose $j_2 \leqslant j_3$. The second condition requires that α be an integer or half-integer so that the third condition allow us to choose $j_1 = 3m$, where m is an integer. This leads to the equation

$$9m(m-1) - 9(m-1) + (m-1)j_2 j_3 = 8. \tag{A15}$$

$m-1$ must thus be a divisor of 8. With this last condition, a case-by-case analysis leads to the only two possible solutions (which are not in principal families),

	j_1	j_2	j_3	α
ii.a	-1	1	6	1
ii.b	-3	2	7	7

Case (ii.a) can be eliminated since the resonance at level $n=1$ signals a movable logarithm.

(iii) $\alpha = 1$,

$$u_0 = 2, \quad u_1 = 0,$$

$$w_0 = 0, \quad w_1 \text{ arbitrary},$$

$$A(n) = (n+1)^2(n-1)(n-4)(n-6)^2.$$

This case is not a principal family solution but all positive resonances are verified.

(iv) $\alpha = 0$,

$$u_0 \text{ not fixed yet}, \quad u_1 = 0,$$

$$w_0 = k\sqrt{\frac{3}{\beta}(u_0 - 2)}, \quad w_1 = 0,$$

$$A(n) = (n+1)n(n-4)\left[n^3 - 12n^2 - \frac{1}{\beta}((3+5\beta)u_0 - 47\beta - 6)n - 9\frac{(1-3\beta)}{\beta}u_0 + 6\frac{(3-10\beta)}{\beta}\right]$$

(recall that $k = \pm i$). To fix the three roots of the cubic polynomial, u_0 must be fixed so that the resonance at level $n=0$ signals the presence of a movable logarithm.

(v) $\alpha = 0$,

$$u_0 = 12\left(\frac{1-\beta}{6-11\beta}\right), \quad u_1 = -(3\beta+2)\sqrt{\frac{3}{10}\left(\frac{1}{6-11\beta}\right)}kw_1,$$

$$w_0\sqrt{\frac{30}{6-11\beta}}k, \quad w_1 \text{ arbitrary},$$

$$A(n) = (n+1)n(n-1)(n-4)\left(n^4 - 11n + \frac{126-336\beta}{6-11\beta}\right).$$

There is a resonance at level $n=0$ but u_0 and w_0 are both fixed.

(vi) $\alpha=\dfrac{(\beta u_0-3)u_0+6}{3u_0}$,

$$u_0 \text{ fixed by the value of } \alpha, \quad u_1=0,$$

$$w_0=ku_0, \quad w_1=0,$$

$$A(n)=(n+1)(n-4)[n^2+(\tfrac{1}{3}\beta u_0^2-2u_0-5)n-\beta u_0^2+6]$$

$$\times[n^2-(\tfrac{1}{3}\beta u_0^2-2u_0+7)n-6u_0+2\beta u_0^2+12].$$

Writing

$$\beta u_0^2=k_1, \quad u_0=\tfrac{1}{2}k_2+\tfrac{1}{6}k_1,$$

the roots of the two quadratic polynomials j_1, j_2, j_3, and j_4 are the integers satisfying

$$j_1+j_2=5+k_2, \quad j_1j_2=6-k_1,$$

$$j_3+j_4=7-k_2, \quad j_3j_4=12+k_1-3k_2, \tag{A16}$$

and we choose $j_1\leqslant j_2$ and $j_3\leqslant j_4$. Introducing the auxiliary integers k_3 and k_4 such that

$$j_1=3+k_2-k_3, \quad j_2=2+k_3,$$

$$j_3=3+k_4-k_2, \quad j_4=4-k_4, \tag{A17}$$

with $2k_4+1\leqslant k_2\leqslant 2k_3-1$. The constraints can be written as

$$k_2(k_3+k_4+1)=0,$$

$$k_3+k_4=k_3^2+k_4^2,$$

$$k_4(k_4+k_4k_3-k_3^2-1)=k_1(1+k_3+k_4), \tag{A18}$$

so that the only possible solution is $(k_1,k_2,k_3,k_4)=(0,0,1,0)$ which correspond to

$$(j_1,j_2,j_3,j_4u_0,\alpha,\beta)=\left(2,3,3,4,0,\sim\frac{1}{u_0},\sim\frac{1}{u_0}\right).$$

However, the compatibility conditions at level $n=3$ are not satisfied.

(vii) $\alpha=\dfrac{3-2u_0}{u_0}$, $\beta=-3\left(\dfrac{u_0-1}{u_0^2}\right)$,

$$u_0 \text{ fixed by } \alpha \text{ and } \beta, \quad u_1=0,$$

$$w_0=ku_0, \quad w_1=0,$$

$$A(n)=(n+1)(n-1)(n-4)(n-m)[n^2+(m-11)n-2(2m-15)]$$

with $m=3(u_0+1)$. The two roots of the quadratic polynomial are

$$j_1,j_2=\frac{8-3u_0}{2}\mp\frac{1}{2}\sqrt{9u_0^2-8}. \tag{A19}$$

Since j_1, j_2 and m are integers, we must have $u_0 = \frac{1}{3}k_1$ with k_1 as an integer. This leads to the condition

$$9u_0^2 - 8 = k_1^2 - 8 = k_2^2, \tag{A20}$$

where k_2 is also an integer but this equation has a solution only when $k_1 = \pm 3$. With $k_1 = -3$, there should be a resonance at level $n = 0$ so that there is a movable logarithm. The only solution is thus $u_0 = 1$, which yields $m = 6$, $j_1 = 2$, $j_2 = 3$ and $\alpha = 1$, $\beta = 0$. All the resonance conditions are verified: φ, w_1, w_2, w_3, u_4, and u_6 are genuine arbitrary functions. Actually, this system is the bosonic core of the SKdV$_{\mathcal{O}}$ equation.

(viii) $$\alpha = \frac{1}{5}\left(\frac{4-u_0}{u_0}\right), \quad \beta = \frac{6}{5}\left(\frac{2u_0-3}{u_0^2}\right),$$

$$u_0 \text{ fixed by } \alpha \text{ and } \beta, \quad u_1 = -2\,\frac{9u_0-11}{9u_0+4}\,kw_1,$$

$$w_0 = ku_0, \qquad w_1 \text{ arbitrary},$$

$$A(n) = (n+1)(n-1)(n-4)(n-m)[n^2-(11-m)n+2m],$$

with $m = \frac{6}{5}(4-u_0)$. Writing the roots of the second order polynomial as j_1 and j_2, we thus have

$$j_1 + j_2 = m - 11, \quad j_1 j_2 = 2m \tag{A21}$$

and we choose $j_1 \leqslant j_2$. Elimination of m leads to the formula,

$$j_2 = \frac{26}{j_1+2} - 2, \tag{A22}$$

so that $2 + j_1$ must be a divisor of 26. We thus find that the only possible solutions are

	m	j_1	j_2	u_0	α	β
viii.a	42	-28	-3	-31	$-\frac{7}{31}$	$-\frac{78}{961}$
viii.b	30	-15	-4	-21	$-\frac{5}{21}$	$-\frac{6}{49}$
viii.c	0	0	11	4	0	$\frac{3}{8}$
viii.d	-12	-1	24	14	$-\frac{1}{7}$	$\frac{15}{98}$

Case (viii.c) can be eliminated since there are movable logarithms at level $n = 0$.

(ix) $$\alpha = \tfrac{1}{3}, \quad \beta = 0,$$

$$u_0 = \tfrac{3}{2}, \quad u_1 = -\tfrac{2}{7}kw_1,$$

$$w_0 = ku_0, \quad w_1 \text{ arbitrary},$$

$$A(n) = (n+1)(n-1)(n-3)(n-4)(n^2-8n+6).$$

$A(n)$ has noninteger roots.

(x) $\beta=0$,

$$u_0=\frac{2}{\alpha+1}, \quad u_1=0,$$

$$w_0=ku_0, \quad w_1=0,$$

$$A(n)=(n+1)(n-3)(n-4)(n-m)(n^2+(m-9)n+6),$$

with $m=2(2-u_0)$. The roots of the quadratic piece are

$$j_1,j_2=\frac{9-m}{2}\mp\frac{1}{2}\sqrt{m^2-18m+57} \tag{A23}$$

with $j_1\leqslant j_2$. We can write the quantity inside the square root as

$$m^2-18m+57=(m-9)^2-24=k_1^2, \tag{A24}$$

where k_1 must be an integer. In consequence, we must have $m=14$ or $m=4$. The choice $m=4$, $j_1=2$, $j_2=3$ leads to $\alpha\sim\infty$ and $u_0=w_0=u_1=0$ so that there are no singularities at all. The only possible case is thus

$$(m,j_1,j_2,u_0,\alpha,\beta)=(14,-3,-2,-5,-\tfrac{7}{5},0). \tag{A25}$$

(xi) $\alpha=0$, $\beta=0$,

$$u_0=2, \quad u_1=0,$$

$$w_0 \text{ arbitrary}, \quad w_1=0,$$

$$A(n)=(n+1)n(n-4)(n^3-12n^2+w_0^2n+37n-6+3w_0^2).$$

There is a resonance at level $n=0$ but u_0 is already fixed and w_0 cannot be arbitrary since it enters in the expression of the other resonances.

(xii) $\alpha=0$, $\beta=0$,

$$u_0=2, \quad u_1 \text{ arbitrary},$$

$$w_0=\sqrt{5}k, \quad w_1=\sqrt{5}ku_1,$$

$$A(n)=(n+1)n(n-1)(n-4)(n^2-11n+21).$$

There is a resonance at level $n=0$ while u_0 and w_0 are both fixed and moreover $A(n)$ has noninteger roots.

For $c=0$, we have thus found only one case in a principal family for which the bosonic core passes the test: this is case (IV) of Sec. IV. Some other possibilities can be identified as cases (XII)–(XVII).

APPENDIX B: LEADING SINGULARITY AND RESONANCE EQUATION FOR FERMIONIC FIELDS

The general recursion equations for the fermionic evolution equations can be written as [cf. (3.3)]

$$B_1^1(n)\xi_n^{(1)}+B_2^1(n)\xi_n^{(2)}=G_n^1,$$
$$B_1^2(n)\xi_n^{(1)}+B_2^2(n)\xi_n^{(2)}=G_n^2, \tag{B1}$$

where

$$B_1^1(n)=B_2^2(n)=-(n-r)(n-r-1)(n-r-2)-2cu_0+(6-c)(n-r)u_0+\beta(n-r-2)w_0^2,$$
$$B_1^2(n)=-B_2^1(n)=[c(n-r)(n-r-1)-(6-c)(n-r)+(\alpha-1)(n-r-1)(n-r-2)]w_0, \tag{B2}$$

r is the leading singularity exponent (so that $r\leqslant 0$ corresponds to no singularity) and G_n^i ($i=1,2$) are functions of $\varphi,u_0,\ldots,u_n,\xi_0^{(1,2)},\ldots,\xi_{n-1}^{(1,2)},w_0,\ldots,w_n$.

With $n=0$, we have

$$G_0^i=0,$$
$$B_1^1(0)=r(r+1)(r+2)-2cu_0-(6-c)ru_0-\beta(r+2)w_0^2, \tag{B3}$$
$$B_1^2(0)=[cr(r+1)+(6-c)r+(\alpha-1)(r+1)(r+2)]w_0.$$

Multiplying the first equation in (B1) with $n=0$ by $\xi_0^{(1)}$ and the second by $\xi_0^{(2)}$ yields (using $G_0^i=0$)

$$B_1^1(0)\xi_0^{(1)}\xi_0^{(2)}=B_1^2(0)\xi_0^{(1)}\xi_0^{(2)}=0. \tag{B4}$$

There are thus two possible types of solutions: either the two B_j^i coefficients vanish or $\xi_0^{(1)}\xi_0^{(2)}=0$, that is,

(1) $B_1^1(0)=B_1^2(0)=0$ (no relation between $\xi_0^{(1)}$ and $\xi_0^{(2)}$);

(2) $\xi_0^{(2)}=k_0\xi_0^{(1)}$ (with k_0 a bosonic constant).

The leading singularity is fixed by introducing the values found in the bosonic-core analysis (corresponding to the "body piece," i.e., without the nilpotent part, of the bosonic components) and verify the possible solutions for r.

Before pursuing, the exact meaning of this computation should be clarified. The goal is to fix the leading singularity of the fermionic field for those 5 particular cases for which the bosonic-core analysis manifestly shows the Painlevé property. We thus look for the solutions [type-(1) or (2)] of (B1) for the special values of the parameters c, α, β, u_0, and w_0 given in Sec. IV, appropriate to each possibility. The solutions with negative resonances will not be considered. Now, let us eliminate a possible source of ambiguity in our procedure; *a priori*, the values of u_0 and w_0 entering in (B1) should be those pertaining to the complete system, incorporating the fermions. However, as mentioned above, only the non-nilpotent parts are considered. The reason for this is that since the nilpotent piece can be eliminated by an appropriate multiplication, the bosonic core must also satisfy (B4).

The solutions to case (1) are

(I) $r=-2$,

(II) $r=0,-2$,

(III) $r=-2$,

(IV) $r=0$,

(V) $r=2,-2,-3$.

For case (2), Eq. (B1) for $n=0$ can be written

$$B_1^1(0)-k_0B_1^2(0)=0, \quad k_0^2B_1^1(0)+k_0B_1^2(0)=0. \tag{B5}$$

The compatibility of these equations forces $k_0^2=-1$ or $k_0=\pm i$. The constant $k=\pm i$ that appear in the expression of the bosonic component w_0 (cf. Sec. IV) can thus be either $k=\pm k_0$; both cases need thus to be considered (the precise relation being fixed by the resonance equations). We then find the following possible solutions for r:

$$\begin{aligned}
&\text{(I)} \quad k=+k_0: \quad r=2,-2,-3,\\
&\qquad k=-k_0: \quad r=0,-1,-2,\\
&\text{(II)} \quad k=+k_0: \quad r=0,-2,-4,\\
&\qquad k=-k_0: \quad r=2,0,-2,\\
&\text{(III)} \quad k=+k_0: \quad r=-1,-2,-3,\\
&\qquad k=-k_0: \quad r=2,0,-2,\\
&\text{(IV)} \quad k=+k_0: \quad r=0,-1,-2,\\
&\qquad k=-k_0: \quad r=2,0,-5,\\
&\text{(V)} \quad r=2,-2,-3.
\end{aligned}$$

Observe that the type-(1) solutions for r are recovered as the intersection of the two set of solutions in each case: this is clear since in case (1) we do not assume any special relation between k and k_0; it should then hold for all possibilities, in particular when $k=k_0$ and $-k_0$. In the following, we can thus restrict ourself to type-(2) solutions.

In order to uniquely fix the value of r (and, thereby, the value of k appropriate to each case), we must consider the resonance equations. Since the bosonic resonances are solutions of $A(n)=\det|A_j^i(n)|=0$, the fermionic resonances are necessarily given by

$$B(n)=\det|B_j^i(n)|=0 \quad (i,j=1,2). \tag{B6}$$

Inserting the values already found for r, u_0 and w_0, the roots of $B(n)$ should then lead to the resonance levels for the fermionic fields. The idea is to select r by requiring the corresponding polynomial $B(n)$ to have only integer roots. The explicit form of these polynomials is

$$\begin{aligned}
&\text{(I)} \quad r=2: \quad B(n)=n(n-2)(n-3)(n-4)^2(n-5),\\
&\qquad r=0: \quad B(n)=(n^5-4n^4-n^3+16n^2-12n+36)(n-2),\\
&\qquad r=-1: \quad B(n)=(n^5+n^4-7n^3-n^2+6n+54)(n-1),\\
&\qquad r=-2: \quad B(n)=(n^5+6n^4+7n^3-6n^2-8n+72)n,\\
&\qquad r=-3: \quad B(n)=(n^5+11n^4+41n^3+61n^2+30n+90)(n+1),\\
&\text{(II)} \quad r=2: \quad B(n)=n(n-2)^2(n-4)^2(n-6),\\
&\qquad r=0: \quad B(n)=(n^4-4n^3-4n^2+52n-54)n(n-2),\\
&\qquad r=-2: \quad B(n)=(n^4+4n^3-4n^2+56n-36)(n+2)n,
\end{aligned}$$

$$r=-4: \quad B(n)=(n^4+12n^3+44n^2+156n+54)(n+4)(n+2),$$

(III) $$r=2: \quad B(n)=n(n-2)(n-3)(n-4)^2(n-5),$$

$$r=0: \quad B(n)=(n^4-2n^3-5n^2+42n-18)(n-2)^2,$$

$$r=-1: \quad B(n)=(n^5+n^4-7n^3+53n^2-48n-\tfrac{81}{2})(n-1),$$

$$r=-2: \quad B(n)=(n^4+7n^3+14n^2+80n+108)n(n-1),$$

$$r=-3: \quad B(n)=(n^5+11n^4+41n^3+151n^2+210n-\tfrac{225}{2})(n+1),$$

(IV) $$r=2: \quad B(n)=n(n-2)^2(n-3)(n-4)(n-7),$$

$$r=0: \quad B(n)=(n+2)n^2(n-1)(n-2)(n-5),$$

$$r=-1: \quad B(n)=(n+3)(n+1)^2(n-1)n(n-4),$$

$$r=-2: \quad B(n)=(n+4)(n+2)^2(n+1)n(n-3),$$

$$r=-5: \quad B(n)=(n+7)(n+5)^2(n+4)(n+3)n,$$

(V) $$r=2: \quad B(n)=n^2(n-4)^2(n-5)^2,$$

$$r=-2: \quad B(n)=(n+4)^2n^2(n-1)^2,$$

$$r=-3: \quad B(n)=(n+5)^2(n+1)^2n^2.$$

We can already eliminate all cases for which there are noninteger roots. This leaves us with $r=2$ as the only possibility for cases (I), (II), and (III) while we have some other possibilities for cases (IV) and (V). However, we argue in Sec. V that for the other possibilities we can restrict to $r=2$ (moreover, this amounts to restrict the study to the principal families).

The situation concerning the leading fermionic singularity is thus somewhat peculiar: we essentially keep track of all possibilities and determine the particular values which ensure integer-valued resonances. Quite interestingly, the same value for r is singled out in all cases when we restrict to principal family solutions. Actually, this value corresponds precisely to the one that follows from a naive consideration where the fermionic terms, in the bosonic evolution equations, have a dominant singular behavior comparable to that of the leading bosonic terms.

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Solitons and almost-intertwining matrices

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We define the algebraic variety of almost intertwining matrices to be the set of triples (X,Y,Z) of $n\times n$ matrices for which $XZ=YX+T$ for a rank one matrix T. A surprisingly simple formula is given for tau functions of the KP hierarchy in terms of such triples. The tau functions produced in this way include the soliton and vanishing rational solutions. The induced dynamics of the eigenvalues of the matrix X are considered, leading in special cases to the Ruijsenaars–Schneider particle system. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379313]

I. INTRODUCTION

The KP hierarchy[1,2] is a well-studied system of integrable nonlinear partial differential equations with Lax form

$$\frac{\partial \mathcal{L}}{\partial t_i}=[\mathcal{L},\mathcal{L}_+^i], \quad i=1,2,3,...$$

for a monic, first-order pseudodifferential operator $\mathcal{L}$. In one of its formulations, the KP hierarchy is a set of bilinear equations for the "tau function" $\tau(t_1,t_2,t_3,t_4,\ldots)$ depending upon infinitely many "time variables" t_i $(i\in\mathbb{Z}_+)$. In this paper we will consider τ functions of the form:

$$\tau_M(t_1,t_2,\ldots):=\det(Xe^{g(Z)}+e^{g(Y)}), \tag{1}$$

where $M=(X,Y,Z)$ is a triple of $n\times n$ constant complex matrices and the function g is defined as

$$g(W):=\sum_{i=1}^{\infty} t_i W^i, \quad t_i\in\mathbb{C}. \tag{2}$$

(To avoid issues of convergence, we will here consider only the case in which all but a finite number of the parameters $t_i\in\mathbb{C}$ are nonzero.)

It is *not* true that (1) always gives the formula for a function which satisfies the KP hierarchy. For instance, as we shall see from Remark 2.2 and Theorem 3.1, in the 2×2 case formula (1) is only a tau function if $\det[(XZ-YX)(Y-Z)]=0$. On the other hand, among the solutions one can obviously write this way are the *one-soliton solutions* which are the natural generalizations in this context of the solitary wave from which the term "soliton" was coined by Zabusky and Kruskal.[3] The *standard* τ function for the one-soliton solution takes the form (1) where $M=(X,Y,Z)\in\mathbb{C}^3$ is any triple of scalar constants. (To exclude the degenerate cases we must further assume that X and $Y-Z$ are nonzero.) This τ function describes a single line soliton of the KP equation. More generally, one may be interested in τ functions of n-soliton solutions ("nonlinear superpositions" of n different line solitons) or their rational degenerations. These τ functions are usually written in a form that looks very different than (1).

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Of course, when X, Y, and Z are scalar as in the one-soliton case, then the determinant which appears in (1) is unnecessary. However, the main result of this paper is that the n-soliton solutions also take the form (1) and that they arise in the case that X, Y, and Z are three $n\times n$ matrices satisfying the condition $\operatorname{rank}(XZ-YX)=1$. In fact, this same rank one condition provides not only the nondegenerate soliton solutions to the KP hierarchy but also their rational degenerations. Thus, we see that the one-soliton τ function is merely a special case of this much more general formula.

II. ALMOST-INTERTWINING MATRICES

It is common to say that an operator X intertwines the operators Y and Z if one has that

$$XZ=YX. \tag{3}$$

Definition 2.1: Given three $n\times n$ matrices X, Y and Z, we define the rank $\kappa(X,Y,Z)$ *to which* X intertwines Y and Z by the formula

$$\kappa(X,Y,Z)=\operatorname{rank}(XZ-YX)=n-\dim\ker(XZ-YX).$$

For fixed $k,n\in\mathbb{N}$ $(0\leqslant k\leqslant n)$ define

$$\mathcal{M}_n^k=\{(X,Y,Z)\,|\,\kappa(X,Y,Z)\leqslant k\}$$

to be the set of all triples of $n\times n$ matrices $M=(X,Y,Z)$ such that $\kappa(M)\leqslant k$.

In most instances, one expects to find that $\kappa(X,Y,Z)=n$, its maximum value. For $\kappa(X,Y,Z)$ to be lower means that X does, in fact, intertwine Y and Z on the positive dimensional subspace $\ker(XZ-YX)$. In particular, when $\kappa(X,Y,Z)=0$, then $XZ=YX$ and so X does actually intertwine the other two matrices. If Y and Z are not intertwined by X, then the best one could ask for would be for $\kappa(X,Y,Z)$ to be equal to one, and so it seems reasonable to say that they are almost intertwined in this case.

Remark 2.1: Note that a triple (X,Y,Z) is in $\mathcal{M}_n^k$ precisely when the $k\times k$ minor determinants of the matrix $XZ-YX$ all vanish. Consequently, $\mathcal{M}_n^k$ has the geometric structure of an affine algebraic variety in the $3n^2$-dimensional vector space of $n\times n$ matrix triples.

The following elementary observations will be used to establish the connection between almost intertwining matrices and solitons:

Lemma 2.1: • There is a natural $GL(n)\times GL(n)$ action on $\mathcal{M}_n^k$ given by

$$(G,H)\in GL(n)\times GL(n):\quad (X,Y,Z)\in\mathcal{M}_n^k\mapsto(GXH^{-1},GYG^{-1},HZH^{-1})\in\mathcal{M}_n^k,$$

which restricts on the diagonal to the natural $GL(n)$ action of simultaneous conjugation

$$G\in GL(n):\quad (X,Y,Z)\in\mathcal{M}_n^k\mapsto(GXG^{-1},GYG^{-1},GZG^{-1})\in\mathcal{M}_n^k.$$

• Let Λ and Ω be $n\times n$ matrices satisfying the commutation relationships

$$[\Lambda,Y]=0,\quad [\Omega,Z]=0,$$

then

$$\kappa(X,Y,Z)=\kappa(\Lambda X\Omega,Y,Z).$$

Proof: Both claims are easily verified by noting that $\kappa(X,Y,Z)\leqslant k$ if and only if

$$XZ=YX+\sum_{i=1}^{k} v_i\otimes w_i \tag{4}$$

for n-vectors $\{v_i\}$ and $\{w_i\}$ and that $\kappa(X,Y,Z)$ is exactly the minimum k for which such an equation exists. □

The main result of this section is the following lemma:

Lemma 2.2: Given three $n\times n$ matrices $\hat{X}$, Y and Z, let $H(a,b,c)\in\mathbb{C}[a,b,c]$ be the polynomial defined by

$$H(a,b,c)=H_1(a)H_2(b,c)-H_1(b)H_2(a,c)+H_1(c)H_2(a,b) \tag{5}$$

with

$$H_1(a)=\det(\hat{X}(aI-Z)+(aI-Y))$$

and

$$H_2(a,b)=(a-b)\det(\hat{X}(aI-Z)(bI-Z)+(aI-Y)(bI-Y)).$$

If $\kappa(\hat{X},Y,Z)\leqslant 1$ then $H(a,b,c)\equiv 0$ is the zero polynomial.

Proof: To say that $\kappa(\hat{X},Y,Z)\leqslant 1$ is equivalent to saying that there exist vectors v and w_1 such that

$$\hat{X}Z-Y\hat{X}=-vw_1^T. \tag{6}$$

[In the case $\kappa(\hat{X},Y,Z)=0$ one of these vectors is the zero vector.] Also, merely for the sake of convenience, we introduce the notation

$$Z_a=(aI-Z),\quad Y_a=(aI-Y)$$

and recall that adj(M) is the classical adjoint matrix [i.e., $\mathrm{adj}(M)=\det(M)M^{-1}$ if M is invertible].

Now, using (6) to eliminate "$\hat{X}Z$," one can rewrite $H_1(a)$, $H_2(a,b)$ as

$$H_1(a)=\det(Y_a(\hat{X}+I)+vw_1^T),\quad H_2(a,b)=(a-b)\det(Y_aY_b(\hat{X}+I)+Y_{a+b}vw_1^T+vw_2^T),$$

where $w_2^T=w_1^TZ$.

Next, since $H(a,b,c)$ depends on $\hat{X}$ polynomially, it is enough to prove that $H(a,b,c)=0$ for almost all $\hat{X}$. Let us assume that $\det(\hat{X}+I)=\gamma\neq 0$. Then we can eliminate reference to $\hat{X}$ by writing

$$H_1(a)=\gamma\det(Y_a+vu_1^T),\quad H_2(a,b)=\gamma(a-b)\det(Y_aY_b+Y_{a+b}vu_1^T+vu_2^T),$$

where

$$u_1^T=w_1\cdot(\hat{X}+I)^{-1},\quad u_2^T=w_2^T\cdot(\hat{X}+I)^{-1}.$$

Let us further rewrite $H_2(a,b)$ as

$$H_2(a,b)=(a-b)\gamma\det(Y_aY_b+Y_avu_1^T+vu_1^TY_b+v(u_2^T+u_1^TY))$$

$$=(a-b)\gamma\det((Y_a+vu_1^T)(Y_b+vu_1^T)+vu_2^T).$$

Finally, denote $Y-vu_1^T$ by M. We obtain

$$H_1(a)=\gamma\det(M_a),\quad H_2(a,b)=\gamma(a-b)\det(M_aM_b+vu_2^T).$$

Note that

$$\det(M_aM_b+vu_2^T)=\det(M_a)\det(M_b)+u_2^T\,\mathrm{adj}(M_aM_b)v=\gamma^{-2}H_1(a)H_1(b)(1+u_2^TM_a^{-1}M_b^{-1}v)$$

and since $[M_a, M_b]=0$ we also have that

$$M_a^{-1}M_b^{-1}=\frac{1}{a-b}(M_b^{-1}-M_a^{-1}).$$

Therefore,

$$\det(M_aM_b+vu_2^T)=\gamma^{-1}H_1(a)H_1(b)+\frac{H_1(a)(u_2^T\,\mathrm{adj}(M_b)v)-H_1(b)(u_2^T\,\mathrm{adj}(M_a)v)}{\gamma(a-b)}.$$

So, using the notation $p(a)=a\gamma^{-2}H_1(a)-\gamma^{-1}u^T\,\mathrm{adj}(M_a)v$, we see that $\det(M_aM_b+vu^T)$ is a Bezoutian of the form

$$\det(M_aM_b+vu^T)=\frac{p(a)H_1(b)-p(b)H_1(a)}{a-b}.$$

Substituting $H_2(a,b)=\gamma(p(a)H_1(b)-p(b)H_1(a))$ into the expression for $H(a,b,c)$ immediately yields $H\equiv 0$. □

Remark 2.2: The special case $n=2$ turns out to be surprisingly simple. A quick calculation verifies that for arbitrary 2×2 matrices $\hat{X}$, Y, and Z the polynomial $H(a,b,c)$ is given by the formula

$$H(a,b,c)=(a-b)(b-c)(c-a)\det[(\hat{X}Z-Y\hat{X})(Y-Z)].$$

III. TAU FUNCTIONS

A. Main theorem

It is easy to check that if $\kappa(M)=0$ then the formula for τ_M defined in (1) is a tau function of the KP hierarchy. In fact, in this case in which (3) is satisfied one has

$$\tau_M(t_1,t_2,t_3,\ldots)=\det(X+I)\exp\left(\sum_{i=1}^{\infty}\sum_{j=1}^{n}(\lambda_j^i)t_i\right),$$

where $\{\lambda_j\}$ are the eigenvalues of Y. Since the function

$$u(x,y,t)=2(\log\tau_M(x,y,t,0,0,\ldots))_{xx}=0$$

is the trivial solution to the KP equation, we say that τ_M is merely a gauge transformation of the trivial tau function.

Moreover, with g defined as in (2) and τ_M defined by (1), we observe that this is still a τ function in the case $\kappa(M)=1$. In fact, it is more interesting in this ''almost-intertwining'' case since we get nontrivial soliton and rational solutions in this way.

Theorem 3.1: If $\kappa(M)\leqslant 1$ for $M=(X,Y,Z)$ then the function

$$\tau_M(t_1,t_2,\ldots)=\det(Xe^{g(Z)}+e^{g(Y)}),\quad g(W)=\sum_{i=1}^{\infty}t_iW^i$$

is a tau function of the KP hierarchy with corresponding (stationary) Baker–Akhiezer function

$$\psi_M(x,z):=\frac{\det(X(zI-Z)e^{xZ}+(zI-Y)e^{xY})}{z^n\det(Xe^{xZ}+e^{xY})}e^{xz}.$$

Proof: Given the semi-infinite vector $\vec{t}=(t_1,t_2,t_3,\ldots)$, we use the notation $\tau_M(\vec{t})=\tau_M(t_1,t_2,\ldots)$. For an arbitrary constant a, we define the semi-infinite vector $[a]=(a,a^2/2,a^3/3,\ldots)$. Then, it is sufficient to prove that the continuous function $\tau(\vec{t})$ defined in (1) satisfies the Hirota equation in Miwa form[4,5]

$$0=(b-c)\tau(\vec{t}-[a^{-1}])\tau(\vec{t}-[b^{-1}]-[c^{-1}])-(a-c)\tau(\vec{t}-[b^{-1}])\tau(\vec{t}-[a^{-1}]-[c^{-1}])$$
$$+(a-b)\tau(\vec{t}-[c^{-1}])\tau(\vec{t}-[a^{-1}]-[b^{-1}]) \tag{7}$$

uniformly in a, b, and c and for all $\vec{t}$.

However, from the definition we see that

$$\begin{aligned}\tau(\vec{t}-[a^{-1}])&=\det(Xe^{g(Z)}e^{\ln(I-a^{-1}Z)}+e^{g(Y)}e^{\ln(I-a^{-1}Y)})\\&=a^{-n}\det(e^{g(Y)})\det(\hat{X}(aI-Z)+(aI-Y))\\&=a^{-n}\det(e^{g(Y)})H_1(a),\end{aligned}$$

where we have chosen $\hat{X}=e^{-g(Y)}Xe^{g(Z)}$ and used the notation of Lemma 2.2. Similarly,

$$(a-b)\tau(\vec{t}-[a^{-1}]-[b^{-1}])=a^{-n}b^{-n}\det(e^{g(Y)})H_2(a,b).$$

Consequently, (7) is equivalent to demonstrating that the polynomial $H(a,b,c)$ in Lemma 2.2 is zero in the case of this $\hat{X}$, Y, and Z. But, according to the second result in Lemma 2.1 we have that $\kappa(\hat{X},Y,Z)=\kappa(X,Y,Z)\leqslant 1$ and so Lemma 2.2 demonstrates that the Hirota equation is satisfied.

Once we know that τ_M is a tau function, the formula for ψ_M is derived from simply using the "famous Japanese formula,"[2]

$$\psi_M(x,z)=\frac{\tau_M(x-z^{-1},-z^{-2}/2,-z^{-3}/3,\ldots)}{\tau_M(x,0,0,\ldots)}e^{xz}.$$

Note that the numerator is simply $\tau_M(\vec{t}-[z^{-1}])$ with $\vec{t}=(x,0,0,\ldots)$. So, again expanding this in terms of the power series for the logarithm we derive the desired expression for ψ_M. □

Remark 3.1: Technically, although the function $\tau\equiv 0$ solves the bilinear equations of the KP hierarchy, it is not generally considered to be a tau function. [In particular, there is no associated operator $\mathcal{L}$ satisfying the Lax equation or function $u(x,y,t)$ satisfying the KP equation.] In the preceding we have not been careful to make certain that τ is nonzero. In fact, one can certainly choose $M\in\mathcal{M}_n^1$ so that $\tau_M=0$. Consequently, Theorem 3.1 should be understood to say that if τ_M is nonzero (which is generally the case) then it is a KP tau function.

Remark 3.2: Since the Baker–Akhiezer function ψ_M in Theorem 3.1 has the property that $z^ne^{-xz}\psi_M$ is a polynomial in z, it must be that τ_M is the tau function of a rank-one KP solution with a (singular) rational spectral curve. In particular, it must be a soliton solution or one of its rational degenerations. Well-known consequences[6–8] of this fact are the following:

Corollary 3.1: Let $K=K_M(t_1,t_2,t_3,\ldots,\partial_x)$ be the ordinary differential operator determined by simply substituting the formal symbol ∂_x in for z in the polynomial

$$K(t_1,t_2,\ldots,z)=\frac{\det(X(zI-Z)e^{g(Z)}+(zI-Y)e^{g(Y)})}{\det(Xe^{(Z)}+e^{g(Y)})}.$$

Then, equating x and t_1, $\mathcal{L}_M=K\partial_xK^{-1}$ satisfies the Lax equations

$$\frac{\partial}{\partial t_i}\mathcal{L}=[\mathcal{L},(\mathcal{L}^i)_+].$$

Moreover, the function

$$u(x,y,t) := \frac{\partial^2}{\partial x^2} \log \tau_M(x,y,t,0,0,\ldots)$$

satisfies the KP equation

$$\tfrac{3}{4} u_{yy} = (u_t - \tfrac{1}{4}(6uu_x + u_{xxx}))_x .$$

Remark 3.3: It is well known and easily verified (cf. Ref. 2) that multiplication by a function of the form $\exp(\Sigma \gamma_i t_i)$ takes one tau function to another having the same corresponding Lax operator $\mathcal{L}$. Such a change is often referred to as a "gauge transformation" in KP theory. Since $\det \exp g(Y)$ is a function of this form with $\gamma_i = \Sigma \lambda_j^i$ (where λ_j are the eigenvalues of Y counted according to multiplicity) it follows that:

Corollary 3.2: For $M = (X,Y,Z) \in \mathcal{M}_n^1$,

$$\hat{\tau}_M(t_1,t_2,\ldots) = \det(Xe^{g(Z)}e^{-g(Y)} + I)$$

is also a KP tau function differing from τ_M by only a gauge transformation.

Remark 3.4: Since the tau function and Baker–Akhiezer function are defined as they are by determinants of X, Y, and Z, simultaneously conjugating all three leaves the corresponding solution unchanged. Consequently, it would be possible to use Lemma 2.1 to take to quotient of $\mathcal{M}_n^1$ by the action of GL and then would be natural to define $\tau_{\overline{M}}$ for $\overline{M} \in \overline{\mathcal{M}_n^1} = \mathcal{M}_n^1 / GL(n)$.

B. Special cases

1. Gelfan'd–Dickii hierarchies (N-KdV)

The N-KdV or Gelfan'd–Dickii hierarchies are special classes of KP solutions for which $\mathcal{L}^N$ is an ordinary differential operator and hence is independent of the KP flows whose indices are multiples of N. In particular, we say a tau function is an N-KdV tau function if it factors as $\tau = f \cdot g$ where

$$\frac{\partial}{\partial t_{iN}} g = 0 \quad \forall i \in \mathbb{N}, \quad \frac{\partial}{\partial t_1} f = 0.$$

In other words, except for a factor independent t_1, τ is independent of t_j for all j that are multiples of N.

Let $\mathcal{M}_n^1(N)$ be the subset of $\mathcal{M}_n^1$,

$$\mathcal{M}_n^1(N) = \{(X,Y,Z) \in \mathcal{M}_n^1 : Y^N = Z^N\}.$$

Theorem 3.2: For $M \in \mathcal{M}_n^1(N)$, the corresponding tau function τ_M is a solution of the N-KdV hierarchy.

Proof: If we consider only the dependence upon t_1 and t_j (j a multiple of N) then

$$\begin{aligned}\tau_M &= \det(Xe^{t_1 Z + t_j Z^j} + e^{t_1 Y + t_j Y^j}) \\ &= \det(Xe^{t_1 Z + t_j Z^j} + e^{t_1 Y + t_j Z^j}) \\ &= \det(Xe^{t_1 Z} + e^{t_1 Y}) \det(e^{t_j Z^j}).\end{aligned}$$

□

For example, if we consider the restriction $Y = -Z$, then we are looking for matrix pairs (X,Z) satisfying

$$\operatorname{rank}(XZ+ZX)=1.$$

In this case, the formula (1) will produce a tau-function solution to the KdV hierarchy (independent of all even time flows). (Note that special cases have been considered elsewhere in the literature in the context of integrable particle systems.[9,10])

2. Solitons

The n-soliton solutions to the KP hierarchy are identified by these properties:

(1) The BA function $\psi(x,z)$ when multiplied by a degree n polynomial $q(z)=z^n+\cdots$ has the form

$$\vec{\psi}(x,z)=q(z)\,\psi(x,z)=\left(\sum_{i=1}^{n} a_i(x)z^i\right)e^{xz}.$$

(2) There are n independent linear ''conditions'' satisfied by $\overline{\psi}(x,z)$ of the form

$$\hat{\alpha}_i\overline{\psi}(x,\lambda_i)+\hat{\beta}_i\overline{\psi}(x,\mu_i)=0,\quad 1\leqslant i\leqslant n$$

(with $\lambda_i\neq\mu_i$).

These solutions can be constructed from $\mathcal{M}_n^1$ by choosing the point $M=(X,Y,Z)$ with

$$X_{ij}=\frac{\alpha_i}{\beta_j(\lambda_j-\mu_i)},\quad Y_{ij}=\mu_i\delta_{ij},\quad Z_{ij}=\lambda_i\delta_{ij}.$$

This can be verified, for instance, by noting that because $[Y,Z]=0$, the tau function $\hat{\tau}_M$ takes the form (cf. Corollary 3.2)

$$\hat{\tau}=\det(Xe^{g(Z)-g(Y)}+I).$$

For any index set $J\subset\{1,\ldots,n\}$, the principal minor of $Xe^{g(Z)-g(Y)}$ can be written as

$$\left(\prod_{i\in J}\frac{\alpha_i}{\beta_i}e^{g(\lambda_i)-g(\mu_i)}\right)\det\left(\frac{1}{\lambda_i-\mu_{i'}}\right)_{i,i'\in J}.$$

The latter determinant is a Cauchy determinant and is equal to

$$\prod_{i,i'\in J;i<i'}\frac{(\lambda_i-\lambda_{i'})(\mu_i-\mu_{i'})}{(\lambda_i-\mu_{i'})(\mu_i-\lambda_{i'})}\prod_{i\in J}\frac{1}{\lambda_i-\mu_i}.$$

Setting

$$c_i=\frac{\alpha_i}{\beta_i(\lambda_i-\mu_i)},$$

we obtain

$$\hat{\tau}=\sum_{J\subset\{1,\ldots,n\}}\prod_{i\in J}c_ie^{g(\lambda_i)-g(\mu_i)}\prod_{i,i'\in J;i<i'}\frac{(\lambda_i-\lambda_{i'})(\mu_i-\mu_{i'})}{(\lambda_i-\mu_{i'})(\mu_i-\lambda_{i'})},$$

which coincides with the known formula for this n-soliton solution of the KP hierarchy.[11]

3. Polynomial τ functions and rational solutions

Clearly, in the case that Y and Z are chosen to be nilpotent, the definition of τ_M produces a *polynomial* in the time variables t_i. It is perhaps of greater interest to note that one may also get tau functions that are—up to a gauge transformation—polynomial in t_1 but an infinite series if all t_i are considered.

For example, choosing

$$X=\begin{pmatrix}1&1&0\\1&0&0\\1&0&0\end{pmatrix},\quad Y=\begin{pmatrix}\lambda&1&0\\0&\lambda&1\\0&0&\lambda\end{pmatrix},\quad Z=\begin{pmatrix}\lambda&0&0\\1&\lambda&0\\0&1&\lambda\end{pmatrix}$$

leads to (after a gauge transformation to remove an exponential factor):

$$\tau(x,y,t,0,0,\ldots)$$

$$=1+(-3\lambda+3\lambda^2)t+\frac{9}{2}\lambda^4t^2+\frac{x^2}{2}+(6\lambda^3t+2\lambda-1)y+2\lambda^2y+(1+3\lambda^2t+2\lambda y)x.$$

Such solutions are well known and have been studied in previous papers.[6,8,12–14] However, one should especially compare the present approach with that of Wilson,[15] where these "vanishing rational KP solutions" are produced from matrix pairs (X,Z) satisfying $\operatorname{rank}(XZ-ZX+I)=1$. The main results in that paper concern the induced dynamics of the eigenvalues which behave as particles in a Calogero–Moser particle system. So, it may be of interest to similarly investigate the dynamics of the eigenvalues associated with almost-intertwining matrices.

IV. EIGENVALUE DYNAMICS

One of the most interesting things about the Ruijsenaars–Schneider (RS) particle system[9,16] is its connection to soliton tau functions. Specifically, certain KP tau functions can be written as

$$\tau(t_1,t_2,\ldots)=\det(X+I),$$

where $X=X(t_1,t_2,t_3,\ldots)$ is a matrix whose eigenvalues move according to the Ruijsenaars–Schneider Hamiltonian.

In this section we similarly study the dynamics of eigenvalues of time-dependent matrices in the context of almost-intertwining matrices to both reproduce and extend known results about the RS system and its connection to solitons.

A. Solitons and a matrix flow

Theorem 4.1: The vector fields V_i on the space of $n\times n$ matrix triples defined by

$$V_i(X_0,Y,Z)=(X_0Z^i-Y^iX_0,0,0) \tag{8}$$

are tangent to the manifold $\mathcal{M}_n^1$ and induce the flows in the variables t_i parametrized as

$$M_t=(X_t,Y,Z)=(e^{-g(Y)}X_0e^{g(Z)},Y,Z). \tag{9}$$

Proof: Note that the flows specified have the stated vector fields and that

$$X_tZ-YX_t=e^{-g(Y)}(X_0Z-YX_0)e^{g(Z)}$$

is a rank one matrix if X_0Z-YX_0 is. □

Remark 4.1: Given a parametrized flow $(X_t,Y,Z)\in\mathcal{M}_n^1$ as previously, the function $\hat{\tau}_M=(X_t+I)$ is another way to write the gauge transformed tau function from Corollary 3.2 with $M=(X_0,Y,Z)$.

B. General equations for eigenvalue dynamics

Given any matrices X_0, Y, Z such that $\kappa(X_0,Y,Z)=1$ let us define $X=X_t$ according to (9). If we denote the eigenvalues of X_t by $\{Q_i(t)\}$ $(1\leqslant i\leqslant n)$, to what extent can we describe their dynamics by intrinsic equations (depending only on Q_i and their derivatives)?

In what follows we will only be considering the flow under the first time parameter t_1, but will write simply t in order to simplify exposition and will use a ''dot'' to indicate differentiation with respect to this parameter.

We define vectors v and w by the formula

$$(X_0Z-YX_0)=vw^T \tag{10}$$

and so we have the equations of motion

$$\dot{X}=vw^T, \quad \dot{Y}=0, \quad \dot{Z}=0. \tag{11}$$

For convenience we introduce the (time-dependent) matrix U which diagonalizes X and the logarithms of the eigenvalues q_i

$$Q=UXU^{-1}=\begin{pmatrix} Q_1 & 0 & 0 & \cdots & \\ 0 & Q_2 & 0 & 0 & \cdots \\ 0 & 0 & Q_3 & 0 & \cdots \\ \vdots & & & \ddots & \end{pmatrix}, \quad q_i=\ln(Q_i) \tag{12}$$

and define in analogy to (10) the matrices and vectors

$$\hat{Y}=UYU^{-1}, \quad \hat{Z}=UZU^{-1}, \quad \hat{v}=Uv, \quad \hat{w}=wU^{-1} \tag{13}$$

so that

$$Q\hat{Z}-\hat{Y}Q=\hat{v}\hat{w}^T. \tag{14}$$

Note, in particular, that looking at an individual element of Eq. (14) yields

$$Q_i\hat{Z}_{ij}-Q_j\hat{Y}_{ij}=\hat{v}_j\hat{w}_i. \tag{15}$$

Now, defining $M=\dot{U}U^{-1}$ we have in analogy to (11)

$$\dot{Q}=[M,Q]+\hat{v}\hat{w}^T, \quad \hat{Y}=[M,\hat{Y}], \quad \hat{Z}=[M,\hat{Z}]. \tag{16}$$

Since Q and $\dot{Q}$ have no off diagonal elements, we get from (16) that

$$\dot{Q}_i=\hat{v}_i\hat{w}_i=\dot{q}_ie^{q_i}, \tag{17}$$

and

$$M_{ij}=\frac{\hat{v}_j\hat{w}_i}{Q_i-Q_j} \quad (i\neq j). \tag{18}$$

It turns out to be especially useful to write the equations of motion in terms of q_i rather than Q_i because then we find by multiplying (16) by Q^{-1} that

$$\begin{pmatrix} \dot{q}_1 & 0 & \cdots \\ \vdots & \ddots & \\ 0 & \cdots & \dot{q}_n \end{pmatrix} = \dot{Q}Q^{-1} = M - QMQ^{-1} + Q\hat{Z}Q^{-1} - \hat{Y}. \tag{19}$$

Since Q is diagonal, $M - QMQ^{-1}$ has no diagonal and $Q\hat{Z}Q^{-1} - \hat{Y}$ has the same diagonal as $\hat{Z} - \hat{Y}$ and so

$$\dot{q}_i = (\hat{Z} - \hat{Y})_{ii}. \tag{20}$$

Finally, we can differentiate (20) and use (15), (17), and (18) to find the equation of motion

$$\ddot{q}_i = ([M, \hat{Z} - \hat{Y}])_{ii} \tag{21}$$

$$= \sum_{k \neq i} (M_{ik}(\hat{Z}_{ki} - \hat{Y}_{ki}) - M_{ki}(\hat{Z}_{ik} - \hat{Y}_{ik})) \tag{22}$$

$$= \sum_{k \neq i} \left(\frac{\dot{Q}_i \dot{Q}_k}{Q_i(Q_i - Q_k)} + \frac{\hat{v}_k \hat{w}_i \hat{Z}_{k,i}}{Q_i} + \frac{\dot{Q}_i \dot{Q}_k}{Q_k(Q_k - Q_i)} + \frac{\hat{v}_i \hat{w}_k \hat{Z}_{ik}}{Q_k} \right) \tag{23}$$

$$= \sum_{k \neq i} \frac{\dot{Q}_i \dot{Q}_k (Q_i + Q_k) - (Q_i - Q_k)(Q_i \hat{v}_i \hat{w}_k \hat{Z}_{ik} - Q_k \hat{v}_k \hat{w}_i \hat{Z}_{ki})}{Q_i Q_k (Q_i - Q_k)}. \tag{24}$$

C. A special case

We can further simplify (24) assuming that $\hat{w}$ has no zero component. In that case, we can utilize additional freedom of conjugation by a diagonal matrix to leave Q unchanged but modify U.

In particular, if $\hat{w}$ is a vector with no zero component, then we can put it in a form where $w = (1,1,1,...,1)$ by multiplying U by the diagonal matrix with w_i's along its diagonal. Now, in this "gauge," we know that $\hat{w}_i = 1$ and so by (17) we know that $\hat{v}_i = \dot{Q}_i$. This then gives us that

$$\ddot{q}_i = \sum_{k \neq i} \frac{\dot{Q}_i \dot{Q}_k (Q_i + Q_k) - (Q_i - Q_k)(Q_i \dot{Q}_i \hat{Z}_{ik} - Q_k \dot{Q}_k \hat{Z}_{ki})}{Q_i Q_k (Q_i - Q_k)}.$$

Ideally, we would like to be able to completely eliminate $\hat{Z}_{ki}$ from this equation and have an "intrinsic" equation for the eigenvalues. It seems that this can only be done when certain additional simplifying assumptions are made.

Suppose that we are in the case that

$$-\lambda \hat{Y} + \hat{Z} = \gamma I \Rightarrow \hat{Z}_{ij} = \lambda \hat{Y}_{ij} \quad (i \neq j). \tag{25}$$

Combining Eqs. (15) and (25) we find that

$$\hat{Z}_{ij} = \frac{\lambda \hat{v}_j \hat{w}_i}{\lambda Q_i + Q_j} \quad (i \neq j).$$

Substituting this into (24) and again using (17) one finds the intrinsic equations of motion

$$\ddot{q}_i = (\lambda - 1)^2 \dot{Q}_i \sum_{k \neq i} \frac{\dot{Q}_k (Q_i + Q_k)}{(Q_i - Q_k)(\lambda Q_i - Q_k)(\lambda Q_k - Q_i)}. \tag{26}$$

Note that the equations are independent of γ. In the case $\lambda=-1$ the dynamics of (26) *is* the Ruijsenaars–Schneider model.[9]

V. COMMENTS AND CONCLUSIONS

It is interesting to note that restrictions on $\kappa(X,Y,Z)$ for triples of square matrices have arisen before in the context of integrable systems. For example, though the notations are different, the key operator identity used by Sakhnovich[17] is such a restriction. Perhaps there is a deep connection between the results of that work and this one, though the relationship is not immediately apparent to us. A more relevant result was obtained by Nijhoff and Chalykh,[18] who used the condition rank $(XZ-qZX)=1$ for invertible X and Z and scalar q to construct solutions to the q-difference KP hierarchy. It is reasonable to suppose that their result could now also be obtained as a discretization of the results in the present work in the special case $Y=qZ$. [Another matrix approach[19] to q-KP made use of the condition rank $(XY-qYX+I)=1$.]

The suggestive appearance of these spaces of matrices in such different contexts within the study of integrable systems might indicate that we should look more carefully at the manifolds $\mathcal{M}_n^k$. For instance, we have implicitly constructed a map from $\mathcal{M}_n^1$ to the infinite dimensional Grassmannian[2] Gr_1, and $\mathcal{M}_n^k$ naturally has the structure of an algebraic variety, but so far we have little understanding of the geometry.

Wilson[15] constructs an adelic Grassmannian and a Hilbert scheme from the set of matrices satisfying rank $([X,Z]+I)=1$. Moreover, the natural symmetry of this set which is manifested as the involution $(X,Z)\mapsto(Z^T,X^T)$ has significance both for the KP hierarchy (bispectrality) and the Calogero–Moser particle system (self-duality). So, it is reasonable to wonder how the obvious symmetries of $\mathcal{M}_n^k$ are reflected in the soliton solutions to the KP hierarchy. We have already noted that multiplying X by a function of Y on the left and a function of Z on the right corresponds to the KP flows. Note also that if $\kappa(X,Y,Z)=1$ and X is invertible then $\kappa(X^{-1},Z,Y)=1$ as well and that this triple corresponds to the same KP solution. (In particular, these two points in $\mathcal{M}_n^1$ get mapped to the same point in $\mathrm{Gr}^{\mathrm{rat}}$.) Similarly, if Y is invertible then $\kappa(Y,X,XZY^{-1})=1$, but it is not immediately apparent what symmetry of KP is analogous.

One alternative characterization of $\mathrm{Gr}^{\mathrm{rat}}$ is as the Grassmannian of finite dimensional subspaces of finitely supported distributions.[6] Specifically, to identify a point $W\in\mathrm{Gr}^{\mathrm{rat}}$ it is sufficient to identify the finitely supported distributions in z which annihilate the normalized Baker–Akhiezer function. We showed in Sec. III B 2 that in the case of nondegenerate solitons, the eigenvalues of Y and Z determine the support of the distributions and X determines the coefficients. We conjecture that this situation holds in general:

Conjecture 5.1: The support of the distributions annihilating $z^n\psi_M$ for $M=(X,Y,Z)\in\mathcal{M}_n^1$ is the set of eigenvalues of the matrices Y and Z with the highest derivative taken at a particular eigenvalue being bounded by the size of the corresponding Jordan blocks.

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A Lax pair for the two dimensional Euler equation

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A Lax pair for the 2D Euler equation is found. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1378305]

I. A LAX PAIR FOR THE TWO DIMENSIONAL (2D) EULER EQUATION

This is to report that a Lax pair for the 2D Euler equation is found. We write the 2D Euler equation in the vorticity form,

$$\frac{\partial \Omega}{\partial t} + \{\Psi, \Omega\} = 0, \tag{1.1}$$

where Ω is the vorticity, Ψ is the stream function, and the bracket $\{\ \}$ is defined as

$$\{f,g\} = (\partial_x f)(\partial_y g) - (\partial_y f)(\partial_x g).$$

Let us denote the x-directional and the y-directional velocities by u and v, respectively. Then

$$u = -\frac{\partial \Psi}{\partial y}, \quad v = \frac{\partial \Psi}{\partial x}, \quad \Omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}, \quad \Delta \Psi = \Omega.$$

The Lax pair is given as

$$\begin{aligned} L\varphi &= \lambda \varphi, \\ \partial_t \varphi + A\varphi &= 0, \end{aligned} \tag{1.2}$$

where

$$L\varphi = \{\Omega, \varphi\}, \ \ A\varphi = \{\Psi, \varphi\},$$

and λ is a complex constant, and φ is a complex-valued function. The compatibility condition of the Lax pair (1.2) gives the 2D Euler equation (1.1), i.e.,

$$\partial_t L = [L, A],$$

where $[L,A] = LA - AL$ gives the Lax representation of the 2D Euler equation (1.1).

Remark 1.1: With the recent development on chaos in partial differential equations,[1–3] *I am interested in building a dynamical system theory for 2D Euler equation under periodic boundary condition.*[4–6] *In particular, I am investigating the existence versus nonexistence of homoclinic structure. For such studies, it will be fundamentally important to find a Lax pair (if it exists) for the 2D Euler equation. Then I started with Zakharov's paper*.[7] *Zakharov proposed the Lax pair,*

$$\lambda D_1 \varphi + \{\Omega, \varphi\} = 0,$$

$$\partial_t \varphi + \lambda D_2 \varphi + \{S, \varphi\} = 0,$$

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where

$$D_1=\alpha\frac{\partial}{\partial x}+\beta\frac{\partial}{\partial y},\quad D_2=\gamma\frac{\partial}{\partial x}+\delta\frac{\partial}{\partial y},$$

α, β, γ, and δ are real constants, λ is a complex constant, S is a real-valued function, and φ is a complex-valued function. The compatibility condition of this Lax pair gives the following equation instead of the 2D Euler equation:

$$\frac{\partial\Omega}{\partial t}+\{S,\Omega\}=0,$$

$$D_1S=D_2\Omega.$$

(Notice the misprints in the English translation of the article.[7]*)*

Remark 1.2: The author is also aware of the Lax pair in the inverse Cauchy–Green tensor variable of the Lagrangian formulations of both 2D and 3D Euler equations found by Susan Friedlander and Misha Vishik.[8,9]

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Finite-dimensional integrable systems related to the *n*-wave interaction equations

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Under a constraint between the potentials and the eigenfunctions, Lax pairs and adjoint Lax pairs of a soliton hierarchy associated with the $n\times n$ generalized Zakharov–Shabat eigenvalue problem are transformed into a spatial finite-dimensional Hamiltonian system and a hierarchy of temporal finite-dimensional Hamiltonian systems. The Lax representations, *r*-matrix structure and integrals of motion are explicitly presented. These integrals of motion are functionally independent and in involution in pairs, which shows that these systems, especially the whole hierarchy of temporal finite-dimensional Hamiltonian systems, are Liouville integrable. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1385565]

I. INTRODUCTION

Since the pioneer work on solitons by Zabusky and Kruskal[1] in the 1960s, many infinite-dimensional integrable systems were found. Flaschka[2] pointed out that finite-dimensional integrable systems can be produced by constraining the infinite-dimensional integrable systems on a finite-dimensional invariant manifold. Motivated by Flaschka's idea and J. Moser's work,[3] the technique of the nonlinearization of Lax pairs, or, more generally, symmetry constraint, was developed during the beginning of the 1990s.[4–7] This method has been applied to various soliton hierarchies associated with matrix eigenvalue problems, from which a considerable number of finite-dimensional Liouville integrable Hamiltonian systems have been obtained.[8–12] Recently, the basic idea was generalized to discuss the binary nonlinearization of Lax pairs and adjoint Lax pairs of soliton hierarchies.[13–15]

The present article is devoted to the binary nonlinearization of the $n\times n$ generalized Zakharov–Shabat eigenvalue problem. The obtained spatial finite-dimensional Hamiltonian system and a hierarchy of temporal finite- dimensional Hamiltonian systems are completely Liouville integrable.[16] In the next section, we construct a soliton hierarchy associated with the eigenvalue problem. In Sec. III, under the Bargmann constraint between the potentials and the eigenfunctions, a spatial finite-dimensional Hamiltonian system and a hierarchy of temporal finite-dimensional Hamiltonian systems are obtained by nonlinearization of Lax pairs and adjoint Lax pairs of the obtained soliton hierarchy. In Sec. IV, the Lax representations are deduced for the resulting finite-dimensional systems. A constant rational *r*-matrix structure is established from the Lax operator. In Sec. V, sufficiently many involutive integrals of motion are obtained; furthermore, they are proved to be functionally independent. Thus the Hamiltonian systems generated from Lax pairs and adjoint Lax pairs are completely integrable in the Liouville sense.

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II. THE SOLITON HIERARCHY

Let us consider the $n\times n$ generalized Zakharov–Shabat eigenvalue problem

$$\phi_x=U(u,\lambda)\phi,\phi=\begin{pmatrix}\phi_1\\ \vdots\\ \phi_n\end{pmatrix},\quad U=\begin{pmatrix}\alpha_1\lambda & u_{12} & \dots & u_{1n}\\ u_{21} & \alpha_2\lambda & \dots & u_{2n}\\ \vdots & \vdots & \ddots & \vdots\\ u_{n1} & u_{n2} & \dots & \alpha_n\lambda\end{pmatrix},\tag{2.1}$$

where the potential vector $u=(u_{12},u_{21},\dots,u_{1n},u_{n1},u_{23},u_{32},\dots,u_{n-1,n},u_{n,n-1})^T$, λ is a constant spectral parameter, and $\alpha_i,1\leqslant i\leqslant n$, are n distinct constants. We will derive the isospectral soliton hierarchy associated with (2.1). To do this we first solve the stationary zero-curvature equation:

$$V_x=[U,V],\quad V=(V_{ij})_{n\times n},\tag{2.2}$$

where $V=\Sigma_{l\geqslant 0}V_l\lambda^{-l},V_l=(V_{ij}^{(l)})_{n\times n}$. Equation (2.2) leads to the following recursion relations:

$$V_{iix}^{(0)}=0,\quad V_{ij}^{(0)}=0,\quad (i\neq j),$$

$$V_{ijx}^{(l)}+u_{ij}(V_{ii}^{(l)}-V_{jj}^{(l)})+\sum_{\substack{k=1\\k\neq i,j}}^{n}(u_{kj}V_{ik}^{(l)}-u_{ik}V_{kj}^{(l)})-(\alpha_i-\alpha_j)V_{ij}^{(l+1)}=0,\quad i\neq j,\tag{2.3}$$

$$V_{iix}^{(l)}=\sum_{\substack{k=1\\k\neq i}}^{n}(u_{ik}V_{ki}^{(l)}-u_{ki}V_{ik}^{(l)}),\quad 1\leqslant i,\quad j\leqslant n,\quad l\geqslant 0.$$

By (2.3) we have

$$V_{ii}^{(0)}=\beta_i,\quad V_{ij}^{(0)}=0,\quad i\neq j,$$

$$V_{ii}^{(1)}=0,\quad V_{ij}^{(1)}=\frac{\beta_i-\beta_j}{\alpha_i-\alpha_j}u_{ij},\quad i\neq j,$$

and require that

$$\beta_i\neq\beta_j(i\neq j),\quad V_{ij}^{(l)}|_{u=0}=0,\quad l\geqslant 1,$$

which means constants of integration are put to be zero. Then $V_{ij}^{(l)}$'s are uniquely determined by (2.3). For instance, it is easy to see that

$$V_{ij}^{(2)}=\frac{\beta_i-\beta_j}{(\alpha_i-\alpha_j)^2}u_{ijx}+\frac{1}{\alpha_i-\alpha_j}\sum_{\substack{k=1\\k\neq i,j}}^{n}\left(\frac{\beta_i-\beta_k}{\alpha_i-\alpha_k}-\frac{\beta_k-\beta_j}{\alpha_k-\alpha_j}\right)u_{ik}u_{kj},\quad i\neq j,$$

$$V_{ii}^{(2)}=\sum_{\substack{k=1\\k\neq i}}^{n}\frac{\beta_k-\beta_i}{(\alpha_k-\alpha_i)^2}u_{ik}u_{ki}.$$

Equations (2.3) can be equivalently written as the Lenard form

$$MG_{l-1}=JG_l,\tag{2.4}$$

$$G_{l-1}=(V_{21}^{(l)},V_{12}^{(l)},\dots,V_{n1}^{(l)},V_{1n}^{(l)},V_{32}^{(l)},V_{23}^{(l)},\dots,V_{n,n-1}^{(l)},V_{n-1,n})^T,\quad l\geqslant 1,$$

$$G_0=\Big(\frac{\beta_2-\beta_1}{\alpha_2-\alpha_1}u_{21},\frac{\beta_1-\beta_2}{\alpha_1-\alpha_2}u_{12},\ldots,\frac{\beta_n-\beta_1}{\alpha_n-\alpha_1}u_{n1},\frac{\beta_1-\beta_n}{\alpha_1-\alpha_n}u_{1n},$$

$$\frac{\beta_3-\beta_2}{\alpha_3-\alpha_2}u_{32},\frac{\beta_2-\beta_3}{\alpha_2-\alpha_3}u_{23},\ldots,\frac{\beta_n-\beta_{n-1}}{\alpha_n-\alpha_{n-1}}u_{n,n-1},\frac{\beta_{n-1}-\beta_n}{\alpha_{n-1}-\alpha_n}u_{n-1,n})^T,$$

with the condition $G_l|_{u=0}=0$. Here J and M are two skew-symmetric operators:

$$J=(J_{ij})_{(n^2-n)\times(n^2-n)}=\begin{pmatrix} J_{12} & & & & & 0\\ & \ddots & & & & \\ & & J_{1n} & & & \\ & & & J_{23} & & \\ & & & & \ddots & \\ 0 & & & & & J_{n-1,n}\end{pmatrix},$$

$$J_{ij}=\begin{pmatrix}0 & \alpha_i-\alpha_j\\ \alpha_j-\alpha_i & 0\end{pmatrix};$$

$M=(M_{ij})_{(n^2-n)\times(n^2-n)}$ with

$$M_{(k-1)(2n-k)+2r-1,(k-1)(2n-k)+2r-1}=2u_{k,k+r}\partial^{-1}u_{k,k+r},$$

$$M_{(k-1)(2n-k)+2r,(k-1)(2n-k)+2r}=2u_{k+r,k}\partial^{-1}u_{k+r,k},$$

$$M_{(k-1)(2n-k)+2r-1,(k-1)(2n-k)+2r}=\partial-2u_{k,k+r}\partial^{-1}u_{k+r,k},$$

$$M_{(k-1)(2n-k)+2r-1,(k-1)(2n-k)+2s-1}=u_{k,k+r}\partial^{-1}u_{k,k+s},$$

$$M_{(k-1)(2n-k)+2r-1,(k-1)(2n-k)+2s}=u_{k+s,k+r}-u_{k,k+r}\partial^{-1}u_{k+s,k},$$

$$M_{(k-1)(2n-k)+2r,(k-1)(2n-k)+2s}=u_{k+r,k}\partial^{-1}u_{k+s,k},$$

$$M_{(k-1)(2n-k)+2r,(k-1)(2n-k)+2s-1}=-u_{k+r,k+s}-u_{k+r,k}\partial^{-1}u_{k,k+s},$$

$$M_{(k-1)(2n-k)+2r-1,(k+p-1)(2n-k-p)+2(r-p)-1}=u_{k,k+r}\partial^{-1}u_{k+p,k+r},$$

$$M_{(k-1)(2n-k)+2r-1,(k+p-1)(2n-k-p)+2(r-p)}=-u_{k,k+p}-u_{k,k+r}\partial^{-1}u_{k+r,k+p},$$

$$M_{(k-1)(2n-k)+2r,(k+p-1)(2n-k-p)+2(r-p)}=u_{k+r,k}\partial^{-1}u_{k+r,k+p},$$

$$M_{(k-1)(2n-k)+2r,(k+p-1)(2n-k-p)+2(r-p)-1}=u_{k+p,k}-u_{k+r,k}\partial^{-1}u_{k+p,k+r},$$

$$M_{(k-1)(2n-k)+2r-1,(k+r-1)(2n-k-r)+2t}=u_{k,k+r}\partial^{-1}u_{k+r+t,k+r},$$

$$M_{(k-1)(2n-k)+2r-1,(k+r-1)(2n-k-r)+2t-1}=-u_{k,k+r+t}-u_{k,k+r}\partial^{-1}u_{k+r,k+r+t},$$

$$M_{(k-1)(2n-k)+2r,(k+r-1)(2n-k-r)+2t-1}=u_{k+r,k}\partial^{-1}u_{k+r,k+r+t},$$

$$M_{(k-1)(2n-k)+2r,(k+r-1)(2n-k-r)+2t}=u_{k+r+t,k}-u_{k+r,k}\partial^{-1}u_{k+r+t,k+r},$$

and

$$M_{ij}^*=-M_{ji},\qquad M_{ij}=0\qquad \text{for other}\quad ij,$$

where

$$k,r,s,p,t\geqslant 1,\quad k+r\leqslant n,\quad k+s\leqslant n,\quad k+r+t\leqslant n,\quad s\neq r,\quad k+p<r.$$

Now we consider the auxiliary problem of the spectral problem (2.1),

$$\phi_{t_m}=V^{(m)}\phi,\quad V^{(m)}=V^{(m)}(u,\lambda)=(\lambda^m V)_+,\quad m\geqslant 1, \tag{2.5}$$

where $()_+$ is the truncation containing only non-negative powers of λ. The compatibility condition between (2.1) and (2.5) leads to the zero-curvature equation, $U_{t_m}-V_x^{(m)}+[U,V^{(m)}]=0$. This implies the following soliton hierarchy,

$$u_{t_m}=K_m=JG_m=J\Phi^m G_0,\quad m\geqslant 1, \tag{2.6}$$

where $\Phi=J^{-1}M$. The first typical nonlinear system in the hierarchy is the famous *n*-wave interaction equations in one spatial dimension:[17]

$$u_{ijt_1}=\frac{\beta_i-\beta_j}{\alpha_i-\alpha_j}u_{ijx}+\sum_{\substack{k=1\\k\neq i,j}}^{n}\left(\frac{\beta_i-\beta_k}{\alpha_i-\alpha_k}-\frac{\beta_k-\beta_j}{\alpha_k-\alpha_j}\right)u_{ik}u_{kj},\quad i\neq j,\quad 1\leqslant i,\quad j\leqslant n.$$

III. FINITE-DIMENSIONAL HAMILTONIAN SYSTEMS

In this section, under the Bargmann constraint between the potentials and the eigenfunctions, the Lax pair and adjoint Lax pair of the soliton hierarchy (2.6) are nonlinearized to a spatial finite-dimensional Hamiltonian system and a hierarchy of temporal finite-dimensional Hamiltonian systems.

The system (2.6) has an adjoint Lax pair

$$\psi_x=-U^T(u,\lambda)\psi, \tag{3.1}$$

$$\psi_{t_m}=-V^{(m)T}(u,\lambda)\psi,\quad m\geqslant 1, \tag{3.2}$$

where $\psi=(\psi_1,\ldots,\psi_n)^T$. In fact, we easily verify that the compatibility condition between (3.1) and (3.2) leads to the same zero-curvature equation as that between Eqs. (2.1) and (2.5).

Let $\lambda_1,\lambda_2,\ldots,\lambda_N$ be N mutual distinct eigenvalues. The systems associated with (2.1) and (3.1) can be written in the form

$$\begin{aligned}(\phi_{1l},\ldots,\phi_{nl})_x&=(\phi_{1l},\ldots,\phi_{nl})U^T(u,\lambda_l),\\(\psi_{1l},\ldots,\psi_{nl})_x&=-(\psi_{1l},\ldots,\psi_{nl})U(u,\lambda_l),\end{aligned} \tag{3.3}$$

where $\phi_{il}=\phi_i(\lambda_l),\psi_{il}=\psi_i(\lambda_l),1\leqslant i\leqslant n,1\leqslant l\leqslant N$, are eigenfunctions. A direct caculation gives the functional gradient of the eigenvalue λ_l with regard to the potential vector u:

$$\begin{aligned}\frac{\delta\lambda_l}{\delta u}&=\left(\frac{\delta\lambda_l}{\delta u_{12}},\frac{\delta\lambda_l}{\delta u_{21}},\ldots,\frac{\delta\lambda_l}{\delta u_{1n}},\frac{\delta\lambda_l}{\delta u_{n1}},\frac{\delta\lambda_l}{\delta u_{23}},\frac{\delta\lambda_l}{\delta u_{32}},\ldots,\frac{\delta\lambda_l}{\delta u_{n-1,n}},\frac{\delta\lambda_l}{\delta u_{n,n-1}}\right)^T\\&=(\phi_{2l}\psi_{1l},\phi_{1l}\psi_{2l},\ldots,\phi_{nl}\psi_{1l},\phi_{1l}\psi_{nl},\phi_{3l}\psi_{2l},\phi_{2l}\psi_{3l},\ldots,\phi_{nl}\psi_{(n-1)l},\phi_{(n-1)l}\psi_{nl})^T.\end{aligned}$$

Such a gradient satisfies the following equation:

$$M\frac{\delta\lambda_l}{\delta u}=\lambda_l J\frac{\delta\lambda_l}{\delta u}. \tag{3.4}$$

Now we consider the Bargmann constraint

$$G_0=\sum_{l=1}^{N}\frac{\delta\lambda_l}{\delta u}, \tag{3.5}$$

which implies

$$u_{ij}=\frac{\alpha_i-\alpha_j}{\beta_i-\beta_j}\langle\Phi_i,\Psi_j\rangle, i\neq j, 1\leqslant i,j\leqslant n, \tag{3.6}$$

where $\langle .,.\rangle$ is the standard inner-product in $\mathcal{R}^N$, and $\Phi_i=(\phi_{i1},\phi_{i2},\ldots,\phi_{iN})^T$, and $\Psi_i=(\psi_{i1},\psi_{i2},\ldots,\psi_{iN})^T$, $1\leqslant i\leqslant n$. Substituting (3.6) in (3.3), we obtain a spatial finite-dimensional Hamiltonian system

$$\Phi_{ix}=\frac{\partial H}{\partial\Psi_i},\quad \Psi_{ix}=-\frac{\partial H}{\partial\Phi_i},\quad 1\leqslant i\leqslant n, \tag{3.7}$$

with the Hamiltonian

$$H=\sum_{i=1}^{n}\alpha_i\langle\Lambda\Phi_i,\Psi_i\rangle+\sum_{1\leqslant i,j\leqslant n}\frac{\alpha_i-\alpha_j}{\beta_i-\beta_j}\langle\Phi_i,\Psi_j\rangle\langle\Phi_j,\Psi_i\rangle,$$

where $\Lambda=\mathrm{diag}(\lambda_1,\lambda_2,\ldots,\lambda_N)$.

In the same way, we discuss the nonlinearization of the auxiliary spectral problem (2.5) and its adjoint one (3.2);

$$\begin{gathered}(\phi_{1l},\ldots,\phi_{nl})_{t_m}=(\phi_{1l},\ldots,\phi_{nl})V^{(m)T}(u,\lambda_l),\\ (\psi_{1l},\ldots,\psi_{nl})_{t_m}=-(\psi_{1l},\ldots,\psi_{nl})V^{(m)}(u,\lambda_l),\quad m\geqslant 1,\quad 1\leqslant l\leqslant N\end{gathered} \tag{3.8}$$

under the constraints (3.6) and the control of the spatial system (3.7).

First we do some caculations. By using (2.4), (3.4) and (3.5), we have

$$G_k=\sum_{l=1}^{N}\lambda_l^k\frac{\delta\lambda_l}{\delta u},$$

which is a special solution of (2.4) and can be written as follows:

$$\tilde{V}_{ij}^{(k)}=\langle\Lambda^{k-1}\Phi_i,\Psi_j\rangle,\quad i\neq j,\quad 1\leqslant i,\quad j\leqslant n,\quad k\geqslant 1. \tag{3.9}$$

Here and hereafter, an overtilde indicates the corresponding nonlinearized quantity. From (3.9) and the last relations of (2.3), we have

$$\tilde{V}_{ii}^{(k)}=\langle\Lambda^{k-1}\Phi_i,\Psi_i\rangle,\quad 1\leqslant i\leqslant n,\quad k\geqslant 1.$$

Thus

$$\tilde{V}_{ij}=V_{ij}^{(0)}+\sum_{k\geqslant 1}\langle\Lambda^{k-1}\Phi_i,\Psi_j\rangle\lambda^{-k},\quad 1\leqslant i,\quad j\leqslant n, \tag{3.10}$$

and

$$(\tilde{V}^{(m)}(\lambda_l))_{ij}=(\lambda_l^m\tilde{V}_{ij})_+=V_{ij}^{(0)}\lambda_l^m+\sum_{k=1}^{m}\langle\Lambda^{k-1}\Phi_i,\Psi_j\rangle\lambda_l^{m-k},\quad m\geqslant 1,\quad 1\leqslant i,\quad j\leqslant n.$$

The nonlinearized temporal systems of (3.8) under the constraints (3.6) and the control of the spatial system (3.7) are a hierarchy of temporal finite-dimensional Hamiltonian systems:

$$\Phi_{it_m}=\frac{\partial H_m}{\partial\Psi_i},\quad \Psi_{it_m}=-\frac{\partial H_m}{\partial\Phi_i},\quad m\geqslant 1,\quad 1\leqslant i\leqslant n,\tag{3.11}$$

with the Hamiltonian

$$H_m=\sum_{i=1}^{n}\beta_i\langle\Lambda^m\Phi_i,\Psi_i\rangle+\frac{1}{2}\sum_{i=1}^{n}\sum_{k=1}^{m}\langle\Lambda^{k-1}\Phi_i,\Psi_i\rangle\langle\Lambda^{m-k}\Phi_i,\Psi_i\rangle$$

$$+\sum_{1\leqslant i<j\leqslant n}\sum_{k=1}^{m}\langle\Lambda^{k-1}\Phi_i,\Psi_j\rangle\langle\Lambda^{m-k}\Phi_j,\Psi_i\rangle,\quad m\geqslant 1.$$

IV. LAX REPRESENTATIONS AND *r*-MATRIX

By (3.10), we have

$$\tilde{V}=\begin{pmatrix}\beta_1+\sum_{l=1}^{N}\frac{\phi_{1l}\psi_{1l}}{\lambda-\lambda_l} & \sum_{l=1}^{N}\frac{\phi_{1l}\psi_{2l}}{\lambda-\lambda_l} & \cdots & \sum_{l=1}^{N}\frac{\phi_{1l}\psi_{nl}}{\lambda-\lambda_l}\\ \sum_{l=1}^{N}\frac{\phi_{2l}\psi_{1l}}{\lambda-\lambda_l} & \beta_2+\sum_{l=1}^{N}\frac{\phi_{2l}\psi_{2l}}{\lambda-\lambda_l} & \cdots & \sum_{l=1}^{N}\frac{\phi_{2l}\psi_{nl}}{\lambda-\lambda_l}\\ \vdots & \vdots & \ddots & \vdots\\ \sum_{l=1}^{N}\frac{\phi_{nl}\psi_{1l}}{\lambda-\lambda_l} & \sum_{l=1}^{N}\frac{\phi_{nl}\psi_{2l}}{\lambda-\lambda_l} & \cdots & \beta_n+\sum_{l=1}^{N}\frac{\phi_{nl}\psi_{nl}}{\lambda-\lambda_l}\end{pmatrix}.\tag{4.1}$$

Under the condition (3.6), the following equations still hold:

$$\tilde{V}_x=[\tilde{U},\tilde{V}],\quad \tilde{V}_{t_m}=[\tilde{V}^{(m)},\tilde{V}],\quad m\geqslant 1,\tag{4.2}$$

which are the Lax representations of the spatial system (3.7) and temporal systems (3.11), respectively. Set $L(\lambda)=\tilde{V}$ and $A_m(\lambda)=\tilde{V}^{(m)}$, thus we have the following theorem.

Theorem 1: Equations (3.7) and (3.11) have the following Lax representations,

$$L(\lambda)_x=[A_0(\lambda),L(\lambda)],\tag{4.3}$$

$$L(\lambda)_{t_m}=[A_m(\lambda),L(\lambda)],\quad m\geqslant 1,\tag{4.4}$$

respectively, where

$$L(\lambda)=(L_{ij}(\lambda))_{n\times n}=\begin{pmatrix} \beta_1+\sum_{l=1}^{N}\frac{\phi_{1l}\psi_{1l}}{\lambda-\lambda_l} & \sum_{l=1}^{N}\frac{\phi_{1l}\psi_{2l}}{\lambda-\lambda_l} & \cdots & \sum_{l=1}^{N}\frac{\phi_{1l}\psi_{nl}}{\lambda-\lambda_l} \\ \sum_{l=1}^{N}\frac{\phi_{2l}\psi_{1l}}{\lambda-\lambda_l} & \beta_2+\sum_{l=1}^{N}\frac{\phi_{2l}\psi_{2l}}{\lambda-\lambda_l} & \cdots & \sum_{l=1}^{N}\frac{\phi_{2l}\psi_{nl}}{\lambda-\lambda_l} \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{l=1}^{N}\frac{\phi_{nl}\psi_{1l}}{\lambda-\lambda_l} & \sum_{l=1}^{N}\frac{\phi_{nl}\psi_{2l}}{\lambda-\lambda_l} & \cdots & \beta_n+\sum_{l=1}^{N}\frac{\phi_{nl}\psi_{nl}}{\lambda-\lambda_l} \end{pmatrix},$$

$$A_0(\lambda)=\begin{pmatrix} \alpha_1\lambda & \frac{\alpha_1-\alpha_2}{\beta_1-\beta_2}\langle\Phi_1,\Psi_2\rangle & \cdots & \frac{\alpha_1-\alpha_n}{\beta_1-\beta_n}\langle\Phi_1,\Psi_n\rangle \\ \frac{\alpha_2-\alpha_1}{\beta_2-\beta_1}\langle\Phi_2,\Psi_1\rangle & \alpha_2\lambda & \cdots & \frac{\alpha_2-\alpha_n}{\beta_2-\beta_n}\langle\Phi_2,\Psi_n\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\alpha_n-\alpha_1}{\beta_n-\beta_1}\langle\Phi_n,\Psi_1\rangle & \frac{\alpha_n-\alpha_2}{\beta_n-\beta_2}\langle\Phi_n,\Psi_2\rangle & \cdots & \alpha_n\lambda \end{pmatrix},$$

and for $m\geqslant 1$, $A_m=((A_m)_{ij})_{n\times n}$ has its entries as follows:

$$(A_m)_{ii}=\beta_i\lambda^m+\sum_{k=1}^{m}\langle\Lambda^{k-1}\Phi_i,\Psi_i\rangle\lambda^{m-k},$$

$$(A_m)_{ij}=\sum_{k=1}^{m}\langle\Lambda^{k-1}\Phi_i,\Psi_j\rangle\lambda^{m-k},\quad i\neq j.$$

Now we deal with the r-matrix relation for the Lax operator $L(\lambda)$. A simple caculation gives rise to

$$\{L_{ik}(\lambda),L_{jl}(\mu)\}=\begin{cases} 0, \text{ when } j\neq k, i\neq l \text{ or } i=j=k=l; \\ \frac{1}{\mu-\lambda}(L_{jk}(\lambda)-L_{jk}(\mu)), \text{ when } j\neq k, i=l; \\ \frac{1}{\mu-\lambda}(L_{il}(\mu)-L_{il}(\lambda)), \text{ when } j=k, i\neq l; \\ \frac{1}{\mu-\lambda}(L_{jj}(\lambda)-L_{jj}(\mu)-L_{ii}(\lambda)+L_{ii}(\mu)), \text{ when } j=k\neq i=l, \end{cases}$$

where the Poisson bracket is defined as

$$\{f,g\}=\sum_{i=1}^{n}\sum_{j=1}^{N}\left(\frac{\partial f}{\partial\phi_{ij}}\frac{\partial g}{\partial\psi_{ij}}-\frac{\partial f}{\partial\psi_{ij}}\frac{\partial g}{\partial\phi_{ij}}\right).$$

Using the notations in Ref. 18, $L_1(\lambda)=L(\lambda)\otimes I, L_2(\mu)=I\otimes L(\mu)$, where I is the $n\times n$ unit matrix, and $\{L_1(\lambda),L_2(\mu)\}$ is a $n^2\times n^2$ matrix composed of various Poisson brackets of the matrix elements of $L_1(\lambda)$ and $L_2(\mu)$, i.e., $\{L_1(\lambda),L_2(\mu)\}_{ij,kl}=\{L_{ik}(\lambda),L_{jl}(\mu)\}, 1\leqslant i,j,k,l\leqslant n$.

A direct computation can give us the following r-matrix formulation.

Theorem 2: Lax operator $L(\lambda)$ satisfies the r-matrix relation as follows:

$$\{L_1(\lambda),L_2(\mu)\}=\left[\frac{1}{\mu-\lambda}P,L_1(\lambda)+L_2(\mu)\right], \tag{4.5}$$

where P is the permutation matrix, $Px\otimes y=y\otimes x$.

It is easy to see that the r-matrix $r_{12}(\lambda,\mu)=[1/(\mu-\lambda)]P$ satisfies the classical Yang–Baxter equation:[18]

$$[r_{12},r_{13}]+[r_{12},r_{23}]+[r_{13},r_{23}]=0.$$

V. INTEGRALS OF MOTION AND THE LIOUVILLE INTEGRABILITY

In this section, we will construct the motion integrals of finite-dimensional Hamiltonian systems (3.7) and (3.11). These integrals of motion are verified to be in involution in pairs and functionally independent, which leads to the complete Liouville integrability of the systems.

Lemma: Let V be a solution of the stationary zero-curvature equation $V_y=[U,V](y=x$ or $t_m)$, then

(1) det$V$ is constant independent of the variable y, and
(2) the matrix $\mu I-V$ is also a solution of the stationary zero-curvature equation $V_y=[U,V]$, where μ is an arbitrary parameter.

Proof: The first result is known (see Ref. 19). The second one can be easily verified.

By the above lemma, we know that $\det(\mu I-L(\lambda))$ is a constant independent of the variables x and t_m. Expanding $\det(\mu I-L(\lambda))$ in power of μ, yields

$$\det(\mu I-L(\lambda))=\mu^n-\sigma_1(\lambda)\mu^{n-1}+\ldots+(-1)^n\sigma_n, \tag{5.1}$$

where

$$\sigma_\nu(\lambda)\equiv\mathrm{tr}\overset{\nu}{\wedge}L(\lambda),\quad 1\leqslant\nu\leqslant n. \tag{5.2}$$

For example,

$$\sigma_1(\lambda)=\mathrm{tr}\,L(\lambda),\quad \sigma_2(\lambda)=\tfrac{1}{2}((\mathrm{tr}L(\lambda))^2-\mathrm{tr}\,L^2(\lambda)),\ \ldots,\sigma_n(\lambda)=\det L(\lambda).$$

Therefore we obtain the following result.

Proposition: The functions $\sigma_\nu(\lambda),1\leqslant\nu\leqslant n$, are integrals of motion of the Hamiltonian systems (3.7) and (3.11).

According to the r-matrix theory,[20] from (4.5) we have

$$\{\mathrm{tr}\,L^i(\lambda),\mathrm{tr}\,L^j(\mu)\}=0,\quad 1\leqslant i,\quad j\leqslant n, \tag{5.3}$$

which insures the involution property of the integrals of motion obtained from expanding $\sigma_\nu(\lambda),1\leqslant\nu\leqslant n$, in powers of λ. Explicity,

$$\sigma_1(\lambda)=\sum_{i=1}^{n}\beta_i+\sum_{m=0}^{\infty}\lambda^{-m-1}F_m^{(1)},$$

$$\sigma_2(\lambda)=\sum_{1\leqslant i<j\leqslant n}\beta_i\beta_j+\sum_{m=0}^{\infty}\lambda^{-m-1}F_m^{(2)},$$

$$\sigma_3(\lambda)=\sum_{1\leqslant i<j<k\leqslant n}\beta_i\beta_j\beta_k+\sum_{m=0}^{\infty}\lambda^{-m-1}F_m^{(3)},$$

$$\ldots,$$

$$\sigma_n(\lambda)=\prod_{i=1}^{n}\beta_i+\sum_{n=0}^{\infty}\lambda^{-m-1}F_n^{(n)},$$

where

$$F_m^{(1)}=\sum_{i=1}^{n}\langle\Lambda^m\Phi_i,\Psi_i\rangle,\quad m\geqslant 0,$$

$$F_0^{(2)}=\sum_{p=1}^{n}\sum_{\substack{i=1\\ i\neq p}}^{n}\beta_i\langle\Phi_p,\Psi_p\rangle,$$

$$F_m^{(2)}=\sum_{p=1}^{n}\sum_{\substack{i=1\\ i\neq p}}^{n}\beta_i\langle\Lambda^m\Phi_p,\Psi_p\rangle+\sum_{1\leqslant i<j\leqslant n}\sum_{l=1}^{m}\begin{vmatrix}\langle\Lambda^{l-1}\Phi_i,\Psi_i\rangle & \langle\Lambda^{m-l}\Phi_i,\Psi_j\rangle\\ \langle\Lambda^{l-1}\Phi_j,\Psi_i\rangle & \langle\Lambda^{m-l}\Phi_j,\Psi_j\rangle\end{vmatrix},\quad m\geqslant 1,$$

$$F_0^{(3)}=\sum_{p=1}^{n}\sum_{\substack{1\leqslant i<j\leqslant n\\ i,j\neq p}}\beta_i\beta_j\langle\Phi_p,\Psi_p\rangle,$$

$$F_1^{(3)}=\sum_{p=1}^{n}\sum_{\substack{1\leqslant i<j\leqslant n\\ i,j\neq p}}\beta_i\beta_j\langle\Lambda\Phi_p,\Psi_p\rangle+\sum_{1\leqslant i<j\leqslant n}\sum_{\substack{k=1\\ k\neq i,j}}^{n}\beta_k\begin{vmatrix}\langle\Phi_i,\Psi_i\rangle & \langle\Phi_i,\Psi_j\rangle\\ \langle\Phi_j,\Psi_i\rangle & \langle\Phi_j,\Psi_j\rangle\end{vmatrix},$$

$$F_m^{(3)}=\sum_{p=1}^{n}\sum_{\substack{1\leqslant i<j\leqslant n\\ i,j\neq p}}\beta_i\beta_j\langle\Lambda^m\Phi_p,\Psi_p\rangle+\sum_{1\leqslant i<j\leqslant n}\sum_{\substack{l+t=m-1\\ l,t\geqslant 0}}\sum_{\substack{k=1\\ k\neq i,j}}^{n}\beta_k\begin{vmatrix}\langle\Lambda^l\Phi_i,\Psi_i\rangle & \langle\Lambda^t\Phi_i,\Psi_j\rangle\\ \langle\Lambda^l\Phi_j,\Psi_i\rangle & \langle\Lambda^t\Phi_j,\Psi_j\rangle\end{vmatrix}$$

$$+\sum_{1\leqslant i<j<k\leqslant n}\sum_{\substack{l+t+s=m-2\\ l,t,s\geqslant 0}}\begin{vmatrix}\langle\Lambda^l\Phi_i,\Psi_i\rangle & \langle\Lambda^t\Phi_i,\Psi_j\rangle & \langle\Lambda^s\Phi_i,\Psi_k\rangle\\ \langle\Lambda^l\Phi_j,\Psi_i\rangle & \langle\Lambda^t\Phi_j,\Psi_j\rangle & \langle\Lambda^s\Phi_j,\Psi_k\rangle\\ \langle\Lambda^l\Phi_k,\Psi_i\rangle & \langle\Lambda^t\Phi_k,\Psi_j\rangle & \langle\Lambda^s\Phi_k,\Psi_k\rangle\end{vmatrix},\quad m\geqslant 2,$$

$$\ldots,$$

$$F_m^{(n)}=\sum_{p=1}^{n}\prod_{\substack{i=1\\ i\neq p}}^{n}\beta_i\langle\Lambda^m\Phi_p,\Psi_p\rangle+\sum_{1\leqslant i<j\leqslant n}\sum_{\substack{l+t=m-1\\ l,t\geqslant 0}}\prod_{\substack{k=1\\ k\neq i,j}}^{n}\beta_k\begin{vmatrix}\langle\Lambda^l\Phi_i,\Psi_i\rangle & \langle\Lambda^t\Phi_i,\Psi_j\rangle\\ \langle\Lambda^l\Phi_j,\Psi_i\rangle & \langle\Lambda^t\Phi_j,\Psi_j\rangle\end{vmatrix}$$

$$+\sum_{1\leqslant i<j<k\leqslant n}\sum_{\substack{l+t+s=m-2\\ l,t,s\geqslant 0}}\prod_{\substack{r=1\\ r\neq i,j,k}}\beta_r\begin{vmatrix}\langle\Lambda^l\Phi_i,\Psi_i\rangle & \langle\Lambda^t\Phi_i,\Psi_j\rangle & \langle\Lambda^s\Phi_i,\Psi_k\rangle\\ \langle\Lambda^l\Phi_j,\Psi_i\rangle & \langle\Lambda^t\Phi_j,\Psi_j\rangle & \langle\Lambda^s\Phi_j,\Psi_k\rangle\\ \langle\Lambda^l\Phi_k,\Psi_i\rangle & \langle\Lambda^t\Phi_k,\Psi_j\rangle & \langle\Lambda^s\Phi_k,\Psi_k\rangle\end{vmatrix}$$

$$+\ldots+\sum_{\substack{l_1+\ldots+l_n=m-n\\ l_1,\ldots,l_n\geqslant 0}}\begin{vmatrix}\langle\Lambda^{l_1}\Phi_1,\Psi_1\rangle & \ldots & \langle\Lambda^{l_n}\Phi_1,\Psi_n\rangle\\ \vdots & \ddots & \vdots\\ \langle\Lambda^{l_1}\Phi_n,\Psi_1\rangle & \ldots & \langle\Lambda^{l_n}\Phi_n,\Psi_n\rangle\end{vmatrix},\quad m\geqslant n.$$

From (5.3) we instantly have the following:

Theorem 3: The functions $F_m^{(i)},1\leqslant i\leqslant n,m\geqslant 0$, are in involution in pairs, i.e., $\{F_k^{(i)},F_l^{(j)}\}=0,1\leqslant i,j\leqslant n,k,l\geqslant 0$.

Now we turn to prove the functional independence of integrals of motion over some region of $\mathcal{R}^{2nN}$. The functional independence means a sufficent number of integrals of motion, which is important but usually difficult to verify. For the case of 2×2 matrix eigenvalue problems, Cao *et al.*[21,22] presented a effective method: straightening Abel-Jacobi coordinates method. But this method cannot be used to the cases of higher order matrix spectral problems, since the ellipic coordinates of Hamiltonian systems resulted from higher order matrix spectral problems are not known yet. Here we use the direct method to prove the functional independence of integrals of motion.

Theorem 4: The nN one-forms $dF_m^{(i)}, 1\leqslant i\leqslant n, 0\leqslant m\leqslant N-1$, are linearly independent over some region of $\mathcal{R}^{2nN}$.

Proof: In the following, we adopt compact forms, for example,

$$\frac{\partial}{\partial \Psi_i}=\left(\frac{\partial}{\partial \psi_{i1}},\ldots,\frac{\partial}{\partial \psi_{iN}}\right)^T,\quad \Psi=(\Psi_1,\ldots,\Psi_n),$$

and denote

$$C_i=\begin{pmatrix} \phi_{i1} & \lambda_1\phi_{i1} & \ldots & \lambda_1^{N-1}\phi_{i1}\\ \phi_{i2} & \lambda_2\phi_{i2} & \ldots & \lambda_2^{N-1}\phi_{i2}\\ \vdots & \vdots & \ddots & \vdots\\ \phi_{iN} & \lambda_N\phi_{iN} & \ldots & \lambda_N^{N-1}\phi_{iN}\end{pmatrix}$$

$$\begin{vmatrix} \frac{\partial F_0^{(1)}}{\partial \Psi_1} & \cdots & \frac{\partial F_{N-1}^{(1)}}{\partial \Psi_1} & \frac{\partial F_0^{(2)}}{\partial \Psi_1} & \cdots & \frac{\partial F_{N-1}^{(2)}}{\partial \Psi_1} & \cdots & \frac{\partial F_0^{(n)}}{\partial \Psi_1} & \cdots & \frac{\partial F_{N-1}^{(n)}}{\partial \Psi_1}\\ \frac{\partial F_0^{(1)}}{\partial \Psi_2} & \cdots & \frac{\partial F_{N-1}^{(1)}}{\partial \Psi_2} & \frac{\partial F_0^{(2)}}{\partial \Psi_2} & \cdots & \frac{\partial F_{N-1}^{(2)}}{\partial \Psi_2} & \cdots & \frac{\partial F_0^{(n)}}{\partial \Psi_2} & \cdots & \frac{\partial F_{N-1}^{(n)}}{\partial \Psi_2}\\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots\\ \frac{\partial F_0^{(1)}}{\partial \Psi_n} & \cdots & \frac{\partial F_{N-1}^{(1)}}{\partial \Psi_n} & \frac{\partial F_0^{(2)}}{\partial \Psi_n} & \cdots & \frac{\partial F_{N-1}^{(2)}}{\partial \Psi_n} & \cdots & \frac{\partial F_0^{(n)}}{\partial \Psi_n} & \cdots & \frac{\partial F_{N-1}^{(n)}}{\partial \Psi_n}\end{vmatrix}_{\Psi=0}$$

$$=\begin{vmatrix} C_1 & \sum_{i=2}^{n}\beta_i C_1 & \sum_{2\leqslant i<j\leqslant n}\beta_i\beta_j C_1 & \cdots & \prod_{i=2}^{n}\beta_i C_1\\ C_2 & \sum_{\substack{i=1\\ i\neq 2}}^{n}\beta_i C_2 & \sum_{\substack{1\leqslant i<j\leqslant n\\ i,j\neq 2}}\beta_i\beta_j C_2 & \cdots & \prod_{\substack{i=1\\ i\neq 2}}^{n}\beta_i C_2\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ C_n & \sum_{i=1}^{n-1}\beta_i C_n & \sum_{1\leqslant i<j\leqslant n-1}\beta_i\beta_j C_n & \cdots & \prod_{i=1}^{n-1}\beta_i C_n\end{vmatrix}$$

$$=\prod_{1\leqslant i<j\leqslant n}(\beta_i-\beta_j)\prod_{1\leqslant i<j\leqslant N}(\lambda_j-\lambda_i)^n\prod_{l=1}^{N}\prod_{k=1}^{n}\phi_{kl}$$

is not zero over the region $\Pi_{l=1}^{N}\Pi_{k=1}^{n}\phi_{kl}\neq 0$ of $\mathcal{R}^{2nN}$. Therefore, the nN one-forms $dF_m^{(i)}, 1\leqslant i\leqslant n, 0\leqslant m\leqslant N-1$, are linearly independent. The proof is finished.

A direct calculation shows that the Hamiltonian functions of systems (3.7) and (3.11) can be rewritten as follows:

$$H=\sum_{i=1}^{n}\gamma_i F_1^{(i)}+\sum_{1\leqslant i<j\leqslant n}\delta_{ij}\left(\sum_{k=1}^{n}(-1)^{k-1}\beta_i^{n-k}F_0^{(k)}\right)\cdot\left(\sum_{k=1}^{n}(-1)^{k-1}\beta_j^{n-k}F_0^{(k)}\right),$$

$$H_m=\sum_{i=1}^{n}\beta_i F_m^{(1)}-F_m^{(2)}+\frac{1}{2}\sum_{k=1}^{m}F_{k-1}^{(1)}F_{m-k}^{(1)},m\geqslant 1,$$

where

$$\gamma_p=\sum_{i=1}^{n}\left((-1)^{p+i}\alpha_i\beta_i^{n-p}\prod_{\substack{1\leqslant k<l\leqslant n\\ k,l\neq i}}(\beta_k-\beta_l)\right)\Big/\prod_{1\leqslant i<j\leqslant n}(\beta_i-\beta_j),$$

$$\delta_{ij}=\frac{\alpha_j-\alpha_i}{(\beta_i-\beta_j)^3\prod_{\substack{k=1\\ k\neq i,j}}^{n}(\beta_i-\beta_k)(\beta_j-\beta_k)}.$$

Hence we have

$$\{H,F_m^{(i)}\}=\{H_j,F_m^{(i)}\}=\{H,H_j\}=0,\quad 1\leqslant i\leqslant n,\quad 0\leqslant m\leqslant N-1,\quad j\geqslant 1.$$

Therefore the integrability of systems (3.7) and (3.11) is established resorting to Theorems 3 and 4.

Theorem 5: The finite-dimensional Hamiltonian systems (3.7) and (3.11) are completely integrable in the Liouville sense and their flows are commuting with each other.

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2+1 gravity, chaos and time machines

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$2+1$ gravity for space–times with topology $\mathbf{R}\times\mathbf{T}^2$ has been much studied. We add a description of how to extend these space–times across a Cauchy horizon into a region where the torus becomes Lorentzian. The result is a one parameter family of tori given by a geodesic in the ''Teichmüller space'' of Lorentzian tori. We describe this in detail. We also point out that if the modular group is regarded as part of the gauge group then these space–times offer a nice toy model for the dynamics of Bianchi IX models; in the region where the tori are spacelike the dynamics is described exactly by a hyperbolic billiard. On the other hand the modular group acts ergodically on the Teichmüller space of Lorentzian tori. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1378302]

I. INTRODUCTION

The subject of $2+1$ dimensional gravity looks *a priori* unpromising since—in the absence of matter—all space–times have constant curvature. Nevertheless it has been the subject of many investigations over the past twenty years or so. Indeed it is now widely recognized that it provides (when handled with taste!) surprisingly illuminating toy models of general relativity. Most of these investigations center on quantum gravity,[1] often from a Hamiltonian point of view, and as a result the space–time properties of the models are receiving somewhat less attention than we think that they deserve. Here we intend to present some properties of $2+1$ space–times with topology $\mathbf{R}\times\mathbf{T}^2$, regarded as quotients of Minkowski space. This perspective enables us to discuss what goes on in that region of space–time where the torus becomes Lorentzian and closed timelike curves appear; existing treatments[2,3] typically use the Hamiltonian ADM formalism and therefore do not go across the Cauchy horizon that bounds this region. The motivation for doing this is partly just curiosity, but partly a feeling that there is structure there which may well illuminate some features occurring in $3+1$ dimensions too—even if it will manifest itself in a different way in the latter case. Be that as it may a nice picture emerges; we can regard the entire space–time as a geodesic in the Teichmüller space of tori. This space is the familiar upper half plane in the Riemannian case, and it is $1+1$ dimensional de Sitter space in the Lorentzian case.

The second point that we wish to bring up is that if the modular group is regarded as part of the gauge group then these space–times offer a nice toy model for the chaotic behavior of Bianchi cosmologies. The dynamics of the latter has attracted attention for quite some time and many of its aspects are by now well understood. (There are many references, old,[4,5] new[6] and very new.[7]) In particular it is well known that the behavior of Bianchi IX models close to the singularity can be approximated by a hyperbolic billiard, which is an archetypical chaotic system. In the literature the situation is often described by saying that chaotic behavior appears when curvature becomes strong, although the precise meaning of the word ''chaotic'' here is a subject of some controversy. It is therefore of some interest that this kind of chaotic behavior appears in $2+1$ gravity with zero curvature, as a kind of global effect. A simplifying feature is that in our case the hyperbolic billiard captures the dynamics exactly.

As additional motivation we note that both the points we raise are important for quantization.

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They also appear to be of interest in string theory—see Ref. 8, but beware of some misunderstandings in that reference.

The organization of the paper is as follows: In Sec. II we construct our space–times by taking quotients of a region of $2+1$ dimensional Minkowski space with the appropriate discrete isometry groups. This construction is well known.[9,10] In Sec. III we describe these space–times as a geodesic in a Teichmüller space; this is a new result as far as the region with closed timelike curves is concerned. Since the Teichmüller space of Lorentzian tori has caused some puzzlement in the past[11] we describe it in detail. In Sec. IV we describe the dynamics which results when taking the quotient of Teichmüller space with the modular group, and stress the analogy to mixmaster cosmology. We focus on the spectrum of closed geodesics since they are the skeleton on which chaos is built; actually a closed geodesic corresponds to a self-similar rather than a periodic space–time. Our account is intended to be pedagogical (and to be helpful in Sec. V); all the hard results are well known to mathematicians[12,13] and to workers in quantum chaos.[14] In Sec. V we discuss the action of the modular group on the Teichmüller space of Lorentzian tori. We show that it is ergodic. (In a general setting involving discrete groups acting on coset spaces formed from noncompact groups such phenomena are known to mathematicians, but our pedestrian treatment is original as far as we know.) In Sec. VI we sketch how our method works for locally de Sitter space–times,[15] and comment on the higher genus case. Our conclusions are in Sec. VII.

II. OUR SPACE–TIMES

Let $\mathbf{M}$ be a region of $2+1$ dimensional Minkowski space and Γ a free discrete isometry group acting in a properly discontinuous way on this region. We want to choose Γ so that the quotient space $\mathbf{M}/\Gamma$ has the topology of a torus cross the real line. For a simply connected M the quotient space has Γ as its fundamental group. Therefore Γ must be a free discrete group with two commuting generators. We also insist that the quotient space should contain a complete spacelike surface that is not crossed by any closed timelike (or null) curve. The solution to this problem is described, e.g., by Louko and Marolf.[10] As generators of the discrete group we choose $g_1=e^{\xi_1}$ and $g_2=e^{\xi_2}$, that is to say exponentials of the two linearly independent commuting Killing vectors,

$$\xi_1=\alpha J_{xt}+\beta P_y; \quad \xi_2=\gamma J_{xt}+\delta P_y; \quad \alpha\delta-\beta\gamma>0. \tag{1}$$

Here J_{xt} is a Lorentz boost, P_y is a translation and α,β,γ and δ are real numbers. This is the most general solution, except for the obvious static case that we ignore. The group Γ will contain all group elements of the form e^{ξ}, where

$$\xi=(n_1\alpha-n_2\gamma)J_{xt}+(n_1\beta-n_2\delta)P_y, \quad n_1,n_2\in\mathbf{Z}. \tag{2}$$

Here n_1 and n_2 are arbitrary integers. We observe that Γ will contain pure boosts if and only if β/δ is rational, and pure translations if and only if α/γ is rational. Note also that in any case the action of Γ on the line $x=t=0$ is problematic; if a pure boost is present it has a line of fixed points there, and if not the action of Γ on this line is ergodic. Hence we see why the covering space M is taken to be a subset of $2+1$ dimensional Minkowski space only.

Since the Killing vectors ξ_1 and ξ_2 commute they form surfaces, namely

$$t^2-x^2=\tau^2\equiv-\sigma^2, \tag{3}$$

where τ^2 is some constant (not necessarily positive; if it is not then σ^2 is positive). These surfaces are left invariant by the group Γ, they foliate Minkowski space, they are intrinsically flat and their mean curvature is constant. They turn into tori when we take the quotient with Γ. From now on we take M to be the union of regions I and II of Minkowski space, as defined in Fig. 1. This means that our quotient spaces will be geodesically incomplete. If we did not restrict M in this way we would obtain what Louko and Marolf[10] accurately describe as a ''modest generalization of Misner space;'' as far as we can see there is nothing interesting to say about this that goes beyond Misner's original observations[16] which is why we make the restriction. Since each invariant

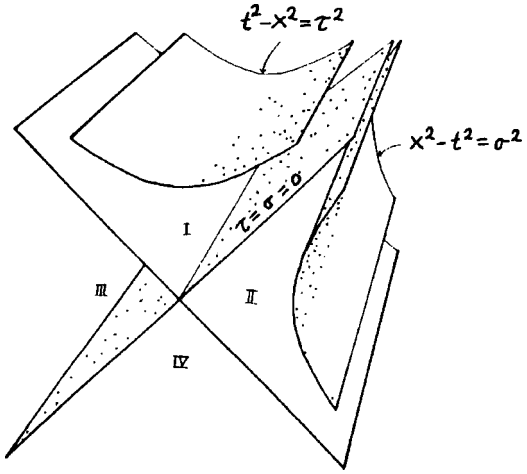

FIG. 1. $2+1$ dimensional Minkowski space divided into four wedge shaped regions, each of which is foliated by flat surfaces left invariant by Γ. Our covering space consists of regions I and II and our quotient space becomes a one parameter family of tori.

surface contributes a torus to the quotient space we now see that our space–times can be described as a one parameter family of flat tori; spacelike tori coming from region I and labeled by τ and Lorentzian tori coming from region II and labeled by σ. The Cauchy horizon $\tau=\sigma=0$ contributes a null torus.

III. A TRIP THROUGH TEICHMÜLLER SPACE

Our task now is to describe the one parameter family of flat tori that constitutes a space–time of the kind that we defined in Sec. II. We use the notation that $\xi_\alpha\xi^\alpha\equiv\|\xi\|^2\equiv\pm|\xi|^2$, where the sign depends on whether the vector is timelike or spacelike and $|\xi|$ is non-negative by definition. Let us first sketch what goes on in the region without closed timelike curves (where a Hamiltonian description is available[2,3]). At fixed τ the tori are built from parallelograms spanned by the generators ξ_1 and ξ_2. The angle between them is given by

$$\cos\theta=\frac{\xi_1\cdot\xi_2}{|\xi_1||\xi_2|}=\frac{\beta\delta+\alpha\gamma\tau^2}{\sqrt{\beta^2+\alpha^2\tau^2}\sqrt{\delta^2+\gamma^2\tau^2}}. \tag{4}$$

Therefore their area is a monotonically increasing function:

$$A=|\xi_1||\xi_2|\sin\theta=(\alpha\delta-\beta\gamma)\tau. \tag{5}$$

(The total area of the torus is the area of a parallelogram times a fixed numerical factor that can be chosen at will.) On the other hand the shape of the torus is changing in an interesting way. To describe it we introduce their Teichmüller space:

Definition: Teichmüller space is the moduli space of marked flat tori.

''Marked'' means that a particular pair of intersecting closed geodesics on the torus (namely the one that corresponds to our generators ξ_1 and ξ_2) has been singled out for special attention. The definition applies equally well to Riemannian and Lorentzian tori; in the former case it is well known that Teichmüller space can be regarded as the upper half plane, and that it is naturally equipped with the Poincaré metric,

$$ds^2=\frac{1}{y^2}(dx^2+dy^2). \tag{6}$$

This is hyperbolic space $\mathbf{H}^2$ and its isometry group is $PSL(2,\mathbf{R})$. We can assign a position in Teichmüller space to our tori if we first normalize our generators so that ξ_1 has length one and lies along the x-axis. Then the tip of ξ_2 will point at a unique point in the upper half plane, namely

$$(x,y)=\frac{|\xi_2|}{|\xi_1|}(\cos\theta,\sin\theta)=\frac{1}{\beta^2+\alpha^2\tau^2}(\beta\delta+\alpha\gamma\tau^2,(\alpha\delta-\beta\gamma)\tau). \tag{7}$$

Note that at this stage we use an auxiliary Euclidean metric on the coordinate plane to assign a point to ξ_2. We now have a curve parametrized by τ and it is elementary to show that this is a semi-circle meeting the boundary at right angles:

$$\left(x-\frac{\beta\gamma+\alpha\delta}{2\alpha\beta}\right)^2+y^2=\left(\frac{\alpha\delta-\beta\gamma}{2\alpha\beta}\right)^2. \tag{8}$$

This is a geodesic with respect to the natural metric. Hence the statement that the torus evolves along a geodesic in Teichmüller space. It should not be forgotten that it also grows in area. A minor calculation informs us that if we move a distance L along the geodesic, as measured by the Poincaré metric, then the area of the torus grows with a factor e^L. Note that this does not depend on the parameters describing the space–time, nor does it depend on where we are on the geodesic.

Now what happens when we pass the Cauchy horizon and enter region II? The first observation is that

$$\|\xi_1\|^2=\beta^2-\sigma^2\alpha^2. \tag{9}$$

Hence (unless ξ_1 is a pure translation or a pure boost) ξ_1 is spacelike in a region where $x^2-t^2=\sigma^2<\beta^2/\alpha^2$ and it is timelike when $x^2-t^2=\sigma^2>\beta^2/\alpha^2$. Let us refer to these regions as region IIa and IIb, respectively. To avoid misunderstandings, because the group Γ contains all the elements listed in Eq. (2) there are closed timelike geodesics through every point in region II, although the existence of closed null geodesics on the Cauchy horizon depends on whether δ/β is rational or not.

If we now try to mimic the construction of the Teichmüller space of Riemannian tori we run into a problem with the first step, which was to use a rotation to bring the generator ξ_1 into a standard position. We cannot use Lorentz transformations for the same purpose here: The Teichmüller space of Lorentzian tori splits into two components depending on whether ξ_1 is spacelike or timelike. We therefore use a different approach at first. By definition the Teichmüller space is the moduli space of marked flat Lorentzian tori.

Theorem 1: The Teichmüller space of Lorentzian tori has the topology $\mathbf{R}\times\mathbf{S}^1$. It is naturally equipped with the de Sitter metric.

Proof: To each oriented dyad of vectors there corresponds a unique flat marked Lorentzian torus. The set of such dyads is isomorphic to the group $SL(2,\mathbf{R})$. If we perform a Lorentz transformation of the dyad the torus is unchanged. Taking this into account we find a one-to-one correspondence between the Teichmüller space and the coset space $SL(2,\mathbf{R})/SO(1,1)$. But it is well known that this space has the stated topology. The de Sitter metric is natural because it is the maximally symmetric metric, and also because it arises if we take the perpendicular distance between the fibers, as measured by the standard metric on $SL(2,\mathbf{R})$.

Although well known the result is not quite trivial. The coset space $SO(2,1)/SO(1,1)$ has the topology of the Möbius strip, even though the group manifolds of $SO(2,1)$ and $SL(2,\mathbf{R})$ have the same topology. Let us give a sketch of the argument: we may, by analogy with the Euler angle parametrization of $\mathbf{S}^3$, introduce local coordinates θ,φ,γ on $SL(2,\mathbf{R})$ (aka $\mathbf{adS}_3$) as

$$X=\cos\frac{\theta}{2}\sinh\frac{\varphi-\gamma}{2},$$

$$Y=\sin\frac{\theta}{2}\sinh\frac{\varphi+\gamma}{2},$$

$$U=\cos\frac{\theta}{2}\cosh\frac{\varphi-\gamma}{2},$$

$$V=\sin\frac{\theta}{2}\cosh\frac{\varphi+\gamma}{2}. \tag{10}$$

The flat metric,

$$ds^2=dX^2+dY^2-dU^2-dV^2, \tag{11}$$

on the embedding space induces the metric

$$ds^2=\tfrac{1}{4}(-d\theta^2+d\varphi^2+d\gamma^2-2\,d\varphi\,d\gamma\cos\theta), \tag{12}$$

on $SL(2,\mathbf{R})$. The coordinate γ runs along the flow lines of the Killing field $J_{XU}+J_{YV}$ which generates $SO(1,1)$ transformations and we want to identify points along these lines. The metric on the resulting space, obtained from the orthogonal distance between the fibers, may be calculated using the threading approach of Boersma and Dray.[17] By identifying the metric in (12) with an Ansatz of the form

$$ds^2=M^2(d\gamma-M_i\,dx^i)^2+h_{ij}\,dx^i\,dx^j, \tag{13}$$

one obtains the metric

$$h=\tfrac{1}{4}(-d\theta^2+\sin^2\theta d\varphi^2), \tag{14}$$

for the quotient space $SL(2,\mathbf{R})/SO(1,1)$. This is precisely the metric for (part of) $\mathbf{adS}_2$ in a reasonably well known coordinate system; anti-de Sitter space and de Sitter space are identical in $1+1$ dimensions. It is also possible to do this calculation in global coordinates, at the expense of their not being adapted to the identification Killing field.

As it stands Theorem 1 is not very useful. To see what kind of curve our tori describe we need to know how to assign a point in Teichmüller space to a given marked torus. This understanding will be provided by the proof of Theorem 2, which will wind its way to the end of this section.

Theorem 2: The Teichmüller space of Lorentzian tori has the topology $\mathbf{R}\times\mathbf{S}^1$. The one parameter family of tori that represents a space–time (defined in Sec. II) is a timelike geodesic in this space provided that it is equipped with the de Sitter metric.

Proof: Our first step is to introduce coordinates (x,t). During the construction we use the flat Minkowski metric on this coordinate plane. Again we normalize the vectors so that ξ_1 points at (1,0). This is always possible provided that $\sigma^2<\beta^2/\alpha^2$. Since we know the scalar product of the vectors we find that the tip of ξ_2 points at the point

$$(x,t)=\frac{1}{\beta^2-\sigma^2\alpha^2}(\beta\delta-\alpha\gamma\sigma^2,-(\alpha\delta-\beta\gamma)\sigma). \tag{15}$$

We have therefore been able to arrange that this component of Teichmüller space is identical to the lower half plane. It is elementary to show that the points on this curve obey

$$\left(x-\frac{\beta\gamma+\alpha\delta}{2\alpha\beta}\right)^2-t^2=\left(\frac{\alpha\delta-\beta\gamma}{2\alpha\beta}\right)^2. \tag{16}$$

This is a hyperbola with its foci on the x-axis and it is a geodesic with respect to the metric,

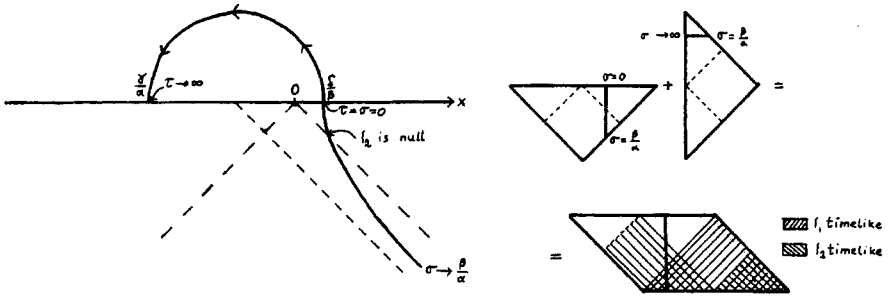

FIG. 2. The curve through Teichmüller space. In the upper half plane the torus is Riemannian. In the lower half plane the torus is Lorentzian but the generator ξ_1 is still spacelike. When ξ_1 is timelike we again obtain a half plane. The latter two half planes are conveniently depicted with conformal diagrams; adding them together so that the curve becomes smooth we obtain the conformal diagram of $1+1$ dimensional de Sitter space.

$$ds^2=\frac{1}{t^2}(dx^2-dt^2). \tag{17}$$

But this is in fact the de Sitter metric on a coordinate patch that covers ''one half'' of de Sitter space.

We can now draw a picture of the geodesic in Teichmüller space, where the Teichmüller space of Riemannian tori has been joined to its counterpart for Lorentzian tori across their conformal boundaries. Note that in the Lorentzian part of the picture the geodesic reaches infinite coordinate values at finite parameter values $\sigma^2=\beta^2/\alpha^2$. This is actually a good thing: We know that the coordinates we are using cover only a part of Teichmüller space. ''Infinity'' in the picture corresponds to a coordinate singularity that is caused by our assumption that ξ_1 is spacelike. (See Fig. 2.)

When ξ_1 is timelike we again introduce an infinite half plane, this time described by the coordinates t' and $x'>0$, and normalize the vectors so that ξ_1 points at $(t',x')=(1,0)$. We then find that ξ_2 points at

$$(t',x')=\frac{1}{\sigma^2\alpha^2-\beta^2}(\beta\delta-\alpha\gamma\sigma^2,(\alpha\delta-\beta\gamma)\sigma). \tag{18}$$

These points lie on the hyperbola,

$$\left(t'+\frac{\beta\gamma+\alpha\delta}{2\alpha\beta}\right)^2-x'^2=\left(\frac{\alpha\delta-\beta\gamma}{2\alpha\beta}\right)^2. \tag{19}$$

This is a geodesic with respect to the metric,

$$ds^2=\frac{1}{x'^2}(dt'^2-dx'^2). \tag{20}$$

This is again the metric on ''one half'' of de Sitter space. Since we now think of the conformal boundary as being timelike it may be more natural to think of it as anti-de Sitter space—but in $1+1$ dimensions de Sitter space and anti-de Sitter space coincide when we switch the meaning of space and time.

It remains to show that the two components of Teichmüller space can be glued together so that they form a de Sitter space, in such a way that the curve becomes a geodesic globally. For this purpose we observe that both $\mathbf{H}^2$ (the Teichmüller space of Riemannian tori) and $1+1$ dimensional de Sitter space can be isometrically mapped into surfaces in a $2+1$ dimensional Minkowski space with the metric

$$ds^2 = dX^2 + dY^2 - dU^2. \tag{21}$$

Explicitly we define an embedding of $\mathbf{H}^2$ by

$$X = \frac{x}{y}, \quad Y + U = \frac{1}{y}, \quad Y - U = -\frac{x^2 + y^2}{y}; \quad y > 0. \tag{22}$$

The surface is the upper sheet of the hyperboloid $X^2 + Y^2 - U^2 = -1$ and the induced metric is the one given in Eq. (6). The first component of the Teichmüller space of Lorentzian tori is embedded through

$$X = \frac{x}{t}, \quad Y + U = \frac{1}{t}, \quad Y - U = \frac{t^2 - x^2}{t}; \quad t > 0. \tag{23}$$

The surface is ''one half'' of the hyperboloid $X^2 + Y^2 - U^2 = 1$ and the induced metric is the one given in Eq. (17). The second component is embedded through

$$X = \frac{t'}{x'}, \quad Y + U = -\frac{1}{x'}, \quad Y - U = \frac{t'^2 - x'^2}{x'}; \quad x' > 0. \tag{24}$$

The surface is ''the other half'' of the hyperboloid $X^2 + Y^2 - U^2 = 1$ and the induced metric is the one given in Eq. (20).

A geodesic in $\mathbf{H}^2$, and a timelike geodesic in de Sitter space, is uniquely defined as the intersection of a hyperboloid with a timelike plane through the origin in the embedding space. The curve in Teichmüller space is given by Eqs. (8), (16) and (19). Therefore, to show that this curve is globally a timelike geodesic in de Sitter space we must find a spacelike vector k_α such that Eqs. (16) and (19) are equivalent to $k \cdot X = 0$. An elementary calculation shows that this is the case for the vector,

$$(k_X, k_Y, k_U) = (\alpha^2\delta^2 - \beta^2\gamma^2, \beta\delta(\alpha^2 + \gamma^2) - \alpha\gamma(\beta^2 + \delta^2), \quad \alpha\gamma(\beta^2 - \delta^2) + \beta\delta(\gamma^2 - \alpha^2)). \tag{25}$$

Equation (8) is also reproduced. This completes the proof that the curve is globally described by a timelike geodesic in de Sitter space.

IV. THE COGWHEELS OF CHAOS

In this section we restrict ourselves to region I (where there are no closed timelike curves), so that the evolution can be regarded as time evolution in a configuration space in the standard sense.[2,3] However, it is a moot point whether the configuration space should be taken to be Teichmüller space or the moduli space of (unmarked) flat tori. The latter space is in fact $\mathbf{H}^2/\Gamma_M$, where Γ_M is the modular group $PSL(2,\mathbf{Z})$ acting on the upper half plane through

$$z \to z' = \frac{az + b}{cz + d}; \quad ad - bc = 1, \tag{26}$$

where a, b, c and d are integers and $z = x + iy$. (To see that z and z' actually correspond to the same torus, consider a pair of intersecting closed geodesics on the torus and choose them to have the shortest circumference possible. The conformal structure can be characterized by the angle and relative lengths of this pair. A little experimentation shows that these are unaffected by a modular transformation.) The quotient space is the famous modular surface, usually described as the fundamental region of the group which is bounded by $r^2 \equiv x^2 + y^2 = 1$ and $x = \pm 1/2$. It is depicted in Fig. 3. Its area is finite and it is a smooth manifold except for two conical singularities occurring at the fixed points of the transformations S and ST, where S and T are the transformations

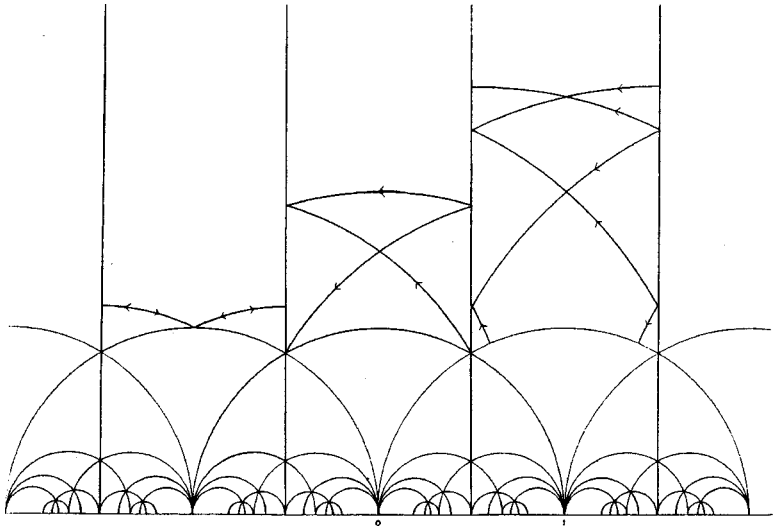

FIG. 3. The modular surface is the fundamental region of the modular group, with sides appropriately identified. The picture shows how the upper half plane is tesselated by copies of the fundamental region. In three of the copies we have drawn examples of closed geodesics ($N=3$ $x_+=[\dot{1}]$, $N=4$ $x_+=[\dot{1},\dot{2}]$ and $N=5$ $x_+=[\dot{1},\dot{3}]$ in the notation introduced below).

$$Sz=-\frac{1}{z},\quad Tz=z+1. \tag{27}$$

S and T generate the group and obey two relations, viz., $S^2=1$ and $(ST)^3=1$. Note that the transformation S acts by switching the elements in the oriented dyad that defines the torus.

The question whether the configuration space is $\mathbf{H}^2$ or $\mathbf{H}^2/\Gamma_M$ matters for the properties of the model but it is not a question of right or wrong, since we do not intend to compare the model to experiment anyway. Technically the modular group does not belong to the connected component of the gauge group so that both options are open as far as consistency is concerned. For thoughtful comments on this issue we refer to papers by Peldán[18] and Matschull;[19] here we choose the second option because it is an interesting one.

As shown by Artin[12] and Hedlund[20] the geodesic flow on the modular surface is ergodic (indeed they showed this at a time when the proper definition of an ergodic system was yet to be found—with today's definition we can say that the flow has the Bernoulli property, which is the strongest ergodic property around). From this point of view it has been much studied; Series has written a nice review with some entries to the technical literature.[13] Here we focus on one aspect of this flow, namely its closed orbits. We take the point of view that one can define ''chaos'' in a dynamical system by the requirement that the number of its unstable closed orbits rises exponentially as a function of length. This is not at all unreasonable; in fact this is the feature of chaotic systems that survives the transition to quantum theory (via the Gutzwiller trace formula, which connects the asymptotic properties of the spectrum of closed geodesics to the spectrum of the Laplacian). Since it is a simple matter of counting it is also a feature that survives the transition to diffeomorphism invariant systems—unlike Lyapounov exponents and the like that can be reparametrized away. To avoid confusion, note that—because the area of our tori is growing—a closed geodesic in moduli space actually corresponds to a self-similar rather than a periodic space–time.

The closed geodesics on the modular surface arise because any hyperbolic Möbius transformation—corresponding to an $SL(2,\mathbf{R})$ matrix whose trace has an absolute value larger than two—has a unique geodesic flowline connecting its pair of fixed points on the real axis. If this Möbius transformation is a modular transformation as well there are points on this geodesic that will be identified with each other, and a closed geodesic results. The distance L between a pair of neighboring identified points is easily computed. It is given by

$$2\cosh\frac{L}{2}=N, \tag{28}$$

where $N=|\mathrm{Tr}\,g|$ and g is the matrix corresponding to the modular transformation, so that $N=a+d$ if the transformation is written as in Eq. (26). Note that N can be used to label the conjugacy classes of $SL(2,\mathbf{R})$. This therefore is the length spectrum of the closed geodesics.

It takes more effort to understand how many closed geodesics there are. In group theoretical terms this is the problem to enumerate the conjugacy classes of $PSL(2,\mathbf{Z})$. There are only two conjugacy classes of elliptic elements, corresponding to the two fixed points on the boundary of the fundamental region. The number of conjugacy classes of hyperbolic elements on the other hand is a rapidly growing function of N. It is in fact known (see for instance Ref. 14) that when L is large the number n of closed geodesics with length l not exceeding L grows like

$$n(l\leqslant L)\sim\frac{e^L}{L}. \tag{29}$$

This settles it: The system is chaotic. It is however an instructive exercise to compute the number of closed geodesics ''from below'' with pedestrian methods, and this we will now proceed to do.

A geodesic in the upper half plane can be conveniently characterized by two real numbers, its starting point x_+ and its end point x_- on the real axis. To each geodesic we can associate a hyperbolic Möbius transformation whose fixed points are these two points. The geodesic projects to a closed geodesic on the modular surface if and only if this Möbius transformation belongs to the modular group, and there will be a unique such Möbius transformation of smallest trace associated to the closed geodesic (if $x=gx$ then $x=g^nx$; if $n>1$ the trace of g^n is greater than the trace of g and the corresponding geodesic is traversed several times—here we count only ''primitive'' closed geodesics). In equations then

$$x_\pm=\frac{ax_\pm+b}{cx_\pm+d}. \tag{30}$$

It follows that $x_\pm$ is a quadratic surd, that is to say a solution to a quadratic algebraic equation with integer coefficients whose discriminant is not a perfect square. The two solutions to this equation are

$$x_\pm=\frac{1}{2c}(a-d\pm\sqrt{N^2-4}), \tag{31}$$

where $N=a+d$ and we made use of the condition $ad-bc=1$. Note that the discriminant $D=N^2-4=4\sinh^2(L/2)$ according to Eq. (28). Since the surds occur in pairs the closed geodesics can in fact be labeled by just one real number, say its ''source'' x_+.

Next we introduce continued fractions.[21] A real number can be uniquely expressed in the form

$$x=a_0+\cfrac{1}{a_1+\cfrac{1}{a_2+\ldots}}\equiv[a_0,a_1,a_2,\ldots], \tag{32}$$

where all the partial quotients a_i are integers and all except possibly a_0 are positive. It is known that x is rational if and only if its continued fraction expansion is finite (i.e., the number of its partial quotients is finite), and it is a quadratic surd if and only if its continued fraction expansion eventually repeats, in which case it is called periodic. The beginning and end of the period is then marked with overdots, so that a quadratic surd of period length k is of the form $x=[a_0;a_1,\ldots a_{n-1},\dot{a}_n,\ldots,\dot{a}_{n+k-1}]$. This nice characterization of quadratic surds is interesting to us.

One piece of the technology of continued fractions should be mentioned, which is that they give rise to a sequence of approximations of x by rational numbers:

$$[a_0]=\frac{p_0}{q_0},\quad [a_0,a_1]=\frac{p_1}{q_1},\quad [a_0,a_1,a_2]=\frac{p_2}{q_2}, \tag{33}$$

and so on. Here p_n and q_n are polynomials in the partial quotients and by induction one can show that

$$p_n=a_n p_{n-1}+p_{n-2},\quad q_n=a_n q_n+q_{n-1}. \tag{34}$$

Note that p_n and q_n are monotonically increasing functions of n.

We want to count equivalence classes of geodesics under the modular group and therefore we will try to fix one member of each equivalence class. Now the modular group acts on a continued fraction in the following way:

$$x=[a_0,a_1,a_2,a_3,\dots]\to ST^{-a_0}x=-[a_1,a_2,a_3,\dots]\to ST^{a_1}ST^{-a_0}x=[a_2,a_3,\dots]. \tag{35}$$

It follows that we can remove the partial quotients in pairs. In particular it follows that we can choose x_+ to be a purely periodic continued fraction since we can always remove the initial sequence. Hence without loss of generality,

$$x_+=[\dot a_0,\dots,\dot a_{k-1}]. \tag{36}$$

If the period length k is even then x_+ is a fixed point of the group element,

$$g=ST^{a_{k-1}}\cdots\ ST^{a_1}ST^{-a_0}. \tag{37}$$

In terms of the polynomials introduced above it can be shown that

$$x_+=gx_+=\frac{q_{k-2}x_+-p_{k-2}}{-q_{k-1}x_++p_{k-1}}\Rightarrow N=|\mathrm{Tr}\,g|=p_{k-1}+q_{k-2}. \tag{38}$$

This is a useful fact since it means that N is a monotonically increasing function of the partial quotients. It also means that N will grow when the length of the period in the continued fraction grows, other things being equal.

The fixed point x_+ is in fact the source of the geodesic associated with g. This is so because g removes one period from the continued fraction, so that when g acts on an approximation to x_+ that is a rational number whose continued fraction expansion consists of a finite number of periods then g moves that rational number away from x_+. If the period length is odd then that g which leaves it fixed and has the smallest value of N is

$$g=ST^{a_{k-1}}\cdot\cdots\cdot ST^{a_0}ST^{-a_{k-1}}\cdot\cdots\cdot ST^{-a_0}. \tag{39}$$

It is convenient to regard continued fractions of odd period lengths as having even periods of twice the original length. According to a theorem of Galois' the corresponding sink (the other root of the quadratic equation) now obeys

$$Sx_-=-\frac{1}{x_-}=[\dot a_{k-1},\dots,\dot a_0]. \tag{40}$$

It is easy to show this since x_- is the source of the group element g^{-1}. The source and sink are now given in reduced form; this means that $x_+>1$ and $-1<x_-<0$.

Two geodesics in reduced form will give rise to the same closed geodesic on the modular surface if one can be obtained from the other by cyclic permutations of the pairs in the continued fraction expansion of their sources. This remaining ambiguity is easy to take care of, so that we

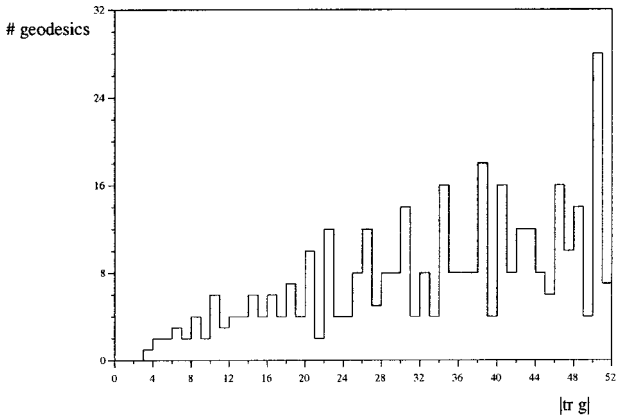

FIG. 4. Degeneracies of the length spectrum: The first 52 levels.

can now make a list of all closed geodesics corresponding to continued fraction expansions of a given period length. Moreover we know from Eq. (38) that the length of the geodesic is a monotonically increasing function of the partial quotients, so it is straightforward to compute the number of primitive closed geodesics of a length not exceeding some chosen reasonable number. The result of such a calculation is given in Fig. 4. Continuing this exercise on a computer one can see how Eq. (29) emerges. (Curiously we were unable to find this calculation in the accessible literature, although it has been done before.[22])

The conclusion is that $2+1$ gravity on the torus is a chaotic system according to the definition that we have adopted. Unlike the case of Bianchi models no approximation was involved. It may be felt that this chaos was introduced by sleight-of-hand since the system was in fact integrable before the modular group was declared to generate gauge symmetries. Indeed we are dealing with chaos of a very special kind, called ''arithmetical chaos.'' Although the system is chaotic in the sense that the number of closed orbits not exceeding a given length grows exponentially, it is also very special because there are huge degeneracies in the length spectrum (caused by the fact that the number of possible lengths grows much more slowly). Closer investigation reveals[14] that in such situations the level statistics of the Laplace operator shows some features that resemble integrable systems much more than they resemble a generic chaotic system (in particular the level repulsion that is typical of the latter is missing here) so the feeling is justified to some extent.

V. A LOOSE END

In the previous section we occupied ourselves with the action of the modular group on the Teichmüller space of Riemannian tori; the quotient space—the moduli space of Riemannian tori—is almost a smooth manifold since the modular group has only two elliptic conjugacy classes, and only the elliptic members of the modular group have fixed points in $\mathbf{H}^2$. The situation is dramatically different for the action of the modular group on the Teichmüller space of Lorentzian tori: Here every hyperbolic element of the modular group has fixed points inside the space, and we have already seen that there is an infinite number of inequivalent elements of this type.

The modular group is a subgroup of $PSL(2,\mathbf{R})=SO(2,1)$ and this is the isometry group of $\mathbf{H}^2$ and $1+1$ dimensional de Sitter space alike. The action of the generators of the modular group is as follows. The generator T gives rise to a ''null rotation'' generated by a Killing vector that becomes null along the coordinate singularity that separates the two parts of de Sitter space in the description we gave above; its fixed points lie on the conformal boundary. In the half plane coordinates it is simply a translation in the x-direction. The generator S is a spatial rotation of de Sitter space; it has no fixed points and cannot be described in a single coordinate patch of the type used above. If we think of S as effecting an interchange of the basis elements in the dyad that defines the torus we see that this must be so whenever one of the elements is spacelike and the

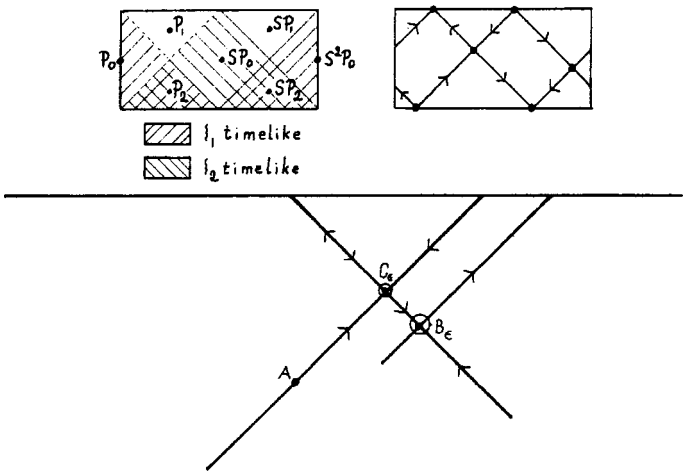

FIG. 5. The action of S on $1+1$ dimensional de Sitter space; also the null flow lines and the fixed points of a hyperbolic transformation; and a sketch of the proof (involving two different hyperbolic transformations) that the action of the modular group is ergodic.

other timelike—the generator S will then transform a point representing a spacelike ξ_1 (say) into a point in the other coordinate patch where ξ_1 is timelike. Figure 5 should be enough to make this clear.

Each hyperbolic element of the modular group has two fixed points inside de Sitter space, and two fixed points on each component of the conformal boundary separated from the fixed points in the interior by null lines that are left invariant by the transformation. The fixed points on the boundary are conjugate pairs of quadratic surds and conversely. This makes it easy to prove the next theorem.

Theorem 3: The action of the modular group on the Teichmüller space of Lorentzian tori is ergodic, in the sense that an arbitrary point can be transformed into an arbitrary coordinate neighborhood of any other point.

Proof: We must show that there is a modular transformation taking an arbitrary point A into a given neighborhood B_ϵ of another arbitrary point B. All neighborhoods are regarded as coordinate neighborhoods and we assume that the pair of points lies within some half plane coordinate patch. (There are exceptional pairs for which this fails, but they can easily be treated with an extension of the argument and will be ignored.)

We need to know that in any neighborhood of any point there is a hyperbolic modular transformation with a fixed point in that neighborhood. This will be so if, given any two points $x_\pm$ on the conformal boundary, we can find a conjugate pair of quadratic surds with one member arbitrarily close to each. But this is easy using the technology of the previous section. First modular transformations are used to show that it is enough to consider the case $x_+ > 1$, $-1 < x_- < 0$. Then one approximates x_+ and $-1/x_-$ with continued fractions to the desired accurary. The sequence of integers that gives the continued fraction approximating $-1/x_-$ is then reversed and added to the sequence that approximates x_+, and the resulting sequence is taken to be the period of a purely periodic continued fraction. Galois' theorem shows that we now have an approximation of x_+ whose conjugate surd approximates x_-. At the end we choose $x_\pm$ to be null separated from the given point. They intersect at a fixed point, and we are done.

With this understanding, draw null lines through A and B meeting each other at the point C. Choose a suitable neighborhood C_ϵ of C and a hyperbolic modular transformation with a fixed point in C_ϵ. Use this transformation to move the point A into C_ϵ. Then choose a hyperbolic modular transformation with a fixed point in B_ϵ and adjust the size of C_ϵ so that the second transformation moves C_ϵ into B_ϵ.

Except for a speculative remark in the conclusions we have nothing to say about what this means.

VI. OTHER SPACE–TIMES

The final issue is to what extent the results described above are peculiar to flat space–times and to the genus one case. We confine our remarks to region I, where there are no closed timelike curves and the tori are spacelike. Consider first locally de Sitter space–times. $2+1$ dimensional de Sitter space–time can be described as the hypersurface,

$$X^2+Y^2+Z^2-U^2=1, \tag{41}$$

embedded in a four dimensional Minkowski space (with U as its time coordinate). Alternatively, it is the maximally symmetric vacuum solution to Einstein's equations with a positive cosmological constant λ. Again we choose two commuting and linearly independent Killing vectors,

$$\xi_1=\alpha J_{ZU}+\beta J_{XY} \quad \xi_2=\gamma J_{ZU}+\delta J_{XY}. \tag{42}$$

They leave invariant the flat surfaces,

$$U^2-Z^2=\sinh^2\tau, \tag{43}$$

whose mean curvature is $K=4\cosh\tau$. Following the same steps as above we find that the invariant flat surfaces are turned into tori and that the evolution of the shape of these tori is given by a geodesic in Teichmüller space, with the interesting difference[15] that the evolution slows down and tends to a definite point in Teichmüller space as the parameter τ goes to infinity (while the area continues to grow). Explicitly,

$$(x,y)=\frac{1}{\alpha^2\tanh^2\tau+\beta^2}(\alpha\gamma\tanh^2\tau+\beta\delta,(\alpha\delta-\beta\gamma)\tanh\tau), \tag{44}$$

$$A=(\alpha\delta-\beta\gamma)\sinh\tau\cosh\tau. \tag{45}$$

The evolution stops because $\tanh\tau\to 1$ as $\tau\to\infty$. Note that this time the change of area as we move a distance L along the geodesic does depend on where we are on the geodesic. A subtlety should be mentioned also, namely that the universal covering space of the quotient spaces considered here is not, in general, de Sitter space itself but a ''larger'' incomplete space–time of constant curvature;[9,23] for the best explanation that we have to offer see Ref. 24.

Why does the evolution stop in the interior of Teichmüller space? The answer is in fact obvious: In the de Sitter case future infinity $\mathcal{J}$ is a spacelike surface transformed into itself by Γ. When we take the quotient we obtain an ''asymptotic torus'' with a definite conformal structure, and this is the endpoint of the geodesic in Teichmüller space. The area of this torus is not defined since $\mathcal{J}$ is equipped with a conformal structure only. At this point the reader may object that $\mathcal{J}$ is a sphere and that a discrete group like our Γ cannot act properly discontinuously on a sphere. This is true but irrelevant; in fact the covering space that we are using is not quite de Sitter space but an incomplete space–time obtained by removing two timelike lines from de Sitter space, and afterwards going to the universal covering space. This means that $\mathcal{J}$ is really a twice punctured sphere that has been ''unrolled'' to form a plane. This is explained in Fig. 7 in Ref. 24, where it can be seen that the invariant flat spacelike surfaces that were defined in the previous section do not encounter the timelike lines that were removed (except on $\mathcal{J}$ itself).

For the genus one case then we find that the chaotic behavior in the moduli space of tori is somehow ''washed away'' by the cosmological constant. It should however be noted that the flat torus universe is quite special in this regard. We can obtain locally flat space–times foliated by Riemann surfaces of higher genus by choosing Γ to be a discrete group—but this time not a free group—generated by noncommuting elements that in general are combinations of boosts and

translations. These space–times are conformally static when Γ consists of pure boosts. As time passes the boost parts will dominate the translations and the solution will tend to a conformally static solution, that is to a definite point inside Teichmüller space. (This has been demonstrated with full rigor.[25]) For the genus one case the evolution never stops for essentially the same reason; it is still true that eventually the boost part of the generators will dominate but now this means that the shape of the torus degenerates so that we approach the boundary of Teichmüller space.

VII. CONCLUSIONS

The main new results of this paper are the explicit description of the moduli space of Lorentzian tori as the union of two half planes constituting a $1+1$ dimensional de Sitter space, and the demonstration that the description of the $2+1$ dimensional locally flat torus universe as a geodesic in Teichmüller space is valid on both sides of the Cauchy horizon. We also emphasized the analogy between these $2+1$ dimensional space–times on the one hand, and mixmaster cosmology on the other. The difference between them is that the BKL approximation is exact in the former case. This is interesting because it shows that chaotic behavior in general relativity should not in general be blamed on strong gravitational fields.

There are some open ends. We did not describe the extension to a geodesically complete space–time, but this was mainly because it appears clear that this would give nothing new (compared to Misner's original work[16]). A more interesting open end is that the analogy to Bianchi IX cosmology holds only in the region where there are no closed timelike curves and the configuration space can be taken to be the moduli space of flat Riemannian tori, which is almost a smooth manifold. In the region with closed timelike curves we have to deal with the moduli space of Lorentzian tori, which is defined as the quotient of $1+1$ dimensional de Sitter space by the modular group. But—as we demonstrated—the action of the modular group is now ergodic, so that the resulting quotient space is not easily described even as a set. It is our understanding that the desire to describe sets of this type is one of the main motivations behind noncommutative geometry.[26] It would be marvelous if one could follow this lead in such a way that an analogy with the singularity in $3+1$ dimensional cosmologies could be drawn.

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Time-dependent automorphism inducing diffeomorphisms in vacuum Bianchi cosmologies and the complete closed form solutions for types II and V

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We investigate the set of space–time general coordinate transformations (GCTs) which leave the line element of a generic Bianchi-type geometry quasiform invariant; i.e., preserve manifest spatial homogeneity. We find that these GCTs, induce special time-dependent automorphic changes, on the spatial scale factor matrix $\gamma_{\alpha\beta}(t)$—along with corresponding changes on the lapse function $N(t)$ and the shift vector $N^{\alpha}(t)$. These changes, which are Bianchi-type dependent, form a group and are, in general, different from those induced by the group SAut(G) advocated in earlier investigations as the relevant symmetry group; they are used to simplify the form of the line element—and thus simplify Einstein's equations as well, without losing generality. As far as this simplification procedure is concerned, the transformations found are proved to be essentially unique. For the case of Bianchi types II and V, where the most general solutions are known, Taub's and Joseph's, respectively, it is explicitly verified that our transformations and only those, suffice to reduce the generic line element to the previously known forms. It thus becomes possible—for these types—to give in closed form the most general solution, containing all the necessary ''gauge'' freedom. © *2001 American Institute of Physics.*
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I. INTRODUCTION

It is well known that spatial homogeneity reduces Einstein's field equations for pure gravity to a system of ten coupled ordinary differential equations (ODEs) with respect to time:[1] one equation quadratic in the velocities $\dot{\gamma}_{\alpha\beta}$ and algebraic in N^2 $(G_{00}=0)$, three linear in velocities and also algebraic in N^{α} $(G_{0i}=0)$, and the six spatial equations $(G_{ij}=0)$ which are linear in $\ddot{\gamma}_{\alpha\beta}$ and also involve $N,\dot{N},N^{\alpha},\dot{N}^{\alpha},\gamma_{\alpha\beta},\dot{\gamma}_{\alpha\beta}$.

In attempting to find solutions to this set of equations, it is natural—although seldom adopted in the literature—to solve the quadratic constraint for N^2 and the linear constraint equations for as many of the N^{α}'s as possible; then substitute into the remaining spatial equations. When this is done, the spatial equations can be solved for only $6-4=2$ independent accelerations $\ddot{\gamma}_{\alpha\beta}$. Only for Bianchi types II and III—a particular VI case—can we solve for $6-3=3$ accelerations, since only two of the three linear constraints are independent; but then in both of these cases, a linear combination of the N^{a}'s remains arbitrary and counterbalances the existence of the third independent acceleration. Thus, the general solution to the above-mentioned system of equations will, in every Bianchi type, involve four arbitrary functions of time, whose specification should, somehow, correspond to a choice of time and space coordinates—in complete analogy to the full pure

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gravity, whereby four arbitrary functions of the space–time coordinates are expected to enter the general solution.

In the literature a different approach is more frequently met. It involves an *a priori* gauge choice of coordinate system: As far as time is concerned, one may set N to be either an explicit function of time, say 1 or t^2 etc., or some combination of $\gamma_{\alpha\beta}$'s—see (2.8). For the spatial coordinates, the depicted situation is more vague. In some works, N^α's are set to zero, in others, some N^α's are retained. In any case, most of these choices are considered as being more or less inequivalent and their connection to the well-known existence of Gauss-normal coordinates ($g_{00}=-1$, $g_{0i}=0$),[2] is not at all clear. When such a gauge choice has been made, the spatial equations can be solved for all six independent $\ddot{\gamma}_{\alpha\beta}(t)$. The constraint equations then become algebraic equations, restricting the initial data—needed to specify a particular solution of the spatial equations.

In both approaches, the ensuing equations are still too difficult to handle; thus further simplifying hypotheses are employed, such as $N^\alpha(t)=0$, leading to $\gamma_{\alpha\beta}=\mathrm{diag}((a^2(t),\, b^2(t),c^2(t)))$ for class A types, etc. For Bianchi types I and IX, the hypothesis $N^\alpha(t)=0$ and $\gamma_{\alpha\beta}=\mathrm{diag}((a^2(t),b^2(t),c^2(t)))$ is known to be linked to kinematics and/or dynamics—although in a, somewhat, vague way, see, e.g. Ref. 3 and Ryan in Ref. 1. In all other cases, this or any other simplifying hypothesis used is interpreted only as an ansatz to be tested at the end, i.e., after having solved all the (further simplified) equations. For example, to take an extreme case, diagonality of $\gamma_{\alpha\beta}(t)$ together with the vanishing of the shift vector is known to lead to incompatibility for Bianchi types IV, VII (class B),[4,5] as well as for the biaxial type VIII cases $(a^2,a^2,c^2),(a^2,b^2,a^2)$.[5] The diversity of the various ansatzen appearing in the literature causes a considerable degree of fragmentation.

It has long been suspected and/or known that automorphisms ought to play an important role in a unified treatment of this problem. The first mention goes back to Heekman and Schücking in Ref. 6. More recently, Jantzen (1979)[6] has used time-dependent automorphism matrices as a convenient parametrization of a general positive definite 3×3 scale factor matrix, $\gamma_{\alpha\beta}(t)$, in terms of a—desired—diagonal matrix. His approach is based on the orthonormal frame bundle formalism, and the main conclusion is (third of Jantzen (1982), p. 1138]:[6] "... *the special automorphism matrix group SAut(G), is the symmetry group of the ordinary differential equations, satisfied by the metric matrix* $\gamma_{\alpha\beta}$, *when no sources are present* ...." Later on, Samuel and Ashtekar[7] saw automorphisms, as a result of general coordinate transformations. Their space–time point of view has led them to consider the so-called "homogeneity preserving diffeomorphisms," and link them to topological considerations.

In this paper, we also take a spacetime point of view, and try to avoid the fragmentation by revealing those general coordinate transformations (GCTs) which enable us to simplify the line element (and therefore Einstein's equations), while at the same time preserving manifest spatial homogeneity. We are, thus, able to identify special automorphic transformations of $\gamma_{\alpha\beta}(t)$, along with corresponding—nontensorial, for the shift vector—changes of N,N^α which allow us to set $N^\alpha=0$ and bring $\gamma_{\alpha\beta}(t)$ to some irreducible, simple—though not unique—form.

The structure of the paper is as follows: In Sec. II, after establishing the existence of time-dependent automorphism inducing diffeomorphisms (AIDs), the general irreducible form of the line element for all Bianchi types is given, and a uniqueness theorem is proven. In Sec. III, attention is focused on Bianchi types II and V. Einstein's equations obtaining from the irreducible form of the line element are explicitly written down and completely integrated. The uniqueness of the transformations given in Sec. II is explicitly verified, with the aid of the well-known Taub's and Joseph's solution, respectively. As a result, we give the closed form of the most general line elements, satisfying Eq. (2.5). Finally, some concluding remarks are included in the discussion.

II. TIME-DEPENDENT AUTOMORPHISM INDUCING DIFFEOMORPHISMS

It is well known that the vacuum Einstein field equations can be derived from an action principle:

$$\mathcal{A}=\frac{-1}{16\pi}\int \sqrt{-{}^{(4)}g}{}^{(4)}R\ \mathrm{d}^4x \tag{2.1}$$

(we use geometrized units, i.e., $G=c=1$).

The standard canonical formalism[8] makes use of the lapse and shift functions appearing in the four-metric:

$$\mathrm{d}s^2=(N^iN_i-N^2)\mathrm{d}t^2+2N_i\ \mathrm{d}x^i\ \mathrm{d}t+g_{ij}\ \mathrm{d}x^i\ \mathrm{d}x^j. \tag{2.2}$$

From this line element the following set of equations obtains, expressed in terms of the extrinsic curvature:

$$K_{ij}=\frac{1}{2N}\left(N_{i|j}+N_{i|j}-\frac{\partial g_{ij}}{\partial t}\right),$$

$$H_0=\sqrt{g}(K_{ij}K^{ij}-K^2+R)=0, \tag{2.3a}$$

$$H_i=2\sqrt{g}(K^j_{i|j}-K_{|i})=0, \tag{2.3b}$$

$$\begin{aligned}\frac{1}{\sqrt{g}}\frac{\mathrm{d}}{\mathrm{d}t}[\sqrt{g}(K^{ij}-Kg^{ij})]=&-N\left(R^{ij}-\frac{1}{2}Rg^{ij}\right)-\frac{N}{2}(K_{kl}K^{kl}-K^2)g^{ij}\\&+2N(K^{ik}K^j_k-KK^{ij})-(N^{|ij}-N^{|l}_{|l}g^{ij})\\&+[(K^{ij}-Kg^{ij})N^l]_{|l}-N^i_{|l}(K^{lj}-Kg^{lj})-N^j_{|l}(K^{li}-Kg^{li}).\end{aligned} \tag{2.3c}$$

This set is equivalent to the ten Einstein's equations.

In cosmology, we are interested in the class of spatially homogeneous space–times, characterized by the existence of an m-dimensional isometry group of motions G, acting transitively on each surface of simultaneity Σ_t. When m is greater than three and there is no proper invariant subgroup of dimension three, the space–time is of the Kantowski–Sachs type[9] and will not concern us further. When m equals the dimension of Σ_t—which is 3—there exist three basis one-forms σ^α_i satisfying

$$\mathrm{d}\sigma^\alpha=C^\alpha_{\beta\gamma}\sigma^\beta\wedge\sigma^\gamma\Leftrightarrow\sigma^\alpha_{i,j}-\sigma^\alpha_{j,i}=2C^\alpha_{\beta\gamma}\sigma^\gamma_i\sigma^\beta_j, \tag{2.4a}$$

where $C^\alpha_{\beta\gamma}$ are the structure constants of the corresponding isometry group.

In this case there are local coordinates $t,\ x^i$ such that the line element in (2.2) assumes the form:

$$\mathrm{d}s^2=(N^\alpha(t)N_\alpha(t)-N^2(t))\mathrm{d}t^2+2N_\alpha(t)\sigma^\alpha_i(x)\ \mathrm{d}x^i\ \mathrm{d}t+\gamma_{\alpha\beta}\sigma^\alpha_i(x)\sigma^\beta_j(x)\ \mathrm{d}x^i\ \mathrm{d}x^j. \tag{2.4b}$$

Italic indices are spatial with range from 1 to 3. Greek indices number the different basis one-forms, take values in the same range, and are lowered and raised by $\gamma_{\alpha\beta}$, and $\gamma^{\alpha\beta}$, respectively.

A commitment concerting the topology of the three-surface is pertinent here, especially in view of the fact that we wish to consider diffeomorphisms;[7] we thus assume that G is simply connected and the three-surface Σ_t can be identified with G by singling out a point p of Σ_t, as the identity e, of G.

If we insert relations (2.4) into Eq. (2.3), we get the following set of ordinary differential equations for the Bianchi-type spatially homogeneous space–times:

$$E_0\doteq K^\alpha_\beta K^\beta_\alpha-K^2+R=0, \tag{2.5a}$$

$$E_\alpha \doteq K^\mu_\alpha C^\epsilon_{\mu\epsilon} - K^\mu_\epsilon C^\epsilon_{\alpha\mu} = 0, \tag{2.5b}$$

$$E^\alpha_\beta \doteq \dot{K}^\alpha_\beta - NKK^\alpha_\beta + NR^\alpha_\beta + 2N^\rho (K^\alpha_\nu C^\nu_{\beta\rho} - K^\nu_\beta C^\alpha_{\nu\rho}), \tag{2.5c}$$

where $K^\alpha_\beta = \gamma^{\alpha\rho} K_{\rho\beta}$ and

$$K_{\alpha\beta} = -\frac{1}{2N}(\dot{\gamma}_{\alpha\beta} + 2\gamma_{\alpha\nu} C^\nu_{\beta\rho} N^\rho + 2\gamma_{\beta\nu} C^\nu_{\alpha\rho} N^\rho), \tag{2.6}$$

$$\begin{aligned} R_{\alpha\beta} = {} & C^\kappa_{\sigma\tau} C^\lambda_{\mu\nu} \gamma_{\alpha\kappa} \gamma_{\beta\lambda} \gamma^{\sigma\nu} \gamma^{\tau\mu} + 2C^\lambda_{\alpha\kappa} C^\kappa_{\beta\lambda} + 2C^\mu_{\alpha\kappa} C^\nu_{\beta\lambda} \gamma_{\mu\nu} \gamma^{\kappa\lambda} \\ & + 2C^\lambda_{\beta\kappa} C^\mu_{\mu\nu} \gamma_{\alpha\lambda} \gamma^{\kappa\nu} + 2C^\lambda_{\alpha\kappa} C^\mu_{\mu\nu} \gamma_{\beta\lambda} \gamma^{\kappa\nu}. \end{aligned} \tag{2.7}$$

When $N^\alpha = 0$, Eq. (2.5c) reduces to the form of the equation given in Ref. 10. Equation set (2.5) forms what is known as a (complete) perfect ideal; that is, there are no integrability conditions obtained from this system. So, with the help of (2.5c), (2.6), and (2.7), it can explicitly be shown that the time derivatives of (2.5a) and (2.5b) vanish identically. The calculation is staightforward—although somewhat lengthy. It makes use of the Jacobi identity $C^\alpha_{\rho\beta} C^\rho_{\gamma\delta} + C^\alpha_{\rho\delta} C^\rho_{\beta\gamma} + C^\alpha_{\rho\gamma} C^\rho_{\delta\beta} = 0$, and its contracted form $C^\alpha_{\alpha\beta} C^\beta_{\gamma\delta} = 0$.

The vanishing of the derivatives of the four constrained equations: $E_0 = 0, E_\alpha = 0$, implies that these equations are first integrals of Eq. (2.5c)—moreover, with vanishing integration constants. Indeed, algebraically solving (2.5a) and (2.5b) for $N(t), N^\alpha(t)$, respectively and substituting in (2.5c), one finds that in all—but types II and III—Bianchi types, Eq. (2.5c) can be solved for only two of the six accelerations $\ddot{\gamma}_{\alpha\beta}$ present. In types II and III, the independent accelerations are three, since E_α are not independent and, thus, can be solved for only two of the three N^α's. But then in both of these cases, a linear combination of the N^a's remains arbitrary, and counterbalances the extra independent acceleration. Thus, in all Bianchi types, four arbitrary functions of time enter the general solution to the set of equations (2.5). Based on the intuition gained from the full theory, one could expect this fact to be a reflection of the only known covariance of the theory, i.e., of the freedom to make arbitrary changes of the time and space coordinates.

The rest of this section is devoted to the investigation of the existence, uniqueness, and properties of general coordinate transformations—containing four arbitrary functions of time, which on the one hand, must preserve the manifest spatial homogeneity of the line element (2.4b), and on the other hand, must be symmetries of Eq. (2.5). As far as time reparametrization is concerned the situation is pretty clear: If a transformation

$$t \to \tilde{t} = g(t) \Leftrightarrow t = f(\tilde{t}) \tag{2.8a}$$

is inserted in the line element (2.4b), it is easily inferred that[ ]

$$\gamma_{\alpha\beta}(t) \to \gamma_{\alpha\beta}(f(\tilde{t})) \equiv \tilde{\gamma}_{\alpha\beta}(\tilde{t}), \tag{2.8b}$$

$$\begin{aligned} N(t) &\to \pm N(f(\tilde{t})) \frac{\mathrm{d}f(\tilde{t})}{\mathrm{d}\tilde{t}} \equiv \tilde{N}(\tilde{t}), \\ N^\alpha(t) &\to N^\alpha(f(\tilde{t})) \frac{\mathrm{d}f(\tilde{t})}{\mathrm{d}\tilde{t}} \equiv \tilde{N}^\alpha(\tilde{t}). \end{aligned} \tag{2.8c}$$

Accordingly, K^α_β transforms under (2.8a) as a scalar and thus (2.5a), (2.5b) are also scalar equations while (2.5c) gets multiplied by a factor $\mathrm{d}f(\tilde{t})/\mathrm{d}\tilde{t}$. Thus, given a particular solution to Eq. (2.5), one can always obtain an equivalent solution by arbitrarily redefining time. Hence, we understand the existence of one arbitrary function of time in the general solution to Einstein's

equations (2.5). In order to understand the presence of the rest three arbitrary functions of time it is natural to turn our attention to the tranformations of the three spatial coordinates x^i. To begin with, consider the transformation:

$$\begin{aligned} &\tilde{t}=t\Leftrightarrow t=\tilde{t},\\ &\tilde{x}^i=g^i(x^j,t)\Leftrightarrow x^i=f^i(\tilde{x}^j,\tilde{t}). \end{aligned} \tag{2.9}$$

It is here understood that our previous assumption concerning the topology of G and the identification of Σ_t with G is valid for all values of the parameter t, for which the transformation is to be well defined.

Under these transformations, the line element (2.4b) becomes

$$\begin{aligned} ds^2=&\left[(N^\alpha N_\alpha-N^2)+\frac{\partial f^i}{\partial\tilde{t}}\frac{\partial f^j}{\partial\tilde{t}}\sigma_i^\alpha(f)\sigma_j^\beta(f)\gamma_{\alpha\beta}(\tilde{t})+2\sigma_i^\alpha(f)\frac{\partial f^i}{\partial\tilde{t}}N_\alpha(\tilde{t})\right]d\tilde{t}^2\\ &+2\sigma_i^\alpha(x)\frac{\partial x^i}{\partial\tilde{x}^m}\left[N_\alpha(\tilde{t})+\sigma_j^\beta(x)\frac{\partial x^j}{\partial\tilde{t}}\gamma_{\alpha\beta}(\tilde{t})\right]d\tilde{x}^m\ d\tilde{t}\\ &+\sigma_i^\alpha(x)\sigma_j^\beta(x)\gamma_{\alpha\beta}(\tilde{t})\frac{\partial x^i}{\partial\tilde{x}^m}\frac{\partial x^j}{\partial\tilde{x}^n}d\tilde{x}^m\ d\tilde{x}^n. \end{aligned} \tag{2.10}$$

Since our aim is to retain manifest spatial homogeneity of the line element (2.4b), we have to refer the form of the line element given in (2.10) to the old basis $\sigma_i^\alpha(\tilde{x})$ at the new spatial point $\tilde{x}^i$. Since σ_i^α (both at x^i and $\tilde{x}^i$) as well as $\partial x^i/\partial\tilde{x}^j$ are invertible matrices, there always exists a nonsingular matrix $\Lambda_\mu^\alpha(\tilde{x},\tilde{t})$ and a triplet $P^\alpha(\tilde{x},\tilde{t})$, such that

$$\begin{aligned} &\sigma_i^\alpha(x)\frac{\partial x^i}{\partial\tilde{x}^m}=\Lambda_\mu^\alpha(\tilde{x},\tilde{t})\sigma_m^\mu(\tilde{x}),\\ &\sigma_i^\alpha(x)\frac{\partial x^i}{\partial\tilde{t}}=P^\alpha(\tilde{x},\tilde{t}). \end{aligned} \tag{2.11}$$

The above-given relations must be regarded as definitions for the matrix Λ_μ^α and the triplet P^α. With these identifications the line element (2.10) assumes the following form:

$$\begin{aligned} ds^2=&[(N^\alpha N_\alpha-N^2)+P^\alpha(\tilde{x},\tilde{t})P^\beta(\tilde{x},\tilde{t})\gamma_{\alpha\beta}(\tilde{t})+2P^\alpha(\tilde{x},\tilde{t})N_\alpha(\tilde{t})]d\tilde{t}^2+2\Lambda_\mu^\alpha(\tilde{x},\tilde{t})\sigma_m^\mu(\tilde{x})[N_\alpha(\tilde{t})\\ &+P^\beta(\tilde{x},\tilde{t})\gamma_{\alpha\beta}(\tilde{t})]d\tilde{x}^m\ d\tilde{t}+\Lambda_\mu^\alpha(\tilde{x},\tilde{t})\Lambda_\nu^\beta(\tilde{x},\tilde{t})\gamma_{\alpha\beta}(\tilde{t})\sigma_m^\mu(\tilde{x})\sigma_n^\nu(\tilde{x})d\tilde{x}^m\ d\tilde{x}^n. \end{aligned} \tag{2.12}$$

If, following the spirit of Ref. 7, we wish the transformation (2.9) to be manifest homogeneity preserving, i.e., to have a well-defined, nontrivial action on $\gamma_{\alpha\beta}(t)$, $N(t)$, and $N^\alpha(t)$, we must impose the condition that $\Lambda_\mu^\alpha(\tilde{x},\tilde{t})$ and $P^\alpha(\tilde{x},\tilde{t})$ do not depend on the spatial point $\tilde{x}$, i.e., $\Lambda_\mu^\alpha=\Lambda_\mu^\alpha(\tilde{t})$ and $P^\alpha=P^\alpha(\tilde{t})$. Then (2.12) is written as

$$\begin{aligned} ds^2=&[(N^\alpha N_\alpha-N^2)+P^\alpha P^\beta\gamma_{\alpha\beta}+2P^\alpha N_\alpha]d\tilde{t}^2+2\Lambda_\mu^\alpha\sigma_m^\mu(\tilde{x})[N_\alpha+P^\beta\gamma_{\alpha\beta}]d\tilde{x}^m\ d\tilde{t}\\ &+\Lambda_\mu^\alpha\Lambda_\nu^\beta\gamma_{\alpha\beta}\sigma_m^\mu(\tilde{x})\sigma_n^\nu(\tilde{x})d\tilde{x}^m\ d\tilde{x}^n\\ \Rightarrow ds^2\equiv&(\tilde{N}^\alpha\tilde{N}_\alpha-\tilde{N}^2)d\tilde{t}^2+2\tilde{N}_\alpha(\tilde{t})\sigma_i^\alpha(\tilde{x})d\tilde{x}^i\ d\tilde{t}+\tilde{\gamma}_{\alpha\beta}(\tilde{t})\sigma_i^\alpha(\tilde{x})\sigma_j^\beta(\tilde{x})d\tilde{x}^i\ d\tilde{x}^j \end{aligned} \tag{2.13}$$

with the allocations

$$\tilde{\gamma}_{\alpha\beta}=\Lambda^{\mu}_{\alpha}\Lambda^{\nu}_{\beta}\gamma_{\mu\nu}, \tag{2.14a}$$

$$\tilde{N}_{\alpha}=\Lambda^{\beta}_{\alpha}(N_{\beta}+P^{\rho}\gamma_{\rho\beta}) \quad \text{and thus} \quad \tilde{N}^{\alpha}=S^{\alpha}_{\beta}(N^{\beta}+P^{\beta}), \tag{2.14b}$$

$$\tilde{N}=N \tag{2.14c}$$

(where $S=\Lambda^{-1}$).

Of course, the demand that Λ^{α}_{β} and P^{α} must not depend on the spatial point $\tilde{x}^{i}$, changes the character of (2.11) from identities to the following set of differential restrictions on the functions defining the transformation:

$$\frac{\partial f^{i}}{\partial\tilde{x}^{m}}=\sigma^{i}_{\alpha}(f)\Lambda^{\alpha}_{\beta}(\tilde{t})\sigma^{\beta}_{m}(\tilde{x}), \tag{2.15a}$$

$$\frac{\partial f^{i}}{\partial\tilde{t}}=\sigma^{i}_{\alpha}(f)P^{\alpha}(\tilde{t}). \tag{2.15b}$$

Equation (2.15) constitutes a set of first-order highly nonlinear PDEs for the unknown functions f^{i}. The existence of local solutions to these equations is guaranteed by Frobenius theorem[11] as long as the necessary and sufficient conditions

$$\frac{\partial}{\partial\tilde{x}^{j}}\left(\frac{\partial f^{i}}{\partial\tilde{x}^{m}}\right)-\frac{\partial}{\partial\tilde{x}^{m}}\left(\frac{\partial f^{i}}{\partial\tilde{x}^{j}}\right)=0,$$

$$\frac{\partial}{\partial\tilde{t}}\left(\frac{\partial f^{i}}{\partial\tilde{x}^{m}}\right)-\frac{\partial}{\partial\tilde{x}^{m}}\left(\frac{\partial f^{i}}{\partial\tilde{t}}\right)=0$$

hold. Through (2.15) and repeated use of (2.4a), these equations reduce, respectively, to

$$\Lambda^{\alpha}_{\mu}C^{\mu}_{\beta\gamma}=\Lambda^{\rho}_{\beta}\Lambda^{\sigma}_{\gamma}C^{\alpha}_{\rho\sigma}, \tag{2.16}$$

$$P^{\mu}C^{\alpha}_{\mu\nu}\Lambda^{\nu}_{\beta}=\tfrac{1}{2}\dot{\Lambda}^{\alpha}_{\beta}. \tag{2.17}$$

It is noteworthy that the solutions to (2.16) and (2.17)—by virtue of (2.14)—form a group, with composition law:

$$(\Lambda_3)^{\alpha}_{\beta}=(\Lambda_1)^{\alpha}_{\varrho}(\Lambda_2)^{\varrho}_{\beta},$$

$$(P_3)^{a}=(\Lambda_1)^{\alpha}_{\beta}(P_2)^{\beta}+(P_1)^{a},$$

where (Λ_1,P_1) and (Λ_2,P_2) are two successive transformations of the form (2.14). Note also that a constant automorphism is always a solution of (2.16), (2.17); indeed, $\Lambda^{a}_{\beta}(t)=\Lambda^{a}_{\beta}$ and $P^{a}(t)=0$ solve these equations. Thus, Λ^{a}_{β} and $P^{a}=0$ can be regarded as the remaining gauge symmetry, after one has fully used the arbitrary functions of time, appearing in a solution $\Lambda^{a}_{\beta}(t)$ and $P^{a}(t)$. Consequently one can, at first sight, regard all the arbitrary constants encountered when integrating (2.17) as absorbable in the shift, since the transformation law for the shift is then tensorial. This is certainly true as long as there is a nonzero initial shift. However, if one has used the independent functions of time, in order to set the shift zero, then the constants remaining within Λ^{a}_{β} are not absorbable. It is these kinds of constants that we explicitly present in the following when we give the solutions to (2.16) and (2.17) for all Bianchi types. A relevant nice discussion, distinguishing between genuine gauge symmetries (cf. arbitrary functions of time) and rigid sym-

metries (cf. arbitrary constants), is presented in Ref. 12. There a different definition of manifest homogeneity preserving diffeomorphisms—stronger than the one adopted in this work—is used, and results in only the inner automorphisms being allowed to acquire t dependence. In connection to this, it is interesting to observe that (2.16) and (2.17) give essentially the same results: Notice that $2P^{\mu}C^{\alpha}_{\mu\beta}$ is, by definition, the generator of inner automorphisms. Thus there is always a $\lambda^{\alpha}_{\beta}(t)\equiv\exp(2P^{\mu}C^{\alpha}_{\mu\beta})\in \mathrm{IAut(G)}$ satisfying (2.17). If we now parametrize the general solution to (2.16) and (2.17) by $\Lambda^{\alpha}_{\beta}(t)=\lambda^{\alpha}_{\varrho}(t)U^{\varrho}_{\beta}(t)$ and substitute in these relations, we deduce that the matrix U is a constant automorphism. This analysis is verified in the explicit solutions to (2.16) and (2.17) presented latter.

Equation (2.16) is satisfied if and only if $\Lambda^{\alpha}_{\beta}(t)$ is an element of the automorphism group of the Lie algebra determined by the $C^{\alpha}_{\beta\gamma}$. Equation (2.17) further restricts the form of $\Lambda^{\alpha}_{\beta}(t)$ and $P^{\alpha}(t)$, so that manifest spatial homogeneity is preserved despite the mixing of the old time and space coordinates in the new spatial coordinates $\tilde{x}^i$. Thus, it is appropriate to call transformations (2.9), satisfying conditions (2.15), (2.16), and (2.17), *time-dependent automorphism inducing diffeomorphisms*. The importance of automorphisms in Bianchi Cosmologies has been stressed in Ref. 6. The symmetry group of the differential equations, satisfied by $\gamma_{\alpha\beta}(t)$, advocated in these works of Jantzen *et al.*, is the unimodular matrices SAut(G). As we shall later see, we find another symmetry group, whose time-dependent part lies essentially in IAut(G) and thus coincides with SAut(G), only for class A Bianchi types VI, VII, VIII, and IX.

At this point it is natural to ask how this difference occurs. It is our opinion that the key elements on which the difference in the symmetry groups found rests are:

(a) The inhomogeneous transformation law (2.14b) for the shift. Indeed, Jantzen (1979), having adopted an orthonormal frame-bundle point of view, naturally assumes as his ''gauge'' transformation laws (2.14a) and (2.14c) and the tensorial law $\overline{N}^a=S^a_{\beta}N^{\beta}$, for the shift p. 221.

(b) The different definition and/or role reserved for the triplet $P^a(t)$; we define it as a sort of ''velocity'' of the transformation (2.9) in (2.15b) and use it in the inhomogeneous law (2.14b). On the other hand, Jantzen [1979), p. 221] uses the corresponding quantity $\omega^a(t)$ (the so called velocity of the automorphism frame to define a new time derivative $\partial/\partial\overline{t}=\partial/\partial t+\omega^a(t)\sigma^i_a(x)\partial/\partial x^i$.

(c) We concentrate on the symmetries of the ODEs (2.5), i.e., of *Eistein's equations written in the invariant base*, while Jantzen, as far as we understand, focuses on the symmetries of the PDEs (2.3), i.e., *of Einstein's equations, written in an arbitrary frame*.

In Ref. 7, the so-called homogeneity preserving diffeomorphisms are considered in relation to the topology of Σ_t. A time-independent version of (2.15), appears in Ref. 13, where all homogeneous three-geometries are classified in equivalence classes with respect to these ''frozen'' transformations. It is straightforward to check that $E_0, E_{\alpha}, E^{\alpha}_{\beta}$ transform—under (2.14)—as follows:

$$\tilde{E}_0=E_0,\quad \tilde{E}_{\alpha}=\Lambda^{\beta}_{\alpha}E_{\beta},\quad \tilde{E}^{\alpha}_{\beta}=S^{\alpha}_{\mu}\Lambda^{\nu}_{\beta}E^{\mu}_{\nu}. \tag{2.18}$$

This fact establishes the covariance of Eq. (2.5) under the ''gauge'' transformation (2.14), and implies that if $(N,N^{\alpha},\gamma_{\alpha\beta})$ is a solution to Einstein's equations, so will be the set $(\tilde{N},\tilde{N}^{\alpha},\tilde{\gamma}_{\alpha\beta})$—provided that (2.16) and (2.17) hold; in fact, as the preceding exposition proves, they will be the same equations expressed in different space–time coordinate systems. Out of the twelve quantities $\Lambda^{\alpha}_{\beta}(t)$ and $P^{\alpha}(t)$, conditions (2.16) and (2.17) leave us, as we are going to see, in every Bianchi type with three arbitrary functions of time. This fact, along with the time reparametrization covariance, completes our understanding of why four arbitrary functions of time enter the general solution to (2.5). Consequently, transformation (2.14), gives us the possibility to simplify the form of the line element, and thus of Einstein's equations without loss of generality. It is obvious that the simplification obtained is different for different Bianchi types, and even within a particular Bianchi type it is not unique—since one may ''spend'' the freedom of the three arbitrary functions in different ways.

A particularly interesting result is that the shift vector $\tilde{N}^\alpha$ can always be put to zero—perhaps at the expense of a more complicated $\tilde{\gamma}_{\alpha\beta}$. For the sake of completeness, we give in the following a detailed analysis of the space of solutions to (2.16) and (2.17), for each and every Bianchi type [solutions to (2.16), have been presented in Ref. 14].

To this end, recall that in three dimensions, the tensor $C^\alpha_{\beta\gamma}$ admits a unique decomposition in terms of a contravariant symmetric tensor density of weight -1, $m^{\alpha\beta}$ and a covariant vector $\nu_\alpha = \frac{1}{2}C^\rho_{\alpha\rho}$ as follows:[15]

$$C^\alpha_{\beta\gamma} = m^{\alpha\delta}\varepsilon_{\delta\beta\gamma} + \nu_\beta\delta^\alpha_\gamma - \nu_\gamma\delta^\alpha_\beta.$$

The contracted Jacobi identities imply that $m^{\alpha\beta}\nu_\beta = 0$, i.e., ν_α is a null eigenvector of the matrix $m^{\alpha\beta}$. Under a $GL(3,\Re)$ linear mixing of the basis one-forms $\sigma^\alpha \to \tilde{\sigma}^\alpha = S^\alpha_\beta\sigma^\beta$, the structure constant tensor transforms as

$$C^\alpha_{\beta\gamma} \to \tilde{C}^\alpha_{\beta\gamma} = S^\alpha_\mu \Lambda^\nu_\beta \Lambda^\rho_\gamma C^\mu_{\nu\rho}.$$

Accordingly, the $m^{\alpha\beta}$ and ν_α transform as

$$\tilde{m}^{\alpha\beta} = |S|^{-1} S^\alpha_\gamma S^\beta_\delta m^{\gamma\delta},$$

$$\tilde{\nu}_\alpha = \Lambda^\beta_\alpha \nu_\beta.$$

Λ (and thus S) is called a Lie algebra automorphism if $C^\alpha_{\beta\gamma} = \tilde{C}^\alpha_{\beta\gamma}$, i.e., if $\tilde{m}^{\alpha\beta}$ and $\tilde{\nu}_\alpha$ are equal to $m^{\alpha\beta}$ and ν_α, respectively. In this case the automorphism conditions become

$$m^{\alpha\beta} = |S|^{-1} S^\alpha_\gamma S^\beta_\delta m^{\gamma\delta}, \tag{2.19a}$$

$$\nu_\alpha = \Lambda^\beta_\alpha \nu_\beta. \tag{2.19b}$$

The different Bianchi types arise according to the rank and signature of $m^{\alpha\beta}$ and the vanishing or not of ν_α. Using (2.19), one can—straightforwardly—solve the system of Eqs. (2.16) and (2.17). We now present the form of $\Lambda^\alpha_\beta(t)$ and $P^\alpha(t)$ satisfying (2.16) and (2.17) as well as some irreducible form for $\gamma_{\alpha\beta}$ for each Bianchi type:

Type I: $m^{\alpha\beta} = 0, \nu_\alpha = 0$. This type has been exhaustively treated in the literature (Refs. 3 and 7). We only note that since all $C^\alpha_{\beta\gamma}$ are zero, (2.17) implies that $P^\alpha(t)$ is arbitrary and $\Lambda^\alpha_\beta(t)$ is constant. Then, (2.16) implies that Λ^α_β is an element of $GL(3,\Re)$. Thus, without loss of generality, one can set $N^\alpha = 0$ using (2.14b). A first integral of Eq. (2.5c) is then $\gamma^{\alpha\rho}\dot{\gamma}_{\rho\beta} = \vartheta^\alpha_\beta$, where ϑ^α_β is an arbitrary constant matrix. From this point, the standard textbooks[3] deduce (using algebraic arguments) a diagonal form: $\gamma_{\alpha\beta} = \mathrm{diag}(e^{\alpha t}, e^{\beta t}, e^{\gamma t})$ and then using Einstein's equations find the general solution, which depends on one essential parameter, as expected—see Table I.

Indeed, from (2.5c), one has 12 initial constants; 6 $\gamma_{\alpha\beta}$, and 6 $\dot{\gamma}_{\alpha\beta}$ at some t_0—according to Peano's theorem. The quadratic constraint equation (2.5a), reduces them to 10, and then, with the usage of constant automorphisms (which contain 9 Λ^α_β's), the number of the remaining essential constants (or essential parameters), is $10-9=1$.

Type II: $\mathrm{rank}(m)=1$ and $\nu_\alpha = 0$. Then, matrix $m^{\alpha\beta}$, can be cast to the form $m^{\alpha\beta} = \mathrm{diag}(1/2,0,0)$. Equations (2.16) and (2.17) give the following form for $\Lambda^\alpha_\beta(t)$:

$$\Lambda^\alpha_\beta(t) = \begin{pmatrix} \varrho_1\varrho_4 - \varrho_2\varrho_3 & x(t) & y(t) \\ 0 & \varrho_1 & \varrho_2 \\ 0 & \varrho_3 & \varrho_4 \end{pmatrix}, \quad (\varrho_1, \varrho_2, \varrho_3, \varrho_4 \text{ constants}).$$

The triplet $P^\alpha(t)$ assumes the following form:

TABLE I. The number of arbitrary constants appearing in general solution for each Bianchi type—vacuum model—is given (depicted in the first reference of Ref. 19, p. 21).

Bianchi type	No. of essential constants
I	1
II	2
VI_0, VII_0	3
VIII, IX	4
IV	3
V	1
VI_h $(h\neq -1/9)$	3
$VI_{-1/9}$	4
VII_h	3

$$P^{\alpha}(t)=\left(P(t), \frac{\varrho_1\dot{y}-\varrho_2\dot{x}}{\varrho_1\varrho_4-\varrho_2\varrho_3}, \frac{\varrho_3\dot{y}-\varrho_4\dot{x}}{\varrho_1\varrho_4-\varrho_2\varrho_3}\right).$$

The general solution to this type is Taub's solution,[16] which contains two essential parameters—see Table I.

Again, we can understand this number, using Peano's theorem and the arbitrary extra constants, appearing in Λ^{α}_{β}. Using $x(t)$ and $y(t)$, we start with 4 $\gamma_{\alpha\beta}$'s (i.e., we set $\gamma_{12}=\gamma_{13}=0$) and no shift. Thus the initial arbitrary constants are $2\times 4=8$. Out of these, the quadratic constraint equation (2.5a), removes 2, and 4 more are eliminated by the 4 ϱ's, contained in Λ^{α}_{β}. So, the remaining arbitrary constants are: $8-2-4=2$, in accordance with the number of expected essential parameters.

Type V: $\mathrm{rank}(m)=0$ and $\nu_{\alpha}\neq 0$. Then $m^{\alpha\beta}=0$ and we may choose $\nu_{\alpha}=-\frac{1}{2}\delta^3_{\alpha}$. Equations (2.16) and (2.17) give the following form for $\Lambda^{\alpha}_{\beta}(t)$:

$$\Lambda^{\alpha}_{\beta}(t)=\begin{pmatrix} \varrho_1P(t) & \varrho_2P(t) & x(t) \\ \varrho_3P(t) & \varrho_4P(t) & y(t) \\ 0 & 0 & 1 \end{pmatrix}, \quad (\varrho_1,\varrho_2,\varrho_3,\varrho_4 \text{ constants})$$

with $\varrho_1\varrho_4-\varrho_2\varrho_3=1$ and the triplet:

$$P^{\alpha}(t)=\left(x\left(\ln\frac{x}{P}\right)^{\cdot}, y\left(\ln\frac{y}{P}\right)^{\cdot}, \left(\ln\frac{1}{P}\right)^{\cdot}\right).$$

The general solution is also known as Joseph's solution (Ref. 17) with one essential parameter.

This number comes naturally within our method; using $x(t)$ and $y(t)$, one can eliminate γ_{13} and γ_{23}. Then, $P(t)$ can serve to set the subdeterminant of $\gamma_{\alpha\beta}$, equal to $(\gamma_{33})^2$. At this stage, we are left with 3 $\gamma_{\alpha\beta}$'s while the linear constraint equations (2.5b), imply that the shift is zero. Again, the quadratic constraint (2.5a) subtracts 2 arbitrary constants, and the constants contained in Λ^{α}_{β}, 3 more. Then, the result is $6-2-3=1$, essential constant.

Type IV: $\mathrm{rank}(m)=1$ and $\nu_{\alpha}\neq 0$. We may choose $m^{\alpha\beta}=\mathrm{diag}(1/2,0,0)$, $\nu_{\alpha}=-\frac{1}{2}\delta^3_{\alpha}$. Equations (2.16) and (2.17) give the following form for $\Lambda^{\alpha}_{\beta}(t)$:

$$\Lambda^{\alpha}_{\beta}(t)=\begin{pmatrix} P(t) & P(t)\ln[\kappa P(t)] & x(t) \\ 0 & P(t) & y(t) \\ 0 & 0 & 1 \end{pmatrix}, \quad (\kappa \text{ constant})$$

and the triplet

$$P^{\alpha}(t)=\left(x\left(\ln\frac{x}{P}\right)^{\cdot}-\dot{y},y\left(\ln\frac{y}{P}\right)^{\cdot},\left(\ln\frac{1}{P}\right)^{\cdot}\right).$$

In this type—which is a class B type—we can set $\gamma_{13}=\gamma_{23}=0$, using $x(t)$ and $y(t)$. At this stage, 2 of the 3 linear constraint equations imply $N^1=N^2=0$, while the third involves $P(t)$. Thus we can further, either set $N^3=0$—through (2.14b)—and retain a nonzero γ_{12}, or eliminate γ_{12}, at the expense of a nonvanishing N^3. It is well known that $N^3=0$ and $\gamma_{12}=0$ lead to incompatibility.[4]

We thus have the following counting of the essential parameters:

(a) When $\gamma_{12}\neq 0$ and $N^3=0$, we have $8-2$ (from the quadratic constraint) -2 (from the remaining linear equation) -1 (from the constant contained in Λ^{α}_{β}) $=3$.

(b) When $\gamma_{12}=0$ and $N^3\neq 0$, we have $6-2$ (from the quadratic constraint) -1 (from the constant contained in Λ^{α}_{β}) $=3$. Notice that here, the remaining linear constraint equation simply serves to define N^3 and thus does not remove any constant.

Type VI: (Including type III[19,18]) rank$(m)=2$, signature$(m)=$Lorentzian, and $\nu_{\alpha}\neq 0$. One convenient choice is $m^{\alpha\beta}=\mathrm{diag}(1,-1,0)$ and $\nu_{\alpha}=h\delta^{3}_{\alpha}$.

Note: In the standard texts, e.g., Ref. 15, the matrix $m^{a\beta}$ is given in a more complicated form, which carries part of the arbitrariness of the magnitude of the vector ν_{α}. In this work, we imply that $C^{\alpha}_{\beta\gamma}$ are given by their defining relation in terms of $\varepsilon_{\alpha\beta\gamma}$, $m^{\alpha\beta}$, ν_{α}.

For all values of $h\neq 0,\pm 1$, Eqs. (2.16) and (2.17) give the following form for $\Lambda^{\alpha}_{\beta}(t)$:

$$\Lambda^{\alpha}_{\beta}(t)=\begin{pmatrix} e^{-hP(t)}\lambda\ \cosh(P(t)) & e^{-hP(t)}\lambda\ \sinh(P(t)) & x(t)\\ e^{-hP(t)}\lambda\ \sinh(P(t)) & e^{-hP(t)}\lambda\ \cosh(P(t)) & y(t)\\ 0 & 0 & 1\end{pmatrix}$$

(λ constant)

while the triplet

$$P^{\alpha}(t)=\left(-\frac{(h^2-1)x(t)\dot{P}(t)+h\dot{x}(t)+\dot{y}(t)}{2(h^2-1)},-\frac{(h^2-1)y(t)\dot{P}(t)+h\dot{y}(t)+\dot{x}(t)}{2(h^2-1)},-\frac{\dot{P}(t)}{2}\right).$$

For $h=0$, class A, there are two solutions:

$$\Lambda^{\alpha}_{\beta}(t)=\begin{pmatrix} \lambda\ \cosh(P(t)) & \lambda\ \sinh(P(t)) & x(t)\\ \epsilon\lambda\ \sinh(P(t)) & \epsilon\lambda\ \cosh(P(t)) & y(t)\\ 0 & 0 & \epsilon\end{pmatrix}$$

(λ constant),

while the triplet

$$P^{\alpha}(t)=\left(\frac{\epsilon\dot{y}(t)-x(t)\dot{P}(t)}{2},\frac{\epsilon\dot{x}(t)-y(t)\dot{P}(t)}{2},-\frac{\epsilon\dot{P}(t)}{2}\right),$$

where $\epsilon=\pm 1$.

For $h=\pm 1$, class B, the solutions are

$$\Lambda^{\alpha}_{\beta}(t)=\begin{pmatrix} e^{-hP(t)}\lambda\ \cosh(P(t)) & e^{-hP(t)}\lambda\ \sinh(P(t)) & x(t)\\ e^{-hP(t)}\lambda\ \sinh(P(t)) & e^{-hP(t)}\lambda\ \cosh(P(t)) & c-hx(t)\\ 0 & 0 & 1\end{pmatrix}$$

$$(\lambda \text{ constant}),$$

while the triplet

$$P^{\alpha}(t)=\left(\Omega(t),\frac{2h\Omega(t)-c\dot{P}(t)+2hx(t)\dot{P}(t)+\dot{x}(t)}{2},\right.$$

$$\left.h\frac{e^{-hP(t)}\lambda\sinh(P(t))\dot{P}(t)-he^{-hP(t)}\lambda\cosh(P(t))\dot{P}(t)}{2e^{-hP(t)}\lambda\cosh(P(t))-2he^{-hP(t)}\lambda\sinh(P(t))}\right).$$

For each of the previously mentioned cases, we have the following.

(a) When $h=0$ (class A), $\gamma_{\alpha\beta}$ can be made diagonal and then the shift vanishes. Thus the counting of the essential parameters is: $6-2$ (from the quadratic constraint) -1 (from the constant, contained in Λ^{α}_{β}) $=3$.

(b) When $h=\pm 1$ (class B), using $x(t)$ and $P(t)$, we can eliminate γ_{13} and γ_{23}. So: $8-2$ (from the quadratic constraint) -2 (from the constants, contained in Λ^{α}_{β}) $=4$ is the number of the essential constants. Notice that the 3 linear constraint equations, are linearly dependent and thus, when $N^3=0$ through (2.14b), there is no linear constraint equation left, to remove any constants, hence the number 4.

(c) When $h\neq 0,\pm 1$, the counting algorithm is exactly the same, as in the type IV case.

Type VII: rank$(m)=2$, signature$(m)=$Euclidean and $\nu_{\alpha}\neq 0$. We may set $m^{\alpha\beta}=\text{diag}(-1,-1,0)$, $\nu_{\alpha}=h\delta^{3}_{\alpha}$. For all values of h, Eqs. (2.16) and (2.17) give the following form for $\Lambda^{\alpha}_{\beta}(t)$:

$$\Lambda^{\alpha}_{\beta}(t)=\begin{pmatrix}\lambda e^{hP(t)}\cos(P(t)) & \lambda e^{hP(t)}\sin(P(t)) & x(t)\\ -\lambda e^{hP(t)}\sin(P(t)) & \lambda e^{hP(t)}\cos(P(t)) & y(t)\\ 0 & 0 & 1\end{pmatrix}$$

$$(\lambda \text{ constant})$$

and the triplet

$$P^{\alpha}(t)=\left(\frac{x(t)\dot{P}(t)+h^2x(t)\dot{P}(t)-h\dot{x}(t)+\dot{y}(t)}{2(1+h^2)},\frac{y(t)\dot{P}(t)+h^2y(t)\dot{P}(t)-h\dot{y}(t)-\dot{x}(t)}{2(1+h^2)},\frac{\dot{P}(t)}{2}\right).$$

For the case $h=0$, there is another solution, except the one deduced from the previous, by setting $h=0$:

$$\Lambda^{\alpha}_{\beta}(t)=\begin{pmatrix}\lambda\cos(P(t)) & \lambda\sin(P(t)) & x(t)\\ \lambda\sin(P(t)) & -\lambda\cos(P(t)) & y(t)\\ 0 & 0 & -1\end{pmatrix}$$

$$(\lambda \text{ constant})$$

and the triplet

$$P^{\alpha}(t)=\left(\frac{x(t)\dot{P}(t)-\dot{y}(t)}{2},\frac{y(t)\dot{P}(t)+\dot{x}(t)}{2},-\frac{\dot{P}(t)}{2}\right).$$

Again, for each of the previously mentioned cases, we have the following.

(a) When $h=0$ (class A), $\gamma_{\alpha\beta}$ can be made diagonal and Eq. (2.5b) gives $N^a=0$. Thus: $6-2$ (from the quadratic constraint) -1 (from the constant, contained in Λ^{α}_{β}) $=3$ is the number of the essential constants.
(b) When $h\neq 0$, the counting algorithm is exactly the same, as in the type IV case.

For Bianchi Types VIII and IX, condition (2.17) does not impose any restriction on $\Lambda^{\alpha}_{\beta}(t)$*, but rather fixes completely the triplet* $P^a(t)$ *to be*

$$P^a=\frac{1}{4|m|}\varepsilon_{\beta\tau\kappa}m^{\alpha\beta}\Lambda^{\tau}_{\gamma}\dot{\Lambda}^{\kappa}_{\delta}m^{\gamma\delta}.$$

Type VIII: rank$(m)=3$, signature$(m)=$Lorentzian. A standard choice is $m^{\alpha\beta}=\eta^{\alpha\beta}=$diag $(-1,1,1)$. Since $|m^{\alpha\beta}|=-1$, (2.19a) implies that $|\Lambda^{\alpha}_{\beta}|=1$ and, thus, Λ^{α}_{β}'s are the isometries of the Minkowski metric, in three dimensions, i.e., the Lorentz boosts, with one timelike and two spacelike directions, times a rotation of the ''space'' plane. Thus, the automorphisms are characterized by the two components of the velocity vector, plus the rotation angle. The triplet, P^a, is

$$P^a=\tfrac{1}{2}(\Lambda^2_{\mu}\dot{\Lambda}^3_{\nu}\eta^{\mu\nu},-\Lambda^3_{\mu}\dot{\Lambda}^1_{\nu}\eta^{\mu\nu},-\Lambda^1_{\mu}\dot{\Lambda}^2_{\nu}\eta^{\mu\nu}).$$

It can be proven—see Appendix—that a positive definite matrix can be diagonalized by this automorphism group, i.e., we can set $\gamma_{\alpha\beta}=\mathrm{diag}(a^2(t),b^2(t),c^2(t))$. Then, from (2.5b), we will have $N^a=0$.

The number 4, of the expected essential parameters—see Table I—can be understood as follows: The time-dependent Lorentz transformation Λ^{α}_{β} can diagonalize $\gamma_{\alpha\beta}$. Thus, the counting: $6-2$ (from the quadratic constraint) $=4$.

Type IX: rank$(m)=3$, signature$(m)=$Euclidean. The standard choice is $m^{\alpha\beta}=\delta^{\alpha\beta}$. Since $|m^{\alpha\beta}|=1$, (2.19a) implies that $|\Lambda^{\alpha}_{\beta}|=1$ and, thus, Λ^{α}_{β}'s are the isometries of the Euclidean metric, in three dimensions, i.e., the orthogonal matrices, which are characterized by three parameters, e.g., the Euler angles. The triplet, P^a, is

$$P^a=\tfrac{1}{2}(\Lambda^2_{\mu}\dot{\Lambda}^3_{\nu}\delta^{\mu\nu},\Lambda^3_{\mu}\dot{\Lambda}^1_{\nu}\delta^{\mu\nu},\Lambda^1_{\mu}\dot{\Lambda}^2_{\nu}\delta^{\mu\nu}).$$

Since a positive definite symmetric matrix can be diagonalized by an element of—the connected to the identity component of—$O(3)$, we have that $\gamma_{\alpha\beta}(t)=\mathrm{diag}(a^2(t),b^2(t),c^2(t))$.[19] Then, from (2.5b), as is well known $N^{\alpha}=0$.

The counting yields—exactly as in type VIII: $6-2$ (from the quadratic constraint) $=4$, essential constants.

From the above-given analysis of the space of solutions to (2.16) and (2.17), we observe that in each Bianchi type, there are 3 arbitrary functions of time, as expected, for two reasons: First, because we are solving the integrability conditions for the existence of a time-dependent spatial diffeomorphism according to (2.9). Second, because as mentioned in the Sec. I, the system of Einstein's equations (2.5) has a gauge freedom of 4 arbitrary functions of time. But one of them, simply corresponds to time reparametrization, while the remaining 3 are the ones we found in the above-given analysis.

In the various Bianchi types, the 3 arbitrary functions are distributed differently among the components of $\Lambda^{a}_{\beta}(t)$ and $P^a(t)$. This fact, together with the different number of arbitrary constants appearing in Λ^{a}_{β} for each type, results in a different number of essential constants—expected by independent arguments[19] to appear in the general solutions to Einstein's equations (2.5)—see Table I.

We now conclude Sec. II by stating the following (uniqueness) Theorem: *"In a given—albeit arbitrary—Bianchi Type, let* γ_1, γ_2, *(in matrix notation) be solutions to Einstein's equations (2.5), then there is a matrix M of the form:* $M=\Lambda_1^{-1}\Sigma\Lambda_2$ *(where* Λ_1 *and* Λ_2 *are solutions to (2.16) and (2.17) and* Σ*, represents the irrelevant symmetries of the solution in its irreducible form) which connects them as:* $\gamma_2=M^T\gamma_1 M$*."*

Note: N, N^a are understood to be given from the quadratic and linear constraint equations (2.5a) and (2.5b).

The proof rests on the previously established facts:

(a) That the solutions to (2.16) and (2.17) suffice to reduce the generic $\gamma_{\alpha\beta}$ to a form that will contain the expected necessary number of essential constants, so as to be regarded as the most general one—for each and every Bianchi type.

(b) That for every given Bianchi type, the solutions to (2.16) and (2.17), form a group. Indeed, let γ_1, γ_2 be solutions to (2.5). Then there are Λ_1, Λ_2—along with P_1, P_2, respectively, if needed—solutions to (2.16) and (2.17), such that

$$\gamma_1 = \Lambda_1^T \gamma_{\text{irreducible}} \Lambda_1,$$

$$\gamma_2 = \Lambda_2^T \gamma_{\text{irreducible}} \Lambda_2,$$

where $\gamma_{\text{irreducible}}$, stands for the solution in a form exhibiting only the essential constants. From the first of these

$$\gamma_{\text{irreducible}} = (\Lambda_1^{-1})^T \gamma_1 \Lambda_1.$$

Since, by definition, $\gamma_{\text{irreducible}}$ is a symmetric matrix there are always nontrivial matrices Σ such that

$$\gamma_{\text{irreducible}} = \Sigma^T \gamma_{\text{irreducible}} \Sigma.$$

Substituting the last two relations for $\gamma_{\text{irreducible}}$ in the expression giving γ_2, we obtain:

$$\gamma_2 = (\Lambda_1^{-1} \Sigma \Lambda_2)^T \gamma_1 \Lambda_1^{-1} \Sigma \Lambda_2.$$

Q.E.D.

III. THE SPACE OF SOLUTIONS FOR TYPE II AND V CASES

In this section, we adopt the more conventional point of view; that of ''gauge'' fixing, before solving. As far as time is concerned, we adopt the ''gauge'' fixing condition $\tilde{N} = \sqrt{\tilde{\gamma}}$, since this simplifies the form of the equations. For the spatial coordinates, as explained in Sec. II, a choice of reference system amounts to a choice of time-dependent automorphism—along with a choice of $P^\alpha(t)$; thus, we select the form of $\tilde{\gamma}_{\alpha\beta}(t)$ to be such that the linear equation would imply $\tilde{N}^\alpha = 0$. In this ''gauge,'' Einstein's equations (2.5) read:

$$-\tilde{\gamma}^{\alpha\kappa}\tilde{\gamma}^{\beta\lambda}\dot{\tilde{\gamma}}_{\kappa\lambda}\dot{\tilde{\gamma}}_{\alpha\beta} + \left(\frac{\dot{\tilde{\gamma}}}{\tilde{\gamma}}\right)^2 - 4\tilde{\gamma}R = 0, \tag{3.1a}$$

$$C^{\epsilon}_{\alpha\mu}\tilde{\gamma}^{\mu\rho}\dot{\tilde{\gamma}}_{\rho\epsilon} - C^{\epsilon}_{\mu\epsilon}\tilde{\gamma}^{\mu\rho}\dot{\tilde{\gamma}}_{\rho\alpha} = 0, \tag{3.1b}$$

$$\ddot{\tilde{\gamma}}_{\alpha\beta} - \tilde{\gamma}^{\mu\nu}\dot{\tilde{\gamma}}_{\alpha\mu}\dot{\tilde{\gamma}}_{\beta\nu} - 2\tilde{\gamma}R_{\alpha\beta} = 0. \tag{3.1c}$$

Note that taking the trace of Eq. (3.1c), one arrives at

$$\left(\frac{\dot{\tilde{\gamma}}}{\tilde{\gamma}}\right)^{\cdot} - 2\tilde{\gamma}R = 0. \tag{3.2}$$

A somewhat useful result deriving from (3.2) is the following: $\tilde{\gamma} = ae^{\beta t}$ implies $\tilde{R} = 0$, which is incompatible for all but I Bianchi types.

We now present a realization of the method developed in Sec. II for the cases of type II and V Bianchi geometries. At this point, a word of caution is pertinent: It is evident—from the previously mentioned counting of the expected number of essential constants—that the well-known Taub's (type II) and Joseph's (type V) solutions are the most general for the respective cases.[18] Thus, we should not expect to find anything new in this respect. However, the thorough investigation of the complete space of solutions requires knowledge of the correct (gauge) symmetry group for Einstein's equations (2.5). In this respect, we shall directly show that transformations (2.14—as specified by conditions (2.16) and (2.16), applied to types II and V—are essentially the only (gauge) symmetries of these Bianchi geometries.

Note: From now on we drop the tildes from the various quantities for simplicity—except in some cases, where misunderstanding could occur.

A. Bianchi type II

As can be seen, from the results concerning type II, we can consider without loss of generality the time-dependent part $\gamma_{\alpha\beta}(t)$, of the three-metric to have the following form:

$$\gamma_{\alpha\beta}(t)=\begin{pmatrix} a(t) & 0 & 0 \\ 0 & b(t) & f(t) \\ 0 & f(t) & c(t) \end{pmatrix}.$$

It is interesting to observe that the freedom in arbitrary functions of time—contained in $\Lambda^{\alpha}_{\beta}(t)$—does not suffice to diagonalize $\gamma_{\alpha\beta}(t)$, i.e., to set $f(t)=0$, *a priori*. Yet, we know [see (3.16) and (3.17) in the following] that the diagonal Taub's metric is the irreducible form of the most general type II solution. The reconciliation of these two, seemingly conflicting facts, obtains only on mass shell; after we have completely solved (3.1), with $\gamma_{\alpha\beta}(t)$ given previously, $f(t)$ becomes linearly dependent upon $b(t)$ and $c(t)$, and we can, thus, gauge it away—utilizing the remaining freedom in arbitrary constants, contained in $\Lambda^{\alpha}_{\beta}(t)$.

Note: From now on, we drop the *t* symbol—for time dependence—from the various quantities, e.g., *a* stands for $a(t)$.

Inserting the form of $\gamma_{\alpha\beta}$ in Eq. (3.1b), we find that they vanish identically. We next consider the following quantity *q*, which is scalar under a general linear mixing $\sigma^{\alpha}\rightarrow\tilde{\sigma}^{\alpha}=S^{\alpha}_{\beta}\sigma^{\alpha}$ with $S^{\alpha}_{\beta}\in GL(3,\Re)$,

$$q=C^{\kappa}_{\mu\nu}C^{\lambda}_{\tau\sigma}\gamma_{\kappa\lambda}\gamma^{\mu\tau}\gamma^{\nu\sigma}=\frac{a^2}{2\gamma}=\frac{a}{2(bc-f^2)},$$

where γ, as usual, denotes the determinant of the matrix $\gamma_{\alpha\beta}$. Then, (2.7) gives the following nonzero components for the Ricci tensor $R_{\alpha\beta}$, and the Ricci scalar, *R:*

$$\begin{aligned} R_{11}&=-q\gamma_{11}, \\ R_{rs}&=q\gamma_{rs} \quad r,s=2,3, \\ R&=q. \end{aligned} \tag{3.3}$$

The (1,1) component of (3.1c) is an autonomous equation for the scale factor *a:*

$$\left(\frac{\dot{a}}{a}\right)^{\cdot}+a^2=0 \tag{3.4}$$

with a first integral

$$\left(\frac{\dot{a}}{a}\right)^2 + a^2 = \omega = \text{constant} > 0. \tag{3.5}$$

Using (3.2), (3.3), and (3.4), we get the equation for *q:*

$$\left(\frac{\dot{q}}{q}\right)^{\cdot} + 3a^2 = 0. \tag{3.6}$$

To obtain first integrals for (3.1c), let us define the new variables:

$$\begin{aligned} &\overline{\gamma}_{11} = q^{-1/3}\gamma_{11}, \quad \overline{\gamma}_{rs} = q^{1/3}\gamma_{rs}, \\ &\overline{\gamma}^{11} = q^{1/3}\gamma^{11}, \quad \overline{\gamma}^{rs} = q^{-1/3}\gamma_{rs}. \end{aligned} \tag{3.7}$$

Then:

$$\overline{\gamma} = \det(\overline{\gamma}_{\alpha\beta}) = q^{1/3}\gamma = \frac{a^2}{2}q^{-2/3}. \tag{3.8}$$

It is straightforward to see that, with the use of (3.7), and (3.3), (3.4), (3.6), the spatial Einstein's equations (3.1c) translate into the following simple, integrable, Kasner-like, equations, in terms of $\overline{\gamma}_{\alpha\beta}$:

$$(\overline{\gamma}^{\alpha\rho}\dot{\overline{\gamma}}_{\rho\beta})^{\cdot} = 0 \tag{3.9}$$

with first integrals:

$$\overline{\gamma}^{\alpha\rho}\dot{\overline{\gamma}}_{\rho\beta} = \vartheta^{\alpha}_{\beta}, \tag{3.10}$$

where

$$\vartheta^{\alpha}_{\beta} = \begin{pmatrix} \theta^1_1 & 0 & 0 \\ 0 & \theta & \varrho \\ 0 & \sigma & \pi \end{pmatrix}.$$

Taking the trace of (3.10), we obtain—by means of (3.8):

$$2\left(\frac{\dot{a}}{a} - \frac{1}{3}\frac{\dot{q}}{q}\right) = \vartheta^a_a = \theta^1_1 + \vartheta^s_s, \tag{3.11}$$

while the (1,1) component of (3.10), gives

$$\frac{\dot{a}}{a} - \frac{1}{3}\frac{\dot{q}}{q} = \theta^1_1. \tag{3.12}$$

Equations (3.11) and (3.12) imply that $\theta^1_1 = \vartheta^s_s = \theta + \pi$, so finally, the matrix ϑ becomes

$$\vartheta^{\alpha}_{\beta} = \begin{pmatrix} \theta + \pi & 0 & 0 \\ 0 & \theta & \varrho \\ 0 & \sigma & \pi \end{pmatrix}. \tag{3.13}$$

Using the relation $\gamma=a^2/(2q)$ (mentioned earlier), as well as (3.5), (3.6), (3.7), and (3.10), it is straightforward to see that the quadratic constraint equation (3.1a), becomes a relation among constants; that is:

$$\omega=2(\vartheta_s^s)^2+|\vartheta_s^r|. \tag{3.14}$$

Integrating (3.5), we get the scale factor *a:*

$$a(t)\doteq a=\frac{\sqrt{\omega}}{\cosh(\pm\sqrt{\omega}t)}. \tag{3.15}$$

From this relation and (3.12), we conclude that

$$q^{-1/3}a=a_0e^{\vartheta_s^s t},\quad a_0>0. \tag{3.16}$$

Now utilizing, in matrix notation, the relation $\overline{\gamma}\vartheta=\vartheta^T\overline{\gamma}$, which is the consistency requirement for (3.10) and (3.16), we deduce that classical solutions exist, only for matrices ϑ, with real eigenvalues and thus diagonalizable. Since (2.16) and (2.17) admit the solutions Λ_β^α=constant, $P^a=0$, we can invoke a constant mixing of ϑ, with a matrix of the form:

$$\Lambda=\begin{pmatrix}1&0&0\\0&\Lambda_2^2&\Lambda_3^2\\0&\Lambda_2^3&\Lambda_3^3\end{pmatrix}$$

and reduce it to a diagonal form. Then, we are essentially led to the diagonal Taub's solution:

$$\begin{aligned}\overline{\gamma}_{22}&=q^{1/3}b=e^{\theta t},\\ \overline{\gamma}_{33}&=q^{1/3}c=e^{\pi t}.\end{aligned} \tag{3.17}$$

At this point, it is interesting to observe that, if for some reason, we had not invoked this diagonalizing Λ, and instead proceeded with the general ϑ_s^r, we would have arrived at a reducible form of the solutions with a nonvanishing $\overline{\gamma}_{23}$. However, this off-diagonal element can be made to vanish through the action of the previously mentioned Λ.

Thus, we have shown that "gauge" transformations (2.14)—with (2.16) and (2.17), holding—suffice to reduce the most general line element, for the type II Bianchi model, to the known Taub's metric. According to the theorem stated at the end of Sec. II, these transformations are, essentially, unique. We are now going to explicitly verify it for the case at hand.

A convenient way to proceed is to start from Taub's form of the solution and ask ourselves; what is the form of the most general time-dependent automorphism $\Lambda_\beta^\alpha(t)$, which retains the form invariance of Einstein's equations (2.5)—written in the invariant basis. Since we know that Λ_2^1 and Λ_3^1 can be time dependent, we focus on a time-dependent matrix Λ, of the form:

$$\Lambda_\beta^\alpha=\begin{pmatrix}\varrho&0&0\\0&\varrho_1&\varrho_2\\0&\varrho_3&\varrho_4\end{pmatrix}, \tag{3.18}$$

where $\varrho=\varrho_1\varrho_4-\varrho_2\varrho_3$ and all ϱ's are time dependent.

Consider the transformation, induced by this Λ_β^α, on $\gamma_{\alpha\beta}^{\text{Taub}}$—in matrix notation:

$$\hat{\gamma}=\Lambda^T\gamma^{\text{Taub}}\Lambda. \tag{3.19}$$

The linear constraint equations (3.1b) still imply $\hat{N}^a=0$. As far as the time gauge fixing condition $N=\sqrt{\gamma}$ is concerned, we have $\sqrt{\hat{\gamma}}=|\Lambda|\sqrt{\gamma^{\text{Taub}}}$, $|\Lambda|>0$, and thus

$$N^{\text{Taub}}\,\mathrm{d}t^{\text{Taub}}=\hat{N}\,\mathrm{d}\hat{t}\Rightarrow \mathrm{d}\hat{t}\,|\Lambda|\sqrt{\gamma^{\text{Taub}}}=\sqrt{\gamma^{\text{Taub}}}\,\mathrm{d}t^{\text{Taub}}\Rightarrow \mathrm{d}\hat{t}\,\varrho^2=\mathrm{d}t^{\text{Taub}}.$$

Since we wish the transformation to be a symmetry of (2.5), and we have secured that $\hat{N}^a=0$, and selected $\hat{N}=\sqrt{\hat{\gamma}}$, the equation satisfied by $\hat{\gamma}_{\alpha\beta}$, would be exactly (3.1) and (3.2). Only the dot—defining the time derivative, with respect to Taub's time—must be replaced by a prime:

$$'\doteq\frac{\mathrm{d}}{\mathrm{d}\hat{t}}=\varrho^2(t^{\text{Taub}})\frac{\mathrm{d}}{\mathrm{d}t^{\text{Taub}}}=\varrho^2(t^{\text{Taub}})\times\dot{}\,. \tag{3.20}$$

Defining the corresponding scale quantities $\hat{\bar{\gamma}}_{\alpha\beta}$, according to (3.7) and (3.8) we must have the analogs of (3.10):

$$\hat{\bar{\gamma}}^{\alpha\rho}\hat{\bar{\gamma}}'_{\rho\beta}=\vartheta^{\alpha}_{\beta}. \tag{3.21}$$

Equation (3.2) reads:

$$\left(\frac{\hat{\gamma}'}{\hat{\gamma}}\right)'-2\hat{\gamma}\hat{R}=0. \tag{3.22}$$

It also holds that

$$\left(\frac{\dot{\gamma}_{\text{Taub}}}{\gamma_{\text{Taub}}}\right)\dot{}\,-2\gamma_{\text{Taub}}R_{\text{Taub}}=0. \tag{3.23}$$

Translating (3.22) in the t^{Taub} variable, and subtracting (3.23), we get

$$2(\varrho^2)\ddot{}+(\varrho^2)\dot{}\,\frac{\dot{\gamma}_{\text{Taub}}}{\gamma_{\text{Taub}}}=0,$$

which, with the help of $\gamma_{\text{Taub}}=a^2_{\text{Taub}}/2q$, (3.12) and $(\theta^1_1)^{\text{Taub}}=(\vartheta^s_s)^{\text{Taub}}$, becomes

$$2(\varrho^2)\ddot{}+(\varrho^2)\dot{}\left(2(\vartheta^s_s)^{\text{Taub}}-\frac{1}{3}\frac{\dot{q}}{q}\right)=0. \tag{3.24}$$

The (1,1) component of (3.21) is

$$\frac{\hat{\bar{\gamma}}_{11}'}{\hat{\bar{\gamma}}_{11}}=\vartheta^s_s,$$

where

$$\hat{\bar{\gamma}}_{11}=q^{-1/3}\hat{\gamma}_{11}=q^{-1/3}\varrho^2\gamma^{\text{Taub}}_{11}$$

and, thus, that component reads:

$$(\varrho^2)\dot{}+\varrho^2(\vartheta^s_s)^{\text{Taub}}=\vartheta^s_s. \tag{3.25}$$

Inserting the derivative of (3.25) into (3.24), we have

$$(\varrho^2)\cdot\frac{\dot{q}}{q}=0,$$

which in conjunction with (3.6) implies $\varrho^2=$constant. Without loss of generality, we can take $\varrho^2=1$. Henceforth, the time variable $\hat{t}$, may—and will—denote Taub's time. It is thus left for us to investigate the unimodular matrices:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & \varrho_1 & \varrho_2 \\ 0 & \varrho_3 & \varrho_4 \end{pmatrix}$$

with $1=\varrho_1\varrho_4-\varrho_2\varrho_3$, and all ϱ's, are time dependent.

It can be proved that a convenient parametrization for this task is

$$\Lambda^{\alpha}_{\beta}=\begin{pmatrix} 1 & 0 & 0 \\ 0 & & \\ 0 & & \Lambda^{r}_{s} \end{pmatrix},$$

where

$$\Lambda^{r}_{s}=R^{r}_{m}L^{m}_{s},$$

$$L^{m}_{s}=\begin{pmatrix} \varphi(t) & \chi(t) \\ 0 & 1/\varphi(t) \end{pmatrix}$$

and R^{r}_{m} are the symmetries of the Taub's metric, i.e., $R^{T}\gamma^{\text{Taub}}R=\gamma^{\text{Taub}}$—in matrix notation—:

$$R=\begin{pmatrix} 1 & 0 & 0 \\ 0 & & \\ 0 & & R^{r}_{m} \end{pmatrix},$$

R^{r}_{m} being

$$R^{r}_{m}=\begin{pmatrix} \cos(\tilde{g}(t)) & \sin(\tilde{g}(t))e^{-(\kappa-\mu)t/2} \\ -\sin(\tilde{g}(t))e^{(\kappa-\mu)t/2} & \cos(\tilde{g}(t)) \end{pmatrix},$$

where $\tilde{g}(t)$ is an unspecified function of time and κ,μ, the eigenvalues of ϑ^{Taub}.

The system (3.21) gives the following equations for $\chi(t)$ and $\varphi(t)$:

$$2\frac{\dot{\varphi}}{\varphi}+\kappa=\theta+\sigma\frac{\chi}{\varphi}, \tag{3.26a}$$

$$\left(\frac{\chi}{\varphi}\right)^{\cdot}=-\sigma\left(\frac{\chi}{\varphi}\right)^{2}+(\pi-\theta)\frac{\chi}{\varphi}+\varrho, \tag{3.26b}$$

$$e^{(\kappa-\mu)t}(\dot{\chi}\varphi-\chi\dot{\varphi})=\frac{\sigma}{\varphi^2}, \tag{3.26c}$$

$$-2\frac{\dot{\varphi}}{\varphi}+\mu=\pi-\sigma\frac{\chi}{\varphi}. \tag{3.26d}$$

Equation (3.25), for the choice $\varrho^2=1$, gives $(\vartheta_s^s)^{\text{Taub}}=\vartheta_s^s$, and hence

$$\pi+\theta=\kappa+\mu. \tag{3.27}$$

It also implies $\hat{\overline{\gamma}}_{11}=\overline{\gamma}_{11}^{\text{Taub}}$, or $a(t)=a^{\text{Taub}}(t)$, as well as $\omega=\omega^{\text{Taub}}$, or, through (3.14),

$$2(\theta+\pi)^2+\pi\theta-\varrho\sigma=2(\kappa+\mu)^2+\kappa\mu \overset{3.27}{\rightarrow} 3.27\kappa\mu=\theta\pi-\varrho\sigma. \tag{3.28}$$

Out of the four differential equations (3.26), only the first three are independent—in view of (3.27). The solution to this system, for $\sigma\neq 0$, is given by

$$\frac{\chi}{\varphi}=k_1-\frac{\lambda^3c^4e^{-\lambda t}}{\sigma(1+\lambda^2c^4e^{-\lambda t})},\quad \lambda=\kappa-\mu \tag{3.29}$$

from Riccati (3.26b), where $k_1=(\pi-\theta+\lambda)/2\sigma$ is the constant special solution and

$$\varphi^2=\frac{\sigma}{\lambda^2c^2}(1+\lambda^2c^4e^{-\lambda t}),\quad \sigma>0. \tag{3.30}$$

Thus, it is easily seen that (3.29) and (3.30) make the matrix L_s^m to be written in the form $L_s^m=\Sigma_n^m\tilde{L}_s^n$, where

$$\Sigma_n^m=\begin{pmatrix}\cos(g(t)) & \sin(g(t))e^{-\lambda t/2}\\ \sin(g(t))e^{\lambda t/2} & -\cos(g(t))\end{pmatrix},$$

$$\tilde{L}_s^n=\begin{pmatrix}\varepsilon_1\dfrac{\sqrt{\sigma}}{\lambda c} & k_1\varepsilon_1\dfrac{\sqrt{\sigma}}{\lambda c}\\ \varepsilon_2c\sqrt{\sigma} & \left(k_1-\dfrac{\lambda}{\sigma}\right)\varepsilon_2c\sqrt{\sigma}\end{pmatrix}$$

with $(\varepsilon_1)^2=(\varepsilon_2)^2=1$, $(\sigma,c)>0$, and

$$\tan(g(t))=\frac{\varepsilon_2c^2\lambda}{\varepsilon_1}e^{-\lambda t/2}.$$

There are the special cases $\sigma=0$, or $\lambda=0$, which are easily seen to fall into the previous case.

Thus, in all cases, there always exist matrices Σ and $\tilde{L}$, such that the transformation matrix Λ_β^α can be written as

$$\Lambda_\beta^\alpha=\begin{pmatrix}1 & 0 & 0\\ 0 & & \\ 0 & R_m^r\Sigma_n^m\tilde{L}_s^n & \end{pmatrix}.$$

This concludes the verification of the Theorem stated at the end of Sec. II, since, indeed, R and Σ have trivial action on $\gamma_{\alpha\beta}^{\text{Taub}}$. It is therefore evident that the most general $\gamma_{\alpha\beta}$, $N(t)$, and $N^a(t)$, satisfying Eq. (2.5), are—in matrix notation:

$$\gamma_{\text{most general}}(t)=\Lambda^{T}(t)\,\gamma^{\text{Taub}}(h(t))\Lambda(t),$$

$$\Lambda=\begin{pmatrix} \varrho_1\varrho_4-\varrho_2\varrho_3 & x(t) & y(t) \\ 0 & \varrho_1 & \varrho_2 \\ 0 & \varrho_3 & \varrho_4 \end{pmatrix},$$

where the ϱ's are constant, and

$$N(t)=\sqrt{|\gamma_{\text{most general}}|}\dot{h}(t),$$

$$N^{\alpha}(t)=S^{\alpha}_{\beta}(t)P^{\beta}(h(t))\dot{h}(t),$$

$$P^{\beta}(h(t))=\left\{P(t),\frac{\varrho_1\dot{y}(t)-\varrho_2\dot{x}(t)}{(\varrho_1\varrho_4-\varrho_2\varrho_3)\dot{h}(t)},\frac{\varrho_3\dot{y}(t)-\varrho_4\dot{x}(t)}{(\varrho_1\varrho_4-\varrho_2\varrho_3)\dot{h}(t)}\right\},$$

$$S=\Lambda^{-1}(t),$$

$$\gamma^{\text{Taub}}(h(t))=\begin{pmatrix} a & 0 & 0 \\ 0 & \dfrac{e^{(2\kappa+\mu)h(t)}}{a} & 0 \\ 0 & 0 & \dfrac{e^{(\kappa+2\mu)h(t)}}{a} \end{pmatrix},$$

$$a=\frac{\sqrt{\omega}}{\cosh(\pm\sqrt{\omega}h(t))},$$

$$\omega=2(\kappa+\mu)^2+\kappa\mu,$$

where the fourth arbitrary function, $h(t)$, accounts for the time reparametrization covariance, i.e., permits us to depart from the time gauge fixing $N=\sqrt{\gamma}$.

B. Bianchi type V

As can be seen from the results of Sec. II concerning type V, we can consider—with the usage of time-dependent AIDs—the time-dependent part $\gamma_{\alpha\beta}(t)$, of the three-metric, to be of the form:

$$\gamma_{\alpha\beta}(t)=\begin{pmatrix} a(t) & b(t) & 0 \\ b(t) & c(t) & 0 \\ 0 & 0 & f(t) \end{pmatrix}$$

with $a(t)c(t)-b^2(t)=f^2(t)$. Again, as happens for type II, the form of the allowed transformation $\Lambda^{\alpha}_{\beta}(t)$ is such that one cannot set $b(t)=0$ *a priori*. Yet, we know—see (3.39) and (3.40) in the following—that the diagonal Joseph's metric is the irreducible form of the most general type V solution. This puzzle finds its resolution only on mass shell; after we have completely solved (3.1) with $\gamma_{\alpha\beta}(t)$ given previously, $b(t)$ becomes linearly dependent upon $a(t)$ and $c(t)$, and we can thus put it to zero—utilizing the remaining freedom in arbitrary constants, contained in $\Lambda^{\alpha}_{\beta}(t)$.

Note: From now on, we drop the t symbol—for time dependence—from the various quantities, e.g., a stands for $a(t)$.

Inserting the form of $\gamma_{\alpha\beta}$ in Eq. (3.1b), we find that they vanish identically. We next define the scalar—under a general linear mixing $\sigma^{\alpha}\to\tilde{\sigma}^{\alpha}=S^{\alpha}_{\beta}\sigma^{\alpha}$, with $S^{\alpha}_{\beta}\in GL(3,\Re)$—quantity *q:*

$$q=C^{\tau}_{\tau\mu}C^{\sigma}_{\sigma\nu}\gamma^{\mu\nu}=\frac{1}{f}.$$

The condition $ac-b^2=f^2$ now reads as: $ac-b^2=1/q^2$, or

$$\gamma=\frac{1}{q^3}. \tag{3.31}$$

Then, (2.7) gives

$$\begin{aligned} R_{\alpha\beta}&=2q\gamma_{\alpha\beta},\\ R&=6q. \end{aligned} \tag{3.32}$$

The (3,3) component of (3.1c) gives an autonomous equation for the scalar quantity *q:*

$$\left(\frac{\dot{q}}{q}\right)^{\cdot}+\frac{4}{q^2}=0 \tag{3.33}$$

with a first integral:

$$\left(\frac{\dot{q}}{q}\right)^2-\frac{4}{q^2}=\omega=\text{constant}. \tag{3.34}$$

Defining the scaled quantities:

$$\begin{aligned} \overline{\gamma}_{\alpha\beta}&=q\gamma_{\alpha\beta},\\ \overline{\gamma}^{\alpha\beta}&=\frac{1}{q}\gamma^{\alpha\beta},\\ |\overline{\gamma}|&=1, \end{aligned} \tag{3.35}$$

and using (3.32) and (3.33), Eq. (3.1c) is translated into the following form:

$$(\overline{\gamma}^{\alpha\rho}\dot{\overline{\gamma}}_{\rho\beta})^{\cdot}=0 \tag{3.36}$$

with first integrals:

$$\overline{\gamma}^{\alpha\rho}\dot{\overline{\gamma}}_{\rho\beta}=\vartheta^{\alpha}_{\beta}, \tag{3.37}$$

where

$$\vartheta^{\alpha}_{\beta}=\begin{pmatrix} \theta & \varrho & 0\\ \sigma & -\theta & 0\\ 0 & 0 & 0 \end{pmatrix}.$$

The form of the matrix, ϑ, has been derived using the form of $\overline{\gamma}_{\alpha\beta}$ and the property that $|\overline{\gamma}|=1$. Using (3.31), (3.34), and (3.37), the quadratic constraint (3.1a) becomes a relation among constants—as was expected—namely:

$$3\omega=\theta^2+\varrho\sigma. \tag{3.38}$$

The property $|\overline{\gamma}|=1$, together with the consistency requirement—in matrix notation—$\overline{\gamma}\vartheta=\vartheta^T\overline{\gamma}$, which follows from (3.37), enables us to conclude that classical solutions, exist only for those values of the parameters, θ, ϱ, σ, for which ϑ is diagonalizable, i.e., when $\theta^2+\varrho\sigma>0$.

Since the matrices Λ^α_β of the form:

$$\Lambda^\alpha_\beta=\begin{pmatrix}\varrho_1 & \varrho_2 & 0\\ \varrho_3 & \varrho_4 & 0\\ 0 & 0 & 1\end{pmatrix}$$

along with $P^a=0$, constitute the remaining gauge freedom, we can invoke such Λ^α_β to diagonalize ϑ^α_β and—at the same time—retain the shift, zero—see (2.14). Now with a diagonal ϑ^α_β, Eq. (3.37) essentially implies that $\overline{\gamma}_{\alpha\beta}$, is diagonal too.

A further integration of (3.34), yields

$$\frac{1}{f(t)}=q(t)=\begin{cases}\dfrac{2}{\sqrt{\omega}}\sinh(\pm\sqrt{\omega}t), & \omega>0\\ \pm 2t, & \omega=0\end{cases}\tag{3.39}$$

and thus we are led to the well-known Joseph's solution—through complete integration of (3.37)—for the diagonal case:

$$\begin{aligned}\overline{\gamma}_{11}&=qa=e^{\lambda t},\\ \overline{\gamma}_{22}&=qc=e^{-\lambda t},\\ 3\omega&=\lambda^2>0\end{aligned}\tag{3.40}$$

or the Milnor's solution,[18] when $\omega=0$—with the corresponding q.

Once again, it is interesting to observe that if, for some reason, we do not invoke this diagonalizing Λ^α_β and, instead, proceed with the general ϑ^α_β, we arrive at a reducible form of the solution, which contains a nonvanishing $\overline{\gamma}_{12}$. However, this off-diagonal element can be made to vanish through the action of the previously mentioned constant automorphism.

Thus, we have shown that the ''gauge'' transformations (2.14)—with (2.16) and (2.17) holding—suffice to reduce the most general line element for the type V Bianchi model to the known Joseph's metric, as predicted from the theorem, stated at the end of Sec. II. As we have done for the type II case, we are now going to explicitly verify that these transformations are essentially unique. To this end, let us consider the most general time-dependent automorphism, complementary to the time-dependent automorphism, described in Sec. II—for the type V case.

$$\Lambda^\alpha_\beta=\begin{pmatrix}A(t) & B(t) & 0\\ C(t) & F(t) & 0\\ 0 & 0 & 1\end{pmatrix}\tag{3.41}$$

with $A(t)F(t)-B(t)C(t)=1$. The action of such automorphism on $\gamma^{\text{Joseph}}_{\alpha\beta}$ is, in matrix notation,

$$\hat{\gamma}=\Lambda^T\gamma^{\text{Joseph}}\Lambda.$$

If we insert $\hat{\gamma}_{\alpha\beta}$ in the linear constraint equations (3.1b), we learn that $\hat{N}^a$ are also zero and, since, $|\hat{\gamma}_{\alpha\beta}|=|\Lambda|^2|\gamma^{\text{Joseph}}_{\alpha\beta}|=|\gamma^{\text{Joseph}}_{\alpha\beta}|$, we conclude that we are in the same temporal, as well as spatial, gauge. Therefore, $\hat{\gamma}_{\alpha\beta}$ will also satisfy Eq. (3.1c). Since Λ^α_β is an automorphism, it is a symmetry of q and, thus, if we define the scaled quantities:

$$\hat{\bar{\gamma}}_{\alpha\beta}=q\hat{\gamma}_{\alpha\beta}$$

they must satisfy the relations analogous to (3.37):

$$\hat{\bar{\gamma}}^{\alpha\rho}\hat{\bar{\gamma}}_{\rho\beta}=\vartheta^{\alpha}_{\beta}, \tag{3.42}$$

where

$$\vartheta^{\alpha}_{\beta}=\begin{pmatrix}\theta & \varrho & 0\\ \sigma & -\theta & 0\\ 0 & 0 & 0\end{pmatrix},$$

while $\bar{\gamma}^{\text{Joseph}}_{\alpha\beta}$ satisfies the following relations:

$$(\bar{\gamma}^{\alpha\rho})_{\text{Joseph}}(\bar{\gamma}_{\rho\beta})_{\text{Joseph}}=(\vartheta^{\alpha}_{\beta})_{\text{Joseph}},$$

where

$$(\vartheta^{\alpha}_{\beta})_{\text{Joseph}}=\begin{pmatrix}\lambda & 0 & 0\\ 0 & -\lambda & 0\\ 0 & 0 & 0\end{pmatrix}.$$

By virtue of (3.34), and since q is invariant, we get that $\omega=\omega^{\text{Joseph}}$, i.e.,

$$\theta^2+\varrho\sigma=\lambda^2. \tag{3.43}$$

In order to proceed with the integration of (3.42), it is convenient to parametrize Λ^{α}_{β} in (3.41) as follows:

$$\Lambda^{\alpha}_{\beta}=\begin{pmatrix}\Lambda^{r}_{s} & & 0\\ & & 0\\ 0 & 0 & 1\end{pmatrix}$$

with $\Lambda^{r}_{s}=R^{r}_{m}L^{m}_{s}$, where R^{r}_{m} is

$$\begin{pmatrix}e^{-\lambda t/2} & 0\\ 0 & e^{\lambda t/2}\end{pmatrix}\cdot\begin{pmatrix}\cos(g(t)) & \sin(g(t))\\ -\sin(g(t)) & \cos(g(t))\end{pmatrix}\cdot\begin{pmatrix}e^{\lambda t/2} & 0\\ 0 & e^{-\lambda t/2}\end{pmatrix},$$

i.e., the symmetries of the Joseph's metric; in matrix notation $R^{T}\gamma^{\text{Joseph}}R=\gamma^{\text{Joseph}}$ and L^{m}_{s} is

$$\begin{pmatrix}\varphi(t) & \tau(t)\\ 0 & 1/\varphi(t)\end{pmatrix}.$$

The system (3.42) gives the following differential equations for $\varphi(t)$ and $\tau(t)$:

$$2\frac{\dot{\varphi}}{\varphi}+\lambda=\theta+\sigma\frac{\tau}{\varphi}, \tag{3.44a}$$

$$\dot{\tau}\varphi-\tau\dot{\varphi}=\varrho\varphi^2-2\theta\varphi\tau-\sigma\tau^2, \tag{3.44b}$$

$$e^{2\lambda t}(\dot{\tau}\varphi-\tau\dot{\varphi})=\frac{\sigma}{\varphi^2}. \tag{3.44c}$$

The solution to this system, for $\sigma\neq 0$, leads to incompatibility of the form $\varphi^2=-e^2$, with e a function of time.

For $\sigma=0$, we get

$$\varphi(t)=c_1\exp\left(\frac{\theta-\lambda}{2}t\right),$$
$$\tau(t)=c_1\frac{\varrho}{2\theta}\exp\left(\frac{\theta-\lambda}{2}t\right) \tag{3.45}$$

with $c_1>0$, and from (3.43), for the case at hand, $\theta=\pm\lambda$. The case $\theta=\lambda$ trivially gives a constant matrix

$$L_s^m=\begin{pmatrix} c_1 & c_1\dfrac{\varrho}{2\lambda} \\ 0 & 1/c_1 \end{pmatrix}$$

while the case $\theta=-\lambda$ gives

$$L_s^m=\begin{pmatrix} 0 & e^{-\lambda t} \\ e^{\lambda t} & 0 \end{pmatrix}\cdot\begin{pmatrix} 0 & 1/c_1 \\ c_1 & -c_1\dfrac{\varrho}{2\lambda} \end{pmatrix}.$$

Since the first matrix in the product is a symmetry of $(\overline{\gamma}_{\alpha\beta})_{\text{Joseph}}$, we again conclude that the nontrivial action of Λ^α_β on $(\overline{\gamma}_{\alpha\beta})_{\text{Joseph}}$, is tantamount to the action of a constant matrix in accordance to the theorem of Sec. II.

Finally, the most general line element $(\gamma_{\alpha\beta},N,N^a)$ satisfying Einstein's equations (2.5) is thus given—in matrix notation—by

$$\gamma_{\text{most general}}(t)=\Lambda^T(t)\,\gamma^{\text{Joseph}}(h(t))\Lambda(t),$$

$$\Lambda=\begin{pmatrix} \varrho_1P(t) & \varrho_2P(t) & x(t) \\ \varrho_3P(t) & \varrho_4P(t) & y(t) \\ 0 & 0 & 1 \end{pmatrix},$$

where the ϱ's are constant, subject to the condition $\varrho_1\varrho_4-\varrho_2\varrho_3=1$ and

$$N(t)=\sqrt{|\gamma_{\text{most general}}|}\dot{h}(t),$$

$$N^\alpha(t)=S^\alpha_\beta P^\beta(h(t)),$$

$$P^\beta(h(t))=\left\{x(t)\left(\ln\frac{x(t)}{P(t)}\right)^{\cdot},y(t)\left(\ln\frac{y(t)}{P(t)}\right)^{\cdot},\left(\ln\frac{1}{P(t)}\right)^{\cdot}\right\},$$

$$S=\Lambda^{-1},$$

$$\gamma^{\text{Joseph}}(h(t))=\begin{pmatrix} \dfrac{e^{\lambda h(t)}}{q} & 0 & 0 \\ 0 & \dfrac{e^{-\lambda h(t)}}{q} & 0 \\ 0 & 0 & f \end{pmatrix},$$

$$\frac{1}{f(h(t))}=q(h(t))=\begin{cases} \dfrac{2}{\sqrt{\omega}}\sinh(\pm\sqrt{\omega}h(t)), & \omega>0 \\ \pm 2h(t), & \omega=0 \end{cases} \tag{3.46}$$

$$3\omega=\lambda^2,$$

where the fourth arbitrary function, $h(t)$, accounts for the time reparametrization covariance.

IV. DISCUSSION

In this work, we present an approach to the problem of solving Einstein's equations for the case of a generic Bianchi-type spatially homogeneous space–time. The approach is not plagued by the fragmentation characterizing the major part of the existing rich literature—which is inherited by the diversity of the various simplifying ansatzen, employed in each case. The key notion for avoiding this fragmentation is that of a time-dependent automorphism inducing diffeomorphism; that is, a general coordinate transformation (2.9), mixing space and time coordinates, whose action on the line element of a Bianchi geometry is described by relations (2.14)—viewed as ''gauge'' transformation laws for the dependent variables $\gamma_{\alpha\beta}(t)$, $N(t)$, and $N^{\alpha}(t)$. The investigation for the existence of such GCTs, leads to the necessary and sufficient conditions (2.16) and (2.17); hence the name time-dependent AIDs. In each and every Bianchi type, these conditions possess a nonempty set of solutions containing precisely three arbitrary functions of time. A choice of these arbitrary functions amounts exactly to a choice for the three spatial coordinates. Thus, the possibility is offered for simplifying Einstein equations—through a simplification of $\gamma_{\alpha\beta}, N^{\alpha}, N$—without running the risk of loss of generality or any sort of incompatibility.

Of course, the possible simplifications differ from one Bianchi type to another; even within the same Bianchi type, there are many possible simplifications—since one, can use the three arbitrary functions at will. This kinematical freedom, when combined with the dynamical information—furnished by the linear constraint equations—considerably simplifies the form of the line-element and thus of Einstein's equations, as well. A useful, in our opinion, irreducible form of the line element for each Bianchi type is given at the balance of Sec. II.

A statement that applies to all types is that, using two of the three arbitrary functions, the scale-factor matrix $\gamma_{\alpha\beta}(t)$ can always—*a priori*; i.e., before solving any classical equations of motion—be put into a so-called ''symmetric''[16] form, i.e., $\gamma_{13}=\gamma_{23}=0$. This applies also for type II, if we take instead of the standard form for the structure constants ($C^1_{23}=-C^1_{32}=1$, all others vanish) the equivalent version $C^3_{12}=-C^3_{21}=1$, all others vanish. If this ''symmetric'' form is then substituted into the linear equations, and the third arbitrariness is used, considerable restrictions among N^{α}'s and the remaining $\gamma_{\alpha\beta}$'s are obtained, as presented in detail at the end of Sec. II. Furthermore, with the help of the essential arbitrary constants in Λ^{α}_{β}, we can diagonalize $\gamma_{\alpha\beta}(t)$, on mass shell. For all Bianchi types, the shift vector N^{α} can always be set to zero—with the help of time-dependent AIDs, and the linear equations. One could, of course, rely on the well-known existence of Gauss-normal coordinates,[2] and argue that this should be true. However, in this work, the explicit realization of this fact is presented; what is more important is that the vanishing of N^{α} is accomplished without spoiling manifest spatial homogeneity. The interplay between line elements with and without shift, established through time-dependent AIDs—see (2.14b)—raises the

need to reexamine the set of existing solutions—with respect to physical equivalence, among each other. In particular, many tilded and untilded fluid solutions,[18] may proven to be GCT related, and thus physically indistinguishable.

Except for the three arbitrary functions of time, of considerable importance are also the (nonabsorbable in the shift) arbitrary constants, appearing in the solutions to (2.16) and (2.17). The number of these constants varies for different Bianchi types. The very interesting fact is that when this number is subtracted from the number of constants, given by Peano's theorem—after the freedom in arbitrary functions of time has been fully exhausted—the resulting number of the (finally) remaining constants equals, for each and every Bianchi type, the number of expected essential constants—see Ref. 19, p. 211. This permits us to conclude that the gauge symmetry transformations (2.14)—with (2.16) and (2.17), holding—are, essentially, unique. It is also noteworthy that the existence of these constant parameters helps to rectify a defect from which the previous approach of Jantzen is suffering; that of an uneven passage, from the lower to the higher Bianchi types, owing to the change of the dimension of the invoked symmetry group;[19] indeed, the arbitrary functions of time are thus varying with dim[SAut(G)], from 8 (type I), to 5 (types II and V), to 3 (higher types). This situation is rather unsatisfactory, since we know that the independent or dynamical degrees of freedom for the gravitational field are 2-per space point. Thus, in cosmology, we expect 2 independent functions of time—irrespective of Bianchi type.

In contrast to this state of affairs, the solutions to (2.16) and (2.17) contain exactly 3 arbitrary functions of time, which together with the arbitrary function—owing to the time reparametrization covariance of Eq. (2.5)—leave us with $6(\gamma_{\alpha\beta})-4=2$ arbitrary functions, in all Bianchi types. The required sensitivity of the method to the particular isometry group is represented by the extra constant parameters—as explained.

It is in this remarkable way that general relativity manages to encode the memory of spatial GCT covariance in the set of the reduced equations (2.5), where only functions of time and their derivatives appear. This encoding also persists in the actions—when these actions exist—and leads to important grouping of $\gamma_{\alpha\beta}$'s into the three solutions: $x^1=C^{\alpha}_{\mu\nu}C^{\beta}_{\rho\sigma}\gamma^{\mu\rho}\gamma^{\nu\sigma}\gamma_{\alpha\beta}$, $x^2=C^{\alpha}_{\beta\delta}C^{\delta}_{\nu\alpha}\gamma^{\beta\nu}$, $x^3=\gamma$ of the quantum linear constraints.[13,20] When a truly scalar Hamiltonian exists,[13,21] the wave function depends only on the q^i's:

$$q^1=\frac{m^{\alpha\beta}\gamma_{\alpha\beta}}{\sqrt{\gamma}},\quad q^2=\frac{(m^{\alpha\beta}\gamma_{\alpha\beta})^2}{2\gamma}-\frac{1}{4}C^{\alpha}_{\mu\nu}C^{\beta}_{\rho\sigma}\gamma^{\mu\rho}\gamma^{\nu\sigma}\gamma_{\alpha\beta},\quad q^3=\frac{m}{\sqrt{\gamma}},$$

which completely and irreducibly determine a spatial three-geometry.

To summarize, the system (2.5), admits solutions containing in each and every Bianchi type exactly four unspecified functions of time. One corresponds to the freedom of changing the time coordinate; three correspond to the freedom of changing the spatial coordinates via time-dependent AIDs. The action of such a transformation on the line element, and on the system of equations (2.5), is described by relations (2.14) and (2.18). Thus, one does not actually need to calculate the simplifying GCTs; one simply uses (2.14), simplifies the equations, solves them completely, and finally inverts the transformation, thereby obtaining the entire space of solutions. It is in this sense that the closed form of the line elements presented in Sec. III, exhaust the space of classical solutions—for the case of Bianchi types II and V.

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APPENDIX

In Ref. 22, the following Theorem is given:

"Let two symmetric forms A and B, be given, on a n-dimensional linear vector space V. If one of them—say A—is non singular, then there is a base in V in which both A and B, are diagonal, if and only if, the mapping $A^{-1}B$, possesses n-real eigenvalues."

Thus, if we take the pair $\gamma_{\alpha\beta}$, $\eta_{\alpha\beta}$, it suffices to prove that $\eta^{\alpha\varrho}\gamma_{\varrho\beta}$, has n-real eigenvalues. In what follows, for the sake of completeness, we give a proof of the entire statement that a positive definite matrix $\gamma_{\alpha\beta}$ can be diagonalized via the Lorentz group.

Theorem: Let γ be a positive definite $n\times n$ real matrix. Then, there exists a Lorentz matrix Λ, such that

$$\Lambda^T\gamma\Lambda=\Delta, \tag{A1}$$

where Δ a diagonal matrix.

Note: Since $\Lambda^T=\eta\Lambda^{-1}\eta$, where η is the Minkowski metric, (A1) may be written as

$$\Lambda^{-1}\eta\gamma\Lambda=\eta\Delta. \tag{A2}$$

In order to prove (A2) it is useful to write it equivalently using the notation employed with linear mappings. To do that, we consider an n-dimensional real linear space V with basis $(e_1,e_2,\ldots,e_n)$. The scalar product in this space is defined as $\langle,\rangle: VV\times V\rightarrow\Re$, with $\langle e_\alpha,e_\beta\rangle=\eta_{\alpha\beta}$. The matrix $\eta\gamma$ defines a mapping $f: V\rightarrow V$ through the relation:

$$f(e_\alpha)=\sum_{\beta=1}^{n}(\eta\gamma)_{\alpha\beta}e_\beta.$$

The following will prove useful later on:

(1) If $M\subseteq V$ then $V=M\oplus M^\perp$.[23]

(2) A mapping $f: V\rightarrow V$ is called self-dual, if $\langle f(x),y\rangle=\langle x,f(y)\rangle$ for every $x,y\in V$. We may prove that the mapping f defined through the matrix $\eta\gamma$ is self-dual. Indeed:

$$\left.\begin{aligned}\langle f(x),y\rangle=\langle y,f(x)\rangle=y^T\eta\eta\gamma x=y^T\gamma x\\ \langle x,f(y)\rangle=x^T\eta\eta\gamma y=x^T\gamma y=y^T\gamma x\end{aligned}\right\}$$

$$\Rightarrow\langle f(x),y\rangle=\langle x,f(x)\rangle.$$

(3) If $M\subseteq V$ is an invariant subspace of V with respect to a self-dual mapping f then $M^\perp$ is also an invariant subspace of V. Indeed, let $b\in M^\perp$ and $m\in M$. Since M is an invariant subspace, it follows that

$$f(m)\in M\Rightarrow\langle f(m),b\rangle=0\Rightarrow\langle m,f(b)\rangle=0\,\forall\, m\in M$$

$$\Rightarrow f(b)\in M^\perp.$$

Equation (A2) states the fact that there exists an orthonormal basis of V consisting of the eigenvalues of f. If (A2) holds then the nonvanishing elements of the real diagonal matrix $\eta\Delta$ will be eigenvalues of $\eta\gamma$. Thus, we have to prove that the eigenvalues of $\eta\gamma$ are real. Indeed, the following theorem holds:

Theorem: If γ is a positive definite symmetric matrix, then $\eta\gamma$ has real eigenvalues.

Proof: Let $\lambda=\alpha+\beta j,\ \beta\neq 0$ be a complex eigenvalue of $\eta\gamma$ and $u\neq 0$ the corresponding complex right eigenvector. Since η is invertible, there exists a $v=x+yj,\ x,y,\in\Re^n$ such that $u=\eta v$. We have

$$\eta\gamma u=\lambda u\Leftrightarrow\eta\gamma\eta v=\lambda\eta v\Leftrightarrow\eta\gamma\eta x=\alpha\eta x-\beta\eta y, \tag{A3}$$

$$\eta\gamma\eta y=\alpha\eta y+\beta\eta x. \tag{A4}$$

Equations (A3) and (A4) imply, respectively,

$$y^T\eta\gamma\eta x=\alpha\langle y,x\rangle-\beta\langle y,y\rangle,$$

$$x^T\eta\gamma\eta y=\alpha\langle x,y\rangle+\beta\langle x,x\rangle.$$

The last two equations have their left-hand sides equal (since $\eta\gamma\eta$ is symmetric), hence

$$\beta(\langle x,x\rangle+\langle y,y\rangle)=0\Rightarrow\langle y,y\rangle=-\langle x,x\rangle. \tag{A5}$$

Since γ is positive definite, $\eta\gamma\eta$ is positive definite as well. Then:

$$x^T\eta\gamma\eta x\geqslant^{(A3)}0\Rightarrow\alpha\langle x,x\rangle-\beta\langle x,y\rangle\geqslant 0, \tag{A6}$$

$$y^T\eta\gamma\eta y\geqslant^{(A4)}0\Rightarrow\alpha\langle y,y\rangle+\beta\langle y,x\rangle\geqslant^{(A5)}0\Rightarrow\alpha\langle x,x\rangle-\beta\langle x,y\rangle\leqslant 0. \tag{A7}$$

From (A6) and (A7) we get

$$\alpha\langle x,x\rangle=\beta\langle x,y\rangle \tag{A8}$$

Through (A5) and (A8), Eqs. (A3) and (A4) imply

$$x^T\eta\gamma\eta x=0,$$

$$y^T\eta\gamma\eta y=0,$$

and since $\eta\gamma\eta$ is positive definite we conclude that $x=0$ and $y=0$, i.e., $u=0$, contradicting our initial assumption $u\neq 0$. Therefore β has to vanish and thus we have proved the reality of λ.

For the eigenvectors of $\eta\gamma$, we can prove that they have a nonzero norm. Indeed, let x be an eigenvector of $\eta\gamma$, i.e.,

$$\eta\gamma x=\lambda x\Rightarrow\gamma x=\lambda\eta x\Rightarrow x^T\gamma x=\lambda x^T\eta x=\lambda\langle x,x\rangle.$$

Since γ is positive definite and $x\neq 0$ we have $x^T\gamma x>0$, so that $\langle x,x\rangle\neq 0$. We are now in position to prove a spectral theorem for a mapping f with real eigenvalues.

Theorem: If $f:V\rightarrow V$ is a self-dual mapping with real eigenvalues, then V has an orthonormal basis consisting of the eigenvectors of f.

Proof: Let λ be an eigenvalue of f, u the corresponding eigenvector, and $M=[u]$ the one-dimensional subspace spanned by u. Obviously, M is an invariant subspace of V with respect to f.

According to (1), we have $V=M\oplus M^{\perp}$. As implied by (2) and (3), $M^{\perp}$ is also an invariant subspace and thus f induces a self-dual mapping onto $M^{\perp}$. Hence, we can apply induction and show that

$$V=M_1\oplus M_2\oplus\ \ldots\ \oplus M_n,$$

where the M_α are one-dimensional invariant subspaces orthogonal to each other. Since u_α is an eigenvector of $\eta\gamma$, it holds that $\langle u,u\rangle\neq 0$, as proved previously. We can thus promote the orthogo-

nal basis to an orthonormal set $(\hat{u}_1,\hat{u}_2,\ldots,\hat{u}_n)$. The transformation connecting this orthonormal basis to the initial orthonormal basis $(e_1,e_2,\ldots,e_n)$ is the matrix Λ sought for in the first theorem, relations (A2) and (A1).

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Ricci-flat warped products and Painlevé analysis

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We apply Painlevé analysis to the Ricci-flat Einstein equations for a warped product with an arbitrary number of factors. We find that, as in the situation of the two factors examined [J. Geom. Phys. **38**, 183–206 (2001)], the cases when the total dimension is 10 or 11 are singled out by the analysis. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1380441]

I. INTRODUCTION

In Ref. 1 we applied Painlevé analysis to investigate the integrability of certain cases of the Ricci-flat Einstein equations, including that of a warped product on two Einstein factors. In this paper, we consider the Ricci-flat equations for warped products with an arbitrary number of Einstein factors. More precisely, we study Riemannian metrics of the form

$$dt^2+f_1^2(t)g_1\oplus\cdots\oplus f_r^2(t)g_r, \tag{1.1}$$

where (Y_i,g_i) are Einstein manifolds with nonzero Einstein constant. We denote the dimension of Y_i by d_i and assume that $d_i>1$. We also let $n=\Sigma_{i=1}^r d_i$, so the metric (1.1) lives on a manifold with dimension $n+1$.

In Ref. 2 we introduced a Hamiltonian formulation of the cohomogeneity one Einstein equations based on a Hamiltonian of ADM type (cf. Ref. 3 or Appendix E of Ref. 4) on the cotangent bundle of the space of all invariant metrics of the principal orbit. This Hamiltonian formalism applies equally well in the special case of r-fold warped product metrics, where the principal orbits are replaced by the product $Y_1\times\cdots\times Y_r$ with *no* symmetry assumptions on the Y_i, as long as (Y_i,g_i) are Einstein. Using changes of variables analogous to those employed in Ref. 1, we deduce that the Ricci-flat Einstein equations for the r-fold warped product metrics (1.1) are equivalent to the Hamiltonian flow of

$$\overline{H}=\sum_{i,j=1}^{r} E_{ij}x_ix_jy_iy_j-\sum_{i=1}^{r} A_ix_i$$

subject to the constraint $\overline{H}=0$. Here A_i is the scalar curvature of the Einstein manifold Y_i, and

$$E_{ij}=1, \quad \text{for } i\neq j,$$

$$E_{ii}=1-\frac{1}{d_i}.$$

Introducing new variables $u_i=x_iy_i$, and rescaling the x_i to make $A_i=1$, Hamilton's equations for $\overline{H}$ now become

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$$x_i' = 2x_i\left(\sum_{j=1}^{r} E_{ij}u_j\right), \tag{1.2}$$

$$u_i' = x_i, \tag{1.3}$$

for $1 \leqslant i \leqslant r$. In the above, a prime denotes differentiation with respect to a variable s which is related to the variable t in (1.1) by

$$\frac{dt}{ds} = f_1(t)^{d_1}\cdots f_r(t)^{d_r},$$

i.e., the distortion of the volume relative to that of the background.

A summary of our analysis of (1.2)–(1.3) is given in Sec. V. We note that the case when (1.1) is replaced by a Lorentz metric with spacelike hypersurfaces is included in our analysis as the special case when all of the A_i are negative.

II. LEADING POWERS

We shall now analyze the equations (1.2)–(1.3). We first find the possible leading terms for a Painlevé expansion around a singularity at $s=0$. We set

$$x_i = \alpha_i s^{M_i} + \cdots, \quad u_i = \beta_i s^{N_i} + \cdots, \quad : \quad (i = 1,..,r),$$

where α_i and β_i are all nonzero. Without loss of generality, let $N_1 = \cdots = N_m < N_{m+1}, \ldots, N_r$.

As E is nondegenerate one of the sums $\Sigma_{j=1}^{m} E_{ij}\beta_j$ is nonzero, so upon examining the corresponding equation in (1.2) we deduce $N_1 \geqslant -1$, with equality if and only if $M_i \neq 0$. On the other hand, if some M_k is nonzero then $N_1 \leqslant -1$. So either $N_1 = -1$ or all $M_k = 0$. The latter possibility implies, from (1.3), that we have $N_k = 0$ or 1, and so we have no singularity at $s=0$, giving a contradiction.

Therefore we must have $N_1 = \cdots = N_m = -1$ and hence, from (1.3)

$$M_1 = \cdots = M_m = -2.$$

Now (1.2) implies

$$\sum_{j=1}^{m} E_{ij}\beta_j = -1 \quad : (i = 1,..., m).$$

These equations have solution

$$\beta_i = \frac{d_i}{1 - \Sigma_{j=1}^{m} d_j} \quad : (i = 1,..., m), \tag{2.1}$$

so for $i > m$ we see that $\Sigma_{j=1}^{m} E_{ij}\beta_j = \Sigma_{j=1}^{m} \beta_j$ is nonzero. Hence, from (1.2), all the M_i are nonzero.

Moreover, for $i = m+1,..., r$ we have

$$2\sum_{j=1}^{m} \beta_j = M_i \geqslant N_i - 1 > -2.$$

Comparing with (2.1) shows that we have a contradiction unless $m = r$.

We have established the following lemma.

Lemma 2.2: The leading terms are given by

$$N_i = -1, \quad M_i = -2 \quad : (i = 1,...,r),$$

$$\alpha_i = d_i/(n-1), \quad \beta_i = -d_i/(n-1) \quad : (i = 1,\ldots, r).$$

□

Remark 2.3: By changing to the variable $1/s$ and doing an analysis similar to that above, we can rule out the existence of Painlevé expansions around a singularity at infinity.

III. RESONANCES

We now look for expansions of the form

$$x_i = \sum_{j=0}^{\infty} \alpha_i^{(j)} s^{-2+j/Q}, \quad u_i = \sum_{j=0}^{\infty} \beta_i^{(j)} s^{-1+j/Q},$$

where Q is an integer to be determined later. Note that $\alpha_i^{(0)} = \alpha_i$, $\beta_i^{(0)} = \beta_i$. We write $\alpha^{(j)}$ for the column vector whose ith entry is $\alpha_i^{(j)}$.

It follows from a straightforward computation that the terms of the expansion must satisfy the recursion relation

$$\begin{pmatrix} \nu I_r & -\left(\frac{2}{n-1}\right)F \\ -I_r & (\nu-1)I_r \end{pmatrix} \begin{pmatrix} \alpha^{(j)} \\ \beta^{(j)} \end{pmatrix} = \begin{pmatrix} \tau^{(j)} \\ 0 \end{pmatrix}, \tag{3.1}$$

where I_r is the identity matrix of size r, $\nu = j/Q$, $F_{ij} = d_i E_{ij}$, and the ith entry of the vector $\tau^{(j)}$ is

$$2\sum_{k=1}^{r} E_{ik} \sum_{p=1}^{j-1} \alpha_i^{(p)} \beta_k^{(j-p)}.$$

We shall denote the matrix in (3.1) by $X(\nu)$.

We can write the recursion as

$$\left(\nu(\nu-1)I_r - \frac{2F}{n-1}\right)\beta^{(j)} = \tau^{(j)},$$

$$\alpha^{(j)} = (\nu-1)\beta^{(j)}.$$

The resonances, that is the values of ν for which the matrix $X(\nu)$ fails to be invertible, are therefore the roots of

$$\nu(\nu-1) = \lambda,$$

where λ ranges over the eigenvalues of $[2/(n-1)]F$. Moreover, the dimension of the kernel of $X(\nu)$ equals the dimension of the λ eigenspace.

Lemma 3.2: The eigenvalues of $[2/(n-1)]F$ *are 2 with multiplicity one and* $-2/(n-1)$ *with multiplicity* $r-1$. *In each case the dimension of the eigenspace equals the multiplicity.*

Proof: Observe that $F = D - I$ where $D_{ij} = d_i$. The eigenvalues of F are therefore -1 with multiplicity $r-1$ and $n-1$ with multiplicity one. The eigenspaces are, respectively, $\{(a_1,\ldots, a_r): \Sigma a_i = 0\}$ and the line spanned by $(d_1,\ldots, d_r)$.

As in Ref. 1 we deduce the following result. □

Lemma 3.3: (i) Two resonances are therefore always -1 *and 2. In these cases,* $\ker(X(\nu))$ *is one dimensional.*

(ii) The remaining resonances, that is, the roots of $\nu(\nu-1) = -2/(n-1)$, *are rational if and only if* $n = 9$ *or* 10 *(cf. Ref. 1).*

If $n = 9$ *these resonances are* 1/2; *if* $n = 10$, *they are* 1/3, 2/3.

For each of these resonances $\ker(X(\nu))$ *has dimension* $r-1$. □

IV. COMPATIBILITY CONDITIONS

We shall now look at the cases $n=9, 10$. To study the compatibility conditions we need to record the kernel of $X(\nu)^T$ where ν is a resonance. The kernel is given by the equations

$$\left(\nu(\nu-1)I_r-\frac{2}{n-1}F^T\right)\alpha=0,$$

$$\beta=\nu\alpha.$$

By Lemma 3.2, the $-2/(n-1)$ eigenspace of $2F^T/(n-1)$ is the hyperplane $\{(a_1,\ldots,a_r):\Sigma d_i a_i=0\}$ and the 2 eigenspace is spanned by $(1,\ldots,1)$. For compatibility, the right-hand side of (3.1) should be orthogonal to the kernel of $X(\nu)^T$.

In particular the compatibility condition at $\nu=2$ is $\Sigma_{i=1}^r \tau_i^{(2Q)}=0$, that is

$$\sum_{i,k=1}^{r} E_{ik}\sum_{p=1}^{2Q-1}\alpha_i^{(p)}\beta_k^{(2Q-p)}=0. \tag{4.1}$$

But using (3.1) we observe that

$$\begin{aligned}\sum_{p=1}^{2Q-1}\alpha_i^{(p)}\beta_k^{(2Q-p)}&=\sum_{p=1}^{2Q-1}\left(\frac{p}{Q}-1\right)\beta_i^{(p)}\beta_k^{(2Q-p)}\\&=\sum_{q=1}^{2Q-1}\left(1-\frac{q}{Q}\right)\beta_i^{(2Q-q)}\beta_k^{(q)}\\&=-\sum_{q=1}^{2Q-1}\alpha_k^{(q)}\beta_i^{(2Q-q)}.\end{aligned}$$

This shows that in (4.1) the terms with $i\neq k$ cancel in pairs and the terms with $i=k$ are 0. Hence the compatibility condition holds at $\nu=2$ if it holds at the earlier resonances.

Note also that at the first positive resonance the compatibility condition always holds because the right-hand side of (3.1) is 0 at that stage of the recursion.

If $n=9$, it is natural to take $Q=2$, so the positive resonances are at $j=1$ and $j=4$. We get one free parameter from the pole position, $r-1$ free parameters from the kernel of $X(1/2)$ and one further parameter from the resonance $j=4$.

If $n=10$, we take $Q=3$, so the positive resonances occur at $j=1, 2, 6$. Since the compatibility condition at $j=1$ automatically holds, we consider $j=2$. Now we have

$$\alpha^{(1)}=-\tfrac{2}{3}\beta^{(1)} \quad \text{and} \quad \sum_{i=1}^{r}\beta_i^{(1)}=0. \tag{4.2}$$

From the description of $\ker(X(2/3)^T)$ it follows that the compatibility condition at $j=2$ is given by

$$\sum_{i,j=1}^{r} v_i\beta_i^{(1)}E_{ij}\beta_j^{(1)}=0$$

for all $(v_1,\ldots,v_r)$ such that $d_1v_1+\cdots+d_rv_r=0$. This simplifies to

$$d_k\tau_i^{(2)}=d_i\tau_k^{(2)}, \quad 1\leqslant i,k\leqslant r,$$

or, equivalently,

$$d_i^2(\beta_k^{(1)})^2 = d_k^2(\beta_i^{(1)})^2.$$

After imposing these conditions we have at most one free parameter at $j=1$. More precisely, we have one free parameter if

$$\{d_1,\ldots,d_r\}=\{5,5\},\ \{5,3,2\},\ \text{or}\ \{3,3,2,2\},$$

and no free parameters otherwise.

The kernel of $X(2/3)$ gives us $r-1$ parameters at $j=2$. The pole position and the resonance at $j=6$ each contribute one further parameter.

Remark 4.3: The majorization argument in Ref. 1 carries over to prove convergence of our formal Painlevé expansion (we now take the constant κ in Ref. 1 to be $2\Sigma_{i,k=1}^{r}E_{ik}$).

V. SUMMARY

We summarize our results as follows.

Theorem 5.1: If $n\neq 9,10$ *then the only rational resonances are* -1 *and* 2.

If $n=9$ *we have a* $(r+1)$*-parameter Painlevé expansion in* $s^{1/2}$ *in a* $2r$*-dimensional system. Here* r *must be less than or equal to 4.*

If $n=10$ *we have an* $(r+2)$*-parameter Painlevé expansion in* $s^{1/3}$ *in a* $2r$*-dimensional system if*

$$\{d_1,\ldots,d_r\}=\{5,5\},\{2,3,5\},\ \text{or}\ \{2,2,3,3\}.$$

Otherwise we have a $(r+1)$*-parameter expansion. Here* r *is less than or equal to 5.* □

Remark 5.2: Recall that the Ricci-flat metric corresponding to a solution of our equations lives on a manifold of dimension $n+1$.

Remark 5.3: In all cases the constraint $\overline{H}=0$ has the effect of fixing the parameter at the top resonance.

Remark 5.4: The two-parameter expansion which always occurs (associated to the resonances $r=-1, 2$) comes from the special family of solutions with $d_j u_i = d_i u_j$ for all i,j. After imposing the Hamiltonian constraint, these solutions are just translations of

$$x_i=\frac{d_i}{(n-1)s^2},\quad u_i=\frac{-d_i}{(n-1)s}.$$

The corresponding Ricci-flat metric is the cone over the product of the Y_i (after the metrics g_i on Y_i have been rescaled by constant factors so that all have the same Einstein constant).

Remark 5.5: In the context of Theorem 4.23 in Ref. 2, the ordered basis $\hat{W}$ for the present case of r-fold warped product metrics may be taken to be $\{(-1, 0, \ldots, 0),\ldots, (0, \ldots, 0, -1)\}$, and one can readily check that when $r\geqslant 3$, all the hypotheses of that theorem are satisfied. Hence the associated Ricci-flat Hamiltonian system does not have nontrivial polynomial generalized first integrals.

On the other hand, the Ricci-flat Einstein equations for the warped product metrics (1.1) with $r=2$ are a subsystem of the system for arbitrary r, provided that the Ricci curvatures A_i/d_i of the factors that are grouped together are chosen to be equal. Therefore the nontrivial polynomial generalized first integrals found in Ref. 5 for the $r=2$ case give rise to explicit Ricci-flat metrics in some of the situations singled out in Theorem 5.1. Of course, these are not generalized integrals of the full system, as was just noted above. Solvability of the Ricci-flat warped product equations in these cases has independently been observed in Ref. 6 using different methods.

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Nonsymmetric gravitation theory in noncommutative geometry

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We propose a reformulation of the nonsymmetric gravitation theory (NGT) in the context of noncommutative geometry. It is shown that all of the Moffat's added terms in his new version of the NGT have a geometric origin. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1385176]

I. INTRODUCTION

Despite the successes of the physical theories describing the fundamental interactions, they remain confronted to several fundamental difficulties which may require the introduction of new mathematical concepts. For this purpose, many theories have been explored like Kaluza–Klein theories, super-gravity, superstrings, etc.

Recently, a geometrical picture has been proposed by Connes[1–4] which consists in generalizing the classical differential geometry to a noncommutative one, and allows the accommodation of other types of spaces like discrete spaces in order to reformulate the standard model of elementary particles.

The success of noncommutative geometry (NCG) comes from the fact that it gives a geometric interpretation for the origin of the Higgs fields (in the standard model), namely as connections on a discrete space.

The reformulation of General Relativity in this framework was done by Chamseddine and collaborators[5,6] where they have considered a space–time given by a product of a 4-dimensional manifold and a two points discrete space. They have generalized the notion of cotangent space to the case of noncommutative geometry, and taken the Cartan structure equations.[7] The resulting action describes a scalar field coupled with gravity.[5,6] General Relativity[8,9] as a classical theory of gravity, was adopted as the correct theory of gravitation in regard to its experimental success, and its simple and elegant mathematical formalism.

Yet Einstein himself attempted to generalize his theory so as to include the fundamental interactions but endowed with a geometrical meaning. In his new theory he considered a more general nonsymmetric metric with the symmetric part corresponding to the metric of General Relativity, and the anti-symmetric one corresponding to the electromagnetic tensor field.

Since then, quite a few other theories inspired by General Relativity and based on a nonsymmetric metric $g_{\mu\nu}$ were proposed. One of those theories which has attracted a sustained interest is certainly the Nonsymmetric Gravitation theory (NGT) propounded by Moffat, and for which the antisymmetric part has a gravitational origin.[10–12]

However, NGT as proposed initially was not self-consistent, but suffered from perturbative problems in the skewon sector where the nonphysical modes happen to be coupled with the physical ones.

Recently, a new more consistent version of NGT was proposed, where the nonphysical modes are no longer coupled to the physical ones. Yet, this problem had been circumvented at the cost of adding by hand new terms to the action without any geometrical origin.[13]

In this work, we propose a new action for NGT which does not suffer from this defect. This

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is done by generalizing the scalar product defining the action as well as the Dirac operator.

In Sec. II, we generalize the formalism of noncommutative geometry for NGT. In Sec. III, we derive the new NGT action, and finally in Sec. IV we discuss our results and give our conclusions.

II. BASICS ON NGT AND NCG

NGT is a geometric theory of gravity based on a nonsymmetric metric $g_{\mu\nu}$. The best formulation of NGT is to use a hyperbolic complex space, where the metric $g_{\mu\nu}$ is written as

$$g_{\mu\nu}=g_{(\mu,\nu)}+g_{[\mu\nu]}=\tilde{g}_{\nu\mu}.$$

Here $\tilde{g}_{\mu\nu}$ stands for the hyperbolic complex conjugate of $g_{\mu\nu}$, $g_{(\mu\nu)}$ and $g_{[\mu\nu]}$ are the symmetric and the antisymmetric parts of $g_{\mu\nu}$, with $\varepsilon^2=1$.

One can also define the inverse $g^{\mu\nu}$ of the metric by[12]

$$g^{\mu\nu}g_{\mu\alpha}=g^{\nu\mu}g_{\alpha\mu}=\delta^{\nu}_{\mu}.$$

The fundamental object in NGT is the connection $W^{\lambda}_{\mu\nu}$ (which is of course nonsymmetric). The latter can be related to another one denoted by $\Gamma^{\lambda}_{\mu\nu}$ through the projective transformation:[12]

$$W^{\lambda}_{\mu\nu}=\Gamma^{\lambda}_{\mu\nu}-\tfrac{2}{3}\delta^{\lambda}_{\mu}W_{\nu},$$

where

$$W_{\mu}=\tfrac{1}{2}(W^{\alpha}_{\mu\alpha}-W^{\alpha}_{\alpha\mu}).$$

It is worth mentioning that the displacement field $\Gamma^{\lambda}_{\mu\nu}$ is defined by the parallel transport law for a vector A^{μ}:

$$\delta A^{\lambda}(x)=\Gamma^{\lambda}_{\mu\nu}A^{\mu}(x)dx^{\nu}.$$

A curvature and contracted curvature tensors $R^{\sigma}_{\mu\nu\rho}$ and $R_{\mu\nu}$, respectively, can be formed from the connection as

$$R^{\sigma}{}_{\mu\nu\rho}=W^{\sigma}{}_{\mu\nu,\rho}-W^{\sigma}{}_{\mu\rho,\nu}+W^{\sigma}{}_{\alpha\rho}W^{\alpha}{}_{\mu\nu}-W^{\sigma}{}_{\alpha\nu}W^{\alpha}{}_{\mu\rho},$$

$$R_{\mu\nu}(W)=W^{\alpha}_{\mu\nu,\alpha}-\tfrac{1}{2}(W^{\alpha}{}_{\mu\alpha,\nu}+W^{\alpha}{}_{\nu\alpha,\mu})+W^{\beta}{}_{\alpha\beta}W^{\alpha}{}_{\mu\nu}-W^{\beta}{}_{\alpha\nu}W^{\alpha}{}_{\mu\beta},$$

where we have used the notation $W^{\sigma}{}_{\mu\nu,\rho}=\partial_{\rho}W^{\sigma}{}_{\mu\nu}$.

As in general relativity, one can introduce a vierbein e^{a}_{μ} such that

$$g_{\mu\nu}=e^{a}_{\mu}\tilde{e}^{b}_{\nu}\eta_{ab},$$

with the orthogonality condition

$$e^{a}_{\mu}e^{\nu}_{a}=\delta_{\mu}{}^{\nu},\quad e_{a}{}^{\mu}e^{b}_{\mu}=\delta_{a}{}^{b},$$

where $\eta_{ab}=\mathrm{diag}(1,-1,-1,-1)$ is the Minkowski metric and $\tilde{e}^{b}_{\nu}$ denotes the hyperbolic complex conjugate of e^{b}_{ν}.

The vierbein satisfies the compatibility condition:

$$\nabla_{\sigma}e^{a}_{\mu}=e^{a}_{\mu,\sigma}+(\omega_{\sigma})^{a}_{b}e^{b}_{\mu}-W^{\nu}_{\sigma\mu}e^{a}_{\nu}=0,$$

where ω_{σ} is the NGT spin connection verifying the following hermiticity condition:[11]

$$(\tilde{\omega}_{\sigma})^{ab}=-(\omega_{\sigma})^{ba}.$$

Notice that in this holonomic coordinates, the curvature tensor $R^{\lambda}_{\sigma\mu\nu}$ is given by[11]

$$R^{\lambda}_{\sigma\mu\nu}=e^{\lambda}_{a}e^{b}_{\sigma}(R_{\mu\nu})^{a}{}_{b},$$

with

$$(R_{\mu\nu})^{a}{}_{b}=(\omega_{\nu})^{a}{}_{b}-(\omega_{\mu})^{a}{}_{b}+[\omega_{\mu},\omega_{\nu}]^{a}{}_{b}.$$

In NCG one can generalize the basic notions of connection, curvature, and torsion. This construction is based on the definition of the metric as an internal product on the cotangent space $T^{*}(M)$ (M is a compact manifold),[8]

$$g:M\to\otimes^{2}T^{*}(M),\quad x\to g_{x}\in T^{*}_{x}(M).$$

By analogy to the algebra of differential forms $\Lambda(M)$ on a manifold M, one can construct from a unitary, associative and involutive algebra $\mathcal{A}$, a Z-graded differential algebra $\Omega(\mathcal{A})$ defined by

$$\Omega(\mathcal{A}):=n\geqslant 0\oplus\Omega^{n}(\mathcal{A}),$$

$$\Omega^{n}(\mathcal{A})=\left\{i\sum\ a_{0}^{(i)}da_{1}^{(i)}\ldots da_{n}^{(i)},\quad a_{0}^{(i)},a_{1}^{(i)},\ldots,a_{n}^{(i)}\in\mathcal{A}\right\},$$

where d is a differential operator:

$$d:\Omega^{n}(\mathcal{A})\to\Omega^{n+1}(\mathcal{A})$$

[here $\Omega^{0}(\mathcal{A})=\mathcal{A}$ and $\Omega^{n}(\mathcal{A})$ is a bilateral A-module].

A connection on a vector fiber bundle $\mathcal{E}$ is by definition a linear application ∇ such that[5]

$$\nabla:\mathcal{E}\to\Omega(\mathcal{A})\otimes_{A}\mathcal{E},$$

with the following property:

$$\nabla(a\sigma)=da\otimes\sigma+a\,\nabla\sigma,\quad\forall a\in\mathcal{A},\quad\forall\sigma\in\mathcal{E}.$$

For each $\mathcal{A}$-left module $\mathcal{E}$, one can define a differential form space by

$$\Omega^{0}(\mathcal{E}):=\Omega(\mathcal{A})\otimes_{A}\mathcal{E}.$$

The curvature of ∇ is given by[5]

$$R(\nabla)=-\nabla^{2}:\mathcal{E}\to\Omega^{2}(\mathcal{A})\otimes_{A}\mathcal{E},$$

with

$$R(\nabla)(a\sigma)=aR(\nabla)(\sigma),\quad\forall a\in A,\quad\forall\sigma\in\mathcal{E}.$$

It is worth mentioning that if $\mathcal{A}$ is involutive then $\Omega(\mathcal{A})$ is involutive too:

$$(da)^{*}=-d(a^{*}),\quad(\alpha\beta)^{*}=\beta^{*}\alpha^{*},\quad\forall a\in A,\quad\forall\alpha,\beta\in\Omega(\mathcal{A}).$$

A connection ∇ is said to be unitary if for $\sigma,\tau\in\mathcal{E}$ one has[5]

$$d\langle\sigma,\tau\rangle=\langle\nabla\sigma,\tau\rangle-\langle\sigma,\nabla\tau\rangle,$$

where $\langle\cdot/\cdot\rangle$ is a Hermitian internal product:

$$\langle \cdot / \cdot \rangle : \mathcal{E} \times \mathcal{E} \to \mathcal{A}.$$

In NCG, the notion of a geodesic distance on M is given by the K-cycles of the algebra $\mathcal{A}$.[6] We remind the reader that a K-cycle $(\mathcal{A}, \mathcal{H}, \rho, \mathcal{D}, \Gamma)$ is defined by the following:

(1) A separable Hilbert space $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$.
(2) A $*$-faithful representation ρ of $\mathcal{A}$ given by bounded operatos on $\mathcal{H}$.
(3) A self-adjoint operator $\mathcal{D}$ on $\mathcal{H}$ with the following properties:
(i) $[\mathcal{D}, \rho(a)] \in \mathrm{End}(\mathcal{H})$: a bounded operator on $\mathcal{H} (\forall a \in \mathcal{A})$.
(ii) The operator $\exp(-\varepsilon \mathcal{D}^2)$ is traceclass, $\forall \varepsilon > 0$.
(4) A self-adjoint operator Γ on $\mathcal{H}$ satisfying

$$\Gamma^* = \Gamma^{-1} = \Gamma, \{\Gamma, \mathcal{D}\} = 0, \quad \rho(a)\Gamma = \Gamma \rho(a), \quad \forall a \in \mathcal{A}.$$

Now, from a K-cycle, one can define an involutive representation π of $\Omega(\mathcal{A})$ as[5,6]

$$\pi(a_0 da_1 \ldots da_p) = \rho(a_0)[D, \rho(a_1)] \cdots [D, \rho(a_p)].$$

Then, we define the algebra of differential forms $\Omega_D(\mathcal{A}.)$ as

$$\Omega_D(\mathcal{A}.) := \pi(\Omega(A))/\pi(d \ \mathrm{Ker}\ \pi) = p \geqslant 0 \oplus \Omega_D^p(\mathcal{A}.),$$

$$\omega_D^p(\mathcal{A}.) := \pi(\omega^p(\mathcal{A}.))/\mathrm{Aux}^p,$$

where Aux^p is the space of auxiliary (junk forms) fields given by

$$\mathrm{Aux}^p) = \{\pi(d\omega) \in \pi(\Omega^p(\mathcal{A}.)); \ \ \omega(\omega) = 0 \ \ \text{and} \ \ \omega \in \Omega^{p-1}(\mathcal{A}.)\}.$$

This allows us to define a metric $\langle \cdot / \cdot \rangle$ as the internal product over the $\mathcal{A}$-left-module $\Omega_D^1(\mathcal{A}.)$ as[6]

$$\langle \cdot / \cdot \rangle : \Omega_D^1(\mathcal{A}) \times \Omega_D^1(\mathcal{A}) \to \mathcal{A}.$$

It is to be noted that $\Omega_D^1(\mathcal{A})$ plays the role of the cotangent space of the noncommutative space.[5]

Since $\Omega_D(\mathcal{A})$ is a Z-graded differential algebra, it can be used to define the connection ∇ on the cotangent space $\Omega_D^1(\mathcal{A})$:

$$\nabla : \Omega_D^1(\mathcal{A}) \to \Omega_D^1(\mathcal{A}) \otimes_A \Omega_D^1(\mathcal{A});$$

the curvature and the torsion are defined by

$$R(\nabla) = -\nabla^2 : \Omega_D^1(\mathcal{A}) \to \Omega_D^2(\mathcal{A}) \otimes_A \otimes_A \Omega_D^1(\mathcal{A})$$

and

$$T(\nabla) = d - m \circ \nabla : \nabla : \Omega_D^1(\mathcal{A}) \to \Omega_D^2(\mathcal{A}),$$

respectively. Here m denotes the forms product:

$$m : \Omega_D^1(\mathcal{A}) \times \Omega_D^1(\mathcal{A}) \to \Omega_D^2(\mathcal{A}), \quad (\omega, \eta) \to \omega, \eta, \quad \forall \omega, \eta \in \Omega_D^1(\mathcal{A}).$$

In order to get the Cartan structure equations, we suppose that $\Omega_D^1(\mathcal{A})$ is a trivial vector fiber space. Let $(E^A)_{1 \leqslant A \leqslant N}$ be a basis of the space $\Omega_D^1 \mathcal{A}$, and define $\Omega^{AB} \in \Omega_D^1(\mathcal{A})$ such that[5,7]

$$\nabla E^A = -B \sum \ \Omega^{AB} \otimes E^B, \quad A, B = 1, 2, \ldots, N.$$

The components R^{AB}, T^A of the curvature $R(\nabla)$ and the torsion $T(\nabla)$ are given by

$$R(\nabla)E^A = B\sum R^{AB}\otimes E^B, \quad A,B=1,2,...,N,$$

$$T^A = T(\nabla).E^A, \quad A=1,2,...,N.$$

Now, using the definition of $R(\nabla)$ and $T(\nabla)$, we get the (noncommutative) Cartan structure equations:[5,7]

$$R^{AB} = d\Omega^{AB} + C\sum \Omega^{AC}\Omega^{CB},$$

$$T^A = dE^A + B\sum \Omega^{AB}E^B.$$

III. GENERALIZED NONCOMMUTATIVE GEOMETRY APPROACH

In order to reformulate NGT in the context of NCG, we have to generalize the Dirac operator with the following form:[6]

$$D = \begin{pmatrix} \gamma^a\otimes E_a^\mu\partial_\mu\otimes 1 & \gamma^5\otimes M_{12}\otimes K_{12} \\ \gamma^5\otimes M_{21}\otimes K_{21} & \gamma^a\otimes E_a^\mu\partial_\mu\otimes 1 \end{pmatrix} = \begin{pmatrix} \gamma^a E_a^\mu\partial_\mu & \gamma^5 M_{12}K_{12} \\ \gamma^5 M_{21}K_{21} & \gamma^a E_a^\mu\partial_\mu \end{pmatrix}. \tag{1}$$

The diagonal elements of the Dirac operator is a compact form which means

$$\gamma^a\otimes E_a^\mu\partial_\mu\otimes 1 = \gamma^a e_a^\mu\partial_\mu\otimes M\otimes 1 + \gamma^a\tilde{e}_a^\mu\partial_\mu\otimes\tilde{M}\otimes 1,$$

with

$$M = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \tilde{M} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},$$

where E_a^μ is a 2×2 matrix characterizing the vierbein and defined by

$$E_a^\mu = (E_a^\mu)^* = E_a^{\mu *} = \begin{pmatrix} 0 & e_a^\mu \\ \tilde{e}_a^\mu & 0 \end{pmatrix}, \tag{2}$$

with M_{12}, M_{21} (resp., K_{12}, K_{21}) are 2×2 (resp., $N\times N$) matrices. It is worth mentioning that the γ^a's are the ordinary Dirac matrices in the flat four-dimensional space–time and are defined as[6]

$$\begin{gathered} \gamma^{a*} = -\gamma^a, \quad \{\gamma^a,\gamma^b\} = \gamma^a\gamma^b + \gamma^b\gamma^a = -2\delta^{ab}, \\ \gamma^{ab} = \tfrac{1}{2}[\gamma^a,\gamma^b], \quad \gamma^{(ab)} = \tfrac{1}{2}\{\gamma^a,\gamma^b\} = -\delta^{ab}. \end{gathered} \tag{3}$$

In order to have a self-adjoint Dirac operator as it is required to be, one has to set the conditions:

$$K_{21}^* = K_{12} = K \tag{4}$$

and

$$M_{12} = M_{21}^* = M. \tag{5}$$

Concerning the algebra $\mathcal{A}$, it is defined as

$$\mathfrak{a}=C^{\infty}_{\mathbb{R}}(X)\otimes(M_2(\mathbb{K})\oplus M_2(\mathbb{K}))=C^{\infty}_{\mathbb{R}}(X,M_2(\mathbb{K}))\oplus C^{\infty}_{\mathbb{R}}(X,M_2(\mathbb{K})), \tag{6}$$

$$\mathcal{A}=\{a^{(1)}+\alpha^{(2)};\alpha^{(i)}\in C^{\infty}_{\mathbb{R}}(X,M_2(\mathbb{K})),\ \ i=1,2\}, \tag{7}$$

with

$$C^{\infty}_{\mathbb{R}}(X,M_2(\mathbb{K}))=C^{\infty}_{\mathbb{R}}(X)\otimes M_2(\mathbb{K}),$$

where $C^{\infty}_{\mathbb{R}}(X)$ denotes the space of infinite differentiable real functions on a manifold X and $M_2(\mathbb{K})$ the set of 2×2 hyperbolic complex matrices. (We can state that the space X is a spin manifold, and replace the Dirac operator $e^{\mu}_a\partial_\mu$ by $e^{\mu}_a\nabla_\mu$, where $\nabla_\mu=\partial_\mu+\omega_\mu$ without changing the results. The reason is that the spin connection ω_μ commutes with the elements of the algebra $\mathcal{A}$.)

In what follows, we restrict ourselves to a subalgebra $\mathcal{B}$ of $\mathcal{A}$ such that

$$\mathcal{B}=\left\{\alpha\in\mathcal{A}/\alpha=\alpha^{(1)}+\alpha^{(2)},\alpha^{(i)}=\begin{pmatrix}a^{(i)} & 0\\ 0 & a^{(i)}\end{pmatrix},\quad a^{(i)}\in C^{\infty}_{\mathbb{R}}(X,\mathbb{K}),\quad i=1,2\right\}. \tag{8}$$

Then one can choose the following representation:

$$\pi(\alpha)=\pi(\alpha^{(1)}+\alpha^{(2)})=\begin{pmatrix}1\otimes\alpha^{(1)}\otimes 1 & 0\\ 0 & 1\otimes\alpha^{(2)}\otimes 1\end{pmatrix}=\begin{pmatrix}\alpha^{(1)} & 0\\ 0 & \alpha^{(2)}\end{pmatrix}. \tag{9}$$

The algebra acts by left multiplication on the following Hilbert space $\mathcal{H}$:[6]

$$\mathcal{H}=\mathcal{H}_1\mathcal{H}_2,$$

where

$$\mathcal{H}_i=L^2(S,dv)\otimes_R K^2\otimes_R K^N, \tag{10}$$

and R, K denote the rings of real and hyperbolic complex numbers, respectively and S is the spinors space, dv is the volume element on X.

For the 1-forms space denoted by $\Omega^1_D(\mathcal{B})$, one has as a representation,

$$\Omega^1_D(\mathcal{B})=\pi(\Omega^1(\mathcal{B}))=\left\{\pi(\omega)=\pi\left(i\sum\ \alpha_i\delta\beta_i\right)=i\sum\ \pi(\alpha_i)[D,\pi(\beta_i)]\right\}. \tag{11}$$

Straightforward calculations give

$$\pi(\omega)=\begin{pmatrix}\gamma^a E^{\mu}_a\omega^{(1)}_{\mu} & \gamma^5 K_{12}\Phi_{12}\\ \gamma^5 K_{21}\Phi_{21} & \gamma^a E^{\mu}_a\omega^{(2)}_{\mu}\end{pmatrix}, \tag{12}$$

where

$$\omega^{(m)}_{\mu}=i\sum\ \alpha^{(m)}_i\,\partial_\mu\beta^{(m)}_i,\quad m=1,2 \tag{13}$$

and

$$\Phi_{mn}=\phi_{mn}M_{mn}, \tag{14}$$

with

$$\phi_{mn}=\sum_i\ (\alpha_i^{(m)}\beta_i^{(n)})-1,\quad m\neq n=1,2, \tag{15}$$

together with the normalization condition:

$$\sum_i\ \alpha_i^{(1)}\beta_i^{(1)}=\sum_i\ \alpha_i^{(2)}\beta_i^{(2)}=1. \tag{16}$$

Now, in order to get a representation $\Omega_D^2(\mathcal{B})$ of the 2-forms space $\Omega^2(\mathcal{B})$ without the junks forms (auxiliary fields), one has to set

$$\Omega_D^2(\mathcal{B})=\pi(\Omega_D^2(\mathcal{B}))/\mathrm{Aux}^2, \tag{17}$$

where Aux^2 is the space of the auxiliary fields defined as

$$\mathrm{Aux}^2=\{\pi(\delta\omega)/\pi(\omega)=0\},\quad \omega\in\Omega^1(\mathcal{B}), \tag{18}$$

with

$$\pi(\delta\omega)=i\sum\ \pi(\delta\alpha_i\,\delta\beta_i)=i\sum\ [D,\pi(\alpha_i)][D,\pi(\beta_i)]. \tag{19}$$

Direct but lengthy calculations lead to

$$\pi(\delta\omega)_{11}=\gamma^a\gamma^bE_a^\mu E_b^\nu(\partial_\mu\omega_\nu^{(1)}-X_{\mu\nu}^{(1)})+K_{12}K_{21}M_{12}M_{21}(\phi_{12}+\phi_{21}),$$

$$\pi(\delta\omega)_{22}=\gamma^a\gamma^bE_a^\mu E_b^\nu(\partial_\mu\omega_\nu^{(2)}-X_{\mu\nu}^{(2)})+K_{21}K_{12}M_{21}M_{12}(\phi_{21}+\phi_{12}),$$

$$\pi(\delta\omega)_{12}=K_{12}\gamma^a\gamma^5(E_a^\mu M_{12}(\partial_\mu\phi_{12}+\omega_\mu^{(1)})-M_{12}E_a^\mu\omega_\mu^{(2)}-[E_a^\mu,M_{12}]Y_\mu^{(12)}),$$

$$\pi(\delta\omega)_{21}=K_{21}\gamma^a\gamma^5(E_a^\mu M_{21}(\partial_\mu\phi_{21}+\omega_\mu^{(2)})-M_{21}E_a^\mu\omega_\mu^{(1)}-[E_a^\mu,M_{21}]Y_\mu^{(21)}),$$

where the hyperbolic complex functions $X_{\mu\nu}^{(m)}$ and $Y_\mu^{(mn)}$ are given by

$$X_{\mu\nu}^{(m)}=i\sum\ \alpha_i^{(m)}\partial_\mu\,\partial_\nu\beta_i^{(m)},\quad m=1,2,$$

and

$$Y_\mu^{(mn)}=i\sum\ \alpha_i^{(m)}\,\partial_\mu\beta_i^{(n)},\quad m\neq n=1,2. \tag{20}$$

After some simplifications, we obtain the following expression for Aux^2:

$$\mathrm{Aux}^2=\begin{pmatrix}\gamma^a\gamma^bE_a^\mu E_b^\nu X_{\mu\nu}^{(1)} & K\gamma^a\gamma^5[E_a^\mu,M_{12}]Y_\mu\\ K^*\gamma^a\gamma^5[E_a^\mu,M_{21}]Z_\mu & \gamma^a\gamma^bE_a^\mu E_b^\nu X_{\mu\nu}^{(2)}\end{pmatrix}, \tag{21}$$

where $X_{\mu\nu}^{(1)}=X_{\nu\mu}^{(1)}$, $X_{\mu\nu}^{(2)}=X_{\nu\mu}^{(2)}$, Y_μ,Z_μ are arbitrary hyperbolic complex functions.

The curvature tensor $R^{AB}(A,B=\overline{1,5})$ is defined by[6,7]

$$R^{AB}=d\Omega^{AB}+C\sum\ \Omega^{AC}\Omega^{CB}, \tag{22}$$

where the components of the connection $\Omega^{AB}\in\Omega_D^1(\mathcal{B})$ are given by

$$(\Omega^{AB})_{mn}=\gamma^a E_a^\mu \omega_\mu^{(m)AB},\quad m=1,2,$$
$$(\Omega^{AB})_{mn}=\gamma^5 K_{mn} M_{mn}^{AB}\phi_{mn},\quad m\neq n=1,2. \tag{23}$$

Setting

$$M_{12}=\begin{pmatrix}0&1\\0&0\end{pmatrix},\quad M_{21}=M_{12}^*=\begin{pmatrix}0&0\\1&0\end{pmatrix},\quad \tau=\begin{pmatrix}1&0\\0&0\end{pmatrix},\quad \overline{\tau}=\begin{pmatrix}0&0\\0&1\end{pmatrix} \tag{24}$$

and

$$E_a^\mu E_b^\nu=\eta_{ab}^{\mu\nu}\mathbf{1}-\varepsilon g_{ab}^{\mu\nu}\tau_3, \tag{25}$$

with:

$$\eta_{ab}^{\mu\nu}=(\alpha_a^\mu\alpha_b^\nu-\beta_a^\mu\beta_b^\nu)=+\eta_{ba}^{\nu\mu},$$
$$g_{ab}^{\mu\nu}=\alpha_a^\mu\beta_b^\nu-\beta_a^\mu\alpha_b^\nu=-g_{ba}^{\nu\mu},$$
$$\tau-\overline{\tau}=\tau_3,$$

and

$$\alpha_a^\mu=\tfrac{1}{2}(e_a^\mu+\tilde{e}_a^\mu),$$
$$\beta_a^\mu=\tfrac{1}{2}\varepsilon(e_a^\mu-\tilde{e}_a^\mu),$$

we obtain the following expressions for the component of R^{AB}:

$$R_{11}^{AB}=\tfrac{1}{2}(\gamma^{ab}\eta_{ab}^{\mu\nu}\mathbf{1}+\varepsilon g_{ab}^{\mu\nu}\delta_{ab}\tau_3)R_{\mu\nu}^{(1)AB}-\tfrac{1}{2}(\mathrm{Tr}(K.K^*)-2(K.K^*)\tau)H_{12}^{AB},$$
$$R_{22}^{AB}=\tfrac{1}{2}(\gamma^{ab}\eta_{ab}^{\mu\nu}\mathbf{1}+\varepsilon g_{ab}^{\mu\nu}\delta_{ab}\tau_3)R_{\mu\nu}^{(2)AB}-\tfrac{1}{2}(\mathrm{Tr}(K.K^*)-2(K^*.K)\overline{\tau})H_{21}^{AB},$$
$$R_{12}^{AB}=\tfrac{1}{2}K.\gamma^a\gamma^5\tilde{e}_a^\mu(\nabla_\mu\phi_{12}^{AB}-(\phi_{12}^{AC}\omega_\mu^{(2)CB}+\omega^{(2)AB})),$$
$$R_{21}^{AB}=\tfrac{1}{2}K.^*\gamma^a\gamma^5 e_a^\mu(\nabla_\mu\phi_{21}^{AB}-(\phi_{21}^{AC}\omega_\mu^{(1)CB}+\omega_\mu^{(1)AB})),$$

where

$$R_{\mu\nu}^{(m)AB}=\partial_\mu\omega_\nu^{(m)AB}+C\sum\ \omega_\mu^{(m)AC}\omega_\nu^{(m)CB}-(\mu\leftrightarrow\nu)=-R_{\nu\mu}^{(m)AB},\quad m=1,2,$$
$$\gamma^{ab}=\tfrac{1}{2}[\gamma^a,\gamma^b],$$
$$H_{12}^{AB}=C\sum\ \phi_{12}^{AC}\phi_{21}^{CB}+\phi_{12}^{AB}+\phi_{21}^{AB},$$
$$H_{21}^{AB}=C\sum\ \phi_{21}^{AC}\phi_{12}^{CB}+\phi_{21}^{AB}+\phi_{12}^{AB},$$
$$\nabla_\mu\phi_{12}^{AB}=\partial_\mu\phi_{12}^{AB}+C\sum\ \omega_\mu^{(1)AC}\phi_{12}^{CB}+\omega_\mu^{(1)AB},$$

$$\nabla_\mu \phi_{21}^{AB} = \partial_\mu \phi_{21}^{AB} + C \sum \omega_\mu^{(2)AC} \phi_{21}^{CB} + \omega_\mu^{(2)AB}.$$

As for the torsion T^A $(A = \overline{1,5})$, it is defined by[6,7]

$$T^A = d\xi^A + B \sum \Omega^{AB}.\xi^B,$$

where the generators ξ^A are

$$\xi^a = \gamma^b E_b^\mu \tilde{e}_\mu^a \otimes \mathbf{1},$$

$$\xi^{a*} = -\gamma^b E_b^\mu e_\mu^a \otimes \mathbf{1} = -\tilde{\xi}$$

and

$$\xi^5 = \begin{pmatrix} 0 & \gamma^5 K M_{21} \\ -\gamma^5 K^* M_{21} & 0 \end{pmatrix} = -\xi^{5*} = -\tilde{\xi}^5.$$

Using the fact that

$$d\xi^a = \gamma^b \gamma^c E_b^\mu E_c^\nu \partial_\mu \tilde{e}_\nu^a \otimes \mathbf{1},$$

$$d\xi^5 = 0,$$

the components of T^A, which are orthogonal to the auxiliary fields space, take the form

$$(T^a)_{11} = (\gamma^{cd} \eta_{cd}^{\mu\nu} \mathbf{1} + \varepsilon g^{\mu\nu} \tau_3)(\partial_\mu \tilde{e}_\nu^a + \omega_\mu^{(1)ab} \tilde{e}_\nu^b) + \tfrac{1}{2}(\mathrm{Tr}(K.K^*) - 2(K.K^*)\tau)\phi_{12}^{a5},$$

$$(T^a)_{22} = (\gamma^{cd} \eta_{cd}^{\mu\nu} \mathbf{1} + \varepsilon g^{\mu\nu} \tau_3)(\partial_\mu \tilde{e}_\nu^a + \omega_\mu^{(2)ab} \tilde{e}_\nu^b) - \tfrac{1}{2}(\mathrm{Tr}(K.K^*) - 2(K^*.K)\overline{\tau})\phi_{21}^{a5},$$

$$(T^a)_{12} = +K.\gamma^d \gamma^5 \tilde{e}_d^\mu \omega_\mu^{(1)a5} - K\gamma^d \gamma^5 \tilde{e}_d^\mu (\omega_\mu^{(1)a5} + \tilde{e}_\mu^b \phi_{12}^{ab})\tau,$$

$$(T^a)_{21} = -K.^* \gamma^d \gamma^5 e_d^\mu \omega_\mu^{(2)a5} + K^* \gamma^d \gamma^5 e_d^\mu (\omega_\mu^{(2)a5} - \tilde{e}_\mu^b \phi_{21}^{ab})\overline{\tau},$$

and

$$(T^5)_{11} = (\gamma^{cd} \eta_{cd}^{\mu\nu} \mathbf{1} + \varepsilon g^{\mu\nu} \tau_3) \omega_\mu^{(1)5b} \tilde{e}_\nu^b + \tfrac{1}{2}(\mathrm{Tr}(K.K^*) - 2(K.K^*)\tau)\phi_{12}^{55},$$

$$(T^5)_{22} = (\gamma^{cd} \eta_{cd}^{\mu\nu} \mathbf{1} + \varepsilon g^{\mu\nu} \tau_3) \omega_\mu^{(2)5b} \tilde{e}_\nu^b - \tfrac{1}{2}(\mathrm{Tr}(K.K^*) - 2(K^*.K)\overline{\tau})\phi_{21}^{55},$$

$$(T^5)_{12} = K\gamma^d \gamma^5 \tilde{e}_d^\mu \omega_\mu^{(1)55} - K\gamma^d \gamma^5 \tilde{e}_d^\mu (\omega_\mu^{(1)55} + \tilde{e}_\mu^b \phi_{12}^{5b})\tau,$$

$$(T^5)_{21} = -K^* \gamma^d \gamma^5 e_d^\mu \omega_\mu^{(2)55} + K^* \gamma^d \gamma^5 e_d^\mu (\omega_\mu^{(2)55} - \tilde{e}_\mu^b \phi_{21}^{5b})\overline{\tau}.$$

IV. THE NEW NGT ACTION

In order to get the action $\mathfrak{I}$, one has to use the following form:[5]

$$\mathfrak{I} = \tfrac{1}{2}(E^A E^{B*} - E^{B*} E^A, R^{BA}), \tag{26}$$

where $(,)$ denotes the generalized scalar product defined as

$$(E^A E^{B*} - E^{B*} E^A, R^{BA}) = \int d^4x \sqrt{e\tilde{e}}\ \mathrm{Tr}_K \cdot \mathrm{tr}((E^B E^{A*} - E^{A*} E^B) R^{BA}), \tag{27}$$

and (Tr_K) is the trace over the K matrices, while (tr) is the trace over the Clifford algebra. The E^A's are the generators of a subspace of the 1-form space $\Omega^1_D(A)$ defined by

$$\pi(\omega) = i \sum \pi(\alpha_i)[D, \pi(\beta_i)], \tag{28}$$

with

$$\alpha_i \in A, \quad \beta_i \in \mathcal{B}, \alpha_i = \alpha_i^{(1)} \oplus \alpha_i^{(2)}, \quad \beta_i = \beta_i^{(1)} \oplus \beta_i^{(2)}.$$

After some simplifications, one obtains

$$\pi(\omega) = \begin{pmatrix} \gamma^a \omega_\mu^{(1)} E_a^\mu & \gamma^5 K \Phi_{12} M_{12} \\ \gamma^5 K^* \Phi_{21} M_{12} & \gamma^a \omega_\mu^{(2)} E_a^\mu \end{pmatrix}, \tag{29}$$

where now the generators of this subspace are expressed by

$$E^a = \gamma^b e_\mu^a \tau E_b^\mu \otimes \mathbf{1} = \gamma^a M_{12} \otimes \mathbf{1},$$

$$\tilde{E}^a = \gamma^b \tilde{e}_\mu^a \overline{\tau} E_b^\mu \otimes \mathbf{1} = \gamma^a M_{21} \otimes \mathbf{1},$$

$$E^5 = \begin{pmatrix} 0 & \gamma^5 K M_{12} \\ -\gamma^5 K^* M_{21} & 0 \end{pmatrix} = \tilde{E}^5.$$

It is worth mentioning that if we use the generators ξ^A of the space $\Omega^1_D(\mathcal{B})$,

$$\xi^a = \gamma^b E_b^\mu \tilde{e}_\mu^a \otimes \mathbf{1} = \begin{pmatrix} 0 & \gamma^b e_b^\mu \tilde{e}_\mu^a \\ \gamma^a & 0 \end{pmatrix} \otimes \mathbf{1},$$

to define the action, we get two contributions to the action: one coming from the term $\gamma^b \tilde{e}_b^\mu \tilde{e}_\mu^a = \gamma^a$ and which gives the NGT action, and the other one from the term $\gamma^b e_b^\mu \tilde{e}_\mu^a$ giving a meaningless contribution. This is however not the case for the generators E^A where the matrix $\tau = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$ in the expression of E^a ensures the absence of such terms in the action.

According to the above mentioned remark, we cannot use only the algebra $\mathcal{B}$ because we need the generators E^A to define the action, which are elements of the space $\Omega^1_D(\mathcal{A})$. Also we can use only the algebra $\mathcal{A}$, but because the matrix E_a^μ in the Dirac operator does not commute with the elements of the algebra $\mathcal{A}$, this will give a complicated expression for the space of 1- and 2-forms, and the elimination of the auxiliary fields will be very tedious. Then, in order to get the usual expression for the tensor $R_{\mu\nu}^{(m)ab}$, we must impose that the connection forms Ω^{AB} lie in the space $\Omega^1_D(\mathcal{B})$. This is why we have used the algebra $\mathcal{B}$ to define the space of 1- and 2-forms, the curvature tensor, the torsion, and using the algebra $\mathcal{A}$ to define the generators E_a^μ.

Using the generalized scalar product (0.27), the equation (26) is rewritten as

$$\begin{aligned} \mathfrak{I} = \int d^4x \sqrt{e\tilde{e}} \Big\{ & -\frac{1}{2}(2\eta_{ab}^{\mu\nu} - \varepsilon \delta_{ab} g^{\mu\nu})(R_{\mu\nu}^{(1)ba} + R_{\mu\nu}^{(2)ba}) + \frac{1}{2}\mathrm{Tr}(K.K^*)(\phi_{12}^{aB}\phi_{21}^{Ba} - \phi_{21}^{aB}\phi_{12}^{Ba}) \\ & + \frac{1}{2}\mathrm{Tr}(K.K^*)\tilde{e}_a^\mu(\nabla_\mu \phi_{12}^{a5} - \phi_{12}^{aB}\omega_\mu^{(2)B5} - \omega_\mu^{(2)a5}) \\ & + \frac{1}{2}\mathrm{Tr}(K.K^*)e_a^\mu(\nabla_\mu \phi_{21}^{5a} - \phi_{21}^{5B}\omega_\mu^{5B}\omega_\mu^{(1)Ba} - \omega_\mu^{(1)5a}) \Big\}. \end{aligned}$$

Imposing the weak conditions

$$\mathrm{Tr}_k(T^a)=0, \quad T^5\neq 0,$$

where Tr denotes the trace over $K^2\otimes K^N$, one gets the following constraints:

$$\omega_\mu^{(1)ab}=\omega_\mu^{(2)ab}, \tag{30}$$

$$\omega_\mu^{(2)a5}=\omega_\mu^{(2)5a}=\omega_\mu^{(1)a5}=\omega_\mu^{(1)5a}=0, \tag{31}$$

$$\phi_{12}^{ab}=\phi_{21}^{ab}=0, \tag{32}$$

$$\phi_{12}^{a5}=\phi_{21}^{5a}\Rightarrow\phi_{21}^{5a}=\phi_{12}^{5a}. \tag{33}$$

Moreover, by making use of the fact that T^A must be orthogonal to the space Aux^2, we get the following relations:

$$\begin{aligned}
&\omega_\mu^{(2)a5}-\tilde{e}_\mu^b\phi_{21}^{ab}=0,\\
&\omega_\mu^{(1)a5}+\tilde{e}_\mu^b\phi_{12}^{ab}=0,\\
&\omega_\mu^{(2)55}-\tilde{e}_\mu^b\phi_{21}^{5b}=0,\\
&\omega_\mu^{(1)55}+\tilde{e}_\mu^b\phi_{12}^{5b}=0,
\end{aligned} \tag{34}$$

which allows us to express the ϕ_{mn}^{Ab} fields in terms of the $\omega_\mu^{(m)A5}$ fields in the action.

Taking into account both the compatibility and the unitarity conditions:

$$\begin{aligned}
&\nabla_\sigma\tilde{e}_\mu^a=\partial_\sigma\tilde{e}_\mu^a+\omega_\sigma^{ab}\tilde{e}_\mu^b-W_{\sigma\mu n}^\lambda\tilde{e}_\lambda^a=0,\\
&(\Omega^{AB})^*=\Omega^{BA},
\end{aligned} \tag{35}$$

we end up with

$$\tilde{\omega}_\mu^{(1)AB}=-\omega_\mu^{(1)BA}, \quad \tilde{\omega}_\mu^{(2)AB}=-\omega_\mu^{(2)BA},$$

$$\tilde{\phi}_{12}^{AB}=\phi_{21}^{BA}, \quad \tilde{\phi}_{21}^{AB}=\phi_{12}^{BA}, \quad \tilde{R}_{\mu\nu}^{AB}=-R_{\mu\nu}^{BA}.$$

Using these various constraints, the action takes the simplified form

$$\mathfrak{I}=\int d^4x\sqrt{e\tilde{e}}\,\mathfrak{L},$$

with

$$\mathfrak{L}=G^{\mu\nu}R_{\mu\nu}-\varepsilon g_{ab}^{\mu\nu}R_{\mu\nu}^{ba}+\tfrac{1}{4}\,\mathrm{Tr}(K.K^*)(G^{(\mu\nu)}W_\mu W_\nu+G^{[\mu\nu]}\partial_\mu W_\nu). \tag{36}$$

Notice that one can also add the following cosmological term J to the action (2.37):

$$J=\frac{\alpha}{2}(E^AE^{B^*}-E^{B^*}E^A,\xi^A\xi^{B^*}), \tag{37}$$

which becomes after simple calculations,

$$J=\alpha\int \sqrt{e\tilde{e}}d^4x(-2G^{[\mu\nu]}G_{[\mu\nu]}-2\ \mathrm{Tr}(K\cdot K^*)-8-G^{\mu\nu}_{ab}G^{ab}_{\nu\mu}). \tag{38}$$

Here α is an arbitrary constant.

Consequently, the total NGT action takes the following form:

$$\mathfrak{I}_{\mathrm{NGT}}=\int d^4x\sqrt{e\tilde{e}}\mathfrak{L}_{\mathrm{NGT}},$$

with

$$\mathfrak{L}_{\mathrm{NGT}}=\mathfrak{L}_{\acute{g}\mathrm{eom}}+\mathfrak{L}_{\mathrm{skew}}+\mathfrak{L}_c+\mathfrak{L}_W,$$

where

$$\text{Body Math}\quad \mathfrak{L}_{\mathrm{geom}}=G^{\mu\nu}R_{\mu\nu}-\tfrac{1}{4}\mathrm{Tr}(K\cdot K^*)G^{[\mu\nu]}W_{[\mu,\nu]}-\varepsilon g^{\mu\nu}_{ab}R^{ba}_{\mu\nu},$$

$$\text{Body Math}\quad \mathfrak{L}_W=\tfrac{1}{4}\mathrm{Tr}(K\cdot K^*)G^{(\mu\nu)}W_\mu W_\nu,$$

$$\text{Body Math}\quad \mathfrak{L}_{\mathrm{skew}}=-2\alpha G^{[\mu\nu]}G_{[\mu\nu]},$$

$$\text{Body Math}\quad \mathfrak{L}_c=-2\alpha\,\mathrm{Tr}(K\cdot K^*)-8\alpha-\alpha G^{\mu\nu}_{ab}G^{ab}_{\nu\mu},$$

and $G^{(\mu\nu)}$ (resp., $G^{[\mu\nu]}$) is the symmetric (resp., antisymmetric) part of $G^{\mu\nu}$. Notice that if one redefines the connection W_μ such that

$$(\tfrac{2}{3}-\tfrac{1}{4}\mathrm{Tr}(K\cdot K^*))W_\mu=\tfrac{2}{3}\overline{W}_\mu, \tag{39}$$

and using the fact that[12,13]

$$R_{\mu\nu}(W)=R_{\mu\nu}(\Gamma)+\tfrac{2}{3}W_{[\mu,\nu]}, \tag{40}$$

one obtains the following geometrical term $\mathfrak{L}_{\mathrm{geom}}$:

$$\mathfrak{L}_{\mathrm{geom}}=G^{\mu\nu}R_{\mu\nu}(\overline{W})-\varepsilon g^{\mu\nu}_{ab}R^{ba}_{\mu\nu},$$

where $\overline{W}^{\lambda}_{\mu\nu}$ is defined as

$$\overline{W}^{\lambda}_{\mu\nu}=\Gamma^{\lambda}_{\mu\nu}-\tfrac{2}{3}\delta^{\lambda}_{\mu}\overline{W}_\nu. \tag{41}$$

Setting $x=-\mathrm{Tr}(K\cdot K^*)$, one can write

$$\mathfrak{L}_W=\tfrac{1}{4}\mathrm{Tr}(K\cdot K^*)G^{(\mu\nu)}W_\mu W_\nu=-f(x)G^{(\mu\nu)}\overline{W}_\mu\overline{W}_\nu, \tag{42}$$

where

$$f(x)=\frac{1}{9}\frac{x}{(\frac{2}{3}+\frac{1}{4}x)^2}. \tag{43}$$

Now, it is worth mentioning that the term $\mathfrak{L}_W$ used in the Moffat's NGT Lagrangian has the form

$$\mathfrak{L}_W=\tfrac{1}{2}\sigma G^{(\mu\nu)}\overline{W}_\mu\overline{W}_\nu, \tag{44}$$

where σ was taken in an *ad-hoc* fashion to be equal to $-1/3$ for consistency with physics.

Notice that in our model, this value of σ comes out rather naturally since $1/2\sigma$ corresponds to the maximum of the $f(x)$ interaction coefficient.

V. CONCLUSIONS

In this work, we have been able to reformulate NGT in the formalism of noncommutative geometry without recourse to an additional scalar field (as it is the case for General Relativity). Moreover, all the terms which were put by hand by Moffat in his modified NGT action for physics consistency, were derived explicitly in our theory, with the added benefit of gaining some deeper geometrical insight. In particular, we have been able to attach a geometrical meaning to the coupling constant:

$$\mathfrak{L}_W = -f(x)G^{(\mu\nu)}\overline{W}_\mu\overline{W}_\nu,$$

where the value which maximizes our $f(x)$ corresponds exactly to the one chosen by Moffat.

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Friedmann limits of rotating hypersurface–homogeneous dust models

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The existence of Friedmann limits is systematically investigated for all the hypersurface–homogeneous rotating dust models, presented in previous papers by this author. Limiting transitions that involve a change of the Bianchi type are included. Except for stationary models that obviously do not allow it, the Friedmann limit expected for a given Bianchi type exists in all cases. Each of the three Friedmann models has parents in the rotating class; the $k=+1$ model has just one parent class, the other two each have several parent classes. The type IX class is the one investigated in 1951 by Gödel. For each model, the consecutive limits of zero rotation, zero tilt, zero shear, and spatial isotropy are explicitly calculated. [DOI: 10.1063/1.1378304]

I. MOTIVATION AND SUMMARY OF THE METHOD

In previous papers[1–3] a complete set of all metric forms was derived that can represent hypersurface–homogeneous rotating dust models. For each case, the generators of the symmetry algebra were found, the Bianchi type determined, and the metric form resulting from the Killing equations was explicitly presented. That classification was more detailed than the Bianchi classification because all possible orientations of the symmetry orbits in the spacetime were allowed, i.e., the orbits could be spacelike, timelike or null.

In a later paper,[4] one of the Bianchi type V models was investigated. Among the problems considered there was the question whether the model can reproduce the $k=-1$ Friedmann model in the limit of zero rotation, $\omega\to 0$. Since the coordinates that are well-suited to the classification are not suitable at all for considering the limit $\omega\to 0$, this limit could be taken only after a coordinate change and reparametrization of the metric.

In the present paper, the existence of the Friedmann limits is systematically investigated for all the other cases found in the classification in Refs. 1–3. The Bianchi type is allowed to change in the limiting transition. In all Bianchi type I cases the velocity field is tangent to the symmetry orbits, i.e., those models have matter density constant along the flow, and no expanding Friedmann model can be a subcase there. The same is true for the Bianchi type II from Ref. 1 and for both the subcases of case 1.1.1.2 in Ref. 2 which are of type III. In all the other cases the Friedmann limits that can be expected for a given Bianchi type do indeed exist.

The specialization to the Friedmann metrics is possible in so many cases because there is a free parameter in them that determines the tilt of the orbits with respect to the velocity field (with various values of the tilt parameter, the orbits may be spacelike, timelike or null). Whenever a Friedmann limit exists, the orbits are made orthogonal to the velocity field (''untilted'') during the limiting transition.

In order to make this paper readable independently of the other ones, the basic facts are briefly recalled here. More details can be found in Ref. 1.

The velocity field of a rotating dust, u^α, defines three scalar functions $\tau(x), \eta(x)$ and $\xi(x)$ such that

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$$u_\alpha = \tau_{,\alpha} + \eta\xi_{,\alpha}. \tag{1.1}$$

These functions (whose existence follows from the equations of motion via the Darboux theorem[1]) are determined up to the transformations:

$$\tau = \tau' - S(\xi', \eta'), \quad \xi = F(\xi', \eta'), \quad \eta = G(\xi', \eta'), \tag{1.2}$$

where the functions F and G obey

$$F_{,\xi'}G_{,\eta'} - F_{,\eta'}G_{,\xi'} = 1, \tag{1.3}$$

and then S is determined by

$$S_{,\xi'} = GF_{,\xi'} - \eta', \quad S_{,\eta'} = GF_{,\eta'}. \tag{1.4}$$

[Eq. (1.3) is the integrability condition of (1.4).]

Then, the continuity equation, $(nu^\alpha)_{;\alpha} = 0$, where n is the number density of the dust particles, implies that there exists one more function $\zeta(x)$ such that

$$\sqrt{-g}nu^\alpha = \varepsilon^{\alpha\beta\gamma\delta}\xi_{,\beta}\eta_{,\gamma}\zeta_{,\delta}, \tag{1.5}$$

where g is the determinant of the metric tensor and $\varepsilon^{\alpha\beta\gamma\delta}$ is the Levi-Civita symbol. The function ζ is determined up to the transformations

$$\zeta = \zeta' + T(\xi', \eta'), \tag{1.6}$$

where T is an arbitrary function.

The following relations hold then:

$$\begin{gathered} u^\alpha\tau_{,\alpha} = 1, \quad u^\beta\xi_{,\beta} = u^\beta\eta_{,\beta} = u^\beta\zeta_{,\beta} = 0, \\ \frac{\partial(\tau, \eta, \xi, \zeta)}{\partial(x^0, x^1, x^2, x^3)} = \sqrt{-g}n \neq 0. \end{gathered} \tag{1.7}$$

This shows that $\{\tau, \xi, \eta, \zeta\}$ can be chosen as coordinates, with τ being the time coordinate. They are called the Plebański coordinates. Denoting $\{\tau, \xi, \eta, \zeta\} = \{x^0, x^1, x^2, x^3\} = \{t, x, y, z\}$, we obtain for the velocity field u^α, the metric tensor $g_{\alpha\beta}$, the rotation tensor $\omega_{\alpha\beta}$ and the rotation vector w^α in these coordinates

$$\begin{gathered} u_\alpha = \delta^\alpha{}_0, \quad u_\alpha = \delta^0{}_\alpha + y\,\delta^1{}_\alpha, \\ g_{00} = 1, \quad g_{01} = y, \quad g_{02} = g_{03} = 0, \quad g \equiv \det(g_{\alpha\beta}) = -n^{-2}, \\ w^\alpha = n\,\delta^\alpha_3, \quad \omega_{\alpha\beta} = -\omega_{\beta\alpha} = \tfrac{1}{2}\,\delta^1{}_\alpha\delta^2{}_\beta. \end{gathered} \tag{1.8}$$

It is the last property that makes the limiting transition $\omega \to 0$ impossible without a coordinate transformation and reparametrization.

In these coordinates, if any Killing field is allowed by the metric it must be of the form

$$k^\alpha = (C + \phi - y\,\phi_{,y})\,\delta^\alpha{}_0 + \phi_{,y}\delta^\alpha{}_1 - \phi_{,x}\delta^\alpha{}_2 + \lambda\,\delta^\alpha{}_3, \tag{1.9}$$

where C is an arbitrary constant and $\phi(x,y)$ and $\lambda(x,y)$ are arbitrary functions. If $\phi_{,\alpha} \neq 0$ (i.e., ϕ is not constant on an open set), then the coordinates can be adapted to k^α within the Plebański class [by Eqs. (1.2)–(1.4) and (1.6)] so that

$$k^\alpha = \delta^\alpha{}_1. \tag{1.10}$$

The metric then becomes independent of x, and the coordinates preserving (1.10) are determined up to the transformations:

$$t'=t-\int yH_{,y}dy+A, \quad x'=x+H(y), \quad y'=y, \quad z'=z+T(y), \tag{1.11}$$

where A is an arbitrary constant and H,T are arbitrary functions.

If $\phi_{,\alpha}=0$, then the form of the Killing field $k^\alpha=C\delta^\alpha{}_0+\lambda\delta^\alpha{}_3$, is invariant under (1.2)–(1.6) and the Plebański coordinates cannot be adapted to k^α. The property $\phi=$const is equivalent to the following invariant relation:

$$k^\alpha=Cu^\alpha+(\lambda/n)w^\alpha, \tag{1.12}$$

i.e., k^α is then spanned on the velocity field and the rotation field.

If three Killing fields exist, then each of them can either be of the special type (1.12) or of the general type (1.9). One of the general-type Killing fields can always be transformed to the form (1.10) by (1.2)–(1.6).

This observation gives rise to a complete classification of all hypersurface–homogeneous space–times that are possible for a rotating dust. When all three Killing fields are of the special type (1.12), the symmetry orbits are two-dimensional, and this case is not considered. When two Killing fields are of the special type, while the third one is general, there exist two classes of metrics (Bianchi types I and II) that were derived in Ref. 1. When one Killing field is of the special type, while the two others are general, all Bianchi types except VIII and IX appear (Ref. 2). When all three Killing fields are of the general type, all the Bianchi types appear, some of them hidden as limits of more general types (Ref. 3). The multitude of cases is a consequence of the many possible alignments or misalignments among the three Killing fields and the velocity and rotation fields.

When the Bianchi classification is introduced, the generators of symmetry are scaled to standard forms such that all nonzero structure constants (except the free parameters in types VI_h and VII_h) become equal either to $+1$ or to -1. In general, though, they are arbitrary constants, and in the general form each of those constants can be allowed to become zero. In this way, the more special Bianchi types can be obtained from the more general ones by going to the zero limit with some of the structure constants. The resulting hierarchy of Bianchi types is well-known, and is shown in Fig. 1 (adapted from Ref. 5) for easy reference. The specializations that are possible can be instantly guessed from the values of the a, n_1, n_2, and n_3 parameters for the different Bianchi types. Type III cannot be specialized to IV or V because, with the arbitrary values of the parameters n_2 and n_3, the parameter a is determined by $a=\sqrt{-n_2n_3}$.

Another well-known result[6] is the placement of different Robertson–Walker geometries within the Bianchi classes. This is also recalled for easy reference. Since we are considering only dust models, we will call these geometries the Friedmann models and Friedmann limits of the rotating models.

The $k=0$ model is a subcase of the Bianchi types I and VII_0 (the two Bianchi algebras have different bases, but share common orbits).

The $k=-1$ model is a subcase of the Bianchi types V and VII_h.

The $k=+1$ model is a subcase of the Bianchi type IX.

When considering each case of the classification from Refs. 1–3, one has to recognize from Fig. 1 which of the four types {I, V, VII_0, VII_h, IX} could possibly be contained in it as a subcase and then the appropriate specialization of the arbitrary constants and functions in the model has to be considered. This procedure will be presented in more detail in Sec. II, later it will be applied without detailed explanations.

It will turn out that only the stationary models have no Friedmann limit. In every nonstationary case, the Friedmann limit indicated by the Bianchi type indeed exists. Note that the limits are found for the metrics, without taking into account the Einstein equations. This is why a nonsta-

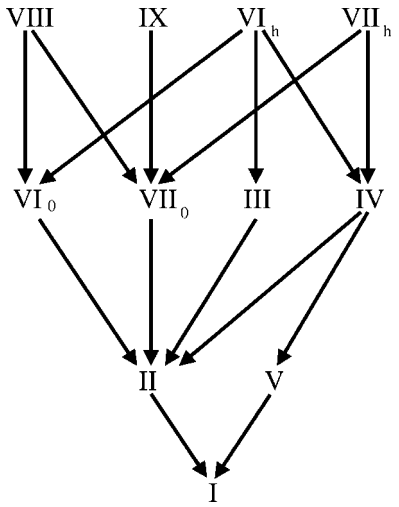

FIG. 1. The diagram shows how the different Bianchi types can be specialized by taking the zero limit of one or more of the structure constants. This allows to recognize (by the rules given at the end of Sec. I), which Friedmann models can possibly be contained as limits in a given class—see text. All the possibilities are actually realized in the collection considered in the paper.

tionary type II metric exists in the collection, and is found to admit the $k=0$ Friedmann limit, even though it is known[7,8] that spatially homogeneous type II dust solutions must have zero rotation, see Sec. III.

Now we shall systematically go over all the cases presented in Refs. 2 and 3. The two cases from Ref. 1 are immediately seen to admit no Friedmann limit: In both of them, the velocity field of the dust is spanned on the Killing fields [see Eqs. (7.7) and (7.8) in Ref. 1], so the particle number density n will obey $n_{,\alpha}u^{\alpha}=0$. Hence, these cases cannot contain any expanding Friedmann model because in the latter $n_{,\alpha}u^{\alpha}\neq 0$.

Each of the models presented in Refs. 2 and 3 that allows a Friedmann limit will be first transformed to the Plebański coordinates (most of them were found in coordinates adapted to the Killing fields that are not in the Plebański class). Then, each model will be transformed by a coordinate transformation and reparametrization of the metric functions and constants to such a form in which the limit of zero rotation can be calculated explicitly. Then, the Friedmann limits will be calculated by consecutively imposing on the metric the conditions of zero rotation, zero tilt, zero shear, and spatial isotropy (i.e., constant curvature in the three-spaces orthogonal to the dust flow). This last condition is not superfluous, even though dust with zero rotation and zero shear must be a Friedmann model in consequence of the Einstein equations.[9] It is conceivable that no Friedmann limit would exist at all in some classes. However, this does not happen, and a spatially isotropic subcase will be found to exist in all cases. The corresponding limits of the Killing fields, where nontrivial, will be also calculated and the Bianchi type of the limit determined.

Since on each of the underlying manifolds five vector fields exist (velocity, rotation, and the three Killing fields), the five vectors must be linearly dependent at each point. This linear relation allows to identify in each case the parameter that determines the tilt of the velocity field with respect to the symmetry orbits—see Sec. V. It turns out that this tilt parameter is always simply proportional to that defined by King and Ellis.[8]

II. THE CASES 1.1.1 OF REF. 2

We begin with case 1.1.1.1., which is of Bianchi type III.

The transformation from the coordinates used in Eq. (2.18) of Ref. 2 (that were adapted to the Killing fields) to the Plebański coordinates is given by Eq. (2.16) in Ref. 2 (where $\{t',x',Y,Z\}$ are

the coordinates of (2.18), and $\{t,x,y,z\}$ are the Plebański coordinates). The transformed metric is

$$
\begin{gathered}
g_{00}=1, \quad g_{01}=y, \quad g_{02}=g_{03}=0, \\
g_{11}=\left(\frac{Y}{2\lambda_3}\right)^2+\frac{1}{2\lambda_3^2}YZ+h_{11}-\frac{b}{\lambda_3}h_{12}Y+\left(\frac{1}{2}bY\right)^2 h_{22}, \\
g_{12}=h_{12}-\tfrac{1}{2}b\lambda_3 Y h_{22}, \quad g_{13}=C_3 h_{13}-\tfrac{1}{2}b^2 C_3 Y h_{23}, \\
g_{22}=\lambda_3^2 h_{22}, \quad g_{23}=bC_3\lambda_3 h_{23}, \quad g_{33}=(bC_3)^2 h_{33},
\end{gathered}
\tag{2.1}
$$

where b, C_3 and λ_3 are arbitrary constants, Y and Z are given by:

$$
Y=-b\lambda_3 t+\lambda_3 y+bC_3 z, \quad Z=b\lambda_3 t+\lambda_3 y-bC_3 z, \tag{2.2}
$$

and all the h_{ij}, $i,j=1,2,3$ are arbitrary functions of Z. The first line of Eq. (2.1) will be the same in all the other metrics transformed to the Plebański coordinates, so it will not be repeated from now on. Since the argument of h_{ij} is determined (by the Killing equations) only up to a constant factor, we are allowed to rescale it by an arbitrary factor. For considering the limit $\omega\to 0$, it will be convenient to assume that the argument of h_{ij} is

$$
T:=Z/(b\lambda_3)=t+y/b-(C_3/\lambda_3)z. \tag{2.3}
$$

This presupposes that $b\lambda_3\neq 0$, but this condition is included in the definition of case 1.1.1.1. The limit $\lambda_3=0$ can be taken into account after a simple reparametrization, and it leads to a stationary solution. The subcase $b=0$ is degenerate, and it belongs to the 1.1.2 family.

As seen from the last formula in (1.8), the simplest way to let $\omega\to 0$ is to transform y as follows:

$$
y=\omega_0\tilde{y}, \tag{2.4}
$$

and then let $\omega_0\to 0$, so that the only nonzero component of rotation in the new coordinates becomes

$$
\omega'_{12}=\omega_0\tilde{y}\xrightarrow[\omega_0\to 0]{}0. \tag{2.5}
$$

Then, however, the components g'_{12}, g'_{22}, and g'_{23} of the transformed metric would simultaneously go to zero, and the metric would become degenerate ($g=0$). To avoid this, h_{22} must be rescaled as follows:

$$
h_{22}=H_{22}/\omega_0^2. \tag{2.6}
$$

Then $g'_{12}=\omega_0 h_{12}-\frac{1}{2}b\lambda_3 Y H_{22}/\omega_0$ would become infinite in the limit $\omega_0\to 0$. To avoid this, h_{12} must be reset so that the infinity is cancelled. Since all h_{ij} depend on T, not on Y, this can be done as follows:

$$
h_{12}=H_{12}/\omega_0-\tfrac{1}{2}(b\lambda_3)^2 T H_{22}/\omega_0^2. \tag{2.7}
$$

The first term in (2.7) contains the ω_0 in the denominator for greater generality, so that $g'_{12}\xrightarrow[\omega_0\to 0]{}H_{12}\neq 0$. Then, to cancel the infinities in g_{11}, the function h_{11} must be reset as follows:

$$
h_{11}=H_{11}-\tfrac{1}{4}b^4(\lambda_3 T)^2 H_{22}/\omega_0^2-b^2 T h_{12}. \tag{2.8}
$$

The reparametrization (2.4), (2.6)–(2.8) would be sufficient to make the limit $\omega_0 \to 0$ of the metric (2.1) nondegenerate. However, the hypersurfaces $t = \text{const}$, that become orthogonal to the velocity field u^α in the limit $\omega_0 \to 0$, would not yet coincide with the hypersurfaces of constant matter density. In the Plebański coordinates, as seen from (1.8), the matter density obeys $g = -n^{-2}$, and so n would depend on $(t - C_3 z/\lambda_3)$ in the limit $\omega_0 \to 0$, i.e., the model would still be tilted. To untilt it, we must let $C_3 \to 0$, and this requires at least one more rescaling. It will be convenient to redefine C_3 as follows

$$C_3 = \omega_0 c, \tag{2.9}$$

so that the untilting occurs simultaneously with $\omega \to 0$. Then we must rescale h_{33}

$$h_{33} = H_{33}/\omega_0^2. \tag{2.10}$$

For greater generality, we will also rescale h_{23}

$$h_{23} = H_{23}/\omega_0^2, \tag{2.11}$$

and then h_{13} must be reset as follows:

$$h_{13} = H_{13}/\omega_0 - \tfrac{1}{2} b^3 \lambda_3 T H_{23}/\omega_0^2. \tag{2.12}$$

The transformation (2.4), applied to (2.1) together with all the subsequent reparametrizations, results in the following metric:

$$\begin{gathered}
g_{00} = 1, \quad g_{01} = \omega_0 \tilde{y}, \quad g_{02} = g_{03} = 0, \\
g_{11} = \frac{1}{4\lambda_3^2}[b\lambda_3 t(-2\lambda_3 \tilde{y} + 2bcz)\omega_0 + (\lambda_3 \tilde{y} + bcz)(3\lambda_3 \tilde{y} - bcz)\omega_0^2] \\
- \frac{1}{4}(bt)^2 + H_{11} - 2b\tilde{y} H_{12} + (b\lambda_3 \tilde{y})^2 H_{22}, \\
g_{12} = H_{12} - b\lambda_3^2 \tilde{y} H_{22}, \quad g_{13} = cH_{13} - b^2 c \lambda_3 \tilde{y} H_{23}, \\
g_{22} = \lambda_3^2 H_{22}, \quad g_{23} = bc\lambda_3 H_{23}, \quad g_{33} = (bc)^2 H_{33},
\end{gathered} \tag{2.13}$$

where the H_{ij} depend only on t. Here, similarly as in (2.1), the first line will be the same for every metric, and so it will not be repeated from now on.

The metric (2.13) still has nonzero shear. If a Friedmann model is to result from it, the shear must be set to zero. The coordinates $\{t,x,y,z\}$ in (2.13) are now comoving and synchronous, so zero shear means that

$$g_{ij} = G_{ij}(x,y,z) R^2(t), \tag{2.14}$$

i.e., all the components of the metric must depend on time only through the same factor $R^2(t)$. This means:

$$\begin{gathered}
H_{11}(t) = \tfrac{1}{4} b^2 t^2 - C_{11} R^2(t), \\
\text{other } H_{ij}(t) = -C_{ij} R^2(t),
\end{gathered} \tag{2.15}$$

where C_{ij} are unknown constants. With no loss of generality, it may be assumed that

$$C_{33} = 1. \tag{2.16}$$

The metric (2.13) with H_{ij} as in (2.15) and (2.16) will represent a Friedmann model when the hypersurfaces $t=\text{const}$ are spaces of constant curvature. In order to calculate this curvature, it is convenient to introduce the new constants D_{11}, D_{12}, and D_{22} by

$$D_{22}{}^2 := C_{22} - C_{23}{}^2, \quad D_{12} := (C_{12} - C_{13}C_{23}/b)/(\lambda_3 D_{22}),$$
$$D_{11}{}^2 := C_{11} - C_{13}{}^2/b^2 - D_{12}{}^2. \tag{2.17}$$

The correct signs for $D_{11}{}^2$ and $D_{22}{}^2$ are guaranteed by the signature of (2.13). Then (2.13) may be written as follows:

$$\begin{aligned} \mathrm{d}s^2 = {} & \mathrm{d}t^2 - (D_{11}R\,\mathrm{d}x)^2 - R^2[(D_{12} - b\lambda_3 D_{22}y)\mathrm{d}x + \lambda_3 D_{22}\mathrm{d}y]^2 \\ & - R^2[(C_{13}/b - b\lambda_3 C_{23}y)\mathrm{d}x + \lambda_3 C_{23}\mathrm{d}y + bc\,\mathrm{d}z]^2, \end{aligned} \tag{2.18}$$

and the curvature tensor for the spaces $t=\text{const}$ may be easily calculated using the orthonormal set of differential forms suggested by (2.18). The curvature tensor is

$$R^{12}{}_{12} = \tfrac{3}{4}F^2G^2 + F^2, \quad R^{13}{}_{13} = R^{23}{}_{23} = -\tfrac{1}{4}F^2G^2, \tag{2.19}$$

where

$$F := b/(D_{11}R), \quad G := C_{23}/D_{22}. \tag{2.20}$$

The Riemann tensor (2.19) will represent constant curvature when $R^{12}{}_{12} = R^{13}{}_{13}$. This implies $b=0$, which seems to be a singular limit of (2.18). However, the limit $b\to 0$ may be easily incorporated into (2.18) by the following reparametrization:

$$C_{13} = D_{13}b, \quad c = C/b. \tag{2.21}$$

After this, the Riemann tensor of the space $t=\text{const}$ still has the same form (2.19)–(2.20). With $b=0$, $R^{ij}{}_{kl} \equiv 0$, i.e., (2.18) represents then the $k=0$ Friedmann model. This is the Friedmann limit of the metric (2.1), as expected for Bianchi type III.

In this case, the coordinates of the Friedmann limit are similar to those usually used (they are the nonorthogonal Cartesian coordinates for the flat space $t=\text{const}$). This will not be so in most other cases—the coordinate representation of the resulting Friedmann limit will be rather exotic, and calculating the Riemann tensor of the subspace $t=\text{const}$ will be the simplest way to check that it is the Friedmann metric indeed.

The Killing fields for the metric (2.1) are (see Ref. 2)

$$k^\alpha_{(1)} = \delta^\alpha_1, \quad k^\alpha_{(2)} = \mathrm{e}^{bx}(\delta^\alpha_0 - b\,\delta^\alpha_2), \quad k^\alpha_{(3)} = C_3\delta^\alpha_0 + \lambda_3\delta^\alpha_3. \tag{2.22}$$

As seen from Fig. 1, the algebra of type III can be specialized only to types II and I, and so the $k=0$ Friedmann limit is the only one of the three that can be expected here. Note that the Killing field $k_{(2)}$ will have a meaningful limit $\omega\to 0$, $b\to 0$ only if the two limits are tuned so that $\omega_0/b \xrightarrow[\omega_0\to 0]{} 0$ (for example, $b = B\sqrt{\omega_0}$). Then $l^\alpha_{(2)} := (\omega_0/b)k^\alpha_{(2)} \xrightarrow[\omega_0\to 0]{} \delta^\alpha{}_2$, which is indeed a Killing field of (2.18) with $b=0$. The algebra $\{k_{(1)}, l_{(2)}, k_{(3)}\}$ becomes then Bianchi type I when $\omega_0 = 0$, as expected.

The reasoning behind the reparametrizations, and the subsequent calculation of the limits of zero rotation, zero tilt, zero shear, and constant curvature of the spaces $t=\text{const}$, follows the same scheme in all the other cases. Therefore, it will be presented in less detail from now on. In some of the cases, the reparametrization that untilts the limit $\omega\to 0$ is a necessary condition for cancelling the infinities introduced by the earlier reparametrizations.

The other two subcases of case 1.1.1 in Ref. 2, i.e., cases 1.1.1.2.1 [Eq. (3.16)] and 1.1.1.2.2 [Eq. (3.32)] are immediately seen to allow no Friedmann limit. For both of them, the Killing fields are given by (2.22) above with $\lambda_3=0$. As seen from (1.8), the Killing field $k_{(3)}$ coincides then with the velocity field of dust, and so both these models are stationary.

In fact, the last of (2.22) is the linear relation among the five vectors mentioned at the end of Sec. I, because it is equivalent to (1.12). Since with $\lambda_3=0$ the velocity becomes one of the Killing fields, i.e., becomes tangent to the symmetry orbits, λ_3 is the tilt parameter. More on this—see Sec. V.

III. CASES 1.1.2 OF REF. 2

The case 1.1.2.1 is again of Bianchi type III. The transformation back from the coordinates of Eq. (4.6) in Ref. 2 (adapted to two Killing fields) to the Plebański coordinates is given by (4.4) in Ref. 2, with the roles of $\{x^\alpha\}$ and $\{x'^\alpha\}$ interchanged. The transformed metric is

$$g_{11}=-2(c/a)y-(c/a)^2+Y^2h_{11}-2(c/a)\lambda_3 Yh_{13}+(c\lambda_3/a)^2h_{33},$$

$$g_{12}=h_{12}-\frac{c\lambda_3}{aY}h_{23},\quad g_{13}=C_3Yh_{13}-(c/a)\lambda_3C_3h_{33}, \tag{3.1}$$

$$g_{22}=h_{22}/Y^2,\quad g_{23}=C_3h_{23}/Y,\quad g_{33}=C_3^2h_{33},\quad Y:=ay+c,$$

where a, c and λ_3 are arbitrary constants and h_{ij} are arbitrary functions of the variable

$$T:=t-C_3z/\lambda_3. \tag{3.2}$$

The reparametrization that will allow setting the rotation and tilt to zero is

$$(y,C_3)=\omega_0(\tilde{y},D),$$

$$h_{11}=H_{11}+(\lambda_3/a)^2H_{33}/\omega_0^2,\quad h_{12}=H_{12}/\omega_0+(\lambda_3/a)H_{23}/\omega_0^2,$$

$$h_{13}=H_{13}+(\lambda_3/a)H_{33}/\omega_0^2,\quad (h_{22},h_{23},h_{33})=(H_{22},H_{23},H_{33})/\omega_0^2. \tag{3.3}$$

The reparametrized metric (without the limit $\omega_0\to 0$ taken yet) is

$$g_{11}=-(c/a)^2-2(c/a)\omega_0\tilde{y}+\tilde{Y}^2H_{11}-2(c/a)\lambda_3\tilde{Y}H_{13}+(\lambda_3\tilde{y})^2H_{33},$$

$$g_{12}=H_{12}+(\lambda_3\tilde{y}/\tilde{Y})H_{23},\quad g_{13}=D\omega_0\tilde{Y}H_{13}+D\lambda_3\tilde{y}H_{33}, \tag{3.4}$$

$$g_{22}=H_{22}/\tilde{Y}^2,\quad g_{23}=DH_{23}/\tilde{Y},\quad g_{33}=D^2H_{33},\quad \tilde{Y}=a\omega_0\tilde{y}+c.$$

Similarly as before, in the limit $\omega_0\to 0$ the H_{ij} will depend only on t, and the subsequent limit of zero shear is $H_{11}=-C_{11}R^2(t)+(c/a)^2$, other $H_{ij}(t)=-C_{ij}R^2(t)$, $C_{33}=1$. Proceeding exactly as in Sec. II, we then find that the hypersurfaces $t=\text{const}$ will have constant curvature when $\lambda_3\to 0$; the resulting limit is the Friedmann $k=0$ model, as expected for type III. The limits $C_3\to 0$ and $\lambda_3\to 0$ should be tuned so that $C_3/\lambda_3 \xrightarrow[\omega_0\to 0]{} 0$, e.g., $\lambda_3=L_3\omega_0{}^{1/2}$.

The case 1.1.2.2 [Eqs. (4.12)–(4.33) in Ref. 2] is of Bianchi type II. It is known from the paper by Ozsváth,[7] and from Theorem 3.1 by King and Ellis,[8] that dust models of type II have zero rotation. However, that thesis was proven with use of the Einstein equations in Ref. 7 and of the Ellis evolution equations[9] in Ref. 8, that include consequences of the Einstein equations. In the approach of Refs. 1–3, the Einstein equations were not used. Moreover, the constant λ_3 plays the role of the tilt parameter here—with $\lambda_3=0$, the metric becomes stationary (the orbits of the symmetry group become timelike and tangent to the velocity field of the dust), and this case is not

covered in Refs. 7 and 8. This is why the case 1.1.2.2 could show up in our consideration. This observation implies a warning: The existence of a Friedmann limit of the metric does not guarantee that the Einstein equations will allow a rotating generalization of a given Bianchi type of the corresponding Friedmann model. A rotating dust solution and the Friedmann solution may turn out to be two disjoint subclasses within that type.

The metric [Eq. (4.13) from Ref. 2] transformed back to the Plebański coordinates [by the inverse of (4.4) from Ref. 2] is

$$\begin{gathered} g_{11}=h_{11}+2\lambda_3 y h_{13}+y^2(1+\lambda_3^2 h_{33}), \\ g_{12}=h_{12}+\lambda_3 y h_{23}, \quad g_{13}=C_3(h_{13}+\lambda_3 y h_{33}), \\ (g_{22},g_{23},g_{33})=(h_{22},C_3 h_{23},C_3^2 h_{33}), \end{gathered} \tag{3.5}$$

where the h_{ij} are arbitrary functions of the T from (3.2). The limit of zero rotation and zero tilt is achieved after the reparametrization

$$\begin{gathered} (y,C_3)=\omega_0(\tilde{y},D), \\ (h_{12},h_{13})=(H_{12},H_{13})/\omega_0, \quad (h_{22},h_{23},h_{33})=(H_{22},H_{23},H_{33})/\omega_0^2, \end{gathered} \tag{3.6}$$

and the reparametrized metric is

$$\begin{gathered} g_{11}=(\omega_0\tilde{y})^2+h_{11}+2\lambda_3\tilde{y}H_{13}+(\lambda_3\tilde{y})^2 H_{33}, \\ g_{12}=H_{12}+\lambda_3\tilde{y}H_{23}, \quad g_{13}=D(H_{13}+\lambda_3\tilde{y}H_{33}), \\ (g_{22},g_{23},g_{33})=(H_{22},DH_{23},D^2H_{33}). \end{gathered} \tag{3.7}$$

The $k=0$ Friedmann limit will result now when $\omega_0=0$, $H_{ij}=-C_{ij}R^2$, and $\lambda_3=0$.

The theorem by King and Ellis mentioned above implies that $\omega_0=0$ will follow when (3.7) is substituted in the Einstein equations.

The Killing fields for the metric (3.1) are

$$\begin{gathered} k^\alpha_{(1)}=\delta^\alpha{}_1, \quad k^\alpha_{(3)}=C_3\delta^\alpha{}_0+\lambda_3\delta^\alpha{}_3, \\ k^\alpha_{(2)}=cx\,\delta^\alpha{}_0+ax\,\delta^\alpha{}_1-(ay+c)\,\delta^\alpha{}_2+(c\lambda_3/C_3)x\,\delta^\alpha{}_3. \end{gathered} \tag{3.8}$$

[The Killing fields for (3.5) result when $a=0$ above.] After the reparametrization (3.3), in the limit $\omega_0\to 0$, the basis (3.8) becomes

$$\begin{gathered} k^\alpha_{(1)}=\delta^\alpha{}_1, \quad l^\alpha_{(3)}:=(1/\lambda_3)k^\alpha_{(3)} \xrightarrow[\omega_0\to 0]{} \delta^\alpha{}_3, \\ l^\alpha_{(2)}=-(\omega_0/c)k^\alpha_{(2)} \xrightarrow[\omega_0\to 0]{} \delta^\alpha{}_2-(\lambda_3/D)x\,\delta^\alpha{}_3. \end{gathered} \tag{3.9}$$

In the Friedmann limit $\lambda_3\to 0$, the generators (3.9) become a Bianchi type I algebra.

IV. CASES 1.2 AND 2 OF REF. 2

All of these allow both the $k=0$ and the $k=-1$ Friedmann limits.

Case 1.2.1.1 is of Bianchi type VI_h with the free parameter $(b^2+f^2)/(b^2-f^2)$ (there is a typo in Ref. 2). In this case [Eqs. (5.6)–(5.7) in Ref. 2], the transformation back to the Plebański coordinates is given by (5.5) from Ref. 2, with the roles of x^α and x'^α interchanged. The resulting metric is

$$g_{11}=h_{11}-2bt(y-bh_{12})-2Zh_{13}+(bt)^2(b^2h_{22}-1)-2b^2tZh_{23}+Z^2h_{33},$$

$$g_{12}=h_{12}+b^2th_{22}-Zh_{23},\quad g_{13}=h_{13}+b^2th_{23}-Zh_{33}, \tag{4.1}$$

$$(g_{22},g_{23},g_{33})=(h_{22},h_{23},h_{33}),\quad Z:=fz,$$

where b and f are arbitrary constants, and h_{ij} are arbitrary functions of

$$T=t+y/b. \tag{4.2}$$

The limit of zero rotation (that will automatically untilt the model) is achieved by the reparametrization

$$y=\omega_0\tilde{y},\quad h_{22}=H_{22}/\omega_0^2,\quad h_{23}=H_{23}/\omega_0,$$

$$h_{11}=H_{11}+(bT)^2-2b^2Th_{12}-b^4T^2H_{22}/\omega_0^2, \tag{4.3}$$

$$h_{12}=H_{12}/\omega_0-b^2TH_{22}/\omega_0^2,\quad h_{13}=H_{13}-b^2TH_{23}/\omega_0,$$

and the reparametrized metric is

$$g_{11}=(\omega_0\tilde{y})^2+H_{11}-2b\tilde{y}H_{12}-2ZH_{13}+(b\tilde{y})^2H_{22}+2b\tilde{y}ZH_{23}+Z^2h_{33},$$

$$g_{12}=H_{12}-b\tilde{y}H_{22}-ZH_{23},\quad g_{13}=H_{13}-b\tilde{y}H_{23}-Zh_{33}, \tag{4.4}$$

$$(g_{22},g_{23},g_{33})=(H_{22},H_{23},h_{33}).$$

With $\omega_0=0$, the shearfree limit will result when all $h_{ij}=-C_{ij}R^2(t)$, and then the $k=-1$ Friedmann model results when $b=f\neq 0$. The $k=0$ Friedmann limit results when $b=f=0$. This is the first instance where the coordinates of the $k=-1$ Friedmann limit come out rather exotic. From now on, this will be the rule.

The Killing fields for the metric (4.1)–(4.2) are

$$k^\alpha_{(1)}=\delta^\alpha{}_1,\quad k^\alpha_{(2)}=e^{bx}(\delta^\alpha{}_0-b\,\delta^\alpha{}_2),\quad k^\alpha_{(3)}=e^{fx}\delta^\alpha{}_3. \tag{4.5}$$

In the $k=-1$ Friedmann limit that will result by the first of (4.3) and $b=f$, $k^\alpha_{(1)}$ remains unchanged, $k^\alpha_{(3)}$ becomes $e^{bx}\delta^\alpha{}_{(3)}$, while $k^\alpha_{(2)}$ is replaced by

$$l^\alpha_{(2)}=(-\omega_0/b)k^\alpha_{(2)}\xrightarrow[\omega_0\to 0]{}\ e^{bx}\delta^\alpha{}_2. \tag{4.6}$$

This is of Bianchi type V, and in the further limit $b=f=0$ it becomes type I.

In the case 1.2.1.2 [Eq. (5.10) in Ref. 2], which is of type IV, the transformation back to the Plebański coordinates is given by Eq. (5.9) there. The whole further calculation is similar to (4.1)–(4.4) above. Instead of the last formula in (4.1) we have

$$Z:=ct+bz, \tag{4.7}$$

where c is one more arbitrary constant, and in (4.3) we have:

$$h_{11}=H_{11}+(bT)^2-2b^2Th_{12}+2cTH_{13}-b^4T^2H_{22}/\omega_0^2+(cT)^2h_{33},$$

$$h_{12}=H_{12}/\omega_0-b^2TH_{22}/\omega_0^2+cTH_{23}/\omega_0,\quad h_{13}=H_{13}-b^2TH_{23}/\omega_0+cTh_{33}. \tag{4.8}$$

The reparametrized metric is

$$g_{11}=(\omega_0\tilde{y})^2(1+c^2h_{33}/b^2)+2c\omega_0\tilde{y}(H_{13}/b-\tilde{y}H_{23}-zh_{33})+H_{11}-2b\tilde{y}H_{12}$$
$$-2bzH_{13}+(b\tilde{y})^2H_{22}+2b^2\tilde{y}zH_{23}+(bz)^2h_{33},$$

$$g_{12}=\omega_0(c/b)\tilde{y}H_{23}+H_{12}-b\tilde{y}H_{22}-bzH_{23}, \tag{4.9}$$

$$g_{13}=\omega_0(c/b)\tilde{y}h_{33}+H_{13}-b\tilde{y}H_{23}-bzh_{33}, \quad (g_{22},g_{23},g_{33})=(H_{22},H_{23},H_{33}).$$

The limit $\omega_0\to 0$ of (4.9) is the same as the limit $\omega_0\to 0$ of (4.4) with $b=f$. Hence, the $k=-1$ Friedmann limit will result from (4.9) when $\omega_0=0$ and $h_{ij}=-C_{ij}R^2(t)$, without any further limitations. The $k=0$ Friedmann limit will result when $b=0$ in addition.

For the case 1.2.2.1 [Eqs. (5.17) and (5.18) in Ref. 2], which is of Bianchi type VI_h, the subcase $C=j+a=0$ is identical to the subcase $c=0$ of case 1.2.2.2, and so the Friedmann limits will be the same (see below).

The case 1.2.2.2 [Eq. (5.19) in Ref. 2], which is of Bianchi type IV, allows the special case $c=0$, where the Bianchi type becomes V. This special case was investigated in detail in Ref. 4, and it was shown there how the $k=-1$ Friedmann limit is obtained. In order to obtain the $k=0$ Friedmann limit, one has to apply the following transformation and rescaling to Eq. (3.5) in Ref. 4:

$$y=\mathrm{e}^{\alpha u}, \quad K=\tilde{K}/\alpha, \tag{4.10}$$

and then take the limit $\alpha\to 0$.

All the subcases of case 2 in Ref. 2 have matter density constant along the dust flow: In case 2.1.1 (type I) and both cases 2.1.2 (types II and I), the velocity field is tangent to the symmetry orbits, in case 2.2 (type I), the velocity field coincides with one of the Killing fields. Therefore, no Friedmann limits will exist there.

With this, all cases of Ref. 2 are exhausted.

V. CASE 1.1.1.1 OF REF. 3

In the cases considered in Ref. 3, each of the three Killing vectors is linearly independent of the velocity and rotation. However, the five vectors existing in each four-dimensional tangent space to the manifold cannot form a linearly independent set. The three-dimensional space spanned by the Killing vectors, K_3, must intersect with the two-dimensional plane spanned by the velocity and rotation, H_2, along at least one direction. In the models of Ref. 1, the whole H_2 plane was a subspace of the K_3 space. In consequence, the velocity was a linear combination of the Killing vectors, and so those models were stationary. In the models of Ref. 2, considered up to now, the plane H_2 and the space K_3 intersected along the direction of the Killing vector $k^\alpha_{(3)}=C_3u^\alpha+(\lambda_3/n)w^\alpha$. From now on, the line of intersection will not coincide with any Killing direction. Hence, in each case an equation of the following form will have to hold:

$$a_1k^\alpha_{(1)}+a_2k^\alpha_{(2)}+a_3k^\alpha_{(3)}=b_1u^\alpha+b_2w^\alpha, \tag{5.1}$$

where a_i and b_i are functions on the manifold. Note that if $b_2=0$, then the velocity field is tangent to the symmetry orbits, and in consequence such a model has zero expansion and matter-density independent of the comoving time (the metric may depend on the time only because in general the metric has shear). Hence, b_2 is a measure of the tilt of the velocity field with respect to the orbits. Its relation to the tilt defined by King and Ellis[8] will be explained below [see after Eq. (5.6)].

The case 1.1.1.1, given by Eqs. (2.28) and (2.29) in Ref. 3, is of Bianchi type VI_h. The transformation back to the Plebański coordinates is given by Eq. (2.27) in Ref. 3, and the result is

$$
\begin{aligned}
g_{11}&=\frac{f^2(b+f)}{b^2(b-f)}U^2-2\frac{f}{b-f}U(ft+y)+h_{11}-2Vh_{12}-2\frac{f\gamma}{b\beta(b-f)}Uh_{13}+V^2h_{22}\\
&\quad+2\frac{f\gamma}{b\beta(b-f)}UVh_{23}+\left[\frac{f\gamma}{b\beta(b-f)}\right]^2U^2h_{33},\\
g_{12}&=V/b^2+h_{12}-Vh_{22}-\frac{f\gamma}{b\beta(b-f)}Uh_{23},\\
g_{13}&=h_{13}-Vh_{23}-\frac{f\gamma}{b\beta(b-f)}Uh_{33},\\
g_{22}&=-1/b^2+h_{22},\quad (g_{23},g_{33})=(h_{23},h_{33}),
\end{aligned}
\tag{5.2}
$$

where b, f, β and γ are arbitrary constants, the h_{ij} are arbitrary functions of the argument:

$$T=t+y/b-\beta(b-f)z/\gamma, \tag{5.3}$$

and U and V stand for

$$U=bt+y,\quad V=bft+(b+f)y. \tag{5.4}$$

The Killing fields for the metric (5.2) are:

$$
\begin{aligned}
k^\alpha_{(1)}&=\delta^\alpha_1,\quad k^\alpha_{(2)}=\mathrm{e}^{fx}\{\delta^\alpha_0-f\delta^\alpha_2+[\gamma/(b\beta)]\delta^\alpha_3\},\\
k^\alpha_{(3)}&=\mathrm{e}^{bx}(-\delta^\alpha_0+b\delta^\alpha_2).
\end{aligned}
\tag{5.5}
$$

From (1.8) it follows then that:

$$b\mathrm{e}^{-fx}k^\alpha_{(2)}+f\mathrm{e}^{-bx}k^\alpha_{(3)}=(b-f)u^\alpha+[\gamma/(n\beta)]w^\alpha. \tag{5.6}$$

This is the Eq. (5.1) specified for the case 1.1.1.1. As remarked above, when $\gamma=0$, the velocity field becomes tangent to the symmetry orbits. [With $\gamma\to0$, the argument of h_{ij} given by (5.2) has to be redefined so that it becomes $Z=\gamma T \xrightarrow[\gamma\to0]{} -\beta(b-f)z$.]

This means that the parameter (γ/β) is a measure of the tilt of the velocity field with respect to the symmetry orbits. Indeed, the measure of tilt defined by King and Ellis[8] is proportional to (γ/β). They defined the hyperbolic angle of tilt $\overline{\beta}$ by

$$\cosh\overline{\beta}=u^\alpha n_\alpha \tag{5.7}$$

(the difference in sign from their paper is a consequence of the difference in signature), where n_α is the unit vector normal to the orbits of symmetry. This definition of $\overline{\beta}$ makes sense only when both u^α and n^α are timelike vectors; the cases of n^α being null or spacelike are not considered in Ref. 8. However, $u^\alpha n_\alpha$ is a measure of the tilt also for nontimelike n^α. In particular, when u^α is tangent to the symmetry orbits, $u^\alpha n_\alpha=0$. The vector n^α is related to the Killing fields by

$$n_\alpha=N_\alpha/\sqrt{-g_{\mu\nu}N^\mu N^\nu}:=N_\alpha/\|N\|, \tag{5.8}$$

where

$$N_\alpha=\frac{1}{\sqrt{-g}}\varepsilon_{\alpha\beta\gamma\delta}k^\beta_{(1)}k^\gamma_{(2)}k^\delta_{(3)}. \tag{5.9}$$

In our case then

$$u^\alpha n_\alpha = \|N\|^{-1} N_\alpha u^\alpha = \frac{1}{\|N\|\sqrt{-g}} \mathrm{e}^{(b+f)x} \gamma/\beta. \tag{5.10}$$

Analogs of (5.1) and (5.6) will exist in every case considered from now on. In the models of Ref. 2, considered up to now, where the Killing field $k^\alpha_{(3)}$ always had the form $k^\alpha_{(3)} = C_3 u^\alpha + (\lambda_3/n) w^\alpha$, λ_3 was a measure of the tilt.

For calculating the limit of zero rotation and zero shear, the following reparametrization is useful:

$$\begin{gathered}
(y,\beta) = \omega_0(\tilde{y},B), \quad h_{22} = H_{22}/\omega_0^2, \quad h_{23} = H_{23}/\omega_0, \\
h_{11} = (fT)^2 + H_{11} + 2bfTh_{12} + 2(f^2/D)Th_{13}/\omega_0 - (bfT)^2 H_{22}/\omega_0^2 \\
- 2(bf^3/D)T^2 H_{23}/\omega_0^2 - (f^4/D^2)T^2 h_{33}/\omega_0^2, \\
h_{12} = H_{12}/\omega_0 + bfTH_{22}/\omega_0^2 + (f^2/D)TH_{23}/\omega_0^2, \\
h_{13} = H_{13} + bfTH_{23}/\omega_0 + (f^2/D)Th_{33}/\omega_0, \\
D := f(b-f)B/\gamma.
\end{gathered} \tag{5.11}$$

The reparametrized metric is

$$\begin{gathered}
g_{11} = -2\,ftW\omega_0 + [(Dz)^2 - 2(f/b)\tilde{y}W]\omega_0^2 + H_{11} - 2bWH_{12} \\
- 2\,fzH_{13} + (bW)^2 H_{22} + 2bfzWH_{23} + (fz)^2 H_{33}, \\
g_{12} = (ft/b)\omega_0 + [(b+f)/b^2]\tilde{y}\omega_0^2 + H_{12} - bWH_{22} - fzH_{23}, \\
g_{13} = H_{13} - bWH_{23} - fzh_{33}, \\
(g_{22}, g_{23}, g_{33}) = (H_{22}, H_{23}, h_{33} = H_{33}), \quad W := y + Dz.
\end{gathered} \tag{5.12}$$

The $k=-1$ Friedmann limit results now from (5.12) when $\omega_0 = 0$ (after which all h_{ij} depend only on t), and

$$H_{ij} = -C_{ij}R^2(t), \quad C_{33} = 1, \quad b = f. \tag{5.13}$$

[The last of (5.13) implies $D=0$.] The $k=0$ Friedmann limit results when in addition

$$b = f = 0. \tag{5.14}$$

The reparametrization (5.11) transforms the Killing fields $k^\alpha_{(2)}$ and $k^\alpha_{(3)}$ from (5.5) as follows:

$$\begin{gathered}
l^\alpha_{(2)} = (b\beta/\gamma)k^\alpha_{(2)} \xrightarrow[\omega_0 \to 0]{} \mathrm{e}^{fx}[-(bf\beta/\gamma)\delta^\alpha{}_{(2)} + \delta^\alpha{}_{(3)}] \\
l^\alpha_{(3)} = (\omega_0/b)k^\alpha_{(3)} \xrightarrow[\omega_0 \to 0]{} \mathrm{e}^{bx}\delta^\alpha{}_{(2)}.
\end{gathered} \tag{5.15}$$

In the $k=-1$ Friedmann limit ($b=f$), together with $k^\alpha_{(1)}$, this becomes a Bianchi type V algebra, and in the $k=0$ Friedmann limit ($b=f=0$), it becomes type I.

VI. CASE 1.1.1.2 OF REF. 3

This case is given by Eqs. (3.7)–(3.11) in Ref. 3. It is of Bianchi type VIII or VI_0 (when $g \neq 0$ or $g=0$, respectively), so only the $k=0$ Friedmann limit may exist here. The limit of zero rotation and zero tilt can be considered without transforming the metric back to the Plebański form, but the three subcases have to be considered separately.

The Killing fields in this case are

$$k^\alpha_{(1)}=\delta^\alpha_1, \quad k^\alpha_{(3)}=\mathrm{e}^{\alpha_1 x}\delta^\alpha_2,$$
$$k^\alpha_{(2)}=\mathrm{e}^{-\alpha_1 x}[2gy\,\delta^\alpha_1+\alpha_1(gy^2+2B)\,\delta^\alpha_2+\delta^\alpha_3]. \tag{6.1}$$

The analog of Eq. (5.1) is

$$k^\alpha_{(2)}-\alpha_1(gy^2+2B)\mathrm{e}^{-2\alpha_1 x}k^\alpha_{(3)}-2gy\mathrm{e}^{-\alpha_1 x}k^\alpha_{(1)}=\mathrm{e}^{-\alpha_1 x}[4Bu^\alpha+(8c\gamma\alpha_1/n)w^\alpha], \tag{6.2}$$

and, consequently, the King–Ellis measure of tilt is

$$\sqrt{-g}N_\alpha u^\alpha=\alpha_1, \tag{6.3}$$

[N_α is given by (5.8)].

The argument of the arbitrary functions in the metric is

$$T=t+y/\alpha_1-\frac{B}{2c\gamma\alpha_1}z. \tag{6.4}$$

In case I ($gB\neq 0$), the reparametrization needed is

$$y=\omega_0\tilde{y}, \quad B=\omega_0{}^{3/4}\tilde{B}, \quad \alpha_1=\omega_0^{1/4}a_1, \tag{6.5}$$

$$(h_{13},k_{13})=(G_{13},K_{13})\omega_0, \quad h_{22}=G_{22}/\omega_0^2. \tag{6.6}$$

The full reparametrized metric, with $\omega_0\neq 0$, is rather complicated here, so only the limit $\omega_0\to 0$ will be quoted:

$$\mathrm{d}s^2=\mathrm{d}t^2+h_{11}\mathrm{d}x^2+G_{22}\mathrm{d}y^2-\frac{h_{33}}{2\tilde{B}a_1}\mathrm{d}y\mathrm{d}z+h_{33}\mathrm{d}z^2. \tag{6.7}$$

The $k=0$ Friedmann limit results when further $h_{11}=G_{22}=h_{33}=-R^2(t)$.

As seen from (6.1), the symmetry group becomes Bianchi type I in the limit $\omega_0\to 0$ after the reparametrization (6.4) [the Killing field $k_{(3)}$ has to be replaced by $l_{(3)}=\omega_0 k_{(3)}$ in order that the limit is nonsingular].

In case II ($B=0$), Eq. (6.5) remains unchanged, while (6.6) is replaced by

$$(h_{12},h_{23})=(G_{12},G_{23})\omega_0, \quad h_{22}=G_{22}/\omega_0^2. \tag{6.8}$$

The limit $\omega_0\to 0$ of the reparametrized metric is:

$$\mathrm{d}s^2=\mathrm{d}t^2+h_{11}\mathrm{d}x^2+2G_{12}\mathrm{d}x\mathrm{d}y+2h_{13}\mathrm{d}x\mathrm{d}z+G_{22}\mathrm{d}y^2+h_{33}\mathrm{d}z^2, \tag{6.9}$$

where all the metric components depend only on t. The $k=0$ Friedmann limit is here

$$G_{12}=h_{13}=0, \quad h_{11}=G_{22}=h_{33}=-R^2(t). \tag{6.10}$$

In case III ($g=0$, Bianchi type VI_0), the $k=0$ Friedmann limit results again by (6.5), (6.8), (6.9) and (6.10).

Note two typos in Sec. III of Ref. 3: In (3.7) the correct formula for w^α is

$$w^\alpha=\frac{n\alpha_1}{2c\gamma\Delta}(-4B\delta_0^\alpha+\delta_3^\alpha)=\frac{n}{8c\gamma\alpha_1}(-4B\delta_0^\alpha+\delta_3^\alpha), \tag{6.11}$$

and in (3.10), the correct formula for g_{23} is

$$g_{23}=-2gzh_{13}+h_{23}-\alpha_1 gz^2h_{33}. \tag{6.12}$$

VII. CASE 1.1.2.1 OF REF. 3

This model is of Bianchi type VII_h, and is given by Eqs. (4.19)–(4.23) in Ref. 3. Two formulas in (4.23) had typos, the correct expressions are

$$\begin{aligned} g_{12}&=\mathrm{e}^{(b+f)x/2}[Wh_{12}-(\gamma/D)(b+f)\cos(Dx/2)h_{13}],\\ g_{22}&=\mathrm{e}^{(b+f)x}\{[\gamma^2(b+f)^2h_{33}/D^2+1]\cos^2(Dx/2)\\ &\quad -2(\gamma/D)(b+f)\cos(Dx/2)Wh_{23}+W^2h_{22}\}. \end{aligned} \tag{7.1}$$

The transformation back to the Plebański coordinates is given by (4.21) in Ref. 3, and the resulting metric is

$$\begin{aligned} g_{11}&=y^2+h_{11}+2Uh_{12}-2(\gamma/D)(b+f)yh_{13}+U^2h_{22}\\ &\quad -2(\gamma/D)(b+f)yUh_{23}+[(\gamma/D)(b+f)y]^2h_{33},\\ g_{12}&=-2h_{12}+2(\gamma/D)h_{13}-2Uh_{22}+2(\gamma/D)Uh_{23}+2(\gamma/D)(b+f)yh_{23}-2(\gamma/D)^2(b+f)yh_{33},\\ g_{13}&=h_{13}+Uh_{23}-(\gamma/D)(b+f)yh_{33}, \end{aligned} \tag{7.2}$$

$$g_{22}=4h_{22}-8(\gamma/D)h_{23}+4(\gamma/D)^2h_{33},\quad g_{23}=-2h_{23}+2(\gamma/D)h_{33},$$

$$g_{33}=h_{33},\quad U:=\tfrac{1}{2}[(b+f)^2+D^2]t+2(b+f)y,$$

where b, f D, and γ are arbitrary constants, and h_{ij} are arbitrary functions of the variable

$$T=t+\frac{2y}{b+f}+\frac{D}{\gamma(b+f)}z. \tag{7.3}$$

The Killing fields for the metric (7.2) are

$$\begin{aligned} k^\alpha_{(1)}&=\delta^\alpha_1,\quad k^\alpha_{(2)}=e^{(b+f)x/2}[\cos(Dx/2)\,\delta^\alpha_0-\tfrac{1}{2}W\delta^\alpha_2-\gamma\sin(Dx/2)\,\delta^\alpha_3],\\ k^\alpha_{(3)}&=e^{(b+f)x/2}[\sin(Dx/2)\,\delta^\alpha_0-\tfrac{1}{2}V\delta^\alpha_2+\gamma\cos(Dx/2)\,\delta^\alpha_3],\\ W&:=(b+f)\cos(Dx/2)-D\sin(Dx/2),\\ V&:=D\cos(Dx/2)+(b+f)\sin(Dx/2). \end{aligned} \tag{7.4}$$

The analog of (5.1) is here

$$Vk^\alpha_{(2)}-Wk^\alpha_{(3)}=De^{(b+f)x/2}u^\alpha-\frac{\gamma}{n}(b+f)e^{(b+f)x/2}w^\alpha, \tag{7.5}$$

and the King–Ellis measure of the tilt is:

$$\sqrt{-g}u^{\alpha}N_{\alpha}=-\tfrac{1}{2}(b+f)\gamma e^{(b+f)x}. \tag{7.6}$$

Equation (7.5) shows that with $\gamma(b+f)=0$, the model should be nonexpanding. This is so indeed, but in order to be able to consider the subcase $\gamma(b+f)\to 0$, we have to take $\gamma(b+f)T$ as the argument of h_{ij} in (7.2) instead of the T given by (7.3).

We define

$$E:=(b+f)^2+D^2, \tag{7.7}$$

and then the reparametrization needed for the limit of zero rotation and zero tilt is

$$\begin{gathered}(y,D)=\omega_0(\tilde{y},d),\quad h_{22}=H_{22}/\omega_0^2,\quad h_{23}=H_{23}/\omega_0,\\ h_{11}=H_{11}-ETH_{12}/\omega_0+(\tfrac{1}{2}ET)^2H_{22}/\omega_0^2,\\ h_{12}=H_{12}/\omega_0-\tfrac{1}{2}ETH_{22}/\omega_0^2,\quad h_{13}=H_{13}-\tfrac{1}{2}ETH_{23}/\omega_0.\end{gathered} \tag{7.8}$$

After the reparametrization we have

$$S_{1,2}:=b+f+\varepsilon_{1,2}(\omega_0 d)^2/(b+f)\xrightarrow[\omega_0\to 0]{} b+f,\quad \varepsilon_1=+1,\varepsilon_2=-1,$$

$$\Sigma:=S_2\tilde{y}-\tfrac{1}{2}(d/\gamma)S_1 z,$$

$$\begin{aligned}g_{11}&=(\omega_0 y)^2+H_{11}+2\Sigma H_{12}-2(\gamma/d)(b+f)\tilde{y}H_{13}+\Sigma^2H_{22}\\&\quad-2(\gamma/d)(b+f)\tilde{y}\Sigma H_{23}+[(\gamma/d)(b+f)\tilde{y}]^2h_{33},\\ g_{12}&=-2H_{12}+2(\gamma/d)H_{13}-2\Sigma H_{22}+2(\gamma/d)\tilde{y}H_{23}\\&\quad+2(\gamma/d)(b+f+\Sigma)H_{23}-2(\gamma/d)^2(b+f)\tilde{y}h_{33},\\ g_{13}&=H_{13}+\tilde{y}\Sigma H_{23}-(\gamma/d)(b+f)\tilde{y}h_{33},\\ g_{22}&=4H_{22}-8(\gamma/d)H_{23}+4(\gamma/d)^2h_{33},\\ g_{23}&=-2H_{23}+2(\gamma/d)h_{33},\quad g_{33}=h_{33}:=H_{33}.\end{aligned} \tag{7.9}$$

In the limit $\omega_0\to 0$, all the H_{ij} will depend only on t. The limit of zero shear is then obtained by

$$H_{ij}=-C_{ij}R^2(t),\quad C_{33}=1. \tag{7.10}$$

To obtain the Friedmann limits, a further reparametrization of the constants C_{ij} is necessary. We define

$$\begin{gathered}C_{23}=D_{23}+\gamma/d,\quad {D_{22}}^2=C_{22}-{C_{23}}^2,\\ D_{12}=(C_{12}-C_{13}C_{23})/D_{22},\quad {D_{11}}^2=C_{11}-{C_{13}}^2-{D_{12}}^2.\end{gathered} \tag{7.11}$$

The metric (7.9) may then be written

$$ds^2=dt^2-(D_{11}R\,dx)^2-R^2\left\{\left[-D_{12}-(b+f)D_{22}\left(\tilde{y}-\frac{d}{2\gamma}z\right)\right]dx+2D_{22}d\tilde{y}\right\}^2$$
$$-R^2\left\{\left[C_{13}+(b+f)D_{23}\tilde{y}-\frac{1}{2}(b+f)\left(1+\frac{d}{\gamma}D_{23}\right)z\right]dx-2D_{23}d\tilde{y}+dz\right\}^2, \qquad (7.12)$$

The $k=-1$ Friedmann limit results now when $d=0$, the $k=0$ limit results when $b+f=0$ in addition. The first of (7.11) was necessary to eliminate γ/d from (7.9) so that the limit $d\to 0$ could be subsequently taken.

We have found above [after Eq. (7.6)] that $b+f=0$ corresponds to zero expansion. This is so when $b+f\to 0$ with other parameters unchanged. In considering the $k=0$ Friedmann limit, $b+f$ is set to zero after the limit $d\to 0$ had already been taken. In order to make these two limits compatible, we have to assume that $b+f\to 0$ slowly enough so that $D/(b+f)\to 0$ and $y/(b+f)\to 0$. With the reparametrization (7.8), this is achieved when $b+f=B\omega_0^{\varepsilon}$, where $0<\varepsilon<1$.

After the reparametrization (7.8), in the limit $\omega_0\to 0$, the Killing fields become

$$k^{\alpha}_{(1)}=\delta^{\alpha}{}_{(1)}, \quad l^{\alpha}_{(2)}=-[2\omega_0/(b+f)]k^{\alpha}_{(2)} \xrightarrow[\omega_0\to 0]{} e^{(b+f)x/2}\delta^{\alpha}{}_{(2)}$$

$$l^{\alpha}_{(3)}=(1/\gamma)k^{\alpha}_{(3)} \xrightarrow[\omega_0\to 0]{} e^{(b+f)x/2}\left\{-\frac{d}{2\gamma}\left[1+\frac{1}{2}(b+f)x\right]\delta^{\alpha}{}_{(2)}+\delta^{\alpha}{}_{(3)}\right\}. \qquad (7.13)$$

This is a Bianchi type IV algebra, and in the Friedmann limits $k=-1$ $(d=0)$ and $k=0$ $(d=b+f=0)$ it becomes type V and I, respectively.

VIII. CASE 1.1.2.2 OF REF. 3, BIANCHI TYPE IX SUBCASE

The case 1.1.2.2 contains three different subcases that are of Bianchi types IX, VIII, and VII_0. The type IX subcase requires some adaptation of the formulas given in Ref. 3.

For type IX, $g/c>0$. Then, as seen from Eq. (5.16) in Ref. 3, $B/c<0$, or else (5.16) would lead to a contradiction. These two inequalities imply that $gB<0$, while Eqs. (5.26) and (5.27) in Ref. 3 are adapted to the case $gB>0$. Hence, a re-adaptation of these formulas to type IX is necessary first. We define

$$B:=-\overline{B}, \quad \lambda=i\overline{\lambda}, \quad k_{12}=i\overline{k_{12}}, \quad k_{23}=i\overline{k_{23}} \qquad (8.1)$$

(the overbars simply denote new symbols that will be real), so that instead of (5.16), (5.23), (5.26), and (5.27) from Ref. 3, we obtain

$$K=\frac{1}{2D}\left(\frac{2\overline{B}-gy^2}{c}\right)^{1/2}, \quad \delta^2:=(\overline{B}/D)^2+(2c\gamma)^2, \quad \overline{\lambda^2}:=\frac{g\overline{B}}{8\delta^4D^2},$$

$$R=2cD^2y/(\overline{B}K), \quad \int K^{-3}R\,dy=\frac{4c^2D^4}{g\overline{B}K^2}, \qquad (8.2)$$

$$v=\overline{B}t+2cD\gamma z, \quad U=h_{12}\sin(2\overline{\lambda}v)+\overline{k_{12}}\cos(2\overline{\lambda}v),$$

$$g_{11}=y^2+K^2H_{11}+4\frac{c\gamma D}{\overline{B}}yKH_{13}+8\frac{(c\gamma D)^2}{g\overline{B}}H_{33},$$

$$g_{12}=H_{12}+2\frac{c\gamma D}{\overline{B}K}yH_{23}, \quad g_{13}=KH_{13}+2\frac{c\gamma D}{\overline{B}}yH_{33}, \qquad (8.3)$$

$$g_{22}=H_{22}/K^2,\quad g_{23}=H_{23}/K,\quad g_{33}=H_{33},$$

$$H_{11}=-\frac{cD^2}{2\delta^2\overline{\lambda}}U+h_{11},\quad H_{12}=h_{12}\cos(2\overline{\lambda}v)-\overline{k_{12}}\sin(2\overline{\lambda}v),$$

$$H_{13}=-\frac{cD^2}{2\delta^2\overline{\lambda}}[h_{23}\sin(\overline{\lambda}v)+\overline{k_{23}}\cos(\overline{\lambda}v)],$$

$$H_{22}=2\frac{\delta^2\overline{\lambda}}{cD^2}U+\frac{g\overline{B}}{2c^2D^6}h_{11}+\frac{8c\gamma^2}{\overline{B}D^2}h_{33},\tag{8.4}$$

$$H_{23}=h_{23}\cos(\overline{\lambda}v)-\overline{k_{23}}\sin(\overline{\lambda}v),\quad H_{33}=h_{33},$$

where $\overline{B}$, c, D, g, and γ are arbitrary constants, and all the h_{ij}, $\overline{k_{12}}$, and $\overline{k_{23}}$ are arbitrary functions of the argument

$$T=t-\frac{\overline{B}}{2cD\gamma}z.\tag{8.5}$$

Equations (8.2)–(8.5) are written in the Plebański coordinates.

The Killing fields for metrics (8.3) and (8.4) are

$$k^\alpha_{(1)}=\delta^\alpha_1,$$

$$k^\alpha_{(2)}=\cos(Dx/2)\left[(K-yK_{,y})\delta^\alpha_0+K_{,y}\delta^\alpha_1+\frac{\gamma}{DK}\delta^\alpha_3\right]+\frac{1}{2}DK\sin(Dx/2)\delta^\alpha_2,$$

$$k^\alpha_{(3)}=\sin(Dx/2)\left[(K-yK_{,y})\delta^\alpha_0+K_{,y}\delta^\alpha_1+\frac{\gamma}{DK}\delta^\alpha_3\right]-\frac{1}{2}DK\cos(Dx/2)\delta^\alpha_2.\tag{8.6}$$

(Note: the first commutator in Eq. (5.20) in Ref. 3 should have a minus on the right-hand side.) The analog of (5.1) here is

$$\cos(Dx/2)k^\alpha_{(2)}+\sin(Dx/2)k^\alpha_{(3)}-K_{,y}k^\alpha_{(1)}=(K-yK_{,y})u^\alpha+[\gamma/(DKn)]w^\alpha.\tag{8.7}$$

In agreement with this, the King–Ellis measure of tilt is here

$$\sqrt{-g}N_\alpha u^\alpha=\gamma/2.\tag{8.8}$$

Note that

$$K_{,y}=-\frac{gy}{4cD^2K},\quad K-yK_{,y}=\frac{\overline{B}}{2cD^2K}.\tag{8.9}$$

The case presently considered is the only one of type IX in the whole classification. Therefore,

(1) This is the only place where the $k=+1$ Friedmann model will appear as a limit;
(2) The models represented by Eqs. (8.2)–(8.6) include those considered by Gödel.[10] (Ours are in fact more general because the tilt of the symmetry orbits with respect to the velocity field is an arbitrary parameter here.) We shall deal with this point further on.

For later considerations, it will be convenient to reparametrize the metric (8.4) once more, as follows:

$$\begin{gathered}\overline{G}:=(h_{12}{}^2+\overline{k_{12}}{}^2)^{1/2},\quad h_{12}=-\overline{G}\sin(2\beta),\quad \overline{k_{12}}=\overline{G}\cos(2\beta),\\ F:=(h_{23}{}^2+\overline{k_{23}}{}^2)^{1/2},\quad h_{23}=F\cos(\alpha),\quad \overline{k_{23}}=F\sin(\alpha),\end{gathered}\tag{8.10}$$

where $\overline{G}$, F, α, and β are new functions of the T given by (8.3); and also to transform the coordinate y by

$$y=\sqrt{2\overline{B}/g}\cos(\vartheta).\tag{8.11}$$

From now on, the x^2-coordinate will be ϑ. Then, in order to set the rotation and the tilt to zero, the following further reparametrization is needed:

$$\overline{B}=b\omega_0^2,\quad \gamma=h\omega_0,\quad \overline{G}=G/\omega_0,\quad h_{11}=G_{11}/\omega_0^2.\tag{8.12}$$

Let us note that

$$\overline{\lambda}v=\frac{\sqrt{bg}D(\omega_0 bt+2cDhz)}{2\sqrt{2}[(\omega_0 b)^2+(2cDh)^2]}\xrightarrow[\omega_0\to 0]{}\frac{\sqrt{bg}}{4\sqrt{2}ch}z.\tag{8.13}$$

The metric (8.5), reparametrized by (8.10)–(8.12), becomes

$$\begin{aligned}g_{11}&=\frac{2b}{g}\cos^2\vartheta\omega_0^2+\frac{2b}{4cD^2}G_{11}\sin^2\vartheta-4\frac{chD^3}{g}\sqrt{\frac{2c}{b}}F\sin(\overline{\lambda}v+\alpha)\sin\vartheta\cos\vartheta\\&\quad-D\sqrt{\frac{b}{2g}}G\cos(2\overline{\lambda}v+2\beta)\sin^2\vartheta+8\frac{(chD)^2}{bg}h_{33},\\ g_{12}&=\sqrt{2b/g}G\sin(2\overline{\lambda}v+2\beta)\sin\vartheta-4\sqrt{2}(chD^2/g)\sqrt{c/b}F\cos(\overline{\lambda}v+\alpha)\cos\vartheta,\\ g_{13}&=2\sqrt{2}\frac{chD}{\sqrt{bg}}h_{33}\cos\vartheta-D^2\sqrt{\frac{c}{g}}F\sin(\overline{\lambda}v+\alpha)\sin\vartheta,\\ g_{22}&=2\frac{b}{cD^4}G_{11}+32\frac{(ch)^2}{bg}h_{33}+2\sqrt{2}\frac{1}{D}\sqrt{\frac{b}{g}}G\cos(2\overline{\lambda}v+2\beta),\\ g_{23}&=-2D\sqrt{\frac{c}{g}}F\cos(\overline{\lambda}v+\alpha),\quad g_{33}=h_{33}.\end{aligned}\tag{8.14}$$

In the limit $\omega_0\to 0$, the velocity field $u^\alpha=\delta^\alpha{}_0$ will have zero shear when

$$\begin{gathered}\alpha=\text{const},\quad \beta=\text{const},\\ (G,F,G_{11},h_{33})=-(C_{12},C_{23},C_{11},1)R^2(t).\end{gathered}\tag{8.15}$$

With use of (8.13) it may be verified now that the $k=+1$ Friedmann limit will result from (8.14) and (8.15) when $\omega_0\to 0$ and

$$C_{12}=C_{23}=C_{11}=0.\tag{8.16}$$

The resulting representation of the Friedmann model (again an exotic one) is identical, up to rescalings of coordinates, to the one derived by Behr[11]

$$ds^2=dt^2-R^2(t)\left[8\frac{(chD)^2}{bg}dx^2+4\sqrt{2}\frac{chD}{\sqrt{bg}}\cos\vartheta\,dx\,dz+32\frac{(ch)^2}{bg}d\vartheta^2+dz^2\right]. \tag{8.17}$$

The $k=0$ Friedmann model will result from this after the transformation–reparametrization

$$\vartheta=\arccos(ky),\quad h=H/k,\quad x=kx', \tag{8.18}$$

in the limit $k\to 0$.

For the $k=+1$ Friedmann limit, the algebra of the Killing fields (8.6), suitably transformed by use of (8.9), (8.11), and (8.12), is still of Bianchi type IX. For the $k=0$ limit, the algebra $\{l_{(1)},l_{(2)},l_{(3)}\}:=k\{k_{(1)},k_{(2)},k_{(3)}\}$ is of Bianchi type I when $k\to 0$.

As stated above, the class of models defined by (8.2)–(8.5) must contain the one considered by Gödel in Ref. 10. This is so because two of Gödel's assumptions (dust source and nonzero rotation) place his class within our collection, and the third assumption (compact spaces $t=\text{const}$, i.e., Bianchi type IX; the Bianchi classification and terminology had not yet been in common use in Gödel's time) uniquely points to the subcase I of our case 1.1.2.2. Gödel presented several properties of these models in the form of theorems, but mostly without proofs and almost without formulas. It would be an interesting exercise to see how Gödel's theorems apply to the explicitly given metric (8.2)–(8.5).

In particular, one of his statements seems to need a refinement. He said that there exist ∞^8 rotating solutions satisfying all his requirements. This means that the collection of all solutions of the Einstein equations for (8.2)–(8.5) should be labeled by eight arbitrary constants. One can understand how this happens from Ref. 4, where the Einstein equations were investigated for an equally general Bianchi type V class. Of the six unknown functions in the initial metric, one (h_{33} in Ref. 4) is determined by an algebraic relation, two of the Einstein equations are of first order and can be used to eliminate two more functions, and then the remaining three functions obey equations of second order. This gives eight constants indeed. However, the tilt parameter [γ in (8.7) and (8.8)] is one more arbitrary constant that is contained in the metric even before the Einstein equations are considered.

Rotating dust models of Bianchi type IX were considered by Behr,[11] with simplifying assumptions about the metric. Similarly as in Ref. 4, the main conclusion seems to be that whatever one does with the Einstein equations, no solution comes within sight.

IX. CASE 1.1.2.2 OF REF. 3, BIANCHI TYPES VIII AND VII$_0$

The subcase of case 1.1.2.2 that corresponds to the Bianchi type VIII is defined by

$$g/c<0, \tag{9.1}$$

in Eqs. (5.16)–(5.27) in Ref. 3. Then, B/c and, consequently, Bg can have any sign at this point. Only the $k=0$ Friedmann model can be contained as a subcase here.

The cases $Bg\neq 0$ and $Bg=0$ have to be considered separately. When $Bg\neq 0$, we take Eqs. (5.23)–(5.28) in Ref. 3 with the following specializations:

$$h_{12}=k_{12}=h_{23}=k_{23}=0,$$

$$B=b\omega_0^2,\quad (\gamma,y)=(h,\tilde{y})\omega_0,\quad h_{11}=G_{11}/\omega_0^2. \tag{9.2}$$

Then

$$K=\omega_0\tilde{K},\quad \tilde{K}=\frac{1}{2D}\sqrt{-\frac{g\tilde{y}^2+2b}{c}},$$

$$g_{11}=(\omega_0\tilde{y})^2-8\frac{(cDh)^2}{bg}h_{33}+\tilde{K}^2G_{11},$$

$$g_{12}=0,\quad g_{13}=-2(cDh/b)\tilde{y}h_{33}, \tag{9.3}$$

$$g_{22}=\tilde{K}^{-2}\left(-\frac{bg}{2c^2D^6}G_{11}-8\frac{ch^2}{bD^2}h_{33}\right),\quad g_{23}=0,\quad g_{33}=h_{33}.$$

It is now seen that the proper signature will result only when

$$b/c>0. \tag{9.4}$$

In order to obtain the $k=0$ Friedmann model from (9.3), we then rescale the constants again as follows:

$$b=b_0\sqrt{g},\quad D=dg^{1/4},\quad h=Hg^{3/4}, \tag{9.5}$$

and take the limit $g\to 0$. The limiting metric is

$$\mathrm{d}s^2=\mathrm{d}t^2+G_{11}\left(\frac{b_0}{2cd^2}\mathrm{d}x^2+\frac{1}{d^4}\mathrm{d}\tilde{y}^2\right)+h_{33}\mathrm{d}z^2, \tag{9.6}$$

and in the limit of zero shear, $G_{11}=C_{11}h_{33}=-C_{11}R^2(t)$, this becomes the $k=0$ Friedmann model indeed.

The Killing fields for this case are given by (8.6). After the rescalings (9.2) and (9.5), the following basis of the symmetry algebra is obtained:

$$k^\alpha_{(1)}=\delta^\alpha{}_1,$$

$$l^\alpha_{(2)}=\sqrt{\frac{b_0}{2cg}}\frac{1}{H}k^\alpha_{(3)}\xrightarrow[g\to 0]{}\frac{1}{4cH}\left(-\frac{\tilde{y}}{d}\delta^\alpha{}_1+\frac{1}{2}b_0dx\,\delta^\alpha{}_2\right)+\delta^\alpha{}_3, \tag{9.7}$$

$$l^\alpha_{(3)}=-2\sqrt{\frac{2c}{b_0}}g^{-1/4}k^\alpha_{(3)}\xrightarrow[g\to 0]{}\delta^\alpha{}_2.$$

This is of Bianchi type VII_0.

When $Bg=0$, and the Bianchi type is VIII, we must have:

$$B=0\neq g. \tag{9.8}$$

The metric is then found from Eqs. (5.28) and (5.23)–(5.26) in Ref. 3, suitably adapted. With $B=0$, the arbitrary functions depend only on t. The metric needs then to be rescaled as follows:

$$(\gamma,y)=(h,\tilde{y})\omega_0,\quad (h_{12},h_{13},h_{23})=(G_{12},G_{13},G_{23})/\omega_0,\quad h_{11}=G_{11}/\omega_0^2 \tag{9.9}$$

and the result of the rescaling is

$$g_{11}=(\omega_0\tilde{y})^2-\frac{g\tilde{y}^2}{4cD^2}G_{11}+\frac{Dg}{8ch}\tilde{y}^2zG_{12}-2\sqrt{-c/g}hG_{13}-\frac{g^2}{2^5c^2h}\sqrt{-c/g}(\tilde{y}z)^2G_{13}$$
$$-\frac{D^4g}{2^6ch^2}(\tilde{y}z)^2h_{22}+\frac{1}{4}D^2\tilde{y}zG_{23}+\left(\frac{Dg}{2^4ch}\right)^2(\tilde{y}z)^3G_{23}+4\left(\frac{cDh}{g\tilde{y}}\right)^2h_{33}$$
$$+\frac{1}{8}(Dz)^2h_{33}+\left(\frac{Dg}{2^5ch}\tilde{y}z^2\right)^2h_{33},$$

$$g_{12}=G_{12}-\frac{g}{2cD}\sqrt{-c/g}zG_{13}-\frac{D^3}{4h}zh_{22}+2\frac{cDh}{g\tilde{y}}G_{23}$$
$$+3\frac{Dg}{2^5ch}\tilde{y}z^2G_{23}+2\frac{cDh}{g\tilde{y}^2}zh_{33}+\frac{Dg}{2^5ch}z^3h_{33},$$

$$g_{13}=\frac{1}{2D}\sqrt{-g/c}\tilde{y}G_{13}+\frac{Dg}{2^5ch}\tilde{y}^2zG_{23}+2\frac{cDh}{g\tilde{y}}h_{33}+\frac{Dg}{2^5ch}\tilde{y}z^2h_{33}, \tag{9.10}$$

$$g_{22}=-4\frac{cD^2}{g\tilde{y}^2}h_{22}+2(z/\tilde{y})G_{23}+(z/\tilde{y})^2h_{33},$$

$$g_{23}=G_{23}+(z/\tilde{y})h_{33},\quad g_{33}=h_{33}.$$

In the limit $\omega_0\to0$ one term in g_{11} disappears and the h_{ij} depend only on t. The shearfree limit is then attained when

$$G_{ij}=-C_{ij}R^2(t),\quad h_{33}=-R^2(t),\quad h_{22}=-C_{22}R^2(t). \tag{9.11}$$

To find the Friedmann limit we then assume that

$$C_{12}=C_{13}=C_{23}=0,\quad h=HD,\quad g=-cG^2D^2, \tag{9.12}$$

where H and G are new constants (the last definition takes into account that $g/c<0$ in type VIII), and let $\omega_0\to0$, $D\to0$. The resulting metric is:

$$\mathrm{d}s^2=\mathrm{d}t^2-C_{11}\left(\frac{1}{2}G\tilde{y}R\right)^2\mathrm{d}x^2-C_{22}\left(2\frac{R}{G\tilde{y}}\right)^2\mathrm{d}\tilde{y}^2-R^2\left(-2\frac{H}{G^2\tilde{y}}\mathrm{d}x+\frac{z}{\tilde{y}}\mathrm{d}\tilde{y}+\mathrm{d}z\right)^2. \tag{9.13}$$

The $k=0$ Friedmann limit results from this when

$$\tilde{y}=\mathrm{e}^{ku},\quad C_{22}=(D_{22}/k)^2,\quad k\to0. \tag{9.14}$$

With (9.8), (9.9), and (9.12), the Killing fields become

$$k^\alpha_{(1)}=\delta^\alpha_1,$$

$$k^\alpha_{(2)}=\frac{1}{2}G\cos(Dx/2)\,\delta^\alpha_1+\frac{1}{4}GD\tilde{y}\sin(Dx/2)\,\delta^\alpha_2+\frac{2H}{G\tilde{y}}\cos(Dx/2)\,\delta^\alpha_3,$$

$$k^\alpha_{(3)}=\frac{1}{2}G\sin(Dx/2)\,\delta^\alpha_1-\frac{1}{4}GD\tilde{y}\cos(Dx/2)\,\delta^\alpha_2+\frac{2H}{G\tilde{y}}\sin(Dx/2)\,\delta^\alpha_3. \tag{9.15}$$

Before the limit $D\to0$ can be taken, $k_{(3)}$ needs to be redefined by $k'_{(3)}=(1/D)k_{(3)}$. The basis in the limit becomes

$$k^{\alpha}_{(1)}=\delta^{\alpha}_{1}, \quad k^{\alpha}_{(2)}=\frac{1}{2}G\,\delta^{\alpha}_{1}+\frac{2H}{G\tilde{y}}\,\delta^{\alpha}_{3},$$

$$k'^{\alpha}_{(3)}=\frac{1}{4}Gx\,\delta^{\alpha}_{1}-\frac{1}{4}G\tilde{y}\,\delta^{\alpha}_{2}+\frac{Hx}{G\tilde{y}}\,\delta^{\alpha}_{3}. \tag{9.16}$$

This is of type VI_0. We now transform $\tilde{y}$ by (9.10), and redefine $k'_{(3)}$ once more

$$l^{\alpha}_{(3)}=-(4k/G)k'^{\alpha}_{(3)}. \tag{9.17}$$

In the limit $k\to 0$, the following basis then results:

$$k^{\alpha}_{(1)}=\delta^{\alpha}_{1}, \quad k^{\alpha}_{(2)}=\frac{1}{2}G\,\delta^{\alpha}_{1}+\frac{2H}{G}\,\delta^{\alpha}_{3}, \quad l^{\alpha}_{(3)}=\delta^{\alpha}_{2} \tag{9.18}$$

(u being now the x^2), which is clearly of Bianchi type I.

Finally, when the Bianchi type is VII_0 (i.e., $g=0$), the metric results by a simple specialization of Eqs. (5.23)–(5.25) and (5.28) in Ref. 3. In this case necessarily $b/c<0$ and

$$K=\frac{1}{D}\sqrt{\frac{-b}{2c}}=\text{const.} \tag{9.19}$$

The rescaling that will allow to calculate the limit $\omega_0\to 0$ is

$$(B,y)=(b,\tilde{y})\omega_0^2, \quad D=d\omega_0,$$

$$(h_{12},h_{23})=(G_{12},G_{23})/\omega_0, \quad h_{22}=G_{22}/\omega_0^2. \tag{9.20}$$

The argument of the arbitrary functions must then be redefined so that it becomes:

$$\tilde{u}=u/(2cD\gamma)=t+\frac{B}{2cD\gamma}z \xrightarrow[\omega_0\to 0]{} t. \tag{9.21}$$

The limit $\omega\to 0$ of the metric is then:

$$\mathrm{d}s^2=\mathrm{d}t^2-\frac{b}{2cd^2}h_{11}\mathrm{d}x^2-2G_{12}\mathrm{d}x\mathrm{d}\tilde{y}+\frac{2}{d}\sqrt{\frac{-b}{2c}}h_{13}\mathrm{d}x\mathrm{d}z$$
$$-2\frac{cd^2}{b}C_{22}\mathrm{d}\tilde{y}^2+2G_{23}\mathrm{d}\tilde{y}\mathrm{d}z+h_{33}\mathrm{d}z^2. \tag{9.22}$$

The $k=0$ Friedmann limit results from here when shear is set to zero, i.e., when $g_{ij}=-C_{ij}R^2(t)$.

The basis of the Killing fields in the limit $\omega_0\to 0$ is found as follows:

$$k^{\alpha}_{(1)}=\delta^{\alpha}_{1}, \quad l^{\alpha}_{(2)}=\lim_{\omega_0\to 0}\left(\frac{K\omega_0}{d\gamma}k^{\alpha}_{2}\right)=\delta^{\alpha}_{3}, \quad l^{\alpha}_{(3)}=\lim_{\omega_0\to 0}\left(-\frac{2}{dK}\omega_0 k^{\alpha}_{3}\right)=\delta^{\alpha}_{2}. \tag{9.23}$$

X. CASES 2.1 OF REF. 3

In the case 2.1.1 the transformation back to the Plebański coordinates is the inverse of (7.16) in Ref. 3, and when applied to (7.18) there, it gives the following metric:

$$g_{11}=y^2-(y+V)^2+h_{11}+(b+f)[(y+V)h_{12}+(\gamma/c)Vh_{13}]$$
$$+\tfrac{1}{4}(b+f)^2[(y+V)^2h_{22}+2(\gamma/c)V(y+V)h_{23}+(\gamma V/c)^2h_{33}],$$

$$g_{12}=\frac{2}{b+f}(y+V)-h_{12}-\frac{1}{2}(b+f)[(y+V)h_{22}+(\gamma/c)Vh_{23}], \tag{10.1}$$

$$g_{13}=h_{13}+\tfrac{1}{2}(b+f)[(y+V)h_{23}+(\gamma/c)Vh_{33}],$$

$$g_{22}=-4/(b+f)^2+h_{22},\quad g_{23}=-h_{23},\quad g_{33}=h_{33},$$

where

$$V:=\tfrac{1}{2}(b+f)t+y, \tag{10.2}$$

and the arbitrary functions h_{ij} depend on

$$T:=t+\frac{2y}{b+f}+\frac{2c}{\gamma(b+f)}z. \tag{10.3}$$

[Note two typos in Ref. 3: In Eq. (7.18), the coefficient of Wh_{23} in g_{22} is 2γ, not $2b$, and in (7.17), in the formula for u^α, there should be a (W/c) in front of $\delta^\alpha{}_0$.] The Killing fields for this metric are

$$k^\alpha_{(1)}=\delta^\alpha_1,\quad k^\alpha_{(2)}=e^{(b+f)x/2}\{cx\,\delta^\alpha_0-c[1+\tfrac{1}{2}(b+f)x]\delta^\alpha_2+\gamma\delta^\alpha_3\},$$
$$k^\alpha_{(3)}=e^{(b+f)x/2}[\delta^\alpha_0-\tfrac{1}{2}(b+f)\delta^\alpha_2], \tag{10.4}$$

and they form a Bianchi type IV algebra.

The analog of (5.5) is

$$k^\alpha_{(2)}-\frac{2c}{b+f}[1+\tfrac{1}{2}(b+f)x]k^\alpha_{(3)}=e^{(b+f)x/2}\left(\frac{2c}{b+f}u^\alpha+\frac{\gamma}{n}w^\alpha\right), \tag{10.5}$$

and the King–Ellis measure of tilt is

$$\sqrt{-g}u^\alpha N_\alpha=-\tfrac{1}{2}(b+f)\gamma e^{(b+f)x}. \tag{10.6}$$

The redefinitions needed to make the limit $\omega_0\to 0$ finite are

$$(y,c)=\omega_0(\tilde{y},C),$$

$$h_{11}=H_{11}-\tfrac{1}{2}(b+f)^2T[h_{12}+(\gamma/c)h_{13}]-\tfrac{1}{16}(b+f)^4T^2[H_{22}/\omega_0^2+2(\gamma/c)H_{23}/\omega_0+(\gamma/c)^2h_{33}],$$

$$h_{12}=H_{12}/\omega_0-\tfrac{1}{4}(b+f)^2T[H_{22}/\omega_0^2+(\gamma/c)H_{23}/\omega_0],$$

$$h_{13}=H_{13}-\tfrac{1}{4}(b+f)^2T[H_{23}/\omega_0+(\gamma/c)h_{33}],$$
$$h_{22}=H_{22}/\omega_0^2,\quad h_{23}=H_{23}/\omega_0, \tag{10.7}$$

and the resulting metric is

$$g_{11}=(\omega_0\tilde{y})^2-[\tfrac{1}{2}(b+f)t+2\omega_0\tilde{y}]^2+H_{11}+(b+f)[YH_{12}-zH_{13}]$$
$$+\tfrac{1}{4}(b+f)^2[Y^2H_{22}-2YzH_{23}+z^2H_{33}],$$

$$g_{12}=\omega_0 t+\frac{4\omega_0^2}{b+f}\tilde{y}-H_{12}-\tfrac{1}{2}(b+f)[YH_{22}-zH_{23}],$$

$$g_{13}=H_{13}+\tfrac{1}{2}(b+f)[YH_{23}-zH_{33}], \tag{10.8}$$

$$g_{22}=H_{22}-4\omega_0^2/(b+f)^2, \quad g_{23}=-H_{23}, \quad g_{33}=h_{33}=H_{33},$$

$$Y:=\tilde{y}-Cz/\gamma.$$

In the limit $\omega_0\to 0$, all H_{ij} become functions of t, and the Killing fields become

$$k^\alpha_{(1)}=\delta^\alpha_1,$$

$$l^\alpha_{(2)}=\lim_{\omega_0\to 0}k^\alpha_{(2)}=e^{(b+f)x/2}\{-C[1+\tfrac{1}{2}(b+f)x]\delta^\alpha_2+\gamma\delta^\alpha_3\}, \tag{10.9}$$

$$l^\alpha_{(3)}=\lim_{\omega_0\to 0}\left(-\frac{2}{b+f}\omega_0 k^\alpha_{(3)}\right)=e^{(b+f)x/2}\delta^\alpha_2,$$

still of type IV.

The shearfree limit of (10.8) is

$$H_{11}=-C_{11}R^2(t)+[\tfrac{1}{2}(b+f)t]^2,$$

$$\text{other} \quad H_{ij}=-C_{ij}R^2(t), \quad C_{33}=1. \tag{10.10}$$

The $k=-1$ Friedmann model will then result when $C=0$ (and, consequently, $Y=\tilde{y}$), the $k=0$ Friedmann model will result when $b+f=0$, with no condition on C. Both limits can be easily taken also in the Killing fields (10.9), with $C=0$ they become of type V, with $b+f=0$ they become of type I.

The case 2.1.2 was shown in Ref. 3 to be included in 2.1.1 as a subcase.

XI. CASE 2.2.1.1 OF REF. 3

This case includes two subcases, $\mathcal{A}\neq 0$ and $\mathcal{A}=0$, given by Eqs. (9.11)–(9.15) in Ref. 3. Both are of Bianchi type VIII. The coordinates used there are those of Plebański.

With $\mathcal{A}\neq 0$, Eqs. (9.14) in Ref. 3 are adapted to the case $\mathcal{A}<0$. However, when $\mathcal{A}<0$, the limit of constant curvature in the spaces $t=\text{const}$ has a wrong signature. Therefore, the formulas must be re-adapted to $\mathcal{A}>0$. This is the result:

$$g_{11}=y^2\left(\frac{U}{\sqrt{2\mathcal{A}}}+\frac{\gamma V}{\mathcal{A}\sqrt{2\mathcal{A}}}+h_{11}\right),$$

$$g_{12}=h_{12}\cos(2\lambda v)-k_{12}\sin(2\lambda v)+\frac{\gamma}{2\mathcal{A}}[h_{23}\cos(\lambda v)-k_{23}\sin(\lambda v)],$$

$$g_{13}=y\left(\frac{V}{\sqrt{2\mathcal{A}}}+\frac{\gamma}{2\mathcal{A}}h_{33}\right), \quad g_{22}=y^{-2}\left(-\sqrt{2\mathcal{A}}U+2\mathcal{A}h_{11}-\frac{\gamma^2}{2\mathcal{A}}h_{33}\right), \tag{11.1}$$

$$g_{23}=y^{-1}[h_{23}\cos(\lambda v)-k_{23}\sin(\lambda v)],\quad g_{33}=H_{33}=h_{33},$$

$$U:=h_{12}\sin(2\lambda v)+k_{12}\cos(2\lambda v),\quad V:=h_{23}\sin(\lambda v)+k_{23}\cos(\lambda v),$$

$$\lambda^2=2\mathcal{A}/(4\mathcal{A}^2+\gamma^2)^2,\quad v=2\mathcal{A}t+\gamma z,$$

and the h_{ij} are arbitrary functions of

$$T=t-2\mathcal{A}z/\gamma. \tag{11.2}$$

The Killing fields for (11.1) are

$$k^\alpha_{(1)}=\delta^\alpha_1,\quad k^\alpha_{(2)}=(2\mathcal{A}/y)\,\delta^\alpha_0+(-\mathcal{A}/y^2+x^2/2)\,\delta^\alpha_1-xy\,\delta^\alpha_2+(\gamma/y)\,\delta^\alpha_3,$$

$$k^\alpha_{(3)}=x\,\delta^\alpha_1-y\,\delta^\alpha_2. \tag{11.3}$$

The analog of (5.1) is

$$(\mathcal{A}/y^2+x^2/2)k^\alpha_{(1)}+k^\alpha_{(2)}-xk^\alpha_{(3)}=(2\mathcal{A}/y)u^\alpha+\frac{\gamma}{yn}w^\alpha, \tag{11.4}$$

and the King–Ellis measure of tilt is

$$\sqrt{-g}u^\alpha N_\alpha=\gamma. \tag{11.5}$$

The redefinitions needed to make the limit $\omega_0\to 0$ of (11.1) finite are

$$(y,\gamma)=\omega_0(\tilde{y},h),\quad \mathcal{A}=\tfrac{1}{2}(a\omega_0)^2,$$

$$h_{11}=H_{11}/\omega_0^2,\quad (h_{12},k_{12})=(H_{12},K_{12})/\omega_0. \tag{11.6}$$

Note that with (11.6) we have

$$\lambda v \xrightarrow[\omega_0\to 0]{} az/h. \tag{11.7}$$

The reparametrized metric is

$$\begin{aligned}
g_{11}&=\tilde{y}^2\{2hV/a^3+H_{11}+a^{-1}[H_{12}\sin(2\lambda v)+K_{12}\cos(2\lambda v)]\},\\
g_{12}&=(h/a^2)[h_{23}\cos(\lambda v)-k_{23}\sin(\lambda v)]+H_{12}\cos(2\lambda v)-K_{12}\sin(2\lambda v),\\
g_{13}&=(\tilde{y}/a)(V+hh_{33}/a),\\
g_{22}&=\tilde{y}^{-2}\{-a[H_{12}\sin(2\lambda v)+K_{12}\cos(2\lambda v)]+a^2H_{11}-(h/a)^2H_{33}\},\\
g_{23}&=\tilde{y}^{-1}[h_{23}\cos(\lambda v)-k_{23}\sin(\lambda v)],\quad g_{33}=H_{33}=h_{33}.
\end{aligned} \tag{11.8}$$

In the limit $\omega_0\to 0$, all the arbitrary functions will depend only on t.

The $k=0$ Friedmann limit follows from (11.8) when the following further specialization and transformation is made:

$$\begin{aligned}
&h_{33}=-R^2(t),\quad H_{11}=-(C_{11}+h^2)R^2(t)/a^4,\\
&H_{12}=K_{12}=h_{23}=k_{23}=0,\quad x=a^2x',\quad \tilde{y}=e^{au},
\end{aligned} \tag{11.9}$$

and then the limit $a\to 0$ is taken. The metric becomes then

$$ds^2=dt^2-R^2[C_{11}(dx'^2+du^2)+(g\,dx+dz)^2], \tag{11.10}$$

which is clearly the $k=0$ Friedmann model.

The rescaling (11.6), followed by $\omega_0\to 0$, and the rescaling (11.9), followed by $a\to 0$ transform the Killing fields (11.3) into an almost-standard Bianchi type I basis ($k^\alpha_{(1)}$ has to be replaced by $l^\alpha_{(1)}=a^2k^\alpha_{(1)}$, and $k^\alpha_{(3)}$ has to be replaced by $l^\alpha_{(3)}=ak^\alpha_{(3)}$ before taking the limit $a\to 0$).

The case $\mathcal{A}=0$ is given by Eqs. (9.11) and (9.15) in Ref. 3. The rescalings needed there are

$$y=\omega_0\tilde{y},\quad h_{11}=G_{11}/\omega_0^2,\quad (h_{12},h_{13})=(G_{12},G_{13})/\omega_0. \tag{11.11}$$

The arbitrary functions h_{ij} depend only on t from the beginning. The limit $\omega_0\to 0$ of the rescaled metric is

$$\begin{aligned}ds^2=&dt^2+\tilde{y}^2G_{11}dx^2+2(zG_{13}+G_{12})dx\,d\tilde{y}+2\tilde{y}G_{13}dx\,dz+\tilde{y}^{-2}(h_{22}+2zh_{23}+z^2h_{33})d\tilde{y}^2\\&+2\tilde{y}^{-1}(h_{23}+zh_{33})d\tilde{y}\,dz+h_{33}dz^2.\end{aligned} \tag{11.12}$$

The $k=0$ Friedmann model results now when

$$\begin{gathered}G_{12}=G_{13}=0,\quad G_{11}=-C_{11}R^2(t),\\ h_{ij}=-C_{ij}R^2,\quad C_{33}=1,\quad C_{22}=1/a^2,\\ \tilde{y}=e^{au},\quad a\to 0.\end{gathered} \tag{11.13}$$

The Killing fields need not be reconsidered because $\mathcal{A}=0$ is an allowed subcase for (11.3).

XII. CASES 2.2.1.2 OF REF. 3

In considering these cases, we first have to correct two errors. The first error is that the arbitrary constant y_0 actually must be equal to zero in all the formulas. The second error is that one subcase was overlooked—it needs special treatment and is not included in the formulas given in Sec. X of Ref. 3. This special case is defined by

$$g=0, \tag{12.1}$$

and consequently $\mu_1=0$ and $\mu_2=j$. It is because of $\mu_1=0$ that some of the formulas do not apply to this case.

The conclusion that

$$a=0,\quad c=1, \tag{12.2}$$

can be achieved by a change of the basis of the Killing fields is still valid. With (12.1) and (12.2), the solutions of Eqs. (10.2) and (10.3) in Ref. 3 are

$$P=-jy+M,\quad L_3=\gamma, \tag{12.3}$$

where j, M, and γ are arbitrary constants. The resulting Killing fields are [by (10.6) from Ref. 3]

$$\begin{gathered}k^\alpha_{(1)}=\delta^\alpha_1,\quad k^\alpha_{(2)}=Mx\,\delta^\alpha_0-jx\,\delta^\alpha_1+(jy-M)\,\delta^\alpha_2+\gamma x\,\delta^\alpha_3,\\ k^\alpha_{(3)}=M\,\delta^\alpha_0-j\,\delta^\alpha_1+\gamma\delta^\alpha_3,\end{gathered} \tag{12.4}$$

and they form a Bianchi type III algebra.

The coordinates are still those of Plebański at this point, so u^α and w^α and $g_{0\alpha}$ have their standard forms. The solution of the Killing equations is

$$g_{11}=(2M/j)y-(M/j)^2+(jy-M)^2h_{11}+2(\gamma/j)(jy-M)h_{13}+(\gamma/j)^2h_{33},$$

$$g_{12}=h_{12}+\frac{\gamma h_{23}}{j(jy-M)},\quad g_{13}=(jy-M)h_{13}+(\gamma/j)h_{33},$$

$$g_{22}=h_{22}/(jy-M)^2,\quad g_{23}=h_{23}/(jy-M),\quad g_{33}=h_{33}, \tag{12.5}$$

where the h_{ij} are arbitrary functions of the argument

$$T=t-(M/\gamma)z. \tag{12.6}$$

The Killing fieds (12.4) are a subcase of the general expression that will apply to the whole case 2.2.1.2 collection. The analog of (5.1) will be given further on for the whole class.

The rescalings needed to find the nonrotating limit of (12.5) and (12.6) are

$$(y,M)=\omega_0(\tilde{y},m),\quad h_{11}=H_{11}/\omega_0^2,$$

$$(h_{12},h_{13})=(H_{12},H_{13})/\omega_0. \tag{12.7}$$

The rescaled metric is

$$g_{11}=(2m/j)\omega_0^2\tilde{y}-(m\omega_0/j)^2+(j\tilde{y}-m)^2H_{11}+2(\gamma/j)(j\tilde{y}-m)H_{13}+(\gamma/j)^2h_{33},$$

$$g_{12}=H_{12}+\frac{\gamma h_{23}}{j(j\tilde{y}-m)},\quad g_{13}=(j\tilde{y}-m)H_{13}+(\gamma/j)h_{33},$$

$$g_{22}=H_{22}/(j\tilde{y}-m)^2,\quad g_{23}=h_{23}/(j\tilde{y}-m),\quad g_{33}=h_{33}. \tag{12.8}$$

The $k=0$ Friedmann limit is now obtained from (12.8) when shear is set to zero [$h_{ij}=-C_{ij}R^2(t)$, $C_{33}=1$], and in addition

$$\gamma=hj,\quad j\to 0. \tag{12.9}$$

In order to make the limits $\omega_0\to 0$ and $j\to 0$ compatible, it has to be assumed that $j\propto\omega_0^\alpha$, where $0<\alpha<1$, e.g., $\alpha=1/2$. The Killing fields (12.4) become then an almost-standard Bianchi type I basis in the limit $\omega_0\to 0$, but $k^\alpha_{(3)}$ has to be replaced by $l^\alpha_{(3)}={\omega_0}^{-1/2}k^\alpha_{(3)}$.

The case 2.2.1.2 consists of three subcases, each of a different Bianchi type. The subcase $g<j^2/4$ is of Bianchi type VI_h, with the free parameter $j/(j^2-4g)^{1/2}$. However, the parametrization of the metric used in Ref. 3 is inconvenient for calculating the Friedmann limit. It will be more convenient to rewrite it in the parametrization in which μ_1 and μ_2 appear symmetrically. Therefore, instead of (10.15)–(10.17) from Ref. 3, we will use the following formulas:

$$U:=M\cosh(DY)+N\sinh(DY),\quad V:=M\sinh(DY)+N\cosh(DY),$$

$$D:=(j^2/4-g)^{1/2},\quad \Gamma:=\frac{\gamma}{D(M^2-N^2)},$$

$$P=\mathrm{e}^{-jY/2}U,\quad y=-\frac{j}{2g}P-\frac{D}{g}\mathrm{e}^{-jY/2}V,$$

$$g_{11}=y^2+h_{11}P^2+2\Gamma\mathrm{e}^{-jY}UVh_{13}+(\gamma\Gamma/D)\mathrm{e}^{-jY}h_{33}, \tag{12.10}$$

$$g_{12}=h_{12}+\Gamma(V/U)h_{23},\quad g_{13}=h_{13}P+\Gamma e^{-jY/2}Vh_{33},$$

$$g_{22}=h_{22}/P^2,\quad g_{23}=h_{23}/P,\quad g_{33}=h_{33},$$

where j, g, M, N, and γ are arbitrary constants, y is one of the coordinates, Y is just a parameter used to represent $P(y)$, and h_{ij} are arbitrary functions of the coordinate z. Since the coordinates used in (12.10) are not those of Plebański, the u^α and $g_{0\alpha}$ do not have their standard forms, they are given by Eqs. (10.9) in Ref. 3. The transformation back to the Plebański coordinates is the inverse of (10.8) in Ref. 3, after which we obtain

$$g_{12}=gth_{11}+h_{12}+\Gamma gt\left(V/U-\frac{1}{2}j/D\right)h_{13}+\Gamma(V/U)h_{23}-\Gamma^2 gt\left(1+\frac{jV}{2DU}\right)h_{33},$$

$$g_{22}=P^{-2}\{(gt)^2h_{11}+2gth_{12}-(j\Gamma g/D)t(gth_{13}+h_{23})+h_{22}+g(\Gamma gt/D)^2h_{33}\},\quad (12.11)$$

$$g_{23}=(1/P)\left\{gth_{13}+h_{23}-\frac{j\Gamma gt}{2D}h_{33}\right\},$$

with g_{11}, g_{13}, and g_{33} being the same as in (12.10). The h_{ij} depend now on

$$T=t+\frac{D}{\Gamma g}z. \quad (12.12)$$

The Killing fields corresponding to (12.11) and (12.12) [and to all the other subcases of case (2.2.1.2)] are

$$k^\alpha_{(1)}=\delta^\alpha_1,\quad k^\alpha_{(2)}=x(P-yP_{,y})\delta^\alpha_0+xP_{,y}\delta^\alpha_1-P\delta^\alpha_2+x(\gamma/P)e^{-jY}\delta^\alpha_3,$$
$$k^\alpha_{(3)}=(P-yP_{,y})\delta^\alpha_0+P_{,y}\delta^\alpha_1+(\gamma/P)e^{-jY}\delta^\alpha_3. \quad (12.13)$$

The analog of (5.1) (again valid for all the subcases) is

$$k^\alpha_{(3)}-P_{,y}k^\alpha_{(1)}=(P-yP_{,y})u^\alpha+\frac{\gamma}{nP}e^{-jY}w^\alpha, \quad (12.14)$$

and the King–Ellis measure of tilt is

$$\sqrt{-g}u^\alpha N_\alpha=-\gamma e^{-jY}. \quad (12.15)$$

The rescalings needed to make the limit $\omega_0\to 0$ finite are

$$(M,N,\gamma)=(m,n,h)\omega_0,\quad h_{11}=H_{11}/\omega_0^2,\quad h_{13}=H_{13}/\omega_0. \quad (12.16)$$

In consequence of this we have

$$(y,P,U,V)=(\tilde{y},\tilde{P},\tilde{U},\tilde{V})\omega_0, \quad (12.17)$$

where the symbols with a tilde are obtained from those on the left by replacing $(M,N)\to(m,n)$, and they do not depend on ω_0. Also, from now on Y will be used as the x^2-coordinate in place of y, so

$$dy=\omega_0\tilde{P}dY. \quad (12.18)$$

The rescalings (12.16) have to be accompanied by the following redefinitions of other functions in the metric:

$$h_{12}=-gTH_{11}/\omega_0^2+H_{12}/\omega_0+\frac{j\Gamma gT}{2D\omega_0}H_{13}+\Gamma^2 gTh_{33},$$

$$h_{22}=-(gT)^2H_{11}/\omega_0^2-2gTh_{12}+H_{22}+\frac{j\Gamma g}{D}(gT^2H_{13}/\omega_0+Th_{23})-g(\Gamma gT/D)^2h_{33},$$

$$h_{23}=-gTH_{13}/\omega_0+H_{23}+\frac{j\Gamma gT}{2D}h_{33}. \tag{12.19}$$

The metric resulting after the redefinitions and the coordinate transformation is

$$\tilde{\Gamma}:=\frac{h}{D(m^2-n^2)},$$

$$g_{11}=(\omega_0\tilde{y})^2+H_{11}\tilde{P}^2+\tilde{\Gamma}e^{-jY}[2\tilde{U}\tilde{V}H_{13}-(h/D)h_{33}],$$

$$g_{12}=\tilde{P}\{H_{12}-(D/\tilde{\Gamma})zH_{11}+(j/2-D\tilde{V}/\tilde{U})zH_{13}+\tilde{\Gamma}[(\tilde{V}/\tilde{U})H_{23}+(D+\tfrac{1}{2}j\tilde{V}/\tilde{U})zh_{33}]\},$$

$$g_{13}=H_{13}\tilde{P}+\tilde{\Gamma}e^{-jY/2}\tilde{V}h_{33}, \tag{12.20}$$

$$g_{22}=(Dz/\tilde{\Gamma})^2H_{11}-(D/\tilde{\Gamma})(2zH_{12}+jz^2H_{13})+H_{22}+jzH_{23}+gz^2h_{33},$$

$$g_{23}=-(D/\tilde{\Gamma})zH_{13}+H_{23}+(j/2)zh_{33},\quad g_{33}=h_{33}=H_{33}.$$

In the limit $\omega_0\to 0$, all the H_{ij} will depend only on t.

The limit of zero shear is then, as usual, $H_{ij}=-C_{ij}R^2(t)$, $C_{33}=1$, and the $k=-1$ Friedmann limit results from (12.20) when, in addition

$$h=HD,\quad C_{13}=0,\quad D\to 0. \tag{12.21}$$

With $D=0$ we have $\tilde{U}=m$, $\tilde{V}=n$. The, again rather exotic, representation of the limiting Friedmann model is

$$\begin{aligned}ds^2=&dt^2-R^2(t)(mD_{11}e^{-jY/2}dx+D_{12}dY)^2-(D_{22}RdY)^2\\&-R^2\left[e^{-jY/2}\frac{Hn}{m^2-n^2}dx+(C_{23}+jz/2)dY+dz\right]^2,\end{aligned} \tag{12.22}$$

where

$$D_{11}{}^2:=C_{11}{}^2-\left(\frac{H}{m^2-n^2}\right)^2,\quad D_{12}:=C_{12}/D_{11},$$

$$D_{22}{}^2:=C_{22}-C_{23}{}^2-D_{12}{}^2. \tag{12.23}$$

The $k=0$ Friedmann limit results from (12.22) when $j=0$.

The rescaling (12.16) and the limit $\omega_0\to 0$ transform the Killing fields as follows:

$$\begin{aligned}k^\alpha_{(1)}&=\delta^\alpha_1,\quad k^\alpha_{(2)}=(-j/2+D\tilde{V}/\tilde{U})x\delta^\alpha_1-\delta^\alpha_2+(h/\tilde{U})xe^{-jY/2}\delta^\alpha_3,\\k^\alpha_{(3)}&=(-j/2+D\tilde{V}/\tilde{U})\delta^\alpha_1+(h/\tilde{U})e^{-jY/2}\delta^\alpha_3,\end{aligned} \tag{12.24}$$

the algebra still being of type VI_h.

The further rescaling (12.21) and the limit $D\to 0$ transform (12.24) into a Bianchi type V algebra, but $k^\alpha_{(3)}$ has to be replaced by

$$l^\alpha_{(3)}=D^{-1}\left(k^\alpha_{(3)}+\frac{j}{2}k^\alpha_{(1)}\right)\xrightarrow[D\to 0]{}(n/m)\,\delta^\alpha_1+(H/m)\mathrm{e}^{-jY/2}\delta^\alpha_3. \tag{12.25}$$

When $j=0$ on top of $D\to 0$, the Bianchi type reduces to I.

The subcase with $g>j^2/4$ (Bianchi type VII_h with the free parameter $j/(4g-j^2)^{1/2}$) is given by Eqs. (10.18) and (10.19) in Ref. 3, with $y_0=0$. It is transformed back to the Plebański coordinates by the inverse of (10.8) there, and the result is very similar to our (12.10) and (12.11). Only the definitions of U, V, and y, and a few signs in the metric are different

$$D=(g-j^2/4)^{1/2},\quad \Gamma:=\frac{\gamma}{D(M^2+N^2)},$$

$$U:=M\cos(DY)+N\sin(DY),\quad V:=M\sin(DY)-N\cos(DY),$$

$$P=e^{-jY/2}U,\quad y=-\frac{j}{2g}P+\frac{D}{g}\mathrm{e}^{-jY/2}V,$$

$$\begin{aligned}
g_{11}&=y^2+h_{11}P^2+2\Gamma e^{-jY}UVh_{13}+(\gamma\Gamma/D)\mathrm{e}^{-jY}h_{33},\\
g_{12}&=gth_{11}+h_{12}+\Gamma gt\left(V/U+\frac{1}{2}j/D\right)h_{13}+(\Gamma V/U)h_{23}+\Gamma^2 gt\left(1+\frac{jV}{2DU}\right)h_{33},\\
g_{13}&=h_{13}P+\Gamma\mathrm{e}^{-jY/2}Vh_{33},\\
g_{22}&=P^{-2}[(gt)^2h_{11}+2gth_{12}+(j\Gamma/D)gt(gth_{13}+h_{23})+h_{22}+g(\Gamma gt/D)^2h_{33}],\\
g_{23}&=P^{-1}\left(gth_{13}+h_{23}+\frac{j\Gamma gt}{2D}h_{33}\right),\quad g_{33}=h_{33}.
\end{aligned} \tag{12.26}$$

The h_{ij} are here functions of the argument

$$T=t-\frac{D}{\Gamma g}z. \tag{12.27}$$

The redefinitions in the constants and functions needed here are again (12.16) and (12.17) together with

$$\begin{aligned}
h_{12}&=-gTH_{11}/\omega_0^2+H_{12}/\omega_0-\frac{j\Gamma gT}{2D\omega_0}H_{13}-\Gamma^2 gTh_{33},\\
h_{22}&=-(gT)^2H_{11}/\omega_0^2-2gTh_{12}+H_{22}-(j\Gamma g/D)(gT^2H_{13}/\omega_0+Th_{23})-g(\Gamma gT/D)^2h_{33},\\
h_{23}&=-gTH_{13}/\omega_0+H_{23}-\frac{j\Gamma gT}{2D}h_{33}.
\end{aligned} \tag{12.28}$$

The metric resulting after all the redefinitions is

$$\tilde{\Gamma} := \frac{h}{D(m^2+n^2)},$$

$$g_{11} = (\omega_0 \tilde{y})^2 + H_{11}\tilde{P}^2 + \tilde{\Gamma} e^{-jY}[2\tilde{U}\tilde{V}H_{13} + (h/D)h_{33}],$$

$$g_{12} = \tilde{P}[(D/\tilde{\Gamma})zH_{11} + H_{12} + (j/2 + D\tilde{V}/\tilde{U})zH_{13} + (\tilde{\Gamma}\tilde{V}/\tilde{U})H_{23} + \tilde{\Gamma}(D + \tfrac{1}{2}j\tilde{V}/\tilde{U})zh_{33}], \tag{12.29}$$

$$g_{13} = H_{13}\tilde{P} + \tilde{\Gamma} e^{-jY/2}\tilde{V}h_{33},$$

$$g_{22} = (Dz/\tilde{\Gamma})^2 H_{11} + (D/\tilde{\Gamma})(2zH_{12} + jz^2 H_{13}) + H_{22} + jzH_{23} + gz^2 h_{33},$$

$$g_{23} = (D/\tilde{\Gamma})zH_{13} + H_{23} + (j/2)zh_{33}, \quad g_{33} = h_{33} = H_{33}.$$

Just as before, in the limit $\omega_0 \to 0$ the H_{ij} will depend only on t, and the shearfree limit is found in the same way: $H_{ij} = -C_{ij}R^2$, $C_{33} = 1$.

The $k = -1$ Friedmann limit is now obtained in two ways: either

$$h = HD, \quad D \to 0, \tag{12.30}$$

or

$$C_{11} = C_{13} = 0. \tag{12.31}$$

In the first case the Friedmann limit is

$$ds^2 = dt^2 - R^2(t)(mD_{11}e^{-jY/2}dx + D_{12}dY)^2 - (D_{22}R\,dY)^2$$
$$- R^2[e^{-jY/2}(mC_{13} + n\tilde{\Gamma})dx + (C_{23} + jz/2)dY + dz]^2, \tag{12.32}$$

where

$$D_{11}{}^2 := C_{11}{}^2 - C_{13}{}^2 + H^2/(m^2+n^2)^2, \tag{12.33}$$

D_{12} and D_{22} being the same as in (12.23).

In the second case, the $k = -1$ Friedmann limit is

$$ds^2 = dt^2 - R^2(t)[D_{11}e^{-jY/2}\tilde{U}dx + (D_{12} + Dz)dY]^2 - (D_{22}R\,dY)^2$$
$$- R^2[e^{-jY/2}\tilde{V}\tilde{\Gamma}dx + (C_{23} + jz/2)dY + dz]^2, \tag{12.34}$$

where D_{11} is defined as in (12.33), but with $C_{11} = C_{13} = 0$.

The Killing fields before redefinitions are still given by (12.13), but, in consequence of the different definitions of P and y in the present subcase, the Bianchi type is VII_h. In the Friedmann limit defined by (12.31), the Killing fields are transformed only by (12.16) and (12.17) followed by $\omega_0 \to 0$, and they still form a type VII_h algebra. When (12.30) is imposed on top of (12.16) and (12.17) and $\omega_0 \to 0$, the Killing fields become the same as the limit $D \to 0$ of (12.24) and (12.25), i.e., the Bianchi type becomes V. This is an illustration of the fact, mentioned in Sec. I, that the $k = -1$ Robertson–Walker geometry is a subcase of two Bianchi types simultaneously, they are exactly V and VII_h.

In both cases, the $k=0$ Friedmann limit follows from (12.32) and (12.34) when $j=0$. In the first case, the algebra of the Killing fields becomes type I, in the second case it becomes type VII_0, which is another illustration of the same kind of duality.

Finally, the third subcase of case 2.2.1.2 is given by Eqs. (10.20) and (10.21) in Ref. 3, with $y_0=0$. There is one more typo there, the correct formula for y is

$$y=-2P/j-4M\mathrm{e}^{-jY/2}/j^2. \tag{12.35}$$

This one is of Bianchi type IV. When transformed back to the Plebański coordinates [by the inverse of (10.8) in Ref. 3], it becomes

$$\begin{gathered}
P=e^{-jY/2}(MY+N),\\
g_{11}=y^2+h_{11}P^2-2(\gamma/M)e^{-jY/2}Ph_{13}+(\gamma/M)^2\mathrm{e}^{-jY}h_{33},\\
g_{12}=(jt/2)^2h_{11}+h_{12}+\frac{j^3\gamma t}{8M^2}h_{13}-\frac{\gamma}{M(MY+N)}\left(\frac{1}{4}j^2th_{13}+h_{23}+\frac{j^3\gamma t}{8M^2}h_{33}\right),\\
g_{13}=h_{13}P-(\gamma/M)\mathrm{e}^{-jY/2}h_{33},\\
g_{22}=P^{-2}\left[\left(\frac{1}{4}j^2t\right)^2h_{11}+\frac{1}{2}j^2th_{12}+\frac{j^5\gamma t^2}{16M^2}h_{13}+h_{22}+\frac{j^3\gamma t}{4M^2}h_{23}+\left(\frac{j^3\gamma t}{8M^2}\right)^2h_{33}\right],\\
g_{23}=P^{-1}\left(\frac{1}{4}j^2th_{13}+h_{23}+\frac{j^3\gamma t}{8M^2}h_{33}\right),\quad g_{33}=h_{33},
\end{gathered} \tag{12.36}$$

where the h_{ij} are arbitrary functions of

$$T=t-\frac{4M^2}{j^2\gamma}z. \tag{12.37}$$

The redefinitions needed to calculate the limit $\omega_0\to 0$ are

$$\begin{gathered}
(M,N,\gamma)=(m,n,h)\omega_0,\quad h_{11}=H_{11}/\omega_0^2,\quad h_{13}=H_{13}/\omega_0,\\
h_{12}=-\frac{1}{4}j^2TH_{11}/\omega_0^2+H_{12}/\omega_0-\frac{j^3hT}{8(m\omega_0)^2}H_{13},\\
h_{22}=-(j^2T/4)^2H_{11}/\omega_0^2-\frac{1}{2}j^2Th_{12}-\frac{j^5hT^2}{(4m\omega_0)^2}H_{13}+H_{22}-\frac{j^3hT}{4m^2\omega_0}h_{23}-\left(\frac{j^3hT}{8m^2\omega_0}\right)^2h_{33},\\
h_{23}=-\frac{1}{4}j^2TH_{13}/\omega_0+H_{23}-\frac{j^3hT}{8m^2\omega_0}h_{33}.
\end{gathered} \tag{12.38}$$

We will denote, as before, $(y,P)=\omega_0(\tilde{y},\tilde{P})$, and choose Y as the new x^2-coordinate, so that $\mathrm{d}y=\omega_0\tilde{P}\mathrm{d}Y$. The metric that results is

$$g_{11}=(\omega_0\tilde{y})^2+H_{11}\tilde{P}^2-2(h/m)\mathrm{e}^{-jY/2}\tilde{P}H_{13}+(h/m)^2\mathrm{e}^{-jY}h_{33},$$

$$g_{12}=\tilde{P}\{(m^2/h)zH_{11}+H_{12}+(j/2)zH_{13}-(mY+n)^{-1}[mzH_{13}+(h/m)H_{23}+\tfrac{1}{2}(jh/m)zh_{33}]\},$$

$$g_{13}=H_{13}\tilde{P}-(h/m)\mathrm{e}^{-jY/2}h_{33}, \tag{12.39}$$

$$g_{22}=(m^2z/h)^2H_{11}+2(m^2/h)zH_{12}+(jm^2/h)z^2H_{13}+H_{22}+jzH_{23}+(jz/2)^2h_{33},$$

$$g_{23}=(m^2/h)zH_{13}+H_{23}+(j/2)zh_{33},\quad g_{33}=h_{33}=H_{33}.$$

In the limit $\omega_0\to 0$, the H_{ij} will depend only on t.

The $k=-1$ Friedmann limit is now obtained when

$$H_{ij}=-C_{ij}R^2(t),\quad h=Hm,\quad m\to 0. \tag{12.40}$$

The $k=0$ limit will result when $j=0$ in addition.

XIII. THE CASES 2.2.2 OF REF. 3

The case 2.2.2.1.1 is given by Eqs. (11.11) and (11.12) in Ref. 3. The transformation back to the Plebańnski coordinates is the inverse of (11.10), and the transformed metric is

$$g_{11}=y^2h_{11},\quad g_{12}=(jt/a)(1-h_{11})+h_{12}-\mathcal{A}jth_{13},$$

$$g_{13}=B(j+a)yh_{13},$$

$$g_{22}=\left(\frac{jt}{ay}\right)^2(h_{11}-1)-2\frac{jt}{ay^2}h_{12}+2\mathcal{A}\frac{(jt)^2}{ay^2}h_{13}+h_{22}/y^2-2(\mathcal{A}jt/y^2)h_{23}+(\mathcal{A}jt/y)^2h_{33}, \tag{13.1}$$

$$g_{23}=B(j+a)\left(-\frac{jt}{ay}h_{13}+h_{23}/y-\frac{\mathcal{A}jt}{y}h_{33}\right),\quad g_{33}=B^2(j+a)^2h_{33},$$

where a, $\mathcal{A}$, B, and j are arbitrary constants, and the h_{ij} are arbitrary functions of the argument

$$T=t+\frac{B(j+a)}{\mathcal{A}a}z. \tag{13.2}$$

The Killing fields for the metric (13.1) are

$$k^\alpha_{(1)}=\delta^\alpha_1,\quad k^\alpha_{(2)}=x\delta^\alpha_1-y\delta^\alpha_2,$$

$$k^\alpha_{(3)}=y^{-j/a}[B(j/a+1)\delta^\alpha_0-Bj(ay)^{-1}\delta^\alpha_1-\mathcal{A}\delta^\alpha_3], \tag{13.3}$$

and they form a Bianchi type VI_h algebra, with the free parameter $(j-a)/(j+a)$. The analog of (5.1) is

$$k^\alpha_{(3)}-Bj(ay)^{-1}k^\alpha_{(1)}=y^{-j/a}[B(j/a+1)u^\alpha-(\mathcal{A}/n)w^\alpha], \tag{13.4}$$

and the King-Ellis measure of tilt is

$$\sqrt{-g}u^\alpha N_\alpha=\mathcal{A}y^{1-j/a}. \tag{13.5}$$

By a simple transformation of the z coordinate we can achieve the same result as if

$$B(j+a)=1, \tag{13.6}$$

and we will assume this now.

The redefinitions needed to calculate the limit $\omega_0 \to 0$ are

$$\begin{gathered} y=\omega_0\tilde{y}, \quad \mathcal{A}=A/\omega_0, \quad h_{11}=H_{11}/\omega_0^2, \quad h_{13}=H_{13}/\omega_0, \\ h_{12}=-(j/a)T+(jT/a)H_{11}/\omega_0^2+H_{12}/\omega_0+AjTH_{13}/\omega_0^2, \\ h_{22}=(jT/a)^2(1-H_{11}/\omega_0^2)+2(jT/a)h_{12}-2(Aj^2T^2/a)H_{13}/\omega_0^2+H_{22} \\ +2AjTh_{23}/\omega_0-(AjT)^2h_{33}/\omega_0^2, \\ h_{23}=(jT/a)H_{13}/\omega_0+H_{23}+AjTh_{33}/\omega_0. \end{gathered} \tag{13.7}$$

The redefined metric is

$$\begin{gathered} g_{11}=\tilde{y}^2H_{11}, \quad g_{12}=\frac{j}{a^2A}z(H_{11}-\omega_0^2)+H_{12}+(j/a)zH_{13}, \quad g_{13}=\tilde{y}H_{13}, \\ g_{22}=\tilde{y}^{-2}\left[\left(\frac{jz}{a^2A}\right)^2(H_{11}-\omega_0^2)+2\frac{j}{a^2A}zH_{12}+2\frac{j^2}{a^3A}z^2H_{13}+H_{22}+2(j/a)zH_{23}+(jz/a)^2h_{33}\right], \\ g_{23}=\tilde{y}^{-1}\left[\frac{j}{a^2A}zH_{13}+H_{23}+(j/a)zh_{33}\right], \quad g_{33}=h_{33}=H_{33}. \end{gathered} \tag{13.8}$$

In the limit $\omega_0 \to 0$, the H_{ij} will depend only on t. The $k=-1$ Friedmann limit will then result when

$$H_{ij}=-C_{ij}R^2(t), \quad j=-a, \quad A\to\infty. \tag{13.9}$$

The $k=0$ Friedmann limit will result when

$$\begin{gathered} H_{ij}=-C_{ij}R^2(t), \quad C_{13}=j=0, \quad C_{22}=(D_{22}/k)^2, \\ \tilde{y}=\mathrm{e}^{ku}, \quad k\to 0. \end{gathered} \tag{13.10}$$

The limit (13.9) transforms the Killing fields (13.3) into a Bianchi type V algebra, provided $k^\alpha_{(3)}$ is redefined to $k'^\alpha_{(3)}=-(\omega_0^{j/a}/\mathcal{A})k^\alpha_{(3)}$, and the limits $A\to\infty$ and $j=-a$ are tuned so that $A(j+a)\to\infty$ [for example, $A=\alpha/(j+a)$ and $\alpha\to\infty$]. The limit (13.10) will transform (13.3) into a type I algebra, but $k^\alpha_{(3)}$ has to be redefined as above, and in addition $k^\alpha_{(2)}$ has to be redefined to $k'^\alpha_{(3)}=kk^\alpha_{(2)}$.

The formulas for the case 2.2.2.1.2 simply follow from those above. This case has a completely different outlook only in the coordinates adapted to the Killing fields that were used in Ref. 3. When transformed to the Plebański coordinates, it becomes the subcase of (13.1) given by

$$B(j+a)=1, \quad j=-a, \quad \mathcal{A}=\mathcal{A}_1/a, \tag{13.11}$$

where the $\mathcal{A}_1$ defined above stands in place of the $\mathcal{A}$ from Eq. (11.17) in Ref. 3. Then the redefinitions needed are (13.7) with $\mathcal{A}_1=A/\omega_0$ and $j=-a$, and the redefined metric is

$$\begin{gathered} g_{11}=\tilde{y}^2H_{11}, \quad g_{12}=-(z/A)(H_{11}-\omega_0^2)+H_{12}-zH_{13}, \quad g_{13}=\tilde{y}H_{13}, \\ g_{22}=\tilde{y}^{-2}[(z/A)^2(H_{11}-\omega_0^2)-2(z/A)H_{12}+2(z^2/A)H_{13}+H_{22}-2zH_{23}+z^2h_{33}], \\ g_{23}=\tilde{y}^{-1}[-(z/a)H_{13}+H_{23}-zh_{33}], \quad g_{33}=h_{33}=H_{33}. \end{gathered} \tag{13.12}$$

The $k=-1$ Friedmann limit results now by (13.9) when $\omega_0=0$, and the $k=0$ Friedmann limit results from (13.12) when

$$\omega_0=0, \quad H_{ij}=-C_{ij}R^2(t), \quad (\tilde{y},z)=(e^{ku},e^{kv}),$$

$$(H_{12},H_{13})=(G_{12},G_{13})/k, \quad (H_{22},H_{23},H_{33})=(G_{22},G_{23},G_{33})/k^2, \quad k\to 0. \tag{13.13}$$

The Killing field $k^\alpha_{(3)}$ is different here

$$k^\alpha_{(3)}=y\,\delta^\alpha{}_0-\ln y\,\delta^\alpha{}_1-\mathcal{A}y\,\delta^\alpha{}_3, \tag{13.14}$$

while the two others are as in (13.3). The case 2.2.2.1.2 required a separate consideration in Ref. 3 only because of the logarithm term in the Killing field. In calculating the limits $\omega_0\to 0$ and $A\to\infty$, this vector field has to be redefined similarly as before. For calculating the $k=0$ Friedmann limit, $k^\alpha_{(3)}$ and $k^\alpha_{(2)}$ have to be redefined by $(k'^\alpha_{(2)},k'^\alpha_{(3)})=k(k^\alpha_{(2)},k^\alpha_{(3)}) \xrightarrow[k\to 0]{} (-\delta^\alpha{}_2,-\mathcal{A}\delta^\alpha{}_3)$.

Finally, the case 2.2.2.2 from Ref. 3 [Eqs. (11.18)–(11.27)] is of Bianchi type I, with the velocity field being tangent to the symmetry orbits, so it has no Friedmann limit at all.

XIV. SUMMARY

All the metrics derived in Refs. 1–3, that correspond to rotating hypersurface–homogeneous dust models, have been checked here for the existence of a Friedmann limit. It was found that such a limit exists for all those cases listed in Refs. 2 and 3, where the matter-density is not constant along the flow. However, in at least one class (see Sec. III), the Friedmann model will have no rotating parent solution, but will instead be a separate subclass.

Along the way, the nonstationary metrics were all transformed to such a form, in which the limit of zero rotation can be explicitly calculated. The transformation–reparametrization leading to this form is nonsingular and invertible in each case, but it becomes singular when $\omega\to 0$. The limits $\omega=0$ all have nonzero shear. Thus, a whole collection of metrics generalizing those of Friedmann was found that can be used in studying spatially homogeneous exact perturbations of the latter.

The Class A Bianchi-type metrics (those in which the structure constants have the property $C^a{}_{ac}=0$) are known to admit a Lagrangian–Hamiltonian formulation.[12] Those of them that obey the Einstein equations with a rotating dust source (types VI_0, VII_0, VIII, and IX) were studied by Ozsváth.[7,13] The Lagrangians and Hamiltonians were explicitly found in Refs. 7 and 13, and the Einstein equations in the Hamiltonian form were then transformed to such variables, in which they become analytic. This should prove the existence of solutions.

Two more papers, specifically devoted to rotating spatially homogeneous dust solutions, are those of Behr[11] (where a subclass of type IX models was investigated) and of this author[4] (discussing a subclass of type V models). In both of these, the Einstein equations were transformed, simplified, investigated for known limiting cases and for Lie symmetries, but no explicit solutions were found. A (hopefully) complete overview of other solutions with rotating matter source is given at the end of Ref. 3.

It is hoped that the present paper will be helpful in picking out those models for future investigation that promise interesting physics or geometry.

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Consequences of 't Hooft's equivalence class theory and symmetry by coarse graining

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According to 't Hooft [Class. Quantum. Grav. **16**, 3263 (1999)], quantum gravity can be postulated as a dissipative deterministic system, where quantum states at the ''atomic scale'' can be understood as equivalence classes of primordial states governed by a dissipative deterministic dynamics law at the ''Planck scale.'' In this paper, it is shown that for a quantum system to have an underlying deterministic dissipative dynamics, the time variable should be discrete if the continuity of its temporal evolution is required. Besides, the underlying deterministic theory also imposes restrictions on the energy spectrum of the quantum system. It is also found that quantum symmetry at the ''atomic scale'' can be induced from 't Hooft's coarse graining classification of primordial states at the ''Planck scale.'' © *2001 American Institute of Physics.* [DOI: 10.1063/1.1380250]

I. INTRODUCTION

Recently, Gerard't Hooft postulated that there should be a dissipative deterministic theory underlying quantum gravity at the so-called ''Planck scale.'' [1,2] In his theory, the generic quantum mechanics is no longer the crucial starting point. Rather, a deterministic theory with dissipation of information at the ''Planck scale'' is needed to derive quantum mechanics at the ''atomic scale.'' It seems that this viewpoint can solve problems concerning locality and causality in the so-called Planck scale physics such as quantum gravity, which are quite different from those in the usual quantum field theories in some flat background space–time based on the holographic principle in quantum gravity theory.[3]

In 't Hooft's opinion, at the ''atomic scale'' quantum states are equivalence classes of primordial states at the ''Planck scale.'' In Ref. 4, this point of view was illustrated through a simple model. According to 't Hooft, if we only care about the temporal evolution of equivalence classes, the information within each equivalence class could be ignored. Then from a non-time-reversible evolution, which characterizes a deterministic process with dissipation at the ''Planck scale,'' we can obtain a time-reversible evolution of the properly defined equivalence classes of primordial states. Taking the equivalence classes to be quantum states we are then able to introduce a reversible evolution law at the ''atomic scale.'' Apparently, here the central problem is how to classify the Planck scale states with respect to a deterministic evolution. 't Hooft's solution to this problem is as follows. He argues that two Planck scale states are equivalent at the ''atomic scale'' if, after some finite time interval, they evolve into the same state. This leads to a natural definition of equivalence classes: Two states are in the same equivalence class if and only if they evolve into the same state after some finite time interval. Then, quantum states are identified with these equivalence classes.

Most recently we made clear the mathematical structure of 't Hooft's theory using quotient space construction and related concepts.[5] Let the primordial states span a linear space. We find that

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the equivalence classes defined by 't Hooft can be identified with the cosets of the invariant subspace spanned by those primordial states annihilated by the time-evolution operator. Thus the Hilbert space of quantum states is just the corresponding quotient space and the time-reversible evolution at the ''atomic scale'' can naturally be induced on the quotient space by the dissipative deterministic evolution operator. Following this line, in this paper, we will make a further analysis of the mathematical aspect of 't Hooft's theory and then discuss some physical consequences implied in the theory. We will also probe the spectral structure of finite dimensional quantum system with an underlying deterministic structure and extend 't Hooft's idea to study quantum symmetry problem.

II. SOME MATHEMATICAL RESULTS

In this section we present some mathematical results closely related to the 't Hooft equivalence class theory. In the following, I, J stand for index sets not necessarily finite; if V_1 is a subspace of $V, v \in V$, the element $v+V_1$ in the quotient space V/V_1 is denoted by $\overline{v}$. All the vector spaces to be considered are over the complex number field. Physically, one should bear in mind that V will be the linear space spanned by so-called primordial states at the ''Planck scale'' (see the following). For convenience, we list the mathematical definitions of some concepts appearing in 't Hooft's theory as follows.

Definition 1: A linear operator $T \in \mathrm{End}(V)$ is called deterministic if there exists a basis $\{v_i | i \in I\}$ of V on which T acts in the following way: $\forall i \in I$, $\exists i' \in I$ s.t. $Tv_i = v_{i'}$. Such a basis is called a T-deterministic basis. If, moreover, T is singular (noninvertible), then it is called dissipative deterministic.

Remark 1: In 't Hooft theory, T represents a deterministic time-evolution process (with dissipation) at the ''Planck scale.''

Definition 2: An injective map from a set to itself is called a permutation of the set. A linear operator $T \in \mathrm{End}(V)$ is called a permutation operator if there exists a basis of V on which T act as a permutation.

Definition 3: A linear operator on a vector space is called unitarizable if there exists an inner product on the vector space such that it is unitary relative to it.

Remark 2: Physically, time-reversible evolution is described by a unitary operator, and a reversible but not unitarizable operator usually does not correspond to any practical evolution in quantum mechanics.

Definition 4: Let V and W be two vector spaces, $T \in \mathrm{End}(V)$ and $S \in \mathrm{End}(W)$. If there exists an isomorphism φ between V and W such that $\varphi T = S\varphi$, T and S are called equivalent.

Having prepared the above-given definitions, we now state one of our central results.

Proposition 1: Let V be a vector space, $T \in \mathrm{End}(V)$ is dissipative deterministic and V_1 is a T-invariant subspace such that the induced operator $\overline{T}$ on the quotient space V/V_1 is nonsingular, then $\overline{T}$ is a permutation operator; conversely, if $S \in \mathrm{End}(V)$ is a permutation operator, then there exists a vector space V', a dissipative deterministic operator $S' \in \mathrm{End}(V')$, and an S'-invariant subspace V_1' of V' such that the induced operator $\overline{S'} \in \mathrm{End}(V'/V_1')$ is equivalent to S.

Proof: Let $\{v_i | i \in I\}$ be a T-deterministic basis. Then there exists a subset $J \subset I$ such that $\{\overline{v_i} | i \in J\}$ is a basis of V/V_1. By definition

$$\overline{T}\,\overline{v_i} = \overline{Tv_i} = \overline{v_{i'}}, \quad (i, i' \in I). \tag{1}$$

As $\overline{T}$ is nonsingular, we clearly see that $\overline{T}$ acts as a permutation on the basis $\{\overline{v_i} | i \in J\}$. This proves the first half of the proposition. For the second half, let $\{v_i | i \in I\}$ be a basis of V on which S acts as a permutation, take an arbitrary element $w \notin V$, and define

$$V' = \mathrm{span}\{v_i, w | i \in I\},$$

$V_1'=V$. Define $S'\in \mathrm{End}(V')$ such that $S'|_V=S$ and $S'w=0$. It is then trivial to verify that S' is dissipative deterministic and $\overline{S'}$ is equivalent to S. The proposition is thus proved.

Remark 3: This proposition, as we will see in the following, tells us that 't Hooft 's underlying dissipative deterministic dynamic law at the ''Planck scale'' can only produce very special time-reversible evolution at the ''atomic scale.''

Keep the notations in the above-given proposition. We have the following corollary.

Corollary: If V/V_1 is finite dimensional, then $\overline{T}$ is unitarizable.

Proof: According to the proposition, there is a basis of V/V_1 on which $\overline{T}$ acts as a permutation. If $\dim V/V_1<\infty$, $\overline{T}$ is periodic, namely, there exists a positive integer n such that $\overline{T}^n=1$. Let p be its period. Choose an arbitrary inner product $(,)$ on V/V_1 and define a new inner product $\langle,\rangle$ as follows:

$$\langle\overline{v},\overline{w}\rangle=\sum_{j=1}^{p}(\overline{T}^j\overline{v},\overline{T}^j\overline{w}),\quad \forall\overline{v},\overline{w}\in V/V_1. \tag{2}$$

It is then easy to show that $\overline{T}$ is unitary relative to the inner product $\langle,\rangle$.

Proposition 1 shows us that an invertible linear operator can be induced from a deterministic operator T if and only if it is a permutation operator. The following proposition characterizes the permutation operator on a finite dimensional space.

Proposition 2: Let V be a finite dimensional vector space, $T\in\mathrm{End}(V)$. T is a permutation operator if and only if it is diagonalizable and its eigenvalues can be grouped into some classes, say, $\Delta_{n_1},\Delta_{n_2},\cdots,\Delta_{n_r}$, such that Δ_{n_j} $(j=1,2,\cdots,r)$ exactly consists of the n_j n_jth roots of unity with the same multiplicity.

Proof: Let $\{v_i|i=1,2,\cdots,n\}$ be a basis on which T acts as a permutation. First, suppose T is a cyclic permutation of the basis, namely, we have

$$Tv_1=v_2,Tv_2=v_3,\cdots,Tv_{n-1}=v_n,Tv_n=v_1. \tag{3}$$

Then T is a periodic operator of period n, and its minimal polynomial is λ^n-1. Consequently, T is diagonalizable and its eigenvalues are $\exp(i\,2k\pi/n)$ $(k=1,2,\cdots,n)$, the nth roots of unity. Now let T act as a general permutation on the basis. We notice that the basis elements can be grouped into some classes on each of which T acts as a cyclic permutation. Thus the ''only if'' part of the proposition easily follows.

Conversely, suppose T is diagonalizable and its eigenvalues can be grouped into some classes $\Delta_{n_1},\Delta_{n_2},\cdots,\Delta_{n_r}$ in such a way that Δ_{n_j} $(j=1,2,\cdots,r)$ exactly consists of the n_j n_jth roots of unity with multiplicity m_j. Then there is a basis $\{v_{k,l}^j|j=1,2,\cdots,r;\ k=1,2,\cdots,n_j;\ l=1,2,\cdots,m_j\}$ such that

$$Tv_{k,l}^j=\exp\left(i\frac{2k\pi}{n_j}\right)v_{k,l}^j. \tag{4}$$

Define the subspace $V_{j,l}$ of V as follows:

$$V_{j,l}=\mathrm{span}\{v_{k,l}^j|k=1,2,\cdots,n_j\}.$$

Clearly, we have

$$V=\sum_{j=1}^{r}\sum_{l=1}^{m_j}\oplus V_{j,l}$$

and from the proof of the "only if" part we know in each subspace $V_{j,l}$ there is a basis on which T acts as a cyclic permutation of order m_j. Put together, these bases of the subspaces form a basis of V on which T acts as a permutation. This proves the "if" part of the proposition.

III. DYNAMICS FROM 'T HOOFT'S THEORY

In this section we focus on the physical aspect of 't Hooft's theory, but our analysis depends on the above-mentioned mathematical results.

In 't Hooft's theory, primordial states at the "Planck scale" need not form a linear space. Generally they can be denoted by a set $\Sigma=\{\phi_i|i\in I\}$. *The underlying deterministic evolution is a transformation U (usually depending on time) of* Σ *to itself. If U has no inverse it is called a dissipative deterministic evolution*. Obviously, it can be represented by a matrix with the entries 0 or 1 if I is a finite set. As U is an evolution operator, we write it as $U=U(t_f,t_i)$ by convention. Physically, it represents the evolution in the time interval $[t_i,t_f]$. Certainly the evolution should satisfy the so-called semigroup condition

$$U(t_f,t_m)U(t_m,t_i)=U(t_f,t_i),$$
$$U(t,t)=1. \tag{5}$$

If U is singular, it describes deterministic process with dissipation. As a matter of fact, under such an evolution some states will disappear and some states will evolve into the same state, or in other words, some states with a different past may have the same deterministic fate. 't Hooft thinks that if two states evolve in such a way that their futures are identical they should represent the same state at the "atomic scale." In this view, he divides the elements of Σ into equivalence classes, ϕ_{i_1} and $\phi_{i_2}(i_1,i_2\in I)$ being in the same equivalence class if they are evolved into the same state after finite time interval. Denote by $\Xi=\{\overline{\phi_j}|j\in J\}$ the set of the equivalence classes. Then 't Hooft postulates that the space of quantum states is spanned by $\{\overline{\phi_j}|j\in J\}$ and claims that the reduced evolution on the space of quantum states is reversible. We can mathematically reformulate 't Hooft's theory as follows.[5] We assume that the evolution operator $U(t_2,t_1)$ only depends on the difference of t_2 and t_1, i.e., we can write $U(t_2,t_1)=U(t_2-t_1)$. This is in the spirit of 't Hooft's original construction. Then the evolution at the "Planck scale" is determined by the operator $U(t,0)\triangleq U(t)$. Let V be the vector space spanned by $\{\phi_i|i\in I\}$. Then $U(t)$ can be extended to a *deterministic operator* on V. We call V the space of primordial states in spite of the fact that generally it contains elements which are not states. Let V_1 denote the subspace of V consisting of the vectors annihilated by $U(t)$ at some t, namely, a vector v belongs to V_1 if and only if there exists some $U(t)$ such that $U(t)v=0$. Then it follows that *the space of quantum states is none other than the quotient space*

$$Q=V/V_1=\{|\phi\rangle\triangleq\phi+V_1|\phi\in V\}$$

and a nonsingular evolution law of the quantum states naturally follows from $U(t)$. Let $\overline{v}\equiv|\nu\rangle$ denote the equivalence class containing v. We notice that V_1 is invariant under $U(t)$. Thus $U(t)$ induces a natural action on the quotient space Q. We denote the induced operator by $\overline{U(t)}$, then we have

$$\overline{U(t)}\,\overline{v}=\overline{U(t)v}. \tag{6}$$

The following simple result is easy to prove.

Proposition 3: $\overline{U(t)}$ is nonsingular.

In fact, if $\overline{U(t)}\,\overline{v}=\overline{0}$, then $U(t)v\in V_1$. Thus there exists some t' such that $U(t')U(t)v=0$. It then follows that

$$U(t')U(t)v=U(t'+t)v=0. \tag{7}$$

By definition this means $v \in V_1$, i.e., $\overline{v}=\overline{0}$. This proves the nonsingularity of $\overline{U(t)}$.

Remark 4: In Refs. 1 and 2, 't Hooft just claims the nonsingularity of the induced evolution operator. But it should be pointed out that if the condition $U(t_2,t_1)=U(t_2-t_1)$ is not satisfied the induced evolution $\overline{U(t_2,t_1)}$ might be singular if we still use 't Hooft's principle to classify the primordial states.

We are now in a position to discuss a consequence of 't Hooft's theory. The basis consisting of the equivalence classes is called the primordial basis by 't Hooft. In our notations, $\{\overline{\phi_j}|j \in J\}$ is the primordial basis and $\overline{U(t)}$ is a (dissipative) deterministic operator on V. As we have proved the nonsingularity of $\overline{U(t)}$, it follows from Proposition 1 that $\overline{U(t)}$ is a permutation operator which acts as a permutation on the primordial basis. Then we easily observe that if we require $\overline{U(t)}$ to be continuous with respect to t, the time variable should be discrete. For example, if J is a finite set, or in other words, the quantum Hilbert space is finite dimensional, the induced evolution operator $\overline{U(t)}$ is represented as a matrix with the entries 0 or 1 with respect to the primordial basis. Clearly, it could not be continuous if the time variable is not discrete.

IV. SPECTRUM AND HAMILTONIAN

Let us turn to consider restrictions on the energy spectrum of quantum system imposed by the underlying determinism. Due to the arguments in the last paragraph, we assume the time variable to be discrete. Without losing generality, let the time t take values in Z^+, the set of non-negative integers. The deterministic evolution and the induced evolution of the quantum system is then completely determined by the operator $U(1)$. Suppose $\overline{U(1)}$ is unitary. It is then can be written as $\overline{U(1)}=e^{-iH}$, where H is a Hermitian operator describing the Hamiltonian of the quantum system. Now if the quantum system is finite dimensional it follows from Proposition 2 that the eigenvalues of $\overline{U(1)}$ are of the form $e(-i\,2k\pi/n)$. Thus we have the following

Proposition 4: The eigenvalues of H corresponding to the induced evolution $\overline{U(1)}=e^{-iH}$ of quantum states lie in the set

$$\left\{ \frac{2k\pi}{n} \pm 2m\pi \middle| k,n,m \in Z^+ \right\}.$$

Remark 5: We have seen that evolutions that can be induced from dissipative deterministic evolutions at the ''Planck scale'' belong to a special class. First, there is a rather strict restriction on the corresponding Hamiltonian H. Second, if a quantum system with an underlying deterministic structure as is described by 't Hooft is initially in the state represented by an element of the primordial basis then the evolution will never cause coherent superposition of quantum states. As these drawbacks are inherent in the theory, to remove them we have to generalize the underlying dynamic law at the ''Planck scale.''

Another conclusion that can be drawn from Proposition 1 is that 't Hooft's theory is closely related to the hidden variable theory. Since $\overline{U(t)}$ acts as a permutation on the primordial basis of the space of quantum states, an operator that is diagonal now with respect to this basis will continue to be diagonal in the future. Such an operator could thus be thought to represent a hidden variable. This suggests that a quantum system with an underlying dissipative deterministic mechanism might permit some kind of hidden variable theory. The corollary to Proposition 2 also shows us that if $U(t)$ is a dissipative deterministic such that the quotient space V/V_1 is finite dimensional $\overline{U(t)}$ can be made unitary by properly introducing an inner product. Then $\overline{U(t)}$ can be regarded as an evolution operator for a quantum system. But on the other hand, such inner product is not at all unique. Since a correct quantum theory requires a Hilbert space with properly defined inner product to define probability, this is really a problem if we wish to derive quantum dynamics from a dissipative deterministic evolution, not just to interpret a given quantum system as governed by an underlying deterministic mechanism. So a gap remains to be bridged between the so-called Planck scale physics and the atomic scale physics in 't Hooft's theory.

Before passing to discuss quantum symmetry we would like to present a simple quantum system which has some characteristics of a deterministic system as shown previously. We consider the following quantum system: A spinless free particle in the one-dimensional region $[0,L]$ with the boundary condition $\psi(0,t)=\psi(L,t)$, where $\psi(x,t)$ is the wave function. The Hilbert space of the system is

$$\mathcal{H}=\{\psi\in\mathcal{L}^2[0,L]\psi(0)=\psi(L)\}.$$

Clearly,

$$\Delta=\left\{\exp\left(i\frac{2k\pi}{L}x\right)k=0,\pm1,\pm2,\cdots\right\}$$

is a basis of $\mathcal{H}$. In the case of extreme relativity, the Hamiltonian of the system is $H=-i\hbar c(d/dx)$, *where c* is the speed of light. Define $\overline{U(t)}=e^{-iHt}$. We have

$$\overline{U(t)}\exp\left(i\frac{2k\pi}{L}x\right)=\exp\left(-i2k\pi\frac{\hbar c}{L}t\right)\exp\left(i\frac{2k\pi}{L}x\right). \tag{8}$$

We observe that if we take the time to be discrete, it is then possible to define a time unit such that the one step evolution acts on Δ in the following way:

$$\overline{U(1)}\exp\left(i\frac{2k\pi}{L}x\right)=\exp\left(i\frac{2k\pi}{L}x\right).$$

We then see that this system might be regarded as a deterministic system and Δ might serve as primordial basis for the system. If we normalize $\hbar c/L$ as one energy unit, then the energy spectrum of the system is $\{2k\pi|k=0,\pm1,\pm2,...\}$. This is consistent with our previous discussion.

Remark 6: It should be pointed out that the above-mentioned simple example is essentially the same as the example of massless neutrinos discussed in Ref. 1.

V. QUANTUM SYMMETRY BY COARSE GRAINING

As shown previously, 't Hooft's classification of primordial states implies a scheme for coarse graining. Usually, for a large close system a coarse graining process can result in quantum dissipation and decoherence in the subsystem.[6] But here the converse seems to be the case: Coarse graining (or classification) can lead to a unitary dynamics for the effective system even if the evolution of primordial system is not time reversible. Since ''symmetry dominates dynamics,'' it is rather natural to probe the role of coarse graining in generating symmetry at the ''atomic scale.''

Let a deterministic system be described by an evolution operator $\overline{U(t)}$, and let $\{\overline{\phi_j}|j\in J\}$ be the primordial basis for the system. Denote by P^J the permutation group of the set J. According to Proposition 1, $\overline{U(t)}$ is a permutation operator and can be identified with an element of P^J. By definition, the group of quantum symmetry consists of those unitary operators on the state space that commute with the evolution operator. If we require that these unitary operators be induced from deterministic operators on the space of primordial states, it then follows from Proposition 1 that they belong to the centralizer of $\overline{U(t)}$ in P^J. If the space of quantum states is finite dimensional, by the trick of redefining inner product as is used in the proof of the corollary to Proposition 1, we can show that there exists an inner product such that both $\overline{U(t)}$ and the operators in its centralizer in P^J are unitary operators. Thus in this case it might be reasonable to take the group of quantum symmetry to be the centralizer of $\overline{U(t)}$ in P^J. Anyway, the symmetry group is a discrete group.

We have seen that if we adhere to the principle that things happening in the space of primordial states bear the mark of determinism, then logically, things happening in the space of quantum states bear the mark of discreteness. To change the situation we need to loosen the restriction of

determinism in the strict sense of this word used by 't Hooft. Let us conclude this paper with a short discussion of quantum symmetry derived from a not necessarily deterministic operator on the space of primordial states. Let V be the space of primordial states and $S \in \mathrm{End}(V)$ satisfies $SV_1 \subset V_1$.

Proposition 5: $\overline{U(t)S} - \overline{SU(t)} = 0$ if and only if there exists some t' such that

$$U(t')(U(t)S - SU(t)) = 0. \tag{9}$$

The proof of this result is immediate. It directly follows from Eq. (9) that $(U(t)S - SU(t))V \subset V_1$ (cf. Sec. III). In other words, we have

$$\overline{U(t)S} - \overline{SU(t)} = 0. \tag{10}$$

This proves the ''if'' part. The ''only if'' part can be proved by reversing the deduction.

If the time is discrete and takes values in Z^+, then the evolution at the ''Planck scale'' is determined by $U(1) \triangleq U$. Notice that $U^n = U(n)$ in this case. It follows that Eq. (9) is equivalent to

$$U^n(US - SU) = 0 \tag{11}$$

for some positive integer n. Let us take 't Hooft's example in Ref. 1 to illustrate the above-mentioned idea. We have

$$U = \begin{pmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{12}$$

Let $e_1 = (1\,0\,0\,0)^T$, $e_2 = (0\,1\,0\,0)^T$, $e_3 = (0\,0\,1\,0)^T$, $e_4 = (0\,0\,0\,1)^T$. Then

$$\overline{U} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

with respect to the basis $\{\overline{e_i} | i = 1,2,3\}$. The general matrix T that commutes with $\overline{U}$ is of the form

$$T = \begin{pmatrix} a & b & c \\ b & a & c \\ j & j & k \end{pmatrix}.$$

Suppose $SV_1 \subset V_1$. Then the general solution of Eq. (11) is

$$S = \begin{pmatrix} a & b & c & b \\ b-m & f & g & f \\ j & j & k & j \\ m & a-f & c-g & a-f \end{pmatrix}.$$

It is clear that for each T commuting with $\overline{U}$ there exists S such that $\overline{S} = T$. In fact, as $\overline{e_2} = \overline{e_4}$, the above S has the representation

$$\overline{S}=\begin{pmatrix} a & b & c \\ b & a & c \\ j & j & k \end{pmatrix} \tag{13}$$

with respect to the basis $\{\overline{e_i}|i=1,2,3\}$. Mathematically, this is a trivial fact. On the other hand, we have

$$US-SU=\begin{pmatrix} 0 & 0 & 0 & 0 \\ a-f & m & c-g & m \\ 0 & 0 & 0 & 0 \\ -a+f & -m & -c+g & -m \end{pmatrix}.$$

This simply means that for $\overline{S}$ to commute with $\overline{U}$, S does not necessarily commute with U.

In the representation where $\overline{U}$ is diagonal we have

$$\overline{U}=\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

Thus the matrix T that commutes with $\overline{U}$ takes a block diagonal form. It then follows that the symmetry group of the system is $U(2)\times U(1)$. But if we impose the restriction that S is a deterministic operator, as is required by determinism, it then turns out that the set of nonsingular $\overline{S}$ commuting with $\overline{U}$ is $\{1,\overline{U}\}$, the centralizer of $\overline{U}$ in P^3.

To sum up, if we loosen the restriction of determinism it is possible to induce quantum symmetry from transformations on the space of primordial states through a procedure of coarse graining as shown previously. On the other hand, quantum symmetry at the ''atomic scale'' does not necessitate symmetry at the ''Planck scale.''

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Soliton asymptotics of nondecaying solutions of the modified Kadomtsev–Petviashvili–I equation

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We prove the existence of nondecaying real solutions of the mKP-I equation, vanishing for $x\to+\infty$, and we obtain asymptotic formulas as $t\to\infty$ in the form of an infinite series of asymptotic solitons with curved lines of constant phase and varying amplitude and width. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Investigations of long-time asymptotic behavior of nondecaying at infinity solutions of nonlinear evolution equations in $2+1$ dimensions (two spatial and one time variables) are closely related to the corresponding investigations in $1+1$ dimensions. A. V. Gurevich and L. P. Pitaevsky studied in 1973 the nondecaying solution of the Korteweg–de Vries (KdV) equation, which describes the evolution of the initial step-function $u(x,0)$:[1,2]

$$u_t-6uu_x+u_{xxx}=0,$$

$$u(x,0)=\begin{cases}0 & \text{if } x>0,\\ -c^2 & \text{if } x\leqslant 0.\end{cases}$$

They applied the Whitham method to construct an approximation of this solution by a cnoidal wave with slowly varying parameters, and detected the presence of many strong solitonlike oscillations on the front of the solution for large time. This approximate solution satisfies the KdV equation with error vanishing for $t\to+\infty$. Thus, they conjectured that solutions of the Cauchy problem with initial steplike data split into an infinite sequence of solitons for $t\to\infty$.

However, this conjecture seemed to contradict the idea that solitons were generated by the discrete spectrum of the L-operator since a Schrödinger operator whose potential is a step-function has no discrete spectrum.

The situation was clarified in 1975 by E. Ya. Khruslov in Ref. 3. He showed that these solitonlike oscillations are not generated by the discrete spectrum but by the continuous spectrum of multiplicity one of the Schrödinger operator, i.e., the L-operator of the KdV equation. Later on, these solitons were called ''asymptotic solitons.'' An analogous phenomenon of splitting of nondecaying at infinity initial data into infinite series of solitons was then found for other integrable nonlinear equations (nonlinear Schrödinger equation, sine–Gordon equation, modified Korteweg–de Vries equation and the Toda lattice).[4–8]

In Refs. 9–12, the method proposed by E. Ya. Khruslov in Ref. 3 was extended to the investigation of the asymptotic behavior of nondecaying solutions of the Kadomtsev–Petviashvili (KP) equation for $t\to\infty$. Within the framework of the Zakharov–Shabat scheme,[13] the solutions of the KP equation, vanishing for $x\to\infty$ and bounded for any fixed x,y,t, were obtained, and their

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large-time asymptotic form was proved to be an infinite series of solitons with curved lines of constant phase in a neighborhood of the front for $t\to\infty$. These asymptotic solitons were called ''curved asymptotic solitons.'' Recently,[14] V. E. Zakharov also considered a curved soliton of the KP–II equation, but in another space-time domain.

Our goal is to prove the phenomenon of splitting of nondecaying solutions of the modified Kadomtsev–Petviashvili–I (mKP-I) equation into an infinite series of solitons for $t\to\infty$. The mKP equation was introduced by B. G. Konopelchenko in Ref. 15 as a natural two-dimensional generalization of the modified Korteweg–de Vries (mKdV) equation, and it has the form

$$v_t+\frac{1}{4}v_{xxx}-\frac{3}{2}\alpha^2\left(v_xv^2-v_x\int_x^\infty v_y\,dx'+\frac{1}{2}\int_x^\infty v_{yy}\,dx'\right)=0,$$

where $v=v(x,y,t)$ and

$$\alpha=\begin{cases}1 & \text{for the mKP-II equation,}\\ i & \text{for the mKP-I equation.}\end{cases}$$

This equation was integrated by the $\overline{\partial}$-method (see Ref. 16), and both ''lump solutions'' [vanishing as $(x^2+y^2)^{-1}$] and ''plane solitons'' were obtained.

A scheme of integration of the mKP equation by the inverse scattering method, which is an analog of the Zakharov–Shabat method for the KP equation, was introduced in Ref. 11. According to this scheme, a solution has the form

$$v(x,y,t)=\frac{1}{\alpha}\frac{\mathrm{d}}{\mathrm{d}x}\ln\left(1+\int_x^\infty K(x,s,y,t)\mathrm{d}s\right),\tag{1.1}$$

where the function $K(x,s,y,t)$ is a solution of the Marchenko integral equation

$$K(x,z,y,t)+F(x,z,y,t)+\int_x^\infty K(x,\xi,y,t)F(\xi,z,y,t)\mathrm{d}\xi=0\tag{1.2}$$

viewed as an equation with respect to z, with x,y,t as parameters. The kernel $F(x,z,y,t)$ of (1.2) satisfies the system of linear differential equations

$$\begin{cases}F_t+F_{xxx}+F_{zzz}=0,\\ \alpha F_y+F_{xx}-F_{zz}=0.\end{cases}\tag{1.3}$$

A large class of solutions of (1.3) for $\alpha=i$ can be found by the Fourier method as follows:

$$F(x,z,y,t)=\int\int_\Omega \exp[ip(x-z)-q(x+z)+2qf(p,q,Y)t]\mathrm{d}\mu(p,q),\tag{1.4}$$

where $f(p,q,Y)=q^2-3p^2+2pY$, $Y=y/t$, and the measure $\mathrm{d}\mu(p,q)$ $(p+iq\in\mathbb{C})$ is defined on a set $\Omega\subset\mathbb{C}$.

In Sec. II we introduce two functions $C(s)$ and $g(s)$, and using them we construct a set Ω and a measure $\mathrm{d}\mu$ of a special form. Then we prove that the scheme (1.1)–(1.4) determines the existence of a nondecaying real solution of the mKP-I equation, vanishing for $x\to\infty$ and bounded for any fixed x,y,t.

In Sec. III we state and prove the theorem about splitting of the solutions in a neighborhood of the front into a series of solitons of the form

$$v_n(x,y,t)=-\frac{2q_0(Y)^2}{p_0(Y)+\sqrt{p_0^2(Y)+q_0^2(Y)}\cosh[2q_0(Y)\kappa_n(x,y,t)]},$$

$$\kappa_n(x,y,t)=x-C(Y)t+\frac{1}{2q_0(Y)}(\ln t^{n+1/2}-\ln g(Y)-\ln \phi_n(Y)),$$

where the domain of investigations and the functions $q_0(Y)$, $p_0(Y)$, $\phi_n(Y)$ are completely determined by the functions $C(Y)$ and $g(Y)$.

In Sec. IV we give two examples of curved asymptotic solitons. For example, if $C(Y)=Y^2/3+b^2$, then $q_0(Y)=b$, $p_0(Y)=Y/3$.

II. EXISTENCE OF SOLUTIONS OF THE mKP–I EQUATION

To construct a mKP-I solution by the scheme (1.1)–(1.4) we must define the set Ω in (1.4) and the measure $d\mu(p,q)$ over this set. For this goal we introduce two positive functions $C(s)$ and $g(s)$ which play an important role in the construction of the solution and in the investigation of its asymptotic behavior. We introduce the following conditions.

Condition A: The function $C(s):\mathbb{R}\to\mathbb{R}^+$ is C^∞ and such that

$$C(s)>s^2/3+\delta^2 \quad (\delta=\text{const}>0),$$
$$C''(s)>0. \tag{2.1}$$

Condition B: The set $\Omega\subset\mathbb{R}^2$ has the form

$$\Omega=\{(p,q)\,|\,-\infty<p<\infty,\ 0<\varepsilon\leqslant q\leqslant h(p)\}, \tag{2.2}$$

where $q=h(p)$ is the envelope of the family of hyperbolas

$$f(p,q,s)=C(s), \tag{2.3}$$

which touch it at the point

$$(p_0(s),q_0(s))=(C'(s)/2,\ \sqrt{C(s)+\tfrac{3}{4}(C'(s))^2-sC'(s)}). \tag{2.4}$$

Remark: Conditions A and B imply that

$$C(s)=\max_{(p,q)\in\Omega} f(p,q,s), \tag{2.5}$$

and for any $s\in\mathbb{R}$ this maximum is attained at a unique point, $(p_0(s),q_0(s))$.

Condition C: The function $g(s):\mathbb{R}\to\mathbb{R}^+$ is of class C^∞ and such that the real positive function $\tilde g(p,q)\in C^\infty$, $\tilde g(p_0(s),q_0(s))=g(s)$, satisfies the inequality

$$\forall a=\text{const}>0:\quad \int\int_\Omega e^{a(q+|p|)}\tilde g(p,q)\,dp\,dq<\infty. \tag{2.6}$$

Condition D: The measure $d\mu$ has the form

$$d\mu(p,q)=\tilde g(p,q)\sqrt{\frac{p-iq}{p+iq}}\,dp\,dq. \tag{2.7}$$

Lemma 1: Assume that Conditions A–D are fulfilled. Then the scheme (1.1)–(1.4) determines a smooth real solution of the mKP-I equation vanishing as $x\to\infty$ and bounded for all fixed x,y,t.

Proof: Define an operator $\hat F$ acting in $L^2[x,\infty)$ by the formula

$$[\hat F h](z)=\int_x^\infty F(s,z,y,t)h(s)\,ds,$$

where the kernel F is given by (1.4). The function $h(s)$ depends on the parameters y,t as well. Since

$$\|\hat{F}\|^2_{L^2[x,\infty)} = \int_x^\infty \int_x^\infty |F(x,z,y,t)|^2 \mathrm{d}s\mathrm{d}z$$
$$\leqslant \frac{1}{4\varepsilon^2} \int \int_\Omega \tilde{g}(p,q)\mathrm{d}p\mathrm{d}q \int \int_\Omega \exp[4q(|x|+f(p,q,Y))t]\tilde{g}(p,q)\mathrm{d}p\mathrm{d}q$$
$$\leqslant \frac{1}{4\varepsilon^2} \int \int_\Omega \tilde{g}(p,q)\mathrm{d}p\mathrm{d}q \int \int_\Omega e^{aq}\tilde{g}(p,q)\mathrm{d}p\mathrm{d}q,$$

condition C gives $\|\hat{F}\|_{L^2[x,\infty)}<\infty$, i.e., $\hat{F}$ is a Hilbert–Schmidt operator. Hence, $\hat{F}$ is a compact operator.[17]

The adjoint operator $\hat{F}^*$ is given by

$$[\hat{F}^*\psi](z) = \int_x^\infty \overline{F(z,s,y,t)}\psi(s)\mathrm{d}s,$$

where

$$\overline{F(z,x,y,t)} = \int \int_\Omega \exp[ip(x-z)-q(x+z)+4pqy-2q(3p^2-q^2)t] \sqrt{\frac{p-iq}{p+iq}}\, \tilde{g}(p,q)\mathrm{d}p\mathrm{d}q.$$

Let us consider the homogeneous equation

$$\psi+\hat{F}^*\psi=0. \tag{2.8}$$

Multiplying (2.8) with $\overline{\psi}$, we obtain by integration

$$\|\psi\|^2 - \int \int_\Omega \tilde{g}(p,q)\frac{p}{\sqrt{p^2+q^2}} e^{-2q(3p^2-q^2)t+4pqy} \left| \int_x^\infty e^{(ip-q)s}\psi(s)\mathrm{d}s \right|^2 \mathrm{d}p\mathrm{d}q$$
$$= i \int \int_\Omega \tilde{g}(p,q)\frac{q}{\sqrt{p^2+q^2}} e^{-2q(3p^2-q^2)t+4pqy} \left| \int_x^\infty e^{(ip-q)s}\psi(s)\mathrm{d}s \right|^2 \mathrm{d}p\mathrm{d}q.$$

Since $q>0$, $\tilde{g}(p,q)>0$, the right-hand side of this equation is $\neq 0$. Therefore, Eq. (2.8) has only the trivial solution. Then, Fredholm's theory[17] implies that Eq. (1.2) is solvable for any x,y,t.

According to (1.4) and conditions C and D, $F(x,z,y,t)$ is a C^∞ function with respect to all variables. We can show[18] that the function $K(x,z,y,t)$ is C^∞, too.

Since the set Ω lies inside the upper half-plane ($q\geqslant\varepsilon>0$), $F(x,z,y,t)$ vanishes exponentially as $x+z\to\infty$. Therefore $K(x,z,y,t)$ and its derivatives vanish exponentially also as $x\to+\infty$.

Now let us address the formula (1.1) for the mKP-1 solution. First of all we will show that $K(\cdot,s,\cdot,\cdot)\in L^1[x,\infty)$. Conditions C and D allow us to show that $\|F(\cdot,s,\cdot,\cdot)\|_{L^1(x,\infty)}<\infty$. Now (1.2) implies that the function

$$\Phi(x,a,y,t) = \int_a^\infty K(x,z,y,t)\mathrm{d}z \quad (a\geqslant x)$$

satisfies

$$\Phi(x,a,y,t) + \int_x^\infty \Phi(x,s,y,t)D(s,a,x,y,t)\mathrm{d}s = B(x,a,y,t) \tag{2.9}$$

with

$$B(x,a,y,t)=-\frac{A(x,a,y,t)}{1+A(x,x,y,t)},$$

$$D(s,a,x,y,t)=A_s(s,a,y,t)-\frac{A(x,a,y,t)}{1+A(x,x,y,t)}A_s(s,x,y,t),$$

$$A(x,a,y,t)=\int_a^\infty F(x,z,y,t)\mathrm{d}z,$$

where $A_s(x,a,y,t)=(\partial/\partial s)\,A(s,a,y,t)$. Since $\mathrm{Re}\,A(x,x,y,t)=0$, the kernel $D(s,a,x,y,t)$ and the right-hand side of (2.9) are well defined. Equation (2.9) is a Volterra equation with respect to a and x,y,t are parameters. Application of the successive approximation method to (2.9) gives

$$|\Phi(x,x,y,t)|<\infty. \tag{2.10}$$

Hence, $K(\cdot,s,\cdot,\cdot)\in L^1[x,\infty)$.

Let us show now that

$$\int_x^\infty K(x,s,y,t)\mathrm{d}s\neq -1.$$

Suppose that $\int_x^\infty K(x,s,y,t)\mathrm{d}s=-1$. Then it follows immediately from (2.9) that $\Phi(x,a,y,t)$ satisfies the homogeneous integral equation

$$\Phi(x,a,y,t)+\int_x^\infty \Phi(x,s,y,t)A_s(s,a,y,t)\mathrm{d}s=0. \tag{2.11}$$

We can easily show by the above method that for any $a\geqslant x$ this equation has only the trivial solution. Therefore, $\int_x^\infty K(x,s,y,t)\mathrm{d}s\neq -1$, and (1.1) has sense.

Now we shall prove that the constructed mKP-I solution is real-valued. Analysis of (1.1) implies that it is sufficient to show that

$$\frac{\partial}{\partial x}(2\,\mathrm{Re}\,\Phi(x,x,y,t)+|\Phi(x,x,y,t)|^2)=0. \tag{2.12}$$

First of all, note that

$$\overline{A(x,z)}=-A(z,x). \tag{2.13}$$

Consider the equation conjugated to (2.9). After multiplication of (2.9) by $(\partial/\partial a)\,\Phi(x,a,y,t)$ and integration with respect to a from x to $+\infty$ we obtain

$$\begin{aligned} g(\Phi)=\Phi(x,x,y,t)(A(x,x,y,t)+1)+A(x,x,y,t)(\overline{\Phi(x,x,y,t)}+1)+A(x,x,y,t)|\Phi(x,x,y,t)|^2 \\ +\left((\hat{A}\Phi(x,a,y,t),\Phi(x,a,y,t))-\int_x^\infty \overline{\Phi(x,a,y,t)}\Phi_a(x,a,y,t)\mathrm{d}a\right)=0, \end{aligned} \tag{2.14}$$

where $\hat{A}:L^2[x,\infty)\to L^2[x,\infty)$ has the form

$$(\hat{A}\varphi)(s)=\int_x^\infty \overline{A_{sa}}(s,a)\,\varphi(a)\mathrm{d}a$$

and $(\cdot,\cdot)$ denotes the scalar product in $L^2[x,\infty)$. It follows from (2.13) and (2.14) that

$$g(\Phi)+\overline{g(\Phi)}=2\,\mathrm{Re}\,\Phi(x,x,y,t)+|\Phi(x,x,y,t)|^2=0.$$

□

III. LARGE-TIME ASYMPTOTIC BEHAVIOR OF NONDECAYING SOLUTIONS OF THE mKP–I EQUATION

Our goal is to investigate the long-time asymptotic behavior of the solution of the mKP-I equation defined in Sec. II.

Definition 1: Let $M>0$. Denote by $G_M(t)\subset\mathbb{R}^2$ the domain

$$G_M(t)=\left\{(x,y)\in\mathbb{R}^2\,\middle|\,-\infty<y<\infty,t>t_0(M),x>C(Y)t-\frac{M}{2q_0(Y)}\ln t;Y=\frac{y}{t}\right\}.$$

We call $G_M(t)$ the neighborhood of the front of the solution.

We shall study the behavior of the mKP-I solution in such domains.

Theorem 1 describes the large-time asymptotic behavior of the solutions of the mKP-I equation defined by Lemma 1.

Theorem 1: *Assume that conditions A–D are fulfilled. Then, in the domain $G_M(t)$, the solution $v(x,y,t)$ of the mKP-I equation constructed by the scheme (1.1)–(1.3) has for $t\to\infty$ the asymptotic behavior*

$$v(x,y,t)=-\sum_{n=1}^{[M-1]}v_n(x,y,t)+O\left(\frac{1}{t^{1/2-\varepsilon_1}}\right)\quad(0<\varepsilon_1<\tfrac{1}{2}),\tag{3.1}$$

where

$$v_n(x,y,t)=-\frac{2q_0(Y)^2}{p_0(Y)+\sqrt{p_0^2(Y)+q_0^2(Y)}\cosh[2q_0(Y)\kappa_n(x,y,t)]},$$

$$\kappa_n(x,y,t)=x-C(Y)t+\frac{1}{2q_0(Y)}(\ln t^{n+1/2}-\ln g(Y)-\ln\phi_n(Y)),$$

$$\phi_n(Y)=\frac{(C(Y)+3(C'(Y))^2-4YC'(Y)+Y^2)^n(C''(Y))^{n-1/2}Q^{(n)}\Gamma^{(n)}}{2^{5n-1/2}((n-1)!)^2(C(Y)+3/4(C'(Y))^2-YC'(Y))^{(10n-5)/4}Q^{(n-1)}\Gamma^{(n-1)}},$$

and $\Gamma^{(n)},Q^{(n)}>0$ are the determinants of the $n\times n$ matrices with the entries

$$\Gamma^{(n)}_{i+1,k+1}=\Gamma\left(\frac{i+k+1}{2}\right)(1+(-1)^{i+k}),$$

$$Q^{(n)}_{i+1,k+1}=\Gamma(i+k+1),\quad i,k=0,\ldots,n-1.$$

The asymptotic behavior (3.1) is uniform with respect to x and y in $G_M(t)$ for any fixed $M>2$.

Proof: Let us indicate the key points of the proof. It consists of three steps.

First we show that for $t\to\infty$ the kernel $F(x,z,y,t)$ of the integral equation (1.2) is represented as the sum of a degenerate kernel and a kernel with a small operator norm in the space $L^2(x,\infty)$.

At the second step we prove that the degenerate kernel gives the main contribution in the asymptotic behavior of the solution of Eq. (1.2).

The third step consists of an analysis of the expression (1.1) for the solution $v(x,y,t)$ as $t\to\infty$, where the function $K(x,z,y,t)$ is a solution of the Marchenko integral equation with degenerate kernel.

To investigate the kernel $F(x,z,y,t)$ of the Marchenko equation for $t\to\infty$ [see (1.4)], we set

$$x=C(Y)t+\xi, \quad z=C(Y)t+\zeta,$$

and define

$$\tilde{F}(\xi,\zeta,y,t)=F(\xi+C(Y)t,\zeta+C(Y)t,y,t).$$

Then

$$\tilde{F}(\xi,\zeta,y,t)=\int\int_{\Omega}\exp[ip(\xi-\zeta)-q(\xi+\zeta)-2q(C(Y)-f(p,q,Y))t]\mathrm{d}\mu.$$

For sufficiently small $\varepsilon'>0$, let us consider the curve

$$2q(f(p,q,Y)-C(Y))+\varepsilon'=0. \tag{3.2}$$

This curve defines a partition of the domain Ω into two subdomains $O_{\varepsilon'}$ and $\Omega_{\varepsilon'}$ so that $\Omega=\overline{O_{\varepsilon'}}\cup\Omega_{\varepsilon'}$. Here $O_{\varepsilon'}$ lies between the curve $q=h(p)$ and curve (3.2), moreover $(p_0(Y),q_0(Y))\in O_{\varepsilon'}$. The set $\Omega_{\varepsilon'}$ is the complementary set of $\overline{O_{\varepsilon'}}$ in Ω. According to this decomposition, the kernel (1.4) is the sum of two kernels which we denote by $F_1(x,z,y,t)$ and $F_2(x,z,y,t)$, respectively.

Let us make a change of variables by setting

$$r=2q(C(Y)-f(p,q,Y)) \tag{3.3}$$

in the kernel $F_1(x,z,y,t)$ related to integration over the set $O_{\varepsilon'}$. Let u be the projection of the radius vector directed from the point $(p_0(Y),q_0(Y))$ to the point $(p,q)\in O_{\varepsilon'}$ on the tangent to the curve $q=h(p)$ at the point $(p_0(Y),q_0(Y))$ or, which is the same, on the tangent to the curve $f(p,q,Y)=C(Y)$ at the same point. We have

$$u=\frac{3p_0(Y)-Y}{\sqrt{q_0^2(Y)+(3p_0(Y)-Y)^2}}(q-q_0(Y))+\frac{q_0(Y)}{\sqrt{q_0^2(Y)+(3p_0(Y)-Y)^2}}(p-p_0(Y)). \tag{3.4}$$

The system (3.3) and (3.4) has a unique solution with respect to $(p,q)\in O_{\varepsilon'}$ for $0<\varepsilon'<\min(4\delta^3,\delta-\varepsilon)$. Therefore the variables p and q can be expressed via the variables r and u in $O_{\varepsilon'}$. We can choose the number ε' such that the following Taylor series converge absolutely:

$$p(r,u)=p_0+k_1r+k_2u+k_3ur+k_4r^2+k_5u^2+\cdots,$$

$$q(r,u)=q_0+\lambda_1r+\lambda_2u+\lambda_3ur+\lambda_4r^2+\lambda_5u^2+\cdots,$$

where k_n and λ_n are the coefficients of the corresponding Taylor series. The first of them have the form

$$k_1(Y)=\frac{3p_0(Y)-Y}{4q_0(Y)(q_0^2(Y)+(3p_0(Y)-Y)^2)},$$

$$k_2(Y)=\frac{q_0(Y)}{\sqrt{q_0^2(Y)+(3p_0(Y)-Y)^2}},$$

$$\lambda_1(Y)=-\frac{1}{4q_0(Y)(q_0^2(Y)+(3p_0(Y)-Y)^2)},$$

$$\lambda_2(Y)=\frac{3p_0(Y)-Y}{\sqrt{q_0^2(Y)+(3p_0(Y)-Y)^2}}.$$

For $n>2$ we can obtain the coefficients k_n and λ_n in an explicit form after n–times differentiation of (3.3) and (3.4) with respect to r and u. The equation $q=h(p)$ can be written in the variables r and u in $O_{\varepsilon'}$. Condition A $[C''(Y)\neq 0]$ implies that the curves $f(p,q,Y)=C(Y)$ and $q=h(p)$ have a contact of the first order. Therefore $q=h(p)$ takes the form $u=u(r)$ with

$$u=\pm a(Y)\sqrt{r}+b(Y)r+\cdots,$$

where

$$\begin{aligned}a(Y)&=\left[\frac{q_0^2(Y)+(3p_0(Y)-Y)^2}{4q_0(Y)(3q_0^2(Y)-(3p_0(Y)-Y)^2-h'(p_0(Y))q_0^3(Y))}\right]^{1/2}\\&=\left(\frac{(C(Y)+3(C'(Y))^2-4YC'(Y)+Y^2)C''(Y)}{8(C(Y)+3/4(C'(Y))^2-YC'(Y))^{3/2}}\right)^{1/2}.\end{aligned}\tag{3.5}$$

With the new variables u and r and the notation

$$E_0(\xi,\zeta,Y)=e^{ip_0(Y)(\xi-\zeta)-q_0(Y)(\xi+\zeta)},$$

we write the function $\tilde{F}_1(\xi,\zeta,y,t)=F_1(\xi+C(Y)t,\zeta+C(Y)t,y,t)$ as follows:

$$\begin{aligned}\tilde{F}_1(\xi,\zeta,y,t)=E_0(\xi,\zeta,Y)\int_0^{\varepsilon}dr\int_{-a\sqrt{r}+\cdots}^{a\sqrt{r}+\cdots}du\,j(r,u,Y)\tilde{g}(r,u,Y)\sqrt{\frac{p-iq}{p+iq}}\\\times e^{i(p-p_0)(\xi-\zeta)-(q-q_0)(\xi+\zeta)-rt},\end{aligned}\tag{3.6}$$

where $j(r,u,Y)=j(p(r,u,Y),q(r,u,Y))$ is the Jacobian corresponding to the change of variables $(p,q)\to(r,u)$.

Let us expand the integrand in (3.6) into a series with respect to the powers of r and u in the neighborhood of the point $(p_0(Y),q_0(Y))$ $(u=0,r=0)$:

$$\begin{aligned}&j(r,u,Y)\tilde{g}(r,u,Y)\sqrt{\frac{p-iq}{p+iq}}e^{i(p-p_0(Y))(\xi-\zeta)-(q-q_0(Y))(\xi+\zeta)}\\&=\sum_{n=0}^{\infty}\sum_{j=0}^{n}\sum_{l=0}^{j}\sum_{m=0}^{n-j}\zeta^j\xi^{n-j}r^{l+m}u^{n-l-m}\varphi_{n,j,l,m}(Y)(1+\psi_n(r,u)),\end{aligned}$$

with

$$\begin{aligned}\varphi_{n,j,l,m}(Y)=\frac{(-1)^{n-m}}{l!m!(n-j-m)!(j-l)!}\sqrt{\frac{p_0(Y)-iq_0(Y)}{p_0(Y)+iq_0(Y)}}(ik_1(Y)+\lambda_1(Y))^l(ik_2(Y)\\+\lambda_2(Y))^{j-l}(ik_1(Y)-\lambda_1(Y))^m(\lambda_2(Y)-ik_2(Y))^{n-j-m}g(Y)j_0(Y),\end{aligned}$$

and

$$\begin{aligned}j_0(Y)=j(0,0,Y)=\frac{1}{4q_0(Y)\sqrt{q_0^2(Y)+(3p_0(Y)-Y)^2}},\\g(Y)=\tilde{g}(0,0,Y),\end{aligned}\tag{3.7}$$

the functions $\psi_n(r,u)$ satisfying the inequalities $|\psi_n(r,u)| \leqslant An(r+|u|)$.

Integrating with respect to u and r, we obtain

$$\tilde{F}_1(\xi,\zeta,y,t) = E_0(\xi,\zeta,Y) \sum_{n=0}^{N-1} \sum_{j=0}^{N-n-1} \zeta^n \xi^j \frac{\psi_{nj}(Y)}{t^{(n+j+3)/2}} (1+\delta_n(t)) + \Delta_N(\xi,\zeta,y,t),$$

where

$$\psi_{nj}(Y) = \sqrt{\frac{p_0(Y)-iq_0(Y)}{p_0(Y)+iq_0(Y)}} \frac{g(Y)j_0(Y)a^{n+j+1}(Y)}{2n!j!} \Gamma\left(\frac{n+j+1}{2}\right)(1+(-1)^{n+j})(ik_2(Y) + \lambda_2(Y))^n(\lambda_2(Y)-ik_2(Y))^j, \tag{3.8}$$

and

$$|\delta_n(t)| \leqslant \frac{B_{nj}}{\sqrt{t}},$$

$$|\Delta_N| \leqslant AE_0(\xi,\zeta,y,t) \sum_{j=0}^{N} \frac{|\zeta^j \xi^{N-j}|}{t^{(N+3)/2}}. \tag{3.9}$$

The bound (3.9) is valid for $|\xi|<|\zeta|<t^{1/4}$.

In the domain $\zeta > \xi > -(1/2q_0)\ln t^M$, we have the following bound for the function $\Delta_N(\xi,\zeta,y,t)$ as $t>t_0(M)$

$$\int_x^\infty \int_x^\infty |\Delta_N(s,z,y,t)|^2 \mathrm{d}s\mathrm{d}z \leqslant \frac{A(N)}{t^{1/2-\varepsilon_1}} \quad (0<\varepsilon_1<\tfrac{1}{2}), \tag{3.10}$$

where $A(N) \leqslant e^{N+3}/(N+3)^{N+3}2^{N+4}$ and $N=[2M-3]$.

Consider the operator

$$[\hat{F}_2 h](z) = \int_x^\infty F_2(s,z,y,t)h(s)\mathrm{d}s$$

in the space $L^2[x,\infty)$. We estimate the function $|F_2(s,z,y,t)|^2$ as follows:

$$\begin{aligned} |F_2(s,z,y,t)|^2 &= \left| \int\int_{\Omega_{\varepsilon'}} e^{ip(x-z)-q(x+z)+4pqy-2q(3p^2-q^2)t} \mathrm{d}\mu \right|^2 \\ &\leqslant \left(\int\int_{\Omega_{\varepsilon'}} g(p,q)\mathrm{d}p\mathrm{d}q \right)\left(\int\int_{\Omega_{\varepsilon'}} e^{-2q(s+z)+4qf(p,q,Y)t} \tilde{g}(p,q)\mathrm{d}p\mathrm{d}q \right) \\ &\leqslant A \int\int_{\Omega_{\varepsilon'}} e^{-2q(s+z)+4qf(p,q,Y)t} \tilde{g}(p,q)\mathrm{d}p\mathrm{d}q. \end{aligned}$$

Taking into account that $C(Y)-f(p,q,Y) \geqslant \varepsilon'/2q$ $[(p,q)\in\Omega_{\varepsilon'},\ q\geqslant\varepsilon>0]$, we have the following estimate for the norm of $\hat{F}_2$ for $x>C(Y)t-(\varepsilon'/2\varepsilon)t$:

$$\int_x^\infty \int_x^\infty |F_2(s,z,y,t)|^2 \mathrm{d}s\mathrm{d}z = O(e^{-\varepsilon' t}). \tag{3.11}$$

Therefore inside the domain

$$\zeta > \xi > -\frac{1}{2q_0(Y)} \ln t^M, \quad Y = \frac{y}{t}, \quad -\infty < y < \infty,$$

and for $t \to \infty$, the kernel $\tilde{F}(\xi,\zeta,y,t)$ has the form

$$\tilde{F}(\xi,\zeta,y,t) = \tilde{F}_N(\xi,\zeta,y,t) + \tilde{G}(\xi,\zeta,y,t),$$

where $(N=[2M-3])$

$$\tilde{F}_N(\xi,\zeta,y,t) = e^{ip_0(\xi-\zeta)-q_0(\xi+\zeta)} \sum_{n=0}^{N-1} \sum_{j=0}^{N-n-1} \zeta^n \xi^j \frac{\psi_{nj}(Y)}{t^{(n+j+3)/2}}, \tag{3.12}$$

and the functions $\psi_{nj}(Y)$ defined in (3.8) are bounded. Taking into account (3.9)–(3.11), we can conclude that the function $G(s,z,y,t)$ admits a uniform estimate with respect to y $(-\infty < y < \infty)$:

$$\int_x^\infty \int_x^\infty |G(s,z,y,t)|^2 ds\,dz = O\left(\frac{1}{t^{1/2-\varepsilon_1}}\right) \quad (0 < \varepsilon_1 < 1/2). \tag{3.13}$$

We show that after replacing the kernel $F(x,z,y,t)$ by the degenerate kernel $F_N(x,z,y,t)$ we can obtain an asymptotic representation of the solution $K(x,z,y,t)$ of the Marchenko integral equation (1.2) up to $O(t^{-1/2+\varepsilon_1})$ $(0 < \varepsilon_1 < \frac{1}{2})$ for $t \to \infty$. Set

$$x = C(Y)t + \xi, \quad z = C(Y)t + \zeta,$$

and consider the domain

$$\zeta > \xi > -\frac{1}{2q_0(Y)} \ln t^M,$$

where M is an arbitrary positive number. Let us introduce the operators

$$(\hat{F}_N f)(z) = \int_x^\infty F_N(s,z,y,t) f(s) ds,$$

$$(\hat{G}_N f)(z) = \int_x^\infty G_N(s,z,y,t) f(s) ds,$$

in the space $L^2[x,\infty)$. The degenerate kernel

$$F_N(x,z,y,t) = \tilde{F}_N(x - C(Y)t, z - C(Y)t, y, t)$$

$(N=[2M-3])$ is defined in (3.12) with $\xi = x - C(Y)t$ and $\zeta = z - C(Y)t$, and $\psi_{nj}(Y)$ are defined by (3.8). The function $G_N(x,z,y,t)$ is the difference between $F(x,z,y,t)$ defined in (1.4) and $F_N(x,z,y,t)$:

$$G_N = F - F_N.$$

Now (1.2) takes the form

$$(I + \hat{F}_N) f + \hat{G}_N f = h_N + g_N, \tag{3.14}$$

where $f=K(x,z,y,t)$, $h_N=-F_N(x,z,y,t)$, and $g_N=-G_N(x,z,y,t)$. According to (3.13) we easily obtain the following estimates for the norms of the operator $\hat{G}_N$ and the vector g_N in $L^2[x,\infty)$ for $\zeta>\xi>-[1/2q_0(Y)]\ln t^M$:

$$\|\hat{G}_N\|\leqslant A_1 t^{-1/2+\varepsilon_1},$$
$$\|\hat{g}_N\|\leqslant A_1 t^{-1/2+\varepsilon_1} \quad (A_1=\text{const},\ 0<\varepsilon_1<\tfrac{1}{2}). \tag{3.15}$$

The operator $I+\hat{F}_N$ is the direct sum of two operators, $I_1+\hat{F}_N$ and I_2. The first one acts in the subspace H_1 of $L^2[x,\infty)$ generated by the vectors $e^{(ip_0-q_0)z}$, $ze^{(ip_0-q_0)z}$, $\ldots$, $z^{N-1}e^{(ip_0-q_0)z}$. The second, I_2 $(I=I_1\oplus I_2)$, acts in the orthogonal complement $H_2=L^2[x,\infty)\ominus H_1$ of H_1. Since we have $\hat{F}_N=\hat{F}-\hat{G}$ and since $I+\hat{F}$ is invertible, we derive that also $I+\hat{F}_N$ is invertible in $L^2[x,\infty)$, and

$$\|(I+\hat{F}_N)^{-1}\|_{L^2[x,\infty)}\leqslant A_2<\infty. \tag{3.16}$$

We shall look for a solution of (3.14) in the form $f=\phi_N+\psi_N$, ϕ_N being the solution of the equation $(I+\hat{F}_N)\phi_N=h_N$. The latter observation implies that ψ_N satisfies the equation

$$(I+\hat{F}_N)\psi_N=g_N-\hat{G}_N\phi_N.$$

According to (3.16), we have

$$\|\psi_N\|\leqslant A_2(\|g_N\|+\|\hat{G}_N\|\cdot\|\psi_N\|).$$

Below we shall show that ϕ_N is uniformly bounded with respect to y, t and $\xi>-[1/2q_0(Y)]\ln t^M$ in the space $L^2[x,\infty)\cap L^1[x,\infty)$. This fact and (3.15) allow us to conclude that

$$f(z)=\phi_N(z)+O(t^{-1/2+\varepsilon_1}), \quad 0<\varepsilon_1<\tfrac{1}{2}. \tag{3.17}$$

The replacement of the kernel F by the degenerate kernel F_N in the equation (1.2) and the substitutions $x=C(Y)t+\xi$ and $z=C(Y)t+\zeta$ allow us to obtain as an integral equation for the function $K_N(\xi,\zeta,y,t)=K(\xi+C(Y)t,\zeta+C(Y)t,y,t)$ $(\zeta>\xi)$,

$$K_N(\xi,\zeta,y,t)+F_N(\xi,\zeta,y,t)+\int_\xi^\infty K_N(\xi,s,y,t)F_N(s,\zeta,y,t)\,ds=0, \tag{3.18}$$

where F_N is given by (3.12).

According to (1.1) and (3.17), we have the following asymptotic expression of $v(x,y,t)$ in the domain $x>C(Y)t-(1/2q_0)\ln t^M$:

$$v(x,y,t)=\left(-i\frac{\partial}{\partial\xi}\ln\left\{1+\int_\xi^\infty K_N(\xi,s,y,t)\,ds\right\}\right)\Bigg|_{\xi=x-C(Y)t}+O(t^{-1/2+\varepsilon_1}). \tag{3.19}$$

We shall look for a solution of the equation (3.18) in the form

$$K_N(\xi,\zeta,y,t)=\sum_{n=0}^{N-1}\gamma_n(\xi,Y,t)\zeta^n e^{-(ip_0+q_0)\zeta}. \tag{3.20}$$

By substituting (3.20) into (3.18) we obtain the system of algebraic equations for the functions $\gamma_n(\xi,Y,t)$ $(n=0,\ldots,N-1)$:

$$\gamma_n+\sum_{m=0}^{N-1}\gamma_m\sum_{j=0}^{N-n-1}\frac{\psi_{nj}(Y)}{t^{(n+j+3)/2}}\int_\xi^\infty s^{j+m}e^{-2q_0s}\mathrm{d}s=-\sum_{j=0}^{N-n-1}\frac{\psi_{nj}(Y)}{t^{(n+j+3)/2}}\xi^j e^{(ip_0-q_0)\xi}. \quad (3.21)$$

The solution of these equations has the form

$$\gamma_n=\frac{\det[I+A(\xi,y,t)]^{(l)}}{\det[I+A(\xi,y,t)]},$$

where I is the identity matrix, $A(\xi,y,t)$ is the matrix with the entries $(n,m=0,\ldots,N-1)$,

$$[A]_{n+1,m+1}=\sum_{j=0}^{N-n-1}\frac{\psi_{nj}}{t^{(n+j+3)/2}}I_{j+m}, \quad (3.22)$$

$$I_{j+m}=\int_\xi^\infty s^{j+m}e^{-2q_0s}\mathrm{d}s.$$

The matrix $[I+A(\xi,y,t)]^{(l)}$ is obtained via the substitution of the column of the right-hand sides of the system (3.21) instead of the lth column of the matrix $[I+A(\xi,y,t)]$. The functions ψ_{nj} are defined by (3.8).

The substitution of $\gamma_n(\xi,Y,t)$ into (3.20) gives

$$K_N(\xi,\zeta,y,t)=\sum_{n=0}^{N-1}\frac{\det(I+A)^{(n)}}{\det(I+A)}\zeta^n e^{-(ip_0+q_0)\zeta}.$$

To obtain $v(x,y,t)$ we calculate the integral

$$\int_\xi^\infty K(\xi,s,y,t)\mathrm{d}s=e^{-(ip_0+q_0)\xi}\sum_{n=0}^{N-1}\gamma_n(\xi,y,t)\sum_{i=0}^{n}\frac{\xi^i n!}{i!(ip_0+q_0)^{n-i+1}}$$

and we substitute it into (3.19). One has

$$v(x,y,t)=-i\frac{\mathrm{d}}{\mathrm{d}\xi}\ln\left(1+\sum_{n=0}^{N-1}\frac{\det(I+A(\xi,y,t))^{(n)}}{\det(I+A(\xi,y,t))}\sum_{i=0}^{n}\frac{\xi^i n!e^{-(ip_0+q_0)\xi}}{i!(ip_0+q_0)^{n-i+1}}\right)\Bigg|_{\xi=x-C(Y)t}+O(t^{-1/2+\varepsilon_1}). \quad (3.23)$$

Hence the investigation of the long-time behavior of $v(x,y,t)$ reduces to the study of the determinant formula (3.23) for $t\to\infty$.

We introduce the following notation:

$$G(\xi,y,t)=\sum_{n=0}^{N-1}\frac{\det(I+A(\xi,y,t))^{(n)}}{\det(I+A(\xi,y,t))}\sum_{i=0}^{n}\frac{\xi^i n!e^{-(ip_0+q_0)\xi}}{i!(ip_0+q_0)^{n-i+1}}.$$

The function G can be represented in the form

$$G(\xi,y,t)=\frac{1}{ip_0+q_0}\frac{\partial}{\partial\xi}\ln\det(I+A(\xi,y,t))+\sum_{n=1}^{N-1}\frac{\det(I+A(\xi,y,t))^{(n)}}{\det(I+A(\xi,y,t))}\sum_{i=0}^{n}\frac{\xi^i n!e^{-(ip_0+q_0)\xi}}{i!(ip_0+q_0)^{n-i+1}}.$$

The asymptotic analysis of the function $\det(I+A(\xi,y,t))$ for $t\to\infty$ gives us

$$\det(I+A(\xi,y,t))=1+\sum_{n=1}^{N}\frac{\Delta_n(\xi,y,t)}{t^{n(n+2)/2}}e^{-2nq_0\xi},$$

where

$$\Delta_n(\xi,y,t)=\frac{P_nW_n}{(2q_0)^n}\left[1+O_N\left(\frac{1}{\sqrt{t}}\right)\right],$$

where P_n are the determinants of the $n\times n$ matrices whose entries are the integrals

$$[P_n]_{jk}=2q_0\int_\xi^\infty s^{j+k}e^{-2q_0s}\mathrm{d}s,$$

and W_n are the determinants of the $n\times n$ matrices with the entries

$$[W_n]_{ik}=\psi_{ik}.$$

Besides,

$$W_n=\frac{(q_2^2+p_2^2)^{n(n-1)/2}a^{n^2}}{2^n\Pi_{k=0}^{n-1}(k!)^2}\left(\frac{ip_0+q_0}{ip_0-q_0}\right)^{n/2}(j_0g)^n\Gamma^{(n)}, \tag{3.24}$$

where

$$[\Gamma^{(n)}]_{i+1,k+1}=(1+(-1)^{k+i})\Gamma\left(\frac{k+i+1}{2}\right).$$

It is easy to verify that P_n and $\Gamma^{(n)}$ are the Gram determinants of the two systems of functions $(k=0,\ldots,n-1)$

$$u_k=e^{-\xi/2}\xi^k,\quad \xi>0,$$

$$u_k=\sqrt{2}x^ke^{-x^2/2},\quad -\infty<x<+\infty,$$

respectively. Therefore $\Gamma^{(n)},\ P_n\neq 0$, and $(0\leqslant i,k\leqslant n-1)$

$$P_n=\det\|\Gamma(i+k+1)(2q_0)^{-i-k}\|.$$

Since in the region $\zeta>\xi>(1/2q_0)\ln t^M$ the determinant Δ_n does not vanish [the operator $(I+\hat{F})^{-1}$ is bounded], it is easy to see that $\Gamma^{(n)},P_n>0$.

Let us cover the domain $G_M(t)$ $(M>2)$ by the subdomains

$$a_1=\left\{(\xi,t)\,\middle|\,\xi>-\frac{1}{2q_0}\ln t^{2+\varepsilon}\right\},$$

$$a_n=\left\{(\xi,t)\,\middle|\,-\frac{1}{2q_0}\ln t^{n+1+\varepsilon}<\xi<-\frac{1}{2q_0}\ln t^{n-\varepsilon}\right\},\quad n=2,\ldots,m-1,$$

$$a_m=\left\{(\xi,t)\,\middle|\,-\frac{1}{2q_0}\ln t^{(N+3)/2}<\xi<-\frac{1}{2q_0}\ln t^{m-\varepsilon}\right\},$$

where $m=[(N+1)/2]$. If (ξ,t) belongs to a_n, one has

$$\det(I+A)=\left(\frac{W_{n-1}P_{n-1}e^{-2(n-1)q_0\xi}}{(2q_0)^{n-1}t^{(n-1)(n+1)/2}}+\frac{W_nP_ne^{-2nq_0\xi}}{(2q_0)^nt^{n(n+2)/2}}\right)\left[1+O\left(\frac{1}{\sqrt{t}}\right)\right] \tag{3.25}$$

as $t\to\infty$.

One can represent $G(\xi,y,t)$ in the form

$$G(\xi,y,t)=\frac{1}{(ip_0+q_0)\det(I+A)}\left\{\frac{\partial}{\partial\xi}\det(I+A(\xi,y,t))+\sum_{n=1}^{N-1}\det(I+A(\xi,y,t))^{(n)}\sum_{i=0}^{n}\frac{\xi^i n!e^{-(ip_0+q_0)\xi}}{i!(ip_0+q_0)^{n-i+1}}\right\}.$$

The analysis of the matrices $(I+A)^{(n)}$ for $t\to\infty$ gives us an asymptotic representation for $G(\xi,y,t)$ inside a_n:

$$G(\xi,y,t)=\frac{2q_0}{(ip_0+q_0)(W_{n-1}P_{n-1}+P_nT_ne^{-2q_0\xi})}\{W_{n-1}S_{n-1}+S_nT_ne^{-2q_0\xi}\},$$

where

$$\begin{aligned}T_n&=\frac{W_n}{2q_0t^{n+1/2}},\\ S_n&=-(R_n+nP_n),\\ R_n&=\sum_{k=1}^{n-1}\frac{k!}{(ip_0+q_0)^k}P_n^{(k)},\\ R_1&=0,\end{aligned}\tag{3.26}$$

$P_n^{(k)}$ being the determinant of the matrix obtained from the matrix P_n by replacing the $(k+1)$th column by the transpose of $(1,0,\ldots,0)$.

It follows from (3.19) that

$$v(x,y,t)=\frac{1}{i}\frac{\partial}{\partial\xi}\ln(1+G(\xi,y,t))\Big|_{\xi=x-C(Y)t}=\frac{1}{i}\frac{G_\xi}{1+G}\Big|_{\xi=x-C(Y)t}.\tag{3.27}$$

Let us calculate the numerator and the denominator in (3.27):

$$\begin{aligned}G_\xi(\xi,y,t)&=\frac{4q_0^2}{ip_0+q_0}\frac{T_nW_{n-1}(P_nS_{n-1}-S_nP_{n-1})e^{-2q_0\xi}}{(W_{n-1}P_{n-1}+T_nP_ne^{-2q_0\xi})^2},\\ 1+G(\xi,y,t)&=\frac{W_{n-1}F_{n-1}+T_nF_ne^{-2q_0\xi}}{(ip_0+q_0)(W_{n-1}P_{n-1}+P_nT_ne^{-2q_0\xi})},\end{aligned}\tag{3.28}$$

where

$$F_n=(ip_0+q_0)P_n+2q_0S_n.\tag{3.29}$$

After substitution of (3.28) into (3.27) we obtain

$$v(x,y,t)\sim-\frac{2iq_0^2(S_nP_{n-1}-P_nS_{n-1})}{\frac{1}{2}(P_nF_{n-1}+F_nP_{n-1})+\sqrt{P_nP_{n-1}F_nF_{n-1}}\cosh\{2q_0(x-C(Y)t)-\ln\varphi_n\}},$$

where

$$\varphi_n=\frac{T_n}{W_{n-1}}\sqrt{\frac{P_nF_n}{P_{n-1}F_{n-1}}}. \tag{3.30}$$

One can prove that

$$(ip_0+q_0)P_{n-1}F_n=(ip_0-q_0)P_nF_{n-1}. \tag{3.31}$$

Equations (3.29) and (3.31) give us the following relations:

$$\begin{aligned} F_nP_{n-1}&=(ip_0-q_0)(S_{n-1}P_n-S_nP_{n-1}),\\ F_{n-1}P_n&=(ip_0+q_0)(S_{n-1}P_n-S_nP_{n-1}). \end{aligned} \tag{3.32}$$

Let us write the sum and the product of the relations in (3.32):

$$F_nP_{n-1}+P_nF_{n-1}=2ip_0(S_{n-1}P_n-S_nP_{n-1}),$$

$$F_nF_{n-1}P_nP_{n-1}=-(q_0^2+p_0^2)(S_{n-1}P_n-S_nP_{n-1})^2.$$

Then the function $v(x,y,t)$ has the following form:

$$v(x,y,t)=-\sum_{n=1}^{[(N+1)/2]}\frac{2q_0^2}{p_0+\sqrt{p_0^2+q_0^2}\cosh[2q_0(x-C(Y)t)-\ln\varphi_n(Y,t)]},$$

where $\varphi_n(Y,t)$ is defined by (3.30).

It follows from (3.26) and (3.31) that

$$\frac{T_n}{W_{n-1}}=\frac{1}{2q_0t^{n+1/2}}\frac{W_n}{W_{n-1}},\quad \frac{P_nF_n}{P_{n-1}F_{n-1}}=\frac{P_n^2}{P_{n-1}^2}\frac{ip_0-q_0}{ip_0+q_0},$$

i.e.,

$$\varphi_n(Y,t)=\frac{1}{2q_0t^{n+1/2}}\sqrt{\frac{ip_0-q_0}{ip_0+q_0}}\ \frac{P_nW_n}{P_{n-1}W_{n-1}}. \tag{3.33}$$

In view of condition D and (3.33), one can represent the function φ_n as

$$\varphi_n(Y,t)=\frac{1}{2q_0(Y)t^{n+1/2}}\frac{g(Y)j_0(Y)a^{2n-1}(Y)(k_2^2+\lambda_2^2)^{n-1}P_n\Gamma^{(n)}}{2P_{n-1}\Gamma^{(n-1)}}.$$

Thus, the asymptotic behavior of the solution $v(x,y,t)$ of the mKP-I equation for $t\to\infty$ is given by

$$v(x,y,t)=-\sum_{n=1}^{[M-1]}v_n(x,y,t)+O\left(\frac{1}{t^{1/2-\varepsilon_1}}\right),$$

with

$$v_n(x,y,t)=\frac{2q_0^2(Y)}{p_0+\sqrt{p_0^2+q_0^2}\cosh[2q_0(Y)(x-C(Y)t+(1/2q_0)(\ln t^{n+1/2}-\ln g(Y)-\ln\phi_n(Y)))]},$$

where

$$\phi_n(Y)=\frac{j_0(Y)a^{2n-1}(Y)Q^{(n)}\Gamma^{(n)}}{2(2q_0(Y))^{2(n-1)}[(n-1)!]^2Q^{(n-1)}\Gamma^{(n-1)}}>0, \tag{3.34}$$

and $Q^{(n)}$, $\Gamma^{(n)}$ are the determinants $(0\leqslant i,k\leqslant n-1)$

$$Q^{(n)}=\det\|\Gamma(i+k+1)\|,$$

$$\Gamma^{(n)}=\det\left\|(1+(-1)^{k+i})\Gamma\left(\frac{k+i+1}{2}\right)\right\|.$$

Using condition B, (3.7) and (3.5) we can also write $\phi_n(Y)$ as

$$\phi_n(Y)=\frac{(C(Y)+3(C'(Y))^2-4YC'(Y)+Y^2)^n(C''(Y))^{n-1/2}Q^{(n)}\Gamma^{(n)}}{2^{5n-1/2}((n-1)!)^2(C(Y)+3/4(C'(Y))^2-YC'(Y))^{(10n-5)/4}Q^{(n-1)}\Gamma^{(n-1)}}.$$

So, the mKP-I equation solution $v(x,y,t)$ determined by (1.1)–(1.3) splits into a series of curved solitons whose width and amplitude depend on Y. Since all the factors in $\phi_n(Y)$ are positive, $v_n(x,y,t)$ are regular. These asymptotic solitons diverge with a velocity proportional to $\ln t$ when t increases. The theorem is proved. □

IV. EXAMPLES OF ASYMPTOTIC SOLITONS FOR THE mKP-I EQUATION

In this section we consider two special examples of solutions of the mKP-I equation, which generate asymptotic solitons of different forms in the neighborhood of the front of the mKP-I solution for $t\to\infty$. First of all we have to choose a function $C(Y)$ satisfying condition A. After that we have to construct a set Ω satisfying condition B.

Suppose

$$C(Y)=aY^2+b^2,\quad a\geqslant\tfrac{1}{3},\quad b>\delta>0. \tag{4.1}$$

The family of hyperbolas $f(p,q,Y)=C(Y)$ has the envelope $q=h(p)=\sqrt{b^2+(3-1/a)p^2}$, and touch it at the point $(p_0(Y),q_0(Y))$ given by $(-\infty<Y<\infty)$

$$p_0(Y)=aY,$$

$$q_0(Y)=\sqrt{b^2+a(3a-1)Y^2}.$$

We choose Ω of the form

$$\Omega=\{(p,q)\in\mathbb{R}^2|-\infty<p<\infty,h(p)\geqslant q\geqslant\varepsilon>0\}.$$

Thus conditions A and B are fulfilled.

Now we have to determine two functions $g(Y)$ and $\tilde{g}(p,q)$ satisfying condition C, and to construct a measure $\mathrm{d}\mu$ satisfying condition D. We choose

$$g(Y)=\exp(-q_0^2(Y)-p_0^2(Y)),\quad \tilde{g}(p,q)=\exp(-q^2-p^2),$$

and

$$\mathrm{d}\mu(p,q)=\exp(-q^2-p^2)\sqrt{\frac{p-iq}{p+iq}}\,\mathrm{d}p\,\mathrm{d}q.$$

Thus all conditions of Theorem 1 are fulfilled.

A. First example

We take $a=\frac{1}{3}$ in (4.1). Then

$$p_0(Y)=Y/3,\quad q_0(Y)=b,$$

$$h(p)=b, \quad g(Y)=\exp(-b^2-Y^2/9).$$

According to Theorem 1, inside the domain ($M\geqslant 2$)

$$G_M(t)=\left\{(x,y)\in\mathbb{R}^2 \middle| t>t_0(M), -\infty<y<\infty, x>\frac{y^2}{3t}+b^2t-\frac{M}{2b}\ln t\right\}$$

the solution of the mKP-I equation constructed by (1.1)–(1.3) has as $t\to\infty$ the asymptotic behavior ($0<\varepsilon_1<\frac{1}{2}$)

$$v(x,y,t)=-\sum_{n=1}^{[M-1]}\frac{6b^2}{Y+\sqrt{Y^2+9b^2}\cosh\psi_n(x,y,t)}+O(t^{-1/2+\varepsilon_1}). \tag{4.2}$$

This is a sequence of $[M-1]$ solitons with constant amplitude and constant phase lines of the form

$$\psi_n(x,y,t)=b\left(x-\frac{y^2}{3t}\left(1-\frac{1}{3bt}\right)-b^2t\right)+\frac{1}{2}(\ln t^{n+1/2}+b^2-\ln\varphi_n), \tag{4.3}$$

where

$$\varphi_n=\frac{Q^{(n)}\Gamma^{(n)}}{2^{4n}3^{n-1/2}b^{(6n-5)/2}((n-1)!)^2Q^{(n-1)}\Gamma^{(n-1)}},$$

and $\Gamma^{(n)}$, $Q^{(n)}$ are the determinants of the $n\times n$ matrices whose entries $(i,k=0,\ldots,n-1)$ are given by

$$\begin{aligned}\Gamma^{(n)}_{i+1,k+1}&=\Gamma\left(\frac{i+k+1}{2}\right)(1+(-1)^{i+k}),\\ Q^{(n)}_{i+1,k+1}&=\Gamma(i+k+1).\end{aligned} \tag{4.4}$$

It is easy to derive from (4.3) that all asymptotic solitons have constant amplitude and shifts of phases, and neighboring solitons diverge with velocity proportional to $\ln t$ when the time increases.

B. Second example

We take $a=1$ in (4.1). Then

$$p_0(Y)=Y, \quad q_0(Y)=\sqrt{b^2+2Y^2},$$

$$h(p)=\sqrt{b^2+2p^2}, \quad g(Y)=\exp(-b^2-3Y^2).$$

According to Theorem 1, as $t\to\infty$ inside the domain ($M>2$)

$$G_M(t)=\left\{(x,y)\in\mathbb{R}^2 \middle| t>t_0(M), -\infty<y<\infty, x>\frac{y^2}{t}+b^2t-\frac{M}{2b}\ln t\right\}$$

the solution of the mKP-I equation given by (1.1)–(1.3) has the asymptotic behavior

$$v(x,y,t)=-\sum_{n=1}^{[M-1]}\frac{2(b^2+2Y^2)}{Y+\sqrt{b^2+3Y^2}\cosh^2\psi_n(x,y,t)}+O(t^{-1/2+\varepsilon_1}), \tag{4.5}$$

where

$$\psi_n(x,y,t)=\sqrt{b^2+2Y^2}\left(x-\frac{y^2}{t}\left(1-\frac{3}{2\sqrt{b^2t^2+2y^2}}\right)-b^2t\right)+\frac{1}{2}(\ln t^{n+1/2}+b^2-\ln\varphi_n(Y))$$

with

$$\varphi_n=\frac{(b^2+6Y^2)^nQ^{(n)}\Gamma^{(n)}}{2^{4n}((n-1)!)^2(b^2+2Y^2)^{(10n-5)/4}Q^{(n-1)}\Gamma^{(n-1)}},$$

and $Q^{(n)}$, $\Gamma^{(n)}$ are given by (4.4).

Therefore in this case the curved asymptotic solitons (4.5) have nonconstant amplitudes, widths and phases.

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On the exact steepest descent method: A new method for the description of Stokes curves[a)]

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In order to determine the region where the Borel sum of a Wentzel–Kramers–Brillouin (WKB) solution ψ of an mth order ($m \geqslant 3$) ordinary differential equation $P\psi = 0$ with polynomial coefficients is well defined, we apply the steepest descent method to the Laplace integral of a WKB solution $\hat{\psi}$ of $\hat{P}\hat{\psi} = 0$, with $\hat{P}$ denoting the Laplace transform of P. As a counterpart of the connection formula for $\hat{\psi}$, we introduce a new notion of the exact steepest descent path, which is the union of bifurcated steepest descent paths. Both theoretical and computer-assisted experimental studies are given to show the importance of this notion. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1368138]

I. INTRODUCTION

No algorithmic way of describing Stokes regions, i.e., domains where the Borel sum of a Wentzel–Kramers–Brillouin (WKB) solution is well defined, is known for higher order ordinary differential equations with a large parameter.[1] The main difficulty lies in the necessity of ''new Stokes curves,'' which emanate from possible crossing points of Stokes curves, as Berk, Nevins, and Roberts[2] first observed in discussing a connection formula for WKB solutions. Berk *et al.* further presented a charming idea of applying the steepest descent method to the inverse Fourier transform of a WKB solution for the Fourier-transformed operator. (See also Watanabe–Sanuki–Watanabe[3] for some related subject.) They have confirmed that this approach is effective near saddle points of the integrand,[4] but they have observed several troubles if a steepest descent path hits a turning point of the Fourier-transformed operator.[5]

The principal aim of this paper is to examine the idea of Berk *et al.* from the viewpoint of the exact WKB analysis, i.e., with the Borel resummation of WKB solutions[6–8] (see also Berry–Howls[9] for a related subject ''hyperasymptotics''), and to propose a new notion, ''an exact steepest descent path,'' which naturally fits in with the Borel resummation method. We then present some examples which illustrate how the previously mentioned troubles are naturally resolved by the use of exact steepest descent paths. We note that the notion of an exact steepest descent path is introduced here to exactly take into account the effect of exponentially small terms pertaining to Stokes phenomena of WKB solutions; this explains why we have succeeded in resolving the troubles that Berk *et al.* encountered far away from saddle points.

II. NOTATIONAL PRELIMINARIES

The operators we study in this paper are supposed to have the following form:

$$P = \sum_{\substack{0 \leqslant j \leqslant m \\ 0 \leqslant k \leqslant n}} a_{jk} x^k \eta^{m-j} \left(\frac{\mathrm{d}}{\mathrm{d}x} \right)^j, \tag{1}$$

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where a_{jk} is a constant and η is a large parameter. Let $\hat{\psi}(\xi,\eta)$ denote the Laplace transform of a function $\psi(x,\eta)$, i.e.,

$$\psi(x,\eta)=\int e^{\eta x\xi}\,\hat{\psi}(\xi,\eta)\mathrm{d}\xi, \tag{2}$$

and let $\hat{P}$ denote the Laplace transform of P, i.e.,

$$\hat{P}=\sum a_{jk}\,\eta^{m-k}\left(-\frac{\mathrm{d}}{\mathrm{d}\xi}\right)^k\xi^j. \tag{3}$$

[For the sake of simplicity of the notations we use the Laplace transform instead of the Fourier transform, that is, we use $e^{\eta x\xi}$ instead of $e^{i\eta x\xi}$. We also assume $m\geqslant n$, as our purpose is to analyze the structure of WKB solutions of a higher order operator P in terms of the exact WKB analysis for $\hat{P}$.] In what follows we let $p(x,\xi)$ denote

$$\sum_{\substack{0\leqslant j\leqslant m\\ 0\leqslant k\leqslant n}} a_{jk}\,x^k\,\xi^j. \tag{4}$$

Solving the equation $p(x,\xi)=0$ in the form $x=x_k(\xi)$ $(k=1,\ldots,n)$, we obtain n WKB solutions $\hat{\psi}_k(\xi,\eta)$ of the equation $\hat{P}\hat{\psi}=0$ so that they have the following form:

$$\hat{\psi}_k=\exp\left(\eta\int^{\xi}(-x_k(\xi))\mathrm{d}\xi+\cdots\right)\Big/\sqrt{\eta}. \tag{5}$$

Here the normalization factor $\eta^{-1/2}$ is introduced for the sake of convenience in handling its Borel transform, and $\cdots$ designates terms with nonpositive powers of η.

Thus the object we are interested in is of the form

$$\varphi=\int\exp\left(\eta\left(x\xi-\int^{\xi}x_k(\xi)\mathrm{d}\xi\right)+\cdots\right)\Big/\sqrt{\eta}\,\mathrm{d}\xi. \tag{6}$$

The specification of the path of integration in (6) will be given in Sec. III. As $\hat{\psi}_k$ and φ are formal series in η^{-1}, their meaning should be given, say, by the Borel resummation. Hence we introduce operators P_B and $\hat{P}_B$, respectively, by

$$P_B=\sum a_{jk}\,x^k\frac{\partial^j}{\partial x^j}\frac{\partial^{m-j}}{\partial y^{m-j}} \tag{7}$$

and

$$\hat{P}_B=\sum a_{jk}\frac{\partial^{m-k}}{\partial\tilde{y}^{m-k}}\left(-\frac{\partial}{\partial\xi}\right)^k\xi^j. \tag{8}$$

It then follows from the definition of the Borel transformation that

$$\hat{P}_B\,\hat{\psi}_{k,B}=0 \tag{9}$$

for the Borel transform $\hat{\psi}_{k,B}$ of $\hat{\psi}_k$. Note that the Borel transform $\hat{\psi}_{k,B}$ is computed after applying the Taylor expansion of $\exp(\cdots)$; it then has the form,

$$\left(\exp\left(-\eta\int^{\xi}x_k(\xi)\mathrm{d}\xi\right)\right)(c_0+c_1\eta^{-1}+c_2\eta^{-2}+\cdots)\Big/\sqrt{\eta} \tag{10}$$

and hence its Borel transform is, by definition,

$$\sum_{l=0}^{\infty} \frac{c_l}{\Gamma(l+1/2)} \left(\tilde{y} - \int^{\xi} x_k(\xi) \mathrm{d}\xi \right)^{l-1/2}. \tag{11}$$

It also follows from the definition that the Borel resummed WKB solution $\hat{\psi}_k$ is given by

$$\hat{\psi}_k = \int \exp(-\eta \tilde{y}) \hat{\psi}_{k,B}(\xi, \tilde{y}) \mathrm{d}\tilde{y}, \tag{12}$$

where the integration is performed along the path

$$\tilde{y} = \int_{\hat{a}}^{\xi} x_k(\xi) \mathrm{d}\xi + v, \quad v \geqslant 0. \tag{13}$$

Here $\hat{a}$ is an arbitrarily fixed point to normalize $\hat{\psi}_k$.[10]

So far we have discussed WKB solutions $\hat{\psi}_k$ of the equation $\hat{P}\hat{\psi} = 0$. It is clear that, if we solve the equation $p(x, \xi) = 0$ in the form $\xi = \xi_j(x)$ $(j = 1, \ldots, m)$ we obtain m WKB solutions $\psi_j(x, \eta)$ $(j = 1, \ldots, m)$ of $P\psi = 0$ in the form

$$\psi_j = \exp\left(\eta \int^{x} \xi_j(x) \mathrm{d}x + \cdots \right) \Big/ \sqrt{\eta}, \tag{14}$$

or possibly with another normalization factor η^{-1} instead of $\eta^{-1/2}$, as we will see in Sec. III. Its Borel transform $\psi_{j,B}$ is obtained in the same manner as shown previously.

III. LOCAL CORRESPONDENCE BETWEEN $\hat{\psi}_{k,B}$ AND $\psi_{j,B}$ NEAR A SADDLE POINT

Let us first fix the path of integration in (6); as $\hat{\psi}_k(\xi, \eta)$ has been given its meaning through the Borel resummation, we have only to fix the path of integration in ξ-space. We stipulate that the ξ-integration should be performed along a steepest descent path for $\mathrm{Re}\, f_k$ that passes through a saddle point of f_k with f_k being $x\xi - \int_{\hat{a}}^{\xi} x_k(\xi) \mathrm{d}\xi$. A saddle point ξ_* of f_k satisfies $x = x_k(\xi_*)$, and hence $\xi_* = \xi_j(x)$ holds for some j. Barring the accidental coincidence of ξ_* with a turning point of $\hat{P}$, we find

$$\left. \frac{\mathrm{d}x_k(\xi)}{\mathrm{d}\xi} \right|_{\xi = \xi_j(x)} \neq 0 \tag{15}$$

and hence

$$\left. \frac{\partial^2 f_k}{\partial \xi^2} \right|_{\xi = \xi_j(x)} \neq 0. \tag{16}$$

Thus the ξ-integration is performed along the path described by

$$f_k(x, \xi) = f_k(x, \xi_j(x)) - u^2, \quad u: \text{ real}, \tag{17}$$

i.e.,

$$\left(x\xi - \int_{\hat{a}}^{\xi} x_k(\xi) \mathrm{d}\xi \right) - \left(x\xi_j(x) - \int_{\hat{a}}^{\xi_j(x)} x_k(\xi) \mathrm{d}\xi \right) = -u^2, \quad u: \text{ real}. \tag{18}$$

Fixing the path of integration in (6) in this way, and substituting the Borel sum of $\hat{\psi}_k$ into the integrand, we rewrite the integral (6), by introducing $y=\tilde{y}-x\xi$, in the following way:

$$\varphi=\int\int \exp(-\eta y)\,\hat{\psi}_{k,B}(\xi,y+x\xi)\mathrm{d}y\,\mathrm{d}\xi. \tag{19}$$

Here the domain of integration is described by relation (18) and

$$y=-x\xi_j(x)+\int_{\hat{a}}^{\xi_j(x)} x_k(\xi)\mathrm{d}\xi+v+u^2, \tag{20}$$

which follows from (13) and (18). To see the geometric meaning of (20), let $s(x)$ denote

$$-x\xi_j(x)+\int_{\hat{a}}^{\xi_j(x)} x_k(\xi)\mathrm{d}\xi. \tag{21}$$

Then we find

$$\frac{\mathrm{d}s(x)}{\mathrm{d}x}=-\xi_j(x)-x\frac{\mathrm{d}\xi_j}{\mathrm{d}x}+x_k(\xi_j(x))\frac{\mathrm{d}\xi_j}{\mathrm{d}x}=-\xi_j(x). \tag{22}$$

Thus (20) is rewritten as

$$y=-\int_a^x \xi_j(x)\mathrm{d}x+v+u^2, \tag{23}$$

where a is a fixed point. If we set $w=v+u^2$, the positivity assumption on v entails $u^2\leqslant w$. Hence ξ obeying relation (18) can range only over a compact set for a fixed pair (x,w) $(w\geqslant 0)$. Therefore the integral

$$\chi(x,y)=\int \hat{\psi}_{k,B}(x,y+x\xi)\mathrm{d}\xi \tag{24}$$

is well defined if y satisfies

$$y=-\int_a^x \xi_j(x)\mathrm{d}x+w,\quad w\geqslant 0 \tag{25}$$

and if the ξ-integration is done along the path described by (18). Thus the integral (6) can be written as

$$\int \exp(-\eta y)\chi(x,y)\mathrm{d}y, \tag{26}$$

where y ranges over the half-line $\{y\in\mathbb{C};y=-\int_a^x\xi_j(x)\mathrm{d}x+w,w\geqslant 0\}$. We shall further confirm that $\chi(x,y)$ is the Borel transform of a WKB solution of the equation $P\psi=0$. In view of the particular form of the integral (26), we will then be convinced that the integral (6) should play an important role in describing the domain on which the Borel sum of a WKB solution of $P\psi=0$ is well defined.

In order to verify that χ is the Borel transform of a WKB solution of $P\psi=0$, let us first show $P_B\chi=0$ by the integration by parts. In fact, we have

$$P_B\chi=\sum a_{jl}x^l\left(\frac{\partial}{\partial x}\right)^j\left(\frac{\partial}{\partial y}\right)^{m-j}\int \hat{\psi}_{k,B}(\xi,y+x\xi)\mathrm{d}\xi$$
$$=\sum a_{jl}\int \xi^j\left(\frac{\partial}{\partial y}\right)^{j+m-j}x^l\,\hat{\psi}_{k,B}(\xi,y+x\xi)\mathrm{d}\xi$$
$$=\sum a_{jl}\int \xi^j\left(\frac{\partial}{\partial y}\right)^{m-l}\left(x\frac{\partial}{\partial y}\right)^l\hat{\psi}_{k,B}(\xi,y+x\xi)\mathrm{d}\xi$$
$$=\sum a_{jl}\left(\frac{\partial}{\partial y}\right)^{m-l}\int \left(\frac{\partial}{\partial\zeta}\right)^l(\xi^j\hat{\psi}_{k,B}(\xi,y+x\zeta))\Big|_{\zeta=\xi}\mathrm{d}\xi. \tag{27}$$

By repeatedly using the following identity

$$\frac{\partial}{\partial\xi}(\xi^j\varphi(\xi,y+x\xi))=\frac{\partial}{\partial\xi}(\xi^j\varphi(\xi,y+x\zeta))\Big|_{\zeta=\xi}+\frac{\partial}{\partial\zeta}(\xi^j\varphi(\xi,y+x\zeta))\Big|_{\zeta=\xi} \tag{28}$$

together with the integration by parts applied to the integral interpreted as contour integral, we find

$$P_B\chi=\sum a_{jl}\left(\frac{\partial}{\partial y}\right)^{m-l}\int \left(-\frac{\partial}{\partial\xi}\right)^l(\xi^j\hat{\psi}_{k,B}(\xi,y+x\zeta))\Big|_{\zeta=\xi}\mathrm{d}\xi=0, \tag{29}$$

as

$$\hat{P}_B\hat{\psi}_{k,B}(\xi,y)=\Sigma a_{jl}\left(\frac{\partial}{\partial y}\right)^{m-l}\left(-\frac{\partial}{\partial\xi}\right)^l\xi^j\hat{\psi}_{k,B}(\xi,y)=0.$$

Furthermore a mathematical theory[11] tells us that $\chi(x,y)$ has a singularity of the form $\alpha(x,y)\log(y+\int_a^x\xi_j(x)\mathrm{d}x)+\beta(x,y)$ with α and β holomorphic near $y=-\int_a^x\xi_j(x)\mathrm{d}x$, as $\hat{\psi}_{k,B}(\xi,\tilde{y})$ has the singularity of the form $\tilde{\alpha}(\xi,\tilde{y})(\tilde{y}-\int_a^\xi x_k(\xi)\mathrm{d}\xi)^{-1/2}+\tilde{\beta}(\xi,\tilde{y})$ with $\tilde{\alpha}$ and $\tilde{\beta}$ holomorphic near $\tilde{y}=\int_a^\xi x_k(\xi)\mathrm{d}\xi$. This result combined with the relation $P_B\chi=0$ entails that χ is the Borel transform of a WKB solution of $P\psi=0$ that has the form $\exp(\eta\int_a^x\xi_j(x)\mathrm{d}x+\cdots)/\eta$.

Summing up, the integral (6) relates $\hat{\psi}_{k,B}$ to $\psi_{j,B}$ unless extra singularities become relevant to the domain of integration specified by (13) and (18). As we will see in Sec. IV, other singularities of $\hat{\psi}_{k,B}(\xi,y)$ really sneak into the domain in question if the steepest descent path (18) crosses a Stokes curve for $\hat{P}$. In this sense, the discussion in this section concerns the local correspondence of $\hat{\psi}_{k,B}$ and $\psi_{j,B}$ near the saddle point $\xi=\xi_j(x)$. It is worth noting that this correspondence is what mathematicians call ''the quantized Legendre transformation'' with a generating function $\delta(y-\tilde{y}+x\xi)\mathrm{d}\xi\,\mathrm{d}\tilde{y}$.[12]

IV. CORRESPONDENCE OF WKB SOLUTIONS IN THE LARGE: INTRODUCTION OF THE NOTION OF EXACT STEEPEST DESCENT PATHS

When the steepest descent path for $\mathrm{Re}\,f_k$ given in Sec. III that passes through the saddle point $\xi=\xi_j(x)$ crosses a Stokes curve for $\hat{P}$, say at $\xi=\xi_0$, the singularity of $\hat{\psi}_{k,B}(\xi,\tilde{y})$ located at $\tilde{y}=\int_a^\xi x_{k'}(\xi)\mathrm{d}\xi(k'\neq k)$ may become relevant to the integral (19) by the definition of a Stokes curve in the exact WKB analysis.[10] If $\hat{\psi}_k$ is dominant over $\hat{\psi}_{k'}$ along the Stokes curve, the integral (19) will acquire an additional exponentially small term as a consequence of the ''connection formula.'' To give the concrete description of the added term is the purpose of this section. Our description is based on a precise computation done for the case where P is a harmonic oscillator.[13]

As the exact WKB analysis is complete only for the second-order operators, we now assume that $n=2$, i.e., $\hat{P}$ is of the second order. (Practically speaking, we can deal with more general

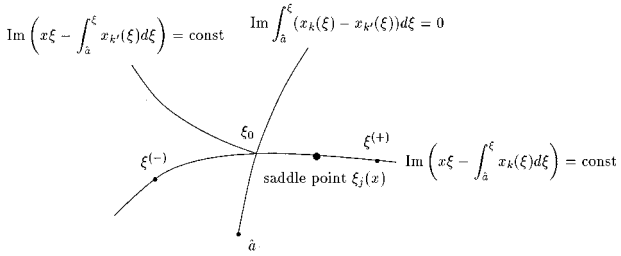


FIG. 1. Crossing of a steepest descent path and a Stokes curve.

operators. See, e.g., example 2 in Sec. V.) When $\hat{P}$ is of second order, we can, and really do, choose $\hat{a}$, the end point of the integral, to be the turning point from which the Stokes curve in question emanates so that $\hat{\psi}_k$ has the form

$$(-\eta x_k(\xi)+\cdots)^{-1/2}\exp\left(\int_{\hat{a}}^{\xi}(-\eta x_k(\xi)+\cdots)\mathrm{d}\xi\right), \tag{30}$$

where $\cdots$ designates terms with odd (and negative) powers of η. We also note that the Stokes curve in question is given by

$$\mathrm{Im}\int_{\hat{a}}^{\xi}(x_k(\xi)-x_{k'}(\xi))\mathrm{d}\xi=0 \tag{31}$$

(cf. Fig. 1). Normalizing $\hat{\psi}_{k'}$ in the same manner as done for $\hat{\psi}_k$, the dominant (Borel resummed) term $\hat{\psi}_k$ acquires an exponentially small term

$$\pm i\hat{\psi}_{k'} \tag{32}$$

when it crosses the Stokes curve (31).[14] The sign depends on the configuration of the steepest descent path and the Stokes curve, and we assume without loss of the generality that the sign is $+$. This exponentially small term appears as a consequence of the fact that at $\xi=\xi_0$ the singularity of $\hat{\psi}_{k,B}(\xi,\tilde{y})$ located at $\tilde{y}=\int_{\hat{a}}^{\xi}x_{k'}(\xi)\mathrm{d}\xi$ hits the path of integration (13) that defines the Borel sum of $\hat{\psi}_k(\xi,\eta)$. Otherwise stated, if we define u_0 and v_0, respectively, by

$$u_0^2=-x\xi_0+\int_{\hat{a}}^{\xi_0}x_k(\xi)\mathrm{d}\xi+x\xi_j(x)-\int_{\hat{a}}^{\xi_j(x)}x_k(\xi)\mathrm{d}\xi \tag{33}$$

and

$$v_0=\int_{\hat{a}}^{\xi_0}(x_{k'}(\xi)-x_k(\xi))\mathrm{d}\xi, \tag{34}$$

then the integrand of (19) finds a new singularity on its domain of integration when $(u,v)=(u_0,v_0)$. Note that $v_0\geqslant 0$ holds because of the fact that ξ_0 is on the Stokes curve in question together with the fact that $\hat{\psi}_k$ is dominant over $\hat{\psi}_{k'}$ there. To fix the configuration of several points to be discussed in the following, we assume $u_0<0$. To analyze the integral (24) with the explicit use of ξ-variable (rather than the u-variable) we introduce the symbol $\xi^{(\pm)}$ to denote the end points of the integral (24). For the sake of definiteness we suppose that $\xi^{(-)}$ corresponds to u that is negative and smaller than u_0. Note also that ξ_0 corresponds to u_0. If we let ξ_* denote the singular point of $\hat{\psi}_{k,B}(\xi,\tilde{y})$ that is described by $\tilde{y}=\int_{\hat{a}}^{\xi}x_{k'}(\xi)\mathrm{d}\xi$, our task is then to describe concretely the integral I obtained by the integration from ξ_0 to ξ_* in Fig. 2(b).

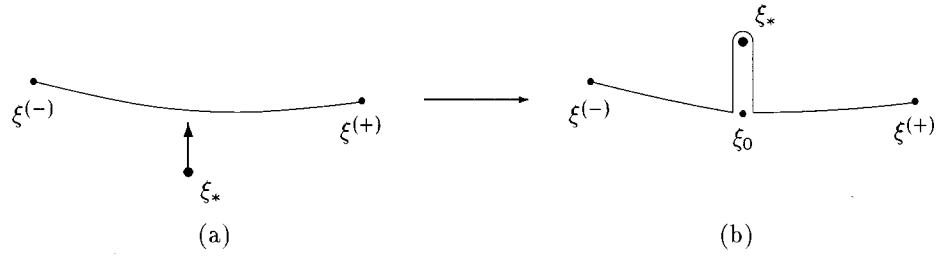


FIG. 2. Singular point ξ_* of $\hat{\psi}_{k,B}(\xi,\tilde{y})$ hitting the path of integration.

In view of the connection formula (32), this integral should be related to $i\hat{\psi}_{k',B}$. To find the precise form of the relation let us consider the following integral (35) with the domain of integration prescribed by (36) and (37) in the following; in what follows we show that the integral I is coincident with the integral (35) with this particular choice of the domain of integration. This integral was first found in the course of concrete computations for harmonic oscillators:[13]

$$i\int\int \exp(\eta(x\xi-\tilde{y}))\hat{\psi}_{k',B}(\xi,\tilde{y})\mathrm{d}\xi\mathrm{d}\tilde{y}=i\int \exp(-\eta y)\left(\int \hat{\psi}_{k',B}(\xi,y+x\xi)\mathrm{d}\xi\right)\mathrm{d}y, \tag{35}$$

where the domain of integration is given by

$$\tilde{y}=\int_{\hat{a}}^{\xi} x_{k'}(\xi)\mathrm{d}\xi+\tilde{v}, \quad \tilde{v}\geqslant 0 \tag{36}$$

and

$$x\xi-\int_{\hat{a}}^{\xi} x_{k'}(\xi)\mathrm{d}\xi-x\xi_0+\int_{\hat{a}}^{\xi_0} x_{k'}(\xi)\mathrm{d}\xi=-\tilde{u}, \quad \tilde{u}\geqslant 0. \tag{37}$$

The geometric meaning of (37) is worth mentioning: ξ obeying (37) is on the steepest descent path for $\mathrm{Re}\, f_{k'}$ with

$$f_{k'}\underset{\mathrm{def}}{=}x\xi-\int_{\hat{a}}^{\xi} x_{k'}(\xi)\mathrm{d}\xi$$

that passes through the point $\xi=\xi_0$. Note that ξ_0 is not a saddle point of $f_{k'}$. Let us now try to find where ξ ranges for fixed x and y; it is clear that

$$y=\tilde{y}-x\xi=-x\xi_0+\int_{\hat{a}}^{\xi_0} x_{k'}(\xi)\mathrm{d}\xi+\tilde{u}+\tilde{v} \tag{38}$$

follows from (36) and (37). Since we know by (22) that

$$-x\xi_j(x)+\int_{\hat{a}}^{\xi_j(x)} x_k(\xi)\mathrm{d}\xi=-\int_a^x \xi_j(x)\mathrm{d}x \tag{39}$$

holds for some a, we can rewrite (38) as follows:

$$y=-\int_a^x \xi_j(x)\mathrm{d}x+x\xi_j(x)-\int_{\hat{a}}^{\xi_j(x)} x_k(\xi)\mathrm{d}\xi-x\xi_0+\int_{\hat{a}}^{\xi_0} x_{k'}(\xi)\mathrm{d}\xi+\tilde{u}+\tilde{v}. \tag{40}$$

On the other hand, (33) and (34) entail

$$-x\xi_0+\int_{\hat{a}}^{\xi_0}x_{k'}(\xi)\mathrm{d}\xi+x\xi_j(x)-\int_{\hat{a}}^{\xi_j(x)}x_k(\xi)\mathrm{d}\xi=u_0^2+v_0. \tag{41}$$

Hence we find

$$y=-\int_a^x\xi_j(x)\mathrm{d}x+w,\quad w=w_0+\tilde{u}+\tilde{v}, \tag{42}$$

where w_0 denotes $u_0^2+v_0$. Since $\tilde{v}$ is supposed to be non-negative, the ξ-integration in (35) is done over the region

$$0\leqslant\tilde{u}\leqslant w-w_0. \tag{43}$$

Let us now consider the geometric meanings of the points corresponding to $\tilde{u}=0$ or $\tilde{u}=w-w_0$. Clearly $\xi=\xi_0$ is the point corresponding to $\tilde{u}=0$. Let ξ'_* denote the point that corresponds to $\tilde{u}=w-w_0$. Then it follows from the definition of $\tilde{u}$ that

$$x\xi'_x-\int_{\hat{a}}^{\xi'_*}x_{k'}(\xi)\mathrm{d}\xi=x\xi_0-\int_{\hat{a}}^{\xi_0}x_{k'}(\xi)\mathrm{d}\xi-(w-w_0). \tag{44}$$

Using the definition of w_0, we find this is equal to

$$x\xi_j(x)-\int_{\hat{a}}^{\xi_j(x)}x_k(\xi)\mathrm{d}\xi-w, \tag{45}$$

which has another expression

$$\int_a^x\xi_j(x)\mathrm{d}x-w \tag{46}$$

by (39). Thus we find

$$x\xi'_*-\int_{\hat{a}}^{\xi'_*}x_{k'}(\xi)\mathrm{d}\xi=\int_a^x\xi_j(x)\mathrm{d}x-w=-y \tag{47}$$

by (42), that is, ξ'_* is a point satisfying the relation (47) on the steepest descent path for $\mathrm{Re}\,f_{k'}$ that emanates from $\xi=\xi_0$. Summing up, we can rewrite the integral (35) as follows:

$$\int_L\exp(-\eta y)\left(\int_{\xi_0}^{\xi'_*}i\hat{\psi}_{k',B}(\xi,y+x\xi)\,\mathrm{d}\xi\right)\mathrm{d}y, \tag{48}$$

where $L=\{y\in\mathbb{C};y=-\int_a^x\xi_j(x)\mathrm{d}x+w,w\geqslant w_0\}$.

Before relating this integral with the connection formula for $\hat{P}$, we note the following property of ξ'_*; relation (47) implies that, at $\xi=\xi'_*$, $\tilde{y}=y+x\xi$ attains the value $\int_{\hat{a}}^{\xi'_*}x_{k'}(\xi)\mathrm{d}\xi$. This is a singular point of $\hat{\psi}_{k',B}(\xi,\tilde{y})$, which coincides with a singular point of $\hat{\psi}_{k,B}(\xi,\tilde{y})$ that is described by $\int_{\hat{a}}^{\xi_*}x_{k'}(\xi)\mathrm{d}\xi$, i.e., the singularity considered in Fig. 2. Thus ξ'_* is actually equal to ξ_*, an end point of the integral I we encountered in Fig. 2. Otherwise stated, the point $\xi=\xi_*$ also lies on the steepest descent path for $\mathrm{Re}\,f_{k'}$ that emanates from ξ_0. Hence the integral I in question is expressed as

$$\int_\gamma\hat{\psi}_{k,B}(\xi,y+x\xi)\mathrm{d}\xi, \tag{49}$$

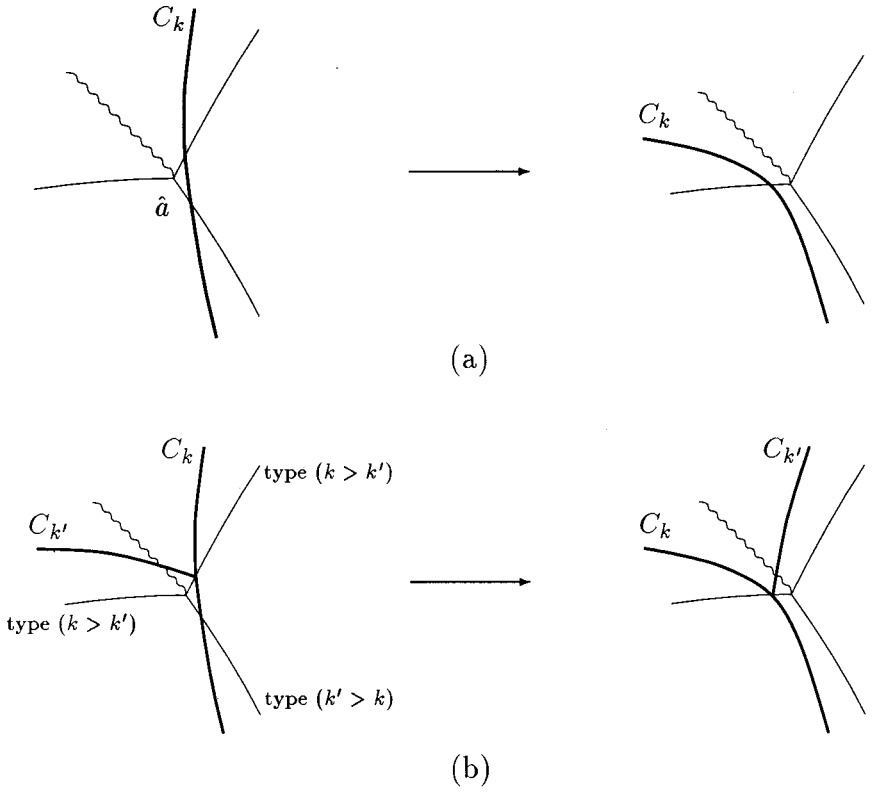


FIG. 3. Schematic illustration of a change of configurations of ordinary steepest descent paths (a) and of exact ones (b) when they hit a simple turning point $\hat{a}$; a lightfaced line and a wiggly line, respectively, designate a Stokes curve and a cut [defining the Riemann surface of $x_k(\xi)$].

where γ denotes a path of integration that starts from ξ_0 and comes back to ξ_0 by encircling the portion of the steepest descent path for $\mathrm{Re}\, f_{k'}$ whose boundaries are ξ_0 and ξ_*. Now let us recall the precise meaning of the connection formula (32) in the exact WKB analysis:[10] if we let $\Delta\hat{\psi}_{k,B}$ denote the discontinuity of $\hat{\psi}_{k,B}(\xi,\tilde{y})$ along the cut $\{\tilde{y}\in\mathbb{C};\tilde{y}=\int_a^\xi x_{k'}(\xi)\mathrm{d}\xi+\tilde{v},\tilde{v}\geqslant 0\}$, then

$$\Delta\hat{\psi}_{k,B}=i\hat{\psi}_{k',B}. \tag{50}$$

Since $(\Delta\hat{\psi}_{k,B})(\xi,y+x\xi)$ is coincident with the integrand of integral (49) because of the choice of the path γ, the integral I is equal to integral (48) by (50). Therefore we conclude that the concrete form of the integral I is given by the integral (35) whose domain of integration is specified by (36) and (37).

The discussion given in this section tells us that, if we consider the integral (24) globally with respect to y, we are forced to consider not only the steepest descent path C_k for $\mathrm{Re}\, f_k$ passing through the saddle point of f_k but also another steepest descent path $C_{k'}$ for $\mathrm{Re}\, f_{k'}$ that is bifurcated from C_k at the crossing point of C_k and a Stokes curve for $\hat{P}$. The necessity of integration over a portion of C_k' and the connection formula for WKB solutions of $\hat{P}\hat{\psi}=0$ are two sides of the same coin, and hence the integral along C_k and that along $C_{k'}$ are, so to speak, equal partners. Therefore, if $C_{k'}$ hits some saddle point, say $\xi=\xi_l(x)$, then some anomalies should be observed in the Borel sum of WKB solutions of the starting equation $P\psi=0$, that is, the point x should be on a Stokes curve for P, ordinary or new. Thus we are led to the ''exact steepest descent path ansatz,'' or ''ESDP ansatz'' for short, which is given in the following. To state the ESDP ansatz,

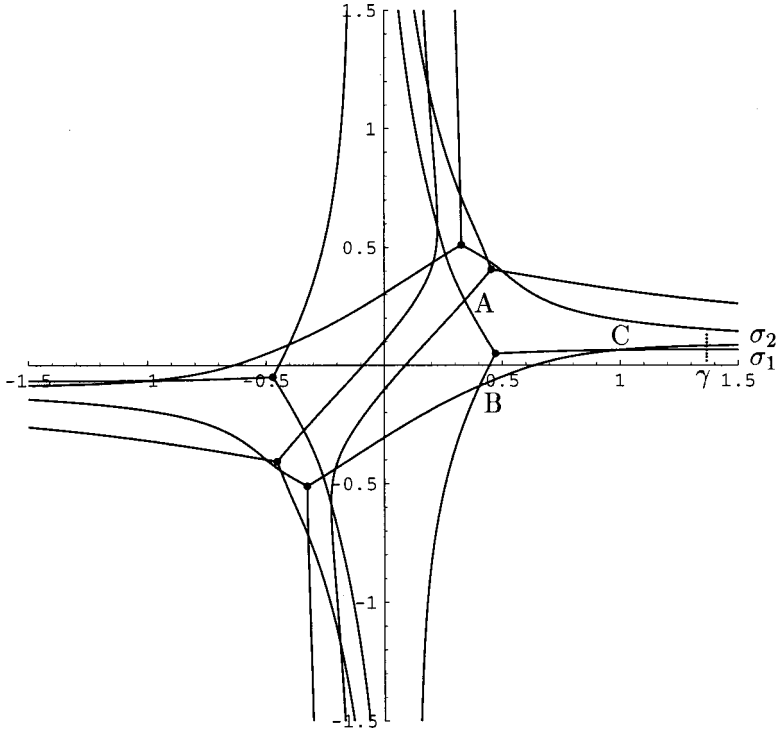


FIG. 4. Stokes curves of Eq. (51).

we prepare the following definition of an exact steepest descent path. There we use the terminology "a Stokes curve of type $(k>k')$" to mean that $\hat{\psi}_k$ is dominant over $\hat{\psi}_{k'}$ along the Stokes curve.

Definition of an exact steepest descent path: Let f_l denote $x\xi-\int_a^\xi x_l(\xi)\mathrm{d}\xi$. An exact steepest descent path C is, by definition, the union of portions of steepest descent paths obtained by the following procedure.

Start with a steepest descent path C_k of $\mathrm{Re}\, f_k$ for some k that passes through a saddle point. If C_k crosses a Stokes curve (for $\hat{P}$) of type $(k>k')$, consider the steepest descent path $C_{k'}$ for $\mathrm{Re}\, f_{k'}$ which starts from the crossing point. If $C_{k'}$ crosses another Stokes curve of type $(k'>k'')$, consider another steepest descent path $C_{k''}$ for $\mathrm{Re}\, f_{k''}$ in the same manner, and so on.

Exact steepest descent path ansatz: *Stokes phenomena for Borel resummed WKB solutions of* $P\psi=0$ *are observed at* x *if and only if an exact steepest descent path connects two saddle points* $\xi_k(x)$ *and* $\xi_l(x)$.

It is evident that this ansatz is a natural generalization of the results[15,16] obtained for a Laplace-type operator P (i.e., an operator whose Laplace transform is of the first order). We also note that the ESDP ansatz is validated by the reasoning given in this section in a most basic situation, that is, when the operator $\hat{P}$ is of the second order and when a steepest descent path passing through a saddle point crosses only one Stokes curve for $\hat{P}$; with this observation we believe that the above-mentioned ansatz should be true in general.

Remark 1: Introduction of exact steepest descent paths automatically resolves the spurious changes of topological configurations of steepest descent paths that occur when they hit a turning

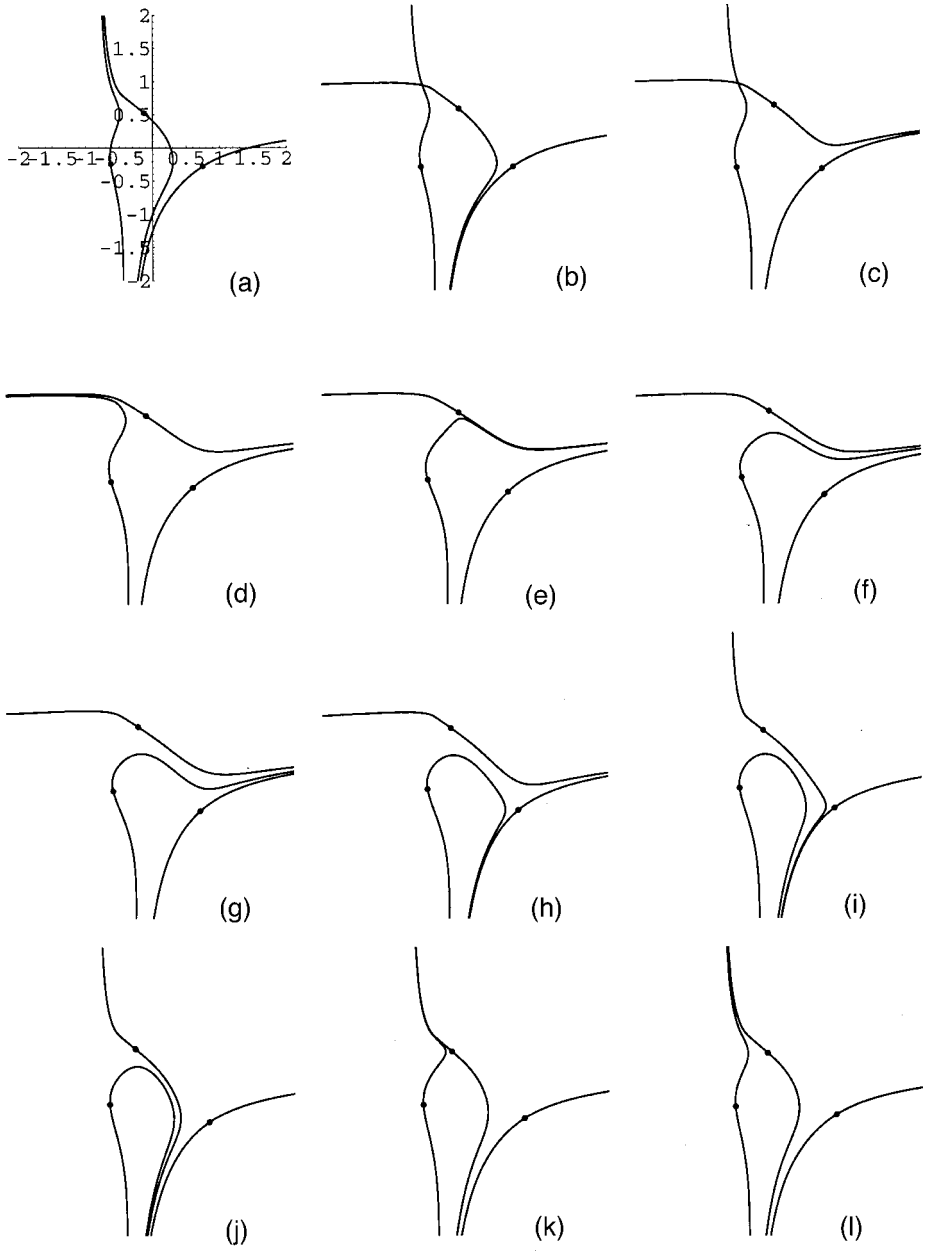


FIG. 5. Ordinary steepest descent paths around the crossing point A.

point of $\hat{P}$. For example, as is shown in Fig. 3, when a steepest descent path C_k hits a simple turning point $\hat{a}$, no topological change of configurations occurs for the exact steepest descent path $C_k \cup C_{k'}$ although the shape of C_k itself changes abruptly.[17]

V. COMPUTER-ASSISTED STUDY OF THE EXACT STEEPEST DESCENT PATH ANSATZ

The purpose of this section is to present a computer-assisted study of the ESDP ansatz in some illuminating examples. See our previous paper[18] for some more detailed explanation of the figures given in the following. We also note that the above-mentioned paper contains discussions on some

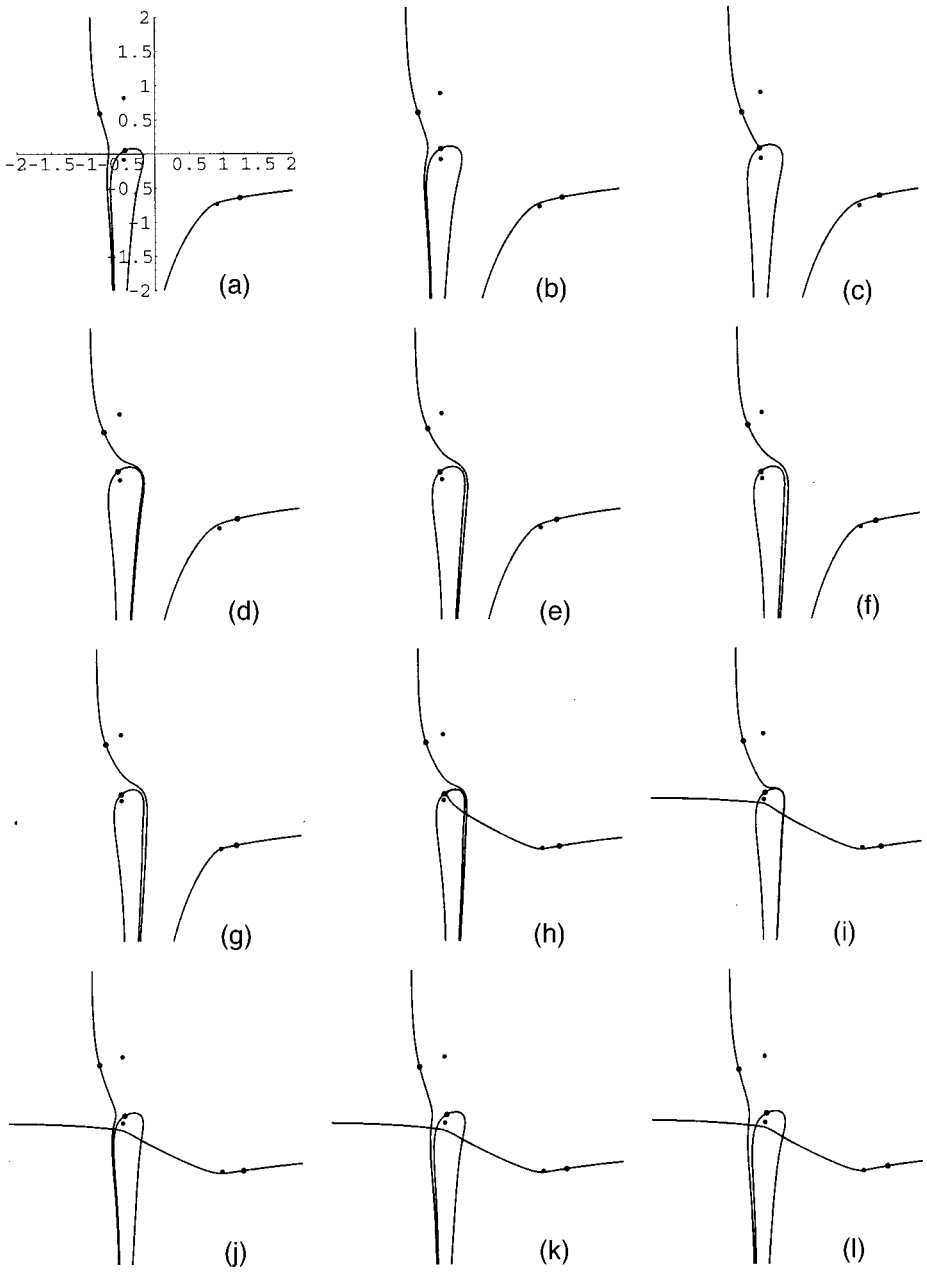


FIG. 6. Ordinary steepest descent paths around the crossing point B.

other less peculiar examples; the examples given in the following are the most illuminating ones among them. All computations are done using MATHEMATICA (ver. 3.0.1 or 4.0.2.1).

Example 1: Consider the following equation:

$$\left(\frac{\mathrm{d}^3}{\mathrm{d}x^3}+\eta^2(i-4x^2)\frac{\mathrm{d}}{\mathrm{d}x}+\eta^3\left(\frac{i}{2}-x^2\right)\right)\psi=0. \tag{51}$$

If we draw ordinary Stokes curves (i.e., if we ignore temporarily new turning points and new Stokes curves), we obtain Fig. 4.

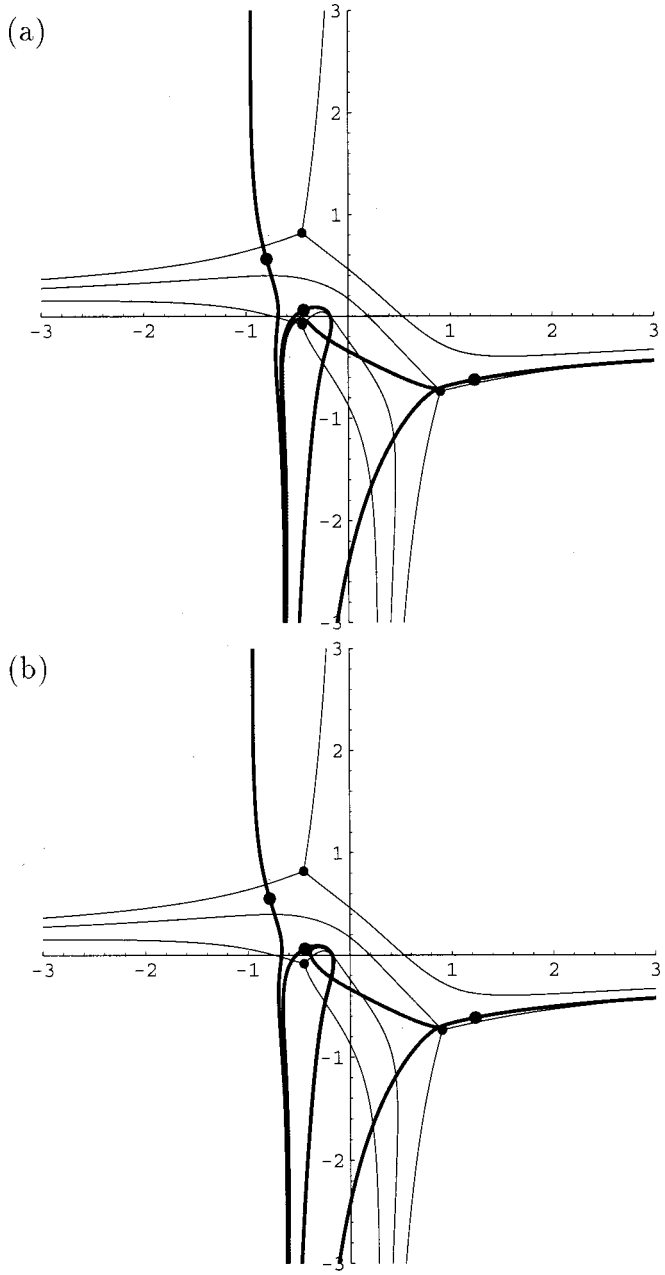


FIG. 7. Exact steepest descent paths for $x=0.459\,36-0.067\,718\,i$ (a) and for $x=0.455\,97-0.060\,089\,4\,i$ (b).

(i) Let us consider the problem near the point A where two Stokes curves cross; let x_k ($k=0,1,\ldots,11$) denote the point

$$c+0.05e^{\pi ik/6}, \tag{52}$$

where c stands for the coordinate of A, and consider the ordinary steepest descent paths for the integral (19) [or rather (6)] with $x=x_k$. With the aid of a computer we find Fig. 5, where Figs. 5(a), 5(b), . . . , 5(l) illustrate the configuration for $x=x_0$, x_1, . . . , x_{11}, respectively. We seek a topological change of configurations which occurs when a steepest descent path hits another saddle point. (The change that occurs when a steepest descent path hits a turning point is spurious

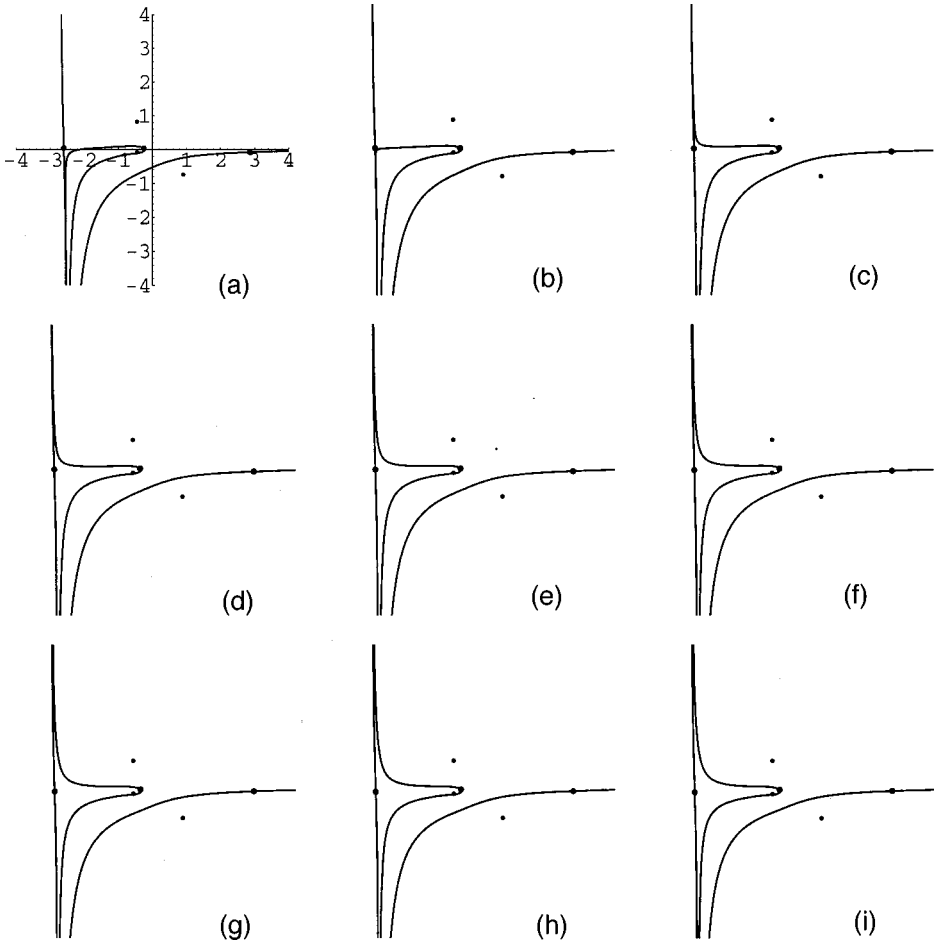


FIG. 8. Ordinary steepest descent paths for the point x_k on the path γ.

and should be ignored; cf. Remark 1 in Sec. IV.) We then observe five changes of the configuration of this kind: between $x=x_1$ and $x=x_2$, around $x=x_4$, between $x=x_7$ and $x=x_8$, around $x=x_{10}$, and between $x=x_6$ and $x=x_7$. Each of the first four corresponds to one of four portions of Stokes curves meeting at the point A, while the fifth change that occurs between $x=x_6$ and $x=x_7$ can be attributed to a new Stokes curve passing through the ordered crossing point A (in the sense of Berk *et al.*[2]). Thus the (ordinary) steepest descent method applied to the integral (6) correctly detects Stokes curves in this case.

(ii) In spite of the success shown in (i), the method fails near B, another crossing point of Stokes curves in Fig. 4. Choosing c to be the coordinate of the point B, we find Fig. 6 that shows the configuration of the ordinary steepest descent paths for the integral (6). In Fig. 6 one can observe only three relevant topological changes of the configuration: around $x=x_2$, around $x=x_7$, and between $x=x_8$ and $x=x_9$. However, the reasoning of Berk *et al.*[19,20] indicates that three Stokes segments meet at a point only if one of them or all of them are actually irrelevant to Stokes phenomena. Otherwise stated, the ordinary steepest descent method applied to the integral (6) cannot correctly detect the Stokes phenomena in this case.

Contrary to this failure, if we use exact steepest descent paths, then we can correctly detect the points where the Stokes phenomena occur, as Fig. 7 shows. Figure 7 visualizes the movement between $x=x_0$ and $x=x_1$ of configuration of the exact steepest descent paths of the integral (19); in order not to make the figures too complicated, some irrelevant paths are omitted. The heavy line designates the *exact* steepest descent path, which plays a crucially important role.

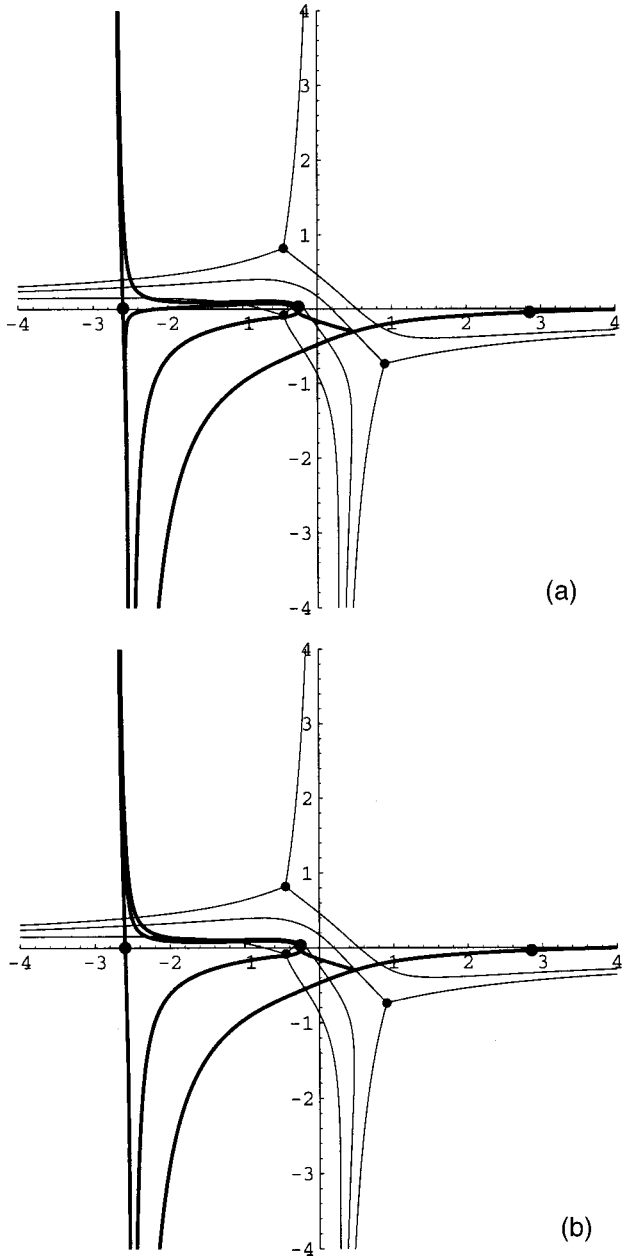
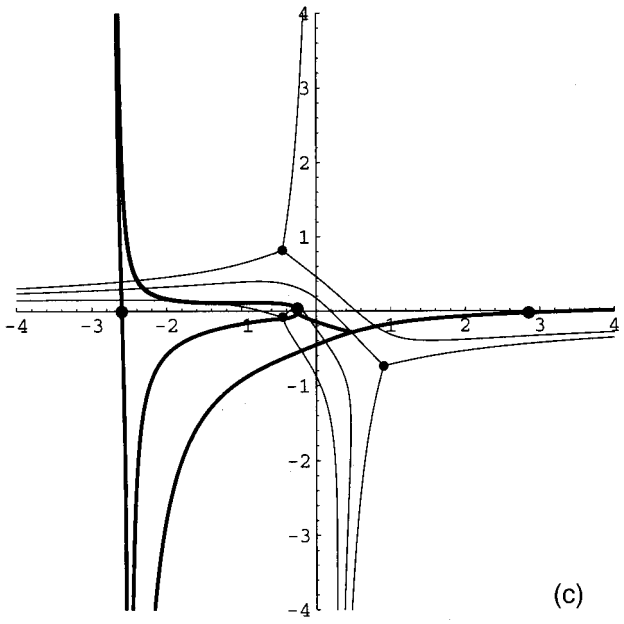


FIG. 9. (i) Exact steepest descent paths for $x=1.37+0.074\,75\,i$ (a) and for $x=1.37+0.08\,i$ (b). (ii) Exact steepest descent paths for $x=1.37+0.085\,25\,i$ (c) and for $x=1.37+0.0905\,i$ (d). (ii bis) Added exact steepest descent paths for $x=1.37+0.085\,25\,i$ (c′) and for $x=1.37+0.0905\,i$ (d′).

(iii) Additional evidence strongly in support of the ESDP ansatz can be found near the point C, where two Stokes curves cross. Let $x_k(k=0,1,\ldots,8)$ denote the point $1.37+\sqrt{-1}(0.059+0.005\,25k)$; these points lie on the path γ that is designated by a dotted line in Fig. 4. Then we find Fig. 8, where Figs. 8(a), . . . , 8(i) describe the configuration of ordinary steepest descent paths for $x=x_0, \ldots, x_8$, respectively. In Fig. 8 we observe a topological change of the configuration only near $x=x_1$, which evidently corresponds to the situation where γ crosses an ordinary Stokes curve σ_1 in Fig. 4; we cannot observe any changes that might be attributed to the crossing of γ and another ordinary Stokes curve σ_2 or a possibly relevant new Stokes curve σ_0 emanating from the crossing point C.



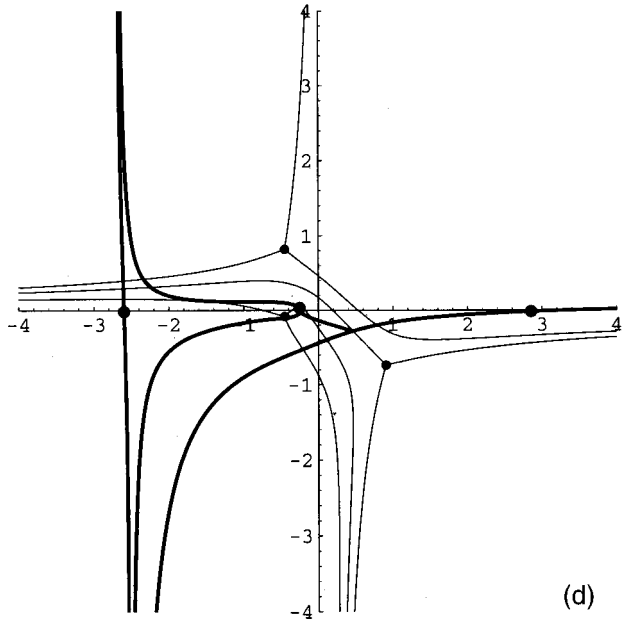


FIG. 9 (*Continued.*)

Let us now add an exact steepest descent path to Figs. 8(d) and 8(e); the resulting figures are, respectively, Figs. 9(a) and 9(b). In contrast with Figs. 8(d) and 8(e), they clearly show a topological difference of configurations. This topological change that occurs between $x=x_3$ and $x=x_4$ corresponds to the crossing of γ and a new Stokes curve σ_0 that emanates from C.

Similarly we find Figs. 9(c) and 9(d) by adding an exact steepest descent path, respectively, to Figs. 8(f) and 8(g). They again show a topological change of configurations, which occurs between $x=x_5$ and $x=x_6$. (As Figs. 9(c) and 9(d) seem to be too complicated to decipher, we also present Fig. 9(c′) and Fig. 9(d′) which contain only the added exact steepest descent path, so that the reader's attention may be concentrated upon it.) This change that occurs between $x=x_5$ and $x=x_6$ corresponds to the crossing of γ and the ordinary Stokes curve σ_2.

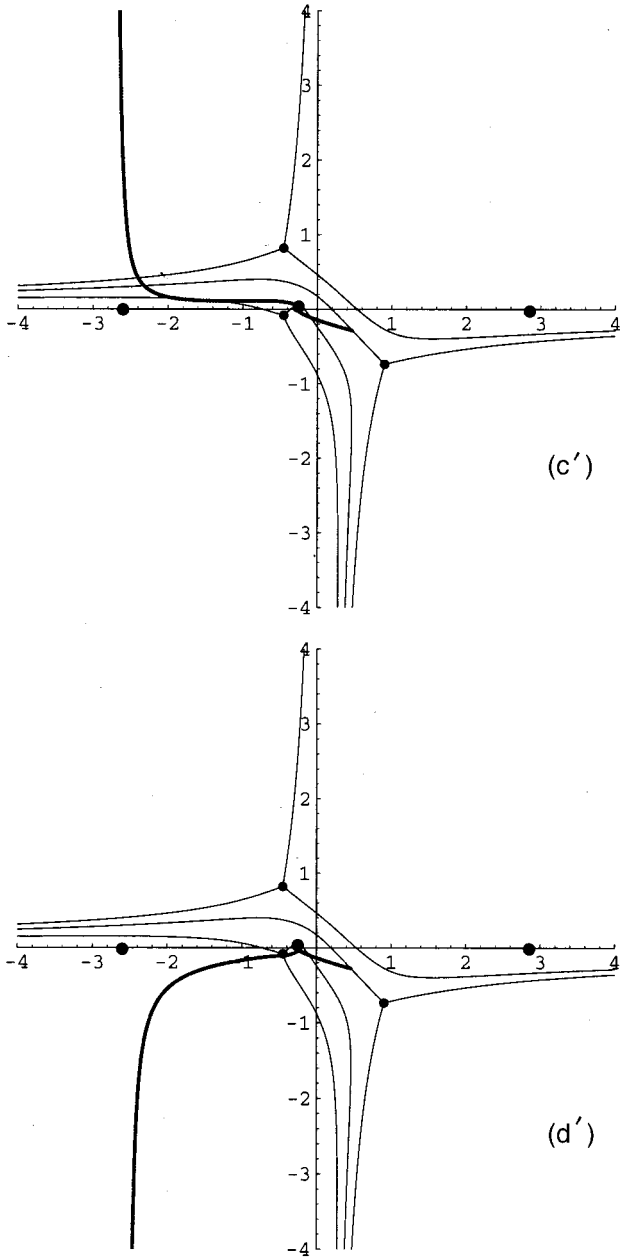


FIG. 9 (*Continued.*)

Thus the addition of an exact steepest descent path neatly explains delicate issues concerning the Stokes phenomena near point C.

Example 2: In order to show that the ESDP ansatz may be valid even if $\hat{P}$ is of higher order, let us study the following Carroll–Hioe equation:

$$\frac{d^3\psi}{dx^3}+2i(r_1+r_2+r_3)\eta x\frac{d^2\psi}{dx^2}+\{-4(r_1r_2+r_2r_3+r_3r_1)\eta^2x^2+2ic_1\eta$$
$$+\tfrac{1}{4}[(\Omega_{12})^2+(\Omega_{23})^2]\eta^2\}\frac{d\psi}{dx}+\{-8ir_1r_2r_3\eta^3x^3-4c_2\eta^2x$$
$$+\tfrac{1}{2}[(\Omega_{12})^2r_3+(\Omega_{23})^2r_1]\eta^3x\}\psi=0, \tag{53}$$

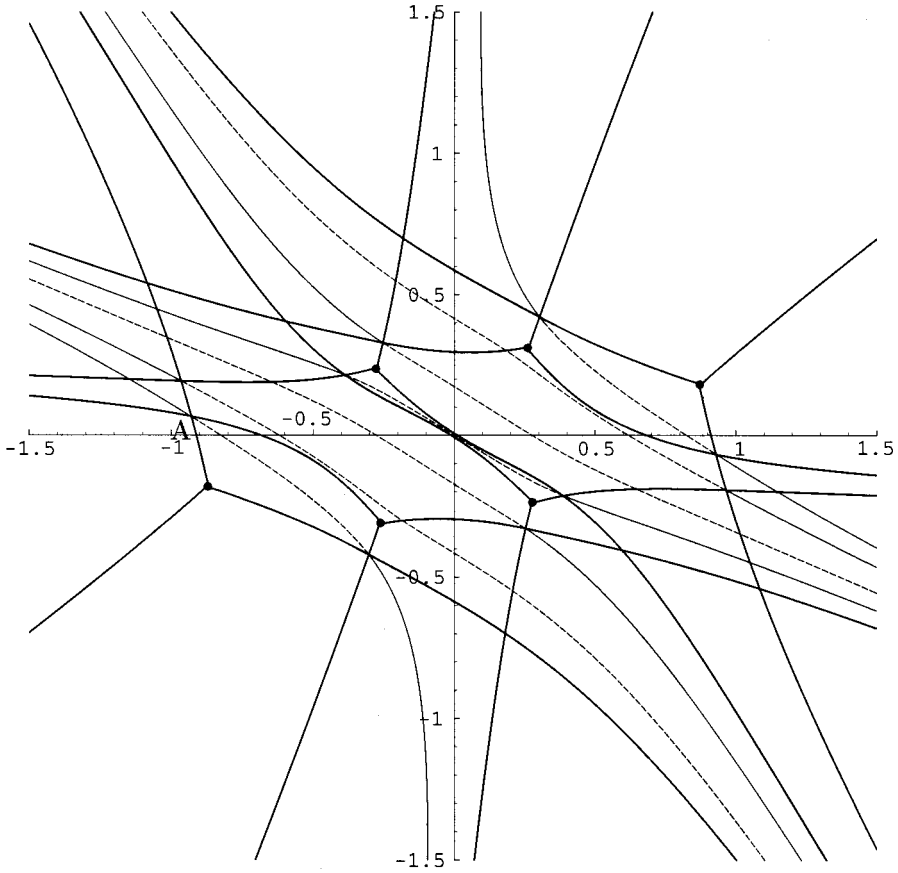


FIG. 10. Stokes geometry for Eq. (53).

where $r_1, r_2, r_3, \Omega_{12}, \Omega_{23}, c_1$, and c_2 are some parameters. In what follows all figures are drawn for the following values of these parameters: (there is no particular meaning in this choice)

$$r_1 = -2+i, \quad r_2 = \tfrac{1}{2}+2i, \quad r_3 = 1-2i, \tag{54}$$

$$\Omega_{12} = -3+4i, \quad \Omega_{23} = 1-3i, \quad \text{and}$$

$$c_1 \text{ and } c_2 \text{ are arbitrarily fixed.}$$

Although $\hat{P}$ is of the third order, Carroll–Hioe ingeniously gave an integral representation of solutions of (53). Hence we can describe the complete Stokes geometry for (53) by analyzing the integral again with the aid of a computer.[21] The result is shown in Fig. 10. (A dotted line indicates that no Stokes phenomena occur across that portion of the curve.)

Choosing c in (52) to be the coordinate of the point A in Fig. 10, we illustrate the configuration of ordinary steepest descent paths for the integral that represents a solution of (53) and the integral (6), respectively, in Figs. 11 and 12. In Fig. 12 we cannot observe any topological change of the configuration caused by the interaction of steepest descent paths and saddle points between $x = x_3$ and $x = x_4$, which is observed in Fig. 11. If we use exact steepest descent paths in addition to ordinary ones, the topological change can be observed in Fig. 13, which describes the behavior between $x = x_3$ and $x = x_4$.

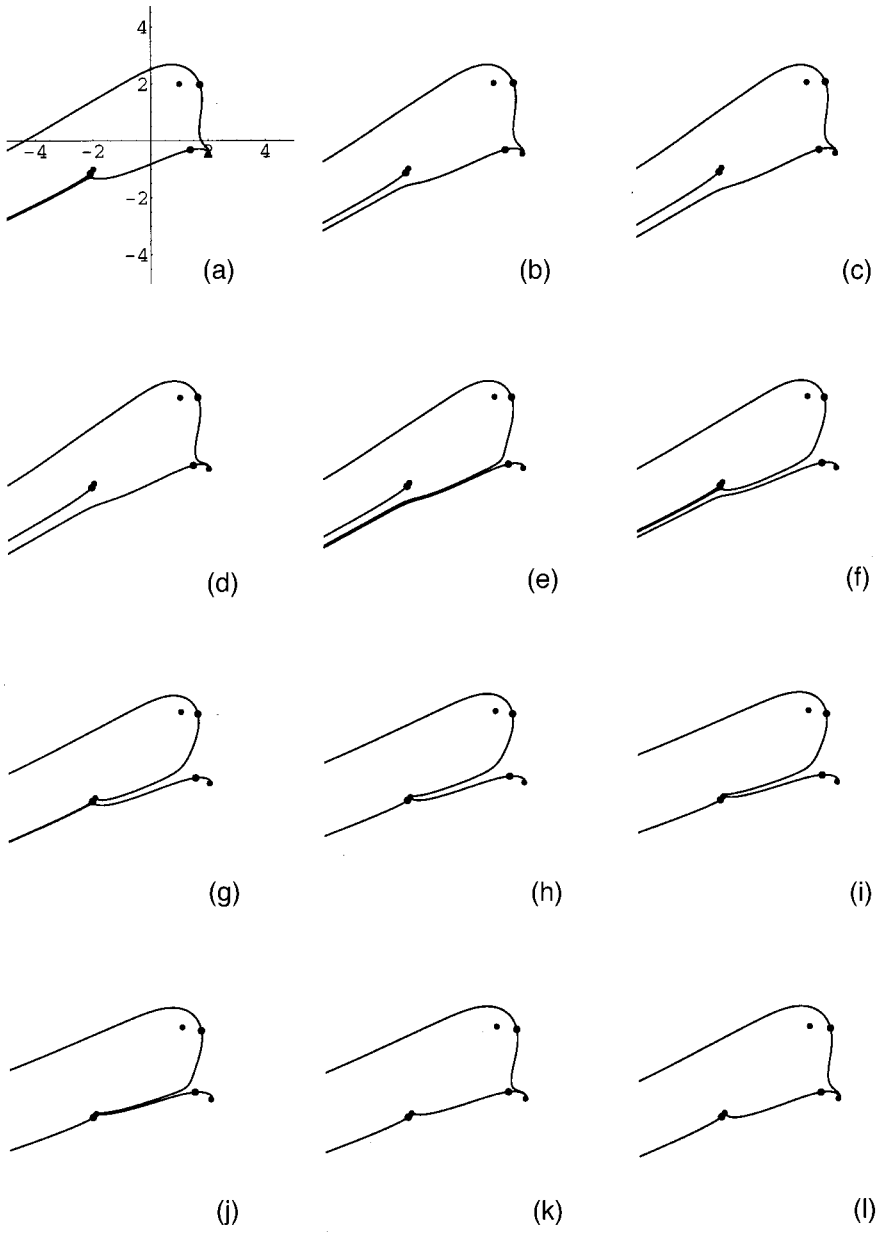


FIG. 11. Ordinary steepest descent paths for the integral representing a solution around the crossing point A.

VI. CONCLUDING REMARKS

As several examples in Sec. V have shown, the ESDP ansatz is a new and powerful proposition in WKB analysis. In particular, we note the disappearance of a pathological change of configurations of steepest descent paths which is observed when an ordinary steepest descent path hits a turning point for $\hat{P}$ (see Remark 1 in Sec. IV), if we use exact steepest descent paths; the effect of a turning point is automatically built in the definition of an exact steepest descent path through its interrelationship with a Stokes curve that emanates from the turning point. This fact nicely fits in with the fact that a turning point is not a singular point of the equation $\hat{P}\hat{\psi}=0$; the singularity at a turning point that appears in the WKB expansion is a spurious one to disappear by the Borel resummation.

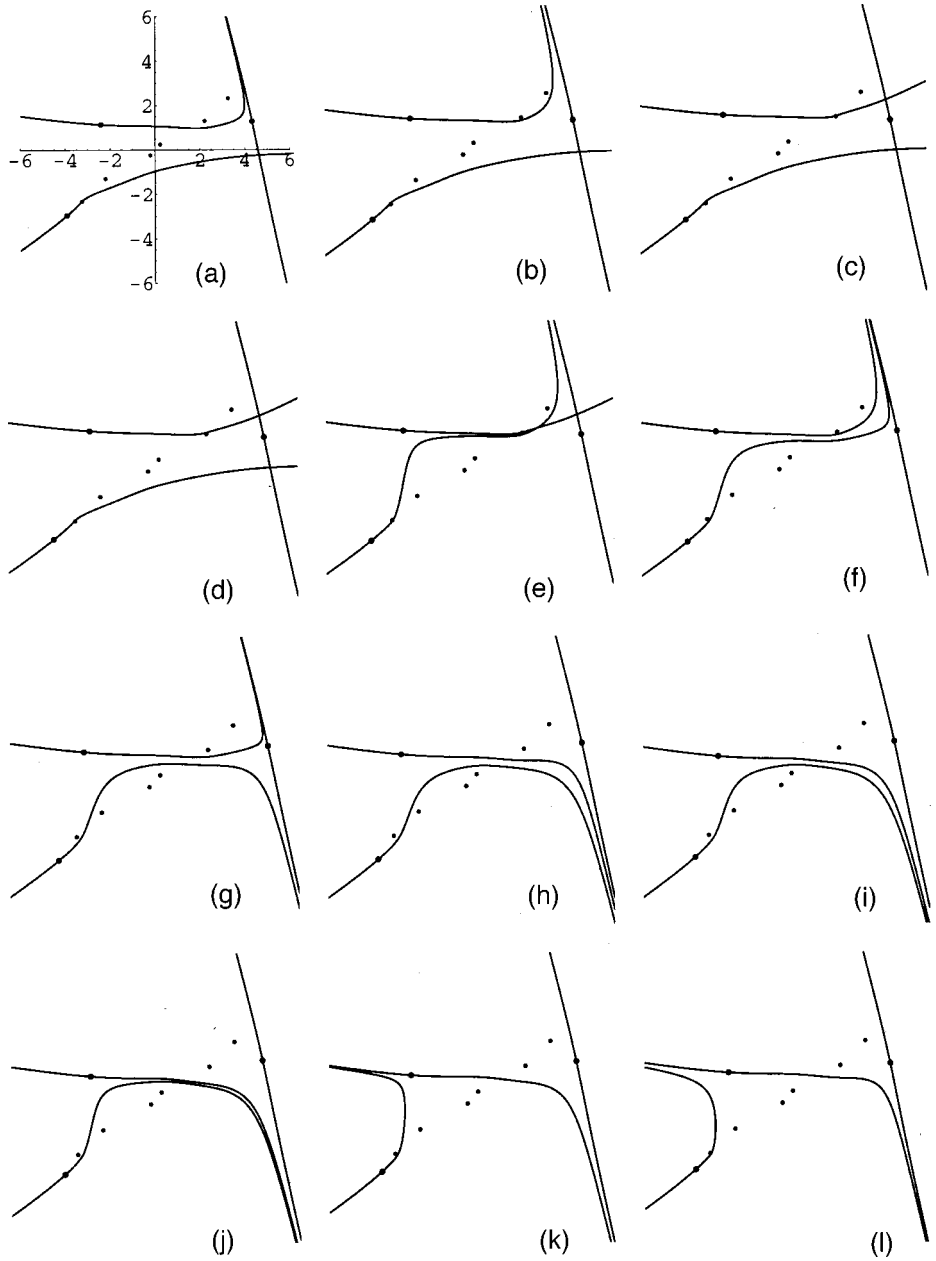


FIG. 12. Ordinary steepest descent paths for the integral (6) around the crossing point A.

Another important implication of the ESDP ansatz is that Stokes phenomena for the operator P occur only on a Stokes curve of the form (62). The reasoning is as follows: Suppose that a Stokes phenomenon is observed at x. The ESDP ansatz then asserts that

$$\mathrm{Im}\left(x\xi_j(x) - \int_{\hat{a}}^{\xi_j(x)} x_k(\xi)\mathrm{d}\xi \right) = \mathrm{Im}\left(x\xi_0 - \int_{\hat{a}}^{\xi_0} x_k(\xi)\mathrm{d}\xi \right), \tag{55}$$

$$\mathrm{Im}\left(x\xi_{j'}(x) - \int_{\hat{a}}^{\xi_{j'}(x)} x_{k'}(\xi)\mathrm{d}\xi \right) = \mathrm{Im}\left(x\xi_0 - \int_{\hat{a}}^{\xi_0} x_{k'}(\xi)\mathrm{d}\xi \right), \tag{56}$$

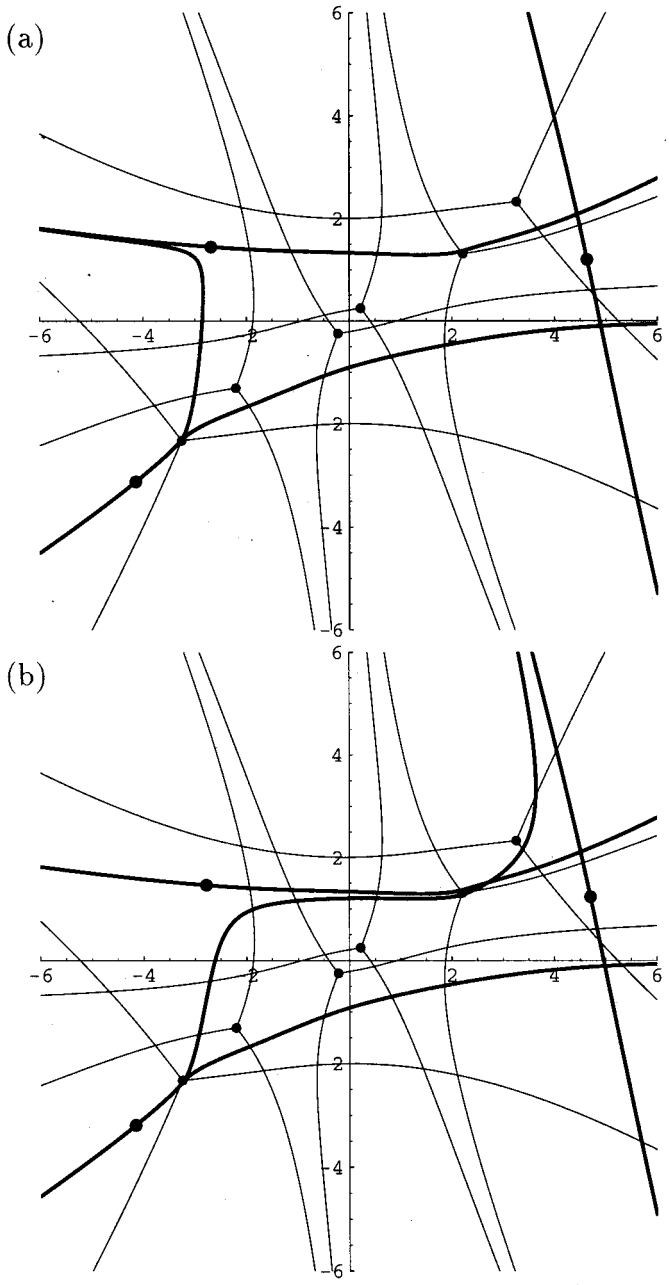


FIG. 13. Exact steepest descent paths for $x=-0.978\,776+0.247\,106\,i$ (a) and for $x=-0.998\,081+0.247\,106\,i$ (b).

and

$$\mathrm{Im}\int_{\hat{a}}^{\xi_0}(x_k(\xi)-x_{k'}(\xi))\mathrm{d}\xi=0 \tag{57}$$

hold for some $j,j',k,$ and k', a turning point $\hat{a}$ and some ξ_0, where $x_k(\xi)$ and $x_{k'}(\xi)$ solve the equation $p(x,\xi)=0$ given by (4) and $\xi_j(x)$ and $\xi_{j'}(x)$ also solve the same equation in ξ. Let us suppose that $\mathcal{R}=\{(x,\xi)\in\mathbb{C}^2:p(x,\xi)=0\}$ is nonsingular and that $x_k(\xi)$, etc., are situated with a turning point a of P as in Fig. 14. Here we note that relations (55) and (56) are slightly weaker

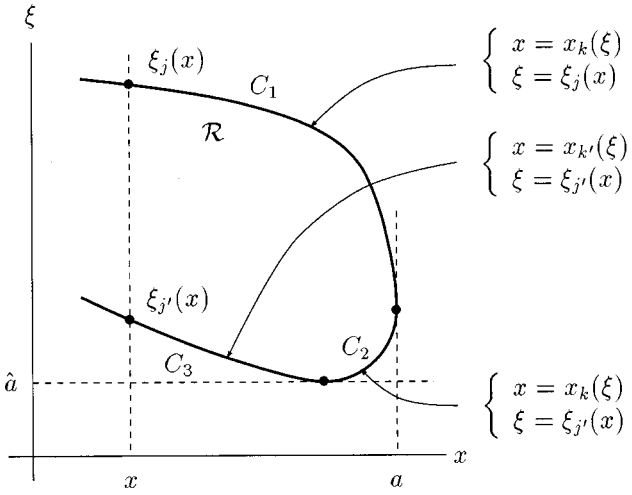


FIG. 14. Schematic illustration of $\mathcal{R}=\{(x,\xi):p(x,\xi)=0\}$.

than the actual situation that the ESDP ansatz requires to occur, because a level surface of $\mathrm{Im}\, f_k$ or $\mathrm{Im}\, f_{k'}$ is not necessarily connected. As we see in the following, these weaker conditions still suffice to entail the required relation (62).

Integration of the one-form $\mathrm{d}(x\xi)=x\mathrm{d}\xi+\xi\mathrm{d}x$ on the portion C_1 in Fig. 14 gives us

$$x\xi_j(x)-a\xi_j(a)=\int_{\xi_j(a)}^{\xi_j(x)}x_k(\xi)\mathrm{d}\xi+\int_a^x\xi_j(x)\mathrm{d}x. \tag{58}$$

Similar calculations on the portions C_2 and C_3, respectively, lead to

$$a\xi_{j'}(a)-x_k(\hat{a})\hat{a}=\int_{\hat{a}}^{\xi_{j'}(x)}x_k(\xi)\mathrm{d}\xi+\int_{x_k(\hat{a})}^{a}\xi_{j'}(x)\mathrm{d}x \tag{59}$$

and

$$x_{k'}(\hat{a})\hat{a}-x\xi_{j'}(x)=\int_{\xi_{j'}(x)}^{\hat{a}}x_{k'}(\xi)\mathrm{d}\xi+\int_x^{x_{k'}(\hat{a})}\xi_{j'}(x)\mathrm{d}x. \tag{60}$$

Combining these relations, we obtain

$$x\xi_j(x)-x\xi_{j'}(x)=\int_{\hat{a}}^{\xi_j(x)}x_k(\xi)\mathrm{d}\xi+\int_{\xi_{j'}(x)}^{\hat{a}}x_{k'}(\xi)\mathrm{d}\xi+\int_a^x\xi_j(x)\mathrm{d}x+\int_x^a\xi_{j'}(x)\mathrm{d}x. \tag{61}$$

Considering the imaginary part of the relation (61) together with (55), (56), and (57), we conclude

$$\mathrm{Im}\int_a^x(\xi_j(x)-\xi_{j'}(x))\mathrm{d}x=0. \tag{62}$$

This relation enhances our belief in the ESDP ansatz.

ACKNOWLEDGMENTS

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An application of solvable structures to classical and nonclassical similarity solutions

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Using exterior differential systems, we extend work by Harrison and Estabrook for deriving similarity solutions of hyperbolic and parabolic partial differential equations (PDEs). We use exterior calculus results to show that a symmetry (isovector) of the differential ideal corresponding to some hyperbolic or parabolic PDE can be used to generate a Cauchy characteristic vector field of a restricted exterior differential system defined on some four-dimensional regular submanifold of the first jet bundle. We then show that this restricted differential ideal has a Frobenius integrable annihilating space, which can be used to yield a similarity solution of the PDE by applying results from Lie and Cartan on integrating Frobenius integrable vector field distributions via symmetry. We also give an extension to conditional symmetries. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1368845]

I. INTRODUCTION

Given a nonlinear partial differential equation (PDE), a so-called ''similarity solution'' is one which is invariant under some group action. Pioneered by Lie,[1] techniques for using symmetries to find similarity solutions have been around for a long time, and in recent times authors such as Bluman and Cole,[2] Bluman and Kumei,[3] Olver,[4–6] and Stephani[7] have provided modern discussions on various aspects of this similarity solution approach to PDEs.

This work considers a single second-order hyperbolic or parabolic PDE of one dependent variable u and two independent variables x^1,x^2 of the form

$$f_1\frac{\partial^2 u}{\partial(x^1)^2}+f_2\frac{\partial^2 u}{\partial(x^2)^2}+f_3\frac{\partial^2 u}{\partial x^1 x^2}=k, \tag{1}$$

where f_1,f_2,f_3,k are smooth functions of $x^1,x^2,u,\partial u/\partial x^1$, $\partial u/\partial x^2$. Although exterior differential systems[8–12] are of most use in studying systems of nonlinear partial differential equations, we examine in this paper their application to similarity solutions of (1) along similar lines to Harrison and Estabrook.[13] We also give an alternative interpretation of the underlying geometric significance of such solutions.

Since this paper is essentially concerned with algorithms based on symmetry for extracting similarity solutions of (1), we assume throughout that given a second-order hyperbolic or parabolic PDE of the form in (1) and symmetry vector field, there exists a local smooth similarity solution. This also means that if we apply the Cartan–Kuranishi theorem,[14] we will obtain after a finite number of prolongations an involutive system of PDEs.

Our work also makes use of results from Lie[15] and Cartan[16,17] for integrating Frobenius integrable vector field distributions with solvable symmetry structures, which has in recent times been extended by Basarab-Horwath,[18] Duzhin and Lychagin,[19] Hartl and Athorne,[20] and Sherring and Prince.[21] With particular emphasis on results in Ref. 21, we establish in Secs. V and VII two algorithms based entirely on symmetry for generating similarity solutions of second order hyperbolic or parabolic PDEs of the type in (1), which avoids the usual requirement of having to solve

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some ordinary differential equation once the similarity variable is known. Finally, we briefly examine conditional symmetries. Using such symmetries we extend earlier results in this paper to give a technique for generating the so-called ''nonclassical'' [6,22,23] similarity solutions, which once again avoids the need to solve any ordinary differential equation.

II. BACKGROUND

It is assumed throughout this paper that for natural numbers n and m, U^n and V^m are, respectively, some open, convex neighborhoods of $\mathbb{R}^n$ and $\mathbb{R}^m$, with coordinates $x^1,\ldots,x^n$ and $z^1,\ldots,z^m$. On the κth jet bundle $J^\kappa(U^n,V^m)$, we say that the set of exterior differential p-forms $\Lambda^p(J^\kappa(U^n,V^m))$ is a section of the bundle of all homogeneous differential forms $\Lambda(J^\kappa(U^n,V^m))$. We define $\mathfrak{X}(J^\kappa(U^n,V^m))$ to be the module of smooth vector fields over $C^\infty(J^\kappa(U^n,V^m))$. Given some $\omega\in\Lambda^p(J^\kappa(U^n,V^m))$, its *kernel* is defined by $\ker(\omega)=\{X\in\mathfrak{X}(J^\kappa(U^n,V^m)):X\lrcorner\omega=0\}$. We assume that on their domains of definition, all vector field distributions are of constant dimension, and unless otherwise stated as in Secs. VI and VII, all mappings and differential one-forms are of constant rank.

The *Cauchy characteristic* space of a differential ideal I generated by some finite collection of differential forms is denoted $A(I)$, and contains all vector fields $X\in\mathfrak{X}(J^\kappa(U^n,V^m))$ such that $X\lrcorner I\subset I$. A vector field $X\in\mathfrak{X}(J^\kappa(U^n,V^m))$ is said to be a *symmetry* (isovector) of I if it satisfies the condition involving the Lie derivative that $\mathcal{L}_X I\subset I$. A vector field $X\in\mathfrak{X}(J^\kappa(U^n,V^m))$ is a *symmetry* of a vector field distribution $D\subset\mathfrak{X}(J^\kappa(U^n,V^m))$ if $\mathcal{L}_X D\subset D$. We say that a vector field is a *nontrivial* symmetry if, in terms of a differential ideal, it is not Cauchy characteristic, or in terms of a vector field distribution, it is not in the distribution.

We also assume throughout this paper that unless otherwise stated, M^q is some open, convex q-dimensional neighborhood of $J^\kappa(U^n,V^m)$. Since by the inverse function theorem, parametrizing immersions mapping onto regular submanifolds are locally diffeomorphic, we also assume all neighborhoods U^n, V^m, and M^q are chosen such that this holds. Thus for the differential map $\Psi_*:\mathfrak{X}(M^r)\to\mathfrak{X}(M^s)$, we can therefore assume for each $Y\in\mathfrak{X}(M^r)$ that Ψ_*Y is a well-defined vector field, and the following property holds:

$$\Psi_*[Y_1,Y_2]=[\Psi_*Y_1,\Psi_*Y_2] \tag{2}$$

for any $Y_1,Y_2\in\mathfrak{X}(M^r)$. We also make use of the following theorem found in Sternberg[24] that we use in Sec. III:

Theorem 1: Let $\Psi:M^r\to M^s$ *be a one-to-one immersion. Then for all* $Y\in\mathfrak{X}(F(M^r))$ *there exists* $X\in\mathfrak{X}(M^r)$ *such that* $\Psi_*X=Y$.

Here we write $\mathfrak{X}(\Psi(M^r))$ to mean the module of vector fields tangent to $\Psi(M^r)$. At Ψ is one-to-one, this notation is unambiguous.

The pull-back map $\Psi^*:\Lambda(M^s)\to\Lambda(M^r)$ has the following properties:

$$(\Psi^*\omega)(Y_1,\ldots,Y_k)=\Psi^*(\omega(\Psi_*Y_1,\ldots,\Psi_*Y_k)), \tag{3}$$

for any $\omega\in\Lambda^k(M^s)$, $Y_1,\ldots,Y_k\in\mathfrak{X}(M^r)$, and

$$\Psi^*\circ\mathrm{d}\omega^1=d\circ\Psi^*\omega^1, \tag{4}$$

$$\Psi^*(\omega^1\wedge\omega^2)=(\Psi^*\omega^1)\wedge(\Psi^*\omega^2), \tag{5}$$

for any $\omega^1,\omega^2\in\Lambda(M^s)$. Given any smooth $\Phi:M^q\to M^r$ and $\omega\in\Lambda^1(M^s)$, we also have the following composition property:

$$(\Psi\circ\Phi)^*\omega=\Phi^*(\Psi^*\omega). \tag{6}$$

III. DIFFERENTIAL IDEAL REPRESENTATION OF PDEs

Working in the second jet bundle $J^2(U^2,V^1)$ with coordinates $x^1,x^2,z^1,z^1_1,z^1_2,\ z^1_{11},z^1_{12},z^1_{22}$, we define

$$F:=f_1z^1_{11}+f_2z^1_{22}+f_3z^1_{12}-k,$$

along with the contact forms

$$C^1:=\mathrm{d}z^1-z^1_1\,\mathrm{d}x^1-z^1_2\,\mathrm{d}x^2,$$

$$C^1_1:=\mathrm{d}z^1_1-z^1_{11}\,\mathrm{d}x^1-z^1_{12}\,\mathrm{d}x^2,$$

$$C^1_2:=\mathrm{d}z^1_2-z^1_{12}\,\mathrm{d}x^1-z^1_{22}\,\mathrm{d}x^2.$$

We can express a solution surface of the PDE in (1) as a two-dimensional integral manifold (immersion) of the differential ideal

$$I_F:=\langle C^1,C^1_1,C^1_2,\mathrm{d}C^1_1,\mathrm{d}C^1_2,F\,\mathrm{d}x^1\wedge\mathrm{d}x^2\rangle,$$

such that the transverse condition $\mathrm{d}x^1\wedge\mathrm{d}x^2\neq 0$ holds on its tangent space. Note that $\mathrm{d}C^1\equiv 0 \mod C^1_1,C^1_2$. Also, Lemma 1.1 in Ref. 25 implies

$$\mathrm{d}(F\,\mathrm{d}x^1\wedge\mathrm{d}x^2)\equiv 0 \mod C^1,C^1_1,C^1_2,\mathrm{d}C^1_1,\mathrm{d}C^1_2.$$

It is well known that an integral manifold in the second jet bundle which annihilates all the contact forms that generate the second-order contact system is the image of the two-jet of some smooth map $f:U^2\to V^1$ if and only if $\mathrm{d}x^1\wedge dx^2\neq 0$ on the tangent space of the integral manifold (see, e.g., Theorem 2.3.1 in Stormark[26]). If, in addition, the integral manifold annihilates F, then the two-jet is that of some local solution of the PDE in (1).

Our principal result of this section is the following:

Theorem 2:

$$I_F=\langle C^1,C^1_1,C^1_2,\mathrm{d}C^1_1,\mathrm{d}C^1_2,L\rangle,$$

where

$$L:=f_1\,\mathrm{d}z^1_1\wedge\mathrm{d}x^2-f_2\,\mathrm{d}z^1_2\wedge\mathrm{d}x^1+f_3\,\mathrm{d}z^1_2\wedge\mathrm{d}x^2-k\,\mathrm{d}x^1\wedge\mathrm{d}x^2.$$

Proof:

$$F\,\mathrm{d}x^1\wedge\mathrm{d}x^2=(f_1z^1_{11}+f_2z^1_{22}+f_3z^1_{12}-k)\mathrm{d}x^1\wedge\mathrm{d}x^2.$$

Now

$$f_1z^1_{11}\,\mathrm{d}x^1\wedge\mathrm{d}x^2=f_1(z^1_{11}\,\mathrm{d}x^1+z^1_{12}\,\mathrm{d}x^2)\wedge\mathrm{d}x^2=f_1(\mathrm{d}z^1_1-C^1_1)\wedge\mathrm{d}x^2,$$

$$f_2z^1_{22}\,\mathrm{d}x^1\wedge\mathrm{d}x^2=-f_2(z^1_{21}\,\mathrm{d}x^1+z^1_{22}\,\mathrm{d}x^2)\wedge\mathrm{d}x^1=-f_2(\mathrm{d}z^1_2-C^1_2)\wedge\mathrm{d}x^1,$$

$$f_3z^1_{12}\,\mathrm{d}x^1\wedge\mathrm{d}x^2=f_3(z^1_{12}\,\mathrm{d}x^1+z^1_{22}\,\mathrm{d}x^2)\wedge\mathrm{d}x^2=f_3(\mathrm{d}z^1_2-C^1_2)\wedge\mathrm{d}x^2.$$

Hence

$$F\,\mathrm{d}x^1\wedge\mathrm{d}x^2\equiv f_1\,\mathrm{d}z^1_1\wedge\mathrm{d}x^2-f_2\,\mathrm{d}z^1_2\wedge\mathrm{d}x^1+f_3\,\mathrm{d}z^1_2\wedge\mathrm{d}x^2-k\,\mathrm{d}x^1\wedge\mathrm{d}x^2 \mod C^1_1,C^1_2\equiv L \mod C^1_1,C^1_2.$$

From this we obtain

$$\mathrm{d}L \equiv \mathrm{d}(F\,\mathrm{d}x^1 \wedge \mathrm{d}x^2) \bmod C_1^1, C_2^1, \mathrm{d}C_1^1, \mathrm{d}C_2^1,$$

$$\equiv 0 \bmod C^1, C_1^1, C_2^1, \mathrm{d}C_1^1, \mathrm{d}C_2^1,$$

■

using Lemma 1.1 in Ref. 25.

Remark: In a similar fashion, it is easy to show that

$$I_F = \langle C^1, C_1^1, C_2^1, \mathrm{d}C_1^1, \mathrm{d}C_2^1, L^\dagger \rangle,$$

where

$$L^\dagger := f_1\,\mathrm{d}z_1^1 \wedge \mathrm{d}x^2 - f_2\,\mathrm{d}z_2^1 \wedge \mathrm{d}x^1 - f_3\,\mathrm{d}z_1^1 \wedge \mathrm{d}x^1 - k\,\mathrm{d}x^1 \wedge \mathrm{d}x^2.$$

In our work, we deal mostly with L, however all results equally apply to $L^\dagger$.

We define

$$I_{\bar{F}} := \langle C^1, C_1^1, C_2^1, \mathrm{d}C_1^1, \mathrm{d}C_2^1, L \rangle.$$

Technically speaking, $I_{\bar{F}} := I_F$ (by Theorem 2), and the notation $I_{\bar{F}}$ might appear redundant. However we will use $I_{\bar{F}}$ as a brief way of referring to the particular choice of generators $C^1, C_1^1, C_2^1, \mathrm{d}C_1^1, \mathrm{d}C_2^1, L$.

Now L (containing all the information specific to the PDE) does not depend on any second-order terms $z_{11}^1, z_{12}^1, z_{22}^1$. Therefore, we may modify our problem to that of finding two-dimensional integral manifolds of a *reduced* differential ideal $I_{\bar{F}}^r$ defined by

$$I_{\bar{F}}^r := \langle C^1, \mathrm{d}C^1, L, \mathrm{d}L \rangle, \tag{7}$$

defined on the first jet bundle $J^1(U^2, V^1)$. We note that since $\mathrm{d}L$ is a three-form, all two-dimensional integral manifolds of $I_{\bar{F}}^r$ will trivially annihilate $\mathrm{d}L$, so this differential form can therefore be ignored in all calculations.

IV. SIMILARITY SOLUTION APPROACHES

Given a Lie point symmetry $X \in \mathfrak{X}(U^2 \times V^1)$ of the PDE in (1), a similarity solution of the PDE is a local solution that remains unchanged under the one-parameter group action of the symmetry. The most well-known procedure for using X to generate a corresponding similarity solution basically involves determining the two functionally independent invariants $\gamma^1, \gamma^2 \in C^\infty(U^2 \times V^1)$ of X and finding a solution of (1) that is some function of these invariants. Doing so, one essentially obtains from (1) a second-order ODE expressed in terms of γ^1, γ^2, known as the ''reduced'' differential equation. In the general case for PDE problems of n independent variables, the reduced equation retains the same order of the PDE but is of $n-1$ independent variables.

An alternative and equivalent approach to finding similarity solutions is discussed by Olver in Ref. 6 where one searches for a common solution of the overdetermined system of PDEs given by (1) and the first-order quasilinear PDE obtained from

$$X^{(1)} \lrcorner C^1 = 0, \tag{8}$$

where z^1 and z_1^1, z_2^1 are replaced with u and its respective first partial derivatives. Here we assume (8) gives a valid PDE and the Lie point symmetry X is not, for example, $\partial/\partial z^1$. The PDE derived from (8) is known as the *characterizing invariance system* (or *invariant surface condition*) corresponding to X, and is typically solved first using invariant coordinates to give a solution in terms

of an arbitrary function. Then, by inserting this solution into (1), a reduced differential equation for the arbitrary function is derived. Once this is solved, a similarity solution is obtained once more.

In this paper we do not follow either of the above-mentioned procedures, but instead choose to adopt another approach formulated by Harrison and Estabrook[13] that uses exterior calculus and differential ideals. This is discussed in the following.

Suppose we are given some differential ideal I_F^r on $J^1(U^2,V^1)$ corresponding to some second-order PDE of the form in (1). If a vector field $V\in\mathfrak{X}(J^1(U^2,V^1))$ is a symmetry of I_F^r, then

$$\mathcal{L}_V C^1=\lambda_1 C^1, \tag{9}$$

and

$$\mathcal{L}_V L=\alpha^1\wedge C^1+\lambda_2\,\mathrm{d}C^1+\lambda_3 L, \tag{10}$$

for some $\lambda_1,\lambda_2,\lambda_3\in C^\infty(J^1(U^2,V^1))$ and $\alpha^1\in\Lambda^1(J^1(U^2,V^1))$. Applying the property that $\mathcal{L}_V(\mathrm{d}\omega)=\mathrm{d}(\mathcal{L}_V\omega)$ for any differential form ω, we can use (9) and (10) to derive corresponding symmetry expressions for the remaining two generators of I_F^r. A key property of the Harrison and Estabrook approach is that the symmetry algebra of I_F^r includes the Lie point symmetry algebra of (1). We state this fact without proof, however in Ref. 27 it is proved for differential ideals where the PDE is left as a zero-form generator of the ideal. Since we are dealing with PDEs of one dependent variable, the determining equations derived from (9) and (10) should also be able to establish any so-called contact symmetries of the PDE in (1).

Suppose then that we are given some symmetry V of I_F^r [or the first prolongation of some Lie point symmetry of (1)]. In the Harrison and Estabrook approach to generating similarity solutions of (1), the differential ideal I_F^r is augmented with $V\lrcorner C^1$, $V\lrcorner\mathrm{d}C^1$, $V\lrcorner L$, and $V\lrcorner\mathrm{d}L$. One then looks for a two-dimensional integral manifold of the augmented ideal

$$\langle C^1,\mathrm{d}C^1,L,\mathrm{d}L,V\lrcorner C^1,V\lrcorner\mathrm{d}C^1,V\lrcorner L,V\lrcorner\mathrm{d}L\rangle, \tag{11}$$

defined on $J^1(U^2,V^1)$, which also satisfies the transverse condition.

The symmetry conditions in (9) and (10) can be used to easily prove that (11) is a differential ideal, and it is clear that V is a Cauchy characteristic vector field of the differential ideal. Though this obvious latter fact has also been noted by Estabrook,[28] we show in Lemma 3 in the following that for hyperbolic and parabolic PDEs of the form in (1), there exists a more useful extension of this result.

Finally, we can simplify (11) in the following way: It is not hard to establish from using (9) and (10) that (11) is equal to

$$\langle C^1,\mathrm{d}C^1,L,\mathrm{d}L,V\lrcorner C^1,\mathrm{d}(V\lrcorner C^1),V\lrcorner L,\mathrm{d}(V\lrcorner L)\rangle. \tag{12}$$

In Sec. V we examine (12) more closely and show that two further reductions are possible.

V. FIRST MAIN RESULT

The class of second-order PDEs we deal with is those for which L is decomposable, or equivalently, $L\wedge L=0$ using Theorem 1.7 in Bryant *et al.*[8] Although L defined in Theorem 2 is obviously not decomposable for some choices of f_1,f_2,f_3, and k, we will see later in Sec. VIII that for all hyperbolic and parabolic PDEs of the form in (1) we are able to add to L some multiple of $\mathrm{d}C^1$ which is then decomposable.

Assuming then without loss that L is decomposable, we have

$$0=Y\lrcorner(L\wedge L)=2(Y\lrcorner L)\wedge L,$$

for any $Y \in \mathfrak{X}(J^1(U^2,V^1))$, so that if $Y \lrcorner L \neq 0$, then $L=(Y \lrcorner L)\wedge\omega$ for some $\omega \in \Lambda^1(J^1(U^2,V^1))$. Therefore, for decomposable L, any integral manifold of

$$\langle C^1, \mathrm{d}C^1, V \lrcorner C^1, \mathrm{d}(V \lrcorner C^1), V \lrcorner L, \mathrm{d}(V \lrcorner L)\rangle \tag{13}$$

is an integral manifold of (12) (the two differential ideals are equal for decomposable L). Here V is the symmetry of I_F^r described in Sec. IV. We shall make use of this condition on L in our two main results, Theorem 4 in this section and Theorem 9 in Sec. VII.

Since $V \lrcorner C^1$ is a smooth function generator of (13), we can make a further simplification to this differential ideal by pulling it back onto the regular submanifold of $J^1(U^2,V^1)$ described by $V \lrcorner C^1=0$, and confine our work to this region of $J^1(U^2,V^1)$. Suppose that the equation $V \lrcorner C^1 =0$ describes a four-dimensional regular submanifold of $J^1(U^2,V^1)$, which we parametrize by the immersion $\Phi: M^4 \to J^1(U^2,V^1)$. Then denoting the pull-back of (13) onto M^4 by

$$J_F^r := \langle \Phi^* C^1, d\circ\Phi^* C^1, \Phi^*(V \lrcorner L), d\circ\Phi^*(V \lrcorner L)\rangle, \tag{14}$$

we have the following lemma:

Lemma 3: Let $V \in \mathfrak{X}(J^1(U^2,V^1))$ be a symmetry of I_F^r. If the equation $V \lrcorner C^1=0$ describes a four-dimensional regular submanifold of $J^1(U^2,V^1)$, which we parametrize by the immersion $\Phi: M^4 \to J^1(U^2,V^1)$, then there exists $W \in \mathfrak{X}(M^4)$ with the property that W is a Cauchy characteristic vector field of J_F^r.

Proof: Let $\Phi: M^4 \to J^1(U^2,V^1)$ be a corresponding immersion mapping onto the regular submanifold of $J^1(U^2,V^1)$ described by $V \lrcorner C^1=0$. It is clear that the tangent space of $\Phi(M^4) \subset J^1(U^2,V^1)$ spans the annihilating space of $\mathrm{d}(V \lrcorner C^1)$. From contracting the symmetry condition in (9) with V we obtain, at any point in $\Phi(M^4)$,

$$V \lrcorner \mathrm{d}(V \lrcorner C^1) = \lambda_1 (V \lrcorner C^1) = 0.$$

Hence V is in the tangent space of $\Phi(M^4)$. Applying Theorem 1, there exists a vector field $W \in \mathfrak{X}(M^4)$ such that $\Phi_* W = V$.

We now proceed to show that W is a Cauchy characteristic vector field of J_F^r by examining each generator of the differential ideal. First,

$$W \lrcorner \Phi^* C^1 = \Phi^*(\Phi_* W \lrcorner C^1) = 0, \tag{15}$$

where for the first equality we have used the property in (3), and for the second, we have made use of the fact that the pull-back of $V \lrcorner C^1$ by Φ is zero.

Next, we have that

$$W \lrcorner \Phi^* \circ \mathrm{d}C^1 = \Phi^*(\Phi_* W \lrcorner \mathrm{d}C^1) = \Phi^*(V \lrcorner \mathrm{d}C^1), \tag{16}$$

once again using (3). Now

$$\begin{aligned} \Phi^*(V \lrcorner \mathrm{d}C^1) &= \Phi^*(\lambda_1 C^1 - \mathrm{d}(V \lrcorner C^1)), \\ &= (\Phi^* \lambda_1)\Phi^* C^1 - d\circ\Phi^*(V \lrcorner C^1), \\ &= (\Phi^* \lambda_1)\Phi^* C^1 \in J_F^r, \end{aligned} \tag{17}$$

where in the first line we have inserted the symmetry condition in (9), and in the second, we have used properties (4) and (5). Combining the end result in (17) with (16) and (4) then gives

$$W \lrcorner d\circ\Phi^* C^1 \in J_F^r. \tag{18}$$

We also have from (3),

$$W \lrcorner \Phi^*(V \lrcorner L) = \Phi^*(\Phi_* W \lrcorner V \lrcorner L) = \Phi^*(V \lrcorner V \lrcorner L) = 0. \tag{19}$$

In a similar fashion,

$$W \lrcorner \Phi^* \circ \mathrm{d}(V \lrcorner L) = \Phi^*(\Phi_* W \lrcorner \mathrm{d}(V \lrcorner L)) = \Phi^*(V \lrcorner \mathrm{d}(V \lrcorner L)). \tag{20}$$

The symmetry condition in (10) yields

$$\begin{aligned} V \lrcorner \mathrm{d}(V \lrcorner L) &= V \lrcorner (\alpha^1 \wedge C^1 + \lambda_2 \, \mathrm{d}C^1 + \lambda_3 L - V \lrcorner \mathrm{d}L), \\ &= (V \lrcorner \alpha^1) C^1 - (V \lrcorner C^1) \alpha^1 + \lambda_2 (V \lrcorner \mathrm{d}C^1) + \lambda_3 (V \lrcorner L). \end{aligned}$$

Pulling this back by Φ, then using (5) and $\Phi^*(V \lrcorner C^1) = 0$ followed by (17) gives

$$\Phi^*(V \lrcorner \mathrm{d}(V \lrcorner L)) = (\Phi^*(V \lrcorner \alpha^1)) \Phi^* C^1 + (\Phi^* \lambda_2) \Phi^*(V \lrcorner \mathrm{d}C^1) + (\Phi^* \lambda_3) \Phi^*(V \lrcorner L) \in J_F^r, \tag{21}$$

so that combining this result with (20) and (4), we obtain

$$W \lrcorner \mathrm{d} \circ \Phi^*(V \lrcorner L) \in J_F^r. \tag{22}$$

Therefore (15), (18), (19), and (22) imply that $W \lrcorner J_F^r \subset J_F^r$. □

From Lemma 3 we obtain the first of our major new results:

Theorem 4: *Given some second-order PDE of the form in* (1) *whose corresponding L is decomposable, let* $V \in \mathfrak{X}(J^1(U^2, V^1))$ *be a symmetry of* I_F^r. *Suppose the equation* $V \lrcorner C^1 = 0$ *describes a four-dimensional regular submanifold of* $J^1(U^2, V^1)$, *and denote* $\Phi : M^4 \to J^1(U^2, V^1)$ *as a corresponding immersion mapping onto this submanifold. With*

$$D_F^r := (\mathrm{sp}\{\Phi^* C^1, \Phi^*(V \lrcorner L)\})^\perp,$$

if $\Phi^*(C^1 \wedge (V \lrcorner L)) \neq 0$, *then* $\Phi_* D_F^r$ *generates a two-dimensional integral manifold of* I_F^r. *If, in addition,* $\mathrm{d}x^1 \wedge \mathrm{d}x^2 \neq 0$ *on* $\Phi_* D_F^r$, *then the integral manifold is the image of the one-jet of some local solution of the PDE in (1).*

Proof: We know from the proof of Lemma 3 that $V = \Phi_* W$ for some $W \in \mathfrak{X}(M^4)$. Since $\Phi^*(C^1 \wedge (V \lrcorner L)) \neq 0$, it follows that D_F^r is two dimensional. From Lemma 3, W is a Cauchy characteristic vector field of the differential ideal J_F^r defined in (14), which implies $[W, Y] \in D_F^r$ for all $Y \in D_F^r$.[29,26] Hence D_F^r is Frobenius integrable. Since it is assumed Φ is diffeomorphic onto its image, $\Phi_* D_F^r$ is well defined. Now let $Z_1, Z_2 \in \Phi_* D_F^r$. This means

$$Z_1 = \Phi_* P_1, \quad Z_2 = \Phi_* P_2,$$

for some $P_1, P_2 \in D_F^r$. Using (2) and the fact that D_F^r is Frobenius integrable, we then get

$$[Z_1, Z_2] = [\Phi_* P_1, \Phi_* P_2] = \Phi_* [P_1, P_2] \in \Phi_* D_F^r,$$

so $\Phi_* D_F^r$ is Frobenius integrable.

Suppose that $\Psi : M^2 \to M^4$ is an immersion mapping onto any leaf of the foliation of M^4 generated by D_F^r. Thus $\Psi^* J_F^r = 0$. Using (6),

$$(\Phi \circ \Psi)^* C^1 = \Psi^*(\Phi^* C^1) = 0, \tag{23}$$

and from (4),

$$(\Phi\circ\Psi)^*(\mathrm{d}C^1)=\mathrm{d}((\Phi\circ\Psi)^*C^1)=0. \tag{24}$$

By assumption, $\Phi^*(C^1\wedge(V\lrcorner L))\neq 0$. This implies $V\lrcorner L\neq 0$. Since L is decomposable, we have $L=(V\lrcorner L)\wedge\omega$ for some $\omega\in\Lambda^1(J^1(U^2,V^1))$. Concentrating on $V\lrcorner L$,

$$0=\Psi^*(\Phi^*(V\lrcorner L))=(\Phi\circ\Psi)^*(V\lrcorner L),$$

which gives

$$\Psi^*(\Phi^*L)=\Psi^*((\Phi^*(V\lrcorner L))\wedge(\Phi^*\omega))=((\Phi\circ\Psi)^*(V\lrcorner L))\wedge((\Phi\circ\Psi)^*\omega)=0. \tag{25}$$

Hence from (23), (24), and (25), it then follows that $(\Phi\circ\Psi)^*I_F^r=0$. If the transverse condition holds, then $\Phi\circ\Psi(M^2)=j^1h(U^2)$ for some $h\in C^\infty(U^2,V^1)$, with h as some local solution of (1). □

Remark: In order to satisfy the transverse requirement, the symmetry V in Theorem 4 must necessarily satisfy the condition $\mathrm{d}(V\lrcorner C^1)\wedge\mathrm{d}x^1\wedge\mathrm{d}x^2\neq 0$. If this is not the case, then $\Phi^*(\mathrm{d}x^1\wedge\mathrm{d}x^2)=0$, and hence *for all* Ψ, $(\Phi\circ\Psi)^*(\mathrm{d}x^1\wedge\mathrm{d}x^2)=0$. Consequently the transverse requirement fails.

We illustrate Theorem 4 with the following example:

Example 5: Consider the heat equation

$$\frac{\partial^2 u}{\partial(x^1)^2}=\frac{\partial u}{\partial x^2}. \tag{26}$$

Defined on $J^1(U^2,V^1)$ we have

$$I_F^r=\langle C^1,\mathrm{d}C^1,L,\mathrm{d}L\rangle,$$

where $F=z^1_{11}-z^1_2$ and $L=(\mathrm{d}z^1_1-z^1_2\,\mathrm{d}x^1)\wedge\mathrm{d}x^2$. Now

$$V:=x^1\frac{\partial}{\partial x^1}+2x^2\frac{\partial}{\partial x^2}$$

is a Lie point symmetry of (26), and we use its first prolongation $V^{(1)}$, where

$$V^{(1)}=x^1\frac{\partial}{\partial x^1}+2x^2\frac{\partial}{\partial x^2}-z^1_1\frac{\partial}{\partial z^1_1}-2z^1_2\frac{\partial}{\partial z^1_2},$$

as our nontrivial symmetry of I_F^r.

Applying Theorem 4, we define the four-dimensional regular submanifold $M^4\subset J^1(U^2,V^1)$ by the locus of

$$V^{(1)}\lrcorner C^1=-x^1z^1_1-x^2z^1_2=0.$$

In a simplified manner without explicitly introducing an immersion, we assume M^4 has coordinates x^1,x^2,z^1,z^1_1 with $x^2\neq 0$, so that on M^4,

$$\begin{aligned} C^1&=\mathrm{d}z^1-z^1_1\,\mathrm{d}x^1+\frac{z^1_1x^1}{2x^2}\mathrm{d}x^2,\\ V^{(1)}\lrcorner L&=-z^1_1x^1\,\mathrm{d}x^1+z^1_1\left(\frac{(x^1)^2}{2x^2}-1\right)\mathrm{d}x^2-2x^2\,\mathrm{d}z^1_1, \end{aligned} \tag{27}$$

with

$$J_{\overline{F}}^{r}=\langle C^1,\mathrm{d}C^1,V^{(1)}\lrcorner L,\mathrm{d}(V^{(1)}\lrcorner L)\rangle,$$

also defined on M^4. From Theorem 4 we have that $D_{\overline{F}}^{r}\subset\mathfrak{X}(M^4)$ generated by the annihilating space of the equations in (27) is Frobenius integrable. It is easy to show that on $D_{\overline{F}}^{r}$, the transverse condition $\mathrm{d}x^1\wedge\mathrm{d}x^2\neq 0$ holds, so we expect to get some local solution to the heat equation. Then applying Proposition 4.7 in Sherring and Prince[21] with a solvable structure of two symmetries, where $X_2:=\partial/\partial z^1\in\mathfrak{X}(M^4)$ is a nontrivial symmetry of $D_{\overline{F}}^{r}$, $X_1:=z_1^1(\partial/\partial z_1^1)\in\mathfrak{X}(M^4)$ is a nontrivial symmetry of $D_{\overline{F}}^{r}\oplus\mathrm{sp}\{X_2\}$, and defining

$$\Omega:=\left(\mathrm{d}z^1-z_1^1\,\mathrm{d}x^1+\frac{z_1^1x^1}{2x^2}\mathrm{d}x^2\right)\wedge\left(-z_1^1x^1\,\mathrm{d}x^1+z_1^1\left(\frac{(x^1)^2}{2x^2}-1\right)\mathrm{d}x^2-2x^2\,\mathrm{d}z_1^1\right),$$

we find

$$\frac{X_2\lrcorner\Omega}{X_1\lrcorner X_2\lrcorner\Omega}=\mathrm{d}\left(\ln(z_1^1\sqrt{x^2})+\frac{(x^1)^2}{4x^2}\right),$$

$$\frac{X_1\lrcorner\Omega}{X_2\lrcorner X_1\lrcorner\Omega}\equiv\mathrm{d}\left(z^1-2z_1^1\sqrt{x^2}\exp\left(\frac{(x^1)^2}{4x^2}\right)\int\exp(-\xi^2)\mathrm{d}\xi\right)\bmod\frac{X_2\lrcorner\Omega}{X_1\lrcorner X_2\lrcorner\Omega},$$

where $\xi:=x^1/(2\sqrt{x^2})$. Putting

$$\ln(z_1^1\sqrt{x^2})+\frac{(x^1)^2}{4x^2}=c^1,$$

and

$$z^1-2z_1^1\sqrt{x^2}\exp\left(\frac{(x^1)^2}{4x^2}\right)\int\exp(-\xi^2)\mathrm{d}\xi=c^2,$$

for any constants c^1,c^2, we obtain

$$u=2\exp(c^1)\int\exp(-\xi^2)\mathrm{d}\xi$$

as our local similarity solution of the heat equation corresponding to V.

We close this section with a warning that there will exist situations when applying Theorem 4 will yield a distribution $\Phi_*D_{\overline{F}}^{r}$ that is not transverse, even with $\mathrm{d}(V\lrcorner C^1)\wedge\mathrm{d}x^1\wedge\mathrm{d}x^2\neq 0$. In such cases we must abandon the above-mentioned approach and look to use elements of $I_{\overline{F}}^{r}$ that are in a sense singular. This is explained in full in Sec. VI.

VI. A SINGULAR APPROACH

Consider a differential ideal $I:=\langle\alpha^1,\alpha^2\rangle$ defined on some open, convex neighborhood $U^4\subset\mathbb{R}^4$ with coordinates $x^1,\ldots,x^4$, generated by two linearly independent one-forms $\alpha^1,\alpha^2\in\Lambda^1(U^4)$. Suppose that for each $i\in\{1,2\}$, $\mathrm{d}\alpha^i\equiv 0\bmod\alpha^1,\alpha^2$, i.e., $\ker(\alpha^1\wedge\alpha^2)$ is Frobenius integrable. Here, we choose to work with a two-dimensional Pfaffian system defined on a four-dimensional space because the material in the following section on second-order hyperbolic or parabolic PDEs of the type in (1) is precisely of this nature, but all results that follow in this section can easily be extended to arbitrary dimensions.

For integrating the Frobenius integrable distribution $\ker(\alpha^1\wedge\alpha^2)$ using solvable symmetry structures, we can use Proposition 4.7 in Sherring and Prince[21] to find some functions $f_1^1,f_2^1,f_1^2,f_2^2,g^1,g^2\in C^\infty(U^4)$ such that

$$f_1^1\alpha^1+f_2^1\alpha^2=\mathrm{d}g^1,$$
$$f_1^2\alpha^1+f_2^2\alpha^2=\mathrm{d}g^2. \tag{28}$$

If, on U^4, the functions g^1,g^2 are of constant maximal rank two, then the equations $g^1=c^1,g^2=c^2$ describe a two-dimensional regular submanifold of U^4. Let $\Psi:M^2\to U^4$ be an immersion mapping onto this submanifold. If, in addition, the determinant

$$\Psi^*\begin{vmatrix} f_1^1 & f_2^1 \\ f_1^2 & f_2^2 \end{vmatrix}\neq 0$$

on M^2, then (28) and the fact that $\Psi^*(\mathrm{d}g^1)=0=\Psi^*(\mathrm{d}g^2)$ imply $\Psi^*\alpha^1=0=\Psi^*\alpha^2$. Hence Ψ is a two-dimensional integral manifold of I, for arbitrary constant functions c^1,c^2.

The problem with the above ''regular'' approach used in Theorem 4 for dealing with a PDE of the form in (1) is that if the submanifold generated by $\Phi_*D_F^r$ is not transverse, then the method fails to give us a local solution with u as some smooth function of x^1,x^2.

Our goal in this section and the next is to provide an alternative approach for finding two-dimensional integral manifolds of I, which includes the above-mentioned situation as a subclass, as well as applies to PDE problems when $\Phi_*D_F^r$ *may or may not* be transverse. We will also see that the trade-off for this extra flexibility is that there is no direct computational approach using solvable symmetry structures, however using the Frobenius integrable nature of $\ker(\alpha^1\wedge\alpha^2)$ (or $\Phi_*D_F^r$ in Theorem 4) we do come close.

Consider then the following obvious extension to the above-given discussion:

Theorem 6: *With α^1,α^2 and I defined as noted previously, let there exist $f_1^1,f_2^1,f_1^2,f_2^2,g^{11},g^{12},g^{21},g^{22}\in C^\infty(U^4)$ such that*

$$f_1^1\alpha^1+f_2^1\alpha^2=g^{11}\,\mathrm{d}g^{12},$$
$$f_1^2\alpha^1+f_2^2\alpha^2=g^{21}\,\mathrm{d}g^{22}. \tag{29}$$

Suppose that for some $p,q\in\{1,2\}$, the equations

$$g^{1p}=\begin{cases} 0 & \text{if } p=1,\\ c^1 & \text{otherwise,}\end{cases}\qquad g^{2q}=\begin{cases} 0 & \text{if } q=1,\\ c^2 & \text{otherwise,}\end{cases}$$

for some constants c^1,c^2 describe a two-dimensional regular submanifold of U^4, and let $\Psi:M^2\to U^4$ be an immersion mapping onto this submanifold. If, on M^2, the determinant

$$\Psi^*\begin{vmatrix} f_1^1 & f_2^1 \\ f_1^2 & f_2^2 \end{vmatrix}\neq 0, \tag{30}$$

then Ψ is a two-dimensional integral manifold of I.

For PDE problems, Theorem 6 will be used to find alternative (hopefully transverse) integral manifolds of I to those found with the usual approach reviewed at the start of this section. Unfortunately there is no algorithmic technique (without involving ODEs) for establishing (29) by means other than following direct one using Proposition 4.7 in Sherring and Prince[21] that incorporates symmetry:

Suppose then we apply Proposition 4.7 with $X_2\in\mathfrak{X}(U^4)$ as a nontrivial symmetry of $\ker(\alpha^1\wedge\alpha^2)$, and $X_1\in\mathfrak{X}(U^4)$ as a nontrivial symmetry of $\mathrm{sp}\{X_2\}\oplus\ker(\alpha^1\wedge\alpha^2)$. We then obtain

$$\frac{X_2 \lrcorner (\alpha^1 \wedge \alpha^2)}{X_1 \lrcorner X_2 \lrcorner (\alpha^1 \wedge \alpha^2)} = \mathrm{d}g^{12},$$
$$\frac{X_1 \lrcorner (\alpha^1 \wedge \alpha^2)}{X_2 \lrcorner X_1 \lrcorner (\alpha^1 \wedge \alpha^2)} = \mathrm{d}g^{22} - X_1(g^{22})\mathrm{d}g^{12}, \tag{31}$$

for some $g^{12}, g^{22} \in C^\infty(U^4)$. This gives integral manifolds of I defined by $g^{12} = c^1$, $g^{22} = c^2$ for constants c^1, c^2. Suppose these are not transverse. Rearranging the equations in (31) gives

$$\begin{aligned}(X_2 \lrcorner \alpha^2)\alpha^1 - (X_2 \lrcorner \alpha^1)\alpha^2 &= (X_2 \lrcorner X_1 \lrcorner (\alpha^1 \wedge \alpha^2))\mathrm{d}g^{12},\\ ((X_1 + X_1(g^{22})X_2) \lrcorner \alpha^2)\alpha^1 - ((X_1 + X_1(g^{22})X_2) \lrcorner \alpha^1)\alpha^2 &= (X_1 \lrcorner X_2 \lrcorner (\alpha^1 \wedge \alpha^2))\mathrm{d}g^{22}.\end{aligned} \tag{32}$$

Now applying Theorem 6 with the equations in (32), we set

$$g^{11} = -g^{21} = X_2 \lrcorner X_1 \lrcorner (\alpha^1 \wedge \alpha^2).$$

We cannot choose $p = 2, q = 2$ since by assumption these integral manifolds of I are not transverse. We also cannot choose $p = 1, q = 1$ because $g^{11} = -g^{21}$ implies we do not obtain a regular two-dimensional submanifold of U^4. This is clearly due to the constant maximal rank two requirement failing. Therefore we require that at least one of the two remaining (p,q) combinations satisfy the rank two condition. Finally, the equation in (30) must also be satisfied, i.e.,

$$\Psi^* \begin{vmatrix} X_2 \lrcorner \alpha^2 & -X_2 \lrcorner \alpha^1 \\ (X_1 + X_1(g^{22})X_2) \lrcorner \alpha^2 & -(X_1 + X_1(g^{22})X_2) \lrcorner \alpha^1 \end{vmatrix} \neq 0.$$

The following is a modification of Theorem 6, which shows that if we are given just one of the equations in (29) (found for example by inspection, or using Proposition 4.7 in Sherring and Prince[21] as in the above), then the other can be determined using a symmetry:

Theorem 7: *With α^1, α^2 and I defined as noted previously, let there exist $f_1^1, f_2^1, g^{11}, g^{12} \in C^\infty(U^4)$ such that*

$$f_1^1 \alpha^1 + f_2^1 \alpha^2 = g^{11}\,\mathrm{d}g^{12}. \tag{33}$$

Suppose that for some $p \in \{1,2\}$, the equation

$$g^{1p} = \begin{cases} 0 & \text{if } p = 1, \\ c^1 & \text{otherwise,} \end{cases} \tag{34}$$

for some constant c^1 describes a three-dimensional regular submanifold of U^4. Let $\Theta: M^3 \to U^4$ denote an immersion mapping onto this submanifold, and let $X \in \mathfrak{X}(M^3)$ be a nontrivial symmetry of $\Theta^*(f_1^2 \alpha^1 + f_2^2 \alpha^2)$, for some $f_1^2, f_2^2 \in C^\infty(U^4)$. Then there exist $\bar{g}^{21}, \bar{g}^{22} \in C^\infty(M^3)$ such that

$$\Theta^*(f_1^2 \alpha^1 + f_2^2 \alpha^2) = \bar{g}^{21}\,\mathrm{d}\bar{g}^{22}.$$

Further suppose that, for some $q \in \{1,2\}$, the equation

$$\bar{g}^{2q} = \begin{cases} 0 & \text{if } q = 1, \\ c^2 & \text{otherwise,} \end{cases}$$

for some constant c^2 describes a two-dimensional regular submanifold of M^3. With $\Psi: M^2 \to M^3$ denoting an immersion mapping onto this submanifold, if

$$(\Theta\circ\Psi)^*\begin{vmatrix} f_1^1 & f_2^1 \\ f_1^2 & f_2^2 \end{vmatrix} \neq 0, \tag{35}$$

on M^2, *then* $\Theta\circ\Psi$ *is a two-dimensional integral manifold of* I.

Proof: Since for each $i\in\{1,2\}$, $\mathrm{d}\alpha^i \equiv 0 \bmod \alpha^1,\alpha^2$, it follows that with

$$\beta^1 := f_1^1\alpha^1 + f_2^1\alpha^2,$$

$$\beta^2 := f_1^2\alpha^1 + f_2^2\alpha^2,$$

we have for each $i\in\{1,2\}$, $d\beta^i \equiv 0 \bmod \beta^1,\beta^2$ for arbitrary choice of $f_1^1, f_2^1, f_1^2, f_2^2 \in C^\infty(U^4)$. Let β^1 satisfy (33) for some f_1^1, f_2^1 and some $g^{11}, g^{12} \in C^\infty(U^4)$, and for some $p\in\{1,2\}$, let the immersion $\Theta: M^3 \to U^4$, defined as in the theorem, map onto the regular submanifold of U^4 given by (34). Then $\Theta^*\beta^1 = 0$, so that

$$\mathrm{d}(\Theta^*\beta^2) = \Theta^*(\mathrm{d}\beta^2) = (\Theta^*\mu_1)\Theta^*\beta^1 + (\Theta^*\mu_2)\Theta^*\beta^2 \equiv 0 \bmod \Theta^*\beta^2,$$

for some $\mu_1,\mu_2 \in C^\infty(U^4)$. Let $X\in\mathfrak{X}(M^3)$ be a nontrivial symmetry of $\Theta^*\beta^2$. Hence from Proposition 4.7 in Sherring and Prince[21] (or even Theorem 2.1 in the same paper), we obtain

$$\mathrm{d}\left(\frac{\Theta^*\beta^2}{X\lrcorner(\Theta^*\beta^2)}\right) = 0.$$

Therefore

$$\Theta^*\beta^2 = (X\lrcorner(\Theta^*\beta^2))\mathrm{d}\overset{2}{g}{}^{22},$$

for some $\overset{2}{g}{}^{22} \in C^\infty(M^3)$. We set $\overset{2}{g}{}^{21} = X\lrcorner(\Theta^*\beta^2)$ and choose $\overset{2}{g}{}^{2q}$ such that it is of constant maximal rank one on M^3. Hence with Ψ defined as in the theorem, we have

$$(\Theta\circ\Psi)^*\beta^1 = 0 = (\Theta\circ\Psi)^*\beta^2.$$

By the assumption in (35), it is then clear that $\Theta\circ\Psi$ is a two-dimensional integral manifold of I. □

Remark: The functions f_1^2, f_2^2 in Theorem 7 are not quite arbitrary: First they must be chosen so that

$$\Theta^*\begin{vmatrix} f_1^1 & f_2^1 \\ f_1^2 & f_2^2 \end{vmatrix} \neq 0,$$

on M^3, or else (35) fails for any Ψ. Then once Ψ is known, (35) must be checked.

Certainly the difficult part in applying Theorem 7 is in establishing (33). Once this is done however, the remaining assumptions in the theorem simply involve two maximal rank conditions, one nonzero determinant condition and one nontrivial symmetry.

Another observation we can make regarding Theorem 7 is that $\ker(\alpha^1\wedge\alpha^2)$ must be Frobenius integrable. Of course, even if $\ker(\alpha^1\wedge\alpha^2)$ is not Frobenius integrable, singular two-dimensional integral manifolds of I may still exist.

The following example illustrates Theorem 7:

Example 8: Suppose on some suitably chosen U^4 where $x^2 \neq 0$, $I := \langle \alpha^1, \alpha^2 \rangle$ with

$$\alpha^1 := \mathrm{d}x^3 + \frac{x^1}{2x^2}\mathrm{d}x^1 - x^4\,\mathrm{d}x^2,$$

$$\alpha^2 := \left(2x^2x^4 - \frac{(x^1)^2}{2x^2} + 1\right)\mathrm{d}x^2.$$

It is easy to show that for all $i \in \{1,2\}$, $d\alpha^i \equiv 0 \bmod \alpha^1, \alpha^2$, and so $\ker(\alpha^1 \wedge \alpha^2)$ is Frobenius integrable.

We begin with the ''regular'' approach to integrating $\ker(\alpha^1 \wedge \alpha^2)$ reviewed at the beginning of this section. Simple inspection (or Proposition 4.7 in Sherring and Prince[21]) yields

$$\alpha^1 \wedge \alpha^2 = \left(2x^2x^4 - \frac{(x^1)^2}{2x^2} + 1 \right) d\left(x^3 + \frac{(x^1)^2}{4x^2} \right) \wedge dx^2.$$

Hence if the equations

$$x^2 = c^1, \quad x^3 + \frac{(x^1)^2}{4x^2} = c^2,$$

for arbitrary constants c^1, c^2 are constant maximal rank two on some suitably chosen neighborhood of U^4, then they describe a two-dimensional foliation of the neighborhood, where each leaf is a regular submanifold that is an integral manifold of I.

We now look to apply Theorem 7 in order to generate different two-dimensional integral manifolds of I. Applying the theorem, suppose we choose $f_1^1 := 0$, $f_2^1 := 1$, and

$$g^{11} := 2x^2x^4 - \frac{(x^1)^2}{2x^2} + 1, \quad g^{12} := x^2,$$

so that (33) holds. We set

$$g^{11} = 0. \tag{36}$$

We also choose $f_1^2 := 1$, $f_2^2 := 0$. Again without explicitly introducing an immersion, and pulling-back α^1 onto M^3 defined by (36) with coordinates for M^3 given by x^1, x^2, x^3, we find (on M^3)

$$\alpha^1 = dx^3 + \frac{x^1}{2x^2} dx^1 + \frac{1}{2x^2} \left(1 - \frac{(x^1)^2}{2x^2} \right) dx^2,$$

which, from Theorem 7, is closed modulo itself. Applying Theorem 2.1 in Ref. 21 with $\partial/\partial x^3$ as a nontrivial symmetry of α^1, we get

$$\alpha^1 = d\left(x^3 + \ln(\sqrt{x^2}) + \frac{(x^1)^2}{4x^2} \right),$$

so

$$\overline{g}^{21} = 1, \quad \overline{g}^{22} = x^3 + \ln(\sqrt{x^2}) + \frac{(x^1)^2}{4x^2}.$$

Hence our only choice is to set

$$\overline{g}^{22} = c^3,$$

where c^3 is an arbitrary constant function. On a suitable neighborhood of U^4 the equations

$$2x^2x^4 - \frac{(x^1)^2}{2x^2} + 1 = 0, \quad x^3 + \ln(\sqrt{x^2}) + \frac{(x^1)^2}{4x^2} = c^3 \tag{37}$$

are of constant maximal rank two, and it is easy to see from above that the nonzero determinant condition in (35) holds. Hence the equations in (37) describe a two-dimensional regular submanifold of the neighborhood of U^4, that is an integral manifold of I. Note that the two-dimensional

leaves described by (37) do not generate a foliation of the neighborhood. Rather, the three-dimensional regular submanifold of the neighborhood described by the equation on the left in (37) is foliated by the two-dimensional leaves generated by the equation on the right.

VII. A SINGULAR APPLICATION

In this section we use Theorem 7 to provide an alternative to Theorem 4 when the transverse requirement fails for $\Phi_* D_F^r$. The following result is the second of our major results:

Theorem 9: *Given some second-order PDE of the form in (1) whose corresponding L is decomposable, let* $V \in \mathfrak{X}(J^1(U^2,V^1))$ *be a symmetry of* I_F^r. *Suppose the equation* $V \lrcorner C^1 = 0$ *describes a four-dimensional regular submanifold of* $J^1(U^2,V^1)$, *and let* $\Phi: M^4 \to J^1(U^2,V^1)$ *denote an immersion mapping onto this submanifold. Further suppose* $\Phi^*(C^1 \wedge (V \lrcorner L)) \neq 0$, *and we have applied Theorem 7, with* $\alpha^1 := \Phi^* C^1$ *and* $\alpha^2 := \Phi^*(V \lrcorner L)$, *thus generating some smooth* $g^{1p}, \overline{g}^{2q}$ *and immersions* $\Theta: M^3 \to J^1(U^2,V^1)$ *and* $\Psi: M^2 \to M^3$, *as in the theorem. If*

$$(\Phi \circ \Theta \circ \Psi)^*(\mathrm{d}x^1 \wedge \mathrm{d}x^2) \neq 0, \tag{38}$$

then $\Phi \circ \Theta \circ \Psi(M^2)$ *is the image of the one-jet of some local solution of the PDE in (1).*

Proof: Using Lemma 3, we have on M^4 that

$$D_F^r := (\mathrm{sp}\{\Phi^* C^1, \Phi^*(V \lrcorner L)\})^\perp$$

is Frobenius integrable. Applying Theorem 7 to J_F^r defined in (14) then generates a two-dimensional integral manifold of J_F^r given by

$$\Theta \circ \Psi: M^2 \to M^4.$$

At this point the proof becomes very similar to that of Theorem 4. As L is decomposable, we find that

$$\Phi \circ \Theta \circ \Psi: M^2 \to J^1(U^2,V^1)$$

is a two-dimensional integral manifold of I_F^r. The condition in (38) is a transverse requirement. It is then clear that the image of $\Phi \circ \Theta \circ \Psi$ is equal to the image of the one-jet of some local solution of the PDE in (1). ■

Remark 1: Theorem 9 can obviously be modified by replacing Theorem 7 with Theorem 6.

Remark 2: While Theorem 9 does not require that $\Phi_* D_F^r$ be transverse, a transverse requirement must still be introduced, but at a later stage.

The following example attempts to clarify Theorem 9:

Example 10: Consider the potential Burgers' equation

$$\frac{\partial u}{\partial x^2} - \frac{\partial^2 u}{\partial (x^1)^2} - \left(\frac{\partial u}{\partial x^1} \right)^2 = 0. \tag{39}$$

Defined on $J^1(U^2,V^1)$ we have

$$I_F^r = \langle C^1, \mathrm{d}C^1, L, \mathrm{d}L \rangle,$$

where $F = z_2^1 - z_{11}^1 - (z_1^1)^2$ and $L = ((z_2^1 - (z_1^1)^2)\mathrm{d}x^1 - \mathrm{d}z_1^1) \wedge \mathrm{d}x^2$. Now

$$V := 2x^2 \frac{\partial}{\partial x^1} - x^1 \frac{\partial}{\partial z^1}$$

is a Lie point symmetry of (39), and we use its first prolongation $V^{(1)}$, where

$$V^{(1)}=2x^2\frac{\partial}{\partial x^1}-x^1\frac{\partial}{\partial z^1}-\frac{\partial}{\partial z_1^1}-2z_1^1\frac{\partial}{\partial z_2^1},$$

as our nontrivial symmetry of I_F^r.

Applying Theorem 9, we define M^4 to be the four-dimensional regular submanifold of $J^1(U^2,V^1)$ given by the locus of

$$V^{(1)}\lrcorner C^1=-x^1-2x^2z_1^1=0.$$

We assume M^4 has coordinates x^1,x^2,z^1,z_2^1 with $x^2\neq 0$, so that on M^4 we have

$$C^1=\mathrm{d}z^1+\frac{x^1}{2x^2}\mathrm{d}x^1-z_2^1\mathrm{d}x^2,$$

$$V^{(1)}\lrcorner L=\left(2x^2z_2^1-\frac{(x^1)^2}{2x^2}+1\right)\mathrm{d}x^2.$$

It is clear that the transverse condition does not hold on the two-dimensional annihilating space of $\mathrm{sp}\{C^1,V^{(1)}\lrcorner L\}$ defined on M^4, so we will look to use Theorem 7. In applying this result, we refer to Example 8 which makes use of the theorem with x^3 replacing z^1 and x^4 replacing z_2^1 so that $\alpha^1=C^1$ and $\alpha^2=V^{(1)}\lrcorner L$. From the example, we then get that

$$u=-\ln(\sqrt{x^2})-\frac{(x^1)^2}{4x^2}+c^3,$$

for any constant c^3 is a similarity solution of (39) corresponding to V.

VIII. DECOMPOSABILITY EXAMINED

Theorems 4 and 9 appear to be restricted by the requirement that L (or $L^\dagger$) be decomposable. However, since $\mathrm{d}C^1$ is in I_F^r, we may look to add some multiple $b\in J^1(U^2,V^1)$ of $\mathrm{d}C^1$ to L so that $L+b\,\mathrm{d}C^1$ is decomposable.

Without loss, working this time with $L^\dagger$, we define the following two-form:

$$\Omega^\dagger:=L^\dagger+b\mathrm{d}C^1,$$

where b is for the moment any smooth function on the first jet bundle $J^1(U^2,V^1)$. The following lemma gives a simple quadratic condition on b in order that $\Omega^\dagger\wedge\Omega^\dagger=0$, so that $\Omega^\dagger$ is decomposable by Theorem 1.7 in Ref. 8.

Lemma 11: With $\Omega^\dagger:=L^\dagger+b\mathrm{d}C^1$, if

$$b=\frac{-f_3\pm\sqrt{f_3^2-4f_1f_2}}{2},$$

with $f_3^2-4f_1f_2\geqslant 0$, *then* $\Omega^\dagger$ *is decomposable.*

Proof:

$$(L^\dagger+b\,\mathrm{d}C^1)^2=(L^\dagger)^2+2b\,\mathrm{d}C^1\wedge L^\dagger+b^2(\mathrm{d}C^1)^2,$$

and

$$(\mathrm{d}C^1)^2 = 2\,\mathrm{d}z_1^1 \wedge \mathrm{d}x^1 \wedge \mathrm{d}z_2^1 \wedge \mathrm{d}x^2,$$

$$(L^\dagger)^2 = -2\,f_1 f_2\,\mathrm{d}z_1^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}z_2^1 \wedge \mathrm{d}x^1,$$

$$\mathrm{d}C^1 \wedge L^\dagger = f_3\,\mathrm{d}z_2^1 \wedge \mathrm{d}x^2 \wedge \mathrm{d}z_1^1 \wedge \mathrm{d}x^1.$$

Hence

$$(L^\dagger + b\,\mathrm{d}C^1)^2 = 2(b^2 + bf_3 + f_1 f_2)\,\mathrm{d}z_1^1 \wedge \mathrm{d}x^1 \wedge \mathrm{d}z_2^1 \wedge \mathrm{d}x^2.$$

It follows that if

$$b = \frac{-f_3 \pm \sqrt{f_3^2 - 4f_1 f_2}}{2},$$

where b is real on $J^1(U^2, V^1)$, then $\Omega^\dagger \wedge \Omega^\dagger = 0$, and therefore by Theorem 1.7 in Ref. 8, $\Omega^\dagger$ is decomposable. □

Proved in a similar way to Lemma 11, we have the following for L:

Lemma 12: With: $\Omega := L + b\,\mathrm{d}C^1$, *if*

$$b = \frac{f_3 \pm \sqrt{f_3^2 - 4f_1 f_2}}{2},$$

with $f_3^2 - 4f_1 f_2 \geqslant 0$, *then* Ω *is decomposable*.

The requirement that the discriminant in Lemmas 11 and 12 remains non-negative on $J^1(U^2, V^1)$ (or on some suitable neighborhood), coincides exactly with the condition found widely in the literature that the second-order PDE in (1) be hyperbolic or parabolic. Hence, if the PDE is of one of these two types, then we are always able to determine a decomposable Ω (or $\Omega^\dagger$). Thus we can apply Theorems 4 and 9 by simply replacing the L in these two theorems with Ω. We illustrate with an example.

Example 13: Consider the nonlinear wave equation:

$$\frac{\partial^2 u}{\partial (x^2)^2} = u \frac{\partial^2 u}{\partial (x^1)^2}. \tag{40}$$

In terms of coordinates of $J^1(U^2, V^1)$, this equation admits the point symmetry

$$V := x^2 \frac{\partial}{\partial x^2} - 2z^1 \frac{\partial}{\partial z^1},$$

whose first prolongation is

$$V^{(1)} = x^2 \frac{\partial}{\partial x^1} - 2z^1 \frac{\partial}{\partial z^1} - 2z_1^1 \frac{\partial}{\partial z_1^1} - 3z_2^1 \frac{\partial}{\partial z_2^1}.$$

Working with L, we have

$$L = -z^1\,\mathrm{d}z_1^1 \wedge \mathrm{d}x^2 - \mathrm{d}z_2^1 \wedge \mathrm{d}x^1,$$

which is clearly not decomposable. From Lemma 12, we find that $L \pm \sqrt{z^1}\,\mathrm{d}C^1$ is decomposable. Taking the positive option gives

$$\Omega_+ := L + \sqrt{z^1}\,\mathrm{d}C^1$$
$$= (\mathrm{d}z_2^1 - \sqrt{z^1}\mathrm{d}z_1^1) \wedge (\sqrt{z^1}\,\mathrm{d}x^2 - \mathrm{d}x^1).$$

Applying Theorem 4, we define the four-dimensional regular submanifold $M^4 \subset J^1(U^2, V^1)$ by the locus of

$$V^{(1)} \lrcorner C^1 = -x^2 z_2^1 - 2z^1 = 0.$$

Let M^4 have coordinates x^1, x^2, z^1, z_1^1 with $x^2 \neq 0$. Then we have on M^4,

$$C^1 = \mathrm{d}z^1 - z_1^1\,\mathrm{d}x^1 + \frac{2z^1}{x^2}\mathrm{d}x^2,$$

$$V^{(1)} \lrcorner \Omega_+ = \left(-\frac{6z^1}{x^2} - 2\sqrt{z^1} z_1^1 \right) \mathrm{d}x^1 + \left(\frac{4(z^1)^{3/2}}{x^2} + 2z^1 z_1^1 \right) \mathrm{d}x^2 + 2\sqrt{z^1}\,\mathrm{d}z^1 + x^2 z^1\,\mathrm{d}z_1^1.$$

It is easy to show that the transverse condition holds on the two-dimensional annihilating space of $\mathrm{sp}\{C^1, V^{(1)} \lrcorner \Omega_+\}$ defined on M^4. By inspection,

$$X_1 := \frac{\partial}{\partial x^1} \in \mathfrak{X}(M^4)$$

is a nontrivial symmetry of $C^1 \wedge (V^{(1)} \lrcorner \Omega_+)$ (pulled-back onto M^4). Using the Lie symmetry analysis software package DIMSYM,[30] we find

$$X_2 := -\frac{1}{(x^2)^2}\frac{\partial}{\partial z^1} \in \mathfrak{X}(M^4)$$

is another nontrivial symmetry of $C^1 \wedge (V^{(1)} \lrcorner \Omega_+)$, which also commutes with X_1. Therefore, taking advantage of this situation and applying Theorems 4.1 and 5.1 in Ref. 21 gives the two closed forms

$$\frac{X_1 \lrcorner (C^1 \wedge (V^{(1)} \lrcorner \Omega_+))}{X_2 \lrcorner X_1 \lrcorner (C^1 \wedge (V^{(1)} \lrcorner \Omega_+))} = \mathrm{d}\left(\frac{(x^2)^4 (z_1^1)^2}{12} - (x^2)^2 z^1 \right),$$

$$\frac{X_2 \lrcorner (C^1 \wedge (V^{(1)} \lrcorner \Omega_+))}{X_1 \lrcorner X_2 \lrcorner (C^1 \wedge (V^{(1)} \lrcorner \Omega_+))} = \mathrm{d}\left(x^1 - \frac{(x^2)^2 z_1^1}{6} \right).$$

Putting

$$\frac{(x^2)^4 (z_1^1)^2}{12} - (x^2)^2 z^1 = c^1, \quad x^1 - \frac{(x^2)^2 z_1^1}{6} = c^2,$$

for any constants c^1, c^2, we obtain

$$u = \frac{3(x^1 - c^2)^2 - c^1}{(x^2)^2}$$

as our similarity solution of the nonlinear wave equation in (40) corresponding to V.

IX. CONDITIONAL SYMMETRIES

Following Olver,[6] Stephani,[7] or Bluman and Cole,[23] a *conditional symmetry* $V \in \mathfrak{X}(U^2 \times V^1)$ of some second-order PDE in (1) is defined as a Lie point symmetry of the overdetermined system of PDEs given by (1) and the first-order quasilinear PDE obtained from

$$V^{(1)} \lrcorner C^1 = 0. \tag{41}$$

In this section we show that all results in the previous sections still hold true if instead of the symmetry being the first prolongation of some point symmetry of (1) it is the first prolongation of some conditional symmetry.

We define

$$\hat{I}^r_F := \langle C^1, \mathrm{d}C^1, L, \mathrm{d}L, (V^{(1)} \lrcorner C^1)\mathrm{d}x^1 \wedge \mathrm{d}x^2, \mathrm{d}(V^{(1)} \lrcorner C^1) \wedge \mathrm{d}x^1 \wedge \mathrm{d}x^2 \rangle,$$

defined on the first jet bundle $J^1(U^2, V^1)$. It is clear from Sec. III that the image of any two-dimensional integral manifold of $\hat{I}^r_F$ that satisfies the transverse condition will be that of some one-jet solution map of the overdetermined system of PDEs given by (1) and (41).

If V is a conditional symmetry of (1), then it follows from the discussion in Sec. IV that

$$\mathcal{L}_{V^{(1)}} \hat{I}^r_F \subset \hat{I}^r_F.$$

Explicitly,

$$\mathcal{L}_{V^{(1)}} C^1 = \lambda_1 C^1, \tag{42}$$

as well as

$$\mathcal{L}_{V^{(1)}} L = \alpha^1 \wedge C^1 + \lambda_2 \, \mathrm{d}C^1 + \lambda_3 L + \lambda_4 ((V^{(1)} \lrcorner C^1)\mathrm{d}x^1 \wedge \mathrm{d}x^2), \tag{43}$$

and finally,

$$\mathcal{L}_{V^{(1)}}((V^{(1)} \lrcorner C^1)\mathrm{d}x^1 \wedge \mathrm{d}x^2) = \alpha^2 \wedge C^1 + \lambda_5 \, \mathrm{d}C^1 + \lambda_6 L + \lambda_7 ((V^{(1)} \lrcorner C^1)\mathrm{d}x^1 \wedge \mathrm{d}x^2), \tag{44}$$

for some $\lambda_1, \ldots, \lambda_7 \in C^\infty(J^1(U^2, V^1))$ and $\alpha^1, \alpha^2 \in \Lambda^1(J^1(U^2, V^1))$.

Suppose in terms of first jet bundle coordinates the equation in (41) describes a four-dimensional regular submanifold of $J^1(U^2, V^1)$, which we parametrize by the immersion $\Phi: M^4 \to J^1(U^2, V^1)$. It is then obvious that

$$\Phi^* \hat{I}^r_F = \Phi^* I^r_F.$$

Without loss, we can assume L is decomposable, so that $L = (V^{(1)} \lrcorner L) \wedge \omega$ for some $\omega \in \Lambda^1(J^1(U^2, V^1))$ (assume $V^{(1)} \lrcorner L \neq 0$). Suppose we now wish to repeat the proof of Lemma 3, where in the lemma,

(1) I^r_F is replaced by $\hat{I}^r_F$,
(2) V is replaced by the first prolongation of our conditional symmetry $V^{(1)}$,
(3) the symmetry conditions in (9) and (10) are replaced by those in (42) and (43).

Now it is not hard to see that the lemma still holds true, since the pull-back of (43) by Φ forces the final term on the right to vanish. Thus when pulled-back by Φ, the two sets of equations given in item (3) are in identical form. Hence from the lemma there exists some Cauchy characteristic vector field $W \in \mathfrak{X}(M^4)$ of J^r_F with the property that $\Phi_* W = V^{(1)}$. Consequently, with the same three substitutions given previously, Theorems 4 and 9 hold.

Finally, the equation in (44) is not used in the proof of any of our results. Therefore it appears that in order for us to use symmetries of $\hat{I}_F^r$ to derive nonclassical similarity solutions, vector fields from the symmetry algebra of $\hat{I}_F^r$ are not strictly necessary. One essentially only requires vector fields that satisfy (42) and (43).

Using a conditional symmetry, we now illustrate Theorem 4 with the following example.

Example 14: Consider the heat equation given in (26). From Stephani,[7] it has the conditional symmetry

$$V := \tan(x^1)\frac{\partial}{\partial x^1} + \frac{\partial}{\partial x^2},$$

whose first prolongation is given by

$$V^{(1)} = \tan(x^1)\frac{\partial}{\partial x^1} + \frac{\partial}{\partial x^2} - z_1^1 \sec^2(x^1)\frac{\partial}{\partial z_1^1}.$$

From Example 5, L is decomposable. Applying Theorem 4, we define the four-dimensional regular submanifold $M^4 \subset J^1(U^2, V^1)$ by the locus of

$$V^{(1)} \lrcorner C^1 = -z_1^1 \tan(x^1) - z_2^1 = 0.$$

Letting M^4 have coordinates x^1, x^2, z^1, z_1^1, we pull-back C^1 and $V^{(1)} \lrcorner L$ so that (on M^4),

$$C^1 = \mathrm{d}z^1 - z_1^1\,\mathrm{d}x^1 + z_1^1 \tan(x^1)\mathrm{d}x^2,$$

$$V^{(1)} \lrcorner L = -z_1^1 \tan x^1\,\mathrm{d}x^1 - z_1^1\,\mathrm{d}x^2 - \mathrm{d}z_1^1.$$

It can be shown that on M^4, $\ker(C^1 \wedge (V^{(1)} \lrcorner L))$ is a two-dimensional Frobenius integrable distribution that satisfies the transverse condition. By inspection,

$$\frac{\partial}{\partial x^2}, \frac{\partial}{\partial z^1} \in \mathfrak{X}(M^4),$$

are two commuting nontrivial symmetries of $C^1 \wedge (V^{(1)} \lrcorner L)$. Hence by Propositions 4.1 and 5.1 in Ref. 21 we obtain the two closed forms

$$\frac{\dfrac{\partial}{\partial x^2} \lrcorner (C^1 \wedge (V^{(1)} \lrcorner L))}{\dfrac{\partial}{\partial z^1} \lrcorner \dfrac{\partial}{\partial x^2} \lrcorner (C^1 \wedge (V^{(1)} \lrcorner L))} = \mathrm{d}(z^1 - z_1^1 \tan(x^1)),$$

$$\frac{\dfrac{\partial}{\partial z^1} \lrcorner (C^1 \wedge (V^{(1)} \lrcorner L))}{\dfrac{\partial}{\partial x^2} \lrcorner \dfrac{\partial}{\partial z^1} \lrcorner (C^1 \wedge (V^{(1)} \lrcorner L))} = \mathrm{d}\left(\ln\left| \frac{z_1^1}{\cos(x^1)} \right| + x^2 \right).$$

Putting

$$z^1 - z_1^1 \tan(x^1) = c^1, \quad \ln\left| \frac{z_1^1}{\cos(x^1)} \right| + x^2 = c^2,$$

for any constants c^1 and c^2 yields

$$u = \sin(x^1)\exp(c^2 - x^2) + c^1$$

as our local nonclassical similarity solution of the wave equation corresponding to the conditional symmetry V.

X. COMMENTS AND CONCLUSIONS

Our main results, Theorems 4 and 9, combined with Lemmas 11 and 12 show how one may use solvable symmetry structures to extract classical and nonclassical similarity solutions of second-order hyperbolic or parabolic PDEs of the form in (1). While the two theorems assume L (or $L^\dagger$) is decomposable, it is hardly a restriction. This is because the discriminant in the two lemmas remains non-negative on some neighborhood precisely when the PDE is hyperbolic or parabolic. Hence, we are always able to apply Theorems 4 and 9 by replacing the given nondecomposable L with a suitable decomposable Ω, which is simply some linear combination of L and $\mathrm{d}C^1$. For Theorem 4 there is a risk that the resulting two-dimensional Frobenius integrable distribution does not satisfy the transverse requirement. If this is the case, then the approach described in the theorem must be abandoned, and we are forced to use the slightly more sophisticated Theorem 9.

Finally, while our work has focused solely on the generation of similarity solutions in the absence of boundary conditions, there is scope for further work with such conditions. As a possible starting point, we know from Theorems 4 and 9 that given a symmetry V, we obtain uniqueness of solution up to two and one arbitrary constants, respectively. We leave such research as the topic of another paper.

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Classical Lie subalgebras of the Lie algebra of matrix differential operators on the circle

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We give a complete description of the anti-involutions of the algebra $\mathcal{D}^N$ of $N \times N$-matrix differential operators on the circle, preserving the principal $\mathbb{Z}$ gradation. We obtain, up to conjugation, two families $\sigma_{\pm,m}$ with $1 \leqslant m \leqslant N$, getting two families $\mathcal{D}^N_{\pm,m}$ of simple Lie subalgebras fixed by $-\sigma_{\pm,m}$. We also give a geometric realization of $\sigma_{\pm,m}$, concluding that $\mathcal{D}^N_{+,m}$ is a subalgebra of $\mathcal{D}^N$ of type $o(m,n)$ and $\mathcal{D}^N_{-,m}$ is a subalgebra of $\mathcal{D}^N$ of type $osp(m,n)$ (ortho-symplectic). Finally, we study the conformal algebras associated with $\mathcal{D}^N_{+,m}$ and $\mathcal{D}^N_{-,m}$. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1380252]

I. INTRODUCTION

Certain subalgebras of the Lie algebra $\mathcal{D}$ of differential operators on the circle were considered in Ref. 1, where they showed that there are two, up to conjugation, anti-involution $\sigma_\pm$ on $\mathcal{D}$, which preserve the principal gradation, and they obtained in this way two different Lie subalgebras fixed by $-\sigma_\pm$. The main goal of the present paper is to extend the results in Ref. 1 to the matrix case, where the picture seems to be rather more complicated and richer.

We give a complete description of the anti-involutions of the algebra $\mathcal{D}^N$ (whose central extension is usually denoted by $W^N_{1+\infty}$), of $N \times N$-matrix differential operators on the circle, preserving the principal $\mathbb{Z}$ gradation. We obtain, up to conjugation, two families $\sigma_{\pm,m}$ with $1 \leqslant m \leqslant N$, getting two families $\mathcal{D}^N_{\pm,m}$ of Lie subalgebras fixed by $-\sigma_{\pm,m}$, and we show that these subalgebras are simple. Then, we give a geometric realization of $\sigma_{\pm,m}$, concluding that $\mathcal{D}^N_{+,m}$ is a subalgebra of $\mathcal{D}^N$ of type $o(m,n)$ and $\mathcal{D}^N_{-,m}$ is a subalgebra of $\mathcal{D}^N$ of type $osp(m,n)$ (ortho-symplectic).

Finally, we study the conformal algebra associated with $\mathcal{D}^N_{+,m}$. Following the notation in Ref. 2, recall that $\mathcal{D}^N$ is a formal distribution algebra with the family of pairwise local formal distributions $\mathcal{F}=\{J^n_A(z)=\delta(t-z)(-\partial_t)^n \otimes A : n \in \mathbb{Z}_+, A \in \mathrm{Mat}_N\mathbb{C}\}$ (see Ref. 2, Example 2.10), and the associated associative (respectively, Lie) conformal algebra is $\mathrm{Cend}_N=\overline{\mathcal{F}}$ (respectively, gc_N). When we try to extend the anti-involutions $\sigma_{+,m}$ on $\mathcal{D}^N$ to the associative conformal algebra Cend_N we find some problems. If we apply $\sigma_{+,m}$ to the fields J^k_A, we have that $\sigma_{+,m}(\mathcal{F}) \not\subset \overline{\mathcal{F}}$, except in the degenerated case $m=0$. Using the notion of Γ-twisted and Γ-formal distribution algebras (Γ is a group) introduced in Refs. 3 and 4, we are able to characterize the conformal subalgebras of gc_N associated with $\mathcal{D}^N_{+,m}$ and $\mathcal{D}^N_{-,m}$. In the case of $\mathcal{D}^N_{+,m}$, we get the conformal orthogonal subalgebra oc_N of gc_N with a $\mathbb{Z}_2$-gradation, and in the other case, $\mathcal{D}^N_{-,m}$, the associated conformal algebra is gc_N with a $\mathbb{Z}_2 \times \mathbb{Z}_2$ action given by a $\mathbb{Z}_2$-gradation and an action of $\mathbb{Z}_2$ (multiplicative) by semilinear automorphisms.

In Ref. 5, the representation theory of the central extension of $\mathcal{D}^N(W^N_{1+\infty})$ was studied and it may be interesting to develop the representation theory for this new family of simple Lie subalgebras (see Ref. 1 for the special case $N=1$).

The paper is organized as follows. In Sec. II we review the Lie algebra $\mathcal{D}^N$ and classify the anti-involutions of $\mathcal{D}^N$ preserving the principal $\mathbb{Z}$-gradation of $\mathcal{D}^N$. In Sec. III, we describe the Lie

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subalgebras $\mathcal{D}^{\mathcal{N}}_{\pm,\mathfrak{m}}$. In Sec. IV we prove that $\mathcal{D}^{\mathcal{N}}_{\pm,\mathfrak{m}}$ are simple. In Sec. V, we obtain a geometric realization of $\sigma_{+,m}$. In Sec. VI we study the conformal subalgebra associated with $\mathcal{D}^{\mathcal{N}}_{+\mathfrak{m}}$, and in Sec. VII, the conformal subalgebra associated with $\mathcal{D}^{\mathcal{N}}_{-,\mathfrak{m}}$.

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II. ANTI-INVOLUTIONS OF $\mathcal{D}^N$

Let N be a positive integer. Denote by $\mathcal{D}^N_{\text{as}}$ the associative algebra of all regular matrix differential operators on $\mathbb{C}^\times$, i.e., the operators on $\mathbb{C}^N[t,t^{-1}]$ of the form

$$E = e_k(t)\partial_t^k + e_{k-1}(t)\partial_t^{k-1} + \cdots + e_0(t),$$

$$\text{where } e_i(t) \in \text{Mat}_N\mathbb{C}[t,t^{-1}]. \tag{2.1}$$

Here and in the following we denote by $\text{Mat}_N R$ the associative algebra of all $N\times N$ matrices over an algebra R. It is more convenient to write the differential operators as linear combinations of elements of the form $t^k f(D)A$, where f is a polynomial, $D = t\partial_t$, $k\in\mathbb{Z}$, and $A\in\text{Mat}_N\mathbb{C}$. The product in $\mathcal{D}^N_{\text{as}}$ is then given by

$$(t^r f(D)A)(t^s g(D)B) = t^{r+s} f(D+s)g(D)AB. \tag{2.2}$$

Let $\mathcal{D}^N$ denote Lie algebra obtained from $\mathcal{D}^N_{\text{as}}$. The bracket in $\mathcal{D}^N$ may be conveniently calculated by the following formula:

$$[t^r f(D)A, t^s g(D)B] = t^{r+s}(f(D+s)g(D)AB - f(D)g(D+r)BA). \tag{2.3}$$

The elements $t^k D^m E_{ij}$ $(k\in\mathbb{Z}, m\in\mathbb{Z}_+, i,j=1,...,N)$ form a basis of $\mathcal{D}^N$. Here and in the following E_{ij} is the standard basis of $\text{Mat}_N\mathbb{C}$. Define the *weight* wt on $\mathcal{D}^N$ by

$$\text{wt}\, t^k f(D)E_{ij} = kN + i - j. \tag{2.4}$$

This gives us the *principal* $\mathbb{Z}$-gradation of $\mathcal{D}^N_{\text{as}}$ and $\mathcal{D}^N$: $\mathcal{D}^N = \oplus_{j\in\mathbb{Z}}\mathcal{D}^N_j$, and so we have the triangular decomposition

$$\mathcal{D}^N = \mathcal{D}^N{}_+ \oplus \mathcal{D}^N{}_0 \oplus \mathcal{D}^N{}_-,$$

where $\mathcal{D}^N{}_\pm = \oplus_{j\in\pm N}\mathcal{D}^N{}_j$.

An *anti-involution* σ of $\mathcal{D}^N_{\text{as}}$ is an involutive antiautomorphism of $\mathcal{D}^N_{\text{as}}$, i.e., $\sigma^2 = I$, $\sigma(aX + bY) = a\sigma(X) + b\sigma(Y)$ and $\sigma(XY) = \sigma(Y)\sigma(X)$, for all $a,b\in\mathbb{C}, X,Y\in\mathcal{D}^N_{\text{as}}$.

In order to classify the anti-involutions of $\mathcal{D}^N_{\text{as}}$ preserving its principal gradation, we shall need the following notation. Define for each $m = 1,...,N$, the permutation π_m in S_N given by

$$\begin{array}{ccccccccccc} 1 & 2 & \dots & m-1 & m & m+1 & \dots & N-1 & N \\ \downarrow & \downarrow & & \downarrow & \downarrow & \downarrow & & \downarrow & \downarrow \\ m & m-1 & \dots & 2 & 1 & N & \dots & m+2 & m+1 \end{array}. \tag{2.5}$$

Let us fix $m = 1,...,N$, $f\in\mathbb{C}$ and $c = \{c_{i,j}\}$, $c_{i,j}\in\mathbb{C}, i>j$, we define $\sigma = \sigma_{\pm,f,c,m}$ by the following formulas:

$$\sigma(E_{ii}) = E_{\pi_m(i),\pi_m(i)},$$

$$\sigma(DE_{ii}) = (-D + f - \delta_{i>m})E_{\pi_n(i),\pi_m(i)},$$

$$\sigma(tE_{ii}) = \pm tE_{\pi_m(i),\pi_m(i)}, \tag{2.6}$$

$$(i>j) \quad \sigma(E_{i,j}) = \begin{cases} c_{i,j}E_{\pi_m(j),\pi_m(i)} & \text{if } \pi_m(i) \leqslant N-i+j \\ tc_{i,j}E_{\pi_m(j),\pi_m(i)} & \text{if } N-i+j < \pi_m(i) \end{cases},$$

$$(i<j) \quad \sigma(E_{i,j}) = \begin{cases} t^{-1}c_{j,i}^{-1}E_{\pi_m(j),\pi_m(i)} & \text{if } \pi_m(i) \leqslant j-i \\ c_{j,i}^{-1}E_{\pi_m(j),\pi_m(i)} & \text{if } \pi_m(i) > j-i \end{cases},$$

where

$$\delta_{i>m} = \begin{cases} 1 & \text{if } i>m, \\ 0 & \text{if } i \leqslant m. \end{cases}$$

Theorem 1: Let $m=1,...,N$, $f \in \mathbb{C}$, and $c=\{c_{i,j}\}$, $c_{i,j} \in \mathbb{C}$, $i>j$. Then $\sigma=\sigma_{\pm,f,c,m}$ defined on generators by (2.6) extends to an anti-involution on $\mathcal{D}_{\text{as}}^N$ which preserves the principal $\mathbb{Z}$-gradation if and only if

$$c_{i,j} = c_{i,i-1}c_{i-1,i-2}\ldots c_{j+1,j}, \tag{2.7a}$$

and

$$\begin{cases} c_{i,j}c_{\pi_m(j),\pi_m(i)} = 1 & \text{if } \pi_m(i) \leqslant N-i+j, \\ c_{i,j}c^{-1}_{\pi_m(i),\pi_m(j)} = \pm 1 & \text{if } \pi_m(i) > N-i+j. \end{cases} \tag{2.7b}$$

Moreover, any anti-involution σ of $\mathcal{D}_{\text{as}}^N$ which preserves the principal $\mathbb{Z}$-gradation is one of them.

The proof of this Theorem is certainly more difficult than the one given in Ref. 1 for $N=1$, and it will be given in several steps. We mainly use the relations between the generators $E_{i,j}$ and the involutive property of σ.

Proof: Step 1. Since σ should preserve the principal $\mathbb{Z}$-gradation, we have $\sigma(E_{i,i}) = \Sigma_{j=1}^N Q_{i,j}(D)E_{j,j}$. But $\sigma(E_{i,i}) = \sigma(E_{i,i}E_{i,i}) = \Sigma_{j=1}^N (Q_{i,j}(D))^2 E_{j,j}$. Therefore, if $Q_{i,j}(D) \neq 0$, then $Q_{i,j}(D) \equiv 1$. Note that $Q_{i,j}$ is independent of D. Now, $E_{i,i} = \sigma^2(E_{i,i}) = \Sigma_{k,j=1}^N Q_{i,j}Q_{j,k}E_{k,k}$, then $\delta_{i,k} = \Sigma_{j=1}^N Q_{i,j}Q_{j,k}$. So, for each i there exist a unique j_i such that $Q_{i,j_i}Q_{j_i,i} = 1$, then $Q_{j_i,i} = 1$. On the other hand, we also have $Q_{j_i,i}Q_{i,k} = 0$ for any $k \neq j_i$, then $Q_{i,k} = 0$ for any $k \neq j_i$, obtaining that $\sigma(E_{i,i}) = E_{j_i,j_i}$. Due to the injectivity of $\sigma, \pi(i) := j_i$ is a permutation in S_N, and since σ is an involution, we have $\pi^2 = id$.

Similar ideas will be used in the following steps.

Step 2. Again, using that σ should preserve the principal $\mathbb{Z}$-gradation, we may assume that $\sigma(DE_{i,i}) = \Sigma_{j=1}^N P_{i,j}(D)E_{j,j}$. We have

$$\begin{aligned} \sigma(DE_{i,i}) &= \sigma(DE_{i,i}E_{i,i}) = \sigma(E_{i,i})\sigma(DE_{i,i}) \\ &= E_{\pi(i),\pi(i)}\left(\sum_{j=1}^N P_{i,j}(D)E_{i,j}\right) \\ &= P_{i,\pi(i)}(D)E_{\pi(i),\pi(i)}. \end{aligned} \tag{2.8}$$

Therefore, $\sigma(DE_{i,i}) = P_i(D)E_{\pi(i),\pi(i)}$ with $P_i(D) = P_{i,\pi(i)}(D)$. Now, let us write $P_i(D) = \overline{P}_i(D) + \dot{P}_i$, where $\dot{P}_i$ stands for the constant term of $P_i(D)$. Thus,

$$\begin{aligned} DE_{i,i} &= \sigma^2(DE_{i,i}) = \sigma(P_i(D)E_{\pi(i),\pi(i)}) \\ &= \sigma((\overline{P}_i(D)+\dot{P}_i)E_{\pi(i),\pi(i)}) \\ &= \overline{P}_i(\sigma(DE_{\pi(i),\pi(i)})) + \dot{P}_i\sigma(E_{\pi(i),\pi(i)}) \\ &= (\overline{P}_i(P_{\pi(i)}(D)) + \dot{P}_i)E_{i,i}. \end{aligned}$$

So, we have $D=\overline{P}_i(P_{\pi(i)}(D))+\dot{P}_i$. Thus, $P_i(D)=a_iD+f_i$ with $a_i\cdot a_{\pi(i)}=1$ and $a_i\cdot f_{\pi(i)}+f_i=0$.

Step 3. Let us suppose that $\sigma(tE_{i,i})=t\Sigma_{l=1}^{N}T_{i,l}(D)E_{l,l}$. Using a similar argument to the one used in (2.8), we can deduce that $T_{i,k}(D)\equiv 0$ if $k\neq\pi(i)$. As before, we denote $T_i(D)=T_{i,\pi(i)}\times(D)$. Again, let us write $T_i(D)=\overline{T}_i(D)+\dot{T}_i$, where $\dot{T}_i$ stands for the constant term of $T_i(D)$. Thus,

$$\begin{aligned} tE_{i,i} = \sigma^2(tE_{i,i}) &= \sigma(tT_i(D)E_{\pi(i),\pi(i)}) \\ &= \sigma((tE_{\pi(i),\pi(i)})(\overline{T}_i(D)+\dot{T}_i)E_{\pi(i),\pi(i)}) \\ &= [\overline{T}_i(\sigma(DE_{\pi(i),\pi(i)})) + \dot{T}_i\sigma E_{\pi(i),\pi(i)}]\sigma(tE_{\pi(i),\pi(i)}) \\ &= (\overline{T}_i(T_{\pi(i)}(a_{\pi(i)}D+f_{\pi(i)})) + \dot{T}_i)tT_{\pi(i)}(D)E_{i,i} \\ &= t((\overline{T}_i(T_{\pi(i)}(a_{\pi(i)}(D+1)+f_{\pi(i)})) + \dot{T}_i)T_{\pi(i)}(D))E_{i,i}. \end{aligned}$$

Thus, $1=T_{\pi(i)}(D)\ (\overline{T}_i(T_{\pi(i)}(a_{\pi(i)}(D+1)+f_{\pi(i)}))+\dot{T}_i)$. Then $\deg(T_i)=0$ for all i, and $T_i\cdot T_{\pi(i)}=1$.

Step 4. Suppose $i>j$. Considering the $\mathbb{Z}$-gradation, we have that $\sigma(E_{i,j})=\Sigma_{l=1}^{N-i+j}C_l^{ij}(D)E_{l+i-j,l}+\Sigma_{l=N-i+j+1}^{N}tC_l^{ij}(D)E_{l+i-j-N,l}$. Since, $\sigma(E_{l,l}E_{i,j})=\sigma(E_{i,j})\sigma(E_{l,l})=\sigma(E_{i,j})E_{\pi(l),\pi(l)}$, we can deduce $C^{i,j}_{\pi(l)}(D)=0$ for all $l\neq i$. Let $C^{i,j}(D)=C^{i,j}_{\pi(i)}(D)$. Therefore, we have

$$\sigma(E_{i,j})=\begin{cases} C^{i,j}(D)E_{\pi(i)+i-j,\pi(i)} & \text{if } \pi(i)\leqslant N-i+j \\ tC^{i,j}(D)E_{\pi(i)+i-j-N,\pi(i)} & \text{if } \pi(i)\geqslant N-i+j+1. \end{cases} \tag{2.9}$$

Similarly, if $i<j$ and

$$\sigma(E_{i,j})=\sum_{l=1}^{j-i}t^{-1}S_l^{ij}(D)E_{N+l+i-j,l}+\sum_{l=j-i+1}^{N}S_l^{ij}(D)E_{l+i-j,l},$$

we deduce that $S^{i,j}_{\pi(l)}(D)=0$ for all $l\neq i$. Thus, denoting $S^{i,j}(D):=S^{ij}_{\pi(i)}(D)$, we have

$$\sigma(E_{i,j})=\begin{cases} S^{i,j}(D)E_{\pi(i)+i-j,\pi(i)} & \text{if } \pi(i)\geqslant j-i+1 \\ t^{-1}S^{i,j}(D)E_{\pi(i)+i-j+N,\pi(i)} & \text{if } \pi(i)\leqslant j-i. \end{cases} \tag{2.10}$$

Let $i>j$ and $k=i-j$, since σ is an involution we have if $\pi(i)\leqslant N-i+j$:

$$E_{i,j}=\sigma^2(E_{i,j})=\sigma(C^{i,j}(D)E_{\pi(i)+k,\pi(i)})=\sigma(C^{i,j}(D)E_{\pi(i)+k,\pi(i)+k}E_{\pi(i)+k,\pi(i)})$$

using (2.9), we must have $\pi(\pi(i)+k)+k\leqslant N-k$, otherwise we get t in the right-hand side above, so $E_{i,j}=C^{\pi(i)+k,\pi(i)}(D)C^{i,j}(a_{\pi(i)+k}D+f_{\pi(i)+k})E_{\pi(\pi(i)+k)+k,\pi(\pi(i)+k)}$. Then, $c_{i,j}:=C^{i,j}(D)$ are constant, $j=\pi(\pi(i)+k)$ and $c_{i,j}\cdot c_{\pi(j),\pi(i)}=1$, using $\pi^2=id$.

If $\pi(i)\geqslant N-i+j+1$, in the same way, using simultaneously (2.9) and (2.10) and taking care of the t that appears in $\sigma(E_{i,j})$ we have $d_{\pi(j),\pi(i)}:=S^{\pi(j),\pi(i)}(D)$ are constant, $j=\pi(\pi(i)+k-N)$, and $1=c_{i,j}\cdot d_{\pi(j),\pi(i)}\cdot b_{\pi(j)}$.

Consider $i<j$ and take $k=i-j$, by the same argument, if $\pi(i)\geqslant -k+1$ then we have $d_{i,j}:=S^{i,j}(D)$ are constant, $j=\pi(\pi(i)+k)$, and $d_{i,j}\cdot d_{\pi(j),\pi(i)}=1$.

And, if $\pi(i)\leqslant -k$ then we have $j=\pi(\pi(i)+N+k)$ and $d_{i,j}\cdot c_{\pi(j),\pi(i)}\cdot b^{-1}_{\pi(j)}=1$.

Step 5. Let $i>j$, then by step 1, $E_{\pi(i),\pi(i)}=\sigma(E_{i,i})=\sigma(E_{i,j}\cdot E_{j,i})=\sigma(E_{j,i})\cdot\sigma(E_{i,j})$, and using (2.9) and (2.10) we get

$$d_{j,i}\cdot c_{i,j}=1. \tag{2.11}$$

Now, let us determine the permutation π. Again, we have for $i=2,\ldots,N$, $E_{\pi(i),\pi(i)}=\sigma(E_{i,i})=\sigma(E_{i,i-1}\cdot E_{i-1,i})=\sigma(E_{i-1,i})\cdot\sigma(E_{i,i-1})$. Now, rewriting (2.9) and (2.10) for this case, we have

$$\sigma(E_{i,i-1})=\begin{cases} c_{i,i-1}E_{\pi(i)+1,\pi(i)} & \text{if } \pi(i)<N \\ tc_{i,i-1}E_{1,N} & \text{if } \pi(i)=N, \end{cases} \tag{2.12}$$

$$\sigma(E_{i-1,i})=\begin{cases} d_{i-1,i}E_{\pi(i-1)-1,\pi(i-1)} & \text{if } \pi(i-1)>1 \\ t^{-1}d_{i-1,i}E_{N,1} & \text{if } \pi(i-1)=1. \end{cases} \tag{2.13}$$

Let i_0 be such that $\pi(i_0)=N$. From these equations, it is easy to see that

$$\pi(i_0-1)=1, \text{ and } \pi(i-1)=\pi(i)+1 \quad \text{for any } i\neq i_0. \tag{2.14}$$

Since π is a bijective map, we conclude that π must be π_m given in (2.5) where $m=i_0-1$.

Step 6. In this step we will characterize the constants a_i, f_i, and b_i defined in steps 2 and 3.

Let us start with a_i. We have

$$\begin{aligned} -b_i tE_{\pi(i),\pi(i)} &= -\sigma(E_{i,i}) \\ &= [\sigma(DE_{i,i}),\sigma(tE_{i,i})] \\ &= [(a_iD+f_i)E_{\pi(i),\pi(i)},b_itE_{\pi(i),\pi(i)}] \\ &= b_ia_itE_{\pi(i),\pi(i)}. \end{aligned}$$

So, $a_i=-1$ for all i. Since $tE_{i+1,i+1}\cdot E_{i+1,i}=E_{i+1,i}\cdot tE_{i,i}$, applying σ to both sides and using (2.12) we deduce that $b_{i+1}=b_i$. In step 3 we showed that $b_i\cdot b_{\pi(i)}=1$, then $b_i=\pm 1$.

Finally, by applying the same argument to $DE_{i+1,i+1}\cdot E_{i+1,i}=E_{i+1,i}\cdot DE_{i,i}$, we get $f_{i_0}=f_{i_{0-1}}-1$, and if $i\neq i_0$ then $f_i=f_{i-1}(1<i)$. Thus $f:=f_1=\cdots=f_{i_{0-1}}$ and $f-1=f_{i_0}=\cdots=f_N$, getting in this way all the conditions in our theorem and all the equations in (2.7).

On the other hand, it is straightforward to check that σ defined by (2.6) is indeed anti-involution of $\mathcal{D}^N_{\text{as}}$, finishing the proof. ■

Let us study conditions (2.7a) and (2.7b) in more detail. By (2.7a), all the coefficients $c_{i,j}$ are completely determined by

$$c_i:=c_{i+1,i}, \quad i=1,\ldots,N-1, \tag{2.15}$$

and condition (2.7b) is equivalent to $c_i\cdot c_{\pi_m(i+1)}=1(i\neq m)$, and $\pm 1=c_m\cdot(c_{N,1})^{-1}=c_m\cdot\Pi_i(c_i)^{-1}=\Pi_{i\neq m}(c_i)^{-1}$. Observe that the permutation π_m is basically given by two simple permutations of the sets $\{1,\ldots,m\}$ and $\{m+1,\ldots,N\}$. Thus Eq. (2.7b) reduces to

$$c_ic_{m-i}=1 \quad (1\leqslant i<m), \quad c_{m+i}c_{N-i}=1 \quad (1\leqslant i<N-m), \quad \pm 1=\prod_{i\neq m} c_i. \tag{2.16}$$

Let $N=n+m$. If m (respectively, n) is even, we have $\Pi_{i<m}c_i=c_{(m-1)/2}$ and $(c_{(m-1)/2})^2=1$ (respectively, $\Pi_{i>m}c_i=c_{m+(n-1)/2}$ and $(c_{m+(n-1)/2})^2=1$); we shall call the coefficient $c_{(m-1)/2}$ (respectively, $c_{m+(n-1)/2}$) a fixed point. If m or n are odd, the corresponding products are equal to 1. Therefore, we have

Case −:

If N is even and

(1) m even, then there are two fixed points and one of them must be 1 and the other one equal to -1.
(2) m odd, then there are no fixed points and the last condition in (2.16) is impossible. Thus *there is no anti-involution in this case*.

If N is odd, then m or n is even and we have only one fixed point that must be equal to -1.

Case +:

For any N, the last condition in (2.16) will be satisfied if we take the (possible) fixed points equal to 1.

III. LIE SUBALGEBRAS $\mathcal{D}^N_{\pm,m}$.

Let $\mathcal{D}^N_{\pm,f,c,m}$ denote the Lie subalgebra of $\mathcal{D}^N$ fixed by $-\sigma_{\pm,f,c,m}$, namely

$$\mathcal{D}^N_{\pm,f,c,m}=\{a\in\mathcal{D}^N|\,\sigma_{\pm,f,c,m}(a)=-a\}. \tag{3.1}$$

Now, we shall study the relation among $\mathcal{D}^N_{\pm,f,c,m}$ for different data $(\pm,f,c,m)$. Let $s\in\mathbb{C}$, denote by Θ_s the automorphism of $\mathcal{D}^N_{\text{as}}$ given by $\Theta_s(A)=A$, $\Theta_s(tI)=tI$ and $\Theta_s(DI)=(D+s)I$, where I stands for the identity matrix. Clearly Θ_s preserves the principal $\mathbb{Z}$-gradation of $\mathcal{D}^N_{\text{as}}$. Let $\sigma_f:=\sigma_{\pm,f,c,m}$, then we have

$$\sigma_f\cdot\Theta_s=\sigma_{f+s}=\Theta_s\cdot\sigma_f. \tag{3.2}$$

Similarly, let $r=\{r_{i,j}\}$ $(i>j)$ satisfying (2.7a) and (2.7b). Denote by Γ_r the automorphism of $\mathcal{D}^N_{\text{as}}$ defined by $\Gamma_r(tI)=tI$, $\Gamma_r(DI)=DI$, $\Gamma_r(E_{i,i})=E_{i,i}$, $\Gamma_r(E_{i,j})=r_{i,j}E_{i,j}$ $(i>j)$, and $\Gamma_r(E_{i,j})=(r_{i,j})^{-1}E_{i,j}$ $(i<j)$. Let $\sigma_c:=\sigma_{\pm,f,c,m}$, then we have

$$\sigma_c\cdot\Gamma_r=\sigma_{c\cdot r}=\Gamma_{r^{-1}}\cdot\sigma_c, \tag{3.3}$$

where $(c\cdot r)_{i,j}:=c_{i,j}r_{i,j}$ and $(r^{-1})_{i,j}=r_{i,j}^{-1}$. Observe that $c\cdot r$ and r^{-1} also satisfy (2.7a) and (2.7b). Using (3.2) and (3.3), we have:

Lemma 1: (cf. Ref. 1, Lemma 2.2) (a) The Lie algebras $\mathcal{D}^N_{\pm,f,c,m}$ are all isomorphic for different $f\in\mathbb{C}$. In fact, we have $\Theta_s(\mathcal{D}^N_{\pm,f,c,m})=\mathcal{D}^N_{\pm,f-2s,c,m}$.

(b) $\Gamma_r(\mathcal{D}^N_{\pm,f,c,m})=\mathcal{D}^N_{\pm,f,c\cdot r^{-2},m}$.

Due to Lemma 1 we may choose a Lie algebra among $\mathcal{D}^N_{\pm,f,c,m}$, but we must keep in mind the analysis of the fixed points for the cases $+$ and $-$ that we made before.

We will fix $f=0$. In this way, we have a normalization similar to the one taken in Ref. 1.

Due to Lemma 1(b), it is possible to change c by $c\cdot r^{-2}$. Thus we can take $c_i=1$, except for the fixed points that are 1 or -1, and they should keep the sign. Denote by $\sigma_{\pm,m}$ and $\mathcal{D}^N_{\pm,m}$ the anti-involution $\sigma_{\pm,f,c,m}$ and the Lie subalgebra $\mathcal{D}^N_{\pm,f,c,m}$, respectively, with this choice of f and c.

Remark 1: Observe that $\mathcal{D}^N_{\pm,m}$ is naturally isomorphic to $\mathcal{D}^N_{\pm,N-m}$.

In order to give an explicit description of this family of subalgebras, we need some notation. For any matrix $A\in\text{Mat}_{m\times n}(\mathbb{C})$, define

$$(A^\dagger)_{i,j}=A_{n+1-j,m+1-i}, \tag{3.4}$$

i.e., the transpose with respect to the other diagonal. Recall the anti-involutions on $\mathcal{D}:=\mathcal{D}^1$ given in Ref. 1:

$$\dot{\sigma}_{\pm,b}(t^k f(D)) = (\pm t)^k f(-D-k+b) \quad (b \in \mathbb{C}). \tag{3.5}$$

We extend $\dot{\sigma}_{\pm,b}$ to a map on $\mathrm{Mat}_{m\times n}(\mathcal{D}) = \mathcal{D} \otimes \mathrm{Mat}_{m\times n}(\mathbb{C})$ by taking $[\dot{\sigma}_{\pm,b}(A)]_{i,j} = \dot{\sigma}_{\pm,b}(A_{i,j})$.

Case +:

We define the following maps on $\mathrm{Mat}_{m\times n}(\mathcal{D})$:

$$\begin{aligned} A^{\dagger_1} &= \dot{\sigma}_{+,0}(A^\dagger), \quad B^{\dagger_2} = t^{-1}\dot{\sigma}_{+,0}(B^\dagger), \\ C^{\dagger_3} &= t\dot{\sigma}_{+,-1}(C^\dagger), \quad F^{\dagger_4} = \dot{\sigma}_{+,-1}(F^\dagger). \end{aligned} \tag{3.6}$$

Then the anti-involution $\sigma_{+,m}$ on $\mathcal{D}^N = \mathcal{D} \otimes \mathrm{Mat}_N(\mathbb{C})$ is explicitly given by

$$\sigma_{+,m}\begin{pmatrix} A & B \\ C & F \end{pmatrix} = \begin{pmatrix} A^{\dagger_1} & C^{\dagger_3} \\ B^{\dagger_2} & F^{\dagger_4} \end{pmatrix}, \tag{3.7}$$

where $A \in \mathrm{Mat}_{m\times m}(\mathcal{D})$, $B \in \mathrm{Mat}_{m\times n}(\mathcal{D})$, $C \in \mathrm{Mat}_{n\times m}(\mathcal{D})$, and $F \in \mathrm{Mat}_{n\times n}(\mathcal{D})$. And

$$\mathcal{D}^N_{+,m} = \left\{ \begin{pmatrix} A & B \\ -B^{\dagger_2} & F \end{pmatrix} : A + A^{\dagger_1} = 0 \ \text{ and } \ F + F^{\dagger_4} = 0 \right\}. \tag{3.8}$$

Observe that condition $\sigma_{+,m}(a) = -a$ implies $C^{\dagger_3} = -B$ and $B^{\dagger_2} = -C$, and these two conditions are equivalent since $(B^{\dagger_2})^{\dagger_3} = B$. It is also possible to prove that $\mathcal{D}^N_{+,m}$ is a Lie subalgebra of $\mathcal{D}^N$ by direct computations, using that $\dagger_1$ and $\dagger_4$ are antiautomorphism, and the identities $B^{\dagger_2} = t^{-1}B^{\dagger_1}$, $F^{\dagger_4} = tF^{\dagger_3}$, $(B^{\dagger_2})^{\dagger_1} = Bt^{-1}$, etc. Observe that ^{†_2} and ^{†_3} are not antiautomorphism. The following identities are also useful

$$\begin{aligned} \dot{\sigma}_{\pm,0}(t^{-1}\dot{\sigma}_{\pm,0}(\cdot)) &= \pm(\cdot)t^{-1}, \\ \dot{\sigma}_{\pm,-1}(t^{-1}\dot{\sigma}_{\pm,0}(\cdot)) &= \pm t^{-1}(\cdot), \end{aligned} \tag{3.9}$$

Case −:

Since the situation N even and m (also n) odd is impossible, we may suppose, due to the symmetry, that n is even.

Now, consider the following maps on $\mathrm{Mat}_{m\times n}(\mathcal{D})$:

$$\begin{aligned} A^{*1} &:= \dot{\sigma}_{-,0}(A^\dagger), \\ B^{*2} = (B_1|B_2)^{*2} &:= t^{-1}\dot{\sigma}_{-,0}\begin{pmatrix} -B_2^\dagger \\ B_1^\dagger \end{pmatrix}, \\ C^{*3} = \begin{pmatrix} C_1 \\ C_2 \end{pmatrix}^{*3} &:= t\dot{\sigma}_{-,-1}(-C_2^\dagger | C_1^\dagger), \\ F^{*4} = \begin{pmatrix} F_1 & F_2 \\ F_3 & F_4 \end{pmatrix}^{*4} &:= \dot{\sigma}_{-,-1}\begin{pmatrix} F_4^\dagger & -F_2^\dagger \\ -F_3^\dagger & F_1^\dagger \end{pmatrix}, \end{aligned} \tag{3.10}$$

where B_i are $m\times p$, with $n = 2p$, C_i are $p\times m$, and F_i are $p\times p$.

Then the anti-involution $\sigma_{-,m}$ on $\mathcal{D}^N$ is explicitly given by

$$\sigma_{-,m}\begin{pmatrix} A & B \\ C & F \end{pmatrix} = \begin{pmatrix} A^{*1} & C^{*3} \\ B^{*2} & F^{*4} \end{pmatrix}, \tag{3.11}$$

where $A \in \mathrm{Mat}_{m\times m}(\mathcal{D})$, $B \in \mathrm{Mat}_{m\times n}(\mathcal{D})$, $C \in \mathrm{Mat}_{n\times m}(\mathcal{D})$, and $F \in \mathrm{Mat}_{n\times n}(\mathcal{D})$. And

$$\mathcal{D}^N_{-,m}=\left\{\begin{pmatrix} A & B \\ -B^{*2} & F\end{pmatrix}: A+A^{*1}=0 \text{ and } F+F^{*4}=0\right\}. \tag{3.12}$$

Note that we have again that condition $\sigma_{-,m}(a)=-a$ implies $C^{*3}=-B$ and $B^{*2}=-C$, and these two conditions are equivalent since $(B^{*2})^{*3}=B$. Again, it is also possible to prove that $\mathcal{D}^N_{-,m}$ is a Lie subalgebra of $\mathcal{D}^N$ by direct computations, using that $*_1$ and $*_4$ are antiautomorphism. Observe that $*_2$ and $*_3$ are not antiautomorphism.

Observe that we may replace † by T (usual transpose) in (3.6)–(3.8) and we get another family of involutions (denoted by $\sigma^T_{+,m}$) that do not preserve the principal $\mathbb{Z}$-gradation, and the corresponding subalgebras are not $\mathbb{Z}$-graded subalgebras of $\mathcal{D}^N$, but they are isomorphic to the others. Namely, using that $A^\dagger=JA^TJ^{-1}$ where

$$J=\begin{pmatrix} 0 & \cdots & 1 \\ \vdots & 1 & \vdots \\ 1 & \cdots & 0\end{pmatrix} \tag{3.13}$$

we get $\mathrm{Ad}_{J_{m,n}}\circ\sigma^T_{+,m}=\sigma_{+,m}$, where

$$J_{m,n}=\begin{pmatrix} J_m & 0 \\ 0 & J_n\end{pmatrix}$$

and J_n is the $n\times n$ matrix J. In the same way, we may replace † by T in (3.10), getting another family of involutions denoted by $\sigma^T_{-,m}$, and they produce subalgebras isomorphic to the others. More precisely, we have $\mathrm{Ad}_{J_{m,p,p}}\circ\sigma^T_{-,m}=\sigma_{-,m}$, where

$$J_{m,p,p}=\begin{pmatrix} J_m & 0 & 0 \\ 0 & J_p & 0 \\ 0 & 0 & J_p\end{pmatrix}.$$

IV. GENERATORS OF $\mathcal{D}^N_{\pm,m}$

In this section we give a detailed description of the generators of $\mathcal{D}^N_{\pm,m}$. Then we show that these subalgebras are simple Lie algebras.

Let us denote by $\mathbb{C}[w]^{(1)}$ the set of all odd polynomials in $\mathbb{C}[w]$, and by $\mathbb{C}[w]^{(0)}$ the set of all even polynomials in $\mathbb{C}[w]$. And let $\overline{k}=0$ if k is an odd integer and $\overline{k}=1$ if k is even.

Note that $\mathcal{D}^N_{\pm,m}=\{x-\sigma_{\pm,m}(x): x\in\mathcal{D}^N\}$ and observe that by (3.5)

$$\dot\sigma_{\pm,b}(t^kf(D_k))=(\pm t)^kf(-D_k),$$

where $D_k=D+(k-b)/2$. Therefore, by (3.6) and (3.10) the following is a set of generators of $\mathcal{D}^N_{\pm,m}$.

From now on we will use the description of the elements in the subalgebras used in (3.8) and (3.12).

- Corresponding to the block A, that is $1\leqslant i,\ j\leqslant m$ and $b=0$ ($D_k=D+k/2$):
  First consider case $+$,
  $$\{t^k(f(D_k)E_{i,m+1-j}-f(-D_k)E_{j,m+1-i}): k\in\mathbb{Z}, f\in\mathbb{C}[x], 1\leqslant i<j\leqslant m\}$$
  for the case $-$,
  $$\{t^k(f(D_k)E_{i,m+1-j}-(-1)^kf(-D_k)E_{j,m+1-i}): k\in\mathbb{Z}, f\in\mathbb{C}[x], 1\leqslant i<j\leqslant m\}$$
  and the generators on the opposite diagonal for the case $+$ are
  $$\{t^kf(D_k)E_{i,m+1-i}: k\in\mathbb{Z}, f\in\mathbb{C}[x]^{(1)}, 1\leqslant i\leqslant m\}$$

and for the case $-$ are

$$\{t^k f(D_k)E_{i,m+1-i} : k\in\mathbb{Z}, f\in\mathbb{C}[x]^{\overline{(k)}}, 1\leqslant i\leqslant m\}.$$

- Corresponding to the blocks $B-C$ $(b=0)$:
  First consider case $+$. Here we have
  $$\{t^k(f(D_k)E_{i,m+j}-t^{-1}f(-D_k)E_{N+1-j,m+1-i}) : k\in\mathbb{Z},\ f\in\mathbb{C}[x],\ 1\leqslant i\leqslant m,\ \text{and}\ 1\leqslant j\leqslant N-m\}.$$
  And for the case $-$,
  $$\{t^k(f(D_k)E_{i,m+j}-(-1)^k t^{-1}f(-D_k)E_{N+1-j,m+1-i}) : k\in\mathbb{Z},\ f\in\mathbb{C}[x],\ 1\leqslant i\leqslant m,\ \text{and}\ 1\leqslant j\leqslant p\},$$
  $$\{t^k(f(D_k)E_{i,m+j}+(-1)^k t^{-1}f(-D_k)E_{N+1-j,m+1-i}) : k\in\mathbb{Z},\ f\in\mathbb{C}[x],\ 1\leqslant i\leqslant m,\ \text{and}\ p+1\leqslant j\leqslant N-m\}.$$
- Corresponding to the blocks F $(b=-1$ and $D_k=D+(k+1)/2)$:
  Case $+$:
  $$\{t^k(f(D_k)E_{m+i,N+1-j}-f(-D_k)E_{m+j,N+1-i}) : k\in\mathbb{Z},\ f\in\mathbb{C}[x],\ 1\leqslant i<j\leqslant N-m\} \tag{4.1}$$

and the generators on the opposite diagonal are

$$\{t^k f(D_k)E_{m+i,N+1-i} : k\in\mathbb{Z},\ f\in\mathbb{C}[x]^{(1)},\ 1\leqslant i\leqslant N-m\}. \tag{4.2}$$

For the case $-$ they are

$$\{t^k(f(D_k)E_{m+i,m+j}-(-1)^k f(-D_k)E_{N+1-j,N+1-i}) : k\in\mathbb{Z},\ f\in\mathbb{C}[x],\ 1\leqslant i,j\leqslant p\},$$

$$\{t^k(f(D_k)E_{m+i,N+1-j}+(-1)^k f(-D_k)E_{m+j,N+1-i}) : k\in\mathbb{Z},\ f\in\mathbb{C}[x],\ 1\leqslant i<j\leqslant p\},$$

$$\{t^k(f(D_k)E_{N+1-i,m+j}+(-1)^k f(-D_k)E_{N+1-j,m+i}) : k\in\mathbb{Z},\ f\in\mathbb{C}[x],\ 1\leqslant i<j\leqslant p\}$$

and the generators on the opposite diagonal are

$$\{t^k f(D_k)E_{m+i,N+1-i} : k\in\mathbb{Z},\ f\in\mathbb{C}[x]^{\overline{(k+1)}},\ 1\leqslant i\leqslant N-m\}.$$

Using the above-given description we can prove the following
Theorem 2: The Lie algebras $\mathcal{D}^N_{\pm,m}$ are simple.
Since this is a rather technical proof, we refer to the Appendix.

V. GEOMETRIC REALIZATION OF $\sigma_{\pm,m}$

In this section we give a geometric realization of $\sigma_{\pm,f,m}$, for arbitrary f. The algebra $\mathcal{D}^N$ acts on the space $V=\mathbb{C}^N[t,t^{-1}]$ and one has two bilinear forms on V:

$$B_\pm(h,g)=\mathrm{Res}_t\, h^T J_\pm g, \tag{5.1}$$

where

$$J_+=\begin{pmatrix} t^{-f-1}J_m & 0 \\ 0 & t^{-f}J_n \end{pmatrix},\quad J_-=\begin{pmatrix} t^{-f-1}J_m & 0 & 0 \\ 0 & 0 & t^{-f}J_p \\ 0 & -t^{-f}J_p & 0 \end{pmatrix}\circ\Phi$$

with $\Phi: V\to V$ given by $\Phi(h(t))=h(-t)$, $h(t)\in V$, and J_m as in (3.13). Observe that $V=\mathbb{C}^m[t,t^{-1}]\times\mathbb{C}^n[t,t^{-1}]$ is an orthogonal decomposition of V. Now, consider the following proposition.

Proposition 1: (a) The bilinear forms $B_{\pm}$ are nondegenerated and B_{+} is symmetric. If f is even (respectively, odd) then B_{-} is symmetric (respectively, skew-symmetric).

(b) For any $L \in \mathcal{D}^N$ and $h,g \in V$ we have

$$B_{\pm}(Lh,g) = B_{\pm}(h,\sigma_{\pm,f,m}(L)g), \tag{5.2}$$

that is, L and $\sigma_{\pm,f,m}(L)$ are adjoint operators with respect to $B_{\pm}$.

Proof: (a) The statements that $B_{\pm}$ are nondegenerated and B_{+} is symmetric are straightforward. Let us see B_{-}:

$$\begin{aligned}
B_{-}(t^k e_i, t^l e_j) &= \mathrm{Res}_t\, e_i^T \begin{pmatrix} (-1)^l t^{k+1-f-1} J_m & 0 & 0 \\ 0 & 0 & (-1)^l t^{k+l-f} J_p \\ 0 & (-1)^l t^{k+l-f}(-J_p) & 0 \end{pmatrix} e_j \\
&= e_i^T \begin{pmatrix} (-1)^l \delta_{k+l-f,0} J_m & 0 & 0 \\ 0 & 0 & (-1)^l \delta_{k+l-f,-1} J_p \\ 0 & (-1)^l \delta_{k+l-f,-1}(-J_p) & 0 \end{pmatrix} e_j \\
&= (-1)^f e_j^T \begin{pmatrix} (-1)^k \delta_{k+l-f,0} J_m & 0 & 0 \\ 0 & 0 & (-1)^k \delta_{k+l-f,-1} J_p \\ 0 & (-1)^k \delta_{k+l-f,-1}(-J_p) & 0 \end{pmatrix} e_i \\
&= (-1)^f B_{-}(t^l e_j, t^k e_i).
\end{aligned}$$

Therefore, if f is even B_{-} is symmetric and if f is odd B_{-} is skew-symmetric.

(b) Let $L = t^k p(D)\left(\begin{smallmatrix} A & B \\ C & F \end{smallmatrix}\right)$, $h = t^r e_p$, and $g = t^s e_q$ be as shown previously. We will consider only the $+$ case. The $-$ case is completely analogous being careful with the definition of J_{-}. Then recall that

$$\sigma_{+,m,f}(L)(g) = t^{s+k} \begin{pmatrix} p(-k-s+f)A^{\dagger} & tp(-k-s+f-1)C^{\dagger} \\ t^{-1}p(-k-s+f)B^{\dagger} & p(-k-s+f-1)F^{\dagger} \end{pmatrix} e^q$$

and $L(h) = t^{k+r} p(r) \left(\begin{smallmatrix} A & B \\ C & F \end{smallmatrix}\right) e_p$. Let us compute,

$$\begin{aligned}
B_{+}(L(t^r e_p), t^s e_q) &= \mathrm{Res}_t\, t^{k+r} p(r) e_p^T \begin{pmatrix} A & B \\ C & F \end{pmatrix}^T \begin{pmatrix} t^{-f-1} J_m & 0 \\ 0 & t^{-f} J_n \end{pmatrix} t^s e_q \\
&= (p,q)\text{entry}\ \ p(r) \begin{pmatrix} \delta_{k+r+s-f,0} A^T J_m & \delta_{k+r+s-f,-1} C^T J_n \\ \delta_{k+r+s-f,0} B^T J_m & \delta_{k+r+s-f,-1} F^T J_n \end{pmatrix}.
\end{aligned} \tag{5.3}$$

On the other hand, we have

$$\begin{aligned}
B_{+}(h, \sigma_{+,f,m}(L)g) &= \mathrm{Res}_t\, t^{r+s+k} e_p^T \begin{pmatrix} t^{-f-1} J_m 0 & \\ 0 & t^{-f} J_n \end{pmatrix} \\
&\quad \cdot \begin{pmatrix} p(-k-s+f)A^{\dagger} & tp(-k-s+f-1)C^{\dagger} \\ t^{-1}p(-k-s+f)B^{\dagger} & p(-k-s+f-1)F^{\dagger} \end{pmatrix} e_q \\
&= \begin{pmatrix} \delta_{k+r+s-f,0} p(-k-s+f) J_m A^{\dagger} & \delta_{k+r+s-f,-1} p(-k-s+f-1) J_m C^{\dagger} \\ \delta_{k+r+s-f,0} p(-k-s+f) J_n B^{\dagger} & \delta_{k+r+s-f,-1} p(-k-s+f-1) J_n F^{\dagger} \end{pmatrix}_{p,q}.
\end{aligned} \tag{5.4}$$

Now, comparing (5.3) with (5.4) we finish the proof. ■

Remark 2: Analogously, we can define the following nondegenerate bilinear forms on V (in this case we consider $f=0$ for simplicity):

$$B_{\pm}^{T}(h,q)=\mathrm{Res}_t\, h^T J_{\pm,T} g,$$

where

$$J_{+,T}=\begin{pmatrix} t^{-1}I_m & 0 \\ 0 & I_n \end{pmatrix}, \quad J_{-,T}=\begin{pmatrix} t^{-1}I_m & 0 & 0 \\ 0 & 0 & I_p \\ 0 & -I_p & 0 \end{pmatrix}\circ\Phi$$

with I_m the $m\times m$ identity matrix, and it is easy to see that they satisfy

$$B_{\pm}(Lh,g)=B_{\pm}(h,\sigma_{\pm,m}^{T}(L)g),$$

where $\sigma_{\pm,m}^{T}$ were defined in (3.13). Therefore, we can claim that $\mathcal{D}_{+,m}^{N}$ is a subalgebra of $\mathcal{D}^N$ of type $o(m,n)$ and $\mathcal{D}_{-,m}^{N}$ is a subalgebra of $\mathcal{D}^N$ of type $osp(m,n)$ (orthogonal-symplectic).

VI. CONFORMAL ALGEBRA ASSOCIATED WITH $\mathcal{D}_{+,m}^{N}$

In this section we will study the conformal algebra associated with $\mathcal{D}_{+,m}^{N}$. We will follow the notation on Ref. 2. Recall that $\mathcal{D}^N=\mathcal{D}^1\otimes_{\mathbb{C}}\mathrm{Mat}_N\mathbb{C}$, viewed as an associative algebra is a formal distribution algebra with the family of pairwise local formal distributions

$$\mathcal{F}=\{J_A^n(z)=J^n(z)\otimes A: n\in\mathbb{Z}_+, A\in\mathrm{Mat}_N\mathbb{C}\},$$

where $J^n(z)=\Sigma_{j\in\mathbb{Z}}t^j(-\partial_t)^n z^{-j-1}=\delta(t-z)(-\partial_t)^n$, cf. Ref. 2, example 2.10. Recall that given a collection of mutually local formal distributions $\mathcal{F}$, the closure $\overline{\mathcal{F}}$ is defined as the minimal $\mathbb{C}[\partial]$-module closed under all nth products, $n\in\mathbb{Z}_+$ (see Ref. 2, pp. 39).

The associated associative conformal algebra is

$$\mathrm{Cend}_N=\oplus_{n\in Z_+}\mathbb{C}[\partial]J^n\otimes\mathrm{Mat}_N\mathbb{C}$$

with λ-product

$$J_{A\,\lambda}^{k}J_B^l=\sum_{j=0}^{k}\binom{k}{j}(\lambda+\partial)^j J_{AB}^{k+l-j}.$$

We will denote by gc_N the conformal (associative) algebra Cend_N viewed as a Lie conformal algebra with the λ-bracket

$$[J_{A\,\lambda}^{k}J_B^l]=\sum_{j=0}^{k}\binom{k}{j}(\lambda+\partial)^j J_{AB}^{k+l-j}-\sum_{j=0}^{l}\binom{l}{j}(-\lambda)^j J_{BA}^{k+l-j}. \tag{6.1}$$

For simplicity, we will introduce the following bijective map that we learn from Kac's lectures at MIT (Spring'98), called the *symbol*,

$$\mathrm{Symb}: \quad gc_N \quad \to\mathrm{Mat}_N[\partial,x],$$

$$\sum_k A_k(\partial)J^k\mapsto\sum_k A_k(\partial)x^k,$$

where $A_k(\partial)\in\mathrm{Mat}_N(\mathbb{C}[\partial])$. The transferred λ-bracket is

$$A(\partial,x)_\lambda B(\partial,x)=A(-\lambda,x+\lambda+\partial)B(\lambda+\partial,x)-B(\lambda+\partial,-\lambda+x)A(-\lambda,x).$$

Now, we will try to extend the anti-involutions $\sigma_{+,m}$ on $\mathcal{D}^N$ to the conformal algebra Cend_N (here we return to our normalization $f=0$ made in Sec. III). When we apply $\sigma_{+,m}$ to the fields J_A^k we find some problems. In order to show this we will need the following formulas:

$$\dot\sigma_{+,0}(\partial_t)=-t\partial_t t^{-1}, \quad \dot\sigma_{+,-1}(\partial_t)=-\partial_t \tag{6.2}$$

and

$$\dot\sigma_{+,b}(\delta(t-z))=\delta(t-z) \quad \text{for any } b. \tag{6.3}$$

If $1\leqslant i,\ j\leqslant m$, using (3.6):

$$\begin{aligned}
\sigma_{+,m}(J^1_{E_{ij}}(z))&=\sigma_{+,m}(\delta(t-z)(-\partial_t)E_{ij})\\
&=\dot\sigma_{+,0}(\delta(t-z)(-\partial_t))E_{m+1-j,m+1-i}\\
&=\dot\sigma_{+,0}(-\partial_t)\dot\sigma_{+,0}(\delta(t-z))E_{m+1-j,m+1-i}\\
&=t\partial_t t^{-1}\delta(t-z)E_{m+1-j,m+1-i}\\
&=(\delta(t-z)\partial_t+t(t^{-1}\delta(t-z))')E_{m+1-j,m+1-i}\\
&=(\delta(t-z)\partial_t-t^{-1}\delta(t-z)+\delta_t'(t-z))E_{m+1-j,m+1-i}\\
&=-J^1_{E_{m+1-j,m+1-i}}(z)-t^{-1}J^0_{E_{m+1-j,m+1-i}}(z)-\partial_z J^0_{E_{m+1-j,m+1-i}}(z).
\end{aligned} \tag{6.4}$$

Warning: The second term in the last line of (6.4) has an extra t^{-1}.
And if $1\leqslant i,\ j\leqslant N-m$,

$$\begin{aligned}
\sigma_{+,m}(J^1_{E_{m+i,m+j}}(z))&=\dot\sigma_{+,-1}(\delta(t-z)(-\partial_t))E_{N+1-j,N+1-i}\\
&=\partial_t\delta(t-z)E_{N+1-j,N+1-i}\\
&=(\delta(t-z)\partial_t+\delta_t'(t-z))E_{N+1-j,N+1-i}\\
&=-J^1_{E_{N+1-j,N+1-i}}(z)-\partial_z J^0_{E_{N+1-j,N+1-i}}(z).
\end{aligned} \tag{6.5}$$

In the same way, for $1\leqslant i\leqslant m$ and $1\leqslant j\leqslant N-m$ we have

$$\sigma_{+,m}(J^1_{E_{i,m+j}}(z))=-t^{-1}(J^1_{E_{N+1-j,m+1-i}}(z)+\partial_z J^0_{E_{N+1-j,m+1-i}}(z)). \tag{6.6}$$

and for $1\leqslant i\leqslant N-m$ and $1\leqslant j\leqslant m$, we get

$$\sigma_{+,m}(J^1_{E_{m+i,j}}(z))=-t(J^1_{E_{m+1-j,N+1-i}}(z)+\partial_z J^0_{E_{m+1-j,N+1-i}}(z))-J^0_{E_{m+1-j,N+1-i}}(z). \tag{6.7}$$

Remark 3: (a) From (6.4) and (6.6) to (6.7), we observe that

$$\sigma_{+,m}(\mathcal{F})\not\subset\overline{\mathcal{F}}.$$

We will return to this point later.

(b) From (6.5) and using symbol, we have that

$$\sigma_{+,m}\begin{pmatrix} 0 & 0 \\ 0 & F(\partial,x) \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & F^{\dagger}(\partial,-\partial-x) \end{pmatrix}.$$

So if we consider the degenerated case $m=0$, we have $\sigma_{+,0}(A)=\dot{\sigma}_{+,-1}(A^{\dagger})$ getting in this way an anti-involution on gc_N. In terms of symbol, the corresponding conformal subalgebra fixed by $-\sigma_{+,0}$, which is usually denoted by oc_N, is the linear $\mathbb{C}$-span of

$$\overline{A(\partial,x)} := A(\partial,x) - \sigma_{+,0}(A(\partial,x)) = A(\partial,x) - A(\partial,-\partial-x)$$

with $A \in \mathrm{Mat}_N$ and the corresponding λ-bracket given by

$$[\overline{A(\partial,x)}_{\lambda}\ \overline{B(\partial,x)}] = \overline{A(-\lambda,\lambda+\partial+x)B(\lambda+\partial,x)} - \overline{B(\lambda+\partial,-\lambda+x)A(-\lambda,-\lambda+x)}$$
$$- \overline{A^{\dagger}(-\lambda,-\partial-x)B(\lambda+\partial,x)} + \overline{B(\lambda+\partial,-\lambda+x)A^{\dagger}(-\lambda,\lambda-x)}.$$

(c) In the case $N=1$ we have the same picture as in Ref. 1, where the fields $W^n(w) := \delta(t-z)(-\partial_t)^n + (-1)^{n+1}(-\partial_t)^n\delta(t-z)$, are introduced. Transferred in terms of symbol, $w^n = x^n - (-\partial-x)^n$ and the λ-bracket is simply (cf. Ref. 1, pp. 131–132)

$$[w^n{}_{\lambda} w^m] = (-\lambda-\partial-w)^n w^m - (\partial-w)^m w^n - (w+\partial)^n w^m + (\lambda-w)^m(-\lambda+w)^n.$$

Let us return to Remark 3(a). Consider the Lie algebra of matrix differential operators with constant coefficients $\mathfrak{g} := \mathrm{Mat}_N\mathbb{C}[\partial]$.

Now, for each $0 \leqslant m \leqslant N$, we have a $\mathbb{Z}_2$-gradation in $\mathfrak{g} = \mathfrak{g}_0 \oplus \mathfrak{g}_1$ where,

$$\mathfrak{g}_0 = \begin{pmatrix} \mathrm{Mat}_m\mathbb{C}[\partial] & 0 \\ 0 & \mathrm{Mat}_{N-m}\mathbb{C}[\partial] \end{pmatrix},$$

$$\mathfrak{g}_1 = \begin{pmatrix} 0 & \mathrm{Mat}_{m\times N-m}\mathbb{C}[\partial] \\ \mathrm{Mat}_{N-m\times m}\mathbb{C}[\partial] & 0 \end{pmatrix}.$$

Let us consider the Lie algebra $\mathcal{D}^{N,1/2}$ of matrix differential operators with coefficients in $\mathbb{C}[t^{1/2},t^{-1/2}]$, which can be seen as

$$\mathcal{D}^{N,1/2} = \mathbb{C}[t^{1/2},t^{-1/2}] \otimes \mathfrak{g}.$$

Consider the following subalgebra of $\mathcal{D}^{N,1/2}$:

$$\mathcal{D}^{N,1/2}_m = \mathbb{C}[t^1,t^{-1}] \otimes \mathfrak{g}_0 \oplus t^{1/2}\mathbb{C}[t^1,t^{-1}] \otimes \mathfrak{g}_1.$$

This is a *twisted* $\mathcal{D}^N$ algebra. Let us define the isomorphism $T_m : \mathcal{D}^{N,1/2} \to \mathcal{D}^{N,1/2}$ given by

$$T_m(A) = \begin{pmatrix} t^{-1/2}I_m & 0 \\ 0 & I_{N-m} \end{pmatrix} A \begin{pmatrix} t^{1/2}I_m & 0 \\ 0 & I_{N-m} \end{pmatrix}.$$

Note that T_m restricted to $\mathcal{D}^N$ gives us an isomorphism between $\mathcal{D}^N$ and $\mathcal{D}^{N,1/2}_m$. Via this isomorphism we translate $\sigma_{+,m}$ to $\mathcal{D}^{N,1/2}_m$, getting $T_m \circ \sigma_{+,m} \circ T_m^{-1} = \sigma_*$ where

$$\sigma_*\begin{pmatrix} A & B \\ C & F \end{pmatrix} = \dot{\sigma}_{+,-1}\begin{pmatrix} A^{\dagger} & C^{\dagger} \\ B^{\dagger} & F^{\dagger} \end{pmatrix}.$$

Observe that σ_* is equivalent to the involution defining oc_N extended to $\mathcal{D}^{N,1/2}_m$. Take the subalgebra $\mathcal{D}^{N,1/2}_{m,\sigma_*}$ of $\mathcal{D}^{N,1/2}_m$ fixed by $-\sigma_*$. This is isomorphic to $\mathcal{D}^N_{+,m}$.

Following the notation in Ref. 3, $\mathcal{D}_m^{N,1/2}$ gives rise to $1/2\mathbb{Z}$-twisted formal distributions algebra with local family

$$\mathcal{F}_m=\left\{ J_{A_i}^{n,i/2}(z):=J^{n,i/2}(z)\otimes A_i:=\sum_{k\in\mathbb{Z}} t^{k+i/2}(-\partial_t)^n z^{-k-1-i/2}A_i : A_i\in(\mathrm{Mat}_N\mathbb{C})_i,\ \ i\in\mathbb{Z}_2\right\}$$

where

$$\begin{aligned}(\mathrm{Mat}_N\mathbb{C})_0&=\left\{\begin{pmatrix} A & 0\\ 0 & F\end{pmatrix}: A\in \mathrm{Mat}_m\mathbb{C}, F\in \ \mathrm{Mat}_{N-m}\mathbb{C}\right\},\\ (\mathrm{Mat}_N\mathbb{C})_1&=\left\{\begin{pmatrix} 0 & B\\ C & 0\end{pmatrix}: B\in \mathrm{Mat}_{m\times N-m}\mathbb{C}, C\in \mathrm{Mat}_{N-m\times m}\mathbb{C}\right\}.\end{aligned}\tag{6.8}$$

Observe that $J_{A_i}^{n,i/2}(z)=\delta_{i/2}(z-t)(-\partial)^n A_i$, where $\delta_{i/2}(z-t)=\Sigma_{k\in\mathbb{Z}} t^{k+i/2}z^{-k-1-i/2}$.

Define $\mathrm{symb}(J_{A_i}^{n,i/2})=xA_i$ where $A_i\in\mathrm{Mat}_N(\mathbb{C})_i, i\in\{0,1\}$. Under this identification, the associated $\mathbb{Z}_2$-graded conformal algebra is

$$gc_{N,m}:=(\mathrm{Mat}_N\mathbb{C}[\partial,x])_0\oplus(\mathrm{Mat}_N\mathbb{C}[\partial,x])_1$$

with λ-product

$$[A_i(\partial,x)_\lambda B_j(\partial,x)]=A_i(-\lambda,\lambda+\partial+x)B_j(\lambda+\partial,x)-B_j(\lambda+\partial,-\lambda+x)A_i(-\lambda,x).$$

Therefore, $gc_{N,m}$ is simply $gc_N=\mathrm{Mat}_N(\mathbb{C}[\partial,x])$ endowed with a $\mathbb{Z}_2$-gradation that comes from the $\mathbb{Z}_2$-gradation in $\mathrm{Mat}_N(\mathbb{C})$ given by (6.8).

It is easy to see that $\sigma_*(\mathcal{F}_m)\subset\mathcal{F}_m$, getting in this way the $\mathbb{Z}_2$-graded conformal subalgebra $oc_{N,m}$ of $gc_{N,m}$ fixed by $-\sigma_*$. Obviously, we can see $oc_{N,m}$ as oc_N with a $\mathbb{Z}_2$-gradation, or as the $\mathbb{Z}_2$-graded conformal algebra associated with the $1/2\mathbb{Z}$-twisted formal distribution algebra $\mathcal{D}_{m,\sigma_*}^{N,1/2}$.

VII. CONFORMAL ALGEBRA ASSOCIATED WITH $\mathcal{D}_{-,m}^N$

In this section we will study the conformal algebra associated with $\mathcal{D}_{-,m}^N$. As in Sec. VI we will follow the notation in Refs. 2 and 3. Recall that in the + case, we first considered the degenerated case $\sigma_{+,0}$ (that is $m=0$) where we obtained a formal distribution algebra structure on $\mathcal{D}_{+,0}^N$, but in the case $1\leqslant m<N$ we obtained a $1/2\mathbb{Z}$-*twisted* formal distribution algebra. Similarly, in the case −, we will first consider the degenerated case $m=N$. Here we are forced to take the Lie algebra $\mathcal{D}_{-,N}^N$ as $\mathbb{Z}_2$-local formal distribution algebra, and in the case $1\leqslant m<N$ we get a double structure, that is $1/2\mathbb{Z}$-*twisted* and $\mathbb{Z}_2$-*local* formal distribution algebra.

Let $m=N$. Here $\sigma_{-,N}(A)=\dot\sigma_{-,0}(A^\dagger)$. In the case of $N=1$ we get the Lie algebra $\mathcal{D}^-$ considered in Ref. 1. In this paper as in our case the most convenient choice is the isomorphic subalgebra $\mathcal{D}_-^N$ which is the subalgebra of $\mathcal{D}^N$ fixed by $-\sigma_-:=-\dot\sigma_{-,-1}(A^\dagger)$ (because $\dot\sigma_{-,-1}(\partial_t)=\partial_t$ and $\dot\sigma_{-,-1}(t)=-t$).

Let us consider as before the fields $J_A^n(z)\in\mathcal{F}$ [cf. (6.1)]. Therefore, we have that

$$\sigma_-(J_A^n(z))=\sigma_-(\delta(z-t)(-\partial_t)^n A)=(-\partial_t)^n\delta(z+t)A^\dagger$$

with $\delta(z+t)=z^{-1}\Sigma_{k\in\mathbb{Z}}(-t/z)^k$. This motivates one to consider the family

$$\mathcal{F}^\pm=\{J_A^{n,\pm1}(z):=\delta(z\pm t)(-\partial_t)^n A: n\in\mathbb{Z}_+ \ \text{ and } \ A\in\mathrm{Mat}_n\mathbb{C}\},$$

which is a family of pairwise $\mathbb{Z}_2$-local formal distributions, (here $\mathbb{Z}_2=\{1,-1\}$), with OPE ($\alpha,\beta\in\mathbb{Z}_2$):

$$[J_A^{m,\alpha}(z),J_B^{n,\beta}(w)]=\sum_{k=0}^{m}\sum_{r=0}^{k}\binom{m}{k}\binom{k}{r}\beta^k(\partial_w^r J_{AB}^{m+n-k,\beta}(w))\partial_w^{k-r}\delta(z-\alpha\beta^{-1}w)$$

$$-\sum_{l=0}^{n}\binom{n}{l}(-\beta)^l J_{BA}^{m+n-l,\beta}(w)\partial_w^l\delta(z-\alpha\beta^{-1}w).$$

As in Sec. VII in Ref. 3, we introduce the following operator on the space of formal distributions: $T_\alpha(a(z))=\alpha a(\alpha z)$, with $\alpha\in\mathbb{Z}_2$. Note that $\mathcal{F}^{\pm}$ is closed under all T_α. Therefore, if we take $\mathrm{symb}(J_A^{1,1})=xA$ and $\mathrm{symb}(J_A^{1,-1})=yA$, then $(\mathcal{D}_-^N,\mathcal{F}^{\pm})$ gives rise to a conformal algebra

$$R=\overline{\mathcal{F}^{\pm}}\simeq gc_N\oplus gc_N=\mathrm{Mat}_N(\mathbb{C}[\partial,x])\oplus\mathrm{Mat}_N(\mathbb{C}[\partial,y]),$$

since the λ-bracket is

$$[A(\partial,x)_\lambda B(\partial,x)]=A(-\lambda,\lambda+\partial+x)B(\lambda+\partial,x)-B(\lambda+\partial,-\lambda+x)A(-\lambda,x),$$

$$[A(\partial,y)_\lambda B(\partial,y)]=A(-\lambda,-\lambda-\partial+y)B(\lambda+\partial,y)-B(\lambda+\partial,\lambda+y)A(-\lambda,y),$$

and $[A(\partial,x)_\lambda B(\partial,y)]=0$. The $\mathbb{Z}_2$-action on it by semilinear automorphisms (this is $\alpha T_\alpha\partial=\partial T_\alpha$ and $T_\alpha([x_\lambda y])=[T_\alpha(x)_{\alpha\lambda}T_\alpha(y)]$), is given by $T_{-1}(A(\partial,x))=A(\partial,y)$ and $T_{-1}(A(\partial,y))=A(\partial,x)$.

Now, we have that

$$\begin{aligned}\sigma_-(A(\partial,x))&=A^\dagger(\partial,y-\partial),\\ \sigma_-(A(\partial,y))&=A^\dagger(\partial,x+\partial).\end{aligned}\tag{7.1}$$

Thus, the subalgebra fixed by $-\sigma_-$ is the $\mathbb{C}$-linear span of $\overline{A(\partial,x)}:=A(\partial,x)-A^\dagger(\partial,y-\partial)$, (observe that $\overline{A(\partial,y)}=-\overline{A(\partial,x+\partial)}$).

The λ-bracket is

$$[\overline{A(\partial,x)}_\lambda B(\partial,x)]=\overline{A(-\lambda,x+\lambda+\partial)B(\lambda+\partial,x)}-\overline{B(\lambda+\partial,-\lambda+x)A(-\lambda,x)}.$$

Note that it is easy to show that

$$T_{-1}(\overline{A(\partial,x)})=-(\overline{A^\dagger(-\partial,x+\partial)}).$$

Therefore, the associated conformal subalgebra is isomorphic to gc_N with a $\mathbb{Z}_2$-action by semilinear automorphisms given by $T_1=id$ and T_{-1}.

Remark 4: Observe that we can collapse to the case $N=1$, getting gc_1 as the $\mathbb{Z}_2$-conformal algebra associated with the Lie algebra $\mathcal{D}_-$ in Ref. 1.

Now, let us consider $1\leqslant m<N$. In this case we need to combine the $1/2\mathbb{Z}$-twisted and the $\mathbb{Z}_2$-local notions.

As in Sec. VI, consider the Lie algebra of matrix differential operators with constant coefficients $\mathfrak{g}:=\mathrm{Mat}_N\mathbb{C}[\partial]$. For each $0\leqslant m\leqslant N$, we take the $\mathbb{Z}_2$-gradation in $\mathfrak{g}=\mathfrak{g}_0\oplus\mathfrak{g}_1$ as before.

Let us consider the Lie algebra $\mathcal{D}^{N,1/2}$ of matrix differential operators with coefficients in $\mathbb{C}[t^{1/2},t^{-1/2}]$, and consider the following subalgebra:

$$\mathcal{D}_m^{N,1/2}=\mathbb{C}[t^1,t^{-1}]\otimes\mathfrak{g}_0\oplus t^{1/2}\mathbb{C}[t^1,t^{-1}]\otimes\mathfrak{g}_1.$$

This is a twisted $\mathcal{D}^N$ algebra. Let us define the isomorphism $T_m:\mathcal{D}^{N,1/2}\to\mathcal{D}^{N,1/2}$ given by

$$T_m(A)=\begin{pmatrix} \sqrt{i}t^{-1/2}I_m & 0 \\ 0 & I_{N-m}\end{pmatrix} A \begin{pmatrix} \frac{1}{\sqrt{i}}t^{1/2}I_m & 0 \\ 0 & I_{N-m}\end{pmatrix}.$$

Note that T_m restricted to $\mathcal{D}^N$ gives us an isomorphism between $\mathcal{D}^N$ and $\mathcal{D}_m^{N,1/2}$. Via this isomorphism we translate $\sigma_{-,m}$ to $\mathcal{D}_m^{N,1/2}$, getting $T_m\circ\sigma_{-,m}\circ T_m^{-1}=\sigma_*$ where

$$\sigma_*(A)=\hat{\sigma}_{-,-1}A^{\ddagger},$$

with $A\in \mathrm{Mat}_N\mathbb{C}$ and

$$A^{\ddagger}=\begin{pmatrix} A_1 & B_1 & B_2 \\ C_1 & F_1 & F_2 \\ C_2 & F_3 & F_4\end{pmatrix}^{\ddagger}=\begin{pmatrix} A_1^{\dagger} & -C_2^{\dagger} & C_1^{\dagger} \\ -B_2^{\dagger} & F_4^{\dagger} & -F_2^{\dagger} \\ B_1^{\dagger} & -F_3^{\dagger} & F_1^{\dagger}\end{pmatrix}.$$

Take the subalgebra $\mathcal{D}_{m,\sigma_*}^{N,1/2}$ of $\mathcal{D}_m^{N,1/2}$ fixed by $-\sigma_*$. This is isomorphic to $\mathcal{D}_{-,m}^N$.

Following the notation in Ref. 3, $\mathcal{D}_m^{N,1/2}$ gives rise to a $1/2\mathbb{Z}$-twisted and $\mathbb{Z}_2$-local formal distributions algebra with the family

$$\mathcal{F}=\left\{ J_{A_i}^{n,i/2,\pm 1}(z):=J^{n,i/2,\pm 1}(z)\otimes A_i:=\sum_{k\in\mathbb{Z}}(\pm t)^{k+i/2}(-\partial_t)^n z^{-k-1-i/2}A_i : A_i\in(\mathrm{Mat}_N\mathbb{C})_i, i\in\mathbb{Z}_2\right\}.$$

Observe that $J_{A_i}^{n,i/2,\pm 1}(z)=\delta_{i/2}(z-(\pm 1)t)(-\partial)^n A_i$ where

$$\delta_{i/2}(z-(\pm 1)t)=\sum_{k\in\mathbb{Z}}((\pm 1)t)^{k+i/2}z^{-k-1-i/2}.$$

Its OPE is ($\alpha,\beta\in\mathbb{Z}_2$):

$$[J_{A_i}^{m,i/2,\alpha}(z),J_{A_j}^{n,i/2,\beta}(w)]=-\sum_{s=0}^{n}\binom{n}{s}(-\beta)^s J_{A_jA_i}^{m+n-s,(i+j)/2,\beta}(w)\partial_w^s\delta_{i/2}(z-\alpha\beta^{-1}w)$$
$$+\sum_{r=0}^{m}\sum_{k=0}^{r}\binom{m}{r}\binom{r}{k}\beta^r(\partial_w^k J_{A_iA_j}^{m+n-r,(i+j)/2,\beta}(w))\partial_w^{r-k}\delta_{i/2}(z-\alpha\beta^{-1}w).$$

Now we also introduce the following operator on the space of $1/2\mathbb{Z}$-twisted and $\mathbb{Z}_2$-local formal distributions: $T_\alpha(a(z))=\alpha a(\alpha z)$, with $\alpha\in\mathbb{Z}_2$. Note that $\mathcal{F}_m$ is closed under all T_α.

Thus, introducing $\mathrm{symb}(J_{A_i}^{1,i/2,1})=xA_i$ and $\mathrm{symb}(J_{A_i}^{1,i/2,-1})=yA_i$ with $A_i\in(\mathrm{Mat}_N\mathbb{C})_i$, $i\in\mathbb{Z}_2=\{0,1\}$, we have that the associated $\mathbb{Z}_2$-graded conformal algebra

$$gc_{N,m}:=\overline{\mathcal{F}_m}=\bigoplus_{i\in\mathbb{Z}_2}((\mathrm{Mat}_N\mathbb{C}[\partial,x])_i\oplus(\mathrm{Mat}_N\mathbb{C}[\partial,y])_i)$$

with λ-bracket

$$[A_i(\partial,x)_\lambda B_j(\partial,x)]=A_i(-\lambda,\lambda+\partial+x)B_j(\lambda+\partial,x)-B_j(\lambda+\partial,-\lambda+x)A_i(-\lambda,x),$$

$$[A_i(\partial,y)_\lambda B_j(\partial,y)]=A_i(-\lambda,-\lambda-\partial+y)B_j(\lambda+\partial,y)-B_j(\lambda+\partial,\lambda+y)A_i(-\lambda,y),$$

and $[A_i(\partial,x)_\lambda B_j(\partial,y)]=0$. Again, the $\mathbb{Z}_2$-action on it by semilinear automorphism is given by $T_{-1}(A_i(\partial,x))=A_i(\partial,y)$ and $T_{-1}(A_i(\partial,y))=A_i(\partial,x)$.

Therefore, $gc_{N,m} \simeq gc_N \oplus gc_N \simeq \mathrm{Mat}_N\mathbb{C}[\partial,x] \oplus \mathrm{Mat}_N\mathbb{C}[\partial,y]$ endowed with a $\mathbb{Z}_2$-gradation and a $\mathbb{Z}_2$-action by semilinear automorphisms given by T_{-1}.

It is easy to see that (in terms of symbol) we have for $i \in \mathbb{Z}_2$,

$$\sigma_*(A_i(\partial,x)) = A_i^{\ddagger}(\partial,y-\partial),$$

$$\sigma_*(A_i(\partial,y)) = A_i^{\ddagger}(\partial,x+\partial).$$

Thus, we consider the $-\sigma_*$-fixed subalgebra which is the $\mathbb{C}$-linear span of $\overline{A_i(\partial,x)} := A_i(\partial,x) - A_i^{\ddagger}(\partial,y-\partial)$.

The λ-bracket is $(i,j \in \mathbb{Z}_2)$

$$[\overline{A_i(\partial,x)}_\lambda \overline{B_j(\partial,x)}] = \overline{A_i(-\lambda,x+\lambda+\partial)B_j(\lambda+\partial,x)} - \overline{B_j(\lambda+\partial,-\lambda+x)A_i(-\lambda,x)}.$$

Therefore, the conformal subalgebra associated with $\mathcal{D}^N_{-,m}$ is isomorphic to gc_N with a $\mathbb{Z}_2 \times \mathbb{Z}_2$-action given by a $\mathbb{Z}_2$-gradation (that comes from the $\mathbb{Z}_2$ gradation in $\mathrm{Mat}_N\mathbb{C}$) and $\mathbb{Z}_2$-action by semilinear automorphism given by $T_1 = id$ and T_{-1}.

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APPENDIX

Here we will prove

Theorem 2: The Lie algebras $\mathcal{D}^N_{\pm,m}$ are simple.

Proof: We will give the proof only for the case $\mathcal{D}^N_{+,m}$, since the other is completely analogous. We are going to use the description in terms of generators given in Sec. IV. Since the proof is rather technical, some details will only be sketched. Assume that $b=1$. Let us define

$$X = \begin{pmatrix} \left(D-\frac{1}{2}\right)I_m & 0 \\ 0 & DI_{N-m} \end{pmatrix} \in \mathcal{D}^N_{+,m}. \tag{A1}$$

Note that $(k \in \mathbb{Z})$

$$\mathrm{ad}(X)\left(t^k f\left(D+\frac{k-1}{2}\right)A = kt^k f\left(D+\frac{k-1}{2}\right)A, \right. \tag{A2a}$$

where $A = \left(\begin{smallmatrix} A_1 & 0 \\ 0 & 0 \end{smallmatrix}\right)$. Similarly, if $F = \left(\begin{smallmatrix} 0 & 0 \\ 0 & F_1 \end{smallmatrix}\right)$, we have that

$$\mathrm{ad}(X)\left(t^k f\left(D+\frac{k}{2}\right)F\right) = kt^k f\left(D+\frac{k}{2}\right)F \tag{A2b}$$

and if $BC = \left(\begin{smallmatrix} 0 & B \\ t^{-1}C & 0 \end{smallmatrix}\right)$, we get

$$\mathrm{ad}(X)\left(t^k f\left(D+\frac{k-1}{2}\right)BC\right) = \left(k-\frac{1}{2}\right)t^k f\left(D+\frac{k-1}{2}\right)BC. \tag{A2c}$$

Let $\mathcal{J}$ be a nonzero ideal of $\mathcal{D}^N_{+,m}$ and let $v\in\mathcal{J}$ and $v=v^A+v^{BC}+v^F$, with v^A+v^F of the form $\left(\begin{smallmatrix}* & 0\\ 0 & *\end{smallmatrix}\right)$, and v^{BC} of the form $\left(\begin{smallmatrix}0 & *\\ * & 0\end{smallmatrix}\right)$.

By [(A2a)–(A2c)] we may assume that $v^A+v^F\in\mathcal{J}$ and $v^{BC}\in\mathcal{J}$. So, since $[I_m,v^A+v^F]\in\mathcal{J}$ we have that $v^A\in\mathcal{J}$ and similarly we can show that $v^F\in\mathcal{J}$.

We are going to show that if $v^A\in\mathcal{J}, v^A\neq 0$, then $E_{i,m+1-j}\pm E_{j,m+1-i}\in\mathcal{J}$ and $E_{i,m+1-i}\in\mathcal{J}$ with $1\leqslant i,j\leqslant m$. Analogous arguments will work finely for the remaining blocks, and the details are left to the reader. Therefore we can conclude that $\mathcal{J}=\mathcal{D}^N_{+,m}$.

Take $v^A\neq 0$ in $\mathcal{J}$. By (A2a), we may suppose $v^A=t^kA(D)=t^k\Sigma_{1\leqslant p,j\leqslant m}\,a_{pj}(D)E_{p,j}$ with A of the form $\left(\begin{smallmatrix}* & 0\\ 0 & 0\end{smallmatrix}\right)$.

Assume that $a_{i,s}(D)\neq 0$. Thus,

$$\left[\left(D-\frac{1}{2}\right)E_{i,m+1-i},t^kA(D)\right]=t^k\sum_{1\leqslant j\leqslant m}\left\{\left(D+k-\frac{1}{2}\right)a_{m+1-i,j}(D)E_{i,j}-\left(D-\frac{1}{2}\right)a_{j,i}(D)E_{j,m+1-i}\right\}. \tag{A3}$$

Now take $Y=t^{-k}(E_{r,s}-E_{m+1-s,m+1-r})\in\mathcal{D}^N_{+,m}$ with $s\neq m+1-r$, $s\neq i$ and $r\neq m+1-i$. Computing $\mathrm{ad}(Y)$ of (A3) we get

$$\begin{aligned}(D-\tfrac{1}{2})[&a_{m+1-i,m+1-s}(D-k)E_{i,m+1-r}-a_{i,s}(D)E_{r,m+1-i}\\&+a_{m+1-r,i}(D)E_{m+1-s,m+1-i}-a_{m+1-i,r}(D-k)E_{i,s}]\end{aligned} \tag{A4}$$

and again, $\mathrm{ad}((D-1/2)E_{m+1-r,r})$ $(r\neq m+1-r,\ r\neq i)$, applied to (A4), gives us

$$-(D-\tfrac{1}{2})^2[a_{m+1-i,m+1-s}(D-k)E_{i,r}+a_{s,i}(D)E_{m+1-r,m+1-i}]\in\mathcal{J} \tag{A5}$$

with $a_{s,i}(D)\neq 0$. In particular, (A5) belongs to $\mathcal{D}^N_{+,m}$, thus we have that

$$a_{m+1-i,m+1-s}(D)=-a_{s,i}(-D-k+1). \tag{A6}$$

Therefore, we may assume that $-(D-1/2)^2[f(D)E_{i,r}+f(-D-k+1)E_{m+1-r,m+1-i}]\in\mathcal{J}$ for some $f\neq 0$.

Note that $E_{pq}-E_{m+1-q,m+1-p}\in\mathcal{D}^N_{+,m}$ for any $1\leqslant p,q\leqslant m$. If we pick different values for p and q it is easy to show that

$$-(D-\tfrac{1}{2})^2[f(D)E_{p,q}+f(-D-k+1)E_{m+1-q,m+1-p}]\in\mathcal{J}, \tag{A7}$$

for arbitrary values of p and q. Note in particular, if $p=m+1-q$ we get an element on the diagonal (cf. with description of generators in Sec. IV).

Now to finish the proof, we only need to show we can lower the degree of $f(D)$ in (A7). But again, since $t(E_{ll}-E_{m+1-l,m+1-l})\in\mathcal{D}^N_{+,m}$ for $1\leqslant l\leqslant m$, and if we compute the bracket between (A7) and $t(E_{p,p}-E_{m+1-p,m+1-p})$, and the bracket between (A7) and $t(E_{q,q}-E_{m+1-q,m+1-q})$ and then the difference between them we have that

$$t((f(D+1)-f(D))E_{p,q}+(g(D)-g(D-1))E_{m+1-q,m+1-p})\in\mathcal{J}.$$

Thus we get an element in the ideal with lower degree in D, but we have increased the degree in t. Using the argument in (A4), we can again lower the degree in t. This process will eventually end, showing that $E_{p,q}\pm E_{m+1-q,m+1-p}$. □

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On completeness of random exponentials in the Bargmann–Fock space

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We study the completeness/incompleteness properties of a system of exponentials $\mathcal{E}_\Lambda=\{e^{\pi\lambda z};\ \lambda\in\Lambda\}$, viewed as elements of the Bargmann–Fock space of entire functions. We assume that the index set Λ is a realization of a random point field in $\mathbb{C}$ (the support of a random measure). We prove that the properties are determined by the density of the field, i.e., by the mean number of the field points per unit area. We also discuss certain implications and motivations of our results, in particular, the jumps of the integrated density of states of the Landau Hamiltonian with the random potential, equal to the sum of point scatters. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379311]

I. INTRODUCTION: PROBLEM AND RESULTS

The probabilistic approach to classical questions on exponential systems gives a new insight and leads to new results combining the methods of probability theory, function theory, and also to some applications. We mention here[1,2] which study the frame property and also completeness of random exponential systems and also[3,4] devoted to expansions in random exponential systems as well as signal analysis applications.

In this paper we study completeness of the random systems of exponentials

$$\mathcal{E}_\Lambda=\{e^{\pi\lambda z};\ \lambda\in\Lambda\}, \tag{1.1}$$

in the Bargmann–Fock space $B^2(\mathbb{C})$ for the case when the index set Λ is a realization of an ergodic point field in $\mathbb{C}$ or is a random perturbation of a periodic lattice in $\mathbb{C}$. Questions of such type appear naturally in time frequency analysis and also in spectral analysis of the Schrödinger operator with random potential. We refer the reader to the end of this introduction for a more detailed survey, now we recall the basic notions and formulate the main results of the article.

We consider the Hilbert space $B^2(\mathbb{C})$ of entire functions defined by the inner product

$$\langle f,g\rangle_{B^2(\mathbb{C})}:=\int_{\mathbb{C}}\int f(z)\overline{g(z)}e^{-\pi|z|^2}\,dm_z, \tag{1.2}$$

where dm_z is the plane Lebesgue measure. We shall consider random sets Λ "uniformly" distributed through the complex plane $\mathbb{C}$. Such sets can be defined in two different ways.

Let $(\Omega,\mathcal{F},\mathbf{P})$ be a probability space and $\mu(\cdot,\omega)$ be an integer-valued random measure in $\mathbb{C}$, i.e., for each Borel set $\Delta\subset\mathbb{C}$, $\mu(\Delta,\cdot)$ is a random variable and also, for $\omega\in\Omega$, $\mu(\cdot,\omega)$ is a locally bounded integer-valued Borel measure.

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To each $\omega\in\Omega$ one may associate the support of $\mu(\cdot,\omega)$, i.e., a discrete set

$$\Lambda_\omega=\{\lambda\in\mathbb{C};\ \mu(\{\lambda\},\omega)>0\},\tag{1.3}$$

such that

$$\mu(\cdot,\omega)=\sum_{\lambda\in\Lambda_\omega}\mu(\{\lambda\},\omega)\,\delta_\lambda(\cdot),\tag{1.4}$$

where δ_λ is the unit measure located at the point λ. In what follows we assume for simplicity that $\mu(\{\lambda\},\omega)=1$ for all $\lambda\in\Lambda_\omega$ with probability 1.

For $g=(m,n)\in\mathbb{Z}^2$ we denote $Q_g=\{x+iy;\ x\in[m,m+1),\ y\in[n,n+1)\}$, and $\mu_g(\omega)=\mu(Q_g,\omega)$. Let **E** and **Var** stand for mathematical expectation and variance in $(\Omega,\mathcal{F},\mathbf{P})$ respectively.

In Sec. III we assume that the family of random variables $\{\mu_g(\omega);\ g\in\mathbb{Z}^2\}$ is a point process in $\mathbb{R}^2$ homogeneous with respect to the group of motions generated by rotations by $\pm\pi/2$ around the origin and translations by integers along the coordinate axis (see, e.g., Ref. 5, Ch. 10, and Ref. 6, p. 17). In particular all random variables μ_g are identically distributed, and we assume that there exists the mathematical expectation

$$\mathbf{E}\mu_g=C<\infty.\tag{1.5}$$

C is called the *density* of the random field $\{\mu_g\}_{g\in\mathbb{Z}^2}$. We also assume that the random field $\{\mu_g\}_{g\in\mathbb{Z}^2}$ satisfies the following decay and mixture conditions:

(**a**) For some $\delta>0$

$$\mathbb{E}\,\mu_{(0,0)}^{2+\delta}<+\infty.\tag{1.6}$$

(**b**) There exist δ, satisfying (1.6), and a positive nondecreasing and slow varying function $h(x)$, $x\geqslant 0$, satisfying the conditions

$$h(0)=1,\quad \sum_{n=1}^{\infty}\frac{1}{n(h(n))^{1/(6+2\delta)}}<\infty,\tag{1.7}$$

and such that

$$\sup_{n\to\infty}\frac{h(n)}{n^{1+\delta}}\mathbf{E}\left|\sum_{j=1}^{n}(\mu_{(j,0)}-C)\right|^{2+\delta}<\infty.\tag{1.8}$$

Recall that a function $h:\mathbb{R}\to\mathbb{R}_+$ is called *slow varying* if, for each $t>0$, $\lim_{x\to\infty}h(tx)/h(x)=1$,

The condition (**b**) looks somewhat cumbersome. Nevertheless it is in fact a mixture condition and seems to be reflecting the general case. This fact is discussed in more details in Sec. V, where we show that the Poisson and generalized Poisson counting measures in $\mathbb{C}$ (see, e.g., Ref. 5, Ch. 10 and Ref. 6, pp. 27–29) having finite moment of order $2+\delta$, measures satisfying ϕ-mixture condition (see definition in Sec. V), as well as measures generated by random independent perturbations of points of a square lattice (see Sec. IV), satisfy this condition.

In Sec. III we prove

Theorem 1.1: *Let Λ_ω be the support of the random measure (1.4) satisfying conditions (1.5)–(1.8). Then the system (1.1) with $\Lambda=\Lambda_\omega$ is complete with probability 1 if $C>1$ and is incomplete with probability 1 if $C<1$.*

Another version of the problem is when the random set Λ_ω is a random perturbation of a lattice in $\mathbb{C}$, i.e., when Λ_ω is of the form

$$\Lambda_\omega=\{\lambda_g(\omega)=ma+ina+\xi_g(\omega);\ g\in\mathbb{Z}^2\},\tag{1.9}$$

where $\{\xi_g; g\in\mathbb{Z}^2\}$ are independent complex-valued centered random variables on a probability space $(\Omega,\mathcal{F},\mathbf{P})$ and $a>0$ is the lattice parameter. Even in the case when all $\{\xi_g; g\in\mathbb{Z}^2\}$ are identically distributed one encounters difficulties when checking condition (**b**) for the corresponding random field (see Theorem 4.1 below). For nonidentically distributed ξ_g's the random point field [i.e., respective measure, defined as in (1.4)] is no longer homogeneous (with respect to the group $\mathbb{Z}^2$). That is why we will consider this case separately.

Theorem 1.2: *Let $\{\xi_g(\omega); g\in\mathbb{Z}\}$ be independent and continuously distributed complex random variables. Assume that $\mathbf{E}\xi_g=0, \forall g\in\mathbb{Z}$ and that for some $\delta>0$*

$$\sup_{g\in\mathbb{Z}^2}\mathbf{E}\,|\xi_g|^{2+\delta}=K<\infty \tag{1.10}$$

[cf. (1.6)]. Then the system (1.1) with $\Lambda=\Lambda_\omega$ and Λ_ω given by (1.9) is complete with probability 1 if $a<1$, and is incomplete with probability 1 if $a>1$.

Remarks: (1) The restriction that all $\xi_g(\omega)$ are continuously distributed may be weakened. We need this condition just to guarantee that with probability 1 the points from Λ_ω are pair-wise different;

(2) this theorem generalizes the well known result for the periodic lattice ($\xi_g=0,\forall g\in\mathbb{Z}^2$), dating back to von Neumann (see Refs. 7 and 8).

As in the classical case (see, e.g., Ref. 9) the completeness theorems for sets of exponential functions can be reduced to constructing and then estimating of entire functions whose zero set is the set of exponents. In the case of the Bargmann–Fock space (1.2) this approach is based on the relation

$$\langle f(\cdot), e^{\pi\bar{\lambda}\cdot}\rangle_{B^2(\mathbb{C})}=f(\lambda), \tag{1.11}$$

valid for each function $f\in B^2(\mathbb{C})$ and $\lambda\in\mathbb{C}$, see, e.g., Ref. 10 (note that unlike[10] we use the inner product (1.2) in which the second factor is complex conjugate). Study of entire functions with randomly located zeros is the main technical content of this article. We believe it has its own intrinsic interest.

Completeness of the exponential system (1.1) in the Bargmann–Fock space $B^2(\mathbb{C})$ defined by (1.2) is equivalent to completeness in $L^2(\mathbb{R})$ of the Gabor system of windowed exponentials

$$\mathcal{G}_\Lambda=\{e_{i\sqrt{2\pi}\lambda}(t);\lambda\in\Lambda\}, \tag{1.12}$$

where, for $\zeta=\mu+i\nu\in\mathbb{C}$

$$e_\zeta(t)=e^{i\mu t-(t-\nu)^2/2},\quad t\in\mathbb{R} \tag{1.13}$$

[see formula (1.17) below]. Since the classic work[7] these systems became a standard tool for time-frequency analysis of nonbandlimited signals. In fact, it was von Neumann who first studied the Gabor systems corresponding to lattices with parameter $a>0$, i.e., to the sets

$$L_a=\{ma+ina;(m,n)\in\mathbb{Z}^2\} \tag{1.14}$$

(see Refs. 7 and 8 for a history survey as well as for various developments and applications). It was proved that such a system is infinitely redundant (overcomplete) in $L^2(\mathbb{R})$ for $a<1$ and is incomplete and has an infinite deficiency if $a>1$. The frame property of $\mathcal{G}_\Lambda$ with Λ given by (1.14) has been considered in Refs. 10–13. The results of Refs. 11 and 13 yield in particular that $\mathcal{G}_{L_a}$ constitute a frame in $L^2(\mathbb{R})$ for all $a<1$. Using the approach from Ref. 1 one can find that the frame property is lost for (generic) random perturbations of the lattice. Below we prove that the completeness–incompleteness property is more robust and survives after random perturbations of the lattice. We refer also to Refs. 14 and 15 where similar question of completeness–incompleteness of (deterministic) exponential systems have been considered.

Systems (1.1) of exponential functions and the Gabor systems (1.12) are connected by the inverse Bargmann transform see, e.g., Ref. 10

$$\mathcal{B}^{-1}: f \mapsto (\mathcal{B}^{-1} f)(t) = -\frac{1}{\pi^{1/4}} \int \int_{\mathbb{C}} f(z) e^{\sqrt{2\pi} t\bar{z} - \pi \bar{z}^2/2 - t^2/2} e^{-\pi |z|^2} dm_z. \tag{1.15}$$

The Bargmann transform itself is defined as

$$\mathcal{B}: \varphi \mapsto (\mathcal{B}\varphi)(z) = \frac{1}{\pi^{1/4}} \int_{\mathbb{R}} \varphi(t) e^{\sqrt{2\pi} tz - \pi z^2/2 - t^2/2} dt. \tag{1.16}$$

It is known (see, e.g., Ref. 10) that $\mathcal{B}^{-1}$ is a unitary mapping between $B^2(\mathbb{C})$ and $L^2(\mathbb{R})$, and for $\lambda = \mu + i\nu \in \mathbb{C}$

$$(\mathcal{B}^{-1} e^{\pi \bar{\lambda} \cdot})(t) = \frac{1}{\pi^{1/4}} e^{i\pi\mu\nu + \pi|\lambda|^2/2} e_{i\sqrt{2\pi}\lambda}(t). \tag{1.17}$$

Relations (1.11), and (1.15)–(1.17) allow one to interpret the previous theorems on the completeness properties of random exponential systems $\mathcal{E}_\omega = \{e^{\pi\lambda z}; \lambda \in \Lambda_\omega\}$, as those on the completeness of random Gabor systems $\mathcal{G}_\omega = \{e_{i\sqrt{2\pi}\lambda}; \lambda \in \Lambda_\omega\}$. Indeed, relation (1.11) identifies the functions $f \in B^2(\mathbb{C})$ annihilating $\mathcal{E}_\omega$ as just the functions vanishing on Λ_ω, while $\mathcal{B}^{-1}$ of (1.15) transforms statements about completeness–incompleteness of $\mathcal{E}_\omega$ into those about $\mathcal{G}_\omega$.

Let $C^\sharp$ denote the density C of the random measure (1.4) or the inverse a^{-2} of the area a^2 of the elementary square of the lattice (1.14). Then we can reformulate our results above as follows.

Theorem 1.3: *Under assumptions of Theorems 1.1 and 1.2 the random Gabor system* $\mathcal{G}_\omega$ *given by (1.12) with* Λ_ω *from (1.3) or from (1.9) is complete with probability 1 in* $L^2(\mathbb{R})$ *if* $C^\sharp > 1$ *and is incomplete if* $C^\sharp < 1$.

Another motivation (application) of the problem studied in this paper is related to the spectral analysis of the Schrödinger operator H with a constant magnetic field and with a random potential V, and to respective branches of the solid-state theory. This operator acts in $L^2(\mathbb{R}^2)$ and one of important problems is to find criteria for the presence of jumps of the integrated density of states (IDS) of the operator at energies equal the Landau levels. The Landau levels comprise the spectrum of the Landau Hamiltonian H_0, the Schrödinger operator with a constant magnetic field and zero potential. The levels are of the form $E_n = n + 1/2$, $n = 0, 1, \ldots$ and all have infinite multiplicity. The IDS of the Landau Hamiltonian is the piece-wise constant function having equal jumps at all E_n. Presence of jumps of the IDS of the Schrödinger operator $H = H_0 + V$ with a constant magnetic field and an electric field given by the potential V depends on the nature of the electric field and on its relative strength with respect to the magnetic field (see Ref. 6 for a general definition of the IDS of random differential operators and Refs. 16–20 for this property of the IDS and its use in solid state theory and in spectral theory).

In the case when the magnetic field is strong enough it is widely accepted that one can replace the Schrödinger operator H acting in $L^2(\mathbb{R}^2)$ by its projection on the eigenspace of the Landau level, that is most close to the energy interval considered. In the case when it is the lowest Landau level E_0 the corresponding eigenfunctions are

$$\psi_m(w) = (2^{m+1}\pi m!)^{-1/2} w^m \exp\{-|w|^2/4\}, \quad m = 0,1,\ldots, w \in \mathbb{C},$$

(see, e.g., Ref. 16), and the orthogonal projection P_0 onto the respective eigenspace $\mathcal{L}_0$ is an integral operator with the kernel

$$P_0(w,\zeta) = (2\pi)^{-1} \exp\{-|w|^2/4 - |\zeta|^2/4 + w\bar{\zeta}/2\}. \tag{1.18}$$

As a result the projection of H onto $\mathcal{L}_0$ has the form $P_0 H P_0 = E_0 P_0 + K$, where the operator K is defined by the kernel

$$K(w_1,w_2)=\int_{\mathbb{R}^2} P_0(w_1,x+iy)V(x,y)P_0(x+iy,w_2)dxdy. \tag{1.19}$$

In the case where V is the sum of contributions of the single site impurity potentials of zero radius, whose positions are $z_j=x_j+y_j, j=1, 2, \ldots$ the operator K becomes

$$K(w_1,w_2)=\sum_{j\geqslant 1} P_0(w_1,z_j)\overline{P_0(w_2,z_j)}. \tag{1.20}$$

Thus, the range of the nontrivial part of the projection P_0HP_0 is the span in $B^2(\mathbb{C})$ of the exponential system indexed by the set $\{z_j\}_{j\geqslant 1}$, and after changing the scale in $\mathbb{C}$ we obtain the system (1.1), where Λ is the set of the coordinates of impurities in this scale. We conclude that in this case the jump in the IDS is present if the system (1.1) is strongly incomplete. More precisely, for Λ_ω given by (1.3) or (1.9) denote

$$\Lambda_\omega(t)=\{\lambda\in\Lambda_\omega;\ |\lambda|<t\},\quad \mathcal{E}_{\omega,t}=\{\exp\{\pi\lambda z\};\ \lambda\in\Lambda_\omega(t)\},\quad X_{\omega,t}=\operatorname{Span}\mathcal{E}_{\omega,t}. \tag{1.21}$$

Set $\nu(t,\omega)=\#\Lambda_\omega(t)$. Then for almost all $\omega\,\nu(t,\omega)<\infty$ for any $t>0$, the system $\mathcal{E}_{\omega,t}$ consists of linearly independent functions, and $\dim X_{\omega,t}=\nu(t,\omega)$. Denote by $P_{\omega,t}$ the orthogonal projection onto $X_{\omega,t}$. Then $\operatorname{Tr}P_{\omega,t}=\dim X_{\omega,t}=\nu(t,\omega)$ and by ergodic theorem

$$\lim_{t\to\infty}\frac{1}{\pi t^2}\operatorname{Tr}P_{\omega,t}=\lim_{t\to\infty}\frac{\nu(t,\omega)}{\pi t^2}=C^\sharp, \tag{1.22}$$

where $C^\sharp=C$ in the case of (1.3) and $C^\sharp=a^{-2}$ in the case of (1.9).

According to Ref. 6 the quantity

$$1-\lim_{t\to\infty}\frac{1}{\pi t^2}\operatorname{Tr}P_{\omega,t},$$

can be interpreted as the jump of the IDS of the projection P_0HP_0 of the Schrödinger operator on the lowest Landau level, i.e., the relative number (per unit area) of those states of the Landau level that are not affected by the random potential. Then the right-hand side of (1.22) tells us that the jump is equal to $1-C^\sharp$, if $C^\sharp<1$. This conclusion is in agreement with the exactly solvable case of the Poisson random measure (1.4)[21] (see also Ref. 18). It was found that in this case the jump is equal to $(1-C)_+$, where $x_+=\max\{x,0\}$. An analogous spectral phenomenon has been known for the long time in the random matrix theory.[22] All these phenomena have the same geometric origin: Nonzero ''relative'' dimension of the null space of respective operator because of homogeneity of the distribution of random points.

All formulas above are written in the dimensionless units. Let us pass for a moment to the dimension-ful units. Then the set Λ_ω induces the length scale L which equals either the reciprocal square root of the (dimension-ful) concentration of points of (1.3) or the lattice parameter a of (1.9). Denote B the magnetic field and $\Phi=BL^2$ the magnetic flux through a piece of the plane of linear size L. Then our criterion implies that the macroscopic number of states of the lowest Landau level unaffected by impurities exists if $\Phi/\Phi_0>1$, where $\Phi_0=hc/e$ is the flux quantum.

For the relation of these questions to the interpretation of the integer Hall effect, see Ref. 16. A similar results for nonrandom sets Λ that are certain perturbations of the periodic lattice were obtained in Ref. 23.

It can be seen from the proof of Theorems 1.1 and 1.2 as well as from arguments of papers[18,23] that the mathematical mechanism of existence of a finite fraction of the Landau states unaffected by the point impurities located at points of a set Λ is that these eigenfunctions have zeros at all points of this set. A similar but simpler phenomenon is known in the case of the one-dimensional Schrödinger operator with the point scatterers (see, e.g., Ref. 20, Sec. 10.3). Since, however, in

this case the spectrum is of multiplicity 1, the only effect that this mechanism produces is coincidence of the asymptotic form of the IDS and of the Lyapunov exponent at the band edges with those of the periodic potential (in particular, the absence of the Lifshitz tails). On the other hand, in the two-dimensional case, according to arguments of Ref. 23, the fraction of states unaffected by the potential consists of delocalized states.

The quantity $C^\sharp$ can be viewed as the relative (per unit area) dimension of the system $\mathcal{E}_\omega$ given by (1.1) with $\Lambda=\Lambda_\omega$ and Λ_ω from (1.3) or from (1.9) or of $\mathcal{G}_\omega$ given by (1.12) with the same Λ_ω. This interpretation allows us to view $|1-C^\sharp|$ as a quantitative characteristic of incompleteness (the relative defect) of systems $\mathcal{E}_\omega$ and $\mathcal{G}_\omega$ in the case when $C^\sharp<1$ and of overcompleteness (the relative redundancy) in the case when $C^\sharp>1$. Indeed, if $\mathcal{E}_\omega$ (or $\mathcal{G}_\omega$) is complete and $C^\sharp>1$, then for any $C_1^\sharp$ such that $1<C_1^\sharp<C^\sharp$ the respective $\mathcal{E}_\omega$ (or $\mathcal{G}_\omega$) is also complete (overcomplete). An analogous statement is valid for $C^\sharp<1$. Thus $C^\sharp$ is also a quantitative characteristic of stability of completeness (overcompleteness) and incompleteness of the random system $\mathcal{E}_\omega$ (or $\mathcal{G}_\omega$), in agreement with the respective results for the case (1.14).[8]

The article is organized as follows. Section II contains some preliminary facts from the probability theory and the function theory. In Sec. III we prove Theorem 1.1 by considering separately the cases when the density of the random field is above and below the threshold $C=1$. In Sec. IV we consider the case (1.9) when the random field is generated by random perturbations of a lattice. In the last Sec. V we discuss various mixing conditions for random fields and compare them with restrictions imposed in this article.

II. AUXILIARY FACTS

In what follows we need to estimate the number of points from Λ_ω of (1.3) in special domains in $\mathbb{C}$. Denote

$$S(t;\theta_1,\theta_2)=\{z;\,|z|<t,\ \theta_1\leqslant\arg z<\theta_2\},\quad (t>0,\,0\leqslant\theta_1<\theta_2\leqslant 2\pi)$$

and

$$N(t;\theta_1,\theta_2)=\#\{Q_g\subset S(t;\theta_1,\theta_2)\}.$$

We have evidently

$$N(t;\theta_1,\theta_2)=\tfrac{1}{2}(\theta_2-\theta_1)t^2+O(t),\quad t\to\infty. \tag{2.1}$$

Given a discrete set $\Lambda\subset\mathbb{C}$ we denote

$$\nu(t,\theta_1,\theta_2;\Lambda)=\#\{\Lambda\cap S(t;\theta_1,\theta_2)\}$$

and

$$\tilde{\nu}(t,\theta_1,\theta_2;\Lambda)=\#\{\Lambda\cap(\cup_{Q_g\subset S(t;\theta_1,\theta_2)}Q_g)\}.$$

Lemma 2.1: Let (1.5)–(1.8) be fulfilled. Then, for each pair (θ_1,θ_2), $0\leqslant\theta_1<\theta_2\leqslant 2\pi$, *we have with probability 1*

$$\lim_{t\to\infty}\frac{1}{N(t;\theta_1,\theta_2)}\tilde{\nu}(t,\theta_1,\theta_2;\Lambda_\omega)=C. \tag{2.2}$$

Proof: It suffices to prove (2.2) only for $t=k$, $k\in\mathbb{N}$. Denote

$$X_k=\tilde{\nu}(k,\theta_1,\theta_2;\Lambda_\omega)/N(k;\theta_1,\theta_2).$$

Consider the random variables

$$Y_m(\omega)=\mu(S(k;\theta_1,\theta_2)\cap\cup_{l\in\mathbb{Z}}Q_{(l,m)},\omega),\quad m\in\mathbb{Z}.$$

We have

$$\tilde{\nu}(k,\theta_1,\theta_2;\Lambda_\omega)=\sum_{m=-k}^{k}Y_m,$$

Since $h(k)$ is a slowly varying function, $f(k):=k^{1+\delta}/h(k)$ is a nondecreasing function for $k\geqslant k_0$, for some $k_0>0$. Conditions (1.5)–(1.8) now yield

$$\mathbf{E}\,|Y_m-\mathbf{E}\,Y_m|^{2+\delta}\leqslant \text{const}\,k^{1+\delta}/h(k),\quad |m|\leqslant k, \tag{2.3}$$

where const does not depend on k. Therefore, for any $\varepsilon>0$

$$\sum_{k=1}^{\infty}\mathbf{P}\,(|X_k-C|>\varepsilon)<\infty. \tag{2.4}$$

Indeed, combining the Chebyshev and Minkowski inequalities (see, e.g., Ref. 24, pp. 190 and 192) with (2.3) we obtain

$$\begin{aligned}(\mathbf{P}(|X_k-C|>\varepsilon))^{1/(2+\delta)}&\leqslant\frac{\text{const}}{\varepsilon k^2}\left(\mathbf{E}\left|\sum_{m=-k}^{k}(Y_m-\mathbf{E}\,Y_m)\right|^{2+\delta}\right)^{1/(2+\delta)}\\&\leqslant\frac{\text{const}}{\varepsilon k^2}\sum_{m=-k}^{k}(\mathbf{E}\,|Y_m-\mathbf{E}\,Y_m|^{2+\delta})^{1/(2+\delta)}\\&\leqslant\frac{\text{const}}{\varepsilon k}\left(\frac{k^{1+\delta}}{h(k)}\right)^{1/(2+\delta)},\end{aligned}$$

so that

$$\mathbf{P}\,(|X_k-C|>\varepsilon)\leqslant\frac{\text{const}}{\varepsilon^{2+\delta}kh(k)},\quad k\in\mathbb{N}.$$

Now (2.4) follows from (1.7) and by the Borel-Cantelli lemma (see, e.g., Ref. 24, p. 254) we obtain that with probability 1 $X_k\to C$ as $k\to\infty$. ■

Remark: In the general case of an ergodic point field the lemma follows directly from the respective ergodic theorem (see, e.g., Ref. 25, Corollary 6.4.2). We give above a proof based on conditions (1.6)–(1.8), because in this case we need not to assume ergodicity.

We also need the following statements from the complex analysis. For $t>0$ we denote $\mathbb{D}_t=\{z\in\mathbb{C};|z|\leqslant t\}$.

Proposition 2.2: (Jensen formula, see, e.g., Ref. 9, p. 14) Let $R_0>0$ and let the function $f(z)$ be holomorphic in $\mathbb{D}_{R_0}$ with $f(0)\neq 0$. Then, for any $R<R_0$, we have

$$\int_0^R\frac{\nu_f(t)}{t}dt=\frac{1}{2\pi}\int_0^{2\pi}\log|f(\mathrm{Re}^{i\theta})|\,d\theta-\log|f(0)|, \tag{2.5}$$

where $\nu_f(t)$ is the number of zeros of $f(z)$ in $\mathbb{D}_t$.

This assertion is used in order to compare the growth of the entire function, whose zero set coincides with the set Λ_ω.

In order to study entire functions with a given zero set we need additional notation. Given a discrete set $\Lambda\subset\mathbb{C}$ we consider its counting functions for disks and sectors:

$$\nu(t)=\#\{\lambda\in\Lambda;\,|\lambda|<t\},\quad \nu(t,\theta,\vartheta)=\#\{\lambda\in\Lambda;\,|\lambda|<t,\,\theta<\arg\lambda<\vartheta\},\tag{2.6}$$

where $t>0$ and $0\leqslant\theta<\vartheta<2\pi$.

Proposition 2.3: Let C be a positive constant and Λ be a point set in $\mathbb{C}$. Assume that for each pair (θ,ϑ), $0\leqslant\theta<\vartheta<2\pi$, there exist the limits

$$\lim_{t\to\infty}\frac{\nu(t,\theta,\vartheta)}{t^2}=C\frac{\vartheta-\theta}{2},\tag{2.7}$$

and

$$\lim_{t\to\infty}\sum_{\lambda\in\Lambda\cap\mathbb{D}_t}\frac{1}{\lambda^2}=:\tau_\Lambda\exp\{i\theta_\Lambda\},\quad \tau_\Lambda>0,\ \theta_\Lambda\in(0,2\pi).\tag{2.8}$$

Then the infinite product

$$f(z)=\prod_{\lambda\in\Lambda}(1-z/\lambda)\exp\{z/\lambda+z^2/2\lambda^2\}$$

converges uniformly on each compact set in $\mathbb{C}$ and

$$r^{-2}\log|f(re^{i\theta})|=\frac{\pi}{2}C+\tau_\Lambda\cos 2(\theta-\theta_\Lambda)+\mathrm{O}(1),\quad r\to\infty$$

for all $z=r\exp\{i\theta\}$ outside of a union of disks of radius ε centered at the points $\lambda\in\Lambda$.

This assertion is a special case of Theorem 2,[9] Ch. 2 for $\rho\equiv 2$ and constant angular density. Existence of the limit (2.8) is a manifestation of a certain isotropy in the distribution of zeros of the entire function f.

III. PROOF OF THEOREM 1.1

We first consider the case when the density is above the threshold $C=1$.

Theorem 3.1: *Assume that conditions of Theorem 1.1 are fulfilled and $C>1$. Then the system $\mathcal{E}_\omega$ defined by (1.1) with $\Lambda=\Lambda_\omega$ is complete in $B^2(\mathbb{C})$ with probability 1.*

Proof: Let Ω' be the set of those Λ_ω for which the limiting relation (2.2) is valid. According to Lemma 2.1 $P(\Omega')=1$. We will prove that the system $\mathcal{E}_\omega$ is complete for all $\omega\in\Omega'$. Assume that the opposite is true. Then, according to (1.11) there exists a nonzero function $g\in B^2(\mathbb{C})$, having Λ_ω as its zero set. Since $f(z)=\overline{g(\overline{z})}\in B^2(\mathbb{C})$ if and only if $g\in B^2(\mathbb{C})$, here and below we ignore transition to conjugate exponents $\overline{\lambda}$, $\lambda\in\Lambda_\omega$.

Assume for simplicity that $0\notin\Lambda_\omega$. Denote $\nu(\tau;\omega)=\nu(0,2\pi,\tau;\omega)$. The Jensen formula (2.5) yields

$$\int_0^t\frac{\nu(\tau,\omega)}{\tau}\,d\tau=\frac{1}{2\pi}\int_0^{2\pi}\log|f(te^{i\theta},\omega)|\,d\theta+\mathrm{O}(1),\quad t\to\infty.\tag{3.1}$$

Combining (2.1) and (2.2) we see that with probability 1

$$\liminf_{t\to\infty}\frac{1}{t^2}\int_0^t\frac{\nu(\tau,\omega)}{\tau}\,d\tau\geqslant C'\pi/2$$

for some $C'>1$. On the other hand the Cauchy inequality yields that, for each $\varepsilon>0$

$$f(z,\omega)\in B^2(\mathbb{C})\Rightarrow|f(z,\omega)|\leqslant\mathrm{const}\exp\{(\pi+\varepsilon)|z|^2/2\},\quad z\in\mathbb{C}.$$

Therefore

$$\limsup_{t\to\infty}\frac{1}{2\pi t^2}\int_0^{2\pi}\log|f(te^{i\theta},\omega)|\,d\theta\leqslant(\pi+\varepsilon)/2 \quad \text{for} \quad \omega\in\Omega'.$$

Fix ε such that $\pi C'>\pi+\varepsilon$. Dividing the both sides of (3.1) by t^2 and passing to the limit as $t\to\infty$, we get a contradiction. ■

Now the case of density below the threshold.

Theorem 3.2: *Assume that the conditions of Theorem 1.1 are fulfilled and $C<1$. Then the system $\mathcal{E}_\omega$ defined by* (1.1) *with $\Lambda=\Lambda_\omega$ is incomplete in $B^2(\mathbb{C})$ with probability 1.*

Proof: We need to construct, for almost all $\omega\in\Omega$, a nonzero function $f_\omega\in B^2(\mathbb{C})$ vanishing on Λ_ω. The construction consists of several steps.

First we will check that the hypothesis of Proposition 2.3 is fulfilled. Indeed, by Lemma 2.1 we have, with probability 1

$$\exists\lim_{t\to\infty}\frac{1}{t^2}\mu(S(t;\theta_1,\theta_2),\omega)=C\frac{\theta_2-\theta_1}{2},$$

for any $0\leqslant\theta_1<\theta_2\leqslant2\pi$. Take a sequence $\{\theta_j\}$ which is dense in $[0,2\pi]$. Then, for almost all $\omega\in\Omega$

$$\exists\lim_{t\to\infty}\frac{\nu(t,\theta_l,\theta_j;\Lambda_\omega)}{t^2}=C\frac{\theta_j-\theta_l}{2} \quad \text{for} \quad \theta_l<\theta_j,$$

which implies that, for almost all $\omega\in\Omega$, the similar relation

$$\exists\lim_{t\to\infty}\frac{\nu(t,\vartheta,\vartheta';\Lambda_\omega)}{t^2}=C\frac{\vartheta'-\vartheta}{2}, \tag{3.2}$$

holds for arbitrary $\vartheta,\vartheta'\in[0,2\pi]$, $\vartheta'>\vartheta$. Indeed,

$$\limsup_{t\to\infty}\frac{\nu(t,\vartheta,\vartheta';\Lambda_\omega)}{t^2}\leqslant\inf_{\theta_l<\vartheta,\ \vartheta'<\theta_j}\lim_{t\to\infty}\frac{\nu(t,\theta_l,\theta_j;\Lambda_\omega)}{t^2}=C\frac{\vartheta'-\vartheta}{2}$$

and

$$\liminf_{t\to\infty}\frac{\nu(t,\vartheta,\vartheta';\Lambda_\omega)}{t^2}\geqslant\sup_{\vartheta<\theta_l,\ \theta_j<\vartheta'}\lim_{t\to\infty}\frac{\nu(t,\theta_l,\theta_j;\Lambda_\omega)}{t^2}=C\frac{\vartheta'-\vartheta}{2}$$

which yields (2.7).

Now denote $\hat{\mathbb{D}}_t=\cup_{Q_g\subset\mathbb{D}_t}Q_g$. We need the following:

Lemma 3.3: Under the conditions of Theorem 1.1 the limit

$$\delta_\omega=\lim_{t\to\infty}\sum_{\lambda\in\Lambda_\omega\cap\hat{\mathbb{D}}_t}\frac{1}{\lambda^2}, \tag{3.3}$$

exists with probability 1.

We mention that relation (3.3) is slightly different from the corresponding statement (2.8) in the hypothesis of Proposition 2.3, in which all points in the disk $\mathbb{D}_t$ (not only those in $\hat{\mathbb{D}}_t$) are taken into account. It is readily seen that the transition from $\mathbb{D}_t$ to $\hat{\mathbb{D}}_t$ does not alter the statement of Proposition 2.3.

Suppose this lemma be already proved. Then, by Proposition 2.3, the product

$$\Pi_\omega(z)=\prod_{\lambda\in\Lambda_\omega}(1-z/\lambda)\exp\left\{\frac{z}{\lambda}+\frac{z^2}{2\lambda^2}\right\},$$

is compact-wise convergent and, for any $\varepsilon>0$, the function

$$f_\omega(z)=\exp\{-\delta_\omega z^2\}\Pi_\omega(z),$$

satisfies with probability 1

$$|f_\omega(z)|\leqslant\exp\left\{\left(\frac{\pi}{2}C+\varepsilon\right)|z|^2\right\}.$$

for sufficiently large $|z|$. Hence, for almost all $\omega\in\Omega$, f_ω belongs to $B^2(\mathbb{C})$.

Clearly $f_\omega(\lambda)=0$ for $\lambda\in\Lambda_\omega$ so that we obtain at least one such function. This proves Theorem 3.2.

Proof of Lemma 3.3: We need an auxiliary fact. For each $n\in\mathbb{Z}$, set

$$h_1(|n|)=(h(|n|))^{1/(6+2\delta)}\quad\text{and}\quad N_n=[|n|/h_1(|n|)]. \tag{3.4}$$

Consider rectangular strips of two kinds:

$$H_{m,s}=\bigcup_{(m-1)N_s\leqslant l<mN_s}Q_{l,s}\quad\text{and}\quad V_{m,s}=\bigcup_{(m-1)N_s\leqslant l<mN_s}Q_{s,l},\quad m,s\in\mathbb{Z}. \tag{3.5}$$

We need those $H_{m,s}$ and $V_{m,s}$ that belong to the sectors

$$D_1:=\{z;\pi/4\leqslant\arg z\leqslant 3\pi/4\}\cup\{z;5\pi/4\leqslant\arg z\leqslant 7\pi/4\} \tag{3.6}$$

and

$$D_2:=\{z;-\pi/4\leqslant\arg z\leqslant\pi/4\}\cup\{z;3\pi/4\leqslant\arg z\leqslant 5\pi/4\}, \tag{3.7}$$

respectively.

The estimate below follows from (1.8).

$$\mathbf{E}\left|\sum_{l=0}^{N_s-1}(\mu_{(l,0)}(\omega)-C)\right|^{2+\delta}\leqslant\text{const}\,(|s|+1)^{1+\delta}/h(|s|),\quad s\in\mathbb{Z}. \tag{3.8}$$

Indeed, for $|s|\geqslant s_0>0$

$$\left(\mathbf{E}\left|\sum_{l=0}^{N_s-1}(\mu_{(l,0)}(\omega)-C)\right|^{2+\delta}\right)^{1/(2+\delta)}\leqslant\left(\mathbf{E}\left|\sum_{l=0}^{|s|}(\mu_{(l,0)}(\omega)-C)\right|^{2+\delta}\right)^{1/(2+\delta)}$$
$$+\left(\mathbf{E}\left|\sum_{l=N_s}^{|s|}(\mu_{(l,0)}(\omega)-C)\right|^{2+\delta}\right)^{1/(2+\delta)}:=\Sigma_1+\Sigma_2.$$

According to (1.8) we have $\Sigma_1\leqslant\text{const}(|s|^{1+\delta}/h(|s|))^{1/(2+\delta)}$. In addition, taking into account that $h(n)$ is a slowly varying function we obtain

$$\Sigma_2=\left(\mathbf{E}\left|\sum_{l=0}^{|s|-N_s}(\mu_{(l,0)}(\omega)-C)\right|^{2+\delta}\right)^{1/(2+\delta)}\leqslant\text{const}\left(\frac{|s|^{1+\delta}}{h(|s|-N_s)}\right)^{1/(2+\delta)}\leqslant\text{const}\left(\frac{|s|^{1+\delta}}{h(|s|)}\right)^{1/(2+\delta)}.$$

We deduce (3.8) from the two last estimates.

For each $m,s\in\mathbb{Z}$ the left-hand side of (3.8) coincides with

$$\mathbf{E}\,|\mu(H_{m,s},\omega)-CN_s|^{2+\delta}. \tag{3.9}$$

The corresponding random variables $\mu(H_{m,s},\omega)$ and $\mu(V_{m,s},\omega)$ satisfy the inequality given by the following:

Lemma 3.4: For all but maybe a finite number of sets $H_{m,s}\subseteq D_1$ defined by (3.5)–(3.7) the inequality

$$|\mu(H_{m,s},\omega)-CN_s|\leqslant(|s|+1)/h_1^2(|s|),$$

holds with probability 1. A similar relation holds for $\mu(V_{m,s},\omega)$, where $V_{m,s}\subseteq D_2$ is defined in (3.5)–(3.7).

Proof: Let $B_{m,s}=\{\omega;|\mu(H_{m,s},\omega)-CN_s|>(|s|+1)/h_1^2(|s|)\}$. The Chebyshev inequality yields

$$\mathbf{P}\,(B_{m,s})\leqslant\frac{h_1^{4+2\delta}(|s|)}{(|s|+1)^{2+\delta}}\mathbf{E}\,|\mu(H_{m,s},\omega)-\mathbf{E}\,\mu(H_{m,s},\omega)|^{2+\delta}. \tag{3.10}$$

Applying (3.8) to the right-hand side of this inequality we obtain

$$\mathbf{P}\,(B_{m,s})\leqslant\text{const}\frac{h_1(|s|)^{4+2\delta}}{(|s|+1)h(|s|)},\quad B_{m,s}\subseteq D_1. \tag{3.11}$$

Since, for each fixed s, the number of the rectangles $H_{m,s}$ under consideration does not exceed $2h_1(|s|)$, we obtain, using (3.11) and (1.7)

$$\sum_{B_{m,s}\subseteq D_1}\mathbf{P}\,(B_{m,s})\leqslant\sum_{s=-\infty}^{\infty}\sum_{|m|\leqslant 2h_1(|s|)}\mathbf{P}\,(B_{m,s})\leqslant\sum_{s=-\infty}^{\infty}\frac{\text{const}}{(|s|+1)(h(|s|))^{1/(6+2\delta)}}<\infty. \tag{3.12}$$

Now the Borel–Cantelli lemma applied to the events $B_{m,s}$ yields the statement of Lemma 3.4 for the random variables $\mu(H_{m,s},\omega)$. The random variables $\mu(V_{m,s},\omega)$ are considered in a similar way. ∎

Now we continue the proof of Lemma 3.3. Denote $K_n=\{z;-n\leqslant\Re z<n,-n\leqslant\Im z<n\}$, $n\in\mathbb{N}$, the square of side length n centered in the origin and let $K_{n(t)}$ be the biggest such square in $\mathbb{D}_t$. Lemma 3.3 follows from the two statements:

(i) For almost all $\omega\in\Omega$ there exists the limit

$$\lim_{t\to\infty}\sum_{\lambda\in\Lambda_\omega\cap K_{n(t)}}\frac{1}{\lambda^2}, \tag{3.13}$$

(ii)

$$\lim_{t\to\infty}\sum_{\lambda\in\Lambda_\omega\cap(\mathbb{D}_t\setminus K_{n(t)})}\frac{1}{\lambda^2}=0. \tag{3.14}$$

In order to prove (3.13) it suffices to pick up a sequence $b_s\geqslant 0$ so that

$$\sum_{s=1}^{\infty}b_s<\infty\quad\text{and, for almost all }\omega\in\Omega,\quad\left|\sum_{\lambda\in\Lambda_\omega\cap(K_{s+1}\setminus K_s)}\frac{1}{\lambda^2}\right|\leqslant b_s. \tag{3.15}$$

Let $H_{m,s}$, $V_{m,s}\subset K_{s+1}\setminus K_s$ and $N(H_{m,s}),N(V_{m,s})$ be the numbers of points from Λ_ω in $H_{m,s},V_{m,s}$ respectively. Let, for definiteness, $N(H_{m,s})\leqslant N(V_{m,s})$. Split the set $\Lambda_\omega\cap V_{m,s}$ into two parts $\Lambda_\omega\cap V_{m,s}=\Lambda_\omega^{(1)}(V_{m,s})\cup\Lambda_\omega^{(2)}(V_{m,s})$ so that $\#\Lambda_\omega^{(1)}(V_{m,s})=N(H_{m,s})$ and $\Lambda_\omega^{(1)}(V_{m,s})\cap\Lambda_\omega^{(2)}(V_{m,s})=\varnothing$.

We estimate the sum

$$\sigma_{m,s,\omega}=\sum_{\lambda\in\Lambda_\omega\cap(H_{m,s}\cup V_{m,s})}\frac{1}{\lambda^2}=\left(\sum_{\lambda\in\Lambda_\omega\cap(H_{m,s}\cup\Lambda_\omega^{(1)}(V_{m,s}))}+\sum_{\lambda\in\Lambda_\omega^{(2)}(V_{m,s})}\right)\frac{1}{\lambda^2}:=\sigma_{m,s,\omega}^{(1)}+\sigma_{m,s,\omega}^{(2)}.$$

If $\lambda_1\in H_{m,s}$ and $\lambda_2\in V_{m,s}$, then

$$\left(\frac{1}{\lambda_1^2}+\frac{1}{\lambda_2^2}\right)\leqslant\frac{A}{(|s|+1)^2h_1(|s|)},\tag{3.16}$$

where A depends on h only. Therefore

$$|\sigma_{m,s,\omega}^{(1)}|\leqslant\frac{AN(H_{m,s})}{(|s|+1)^2h_1(|s|)}.\tag{3.17}$$

By Lemma 3.4 we have for almost all $\omega\in\Omega$

$$N(H_{m,s})\leqslant CN_s+(|s|+1)/h_1^2(|s|)\leqslant(C+1)(|s|+1)/h_1(|s|)\tag{3.18}$$

and

$$|\sigma_{m,s,\omega}^{(1)}|\leqslant A(C+1)/((|s|+1)h_1^2(|s|)).\tag{3.19}$$

Applying Lemma 3.4 once again we obtain that the number of summands in $\sigma_{m,s,\omega}^{(2)}$ does not exceed $2(|s|+1)/h_1^2(|s|)$. Therefore

$$|\sigma_{m,s,\omega}^{(2)}|\leqslant\sum_{\lambda\in\Lambda_\omega^{(2)}(V_{m,s})}\frac{1}{|\lambda|^2}\leqslant 8/((|s|+1)h_1^2(|s|)).\tag{3.20}$$

Consider the sum $\Sigma_{m,s}\sigma_{m,s,\omega}$, where the summation is taken over all (m,s) satisfying $H_{m,s}\subset K_{s+1}\backslash K_s$. Inequalities (3.19) and (3.20) yield

$$\left|\sum_{m,s}\sigma_{m,s,\omega}\right|\leqslant 4h_1(|s|)\left(\frac{A(C+1)}{(|s|+1)h_1^2(|s|)}+\frac{8}{(|s|+1)h_1^2(|s|)}\right)=\frac{4A(C+1)+32}{(|s|+1)h_1(|s|)}\tag{3.21}$$

for almost all $\omega\in\Omega$. It remains to remark that the domain $K_{s+1}\backslash K_s$ is covered by the strips $H_{m,s}$ and $V_{m,s}$ up to for ''angles'' whose contribution may be estimated in a similar way.

Now (3.15) holds with

$$b_s=(4A(C+1)+32)((|s|+1)h_1(|s|))^{-1},$$

which, in turn, yields (3.13). The proof of (3.14) is similar, and we omit it. Lemma 3.3 is proved.

IV. RANDOM PERTURBATIONS OF A LATTICE

In this section we consider the case when the random set of points is generated by independent random perturbation of a periodic lattice, i.e., we prove Theorem 1.2. We will follow the same strategy as in the proof of Theorem 1.1. In addition in this section we do not demand random perturbations to be identically distributed.

Proof of Theorem 1.2: Denote $z_g=ma+ina$, $g=(m,n)\in\mathbb{Z}^2$, take $\alpha=1-\delta/(3+\delta)$, and consider the truncated random variables

$$\xi_g^*=\begin{cases}\xi_g, & \text{if} \quad |\xi_g|\leqslant|z_g|^\alpha\\ 0, & \text{if} \quad |\xi_g|>|z_g|^\alpha.\end{cases}$$

The Chebyshev inequality yields

$$\mathbf{P}(|\xi_g|>|z_g|^{\alpha})\leqslant \frac{\mathbf{E}\,|\xi_g|^{2+\delta}}{|z_g|^{2+\delta/(3+\delta)}},$$

whence, by (1.10)

$$\sum_{g\in\mathbb{Z}^2}\mathbf{P}(|\xi_g|>|z_g|^{\alpha})<\infty. \tag{4.1}$$

Now by the Borel–Cantelli lemma for almost all $\omega\in\Omega$ we have that $\xi_g^*=\xi_g$ for all but maybe a finite number of g's.

Next we have to check the hypothesis of Proposition 2.3 in our setting. That is, that the limits in (3.2) and (3.3) exist with probability 1. Then the function

$$f(z,\omega)=\exp\{-\delta_\omega z^2\}\prod_{\lambda\in\Lambda_\omega}G(z/\lambda;2),$$

belongs to $B^2(\mathbb{C})$. It suffices to check (3.2) and (3.3) for $\lambda_g^*(\omega)=ma+ina+\zeta_g^*$ instead of λ_g. The first of these relations comes from a direct calculation. The second one follows from:

$$\sum_{|\lambda_g^*|<t}\frac{1}{(\lambda_g^*)^2}-\sum_{|z_g|<t-t^a}\frac{1}{z_g^2}=\sum_{|z_g|<t-t^a}\left\{\frac{1}{(\lambda_g^*)^2}-\frac{1}{z_g^2}\right\}+\sum_{|z_g|>t-t^a,\ |\lambda_g^*|<t}\frac{1}{(\lambda_g^*)^2}:=S_1(t)+S_2(t).$$

It is easy to see that with probability 1 $S_2\to 0$ as $t\to\infty$. Besides, $S_1(t)$ approaches with probability 1 a limit as $t\to\infty$. This follows from the fact that the corresponding limit for unperturbed points (clearly) exists and from estimates of the perturbations. The proof of the second part is, in essence, a repetition of the proof of Theorem 1.1. Theorem 1.2 is proved.

We formulate now without proof a statement about a general property of a random field generated by a random perturbations of a lattice. In this statement restrictions on the sequence of random perturbations $\{\xi_g\}$ are more strict than in Theorem 1.2, but even then the proof is rather complicated. We do not know whether it is possible to weaken these restrictions. We formulate this result because (we believe) the study of random perturbations of deterministic sets has its own interest.

Theorem 4.1: *Let $\{\xi_g\,;\,g\in\mathbb{Z}^2\}$ be a sequence of independent, identically, and continuously distributed complex-valued random variables and*

$$\mathbf{E}\,|\xi_g|^{5+\Delta}<\infty,$$

for some $\Delta>0$. Consider the random set of points

$$\Lambda_\omega=\{\lambda=z_g+\xi_g\,;\,g\in\mathbb{Z}^2\}\subset\mathbb{C}, \tag{4.2}$$

here $z_g=ma+ina$ for $g=(m,n)$. Then the corresponding random field $\{\mu_g(\omega),g\in\mathbb{Z}^2\}$, $\mu_g(\omega)=\#\{\Lambda_\omega\cap Q_g\}$ satisfies condition (**b**) *of Section 1 with $\delta=2$ and $h(x)=\exp\{(\log_+x)^{1/2}\}$.*

Recall that $\log_+x:=\max(0,\log x)$.

V. RANDOM FIELDS WITH MIXING CONDITION

In this section we study conditions (**a**), (**b**) on the random field, which were imposed in Secs. I and II. Our goal is to show that in essence these are conditions of mixing and also that, in the most of typical situations, they are satisfied. We use here the notation of Sec. I. Thus, everywhere below we assume that $(\Omega,\mathcal{F},\mathbf{P})$ is a probability space and $\{\mu(\cdot,\omega);\,g\in\mathbb{Z}^2\}$ is defined by the relations

$$\mu_g(\omega)=\mu(Q_g,\omega),\quad g=m+in\in\mathbb{Z}^2,$$

$$Q_g:=\{x+iy;\, x\in[m,m+1),\, m\in[n,n+1)\}.$$

Theorem 5.1: *Let a random field* $\{\mu_g;\, g\in\mathbb{Z}^2\}$ *be homogeneous with respect to translations by integers along the coordinate axis and rotations by* $\pm\pi/2$. *Assume that the* μ_g*'s satisfy (1.6) and are independent. Then condition (***b***) is also valid.*

The theorem is a direct consequence of the following

Proposition 5.2: (Rosental, see e.g., Ref. 26, Ch. 3) Let $X_1,\ldots,X_n$ *be independent random variables with* $\mathbf{E}\,X_k=0, k=1,\ldots,n$ *and* $p>0$. *Denote*

$$M_{n,p}=\sum_{k=1}^{n}\mathbf{E}\,|X_k|^p,\quad B_n=\sum_{k=1}^{n}\mathbf{E}\,X_k^2.$$

Then

$$\mathbf{E}\left|\sum_{k=1}^{n}X_k\right|^p\leqslant C(p)(M_{n,p}+B_n^{p/2}),$$

where $C(p)$ *depends on p only.*

Proof of Theorem 5.1: Condition (**b**) with $h(x)=\exp\{(\log_+x)^{1/2}\}$ follows directly if one applies the proposition to the random variables $X_k=\mu_{(k,0)}-\mathbf{E}\,\mu_{(k,0)}$ and $p=2+\delta$, where δ is given in (1.6). ■

Remark: In particular all the Poisson and generalized the Poisson measures in $\mathbb{C}$ (see, e.g., Ref. 6, pp. 27–29) with a finite moment of order $2+\delta$ satisfy conditions (**a**) and (**b**) of Section I.

Now we compare condition (**b**) with the standard mixture condition. Denote by Σ the σ-algebra generated by all Q_g, $g\in\mathbb{Z}^2$. For each $Q^{(1)},Q^{(2)}\in\Sigma$ we denote by $\mathcal{F}_1,\mathcal{F}_2$ the σ-algebras generated by $\mu(Q^{(1)},\cdot)$ and $\mu(Q^{(2)},\cdot)$, respectively. We say that the random field $\{\mu_g(\omega);\, g\in\mathbb{Z}^2\}$ satisfies the ϕ-mixture condition, if

$$\phi(\tau):=\sup_{\operatorname{dist}(Q^{(1)},Q^{(2)})\geqslant\tau}\{|\mathbf{P}(B/A)-\mathbf{P}(B)|;\, A\in\mathcal{F}_1,B\in\mathcal{F}_2\}\to 0,\quad \text{as}\quad \tau\to\infty,$$

here "dist" denotes the usual Euclidean distance in $\mathbb{C}$.

Theorem 5.3: *Let the random field* $\{\mu_g(\omega);\, g\in\mathbb{Z}^2\}$ *be homogeneous with respect to integer translations along the coordinate axis and rotations by* $\pm\pi/2$. *Assume that the field satisfies condition* (**a**) *the* ϕ*-mixture condition, and also that*

$$\mathbf{Var}\,\mu(\Delta_n)\to\infty\quad \text{as}\quad n\to\infty,$$

for any sequence $\{\Delta_n\}$ *of Borelian sets in* $\mathbb{C}$ *such that* $mes(\Delta_n)\to\infty$. *Then the random field* $\{\mu_g(\omega);\, g\in\mathbb{Z}^2\}$ *satisfies condition* (**b**).

This statement is an immediate consequence of the following facts.

Proposition 5.4: (Ref. 27, Ch. 18) Let a stationary sequence $\{X_k\}$ *satisfy the* ϕ*-mixing condition. Assume that* $\mathbf{E}\,|X_k|^{2+\delta}<\infty$, *for some* $\delta>0$, *and also that* $\mathbf{Var}\,(X_1+\cdots+X_n)\to\infty$ *as* $n\to\infty$. *Then, for some constant* A_1

$$\mathbf{E}\left|\sum_{k=1}^{n}X_k-\sum_{k=1}^{n}\mathbf{E}\,X_k\right|^{2+\delta}\leqslant A_1(\mathbf{Var}(X_1+\cdots+X_n))^{1+\delta/2}. \tag{5.1}$$

Proposition 5.5: (Ref. 27, Ch. 18) Let a stationary sequence $\{X_k\}$ *satisfy the* ϕ*-mixing condition and also* $\lim_{n\to\infty}\mathbf{Var}\,(X_1+\cdots+X_n)\to\infty$ *as* $n\to\infty$. *Then*

$$\mathbf{Var}\,(X_1+\cdots+X_n)=nh(n), \tag{5.2}$$

where $h(n)$ is slowly varying function with respect to the argument $n \in \mathbb{Z}_+$. The function f can be continued to the whole real axis as a slowly varying one.

It can be mentioned that the ϕ-mixing condition for the random field $\{\mu_g(\omega); g \in \mathbb{Z}^2\}$ yields the ϕ-mixing condition for the random variables $\mu_{(1,0)}, \mu_{(2,0)}, \ldots$ and thus deduce condition (**b**) with $h(x) = \exp\{(\log_+ x)^{1/2}\}$ directly from these theorems.

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Discrete approximations to integrals over unparametrized paths

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We discuss measures on spaces of unparametrized paths related to the Wiener measure. These measures arise naturally in the study of one-dimensional gravity coupled to scalar fields. Two kinds of discrete approximations are defined, the piecewise linear and the hypercubic approximations. The convergence of these approximations in the sense of weak convergence of measures is proven. We describe a family of sets of unparametrized paths that are analogous to cylinder sets of parametrized paths. Integrals over some of these sets are evaluated in terms of Dirichlet propagators in bounded regions. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1368367]

I. INTRODUCTION

In quantum field theory and string theory one frequently encounters the problem of integrating over geometrical objects, e.g., Riemannian manifolds or Riemannian manifolds with some additional structure. One wishes to define a measure on sets of geometrical objects and integrate functions that are independent of the coordinates used to describe the objects. The prime example of a theory where this problem arises is the path integral quantization of general relativity where one attempts to give meaning to expressions of the form

$$\langle F\rangle = \int e^{-S(g)} F([g]) D[g],$$

where g is a Riemannian metric on a manifold M, $[g]$ is the equivalence class of g under diffeomorhisms of M,F is a function, and $S(g)$ is a diffeomorphism invariant action functional, e.g., the Einstein–Hilbert action.[1,2] Giving a mathematical meaning to expressions of this form is largely an unsolved problem but some headway has been made, mainly in two dimensions, see Ref. 3 and references therein.

One of the strategies used in physics to deal with functional integrals of this type is to introduce discretizations of the geometrical objects under consideration and try to prove convergence of the discretization as a cutoff parameter, e.g., a lattice spacing, is taken to zero. It inspires confidence in the results obtained when different discretizations lead to identical continuum results. This approach is described in detail in the monograph.[3]

For one-dimensional objects, i.e., when the functional integral is over paths, the situation is radically different from the higher dimensional analogs, since we have measures on parametrized paths in $\mathbb{R}^d$ (e.g., the Wiener measure) that are mathematically well understood and give rise to measures on unparametrized paths as we shall discuss in the following. We study two different discretizations of integrals over unparametrized paths and show that the discrete measures converge to the appropriate continuum measure.

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In ordinary quantum field theory applications of random paths it is often the convergence of regularized propagators that is of main interest and various results in this vein have been known for a long time. Our main interest is the convergence of the underlying measures on unparametrized paths, whereas convergence of propagators merely means convergence of the total volume of the measures. Corresponding problems in nonrelativistic quantum mechanics normally involve only parametrized paths. In this case various aspects of discrete approximations pertaining to the Wiener measure on paths parametrized by a finite time interval have been discussed by many authors, see, e.g., Ref. 4 and references therein. For recent related work on discrete approximations to Wiener measure on Riemannian manifolds we refer to Refs. 5 and 6.

This paper is organized as follows. In Sec. II we introduce the models of discretized random paths we wish to study and give a proof of pointwise convergence of the lattice propagator to the continuum propagator, that will be needed later. In Sec. III we define the appropriate path spaces, the continuum measures and the discretized measures. In Sec. IV we use standard tools of probability theory to prove the convergence of the discretized measures. In Sec. V we determine a family of sets of unparametrized paths that generates the Borel sets of unparametrized paths and plays a role similar to the one played by cylinder sets for the Wiener measure. Finally, in Sec. VI we apply the results of the previous sections to evaluate the measure of some of these sets.

II. PROPAGATORS

Let Δ denote the Laplacian in $\mathbb{R}^d$. It is well known that the Euclidean propagator

$$G(x,y)=2(-\Delta+m^2)^{-1}(x,y) \tag{1}$$

of a scalar particle of mass $m>0$ in $\mathbb{R}^d$ has the path integral representation

$$G(x,y)=\int_{\omega:x\to y} e^{-m|\omega|}D\omega, \tag{2}$$

where ω is a path from x to y in $\mathbb{R}^d$ and $|\omega|$ denotes its length. The most straightforward interpretation of the formal expression on the right-hand side of Eq. (2) is obtained by regarding it as a limit of lattice propagators. We replace $\mathbb{R}^d$ by the hypercubic lattice $a\mathbb{Z}^d$ with lattice spacing a and define a lattice propagator as

$$G^a(x,y)=a^{2-d}\sum_{\omega:x\to y} e^{-m(a)|\omega|} \tag{3}$$

for $x,y\in a\mathbb{Z}^d$ where the sum is over all lattice paths from x to y. The prefactor a^{2-d} is dictated by dimensional considerations and the dependence of the parameter $m(a)$ (lattice mass) on a is determined by the requirement that $G^a(x,y)$ converge to $G(x,y)$ as $a\to 0$.

Using translation invariance we may set $G(x,y)=G(x-y)$ and $G^a(x,y)=G^a(x-y)$. The Fourier transform of the lattice propagator is then

$$\widehat{G^a}(k)=a^d\sum_{x\in a\mathbb{Z}^d} G^a(x)e^{-ik\cdot x}=e^{am(a)}\left(m^2+2a^{-2}\sum_{j=1}^{d}(1-\cos(ak_j))\right)^{-1}, \tag{4}$$

where $k\in[-\pi/a,\pi/a]^d$ and $m(a)$ is given by

$$e^{am(a)}=2d+m^2a^2. \tag{5}$$

Evidently this implies the desired uniform convergence in momentum space

$$d^{-1}\widehat{G^a}(k)\to 2(k^2+m^2)^{-1}=\hat{G}(k) \tag{6}$$

as $a\to 0$, for any $k\in\mathbb{R}^d$.

Pointwise convergence in space–time can be obtained as follows. We extend the lattice propagator from $a\mathbb{Z}^d$ to a smooth function on $\mathbb{R}^d$ by setting

$$G^a(x)=\frac{1}{(2\pi)^d}\int_{[-\pi/a,\pi/a]^d}\widehat{G^a}(k)e^{-ik\cdot x}\,\mathrm{d}k \tag{7}$$

for any $x\in\mathbb{R}^d$. For $\alpha=(\alpha_1,\ldots,\alpha_d)$, where the α_i's are non-negative integers, let

$$\partial^\alpha=\prod_{i=1}^{d}\frac{\partial^{\alpha_i}}{\partial x_i^{\alpha_i}}.$$

Defining $\widehat{G^a}(k)=0$ outside $[-\pi/a,\pi/a]^d$ it is easily verified that

$$\partial^\alpha\widehat{G^a}(k)\to\partial^\alpha\hat{G}(k)$$

uniformly on $\mathbb{R}^d$ for any multi-index α. Moreover, there is a constant c_α such that

$$|\partial^\alpha\widehat{G^a}(k)|\leqslant c_\alpha(k^2+m^2)^{-1-|\alpha|/2}, \tag{8}$$

where $|\alpha|=\alpha_1+\cdots+\alpha_d$. Thus, choosing $|\alpha|>d$, the right-hand side of Eq. (8) is integrable so the dominated convergence theorem together with Fourier inversion implies that

$$d^{-1}x^\alpha G^a(x)\to x^\alpha G(x) \tag{9}$$

as $a\to 0$, where $x^\alpha=x_1^{\alpha_1}\ldots x_d^{\alpha_d}$. In particular,

$$d^{-1}G^a(x)\to G(x) \tag{10}$$

for $x\neq 0$.

There is another path integral representation of the propagator $G(x,y)$ introduced in Ref. 7 whose analog for surfaces has played an important role in string theory in recent years.[8] The alternative representation is given by

$$G(x,y)=\int_{\omega:x\to y}\exp\left(-\frac{1}{2}\int(|\dot{\omega}|^2e^{-1}+m^2e)\mathrm{d}t\right)D\omega De, \tag{11}$$

where the integration is over paths ω in $\mathbb{R}^d$ from x to y and over intrinsic metrics e on the paths. An intrinsic metric on the path is simply a positive definite function defined on the path. In order to give a meaning to Eq. (11), we note an important common feature of the two action functionals

$$S_1(\omega)=m|\omega|=m\int|\dot{\omega}|\mathrm{d}t \tag{12}$$

and

$$S_2(\omega,e)=\frac{1}{2}\int(|\dot{\omega}|^2e^{-1}+m^2e)\mathrm{d}t, \tag{13}$$

which occur in the path integrals (2) and (11). The actions are invariant under reparametrizations

$$t'=\varphi(t),\quad \omega'(t')=\omega(t),\quad e'(t')=\frac{e(t)}{\dot{\varphi}(t)}, \tag{14}$$

where φ is an increasing diffeomorphism between intervals. Thus the path integrations in Eqs. (2) and (11) should be regarded as being taken over diffeomorphism classes of paths in the first case

and over diffeomorphism classes of paths and metrics in the second one. The standard method for dealing with functional integration over such orbit spaces is the so-called Faddeev–Popov procedure. We discuss the orbit spaces and the appropriate measures on them more thoroughly in Sec. III. For the moment we note that any pair (ω,e) can uniquely be reparametrized to (ω',e') such that the parameter interval of the latter is $[0, 1]$ and the metric e' is constant on $[0, 1]$ and equal to the volume

$$T\equiv\int e(t)\mathrm{d}t \tag{15}$$

of e, which is parametrization independent. It follows that the path integral (11) is effectively an integral over T and over paths ω parametrized on $[0, 1]$. An interpretation of (11) is then obtained by subdividing $[0,1]$ into N subintervals of length N^{-1} and letting ω be an N-step piecewise linear path $x=x_0\to x_1\to\cdots\to x_N=y$ for which

$$\int_0^1|\dot\omega|^2\,\mathrm{d}t=\frac{1}{N}\sum_{i=0}^{N-1}\left(\frac{x_{i+1}-x_i}{N^{-1}}\right)^2=N\sum_{i=0}^{N-1}(x_{i+1}-x_i)^2.$$

Setting

$$a^2=\frac{T}{N}$$

we have

$$\begin{aligned}H^a(x,y)&\equiv\frac{a^2}{(2\pi a^2)^{d/2}}\sum_{N=1}^{\infty}\int\prod_{i=1}^{N-1}\frac{dx_i}{(2\pi a^2)^{d/2}}\exp\left(-\frac{1}{2}\sum_{i=0}^{N-1}\frac{|x_{i+1}-x_i|^2}{a^2}-\frac{1}{2}m^2a^2N\right)\\&=a^2\sum_{N=1}^{\infty}(2\pi a^2N)^{-d/2}\exp\left(-\frac{|x-y|^2}{2a^2N}-\frac{1}{2}m^2a^2N\right)\\&\to\int_0^{\infty}(2\pi T)^{-d/2}\exp\left(-\frac{|x-y|^2}{2T}-\frac{1}{2}m^2T\right)dT=G(x,y)\end{aligned}\tag{16}$$

for $x\neq y$, as $a\to0$. Hence, the function $H^a(x,y)$ defined here provides a discrete approximation to $G(x,y)$. In the same way as for the hypercubic lattice approximation we show in Sec. IV that the measures on piecewise linear paths defined by the approximation H^a converge to a continuum path measure which attributes a proper meaning to Eq. (11).

III. THE CONTINUUM MEASURES AND DISCRETE APPROXIMATIONS

As noted in Sec. II the appropriate space to integrate over in Eqs. (2) and (11) consists of equivalence classes of paths under reparametrizations. In this section we define those orbit spaces and the relevant measures.

A. Piecewise linear paths

It is convenient to start with Eq. (11) and for notational and technical simplicity to consider first paths with only one fixed end point x. Let $\Gamma(x)$ be the space consisting of pairs (e,ω) where $e:[0,1]\to\mathbb{R}$ is a positive continuous function and $\omega:[0,1]\to\mathbb{R}^d$ is continuous with $\omega(0)=x$. Let $\mathrm{Diff}_+[0,1]$ denote the set of all increasing diffeomorphisms of the unit interval. As remarked in Sec. II there is a unique $\varphi\in\mathrm{Diff}_+[0,1]$ such that the reparameterized pair (e',ω') defined by Eq. (14) has $e'=T$ where T is a constant. Hence we conclude that

$$\tilde\Gamma(x)\equiv\Gamma(x)/\mathrm{Diff}_+[0,1]=\mathbb{R}_+\times\Omega(x),$$

where $\Omega(x)$ denotes the set of continuous paths $\omega:[0,1]\to\mathbb{R}^d$ with $\omega(0)=x$.

Let us define a metric $\tilde{d}$ on $\tilde{\Gamma}(x)$ by

$$\tilde{d}((T,\omega),(T',\omega'))=|T-T'|+d(\omega,\omega'),$$

where d is the standard uniform metric on $\Omega(x)$ defined by

$$d(\omega,\omega')=\sup\{|\omega(s)-\omega'(s)|:s\in[0,1]\}.$$

Equipped with $\tilde{d}$ the set $\tilde{\Gamma}(x)$ becomes a separable metric space. The discussion of probability measures and their convergence properties is particularly convenient on complete metric spaces (see, e.g., Ref. 9). Since $\Omega(x)$ with the metric d is complete we can complete $\tilde{\Gamma}(x)$ by adjoining $0\times\Omega(x)$. This will be assumed in the following. All measures on $\tilde{\Gamma}(x)$ that will be considered vanish identically on $0\times\Omega(x)$.

On $\Omega(x)$ we have the family of Wiener measures $W_x^t, t>0$, defined on the Borel subsets of $\Omega(x)$. Here t denotes the variance of the measure. We note that W_x^t is uniquely defined by the characteristic functions of its finite dimensional distributions which are given for $0<t_1<t_2<\cdots<t_n\leqslant 1$ by

$$\begin{aligned}p^t_{t_1,\ldots,t_n}(\xi_1,\ldots,\xi_n)&=\int \exp(i\xi_1\cdot\omega(t_1)+\cdots+i\xi_n\cdot\omega(t_n))\,\mathrm{d}W_x^t(\omega)\\&=\int\prod_{i=1}^n \mathrm{d}x_i(2\pi t(t_i-t_{i-1}))^{-d/2}\exp\left(-\frac{|x_i-x_{i-1}|^2}{2t(t_i-t_{i-1})}+i\xi_i\cdot x_i\right)\\&=\exp\left(-\frac{t}{2}\sum_{i=1}^n (t_i-t_{i-1})(\xi_i+\cdots+\xi_n)^2+ix\cdot(\xi_1+\cdots+\xi_n)\right),\end{aligned}\tag{17}$$

where $\xi_1,\ldots,\xi_n\in\mathbb{R}^d$, $t_0=0$, and $x_0=x$.

For a Borel set $B\subseteq\tilde{\Gamma}(x)$ we let

$$B_t=\{\omega:(t,\omega)\in B\}\quad\text{for}\quad t>0,$$

and define the measure W_x on $\tilde{\Gamma}(x)$ by

$$W_x(B)=\int_0^\infty e^{-(1/2)m^2t}W_x^t(B_t)\,\mathrm{d}t.$$

The above-given definition requires $t\to W_x^t(B_t)$ to be a measurable function. Rather than proving this directly we show that this must be the case by giving an alternative definition of W_x. First, let $x=0$ and consider the product M of Lebesgue measure on $\mathbb{R}_+$ and W_0^1 on $\Omega(0)$, i.e.,

$$\mathrm{d}M(t,\omega)=\mathrm{d}t\,\mathrm{d}W_0^1(\omega).$$

Defining a homeomorphism h of $\mathbb{R}_+\times\Omega(0)$ onto itself by $h(t,\omega)=(t,t^{-1/2}\omega)$ and observing that

$$W_0^t(A)=W_0^1(t^{-1/2}A)$$

for Borel sets $A\subseteq\Omega(0)$, it follows that we have a measure W_0 on $\tilde{\Gamma}(0)$ given by

$$W_0(B)=\int_B e^{-(1/2)m^2t}d(M\circ h)(t,\omega),$$

where the measure $M\circ h$ on $\mathbb{R}_+\times\Omega(0)$ is defined by $(M\circ h)(B)=M(h(B))$ for Borel sets $B\subseteq\mathbb{R}_+\times\Omega(0)$. This shows that W_0 is well defined. For arbitrary x we obtain W_x as the translation of W_0 by x.

To set up the discrete approximation to W_x, given by Eq. (16) for the propagator, let $\tilde{\Gamma}_{a,N}(x)\subseteq\tilde{\Gamma}(x)$ be the set of pairs (T,ω), where $T=a^2N$ and ω is an N-step piecewise linear path $x=x_0\to x_1\to\cdots\to x_N$ such that the step $x_{i-1}\to x_i$ is parametrized linearly by the interval $[(i-1)/N,i/N]$. Define the measure $W_{x,a,N}$ on $\tilde{\Gamma}(x)$ supported on $\tilde{\Gamma}_{a,N}(x)$ by

$$dW_{x,a,N}(T,\omega)=\prod_{i=1}^{N} dx_i(2\pi a^2)^{-d/2}\exp\left(-\frac{1}{2a^2}|x_i-x_{i-1}|^2\right). \tag{18}$$

For $N=0$ we let $W_{x,a,0}$ be the Dirac measure at the trivial (constant) path. The approximating measure $W_{x,a}$ on $\tilde{\Gamma}(x)$ is supported on the set

$$\tilde{\Gamma}_a(x)\equiv\bigcup_{N=0}^{\infty}\tilde{\Gamma}_{a,N}(x)$$

and defined by

$$W_{x,a}=(1-e^{-(1/2)m^2a^2})\sum_{N=0}^{\infty}e^{-(1/2)m^2a^2N}W_{x,a,N}. \tag{19}$$

The normalization factor in Eq. (19) has been chosen such that $W_{x,a}$ is a probability measure, whereas the volume of W_x is $W_x(\tilde{\Gamma}(x))=2/m^2$. We prove the following result in the next section.

Theorem III.1: $W_{x,a}\to m^2/2W_x$ as $a\to 0$.

Here and in the following convergence of measures is in the sense of *weak convergence*, i.e.,

$$\int f\,dW_{x,a}\to\int f\,dW_x \quad \text{as} \quad a\to 0,$$

for all bounded continuous functions f on $\tilde{\Gamma}(x)$.

B. Lattice paths

Next let us discuss the measure pertaining to Eq. (2). The relevant orbit space is now

$$\tilde{\Omega}(x)=\Omega(x)/\mathrm{Diff}_+[0,1]=\{[\omega]:\omega\in\Omega(x)\},$$

where $[\omega]=\{\omega\circ\varphi|\varphi\in\mathrm{Diff}_+[0,1]\}$. The quotient space $\tilde{\Omega}(x)$ inherits in a standard fashion a pseudometric $\bar{d}$ from the metric d on $\Omega(x)$, given by

$$\bar{d}([\omega],[\omega'])=\inf\{d(\omega,\omega'\circ\varphi):\varphi\in\mathrm{Diff}_+[0,1]\}.$$

Here the term pseudometric means that $\bar{d}([\omega],[\omega'])=0$ may occur even if $[\omega]\neq[\omega']$. For example, we have $\bar{d}([\omega],[\omega\circ f])=0$ whenever $f:[0,1]\to[0,1]$ is a uniform limit of increasing diffeomorphisms. This defect is eliminated by taking a further quotient setting

$$\bar{\Omega}(x)=\{\bar{\omega}:\omega\in\Omega(x)\},$$

where $\bar{\omega}=\{[\omega']:\bar{d}([\omega],[\omega'])=0\}$. Then $\bar{d}$ defines a metric on $\bar{\Omega}(x)$, and it is straightforward to verify that $\bar{\Omega}(x)$ is a complete separable metric space.

It is not hard to see that the same space $\overline{\Omega}(x)$ results from the above-mentioned construction if, e.g., we replace $\mathrm{Diff}_+[0,1]$ by the group $\mathrm{Homeo}_+[0,1]$ of increasing homeomorphisms of the unit interval. Let us also note that evidently the quotient map $\pi:\Omega(x)\to\overline{\Omega}(x)$ is continuous.

The measure W_x on $\tilde{\Gamma}(x)=\mathbb{R}_+\times\Omega(x)$ constructed in Sec. III A gives rise to a measure V'_x on $\Omega(x)$ by integration over the t variable,

$$V'_x(A)=W_x(\mathbb{R}_+\times A)=\int_0^\infty e^{-(1/2)m^2t}W_x^t(A)\,dt$$

for Borel sets $A\subseteq\Omega(x)$. Transporting this measure to $\overline{\Omega}(x)$ by π we obtain a measure V_x given by

$$V_x(\overline{A})=V'_x(\pi^{-1}(\overline{A})).$$

This measure is defined on those sets $\overline{A}$ for which $\pi^{-1}(\overline{A})$ is a Borel set. This σ-algebra contains the Borel algebra of $\overline{\Omega}(x)$ since π is continuous and we claim that the measure so defined is the appropriate one to associate to Eq. (2).

In order to define the corresponding lattice approximation let $\Omega_{a,N}(x)$ denote the set of parametrized paths in $x+a\mathbb{Z}^d$ with N steps, such that the ith step is linearly parametrized by $[(i-1)/N,i/N]$. Here x is an arbitrary point in $\mathbb{R}^d$. We let the discrete measure $V'_{x,a,N}$ on $\Omega(x)$, supported on $\Omega_{a,N}(x)$ be defined by

$$V'_{x,a,N}(\omega)=e^{-\beta_0 N}\quad\text{for}\quad\omega\in\Omega_{a,N}(x),\tag{20}$$

where $\beta_0=\log 2d$, i.e., $V'_{x,a,N}$ is a normalized counting measure.

Furthermore, in correspondence with Eqs. (3) and (5) we define the measure $V'_{x,a}$ on $\Omega(x)$ supported on

$$\Omega_a(x)\equiv\bigcup_{N=0}^{\infty}\Omega_{a,N}(x)$$

by

$$V'_{x,a}=(1-e^{-(1/2d)m^2a^2})\sum_{N=0}^{\infty}e^{-(1/2d)m^2a^2N}V'_{x,a,N}.\tag{21}$$

Here, $V'_{x,a,0}$ denotes the Dirac measure at the trivial path in $\Omega(x)$, and the normalization has been chosen such that $V'_{x,a}$ is a probability measure.

Similarly, we define

$$\overline{\Omega}_{a,N}(x)=\pi(\Omega_{a,N}(x))$$

and

$$\overline{\Omega}_a(x)=\pi(\Omega_a(x))=\bigcup_{N=0}^{\infty}\overline{\Omega}_{a,N}(x).$$

Correspondingly we define the transported measures $V_{x,a,N}$ and $V_{x,a}$ given by

$$V_{x,a,N}(\overline{A})=V'_{x,a,N}(\pi^{-1}(\overline{A}))\tag{22}$$

and

$$V_{x,a}(\overline{A}) = (1-e^{-(1/2d)m^2a^2}) \sum_{N=0}^{\infty} e^{-(1/2d)m^2a^2N} V_{x,a,N}(\overline{A}) \tag{23}$$

for Borel sets $\overline{A} \subseteq \overline{\Omega}(x)$. With these definitions we then have

Theorem III.2: $V_{x,a} \to (m^2/2)V_x$ as $a \to 0$.

This result is proven in the subsequent section as a consequence of the stronger result $V'_{x,a} \to (m^2/2)V'_x$ as $a \to 0$.

C. Paths with two fixed end points

Let us briefly discuss paths with both end points x,y fixed. It is straightforward to introduce analogs to the spaces defined previously for paths with one fixed end point. We shall use the same notation except that x is everywhere replaced by x,y. On $\Omega(x,y)$ the family of Wiener measures $W^t_{x,y}, t>0$, is defined by the characteristic functions

$$\begin{aligned} q^t_{t_1,\ldots,t_n}(\xi_1,\ldots,\xi_n) &= \int \exp(i\xi_1\cdot\omega(t_1)+\cdots+i\xi_n\cdot\omega(t_n))\mathrm{d}W^t_{x,y}(\omega) \\ &= \int \prod_{i=1}^{n} \mathrm{d}x_i (2\pi t(t_i-t_{i-1}))^{-d/2} \exp\left(-\frac{|x_i-x_{i-1}|^2}{2t(t_i-t_{i-1})} + i\xi_i\cdot x_i\right) \\ &\quad \times (2\pi t(1-t_n))^{-d/2} \exp\left(-\frac{|y-x_n|^2}{2t(1-t_n)}\right) \\ &= Z^t_{x,y} \exp\left(-\frac{t}{2}\sum_{i=1}^{n}(t_i-t_{i-1})(\xi_i+\cdots+\xi_n)^2 - \left(\sum_{i=1}^{n} t_i\xi_i\right)^2 \right. \\ &\quad \left. + i\sum_{i=1}^{n}(t_iy+(1-t_i)x)\xi_i\right), \end{aligned} \tag{24}$$

where

$$Z^t_{x,y} = (2\pi t)^{-d/2} e^{-|x-y|^2/2t},$$

the volume of $W^t_{x,y}$, is simply the heat kernel.

We then define the measure $W_{x,y}$ on $\tilde{\Gamma}(x,y)$ for $x \neq y$ by

$$W_{x,y}(B) = \int_0^\infty e^{-(1/2)m^2t} W^t_{x,y}(B_t)\mathrm{d}t,$$

where $B \subseteq \tilde{\Gamma}(x,y)$ is a Borel set and $B_t \subseteq \Omega(x,y)$ is defined as previously. The fact that this expression is well defined is shown in a similar way as for W_x by first noting that

$$W^t_{0,0}(A) = t^{-d/2} W^1_{0,0}(t^{-1/2}A)$$

for Borel sets $A \subseteq \Omega(0,0)$, and then using

$$W^t_{x,y}(A) = \exp\left(-\frac{|x-y|^2}{2t}\right) W^1_{0,0}(A-\omega_{x,y}),$$

where $\omega_{x,y}$ is the linear path from x to y and A is a Borel subset of $\Omega(x,y)$. The last relation is a direct consequence of Eq. (24).

Having defined $W_{x,y}$ the measures $V'_{x,y}$ and $V_{x,y}$ are defined in a similar way as V'_x and V_x.

The piecewise linear approximation is defined in analogy with Eq. (19) by

$$W_{x,y,a}=(1-e^{-(1/2)m^2a^2})\sum_{N=0}^{\infty} e^{-(1/2)m^2a^2N}W_{x,y,a,N}, \tag{25}$$

where

$$\mathrm{d}W_{x,y,a,N}(T,\omega)=\prod_{i=1}^{N} \mathrm{d}x_i(2\pi a^2)^{-d/2}\exp\left(-\frac{1}{2a^2}|x_i-x_{i-1}|^2\right) \tag{26}$$

for an N-step piecewise linear path $\omega: x=x_0\to x_1\to\cdots\to x_{N-1}\to x_N=y$. Here $W_{x,y,a,1}$ is the Dirac measure $\delta_{(1,\omega_0)}$, where ω_0 is the linear path from x to y, and $T=a^2N$ as before.

Similarly, the hypercubic approximation is defined for $x\neq y, x-y\in a\mathbb{Z}^d$ by

$$V'_{x,y,a}=(1-e^{-m^2a^2})\sum_{N=1}^{\infty} e^{-m^2a^2N}V'_{x,y,a,N}, \tag{27}$$

where

$$V'_{x,y,a,N}(\omega)=a^{-d}e^{-\beta_0 N} \quad \text{for} \quad \omega\in\Omega_{a,N}(x,y), \tag{28}$$

and $V_{x,y,a}$ is obtained by transporting to $\overline{\Omega}(x,y)$ by the quotient map π. Since in all cases we are interested in the limit $a\to 0$ we shall assume $0<a<1$.

It should be noted that in contrast to the case of paths with one fixed end point, the approximating measures defined here are not probability measures. The volume of $W_{x,y,a,N}$ is obtained by explicit computation and equals

$$Z_{x,y}^{a^2N}=(2\pi a^2N)^{-d/2}e^{-|x-y|^2/2a^2N}, \tag{29}$$

which by insertion into (25) immediately shows that the volume of $W_{x,y,a}$ equals $(1-e^{-(1/2)m^2a^2})a^{-2}H^a(x,y)$ and converges to $(m^2/2)G(x,y)$ as $a\to 0$ according to Eq. (16). Similarly, the volume of $V_{x,y}$ equals $(1-e^{-(1/2d)m^2a^2})a^{-2}G^a(x,y)$ and converges to $(m^2/2)G(x,y)$ as $a\to 0$ according to Eq. (10). On the other hand, the volume of $W_{x,y}$ and of $V_{x,y}$ both equal $G(x,y)$. The convergence of volumes extends to the following result.

Theorem III.3: $W_{x,y,a}\to(m^2/2)W_{x,y}$ and $V_{x,y,a}\to(m^2/2)V_{x,y}$ as $a\to 0$ for $x\neq y$.

The proof is given in Sec. IV.

IV. CONVERGENCE OF THE APPROXIMATIONS

In a complete separable metric space M there is a standard two-step procedure for proving convergence of a family $m_a, a>0$, of Borel probability measures to a measure m. The first step is to verify that $m_a, a>0$, is a *tight* (or *precompact*) family. This means that for every $\eta>0$ there exists a compact set $K\subseteq M$ such that $m_a(K)\geqslant 1-\eta$ for all $a>0$. The second step is to show that

$$\int_M f\,\mathrm{d}m_a\to\int_M f\,\mathrm{d}m \tag{30}$$

as $a\to 0$ for a collection of functions that determine the measure in the sense that if the integrals of these functions coincide for two measures then the measures coincide. Of course, the first step is superfluous if one can establish the convergence (30) for all bounded continuous functions f. But this only happens rarely. Generally, the first step ensures that every sequence m_{a_n} from the given family has a convergent subsequence, and the second step then implies that its limit is independent of the chosen sequence or subsequence. For the spaces $\Omega(x)$ and $\Omega(x,y)$ the second step can be

accomplished by proving convergence of the characteristic functions of the finite dimensional distributions. For the spaces $\tilde{\Gamma}(x)$ and $\tilde{\Gamma}(x,y)$ a little more is required as we discuss in the following.

In the following four lemmas we show that the approximations introduced in Sec. III form tight families.

Lemma IV.1: $W_{x,a}, 0<a<1$, is a tight family of measures on $\tilde{\Gamma}(x)$.

Proof: The following is an adaptation of the corresponding argument for the piecewise linear approximations to the measure W_x^t (see Ref. 9). According to the Arzela–Ascoli theorem the sets of compact closure in $\Omega(x)$ are the equicontinuous ones. Defining the modulus of continuity

$$m(\omega,\delta)=\sup\{|\omega(s)-\omega(t)|:|s-t|<\delta\} \quad \text{for} \quad \delta>0, \quad \omega\in\Omega(x),$$

it follows that complements to sets of the form

$$C=\bigcup_{n=1}^{\infty}\left\{\omega: m(\omega,\delta_n)>\frac{1}{n}\right\} \tag{31}$$

have compact closures in $\Omega(x)$ for an arbitrary sequence $\{\delta_n\}$ of positive numbers. We observe that by Eq. (19)

$$W_{x,a}([t_0,+\infty)\times\Omega(x))<\eta \quad \text{if} \quad t_0>-m^{-2}\log\eta \tag{32}$$

for any $\eta>0$ and all $a>0$. In order to prove the lemma it therefore suffices to show that for any $\eta,\varepsilon,t_0>0$ there exists a $\delta>0$ such that

$$W_{x,a}([0,t_0]\times\{\omega\in\Omega(x):m(\omega,\delta)>\varepsilon\})<\eta \tag{33}$$

for all $a>0$.

By Eq. (19) it follows that Eq. (33) holds if

$$W_{x,a,N}(\{(a^2N,\omega)\in\tilde{\Gamma}(x):m(\omega,\delta)>\varepsilon\})<\eta \quad \text{for} \quad a^2N\leq t_0. \tag{34}$$

But for a,N as in Eq. (34) we have

$$\begin{aligned} W_{x,a,N}(\{(a^2N,\omega):m(\omega,\delta)>\varepsilon\}) &= W_{x,1,N}\left(\left\{(N,\omega):m(\omega,\delta)>\frac{\varepsilon}{a}\right\}\right) \\ &\leq W_{x,1,N}\left(\left\{(N,\omega):m(\omega,\delta)>\frac{\varepsilon\sqrt{N}}{\sqrt{t_0}}\right\}\right). \end{aligned} \tag{35}$$

Hence, it suffices to show, for given $\eta,\varepsilon>0$, that

$$W_{x,1,N}(\{(N,\omega):m(\omega,\delta)>\varepsilon\sqrt{N}\})<\eta, \tag{36}$$

if δ is small enough. This is a well-known result (see, e.g., Ref. 9, pp. 62–63). For later reference we briefly recall the argument.

First, note that since paths contributing to (36) are linear on each interval $[(i-1)/N,i/N]$ we have

$$m_N(\omega,\delta)\equiv\max\left\{\left|\omega\left(\frac{i}{N}\right)-\omega\left(\frac{j}{N}\right)\right|:0\leq i,j\leq N,\left|\frac{i}{N}-\frac{j}{N}\right|<\delta\right\}\geq\frac{1}{3}m(\omega,\delta)$$

for $N \geqslant \delta^{-1}$. Note also that by uniform continuity of $\omega \in \Omega(x)$ the inequality (36) is fulfilled for sufficiently small δ for each individual N, so we need not worry about small N. Hence we may replace $m(\omega,\delta)$ in (36) by $m_N(\omega,\delta)$, and we may assume $\delta = M^{-1}$, where $M \in \mathbb{N}$ and $N \geqslant M$.

Next, given $N \geqslant M$, we choose integers $0 = k_0 < k_1 < \cdots < k_M = N$ such that any subinterval $[i/N, j/N]$ of $[0,1]$ of length $\leqslant \delta$ is contained in one of the intervals $[k_l/N, (k_{l+2}/N]$ and such that the latter intervals are all of length $\leqslant 3\delta$. It follows that

$$
\begin{aligned}
&W_{x,1,N}(\{(N,\omega): m(\omega,\delta) > \varepsilon\sqrt{N}\}) \\
&\qquad \leqslant \sum_{l=0}^{M-2} W_{x,1,N}\left(\left\{(N,\omega): \max_{k_l \leqslant k \leqslant l+2} \left|\omega\left(\frac{k_l}{N}\right) - \omega\left(\frac{k}{N}\right)\right| > \frac{\varepsilon}{6}\sqrt{N}\right\}\right) \\
&\qquad \leqslant \sum_{l=0}^{M-2} W_{x,1,N}\left(\left\{(N,\omega): \max_{k_l \leqslant k \leqslant k_{l+2}} \left|\omega\left(\frac{k_l}{N}\right) - \omega\left(\frac{k}{N}\right)\right| \right.\right. \\
&\qquad\qquad \left.\left. > \frac{\delta^{-1/2}\varepsilon}{6\sqrt{3}}\sqrt{k_{l+2} - k_l}\right\}\right).
\end{aligned}
$$

Due to statistical independence of the steps in ω and translation invariance, we have

$$
\begin{aligned}
&W_{x,1,N}\left(\left\{(N,\omega) \in \tilde{\Gamma}(x): \max_{k_l \leqslant k \leqslant k_{l+2}} \left|\omega\left(\frac{k_l}{N}\right) - \omega\left(\frac{k}{N}\right)\right| > \alpha\right\}\right) \\
&\qquad = W_{0,1,k_{l+2}-k_l}\left(\left\{(k_{l+2}-k_l,\omega) \in \tilde{\Gamma}(0): \max_{k_l \leqslant k \leqslant k_{l+2}} \left|\omega\left(\frac{k}{k_{l+2}-k_l}\right)\right| > \alpha\right\}\right)
\end{aligned}
$$

for $\alpha > 0$. Combining this with the previous inequality we conclude that it is sufficient to show for given $\eta > 0$ the existence of $\delta > 0$ such that for all $N \in \mathbb{N}$,

$$
\delta^{-1} W_{0,1,N}\left(\left\{(N,\omega): \max\left\{\left|\omega\left(\frac{i}{N}\right)\right| \middle| 0 \leqslant i \leqslant N\right\} > \delta^{-1/2}\sqrt{N}\right\}\right) < \eta.
$$

This inequality is a consequence of the Chebychev inequality and the uniform boundedness in N of the moments of $N^{-1/2}|\omega(1)|$ with respect to the measure $W_{0,1,N}$. The details may be found in Ref. 9 □

Lemma IV.2: $V'_{x,a}, 0 < a < 1$, is a tight family of measures on $\Omega(x)$.

Proof: This is obtained by an argument similar to the one given previously. First, applying the Arzela–Ascoli theorem one concludes that it is sufficient to prove for given $\eta, \varepsilon > 0$ that

$$
V'_{x,a}(\{\omega \in \Omega(x): m(\omega,\delta) > \varepsilon\}) < \eta \tag{37}
$$

for small enough δ. Second, since the contribution of terms with $a^2 N \geqslant t_0$ in (21) is less than or equal to $\eta/2$ if $t_0 \geqslant -m^2 \log \eta/2$ we conclude as previously that it is sufficient to show the existence of a $\delta > 0$ such that for all $N \in \mathbb{N}$,

$$
V'_{x,1,N}(\{\omega \in \Omega(x): m(\omega,\delta) > \varepsilon\sqrt{N}\}) < \eta. \tag{38}
$$

The proof of this fact parallels the one for piecewise linear paths referred to previously, and uses only the statistical independence of the steps in a path together with the uniform boundedness in N of the moments of $N^{-1/2}|\omega(1)|$ with respect to the measure $V'_{x,1,N}$. We omit the details of the argument. □

Lemma IV.3: $W_{x,y,a}, 0 < a < 1$, is a tight family of measures on $\tilde{\Gamma}(x,y)$ for $x \neq y$.

Proof: By definition tightness of the family $W_{x,y,a}, a>0$, means tightness of the corresponding family of normalized measures. Since, however, the volume of $W_{x,y,a}$ converges to the volume of $\frac{1}{2}m^2 W_{x,y}$ as $a\to 0$, as noted previously, we need not worry about normalization.

We note first that the volume of $W_{x,y,a,N}$ given by (29) is uniformly bounded in a and N. Hence, in (25) the sum over $N\leqslant s_0 a^{-2}$ or over $N\geqslant t_0 a^{-2}$ can be made arbitrarily small for sufficiently small s_0 or sufficiently large t_0, respectively. By the same arguments as in the first part of the proof of Lemma IV.1 it is sufficient to demonstrate the existence of a $\delta>0$ such that

$$W_{x,y,a,N}(\{(a^2N,\omega)\in\tilde{\Gamma}(x,y): m(\omega,\delta)>\varepsilon\})<\eta \quad \text{for} \quad s_0\leqslant a^2N\leqslant t_0, \tag{39}$$

for given $\eta,\varepsilon,s_0,\ t_0>0$.

We may as before replace $m(\omega,\delta)$ by $m_N(\omega,\delta)$. Assuming $\delta<\frac{1}{3}$ and setting $N_1=[\frac{2}{3}N]+1$, $N_2=[\frac{1}{3}N]$ (where $[\alpha]$ denotes the integer part of α), any subinterval of $[0,\ 1]$ of length δ is contained in either $[0,N_1/N]$ or in $[N_2/N,1]$. Hence, we have

$$\begin{aligned} &W_{x,y,a,N}(\{(a^2N,\omega): m_N(\omega,\delta)>\varepsilon\}) \\ &\quad\leqslant W_{x,y,a,N}(\{(a^2N,\omega): m_N^1(\omega,\delta)>\varepsilon\}) + W_{x,y,a,N}(\{(a^2N,\omega): m_N^2(\omega,\delta)>\varepsilon\}), \end{aligned} \tag{40}$$

where we have set

$$m_N^1(\omega,\delta)=\max\left\{\left|\omega\left(\frac{i}{N}\right)-\omega\left(\frac{j}{N}\right)\right|: 0\leqslant i,j\leqslant N_1, \left|\frac{i}{N}-\frac{j}{N}\right|<\delta\right\}$$

and

$$m_N^2(\omega,\delta)=\max\left\{\left|\omega\left(\frac{i}{N}\right)-\omega\left(\frac{j}{N}\right)\right|: N_2\leqslant i,j\leqslant N, \left|\frac{i}{N}-\frac{j}{N}\right|<\delta\right\}.$$

By definition of $W_{x,y,a,N}$ we have

$$W_{x,y,a,N}(\{(a^2N,\omega): m_N^1(\omega,\delta)>\varepsilon\})=\int_{\mathbb{R}^d} \mathrm{d}u\ Z_{u,y}^{a^2(N-N_1)} W_{x,u,a,N_1}(\{(a^2N_1,\omega): m_{N_1}(\omega,\delta)>\varepsilon\}). \tag{41}$$

Here $a^2(N-N_1)\geqslant a^2(\frac{1}{3}N-1)\geqslant\frac{1}{6}s_0$ (assuming $N\geqslant 6$) so

$$Z_{u,y}^{a^2(N-N_1)}\leqslant(\tfrac{1}{3}\pi s_0)^{-d/2}.$$

Using this estimate together with

$$\mathrm{d}W_{x,a,N}(a^2N,\omega)=\mathrm{d}\omega(1)\mathrm{d}W_{x,\omega(1),a,N}(\omega) \quad \text{for} \quad \omega\in\Omega(x)$$

in Eq. (41) we obtain

$$W_{x,y,a,N}(\{(a^2N,\omega): m_N^1(\omega,\delta)>\varepsilon\})\leqslant(\tfrac{1}{3}\pi s_0)^{-d/2} W_{x,a,N_1}(\{(a^2N_1,\omega): m_{N_1}(\omega,\delta)>\varepsilon\}).$$

Finally, using $a^2N_1\leqslant\frac{2}{3}t_0$ we conclude from the proof of Lemma IV.1 that $W_{x,a,N_1}(\{(a^2N_1,\omega): m_{N_1}(\omega,\delta)>\varepsilon\})$ can be made arbitrarily small for $a^2N\leqslant t_0$ if δ is chosen small enough.

The second term in (40) can be treated similarly, and the lemma is proven. □

Lemma IV.4: $V'_{x,y,a}, 0<a<1$, is a tight family of measures on $\Omega(x,y)$ for $x\neq y$.

Proof: Only a few modifications of the previous proof are needed.

For the volume $Z_{x,y,1,N}$ of $W_{x,y,1,N}$ we have the following result, which is rather easily derived from its Fourier representation (see, e.g., Ref. 10, pp. 76–77):

$$\lim_{N\to\infty}((2\pi N/d)^{d/2}Z_{x,y,1,N}-e^{-|x-y|^2/2N/d})=0$$

uniformly in $x-y\in\mathbb{Z}^d$. For the volume $Z_{x,y,a,N}$ of $W_{x,y,a,N}$ this means

$$\lim_{N\to\infty}((2\pi a^2N/d)^{d/2}Z_{x,y,a,N}-e^{-|x-y|^2/2Nd^2/d})=0 \tag{42}$$

uniformly in $x-y\in a\mathbb{Z}^d$ and $0<a<1$.

As a first consequence of (42) we note that $Z_{x,y,a,N}$ is uniformly bounded in a,N for $a^2N\geqslant t_0$ for any given $t_0>0$ large enough. It follows that in Eq. (25) the sum over $N\geqslant t_0a^{-2}$ can be made arbitrarily small [when applied to any Borel set in $\Omega(x,y)$] by choosing t_0 large enough.

A second consequence is that for any $s_0>0$

$$(1-e^{-(1/2d)m^2a^2})\sum_{a^2N\geqslant s_0}^{\infty}e^{-(1/2d)m^2a^2N}Z_{x,y,a,N}\to\frac{m^2}{2d}\int_{s_0}^{\infty}Z_{x,y}^{t/d}e^{-(1/2d)m^2t}\mathrm{d}t$$
$$=\frac{m^2}{2}\int_{s_0/d}^{\infty}Z_{x,y}^{t}e^{-(1/2)m^2t}\,\mathrm{d}t$$

as $a\to0$. On the other hand, as we know from Sec. II,

$$(1-e^{-(1/2d)m^2a^2})\sum_{N=0}^{\infty}e^{-(1/2d)m^2a^2N}Z_{x,y,a,N}\to\frac{m^2}{2}G(x,y)=\frac{m^2}{2}\int_{0}^{\infty}Z_{x,y}^{t}e^{-(1/2)m^2t}\,\mathrm{d}t$$

as $a\to0$. Hence we conclude that the sum in Eq. (25) over $a^2N\leqslant s_0$ can be made arbitrarily small for all $a<a_0$ for some $a_0>0$. Replacing s_0 by $\min\{s_0,a_0^2\}$ we can arrange that $a_0=1$.

It now follows as in the previous proof that it suffices to show for given $\eta,\varepsilon,s_0,t_0>0$ that there exists $\delta>0$ such that

$$V'_{x,y,a,N}(\{\omega:m_N(\omega,\delta)>\varepsilon\})<\eta\quad\text{for}\quad s_0<a^2N<t_0.$$

Following the proof of Lemma 4.3 we have the estimate

$$V'_{x,y,a,N}(\{(a^2N,\omega):m_N(\omega,\delta)>\varepsilon\})$$
$$\leqslant V'_{x,y,a,N}(\{(\omega):m_N^1(\omega,\delta)>\varepsilon\})+V'_{x,y,a,N}(\{(\omega):m_N^2(\omega,\delta)>\varepsilon\}). \tag{43}$$

By definition of $V'_{x,y,a,N}$ we can write

$$V'_{x,y,a,N}(\{(\omega):m_N^1(\omega,\delta)>\varepsilon\}=\sum_{u\in a\mathbb{Z}^d}Z_{u,y,a,N-N_1}V'_{x,u,a,N_1}(\{(\omega):m_{N_1}(\omega,\delta)>\varepsilon\}.$$

From Eq. (42) and $a^2(N-N_1)\geqslant\frac{1}{6}s_0$ it follows that $Z_{u,y,a,N-N_1}$ is uniformly bounded in x,y,a,N for $a^2N\geqslant s_0$ and $n\geqslant N_0$ for some $N_0\in\mathbb{N}$. Letting C denote such an upper bound, we have

$$V'_{x,y,a,N}(\{(\omega):m_N^1(\omega,\delta)>\varepsilon\}\leqslant C\sum_{u\in a\mathbb{Z}^d}V'_{u,x,a,N_1}((\{(\omega)m_{N_1}(\omega,\delta)>\varepsilon\}$$
$$=CV'_{x,a,N_1}((\{(\omega):m_{N_1}(\omega,\delta)>\varepsilon\}. \tag{44}$$

From the proof of Lemma 4.2 it now follows as previously that the right-hand side of (44) can be made arbitrarily small for $a^2N \leq t_0$ if δ is chosen sufficiently small. Estimating the second term in (43) similarly and noting again that the case $N<N_0$ can be taken care of separately, the proof of the lemma is complete. □

We are now ready to give proofs of the convergence theorems stated in Sec. III. In view of the preceding lemmas and the remarks at the beginning of this section it is sufficient in each case to prove convergence on a measure determining class of functions.

Proof of Theorem III.1: For $0<t_1<\cdots<t_n\leq 1$ and $s\in\mathbb{R}$, $\xi_1,\ldots,\xi_n\in\mathbb{R}^d$ we define the characteristic function $p_{a;t_1,\ldots,t_n}$ of $W_{x,a}$ by

$$p_{a;t_1,\ldots,t_n}(s,\xi_1,\ldots,\xi_n)=\int_{\tilde{\Gamma}(x)} e^{i(st+\xi_1\cdot\omega(t_1)+\cdots+\xi_n\cdot\omega(t_1))}\mathrm{d}W_{x,a}(t,\omega), \tag{45}$$

and similarly the characteristic function $p_{t_1,\ldots,t_n}$ of W_x. We claim it is sufficient to show that $p_{a;t_1,\ldots,t_n}\to(m^2/2)p_{t_1,\ldots,t_n}$ pointwise as $a\to 0$, for arbitrary $0<t_1<\cdots<t_n\leq 1$. In order to see this, it is enough to verify that the measure W_x on $\tilde{\Gamma}(x)$ is determined by its characteristic functions. Let f be a smooth function on $\mathbb{R}_+\times R^{nd}$ with compact support. Multiplying $p_{t_1,\ldots,t_n}$ by the Fourier transform of f at $(s,\xi_1,\ldots,\xi_n)$ and integrating over $(s,\xi_1,\ldots,\xi_n)\in\mathbb{R}^{nd+1}$ gives by Fubini's theorem $\int_{\tilde{\Gamma}(x)} f(t,\omega(t_1),\ldots,\omega(t_n))\mathrm{d}W_{x,a}(t,\omega)$. A simple limiting argument then shows that measures of sets of the form $\{(t,\omega):(t,\omega(t_1),\ldots,\omega(t_n))\in C\}$, where $C\subseteq\mathbb{R}_+\times\mathbb{R}^{nd}$ is closed, are determined by the characteristic functions. Since sets of this form generate the Borel algebra in $\tilde{\Gamma}(x)$ the claim follows.

Given N let $1\leq N_1\leq\ldots\leq N_n\leq N$ be such that $t_i\in](N_i-1)/N,N_i/N]$ and set $t_i'=N_i/N$. By an explicit computation, replacing the intermediate times t_i by t_i' in the piecewise linear paths, one finds

$$\int_{\tilde{\Gamma}(x)} e^{i(st+\xi_1\cdot\omega(t_1)+\cdots+\xi_n\cdot\omega(t_n))}\mathrm{d}W_{x,a,N}(t,\omega)=C_{a,N}p^{a^2N}_{t_1',\ldots,t_n'}(s,\xi_1,\ldots,\xi_n).$$

The quantity $C_{a,N}$ which depends on the time differences t_i-t_i' tends to 1 uniformly in N as $a\to 0$. Using the expression (17) for $p^t_{t_1,\ldots,t_n}(s,\xi_1,\ldots,\xi_n)$ it follows easily that

$$\begin{aligned}p_{a;t_1,\ldots,t_n}(s,\xi_1,\ldots,\xi_n)&=(1-e^{-(1/2)m^2a^2})\sum_{N=0}^{\infty} C_{a,N}e^{-(1/2)m^2a^2N}e^{isa^2N}p^{a^2N}_{t_1',\ldots,t_n'}(s,\xi_1,\ldots,\xi_n)\\&\to\frac{m^2}{2}p_{t_1,\ldots,t_n}(s,\xi_1,\ldots,\xi_n)\end{aligned}$$

as $a\to 0$.

Proof of Theorem III.2: We do this by proving the stronger result that $V'_{x,a}\to(m^2/2)V'_x$ as $a\to 0$. It follows by the same argument as given in the beginning of the previous proof that it is enough to prove convergence of the characteristic function

$$\begin{aligned}p'_{\alpha;t_1,\ldots,t_n}(\xi_1,\ldots,\xi_n)&=\int_{\Omega(x)} e^{i(\xi_1\cdot\omega(t_1)+\cdots+\xi_n\cdot\omega(t_n))}\mathrm{d}V'_{x,a}(t,\omega)\\&=(1-e^{-(1/2)m^2a^2})\sum_{N=0}^{\infty} e^{-(1/2)m^2a^2N}\sum_{\omega\in\Omega_{a,N}(x)} e^{-\beta_0 N}e^{i(\xi_1\cdot\omega(t_1)+\cdots+\xi_n\cdot\omega(t_n))}\end{aligned}$$

to $(m^2/2)p_{t_1,\ldots,t_n}$ as $a\to 0$ for arbitrary $0<t_1<\cdots<t_n\leq 1$. Furthermore, we can assume $x=0$, since translation by x only gives rise to a factor $e^{ix\cdot(\xi_1+\cdots+\xi_n)}$ in the characteristic functions. Defining N_i and t_i' as in the preceding proof we have

$$
\begin{aligned}
&p'_{a;t_1,\ldots,t_n}(\xi_1,\ldots,\xi_n)\\
&\quad=(1-e^{-(1/2d)m^2a^2})\sum_{N=0}^{\infty} e^{-(1/2d)m^2a^2N}\prod_{i=1}^{n}\left(\frac{1}{d}\sum_{\nu=1}^{d}\cos a(\xi_i+\cdots+\xi_n)_\nu\right)^{N_i-N_{i-1}}\\
&\quad=(1-e^{-(1/2d)m^2a^2})\sum_{N=0}^{\infty} e^{-(1/2d)m^2a^2N}\prod_{i=1}^{n}\left(\frac{1}{d}\sum_{\nu=1}^{d}\cos a(\xi_i+\cdots+\xi_n)_\nu\right)^{(t'_i-t'_{i-1})N},
\end{aligned}
$$

where ν labels the components of the ξ variables and $N_0=0$. Finally, using

$$
\left(\frac{1}{d}\sum_{\nu=1}^{d}\cos a(\xi_i+\cdots+\xi_n)_\nu\right)^{s/a^2}\to e^{-(s/2d)(\xi_i+\cdots+\xi_n)^2}
$$

as $a\to 0$, an application of the dominated convergence theorem shows that

$$
p'_{a;t_1,\ldots,t_n}(\xi_1,\ldots,\xi_n)\to\frac{m^2}{2}\int_0^\infty \mathrm{d}t\, e^{(1/2)m^2t}\exp\left(-\frac{t}{2}\sum_{i=1}^{n}(t_i-t_{i-1})(\xi_i+\cdots+\xi_n)^2\right)
$$

as $a\to 0$, which is the desired result.

Proof of Theorem III.3: The convergence $W_{x,y,a}\to W_{x,y}$ follows by essentially the same proof as of Theorem III.1. Similarly the convergence $V_{x,y,a}\to V_{x,y}$ is obtained by trivial modifications of the proof of Theorem III.2. Details are left to the reader.

V. CYLINDER SETS

In this section we define a class of sets of geometric paths which generate the Borel algebra and play a role similar to the one played by cylinder sets in the theory of parametrized paths. We will see in Sec. VI that the measure of these sets can be calculated in a particularly simple way.

A natural condition to put on a parametrized path ω is that the path be located in a particular subset A of $\mathbb{R}^d$ at a given time t, i.e., $\omega(t)\in A$. For geometric paths a condition of this type is meaningless but a similar one which has a well-defined meaning is the condition that a geometric path $\overline{\omega}$ hit a set A. This means that $\overline{\omega}\cap A\neq\varnothing$, i.e., if ω is a parametrization of $\overline{\omega}$ then there is a time t such that $\omega(t)\in A$. More generally, we can require that a geometric path hit a number of sets in a particular order and/or stay away from other sets. In the following we define a certain class of sets defined by such conditions. Other definitions are possible but we find this class simple to work with.

We consider paths with two fixed end points x and y. Let $A_1,\ldots,A_n$ be subsets of $\mathbb{R}^d$ and let $\overline{\omega}\in\overline{\Omega}(x,y)$ with parametrization $\omega:[0,1]\to\mathbb{R}^d$. Define

$$
\begin{aligned}
\tau_1&=\sup\{t\geqslant 0:\omega([0,t])\subseteq A_1\},\\
\tau_2&=\sup\{t\geqslant \tau_1:\omega([\tau_1,t])\subseteq A_2\},\\
&\vdots\\
\tau_n&=\sup\{t\geqslant \tau_{n-1}:\omega([\tau_{n-1},t])\subseteq A_n\},
\end{aligned}
$$

where by convention $\sup\varnothing=1$. We then define $Z(A_1,\ldots,A_n)$ as the set of all geometric paths $\overline{\omega}\in\overline{\Omega}(x,y)$ such that

$$
\tau_1<\tau_2<\cdots<\tau_{n-1}<\tau_n=1.
$$

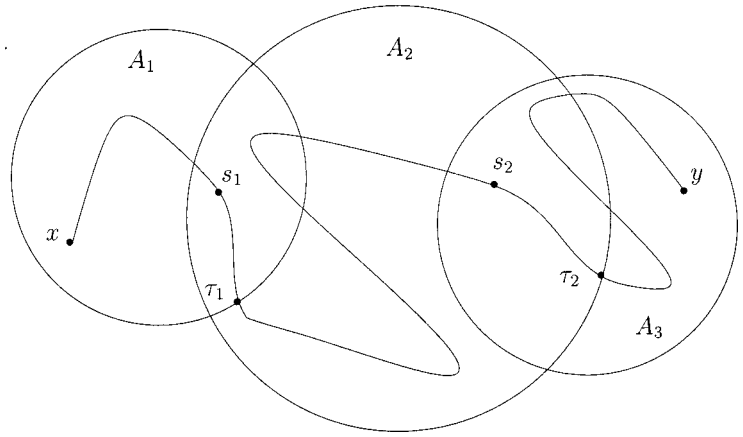

FIG. 1. An illustration of the times s_i and τ_i in the case of $n=3$.

This defining property is easily seen to be independent of the parametrization ω chosen for $\overline{\omega}$. In fact, $\overline{\omega}\in Z(A_1,\ldots,A_n)$ exactly if it starts at $x\in A_1$, stays inside A_1 until it leaves A_1 at a point $x_1=\omega(\tau_1)\in A_2$, then stays in A_2 until it leaves at a point $x_2=\omega(\tau_2)\in A_3$ and so on until it leaves A_{n-1} at a point $x_{n-1}=\omega(\tau_{n-1})\in A_n$ and then finally stays in A_n until it ends at $y\in\overline{A_n}$. The values of the escape times τ_i depend of course on the parametrization but their ordering and the points x_i are independent of parametrization.

Proposition 5.1: Let $A_1,\ldots,A_n\subseteq\mathbb{R}^d$ be open sets such that $x\in A_1$ and $y\in A_n\backslash\overline{A}_{n-1}$. Furthermore, assume

$$A_{i-1}\cap\partial A_i\cap A_{i+1}=\varnothing \tag{46}$$

for $i=2,\ldots,n-1$. Then $Z(A_1,\ldots,A_n)$ is an open subset of $\overline{\Omega}(x,y)$.

Proof: Let $\overline{\omega}\in Z(A_1,\ldots,A_n)$. Choose a parametrization ω for $\overline{\omega}$. Since the sets A_i are open we can choose $s_i<\tau_i$ such that $\omega([s_i,\tau_i])\subseteq A_{i+1}$, see Fig. 1. By the definition of the τ_i's it follows that $\omega([s_i,s_{i+1}])\subseteq A_{i+1}$ for $i=0,1,\ldots,n-1$, setting $s_0=0$.

Let $r_i>0$ be the distance from the compact set $\omega([s_i,s_{i+1}])$ to the boundary of A_{i+1}, $i=0,1,\ldots,n-1$, and set $r=\min_i r_i$. Now take a geometric path $\overline{\omega'}$ at a distance smaller than r from $\overline{\omega}$. Then there exists a parametrization $\omega':[0,1]\to\mathbb{R}^d$ of $\overline{\omega'}$ such that

$$\sup_{t\in[0,1]}|\omega(t)-\omega'(t)|<r.$$

In particular it follows that

$$\omega'([s_i,s_{i+1}])\subseteq A_{i+1}.$$

By the assumption (46) we may from the outset choose the s_i's such that $\omega(s_{i+1})\notin A_i$. Choosing r smaller, if necessary, we can also assume that r is smaller than the smallest of the distances from $\omega(s_{i+1})$ to A_i, $i=1,2,\ldots,n$. Hence, $\omega'(s_{i+1})\notin A_i$. On the other hand $\omega'(s_i)\in A_i$ so ω' leaves the set A_i at a time $\tau_i'\in[s_i,s_{i+1}]$. It follows that $\tau_1'<\tau_2'<\ldots\tau_n'=1$ so $\overline{\omega'}\in Z(A_1,\ldots,A_n)$. □

The condition (46) was essential in the above-given argument because otherwise the paths might never enter the interior of $A_i\backslash A_{i-1}$ for some i. But (46) can be replaced by a weaker condition as we now explain.

Let A be an open set in $\mathbb{R}^d$. We say that a geometric path $\overline{\omega}$ is *tangent to the boundary of A* at $x\in\partial A$ if there is a parametrization ω of $\overline{\omega}$ such that $\omega(t_0)=x$ and there is an $\varepsilon>0$ such that $\omega(t)\in\overline{A}$ for $0<|t-t_0|<\varepsilon$. We claim that any path in $Z(A_1,\ldots,A_n)$ which is nowhere tangent to

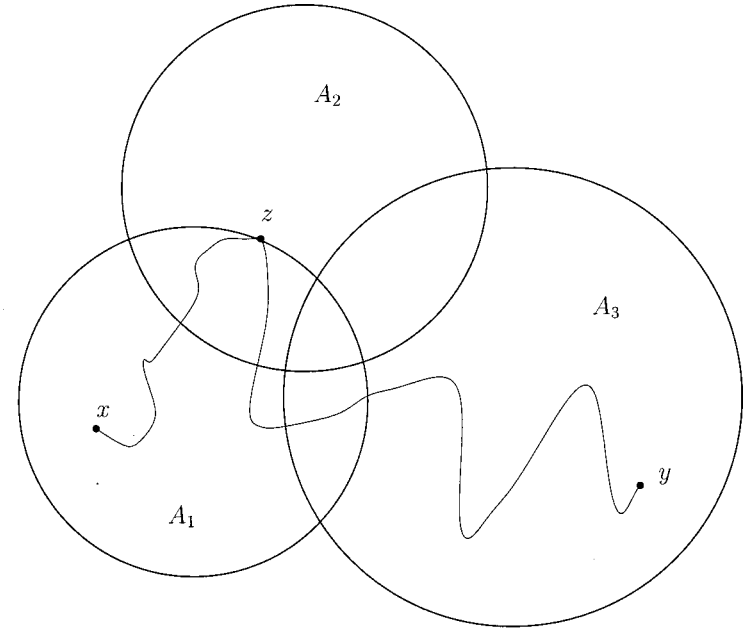

FIG. 2. A path from x to y which is tangent to A_1 at the point z. There are paths arbitrarily close to this path which are not in $Z(A_1,A_2,A_3)$.

any of the boundaries ∂A_i is an interior point of the set $Z(A_1,\ldots,A_n)$. This can be seen as follows: In addition to the s_i's, choose numbers $s_i' \in [0,1]$ such that $\tau_i < s_i' < s_i$ and $\omega(s_i') \notin \overline{A_i}$. Now choose $r>0$ smaller than each of the distances from $\omega(s_i')$ to $\overline{A_i}$. It then follows that a path $\overline{\omega'}$ within a distance r from $\overline{\omega}$ leaves A_i somewhere between s_i and s_i' and hence $\overline{\omega'} \in Z(A_1,\ldots,A_n)$ as before.

It is not hard to see that if $\overline{\omega} \in Z(A_1,\ldots,A_n)$ is tangent to one of the ∂A_i's then $\overline{\omega} \in \partial Z(A_1,\ldots,A_n)$, i.e., there are paths arbitrarily close to $\overline{\omega}$ that are not in $Z(A_1,\ldots,A_n)$, see Fig. 2.

We do not have a proof that the sets $Z(A_1,\ldots,A_n)$ are measurable for general open sets $A_1,\ldots,A_n$. We avoid this problem simply by taking the closures of these sets. We denote the closures by $\overline{Z}(A_1,\ldots A_n)$.

Proposition 5.2: The sets $\overline{Z}(A_1,\ldots,A_n)$ where the A_i's are open balls generate the Borel algebra of geometric paths.

Proof: We will show that any open set in $\overline{\Omega}(x,y)$ can be written as a countable union of $\overline{Z}$ sets. Given $\overline{\omega} \in \overline{\Omega}(x,y)$ and $\varepsilon>0$ we show that there are open balls $A_1,\ldots,A_n$ such that $\overline{\omega} \in \overline{Z}(A_1,\ldots,A_n)$ and $\overline{Z}(A_1,\ldots,A_n)$ is contained in a ball in $\overline{\Omega}(x,y)$ of radius ε centered on $\overline{\omega}$. Moreover, the A_i's can be taken to have rational centers and radii. It follows then by a standard argument that the $\overline{Z}$ sets generate the Borel algebra.

Let $\overline{\omega} \in U$ where $U \subseteq \overline{\Omega}(x,y)$ is open. Choose a rational number ε so that $\varepsilon < \frac{1}{2}\overline{d}(\overline{\omega},\partial U)$. Let A_1 be an open ball of radius ε centered at x. If $\overline{\omega}$ is not contained in A_1 let $x_1 \in \mathbb{R}^d$ be the point where $\overline{\omega}$ leaves A_1 for the first time, i.e., if $\omega:[0,1]\to\mathbb{R}^d$ is a parametrization of $\overline{\omega}$, then $x_1 = \omega(\tau_1)$, where

$$\tau_1 = \sup\{t \in [0,1]: \omega([0,t]) \subseteq A_1\}$$

as before. Take a point y_1 with rational coordinates such that $|x_1 - y_1| < \varepsilon/3$. Let A_2 be a ball of radius ε centered at y_1. If $\overline{\omega}$ stays inside A_2 after it leaves A_1 at x_1 the construction is finished; otherwise let x_2 be the point where $\overline{\omega}$ leaves A_2 for the first time after it left A_1 and x_1 and define

y_2 and A_3 in a way analogous to the one used to define y_1 and A_2. The construction continues in this way until we obtain a set A_n inside which $\overline{\omega}$ stays after it leaves A_{n-1}. The construction has to end after a finite number of steps since any parametrization ω of $\overline{\omega}$ is a uniformly continuous map.

From the above-given construction it is clear that $\overline{\omega} \in Z(A_1,\ldots,A_n)$. Moreover, if $\overline{\omega'}$ is another path in $Z(A_1,\ldots,A_n)$ then $\overline{d}(\overline{\omega},\overline{\omega'}) \leqslant 2\varepsilon$ because we can choose a parametrization ω' of $\overline{\omega'}$ such that the τ_i's coincide for ω and ω' and hence, for any $t \in [0,1]$, $\omega(t)$ and $\omega'(t)$ both belong to the same $A_j, j=1,\ldots,n$. We conclude that $Z(A_1,\ldots,A_n)$ and hence $\overline{Z}(A_1,\ldots,A_n)$ is contained in a closed ball in $\overline{\Omega}(x,y)$ of radius 2ε centered on $\overline{\omega}$. This ball is contained in U and the proof is complete. □

We remark that the proof of the above-mentioned result can of course be adapted to the case where the sets A_i are boxes in $\mathbb{R}^d$ rather than balls.

VI. INTEGRATING OVER CYLINDER SETS

In this section we show that the lattice approximation to the measure of the $\overline{Z}$ sets converges and we derive some formulas for the measure of these sets in terms of Dirichlet propagators.

Let A be a bounded set in $\mathbb{R}^d$ with a smooth boundary. Let x and y be two different points in the interior of A. We recall that the Dirichlet Green function for $\frac{1}{2}(-\Delta + m^2)$ with data on ∂A, denoted $G_A^D(x,y)$, is given by the Wiener integral over all paths from x to y that avoid ∂A. This fact is established in, e.g., Ref. 11 for the corresponding heat kernel and hence follows for the propagator by integrating over time.

In the following discussion the end points x and y will be kept fixed and for simplicity we denote the measure $V_{x,y}$ by μ. Accordingly we can write

$$G_A^D(x,y) = \int_{\overline{Z}(A)} \mathrm{d}\mu = \mu(\overline{Z}(A)). \tag{47}$$

We are interested in generalizing this formula to the case of $\overline{Z}(A_1,\ldots,A_n)$ with $n>1$ and showing that

$$\lim_{a\to 0} V_{x,y,a}(\overline{Z}(A_1,\ldots,A_n)) = \mu(\overline{Z}(A_1,\ldots,A_n)). \tag{48}$$

In order to minimize technical complications let us assume that the sets A_i are boxes so their boundaries are contained in hyperplanes.

Let us consider a family of boxes $A_1,\ldots,A_n$ in $\mathbb{R}^d$ with the property that the intersection of any two different boundaries ∂A_i and ∂A_j has codimension 2 or greater, i.e., the boundaries never overlap. Let us define O_1 as the collection of all paths in $\overline{\Omega}(x,y)$ that are somewhere tangent to one of the hyperplanes that make up the boundaries of the A_i's. Let O_2 be the collection of all paths in $\overline{\Omega}(x,y)$ that meet one or more of the intersections $\partial A_i \cap \partial A_j$, $i \neq j$. Put $O = O_1 \cup O_2$. It can be checked that the set of paths that are somewhere tangent to a given hyperplane is a measurable set with measure zero. It has measure zero since the probability that a Wiener path intersects a hyperplane exactly once in a time interval is zero, see, e.g., Ref. 12, Chap. 12. The set O_2 is easily seen to be closed and hence measurable. Its measure is zero since the codimension of the intersections $\partial A_i \cap \partial A_j$ is greater than 1. Thus, O is a measurable set with measure 0. The boundary of $Z(A_1,\ldots,A_n)$ consists of paths for which either two of the τ_i 's coincide or the path is tangent to one of the boundaries ∂A_i. Hence, $\partial\overline{Z}(A_1,\ldots,A_n) \subseteq \partial Z(A_1,\ldots,A_n) \subseteq O$. *We can therefore conclude from Ref. 9 Theorem 2.1 that the convergence (48) takes place for boxes* and the argument can be extended to the case of A_i's with piecewise smooth boundaries.

Let us now turn to the calculation of the measure of the $\overline{Z}$ sets. Let A be as before. Since $G_A^D(x,z) = 0$ for $z \in \partial A$ we have

$$\int_{\partial A}\frac{\partial}{\partial n}(G_A^D(x,z)G(z,y))\mathrm{d}S=\int_{\partial A}\frac{\partial G_A^D}{\partial n}(x,z)G(z,y)\mathrm{d}S, \tag{49}$$

where $\partial/\partial n$ is the normal derivative to ∂A with respect to z. Let Y_A be the collection of all paths from x to y which hit the boundary ∂A. An application of the divergence theorem and Eq. (47) lead to

$$\mu(Y_A)=\int_{\partial A}\frac{\partial G_A^D}{\partial n}(x,z)G(z,y)\mathrm{d}S. \tag{50}$$

More generally, it can be argued that

$$P_A(z)=\frac{\partial G_A^D}{\partial n}(x,z)G(z,y) \tag{51}$$

is [up to the constant factor $\mu(Y_A)$] the *conditional probability density* that a path from x to y which hits the boundary ∂A hits it for the first time at the point $z\in\partial A$, and $P_A(z)$ is given by an integral over all paths from x to y which hit the boundary of A and hit it for the first time in z.

It is convenient to extend the Dirichlet Green functions G_A^D to all of $\mathbb{R}^d$ such that they are 0 outside A. Let us now consider the case $x\in A_1$, $y\in A_2\backslash A_1$, $A_1\cap A_2\neq\varnothing$. Then the measure of $\overline{Z}(A_1,A_2)$ is the integral over all paths from x to y which leave A_1 for the first time at a point $z\in\partial A_1\cap A_2$ and stay in A_2 after they leave A_1. The integral over these paths is obtained by analogy with Eq. (50) as

$$\mu(\overline{Z}(A_1,A_2))=\int_{\partial A_1}\frac{\partial G_{A_1}^D}{\partial n}(x,z)G_{A_2}^D(z,y)\mathrm{d}S \tag{52}$$

and

$$\frac{\partial G_{A_1}^D}{\partial n}(x,z)\frac{G_{A_2}^D(z,y)}{\mu(\overline{Z}(A_1,A_2)}} \tag{53}$$

is the conditional probability density that a path in $\overline{Z}(A_1,A_2)$ leaves A_1 for the first time in the point z.

It is straightforward to generalize the above-mentioned considerations to the case of arbitrary n, i.e., $\overline{Z}(A_1,\ldots,A_n)$. By the Markov property of the Brownian paths we have

$$\mu(\overline{Z}(A_1,\ldots,A_n))=\int_{\partial A_1}\cdots\int_{\partial A_{n-1}}\prod_{i=1}^{n-1}\frac{\partial G_{A_i}^D}{\partial n_i}(z_{i-1},z_i)G_{A_n}^D(z_{n-1},y)\mathrm{d}S_1\ldots\mathrm{d}S_{n-1}, \tag{54}$$

where we have set $z_0=x$ and $\partial/\partial n_i$ denotes the normal derivative to ∂A_i with respect to z_i. In this integral formula z_i is the point where the path first leaves A_i after hitting $A_1,\ldots,A_{i-1}$ in that order.

We note that for $n=1$ the convergence (48), i.e., the convergence of the lattice approximations to the Dirichlet propagators is well known for sufficiently nice sets A. This convergence can also be proved directly without the use of measure theory. We also note that all the integration formulas given previously have clear lattice analogs for arbitrary n.

VII. CONCLUSION

We have in this paper defined integration over geometric paths and studied natural discretized measures on spaces of such paths. Two different discretizations were discussed, one with a metric degree of freedom and one without. We have proven the convergence of the discretized measures

and thereby in particular established the convergence of the discrete approximations to the integrals over paths that one is normally interested in for physics applications. We furthermore introduced, in the case without a metric degree of freedom, a natural class of sets of geometric paths which play the role of cylinder sets and generate the Borel algebra and we have shown how to calculate the measure of these sets in terms of Dirichlet propagators.

One, perhaps disappointing but not entirely unexpected, outcome of our analysis is that no technical simplifications are obtained by considering only parametrization independent quantities, i.e., by restricting to inherently physical degrees of freedom. In particular, it is hard to get a technical handle on geometric paths without introducing parametrizations to calculate with as is usually done in theories with a local gauge invariance.

One of the main motivations for this study was to obtain some insight into the corresponding problem for random surfaces. The random surface case is far more difficult than the one considered in this paper since the measures on parametrized surfaces which correspond to Wiener measure on paths are not well understood. Some of the ideas we have discussed here can be carried over to embedded surfaces but modifications would be needed since points on a geometric surface cannot be ordered like the points on a geometric path. For nonimbedded surfaces a new approach is required. In the absence of imbedding degrees of freedom, points on the surface have to be identified in terms of intrinsic geometric degrees of freedom like curvature. How to do this in a systematic fashion is far from obvious.

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Relativistic Lagrange formulation

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It is well-known that the equations for a simple fluid can be cast into what is called their Lagrange formulation. We introduce a notion of a generalized Lagrange formulation, which is applicable to a wide variety of systems of partial differential equations. These include numerous systems of physical interest, in particular, those for various material media in general relativity. There is proved a key theorem, to the effect that, if the original (Euler) system admits an initial-value formulation, then so does its generalized Lagrange formulation. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1364502]

I. INTRODUCTION

Consider a simple perfect fluid in general relativity. That is, fix a space-time—a 4-dimensional manifold M with metric g_{ab} of Lorentz signature $(-,+,+,+)$. The fluid is described thereon by two fields, a unit timelike vector field u^a (which is interpreted as the velocity field of the fluid), and a scalar field ρ (which is interpreted as its mass density). These fields must satisfy the fluid equations,

$$(\rho+p)u^m\nabla_m u^a=-(g^{am}+u^a u^m)\nabla_m p, \tag{1}$$

$$\nabla_m(\rho u^m)=-p\nabla_m u^m. \tag{2}$$

Here p is specified as some fixed function of ρ, the function of state.

This treatment is usually called the Euler formulation of a fluid. Its characteristic feature is that the fluid is described by means of fields on space–time. That is, the ''independent variable'' in this formulation—the thing the fields are functions of—is the event of space-time. There is an alternative treatment of a fluid, called the Lagrange formulation, in which we ''move with the fluid, rather than remain fixed in space–time.'' In other words, the independent variable in this formulation is the fluid-element, and so the fluid is described by fields that are functions on the manifold of fluid-elements.[1]

Each of these two formulations has its advantages. The Euler formulation is less tightly tied down to the fluid itself, and so is usually more convenient when other systems—which would naturally be described with reference to space–time—are involved. In particular, the Euler formulation is normally used for a fluid in interaction with other fields, as, for example, in the Einstein-fluid system. The Lagrange formulation, by contrast, tends to be more convenient when one wishes to identify and follow individual fluid elements. For example, the Lagrange formulation might be used to describe a fluid object with a boundary. The boundary, in this formulation,

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would be fixed once and for all at the beginning (by designating those fluid-elements that constitute the boundary) as part of the kinematical structure. In the Euler formulation of such an object, by contrast, the boundary would be ''dynamical.''

How are the Euler and Lagrange formulations related to each other? Certainly, the two are physically equivalent, i.e., they represent mere mathematical reformulations of the same physics. That is, all physical predictions will be the same, no matter which formulation is used; and, at least in principle, either formulation could be used to solve any given problem. Indeed, one might be tempted to go further than this, to view them as related by a mere coordinate transformation on the manifold of independent variables. But such a viewpoint would be misleading, for the ''coordinate transformation'' between the two sets of variables involves the dynamics of the system. Thus, for example, from the standpoint of the Euler formulation the Lagrange formulation represents a curious mixing of kinematics with dynamics.

These mathematical differences in fact go even deeper. It is well-known that the equations for a perfect fluid in the Euler formulation, Eqs. (1)–(2), have a well-posed initial-value formulation.[3] But the corresponding equations in the Lagrange formulation—at least, those obtained directly, by simply ''transforming'' the Euler equations—do not.[5] However, it has been shown by Friedrich, in Ref. 17, that, at least for a certain fluid system in general relativity, there *can* be introduced a Lagrange formulation having also an initial-value formulation. It is necessary, in Friedrich's treatment, to introduce a substantial number of additional fields (including a frame-field) together with additional equations on those fields. What is not so transparent, however, is the mechanism behind this treatment. Precisely what features of these fluid systems are needed for such a deterministic Lagrange formulation?

Our purpose in this paper is to introduce and explore a certain, broad, geometrical setting for the Lagrange formulation of systems of partial differential equations.

In Sec. II, we introduce that setting. Our framework is systems of partial differential equations that are first-order and quasi-linear (i.e., involving only first derivatives of the fields, and those only linearly)—a framework that includes virtually every partial differential equation in physics. Given any such system—provided only that it has among its fields a distinguished vector field—we write out a new system, its ''Lagrange formulation.'' The key idea of this scheme is what one might expect: Include, among the dynamical variables of the new system, what were the independent variables of the original system. It turns out that, in order to execute this scheme, it is normally necessary to introduce additional dynamical variables and equations. We give a general scheme for choosing these variables. The key result of this section is the following: Given any system of partial differential equations having a distinguished vector field as above, and also having an initial-value formulation, then a certain version of its Lagrange formulation also has an initial-value formulation.

In Sec. III, we give some examples of this scheme. We apply the present scheme not only to ordinary fluids, but also to various other types of material systems, including dissipative fluids and elastic solids. This scheme is also applicable when such material systems are undergoing interaction, e.g., when they are coupled to an electromagnetic or gravitational field. Finally, we show in Sec. III how Friedrich's original system fits within the present framework.

A number of related mathematical issues are discussed in the appendices. In Appendix A, we describe a general procedure for modifying any system of partial differential equations by ''taking derivatives'' of the fields of that system. This procedure, it turns out, is crucial for casting systems into a form in which our Lagrange formulation can be applied. In Appendix B, we review a few facts about the initial-value formulation of systems of partial differential equations. (For a more detailed treatment, see, for example, Ref. 2.)

II. LAGRANGE FORMULATION

Fix a first-order, quasilinear system of partial differential equations. That is, let there be given a fiber bundle, consisting of some base manifold M, some bundle manifold $\mathcal{B}$, and some smooth projection mapping $\mathcal{B}\overset{\pi}{\to}M$. Typically, M will be the 4-dimensional manifold of space–time

events (but it could be any smooth manifold). By the *fiber* over a point x of M, we mean the set of all points y of $\mathcal{B}$ such that $\pi(y)=x$. Think of the fiber over $x\in M$ as ''the set of possible field-values at x.'' Then $\mathcal{B}$ is interpreted as the set of ''all possible choices of field-values at all points of M,'' and π as the mapping that assigns, to each such choice, the underlying point of M. Thus, point y of $\mathcal{B}$ could be written as $y=(x,\phi)$, with $x\in M$ and ϕ in the fiber over x. The action of the projection mapping would then be given by $\pi(x,\phi)=x$. Typically, the fiber over a point $x\in M$ will be some collection of tensors, with given index structure (possibly subject to various algebraic conditions), at x, whence $\mathcal{B}$ will be a manifold of all such tensor-collections at all points of M. In this case, $\mathcal{B}$ is called a *tensor bundle*. However, $\mathcal{B}$ could in general be any smooth manifold, subject only to the local-product condition in the definition of a fiber bundle.[6]

By a *cross-section* of such a bundle we mean a smooth mapping $M\overset{\phi}{\rightarrow}\mathcal{B}$ such that $\pi\circ\phi$ is the identity map on M. In other words, a cross-section assigns, to each point x of M, a point of the fiber over x; i.e., it assigns a ''field-value'' at each point of M. In the case of a tensor bundle, a cross-section is simply a certain collection of smooth tensor fields on M. Our partial differential equation will be an equation on this map, linear in its first derivative. In order to write out this equation, we introduce two smooth fields, ${k^{Aa}}_{\alpha}$ and j^{A}, on $\mathcal{B}$. Since these are fields on $\mathcal{B}$, they depend on point $y=(x,\phi)$ of $\mathcal{B}$, i.e., they depend on a choice of ''point x of the base manifold, as well as field-value ϕ at that point.'' The index ''α'' on ${k^{Aa}}_{\alpha}$ is a tensor index in $\mathcal{B}$ at the point, $y\in\mathcal{B}$, at which this field is evaluated; the index ''a'' is a tensor index in M at the corresponding point, $\pi(y)$, of the base manifold. The index ''A,'' on both ${k^{Aa}}_{\alpha}$ and j^{A}, lies in some new vector space (which will turn out, shortly, to be the vector space of equations). Finally, our partial differential equation, on a cross-section ϕ, is

$$ {k^{Aa}}_{\alpha}(\nabla\phi)_{a}{}^{\alpha}=j^{A}. \tag{3}$$

This equation is to be imposed at each point $x\in M$, with the fields k and j evaluated at $\phi(x)\in\mathcal{B}$, i.e., on the cross-section. Here, $(\nabla\phi)_{a}{}^{\alpha}$ denotes the derivative of the map ϕ [i.e., a map from tangent vectors in M at x to tangent vectors in $\mathcal{B}$ at $\phi(x)$]. The index ''A'' in Eq. (3) is free, i.e., Eq. (3) represents a number of scalar equations equal to the dimension of the vector space in which ''A'' lies.

Here is an example. Fix a 4-dimensional manifold M, together with a Lorentz-signature metric g_{ab} on this M. Let $\mathcal{B}$ be the 8-manifold consisting of triples, (x,u^{a},ρ), where x is a point of M, u^{a} is a unit timelike vector at x, and ρ is a number. Let $\pi(x,u^{a},\rho)=x$. This is a fiber bundle; in fact, a tensor bundle. The fiber over a point $x\in M$ consists of (u^{a},ρ), a vector at x together with a number. A cross-section of this bundle is represented by smooth fields, u^{a} and ρ, on M. Let the equations, on such a cross-section, be (1)–(2), where $p(\rho)$ is some given, fixed function of one variable, and ∇_{a} is the derivative operator defined by the space–time metric g_{ab}. This is a first-order, quasilinear system of partial differential equations, i.e., the equations are linear in the first derivatives of the fields. The vector space of equations, in this example, has dimension four. This system, of course, describes a simple perfect fluid in general relativity.

We shall now introduce a technique that transforms a given first-order, quasilinear system of partial differential equations—provided that system lies within a certain class—into a new first-order, quasilinear system of partial differential equations. This new system will be called the *Lagrange formulation* of the original. While the new system will differ in many respects from the original one—e.g., it will have a different base manifold, a different bundle manifold, and a different number of equations—the two will be intimately related to each other. In particular, it will turn out that there is a natural correspondence between the solutions of the original system and those of its Lagrange formulation.

In order to apply this technique to a given system of equations, it is necessary that that system satisfy the following condition: Among the various fields of the system there must be distinguished one consisting of a nowhere-vanishing vector field on the base manifold M. This condition means, then, that the fields of our system take the form (u^{a},φ), where u^{a} represents the

nowhere-vanishing vector field on M, and φ represents ''the rest of the fields.'' Thus, given a system that has, among its various fields, no vector field at all, then we shall be unable to write out any Lagrange formulation for it; and if it has several vector fields, then we must, at this stage, distinguish a particular one. We shall denote by $B \overset{\pi}{\to} M$ the bundle in which the rest of the fields, the φ, lie, and use Greek indices for tensors in the manifold B. Note that these are *different* from the Greek indices, e.g., in Eq. (3), for tensors in the manifold $\mathcal{B}$. The equation for our system may now be written as

$$k'^{Aa}{}_{b}\nabla_a u^b + k''^{Aa}{}_{\alpha}(\nabla\varphi)_a{}^{\alpha} = j^A, \tag{4}$$

where $k'^{Aa}{}_{b}$, $k''^{Aa}{}_{\alpha}$, and j^A are all functions of u^a, φ, and point of M. In Eq. (4), the ∇_a in the first term can be any derivative operator on M; and the form of j^A depends, of course, on what operator has been chosen. We could, for example, simply fix, once and for all, some derivative operator ∇_a, and use it to write Eq. (4). Should it happen that the manifold M comes equipped with a kinematical metric (i.e., one not included among the physical fields φ), then it is often convenient to use its derivative operator in Eq. (4). This possibility is available, e.g., for systems representing fluids in special relativity, or in general relativity with a fixed background metric. In fact, we could even choose the derivative operator ∇_a in Eq. (4) to depend on the fields (u^a, φ) themselves, provided only that its dependence on these fields is algebraic, rather than through their derivatives. We now obtain the Lagrange formulation of this system.

For the base manifold of the Lagrange formulation, we choose any manifold $\hat{M}$ having the same dimension as M. Tensors over this $\hat{M}$ will be denoted by lower-case Latin indices with hats. We also fix, once and for all on this manifold $\hat{M}$, a nowhere-vanishing vector field, $\hat{u}^{\hat{a}}$. This $\hat{u}^{\hat{a}}$ is a purely kinematical object, i.e., it is fixed right at the beginning, and will not be subject to any dynamical equations.

We next specify the bundle manifold, $\hat{\mathcal{B}}$, of the Lagrange formulation. Fix a point, $\hat{x}$, of the base manifold $\hat{M}$. Let the fiber over this point consist of a triple, $(x, \varphi, \kappa_{\hat{a}}{}^{b})$, where (i) x is a point of M, the base manifold of the original system, (ii) φ is a point of the fiber over x in B, the bundle manifold for the original system, and (iii) $\kappa_{\hat{a}}{}^{b}$ is an invertible tensor, where the index ''$\hat{a}$'' refers to tensors in $\hat{M}$ at the point $\hat{x} \in \hat{M}$ and the index ''b'' refers to tensors in M at the point $x \in M$. A more detailed discussion of these three objects follows.

(i) The points (x) of the base manifold M of the original system become, in its Lagrange formulation, *field-values*. In the case of a simple perfect fluid, for example, each point of the original base manifold M represents an event of space–time; while each point of the new base manifold $\hat{M}$ represents ''a particular fluid-element at a particular moment of its life.'' Thus, in the Lagrange formulation of such a fluid, x will be a field over $\hat{x}$, a field that specifies ''which event in space–time that particular fluid-element occupies at that particular moment.''

(ii) The field-values, the φ, of the original system become field-values also in its Lagrange formulation. But there is one important change: What were fields over M in the original system become, in its Lagrange formulation, fields over $\hat{M}$. Thus, were the fields collected in φ all tensor fields on M, then the corresponding fields in the Lagrange formulation would depend on point $\hat{x}$ of $\hat{M}$, but would continue to be tensors in the tangent space at the point x of M.[7] In the case of a simple perfect fluid, this step amounts, physically, to ''attaching the density ρ to the fluid element, rather than to the point of space–time.''

(iii) There is introduced a new object, $\kappa_{\hat{a}}{}^{b}$, an invertible two-point tensor, with one index at $\hat{x} \in \hat{M}$, the other at $x \in M$. Nothing analogous was present in the original system. Denote the inverse of $\kappa_{\hat{a}}{}^{b}$ by $\overline{\kappa}_{b}{}^{\hat{a}}$, so we have $\kappa_{\hat{a}}{}^{b}\overline{\kappa}_{b}{}^{\hat{c}} = \delta_{\hat{a}}{}^{\hat{c}}$ and $\overline{\kappa}_{b}{}^{\hat{a}}\kappa_{\hat{a}}{}^{c} = \delta_{b}{}^{c}$. The role of this tensor $\kappa_{\hat{a}}{}^{b}$ is, as we shall see, to preserve the first-order character of the final system of

equations. Note that the dynamical field u^a in the original system has disappeared entirely: There is no analog of it as a dynamical field in the Lagrange formulation.

Next note that the pair (x,φ), where x is a point of M and φ is a point of the fiber in B over x, is precisely the same thing as a point of the bundle manifold B. Call that point (for later convenience) $\hat{\varphi}$, so we have $\hat{\varphi}=(x,\varphi)\in B$. Then we may recover the point x of the original base-manifold from the point $\hat{\varphi}\in B$ using the projection π: We have $x=\pi(\hat{\varphi})$. Thus, our construction of the bundle manifold $\hat{\mathcal{B}}$ for the Lagrange formulation could have been stated as follows: The fiber over point $\hat{x}\in\hat{M}$ consists of a pair, $(\hat{\varphi},\kappa_{\hat{a}}{}^{b})$, where $\hat{\varphi}$ is a point of the manifold B, and $\kappa_{\hat{a}}{}^{b}$ is an invertible tensor with one index at $\hat{x}\in\hat{M}$, the other at $\pi(\hat{\varphi})\in M$.

We have now completed the specification of the fiber bundle in which the Lagrange formulation of our system will be written. The base manifold, $\hat{M}$, is some new manifold, of the same dimension as M, while the bundle manifold $\hat{\mathcal{B}}$ is such that the fiber over $\hat{x}\in\hat{M}$ consists of a pair, $(\hat{\varphi},\kappa_{\hat{a}}{}^{b})$, where $\hat{\varphi}\in B$, and $\kappa_{\hat{a}}{}^{b}$ is a certain 2-point tensor. A cross-section of this bundle, then, is a smooth map (a map we also denote by $\hat{\varphi}$) that assigns, to each point $\hat{x}\in\hat{M}$, a point $\hat{\varphi}$ of B together with a suitable tensor $\kappa_{\hat{a}}{}^{b}$. On such a cross-section, we now impose the following equations:

$$(\nabla(\pi\circ\hat{\varphi}))_{\hat{a}}{}^{b}=\kappa_{\hat{a}}{}^{b}, \tag{5}$$

$$\nabla_{[\hat{c}}(\kappa_{\hat{a}]}{}^{b})=f_{\hat{c}\hat{a}}{}^{b}, \tag{6}$$

$$k'^{Aa}{}_{b}\overline{\kappa}_{a}^{\hat{d}}\nabla_{\hat{d}}(\kappa_{\hat{c}}{}^{b}\hat{u}^{\hat{c}})+k''^{Aa}{}_{\alpha}\overline{\kappa}_{a}^{\hat{c}}(\nabla\hat{\varphi})_{\hat{c}}{}^{\alpha}=j^{A}. \tag{7}$$

These are the equations of the Lagrange formulation. In Eq. (5), the combination $\pi\circ\hat{\varphi}$ is a map from $\hat{M}$ to M, for $\hat{\varphi}$ goes from $\hat{M}$ to B, and π from B down to M. Equation (5) asserts that the derivative of this map is precisely the tensor $\kappa_{\hat{a}}{}^{b}$. Thus, this equation provides the geometrical meaning of the field $\kappa_{\hat{a}}{}^{b}$. Note that invertibility of $\kappa_{\hat{a}}{}^{b}$ in Eq. (5) implies that the map $\pi\circ\hat{\varphi}$ from $\hat{M}$ to M is a local diffeomorphism between these two manifolds. It was to achieve this feature that we originally choose $\hat{M}$ to have the same dimension as M. Equation (6) is merely the curl[8] of Eq. (5). Any derivative[9] may be used on the left in Eq. (6), but the exact form of the function $f_{\hat{c}\hat{a}}{}^{b}$ [of $(\hat{\varphi},\kappa_{\hat{a}}{}^{b})$] that appears on the right will depend on which derivative was chosen. This situation is analogous to that of Eq. (4). Equation (7) is the translation of the equation of the original system (4) to our new system. Here, everywhere in the fields $f_{\hat{c}\hat{a}}{}^{b}$, $k'^{Aa}{}_{b}$, $k''^{Aa}{}_{\alpha}$, and j^{A} there is to be substituted the combination ''$\kappa_{\hat{a}}{}^{b}\hat{u}^{\hat{a}}$'' for ''$u^{b}$;'' and ''$\hat{\varphi}$'' for ''$\varphi$.'' In Eq. (7), this ''replacement'' takes place even inside the derivative. Note that the field u^{b} of the original system has now disappeared entirely, having been replaced by the image of the kinematical field $\hat{u}^{\hat{b}}$ under the mapping $\pi\circ\hat{\varphi}$.

Thus, beginning with any first-order, quasilinear system of partial differential equations of the form (4), we obtain a new system of equations, its Lagrange formulation, of the form (5)–(7). The Lagrange formulation has a completely new base space, but fields and equations that echo those of the original system.

We now claim the following: Every solution of the Lagrange formulation gives rise, at least locally, to a solution of the original system. Indeed, let $(\hat{\varphi},\kappa_{\hat{a}}{}^{b})$ be fields satisfying (5)–(7). Then, as we have seen, $\pi\circ\hat{\varphi}$ is a local diffeomorphism between $\hat{M}$ and M. We now introduce the following two fields on M: $u^{b}=(\nabla(\pi\circ\hat{\varphi}))_{\hat{a}}{}^{b}\hat{u}^{\hat{a}}$, and $\varphi=\hat{\varphi}\circ(\pi\circ\hat{\varphi})^{-1}$. That is, we let u^{b} and φ be the images of $\hat{u}^{\hat{b}}$ and $\hat{\varphi}$, respectively, under the diffeomorphism $\pi\circ\hat{\varphi}$. Then these fields, (u^{b},φ), on M satisfy the system (4), as is immediate from Eqs. (5), (7). We next claim that the converse also holds: Every solution of the original system gives rise, at least locally, to a solution of its Lagrange formulation. Indeed, let (u^{b},φ) be fields satisfying (4). Choose any manifold $\hat{M}$ with the same dimension as that of M, and any nowhere-vanishing vector field $\hat{u}^{\hat{a}}$ thereon. Now let $\hat{\varphi}$ be

a diffeomorphism between $\hat{M}$ and the cross-section, $\varphi[M]$, such that $(\pi\circ\hat{\varphi})$ sends $\hat{u}$ to u; and then define $\kappa_{\hat{a}}{}^{b}$ by Eq. (5). Then these fields $(\hat{\varphi},\kappa_{\hat{a}}{}^{b})$ on $\hat{M}$ will satisfy Eqs. (5)–(7) [the first two by construction, the last by Eq. (4)].

Thus, the original system and its Lagrange formulation are identical as to solutions. But the two systems are quite different as to form. Their base manifolds, $\hat{M}$ and M, although of the same dimension, differ in their geometry. The manifold $\hat{M}$ must be endowed with a fixed, kinematical ''velocity field,'' $\hat{u}^{\hat{a}}$, while M has no such kinematical field. On the other hand, various kinematical fields that might have been specified over M (such as a Lorentz metric) yield no analogous kinematical fields[10] on $\hat{M}$. Furthermore, the fields of the two systems differ in several respects. Beginning with the fields of the original system, we must delete the dynamical field u^{a}, while adding ''point of M'' as well as the invertible tensor $\kappa_{\hat{a}}{}^{b}$, to obtain the fields of the Lagrange formulation. Finally, the equations for the two systems differ in that, for the Lagrange formulation, there must be introduced one new equation (5) on the derivative of the ''point of M,'' as well as is the curl (6) of this new equation.

What we have described above is precisely what is usually done in writing down the Lagrange formulation for a fluid. For example, consider again the simple perfect fluid, with fields (u^{a},ρ) on M and Eqs. (1)–(2). Its Lagrange formulation consists of fields[11,12] $(x,\kappa_{\hat{b}}{}^{a},\hat{\rho})$ on $\hat{M}$, with equations consisting of (5), (6), and

$$(\hat{\rho}+p(\hat{\rho}))\hat{u}^{\hat{c}}\nabla_{\hat{c}}(\kappa_{\hat{m}}{}^{a}\hat{u}^{\hat{m}})+(g^{am}+\hat{u}^{\hat{c}}\kappa_{\hat{c}}{}^{a}\hat{u}^{\hat{n}}\kappa_{\hat{n}}{}^{m})\overline{\kappa}_{m}{}^{\hat{b}}\nabla_{\hat{b}}p(\hat{\rho})=0, \tag{8}$$

$$\hat{u}^{\hat{b}}\nabla_{\hat{b}}\hat{\rho}+(\hat{\rho}+p(\hat{\rho}))\overline{\kappa}_{a}{}^{\hat{b}}\nabla_{\hat{b}}(\kappa_{\hat{m}}{}^{a}\hat{u}^{\hat{m}})=0. \tag{9}$$

We now return to the general case. It turns out that the procedure given above—starting with a system and ending with its Lagrange formulation—suffers from a serious difficulty. In general, the equations of the Lagrange formulation, (5)–(7), will fail to have an initial-value formulation, even if the original system, (4), did have such a formulation. For example, the system (5)–(6), (8)–(9) has no initial-value formulation, although the system (1)–(2) of course does. But it turns out that this difficulty does not arise—i.e., the Lagrange formulation does inherit an initial-value formulation from the original system—provided the original system satisfies the following condition: There can be derived from Eq. (4) an expression for the derivative of the vector field u^{a}, without contractions, back in terms of the various fields of the system. In other words, it must be possible to cast Eq. (4) into the form

$$\nabla_{a}u^{b}=w_{a}{}^{b}, \tag{10}$$

$$k''^{Aa}{}_{\alpha}(\nabla\varphi)_{a}{}^{\alpha}=j'^{A}, \tag{11}$$

where $w_{a}{}^{b}$, $k''^{Aa}{}_{\alpha}$, and j'^{A} are functions of (x,u^{a},φ), i.e., are functions of the point of B and the vector u^{a}. In Eq. (10), ∇_{a} can, again, be any derivative operator on the manifold M; and the form of $w_{a}{}^{b}$ depends, of course, on what operator has been chosen. Note that, once we have derived from Eq. (4) an equation of the form (10), then it is easy to cast the equations that remain into the form (11): Simply use Eq. (10) to remove all u-derivatives from Eq. (4). Indeed, we have $j'^{A}=j^{A}-k'^{Aa}{}_{b}w_{a}{}^{b}$.

The equations for systems of physical interest typically do *not* take the form of Eqs. (10)–(11), i.e., they do not express the derivative of u^{a} in terms of the other fields. For example, Eqs. (1)–(2) do not have this form. But it turns out that there is a simple, general procedure by which *any* first-order, quasilinear system of partial differential equations having a preferred vector field u^{a} can be recast so as to take the form (10)–(11). This procedure, called taking the *derivative system*, is spelled out in Appendix A. It consists of modifying the original system by introducing additional fields, which represent the derivatives of the original fields, as well as additional equations on those fields. The result of taking the derivative system is to produce a new system of

partial differential equations, having, in an appropriate sense, identical solutions to the original. Applied to a system in which a preferred vector field u^a has been distinguished, it produces a system in which $\nabla_a u^b$ is expressed back in terms of the fields of the system. Furthermore, applied to any system having an initial-value formulation, the derivative system also has an initial-value formulation.

As an example of this procedure, we return to the system, (1)–(2), for a simple perfect fluid in general relativity. For the distinguished nowhere-vanishing vector field in this case, we choose, of course, the velocity field u^a of the fluid. The result of taking the derivative system of this system is the following. The fields consist of $(u^a,\rho,w_a{}^b,v_a)$, where u^a is a unit timelike vector field, ρ a positive scalar field, $w_a{}^b$ a tensor field satisfying $g_{ab}u^a w_c{}^b=0$, and v_a a vector field, all subject to the algebraic conditions

$$(\rho+p)u^m w_m{}^a+(g^{am}+u^a u^m)(\partial p/\partial\rho)v_m=0, \tag{12}$$

$$u^m v_m+(\rho+p)w_m{}^m=0. \tag{13}$$

On these fields is imposed the following system of first-order, quasilinear partial differential equations:

$$\nabla_a u^b=w_a{}^b, \tag{14}$$

$$\nabla_{[a}w_{b]}{}^c=R_{abm}{}^c u^m, \tag{15}$$

$$\nabla_a\rho=v_a, \tag{16}$$

$$\nabla_{[a}v_{b]}=0. \tag{17}$$

Note what has happened here. We have introduced two new fields, $w_a{}^b$ and v_a. The ''interpretation'' of $w_a{}^b$ [via (14)] is as the derivative of u^b; and of v_a [via (16)] as the derivative of ρ. The original fluid equations, (1)–(2), have been converted into algebraic conditions, (12)–(13), on these new fields. That is, the original fluid equations serve merely to define the bundle of fields for this new system. Finally, the new system contains two other equations, Eqs. (15) and (17), that are merely the curls of Eqs. (14) and (16), respectively.

In short, our ''procedure'' has done nothing of substance. But note that, starting with a system (1)–(2), which fails to express $\nabla_a u^b$ in terms of the fields of the system, our procedure produces a new system satisfying, via (14), this condition. Furthermore—and this is perhaps the striking feature—the system (14)–(17) inherits from the original fluid system, (1)–(2), its initial-value formulation.

The key result of this section is the following: *Consider any system (4) of partial differential equations in which there has been selected a preferred vector field u^a. Let (i) that system have an initial-value formulation, and (ii) the equations of that system express the derivative of u^a in terms of the fields of the system [as in (10)–(11)]. Then the Lagrange formulation of that system also admits an initial-value formulation.*

First note that the Lagrange formulation of the system (10)–(11) consists of Eqs. (5)–(6), together with

$$\overline{\kappa}_a{}^{\hat{c}}\nabla_{\hat{c}}(\kappa_{\hat{m}}{}^b\hat{u}^{\hat{m}})=w_a{}^b, \tag{18}$$

$$k''^{Aa}{}_{\alpha}\overline{\kappa}_a{}^{\hat{b}}(\nabla\hat{\varphi})_{\hat{b}}{}^{\alpha}=j'^A. \tag{19}$$

As discussed in Appendix B, in order that a general first-order, quasilinear system of partial differential equations have an initial-value formulation it is necessary that it satisfy three conditions: (i) the system admits a hyperbolization; (ii) all the constraints of the system are integrable,

and (iii) the system has the correct number of equations relative to the number of its unknowns. What these conditions mean is also explained in Appendix B. We check these three conditions in turn.

Let the original system, Eqs. (10)–(11), admit a hyperbolization. Then the construction that, applied to Eqs. (10)–(11) to obtain a bilinear expression in $\delta\varphi^{\alpha}$ yields, when applied to Eqs. (18)–(19), a corresponding bilinear expression in $\delta\hat{\varphi}^{\hat{\alpha}}$. Next, contract Eq. (6) with $\hat{u}^{\hat{c}}$ and use Eq. (18) to obtain an equation expressing $\hat{u}^{\hat{m}}\nabla_{\hat{m}}\kappa_{\hat{a}}{}^{b}$ algebraically in terms of the fields. From this there follows immediately an appropriate bilinear expression in $\delta\kappa_{\hat{a}}{}^{b}$. Finally, a bilinear expression in δx arises from Eq. (5). These three bilinear expressions, taken together, represent a hyperbolization for the system (5)–(6), (18)–(19).

Every constraint of the original system (10)–(11) gives rise to a constraint of its Lagrange formulation; and, furthermore, if these constraints of the original system are integrable, then so are the corresponding constraints of the Lagrange formulation.[13] This assertion is immediate from the fact that Eqs. (18) and (19) mimic Eqs. (10) and (11), respectively. But, it turns out, there are two additional classes of constraints for the system of the Lagrange formulation. The first class arises from taking the curl of each side of Eq. (5). These constraints are certainly integrable, and, indeed, the corresponding integrability conditions are precisely Eq. (6). The second class of constraints arises from taking the curl of each side of Eq. (6). These constraints are also integrable, and indeed their integrability conditions are identities, simply from the way Eq. (6) was obtained. We conclude, thus, that a system of the form (10)–(11) having all its constraints integrable leads to a Lagrange formulation (5)–(6) (18)–(19), also having all its constraints integrable.

Finally, in order to check the third condition, we introduce the following integers. Denote by n the dimension of the base space M (the number of independent variables of the system), by u the dimension of the fibers in the bundle B (the number of unknowns represented by φ), by e the dimension of the vector space in which the index ''A'' of Eq. (11) lies, and by c the dimension of the space of vectors of the form $w_m c^m{}_A$, as $c^m{}_A$ runs over constraints for Eq. (11). Then, for the original system, we have the number of unknowns is given by $u_0=u+n$ (the term ''n'' arising from the field u^a); the number of equations is given by $e_0=n^2+e$ [these terms arising from Eqs. (10) and (11), respectively]; and the number of effective constraints is given by $c_0=n(n-1)+c$ [these terms arising from the constraints of Eqs. (10) and (11), respectively]. For the Lagrange formulation, on the other hand, we have: the number of unknowns is given by $u_L=u+n+n^2$ (the term ''n'' arising from the field ''point of M,'' the term ''n^2'' from the field $\kappa_{\hat{a}}{}^{b}$); the number of equations is given by $e_L=n^2+n^2(n-1)/2+n^2+e$ [these terms arising from Eqs. (5)–(6), (18)–(19), respectively]; and the dimension of the space of effective constraints is given by $c_L=n(n-1)+n(n-1)(n-2)/2+n(n-1)+c$ [these terms arising from the constraints of Eqs. (5)–(6), (18)–(19), respectively]. It is easy to check from these formulas that $e_0-c_0=u_0$ implies $e_L-c_L=u_L$. In other words, if the original system has the appropriate number of equations relative to its number of unknowns, then so does its Lagrange formulation.

Thus, we have shown a system of the form (10)–(11) having an initial-value formulation gives rise to a Lagrange formulation also with an initial-value formulation.

III. EXAMPLES

In this section, we introduce various examples of physical systems, the partial differential equations that describe them, and the Lagrange formulations of those partial differential equations.

One such example, the simple perfect fluid, has been discussed already in Sec. II. The fields, on space–time, M, g_{ab}, consist of a unit timelike vector field u^a (interpreted as the fluid velocity) and a positive scalar field ρ (interpreted as the mass density); and the equations are (1)–(2), where $p(\rho)$ is some fixed function (the function of state), which specifies the type of fluid under consideration. This is the Euler formulation. In order to achieve a Lagrange formulation for this system, the first step is to modify these equations so that the derivative of u^a, without contractions, is expressed in terms of the other fields. This was achieved by taking the derivative system: We introduced two new (tensor) fields, $w_a{}^b$ and v_a, subject to the algebraic conditions (12)–(13). We

then imposed on the total set of fields, $(u^a, \rho, w_a{}^b, v_a)$, the partial differential equations (14)–(17). This new system (14)–(17) is, by virtue of Eq. (14), of the required form, and, in addition, it inherits from the original system, (1)–(2), its initial-value formulation. To this system, (14)–(17), we may therefore apply the methods of Sec. II to obtain its Lagrange formulation. There result fields $(x, \hat{\rho}, \hat{w}_a{}^b, \hat{v}_a, \kappa_{\hat{a}}{}^b)$ on $\hat{M}$, subject to the equations (5)–(7). This new system, as demonstrated in Sec. II, again has an initial-value formulation.

There is a natural generalization of this simple perfect-fluid system to a much broader class of fluids. Fix some smooth manifold S, the points of which will, shortly, be interpreted as representing ''local, internal, states of the fluid.'' Also fix any space–time (M, g_{ab}). Let the fields, on this space–time, consist of a unit, timelike vector field, u^a (again interpreted as the velocity field of the fluid), together with a second field, φ, which is valued in S (and which is interpreted as giving the local state of the fluid at each point of space–time). Thus, φ is a mapping, $M \stackrel{\varphi}{\rightarrow} S$. As an example, the simple perfect-fluid system discussed above is the special case in which S is a 1-manifold (whose points are labeled by a coordinate ρ, whence φ reduces to the density field ρ). That is, our simple perfect fluid is one whose local state is completely characterized by the value of the density.

We next wish to write equations on these fields. To this end, fix two tangent vector fields, V^α and T^α, and one covector field, F_α, on the manifold S, where we have introduced Greek indices[14] to represent tensors in S. The physical interpretations of these fields will be given shortly. Let the equations for this system be

$$u^a \nabla_a u^b + (g^{ab} + u^a u^b)(\nabla \varphi)_a{}^\alpha F_\alpha = 0, \tag{20}$$

$$u^a (\nabla \varphi)_a{}^\alpha + V^\alpha \nabla_a u^a + T^\alpha = 0. \tag{21}$$

The first equation gives the fluid acceleration in terms of the derivative of the fluid state. We may interpret the field F_α, which acts by driving the fluid, as an ''effective force.'' The second equation gives the time rate of change of the fluid state in terms of that state and the divergence of u^a.[15] We may interpret the fields V^α and T^α, respectively, as giving the rate of change of fluid state under small volume-changes of a sample of that fluid, and under allowing a sample of that fluid to evolve in time. The simple perfect fluid, for example, has $F_\alpha = (\rho + p)^{-1} \nabla_\alpha p$, $V^\alpha = (\rho + p) \partial/\partial\rho$, and $T^\alpha = 0$ [for these choices reproduce Eqs. (1)–(2)]. Another familiar example is the perfect fluid with 2-dimensional manifold S of internal states, where the additional degree of freedom is represented by a conserved particle-number n. In this case, F_α is given by the same expression as above, V^α by $(\rho + p) \partial/\partial\rho|_n + n\, \partial/\partial n|_\rho$, and again T^α by 0. A more exotic example is that of a fluid consisting of several species of particles, between which chemical reactions can take place as the fluid evolves. In this case, we would have $\dim(S) > 2$ (the additional degrees of freedom describing the chemical composition of the fluid) and T^α nonzero (representing the rate and direction of the chemical reactions).

When does the system above satisfy the three properties, as discussed in Appendix B, for having an initial-value formulation? Two of these properties are immediate: Clearly, this system has no constraints, and the dimension of its space of equations is the same [namely, $\dim(S) + 3$] as the dimension of its space of fields. As for the third condition, this system, it turns out, admits a hyperbolization if and only if[16] $V^\alpha F_\alpha > 0$ everywhere on S. Note that, in the explicit examples given above, the combination $V^\alpha F_\alpha$ is precisely the square of the sound speed.

We now have a system of equations (20)–(21), having a preferred vector field, u^a, and, subject only to the inequality $V^\alpha F_\alpha > 0$, having an initial-value formulation. So, we may apply to this system the results of Appendix A and Sec. II. The first step is to take the derivative system (Appendix A). The result of this step is to include, in addition to the fields u^a, φ above, two new fields, $w_a{}^b$ (with $u_b w_a{}^b = 0$) and $\zeta_a{}^\alpha$, subject to the algebraic conditions $u^a w_a{}^b + (g^{ab} + u^a u^b) \zeta_a{}^\alpha F_\alpha = 0$ and $u^a \zeta_a{}^\alpha + V^\alpha w_a{}^a + T^\alpha = 0$. [These algebraic conditions reflect Eqs. (20)–(21).] The equations on these fields for the derivative system are given by

$$\nabla_a u^b = w_a{}^b, \tag{22}$$

$$\nabla_{[a} w_{b]}{}^c = R_{abd}{}^c u^d, \tag{23}$$

$$(\nabla \varphi)_a{}^\alpha = \zeta_a{}^\alpha, \tag{24}$$

$$\nabla_{[a} \zeta_{b]}{}^\alpha = 0. \tag{25}$$

This system indeed has a preferred vector field, u^a; has among its equations one [Eq. (22)] that expresses the derivative of this u^a algebraically in terms of the fields; and has an initial-value formulation [by virtue of that for Eqs. (20)–(21)]. So, we may, as described in Sec. II, take the Lagrange formulation of this system. There results a new system of partial differential equations, (5)–(7), again having an initial-value formulation.

Even the broad class of generalized fluids above does not include all possible types. For example, there exist fluids manifesting dissipative effects, such as heat-flow and viscosity. One description of such a fluid in relativity (Refs. 18–21) proceeds as follows. The fields consist of a unit timelike vector field u^a (interpreted as the fluid 4-velocity), two scalar fields, ρ and n (interpreted, respectively, as the fluid mass density and particle-number density), a vector field q_a satisfying $u^a q_a = 0$ (interpreted as the heat-flow vector), and a symmetric tensor field τ_{ab} satisfying $u^a \tau_{ab} = 0$ (interpreted as the stress tensor). Thus, the space of field-values at each point of M is 14-dimensional. The equations on these fields consist of (i) vanishing of the divergence of nu^a (conservation of particle number), (ii) vanishing of the divergence of $(\rho + p)u^a u^b + pg^{ab} + 2u^{(a} q^{b)} + \tau^{ab}$ (conservation of stress-energy), and (iii) a certain system of nine additional equations that, effectively, governs the dynamical evolution of q^a and τ^{ab}. It turns out that the resulting system, consisting of (i)–(iii), has an initial-value formulation: Specifically, it has a hyperbolization and no constraints. Furthermore—and this is perhaps surprising—this system of equations can be so chosen that it reduces, in an appropriate limit, to the familiar Navier–Stokes system for a dissipative fluid. [The Navier–Stokes dissipation coefficients—the thermal conductivity and viscosity—arise from within the nine equations (iii).] Here, in any case, is a system of equations with a preferred vector field u^a—a system, therefore, to which the present methods can be applied. Thus, we take the derivative system, as described in Appendix A, and then the Lagrange formulation, as described in Sec. II. There results a Lagrange formulation for a dissipative, relativistic fluid.

There exist still other types of material systems, e.g., some that are not fluids at all. Consider, for example, the elastic solid. In one treatment[22] of such a system in relativity, the fields consist of a unit timelike vector field u^a (the material 4-velocity), a positive function ρ (the mass density of the material), and a symmetric tensor field h_{ab} satisfying $h_{ab} u^b = 0$. This h_{ab} represents the geometry of the material as it was ''frozen in'' at the time the material originally solidified: It describes the shape to which the material would ''like to return.'' Thus, the combination $h_{ab} - (g_{ab} + u_a u_b)$, the difference between this natural geometry and the actual spatial geometry in which the material currently finds itself, is interpreted as the strain of the solid material. The equations on these fields are $\mathcal{L}_u h_{ab} = 0$ (the vanishing of the Lie derivative of h_{ab}, interpreted as asserting that the material remembers, over time, its frozen-in geometry), and $\nabla_b(\rho u^a u^b + \tau^{ab}) = 0$, (interpreted as the conservation of stress-energy, whence τ^{ab} is interpreted as the stress of the material). Here, τ^{ab} is to be given as some fixed function of h_{ab}, g_{ab}, and u^a. This is the stress–strain relation. Provided this stress–strain relation is chosen appropriately, the final system, it turns out, has an initial-value formulation: Specifically, it has a hyperbolization and no constraints. Again, we have a system to which the present methods can be applied. There results a Lagrange formulation for an elastic solid.

There are, presumably, a variety of other systems of equations, representing ''materials'' of various sorts, having, among their fields, a preferred 4-velocity. Examples might include the systems for a plasma, for a superconductor, or for a solid (such as ice) that is able to flow. These systems, too, will have Lagrange formulations.

These various material systems may, of course, interact with their environment in a variety of ways, e.g., electromagnetically, gravitationally, or through contact forces. What impact do such interactions have on their Lagrange formulations?

Consider, as an example, the fluid of Eqs. (20)–(21) interacting electromagnetically. This charged-fluid system is described by fields consisting of the original fluid variables, u^a and φ, together with an antisymmetric (electromagnetic) tensor field F_{ab}. The equations on these fields consist of Eq. (20), modified by the inclusion of a term on the right of the form $\mu F^b{}_a u^a$, Eq. (21)[23] and Maxwell's equations,

$$\nabla^b F_{ab} = \sigma u_a , \tag{26}$$

$$\nabla_{[a} F_{bc]} = 0. \tag{27}$$

Here, the μ in the first equation and the σ in Eq. (26) must be given as fixed fields on the manifold S of fluid states. The field σ describes how the fluid drives the electromagnetic field, and so is interpreted as the charge density. We require that it satisfy charge conservation: $V^\alpha \nabla_\alpha \sigma = \sigma$, $T^\alpha \nabla_\alpha \sigma = 0$. The field μ, which describes how the electromagnetic field drives the fluid, might be called the specific charge density. [For a normal fluid, σ and μ are in ratio $(\rho + p)$.] Here, in any case, is a list of fields, together with a system of equations on those fields. This system has an initial-value formulation, which it inherits from the separate initial-value formulations for the original fluid system [(20)–(21)] and for Maxwell's equations. We wish to take the Lagrange formulation for this system. Since the system does not express the derivative of u^a in terms of the other fields, the first step is to take the derivative system. But note that, in taking the derivative system, it is necessary to introduce, not only the new fields $w_a{}^b$ and $\zeta_a{}^\alpha$ that represent [via Eqs. (22) and (24), respectively] the derivatives of u^b and φ, but also the field ζ_{abc} that represents [via Eq. (A5)] the derivative of F_{ab}. One might have hoped that it would be possible, exploiting somehow the fact that our system of equations splits naturally into ''fluid equations'' and ''Maxwell-field equations,'' to avoid introducing the additional field ζ_{abc}. Unfortunately, this seems not to be the case. This issue is discussed briefly in Appendix A. In any case, this derivative system has the appropriate form (a preferred vector field u^a, whose derivative is expressed in terms of the fields of the system), and an initial-value formulation (which it inherits from that of the original coupled system). So, we may apply the methods of Sec. II. Thus, there is a Lagrange formulation for a charged fluid, but it requires the introduction of a further field ζ_{abc}, representing the derivative of the Maxwell field.

In a similar way, we may write down the Lagrange formulation for a charged dissipative fluid, a charged elastic solid, etc. In each of these cases, it is necessary to introduce the auxiliary field ζ_{abc}.

The situation for gravitational interactions is similar. Consider, again, the fluid of (20)–(21), now interacting gravitationally. The interacting system is described by fields consisting of the original fluid variables, u^a and φ, together with the variables for gravitation: a Lorentz-signature metric g_{ab}, and a derivative operator, ∇_a. The equations of this system consist of Eqs. (20)–(21),[24] the equation $\nabla_a g_{bc} = 0$, and Einstein's equation,

$$G_{ab} = T_{ab} , \tag{28}$$

where G_{ab} is the Einstein tensor. Here, T_{ab} is some fixed symmetric tensor function of g_{ab} and the fluid variables (which we interpret as the stress-energy tensor of the fluid). It plays a role analogous to that of the functions μ and σ for electromagnetic interactions. We demand of this tensor function that, as a consequence of Eqs. (20)–(21), it be conserved.[25] This system of equations does *not* have an initial-value formulation, in the sense we are using this term. But this is merely a consequence of the fact that our sense of this term is overly restrictive, in that it does not tolerate the diffeomorphism freedom characteristic of all systems in general relativity. In a physical sense, i.e., once the diffeomorphism freedom has been treated properly, the fluid-Einstein system does, of course, have an initial-value formulation. Now take the derivative system of this system. Note that

in doing so we must, as in the electromagnetic case, include also fields to represent the derivatives of the gravitational fields.[26] Take the Lagrange formulation of the result. The resulting system, again, will not have an initial-value formulation in our restrictive sense, but it will have such a formulation when the diffeomorphism-freedom is properly taken into account. We conclude, then, that there does exist a Lagrange formulation for a gravitating fluid, but that it requires that we introduce further fields to represent the derivatives of the gravitational fields.

In a similar way, we may write down the Lagrange formulation for a gravitating dissipative fluid, a gravitating elastic solid, etc. In each case, it is necessary to introduce fields representing the derivatives of the gravitational fields; and in each case the Lagrange formulation retains the initial-value formulation of the original system.

A similar treatment is available for systems consisting of two or more different materials in interaction. In these cases, there will be two or more 4-velocity fields present, and we shall have to select one to be that with respect to which the Lagrange formulation is taken.

The treatment of systems in which several interactions are turned on simultaneously, e.g., the charged gravitating fluid, is similar.

Finally, we briefly characterize, within the present framework, Friedrich's[17] original example of a relativistic Lagrange formulation. Begin with the system for a gravitating fluid, as described above, for the case in which the fluid has a 2-dimensional manifold S of local states, i.e., that in which $T^\alpha = 0$ and $V^\alpha = (\rho + p)\partial/\partial\rho|_n + n\partial/\partial n|_\rho$. For this system, first take the derivative system, and then the Lagrange formulation. The result of this process—after three, essentially cosmetic, further modifications—is precisely Friedrich's original example. The three further modifications are the following.

(1) Introduce, already in the original Einstein-fluid system, before taking the derivative system, a 3-dimensional space of additional variables, consisting of three unit vector fields, x^a, y^a, and z^a, that are required to be orthogonal to each other and to the 4-velocity u^a. On these fields, impose the equations that they be Fermi-transported by u^a. The introduction of these fields with these equations does not interfere with the initial-value formulation. These fields, which have no direct physical significance, are introduced to facilitate the writing of various equations.
(2) After taking the derivative system, but before passing to the Lagrange formulation, suppress half of the field $\zeta_a{}^\alpha$, which represents the derivative of the fluid state.[27] While such suppression of variables will in general destroy the initial-value formulation for a system, it turns out that, in this particular instance, it does not. Thus, the essential effect of this modification is to reduce by four the number of independent variables.
(3) Write the final equations, after passing to the Lagrange formulation, not in terms of the specific fields listed above, but rather in terms of others that are algebraic functions of these. This choice of variables—choice of ''coordinates'' on the bundle space—is, of course, a matter of convenience.

IV. CONCLUSION

We have introduced a scheme that takes a first-order, quasilinear system of partial differential equations and produces from it a new first-order, quasilinear system, its ''Lagrange formulation.'' The key requirement, on a given system of equations, in order that this scheme be applicable to it is that that system have, among its fields, some nowhere-vanishing vector field. Why this special role of a vector field? Could, for example, a similar scheme be developed based on some other geometrical object(s)? It turns out that there are two special features of vector fields that we used in the construction of the Lagrange formulation.

First, nowhere-vanishing vector fields on manifolds are locally homogeneous. This means the following. Let there be given any manifold M, any nowhere-vanishing vector field u^a thereon, and any point $x \in M$; and, similarly, some other manifold $\hat{M}$ (of the same dimension), vector field $\hat{u}^{\hat{a}}$ and point $\hat{x} \in \hat{M}$. Then there always exists a diffeomorphism between neighborhoods of x and $\hat{x}$

that sends u^a to $\hat{u}^{\hat{a}}$. In other words, nowhere-vanishing vector fields are ''locally all the same:'' They carry no local structure. We used this fact in Sec. II in order to replace u^a on M by some kinematical field $\hat{u}^{\hat{a}}$ on $\hat{M}$.

Second, by virtue of the appearance of the vector field $\hat{u}^{\hat{a}}$ on the left in Eq. (18), the system (6), (18) for the two-point tensor $\kappa_{\hat{a}}{}^{b}$ admits a hyperbolization. We used this fact in Sec. II in order to achieve a hyperbolization, and consequently an initial-value formulation, for the entire system (5)–(6), (18)–(19).

It appears that, given any other geometrical structure manifesting these two features, then there could be developed a ''Lagrange formulation'' based on it. It is only necessary to make three key modifications in Sec. II (all involving replacing the vector field by the totality of fields in the new geometrical structure): (i) Replace Eq. (10) by equations for the derivatives of all the fields of the geometrical structure; (ii) endow the base manifold $\hat{M}$ of the Lagrange formulation with kinematical fields consisting of all the fields of the geometrical structure; and (iii) replace Eq. (18) by the corresponding equation involving all the fields of the geometrical structure. Unfortunately, it is not so easy to find geometrical structures having the two features described above, in part because they are somewhat in opposition to each other: The first feature, local homogeneity, prefers fewer fields, relatively devoid of structure; while the second feature, hyperbolicity of (6), (18), prefers many fields, of rich structure.

There are a variety of geometrical structures that are locally homogeneous. Examples include: two commuting, pointwise independent vector fields; a nowhere-vanishing, curl-free 1-form; a symplectic structure; a flat, Lorentz-signature metric. Examples of geometrical structures that yield a hyperbolization for (6), (18) are somewhat less plentiful. One simple class consists of those in which the geometrical structure is comprised of a nowhere-vanishing vector field u^a, together with any additional fields of whatever type. For structures in this class, a hyperbolization for (6), (18) (suitably generalized) is guaranteed already by the presence of the vector field u^a in the structure.

Here is an application of these ideas. Consider the geometrical structure consisting of a nowhere-vanishing vector field u^a, together with a nowhere-vanishing 3-form, ω_{abc}, that has zero curl and is annihilated by u^a. This structure satisfies both of the features above—it is locally homogeneous, and it gives rise to a hyperbolization for (6), (18). So, this geometrical structure could serve as the basis for a Lagrange formulation. In fact, this formulation is appropriate for a physical system, namely that of a fluid with a 2-dimensional manifold of internal states, as discussed in Sec. III. Identify u^a with the velocity field of the fluid, and ω_{abc} with the particle-number density, via $\omega_{abc}=n\epsilon_{abcd}u^d$.

It is curious that the original system and its Lagrange formulation, while so similar with regard to their solutions, are completely different with regard to their initial-value formulations. Indeed, as we have seen in Sec. II, it is frequently the case that the original system of equations (4) has an initial-value formulation, while its Lagrange formulation, (5)–(7), does not. Perhaps there is some more natural or more general notion of ''initial-value formulation'' that would resolve this disparity.

APPENDIX A: DERIVATIVE SYSTEMS

Fix, once and for all, a first-order, quasilinear system of partial differential equations, as described in Sec. II. That is, fix a fiber bundle, with bundle manifold $\mathcal{B}$, base manifold M, and projection mapping $\mathcal{B}\overset{\pi}{\rightarrow}M$, together with smooth fields $k^{Aa}{}_{\alpha}, j^A$ on the bundle manifold $\mathcal{B}$. Our system of equations, on a cross-section, $M\overset{\phi}{\rightarrow}\mathcal{B}$, of this fiber bundle, is given by

$$k^{Aa}{}_{\alpha}(\nabla\phi)_a{}^{\alpha}=j^A. \tag{A1}$$

We shall now construct from this system a new first-order, quasilinear system of partial differential equations. The idea is to "take one derivative" (with respect to the point of M) of Eq. (A1).

The first step is to introduce the appropriate bundle of fields for the new system. Let the base manifold again be M. But now let the fiber, over a point $x \in M$, consist of all pairs, $(\phi, \zeta_a{}^\alpha)$, where ϕ is point of $\mathcal{B}$ satisfying $\pi(\phi) = x$ and $\zeta_a{}^\alpha$ is a tensor at ϕ satisfying

$$k^{Aa}{}_\alpha \zeta_a{}^\alpha = j^A. \tag{A2}$$

Thus, ϕ is merely a point of the fiber over $x \in M$, in the original bundle $\mathcal{B}$. It represents a set of "values for the original fields" at x. The tensor $\zeta_a{}^\alpha$ represents a set of "values for the derivatives of the original fields." In order that a given $\zeta_a{}^\alpha$ be a viable candidate for these derivatives, it must satisfy Eq. (A2), the algebraic equation that results from replacing $(\nabla\phi)_a{}^\alpha$ in Eq. (A1) by $\zeta_a{}^\alpha$. We impose this algebraic condition on ζ in the very construction of the new bundle (as opposed, e.g., to introducing it later as an "algebraic constraint"). In short, the *dynamics* [Eq. (A1)] of the original system goes into the *kinematics* [Eq. (A2)] of the new system. Call the bundle space of this new fiber bundle $\mathcal{B}'$. Thus, the dimension of the fibers of $\mathcal{B}'$ is given by: (dim fibers of $\mathcal{B}$) $(1 + \dim(M))$-(dim vector space of equations in $\mathcal{B}$).

Consider, as an example, Maxwell's equations. Then M is a 4-dimensional manifold, with fixed smooth metric g_{ab} of Lorentz signature. For the bundle $\mathcal{B}$, the fiber over $x \in M$ consists of all antisymmetric tensors, F_{bc}, at x. Equation (A1) is Maxwell's equations: $g^{ab}\nabla_a F_{bc} = 0$, $\nabla_{[a}F_{bc]} = 0$. For this example, the new bundle, $\mathcal{B}'$, has, as its fiber over $x \in M$, the collection of all pairs, (F_{bc}, ζ_{abc}), with symmetries $F_{bc} = F_{[bc]}, \zeta_{abc} = \zeta_{a[bc]}$, and with ζ satisfying the algebraic conditions [Eq. (A2)] $g^{ab}\zeta_{abc} = 0, \zeta_{[abc]} = 0$. Thus, the fibers of $\mathcal{B}$ have dimension six, those of $\mathcal{B}'$ dimension twenty-two.

Returning to the general case, the second step is to introduce appropriate equations on this bundle. A cross-section of the bundle $\mathcal{B}'$ consists of fields $\phi, \zeta_a{}^\alpha$ on M. On such a cross-section, we impose the following system of partial differential equations:

$$(\nabla\phi)_a{}^\alpha = \zeta_a{}^\alpha, \tag{A3}$$

$$\nabla_{[a}\zeta_{b]}{}^\alpha = f_{ab}{}^\alpha. \tag{A4}$$

Equation (A3) provides the "interpretation" of ζ, as the derivative of ϕ. The $f_{ab}{}^\alpha$ on the right of (A4) is some field on $\mathcal{B}'$ [i.e., some function of (x, ϕ, ζ)], whose exact form depends on what derivative operator is used on the left side of that equation. The general rule is that Eq. (A4) to be the result of taking the curl of Eq. (A3). For example, if ϕ is represented by tensor fields over M, if ζ is represented by the tensor fields obtained by taking the covariant derivatives (with respect to some fixed derivative operator on M) of those fields, and if that same derivative operator is used on the left in Eq. (A4), then f will consist of certain terms involving ϕ and the curvature tensor of that derivative operator. If, on the other hand, all bundles are taken as simple products, and all derivatives are taken using the corresponding (flat) connection, then $f_{ab}{}^\alpha = 0$. Note that we have *not* included in our system the derivative of Eq. (A2). The reason is that Eq. (A2) has already been included at the algebraic level in the construction of the bundle $\mathcal{B}'$. Its derivative is thus an identity in $\mathcal{B}'$. On the other hand, we *do* include in our system Eq. (A4), even though it merely results from taking a derivative of Eq. (A3). In short, all algebraic conditions on fields are included in the construction of the bundle,[28] while all differential conditions on fields are included in the equations on a cross-section of that bundle. We note that the system of Eqs. (A3)–(A4) is indeed first-order and quasilinear.

Consider again the example, above, of Maxwell's equations. Then a cross-section of bundle $\mathcal{B}'$ consists of smooth fields, F_{bc}, ζ_{abc}, satisfying everywhere the symmetries and algebraic conditions given above. The equations, (A3)–(A4), on such a cross-section become, respectively,

$$\nabla_a F_{bc} = \zeta_{abc}, \tag{A5}$$

$$\nabla_{[d}\zeta_{a]bc} = 2R_{da[b}{}^{m}F_{c]m}. \tag{A6}$$

Given a system, consisting of bundle $\mathcal{B}$ and partial differential equations (A1), then by its *derivative system* we mean the system, consisting of bundle $\mathcal{B}'$ and partial differential equations (A3)–(A4), constructed above. Note that every solution of the original system gives rise to a solution of its derivative system [by merely setting $\zeta_a{}^{\alpha} = (\nabla\phi)_a{}^{\alpha}$]. Conversely, every solution of the derivative system gives rise to a solution of the original system (by merely ignoring ζ). The two systems of partial differential equations are, in this sense, ''equivalent as to solutions.'' But they are not ''equivalent as to form,'' a feature we exploit in Sec. II.

We next turn to the issue of the existence of an initial-value formulation for these systems. As discussed in Appendix B, we say that a general first-order quasilinear system (A1) of partial differential equations admits an *initial-value formulation* provided it satisfies the following three conditions: (i) the system admits a hyperbolization; (ii) all constraints of the system are integrable; and (iii) the system has the correct number of equations relative to the number of its unknowns. See Appendix B for the details of what these conditions mean. A key property of the derivative system is the following: *If the original system, (A1) admits an initial-value formulation, then so does its derivative system, (A3)–(A4).* We check the three conditions in turn.

Let the original system (A1) admit a hyperbolization (say, $h_{\beta A}$, with w_a). Then, we claim, so does its derivative system. Indeed, the corresponding bilinear expression [on a pair of tangent vectors, represented as $(\delta\phi^{\alpha}, \delta\zeta_a{}^{\alpha})$ and $(\delta'\phi^{\alpha}, \delta'\zeta_a{}^{\alpha})$] is given by

$$w_m h_{\alpha A} k^{Am}{}_{\beta}[\overset{+}{g}{}^{ab}\delta\zeta_a{}^{\alpha}\delta'\zeta_b{}^{\beta} + \delta\phi^{\alpha}\delta'\phi^{\beta}], \tag{A7}$$

where $\overset{+}{g}{}^{ab}$ is any positive-definite metric field on M. It is apparently not known whether the converse is true, i.e., whether the existence of a hyperbolization for the derivative system, (A3)–(A4), implies the existence of a hyperbolization for the original system (A1). Simple examples suggest that this is a reasonable conjecture.

Integrable constraints of the system (A1) do *not* lead to constraints of the corresponding derivative system. Rather, they lead to a reduction in the number of effective equations. Indeed, let $c^b{}_A$ be any constraint. Then the result of contracting Eq. (A4) with $c^a{}_A k^{Ab}{}_{\alpha}$ is an identity: It holds automatically, by virtue of Eq. (A2). Thus, each constraint for the system (A1) reduces by one the number of effective equations represented by Eqs. (A3)–(A4).

What, then, *are* the constraints of the derivative system (A3)–(A4)? These fall into two classes. The first class consists of those constraints that correspond to taking the curl of Eq. (A3). These constraints are of course integrable: Their integrability conditions are precisely (A4). The second class of constraints consists of those that correspond to taking the curl of Eq. (A4). These constraints, too, are integrable, by virtue of the fact that Eq. (A4) is itself a curl. Not all of these constraints, it turns out, are in general algebraically independent.

Let us return to our original partial differential equation (A1). Denote by n the dimension of the base manifold M (the ''number of independent variables''), by u the dimension of the fibers in the bundle $\mathcal{B}$ (the ''number of unknown functions''), and by e the dimension of the vector space of equations, (A1). Further, denote by $\hat{c}$ the dimension of the vector space of constraints, and, for fixed nonzero covector w_a, by c the dimension of the space of vectors of the form $w_a c^a{}_A$, as $c^a{}_A$ runs over the constraints. Then, as discussed in Appendix B, the condition that the original system (A1) have the ''correct number of equations'' becomes $e - c = u$. We turn now to the derivative system (A3)–(A4). The number of its unknowns is given by $u' = u + (nu - e)$ (the two terms representing the numbers of unknowns contained in the fields ϕ and ζ, respectively). The number of its equations is given by $e' = nu + [un(n-1)/2 - \hat{c}]$ [the two terms representing the number of effective equations in (A3) and (A4)], respectively. Finally, the number of effective constraints of the derivative system is given by $c' = u(n-1) + [(n-1)(n-2)u/2 + c - \hat{c}]$, (the two terms rep-

resenting the number of effective constraints in (A3) and (A4), respectively[29]). From these formulas, it is easy to check: If $e-c=u$, then $e'-c'=u'$. In other words, if the original system has the correct number of equations, then so does the derivative system.

We conclude, then, that, beginning with a system (A1) having an initial-value formulation, its derivative system, (A3)–(A4), also has an initial-value formulation.

The construction above of the derivative system is useful because it permits a large class of systems of partial differential equations to be cast into a form to which the Lagrange formulation of Sec. II can be applied. But, unfortunately, passing to the derivative system and then to the Lagrange formulation is often a cumbersome procedure. The reason is that the derivative system requires the introduction of additional fields to represent the derivatives of *all* the fields of the original system—even of those fields only remotely related to the one real interest: the velocity field. The result is a large number of extraneous fields. More useful would be a construction that goes only part way to the full derivative system—one that introduces additional fields to represent the derivatives of only *some* of the original fields, leaving the remaining ones intact. It turns out that, while there are one or two systems (e.g., that for dust) for which a smaller derivative system along these lines is available, for the vast majority of systems of partial differential equations of physical interest there is none. Here, briefly, is why.

First, we must designate which of the dependent variables (the fields represented by ϕ) are to be derived and which not. This is done by writing the original bundle, $\mathcal{B}$, as a product of two bundles, $\mathcal{B}'$ and $\mathcal{B}''$, with the same base space[30] M. The bundle $\mathcal{B}'$ carries the fields whose derivatives will be represented by new variables, while $\mathcal{B}''$ carries the remaining fields. A cross-section ϕ of $\mathcal{B}$ consists precisely of a pair, (ϕ',ϕ''), where ϕ' is a cross-section of the bundle $\mathcal{B}'$, and ϕ'' is a cross-section of the bundle $\mathcal{B}''$. In terms of these variables, Eq. (A1) becomes

$$k'^{Aa}{}_{\alpha'}(\nabla\phi')_a{}^{\alpha'}+k''^{Aa}{}_{\alpha''}(\nabla\phi'')_a{}^{\alpha''}=j^A, \tag{A8}$$

where primed Greek indices denote tensors in $\mathcal{B}'$, and double-primed in $\mathcal{B}''$. Here, the fields k', k'' and j are all functions on $\mathcal{B}$, i.e., are functions of (x,ϕ',ϕ''). We now proceed just as with the derivative system. Introduce a new fiber bundle, with base manifold again M, but with fiber over $x\in M$ consisting of certain triples, $(\phi',\zeta_a{}^{\alpha'},\phi'')$. There must now be imposed on such triples all those algebraic conditions that flow from (A8). This is done as follows. At each point, denote by V the vector space of μ_A satisfying $\mu_A k''^{Aa}{}_{\alpha''}=0$. That is, V captures "those equations in (A8) that contain no derivative of ϕ''." We now demand, in order that a triple $(\phi',\zeta_a{}^{\alpha'},\phi'')$ give rise to a point of the fiber, the following: For every $\mu_A\in V$, $\mu_A k'^{Aa}{}_{\alpha'}\zeta_a{}^{\alpha'}=\mu_A j^A$. This is the fiber bundle for our new system. Let the equations of the new system be

$$(\nabla\phi)_a{}^{\alpha'}=\zeta_a{}^{\alpha'}, \tag{A9}$$

$$\nabla_{[a}\zeta_{b]}{}^{\alpha'}=f_{ab}{}^{\alpha'}, \tag{A10}$$

$$\nu_A k'^{Aa}{}_{\alpha'}\zeta_a{}^{\alpha'}+\nu_A k''^{Aa}{}_{\alpha''}(\nabla\phi'')_a{}^{\alpha''}=\nu_A j^A. \tag{A11}$$

In (A11), ν_A is any vector in some fixed subspace complementary to the subspace V. In other words, Eq. (A11) reflects those equations of (A8) that do involve the derivative of ϕ''.

The system (A9)–(A11) is, certainly, a first-order, quasilinear system of partial differential equations; and it has as its variables precisely the ones we intended, namely $(\phi',\zeta_a{}^{\alpha'},\phi'')$. But, unfortunately, this system is subject to a variety of maladies—and these can arise even if the original system was quite well-behaved. For example—and this happens frequently—there can be constraints for the system (A9)–(A11) that are hidden in Eq. (A11), and thus do not arise from any constraints for the original system, (A8). Furthermore, these new constraints are not in general integrable. One could attempt to include the integrability conditions of these new constraints as new equations for the system. But two further problems can arise. First, some integrability con-

ditions can turn out to be mere algebraic equations on the fields, $(\phi', \zeta_a{}^{\alpha'}, \phi'')$. The only way to ''include'' such equations is to start over, introducing a new bundle right from the beginning. Second, some integrability conditions can turn out to be quadratic, rather than linear, in the field-derivatives. These cannot simply be ''included''—at least, not if we wish to retain a quasilinear system. The system (A9)–(A11) can also manifest a number of other types of difficulties, e.g., the absence of a hyperbolization or the wrong number of equations. There appears to be no simple, general condition that guarantees that Eqs. (A9)–(A11) lead to a system with an initial-value formulation.

As an example of this construction consider again the simple fluid, (1)–(2). Let $\mathcal{B}'$ be the bundle whose fiber consists only of the variable u^a; and $\mathcal{B}''$ the bundle whose fiber consists only of the variable ρ. In this example, the vector space V, capturing those equations in (1)–(2) involving no derivative of ρ, is zero-dimensional. The corresponding new bundle space, then, is that whose fiber, over $x \in M$, consists of $(u^a, w_b{}^a, \rho)$, with u^a unit timelike and $w_b{}^a$ satisfying $g_{ac}u^c w_b{}^a = 0$ (unit-ness of u^a). The equations for the new system, in this example, are

$$\nabla_b u^a = w_b{}^a, \tag{A12}$$

$$\nabla_{[a} w_{b]}{}^c = R_{abd}{}^c u^d, \tag{A13}$$

$$(g^{am} + u^a u^m)\nabla_m p + (\rho + p) u^m w_m{}^a = 0, \tag{A14}$$

$$u^m \nabla_m \rho + (\rho + p) w_m{}^m = 0. \tag{A15}$$

This system has a new constraint [obtained by combining Eqs. (A14) and (A15) to obtain an expression for $\nabla_m \rho$, and then taking its curl], which turns out not to be integrable. But its integrability condition turns out to be quasilinear in field-derivatives, and so may be included as a further equation of the system. The resulting system in this case (but not for the case of an even slightly more complicated fluid) actually admits a hyperbolization.

APPENDIX B: INITIAL-VALUE FORMULATION

Consider a first-order, quasilinear system of partial differential equations, as described in Sec. II. That is, we have a fiber bundle, with base manifold M, bundle manifold $\mathcal{B}$, and projection mapping $\mathcal{B} \overset{\pi}{\to} M$. The system of partial differential equations, on a cross-section, $M \overset{\phi}{\to} \mathcal{B}$, of this bundle, is given by Eq. (3). We are concerned here with the issue of under what circumstances such a system admits an initial-value formulation, i.e., a formulation in which the fields are first specified on some ''initial surface'' in M, and are then determined elsewhere in M by Eq. (3) itself.

The key to achieving such a formulation is an object called a *hyperbolization* of the system (3), a field $h_{\beta A}$ on the bundle manifold $\mathcal{B}$ having the properties described below. Consider, for (x, ϕ) any point of the bundle manifold $\mathcal{B}$, w_m any covector at $x \in M$, and $\delta\phi^\alpha, \delta'\phi^\alpha$ any two vectors at $(x, \phi) \in \mathcal{B}$ tangent to the fiber (''vertical''), the expression

$$w_m h_{\beta A} k^{Am}{}_\alpha \delta\phi^\alpha \delta'\phi^\beta. \tag{B1}$$

We demand, in order that this $h_{\beta A}$ be a hyperbolization, that, everywhere in $\mathcal{B}$, this expression be symmetric in $\delta\phi^\alpha, \delta'\phi^\alpha$ for all w_m, and positive-definite (i.e., positive for any nonzero $\delta'\phi^\beta = \delta\phi^\beta$) for some w_m. The most direct way to specify a hyperbolization for a system of partial differential equations is simply to give the bilinear expression (B1). Such an expression indeed defines a hyperbolization provided it is symmetric and positive-definite, as described above, and furthermore, that it is some multiple of the result of replacing, in the left side of Eq. (3), ''$(\nabla\phi)_a{}^\alpha$'' by ''$w_a\, \delta\phi^\alpha$.'' As an example, consider the system, (1)–(2), for a simple perfect fluid. Consider the bilinear expression

$$\delta' u^a[(\rho+p)(u^m w_m) g_{ab}\delta u^b + (\partial p/\partial\rho) w_a \delta\rho] + (\partial p/\partial\rho)(\rho+p)^{-1}\delta'\rho[(\rho+p)\delta u^m w_m + u^m w_m \delta\rho]. \tag{B2}$$

We note that this expression is symmetric under interchange of the two vectors $(\delta\rho, \delta u^a)$ and $(\delta'\rho, \delta' u^a)$, and that [provided $(\rho+p)>0$ and $1\geqslant(\partial p/\partial\rho)>0$] it is positive-definite whenever w_m is future-directed timelike. Furthermore, this expression arises, as described above, from Eqs. (1)–(2). This bilinear expression, then, specifies a hyperbolization for this system.

Let there be given a hyperbolization, $h_{\alpha A}$, for the system (3). Then this object gives rise to an initial-value formulation for a portion of that system, in the following manner. Fix initial data, consisting of a submanifold T of M of codimension one (an ''initial surface'') together with a cross-section ϕ_0 over this submanifold (''data'' on that surface), such that at each point of T, the normal to T is one of the vectors w_m for which the bilinear expression (B1) is positive-definite (the surface is ''noncharacteristic''). Then, in some neighborhood of the submanifold T, there exists one and only one solution ϕ of the system

$$h_{\beta A} k^{Aa}{}_{\alpha} (\nabla\phi)_a{}^{\alpha} = h_{\beta A} j^A, \tag{B3}$$

such that $\phi=\phi_0$ on T. Note that we do not guarantee a solution of the entire system (3), but rather only of those components that are involved in the hyperbolization. While the proof of this theorem is technically difficult, the key idea is to construct, using the hyperbolization, an energy integral, which is positive-definite, and, effectively, conserved.

Denote by u the number of unknowns of the system (3) (i.e., the dimension of the fibers in $\mathcal{B}$), and by e the number of equations (i.e., the dimension of the vector space in which the index ''A'' lies). Then the mere existence of a hyperbolization for this system already implies $e\geqslant u$ (i.e., that there are at least as many equations as unknowns). Should it happen that this inequality is an equality, i.e., that $e=u$, then it follows that the hyperbolization tensor $h_{\alpha A}$ is invertible, and so that the system (B3) exhausts the original system of equations (3). Thus, in this case we are done: We have achieved our full initial-value formulation. In the example of the simple perfect fluid above, for instance, we have $e=u=4$, and so the hyperbolization (B2) gives rise to an initial-value formulation for the fluid system (1)–(2). Unfortunately, in many cases of interest we have the strict inequality $e>u$, i.e., there are additional equations in (3) that are not accounted for in (B3). Such ''additional equations'' are dealt with in the following manner.

By a *constraint* of the system, (3), of partial differential equations, at a point of $\mathcal{B}$, we mean a tensor $c^a{}_A$ at that point such that the tensor $c^a{}_A k^{Ab}{}_{\alpha}$ is antisymmetric in the indices ''a,b.'' This definition has two facets. First, each constraint gives rise to an integrability condition. Fix a constraint field, $c^a{}_A$, and a solution ϕ of Eq. (3). Contract both sides of Eq. (3) with $c^b{}_A$, and apply to both sides some derivative operator, ∇_b, on M. Then, by the constraint-condition, terms involving second derivatives of ϕ vanish, leaving an algebraic equation (indeed, a polynomial of degree at most two) in the first derivative, $(\nabla\phi)_a{}^{\alpha}$, of ϕ. The constraint field is said to be *integrable* if this equation is an algebraic consequence of Eq. (3), i.e., if the difference of its two sides is the product of some expression (at most linear in field-derivatives) and the difference of the two sides of (3). The lack of integrability of a constraint generally indicates that ''not all the equations have been included in the original system (3).'' As to the second facet, each constraint gives rise to a compatibility condition on initial data. Fix constraint field, $c^a{}_A$, solution ϕ of Eq. (3), and submanifold T of M of codimension one. Then, at each point of T, we have

$$n_m c^m{}_A k^{Aa}{}_{\alpha} (\nabla\phi)_a{}^{\alpha} = n_m c^m{}_A j^A, \tag{B4}$$

where n_m is the normal to T at that point. But, by virtue of the constraint-condition, the index ''a'' in the tensor $n_m c^m{}_A k^{Aa}{}_{\alpha}$ is tangent to T. Thus, Eq. (B4) takes the derivative of ϕ only in directions tangent to T, and so it refers only to the value of ϕ on T, i.e., only to the initial data on T. In short, Eq. (B4) represents a compatibility condition on initial data. If these compatibility conditions were not satisfied, then we would have have no hope of finding a corresponding

solution of Eq. (3). As an example, consider the Maxwell equation $\nabla_{[a}F_{bc]}=0$. This equation has a constraint. The corresponding integrability condition, obtained by taking the curl of this equation, is an identity, and so this constraint is integrable. The compatibility condition (B4) on initial data becomes, in this example, $\nabla\cdot B=0$.

In the case in which $e>u$, i.e., in which the system (3) has more equations than unknowns, two further conditions must be imposed on the system. The first is that all the constraints be integrable. The second is that $e-c=u$, where c denotes the dimension of the vector space of vectors of the form $w_m c^m{}_A$, for fixed w_m, as $c^m{}_A$ runs through all the constraints. This last condition means that any additional equations in (3) that are not included already in (B3) are accounted for, effectively, by constraints. It states that (3) has the ''correct number of equations'' for its unknowns. In the case of Maxwell's equations, for example, all the constraints are integrable, as we have already remarked; and we have $e=8$, $c=2$, and $u=6$, so there is indeed the correct number of equations. That is, the two further conditions above are satisfied in this example.

Consider now a first-order, quasilinear system of partial differential equations that satisfies the three conditions given above. That is, let the system (i) admit a hyperbolization, (ii) have all its constraints integrable, and (iii) have the correct number of equations, as described above. It seems likely that such a system—possibly with some mild further conditions—must always manifest an initial-value formulation in some suitable sense. That is, we would expect that, given initial data for the system on a suitable surface T, satisfying on T the compatibility conditions (B4), then there exists a unique corresponding solution of Eq. (3) in a neighborhood of T. A key piece of evidence prompting this expectation is the following. There certainly exists a solution of Eq. (B3) manifesting the initial data, as we have already seen. Consider next the left sides of Eq. (B4) (as $c^m{}_A$ varies over all constraints). These expressions of course vanish on T, and, by virtue of the conditions (ii) and (iii) above, satisfy a system of equations that express the ''time-derivatives'' (off T) of these expressions in terms of their ''space-derivatives'' (within T). Naively, we might expect that, as a consequence, these expressions must vanish in a neighborhood of T. But the vanishing of these expressions implies, again by condition (iii) above, that Eq. (3) itself is satisfied everywhere in a neighborhood of T. Indeed, in all physical examples of which we are aware—including all those discussed in this paper—this naive expectation is in fact borne out. Unfortunately, there is, apparently, no general theorem to this effect. Nevertheless, we shall, for convenience, use the expression ''having an initial-value formulation'' to describe systems of partial differential equations that satisfy the three conditions, (i)–(iii), above.

[1] See, for example, R. Courant and K. O. Friedrichs, *Supersonic Flow and Shock Waves* (Interscience, New York, 1948), for the Euler and Lagrange formulations of non-relativistic perfect fluids, and Appendix A of Ref. 2 for the Euler formulation of a relativistic perfect fluid.

[2] R. Geroch, ''Partial differential equations of physics,'' in *General Relativity*, Proceedings of the 46th Scottish Universities Summer School in Physics, edited by G. S. Hall and J. R. Pulham (SUSSP Publications, Edinburgh; IOP, London, 1996). Available as gr-qc/9602055.

[3] For the case of the Einstein-Euler system, for example, see Sec. 4.2 of Ref. 4, and references therein.

[4] H. Friedrich and A. Rendall, ''The Cauchy problem for the Einstein equations,'' in *Einstein's Field Equations and their Physical Interpretation*, edited by B. G. Schmidt (Springer-Verlag, Berlin, 2000), available as gr-qc/0002074.

[5] In fact, some care must be taken, in the Lagrange formulation, even to say what ''initial-value formulation'' means, in light of the fact that the independent variables are not the usual space-time events, through which evolution normally proceeds.

[6] Recall that this condition requires, essentially, that, locally in M, $\mathcal{B}$ can be written as a product, $M\times F$, of M with some other fixed manifold F, in such a way that the projection mapping π becomes the projection to the M-factor in this product. This condition guarantees, e.g., that, locally, all the fibres of the bundle are diffeomorphic with this fixed manifold F, and so with each other.

[7] Note that we can, in this case, convert these to ordinary tensors on the manifold $\hat{M}$ by using $\kappa_{\hat{a}}{}^b$ and its universe. This, a mere ''coordinate transformation'' on the fibres, changes nothing, in particular, not the final partial differential equations of the Lagrange formulation.

[8] For convenience, we shall always include within our system *all* first-order equations on the fields of the system, even those that arise from differentiating other equations of the system.

[9] These derivatives may be characterized in the following manner. Consider the bundle with base space $\hat{M}$ and fibre over $\hat{x}\in\hat{M}$ consisting of a pair, $(x,\kappa_{\hat{a}}{}^b)$, where $x\in M$ and $\kappa_{\hat{a}}{}^b$ is a tensor with indices at x and $\hat{x}$. Then a choice of connection in this bundle gives rise to an operator $\nabla_{\hat{a}}$ for use in the left side of Eq. (6).

[10] A Lorentz metric on M, for example, becomes, on $\hat{M}$, an algebraic function of the fields (namely, just of x) of the Lagrange formulation.

[11] In the notation of (5)–(7), we have $\varphi=(x,\rho)$, and $\hat{\varphi}=(x,\hat{\rho})$.

[12] There is an unfortunate complication here, involving the normalization condition, $u^a u^b g_{ab}=-1$, on u^a. It is awkward simply to carry this condition through the Lagrange formulation. But there are several other ways—none very elegant—to deal with it. Perhaps the simplest is to rewrite the fluid equations from the outset [by inserting, strategically, factors of $(u^a u^b g_{ab})$] in such a way that, while retaining their initial-value formulation, they no longer require this normalization condition. Then take the Lagrange formulation of these new equations.

[13] Note in particular that the original system, (10)–(11), always possesses the constraints arising from the curl of Eq. (10). Thus, if the constraints of this system are to be integrable, this curl-equation must have been included in the system (10)–(11).

[14] These are not to be confused with the indices for tensors on the bundle space, used extensively in Sec. II.

[15] Note that the last two terms on the left in Eq. (21) constitute the most general expression (involving u^a and φ) quasilinear in the derivative of u^a.

[16] For "if," suppose that $V^\alpha F_\alpha>0$ everywhere on S. It follows that there exists a positive-definite metric field, $g_{\alpha\beta}$, on the manifold S such that $V^\alpha g_{\alpha\beta}=F_\beta$ everywhere. Choose one (e.g., the sum of $F_\alpha F_\beta/(F_\gamma V^\gamma)$ and a suitable positive semi-definite tensor $h_{\alpha\beta}$ that annihilates V^α) and consider the bilinear expression

$$-(w_m u^m)[g_{ab}\delta u^a \delta' u^b + g_{\alpha\beta}\delta\varphi^\alpha \delta'\varphi^\beta] - w_m F_\alpha [\delta u^m \delta'\varphi^\alpha + \delta' u^m \delta\varphi^\alpha].$$

This bilinear expression indeed arises, as described in Appendix B, from Eqs. (20)–(21), and is indeed positive-definite (for w_m sufficiently close to u_m). So, this bilinear expression gives rise to a hyperbolization. The converse is easy.

[17] H. Friedrich, "Evolution equations for gravitating ideal fluid bodies in general relativity," Phys Rev. D **57**, 2317–2322 (1998).

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[23] There could also be included on the right side of this equation terms algebraic in the electromagnetic and other fields. Such terms would represent, e.g., an effect of the electromagnetic field on the rates of chemical reactions.

[24] Note that there are no expressions, algebraic in the gravitational fields, that could be introduced on the right in these equations. This is a reflection of "the equivalence principle."

[25] The most general candidate for such a stress-energy (i.e., the most general algebraic function of our fields, having the correct index-structure) is given by $T_{ab}=(\rho+p)u_a u_b + p g_{ab}$, where ρ,p are some functions on the manifold S of fluid states. When does there exist such a T^{ab} that, in addition, is conserved, $\nabla_b T^{ab}=0$, by virtue of the field equations (20)–(21)? It is not difficult to check that (assuming $V^\alpha F_\alpha>0$; and demanding $\rho+p>0$) a necessary and sufficient condition is that the fields F_α, V^α, and T^α on S satisfy the following three equations: $F_{[\alpha}\nabla_\beta F_{\gamma]}=0$, $T^\alpha K_\alpha=0$, and $\nabla_{[\alpha}(K_{\beta]}+F_{\beta]}=0$, where we have set $K_\alpha=(2V^\beta\nabla_{[\beta}F_{\alpha]}+F_\alpha)/(V^\gamma F_\gamma)$.

[26] In the resulting system, there will initially be two versions of "the derivative of the metric g_{ab}," one being the original derivative operator ∇_a, and the other arising (via g_{ab}) through passage to the derivative system. These two versions are then to be set equal to each other, via Eq. (A2). A similar phenomenon occurs, e.g., on taking the derivative system of the Klein-Gordon system.

[27] This "suppression" proceeds, in more detail, as follows. Choose on the 2-manifold S, a function s (which is interpreted in Ref. 17 as the entropy per particle) satisfying $V^\alpha\nabla_\alpha s=0$. Now delete the field $\zeta_a{}^\alpha$ everywhere, by replacing the component $\zeta_a{}^\alpha\nabla_\alpha s$ of $\zeta_a{}^\alpha$ by some new field f_a, and the remaining components of $\zeta_a{}^\alpha$ by $(\nabla\varphi)_a{}^\alpha$. To the resulting system add those further equations that are required for integrability of the constraints.

[28] In fact, there is, at this level of generality, a possible anomaly with the system (A3)–(A4). In some cases, further *algebraic* conditions on the fields can follow from Eq. (A4). In fact, this anomaly will never arise in systems of interest, because it is precluded by the requirement, which we shall impose shortly, that all constraints of the original system (A1), be integrable.

[29] The number of effective constraints of Eq. (A4) is the dimension of the vector space of tensors $\Lambda^{ab}{}_\alpha$ satisfying $\Lambda^{ab}{}_\alpha=\Lambda^{[ab]}{}_\alpha$ and $w_a\Lambda^{ab}{}_\alpha=0$ (namely, $(n-1)(n-2)u/2$), minus the dimension of the vector space of such tensors of the form $c^a{}_A k^{Ab}{}_\alpha$ for $c^a{}_A$ a constraint (namely, $\hat{c}-c$).

[30] Recall that the product of two bundles, with the same base space M, is the bundle, again with the base space M, whose fibre, over point $x\in M$, is given by the product of the fibres, over x, in the separate bundles.

Reduction of Sasakian manifolds

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We show that the contact reduction can be specialized to Sasakian manifolds. We prove that the Sasakian reduction is compatible with the Kähler reduction both in the cone construction and in the Boothby–Wang fibration. In particular, applying Futaki's results, we obtain a sufficient condition for the reduced space of a regular Sasakian–Einstein manifold to be Sasakian–Einstein. We present examples of Sasakian–Einstein manifolds obtained by S^1 reduction of standard Sasakian spheres. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1386636]

I. INTRODUCTION

The reduction technique was naturally extended from symplectic to contact structures by Geiges in Ref. 1 and Albert in Ref. 2. On the other hand, Boyer, Galicki and B. Mann defined in Ref. 3 a moment map for 3-Sasakian manifolds, thus extending the reduction procedure for nested metric contact structures. Quite surprisingly, a reduction scheme for Sasakian manifolds (contact manifolds endowed with a compatible Riemannian metric satisfying a curvature condition), was still missing.

In this note, based on the preprint,[4] we fill the gap by defining a Sasakian moment map and constructing the associated reduced space (compare with Ref. 5; here we focus on the Riemannian aspects). We then relate Sasakian reduction to Kähler reduction *via* the Kähler cone over a Sasakian manifold and *via* the Boothby–Wang fibration. Further, we derive a condition, similar to Futaki's, for the reduced manifold of a regular Sasakian–Einstein manifold to be Sasakian–Einstein. We end this paper with some completely worked examples of the S^1-reduction of standard Sasakian spheres. Most of the reduced Sasakian structures that we obtain are Einstein. Some of them are among the examples considered in Ref. 6, however our methods allow a much simpler check of the Einstein condition.

Sasakian manifolds seem to be more and more important in superconformal field theories, being connected with the Maldacena conjecture. One of our examples, a S^1 bundle over $S^2 \times S^2$, already appeared in Ref. 7, where the Kähler reduction of the cone over a Sasakian manifold is implicitly used.

II. SASAKIAN MANIFOLDS

In this section we briefly recall the notion of a Sasakian manifold. The definition we give is not the standard one, but is suited for our purpose. For more details, we refer to Refs. 8 and 9.

Definition 2.1: A *Sasakian* manifold is a $(2n+1)$-dimensional Riemannian manifold (N,g) endowed with a unitary Killing vector field ξ such that the curvature tensor of g satisfies the equation

$$R(X,\xi)Y = \eta(Y)X - g(X,Y)\xi, \tag{2.1}$$

where η is the metric dual 1-form of ξ: $\eta(X) = g(\xi,X)$.

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Let $\varphi=\nabla\xi$, where ∇ is the Levi-Civita connection of g. The following formulas are then easily deduced:

$$\varphi\xi=0, \quad g(\varphi Y,\varphi Z)=g(Y,Z)-\eta(Y)\eta(Z), \quad d\eta(X,Y)=g(\phi X,Y). \tag{2.2}$$

It can be seen that η is a contact form on N, whose Reeb field is ξ (it is also called the characteristic vector field). Moreover, the restriction of φ to the contact distribution $\eta=0$ is an almost complex structure satisfying the ''integrability'' condition (called normality) $[\varphi,\varphi]+2\,d\eta\otimes\xi=0$.

The simplest example is the standard sphere $S^{2n+1}\subset\mathbb{C}^{n+1}$, with the metric induced by the flat one of $\mathbb{C}^{n+1}$. The characteristic Killing vector field is $\xi_p=-i\vec{p}$, i being the imaginary unit; this is the standard Sasakian structure of the odd sphere. Other Sasakian structures on the sphere can be obtained by D-homothetic transformations (cf. Ref. 10). Also, the unit sphere bundle of any real space form is Sasakian.

More generally, the quantization bundle of a compact Kähler manifold naturally carries a Sasakian structure. The converse construction, possible when the characteristic field is regular, is known as the Boothby–Wang fibration. Precisely, the following result (the metric part is due to Morimoto and Hatakeyama) is available (cf. Refs. 11 or 9).

Theorem 2.1: Let (P,h) be a Hodge manifold. There exists a principal circle bundle $\pi:N\to P$ and a connection form η in it, with curvature from the pull-back of the Kähler form of P, which is a contact form on S. Let ξ be the vector field dual to η with respect to the metric $g=\pi^*h+\eta\otimes\eta$. Then (N,g,ξ) is Sasakian.

The following equivalent definition puts Sasakian geometry into the framework of holonomy groups. Let $C(N)=N\times\mathbb{R}_+$ be the cone over (N,g). Endow it with the warped-product cone metric $C(g)=r^2g+dr^2$. Let $R_0=r\,\partial r$ and define on $C(N)$ the complex structure J acting like this (with obvious identifications): $JY=\varphi Y-\eta(Y)R_0$, $JR_0=\xi$. We have the following.

Theorem 2.2 Ref. 9: (N,g,ξ) is Sasakian if and only if the cone over N $(C(N),C(g),J)$ is Kählerian.

III. MAIN RESULTS

A. Direct construction

In this section we show that the contact map defined in Ref. 1 is compatible with the Sasakian metric and the contact reduced space is indeed Sasakian.

Theorem 3.1: Let (N,g,ξ) be a compact $2n+1$-dimensional Sasakian manifold and G a compact d-dimensional Lie group acting on N by contact isometries. Suppose $0\in\mathfrak{g}^*$ is a regular value of the associated moment map μ. Then the reduced space $M=N//G:=\mu^{-1}(0)/G$ is a Sasakian manifold of dimension $2(n-d)+1$.

Proof: By Ref. 1, the contact moment map $\mu:N\to\mathfrak{g}^*$ is defined by

$$<\mu(x),\underline{X}>=\eta(X),$$

for any $\underline{X}\in\mathfrak{g}$ and X the corresponding field on N. We know that the reduced space is a contact manifold, *loc. cit.* Hence we only need to check that (1) the Riemannian metric is projected on M and (2) the field ξ projects to a unitary Killing field on M such that the curvature tensor of the projected metric satisfies formula (2.1).

To this end, we first describe the metric geometry of the Riemannian submanifold $\mu^{-1}(0)$.

Let $\{\underline{X}_1,\ldots,\underline{X}_d\}$ be a basis of $\mathfrak{g}$ and let $\{X_1,\ldots,X_d\}$ be the corresponding vector fields on N. Since 0 is a regular value of μ, $\{X_{ix}\}$ is a linearly independent system in each $T_x\mu^{-1}(0)$. From the very definition of the moment map we have $\eta_p(X_i)=\mu(p)(X_i)=0$, hence $X_i\perp\xi$. As G acts by contact isometries, we have

$$\mathcal{L}_{X_i}g=0, \quad \mathcal{L}_{X_i}\eta=0 \quad i=1,\ldots,d. \tag{3.1}$$

Note that these also imply $[X_i,\xi]=\mathcal{L}_{X_i}\xi=0$.

We observe that $\mu^{-1}(0)$ is an isometrically immersed submanifold of N (we denote the induced metric also with g) whose tangent space in each point is described by $Y\in T_x\mu^{-1}(0)$ if and only if $d\mu_x(Y)=0$. Hence, by the definition of the moment map, the vector fields ξ and X_i are tangent to $\mu^{-1}(0)$. Moreover, for any Y tangent to $\mu^{-1}(0)$, one has $g(\varphi X_i,Y)=d\eta(Y,X_i)=d\mu(Y)=0$; hence the vector fields $\{X_i\}$ produce a local basis (not necessarily orthogonal) of the normal bundle of $\mu^{-1}(0)$. The shape operators $A_i:=A_{\varphi X_i}$ of this submanifold in N are computed as follows [we let ∇, ∇^N be the Levi Civita covariant derivatives of $\mu^{-1}(0)$, resp. N]:

$$\begin{aligned} g(A_iY,Z)&=-g(\nabla^N_Y(\|X_i\|^{-1}\varphi X_i),Z)=-g(Y(\|X_i\|^{-1})\varphi X_i,Z)-g(\|X_i\|^{-1}\nabla^N_Y(\varphi X_i),Z)\\ &=-\|X_i\|^{-1}g(\nabla^N_Y(\varphi X_i),Z)=-\|X_i\|^{-1}g(\nabla^N_Y(\varphi)X_i+\varphi\nabla^N_YX_i,Z)\\ &=-\|X_i\|^{-1}g(\eta(X_i)Y-g(X_i,Y)\xi+\varphi\,\nabla^N_YX_i,Z)\\ &=\|X_i\|^{-1}\{g(X_i,Y)\,\eta(Z)-g(\varphi\,\nabla^N_YX_i,Z\}. \end{aligned}\tag{3.2}$$

In particular, for the corresponding quadratic second fundamental forms we get

$$h_i(Y,\xi)=\|X_i\|^{-1}g(X_i,Y),\quad h_i(\xi,\xi)=0.\tag{3.3}$$

Consequently, one easily obtains the following: *the restriction of the vector field ξ is Killing on $\mu^{-1}(0)$ too*.

Using the Gauss equation of a submanifold,

$$R^N(X,Y,Z,W)=R^{\mu^{-1}(0)}(X,Y,Z,W)+g(h(X,Z),h(Y,W))-g(h(X,W),h(Y,Z)),$$

and the formula (3.2) we now compute the needed part of the curvature tensor of $\mu^{-1}(0)$ at a fixed point $p\in\mu^{-1}(0)$. We take X,Y,Z orthogonal to ξ_p and obtain

$$\begin{aligned} g(R^{\mu^{-1}(0)}(X,\xi)Y,Z)-g(R^N(X,\xi)Y,Z)&=-\sum_{i=1}^{d}\|X_i\|^{-2}\{h_i(X,Y)h_i(\xi,Z)-h_i(X,Z)h_i(\xi,Y)\}\\ &=-\sum_{i=1}^{d}\|X_i\|^{-2}\{g(X_i,Z)g(\nabla^N_XX_i,\varphi Y)\\ &\quad-g(X_i,Y)g(\nabla^N_XX_i,\varphi Z)\} \end{aligned}\tag{3.4}$$

(note that $\nu_i=\|X_i\|^{-1}\varphi X_{ip}$ are chosen to be orthonormal in p; this is always possible pointwise by an appropriate choice of the initial $\underline{X}_i$).

Now let $\pi:\mu^{-1}(0)\to M$ and endow M with the projection g^M of the metric g such that π becomes a Riemannian submersion. This is possible because G acts by isometries. In this setting, the vector fields X_i span the vertical distribution of the submersion, while ξ is horizontal and projectable (because $\mathcal{L}_{X_i}\xi=0$). Denote with ζ its projection on M. ζ is obviously unitary. To prove that ζ is Killing on M, we just observe that $\mathcal{L}_\zeta g(Y,Z)=\mathcal{L}_\xi g(Y^h,Z^h)$, where Y^h denotes the horizontal lift of Y. Finally, to compute the values $R^M(X,\zeta)Y$ of the curvature tensor of g^M, we use the O'Neill formula [cf. Ref. 12 Eq. (9.28f)]:

$$\begin{aligned} g^M(R^M(X,\zeta)Y,Z)&=g(R^{\mu^{-1}(0)}(X^h,\xi)Y^h,Z^h)+g(A(X^h,\xi),A(Y^h,Z^h))-g(A(\xi,Y^h),A(X^h,Z^h))\\ &\quad+g(A(X^h,Z^h),A(\xi,Z^h)), \end{aligned}$$

where X,Y,Z are unitary, normal to ζ and the O'Neill (1,2) tensor A is defined as: $A(Z^h,X^h)$ = vertical part of $\nabla_{Z^h}X^h$. Using the Gauss formula and (3.3), we obtain

$$g(\nabla_{Z^h}\xi, X_i) = g(\varphi Z^h, X_i) = -g(Z^h, \varphi X_i) = 0;$$

hence $\nabla_{Z^h}\xi$ has no vertical part and $A(Z^h,\xi)=0$. Thus

$$R^M(X,\zeta)Y = R^{\mu^{-1}(0)}(X^h,\xi)Y^h = R^N(X^h,\xi)Y^h$$

because of (3.4) and the fact that X^h, Y^h are normal to all X_i. Hence

$$R^M(X,\zeta)Y = g(\xi,Y^h)X^h - g(X^h,y^h)\xi = g^M(\zeta,Y)X - g^M(X,Y)\zeta,$$

which proves that (M,g^M,ζ) is a Sasakian manifold. □

B. Compatibility with the cone construction

In the following we relate Sasakian reduction to Kähler reduction by using the cone construction. Roughly speaking, we prove that reduction and taking the cone are commuting operations.

Let $\omega = dr \wedge \eta + r^2\, d\eta$ be the Kähler form of the cone $C(N)$ over a Sasakian manifold (N,g,ξ). If ρ_t are the translations acting on $C(N)$ by $(x,r)\mapsto(x,tr)$, then the vector field $R_0 = r\,\partial r$ is the one generated by $\{\rho_t\}$. Moreover, the following two relations are useful:

$$\mathcal{L}_{R_0}\omega = \omega, \quad \rho_t^*\omega = t\omega. \tag{3.5}$$

Suppose that a compact Lie group G acts on $C(N)$ by holomorphic isometries, commuting with ρ_t. This ensures a corresponding action of G on N. In fact, we can consider $G \cong G\times\{Id\}$ acting as $(g,(x,r))\times(gx,r)$.

Suppose that a moment map $\Phi: C(N)\to\mathfrak{g}$ exists.

As above, let $\{\underline{X}_1,\ldots,\underline{X}_d\}$ be a basis of $\mathfrak{g}$ and let $\{X_1,\ldots,X_d\}$ be the corresponding vector fields on $C(N)$. We see that X_i are independent on r, hence can be considered as vector fields on N. Furthermore, the commutation of G with ρ_t implies

$$\Phi(\rho_t(p)) = t\Phi(p). \tag{3.6}$$

Now we imbed N in the cone as $N\times\{1\}$ and let $\mu := \Phi|_{N\times\{1\}}$. This is the moment map of the action of G on N. To see this, recall the definition of the symplectic moment map $\Phi = (\Phi_1,\ldots,\Phi_d)$: Φ_i is given up to constant by $d\Phi_i(Y) = \omega(X_i,Y)$. Here we uniquely determine Φ_i by imposing the condition $\eta(X_i) = \Phi|_{N\times\{1\}}$. This immediately implies that the Reeb field of N is orthogonal to the vector fields X_i since $g(\xi,X_i) = \eta(X_i) = 0$. As G acts by isometries on $C(N)$, we may project the cone metric to a metric on $N//G\times\mathbb{R}_+$ which we denote by g_0. Then $g_0(Y,Z) = C(g)(Y^h,Z^h)$, where Y^h, Z^h are the unique vector fields on $\Phi^{-1}(0)$ orthogonal to all of X_i which project on Y, Z (we call them horizontal).

Let $P = \Phi^{-1}(0)/G$ be the reduced Kähler manifold. The key remark is that because of (3.6), $\Phi^{-1}(0)$ is the cone $N'\times\mathbb{R}_+$ over $N' = \{x\in N; (x,1)\in\Phi^{-1}(0)\}$. Moreover, since the actions of G and ρ_t commute, one has an induced action of G on N'. Then

$$\Phi^{-1}(0)/G \cong (N'\times\mathbb{R}_+)/G \cong N'/G\times\mathbb{R}_+.$$

The manifold $N'//G\times\mathbb{R}_+$ is Kähler, as the reduction of a Kähler manifold, but we still have to check that this Kähler structure is a cone one. For the more general, symplectic case, this was done in Ref. 13. Let g_0 be the reduced Kähler metric and g' be the Sasakian reduced metric on $N'//G$. It is easily seen that the lift of g_0 to $\Phi^{-1}(0)$ coincides with the lift of the cone metric $r^2g' + dr^2$ on horizontal fields. This implies that the cone metric coincides with g_0.

Summing up we have proved the following.

Theorem 3.2: Let (N,g,ξ) be a Sasakian manifold and let $(C(N),\ C(g),J)$ be the Kähler cone over it. Let a compact Lie group G act by holomorphic isometries on $C(N)$ and commuting with the action of the 1-parameter group generated by the field R_0. If a moment map with regular

value 0 exists for this action, then a moment map with regular value 0 exists also for the induced action of G on N. Moreover, the reduced space $C(N)//G$ is the Kähler cone over the reduced Sasakian manifold $N//G$.

The advantage of defining the Sasakian reduction *via* Kähler reduction, as done in Ref. 3 for 3-Sasakian manifolds, is the avoiding of curvature computations. However, as we shall see, the direct construction is easily applicable.

C. Compatibility with the Boothby–Wang fibration and obtaining Sasakian–Einstein spaces by reduction

Let (N,g,ξ) be a compact Sasakian manifold with a regular characteristic vector field and let $\pi:N\to P$ be the corresponding Boothby–Wang fibration over the Hodge base P. Let G be a compact Lie group acting on N by Sasakian transformations. By (3.1), it preserves the fibers of π; hence it induces an action by Kähler transformations on P. If we denote with ${}^N\mu$, ${}^P\mu$ the corresponding moment maps, using the relation (cf. Theorem 2.1) $g(X,\varphi Y)=\pi^*\omega(X,Y)$ and the definitions of the respective moment maps, it is easy to see that we have an S^1 subbundle ${}^N\mu^{-1}(0)\to{}^P\mu^{-1}(0)$ and an S^1 bundle $N//G\to P//G$. Finally one can check that 0 is a regular value for an induced moment map on the base using the relation

$$d\,{}^N\mu(X)=d\,\eta(X,\cdot)=\pi^*\omega(X,\cdot)=\pi^*d\,{}^P\mu$$

The details being easily settled, we can state the following.

Proposition 3.1: Let G be a compact Lie group acting by Sasakian transformations on the total space of a Boothby–Wang fibration $\pi:N\to P$. Then there exists a Boothby–Wang fibration of the reduced spaces $N//G\to P//G$.

On the other hand, if the Hodge base of a Boothby–Wang fibration is Kähler–Einstein, then the total space is Sasakian–Einstein, as proved in Ref. 9. According to Futaki (cf. Ref. 14, Corollary 7.3.4), if one reduces a Kähler–Einstein manifold, the reduced space is still Einstein if and only if the length of the multivector $X_1\wedge\cdots\wedge X_d$ is constant on the level set of the moment map. Hence, one way to obtain Sasakian–Einstein metrics *via* reduction is to start with a regular Sasakian–Einstein manifold and with a Sasakian action inducing on the Hodge base a Kähler action of Futaki's type. The precise result is the following.

Theorem 3.3: Let G be a compact Lie group acting by Sasakian transformations on the regular Sasakian–Einstein manifold N having 0 as a regular value of the corresponding moment map μ. If the length of the multivector $X_1\wedge\cdots\wedge X_d$ is constant on $\mu^{-1}(0)$ then the reduced space is Sasakian–Einstein.

Proof: First observe that the Boothby–Wang fibration $\pi:N\to P$ has a Kähler–Einstein base, with positive Ricci curvature, according to Ref. 9, Theorem 2.5(iv). Now, from the equations (3.1) we see that the S^1 action on $\mu^{-1}(0)$ commutes with the G-action. In particular the multivector $X_1\wedge\cdots\wedge X_d$ is projectable to $\mu^{-1}(0)/S^1$ for the projection $\pi:\mu^{-1}(0)\to\mu^{-1}(0)/S^1$. In view of the preceding section, this is a restriction of the Boothby–Wang fibration to the corresponding zero-sets of the moment maps on N and P, respectively. Since it is a Riemannian submersion and X_i are orthogonal to ξ, the lengths of the projected vectors are preserved, as well as the length of the projected multivector. Now we can apply Futaki's result (Ref. 14, Corollary 7.3.4) in order to conclude that the base for the reduced Boothby–Wang fibration $N//G\to P//G$ is Kähler–Einstein. Then, again according to Ref. 9, Theorem 2.5(iv), the reduced Sasakian manifold is Sasakian–Einstein. □

We apply this result in the examples of the last section.

In the same spirit, combining Ref. 9, Theorem 2.5(iii) (stating that the base of the Boothby–Wang fibration is Fano if and only if the Ricci curvature of the total space is >-2) and Ref. 14, Corollary 7.3.3 (asserting that the reduced space of a Fano manifold is again Fano), we obtain the following.

Proposition 3.2: Let G be a compact Lie group acting by Sasakian transformations on the regular Sasakian–Einstein manifold N having 0 as a regular value of the corresponding moment map μ. Then N has Ricci curvature Ric>-2 if and only if $N//G$ has Ricci curvature Ric>-2.

IV. EXAMPLES: S^1 ACTIONS ON SASAKIAN SPHERES

Example 4.1: Let us start with $S^7\subset\mathbb{C}^4$ with its standard Sasakian structure. Let the complex coordinates of $\mathbb{C}^4$ be $(z_0,\ldots,z_3)$, with $z_j=x_j+iy_j$. The contact form on S^7 can then be written as

$$\eta=\sum_{j=0}^{3}(x_j\,dy_j-y_j\,dx_j),$$

and its Reeb field is

$$\xi=\sum_{j=0}^{3}(x_j\,\partial y_j-y_j\,\partial x_j).$$

Let S^1 act on S^7 by $e^{it}\mapsto(e^{-it}z_0,e^{-it}z_1,e^{it}z_2,e^{it}z_3)$. The associated field of this action is (in real coordinates)

$$X_0=-(x_0\,\partial y_0-y_0\,\partial x_0)-(x_1\,\partial y_1-y_1\,\partial x_1)+(x_2\,\partial y_2-y_2\,\partial x_2)+(x_3\,\partial y_3-y_3\,\partial x_3).$$

The moment map $\mu:S^7\to\mathbb{R}$ reads as

$$\mu(z)=\eta_z(X_0)=-|z_0|^2-|z_1|^2+|z_2|^2+|z_3|^2,$$

with zero level set

$$\{z\in S^7;\ \ |z_0|^2+|z_1|^2=|z_2|^2+|z_3|^2\}=S^3\left(\frac{1}{\sqrt{2}}\right)\times S^3\left(\frac{1}{\sqrt{2}}\right).$$

Clearly μ is nondegenerate on $\mu^{-1}(0)$.

The reduced space can be identified with $S^3\times S^3/S^1$ which, by Ref. 6, is diffeomorphic with $S^2\times S^3$. [In this case, one can also avoid the topological arguments in Ref. 6 and identify the reduced space by observing that the following diffeomorphism of $S^3\times S^3$: $(z_0,z_1,z_2,z_3)\mapsto(z_0z_3+\overline{z_1z_2},z_0z_2-\overline{z_1z_3},z_2,z_3)$ is equivariant with respect to the previous S^1 action which, restricted to the second factor of the product, is the usual action inducing the Hopf fibration; *mille grazie* to Rosa Gini and Maurizio Parton for letting us know it (Ref. 15).]

The reduced Sasakian structure obtained in this way on $S^2\times S^3$ is directly checked to be Einstein and to project on the Kähler Einstein metric of $\mathbb{C}P^1\times\mathbb{C}P^1$ making the fiber map be a Riemannian submersion. As by Ref. 6 such an Einstein metric is unique, our reduced Sasakian structure coincides with the Sasakian structure found in Ref. 16 viewing $S^2\times S^3$ as a minimal submanifold of S^7, the total space of the pull-back over $\mathbb{C}P^1\times\mathbb{C}P^1$ of the Hopf bundle $S^7\to\mathbb{C}P^3$. The same Einstein–Sasakian metric on $S^2\times S^3$ also appears in Ref. 10, constructed by a different approach. In Example 4.3 we will generalize this structure by making use of Theorem 3.2.

Example 4.2: Consider again S^7 as the starting Sasakian manifold, but let S^1 act by $e^{it}\mapsto(e^{-kit}z_0,e^{it}z_1,e^{it}z_2,e^{it}z_3)$, $k\in\mathbb{Z}_+$. Now $\mu^{-1}(0)\cong S^1(\sqrt{k/k+1})\times S^5(\sqrt{1/k+1})$. In order to identify the reduced space, we regard the k:1 mapping,

$$S^1\times S^5\ni(z_0,z_1,z_2,z_3)\mapsto((z_0)^{-k},z_1,z_2,z_3)\in S^1\times S^5.$$

It induces a k:1 map from $M=S^1\times S^5/S^1$, where S^1 acts diagonally, to the reduced space $\mu^{-1}(0)/S^1$ with the action given above. As in Ref. 15, the map

$$(z_0,\ldots,z_3)\mapsto(z_0,\overline{z_0}z_1,\overline{z_0}z_2,\overline{z_0}z_3)$$

is an equivariant diffeomorphism of $S^1\times S^5$, equivariant with respect to the diagonal action of S^1 and the action of S^1 on the first factor. Hence M is diffeomorphic to S^5 and the reduced Sasakian space is $S^5/\mathbb{Z}_k$. Again, we shall see below that the metric is actually Sasakian–Einstein and it is the same as that found in Ref. 6.

Example 4.3: In general, consider the weighted action of S^1 on $S^{2n-1}\subset\mathbb{C}^n$ by

$$(e^{it},(z_0,\ldots,z_{n-1}))\mapsto(e^{\lambda_0 it}z_0,\ldots,e^{\lambda_n it}z_{n-1}),$$

where $(\lambda_0,\ldots,\lambda_{n-1})\in\mathbb{Z}^n$. The associated moment map,

$$\mu(z)=\lambda_0|z_0|^2+\cdots+\lambda_n|z_{n-1}|^2,$$

is regular on $\mu^{-1}(0)$ for any $(\lambda_0,\ldots,\lambda_{n-1})$ such that $\lambda_0\cdots\lambda_{n-1}\neq 0$, $(\lambda_0,\ldots,\lambda_{n-1})=1$ and at least two λ's have different signs (compare with the 3-Sasakian case where the weights obey to more restrictions; cf. Ref. 3).

Now take $\lambda_0=\cdots=\lambda_k=a$ and $\lambda_{k+1}=\cdots=\lambda_{n-1}=-b$, $a,b\in\mathbb{Z}_+$ relatively prime. Then $\mu^{-1}(0)\cong S^{2k+1}(\sqrt{a/a+b})\times S^{2(n-k)-1}(\sqrt{b/a+b})$. Moreover the length of the induced vector field X_0 on μ^{-1} is easily calculated to be $(a^2+b^2)/2$. Now we can apply Theorem 3.2 to deduce that the reduced metric is Sasakian–Einstein. Note that the induced metric on $\mu^{-1}(0)$ coincides with the product metric of the standard metrics of the two factors. Moreover we see that the reduced space is diffeomorphic with an S^1 factor of the above product of spheres given by the following action:

$$(e^{it},(x,y))\mapsto(e^{iat}x,e^{-ibt}y).$$

One can now adapt the arguments of Ref. 6, Corollary 2.2 and prove that the reduced spaces are S^1 bundles over $\mathbb{C}P^k\times\mathbb{C}P^{n-k-1}$ and, for $1\leqslant k$, $4<n$, they are not homeomorphic to each other in general. These are the examples considered in Ref. 6. However, for $k=1$, $n=2$, the reduced space is always diffeomorphic with $S^2\times S^3$. Hence, one obtains an infinite family of Sasakian structures on $S^2\times S^3$.

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Unitary irreducible representations of a Lie algebra for matrix chain models

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There is a decomposition of a Lie algebra for open matrix chains akin to the triangular decomposition. We use this decomposition to construct unitary irreducible representations. All multiple meson states can be retrieved this way. Moreover, they are the only states with a finite number of non-zero quantum numbers with respect to a certain set of maximally commuting linearly independent quantum observables. Any other state is a tensor product of a multiple meson state and a state coming from a representation of a quotient algebra that extends and generalizes the Virasoro algebra. We expect the representation theory of this quotient algebra to describe physical systems at the thermodynamic limit. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1384866]

I. INTRODUCTION

Theories with matrix degrees of freedom are of wide interest in physics. Quantum chromodynamics (QCD) is an important example. Each gluon field carries two color indices. They can be treated as row and column indices of a matrix field. A typical term in the action of a physical theory is constructed by multiplying matrix fields together and taking the trace of the resulting product; this serves to preserve gauge invariance. M(atrix)-theory,[1] a candidate for a unified theory of gravitational, strong and electroweak interactions, is another major example. In this model, the matrices describe the positions of D0-branes and their relative distances noncommutatively.[2]

So far, the most successful calculational tool for both theories is perturbative analysis, whose approximation assumptions are valid in the high-energy regime of QCD and the classical limit of M-theory. Indeed, there is an excellent agreement between perturbative QCD predictions and measurements of high-energy scattering experiments among quarks and gluons. (See Ref. 3, for instance, for a general introduction and further literature on the subject.) Perturbative M-theory calculations of scattering processes among M-theory objects are, by and large, in good agreement with classical supergravity, too. (References 4 and 5 are two recent reviews on the subject. Additional literature can be found therein.) To study important low-energy phenomena of QCD like color confinement, hadron spectrum or the parton distribution of a nucleon, or large quantum effects of supergravity, however, it is necessary to develop nonperturbative methods.

As we have just noted, both QCD and M-theory are intrinsically matrix models. Little is known about the ramifications of the matrix nature, though many researchers believe that this is the key to a deeper understanding of the physics of a matrix model. One approach is to study its symmetry. This consists in identifying a symmetry of a generic matrix model, expressing the symmetry in terms of a Lie algebra (or quantum group) and developing a representation theory for the Lie algebra.

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Numerous examples have demonstrated the fruitfulness of studying representation theories. To name but a few, the representation theory of so(3) shapes the energy spectra of physical systems with rotational symmetry; the representation theory of the Poincaré algebra enables us to classify massless fundamental particles;[3] even more remarkably, the so(4) symmetry of the hydrogenic atom dictates its energy spectrum completely.[6]

Perhaps the most prominent example in recent years is the Virasoro algebra, a Lie algebra describing two-dimensional conformal symmetry. Its representation theory reveals how the reducibility of a highest weight representation depends on the values of c, the central charge, and h, the eigenvalue of the highest weight state under the action of L_0, the energy operator. We can use these irreducible representations to describe compactified string theory.[7] We can also use a small number of highest weight reducible representations to build up a so-called minimal model describing a physical system at criticality like the Ising model and the three-state Potts model.[8] In addition, the representation theory renders us a character formula

$$\mathrm{Tr}\exp\left[2\pi\mathrm{i}\tau\left(L_0-\frac{c}{24}\right)\right]=\frac{q^{h+(1-c)/24}}{\eta(\tau)},$$

where τ is a complex variable, Tr means a sum over all states of highest weight representation and $\eta(\tau)$ is the Dedekind function

$$\eta(\tau)=\exp\left(\frac{\pi\mathrm{i}\tau}{12}\right)\prod_{n=1}^{\infty}(1-\exp(2\pi\mathrm{i}n\tau)).$$

If we interpret τ as the ratio between two complex periods along two linearly independent directions on a torus, this character formula becomes nothing but the holomorphic part of the partition function of a conformal field theory on a torus.[9] Thus we can solve for the thermodynamics of this system.

In Ref. 10, Rajeev and one of us gave an exposition on the basic properties of a newly discovered Lie algebra $\hat{G}_{\Lambda,\Lambda_F}$ for open matrix chains in the large-N limit.[11] (By an open matrix chain we mean a state produced by the action of a product of a row vector, several square matrices and a column vector of creation operators on the vacuum.) They can be interpreted as mesons in QCD, discretized open strings in a string-bit model[12] or one-dimensional open quantum spin chain systems. The relation of this Lie algebra with another Lie algebra for closed matrix chains was discussed at length in Ref. 13. We would like to build upon the results of Ref. 10, and work out a representation theory for it. In this article, we will present first results on the subject.

As noted in Ref. 13, $\hat{G}_{\Lambda,\Lambda_F}$ can be broken down into a direct sum of subalgebras in a manner similar to the triangular decomposition of a semi-simple Lie algebra. Just as a traditional triangular decomposition gives rise to lowest weight representations, this decomposition for $\hat{G}_{\Lambda,\Lambda_F}$ leads to interesting representations generated by a weight vector, which we will call a lowest weight vector. The corresponding representation will be called a lowest weight representation. It can be made irreducible by quotienting out the maximal subrepresentation. Some lowest weight vectors produce unitary representations.

Since the Cartan subalgebra we have found for $\hat{G}_{\Lambda,\Lambda_F}$ is simultaneously a maximally commutative subalgebra, we can treat it as a linear space generated by a maximally commuting set of linearly independent quantum observables. A lowest weight vector is then a quantum eigenstate of this set of quantum observables, and the lowest weight a set of quantum numbers. An interesting result we are going to show is that *if only a finite number of these quantum numbers are nonzero, then this eigenstate must be, in the context of QCD, a multiple meson state. Any state with an infinite number of nonzero quantum numbers must be a tensor product of a multiple meson and a state coming from an irredicible representation of a certain quotient algebra which extends and generalizes the Virasoro algebra*. Already for the case $\Lambda=1$ the quotient algebra is quite inter-

TABLE I. Some basis vectors of the grand string algebra. They form an overcomplete set of generators for the open string algebra. Λ and Λ_F are positive integers. λ_1, λ_2, λ_3 and λ_4 are positive integers between 1 and Λ_F inclusive. $\dot{I}$ and $\dot{J}$ are finite empty or nonempty sequences of integers, each of which is between 1 and Λ inclusive. I and J are finite nonempty sequences of integers, each of which is between 1 and Λ inclusive. $\bar{\Xi}$ and Ξ are operators acting on two different Λ_F-dimensional Hilbert spaces, and f, l, r and σ are operators acting on the same infinite-dimensional Hilbert spaces. All three Hilbert spaces were introduced in Ref. 10. (There is some abuse of notations here for the sake of future convenience; strictly speaking, the more proper notations $\bar{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot{I}}_{\dot{J}}\otimes 1$, $1\otimes r^{\dot{I}}_{\dot{J}}\otimes \Xi^{\lambda_1}_{\lambda_2}$ and $1\otimes\sigma^{I}_{J}\otimes 1$ for the operators of the second, third and fourth kind, respectively, refer to the defining representation.)

Operator of which kind	Expression
first	$\bar{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot{I}}_{\dot{J}}\otimes \Xi^{\lambda_3}_{\lambda_4}$
second	$\bar{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot{I}}_{\dot{J}}$
third	$r^{\dot{I}}_{\dot{J}}\otimes \Xi^{\lambda_1}_{\lambda_2}$
fourth	σ^{I}_{J}
any	X, $X^{\dot{I}}_{\dot{J}}$ or $Y^{\dot{I}}_{\dot{J}}$

esting. Specifically, it is an extension of the Virasoro algebra by an infinite Heisenberg algebra.[14] We expect the representation theory of the quotient algebra to describe physical systems at the thermodynamic limit.

This article is organized as follows. We will review without proofs the definition of $\hat{G}_{\Lambda,\Lambda_F}$ and its basis properties in Sec. II, further details of which can be found in Refs. 10 and 13. We will work out two useful bases for the Lie algebra in Sec. III, and its Cartan subalgebra and root vectors in Sec. IV. (The reader is advised to read only the statements of the propositions in these two sections on a first reading, and return to them later on if he or she is interested in the details.) We will define the notion of a Verma-like module and the associated Hermitian form in Sec. V, and use this to identify the representation spaces of multiple meson states in Sec. VI and other states which are related to the quotient algebra in Sec. VII.

We follow Refs. 15 and 16 in the usage of Lie algebra terminologies.

II. DEFINITIONS

Two Lie algebras were defined in Ref. 13: the grand string algebra and the open string algebra. The latter is our major interest in this article, and was defined as a quotient of the former. We will briefly review them in this section. Further details of the notations and formalism can be found in Refs. 10 and 13. One agreement we need to make with the reader now is that *unless otherwise specified, the summation convention will not be adopted.*

The elements of the grand string algebra were originated from operators acting on closed or open matrix chains (which are sometimes called closed or open singlet states). Some of them are shown in Table I. A physical observable is a linear combination of such operators. An operator of the first kind replaces a whole open singlet state with a finite linear combination of open single states; an operator of the second kind replaces the conjugate and the adjacent adjoint partons of an open singlet state with a finite linear combination of open singlet states with possibly other conjugate and adjoint partons; an operator of the third kind is similar to the second kind in action except that it acts on the end with a fundamental parton; an operator of the fourth kind propagates

an open singlet state to a finite linear combination of open singlet states in each of which a middle segment of adjacent adjoint partons in the original state is replaced with a possibly different sequence of adjoint partons.

Note that *as operators acting on closed or open matrix chains, the operators tabulated are not linearly independent; as elements of the grand string algebra, however, they are linearly independent*. Listed below are the Lie brackets of the grand string algebra between

(1) an operator of the first kind and any operator:

$$[\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot I}_{\dot J}\otimes\Xi^{\lambda_3}_{\lambda_4},\overline{\Xi}^{\lambda_5}_{\lambda_6}\otimes f^{\dot K}_{\dot L}\otimes\Xi^{\lambda_7}_{\lambda_8}]=\delta^{\lambda_5}_{\lambda_2}\delta^{\dot K}_{\dot J}\delta^{\lambda_7}_{\lambda_4}\overline{\Xi}^{\lambda_1}_{\lambda_6}\otimes f^{\dot I}_{\dot L}\otimes\Xi^{\lambda_3}_{\lambda_8}-\delta^{\lambda_1}_{\lambda_6}\delta^{\dot I}_{\dot L}\delta^{\lambda_3}_{\lambda_8}\overline{\Xi}^{\lambda_5}_{\lambda_2}\otimes f^{\dot K}_{\dot J}\otimes\Xi^{\lambda_7}_{\lambda_4},\quad(1)$$

$$[\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot I}_{\dot J}\otimes\Xi^{\lambda_3}_{\lambda_4},\overline{\Xi}^{\lambda_5}_{\lambda_6}\otimes l^{\dot K}_{\dot L}]=\delta^{\lambda_5}_{\lambda_2}\overline{\Xi}^{\lambda_1}_{\lambda_6}\otimes\sum_{\dot J_1\dot J_2=\dot J}\delta^{\dot K}_{\dot J_1}f^{\dot I}_{\dot L\dot J_2}\otimes\Xi^{\lambda_3}_{\lambda_4}-\delta^{\lambda_1}_{\lambda_6}\overline{\Xi}^{\lambda_5}_{\lambda_2}\otimes\sum_{\dot I_1\dot I_2=\dot I}\delta^{\dot I_1}_{\dot L}f^{\dot K\dot I_2}_{\dot J}\otimes\Xi^{\lambda_3}_{\lambda_4},\quad(2)$$

$$[\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot I}_{\dot J}\otimes\Xi^{\lambda_3}_{\lambda_4},r^{\dot K}_{\dot L}\otimes\Xi^{\lambda_5}_{\lambda_6}]=\delta^{\lambda_5}_{\lambda_4}\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes\sum_{\dot J_1\dot J_2=\dot J}\delta^{\dot K}_{\dot J_2}f^{\dot I}_{\dot J_1\dot L}\otimes\Xi^{\lambda_3}_{\lambda_6}-\delta^{\lambda_3}_{\lambda_6}\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes\sum_{\dot I_1\dot I_2=\dot I}\delta^{\dot I_2}_{\dot L}f^{\dot I_1\dot K}_{\dot J}\otimes\Xi^{\lambda_5}_{\lambda_4},\quad(3)$$

and

$$[\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot I}_{\dot J}\otimes\Xi^{\lambda_3}_{\lambda_4},\sigma^{K}_{L}]=\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes\left(\sum_{\dot J_1\dot J_2\dot J_3=\dot J}\delta^{K}_{\dot J_2}f^{\dot I}_{\dot J_1L\dot J_3}-\sum_{\dot I_1\dot I_2\dot I_3=\dot I}\delta^{\dot I_2}_{L}f^{\dot I_1K\dot I_3}_{\dot J}\right)\otimes\Xi^{\lambda_3}_{\lambda_4};\quad(4)$$

(2) an operator of the second kind and an operator of the second, third or fourth kind:

$$\begin{aligned}[\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot I}_{\dot J},\overline{\Xi}^{\lambda_3}_{\lambda_4}\otimes l^{\dot K}_{\dot L}]=&\delta^{\lambda_3}_{\lambda_2}\overline{\Xi}^{\lambda_1}_{\lambda_4}\otimes\left(\delta^{\dot K}_{\dot J}l^{\dot I}_{\dot L}+\sum_{\dot J_1\dot J_2=\dot J}\delta^{\dot K}_{\dot J_1}l^{\dot I}_{\dot L\dot J_2}+\sum_{\dot K_1\dot K_2=\dot K}\delta^{\dot K_1}_{\dot J}l^{\dot I\dot K_2}_{\dot L}\right)\\&-\delta^{\lambda_1}_{\lambda_4}\overline{\Xi}^{\lambda_3}_{\lambda_2}\otimes\left(\delta^{\dot I}_{\dot L}l^{\dot K}_{\dot J}+\sum_{\dot L_1\dot L_2=\dot L}\delta^{\dot I}_{\dot L_1}l^{\dot K}_{\dot J\dot L_2}+\sum_{\dot I_1\dot I_2=\dot I}\delta^{\dot I_1}_{\dot L}l^{\dot K\dot I_2}_{\dot J}\right),\end{aligned}\quad(5)$$

$$[\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot I}_{\dot J},r^{\dot K}_{\dot L}\otimes\Xi^{\lambda_3}_{\lambda_4}]=\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes\left(\sum_{\substack{\dot J_1\dot J_2=\dot J\\ \dot K_1\dot K_2=\dot K}}\delta^{\dot K_1}_{\dot J_2}f^{\dot I\dot K_2}_{\dot J_1\dot L}-\sum_{\substack{\dot I_1\dot I_2=\dot I\\ \dot L_1\dot L_2=\dot L}}\delta^{\dot I_2}_{\dot L_1}f^{\dot I_1\dot K}_{\dot J\dot L_2}\right)\otimes\Xi^{\lambda_3}_{\lambda_4},\quad(6)$$

and

$$\begin{aligned}[\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot I}_{\dot J},\sigma^{K}_{L}]=\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes\Bigg(&\delta^{K}_{\dot J}l^{\dot I}_{L}+\sum_{K_1K_2=K}\delta^{K_1}_{\dot J}l^{\dot I K_2}_{L}+\sum_{\dot J_1\dot J_2=\dot J}\delta^{K}_{\dot J_2}l^{\dot I}_{\dot J_1L}+\sum_{\dot J_1\dot J_2=\dot J}\delta^{K}_{\dot J_1}l^{\dot I}_{\dot L\dot J_2}+\sum_{\substack{\dot J_1\dot J_2=\dot J\\ K_1K_2=K}}\delta^{K_1}_{\dot J_2}l^{\dot I K_2}_{\dot J_1L}\\&+\sum_{\dot J_1\dot J_2\dot J_3=\dot J}\delta^{K}_{\dot J_2}l^{\dot I}_{\dot J_1L\dot J_3}-\delta^{\dot I}_{L}l^{K}_{\dot J}-\sum_{L_1L_2=L}\delta^{\dot I}_{L_1}l^{K}_{\dot J L_2}-\sum_{\dot I_1\dot I_2=\dot I}\delta^{\dot I_2}_{L}l^{\dot I_1K}_{\dot J}-\sum_{\dot I_1\dot I_2=\dot I}\delta^{\dot I_1}_{L}l^{K\dot I_2}_{\dot J}\\&-\sum_{\substack{L_1L_2=L\\ \dot I_1\dot I_2=\dot I}}\delta^{\dot I_2}_{L_1}l^{\dot I_1K}_{\dot J\dot L_2}-\sum_{\dot I_1\dot I_2\dot I_3=\dot I}\delta^{\dot I_2}_{L}l^{\dot I_1K\dot I_3}_{\dot J}\Bigg);\end{aligned}\quad(7)$$

(3) an operator of the third kind and an operator of the third or fourth kind:

$$[r^{\dot I}_{\dot J}\otimes\Xi^{\lambda_1}_{\lambda_2},r^{\dot K}_{\dot L}\otimes\Xi^{\lambda_3}_{\lambda_4}]=\delta^{\lambda_3}_{\lambda_2}\Bigg(\delta^{\dot K}_{\dot J}r^{\dot I}_{\dot L}+\sum_{J_1J_2=\dot J}\delta^{\dot K}_{J_2}r^{\dot I}_{J_1\dot L}+\sum_{K_1K_2=\dot K}\delta^{\dot K_2}_{\dot J}r^{K_1\dot I}_{\dot L}\Bigg)\otimes\Xi^{\lambda_1}_{\lambda_4}$$
$$-\delta^{\lambda_1}_{\lambda_4}\Bigg(\delta^{\dot I}_{\dot L}r^{\dot K}_{\dot J}+\sum_{L_1L_2=\dot L}\delta^{\dot I}_{L_2}r^{\dot K}_{L_1\dot J}+\sum_{I_1I_2=\dot I}\delta^{\dot I_2}_{\dot L}r^{I_1\dot K}_{\dot J}\Bigg)\otimes\Xi^{\lambda_3}_{\lambda_2}\tag{8}$$

and

$$[r^{\dot I}_{\dot J}\otimes\Xi^{\lambda_1}_{\lambda_2},\sigma^K_L]=\Bigg(\delta^K_{\dot J}r^{\dot I}_L+\sum_{K_1K_2=K}\delta^{K_2}_{\dot J}r^{K_1\dot I}_L+\sum_{J_1J_2=\dot J}\delta^K_{J_2}r^{\dot I}_{J_1L}+\sum_{J_1J_2=\dot J}\delta^K_{J_1}r^{\dot I}_{LJ_2}+\sum_{\substack{J_1J_2=\dot J\\K_1K_2=K}}\delta^{K_2}_{J_1}r^{K_1\dot I}_{LJ_2}$$
$$+\sum_{J_1J_2J_3=\dot J}\delta^K_{J_2}r^{\dot I}_{J_1LJ_3}-\delta^{\dot I}_Lr^K_{\dot J}-\sum_{L_1L_2=L}\delta^{\dot I}_{L_2}r^K_{L_1\dot J}-\sum_{I_1I_2=\dot I}\delta^{I_2}_Lr^{I_1K}_{\dot J}-\sum_{I_1I_2=\dot I}\delta^{I_1}_Lr^{KI_2}_{\dot J}$$
$$-\sum_{\substack{L_1L_2=L\\I_1I_2=\dot I}}\delta^{I_1}_{L_2}r^{KI_2}_{L_1\dot J}-\sum_{I_1I_2I_3=\dot I}\delta^{I_2}_Lr^{I_1KI_3}_{\dot J}\Bigg)\otimes\Xi^{\lambda_1}_{\lambda_2};\tag{9}$$

(4) two operators of the fourth kind:

$$[\sigma^I_J,\sigma^K_L]=\delta^K_J\sigma^I_L+\sum_{J_1J_2=J}\delta^K_{J_2}\sigma^I_{J_1L}+\sum_{K_1K_2=K}\delta^{K_1}_J\sigma^{IK_2}_L$$
$$+\sum_{\substack{J_1J_2=J\\K_1K_2=K}}\delta^{K_1}_{J_2}\sigma^{IK_2}_{J_1L}+\sum_{J_1J_2=J}\delta^K_{J_1}\sigma^I_{LJ_2}+\sum_{K_1K_2=K}\delta^{K_2}_J\sigma^{K_1I}_L+\sum_{\substack{J_1J_2=J\\K_1K_2=K}}\delta^{K_2}_{J_1}\sigma^{K_1I}_{LJ_2}$$
$$+\sum_{J_1J_2J_3=J}\delta^K_{J_2}\sigma^I_{J_1LJ_3}+\sum_{K_1K_2K_3=K}\delta^{K_2}_J\sigma^{K_1IK_3}_L-(I\leftrightarrow K,J\leftrightarrow L)+\cdots.\tag{10}$$

The ellipses in the last equation represent terms which cannot be written in terms of the operators listed in Table I; they play no role in the open string algebra, to be introduced immediately.

As the elements of the grand string algebra come from phyiscal observables of open matrix chains, it should not be surprising the open matrix chains provide a representation of the grand string algebra, albeit not a faithful one. As we mentioned in the Introduction, an open matrix chain can be abstractly written as $\overline{\phi}^{\lambda_1}\otimes s^{\dot K}\otimes\phi^{\lambda_2}$. $\overline{\phi}^1$, $\overline{\phi}^2$,…, and $\overline{\phi}^{\Lambda_F}$ span a Λ_F-dimensional vector space; ϕ^1, ϕ^2,…, and ϕ^{Λ_F} span another Λ_F-dimensional vector space; and all vectors of the form s^K span an infinite-dimensional vector space. Let $\mathcal{T}_o$ be the vector space consisting of finite linear combinations of open matrix chains. The actions of the four kinds of operators on an open matrix chain are given by

$$\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot I}_{\dot J}\otimes\Xi^{\lambda_3}_{\lambda_4}(\overline{\phi}^{\lambda_5}\otimes s^{\dot K}\otimes\phi^{\lambda_6})=\delta^{\lambda_5}_{\lambda_2}\delta^{\dot K}_{\dot J}\delta^{\lambda_6}_{\lambda_4}\overline{\phi}^{\lambda_1}\otimes s^{\dot I}\otimes\phi^{\lambda_3},\tag{11}$$

$$\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot I}_{\dot J}(\overline{\phi}^{\lambda_3}\otimes s^{\dot K}\otimes\phi^{\lambda_4})=\delta^{\lambda_3}_{\lambda_2}\sum_{\dot K_1\dot K_2=\dot K}\delta^{\dot K_1}_{\dot J}\overline{\phi}^{\lambda_1}\otimes s^{\dot I\dot K_2}\otimes\phi^{\lambda_4},\tag{12}$$

$$r^{\dot I}_{\dot J}\otimes\Xi^{\lambda_1}_{\lambda_2}(\overline{\phi}^{\lambda_3}\otimes s^{\dot K}\otimes\phi^{\lambda_4})=\delta^{\lambda_4}_{\lambda_2}\sum_{\dot K_1\dot K_2=\dot K}\delta^{\dot K_2}_{\dot J}\overline{\phi}^{\lambda_3}\otimes s^{\dot K_1\dot I}\otimes\phi^{\lambda_1},\tag{13}$$

and

$$\sigma_J^I(\overline{\phi}^{\lambda_1}\otimes s^{\dot{K}}\otimes\phi^{\lambda_2})=\overline{\phi}^{\lambda_1}\otimes\left(\sum_{\dot{K}_1K_2\dot{K}_3=\dot{K}}\delta_J^{K_2}s^{\dot{K}_1I\dot{K}_3}\right)\otimes\phi^{\lambda_2}. \tag{14}$$

$\mathcal{T}_o$ is a representation space for the grand string algebra.

Definition 1: The Lie algebra denoted as $\hat{G}_{\Lambda,\Lambda_F}$ in Ref. 10 and later on called the open string algebra in Ref. 13 is defined as the quotient of the grand string algebra by the annihilator of the representation $\mathcal{T}_o$. We will call $\mathcal{T}_o$ the defining representation.

Equations (1), (5), (8) and (10) show that the space generated by each kind of operator forms a subalgebra of the open string algebra. The four subalgebras were denoted by $F_{\Lambda,\Lambda_F}=\mathrm{gl}(\Lambda_F)\otimes F_\Lambda\otimes\mathrm{gl}(\Lambda_F)$, $\mathrm{gl}(\Lambda_F)\otimes\hat{L}_\Lambda$, $\hat{R}_\Lambda\otimes\mathrm{gl}(\Lambda_F)$ and $\hat{\Sigma}_\Lambda$, respectively, in Ref. 10. In addition, Eqs. (1)–(4) tell us that $\mathrm{gl}(\Lambda_F)\otimes F_\Lambda\otimes\mathrm{gl}(\Lambda_F)$ is a proper ideal isomorphic to $\mathrm{gl}(\infty)$, and Eqs. (1)–(9) tell us that all the operators of the first three kinds together span a bigger proper ideal $\hat{M}_{\Lambda,\Lambda_F}$.

For future convenience, let us introduce some more operators of the fourth kind acting on the defining representation space. They are $\sigma_\varnothing^\varnothing$, $\sigma_\varnothing^I$ and $\sigma_J^\varnothing$, and are defined by

$$\sigma_\varnothing^\varnothing(\overline{\phi}^{\lambda_1}\otimes s^{\dot{K}}\otimes\phi^{\lambda_2})\equiv(\#(\dot{K})+1)\,\overline{\phi}^{\lambda_1}\otimes s^{\dot{K}}\otimes\phi^{\lambda_2}, \tag{15}$$

$$\sigma_\varnothing^I(\overline{\phi}^{\lambda_1}\otimes s^{\dot{K}}\otimes\phi^{\lambda_2})\equiv\sum_{\dot{K}_1\dot{K}_2=\dot{K}}\overline{\phi}^{\lambda_1}\otimes s^{\dot{K}_1I\dot{K}_2}\otimes\phi^{\lambda_2} \tag{16}$$

and

$$\sigma_J^\varnothing(\overline{\phi}^{\lambda_1}\otimes s^{\dot{K}}\otimes\phi^{\lambda_2})\equiv\sum_{\dot{K}_1K_2\dot{K}_3=\dot{K}}\delta_J^{K_2}\overline{\phi}^{\lambda_1}\otimes s^{\dot{K}_1\dot{K}_3}\otimes\phi^{\lambda_2}. \tag{17}$$

Though these operators look completely new, they are actually elements of the open string algebra, as can be seen from the following identities which are now fully general:

$$\sigma_{\dot{J}}^{\dot{I}}=\sum_{i=1}^{\Lambda}\sigma_{i\dot{J}}^{i\dot{I}}+\sum_{\lambda=1}^{\Lambda_F}\overline{\Xi}_\lambda^\lambda\otimes l_{\dot{J}}^{\dot{I}}=\sum_{j=1}^{\Lambda}\sigma_{\dot{J}j}^{\dot{I}j}+\sum_{\lambda=1}^{\Lambda_F}r_{\dot{J}}^{\dot{I}}\otimes\Xi_\lambda^\lambda. \tag{18}$$

The reader can check the validity of Eq. (18) by verifying that the left and right hand sides have the same action on any open matrix chain.

Without recourse to Eq. (18), there is a representation of $\sigma_J^\varnothing$ directly in terms of matrix annihilation operators as shown in the following formula, where the summation convention for color indices is adopted:

$$\sigma_J^\varnothing=\frac{1}{N^{(b-2)/2}}a_{\nu_b}^{\nu_{b-1}}(j_b)a_{\nu_{b-1}}^{\nu_{b-2}}(j_{b-1})\cdots a_{\nu_1}^{\nu_b}(j_1). \tag{19}$$

We know of no representation of $\sigma_\varnothing^\varnothing$ or $\sigma_\varnothing^I$ in terms of matrix annihilation or creation operators without using Eq. (18).

Sometimes we will use the generic notation $X_{\dot{J}}^{\dot{I}}$ or $Y_{\dot{J}}^{\dot{I}}$ to refer to $\overline{\Xi}_{\lambda_2}^{\lambda_1}\otimes f_{\dot{J}}^{\dot{I}}\otimes\Xi_{\lambda_4}^{\lambda_3}$, $\overline{\Xi}_{\lambda_2}^{\lambda_1}\otimes l_{\dot{J}}^{\dot{I}}$, $r_{\dot{J}}^{\dot{I}}\otimes\Xi_{\lambda_2}^{\lambda_1}$ or $\sigma_{\dot{J}}^{\dot{I}}$, ignoring λ_1, λ_2, λ_3 and λ_4.

III. BASES

The operators listed in Table I do not form a basis for the open string algebra because they are overcomplete. In this section, we will work out two bases which will be of use in future discussions. Readers who are not interested in the details may read only the statements of Propositions 1 and 2, and then move on directly to the next section.

Before we start, we need to recall a lexicographic ordering for integer sequences from Ref. 13. We will use it to construct another one for a basis of the open string algebra. (Both orderings are denoted as $>$ as there is no danger of confusion.)

Definition 2: We designate $\dot{I}>\dot{J}$ *if either*

(1) $\#(\dot{I})>\#(\dot{J})$*; or*
(2) $\#(\dot{I})=\#(\dot{J})=a\neq 0$*, and there exists an integer* $r\leqslant a$ *such that* $i_1=j_1$, $i_2=j_2,\ldots,$ $i_{r-1}=j_{r-1}$ *and* $i_r>j_r$.

Definition 3: Here is a lexicographic ordering for a basis of the open string algebra.

(1) $X^{\dot{I}}_{\dot{J}}>Y^{\dot{K}}_{\dot{L}}$ *if*
  (a) $\#(\dot{I})-\#(\dot{J})>\#(\dot{K})-\#(\dot{L})$*; or*
  (b) $\#(\dot{I})-\#(\dot{J})=\#(\dot{K})-\#(\dot{L})$ *and* $\#(\dot{I})+\#(\dot{J})>\#(\dot{K})+\#(\dot{L})$*; or*
  (c) $\#(\dot{I})=\#(\dot{K})$, $\#(\dot{J})=\#(\dot{L})$ *and* $\dot{J}>\dot{L}$*; or*
  (d) $\dot{J}=\dot{L}$, $\#(\dot{I})=\#(\dot{K})$ *and* $\dot{I}>\dot{K}$*;*
(2) $\sigma^{\dot{I}}_{\dot{J}}>r^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2}>\overline{\Xi}^{\lambda_3}_{\lambda_4}\otimes l^{\dot{I}}_{\dot{J}}>\overline{\Xi}^{\lambda_5}_{\lambda_6}\otimes f^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_7}_{\lambda_8}$*;*
(3) $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_3}_{\lambda_4}>\overline{\Xi}^{\lambda_5}_{\lambda_6}\otimes f^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_7}_{\lambda_8}$ *if*
  (a) $\lambda_2\lambda_4>\lambda_6\lambda_8$ *as concatenated sequences; or*
  (b) $\lambda_2\lambda_4=\lambda_6\lambda_8$ *and* $\lambda_1\lambda_3>\lambda_5\lambda_7$*;*
(4) $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot{I}}_{\dot{J}}>\overline{\Xi}^{\lambda_3}_{\lambda_4}\otimes l^{\dot{I}}_{\dot{J}}$ *if*
  (a) $\lambda_2>\lambda_4$*; or*
  (b) $\lambda_2=\lambda_4$ *and* $\lambda_1>\lambda_3$*;*
(5) $r^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2}>r^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_3}_{\lambda_4}$ *if*
  (a) $\lambda_2>\lambda_4$*; or*
  (b) $\lambda_2=\lambda_4$ *and* $\lambda_1>\lambda_3$.

Note that changing the basis changes the lexicographic ordering also.

Proposition 1: The following set $\mathcal{B}_0$ *of elements forms a basis for the open string algebra:*

(1) all $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_3}_{\lambda_4}$ *such that* $\lambda_1+\lambda_2>2$ *and* $\lambda_3+\lambda_4>2$*;*
(2) all $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot{I}}_{\dot{J}}$ *such that* $\lambda_1\neq 1$ *or* $\lambda_2\neq 1$*;*
(3) all $r^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2}$ *such that* $\lambda_1\neq 1$ *or* $\lambda_2\neq 1$*; and*
(4) all $\sigma^{\dot{I}}_{\dot{J}}$.

This proposition is a consequence of the following two lemmas.

Lemma 1: $\mathcal{B}_0$ *is a linearly independent set.*

Proof: We will prove this by *ad absurdum*. Consider an arbitrary sum X of a finite number of the elements listed in Proposition 1. Write down X according to the following

Convention: The numerical coefficient of $\sigma^{\dot{I}}_{\dot{J}}$ in X is written as $c(\sigma^{\dot{I}}_{\dot{J}})$. The coefficients of other operators are written similarly. (By definition, only a finite number of the coefficients are nonzero.)

Assume that this sum X is identically equal to zero. There are now several possibilities.

Consider first the case in which some $c(\sigma^{\dot{I}}_{\dot{J}})\neq 0$ in the sum X, which can then be written as

$$\sum_{i=1}^{p} c(\sigma^{\dot{I}_i}_{\dot{J}_i})\sigma^{\dot{I}_i}_{\dot{J}_i}+\cdots,$$

where p is a finite positive integer, $\dot{J}_1=\dot{J}_2=\cdots=\dot{J}_q<\dot{J}_{q+1}\leqslant\cdots\leqslant\dot{J}_p$ for some integer $q\leqslant p$, $\dot{I}_r\neq\dot{I}_s$ for $1\leqslant r,s\leqslant q$ such that $r\neq s$, and the ellipses denote terms involving operators of other kinds. Then acting the sum on $\overline{\phi^1}\otimes s^{\dot{J}_1}\otimes\phi^1$ yields

$$\sum_{i=1}^{q} c(\sigma^{\dot{I}_i}_{\dot{J}_1})\overline{\phi^1}\otimes s^{\dot{I}_i}\otimes\phi^1+\cdots,$$

where the ellipses consist of terms proportional to $\overline{\phi^{\lambda_1}}\otimes s^{\dot{K}}\otimes\phi^{\lambda_2}$, where $\lambda_1>1$ or $\lambda_2>1$. This is manifestly nonzero, a contradiction. Hence there is no operator of the form $\sigma^{\dot{I}}_{\dot{J}}$ in the sum.

Similarly, considering the action of the sum on a state of the form $\overline{\phi^\rho}\otimes s^K\otimes\phi^1$ will rule out the presence of any $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot{I}}_{\dot{J}}$ in the sum. Then considering $\overline{\phi^1}\otimes s^{\dot{K}}\otimes\phi^\rho$ will rule out any $r^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2}$. Finally, considering $\overline{\phi^{\rho_1}}\otimes s^{\dot{K}}\otimes\phi^{\rho_2}$ will eliminate all $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_3}_{\lambda_4}$. Consequently, no element of $\mathcal{B}_0$ can appear in the sum to make it identically zero, and $\mathcal{B}_0$ is linearly independent. Q.E.D.

Lemma 2: Any element of the open string algebra can be written as a finite sum of the elements listed in Proposition 1.

Proof: This follows from the following formulas, which the reader can check one by one by verifying that the actions of the left and right hand sides of any equation below on any open matrix chain are the same:

$$\sum_{\lambda=1}^{\Lambda_F}\overline{\Xi}^{\lambda}_{\lambda}\otimes r^I_J=\sigma^I_J-\sum_{j=1}^{\Lambda}\sigma^{Ij}_{Jj};\tag{20}$$

$$\sum_{\lambda=1}^{\Lambda_F} l^I_J\otimes\Xi^{\lambda}_{\lambda}=\sigma^I_J-\sum_{i=1}^{\Lambda}\sigma^{iI}_{iJ};\tag{21}$$

$$\sum_{\lambda_3=1}^{\Lambda_F}\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_3}_{\lambda_3}=\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot{I}}_{\dot{J}}-\sum_{j=1}^{\Lambda}\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot{I}\dot{j}}_{\dot{J}j};\tag{22}$$

and

$$\sum_{\lambda_1=1}^{\Lambda_F}\overline{\Xi}^{\lambda_1}_{\lambda_1}\otimes f^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_2}_{\lambda_3}=r^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_2}_{\lambda_3}-\sum_{i=1}^{\Lambda} r^{i\dot{I}}_{i\dot{J}}\otimes\Xi^{\lambda_2}_{\lambda_3}.\tag{23}$$

Q.E.D.

Remark 1: Equations (20)–(23) may now be taken as a set of defining relations for the open string algebra, though there is a little redundancy in them.

We now give a different basis for the open string algebra. We will use it to construct ''Verma-like modules.''

Proposition 2: The following set $\mathcal{B}_4$ of elements form a basis for the open string algebra:

(1) all $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_3}_{\lambda_4}$;

(2) all $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot{I}}_{\dot{J}}$ such that the last integers in $\dot{I}$ *and* $\dot{J}$ *are not simultaneously 1;*

(3) all $r^{\varnothing}_{\varnothing}\otimes\Xi^{\lambda_1}_{\lambda_2}$ *such that* $\lambda_1\neq 1$ *or* $\lambda_2\neq 1$*;*
(4) all $r^{I}_{\varnothing}\otimes\Xi^{\lambda_1}_{\lambda_2}$ *such that* $\lambda_1\neq 1$, $\lambda_2\neq 1$ *or the first integer of* I *is not 1;*
(5) all $r^{\varnothing}_{J}\otimes\Xi^{\lambda_1}_{\lambda_2}$ *such that* $\lambda_1\neq 1$, $\lambda_2\neq 1$ *or the first integer of* J *is not 1;*
(6) all $r^{I}_{J}\otimes\Xi^{\lambda_1}_{\lambda_2}$ *such that the first integers in* I *and* J *are not simultaneously 1; and*
(7) all $\sigma^{\dot{I}}_{\dot{J}}$ *such that the first integers in* I *and* J *are not simultaneously 1 and the last integers in* I *and* J *are not simultaneously 1 either.*

Proof (sketched): This follows from Lemma 1 by extensive use of Eqs. (20)–(23) and by insisting that all the elements $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_3}_{\lambda_4}$ should occur in the basis. Observe that the recundancy in the mentioned equations in the present setting is due to the fact that the elements $\sigma^{1\dot{I}1}_{\varnothing}$, $\sigma^{\varnothing}_{1\dot{J}1}$, and $\Sigma_i\sigma^{i}_{i}$ occur both in Eq. (20) and in Eq. (21). The reader can find a more detailed and thoroughly rigorous proof in Ref. 17.

IV. CARTAN SUBALGEBRA AND ROOT VECTORS

We are going to work out a Cartan subalgebra and the root vectors associated with it for the open string algebra. We will need these results in future sections. Once again those who are not interested in details may only read the statements of the propositions in this section, and move on to the next section directly.

Proposition 3: All $\overline{\Xi}^{\lambda_1}_{\lambda_1}\otimes f^{\dot{I}}_{\dot{I}}\otimes\Xi^{\lambda_2}_{\lambda_2}$, *all* $\overline{\Xi}^{\lambda}_{\lambda}\otimes l^{\dot{I}}_{\dot{I}}$, *all* $r^{\dot{I}}_{\dot{I}}\otimes\Xi^{\lambda}_{\lambda}$ *and all* $\sigma^{\dot{I}}_{\dot{I}}$ *form an overcomplete set of generators of a Cartan subalgebra* G^{00} *of the open string algebra.*[18]

Proof: In terms of the basis $\mathcal{B}_0$, what we need to show is that

(1) all $\overline{\Xi}^{\lambda_1}_{\lambda_1}\otimes f^{\dot{I}}_{\dot{I}}\otimes\Xi^{\lambda_2}_{\lambda_2}$ such that $\lambda_1\neq 1$ and $\lambda_2\neq 1$,
(2) all $\overline{\Xi}^{\lambda}_{\lambda}\otimes l^{\dot{I}}_{\dot{I}}$, such that $\lambda\neq 1$,
(3) all $r^{\dot{I}}_{\dot{I}}\otimes\Xi^{\lambda}_{\lambda}$ such that $\lambda\neq 1$, and
(4) all $\sigma^{\dot{I}}_{\dot{I}}$

form a basis for this Cartan subalgebra. It is obvious that G^{00} is commutative and, *a fortiori*, nilpotent. Consider an element X of the normalizer of G^{00}. Let us express X in terms of the basis $\mathcal{B}_0$ using the Convention in the proof of Lemma 1. Consider the following.

Case 1: There exist in X *terms of the form* $c(\sigma^{\dot{I}_i}_{\dot{J}_i})\sigma^{\dot{I}_i}_{\dot{J}_i}$ *such that* i *is a positive integer not larger than* p, $\dot{I}_i\neq\dot{J}_i$, $c(\sigma^{\dot{I}_i}_{\dot{J}_i})\neq 0$ *for each* i *and* $c(\sigma^{\dot{I}}_{\dot{J}})=0$ *for any other* $\dot{I}$ *and* $\dot{J}$ *such that* $\dot{I}\neq\dot{I}_i$ *or* $\dot{J}\neq\dot{J}_i$ *for each* i. *Without loss of generality, we can further assume that either*

$$\dot{I}_1\leqslant\dot{I}_i \quad and \quad \dot{I}_1\leqslant\dot{J}_i \tag{24}$$

for each value of i, *or*

$$\dot{J}_1\leqslant\dot{I}_i \quad and \quad \dot{J}_1\leqslant\dot{J}_i \tag{25}$$

for each value of i.

If Eq. (24) is true, then

$$[\overline{\Xi}^{1}_{1}\otimes f^{\dot{I}_1}_{\dot{I}_1}\otimes\Xi^{1}_{1},X]=c(\sigma^{\dot{I}_1}_{\dot{J}_1})\overline{\Xi}^{1}_{1}\otimes f^{\dot{I}_1}_{\dot{J}_1}\otimes\Xi^{1}_{1}+\cdots, \tag{26}$$

which clearly does not belong to G^{00}. If instead Eq. (25) is true, then

$$[\bar{\Xi}^1_1 \otimes f^{\dot{J}_1}_{\dot{J}_1} \otimes \Xi^1_1, X] = -c(\sigma^{\dot{I}_1}_{\dot{J}_1})\bar{\Xi}^1_1 \otimes f^{\dot{I}_1}_{\dot{J}_1} \otimes \Xi^1_1 + \cdots, \tag{27}$$

which clearly does not belong to G^{00} either. Thus there is no term proportional to $\sigma^{\dot{I}}_{\dot{J}}$ in X such that $\dot{I} \neq \dot{J}$.

Similar arguments by contradiction enable us to rule out all other cases listed below.

Case 2: There exist in X terms of the form $c(r^{\dot{I}_i}_{\dot{J}_i} \otimes \Xi^{\lambda_i}_{\rho_i}) r^{\dot{I}_i}_{\dot{J}_i} \otimes \Xi^{\lambda_i}_{\rho_i}$ *such that the following four conditions hold:*

(1) i *is a positive integer not larger than p;*
(2) $\dot{I}_i \lambda_i \neq \dot{J}_i \rho_i$ *for each i;*
(3) $c(r^{\dot{I}_i}_{\dot{J}_i} \otimes \Xi^{\lambda_i}_{\rho_i}) \neq 0$ *for each i; and*
(4) $c(r^{\dot{I}}_{\dot{J}} \otimes \Xi^{\lambda}_{\rho}) = 0$ *for any other* $\dot{I}$, $\dot{J}$, λ *and* ρ *such that* $\dot{I}\lambda \neq \dot{I}_i \lambda_i$ *or* $\dot{J}\rho \neq \dot{J}_i \rho_i$ *for each i.*

Without loss of generality, we can further assume that for all values of i, either

$$\dot{I}_1 \lambda_1 \leqslant \dot{I}_i \lambda_i \quad \text{and} \quad \dot{I}_1 \lambda_1 \leqslant \dot{J}_i \rho_i \tag{28}$$

for each value of i, *or*

$$\dot{J}_1 \rho_1 \leqslant \dot{I}_i \lambda_i \quad \text{and} \quad \dot{J}_1 \rho_1 \leqslant \dot{J}_i \rho_i \tag{29}$$

for each value of i.

Case 3: There exist in X terms of the form $c(\bar{\Xi}^{\lambda_i}_{\rho_i} \otimes l^{\dot{I}_i}_{\dot{J}_i}) \bar{\Xi}^{\lambda_i}_{\rho_i} \otimes l^{\dot{I}_i}_{\dot{J}_i}$ *such that the following four conditions hold:*

(1) i *is a positive integer not larger than p;*
(2) $\dot{I}_i \lambda_i \neq \dot{J}_i \rho_i$ *for each i;*
(3) $c(\bar{\Xi}^{\lambda_i}_{\rho_i} \otimes l^{\dot{I}_i}_{\dot{J}_i}) \neq 0$ *for each i; and*
(4) $c(\bar{\Xi}^{\lambda}_{\rho} \otimes l^{\dot{I}}_{\dot{J}}) = 0$ *for any other* $\dot{I}$, $\dot{J}$, λ *and* ρ *such that* $\dot{I}\lambda \neq \dot{I}_i \lambda_i$ *or* $\dot{J}\rho \neq \dot{J}_i \rho_i$ *for each i.*

(5) Case 4: There exist in X terms of the form $c(\bar{\Xi}^{\lambda_i}_{\rho_i} \otimes f^{\dot{I}_i}_{\dot{J}_i} \otimes \Xi^{\alpha_i}_{\beta_i}) \bar{\Xi}^{\lambda_i}_{\rho_i} \otimes f^{\dot{I}_i}_{\dot{J}_i} \otimes \Xi^{\alpha_i}_{\beta_i}$ *such that the following four conditions hold:*

(1) i *is a positive integer not larger than p;*
(2) $\dot{I}_i \lambda_i \alpha_i \neq \dot{J}_i \rho_i \beta_i$ *for each i;*
(3) $c(\bar{\Xi}^{\lambda_i}_{\rho_i} \otimes f^{\dot{I}_i}_{\dot{J}_i} \otimes \Xi^{\alpha_i}_{\beta_i}) \neq 0$ *for each i; and*
(4) $c(\bar{\Xi}^{\lambda}_{\rho} \otimes f^{\dot{I}}_{\dot{J}} \otimes \Xi^{\alpha}_{\beta}) = 0$ *for any other* $\dot{I}$, $\dot{J}$, λ, ρ, α *and* β *such that* $\dot{I}\lambda\alpha \neq \dot{I}_i \lambda_i \alpha_i$ *or* $\dot{J}\rho\beta \neq \dot{J}_i \rho_i \beta_i$ *for each i.*

Q.E.D.

Proposition 4: A necessary and sufficient condition for a vector of the open string algebra to be an eigenvector with respect to the Cartan subalgebra G^{00} *is that this vector is proportional to* $\bar{\Xi}^{\lambda_1}_{\lambda_2} \otimes f^{\dot{I}}_{\dot{J}} \otimes \Xi^{\lambda_3}_{\lambda_4}$, *where* $\dot{I}\lambda_1\lambda_3 \neq \dot{J}\lambda_2\lambda_4$.[19]

Proof: The sufficient part is obvious. Let us prove the necessary part. Write down the eigenvector V in terms of the basis set $\mathcal{B}_0$ according to the Convention in the proof of Lemma 1. It is

clear that V contains no term proportional to an element in $\mathcal{B}_0$. Now consider Case 1 in the proof of Proposition 3. If Eq. (24) is true, then Eq. (26) tells us that $V \in F_{\Lambda,\Lambda_F}$; if Eq. (25) is true instead, then Eq. (27) still yields the same conclusion that $V \in F_{\Lambda,\Lambda_F}$.

Next consider Case 2 in the proof of Proposition 3 together with the additional assumption that $c(\sigma^{\dot{I}}_{\dot{J}})=0$ for all $\dot{I}$ and $\dot{J}$. An argument similar to the one in the preceding paragraph shows that $V \in F_{\Lambda,\Lambda_F}$. We reach the same conclusion even if we consider Case 3 in the proof of Proposition 3 together with the additional assumptions that $c(\sigma^{\dot{I}}_{\dot{J}})=0$ and $c(r^{\dot{I}}_{\dot{J}} \otimes \Xi^{\lambda}_{\rho})=0$ for all $\dot{I}$, $\dot{J}$, λ and ρ.

We therefore conclude that in all cases, $V \in F_{\Lambda,\Lambda_F}$. Now, we know that F_{Λ,Λ_F} is isomorphic to gl(∞) whose properties then lead to the necessary part of this proposition. Q.E.D.

V. VERMA-LIKE MODULES

Verma modules are a valuable tool for constructing nontrivial unitary lowest weight irreducible representations of familiar Lie algebras like the Virasoro algebra. We are going to adopt the same approach to construct unitary lowest weight irreducible representations for the open string algebra. This algebra, however, differs from the Virasoro algebra in one important aspect—its Cartan subalgebra and the associated root vectors do not span the whole open string algebra. This implies there cannot be any triangular decomposition of the open string algebra in the traditional sense. Nevertheless, there is still a decomposition very similar to the triangular decomposition, and we can use this other decomposition as a starting point to define a module which resembles a Verma module. We will call this a Verma-like module.

It was noted in Ref. 13 that the subalgebra $\hat{\Sigma}_{\Lambda}$ admits a decomposition into subalgebras of ''raising,'' ''diagonal'' and ''lowering'' operators. Indeed, we will see shortly that the open string algebra can be $\mathbb{Z}$-graded.

Let $\#(\dot{I})$ be the number of integers in $\dot{I}$ and $\tilde{G}^m$ be a subspace of the grand string algebra spanned by all operators of any form shown in Table I (and all operators of the fifth kind not mentioned in Sec. II) such that $\#(\dot{I})-\#(\dot{J})=m$ or $\#(I)-\#(J)=m$. Then the grand string algebra is a direct sum of $\tilde{G}^m$ for all integral values of m. Furthermore, the reader can check from the Lie brackets of the grand string algebra, all of which can be found in Ref. 13 and most of which were reproduced in Sec. II, that

$$[\tilde{G}^m,\tilde{G}^n] \subseteq \tilde{G}^{m+n}.$$

Hence, the set of all $\tilde{G}^m$ provides a $\mathbb{Z}$-grading for the grand string algebra. Moreover, the defining representation is, in a natural way, a graded representation for the grand string algebra with the grade of $\overline{\phi}^{\lambda_1} \otimes s^{\dot{K}} \otimes \phi^{\lambda_2}$ equal to $\#(\dot{K})$. Recall from Definition 1 that the open string algebra is the quotient of the grand string algebra by the annihilator of this graded representation. It follows that the open string algebra is also $\mathbb{Z}$-graded:

$$\hat{G}_{\Lambda,\Lambda_F} = \bigoplus_{m=-\infty}^{\infty} G^m \tag{30}$$

with G^m being the image of $\tilde{G}^m$ under the quotient operation and satisfying

$$[G^m,G^n] \subseteq G^{m+n}. \tag{31}$$

The Cartan subalgebra G^{00} is a subalgebra of G^0. Let G^{0+} be the subspace of G^0 spanned by all operators of any form shown in Table I such that $\dot{I}\lambda_1\lambda_3 > \dot{J}\lambda_2\lambda_4$, $\dot{I}\lambda_1 > \dot{J}\lambda_2$, $\dot{I} > \dot{J}$ or $I > J$. Then G^{0+} is a subalgebra of G^0.[13] Likewise, let G^{0-} be the subspace of G^0 spanned by all

operators of any form shown in Table I such that $\dot{J}\lambda_2\lambda_4 > \dot{I}\lambda_1\lambda_3$, $\dot{J}\lambda_2 > \dot{I}\lambda_1$, $\dot{J} > \dot{I}$ or $J > I$. Then G^{0-} is another subalgebra of G^0. Moreover, we have $G^0 = G^- \oplus G^{00} \oplus G^+$. Consider

$$G^+ \equiv G^{0+} \oplus \left(\bigoplus_{m=1}^{\infty} G^m \right) \tag{32}$$

and

$$G^- \equiv G^{0-} \oplus \left(\bigoplus_{m=-\infty}^{-1} G^m \right). \tag{33}$$

It follows from the fact that G^{0+} is a subalgebra of G^0 and Eq. (31) that G^+ is a subalgebra of the open string algebra. Likewise, G^- is another subalgebra of $\hat{G}_{\Lambda,\Lambda_F}$. Then

$$\hat{G}_{\Lambda,\Lambda_F} = G^+ \oplus G^{00} \oplus G^-. \tag{34}$$

Let us now construct a module for the open string algebra using Eq. (34). Consider the universal enveloping algebra $\mathcal{U}(\hat{G}_{\Lambda,\Lambda_F})$ of the open string algebra. Let $h_I(\lambda_1;\dot{I};\lambda_2)$, $h_{II}(\lambda;\dot{I})$, $h_{III}(\dot{I};\lambda)$ and $h_{IV}(\dot{I})$ be fixed functions on an integer sequence $\dot{I}$ and, with the exception of h_{IV}, the positive integer(s) λ_1, λ_2 or λ also. The subscripts tell us the kinds of operators with which the functions are associated. Construct the left ideal $\mathcal{I}$ of $\mathcal{U}(\hat{G}_{\Lambda,\Lambda_F})$ generated by

(1) all elements in G^-,
(2) all $\overline{\Xi}^{\lambda_1}_{\lambda_1} \otimes f^{\dot{I}}_{I} \otimes \Xi^{\lambda_2}_{\lambda_2} - h_I(\lambda_1;\dot{I};\lambda_2)\cdot \mathbf{1}$ with $\mathbf{1}$ being the identity element of $\mathcal{U}(\hat{G}_{\Lambda,\Lambda_F})$,
(3) all $\overline{\Xi}^{\lambda}_{\lambda} \otimes l^{\dot{I}}_{I} - h_{II}(\lambda;\dot{I})\cdot \mathbf{1}$ such that $\overline{\Xi}^{\lambda}_{\lambda} \otimes l^{\dot{I}}_{I} \in \mathcal{B}_4$,
(4) all $r^{\dot{I}}_{I} \otimes \Xi^{\lambda}_{\lambda} - h_{III}(\dot{I};\lambda)\cdot \mathbf{1}$ such that $r^{\dot{I}}_{I} \otimes \Xi^{\lambda}_{\lambda} \in \mathcal{B}_4$ and
(5) all $\sigma^{\dot{I}}_{I} - h_{IV}(\dot{I})\cdot \mathbf{1}$ such that $\sigma^{\dot{I}}_{I} \in \mathcal{B}_4$.

The values of all h_I, h_{II}, h_{III} and h_{IV} listed above can be freely chosen. Fix the values of these four functions on other arguments by the succeeding equations in all of which $\dot{K}_0$ stands for the empty sequence and $\dot{K}_n = K_n$ stands for the sequence 11...1 with n integers for $n > 0$:

$$h_{II}(\lambda_1;\dot{I}K_n) = h_{II}(\lambda_1;\dot{I}) - \sum_{p=0}^{n-1} \sum_{j=2}^{\Lambda} h_{II}(\lambda_1;\dot{I}\dot{K}_p j) - \sum_{p=0}^{n-1} \sum_{\lambda_2=1}^{\Lambda_F} h_I(\lambda_1;\dot{I}\dot{K}_p;\lambda_2), \tag{35}$$

where λ_1 is any positive integer not larger than Λ_F, n is any positive integer, and $\dot{I}$ is any integer sequence such that either it is empty or its last integer is larger than 1 [cf. Eq. (22)];

$$h_{III}(K_n\dot{I};\lambda_2) = h_{III}(\dot{I};\lambda_2) - \sum_{p=0}^{n-1} \sum_{i=2}^{\Lambda} h_{III}(i\dot{K}_p\dot{I};\lambda_2) - \sum_{p=0}^{n-1} \sum_{\lambda_1=1}^{\Lambda_F} h_I(\lambda_1;\dot{K}_p\dot{I};\lambda_2), \tag{36}$$

where n is positive, and either

(1) $\dot{I}$ is empty and $\lambda_2 \neq 1$, or
(2) $\dot{I}$ is nonempty and the first integer of $\dot{I}$ is not 1

[cf. Eq. (23)];

$$h_{III}(\dot{K}_n;1)=\sum_{\lambda=1}^{\Lambda_F} h_{II}(\lambda;\varnothing)-\sum_{\lambda=2}^{\Lambda_F} h_{III}(\varnothing;\lambda)-\sum_{p=0}^{n-1}\sum_{i=2}^{\Lambda} h_{III}(i\dot{K}_p;1)-\sum_{p=0}^{n-1}\sum_{\lambda=1}^{\Lambda_F} h_I(\lambda_1;\dot{K}_p;1), \tag{37}$$

where n is any non-negative integer [cf. Eqs. (22) and (23)];

$$h_{IV}(K_n\dot{I})=h_{IV}(\dot{I})-\sum_{p=0}^{n-1}\sum_{i=2}^{\Lambda} h_{IV}(i\dot{K}_p\dot{I})-\sum_{p=0}^{n-1}\sum_{\lambda=1}^{\Lambda_F} h_{II}(\lambda;\dot{K}_p\dot{I}), \tag{38}$$

where n is any positive integer, $\dot{I}$ is either empty or has both its first and last integers larger than 1, and the values of h_{II} can either be freely chosen or determined from Eq. (35) [cf. Eq. (20)];

$$h_{IV}(IK_n)=h_{IV}(I)-\sum_{p=0}^{n-1}\sum_{j=2}^{\Lambda} h_{IV}(I\dot{K}_pj)-\sum_{p=0}^{n-1}\sum_{\lambda=1}^{\Lambda_F} h_{III}(I\dot{K}_p;\lambda), \tag{39}$$

where n is a positive integer, I is a nonempty sequence whose first and last integers are both larger than 1, and the values of h_{III} can either be freely chosen or determined from Eq. (36) or (37) [cf. Eq. (21)];

$$h_{IV}(K_m\dot{I}K_n)=h_{IV}(K_m\dot{I})-\sum_{p=0}^{n-1}\sum_{j=2}^{\Lambda} h_{IV}(K_m\dot{I}\dot{K}_pj)-\sum_{p=0}^{n-1}\sum_{\lambda=1}^{\Lambda_F} h_{III}(K_m\dot{I}\dot{K}_p;\lambda), \tag{40}$$

where both m and n are positive integers, $\dot{I}$ is a nonempty integer sequence whose first and last integers are both larger than 1, the values of h_{III} could be determined from Eq. (36) or (37), and those of h_{IV} could be determined from Eq. (38) [cf. Eqs. (20)–(23)]. The four functions $h=(h_I,h_{II},h_{III},h_{IV})$ determined in this way will be called a *lowest weight*. (Clearly, the four functions are *not* linearly indepedent.) That $\mathcal{B}_4$ is a basis of the open string algebra then implies that $\mathcal{I}$ is spanned by G^- and all elements of the form

$$\bar{\Xi}^{\lambda_1}_{\lambda_1}\otimes f^{\dot{I}}_{\dot{I}}\otimes\Xi^{\lambda_2}_{\lambda_2}-h_I(\lambda_1;\dot{I};\lambda_2)\cdot\mathbf{1},$$

$$\bar{\Xi}^{\lambda}_{\lambda}\otimes l^{\dot{I}}_{\dot{I}}-h_{II}(\lambda_1;\dot{I})\cdot\mathbf{1},$$

$$r^{\dot{I}}_{\dot{I}}\otimes\Xi^{\lambda}_{\lambda}-h_{III}(\dot{I};\lambda)\cdot\mathbf{1}$$

or

$$\sigma^{\dot{I}}_{\dot{I}}-h_{IV}(\dot{I})\cdot\mathbf{1}.$$

Define $\mathcal{M}$ to be $\mathcal{U}/\mathcal{I}$. $\hat{G}_{\Lambda,\Lambda_F}$ acts on $\mathcal{M}$ by left multiplication and so $\mathcal{M}$ is a valid representation of $\hat{G}_{\Lambda,\Lambda_F}$. Let $|v_h\rangle$ be the image of $\mathbf{1}$ in $\mathcal{M}$. Then

$$G^-|v_h\rangle=0;$$

$$\bar{\Xi}^{\lambda_1}_{\lambda_1}\otimes f^{\dot{I}}_{\dot{I}}\otimes\Xi^{\lambda_2}_{\lambda_2}|v_h\rangle=h_I(\lambda_1;\dot{I};\lambda_2)|v_h\rangle;$$

$$\bar{\Xi}^{\lambda}_{\lambda}\otimes l^{\dot{I}}_{\dot{I}}|v_h\rangle=h_{II}(\lambda;\dot{I})|v_h\rangle; \tag{41}$$

$$r_{I}^{\dot{I}}\otimes\Xi_{\lambda}^{\lambda}|v_h\rangle=h_{III}(\dot{I};\lambda)|v_h\rangle;$$

$$\sigma_{I}^{\dot{I}}|v_h\rangle=h_{IV}(\dot{I})|v_h\rangle.$$

We will call any $|v_h\rangle$ satisfying Eq. (41) a *lowest weight vector*. (Note that not all elements in G^+ can be written as finite linear combinations of root vectors of G^{00} and so this notion of a lowest weight vector is different from the traditional one.) The Poincaré–Birkhoff–Witt theorem implies that $|v_h\rangle$ together with all the elements in $\mathcal{M}$ of the form

$$E(v_h)=\prod_{p=1}^{n} X_{J_p}^{\dot{I}_p}|v_h\rangle, \tag{42}$$

where n is any positive integer, $X_{J_p}^{\dot{I}_p}\in G^+$ for each value of p and the product is arranged in the reverse of the lexicographic ordering in Definition 3, forms a basis for $\mathcal{M}$. The *expectation value* of $E(v_h)$, which we will denote as $\langle E(v_h)\rangle$, is the coefficient of $|v_h\rangle$ in the expression for $E(v_h)$ written in this basis. We will call $\mathcal{M}$ a *Verma-like module*. (Again if G^+ and G^- were spanned by root vectors, $\mathcal{M}$ would be a Verma module.)

A *lowest weight representation* of the open string algebra is a Verma-like module or a quotient of it. (We called it a highest weight representation in Ref. 20.) In general, a lowest weight representation is not irreducible. If there is a maximal subrepresentation of a Verma-like module, the resulting quotient representation will be an irreducible lowest weight representation.

To establish the notion of unitarity for lowest weight representations, we introduce a number of auxiliary notions as follows. Define an antilinear anti-involution ω on $\hat{G}_{\Lambda,\Lambda_F}$ by

$$\begin{aligned}
\omega(\overline{\Xi}_{\lambda_2}^{\lambda_1}\otimes f_{J}^{\dot{I}}\otimes\Xi_{\lambda_4}^{\lambda_3})&=\overline{\Xi}_{\lambda_1}^{\lambda_2}\otimes f_{I}^{\dot{J}}\otimes\Xi_{\lambda_3}^{\lambda_4};\\
\omega(\overline{\Xi}_{\lambda_2}^{\lambda_1}\otimes l_{J}^{\dot{I}})&=\overline{\Xi}_{\lambda_1}^{\lambda_2}\otimes l_{I}^{\dot{J}};\\
\omega(r_{j}^{\dot{I}}\otimes\Xi_{\lambda_2}^{\lambda_1})&=r_{I}^{\dot{j}}\otimes\Xi_{\lambda_1}^{\lambda_2};\\
\omega(\sigma_{J}^{I})&=\sigma_{I}^{J}.
\end{aligned} \tag{43}$$

(Readers who know how these four kinds of operators were introduced in Refs. 10 and 13 should be aware that this antilinear anti-involution is nothing but the Hermitian conjugation of creation and annihilation operators of partons.) This antilinear anti-involution of $\hat{G}_{\Lambda,\Lambda_F}$ extends straightforwardly to an antilinear anti-involution of its universal enveloping algebra $\mathcal{U}(\hat{G}_{\Lambda,\Lambda_F})$.

From now on, we assume all the weight functions to be real. This allows us to define a sesquilinear form $\langle\cdot|\cdot\rangle$ on two elements $E_1(v_h)$ and $E_2(v_h)$ of $\mathcal{M}$, both of which are of the form Eq. (42), by

$$\langle E_1(v_h)|E_2(v_h)\rangle\equiv\langle(\omega(E_1)E_2)(v_h)\rangle. \tag{44}$$

Since $\langle\omega(E)(v_h)\rangle$ is the complex conjugate of $\langle E(v_h)\rangle$, $\langle\cdot|\cdot\rangle$ is a Hermitian form of $\mathcal{M}$. Moreover, it is clearly contravariant.

A lowest weight representation is *unitary* if its Hermitian form is positive definite. Of course, a Verma-like module is not unitary in general. Nevertheless, by a judicious choice of weight functions, it is possible to obtain unitary quotient representations with the help of this Hermitian form. In this case we call the Verma-like module *unitarizable*.

VI. TENSOR PRODUCTS OF THE DEFINING REPRESENTATION

Recall the defining representation in Sec. II. It is unitary and irreducible. More unitary irreducible representations can be obtained from the defining representation by taking its tensor products. Can they be obtained from Verma-like modules? We will answer this question in the form of a theorem. To state it, we need the following.

Definition 4: A Verma-like module is said to be approximately finite if its lowest weight function h satisfies the following conditions:[21]

(1) $h_I(\lambda_1;\dot{I};\lambda_2)-h_I(\lambda_3;\dot{J};\lambda_4)$ *is a non-negative integer if* $J\lambda 3\lambda 4>I\lambda 1\lambda 2$*;*
(2) $h_{II}(\lambda;\dot{I})=\Sigma_{i_1,\lambda_1}h_I(\lambda;\dot{I}\dot{I}_1;\lambda_1)$*;*
(3) $h_{III}(\dot{I};\lambda)=\Sigma_{\lambda_1,i_1}h_I(\lambda_1;\dot{I}_1\dot{I};\lambda)$*; and*
(4) $h_{IV}(\dot{I})=\Sigma_{\lambda_1,i_1,i_2,\lambda_2}h_I(\lambda_1;\dot{I}_1\dot{I}\dot{I}_2;\lambda_2)$.

(By convergence and unitarity, only a finite number of summands can be nonzero in each of the last three equations.)

Theorem 1: *The following statements pertaining to a unitary irreducible representation of open string algebra are equivalent:*

(1) The representation is a tensor product of the defining representation.
(2) The representation is the quotient of an approximately finite Verma-like module by its maximal subrepresentation.
(3) The representation is the quotient of a Verma-like module in which h_I, h_{II}, h_{III} *and* h_{IV} *are all nonzero only on a finite number of arguments by its maximal subrepresentation.*
(4) The representation is the quotient of a Verma-like module in which h_{IV} *is nonzero only on a finite number of arguments by its maximal subrepresentation.*[22]

Moreover, the maximal subrepresentations in the above statements are the radical of the Hermitian form of the Verma-like module.

There are some interesting physical interpretations of this theorem. In the context of QCD, a tensor product of the defining representation is a space consisting of multiple meson states. Theorem 1 thus reflects once again a long-established fact that in the large-N limit, one cannot break an open string into several, or combine several open strings to one.[23] Furthermore, the proof of Proposition 3 clearly shows that G^{00} is a maximally commutative subalgebra of $\hat{G}_{\Lambda,\Lambda_F}$. We may thus think of G^{00} as a linear space generated by a maximally commuting set of linearly independent quantum observables, of which the lowest weight state is an eigenstate with all its eigenvalues, or quantum numbers, given by the weight functions. If this state has only a finite number of nonzero quantum numbers, any other state generated by it will have a finite number of nonzero quantum numbers, too. Consequently, the above theorem implies that if an eigenstate, lowest weight or not, has only a finite number of nonzero quantum numbers with respect to these quantum observables, then this eigenstate must be a multiple meson state.

Before embarking on the proof of the equivalences, let us make some simple observations which have, as consequences, among other things, the statements about the Hermitian form in the theorem.

Lemma 3: The maximal subrepresentation of a unitarizable Verma-like module is the radical of the Hermitian form.

Proof: If we quotient out by the radical of the Hermitian form in the Verma module we get a representation with a nondegenerate Hermitian form (still contravariant of course). *A priori* it might seem possible that this representation could have a proper unitary quotient. However, exactly due to the unitarity assumption, if there exists a nonzero maximal proper invariant subspace I such that the quotient by it is unitary, then in fact the quotient must be equivalent to $I^{\perp}$. But since the space is cyclic, this is possible only if $I=0$, which is a contradiction. Q.E.D.

Lemma 4: If for a given weight h there exists a contravariant unitary lowest (or highest) weight module V_h, then it is unique.

Proof: Let $|v_h\rangle$ denote the lowest weight vector and let A_h denote the annihilator of $|v_h\rangle$ in the envelopping algebra $\mathcal{U}$. Then $V_h \simeq \mathcal{U}/A_h$ and by Lemma 3, A_h is equal to the set of $Y \in \mathcal{U}$ for which $Y|v_h\rangle = 0 \Leftrightarrow \langle Y(v_h)|Y(v_h)\rangle = 0$. By contravariance, the latter condition is expressible entirely in terms of the Lie algebra structure and h. Q.E.D.

We will now prove Theorem 1 by a series of lemmas in which (*1*), (*2*), (*3*), and (*4*), stand for the four enumerated statements in Theorem 1.

Lemma 5: (1)⇒(2).

Proof: First of all we observe that the defining representation $\mathcal{T}_o$ is obviously approximately finite. Indeed, it is elementary to verify that the following identities hold in $\mathcal{T}_o$:

$$\overline{\Xi}^{\lambda_1}_{\lambda_2} \otimes l^{\dot{I}}_{\dot{J}} = \sum_{\lambda_3=1}^{\Lambda_F} \sum_{\dot{K}} \overline{\Xi}^{\lambda_1}_{\lambda_2} \otimes f^{\dot{I}\dot{K}}_{\dot{J}\dot{K}} \otimes \Xi^{\lambda_3}_{\lambda_3}, \tag{45}$$

$$r^{\dot{I}}_{\dot{J}} \otimes \Xi^{\lambda_3}_{\lambda_4} = \sum_{\lambda_1=1}^{\Lambda_F} \sum_{\dot{K}} \overline{\Xi}^{\lambda_1}_{\lambda_1} \otimes f^{\dot{K}\dot{I}}_{\dot{K}\dot{J}} \otimes \Xi^{\lambda_3}_{\lambda_4} \tag{46}$$

and

$$\sigma^{\dot{I}}_{\dot{J}} = \sum_{\lambda_1,\lambda_2=1}^{\Lambda_F} \sum_{\dot{K}_1,\dot{K}_2} \overline{\Xi}^{\lambda_1}_{\lambda_2} \otimes f^{\dot{K}_1\dot{I}\dot{K}_2}_{\dot{K}_1\dot{J}\dot{K}_2} \otimes \Xi^{\lambda_2}_{\lambda_2} \tag{47}$$

for all $\dot{I}$, $\dot{J}$, λ_1, λ_2, λ_3, and λ_4. It is clear that the tensor product $\mathcal{T}_o^d = \mathcal{T}_o \otimes \mathcal{T}_o \otimes \cdots \otimes \mathcal{T}_o$ (d copies) will have the same property. Furthermore, any Young symmetrizer c_γ will define an invariant subspace and a nonzero weight vector v_γ which is annihilated by any subalgebra $gl(N)^- \subset gl(\infty) \equiv gl(\Lambda_F) \otimes F_\Lambda \otimes gl(\Lambda_F)$.

Let

$$\gamma = (\gamma_1, \gamma_2, \dots) \quad \text{with } \gamma_1 \geqslant \gamma_2 \geqslant \cdots \geqslant \gamma_n \geqslant 0 = \gamma_{n+1} = \gamma_{n+2} = \cdots$$

such that $d = \gamma_1 + \gamma_2 + \cdots + \gamma_n$. Again, by looking at the subalgebras gl(N) it follows that $c_\gamma(\mathcal{T}_o)$ carries an irreducible representation. That v_γ is annihilated by all of G^- and forms a one-dimensional representation for G^{00} is equally clear. The lowest weight is given by the formulas

$$h_I(1;\varnothing;1) = \gamma_1,$$

$$h_I(1;\varnothing;2) = \gamma_2,$$

$$\vdots$$

$$h_I(1;\varnothing;\Lambda_F) = \gamma_{\Lambda_F},$$

$$h_I(2;\varnothing;1) = \gamma_{\Lambda_F+1},$$

$$\vdots$$

$$h_I(\Lambda_F;\varnothing;\Lambda_F) = \gamma_{\Lambda_F\Lambda_F},$$

$$h_I(1;1;1) = \gamma_{\Lambda_F\Lambda_F+1},$$

$$\vdots$$

$$h_I(1;1;\Lambda_F)=\gamma_{\Lambda_F\Lambda_F+\Lambda_F},$$

$$h_I(2;1;1)=\gamma_{\Lambda_F\Lambda_F+\Lambda_F+1},$$

$$\vdots$$

$$h_I(\Lambda_F;1;\Lambda_F)=\gamma_{2\Lambda_F\Lambda_F},$$

$$h_I(1;2;1)=\gamma_{2\Lambda_F\Lambda_F+1},$$

$$\vdots$$

$$h_I(\Lambda_F;\Lambda;\Lambda_F)=\gamma_{\Lambda\Lambda_F\Lambda_F},$$

$$h_I(1;11;1)=\gamma_{\Lambda\Lambda_F\Lambda_F+1},$$

$$\vdots$$

$$h_I(\rho_1;\dot{K};\rho_2)=\gamma_n$$

and (48)

$$h_I(\lambda_1;\dot{I};\lambda_2)=0 \quad \text{if} \quad \dot{I}\lambda_1\lambda_2>\dot{K}\rho_1\rho_2.$$

Equations (45)–(47) clearly also hold in $c_\gamma(\mathcal{T}_o)$. Q.E.D.

Lemma 6: (2)⇒(1).

Proof: Let h_I be given in terms of a γ as in Eq. (48). Then, since it is nonzero only on a finite number of arguments, γ defines a Young symmetrizer c_γ. Consider $c_\gamma(\mathcal{T}_o)$. It is easy to see that this space has the right lowest weight. By Lemma 4 it is unique. Q.E.D.

Lemma 7: (2)⇒(3).

Proof: According to Definition 4, only a finite number of the summands in the formula

$$h_{IV}(\varnothing)=\sum_{\lambda_1,\dot{I}_1,\dot{I}_2,\lambda_2} h_I(\lambda_1;\dot{I}_1\dot{I}_2;\lambda_2)$$

are nonzero, so there exists an integer sequence $\dot{K}$ such that $h_I(\lambda_1;\dot{I};\lambda_2)=0$ for any λ_1 and λ_2 if $\dot{I}>\dot{K}$. Then $h_{II}(\lambda;\dot{I})=h_{III}(\dot{I};\lambda)=h_{IV}(I)=0$ if $\dot{I}>\dot{K}$. In particular, h_{II}, h_{III} and h_{IV} are nonzero on a finite number of arguments only. Q.E.D.

Lemma 8: If $\dot{I}\lambda_1\lambda_3>\dot{J}\lambda_2\lambda_4$, then $h_I(\lambda_2;\dot{J};\lambda_4)-h_I(\lambda_1;\dot{I};\lambda_3)$ is a non-negative integer.

Observe that this result is completely general: any unitary irreducible representation of the open string algebra constructed from a Verma-like module satisfies the first condition in Definition 4.

Proof: Let $\dot{I}$ and $\dot{J}$ be arbitrarily chosen integer sequences, and λ_1, λ_2, λ_3 and λ_4 arbitrarily chosen positive integers not greater than Λ_F. Notice that

$$\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_3}_{\lambda_4},\ \overline{\Xi}^{\lambda_1}_{\lambda_1}\otimes f^{\dot{I}}_{\dot{I}}\otimes\Xi^{\lambda_3}_{\lambda_3}-\overline{\Xi}^{\lambda_2}_{\lambda_2}\otimes f^{\dot{J}}_{\dot{J}}\otimes\Xi^{\lambda_4}_{\lambda_4} \text{ and } \overline{\Xi}^{\lambda_2}_{\lambda_1}\otimes f^{\dot{J}}_{\dot{I}}\Xi^{\lambda_4}_{\lambda_3},$$

where $\dot{I}\lambda_1\lambda_3>\dot{J}\lambda_2\lambda_4$, span a subalgebra of the open string algebra. This subalgebra is isomorphic to sl(2,$\mathbb{C}$). We therefore deduce from the representation theory of sl(2,$\mathbb{C}$) that $h_I(\lambda_2;\dot{J};\lambda_4)-h_I(\lambda_1;\dot{I};\lambda_3)$ must be a nonnegative integer. Q.E.D.

Lemma 9: (3)⇒(2).

Proof: Since there are only a finite number of arguments on which h_I does not vanish, Lemma 8 implies that there exists an integer sequence $\dot{K}\rho_1\rho_2$ such that

(1) $h_I(\rho_1;\dot{K};\rho_2)>0$;
(2) $h_I(\lambda_1;\dot{I};\lambda_2)=0$ if $\dot{I}\lambda_1\lambda_2>\dot{K}\rho_1\rho_2$; and
(3) $0<h_I(\lambda_1;\dot{I};\lambda_2)\leqslant h_I(\lambda_3;\dot{J};\lambda_4)$ if $\dot{K}\rho_1\rho_2>\dot{I}\lambda_1\lambda_2>\dot{J}\lambda_3\lambda_4$.

In other words, Eq. (48) with the partition γ holds.

We will move on to show that h_{II} satisfies Definition 4. The proofs for h_{III} and h_{IV} are similar. Let $\dot{K}_1\rho_3$ be the integer sequence such that $h_{II}(\rho_3;\dot{K}_1)>0$ and $h_{II}(\lambda;\dot{I})=0$ if $\dot{I}\lambda>\dot{K}_1\rho_3$. Then Eq. (22) implies that

$$\sum_{\lambda} h_I(\rho_3;\dot{K}_1;\lambda)=h_{II}(\rho_3;\dot{K}_1)-\sum_{i} h_{II}(\rho_3;\dot{K}_1 i)>0.$$

Hence $\dot{K}_1\rho_3\leqslant\dot{K}\rho_1$. $\dot{K}_1\rho_3<\dot{K}\rho_1$ is impossible or else

$$\sum_{\lambda} h_I(\rho_1;\dot{K};\lambda)=h_{II}(\rho_1;\dot{K})-\sum_{i} h_{II}(\rho_1;\dot{K}i)=0,$$

a contradiction. Thus $\rho_3=\rho_1$ and $\dot{K}_1=\dot{K}$. That h_{II} satisfies Definition 4 now follows from the fact that $h_{II}(\lambda;\dot{I})$ is a sum of

(1) all $h_I(\lambda;\dot{I}\dot{I}_1;\lambda_1)$ where λ_1 can take on any value and $\dot{I}_1$ is an integer sequence such that $\dot{I}\dot{I}_1\lambda<\dot{K}\rho_1$,
(2) all $h_{II}(\lambda;\dot{I}\dot{I}_1 i)$ where $\dot{I}_1 i$ is any integer sequence such that $\dot{I}\dot{I}_1\lambda<\dot{K}\rho_1$ but $\dot{I}\dot{I}_1 i\lambda>\dot{K}\rho_1$,

and the fact that the summands in the second family vanish identically. Q.E.D.

Lemma 10: (3)⇒(4).

Proof: Trivial. Q.E.D.

Lemma 11: $h_{II}(\lambda_2;\dot{J})-h_{II}(\lambda_1;\dot{I})\geqslant 0$ *and* $h_{III}(\dot{J};\lambda_2)-h_{III}(\dot{I};\lambda_1)\geqslant 0$ *if* $\dot{I}\lambda_1>\dot{J}\lambda_2$.

Proof: This comes from the inequalities

$$\langle v_h|(\bar{\Xi}^{\lambda_2}_{\lambda_1}\otimes l^{\dot{J}}_{\dot{I}})(\bar{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot{I}}_{\dot{J}})|v_h\rangle\geqslant 0$$

and

$$\langle v_h|(r^{\dot{J}}_{\dot{I}}\otimes\Xi^{\lambda_2}_{\lambda_1})(r^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2})|v_h\rangle\geqslant 0.$$

Q.E.D.

Lemma 12: (4)⇒(3).

Proof: Let $\dot{K}$ be an integer sequence such that $h_{IV}(\dot{K})>0$ and $h_{IV}(\dot{I})=0$ for any $\dot{I}>\dot{K}$. Equations (20)–(23) imply that for this $\dot{I}$,

$$\sum_{\lambda_1,\lambda_2=1}^{\Lambda_F} h_I(\lambda_1;\dot{I};\lambda_2)=h_{IV}(\dot{I})-\sum_{i=1}^{\Lambda} h_{IV}(i\dot{I})-\sum_{j=1}^{\Lambda} h_{IV}(\dot{I}j)+\sum_{i,j=1}^{\Lambda} h_{IV}(i\,\dot{I}j)=0. \tag{49}$$

Assume that some $h_I(\lambda_1;\dot{I};\lambda_2)\neq 0$ in Eq. (49). Then there exist two integers ρ_1 and ρ_2 such that $h_I(\rho_1;\dot{I};\rho_2)<0$. By Lemma 8, $h_I(\lambda_3;\dot{J};\lambda_4)<0$ if $\dot{J}>\dot{I}$. Hence for this $\dot{J}$,

$$0>\sum_{\lambda_3,\lambda_4=1}^{\Lambda_F} h_I(\lambda_3;\dot{J};\lambda_4)=h_{IV}(\dot{J})-\sum_{i=1}^{\Lambda} h_{IV}(i\dot{J})-\sum_{j=1}^{\Lambda} h_{IV}(\dot{J}j)+\sum_{i,j=1}^{\Lambda} h_{IV}(i\dot{J}j)=0,$$

a contradiction. We thus conclude that $h_I(\lambda_1;\dot{I};\lambda_2)=0$ for any integer sequence $\dot{I}$ such that $\dot{I}>\dot{K}$ and any integers λ_1 and λ_2. In particular, h_I is nonzero on a finite number of arguments only. A similar argument using Lemma 11 shows that h_{II} and h_{III} are nonzero on a finite number of arguments only. Q.E.D.

VII. OTHER UNITARY IRREDUCIBLE REPRESENTATIONS

Now that we have identified a class of unitary irreducible representations, it is natural for us to ask what other unitary irreducible representations look like. One crucial observation is that not only are the above tensor product representations faithful representations of the full open string algebra, but also they are completely determined by the ideal $\mathrm{sl}(\infty)=[\mathrm{gl}(\infty),\mathrm{gl}(\infty)]$, where $\mathrm{gl}(\infty)=F_{\Lambda,\Lambda_F}$, and are the only representations that remain faithful and unitary as representations of this ideal. This suggests that other unitary irreducible representations can be obtained as unitary lowest weight representations from the quotient algebra by $\mathrm{sl}(\infty)$, i.e., as "truly infinite" (t.i.) representations of the open string algebra—lowest weight representations in which $\mathrm{sl}(\infty)$ acts trivially. Indeed, it turns out that we have the following.

Theorem 2: *Any unitary irreducible lowest weight representation of the open string algebra is a tensor product of a unitary irreducible approximately finite representation and a unitary irreducible lowest weight representation in which any element of* $\mathrm{sl}(\infty)$ *acts as the* 0 *operator*.[24]

Together with the physical interpretation of Theorem 1, this result implies that if a lowest weight state has an infinite number of nonzero quantum numbers, it must be a tensor product of a multiple meson state and a state in a representation of the quotient algebra. As remarked in the Introduction, the quotient algebra extends and generalizes the Virasoro algebra. Already for the case $\Lambda=1$ the quotient algebra is quite interesting. Specifically, it is an extension of the Virasoro algebra by an infinite Heisenberg algebra.[14] Physically speaking, $\mathrm{sl}(\infty)$ consists of finite-size-effect operators. Studying the quotient algebra is thus equivalent to studying a physical system which is free of finite-size effects. Hence, we expect the representation theory of the quotient algebra to describe the physics of open matrix chains at the thermodynamic limit.

Let h be the weight function of an arbitrary unitary lowest weight representation $\mathcal{R}$ of the open string algebra, and $|v_h\rangle$ its lowest weight vector (somewhat abusing notation, we do not distinguish between the space and the representation). Our task is to produce two representations $\mathcal{R}_{a.f.}$ and $\mathcal{R}_{t.i.}$ such that $\mathcal{R}_{a.f.}$ is approximately finite, $\mathcal{R}_{t.i.}$ comes from the quotient algebra [is trivial on $\mathrm{sl}(\infty)$], and $\mathcal{R}=\mathcal{R}_{t.i.}\otimes\mathcal{R}_{a.f.}$. As usual, we do this by proving a succession of lemmas.

Lemma 13: In the first two equations below, assume that $\dot{I}\lambda_1>\dot{J}\lambda_2$, *and in the third assume that* $\dot{I}>\dot{J}$. *Let*

$$\bar{\Xi}^{\lambda_1}_{\lambda_2}\otimes\tilde{l}^{\dot{I}}_{\dot{J}}\equiv\bar{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot{I}}_{\dot{J}}-\sum_{\lambda_3=1}^{\Lambda_F}\sum_{\dot{K}}\bar{\Xi}^{\lambda_1}_{\lambda_2}\otimes f^{\dot{I}\dot{K}}_{\dot{J}\dot{K}}\otimes\Xi^{\lambda_3}_{\lambda_3}, \tag{50}$$

$$\tilde{r}^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2}\equiv r^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2}-\sum_{\lambda_3=1}^{\Lambda_F}\sum_{\dot{K}}\bar{\Xi}^{\lambda_3}_{\lambda_3}\otimes f^{\dot{K}\dot{I}}_{\dot{K}\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2}, \tag{51}$$

and

$$\tilde{\sigma}^{\dot{I}}_{\dot{J}}\equiv\sigma^{\dot{I}}_{\dot{J}}-\sum_{\lambda_1,\lambda_2=1}^{\Lambda_F}\sum_{\dot{K},\dot{L}}\bar{\Xi}^{\lambda_1}_{\lambda_1}\otimes f^{\dot{K}\dot{I}\dot{L}}_{\dot{K}\dot{J}\dot{L}}\otimes\Xi^{\lambda_2}_{\lambda_2}. \tag{52}$$

Then $\bar{\Xi}^{\lambda_1}_{\lambda_2}\otimes\tilde{l}^{\dot{I}}_{\dot{J}}|v_h\rangle$, $\tilde{r}^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2}|v_h\rangle$ *and* $\tilde{\sigma}^{\dot{I}}_{\dot{J}}|v_h\rangle$ *have finite norms.*

Proof: We will show that $\tilde{\sigma}^{\dot{I}}_{\dot{J}}|v_h\rangle$ has a finite norm. The rest of the lemma can be proved by a simpler version of the following argument.

For any non-negative integer p, consider the operator

$$\tilde{\sigma}^{\dot{I}}_{\dot{J}}(p)=\sigma^{\dot{I}}_{\dot{J}}-\sum_{\lambda_1,\lambda_2=1}^{\Lambda_F}\sum_{\substack{\dot{K},\dot{L}\\ \#(\dot{K}\dot{L})\leqslant p}}\bar{\Xi}^{\lambda_1}_{\lambda_1}\otimes f^{\dot{K}\dot{I}\dot{L}}_{\dot{K}\dot{J}\dot{L}}\otimes\Xi^{\lambda_2}_{\lambda_2}. \tag{53}$$

Certainly it is well defined because there are only a finite number of summands in Eq. (53). [We can define $\tilde{l}^{\dot{I}}_{\dot{J}}(p)$ and $\tilde{r}^{\dot{I}}_{\dot{J}}(p)$ similarly.] Let

$$s(\dot{I},\dot{J},\dot{K},\dot{L})=\sum_{\dot{K}',\dot{L}'}\delta^{\dot{K}\dot{I}\dot{L}}_{\dot{K}'\dot{I}\dot{L}'}\delta^{\dot{K}\dot{J}\dot{L}}_{\dot{K}'\dot{J}\dot{L}'}.$$

Clearly, s is a positive integer. Since

$$[\tilde{\sigma}^{\dot{I}}_{\dot{J}}(p),f^{\dot{K}'\dot{J}\dot{L}'}_{\dot{K}'\dot{I}\dot{L}'}]=0 \tag{54}$$

for $\#(\dot{K}'\dot{L}')\leqslant p$,

$$\langle v_h|\tilde{\sigma}^{\dot{J}}_{\dot{I}}(p)\tilde{\sigma}^{\dot{I}}_{\dot{J}}(p)|v_h\rangle=\langle v_h|\sigma^{\dot{J}}_{\dot{I}}\sigma^{\dot{I}}_{\dot{J}}|v_h\rangle-\sum_{\lambda_1,\lambda_2=1}^{\Lambda_F}\sum_{\substack{\dot{K},\dot{L}\\ \#(\dot{K}\dot{L})\leqslant p}}s(\dot{I},\dot{J},\dot{K},\dot{L})(h_I(\lambda_1;\dot{K}\dot{J}\dot{L};\lambda_2)$$

$$-h_I(\lambda_1;\dot{K}\dot{I}\dot{L};\lambda_2)), \tag{55}$$

which, in turn, is non-negative owing to unitarity. That p can be arbitrarily large and Lemma 8 together then imply that for any fixed nonempty integer sequences $\dot{I}$ and $\dot{J}$, only a finite number of

$$h_I(\lambda_1;\dot{K}\dot{J}\dot{L};\lambda_2)-h_I(\lambda_1;\dot{K}\dot{I}\dot{L};\lambda_2),$$

where λ_1 and λ_2 are arbitrary positive integers not larger than Λ_F, and $\dot{K}$ and $\dot{L}$ are empty or nonempty integer sequences, are nonzero. As a result,

$$\sum_{\substack{\dot{K},\dot{L}\\ \#(\dot{K}\dot{L})>q_0}}\bar{\Xi}^{\lambda_1}_{\lambda_1}\otimes f^{\dot{K}\dot{I}\dot{L}}_{\dot{K}\dot{J}\dot{L}}\otimes\Xi^{\lambda_2}_{\lambda_2}|v_h\rangle=0 \tag{56}$$

for some positive integer q_0 because its norm vanishes. Thus $\tilde{\sigma}^{\dot{I}}_{\dot{J}}|v_h\rangle$ has a finite norm. Q.E.D.

Define $\mathcal{R}_f$ to be the subspace of $\mathcal{R}$ generated by the actions of elements of $\mathrm{gl}(\Lambda_F)\otimes F_\Lambda\otimes\mathrm{gl}(\Lambda_F)$ on the lowest weight vector $|v_h\rangle$. For brevity, let $\tilde{X}$ denote any one of the operators defined in Eqs. (50)–(52). It now follows easily that $\tilde{X}v$ is well defined for any $v\in\mathcal{R}_f$.

Lemma 14: For any $v\in\mathcal{R}_f$ and any $F\in\mathrm{gl}(\Lambda_F)\otimes F_\Lambda\otimes\mathrm{gl}(\Lambda_F)$,

$$\tilde{X}Fv=F\tilde{X}v.$$

Proof: Any $F\in\mathrm{gl}(\Lambda_F)\otimes F_\Lambda\otimes\mathrm{gl}(\Lambda_F)$ commutes, for fixed $\dot{I},\dot{J}$, with everything in $\mathrm{gl}(\Lambda_F)\otimes F_\Lambda\otimes\mathrm{gl}(\Lambda_F)$ of the form $\bar{\Xi}^{\lambda_1}_{\lambda_1}\otimes f^{\dot{K}\dot{I}\dot{L}}_{\dot{K}\dot{J}\dot{L}}\otimes\Xi^{\lambda_2}_{\lambda_2}$ except possibly finitely many. The claim now follows by a simple computation as in the proof of the previous lemma. Q.E.D.

Corollary 1: Let $\tilde{X}^{\dot{I}_p}_{\dot{J}_p}$ *stand for either* $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes\tilde{l}^{\dot{I}}_{\dot{J}}$, $\tilde{r}^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2}$ or $\tilde{\sigma}^{\dot{I}}_{\dot{J}}$. *Then*

$$\prod_{p=1}^{n}\tilde{X}^{\dot{I}_p}_{\dot{J}_p}|v_h\rangle \tag{57}$$

has a finite norm for any value of n.

Proof: This follows directly from Lemmas 13 and 14. Q.E.D.

It follows from Lemmas 13 and 14 and Corollary 1 that $\tilde{l}$, $\tilde{r}$ and $\tilde{\sigma}$ are well-defined operators on a lowest weight module.

Lemma 15: There exist $\alpha\in\mathbb{R}$ *and* $N\in\mathbb{N}$ *such that* $h_I(\lambda_1;I;\lambda_2)=\alpha$ *for all* λ_1 *and* λ_2 *provided* $\#(I)\geqslant N$.

Proof: Observe that since $\dot{I}>\dot{J}$, (55) implies more generally for any $\lambda_1,\lambda_2,\lambda_3,\lambda_4$ that (the non-negative integer)

$$(h_I(\lambda_1;\dot{K}\dot{J}\dot{L};\lambda_2)-h_I(\lambda_3;\dot{K}\dot{I}\dot{L};\lambda_4))$$

can be nonzero for at most finitely many $\dot{K},\dot{L}$. As a special case of this, notice that for any $i=1,\ldots,\Lambda_F$, only a finite number of

$$h_I(\lambda_1;\dot{K}\dot{L};\lambda_2)-h_I(\lambda_3;\dot{K}\{i\}\dot{L};\lambda_4)$$

are nonzero. Hence, there exists an $N\in\mathbb{N}$ such that for any U with $\#(U)\geqslant N$, any $\lambda_1,\lambda_2,\lambda_3,\lambda_4,\lambda_5,\lambda_6$, and any indices $1\leqslant i,j\leqslant\Lambda_F$, $h_I(\lambda_1;U;\lambda_2)=h_I(\lambda_3;U\{i\};\lambda_4)=h_I(\lambda_5;\{j\}U;\lambda_6)$. But since for any two sequences U,V with $\#(U)=\#(V)=N$ there is a sequence W such that both U and V occur as segments of W, it follows that we must have $h_I(\lambda_1;U;\lambda_2)=h_I(\lambda_3;V;\lambda_4)$. Q.E.D.

We can now define the two spaces $\mathcal{R}_{t.i.}$ (the truly infinite) and $\mathcal{R}_{a.f.}$ (the almost finite).

Definition 5: Let α *be as in Lemma 15, set* $h^{a.e.}_I=h_I-\alpha$, *and let* $h^{a.e.}_{II}$, $h^{a.e.}_{III}$, *and* $h^{a.e.}_{IV}$ *be defined from* $h^{a.e.}_I$ *as in Definition 4.* $\mathcal{R}_{a.f.}$ *then is defined as the lowest weight representation having this lowest weight. Similarly,* $\mathcal{R}_{t.i.}$ *is defined to be the lowest weight representation given by the lowest weight* $(h^q_I,h^q_{II},h^q_{III},h^q_{IV})$ *with* $h^q_I\equiv\alpha$, *and* $h^q_W=h_W-h^{a.e.}_W$ *for* $W=II,III,IV$.

In the following we shall, among other things, consider elements $f^{\dot{I}}_{\dot{J}}$, with $\dot{I}>\dot{J}$ acting in $\mathcal{R}_f$ or in $\mathcal{R}_{a.f.}$. We will use the same symbol for these actions since the two spaces are, in fact, equal as vector spaces. As representations of $\mathrm{gl}(\Lambda_F)\otimes F_\Lambda\otimes\mathrm{gl}(\Lambda_F)$ they differ by a tensor product of a one-dimensional representation (defined by α) and this is trivial on said elements. Furthermore, in the representation $\mathcal{R}_{t.i.}$ each $f^{\dot{I}}_{\dot{J}}$, with $\dot{I}>\dot{J}$, acts trivially since by construction they must annihilate the lowest weight vector while at the same time having commutators with the other generators that again yield elements $f^{\dot{K}}_{\dot{L}}$, with $\dot{K}>\dot{L}$.

Proof of Theorem 2: Let $X^{\dot{I}_p}_{\dot{J}_p}$ stand for either $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes l^{\dot{I}}_{\dot{J}}$, $r^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2}$ or $\sigma^{\dot{I}}_{\dot{J}}$ and likewise $\tilde{X}^{\dot{I}_p}_{\dot{J}_p}$ stand for either $\overline{\Xi}^{\lambda_1}_{\lambda_2}\otimes\tilde{l}^{\dot{I}}_{\dot{J}}$, $\tilde{r}^{\dot{I}}_{\dot{J}}\otimes\Xi^{\lambda_1}_{\lambda_2}$ or $\tilde{\sigma}^{\dot{I}}_{\dot{J}}$. It follows that $\mathcal{R}_{t.i.}$ is generated by operators from $X^{\dot{I}_p}_{\dot{J}_p}$. Further, it follows from Lemmas 13 and 14 and Corollary 1 that any element of $\mathcal{R}$ can be written as a finite linear combination of elements of the form

$$\prod_{p=1}^{n}\tilde{X}^{\dot{I}_p}_{\dot{J}_p}\prod_{p=1}^{n_I}\overline{\Xi}^{\lambda^{(I)}_p}_{\rho^{(I)}_p}\otimes f^{\dot{I}^{(I)}_p}_{\dot{J}^{(I)}_p}\otimes\Xi^{\eta^{(I)}_p}_{\zeta^{(I)}_p}|v_h\rangle, \tag{58}$$

where the two products are arranged in such a way that in each product, the factors follow the lexicographic ordering from Definition 3 with σ, r and l replaced with $\tilde{\sigma}$, $\tilde{r}$ and $\tilde{l}$, respectively.

Denote the lowest weight vector of $\mathcal{R}_{t.i.}$ by $v_{t.i.}$ and the lowest weight vector of $\mathcal{R}_{a.f.}$ by $v_{a.f.}$. Assume they are both unit vectors in their respective spaces. We can then define a surjection from $\mathcal{R}_{t.i.}\otimes\mathcal{R}_f$ to $\mathcal{R}$ by mapping

$$\left(\prod_{p=1}^{n} X^{\dot{I}_p}_{\dot{J}_p} v_{t.i.}\right)\otimes\left(\prod_{p=1}^{n_I} \overrightarrow{\Xi}^{(I)}_{\rho^{(I)}_p p}\otimes f^{\dot{I}^{(I)}_p}_{\dot{j}^{(I)}_p}\otimes \Xi^{\eta^{(I)}_p}_{\zeta^{(I)}_p} v_{a.f.}\right) \tag{59}$$

to the one shown in Eq. (58). Because of Lemma 14 and the above remarks, this is easily seen to be a map that preserves the respective inner products. By looking at the images of $\mathcal{R}_{t.i.}\otimes v_{a.f.}$ and $v_{t.i.}\otimes\mathcal{R}_{a.f.}$ it follows that $\mathcal{R}_{t.i.}$ and $\mathcal{R}_{a.f.}$ are unitary. The irreducibility is obvious, cf. Lemma 4. Q.E.D.

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Fine gradings of o(5, $\mathbb{C}$), sp(4, $\mathbb{C}$) and of their real forms

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There are three fine gradings of the simple Lie algebra of type B_2 over the complex number field. They provide a basic information about the structure of the algebra. In the paper an explicit description of all fine gradings is given in terms of the four-dimensional symplectic [sp(4, $\mathbb{C}$)] and five-dimensional orthogonal [o(5, $\mathbb{C}$)] representations of the algebra. In addition, the real forms of B_2 are considered. It is shown which of the fine gradings survive the restriction to each of the real forms. These results should be useful in defining various sets of additive quantum numbers for systems with such symmetries, for systematic study of grading preserving contractions of this Lie algebra, and generally for choosing bases which reflect structural properties of the Lie algebra.
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I. INTRODUCTION

The motivation for studying specific gradings of simple Lie algebras with complex or real parameters is often linked with applications. Among the infinity of possible decompositions of the algebra as a linear space into the direct sum of subspaces, there are a few decompositions particularly ''compatible'' with the structure of the given algebra, the so-called grading decompositions.[1] (Two decompositions are considered to be different only if they are nonconjugate under the action of the automorphism group of the Lie algebra.) Some of the gradings are coarse: the Lie algebra is decomposed in a small number of grading subspaces. The coarsest nontrivial ones are the $\mathbb{Z}_2$ gradings. Their role, for example, in defining the compact and noncompact part of real forms of complex algebras is well known. The opposite extreme are the fine gradings decomposing the algebra into as many subspaces as possible. Every simple Lie algebra with complex parameters admits a fine grading called root or Cartan decomposition. Corresponding bases of the algebra and of its representation spaces (defined up to a normalization by the grading) have been the work horses of the theory and applications even if the underlying grading property is usually not emphasized. For example, the Lie algebra sl(2, $\mathbb{C}$) has precisely two such gradings, each defining one basis (called also generators) of sl(2, $\mathbb{C}$). Practically no other bases are used in the theory or in the numerous applications. The basis of the root decomposition is often denoted by L_+, L_0, L_-, the other ones are the Pauli matrices. In both cases the generators are determined by the grading up to a nonzero normalization constant.

For simple Lie algebras of higher ranks fine gradings may not decompose the algebra into subspaces which are all of dimension one. Then the corresponding bases are defined only partially

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by the grading. Well known is the example of the root decomposition/grading of sl(3, $\mathbb{C}$). Two ''diagonal'' generators have to be chosen by other considerations, while the remaining six are given by the grading. Possible choice of additive quantum numbers is another use of the fine gradings. The grading subspaces are eigenspaces of the grading group, the eigenvalues being the quantum numbers. A maximal set of additive quantum numbers is given by several elements of the grading group which have sufficiently many distinct eigenvalues to label the grading subspaces.

A grading of a Lie algebra L is a structural property of L resulting from the presence of an Abelian subgroup of diagonable automorphisms in the group of automorphism of L. Between the coarsest trivial grading, corresponding to the identity element of the automorphism group, to the finest gradings, there are many intermediate gradings. A complete list of such gradings has not been put together even for the rank 2 simple Lie algebras. Description of fine gradings makes such a task much simpler.

There are other motivations for studying the gradings of simple Lie algebras one can bring forward besides the choice of bases and the additive quantum numbers.

Our motivation originated in the study of graded contractions of simple Lie algebras.[2] Unlike the standard Wigner–Inonü contractions,[3] here one requires that a suitably chosen grading is preserved during the contraction/deformation process. It allows one to consider, separately from the general problem of all deformations of a given Lie algebra, only those deformations which are of interest for a problem at hand. Typically it makes it easy to keep any subalgebra of importance free of deformations (see, for example, Ref. 4). Finally it makes it possible to deform the action of the Lie algebra in the representation spaces so that one has a representation of the deformed algebra.[5] Another possible application of graded contractions allows one to link the very difficult task of classification of isomorphism classes of solvable Lie algebras to much simpler (though also difficult) problems of classification of isomorphism classes of equidimensional nilpotent Lie algebras.[6]

Yet another curious possibility of applications of fine gradings is implied in Ref. 7. The relevant observation made there is that the Drinfel–Jimbo quantum algebra arises as a q-deformation of the universal enveloping algebra U(so(n)) in the basis given by the root decomposition (see, for example, Ref. 8). In Ref. 7 an analogous but very different deformation is based on another fine grading of so(n). It is quite natural to ask the question about q-deformations for every fine grading of so(n), not only the two mentioned in Ref. 7.

In this paper we consider the rank 2 simple Lie algebra B_2 (equivalently also denoted C_2). In the physics literature it is frequently specified by one of its two lowest dimensional representations. It then is called either sp(4, $\mathbb{C}$) or o(5, $\mathbb{C}$). Our notations for the real forms of B_2 are the following. The compact one is written either as usp(4) or as o(5); the real form with 6 compact and 4 noncompact generators is shown as usp(2, 2) and o(4, 1); the last real form with 4 compact and 6 non-compact generators is denoted either by sp(4, $\mathbb{R}$) or by o(3, 2). According to Ref. 9 there are three fine gradings of B_2 which are not equivalent under the group of automorphisms of B_2. One of them is the well known root decomposition, the second one in our list is new, the basis given by the third fine grading in our list, at least in its o(5, $\mathbb{C}$)-version, has been often used in physics literature without reference to any grading. The second and third gradings each define an orthogonal (with respect to the Killing form) basis of B_2. In the first case, the root decomposition goes far in defining a basis but there is one subspace (Cartan subalgebra) which is of dimension 2. There is no grading of the algebra which would allow one to split the two-dimensional subspace into two one-dimensional ones. Any such splitting is not a grading.

Applications of the real forms of B_2 are too numerous to be mentioned here. Let us just mention that among their orthogonal realizations there are the Lie algebras of the de Sitter groups, that some real forms of the symplectic realization have been intensively applied in the recent years in nuclear physics, and also in quantum optics.[10–13]

Fine gradings are in correspondence with the maximal Abelian diagonable (MAD) subgroups of the automorphism groups of Lie algebras. The MAD-groups of B_2 as well as of other classical Lie algebras were classified in Ref. 14. Similar results for the real forms are found in Ref. 15. Given the 1–1 correspondence between the MAD-groups and the fine gradings, the existence of

the fine gradings which we are to describe here can be inferred from there. However, such a task is relatively laborious. Therefore we are undertaking to provide an explicit description of the fine gradings for the low rank simple Lie algebras which are most often encountered in applications. Fine gradings of sl(3, $\mathbb{C}$) are found in Ref. 9; there are four of them.

The paper is organized as follows: After the preliminaries in Sec. II, we consider the two representations of B_2 one by one and derive explicitly the fine gradings in terms of matrices $\mathbb{C}^{5\times5}$ for o(5, $\mathbb{C}$) (Sec. III) and matrices $\mathbb{C}^{4\times4}$ for sp(4, $\mathbb{C}$) (Sec. IV). The gradings for both representations are given in Tables II, IV, and VI. In Sec. V we consider the real forms of the Lie algebra. There are 3 fine gradings of o(3, 2) and sp(4, $\mathbb{R}$), two fine gradings of o(4, 1) and usp(2, 2), and only one fine grading for the compact algebras o(5) and usp(4). The gradings are presented in Tables IX–XX. Note that we use the same letters for corresponding basis elements of the Lie algebra in 4 and 5 dimensions; their normalizations are not the same [cf. (2) below].

II. PRELIMINARIES

A grading of Lie algebra L is a decomposition of L into a direct sum of linear subspaces $\Gamma: L=\oplus_{i\in I}L_i$ which satisfies the following property:

$$\text{For any pair of indices } i,j\in I \text{ there exists } k\in I \text{ such that } 0\subseteq[L_i,L_j]\subseteq L_k. \tag{1}$$

Throughout the paper we use a shorthand notation when writing expressions like $[L_i,L_j]$. It should be read as the commutator of any element of L_i with any element of L_j. It is often convenient to set up the indices additively, so that $k=i+j$. Note that if $[L_i,L_j]=0$, then $k\in I$ is not defined.[16,17]

A grading which cannot be further refined is called *fine*. In this article we describe explicitly the fine gradings of two isomorphic simple algebras over $\mathbb{C}$, namely, o(5, $\mathbb{C}$) and sp(4, $\mathbb{C}$). More precisely we are dealing here with three irreducible representations of the Lie algebra B_2: the four-dimensional one which we call sp(4, $\mathbb{C}$), the one of dimension five calling it o(5, $\mathbb{C}$), and the adjoint representation of dimension ten, namely, the algebra acting on itself.

As long as one is interested only in the gradings of B_2, i.e., decomposition into the direct sums of grading subspaces, particular normalization of basis elements of each subspace is of little importance. However, in applications one often needs to fix a normalization of bases. It is done using the scalar product in the Lie algebra (Killing form). For any $x,y\in B_2$ and for any matrix representation $\phi(B_2)$, one has the scalar product of (x,y),

$$(x,y)l_\phi=\mathrm{tr}\ \phi(x)\phi(y), \tag{2}$$

where l_ϕ is a representation-dependent integer-valued numerical constant called the (second) index of the representation ϕ. Values of l_ϕ for the representations of simple Lie algebras are generally well known.[18] In particular, for the irreducible representations of B_2 of dimensions 4, 5, and 10, they are 2, 4, 12, respectively.

Skew-symmetric 5×5 matrices represent the 10-dimensional complex vector space of o(5, $\mathbb{C}$),

$$\mathrm{o}(5,\mathbb{C})=\{X\in\mathbb{C}^{5\times5}\,|\,X+X^T=0\}=\left\{\left.\begin{pmatrix}0&a&b&c&d\\-a&0&e&f&g\\-b&-e&0&h&j\\-c&-f&-h&0&k\\-d&-g&-j&-k&0\end{pmatrix}\right|\ a,\ldots,k\in\mathbb{C}\right\}. \tag{3}$$

The isomorphic Lie algebra sp(4, $\mathbb{C}$) can be realized as the complex vector space of matrices,

$$\mathrm{sp}(4,\mathbb{C})=\left\{X\in\mathbb{C}^{4\times4}\middle|X\begin{pmatrix}0&I_2\\-I_2&0\end{pmatrix}+\begin{pmatrix}0&I_2\\-I_2&0\end{pmatrix}X^T=0\right\}$$

$$=\left\{\begin{pmatrix}m&n&p&q\\r&s&q&t\\u&v&-m&-r\\v&w&-n&-s\end{pmatrix}\middle|\,m,\ldots,w\in\mathbb{C}\right\}.$$

Since our algebras are simple, we can use results deduced in Ref. 1. If L is a simple Lie algebra over $\mathbb{C}$, then fine gradings of L are in the one-to-one correspondence with the maximal Abelian groups of diagonable automorphisms (MAD-groups). It is known that groups of automorphisms of $\mathrm{o}(5,\mathbb{C})$ and $\mathrm{sp}(4,\mathbb{C})$ are formed by inner automorphisms only, i.e., by automorphisms of the form,

$$\mathrm{Ad}_A X := A^{-1}XA \tag{4}$$

for any X belonging to the Lie algebra, and where A is an element of the corresponding Lie group. Technically our problem in this paper is to find, for suitably chosen A, the eigenvalues and eigenvectors of the transformations (4) of $X\in B_2$. In order to describe the group of automorphisms Aut $\mathrm{o}(5,\mathbb{C})$ and Aut $\mathrm{sp}(4,\mathbb{C})$, we introduce the Lie groups of orthogonal and symplectic matrices,

$$\mathrm{O}(5,\mathbb{C})=\{A\in\mathbb{C}^{5\times5}|AA^T=I\},\quad \mathrm{Sp}(4,\mathbb{C})=\{A\in\mathbb{C}^{4\times4}|AJA^T=J\},$$

where $J=\left(\begin{smallmatrix}0&I_2\\-I_2&0\end{smallmatrix}\right)$.

The automorphism groups are formed by the transformations (4),

$$\text{Aut }\mathrm{o}(5,\mathbb{C})=\{\mathrm{Ad}_A|A\in\mathrm{O}(5,\mathbb{C})\},\quad \text{Aut }\mathrm{sp}(4,\mathbb{C})=\{\mathrm{Ad}_A|A\in\mathrm{Sp}(4,\mathbb{C})\}. \tag{5}$$

In Ref. 14 it is shown that there exist three nonconjugate MAD-groups in Aut $\mathrm{o}(5,\mathbb{C})$, and similarly in Aut $\mathrm{sp}(4,\mathbb{C})$. In order to describe the three MAD-groups explicitly, we have to provide A in (4) as the matrices $\mathbb{C}^{5\times5}$ and $\mathbb{C}^{4\times4}$ respectively.

The MAD-groups $\mathcal{G}_1,\mathcal{G}_2,\mathcal{G}_3$ of Aut $\mathrm{o}(5,\mathbb{C})$ are given as subgroups of Aut $\mathrm{o}(5,\mathbb{C})$, where the following matrices A are used in (4):

$$\mathcal{G}_1:\quad A=(\varepsilon)\oplus\begin{pmatrix}\cos\varphi_1&\sin\varphi_1\\-\sin\varphi_1&\cos\varphi_1\end{pmatrix}\oplus\begin{pmatrix}\cos\varphi_2&\sin\varphi_2\\-\sin\varphi_2&\cos\varphi_2\end{pmatrix},\quad \varepsilon=\pm1,\ \varphi_1,\varphi_2\in\mathbb{C},$$

$$\mathcal{G}_2:\quad A=\mathrm{diag}(\varepsilon_1,\varepsilon_2,\varepsilon_3)\oplus\begin{pmatrix}\cos\varphi&\sin\varphi\\-\sin\varphi&\cos\varphi\end{pmatrix},\qquad \varepsilon_i=\pm1,\ \varphi\in\mathbb{C},$$

$$\mathcal{G}_3:\quad A=\mathrm{diag}(\varepsilon_1,\varepsilon_2,\varepsilon_3,\varepsilon_4,\varepsilon_5),\qquad \varepsilon_i=\pm1.$$

Correspondingly, the MAD-groups $\mathcal{H}_1,\mathcal{H}_2,\mathcal{H}_3$ of Aut $\mathrm{sp}(4,\mathbb{C})$ are given by

$$\mathcal{H}_1:\quad A=\mathrm{diag}(\alpha,\beta,\alpha^{-1},\beta^{-1}),\qquad \alpha,\beta\in\mathbb{C},$$

$$\mathcal{H}_2:\quad A=\begin{pmatrix}\alpha&0\\0&\alpha^{-1}\end{pmatrix}\otimes\sigma_k=\begin{pmatrix}\alpha\sigma_k&0\\0&\alpha^{-1}\sigma_k\end{pmatrix},\quad k=0,1,2,3,\ \alpha\in\mathbb{C},$$

$$\mathcal{H}_3:\quad A=\sigma_j\otimes\sigma_k,\qquad j,k=0,1,2,3,$$

where $\sigma_0=\left(\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right)$, $\sigma_1=\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$, $\sigma_2=\left(\begin{smallmatrix}0&1\\-1&0\end{smallmatrix}\right)$, $\sigma_3=\left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)$.

According to Ref. 1, a grading $\Gamma: L=\oplus_{i\in I}L_i$ is fine iff Γ is a decomposition into eigenspaces of elements of a MAD-group $\mathcal{G}$. Since the decomposition of a finite-dimensional Lie algebra has only finite number of nonempty subspaces, we need only one or several elements of $\mathcal{G}$ even if the group $\mathcal{G}$ is infinite. The choice of such "grading elements" is far from unique. Our choice of grading elements is shown later.

It follows from the definition of a grading, that there is a partial binary operation defined on the index set I,

$$(i,j)\to k \quad \text{if} \quad 0\neq[L_i,L_j]\subseteq L_k. \tag{6}$$

Clearly this operation is closely related to the choice of labeling subscripts of the grading subspaces L_j. Since the grading subspaces are eigenspaces of the chosen grading elements, it is natural to use their eigenvalues for the labeling. Thus if L_i is the eigenspace of $\mathrm{Ad}_A\in\mathcal{G}$ corresponding to λ_i and L_j is the eigenspace corresponding to λ_j, and $[L_i,L_j]\neq 0$, then $[L_i,L_j]$ is the eigenspace corresponding to the eigenvalue $\lambda_i\lambda_j$. This fact enables one to embed I, equipped with operation (6), into an Abelian group. The multiplicative group is replaced by an additive one by putting $\lambda_j=e^{a_j}$ and using just the exponents as labels.

III. FINE GRADINGS OF o(5, $\mathbb{C}$)

For easier recording of the results, we use constant matrices E_{ij} and $M_{ij}\in\mathbb{C}^{5\times 5}$,

$$(E_{ij})_{rs}=\delta_{ir}\delta_{js}, \quad M_{ij}=E_{ij}-E_{ji}. \tag{7}$$

Their commutation relations are

$$[E_{jk},E_{mn}]=\delta_{km}E_{jn}-\delta_{jn}E_{mk},$$

$$[M_{pq},M_{rs}]=\delta_{qr}M_{ps}+\delta_{ps}M_{qr}-\delta_{qs}M_{pr}-\delta_{pr}M_{qs}.$$

A. The fine grading of o(5, $\mathbb{C}$) corresponding to $\mathcal{G}_1$

Since $\mathcal{G}_1$ is an Abelian group depending on two continuous complex parameters φ_1 and φ_2, it is a maximal torus of O(5, $\mathbb{C}$) so that the corresponding grading is a root decomposition of o(5, $\mathbb{C}$). If $\mathrm{Ad}_{A_1}\in\mathcal{G}_1$ is used in (4),

$$A_1=(1)\oplus\begin{pmatrix}\cos\varphi_1 & \sin\varphi_1\\ -\sin\varphi_1 & \cos\varphi_1\end{pmatrix}\oplus\begin{pmatrix}\cos\varphi_2 & \sin\varphi_2\\ -\sin\varphi_2 & \cos\varphi_2\end{pmatrix},$$

then the Lie algebra o(5, $\mathbb{C}$) is decomposed into nine subspaces: one two-dimensional (Cartan subalgebra) and 8 one-dimensional (root) subspaces.

The eigenvectors $X_1,\ldots,X_{10}$ are given in terms of matrices M_{jk},

$$X_1=\iota M_{23}+\iota M_{45}, \qquad X_2=\iota M_{23}-\iota M_{45},$$

$$X_3=M_{14}-\iota M_{15}, \qquad X_4=M_{24}+M_{35}+\iota(M_{25}-M_{34}),$$

$$X_5=M_{12}-\iota M_{13}, \qquad X_6=M_{24}-M_{35}+\iota(-M_{25}-M_{34}),$$

$$X_7=M_{24}-M_{35}+\iota(M_{25}+M_{34}), \quad X_8=M_{12}+\iota M_{13},$$

TABLE I. The correspondence between eigenvectors X_k from (8) and the eigenvalues λ of Ad_{A_1}.

λ	1	1	$e^{\iota\varphi_2}$	$e^{\iota(\varphi_1-\varphi_2)}$	$e^{\iota\varphi_1}$	$e^{\iota(\varphi_1+\varphi_2)}$	$e^{-\iota(\varphi_1+\varphi_2)}$	$e^{-\iota\varphi_1}$	$e^{-\iota(\varphi_1-\varphi_2)}$	$e^{-\iota\varphi_2}$
X_k	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}

TABLE II. Grading subspaces for $\mathbb{Z}_9$-grading of o(5, $\mathbb{C}$) and sp(4, $\mathbb{C}$). For definition of X_i see (8) and (11), respectively.

L_0	L_1	L_2	L_3	L_4	L_5	L_6	L_7	L_8
$\mathbb{C}X_1+\mathbb{C}X_2$	$\mathbb{C}X_3$	$\mathbb{C}X_4$	$\mathbb{C}X_5$	$\mathbb{C}X_6$	$\mathbb{C}X_7$	$\mathbb{C}X_8$	$\mathbb{C}X_9$	$\mathbb{C}X_{10}$

$$X_9=M_{24}+M_{35}+\iota(-M_{25}+M_{34}),\quad X_{10}=M_{14}+\iota M_{15}. \tag{8}$$

Any linear combinations of X_1 and X_2 with coefficients in $\mathbb{C}$ are compatible with this grading. The presence of $\iota=\sqrt{-1}$ in the linear combinations (8) cannot be avoided as long as o(5, $\mathbb{C}$) is spanned by antisymmetric matrices [cf. (3)].

Putting $\varphi_1=2\pi/3$ and $\varphi_2=2\pi/9$ in Table I, we can see that the index set I is the additive group $\mathbb{Z}_9$. Thus we get the decomposition and the commutation relations,

$$\text{o}(5,\mathbb{C})=\oplus_{k=0}^{8}L_k,\quad 0\neq[L_k,L_j]\subseteq L_{k+j\ (\mathrm{mod}\ 9)}$$

with the grading subspaces L_k given in Table II.

The Cartan subalgebra in this case is L_0. In order to recognize the root spaces among $L_1,\ldots,L_8$, we have to fix a choice of simple roots of the Lie algebra B_2 and identify the correspondence between the eigenvalues λ_k of Ad_{A_1} and the roots. Let γ_1,γ_2 denote the short and long simple root respectively. A possible choice is $\gamma_1=\varphi_2$ and $\gamma_2=\varphi_1-\varphi_2$. The two nonsimple positive roots are then $\gamma_1+\gamma_2=\varphi_1$ and $2\gamma_1+\gamma_2=\varphi_1+\varphi_2$.

B. The fine grading of o(5, $\mathbb{C}$) corresponding to $\mathcal{G}_2$

Decomposing o(5, $\mathbb{C}$) simultaneously into eigenspaces of $\mathrm{Ad}_{A_1},\mathrm{Ad}_{A_2}\in\mathcal{G}_2$, where

$$A_1=\mathrm{diag}(1,1,-1)\oplus\begin{pmatrix}\cos\varphi & \sin\varphi\\ -\sin\varphi & \cos\varphi\end{pmatrix},\quad A_2=\mathrm{diag}(1,-1,-1)\oplus\begin{pmatrix}\cos\varphi & \sin\varphi\\ -\sin\varphi & \cos\varphi\end{pmatrix},$$

we obtain a grading into 10 one-dimensional subspaces which are the linear hulls of matrices,

$$Y_1=M_{45},\quad Y_2=M_{12},\quad Y_3=M_{23},\quad Y_4=M_{13},$$

$$Y_5=M_{14}+\iota M_{15},\quad Y_6=M_{24}+\iota M_{25},\quad Y_7=M_{34}+\iota M_{35},$$

$$Y_8=M_{14}-\iota M_{15},\quad Y_9=M_{24}-\iota M_{25},\quad Y_{10}=M_{34}-\iota M_{35}, \tag{9}$$

which correspond to the pair λ_1 and λ_2 of eigenvalues of Ad_{A_1} and Ad_{A_2}, respectively (Table III).

Putting $\varphi=2\pi/3$, we embed the index set I into the additive group $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_3$, see Table IV. The commutation relations thus are

$$\text{o}(5,\mathbb{C})=\oplus_{(i,j,k)}L_{(i,j,k)},$$

$$0\neq[L_{(i,j,k)},L_{(p,q,r)}]=L_{(i+p,j+q,k+r)}\ (\mathrm{mod}\ 2,\mathrm{mod}\ 2,\mathrm{mod}\ 3).$$

TABLE III. The correspondence between eigenvectors Y_k from (9) and eigenvalues of Ad_{A_1} and Ad_{A_2}.

λ_1	1	1	-1	-1	$e^{-\iota\varphi}$	$e^{-\iota\varphi}$	$-e^{-\iota\varphi}$	$e^{\iota\varphi}$	$e^{\iota\varphi}$	$-e^{-\iota\varphi}$
λ_2	1	-1	1	-1	$e^{-\iota\varphi}$	$-e^{-\iota\varphi}$	$-e^{-\iota\varphi}$	$e^{\iota\varphi}$	$-e^{\iota\varphi}$	$-e^{\iota\varphi}$
Eigenvectors	Y_1	Y_2	Y_3	Y_4	Y_5	Y_6	Y_7	Y_8	Y_9	Y_{10}

TABLE IV. $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_3$-labeling of grading subspaces for gradings given by MAD groups $\mathcal{G}_2$ and $\mathcal{H}_2$. For $Y_i\in$ o(5, $\mathbb{C}$) see (9), for $Y_i\in$ sp(4, $\mathbb{C}$) see (12).

$L_{(0,0,0)}$	$L_{(0,1,0)}$	$L_{(1,0,0)}$	$L_{(1,1,0)}$	$L_{(0,0,1)}$	$L_{(0,1,1)}$	$L_{(1,1,1)}$	$L_{(0,0,2)}$	$L_{(0,1,2)}$	$L_{(1,1,2)}$
$\mathbb{C}Y_1$	$\mathbb{C}Y_2$	$\mathbb{C}Y_3$	$\mathbb{C}Y_4$	$\mathbb{C}Y_5$	$\mathbb{C}Y_6$	$\mathbb{C}Y_7$	$\mathbb{C}Y_8$	$\mathbb{C}Y_9$	$\mathbb{C}Y_{10}$

C. The fine grading of o(5, $\mathbb{C}$) corresponding to $\mathcal{G}_3$

Another way to obtain a decomposition of o(5, $\mathbb{C}$) into 10 one-dimensional grading subspaces is using $\mathrm{Ad}_{A_1},\mathrm{Ad}_{A_2},\mathrm{Ad}_{A_3},\mathrm{Ad}_{A_4}\in\mathcal{G}_3$. We set

$$A_1=\mathrm{diag}(1,-1,-1,1,1),\quad A_2=\mathrm{diag}(1,1,1,1,-1),$$

$$A_3=\mathrm{diag}(1,1,1,-1,1),\quad A_4=\mathrm{diag}(1,1,-1,-1,-1).$$

We have the eigenvectors

$$Z_1=M_{23},\quad Z_2=M_{14},\quad Z_3=M_{15},\quad Z_4=M_{45},\quad Z_5=M_{35},$$

$$Z_6=M_{25},\quad Z_7=M_{12},\quad Z_8=M_{34},\quad Z_9=M_{13},\quad Z_{10}=M_{24}, \tag{10}$$

which correspond to the tetrads of eigenvalues $\lambda_1,\ldots,\lambda_4$ shown in Table V. The tetrads are subsets of the multiplicative form of the group $(\mathbb{Z}_2)$.[4] Labeling of grading subspaces by additive form of this group is in Table VI.

The grading decomposition and the commutation relation thus are

$$\text{o}(5,\mathbb{C})=\oplus_{(i,j,k,m)}L_{(i,j,k,m)},$$

$$0\neq[L_{(i,j,k,m)},L_{(p,q,r,s)}]=L_{(i+p,j+q,k+r,m+s)\ (\mathrm{mod}\ 2,\mathrm{mod}\ 2,\mathrm{mod}\ 2,\mathrm{mod}\ 2)}.$$

IV. FINE GRADINGS OF sp(4, $\mathbb{C}$)

Since Lie algebra sp(4, $\mathbb{C}$) is isomorphic to the algebra o(5, $\mathbb{C}$), their fine gradings are isomorphic as well. We shall denote the subspaces of the three fine gradings of sp(4, $\mathbb{C}$) again by $\mathbb{C}X_i$, $\mathbb{C}Y_i$, and $\mathbb{C}Z_i$ respectively, in such a way that the subspaces in sp(4, $\mathbb{C}$) and o(5, $\mathbb{C}$) with the same notation correspond to each other via isomorphism between these two algebras. Therefore the assignment of indices for subspaces of the gradings in Tables II, IV, and VI is valid for fine gradings of sp(4, $\mathbb{C}$) as well.

A. The fine grading of sp(4, $\mathbb{C}$) corresponding to $\mathcal{H}_1$

A decomposition of sp(4, $\mathbb{C}$) into one two-dimensional and eight one-dimensional subspaces is obtained using $\mathrm{Ad}_{A_1}\in\mathcal{H}_1$, $A_1=\mathrm{diag}(\alpha,\beta,\alpha^{-1},\beta^{-1})$. The presence of two continuous parameters α and β reveals that A_1 stands for the maximal torus. Hence the grading we find in this case is the root decomposition. The eigenvectors are

TABLE V. Four eigenvalues labeling multiplicatively the basis (10) in o(5, $\mathbb{C}$) and the basis (13) in sp(4, $\mathbb{C}$).

λ_1	1	1	1	1	−1	−1	−1	−1	−1	−1
λ_2	1	1	−1	−1	−1	−1	1	1	1	1
λ_3	1	−1	1	−1	1	1	1	−1	1	−1
λ_4	−1	−1	−1	1	1	−1	1	1	−1	−1
Eigenvectors	Z_1	Z_2	Z_3	Z_4	Z_5	Z_6	Z_7	Z_8	Z_9	Z_{10}

TABLE VI. $(\mathbb{Z}_2)^4$-labeling of grading subspaces for gradings given by MAD-groups $\mathcal{G}_3$ and $\mathcal{H}_3$. For $Z_i \in o(5, \mathbb{C})$, see (10), and for $Z_i \in sp(4, \mathbb{C})$, see (13).

$L_{(0,0,0,1)}$	$L_{(0,0,1,1)}$	$L_{(0,1,0,1)}$	$L_{(0,1,1,0)}$	$L_{(1,1,0,0)}$	$L_{(1,1,0,1)}$	$L_{(1,0,0,0)}$	$L_{(1,0,1,0)}$	$L_{(1,0,0,1)}$	$L_{(1,0,1,1)}$
$\mathbb{C}Z_1$	$\mathbb{C}Z_2$	$\mathbb{C}Z_3$	$\mathbb{C}Z_4$	$\mathbb{C}Z_5$	$\mathbb{C}Z_6$	$\mathbb{C}Z_7$	$\mathbb{C}Z_8$	$\mathbb{C}Z_9$	$\mathbb{C}Z_{10}$

$$X_1=\begin{pmatrix}1&0&0&0\\0&0&0&0\\0&0&-1&0\\0&0&0&0\end{pmatrix},\quad X_2=\begin{pmatrix}0&0&0&0\\0&1&0&0\\0&0&0&0\\0&0&0&-1\end{pmatrix},\quad X_3=\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&1&0&0\\1&0&0&0\end{pmatrix},$$

$$X_4=\begin{pmatrix}0&0&0&0\\0&0&0&1\\0&0&0&0\\0&0&0&0\end{pmatrix},\quad X_5=\begin{pmatrix}0&0&0&0\\1&0&0&0\\0&0&0&-1\\0&0&0&0\end{pmatrix},\quad X_6=\begin{pmatrix}0&0&0&0\\0&0&0&0\\1&0&0&0\\0&0&0&0\end{pmatrix},$$

$$X_7=\begin{pmatrix}0&0&1&0\\0&0&0&0\\0&0&0&0\\0&0&0&0\end{pmatrix},\quad X_8=\begin{pmatrix}0&1&0&0\\0&0&0&0\\0&0&0&0\\0&0&-1&0\end{pmatrix},\quad X_9=\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&0&0&0\\0&1&0&0\end{pmatrix},$$

$$X_{10}=\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&0&0&0\\0&0&0&0\end{pmatrix}. \tag{11}$$

Corresponding eigenvalues are shown in Table VII.

Putting $\alpha=\exp((4\pi/9)\iota), \beta=\exp((16\pi/9)\iota)$, and having the same dependence of L_i on X_j as in the case of $o(5, \mathbb{C})$-decomposition under $\mathcal{G}_1$, the index set I is again embedded into $\mathbb{Z}_9$ (see Table II). Let us now make explicit the relation between the eigenvalues and the roots of B_2. Suppose again γ_1 and γ_2 are, respectively, the short and long simple root of B_2. Then a possible choice is to put

$$\gamma_1=\ln(\alpha\beta)=\ln\alpha+\ln\beta,\quad \gamma_2=\ln\beta^{-2}=-2\ln\beta.$$

The two nonsimple short and long positive roots are then, respectively,

$$\gamma_1+\gamma_2=\ln(\alpha\beta\cdot\beta^{-2})=\ln\alpha-\ln\beta,\quad 2\gamma_1+\gamma_2=\ln(\alpha^2\beta^2\cdot\beta^{-2})=2\ln\alpha.$$

Similarly one finds the negative roots. Cartan subalgebra is generated by X_1 and X_2.

TABLE VII. The correspondence between eigenvectors X_k from (11) and the eigenvalues of Ad_{A_1}.

λ	1	1	$\alpha\beta$	β^{-2}	$\alpha\beta^{-1}$	α^2	α^{-2}	$\alpha^{-1}\beta$	β^2	$\alpha^{-1}\beta^{-1}$
Eigenvectors	X_1	X_2	X_3	X_4	X_5	X_6	X_7	X_8	X_9	X_{10}

TABLE VIII. Correspondence between eigenvalues of Ad_{A_1} and Ad_{A_2} and eigenvectors (12).

λ_1	1	1	−1	−1	α^{-2}	α^{-2}	$-\alpha^{-2}$	α^2	α^2	$-\alpha^2$
λ_2	1	−1	1	−1	α^{-2}	$-\alpha^{-2}$	$-\alpha^{-2}$	α^2	$-\alpha^2$	$-\alpha^2$
Eigenvectors	Y_1	Y_2	Y_3	Y_4	Y_5	Y_6	Y_7	Y_8	Y_9	Y_{10}

B. The fine grading of sp(4, $\mathbb{C}$) corresponding to $\mathcal{H}_2$

Now let us put $A_1=\left(\begin{smallmatrix}\alpha & 0\\ 0 & \alpha^{-1}\end{smallmatrix}\right)\otimes\sigma_3$, and $A_2=\left(\begin{smallmatrix}\alpha & 0\\ 0 & \alpha^{-1}\end{smallmatrix}\right)\otimes\sigma_2$. A pair of automorphisms $\mathrm{Ad}_{A_1},\mathrm{Ad}_{A_2}\in\mathcal{H}_2$ decomposes sp(4, $\mathbb{C}$) again into ten one-dimensional subspaces. The eigenvectors are the following:

$$Y_1=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix},\quad Y_2=\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix},\quad Y_3=\begin{pmatrix}0&1&0&0\\-1&0&0&0\\0&0&0&1\\0&0&-1&0\end{pmatrix},$$

$$Y_4=\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&-1\\0&0&-1&0\end{pmatrix},\quad Y_5=\begin{pmatrix}0&0&1&0\\0&0&0&1\\0&0&0&0\\0&0&0&0\end{pmatrix},\quad Y_6=\begin{pmatrix}0&0&1&0\\0&0&0&-1\\0&0&0&0\\0&0&0&0\end{pmatrix},$$

$$Y_7=\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&0&0&0\\0&0&0&0\end{pmatrix},\quad Y_8=\begin{pmatrix}0&0&0&0\\0&0&0&0\\1&0&0&0\\0&1&0&0\end{pmatrix},\quad Y_9=\begin{pmatrix}0&0&0&0\\0&0&0&0\\1&0&0&0\\0&-1&0&0\end{pmatrix},$$

$$Y_{10}=\begin{pmatrix}0&0&0&0\\0&0&0&0\\0&1&0&0\\1&0&0&0\end{pmatrix}. \tag{12}$$

Corresponding eigenvalues are shown in Table VIII.

Putting $\alpha=\exp((\pi/3)\iota)$ enables us to label eigenspaces by indices from the group $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_3$ as found in Table IV.

C. The fine grading of sp(4, $\mathbb{C}$) corresponding to $\mathcal{H}_3$

The second way to decompose sp(4, $\mathbb{C}$) into ten one-dimensional eigenspaces is using four automorphisms $\mathrm{Ad}_{A_1},\mathrm{Ad}_{A_2},\mathrm{Ad}_{A_3},\mathrm{Ad}_{A_4}\in\mathcal{H}_3$, where $A_1=\sigma_3\otimes\sigma_0$, $A_2=\sigma_0\otimes\sigma_3$, $A_3=\sigma_0\otimes\sigma_1$, and $A_4=\sigma_1\otimes\sigma_0$. We get the eigenvectors

$$Z_1=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix},\quad Z_2=\begin{pmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix},\quad Z_3=\begin{pmatrix}0&1&0&0\\1&0&0&0\\0&0&0&-1\\0&0&-1&0\end{pmatrix},$$

$$Z_4=\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix},\quad Z_5=\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},\quad Z_6=\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix},$$

$$Z_7=\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},\quad Z_8=\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix},\quad Z_9=\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix},$$

$$Z_{10}=\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{13}$$

The correspondence with the tetrads of eigenvalues is given in Table V.

The relation between eigenvectors Z_i and grading subspaces labeled by elements of the group $\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2\times\mathbb{Z}_2$ is shown in Table VI.

V. FINE GRADINGS OF REAL FORMS OF o(5, $\mathbb{C}$) AND sp(4, $\mathbb{C}$)

The real forms of o(5, $\mathbb{C}$) are determined by nonsingular Hermitian matrices $E\in \mathrm{O}(5,\mathbb{C})$ as follows:

$$\mathrm{o}(5-k,k)=\{X\in \mathrm{o}(5,\mathbb{C})\,|\,XE=-EX^{+}\}, \tag{14}$$

where E has $5-k$ positive and k negative eigenvalues, $k=0,1,2$. Two Hermitian orthogonal matrices with the same number of positive and negative eigenvalues (i.e., matrices with the same signatures) give two isomorphic real forms.

Real forms of sp(4, $\mathbb{C}$) are of two types. The first one is

$$\mathrm{sp}(4,\mathbb{R})=\{X\in \mathrm{sp}(4,\mathbb{C})\,|\,X=\overline{X}\},$$

where the overbar denotes complex conjugation, and the second type of real forms corresponds to Hermitian matrices $E\in \mathrm{Sp}(4,\mathbb{C})$,

$$\mathrm{usp}(4-2k,2k)=\{X\in \mathrm{sp}(4,\mathbb{C})\,|\,XE=-EX^{+}\}, \tag{15}$$

where E has $4-2k$ positive and $2k$ negative eigenvalues, $k=0,1$.

Since o(5, $\mathbb{C}$) and sp(4, $\mathbb{C}$) are isomorphic Lie algebras, we have the isomorphic pairs of real forms. More precisely,

$$\mathrm{o}(5)\sim\mathrm{usp}(4),\quad \mathrm{o}(4,1)\sim\mathrm{usp}(2,2),\quad \mathrm{o}(3,2)\sim\mathrm{sp}(4,\mathbb{R}). \tag{16}$$

Let us consider a MAD-group $\mathcal{K}$ on a real form $L_{\mathbb{R}}$ of a complex Lie algebra L. Any automorphism $g\in\mathcal{K}$ can be uniquely extended from $L_{\mathbb{R}}$ to L. Obviously such extensions are diagonable, their spectrum is real, and they mutually commute. Therefore $\mathcal{K}$ is a subgroup of some MAD-group $\mathcal{G}$ of complex Lie algebra L. If we denote by $\mathcal{G}^{\mathbb{R}}$ those automorphisms of $\mathcal{G}$ which have real spectrum, then $\mathcal{K}\subseteq\mathcal{G}^{\mathbb{R}}\subseteq\mathcal{G}$. It is proven in Ref. 15 that for any MAD-group $\mathcal{K}$ on a real form of classical Lie algebra L with the exception of o(8, $\mathbb{C}$) there exists a MAD-group $\mathcal{G}$ on L such that $\mathcal{K}=\mathcal{G}^{\mathbb{R}}$.

For any MAD-group $\mathcal{G}$ on o(n, $\mathbb{C}$) with n odd there exists a simple criteria how to decide for which real form o($n-k,k$) the group $\mathcal{G}^{\mathbb{R}}$ is a MAD-group on o($n-k,k$).

Theorem: *Let $\mathcal{G}$ be a MAD-group on* o(n, $\mathbb{C}$), *n odd, and let E be a Hermitian orthogonal matrix with $n-k$ positive and k negative eigenvalues. Then $\mathcal{G}^{\mathbb{R}}$ is a MAD-group on* $\mathrm{o}(n-k,k)=\{X\in\mathrm{o}(n,\mathbb{C})\,|\,XE=-EX^{+}\}$ *if and only if*

$$AEA^{+}=E \quad \text{for any} \quad \mathrm{Ad}_A\in\mathcal{G}^{\mathbb{R}}. \tag{17}$$

Note that automorphisms Ad_A of Aut o(n, $\mathbb{C}$) with

$$A=\mathrm{diag}(\varepsilon_1,\ldots,\varepsilon_s)\oplus\begin{pmatrix}\cos\varphi_1 & \sin\varphi_1\\ -\sin\varphi_1 & \cos\varphi_1\end{pmatrix}\oplus\cdots\oplus\begin{pmatrix}\cos\varphi_p & \sin\varphi_p\\ -\sin\varphi_p & \cos\varphi_p\end{pmatrix},\quad \varepsilon_j=\pm1,\quad \varphi_j\in\mathbb{C}$$

has the real spectrum if and only if $\varphi_j=\iota\psi_j$, $\psi_j\in\mathbb{R}$ for all $j=1,...,p$. In this case the matrix A has the form,

$$A=\mathrm{diag}(\varepsilon_1,\ldots,\varepsilon_3)\oplus\begin{pmatrix}\cosh\psi_1 & \iota\sinh\psi_1\\ -\iota\sinh\psi_1 & \cosh\psi_1\end{pmatrix}\oplus\cdots\oplus\begin{pmatrix}\cosh\psi_p & \iota\sinh\psi_p\\ -\iota\sinh\psi_p & \cosh\psi_p\end{pmatrix},$$

where $\varepsilon_j=\pm1$, $\psi_j\in\mathbb{R}$.

Therefore, $\mathcal{G}_3^{\mathbb{R}}=\mathcal{G}_3$, and for the description $\mathcal{G}_1^{\mathbb{R}}$ and $\mathcal{G}_2^{\mathbb{R}}$ we have to choose those automorphisms from $\mathcal{G}_1,\mathcal{G}_2$, for which parameters φ_1,φ_2, and φ, resp., belong to $\iota\mathbb{R}$.

A. Fine gradings of o(3, 2)

Let us apply the theorem to o(5, $\mathbb{C}$) and MAD-groups $\mathcal{G}_1,\mathcal{G}_2,\mathcal{G}_3$. If we choose $E=\mathrm{diag}(1,1,-1,1,-1)$, then the condition (17) is satisfied for $\mathcal{G}_1^{\mathbb{R}},\mathcal{G}_2^{\mathbb{R}},\mathcal{G}_3^{\mathbb{R}}$. Hence we can conclude that o(3, 2) has three MAD-groups.

Thus we find three find gradings of o(3, 2). Using $E=\mathrm{diag}(1,1,-1,1,-1)$ in (14),

$$\mathrm{o}(3,2)=\left\{\begin{pmatrix}0 & a & \iota b & c & \iota d\\ -a & 0 & \iota e & f & \iota g\\ -\iota b & -\iota e & 0 & \iota h & j\\ -c & -f & -\iota h & 0 & \iota k\\ -\iota d & -\iota g & -j & -\iota k & 0\end{pmatrix}\;\middle|\; a,\ldots,k\in\mathbb{R}\right\}.$$

Indeed, all subspaces of gradings of complex Lie algebra o(5, $\mathbb{C}$) corresponding to $\mathcal{G}_i$ contain elements belonging to o(3, 2). The gradings of the real form o(3, 2) are found in Tables IX, X, XI in terms of the bases (8), (9), and (10) of o(5, $\mathbb{C}$).

B. Fine gradings of o(4, 1)

The groups $\mathcal{G}_2^{\mathbb{R}}$ and $\mathcal{G}_3^{\mathbb{R}}$ satisfy (17) with the matrix $E=\mathrm{diag}(1,1,1,1,-1)$, but there exists no orthogonal Hermitian matrix E with one negative and four positive eigenvalues such that $\mathcal{G}_1^{\mathbb{R}}$ and E fulfill (17). Therefore the real form o(4, 1) has only two fine gradings corresponding to $\mathcal{G}_2^{\mathbb{R}}$ and $\mathcal{G}_3^{\mathbb{R}}$. For the definition of the real form o(4, 1) we use the matrix $E=\mathrm{diag}(1,1,1,1,-1)$, and thus the real form is given as

TABLE IX. Grading of o(3, 2) corresponding to $\mathcal{G}_1^{\mathbb{R}}$; X_i are form (8).

L_0	L_1	L_2	L_3	L_4	L_5	L_6	L_7	L_8
$\mathbb{R}X_1+\mathbb{R}X_2$	$\mathbb{R}X_3$	$\mathbb{R}X_4$	$\mathbb{R}X_5$	$\mathbb{R}X_6$	$\mathbb{R}X_7$	$\mathbb{R}X_8$	$\mathbb{R}X_9$	$\mathbb{R}X_{10}$

TABLE X. Grading of o(3, 2) corresponding to $\mathcal{G}_2^{\mathbb{R}}$; Y_i are from (9).

$L_{(0,0,0)}$	$L_{(0,1,0)}$	$L_{(1,0,0)}$	$L_{(1,1,0)}$	$L_{(0,0,1)}$	$L_{(0,1,1)}$	$L_{(1,1,1)}$	$L_{(0,0,2)}$	$L_{(0,1,2)}$	$L_{(1,1,2)}$
$\iota\mathbb{R}Y_1$	$\mathbb{R}Y_2$	$\iota\mathbb{R}Y_3$	$\iota\mathbb{R}Y_4$	$\mathbb{R}Y_5$	$\mathbb{R}Y_6$	$\iota\mathbb{R}Y_7$	$\mathbb{R}Y_8$	$\mathbb{R}Y_9$	$\iota\mathbb{R}Y_{10}$

$$\mathrm{o}(4,1)=\left\{\left.\begin{pmatrix} 0 & a & b & c & \iota d \\ -a & 0 & e & f & \iota g \\ -b & -e & 0 & h & \iota j \\ -c & -f & -h & 0 & \iota k \\ -\iota d & -\iota g & -\iota j & -\iota k & 0 \end{pmatrix}\right| a,\ldots,k\in\mathbb{R}\right\}.$$

The fine gradings of o(4, 1) are found in Tables XII and XIII.

C. Fine gradings of o(5)

The compact real form o(5) has only one fine grading, since only $\mathcal{G}_3^{\mathbb{R}}$ with $E=\mathrm{diag}(1,1,1,1,1)$ satisfies the condition (17).

For the definition of the compact real form o(5) we use the matrix $E=\mathrm{diag}(1,1,1,1,1)$, and thus the real form is given as

$$\mathrm{o}(5)=\{X\in\mathbb{R}^{5\times 5}\,|\,X+X^T=0\}.$$

The only fine grading possible on this real form is in Table XIV.

D. Fine gradings of real forms of sp(4, $\mathbb{C}$)

In order to describe the fine gradings of the real forms of sp(4, $\mathbb{C}$), we make use of the isomorphisms (16). It follows from the description of gradings of real forms of o(5, $\mathbb{C}$) that there exist three nonconjugate MAD-groups in the case of sp(4, $\mathbb{R}$), two MAD-groups for usp(2, 2), and one MAD-group for the compact real form usp(4). All the fine gradings of the real forms of sp(4, $\mathbb{C}$) are presented in Tables XV–XX, respectively.

We realize the real form sp(4, $\mathbb{R}$) as

$$\mathrm{sp}(4,\mathbb{R})=\left\{\left.\begin{pmatrix} m & n & p & q \\ r & s & q & t \\ u & v & -m & -r \\ v & w & -n & -s \end{pmatrix}\right| m,\ldots,w\in\mathbb{R}\right\}=\{X\in\mathbb{R}^{4\times 4}\,|\,XJ+JX^T=0\}.$$

Choosing $E=\begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$ in (15), we obtain

TABLE XI. Grading of o(3, 2) corresponding to $\mathcal{G}_3^{\mathbb{R}}$; Z_i are from (10).

$L_{(0,0,0,1)}$	$L_{(0,0,1,1)}$	$L_{(0,1,0,1)}$	$L_{(0,1,1,0)}$	$L_{(1,1,0,0)}$	$L_{(1,1,0,1)}$	$L_{(1,0,0,0)}$	$L_{(1,0,1,0)}$	$L_{(1,0,0,1)}$	$L_{(1,0,1,1)}$
$\iota\mathbb{R}Z_1$	$\mathbb{R}Z_2$	$\iota\mathbb{R}Z_3$	$\iota\mathbb{R}Z_4$	$\mathbb{R}Z_5$	$\iota\mathbb{R}Z_6$	$\mathbb{R}Z_7$	$\iota\mathbb{R}Z_8$	$\iota\mathbb{R}Z_9$	$\mathbb{R}Z_{10}$

TABLE XII. Grading of o(4, 1) corresponding to $\mathcal{G}_2^{\mathbb{R}}$; Y_i are from (9).

$L_{(0,0,0)}$	$L_{(0,1,0)}$	$L_{(1,0,0)}$	$L_{(1,1,0)}$	$L_{(0,0,1)}$	$L_{(0,1,1)}$	$L_{(1,1,1)}$	$L_{(0,0,2)}$	$L_{(0,1,2)}$	$L_{(1,1,2)}$
$\imath\mathbb{R}Y_1$	$\mathbb{R}Y_2$	$\mathbb{R}Y_3$	$\mathbb{R}Y_4$	$\mathbb{R}Y_5$	$\mathbb{R}Y_6$	$\mathbb{R}Y_7$	$\mathbb{R}Y_8$	$\mathbb{R}Y_9$	$\mathbb{R}Y_{10}$

TABLE XIII. Grading of o(4, 1) corresponding to $\mathcal{G}_3^{\mathbb{R}}$; Z_i are from (10).

$L_{(0,0,0,1)}$	$L_{(0,0,1,1)}$	$L_{(0,1,0,1)}$	$L_{(0,1,1,0)}$	$L_{(1,1,0,0)}$	$L_{(1,1,0,1)}$	$L_{(1,0,0,0)}$	$L_{(1,0,1,0)}$	$L_{(1,0,0,1)}$	$L_{(1,0,1,1)}$
$\mathbb{R}Z_1$	$\mathbb{R}Z_2$	$\imath\mathbb{R}Z_3$	$\imath\mathbb{R}Z_4$	$\imath\mathbb{R}Z_5$	$\imath\mathbb{R}Z_6$	$\mathbb{R}Z_7$	$\mathbb{R}Z_8$	$\mathbb{R}Z_9$	$\mathbb{R}Z_{10}$

TABLE XIV. Grading of o(5) corresponding to $\mathcal{G}_3^{\mathbb{R}}$; Z_i are from (10).

$L_{(0,0,0,1)}$	$L_{(0,0,1,1)}$	$L_{(0,1,0,1)}$	$L_{(0,1,1,0)}$	$L_{(1,1,0,0)}$	$L_{(1,1,0,1)}$	$L_{(1,0,0,0)}$	$L_{(1,0,1,0)}$	$L_{(1,0,0,1)}$	$L_{(1,0,1,1)}$
$\mathbb{R}Z_1$	$\mathbb{R}Z_2$	$\mathbb{R}Z_3$	$\mathbb{R}Z_4$	$\mathbb{R}Z_5$	$\mathbb{R}Z_6$	$\mathbb{R}Z_7$	$\mathbb{R}Z_8$	$\mathbb{R}Z_9$	$\mathbb{R}Z_{10}$

TABLE XV. Grading of sp(4, $\mathbb{R}$) corresponding to $\mathcal{H}_1^{\mathbb{R}}$; X_i are from (11).

L_0	L_1	L_2	L_3	L_4	L_5	L_6	L_7	L_8
$\mathbb{R}X_1+\mathbb{R}X_2$	$\mathbb{R}X_3$	$\mathbb{R}X_4$	$\mathbb{R}X_5$	$\mathbb{R}X_6$	$\mathbb{R}X_7$	$\mathbb{R}X_8$	$\mathbb{R}X_9$	$\mathbb{R}X_{10}$

TABLE XVI. Grading of sp(4, $\mathbb{R}$) corresponding to $\mathcal{H}_2^{\mathbb{R}}$; Y_i are from (12).

$L_{(0,0,0)}$	$L_{(0,1,0)}$	$L_{(1,0,0)}$	$L_{(1,1,0)}$	$L_{(0,0,1)}$	$L_{(0,1,1)}$	$L_{(1,1,1)}$	$L_{(0,0,2)}$	$L_{(0,1,2)}$	$L_{(1,1,2)}$
$\mathbb{R}Y_1$	$\mathbb{R}Y_2$	$\mathbb{R}Y_3$	$\mathbb{R}Y_4$	$\mathbb{R}Y_5$	$\mathbb{R}Y_6$	$\mathbb{R}Y_7$	$\mathbb{R}Y_8$	$\mathbb{R}Y_9$	$\mathbb{R}Y_{10}$

TABLE XVII. Grading of sp(4, $\mathbb{R}$) corresponding to $\mathcal{H}_3^{\mathbb{R}}$; Z_i are from (13).

$L_{(0,0,0,1)}$	$L_{(0,0,1,1)}$	$L_{(0,1,0,1)}$	$L_{(0,1,1,0)}$	$L_{(1,1,0,0)}$	$L_{(1,1,0,1)}$	$L_{(1,0,0,0)}$	$L_{(1,0,1,0)}$	$L_{(1,0,0,1)}$	$L_{(1,0,1,1)}$
$\mathbb{R}Z_1$	$\mathbb{R}Z_2$	$\mathbb{R}Z_3$	$\mathbb{R}Z_4$	$\mathbb{R}Z_5$	$\mathbb{R}Z_6$	$\mathbb{R}Z_7$	$\mathbb{R}Z_8$	$\mathbb{R}Z_9$	$\mathbb{R}Z_{10}$

TABLE XVIII. Grading of usp(2, 2) corresponding to $\mathcal{H}_2^{\mathbb{R}}$; Y_i are from (12).

$L_{(0,0,0)}$	$L_{(0,1,0)}$	$L_{(1,0,0)}$	$L_{(1,1,0)}$	$L_{(0,0,1)}$	$L_{(0,1,1)}$	$L_{(1,1,1)}$	$L_{(0,0,2)}$	$L_{(0,1,2)}$	$L_{(1,1,2)}$
$\mathbb{R}Y_1$	$\imath\mathbb{R}Y_2$	$\mathbb{R}Y_3$	$\imath\mathbb{R}Y_4$	$\mathbb{R}Y_5$	$\imath\mathbb{R}Y_6$	$\imath\mathbb{R}Y_7$	$\mathbb{R}Y_8$	$\imath\mathbb{R}Y_9$	$\imath\mathbb{R}Y_{10}$

TABLE XIX. Grading of usp(2, 2) corresponding to $\mathcal{H}_3^{\mathbb{R}}$; Z_i are from (13).

$L_{(0,0,0,1)}$	$L_{(0,0,1,1)}$	$L_{(0,1,0,1)}$	$L_{(0,1,1,0)}$	$L_{(1,1,0,0)}$	$L_{(1,1,0,1)}$	$L_{(1,0,0,0)}$	$L_{(1,0,1,0)}$	$L_{(1,0,0,1)}$	$L_{(1,0,1,1)}$
$\mathbb{R}Z_1$	$\imath\mathbb{R}Z_2$	$\imath\mathbb{R}Z_3$	$\mathbb{R}Z_4$	$\imath\mathbb{R}Z_5$	$\imath\mathbb{R}Z_6$	$\mathbb{R}Z_7$	$\imath\mathbb{R}Z_8$	$\mathbb{R}Z_9$	$\imath\mathbb{R}Z_{10}$

TABLE XX. Grading of usp(4) corresponding to $\mathcal{H}_3^{\mathbb{R}}$; Z_i are from (13).

$L_{(0,0,0,1)}$	$L_{(0,0,1,1)}$	$L_{(0,1,0,1)}$	$L_{(0,1,1,0)}$	$L_{(1,1,0,0)}$	$L_{(1,1,0,1)}$	$L_{(1,0,0,0)}$	$L_{(1,0,1,0)}$	$L_{(1,0,0,1)}$	$L_{(1,0,1,1)}$
$\iota\mathbb{R}Z_1$	$\iota\mathbb{R}Z_2$	$\iota\mathbb{R}Z_3$	$\mathbb{R}Z_4$	$\iota\mathbb{R}Z_5$	$\mathbb{R}Z_6$	$\iota\mathbb{R}Z_7$	$\iota\mathbb{R}Z_8$	$\mathbb{R}Z_9$	$\mathbb{R}Z_{10}$

$$\mathrm{usp}(2,2)=\left\{\begin{pmatrix} m+\iota s & n+\iota r & p+\iota t & \iota q \\ -n+\iota r & m-\iota s & \iota q & p-\iota t \\ u+\iota w & \iota v & -m-\iota s & n-\iota r \\ \iota v & u-\iota w & -n-\iota r & -m+\iota s \end{pmatrix} \middle| \; m,\ldots,w\in\mathbb{R}\right\}.$$

Finally, the compact form (corresponding to $E=I$ in (15)) is written as

$$\mathrm{usp}(4)=\left\{\begin{pmatrix} \iota m & n+\iota r & p+\iota u & q+\iota v \\ -n+\iota r & \iota s & q+\iota v & t+\iota w \\ -p+\iota u & -q+\iota v & -\iota m & n-\iota r \\ -q+\iota v & -t+\iota w & -n-\iota r & -\iota s \end{pmatrix} \middle| \; m,\ldots,w\in\mathbb{R}\right\}.$$

VI. CONCLUDING REMARKS

Let us add the following remarks to the applications and problems mentioned in the Introduction.

(1) The way from the general classification of MAD-groups[15,14] to specific gradings of Lie algebras is relatively laborious, as we have exemplified in this paper. It would be interesting to provide explicit fine gradings for several other low rank Lie algebras of interest in physics besides the one or two which are well known. It is known that there are four fine gradings of sl(3, $\mathbb{C}$),[9] five for the nonsimple o(4, $\mathbb{C}$), eight in the case of sl(4, $\mathbb{C}$) or o(6, $\mathbb{C}$), and something up to that number for their real forms.

(2) The intermediate gradings found between the extremes of a fine grading and the trivial grading (by the identity element), are also useful. Most of the gradings used in graded contractions of Lie and superalgebras[2,5] are not the fine ones. The intermediate gradings should be useful in typical symmetry breaking situations where an important subalgebra needs to be preserved. This is a situation which often arises in graded contractions. There all deformations other than those of the subalgebra are admissible for consideration (see, for example, Ref. 4).

A full list of possible ''minimal'' refinements of gradings, starting from no grading at all (grading by the identity of the automorphism group) and proceeding step-by-step to the fine ones, is nowhere to be found for any simple Lie algebra of rank$\geqslant 2$ over $\mathbb{C}$. Closest to that are the coarsenings of the root decomposition of sl(3, $\mathbb{C}$) in Ref. 19.

(3) A comprehensive description of gradings of representation spaces by MAD-groups would be very useful. Here we have dealt with the three lowest representations of B_2. Note that for grading of an algebra and for a few of its representations, one does not need to use the whole MAD-group; suitably chosen elements of it provide enough of eigenvalues to distinguish grading subspaces. We have seen, for example, that for the root decomposition of B_2, it was sufficient to use a cyclic subgroup $\mathbb{Z}_9$ of the torus instead of the whole maximal torus. Generally one has to use the whole MAD-group for grading of all the representation spaces.

There is an additional complication to that in case of the simple Lie algebras of types A_n, B_n, C_n, D_n when $n>1$, and for E_6, and E_7. In those cases any MAD-group has to be Abelian in its action on the Lie algebra (adjoint action), and on the representations of the congruence class zero. On other irreducible representations, elements of a MAD-group may commute only up to the center of the corresponding Lie group. Consequently, not all elements of some MAD-groups can be simultaneously diagonalized in such representations. However, even then one could consider

reducible representations formed by the direct sum of pairs of irreducible contragredient representations (the only exception would be o(8, $\mathbb{C}$)) and diagonalize the whole MAD-group on it.

Gradings of representation spaces by a maximal torus are well known. They are called weight decompositions.

(4) For a given grading of a simple Lie algebra, in particular for the fine gradings, it is interesting to find also its normalizer in the group of automorphisms. Except for the root decomposition, little was known about the normalizers until recently.[9] Clearly the MAD-group is part of the normalizer which transforms each grading subspace into itself. More interesting are the elements of the normalizer which permute the grading subspaces.[16,17] They would, for example, transform equal valued Clebsch–Gordan coefficients among themselves provided one uses bases consisting of eigenvectors of the grading group in representation spaces.

(5) It is known that B_2 has two independent Casimir operators, one of degree 2 and one of degree 4. It would be interesting to compare their expressions written in the three bases provided by fine gradings. Perhaps one could get some better information about the spectrum of the operator of degree 4.

(6) One of the basic structures underlying the theory of semisimple Lie algebras and their representations are the root and weight lattices.[20] They are defined using the maximal torus which is one of the MAD-groups. What would be the analog of the lattices for some other MAD-groups?

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Similarity reduction, generalized symmetries and integrability of Belov–Chaltikian and Blaszak–Marciniak lattice equations

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The Lie point symmetries of Belov–Chaltikian (BC) and Blaszak–Marciniak (BM) lattice equations is derived. Using the symmetries similarity reduction for both BC and BM lattice equations is obtained and show that each of the reduced equation possesses Lax representation and satisfies the singularity confinement criteria (a discrete version of the Painlevé property) indicating their integrability. Two particular solutions of both the reduced equations are given explicitly. A systematic investigation for nonclassical symmetries of BC and BM lattice equations is carried out. Further, a sequence of conserved densities and generalized symmetries of both BC and BM lattice equation are derived explicitly. The existence of a sequence of such symmetries is a predictor for integrability. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1378306]

I. INTRODUCTION

The study of discrete nonlinear systems governed by differential–difference, difference, lattice equations, and mappings has attracted considerable attention in recent years.[1–5] Several analytical but adhoc methods such as inverse scattering technique,[1,6] singularity confinement criteria,[7] symmetries approach,[5,8–12] Hirota bilinearization,[13] symplectic structure and construction of integrals of motion,[14] etc.[15] have been proposed to deal with discrete nonlinear systems towards its complete integrability, linearizability, and solvability. Among them the extended algorithmic Lie symmetries approach initiated by Maeda[8] and others[5,9,10,16] provides an efficient tool to construct similarity as well as exact solution of discrete nonlinear equations besides deriving its group theoretical aspects. Also, the Lie symmetries approach enables one to determine conditions at which the autonomous nonlinear difference equation can be transformed into linear difference equations. It was shown that an autonomous difference equation of arbitrary order and with one or more independent variables can be linearized by a point transformation if and only if it admits a symmetry vector field whose coefficient is the product of two functions, one of the dependent variable and one of the independent variables.[17] Furthermore the symmetry approach provides an effective tool to determine conditions on the parameters at which the nonlinear partial differential–difference or lattice equations possess a sequence of generalized or higher order or Lie Backlund symmetries. If a nonlinear partial differential–difference or lattice equations admits a sequence of generalized symmetries then it is expected to be integrable. Once the generalized symmetries are explicitly known it is quite often possible to find the recursion operator. If the recursion operator is hereditary then the equation will possess infinitely many symmetries. If the operator is hereditary and factorizable then the equation has infinitely many conserved quantities.

In this article we consider two new interesting integrable coupled lattice equations namely, Belov–Chaltikian (BC) lattice equation[18] given by

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$$\frac{du_n}{dt}=u_n(u_{n+1}-u_{n-1})+v_{n-1}-v_n, \tag{1a}$$

$$\frac{dv_n}{dt}=v_n(u_{n+2}-u_{n-1}), \tag{1b}$$

and Blaszak–Marciniak (BM) lattice equation[19] defined by

$$\frac{du_n}{dt}=w_{n+1}-w_{n-1}, \tag{2a}$$

$$\frac{dv_n}{dt}=u_{n-1}w_{n-1}-u_nw_n, \tag{2b}$$

$$\frac{dw_n}{dt}=w_n(v_n-v_{n+1}), \tag{2c}$$

where $u_n=u(n,t)$, $v_n=v(n,t)$, $w_n=w(n,t)$, t is a continuous variable and n is a discrete variable. It is appropriate to mention that the BC lattice equation (1) was first found in the study of lattice analogues of W-algebras[20] while the BM lattice equation (2) was derived as an application of r-matrix formalism to the algebra of shift operators.[21,22] Also both BC and BM lattice equations (1) and (2) have rich mathematical structures such as biHamiltonian structure, Backlund transformation, bilinear form, soliton solution, and nonlinear superposition formula. The purpose of this paper is to derive group theoretical properties of BC and BM lattice equations (1) and (2) and investigate its relation with integrability.

The plan of the paper is as follows: In Sec. II, the Lie point symmetries of Belov–Chaltikian (BC) and Blaszak–Marciniak (BM) lattice equations is derived. Using the symmetries similarity reduction for both BC and BM lattice equations is obtained and show that each of the reduced equation possesses Lax representation and satisfies the singularity confinement criteria (a discrete version of the Painlevé property) indicating their integrability. Two particular solutions of both the reduced equations is given explicitly. In Sec. III, a systematic investigation for nonclassical symmetries of BC and BM lattice equations is carried out. In Sec. IV, a sequence of conserved densities and generalized symmetries of both BC and BM lattice equation are derived explicitly. The existence of a sequence of such symmetries is a predictor for integrability. In Sec. V, we give a brief details of our results.

II. SIMILARITY REDUCTION, LAX REPRESENTATION, AND SINGULARITY CONFINEMENT CRITERIA

A. Belov–Chaltikian lattice equation

Consider a one parameter (ϵ) continuous local Lie group of transformations,

$$n^*=n+\epsilon\xi_1+O(\epsilon^2), \quad t^*=t+\epsilon\xi_2+O(\epsilon^2), \tag{3a}$$

$$u^*_{n^*}=u_n+\epsilon\xi_3+O(\epsilon^2), \quad v^*_{n^*}=v_n+\epsilon\xi_4+O(\epsilon^2), \tag{3b}$$

where $\xi_i=\xi_i(n,t,u_n,v_n)$, $i=1,2,3,4$, are infinitesimals and the associated infinitesimal generator is

$$Y=\xi_1(n,t)\frac{\partial}{\partial n}+\xi_2(n,t)\frac{\partial}{\partial t}+\xi_3(n,t)\frac{\partial}{\partial u_n}+\xi_4(n,t)\frac{\partial}{\partial v_n}, \tag{3c}$$

where we have not indicated the explicit dependence of u_n and v_n in ξ_i's. The reader should realize that although usually the independent variable n in this equation is taken to be integer, here we allow n to be any real number. BC equation (1) is invariant under the transformations (3) if

$$\frac{du^*_{n^*}}{dt^*} = u^*_{n^*}(u^*_{n^*+1} - u^*_{n^*-1}) + v^*_{n^*-1} - v^*_{n^*}, \tag{4a}$$

$$\frac{dv^*_{n^*}}{dt^*} = v^*_{n^*}(u^*_{n^*+2} - u^*_{n^*-1}) \tag{4b}$$

provided u_n and v_n satisfy Eqs. (1a) and (1b). Making use of the expressions for $du^*_{n^*}/dt^*$, $dv^*_{n^*}/dt^*$, $u^*_{n^*+1}$, $u^*_{n^*-1}$, $u^*_{n^*+2}$, and $v^*_{n^*-1}$[10,12] in Eq. (4) we obtain the following invariance equation:

$$\xi_{3t} + (\xi_{3u_n} - \xi_{2t})\frac{du_n}{dt} = (u_{n+1} - u_{n-1})\xi_3 + u_n(\xi_3(n+1) - \xi_3(n-1)) + \xi_4(n-1) - \xi_4(n) \tag{5a}$$

and

$$\xi_{4t} + (\xi_{4v_n} - \xi_{2t})\frac{dv_n}{dt} = v_n(\xi_3(n+2) - \xi_3(n-1)) + (u_{n+2} - u_{n-1})\xi_4(n), \tag{5b}$$

where $\xi_{3t} = \partial\xi_3/\partial t$, $\xi_{3u_n} = \partial\xi_3/\partial u_n$, etc.

Substituting Eqs. (1a) and (1b) into (5a) and (5b) we obtained a overdetermined system of equations and solving we get

$$\xi_1(n,t) = \alpha, \quad \xi_2(n,t) = -\beta t + \gamma, \quad \xi_3(n,t) = \beta u_n, \quad \xi_4(n,t) = 2\beta v_n, \tag{6}$$

where α, β, γ are arbitrary constants and so the infinitesimal generator (3c) takes the following form:

$$Y = \alpha\frac{\partial}{\partial n} + (-\beta t + \gamma)\frac{\partial}{\partial t} + \beta u_n\frac{\partial}{\partial u_n} + 2\beta v_n\frac{\partial}{\partial v_n}. \tag{7}$$

Here the generators Y_1, Y_2, Y_3 become

$$Y_1 = -t\frac{\partial}{\partial t} + u_n\frac{\partial}{\partial u_n} + 2v_n\frac{\partial}{\partial v_n}, \quad Y_2 = \frac{\partial}{\partial t}, \quad Y_3 = \frac{\partial}{\partial n}$$

and the commutator relation satisfies

$$[Y_1, Y_2] = Y_2, \quad [Y_1, Y_3] = 0, \quad [Y_2, Y_3] = 0$$

indicating that the underlying symmetry algebra of (1) is nilpotent.

Next, the similarity variable and the similarity transformation associated with the above set of symmetries $(\xi_1, \xi_2, \xi_3, \xi_4)$, given in (6) can be obtained by solving the characteristic equation

$$\frac{dn}{\xi_1} = \frac{dt}{\xi_2} = \frac{du_n}{\xi_3} = \frac{dv_n}{\xi_4}. \tag{8}$$

The similarity variable η and similarity transformations $v(\eta)$ and $\omega(\eta)$ are

$$\eta = n + \frac{\alpha}{\beta}\log(-\beta t + \gamma), \tag{9a}$$

$$v(\eta) = (-\beta t + \gamma)u_n, \quad \omega(\eta) = (-\beta t + \gamma)^2 v_n, \tag{9b}$$

and so the BC lattice equation (1) reduces into

$$\beta v(\eta) - \alpha \frac{dv}{d\eta} = v(\eta)[v(\eta+1) - v(\eta-1)] + \omega(\eta-1) - \omega(\eta) \tag{10a}$$

and

$$2\beta\omega(\eta) - \alpha \frac{d\omega}{d\eta} = \omega(\eta)[v(\eta+2) - v(\eta-1)]. \tag{10b}$$

It is straightforward to check that the Lax representation for BC lattice equation takes the following form

$$\frac{dQ(n,t)}{dt} = -u_{n-1}Q(n,t) + Q(n-1,t), \tag{11a}$$

$$\lambda Q(n,t) = Q(n+1,t) + u_n Q(n+2,t) + v_n Q(n+3,t), \tag{11b}$$

where λ is a spectral parameter. It is easy to check that the compatibility condition leads to BC lattice equation. After some calculation we find that the reduced equation (10) admits the following Lax representation:

$$\left(-\alpha\frac{d}{d\eta} + \beta\zeta\frac{d}{d\zeta}\right)R(\eta,\zeta) = (\beta\eta - v(\eta-1))R(\eta,\zeta) + R(\eta-1,\zeta), \tag{12a}$$

$$\zeta R(\eta,\zeta) = R(\eta+1,\zeta) + v(\eta)R(\eta+2,\zeta) + \omega(\eta)R(\eta+3,\zeta), \tag{12b}$$

where ζ is a spectral parameter. The compatibility condition of Eqs. (12a) and (12b) gives the reduced equations (10a) and (10b).

It was conjectured that every ordinary differential equation obtained by an exact reduction of nonlinear partial differential equation solvable by inverse scattering transform is of Painlevé type or satisfies the Painlevé property.[23] The above conjecture also holds good for integrable nonlinear partial differential difference equations as well.[10,24] We show below that the reduced equations (10) of BC lattice equation (1) satisfies the singularity confinement criteria[7] which can be viewed as a discrete version of the Painlevé property. Rewriting Eqs. (10a) and (10b) as

$$\omega(\eta) = \omega(\eta-1) + v(\eta)[v(\eta+1) - v(\eta-1) - \beta] + \alpha\frac{dv}{d\eta} \tag{13a}$$

and

$$v(\eta+2) = v(\eta-1) + 2\beta - \frac{c}{\omega}\frac{d\omega}{d\eta}. \tag{13b}$$

From Eqs. (13a) and (13b) it is clear that there exists three distinct singularities:

(i) $\omega(\eta) = 0, \quad v(\eta) \neq 0;$
(ii) $\omega(\eta) = 0, \quad v(\eta) = 0;$
(iii) $\omega(\eta) \neq 0, \quad v(\eta) = 0.$

Let us first consider case (i). For a given value of η_0, $\omega(\eta_0)=0$, $v(\eta_0)\neq 0$, $v(\eta_0+1)\neq 0$, $v(\eta_0-1)\neq 0$, $\omega(\eta_0-1)\neq 0$. In order to derive various iterations of $v(\eta)$ and $\omega(\eta)$ we choose $\omega(\eta)=C_1(\eta)\tau(\eta)$ and expand equations for $\omega(\eta_0+1)$, $\omega(\eta_0+2)$, $v(\eta_0+3)$, $v(\eta_0+4)$ in a Laurent series. After a detailed calculation we find the following:

$$v(\eta_0+1)=finite, \omega(\eta_0+1)=finite+O\left(\frac{1}{\tau}\right),$$

$$v(\eta_0+2)=O\left(\frac{1}{\tau}\right), \quad \omega(\eta_0+2)=finite,$$

$$v(\eta_0+3)=O\left(\frac{1}{\tau}\right), \quad \omega(\eta_0+3)=finite,$$

$$v(\eta_0+4)=finite, \quad \omega(\eta_0+4)=finite.$$

Hence the singularity confinement criteria is satisfied for the case (i). Similar conclusion can also be arrived at for the cases (ii) and (iii). Thus the similarity reduction of BC lattice equation (1) is expected to be integrable.

Moreover equations (10a,b) admit the following two particular solutions for the case $\beta=0$:

(i) Soliton solution

$$v(\eta)=\frac{B^2k}{\alpha(e^{-k}-e^{k})}\frac{[1+e^{k\left(\eta+\frac{(2\delta-1)}{2}+\frac{A}{2B}\right)}][1+e^{k\left(\eta+\frac{(2\delta-1)}{2}-\frac{A}{2B}\right)}]}{[1+e^{k(\eta+\delta)}][1+e^{k(\eta-1+\delta)}]}, \tag{14a}$$

$$\omega(\eta)=\frac{(A^2+B^2-10\alpha^2)k}{3(e^{k}-e^{-k})}\frac{[1+e^{k(\eta+2+\delta)}][1+e^{k(\eta-2+\delta)}]}{[1+e^{k(\eta+1+\delta)}][1+e^{k(\eta-1+\delta)}]}. \tag{14b}$$

(ii) Rational solution

$$v(\eta)=\frac{-B^2\left(2\eta+2\delta-1+\frac{A}{B}\right)\left(2\eta+2\delta-1-\frac{A}{B}\right)}{8\alpha(\eta+\delta)(\eta+\delta-1)}, \tag{15a}$$

$$\omega(\eta)=\frac{(A^2+B^2-10\alpha^2)[(\eta+\delta)^2-4]}{6[(\eta+\delta)^2-1]}, \tag{15b}$$

where $A^2=9\alpha^2+3\beta_1$, $B^2=\alpha^2+3\beta_1$ and k, δ are arbitrary parameters.

B. Blaszak–Marciniak (BM) lattice equation

Consider a one parameter (ϵ) continuous local Lie group of tansformations

$$n^*=n+\epsilon\phi_1+O(\epsilon^2), \quad t^*=t+\epsilon\phi_2+O(\epsilon^2), \tag{16a}$$

$$u_{n^*}^*=u_n+\epsilon\phi_3+O(\epsilon^2), \quad v_{n^*}^*=v_n+\epsilon\phi_4+O(\epsilon^2), \quad w_{n^*}^*=w_n+\epsilon\phi_5+O(\epsilon^2), \tag{16b}$$

where $\phi_i=\phi_i(n,t,u_n,v_n,w_n)$, $i=1,2,3,4,5$ are infinitesimals and the associated infinitesimal generator is

$$Z=\phi_1(n,t)\frac{\partial}{\partial n}+\phi_2(n,t)\frac{\partial}{\partial t}+\phi_3(n,t)\frac{\partial}{\partial u_n}+\phi_4(n,t)\frac{\partial}{\partial v_n}+\phi_5(n,t)\frac{\partial}{\partial w_n}. \tag{17}$$

The BM lattice (2) is invariant under the transformations (16) if

$$\frac{du_{n*}^{*}}{dt^{*}}=w_{n*+1}^{*}-w_{n*-1}^{*}, \tag{18a}$$

$$\frac{dv_{n*}^{*}}{dt^{*}}=u_{n*-1}^{*}w_{n*-1}^{*}-u_{n*}^{*}w_{n*}^{*}, \tag{18b}$$

$$\frac{dw_{n*}^{*}}{dt^{*}}=w_{n*}^{*}(v_{n*}^{*}-v_{n*+1}^{*}), \tag{18c}$$

provided u_n, v_n, w_n satisfy Eqs. (2a)–(2c). Making use of the experssions for du_{n*}^{*}/dt^{*}, dv_{n*}^{*}/dt^{*}, dw_{n*}^{*}/dt^{*}, w_{n*+1}^{*}, w_{n*-1}^{*}, u_{n*-1}^{*}, and v_{n*+1}^{*} [10,12] in Eq. (18) we obtain the following invariance equation:

$$\phi_{3t}+(\phi_{3u_n}-\phi_{2t})\frac{du_n}{dt}=\phi_5(n+1)-\phi_5(n-1), \tag{19a}$$

$$\phi_{4t}+(\phi_{4v_n}-\phi_{2t})\frac{dv_n}{dt}=u_{n-1}\phi_5(n-1)+\phi_3(n-1)w_{n-1}-u_n\phi_5(n)-\phi_3(n)w_n, \tag{19b}$$

and

$$\phi_{5t}+(\phi_{5w_n}-\phi_{2t})\frac{dw_n}{dt}=w_n(\phi_4(n)-\phi_4(n+1))+(v_n-v_{n+1})\phi_5(n), \tag{19c}$$

where $\phi_{3t}=\partial\phi_3/\partial t$, $\phi_{3u_n}=\partial\phi_3/\partial u_n$, etc.

Substituting Eqs. (2a)–(2c) in (19a)–(19c) we obtained a overdetermined system of equations and solving we get

$$\phi_1(n,t)=\alpha_1, \quad \phi_2(n,t)=-\beta_1 t+\gamma_1, \tag{20a}$$

$$\phi_3(n,t)=\frac{\beta_1}{2}u_n, \quad \phi_4(n,t)=\beta_1 v_n, \quad \phi_5(n,t)=\frac{3\beta_1}{2}w_n, \tag{20b}$$

where α_1, β_1, γ_1 are arbitrary constants and so the infinitesimal generator (17) becomes

$$Z=\alpha_1\frac{\partial}{\partial n}+(-\beta_1 t+\gamma_1)\frac{\partial}{\partial t}+\frac{\beta_1}{2}u_n\frac{\partial}{\partial u_n}+\beta_1 v_n\frac{\partial}{\partial v_n}+\frac{3\beta_1}{2}w_n\frac{\partial}{\partial w_n}. \tag{21}$$

Here the generators Z_1, Z_2, Z_3 become

$$Z_1=-t\frac{\partial}{\partial t}+\frac{1}{2}u_n\frac{\partial}{\partial u_n}+v_n\frac{\partial}{\partial v_n}+\frac{3}{2}w_n\frac{\partial}{\partial w_n}, \quad Z_2=\frac{\partial}{\partial t}, \quad Z_3=\frac{\partial}{\partial n}, \tag{22}$$

and the commutator relation satisfies

$$[Z_1,Z_2]=Z_2, \quad [Z_1,Z_3]=0, \quad [Z_2,Z_3]=0,$$

indicating that the underlying symmetry algebra of (2) is nilpotent.

Proceeding as before for the BC lattice equation, we obtain the following similarity variable θ and the similarity transformations $\mu(\theta)$, $v(\theta)$, and $\omega(\theta)$

$$\theta = n + \frac{\alpha_1}{\beta_1}\log(-\beta_1 t + \gamma_1), \tag{23a}$$

$$\mu(\theta) = (-\beta_1 t + \gamma_1)^{1/2} u_n, \quad v(\theta) = (-\beta_1 t + \gamma_1) v_n, \quad \omega(\theta) = (-\beta_1 t + \gamma_1)^{3/2} w_n \tag{23b}$$

and so the BM lattice equation (2) reduces to

$$\frac{\beta_1}{2}\mu(\theta) - \alpha_1 \frac{d\mu}{d\theta} = \omega(\theta+1) - \omega(\theta-1), \tag{24a}$$

$$\beta_1 v(\theta) - \alpha_1 \frac{dv}{d\theta} = \mu(\theta-1)\omega(\theta-1) - \mu(\theta)\omega(\theta), \tag{24b}$$

and

$$\frac{3\beta_1}{2}\omega(\theta) - \alpha_1 \frac{d\omega}{d\theta} = \omega(\theta)(v(\theta) - v(\theta+1)). \tag{24c}$$

The Lax representation for BM lattice equation is

$$\frac{dQ_1(n,t)}{dt} = -\frac{1}{2} v_{n+1} Q_1(n,t) + w^{1/2}(n+1) Q_1(n+1,t), \tag{25a}$$

$$\begin{aligned}(\lambda_1 + v_{n+1}) Q_1(n,t) = {} & w^{1/2}(n) u_n Q_1(n-1,t) + w^{1/2}(n+1) Q_1(n+1,t) \\ & + w^{1/2}(n) w^{1/2}(n-1) Q_1(n-2,t),\end{aligned} \tag{25b}$$

where λ_1 is a spectral parameter. This leads to the following Lax representation for the reduced equation (24):

$$\left(\alpha_1 \frac{d}{d\theta} + \beta_1 \zeta_1 \frac{d}{d\zeta_1}\right) R_1(\theta,\zeta_1) = \frac{\beta_1 \theta}{4} R_1(\theta,\zeta_1) + \frac{1}{2} v(\theta+1) R_1(\theta,\zeta_1) - \omega^{1/2}(\theta+1) R_1(\theta+1,\zeta_1), \tag{26a}$$

$$\begin{aligned}(\zeta_1 + v(\theta+1)) R_1(\theta,\zeta_1) = {} & \omega^{1/2}(\theta)\mu(\theta) R_1(\theta-1,\zeta_1) + \omega^{1/2}(\theta+1) R_1(\theta+1,\zeta_1) \\ & + \omega^{1/2}(\theta)\omega^{1/2}(\theta-1) R_1(\theta-2,\zeta_1),\end{aligned} \tag{26b}$$

where ζ_1 is a spectral parameter. The compatibility condition of Eqs. (26a) and (26b) gives the reduced equation (24).

In order to check the singularity confinement criterion we rewrite the reduced Eqs. (24a)–(24c) into

$$v(\theta+1) = v(\theta) - \frac{3\beta_1}{2} + \frac{\alpha_1}{\omega}\frac{d\omega}{d\theta}, \tag{27a}$$

$$\omega(\theta+1) = \omega(\theta-1) + \frac{\beta_1}{2}\mu(\theta) - \alpha_1 \frac{d\mu}{d\theta}, \tag{27b}$$

$$\mu(\theta+1) = \frac{1}{\omega(\theta+1)}\left[\mu(\theta)\omega(\theta) - \beta_1 v(\theta+1) + \alpha_1 \frac{dv(\theta+1)}{d\theta}\right]. \tag{27c}$$

It is clear from the above equations that there exist seven distinct singularities. We have checked that the singularity confinement criteria is satisfied in all the seven cases. Thus the similarity reduction of BM lattice equation (2) is expected to be integrable.

Equations (24a)–(24c) also admit the following two particular solutions ($\beta_1=0$):

(i) Soliton solution

$$\mu(\theta)=\frac{2\alpha_1^2k_1}{A_2B_1^2(e^{k_1}-e^{-k_1})}\frac{[1+e^{k_1(\theta+\delta_1-B_1)}][1+e^{k_1(\theta+\delta_1+B_1)}]}{[1+e^{k_1(\theta+\delta_1+1)}][1+e^{k_1(\theta+\delta_1-1)}]}, \tag{28a}$$

$$v(\theta)=\frac{2\alpha_1k_1}{(B_2^2-1)(e^{k_1}-e^{-k_1})}\frac{\left[1+e^{k_1\frac{(\theta+2\delta_1-B_2+1)}{2}}\right]\left[1+e^{k_1\frac{(\theta+2\delta_1+B_2+1)}{2}}\right]}{[1+e^{k_1(\theta+\delta_1)}][1+e^{k_1(\theta+\delta_1-1)}]}, \tag{28b}$$

$$\omega(\theta)=\frac{2A_2k_1}{(e^{k_1}-e^{-k_1})}\frac{[1+e^{k_1(\theta+\delta_1+1)}][1+e^{k_1(\theta+\delta_1-1)}]}{[1+e^{k_1(\theta+\delta_1)}][1+e^{k_1(\theta+\delta_1)}]}. \tag{28c}$$

(ii) Rational solution

$$\mu(\theta)=\frac{\alpha_1^2}{A_2B_1^2}\frac{(\theta+\delta_1-B_1)(\theta+\delta_1+B_1)}{(\theta+\delta_1-1)(\theta+\delta_1+1)}, \tag{29a}$$

$$v(\theta)=\frac{\alpha_1(2\theta+2\delta_1-B_2+1)(2\theta+2\delta_1+B_2+1)}{(B_2^2-1)(\theta+\delta_1)(\theta+\delta_1-1)}, \tag{29b}$$

$$\omega(\theta)=\frac{A_2[(\theta+\delta_1)^2-1]}{(\theta+\delta_1)^2}, \tag{29c}$$

where $B_1^2=\alpha_1^3/\alpha_1^3+2A_2^2$, $B_2^2=1+4\alpha_1/A_1$ and k_1, δ_1 are arbitrary parameters.

III. NONCLASSICAL SYMMETRIES

A. Belov–Chaltikian lattice equation (BC)

In this section we investigate whether nonclassical symmetries (also referred to as conditional symmetries) for BC lattice equation (1) exists or not. In order to derive the nonclassical symmetries we consider two conditional constrained equations at first

$$T\frac{du_n}{dt}+X\frac{du_n}{dn}-U=0, \tag{30a}$$

$$T\frac{dv_n}{dt}+X\frac{dv_n}{dn}-V=0, \tag{30b}$$

where T,X,U,V are some undetermined functions of t, n, u_n, and v_n. Now we apply the standard algorithm that provides the symmetry algebra. The vector field has the form

$$S=T\frac{\partial}{\partial t}+X\frac{\partial}{\partial n}+U\frac{\partial}{\partial u_n}+V\frac{\partial}{\partial v_n}. \tag{31}$$

We consider two different cases: $T\neq0$, $X=0$, and $T\neq0$, $X\neq0$

Case 1: $T\neq0,X\neq0$

With no loss of generality we put $T=1$ in Eqs. (30) and (31). Making use of Eq. (1) we write Eqs. (30a) and (30b) as

$$U-X\frac{du_n}{dn}=u_n[u_{n+1}-u_{n-1}]+v_{n-1}-v_n, \tag{32a}$$

$$V-X\frac{dv_n}{dn}=v_n[u_{n+2}-u_{n-1}]. \tag{32b}$$

Proceeding further we obtain the following invariance equation

$$\left(X\frac{\partial U}{\partial t}-U\frac{\partial X}{\partial t}\right)+\left(\frac{\partial X}{\partial t}+X\frac{\partial U}{\partial u_n}\right)[u_n(u_{n+1}-u_{n-1})+v_{n-1}-v_n]$$
$$=X[u_n(U_{n+1}-U_{n-1})+U_n(u_{n+1}-u_{n-1})+V_{n-1}-V_n], \tag{33a}$$

$$\left(X\frac{\partial V}{\partial t}-V\frac{\partial X}{\partial t}\right)+\left(\frac{\partial X}{\partial t}+X\frac{\partial V}{\partial v_n}\right)[v_n(u_{n+2}-u_{n-1})]$$
$$=X[v_n(U_{n+2}-U_{n-1})+V_n(u_{n+2}-u_{n-1})]. \tag{33b}$$

We then obtain an overdetermined system of equations and solving them yields

$$X=\frac{1}{-at+b},\quad U=\frac{au_n}{-at+b},\quad V=\frac{2av_n}{-at+b}, \tag{34}$$

where a,b are arbitrary constants and so the vector field S becomes

$$S=\frac{1}{-at+b}\frac{\partial}{\partial n}+\frac{au_n}{-at+b}\frac{\partial}{\partial u_n}+\frac{2av_n}{-at+b}\frac{\partial}{\partial v_n}+\frac{\partial}{\partial n}.$$

Let us compare the nonclassical symmetries of BC lattice equation with classical ones. We now multiply Eq. (30) and the corresponding vector field (31) by $(-at+b)$ and obtain

$$S_1=\frac{\partial}{\partial n}+(-at+b)\frac{\partial}{\partial t}+au_n\frac{\partial}{\partial u_n}+2av_n\frac{\partial}{\partial v_n}. \tag{35}$$

Case 2: $T\neq 0, X=0$

Here the invariant surface conditions (30a) and (30b) becomes

$$T\frac{du_n}{dt}=U,\quad T\frac{dv_n}{dt}=V. \tag{36}$$

Substituting the above equation (36) in (1) we obtain

$$U=Tu_n(u_{n+1}-u_{n-1})+v_{n-1}-v_n, \tag{37a}$$

$$V=Tv_n(u_{n+2}-u_{n-1}). \tag{37b}$$

Applying classical Lie algorithm to the above equation (37) yields

$$T\frac{\partial U}{\partial t}+U\left(\frac{\partial U}{\partial u_n}-\frac{\partial T}{\partial t}\right)=T[u_n(U_{n+1}-U_{n-1})+U_n(u_{n+1}-u_{n-1})+V_{n-1}-V_n], \tag{38a}$$

$$T\frac{\partial V}{\partial t}+V\left(\frac{\partial V}{\partial v_n}-\frac{\partial T}{\partial t}\right)=T[v_n(U_{n+2}-U_{n-1})+V_n(u_{n+2}-u_{n-1})]. \tag{38b}$$

Solving the above equation (38), we obtain

$$T=-a_1t+b_1,\quad U=a_1u_n,\quad V=2a_1v_n, \tag{39}$$

where a_1,b_1 are arbitrary constants and so the conditional symmetry generator is

$$S_1=(-a_1t+b_1)\frac{\partial}{\partial t}+a_1u_n\frac{\partial}{\partial u_n}+2a_1v_n\frac{\partial}{\partial v_n}. \tag{40}$$

For cases (1) and (2) we conclude that no nonclassical symmetries exist for BC lattice equation (1).

B. Blaszak–Marciniak lattice

We also investigate the nonclassical symmetries for BM lattice by proceeding in a similar manner as for BC lattice. There are two different cases: $\tilde{T}\neq 0,\tilde{X}\neq 0$ and $\tilde{T}\neq 0,\tilde{X}=0$.

Case 1: $\tilde{T}\neq 0,\tilde{X}\neq 0$

Invariant surface condition is

$$\tilde{T}\frac{du_n}{dt}+\tilde{X}\frac{du_n}{dn}-\tilde{U}=0, \tag{41a}$$

$$\tilde{T}\frac{dv_n}{dt}+\tilde{X}\frac{dv_n}{dn}-\tilde{V}=0, \tag{41b}$$

$$\tilde{T}\frac{dw_n}{dt}+\tilde{X}\frac{dw_n}{dn}-\tilde{W}=0. \tag{41c}$$

With no loss of generality we put $\tilde{T}=1$ in Eq. (41). Making use of Eq. (2) we write Eq. (41) as

$$\tilde{U}-\tilde{X}\frac{du_n}{dn}=w_{n+1}-w_{n-1}, \tag{42a}$$

$$\tilde{V}-\tilde{X}\frac{dv_n}{dn}=u_{n-1}w_{n-1}-u_nw_n, \tag{42b}$$

$$\tilde{W}-\tilde{X}\frac{dw_n}{dn}=w_n(v_n-v_{n+1}). \tag{42c}$$

Proceeding further we obtain the following invariance equation:

$$\left[\tilde{X}\frac{\partial\tilde{U}}{\partial t}-\tilde{U}\frac{\partial\tilde{X}}{\partial t}\right]+\left(\frac{\partial\tilde{X}}{\partial t}+\tilde{X}\frac{\partial\tilde{U}}{\partial u_n}\right)(w_{n+1}-w_{n-1})=\tilde{X}[\tilde{W}(n+1)-\tilde{W}(n-1)], \tag{43a}$$

$$\left(\tilde{X}\frac{\partial\tilde{V}}{\partial t}-\tilde{V}\frac{\partial\tilde{X}}{\partial t}\right)+\left(\frac{\partial\tilde{X}}{\partial t}+\tilde{X}\frac{\partial\tilde{V}}{\partial v_n}\right)(u_{n-1}w_{n-1}-u_nw_n)$$
$$=\tilde{X}[\tilde{U}(n-1)w_{n-1}+u_{n-1}\tilde{W}(n-1)-\tilde{U}(n)w_n-u_n\tilde{W}(n)], \tag{43b}$$

$$\left(\tilde{X}\frac{\partial\tilde{W}}{\partial t}-\tilde{W}\frac{\partial\tilde{X}}{\partial t}\right)+\left(\frac{\partial\tilde{X}}{\partial t}+\tilde{X}\frac{\partial\tilde{W}}{\partial w_n}\right)[w_n(v_n-v_{n+1})]=\tilde{X}[\tilde{W}(v_n-v_{n+1})+w_n(\tilde{V}(n)-\tilde{V}(n+1))]. \tag{43c}$$

We then obtain an overdetermined system of equations and solving them yields

$$\tilde{X}=\frac{1}{-a_2t+b_2},\quad \tilde{U}=\frac{a_2u_n}{2(-a_2t+b_2)},\quad \tilde{V}=\frac{a_2v_n}{-a_2t+b_2},\quad \tilde{W}=\frac{3a_2w_n}{2(-a_2t+b_2)}, \tag{44a}$$

where a_2,b_2 are arbitrary constants and so the vector field S_2 becomes

$$S_2=\frac{1}{-a_2t+b_2}\frac{\partial}{\partial n}+\frac{a_2u_n}{2(-a_2t+b_2)}\frac{\partial}{\partial u_n}+\frac{a_2v_n}{-a_2t+b_2}\frac{\partial}{\partial v_n}+\frac{3a_2w_n}{2(-a_2t+b_2)}\frac{\partial}{\partial w_n}\frac{\partial}{\partial t}. \tag{44b}$$

We compare the nonclassical symmetries of BM lattice equation with the classical one (20a) and (20b). Multiplying Eq. (41) by $(-a_2t+b_2)$ we see that the vector field (44b) reduces into

$$S_2=\frac{\partial}{\partial n}+(-a_2t+b_2)\frac{\partial}{\partial t}+\frac{1}{2}a_2u_n\frac{\partial}{\partial u_n}+a_2v_n\frac{\partial}{\partial v_n}+\frac{3}{2}a_2w_n\frac{\partial}{\partial w_n}. \tag{45}$$

Case 2: $\tilde{T}\neq 0,\tilde{X}=0$

Here the invariant surface condition (41) becomes

$$\tilde{T}\frac{du_n}{dt}-\tilde{U}=0,\quad \tilde{T}\frac{dv_n}{dt}-\tilde{V}=0,\quad \tilde{T}\frac{dw_n}{dt}-\tilde{W}=0. \tag{46}$$

As a result Eq. (2) becomes

$$\tilde{U}=\tilde{T}[w_{n+1}-w_{n-1}], \tag{47a}$$

$$\tilde{V}=\tilde{T}[u_{n-1}w_{n-1}-u_nw_n], \tag{47b}$$

$$\tilde{W}=\tilde{T}[w_n(v_n-v_{n+1})]. \tag{47c}$$

Applying classical Lie algorithm we obtain the following invariant equation:

$$\tilde{T}\frac{\partial\tilde{U}}{\partial t}+\tilde{U}\left(\frac{\partial\tilde{U}}{\partial u_n}-\frac{\partial\tilde{T}}{\partial t}\right)=\tilde{T}[\tilde{W}(n+1)-\tilde{W}(n-1)], \tag{48a}$$

$$\tilde{T}\frac{\partial\tilde{V}}{\partial t}+\tilde{V}\left(\frac{\partial\tilde{V}}{\partial v_n}-\frac{\partial\tilde{T}}{\partial t}\right)=\tilde{T}[u(n-1)\tilde{W}(n-1)+\tilde{U}(n-1)w(n-1)-\tilde{U}(n)w_n-u_n\tilde{W}(n)], \tag{48b}$$

$$\tilde{T}\frac{\partial\tilde{W}}{\partial t}+\tilde{W}\left(\frac{\partial\tilde{W}}{\partial w_n}-\frac{\partial\tilde{T}}{\partial t}\right)=\tilde{T}[\tilde{W}(v_n-v_{n+1})+w_n(\tilde{V}(n)-\tilde{V}(n+1))]. \tag{48c}$$

Solving the above equation (48) gives

$$\tilde{T}=-a_3t+b_3,\quad \tilde{U}=\frac{a_3u_n}{2},\quad \tilde{V}=a_3v_n,\quad \tilde{W}=\frac{3a_3w_n}{2}, \tag{49}$$

where a_3 and b_3 are arbitrary constants and so the conditional symmetry generator is

$$S_2=(-a_3t+b_3)\frac{\partial}{\partial t}+\frac{a_3u_n}{2}\frac{\partial}{\partial u_n}+a_3v_n\frac{\partial}{\partial v_n}+\frac{3}{2}a_3w_n\frac{\partial}{\partial w_n}. \tag{50}$$

Thus it is clear from the cases (1) and (2) that there exists no nonclassical symmetries for BM lattice equation (2) as well.

IV. CONSERVED DENSITIES AND GENERALIZED SYMMETRIES

A. Belov–Chaltikian (BC) lattice equation

It is known that there exists a deep connection between the generalized symmetries and integrability of nonlinear evolution equations.[5] More precisely, if a nonlinear partial differential difference or lattice equations admits a sequence of generalized symmetries, then it is expected to be integrable. The generalized or higher order or Lie Backlund symmetries were computed for nonlinear partial differential equations by different authors in different context[25] and demonstrated

its relation with integrability. For nonlinear partial differential–difference or lattice equations attempt was made to derive polynomial generalized symmetries by different groups.[5,26–28] However, it is not clear how to compute nonpolynomial generalized symmetries. Yet the nonexistence of polynomial generalized symmetries or conserved quantities does not preclude integrability. We wish to note that the evaluation of generalized symmetries for nonlinear differential difference equations is a tedious and cumbersome work. In fact, there exists several software to compute polynomial generalized symmetries and conserved densities. For example, using a package in Mathematica, Goktas, and Hereman[5] have demonstrated that under what conditions on the parameters given nonlinear evolution equations including lattice equations admit a sequence of generalized symmetries and conserved densities.[5,28,29] In this paper we derive, the generalized symmetries and conserved densities for BC and BM lattice equations (1) and (2) without using any software package.

Let us first derive the conserved densities for the BC lattice equation (1) which is invariant under the scaling symmetry

$$(t,u_n,v_n)\rightarrow(\lambda t,\lambda^{-1}u_n,\lambda^{-2}v_n), \tag{51}$$

where λ is an arbitrary parameter. Thus u_n and v_n corresponds to one and two derivatives with respect to t, respectively. In otherwords

$$u_n\sim\frac{d}{dt},\quad v_n\sim\frac{d^2}{dt^2}.$$

In order to derive the conserved densities, Eqs. (1a) and (1b) should have the same rank. To start with we consider the form of conserved density with rank 2. We remind that if ρ_n is a conserved density for a nonlinear differential–difference, difference, or lattice equation then

$$\frac{d\rho_n}{dt}=J_n-J_{n+1}, \tag{52}$$

where J_n is the flux.

Forming all monomials of u_n,v_n with rank 2 yields the list $\Phi=\{u_n,u_n^2,v_n\}$. Introducing the necessary t derivatives leads to $\{u_n^2,v_n,u_nu_{n+1},u_nu_{n-1},v_{n-1}\}$. Using $u_nu_{n+1}\equiv u_nu_{n-1}$, $v_n\equiv v_{n-1}$, we obtain $I=\{u_n^2,v_n,u_nu_{n+1}\}$. Then the conserved density can be obtained by considering a linear combination of the terms in I

$$\rho_n=c_1u_n^2+c_2v_n+c_3u_nu_{n+1}, \tag{53}$$

where c_1,c_2,c_3 are constants. Differentiating equation (53) with respect to t and making use of Eqs. (1a) and (1b) we get

$$\begin{aligned}\frac{d\rho_n}{dt}=&(2c_1-c_3)u_n^2u_{n+1}+(2c_1-c_3)u_{n+1}v_n+(c_3-2c_1)u_nv_n-(c_2+c_3)u_nv_{n+1}+(c_2\\&+c_3)u_{n+2}v_n+(c_3-2c_1)u_nu_{n+1}^2+[J_n-J_{n+1}],\end{aligned} \tag{54}$$

with flux

$$J_n=2c_1u_nv_{n-1}-c_3u_nu_{n+1}u_{n-1}+c_3u_{n+1}v_{n-1}-c_2v_nu_{n-1}-2c_1u_n^2u_{n-1}. \tag{55}$$

By definition (52), the monomials outside the square brackets in (54) must vanish. This yields $2c_1-c_3=0$,$c_2+c_3=0$. We see that there are two equations for three unknowns. Choosing $c_1=1/2$, we obtain $c_2=-1$, $c_3=1$ and so the conserved density with rank 2, $\rho_n^{(2)}$ and the associated flux becomes

$$\rho_n^{(2)}=\tfrac{1}{2}u_n^2-v_n+u_nu_{n+1},$$

$$J_n^{(2)}=u_nv_{n-1}-u_nu_{n+1}u_{n-1}+u_{n+1}v_{n-1}+v_nu_{n-1}-u_n^2u_{n-1}.$$

Next we compute the conserved density of rank 3. As before forming all monomials of u_n and v_n with rank 3 yields the list $\phi=\{u_n,u_n^2,u_n^3,v_n,u_nv_n\}$. Introducing the necessary t derivatives and rescaling we obtain

$$I=\{u_n^3,u_nv_n,u_n^2u_{n+1},u_{n+1}^2u_n,u_{n+1}v_n,u_nu_{n+1}u_{n+2},u_nv_{n+1},u_{n+2}v_n,u_{n+1}v_{n-1},v_nu_{n-1}\}.$$

Then the conserved density can take the form

$$\rho_n=c_4u_n^3+c_5u_nv_n+c_6u_n^2u_{n+1}+c_7u_nu_{n+1}^2+c_8u_{n+1}v_n+c_9u_nu_{n+1}u_{n+2}+c_{10}u_nv_{n+1}+c_{11}u_{n+2}v_n+c_{12}u_{n+1}v_{n-1}+c_{13}v_nu_{n-1}. \tag{56}$$

Differentiating equation (56) with respect to t, making use of Eqs. (1a) and (1b) and by definition (52), we obtain $c_4=1/3,c_5=-1,c_6=1,c_7=1,c_8=-1,c_9=1,c_{10}=-1,c_{11}=-1,c_{12}=c_{13}=0$, and so the conserved density with rank 3, $\rho_n^{(3)}$ and the associated flux is

$$\rho_n^{(3)}=\tfrac{1}{3}u_n^3+(u_nu_{n+1}-v_n)(u_n+u_{n+1}+u_{n+2})-u_nv_{n+1},$$

$$\begin{aligned}J_n^{(3)}=&u_{n-1}(2u_n+u_{n+1}+u_{n+2})(v_n-u_nu_{n+1})+u_nv_{n-1}(u_n+2u_{n+1})-v_{n-1}(v_n+v_{n+1})\\&+u_{n+1}v_{n-1}(u_{n+2}+u_{n+1})+u_nu_{n-1}(v_{n+1}-u_n^2).\end{aligned}$$

Since the derivation of the conserved density of rank 4 involves more number of terms we give below only the result

$$\begin{aligned}\rho_n^{(4)}=&\tfrac{1}{4}u_n^4+u_n^3u_{n+1}+\tfrac{3}{2}u_n^2u_{n+1}^2+u_nu_{n+1}^2(u_{n+1}+u_{n+2})+u_nu_{n+1}u_{n+2}(u_n+u_{n+1}+u_{n+2}+u_{n+3})\\&+\tfrac{1}{2}v_n^2+v_nv_{n-1}-u_nv_n(u_n+u_{n+1}+u_{n-1}+u_{n+2})-u_nv_{n-1}(u_n+u_{n+1}+u_{n-2})\\&-v_nu_{n-1}(u_n+u_{n-2}+u_{n+2})-u_nu_{n+1}(v_n+v_{n-1})-u_n^2(v_{n+1}+v_{n-2})\\&+v_n(v_{n+2}-u_{n+2}u_{n+3}),\end{aligned}$$

$$\begin{aligned}J_n^{(4)}=&u_n^3v_{n-1}-u_n^4u_{n-1}-u_n^3v_{n-2}-2v_{n-1}^2u_n-v_{n-1}^2u_{n+1}-v_{n-1}^2u_{n-2}-u_nu_{n-1}u_{n+1}u_{n+2}u_{n+3}\\&-u_{n+1}^3u_nu_{n-1}-2u_n^2u_{n+1}v_{n-2}-3u_n^2u_{n+1}^2u_{n-1}+2u_n^2u_{n-1}v_{n-1}+u_{n-1}u_{n-2}u_{n-3}v_n\\&+u_nu_{n-1}u_{n-2}v_{n+1}+u_{n+1}u_nu_{n-1}v_{n+2}+u_nu_{n-1}u_{n-2}v_n+u_nu_{n-1}u_{n+1}v_{n+1}\\&+u_{n+1}u_{n-1}u_{n-2}v_n+u_nu_{n+2}u_{n-1}v_{n+1}+2u_nu_{n+1}u_{n-1}v_n-u_nu_{n-1}u_{n+2}v_n\\&-2u_nu_{n-1}u_{n+2}u_{n+1}^2-2u_n^2u_{n+2}u_{n+1}u_{n-1}-u_{n+2}^2u_nu_{n+1}u_{n-1}+2u_nu_{n+1}u_{n-1}v_{n-1}\\&+u_{n+1}u_{n+2}u_{n+3}v_{n-1}+u_{n+1}u_{n+2}u_{n-1}v_n+u_{n-2}^2u_{n-1}v_n-v_nv_{n-2}u_{n-2}-v_{n+1}v_{n-1}u_{n-1}\\&+u_{n-1}^2u_nv_{n+1}+u_n^2u_{n-1}v_n-v_{n-1}v_{n-3}u_n-v_nv_{n-2}u_{n+1}-v_{n+1}v_{n-1}u_{n+2}+u_{n+2}v_nv_{n-1}\\&-v_nv_{n-3}u_{n-1}-v_{n+1}v_{n-2}u_n-v_{n+2}v_{n-1}u_{n+1}+u_{n+2}^2u_{n+1}v_{n-1}-v_nv_{n-2}u_{n+2}\\&-v_{n+1}v_{n-1}u_{n+3}+u_{n-1}^2u_{n+2}v_n+u_n^2u_{n-3}v_{n-2}+u_{n+1}^2u_{n-2}v_{n-1}+u_nu_{n-2}^2v_{n-1}\\&+u_{n+1}u_{n-1}^2v_n+2u_n^2u_{n-1}v_{n-2}+u_{n+1}^2u_nv_{n-1}-u_nv_{n-1}v_{n-2}+v_nv_{n-1}u_{n-2}+v_nv_{n-2}u_{n-1}\\&+v_{n-1}v_{n+1}u_n+4u_{n-1}^2u_nv_n-3v_nv_{n-1}u_{n-1}+u_n^2u_{n-2}v_{n-1}+v_nu_{n+1}^2u_{n-1}+2u_n^2u_{n+1}v_{n-1}\end{aligned}$$

$$+2u_n^2u_{n-1}v_{n-1}+4u_n^2u_{n-1}v_{n+1}.$$

Proceeding in a similar manner one can compute conserved densities ρ_n with rank $\geqslant 5$.

Next we derive the generalized symmetries for the BC lattice equation (1) which is invariant under the dilation symmetry

$$(t,u_n,v_n)\rightarrow(\lambda^{-1}t,\lambda u_n,\lambda^2 v_n),$$

where λ is an arbitrary parameter. Thus u_n and v_n corresponds to one and two derivatives with respect to t, respectively. We first derive generalized symmetries of BC lattice equation with ranks (2) and (3) denoted by $G_1^{(1)}$ and $G_1^{(2)}$. Forming all the monomials in u_n and v_n of rank 2 and 3 gives the following:

$L_1=\{u_n,u_n^2,v_n\}, L_2=\{u_n,u_n^2,u_n^3,v_n,u_nv_n\}$.

We then introduce the necessary t derivatives in each monomial of L_1. Making use of Eqs. (1a) and (1b) we obtain

$$\frac{d^0}{dt^0}(u_n^2)=u_n^2,\quad \frac{d^0}{dt^0}(v_n)=v_n,\quad \frac{d}{dt}(u_n)=u_n(u_{n+1}-u_{n-1})+v_{n-1}-v_n,$$

and a set:

$$R_1=\{u_n^2,v_n,u_nu_{n+1},u_nu_{n-1},v_{n-1}\}.$$

Similarly, based on the monomials in L_2, we get

$$\begin{aligned}R_2=\{&u_n^3,u_nv_n,v_nu_{n+2},v_nu_{n-1},u_n^2u_{n+1},u_n^2u_{n-1},u_nv_{n-1},u_nu_{n+1}u_{n+2},\\&u_nv_{n+1},u_nu_{n-1}u_{n-2},u_nv_{n-2},u_nu_{n+1}^2,u_nu_{n+1}u_{n-1},u_{n+1}v_{n-1},\\&u_{n+1}v_n,u_nu_{n-1}^2,u_{n-1}v_{n-1},v_{n-1}u_{n-2}\}.\end{aligned}$$

Then the generalized symmetry can be obtained by considering linear combination of the terms in R_1 and R_2

$$G_1^{(1)}=c_1u_n^2+c_2v_n+c_3u_nu_{n+1}+c_4u_nu_{n-1}+c_5v_{n-1}, \tag{57a}$$

$$\begin{aligned}G_1^{(2)}=&c_6u_n^3+c_7u_nv_n+c_8v_nu_{n+2}+c_9v_nu_{n-1}+c_{10}u_n^2u_{n+1}+c_{11}u_n^2u_{n-1}+c_{12}u_nv_{n-1}\\&+c_{13}u_nu_{n+1}u_{n+2}+c_{14}u_nv_{n+1}+c_{15}u_nu_{n-1}u_{n-2}+c_{16}u_nv_{n-2}+c_{17}u_nu_{n+1}^2\\&+c_{18}u_nu_{n+1}u_{n-1}+c_{19}u_{n+1}v_{n-1}+c_{20}u_{n+1}v_n+c_{21}u_nu_{n-1}^2+c_{22}u_{n-1}v_{n-1}+c_{23}v_{n-1}u_{n-2},\end{aligned} \tag{57b}$$

where c_i, $i=1,2,\ldots,23$ are arbitrary constants.

To determine the coefficients c_i, $i=1,2,\ldots,23$ we introduce a lattice equation

$$\frac{du}{d\tau}=G_1^{(1)},\quad \frac{dv}{d\tau}=G_2^{(1)}. \tag{58}$$

Now by the compatibility condition of (1) and (58) we obtain

$$D_tG_1^{(1)}=D_\tau F_1,\quad D_tG_2^{(1)}=D_\tau F_2, \tag{59}$$

where $D_t=d/dt$, F_1, and F_2 are the right-hand side terms of Eqs. (1a) and (1b). We solve the above equation (59) and eliminate $\dot{u}_{n+1}$, $\dot{u}_{n-1}$, $\dot{v}_{n+1}$, $\dot{v}_{n-1}$, etc. then using Eq. (1) the nonzero coefficients are

$$c_2=-c_3=c_4=-c_5=c_9=-c_8,$$

we choose $c_8=1$ the symmetry is

$$G_1^{(1)}=u_n(u_{n+1}-u_{n-1})+v_{n-1}-v_n,$$
$$G_2^{(1)}=v_n(u_{n+2}-u_{n-1}).$$

Proceeding in a similar fashion described earlier we computed the generalized symmetries with ranks (3) and (4)

$$\begin{aligned}
G_2^{(1)}=&c_1u_n^3+c_2u_nv_n+c_3u_{n+2}v_n+c_4u_{n-1}v_n+c_5u_n^2u_{n+1}+c_6u_n^2u_{n-1}+c_7u_nv_{n-1}\\
&+c_8u_nu_{n+1}u_{n+2}+c_9u_nv_{n+1}+c_{10}u_nu_{n-1}u_{n-2}+c_{11}u_nv_{n-2}+c_{12}u_nu_{n+1}^2+c_{13}u_nu_{n+1}u_{n-1}\\
&+c_{14}u_{n+1}v_{n-1}+c_{15}u_{n+1}v_n+c_{16}u_nu_{n-1}^2+c_{17}u_{n-1}v_{n-1}+c_{18}v_{n-1}u_{n-2},\\
G_2^{(2)}=&c_{19}u_n^4+c_{20}v_n^2+c_{21}u_n^2v_n+c_{22}u_n^3u_{n+1}+c_{23}u_n^3u_{n-1}+c_{24}u_n^2v_{n-1}+c_{25}u_nu_{n+2}v_n\\
&+c_{26}u_nu_{n-1}v_n+c_{27}u_nu_{n+1}v_n+c_{28}v_nv_{n-1}+c_{29}u_n^2u_{n+1}^2+c_{30}u_n^2u_{n-1}^2+c_{31}u_n^2u_{n+1}u_{n-1}\\
&+c_{32}u_nu_{n+1}v_{n-1}+c_{33}u_nu_{n-1}v_{n-1}+c_{34}u_n^2u_{n+1}u_{n+2}+c_{35}u_n^2v_{n+1}+c_{36}u_n^2u_{n-1}u_{n-2}\\
&+c_{37}u_n^2v_{n-2}+c_{38}v_{n-1}^2+c_{39}u_nu_{n-2}v_{n-1}+c_{40}u_{n+2}^2v_n+c_{41}u_{n-1}^2v_n+c_{42}u_{n+2}u_{n-1}v_n\\
&+c_{43}u_{n+2}u_{n+3}v_n+c_{44}u_{n+1}u_{n+2}v_n+c_{45}v_nv_{n+1}+c_{46}v_nv_{n+2}+c_{47}u_{n-1}u_{n-2}v_n\\
&+c_{48}v_nv_{n-2}+c_{49}u_nu_{n+1}^3+c_{50}u_nu_{n+1}^2u_{n-1}+c_{51}u_{n+1}^2v_{n-1}+c_{52}u_{n+1}^2v_n+c_{53}u_nu_{n-1}^2u_{n+1}\\
&+c_{54}u_{n+1}u_{n-1}v_{n-1}+c_{55}u_{n+1}u_{n-1}v_n+c_{56}u_nu_{n-1}^3+c_{57}u_{n-1}^2v_{n-1}+c_{58}u_nu_{n+1}^2u_{n+2}\\
&+c_{59}u_nu_{n+1}v_{n+1}+c_{60}u_nu_{n+1}u_{n-1}u_{n-2}+c_{61}u_nu_{n+1}v_{n-2}+c_{62}u_nu_{n+1}u_{n-1}u_{n+2}\\
&+c_{63}u_nu_{n-1}v_{n+1}+c_{64}u_nu_{n-1}^2u_{n-2}+c_{65}u_nu_{n-1}v_{n-2}+c_{66}u_{n+1}u_{n-2}v_{n-1}\\
&+c_{67}u_{n-1}u_{n-2}v_{n-1}+c_{68}u_nu_{n+1}u_{n+2}u_{n+3}+c_{69}u_nu_{n+1}v_{n+2}+c_{70}u_{n+1}u_{n+2}v_{n-1}\\
&+c_{71}u_nu_{n+2}^2u_{n+1}+c_{72}u_nu_{n+2}v_{n+1}+c_{73}u_nu_{n+3}v_{n+1}+c_{74}v_{n+1}v_{n-1}\\
&+c_{75}u_nu_{n-1}u_{n-2}u_{n-3}+c_{76}u_nu_{n-1}v_{n-3}+c_{77}u_nu_{n-1}v_{n-2}+c_{78}u_nu_{n-2}^2u_{n-1}\\
&+c_{79}u_nu_{n-2}v_{n-2}+c_{80}v_{n-1}v_{n-2}+c_{81}u_nu_{n-3}v_{n-2}+c_{82}u_{n-2}^2v_{n-1}+c_{83}u_{n-2}u_{n-3}v_{n-1}\\
&+c_{84}v_{n-1}v_{n-3}.
\end{aligned}$$

As before replacing $G_1^{(1)}$ by $G_2^{(1)}$ and $G_2^{(1)}$ by $G_2^{(2)}$ in the compatibility condition (59) we find the nonzero coefficients,

$$\begin{aligned}
-c_2=&-c_3=c_5=-c_6=c_7=c_8=-c_9=-c_{10}=c_{11}=c_{12}=-c_{15}=-c_{16}=c_{17}=c_{18}=-c_{26}\\
&=c_{28}=c_{40}=-c_{41}=c_{44}=-c_{45}=-c_{46}=-c_{47}=c_{48}=c_{43}.
\end{aligned}$$

By choosing $c_{43}=-1$, we obtain the symmetry as

$$\begin{aligned}
G_2^{(1)}=&(v_n-u_nu_{n+1})(u_n+u_{n+1}+u_{n+2})+(u_nu_{n-1}-v_{n-1})(u_n+u_{n-1}+u_{n-2})\\
&-u_n(v_{n-2}-v_{n+1}),\\
G_2^{(2)}=&u_{n-1}v_n(u_n+u_{n-1}+u_{n-2})-u_{n+2}v_n(u_{n+1}+u_{n+2}+u_{n+3})\\
&+v_n(v_{n+1}+v_{n+2}-v_{n-1}-v_{n-2}).
\end{aligned}$$

It is straightforward to compute the generalized symmetries of higher order and, therefore, we refrain from presenting details of the symmetries.

B. Blaszak–Marciniak (BM) lattice equation

Following the procedure adopted for BC lattice equation we find that BM lattice equation also admits a sequence of conserved densities and generalized symmetries. The results are

$$\rho_n^{(1)}=v_n, J_n^{(1)}=u_{n-1}w_{n-1},$$

$$\rho_n^{(2)}=\tfrac{1}{2}v_n^2+u_nw_n, J_n^{(2)}=u_{n-1}w_{n-1}v_n-w_nw_{n-1},$$

$$\rho_n^{(3)}=\tfrac{1}{3}v_n^3+u_nv_nw_n+u_nw_nv_{n+1}-w_nw_{n-1},$$

$$J_n^{(3)}=v_n^2u_{n-1}w_{n-1}-w_nw_{n-1}v_{n-1}-w_nw_{n-1}v_n+u_nu_{n-1}w_nw_{n-1},$$

$$\rho_n^{(4)}=\tfrac{1}{4}v_n^4+\tfrac{1}{2}u_n^2w_n^2+u_nu_{n-1}w_nw_{n-1}-w_nw_{n+1}v_n-w_nw_{n+1}v_{n+1}-w_nw_{n-1}v_{n+1}+u_nw_nv_nv_{n+1}$$
$$+u_nw_nv_{n+1}^2+u_nv_n^2w_n,$$

$$J_n^{(4)}=2u_nu_{n-1}w_nw_{n-1}v_n-w_nw_{n-1}v_n^2+v_n^3u_{n-1}w_{n-1}-w_{n-1}^2u_{n-1}w_n-u_nw_nw_{n-1}w_{n-2}$$
$$+u_nu_{n-1}w_nw_{n-1}v_{n-1}-v_{n-1}v_{n+1}w_nw_{n-1}-w_nw_{n-1}v_nv_{n+1}-w_n^2w_{n-1}u_n,$$

$$G_3^{(1)}=w_{n+1}-w_{n-1},\quad G_3^{(2)}=u_{n-1}w_{n-1}-u_nw_n,\quad G_3^{(3)}=w_n(v_n-v_{n+1}),$$

and

$$G_4^{(1)}=w_{n-1}(v_n+v_{n-1})-w_{n+1}(v_{n+1}+v_{n+2}),$$

$$G_4^{(2)}=u_nw_n(v_n+v_{n+1})-u_{n-1}w_{n-1}(v_n+v_{n-1})+w_{n-1}w_{n-2}-w_nw_{n+1},$$

$$G_4^{(3)}=w_n(v_{n+1}^2-v_n^2)+w_n(w_{n+1}u_{n+1}-w_{n-1}u_{n-1}).$$

V. CONCLUSION

Using classical Lie symmetry approach we derive Lie symmetries and similarity reduction of BC and BM lattice equations. We have also shown that the reduced equation possesses different integrability properties such as Lax representation, singularity confinement criterion. Moreover, the reduced equations admit two interesting particular solutions. Also we have checked that both BC and BM lattice equation do not admit nonclassical symmetries. Furthermore, we have shown for both BC and BM lattice equations that there exists a sequence of conserved densities and generalized symmetries a characteristic of integrable systems governed by nonlinear partial differential, differential–difference equations. It is of interest to investigate whether any other integrability properties such as master symmetries, hereditary operators, etc. of BC and BM lattice equations exists or not which is under investigation.

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Invariant integration on classical and quantum Lie supergroups

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Invariant integrals on Hopf superalgebras, in particular, the classical and quantum Lie supergroups, are studied. The uniqueness (up to scalar multiples) of a left integral is proved, and a $\mathbb{Z}_2$-graded version of Maschke's theorem is discussed. A construction of left integrals is developed for classical and quantum Lie supergroups. Applied to several classes of examples the construction yields the left integrals in explicit form. © *2001 American Institute of Physics.*
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I. INTRODUCTION

This article studies invariant integrals on Hopf superalgebras. We shall focus on the Hopf superalgebras of functions on classical Lie supergroups and their quantum counterparts, developing aspects of the general theory of integrals on them, and also establishing an explicit construction of such integrals.

An important feature of classical and quantum Lie superalgebras is that their finite-dimensional representations are not completely reducible. This imposes severe restrictions on the possible integrals on the corresponding classical and quantum Lie supergroups. We shall extensively investigate this fact, arriving at a result which may be regarded as a $\mathbb{Z}_2$-graded version of Maschke's theorem in an infinite-dimensional setting.

Recall that if the dual of a given finite-dimensional Hopf algebra is semisimple, then a generalization of Maschke's theorem (see Refs. 1 and 2) applies, and the invariant integral on the Hopf algebra can be obtained by considering a Peter–Weyl type basis of the Hopf algebra. Such a construction of integrals fails badly in the supersymmetric setting [except for $\mathrm{OSP}(1|2n)$ and $\mathrm{OSP}_q(1|2n)$]. Here we develop an explicit construction of integrals, which can be implemented on classical Lie supergroups and also on type I quantum supergroups. The construction can also be adapted to produce integrals on quantum groups at roots of unity.

The study of this article is motivated by the great importance of the Haar measure in the theory of locally compact Lie groups. The first place we know of where integrals in the sense of Hopf algebra theory have shown up is Hochschild's proof of Tannaka's duality theorem for compact groups.[3] Later on they played an important role in the structure theory of finite-dimensional Hopf algebras (for example, see Refs. 4–7).

With the appearance of quantum groups and quantum algebras, it became obvious that integrals have to play an important role there, too. In fact, the quantum Haar functional is a basic tool in the C^*-algebra approach to quantum groups,[8] and it can also be used to introduce topologies on Hopf algebras which originally are defined by purely algebraic means.[9] Correspondingly, there are various attempts to define integration on quantum groups, quantum spaces and their braided generalizations (see Ref. 10 and the references therein).

In principle, the braided case includes Hopf superalgebras as a special example, but it seems worthwhile to investigate the super case separately. Needless to say, there is a huge literature dealing with the integration on supermanifolds and supergroups, but a theory of integrals on Hopf

superalgebras seems to be missing. This will be the topic of the present work. We hope that integrals will also prove to be useful in the further investigation of the structure and representations of quantum supergroups, and that our results will shed some new light on the integration over classical, i.e., undeformed Lie supergroups.

At present, we know of only one related work.[11] In that reference, integrals on quantum supergroups of the special linear type are constructed by means of the R-matrix formalism. However, even for the $\mathrm{SL}_q(m|n)$ quantum supergroups the techniques used and the results derived in that paper are totally different from those to be presented here [even though, because of the uniqueness theorem to be proved in Sec. II, the integrals on $\mathrm{SL}_q(m|n)$ constructed here and in Ref. 11 must be proportional].

The organization of the article is as follows. In Sec. II we develop some general theory of integrals on Hopf superalgebras and establish results generalizing Maschke's theorem. In Sec. III we study classical Lie supergroups. A general construction of integrals is developed, and applied to the type I Lie supergroups, and also the type II Lie supergroups $\mathrm{OSP}(1|2n)$ and $\mathrm{OSP}(3|2)$. In Sec. IV we extend the results to the quantum setting, obtaining a method for constructing integrals on quantum supergroups. As examples, the type I quantum supergroups are studied in detail. Section V contains a brief discussion of our results. Finally, in the Appendix we have collected some information on the finite dual of $U(\mathfrak{gl}(1))$.

We close this introduction by recalling some conventions related to $\mathbb{Z}_2$-graded algebraic structures. The two elements of $\mathbb{Z}_2$ are denoted by $\overline{0}$ and $\overline{1}$. Unless stated otherwise, all gradations considered in this work will be $\mathbb{Z}_2$-gradations. For any superspace, i.e., $\mathbb{Z}_2$-graded vector space $V=V_{\overline{0}}\oplus V_{\overline{1}}$, we define the gradation index $[\,]$: $V_{\overline{0}}\cup V_{\overline{1}}\to\mathbb{Z}_2$ by $[x]=\alpha$ if $x\in V_\alpha$, where $\alpha\in\mathbb{Z}_2$. All algebraic notions and constructions are to be understood in the super sense, i.e., they are assumed to be consistent with the $\mathbb{Z}_2$-gradations and to include the appropriate sign factors.

II. INTEGRALS ON HOPF SUPERALGEBRAS

Let $\mathcal{A}$ be a Hopf superalgebra with comultiplication Δ, counit ε, and antipode S. A left integral $\int^l$ on $\mathcal{A}$ is an element of $\mathcal{A}^*$, such that

$$\left(\mathrm{id}_{\mathcal{A}}\otimes\int^l\right)\Delta=\mathbb{1}_{\mathcal{A}}\int^l. \tag{1}$$

Equivalently, this means that

$$a^*\cdot\int^l=a^*(\mathbb{1}_{\mathcal{A}})\int^l,\quad \forall a^*\in\mathcal{A}^*, \tag{2}$$

where the dot denotes the multiplication in $\mathcal{A}^*$ deduced from Δ. A right integral $\int^r\in\mathcal{A}^*$ on $\mathcal{A}$ is defined by a similar requirement

$$\left(\int^r\otimes\ \mathrm{id}_{\mathcal{A}}\right)\Delta=\mathbb{1}_{\mathcal{A}}\int^r. \tag{3}$$

Let $\mathcal{A}^{\mathrm{aop,cop}}$ be the Hopf superalgebra opposite to $\mathcal{A}$ both regarded as an algebra and a coalgebra. Then a linear form $\int\in\mathcal{A}^*$ is a left/right integral on $\mathcal{A}$ if and only if it is a right/left integral on $\mathcal{A}^{\mathrm{aop,cop}}$. In particular, if the antipode S of $\mathcal{A}$ (and hence of $\mathcal{A}^{\mathrm{aop,cop}}$) is invertible, then $S^{\pm1}$ are isomorphisms of $\mathcal{A}$ onto $\mathcal{A}^{\mathrm{aop,cop}}$, and hence $\int$ is a left integral on $\mathcal{A}$ if and only if $\int S^{\pm1}$ are right integrals on $\mathcal{A}$. Thus we only need to consider left integrals (or right integrals).

We have the following result:

Theorem 1: *The dimension of the space of left integrals on $\mathcal{A}$ is not greater than 1. In particular, any integral on $\mathcal{A}$ is even or odd.*

Proof: The proof is carried out by reducing the problem to the classical nongraded case. In principle, this can be viewed as an application of Majid's bosonization,[12] but for the present simple case the technique has been known for quite some time.

For notational convenience (and for reasons that will become obvious at the end of this proof) we define a map

$$\tau:\mathbb{Z}_2\times\mathbb{Z}_2\to\mathbb{C}$$

by

$$\tau(\alpha,\beta)=(-1)^{\alpha\beta},\quad \forall\,\alpha,\beta\in\mathbb{Z}_2.$$

Let $\mathbb{C}\mathbb{Z}_2$ be the group Hopf algebra of $\mathbb{Z}_2$. The canonical basis elements will be denoted by g_α, $\alpha\in\mathbb{Z}_2$. In particular, we have

$$g_\alpha g_\beta=g_{\alpha+\beta},\quad \forall\,\alpha,\beta\in\mathbb{Z}_2.$$

Then

$$\overline{\mathcal{A}}=\mathcal{A}\otimes\mathbb{C}\mathbb{Z}_2$$

is made into a usual Hopf algebra by means of the following definitions (where $a,b\in\mathcal{A}$ and $\alpha,\beta\in\mathbb{Z}_2$):
product:

$$(a\otimes g_\alpha)(b\otimes g_\beta)=\tau(\alpha,[b])\,ab\otimes g_{\alpha+\beta},$$

coproduct (in Sweedler's notation):

$$\overline{\Delta}(a\otimes g_\alpha)=\sum_{(a)}(a_{(1)}\otimes g_{[a_{(2)}]+\alpha})\otimes(a_{(2)}\otimes g_\alpha),$$

counit:

$$\overline{\varepsilon}(a\otimes g_\alpha)=\varepsilon(a),$$

antipode:

$$\overline{S}(a\otimes g_\alpha)=\tau([a],\alpha+[a])\,S(a)\otimes g_{-\alpha-[a]}.$$

Now let s be a left integral on $\mathcal{A}$, i.e., a linear form $s\in\mathcal{A}^*$ such that

$$(\mathrm{id}_{\mathcal{A}}\otimes s)\Delta=\mathbb{1}_{\mathcal{A}}\,s,$$

and let us assume that s is homogeneous of degree σ. Recall that $\otimes$ denotes the tensor product in the *graded* sense. Nevertheless, it is easy to see that the equation above is equivalent to

$$\sum_{(a)}a_{(1)}s(a_{(2)})=s(a)\,\mathbb{1}_{\mathcal{A}},\quad \forall\,a\in\mathcal{A},$$

i.e., it takes the same form as in the nongraded case.

Define the linear form t_σ on $\mathbb{C}\mathbb{Z}_2$ by

$$t_\sigma(g_\alpha)=\delta_{\sigma,\,\alpha},\quad \forall\,\alpha\in\mathbb{Z}_2.$$

Then

$$\overline{s} = s \otimes t_\sigma$$

(nongraded tensor product) is a left integral on $\overline{\mathcal{A}}$. We prove this by showing that $\overline{s}$ satisfies the equation analogous to that given above for s: For all $a \in \mathcal{A}$ and $\alpha \in \mathbb{Z}_2$, we have

$$\begin{aligned}
(\mathrm{id}_{\overline{\mathcal{A}}} \otimes \overline{s})(\overline{\Delta}(a \otimes g_\alpha)) &= (\mathrm{id}_{\overline{\mathcal{A}}} \otimes \overline{s}) \sum_{(a)} (a_{(1)} \otimes g_{[a_{(2)}]+\alpha}) \otimes (a_{(2)} \otimes g_\alpha) \\
&= \sum_{(a)} (a_{(1)} \otimes g_{[a_{(2)}]+\alpha})\, s(a_{(2)})\, t_\sigma(g_\alpha) \\
&= \sum_{(a)} (a_{(1)} \otimes g_{-\sigma+\alpha})\, s(a_{(2)})\, t_\sigma(g_\alpha) \\
&= \left(\sum_{(a)} a_{(1)} s(a_{(2)}) \right) \otimes g_0\, t_\sigma(g_\alpha) \\
&= s(a) t_\sigma(g_\alpha)\, 1\!\!1_{\mathcal{A}} \otimes g_0 \\
&= \overline{s}(a \otimes g_\alpha)\, 1\!\!1_{\mathcal{A}} \otimes g_0,
\end{aligned}$$

as required.

Now let us suppose that $s \neq 0$ and that s' is a second nonzero integral on $\mathcal{A}$ which is homogeneous of degree σ'. Then $\overline{s} = s \otimes t_\sigma$ and $\overline{s'} = s' \otimes t_{\sigma'}$ are nonzero integrals on $\overline{\mathcal{A}}$. According to Sullivan's theorem on the uniqueness of integrals on ordinary (nongraded) Hopf algebras (see Refs. 13 and 2) these integrals must be proportional. This implies that $\sigma = \sigma'$ (otherwise, t_σ and $t_{\sigma'}$ would be linearly independent) and hence that s and s' are proportional.

Finally, let $s \in \mathcal{A}^*$ be an arbitrary linear form on $\mathcal{A}$, and let $s = \Sigma_{\sigma \in \mathbb{Z}_2} s_\sigma$, with $s_\sigma \in (\mathcal{A}^*)_\sigma$, be its decomposition into homogeneous components. Obviously, s is a left integral on $\mathcal{A}$ if and only if all of the s_σ are. Applying the foregoing result to the s_σ, we conclude that, for a left integral s, at most one of the s_σ can be different from zero, i.e., that s is homogeneous. This proves the theorem.

The reader will notice that the same proof applies to arbitrary color Hopf algebras (and this was the other reason to introduce the map τ).

The uniqueness result of the theorem enables us to investigate how a left integral behaves under ''right translations.'' Thus, let $\int$ be a nontrivial left integral on $\mathcal{A}$. We know that the linear form $\int$ is homogeneous, let γ be its degree. We consider the linear map

$$g: \mathcal{A} \to \mathcal{A}, \quad g = \left(\int \otimes \mathrm{id} \right) \Delta.$$

Obviously, it is homogeneous of degree γ and not equal to zero (otherwise, $\varepsilon\, g = \int$ would be equal to zero). Using the coassociativity of the coproduct, it is easy to check that

$$(g \otimes \mathrm{id})\Delta = \Delta\, g, \tag{4}$$

$$(\mathrm{id} \otimes g)\Delta = j\, g, \tag{5}$$

where

$$j: \mathcal{A} \to \mathcal{A} \otimes \mathcal{A}, \quad j(a) = 1\!\!1_{\mathcal{A}} \otimes a$$

is the right canonical injection of $\mathcal{A}$ into $\mathcal{A} \otimes \mathcal{A}$.

Now let $a^* \in \mathcal{A}^*$ be an arbitrary homogeneous linear form on $\mathcal{A}$. Equation (5) implies that $a^*\, g$ is a left integral on $\mathcal{A}$ and hence proportional to $\int$. In particular, $a^*\, g$ vanishes on the kernel

of $\int$. Since this is true for all homogeneous elements $a^* \in \mathcal{A}^*$, it follows that g itself vanishes on the kernel of $\int$. Consequently, there exists a unique element $a_0 \in \mathcal{A}$ such that

$$g(a) = \left\langle \int , a \right\rangle a_0, \quad \forall a \in \mathcal{A},$$

and a_0 is even. Equation (4) now means that

$$\Delta(a_0) = a_0 \otimes a_0 .$$

Since a_0 is nonzero (because g is nonzero), we see that a_0 is a grouplike element of $\mathcal{A}$. Thus we have proved the following proposition.

Proposition 1: Let $\int$ be a nontrivial left integral on a Hopf superalgebra $\mathcal{A}$. Then there exists a unique even grouplike element $a_0 \in \mathcal{A}$ such that

$$\left(\int \otimes \mathrm{id} \right) \Delta = a_0 \int .$$

In particular, $\int$ is also a right integral if and only if $a_0 = \mathbb{1}_{\mathcal{A}}$.

Let V be a finite-dimensional $\mathbb{Z}_2$-graded right $\mathcal{A}$-comodule, and let

$$\omega : V \to V \otimes \mathcal{A}$$

be its structure map (which, according to our general conventions, is supposed to be even). The antipode of $\mathcal{A}$ enables one to introduce a right $\mathcal{A}$-comodule structure on the dual space V^* of V, with the structure map

$$\overline{\omega} : V^* \to V^* \otimes \mathcal{A}$$

uniquely defined by

$$\langle v^*, w \rangle \mathbb{1}_{\mathcal{A}} = (\langle , \rangle \otimes M)(\mathrm{id}_{V^*} \otimes T \otimes \mathrm{id}_{\mathcal{A}}) \overline{\omega}(v^*) \otimes \omega(w), \quad \forall v^* \in V^*, w \in V,$$

where T is the flipping map, M denotes the multiplication in $\mathcal{A}$ and $\langle , \rangle$ is the dual space pairing. It follows that $\mathrm{End}(V) = V \otimes V^*$ has a natural right $\mathcal{A}$-comodule structure

$$\delta : \mathrm{End}(V) \to \mathrm{End}(V) \otimes \mathcal{A}.$$

For later use we note that a map $g \in \mathrm{End}(V)$ is a comodule endomorphism of V if and only if it is even and coinvariant, i.e., it satisfies

$$\delta(g) = g \otimes \mathbb{1}_{\mathcal{A}} .$$

If $\int$ is a left integral on $\mathcal{A}$, we define the linear map

$$\Phi = \left(\mathrm{id} \otimes \int \right) \delta : \mathrm{End}(V) \to \mathrm{End}(V).$$

Consider $\Phi(m) \in \mathrm{End}(V)$ for any $m \in \mathrm{End}(V)$. Left invariance of $\int$ immediately leads to

$$\delta(\Phi(m)) = \Phi(m) \otimes \mathbb{1}_{\mathcal{A}};$$

that is, we have the following.

Lemma 1: $\mathrm{Im}\,\Phi$ *is contained in the subspace of coinvariant elements of* $\mathrm{End}(V)$.

Now we consider the case when V contains a sub-comodule V_1. Let $P \in \mathrm{End}(V)$ be a projection onto V_1, i.e., $\mathrm{Im}\,P = V_1$ and $P^2 = P$. It can be easily shown that $\Phi(P)$ satisfies

$$\Phi(P)V\subset V_1 \quad \text{and} \quad \Phi(P)v_1=v_1\int 1_{\mathcal{A}}, \quad \forall v_1\in V_1.$$

Suppose now that $\int 1_{\mathcal{A}}\neq 0$. This implies that $\int$ is even. Thus $\Phi(P)$ is even as well, and hence it is a comodule endomorphism of V. It follows that $\mathrm{Ker}\,\Phi(P)$ is a comodule complement of V_1 in V. Since this holds for any finite-dimensional right $\mathcal{A}$-comodule V and any of its subcomodules, we conclude that all finite-dimensional right $\mathcal{A}$-comodules are completely reducible. Using the basic fact that all finitely generated comodules are finite-dimensional, it follows by means of standard arguments (known, for example, from the general theory of semisimple modules over rings) that all (not necessarily finite-dimensional) right $\mathcal{A}$-comodules are completely reducible.

Conversely, let $\mathcal{A}$ be a Hopf superalgebra such that all right $\mathcal{A}$-comodules are completely reducible. In particular, $\mathcal{A}$ regarded as a right $\mathcal{A}$-comodule with structure map Δ is completely reducible. Let $\mathcal{A}_0$ be a comodule complement of $\mathbb{C}1_{\mathcal{A}}$ in $\mathcal{A}$. Then any linear form $\int^r$ on $\mathcal{A}$ with kernel $\mathcal{A}_0$ is a right(!) integral on $\mathcal{A}$ such that $\int^r 1_{\mathcal{A}}\neq 0$. Applying the foregoing to $\mathcal{A}^{\mathrm{aop,cop}}$ and $\int^r$ (which is a left integral on $\mathcal{A}^{\mathrm{aop,cop}}$) we conclude that all left $\mathcal{A}$-comodules are completely reducible and that $\mathcal{A}$ also has a left integral $\int^l$ such that $\int^l 1_{\mathcal{A}}\neq 0$. It should be noted that according to Larson[6] analogous results hold for Hopf algebras, comodules and integrals living in an arbitrary tensor category.

Actually, much more can be said. Let $\{V(\lambda)|\lambda\in\Lambda\}$ be a complete representative set of all finite-dimensional right $\mathcal{A}$-comodules, where Λ is some index set. Among these, there is a one-dimensional comodule, $V(0)$, say, such that under the coaction, $v\mapsto v\otimes 1_{\mathcal{A}}$. We call $V(0)$ the trivial $\mathcal{A}$-comodule. For each $V(\lambda)$, we choose a basis $\{v_a^{(\lambda)}|a=1,2,\ldots,\dim V(\lambda)\}$. Then under the coaction of $\mathcal{A}$, we have

$$\omega(v_a^{(\lambda)})=\sum_b v_b^{(\lambda)}\otimes t_{ba}^{(\lambda)},$$

and the $t_{ab}^{(\lambda)}$ form a Peter-Weyl type of basis for $\mathcal{A}$. If $\int$ denotes the linear form on $\mathcal{A}$ defined by

$$\int 1_{\mathcal{A}}=1, \quad \int t_{ab}^{(\lambda)}=0, \quad \forall\lambda\neq 0,$$

then $\int$ is both a left and right integral on $\mathcal{A}$ and, obviously, it is even.

Summarizing part of our results, we have proved the following generalization of the well-known Maschke's theorem to the case of Hopf superalgebras (see Refs. 1, 6, and 2).

Proposition 2: The Hopf superalgebra $\mathcal{A}$ admits a left integral $\int$ with $\int 1_{\mathcal{A}}\neq 0$ if and only if all right $\mathcal{A}$-comodules are completely reducible.

In the present work we are mainly interested in the case where $\mathcal{A}$ is a sub-Hopf-superalgebra of the finite dual $\mathcal{U}^\circ$ of a Hopf superalgebra $\mathcal{U}$. The comultiplication, counit, and antipode of $\mathcal{U}$ will also be denoted by Δ, ε, and S, respectively. In this case, if V is a right $\mathcal{A}$-comodule, then V also has a natural left $\mathcal{U}$-module structure defined by

$$x\,v=(-1)^{[x][v]}(\omega(v))(x), \quad \forall x\in\mathcal{U}, v\in V.$$

We denote by $\mathcal{U}-\mathrm{Mod}_r$ the collection of all the left $\mathcal{U}$-modules obtained from finite-dimensional right $\mathcal{A}$-comodules, which forms a monoidal category. The above proposition is equivalent to the following statement: The category $\mathcal{U}-\mathrm{Mod}_r$ is semisimple if and only if $\mathcal{A}$ admits a left integral which does not vanish on the identity.

Let us close this section by the following simple remark. As above, let $\mathcal{A}$ be a sub-Hopf-superalgebra of $\mathcal{U}^\circ$. The even grouplike elements of $\mathcal{U}^\circ$ are exactly the characters of $\mathcal{U}$, i.e., the superalgebra homomorphisms of $\mathcal{U}$ into $\mathbb{C}$. By convention, $\mathcal{A}$ always contains the unit element of $\mathcal{U}^\circ$, i.e., the counit $\varepsilon_{\mathcal{U}}$ of $\mathcal{U}$. This is the so-called trivial character of $\mathcal{U}$. Now Proposition 1 implies the following lemma.

Lemma 2: Suppose that $\mathcal{A}$ does not contain any non-trivial character of $\mathcal{U}$. Then every left integral on $\mathcal{A}$ is also a right integral.

III. INTEGRALS ON CLASSICAL SUPERGROUPS

Let $\mathfrak{g}=\mathfrak{g}_{\bar{0}}\oplus\mathfrak{g}_{\bar{1}}$ be a finite-dimensional Lie superalgebra,[14,15] where $\mathfrak{g}_{\bar{0}}$ and $\mathfrak{g}_{\bar{1}}$ are the even and odd subspaces respectively. We take $\mathcal{U}$ to be the enveloping algebra $U(\mathfrak{g})$ of $\mathfrak{g}$. $U(\mathfrak{g})$ contains the enveloping algebra $U(\mathfrak{g}_{\bar{0}})$ of the Lie subalgebra $\mathfrak{g}_{\bar{0}}$ as a subalgebra. We denote $U(\mathfrak{g}_{\bar{0}})$ by $\mathcal{U}_e$, and let

$$\mathcal{I}: \mathcal{U}_e \to \mathcal{U}$$

be the embedding, which is a Hopf superalgebra map. It is well-known that the dual $\mathcal{I}^*$ of $\mathcal{I}$ induces a Hopf superalgebra map

$$\mathcal{P}: \ \mathcal{U}^\circ \to \mathcal{U}_e^\circ,$$

which is given by

$$\langle \mathcal{P}(a), u\rangle = \langle a\,, \mathcal{I}(u)\rangle, \quad \forall a \in \mathcal{U}^\circ, \quad u \in \mathcal{U}_e\,.$$

In the present work, a Lie supergroup will be defined in terms of its Hopf superalgebra of functions, i.e., we proceed as in the usual definition of quantum groups[16] or quantum supergroups[17] (for a related treatment of supergroups, see Refs. 18 and 19). More precisely, if $\mathfrak{g}$ is a Lie superalgebra, the superalgebra of functions on a Lie supergroup associated to $\mathfrak{g}$ will be a sub-Hopf-superalgebra $\mathcal{A}$ of $\mathcal{U}^\circ = U(\mathfrak{g})^\circ$, subject to the condition that $\mathcal{A}$ be dense in $U(\mathfrak{g})^*$. Actually, in our discussion of integrals, this latter property will not be used.

Thus, let $\mathcal{A}$ be a sub-Hopf-superalgebra of $\mathcal{U}^\circ$. We set

$$\mathcal{P}(\mathcal{A}) = \mathcal{A}_e\,,$$

which is a Hopf subalgebra of $\mathcal{U}_e^\circ$. Then there exist the following natural Hopf superalgebra maps (which are injective if $\mathcal{A}$ is dense in $\mathcal{U}^*$ and, consequently, $\mathcal{A}_e$ is dense in $\mathcal{U}_e^*$):

$$\nu: U(\mathfrak{g}) \to \mathcal{A}^\circ,$$

$$x \mapsto \nu(x), \ \ \langle \nu(x), a\rangle = (-1)^{[x][a]}\langle a, x\rangle, \quad \forall a \in \mathcal{A}; \tag{6}$$

$$\nu_e : \mathcal{U}_e \to \mathcal{A}_e^\circ,$$

$$u \mapsto \nu_e(u) = \tilde{u}\,, \ \ \langle \tilde{u}, a_0\rangle = \langle a_0\,, u\rangle, \quad \forall a_0 \in \mathcal{A}_e\,;$$

$$\hat{\mathcal{I}} = \nu\mathcal{I}: \mathcal{U}_e \to \mathcal{A}^\circ,$$

$$u \mapsto \hat{u}\,, \ \ \langle \hat{u}, a\rangle = \langle \tilde{u}, \mathcal{P}(a)\rangle = \langle \mathcal{P}(a), u\rangle = \langle a, \mathcal{I}(u)\rangle, \quad \forall a \in \mathcal{A}. \tag{7}$$

Let

$$\int_0 : \mathcal{A}_e \to \mathbb{C}$$

be a left integral on $\mathcal{A}_e$ with $\int_0 \mathbb{1}_{\mathcal{A}_e} = 1$. The existence of $\int_0$ depends on properties of $\mathfrak{g}_{\bar{0}}$ and $\mathcal{A}_e$. In the case when $\mathfrak{g}_{\bar{0}}$ is semisimple or reductive as a Lie algebra, such an $\int_0$ is known to exist and is right invariant as well. (However, see the Appendix about the reductive case.)

Lemma 3: The linear form $\int_0 \mathcal{P}: \mathcal{A} \to \mathbb{C}$ is left invariant with respect to $\mathcal{U}_e$ in the sense that

$$\hat{\mathcal{I}}(u)\cdot\left(\int_0\mathcal{P}\right)=\varepsilon(u)\int_0\mathcal{P},\quad \forall u\in\mathcal{U}_e.$$

Proof: Lemma 3 can be confirmed by a direct calculation. For any $u\in\mathcal{U}_e$ and $a\in\mathcal{A}$, we have

$$\begin{aligned}\left\langle \hat{u}\cdot\left(\int_0\mathcal{P}\right),a\right\rangle&=\sum_{(a)}\langle\hat{u},a_{(1)}\rangle\int_0\mathcal{P}(a_{(2)})\\&=\sum_{(a)}\langle\tilde{u},\mathcal{P}(a_{(1)})\rangle\int_0\mathcal{P}(a_{(2)})\\&=\left\langle\tilde{u}\otimes\int_0,\Delta\mathcal{P}(a)\right\rangle\\&=\left\langle\tilde{u}\cdot\int_0,\mathcal{P}(a)\right\rangle=\varepsilon(u)\int_0\mathcal{P}(a).\end{aligned}$$

Let $J=\mathcal{U}\mathfrak{g}_0^-$. By using the Poincaré–Birkhoff–Witt theorem for Lie superalgebras,[15] one immediately sees the following.

Lemma 4: The subspace J is a left ideal of $\mathcal{U}$ with finite codimension.

Consequently, the quotient space $\mathcal{U}/J$ is a left $\mathcal{U}$-module in the standard fashion:

$$x(y+J)=xy+J,\quad \forall x\in\mathcal{U},\ \ y+J\in\mathcal{U}/J.$$

Note that this module is isomorphic to the $\mathcal{U}$-module induced from the trivial $\mathcal{U}_e$-module. According to the usual definition, an element $z+J\in\mathcal{U}/J$, with $z\in\mathcal{U}$, is said to be invariant (under the action of $\mathcal{U}$) if

$$x(z+J)=\varepsilon(x)z+J,\quad \forall x\in\mathcal{U}.$$

Let $z+J$ be any invariant of this type, and let $\nu(z)$ be the image of z in $\mathcal{A}^\circ$ under the natural Hopf superalgebra map (6). Then we have the following theorem.

Theorem 2: *The linear form $\int=\nu(z)\cdot\int_0\mathcal{P}$ is a left integral on $\mathcal{A}$ and does not depend on the choice of the representative for $z+J$. If $z\notin J$ and if the matrix elements of the $\mathcal{U}$-module $\mathcal{U}/J$ belong to $\mathcal{A}$, the integral $\int$ is not equal to zero.*

Remark: The definition of $\int$ involves implicitly the comultiplication of $\mathcal{A}$. For any $a\in\mathcal{A}$,

$$\int a=\left\langle\nu(z)\otimes\int_0\mathcal{P},\ \ \Delta(a)\right\rangle.$$

Proof of Theorem 2: It follows from Lemma 3 that for any $X_0\in\mathfrak{g}_0^-$, $\nu(X_0)\cdot\int_0\mathcal{P}=0$. As ν is an algebra homomorphism, $\nu(y)\cdot\int_0\mathcal{P}=0$ for all $y\in J$. This proves the second part of the theorem. Now the invariance property of $z+J$ leads to

$$\nu(x)\cdot\int=\varepsilon(x)\int,\quad \forall x\in\mathcal{U}.$$

This implies Eq. (1). [Indeed, since $\mathcal{A}$ is contained in $\mathcal{U}^*$, it is sufficient to check Eq. (2) for all $a^*=\nu(x),\ x\in\mathcal{U}$.]

To prove the last part of the theorem, we choose a homogeneous basis $(v_i)_{1\leqslant i\leqslant r}$ of $\mathcal{U}/J$ such that $v_1=1_{\mathcal{U}}+J$. Let π be the representation of $\mathcal{U}$ in $\mathcal{U}/J$, and let $\pi_{i,j}$ be the matrix elements of π with respect to the basis (v_i), i.e.,

$$\pi(x)v_j=\sum_{i=1}^{r}\pi_{i,j}(x)v_i \quad \text{if } x\in\mathcal{U},\ 1\leqslant j\leqslant r.$$

Since v_1 is $\mathcal{U}_e$-invariant, we have

$$\pi_{i,1}(x)=\varepsilon_{\mathcal{U}_e}(x)\,\delta_{i,1} \quad \text{if } x\in\mathcal{U}_e,\ 1\leqslant i\leqslant r.$$

This implies that

$$\int\pi_{i,1}=(-1)^{[v_i]}\pi_{i,1}(z), \quad 1\leqslant i\leqslant r$$

(recall that we are assuming that $\int_0\mathbb{1}_{\mathcal{A}_e}=1$). Since $z\notin J$ and since

$$z+J=\pi(z)v_1=\sum_{i=1}^{r}\pi_{i,1}(z)v_i,$$

at least one of the matrix elements $\pi_{i,1}(z)$ must be different from zero. This proves the theorem.

We notice that

$$\int\mathbb{1}_{\mathcal{A}}=\varepsilon(z)\int_0\mathbb{1}_{\mathcal{A}_e}.$$

Taking for granted that $\int_0\mathbb{1}_{\mathcal{A}_e}$ is different from zero, we see that $\int\mathbb{1}_{\mathcal{A}}\neq 0$ if and only if $\varepsilon(z)\neq 0$.

Remark: Suppose that the Lie algebra $\mathfrak{g}_0^-$ is reductive, and that the adjoint representation of the center of $\mathfrak{g}_0^-$ in $\mathfrak{g}_1^-$ is diagonalizable. Then the subspace of $\mathcal{U}$-invariant elements of $\mathcal{U}/J$ is at most one-dimensional. This follows at once from Theorems 1 and 2, applied to a suitable sub-Hopf-superalgebra $\mathcal{A}$ of $\mathcal{U}^\circ$ (see the Appendix).

Let us now consider examples.

Example 1: The Berezin integral

Consider the purely odd Lie superalgebra $\mathfrak{g}=\mathfrak{g}_1^-$ with the basis $\{\xi_i,\ i=1,2,\ldots,n\}$ and with the super bracket

$$[\xi_i,\xi_j]=0, \quad \forall i,j.$$

Obviously, $\mathcal{U}=U(\mathfrak{g})$ is the Grassmann algebra on the n generators ξ_i, and $\mathcal{U}_e=\mathbb{C}\mathbb{1}_{\mathcal{U}}$. It is well-known that $\mathcal{U}$ has the basis

$$\Xi_{j_1\cdots j_l}=\xi_{j_1}\cdots\xi_{j_l}, \quad 1\leqslant j_1<\cdots<j_l\leqslant n,$$

where the $l=0$ element is understood to be the unity. The Hopf structure of $\mathcal{U}$ is the standard one for enveloping algebras of Lie superalgebras.

Introduce a basis $\{\Theta_{i_1\cdots i_k},\ 1\leqslant i_1<\cdots<i_k\leqslant n,\ 0\leqslant k\leqslant n\}$ for $\mathcal{U}^*$ (the $k=0$ case corresponds to the unit element) such that

$$\langle\Theta_{i_1\cdots i_k},\Xi_{j_1\cdots j_l}\rangle=(-1)^{(1/2)\,k(k-1)}\delta_{kl}\,\delta_{i_1j_1}\cdots\delta_{i_kj_k},$$

and set

$$\theta_i=\Theta_i, \quad i=1,2,\ldots,n.$$

The cocommutativity of $\mathcal{U}$ implies that

$$\theta_i\theta_j+\theta_j\theta_i=0, \quad \forall i,j.$$

It is also easy to show that

$$\Theta_{i_1\cdots i_k}=\theta_{i_1}\cdots\theta_{i_k},\quad i_1<\cdots<i_k.$$

As a Hopf superalgebra, $\mathcal{U}^*$ has the unique comultiplication such that

$$\Delta(\theta_i)=\theta_i\otimes\mathbb{1}+\mathbb{1}\otimes\theta_i,$$

the counit is fixed by

$$\varepsilon(\theta_i)=0,$$

and the antipode is specified by

$$S(\theta_i)=-\theta_i.$$

Since $(\mathcal{U}^*)^*\cong\mathcal{U}$ in this case, we make the identification. It is obvious that $\int_0\mathcal{P}=\mathbb{1}_{\mathcal{U}}$. Moreover, the $\mathcal{U}$-invariant elements of $\mathcal{U}$ are the scalar multiples of $\Xi_{1\,2\,\cdots\,n}$. Thus upon choosing an appropriate normalization we obtain the unique integral

$$\int=(-1)^{(1/2)\,n(n-1)}\xi_1\xi_2\cdots\xi_n,$$

which yields the standard Berezin integral on the Grassmanian algebra $\mathcal{U}^*$:

$$\int\theta_{i_1}\theta_{i_2}\cdots\theta_{i_k}=0,\quad \text{if } k<n,$$

$$\int\theta_1\theta_2\cdots\theta_n=1.$$

To explain the left (and right) invariance of $\int$ in more familiar terms, note that if $P(\theta)$ is any polynomial in the θ_i's, then

$$\Delta P(\theta)=P(\theta\otimes\mathbb{1}+\mathbb{1}\otimes\theta).$$

Left invariance of the integral means

$$\left(\mathrm{id}\otimes\int\right)\Delta(P(\theta))=\int P(\theta).$$

One may write $\mathbb{1}\otimes\theta_i$ as θ_i, and denote $\theta_i\otimes\mathbb{1}$ by λ_i, which is regarded as an independent Grassmann number. The above equation states that

$$\int_\theta P(\theta+\lambda)=\int P(\theta),$$

where the subscript θ on the left hand side indicates the fact that the ''integration'' is carried out over the θ's. The last equation is nothing but the translational invariance of the Berezin integral.

Example 2: The Lie supergroup $\mathrm{SL}(m|n)$

Let $\mathfrak{g}$ denote the Lie superalgebra $\mathfrak{sl}(m|n)$, which we shall regard as a subalgebra of the general linear Lie superalgebra $\mathfrak{gl}(m|n)$. Let $\{E_{ab}\,|\,a,b=1,2,\ldots,m+n\}$ be the standard homogeneous basis of $\mathfrak{gl}(m|n)$, which satisfies the commmutation relations

$$[E_{ab},E_{cd}]=\delta_{bc}E_{ad}-(-1)^{[E_{ab}][E_{cd}]}\delta_{da}E_{cb},$$

where $[\cdot,\cdot]$ should be understood as the graded brackets, namely, it is symmetric when both arguments are odd, and antisymmetric otherwise.

The standard basis for $\mathfrak{g}$ then is given by

$$E_{ab}, \quad a\neq b; \quad h_a=E_{aa}-(-1)^{\delta_{am}}E_{a+1,\,a+1}, \quad a<m+n.$$

The maximal even subalgebra of $\mathfrak{g}$ is $\mathfrak{g}_{\bar{0}}=\mathfrak{sl}(m)\oplus\mathfrak{sl}(n)\oplus\mathfrak{gl}(1)$. Let $\mathfrak{g}_{\bar{1}+}$ be the odd subalgebra spanned by $E_{i\mu}$, $i\leqslant m$, $\mu>m$, and $\mathfrak{g}_{\bar{1}-}$ be that spanned by $E_{\mu i}$. Then $\mathfrak{g}$ is the direct sum $\mathfrak{g}=\mathfrak{g}_{\bar{1}-}\oplus\mathfrak{g}_{\bar{0}}\oplus\mathfrak{g}_{\bar{1}+}$ (as vector spaces). Under the Lie superbracket,

$$\begin{gathered}[\mathfrak{g}_{\bar{1}+},\mathfrak{g}_{\bar{1}+}]=\{0\}, \quad [\mathfrak{g}_{\bar{1}-},\mathfrak{g}_{\bar{1}-}]=\{0\},\\ [\mathfrak{g}_{\bar{0}},\mathfrak{g}_{\bar{1}\pm}]\subset\mathfrak{g}_{\bar{1}\pm}, \quad [\mathfrak{g}_{\bar{1}+},\mathfrak{g}_{\bar{1}-}]\subset\mathfrak{g}_{\bar{0}}.\end{gathered} \tag{8}$$

Next, we observe that $U(\mathfrak{g}_{\bar{1}+})$ and $U(\mathfrak{g}_{\bar{1}-})$ are both isomorphic to the Grassmann algebra on mn generators. The subspaces of the highest Grassmann degree in $U(\mathfrak{g}_{\bar{1}+})$ and $U(\mathfrak{g}_{\bar{1}-})$ are both one-dimensional. We choose the following bases for them, respectively,

$$\mathbb{E}=\mathbb{E}_m\,\mathbb{E}_{m-1}\cdots\mathbb{E}_1, \quad \mathbb{F}=\mathbb{F}_1\,\mathbb{F}_2\cdots\mathbb{F}_m,$$

where

$$\mathbb{E}_i=E_{i,m+1}\,E_{i,m+2}\cdots E_{i,m+n},$$

$$\mathbb{F}_i=E_{m+n,i}\,E_{m+n-1,i}\cdots E_{m+1,i}.$$

Then we have

$$[X,\mathbb{E}]=[X,\mathbb{F}]=0, \quad \forall X\in\mathfrak{g}_{\bar{0}},$$

$$\xi_+\mathbb{E}=0, \quad \forall\xi_+\in\mathfrak{g}_{\bar{1}+},$$

$$\xi_-\mathbb{F}=0, \quad \forall\xi_-\in\mathfrak{g}_{\bar{1}-},$$

$$\xi_-\mathbb{E}-(-1)^{mn}\mathbb{E}\,\xi_-\in U(\mathfrak{g})\mathfrak{g}_{\bar{0}}, \quad \forall\xi_-\in\mathfrak{g}_{\bar{1}-}.$$

Defining

$$\Gamma=\mathbb{E}\,\mathbb{F},$$

it follows that

$$X\Gamma\in U(\mathfrak{g})\mathfrak{g}_{\bar{0}}, \quad \forall X\in\mathfrak{g}.$$

Let t be the defining representation of $\mathfrak{sl}(m|n)$, with

$$t(E_{ab})=e_{ab}, \quad a\neq b,$$

$$t(h_a)=e_{aa}-(-1)^{\delta_{am}}e_{a+1,\,a+1},$$

where the e_{ab}'s are the matrix units, and let t_{ab}, $a,b=1,2,\ldots,m+n$, be the elements of $\mathcal{U}^\circ = U(\mathfrak{g})^\circ$ defined by

$$(t_{ab}(x))_{a,\,b=1}^{m+n} = t(x), \quad \forall x \in U(\mathfrak{g}).$$

Moreover, let $\overline{t}$ be the dual representation of t, and let us similarly introduce the matrix elements $\overline{t}_{ab} \in U(\mathfrak{g})^\circ$ of $\overline{t}$. We note that

$$\sum_c \overline{t}_{ca} t_{cb} (-1)^{([a]+[c])([b]+\overline{1})} = \delta_{ab}.$$

The standard comultiplication on $U(\mathfrak{g})$ is super cocommutative. Therefore the finite dual $U(\mathfrak{g})^\circ$ is a super commutative Hopf superalgebra. The matrix elements t_{ab} and $\overline{t}_{ab}$ of the vector representation and the dual vector representation generate a sub-Hopf-superalgebra $\mathcal{A}$ of $U(\mathfrak{g})^\circ$, with the comultiplication

$$\Delta(t_{ab}) = \sum_c t_{ac} \otimes t_{cb} (-1)^{([a]+[c])([c]+[b])},$$

$$\Delta(\overline{t}_{ab}) = \sum_c \overline{t}_{ac} \otimes \overline{t}_{cb} (-1)^{([a]+[c])([c]+[b])},$$

the counit $\varepsilon(t_{ab}) = \varepsilon(\overline{t}_{ab}) = \delta_{ab}$, and the involutary antipode $S(t_{ab}) = (-1)^{[a]([a]+[b])} \overline{t}_{ba}$, where

$$[a] = \begin{cases} \overline{0}, & a \leqslant m, \\ \overline{1}, & a > m. \end{cases}$$

An important fact is the following.

Proposition 3: The subspace $\mathcal{A}$ is dense in $U(\mathfrak{sl}(m|n))^*$.

Proof: This follows from a slight strengthening of a theorem which in the nongraded case is due to Harish-Chandra. Let V be a finite-dimensional graded vector space and let $\mathfrak{g}$ be a graded subalgebra of the Lie superalgebra $\mathfrak{sl}(V)$. We regard V as a $\mathfrak{g}$-module. Arguing as in the nongraded case (see the proof of Theorem 2.5.7 in Ref. 20) one can easily prove that for any nonzero element $x \in U(\mathfrak{g})$ there exists an integer $r \geqslant 0$ such that x acts nontrivially on $V^{\otimes r}$. Actually, there is a minor complication: Dixmier's proof only applies if $\dim V_{\overline{0}} \neq \dim V_{\overline{1}}$. But if $\dim V_{\overline{0}} = \dim V_{\overline{1}}$, we can embed V into $W = V \oplus \mathbb{C}$, where $\mathbb{C}$ is regarded as a trivial $\mathfrak{g}$-module. Then his arguments apply to W, and the tensorial powers of W are isomorphic to direct sums of tensorial powers of V. This proves the proposition.

As at the beginning of this section, let $\mathcal{P}$ be the dual of the embedding of $U(\mathfrak{g}_{\overline{0}})$ in $U(\mathfrak{g})$. We have

$$\mathcal{P}(t_{i\mu}) = \mathcal{P}(t_{\mu i}) = \mathcal{P}(\overline{t}_{i\mu}) = \mathcal{P}(\overline{t}_{\mu i}) = 0, \quad 1 \leqslant i \leqslant m, \quad m < \mu \leqslant m+n.$$

Set

$$\mathcal{A}_e = \mathcal{P}(\mathcal{A}).$$

Then $\mathcal{A}_e$ has a Peter-Weyl type basis in terms of the matrix elements of irreducible finite-dimensional representations of $\mathfrak{sl}(m) \oplus \mathfrak{sl}(n) \oplus \mathfrak{gl}(1)$. Thus it follows from the discussion of the last section that there exists a unique normalized left integral

$$\int_0 : \ \mathcal{A}_e \to \mathbb{C},$$

which also turns out to be right invariant (see the Appendix). Denote by $\nu(\Gamma) \in \mathcal{A}^\circ$ the image of Γ under the natural embedding $U(\mathfrak{g}) \to \mathcal{A}^\circ$. Recalling Lemma 2, we have the following theorem.

Theorem 3: *The linear form $\int = \nu(\Gamma) \cdot \int_0 \mathcal{P}$ is a nontrivial left and right integral on $\mathcal{A}$.*

To see that $\int$ is indeed nontrivial, we consider $\int \Theta \overline{\Theta}$, where

$$\Theta_i = t_{i,m+n} t_{i,\, m+n-1} \cdots t_{i,m+1},$$

$$\overline{\Theta}_i = \overline{t}_{i,m+n} \overline{t}_{i,m+n-1} \cdots \overline{t}_{i,m+1}, \quad i = 1, 2, \ldots, m,$$

$$\Theta = \Theta_m \Theta_{m-1} \cdots \Theta_1,$$

$$\overline{\Theta} = \overline{\Theta}_m \overline{\Theta}_{m-1} \cdots \overline{\Theta}_1.$$

We have

$$\int \Theta \overline{\Theta} = \langle \Theta \overline{\Theta}, \mathbb{E}\mathbb{F} \rangle \int_0 \mathcal{P}(\det(t_{\mu\nu}) \det(\overline{t}_{\mu\nu}))^m.$$

As

$$\det(t_{\mu\nu}) \det(\overline{t}_{\mu\nu})(u) = \varepsilon(u), \quad \forall u \in U(\mathfrak{g}_0^-),$$

we immediately obtain

$$\int_0 \mathcal{P}(\det(t_{\mu\nu}) \det(\overline{t}_{\mu\nu}))^m = 1.$$

By induction we can show that

$$\langle \Theta \overline{\Theta}, \mathbb{E}\mathbb{F} \rangle = (-1)^{mn(mn+1)/2},$$

hence

$$\int \Theta \overline{\Theta} = (-1)^{mn(mn+1)/2}.$$

Example 3: The Lie supergroup $\mathrm{OSP}(2|2n)$

The Lie superalgebras $\mathfrak{g} = \mathfrak{osp}(2|2n)$ form the other series of type I (basic classical) Lie superalgebras besides $\mathfrak{sl}(m|n)$. They share many properties with the latter. In particular, the odd subspace of $\mathfrak{osp}(2|2n)$ is a direct sum of $\mathfrak{g}_{1+}^-$ and $\mathfrak{g}_{1-}^-$. Both $U(\mathfrak{g}_{1+}^-)$ and $U(\mathfrak{g}_{1-}^-)$ are isomorphic to the Grassmann algebra on $2n$ generators. The maximal even subalgebra of $\mathfrak{osp}(2|2n)$ is $\mathfrak{sp}(2n) \oplus \mathfrak{gl}(1)$, and $\mathfrak{g}_0^-$ and $\mathfrak{g}_{1\pm}^-$ satisfy relations of the same form as (8).

The subspaces of $U(\mathfrak{g}_{1\pm}^-)$ of the highest Grassmann degree are both one-dimensional. We choose bases $\mathbb{E}$ and $\mathbb{F}$ for them, respectively, and set $\Gamma = \mathbb{E}\mathbb{F}$. Then

$$X\Gamma \in U(\mathfrak{g})\mathfrak{g}_0^-, \quad \forall X \in \mathfrak{g}.$$

Let t be the defining representation of $\mathfrak{osp}(2|2n)$. It is known that t is self-dual. Introduce the matrix elements of t,

$$t_{ab} \in U(\mathfrak{g})^\circ, \quad a, b = 1,2,\ldots,2n+2,$$

with t_{ij} and $t_{\mu\nu}$ being even, and $t_{i\mu}$ and $t_{\mu i}$ odd, where $i,j=1,2$; $\mu,\nu=3,4,\ldots,2n+2$.

Proposition 4: The elements t_{ab} generate a sub-Hopf-superalgebra $\mathcal{A}$ of $U(\mathfrak{osp}(2|2n))^\circ$, and $\mathcal{A}$ is dense in $U(\mathfrak{osp}(2|2n))^*$.

Proof: This follows from the proof of Proposition 3.

Set $\mathcal{A}_e=\mathcal{P}(\mathcal{A})$. Then $\mathcal{A}_e$ admits a unique (up to scalar multiples) left integral $\int_0$. Denoting by $\nu(\Gamma)$ the canonical image of Γ in $\mathcal{A}^\circ$, we have

Theorem 4: *The linear form $\int=\nu(\Gamma)\cdot\int_0\mathcal{P}$ is a nontrivial left and right integral on $\mathcal{A}$.*

The $t_{i\mu}$ and $t_{\mu i}$ generate a Grassmann algebra contained in $\mathcal{A}$. We take Θ to be a nonzero element of the highest degree in this Grassmann algebra. Then direct computations can show that

$$\int\Theta\neq 0.$$

Example 4: The Lie supergroup OSP$(1|2n)$

Let us start with the simplest case, $n=1$. The Dynkin diagram of $\mathfrak{osp}(1|2)$ is just ●, and the simple Chevalley generators are $\{e,f,h\}$, where e and f are odd while h is even, with the commutation relations

$$[h,e]=e,\ [h,f]=-f,\ [e,f]=h.$$

It is important to observe that $[e,e]=E$, $[f,f]=F$ and h span an $\mathfrak{sl}(2)$ subalgebra, which is the maximal even subalgebra $\mathfrak{osp}(1|2)_{\bar 0}$. This is a general feature of any type II superalgebra, where some simple generators of the maximal even subalgebra are generated by odd elements. We denote $\mathfrak{g}=\mathfrak{osp}(1|2)$, $\mathfrak{g}_{\bar 0}=\mathfrak{sl}(2)\subset\mathfrak{osp}(1|2)$, $\mathcal{U}=U(\mathfrak{g})$ and $\mathcal{U}_e=U(\mathfrak{g}_{\bar 0})$.

Now

$$\mathbb{1}+ef+\mathcal{U}\mathfrak{g}_{\bar 0}^-$$

is an invariant of the left $\mathcal{U}$-module $\mathcal{U}/\mathcal{U}\mathfrak{g}_{\bar 0}^-$, and we have the left and right integral

$$\int\ =\nu(\mathbb{1}+ef)\cdot\int_0\mathcal{P}:\mathcal{U}^\circ\to\mathbb{C},$$

where $\int_0:\mathcal{U}_e^\circ\to\mathbb{C}$ is the standard Haar functional on $\mathcal{U}_e^\circ$. Consider $\int\mathbb{1}_{\mathcal{U}^\circ}$. We have

$$\int\mathbb{1}_{\mathcal{U}^\circ}=\langle\mathbb{1}_{\mathcal{U}^\circ},\mathbb{1}+ef\rangle\int_0\mathcal{P}(\mathbb{1}_{\mathcal{U}^\circ})=\int_0\mathbb{1}_{\mathcal{U}_e^\circ}\neq 0.$$

That is, the integral does not vanish on the identity element of $\mathcal{U}^\circ$. It follows from the discussion of Sec. II that all finite-dimensional representations of $\mathfrak{osp}(1|2)$ are completely reducible, which, of course, is a well-known fact.

The general case can be treated similarly. We do not go into details but only mention that an even element $u_0\in\mathcal{U}=U(\mathfrak{osp}(1|2n))$ such that $\varepsilon(u_0)\neq 0$ and such that $u_0+\mathcal{U}\mathfrak{g}_{\bar 0}^-$ is invariant in $\mathcal{U}/\mathcal{U}\mathfrak{g}_{\bar 0}^-$ has been constructed by Djoković and Hochschild in Ref. 21. Moreover, they have proved the following theorem:

Let $\mathfrak{g}$ be a finite-dimensional Lie superalgebra over a field of characteristic zero. Then all finite-dimensional representations of $\mathfrak{g}$ are completely reducible if and only if the following two conditions are satisfied.

(1) The Lie algebra $\mathfrak{g}_{\bar 0}^-$ is semisimple.
(2) There is an element u_0 in $U(\mathfrak{g})$ such that $u_0+U(\mathfrak{g})\mathfrak{g}_{\bar 0}^-$ is an invariant element of $U(\mathfrak{g})/U(\mathfrak{g})\mathfrak{g}_{\bar 0}^-$ and satisfies $\varepsilon(u_0)\neq 0$.

Visibly, in the cited reference the element u_0 has been a decisive tool in the proof that all finite-dimensional representations of $\mathfrak{osp}(1|2n)$ are completely reducible. It is remarkable that in

the present work it serves to construct a left integral on $\mathcal{U}^\circ$ which does not vanish on the unit element, a result which, in turn, implies the complete reducibility of the $\mathcal{U}^\circ$-comodules and hence of the finite-dimensional $\mathcal{U}$-modules.

Example 5: The Lie supergroup OSP$(3|2)$

Let $\mathfrak{g}$ denote the Lie superalgebra $\mathfrak{osp}(3|2)$. It is the simplest of those orthosymplectic Lie superalgebras which are not of type I and not one of the special algebras $\mathfrak{osp}(1|2n)$. Its maximal even subalgebra is $\mathfrak{g}_{\bar{0}}=\mathfrak{so}(3)\oplus\mathfrak{sp}(2)$. The $\mathfrak{g}$-module $U(\mathfrak{g})/U(\mathfrak{g})\mathfrak{g}_{\bar{0}}$ will be denoted by W. We shall also need the quadratic Casimir element $C\in U(\mathfrak{g})$ and the corresponding Casimir operator C_W acting on W.

In the subsequent investigation of the $\mathfrak{g}$-module W we are going to use the classification of finite-dimensional irreducible $\mathfrak{g}$-modules obtained by Van der Jeugt in Ref. 22. Both the $\mathfrak{g}$-modules and the $\mathfrak{g}_{\bar{0}}$-modules are characterized by a pair of numbers $p,q\in\{0,\frac{1}{2},1,\frac{3}{2},\ldots\}$. By a slight abuse of notation, we denote the corresponding $\mathfrak{g}$-module by $[p,q]$, and the corresponding $\mathfrak{g}_{\bar{0}}$-module by (p,q). [We remark that p is associated in the obvious way to $\mathfrak{so}(3)$ and q to $\mathfrak{sp}(2)$.]

A version of the Poincaré–Birkhoff–Witt theorem implies that W, regarded as a $\mathfrak{g}_{\bar{0}}$-module, is isomorphic to the Grassmann algebra constructed over $\mathfrak{g}_{\bar{1}}$. Using the representation theory of $\mathfrak{sl}(2)$, we conclude that the $\mathfrak{g}_{\bar{0}}$-module W decomposes into the direct sum of the modules contained in the following list, where the first line gives the Grassmann degree to which the modules underneath belong.

$$
\begin{array}{ccccccc}
0 & 1 & 2 & 3 & 4 & 5 & 6 \\
(0,0) & (1,\tfrac{1}{2}) & (1,1) & (2,\tfrac{1}{2}) & (1,1) & (1,\tfrac{1}{2}) & (0,0) \\
 & & (2,0) & (1,\tfrac{1}{2}) & (2,0) & & \\
 & & (0,0) & (0,\tfrac{3}{2}) & (0,0) & &
\end{array}
$$

Comparison with the lower-dimensional irreducible $\mathfrak{g}$-modules then shows that for a Jordan-Hölder sequence of the $\mathfrak{g}$-module W the irreducible quotients must be isomorphic to the following modules:

$$
[0,\tfrac{3}{2}],\ [1,1],\ [1,\tfrac{1}{2}],\ [0,0],\ [0,0].
$$

For the convenience of the reader and for later use, we also note how these modules decompose into irreducible $\mathfrak{g}_{\bar{0}}$-submodules, moreover, in the first column we give the eigenvalue of the quadratic Casimir operator (normalized as in Ref. 22) in these modules:

$$
\begin{aligned}
-6 \quad & [0,\tfrac{3}{2}]\cong(0,\tfrac{3}{2})\oplus(1,1)\oplus(1,\tfrac{1}{2})\oplus(0,0) \\
0 \quad & [1,1]\cong(1,1)\oplus(1,\tfrac{1}{2})\oplus(2,\tfrac{1}{2})\oplus(2,0) \\
2 \quad & [1,\tfrac{1}{2}]\cong(1,\tfrac{1}{2})\oplus(2,0)\oplus(0,0) \\
0 \quad & [0,0]\cong(0,0)
\end{aligned}
$$

Note that at this point it is obvious that the $\mathfrak{g}$-module W is not completely reducible: It is generated, as a $\mathfrak{g}$-module, by a $\mathfrak{g}_{\bar{0}}$-invariant element; the multiplicity of $(0,0)$ in the $\mathfrak{g}_{\bar{0}}$-module W is equal to 4, but the length of the $\mathfrak{g}$-module W (i.e., the number of irreducible quotients of a Jordan-Hölder sequence) is equal to 5.

The eigenvalues given previously imply that the primary decomposition of W with respect to C_W takes the following form:

$$
W=W_{-6}\oplus W_2\oplus W_0, \tag{9}
$$

where W_r, $r\in\{-6,2,0\}$, is the primary subspace of W corresponding to the eigenvalue r of C_W. Of course, the W_r's are $\mathfrak{g}$-submodules of W. Regarded as $\mathfrak{g}$-modules, we have

$$W_{-6}\cong[0,\tfrac{3}{2}],\quad W_2\cong[1,\tfrac{1}{2}],$$

whereas W_0 has a Jordan-Hölder sequence of the form

$$W_0\supset W_0'\supset W_0''\supset\{0\},$$

where one of the three modules W_0/W_0', W_0'/W_0'', W_0'' is isomorphic to $[1,1]$, while the other two are trivial one-dimensional. In any case we have

$$C_W(W_0)\subset W_0', \tag{10}$$

$$C_W(W_0')\subset W_0'', \tag{11}$$

$$C_W(W_0'')=\{0\}. \tag{12}$$

We stress that while W_{-6} and W_2 are eigenspaces of C_W, this is not so for W_0. In fact, we shall see that the restriction of C_W to W_0 is not equal to zero but only nilpotent.

Lemma 5: The subspace $C_W(W_0)$ of W_0 is either a trivial one-dimensional $\mathfrak{g}$-submodule of W_0 or else it is equal to $\{0\}$.

Proof: In the subsequent discussion, it is important to keep the following fact in mind:
(*) The $\mathfrak{g}$-module $[1,1]$ does not contain a trivial $\mathfrak{g}_0^-$-submodule.
There are three cases to consider.

(a) The module W_0/W_0' is isomorphic to $[1,1]$. This case is not possible since W_0, like W_2, is generated by a $\mathfrak{g}_0^-$-invariant element which, under the present assumption and because of (*), would have to belong to W_0'.

(b) The module W_0'/W_0'' is isomorphic to $[1,1]$. In this case, W_0'' consists of $\mathfrak{g}$-invariant elements, hence the existence of nonzero $\mathfrak{g}$-invariant elements in W_0 is obvious. However, we want to find an explicit expression for them, and a first step towards this end is the lemma. According to Eq. (11) we have $C_W(W_0')\subset W_0''$. Using Eq. (12) and recalling (*), we can even conclude that $C_W(W_0')=\{0\}$. Thus C_W induces a $\mathfrak{g}$-module map $W_0/W_0'\to W_0$, and this implies our claim. Actually, it is easy to see that $C_W(W_0)\subset W_0''$.

(c) The module W_0'' is isomorphic to $[1,1]$. Equation (12) says that $C_W(W_0'')=\{0\}$, hence C_W induces a $\mathfrak{g}$-module map $W_0'/W_0''\to W_0'$ which, according to Eq. (11), is even a map into W_0''. Invoking (*) we conclude that $C_W(W_0')=\{0\}$, and our claim follows as in part (b). This proves the lemma.

Let us now recall the decomposition (9) of W and also the fact that the $\mathfrak{g}$-module W is generated by the element $\mathbb{1}_{U(\mathfrak{g})}+U(\mathfrak{g})\mathfrak{g}_0^-$. Then the lemma above can be rephrased as follows: Either the element

$$z=C(C-2)(C+6)\in U(\mathfrak{g})$$

belongs to $U(\mathfrak{g})\mathfrak{g}_0^-$, or else $z+U(\mathfrak{g})\mathfrak{g}_0^-$ is a nontrivial invariant element of $U(\mathfrak{g})/U(\mathfrak{g})\mathfrak{g}_0^-$.

Thus all that remains to be shown is that z does not belong to $U(\mathfrak{g})\mathfrak{g}_0^-$. This is an easy consequence of the Poincaré–Birkhoff–Witt (PBW) theorem, which allows us to construct a suitable basis of W. Actually, the task can be simplified, as follows. The Casimir element C can be decomposed (in various ways) into the sum of two pieces,

$$C=C_o+C_e,$$

where C_o is quadratic in the elements of $\mathfrak{g}_{\bar{1}}^-$, and where C_e belongs to $U(\mathfrak{g}_{\bar{0}}^-)$. Since C commutes with all elements of $U(\mathfrak{g})$, it follows that

$$z \in C_o(C_o-2)(C_o+6)+U(\mathfrak{g})\mathfrak{g}_{\bar{0}}^-,$$

and hence we can replace z by

$$z_o=C_o(C_o-2)(C_o+6).$$

Applying Theorem 2 to z or z_o and recalling Lemma 2 we obtain a nonzero left and right integral on $U(\mathfrak{osp}(3|2))^\circ$.

IV. INTEGRALS ON QUANTUM SUPERGROUPS

We shall extend the construction of integrals on classical supergroups to quantum supergroups at generic q. Recall that the Drinfeld-Jimbo quantum superalgebra $U_q(\mathfrak{g})$ associated with a simple basic classical Lie superalgebra $\mathfrak{g}$ is usually defined with respect to the distinguished simple root system of $\mathfrak{g}$ where only one odd simple root exists. By removing the odd simple generators (but retaining the corresponding Cartan generator), one obtains a graded quantum subalgebra $U_q(\mathfrak{g}_0)\subset U_q(\mathfrak{g})$, where $\mathfrak{g}_0\subset\mathfrak{g}$ is an even subalgebra of $\mathfrak{g}$, which is a reductive Lie algebra. We stress that while for the basic classical Lie superalgebras of type I we have $\mathfrak{g}_0=\mathfrak{g}_{\bar{0}}^-$, this is *not* the case for type II.

An important fact is that $U_q(\mathfrak{g}_0)$ forms a Hopf subalgebra of $U_q(\mathfrak{g})$, with its structure inherited from the latter. We have the following Hopf superalgebra maps:

$$\mathcal{I}:\ U_q(\mathfrak{g}_0)\to U_q(\mathfrak{g}),$$

$$\mathcal{P}:\ U_q(\mathfrak{g})^\circ\to U_q(\mathfrak{g}_0)^\circ,$$

where $\mathcal{I}$ is the natural embedding and $\mathcal{P}$ is induced from its dual $\mathcal{I}^*$.

A quantum supergroup associated with $U_q(\mathfrak{g})$ is defined by specifying its superalgebra of functions $\mathcal{A}$, where $\mathcal{A}$ should meet two basic requirements, namely, it forms a sub-Hopf-superalgebra of $U_q(\mathfrak{g})^\circ$, and it is dense in $U_q(\mathfrak{g})^*$. In general, $\mathcal{A}$ is generated by the matrix elements of some finite-dimensional irreducible representations of $U_q(\mathfrak{g})$. The structure of $\mathcal{A}$ associated with a type I quantum superalgebra has been extensively studied. The fact that $\mathcal{A}$ is dense in $U_q(\mathfrak{g})^*$ implies that the natural Hopf superalgebra maps

$$\nu:\ U_q(\mathfrak{g})\to\mathcal{A}^\circ,$$

$$\hat{\mathcal{I}}=\nu\mathcal{I}:\ U_q(\mathfrak{g}_0)\to\mathcal{A}^\circ,$$

are embeddings.

Denote $\mathcal{A}_e=\mathcal{P}(\mathcal{A})$. Then $\mathcal{A}_e$ separates points of $U_q(\mathfrak{g}_0)$, i.e., it is dense in $U_q(\mathfrak{g}_0)^*$. Furthermore, $\mathcal{A}_e$ admits a Peter-Weyl type basis in terms of the matrix elements of finite-dimensional irreducible representations of $U_q(\mathfrak{g}_0)$, and there exists a unique (up to scalar multiples) left integral

$$\int_0:\ \mathcal{A}_e\to\mathbb{C},$$

which also turns out to be right invariant, and it is nonvanishing on $1_{\mathcal{A}_e}$.

Similar to the classical case, we consider

$$\int_0\mathcal{P}:\ \mathcal{A}\to\mathbb{C},$$

which is clearly left invariant with respect to $U_q(\mathfrak{g}_0)$, i.e.,

$$\hat{\mathcal{I}}(u)\cdot\int_0\mathcal{P}=\varepsilon(u)\int_0\mathcal{P},\quad \forall u\in U_q(\mathfrak{g}_0).$$

Let K denote the ideal of $U_q(\mathfrak{g}_0)$ defined by

$$K=\{u\in U_q(\mathfrak{g}_0)|\ \varepsilon(u)=0\},$$

where ε is the counit of $U_q(\mathfrak{g})$. Then

$$J=U_q(\mathfrak{g})K \tag{13}$$

is a left ideal of $U_q(\mathfrak{g})$.

Lemma 6: If $\mathfrak{g}$ *is one of the Lie superalgebras* $\mathfrak{sl}(m|n)$ *or* $\mathfrak{osp}(2|2n)$ (*i.e., if* $\mathfrak{g}$ *is basic classical of type I*), *the left ideal* J *has finite codimension in* $U_q(\mathfrak{g})$.

Proof: This follows immediately from the PBW theorems for these quantum superalgebras established in Refs. 23 and 24.

Clearly $U_q(\mathfrak{g})/J$ forms a left $U_q(\mathfrak{g})$-module under the natural action

$$x(y+J)=xy+J,\quad \forall x,y\in U_q(\mathfrak{g}).$$

Let $z+J$ be an invariant of $U_q(\mathfrak{g})/J$, i.e., $x(z+J)=\varepsilon(x)z+J$, $\forall x\in U_q(\mathfrak{g})$. Nontrivial invariants of this kind exist for type I quantum superalgebras, as we will see later. However, we doubt that the type II quantum superalgebras admit such invariants, as in this case J is expected to have infinite codimension.

Theorem 5: *Let* $\int=\nu(z)\cdot\int_0\mathcal{P}$. *Then* $\int$ *is a left integral on* $\mathcal{A}$, *that does not depend on the representative of* $z+J$. *As before,* $\nu(z)$ *is the image of* z *under the natural embedding* $U_q(\mathfrak{g})\rightarrow\mathcal{A}^\circ$.

Proof: The proof goes in the same way as in the classical case.

Example 6: *The quantum supergroup* $\mathrm{SL}_q(m|n)$

We study the quantum supergroup $\mathrm{SL}_q(m|n)$. The quantum superalgebra $U_q(\mathfrak{sl}(m|n))$ is generated by the simple and the Cartan generators

$$E_{a,a+1},\quad E_{a+1,a},\quad k_a^{\pm1},\quad a=1,2,\ldots,m+n-1,$$

subject to the standard relations. (Here $k_a=K_aK_{a+1}^{-1}$ in the notation of Ref. 23.) The generators $E_{m,m+1}$ and $E_{m+1,m}$ are odd, while all the others are even. Define recursively

$$E_{ab}=E_{ac}E_{cb}-q_c^{-1}E_{cb}E_{ac},$$

$$E_{ba}=E_{bc}E_{ca}-q_cE_{ca}E_{bc},\quad a<c<b,$$

where $q_c=q^{(-1)^{[c]}}$. The vector representation t of $U_q(\mathfrak{sl}(m|n))$ is given by

$$t(E_{a,a\pm1})=e_{a,a\pm1},$$

$$t(k_a)=q_a^{e_{aa}}q_{a+1}^{-e_{a+1,a+1}}=1+(q_a-1)e_{aa}+(q_{a+1}^{-1}-1)e_{a+1,a+1}.$$

We shall denote the dual vector representation by $\overline{t}$, and let

$$t_{ab},\ \overline{t}_{ab}\in U_q(\mathfrak{sl}(m|n))^\circ,\quad a,b=1,2,\ldots,m+n,$$

be the matrix elements of t and $\bar{t}$, respectively. Then the superalgebra $\mathcal{A}$ of functions on the quantum supergroup $\mathrm{SL}_q(m|n)$ is defined to be the subalgebra of $U_q(\mathfrak{sl}(m|n))^\circ$ generated by the t_{ab}, $\bar{t}_{ab}$. In Ref. 25 the following was shown.

Proposition 5: The algebra $\mathcal{A}$ is a sub-Hopf-superalgebra of $U_q(\mathfrak{sl}(m|n))^\circ$ and is dense in $U_q(\mathfrak{sl}(m|n))^*$.

The quantum even subalgebra $U_q(\mathfrak{g}_0)$ is $U_q(\mathfrak{sl}(m)\oplus\mathfrak{gl}(1)\oplus\mathfrak{sl}(n))$ with generators

$$k_a^{\pm 1},\ E_{b,b+1},\ E_{b+1,b},\quad a,b=1,2,\ldots,m+n-1,\quad b\neq m.$$

The images of t and $\bar{t}$ under $\mathcal{P}$ give rise to representations of $U_q(\mathfrak{g}_0)$, with

$$\mathcal{P}(t)=\begin{pmatrix}\mathcal{P}(t_{ij}) & 0\\ 0 & \mathcal{P}(t_{\mu\nu})\end{pmatrix},\quad \mathcal{P}(\bar{t})=\begin{pmatrix}\mathcal{P}(\bar{t}_{ij}) & 0\\ 0 & \mathcal{P}(\bar{t}_{\mu\nu})\end{pmatrix}.$$

The matrix elements of these representations generate $\mathcal{A}_e$, which forms a Hopf subalgebra of $U_q(\mathfrak{g}_0)^\circ$. On $\mathcal{A}_e$ there exists a unique left integral $\int_0$ which annihilates the matrix elements of all nontrivial irreducible representations and satisfies

$$\int_0 \mathbb{1}_{\mathcal{A}_e}=1.$$

Introduce

$$\mathbb{E}_i=E_{i,m+1}\ E_{i,m+2}\cdots E_{i,m+n},$$

$$\mathbb{F}_i=E_{m+n,i}\ E_{m+n-1,i}\cdots E_{m+1,i},$$

$$\mathbb{E}=\mathbb{E}_m\,\mathbb{E}_{m-1}\cdots\mathbb{E}_1,$$

$$\mathbb{F}=\mathbb{F}_1\,\mathbb{F}_2\cdots\mathbb{F}_m,$$

$$\Gamma=\mathbb{E}\,\mathbb{F}.$$

Lemma 7: Let J be defined as in (13). Then the image of Γ under the canonical map $U_q(\mathfrak{sl}(m|n))\to U_q(\mathfrak{sl}(m|n))/J$ is an invariant.

Proof: In Ref. 23 it was shown that

$$k_a\Gamma=\Gamma\,k_a,\quad \forall a,$$

$$[E_{c,c+1},\mathbb{E}]=[E_{c,c+1},\mathbb{F}]=0,\quad c\neq m,$$

$$[E_{c+1,c},\mathbb{E}]=[E_{c+1,c},\mathbb{F}]=0,\quad c\neq m.$$

It is also clear that

$$E_{m,m+1}\Gamma=0.$$

This immediately leads to

$$E_{i,m+1}\Gamma=0,\quad \forall i\leqslant m.$$

What remains to be shown is that

$$E_{m+1,m}\Gamma\in J. \tag{14}$$

By using the fact that $E_{m+1,m}$ q-anticommutes with all $E_{\mu,i}$, $\mu \geqslant m+1$, $i \leqslant m$, and $(E_{m+1,m})^2 = 0$, we have

$$E_{m+1,m}\,\mathbb{F} = 0.$$

Thus

$$E_{m+1,m}\Gamma = [E_{m+1,m}, \mathbb{E}]\,\mathbb{F}.$$

To determine the right hand side, we need the following commutation relations:

$$[E_{m+1,m}, \mathbb{E}_i] = q^{m+n-2} E_{i,m+2} E_{i,m+3} \cdots E_{i,m+n} k_m E_{i,m}, \quad i < m,$$

$$[E_{i,m}, \mathbb{E}_j] = 0, \quad i > j.$$

Now

$$[E_{m+1,m}, \Gamma] = [E_{m+1,m}, \mathbb{E}_m]\,\mathbb{E}_{m-1} \cdots \mathbb{E}_1\,\mathbb{F},$$

where $[E_{m+1,m}, \mathbb{E}_m]$ can be easily calculated to yield

$$[E_{m+1,m}, \mathbb{E}_m] = \frac{k_m - k_m^{-1}}{q - q^{-1}} E_{m,m+2} \cdots E_{m,m+n} + \sum_{\alpha=2}^{n} (-1)^{\alpha} q^{-(n-\alpha)} E_{m,m+1} \cdots \hat{E}_{m,m+\alpha} \cdots E_{m,m+n} E_{m+1,m+\alpha} k_\alpha^{-1},$$

with $\hat{E}_{m,m+\alpha}$ indicating that $E_{m,m+\alpha}$ is removed from the second term. By using

$$E_{m+1,m+\alpha}\,\mathbb{E}_i - q^{-2}\,\mathbb{E}_i\,E_{m+1,m+\alpha} = 0, \quad i = 1,2,\ldots,m, \quad \alpha = 2,3,\ldots,n,$$

we immediately see that (14) indeed holds.

Let $\nu: U_q(\mathfrak{g}) \to \mathcal{A}^\circ$ be the natural embedding.

Theorem 6: *There exists the following nontrivial left integral on* $\mathcal{A}$*:*

$$\int = \nu(\Gamma) \cdot \int_0 \mathcal{P}.$$

Example 7: The quantum supergroup $\mathrm{OSP}_q(2|2n)$.

We denote by $\mathfrak{g}$ the Lie superalgebra $\mathfrak{osp}(2|2n)$ and recall that in this case $\mathfrak{g}_0 = \mathfrak{g}_0^-$ is the maximal even subalgebra $\mathfrak{sp}(2n) \oplus \mathfrak{gl}(1)$ of $\mathfrak{g}$. Introduce the $(n+1)$-dimensional Minkowski space $\mathfrak{h}^*$ with a basis $\{\delta_i \mid i = 0,1,2,\ldots,n\}$ and the bilinear form $(,): \mathfrak{h}^* \times \mathfrak{h}^* \to \mathbb{C}$ defined by

$$(\delta_i, \delta_j) = -(-1)^{\delta_{0,i}}\,\delta_{i,j}, \quad \forall i,j.$$

Then the simple roots can be expressed as $\alpha_i = \delta_i - \delta_{i+1}$, $0 \leqslant i < n$, $\alpha_n = 2\delta_n$, with α_0 being the unique odd simple root. A convenient version of the Cartan matrix $A = (a_{ij})_{i,j=0}^{n}$ is $a_{ij} = 2(\alpha_i, \alpha_j)/(\alpha_i, \alpha_i)$, $\forall i > 0$, $a_{0,j} = (\alpha_0, \alpha_j)$. The quantum superalgebra $U_q(\mathfrak{g})$ is the universal complex superalgebra with generators $\{k_i^{\pm 1}, e_i, f_i, i \in \mathbb{N}_n\}$, $\mathbb{N}_n = \{0,1,2,\ldots,n\}$, where e_0 and f_0 are odd and the rest are even. The defining relations are

$$k_i k_j = k_j k_i, \quad k_i k_i^{-1} = k_i^{-1} k_i = \mathbb{1},$$

$$k_i e_j k_i^{-1} = q_i^{a_{ij}/2} e_j, \quad k_i f_j k_i^{-1} = q_i^{-a_{ij}/2} f_j,$$

$$[e_i,f_j]=\delta_{ij}(k_i^2-k_i^{-2})/(q_i-q_i^{-1}),\quad i,j\in\mathbb{N}_n,$$

$$(e_0)^2=(f_0)^2=0,$$

$$\sum_{\mu=0}^{1-a_{ij}}(-1)^\mu\begin{bmatrix}1-a_{ij}\\ \mu\end{bmatrix}_{q_i}e_i^{1-a_{ij}-\mu}e_je_i^\mu=0,\quad i\neq 0,$$

$$\sum_{\mu=0}^{1-a_{ij}}(-1)^\mu\begin{bmatrix}1-a_{ij}\\ \mu\end{bmatrix}_{q_i}f_i^{1-a_{ij}-\mu}f_jf_i^\mu=0,\quad i\neq 0,$$

where $\left[\begin{smallmatrix}m\\ n\end{smallmatrix}\right]_q$ is a q-binomial coefficient. As is well-known, the quantum superalgebra $U_q(\mathfrak{g})$ has the structure of a Hopf superalgebra. Note that $\{e_i, f_i, k_i^{\pm 1}\mid i=1,2,\ldots,n\}$ generate a Hopf subalgebra $U_q(\mathfrak{sp}(2n))\subset U_q(\mathfrak{g})$. Together with $\{k_0^{\pm 1}\}$, they generate $U_q(\mathfrak{g}_0)=U_q(\mathfrak{sp}(2n)\oplus\mathfrak{gl}(1))$.

Define the odd elements

$$\psi_1=e_0,$$

$$\psi_{i+1}=\psi_ie_i-qe_i\psi_i,\quad 1\leqslant i<n,$$

$$\psi_{-n}=\psi_ne_n-q^2e_n\psi_n,$$

$$\psi_{-i}=\psi_{-i-1}e_i-qe_i\psi_{-i-1},\quad 1\leqslant i<n;$$

$$\phi_0=f_0,$$

$$\phi_{i+1}=f_i\phi_i-q^{-1}\phi_if_i,\quad 1\leqslant i<n,$$

$$\phi_{-n}=f_n\phi_n-q^{-2}\phi_nf_n,$$

$$\phi_{-i}=f_i\phi_{-i-1}-q^{-1}\phi_{-i-1}f_i,\quad 1\leqslant i<n,$$

which satisfy the following relations

$$\psi_{\pm i}\psi_{\pm j}+q^{\pm 1}\psi_{\pm j}\psi_{\pm i}=0,\quad i\leqslant j,$$

$$\psi_i\psi_{-j}+q\psi_{-j}\psi_i=0,\quad \forall i\neq j,$$

$$\psi_n\psi_{-n}+q^2\psi_{-n}\psi_n=0,$$

$$\psi_{-i-1}\psi_{i+1}+\psi_{i+1}\psi_{-i-1}+q\psi_{-i}\psi_i+q^{-1}\psi_i\psi_{-i}=0,\quad i<n;$$

$$\psi_je_i-q^{(\alpha_i,\delta_0-\delta_j)}e_i\psi_j=\delta_{ij}\psi_{i+1},\quad \forall i,j,$$

$$\psi_{-j}e_i-q^{(\alpha_i,\delta_0+\delta_j)}e_i\psi_{-j}=\delta_{i+1,j}\psi_{-i+1},\quad i>1,$$

and also similar relations for $\phi_{\pm i}$, where ψ_{n+1} and ϕ_{n+1} are understood as ψ_{-n} and ϕ_{-n}, respectively. Let

$$E_{1,2}=e_1,$$

$$E_{1,i+1}=E_{1,i}e_i-qe_iE_{1,i},\quad 1<i<n,$$

$$E_{1,\bar{n}}=E_{1,n}e_n-q^2e_nE_{1,n},$$

$$E_{1,\bar{i}}=E_{1,\overline{i+1}}e_i-qe_iE_{1,\overline{i+1}},\quad 1<i<n,$$

$$E_{1,\bar{1}}=E_{1,\bar{2}}e_1q^{-1}-qe_1E_{1,\bar{2}},$$

where we have introduced the notation $\bar{\bar{i}}=-i$. Then

$$\{\psi_i,f_0\}=E_{1,i}k_0^{-2},\quad \{\psi_{-i},f_0\}=E_{1,\bar{i}}k_0^{-2}.$$

Define

$$\mathbb{E}=\psi_1\psi_2\cdots\psi_n\psi_{-n}\psi_{-n+1}\cdots\psi_{-1},$$

$$\mathbb{F}=\phi_{-1}\phi_{-2}\cdots\phi_{-n}\phi_n\phi_{n-1}\cdots\phi_1,$$

$$\Gamma=\mathbb{E}\,\mathbb{F}.$$

We have the following lemma.

Lemma 8: Let J be defined as in (13). Then

(i) $[v,\mathbb{E}]=[v,\mathbb{F}]=0,\ \forall v\in U_q(\mathfrak{sp}(2n))\subset U_q(\mathfrak{g}_0)$,
(ii) $[u,\Gamma]=0,\ \forall u\in U_q(\mathfrak{g}_0)$,
(iii) $x\Gamma\in\varepsilon(x)\Gamma+J,\ \forall x\in U_q(\mathfrak{g})$.

Of particular importance for us is the vector representation t of $U_q(\mathfrak{g})$. Introduce the index $a=i$ or $\bar{i}$, with $i=0,1,\ldots,n$, $\bar{i}=\bar{0},\bar{1},\ldots,\bar{n}$. We have

$$t(e_0)=e_{0,1}+e_{\bar{1},\bar{0}},\quad t(f_0)=e_{1,0}-e_{\bar{0},\bar{1}},$$

$$t(e_i)=e_{i,i+1}-e_{\overline{i+1},\bar{i}},\quad t(f_i)=e_{i+1,i}-e_{\bar{i},\overline{i+1}},\quad 1\leqslant i<n,$$

$$t(e_n)=e_{n,\bar{n}},\quad t(f_n)=e_{\bar{n},n},$$

$$t(k_i)=q_i^{H_i/2},\quad 0\leqslant i\leqslant n,$$

where

$$H_0=\delta_0^*+\delta_1^*,$$

$$H_i=\delta_i^*-\delta_{i+1}^*,\quad 0<i<n,$$

$$H_n=\delta_n^*;$$

$$\delta_i^*=e_{i,i}-e_{\bar{i},\bar{i}},\quad 0\leqslant i\leqslant n.$$

Let $t_{ab}\in U_q(\mathfrak{g})^\circ,\ a,b=0,1,\ldots,n,\bar{0},\bar{1},\ldots,\bar{n},$ be the matrix elements of the vector representation t,

$$\langle t_{ab},x\rangle=t(x)_{ab},\quad \forall x\in U_q(\mathfrak{g}).$$

We will take the algebra $\mathcal{A}$ of functions on $\mathrm{OSP}_q(2|2n)$ to be the subalgebra of $U_q(\mathfrak{g})^\circ$ generated by the elements t_{ab}. In Ref. 26 we have shown the following.

Proposition 6: The algebra $\mathcal{A}$ is a sub-Hopf-superalgebra of $\mathcal{U}_q(\mathfrak{osp}(2|2n))^\circ$ and is dense in $\mathcal{U}_q(\mathfrak{osp}(2|2n))^*$.

As usual, let $\mathcal{P}: U_q(\mathfrak{g})^\circ \to U_q(\mathfrak{g}_0)^\circ$ be the map induced by the dual of the embedding $\mathcal{I}: U_q(\mathfrak{g}_0) \to U_q(\mathfrak{g})$, let $\nu: U_q(\mathfrak{g}) \to \mathcal{A}^\circ$ be the canonical map, and let $\hat{\mathcal{I}} = \nu \mathcal{I}$. Set $\mathcal{A}_e = \mathcal{P}(\mathcal{A})$. Then $\mathcal{A}_e$ admits a left integral $\int_0$, which we normalize by setting $\int_0 1_{\mathcal{A}_e} = 1$. Now

$$\int_0 \mathcal{P}: \mathcal{A} \to \mathbb{C}$$

is a well-defined linear map, which is left invariant with respect to $U_q(\mathfrak{g}_0) \subset U_q(\mathfrak{g})$:

$$\hat{\mathcal{I}}(u) \cdot \int_0 \mathcal{P} = \varepsilon(u) \int_0 \mathcal{P}, \quad \forall u \in U_q(\mathfrak{g}_0).$$

We define

$$\int = \nu(\Gamma) \cdot \int_0 \mathcal{P}.$$

Theorem 7: *The linear form $\int: \mathcal{A} \to \mathbb{C}$ is a left integral on $\mathcal{A}$.*
Consider $\int \Lambda$, where

$$\Lambda = t_{\bar{1}\,0} \cdots t_{\bar{n}\,0} t_{n\,\bar{0}} \cdots t_{1\,\bar{0}} t_{\bar{1}\,0} \cdots t_{\bar{n}\,0} t_{n\,0} \cdots t_{1\,0}.$$

Using the following property of the Hopf superalgebra homomorphism $\mathcal{P}$,

$$\mathcal{P}(t_{a\,0}) = \mathcal{P}(t_{a\,\bar{0}}) = 0, \quad \forall a \neq 0, \bar{0},$$

$$\mathcal{P}(t_{0\,\bar{0}}) = \mathcal{P}(t_{\bar{0}\,0}) = 0,$$

we have

$$\int \Lambda = \langle \Lambda, \Gamma \rangle \int_0 \mathcal{P}((t_{\bar{0}\,\bar{0}})^{2n} (t_{0\,0})^{2n}).$$

Now

$$\mathcal{P}(t_{\bar{0}\,\bar{0}} t_{0\,0}) = \mathcal{P}(t_{0\,0} t_{\bar{0}\,\bar{0}}) = 1_{U_q(\mathfrak{g}_0)^\circ},$$

thus

$$\int \Lambda = \langle \Lambda, \Gamma \rangle,$$

which does not vanish if its $q \to 1$ limit is nonzero. A brute force calculation shows

$$|\langle \Lambda, \Gamma \rangle| \to 1, \text{ as } q \to 1.$$

V. DISCUSSION

In the present work we have introduced and investigated the integrals on Hopf superalgebras, with special emphasis on the classical and quantum supergroups. In the undeformed case, there is obviously one problem that we have not solved completely, namely, to prove the existence of nonzero integrals for all of the basic classical Lie supergroups. However, in the meantime we have shown that nonzero integrals exist for a large class of Lie supergroups, including the classical simple ones. For further details, we refer the reader to Ref. 27.

In the quantum case, we have only been able to treat the type I supergroups. In particular, we could not say anything about most of the orthosymplectic quantum supergroups. There are clear indications that our method will not work (or, at least, has to be modified) in this case. However, one should remember that, at present, only very little is known about the orthosymplectic quantum supergroups anyway.

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APPENDIX: DESCRIPTION OF $U(\mathfrak{gl}(1))^\circ$

In Example 2 of Sec. III we need to choose a (left) integral on

$$\mathcal{A}_e \subset \mathcal{U}_e^\circ,$$

where

$$\mathcal{U}_e = U(\mathfrak{g}_{\bar{0}}) = U(\mathfrak{sl}(m) \oplus \mathfrak{sl}(n) \oplus \mathfrak{g}(1)) \cong U(\mathfrak{sl}(m)) \otimes U(\mathfrak{sl}(n)) \otimes U(\mathfrak{gl}(1)),$$

and hence

$$\mathcal{U}_e^\circ \cong U(\mathfrak{sl}(m))^\circ \otimes U(\mathfrak{sl}(n))^\circ \otimes U(\mathfrak{gl}(1))^\circ$$

(the isomorphisms are to be interpreted in the Hopf algebra sense). According to the discussion in Sec. II, the Hopf algebras $U(\mathfrak{sl}(n))^\circ$ are sufficiently well understood. In particular, there is a unique (up to scalar multiples) left integral on $U(\mathfrak{sl}(n))^\circ$, which turns out to be right invariant as well. For $\mathfrak{osp}(2|2n)$ and for the quantum counterparts the situation is similar. Correspondingly, in the present appendix we would like to comment on $U(\mathfrak{gl}(1))^\circ$. Needless to say, the results to be presented are well-known,[28,29] and we summarize them here in order to clarify some slightly subtle issues.

The Lie algebra $\mathfrak{gl}(1)$ is one-dimensional, hence $U(\mathfrak{gl}(1))$ is isomorphic (as a Hopf algebra) to the polynomial algebra $\mathbb{C}[X]$ in one indeterminate X. The Hopf algebra structure is the one known from enveloping algebras: The structure maps are uniquely fixed by the equations

$$\Delta(X) = X \otimes 1 + 1 \otimes X,$$

$$\varepsilon(X) = 0,$$

$$S(X) = -X.$$

It follows that

$$\Delta(X^r) = \sum_{s=0}^{r} \binom{r}{s} X^s \otimes X^{r-s},$$

for all integers $r \geqslant 0$.

The finite dual $\mathbb{C}[X]^\circ$ of $\mathbb{C}[X]$ can be described as follows. Define, for any element $a \in \mathbb{C}$ and any integer $r \geqslant 0$, the linear form u_a^r on $\mathbb{C}[X]$ by

$$\langle u_a^r, P\rangle = \left.\frac{d^r P}{dX^r}\right|_{X=a}, \quad \forall P \in \mathbb{C}[X].$$

Using some elementary algebra, it is not difficult to prove that these linear forms, with a and r as described above, form a basis of the vector space $\mathbb{C}[X]^\circ$. The multiplication in $\mathbb{C}[X]^\circ$ is given by

$$u_a^r u_b^s = u_{a+b}^{r+s},$$

in particular, the unit element is equal to u_0^0 (which is the counit of $\mathbb{C}[X]$), the coproduct is given by

$$\Delta(u_a^r) = \sum_{s=0}^{r} \binom{r}{s} u_a^s \otimes u_a^{r-s},$$

the counit by

$$\varepsilon(u_a^r) = \delta_{r,0},$$

and the antipode by

$$S(u_a^r) = (-1)^r u_{-a}^r,$$

where, in all cases, $a, b \in \mathbb{C}$ and $r, s \geqslant 0$ are integers.

Let us next recall that the dual $\mathbb{C}[X]^*$ of the vector space $\mathbb{C}[X]$ can be identified (in various ways) with the space of formal power series $\mathbb{C}[[Y]]$ in one indeterminate Y. If the dual pairing

$$\langle\,,\rangle : \mathbb{C}[[Y]] \times \mathbb{C}[X] \to \mathbb{C}$$

is chosen such that

$$\left\langle \sum_{n\geqslant 0} c_n Y^n, X^r \right\rangle = r!\, c_r, \quad \forall r,$$

then the coalgebra structure of $\mathbb{C}[X]$ induces just the usual algebra structure on $\mathbb{C}[[Y]]$. Using this identification, the corresponding injection

$$\mathbb{C}[X]^\circ \to \mathbb{C}[[Y]]$$

is given by

$$u_a^r \to Y^r \exp(aY),$$

which immediately gives the product rule for the u_a^r's. Similarly, we find

$$\Delta(Y^r \exp(aY)) = (Y\otimes 1 + 1\otimes Y)^r (\exp(aY)\otimes \exp(aY)).$$

Under the canonical embedding of $\mathbb{C}[[Y]]\otimes\mathbb{C}[[Y]]$ into $\mathbb{C}[[Y\otimes 1, 1\otimes Y]]$, the algebra of formal power series in $Y\otimes 1$ and $1\otimes Y$, the right hand side of this equation can be written in the form

$$(Y\otimes 1 + 1\otimes Y)^r \exp(a(Y\otimes 1 + 1\otimes Y)).$$

In this sense, the coproduct in $\mathbb{C}[X]^\circ$ is fixed by the simple rule

$$\Delta(Y) = Y\otimes 1 + 1\otimes Y,$$

just as for $\mathbb{C}[X]$.

Let us now turn to the object of our main concern, the integrals. It is easy to see that on $\mathbb{C}[X]^\circ$ a nontrivial integral does not exist. However, there is a way out. Obviously, the elements u_a^0, $a \in \mathbb{C}$, span a Hopf subalgebra $\mathcal{K}$ of $\mathbb{C}[X]^\circ$, and the linear form $\int$ on $\mathcal{K}$, defined by

$$\int u_a^0 = \delta_{a,0}, \quad \forall a \in \mathbb{C},$$

is a left and right integral on $\mathcal{K}$. Note that the u_a^0's are exactly the characters of the algebra $\mathbb{C}[X]$, i.e., the grouplike elements of $\mathbb{C}[X]^\circ$, and that $\mathcal{K}$ is isomorphic to the group Hopf algebra of the additive group $\mathbb{C}$.

Now we recall that, for an arbitrary algebra A (associative, with unit element), the finite dual A° consists exactly of the matrix elements (regarded as linear forms on A) of the representations of A. (Here and in the following, all representations are assumed to be finite-dimensional.) It is easy to see that the matrix elements of the completely reducible representations of $\mathbb{C}[X]$ (i.e., the representations for which the image of X is diagonalizable) belong to $\mathcal{K}$, whereas the other elements of $\mathbb{C}[X]^\circ$ stem from those representations which are not completely reducible. Note that, once again, the close relationship between complete reducibility and the existence of nontrivial integrals shows up.

Returning to the situation at the beginning of this appendix, we have to assume that

$$\mathcal{A}_e \subset U(\mathfrak{sl}(m))^\circ \otimes U(\mathfrak{sl}(n))^\circ \otimes \mathcal{K}.$$

According to the foregoing discussion, this corresponds to the requirement to consider only those representations of $\mathfrak{g} = \mathfrak{sl}(m|n)$ for which the one-dimensional center of $\mathfrak{g}_0^-$ is represented by diagonalizable operators, which is usually assumed anyway.

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Geodesic hierarchies and involutivity

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We consider a special class of pseudo-Riemannian metrics that admit integrals in involution. A necessary and sufficient conditions for the complete integrability of the geodesic flows of the corresponding metrics is proved. Any of the metrics we consider lies in a big family (hierarchy) of metrics that also admit integrals in involution. Many classical and new examples of completely integrable metrics lie in such hierarchies. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The main purpose of the present paper is to prove the Liouville integrability of a class of pseudo-Riemannian metrics. The main idea of the proof of the involutivity of the corresponding first integrals is based on the observation that the metrics we consider lie in a big family (hierarchy) of metrics that also admit first integrals. The technique we use allows us to extend the main results proven in Refs. 1–5 to the case of pseudo-Riemannian metrics. In the present paper the word ''metric'' means *pseudo-Riemannian metric*, i.e., nondegenerate symmetric tensor field of type (0,2). The positive definite metrics are called Riemannian metrics.

Suppose that g and $\overline{g}$ are smooth metrics given on the smooth n-dimensional manifold M^n.

Definition 1: The metrics g and $\overline{g}$ are called geodesically equivalent *if they have the same geodesics (considered as unparemetrized curves).*

Having the metric g and $\overline{g}$ on M^n define the operator,

$$A(g,\overline{g})_j^i \stackrel{\text{def}}{=} \left|\frac{\det \overline{g}}{\det g}\right|^{1/(n+1)} \overline{g}^{i\alpha} g_{\alpha j}. \tag{1}$$

Consider the one-parameter family of functions on the tangent bundle TM^n given by the formula

$$K_c(g,\overline{g})(\xi) \stackrel{\text{def}}{=} \det(A+c\mathbf{1})g((A+c\mathbf{1})^{-1}\xi,\xi), \tag{2}$$

where c is a real parameter $A \stackrel{\text{def}}{=} A(g,\overline{g})$ and $\xi \in TM^n$. The functions K_c are well-defined on the whole manifold M^n for all real parameters c. Moreover, it can be easily seen that

$$K_c(\xi) = I_{n-1}(\xi)c^{n-1} + I_{n-2}(\xi)c^{n-2} + \cdots + I_0(\xi) \tag{3}$$

and $I_{n-1}(\xi) = g(\xi,\xi)$.

Theorem 1: *If the metrics g and $\overline{g}$ are geodesically equivalent, then the functions from the one-parameter family (2) are in involution with respect to the symplectic structure $\omega_g \stackrel{\text{def}}{=} FL_g^* \omega$, where $FL_g: TM \to T^*M$ is the Legendre transformation corresponding to the metric g and ω is the canonical symplectic structure on the cotangent bundle T^*M^n.*

Remark 1: Formula (3) shows that if some function F commutes with K_c for n different values of the parameter c, then these functions commute for all values of the parameter c. Moreover, F commutes with the coefficients $I_k (k=0,\ldots,n-1)$. As a corollary we obtain that the functions I_k $(k=0,\ldots,n-1)$ are in involution, and therefore, they are integrals of the geodesic flow of the metric g.

Suppose that the the metrics g and $\overline{g}$ are geodesically equivalent.

Definition 2: The number

$$r(g,\overline{g})\overset{\text{def}}{=}\max_{\xi\in TM^n}\ \mathrm{rk}\{d_\xi I_0,\ldots,d_\xi I_{n-1}\} \tag{4}$$

is called rank of the geodesic equivalence of the pair g and $\overline{g}$.

An equivalent definition in terms of the invariants of the operator $A(g,\overline{g})$ is given in Sec. III B (Definition 4). Indeed, denote by $r(g,\overline{g})(x)$ the degree of the minimal polynomial of the operator $A(g,\overline{g})|_x$. We prove in Sec. III B that $r(g,\overline{g})=\max_{x\in M^n} r(g,\overline{g})(x)$.

The smooth functions $F_1,\ldots,F_k$ given on the manifold V^m are called *functionally independent* if the set of points $x\in V^m$ where the differentials $d_xF_1,\ldots,d_xF_k$ are linearly independent is dense in V^m.

Theorem 2: *Suppose that the manifold M^n is connected and let the rank of the geodesic equivalence of the pair of geodesically equivalent metrics g and $\overline{g}$ is r; then there exist r quadratic in velocities functions $B_1(\xi),\ldots,B_r(\xi)$, $\xi\in TM$, such that the next three conditions are satisfied:*

(a) the functions $B_1,\ldots,B_r$ are pairwise commuting integrals of the geodesic flow of the metric g;

(b) the functions $B_1,\ldots,B_r$ are functionally independent on TM;

(c) for every fixed value of the parameter c there exist r constants $\alpha_1,\ldots,\alpha_r$ (depending on c) such that $K_c(\xi)=\Sigma_{i=1}^r\alpha_iB_i(\xi)$.

The functions $B_1,\ldots,B_r$ can be taken in the form $B_k=^{\text{def}}I_{i_k}$ where $0\leqslant i_k\leqslant n-1$ are some specially chosen different integer numbers.

Remark 2: Actually, in Theorem 2 we can take $B_1=^{\text{def}}I_{n-1},\ldots,B_r=^{\text{def}}I_{n-r}$. Another system of functions that satisfy conditions (a), (b), and (c) of Theorem 2 can be obtained if we put $B_1=^{\text{def}}K_{c_1},\ldots,B_r=^{\text{def}}K_{c_r}$ where $c_1,\ldots,c_r$ are arbitrary taking different real constants such that the integrals $K_{c_k}(k=1,\ldots,r)$ are not identically equal to zero.

Remark 3: It follows from Theorem 2 that the set of the points $x\in M^n$, where the degree of the minimal polynomial of the operator $A(g,\overline{g})|_x$ coincides with the rank of the geodesic equivalence $r(g,\overline{g})$ is open and dense in M^n.

Remark 4: Theorem 1 generalizes the classical results proved by Dini, Painlevé, Levi-Civita, and Liouville that the geodesic flows of the geodesically equivalent metrics g and $\overline{g}$ admit first integrals (see Refs. 6 and 7). The fact that the geodesic flows of the metrics g and $\overline{g}$ admit globally defined functionally independent integrals in involution (provided the metric g is positive definite) was first proven in Refs. 1 and 2 (see also Refs. 3, 4, and 5). Theorem 1 and Theorem 2 generalize all these results.

Corollary 1: Suppose that the metrics g and $\overline{g}$ are geodesically equivalent. If the differentials $d_{\xi_0}I_{n-1},\ldots,d_{\xi_0}I_0$ are linearly independent at some point $\xi_0\in TM^n$, then the rank of the geodesic equivalence of the pair g and $\overline{g}$ is equal to n and the geodesics flow of the metrics g and $\overline{g}$ are completely integrable.

Theorem 3: *Suppose that the metrics g and $\overline{g}$ are nontrivially geodesically equivalent (i.e., $g\neq\mathrm{const}\,\overline{g}$); then the rank $r(g,\overline{g})$ of the geodesic equivalence of the pair g and $\overline{g}$ is greater than or equal to two and any of the geodesic flows of the metrics g and $\overline{g}$ admits a first integral that is functionally independent of the energy almost everywhere on TM^n.*

The paper is organized as follows: In Sec. II we give the definition of the geodesic hierarchies and prove that the functions given by formula (2) are integrals of the geodesic flow of the metric g. In Sec. III we prove theorems 1, 2, and 3. Combining all these results we prove in Sec. III C Theorem 7 that assigns to any pair of geodesically equivalent metrics a hierarchy of functions in involution. In Sec. IV we apply the results obtained in the previous sections to a special case of geodesic equivalence in $\mathbf{R}^n$. Constructing the corresponding *projective hierarchy* we prove Theorems 8, 9, 10, and 11. As a corollary from Theorem 9 we obtain the theorem that was proven in

Ref. 1 (and independently in Ref. 8) that the standard ellipsoid admits a nontrivial geodesic equivalence. Theorem 9 shows that the same result is true also for the hyperboloids. Moreover, there exists a geodesic family of metrics dg_c^2 [given by formula (60)] having the property that the restriction of dg_c^2 to any of the quadrics from a fixed confocal family gives a metric that is geodesically equivalent to the restriction of the standard Euclidean metric on the same quadric. In Sec. IV we prove that the Euclidean metric in $\mathbf{R}^n$, the hyperbolic plane, and the analog of the Poisson sphere that corresponds to the Clebsch case of motion of the rigid body lie in the projective hierarchy. As corollaries we obtain the results proven in Ref. 4. A pseudo-Riemannian analog of the results proven in Ref. 4 is given. In Sec. IV B we find a family of functions in involution in $T^*\mathbf{R}^n$. The family contains the integrals obtained by Uhlenbeck in Ref. 9 and Moser in Ref. 10 as a particular case.

Throughout the paper together with the common tensor notations (with or without indices) we use the next convention. Let b be a bilinear form given on the manifold M^n. The formula $\xi \mapsto b(.,\xi)$ $(\xi \in TM^n)$ gives a fiberwise transformation of the bundles $TM^n \to T^*M^n$ that we denote by the same letter. Vice versa, any fiberwise linear transformation $K: TM^n \to T^*M^n$ gives a bilinear form by the formula $K(\xi,\eta) = {}^{\text{def}}\langle K\eta, \xi\rangle$, where the brackets $\langle .,. \rangle$ denote the standard pairing between vectors and covectors. If b is nondegenerate, then b^{-1} denotes the inverse transformation, i.e., $b^{-1}: T^*M^n \to TM^n$. Let A be a fiberwise linear transformation of the tangent bundle, i.e., $A \in \Gamma(\mathrm{Hom}(TM^n, TM^n))$. Denote by A' the transformation of the cotangent bundle T^*M^n given by the formula $p \mapsto \langle p, A(.)\rangle$. Let a be a nondegenerate bilinear form given on the manifold M^n. Using the previous duality we treat the compositions bA, $A'b$ or Aa^{-1} as bilinear forms on the corresponding bundles.

II. GEODESIC FAMILIES AND HIERARCHIES

This section has an informative character. In the first part we prove that the functions given by formula (2) are integrals of the geodesic flow of the metric g. In the second part we give the notion of the geodesic hierarchy. The existence of hierarchies is essential in the proof of the commutativity of the integrals given by formula (2).

A. Geodesic families

We follow the ideas presented in Ref. 11. Consider the one-parameter family of metrics

$$g_c(g,\overline{g})(\xi,\eta) = {}^{\text{def}} \frac{1}{\det(A + c\mathbf{1})} g((A + c\mathbf{1})^{-1}\xi, \eta), \tag{5}$$

where c is a real parameter $A = {}^{\text{def}} A(g,\overline{g})$ and $\xi, \eta \in TM^n$. The metric g_c is well-defined at the points of M^n where the operator $(A + c\mathbf{1})$ is invertible.

Theorem 4: *Suppose that the metric g_c is well-defined on some open subset $U \subset M^n$ for some fixed value of the parameter c; then the metrics g and g_c are geodesically equivalent on U.*

Remark 5: If the manifold M^n is compact, then the operator $(A + c\mathbf{1})$ is invertible on M^n for all sufficiently big parameters c.

Proof of Theorem 4: To prove the theorem we need the next lemma.

Lemma 1:

(1) Suppose that the pseudo-Riemannian metrics g and $\overline{g}$ are geodesically equivalent; then the tensors a_{ij} and λ_i,

$$a_{ij} = {}^{\text{def}} A_i^\alpha g_{\alpha j}, \tag{6}$$

$$\lambda_i = {}^{\text{def}} -A_i^\alpha \psi_\alpha, \tag{7}$$

where $(n+1)\psi_i=\frac{1}{2}\partial_i \ln|\overline{g}/g|$, $g=\det(g_{ij})$, *and the operator A is given by formula (1) satisfy the equation*

$$a_{ij,k}=\lambda_i g_{jk}+\lambda_j g_{ik}. \tag{8}$$

Here $a_{ij,k}$ *denotes the covariant derivative* $\nabla_k a_{ij}$, *where* ∇ *is the Levi-Civita connection corresponding to the metric g.*

(2) Conversely, if a nondegenerate symmetric tensor field a_{ij} *and an 1-form* λ_i *satisfy Eq. (8), then the metric*

$$\overline{g}_{ij}\overset{\text{def}}{=}\left(\frac{\hat{g}}{g}\right)\hat{g}_{ij}, \tag{9}$$

where $\hat{g}_{ij}\overset{\text{def}}{=}g_{i\alpha}a^{\alpha\beta}g_{\beta j}$, *is geodesically equivalent to g.*

The statement of this lemma is proven (under the condition of ''nontriviality'' of the geodesic equivalence) in Ref. 12. A geodesic equivalence is said to be ''nontrivial'' if the covector field ψ_k is not identically equal to zero. Nevertheless, the proof proposed in Ref. 12 passes also in our case.

Remark 6: To avoid any confusion recall that we use the expression "nontrivial geodesic equivalence" in a slightly different sense. In our terminology the metrics g and $\overline{g}$ *are "nontrivially geodesically equivalent" if* $g\neq \text{const}\,\overline{g}$.

Let us return to the proof of Theorem 4. Suppose that the metrics g and $\overline{g}$ are geodesically equivalent. It follows from Lemma 1 that the form a_{ij} given by formula (6) satisfies Eq. (8). Using the obvious relation that $\nabla g=0$ we see that the tensor field $a_c\overset{\text{def}}{=}a+cg$, where the constant c is the same as in the statement of the theorem, also satisfies Eq. (8). Moreover, $a_c\overset{\text{def}}{=}g(A+c\mathbf{1})$ is nondegenerate and applying the inverse part of Lemma 1 we obtain that the metrics g and

$$\overline{g}_c\overset{\text{def}}{=}\frac{\det \hat{g}_c}{\det g}\hat{g}_c \tag{10}$$

$$=\frac{\det(g(A+c\mathbf{1})^{-1})}{\det g}g(A+c\mathbf{1})^{-1} \tag{11}$$

$$=\frac{1}{\det(A+c\mathbf{1})}g(A+c\mathbf{1})^{-1} \tag{12}$$

are geodesically equivalent. Theorem 4 is proved.

As a corollary of Theorem 4 we obtain the next proposition.

Proposition 1: If the metrics g and $\overline{g}$ *are geodesically equivalent, then the functions given by formula (2) are integrals of the geodesic flow of the metric g.*

This theorem was proven by Levi-Civita in the case of positive definite metric g under some additional assumption (see Ref. 6). Actually, he proved the result under the assumption that the number of the roots (without their multiplicities) of the characteristic polynomial $\det(\overline{g}-\lambda g)=0$ is a constant. Remark that in the case of positive definite metric g all roots of the characteristic polynomial are real. Another proof was given by Liouville (see Ref. 6). A proof from a symplectic point of view is given in Refs. 1 and 2 (see also Ref. 13).

Proof of Proposition 1: We follow Ref. 11. Let us fix some point $x_0\in M^n$. It is clear that there exists an open neighborhood $U(x_0)$ of the point x_0 and an interval $(-\epsilon,\epsilon)$ such that the metric g_c given by formula (5) is well-defined on $U(x_0)$ for $c\in(-\epsilon,\epsilon)$. It follows from Theorem 4 that the metrics g and $\overline{g}_c$ are geodesically equivalent. We need the next proposition proved by Painlevé (see Ref. 6).

Proposition 2: If the metrics g and $\overline{g}$ *are geodesically equivalent, then the function given by the formula,*

$$I_0(g,\overline{g})(\xi)\overset{\text{def}}{=}\left|\frac{\det g}{\det \overline{g}}\right|^{2/(n+1)}\overline{g}(\xi,\xi), \tag{13}$$

where $\xi\in TM^n$, *is an integral of the geodesic flow of the metric* g.

One can find the proof of this proposition in Ref. 14 (see Sec. IV A).

Let us return to the proof of Proposition 1. The metrics g and g_c are geodesically equivalent. It follows from Proposition 2 that the function,

$$I_0(g,g_c)\overset{\text{def}}{=}\left|\frac{\det g}{\det g_c}\right|^{2/n+1} g_c \tag{14}$$

$$=\det(A+c\mathbf{1})^2\frac{1}{\det(A+c\mathbf{1})}g(A+c\mathbf{1})^{-1} \tag{15}$$

$$=\det(A+c\mathbf{1})g(A+c\mathbf{1})^{-1} \tag{16}$$

is an integral of the geodesic flow of the metric g on $U(x_0)$ for all $c\in(-\epsilon,\epsilon)$. It follows from Remark 1 that the functions given by formula (2) are integrals of the geodesic flow of the metric g on $U(x_0)$. Finally, recall that the point x_0 was arbitrary chosen. This completes the proof of Proposition 1.

B. Geodesic hierarchies

Suppose that g and $\overline{g}$ are metrics given on the manifold M^n. Denote by A the operator $A=^{\text{def}}A(g,\overline{g})$ given by formula (1). We need the next theorem proven in Ref. 15.

Theorem 5: *If the metrics* g *and* $\overline{g}$ *are geodesically equivalent, then for any integer number* k *the metrics* gA^k *and* $\overline{g}A^k$ *are also geodesically equivalent.*

Therefore, having a pair of geodesically equivalent metrics g and $\overline{g}$ we obtain a sequence of pairs of geodesically equivalent metrics that is called *geodesic hierarchy* of the pair g and $\overline{g}$. To describe the hierarchy we use the next formal diagram,

$$\begin{array}{ccc}
\downarrow & & \downarrow \\
g^{(-1)} & \overset{g.e.}{\leftrightarrow} & \overline{g}^{(-1)} \\
\downarrow & & \downarrow \\
g & \overset{g.e.}{\leftrightarrow} & \overline{g} \\
\downarrow & & \downarrow \\
g^{(1)} & \overset{g.e.}{\leftrightarrow} & \overline{g}^{(1)} \\
\downarrow & & \downarrow \\
g^{(2)} & \overset{g.e.}{\leftrightarrow} & \overline{g}^{(2)} \\
\downarrow & & \downarrow ,
\end{array}$$

where $g^{(k)}=^{\text{def}}gA^k$ and $\overline{g}^{(k)}=^{\text{def}}\overline{g}A^k$ $(k\in\mathbf{Z})$. The main properties of the geodesic hierarchies are investigated in Ref. 11. Some generalizations of the construction are given in Ref. 3. In Refs. 4, 5 the construction of the geodesic hierarchy is applied for constructing new examples of geodesically equivalent metrics and completely integrable systems.

III. INVOLUTIVITY OF THE INTEGRALS

The main purpose of the present section is to prove the involutivity of the integrals given by formula (2), provided the metrics g and $\overline{g}$ are geodesically equivalent. We prove Theorem 1 and 2.

A. Hierarchies and involutivity

Suppose that the metrics g and $\overline{g}$ are geodesically equivalent. Let us fix an arbitrary point $x_0 \in M^n$. It is clear that there exist an open neighborhood $U(x_0)$ of the point x_0 and an interval $(-\epsilon,\epsilon)$, $\epsilon>0$, such that the operator $(A+c\mathbf{1})|_x$ is invertible if $x \in U(x_0)$ and $c \in (-\epsilon,\epsilon)$. Consider the one-parameter family $g_c \stackrel{\text{def}}{=} g_c(g,\overline{g})$, $c \in (-\epsilon,\epsilon)$ [see formula (5)], of geodesically equivalent metrics on $U(x_0)$. Let us fix some $\kappa \in (-\epsilon,\epsilon)$. The metrics g and g_κ are geodesically equivalent on $U(x_0)$. Consider the next subsequence from the geodesic hierarchy of the pair g and g_κ,

$$\begin{array}{ccc}
\downarrow & & \downarrow \\
g & \overset{g.e.}{\leftrightarrow} & g_\kappa \\
\downarrow & & \downarrow \\
g^{(1)} & \overset{g.e.}{\leftrightarrow} & g_\kappa^{(1)} \\
\downarrow & & \downarrow \\
g^{(2)} & \overset{g.e.}{\leftrightarrow} & g_\kappa^{(2)} \\
\downarrow & & \downarrow,
\end{array}$$

where $g^{(l)} \stackrel{\text{def}}{=} gA(g,g_\kappa)^l$ and $g_\kappa^{(l)} \stackrel{\text{def}}{=} g_\kappa A(g,g_\kappa)^l$. The metrics $g^{(2)}$ and $g_\kappa^{(2)}$ are geodesically equivalent. It can be easily seen that $A(g,g_\kappa)=A+\kappa\mathbf{1}$. Hence, $g_\kappa^{(2)} \stackrel{\text{def}}{=} g_\kappa A(g,g_\kappa)^2 = 1/\det(A+\kappa\mathbf{1})\, g(A+\kappa\mathbf{1})$. Let us consider the one-parameter family of integrals $K_\alpha(g_\kappa^{(2)},g^{(2)})$ of the geodesic flow of the metric $g_\kappa^{(2)}$. A direct computation shows that $A(g_\kappa^{(2)},g^{(2)})=(A+\kappa\mathbf{1})^{-1}$. Applying the Legendre transformation corresponding to the metric $g_\kappa^{(2)}$ we obtain that the functions,

$$g_\kappa^{(2)-1} = \det(A+\kappa\mathbf{1})(A+\kappa\mathbf{1})^{-1} g^{-1} \tag{17}$$

and

$$K_\alpha(g_\kappa^{(2)},g^{(2)}) \stackrel{\text{def}}{=} \det((A+\kappa\mathbf{1})^{-1}+\alpha\mathbf{1})((A+\kappa)^{-1}+\alpha\mathbf{1})^{-1} g_\kappa^{(2)-1} \tag{18}$$

$$= \det(\alpha A+(\kappa\alpha+1)\mathbf{1})(\alpha A+(\kappa\alpha+1)\mathbf{1})^{-1} g^{-1} \tag{19}$$

are in involution with respect to the canonical symplectic structure on T^*M^n. Remark that after applying the Legendre transformation corresponding to the metric g the family of integrals (2) takes the form $K_c(g,\overline{g})=\det(A+c)(A+c)^{-1}g^{-1}$, where c is an arbitrary real parameter. Hence, the Poisson bracket $\{K_\kappa,K_{\kappa+1/\alpha}\}$ vanishes for all $\alpha\neq 0$ and $\kappa \in (-\epsilon,\epsilon)$. Fixing n different real numbers $\kappa_i \in (\epsilon,\epsilon)$, $i=1,\ldots,n$, $\kappa_i \neq \kappa_j$ $(i\neq j)$, we obtain that $\{K_{\kappa_i},K_c\}=0$ for all real values of the parameter c. Finally, recall that $K_\mu = I_{n-1}\mu^{n-1}+I_{n-2}\mu^{n-2}+\cdots+I_0$. The last equality and the nondegeneracy of the corresponding Vandermonde determinant show that the functions I_l $(l=1,\ldots,n)$ are linear combinations with constant coefficients of the functions K_{κ_i} $(i=1,\ldots,n)$. Therefore, the integrals given by formula (2) are in involution on $T^*U(x_0)$. The point x_0 was taken arbitrary. This proves Theorem 1.

B. The rank of the family of integrals

Suppose that the metrics g and $\overline{g}$ are geodesically equivalent. Consider the family of integrals $K_c=K_c(g,\overline{g})$ given by formula (2).

Remark 7: Let V be a vector space. It is useful for us to identify the linear space of the quadratic forms on V and the space of the symmetric bilinear forms on V.

For every fixed c the integral K_c gives a smooth section of the vector bundle $\mathrm{Symm}(T^*M^n \otimes T^*M^n)$. Let us fix a point $x\in M^n$ and a vector $\xi\in T_xM^n$. Consider the curves $\gamma_x:\mathbf{R} \to \mathrm{Symm}(T_x^*M^n\otimes T_x^*M^n)$ and $\gamma_x(\xi):\mathbf{R}\to T_x^*M^n$ given by the formulas

$$\gamma_x : c\mapsto K_c|_x \in \mathrm{Symm}(T_x^*M^n\otimes T_x^*M^n) \tag{20}$$

and

$$\gamma_x(\xi): c\mapsto K_c(.,\xi)\in T_x^*M^n. \tag{21}$$

Denote by $\mathrm{Span}(\gamma_x)$ the linear subspace in $\mathrm{Symm}(T_x^*M^n\otimes T_x^*M^n)$ of minimal dimension that contains the image of the curve γ_x. Denote by $\mathrm{Span}(\gamma_x(\xi))$, $\xi\in T_xM^n$, the linear subspace in $T_x^*M^n$ of minimal dimension that contains the image of the curve $\gamma_x(\xi)$. Consider the numbers

$$r_\gamma(x) \overset{\text{def}}{=} \max_{\xi\in T_xM^n} \dim \mathrm{Span}(\gamma_x(\xi)) \tag{22}$$

and

$$R_\gamma(x) \overset{\text{def}}{=} \dim \mathrm{Span}(\gamma_x). \tag{23}$$

Recall that $K_c=I_{n-1}c^{n-1}+I_{n-2}c^{n-2}+\cdots+I_0$.

Lemma 2: The next two statements are satisfied:

(1)

$$R_\gamma(x)=\mathrm{rk}\{I_{n-1}|_x,\ldots,I_0|_x\} \tag{24}$$

and

$$r_\gamma(x)=\max_{\xi\in T_xM^n} \mathrm{rk}\{I_{n-1}|_x(.,\xi),\ldots,I_0|_x(.,\xi)\}; \tag{25}$$

(2) the equality $r_\gamma(x)=\mathrm{rk}\{I_{n-1}|_x(.,\xi),\ldots,I_0|_x(.,\xi)\}$ *is satisfied in an open dense subset in* T_xM^n.

Proof of Lemma 2: The first item of the lemma is obvious. Indeed, it follows from formula (3) that the vector space spanned on the forms $I_{n-1}|_x,\ldots,I_0|_x\in\mathrm{Symm}(T_x^*M^n \otimes T_x^*M^n)$ contains $\mathrm{Span}(\gamma_x)$. Let us fix n different real numbers $c_1,\ldots,c_n$ and consider the forms $K_{c_1}|_x,\ldots,K_{c_n}|_x\in\mathrm{Span}(\gamma_x)$. Using formula (3) and the nondegeneracy of the Vandermonde determinant corresponding to the numbers $c_1,\ldots,c_n$ we see that $I_k|_x\in\mathrm{Span}(\gamma_x)$. Therefore, $\mathrm{Span}(I_{n-1}|_x,\ldots,I_0|_x)=\mathrm{Span}(\gamma_x)$. The same arguments show that $\mathrm{Span}(I_{n-1}|_x(.,\xi),\ldots,I_0|_x(.,\xi))=\mathrm{Span}(\gamma_x(\xi))$.

Let us prove the second item of the lemma. Fixing a basis in T_xM^n consider the $n\times n$-matrix constructing from the coefficients of the linear forms $I_{n-1}|_x(.,\xi),\ldots,I_0|_x(.,\xi)\in T_x^*M^n$. Formula (25) shows that there exists a nondegenerate minor of size $r_\gamma(x)\times r_\gamma(x)$ of this matrix. The corresponding determinant is a homogeneous polynomial of degree $r_\gamma(x)$ in the variables $(\xi_1,\ldots,\xi_n)$, where ξ_i are the coordinates of the vector $\xi\in T_xM^n$. Therefore, the considered minor is nondegenerate in an open dense subset in T_xM^n. Lemma 2 is proved.

Let λ be an eigenvalue of the operator $A|_x$ [see formula (1)]. Denote by $J_{r_1}(\lambda),\ldots,J_{r_k}(\lambda)$ $(1\leqslant r_1\leqslant\cdots\leqslant r_k)$ the Jordan's blocks corresponding to this eigenvalue. The numbers r_i $(i=1,\ldots,k)$ denote the size of the Jordan's blocks. By definition, the Jordan's blocks of size one are numbers, i.e., $J_1(\lambda)=\lambda$. The maximal size r_k of the Jordan's blocks is called *r-number of the eigenvalue* λ [we will denote it by $r(\lambda)$.]

Proposition 3:

(1) The numbers $r_\gamma(x)$ *and* $R_\gamma(x)$ *coincide. Denote by* $r(g,\overline{g})(x)$ *the number* $r(x)=^{\text{def}}r_\gamma(x)=R_\gamma(x)$*;*

(2) Denote by $\lambda_1,\ldots,\lambda_m$ *the eigenvalues of the operator* $A|_x$ *(i.e., the roots of the characteristic polynomial* $\chi_{A|_x}(\lambda)=^{\text{def}}\det(A|_x-\lambda\mathbf{1})$ *without their multiplicities). Then,*

$$r(x)=\sum_{i=1}^{m} r(\lambda_i). \tag{26}$$

In other words $r(x)$ *coincides with the degree of the minimal polynomial of the operator* $A|_x$.

Definition 3: The number $r(x)=r(g,\overline{g})(x)$ *is called* rank of the geodesic equivalence of the pair g and $\overline{g}$ at the point x.

Definition 4: The number $r(g,\overline{g})=^{\text{def}}\max_{x\in M^n} r(g,\overline{g})(x)$ *is called* rank of the geodesic equivalence of the pair g and $\overline{g}$.

Proof of Proposition 3: Without loss of generality it can be assumed that the curves γ_x and $\gamma_x(\xi)$ are given by the formulas

$$c\mapsto(A|_x+c\mathbf{1}_x)^{-1}\in\mathrm{Hom}(T_xM^n,T_xM^n) \tag{27}$$

and

$$c\mapsto(A|_x+c\mathbf{1}_x)^{-1}(\xi)\in T_xM^n, \tag{28}$$

respectively. Moreover, instead of these curves consider their "complexifications" $\gamma_x^{\mathbf{C}}: c\mapsto(A|_x^{\mathbf{C}}+c\mathbf{1}_x)^{-1}\in\mathrm{Hom}^{\mathbf{C}}(T_x^{\mathbf{C}}M^n,T_x^{\mathbf{C}}M^n)$ and $\gamma_x^{\mathbf{C}}(\xi): c\mapsto(A|_x^{\mathbf{C}}+c\mathbf{1}_x)^{-1}(\xi)\in T_x^{\mathbf{C}}M^n$, $\xi\in T_x^{\mathbf{C}}M^n$, where $c\in\mathbf{C}\backslash\{-\lambda_1,\ldots,-\lambda_m\}$ and $A|_x^{\mathbf{C}}$ is the complexification of the operator $A|_x$. By $\mathbf{1}_x$ we denote the identity operator in T_xM^n and $T_x^{\mathbf{C}}M^n$. It is clear that $R_\gamma(x)$ coincides with the complex dimension of the minimal (complex)linear subspace in $\mathrm{Hom}^{\mathbf{C}}(T_x^{\mathbf{C}}M^n,T_x^{\mathbf{C}}M^n)$ that contains the image of the curve $\gamma_c^{\mathbf{C}}$. Analogically, $r_\gamma(x)=\max_{\xi\in T_x^{\mathbf{C}}M^n}\dim_{\mathbf{C}}\mathrm{Span}^{\mathbf{C}}(\gamma_c^{\mathbf{C}}(\xi))$, where $\mathrm{Span}^{\mathbf{C}}(\gamma_c^{\mathbf{C}}(\xi))$ denotes the linear subspace in $T_x^{\mathbf{C}}M^n$ of minimal dimension that contains the image of the curve $\gamma_x^{\mathbf{C}}(\xi)$. Let us fix a basis in $T_x^{\mathbf{C}}M^n$ such that the operator $A|_x^{\mathbf{C}}$ has a Jordan's normal form, i.e., in coordinates, $A|_x^{\mathbf{C}}=\mathrm{diag}(J_\alpha(\lambda_1),\ldots,J_\beta(\lambda_m))$, where $\lambda_1,\ldots,\lambda_m$ are the eigenvalues of the operator and $J_r(\lambda)$ denotes a Jordan's block of size r corresponding to the eigenvalue λ. We have that

$$(A|_x^{\mathbf{C}}+c\mathbf{1}_x)^{-1}=\mathrm{diag}(J_\alpha(\lambda_1+c)^{-1},\ldots,J_\beta(\lambda_m+c)^{-1}). \tag{29}$$

Remark that

$$J_r(\lambda)^{-1}=\begin{bmatrix} 1/\lambda & -1/\lambda^2 & \cdots & (-1)^{r+1}/\lambda^r \\ 0 & 1/\lambda & \cdots & (-1)^r/\lambda^{r-1} \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & 1/\lambda \end{bmatrix}.$$

Let ω_k $(k=1,\ldots,m)$ be a small circle around the eigenvalue λ_k such that the corresponding disk doesn't contain other eigenvalues. Consider the operators

$$M_k^l=(-1)^{l+1}\frac{1}{2\pi i}\oint_{\omega_k}(\lambda_k-z)^l(A|_x^{\mathbf{C}}-z\mathbf{1})^{-1}dz, \tag{30}$$

where $k=1,\dots,m;\ l=0,\dots,r(\lambda_k)-1$.

Lemma 3: The operators M_k^l $(k=1,\dots,m;\ l=0,\dots,r(\lambda_k)-1)$ form a basis of the linear space of minimal dimension that contains the image of the curve $\gamma_x^{\mathbf{C}}$.

Proof of Lemma 3: It follows from the form of the integrand in formula (30) that the operators M_k^l lie in any linear space that contains the image of the curve $\gamma_x^{\mathbf{C}}$. Formula (29) and Cauchy formula show that M_k^l $(k=1,\dots,m;\ l=1,\dots,r(\lambda_k))$ are linearly independent and the vector space spanned on them contains the image of the curve $\gamma_x^{\mathbf{C}}$. Lemma 3 is proved.

It follows from Lemma 3 that $R_\gamma(x)=\Sigma_{i=1}^m r(\lambda_i)$. The second item of Proposition 3 is proved. The first item can be easily proved by direct calculations using the simple form of the operators M_k^l in the Jordan's basis. Proposition 3 is proved.

Remark 8: Suppose that $r=r(g,\overline{g})(x)$. It follows from formula (29) that

$$T(c)|_x\overset{\text{def}}{=}(\lambda_1+c)^{r(\lambda_1)}\ \cdots(\lambda_m+c)^{r(\lambda_m)}(A|_x^{\mathbf{C}}+c\mathbf{1}_x)^{-1} \tag{31}$$

$$=P_{r-1}|_x c^{r-1}+P_{r-2}|_x c^{r-2}\cdots+P_0|_x. \tag{32}$$

It is clear that the forms $P_{r-1}|_x,\dots,P_0|_x$ are linearly independent. Therefore, if we take r real constants $c_1,\dots,c_r$ $(c_i\neq c_j(i\neq j))$, then the forms $T(c_1)|_x,\dots,T(c_r)|_x$ are linearly independent. Formula (2) shows that

$$K_c|_x=(\lambda_1+c)^{n_1-r(\lambda_1)}\ \cdots(\lambda_m+c)^{n_m-r(\lambda_m)}gT(c)|_x, \tag{33}$$

where n_k denotes the multiplicity of λ_k in the characteristic polynomial of the operator $A|_x$. Hence, if $K_{c_i}|_x\neq 0$ $(i=1,\dots,r)$, then the forms $K_{c_1}|_x,\dots,K_{c_r}|_x$ give a basis of the linear space of minimal dimension that contains the image of the curve $\gamma_x^{\mathbf{C}}$. It follows from formula (33) that the forms $I_{n-1}|_x,\dots,I_{n-r}|_x$ give another basis.

Theorem 6: *Suppose that the manifold M^n is connected and the rank of the geodesic equivalence of the pair g and $\overline{g}$ (given by Definition 4) is r; then there exist r quadratic in velocities functions $B_1(\xi),\dots,B_r(\xi)$, $\xi\in TM$, such that the next three conditions are satisfied:*

(a) The functions $B_1,\dots,B_r$ are pairwise commuting integrals of the geodesic flow of the metric g;

(b) The functions $B_1,\dots,B_r$ are functionally independent on TM;

(c) For every fixed value of the parameter c there exists r constants $\alpha_1,\dots,\alpha_r$ (depending on c) such that $K_c(\xi)=\Sigma_{i=1}^r\alpha_i B_i(\xi)$.

The functions $B_1,\dots,B_r$ can be taken in the form $B_k\overset{\text{def}}{=}I_{i_k}$, where $0\leqslant i_k\leqslant n-1$ are some specially chosen different integer numbers.

Remark 9: Actually, in Theorem 6 we can take $B_1\overset{\text{def}}{=}I_{n-1},\dots,B_r\overset{\text{def}}{=}I_{n-r}$. Another system of functions that satisfy conditions (a), (b), and (c) of Theorem 6 can be obtained if we put $B_1\overset{\text{def}}{=}K_{c_1},\dots,B_r\overset{\text{def}}{=}K_{c_r}$ where $c_1,\dots,c_r$ are arbitrarily taking different real constants such that the integrals K_{c_k} $(k=1,\dots,r)$ are not identically equal to zero.

Remark 10: It follows from Theorem 6 and Remark 8 that for every point x on the manifold M^n the dimension of the linear space spanned on the quadratic forms $B_1|_x,\dots,B_r|_x$ coincides with the rank of the geodesic equivalence of the pair g and $\overline{g}$ at x. Indeed, it follows from item (c) of Theorem 6 that $I_{n-i}=\Sigma_{i=1}^r\alpha_i^l B_l$ $(i=1,\dots,r)$, where (α_i^l) is a constant matrix. If x is a point of maximal rank [i.e., $r(g,\overline{g})(x)=r$], then $I_{n-1}|_x,\dots,I_{n-r}|_x$ are linearly independent. Therefore, $B_1|_x,\dots,B_r|_x$ are also linearly independent and the matrix (α_i^l) is nondegenerate.

Proof of Theorem 6: Suppose that the metrics g and $\overline{g}$ are geodesically equivalent.

Definition 5: A point $x_0 \in M^n$ is called stable *if the rank of the geodesic equivalence $r(g,\overline{g})\times(x)$ is equal to some constant s in an open neighborhood of the point x_0. In this case we say that x_0 is a stable point of rank s.*

Definition 6: A point $x_0 \in M^n$ is called singular *if it is not stable.*

Denote by $\mathcal{M}(g,\overline{g})$ the set of the stable points on M^n.

Lemma 4: The set of the stable points $\mathcal{M}(g,\overline{g})$ is everywhere dense in M^n.

Proof of Lemma 4: Let us fix a point $x_0 \in M^n$. It follows from Lemma 2 that $r(x)$ coincides with the dimension of the vector space spanned on the forms $I_{n-1}|_x, \ldots, I_0|_x \in \mathrm{Symm}(T_x^* M^n \otimes T_x^* M^n)$. It gives that the inequality $r(x) \geqslant r(x_0)$ is satisfied in an open neighborhood of x_0. Therefore, *if x_0 is a singular point, then every open neighborhood of x_0 contains a point y such that $r(y) > r(x_0)$.*

Suppose that the open set V consists of singular points. Let us take a point $p_1 \in V$. The point p_1 is singular. Hence, there is a point $p_2 \in V$ such that $r(p_2) > r(p_1)$. But the point p_2 is also singular. Applying the last argument several times we see that there exists a singular point $p_k \in V$ such that $r(p_k) = n$. From another side it is clear that the points of maximal rank are stable. This is a contradiction. Lemma 4 is proved.

Let us return to the proof of Theorem 6. Denote by r the rank of the geodesic equivalence of the pair g and $\overline{g}$. First of all, let us prove a local variant of Theorem 6.

Lemma 5: Suppose that x_0 is a stable point of rank s; then there exists an open neighborhood $U(x_0)$ of the point x_0 and quadratic in velocities functions $B_1, \ldots, B_s$ such that statements (a), (b), and (c) of Theorem 6 are satisfied. Moreover, for every point $x \in U(x_0)$, the set of the points $\xi \in T_x M^n$, are linearly independent is open and dense in $T_x M^n$.

Proof of Lemma 5: Suppose that $x_0 \in M^n$ is a stable point of rank s. It follows from Lemma 2 that we can choose s different integer numbers $0 \leqslant i_k \leqslant n-1$ $(k=1,\ldots,s)$ (see also Remark 8) such that the forms $I_{i_1}|_{x_0}, \ldots, I_{i_s}|_{x_0}$ are linearly independent. Let us define $B_1 = {}^{\mathrm{def}} I_{i_1}, \ldots, B_s = {}^{\mathrm{def}} I_{i_s}$. It is clear that the forms $B_k|_x$ $(k=1,\ldots,s)$ are linearly independent for every x from an open neighborhood $U(x_0)$ of the point x_0. We can take $U(x_0)$ such that $r(g,\overline{g})(x) = r$ on $U(x_0)$. Remark that the set of the points $\xi \in TU(x_0)$ where the differentials $d_\xi B_k$ $(k=1,\ldots,s)$ are linearly independent is open and dense in $TU(x_0)$. Moreover, the intersection of this set with any tangent plane $T_x U(x_0)$ is open and dense in $T_x U(x_0)$. Indeed, it follows from Lemma 2 that the set of the points $\xi \in T_x M^n$ where the differentials $d_\xi(B_k|_{T_x M^n}) = 2B_k(.,\xi)$ $(k=1,\ldots,s)$ are linearly independent is open and dense subset in $T_x M^n$.

Let us fix a real constant c and consider the form K_c. We have that $K_c(\xi) = \Sigma_{k=1}^s \alpha_k(x) B_k(\xi)$, $\xi \in TU(x_0)$, where $\alpha_k(x)$ are smooth functions on $U(x_0)$. Denote by E_g the energy function $E_g(\xi) = {}^{\mathrm{def}} \frac{1}{2} g(\xi,\xi)$. We have $0 = \{E_g, K_c\} = \Sigma_{k=1}^s \{E_g, \alpha_k\} B_k$. Hence, the Poisson brackets $\{E_g, \alpha_k\}$ vanish. It gives that α_k $(k=1,\ldots,s)$ are constants. Lemma 5 is proved.

Let us prove item (b) of Theorem 6.

Lemma 6: Let x and y be two points on M^n connected by a geodesic line and let $D(y)$ be an open neighborhood of the point y. Suppose that the set of the points $\xi \in T_x M^n$, where the differentials $d_\xi B_1, \ldots, d_\xi B_r$ are linearly independent is open and dense in $T_x M^n$; then there exists a point $y' \in D(y)$ such that the set of the points $\eta \in T_{y'} M^n$ where the differentials $d_\eta B_1, \ldots, d_\eta B_r$ are linearly independent is open and dense in $T_{y'} M^n$.

Proof of Lemma 6: Without loss of generality it can be assumed that y is a stable point of rank $r(y) = r_1$. Therefore, we can find an open neighborhood $V(y) \subset D(y)$ of the point y where the rank $r(u) = r_1$ $(u \in V(y))$ and the statements of Lemma 5 are satisfied. In particular, there exist functionally independent on $TV(y)$ functions $Q_1, \ldots, Q_{r_1}$ such that $B_k = \Sigma_{i=1}^{r_1} \beta_k^i Q_i$, where β_k^i are some constants. Therefore,

$$dB_k = \sum_{i=1}^{r_1} \beta_k^i dQ_i. \tag{34}$$

The points x and y can be connected by a geodesic. It can be easily seen that there exists a vector

$\xi \in T_x M^n$ such that $\exp(\xi) \in V(y)$ and the differentials $d_\xi B_k$ $(k=1,\ldots,r)$ are linearly independent. Using the fact that the functions B_k are integrals of the geodesic flow of the metric g we see that the differentials $d_w B_k$, where $w =^{\text{def}} d/dt\,|_{t=1} \exp(t\xi) \in TV(y)$, are linearly independent. Let us take $y' =^{\text{def}} \exp(\xi)$. It follows from formula (34) that $d_w B_k = \Sigma_{i=1}^{r_1} \beta_k^i d_w Q_i$. The last equality is possible only if the rank of the matrix (β_k^i) is equal to r and $r_1 \geqslant r$. By definition $r \geqslant r_1$. Hence, the square matrix (β_k^i) is nondegenerate. Therefore, dB_k $(k=1,\ldots,r)$ are linearly independent at the same points where dQ_k $(k=1,\ldots,r_1)$ are linearly independent. Finally, the statement of Lemma 6 follows from Lemma 5. Lemma 6 is proved.

Let us fix a point $x_0 \in M^n$. Suppose that x_0 is a stable point of rank r. Consider the functions $B_1,\ldots,B_r$ given by Lemma 5. These functions are invariantly defined on the whole manifold M^n (by definition, $B_k =^{\text{def}} I_{i_k}$). Assume that there exists an open set W in TM^n such that if $\xi \in W$ then the differentials $d_\xi B_k$ $(k=1,\ldots,r)$ are linearly dependent. Let us take a point $y_0 \in \pi(W)$, where $\pi: TM^n \to M^n$ denotes the natural projection on M^n. Provided the manifold M^n is connected, we can choose a sequence of points $x_0, x_1, \ldots, x_N = y_0$ and open neighborhoods $W(x_0), W(x_1), \ldots, W(x_N), W(x_N) \subseteq \pi(W)$ of these points such that any two points $u \in W(x_i)$ and $v \in W(x_{i+1})$ can be connected by a geodesic $(0 \leqslant i \leqslant N-1)$. Applying Lemma 6 successively we obtain that there exists a point $y_0' \in \pi(W)$ such that the set of the points $\eta \in T_{y_0'} M^n$ where the differentials $d_\eta B_1, \ldots, d_\eta B_r$ are linearly independent is open and dense in $T_{y_0'} M^n$. This is a contradiction. Item (b) is proved.

It follows from item (b) and Lemma 5 that the forms $B_k|_x$ $(k=1,\ldots,r)$ are linearly independent for every fixed x from an open and dense subset $\mathcal{K}$ in M^n. Indeed, the assumption that these forms are linearly dependent for every fixed x from an open subset in M^n implies (see Lemma 5) that there exists an open subset U in M^n such that $\Sigma_{i=1}^r \beta_i B_i = 0$ on U, where β_i are some constants. This contradicts to item (b). It is clear that for any two points $x \in \mathcal{K}$ and $y \in \mathcal{K}$ there exists a sequence $\{\xi_i\}_{i=1}^{N-1} \subset T\mathcal{K}$, $\xi_1 \in T_x M^n$, such that for every fixed $1 \leqslant i \leqslant N-1$ the differentials $d_{\xi_i} B_1, \ldots, d_{\xi_i} B_r$ are linearly independent and $\exp(\xi_i) = x_{i+1}$ $(i=1,\ldots,N-1)$, $x_N = y_0$. Let us fix a value c and consider the integral K_c given by formula (2). As in the proof of Lemma 5 we see that there exist open neighborhoods $U(x_1), \ldots, U(x_N)$ of the points $x_1, \ldots, x_N$, respectively, such that $K_c(\xi) = \Sigma_{s=1}^r \alpha_i^s B_s(\xi)$, where α_i^k are constants and $\xi \in TU(x_i)$ $(i=1,\ldots,N)$. We have $d_{\xi_1} K_c = \Sigma_{s=1}^r \alpha_1^s d_{\xi_1} B_s$. From another side,

$$d_{\xi_1} K_c = d_{\zeta^1(\xi_1)} K_c \circ \zeta_*^1 \tag{35}$$

$$= \sum_{s=1}^r \alpha_2^s d_{\zeta^1(\xi_1)} B_s \circ \zeta_*^1 \tag{36}$$

$$= \sum_{s=1}^r \alpha_2^s d_{\xi_1} B_s, \tag{37}$$

where $\zeta^t: TM^n \to TM^n$ denotes the geodesic flow corresponding to the metric g. The linear independence of the differentials $dB_1, \ldots, dB_r$ at ξ_1 shows that $\alpha_1^s = \alpha_2^s$ $(s=1,\ldots,r)$. Applying this constriction successively we obtain that $\alpha_1^s = \alpha_2^s = \cdots = \alpha_N^s$ $(s=1,\ldots,r)$. Therefore, $K_c = \Sigma_{s=1}^r \alpha_1^s B_s$ on $\mathcal{K}$. Using the fact that $\mathcal{K}$ is open and dense in M^n we prove item (c). This completes the proof of Theorem 6.

Remark 11: It follows from Theorem 6 that all stable points on M^n have the same rank.

As a simple corollary from Theorem 6 we obtain the next proposition.

Proposition 4: The rank of the geodesic equivalence of the pair g and $\overline{g}$ coincides with the number,

$$\rho \overset{\text{def}}{=} \max_{\xi \in TM^n} \operatorname{rk}\{d_\xi I_0, \ldots, d_\xi I_{n-1}\}. \tag{38}$$

Finally, Theorem 2 and Theorem 3 follow directly from Theorem 6 and Proposition 4.

Remark 12: Let g be a metric and $A \in \Gamma(\operatorname{Hom}(TM^n, TM^n))$ be an operator given on the manifold M^n. Suppose that the one-parameter family of functions on TM^n,

$$K_c(g,A) = \text{def}\det(A + c\mathbf{1})g(A + c\mathbf{1})^{-1} \tag{39}$$

$$= I_{n-1}(g,A)c^{n-1} + I_{n-2}(g,A)c^{n-2} + \cdots + I_0(g,A) \tag{40}$$

are integrals of the geodesic flow of the metric g. Denote by $r(g,A)(x)$ the degree of the minimal polynomial of the operator $A|_x$. Let $r = r(g,A) = \overset{\text{def}}{} \max_{x \in M^n} r(g,A)(x)$. It can be easily seen that statements (b) and (c) of Theorem 6 still hold. Moreover, the number $r(g,A)$ coincides with the number,

$$\rho(g,A) \overset{\text{def}}{=} \max_{\xi \in TM^n} \operatorname{rk}\{d_\xi I_0, \ldots, d_\xi I_{n-1}\}. \tag{41}$$

Theorem 6 admits us to prove the next corollary.

Corollary 2: Suppose that the metrics g and $\overline{g}$ are geodesically equivalent. Suppose in addition that the manifold M^n is connected and let $x_0 \in M^n$ be a point of maximal rank [i.e., $r(g,\overline{g}) \times (x_0) = r(g,\overline{g})$]. Denote by $m(\lambda)$ the multiplicity of the eigenvalue λ of the operator $A(g,\overline{g})|_{x_0}$ and let $r(\lambda)$ be the corresponding r-number (see Sec. III B); then if $m(\lambda) - r(\lambda) > 0$ the value λ is an eigenvalue of the operator $A(g,\overline{g})|_x$ for every point x on M^n.

Proof of Corollary 2: Let $\lambda \in \mathbf{C}$ be an eigenvalue of the operator $A(g,\overline{g})|_{x_0}$ such that $m(\lambda) - r(\lambda) > 0$. It follows from Theorem 6 that

$$K_\lambda = \sum_{k=1}^{r} \alpha_k I_{n-k}, \tag{42}$$

where $\alpha_1, \ldots, \alpha_r$ are constants. Formula (33) shows that $K_\lambda|_{x_0} = 0$. From another side, the forms $I_{n-1}|_{x_0}, \ldots, I_{n-r}|_{x_0}$ are linearly independent (see Remark 8). Therefore, $\alpha_i = 0$ $(i = 1, \ldots, r)$ and $K_\lambda \equiv 0$ on M^n. Finally, the statement of the corollary follows from formula (33). Corollary 2 is proved.

Combining Corollary 2 and Theorem 6 we obtain the next criterion.

Proposition 5: The integrals given by formula (2) are enough for the complete integrability of the geodesic flow of the metric g iff the equation $K_\lambda \equiv 0$ (on M^n) does not have a constant solution $\lambda \in \mathbf{C}$.

C. Associated hierarchy of functions in involution

Combining theorems 1, 2, and 5 we obtain the next theorem.

Theorem 7: *Suppose that the metrics g and $\overline{g}$ are geodesically equivalent. For every integer l consider the family of functions on T^*M^n,*

$$K_\alpha^{(l)}(g,\overline{g}) \overset{\text{def}}{=} \det(A + \alpha\mathbf{1})(A + \alpha\mathbf{1})^{-1} A^{-l} g^{-1} \tag{43}$$

$$= I_{n-1}^{(l)} \alpha^{n-1} + I_{n-2}^{(l)} \alpha^{n-2} + \cdots + I_0^{(l)}, \tag{44}$$

where $A=A(g,\overline{g})$ is given by formula (1). Then the functions $I^{(l)}_{n-1},\dots,I^{(l)}_0$ are in involution with respect to the canonical symplectic structure on T^*M^n. If the rank of the geodesic equivalence of the pair g and $\overline{g}$ is r, then the functions $I^{(l)}_{n-1},\dots,I^{(l)}_{n-r}$ are functionally independent.

Proof of Theorem 7: Let us consider the geodesic hierarchy of the pair g and $\overline{g}$,

$$\begin{array}{ccc} \downarrow & & \downarrow \\ g^{(l-1)} & \overset{g.e.}{\leftrightarrow} & \overline{g}^{(l-1)} \\ \downarrow & & \downarrow \\ g^{(l)} & \overset{g.e.}{\leftrightarrow} & \overline{g}^{(l)} \\ \downarrow & & \downarrow, \end{array}$$

where $g^{(l)}=^{\text{def}}gA^l$, $\overline{g}^{(l)}=^{\text{def}}\overline{g}A^l$, and l is a fixed integer number. It follows from formula (1) that $A(g^{(l)},\overline{g}^{(l)})=A(g,\overline{g})$. Therefore, the one-parameter family of functions

$$K_\alpha(g^{(l)},\overline{g}^{(l)})\overset{\text{def}}{=}\det(A+\alpha\mathbf{1})(A+\alpha\mathbf{1})^{-1}g^{(l)-1} \tag{45}$$

$$=\det(A+\alpha\mathbf{1})(A+\alpha\mathbf{1})^{-1}A^{-l}g^{-1} \tag{46}$$

are in involution with respect to the canonical symplectic structure on T^*M^n. It is clear that the rank of the geodesic equivalence of the pair $g^{(l)}$ and $\overline{g}^{(l)}$ is the same as the rank of the geodesic equivalence of the initial pair g and $\overline{g}$. Theorem 7 is proved.

IV. PROJECTIVE HIERARCHY

Let us consider the projective space $\mathbf{RP}^n=^{\text{def}}\{(x_1:\cdots:x_{n+1})\}$ and fix the affine chart $\mathbf{R}^n\cong\{x_{n+1}=1\}\hookrightarrow\mathbf{R}^{n+1}$. Any nondegenerate linear transformation L of $\mathbf{R}^{n+1}$ gives a projective transformation of $\mathbf{RP}^n$ that acts on the affine chart $\mathbf{R}^n$ as a linear-fractional transformation that we denote by μ_L. If the projective transformation μ_L is not an affine transformation, then it is a partially defined transformation that is not defined over a hyperplane Z_L in $\mathbf{R}^n$. It is clear that if a straight line l is not contained in Z_L, then the image $\mu_L(l)$ is a straight line.

Let us consider the projective transformation of the plane $\mathbf{R}^n$ given by the formula,

$$\mu:\begin{cases} x_1 & \mapsto & (\lambda_1x_1)/x_n \\ & \vdots & \\ x_{n-1} & \mapsto & (\lambda_{n-1}x_{n-1})/x_n \\ x_n & \mapsto & \lambda_n-\lambda_n/x_n \end{cases},$$

where λ_i $(i=1,\dots,n)$ are nonzero constants. Consider the metric $dg^2=^{\text{def}}\epsilon_1dx_1^2+\cdots\epsilon_ndx_n^2$ on $\mathbf{R}^n$, where $\epsilon_i=\pm1$. The geodesics of the metric g are straight lines. Denote by $\overline{g}$ the pullback μ^*g. Remark that the metric $\overline{g}$ is not defined over the hyperplane $Z=^{\text{def}}\{x_n=0\}$. It is clear that the metrics g and $\overline{g}$ are geodesically equivalent on $\mathcal{D}=^{\text{def}}\mathbf{R}^n\backslash Z$. Our aim is to compute the geodesic hierarchy corresponding to the pair of geodesically equivalent metrics g and $\overline{g}$. We have

$$d\overline{g}^2\overset{\text{def}}{=}\mu^*(dg^2)=\epsilon_1\lambda_1^2\left(\frac{x_ndx_1-x_1dx_n}{x_n^2}\right)^2+\cdots\epsilon_{n-1}\lambda_{n-1}^2\left(\frac{x_ndx_{n-1}-x_{n-1}dx_n}{x_n^2}\right)^2+\epsilon_n\lambda_n^2\left(\frac{dx_n}{x_n^2}\right)^2. \tag{47}$$

Let us compute the operator $A=^{\text{def}}A(g,\overline{g})$. We need the next simple lemmas.

Lemma 7: Consider the matrix,

$$C \overset{\text{def}}{=} \overline{a} \otimes \overline{a} + b, \tag{48}$$

where $b = {}^{\text{def}}\mathrm{diag}(b_1, \ldots, b_n)$, $b_i \neq 0$ $(i = 1, \ldots, n)$, $\overline{a} = {}^{\text{def}}(a_1, \ldots, a_n)'$ *(the symbol* $'$ *denotes the transposition of a matrix) and* $\overline{a} \otimes \overline{a}$ *stands for the matrix* $\overline{a}\overline{a}'$. *Then the inverse matrix* C^{-1} *is given by the formula*

$$C^{-1} = b^{-1} - \frac{1}{D}(b^{-1}\overline{a}) \otimes (b^{-1}\overline{a}), \tag{49}$$

where $D = {}^{\text{def}}\langle b^{-1}\overline{a}, \overline{a}\rangle + 1$ *and* $\langle \overline{x}, \overline{y}\rangle = {}^{\text{def}}\sum_{i=1}^{n} x_i y_i$. *Moreover,* $\det C = (\Pi_{k=1}^{n} b_k) D$.

Proof of Lemma 7: The proof is by direct calculation. We have

$$(\overline{a}\overline{a}' + b)\left(b^{-1} - \frac{1}{D}(b^{-1}\overline{a})(b^{-1}\overline{a})' \right) \tag{50}$$

$$= \overline{a}(\overline{a}' b^{-1}) + E - \frac{\langle \overline{a}, b^{-1}\overline{a}\rangle}{D}\overline{a}(b^{-1}\overline{a})' - \frac{1}{D}\overline{a}(b^{-1}\overline{a})' = E, \tag{51}$$

where E denotes the unit matrix. Lemma 7 is proved.

Lemma 8: Consider the matrix,

$$C_0 \overset{\text{def}}{=} \overline{a} \otimes \overline{a} + \mathrm{diag}(b_1, \ldots, b_{n-1}, 0), \tag{52}$$

where $b_i \neq 0$ $(i = 1, \ldots, n-1)$. *Then the inverse matrix* C_0^{-1} *is given by the formula,*

$$C_0^{-1} = \frac{1}{a_n^2}\left\{ \sum_{i=1}^{n-1} \frac{a_n^2}{b_i} E_{ii} + \left(\sum_{i=1}^{n-1} \frac{a_i^2}{b_i} + 1 \right) E_{nn} - \sum_{i=1}^{n-1} \frac{a_n a_i}{b_i} E_{in} - \sum_{i=1}^{n-1} \frac{a_n a_i}{b_i} E_{ni} \right\}, \tag{53}$$

where the matrix E_{ij} *has elements* $e_{kl} = {}^{\text{def}}\delta_{ki}\delta_{lj}$ $(k, l = 1, \ldots, n)$. *We have that* $\det C_0 = (\Pi_{k=1}^{n-1} b_k) a_n^2$.

Lemma 8 easily follows from Lemma 7 and the formula $C_0^{-1} = \lim_{\alpha \to +0}(C_0 + \alpha)^{-1}$.

Denote by $\overline{G}$ the matrix corresponding to the metric $\overline{g}$, i.e., the Gramian of the metric g. Taking $\overline{a} = \overline{x}$ $(\overline{x} = {}^{\text{def}}(x_1, \ldots, x_n))$, $b_i = (\epsilon_n \lambda_n^2)/(\epsilon_i \lambda_i^2)$ $(i = 1, \ldots, n-1)$, and applying Lemma 8 we see that

$$\overline{G}^{-1} = \frac{x_n^2}{\epsilon_n \lambda_n^2}\left(\overline{x} \otimes \overline{x} + \mathrm{diag}\left(\frac{\epsilon_n \lambda_n^2}{\epsilon_1 \lambda_1}, \ldots, \frac{\epsilon_n \lambda_n^2}{\epsilon_{n-1}\lambda_{n-1}}, 0 \right) \right). \tag{54}$$

As a corollary we obtain that $\det \overline{G} = (-1)^s (\Pi_{i=1}^{n} \lambda_i^2)/x_n^{2n+2}$, where s is the signature of the metric g. Finally, combining (1) and (54) we obtain (up to a multiplication on a constant) that

$$A(g, \overline{g}) = \left(\overline{x} \otimes \overline{x} + \mathrm{diag}\left(\frac{\epsilon_n \lambda_n^2}{\epsilon_1 \lambda_1^2}, \ldots, \frac{\epsilon_n \lambda_n^2}{\epsilon_{n-1}\lambda_{n-1}^2}, 0 \right) \right) \mathcal{E}, \tag{55}$$

where $\mathcal{E} = {}^{\text{def}}\mathrm{diag}(\epsilon_1, \ldots, \epsilon_n)$. Denote for simplicity,

$$\mathcal{A} \overset{\text{def}}{=} \overline{x} \otimes \overline{x} + \mathrm{diag}\left(\frac{\epsilon_n \lambda_n^2}{\epsilon_1 \lambda_1^2}, \ldots, \frac{\epsilon_n \lambda_n^2}{\epsilon_{n-1}\lambda_{n-1}^2}, 0 \right). \tag{56}$$

We have $A = \mathcal{A}\mathcal{E}$.

It follows from Theorem 4 that the one-parameter family of metrics $g_c(g,\overline{g})=^{\text{def}}1/[\det(A+c\mathbf{1})]\,g(A+c\mathbf{1})^{-1}$ are geodesically equivalent to g. We have

$$G_c=^{\text{def}}\frac{1}{\det(\mathcal{A}\mathcal{E}+cE)}\,\mathcal{E}(\mathcal{A}\mathcal{E}+cE)^{-1} \tag{57}$$

$$=\frac{(-1)^s}{\det(\mathcal{A}+c\mathcal{E})}(\mathcal{A}+c\mathcal{E})^{-1}, \tag{58}$$

where G_c denotes the Gramian of the metric g_c. It follows from Lemma 7 that up to a multiplication on a constant we have

$$dg_c^2=\left\{D_c\left(\frac{\epsilon_1 dx_1^2}{d_1+c}+\cdots+\frac{\epsilon_{n-1}dx_{n-1}^2}{d_{n-1}+c}+\frac{\epsilon_n dx_n^2}{c}\right)-\left(\frac{\epsilon_1 x_1 dx_1}{d_1+c}+\cdots+\frac{\epsilon_{n-1}x_{n-1}dx_{n-1}}{d_{n-1}+c}+\frac{\epsilon_n x_n dx_n}{c}\right)^2\right\}/D_c^2, \tag{59}$$

where $d_k=^{\text{def}}\epsilon_n\lambda_n^2/\lambda_k^2$ and

$$D_c=^{\text{def}}\frac{\epsilon_1 x_1^2}{d_1+c}+\cdots+\frac{\epsilon_{n-1}x_{n-1}^2}{d_{n-1}+c}+\frac{\epsilon_n x_n^2}{c}+1. \tag{60}$$

Remark 13: The metric dg_c^2 is not defined on the quadric $Z_c=^{\text{def}}\{D_c=0\}$. The most of the metrics we consider in the present section are not defined on a hypersurface. Nevertheless, from now on when we say that some metrics are geodesically equivalent we mean they are geodesically equivalent in the domain where both of them are defined.

It follows from Theorem 1 that the quadratic forms

$$dK_c^2=D_c\left(\frac{\epsilon_1 dx_1^2}{d_1+c}+\cdots+\frac{\epsilon_{n-1}dx_{n-1}^2}{d_{n-1}+c}+\frac{\epsilon_n dx_n^2}{c}\right)-\left(\frac{\epsilon_1 x_1 dx_1}{d_1+c}+\cdots+\frac{\epsilon_{n-1}x_{n-1}dx_{n-1}}{d_{n-1}+c}+\frac{\epsilon_n x_n dx_n}{c}\right)^2 \tag{61}$$

are pairwise commuting integrals of the geodesic flow of the metric dg^2 on every of the half-planes $\{x_n>0\}$ and $\{x_n<0\}$. The quadratic forms K_c are smoothly defined on the whole $\mathbf{R}^n$. Therefore, they are pairwise commuting integrals of the geodesic flow the metric dg^2 on $\mathbf{R}^n$.

Let us compute the rank of the geodesic equivalence of the pair g and $\overline{g}$. Suppose that $d_i\neq d_j$ $(i\neq j)$ and $d_i\neq 0$ $(i=1,\ldots,n-1)$. Consider the characteristic polynomial,

$$\chi_A(c)=^{\text{def}}\det(\mathcal{A}\mathcal{E}+cE) \tag{62}$$

$$=\prod_{k=1}^{n}(d_k+c)\left\{\frac{\epsilon_1 x_1^2}{d_1+c}+\cdots+\frac{\epsilon_{n-1}x_{n-1}^2}{d_{n-1}+c}+\frac{\epsilon_n x_n^2}{c}+1\right\}, \tag{63}$$

where we put $d_n=0$. It is clear that the polynomial $\chi_A(c)|_{(x=0)}$ has n different roots. Therefore, the rank of the geodesic equivalence of the pair dg^2 and $d\overline{g}^2$ is n (see Remark 12). Let us fix some real constant c and consider the metric dg_c^2 given by formula (59). The formula $A(g,g_c)=A(g,\overline{g})+c$ shows that the rank of the geodesic equivalence of the pair g and g_c is also n. We have proved the next theorem.

Theorem 8: *The metric $dg^2=^{\text{def}}\Sigma_{i=1}^n\epsilon_i dx_i^2$ and the metrics given by formula (59) are geodesically equivalent. If $d_i\neq d_j$ $(i\neq j)$ and $d_i\neq 0$ $(i=1,\ldots,n-1,)$, then the rank of the geodesic equivalence of the pair dg^2 and dg_c^2 is n.*

The metrics dg_c^2 given by formula (59) have a very special property given by the next theorem.

Theorem 9: *Consider the Euclidean case, i.e.* $\epsilon_i=1$ $(i=1,\dots,n)$. *Suppose that* $d_i\neq d_j$ $(i\neq j)$ *and* $d_i\neq 0$ $(i=1,\dots,n-1)$. *Then the restriction of the metrics* dg_c^2 *given by formula (59) on every quadric* Q_α $(\alpha\neq c)$ *from the confocal family* $Q_\alpha=^{\text{def}}\{D_\alpha=0\}$ *is geodesically equivalent to the restriction of the standard Euclidean metric* dg^2 *on* Q_α.

As a corollary we obtain the theorem proved in Ref. 1 and independently in Ref. 8 that the standard ellipsoid admits a nontrivial geodesic equivalence. Theorem 9 shows that the same result is true for the hyperboloids.

Proof of Theorem 9: Suppose that $dg^2=\Sigma_{i=1}^n dx_i^2$. Let us fix a point $\overline{x_0}=(x_1^0,\dots,x_n^0)\in\mathbf{R}^n$ such that $x_1^0\cdots x_n^0\neq 0$. It can be easily seen that there exists n different real constants $\alpha_1,\dots,\alpha_n$ such that $Q_{\alpha_1}(\overline{x_0})=0,\dots,Q_{\alpha_n}(\overline{x_0})=0$. It follows from formula (61) that

$$K_{\alpha_l}|_{\overline{x}_0}=-(d_{\overline{x}_0}Q_{\alpha_l})^2/4. \tag{64}$$

The forms $d_{\overline{x}_0}Q_{\alpha_l}$ are linearly independent. Therefore, $r(g,\overline{g})(\overline{x_0})=n$. Formula (3) and the nondegeneracy of the corresponding Vandermonde determinant show that the forms $I_0|_{\overline{x}_0},\dots,I_{n-1}|_{\overline{x}_0}$ are simultaneously diagonalizable in the dual to the forms $d_{\overline{x}_0}Q_{\alpha_l}$ $(l=1,\dots,n)$ frame. The form I_{n-1} is conformally equivalent to the metric g and the form I_0 is conformally equivalent to $\overline{g}$. Hence, the gradients (with respect to the metric g) $\nabla_{\overline{x}_0}Q_{\alpha_1},\dots,\nabla_{\overline{x}_0}Q_{\alpha_n}$ coincide with the principal directions of the metrics $g|_{\overline{x}_0}$ and $\overline{g}|_{\overline{x}_0}$. Finally, the statement of the theorem follows from Levi-Civita's theorem about the local form of the Riemannian metrics that permit geodesic equivalence (see Refs. 6, 11, 3). Theorem 9 is proved.

A. Projective hierarchy of geodesically equivalent metrics

Let $\{(x_1,\dots,x_n)\}$ be the coordinates in $\mathbf{R}^n$. Let us fix a value κ of the parameter c in formula (57). Using Theorem 5 we obtain that for every integer k the metrics given by the formulas,

$$dg_\kappa^{(k)2}=^{\text{def}}\langle\mathcal{E}(\mathcal{A}\mathcal{E}+\kappa E)^k d\overline{x},d\overline{x}\rangle \tag{65}$$

and

$$d\overline{g}_\kappa^{(k)2}=^{\text{def}}\frac{1}{\det(\mathcal{A}\mathcal{E}+\kappa E)}\langle\mathcal{E}(\mathcal{A}\mathcal{E}+\kappa E)^{k-1}d\overline{x},d\overline{x}\rangle, \tag{66}$$

where $d\overline{x}=(dx_1,\dots,dx_n)$, $\langle\overline{\xi},\overline{\eta}\rangle=^{\text{def}}\Sigma_{i=1}^n\xi_i\eta_i$,

$$\mathcal{A}=^{\text{def}}\overline{x}\otimes\overline{x}+\operatorname{diag}(\epsilon_1 d_1,\dots,\epsilon_{n-1}d_{n-1},0), \tag{67}$$

$$\mathcal{E}=^{\text{def}}\operatorname{diag}(\epsilon_1,\dots,\epsilon_n),\quad \epsilon_i=\pm 1, \tag{68}$$

are geodesically equivalent.

Theorem 10: *Let* κ *be a fixed real constant. For every fixed integer* k *the metrics given by formulas (65) and (66) are geodesically equivalent. Provided that* $d_i\neq d_j$ $(i\neq j)$ *and* $d_i\neq 0$ $(i=1,\dots,n-1)$ *the rank of the geodesic equivalence is* n.

Remark 14: The metric $d\overline{g}_\kappa^{(2)2}$, *provided* $\mathcal{E}=E$, *is isometric to the analog of the Poisson sphere corresponding to the Clebsch case of motion of the rigid body (see Sec. III B in Ref. 4).*

Remark 15: Using Lemma 8 we obtain that up to a multiplication on a constant,

$$d\overline{g}_\kappa^{(1)2}|_{(\kappa=0)}=\frac{1}{x_n^2}\sum_{i=1}^n\epsilon_i dx_i^2. \tag{69}$$

This is a canonical form of the metrics with constant negative curvature. The metric $dg_{\kappa}^{(1)2}|_{(\kappa=0)}=\langle \mathcal{E}\mathcal{A}\mathcal{E}d\overline{x},d\overline{x}\rangle$ *is geodesically equivalent to* $d\overline{g}_{\kappa}^{(1)2}|_{(\kappa=0)}$. *The metric* $dg_{\kappa}^{(1)2}|_{(\kappa=0)}$ *is smoothly defined on the whole* $\mathbf{R}^n$.

B. Projective hierarchy of functions in involution

Let $\{(x_1,\ldots,x_n)\}$ be the coordinates in $\mathbf{R}^n$. Denote by $(x_1,\ldots,x_n;p_1,\ldots,p_n)$ the corresponding coordinates in $T^*\mathbf{R}^n$. Applying Theorem 7 we obtain the next theorem.

Theorem 11: *For every fixed real* κ *and every fixed integer number* l *the one-parameter family of functions on* $T^*\mathbf{R}^n$ *given by the formula* $K_{\alpha}^{(l)}(\overline{p})=^{\text{def}}\langle K_{\alpha}^{(l)}\overline{p},\overline{p}\rangle$, *where* $\overline{p}=^{\text{def}}(p_1,\ldots,p_n)$, $\langle\overline{\xi},\overline{\eta}\rangle=^{\text{def}}\Sigma_{i=1}^{n}\xi_i\eta_i$,

$$K_{\alpha}^{(l)}\overset{\text{def}}{=}\det(\mathcal{A}\mathcal{E}+\alpha E)(\mathcal{A}\mathcal{E}+\alpha E)^{-1}(\mathcal{A}\mathcal{E}+\kappa E)^{-l}\mathcal{E} \tag{70}$$

$$=I_{n-1}^{(l)}(\kappa)\alpha^{n-1}+I_{n-2}^{(l)}(\kappa)\alpha^{n-2}+\cdots+I_{0}^{(l)}(\kappa) \tag{71}$$

and the matrices $\mathcal{A}$ *and* $\mathcal{E}$ *are given by formulas (67) and (68), are in involution with respect to the canonical symplectic structure on* $T^*\mathbf{R}^n$. *If* $d_i\neq d_j$ $(i\neq j)$ *and* $d_i\neq 0$ $(i=1,\ldots,n-1)$, *then the functions* $I_0^{(l)},\ldots,I_{n-1}^{(l)}$ *are functionally independent on* $T^*\mathbf{R}^n$.

Remark 16: If we take $l=0$ *and* $\mathcal{E}=E$ *we derive the integrals obtained by Uhlenbeck in Ref. 9. Another way of obtaining these integrals was proposed by Moser in Ref. 10. The families of functions in involution given by Theorem 11 generalize all these results.*

Remark 17: The case $l=-1$, $\kappa=0$, *gives a family of pairwise commuting functions* $I_0^{(-1)},\ldots,I_{n-1}^{(-1)}$ *on* T^*M^n. *The function* $I_{n-1}^{(-1)}$ *coincides with the Hamiltonian of the metric given by formula (69). Therefore, the functions* $I_0^{(-1)},\ldots,I_{n-1}^{(-1)}$ *on* T^*M^n *are complete family of integrals of the geodesic flow of the hyperbolic plane.*

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Trefoil symmetries I. Clover extensions beyond Coleman–Mandula theorem

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A graded minimal Lie algebraic extension of the space–time symmetry is constructed involving only spin-1 multiplets as novel generators. The extension involves $\mathbb{Z}_4\times\mathbb{Z}_4$ graded parameters and generators. It provides a bosonic analog to supersymmetry since the composition of *three* symmetric vector charges produces a space–time translation. There arise three noncommutative four-dimensional manifolds with pseudometric. © *2001 American Institute of Physics.*
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I. INTRODUCTION

A thorough analysis and account of the algebraic manipulations leading to symmetry transformations with desired invariant properties can reveal unexpected underlying grading structures. These gradings in turn can enable noncommutative (and even nonassociative) novel extensions whose plausibility has been largely overlooked[1,2]

In theoretical physics, the addition is sometimes tacitly constrained to elements of the ''same type.'' Besides the account of involved units of measure (dimensional analysis), eventually certain ''apparently ad hoc'' constraints play a role. Such constraints are called superselection rules. We will observe that to a certain extent such constraints might be casted by requiring a fixed underlying grading structure.

The extension of the real numeric field $\mathbb{R}$ to the complex, quaternion, octonion, and Cayley numbers abandons sequentially linear ordered field, commutativity, associativity, and division ring property. This line of extension maintains the addition operation between any two numbers. The addition in physical models can be, nevertheless, constrained to parameters of the ''same type,'' i.e., to ''homogeneous sums'' in a certain sense. Accordingly, certain desirable properties can be maintained for constrained use of the addition operation. We land in the realm of some sort of graded projective rings in which certain properties might be relaxed while maintaining all desirable features of the underlying ''number structure.''

The latter considerations lead to the introduction of graded parameters (parameter≡measure of a symmetry transformation, i.e., an angle, a length, etc.)[3] and to graded groups of transformations and graded Lie algebras.[1,2] In this case, the numbers will be replaced by parameters which will be ''designed'' for matching the features of the observed symmetries.

We are aware of the powerful connection among continuous symmetries and conserved quantities. The most general extensions of the external or space–time symmetries of the S matrix have been studied by Coleman and Mandula[4] and by Haag, Łopuszańnski, and Sohnius[5] using, respectively, group and supergroup structures and quite general and well-motivated assumptions in the quantum field theory realm. We are going to relax one underlying assumption to obtain an extension of the Coleman–Mandula theorem: *We do not assume that all symmetry generators should be acted on through commutators under Poincaré transformations*. We will find, already at this step, traces of the would-be internal symmetries (perhaps after a breaking of the obtained graded

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symmetry). This work is a continuation of the program started in Ref. 6 where several technical difficulties could be overcome. In fact, there seems to exist multiple possible paths for constructing novel extensions. We have stated in *italics* each of the assumptions characterizing the extension presented here.

The careful study of the underlying grading structure of the Poincaré group (Sec. III) has opened the possibility of considering gradings of a different sort than those used by supersymmetry. It has been found that besides $\mathbb{Z}_2$-gradings there are $\mathbb{Z}_2\times(\mathbb{Z}_{4N}\times\mathbb{Z}_{4N})$-gradings ($N\in\mathbb{N}$) compatible with the symmetries of the Poincaré group of special relativity.[1] Here we will study exhaustively a particular line of extension which is self-bosonic, i.e., we select here *only the bosonic part of the* $\mathbb{Z}_2$*-grading factor*. In this sense, we consider that our results go beyond Coleman–Mandula no-go theorem.

We consider here a $\mathbb{Z}_4\times\mathbb{Z}_4$ graded extension of the Poincaré algebra in which there are three symmetric-vector generators $P_{(1)}$, $P_{(2)}$, $P_{(3)}$ which can be composed via $(\frac{1}{2},\frac{1}{2})\otimes(\frac{1}{2},\frac{1}{2})\otimes(\frac{1}{2},\frac{1}{2})=(\frac{1}{2},\frac{1}{2})\oplus\cdots$ to produce the (standard) space–time translation multiplet $P_{(0)}$,

$$[\![P_{(1)},[\![P_{(2)},P_{(3)}]\!]]\!]\sim P_{(0)}.$$

The double brackets stand for q-commutators respecting the grading assignments of their entries, and $P_{(0)}=(P_0,P_1,P_2,P_3)$ is the translation four-vector.

To a certain extent, this is a bosonic counterpart of the supersymmetric extensions in which two fermionic charges are composed via $(\frac{1}{2},0)\otimes(0,\frac{1}{2})=(\frac{1}{2},\frac{1}{2})$ to produce the translation $P_{(0)}$,

$$[\![Q_{(0)},\overline{Q}_{(0)}]\!]\sim P_{(0)}.$$

The introduction of graded fermionic charges in a $\mathbb{Z}_2\times(\mathbb{Z}_4\times\mathbb{Z}_4)$-graded extension is done in a forthcoming paper, where the graded fermionic charges $\overline{Q}_{(1)}$, $Q_{(2)}$, $\overline{Q}_{(3)}$ can be composed to produce a susy generator $Q_{(0)}$,

$$[\![\overline{Q}_{(1)},[\![Q_{(2)},\overline{Q}_{(3)}]\!]]\!]\sim Q_{(0)}.$$

We call *trefoil symmetries* all the graded Lie algebras with involution that extend the Poincaré algebra. Those trefoil symmetries involving only $\mathbb{Z}_4\times\mathbb{Z}_4$-graded parameters and only novel multiplets of integer spin will be called *clover extensions*, and correspond to the simplest extensions beyond the Coleman–Mandula no-go theorem. The new ingredient leading to supersymmetry was the spin-$\frac{1}{2}$ irreps. The new ingredients leading to the clover extensions are the integer spin irreps of novel graded classes. Supersymmetry results from the nontrivial cohomology of the odd supertranslation group. The trefoil and clover extensions result from the nontrivial cohomology of a group grading which extends a grading of the Poincaré algebra.

We explore here a *minimal* $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$*-graded extension in which the new symmetry generators build up symmetric and antisymmetric vector multiplets*. Such an extension will be called *minimal vector clover extension*. In the second paper of this series another minimal extension will be obtained in which the new generators are symmetric vectors and scalar charges. In the third paper of this series we will explore an extension simultaneously involving the previous minimal extensions as particular cases and address the introduction of dimensionless symmetry charges which are candidates for internal symmetries after graded symmetry breaking. In the fourth paper we study the graded superspace formalism for building concrete representations. In the fifth paper we study covariant constraints, the diverse representations, and their relations. The last two papers of this series address the simplest supermultiplets and their possible quantum actions, and study Casimir operators associated with the extensions. An immediate aim there is to present a natural relation between spin one (Yang–Mills?) and spin zero (Higgs?) fields. Further stages of this research will be devoted to the introduction of spin $\frac{1}{2}$ multiplets of generators, their connection to internal symmetry groups, the local realization of the presented symmetries and graded supergravity.

This paper is structured in the following way. Section II provides a quick introduction to graded continuous symmetries. Section III reviews the features of the suited group gradings for extending the Poincaré algebra. Section IV introduces the irreducible multiplets we need for constructing the extended Poincaré algebra and gives the corresponding self-, dual-, and complex-conjugated representations. In Sec. V we present the general structure of the searched extension, its underlying assumptions, and the strategy for its obtention. In Sec. VI we study the Jacobi identities and obtain the desired $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded Lie algebraic extension of the Poincaré algebra. Section VII gives the concluding remarks.

II. GRADED CONTINUOUS SYMMETRIES

To each parameter (or generator) we associate an index which is a group element that reveals the properties of these type of parameters (or generators) under addition, product (q-commutators), permutation of factors (or q-commutator entries), and alteration of parentheses (or q-commutators). A couple $(\mathbb{I};q)$ is called a *faithful associative group grading over* $\mathbb{C}$ if it satisfies that $\mathbb{I}$ is an Abelian group[2] and

$$q:\mathbb{I}\times\mathbb{I}\to\mathbb{C}\backslash\{0\}:\quad(\tilde a,\tilde e)\mapsto q_{(\tilde a,\tilde e)}=:q_{\tilde a,\tilde e}\in\mathbb{C}\{0\},\tag{2.1}$$

$$q_{\tilde a,\tilde e}=(q_{\tilde e,\tilde a})^{-1},\quad q_{\tilde a+\tilde e,\tilde c}=q_{\tilde a,\tilde c}q_{\tilde e,\tilde c}\quad\forall\tilde a,\tilde e,\tilde c\in\mathbb{I},\tag{2.2}$$

$$q_{\tilde o,\tilde a}=1,\quad\tilde o\text{ neutral element of }\mathbb{I},\quad\forall\tilde a\in\mathbb{I},\tag{2.3}$$

$$\tilde a\neq\tilde e\Rightarrow\exists\tilde c\in\mathbb{I}:q_{\tilde a,\tilde c}\neq q_{\tilde e,\tilde c}.\tag{2.4}$$

If additionally, the couple $(\mathbb{I};q)$ satisfies that there exists an involution $(\,.\,)^\star$ in $\mathbb{I}$ such that

$$q_{\tilde a^\star,\tilde e^\star}=(q^*_{\tilde a,\tilde e})^{-1},$$

where $(.)^*$ is complex conjugation, then we call $(\mathbb{I};q)$ a faithful associative group grading *with involution*. Some examples thereof are given as follows.

Example 1. $(\mathbb{Z}_2;q^{\mathbb{Z}_2})$-grading or supergrading:

$$\{\mathbb{Z}_2;+\},\quad\mathbb{Z}_2=\{0,1\},$$

$$+:\mathbb{Z}_2\times\mathbb{Z}_2\to\mathbb{Z}_2;\quad(a_0,e_0)\mapsto(a_0+e_0)\bmod 2,$$

$$q^{\mathbb{Z}_2}:\mathbb{Z}_2\times\mathbb{Z}_2\to\mathbb{C}\backslash\{0\};\quad(a_0,e_0)\mapsto q^{\mathbb{Z}_2}_{a_0,e_0}=\mathrm{e}^{\mathrm{i}\pi a_0e_0}.$$

Example 2. $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-grading:

$$\{\mathbb{Z}_4\times\mathbb{Z}_4;+\},\quad\mathbb{Z}_4\times\mathbb{Z}_4=\{(m,n);\quad n,m=0,1,2,3\}$$

$$(n,m)+(n',m'):=((n+n')\bmod 4,(m+m')\bmod 4)$$

$$q_{(n,m),(n',m')}:=\mathrm{e}^{(\mathrm{i}\pi/2)(nm'-n'm)}.$$

This type of grading has been called Weil grading[3] since it reproduces the structure of the Weil pairings used in the arithmetic of elliptic curves. It manifests close resemblance to the Dirac–Schwinger–Zwanziger condition,[7] which will be discussed elsewhere.

Example 3. $(\mathbb{Z}_2\times(\mathbb{Z}_4\times\mathbb{Z}_4);q^{\mathbb{Z}_2}q)$-grading:

$$(q^{\mathbb{Z}_2}q)_{(a_0,(n,m)),(a_0',(n',m'))}:=q^{\mathbb{Z}_2}_{a_0,a_0'}q_{(n,m),(n',m')}.$$

We consider now a set of parameters $\mathbb{P}=\{\beta_{\tilde{a}},\beta'_{\tilde{e}},\dots\}$ which builds up an $(\mathbb{I};q)$-*graded parameter algebra*, i.e., the parameters are $\mathbb{I}$-graded, and have a binary product which is q-commutative and associative (for more general cases see Ref. 2): $(\mathbb{I};q)$ is a faithful associative group grading,

$$(\beta_{\tilde{a}}\beta'_{\tilde{e}}) \text{ has index } \tilde{a}+\tilde{e} \quad \forall \beta_{\tilde{a}},\beta'_{\tilde{e}}\in\mathbb{P} \quad (\mathbb{I}\text{-grading}),$$

$$(\beta_{\tilde{a}}\beta'_{\tilde{e}})=q_{\tilde{a},\tilde{e}}(\beta'_{\tilde{e}}\beta_{\tilde{a}}) \quad \forall \beta_{\tilde{a}},\beta'_{\tilde{e}}\in\mathbb{P} \quad (q\text{-commutative}),$$

$$(\beta_{\tilde{a}}(\beta'_{\tilde{e}}\beta''_{\tilde{c}}))=((\beta_{\tilde{a}}\beta'_{\tilde{e}})\beta''_{\tilde{c}}) \quad \forall \beta_{\tilde{a}};\beta'_{\tilde{e}},\beta''_{\tilde{c}}\in\mathbb{P} \quad (\text{associative}).$$

The $(\mathbb{I};q)$-graded parameters are the measures (i.e., angles, lengths, etc.) of graded continuous symmetry transformations

$$g(\beta)=g(\beta_{-\tilde{a}_1},\beta_{-\tilde{a}_2},\dots,\beta_{-\tilde{a}_n})=\exp(\mathrm{i}\beta_{-\tilde{a}_j}Q_{\tilde{a}_j}). \tag{2.5}$$

The graded symmetry generators $Q_{\tilde{a}_j}$ constitute a novel structure known as ϵ-colored,[8] or $(\mathbb{I};q)$-graded Lie algebra.[1] (For more general extensions involving nonassociative parameters see Ref. 2). We call $\{\mathbb{L};+,[\![.,.]\!]\}$ an $(\mathbb{I};q)$-*graded Lie algebra over* $\mathbb{C}$ iff $0\in\mathbb{L}\neq\{0\}$, $(\mathbb{I};q)$ is a faithful associative group grading, and there exist an application S_t and a binary operation $[\![.,.]\!]$ satisfying the following five axioms.

Axiom 1: S_t assigns an index to each nonvanishing generator in $\mathbb{L}$, the generators carrying the same index build up a vector space, $(\mathbb{I};q)$ is the minimal allowed group grading:

$$S_t:\mathbb{L}\backslash\{0\}\to\mathbb{I}, \quad Q_{\tilde{a}}\mapsto S_t(Q_{\tilde{a}})=\tilde{a},$$

$$\mathbb{I} \text{ is generated by } S_t(\mathbb{L}\backslash\{0\}),$$

$$\mathbb{L}_{\tilde{a}}=\{0\}\cup S_t^{-1}(\tilde{a}) \text{vector space over } \mathbb{C} \quad \forall\tilde{a}\in\mathbb{I},$$

$$\mathbb{L}=\cup_{\tilde{a}\in\mathbb{I}}\ \mathbb{L}_{\tilde{a}}.$$

Axiom 2: $[\![.,.]\!]$ is a closed binary, $\mathbb{I}$-graded operation:

$$[\![.,.]\!]:\mathbb{L}\times\mathbb{L}\to\mathbb{L}, \quad (Q_{\tilde{a}},Q'_{\tilde{e}})\mapsto[\![Q_{\tilde{a}},Q'_{\tilde{e}}]\!]\in\mathbb{L},$$

$$[\![\mathbb{L}_{\tilde{a}},\mathbb{L}_{\tilde{e}}]\!]\subseteq\mathbb{L}_{\tilde{a}+\tilde{e}} \quad (\mathbb{I}\text{-grading}).$$

Axiom 3: $[\![.,.]\!]$ is q-antisymmetric:

$$[\![Q_{\tilde{a}},Q'_{\tilde{e}}]\!]=-q_{\tilde{a},\tilde{e}}[\![Q'_{\tilde{e}},Q_{\tilde{a}}]\!], \quad \forall Q_{\tilde{a}},Q'_{\tilde{e}}\in\mathbb{L}.$$

Axiom 4: $[\![.,.]\!]$ is bilinear with respect to the vector space structures:

$$[\![Q_{\tilde{a}}+yQ''_{\tilde{a}},Q'_{\tilde{e}}]\!]=[\![Q_{\tilde{a}},Q'_{\tilde{e}}]\!]+y[\![Q''_{\tilde{a}},Q'_{\tilde{e}}]\!], \quad \forall Q_{\tilde{a}},Q''_{\tilde{a}},Q'_{\tilde{e}}\in\mathbb{L}, \quad \forall y\in\mathbb{C}.$$

Axiom 5: $[\![.,.]\!]$ is q-Jacobi associative (q-Leibnitz rule):

$$[\![Q_{\tilde{a}},[\![Q'_{\tilde{e}},Q''_{\tilde{c}}]\!]]\!]=[\![[\![Q_{\tilde{a}},Q'_{\tilde{e}}]\!],Q''_{\tilde{c}}]\!]+q_{\tilde{a},\tilde{e}}[\![Q'_{\tilde{e}},[\![Q_{\tilde{a}},Q''_{\tilde{c}}]\!]]\!], \quad \forall Q_{\tilde{a}},Q'_{\tilde{e}},Q''_{\tilde{c}}\in\mathbb{L}.$$

If we adopt an extra axiom:

Axiom 6: There exist involutions $(.)^*$, $(.)^\star$, $\overline{(.)}$, in $\mathbb{C}$, $\mathbb{I}$, and $\mathbb{L}$, respectively, such that $(\mathbb{I};q)$ is a group grading with involution, and fulfilling

$$\overline{(yQ_a)}=y^*\overline{Q}_{a^\star},$$

$$\overline{[\![Q_{\tilde a},Q'_{\tilde e}]\!]}=[\![\overline{Q}'_{\tilde e^\star},\overline{Q}_{\tilde a^\star}]\!] \quad \forall Q_{\tilde a},Q'_{\tilde e}\in\mathbb{L},$$

$$\overline{(y\beta_{-\tilde a}Q_{\tilde a})}=y^*\overline{Q}_{\tilde a^\star}\overline{\beta}_{-\tilde a^\star} \quad \forall Q_{\tilde a}\in\mathbb{L},\ \forall\beta_{-\tilde a}\in\mathbb{P},$$

then the $\mathbb{L}$ is called an $(\mathbb{I};q)$-graded Lie algebra over $\mathbb{C}$ **with involution**. *We adopt here the trivial involution* $(.)^\star$ in $\mathbb{I}$, i.e. $(.)^\star=$identity. Obviously $(\tilde a^\star)^\star=\tilde a$.

The products $\beta_{-\tilde a}Q_{\tilde a}$ of an $(\mathbb{I};q)$-graded parameter $\beta_{-\tilde a}$ by an $(\mathbb{I};q)$-graded Lie algebra generator $Q_{\tilde a}$ are (plain) Lie algebra generators in an analogous way as the product $\theta^\alpha Q_\alpha$ of a Grassmann parameter by a fermionic supersymmetry charge constitutes a Lie algebra generator. The mixture of parameters and generators is governed by

$$\begin{aligned}\beta_{-\tilde a}Q'_{\tilde e}&=q_{-\tilde a,\tilde e}Q'_{\tilde e}\beta_{-\tilde a},\\ [\beta_{-\tilde a}Q_{\tilde a},\beta'_{-\tilde e}Q'_{\tilde e}]&=\beta'_{-\tilde e}\beta_{-\tilde a}[\![Q_{\tilde a},Q'_{\tilde e}]\!].\end{aligned} \tag{2.6}$$

III. GROUP GRADINGS FOR EXTENDING POINCARÉ ALGEBRA

A given Lie algebra can be extended to an $(\mathbb{I};q)$-graded Lie algebra in which the group $\mathbb{I}$ respects the underlying gradings of the given Lie algebra. The underlying gradings are in close relation to the Levi decomposition and the roots of the Lie algebra. The underlying gradings of the Poincaré algebra and their suited graded extensions have been studied in Ref. 1. We briefly illustrate these results. The Lorentz algebra M can be written

$$[M_{\mu\nu},M_{\rho\sigma}]=\mathrm{i}(g_{\mu\sigma}M_{\nu\rho}+g_{\nu\rho}M_{\mu\sigma}-g_{\mu\rho}M_{\nu\sigma}+g_{\nu\sigma}M_{\mu\rho}), \tag{3.1}$$

where $g=\mathrm{diag}\,(1,-1,-1,-1)$ is the Minkowski pseudometric. Changing variables we can write

$$\begin{aligned}J_i&\equiv\tfrac{1}{2}\epsilon_{ijk}M^{jk},\quad \hat J_i\equiv M^{0i}\\ [J_i,J_j]&=\mathrm{i}\epsilon_{ijk}J_k,\\ [J_i,\hat J_j]&=\mathrm{i}\epsilon_{ijk}\hat J_k,\\ [\hat J_i,\hat J_j]&=-\mathrm{i}\epsilon_{ijk}J_k.\end{aligned} \tag{3.2}$$

After a complexification we obtain the decomposition of this semisimple Lie algebra M into simple factors

$$\begin{aligned}T_{(0)i}&\equiv\tfrac{1}{2}(J_i+\mathrm{i}\hat J_i),\quad \overline{T}_{(0)i}\equiv\tfrac{1}{2}(J_i-\mathrm{i}\hat J_i),\\ [T_{(0)i},T_{(0)j}]&=\mathrm{i}\epsilon_{ijk}T_{(0)k},\\ [T_{(0)i},\overline{T}_{(0)j}]&=0,\\ [\overline{T}_{(0)i},\overline{T}_{(0)j}]&=\mathrm{i}\epsilon_{ijk}\overline{T}_{(0)k}.\end{aligned} \tag{3.3}$$

$$M\approx su(2)\oplus su(2).$$

To study the underlying grading of the Poincaré algebra we assume that *both the generators* $M_{\mu\nu}$ *and the generators* $T_{(0)i}$ *and* $\overline{T}_{(0)i}$ *can be adopted for generating the Lorentz group, and also that both Casimir operators of the Poincaré algebra carry the trivial index*. This leads to the following index assignment:

$$
\begin{gathered}
S_t(P^0_{(0)})=\tilde{a}_0,\\
S_t(M_{23})=S_t(J_1)=S_t(\hat{J}_1)=S_t(M_{01})=S_t(P^1_{(0)})=\tilde{a}_1,\\
S_t(M_{31})=S_t(J_2)=S_t(\hat{J}_2)=S_t(M_{02})=S_t(P^2_{(0)})=\tilde{a}_2\\
S_t(M_{12})=S_t(J_3)=S_t(\hat{J}_3)=S_t(M_{03})=S_t(P^3_{(0)})=\tilde{a}_3,
\end{gathered}
\tag{3.4}
$$

where $P^\mu_{(0)}$ are the translation generators and $\tilde{a}_0=\tilde{o}$ is the neutral element of the grading group $\mathbb{I}$. From the algebraic relations (3.1)–(3.3) and the Poincaré algebra relations involving the translation generators we obtain

$$
\begin{gathered}
q_{\tilde{a}_\mu,\tilde{a}_\nu}=1, \quad \forall \quad \mu,\nu=0,1,2,3,\\
\tilde{a}_1+\tilde{a}_2=\tilde{a}_3, \quad \tilde{a}_2+\tilde{a}_3=\tilde{a}_1, \quad \tilde{a}_3+\tilde{a}_1=\tilde{a}_2.
\end{gathered}
\tag{3.5}
$$

This implies that the grading group $\{\tilde{a}_0,\tilde{a}_1,\tilde{a}_2,\tilde{a}_3\}$ underlying the Poincaré algebra (with the adopted assumptions) is $\mathbb{Z}_2\times\mathbb{Z}_2$, the Klein group. This coincides with the group of discrete transformations that builds the full Poincaré group. Now,

$$
\tilde{a}_\mu+\tilde{a}_\mu=\tilde{o}\Rightarrow\tilde{a}_\mu=-\tilde{a}_\mu \quad \forall\mu=0,1,2,3. \tag{3.6}
$$

From (2.2) and (2.3) we obtain

$$
1=q_{\tilde{o},\tilde{c}}=q_{\tilde{a}_\nu+\tilde{a}_\nu,\tilde{c}}=q_{\tilde{a}_\nu,\tilde{c}}q_{\tilde{a}_\nu,\tilde{c}}=1 \quad \forall\tilde{c}\in\mathbb{I},
$$

hence

$$
q_{\tilde{a}_\nu,\tilde{c}}\in\{+1,-1\}, \quad \forall \quad \tilde{c}\in\mathbb{I}, \quad \forall \quad \nu=0,1,2,3. \tag{3.7}
$$

Accordingly, *the algebraic relations involving Poincaré generators can only be of commutator type or anticommutator type*.

We adopt a model for the q-application in which the indices with a tilde have the form

$$
\begin{gathered}
\tilde{c}=(c_0,[(c_1,c_2)]), \quad \tilde{u}=(u_0,[(u_1,u_2)]),\\
q_{\tilde{c},\tilde{u}}:=\exp\{\mathrm{i}\pi c_0u_0\}\exp\left\{\frac{\mathrm{i}\pi}{2N}(c_1u_2-c_2u_1)\right\}.
\end{gathered}
\tag{3.8}
$$

The first components c_0, u_0 turn out to belong to $\mathbb{Z}_2$ and the last components $[(c_1,c_2)]$, $[(u_1,u_2)]$ constitute equivalence classes of bivectors in a plane which satisfy quantization relations in the areas they subtend. Relations (3.3)–(3.5) lead to the conclusion that the allowed group gradings have the form $\mathbb{Z}_2\times(\mathbb{Z}_{4N}\times\mathbb{Z}_{4N})$, $N\in\mathbb{N}$ and the previously mentioned example 3 is just the simplest ($N=1$) novel grading compatible with the Poincaré algebra.[1] In this study we will leave the $\mathbb{Z}_2$ factor aside since we are looking for a self-bosonic extension beyond the Coleman–Mandula no-go theorem. A future paper will study an extension beyond the Haag–Lopuszański–Sohnius no-go theorem. Since we are not considering here the $\mathbb{Z}_2$-grading factor we adopt as indices with a tilde the elements associated with the group $\mathbb{Z}_4\times\mathbb{Z}_4$. The group elements associated with the Poincaré group turn out to build the $\mathbb{Z}_2\times\mathbb{Z}_2$ subgroup:

TABLE I. Addition table of the group $\mathbb{Z}_4\times\mathbb{Z}_4$.

+	(0)0	(0)1	(0)2	(0)3	(1)0	(1)1	(1)2	(1)3	(2)0	(2)1	(2)2	(2)3	(3)0	(3)1	(3)2	(3)3
(0,0)≡(0)0	(0)0	(0)1	(0)2	(0)3	(1)0	(1)1	(1)2	(1)3	(2)0	(2)1	(2)2	(2)3	(3)0	(3)1	(3)2	(3)3
(2,0)≡(0)1	(0)1	(0)0	(0)3	(0)2	(1)1	(1)0	(1)3	(1)2	(2)3	(2)2	(2)1	(2)0	(3)2	(3)3	(3)0	(3)1
(0,2)≡(0)2	(0)2	(0)3	(0)0	(0)1	(1)2	(1)3	(1)0	(1)1	(2)1	(2)0	(2)3	(2)2	(3)3	(3)2	(3)1	(3)0
(2,2)≡(0)3	(0)3	(0)2	(0)1	(0)0	(1)3	(1)2	(1)1	(1)0	(2)2	(2)3	(2)0	(2)1	(3)1	(3)0	(3)3	(3)2
(1,0)≡(1)0	(1)0	(1)1	(1)2	(1)3	(0)1	(0)0	(0)3	(0)2	(3)1	(3)2	(3)0	(3)3	(2)1	(2)3	(2)2	(2)0
(3,0)≡(1)1	(1)1	(1)0	(1)3	(1)2	(0)0	(0)1	(0)2	(0)3	(3)3	(3)0	(3)2	(3)1	(2)2	(2)0	(2)1	(2)3
(1,2)≡(1)2	(1)2	(1)3	(1)0	(1)1	(0)3	(0)2	(0)1	(0)0	(3)2	(3)1	(3)3	(3)0	(2)0	(2)2	(2)3	(2)1
(3,2)≡(1)3	(1)3	(1)2	(1)1	(1)0	(0)2	(0)3	(0)0	(0)1	(3)0	(3)3	(3)1	(3)2	(2)3	(2)1	(2)0	(2)2
(0,1)≡(2)0	(2)0	(2)3	(2)1	(2)2	(3)1	(3)3	(3)2	(3)0	(0)2	(0)0	(0)1	(0)3	(1)1	(1)2	(1)0	(1)3
(0,3)≡(2)1	(2)1	(2)2	(2)0	(2)3	(3)2	(3)0	(3)1	(3)3	(0)0	(0)2	(0)3	(0)1	(1)3	(1)0	(1)2	(1)1
(2,3)≡(2)2	(2)2	(2)1	(2)3	(2)0	(3)0	(3)2	(3)3	(3)1	(0)1	(0)3	(0)2	(0)0	(1)2	(1)1	(1)3	(1)0
(2,1)≡(2)3	(2)3	(2)0	(2)2	(2)1	(3)3	(3)1	(3)0	(3)2	(0)3	(0)1	(0)0	(0)2	(1)0	(1)3	(1)1	(1)2
(3,3)≡(3)0	(3)0	(3)2	(3)3	(3)1	(2)1	(2)2	(2)0	(2)3	(1)1	(1)3	(1)2	(1)0	(0)3	(0)0	(0)2	(0)1
(1,1)≡(3)1	(3)1	(3)3	(3)2	(3)0	(2)3	(2)0	(2)2	(2)1	(1)2	(1)0	(1)1	(1)3	(0)0	(0)3	(0)1	(0)2
(1,3)≡(3)2	(3)2	(3)0	(3)1	(3)3	(2)2	(2)1	(2)3	(2)0	(1)0	(1)2	(1)3	(1)1	(0)2	(0)1	(0)3	(0)0
(3,1)≡(3)3	(3)3	(3)1	(3)0	(3)2	(2)0	(2)3	(2)1	(2)2	(1)3	(1)1	(1)0	(1)2	(0)1	(0)2	(0)0	(0)3

$$
\begin{aligned}
&S_t(x^0)=S_t(P^0_{(0)})=\tilde{o}=\tilde{a}_0=(0,0)\equiv(0)_0,\\
&S_t(x^1)=S_t(P^1_{(0)})=S_t(M^{01})=S_t(M^{23})=\tilde{a}_1=(2,0)\equiv(0)_1,\\
&S_t(x^2)=S_t(P^2_{(0)})=S_t(M^{02})=S_t(M^{31})=\tilde{a}_2=(0,2)\equiv(0)_2,\\
&S_t(x^3)=S_t(P^3_{(0)})=S_t(M^{03})=S_t(M^{12})=\tilde{a}_3=(2,2)\equiv(0)_3.
\end{aligned}
\tag{3.9}
$$

It is easy to verify that this choice satisfies relations (3.5)–(3.7) under the group grading given in example 2. Observe that the index assignment does not enter into conflict with the relations used in special relativity, quantum mechanics, and QFT. For instance,

$$S_t(x^2P^3_{(0)}-x^3P^2_{(0)})=\tilde{a}_2+\tilde{a}_3=\tilde{a}_1=S_t(M^{23}).$$

Notice that we have two different ways for designating group elements: the first way are couples (n,m), where $n,m=0,1,2,3$; the second way which will become clear shortly, has the form $(f)_s$ where f indicates the class, and s indicates the element of the class. In order to visualize the grading structure we provide in Table I the addition table of the group $\mathbb{Z}_4\times\mathbb{Z}_4$ and in Table II the q-function for every couple of group elements. The values in Table II have to be identified with q (line, column).

In Tables I and II we have divided the 16 group elements into four classes. The class (0) contains the indices associated with the Poincaré generators $\{\tilde{a}_0,\tilde{a}_1,\tilde{a}_2,\tilde{a}_3\}=\{(0)_0,(0)_1,(0)_2,(0)_3\}$. Classes (1), (2), and (3) contain indices which remain in the same class when you add elements of class (0). This fact indicates that classes (0)–(3) provide the sets of indices available for building novel invariant multiplets of generators.

From Table I we obtain Table III for the addition of class indices $(\mathbb{Z}_4\times\mathbb{Z}_4)/(\mathbb{Z}_2\times\mathbb{Z}_2)\approx\mathbb{Z}_2\times\mathbb{Z}_2$. We write $(i\dagger j)$ instead of $(i)\dagger(j)$.

IV. GRADED SPIN IRREPS OF GENERATORS

We consider an extension $\mathbb{L}$ of the Poincaré algebra. The generators of $\mathbb{L}$ are assumed to be arranged into multiplets which transform linearly under the action of the generators of the Lorentz Lie subalgebra. Candidates for defining invariant multiplets are divided into four classes since the

TABLE II. q-function for $\mathbb{Z}_4\times\mathbb{Z}_4$.

$q^{\mathbb{Z}_4\times\mathbb{Z}_4}$	(0)0	(0)1	(0)2	(0)3	(1)0	(1)1	(1)2	(1)3	(2)0	(2)1	(2)2	(2)3	(3)0	(3)1	(3)2	(3)3
(0,0)≡(0)0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
(2,0)≡(0)1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1
(0,2)≡(0)2	1	1	1	1	−1	−1	−1	−1	1	1	1	1	−1	−1	−1	−1
(2,2)≡(0)3	1	1	1	1	−1	−1	−1	−1	−1	−1	−1	−1	1	1	1	1
(1,0)≡(1)0	1	1	−1	−1	1	1	−1	−1	i	−i	−i	i	−i	i	−i	i
(3,0)≡(1)1	1	1	−1	−1	1	1	−1	−1	−i	i	i	−i	i	−i	i	−i
(1,2)≡(1)2	1	1	−1	−1	−1	−1	1	1	i	−i	−i	i	i	−i	i	−i
(3,2)≡(1)3	1	1	−1	−1	−1	−1	1	1	−i	i	i	−i	−i	i	−i	i
(0,1)≡(2)0	1	−1	1	−1	−i	i	−i	i	1	1	−1	−1	i	−i	−i	i
(0,3)≡(2)1	1	−1	1	−1	i	−i	i	−i	1	1	−1	−1	−i	i	i	−i
(2,3)≡(2)2	1	−1	1	−1	i	−i	i	−i	−1	−1	1	1	i	−i	−i	i
(2,1)≡(2)3	1	−1	1	−1	−i	i	−i	i	−1	−1	1	1	−i	i	i	−i
(3,3)≡(3)0	1	−1	−1	1	i	−i	−i	i	−i	i	−i	i	1	1	−1	−1
(1,1)≡(3)1	1	−1	−1	1	−i	i	i	−i	i	−i	i	−i	1	1	−1	−1
(1,3)≡(3)2	1	−1	−1	1	i	−i	−i	i	i	−i	i	−i	−1	−1	1	1
(3,1)≡(3)3	1	−1	−1	1	−i	i	i	−i	−i	i	−i	i	−1	−1	1	1

sets of indices $\{(0)_0,(0)_1,(0)_2,(0)_3\}$, $\{(1)_0,(1)_1,(1)_2,(1)_3\}$, $\{(2)_0,(2)_1,(2)_2,(2)_3\}$, $\{(3)_0,(3)_1,(3)_2,(3)_3\}$ remain invariant under addition of indices of the set $\{(0)_0,(0)_1,(0)_2,(0)_3\}$ associated with the Poincaré generators. That is why *we will consider for each spin four types of multiplets*. There arise three novel four-dimensional manifolds besides the Minkowski manifold. The coordinates of the Minkowski space carry indices of the class (0) according to (3.9). The three novel manifolds are noncommutative and have a metric structure (also spin-$\frac{1}{2}$ structures can be defined in those novel manifolds). *We assume here that a generalized spin-statistics theorem holds, in which self-bosonic generators transform under integer spin representations*. We consider multiplets of generators $a_{(f)s}$ of classes $(f)=(0),(1),(2),(3)$. The index s stands for the different components of each multiplet (except for spin-0 singlets not to be discussed here). The corresponding dual multiplets are written $a_{(f)}{}^{s}$, and the complex-conjugated and dual complex-conjugated multiplets are given by $\overline{a}_{(f)\dot{s}}$ and $\overline{a}_{(f)}{}^{\dot{s}}$. All these multiplets transform linearly under Lorentz generators:

$$[\![T_{(0)i},a_{(f)s}]\!]=-\mathrm{i}\sigma^{a}(i,f)_{s}{}^{t}a_{(f)t}, \tag{4.1}$$

$$[\![T_{(0)i},a_{(f)}{}^{s}]\!]=\mathrm{i}q_{(0)i,(f)s}\,a_{(f)}{}^{t}\,\sigma^{a}(i,f)_{t}{}^{s}, \tag{4.2}$$

$$[\![\overline{T}_{(0)i},\overline{a}_{(f)\dot{s}}]\!]=-\mathrm{i}q_{(0)i,(f)s}\,\overline{a}_{(f)\dot{t}}\,\overline{\sigma^{a}}(i,f)^{\dot{t}}{}_{\dot{s}}, \tag{4.3}$$

$$[\![\overline{T}_{(0)i},\overline{a}_{(f)}{}^{\dot{s}}]\!]=\mathrm{i}\overline{\sigma^{a}}(i,f)^{\dot{s}}{}_{\dot{t}}\,\overline{a}_{(f)}{}^{\dot{t}}, \tag{4.4}$$

TABLE III. Addition of class indices $\mathbb{Z}_2\times\mathbb{Z}_2$.

†	(0)	(1)	(2)	(3)
(0)	(0)	(1)	(2)	(3)
(1)	(1)	(0)	(3)	(2)
(2)	(2)	(3)	(0)	(1)
(3)	(3)	(2)	(1)	(0)

where $\overline{a_{(f)s}}=\overline{a}_{(f)\dot{s}}$, $\overline{a_{(f)}{}^{s}}=\overline{a}_{(f)}{}^{\dot{s}}$ and we have adopted the already described notation for the indices. We write $(f)s$ to indicate the sth index of the class (f). From the involution of (4.1) we obtain (using the property of q-commutators under involution, Axiom 6)

$$\overline{[\![T_{(0)i},a_{(f)s}]\!]}=[\![\overline{a}_{(f)\dot{s}},\overline{T}_{(0)i}]\!]$$

$$=\mathrm{i}\overline{a}_{(f)\dot{t}}\sigma^{a}(i,f)_{s}^{*t}.$$

Using (4.3) we conclude finally

$$\overline{\sigma^{a}}(i,f)^{\dot{t}}{}_{\dot{s}}=\sigma^{a}(i,f)_{s}^{*\,t}. \tag{4.5}$$

Analogously, under involution of (4.2) we again obtain (4.5). We now study which shall be the structure of the σ-matrices. We use the following Jacobi identity

$$[\![T_{(0)j},[\![T_{(0)k},a_{(f)s}]\!]]\!]=[\![[\![T_{(0)j},T_{(0)k}]\!],a_{(f)s}]\!]+q_{(0)j,(0)k}[\![T_{(0)k},[\![T_{(0)j},a_{(f)s}]\!]]\!].$$

Using (3.3) and (4.1) we obtain

$$[\mathrm{i}\sigma^{a}(j,f),\mathrm{i}\sigma^{a}(k,f)]=\mathrm{i}\epsilon_{jkl}(\mathrm{i}\sigma^{a}(l,f)), \tag{4.6}$$

where the commutator has the usual meaning. Accordingly, the matrices $\mathrm{i}\sigma^{a}(j,f)_{s}{}^{t}$ and $-\mathrm{i}[\sigma^{a}(j,f)^{\mathrm{tr}}]^{t}{}_{s}$ are standard representations of angular momenta. Analogously, using the Jacobi identity for the triple $\overline{T}_{(0)j}$, $\overline{T}_{(0)k}$, $\overline{a}_{(f)\dot{s}}$ we obtain

$$[-\mathrm{i}q_{(0)j,(f)}\overline{\sigma^{a}}(j,f),-\mathrm{i}q_{(0)k,(f)}\overline{\sigma^{a}}(k,f)]=\mathrm{i}\epsilon_{jkl}(-\mathrm{i}q_{(0)l,(f)}\overline{\sigma^{a}}(l,f)). \tag{4.7}$$

Hence, $-\mathrm{i}q_{(0)j,(f)}\overline{\sigma^{a}}(j,f)$ and $\mathrm{i}q_{(0)j,(f)}\overline{\sigma^{a}}(j,f)^{\mathrm{tr}}$ are also standard representations of angular momenta. We write $q_{(0)j,(f)}$ instead of $q_{(0)j,(f)s}$ since they are independent of the index s. It is easy to verify that $a_{(f)}{}^{s}a_{(f)s}$ (summation only over s throughout the multiplet) and $\overline{a}_{(f)\dot{s}}\overline{a}_{(f)}{}^{\dot{s}}$ are invariant quadratic products. For example:

$$[\![T_{(0)j},a_{(f)}{}^{s}a_{(f)s}]\!]=[\![T_{(0)j},a_{(f)}{}^{s}]\!]a_{(f)s}+q_{(0)j,(f)}\,a_{(f)}{}^{s}[\![T_{(0)j},a_{(f)s}]\!]=0.$$

We study now the "metric" structure $\epsilon^{a}(f)^{us}$, $\epsilon^{a}(f)_{us}$ connecting the self-representation $a_{(f)s}$ and the dual-self-representation $a_{(f)}{}^{s}$:

$$\epsilon^{a}(f)^{us}\,a_{(f)s}=a_{(f)}{}^{u}, \tag{4.8}$$

$$\epsilon^{a}(f)_{ds}\,a_{(f)}{}^{s}=a_{(f)d}. \tag{4.9}$$

We *assume* that these "metrics" carry trivial index $\tilde{o}$ and thus:

$$[\![T_{(0)j},a_{(f)}{}^{u}]\!]=\epsilon^{a}(f)^{ud}[\![T_{(0)j},a_{(f)d}]\!]$$

$$=\mathrm{i}a_{(f)}{}^{v}(-\epsilon^{a}(f)^{ud}\,\sigma^{a}(j,f)_{d}{}^{t}\,\epsilon^{a}(f)_{tv}).$$

Comparing this with Eq. (4.2) we obtain

$$\sigma^{a}(j,f)_{v}{}^{u}=-q_{(f),(0)j}\,\epsilon^{a}(f)^{ud}\sigma^{a}(j,f)_{d}^{t}\epsilon^{a}(f)_{tv}.$$

In matricial notation

$$\sigma^{a}(j,f)^{\mathrm{tr}}=-q_{(f),(0)j}\epsilon^{\uparrow a}(f)\sigma^{a}(j,f)\epsilon^{\downarrow a}(f), \tag{4.10}$$

where $\epsilon^{\uparrow a}(f)$ and $\epsilon^{\downarrow a}(f)$ stand for the metric with indices up and down respectively. Analogously, we define a ''metric'' structure among the complex-conjugated representation and its dual:

$$\overline{\epsilon^{a}}(f)^{\dot{u}\dot{s}}\,\overline{a}(f)_{\dot{s}}=\overline{a}(f)^{\dot{u}}, \tag{4.11}$$

$$\overline{\epsilon^{a}}(f)_{\dot{d}\dot{s}}\,\overline{a}_{(f)}{}^{\dot{s}}=\overline{a}_{(f)\dot{d}}, \tag{4.12}$$

which leads in matricial notation to

$$\overline{\sigma^{a}}(j,f)^{\mathrm{tr}}=-q_{(0)j,(f)}\overline{\epsilon^{\downarrow a}}(f)^{\mathrm{tr}}\overline{\sigma^{a}}(j,f)\overline{\epsilon^{\uparrow a}}(f)^{\mathrm{tr}}. \tag{4.13}$$

We classify now the spin representations according to their eigenvalues with respect to the Casimir operators of the Lorentz algebra: $\Sigma T_{(0)i}T_{(0)i}$ and $\Sigma\overline{T}_{(0)i}\overline{T}_{(0)i}$. A multiplet $a_{(f)s}$ is said to be in the (s_l,s_r)-spin representation if

$$\begin{aligned}\left[\!\left[\sum_{i=1}^{3} T_{(0)i}T_{(0)i}, a_{(f)s}\right]\!\right]&=s_l(s_l+1)a_{(f)s},\\ \left[\!\left[\sum_{i=1}^{3} \overline{T}_{(0)i}\overline{T}_{(0)i}, a_{(f)s}\right]\!\right]&=s_r(s_r+1)a_{(f)s}.\end{aligned} \tag{4.14}$$

The total spin is given by s_l+s_r. We are now going to list the irreps of integer total spin one.

A. Spin (1,0) and (0,1) irreps

An example of a multiplet of spin (1,0) and spin (0,1) of class (0) is given by the triplets $T_{(0)i}$ and $\overline{T}_{(0)i}$, respectively. We have to select then triples of indices of each one of the three remaining classes to define their spin (1,0) and (0,1) irreps. There are in principle no *a priori* reasons for selecting three indices out of the four available in each class. The metric structure they lead to is not the main aspect for making the choice. In fact, it is easy to check that the actual choice of the representation is responsible for the resulting metric. In the case of the class (0) triplets we see that the underlying metric is Euclidean. In the zero class we adopt the last three indices of the class (0) for the triplet. We adopt the same choice of the remaining three classes. Hence we adopt indices $\{(0)_1,(0)_2,(0)_3\}$, $\{(1)_1,(1)_2,(1)_3\}$, $\{(2)_1,(2)_2,(2)_3\}$, $\{(3)_1,(3)_2,(3)_3\}$ for the multiplets, i.e.,

$$S_t(T_{(f)j})=S_t(\overline{T}_{(f)j})=(f)j;\quad j=1,2,3, \tag{4.15}$$

where we denote the generic multiplet of spin (1,0) and class (f) by $T_{(f)}$ and the generic multiplet of spin (0,1) and class (f) by $\overline{T}_{(f)}$. The Lorentz generators $T_{(0)}$ and $\overline{T}_{(0)}$ form triplets for which

$$\sigma^{T}(j,0)_{k}{}^{l}=-\epsilon_{jkl},\quad \overline{\sigma^{T}}(j,0)^{l}{}_{k}=-\epsilon_{jkl}. \tag{4.16}$$

In order to match the grading properties according to Axiom 2 of $(\mathbb{I};q)$-graded Lie algebras, the texture of the σ-matrices is not free, and has to account for the equality of the indices in both sides of the q-commutator relations (4.1)–(4.4). An adequate choice for the σ^{T}-matrices is given in Table IV with $\overline{\sigma^{T}}(j,f)=\sigma^{T}(j,f)^{*\,\mathrm{tr}}$.

We can determine candidates for the metric in each one of these spin-1 multiplets. From relation (4.10) we have

$$\begin{aligned}\sigma^{T}(j,f)^{\mathrm{tr}}&=-q_{(f),(0)j}\epsilon^{\uparrow T}(f)\sigma^{T}(j,f)\epsilon^{\downarrow T}(f)\\ &=-(2\delta_{f0}+2\delta_{fj}-1)\epsilon^{\uparrow T}(f)\sigma^{T}(j,f)\epsilon^{\downarrow T}(f).\end{aligned} \tag{4.17}$$

It is easy to verify that a possible choice is given by

TABLE IV. σ^T matrices.

(f)	Spin(1,0)	$\sigma^T(1,f)$	$\sigma^T(2,f)$	$\sigma^T(3,f)$
(0)	$T_{(0)}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
(1)	$T_{(1)}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
(2)	$T_{(2)}$	$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}$
(3)	$T_{(3)}$	$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$

$$\epsilon^{\uparrow T}(0)=\epsilon^{\downarrow T}(0)=\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \tag{4.18}$$

$$\epsilon^{\uparrow T}(i)=\epsilon^{\downarrow T}(i)=\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \tag{4.19}$$

for $i=1,2,3$. Anagously, by using Eq. (4.13) we obtain

$$\overline{\epsilon}^{\uparrow \overline{T}}(0)=\overline{\epsilon}^{\downarrow \overline{T}}(0)=\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \tag{4.20}$$

$$\overline{\epsilon}^{\uparrow \overline{T}}(i)=\overline{\epsilon}^{\downarrow \overline{T}}(i)=\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \tag{4.21}$$

for $i=1,2,3$. Here we find a curious difference between the familiar class (0) triplets and the triplets for the novel three classes. This difference could be avoided by an alternative representation presented in Table VII. Although the metrics turn out to be Euclidean in this case, it is found that these alternative irreps are not suited for allowing the desired extensions. We come latter to this point.

B. Spin $(\frac{1}{2},\frac{1}{2})$ irreps

An example of spin $(\frac{1}{2},\frac{1}{2})$ irrep of class (0) is given by the translation multiplet $P_{(0)\mu}$, which leads to

$$\sigma^P(j,0)_\mu{}^\nu=-\frac{i}{2}(\delta_{0\mu}\delta_j^\nu+\delta_{j\mu}\delta_0^\nu)+\frac{1}{2}(\epsilon^{mkl}\delta_{l\mu}\delta_k^\nu\delta_{mj}), \tag{4.22}$$

TABLE V. σ^P-matrices.

(f)	Spin $(\frac{1}{2},\frac{1}{2})$	$\sigma^P(1,f)$	$\sigma^P(2,f)$	$\sigma^P(3,f)$
(0)	$P_{(0)}$	$\frac{1}{2}\begin{bmatrix} 0 & -\mathrm{i} & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & -\mathrm{i} & 0 \\ 0 & 0 & 0 & 1 \\ -\mathrm{i} & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \end{bmatrix}$
(1)	$P_{(1)}$	$\frac{1}{2}\begin{bmatrix} 0 & -\mathrm{i} & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & -\mathrm{i} & 0 \\ 0 & 0 & 0 & 1 \\ -\mathrm{i} & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \end{bmatrix}$
(2)	$P_{(2)}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & -\mathrm{i} & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & -\mathrm{i} & 0 \\ 0 & 0 & 0 & 1 \\ -\mathrm{i} & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$
(3)	$P_{(3)}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & -\mathrm{i} & 0 \\ 0 & 0 & 0 & 1 \\ -\mathrm{i} & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & -\mathrm{i} & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

$$q_{(0)j,(0)}\overline{\sigma^P}(j,0)^{\nu}{}_{\mu}=\frac{\mathrm{i}}{2}(\delta_{0\mu}\delta^{\nu}_{j}+\delta_{j\mu}\delta^{\nu}_{0})+\frac{1}{2}(\epsilon^{mkl}\delta_{l\mu}\delta^{\nu}_{k}\delta_{mj}). \tag{4.23}$$

Again, the textures of the $\sigma^P(j,f)$ and $\overline{\sigma^P}(j,f)$ matrices are imposed by the addition Table I and a suited choice of spin $(\frac{1}{2},\frac{1}{2})$ irreps for the different classes is given in Table V for generic spin $(\frac{1}{2},\frac{1}{2})$ four-vectors $P_{(f)}$ with $\overline{\sigma^P}(j,f)=\sigma^P(j,f)^{*\mathrm{tr}}$.

We observe again that the $\sigma^P(j,f)$ and $\overline{\sigma^P}(j,f)$ matrices are obtained by suited permutations of the matrices obtained for the class (0) in order to match the adequate textures. We can determine candidates for the metric in each one of these spin $(\frac{1}{2},\frac{1}{2})$ irreps. From relation (4.10) we have

$$\begin{aligned}\sigma^P(j,f)^{\mathrm{tr}}&=-q_{(f),(0)j}\epsilon^{\uparrow P}(f)\sigma^P(j,f)\epsilon^{\downarrow P}(f)\\&=-(2\delta_{f0}+2\delta_{fj}-1)\epsilon^{\uparrow P}(f)\sigma^P(j,f)\epsilon^{\downarrow P}(f).\end{aligned} \tag{4.24}$$

From this we can adopt

$$\epsilon^{\uparrow P}(0)=\epsilon^{\downarrow P}(0)=\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \tag{4.25}$$

$$\epsilon^{\uparrow P}(i)=\epsilon^{\downarrow P}(i)=\begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \tag{4.26}$$

for $i=1,2,3$. This is consistent with the $P_{(f)}$ multiplets as real representations [a further metric can accomplish (4.24) for $j=1,2,3$, $\epsilon^{\uparrow P}(j)=\sigma_2\otimes\mathrm{i}\sigma_2$, with σ_2 the standard Pauli matrix, but this leads

TABLE VI. Structure of the extension. $j=1,2,3$; $\mu=0,1,2,3$.

Spin → / ↓ Naive dim	(1,0)	$(\frac{1}{2},\frac{1}{2})$	(0,1)
1		$P_{(0)\mu}$	
2/3	$T_{(1)j}, T_{(2)j}, T_{(3)j}$		$\overline{T}_{(1)j}, \overline{T}_{(2)j}, \overline{T}_{(3)j}$
1/3		$P_{(1)\mu}, P_{(2)\mu}, P_{(3)\mu}$	
0	$T_{(0)j}$		$\overline{T}_{(0)j}$

to a nonreal invariant metric]. The pseudometrics in (4.25) and (4.26) reveal that the difference between the familiar class (0) multiplets and the novel multiplets persists. The difference could be again avoided by an alternative representation presented in the Appendix, table VIII. In this case, the ''metrics'' turn out to be Minkowskian, but it is found that these alternative irreps are not suited for the desired extensions.

V. GENERAL STRUCTURE OF THE EXTENSION

In this section we are going to give an outline of the structure of the aimed extension. We are looking for a novel extension of the Poincaré algebra in which, in analogous fashion as accomplished by supersymmetry, a translation can be composed by iteration of further symmetry transformations. We are going to *assume* all throughout this work that the *Clebsch–Gordan theorem* holds for graded multiplets. In order to produce a spin $(\frac{1}{2},\frac{1}{2})$ class (0) charge $P_{(0)}$ we can use three spin $(\frac{1}{2},\frac{1}{2})$-irreps, since

$$(\tfrac{1}{2},\tfrac{1}{2})\otimes(\tfrac{1}{2},\tfrac{1}{2})\otimes(\tfrac{1}{2},\tfrac{1}{2})=(\tfrac{1}{2},\tfrac{1}{2})\otimes((0,0)\oplus(1,0)\oplus(0,1)\oplus(1,1))$$

$$=(\tfrac{1}{2},\tfrac{1}{2})\oplus\ldots.$$

We will start with three spin $(\frac{1}{2},\frac{1}{2})$-irreps $P_{(1)}, P_{(2)}, P_{(3)}$ of naive dimension 1/3 so that they can compose a spin $(\frac{1}{2},\frac{1}{2})$-irrep $P_{(0)}$ of naive dimension 1: the translation multiplet. We introduce spin-1 multiplets necessary for some nontrivial minimal extension accomplishing

$$[\![P_{(1)},[\![P_{(2)},P_{(3)}]\!]]\!]\sim P_{(0)}. \tag{5.1}$$

We are going to implement three steps for building the extension. In order to have (5.1) we need to have a nontrivial result for $[\![P_{(i)},P_{(j)}]\!]$ with $i\neq j$; $i,j=1,2,3$. This implies that we need multiplets in the following direct sum of representations:

$$(\tfrac{1}{2},\tfrac{1}{2})\otimes(\tfrac{1}{2},\tfrac{1}{2})=(0,0)\oplus(1,0)\oplus(0,1)\oplus(1,1).$$

In a forthcoming paper we discuss the introduction of spin (0,0) singlets at this point. We will adopt in the first step only candidates of spin (1,0) and (0,1) of naive dimension 2/3: the spin (1,0)-triplets $T_{(i)}$; $i=1,2,3$, and the spin (0,1)-triplets $\overline{T}_{(i)}$; $i=1,2,3$. We can picture the structure of the aimed extension in the diagram given in Table VI.

In the second step we consider the composition of a space–time translation via $[\![T_{(k)},P_{(k)}]\!]\sim P_{(0)}$ or $[\![\overline{T}_{(k)},P_{(k)}]\!]\sim P_{(0)}$. In the last step we study the consistency of the previous two steps using the graded Jacobi identities.

VI. GRADED EXTENSION OF THE POINCARÉ ALGEBRA

We already observed that the Lie product of two spin $(\frac{1}{2},\frac{1}{2})$-irreps will be expressed in terms of spin (1,0)-triplets $T_{(1)}, T_{(2)}, T_{(3)}$ and (0,1)-triplets $\overline{T}_{(1)}, \overline{T}_{(2)}, \overline{T}_{(3)}$ all of them of naive dimension 2/3:

TABLE VII. $\sigma^{\tilde{T}}$-matrices.

(f)	Spin(1,0)	$\sigma^{\tilde{T}}(1,f)$	$\sigma^{\tilde{T}}(2,f)$	$\sigma^{\tilde{T}}(3,f)$
(1)	$\tilde{T}_{(1)}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 \\ -\mathrm{i} & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & -\mathrm{i} & 0 \\ -\mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$
(2)	$\tilde{T}_{(2)}$	$\begin{bmatrix} 0 & -\mathrm{i} & 0 \\ -\mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 \\ -\mathrm{i} & 0 & 0 \end{bmatrix}$
(3)	$\tilde{T}_{(3)}$	$\begin{bmatrix} 0 & 0 & -\mathrm{i} \\ 0 & 0 & 0 \\ -\mathrm{i} & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & -\mathrm{i} & 0 \\ -\mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$

$$[\![P_{(i)\mu},P_{(j)\nu}]\!]=\eta^{r}(i,j)_{\mu\nu}T_{(i\dagger j)r}+\hat{\eta}^{\dot{r}}(i,j)_{\mu\nu}\overline{T}_{(i\dagger j)\dot{r}} \tag{6.1}$$

for $i\neq j$. Now, using the involution and q-antisymmetry, and the reality of the $P_{(i)}$-irreps

$$\overline{[\![P_{(i)\mu},P_{(j)\nu}]\!]}=[\![P_{(j)\nu},P_{(i)\mu}]\!]=-q_{(j)\nu,(i)\mu}[\![P_{(i)\mu},P_{(j)\nu}]\!]$$

we obtain

$$\begin{aligned} -q_{(j)\nu,(i)\mu}\eta^{r}(i,j)_{\mu\nu}&=\eta^{r}(j,i)_{\nu\mu}=\hat{\eta}^{\dot{r}}(i,j)^{*}_{\mu\nu},\\ -q_{(j)\nu,(i)\mu}\hat{\eta}^{\dot{r}}(i,j)_{\mu\nu}&=\hat{\eta}^{\dot{r}}(j,i)_{\nu\mu}=\eta^{r}(i,j)^{*}_{\mu\nu}. \end{aligned} \tag{6.2}$$

Consider now the Jacobi identities obtained from the triple $T_{(0)l}$, $P_{(i)\mu}$, $P_{(j)\nu}$:

$$[\![T_{(0)l},[\![P_{(i)\mu},P_{(j)\nu}]\!]]\!]=[\![[\![T_{(0)l},P_{(i)\mu}]\!],P_{(j)\nu}]\!]+q_{(0)l,(i)}[\![P_{(i)\mu},[\![T_{(0)l},P_{(j)\nu}]\!]]\!]. \tag{6.3}$$

Using the identities (6.1) and (4.1) we obtain

$$\begin{aligned} \eta^{r}(i,j)_{\mu\nu}(-\mathrm{i}\sigma^{T}(l,i\dagger j)_{r}{}^{n}T_{(i\dagger j)n})=&-\mathrm{i}\sigma^{P}(l,i)_{\mu}{}^{\rho}(\eta^{n}(i,j)_{\rho\nu}T_{(i\dagger j)n}+\hat{\eta}^{\dot{n}}(i,j)_{\rho\nu}\overline{T}_{(i\dagger j)\dot{n}})\\ &+-\mathrm{i}q_{(0)l,(i)}\sigma^{P}(l,j)_{\nu}{}^{\delta}(\eta^{n}(i,j)_{\mu\delta}T_{(i\dagger j)n}+\hat{\eta}^{\dot{n}}(i,j)_{\mu\delta}\overline{T}_{(i\dagger j)\dot{n}}). \end{aligned}$$

With $T_{(i\dagger j)\dot{n}}$ and $\overline{T}_{(i\dagger j)\dot{n}}$ being linearly independent we obtain:

$$\begin{aligned} \sigma^{P}(l,i)_{\mu}{}^{\rho}\hat{\eta}^{\dot{n}}(i,j)_{\rho\nu}+(2\delta_{li}-1)\hat{\eta}^{\dot{n}}(i,j)_{\mu\rho}\sigma^{P}(l,j)_{\nu}{}^{\rho}&=0,\\ \sigma^{P}(l,i)_{\mu}{}^{\rho}\eta^{n}(i,j)_{\rho\nu}+(2\delta_{li}-1)\eta^{n}(i,j)_{\mu\rho}\sigma^{P}(l,j)_{\nu}{}^{\rho}&=\eta^{r}(i,j)_{\mu\nu}\sigma^{T}(l,i\dagger j)_{r}{}^{n}. \end{aligned} \tag{6.4}$$

In analogous fashion, for the triple $\overline{T}_{(0)l}$, $P_{(i)\mu}$, $P_{(j)\nu}$ we obtain further equations:

$$\begin{aligned} \overline{\sigma}^{P}(l,i)^{\rho}{}_{\mu}\eta^{n}(i,j)_{\rho\nu}+(2\delta_{lj}-1)\eta^{n}(i,j)_{\mu\rho}\overline{\sigma}^{P}(l,j)^{\rho}{}_{\nu}&=0,\\ \overline{\sigma}^{P}(l,j)^{\rho}{}_{\nu}\hat{\eta}^{\dot{n}}(i,j)_{\mu\rho}+(2\delta_{lj}-1)\hat{\eta}^{\dot{n}}(i,j)_{\rho\nu}\overline{\sigma}^{P}(l,i)^{\rho}{}_{\mu}&=\hat{\eta}^{\dot{r}}(i,j)_{\mu\nu}\overline{\sigma^{T}}(l,i\dagger j)^{\dot{n}}{}_{\dot{r}}. \end{aligned} \tag{6.5}$$

Using Table I we can determine the allowed textures for the arrays $\eta^{n}(i,j)$ and $\hat{\eta}^{\dot{n}}(i,j)$. We can now use Eqs. (6.2)–(6.5) and use the matrices $\sigma^{\tilde{T}}$ and $\overline{\sigma^{\tilde{T}}}$ for the triplets $\tilde{T}_{(i)}$ and $\tilde{\tilde{T}}_{(i)}$ in Table VII and obtain that using these alternative irreps there are not nontrivial η and $\hat{\eta}$ matrices. This fact is independent of the usage of irreps $P_{(i)}$ in Table V or the alternative $\tilde{P}_{(i)}$ in

Table VIII in the Appendix. Hence, in order *to allow for nontrivial* η and $\hat{\eta}$ matrices *we adopt* triplets $T_{(i)}$ and $\overline{T}_{(i)}$ given by the irreps in Table IV and irreps $P_{(i)}$ given in Table V. Using these multiplets and Eqs. (6.2)–(6.5), for $ijk \in \{123,231,312\}$, we obtain

$$\eta^1(i,j)=a_k\begin{bmatrix}1&0&0&0\\0&0&0&1\\0&-1&0&0\\0&0&1&0\end{bmatrix},\quad \eta^2(i,j)=a_k\begin{bmatrix}0&\mathrm{i}&0&0\\0&0&1&0\\-\mathrm{i}&0&0&0\\0&0&0&-1\end{bmatrix},$$
$$\eta^3(i,j)=a_k\begin{bmatrix}0&0&0&\mathrm{i}\\\mathrm{i}&0&0&0\\0&0&1&0\\0&1&0&0\end{bmatrix}, \tag{6.6}$$

and the further matrices are obtained using (6.2).

We could consider the composition of repeated $P_{(i)}$ charges: $[\![P_{(i)\mu},P_{(i)\nu}]\!]$. These would lead to the consideration of spin (1,0) and spin(0,1) multiplets of class (0), but they are excluded by the Coleman–Mandula theorem.

We are now ready to go to the second step of our extension. Since we want (5.1) to hold, we have

$$[\![T_{(k)r},P_{(l)\mu}]\!]=\delta_{kl}K_r(l)^{\nu}_{\mu}P_{(0)\nu}, \tag{6.7}$$

$$[\![\overline{T}_{(k)\dot{r}},P_{(l)\mu}]\!]=\delta_{kl}\hat{K}_{\dot{r}}(l)^{\nu}_{\mu}P_{(0)\nu}. \tag{6.8}$$

From the properties of involution and q-anticommutation it follows

$$\hat{K}_{\dot{r}}(l)^{\nu}_{\mu}=-q_{(l)r,(l)\mu}K_r(l)^{\nu}_{\mu}{}^*. \tag{6.9}$$

From the triples $T_{(0)l}$, $T_{(k)j}$, $P_{(k)\mu}$ and $\overline{T}_{(0)l}$, $T_{(k)j}$, $P_{(k)\mu}$ we obtain

$$K_j(k)^{\nu}_{\mu}\overline{\sigma}^{P}(l,0)^{\rho}{}_{\nu}=\overline{\sigma}^{P}(l,k)^{\nu}{}_{\mu}K_j(k)^{\rho}_{\nu}, \tag{6.10}$$

$$K_j(k)^{\nu}_{\mu}\sigma^{P}(l,0)_{\nu}{}^{\rho}=(2\delta_{lk}-1)\sigma^{P}(l,k)_{\mu}{}^{\nu}K_j(k)^{\rho}_{\nu}+\sigma^{T}(l,k)_j{}^{m}K_m(k)^{\rho}_{\mu}. \tag{6.11}$$

Using Eqs. (6.9)–(6.11) we obtain

$$K_1(1)=b_1\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix},\quad K_2(1)=b_1\begin{bmatrix}0&0&0&\mathrm{i}\\0&0&1&0\\0&-1&0&0\\\mathrm{i}&0&0&0\end{bmatrix},$$
$$K_3(1)=b_1\begin{bmatrix}0&0&-\mathrm{i}&0\\0&0&0&1\\-\mathrm{i}&0&0&0\\0&-1&0&0\end{bmatrix},$$

$$K_1(2)=b_2\begin{bmatrix}1&0&0&0\\0&0&1&0\\0&0&0&1\\0&1&0&0\end{bmatrix},\quad K_2(2)=b_2\begin{bmatrix}0&\mathrm{i}&0&0\\0&0&0&1\\0&0&-1&0\\\mathrm{i}&0&0&0\end{bmatrix},$$

$$K_3(2)=b_2\begin{bmatrix}0&0&0&-\mathrm{i}\\0&1&0&0\\-\mathrm{i}&0&0&0\\0&0&-1&0\end{bmatrix},$$

$$K_1(3)=b_3\begin{bmatrix}1&0&0&0\\0&0&0&1\\0&1&0&0\\0&0&1&0\end{bmatrix},\quad K_2(3)=b_3\begin{bmatrix}0&0&\mathrm{i}&0\\0&1&0&0\\0&0&0&-1\\\mathrm{i}&0&0&0\end{bmatrix},\tag{6.12}$$

$$K_3(3)=b_3\begin{bmatrix}0&-\mathrm{i}&0&0\\0&0&1&0\\-\mathrm{i}&0&0&0\\0&0&0&-1\end{bmatrix},$$

the $\hat{K}$-matrices are obtained using (6.9).

We are now ready to go to the last consistency condition. We use the triple $P_{(1)\rho}$, $P_{(2)\mu}$, $P_{(3)\nu}$ and the corresponding Jacobi identity to obtain

$$\begin{aligned}0=&q_{(1)\rho,(2)\mu+(3)\nu}\eta^r(2,3)_{\mu\nu}K_r(1)^\sigma_\rho+q_{(2)\mu,(3)\nu}\eta^{r*}(2,3)_{\mu\nu}K^*_r(1)^\sigma_\rho+\eta^r(1,2)_{\rho\mu}K_r(3)^\sigma_\nu\\&+q_{(1)\rho,(2)\mu+(3)\nu}q_{(2)\mu,(3)\nu}\eta^{r*}(1,2)_{\rho\mu}K^*_r(3)^\sigma_\nu+q_{(1)\rho+(2)\mu,(3)\nu}\eta^r(3,1)_{\nu\rho}K_r(2)^\sigma_\mu\\&+q_{(1)\rho,(2)\mu}\eta^{r*}(3,1)_{\nu\rho}K^*_r(2)^\sigma_\mu.\end{aligned}\tag{6.13}$$

From Table II we see that

$$q_{(2)\mu,(3)\nu}=q_{(3)\mu,(1)\nu}=q_{(1)\mu,(2)\nu}=\begin{bmatrix}\mathrm{i}&-\mathrm{i}&-\mathrm{i}&\mathrm{i}\\-\mathrm{i}&\mathrm{i}&\mathrm{i}&-\mathrm{i}\\\mathrm{i}&-\mathrm{i}&-\mathrm{i}&\mathrm{i}\\-\mathrm{i}&\mathrm{i}&\mathrm{i}&-\mathrm{i}\end{bmatrix}_{\mu\nu}.\tag{6.14}$$

Using (6.13) and (6.14) we obtain the following consistency conditions:

$$a_1b_1+a_2b_2+a_3b_3+\mathrm{i}(a_1^*b_1^*+a_2^*b_2^*+a_3^*b_3^*)=0,\tag{6.15}$$

$$a_1b_1-\mathrm{i}a_1^*b_1^*=a_2b_2-\mathrm{i}a_2^*b_2^*=a_3b_3-\mathrm{i}a_3^*b_3^*.\tag{6.16}$$

We can parametrize these constraints in the following way

$$a_1b_1+a_2b_2+a_3b_3=\frac{3}{2}r_0(1-\mathrm{i}),\quad r_0\in\mathbb{R},\tag{6.17}$$

$$a_jb_j-\mathrm{i}a_j^*b_j^*=r_0(1-\mathrm{i}),\quad j=1,2,3.\tag{6.18}$$

A particular nontrivial solution to the constraints is given by

$$a_j=a, \quad b_j=b(1-\mathrm{i}), \quad a,b\in\mathbb{R}\backslash\{0\}, \quad r_0=2ab, \quad j=1,2,3. \tag{6.19}$$

The reader might find it surprising that nontrivial solutions of the structure constants have to be strictly complex, and might expect some conflict with the reality of the compounded translations. Consider for instance the following two triple q-commutators leading to nontrivial translations:

$$[\![P_{(1)0},[\![P_{(2)2},P_{(3)1}]\!]]\!]=(a_1b_1-\mathrm{i}a_1^*b_1^*)P_{(0)0}, \tag{6.20}$$

$$[\![P_{(3)2},[\![P_{(1)2},P_{(2)0}]\!]]\!]=(\mathrm{i}a_3b_3+a_3^*b_3^*)P_{(0)3}. \tag{6.21}$$

The resulting complex coefficients have exactly the required shape, since involution produces the same changes in both sides of (6.20) and (6.21):

$$\overline{[\![P_{(1)0},[\![P_{(2)2},P_{(3)1}]\!]]\!]}=[\![[\![P_{(3)1},P_{(2)2}]\!],P_{(1)0}]\!]=\mathrm{i}[\![P_{(1)0},[\![P_{(2)2},P_{(3)1}]\!]]\!], \tag{6.22}$$

$$\overline{[\![P_{(3)2},[\![P_{(1)2},P_{(2)0}]\!]]\!]}=[\![[\![P_{(2)0},P_{(1)2}]\!],P_{(3)2}]\!]=-\mathrm{i}[\![P_{(3)2},[\![P_{(1)2},P_{(2)0}]\!]]\!]. \tag{6.23}$$

Now, the corresponding (q-commuting) parameters for transformations (6.20) and (6.21) can be found recalling (2.5) and (2.6) and fulfill under involution:

$$\overline{\beta_{-(3)1}\beta_{-(2)2}\beta_{-(1)0}}=-\mathrm{i}\beta_{-(3)1}\beta_{-(2)2}\beta_{-(1)0}, \tag{6.24}$$

$$\overline{\beta_{-(2)0}\beta_{-(1)2}\beta_{-(3)2}}=\mathrm{i}\beta_{-(2)0}\beta_{-(1)2}\beta_{-(3)2}. \tag{6.25}$$

It is curious that due to the noncommutativity, the product of ''real'' (self-involutive) parameters produce complex behavior. The products

$$\beta_{-(3)1}\beta_{-(2)2}\beta_{-(1)0}[\![P_{(1)0},[\![P_{(2)2},P_{(3)1}]\!]]\!],$$

$$\beta_{-(2)0}\beta_{-(1)2}\beta_{-(3)2}[\![P_{(3)2},[\![P_{(1)2},P_{(2)0}]\!]]\!],$$

provide actually real (self-involutive) contributions, as required.

VII. CONCLUSIONS

We have started the construction of graded Lie algebraic extensions with involution of the Poincaré algebra, which we call generically *trefoil symmetries*. Those trefoil symmetries which involve only $\mathbb{Z}_4\times\mathbb{Z}_4$-graded parameters and novel generators of integer spin have been called *clover extensions*. We have obtained a $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded Clover extension $\mathbb{L}$ of the Poincaré algebra. In particular we call this extension *minimal vector clover extension*, for very apparent reasons. In this extension a space–time translation is obtained through the composition of three symmetric vectors which might be interpreted as translations in three novel noncommutative four-dimensional manifolds with a pseudometric.

The Poincaré algebra:

$$\begin{gathered}[\![T_{(0)i},T_{(0)j}]\!]=\mathrm{i}\epsilon_{ijk}T_{(0)k}, \quad [\![T_{(0)i},\overline{T}_{(0)j}]\!]=0, \quad [\![\overline{T}_{(0)i},\overline{T}_{(0)j}]\!]=\mathrm{i}\epsilon_{ijk}\overline{T}_{(0)k},\\ [\![T_{(0)i},P_{(o)\nu}]\!]=-\mathrm{i}\sigma^P(i,0)_\nu{}^\rho P_{(0)\rho}, \quad [\![\overline{T}_{(0)i},P_{(0)\nu}]\!]=-\mathrm{i}q_{(0)i,(0)\nu}P_{(0)\rho}\,\overline{\sigma}^P(i,0)^\rho{}_\nu, \qquad (7.1)\\ [\![P_{(0)\mu},P_{(0)\nu}]\!]=0,\end{gathered}$$

for which the q-commutators coincide with commutators, extends for $f,i,j,k,l=1,2,3$ through the *minimal vector clover extension:*

$$[\![T_{(0)i},P_{(f)\nu}]\!]=-\mathrm{i}\sigma^{P}(i,f)_{\nu}{}^{\rho}P_{(f)\rho},\quad [\![\overline{T}_{(0)i},P_{(f)\nu}]\!]=-\mathrm{i}q_{(0)i,(f)\nu}P_{(f)\rho}\,\overline{\sigma}^{P}(i,f)^{\rho}{}_{\nu},\quad (7.2)$$

$$[\![T_{(0)i},T_{(f)s}]\!]=-\mathrm{i}\sigma^{T}(i,f)_{s}{}^{t}T_{(f)t},\quad [\![\overline{T}_{(0)i},T_{(f)s}]\!]=0,$$

$$[\![T_{(0)i},\overline{T}_{(f)\dot{s}}]\!]=0,\quad [\![\overline{T}_{(0)i},\overline{T}_{(f)\dot{s}}]\!]=-\mathrm{i}q_{(0)i,(f)s}\,\overline{T}_{(f)}{}^{\dot{t}}\,\overline{\sigma^{T}}(i,f)^{\dot{t}}{}_{\dot{s}},\quad (7.3)$$

$$[\![P_{(0)\mu},P_{(f)\nu}]\!]=0,\quad [\![P_{(f)\mu},P_{(f)\nu}]\!]=0,\quad (7.4)$$

$$[\![P_{(0)\mu},T_{(f)t}]\!]=0,\quad [\![P_{(0)\mu},\overline{T}_{(f)s}]\!]=0,\quad (7.5)$$

$$[\![T_{(i)s},T_{(j)t}]\!]=0,\quad [\![T_{(i)s},\overline{T}_{(j)\dot{t}}]\!]=0,\quad [\![\overline{T}_{(i)\dot{s}},\overline{T}_{(j)\dot{t}}]\!]=0,\quad (7.6)$$

$$[\![P_{(i)\mu},P_{(j)\nu}]\!]=\eta^{r}(i,j)_{\mu\nu}T_{(i\dagger j)r}+\hat{\eta}^{\dot{r}}(i,j)_{\mu\nu}\overline{T}_{(i\dagger j)\dot{r}};\quad i\neq j,\quad (7.7)$$

$$\begin{aligned}[\![T_{(k)r},P_{(l)\mu}]\!]&=\delta_{kl}K_{r}(l)_{\mu}^{\nu}P_{(0)\nu},\\ [\![\overline{T}_{(k)\dot{r}},P_{(l)\mu}]\!]&=\delta_{kl}\hat{K}_{\dot{r}}(l)_{\mu}^{\nu}P_{(0)\nu}.\end{aligned}\quad (7.8)$$

The σ-matrices are given in Table IV and V. The η-matrices are given in (6.6). The K-matrices are given in (6.12). These matrices are constrained by the conditions (6.17) and (6.18). A particular choice respecting the symmetry among the novel classes is given by (6.19).

Relations (7.1)–(7.8) provide a $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded Lie algebra $\mathbb{L}$ with involution, which extends nontrivially the Poincaré algebra.

A very important feature of the obtained extension is that *this extension does not correspond to any cumbersome deformation of the conformal extension and related series since there the (scalar) dilatation operator cannot be excluded.*

This extension is minimal in the sense that no extra generators are needed for the closure of the algebra, and the omission of some generator would either damage the closure of the graded algebra, or would not provide an actual nontrivial extension of the Poincaré algebra.

The obtained constraints on the structure constants reveal that the isotropy and homogeneity of the space–time can be maintained in this extension: there are particular choices of the structure constants that maintain the profound symmetry behind the three novel classes.

The grading indices used by the novel generators provide a sort of triple replication of the way in which the class (0) indices are used by the Poincaré algebra: The Poincaré algebra uses once the index $(0)_0$ and three times each index $(0)_j$, for $j=1,2,3$. The novel generators of class (i) use once the index $(i)_0$ and three times each index $(i)_j$, for $j=1,2,3$. The Poincaré algebra has ten parameters (and generators) and the obtained extension has $10+3\times10=40$ parameters (and generators). There are further minimal extensions that can be nontrivially coupled to generators of this extension.

The index structure has certain attractive patterns. The class (0) builds up a $\mathbb{Z}_2\times\mathbb{Z}_2$ group, which might be connected to the discrete transformations of time reversal and space inversion. According to Table III the novel classes reproduce this Klein group structure as well. The three novel classes can be composed to arrive at the class (0). We discuss in further stages of this series the extent to which we could expect a connection to color charges, to the 1/3 electric charges of quarks, to the lepton and quarks family structure, or to the family generations. Observe for now that we have 16 Weyl fermions in each family, 12 of them are quarks and 4 leptons, which maintain some analogy with the structure of the $\mathbb{Z}_4\times\mathbb{Z}_4$-grading and its classes. The naive extensions of these symmetries, and the study of inner automorphism will provide the way for relating internal and external symmetries. The presence of spin 1 generators in the extension suggest superfields that might connect gauge and Higgs fields. Gravitation will be involved in this research

TABLE VIII. $\sigma^{\tilde{P}}$-matrices.

(f)	Spin $(\frac{1}{2},\frac{1}{2})$	$\sigma^{\tilde{P}}(1,f)$	$\sigma^{\tilde{P}}(2,f)$	$\sigma^{\tilde{P}}(3,f)$
(1)	$\tilde{P}_{(1)}$	$\frac{1}{2}\begin{bmatrix} 0 & -\mathrm{i} & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \\ -1 & 0 & 0 & 0 \\ 0 & -\mathrm{i} & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -\mathrm{i} & 0 \\ 0 & -\mathrm{i} & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$
(2)	$\tilde{P}_{(2)}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -\mathrm{i} & 0 \\ 0 & -\mathrm{i} & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & -\mathrm{i} & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \\ -1 & 0 & 0 & 0 \\ 0 & -\mathrm{i} & 0 & 0 \end{bmatrix}$
(3)	$\tilde{P}_{(3)}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \\ -1 & 0 & 0 & 0 \\ 0 & -\mathrm{i} & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -\mathrm{i} & 0 \\ 0 & -\mathrm{i} & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & -\mathrm{i} & 0 & 0 \\ -\mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

by considering further extensions or local versions of flat graded symmetries. The reader might inquire for a sort of echo of grading in the Kepler symmetry relating the cube of the semimajor axes with the square of the periods of revolution in planetary motion.

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APPENDIX

Here we present some spin representations whose metrics are formally identical to those of the class (0). Nevertheless, it turns out that these representations are not suited for allowing nontrivial extensions of the Poincaré algebra.

1. Alternative spin (1,0) and (0,1) irreps

We can construct an alternative representation to the spin (1,0) and (0,1) irreps presented in Table IV. Consider for instance the allowed choice given in Table VII with $\overline{\sigma^{\tilde{T}}}(j,f) = \sigma^{\tilde{T}}(j,f)^{*\mathrm{tr}}$. In this case the metrics turn out to be Euclidean. $\epsilon^{\uparrow\tilde{T}}(f) = \overline{\epsilon^{\uparrow\tilde{T}}}(f) = \mathrm{diag}(-1,-1,-1)$. Nevertheless, it is found in the main text that these alternative irreps are not suited for allowing nontrivial extensions of external symmetries.

2. Alternative spin $(\frac{1}{2},\frac{1}{2})$ irreps

We can construct an alternative representation to the spin $(\frac{1}{2},\frac{1}{2})$ irreps presented in Table V. Consider for instance the choice given in Table VIII with $\overline{\sigma^{\tilde{P}}}(j,f) = \sigma^{\tilde{P}}(j,f)^{*\mathrm{tr}}$. In this case, the "metrics" turn out to be Minkowskian: $\epsilon^{\uparrow\tilde{P}}(f) = \mathrm{diag}(1,-1,-1,-1) = \epsilon^{\downarrow\tilde{P}}(f)$. Again, it is found that these alternative irreps are not suited for the desired symmetry extensions.

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Trefoil symmetry II. Another clover extension

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We construct a novel graded extension of the Poincaré group with integer spin multiplets as novel generators. The extension involves $\mathbb{Z}_4\times\mathbb{Z}_4$ graded parameters and produce space–time translations through the composition of novel symmetric vector and scalar multiplets. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Grading structures suited for extending the Poincaré group were determined long ago[1] and even more general realms have been found for constructing continuous symmetries.[2] This is the second paper in a series on graded extensions of the Poincaré group beyond the Coleman–Mandula no-go theorem.[3] The study of novel symmetries beyond those of special relativity and supersymmetry has started addressing graded Lie algebraic extensions with involution which have been called *trefoil symmetries*.[4] Those trefoil symmetries which are $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded and involve only multiplets of generators of integer spin have been called *clover symmetries* and correspond to the simplest extensions beyond the Coleman–Mandula no-go theorem.

In Ref. 4 the reader can find a review on grading groups, graded parameter, and graded Lie algebras, on the grading groups suited for extending the external symmetries of the special relativity, and a minimal $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded extension of the Poincaré algebra which involved only spin-1 multiplets as novel generators, which has been called *minimal vector clover symmetry*. Our aim is to present another extension called *minimal scalar clover symmetry*, since the novel generators are only symmetric vector and scalar multiplets. *We will maintain all throughout this work all the conventions stated in Ref. 4*. We look for a $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded Lie algebra with involution which contains the Poincaré algebra. The novel algebra has three symmetric-vector generators $P_{(1)}$, $P_{(2)}$, $P_{(3)}$ of naive dimension 1/3. We want them to compose via

$$(\tfrac{1}{2},\tfrac{1}{2})\otimes(\tfrac{1}{2},\tfrac{1}{2})\otimes(\tfrac{1}{2},\tfrac{1}{2})=(\tfrac{1}{2},\tfrac{1}{2})\oplus\ \ldots \tag{1.1}$$

to produce the (standard) space–time translation multiplet $P_{(0)}$,

$$[\![P_{(1)},[\![P_{(2)},P_{(3)}]\!]]\!]\sim P_{(0)}\,. \tag{1.2}$$

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The double brackets stand for q-commutators respecting the grading assignments of its entries, and $P_{(0)}=(P_0,P_1,P_2,P_3)$ stands for the translation four-vector. The Lorentz generators will be written in terms of the spin (1,0) triplet $T_{(0)}$ and the spin (0,1) triplet $\overline{T}_{(0)}$ as presented in Ref. 4. In order to have (1.2) we need a nontrivial result for $[\![P_{(i)},P_{(j)}]\!]$ with $i\neq j$; $i,j=1,2,3$. Hence, we need multiplets in the following direct sum of representations:

$$(\tfrac{1}{2},\tfrac{1}{2})\otimes(\tfrac{1}{2},\tfrac{1}{2})=(0,0)\oplus(1,0)\oplus(0,1)\oplus(1,1).$$

We will discuss here the introduction of spin (0,0) singlets at this point:

$$[\![P_{(i)},P_{(j)}]\!]\sim E_{(i\dagger j)}+\overline{E}_{(i\dagger j)};\quad i\neq j;\quad i,j=1,2,3. \tag{1.3}$$

The novel scalars $E_{(f)s}$ have naive dimension 2/3.

This work is structured in the following way. Section II introduces the required novel irreducible multiplets. Section III gives an outline of the general structure of the aimed extension. In Sec. IV we study the Jacobi identities and obtain the desired $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded Lie algebraic extension of the Poincaré algebra. Section V inquires about the introduction of dimensionless scalar charges. Section VI gives the concluding remarks.

II. GRADED SPIN IRREPS OF GENERATORS

We consider multiplets of generators $a_{(f)s}$ of classes $(f)=(0),(1),(2),(3)$. The index s stands for the different components of each multiplet except for spin-0 singlets. The dual multiplets are written $a_{(f)}{}^{s}$, and the corresponding complex-conjugated and dual complex-conjugated-multiplets are given by $\overline{a}_{(f)\dot{s}}$ and $\overline{a}_{(f)}{}^{\dot{s}}$. All these multiplets transforms linearly under Lorentz generators:

$$[\![T_{(0)i},a_{(f)s}]\!]=-\mathrm{i}\sigma^a(i,f)_s{}^t a_{(f)t}, \tag{2.1}$$

$$[\![T_{(0)i},a_{(f)}{}^{s}]\!]=\mathrm{i}q_{(0)i,(f)s}\,a_{(f)}{}^{t}\,\sigma^a(i,f)_t{}^{s}, \tag{2.2}$$

$$[\![\overline{T}_{(0)i},\overline{a}_{(f)\dot{s}}]\!]=-\mathrm{i}q_{(0)i,(f)s}\,\overline{a}_{(f)\dot{t}}\,\overline{\sigma^a}(i,f)^{\dot{t}}{}_{\dot{s}}, \tag{2.3}$$

$$[\![\overline{T}_{(0)i},\overline{a}_{(f)}{}^{\dot{s}}]\!]=\mathrm{i}\overline{\sigma^a}(i,f)^{\dot{s}}{}_{\dot{t}}\,\overline{a}_{(f)}{}^{\dot{t}}, \tag{2.4}$$

where $\overline{a_{(f)s}}=\overline{a}_{(f)\dot{s}}$, $\overline{a_{(f)}{}^{s}}=\overline{a}_{(f)}{}^{\dot{s}}$. From the involution we obtain

$$\overline{\sigma^a}(i,f)^{\dot{t}}{}_{\dot{s}}=\sigma^a(i,f)^{*\,t}_{s}. \tag{2.5}$$

From the Jacobi identity

$$[\![T_{(0)j},[\![T_{(0)k},a_{(f)s}]\!]]\!]=[\![[\![T_{(0)j},T_{(0)k}]\!],a_{(f)s}]\!]+q_{(0)j,(0)k}[\![T_{(0)k},[\![T_{(0)j},a_{(f)s}]\!]]\!]$$

we obtain

$$[\mathrm{i}\sigma^a(j,f),\mathrm{i}\sigma^a(k,f)]=\mathrm{i}\epsilon_{jkl}(\mathrm{i}\sigma^a(l,f)), \tag{2.6}$$

where the commutator has the usual meaning. Accordingly, the matrices $\mathrm{i}\sigma^a(j,f)_s{}^t$ and $-\mathrm{i}[\sigma^a(j,f)^{\mathrm{tr}}]^t{}_s$ are standard representations of angular momenta. Analogously, using the Jacobi identity for the triple $\overline{T}_{(0)j}$, $\overline{T}_{(0)k}$, $\overline{a}_{(f)\dot{s}}$ we obtain

$$[-\mathrm{i}q_{(0)j,(f)}\overline{\sigma^a}(j,f),-\mathrm{i}q_{(0)k,(f)}\overline{\sigma^a}(k,f)]=\mathrm{i}\epsilon_{jkl}(-\mathrm{i}q_{(0)l,(f)}\overline{\sigma^a}(l,f)). \tag{2.7}$$

Hence, $-\mathrm{i}q_{(0)j,(f)}\overline{\sigma^a}(j,f)$ and $\mathrm{i}q_{(0)j,(f)}\overline{\sigma^a}(j,f)^{\mathrm{tr}}$ are also standard representations of angular momenta. It is easy to verify that $a_{(f)}{}^s a_{(f)_s}$ (summation only over s through the multiplet) and $\overline{a}_{(f)\dot{s}}\overline{a}_{(f)}{}^{\dot{s}}$ are invariant quadratic products.

The "metrics" $\epsilon^a(f)^{us}$ and $\epsilon^a(f)_{us}$ connect the self-representation $a_{(f)s}$ and the dual-self-representation $a_{(f)}{}^s$:

$$\epsilon^a(f)^{us}\, a_{(f)s} = a_{(f)}{}^u, \tag{2.8}$$

$$\epsilon^a(f)_{ds}\, a_{(f)}{}^s = a_{(f)d}. \tag{2.9}$$

These "metrics" carry trivial index $\tilde{o}$, and fulfill in matricial notation

$$\sigma^a(j,f)^{\mathrm{tr}} = -q_{(f),(0)j}\epsilon^{\uparrow a}(f)\sigma^a(j,f)\epsilon^{\downarrow a}(f), \tag{2.10}$$

where $\epsilon^{\uparrow a}(f)$ and $\epsilon^{\downarrow a}(f)$ stand for the metric with indices up and down, respectively. Analogously, we define a "metric" between the complex-conjugated-representation and its dual:

$$\overline{\epsilon^a}(f)^{\dot{u}\dot{s}}\overline{a}(f)_{\dot{s}} = \overline{a}(f)^{\dot{u}}, \tag{2.11}$$

$$\overline{\epsilon^a}(f)_{\dot{d}\dot{s}}\overline{a}_{(f)}{}^{\dot{s}} = \overline{a}_{(f)\dot{d}}, \tag{2.12}$$

which leads in matricial notation to

$$\overline{\sigma^a}(j,f)^{\mathrm{tr}} = -q_{(0)j,(f)}\overline{\epsilon}^{\downarrow\overline{a}}(f)^{\mathrm{tr}}\overline{\sigma^a}(j,f)\overline{\epsilon}^{\uparrow\overline{a}}(f)^{\mathrm{tr}}. \tag{2.13}$$

We classify now the spin representations according to their eigenvalues with respect to the Casimir operators of the Lorentz algebra: $\Sigma T_{(0)i}T_{(0)i}$ and $\Sigma\overline{T}_{(0)i}\overline{T}_{(0)i}$. A multiplet $a_{(0)s}$ is said to be in the (s_l,s_r)-spin representation if

$$\begin{aligned}\left[\!\left[\sum_{i=1}^{3} T_{(0)i}T_{(0)i}, a_{(f)s}\right]\!\right] &= s_l(s_l+1)a_{(f)s},\\ \left[\!\left[\sum_{i=1}^{3} \overline{T}_{(0)i}\overline{T}_{(0)i}, a_{(f)s}\right]\!\right] &= s_r(s_r+1)a_{(f)s}.\end{aligned} \tag{2.14}$$

The total spin is given by s_l+s_r. We are now going to list the irreps of integer total spin not greater than one.

A. Spin $(\frac{1}{2},\frac{1}{2})$ irreps

We consider spin $(\frac{1}{2},\frac{1}{2})$ multiplets $P_{(f)s}$; $f=0,1,2,3$. The four-vector $P_{(0)s}$ is the space–time translation. The textures of the $\sigma^P(j,f)$ and $\overline{\sigma^P}(j,f)$ matrices are fixed by the graded structure and a suited choice of spin $(\frac{1}{2},\frac{1}{2})$ irreps for the different classes is given in Table I for generic spin $(\frac{1}{2},\frac{1}{2})$ four-vectors $P_{(f)}$ with $\overline{\sigma^P}(i,f)=\sigma^P(i,f)^{*\mathrm{tr}}$.

From relation (2.10) we can adopt

$$\epsilon^{\uparrow P}(0)=\epsilon^{\downarrow P}(0)=\begin{bmatrix}1&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix}, \tag{2.15}$$

TABLE I. σ^P-matrices.

(f)	Spin $(\frac{1}{2},\frac{1}{2})$	$\sigma^P(1,f)$	$\sigma^P(2,f)$	$\sigma^P(3,f)$
(0)	$P_{(0)}$	$\frac{1}{2}\begin{bmatrix} 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 1 \\ -i & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -i & 0 & 0 & 0 \end{bmatrix}$
(1)	$P_{(1)}$	$\frac{1}{2}\begin{bmatrix} 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 1 \\ -i & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -i & 0 & 0 & 0 \end{bmatrix}$
(2)	$P_{(2)}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -i & 0 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 1 \\ -i & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$
(3)	$P_{(3)}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 1 \\ -i & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -i & 0 & 0 & 0 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

$$\epsilon^{\uparrow P}(i)=\epsilon^{\downarrow P}(i)=\begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}, \quad i=1,2,3, \tag{2.16}$$

which is consistent with the $P_{(f)}$ multiplets as real representations.

B. Spin (0,0) irreps

The spin (0,0) irreps are one-dimensional and are just characterized by vanishing σ-matrices, i.e., they are Lorentz invariant. A scalar siglet $E_{(\mu)\rho}$ means just that it carries index $(\mu)\rho$. In this case the subindex ρ *is not to be interpreted as a multiplet index.*

III. GENERAL STRUCTURE OF THE EXTENSION

We are going to implement three steps for building a novel extension. We will consider in the first step the composition of spin (0,0) singlets $E_{(f)s}$ of naive dimension 2/3 via $[\![P_{(i)},P_{(j)}]\!] \sim E_{(i\dagger j)}+\overline{E}_{(i\dagger j)}$ with $i\neq j$; $i,j=1,2,3$. We can picture the structure of the aimed extension in the diagram given in Table II.

In the second step we consider the composition of a space–time translation via $[\![E_{(k)},P_{(k)}]\!] \sim P_{(0)}$ or $[\![\overline{E}_{(k)},P_{(k)}]\!]\sim P_{(0)}$. In the last step we study the consistency of the previous two steps using the graded Jacobi-identities.

IV. GRADED EXTENSION OF THE POINCARÉ ALGEBRA

We already observed that the product of two spin-$(\frac{1}{2},\frac{1}{2})$ irreps will be expressed in terms of scalar singlets $E_{(k)\sigma},\overline{E}_{(k)\sigma}$ of naive dimension 2/3:

$$[\![P_{(i)\mu},P_{(j)\nu}]\!]=C^{\sigma}(i,j)_{\mu\nu}E_{(i\dagger j)\sigma}+\hat{C}^{\sigma}(i,j)_{\mu\nu}\overline{E}_{(i\dagger j)\sigma}, \tag{4.1}$$

TABLE II. Structure of the extension. $j=1,2,3$; μ, $s=0,1,2,3$.

	Spin		
Naive dim	(1,0)	$(\frac{1}{2},\frac{1}{2})$ / (0,0)	(0,1)
1		$P_{(0)\mu}$	
2/3		$E_{(1)0},E_{(2)0},E_{(3)0},\overline{E}_{(1)0},\overline{E}_{(2)0},\overline{E}_{(3)0}$	
1/3		$P_{(1)\mu},P_{(2)\mu},P_{(3)\mu}$	
0	$T_{(0)j}$	$(G_{(0)0},\overline{G}_{(0)0})$	$\overline{T}_{(0)j}$

for $i\neq j$, $i,j=1,2,3$. Now, using the involution and q-antisymmetry, and the reality of the $P_{(i)}$- irreps

$$\overline{[\![P_{(i)\mu},P_{(j)\nu}]\!]}=[\![P_{(j)\nu},P_{(i)\mu}]\!]=-q_{(j)\nu,(i)\mu}[\![P_{(i)\mu},P_{(j)\nu}]\!]$$

we obtain

$$-q_{(j)\nu,(i)\mu}C^{\sigma}(i,j)_{\mu\nu}=C^{\sigma}(j,i)_{\nu\mu}=\hat{C}^{\sigma}(i,j)^{*}_{\mu\nu}. \tag{4.2}$$

Consider now the Jacobi identities obtained from the triple $T_{(0)l}$, $P_{(i)\mu}$, $P_{(j)\nu}$:

$$[\![T_{(0)l},[\![P_{(i)\mu},P_{(j)\nu}]\!]]\!]=[\![[\![T_{(0)l},P_{(i)\mu}]\!],P_{(j)\nu}]\!]+q_{(0)l,(i)}[\![P_{(i)\mu},[\![T_{(0)l},P_{(j)\nu}]\!]]\!]. \tag{4.3}$$

Using the identities (4.1) and (2.1) we obtain

$$\begin{aligned}0=&-\mathrm{i}\sigma^{P}(l,i)_{\mu}{}^{\rho}(C^{\sigma}(i,j)_{\rho\nu}E_{(i\dagger j)\sigma}+\hat{C}^{\sigma}(i,j)_{\rho\nu}\overline{E}_{(i\dagger j)\sigma})\\&+-\mathrm{i}q_{(0)l,(i)}\sigma^{P}(l,j)_{\nu}{}^{\delta}(C^{\sigma}(i,j)_{\mu\delta}E_{(i\dagger j)\sigma}+\hat{C}^{\sigma}(i,j)_{\mu\delta}\overline{E}_{(i\dagger j)\sigma}).\end{aligned}$$

With $E_{(i\dagger j)s}$ and $\overline{E}_{(i\dagger j)s}$ being linearly independent we obtain

$$\sigma^{P}(l,i)_{\mu}{}^{\rho}C^{\sigma}(i,j)_{\rho\nu}+(2\delta_{li}-1)C^{\sigma}(i,j)_{\mu\rho}\sigma^{P}(l,j)_{\nu}{}^{\rho}=0. \tag{4.4}$$

In analogous fashion, for the triple $\overline{T}_{(0)l}$, $P_{(i)\mu}$, $P_{(j)\nu}$ we obtain further equations:

$$\overline{\sigma}^{P}(l,i)^{\rho}{}_{\mu}C^{\sigma}(i,j)_{\rho\nu}+(2\delta_{lj}-1)C^{\sigma}(i,j)_{\mu\rho}\overline{\sigma}^{P}(l,j)^{\rho}{}_{\nu}=0. \tag{4.5}$$

Using the table of the grading group $\mathbb{Z}_4\times\mathbb{Z}_4$ we can determine the allowed textures for the arrays $C^{\sigma}(i,j)$, $\hat{C}^{\sigma}(i,j)$. We can now use Eqs. (4.2)–(4.5) and the σ-matrices in Table I to obtain for $ijk\in\{123,231,312\}$:

$$C^0(i,j)=c_{k0}\begin{bmatrix}0&0&1&0\\0&\mathrm{i}&0&0\\0&0&0&\mathrm{i}\\1&0&0&0\end{bmatrix},\quad C^1(i,j)=c_{k1}\begin{bmatrix}1&0&0&0\\0&0&0&-1\\0&1&0&0\\0&0&1&0\end{bmatrix},$$
$$C^2(i,j)=c_{k2}\begin{bmatrix}0&1&0&0\\0&0&-\mathrm{i}&0\\1&0&0&0\\0&0&0&-\mathrm{i}\end{bmatrix},\quad C^3(i,j)=c_{k3}\begin{bmatrix}0&0&0&1\\-1&0&0&0\\0&0&-\mathrm{i}&0\\0&\mathrm{i}&0&0\end{bmatrix}. \tag{4.6}$$

The further matrices are obtained using (4.2).

We are now ready to go to the second step of our extension. Since we want (1.2) to hold, we have two ways for arriving at this stage:

$$[\![E_{(f)\sigma},P_{(l)\mu}]\!]=\delta_{fl}S_\sigma(l)^\nu_\mu P_{(0)\nu}, \tag{4.7}$$

$$[\![\overline{E}_{(f)\sigma},P_{(l)\mu}]\!]=\delta_{fl}\hat{S}_\sigma(l)^\nu_\mu P_{(0)\nu}, \tag{4.8}$$

for $l\in 1,2,3$. From the properties of involution and q-anticommutation it follows

$$\hat{S}_\sigma(l)^\nu_\mu=-q_{(l)\sigma,(l)\mu}S_\sigma(l)^{\nu *}_\mu. \tag{4.9}$$

From the triples $T_{(0)l}$, $E_{(k)s}$, $P_{(k)\mu}$ and their corresponding Jacobi identities we obtain

$$S_\sigma(k)^\nu_\mu\sigma^P(l,0)_\nu{}^\rho=(2\delta_{lk}-1)\sigma^P(l,k)_\mu{}^\delta S_\sigma(k)^\rho_\delta, \tag{4.10}$$

$$S_\sigma(k)^\nu_\mu\overline{\sigma}^P(l,0)^\rho{}_\nu=\overline{\sigma}^P(l,k)^\delta{}_\mu S_\sigma(k)^\rho_\delta. \tag{4.11}$$

Using Eqs. (4.10) and (4.11) we obtain

$$S_i(k)=0\quad\forall i\neq 0, \tag{4.12}$$

$$S_0(1)=s_{10}\begin{bmatrix}0&1&0&0\\1&0&0&0\\0&0&0&-\mathrm{i}\\0&0&\mathrm{i}&0\end{bmatrix},\quad S_0(2)=s_{20}\begin{bmatrix}0&0&1&0\\1&0&0&0\\0&-\mathrm{i}&0&0\\0&0&0&-\mathrm{i}\end{bmatrix},$$
$$S_0(3)=s_{30}\begin{bmatrix}0&0&0&1\\1&0&0&0\\0&0&-\mathrm{i}&0\\0&\mathrm{i}&0&0\end{bmatrix}. \tag{4.13}$$

Accordingly, only through the singlets $E_{(l)0}$; $l=1,2,3$ we might expect to produce a space–time translation. *Since we are looking for a minimal extension, we leave aside from now on the scalars* $E_{(l)j}$; $l,j=1,2,3$.

We are now ready to go to the last consistency condition. We use the triple $P_{(1)\rho}$, $P_{(2)\mu}$, $P_{(3)\nu}$ and the corresponding Jacobi identity to obtain

$$\begin{aligned}0=&q_{(1)\rho,(2)\mu+(3)\nu}C^\delta(2,3)_{\mu\nu}S_\delta(1)^\sigma_\rho+C^\delta(1,2)_{\rho\mu}S_\delta(3)^\sigma_\nu\\&+q_{(1)\rho+(2)\mu,(3)\nu}C^\delta(3,1)_{\nu\rho}S_\delta(2)^\sigma_\mu.\end{aligned} \tag{4.14}$$

From the group grading $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$ we have:[4]

$$q_{(2)\mu,(3)\nu}=q_{(3)\mu,(1)\nu}=q_{(1)\mu,(2)\nu}=\begin{bmatrix} \mathrm{i} & -\mathrm{i} & -\mathrm{i} & \mathrm{i} \\ -\mathrm{i} & \mathrm{i} & \mathrm{i} & -\mathrm{i} \\ \mathrm{i} & -\mathrm{i} & -\mathrm{i} & \mathrm{i} \\ -\mathrm{i} & \mathrm{i} & \mathrm{i} & -\mathrm{i} \end{bmatrix}_{\mu\nu}. \tag{4.15}$$

Equations (4.14) and (4.15) lead to the consistency conditions

$$c_{j0}s_{j0}-\mathrm{i}c^*_{j0}s^*_{j0}=0, \quad j\in 1,2,3. \tag{4.16}$$

We can parametrize these constraints in the following way:

$$c_{10}\ \ s_{10}=t_1(1+\mathrm{i}), \quad c_{20}s_{20}=t_2(1+\mathrm{i}), \quad c_{30}s_{30}=t_3(1+\mathrm{i}), \tag{4.17}$$

$$t_1,t_2,t_3\in\mathbb{R}.$$

It is easy to construct particular solutions that maintain the symmetry among the novel multiplet classes (and thus the homogeneity and isotropy of space–time). Consider for instance the particular choice satisfying the constraints in (4.17):

$$c_{j0}=c, \quad s_{j0}=s(1+\mathrm{i}), \quad c,s\in\mathbb{R}\backslash\{0\}, \quad j=1,2,3\,. \tag{4.18}$$

Hence, there exist nontrivial solutions to the coefficients c_{j0},s_{j0}; $j=1,2,3$. This *does not imply* that we can compose a space–time translation $P_{(0)}$ just with the symmetric four-vectors $P_{(i)}$ (and the scalar fields $E_{(i)0}$) via the triple composition $[\![P_{(1)},[\![P_{(2)},P_{(3)}]\!]]\!]$ as originally aimed in (1.2). The contributions to this triple q-commutator turn out to be proportional to $c_{10}s_{10}-\mathrm{i}c^*_{10}s^*_{10}$, which vanish according to (4.16). We *can* nevertheless compose a space–time translation via $[\![E_{(l)0},P_{(l)}]\!]$ or via $[\![\overline{E}_{(l)0},P_{(l)}]\!]$, and this fact provides authentically a minimal extension of the Poincaré algebra by itself.

The class (0)-indices are used by the Poincaré algebra in the following way: once the index $(0)_0$ and three times each index $(0)_j$, for $j=1,2,3$. The novel generators of the class (i), $i=1,2,3$ use three times the index $(i)_0$ (since $E_{(i)0}$ is complex) and once each index $(i)_j$, for $j=1,2,3$. The Poincaré algebra has ten parameters (and generators) and the minimal extension presented here has $10+3\times3+3\times3=28$ parameters (and generators).

In order to maintain a symmetric usage of the indices of the different classes for the spin (0,0) and spin $(\frac{1}{2},\frac{1}{2})$ multiplets, the previous considerations suggest the introduction of two charges of index (0)0 of spin (0,0). This question will be addressed in Sec. V.

V. INTRODUCING DIMENSIONLESS SCALAR GENERATORS

A very appealing idea arises when considering novel extensions of the Poincaré algebra, since elusive connections between internal and external symmetries might be revealed. Particularly interesting is the introduction of dimensionless scalar generators since they are naively the most expedite candidates for internal symmetry generators. We introduce scalar dimensionless singlets $G_{(\rho)\mu}$, where $\rho,\mu=0,1,2,3$ and we will select only the ones which are effectively nontrivially connected to the extension obtained Sec. IV.

The generators $G_{(\rho)\mu}$ are scalar, and thus have trivial q-commutation relations with the Lorentz generators. If these scalar generators have nontrivial q-commutation relations with the mentioned extension, they have nontrivial relations with the multiplets $P_{(i)}$; $i=1,2,3$, since *all* the novel generators of the extension as well as the space–time translations are obtained from compositions of objects obtained in turn from the composition of the multiplets $P_{(i)}$.

We expect that the multiplets $P_{(i)}$; $i=1,2,3$ might constitute representations of the subgroup built by the novel scalar singlets. These scalars satisfy the q-commutation relations

$$[\![G_{(\rho)\mu},G_{(\sigma)\nu}]\!]=-\mathrm{i}\zeta_{\mu}(\rho,\sigma)_{\nu}{}^{\kappa}G_{(\rho\dagger\sigma)\kappa}. \tag{5.1}$$

The structure constants build up the adjoint representation, hence the matrix

$$D^{G}(G_{(\rho)\mu})=-\mathrm{i}\zeta_{\mu}(\rho,\sigma)^{\mathrm{tr}} \tag{5.2}$$

constitutes a representation D^{G} of the generator $G_{(\rho)\mu}$. Now, the multiplets $P_{(i)}$; $i=1,2,3$ build up representations of the group generated by $G_{(\rho)\mu}$. We should have

$$[\![G_{(\rho)\mu},P_{(i)\nu}]\!]=-\mathrm{i}\Lambda_{\mu}(\rho,i)_{\nu}{}^{\sigma}P_{(\rho\dagger i)\sigma}. \tag{5.3}$$

Using the Jacobi identities associated with the triples $G_{(\rho)\mu}$, $G_{(\alpha)\xi}$, $P_{(j)\nu}$, we obtain

$$\Lambda_{\mu}(\rho,\alpha\dagger j)^{\mathrm{tr}}\Lambda_{\xi}(\alpha,j)^{\mathrm{tr}}-q_{(\rho)\mu,(\alpha)\xi}\Lambda_{\xi}(\alpha,\rho\dagger j)^{\mathrm{tr}}\Lambda_{\mu}(\rho,j)^{\mathrm{tr}}=\zeta_{\mu}(\rho,\alpha)_{\xi}{}^{\kappa}\Lambda_{\kappa}(\rho\dagger\alpha,j)^{\mathrm{tr}}. \tag{5.4}$$

Hence, $-\mathrm{i}\Lambda_{\mu}(\rho,i)^{\mathrm{tr}}$ constitutes a representation D^{P} of the algebra generated by $G_{(\rho)\mu}$:

$$D^{P}(G_{(\rho)\mu})=-\mathrm{i}\Lambda_{\mu}(\rho,i)^{\mathrm{tr}}. \tag{5.5}$$

Using the Jacobi identity associated with the triples $T_{(0)r}$, $G_{(\rho)\mu}$, $P_{(i)\nu}$ and $\overline{T}_{(0)r}$, $G_{(\rho)\mu}$, $P_{(i)\nu}$ we obtain, respectively, for $\mu=0,1,2,3$:

$$\Lambda_{\mu}(0,i)=l(0i)_0\begin{bmatrix}\mathrm{i}&0&0&0\\0&\mathrm{i}&0&0\\0&0&\mathrm{i}&0\\0&0&0&\mathrm{i}\end{bmatrix},\quad l(0i)_1\begin{bmatrix}0&\mathrm{i}&0&0\\\mathrm{i}&0&0&0\\0&0&0&-1\\0&0&1&0\end{bmatrix},$$
$$l(0i)_2\begin{bmatrix}0&0&\mathrm{i}&0\\0&0&0&1\\\mathrm{i}&0&0&0\\0&-1&0&0\end{bmatrix},\quad l(0i)_3\begin{bmatrix}0&0&0&\mathrm{i}\\0&0&-1&0\\0&1&0&0\\\mathrm{i}&0&0&0\end{bmatrix}. \tag{5.6}$$

For $(i,j)\in\{12,23,31\}$ we obtain, respectively, for $\mu=0,1,2,3$:

$$\Lambda_{\mu}(i,j)=l(ij)_0\begin{bmatrix}0&\mathrm{i}&0&0\\0&0&-1&0\\-\mathrm{i}&0&0&0\\0&0&0&-1\end{bmatrix},\quad l(ij)_1\begin{bmatrix}0&0&0&\mathrm{i}\\-\mathrm{i}&0&0&0\\0&0&1&0\\0&1&0&0\end{bmatrix},$$
$$l(ij)_2\begin{bmatrix}0&0&\mathrm{i}&0\\0&1&0&0\\0&0&0&-1\\\mathrm{i}&0&0&0\end{bmatrix},\quad l(ij)_3\begin{bmatrix}\mathrm{i}&0&0&0\\0&0&0&-\mathrm{i}\\0&-\mathrm{i}&0&0\\0&0&\mathrm{i}&0\end{bmatrix}, \tag{5.7}$$

$$\Lambda_\mu(j,i)=l(ji)_0\begin{bmatrix}0&\mathrm{i}&0&0\\0&0&0&1\\0&0&1&0\\-\mathrm{i}&0&0&0\end{bmatrix},\quad l(ji)_1\begin{bmatrix}0&0&\mathrm{i}&0\\-\mathrm{i}&0&0&0\\0&-1&0&0\\0&0&0&-1\end{bmatrix},$$
$$l(ji)_2\begin{bmatrix}\mathrm{i}&0&0&0\\0&0&-\mathrm{i}&0\\0&0&0&\mathrm{i}\\0&-\mathrm{i}&0&0\end{bmatrix},\quad l(ji)_3\begin{bmatrix}0&0&0&\mathrm{i}\\0&-1&0&0\\\mathrm{i}&0&0&0\\0&0&1&0\end{bmatrix}. \tag{5.8}$$

We now consider the introduction of $G_{(\rho)\mu}$ generators in the presence of $P_{(i)}$ and $E_{(\alpha)0}$ multiplets. According to (4.1) and (5.3), the scalar charges $E_{(\alpha)0}$ should transform as a (product) representation, hence we have

$$[\![G_{(\rho)\mu},E_{(\alpha)0}]\!]=-\mathrm{i}\epsilon_\mu(\rho,\alpha)E_{(\rho\dagger\alpha)0}. \tag{5.9}$$

Using Eq. (4.1) and the Jacobi identity for the triple $G_{(\rho)\mu}$, $P_{(i)\sigma}$, $P_{(j)\nu}$ we obtain

$$C^0(i,j)_{\sigma\nu}\epsilon_\mu(\rho,i\dagger j)=\Lambda_\mu(\rho,i)_\sigma{}^\tau C^0(i\dagger\rho,j)_{\tau\nu}+q_{(\rho)\mu,(i)\sigma}C^0(i,\rho\dagger j)_{\sigma\omega}\Lambda_\mu(\rho,j)_\nu{}^\omega. \tag{5.10}$$

The relation (5.10) provides nontrivial solutions only for the complex singlet $G_{(0)0}$ [and since we want to determine dimensionless scalars with a nontrivial relation with the extension, we exclude the further (decoupled) scalars from now on]:

$$[\![G_{(0)0},P_{(i)\nu}]\!]=l(0i)_0P_{(i)\nu}, \tag{5.11}$$

$$[\![G_{(0)0},E_{(k)0}]\!]=-l(0k)_0E_{(k)0}, \tag{5.12}$$

$$[\![G_{(0)0},\overline{E}_{(k)0}]\!]=-l(0k)_0\overline{E}_{(k)0}. \tag{5.13}$$

Now, the charge $G_{(0)0}$ is complex, and in terms of its components (5.11)–(5.13) read

$$\begin{aligned}[\![\mathrm{Re}\,G_{(0)0},P_{(i)\nu}]\!]&=\mathrm{i}\,\mathrm{Im}(l(0i)_0)P_{(i)\nu},\\ [\![\mathrm{Im}\,G_{(0)0},P_{(i)\nu}]\!]&=-\mathrm{i}\,\mathrm{Re}(l(0i)_0)P_{(i)\nu},\end{aligned} \tag{5.14}$$

$$\begin{aligned}[\![\mathrm{Re}\,G_{(0)0},E_{(k)0}]\!]&=-\mathrm{i}\,\mathrm{Im}(l(0k)_0)E_{(k)0},\\ [\![\mathrm{Im}\,G_{(0)0},E_{(k)0}]\!]&=\mathrm{i}\,\mathrm{Re}(l(0k)_0)E_{(k)0},\end{aligned} \tag{5.15}$$

$$\begin{aligned}[\![\mathrm{Re}\,G_{(0)0},\overline{E}_{(k)0}]\!]&=-\mathrm{i}\,\mathrm{Im}(l(0k)_0)\overline{E}_{(k)0},\\ [\![\mathrm{Im}\,G_{(0)0},\overline{E}_{(k)0}]\!]&=\mathrm{i}\,\mathrm{Re}(l(0k)_0)\overline{E}_{(k)0}.\end{aligned} \tag{5.16}$$

The nontrivial coupling constants associated with the surviving scalar dimensionless complex charge $G_{(0)0}$ satisfy

$$l(01)_0+l(02)_0+l(03)_0=0. \tag{5.17}$$

This indicates just that according to relations (4.7) and (4.8), the charge of $P_{(0)}$ is vanishing as is required by the Coleman–Mandula theorem. Hence, we can think on the charge $G_{(0)0}$ as an additive charge.

We can now give an explicit and particular choice of the charges $\mathrm{Im}\, l(0i)_0$ and $\mathrm{Re}\, l(0i)_0$ that maintains the symmetries among the multiplets $P_{(1)}$, $P_{(2)}$, $P_{(3)}$. We can adopt for the values of $l(0i)_0$ three complex numbers symmetrically oriented in the complex plane:

$$l(01)_0 = l, \quad l(02)_0 = l e^{i2\pi/3}, \quad l(03)_0 = l e^{i4\pi/3}, \quad l \in \mathbb{R}. \tag{5.18}$$

We observe that the relations (5.14)–(5.16) could be interpreted as presenting $\mathrm{Re}\, G_{(0)0}$ and $\mathrm{Im}\, G_{(0)0}$ as a sort of U(1)-generators. The charges $G_{(0)0}$ and $\overline{G}_{(0)0}$ swap under involution. It is, nevertheless, not excluded that these generators might have nontrivial relations with further scalar charges. From relations (5.4) we conclude in particular,

$$[\![\mathrm{Re}\, G_{(0)0}, \mathrm{Im}\, G_{(0)0}]\!] = 0. \tag{5.19}$$

We observe that only the scalar charges $G_{(0)0}$, $\overline{G}_{(0)0}$ provide an authentic further enhancement of the clover extension obtained in Sec. IV.

VI. CONCLUSIONS

We have continued the study of graded Lie algebraic extensions with involution of the space–time symmetries, which has been called generically *trefoil symmetries*. We have inquired for a novel *clover extension*, i.e., a trefoil symmetry which is $\mathbb{Z}_4 \times \mathbb{Z}_4$-graded and involve only novel generators of integer spin. We have obtained a $(\mathbb{Z}_4 \times \mathbb{Z}_4; q)$-graded clover extension $\mathbb{L}'$ of the Poincaré algebra in which a space–time translation can be obtained through the composition of symmetric vectors (which might be interpreted as translations in three novel noncommutative four-dimensional manifolds with a pseudometric) and scalar fields. In particular, call this extension the *minimal scalar clover Extension*.

The Poincaré algebra:

$$\begin{gathered}
[\![T_{(0)i}, T_{(0)j}]\!] = i\epsilon_{ijk} T_{(0)k}, \quad [\![T_{(0)i}, \overline{T}_{(0)j}]\!] = 0, \quad [\![\overline{T}_{(0)i}, \overline{T}_{(0)j}]\!] = i\epsilon_{ijk} \overline{T}_{(0)k}, \\
[\![T_{(0)i}, P_{(0)\nu}]\!] = -i\sigma^P(i,0)_\nu{}^\rho P_{(0)\rho}, \quad [\![\overline{T}_{(0)i}, P_{(0)\nu}]\!] = -i q_{(0)i,(0)\nu} P_{(0)\rho} \overline{\sigma}^P(i,0)^\rho{}_\nu, \\
[\![P_{(0)\mu}, P_{(0)\nu}]\!] = 0,
\end{gathered} \tag{6.1}$$

extends for $f,i,j,k,l = 1,2,3$ through the *minimal scalar clover extension*

$$[\![T_{(0)i}, P_{(f)\nu}]\!] = -i\sigma^P(i,f)_\nu{}^\rho P_{(f)\rho}, \quad [\![\overline{T}_{(0)i}, P_{(f)\nu}]\!] = -i q_{(0)i,(f)\nu} P_{(f)\rho} \overline{\sigma}^P(i,f)^\rho{}_\nu,$$

$$[\![T_{(0)i}, E_{(f)0}]\!] = 0, \quad [\![\overline{T}_{(0)i}, E_{(f)0}]\!] = 0, \tag{6.2}$$

$$[\![T_{(0)i}, \overline{E}_{(f)0}]\!] = 0, \quad [\![\overline{T}_{(0)i}, \overline{E}_{(f)0}]\!] = 0,$$

$$[\![P_{(0)\mu}, P_{(f)\nu}]\!] = 0, \quad [\![P_{(f)\mu}, P_{(f)\nu}]\!] = 0, \tag{6.3}$$

$$[\![P_{(0)\mu}, E_{(f)0}]\!] = 0, \quad [\![P_{(0)\mu}, \overline{E}_{(f)0}]\!] = 0, \tag{6.4}$$

$$\begin{gathered}
[\![E_{(i)0}, E_{(j)0}]\!] = 0, \quad [\![E_{(i)0}, \overline{E}_{(j)0}]\!] = 0, \\
[\![\overline{E}_{(i)0}, \overline{E}_{(j)0}]\!] = 0,
\end{gathered} \tag{6.5}$$

$$[\![P_{(i)\mu}, P_{(j)\nu}]\!] = C^0(i,j)_{\mu\nu} E_{(i\dagger j)0} + \hat{C}^0(i,j)_{\mu\nu} \overline{E}_{(i\dagger j)0}, \quad i \neq j, \tag{6.6}$$

$$[\![E_{(f)0}, P_{(l)\mu}]\!] = \delta_{fl} S_0(l)^\nu_\mu P_{(0)\nu}, \tag{6.7}$$

$$[\![\overline{E}_{(f)0},P_{(l)\mu}]\!]=\delta_{fl}\hat{S}_0(l)^{\nu}_{\mu}P_{(0)\nu}. \tag{6.8}$$

The σ-matrices are given in Table I. The C^0-matrices are given in (4.6). The S_0-matrices are given in (4.13). These matrices are constrained by the consistency conditions (4.16) and (4.17). A particular choice respecting the symmetry among the novel classes is given by (4.18). Relations (6.1)–(6.8) provide a $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded Lie algebra $\mathbb{L}'$ with involution, which extends nontrivially the Poincaré algebra.

The obtained extension does not correspond to any cumbersome deformation of the conformal extension and related series since there the scalar dilatation operator *does not* commute with the space–time translation.

The obtained extension is minimal in the sense that no extra generators are needed for the closure of the algebra, and the omission of some generator would either damage the closure of the graded algebra, would damage the symmetry among the novel classes, or would not provide an actual nontrivial extension of the Poincaré algebra. The structure constants can be chosen so that no anisotropy or inhomogeneity is introduced to the space–time.

The obtained extension *cannot* compose a space–time translation $P_{(0)}$ via the triple composition $[\![P_{(1)},[\![P_{(2)},P_{(3)}]\!]]\!]$ as originally aimed since the parameter constraints (4.16) annihilate their contributions. Nevertheless, we *can* compose a space–time translation via $[\![E_{(l)0},P_{(l)}]\!]$ or via $[\![\overline{E}_{(l)0},P_{(l)}]\!]$, and this provides an authentic extension of the Poincaré algebra.

The introduction of dimensionless scalar charges has been also addressed and it has been found that scalar charges $\mathrm{Re}\,G_{(0)0}$ and $\mathrm{Im}\,G_{(0)0}$ can have nontrivial relations with the novel generators of the obtained minimal scalar clover extension. This constitutes the *dimensionless scalar enhancement*:

$$[\![\mathrm{Re}\,G_{(0)0},\mathrm{Im}\,G_{(0)0}]\!]=0, \tag{6.9}$$

$$\begin{aligned}[\![\mathrm{Re}\,G_{(0)0},P_{(i)\nu}]\!]&=\mathrm{i}\,\mathrm{Im}(l(0i)_0)P_{(i)\nu},\\ [\![\mathrm{Im}\,G_{(0)0},P_{(i)\nu}]\!]&=-\mathrm{i}\,\mathrm{Re}(l(0i)_0)P_{(i)\nu},\end{aligned} \tag{6.10}$$

$$\begin{aligned}[\![\mathrm{Re}\,G_{(0)0},E_{(k)0}]\!]&=-\mathrm{i}\,\mathrm{Im}(l(0k)_0)E_{(k)0},\\ [\![\mathrm{Im}\,G_{(0)0},E_{(k)0}]\!]&=\mathrm{i}\,\mathrm{Re}(l(0k)_0)E_{(k)0},\end{aligned} \tag{6.11}$$

$$\begin{aligned}[\![\mathrm{Re}\,G_{(0)0},\overline{E}_{(k)0}]\!]&=-\mathrm{i}\,\mathrm{Im}(l(0k)_0)\overline{E}_{(k)0},\\ [\![\mathrm{Im}\,G_{(0)0},\overline{E}_{(k)0}]\!]&=\mathrm{i}\,\mathrm{Re}(l(0k)_0)\overline{E}_{(k)0}.\end{aligned} \tag{6.12}$$

The nontrivial structure constants satisfy:

$$l(01)_0+l(02)_0+l(03)_0=0, \tag{6.13}$$

According to relations (4.7) and (4.8), the charge of $P_{(0)}$ is vanishing as required by the Coleman–Mandula theorem. Clearly, the charge $G_{(0)0}=\mathrm{Re}\,G_{(0)0}+\mathrm{i}\,\mathrm{Im}\,G_{(0)0}$ is an additive charge.

The class (0)-indices are used by the Poincaré algebra in the following way: once the index $(0)_0$ and three times each index $(0)_j$, for $j=1,2,3$. The novel generators of the minimal scalar clover extension (6.2)–(6.8) of the class (i), $i=1,2,3$ use three times the index $(i)_0$ (since $E_{(i)0}$ is complex) and once each index $(i)_j$, for $j=1,2,3$. The Poincaré algebra has ten parameters (and generators) and the minimal extension presented here has $10+3\times3+3\times3=28$ parameters (and generators). The enhancement of the minimal scalar clover extension using scalar dimensionless charges (6.9)–(6.12) makes symmetric the usage of indices for spin (0,0) and spin $(\frac{1}{2},\frac{1}{2})$ multiplets in the four different classes and completes an algebra with 30 generators. Nevertheless, only class (0) indices are used for spin (1,0) and (1,0) multiplets.

This situation allows one to conjecture an extension that makes symmetric usage of spin multiplets in all the classes. Such an extension would use exactly three times each one of the elements of the grading group $\mathbb{Z}_4 \times \mathbb{Z}_4$, and would involve the minimal vector clover and minimal scalar clover extensions as particular cases. This is exactly the content of the next contribution in this paper series. The connection of the already obtained extensions with known internal symmetries will be discussed as well in the further parts of this paper series.

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Trefoil symmetry III. The full clover extension

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We aim to approach a trefoil symmetry involving $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded parameters, multiplets of generators of integer spin <2 with naive dimensions in the interval $[0,1]$. The resulting full clover extension involves as particular subalgebras the minimal clover extensions previously obtained. We address the introduction of further scalar, dimensionless multiplets, and central charges. They could provide connections among external and internal symmetries, perhaps after some graded symmetry breaking. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The isospin interaction distinguishes between left and right $\frac{1}{2}$-spin multiplets. This observation suggests deep connections among external and internal symmetries. The present work addresses a possible channel for relating nontrivially internal and external symmetries.

There have been found two minimal nontrivial extensions[1,2] of the external symmetries of special relativity using $\mathbb{Z}_4\times\mathbb{Z}_4$-gradings and novel multiplets of integer spin. They correspond to extensions beyond the the Coleman–Mandula no-go theorem[3] since some of its assumptions were relaxed: On the one hand the novel symmetries are governed by $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded Lie groups, with generator structure given by a $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded Lie algebra with involution. On the other hand, the algebraic relations combining the generators of the Poincaré algebra and the novel generators can be either of commutator or anticommutator type.[4,1]

In the present work we are going to study a more general extension involving the previously obtained as particular cases. We aim in particular at the trefoil symmetry involving $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded parameters, multiplets of generators of integer spin <2 with naive dimensions in the interval $[0,1]$. We introduce novel generators that match naturally with the leitmotif of the previous extensions: the production of space–time translations $P_{(0)}$ via the composition of three symmetric vector charges:

$$[\![P_{(1)},[\![P_{(2)},P_{(3)}]\!]]\!]\sim P_{(0)}. \tag{1.1}$$

The double brackets stand for q-commutators[5] respecting the grading assignments of its entries, and $P_{(0)}=(P_0,P_1,P_2,P_3)$ translation four-vector. The Lorentz generators will be written in terms of the spin (1,0) triplet $T_{(0)}$ and the spin (0,1) triplet $\overline{T}_{(0)}$ as presented in Ref. 1.

We will maintain all throughout this work all the conventions stated in Refs. 1 and 2. In the first of these works we made a review on grading groups, graded parameter and graded Lie algebras, on the grading groups suited for extending the external symmetries of the special relativity. There, we constructed the so-called minimal vector clover extension, which is a $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded extension of the Poincaré algebra which involved only spin-1 multiplets as novel generators. This minimal extension succeeded in producing a space–time translation through the composition of three symmetric vector multiplets as in Eq. (1.1). In the second refereed work the

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so-called minimal scalar clover extension was obtained, which can produce a space–time translation through the composition of a symmetric vector generator and scalar generators.

We are interested now mainly in two aspects: First, we want to identify the constraints on the structure constants due to the simultaneous presence of the minimal extensions obtained so far. Second, we want to determine candidates for the would-be internal symmetries after a graded symmetry breaking. This is actually the most appealing aim of this paper: the identification of clues that might present more naturally the internal symmetries we observe in nature.

This work is structured in the following way. In Sec. II we study an extension involving simultaneously the novel multiplets of generators of the previously determined minimal extensions and study the constraints arising on their structure constants. In Sec. III we discuss the introduction of generators that could induce internal symmetries after a breaking of the graded symmetry. Section IV studies the introduction of scalar multiplets naively dimensionless, which are naturally candidates for would-be generators of internal symmetries after graded symmetry breaking. In Sec. V we study the introduction of nondimensionless scalar multiplets and discuss their relations with dimensionless scalar multiplets. In Sec. VI we consider the introduction of dimensionless antisymmetric vector multiplets. In Sec. VII we review the obtained results and give the concluding remarks.

II. MERGED EXTENSION

In analogous fashion as accomplished by supersymmetry, we are looking here for a novel extension of the Poincaré algebra in which a translation can be composed by the iteration of further symmetry transformations. In order to produce a spin-$(\frac{1}{2},\frac{1}{2})$ class (0) space–time translation multiplet $P_{(0)}$ we can use three spin-$(\frac{1}{2},\frac{1}{2})$ irreps $P_{(1)},P_{(2)},P_{(3)}$ as in Eq. (1.1), since

$$(\tfrac{1}{2},\tfrac{1}{2})\otimes(\tfrac{1}{2},\tfrac{1}{2})\otimes(\tfrac{1}{2},\tfrac{1}{2})=(\tfrac{1}{2},\tfrac{1}{2})\oplus\ldots. \tag{2.1}$$

In order to have a nontrivial right-hand side of (1.1) we need a nontrivial result for $[\![P_{(i)},P_{(j)}]\!]$ with $i\neq j$; $i,j=1,2,3$. Accordingly, such extension has to involve multiplets of generators in the right-hand side direct summation:

$$(\tfrac{1}{2},\tfrac{1}{2})\otimes(\tfrac{1}{2},\tfrac{1}{2})=(0,0)\oplus(1,0)\oplus(0,1)\oplus(1,1). \tag{2.2}$$

In Ref. 1 we studied the minimal extension involving generators with representations $(1,0)\oplus(0,1)$ of dimension 2/3 at this point, while in Ref. 2 we studied the introduction of spin (0,0) singlets of dimension 2/3. We study now the simultaneous introduction of both spin 1 and spin 0 multiplets. The fist step will study the constraints on the algebraic relation:

$$[\![P_{(i)\mu},P_{(j)\nu}]\!]=C^{\sigma}(i,j)_{\mu\nu}E_{(i\dagger j)\sigma}+\hat{C}^{\sigma}(i,j)_{\mu\nu}\overline{E}_{(i\dagger j)\sigma}+\eta^{r}(i,j)_{\mu\nu}T_{(i\dagger j)r}+\hat{\eta}^{\dot{r}}(i,j)_{\mu\nu}\overline{T}_{(i\dagger j)\dot{r}},\quad i\neq j. \tag{2.3}$$

Now, using the involution and q-antisymmetry, and the reality of the $P_{(i)}$-irreps

$$\overline{[\![P_{(i)\mu},P_{(j)\nu}]\!]}=[\![P_{(j)\nu},P_{(i)\mu}]\!]=-q_{(j)\nu,(i)\mu}[\![P_{(i)\mu},P_{(j)\nu}]\!] \tag{2.4}$$

we obtain

$$\begin{aligned}
-q_{(j)\nu,(i)\mu}C^{\sigma}(i,j)_{\mu\nu}&=C^{\sigma}(j,i)_{\nu\mu}=\hat{C}^{\sigma}(i,j)^{*}_{\mu\nu},\\
-q_{(j)\nu,(i)\mu}\eta^{r}(i,j)_{\mu\nu}&=\eta^{r}(j,i)_{\nu\mu}=\hat{\eta}^{\dot{r}}(i,j)^{*}_{\mu\nu},\\
-q_{(j)\nu,(i)\mu}\hat{\eta}^{\dot{r}}(i,j)_{\mu\nu}&=\hat{\eta}^{\dot{r}}(j,i)_{\nu\mu}=\eta^{r}(i,j)^{*}_{\mu\nu}.
\end{aligned} \tag{2.5}$$

Consider now the Jacobi identities obtained from the triple $T_{(0)l}$, $P_{(i)\mu}$, $P_{(j)\nu}$:

$$[\![T_{(0)l},[\![P_{(i)\mu},P_{(j)\nu}]\!]]\!]=[\![[\![T_{(0)l},P_{(i)\mu}]\!],P_{(j)\nu}]\!]+q_{(0)l,(i)}[\![P_{(i)\mu},[\![T_{(0)l},P_{(j)\nu}]\!]]\!]. \tag{2.6}$$

Using the identities (2.3) and the σ-matrices associated with the Lorentz transformations of the novel multiplets irreps, we obtain

$$\begin{aligned}\eta^r(i,j)_{\mu\nu}(-\mathrm{i}\sigma^T(l,i\dagger j)_r{}^n T_{(i\dagger j)n})=&-\mathrm{i}\sigma^P(l,i)_\mu{}^\rho(C^\sigma(i,j)_{\rho\nu}E_{(i\dagger j)\sigma}+\hat{C}^\sigma(i,j)_{\rho\nu}\overline{E}_{(i\dagger j)\sigma}\\&+\eta^n(i,j)_{\rho\nu}T_{(i\dagger j)n}+\hat{\eta}^{\dot n}(i,j)_{\rho\nu}\overline{T}_{(i\dagger j)\dot n})-\mathrm{i}q_{(0)l,(i)}\sigma^P(l,j)_\nu{}^\delta\\&\times(C^\sigma(i,j)_{\mu\delta}E_{(i\dagger j)\sigma}+\hat{C}^\sigma(i,j)_{\mu\delta}\overline{E}_{(i\dagger j)\sigma}+\eta^n(i,j)_{\mu\delta}T_{(i\dagger j)n}\\&+\hat{\eta}^{\dot n}(i,j)_{\mu\delta}\overline{T}_{(i\dagger j)\dot n}).\end{aligned}$$

With $E_{(i\dagger j)s}$, $\overline{E}_{(i\dagger j)s}$, $T_{(i\dagger j)n}$, and $\overline{T}_{(i\dagger j)n}$ being linearly independent we obtain

$$\begin{aligned}&\sigma^P(l,i)_\mu{}^\rho C^\sigma(i,j)_{\rho\nu}+(2\delta_{li}-1)C^\sigma(i,j)_{\mu\rho}\sigma^P(l,j)_\nu{}^\rho=0,\\&\sigma^P(l,i)_\mu{}^\rho\hat{\eta}^{\dot n}(i,j)_{\rho\nu}+(2\delta_{li}-1)\hat{\eta}^{\dot n}(i,j)_{\mu\rho}\sigma^P(l,j)_\nu{}^\rho=0,\\&\sigma^P(l,i)_\mu{}^\rho\eta^n(i,j)_{\rho\nu}+(2\delta_{li}-1)\eta^n(i,j)_{\mu\rho}\sigma^P(l,j)_\nu{}^\rho=\eta^r(i,j)_{\mu\nu}\sigma^T(l,i\dagger j)_r{}^n.\end{aligned} \tag{2.7}$$

In analogous fashion, for the triple $\overline{T}_{(0)l}$, $P_{(i)\mu}$, $P_{(j)\nu}$ we obtain further equations:

$$\begin{aligned}&\overline{\sigma}^P(l,i)^\rho{}_\mu C^\sigma(i,j)_{\rho\nu}+(2\delta_{lj}-1)C^\sigma(i,j)_{\mu\rho}\overline{\sigma}^P(l,j)^\rho{}_\nu=0,\\&\overline{\sigma}^P(l,i)^\rho{}_\mu\eta^n(i,j)_{\rho\nu}+(2\delta_{lj}-1)\eta^n(i,j)_{\mu\rho}\overline{\sigma}^P(l,j)^\rho{}_\nu=0,\\&\overline{\sigma}^P(l,j)^\rho{}_\nu\hat{\eta}^{\dot n}(i,j)_{\mu\rho}+(2\delta_{lj}-1)\hat{\eta}^{\dot n}(i,j)_{\rho\nu}\overline{\sigma}^P(l,i)^\rho{}_\mu=\hat{\eta}^{\dot r}(i,j)_{\mu\nu}\overline{\sigma^T}(l,i\dagger j)^{\dot n}{}_{\dot r}.\end{aligned} \tag{2.8}$$

We observe that these equations do not differ from those obtained for the C- and η-arrays at this step in the previously obtained minimal extensions,[1,2] hence for $ijk\in\{213,321,132\}$:

$$C^0(i,j)=c_{k0}\begin{bmatrix}0&0&1&0\\0&\mathrm{i}&0&0\\0&0&0&\mathrm{i}\\1&0&0&0\end{bmatrix}, \tag{2.9}$$

$$\begin{aligned}&\eta^1(i,j)=a_k\begin{bmatrix}1&0&0&0\\0&0&0&1\\0&-1&0&0\\0&0&1&0\end{bmatrix},\quad \eta^2(i,j)=a_k\begin{bmatrix}0&\mathrm{i}&0&0\\0&0&1&0\\-\mathrm{i}&0&0&0\\0&0&0&-1\end{bmatrix},\\&\eta^3(i,j)=a_k\begin{bmatrix}0&0&0&\mathrm{i}\\\mathrm{i}&0&0&0\\0&0&1&0\\0&1&0&0\end{bmatrix}.\end{aligned} \tag{2.10}$$

The further matrices are obtained using (2.5).

We are now ready to go to the second step of our extension. Since we want (1.1) to hold, we have two ways for arriving at this stage—through the singlets E or through the triplets T:

$$[\![E_{(f)\sigma},P_{(l)\mu}]\!]=\delta_{fl}S_\sigma(l)^\nu_\mu P_{(0)\nu}, \tag{2.11}$$

$$[\![\overline{E}_{(f)\sigma},P_{(l)\mu}]\!]=\delta_{fl}\hat{S}_{\sigma}(l)^{\nu}_{\mu}P_{(0)\nu}, \tag{2.12}$$

$$[\![T_{(k)r},P_{(l)\mu}]\!]=\delta_{kl}K_{r}(l)^{\nu}_{\mu}P_{(0)\nu}, \tag{2.13}$$

$$[\![\overline{T}_{(k)r},P_{(l)\mu}]\!]=\delta_{kl}\hat{K}_{r}(l)^{\nu}_{\mu}P_{(0)\nu}. \tag{2.14}$$

From the properties of involution and q-anticommutation it follows

$$\hat{S}_{\sigma}(l)^{\nu}_{\mu}=-q_{(l)\sigma,(l)\mu}S_{\sigma}(l)^{\nu}_{\mu}{}^{*}, \tag{2.15}$$

$$\hat{K}_{r}(l)^{\nu}_{\mu}=-q_{(l)r,(l)\mu}K_{r}(l)^{\nu}_{\mu}{}^{*}. \tag{2.16}$$

From the triples $T_{(0)l}$, $E_{(k)s}$, $P_{(k)\mu}$ and $\overline{T}_{(0)l}$, $E_{(k)s}$, $P_{(k)\mu}$ and their corresponding Jacobi identities we obtain

$$\begin{aligned} &S_{\sigma}(k)^{\nu}_{\mu}\sigma^{P}(l,0)_{\nu}{}^{\rho}=(2\delta_{lk}-1)\sigma^{P}(l,k)_{\mu}{}^{\delta}S_{\sigma}(k)^{\rho}_{\delta},\\ &S_{\sigma}(k)^{\nu}_{\mu}\overline{\sigma}^{P}(l,0)^{\rho}{}_{\nu}=\overline{\sigma}^{P}(l,k)^{\delta}{}_{\mu}S_{\sigma}(k)^{\rho}_{\delta}. \end{aligned} \tag{2.17}$$

From the triples $T_{(0)l}$, $T_{(k)j}$, $P_{(k)\mu}$ and $\overline{T}_{(0)l}$, $T_{(k)j}$, $P_{(k)\mu}$ we obtain

$$K_{j}(k)^{\nu}_{\mu}\overline{\sigma}^{P}(l,0)^{\rho}{}_{\nu}=\overline{\sigma}^{P}(l,k)^{\nu}{}_{\mu}K_{j}(k)^{\rho}_{\nu}, \tag{2.18}$$

$$K_{j}(k)^{\nu}_{\mu}\sigma^{P}(l,0)_{\nu}{}^{\rho}=(2\delta_{lk}-1)\sigma^{P}(l,k)_{\mu}{}^{\nu}K_{j}(k)^{\rho}_{\nu}+\sigma^{T}(l,k)_{j}{}^{m}K_{m}(k)^{\rho}_{\mu}. \tag{2.19}$$

We observe that the obtained equations coincide with the constraints for the S- and K-arrays at this step in the previously obtained minimal extensions,[1,2] hence we have

$$S_{i}(k)=0 \quad \forall i\neq 0, \tag{2.20}$$

$$\begin{aligned} &S_{0}(1)=s_{10}\begin{bmatrix}0&1&0&0\\1&0&0&0\\0&0&0&-\mathrm{i}\\0&0&\mathrm{i}&0\end{bmatrix}, \quad S_{0}(2)=s_{20}\begin{bmatrix}0&0&1&0\\1&0&0&0\\0&-\mathrm{i}&0&0\\0&0&0&-\mathrm{i}\end{bmatrix},\\ &S_{0}(3)=s_{30}\begin{bmatrix}0&0&0&1\\1&0&0&0\\0&0&-\mathrm{i}&0\\0&\mathrm{i}&0&0\end{bmatrix}, \end{aligned} \tag{2.21}$$

$$K_1(1)=b_1\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix},\quad K_2(1)=b_1\begin{bmatrix}0&0&0&\mathrm{i}\\0&0&1&0\\0&-1&0&0\\\mathrm{i}&0&0&0\end{bmatrix},$$

$$K_3(1)=b_1\begin{bmatrix}0&0&-\mathrm{i}&0\\0&0&0&1\\-\mathrm{i}&0&0&0\\0&-1&0&0\end{bmatrix},$$

$$K_1(2)=b_2\begin{bmatrix}1&0&0&0\\0&0&1&0\\0&0&0&1\\0&1&0&0\end{bmatrix},\quad K_2(2)=b_2\begin{bmatrix}0&\mathrm{i}&0&0\\0&0&0&1\\0&0&-1&0\\\mathrm{i}&0&0&0\end{bmatrix},\tag{2.22}$$

$$K_3(2)=b_2\begin{bmatrix}0&0&0&-\mathrm{i}\\0&1&0&0\\-\mathrm{i}&0&0&0\\0&0&-1&0\end{bmatrix},$$

$$K_1(3)=b_3\begin{bmatrix}1&0&0&0\\0&0&0&1\\0&1&0&0\\0&0&1&0\end{bmatrix},\quad K_2(3)=b_3\begin{bmatrix}0&0&\mathrm{i}&0\\0&1&0&0\\0&0&0&-1\\\mathrm{i}&0&0&0\end{bmatrix},$$

$$K_3(3)=b_3\begin{bmatrix}0&-\mathrm{i}&0&0\\0&0&1&0\\-\mathrm{i}&0&0&0\\0&0&0&-1\end{bmatrix}.$$

The $\hat{S}$- and $\hat{K}$-matrices are obtained using (2.15) and (2.16). We are now ready to go to the last consistency condition. We use the triplet $P_{(1)\rho}$, $P_{(2)\mu}$, $P_{(3)\nu}$ and the corresponding Jacobi identity to obtain:

$$\begin{aligned}0=&q_{(1)\rho,(2)\mu+(3)\nu}\eta^r(2,3)_{\mu\nu}K_r(1)^\sigma_\rho+q_{(2)\mu,(3)\nu}\eta^{r*}(2,3)_{\mu\nu}K^*_r(1)^\sigma_\rho\\&+q_{(1)\rho,(2)\mu+(3)\nu}C^\delta(2,3)_{\mu\nu}S_\delta(1)^\sigma_\rho+\eta^r(1,2)_{\rho\mu}K_r(3)^\sigma_\nu\\&+q_{(1)\rho,(2)\mu+(3)\nu}q_{(2)\mu,(3)\nu}\eta^{r*}(1,2)_{\rho\mu}K^*_r(3)^\sigma_\nu+C^\delta(1,2)_{\rho\mu}S_\delta(3)^\sigma_\nu\\&+q_{(1)\rho+(2)\mu,(3)\nu}\eta^r(3,1)_{\nu\rho}K_r(2)^\sigma_\mu+q_{(1)\rho,(2)\mu}\eta^{r*}(3,1)_{\nu\rho}K^*_r(2)^\sigma_\mu\\&+q_{(1)\rho+(2)\mu,(3)\nu}C^\delta(3,1)_{\nu\rho}S_\delta(2)^\sigma_\mu.\end{aligned}\tag{2.23}$$

From the q-application of the $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$ group grading,[4,1] we have

$$q_{(2)\mu,(3)\nu}=q_{(3)\mu,(1)\nu}=q_{(1)\mu,(2)\nu}=\begin{bmatrix} \mathrm{i} & -\mathrm{i} & -\mathrm{i} & \mathrm{i} \\ -\mathrm{i} & \mathrm{i} & \mathrm{i} & -\mathrm{i} \\ \mathrm{i} & -\mathrm{i} & -\mathrm{i} & \mathrm{i} \\ -\mathrm{i} & \mathrm{i} & \mathrm{i} & -\mathrm{i} \end{bmatrix}_{\mu\nu}. \tag{2.24}$$

Equations (2.23) and (2.24) lead to the following set of independent constraints:

$$a_1b_1+a_2b_2+a_3b_3+\mathrm{i}(a_1^*b_1^*+a_2^*b_2^*+a_3^*b_3^*)=0, \tag{2.25}$$

$$c_{10}s_{10}-\mathrm{i}c_{10}^*s_{10}^*=a_2b_2-\mathrm{i}a_2^*b_2^*-a_3b_3+\mathrm{i}a_3^*b_3^*, \tag{2.26}$$

$$c_{20}s_{20}-\mathrm{i}c_{20}^*s_{20}^*=a_3b_3-\mathrm{i}a_3^*b_3^*-a_1b_1+\mathrm{i}a_1^*b_1^*, \tag{2.27}$$

$$c_{30}s_{30}-\mathrm{i}c_{30}^*s_{30}^*=a_1b_1-\mathrm{i}a_1^*b_1^*-a_2b_2+\mathrm{i}a_2^*b_2^*. \tag{2.28}$$

Adding the last three constraints we obtain

$$c_{10}s_{10}+c_{20}s_{20}+c_{30}s_{30}-\mathrm{i}(c_{10}^*s_{10}^*+c_{20}^*s_{20}^*+c_{30}^*s_{30}^*)=0. \tag{2.29}$$

The constraints (2.25)–(2.28) can be parametrized in the following way;

$$a_1b_1-\mathrm{i}a_1^*b_1^*=\tfrac{1}{3}(3r_0-r_2+r_3)(1-\mathrm{i}), \tag{2.30}$$

$$a_2b_2-\mathrm{i}a_2^*b_2^*=\tfrac{1}{3}(3r_0-r_3+r_1)(1-\mathrm{i}), \tag{2.31}$$

$$a_3b_3-\mathrm{i}a_3^*b_3^*=\tfrac{1}{3}(3r_0-r_1+r_2)(1-\mathrm{i}), \tag{2.32}$$

$$c_{10}s_{10}-\mathrm{i}c_{10}^*s_{10}^*=r_1(1-\mathrm{i}), \tag{2.33}$$

$$c_{20}s_{20}-\mathrm{i}c_{20}^*s_{20}^*=r_2(1-\mathrm{i}), \tag{2.34}$$

$$c_{30}s_{30}-\mathrm{i}c_{30}^*s_{30}^*=r_3(1-\mathrm{i}), \tag{2.35}$$

$$r_1+r_2+r_3=0, \quad r_0,r_1,r_2,r_3\in\mathbb{R}. \tag{2.36}$$

These constraints show that we have actually choices of structure constants that go beyond the naive superposition of the two minimal extensions in Refs. 1 and 2. It is easy to get convinced that the presence of scalar fields can lead to an apparent asymmetry among the structure constants associated with the three classes (1), (2), and (3) unless we take $r_1=r_2=r_3=0$. This suggests that we can exhibit a particular choice of structure constants that maintain the symmetry among the three novel families, which is exactly a superposition of the particular choices presented in the minimal extensions:[1,2]

$$a_j=a, \quad b_j=b(1-\mathrm{i}), \quad a,b\in\mathbb{R}\backslash\{0\}, \quad j=1,2,3. \tag{2.37}$$

$$c_{j0}=c, \quad s_{j0}=s(1+\mathrm{i}), \quad c,s\in\mathbb{R}\backslash\{0\}, \quad j=1,2,3. \tag{2.38}$$

We observe that although the scalar fields are not strictly necessary for a consistent algebraic extension with a nontrivial generation of a space–time translation via (1.1), they can be involved without introducing any asymmetry between the novel classes, and therefore without introducing any anisotropy or inhomogeneity. In future stages of this research the presence of the scalar fields might be relevant for the cancellation of anomalies or for obtaining would-be internal symmetries. As already noticed in Refs. 1 and 2, since the scalar fields can be consistently excluded from the

TABLE I. Structure of the merged extension. $j=1,2,3$; $\mu=0,1,2,3$.

	Spin		
Naive dim	(1,0)	$(\frac{1}{2},\frac{1}{2})$ / (0,0)	(0,1)
1		$P_{(0)\mu}$	
2/3	$T_{(1)j}, T_{(2)j}, T_{(3)j}$	$E_{(1)0}, E_{(2)0}, E_{(3)0}, \overline{E}_{(1)0}, \overline{E}_{(2)0}, \overline{E}_{(3)0},$	$\overline{T}_{(1)j}, \overline{T}_{(2)j}, \overline{T}_{(3)j}$
1/3		$P_{(1)\mu}, P_{(2)\mu}, P_{(3)\mu}$	
0	$T_{(0)j}$		$\overline{T}_{(0)j}$

extension and the novel scalar generators q-commute with the space–time translations then *the merged extension does not correspond to any cumbersome deformation of the conformal extension*.

We can picture the structure of the merged extension in the diagram given in Table I. One latter comment is in order about the obtained extension. The elements of the group $\mathbb{Z}_4\times\mathbb{Z}_4$ are used as indices for generators in the following way: Each index of the classes (1), (2), and (3) has been used three times. In the class (0) all the indices have been used three times except the neutral index $(0)_0$ which was used just once. We observe also that the antisymmetric vectors $T_{(j)}$, $\overline{T}_{(j)}$ for $j=1,2,3$ are accompanied by a couple of scalars $E_{(j)0}$, $\overline{E}_{(j)0}$ also of dimension 2/3. The dimensionless antisymmetric vector $T_{(0)}$, $\overline{T}_{(0)}$ might have an associated complex couple of scalars $G_{(0)0}$, $\overline{G}_{(0)0}$. This question will be answered in Sec. IV.

III. SEARCHING FOR CANDIDATES FOR INTERNAL SYMMETRIES

We now turn the attention to the inclusion of further generators to the extension previously obtained. We recognize different candidates for the would-be internal symmetry generators perhaps after some sort of graded symmetry breaking (analogous to supersymmetry breaking):

(1) the dimensionless scalar generators,
(2) the nondimensionless scalar generators,
(3) invariant forms of nonscalar generators (such as $T_{(i)1}T_{(i)1}-T_{(i)2}T_{(i)2}-T_{(i)3}T_{(i)3}$; $i=1,2,3$) that might survive as symmetry generators after graded symmetry breaking.

We will investigate in Sec. IV the introduction of scalar dimensionless singlets $G_{(\rho)\mu}$, where $\rho,\mu=0,1,2,3$. We will ask in Sec. V for the introduction of nondimensionless scalar central charges $Z_{(\rho)\mu}$, where $\rho,\mu=0,1,2,3$. In Sec. VI we ask for the introduction of dimensionless antisymmetric vectors $\mathbf{T}_{(i)}$ and $\overline{\mathbf{T}}_{(i)}$. This will finish our survey of enhancements of the obtained extension.

IV. DIMENSIONLESS SCALAR GENERATORS

Particular interest is paid to the dimensionless scalar generators since they are naively the most expedite candidates for internal symmetry generators perhaps after some sort of graded symmetry breaking. We introduce scalar dimensionless singlets $G_{(\rho)\mu}$, where $\rho,\mu=0,1,2,3$ and we will select the ones which are effectively nontrivially connected to the extension obtained in Sec. III.

The generators $G_{(\rho)\mu}$ have trivial q-commutation relations with the Lorentz generators, since they are scalar. If these scalar generators have nontrivial q-commutation relations with the mentioned extension, they have nontrivial relations with the multiplets $P_{(i)}$; $i=1,2,3$, since *all* the novel generators of the extension as well as the space–time translations are obtained from the composition of the multiplets $P_{(i)}$.

We expect that the multiplets $P_{(i)}$; $i=1,2,3$ might constitute representations of the subgroup built by the novel scalar singlets. These scalars satisfy the q-commutation relations

$$[\![G_{(\rho)\mu},G_{(\sigma)\nu}]\!]=-\mathrm{i}\zeta_{\mu}(\rho,\sigma)_{\nu}{}^{\kappa}G_{(\rho\dagger\sigma)\kappa}. \tag{4.1}$$

The structure constants build up the adjoint representation, hence the matrix

$$D^{G}(G_{(\rho)\mu})=-\mathrm{i}\zeta_{\mu}(\rho,\sigma)^{\mathrm{tr}} \tag{4.2}$$

constitutes a representation D^{G} of the generator $G_{(\rho)\mu}$. Now, the multiplets $P_{(i)}$; $i=1,2,3$ build up representations of the group generated by $G_{(\rho)\mu}$. We should have

$$[\![G_{(\rho)\mu},P_{(i)\nu}]\!]=-\mathrm{i}\Lambda_{\mu}(\rho,i)_{\nu}{}^{\sigma}P_{(\rho\dagger i)\sigma}. \tag{4.3}$$

Using the Jacobi identities associated with the triples $G_{(\rho)\mu}$, $G_{(\alpha)\xi}$, $P_{(j)\nu}$, we obtain

$$\Lambda_{\mu}(\rho,\alpha\dagger j)^{\mathrm{tr}}\Lambda_{\xi}(\alpha,j)^{\mathrm{tr}}-q_{(\rho)\mu,(\alpha)\xi}\Lambda_{\xi}(\alpha,\rho\dagger j)^{\mathrm{tr}}\Lambda_{\mu}(\rho,j)^{\mathrm{tr}}=\zeta_{\mu}(\rho,\alpha)_{\xi}{}^{\kappa}\Lambda_{\kappa}(\rho\dagger\alpha,j)^{\mathrm{tr}}. \tag{4.4}$$

Hence, $-\mathrm{i}\Lambda_{\mu}(\rho,i)^{\mathrm{tr}}$ constitutes a representation D^{P} of the algebra generated by $G_{(\rho)\mu}$:

$$D^{P}(G_{(\rho)\mu})=-\mathrm{i}\Lambda_{\mu}(\rho,i)^{\mathrm{tr}}. \tag{4.5}$$

Using the Jacobi identity associated with the triples $T_{(0)r}$, $G_{(\rho)\mu}$, $P_{(i)\nu}$ and $\overline{T}_{(0)r}$, $G_{(\rho)\mu}$, $P_{(i)\nu}$ we obtain, respectively, for $\mu=0,1,2,3$:

$$\begin{aligned}&\Lambda_{\mu}(0,i)=l(0i)_0\begin{bmatrix}\mathrm{i}&0&0&0\\0&\mathrm{i}&0&0\\0&0&\mathrm{i}&0\\0&0&0&\mathrm{i}\end{bmatrix},\quad l(0i)_1\begin{bmatrix}0&\mathrm{i}&0&0\\\mathrm{i}&0&0&0\\0&0&0&-1\\0&0&1&0\end{bmatrix},\\&l(0i)_2\begin{bmatrix}0&0&\mathrm{i}&0\\0&0&0&1\\\mathrm{i}&0&0&0\\0&-1&0&0\end{bmatrix},\quad l(0i)_3\begin{bmatrix}0&0&0&\mathrm{i}\\0&0&-1&0\\0&1&0&0\\\mathrm{i}&0&0&0\end{bmatrix}.\end{aligned} \tag{4.6}$$

For $(i,j)\in\{12,23,31\}$ we obtain, respectively, for $\mu=0,1,2,3$:

$$\begin{aligned}&\Lambda_{\mu}(i,j)=l(ij)_0\begin{bmatrix}0&\mathrm{i}&0&0\\0&0&-1&0\\-\mathrm{i}&0&0&0\\0&0&0&-1\end{bmatrix},\quad l(ij)_1\begin{bmatrix}0&0&0&\mathrm{i}\\-\mathrm{i}&0&0&0\\0&0&1&0\\0&1&0&0\end{bmatrix},\\&l(ij)_2\begin{bmatrix}0&0&\mathrm{i}&0\\0&1&0&0\\0&0&0&-1\\\mathrm{i}&0&0&0\end{bmatrix},\quad l(ij)_3\begin{bmatrix}\mathrm{i}&0&0&0\\0&0&0&-\mathrm{i}\\0&-\mathrm{i}&0&0\\0&0&\mathrm{i}&0\end{bmatrix},\end{aligned} \tag{4.7}$$

$$\Lambda_\mu(j,i)=l(ji)_0\begin{bmatrix}0&\mathrm{i}&0&0\\0&0&0&1\\0&0&1&0\\-\mathrm{i}&0&0&0\end{bmatrix},\quad l(ji)_1\begin{bmatrix}0&0&\mathrm{i}&0\\-\mathrm{i}&0&0&0\\0&-1&0&0\\0&0&0&-1\end{bmatrix},$$
$$l(ji)_2\begin{bmatrix}\mathrm{i}&0&0&0\\0&0&-\mathrm{i}&0\\0&0&0&\mathrm{i}\\0&-\mathrm{i}&0&0\end{bmatrix},\quad l(ji)_3\begin{bmatrix}0&0&0&\mathrm{i}\\0&-1&0&0\\\mathrm{i}&0&0&0\\0&0&1&0\end{bmatrix}. \tag{4.8}$$

We will study first the compatibility of this group structure $G_{(\rho)\mu}$ with the triplets $T_{(i)}$ and $\overline{T}_{(i)}$ and afterwards we study the compatibility with the scalar singlets $E_{(\alpha)\xi}$. Since the triplets $T_{(i)}$ and $\overline{T}_{(i)}$ are obtained by the composition of multiplets $P_{(i)}$, we expect that the triplets $T_{(i)}$ and $\overline{T}_{(i)}$ constitute representations of the algebra generated by $G_{(\rho)\mu}$:

$$[\![G_{(\rho)\mu},T_{(i)a}]\!]=-\mathrm{i}\tau_\mu(\rho,i)_a{}^bT_{(\rho\dagger i)b}, \tag{4.9}$$

$$[\![G_{(\rho)\mu},\overline{T}_{(i)a}]\!]=-\mathrm{i}\hat{\tau}_\mu(\rho,i)^b{}_a\overline{T}_{(\rho\dagger i)b}. \tag{4.10}$$

Using the Jacobi identity for the triples $T_{(l)c}$, $G_{(\rho)\mu}$, $\overline{T}_{(k)a}$ we obtain, respectively, for $\mu=0,1,2,3$:

$$\tau_\mu(0,1)=t(01)_0\begin{bmatrix}\mathrm{i}&0&0\\0&\mathrm{i}&0\\0&0&\mathrm{i}\end{bmatrix},\quad t(01)_1\begin{bmatrix}0&0&0\\0&0&-1\\0&1&0\end{bmatrix},$$
$$t(01)_2\begin{bmatrix}0&0&1\\0&0&0\\-1&0&0\end{bmatrix},\quad t(01)_3\begin{bmatrix}0&-1&0\\1&0&0\\0&0&0\end{bmatrix}, \tag{4.11}$$

$$\tau_\mu(0,2)=t(02)_0\begin{bmatrix}\mathrm{i}&0&0\\0&\mathrm{i}&0\\0&0&\mathrm{i}\end{bmatrix},\quad t(02)_1\begin{bmatrix}0&-1&0\\1&0&0\\0&0&0\end{bmatrix},$$
$$t(02)_2\begin{bmatrix}0&0&0\\0&0&-1\\0&1&0\end{bmatrix},\quad t(02)_3\begin{bmatrix}0&0&1\\0&0&0\\-1&0&0\end{bmatrix}, \tag{4.12}$$

$$\tau_\mu(0,3)=t(03)_0\begin{bmatrix}\mathrm{i}&0&0\\0&\mathrm{i}&0\\0&0&\mathrm{i}\end{bmatrix},\quad t(03)_1\begin{bmatrix}0&0&1\\0&0&0\\-1&0&0\end{bmatrix},$$
$$t(03)_2\begin{bmatrix}0&-1&0\\1&0&0\\0&0&0\end{bmatrix},\quad t(03)_3\begin{bmatrix}0&0&0\\0&0&-1\\0&1&0\end{bmatrix}. \tag{4.13}$$

For $(ij)\in\{12,23,31\}$:

$$\tau_\mu(i,j)=t(ij)_0\begin{bmatrix}0&-1&0\\0&0&0\\0&0&-1\end{bmatrix},\quad t(ij)_1\begin{bmatrix}0&0&0\\0&1&0\\-1&0&0\end{bmatrix},$$
$$t(ij)_2\begin{bmatrix}1&0&0\\0&0&-1\\0&0&0\end{bmatrix},\quad t(ij)_3\begin{bmatrix}0&0&-\mathrm{i}\\-\mathrm{i}&0&0\\0&\mathrm{i}&0\end{bmatrix}, \tag{4.14}$$

$$\tau_\mu(j,i)=t(ji)_0\begin{bmatrix}0&0&1\\0&1&0\\0&0&0\end{bmatrix},\quad t(ji)_1\begin{bmatrix}0&0&0\\-1&0&0\\0&0&-1\end{bmatrix},$$
$$t(ji)_2\begin{bmatrix}0&-\mathrm{i}&0\\0&0&\mathrm{i}\\-\mathrm{i}&0&0\end{bmatrix},\quad t(ji)_3\begin{bmatrix}-1&0&0\\0&0&0\\0&1&0\end{bmatrix}. \tag{4.15}$$

Observe that these results are analogous to the down-right 3×3 submatrices of the corresponding Λ_μ matrices in Eqs. (4.6)–(4.8). Using the identity (2.3) we obtain for the Jacobi identity associated with the triple $G_{(\rho)\mu}$, $P_{(i)\mu}$, $P_{(j)\nu}$ the constraints

$$\Lambda_\sigma(\rho,i)_\mu{}^\lambda\eta^r(\rho\dagger i,j)_{\lambda\nu}-q_{(\rho)\sigma,(i)\mu}\eta^r(i,j\dagger\rho)_{\mu\lambda}\Lambda_\sigma(\rho,j)_\nu{}^\lambda=\eta^s(i,j)_{\mu\nu}\tau_\sigma(\rho,i\dagger j)_s{}^r, \tag{4.16}$$

$$\Lambda_\sigma(\rho,i)_\mu{}^\lambda\hat\eta^r(\rho\dagger i,j)_{\lambda\nu}-q_{(\rho)\sigma,(i)\mu}\hat\eta^r(i,j\dagger\rho)_{\mu\lambda}\Lambda_\sigma(\rho,j)_\nu{}^\lambda=\hat\eta^s(i,j)_{\mu\nu}\hat\tau_\sigma(\rho,i\dagger j)_s{}^r. \tag{4.17}$$

From (4.16) we obtain the independent constraints

$$l(01)_0+l(02)_0=t(03)_0,$$
$$l(02)_0+l(03)_0=t(01)_0, \tag{4.18}$$
$$l(03)_0+l(01)_0=t(02)_0,$$

$$l(01)_1=-l(02)_1=-l(03)_1,$$
$$l(01)_2=-l(02)_2=l(03)_2, \tag{4.19}$$
$$l(01)_3=l(02)_3=-l(03)_3,$$

$$t(0i)_j=0;\quad \text{for } i,j=1,2,3, \tag{4.20}$$

$$l(12)_\sigma=l(23)_\sigma=l(31)_\sigma=0\quad\text{for } \sigma\neq2,$$
$$l(21)_\sigma=l(32)_\sigma=l(13)_\sigma=0\quad\text{for } \sigma\neq3, \tag{4.21}$$

$$t(12)_\sigma=t(23)_\sigma=t(31)_\sigma=0\quad\text{for } \sigma\neq3,$$
$$t(21)_\sigma=t(32)_\sigma=t(13)_\sigma=0\quad\text{for } \sigma\neq2, \tag{4.22}$$

$$a_2 l(12)_2 = a_3 t(13)_2,$$
$$a_3 l(23)_2 = a_1 t(21)_2, \tag{4.23}$$
$$a_1 l(31)_2 = a_2 t(32)_2,$$
$$a_3 l(13)_3 = a_2 t(12)_3,$$
$$a_1 l(21)_3 = a_3 t(23)_3, \tag{4.24}$$
$$a_2 l(32)_3 = a_1 t(31)_3.$$

Now using Eqs. (2.12) and (2.14) and the Jacobi identities for the triple $G_{(\rho)\sigma}$, $T_{(k)j}$, $P_{(l)\mu}$ we obtain the constraint

$$\tau_\sigma(\rho,k)_j{}^n \delta_{\rho\dagger k,l} K_n(l)^r_\mu + q_{(\rho)\sigma,(k)j} \Lambda_\sigma(\rho,l)_\mu{}^\nu \delta_{\rho\dagger l,k} K_j(k)^r_\nu = 0, \tag{4.25}$$

where we *assumed* that $P_{(0)}$ should be a invariant (q-commute) under the algebra generated by the $G_{(\rho)\sigma}$ according to an extrapolation of Coleman–Mandula theorem. (This is strictly a part of this theorem for the charges $G_{(0)\sigma}$). From the constraints (4.25) we obtain

$$t(0i)_0 = -l(0i)_0; \quad \text{for } i=1,2,3, \tag{4.26}$$

$$b_j l(0i)_j = t(0i)_j = 0 \quad \text{for } i,j=1,2,3, \tag{4.27}$$

$$b_3 l(12)_2 = -b_2 t(13)_2,$$
$$b_1 l(23)_2 = -b_3 t(21)_2, \tag{4.28}$$
$$b_2 l(31)_2 = -b_1 t(32)_2,$$
$$b_2 l(13)_2 = -b_3 t(12)_3,$$
$$b_3 l(21)_2 = -b_1 t(23)_3, \tag{4.29}$$
$$b_1 l(32)_2 = -b_2 t(31)_3.$$

From Eqs. (4.18)–(4.24) and (4.26)–(4.29) we obtain, for a nontrivial extension with $a_i b_i \neq 0$; $i=1,2,3$, the result:

$$l(ij)_\rho = t(ij)_\rho = 0, \quad i,j=1,2,3, \quad i \neq j, \quad \rho = 0,1,2,3, \tag{4.30}$$

$$l(0j)_k = 0, \quad j,k=1,2,3. \tag{4.31}$$

Hence, the only scalar dimensionless charge nontrivially related to the self-bosonic extension with $T_{(i)}$ ($\overline{T}_{(i)}$) triplets is just the singlet $G_{(0)0}$ ($\overline{G}_{(0)0}$). The nontrivial coupling constants associated with the surviving scalar dimensionless complex charge $G_{(0)0}$ satisfy

$$l(01)_0 + l(02)_0 + l(03)_0 = 0, \tag{4.32}$$

$$t(0i)_0 = -l(0i)_0, \quad i=1,2,3. \tag{4.33}$$

Hence, we can think on the charge $G_{(0)0}$ as an additive charge. The resulting relations

$$[\![G_{(0)0}, P_{(i)\nu}]\!] = l(0i)_0 P_{(i)\nu}, \tag{4.34}$$

$$[\![G_{(0)0}, T_{(k)a}]\!] = -l(0k)_0 T_{(k)a}, \tag{4.35}$$

$$[\![G_{(0)0}, \overline{T}_{(k)a}]\!] = -l(0k)_0 \overline{T}_{(k)a}, \tag{4.36}$$

indicate just that according to relation (1.1), the charge of $P_{(0)}$ is vanishing as it was required. Now, the charge $G_{(0)0}$ is complex $G_{(0)0}=\mathrm{Re}\,G_{(0)0}+\mathrm{i}\,\mathrm{Im}\,G_{(0)0}$, and in terms of its components (4.34)–(4.36) read

$$\begin{aligned}[\![\mathrm{Re}\,G_{(0)0},P_{(i)\nu}]\!]&=\mathrm{i}\,\mathrm{Im}(l(0i)_0)P_{(i)\nu},\\ [\![\mathrm{Im}\,G_{(0)0},P_{(i)\nu}]\!]&=-\mathrm{i}\,\mathrm{Re}(l(0i)_0)P_{(i)\nu},\end{aligned}\tag{4.37}$$

$$\begin{aligned}[\![\mathrm{Re}\,G_{(0)0},T_{(k)a}]\!]&=-\mathrm{i}\,\mathrm{Im}(l(0k)_0)T_{(k)a},\\ [\![\mathrm{Im}\,G_{(0)0},T_{(k)a}]\!]&=\mathrm{i}\,\mathrm{Re}(l(0k)_0)T_{(k)a},\end{aligned}\tag{4.38}$$

$$\begin{aligned}[\![\mathrm{Re}\,G_{(0)0},\overline{T}_{(k)a}]\!]&=-\mathrm{i}\,\mathrm{Im}(l(0k)_0)\overline{T}_{(k)a},\\ [\![\mathrm{Im}\,G_{(0)0},\overline{T}_{(k)a}]\!]&=\mathrm{i}\,\mathrm{Re}(l(0k)_0)\overline{T}_{(k)a}.\end{aligned}\tag{4.39}$$

We now consider the introduction of $G_{(\rho)\mu}$ generators in the presence of $P_{(i)}$ and $E_{(\alpha)0}$ multiplets. We expect that according to (2.3) and (2.10) we have

$$[\![G_{(\rho)\mu},E_{(\alpha)0}]\!]=-\mathrm{i}\epsilon_{\mu}(\rho,\alpha)E_{(\rho\dagger\alpha)0}.\tag{4.40}$$

Using Eq. (2.3) and the Jacobi identity for the triple $G_{(\rho)\mu}$, $P_{(i)\sigma}$, $P_{(j)\nu}$ we obtain

$$C^0(i,j)_{\sigma\nu}\epsilon_{\mu}(\rho,i\dagger j)=\Lambda_{\mu}(\rho,i)^{\tau}_{\sigma}C^0(i\dagger\rho,j)_{\tau\nu}+q_{(\rho)\mu,(i)\sigma}C^0(i,\rho\dagger j)_{\sigma\omega}\Lambda_{\mu}(\rho,j)^{\omega}_{\nu}.\tag{4.41}$$

Again, we obtain nontrivial relations only for the complex singlet $G_{(0)0}$:

$$[\![G_{(0)0},E_{(k)0}]\!]=-l(0k)_0E_{(k)0},\tag{4.42}$$

$$[\![G_{(0)0},\overline{E}_{(k)0}]\!]=-l(0k)_0\overline{E}_{(k)0},\tag{4.43}$$

which in terms of its components read

$$\begin{aligned}[\![\mathrm{Re}\,G_{(0)0},E_{(k)0}]\!]&=-\mathrm{i}\,\mathrm{Im}(l(0k)_0)E_{(k)0},\\ [\![\mathrm{Im}\,G_{(0)0},E_{(k)0}]\!]&=\mathrm{i}\,\mathrm{Re}(l(0k)_0)E_{(k)0},\end{aligned}\tag{4.44}$$

$$\begin{aligned}[\![\mathrm{Re}\,G_{(0)0},\overline{E}_{(k)0}]\!]&=-\mathrm{i}\,\mathrm{Im}(l(0k)_0)\overline{E}_{(k)0},\\ [\![\mathrm{Im}\,G_{(0)0},\overline{E}_{(k)0}]\!]&=\mathrm{i}\,\mathrm{Re}(l(0k)_0)\overline{E}_{(k)0}.\end{aligned}\tag{4.45}$$

We can now give an explicit and particular choice of the charges $\mathrm{Im}\,l(0i)_0$ and $\mathrm{Re}\,l(0i)_0$ that maintains the symmetries among the multiplets $P_{(1)}$, $P_{(2)}$, $P_{(3)}$. We can adopt for the values of $l(0i)_0$ three complex numbers symmetrically oriented in the complex plane:

$$l(01)_0=l,\quad l(02)_0=l\mathrm{e}^{\mathrm{i}2\pi/3},\quad l(03)_0=l\mathrm{e}^{\mathrm{i}4\pi/3},\quad l\in\mathbb{R}.\tag{4.46}$$

We observe that the relations (4.34) and (4.45) could be interpreted as presenting $\mathrm{Re}\,G_{(0)0}$ and $\mathrm{Im}\,G_{(0)0}$ as a sort of U(1)-generators. The charges $G_{(0)0}$ and $\overline{G}_{(0)0}$ swap under involution. It is, nevertheless, not excluded that these generators might have nontrivial relations with further scalar charges. From relation (4.5) we conclude that this scalar charges commute among them. In particular

$$[\![\mathrm{Re}\,G_{(0)0},\mathrm{Im}\,G_{(0)0}]\!]=0.\tag{4.47}$$

TABLE II. Full clover extension. $j=1,2,3;\ \mu=0,1,2,3$.

Naive dim	Spin (1,0)	Spin $(\frac{1}{2},\frac{1}{2})$	Spin (0,1)
1		$P_{(0)\mu}$	
2/3	$T_{(1)j}, T_{(2)j}, T_{(3)j}$	$E_{(1)0}, E_{(2)0}, E_{(3)0}, \overline{E}_{(1)0}, \overline{E}_{(2)0}, \overline{E}_{(3)0},$	$\overline{T}_{(1)j}, \overline{T}_{(2)j}, \overline{T}_{(3)j}$
1/3		$P_{(1)\mu}, P_{(2)\mu}, P_{(3)\mu}$	
0	$T_{(0)j}$	$G_{(0)0}, \overline{G}_{(0)0}$	$\overline{T}_{(0)j}$

A more explicit role of these scalar charges might be exhibited when introducing graded spinor charges for instance. We discuss possible interpretations of the novel scalar charges in the last section.

We observe that only the scalar charges $G_{(0)0}$, $\overline{G}_{(0)0}$ provide an authentic further enhancement of the merged extension obtained in the Sec. III. The structure of the obtained extension is presented graphically in Table II below, this extension will be called the **full clover extension**. The usage of the grading group elements for this symmetry presents a truly democratic pattern: each group element in $\mathbb{Z}_4\times\mathbb{Z}_4$ is used as generator index three times, and there is the same number spin representations (multiplets of generators) in each class.

V. CENTRAL CHARGES

We consider first extra scalar charges $Z_{(k)\nu}$, with $k=1,2,3;\ \mu=0,1,2,3$ produced by the combination of the multiplets $P_{(1)}$, $P_{(2)}$, $P_{(3)}$:

$$[\![P_{(i)\mu},P_{(j)\nu}]\!]=C^{\sigma}(i,j)_{\mu\nu}E_{(i\dagger j)\sigma}+\hat{C}^{\sigma}(i,j)_{\mu\nu}\overline{E}_{(i\dagger j)\sigma}+\eta^{r}(i,j)_{\mu\nu}T_{(i\dagger j)r}+\hat{\eta}^{\dot{r}}(i,j)_{\mu\nu}\overline{T}_{(i\dagger j)\dot{r}}$$
$$+D^{\sigma}(i,j)_{\mu\nu}Z_{(i\dagger j)\sigma}+\hat{D}^{\sigma}(i,j)_{\mu\nu}\overline{Z}_{(i\dagger j)\sigma},\quad i\neq j. \tag{5.1}$$

Using relation (2.4), we obtain

$$-q_{(j)\nu,(i)\mu}D^{\sigma}(i,j)_{\mu\nu}=D^{\sigma}(j,i)_{\nu\mu}=\hat{D}^{\sigma}(i,j)^{*}_{\mu\nu}. \tag{5.2}$$

Using the Jacobi identities for the triple $T_{(0)l}$, $P_{(i)\mu}$, $P_{(j)\nu}$ and the triple $\overline{T}_{(0)l}$, $P_{(i)\mu}$, $P_{(j)\nu}$ we obtain

$$\sigma^{P}(l,i)^{\rho}_{\mu}D^{\sigma}(i,j)_{\rho\nu}+(2\delta_{li}-1)D^{\sigma}(i,j)_{\mu\rho}\sigma^{P}(l,j)^{\rho}_{\nu}=0, \tag{5.3}$$

$$\overline{\sigma}^{P}(l,i)^{\rho}{}_{\mu}D^{\sigma}(i,j)_{\rho\nu}+(2\delta_{lj}-1)D^{\sigma}(i,j)_{\mu\rho}\overline{\sigma}^{P}(l,j)^{\rho}{}_{\nu}=0. \tag{5.4}$$

The grading structure determines the allowed textures for the arrays $D^{\sigma}(i,j)$, $\hat{D}^{\sigma}(i,j)$. From Eqs. (5.2)–(5.4) for $ijk\in\{123,231,312\}$, we obtain:

$$D^0(i,j)=d_{k0}\begin{bmatrix}0&0&1&0\\0&\mathrm{i}&0&0\\0&0&0&\mathrm{i}\\1&0&0&0\end{bmatrix},\quad D^1(i,j)=d_{k1}\begin{bmatrix}1&0&0&0\\0&0&0&-1\\0&1&0&0\\0&0&1&0\end{bmatrix},$$
$$D^2(i,j)=d_{k2}\begin{bmatrix}0&1&0&0\\0&0&-\mathrm{i}&0\\1&0&0&0\\0&0&0&-\mathrm{i}\end{bmatrix},\quad D^3(i,j)=d_{k3}\begin{bmatrix}0&0&0&1\\-1&0&0&0\\0&0&-\mathrm{i}&0\\0&\mathrm{i}&0&0\end{bmatrix}. \tag{5.5}$$

The further matrices are obtained using (5.2).

The central charges $Z_{(k)\nu},\overline{Z}_{(k)\nu}$ q-commute with all the generators of the clover extension obtained in Sec. II since the scalars that have nontrivial relations have been taken into account by the scalar couples $E_{(j)0},\overline{E}_{(j)0}$. Therefore their name of central charges:

$$[\![Z_{(k)\nu},Y]\!]=0,\quad [\![\overline{Z}_{(k)\nu},Y]\!]=0,$$
$$\forall Y=P_{(\mu)\nu},T_{(\mu)j},\overline{T}_{(\mu)j},E_{(j)0},\overline{E}_{(j)0},\quad \mu,\nu=0,1,2,3,\quad j,k=1,2,3. \tag{5.6}$$

Nevertheless, under the presence of the dimensionless scalars $G_{(0)0},\overline{G}_{(0)0}$ introduced in Sec. IV, these central charges acquire some nontrivial q-commutation relations:

$$[\![G_{(0)0},Z_{(k)\nu}]\!]=-l(0k)_0Z_{(k)\nu}, \tag{5.7}$$

$$[\![G_{(0)0},\overline{Z}_{(k)\nu}]\!]=-l(0k)_0\overline{Z}_{(k)\nu},\quad k=1,2,3. \tag{5.8}$$

The production of a scalar singlets $Z_{(0)\mu}$, with $\mu=0,1,2,3$ is considered when we compose repeated $P_{(i)}$ charges:

$$[\![P_{(i)\mu},P_{(i)\nu}]\!]=D^\sigma(i,i)_{\mu\nu}Z_{(0)\sigma}+\hat{D}^\sigma(i,i)_{\mu\nu}\overline{Z}_{(0)\sigma}. \tag{5.9}$$

We do not consider spin (1,0) and spin(0,1) multiplets of class (0) in (5.9) since they are excluded by the Coleman–Mandula theorem. We observe that the introduction of the scalar $Z_{(0)\mu}$ endanger the interpretation of the $P_{(i)}$ charges as translations in the novel four-dimensional noncommutative manifolds. From the Jacobi identities we obtain equations identical to (5.3) and (5.4) with $i=j$, whose solutions are

$$D^0(i,i)=\overline{d}_{i0}\begin{bmatrix}0&1&0&0\\-1&0&0&0\\0&0&0&-\mathrm{i}\\0&0&\mathrm{i}&0\end{bmatrix},\quad D^1(i,i)=\overline{d}_{i1}\begin{bmatrix}1&0&0&0\\0&-1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix},$$
$$D^2(i,i)=\overline{d}_{i2}\begin{bmatrix}0&0&0&1\\0&0&\mathrm{i}&0\\0&\mathrm{i}&0&0\\1&0&0&0\end{bmatrix},\quad D^3(i,i)=\overline{d}_{i3}\begin{bmatrix}0&0&1&0\\0&0&0&-\mathrm{i}\\1&0&0&0\\0&-\mathrm{i}&0&0\end{bmatrix}. \tag{5.10}$$

The further matrices are obtained using (5.2).

The central charges $Z_{(0)\nu}$, $\overline{Z}_{(k)\nu}$ also q-commute with all the generators of the merged extension obtained in Sec. II:

$$[\![Z_{(0)\nu},Y]\!]=0, \quad [\![\overline{Z}_{(0)\nu},Y]\!]=0,$$
$$\forall Y=P_{(\mu)\nu},T_{(\mu)j},\overline{T}_{(\mu)j},E_{(j)0},\overline{E}_{(j)0}, \quad \mu,\nu=0,1,2,3,j=1,2,3. \tag{5.11}$$

Nevertheless, under the presence of the dimensionless scalars $G_{(0)0}$, $\overline{G}_{(0)0}$ introduced in Sec. IV, the central charges $Z_{(0)\nu}$, $\overline{Z}_{(0)\nu}$ for $D^{\mu}(i,i)$ nonvanishing for $\mu=0,1,2,3;i=1,2,3$ imply:

$$[\![G_{(0)0},Z_{(0)\nu}]\!]=2\,l(0i)_0 Z_{(0)\nu}, \tag{5.12}$$

$$[\![G_{(0)0},\overline{Z}_{(0)\nu}]\!]=2\,l(0i)_0 \overline{Z}_{(0)\nu}, \tag{5.13}$$

$$2\,l(01)_0=2\,l(02)_0=2\,l(03)_0=0. \tag{5.14}$$

In order to circumvent this fact, we could introduce central charges $Z^i_{(0)\nu}$ with $i=1,2,3$ in Eq. (5.9) instead of the charges $Z_{(0)\nu}$. In this case, Eqs. (5.12) and (5.13) for $Z^i_{(0)\nu}$ instead of $Z_{(0)\nu}$ do not lead to Eq. (5.14).

We conclude this section observing that it is possible to introduce central charges $Z_{(k)\nu}$, $\overline{Z}_{(k)\nu}$ with $k=1,2,3$; $\nu=0,1,2,3$ and central charges $Z^i_{(0)\nu}$, $\overline{Z^i}_{(0)\nu}$ with $i=1,2,3$; $\mu=0,1,2,3$ of naive dimension 2/3 in the enhanced merged extension of Sec. IV. Nevertheless, we do not recognize so far a systematic in the usage of group grading indices by such central charges (at least as clear as it was obtained by the enhanced merged extension). The presence of the central charges $Z^i_{(0)\nu}$ would damage the interpretation of the charges $P_{(i)\mu}$ as translations in flat noncommutative four-dimensional manifolds. The role of the central charges might become clear when studying local versions of these symmetries toward novel gravity models.

VI. DIMENSIONLESS ANTISYMMETRIC VECTORS

We can also consider the introduction of dimensionless triplets $\mathbf{T}_{(i)}$ and $\overline{\mathbf{T}}_{(i)}$ of spin (1,0) and spin (0,1), respectively, such that they satisfy relations of the sort:

$$[\![\mathbf{T}_{(f)i},\mathbf{T}_{(g)j}]\!]=\Sigma^k(f,g)_{ij}\mathbf{T}_{(f\dagger g)k}.$$

Using the q-commutativity property we have

$$-q_{(f)j,(g)k}\Sigma^l(g,f)_{kj}=\Sigma^l(f,g)_{jk}.$$

After considering the necessary Jacobi identities associated with the triple $T_{(0)i}$, $\mathbf{T}_{(f)j}$, $\mathbf{T}_{(g)k}$ we obtain

$$\Sigma^l(f,g)\sigma^T(i,h)_l{}^n=\sigma^T(i,f)\Sigma^n(f,g)+q_{(0)i,(f)j}\Sigma^n(f,g)\sigma^T(i,g)^{\mathrm{tr}}. \tag{6.1}$$

Solving the equations above we obtain that there are no nontrivial connections between the proposed dimensionless antisymmetric vector generators:

$$\Sigma^k(f,g)_{ij}=0, \quad \forall i,j,k,f,g=1,2,3.$$

Hence, there is no place for extra dimensionless antisymmetric vectors.

VII. CONCLUSIONS

We have completed the construction of a very particular type of graded Lie algebraic extension of the Poincaré algebra with involution. The obtained trefoil symmetry is a $(\mathbb{Z}_4\times\mathbb{Z}_4;q)$-graded extension with multiplets of generators of spin <2 which belong to what has been called clover extensions. The obtained extension will be called the *full clover extension*, or simply the *clover extension*. It includes as particular cases the minimal vector clover extension and

the minimal scalar clover extension (also with dimensionless scalars). The clover extension corresponds to what would be $N=1$ supersymmetry for the $\mathbb{Z}_2$-supergradings. Replication of the clover extensions can also be considered but lie outside of the scope of the present work.

The Poincaré algebra:

$$\begin{gathered}
[\![T_{(0)i},T_{(0)j}]\!]=\mathrm{i}\epsilon_{ijk}T_{(0)k},\quad [\![T_{(0)i},\overline{T}_{(0)j}]\!]=0,\quad [\![\overline{T}_{(0)i},\overline{T}_{(0)j}]\!]=\mathrm{i}\epsilon_{ijk}\overline{T}_{(0)k},\\
[\![T_{(0)i},P_{(o)\nu}]\!]=-\mathrm{i}\sigma^{P}(i,0)_{\nu}{}^{\rho}P_{(0)\rho},\quad [\![\overline{T}_{(0)i},P_{(0)\nu}]\!]=-\mathrm{i}q_{(0)i,(0)\nu}P_{(0)\rho}\overline{\sigma}^{P}(i,0)^{\rho}{}_{\nu},\qquad (7.1)\\
[\![P_{(0)\mu},P_{(0)\nu}]\!]=0,
\end{gathered}$$

for which the q-commutators coincide with commutators, extends for $f,i,j,k,l=1,2,3$ through the *full clover extension*:

$$\begin{gathered}
[\![T_{(0)i},P_{(f)\nu}]\!]=-\mathrm{i}\sigma^{P}(i,f)_{\nu}{}^{\rho}P_{(f)\rho},\quad [\![\overline{T}_{(0)i},P_{(f)\nu}]\!]=-\mathrm{i}q_{(0)i,(f)\nu}P_{(f)\rho}\overline{\sigma}^{P}(i,f)^{\rho}{}_{\nu},\\
[\![T_{(0)i},T_{(f)s}]\!]=-\mathrm{i}\sigma^{T}(i,f)_{s}{}^{t}T_{(f)t},\quad [\![\overline{T}_{(0)i},T_{(f)s}]\!]=0,
\end{gathered}\qquad (7.2)$$

$$[\![T_{(0)i},\overline{T}_{(f)\dot{s}}]\!]=0,\quad [\![\overline{T}_{(0)i},\overline{T}_{(f)\dot{s}}]\!]=-\mathrm{i}q_{(0)i,(f)s}\overline{T}_{(f)\dot{t}}\overline{\sigma^{T}}(i,f)^{\dot{t}}{}_{\dot{s}},\qquad (7.3)$$

$$[\![T_{(0)i},E_{(f)0}]\!]=0,\quad [\![\overline{T}_{(0)i},E_{(f)0}]\!]=0,\qquad (7.4)$$

$$[\![T_{(0)i},\overline{E}_{(f)0}]\!]=0,\quad [\![\overline{T}_{(0)i},\overline{E}_{(f)0}]\!]=0,\qquad (7.5)$$

$$[\![T_{(0)i},G_{(0)0}]\!]=0,\quad [\![\overline{T}_{(0)i},G_{(0)0}]\!]=0,\qquad (7.6)$$

$$[\![T_{(0)i},\overline{G}_{(0)0}]\!]=0,\quad [\![\overline{T}_{(0)i},\overline{G}_{(0)0}]\!]=0,\qquad (7.7)$$

$$[\![P_{(0)\mu},P_{(f)\nu}]\!]=0,\qquad (7.8)$$

$$[\![P_{(0)\mu},T_{(f)t}]\!]=0,\quad [\![P_{(0)\mu},\overline{T}_{(f)s}]\!]=0,\qquad (7.9)$$

$$[\![P_{(0)\mu},E_{(f)0}]\!]=0,\quad [\![P_{(0)\mu},\overline{E}_{(f)0}]\!]=0,\qquad (7.10)$$

$$[\![P_{(0)\mu},G_{(0)0}]\!]=0,\quad [\![P_{(0)\mu},\overline{G}_{(0)0}]\!]=0,\qquad (7.11)$$

$$[\![T_{(i)s},T_{(j)t}]\!]=0,\quad [\![T_{(i)s},\overline{T}_{(j)\dot{t}}]\!]=0,\quad [\![\overline{T}_{(i)\dot{s}},\overline{T}_{(j)\dot{t}}]\!]=0,\qquad (7.12)$$

$$[\![E_{(i)0},E_{(j)0}]\!]=0,\quad [\![E_{(i)0},\overline{E}_{(j)0}]\!]=0,\quad [\![\overline{E}_{(i)0},\overline{E}_{(j)0}]\!]=0,\qquad (7.13)$$

$$[\![T_{(i)s},E_{(j)0}]\!]=0,\quad [\![T_{(i)s},\overline{E}_{(j)0}]\!]=0,\qquad (7.14)$$

$$[\![\overline{T}_{(i)\dot{s}},E_{(j)0}]\!]=0,\quad [\![\overline{T}_{(i)\dot{s}},\overline{E}_{(j)0}]\!]=0,\qquad (7.15)$$

$$[\![P_{(f)\mu},P_{(f)\nu}]\!]=0,\qquad (7.16)$$

$$[\![P_{(i)\mu},P_{(j)\nu}]\!]=C^{\sigma}(i,j)_{\mu\nu}E_{(i\dagger j)\sigma}+\hat{C}^{\sigma}(i,j)_{\mu\nu}\overline{E}_{(i\dagger j)\sigma}+\eta^{r}(i,j)_{\mu\nu}T_{(i\dagger j)r}+\hat{\eta}^{\dot{r}}(i,j)_{\mu\nu}\overline{T}_{(i\dagger j)\dot{r}},\quad i\neq j\qquad (7.17)$$

$$[\![T_{(k)r},P_{(l)\mu}]\!]=\delta_{kl}K_{r}(l)_{\mu}^{\nu}P_{(0)\nu},\qquad (7.18)$$

$$[\![\overline{T}_{(k)\dot{r}},P_{(l)\mu}]\!]=\delta_{kl}\hat{K}_{\dot{r}}(l)^{\nu}_{\mu}P_{(0)\nu}. \tag{7.19}$$

$$[\![E_{(f)\sigma},P_{(l)\mu}]\!]=\delta_{fl}S_{\sigma}(l)^{\nu}_{\mu}P_{(0)\nu}, \tag{7.20}$$

$$[\![\overline{E}_{(f)\sigma},P_{(l)\mu}]\!]=\delta_{fl}\hat{S}_{\sigma}(l)^{\nu}_{\mu}P_{(0)\nu}, \tag{7.21}$$

$$[\![G_{(0)0},\overline{G}_{(0)0}]\!]=0, \tag{7.22}$$

$$[\![G_{(0)0},P_{(i)\nu}]\!]=l(0i)_0P_{(i)\nu},\quad [\![\overline{G}_{(0)0},P_{(i)\nu}]\!]=-l(0i)^{*}_0P_{(i)\nu}, \tag{7.23}$$

$$[\![G_{(0)0},T_{(k)a}]\!]=-l(0k)_0T_{(k)a},\quad [\![\overline{G}_{(0)0},T_{(k)a}]\!]=l(0k)^{*}_0T_{(k)a}, \tag{7.24}$$

$$[\![G_{(0)0},\overline{T}_{(k)a}]\!]=-l(0k)_0\overline{T}_{(k)a},\quad [\![\overline{G}_{(0)0},\overline{T}_{(k)a}]\!]=l(0k)^{*}_0\overline{T}_{(k)a}. \tag{7.25}$$

The σ-matrices associated with the different spin representations were given in Ref. 1 The η- and C-matrices are given in (2.9) and (2.10). The K- and S-matrices are given in (2.21) and (2.22). These matrices are constrained by the conditions (2.25)–(2.28), or equivalently to the constraints (2.30)–(2.36). A particular choice respecting the symmetry among the novel classes is given by (2.37) and (2.38). The l-structure constants fulfill the constraint (4.32). A particular choice respecting the symmetry among the novel classes is given in (4.46). The obtained constraints on the structure constants reveal that no anisotropy or inhumogeneity should be introduced to the space–time through this extension since there are particular choices of the structure constants that maintain the profound symmetry behind the three novel classes.

The naive dimensions and spin representations of the full clover extension are presented diagramatically in Table II. This extension has 48 generators, three for each one of the 16 elements of the grading group $\mathbb{Z}_4\times\mathbb{Z}_4$. Both the minimal vector clover extension and the full clover extension make a democratic usage of the grading indices.

In the full clover extension each class has exactly a couple (conjugate pair) of scalar singlets, a symmetric vector and a couple (conjugate pair) of antisymmetric vectors. This structure gives a taste of what could be the structure of graded superfields. The minimal vector clover extension exhibits what might be a constrained version of such graded superfields, each class involving only a symmetric vector and a couple (conjugate pair) of antisymmetric vectors. The same type of comment might be done for the minimal scalar clover extension. We observe already that a relation among vector and scalar multiplets is suggested, whose relevance for a relation among gauge and Higgs fields is discussed in a forthcomming publication.

Since the product of each generator by its corresponding graded parameter builds a Lie algebra generator, we might inquire about which could be the Lie algebra and Lie groups associated with the presented extensions. The full clover extension has 48 generators, so it might be related to the Lie algebras A_6 $(u(7),su(7),su(p,q)$ for $p+q=7$, $sl(7,\mathbb{R}))$ or with $sl(5,\mathbb{C})$. The minimal vector clover extension enhanced with the two dimensionless scalars is a subalgebra of dimension 42, so it might be related to the Lie algebras $so(7,\mathbb{C}),o(7,\mathbb{C})$ or $sp(3,\mathbb{C})$. The minimal vector clover extension with dimension 40 has the same dimension of the supergraded de Sitter algebra $osp(5|4)$, but there the space–time translations no longer commute, while here they do. The minimal scalar clover extension enhanced with the two dimensionless scalars has dimension 30, so it might be related to the Lie algebra $sl(4,\mathbb{C})$. The minimal scalar clover extension has dimension 28, so it might be related to the Lie algebras $D_4(o(8),so(8),so(p,q)$ for $p+q=8,so^{*}(8))$ or $so(6,\mathbb{C}),o(6,\mathbb{C})$.

The introduction of central charges has also been addressed, although all scalar charges in the full clover extension might be seen as central charges as well. In particular we considered the introduction of scalar charges $Z_{(k)\nu},\overline{Z}_{(k)\nu}$ with $k=1,2,3$; $\nu=0,1,2,3$ and $Z^{i}_{(0)\nu}$, $\overline{Z}^{i}_{(0)\nu}$ with $i=1,2,3$; $\mu=0,1,2,3$ of naive dimension 2/3, by replacing relations (7.16) and (7.17) with

$$[\![P_{(i)\mu},P_{(i)\nu}]\!]=D^{\sigma}(i,i)_{\mu\nu}Z^{i}_{(0)\sigma}+\hat{D}^{\sigma}(i,i)_{\mu\nu}\overline{Z}^{i}_{(0)\sigma}, \tag{7.26}$$

$$[\![P_{(i)\mu},P_{(j)\nu}]\!]=C^{\sigma}(i,j)_{\mu\nu}E_{(i\dagger j)\sigma}+\hat{C}^{\sigma}(i,j)_{\mu\nu}\overline{E}_{(i\dagger j)\sigma}+\eta^{r}(i,j)_{\mu\nu}T_{(i\dagger j)r}+\hat{\eta}^{\dot{r}}(i,j)_{\mu\nu}\overline{T}_{(i\dagger j)\dot{r}}$$
$$+D^{\sigma}(i,j)_{\mu\nu}Z_{(i\dagger j)\sigma}+\hat{D}^{\sigma}(i,j)_{\mu\nu}\overline{Z}_{(i\dagger j)\sigma}, \quad i\neq j, \tag{7.27}$$

where the D-matrices are given in (5.5) and (5.10). These central charges q-commute with all the generators of the full clover extension with the exception of the dimensionless scalars:

$$[\![G_{(0)0},Z_{(k)\nu}]\!]=-l(0k)_{0}Z_{(k)\nu}, \tag{7.28}$$

$$[\![G_{(0)0},\overline{Z}_{(k)\nu}]\!]=-l(0k)_{0}\overline{Z}_{(k)\nu}, \quad k=1,2,3. \tag{7.29}$$

$$[\![G_{(0)0},Z^{i}_{(0)\nu}]\!]=2\,l(0i)_{0}Z^{i}_{(0)\nu}, \tag{7.30}$$

$$[\![G_{(0)0},\overline{Z}^{i}_{(0)\nu}]\!]=2\,l(0i)_{0}\overline{Z}^{i}_{(0)\nu}, \quad i=1,2,3. \tag{7.31}$$

It was remarked that the introduction of the central charges $Z^{i}_{(0)\nu}$, $\overline{Z}^{i}_{(0)\nu}$ damage or at least modify the interpretation of the $P_{(i)\mu}$ multiplets as translations in the noncommutative manifold, since they would no longer q-commute among them, as naively expected from a translation. It was also remarked that there is no place for introducing extra dimensionless antisymmetric vectors nontrivially connected with the clover extension. We do not recognize either any naive ''democratic'' pattern in the usage of group indices for these central charges.

Note added in proof. Central charges q-commuting with all the full clover extension generators can be included in the right-hand side of Eqs. (4.47) and (7.22).

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Space-like hypersurfaces in the de Sitter spaces

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By using Cheng–Yau's self-adjoint operator $\Box$, we study the space-like hypersurfaces in the de Sitter spaces and obtain some general rigidity results. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1386638]

I. INTRODUCTION

Let $M_p^{n+p}(c)$ be an $(n+p)$-dimensional connected semi-Riemannian manifold of constant curvature c whose index is p. It is called an indefinite space form of index p and simply a space form when $p=0$. If $c>0$, we call it a de Sitter space of index p, and denote it by $S_p^{n+p}(c)$. The study of space-like hypersurfaces in de Sitter space has recently been of substantial interest from both physics and mathematical points of view. Akutagawa[1] and Ramanathan[2] investigated space-like hypersurfaces in a de Sitter space and proved independently that a complete space-like hypersurface in a de Sitter space with constant mean curvature is totally umbilical if the mean curvature H satisfies $H^2 \leqslant c$ when $n=2$ and $n^2H^2<4(n-1)c$ when $n\geqslant 3$. Later, Cheng[3] generalized this result to general submanifolds in a de Sitter space.

On the other hand, Cheng and Ishikawa[4] have recently shown that the totally umbilical round spheres are the only compact space-like hypersurfaces in $S_1^{n+1}(1)$ with constant scalar curvature $R<n(n-1)$. Some other authors, such as Liu,[5] Li,[6] and Zheng,[7,8] have also obtained interesting results related to the characterization of the totally umbilical round spheres as the only compact space-like hypersurfaces in the de Sitter space with constant scalar curvature.

In the present paper, we would like to use Cheng-Yau's self-adjoint operator $\Box$ to study the space-like hypersurfaces in the de Sitter spaces and get some very interesting general rigidity results.

II. PRELIMINARIES

Let S_1^{n+1} be an $(n+1)$-dimensional de Sitter space of constant curvature 1 whose index is 1. Let M be an n-dimensional compact space-like hypersurface in S_1^{n+1}. We choose a local field of semi-Riemannian orthonormal frames $e_1, \ldots, e_{n+1}$ in S_1^{n+1} such that at each point of M, $e_1, \ldots, e_n$ span the tangent space of M and form an orthonormal frame there. We use the following convention on the range of indices:

$$1\leqslant A,B,C, \ldots \leqslant n+1; \quad 1\leqslant i,j,k, \ldots \leqslant n.$$

Let $\omega_1, \ldots, \omega_{n+1}$ be its dual frame field so that the semi-Riemannian metric of S_1^{n+1} is given by $d\overline{s^2}=\Sigma_i \omega_i^2-\omega_{n+1}^2=\Sigma_A \epsilon_A \omega_A^2$, where $\epsilon_i=1$ and $\epsilon_{n+1}=-1$. Then the structure equations of S_1^{n+1} are given by

$$d\omega_A=\sum_B \epsilon_B \omega_{AB} \wedge \omega_B, \quad \omega_{AB}+\omega_{BA}=0, \tag{1}$$

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$$d\omega_{AB}=\sum_{C}\ \epsilon_C\omega_{AC}\wedge\omega_{CB}-\frac{1}{2}\sum_{C,D}\ K_{ABCD}\omega_C\wedge\omega_D\,, \tag{2}$$

$$K_{ABCD}=\epsilon_A\epsilon_B(\,\delta_{AC}\delta_{BD}-\delta_{AD}\delta_{BC}). \tag{3}$$

Restrict these form to M^n, we have

$$\omega_{n+1}=0, \tag{4}$$

the Riemannian metric of M^n is written as $ds^2=\Sigma_i\,\omega_i^2$. From Cartan's lemma we can write

$$\omega_{n+1i}=\sum_{j}\ h_{ij}\omega_j\,,\quad h_{ij}=h_{ji}\,. \tag{5}$$

From these formulas, we obtain the structure equations of M:

$$\mathrm{d}\omega_i=\sum_{j}\ \omega_{ij}\wedge\omega_j\,,\quad \omega_{ij}+\omega_{ji}=0, \tag{6}$$

$$\mathrm{d}\omega_{ij}=\sum_{k}\ \omega_{ik}\wedge\omega_{kj}-\frac{1}{2}\sum_{k,l}\ R_{ijkl}\omega_k\wedge\omega_l\,, \tag{7}$$

$$R_{ijkl}=(\,\delta_{ik}\delta_{jl}-\delta_{il}\delta_{jk})-(h_{ik}h_{jl}-h_{il}h_{jk}), \tag{8}$$

where R_{ijkl} are the components of the curvature tensor of M and

$$h=\sum_{i,j}\ h_{ij}\omega_i\otimes\omega_j \tag{9}$$

is the second fundamental form of M. We also have

$$R_{ij}=(n-1)\,\delta_{ij}-nHh_{ij}+\sum_{k}\ h_{ik}h_{kj}\,, \tag{10}$$

$$n(n-1)(R-1)=-n^2H^2+|h|^2, \tag{11}$$

where R is the normalized scalar curvature, and H the mean curvature.

Define the first and the second covariant derivatives of h_{ij}, say h_{ijk} and h_{ijkl} by

$$\sum_{k}\ h_{ijk}\omega_k=dh_{ij}+\sum_{k}\ h_{kj}\omega_{ki}+\sum_{k}\ h_{ik}^{\alpha}\omega_{kj}\,, \tag{12}$$

$$\sum_{l}\ h_{ijkl}\omega_l=dh_{ijk}+\sum_{m}\ h_{mjk}\omega_{mi}+\sum_{m}\ h_{imk}\omega_{mj}+\sum_{m}\ h_{ijm}\omega_{mk}\,. \tag{13}$$

Then we have the Codazzi equation

$$h_{ijk}=h_{ikj}\,, \tag{14}$$

and the Ricci's identity

$$h_{ijkl}-h_{ijlk}=\sum_{m}\ h_{mj}R_{mikl}+\sum_{m}\ h_{im}R_{mjkl}\,. \tag{15}$$

For indefinite Riemannian manifolds in detail, refer to O'Neill.[9]

For a C^2-function f defined on M^n, we defined its gradient and Hessian f_{ij} by

$$df=\sum_i f_i\omega_i, \quad \sum_j f_{ij}\omega_j=df_i+\sum_j f_j\omega_{ji}. \tag{16}$$

We know that $f_{ij}=f_{ji}$ by exterior differentiation of (16).

Let $\phi=\Sigma_{ij}\phi_{ij}\omega_i\otimes\omega_j$ be a symmetric tensor defined on M^n, where

$$\phi_{ij}=nH\delta_{ij}-h_{ij}. \tag{17}$$

Following Cheng–Yau,[10] we introduce an operator $\Box$ associated with ϕ acting on any C^2-function f by

$$\Box f=\sum_{i,j}\phi_{ij}f_{ij}=\sum_{i,j}(nH\delta_{ij}-h_{ij})f_{ij}. \tag{18}$$

Since ϕ_{ij} is divergence-free, it follows[10] that the operator $\Box$ is self-adjoint relative to the L^2 inner product of M^n, i.e.,

$$\int_M f\Box g=\int_M g\Box f. \tag{19}$$

We can choose a local frame field $e_1,\ldots,e_n$ at any point $p\in M$, such that $h_{ij}=\lambda_i\delta_{ij}$ at p, by use of (18) and (11), we have

$$\Box(nH)=nH\Delta(nH)-\sum_i\lambda_i(nH)_{ii}$$

$$=\frac{1}{2}\Delta(nH)^2-\sum_i(nH)_i^2-\sum_i\lambda_i(nH)_{ii}$$

$$=-\frac{1}{2}n(n-1)\Delta R+\frac{1}{2}\Delta|h|^2-n^2|\nabla H|^2-\sum_i\lambda_i(nH)_{ii}. \tag{20}$$

On the other hand, through a standard calculation by use of (14) and (15), we get

$$\frac{1}{2}\Delta|h|^2=\sum_{i,j,k}h_{ijk}^2+\sum_i\lambda_i(nH)_{ii}+\frac{1}{2}\sum_{i,j}R_{ijij}(\lambda_i-\lambda_j)^2. \tag{21}$$

Putting (21) into (20), we have

$$\Box(nH)=-\frac{1}{2}n(n-1)\Delta R+|\nabla h|^2-n^2|\nabla H|^2+\frac{1}{2}\sum_{i,j}R_{ijij}(\lambda_i-\lambda_j)^2. \tag{22}$$

Now we assume that M^n is compact (without boundary) and we obtain the following formula by integrating (22) and by noting $\int_M\Delta R=0$ and $\int_M\Box(nH)=0$

$$\int_{M^n}\left[|\nabla h|^2-n^2|\nabla H|^2+\frac{1}{2}\sum_{i,j}R_{ijij}(\lambda_i-\lambda_j)^2\right]=0. \tag{23}$$

From (8), we have $R_{ijij}=1-\lambda_i\lambda_j$, $i\neq j$, and by putting this into (23), we obtain

$$\int_{M^n}\left[|\nabla h|^2-n^2|\nabla H|^2+n|h|^2-n^2H^2+|h|^4-nH\sum_i \lambda_i^3\right]=0. \tag{24}$$

Let $\mu_i=\lambda_i-H$ and $|Z|^2=\Sigma_i \mu_i^2$, we have

$$\sum_i \mu_i=0, \quad |Z|^2=|h|^2-nH^2, \tag{25}$$

$$\sum_i \lambda_i^3=\sum_i \mu_i^3+3H|Z|^2-nH^3. \tag{26}$$

From (24) to (26), we get

$$\int_{M^n}\left[|\nabla h|^2-n^2|\nabla H|^2+|Z|^2(n-nH^2+|Z|^2)-nH\sum_i \mu_i^3\right]=0. \tag{27}$$

We need the following algebraic lemma due to M. Okumura.[11,12]

Lemma 2.1: Let μ_i, $i=1,\ldots,n$, be real numbers such that $\Sigma_i \mu_i=0$ and $\Sigma_i \mu_i^2=\beta^2$, where $\beta=$constant$\geqslant 0$. Then

$$-\frac{n-2}{\sqrt{n(n-1)}}\beta^3\leqslant\sum_i \mu_i^3\leqslant\frac{n-2}{\sqrt{n(n-1)}}\beta^3, \tag{28}$$

and the equality holds in (28) if and only if at least $(n-1)$ of the μ_i are equal.

By use of Lemma 2.1, we have

$$\int_{M^n}\left[|\nabla h|^2-n^2|\nabla H|^2+(|h|^2-nH^2)\left(n-2nH^2+|h|^2-\frac{n(n-2)}{\sqrt{n(n-1)}}H\sqrt{|h|^2-nH^2}\right)\right]\leqslant 0. \tag{29}$$

III. MAIN RESULTS

Now consider the quadratic form

$$Q(u,t)=u^2-\frac{n-2}{\sqrt{n-1}}ut-t^2.$$

By the orthogonal transformation

$$\begin{cases}\overline{u}=\dfrac{1}{\sqrt{2n}}\{(1+\sqrt{n-1})u+(1-\sqrt{n-1})t\},\\ \overline{t}=\dfrac{1}{\sqrt{2n}}\{(\sqrt{n-1}-1)u+(\sqrt{n-1}+1)t\},\end{cases}$$

$Q(u,t)$ turns into

$$Q(u,t)=\frac{n}{2\sqrt{n-1}}(\overline{u}^2-\overline{t}^2),$$

where $\overline{u}^2+\overline{t}^2=u^2+t^2$.

Take $u=|Z|$, $t=\sqrt{n}H$, then

$$
\begin{aligned}
&n-nH^2-\frac{n(n-2)}{\sqrt{n(n-1)}}H|Z|+|Z|^2\\
&\quad=n+Q(u,t)=nc+\frac{n(\overline{u^2}-\overline{t^2})}{2\sqrt{n-1}}\\
&\quad=n+\frac{n(-\overline{u^2}-\overline{t^2})}{2\sqrt{n-1}}+\frac{n\overline{u^2}}{\sqrt{n-1}}\\
&\quad\geqslant n-\frac{n}{2\sqrt{n-1}}|h|^2. \qquad (30)
\end{aligned}
$$

From (30) and (29) we have

$$
0\geqslant\int_{M^n}\left\{(|\nabla h|^2-n^2|\nabla H|^2)+|Z|^2\left[n-\frac{n}{2\sqrt{n-1}}|h|^2\right]\right\}. \qquad (31)
$$

Therefore we have the following result.

Theorem 3.1: Let M be an n-dimensional ($n\geqslant 3$) compact space-like hypersurface in an $(n+1)$-dimensional de Sitter space S_1^{n+1}. If

$$
|\nabla h|^2\geqslant n^2|\nabla H|^2, \qquad (32)
$$

and

$$
0\leqslant|h|^2\leqslant 2\sqrt{n-1}, \qquad (33)
$$

then M is a totally umbilical hypersurface.

Proof: By the assumption of theorem, the right-hand side is non-negative. Thus, either $|Z|^2\equiv 0$, that is , M is totally umbilical; or

$$
|h|^2=2\sqrt{n-1}. \qquad (34)
$$

In the latter case, equality holds in Lemma 2.1, and it follows that M has at most two distinct constant principle curvatures. We conclude that M is totally umbilical from the compactness of M. This completes the proof of Theorem 3.1.

Lemma 3.1: Let M be an n-dimensional compact space-like hypersurface in an $(n+1)$-dimensional de Sitter space S_1^{n+1}. Suppose that the normalized scalar curvature $R=$constant and $R\leqslant 1$. Then $|\nabla h|^2\geqslant n^2|\nabla H|^2$.

Proof: From (11),

$$
-n^2H^2+\sum_{i,j}h_{ij}^2=n(n-1)(R-1).
$$

Taking the covariant derivative of the above-given expression, and using the fact $R=$constant, we get

$$
n^2HH_k=\sum_{i,j}h_{ij}h_{ijk}.
$$

By Cauchy–Schwarz inequality, we have

$$\sum_k n^4H^2(H_k)^2=\sum_k\left(\sum_{i,j}h_{ij}h_{ijk}\right)^2\leqslant\left(\sum_{i,j}h_{ij}^2\right)\sum_{i,j,k}h_{ijk}^2, \tag{35}$$

that is

$$n^4H^2\|\nabla H\|^2\leqslant|h|^2|\nabla h|^2. \tag{36}$$

On the other hand, from $R\leqslant 1$, we have $n^2H^2-|h|^2\geqslant 0$. Thus

$$H^2|\nabla h|^2\geqslant n^2H^2|\nabla H|^2$$

and Lemma 3.1 follows.

From Theorem 3.1 and Lemma 3.1, we have

Corollary 3.1: Let M be an n-dimensional ($n\geqslant 2$) compact space-like hypersurface with constant normalized scalar curvature R in an $(n+1)$-dimensional de Sitter space S_1^{n+1}. If $R\leqslant 1$ and

$$0\leqslant|h|^2\leqslant 2\sqrt{n-1}, \tag{37}$$

then M is a totally umbilical hypersurface.

Lemma 3.2: Let M be an n-dimensional compact space-like hypersurface in an $(n+1)$-dimensional de Sitter space S_1^{n+1}. Suppose that the normalized scalar curvature R is proportional to the mean curvature H of M, that is

$$R=aH, \tag{38}$$

where a is any constant. Then $|\nabla h|^2\geqslant n^2|\nabla H|^2$.

Proof: By use of Gauss equation $-n^2H^2+|h|^2=n(n-1)(R-1)$ and the assumption (38), we have

$$|h|^2=n^2H^2-n(n-1)(1-aH). \tag{39}$$

Taking the covariant derivative of (39), we have for every k

$$2\sum_{i,j}h_{ij}h_{ijk}=(2n^2H+n(n-1)a)H_k.$$

It follows that

$$4|h|^2|\nabla h|^2\geqslant 4\sum_k\left(\sum_{i,j}h_{ij}h_{ijk}\right)^2=(2n^2H+n(n-1)a)^2|\nabla H|^2. \tag{40}$$

By (38) and (39), we have

$$\begin{aligned}&(2n^2H+n(n-1)a)^2-4n^2|h|^2\\&\quad=(4n^4H^2+n^2(n-1)^2a^2+4n^3(n-1)Ha)-n^2(4n^2H^2-4n(n-1)(1-aH))\\&\quad=n^2(n-1)((n-1)a^2+4n)>0.\end{aligned} \tag{41}$$

Combining (40) with (41), we have $|\nabla h|^2\geqslant n^2|\nabla H|^2$. This completes the proof of Lemma 3.2.

From Theorem 3.1 and Lemma 3.2, we have

Corollary 3.2: Let M be an n-dimensional ($n\geqslant 2$) compact space-like hypersurface in an $(n+1)$-dimensional de Sitter space S_1^{n+1}. Suppose that the normalized scalar curvature R is proportional to the mean curvature H of M, that is, there exists a constant a such that

$$R=aH, \tag{42}$$

If

$$0\leqslant|h|^2\leqslant 2\sqrt{n-1}, \tag{43}$$

then M is a totally umbilical hypersurface.

Theorem 3.2: Let M be an n-dimensional ($n\geqslant 3$) compact space-like hypersurface in an $(n+1)$-dimensional de Sitter space S_1^{n+1}. If M has non-negative sectional curvature and

$$|\nabla h|^2\geqslant n^2|\nabla H|^2, \tag{44}$$

then M is a totally umbilical hypersurface.

Proof: If M has non-negative sectional curvature, $R_{ijij}\geqslant 0$, so the assumptions of Theorem 3.2 imply that the right-hand side of (23) is non-negative, thus we have

$$\frac{1}{2}\sum_{i,j} R_{ijij}(k_i-k_j)^2=0. \tag{45}$$

In the same way as Nomizu–Smyth's,[13] it follows that M has at most two distinct constant principle curvatures. We conclude that M is totally umbilical from the compactness of M. This completes the proof of Theorem 3.2.

From Theorem 3.2 and Lemma 3.1, we have

Corollary 3.3 (Ref. 8): Let M be an n-dimensional ($n\geqslant 2$) compact space-like hypersurface with constant normalized scalar curvature R and $R\leqslant 1$ in an $(n+1)$-dimensional de Sitter space S_1^{n+1}. If M has non-negative sectional curvature, then M is a totally umbilical hypersurface.

From Theorem 3.2 and Lemma 3.2, we have

Corollary 3.4: Let M be an n-dimensional ($n\geqslant 2$) compact space-like hypersurface in an $(n+1)$-dimensional de Sitter space S_1^{n+1}. If M has non-negative sectional curvature and the normalized scalar curvature R is proportional to the mean curvature H of M, that is, there exists a constant a such that

$$R=aH, \tag{46}$$

then M is a totally umbilical hypersurface.

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Comment on "Method of handling the divergences in the radiation theory of sources that move faster than their waves" [J. Math. Phys. 40, 4331 (1999)]

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The "method" in question[1] has repeatedly led to results which I proved false in 1996 by a short, transparent, and rigorous theorem.[2] Even shorter is the remark here that inspection of the standard formula for the electromagnetic field suffices to prove the results of the "method" false. © *2001 American Institute of Physics.*
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The "method of handling the divergences in the radiation theory of sources that move faster than their waves"[1] has repeatedly led to results claiming unexpectedly strong waves from such sources.[2–8] In response to these claims I noted in 1996 a rigorous upper bound on the intensity of such waves which they violated.[9] My disproof is, in turn, referenced several times in Ref. 1, with comment as to where I must have erred. That I have not could be demonstrated by reproducing my bound theorem here. It is short and transparent, but I have repeated it before.[10] Even shorter is the following remark exploiting standard electromagnetism.[11] It shows that if, as is assumed in the "method,"[1–9] the source distribution in question is *finite in extent, bounded in magnitude, and smooth*, then the intensity of waves from it cannot possibly decay less slowly than $1/r^2$. This therefore proves that the $1/r$ intensity decay claimed to result from the "method" must be false.

The standard electromagnetic formula for the magnetic field at the origin as an integral over all space is[11]

$$\mathbf{B}=\frac{\mu_0}{4\pi}\int\frac{[\operatorname{curl}\mathbf{j}]}{r}\mathrm{d}^3\mathbf{r} \tag{1}$$

where the square brackets $[\bullet]$ stand for "retarded value of." (Importantly $[\operatorname{curl}\mathbf{j}]\neq\operatorname{curl}[\mathbf{j}]$.) Rigorously then, if the origin is outside some fixed ball enclosing all source currents $\mathbf{j}$, we have

$$|\mathbf{B}|\leqslant\frac{\mu_0}{4\pi}(\max|\operatorname{curl}\mathbf{j}|)\times\frac{(\text{Volume of ball})}{(\text{Min distance } r \text{ from the origin to the ball surface})}. \tag{2}$$

That is $|\mathbf{B}|\leqslant\text{const}/r$, or the intensity $|\mathbf{B}^2|\leqslant\text{const}/r^2$. The assumption of smoothness of $\mathbf{j}$ ensures that the constant is finite, not infinite, and the inverse square law is thus proved on this basis, contrary to the $1/r$ claim. No mention of the nature of the source "motion" (fast or slow) is necessary; the source distribution variation is smooth but otherwise general.

If (1) is considered in need of justification, then this is supplied by my earlier disproof.[9,10] Finally, the only criticism in Ref. 1 of my disproof which was not already refuted in Ref. 10 is the note of Ref. 11 of Ref. 1. This note gets the logic backwards; justification is required to make any *restriction* on the domain of integration, not the other way round.

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Comment on "Uncertainty principle for proper time and mass" [J. Math. Phys 40, 1237 (1999)]

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Kudaka and Matsumoto derive the uncertainty relation $c^2\Delta m\Delta\tau\approx h$ between the proper time τ and rest mass m of a material particle by adopting for the description of the particle the Lagrangian $L=M(\dot{\tau}-c^{-1}\sqrt{-g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu})+eA_\mu(x)\dot{x}^\mu$, defined on the enlarged space (x^μ,τ,M), where M is an additional dynamical variable. A key step in the derivation of their uncertainty relation is the identification of the variable M with the rest mass m. Adopting the point of view of variational analysis, we show that such an identification goes against the relativistic requirement of the path dependence of proper time. © *2001 American Institute of Physics.*
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In a recent paper entitled "Uncertainty principle for proper time and mass," Kudaka and Matsumoto[1] contend that the uncertainty relation

$$c^2\Delta m\Delta\tau\approx h \tag{1}$$

between the rest mass m and the proper time τ of a particle can be derived if, instead of the usual relativistic Lagrangian

$$\mathrm{L}_o=-mc\sqrt{-g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu}+eA_\mu(x)\dot{x}^\mu, \tag{2}$$

one uses for the description of the particle a Lagrangian L which, besides the space–time coordinates $x^\mu(\mu=1,2,3,4)$, is dependent on both the proper time τ and an additional dynamical variable denoted M, and is defined by

$$\mathrm{L}=M(\dot{\tau}-c^{-1}\sqrt{-g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu})+eA_\mu(x)\dot{x}^\mu, \tag{3}$$

the dot denoting differentiation with respect to an arbitrary parameter λ. A key step in their derivation of the uncertainty relation (1) is the identification of the dynamical variable M with the rest mass m. For this purpose, the authors consider the following Euler–Lagrange (EL) equations

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\frac{\partial\mathrm{L}}{\partial\dot{X}^A}-\frac{\partial\mathrm{L}}{\partial X^A}=0,\quad X^A=(x^\mu,\tau,M),\quad (A=1,\ldots,6), \tag{4}$$

or equivalently in explicit form

$$\dot{M}=0, \tag{5}$$

$$\dot{\tau}=c^{-1}\sqrt{-g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu}, \tag{6}$$

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\left(\frac{M}{c}\frac{g_{\rho\mu}\dot{x}^\mu}{\sqrt{-g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu}}+eA_\rho(x)\right)-\frac{M}{2c}\frac{g_{\mu\nu,\rho}\dot{x}^\mu\dot{x}^\nu}{\sqrt{-g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu}}-eA_{\mu,\rho}(x)\dot{x}^\mu=0 \tag{7}$$

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and note that Eq. (7), with the aid of Eqs. (5) and (6), may be written in the form

$$\frac{M}{c^2}[\ddot{x}^\rho+\Gamma^\rho_{\mu\nu}\dot{x}^\mu\dot{x}^\nu]=ef^{\rho\mu}\dot{x}_\mu, \tag{8}$$

where $\Gamma^\rho_{\mu\nu}$ and $f_{\mu\nu}=A_{\nu,\mu}-A_{\mu,\nu}$ are respectively the Christoffel symbols of the second kind and the skew-symmetric electromagnetic tensor, the dot denoting now differentiation with respect to proper time τ. Comparison with the equation of motion

$$m[\ddot{x}^\rho+\Gamma^\rho_{\mu\nu}\dot{x}^\mu\dot{x}^\nu]=ef^{\rho\mu}\dot{x}_\mu \tag{9}$$

derived from the relativistic Lagrangian L_o shows that the two equations coincide if the dynamical variable M is identified with the rest energy mc^2 of the particle. From Eq. (5) it follows that the above identification is justified only in the case where M is a non-null constant. This fact is taken for granted by the authors and no discussion of the conditions ensuring this demand is presented. Moreover, from the point of view of variational analysis the EL equations, as a necessary condition for an extremum, are deduced from the first variation of a functional. The formal application, by the authors, of the EL equations (5)–(7) without specifying the form of the functional defined by the Lagrangian L and without saying precisely what extremum problem or variational principle is being considered, raises the question of the meaning and validity of this identification. The purpose of this comment is to show that the identification of the dynamical variable M with the rest mass goes against the relativistic requirement of the path dependence of proper time. Such a conclusion is reached if, by analogy with Hamilton's principle, we suppose that the Lagrangian L, as integrand, serves to define the parametric integral on the enlarged space (x^μ,τ,M)

$$J_{\mathrm{L}}=\int_{\lambda_1}^{\lambda_2}[M(\dot{\tau}-c^{-1}\sqrt{-g_{\mu\nu}\dot{x}^\mu\dot{x}^\nu})+eA_\mu(x)\dot{x}^\mu]d\lambda. \tag{10}$$

The integral is taken along the curve C joining the points P_1, P_2 corresponding to the parameter values λ_1 and λ_2, respectively, and which is representable in the form of the sextuple $X^A(\lambda)=(x^\mu(\lambda),\tau(\lambda),M(\lambda))$, with $\dot{X}^A(\lambda)$ vanishing nowhere on $[\lambda_1,\lambda_2]$, i.e., regular representation of the curve C. An important property of the functional J_L is that its value is independent of the particular parameter chosen. The Euler condition for the functional J_L assumes the form of the EL equations (5)–(7), in the absence of side conditions. This result is established by considering the problem of extremizing J_L as a nonparametric problem in the space (λ,x^μ,τ,M).[2,3] The Euler condition ensures that the extremizing curve g defined by the sextuple $\overline{X^A}(\lambda)=(\overline{x^\mu}(\lambda),\overline{\tau}(\lambda),\overline{M}(\lambda))$ lies entirely on the hypersurface $M=\text{const}$. It remains to specify under which end conditions the functional J_L is to be extremized. We shall see that in order to comply with the relativistic demand of the path dependence of proper time we must treat an extremum problem with variable end point. For such a problem, besides the Euler necessary condition, a second necessary condition, known as the transversality condition, must be satisfied.

For purpose of reference let us briefly recall Morse's formulation of this condition[2a,b]. Let points P_1, P_2 near the intial and final end points $\overline{P}_1$, $\overline{P}_2$ of the extremal g be given by functions

$$X^{AS}=(x^{\mu s},\tau^s,M^s)=X^{AS}(\alpha_1,\ldots,\alpha_r)\quad(s=1,2;1\leqslant r\leqslant 2m,m=4+2) \tag{11}$$

for values of the parameters (α) near (0). The functions appearing in Eq. (11) are assumed to be of class C^2 near $(\alpha)=(0)$. The end points $\overline{P}_1$, $\overline{P}_2$ of g being given by the values of the functions (11) for $(\alpha)=(0)$, i.e., $\overline{X^A}(\lambda_s)=X^{AS}(0)$ $(s=1.2)$. Curves neighboring the extremal g whose end points are given by the functions (11) are called terminally admissible or just admissible, in the absence of side conditions. The regular r dimensional manifold $X^{AS}=X^{AS}(\alpha)$ is known as the terminal manifold. The assumption of regularity meaning that the functional matrix

$$\left|\frac{\partial X^{AS}(0)}{\partial \alpha_h}\right| \quad (s=1,2;h=1,\ldots,r) \tag{12}$$

is of rank r. In the case of two end point manifolds M_1 and M_2 with respective dimensions p and q with $r=p+q$, meeting g at $\overline{P}_1$, $\overline{P}_2$, respectively, one sets

$$(\alpha_1,\ldots,\alpha_r)=(\rho_1,\ldots,\rho_p;\sigma_1,\ldots,\sigma_q), \tag{13}$$

and condition (11) takes the form

$$X^{A1}=X^{A1}(\rho_1,\ldots,\rho_p), \quad X^{A2}=X^{A2}(\sigma_1,\ldots,\sigma_q). \tag{14}$$

The curve g defined by the sextuple $\overline{X}^A(\lambda)$ and the set $(\alpha)=(0)$ will afford an extremum to the functional J_L relative to the neighboring curves of class C^1 if, besides the EL equations (5)–(7), the transversality condition (15) is satisfied:

$$[\mathrm{L}_{\dot{X}^A} dX^{AS}]_{s=1}^{s=2}=0, \quad (\alpha)=0, \tag{15}$$

where $(X,\dot{X})$ must be taken on g at the respective end points of g. Condition (15) is an identity in $d\alpha_h$ when the differentials dX^{AS} are expressed in terms of $d\alpha_h$. Without loss of generality we may assume that the end condition, at the first end point, fixes X^{A1} at $\overline{P}_1$. In this case the tranversality condition (15) reduces to

$$\left[\mathrm{L}_{\dot{X}^A}\frac{\partial X^{AS}(0)}{\partial \sigma_q}\right]^{s=2}=0. \tag{16}$$

Substitution of the expression of $\mathrm{L}_{\dot{X}}$ in (16) gives

$$\overline{M}(\lambda_2)\tau_q^2(0)+\left(\frac{\overline{M}(\lambda)g_{\mu\nu}\dot{\overline{x}}^{\nu}(\lambda)}{\sqrt{-g_{\mu\nu}\dot{\overline{x}}^{\mu}(\lambda)\dot{\overline{x}}^{\nu}(\lambda)}}+eA_{\mu}(\overline{x}(\lambda))\right)_{\lambda=\lambda_2} x_q^{\mu 2}(0)=0, \tag{17}$$

where the subscript q attached to τ^2 or $x^{\mu 2}$ means differentiation with respect to σ_q.

The second end point X^{A2} cannot be fixed at $\overline{P}_2$ otherwise the space–time projections of the admissible curves $X^A(\lambda)$, $\lambda_1\leqslant\lambda\leqslant\lambda_2$, contained within the future sheet of the null cone with vertex E_1, projection of the point $\overline{P}_1$, would all have the prescribed value $\overline{\tau}(\lambda_2)$ at their second end point; this would contradict the relativistic demand of the path dependence of proper time. Accordingly τ^2 must be left undetermined while $x^{\mu 2}$ can be set equal to the space–time coordinates $\overline{x}^{\mu}(\lambda_2)$ of $\overline{P}_2$. On account of this result it follows that along the extremal g the constant value taken by the dynamical variable M is equal to zero and thus it cannot be identified with the rest mass m. This conclusion remains valid in the general case where both τ^2 and $x^{\mu 2}$ are left undetermined at the second end point.

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Response to "Comment on 'Uncertainty principle for proper time and mass'" [J. Math. Phys. 42, 3975 (2001)]

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Krikorian asserts the following.

(1) The Lagrangian

$$\mathrm{L}=M(\dot{\tau}-c^{-1}\sqrt{-g_{\mu\nu}\dot{x}^{\mu}\dot{x}^{\nu}})+eA_{\mu}(x)\dot{x}^{\mu} \tag{1}$$

which we used for the description of a clock[1] is singular in a sense.

(2) When one considers the variational problem for such a singular Lagrangian, "the transversality condition"[2] must be taken into account in addition to the Euler condition.

(3) If both of these two conditions are taken into account for the Lagrangian L, it follows that the value of the variable M must be equal to zero along extremal curves. Therefore our conclusion[1] that the variable M can be identified with the rest mass of the particle is not correct. The objective of this response is to question the second of his assertions.

Let us consider a simple Lagrangian

$$\mathrm{L}'=-mc\sqrt{(\dot{x}^0)^2-(\dot{x}^1)^2} \tag{2}$$

for the description of a particle with rest mass m, where the dynamical variables are the space–time coordinates (x^0,x^1) (assuming one-dimensional space for simplicity) and the dot denotes the differential with respect to the proper time τ. The Euler–Lagrange equations are

$$\ddot{x}^0=\ddot{x}^1=0. \tag{3}$$

The Lagrangian L' is singular in the sense that

$$\det(\partial^2\mathrm{L}'/\partial\dot{x}^{\mu}\partial\dot{x}^{\nu})=0. \tag{4}$$

The Lagrangian L is also singular in this sense, and, in our judgment, this is the reason Krikorian asserts that the transversality condition must be taken into account when we consider the variational problem for the Lagrangian L.

Following his assertion, let us consider an extremal $x^{\mu}(\tau)(\tau_1\leqslant\tau\leqslant\tau_2)$ for the Lagrangian L' which, besides the Euler condition, satisfies the transversality condition. Without loss of generality we may assume that the first end point is fixed. In this case the transversality condition reduces to

$$\dot{x}^0(\tau_2)=0 \quad \text{or} \quad \dot{x}^1(\tau_2)=0. \tag{5}$$

Combining the condition (5) with the Euler condition (3), we are led to the conclusion that

$$\dot{x}^1(\tau)=0 \quad (\text{for all } \tau). \tag{6}$$

That is to say, only a very limited class of motions is admissible if we consider the variational problem for the Lagrangian L' under the transversality condition.

On the other hand, there is a general method[3] by which we can formulate Hamilton's principle for such a singular Lagrangian. When we apply the method to the Lagrangian L', we can actually describe all free motions of the relativistic particle. That is to say, at least for the Lagrangian L', there is no need to introduce the transversality condition and to limit the extent of the admissible motions. We dealt with the variational problem for the Lagrangian L by this method and got a set of motion equations which seems to be very reasonable.

Our question is then why we have to introduce an extra condition which limits the extent of the admissible motions when there is a method by which we can adequately represent Hamilton's principle and derive a set of reasonable motion equations.

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From classical to quantum mechanics: "How to translate physical ideas into mathematical language"

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Following previous works by E. Prugovečki [Physica A **91A**, 202 (1978) and *Stochastic Quantum Mechanics and Quantum Space–time* (Reidel, Dordrecht, 1986)] on common features of classical and quantum mechanics, we develop a unified mathematical framework for classical and quantum mechanics (based on L^2-spaces over classical phase space), in order to investigate to what extent quantum mechanics can be obtained as a simple modification of classical mechanics (on both logical and analytical levels). To obtain this unified framework, we split quantum theory in two parts: (i) general quantum axiomatics (a system is described by a state in a Hilbert space, observables are self-adjoints operators, and so on) and (ii) quantum mechanics proper that specifies the Hilbert space as $L^2(\mathbf{R}^n)$; the Heisenberg rule $[\mathbf{p}_i,\mathbf{q}_j]=-i\hbar\delta_{ij}$ with $\mathbf{p}=-i\hbar\nabla$, the free Hamiltonian $\mathbf{H}=-\hbar^2\Delta/2m$ and so on. We show that general quantum axiomatics (up to a supplementary "axiom of classicity") can be used as a nonstandard mathematical ground to formulate physical ideas and equations of ordinary classical statistical mechanics. So, the question of a "true quantization" with "$\hbar$" must be seen as an independent physical problem not directly related with quantum formalism. At this stage, we show that this nonstandard formulation of classical mechanics exhibits a new kind of operation that has no classical counterpart: this operation is related to the "quantization process," and we show why quantization physically depends on group theory (the Galilei group). This analytical procedure of quantization replaces the "correspondence principle" (or canonical quantization) and allows us to map classical mechanics into quantum mechanics, giving all operators of quantum dynamics and the Schrödinger equation. The great advantage of this point of view is that quantization is based on concrete physical arguments and not derived from some "pure algebraic rule" (we exhibit also some limit of the correspondence principle). Moreover spins for particles are naturally generated, including an approximation of their interaction with magnetic fields. We also recover by this approach the semi-classical formalism developed by E. Prugovečki [*Stochastic Quantum Mechanics and Quantum Space–time* (Reidel, Dordrecht, 1986)]. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1386410]

I. INTRODUCTION

From the beginning of quantum mechanics, different methods have been developed to link classical and quantum formalisms. One of the most famous is the Wigner–Weyl transformation that allows one to recover the semi-classical limit of quantum mechanics in phase space.[1] This operation associates to each quantum operator **a** a function in phase space $a(p,q)$ in such a way that at the lowest order in $\hbar$ (zeroth order), the quantum evolution of $a(p,q)$ reduces to the classical one.

From this point of view, quantization is mathematically a deformation of the Abelian algebra of functions in phase space into a noncommutative algebra using the so-called $*_h$-product that replaces standard multiplication[2] [$a(p,q)*_h b(p,q)$ corresponds to the operator product $\mathbf{a}\cdot\mathbf{b}$].

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Although the Wigner–Weyl transformation is algebraically very powerful, it is not completely satisfactory from a physical point of view, because all quantum densities **D** are not mapped into true probability densities[3] $\rho(p,q)$ (positive functions). Nevertheless, this formalism is very useful, and not only in nonrelativistic mechanics, since it can be extended to special relativity.[4]

The Wigner–Weyl transformation is not the unique way to obtain a semi-classical formula. Such kind of formula also occurs using a coherent state splitting.[5,6] Moreover, we have already proved that we can define Hamiltonian-dependent coherent states that allow us to obtain exact quantum results with a semi-classical formula,[7] and this approach preserves positivity [a quantum density **D** is associated with a true classical probability density $\rho(p,q)$]. This formalism with coherent states can be also extended to relativity.[6,8]

All these procedures have the nice property of giving an analytical connection between classical and quantum formalisms, overcoming the apparent discontinuity between classical and quantum pictures. Nevertheless, we always have to assume first quantum operators to obtain semi-classical results, while at the same time, quantum operators (and specially quantum Hamiltonian) are themselves derived from the correspondence principle. So, quantum operators are in fact deduced from classical ones by some ''pure algebraic rule.'' Then, at a logical level, the relationship between classical and quantum mechanics remains not so clear, since we need both of them at the same time, although only quantum mechanics is assumed in principle to be the ''true theory.''

This shows that the logical relationship between quantum mechanics and classical mechanics is more complicated than, for example, the relationship between classical mechanics and special relativity; while quantum mechanics only needs a new constant ''$\hbar$,'' exactly as special relativity needs the new constant ''c.'' We mean that classical and relativistic mechanics are formulated on the same mathematical ground (basic mathematical objects) in such a way that taking the limit $c\to\infty$ into any relativistic formula, we obtain the standard classical result. But this cannot be done directly in the same way ($\hbar\to 0$) in the case of quantum mechanics because the Hilbert space formalism is not the mathematical formalism of classical mechanics.

For the same reason, in special relativity we do not need a general procedure to lift up a classical quantity into the relativistic framework, while in quantum mechanics, we need the correspondence principle.

Of course, different studies have been led, not on a purely analytical level, but on a logical level, to find an *a priori* justification of the quantum picture and these attempts go back to von Neumann.[9]

More recently, in the 1960s, Mackey[10,11] has presented a general mathematical description of a statistical system based on an abstract structure called ''orthocomplemented lattice'' that unifies classical and quantum statistics: adding an *ad hoc* postulate to the basic lattice picture allows us to recover either classical formalism or a quantum one.

This shows that the mathematical representations of classical and quantum theories share some general common structure, but this does not explain the special realization leading to quantum mechanics, namely the choice of the Hilbert space as $L^2(\mathbf{R}^n)$ with $\mathbf{p}=-i\hbar\nabla$ and the free Hamiltonian $\mathbf{H}=-\hbar^2\Delta/2m$. In fact, different studies show that these special realizations are connected to group theory, namely Euclidean invariance and Galilean invariance.[11,12]

Among the contributions to these ''first level'' foundations of quantum mechanics (see Ref. 13 for a nonexhaustive list of references), we shall give some details about the results obtained by Prugovečki[6,14] that are in direct relation with the present article.

The common structure shared by classical and quantum theories suggests that it may exist a possible unified mathematical framework based on L^2-spaces over classical phase space, and the work of Prugovečki in Refs. 14 and 6 (Chaps. 1 and 3) deals with this problem. In fact, this unification is obtained by a change of representation of quantum mechanics and a recasting of classical statistical mechanics. Coherent states obtained from the Galilei group allows us to formulate quantum mechanics into a subspace of the Hilbert space $L^2(\Gamma)$ on the phase space Γ, while classical statistical mechanics can be also formulated in the Hilbert space $L^2(\Gamma)$. Moreover, as indicated in Ref. 14 ''the classical theory emerges as an approximation to the first order of $\hbar$ of the

quantum theory once both of these theories are formulated in terms of superoperators acting in the Liouville space over $L^2(\Gamma)$.''

Now, let us situate our article and its goals.

As noticed previously, the difficulty to connect classical and quantum mechanics on both logical and analytical levels is essentially due to the great difference of mathematical language that confuses physical intuition. In this article, we develop a precise mathematical ground based on some axiomatics, in which classical mechanics and quantum mechanics can be expressed using the same tools. Our goal is not only to unify classical and quantum formalism, but also to rebuild quantum mechanics only starting with classical mechanics, using physical ideas and logical arguments instead of ''simple algebraic rules.'' Moreover, we want to obtain a precise status (classical or quantum) for each ingredient of quantum mechanics.

This question of the classical or purely quantum nature of the ingredients of quantum mechanics is legitimate by at least two arguments:

(i) First, most of quantum operators are deduced from classical quantities (correspondence principle).

(ii) Second, taking the limit $\hbar \to 0$, quantum mechanics must degenerate into classical mechanics. Unfortunately, this limit only says that $\mathbf{p}$ and $\mathbf{q}$ are now commuting operators: the general quantum formalism with wave functions, operators, and so on remains unchanged.

The only possible explanation of this last result is that quantum formalism with commuting operators describes the ideas of classical statistical mechanics as well as the usual formalism in phase space. This means that we have in fact two possible mathematical formalisms to represent the same physical ideas of classical statistical mechanics. Then it must be possible to formulate the ideas and the equations of standard classical statistical mechanics using only the general quantum formalism (axiomatics) and then the question of the true quantization with $\hbar$ must be seen as an independent problem not directly related with the formalism.

In this article, we present such a ''nonstandard axiomatic formulation'' of classical statistical mechanics and we show how (and why) it is equivalent to the usual one. Of course this new picture is not a true quantum theory, since it represents always classical ideas, but it works with general quantum formalism. The use of Hilbert space techniques into classical mechanics is not new and goes back to Koopman.[15] Even the concept of ''classical amplitude'' is not new and has been introduced by Schönberg.[16] But in this article we do not look at these techniques with the same point of view: we consider the Hilbert space formalism as a true logical and analytical representation of classical mechanics, and not only as a mathematical trick. Of course, even if our starting point is different, we recover most of the formula obtained by Prugovečki in Refs. 14 and 6 (Chap. 3).

Then, we show that our nonstandard formalism exhibits a new operation (projection) that has no classical counterpart: this operation is related to the ''quantization process,'' and we show why quantization physically depends on group theory (Galilei group). We cross again the results obtained in Ref. 6, since the procedure of projection gives a subspace of $L^2(\Gamma)$ where quantum mechanics can be formulated, and then many results are common.

But the important result is that this procedure of projection replaces the correspondence principle and allows us to recover all operators of quantum mechanics and the Schrödinger equation.

The great advantage of this point of view is that now, quantization is explicitly based on concrete physical arguments and not derived from some ''pure algebraic rule.'' Moreover, spins for particles are naturally generated, including an approximation of their interaction with magnetic fields. We also recover the natural semi-classical formalism due to coherent states of Galilei group: some exact quantum results are obtained with classicallike formula.

As indicated, many formulas obtained in this article can be found in the previous works of Prugovečki, but they are obtained from another point of view (and our formalism does not use superoperators and Liouville space). The necessary parallels are done in the remainder of the text.

To conclude this introduction, let us specify two points.

First, we do not situate our article in the framework of the question: why does the macroscopic world appear essentially classical, while the microscopic world is quantum? It is well known that this effect is due to decoherence (for details see the nonexhaustive list of references in Ref. 17). Our article is not any more in the field of ''consistent interpretations of quantum mechanics'' or ''consistent histories'' that looks for the logical problems raised by quantum mechanics (Omnès,[18] Gell-Mann–Hartle,[19] Griffiths[20]), even if our article contains consequences on the interpretation of quantization.

Second, there exists one important aspect of our point of view that is not developed in this article: this concerns our previous remark on the equivalence of quantum formalism with commuting operators and the usual classical formalism. If this equivalence is true, this means that any one of these formalisms can be (logically and physically) rebuilt from the other one, and more specially that the full general quantum framework (axiomatics) can be found (as a change of mathematical language) only starting with classical formalism. Of course, on a logical level, it should be more enlightening to recover first general quantum formalism, before any further development. But this would be too long for a single article. So, this special point will be published later in an article devoted to this question.

II. CLASSICAL MECHANICS IN PHASE SPACE (ONE PARTICLE)

A. Phase space structure and Poisson brackets

We only present in this section the main features that we need. For more details, see Ref. 21.

Phase space represents configuration space and it is the set of pairs $(\vec{p},\vec{q})$ of momenta and positions, where $(\vec{p},\vec{q})$ represents the (pure) state of the system. Physical observables are functions $f(\vec{p},\vec{q})$ on phase space.

Now, from a mathematical point of view, if we call M the $\mathbf{R}^3$ space manifold, phase space is the cotangent bundle TM^*. It possesses a natural geometry (namely, a symplectic geometry) that allows us to define the Poisson brackets (PB), $\{f,g\}$ of two functions by

$$\{f,g\}=\vec{\nabla}_p f\cdot\vec{\nabla}_q g-\vec{\nabla}_p g\cdot\vec{\nabla}_q f. \tag{1}$$

The PB is the basic algebraic component of classical mechanics and the physical content of PBs can be related to group theory. Namely, any classical observable f can be seen as the generator of a one-parameter group of transformations acting on observables. Any g is transformed into g_α through

$$\frac{\partial g_\alpha}{\partial\alpha}=\{f,g_\alpha\}. \tag{2}$$

Equivalently, we have trajectories of states $(\vec{p_\alpha},\vec{q_\alpha})$ generated by f following the equations

$$\begin{aligned}\frac{\partial}{\partial\alpha}\vec{q_\alpha}&=\vec{\nabla}_p f(\vec{q_\alpha},\vec{p_\alpha}),\\ \frac{\partial}{\partial\alpha}\vec{p_\alpha}&=-\vec{\nabla}_q f(\vec{q_\alpha},\vec{p_\alpha}).\end{aligned} \tag{3}$$

Then, on a mathematical level, all classical observables play the same role and this role is summarized by the algebra due to Poisson brackets.

B. Classical dynamics

1. Equations of motion for a pure state

Dynamics on phase space is defined by the Hamiltonian equations that are a special case of (3):

$$\frac{d}{dt}\vec{q}=\vec{\nabla}_p H(\vec{q},\vec{p},t),$$
$$\frac{d}{dt}\vec{p}=-\vec{\nabla}_q H(\vec{q},\vec{p},t), \tag{4}$$

where H is the Hamiltonian (eventually time dependent).

2. Dynamics and statistics

These equations (4) correspond to the ideal case of a particle perfectly localized in phase space and we can represent this situation by the probability density $\rho(\vec{p},\vec{q},t)=\delta(\vec{p}-\vec{p_0}(t))\delta(\vec{q}-\vec{q_0}(t))$. Now, if we build a general density ρ as superpositions of "δ" as $\rho=\Sigma_i p_i \delta_{\vec{p_i}(t),\vec{q_i}(t)}$, we find that ρ verifies the Liouville equation:

$$\frac{\partial\rho}{\partial t}=-\{H,\rho\}. \tag{5}$$

So we say classically that (5) describes the evolution of any probability density ρ.

Now, starting from a density ρ that verifies (5), we can look at the evolution of the expectation value $\langle f\rangle_t$ of an observable $f(\vec{p},\vec{q},t)$ defined as $\langle f\rangle_t=\int d^3\vec{p}\,d^3\vec{q}\,\rho(\vec{q},\vec{p},t)\ f(\vec{p},\vec{q},t)$. We find

$$\frac{d}{dt}\langle f\rangle_t=\left\langle\frac{\partial f}{\partial t}\right\rangle_t+\langle\{H,f\}\rangle_t. \tag{6}$$

Applied to the special case of the two fundamental observables $\vec{p}$ and $\vec{q}$, Eq. (6) gives

$$\frac{d}{dt}\langle\vec{q}\rangle_t=\langle\vec{\nabla}_p H\rangle_t,$$
$$\frac{d}{dt}\langle\vec{p}\rangle_t=-\langle\vec{\nabla}_q H\rangle_t. \tag{7}$$

3. Strong and weak dynamical equations

In this section we want to point out some important remarks on the dynamical equations in the framework of statistical mechanics.

Let us assume that the evolution of the probability density $\rho(\vec{p},\vec{q},t)$ is unknown, and that we only know the evolution of expectation values of $\vec{p}$ and $\vec{q}$ through the equations (7). We want to see if it is possible to rebuild the equations (4) on pure states and to find the Liouville equation, only starting with (7).

Basically, if we assume that "δ" densities are allowed such as $\rho(\vec{p},\vec{q},t)=\delta(\vec{p}-\vec{p_0}(t))\delta(\vec{q}-\vec{q_0}(t))$, we find that the equations (7) on expectation values imply that the trajectory $(\vec{p_0}(t),\vec{q_0}(t))$ follows the Hamiltonian equations (4), then we deduce in the same way that a general density must verify the Liouville equation.

But if "δ" densities are not allowed, we cannot directly deduce the evolution of states only starting with expectation value equations, and then we cannot recover Liouville equation. This means that we can find other possible laws of evolution for the density $\rho(\vec{q},\vec{p},t)$ that are compatible with the equations (7) on expectation values.

So we call Eqs. (4) on states "*strong dynamical equations*" and Eqs. (7) on expectation values "*weak dynamical equations*."

Now, as argued by Born,[22] the true mathematical representation of any physical measure is an expectation value associated with some probability density, because a real result of a physical

experiment always contains some uncertainty. Therefore, physical observables (classical or quantum) are always stochastic. This important remark is also the starting point of Prugovečki's monograph.[6]

So weak dynamical equations (7) are a better mathematical description of our physical knowledge about classical dynamics. When we say that strong dynamical equations (4) are realized, in fact we extrapolate our real knowledge by assuming that we can use "δ" densities. Of course this procedure is natural, but not logically necessary. We will use this remark in Sec. V A.

C. Physical symmetries in phase space

We will see later in Sec. VI that our quantization principle is based on the representation of symmetries. Symmetries are defined as the set of physical transformations allowing us to look at the same system from different but equivalent frames. Then let us specify in this section the symmetries involved in phase space.

At first sight, the Poisson brackets defined previously seem to prove that each observable defines a generator of such a symmetry, so the set of symmetries is generated by the full set of classical observables.

But this is only true on a mathematical level: it is false on a physical point of view, because any of these transformations cannot be realized in practice as a real change of frame. The only real continuous transformations that can be realized are space translations, space rotations and Galilean transformations. They constitute the Galilei group. We can also add two discrete transformations: parity and time reversal.

So the true set of classical symmetries can be divided as follows:

(i) the space transformations: translations, rotations and parity,
(ii) the kinematical transformations: Galilei boosts, and
(iii) time reversal.

III. NEW FRAMEWORK FOR CLASSICAL MECHANICS

As indicated in the Introduction, our point of view is to use standard quantum formalism applied to the case of classical mechanics.

So, we introduce the "continuous orthonormal basis" $\{|\vec{p},\vec{q}\rangle\}$ that diagonalizes at the same time the operators $\vec{\mathbf{p}}$ and $\vec{\mathbf{q}}$ ($[\vec{\mathbf{p}},\vec{\mathbf{q}}]=0$). In the remainder of the text, we often use this notation $|\vec{p},\vec{q}\rangle$, but only in circumstances that do not introduce mathematical ambiguity.

It is well known that these $|\vec{p},\vec{q}\rangle$ vectors do not belong to the Hilbert space defined later, but rather to corresponding rigged or equipped Hilbert space.[23]

Now we list the basic axioms[24] (since we do not try to obtain a minimal list, some axioms can be redundant).

A. The basic elements

1. Primary axioms

(i) The mathematical framework is the Hilbert space $\mathcal{H}=L^2(\mathbf{R}^6)$ over classical phase space with the inner product: $(\phi|\psi)=\int d^3\vec{p}\,d^3\vec{q}\,\phi^*(\vec{p},\vec{q})\,\psi(\vec{p},\vec{q})$.
(ii) A particle is represented at a given time by a normalized vector ϕ_t in $\mathcal{H}$ called the state of the system.
(iii) An observable $\mathbf{F}$ is a self-adjoint operator on $\mathcal{H}$ and the possible values of this observable are the eigenvalues of $\mathbf{F}$.

Remarks: Orthogonal projectors are special observables with eigenvalues 0 and 1, corresponding to experiments of the true–false type, and by the spectral theorem[25] we know that general observables are related to orthogonal projectors thanks to projection valued measures (pvm).

2. Statistical axioms

(i) A statistical situation is described by a density operator **D** (a positive trace class operator with $\mathrm{Tr}\mathbf{D}=1$); in particular a system in the state ϕ is statistically represented by the density $\mathbf{D}=|\phi\rangle\langle\phi|$.

(ii) The expectation value of an observable **F** is given by $\langle\mathbf{F}\rangle=\mathrm{Tr}(\mathbf{D}.\mathbf{F})$; the standard error ΔF is given by $\Delta F^2=\langle\mathbf{F}^2\rangle-\langle\mathbf{F}\rangle^2$.

3. Collapse axiom

• Let a system be in a situation described by the density **D** and consider a measure of the observable **F** associated with its projection valued measure **P**. Now, assume that a measure of the observable specifies that the numerical outcomes f are in the range $f\in A$, where A is some interval. Then after the experiment, the system is described by the new density operator $\mathbf{D}'$ with

$$\mathbf{D}'=\frac{1}{\mathrm{Tr}(\mathbf{DP}(A))}\mathbf{P}(A)\mathbf{DP}(A). \tag{8}$$

More precisely, if the system is initially in the state $|\phi\rangle$, after the experiment the system is in the state $|\phi'\rangle$:

$$|\phi'\rangle=\frac{1}{\sqrt{\langle\phi|\mathbf{P}(A)|\phi\rangle}}\mathbf{P}(A)|\phi\rangle. \tag{9}$$

This means that after the experiment, the system is in a state that belongs to the subspace of $\mathcal{H}$ associated with the orthogonal projector $\mathbf{P}(A)$.

4. Axiom of evolution

• The evolution of a state ϕ_t is given by a unitary operator $\mathbf{U}_{t_1,t_2}$ such that $\phi_t=\mathbf{U}_{t,t_0}(\phi_{t_0})$.

Now, to specify the situation of classical mechanics, we must add a new axiom of "classicity."

5. Axiom of classicity

• The true physical observables are always "diagonal in the $|\vec{p},\vec{q}\rangle$ basis," and then a classical observable **f** can be written

$$\forall\,\phi\in\mathcal{H},\mathbf{f}(\phi)(\vec{p},\vec{q})=f(\vec{p},\vec{q})\,\phi(\vec{p},\vec{q}), \tag{10}$$

or $\mathbf{f}=f(\vec{\mathbf{p}},\vec{\mathbf{q}})$ as a function of operators.

This axiom is equivalent to the classical hypothesis specifying that all observables are functions of $\vec{p}$ and $\vec{q}$.

Remark: Density operators **D** are not considered as observables, so they do not need to be "diagonal in the $\{|\vec{p},\vec{q}\rangle\}$ basis" (in fact this is impossible for a trace class operator).

Now, we claim that this new mathematical framework constitutes a complete alternative formulation of classical statistical mechanics.

B. Equivalence of the new framework with the standard formalism

1. The mathematical basis of statistical mechanics

Classical statistical mechanics is based on ordinary probability theory[26] that employs a sample space $\mathcal{C}$. An event is a set of sample points, and the events, under the operations on sets form a Boolean algebra. The set $\mathcal{E}$ of events is a σ-field, and a probability law μ on $\mathcal{C}$ is a positive function acting on events as prescribed by the mathematical theory of measure.[27]

In our case, the sample space $\mathcal{C}$ is phase space and a sample point is a state $(\vec{p},\vec{q})$. The set $\mathcal{E}$ of events is given by the family $\mathcal{B}(\mathcal{C})$ of Borel sets in $\mathcal{C}$. Each probability law μ is associated with a positive density $\rho(\vec{p},\vec{q})$ such that $\mu(A)=\int_A \rho d^3\vec{p}\, d^3\vec{q}$.

2. Equivalence of primary axioms

(i) Now let us call Ω the set of orthogonal projectors of $\mathcal{H}=L^2(\mathcal{C})$ and define the mapping Π from the set of events $\mathcal{E}$ to Ω by

$$\forall \phi \in \mathcal{H}, \forall A \in \mathcal{E}, \Pi(A)(\phi)(\vec{p},\vec{q}) = \chi_A(\vec{p},\vec{q})\phi(\vec{p},\vec{q}), \tag{11}$$

where $\chi_A(\vec{p},\vec{q})$ is the characteristic function of the set A.

The family $\{\Pi(A)\}_{A\in\mathcal{E}}$ gives a representation of the Boolean algebra of events in the quantum mathematical framework as an Abelian algebra of orthogonal projectors [and the $\Pi(A)$ become classical observables according to our previous definition].

(ii) In the ordinary formalism a particle is assumed to be represented by a point $(\vec{p},\vec{q})$ at a given time; but as remarked previously, a true physical experiment always has some uncertainty, so the mathematical representation of a physical result is an expectation value associated with some probability density ρ. Of course in principle, ρ can be as close as possible to a "δ," but "δ" is never reached. This means that we can never really know that a particle is at the point $(\vec{p},\vec{q})$. It is much more realistic to say that a single particle is represented by a true (sharp) density ρ. In the language of statistical sets, this means that we look at a single particle as an element of the class of all particles "prepared" in the same way, the preparation being such that the uncertainty on $\vec{p}$ and $\vec{q}$ can be reduced, but cannot be cancelled.

If we start with this new hypothesis, this means that now, a single particle always exhibits some uncertainty. Moreover, this hypothesis allows us to associate to each particle the object $\phi(\vec{p},\vec{q})=\sqrt{\rho(\vec{p},\vec{q})}$ that defines a normalized wave function of $\mathcal{H}$.

This result can also be found using some extremum property. In the ordinary formalism, the one-point sets $\{(\vec{p},\vec{q})\}$ can be seen as the smallest (more precise) events for the ordering relation "$\subset$" on sets. Using the mapping Π on events, we see that $A\subset B \Leftrightarrow \Pi(A)\leqslant\Pi(B)$ where "$\leqslant$" is the inegality between self-adjoint operators. So a new representation of points can be given by using Π directly or using the extremum property. Since the projector associated to a point x is $\Pi(\{x\})=0$, a point x cannot be associated with a true projector, and then we can only use the extremum property to look for the minimal orthogonal projectors. Of course these minimal projectors are given by $|\phi\rangle\langle\phi|$, where ϕ is a normalized vector in $\mathcal{H}$. So we recover that the most precise events are associated with a normalized vector ϕ in $\mathcal{H}$, and then a particle must be described by ϕ. We remark that the real equivalent of the point $(\vec{p},\vec{q})$ is the unbounded state $|\vec{p},\vec{q}\rangle$ or pseudo-projector $|\vec{p},\vec{q}\rangle\langle\vec{p},\vec{q}|$ that cannot be seen as a "true state" in this formalism.

To finish, let us say that we recover through $\rho(\vec{p},\vec{q})=|\phi(\vec{p},\vec{q})|^2$ the idea of "confidence measures" introduced by Prugovecki[6] in order to build the "stochastic phase space."

(iii) Now if we look at observables, each classical quantity $f(\vec{p},\vec{q})$ can be approximated by step functions $\Sigma_i f_i \chi_{A_i}$ where χ_{A_i} are characteristic functions of sets A_i. So we can extend by linearity the mapping Π to lift up any classical observable into its quantum representation as

$$\forall \phi \in \mathcal{H}, \mathbf{f}(\phi)(\vec{p},\vec{q}) = f(\vec{p},\vec{q})\phi(\vec{p},\vec{q}). \tag{12}$$

Of course we recover the "axiom of classicity" and the fact that the possible values of the observable are its eigenvalues.

3. Equivalence of statistical axioms

(i) A probability law on the ordinary framework is given by a mapping μ acting on events following some precise rules. If we look for a mapping μ_Q acting on the representation of events (that is, on orthogonal projectors) with the same rules, a theorem due to Gleason[28] proves that μ_Q

is given by a density operator $\mathbf{D}$ such that $\mu_Q(\Pi(A))=\mathrm{Tr}(\mathbf{D}\cdot\Pi(A))$. This means that we can associate to each classical probability law μ a density operator $\mathbf{D}$ such that $\mu(A)=\mathrm{Tr}(\mathbf{D}\cdot\Pi(A))$. If we develop this formula, we find

$$\mu(A)=\mathrm{Tr}(\mathbf{D}\cdot\Pi(A))=\int_A d^3\vec{p}\,d^3\vec{q}\,\langle\vec{p},\vec{q}|\mathbf{D}|\vec{p},\vec{q}\rangle. \tag{13}$$

So the classical density $\rho(\vec{p},\vec{q})$ is given by the diagonal element $\rho(\vec{p},\vec{q})=\langle\vec{p},\vec{q}|\mathbf{D}|\vec{p},\vec{q}\rangle$ (this quantity is positive since $\mathbf{D}$ is a positive operator).

Now for a particle "in the state ϕ," if we assume that $\mathbf{D}=|\phi\rangle\langle\phi|$, the corresponding classical density ρ is given by

$$\rho(\vec{p},\vec{q})=\langle\vec{p},\vec{q}|\mathbf{D}|\vec{p},\vec{q}\rangle=|\langle\vec{p},\vec{q}|\phi\rangle|^2. \tag{14}$$

So we recover the formula introduced for justifying the existence of states.

(ii) Now, if we use the relation $\rho(\vec{p},\vec{q})=\langle\vec{p},\vec{q}|\mathbf{D}|\vec{p},\vec{q}\rangle$ for computing classical expectation value, we find

$$\langle f\rangle=\int d^3\vec{p}\,d^3\vec{q}\,\rho f=\mathrm{Tr}(\mathbf{D}\cdot\mathbf{f}). \tag{15}$$

Remark: We see that it is impossible to distinguish the statistical effects due to a general density $\mathbf{D}$ from those due to a pure state, because only the diagonal elements $\langle\vec{p},\vec{q}|\mathbf{D}|\vec{p},\vec{q}\rangle$ are relevant in our case: the pure state $\langle\vec{p},\vec{q}|\phi\rangle=\sqrt{\langle\vec{p},\vec{q}|\mathbf{D}|\vec{p},\vec{q}\rangle}$ gives exactly the same results as $\mathbf{D}$ (in our classical framework). So pure states and general densities $\mathbf{D}$ are different on a logical level, but they are physically undistinguishable. Physical results only depend on an equivalence class of densities $\mathbf{D}$ such that $\langle\vec{p},\vec{q}|\mathbf{D}|\vec{p},\vec{q}\rangle=\rho(\vec{p},\vec{q})$ for a given density ρ. We also find this remark in Prugovečki's monograph[6] (p. 154).

4. Equivalence of the collapse axiom with conditional probability

In ordinary probability theory, we use conditional probability to take into account new results to modify a probability law. Namely, if we have a probability law μ and if we know that some event E is realized, the new probability law μ_E is

$$\mu_E(A)=\frac{\mu(A\cap E)}{\mu(E)}. \tag{16}$$

In our case, if μ is associated with a density $\mathbf{D}$, we have

$$\mu_E(A)=\frac{\mathrm{Tr}(\mathbf{D}\cdot\Pi(A\cap E))}{\mathrm{Tr}(\mathbf{D}\cdot\Pi(E))}. \tag{17}$$

If we use the fact that $\Pi(A\cap E)=\Pi(A)\cdot\Pi(E)=\Pi(E)\cdot\Pi(A)$, we find

$$\mu_E(A)=\frac{\mathrm{Tr}(\Pi(E)\cdot\mathbf{D}\cdot\Pi(E)\Pi(A))}{\mathrm{Tr}(\mathbf{D}\cdot\Pi(E))}. \tag{18}$$

If we introduce the operator $\mathbf{D}_E$ defined as

$$\mathbf{D}_E=\frac{1}{\mathrm{Tr}(\mathbf{D}\cdot\Pi(E))}\Pi(E)\cdot\mathbf{D}\cdot\Pi(E), \tag{19}$$

$\mathbf{D}_E$ is a true density operator and $\mu_E(A)=\mathrm{Tr}(\mathbf{D}_E\cdot\Pi(A))$. So $\mathbf{D}_E$ is the density operator associated with μ_E.

So, we find that conditional probability is implemented in the quantum framework with the formula of the ''collapse axiom.'' Now, let us apply this result to the case of some measure of a classical observable $F(\vec{p},\vec{q})$ that specifies that the possible numerical outcomes f belong to a set $V\subset\mathbf{R}$. This means that after the measure, we know that the particle ''is'' in the region $F^{-1}(V)$ of phase space. This means that we know that the event $F^{-1}(V)$ is realized. So the initial probability law μ associated with the density $\mathbf{D}$ must be changed and the new density $\mathbf{D}'$ is

$$\mathbf{D}'=\frac{1}{\mathrm{Tr}(\mathbf{D}\cdot\mathbf{P}(V))}\mathbf{P}(V)\cdot\mathbf{D}\cdot\mathbf{P}(V) \quad \text{with} \quad \mathbf{P}=\Pi\circ F^{-1}. \tag{20}$$

It is not hard to see that $\mathbf{P}=\Pi\circ F^{-1}$ is exactly the projection valued measure associated with the quantum version $\mathbf{F}$ of the classical observable F. This shows that the collapse axiom is (in our case) a translation of conditional probability.

5. Axiom of evolution

We will see in the following that this axiom allows us to recover classical dynamics.

C. Conclusion

This new mathematical framework for classical mechanics is completely equivalent to the ordinary one. But, while the usual framework is mathematically and physically closed (all things that you can write possess a classical meaning), now this new formalism can be extended by removing some axiom, more specially the ''axiom of classicity,'' by assuming that, perhaps, some unclassical observables also have a physical meaning. As we will see later, quantization corresponds to such a process. We finish with some remarks.

(i) Interference effect: Usually, interferences are seen as one of the main consequences of quantum formalism. We want to point out that they cannot be observed in our case, thanks to our ''axiom of classicity.'' Actually, to see interferences, we need at least two physical observables that are not diagonal in the same basis, and this case is excluded by our axiom. This can be seen also by the fact that pure states cannot be distinguished from general densities.

(ii) Delocalization of states: We have introduced the state ϕ that describes a particle by assuming that $\rho(\vec{p},\vec{q})=|\langle\vec{p},\vec{q}|\phi\rangle|^2$ is a sharp density in phase space. But nothing forbids ϕ to be very delocalized, and, in principle, we must look at this delocalization as being intrinsic (not due to a lack of information as in the case of a general density $\mathbf{D}$). So the question that arises is: why do classical objects have to be described in practice with only very sharp densities? The answer to this question is contained in our previous remark on the physical impossibility (in this framework) to distinguish states from general densities (the physical effects of a density can always be represented by a state). So, it is only a matter of convenience (and consistency) to decide that ''true states'' correspond to very small delocalization. Of course, it must also be possible to develop some argumentation based on ''decoherence.''

(iii) Equivalence-class of densities: We have seen that physical results only depend on some equivalence class of densities $\mathbf{D}$. At first sight, this can be thought as a weakness of our formalism, since this introduces some degeneracy into the representation. But this is in fact a richness of the formalism, because breaking the degeneracy we can recover quantum mechanics.

(iv) Local $U(1)$ invariance: Since the computation of any physical quantity only depends on $\rho(\vec{p},\vec{q})=|\langle\vec{p},\vec{q}|\phi\rangle|^2$, we can modify the state $\phi(\vec{p},\vec{q})$ by any phase factor $\exp(i\,\theta(\vec{p},\vec{q}))$ without changing physical results.

Now, we can analyze how the classical structure of Poisson brackets can be implemented in this new framework, and how we can recover classical dynamics.

IV. REPRESENTATION OF POISSON BRACKETS IN THE NEW FRAMEWORK

Let $f(\vec{p},\vec{q})$ be an observable (real function). We associate to f a self-adjoint operator $\mathbf{X}_f$ acting on states $\phi \in \mathcal{H}$ by

$$\mathbf{X}_f \phi = -i\{f,\phi\}. \tag{21}$$

Here $\mathbf{X}_f$ defines a generator of a one-parameter unitary group $\mathbf{U}_\alpha$ with

$$\mathbf{U}_\alpha = \exp[-i\alpha \mathbf{X}_f]. \tag{22}$$

Furthermore, if we define the state $|\phi_\alpha\rangle = \mathbf{U}_\alpha |\phi\rangle$, we have

$$i\frac{\partial}{\partial \alpha}|\phi_\alpha\rangle = \mathbf{X}_f|\phi_\alpha\rangle \quad \text{or} \quad \frac{\partial}{\partial \alpha}\phi_\alpha = -\{f,\phi_\alpha\}. \tag{23}$$

Now it is obvious that $\mathbf{U}_\alpha$ acts on unbounded states $|\vec{p},\vec{q}\rangle$ exactly as the classical transformation (3):

$$\mathbf{U}_\alpha |\vec{p},\vec{q}\rangle = |\vec{p_\alpha},\vec{q_\alpha}\rangle, \tag{24}$$

where $(\vec{p_\alpha},\vec{q_\alpha})$ is the trajectory with initial conditions $(\vec{p},\vec{q})$.

So $\mathbf{U}_\alpha$ maps states into states.

For a classical observable g, and the associated operator $\mathbf{g}$, the transformed operator $\mathbf{g}_\alpha$ is $\mathbf{U}_\alpha^\dagger \mathbf{g} \mathbf{U}_\alpha$.

Due to (24), $\mathbf{g}_\alpha$ is also a self-adjoint operator associated with a classical observable g_α and

$$\frac{\partial}{\partial \alpha}\mathbf{g}_\alpha = i[\mathbf{X}_f,\mathbf{g}_\alpha] \quad \text{or} \quad \frac{\partial}{\partial \alpha} g_\alpha = \{f,g_\alpha\}. \tag{25}$$

Moreover, the commutator $[\mathbf{X}_f,\mathbf{X}_g]$ of two operators $\mathbf{X}_f$ and $\mathbf{X}_g$ is given by

$$i[\mathbf{X}_f,\mathbf{X}_g] = \mathbf{X}_{\{f,g\}}. \tag{26}$$

So the linear mapping $f \to \mathbf{X}_f$ is a representation of the action induced by f through Poisson brackets. The equation (26) shows that $i[\cdot,\cdot]$ is a representation of $\{\cdot,\cdot\}$.

Nevertheless, since $\mathbf{X}_f = 0$ for $f = \text{const}$, we cannot recover the special value $\{p_i,q_j\} = \delta_{ij}$.

Remark on the "active" and "passive" representations of observables: From general quantum axiomatics, each $\mathbf{X}_f$ as a self-adjoint operator defines mathematically a possible observable (even if physically $\mathbf{X}_f$ is not a classical object because of our axiom of classicity). Then, on a purely mathematical point of view, we have two possible self-adjoint operators deducible from the classical quantity $f(x)$:

(i) $\mathbf{f} = \int dx\ f(x)|x\rangle\langle x|$,
(ii) $\mathbf{X}_f$.

Here $\mathbf{f}$ defines the observable as a ''passive object,'' which is a datum, while $\mathbf{X}_f$ is the ''active version'' of f as the action induced by f through Poisson brackets. Moreover $\mathbf{f}$ and $\mathbf{X}_f$ are independent, because $[\mathbf{f},\mathbf{X}_f] = 0$.

Then, while in the ''passive representation,'' all classical observables $\mathbf{f}$ commute; in the ''active representation'' commutators are related to Poisson brackets [Eq. (26)].

So, from the mathematical point of view, $\mathbf{X}_f$ is an alternative representation of the classical quantity $f(x)$. Unfortunately, on a physical level, $\mathbf{f}$ and $\mathbf{X}_f$ do not have the same homogeneity: $\mathbf{X}_f$ is homogeneous to $\mathbf{f}$ divided by an action. So, as long as we do not have a specific unit of action, we cannot follow up this process.

To end this remark, we want to indicate that this idea of representing classical observables by a pair of operators has already been used by George and Prigogine[29] using the superoperator formalism.

V. CLASSICAL DYNAMICS IN THE NEW FRAMEWORK

A. New formulation of equations of motion

From the general axioms, we know that the evolution of states is given by the unitary operators $\mathbf{U}_{t,t_0}$ such that $\phi_t=\mathbf{U}_{t,t_0}(\phi_{t_0})$. Moreover, Sec. II B 1 specifies that dynamics is defined by the data of the classical Hamiltonian H (eventually time dependent), and we have seen in Secs. II B 2 and 3 that ''weak dynamical equations'' (7) are a more general formula to specify dynamics. So, we assume in the following that Eqs. (7) are our basic equations of motion.

Since we have seen in Sec. III B 3 the equivalence between quantum and classical formula for expectation values of classical observables using the classical density $\rho(\vec{p},\vec{q},t)=|\langle\vec{p},\vec{q}|\phi_t\rangle|^2$, equations (7) can be written

$$\frac{d}{dt}\langle\phi_t|\vec{\mathbf{q}}|\phi_t\rangle=\langle\phi_t|\overrightarrow{\nabla}_p H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)|\phi_t\rangle,$$

$$\frac{d}{dt}\langle\phi_t|\vec{\mathbf{p}}|\phi_t\rangle=-\langle\phi_t|\overrightarrow{\nabla}_q H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)|\phi_t\rangle, \tag{27}$$

where $\overrightarrow{\nabla}_p H$ and $\overrightarrow{\nabla}_q H$ can be seen as functions of the operators $\vec{\mathbf{p}}$ and $\vec{\mathbf{q}}$, since $\vec{\mathbf{p}}$ and $\vec{\mathbf{q}}$ commute.

Equations (27) are our new basic dynamical equations.

B. Classical dynamics

1. Primary equations

Any operator $\mathbf{f}$ associated with the classical observable $f(\vec{p},\vec{q})$ can be written as $\mathbf{f}=f(\vec{\mathbf{p}},\vec{\mathbf{q}})$, since $\vec{\mathbf{p}}$ and $\vec{\mathbf{q}}$ commute. So the expectation value $\langle\mathbf{f}\rangle_t$ verifies

$$\langle\mathbf{f}\rangle_t=\langle\phi_t|f(\vec{\mathbf{p}},\vec{\mathbf{q}})|\phi_t\rangle=\langle\phi_0|f(U^\dagger_{t,t_0}\vec{\mathbf{p}}U_{t,t_0},U^\dagger_{t,t_0}\vec{\mathbf{q}}U_{t,t_0})|\phi_0\rangle. \tag{28}$$

Now we introduce the operators $\vec{\mathbf{q}}(t)$ and $\vec{\mathbf{p}}(t)$ defined as

$$\begin{aligned}\vec{\mathbf{q}}(t)&=U^\dagger_{t,t_0}\vec{\mathbf{q}}U_{t,t_0},\\ \vec{\mathbf{p}}(t)&=U^\dagger_{t,t_0}\vec{\mathbf{p}}U_{t,t_0}.\end{aligned} \tag{29}$$

Equations for expectation values (27) become

$$\begin{aligned}\langle\phi_0|\frac{d}{dt}\vec{\mathbf{q}}(t)|\phi_0\rangle&=\langle\phi_0|\overrightarrow{\nabla}_p H(\vec{\mathbf{p}}(t),\vec{\mathbf{q}}(t),t)|\phi_0\rangle,\\ \langle\phi_0|\frac{d}{dt}\vec{\mathbf{p}}(t)|\phi_0\rangle&=-\langle\phi_0|\overrightarrow{\nabla}_q H(\vec{\mathbf{p}}(t),\vec{\mathbf{q}}(t),t)|\phi_0\rangle.\end{aligned} \tag{30}$$

Since Eqs. (30) **must be valid for any state** ϕ_0, we deduce the following equations of evolution for the operators $\vec{\mathbf{q}}(t)$ and $\vec{\mathbf{p}}(t)$:

$$\begin{aligned}\frac{d}{dt}\vec{\mathbf{q}}(t)&=\overrightarrow{\nabla}_p H(\vec{\mathbf{p}}(t),\vec{\mathbf{q}}(t),t),\\ \frac{d}{dt}\vec{\mathbf{p}}(t)&=-\overrightarrow{\nabla}_q H(\vec{\mathbf{p}}(t),\vec{\mathbf{q}}(t),t),\end{aligned} \tag{31}$$

which are the natural formulation of the equations of motion in the new framework, and they can be symbolically identified with the Hamiltonian equations (4).

2. Operator of evolution and Liouville equation

Now if we look at the operator $\mathbf{X}_H(t)$ as defined in Sec. III C,

$$\mathbf{X}_H(t) = -i(\overrightarrow{\nabla}_p H \cdot \overrightarrow{\nabla}_q - \overrightarrow{\nabla}_q H \cdot \overrightarrow{\nabla}_p). \tag{32}$$

We have

$$\begin{aligned} [\mathbf{X}_H(t), \vec{\mathbf{q}}] &= -i\overrightarrow{\nabla}_p H(\vec{\mathbf{p}}, \vec{\mathbf{q}}, t), \\ [\mathbf{X}_H(t), \vec{\mathbf{p}}] &= i\overrightarrow{\nabla}_q H(\vec{\mathbf{p}}, \vec{\mathbf{q}}, t). \end{aligned} \tag{33}$$

Let us define $\mathbf{U}_{t,t_0}$ as the unitary operator generated by $\mathbf{X}_H(t)$:

$$\begin{aligned} i\frac{d}{dt}\mathbf{U}_{t,t_0} &= \mathbf{X}_H(t)\mathbf{U}_{t,t_0}, \\ \mathbf{U}_{t_0,t_0} &= \mathbf{1}. \end{aligned} \tag{34}$$

A simple checking shows that now the operators $\vec{\mathbf{q}}(t)$ and $\vec{\mathbf{p}}(t)$ defined by (29) verify Eqs. (31) and then $\mathbf{U}_{t,t_0}$ is the operator of evolution. We deduce that for any state ϕ_0 at time t_0 we have

$$\phi(t) = \mathbf{U}_{t,t_0}(\phi_0). \tag{35}$$

Then using the definition of $\mathbf{U}_{t,t_0}$, the wave function $\phi(\vec{p},\vec{q},t)$ verifies the Liouville equation:

$$\frac{\partial \phi}{\partial t} = -\{H, \phi\}. \tag{36}$$

Because this differential equation is of order one with real coefficients, we recover that the probability density $\rho(\vec{p},\vec{q},t) = |\phi(\vec{p},\vec{q},t)|^2$ must also verify the Liouville equation. Now, since any density operator $\mathbf{D}$ can be split as $\mathbf{D} = \Sigma_n p_n |\phi_n\rangle\langle\phi_n|$, we recover that any classical density $\rho(\vec{p},\vec{q},t) = \langle \vec{p},\vec{q}|D_t|\vec{p},\vec{q}\rangle$ must verify also the Liouville equation. Prugovečki also finds equation (36) in his monograph Ref. 6, (Chap. 3) for a ''classical wave function,'' but our procedure based on ''weak dynamical equations'' is completely different.

We see that starting only from equations for expectation values, and even if ''δ'' densities are excluded, we recover completely the equations of standard classical mechanics. This result is due to the fact that we can find densities as close as possible to ''δ.''

VI. THE QUANTIZATION PROCESS

A. The problem of unclassical observables: What is quantization?

Our framework of classical mechanics is based on the ''axiom of classicity'' that limits the range of physical observables. We analyze here the possibility of giving a physical meaning to some unclassical observable (and then breaking down our axiom).

The starting point of our procedure is the representation of classical events given by our mapping Π. As we can verify easily, for each classical event ''A'' that gives a nonzero projector $\Pi(A)$, $\Pi(A)$ corresponds in fact to an infinite dimensional subspace of $\mathcal{H}$. This means that the one-dimensional projectors $\boldsymbol{\pi}_\phi = |\phi\rangle\langle\phi|$ that represent the ''minimal events'' and define states are not classical events. Since we only possess the projectors $\Pi(A)$ to select particles, we can never decide if a particle is in a given state ϕ (this is because we cannot distinguish states from general densities). So in this classical picture, a particle is described by a mathematical object that cannot be completely specified from experiment (exactly as points in phase space that cannot be experi-

mently reached). But this means that we cannot specify any more what is really the full space $\mathcal{S}$ of all ϕ. So we can imagine two different situations:

(i) The space $\mathcal{S}=\mathcal{H}$, and then all states are possible.
(ii) The space $\mathcal{S}$ is only a proper subspace of $\mathcal{H}$.

In the latter case, we can define the orthogonal projector $\boldsymbol{\pi}_{\mathcal{S}}$ on $\mathcal{S}$. By definition $\boldsymbol{\pi}_{\mathcal{S}}$ cannot be a classical event, but nevertheless $\boldsymbol{\pi}_{\mathcal{S}}$ has a physical meaning as the projector on all physical states. So we can give a physical meaning to an unclassical object and, moreover this ''unclassical event'' must always be realized since all physical states ϕ must verify $\boldsymbol{\pi}_{\mathcal{S}}\phi=\phi$.

Another way to present the problem is to look at the full set of orthogonal projectors as the set of all symbolic logical questions on a system. In the framework of classical mechanics, only a subset of questions [the projectors $\Pi(A)$] possesses a physical answer (true or false). The remainder must be either unphysical questions, or *undecidable* questions. The ''question $\boldsymbol{\pi}_{\mathcal{S}}$'' is undecidable.

So we have the opportunity of ''creating'' a new logical framework by postulating that some ''question $\boldsymbol{\pi}_{\mathcal{S}}$'' has a positive answer. Of course, we need physical arguments to choose $\boldsymbol{\pi}_{\mathcal{S}}$ in order to preserve basic physical results. In our point of view, quantization corresponds to this kind of postulate.

In the following, we assume that some proper subspace $\mathcal{S}$ of $\mathcal{H}$ (represented by $\boldsymbol{\pi}_{\mathcal{S}}$) contains all possible states.

We analyze first the consequences of this postulate and then we give the arguments to choose $\boldsymbol{\pi}_{\mathcal{S}}$.

B. Consequences of a quantization

Of course, we must assume that all general axioms listed in Secs. III A 1–4 are always valid, but on the Hilbert space $\mathcal{S}$. Moreover, we must analyze separately how to take into account our axiom of classicity.

First of all, since the basic objects of our formalism are now operators on $\mathcal{S}$ which is a subspace of $\mathcal{H}$, we want to specify the relation between self-adjoint operators on $\mathcal{H}$ and self-adjoint operators on $\mathcal{S}$. Since $\boldsymbol{\pi}_{\mathcal{S}}$ is a projector, a self-adjoint operator $\mathbf{a}$ on $\mathcal{H}$ corresponds to a self-adjoint operator on $\mathcal{S}$ if and only if

$$\boldsymbol{\pi}_{\mathcal{S}}\cdot\mathbf{a}\cdot\boldsymbol{\pi}_{\mathcal{S}}=\mathbf{a}. \tag{37}$$

So this relation (37) must now be verified for both observables and densities. Now we analyze how classical observables are modified.

1. The "correspondence principle"

Let f be a classical observable and $\mathbf{f}=\int f(x)|x\rangle\langle x|dx$ be the corresponding operator. For any density $\mathbf{D}$, we have seen that the expectation value of f is given by $\langle f\rangle=\mathrm{Tr}(\mathbf{D}\cdot\mathbf{f})$. But now the only possible densities verify Eq. (37) and then $\langle f\rangle$ can be written as $\langle f\rangle=\mathrm{Tr}(\mathbf{D}\cdot\boldsymbol{\pi}_{\mathcal{S}}\cdot\mathbf{f}\cdot\boldsymbol{\pi}_{\mathcal{S}})$. So in any physical situation, we only need the self-adjoint operator $\mathbf{f}_{\mathcal{S}}=\pi_{\mathcal{S}}\mathbf{f}\pi_{\mathcal{S}}$, and by construction $\mathbf{f}_{\mathcal{S}}$ defines a true observable on the physical Hilbert space $\mathcal{S}$.

So it is natural to assume that the operator $\mathbf{f}_{\mathcal{S}}=\boldsymbol{\pi}_{\mathcal{S}}\cdot\mathbf{f}\cdot\boldsymbol{\pi}_{\mathcal{S}}$ *defines the new version of the classical observable* **f:** *we call* $\mathbf{f}_{\mathcal{S}}$ *the quantized observable associated with* **f**.

This allows us to justify and not to postulate the famous ''correspondence principle'' that gives quantized version of classical observable. We will see later that *almost* all these quantized observables correspond effectively to the usual quantum operators.

2. Remarks on quantized observables

Of course, the simplest quantized observables are $\boldsymbol{\pi}_{\mathcal{S}}\vec{\mathbf{p}}\boldsymbol{\pi}_{\mathcal{S}}$ and $\boldsymbol{\pi}_{\mathcal{S}}\vec{\mathbf{q}}\boldsymbol{\pi}_{\mathcal{S}}$. Since $\vec{\mathbf{p}}$ and $\vec{\mathbf{q}}$ are the basic objects of our classical framework, $\boldsymbol{\pi}_{\mathcal{S}}\vec{\mathbf{p}}\boldsymbol{\pi}_{\mathcal{S}}$ and $\boldsymbol{\pi}_{\mathcal{S}}\vec{\mathbf{q}}\boldsymbol{\pi}_{\mathcal{S}}$ must become the new fundamental observables; and these new operators do not commute in general.

In the case of more complex classical observables, some ambiguity may exist in the definition of the quantized version.

For example, if we look at the quantized observable $\vec{\mathbf{L}}$ associated with the classical orbital momentum $\vec{l}=\vec{p}\wedge\vec{q}$, we can say that $\vec{\mathbf{L}}=\overrightarrow{\mathbf{L_1}}=\boldsymbol{\pi}_{\mathcal{S}}\vec{\mathbf{p}}\wedge\vec{\mathbf{q}}\boldsymbol{\pi}_{\mathcal{S}}$ according to our procedure, but we can also define $\vec{\mathbf{L}}=\overrightarrow{\mathbf{L}_2}=1/2(\boldsymbol{\pi}_{\mathcal{S}}\vec{\mathbf{p}}\boldsymbol{\pi}_{\mathcal{S}}\wedge\boldsymbol{\pi}_{\mathcal{S}}\vec{\mathbf{q}}\boldsymbol{\pi}_{\mathcal{S}}-\boldsymbol{\pi}_{\mathcal{S}}\vec{\mathbf{q}}\boldsymbol{\pi}_{\mathcal{S}}\wedge\boldsymbol{\pi}_{\mathcal{S}}\vec{\mathbf{p}}\boldsymbol{\pi}_{\mathcal{S}})$. In both cases we have a well-defined self-adjoint operator, and then a possible observable associated with the classical quantity $\vec{l}$ (in general $\overrightarrow{\mathbf{L_1}}$ and $\overrightarrow{\mathbf{L_2}}$ define two different operators). Of course only $\overrightarrow{\mathbf{L_1}}$ is a direct quantization (according to our procedure); but it is not sufficient to prove that $\overrightarrow{\mathbf{L_1}}$ is the right answer, because orbital momentum is classically the generator of rotations and we can demand that this general physical property remains unchanged. This means that, for complex observables, we need generally some external arguments on the physical role played by the observable (for example, as generator of symmetry) to decide which is the right quantized object. We will see in Sec. X B, precisely in the case of $\vec{l}=\vec{p}\wedge\vec{q}$, that we must examine carefully different possible observables to deduce the right one.

3. Quantization of classical events

As seen before, classical events are represented by the projectors $\Pi(A)$. Our quantization transforms $\Pi(A)$ into $\Pi_{\mathcal{S}}(A)=\boldsymbol{\pi}_{\mathcal{S}}\Pi(A)\boldsymbol{\pi}_{\mathcal{S}}$. But now $\Pi_{\mathcal{S}}(A)$ is no longer an orthogonal projector and cannot be associated with a ''true-false type question.'' $\Pi_{\mathcal{S}}(A)$ must be interpreted as a ''semi-classical event'' or as a quasiprojector. This label becomes more obvious if we remark that

$$\Pi_{\mathcal{S}}(A)=\int_A d^3\vec{p}\,d^3\vec{q}\,\boldsymbol{\pi}_{\mathcal{S}}|\vec{p},\vec{q}\rangle\langle\vec{p},\vec{q}|\,\boldsymbol{\pi}_{\mathcal{S}}, \tag{38}$$

while

$$\mathbf{1}_{\mathcal{S}}=\boldsymbol{\pi}_{\mathcal{S}}=\int d^3\vec{p}\,d^3\vec{q}\,\boldsymbol{\pi}_{\mathcal{S}}|\vec{p},\vec{q}\rangle\langle\vec{p},\vec{q}|\,\boldsymbol{\pi}_{\mathcal{S}}. \tag{39}$$

The states $\{|\xi_{\vec{p},\vec{q}}\rangle=\boldsymbol{\pi}_{\mathcal{S}}|\vec{p},\vec{q}\rangle\}$ are no longer a ''continuous orthogonal basis,'' but they verify the previous closure relation on the physical Hilbert space $\mathcal{S}$. So, these states define in fact an overcomplete basis and can be seen as ''semi-classical states.'' In Sec. XI, we detail this point in direct connection with Prugovečki's work.

Now, we can analyze what kind of arguments can be used to specify the projector $\boldsymbol{\pi}_{\mathcal{S}}$.

C. Our arguments to choose a quantization

Our arguments for quantization are based on the physical existence of a fundamental group of transformations acting on phase space, namely the symmetry group. As indicated in Sec. II C, the symmetry group is the Galilei group G (up to some discrete transformations). So we look for a representation of the group G on the Hilbert space $\mathcal{H}$ in such a way that classical objects are always transformed in the same way.

1. How to represent the Galilei group

Classically an observable $f(\vec{p},\vec{q})$ is transformed into $f_u=f\circ u^{-1}$ in a symmetry $u\in G$. Now, the operator associated with f_u is

$$\mathbf{f}_u=\int d^3\vec{p}\,d^3\vec{q}\,(f\circ u^{-1})(\vec{p},\vec{q})|\vec{p},\vec{q}\rangle\langle\vec{p},\vec{q}|. \tag{40}$$

Since any symmetry u preserves the element of volume in phase space, we have

$$\mathbf{f}_u=\int d^3\vec{p}\,d^3\vec{q}\,f(\vec{p},\vec{q})|u(\vec{p},\vec{q})\rangle\langle u(\vec{p},\vec{q})|. \tag{41}$$

Then we can write

$$\mathbf{f}_u = \mathbf{T}_u \cdot \mathbf{f} \cdot \mathbf{T}_u^{\dagger} \tag{42}$$

if we define the action of the operator $\mathbf{T}_u$ on $\mathcal{H}$ as

$$\mathbf{T}_u |\vec{p},\vec{q}\rangle = \exp(i\theta_u(\vec{p},\vec{q}))|u(\vec{p},\vec{q})\rangle, \tag{43}$$

where $\theta_u(\vec{p},\vec{q})$ is an unspecified phase factor [in fact we use the local $U(1)$ invariance].

This means that any projective representation of G preserves classical properties. Of course the choice $\theta_u = 0$ gives a right representation, but this solution is not necessarily the unique one. Moreover, if there exist different nonequivalent representations, we have to make a choice: if this picture is really the right mathematical framework, we must say that only one of these representations is realized.

In the following, we assume that this choice has been done, and then the functions θ_u are specified.

Now, we are ready to develop our arguments for quantization.

2. Arguments for quantization

We remark first that "*phase space is connected by symmetries*": given two points x_0 and x_1 in phase space, we can always find some symmetry $u \in G$ such that $x_1 = u(x_0)$ (the group G is transitive). So, starting from any point x_0, the action of the full symmetry group G generates phase space. This means that the set of physical states is generated by the symmetry group: to specify dynamical properties of a particle, we do not need a larger space than a space generated by G.

Now in the new framework, the points x of phase space are used to build the "continuous orthogonal basis" $\{|x\rangle\}$, so this complete orthogonal basis of $\mathcal{H}$ is generated by the action G (or its representation) on some ket $|x_0\rangle$. But, in general, we can build other (orthogonal) bases with this property: we can find orthogonal basis $\{|y,n\rangle\}$ (where y specifies continuous variables and n is an integer parameter) such that the action of the representation $\{\mathbf{T}_u\}$ on some ket $|y_0,n\rangle$ generates the full set $\{|y,n\rangle\}$ for a fixed n. So each subspace $\mathcal{H}_n$ associated with the projector $\Pi_n = \int dy |y,n\rangle\langle y,n|$ possesses exactly the same property as the initial Hilbert space $\mathcal{H}$. Moreover, two states ϕ_0 and ϕ_1 belonging to two different subspaces $\mathcal{H}_{n_0}$ and $\mathcal{H}_{n_1}$ can never be connected by a symmetry $\mathbf{T}_u$. So it is logical to assume that only one of these subspaces $\mathcal{H}_n$ is sufficient to specify the dynamical properties of a particle.

3. Conclusion

If we demand that the Hilbert space of states verifies the same property as classical phase space, then it is sufficient to assume that the physical Hilbert space $\mathcal{S}$ is a subspace of irreducible representation of the $\{\mathbf{T}_u\}$: this specifies our quantization.

So, logically, we must first analyze all possible projective representations of the Galilei group, before looking for quantization. Nevertheless, since in this article we want to focus on the "right choice," we only develop in the following paragraphs the intuitive arguments leading to the "right" representation compatible with quantum mechanics (there is no mathematical reason to choose this special representation).

VII. REPRESENTATIONS OF THE GALILEI GROUP

The quantum phase space representation of the Galilei group developed in this section can be found in Prugovečki's monograph (Ref. 6 Chap. 1). This representation has been obtained in the context of positive operator value (POV) measures that constitute a "system of covariance" for the Galilei group, and the method was originally developed in the configuration representation.[30]

But, as indicated at the end of the last section, we have no mathematical reason to choose a special representation, starting from our point of view. So we will prove in the following that

assuming the physical existence of some "unit of action" implies the existence of some new symmetry with no classical equivalent, and taking into account this new symmetry, we can guess the representation we look for.

To begin, we look first at the classical situation corresponding to a cancellation of all the coefficients $\theta_u(x)$ introduced in Sec. VI.

A. The classical representation

We can use the generators $\mathbf{X}_f$ induced by Poisson brackets (Sec. IV) to build this classical representation of the Galilei group.

The continuous transformations of the group are space translations, Galilei boosts and rotations that are respectively associated with the observables $\vec{p}$, $\vec{q}$ and $\vec{l}=\vec{q}\wedge\vec{p}$. Namely, using the notations of Sec. IV,

$$\begin{aligned}\exp[-i\vec{q_0}\cdot\mathbf{X}_{\vec{p}}]|\vec{p},\vec{q}\rangle&=|\vec{p},\vec{q}+\vec{q_0}\rangle,\\ \exp[i\vec{p_0}\cdot\mathbf{X}_{\vec{q}}]|\vec{p},\vec{q}\rangle&=|\vec{p}+\vec{p_0},\vec{q}\rangle,\\ \exp[-i\vec{\omega}\cdot\mathbf{X}_{\vec{l}}]|\vec{p},\vec{q}\rangle&=|\mathcal{R}_{\vec{\omega}}(\vec{p}),\mathcal{R}_{\vec{\omega}}(\vec{q})\rangle,\end{aligned}\tag{44}$$

where $\mathcal{R}_{\vec{\omega}}$ is the geometrical rotation.

B. First consequences of a unit of action

In the remainder, we assume that there exists some natural unit of action, namely, the Planck constant h (or the reduced value $\hbar=h/2\pi$), and we are interested in the consequences of this hypothesis for the objects defined on $\mathcal{H}$.

1. New physical symmetry: The symplectic transform

Taking into account the data of $\hbar$, we can define a set of linear operators $\{\mathbf{K}_S(\alpha)\}_{\alpha\in\mathbf{R}}$ (symplectic involutions) depending on the undimensional real parameter α by

$$\langle\vec{p},\vec{q}|\mathbf{K}_S(\alpha)|\vec{p_1},\vec{q_1}\rangle=(\alpha/h)^3\exp[(i\alpha/\hbar)(\vec{q}\cdot\vec{p_1}-\vec{p}\cdot\vec{q_1})].\tag{45}$$

A simple checking proves that

$$\mathbf{K}_S^\dagger(\alpha)=\mathbf{K}_S(\alpha)\quad\text{and}\quad\mathbf{K}_S(\alpha)^2=\mathbf{1}_{\mathcal{H}}.\tag{46}$$

So each $\mathbf{K}_S(\alpha)$ is a self-adjoint unitary operator, that is, an involution, and $\mathbf{K}_S(\alpha)$ depends on the symplectic product $\vec{q}\cdot\vec{p_1}-\vec{p}\cdot\vec{q_1}$.

On the other hand, we can also define the unitary gauge transforms $\mathbf{U}_G(\xi)$ depending on the undimensional real parameter ξ as

$$\mathbf{U}_G(\xi)|\vec{p},\vec{q}\rangle=\exp[-(i\xi/\hbar)\vec{p}\cdot\vec{q}]|\vec{p},\vec{q}\rangle,\tag{47}$$

or

$$\mathbf{U}_G(\xi)=\exp[-(i\xi/\hbar)\vec{\mathbf{p}}\cdot\vec{\mathbf{q}}].\tag{48}$$

These operators $\mathbf{K}_S(\alpha)$ and $\mathbf{U}_G(\xi)$ are the simplest "new symmetries" induced by the existence of $\hbar$.

Combining $\mathbf{K}_S(\alpha)$ and $\mathbf{U}_G(\xi)$, we extend the set $\{\mathbf{K}_S(\alpha)\}_{\alpha\in\mathbf{R}}$ of involutions (unitary self-adjoint operators) to $\{\mathbf{K}_S(\alpha,\xi)\}_{(\alpha,\xi)\in\mathbf{R}^2}$ with

$$\mathbf{K}_S(\alpha,\xi)=\mathbf{U}_G(\xi)^\dagger\mathbf{K}_S(\alpha)\mathbf{U}_G(\xi).\tag{49}$$

Now, each $\mathbf{K}_S(\alpha,\xi)$ is mathematically a new symmetry. But is it really possible that different nonequivalent $\mathbf{K}_S(\alpha,\xi)$ physically exist at the same time?

In fact, we see that modifying α and ξ corresponds to a scaling on $\hbar$. If we say that there exists a **unique** unit of action, only one of these $\mathbf{K}_S(\alpha,\xi)$ must be taken as fundamental. Of course, this is not sufficient to specify the value of α and ξ, so we have to make a choice.

a. Conclusion. We postulate in all the following that **the fundamental symplectic transform** is $\mathbf{K}_S$ defined as

$$\mathbf{K}_S=\mathbf{K}_S(\tfrac{1}{2},\tfrac{1}{2}) \tag{50}$$

or

$$\langle\vec{p},\vec{q}|\mathbf{K}_S|\vec{p_1},\vec{q_1}\rangle=(1/2h)^3\exp[(i/2\hbar)(\vec{q}-\vec{q_1})\cdot(\vec{p}+\vec{p_1})]. \tag{51}$$

(Of course this choice contains some arbitrariness due to other possible unitary equivalent possibilities.)

Now, $\mathbf{K}_S$ must be seen as a new physical symmetry (unclassical) induced by the existence of "h," and then it must be added to the Galilei group.

2. "Passive" and "active" representations of observables

We have seen in Sec. IV that we can mathematically associate to each classical observable f two self-adjoint operators $\mathbf{f}$ and $\mathbf{X}_f$, $\mathbf{X}_f$ being homogeneous to f divided by an action.

So $\mathbf{f}$ and $\hbar\mathbf{X}_f$ are now two possible representations of f with the same physical homogeneity, but $\hbar\mathbf{X}_f$ is a nonclassical observable. Moreover, $\mathbf{f}$ and $\hbar\mathbf{X}_f$ are independent since $[\mathbf{f},\hbar\mathbf{X}_f]=0$. Then, introducing $\hbar$ generates some apparent mathematical ambiguity into the representation of observables: each observable can be defined as a datum or as a generator of a one-parameter group.

We will see in the remainder that our procedure of quantization allows us to remove this ambiguity.

C. New representation of the Galilei group

Now, we consider $\mathbf{K}_S$ as a new physical symmetry, but without any classical equivalent. So it is natural to assume that $\mathbf{K}_S$ does not interfere with the unitary operators $\mathbf{U}_\beta$ that represent the Galilei group, in other words $[\mathbf{K}_S,\mathbf{U}_\beta]=0$. This means that the (self-adjoint) generators $\mathbf{Y}\alpha$ of the Galilei group must verify $[\mathbf{K}_S,\mathbf{Y}\alpha]=0$. Since $\mathbf{K}_S$ is an involution, this last requirement can be written as

$$\mathbf{K}_S\mathbf{Y}\alpha\mathbf{K}_S=\mathbf{Y}\alpha \quad\text{or}\quad \mathbf{Y}\alpha=\tfrac{1}{2}(\mathbf{Y}\alpha+\mathbf{K}_S\mathbf{Y}\alpha\mathbf{K}_S). \tag{52}$$

Now, as seen in Sec. VII A, the classical generators of the Galilei group are $\mathbf{X}_{\vec{p}}=-i\overrightarrow{\nabla}_q$, $\mathbf{X}_{\vec{q}}=i\overrightarrow{\nabla}_p$ and $\mathbf{X}_{\vec{q}\wedge\vec{p}}=(-i)(\vec{q}\wedge\overrightarrow{\nabla}_q+\vec{p}\wedge\overrightarrow{\nabla}_p)$. Using (51) and the fact that $\mathbf{K}_S$ is an involution, we find, after some algebra,

$$\begin{aligned}
\mathbf{K}_S\mathbf{X}_{\vec{p}}\mathbf{K}_S&=(1/2\hbar)(\vec{\mathbf{p}}+\mathbf{K}_S\vec{\mathbf{p}}\mathbf{K}_S)=\mathbf{X}_{\vec{p}},\\
\mathbf{K}_S\mathbf{X}_{\vec{q}}\mathbf{K}_S&=(1/2\hbar)(\vec{\mathbf{q}}-\mathbf{K}_S\vec{\mathbf{q}}\mathbf{K}_S)=-\mathbf{X}_{\vec{q}},\\
\mathbf{K}_S\mathbf{X}_{\vec{q}\wedge\vec{p}}\mathbf{K}_S&=\mathbf{X}_{\vec{q}\wedge\vec{p}}.
\end{aligned} \tag{53}$$

So, $\mathbf{X}_{\vec{p}}$ and $\mathbf{X}_{\vec{q}\wedge\vec{p}}$ (generators of translation and rotations) are effectively invariant under $\mathbf{K}_S$, but not $\mathbf{X}_{\vec{q}}$ (generator of Galilei boosts). So we must modify $\mathbf{X}_{\vec{q}}$ and we define the new generator $\mathbf{X}^{(1)}_{\vec{q}}$ of Galilei boosts as

$$\mathbf{X}_{\vec{q}}^{(1)}=(1/2\hbar)(\vec{\mathbf{q}}+\mathbf{K}_S\vec{\mathbf{q}}\mathbf{K}_S)=\hbar^{-1}\vec{\mathbf{q}}+\mathbf{X}_{\vec{q}}. \tag{54}$$

Now we have

$$\mathbf{K}_S\mathbf{X}_{\vec{q}}^{(1)}\mathbf{K}_S=\mathbf{X}_{\vec{q}}^{(1)}. \tag{55}$$

This new generator $\mathbf{X}_{\vec{q}}^{(1)}$ is invariant under $\mathbf{K}_S$ and the new representation of Galilei boosts becomes

$$\exp[i\vec{p_0}\cdot\mathbf{X}_{\vec{q}}^{(1)}]|\vec{p},\vec{q}\rangle=\exp[(i/\hbar)\vec{p_0}\cdot\vec{q}]|\vec{p}+\vec{p_0},\vec{q}\rangle. \tag{56}$$

As expected from the general arguments of Sec. VI C, we find a supplementary phase factor $\theta=(i/\hbar)\vec{p_0}\cdot\vec{q}$ that modifies the classical representation, but only for Galilei boosts. The representation of translations and rotations is unchanged.

To conclude, taking into account the remarks of Sec. VII B 2 on the representation of observables, we introduce the ''prequantum'' operators $\overrightarrow{\mathbf{P}_*}$, $\overrightarrow{\mathbf{Q}_*}$ and $\overrightarrow{\mathbf{J}_*}$, homogeneous, respectively, to $\vec{p}$, $\vec{q}$ and $\vec{q}\wedge\vec{p}=\vec{l}$:

$$\begin{aligned}
\overrightarrow{\mathbf{P}_*}&=\hbar\mathbf{X}_{\vec{p}}=-i\hbar\overrightarrow{\nabla}_q=(\tfrac{1}{2})(\vec{\mathbf{p}}+\mathbf{K}_S\vec{\mathbf{p}}\mathbf{K}_S),\\
\overrightarrow{\mathbf{Q}_*}&=\hbar\mathbf{X}_{\vec{q}}^{(1)}=\vec{q}+i\hbar\overrightarrow{\nabla}_p=(\tfrac{1}{2})(\vec{\mathbf{q}}+\mathbf{K}_S\vec{\mathbf{q}}\ \ \mathbf{K}_S),\\
\overrightarrow{\mathbf{J}_*}&=\hbar\mathbf{X}_{\vec{l}}=-i\hbar(\vec{q}\wedge\overrightarrow{\nabla}_q+\vec{p}\wedge\overrightarrow{\nabla}_p).
\end{aligned} \tag{57}$$

These operators are the generators of the new representation of the Galilei group through the equations

$$\begin{aligned}
&\exp[-(i/\hbar)\vec{q_0}\cdot\overrightarrow{\mathbf{P}_*}]|\vec{p},\vec{q}\rangle=|\vec{p},\vec{q}+\vec{q_0}\rangle,\\
&\exp[(i/\hbar)\vec{p_0}\cdot\overrightarrow{\mathbf{Q}_*}]|\vec{p},\vec{q}\rangle=\exp[(i/\hbar)\vec{p_0}\cdot\vec{q}]|\vec{p}+\vec{p_0},\vec{q}\rangle,\\
&\exp[-(i/\hbar)\vec{\omega}\cdot\overrightarrow{\mathbf{J}_*}]|\vec{p},\vec{q}\rangle=|\mathcal{R}_{\vec{\omega}}(\vec{q}),\mathcal{R}_{\vec{\omega}}(\vec{p})\rangle,
\end{aligned} \tag{58}$$

where $\mathcal{R}_{\vec{\omega}}$ is the geometrical rotation.

The index ''*'' on $\overrightarrow{\mathbf{P}_*}$, $\overrightarrow{\mathbf{Q}_*}$ and $\overrightarrow{\mathbf{J}_*}$ is used to distinguish these ''prequantum operators'' from the true quantum ones that will be obtained by our procedure of quantization.

Now, while the old generators $\mathbf{X}_{\vec{p}}$ and $\mathbf{X}_{\vec{q}}$ were commuting, the new ones $\overrightarrow{\mathbf{P}_*}$ and $\overrightarrow{\mathbf{Q}_*}$ verify

$$[\mathbf{P}_{*i},\mathbf{Q}_{*j}]=-i\hbar\,\delta_{ij}. \tag{59}$$

In fact, for any component of the operators $\overrightarrow{\mathbf{P}_*}$, $\overrightarrow{\mathbf{Q}_*}$, and $\overrightarrow{\mathbf{J}_*}$, the expression of the commutator $(i/\hbar)[\mathbf{A},\mathbf{B}]$ exactly corresponds to the Poisson bracket of the associated classical observables ($\vec{p}$, $\vec{q}$, $\vec{l}$):

$$\begin{aligned}
&[\mathbf{P}_{*i},\mathbf{P}_{*j}]=[\mathbf{Q}_{*i},\mathbf{Q}_{*j}]=0,\\
&[\mathbf{P}_{*i},\mathbf{Q}_{*j}]=-i\hbar\,\delta_{ij},\\
&[\mathbf{J}_{*i},\mathbf{J}_{*j}]=i\hbar\,\epsilon_{ijk}\mathbf{J}_{*k},\\
&[\mathbf{J}_{*i},\mathbf{Q}_{*j}]=i\hbar\,\epsilon_{ijk}\mathbf{Q}_{*k},\\
&[\mathbf{J}_{*i},\mathbf{P}_{*j}]=i\hbar\,\epsilon_{ijk}\mathbf{P}_{*k}.
\end{aligned} \tag{60}$$

So, independent of our specific procedure of quantization of observables based on projection, it is natural to expect that these operators $\vec{\mathbf{P}}_*$, $\vec{\mathbf{Q}}_*$, and $\vec{\mathbf{J}}_*$ are the right representations of momentum, position and angular momentum.

We will find that our procedure of quantization confirms this hypothesis.

D. Angular momentum and spin

Starting from $\vec{\mathbf{P}}_*$, $\vec{\mathbf{Q}}_*$, and $\vec{\mathbf{J}}_*$, we define two new generators called $\vec{\mathbf{L}}_*$ and $\vec{\mathbf{S}}_*$:

$$\begin{aligned} \vec{\mathbf{L}}_* &= \vec{\mathbf{Q}}_* \wedge \vec{\mathbf{P}}_*, \\ \vec{\mathbf{S}}_* &= \vec{\mathbf{J}}_* - \vec{\mathbf{L}}_* = -i\hbar \vec{p} \wedge \vec{\nabla}_p - \hbar^2 \vec{\nabla}_p \wedge \vec{\nabla}_q. \end{aligned} \tag{61}$$

$\vec{\mathbf{L}}_*$ and $\vec{\mathbf{S}}_*$ are generators of rotations since their components verify $[\mathbf{A}_i, \mathbf{A}_j] = i\hbar \epsilon_{ijk} \mathbf{A}_k$. But, moreover, we have

$$[\mathbf{S}_{*i}, \mathbf{Q}_{*j}] = [\mathbf{S}_{*i}, \mathbf{P}_{*j}] = 0. \tag{62}$$

So, anticipating on the remainder, $\vec{\mathbf{L}}_*$ generates orbital rotations, while $\vec{\mathbf{S}}_*$ defines internal rotations: we find some spin representation.

Nevertheless, since $\vec{\mathbf{S}}_*$ is built with true vectors, it only generates integer spins.

This means that we cannot recover half-integer spins only starting with our configuration space $\mathcal{H} = L^2(\mathcal{C})$. If we want to recover all possible values of spin, we must add some external degrees of freedom to our Hilbert space.

More precisely, we must assume that the basis of $\mathcal{H}$ is $\{|\vec{p}, \vec{q}\rangle \otimes |\epsilon\rangle\}$ with $\epsilon = 0, \pm 1$. The value $\epsilon = 0$ corresponds to the previous case of integer spins, while the new values $\epsilon = \pm 1$ describe the half-integer components. We must also modify the generator $\vec{J}_*$ of rotations to take into account rotations of new degrees of freedom:

$$\vec{\mathbf{J}}_* = \hbar \vec{\mathbf{X}}_I + \frac{\hbar}{2} \vec{\Sigma}, \tag{63}$$

where $\vec{\Sigma}$ applied to $|\epsilon = 0\rangle$ gives 0, and applied to $|\epsilon = \pm 1\rangle$, $\vec{\Sigma}$ reduces to Pauli matrices.

Of course the operators $\vec{\mathbf{P}}_*$, $\vec{\mathbf{Q}}_*$, and $\vec{\mathbf{L}}_*$ are unchanged, and only $\vec{\mathbf{S}}_*$ is modified.

In the remainder we do not develop any further this extended framework, because the heaviness of the formalism hides the ideas involved in our procedure of quantization. So we continue to use our Hilbert space generated by the basis $\{|\vec{p}, \vec{q}\rangle\}$, but now we know that this framework can only generate integer spins, and so all the following is devoted to bosonic particles.

E. Discrete symmetries

1. Parity

Parity is defined as the linear operator $\mathbf{K}_P$ acting on states $|\vec{p}, \vec{q}\rangle$ as

$$\mathbf{K}_P |\vec{p}, \vec{q}\rangle = |-\vec{p}, -\vec{q}\rangle. \tag{64}$$

2. Time reversal

Classically speaking, time reversal transforms a state $(\vec{p}, \vec{q})$ into $(-\vec{p}, \vec{q})$. Then we can try to represent time reversal as a linear operator acting on states $|\vec{p}, \vec{q}\rangle$, such that $\mathbf{K}_T |\vec{p}, \vec{q}\rangle = |-\vec{p}, \vec{q}\rangle$. But if we take this definition, the linear condition is incompatible with Galilei boosts, because of the supplementary phase factor introduced into the representation. To obtain a consistent result, we must assume that $\mathbf{K}_T$ is an antilinear operator. So, we define $\mathbf{K}_T$ as an antilinear operator such that

$$\mathbf{K}_T |\vec{p}, \vec{q}\rangle = |-\vec{p}, \vec{q}\rangle. \tag{65}$$

3. Symplectic transform

The symmetry $\mathbf{K}_S$ has been defined in Sec. VII B 1, and by construction $\mathbf{K}_S$ commutes with all the previous symmetries.

VIII. IRREDUCIBLE REPRESENTATION OF THE GALILEI GROUP

Computations on the irreducible representations of the Galilei group in phase space have already been published[31] (for the Poincaré group, see Ref. 32); for the case of scalar particles (see Ref. 6, Chap. 1).

We recall here this analysis in order to prove the consistency of our approach and also to introduce specific notations.

A. Subspaces of irreducible representation of P_* and Q_*

We have seen that the generators $\overrightarrow{\mathbf{P}_*}$ and $\overrightarrow{\mathbf{Q}_*}$ verify $[\mathbf{P}_{*i},\mathbf{Q}_{*j}]=-i\hbar\,\delta_{ij}$ and we know that irreducible representations of these relations are obtained by $\overrightarrow{\mathbf{P}_*}\equiv -i\hbar\overrightarrow{\nabla}_x$ and $\overrightarrow{\mathbf{Q}_*}\equiv\vec{x}$ (for the moment $\vec{x}$ must be only seen as a parameter). So we look for (unbounded) states "$|\vec{x},\alpha\rangle$" such that

$$\begin{aligned}\langle\vec{x},\alpha|\overrightarrow{\mathbf{P}_*}|\vec{p},\vec{q}\rangle&=-i\hbar\overrightarrow{\nabla}_x\langle\vec{x},\alpha|\vec{p},\vec{q}\rangle,\\ \langle\vec{x},\alpha|\overrightarrow{\mathbf{Q}_*}|\vec{p},\vec{q}\rangle&=\vec{x}\langle\vec{x},\alpha|\vec{p},\vec{q}\rangle.\end{aligned}\tag{66}$$

If we call $\phi=\langle\vec{p},\vec{q}|\vec{x},\alpha\rangle$, using the explicit expression of $\overrightarrow{\mathbf{P}_*}$ and $\overrightarrow{\mathbf{Q}_*}$, we obtain

$$\begin{aligned}(\overrightarrow{\nabla}_q+\overrightarrow{\nabla}_x)\,\phi&=0,\\ i\hbar\overrightarrow{\nabla}_p\phi&=(\vec{x}-\vec{q})\,\phi.\end{aligned}\tag{67}$$

The general solution of this system is

$$\phi=\Phi(\vec{x}-\vec{q})\exp[-(i/\hbar)\vec{p}\cdot(\vec{x}-\vec{q})],\tag{68}$$

where Φ is an arbitrary function.

So the states' $\{|\vec{x},\alpha\rangle\}$ solutions of the problem are given by

$$\langle\vec{p},\vec{q}|\vec{x},\alpha\rangle=\Phi_\alpha(\vec{x}-\vec{q})\exp[-(i/\hbar)\vec{p}\cdot(\vec{x}-\vec{q})].\tag{69}$$

Computing the scalar product $\langle\vec{y},\beta|\vec{x},\alpha\rangle$ we obtain

$$\begin{aligned}\langle\vec{y},\beta|\vec{x},\alpha\rangle&=\langle\langle\beta|\alpha\rangle\rangle\,\delta(\vec{y}-\vec{x})\\ \langle\langle\beta|\alpha\rangle\rangle&=h^3\int d^3\vec{q}\,\Phi^*_\beta(\vec{q})\Phi_\alpha(\vec{q}),\end{aligned}\tag{70}$$

where $h=2\pi\hbar$ is the Planck constant and $\langle\langle\beta|\alpha\rangle\rangle$ defines a reduced scalar product on the fields Φ_α.

Now, if we take a complete orthonormal basis $\{\Phi_n\}$ for the reduced scalar product ($\langle\langle n|m\rangle\rangle=\delta_{n,m}$), the states $\{|\vec{x},n\rangle\}$ define a complete orthogonal basis for our configuration space and we can define the bounded projectors Π_n onto each subspace generated by the states $\{|\vec{x},n\rangle\}_{\vec{x}\in\mathbf{R}^3}$:

$$\Pi_n=\int d^3\vec{x}|\vec{x},n\rangle\langle\vec{x},n|.\tag{71}$$

Moreover, we have also the closure relation

$$\sum_n \Pi_n = \mathbf{1}_{\mathcal{H}}. \tag{72}$$

Each of these Π_n defines a subspace of irreducible representation of the commutation relations between $\overrightarrow{\mathbf{P}_*}$ and $\overrightarrow{\mathbf{Q}_*}$, so

$$[\overrightarrow{\mathbf{P}_*}, \Pi_n] = [\overrightarrow{\mathbf{Q}_*}, \Pi_n] = 0. \tag{73}$$

The action of space translations and Galilei boosts generated by $\overrightarrow{P_*}$ and $\overrightarrow{Q_*}$ on each subspace is given by

$$\begin{aligned} \exp[-(i/\hbar)\vec{q_0}\cdot\overrightarrow{\mathbf{P}_*}]|\vec{x},n\rangle &= |\vec{x}+\vec{q_0},n\rangle, \\ \exp[(i/\hbar)\vec{q_0}\cdot\overrightarrow{\mathbf{Q}_*}]|\vec{x},n\rangle &= \exp[(i/\hbar)\vec{p_0}\cdot\vec{x}]|\vec{x},n\rangle. \end{aligned} \tag{74}$$

Now, we look at irreducible representations of the rotation group, taking into account the previous results.

B. Irreducible representations of rotations

We have previously seen that the generator of rotations is $\overrightarrow{\mathbf{J}_*} = \overrightarrow{\mathbf{L}_*} + \overrightarrow{\mathbf{S}_*}$ with $[\overrightarrow{\mathbf{L}_*}, \overrightarrow{\mathbf{S}_*}] = 0$. Then,

$$\exp[-(i/\hbar)\vec{\omega}\cdot\overrightarrow{\mathbf{J}_*}] = \exp[-(i/\hbar)\vec{\omega}\cdot\overrightarrow{\mathbf{L}_*}]\exp[-(i/\hbar)\vec{\omega}\cdot\overrightarrow{\mathbf{S}_*}]. \tag{75}$$

Since by construction $\overrightarrow{\mathbf{L}_*} = \overrightarrow{\mathbf{Q}_*} \wedge \overrightarrow{\mathbf{P}_*}$ acts on each subspace Π_n as the usual quantum operator of orbital angular momentum, we have

$$\exp[-(i/\hbar)\vec{\omega}\cdot\overrightarrow{\mathbf{J}_*}]|\vec{x},n\rangle = \exp[-(i/\hbar)\vec{\omega}\cdot\overrightarrow{\mathbf{S}_*}]|\mathcal{R}_{\vec{\omega}}(\vec{x}),n\rangle. \tag{76}$$

Then irreducible representations of rotations are only dependent on the generators $\overrightarrow{\mathbf{S}_*}$. Moreover, we know that these representations are obtained by states $|S,m_S\rangle$ such that $\overrightarrow{\mathbf{S}_*}^2|S,m_S\rangle = \hbar^2 S(S+1)$ and $\mathbf{S}_{*z}|S,m_S\rangle = \hbar m_S|S,m_S\rangle$. Then we look for states $|\vec{x},S,m_S\rangle$ solving the problem.

The action of $\overrightarrow{\mathbf{S}_*}$ on $|\vec{x},n\rangle$ is given by

$$\langle\vec{p},\vec{q}|\overrightarrow{\mathbf{S}_*}|\vec{x},n\rangle = i\hbar\overrightarrow{\nabla}_p \wedge (\vec{p} + i\hbar\overrightarrow{\nabla}_q)\langle\vec{p},\vec{q}|\vec{x},n\rangle. \tag{77}$$

Taking the explicit expression (69) of $\langle\vec{p},\vec{q}|\vec{x},n\rangle$ we obtain

$$\langle\vec{p},\vec{q}|\overrightarrow{\mathbf{S}_*}|\vec{x},n\rangle = -i\hbar(\vec{x}-\vec{q}) \wedge \vec{\nabla}\Phi_n(\vec{x}-\vec{q})\exp[-(i/\hbar)\vec{p}\cdot(\vec{x}-\vec{q})]. \tag{78}$$

So $\overrightarrow{\mathbf{S}_*}$ only acts on the field Φ_n as the usual quantum orbital angular operator. Then we know that irreducible representations are obtained by spherical harmonics and the states $|\vec{x},S,m_S\rangle$ are defined by

$$\begin{aligned} \langle\vec{p},\vec{q}|\vec{x},S,m_S\rangle &= \Phi_{S,m_S}(\vec{x}-\vec{q})\exp[-(i/\hbar)\vec{p}\cdot(\vec{x}-\vec{q})], \\ \Phi_{S,m_S}(\vec{x}) &= \Psi(\|\vec{x}\|)Y_S^{m_S}(\vec{x}/\|\vec{x}\|). \end{aligned} \tag{79}$$

Here Ψ is an arbitrary function normalized with the reduced scalar product defined in (70):

$$\int_0^\infty x^2 dx |\Psi(x)|^2 = h^{-3}. \tag{80}$$

Now the action of the rotation group on the orthogonal basis $|\vec{x},S,m_S\rangle$ can be deduced from (76):

$$\exp[-(i/\hbar)\vec{\omega}\cdot\overrightarrow{\mathbf{J}_*}]|\vec{x},S,m\rangle = \sum_{m_1} R^S_{m_1,m}(\vec{\omega})|\mathcal{R}_{\vec{\omega}}(\vec{x}),S,m_1\rangle, \tag{81}$$

where $R^S_{m_1,m}(\vec{\omega})$ is the irreducible matrix of rotation.

C. Conclusion

The final result is that irreducible subspaces of the Galilei group are given by the projectors Π_S on the states generated by the orthogonal basis $\{|\vec{x},S,m\rangle\}$, that is,

$$\Pi_S = \sum_m \int d^3\vec{x}|\vec{x},S,m\rangle\langle\vec{x},S,m|. \tag{82}$$

Each of these subspaces depends of course on the value of S (integer), but also depends on an arbitrary function Ψ normalized in (80).

D. Action of discrete symmetries on an irreducible subspace

1. Parity

Following the definition (64) of the operator $\mathbf{K}_P$ we find

$$\langle\vec{p},\vec{q}|\mathbf{K}_P|\vec{x},S,m_S\rangle = \Phi_{S,m_S}(\vec{x}+\vec{q})\exp[(i/\hbar)\vec{p}\cdot(\vec{x}+\vec{q})]. \tag{83}$$

Now, using the parity of the spherical harmonics, we find

$$\mathbf{K}_P|\vec{x},S,m_S\rangle = (-1)^S|-\vec{x},S,m_S\rangle. \tag{84}$$

2. Time reversal

Following the definition (65) of the antilinear operator $\mathbf{K}_T$ we find

$$\langle\vec{p},\vec{q}|\mathbf{K}_T|\vec{x},S,m_S\rangle = \Phi^*_{S,m_S}(\vec{x}-\vec{q})\exp[-(i/\hbar)\vec{p}\cdot(\vec{x}-\vec{q})]. \tag{85}$$

Using the definition of Φ_{S,m_S} and the relation between spherical harmonics and its conjugate, we find

$$\langle\vec{p},\vec{q}|\mathbf{K}_T|\vec{x},S,m\rangle = (-1)^m\Psi^*(|\vec{x}-\vec{q}|)Y_S^{-m}\exp[-(i/\hbar)\vec{p}\cdot(\vec{x}-\vec{q})]. \tag{86}$$

We deduce that each subspace Π_S is invariant by time reversal, only if the unknown function Ψ verifies $\Psi^* = \alpha\Psi$.

Since Ψ is always defined up to a constant phase factor, **we assume in the remainder that Ψ is real**.

Then $\mathbf{K}_T$ is an antilinear operator that verifies

$$\mathbf{K}_T|\vec{x},S,m_S\rangle = (-1)^{m_S}|\vec{x},S,-m_S\rangle. \tag{87}$$

3. Symplectic transform

Using the definition (51) of the operator $\mathbf{K}_S$ we find

$$\langle \vec{p},\vec{q}|\mathbf{K}_S|\vec{x},S,m_S\rangle = \Phi_{S,m_S}(\vec{q}-\vec{x})\exp[-(i/\hbar)\vec{p}\cdot(\vec{x}-\vec{q})]. \tag{88}$$

Because of the parity of spherical harmonics, we find

$$\mathbf{K}_S|\vec{x},S,m_S\rangle = (-1)^S|\vec{x},S,m_S\rangle. \tag{89}$$

Then the nonclassical symmetry $\mathbf{K}_S$ acts on $|\vec{x},S,m_S\rangle$ as an intrinsic parity.

We conclude that the discrete symmetries $\mathbf{K}_P$, $\mathbf{K}_T$, and $\mathbf{K}_S$ are represented on each subspace Π_S, if we assume the unknown function Ψ to be real.

This condition on Ψ can be found in Ref. 6 (Chap. 1) in the study of ''stochastic probability currents,'' but it is not deduced from symmetry arguments as in our case.

IX. AXIOM OF QUANTIZATION

Any subspace $\mathcal{H}_S = \mathrm{Ran}(\Pi_S)$ corresponds to our requirements defined in Sec. VI C and a quantization is the projection from the global Hilbert space $\mathcal{H}$ on one of these subspaces $\mathcal{H}_S$.

As expected, the action of all symmetries on the states ''$|\vec{x},S,m_S\rangle$'' corresponds exactly with the quantum definition. But for the moment the quantities $\vec{x},S,m_S$ are only mathematical parameters and are not related to physical observables (even if we can guess their meaning).

On the other hand, each $\mathcal{H}_S$ is defined by the integer parameter S and the real function $\Psi(x)$. The essential effect of this function is to introduce a specific length scale λ as a characteristic of the representation. To make explicit this dependence, we reduce $\Psi(x)$ to a purely mathematical (dimensionless) function Ψ_0 by the scaling

$$\Psi(x) = (\lambda h)^{-3/2}\Psi_0(x/\lambda). \tag{90}$$

The condition of normalization (80) becomes

$$\int_0^\infty u^2 du \Psi_0(u)^2 = 1. \tag{91}$$

Finally, if we look at the main physical consequences of our procedure of quantization, we see that the important result is that a particle associated with a subspace $\mathcal{H}_S$ possesses an internal structure. This structure is defined by the intrinsic properties for rotations (spin S), and by a specific length scale λ. Through λ and Ψ, we recover the old idea of ''proper wave function'' first introduced by Landé[33] and Born[34] to describe elementary particles that are not pointlike. This result (and the consequences on measurement) is also obtained by Prugovečki (Ref. 6, Chap. 1, pp. 25 and 60). In fact, our idea of quantization can be seen as the reverse procedure of Prugovečki's approach (obtaining phase space representation of quantum mechanics).

At this stage, if we want to give a physical meaning to λ, we must specify what we mean by ''particles.'' Of course, elementary objects such as electrons or protons (in nonrelativistic mechanics) are particles, but atoms with frozen internal degrees of freedom can be also seen as particles.

A. The case of elementary particles

In nonrelativistic quantum mechanics, we cannot build a natural length scale λ for a true particle, but in relativistic quantum mechanics the Compton wave length $\lambda_c = h/Mc$ defines such intrinsic length scale. So it is natural to look at λ as the preceding of the relativistic quantity λ_c. This means that λ must always be a very small quantity (in regard to all other classical length scales).

B. The case of complex particles (atoms)

First, we must assume that all internal degrees of freedom are frozen, to be able to describe the system only using external dynamical quantities. In this case λ simply represents the geometrical size of the system. Moreover, we must always assume that λ is very small in regard to all other classical length scales of the problem, because the existence of some length scale of order of λ implies a dynamical effect on the internal degrees of freedom of the system.

X. THE BASIC QUANTIZED OBSERVABLES

In all the remainder the subspace $\mathcal{H}_S$ is assumed to be fixed, and following always our procedure of Sec. VI C, we can look how classical observables are transformed through quantization.

We recall that, starting from a classical quantity $f(\vec{p},\vec{q})$, we build first the associated classical operator **f**, and then we quantify **f** by taking the projection $\Pi_S \cdot \mathbf{f} \cdot \Pi_S$. The idea of projecting classical operators (stochastic observables) on irreducible subspaces in order to obtain quantum equations can be also found in Ref. 6, but it is not used as a general procedure to replace the correspondence principle and rebuild quantum mechanics.

A. Quantum operators of position and momentum

So, we define the quantum operator of position $\vec{\mathbf{Q}}$ and momentum $\vec{\mathbf{P}}$ as

$$\begin{aligned} \vec{\mathbf{Q}} &= \Pi_S \vec{\mathbf{q}} \Pi_S, \\ \vec{\mathbf{P}} &= \Pi_S \vec{\mathbf{p}} \Pi_S. \end{aligned} \tag{92}$$

First, we remark that the action of the symplectic transform K_S on the states $|\vec{x},S,m_S\rangle$ (89) implies

$$K_S \Pi_S = \Pi_S K_S = (-1)^S \Pi_S. \tag{93}$$

Now, we have the definitions (57) of $\overrightarrow{P_*}$ and $\overrightarrow{Q_*}$:

$$\begin{aligned} \overrightarrow{P_*} &= (\tfrac{1}{2})(\vec{\mathbf{p}} + K_S \vec{\mathbf{p}} K_S), \\ \overrightarrow{Q_*} &= (\tfrac{1}{2})(\vec{\mathbf{q}} + K_S \vec{\mathbf{q}} K_S). \end{aligned} \tag{94}$$

Projecting these relations with Π_S and taking into account (93), we obtain

$$\begin{aligned} \Pi_S \overrightarrow{P_*} &= \Pi_S \overrightarrow{P_*} \Pi_S = \Pi_S \vec{\mathbf{p}} \Pi_S = \vec{\mathbf{P}}, \\ \Pi_S \overrightarrow{Q_*} &= \Pi_S \overrightarrow{Q_*} \Pi_S = \Pi_S \vec{\mathbf{q}} \Pi_S = \vec{\mathbf{Q}} \end{aligned} \tag{95}$$

(we recall that by construction Π_S commutes with $\overrightarrow{P_*}$ and $\overrightarrow{Q_*}$).

So,

$$\begin{aligned} \langle \vec{x},S,m|\vec{\mathbf{P}}|\vec{y},S,m_1\rangle &= -i\hbar(\vec{\nabla}\delta)(\vec{x}-\vec{y})\,\delta_{m,m_1}, \\ \langle \vec{x},S,m|\vec{\mathbf{Q}}|\vec{y},S,m_1\rangle &= \vec{x}\,\delta(\vec{x}-\vec{y})\,\delta_{m,m_1}. \end{aligned} \tag{96}$$

Conclusion

We find that the quantized version $\vec{\mathbf{P}}$ and $\vec{\mathbf{Q}}$ of the classical observables $\vec{p}$ and $\vec{q}$ correspond precisely with the usual quantum operators.

Moreover, these operators are also the restriction of the generators of translations and Galilei boosts. This means that, in the ''quantum world,'' these observables are exactly the generators of symmetries (translation and Galilei boosts) as in the classical picture through Poisson brackets. (We also notice that our procedure allows us to remove the ambiguity between ''passive and active'' representations of $\vec{p}$ and $\vec{q}$.)

But, we will see in the following section, that this conclusion cannot be extended to angular momentum because of spin: the projection of the classical angular momentum $\vec{\mathbf{q}}\wedge\vec{\mathbf{p}}$ is not in general the restriction of the generator of rotations $\overrightarrow{J_*}$. In this case we must use other arguments to choose the quantum observable associated with angular momentum.

B. Quantum angular momentum and spin

We know from (57) that the generator of rotations is $\overrightarrow{\mathbf{J}_*}=-i\hbar(\vec{q}\wedge\overrightarrow{\nabla_q}+\vec{p}\wedge\overrightarrow{\nabla_p})$ and by construction Π_S commutes with $\overrightarrow{\mathbf{J}_*}$. Moreover, we have seen in (60) that the commutators of $\overrightarrow{\mathbf{P}_*}$, $\overrightarrow{\mathbf{Q}_*}$, and $\overrightarrow{\mathbf{J}_*}$ correspond exactly to the expression of the Poisson brackets of the classical quantities $\vec{p}$, $\vec{q}$ and $\vec{l}=\vec{q}\wedge\vec{p}$. Now, since we have proved that the restrictions $\vec{\mathbf{P}}$ and $\vec{\mathbf{Q}}$ of $\overrightarrow{\mathbf{P}_*}$ and $\overrightarrow{\mathbf{Q}_*}$ are the quantum operators of momentum and position, we can also guess that the ''quantum angular momentum'' $\vec{\mathbf{J}}$ is the restriction of the generator $\overrightarrow{\mathbf{J}_*}$. So we define

$$\vec{\mathbf{J}}=\Pi_S\overrightarrow{\mathbf{J}_*}=\overrightarrow{\mathbf{J}_*}\Pi_S=\Pi_S\overrightarrow{\mathbf{J}_*}\Pi_S. \tag{97}$$

Of course the general definitions of Sec. III for observables attest that $\vec{\mathbf{J}}$ (as a self-adjoint operator commuting with Π_S) is mathematically a possible observable. But up to now, we have only defined the quantum version of classical observables by our procedure of quantization. So we must first find the relation connecting $\vec{\mathbf{J}}$ to the quantized version $\Pi_S\vec{l}\Pi_S$ of the classical angular momentum $\vec{l}=\vec{q}\wedge\vec{p}$. The following lines are devoted to this question.

Taking into account the explicit expression of $\overrightarrow{\mathbf{P}_*}$ and $\overrightarrow{\mathbf{Q}_*}$, we rewrite $\overrightarrow{\mathbf{J}_*}$ as

$$\overrightarrow{\mathbf{J}_*}=\vec{\mathbf{q}}\wedge\overrightarrow{\mathbf{P}_*}+\overrightarrow{\mathbf{Q}_*}\wedge\vec{\mathbf{p}}-\vec{\mathbf{q}}\wedge\vec{\mathbf{p}}. \tag{98}$$

Using the equations (95) related to $\vec{\mathbf{P}}$ and $\vec{\mathbf{Q}}$ we find

$$\vec{\mathbf{J}}=2\vec{\mathbf{Q}}\wedge\vec{\mathbf{P}}-\Pi_S\vec{\mathbf{q}}\wedge\vec{\mathbf{p}}\Pi_S. \tag{99}$$

But we know also that the generator of rotations $\overrightarrow{\mathbf{J}_*}$ can be divided into $\overrightarrow{\mathbf{J}_*}=\overrightarrow{\mathbf{L}_*}+\overrightarrow{\mathbf{S}_*}$ with $\overrightarrow{\mathbf{L}_*}=\overrightarrow{\mathbf{Q}_*}\wedge\overrightarrow{\mathbf{P}_*}$, and by construction Π_S commutes with $\overrightarrow{\mathbf{L}_*}$ and $\overrightarrow{\mathbf{S}_*}$. So we can define two new quantum observables $\vec{\mathbf{L}}$ and $\vec{\mathbf{S}}$ as the restriction of $\overrightarrow{\mathbf{L}_*}$ and $\overrightarrow{\mathbf{S}_*}$**:**

$$\begin{aligned}\vec{\mathbf{L}}&=\Pi_S\overrightarrow{\mathbf{L}_*}=\overrightarrow{\mathbf{L}_*}\Pi_S=\vec{\mathbf{Q}}\wedge\vec{\mathbf{P}},\\ \vec{\mathbf{S}}&=\Pi_S\overrightarrow{\mathbf{S}_*}=\overrightarrow{\mathbf{S}_*}\Pi_S,\\ \vec{\mathbf{J}}&=\vec{\mathbf{L}}+\vec{\mathbf{S}}.\end{aligned} \tag{100}$$

We call $\vec{\mathbf{L}}$ ''orbital angular momentum'' and $\vec{\mathbf{S}}$ ''spin momentum.'' Now using Eqs. (99) and (100) we find finally

$$\Pi_S\vec{\mathbf{q}}\wedge\vec{\mathbf{p}}\Pi_S=\vec{\mathbf{L}}-\vec{\mathbf{S}}=\vec{\mathbf{Q}}\wedge\vec{\mathbf{P}}-\vec{\mathbf{S}}. \tag{101}$$

This shows that the quantized version of the classical angular momentum $\vec{l}=\vec{q}\wedge\vec{p}$ does not correspond in general to the generator $\vec{\mathbf{J}}$ (or $\vec{\mathbf{L}}$).

In fact, we find that $\Pi_S\vec{\mathbf{q}}\wedge\vec{\mathbf{p}}\Pi_S=\vec{\mathbf{L}}=\vec{\mathbf{J}}$ only in the case of scalar particles ($S=0$).

Then, for $S=0$, it is true that the quantized version of the classical angular momentum $\vec{l}=\vec{q}\wedge\vec{p}$ is the generator $\vec{\mathbf{J}}=\vec{\mathbf{L}}=\vec{\mathbf{Q}}\wedge\vec{\mathbf{P}}$ of rotations. This is because we call $\vec{\mathbf{L}}$ ''orbital angular momentum.'' But this correspondence fails for $S\neq 0$, because of the spin variables.

This result is very simple to understand, if we recall that $\vec{\mathbf{S}}$ cannot be obtained as the quantization of any classical observable. So, introducing spins in our formalism is equivalent to defining nonclassical observables. Then each subspace Π_S, for $S\neq 0$, cannot be described using only quantized version of classical observables, and this generates the nonequivalence between $\Pi_S\vec{\mathbf{I}}\Pi_S$ and $\vec{\mathbf{J}}$ (or $\vec{\mathbf{L}}$).

Nevertheless, if we look at the case $S\neq 0$ as an extension of $S=0$, we **must postulate** that $\vec{\mathbf{J}}$ is the physical quantum observable of angular momentum, precisely because $\vec{\mathbf{J}}$ is always the generator of rotations. Moreover, $\vec{\mathbf{L}}$ and $\vec{\mathbf{S}}$ are also quantum observables as the generator of orbital rotations and as the generator of spin rotations.

Finally, the parameter S and the nonclassical observable $\vec{\mathbf{S}}$ only appear because we look for irreducible representations of the Galilei group, in order to apply our general procedure of quantization. Then we recover the usual result that spins are ''purely quantum objects.''

Conclusion

We summarize the previous discussion in two points:

(i) In the case of scalar particles ($S=0$), it is true that the generator of rotations $\vec{\mathbf{J}}=\vec{\mathbf{L}}=\vec{\mathbf{Q}}\wedge\vec{\mathbf{P}}$ is the quantized version of the classical angular momentum $\vec{l}=\vec{q}\wedge\vec{p}$. This is because we call $\vec{\mathbf{L}}$ ''orbital angular momentum.''

(ii) In the case of nonscalar particles ($S\neq 0$), it is false that the generator of rotations $\vec{\mathbf{J}}=\vec{\mathbf{L}}+\vec{\mathbf{S}}=\vec{\mathbf{Q}}\wedge\vec{\mathbf{P}}+\vec{\mathbf{S}}$ is the quantized version of $\vec{l}=\vec{q}\wedge\vec{p}$. We must postulate that $\vec{\mathbf{J}}$ is the physical observable of angular momentum precisely because $\vec{\mathbf{J}}$ is always the generator of rotations. The operators $\vec{\mathbf{L}}$ and $\vec{\mathbf{S}}$ are also quantum observables as generators of orbital rotations and spin rotations (in fact $\vec{\mathbf{L}}=\Pi_S\vec{\mathbf{q}}\Pi_S\wedge\Pi_S\vec{\mathbf{p}}\Pi_S\neq\Pi_S\vec{\mathbf{q}}\wedge\vec{\mathbf{p}}\Pi_S$).

XI. SEMI-CLASSICAL PROPERTIES

This section is certainly the closest to Prugovečki's monograph,[6] because we recover the central part played by coherent states of the Galilei group to connect quantum operators with classical formulas. In fact, we recover the positive operator value (POV) measure that constitutes a ''stochastic phase-space system of covariance'' for the Galilei group. So, we do not develop in details the consequences on the stochastic level and measurements that can be found in Ref. 6.

A. Semi-classical states and semi-classical events

1. Semi-classical states

In the global Hilbert space $\mathcal{H}$, we have the closure relation

$$\mathbf{1}_{\mathcal{H}}=\int d^3\vec{p}\,d^3\vec{q}\,|\vec{p},\vec{q}\rangle\langle\vec{p},\vec{q}|. \tag{102}$$

Then,

$$\Pi_S=\int d^3\vec{p}\,d^3\vec{q}\,\Pi_S|\vec{p},\vec{q}\rangle\langle\vec{p},\vec{q}|\Pi_S. \tag{103}$$

We deduce that the states $|\xi_{\vec{p},\vec{q}},S\rangle=\Pi_S|\vec{p},\vec{q}\rangle$ define an overcomplete basis of our physical Hilbert space $\mathcal{H}_S$ (cf. Sec. VI B 3).

Moreover, using (79),

$$\langle\xi_{\vec{p},\vec{q}},S|\xi_{\vec{p},\vec{q}},S\rangle=\sum_m\int d^3\vec{x}\,|\Phi_{S,m}(\vec{x})|^2=(2S+1)h^{-3}. \tag{104}$$

These coherent states for the Galilei group have many applications in standard quantum dynamics (Omnès,[18] Perelomov or Klauder[5]). In Prugovečki's work,[6] these states introduce the "resolution generator" that represents the "proper wave function" of an extended test particle and allow us to give a concrete connection between standard quantum mechanics and its "stochastic phase-space" representation.

2. Semi-classical configuration events

If we take a classical event "A" in phase space, it is represented in $\mathcal{H}$ by the projector $\Pi(A)$:

$$\Pi(A)=\int_A d^3\vec{p}\,d^3\vec{q}\,|\vec{p},\vec{q}\rangle\langle\vec{p},\vec{q}|. \tag{105}$$

Quantizing $\Pi(A)$, we obtain $\Pi_S(A)$:

$$\Pi_S(A)=\Pi_S\Pi(A)\Pi_S=\int_A d^3\vec{p}\,d^3\vec{q}\,|\xi_{\vec{p},\vec{q}},S\rangle\langle\xi_{\vec{p},\vec{q}},S|. \tag{106}$$

As indicated in Sec. VI B 3, $\Pi_S(A)$ is no longer a true projector, and then $\Pi_S(A)$ must be seen as a "fuzzy" quantum event (quasiprojector), or a semi-classical event (Omnès[18]). In Prugovečki's monograph,[6] $\Pi_S(A)$ is exactly the POV measure that gives a system of covariance for the Galilei group.

Now, taking the trace of $\Pi_S(A)$, we obtain

$$\mathrm{Tr}(\Pi_S(A))=(2S+1)\mathcal{V}(A)h^{-3}, \tag{107}$$

where $\mathcal{V}(A)$ is the volume of "A" in phase space.

Then $\mathrm{Tr}(\Pi_S(A))$ gives exactly the semi-classical number of quantum states contained in the volume "A" of phase space.

B. Semi-classical states and quantum observables

1. Expectation values

For $\vec{\mathbf{P}}$, $\vec{\mathbf{Q}}$, $\vec{\mathbf{L}}=\vec{\mathbf{Q}}\wedge\vec{\mathbf{P}}$ and $\vec{\mathbf{S}}$, we find after some algebra

$$\begin{aligned}
\langle\xi_{\vec{p},\vec{q}},S|\vec{\mathbf{P}}|\xi_{\vec{p},\vec{q}},S\rangle&=\mathcal{N}\vec{p},\\
\langle\xi_{\vec{p},\vec{q}},S|\vec{\mathbf{Q}}|\xi_{\vec{p},\vec{q}},S\rangle&=\mathcal{N}\vec{q},\\
\langle\xi_{\vec{p},\vec{q}},S|\vec{\mathbf{L}}|\xi_{\vec{p},\vec{q}},S\rangle&=\mathcal{N}\vec{q}\wedge\vec{p},\\
\langle\xi_{\vec{p},\vec{q}},S|\vec{\mathbf{S}}|\xi_{\vec{p},\vec{q}},S\rangle&=0,
\end{aligned} \tag{108}$$

where $\mathcal{N}=\langle\xi_{\vec{p},\vec{q}},S|\xi_{\vec{p},\vec{q}},S\rangle=(2S+1)h^{-3}$.

These results are precisely what we expect for semi-classical states.

2. Splitting of observables on semi-classical states

Moreover, since $\vec{\mathbf{P}}=\Pi_S\vec{\mathbf{p}}\Pi_S$ and $\vec{\mathbf{Q}}=\Pi_S\vec{\mathbf{q}}\Pi_S$, we have

$$\begin{aligned}
\vec{\mathbf{P}}&=\int d^3\vec{p}\,d^3\vec{q}\,\vec{p}\,|\xi_{\vec{p},\vec{q}},S\rangle\langle\xi_{\vec{p},\vec{q}},S|,\\
\vec{\mathbf{Q}}&=\int d^3\vec{p}\,d^3\vec{q}\,\vec{q}\,|\xi_{\vec{p},\vec{q}},S\rangle\langle\xi_{\vec{p},\vec{q}},S|.
\end{aligned} \tag{109}$$

More generally, the quantized version $\mathbf{F}$ of any classical observable $f(\vec{p},\vec{q})$ possesses the splitting

$$\mathbf{F}=\Pi_S f(\vec{\mathbf{p}},\vec{\mathbf{q}})\Pi_S=\int d^3\vec{p}\,d^3\vec{q}\,f(\vec{p},\vec{q})|\xi_{\vec{p},\vec{q}},S\rangle\langle\xi_{\vec{p},\vec{q}},S|. \tag{110}$$

C. Quantized observables and statistics

The following formulas are also found in Refs. 6 and 14 (they are obtained in order to complete the formulation of quantum statistical mechanics on stochastic phase space).

For statistics, Sec. VI B shows that we must introduce a density operator $\mathbf{D}$ with $\Pi_S\mathbf{D}=\mathbf{D}\Pi_S=\mathbf{D}$.

Moreover, the expectation values of position and momentum are given by $\langle\vec{\mathbf{P}}\rangle=\mathrm{Tr}(\mathbf{D}\cdot\vec{\mathbf{P}})$, and $\langle\vec{\mathbf{Q}}\rangle=\mathrm{Tr}(\mathbf{D}\cdot\vec{\mathbf{Q}})$.

But because $\vec{\mathbf{P}}=\Pi_S\vec{\mathbf{p}}\Pi_S$, $\vec{\mathbf{Q}}=\Pi_S\vec{\mathbf{q}}\Pi_S$, and $\mathbf{D}=\Pi_S\mathbf{D}\Pi_S$, we also have $\langle\vec{\mathbf{P}}\rangle=\mathrm{Tr}(\mathbf{D}\cdot\vec{\mathbf{p}})$, and $\langle\vec{\mathbf{Q}}\rangle=\mathrm{Tr}(\mathbf{D}\cdot\vec{\mathbf{q}})$. So we can use our results of Sec. III B 3 on classical observables to obtain

$$\begin{aligned}1=\mathrm{Tr}(\mathbf{D})&=\int d^3\vec{p}\,d^3\vec{q}\,\rho(\vec{p},\vec{q}),\\ \langle\vec{\mathbf{P}}\rangle&=\int d^3\vec{p}\,d^3\vec{q}\,\vec{p}\,\rho(\vec{p},\vec{q}),\\ \langle\vec{\mathbf{Q}}\rangle&=\int d^3\vec{p}\,d^3\vec{q}\,\vec{q}\,\rho(\vec{p},\vec{q}),\end{aligned} \tag{111}$$

where $\rho(\vec{p},\vec{q})=\langle\vec{p},\vec{q}|\mathbf{D}|\vec{p},\vec{q}\rangle$ is a positive function since $\mathbf{D}$ is a positive operator.

As mentioned in Sec. III B 3, we recover that $\rho(\vec{p},\vec{q})$ is a true classical probability density, but $\hbar$ dependent, because $\mathbf{D}=\Pi_S\mathbf{D}\Pi_S$ depends in general on $\hbar$ through Π_S. Moreover, Eqs. (111) show that the quantum expectation values of $\vec{\mathbf{P}}$ and $\vec{\mathbf{Q}}$ can always be expressed with a classical formula, using a $\hbar$-dependent density of probability.

More generally, any expectation value $\langle\mathbf{F}\rangle=\mathrm{Tr}(\mathbf{D}\cdot\mathbf{F})$ of a quantized observable $\mathbf{F}$ obtained from a classical quantity $f(\vec{p},\vec{q})$ by $\mathbf{F}=\Pi_S f(\vec{\mathbf{p}},\vec{\mathbf{q}})\Pi_S$ verifies

$$\langle\mathbf{F}\rangle=\int d^3\vec{p}\,d^3\vec{q}\,f(\vec{p},\vec{q})\rho(\vec{p},\vec{q}). \tag{112}$$

So, for any quantum observable $\mathbf{F}$ deducible from a classical one $f(\vec{p},\vec{q})$ by our procedure of quantization, the expectation value is obtained by a classical formula, using the density $\rho(\vec{p},\vec{q})=\langle\vec{p},\vec{q}|\mathbf{D}|\vec{p},\vec{q}\rangle$.

Nevertheless, these semi-classical expressions cannot be extended to nonclassical observables like $\vec{\mathbf{S}}$ because we cannot find any classical quantity associated with $\vec{\mathbf{S}}$.

XII. QUANTUM DYNAMICS

As mentioned in Sec. II B 1 and developed in Secs. II B 3 and V, classical dynamics on $\mathcal{H}$ is induced by a classical observable H through the weak dynamical equations (7) which give the evolution of expectation values. Moreover, the evolution of a state ϕ is defined by a unitary operator U_{t_1,t_0} such that $\phi_{t_1}=U_{t_1,t_0}(\phi_{t_0})$ and Eqs. (7) can be written as Eqs. (27) that we recall here:

$$\begin{aligned}\frac{d}{dt}\langle\phi_t|\vec{\mathbf{q}}|\phi_t\rangle&=\langle\phi_t|\overrightarrow{\nabla}_p H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)|\phi_t\rangle,\\ \frac{d}{dt}\langle\phi_t|\vec{\mathbf{p}}|\phi_t\rangle&=-\langle\phi_t|\overrightarrow{\nabla}_q H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)|\phi_t\rangle.\end{aligned} \tag{113}$$

Remark: We can find in Ref. 6 (Chap. 3) the reverse procedure, that is, the method to recover classical equations, starting from quantum equations on stochastic phase space.

A. The quantum operator of evolution: Schrödinger equation

Now, since the physical Hilbert space is $\mathcal{H}_S$, $\mathcal{H}_S$ must be invariant under evolution and then $\Pi_S U_{t_1,t_0} = U_{t_1,t_0}\Pi_S$. So for any trajectory of states $\phi_t = U_{t,t_0}(\phi_{t_0}) \in \mathcal{H}_S$. Equations (113) of Sec. V A (where quantization is missing) have not to be changed, but now we must make explicit the condition $|\phi_t\rangle = \Pi_S|\phi_t\rangle$:

$$\begin{aligned}\frac{d}{dt}\langle\phi_t|\Pi_S\vec{\mathbf{q}}\Pi_S|\phi_t\rangle &= \langle\phi_t|\Pi_S\overrightarrow{\nabla}_p H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)\Pi_S|\phi_t\rangle,\\ \frac{d}{dt}\langle\phi_t|\Pi_S\vec{\mathbf{p}}\Pi_S|\phi_t\rangle &= -\langle\phi_t|\Pi_S\overrightarrow{\nabla}_q H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)\Pi_S|\phi_t\rangle.\end{aligned} \tag{114}$$

Using the definition of $\vec{\mathbf{P}}$ and $\vec{\mathbf{Q}}$, Eqs. (114) become

$$\begin{aligned}\frac{d}{dt}\langle\phi_t|\vec{\mathbf{Q}}|\phi_t\rangle &= \langle\phi_t|\Pi_S\overrightarrow{\nabla}_p H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)\Pi_S|\phi_t\rangle,\\ \frac{d}{dt}\langle\phi_t|\vec{\mathbf{P}}|\phi_t\rangle &= -\langle\phi_t|\Pi_S\overrightarrow{\nabla}_q H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)\Pi_S|\phi_t\rangle.\end{aligned} \tag{115}$$

Before any further computation, we want first to point out that, by construction, our new dynamical equations (115) for expectation values of $\vec{\mathbf{P}}$ and $\vec{\mathbf{Q}}$ always have the same semi-classical expression given by (7) where the classical density ρ_t is given by $\rho_t(\vec{p},\vec{q}) = |\langle\vec{p},\vec{q}|\phi_t\rangle|^2$.

Now, in order to write (115) in a simplified manner, we need the following technical remarks.

Remark: General relations between commutators and derivation. We have seen that any classical quantity $f(\vec{p},\vec{q})$ is represented on $\mathcal{H}$ by the operator $\mathbf{f} = f(\vec{\mathbf{p}},\vec{\mathbf{q}})$. Taking the definition (57) of the generators $\overrightarrow{\mathbf{P}_*}$ and $\overrightarrow{\mathbf{Q}_*}$ we have

$$\begin{aligned}[\overrightarrow{\mathbf{P}_*}, f(\vec{\mathbf{p}},\vec{\mathbf{q}})] &= -i\hbar\overrightarrow{\nabla}_q f(\vec{\mathbf{p}},\vec{\mathbf{q}}),\\ [\overrightarrow{\mathbf{Q}_*}, f(\vec{\mathbf{p}},\vec{\mathbf{q}})] &= i\hbar\overrightarrow{\nabla}_p f(\vec{\mathbf{p}},\vec{\mathbf{q}}).\end{aligned} \tag{116}$$

If we project these equations on $\mathcal{H}_S$, we obtain

$$\begin{aligned}[\vec{\mathbf{P}}, \Pi_S f(\vec{\mathbf{p}},\vec{\mathbf{q}})\Pi_S] &= -i\hbar\Pi_S\overrightarrow{\nabla}_q f(\vec{\mathbf{p}},\vec{\mathbf{q}})\Pi_S,\\ [\vec{\mathbf{Q}}, \Pi_S f(\vec{\mathbf{p}},\vec{\mathbf{q}})\Pi_S] &= i\hbar\Pi_S\overrightarrow{\nabla}_p f(\vec{\mathbf{p}},\vec{\mathbf{q}})\Pi_S.\end{aligned} \tag{117}$$

This shows how commutators between $\vec{\mathbf{P}}$, $\vec{\mathbf{Q}}$ and quantized observables $\Pi_S\mathbf{f}\Pi_S$ are connected to derivations.

We are ready now to write Eqs. (115) in a simplified way, using (117):

$$\begin{aligned}\frac{d}{dt}\langle\phi_t|\vec{\mathbf{Q}}|\phi_t\rangle &= i\hbar^{-1}\langle\phi_t|[\Pi_S H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)\Pi_S, \vec{\mathbf{Q}}]|\phi_t\rangle,\\ \frac{d}{dt}\langle\phi_t|\vec{\mathbf{P}}|\phi_t\rangle &= i\hbar^{-1}\langle\phi_t|[\Pi_S H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)\Pi_S, \vec{\mathbf{P}}]|\phi_t\rangle.\end{aligned} \tag{118}$$

So, if we introduce the quantized observable $\mathbf{H}(t) = \Pi_S H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)\Pi_S$ associated with the classical Hamiltonian $H(\vec{p},\vec{q},t)$, previous equations become

$$\frac{d}{dt}\langle\phi_t|\vec{\mathbf{Q}}|\phi_t\rangle = i\hbar^{-1}\langle\phi_t|[\mathbf{H}(t),\vec{\mathbf{Q}}]|\phi_t\rangle,$$
$$\frac{d}{dt}\langle\phi_t|\vec{\mathbf{P}}|\phi_t\rangle = i\hbar^{-1}\langle\phi_t|[\mathbf{H}(t),\vec{\mathbf{P}}]|\phi_t\rangle, \tag{119}$$

or, for any initial state $\phi_0 \in \mathcal{H}_S$,

$$\frac{d}{dt}\langle\phi_0|U^\dagger_{t,t_0}\vec{\mathbf{Q}}U_{t,t_0}|\phi_0\rangle = i\hbar^{-1}\langle\phi_0|U^\dagger_{t,t_0}[\mathbf{H}(t),\vec{\mathbf{Q}}]U_{t,t_0}|\phi_0\rangle,$$
$$\frac{d}{dt}\langle\phi_0|U^\dagger_{t,t_0}\vec{\mathbf{P}}U_{t,t_0}|\phi_0\rangle = i\hbar^{-1}\langle\phi_0|U^\dagger_{t,t_0}[\mathbf{H}(t),\vec{\mathbf{P}}]U_{t,t_0}|\phi_0\rangle. \tag{120}$$

We know that these equations are solved if U_{t,t_0} is the unitary group generated by $\mathbf{H}(t)$:

$$i\hbar\frac{d}{dt}U_{t,t_0} = \mathbf{H}(t)U_{t,t_0},$$
$$U_{t_0,t_0} = \mathbf{1}. \tag{121}$$

So any trajectory of states $|\phi_t\rangle$ verifies the equation

$$i\hbar\frac{d}{dt}|\phi_t\rangle = \mathbf{H}(t)|\phi_t\rangle. \tag{122}$$

This is precisely the general form of Schrödinger equation.

So, symbolically speaking, we have solved the problem of quantum dynamics.

To finish, let us remark that the expectation value $\langle\phi_t|\mathbf{H}(t)|\phi_t\rangle$ possesses also a semi-classical expression:

$$\langle\phi_t|\mathbf{H}(t)|\phi_t\rangle = \int d^3\vec{p}\,d^3\vec{q}\,\rho_t H(\vec{p},\vec{q},t), \tag{123}$$

where $\rho_t(\vec{p},\vec{q}) = |\langle\vec{p},\vec{q}|\phi_t\rangle|^2$, because $\mathbf{H}(t) = \Pi_S H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)\Pi_S$ is the quantized version of the classical Hamiltonian (cf. Sec. X E).

Conclusion

Of course we have recovered that the evolution of states is given by Schrödinger equation. But we want to remark that our starting point for dynamics was uniquely the "weak dynamical equations" introduced early in Sec. II B 3, and by construction they are always valid using the pseudo-classical density $\rho_t(\vec{p},\vec{q}) = |\langle\vec{p},\vec{q}|\phi_t\rangle|^2$. So, we have shown, in fact, that weak dynamical equations possess solutions in $\rho_t(\vec{p},\vec{q})$ that do not follow the Liouville equation, and these other solutions are those given by quantum dynamics.

Of course, it remains to make explicit the quantum Hamiltonian $\mathbf{H}(t)$ to prove that we recover the usual expression of the Schrödinger equation. This is done in the last paragraph.

B. The quantum Hamiltonian

The general form of the classical Hamiltonian $H(\vec{p},\vec{q},t)$ is

$$H = \frac{1}{2M}(\vec{p} - e\vec{A}(\vec{q},t))^2 + V(\vec{q},t), \tag{124}$$

the quantum Hamiltonian being $\mathbf{H}(t)=\Pi_S H(\vec{\mathbf{p}},\vec{\mathbf{q}},t)\Pi_S$. The idea of using projection of the external fields as $\Pi_S V(\vec{\mathbf{q}},t)\Pi_S$ to describe the interaction of an ''extended particle'' can be found in Ref. 6, but it is not deduced from a general procedure as in our point of view. It is rather induced from external arguments. Of course some of the following computations are in the previous reference, but we prefer to recall the full procedure to obtain a global result.

To simplify computations, we study independently the free Hamiltonian, the case of interaction with a potential energy and the case of interaction with a magnetic field.

1. The free quantum Hamiltonian

The quantum Hamiltonian **H** reduces to

$$\mathbf{H}=\frac{1}{2M}\Pi_S\vec{\mathbf{p}}^2\Pi_S. \tag{125}$$

Taking into account the expression of $\langle\vec{p},\vec{q}|\vec{x},S,m\rangle$, we compute the matrix element $\langle\vec{x},S,m|\vec{\mathbf{p}}^2|\vec{y},S,m_1\rangle$ and we find

$$\langle\vec{x},S,m|\vec{\mathbf{p}}^2|\vec{y},S,m_1\rangle=-\hbar^2(\Delta\delta)(\vec{x}-\vec{y})h^3\int d^3\vec{q}\,\Phi^*_{S,m}(\vec{x}-\vec{q})\Phi_{S,m_1}(\vec{y}-\vec{q}). \tag{126}$$

From the properties of $\Delta\delta$, this expression can be split into

$$\begin{aligned}
&\langle\vec{x},S,m|\vec{\mathbf{p}}^2|\vec{y},S,m_1\rangle=A+B+C,\\
&A=-\hbar^2(\Delta\delta)(\vec{x}-\vec{y})h^3\int d^3\vec{q}\,\Phi^*_{S,m}(\vec{x}-\vec{q})\Phi_{S,m_1}(\vec{x}-\vec{q}),\\
&B=-2\hbar^2(\vec{\nabla}\delta)(\vec{x}-\vec{y})h^3\int d^3\vec{q}\,\Phi^*_{S,m}(\vec{x}-\vec{q})(\vec{\nabla}\Phi_{S,m_1})(\vec{x}-\vec{q}),\\
&C=-\hbar^2\delta(\vec{x}-\vec{y})h^3\int d^3\vec{q}\,\Phi^*_{S,m}(\vec{x}-\vec{q})(\Delta\Phi_{S,m_1})(\vec{x}-\vec{q}).
\end{aligned} \tag{127}$$

Taking into account the properties of orthogonality and normalization of the fields $\Phi_{S,m}$, we first obtain

$$A=-\hbar^2(\Delta\delta)(\vec{x}-\vec{y})\,\delta_{m,m_1}. \tag{128}$$

Now, because of the parity of $\Phi_{S,m}$, we have

$$B=0. \tag{129}$$

Finally, if we use the explicit expression (79) of $\Phi_{S,m}$ and the expression of Δ in spherical coordinates, we find

$$\begin{aligned}
&C=K\delta(\vec{x}-\vec{y})\,\delta_{m,m_1},\\
&K=\hbar^2h^3\int_0^\infty dr\{[(r\Psi)']^2+S(S+1)\Psi^2\}.
\end{aligned} \tag{130}$$

Now, we want to use the scaling on the function $\Psi(x)$ introduced in Sec. IX to exhibit the dependence of the representation in a scale length λ. We recall that we take a dimensionless mathematical function Ψ_0 such that $\Psi(x)=(\lambda h)^{-3/2}\Psi_0(x/\lambda)$. Using this scaling, we find that the previous constant K is

$$K=(\hbar\chi/\lambda)^2,$$
$$\chi^2=\int_0^\infty du\{[(u\Psi_0)']^2+S(S+1)\Psi_0^2\}, \tag{131}$$

where χ^2 is a dimensionless positive coefficient.

If we summarize this computation, we have

$$\langle\vec{x},S,m|\mathbf{H}|\vec{y},S,m_1\rangle=-(\hbar^2/2M)(\Delta\delta)(\vec{x}-\vec{y})\,\delta_{m,m_1}+E_0\,\delta(\vec{x}-\vec{y})\,\delta_{m,m_1},$$
$$E_0=\hbar^2\chi^2\lambda^{-2}/2M, \tag{132}$$

or in the operator formalism

$$\mathbf{H}=\frac{1}{2M}\vec{\mathbf{P}}^2+E_0. \tag{133}$$

We recover the usual quantum Hamiltonian of the free particle with a supplementary constant E_0. Of course this constant does not modify dynamical properties and we can simply ignore it.

But if we want to give a physical meaning to this term, we must say that the particle possesses an intrinsic proper energy. So, exactly as in Sec. IX, we must distinguish the case of true elementary particles from the case of more complex systems.

a. The case of elementary particles. For a true particle, the only possible definition of E_0 is the mass energy of the particle. Of course, we cannot directly find E_0 in the framework of nonrelativistic mechanics and then $E_0=Mc^2$ must be induced from external arguments. But if we assume this formula, we find that the scale length λ verifies

$$\lambda=\lambda_c\frac{\chi}{2\sqrt{2}\,\pi}, \tag{134}$$

where $\lambda_c=h/Mc$ is the Compton wave length.

So we recover the intuitive result of Sec. IX, where we have recognized in λ the Compton wave length. Since we are in nonrelativistic mechanics, λ must always be a very small quantity in regard to all other length scales.

b. The case of complex systems. As mentioned in Sec. IX, if the particle possesses an internal structure, we must assume that all internal degrees of freedom are frozen, and then E_0 represents the internal energy.

2. Quantum Hamiltonian with a potential energy

The quantum Hamiltonian $\mathbf{H}(t)$ reduces to

$$\mathbf{H}(t)=\frac{1}{2M}\Pi_S\vec{\mathbf{p}}^2\Pi_S+\Pi_S V(\vec{\mathbf{q}},t)\Pi_S. \tag{135}$$

Taking into account the result on the free case, we have

$$\mathbf{H}(t)=\frac{1}{2M}\vec{\mathbf{P}}^2+E_0+\Pi_S V(\vec{\mathbf{q}},t)\Pi_S. \tag{136}$$

So we have only to specify the matrix element $\langle\vec{x},S,m|V(\vec{\mathbf{q}},t)|\vec{y},S,m_1\rangle$.

After some algebra, we find

$$\langle \vec{x},S,m|V(\vec{\mathbf{q}},t)|\vec{y},S,m_1\rangle = \delta(\vec{x}-\vec{y})h^3 \int d^3\vec{q}\,V(\vec{x}-\vec{q},t)\Phi^*_{S,m}(\vec{q})\Phi_{S,m_1}(\vec{q}). \tag{137}$$

Using our scaling on the function Ψ in $\Phi_{S,m}$, we have

$$\langle \vec{x},S,m|V(\vec{\mathbf{q}},t)|\vec{y},S,m_1\rangle = \delta(\vec{x}-\vec{y}) \int d^3\vec{u}\,V(\vec{x}-\lambda\vec{u},t)\Psi_0(u)^2 Y^m_S(\hat{u})^* Y^{m_1}_S(\hat{u}), \tag{138}$$

where $\hat{u}=\vec{u}/|\vec{u}|$.

Now, if we want to simplify the previous expression, we must take into account the magnitude of λ in comparison with the length scale of variation of $V(\vec{x})$. We have seen in the previous section that λ must always be very small in regard to all other length scales, so we can use the following development in the equation (138):

$$V(\vec{x}-\lambda\vec{u},t) \simeq V(\vec{x},t) - \lambda\vec{u}\cdot\vec{\nabla}V(\vec{x},t) + \lambda^2\epsilon. \tag{139}$$

Taking into account the parity of the spherical harmonics, we obtain that the first order in λ vanishes and

$$\langle \vec{x},S,m|V(\vec{\mathbf{q}},t)|\vec{y},S,m_1\rangle = (V(\vec{x},t)\,\delta_{m,m_1} + \lambda^2\epsilon)\delta(\vec{x}-\vec{y}). \tag{140}$$

Then, up to the second order in λ, the operator $\Pi_S V(\vec{\mathbf{q}},t)\Pi_S$ can be identified with $V(\vec{\mathbf{Q}},t)$. So if we neglect the corrections in λ^2, we conclude that the quantum Hamiltonian $\mathbf{H}(t)$ is

$$\mathbf{H}(t) = \frac{1}{2M}\vec{\mathbf{P}}^2 + E_0 + V(\vec{\mathbf{Q}},t). \tag{141}$$

We recover the usual Hamiltonian of quantum mechanics.

a. The harmonic case. In the particular case where $V(\vec{\mathbf{q}}) = \frac{1}{2}m\omega^2\vec{\mathbf{q}}^2$, we can compute completely the operator $\Pi_S V(\vec{\mathbf{q}})\Pi_S$ and we obtain

$$\Pi_S V(\vec{\mathbf{q}})\Pi_S = V(\vec{\mathbf{Q}}) + E_1, \tag{142}$$

where E_1 is a supplementary constant energy given by

$$E_1 = \frac{1}{2}m\omega^2\lambda^2\eta^2 \quad \text{with} \quad \eta^2 = \int_0^\infty u^4 du\,\Psi_0(u)^2. \tag{143}$$

b. Conclusion. We recover the quantum operator of potential energy, but we see that the operator $V(\vec{\mathbf{Q}},t)$ is only an approximation (up to second order in λ) of the true quantized operator $\Pi_S V(\vec{\mathbf{q}},t)\Pi_S$. So, the prescription of the correspondence principle corresponds in fact to the limiting case $\lambda \to 0$. But, if it is possible to take this limit for $\Pi_S V(\vec{\mathbf{q}},t)\Pi_S$, we cannot do so directly with the free part of the Hamiltonian because $E_0 \propto 1/\lambda^2$: we need first to renormalize the free Hamiltonian. Moreover, if we take this limit, we lose our ''connection with the classical world'' because the value $\lambda = 0$ is forbidden for reasons of normalization: λ can be as small as you want but never cancelled.

To conclude, we can say that this approach specifies the limit of the usual correspondence principle which postulates that the classical potential $V(\vec{q},t)$ must be directly lifted into quantum Hamiltonian. In fact, mathematically speaking, the true operator $\Pi_S V(\vec{\mathbf{q}},t)\Pi_S$ depends on S and λ, but because λ is always very small (in nonrelativistic mechanics), we can physically ignore it.

The idea of using the projected field $\Pi_S V(\vec{\mathbf{q}},t)\Pi_S$ for an extended particle and the corresponding computation can be found in Ref. 6.

3. Quantum Hamiltonian with a magnetic field

To simplify computations, we only study the case of a uniform magnetic field $\vec{B}$ associated with the potential vector $\vec{A}(\vec{q})=\frac{1}{2}\vec{B}\wedge\vec{q}$. The quantum Hamiltonian $\mathbf{H}$ is

$$\mathbf{H}=\frac{1}{2M}\Pi_S[\vec{\mathbf{p}}-e\vec{A}(\vec{\mathbf{q}})]^2\Pi_S. \tag{144}$$

Developing the previous expression, we have

$$\mathbf{H}=\frac{1}{2M}\Pi_S\vec{\mathbf{p}}^2\Pi_S-\frac{e}{M}\Pi_S\vec{\mathbf{p}}\cdot\vec{A}(\vec{\mathbf{q}})\Pi_S+\frac{e^2}{2M}\Pi_S\vec{A}(\vec{\mathbf{q}})^2\Pi_S. \tag{145}$$

Using the expression of the free Hamiltonian we obtain

$$\mathbf{H}=\frac{1}{2M}\vec{\mathbf{P}}^2+E_0+\mathbf{H}_1+\mathbf{H}_2,$$

$$\mathbf{H}_1=-\frac{e}{M}\Pi_S\vec{\mathbf{p}}\cdot\vec{A}(\vec{\mathbf{q}})\Pi_S, \tag{146}$$

$$\mathbf{H}_2=\frac{e^2}{2M}\Pi_S\vec{A}(\vec{\mathbf{q}})^2\Pi_S.$$

We first look at $\mathbf{H}_1$, using the explicit form of $\vec{A}(\vec{q})$:

$$\mathbf{H}_1=-\frac{e}{2M}\Pi_S\vec{\mathbf{p}}\cdot(\vec{B}\wedge\vec{\mathbf{q}})\Pi_S=-\frac{e}{2M}\vec{B}\cdot\Pi_S\vec{\mathbf{q}}\wedge\vec{\mathbf{p}}\Pi_S. \tag{147}$$

But we have seen in Sec. X B that $\Pi_S\vec{\mathbf{q}}\wedge\vec{\mathbf{p}}\Pi_S=\vec{\mathbf{Q}}\wedge\vec{\mathbf{P}}-\vec{\mathbf{S}}$. Then,

$$\mathbf{H}_1=-\frac{e}{2M}\vec{B}\cdot(\vec{\mathbf{Q}}\wedge\vec{\mathbf{P}})+\frac{e}{2M}\vec{B}\cdot\vec{\mathbf{S}}. \tag{148}$$

We can transform again the first term to obtain

$$\mathbf{H}_1=-\frac{e}{M}(\vec{A}(\vec{\mathbf{Q}})\cdot\vec{\mathbf{P}}+\vec{\mathbf{P}}\cdot\vec{A}(\vec{\mathbf{Q}}))+\frac{e}{2M}\vec{B}\cdot\vec{\mathbf{S}}. \tag{149}$$

Since $\mathbf{H}_2$ can be seen as a harmonic potential energy, we can use the result of the previous paragraph to obtain

$$\mathbf{H}_2=\frac{e^2}{2M}\vec{A}(\vec{\mathbf{Q}})^2+E_1. \tag{150}$$

If we collect all the results, we conclude that the quantum Hamiltonian is

$$\mathbf{H}=\frac{1}{2M}[\vec{\mathbf{P}}-e\vec{A}(\vec{\mathbf{Q}})]^2+\frac{e}{2M}\vec{B}\cdot\vec{\mathbf{S}}+E_0+E_1. \tag{151}$$

So we find that our projection of the classical Hamiltonian (where spin is missing) generates directly an interaction between spin and magnetic field. Of course, if we believe in this formula,

we must say that the particle possesses a magnetic momentum $\vec{\boldsymbol{\mu}}_0 = -(e/2M)\vec{\mathbf{S}}$. Unfortunately $\vec{\boldsymbol{\mu}}_0$ does not correspond in general to the true value of $\vec{\boldsymbol{\mu}}$. The reason is that $\vec{\boldsymbol{\mu}}_0$ only describes the part of $\vec{\boldsymbol{\mu}}$ deducible from our classical Hamiltonian.

In fact, when $\vec{B}$ is uniform, we can add to $\mathbf{H}$ any supplementary term as $\mathbf{H}_I = -(g+1)(e/2M)\vec{B}\cdot\vec{\mathbf{S}}$ without changing the equations of motion for $\vec{\mathbf{P}}$ and $\vec{\mathbf{Q}}$. So, because $\vec{\mathbf{S}}$ is not a classical observable, the part of $\mathbf{H}$ that specifies the evolution of $\vec{\mathbf{S}}$ is not given by our procedure, which is only based on the classical observables $\vec{\mathbf{P}}$ and $\vec{\mathbf{Q}}$. The term $-\vec{\boldsymbol{\mu}}_0\cdot\vec{B}$ must be only seen as an indication on the form of interaction between $\vec{\mathbf{S}}$ and $\vec{B}$. Of course, adding $\mathbf{H}_I$ to our Hamiltonian allows us to recover the usual formula for $\vec{\boldsymbol{\mu}}$.

Finally, if we assume $\vec{B}$ to be nonuniform, we see that the new Hamiltonian $\mathbf{H}_I$ introduces a new dynamical coupling between classical observables and $\vec{\mathbf{S}}$. This purely quantum effect (on expectation values) cannot be reproduced by our procedure.

XIII. CONCLUSION

This analysis shows how the overlapped components of classical and quantum mechanics can be separated to give a complete sequential structure that allows a better understanding of the role of each ingredient. Moreover, we can get rid of too crude rules of quantization based only on pairs of canonical coordinates, which do not explain why only one system of canonical coordinates gives the right quantization. Our procedure also allows one to give a satisfactory explanation of the apparent illogical process that consists in building quantum dynamical equations only using classical quantities (the classical potential energy, for example). Moreover, we recover the central part played by coherent states to connect classical and quantum objects.

As specified in the Introduction and all through the text, Prugovečki's work contains a great number of key points common with this article. The main differences with this article are in the point of view (leading idea) and the way of putting together the mathematical elements. But in both cases we find the same important physical result: in general, a particle must be dressed with a ''proper wave function'' that introduces a specific length scale. All the consequences on the localizability of particles are not developed in this article, since they can be found in Prugovečki's monograph.[6]

Nevertheless, as indicated in the Introduction, this article is not ''logically complete'' because general quantum axiomatics are not rebuilt (as a change of mathematical language) from ideas of classical mechanics. So, we can look at the beginnning of this article as a ''middle-point,'' the first part will be published later.

To conclude, we can consider two natural directions of generalizations of our procedure: the first one concerns the multiparticle case and second quantization, the second one is of course special relativity (that should be intimately related to Prugovečki's work).

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Classical limit of fermions in phase space

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Using the mathematical structure of the Grassmann algebra, studied by Schönberg, we write down the Pauli equation and the Dirac equation in phase space. In addition, in order to investigate the physical nature of the spin degree of freedom inherent in these equations we set up a novel classical limiting process $\hbar \to 0$. Thus we are able to derive relativistic and nonrelativistic classical statistical mechanics, for particle with spin 1/2, within a geometric algebra framework. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1386411]

I. INTRODUCTION

Alternative formulations of the Dirac equation aim to reveal new mathematical and physical interpretations hidden in the ordinary formulation. Following this spirit, attempts of expressing the Dirac theory using a quaternionic algebra[1–4] or in terms of geometric algebra, *à la* Hestenes,[5–7] show some nontrivial results:

(i) the usual Schrödinger equation presents spin;[5,6,1]
(ii) the Dirac equation can be formulated without making reference to matrices and complex numbers;[7,8]
(iii) one avoids anomalies, ambiguities, and inconsistencies with regard to the conservation laws once calculated by using the usual methods.[9]

It is worth noticing that these algebraic versions of the Dirac equation lie on configuration space. Another way to formulate the Dirac theory is in terms of the geometric algebra, *à la* Schönberg,[10–12] initiated by Bohm and Hiley[13] and developed by Holland.[14] Here the Dirac theory lies on phase space. It is important therefore to explore some possible relations between these two algebraic-geometrical approaches. To this end, following the Bohm–Hiley–Holland method, we obtain the Pauli equation in *phase space* and point out its relationship with the Schrödinger equation (in phase space, as well). Thus we answer in a natural way how the spin may appear in the Schrödinger theory.

The present work aims also to connect the quantum theory with the classical one. We define in Sec. II a classical limiting method and apply it to the Schrödinger equation in terms of wave function $\psi(q,t)$ and Wigner function $W(q,p,t)$; we also apply this method to the usual Dirac equation. After presenting some elements of the Schönberg geometric algebra (Sec. III), in Secs. IV and V we evaluate the classical limit of the Dirac and Pauli equations in phase space, respectively. In Sec. VI final remarks are included.

II. THE CLASSICAL LIMIT $\hbar \to 0$

In order to define a classical limiting method of quantum dynamics we inspire ourselves on the purely formal works by Hermann.[15,16] The fundamental idea is to start from a given (quantum) differential equation

$$\mathcal{O}_\hbar \Xi_\hbar = 0 \tag{1}$$

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and to perform the transformation

$$\Xi'_\hbar = e^{\alpha\xi/\hbar}\Xi_\hbar \tag{2}$$

characterized by the arbitrary parameter α and by the function ξ (without $\hbar$); thus Eq. (1) turns to be

$$\overline{\mathcal{O}}^{\xi}_{\hbar}\Xi'_\hbar = 0. \tag{3}$$

By taking $\hbar \to 0$ in Eq. (3) we obtain an equation of motion only for ξ, so that any quantal information contained in Eq. (1) or (3) disappears in the classical domain. Provided asymptotic conditions are obeyed by the function $\Xi'_\hbar$ and its derivatives in the limit $\hbar \to 0$, the resulting equation for ξ is called the classical limit of Eq. (1). In other words, in our method the classical limit of quantum dynamics occurs without requiring the convergence of the function $\Xi'_\hbar$ as $\hbar \to 0$.

Below we are going to apply this method to the usual Schrödinger and Dirac equations.

A. Classical limit of the Schrödinger equation in configuration space

Let us consider a particle (an electron, for example) with mass m, charge $|e|$ under the influence of an external scalar potential $V(q^k,t)$ and of electromagnetic fields described by the equation $(k=1,2,3)$

$$\imath\hbar\frac{\partial\psi}{\partial t} + \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q^k \partial q^k} - \frac{e\hbar\imath}{c}A_K\frac{\partial\psi}{\partial q^k} - \left[\frac{e\hbar\imath}{2mc}\frac{\partial A_k}{\partial q^k} + \frac{e^2}{2mc^2}A_k^2 - e\phi - V\right]\psi = 0 \tag{4}$$

[$A_k(q^k,t)$ being the components of the vector potential and $\phi(q^k,t)$ a scalar potential; c is the speed of light]. The transformation (2), with $\Xi = \psi(q^k,t)$, leads Eq. (4) to

$$\mathcal{O}^{\xi}\psi' + \hbar\mathcal{O}^{\xi}_{(1)}\psi' + \hbar^2\mathcal{O}^{\xi}_{(2)}\psi' = 0, \tag{5}$$

where

$$\mathcal{O}^{\xi} = -\imath\alpha\frac{\partial\xi}{\partial t} - \frac{\alpha^2}{2m}\left(\frac{\partial\xi}{\partial q^k}\right)^2 + \frac{\imath e\alpha}{mc}A_k\frac{\partial\xi}{\partial q^k} + \frac{e^2}{2mc^2}A_k^2 + e\phi + V, \tag{6}$$

$$\mathcal{O}^{\xi}_{(1)} = \imath\frac{\partial}{\partial t} - \left[\frac{\alpha}{m}\frac{\partial\xi}{\partial q^k} - \frac{\imath e}{mc}A_k\right]\frac{\partial}{\partial q^k} - \left[\frac{\alpha}{2mc}\frac{\partial^2\xi}{\partial q^k\partial q^k} + \frac{\imath e}{2mc}\frac{\partial A_k}{\partial q^k}\right], \tag{7}$$

$$\mathcal{O}^{\xi}_{(2)} = \frac{1}{2m}\frac{\partial^2}{\partial q^k\partial q^k}. \tag{8}$$

Now by making $\hbar \to 0$ in Eq. (5) we arrive at

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial q^k} - \frac{e}{c}A_k\right)^2 + e\phi + V = 0, \tag{9}$$

which is the classical Hamilton–Jacobi equation, since

$$\lim_{\hbar\to 0}\psi' \sim \psi'' \neq 0, \tag{10}$$

$$\lim_{\hbar\to 0}\hbar\psi' \sim 0, \tag{11}$$

$$\lim_{\hbar\to 0} \hbar \frac{\partial \psi'}{\partial x} \sim 0 \quad (x=t,q^k), \tag{12}$$

$$\lim_{\hbar\to 0} \hbar^2 \frac{\partial^2 \psi'}{\partial q^k \partial q^k} \sim 0. \tag{13}$$

The symbol $\sim$ denotes asymptotics and therefore one does not require the existence of the classical limit of ψ'. It is important to remark that the parameter α in Eq. (5) has to be equal to ι. The identification $\xi \equiv S$ is only possible because

$$\lim_{\hbar\to 0} \hat{p}'_k = \lim_{\hbar\to 0} \left[e^{-\iota\xi/\hbar} \left(\frac{\hbar}{\iota} \frac{\partial}{\partial q^k} \right) e^{\iota\xi/\hbar} \right] = \frac{\partial \xi}{\partial q^k} = p_k . \tag{14}$$

[In the Wentzel–Kramers–Brillouin (WKB) method[17,18] such identification is introduced *ad hoc*.] It follows also that the classical limit of the commutator, i.e.,

$$\lim_{\hbar\to 0} [e^{-\iota\xi/\hbar} (\hat{q}^k \hat{p}_k - \hat{p}_k \hat{q}^k) e^{\iota\xi/\hbar} = \iota\hbar], \tag{15}$$

is $q^k p_k - p_k q^k = 0$. So we are able to answer the question: "How do noncommuting observables disappear in the classical limit." [19] (The WKB method[17,18] does not answer this question.)

As an example of the asymptotic behavior (10)–(13) let us consider the function $\psi = e^{\iota[S+(\hbar/\iota)S_1+(\hbar/\iota)^2 S_2+\cdots]/\hbar}$ and perform the transformation (2). It follows then that with this ψ' conditions (11)–(13) are obeyed, while by using the WKB approximation ($\hbar\to 0$)[17,18] about ψ' we obtain an asymptotic function $\psi'' = e^{S_1+(\hbar/\iota)S_2}$ satisfying the condition (10). Here an important point to be emphasized is that the superposition of two WKB functions, which in turn is not a WKB one, also does obey all Eqs. (10)–(13). This means that the validity conditions of the WKB method are only sufficient, but not necessary, for the classical limit of the Schrödinger equation.

B. Classical limit of the Schrödinger equation in phase space

Our classical limiting process is not constrained to configuration space. Starting with the Schrödinger equation (4) at point $q_1^k = q^k + \eta^k \hbar/2$ and its complex-conjugate at point $q_2^k = q^k - \eta^k \hbar/2$, and using the Wigner function[20]

$$W(q^k, p_k, t) = \frac{1}{(2\pi)^3} \int \rho(q_1^k, q_2^k, t) e^{-\iota p_k \eta^k} d^3\eta, \tag{16}$$

ρ being the density matrix, we obtain the Schrödinger equation in phase space

$$\iota\hbar \frac{\partial W}{\partial t} + \frac{\iota\hbar}{m} \left(p_k - \frac{e}{c} A_k \right) \frac{\partial W}{\partial q^k} + \frac{\iota e\hbar}{mc} \left(p_k - \frac{e}{c} A_k \right) \frac{\partial A_k}{\partial q^i} \frac{\partial W}{\partial p_i} + \mathcal{I} = 0 \tag{17}$$

with

$$\mathcal{I} = \int e \left[\phi\left(q^i + \frac{\hbar\eta^i}{2} \right) - \phi\left(q^i - \frac{\hbar\eta^i}{2} \right) \right] + \left[V\left(q^i + \frac{\hbar\eta^i}{2} \right) - V\left(q^i - \frac{\hbar\eta^i}{2} \right) \right] e^{-\iota p^k \eta_k} d^3\eta. \tag{18}$$

We expand the potentials ϕ and V in a Taylor series and next perform the transformation (2) with $\alpha^2 \approx 0$; by taking into account the conditions

$$\lim_{\hbar\to 0} W' \sim W'' \neq 0, \tag{19}$$

$$\lim_{\hbar\to 0}\hbar^n W'\sim 0 \quad (n=2,4,6,...,\infty), \tag{20}$$

$$\lim_{\hbar\to 0}\hbar\frac{\partial W'}{\partial x}\sim 0 \quad (x=t,q^k), \tag{21}$$

$$\lim_{\hbar\to 0}\hbar^j\frac{\partial^n W'}{\partial q^n\partial q^n}\sim 0 \quad (j,n=1,2,3,...,\infty) \tag{22}$$

[in expression (22) $n\leqslant j$ for j even and $n=j$ for j odd], we find the classical Liouville equation

$$\frac{\partial F}{\partial t}+\frac{1}{m}\left(p_k-\frac{e}{c}A_k\right)\frac{\partial F}{\partial q^k}+\left[\frac{e}{mc}\left(p_k-\frac{e}{c}A_k\right)\frac{\partial A_k}{\partial q^i}-\frac{\partial V}{\partial q^i}-e\frac{\partial\phi}{\partial q^i}\right]\frac{\partial F}{\partial p_i}=0, \tag{23}$$

where $\xi\equiv F(q^k,p_k,t)\geqslant 0$ is the probability density function. Even though our procedure of calculating the classical limit is mathematically admissible, we may justify its physical consistence only operationally. The physical significance behind the condition $\alpha^2\approx 0$ is not still clear for us.

C. Classical limit of the Dirac equation in configuration space

We perform upon the Dirac equation[21] describing a particle with spin 1/2,

$$\gamma^\mu\left(\hbar\frac{\partial}{\partial q^\mu}-\frac{\iota e}{c}A_\mu\right)\psi+mc\psi=0, \tag{24}$$

the transformation (2) with $\alpha=\iota$, take $\hbar\to 0$, and obtain

$$\gamma^\mu\left(\frac{\partial\xi}{\partial q^\mu}+\frac{\iota e}{c}A_\mu\right)+\iota mc=0 \tag{25}$$

since

$$\lim_{\hbar\to 0}\psi'\sim\psi''\neq 0, \tag{26}$$

$$\lim_{\hbar\to 0}\hbar\frac{\partial\psi'}{\partial q^\mu}\sim 0. \tag{27}$$

By squaring Eq. (25) we arrive at the relativistic Hamilton–Jacobi equation without spin:[22]

$$\left(\frac{\partial S}{\partial q^\mu}+\frac{\iota e}{c}A_\mu\right)^2+m^2c^2=0. \tag{28}$$

In the next section we present some elements of the Grassmann algebra using the Schönberg approach[10–12] in order to reformulate the algebraic content of the Dirac and Pauli equations.

III. THE GRASSMANN–SCHÖNBERG ALGEBRA G_n

Here we want to show only how the Clifford and Grassmann algebras appear connected in the Schönberg works.[10–12] Let us start with n-dimensional two Clifford algebras given by

$$[\gamma_i^{(+)},\gamma_j^{(+)}]_+=+2\eta_{ij}1_{C_n},\quad [\gamma_i^{(-)},\gamma_j^{(-)}]_+=-2\eta_{ij}1_{C_n}, \tag{29}$$

where $[A,B]_+ = AB + BA$ and 1_{C_n} is the unity of the algebra. The $\gamma_i^{(+)}$'s generate a Clifford algebra C_n^+ associated with the positive metric $+\eta_{ij}$ and the $\gamma_i^{(-)}$'s generate a Clifford algebra corresponding to the negative metric $-\eta_{ij}$ such that

$$[\gamma_i^{(+)}, \gamma_j^{(-)}]_+ = 0. \tag{30}$$

Defining the element

$$\omega = \gamma_1^{(+)} \cdots \gamma_n^{(+)} \gamma_1^{(-)} \cdots \gamma_n^{(-)}, \tag{31}$$

which anticommutes with the $\gamma_i^{(+)}$'s and $\gamma_i^{(-)}$'s, i.e.,

$$[\omega, \gamma_i^{(+)}]_+ = 0, \quad [\omega, \gamma_j^{(-)}]_+ = 0, \tag{32}$$

and also the elements

$$\overline{\gamma_i} = \gamma_i^{(+)}, \quad \bar{\bar{\gamma}}_i = \omega \gamma_i^{(-)}, \tag{33}$$

it is straightforward to verify that $\overline{\gamma_i}$ and $\bar{\bar{\gamma}}_i$ generate two Clifford algebras with the same metric η_{ij}:

$$[\overline{\gamma_i}, \overline{\gamma_j}]_+ = 2\eta_{ij} 1_{C_n} = [\bar{\bar{\gamma}}_i, \bar{\bar{\gamma}}_j]_+, \quad [\overline{\gamma_i}, \bar{\bar{\gamma}}_j]_- = 0. \tag{34}$$

The derivation of (29) and (30) from (34) is obtained by defining the element $\overline{\omega} = \overline{\gamma_1} \cdots \overline{\gamma_n} \bar{\bar{\gamma}}_1 \cdots \bar{\bar{\gamma}}_n = \omega$ and using $\overline{\gamma_i} = \gamma_i^{(+)}$ and $\gamma_i^{(-)} = \omega \bar{\bar{\gamma}}_i$ with $\omega^2 = 1_{C_n}$.

The connection with the Grassmann algebra is realized by introducing the terms $\hat{a}_i$ and $\hat{b}_i$ defined by

$$\hat{a}_1 = \frac{\gamma_i^{(+)} + \gamma_i^{(-)}}{2}, \quad \hat{b}_i = \frac{\gamma_i^{(+)} - \gamma_i^{(-)}}{2}, \tag{35}$$

which obey the following anticommutative relations:

$$[\hat{a}_i, \hat{a}_j]_+ = 0 = [\hat{b}_i, \hat{b}_j]_+, \quad [\hat{a}_i, \hat{b}_j]_+ = \eta_{ij} 1_{G_n}, \tag{36}$$

1_{G_n} being the unity of the n-dimensional Grassmann algebra G_n. In this algebra one can build the idempotent P

$$P = \hat{a}_1 \hat{b}_1 \cdots \hat{a}_n \hat{b}_n \Rightarrow P^2 = P \tag{37}$$

such that

$$\hat{a}_i P = 0 = P \hat{b}_i. \tag{38}$$

With the introduction of the algebraic elements $\mathbf{e}_{j_1 \cdots j_r}^{k_1 \cdots k_r}$ (Ref. 12)

$$\mathbf{e}_{j_1 \cdots j_r}^{k_1 \cdots k_v} = \hat{b}_{k_1} \cdots \hat{b}_{k_v} P \hat{a}_{j_r} \cdots \hat{a}_{j_1}, \tag{39}$$

it follows from the ortogonality rule

$$\mathbf{e}_{j_1 \cdots j_r}^{k_1 \cdots k_v} \mathbf{e}_{h_1 \cdots h_s}^{i_1 \cdots i_u} = \delta_{r,u} \delta_{j_1 \cdots j_r}^{i_1 \cdots i_u} \mathbf{e}_{h_1 \cdots h_s}^{k_1 \cdots k_v} \tag{40}$$

$(r,s,u,v=0,...,n;i_1,j_1,k_1,h_1<\cdots<i_u,j_r,k_v,h_s;i,j,k,h=1,...,n)$ that Eq. (39) does form a set of 2^{2n} linearly independent elements and therefore it does constitute a basis for G_n. Hence the general element $\Gamma\in G_n$ reads

$$\Gamma=\sum_{r,v}^{0,...,n}\frac{1}{r!v!}[A]^{j_1\cdots j_r}_{k_1\cdots k_v}\mathbf{e}^{k_1\cdots k_v}_{j_1\cdots j_r}, \tag{41}$$

where the coefficients $[A]$'s are antisymmetrical with respect to the j's and k's separately. P is a primitive idempotent because $\Gamma P\Gamma=[A]\Gamma$, $\forall\Gamma\in G_n$. The unity element of G_n is given by

$$1_{G_n}=\sum_{r}^{0,...,n}\frac{1}{r!}\mathbf{e}^{j_1\cdots j_r}_{j_1\cdots j_r} \tag{42}$$

with implicit sum in $j(=1,...,n)$. Multiplying (41) to the left by P we obtain the Schönberg spinor

$$\Psi=\sum_{r}^{0,...,n}\frac{1}{r!}[A]_{k_1\cdots k_r}\mathbf{e}^{k_1\cdots k_r} \tag{43}$$

as a general element of G_nP (the minimal left ideal of G_n) which is an n-dimensional linear space with 2^n linearly independent elements.

IV. CLASSICAL LIMIT OF THE DIRAC EQUATION IN PHASE SPACE

We initially start from the Dirac equation and its adjoint for the wave function ψ of an electron with mass m and charge $|e|$ at two points q_1^μ and q_2^μ of space–time:

$$[\gamma^\mu\pi_\mu(q_1^\alpha)+mc]\psi(q_1^\alpha)=0, \tag{44}$$

$$\overline{\psi}(q_2^\nu)[\pi_\mu^\dagger(q_2^\alpha)\gamma^\mu-mc]=0. \tag{45}$$

Here $\pi_\mu(q_1^\alpha)=\hbar(\partial/\partial q_1^\mu)-(\imath e/c)A_\mu(q_1^\alpha)$, $\pi_\mu^\dagger(q_2^\alpha)=\hbar(\partial/\partial q_2^\mu)+(\imath e/c)A_\mu(q_2^\alpha)$, $\overline{\psi}=\psi^\dagger\gamma^4$, and $A_\mu=(\mathbf{A},\imath A_0)$, where $\mathbf{A}$ is the potential vector and A_0 the scalar potential. The Dirac matrices γ^μ generate the Clifford algebra C_4 with unity 1_{C_4}:

$$[\gamma^\mu,\gamma^\nu]_+=2g^{\mu\nu}1_{C_4} \tag{46}$$

$[g^{\mu\nu}=\mathrm{diag}(1,1,1,-1)]$. We multiply (44) by $\overline{\psi}(q_2^\alpha)$ and (45) by $\psi(q_1^\alpha)$ and obtain two equations for the density matrix $\rho(q_1^\alpha,q_2^\alpha)=\psi(q_1^\alpha)\overline{\psi}(q_2^\alpha)$, interpreted here as a general element of the Clifford algebra, i.e.,

$$\rho=C_0.1_{C_4}+C_\mu\gamma^\mu+C_{\mu\nu}\gamma^\mu\gamma^\nu+C_{\mu\nu\lambda}\gamma^\mu\gamma^\nu\gamma^\lambda+C_{\mu\nu\lambda\alpha}\gamma^\mu\gamma^\nu\gamma^\lambda\gamma^\alpha, \tag{47}$$

where the C's are coefficients of q_1^α and q_2^α. We now lift these two equations to a higher dimension space that we call *superspace*,[13,14]

$$[\tilde{\gamma}^\mu\pi_\mu(q_1^\alpha)+mc]\xi=0, \tag{48}$$

$$[\tilde{\gamma}^\mu\pi_\mu^\dagger(q_2^\alpha)-mc]\xi=0, \tag{49}$$

with

$$\tilde{\gamma}^\mu=\gamma^\mu\otimes 1_{C_4},\quad \tilde{\gamma}^\mu=1_{C_4}\otimes\gamma^\mu,\quad \xi\equiv\xi(q_1^\alpha,q_2^\alpha)=(\rho\otimes 1_{C_4})\Lambda. \tag{50}$$

The symbol $\otimes$ denotes the direct product. The arrows above γ^{μ} indicate the sense in which the multiplication is realized about ξ. The element Λ is a primitive idempotent belonging to the algebra of *superspace* $G_4 = C_4 \otimes C_4$. The density supermatrix $\rho(q_1^{\alpha}, q_2^{\alpha}) \otimes 1_{C_4}$ then should be associated with two Clifford algebras with the same metric

$$\rho \otimes 1_{C_4} = d_0 . 1_{C_4} + \cdots + d_{\mu\nu\lambda\alpha} \vec{\gamma}^{\mu} \vec{\gamma}^{\nu} \vec{\gamma}^{\lambda} \vec{\gamma}^{\alpha} = \sum_{A}^{16} d_A \vec{\gamma}^{A}, \tag{51}$$

$$\rho \otimes 1_{C_4} = d_0 . 1_{C_4} + \cdots + d_{\mu\nu\lambda\alpha} \tilde{\gamma}^{\mu} \tilde{\gamma}^{\nu} \tilde{\gamma}^{\lambda} \tilde{\gamma}^{\alpha} = \sum_{A}^{16} d_A \tilde{\gamma}^{A}. \tag{52}$$

With $\Lambda \equiv P$ the function ξ is considered as the Schönberg spinor $\Psi \in G_4 P$ given by (43), i.e., ξ is an element belonging to the minimal left ideal of the algebra G_4 because defining

$$\vec{\gamma}^{\mu} = \hat{a}^{\mu} + \hat{b}^{\mu} \tag{53}$$

and

$$\tilde{\gamma}^{\mu} = \omega(\hat{a}^{\mu} - \hat{b}^{\mu}) \tag{54}$$

we have

$$\vec{\gamma}^{j_1} \cdots \vec{\gamma}^{j_k} P = \hat{a}^{j_1} \cdots \hat{a}^{j_k} P, \quad \tilde{\gamma}^{j_1} \cdots \tilde{\gamma}^{j_k} P = \hat{a}^{g_1} \cdots \hat{a}^{j_k} P. \tag{55}$$

Using (53), (54), and $\omega^2 = 1_{G_4}$, Eqs. (48) and (49) can be written in terms of $\hat{a}^{\mu}$, $\hat{b}^{\mu}$ as

$$[(\hat{a}^{\mu} + \hat{b}^{\mu}) \pi_{\mu}(q_1^{\alpha}) + mc] \Psi = 0, \tag{56}$$

$$[(\hat{a}^{\mu} - \hat{b}^{\mu}) \pi_{\mu}^{\dagger}(q_2^{\alpha}) - \omega mc] \Psi = 0. \tag{57}$$

Adding and subtracting (56) and (57), changing the variables

$$q^{\alpha} = \frac{q_1^{\alpha} + q_2^{\alpha}}{2}, \quad \eta^{\alpha} = \frac{q_1^{\alpha} - q_2^{\alpha}}{\hbar}, \tag{58}$$

and performing the relativistic Wigner transformation

$$\mathcal{W}(q^{\alpha}, p_{\alpha}) = \frac{1}{(2\pi)^4} \int \Psi\left(q^{\alpha} + \frac{\hbar \eta^{\alpha}}{2}, q^{\alpha} - \frac{\hbar \eta^{\alpha}}{2} \right) e^{-\iota p_{\alpha} \eta^{\alpha}} d^4 \eta, \tag{59}$$

we obtain two Dirac equations in relativistic quantum phase space

$$O^{\mu} \mathcal{W} \equiv \hat{a}^{\mu} \hbar \left(\frac{\partial}{\partial q^{\mu}} - \frac{e}{c} \frac{\partial A_{\mu}}{\partial q^{\alpha}} \frac{\partial}{\partial p_{\alpha}} \right) \mathcal{W} - 2\iota \hat{b}^{\mu} \left(p_{\mu} + \frac{e}{c} A_{\mu} \right) \mathcal{W} = mc(\omega - 1) \mathcal{W}, \tag{60}$$

$$\overline{O}^{\mu} \mathcal{W} \equiv \hat{b}^{\mu} \hbar \left(\frac{\partial}{\partial q^{\mu}} - \frac{e}{c} \frac{\partial A_{\mu}}{\partial q^{\alpha}} \frac{\partial}{\partial p_{\alpha}} \right) \mathcal{W} - 2\iota \hat{a}^{\mu} \left(p_{\mu} + \frac{e}{c} A_{\mu} \right) \mathcal{W} = -mc(\omega + 1) \mathcal{W}, \tag{61}$$

with the following approximation:

$$A_{\mu}\left(q^{\alpha} \pm \frac{\hbar}{2} \eta^{\alpha} \right) \approx A_{\mu}(q^{\alpha}) \pm \frac{\hbar}{2} \eta^{\alpha} \frac{\partial A_{\mu}}{\partial q^{\alpha}}. \tag{62}$$

Now squaring Eqs. (60) and (61), i.e., evaluating the relations

$$(O^{\beta}O^{\mu}+O^{\mu}O^{\beta})\mathcal{W}=4m^2c^2(1-\omega)^2\mathcal{W}, \tag{63}$$

$$(\overline{O}^{\beta}\overline{O}^{\mu}+\overline{O}^{\mu}\overline{O}^{\beta})\mathcal{W}=4m^2c^2(1+\omega)^2\mathcal{W}, \tag{64}$$

we obtain, after adding (63) and (64), the Dirac equation in Liouvillian form

$$\frac{\iota\hbar}{m}g^{\beta\mu}\left(p_{\mu}+\frac{e}{c}A_{\mu}\right)\frac{\partial\mathcal{W}}{\partial q^{\beta}}+\left[\frac{\hbar\mu_0}{4}S^{\beta\mu}_{(+)}\frac{\partial F_{\beta\mu}}{\partial q^{\alpha}}-\frac{\iota\hbar e}{mc}g^{\beta\mu}\left(p_{\mu}+\frac{e}{c}A_{\mu}\right)\frac{\partial A_{\beta}}{\partial q^{\alpha}}\right]\frac{\partial\mathcal{W}}{\partial p^{\alpha}}=\Delta\mathcal{W} \tag{65}$$

with

$$\Delta=mc^2-\iota\mu_0 S^{\beta\mu}_{(-)}F_{\beta\mu}. \tag{66}$$

Here $\mu_0=e\hbar/2mc$ is the magnetic moment of the electron spin, whereas

$$S^{\beta\mu}_{(+)}=\hat{a}^{\beta}\hat{a}^{\mu}+\hat{b}^{\beta}\hat{b}^{\mu},\quad S^{\beta\mu}_{(-)}=\hat{a}^{\mu}\hat{b}^{\beta}-\hat{a}^{\beta}\hat{b}^{\mu} \tag{67}$$

are spin terms coupled to the electromagnetic field. [Without these terms (67) the function $\mathcal{W}$ cannot be interpreted as a constant of the motion due to the presence of mass in Eq. (65). This detail is neglected in Refs. 13 and 14.] The relativistic Wigner function $\mathcal{W}(q^{\alpha},p_{\alpha})$ is an algebraic spinor of the form (43) due to the fact that

$$\mathcal{W}(q^{\alpha},p_{\alpha})=\sum_{s}^{0,\ldots,4}\frac{1}{s!}W_{j_i\cdots j_s}\mathbf{e}^{j_1\cdots j_s}, \tag{68}$$

where the coefficients W are the following functions of q^{μ},p_{μ}:

$$W_{j_1\cdots j_s}=\frac{1}{(2\pi)^4}\int A_{j_1\cdots j_s}e^{-\iota p_{\alpha}\eta^{\alpha}}d^4\eta. \tag{69}$$

It follows then that the information about the spin degree of freedom should also appear in the tensorial structure of $\mathcal{W}$ because we believe that in the absence of field ($A_{\mu}=0$) the particle still has *objectively* spin. Without the spin freedom we have a relativistic equation in phase space for a scalar function $W(q_{\alpha},p_{\alpha})$ describing a fermion.

Now performing the transformation (2) in relativistic quantum phase space given by

$$\mathcal{W}'=T_{\mathcal{F}}\mathcal{W},\quad T_{\mathcal{F}}=e^{\iota\mathcal{F}/\hbar}, \tag{70}$$

and making $\hbar\to 0$ we obtain

$$\frac{1}{m}g^{\beta\mu}\left(p_{\mu}+\frac{e}{c}A_{\mu}\right)\frac{\partial\mathcal{F}}{\partial q^{\beta}}+\left[\frac{e}{mc}g^{\beta\mu}\left(p_{\mu}+\frac{e}{c}A_{\mu}\right)\frac{\partial A_{\beta}}{\partial q^{\alpha}}\right]\frac{\partial\mathcal{F}}{\partial p^{\alpha}}=mc^2\mathcal{F}, \tag{71}$$

since $\lim_{\hbar\to 0}\mathcal{W}'\sim\mathcal{W}''\neq 0$, $\lim_{\hbar\to 0}\hbar\partial\mathcal{W}'/\partial x\sim 0(x=q^{\alpha},p_{\alpha})$. Here $\mathcal{F}$ is the element

$$\mathcal{F}=\sum_{t}^{0,\ldots,4}\frac{1}{t!}F^{k_1\cdots k_t}_{k_1\cdots k_t}\mathbf{e}^{k_1\cdots k_t}_{k_1\cdots k_t} \tag{72}$$

of the algebra G_4 because $T_{\mathcal{F}}^{-1}T_{\mathcal{F}}=T_{\mathcal{F}}T_{\mathcal{F}}^{-1}=1_{G_4}\Rightarrow\mathcal{F}\in G_4$ [see Eq. (40)].

Equation (71) is the relativistic Liouville equation for the probability distribution function $\mathcal{F}(q^{\mu},p_{\mu})$ for a classical system with spin 1/2.

V. CLASSICAL LIMIT OF THE PAULI EQUATION IN PHASE SPACE

It is well known that the nonrelativistic limit of the Dirac equation is the Pauli equation. Our objective in this section is also to write down the Pauli equation in phase space within the Schönberg geometric algebra. Starting from the usual Pauli equation[23] at point q_1^k,

$$\imath\hbar\frac{\partial\psi}{\partial t}+\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q_1^k\partial q_1^k}-\frac{e\hbar\imath}{c}A_k\frac{\partial\psi}{\partial q_1^k}-\frac{e\hbar\imath}{2mc}\frac{\partial A_k}{\partial q_1^k}\psi-\frac{e^2}{2mc^2}A_k^2\psi-e\phi\psi+\frac{e\hbar}{2mc}\sigma_kB^k\psi=0, \tag{73}$$

where B^k are the magnetic field components, and its complex conjugate at point q_2^k, following the Bohm–Hiley–Holland method presented in Sec. IV, we arrive at the Pauli equation in *superspace*,

$$\begin{aligned}\imath\hbar\frac{\partial\xi}{\partial t}-\frac{\hbar^2}{2m}\left[\frac{\partial^2\xi}{\partial q_2^k\partial q_2^k}-\frac{\partial^2\xi}{\partial q_1^k\partial q_1^k}\right]-\frac{\imath e\hbar}{mc}\left[A_k(q_1^i)\frac{\partial\xi}{\partial q_1^i}+A_k(q_2^i)\frac{\partial\xi}{\partial q_2^i}\right]-\frac{e\imath\hbar}{2mc}\left(\frac{\partial A_k}{\partial q_1^k}+\frac{\partial A_k}{\partial q_2^k}\right)\xi\\ -\frac{e^2}{2mc^2}[A_k^2(q_1^i)-A_k^2(q_2^i)]\xi-e[\phi(q_1^i)-\phi(q_2^i)]\xi-\frac{e\hbar}{2mc}[B^k(q_2^k)\xi\tilde{\sigma}_k-B^k(q_1^k)\vec{\sigma}_k\xi]\end{aligned} \tag{74}$$

with

$$\xi(q_1^k,q_2^k,t)=[\rho(q_1^k,q_2^k,t)\otimes 1_{C_3}\otimes 1_{C_3}]\Lambda, \tag{75}$$

$$\vec{\sigma}_k=(\sigma_k\otimes 1_{C_3}\otimes 1_{C_3}),\quad \tilde{\sigma}_k=(1_{C_3}\otimes 1_{C_3}\otimes\sigma_k). \tag{76}$$

In phase space we find

$$\begin{aligned}\imath\hbar\frac{\partial\mathcal{W}}{\partial t}+\frac{\imath\hbar}{m}\left(p_k-\frac{e}{c}A_k\right)\frac{\partial\mathcal{W}}{\partial q^k}+\frac{\imath e\hbar}{mc}\left(p_k-\frac{e}{c}A_k\right)\frac{\partial A_k}{\partial q^i}\frac{\partial\mathcal{W}}{\partial p_i}\\ +\int e\left[\phi\left(q^i+\frac{\hbar\eta^i}{2}\right)-\phi\left(q^i-\frac{\hbar\eta^i}{2}\right)\right]\Psi e^{-\imath p_k\eta^k}d^3\eta+\mathcal{N}\mathcal{W}=0,\end{aligned} \tag{77}$$

with

$$\mathcal{N}=\mu_0S_{(-)}^kB_k=\mu_0[(\hat{a}^k+\hat{b}^k)-\omega(\hat{a}^k-\hat{b}^k)]B_k. \tag{78}$$

The solution of (77), $\mathcal{W}\in G_3P$, has the form

$$\mathcal{W}(q^k,p_k,t)=W+W_i\mathbf{e}^i+W_{ij}\mathbf{e}^{ij}+W_{ijl}\mathbf{e}^{ijl}. \tag{79}$$

Again the spin appears generating a coupling between its magnetic moment and the magnetic field and also in the tensorial structure of $\mathcal{W}$ (79). Neglecting the magnetic moment ($\mu_0=0$) we note that Eq. (77) is the Schrödinger equation (with spin) in phase space. Considering only the scalar part of $\mathcal{W}$, i.e., $\mathcal{W}\equiv W$, we reobtain Eq. (17) which does not contain spin. Thus with the reformulation of the Pauli equation in phase space on the basis of the geometric algebra we conclude that the spin freedom *may* be present in the Schrödinger theory. Therefore Hestenes' statement[5] ''spin is already in the Schrödinger equation'' seems to us very strong.

When we calculate the classical limit of Eq. (77), after performing the transformation (2), for $\Psi\equiv\mathcal{W}$ and $\alpha^2\approx 0$, and taking the limit $\hbar\to 0$, we get

$$\frac{\partial\mathcal{F}}{\partial t}+\frac{1}{m}\left(p_k-\frac{e}{c}A_k\right)\frac{\partial\mathcal{F}}{\partial q^k}+\left[\frac{e}{mc}\left(p_k-\frac{e}{c}A_k\right)\frac{\partial A_k}{\partial q^i}-e\frac{\partial\phi}{\partial q^i}\right]\frac{\partial\mathcal{F}}{\partial p_i}=0 \tag{80}$$

with $\mathcal{F}\in G_3$, that is, Eq. (80) is the Liouville equation with spin 1/2 in the nonrelativistic domain. If this degree of freedom is neglected we obtain Eq. (23) (without spin).

VI. CONCLUDING REMARKS

It is common (in the textbook literature) to find, associated with the problem of the classical limit of quantum mechanics, the well-known Ehrenfest theorem. Although Pauli[22] emphasized in 1933 that the transition *quantum→classical* is not complete using such a theorem, only recently[24] one has shown definitely that the validity conditions of the Ehrenfest theorem are neither necessary nor sufficient to characterize the classical domain. Alternatively, in this article we have defined a general method of evaluating the classical limit $\hbar\to 0$ of quantum-mechanical equations of motion depending on the asymptotic (or semiclassical) behavior of the quantum state, thus avoiding the question whether the classical limit of a quantum statum is an ensemble of classical trajectories or a single classical trajectory.[24] Applying it to the Schrödinger equation we showed that the validity conditions of the WKB approximation are only sufficient, but not necessary, to obtain the classical Hamilton–Jacobi equation, while the classical limit of the Schrödinger equation in terms of Wigner function leads correctly to the Liouville equation without using the high-temperature condition of Ref. 25.

In Refs. 13 and 14 Bohm, Hiley, and Holland studied the Dirac equation in phase space by means of geometric algebra. In the present article we were also able to put the Pauli equation (and consequently the Schrödinger equation) within this same algebraic structure. In our approach spin is seen as giving rise to a magnetic moment which couples with the external magnetic field and as a tensorial property inherent in the Schönberg–Grassmann algebra. This interpretation is different from that given in Refs. 13 and 14 where in the absence of spin the Schönberg spinor $\mathcal{W}$, solution of Eq. (65), is considered as a constant of the motion.

When we calculate the classical limit of the Pauli equation and the Dirac equation in phase space we get two peculiar results from our classical limiting process. The first one concerns the physical nature of spin: this degree of freedom is a property hidden in the antisymmetric tensors; this occurs both in the classical domain and the quantum one. The other result supports the view that the coupling between the magnetic moment, generated by the spin, and electromagnetic field is the intrinsically quantum feature.

Finally we point out that our present work leaves two questions open:

(α) What is the physical reason for the assumption that the parameter α, in the definition of the classical limiting process (2), should be considered arbitrary?

(β) What are the advantages of formulating (relativistic and nonrelativistic) classical statistical mechanics in terms of geometric algebra?

We hope that future papers can clarify these questions.

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The absolute definition of the phase-shift in potential scattering[a)]

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The variable phase approach to potential scattering with regular spherically symmetric potentials satisfying Eq. (1), and studied by Calogero in his book [*Variable Phase Approach to Potential Scattering* (Acadamic, New York, 1967)] is revisited, and we show directly that it gives the absolute definition of the phase-shifts, i.e., the one which defines $\delta_\ell(k)$ as a continuous function of k for all $k \geqslant 0$, up to infinity, where $\delta_\ell(\infty)=0$ is automatically satisfied. This removes the usual ambiguity $\pm n\pi$, n integer, attached to the definition of the phase-shifts through the partial wave scattering amplitudes obtained from the Lippmann–Schwinger integral equation, or via the phase of the Jost functions. It is then shown rigorously, and also on several examples, that this definition of the phase-shifts is very general, and applies as well to all potentials which have a strong repulsive singularity at the origin, for instance those which behave like gr^{-m}, $g>0$, $m \geqslant 2$, etc. We also give an example of application to the low-energy behavior of the S-wave scattering amplitude in two dimensions, which leads to an interesting result. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1389090]

I. INTRODUCTION

In quantum scattering theory with a spherically symmetric potential $V(r)$, the phase-shift, defined for each partial-wave by the asymptotic behavior of the radial wave function at large distances, has the usual ambiguity of $\pm \pi n$, n integer. When the potential is regular, i.e., is $L^1(a,\infty)$, and satisfies the Bargmann–Jost–Kohn condition[1–3]

$$\int_0^\infty r|V(r)|\,dr<\infty, \tag{1}$$

one can show that the phase-shift $\delta_\ell(k)$ at infinite energy satisfies the condition

$$\mathrm{tg}\,\delta_\ell(\infty)=0, \quad \text{or} \quad \sin\delta_\ell(\infty)=0, \tag{2}$$

so that one can make the ''canonical'' choice

$$\delta_\ell(\infty)=0, \tag{3}$$

and then proceed downwards by continuity for finite values of k.

The same ambiguity exists, of course, when the phase-shift is defined through the phase of the Jost function[1–3]. The problem becomes even more serious when the potential is singular and repulsive near $r=0$, and short-range otherwise:

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$$V(r) \underset{r\to 0}{\simeq} g r^{-m}, \quad g>0, \quad m>2; \quad \underset{r\to 0}{\simeq} g \exp(\alpha/r), \quad g>0, \quad \alpha>0; \quad \text{etc.} \tag{4}$$

In these cases, one can still define the S-matrix, $S_\ell = \exp(2i\delta_\ell(k))$, with a continuous phase-shift $\delta_\ell(k)$, which is again given by the asymptotic behavior of the wave function for $r\to\infty$. However, now, one has[4–6]

$$\delta_\ell(\infty) = -\infty, \tag{5}$$

and this adds to the difficulty of finding a unique phase-shift.

From the above remarks, it would seem therefore satisfactory to find a unique definition of the phase-shift itself by some formula containing $V(r)$ and the wave function, and such that (3) is automatically satisfied when the potential satisfies (1), and then, to see whether such a definition can be extended, eventually with some modification, to potentials which are singular at $r=0$ or at $r=\infty$ (long range).

The answer to the above quest has already been found, although not written down explicitly in the form (20) we give later. It is given by the variable phase method.[7] To simplify the algebra, and see what is essential, let us take the case of the S-wave, $\ell=0$. We have the radial Schrödinger equation

$$\begin{gathered} \varphi''(k,r) + k^2 \varphi(k,r) = V(r)\varphi(k,r) \\ r \in [0,\infty), \quad \varphi(0)=0, \quad \varphi'(0)=1. \end{gathered} \tag{6}$$

If we write now the wave function as

$$\begin{gathered} \varphi = A(k,r)\sin[kr+\delta(k,r)], \\ A(k,r) \geqslant 0, \quad A(k,0)\neq 0, \quad \delta(k,0)=0, \end{gathered} \tag{7}$$

it can be shown that one has formally the differential equation[7]

$$\begin{gathered} \frac{d}{dr}\delta(k,r) = -\frac{1}{k}V(r)\sin^2[kr+\delta(k,r)], \\ \delta(k,0)=0, \end{gathered} \tag{8}$$

and then

$$A(k,r) = \frac{1}{k}\exp\frac{1}{2}k\int_0^r V(t)\sin 2[kt+\delta(k,t)]\,dt, \tag{9}$$

provided (8) has a solution, and the integral in (9) is finite. We shall see this in a moment. In essence, A is the amplitude of the wave function φ, whose oscillations are given by $\sin[kr+\delta(k,r)]$. The function $\delta(k,r)$ can be interpreted as the local phase-shift since $\delta(k,R)$ is the phase-shift due to the cut potential $V(r)\theta(R-r)$. The total phase-shift is defined as

$$\delta(k) = \lim_{r\to\infty} \delta(k,r). \tag{10}$$

In order to see whether (8) has a unique solution, we can write it as

$$\delta(k,r) = -\frac{1}{k}\int_0^r V(t)\sin^2[kt+\delta(k,t)]\,dt. \tag{11}$$

One can then try to solve this nonlinear integral equation by iteration, starting from the zeroth order approximation

$$\delta^{(0)}(k,r)=0. \tag{12}$$

Numerical calculations show that this process is fast converging for usual regular potentials used in nuclear physics, and indeed has been used in practice.

From (11), it is obvious that the phase-shift is given by

$$\delta(k)=-\frac{1}{k}\int_0^\infty V(r)\sin^2[kr+\delta(k,r)]dr. \tag{13}$$

This formula shows that, for short-range potentials, the tail of the integral,

$$\left|-\frac{1}{k}\int_R^\infty V(r)\sin^2[kr+\delta(k,r)]dr\right|\leqslant\frac{1}{k}\int_R^\infty|V(r)|dr, \tag{14}$$

can be made very small if we choose R larger than the ''range'' of the potential.

In order to study the nonlinear integral equation (11) in a rigorous way, we can use the inequality[1,3]

$$|\sin x|\leqslant C\frac{|x|}{1+|x|},\quad x\ \text{real}, \tag{15}$$

where C is an appropriate constant. Noting that $x/(1+x)$ is an increasing function of x for x positive, we have

$$|\sin(x+y)|\leqslant C\frac{|x+y|}{1+|x+y|}\leqslant C\frac{|x|+|y|}{1+|x|+|y|}. \tag{16}$$

Using this in the integral equation (11), we find

$$|\delta(k,r)|\leqslant\frac{C^2}{k}\int_0^r|V(t)|\left[\frac{kt+|\delta(k,t)|}{1+kt+|\delta(k,t)|}\right]^2dt,\quad k>0. \tag{17}$$

It is then obvious that an upper bound $\Delta(k,r)$ for $|\delta(k,r)|$ is obtained from the solution of the integral equation

$$\Delta(k,r)=\frac{C^2}{k}\int_0^r|V(t)|\left[\frac{kt+\Delta(k,t)}{1+kt+\Delta(k,t)}\right]^2dt. \tag{18}$$

We can again solve this integral equation by iteration, starting from $\Delta^{(0)}=0$. It is obvious here that the solution cannot become infinite at any point on $[0,\infty)$. Indeed, if $\Delta(k,r)$ becomes infinite at $r=r_1$, then, as $r\uparrow r_1$, the fraction in (18) becomes one, and since V is supposed to be L^1, we get a contradiction.

We show in Appendix A that the equation (18) has always a unique solution for all values of $k>0$, provided V satisfies (1), and therefore that (11) also has a unique solution. We show also that $\lim_{k\to\infty}\Delta(k,\infty)=0$, from which we conclude then directly that we have (3). However, it is not really necessary to use the integral equation. Indeed, as we shall see in the next section, we can express the right-hand side of (11) in terms of the regular solution φ given by (6), and its derivative φ', to obtain the new formulas

$$\delta(k,r)=-k\int_0^r V(t)\frac{\varphi^2(k,t)}{\varphi'^2(k,t)+k^2\varphi^2(k,t)}dt, \tag{19}$$

and

$$\delta(k) = -k \int_0^\infty V(r) \frac{\varphi^2}{\varphi'^2 + k^2 \varphi^2} dr. \tag{20}$$

We shall see in the next section how to generalize these equations to higher ℓ. Likewise, the amplitude $A(k,r)$ can also be written as[7]

$$A(k,r) = \frac{1}{k} \sqrt{\varphi'^2 + k^2 \varphi^2}. \tag{21}$$

Now, we know, quite generally, that for potentials satisfying (1), the wave function $\varphi(k,r)$ exists for all values of k, real or complex, and all values of $r \geqslant 0$.[1–3] Likewise for $\varphi'(k,r)$, and we have, of course,

$$\varphi'(k,0) = 1, \quad \varphi(k,r) \underset{r \to 0}{=} r + r o(1). \tag{22}$$

Moreover, we have also that φ and φ', for any fixed real $k > 0$, are real and continuous function of r, and bounded as $r \to \infty$. Also, from the general theory of differential equations, we know that, for any k, φ and φ' cannot vanish simultaneously at any point $r = r_0 \geqslant 0$, since this would entail that $\varphi \equiv 0$, a contradiction with $\varphi'(k,0) = 1$. It follows that, because of (1), the integrals in (19) and (20) are absolutely convergent for all real values of $k > 0$, and define continuous functions of k. Therefore, (19) and (20) define, in a very nice and simple way, the ''local'' and the total phase-shift, respectively. We shall come in the third section to the case $k = 0$.

Several remarks are now in order. First of all, (20) shows that, for a potential of a given sign, the phase-shift has the opposite sign, something well-knowna,[1,2] and also obvious on (11) and (13). Second, it is obvious on (19) and (20) that the phase-shift is independent of the amplitude of φ. Multiplying φ by a constant factor $\lambda(k)$ independent of r leaves (19) and (20) invariant. This is as expected, of course. Finally, from (21) we find

$$A(k,r) > 0, \quad A(k,0) = \frac{1}{k} \neq 0, \tag{23}$$

which was assumed in (7). Now, for $r \to \infty$, the asymptotic behavior of φ and φ' are given by[1–3]

$$\varphi(k,r) \underset{r \to \infty}{\simeq} \frac{|F(k)|}{k} \sin(kr + \delta) + o(1), \tag{24}$$

and

$$\varphi'(k,r) \underset{r \to \infty}{\simeq} |F(k)| \cos(kr + \delta) + o(1), \tag{25}$$

where $F(k)$ is the Jost function, which never vanishes for $k > 0$.[1–3] Using now (24) and (25) in (21), we find

$$A(k,\infty) = \frac{|F(k)|}{k}, \tag{26}$$

and this, used in (7), leads again to (24), a consistency check.

We have now to see whether, for regular potentials satisfying (1), the phase-shift defined by (20) satisfies (3): $\delta(\infty) = 0$. This is very easy to check. Indeed, for k real and going to infinity, we have uniformly in r,[1,3] for any $r \in [0,R]$, $R < \infty$,

$$\varphi(k,r) \underset{k\to\infty}{=} \frac{\sin kr}{k} + \frac{1}{k}o(1), \tag{27}$$

and

$$\varphi'(k,r) \underset{k\to\infty}{=} \cos kr + o(1). \tag{28}$$

Using these in (20), together with (14), leads to

$$\delta(k) \underset{k\to\infty}{\simeq} -k\int_0^R V(r)\frac{\sin^2 kr}{k^2}dr = -\int_0^R V(r)\frac{1-\cos 2kr}{2k}dr = -\int_0^R V(r)dr\int_0^r \sin 2ktdt$$
$$= -\int_0^R \sin 2ktdt\left(\int_t^R V(r)dr\right). \tag{29}$$

Now, in general, $W(t)=\int_t^\infty V(r)dr$ is $L^1(0,\infty)$. Indeed

$$\int_0^\infty |W(t)|\,dt = \int_0^\infty dt\left|\int_t^\infty V(r)dr\right| \leq \int_0^\infty dt\int_t^\infty |V(r)|\,dr = \int_0^\infty |V(r)|\,dr\int_0^r dt = \int_0^\infty r|V(r)|\,dr < \infty \tag{30}$$

by virtue of (1). Therefore, in the last integral in (29) we have a Fourier sine transform of an L^1 function. From the Riemann–Lebesgue lemma, it follows that, as $k\to\infty$, it vanishes. Therefore, $\delta(k\to\infty)=0$. This argument, which is quite general, can be made more precise (see Appendix B). It follows that the definition of the phase-shift given by (20) in terms of the well-defined regular solution φ, (6), is indeed an absolute definition of $\delta(k)$ for all $k>0$ satisfying automatically (3).

We shall see later that (20) can be extended to potentials which are outside the Bargmann–Jost–Kohn class, especially to those potentials which are strongly repulsive at $r=0$. We are going now to give first the derivation of (8), (9) and (21). These are found essentially in Ref. 7, except for the integral forms (19) and (20), which are the basic equations of our article. We reproduce the proofs for the convenience of the reader.

II. DERIVATION OF (19) AND (20)

We follow the usual method given in Ref. 7 for deriving the differential equation (8). Differentiating (7), we find

$$\varphi' = A'\sin(kr+\delta) + A(k+\delta')\cos(kr+\delta). \tag{31}$$

We have here two unknown functions A and δ, and only one equation, the Schrödinger equation (6), at our disposal. We can therefore impose a relation between A and δ. We impose

$$A'\sin(kr+\delta) + A\delta'\cos(kr+\delta) = 0. \tag{32}$$

It follows that (31) becomes simply

$$\varphi' = Ak\cos(kr+\delta). \tag{33}$$

Differentiating now this, and using the Schrödinger equation (6), we find the new equation

$$A'k\cos(kr+\delta) - Ak\delta'\sin(kr+\delta) = VA\sin(kr+\delta). \tag{34}$$

Combining this with (32), we find the differential phase equation (8) and the amplitude equation (9), a complete set equivalent to the Schrödinger equation (6).

However, we can go back again to φ and φ', using (7) and (33). Adding their squares, we find[4]

$$A^2(k,r)=\frac{1}{k^2}(\varphi'^2+k^2\varphi^2). \tag{35}$$

It follows that (8) can be written

$$\delta'=-\frac{1}{k}V\sin^2(kr+\delta)=-\frac{1}{k}V\frac{\varphi^2}{A^2}$$

$$=-kV\frac{\varphi^2}{\varphi'^2+k^2\varphi^2}. \tag{36}$$

This is the basic equation, giving the ''local'' phase-shift $\delta(k,r)$ in terms of φ and φ'. Integrating it, we find

$$\delta(k,r)=-k\int_0^r V(t)\frac{\varphi^2(k,t)}{\varphi'^2(k,t)+k^2\varphi^2(k,t)}dt, \tag{37}$$

where the initial condition $\delta(k,0)=0$ has been used. Making now $r\to\infty$, we get the total phase-shift, (20). We have already checked that in (19) and (20) the integrals are absolutely convergent, and define continuous functions of k for all $k>0$.

A. Higher waves

The method for $\ell\neq 0$ is quite similar.[7] We have to deal now with the radial Schrödinger equation

$$\varphi_\ell''(k,r)+k^2\varphi_\ell(k,r)=\left[\frac{\ell(\ell+1)}{r^2}+V(r)\right]\varphi_\ell(k,r), \tag{38a}$$

and its free counterpart when $V=0$:

$$\frac{d^2}{dr^2}\begin{pmatrix}u_\ell\\ v_\ell\end{pmatrix}+k^2\begin{pmatrix}u_\ell\\ v_\ell\end{pmatrix}=\frac{\ell(\ell+1)}{r^2}\begin{pmatrix}u_\ell\\ v_\ell\end{pmatrix}. \tag{38b}$$

These free solutions are given by[1–3,7,8]

$$u_\ell(kr)=\sqrt{\frac{\pi kr}{2}}J_{\ell+1/2}(kr)\underset{r\to 0}{=}\frac{(kr)^{\ell+1}}{(2\ell+1)!!}+\cdots,$$

$$v_\ell(kr)=\sqrt{\frac{\pi kr}{2}}N_{\ell+1/2}(kr)\underset{r\to 0}{=}\frac{(2\ell-1)!!}{(kr)^\ell}+\cdots, \tag{39a}$$

$$(2\ell+1)!!=\frac{\Gamma(2\ell+2)}{2^\ell\Gamma(\ell+1)},\quad \ell>-\frac{1}{2}.$$

We have also

$$u_\ell(kr) \underset{r\to\infty}{=} \sin(kr-\tfrac{1}{2}\ell\pi)+\cdots,$$
$$v_\ell(kr) \underset{r\to\infty}{=} \cos(kr-\tfrac{1}{2}\ell\pi)+\cdots. \tag{39b}$$

Their Wronkian is given by

$$W(u_\ell,v_\ell)\equiv u'_\ell v_\ell - u_\ell v'_\ell = k. \tag{40}$$

As for the regular solution $\varphi_\ell(k,r)$, it is customary to normalize it such that[1–3]

$$\varphi_\ell(k,r) \underset{r\to 0}{\simeq} \frac{r^{\ell+1}}{(2\ell+1)!!}+\cdots. \tag{41}$$

Now, again, under the condition (1) on the potential, one can show that both φ and φ' exist for all real or complex values of k, all $r\geqslant 0$, and are continuous in both variables.[1–3] Moreover, one has the asymptotic behaviors

$$\varphi_\ell(k,r) \underset{r\to\infty}{=} \frac{|F_\ell(k)|}{k^{\ell+1}}\sin\left(kr-\frac{1}{2}\ell\pi+\delta_\ell(k)\right)+o(1),$$
$$\varphi'_\ell(k,r) \underset{r\to\infty}{=} \frac{|F_\ell(k)|}{k^{\ell}}\cos\left(kr-\frac{1}{2}\ell\pi+\delta_\ell(k)\right)+o(1), \tag{42}$$

where $F_\ell(k)$ is the Jost function, well-defined and continuous for all $k\geqslant 0$. For k real, one has also, uniformly in r for any $r\in[0,R]$, $R<\infty$,

$$\varphi_\ell(k,r) \underset{k\to\infty}{=} \frac{\sin kr}{k^{\ell+1}}+\frac{o(1)}{k^{\ell+1}},$$
$$\varphi'_\ell(k,r) \underset{k\to\infty}{=} \frac{\cos kr}{k^{\ell}}+\frac{o(1)}{k^{\ell}}. \tag{43}$$

We write now

$$\varphi_\ell(k,r)=A_\ell(k,r)[u_\ell(kr)\cos\delta_\ell(k,r)+v_\ell(kr)\sin\delta_\ell(k,r)], \tag{44}$$

$A_\ell(k,r)\neq 0$ for all $r\geqslant 0$, $\delta_\ell(k,0)=0$. We have now again two unknown functions A_ℓ and δ_ℓ, and only one (differential) equation to determine them. We can therefore impose a relation between A_ℓ and δ_ℓ. Simplifying the writing, we impose

$$A'[u\cos\delta+v\sin\delta]+A[-u\sin\delta+v\cos\delta]\delta'=0. \tag{45}$$

Differentiating now (44) and taking into account (45), we find

$$\varphi'=A[u'\cos\delta+v'\sin\delta]. \tag{46}$$

One more differentiation gives us now

$$\varphi''=A'[u'\cos\delta+v'\sin\delta]+A[u''\cos\delta+v''\sin\delta]+A[-u'\sin\delta+v'\cos\delta]\delta'. \tag{47}$$

Using now (38a) for φ'', and (38b) for u'' and v'', we find from (47)

$$A'[u'\cos\delta+v'\sin\delta]+A[-u'\sin\delta+v'\cos\delta]\delta'=VA[u\cos\delta+v\sin\delta]. \tag{48}$$

We have now two equations, namely (45) and (48), to determine A and δ. We can write them, symbolically, as

$$aA' + bA\delta' = 0, \tag{49}$$

$$cA' + dA\delta' = aVA. \tag{50}$$

Eliminating A', and using $A \neq 0$ and (40), we find

$$ad - bc = -(u'v - uv') = -k \tag{51}$$

and

$$\delta'_\ell = -\frac{1}{k} V(r)[u_\ell \cos \delta_\ell + v_\ell \sin \delta_\ell]^2, \tag{52}$$

to which we have to add $\delta_\ell(k,0) = 0$. Likewise, eliminating δ', we find

$$kA'_\ell = V(r)A_\ell[u_\ell \cos \delta_\ell + v_\ell \sin \delta_\ell][-u_\ell \sin \delta_\ell + v_\ell \cos \delta_\ell]. \tag{53}$$

As it is easily seen, we have again equations very similar to the equations for $\ell = 0$. Once (52) is solved, with the boundary condition $\delta_\ell(k,0) = 0$, we can replace its solution δ_ℓ in (53), and integrate it to get A_ℓ:

$$A_\ell(k,r) = A_\ell(k,0) \exp\left[\frac{1}{k}\int_0^r \cdots\right]. \tag{54}$$

However, as we saw previously, we can write both δ_ℓ and A_ℓ in terms of φ_ℓ. From (44) and (46), we can calculate $\sin \delta_\ell$ and $\cos \delta_\ell$:

$$\sin \delta = \frac{u'\varphi - u\varphi'}{kA}, \tag{55}$$

$$\cos \delta = \frac{v\varphi' - v'\varphi}{kA}. \tag{56}$$

Using now $\sin^2 \delta + \cos^2 \delta = 1$, we get

$$A_\ell^2 = \frac{1}{k^2}[(u_\ell \varphi'_\ell - u'_\ell \varphi_\ell)^2 + (v_\ell \varphi'_\ell - v'_\ell \varphi_\ell)^2]. \tag{57}$$

Using also (55) and (56) in (52) and remembering (40), we get

$$\delta'_\ell = -\frac{1}{k} V(r) \frac{\varphi_\ell^2(k,r)}{A_\ell^2(k,r)}. \tag{58}$$

Integrating this now, we have

$$\delta_\ell(k,r) = -k\int_0^r V(t) \frac{\varphi_\ell^2(k,t)}{[(u_\ell \varphi'_\ell - u'_\ell \varphi_\ell)^2 + (v_\ell \varphi'_\ell - v'_\ell \varphi_\ell)^2]} dt. \tag{59}$$

All these formulas, so far purely formal, are very similar to those for $\ell = 0$. However, using now the behaviors of φ, φ', u, u', v, v' for $r \to 0$, we can check that all our above formulas are meaningful, i.e., the integrals are convergent at $r = 0$. Again, it is clear from (57) that $A_\ell(k,r) \neq 0$ for all $r \geqslant 0$. Indeed, if A_ℓ is zero at $r = r_0$, we must have, according to (57), $u\varphi' - u'\varphi$

$=0$ and $v\varphi'-v'\varphi=0$ at this point. Calculating again φ and φ' from these two equations, we find that, if $k\neq 0, \varphi=\varphi'=0$ at $r=r_0$. And this entails that $\varphi\equiv 0$ everywhere, a contradiction with (41). Therefore, our assumption on A_ℓ is satisfied: $A_\ell(k,r)$, for $k>0$, never vanishes for $r\in[0,\infty)$.

Let us now look at the behavior of $\delta_\ell(k,r)$, (59), $k>0$ for $r\to 0$, $\ell>-\frac{1}{2}$. From (39a) and (41), it is easily seen that the numerator behaves like $r^{2\ell+2}$ whereas the denominator becomes a positive constant. Therefore, we have, for $k>0$,

$$\delta_\ell(k,r)\underset{r\to 0}{\simeq}\text{const}\int_0^r t^{2\ell+2}V(t)\,dt=r^{2\ell+1}o(1). \tag{60}$$

This shows that our assumption on $\delta_\ell(k,r)$ is also satisfied: $\delta_\ell(k,0)=0$. Using (60) in (53), we find also that we have a convergent integral in (54). This completes the validity of the method and its consistency.

We have now to look at (57) and (59) for $r\to\infty$. From (39b) and (42), we find easily, for all $k>0$, that we have

$$A_\ell^2(k,\infty)=\frac{|F_\ell(k)|^2}{k^{2\ell+2}}\Rightarrow A_\ell(k,\infty)=\frac{|F_\ell(k)|}{k^{\ell+1}}, \tag{61}$$

where $F_\ell(k)$ is the Jost function, finite and continuous for all $k\geqslant 0$.[1–3] From (59) for $r\to\infty$, we find

$$\delta_\ell(k)=-k\int_0^\infty V(r)\frac{\varphi_\ell^2(k,r)}{[(u_\ell'\varphi_\ell-u_\ell\varphi_\ell')^2+(v_\ell'\varphi_\ell-v_\ell\varphi_\ell')^2]}dr, \tag{62}$$

and it is easily checked from (39b) and (42) that the integral here is well-defined and absolutely convergent, and since φ, φ', u, u', v and v' are all continuous functions of k for all $k>0$,[8] the same is true for $\delta_\ell(k)$: the phase-shift is a continuous function of k for all $k>0$. To check (3), we can use (43) in (62), and we find, as for the case $\ell=0$, that $\delta_\ell(\infty)=0$. Moreover, $k^{\ell+1}A_\ell$ and δ_ℓ are also continuous functions of k for all $k>0$. They are given, respectively, by (57) and (59). The physical phase-shift is given by (62), an absolutely convergent integral for all $k>0$ under the assumption (1), and one has also (3). Therefore, (62) gives an absolute definition of the phase-shift $\delta_\ell(k)$ in general for all k, and for potentials satisfying (1). We shall see in the next section that (20) and (62) are valid also for singular repulsive potentials as well. The case $k=0$ will be considered at the end of the next section.

Remark: Making $\ell=0$, one finds, as expected, all the formulas we found previously for the S-wave. Before ending this section, let us mention that by combining (38a) and (38b), and integrating from 0 to r, using the appropriate boundary conditions at $r=0$, namely (39a), (40), and (41), to evaluate the integrated terms, one can calculate $u'\varphi-u\varphi'$ and $v'\varphi-v\varphi'$, so that (62) can be written, for $\ell>-\frac{1}{2}$, also as

$$\delta_\ell(k)=-k\int_0^\infty V(r)\frac{\varphi_\ell^2(k,r)}{(\int_0^r u_\ell\varphi_\ell V dt)^2+(k^{-\ell}+\int_0^r v_\ell\varphi_\ell V dt)^2}dr. \tag{63}$$

Note here that we have now precise boundary conditions at $r=0$ for all the functions entering in (63), so that care must be taken in using it, whereas in (20) and (62), the normalization of φ at $r=0$ does not matter. For $-\frac{1}{2}\leqslant\ell<0$, as we shall see in the next section, (62) and (63) are valid provided we use there the ''distinguished'' pure Bessel solution for φ, given by the integral equation (68). Indeed, now, both free solutions $u_\ell=\sqrt{r}J_{\ell+1/2}(kr)$ and $v_\ell=\sqrt{r}N_{\ell+1/2}(kr)$ vanish at $r=0$, and so, as free solution, we can start from any combination $au_\ell+bv_\ell$, and use it as the inhomogeneous term in (68). We get then always a solution φ_ℓ with $\varphi(k,0)=0$. The ''distinguished'' solution is the one with $b=0$.

III. DOMAIN OF VALIDITY OF (20) AND (62)

As we have seen, formulas (20) for the S-wave, or its generalization (62) for higher waves, are valid for all $k>0$ and all $\ell \geqslant 0$, provided the potential satisfies the integrability condition (1): $rV(r) \in L^1(0,\infty)$. Roughly speaking, this means that V is less singular than r^{-2} at the origin. We may now ask whether they are also valid for potentials having stronger singularity there, for instance $V(r) \sim g r^{-m}$, $m \geqslant 2$, $g>0$, or $g \exp(\alpha/r^n)$, $g>0$, $\alpha>0$, $n>0$, etc., as $r \to 0$. Rather than developing the general formalism for such general singular potentials (singular and repulsive at the origin), we shall consider explicit examples, and leave the full theory for a forthcoming paper.

(i) We consider the formula (20) for the S-wave, and take boldly the potential to be the centrifugal barrier

$$V(r) = \frac{\ell(\ell+1)}{r^2}, \quad \ell>0, \tag{64}$$

in the Schrödinger equation (6). The wave function is now just, up to an unimportant constant multicative factor, $\varphi = \sqrt{kr} J_{\ell+1/2}(kr)$ which is of the form $\phi(kr)$. It is easily seen that (20) is well-defined because the integral is convergent (absolutely) both at $r=0$ and $r=\infty$. If we make the change of variable $z=kr$ in it, we find, by writing $\varphi' = k\,(d/dz)\,\phi = k\dot{\phi}(z)$, $\dot{} = d/dz$,

$$\delta = -\ell(\ell+1) \int_0^\infty \frac{\phi^2(z)}{[\dot{\phi}^2(z) + \phi^2(z)]} dz, \tag{65}$$

where $\phi = \sqrt{z} J_{\ell+1/2}(z)$. This last formula is now independent of k. The same is therefore true for the original formula (20) with our $\varphi(k,r)$. We can therefore calculate it at any value of k, for instance, for $k=0$. Using (39a), we find

$$\delta = -\ell(\ell+1) \int_0^\infty \frac{dz}{[(\ell+1)^2 + z^2]} = -\ell \int_0^\infty \frac{dt}{1+t^2} = -\ell \frac{\pi}{2}. \tag{66}$$

This is exactly the phase-shift of the centrifugal barrier $\ell(\ell+1)/r^2$ since, without this potential, the wave function is $\sin kr$, and with the potential, $\varphi \cong \text{const} \times \sin(kr - \frac{1}{2}\ell\pi)$, as $r \to \infty$, according to (42).

In conclusion, our formula (20) is valid for repulsive singular potentials g/r^2, $g>0$, which violate (1) both at $r=0$ and $r=\infty$.

(ii) We consider now the previous example, but with $-\frac{1}{2} \leqslant \ell < 0$. Here, proceeding as before, we find, as expected, again (66). Note that δ is now positive because the potential $\ell(\ell+1)/r^2$ is negative. For $\ell = -\frac{1}{2}$, the full solution is $\varphi = \sqrt{kr} J_0(kr)$, so that $\varphi \sim \sqrt{r}$ and $\varphi' \sim 1/(2\sqrt{r})$ as $r \to 0$.

Remark: Formula (20) was proved for regular potentials. In all rigor, in order to apply it to the centrifugal barrier potential $\ell(\ell+1)/r^2$, we must first regularize this at the origin, for instance by cutting it by $\theta(r-\varepsilon)$, and then make $\varepsilon \downarrow 0$, or by replacing r in the denominator by $(r+\varepsilon)$, and again take the limit $\varepsilon \downarrow 0$. However, as we saw, at the limit, we have already an absolutely convergent integral for all $\ell \geqslant -\frac{1}{2}$. Also, the derivation of (20) was based on the assumption $\varphi'(0)=1$, i.e., $\varphi(r) \simeq r + \cdots$ for $r \to 0$. However, for $\ell \neq 0$, we have rather $\varphi_\ell \simeq r^{\ell+1} + \cdots$. The extra factor r^ℓ comes from the regularized formula for the amplitude A in the limit $\varepsilon \downarrow 0$, as can easily be seen.[7]

(iii) We consider now (13) with

$$V(r) = \frac{\ell(\ell+1)}{r^2} + V_1(r), \quad \ell \geqslant -\frac{1}{2}, \tag{67}$$

assuming that $rV_1(r)\in L^1(0,\infty)$. Consider first $\ell>-\frac{1}{2}$. As we saw, the presence of this "weak perturbation," as compared to $\ell(\ell+1)/r^2$, does not modify the behavior of the regular solution φ_ℓ at $r=0$, given by (41), to be compared with (39a).[1–3] And since (20), as we just saw, works with $\ell(\ell+1)/r^2$, $\ell\geqslant-\frac{1}{2}$, applied to the regular solution φ_ℓ, it should work also when we add V_1, provided we use always pure Bessel functions as free solutions. This means that the Volterra integral equation which combines the Schrödinger equation and the boundary condition at $r=0$ is

$$\varphi_\ell(k,r)=\frac{1}{k^{\ell+1}}u_\ell(kr)+\int_0^r G_\ell(k;r,r')V(r')\varphi_\ell(k,r')dr',$$
$$G_\ell(k;r,r')=\frac{1}{k}[u_\ell(kr)v_\ell(kr')-u_\ell(kr')v_\ell(kr)]. \tag{68}$$

We consider now $\ell=-\frac{1}{2}$. As has been shown in Ref. 9, in order to formulate a decent scattering theory leading to the asymptotic form (42) with a well-defined Jost function $F_\ell(k)$ and a well-defined phase-shift δ_ℓ, one has to make stronger assumptions on V than (1), namely,

$$\int_0^\infty r|V(r)|(1+|\log r|)\,dr<\infty,$$
$$\int_a^\infty r|V(r)|(\log r)^2\,dr<\infty,\quad a>0. \tag{69}$$

This will be used later for $\ell=-\frac{1}{2}$, and $k\to0$, where we give more details.

In conclusion, formula (20) is valid for (67) and the regular solution φ_ℓ. Therefore, we have now two methods to deal with (67). The first one is to apply (62) to V_1, and the second one to apply (20) to the full potential (67). In any case, we get, of course, the full phase-shift

$$\delta_\ell^{\text{total}}=\delta_\ell-\tfrac{1}{2}\ell\pi, \tag{70}$$

δ_ℓ being the physical phase-shift due to V_1, which is what interests us in scattering theory. Remember that, in (20) or (62), φ is always the full solution: solution of (38a) with $V=V_1$, or (6) with (67), always together with (41).

(iv) We consider now more singular potentials, namely $V(r)=g/r^m$, $m>2$, $g>0$. Here, it is known that the solution of the Schrödinger equation (1) which vanishes at $r=0$ behaves there as[1–6]

$$\varphi_\ell(k,r)\underset{r\to0}{\simeq}[V(r)]^{-1/4}\exp\left(-\int_r^\infty[V(t)]^{1/2}dt\right)=\phi_0(r)=g^{-1/4}r^{m/4}\exp\left[-\sqrt{g}\frac{2}{m-2}\frac{1}{r^{(m-2)/2}}\right], \tag{71}$$

independent of k and ℓ. The wave function φ and all of its derivatives $\varphi^{(n)}$ vanish exponentially at $r=0$. Notice that we can omit the factor $g^{-1/4}$ in front of the last expression since our formulas for the phase-shifts are homogeneous in φ. In fact, at $k=0$, the Schrödinger equation is soluble exactly, and its solution is,[4] up to an unimportant constant multiplicative factor,

$$\varphi_\ell(k=0,r)=\sqrt{r}K_{(2\ell+1)/(m-2)}\left(\frac{2\sqrt{g}}{m-2}r^{-(m-2)/2}\right), \tag{72}$$

where K_ν is the modified Hankel function.[8] Using the asymptotic behavior of $K_\nu(x)$ for $x\to\infty$, we find indeed, up to constant multiplicative factors, the behavior shown in (71). On the other hand,

we know that now, because of the strong singularity of V at $r=0$, the phase-shift does not go to zero as $k\to\infty$, contrary to the case of regular potentials satisfying (1). Rather, one has the high energy behavior[5,6]

$$\delta_{\ell}(k) \underset{k\to\infty}{=} -Ag^{1/m}k^{(m-2)/m}+\cdots, \tag{73}$$

where

$$A=\frac{\sqrt{\pi}}{2}\frac{\Gamma(1-1/m)}{\Gamma(3/2-1/m)}. \tag{74}$$

Since the main term in (73) is independent of ℓ, we shall consider the case $\ell=0$ to simplify the algebra, and therefore use (20). In this formula, the integral can be split into $\int_0^R+\int_R^\infty$. For the second integral, we have

$$\left|k\int_R^\infty \cdots\right| < \frac{g}{k}\int_R^\infty \frac{dr}{r^m} = O(k^{(m-2)/m+\varepsilon}), \tag{75}$$

ε very small (>0), as $k\to\infty$, provided $R=O(k^{-2/m+\varepsilon})$. The contribution of (75) can therefore be neglected if we compare with (73). Note that $R\to 0$ as $k\to\infty$. In the first integral, we can therefore replace, in first approximation, φ by ϕ_0 given in (71), and independent of k. We find then

$$-gk\int_0^R \frac{1}{r^m}\frac{\phi_0^2}{\phi_0'^2+k^2\phi_0^2}dr = -gk\int_0^R \frac{1}{((m/4)\,r^{m/2-1}+\sqrt{g})^2+k^2r^m}dr. \tag{76}$$

Making now the change of variable $x=k^{2/m}r$, letting $k\to\infty$, and noting that $k^{2/m}R\to\infty$, we find

$$-gk\int_0^R \cdots \underset{k\to\infty}{\simeq} -gk^{(m-2)/m}\int_0^\infty \frac{dx}{g+x^m} = -g^{1/m}k^{(m-2)/m}\int_0^\infty \frac{dt}{1+t^m}. \tag{77}$$

It follows that the approximate value of $\delta(k)$ behaves asymptotically as

$$\delta_{\text{app}}(k) \underset{k\to\infty}{\simeq} -Bg^{1/m}k^{(m-2)/m},\quad B=\int_0^\infty \frac{dt}{1+t^m}. \tag{78}$$

This coincides with (73) up to a numerical factor, and is obtained without much effort, as we see.

The above argument to obtain (78) is, of course, heuristic because (71) is uniform in k only for $k\in[0,K]$, $K<\infty$. But it can be made more precise and quite rigorous. In a forth-coming paper, we shall develop a technique to deal with all these problems in a unified way.

Remark: The remark at the end of (*ii*) applies here, too. We must regularize first the potential, and then let $\varepsilon\downarrow 0$. The exponential decrease of φ as $r\to 0$ comes then from the amplitude A in the limit $\varepsilon\downarrow 0$.

A. A low-energy example

Our last example is the low energy behavior of the phase-shift for $\ell=-\frac{1}{2}$, where the potential is assumed to be repulsive ($V\geqslant 0$), and to satisfy the integrability conditions

$$\int_0^\infty r|V(r)|(1+|\log r|)\,dr<\infty, \tag{79}$$

and

$$\int_a^\infty r|V(r)|(\log r)^2\,dr<\infty,\quad a>0. \tag{80}$$

This corresponds to the S-wave Schrödinger equation in two space dimensions, and is interesting to study.[9]

As we saw in (iii), we must use here only the pure "Bessel" solutions. This means that the solution φ is the solution of the integral equation (68) for $\ell=-\frac{1}{2}$:

$$\varphi(k,r)=\sqrt{kr}J_0(kr)+\int_0^r G(k,r,r')V(r')\varphi(k,r')dr', \tag{81}$$

where the Green's function is given by

$$G=\frac{\pi}{2}\sqrt{rr'}[J_0(kr)N_0(kr')-J_0(kr')N_0(kr)]. \tag{82}$$

The occurrence of $\log r$ in (79) is due to the presence of $\log(kr)$ in N_0. Here, φ is normalized somewhat differently, but we know that the normalization of φ does not matter in (20) and (62). In (63), φ is normalized now as to $\varphi\simeq\sqrt{r}$ for $r\to 0$.

It is then shown in the above reference that the phase-shift, i.e., the phase-shift $\delta_0(k)$ of the S-wave in the two dimensional space problem, has the universal behavior

$$\delta_0(k)\underset{k\to 0}{\simeq}\frac{-\pi/2}{|\log k|}+\cdots, \tag{83}$$

i.e., the main term is independent of the potential.

We are going to find (83) by using the formula (63) for $\ell=-\frac{1}{2}$, in which φ_ℓ is given as above, and, for $z\to 0$,[8]

$$\begin{aligned} J_0(z)&=1-\frac{z^2}{4}+\cdots,\\ N_0(z)&=\frac{2}{\pi}\left[\log\frac{z}{2}+\gamma\right]J_0(z)+O(z^2). \end{aligned} \tag{84}$$

From the integral equation for φ, it can be easily shown that, under the assumptions (79) and (80), the low-energy behavior of φ is given by $\varphi\underset{k\to 0}{\simeq}\sqrt{kr}J_0(kr)\simeq\sqrt{kr}+\cdots$, which we have to normalize to $\varphi\simeq\sqrt{r}$, and, for u and v, in order to comply with (40), we must take

$$\begin{aligned} u&\simeq\sqrt{kr}+\cdots,\\ v&\simeq-\sqrt{kr}\log kr+\cdots. \end{aligned} \tag{85}$$

Using now the above low energy behaviors in (63), we find

$$\delta(k)\underset{k\to 0}{\simeq}-\int_0^\infty\frac{rV(r)}{(\int_0^r tV(t)\,dt)^2+(1-\int_0^r tV(t)\log kt\,dt)^2}dr. \tag{86}$$

Since V was assumed to be positive, we can introduce the new variable $X=X(r)$ by

$$X(r)=|\log k|\int_0^r tV(t)dt,\quad dX=|\log k|rVdr, \tag{87}$$

which is a one-to-one mapping from $r\in[0,\infty)$ to $X\in[0,|\log k|A]$, where $A=\int_0^\infty r|V(r)|dr$. Letting now $k\to 0$, we find easily from (86)

$$\delta(k)\underset{k\to 0}{\simeq}-\frac{1}{|\log k|}+\cdots. \tag{88}$$

Here again, as for the case of singular potentials, we do not get the exact constant $\pi/2$ because we use $\varphi\simeq\sqrt{r}$, which is not uniform on the entire r-axis. We shall come back to this in more detail in a forthcoming paper.

B. The case $k=0$

Let us consider now $k=0$ in (20). It is known that, under (1), one has[1–3]

$$\varphi(0,r)\underset{r\to\infty}{=}\varphi'(0,\infty)r+D+o(1), \tag{89}$$

where $\varphi'(0,\infty)$ is finite or zero, and D is finite also. Making now $k=0$ in (20), we find, for the S-wave scattering length[1,2]

$$a_0=\lim_{k\to 0}\frac{-\delta_0(k)}{k}=\int_0^\infty\frac{\varphi^2(0,r)}{\varphi'^2(0,r)}V(r)\,dr. \tag{90}$$

At the origin $r=0$, there is no convergence problem since $\varphi'(k,0)=1$ for all k. However, at $r=\infty$, because of (89), we must assume

$$\int_R^\infty r^2|V(r)|\,dr<\infty \tag{91}$$

in order to secure proper convergence, which is also well-known.[1,2] But this is not yet the end. We must also be sure that $\varphi'(0,r)$ does not vanish for $r>0$. This is surely the case if V is positive,[1,2] but cannot be guaranteed otherwise. In conclusion, (91) is valid only when $\varphi'(0,r)\neq 0$ for all $r>0$. For higher waves, in order to have proper convergence at $r=\infty$, one needs[1,2]

$$\int_0^\infty r^{2\ell+2}|V(r)|\,dr<\infty \tag{92}$$

and again the nonvanishing of the denominators in (20) or (62). We shall see in a forthcoming paper, how to modify these formulas in the presence of bound states. However, we know that in all cases, $\delta_\ell(k)$ is continuous down to $k+0$, and one has the Levinson theorem $\delta(+0)=n\pi$, where n is the number of bound states.[1–3,7]

C. Two-potential case

Formulas (62) and (63), as it is obvious, can of course be applied in the case where we have two potentials:

$$V=V_1+V_2, \tag{93}$$

both satisfying (1). Here, we can apply either (20) to V, or (62) and (63) to V_2, where u_ℓ and v_ℓ are now replaced by two appropriate independent solutions of the Schrödinger equation φ_1 and ψ_1, normalized according to (40):

$$W[\varphi_1,\psi_1]=\varphi_1'\psi_1-\varphi_1\psi_1'=k. \tag{94}$$

With (20), we would get the full phase-shift, and with (62) or (63), the phase-shift δ_2 due to V_2.

APPENDIX A

We have to study here the integral equation (18):

$$\Delta(k,r)=\frac{D}{k}\int_0^r|V(t)|\left[\frac{kt+\Delta(k,t)}{1+kt+\Delta(k,t)}\right]^2dt. \tag{A1}$$

We solve it by iteration, starting from

$$\Delta^{(0)}(k,r)=0. \tag{A2}$$

Since $x/(1+x)$ is an increasing function of x for $x\geqslant 0$, we get the increasing sequence of iterations

$$\Delta^{(1)}(k,r)<\Delta^{(2)}(k,r)<\cdots, \tag{A3}$$

where

$$\begin{aligned}\Delta^{(1)}(k,r)&=\frac{D}{k}\int_0^r|V(t)|\left(\frac{kt}{1+kt}\right)^2dt,\\ \Delta^{(n)}(k,r)&=\frac{D}{k}\int_0^r|V(t)|\left(\frac{kt+\Delta^{(n-1)}(k,t)}{1+kt+\Delta^{(n-1)}(k,t)}\right)^2dt.\end{aligned} \tag{A4}$$

(i) Assume now first that V is integrable at $r=0$ and therefore is $L^1(0,\infty)$. It is then obvious that the increasing sequence of iterations is bounded by

$$\overline{\Delta}(k,r)=\frac{D}{k}\int_0^r|V(t)|dt,\quad r\geqslant 0,\quad k>0. \tag{A5}$$

It has therefore a limit, and one has the solution

$$\Delta(k,r)=\lim_{n\to\infty}\Delta^{(n)}(k,r)\leqslant\overline{\Delta}(k,r) \tag{A6a}$$

for all $r\geqslant 0$, and all $k>0$. For $r\to\infty$, the same statement is valid. Indeed, if we note that both $\Delta(k,r)$ and $\overline{\Delta}(k,r)$ are increasing functions of r, it follows that we have, when $r\to\infty$,

$$\Delta(k)=\lim_{r\to\infty}\Delta(k,r)\leqslant\overline{\Delta}(k)=\lim_{r\to\infty}\overline{\Delta}(k,r)=\frac{D}{k}\int_0^\infty|V(t)|dt. \tag{A6b}$$

It is then obvious from (A5) that we have $\Delta(k\to\infty)=0$, which gives in turn (3), as expected.

(ii) If we have only (1): $rV(r)\in L^1$, we must refine slightly our argument. Since our problem is now the convergence of the integral in $\Delta^{(n)}(k,r)$ at $r=0$, we consider r very small. Now, as it is obvious, another sequence of upper bounds for $\Delta^{(n)}(k,r)$ is obtained by using the drastic inequality $x/(1+x)<x$ in (A1). We obtain in this way a sequence of upper bounds for $\Delta^{(n)}$ from the sequence of iterations of

$$\bar{\bar{\Delta}}(k,r)=\frac{D}{k}\int_0^r|V(t)|[kt+\bar{\bar{\Delta}}(k,t)]^2dt. \tag{A7}$$

Putting $\bar{\Delta}=k\omega$, we get

$$\omega(k,r)=D\int_0^r|V(t)|(t+\omega)^2dt, \tag{A8}$$

which is in fact independent of k, and must be iterated now. The above equation is nothing else than the integral equation for minus the local scattering length

$$a(r)=\lim_{k\to 0}\frac{-\delta(k,r)}{k} \tag{A9}$$

for the potential $-D|V(r)|$, and has been studied in the book of Calogero,[7] Chaps. 11 and 12, where it is shown that the iteration of (A8) leads to an absolutely convergent series expansion for the solution, provided r is small enough and $rV(r)\in L^1$. Alternatively, (A8) is nothing else than the Riccati equation

$$\omega'(r)=D|V(r)|[r+\omega(r)]^2 \tag{A10}$$

with $\omega(0)=0$, which has also been thoroughly studied in the books of Hille[10] and Coddington and Levinson,[11] to which we refer the reader, with the same conclusion.

Once we secure the solution of (A7) in a small interval $[0,r_0]$, with $\Delta(k,0)=0$, we can then start at $r=r_0$. Consider instead of (A1) the integral equation,

$$\Delta(k,r)=\Delta(k,r_0)+\frac{D}{k}\int_{r_0}^r|V(t)|\left[\frac{kt+\Delta(k,t)}{1+kt+\Delta(k,t)}\right]^2dt, \tag{A11}$$

and proceed as before, by iteration. Here, we need only $V\in L^1(r_0,\infty)$. We get then again an increasing sequence bounded by

$$\Delta(k,r_0)+\frac{D}{k}\int_{r_0}^\infty|V(t)|dt, \tag{A12}$$

with the same conclusions as before for the existence of the limit of the iterations, etc. However, the high-energy behavior of $\delta(k,r)$ cannot be obtained from the above analysis.

A different method, which supercedes the above considerations, and provides at the same time the high-energy limit of $\delta(k,r)$ and of $\delta(k)=\delta(k,\infty)$ is as follows. It consists in neglecting Δ in the denominator of the right-hand side of (A1):

$$\Delta(k,r)\leqslant\frac{D}{k}\int_0^r|V(t)|\left[\frac{kt+\Delta(k,t)}{1+kt}\right]^2dt\leqslant\frac{D}{k}\int_0^r\frac{r}{t}|V(t)|\left[\frac{kt+\Delta}{1+kt}\right]^2dt. \tag{A13}$$

Writing now $\Delta=r\omega$, the two ends of (A13) lead us to the integral equation

$$\omega=\frac{D}{k}\int_0^r t|V(t)|\frac{(k+\omega)^2}{(1+kt)^2}dt \tag{A14}$$

whose solution provides still a stronger upper bound for $\Delta(k,r)$. Now, it is trivial to solve (A14). We just differentiate it, and integrate the differential equation, taking into account $\omega(k,0)=0$. This solution is just

$$\omega(k,r)=\frac{kI(k,r)}{1-I(k,r)},$$
$$I(k,r)=D\int_0^r \frac{t|V(t)|}{(1+kt)^2}dt. \tag{A15}$$

The solutions exists as long as $I(k,r)<1$, that is, in the interval $[0,r_0)$, where $r_0(k)$ is given by

$$D\int_0^{r_0} \frac{r|V(r)|}{(1+kr)^2}dr=1. \tag{A16}$$

Note that, in any fixed interval $[0,R]$, $R\leqslant\infty$, we have

$$\lim_{k\to\infty} I(k,r)=0. \tag{A17}$$

Indeed, from (A15), and using $1+kt\geqslant 1$ and $1+kt>kt$, we have

$$I(k,r)\leqslant I(k,\infty)\leqslant D\int_0^\infty \frac{t|V(t)|}{1+kt}dt=J(k,\infty)\leqslant \int_0^\varepsilon t|V(t)|dt+\frac{1}{k}D\int_\varepsilon^\infty |V(t)|dt, \tag{A18}$$

where, in obvious notations, $J(k,r)$ is defined by $D\int_0^r[t|V(t)|/(1+kt)]dt$. Now, we can first make ε small enough, independent of k, in order to make the first integral on the right-hand side as small as we wish. Once ε is fixed, we can then make k large enough in order to make also the second integral as small as we wish. This proves (A17).

Remark: It is obvious that (A17) is uniform in any finite interval $0\leqslant r\leqslant R$.

As a consequence of (A17), $r_0(k)$ defined by (A16) satisfies

$$\lim_{k\to\infty} r_0(k)=\infty, \tag{A19}$$

so that, the larger k is, the larger is the domain of validity of (A15). In any case, by making k large enough, and combining (A15) and (A17), we can have, uniformly in r in $[0,R]$,

$$\omega(k,r)\leqslant 2kI(k,r),\quad k>K, \tag{A20}$$

and we know that $r\omega(k,r)$ is an upper bound for $\Delta(k,r)$. We can therefore, for k large enough, use (A20) in (A1):

$$\Delta(k,r)=\frac{D}{k}\int_0^r |V(t)|[\cdots]^2dt\leqslant\frac{D}{k}\int_0^r |V(t)|[\cdots]^1dt\leqslant\frac{D}{k}\int_0^r |V(t)|,$$
$$\frac{kt+2ktI(k,t)}{1+kt}dt=J(k,r)+2D\int_0^r\frac{t|V(t)|}{1+kt}I(k,t)dt\leqslant J(k,r)+2I(k,r)J(k,r). \tag{A21}$$

Now, as we saw for (A19), both I and J go to zero as $k\to\infty$, uniformly in r for r in any finite interval $[0,R]$. Therefore,

$$\lim_{k\to\infty}\Delta(k,r)=0,\quad 0\leqslant r\leqslant R. \tag{A22}$$

Once we have shown the existence of the solution $\Delta(k,r)$ in $[0,R]$, we can proceed as for (A11), write, for $r>R$,

$$\Delta(k,r)=\Delta(k,R)+\frac{D}{k}\int_R^r|V(t)|\left[\frac{kt+\Delta(k,t)}{1+kt+\Delta(k,t)}\right]^2dt, \tag{A23}$$

and proceed again by iteration. This way of proceeding is legitimate since (A1), or (18), was obtained from the differential equation (8) and the bound (16). We can therefore start at any point $r=R$, and integrate after, provided we know $\delta(k,R)$. And we obtain a bigger upper bound if we replace $|\delta(k,R)|$ by $\Delta(k,R)$. The process is now very similar to what we had in (i). We get an increasing sequence of iterations $\Delta^{(n)}(k,r)$, with $\Delta^{(0)}(k,r)=\Delta(k,R)$, and a global upper bound for all $\Delta^{(n)}(k,r)$:

$$\Delta^{(n)}(k,r)\leqslant\Delta_0(k)=\Delta(k,R)+\frac{D}{k}\int_R^\infty|V(t)|dt, \tag{A24}$$

valid for all $r>R$, including $r=\infty$, and all n. The sequence has therefore a limit, and this limit provides the solution $\Delta(k,r)$ of (A1) for all $r\geqslant R$, including $r=\infty$, with $R<r_0(k)$, and $r_0(k)$ given by (A16). Since we have also proved the existence of the solution in $[0,r_0]$, we have therefore proved the existence of the solution of (A1) for all $r\geqslant 0$. Obviously, we have

$$\Delta(k,0)=0. \tag{A25a}$$

Therefore, we have, for $r>R$,

$$\Delta(k,r)\leqslant\Delta(k,R)+\frac{D}{k}\int_R^\infty|V(t)|dt. \tag{A25b}$$

If we note also that $\Delta(k,r)$ is an increasing function of r, we secure the existence of $\Delta(k)=\Delta(k,\infty)$, and from (A22) and (A24), we obviously have, for the phase-shift

$$\lim_{k\to\infty}\delta(k)\leqslant\lim_{k\to\infty}\Delta(k)=\lim_{k\to\infty}\Delta(k,\infty)=0. \tag{A26}$$

This completes our proof for the general case where $rV(r)\in L^1(0,\infty)$.

APPENDIX B

Here, we shall show that, for regular potentials satisfying (1), one can make (3) more precise if one knows the detail behavior of the potential when $r\to 0$. One has, indeed, the following:

Theorem 1:[12] Let us assume that V is continuous and bounded, away from the origin, in $[0,R]$, $R<\infty$, and is such that

$$\lim_{r\to 0}r^{1+\alpha}V(r)=V_0,\quad 0<\alpha<1. \tag{B1}$$

We have then, as $k\to\infty$,

$$\delta(k)=\frac{-V_0}{\alpha}\cos\left(\frac{\pi\alpha}{2}\right)\Gamma(1-\alpha)\frac{1}{(2k)^{1-\alpha}}+\cdots, \tag{B2}$$

and, conversely, (B2) entails (B1).

We shall give the proof for the S-wave, $\ell=0$. The proof for higher waves is quite similar. Because of (14), we can just limit ourselves to (29):

$$\delta(k)\cong-\int_0^R dt\sin 2kt\left(\int_t^R V(r)dr\right). \tag{B3}$$

For the asymptotic behavior of this integral (as $k\to\infty$,) we can now use the following theorem of Titchmarsh.[13]

Theorem 2: Let $f(x)$ and $f'(x)$ be integrable over any finite interval not ending at $x=0$; let $x^{1+\alpha}f'(x)$ be bounded for all x, and let $f(x)\sim x^{-\alpha}$ as $x\to 0$. Then, denoting by F_0 the limit of $x^{1+\alpha}f'(x)$ as $x\to 0$, we have

$$\int_0^\infty f(x)\sin kx\,dx = F_0\Gamma(1-\alpha)\cos\frac{\pi\alpha}{2}\,\frac{1}{k^{1-\alpha}}(1+o(1)), \tag{B4}$$

as $k\to\infty$. The converse theorem is also true if we deal with finite intervals in (B4) since we can define the Fourier inverse transforms in a straightforward manner. This is indeed the case in (B3).

Our Theorem 1 follows now immediately from the theorem of Titchmarsh applied to (B3). Moreover, it is a Tauberian kind theorem, i.e., its converse is also true if we remember that the Fourier transform of an L^1 function $f(x)$ is a continuous function $F(k)$ of k. More refined theorems containing logarithmic terms can also be proved. Examples are treated in Calogero's book.[7] For higher waves, the proof is similar by using (39b) and (43) in (62).

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A single-mode quantum transport in serial-structure geometric scatterers

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We study transport in quantum systems consisting of a finite array of N identical single-channel scatterers. A general expression of the S matrix in terms of the individual-element data obtained recently for potential scattering is rederived in this wider context. It shows in particular how the band spectrum of the infinite periodic system arises in the limit $N\to\infty$. We illustrate the result on two kinds of examples. The first are serial graphs obtained by chaining loops or T-junctions. Another example concerns geometric scatterers where the individual element consists of a surface with a pair of leads; we show that apart from the resonances coming from the decoupled-surface eigenvalues, such scatterers exhibit the high-energy behavior typical for the δ' interaction for the physically interesting couplings. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1389287]

I. INTRODUCTION

A rapid progress in experimental solid state physics has expanded dramatically the list of situations in which consequences of the basic equations of quantum mechanics may be tested, since the interaction is prescribed by the experimentalist by the shape design of the structure in question, material choice, etc. One of the frequently occuring cases in mesoscopic transport involves a passage of a quantum particle through a *serial*—or finitely periodic—structure obtained by arraying a certain number N of identical scatterers.

Our aim in the present article is to study this situation under the assumption that the individual scatterers have a single transport mode. For a collection of mesoscopic elements connected by quantum wires, this is certainly an idealization. We can adopt this approximation provided the transverse modes in the wires are well separated and the distances between the scatterers are large enough so that the intermode coupling and influence of the evanescent modes can be neglected.

Such a single-mode transport is often investigated in literature, with the S-matrix obtained either ''inductively'' by adding the scatterers successively or by means of the transfer matrix method. It is difficult to collect all relevant references but a representative sample is given in Ref. 1; an extension of this ''factorization'' method to scattering on graphs was proposed recently in Ref. 2. On the other hand, the mentioned methods are typically used to evaluate the S-matrix

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numerically and give little insight, say, into its dependence on the number N of the scatterers. To this purpose a transparent expression for the S-matrix is needed.

Such closed-form formulas were derived recently in one-dimensional potential scattering, first for an array of δ interactions[3–5] and then for an arbitrary finitely periodic potential;[6,7] also the number of bound states has been discussed in this setting.[8,9] When this work was in its final stage, another analysis of this situation appeared[3] which investigated in detail the distribution of scattering resonances and the corresponding time delay. Our main observation is that the input for the S-matrix expression are the individual-element scattering data, and thus the result can be applied to scattering on an array of arbitrary ''black boxes.'' The aim of the present paper is to rederive the result of Refs. 6 and 7 in this more general context and to illustrate it on several examples of nonpotential scattering.

They fall into two categories. First, in Sec. III, we consider two cases of serial graphs, an array of loops joined by leads and exposed to a homogeneous magnetic field, and a ''comb-shaped'' graph, i.e., a line with a family of identical appendices. A less conventional example is discussed in Sec. IV, where scatterers of dimension two are coupled by single mode leads. We derive a general S-matrix expression and analyze in detail the particular case when the scatterers are spheres. The latter was previously discussed in Ref. 10; in distinction to this paper we use a physically reasonable coupling between the spheres and the leads. For a single scatterer we prove existence of resonance peaks and the background which dominates at large energies and decays not slower than E^{-1} as $E\to\infty$. Furthermore, we conjecture that the ''coarse grained'' transmission probability (averaged locally over the resonances) has the E^{-1} decay typical for the δ' interaction. In all three examples we analyze the dependence of scattering quantities on the parameters. In particular, we illustrate how the band spectrum arises when the number of arrayed scatterers tends to infinity.

II. SERIAL STRUCTURE TRANSPORT

A. Preliminaries

Consider an equidistant array $\{\mathcal{S}_j : j=0,\dots,N-1\}$ of identical scatterers placed at the line points $x_0+j\mathrm{l}$. The spacing $\mathrm{l}\geqslant 0$ in this convention includes only the distance between $\mathcal{S}_j$ and $\mathcal{S}_{j+1}$, not the possible size of the scatterers themselves.

Let us review briefly basic notions concerning a single-mode scattering on a sole scatterer $\mathcal{S}$ placed conventionally at the point $x_0=0$. On the two halflines attached to $\mathcal{S}$ the particle moves as free, so the on-shell S-matrix at energy k^2,

$$\begin{pmatrix} B_+ \\ B_- \end{pmatrix} = S \begin{pmatrix} A_+ \\ A_- \end{pmatrix}, \tag{2.1}$$

couples the coefficients of the asymptotic solutions

$$\psi(x) = \begin{cases} A_+ e^{ikx} + B_- e^{-ikx} + \cdots, & x<0, \\ B_+ e^{ikx} + A_- e^{-ikx} + \cdots, & x>0. \end{cases} \tag{2.2}$$

In particular, we have

$$S = \begin{pmatrix} t & \tilde{r} \\ r & \tilde{t} \end{pmatrix}, \tag{2.3}$$

where r,t and $\tilde{r},\tilde{t}$ are the left-to-right and right-to-left reflection and transmission amplitudes, respectively. We shall consider only the nondissipative situation when S is unitary; its dependence on the momentum k will be indicated only if necessary.

Since the interaction responsible for the scattering is localized by assumption, solutions to the Schrödinger equation acquire the asymptotic form outside the scatterer. Hence S may be expressed

alternatively in terms matrices used in the theory of ordinary differential equations. One is the ''coefficient'' transfer matrix M relating the solutions to the left and to the right of the scatterer by

$$\begin{pmatrix} B_+ \\ A_- \end{pmatrix} = M \begin{pmatrix} A_+ \\ B_- \end{pmatrix}. \tag{2.4}$$

It is straightforward to see that

$$M = \frac{1}{\tilde{t}} \begin{pmatrix} t\tilde{t} - r\tilde{r} & \tilde{r} \\ -r & 1 \end{pmatrix}, \tag{2.5}$$

and, vice versa,

$$r = -\frac{M_{21}}{M_{22}}, \quad t = M_{11} - \frac{M_{12}M_{21}}{M_{22}}, \quad \tilde{r} = \frac{M_{12}}{M_{22}}, \quad \tilde{t} = \frac{1}{M_{22}}. \tag{2.6}$$

Another one is the transfer matrix which relates the values and derivatives of the two solutions,

$$\begin{pmatrix} u(0+) \\ u'(0+) \end{pmatrix} = L \begin{pmatrix} u(0-) \\ u'(0-) \end{pmatrix}. \tag{2.7}$$

Substituting the boundary values of $u(x) = e^{ikx} + re^{-ikx}$ for $x<0$ and $u(x) = te^{ikx}$ for $x>0$ into this relation, we get a pair of equations for r,t which is solved by

$$\begin{aligned} r &= -\frac{L_{21} + ik(L_{22} - L_{11}) + k^2 L_{12}}{L_{21} - ik(L_{22} + L_{11}) - k^2 L_{12}}, \\ t &= -\frac{2ik \det L}{L_{21} - ik(L_{22} + L_{11}) - k^2 L_{12}}. \end{aligned} \tag{2.8}$$

In the same way we get the right-to-left amplitudes,

$$\begin{aligned} \tilde{r} &= -\frac{L_{21} + ik(L_{11} - L_{22}) + k^2 L_{12}}{L_{21} - ik(L_{22} + L_{11}) - k^2 L_{12}}, \\ \tilde{t} &= -\frac{2ik}{L_{21} - ik(L_{22} + L_{11}) - k^2 L_{12}}. \end{aligned} \tag{2.9}$$

Combining (2.5) with (2.8) and (2.9) we can express the ''coefficient'' transfer matrix as

$$M = \frac{1}{2ik} \begin{pmatrix} L_{21} + ik(L_{11} + L_{22}) - k^2 L_{12} & L_{21} + ik(L_{11} - L_{22}) + k^2 L_{12} \\ -L_{21} + ik(L_{11} - L_{22}) - k^2 L_{12} & -L_{21} + ik(L_{11} + L_{22}) + k^2 L_{12} \end{pmatrix}. \tag{2.10}$$

The class of admissible transfer matrices is restricted by the S-matrix unitarity. In particular, the conservation of probability current, $|r|^2 + |t|^2 = |\tilde{r}|^2 + |\tilde{t}|^2 = 1$, implies $|\det L| = 1$; we shall write therefore

$$\det L = \frac{t}{\tilde{t}} =: e^{2i\varphi}. \tag{2.11}$$

One can also express L by means of the other two matrices. For instance, suppose that (2.3) is given. Using the relation (2.7) with the boundary values for the left-to-right scattering, the same for the right-to-left case with the explicitly written L^{-1} and $t=\tilde{t}\det L$, we get a system of four linear equations for L_{jk},

$$\begin{aligned} &L_{11}(1+r)+ikL_{12}(1-r)=t, \quad L_{21}(1+r)+ikL_{22}(1-r)=ikt, \\ &L_{22}(1+\tilde{r})+ikL_{12}(1-\tilde{r})=t, \quad L_{21}(1+\tilde{r})+ikL_{11}(1-\tilde{r})=ikt. \end{aligned} \tag{2.12}$$

Only three of them are independent; it is straightforward to see that the first with the third equation, and the second with the fourth equation lead to the same relation which is solved by

$$L_{22}=L_{11}\frac{(1+r)(1-\tilde{r})}{(1-r)(1+\tilde{r})}-\frac{t(r-\tilde{r})}{(1-r)(1+\tilde{r})}.$$

The same pairs of equations allow us to express L_{12} and L_{21} in terms of L_{11} and L_{22}; in combination with the last relation we find

$$L_{12}=-L_{11}\frac{(1+r)}{ik(1-r)}+\frac{t}{ik(1+\tilde{r})}, \quad L_{21}=-ikL_{11}\frac{(1-\tilde{r})}{ik(1+\tilde{r})}+\frac{ikt}{(1+\tilde{r})}.$$

We have still the condition (2.11). Computing the determinant with the help of the above relations, we get

$$\det L=\frac{t(2L_{11}-t)}{(1-r)(1+\tilde{r})}=\frac{t}{\tilde{t}}.$$

One can express L_{11} from here and substitute into the formulas for the other elements; this yields finally

$$L=\frac{1}{2\tilde{t}}\begin{pmatrix} t\tilde{t}+(1+r)(1-\tilde{r}) & \dfrac{1}{ik}[t\tilde{t}-(1+r)(1+\tilde{r})] \\ ik[t\tilde{t}-(1-r)(1-\tilde{r})] & t\tilde{t}+(1-r)(1+\tilde{r}) \end{pmatrix}. \tag{2.13}$$

The determinant of this matrix is equal to the middle expression of (2.11) and, substituting into (2.8) and (2.9), one can check that (2.13) indeed represents the inverse transformation.

Furthermore, the unitarity of S has a stronger consequence. It is well known that a general 2×2 unitary matrix can be parametrized by four real numbers as

$$e^{i\xi}\begin{pmatrix} e^{i(\alpha+\delta)}\cos\beta & e^{i(\delta-\alpha)}\sin\beta \\ -e^{i(\alpha-\delta)}\sin\beta & e^{-i(\alpha+\delta)}\cos\beta \end{pmatrix}.$$

Using this for S given by (2.3) and substituting into (2.13) we find that

$$L=e^{i\varphi}\mathcal{L}, \quad \mathcal{L} \text{ real with } \det\mathcal{L}=1, \tag{2.14}$$

where $\varphi:=\alpha+\delta$. Notice that M given by (2.10) has then the following property:

$$\overline{M}_{11}=e^{-2i\varphi}M_{22}, \quad \overline{M}_{12}=e^{-2i\varphi}M_{21}. \tag{2.15}$$

B. Recursive relations for scattering amplitudes

Before we derive the mentioned closed-form expression, let us recall the usual factorization technique. We index the transmission and reflection amplitudes for the array by N. In analogy with (2.3) we have

$$\begin{pmatrix} B_-^N \\ B_+^N \end{pmatrix} = \begin{pmatrix} r_N & \tilde{t}_N \\ t_N & \overline{\varepsilon}^{2(N-1)}\tilde{r}_N \end{pmatrix} \begin{pmatrix} A_+^N \\ A_-^N \end{pmatrix}, \tag{2.16}$$

where $\varepsilon := e^{ikl}$. Next we add the $(N+1)$-th scatterer to the right side of the array for which

$$\begin{pmatrix} B_- \\ B_+ \end{pmatrix} = \begin{pmatrix} \varepsilon^{2N} r & \tilde{t} \\ t & \overline{\varepsilon}^{2N}\tilde{r} \end{pmatrix} \begin{pmatrix} A_+ \\ A_- \end{pmatrix}, \tag{2.17}$$

where, of course, $B_+^N = A_+$ and $B_- = A_-^N$. In analogy with (2.5) we rewrite the last two relations in the "coefficient" transfer matrix form. Multiplying the two matrices we get

$$\begin{pmatrix} B_+ \\ A_- \end{pmatrix} = M \begin{pmatrix} A_+^N \\ B_-^N \end{pmatrix}$$

with

$$M := \begin{pmatrix} \dfrac{1}{\tilde{t}\tilde{t}_N}((t\tilde{t} - r\tilde{r})(t_N\tilde{t}_N - r_N\tilde{r}_N\overline{\varepsilon}^{2(N-1)}) - r_N\tilde{r}\overline{\varepsilon}^{2N}) & \dfrac{1}{\tilde{t}\tilde{t}_N}((t\tilde{t} - r\tilde{r})\tilde{r}_N + \overline{\varepsilon}^{2N}\tilde{r}) \\ \dfrac{1}{\tilde{t}\tilde{t}_N}(-\varepsilon^{2N} r(t_N\tilde{t}_N - r_N\tilde{r}_N) - r_N) & \dfrac{1}{\tilde{t}\tilde{t}_N}(1 - \varepsilon^{2N} r\tilde{r}_N) \end{pmatrix}.$$

Comparing this with (2.6) we find the sought-after recursive relations

$$\tilde{r}_{N+1} = \overline{\varepsilon}^{2N}\tilde{r} + \frac{\tilde{r}_N\tilde{t}t}{1 - \varepsilon^{2N}\tilde{r}_N r}, \quad \tilde{t}_{N+1} = \frac{\tilde{t}\tilde{t}_N}{1 - \varepsilon^{2N} r\tilde{r}_N}. \tag{2.18}$$

If we modify the argument by adding the $(N+1)$-th scatterer to the left of the array, we get in the same way

$$r_{N+1} = \varepsilon^{2N} r + \frac{r_N\tilde{t}t}{1 - \overline{\varepsilon}^{2N}\tilde{r}r_N}, \quad t_{N+1} = \frac{tt_N}{1 - \overline{\varepsilon}^{2N} r_N\tilde{r}}. \tag{2.19}$$

Since the "component" S-matrices are unitary, it is straightforward to check by induction that the same is true for the total S-matrix. The relations (2.18) and (2.19) have a transparent meaning: expanding the fractions into geometric series we obtain expressions containing sums of contributions from various scattering processes.

C. The S-matrix expression

While the factorization technique described above is general, it does not relate directly the S-matrices of an individual scatterer and that of the whole array. Such a formula is particularly useful when the scatterers involved are identical. To deal with this situation, notice first that in view of (2.15) we can write the M matrix of the jth scatterer as

$$M_j = e^{i\varphi} \begin{pmatrix} \overline{R} & \overline{\varepsilon}^{2j}\overline{S} \\ \varepsilon^{2j} S & R \end{pmatrix}, \tag{2.20}$$

where $\varepsilon := e^{ikl}$ as above and

$$R := e^{-i\varphi} M_{22} = \frac{e^{-i\varphi}}{\tilde{t}} = \frac{e^{i\varphi}}{t} = \frac{\mathcal{L}_{11}+\mathcal{L}_{22}}{2} + i\left(\frac{\mathcal{L}_{21}}{2k} - \frac{k}{2}\mathcal{L}_{12}\right),$$
$$S := e^{-i\varphi} M_{21} = -\frac{e^{-i\varphi} r}{\tilde{t}} =: -\frac{e^{i\varphi} r}{t} = \frac{\mathcal{L}_{11}-\mathcal{L}_{22}}{2} + i\left(\frac{\mathcal{L}_{21}}{2k} + \frac{k}{2}\mathcal{L}_{12}\right). \tag{2.21}$$

By definition the ''coefficient'' transfer matrix of the array is obtained by multiplying successively the matrices (2.20). We denote $M^{(n)} := M_n M_{n-1} \cdots M_0$. It is easy to compute the first few matrices $M^{(n)}$; this inspires us to look for the general product in the form

$$M^{(n)} = e^{i(n+1)\varphi} \begin{pmatrix} \overline{\varepsilon}^{n+1} |S|^{n+1} \overline{\gamma_n} & \overline{\varepsilon}^n \overline{S} |S|^n \overline{\delta_n} \\ \varepsilon^n S |S|^n \delta_n & \varepsilon^{n+1} |S|^{n+1} \gamma_n \end{pmatrix}, \tag{2.22}$$

where the coefficients have to satisfy the recursive relations

$$\gamma_{n+1} = \zeta \gamma_n + \overline{\delta_n}, \quad \delta_{n+1} = \zeta \delta_n + \overline{\gamma_n} \tag{2.23}$$

with $\delta_0 = 1$ and

$$\gamma_0 = \zeta := \frac{\overline{\varepsilon} R}{|S|}, \tag{2.24}$$

which follows from $M^{(n+1)} = M_{n+1} M^{(n)}$. Since

$$\det M_j = e^{2i\varphi}(|R|^2 - |S|^2) = e^{2i\varphi} \frac{1-|r|^2}{|\tilde{t}|^2} = e^{2i\varphi}, \tag{2.25}$$

and, consequently, $\det M^{(n)} = e^{2i(n+1)\varphi} |S|^{2n+2} (|\gamma_n|^2 - |\delta_n|^2) = e^{2i(n+1)\varphi}$, we have

$$\gamma_n = e^{i\theta_n} \sqrt{|\delta_n|^2 + |S|^{-2n-2}} \tag{2.26}$$

with a phase factor to be determined. Substituting into the relations (2.23) we get

$$e^{i\theta_{n+1}} \sqrt{|\delta_{n+1}|^2 + |S|^{-2n-4}} = \zeta e^{i\theta_n} \sqrt{|\delta_n|^2 + |S|^{-2n-2}} + \delta_n,$$
$$\delta_{n+1} = \zeta \delta_n + e^{-i\theta_n} \sqrt{|\delta_n|^2 + |S|^{-2n-2}}. \tag{2.27}$$

We express $e^{i\theta_n}$ from the second equation and substitute into the first one; this yields

$$\delta_{n+2} - (\zeta + \overline{\zeta}) \delta_{n+1} + (|\zeta|^2 - 1) \delta_n = 0. \tag{2.28}$$

Now $\delta_0 = 1$ and $\delta_1 = \zeta + \overline{\zeta}$, so (2.28) is solved by

$$\delta_n = (|\zeta|^2 - 1)^{n/2} U_n\left(\frac{\zeta + \overline{\zeta}}{2\sqrt{|\zeta|^2 - 1}}\right),$$

where U_n is the Chebyshev polynomial of the second kind. Since $|\zeta|^2 - 1 = |S|^{-2}$ by (2.25), its argument can be more compactly written as $\mathrm{Re}(\overline{\varepsilon} R)$. Using (2.26) and (2.27) again, we find $M^{(n)} = e^{2i(n+1)\varphi} \mathcal{M}^{(n)}$ with

$$\mathcal{M}^{(n)}=\begin{pmatrix} \overline{\varepsilon}^{n+1}e^{-i\theta_n}\sqrt{1+|S|^2U_n(\mathrm{Re}(\overline{\varepsilon}R))^2} & \overline{\varepsilon}^{n}\overline{S}U_n(\mathrm{Re}(\overline{\varepsilon}R)) \\ \varepsilon^{n}SU_n(\mathrm{Re}(\overline{\varepsilon}R)) & \varepsilon^{n+1}e^{i\theta_n}\sqrt{1+|S|^2U_n(\mathrm{Re}(\overline{\varepsilon}R))^2} \end{pmatrix}, \quad (2.29)$$

where

$$e^{i\theta_n}=\frac{U_{n+1}(\mathrm{Re}(\overline{\varepsilon}R))-\varepsilon\overline{R}U_n(\mathrm{Re}(\overline{\varepsilon}R))}{\sqrt{1+|S|^2U_n^2(\mathrm{Re}(\overline{\varepsilon}R))}}. \quad (2.30)$$

Now we may employ (2.5) and (2.11) to find the sought-after formulas for the array of N scatterers; it is sufficient to put $n=N-1$. We arrive at the following conclusion:

Theorem II.1: *With the given notation, the transmission and reflection amplitudes of an N-element serial structure express as*

$$t_N=\frac{\overline{\varepsilon}^{N}e^{-i\theta_{N-1}}}{\sqrt{1+|S|^2U_{N-1}(\mathrm{Re}(\overline{\varepsilon}R))^2}} \quad (2.31)$$

$$r_N=-\frac{\overline{\varepsilon}e^{-i\theta_{N-1}}SU_{N-1}(\mathrm{Re}(\overline{\varepsilon}R))}{\sqrt{1+|S|^2U_{N-1}(\mathrm{Re}(\overline{\varepsilon}R))^2}}, \quad (2.32)$$

where the phase factor is given by (2.30). In the same way the right-to-left amplitudes are $\tilde{t}_N=t_Ne^{-2iN\varphi}$ *and*

$$\tilde{r}_N=-\frac{\overline{\varepsilon}^{2N-1}e^{-i\theta_{N-1}}\overline{S}U_{N-1}(\mathrm{Re}(\overline{\varepsilon}R))}{\sqrt{1+|S|^2U_{N-1}(\mathrm{Re}(\overline{\varepsilon}R))^2}}.$$

In particular, the transmission and reflection probabilities are the same in both directions and equal

$$|t_N|^2=\frac{1}{1+|S|^2U_{N-1}(\mathrm{Re}(\overline{\varepsilon}R))^2}, \quad |r_N|^2=\frac{|S|^2U_{N-1}(\mathrm{Re}(\overline{\varepsilon}R))^2}{1+|S|^2U_{N-1}(\mathrm{Re}(\overline{\varepsilon}R))^2}. \quad (2.33)$$

Recall that

$$|S|^2=\left|\frac{r}{t}\right|^2, \quad \mathrm{Re}(\overline{\varepsilon}R)=\mathrm{Re}\left(\frac{e^{-i(kl+\varphi)}}{\tilde{t}}\right)=\mathrm{Re}\left(\frac{e^{-i(kl-\varphi)}}{t}\right);$$

it is obvious from (2.33) that the probability current is preserved.

D. Relation to band spectra of periodic systems

An advantage of the above formula is that it makes clear the relation between serial structure and their infinite analogs. Consider an infinite periodic array of identical scatterers $\mathcal{S}$ joined by line segments of length l. The one-period transfer matrix is $T=L\,\mathcal{U}_l(k)$, where

$$\mathcal{U}_l(k):=\begin{pmatrix} \cos kl & \frac{1}{k}\sin kl \\ -k\sin kl & \cos kl \end{pmatrix}$$

coresponds to the segment. The band spectrum of the problem is given by the Bloch condition, $\det(T-e^{i\theta})=0$, or

$$e^{2i\theta}-e^{i\theta}\mathrm{tr}\,T+\det T=0. \quad (2.34)$$

In view of (2.11), $\det T=\det L=e^{2i\varphi}$, so the condition may be written as

$$e^{-i\varphi}\mathrm{tr}\, T=2\cos(\theta-\varphi).$$

To express the lhs, we employ (2.13) which yields

$$\mathrm{tr}\, T=\mathrm{tr}\, T\cos kl+\left(\frac{1}{k}L_{21}-kL_{12}\right)\sin kl=\frac{t\tilde{\bar{t}}-r\tilde{\bar{r}}}{\tilde{t}}e^{ikl}+\frac{1}{\tilde{t}}e^{-ikl},$$

and since

$$\frac{t\tilde{\bar{t}}-r\tilde{\bar{r}}}{\tilde{t}}=\frac{e^{2i\varphi}}{\bar{\tilde{t}}}$$

by (2.5) and (2.15), we arrive finally at

$$\mathrm{Re}(\bar{\varepsilon}R)=\frac{e^{i(kl+\varphi)}}{2\bar{\tilde{t}}}+\frac{e^{-i(kl+\varphi)}}{2\tilde{t}}=\cos(\theta-\varphi). \tag{2.35}$$

The lhs as a function of k is typically oscillating. Since the amplitude $|t|^{-1}>1$ unless the single-element scattering is reflectionless, the periodic spectrum has gaps in general.

The relations (2.33) show how the band spectrum arises in the limit $N\to\infty$ of the serial-structure scattering. The Chebyshev polynomials

$$U_n(x)=\sum_{m=0}^{[n/2]}(-1)^m\frac{(n-m)!}{m!(n-2m)!}(2x)^{n-2m} \tag{2.36}$$

are oscillating within the interval $[-1,1]$. The easiest way to see that is to use the representation

$$U_n(x)=\frac{\sin(n+1)\xi}{\sin\xi},\quad \xi:=\arccos x. \tag{2.37}$$

Thus U_{N-1} has $N-1$ roots in $[-1,1]$ and each band contains at least $N-1$ points where $|t_N(k)|^2=1$. Possible additional points with this property can come from zeros of the single-element reflection coefficient. Properties of Chebyshev polynomials yield also lower bounds to the envelope of the transmission probability oscillations. The representation (2.37) implies $|U_n(x)|\leqslant(1-x^2)^{-1/2}$ for $|x|<1$, and therefore

$$|t_N(k)|^2\geqslant\frac{1-(\mathrm{Re}(\bar{\varepsilon}R))^2}{1+|S|^2-(\mathrm{Re}(\bar{\varepsilon}R))^2}=\frac{|t(k)|^2-(\mathrm{Re}(\tilde{t}(k)e^{i(kl+\varphi)}))^2}{1-(\mathrm{Re}(\tilde{t}(k)e^{i(kl+\varphi)}))^2}. \tag{2.38}$$

If $|t(\cdot)|^2$ is a slowly varying function, the rhs reaches its maximum $|t(k)|^2$ in the middle of the band; it is zero at the band edges. However, the transmission can vanish within a band only due to a single-element full reflection. This follows from another upper bound,[11] $|U_n(x)|\leqslant(n+1)$ for $|x|\leqslant 1$, which yields $|t_N|^2\geqslant(1+N^2|S|^2)^{-1}$ or

$$|t_N(k)|^2\geqslant\frac{|t(k)|^2}{1+(N-1)|r(k)|^2}. \tag{2.39}$$

On the other hand, to see the behavior of the reflection and transmission amplitudes in the gaps of the periodic spectrum, we have to estimate the Chebyshev polynomials outside $[-1,1]$. By analytical continuation, the relation (2.37) gives $U_n(x)=\sinh((n+1)\operatorname{arcosh} x)/\sinh(\operatorname{arcosh} x)$, so

$$U_n(x)=\sum_{k=0}^{n}(x+\sqrt{x^2-1})^{n-2k}.$$

Then we have, for instance, the following estimates

$$n+x^n\leqslant U_n(x)\leqslant(n+1)(x+\sqrt{x^2-1})^n. \tag{2.40}$$

The first inequality yields an upper bound,

$$|t_N(k)|^2\leqslant\frac{1}{1+(N-1+(\mathrm{Re}(\overline{\varepsilon}R))^{N-1})^2}. \tag{2.41}$$

It is clear that $|t_N(k)|^2=1$ holds only if the same is true for $|t(k)|^2$; in all the other cases it behaves as $o((\mathrm{Re}(\overline{\varepsilon}R))^{2N-2})$ as $N\to\infty$. On the other hand, $|t_N(k)|^2=0$ holds only if a single scatterer has a full reflection at this energy, otherwise the second inequality of (2.40) together with $|\mathrm{Re}(\overline{\varepsilon}R)|\leqslant|t(k)|^{-1}$ and the unitarity relation gives

$$|t_N(k)|^2\geqslant\frac{|t(k)|^{2N}}{|t(k)|^{2N}+N^2|r(k)|^2(1+|r(k)|)^{2N-2}}. \tag{2.42}$$

III. SERIAL GRAPHS

As we have said we want now to illustrate the above results on several examples which go beyond the usual one-dimensional potential scattering. In this section we shall discuss the situation where the serial structure is a graph.

Although nonrelativistic quantum mechanics for quantum particles confined to a graph has been considered already several decades ago in connection with the free-electron models of hydrocarbons.[12] it became a subject of intense interest only recently as a tool to describe systems of quantum wires—see Refs. 13–29 and references therein. There are also other systems for which graph description could prove to be useful, such as objects composed of carbon nanotubes.[30,31]

Graph systems are attractive because they are often explicitly solvable; on the mathematical level they represent systems of ordinary differential equations in contrast to partial differential equations with nontrivial boundary conditions needed to describe quantum wire systems in higher dimensions. At the same time, the simplified description may still preserve basic features of the real system. Of course, replacing a branched waveguide system by its skeleton graph is a nontrivial approximation, but we shall avoid discussing this point here; some comments can be found in Refs. 19 and 32 and references given there.

A. Loop arrays

In our first example an individual scatterer is a planar loop $\mathcal{L}$ with a pair of external leads placed into a homogeneous magnetic field cf. Fig. 1.

We suppose that the field is perpendicular to the graph plane. The corresponding vector potential in the circular gauge is $\vec{A}(\vec{x})=(-\frac{1}{2}By,\frac{1}{2}Bx,0)$ and

$$\int_{\mathcal{L}}\vec{A}(\vec{x})\,d\vec{x}=\frac{BS}{L_1+L_2}=\frac{\Phi}{L_1+L_2},$$

where S is the loop area, L_j are the lengths of its two branches, and Φ is the corresponding magnetic flux.

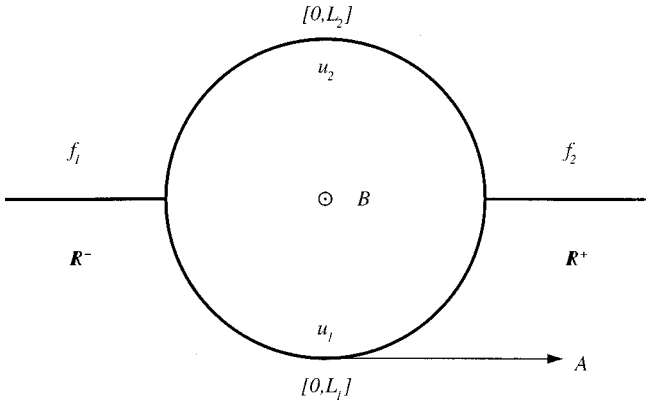

FIG. 1. A loop–graph scatterer in a magnetic field.

Such a scattering system has been considered earlier—see Refs. 33, 17 and 27 and references therein. The Hilbert space for the graph of Fig. 1 is the orthogonal sum of four L^2 spaces referring to the graph links; its elements will be denoted as (f_1,u_1,u_2,f_2) with the coordinates at the loop taken anticlockwise. We suppose that the particle has a unit charge and apart from the magnetic field it moves as free on the graph. There are various ways how to couple the operators $(-i\partial_x - A)^2$ from different graph links in a self-adjoint way.[28,24,29] For the sake of simplicity we restrict ourselves to the usual δ coupling, i.e., we impose the boundary conditions

$$\begin{aligned} f_1(0)=u_1(0)=u_2(L_2), \quad -f_1'(0)+u_1'(0)-u_2'(L_2)=\alpha_1 f_1(0), \\ f_2(0)=u_2(0)=u_1(L_1), \quad f_2'(0)-u_1'(L_1)+u_2'(0)=\alpha_2 f_2(0), \end{aligned} \tag{3.1}$$

where the function and derivative values mean the appropriate one-sided limits. On the other hand, we do not suppose in general that α_1,α_2 and L_1,L_2 are the same.

Substituting into (3.1) the boundary values of the generalized eigenfunctions on the loop, $u_j(x)=A_j e^{-i(A-k)x}+B_j e^{-i(A+k)x}$, $j=1,2$, we get a system of six equations. Eliminating from here A_j,B_j we arrive at the relations

$$f_2(0)=\frac{1}{2kD}((i\alpha_1 B+2kC)f_1(0)+iBf_1'(0))$$

$$f_2'(0)=\frac{1}{2kD}((i\alpha_1\alpha_2 B+2(\alpha_1+\alpha_2)kC-4ik^2E_-E_+)f_1(0)+(2kC+i\alpha_2 B)f_1'(0)),$$

determining the transfer matrix, where

$$B=(\varepsilon_{1+}-\varepsilon_{1-})(\varepsilon_{2-}-\varepsilon_{2+})=4e^{-i\Phi}\sin kL_1\sin kL_2,$$

$$C=-\varepsilon_{1-}\varepsilon_{2-}+\varepsilon_{1+}\varepsilon_{2+}=2ie^{-i\Phi}\sin k(L_1+L_2),$$

$$D=\varepsilon_{2+}-\varepsilon_{2-}+\varepsilon_{2+}\varepsilon_{2-}(\varepsilon_{1+}-\varepsilon_{1-}),$$

$$E_\pm=1-\varepsilon_{1\pm}\varepsilon_{2\pm}=2i\,e^{-i\Phi/2}e^{\pm ik(L_1+L_2)/2}\sin\left(\frac{\pm k(L_1+L_2)-\Phi}{2}\right),$$

$$\varepsilon_{j\pm}=e^{i(-A\pm k)L_j},\quad j=1,2.$$

The reflection and transmission amplitudes are given by

$$r(k)=\frac{-i\alpha_1\alpha_2 B+k((\alpha_2-\alpha_1)B-2(\alpha_1+\alpha_2)C)+ik^2(4E_-E_+-B)}{i\alpha_1\alpha_2 B+k(\alpha_2+\alpha_1)(2C+B)-ik^2(4E_-E_++B+4C)},$$
$$t(k)=\frac{4ik^2De^{-2i\Phi}}{i\alpha_1\alpha_2 B+k(\alpha_2+\alpha_1)(2C+B)-ik^2(4E_-E_++B+4C)}, \tag{3.2}$$

respectively. Since $B,C,E_\pm$ as well as D^2 are 2π-periodic functions of the magnetic flux, the same is valid for the reflection and transmission *probabilities*. Recall that if we put $e=\hbar=c=1$, then 2π is the magnetic flux quantum in these units.

B. Band spectrum of an infinite loop array

We illustrate the relation of transmission probabilities of a finite array of loops and the spectrum of the corresponding infinite system on Fig. 2. As already mentioned $|t_N(k)|^2$ is a 2π-periodic function and, because the condition (2.35) determining the band spectrum of the infinite system can be reformulated as $0<|\mathrm{Re}(\overline{\varepsilon R})|<1$, we show dependence on Φ only in the range $[0,2\pi]$ {$|\mathrm{Re}(\overline{\varepsilon R})|$ is also a 2π-periodic function}. We choose loops with different L_1, L_2 and α_1, α_2. Even for a relatively small number of loops $N=6$ the values of $|t_N(k)|^2$ are clearly nonzero in areas of parameters Φ and k where there are bands of the infinite system and negligible where there are gaps.

C. Comb graphs

Our next example concerns the case of a comb-shaped graph, i.e., a line with a finite number N of identical appendices attached to it at equally spaced points. Such systems have been discussed recently[34] following earlier studies of a single-stub waveguide.[35–38]

Comparing to the previous work and the preceding example, we shall discuss comb-shaped graphs in a more thorough way. First of all, instead of the δ-coupling used above (or the Griffith's boundary conditions in the terminology of Ref. 34) we allow for the most general self-adjoint way in which the stubs can be attached to continuous wavefunctions on the line. This amounts to imposing at the junctions the boundary conditions adopted from an earlier treatment of the T-shaped graph.[24] Should the Hamiltonian be time-reversal invariant, the junction is then characterized by three real parameters. In this framework we are able to handle imperfect contacts;[20] moreover, it is straightforward to modify the results derived below to graphs with a δ'-coupling which corresponds to the situation where the junction itself represents a complicated geometric scatterer (see Refs. 15 and 19; more about that will be said in the next section). Computing the S-matrix we also assume that the particle is under the influence of a potential on the stubs; this makes it possible to investigate how the band-form zones of high transmission which arise for $N\gg 1$ change when an external field is applied.

The formula derived in the previous section allows us to express the transmission and reflection probabilities. In addition to them, one is able to generalize the result of Ref. 24 to the present situation and to find an explicit Krein-formula expression for the resolvent of the comb-graph Hamiltonian. This allows us to study their resonance structure of the problem which arises from perturbation of the disconnected-stub discrete spectrum embedded into the continuum of the line motion. The mentioned expression yields an equation from which the resolvent singularities on the second sheet can be found.

After this introduction, let us describe the model. For a greater generality we suppose first that the appendices are not necessarily identical. The graph Γ_N will therefore consist of a line with a finite sequence $\{(s-1)\mathrm{l}\}_{s=1}^N$ of points at which appendices of finite lengths L_s are attached (see Fig. 3).

The state Hilbert space of the problem is then $\mathcal{H}\equiv L^2(\Gamma_N):=L^2(\mathbb{R})\oplus(\oplus_{s=1}^N L^2(0,L_s))$; we shall write its elements as columns

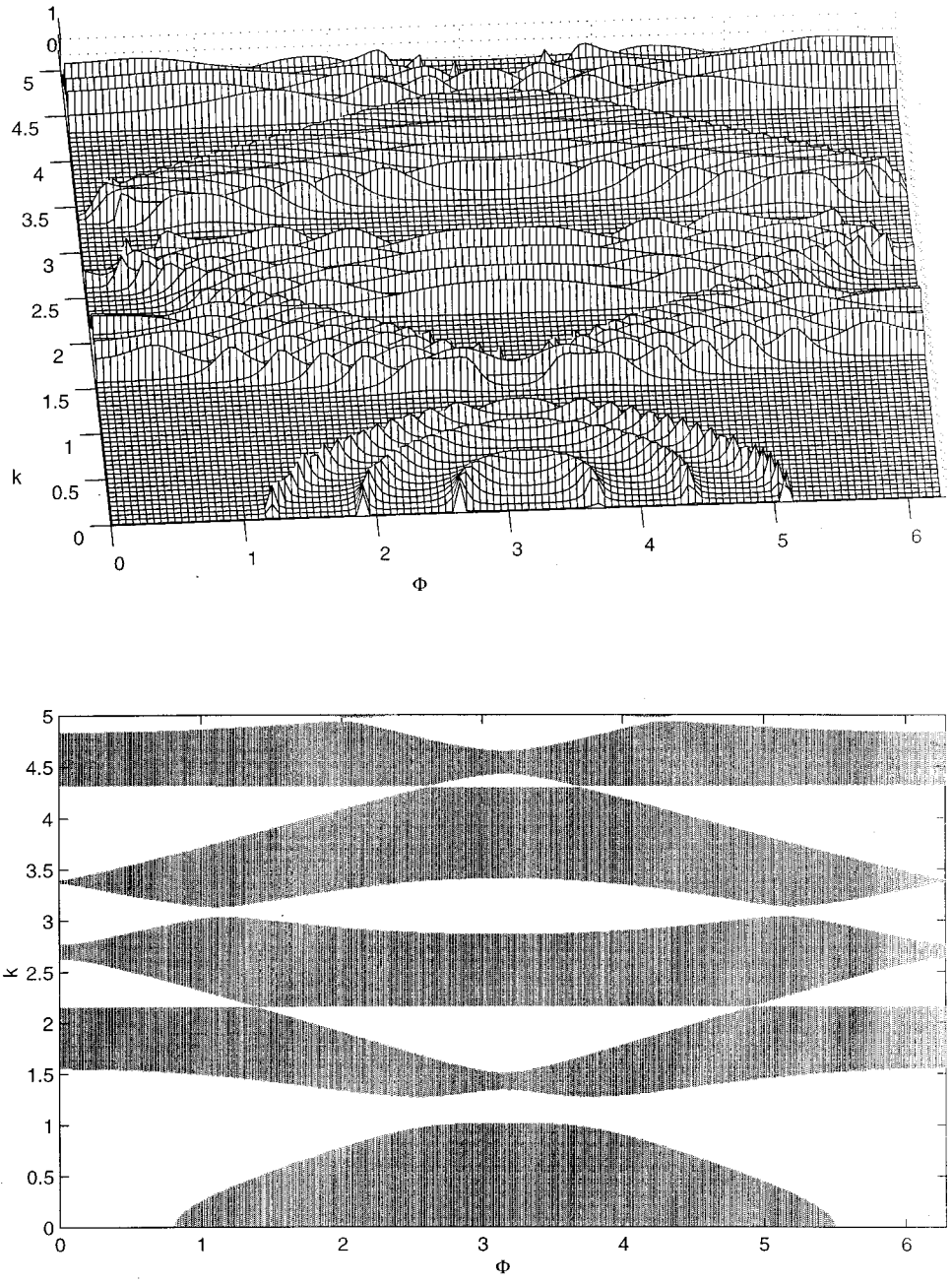

FIG. 2. The relation of transmission probabilities of a finite array of loops ($N=6$) and the spectrum of the corresponding infinite system, $L_1=0.5$, $L_2=1.5$, $l=\sqrt{2}$, $\alpha_1=-1$, and $\alpha_2=-2$. The upper figure shows $|t(k,\Phi)|^2$ (varying from 0 to 1), while the lower one show the band spectrum of the infinite periodic system.

$$\psi=\begin{pmatrix} f \\ u_1 \\ \vdots \\ u_N \end{pmatrix}.$$

We suppose that the motion at the backbone line is free while the particle is exposed to potentials V_s on the "teeth;" hence the Hamiltonian of a nonrelativistic particle of mass $m=\frac{1}{2}$ living on Γ_N acts as

FIG. 3. A comb-shaped graph.

$$(H\psi)_1(x) := -f''(x), \quad (H\psi)_{s+1}(x) := (-u_s'' + V_s u_s)(x), \quad s = 1, \ldots, N, \tag{3.3}$$

out of the junctions. To make it a self-adjoint operator one has to choose again properly the boundary conditions which couple the wavefunctions at the branching points of the graph in such a way that the probability current conservation at the vertices is conserved. As we have said, we shall require continuity of the line component f of ψ at the junctions; to keep a manageable number of parameters we assume the Dirichlet conditions at the end of the stubs. Consequently, the domain of the Hamiltonian consists of all $\psi \in \mathcal{H}$ with $f \in AC^2(\mathbb{R})$ and $u_s \in AC^2(0, L_s)$ satisfying the conditions[24]

$$\begin{gathered} f((s-1)\mathrm{l}+) = f((s-1)\mathrm{l}-) =: f((s-1)\mathrm{l}), \\ u_s(0) = b_s f((s-1)\mathrm{l}) + c_s u_s'(0), \\ f'((s-1)\mathrm{l}+) - f'((s-1)\mathrm{l}-) = d_s f((s-1)\mathrm{l}) - b_s u_s'(0), \\ u_s(L_s) = 0 \end{gathered} \tag{3.4}$$

for $s = 1, \ldots, N$. In general, b_s may be complex, however, we restrict from the start to Hamiltonians which are time-reversal invariant and suppose that the coefficient matrices $\mathbb{K}_s = \left(\begin{smallmatrix} b_s & c_s \\ d_s & -b_s \end{smallmatrix}\right)$ are real. The sth appendix is decoupled from the line by putting $b_s = 0$; it is then described by the operator $h_{c_s} := -d^2/dx^2 + V_s$ specified by the decoupled condition

$$u_s(0) - c_s u_s'(0) = 0 \tag{3.5}$$

at the junction.

In what follows we concentrate on the finite periodic case where $L_s = L$, $V_s = V$, and $\mathbb{K}_s = \mathbb{K}$; the operator specified by the boundary conditions (3.4) will be denoted as $H_N \equiv H_N(\mathbb{K}, V)$. The potential V is supposed to belong to $L^1(0, L)$.

D. Scattering on a comb graph

To write the scattering matrix we need some notation. Let u_L be the unique solution to the appendix Schrödinger equation,

$$-u_L'' + V u_L = k^2 u_L \tag{3.6}$$

with the energy k^2 and the normalized Dirichlet condition at the outer endpoint, $u_L(L) = 1$ $-u_L'(L) = 0$. If all the junctions are described by the parameters b, c, d in (3.4), we put

$$\beta := \frac{d}{2k} + \frac{b^2}{2k}\left(\frac{u_L'}{c u_L' - u_L}\right)(0), \quad \zeta := \cos k\mathrm{l} + \beta \sin k\mathrm{l}, \tag{3.7}$$

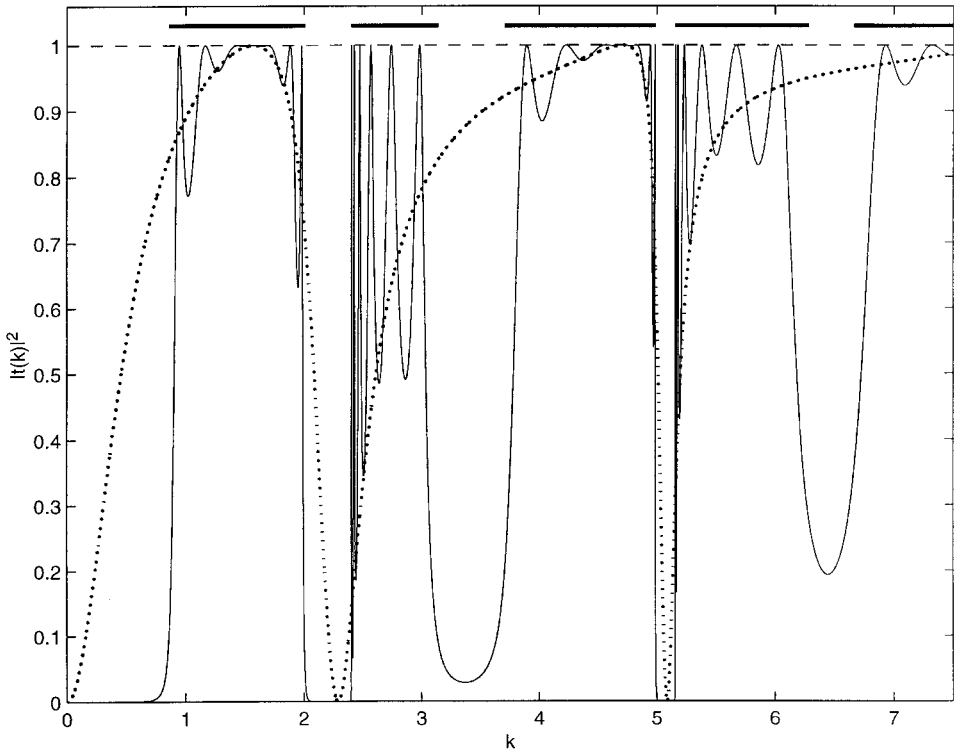

FIG. 4. The relation of transmission probabilities of a single appendix (dotted line), a finite array of appendices ($N=7$) (full line), and the spectrum of the corresponding infinite system (thick lines above). The parameters are $b=1.2$, $c=0.5$, $d=0$, $L=1$, and $\mathrm{l}=1$.

and denote again $\varepsilon := e^{ik\mathrm{l}}$. For a single stub, $s=N=1$, we insert a generalized eigenvector of the form $\binom{f}{\alpha u_1}$ into the boundary conditions (3.4) and express $f(0+), f'(0+)$ by means of the left-sided limits; this yields the single-element transfer matrix which can be written with the help of (3.7) as

$$L_\beta = \begin{pmatrix} 1 & 0 \\ 2k\beta & 1 \end{pmatrix},$$

so $R=1+i\beta$ and $S=i\beta$. Furthermore, $\mathrm{Re}(\overline{\varepsilon}\overline{R})=\zeta$. Using then the explicit expression (2.30) of the phase factor together with (2.31) and (2.32), we may write the left-to-right scattering amplitudes as

$$r_N = \frac{i\beta U_{N-1}(\zeta)}{\varepsilon U_{N-2}(\zeta) - (1+i\beta)U_{N-1}(\zeta)}, \quad t_N = -\frac{\varepsilon^{1-N}}{\varepsilon U_{N-2}(\zeta) - (1+i\beta)U_{N-1}(\zeta)}. \tag{3.8}$$

In particular, the reflection and transmission probabilities are

$$|t_N(k)|^2 = 1 - |r_N(k)|^2 = \frac{1}{1+\beta^2 U_{N-1}(\zeta)^2}. \tag{3.9}$$

Let us now illustrate how the the transmission probability depends on the number of the teeth and the parameters of the junctions. Figure 4 shows a typical example of the situation. For a certain set of parameters b, c, and d we compare $|t(k)|^2$ for one and seven appendices with an infinite array of them. The band spectrum is marked by thick lines above. The suppression of the

transmission coefficient at those values of k where the infinite system shows gaps is evident even for a relatively small number of elementary scatterers, $N=7$. In each band we distinguish $N-1$, i.e., six values of k_i when $|t(k_i)|^2=1$ as it should be—cf.(2.37). In addition the first and third band contain an additional value of k_a for which $|t(k_a)|^2=1$ and these values coincide with the values of k for which a single appendix allows a perfect transmission. The values of k for which the reflection is total fall into gaps of the infinite system as it should be (cf. the end of Sec. II D).

In addition to the S-matrix one can ask about scattering resonances for the comb graphs. The particular character of the coupling (3.4) makes it possible to find the resonance condition as a direct generalization of the argument given in Ref. 24. It turns out that the corresponding poles of the analytically continued resolvent appear at the points where the denominators in (3.8) vanish.

E. Band spectrum of an infinite comb and resonances

We discuss only the case of free appendices here, i.e., $V_s=0$. Investigation of nonzero potentials represents no complication in general conception. Typical spectra of an infinite comb are presented on Fig. 5. The parameters of such a structure could be divided into two groups, viz. l,L and b,c,d. The dependence on l is rather simple; a change of l results in scaling of spectrum in k. This is the consequence of the fact that the transfer matrix T depends only on the product $k\mathrm{l}$. This is the reason why we show all the spectra for $\mathrm{l}=1$ only. The dependence on L is more complicated as can be inferred from Fig. 5.

A striking feature of such a spectrum are sudden transitions of bands to gaps or vice versa at $k\mathrm{l}=n\pi$, $n\in\mathbb{Z}$ for almost all L. This can be understood, if we write down the Bloch condition explicitly as

$$\beta(k)\sin(k\mathrm{l})+\cos(k\mathrm{l})=\cos(\theta).$$

Clearly, this is always fulfilled for $k\mathrm{l}=n\pi$, unless β has a singularity at $n\pi/\mathrm{l}$. Therefore $k=n\pi/\mathrm{l}$ belongs always to the band in this case. The situations when $\beta(n\pi/\mathrm{l})$ is infinite requires a further analysis. An effect of a small change ϵ in k can be estimated from $\beta(k+\epsilon)\epsilon\mathrm{l}+1=(-1)^n\cos(\theta)$. With the exception of points where $\beta(n\pi/\mathrm{l})=0$, small change of ϵ does not change the sign of β, while the change of sign of ϵ leads to the change of sign of $\beta(k+\epsilon)\epsilon\mathrm{l}$. Only in the vicinity of points where $\beta(n\pi/\mathrm{l})=0$ can the sign of $\beta(k+\epsilon)\epsilon\mathrm{l}$ rest unchanged, cf. Fig 5.

Of the three parameters determining the coupling of an appendix to the backbone line, i.e., b,c,d, we find b as the most suitable to begin with. Putting $b=0$ effectively switches off the appendices as already mentioned in Sec. III B. This implies that we have eigenvalues k_n^2 embedded in the continuum, where k_n are solutions of (3.5). These values of momentum play an important role from three points of view. First, k_n's are the values for which $u_L(0)=0$ and the number of zeros of u increases by one when k passes to higher values; this means that the whole $\mathbb{R}^+$ is divided into disjoint intervals by these values (for a given L). On the other hand, a band can belong to two intervals (although this happens only for some L) and states of the same band can be described by wave functions with different numbers of zeros of u's. Also, and this situation is far more frequent, one interval can contain two or more bands, so that the number of zeros of u is not directly related to the ordinal number of a band.

In order to reveal the second role of these values of k_n's, we have to a return to finite number of appendices attached to the line. If we begin with one appendix only, direct calculation shows that $t(k_n)=0$ and $r(k_n)=-1$. Therefore, regardless of the number of appendices N, the full reflection takes place, i.e., $t_N=0, r_N=-1$.

We close this section with discussion of scattering resonances of our system. Recently, it was shown[3] that there is a certain "band" structure in the spectrum of resonances and that this spectrum converges to the energy band spectrum of the infinite periodic system in the limit of an infinite number of scatterers. The authors also show that one should expect $N-1$ resonances in each band if the system consists of N identical cells. These conclusions are in accordance with our results but for one difference—the number of resonances in a band is $2N-1$. It is a consequence of the fact that the origin of resonances is twofold here. $N-1$ resonances comes from the spacial

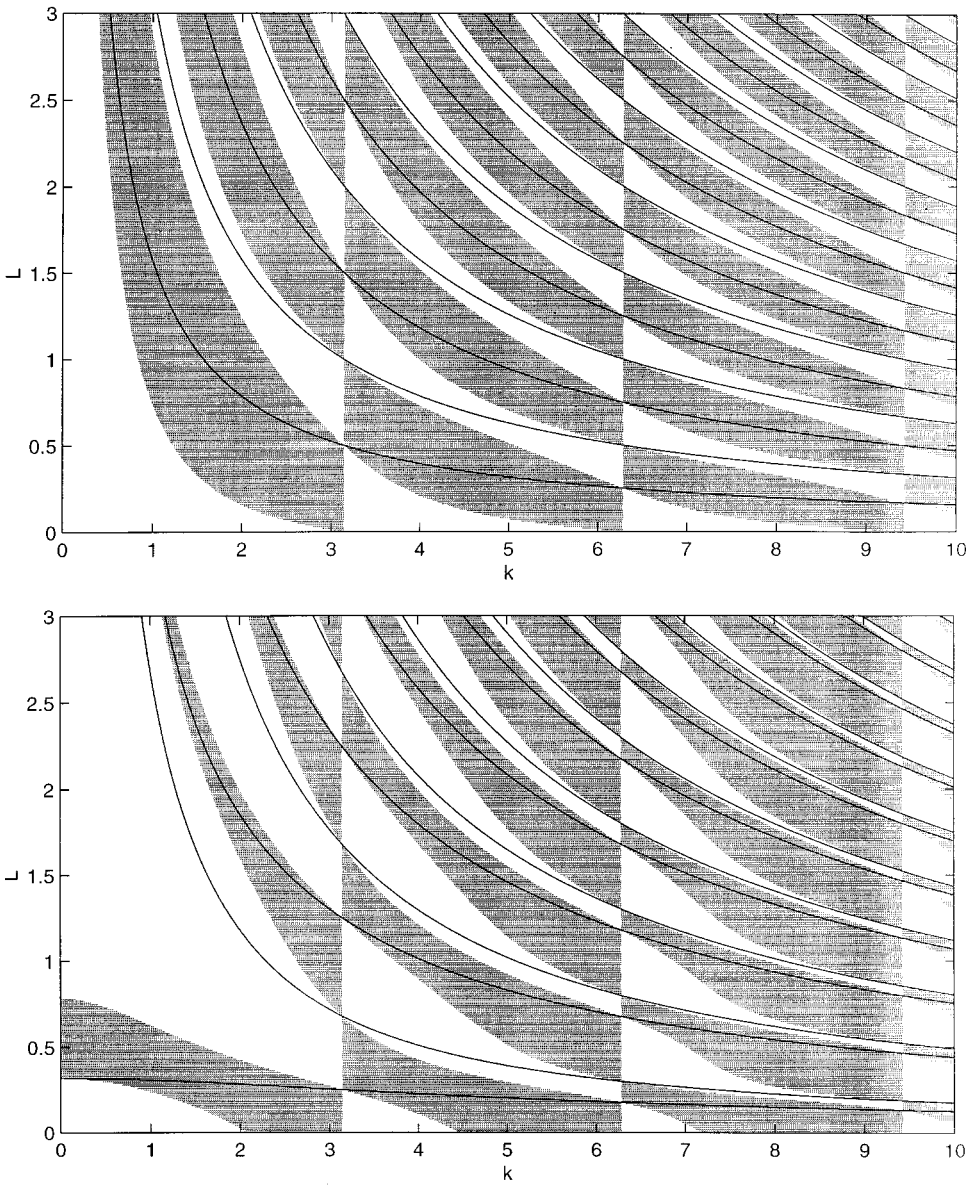

FIG. 5. The band spectra of infinite arrays of appendices. The upper figure is for $b=1$, $c=d=0$, and the lower one for $b=3$, $c=0.5$, and $d=-11$. The spacing is chosen $l=1$ in both cases. The full lines show the role of perfect transmission (the lines in the bands) and total reflection (the lines in the gaps) for a single appendix.

order of our periodical structure as in Ref. 3 and the remaining N ones have their origin in k_n^2, which is an N-fold eigenvalue for the case of $b=0$. As $|b|$ grows this degenercy is lifted and we find N resonances in the vicinity of k_n^2. This is the third role of k_n. The $N-1$ resonances related to the spatial setting travel from $-\infty$, and for small b these two sets are well separated as is shown on Fig. 6.

There are situations when a resonance or a bound state appears at $k=0$. The manifestation of this instance is that $|t(0)|^2=1$. This can take place even in the case of one appendix. The expression (5) of Ref. 24 with explicit form of $u_L(0)$ shows that this can happen as soon as the condition

$$d(c+L)+b^2=0$$

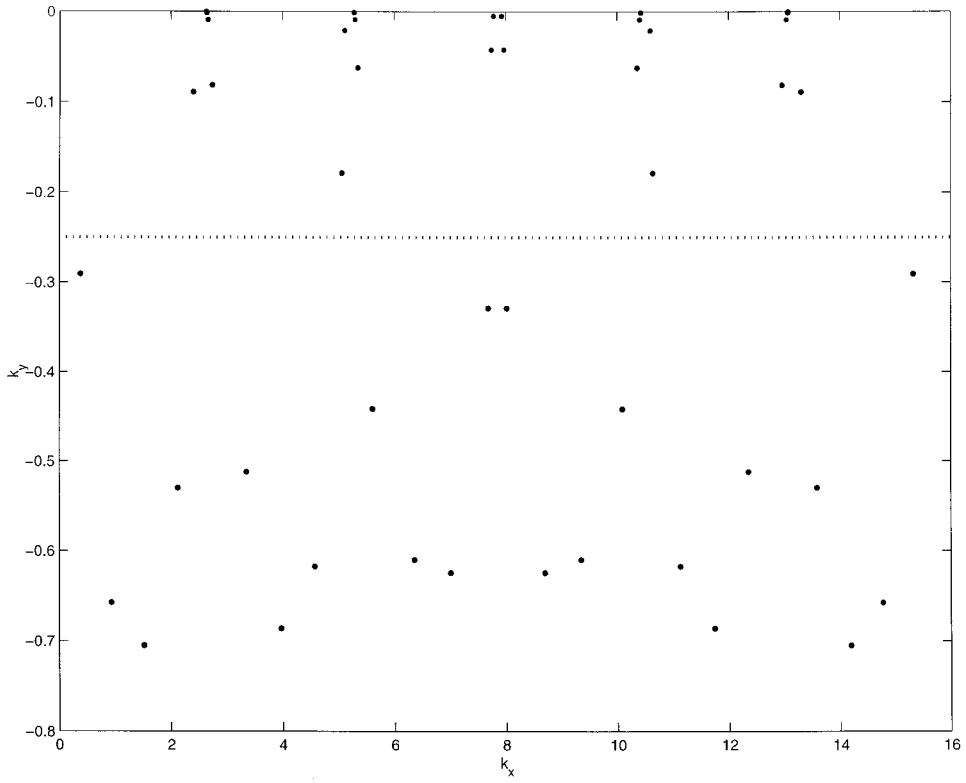

FIG. 6. This figure shows positions of resonances for $N=5$ appendices and $b=0.4$, $c=d=0$, and $L=1.2$. The dotted line separates the two sets of resonances. The resonances closer to the real axis have their origin in N-fold eigenvalues for $b=0$; increasing $|b|$ lifts the degeneracy and pushes the resonances from the real line. The rest of the resonances (below the dotted line) has the origin in the serial arrangement of individual scatterers.

is fulfilled. Provided that this condition holds, there is perfect transmission at $k=0$ for any number of appendices, i.e., $t_N(0)=1$. Besides this there could be other situations when $t_N(0)=1$ for $N>1$. If there exists such an $n=1,\ldots,N-1$ that

$$\cos\left(\frac{n\pi}{N}\right)=1+\frac{(dc+dL+b^2)\mathrm{l}}{2(c+L)},$$

we have again $t_N(0)=1$. This corresponds to $U_{N-1}(\zeta(0))=0$ in (3.9). Direct inspection confirms that the wavefunction does not belong to $L^2(\Gamma_N)$ and that these states are resonances (and not bound states).

IV. SERIAL STRUCTURES OF MIXED DIMENSIONALITY

In this section we want to treat the situation when the scatterers connected by single-mode leads have a higher dimension. For the sake of simplicity, we shall consider only the simplest possibility when the dimension is two, i.e., the scatterer is a surface. Such systems can be realized in both the solid state (recall, e.g., the ''bamboo defects'' in nanotubes[39]) and electromagnetism (for flat resonators), but we avoid discussing examples and the conditions under which these models are realistic. We suppose that the surface is smooth, bounded, and connected, with or without the boundary. Although it makes no difficulty to let the particle on the surface interact with an external potential field, we will regard it as free, i.e., its Hamiltonian will be (in appropriate units) just the corresponding Laplace-Beltrami operator.

A. Coupling of leads to a surface

The basic question for the described serial structures is the way in which the leads are coupled to the scatterers. The physical condition is again a conservation of the probability current, which translates into the self-adjointness requirement of the corresponding Hamiltonian. Since the coupling is local, we may disregard geometrical peculiarities of the lead and the surface and consider the setting when a halfline is attached to a plane. The state Hilbert space is then $L^2(\mathbb{R}^-) \oplus L^2(\mathbb{R}^2)$ and the Hamiltonian acts on its elements $\binom{\phi_1}{\phi_2}$ as $\binom{-\phi_1''}{-\Delta\phi_2}$. To make it self-adjoint one has to impose suitable boundary conditions which couple the wavefunctions at the junction. A general solution to this problem is given in Ref. 23. The conditions are of the form

$$\phi_1'(0-) = A\phi_1(0-) + BL_0(\phi_2), \quad L_1(\phi_2) = C\phi_2(0-) + DL_0(\phi_2), \tag{4.1}$$

together with several ''exceptional'' classes, where

$$L_0(\phi_2) = \lim_{r\to 0+} \frac{\phi_2(\vec{x})}{\ln r},$$

$$L_1(\phi_2) = \lim_{r\to 0+} (\phi_2(\vec{x}) - L_0(\phi_2)\ln r)$$

with $r := |\vec{x}|$ are the generalized boundary values in the plane, and the coefficients A, B, C, D depend on four real parameters; evaluating the boundary form, it is straightforward to see that they satisfy restrictions

$$A, D \in \mathbb{R}, \quad B = 2\pi\overline{C}. \tag{4.2}$$

A disadvantage of this result is that it tells us nothing about physical relevance of the coefficients values in the boundary conditions (4.1). The choice of the coupling depends on particular properties of the junction it models, of course, but one would like to select a subclass representing a ''natural'' coupling. One way to achieve this goal was suggested in Ref. 40: comparing the scattering matrix of the junction given by (4.1) with the low-energy behavior of scattering in the system of a plane to which a cylindrical ''tube'' is attached, and taking into account the condition (4.2), we arrive at the identification

$$A = \frac{1}{2\rho}, \quad B = \sqrt{\frac{2\pi}{\rho}}, \quad C = \frac{1}{\sqrt{2\pi\rho}}, \quad D = -\ln\rho, \tag{4.3}$$

where ρ is the contact radius. Physical relevance of these conditions was illustrated in Ref. 40 by explaining the experimentally observed distribution of resonances in a microwave resonator with a thin antenna. Motivated by this, we will use in the following (4.1) and (4.3) to describe the coupling between the leads and the scatterers.

B. The single-element S-matrix

Using the local character of the boundary conditions derived above we apply them to coupling of a pair of halfline leads to an arbitrary surface G. The only restriction is that that the junction may not belong to the boundary of G if it has any. We shall compute the transfer and scattering matrices for such a system.

As we have said, the Hamiltonian is a Laplace-Beltrami operator on the state Hilbert space $L^2(G)$ of the scatterer. We shall characterize it by its Green's function $G(.,.;k)$, i.e., the integral kernel of its resolvent which exists whenever k^2 does not belong to the spectrum. Its actual form

depends on the geometry of G but we shall not need it. What is important is the character of its singularity. As a smooth manifold, G admits in the vicinity of any point a local Cartesian chart and the Green's function behaves as that of Laplacian in the plane,

$$G(x,y;k)=-\frac{1}{2\pi}\ln|x-y|+\mathcal{O}(1), \quad |x-y|\to 0. \tag{4.4}$$

Looking for scattering solutions to the Schrödinger equation, we need a general solution to the Laplace-Beltrami equation on G for the energy k^2. Without loss of generality, we may write it as

$$u(x)=a_1G(x,x_1;k)+a_2G(x,x_2;k), \tag{4.5}$$

where x_1,x_2 are two different points of G at which the leads are attached. The generalized boundary values (labeled by the point at which they are taken) of this solution are then

$$L_0[x_j]=-\frac{a_j}{2\pi}, \quad L_1[x_j]=a_j\xi(x_j,k)+a_{3-j}G(x_1,x_2;k) \tag{4.6}$$

for $j=1,2,$ where

$$\xi(x_j;k)=\lim_{x\to x_j}\left[G(x,x_j;k)+\frac{\ln|x-x_j|}{2\pi}\right]. \tag{4.7}$$

Next we denote the wavefunction on the jth lead as u_j. For simplicity we use the abbreviations u_j,u_j' for its boundary values; then the boundary conditions (4.1) yield

$$u_1'=A_1u_1-\frac{B_1a_1}{2\pi}, \quad a_1\xi_1+a_2g=C_1u_1-\frac{D_1a_1}{2\pi},$$

$$u_2'=-A_2u_2+\frac{B_2a_2}{2\pi}, \quad a_2\xi_2+a_1g=C_2u_2-\frac{D_2a_2}{2\pi},$$

where $g:=G(x_1,x_2;k)$. In the the first equation of the second pair we have changed sign, because the second lead is identified with $\mathbb{R}^+$. It is straightforward to rewrite these equations as a linear system with the unknown u_2,u_2',a_1,a_2 and to solve it; this gives, in particular, the transfer matrix,

$$L=\frac{1}{gC_2}\begin{pmatrix} C_1Z_2+2\pi\dfrac{A_1}{B_1}\Delta & -2\pi\dfrac{\Delta}{B_1} \\ B_2C_2\left(\dfrac{C_1}{2\pi}-Z_1\dfrac{A_1}{B_1}\right)-C_1A_2Z_2-2\pi\dfrac{A_1A_2}{B_1}\Delta & 2\pi\dfrac{A_2}{B_1}\Delta+\dfrac{B_2C_2Z_1}{B_1} \end{pmatrix}, \tag{4.8}$$

where $Z_j:=D_j/2\pi+\xi_j$ and $\Delta:=g^2-Z_1Z_2$. Using (4.2) we find easily

$$\det L=-\frac{B_2C_1}{B_1C_2}=-\frac{\overline{C_2}C_1}{\overline{C_1}C_2}, \tag{4.9}$$

so $\det L=1$ if the junctions are identical or the coefficients C_j are real. The second possibility is if the couplings are invariant with respect to the time reflection, which we shall suppose in the following. In that case the transfer matrix simplifies to the form

$$L=\frac{1}{g}\begin{pmatrix} Z_2+\dfrac{A}{C^2}\Delta & -2\dfrac{\Delta}{C^2} \\ C^2-A(Z_1+Z_2)-\dfrac{A^2}{C^2}\Delta & \dfrac{A}{C^2}\Delta+Z_1 \end{pmatrix}, \tag{4.10}$$

in particular,

$$L=\frac{1}{g}\begin{pmatrix} Z_1+\pi\Delta & -2\pi\rho\Delta \\ \dfrac{1}{2\rho}\left(\dfrac{1}{\pi}-Z_1-Z_2-\pi\Delta\right) & Z_1+\pi\Delta \end{pmatrix} \tag{4.11}$$

for the physically most interesting class of couplings (4.3). The S-matrix of our geometric scatterer is then given by the relations (2.31) and (2.32); in the case (4.11) we have

$$\begin{aligned} r(k)&=-\frac{\pi\Delta+Z_1+Z_2-\pi^{-1}+2ik\rho(Z_2-Z_1)+4\pi k^2\rho^2\Delta}{\pi\Delta+Z_1+Z_2-\pi^{-1}+2ik\rho(Z_1+Z_2+2\pi\Delta)-4\pi k^2\rho^2\Delta}, \\ t(k)&=-\frac{4ik\rho g}{\pi\Delta+Z_1+Z_2-\pi^{-1}+2ik\rho(Z_1+Z_2+2\pi\Delta)-4\pi k^2\rho^2\Delta}. \end{aligned} \tag{4.12}$$

To make use of these formulas, we need to know g,Z_1,Z_2,Δ as functions of the momentum k. By assumption the manifold G is compact, so the spectrum $\{\lambda_n\}_{n=1}^{\infty}$ of the Hamitonian is purely discrete and the corresponding eigenfunctions $\{\phi(x)_n\}_{n=1}^{\infty}$ form an orthonormal basis in $L^2(G)$. The usual Green's function expression then gives

$$g(k)=\sum_{n=1}^{\infty}\frac{\phi_n(x_1)\overline{\phi_n(x_2)}}{\lambda_n-k^2}. \tag{4.13}$$

To express the remaining three values we have to compute the regularized limit (4.7). Expanding the logarithm into the Taylor series, we can rewrite the sublimit expression as

$$G(x_j+\sqrt{\varepsilon}n,x_j;k)+\frac{\ln\sqrt{\varepsilon}}{2\pi}=\sum_{n=1}^{\infty}\left(\frac{\phi_n(x_j+\sqrt{\varepsilon}n)\phi_n(x_j)}{\lambda_n-k^2}-\frac{(1-\varepsilon)^n}{4\pi n}\right),$$

where n is a unit vector in the local chart around the point x_j. Unfortunately, interchanging the limit with the sum is not without risk since the latter does not converge uniformly. To see that the result may indeed depend on the regularization procedure, it is sufficient to replace $\sqrt{\varepsilon}$ by $c\sqrt{\varepsilon}$ on the lhs. To form the idea about this nonuniqueness, let us compute the difference

$$\xi(x_j,k)-\xi(x_j,k')=\lim_{\varepsilon\to 0+}\sum_{n=1}^{\infty}\left(\frac{\phi_n(x_j+\sqrt{\varepsilon n})\overline{\phi_n(x_j)}}{\lambda_n-k^2}-\frac{\phi_n(x_j+\sqrt{\varepsilon n})\overline{\phi_n(x_j)}}{\lambda_n-k'}\right).$$

This sum is already uniformly convergent, because by standard semiclassical estimates (Ref. 41, XIII.16) the sequence $\{\|\phi_n\|_\infty\}_{n=1}^{\infty}$ is bounded with our assumptions and $\lambda_n=4\pi|G|^{-1}n+\mathcal{O}(1)$ as $n\to\infty$, so

$$\frac{1}{\lambda_n-k^2}-\frac{1}{\lambda_n-k'^2}\sim\frac{1}{n^2},$$

and therefore

$$\xi(x_j,k)-\xi(x_j,k')=\sum_{n=1}^{\infty}\left(\frac{|\phi_n(x_j)|^2}{\lambda_n-k^2}-\frac{|\phi_n(x_j)|^2}{\lambda_n-k'^2}\right). \tag{4.14}$$

From the same reason

$$\tilde{\xi}(x_j,k):=\sum_{n=1}^{\infty}\left(\frac{|\phi_n(x_j)|^2}{\lambda_n-k^2}-\frac{1}{4\pi n}\right) \tag{4.15}$$

makes sense and $\xi(x_j,k)-\tilde{\xi}(x_j,k)$ is independent of k. We have therefore

$$\xi(x_j,k)=\sum_{n=1}^{\infty}\left(\frac{|\phi_n(x_j)|^2}{\lambda_n-k^2}-\frac{1}{4\pi n}\right)+c(G). \tag{4.16}$$

The constant depends only on the manifold G. We will neglect it in the following, because its nonzero value means just a coupling constant renormalization: D_j has to be changed to $D_j+2\pi c(G)$. For a flat rectangular G, we found in Ref. 40 an agreement with the experiment using $c(G)=0$.

C. A "bubble" on the line

To make the above consideration more concrete, we shall concentrate in the rest of this section on a single example. We are going to consider the case when G is a sphere of radius R with the leads attached at the poles, which is the system proposed by Kiselev.[10] The most important result of this paper was that apart from the resonances coming from the bound states on the sphere, such a scatterer has the high-energy behavior similar to that of the so-called δ' interaction,[42,15,43] i.e., the transmission probability *decays* as E^{-1} for $E\to\infty$. This was established in Ref. 10 up to a logarithmic correction. The difference here is that we shall use the physically interesting coupling (4.3), while Ref. 10 employed a two-dimensional subset of the conditions (4.1) disjoint with the above one. This leads to a different S-matrix, and while the indicated high-energy behavior remains preserved, the argument used in Ref. 10 to demonstrate it has to be changed in numerous places; this is why we present its modified version here.

The sphere Hamiltonian is chosen in the standard way. Using the spherical coordinates, we write it as

$$H_G=\frac{1}{R^2}\frac{\partial^2}{\partial\theta^2}+\frac{\cot\theta}{R^2}\frac{\partial}{\partial\theta}+\frac{1}{R^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \tag{4.17}$$

with the usual domain. For the sake of simplicity we put $R=1$ in the following; the results for a general R can be obtained by a scaling transformation. The spectrum of H_G then consists of the eigenvalues $\lambda_{l,m}=l(l+1)$, $l=0,1,\ldots$, $m=-l,-l+1,\ldots,l$ of multiplicity $2l+1$ to which the eigenfunctions

$$\phi_l^m(\theta,\psi)=\sqrt{\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!}}P_l^{|m|}(\cos\theta)e^{im\varphi}$$

correspond. The junctions x_1,x_2 we place at the points $\theta=0$ and $\theta=\pi$, respectively, where

$$P_l^{|m|}(\pm1)=(-1)^l\delta_{0,|m|},$$

so only states with $m=0$ can be coupled to the leads. To express the S-matrix, we need the quantities

$$g(k)=\frac{1}{4\pi}\sum_{l=1}^{\infty}\frac{2l+1}{l(l+1)-k^2}(-1)^l, \tag{4.18}$$

$$Z_j(k)=Z(k):=\frac{1}{4\pi}\sum_{l=1}^{\infty}\left(\frac{2l+1}{l(l+1)-k^2}-\sum_{j=0}^{2l}\frac{1}{l^2+j+1}\right)-\frac{\ln\rho}{2\pi}+c(G), \tag{4.19}$$

where ρ is the junction diameter which is supposed to be the same for $j=1,2$. The relations (4.12) yield, in particular, the transmission probability in the form

$$t(k)=\frac{4\pi ik\rho g(k)}{1-2\pi Z(k)(1+2ik\rho)-\pi^2\Delta(k)(1+2ik\rho)^2}, \tag{4.20}$$

where $\Delta(k)=(g(k)-Z(k))(g(k)+Z(k))$.

To prove that (4.20) behaves as indicated above at large values of $E=k^2$, we need several auxiliary results.

Lemma IV.1: The function $Z(\cdot)+(-1)^l g(\cdot)$ is strictly increasing on the intervals $(l(l-1),l(l+1))$.

Proof: We have

$$Z'(k)+(-1)^l g'(k)=2k\sum_{j=0}^{\infty}\frac{2j+1}{(j(j+1)-E)^2}(1+(-1)^{j+l})>0.$$

■

Lemma IV.2: We have

$$g(k)=\frac{(-1)^l}{4\pi}\left(-\frac{2l-1}{l(l-1)-E}+\frac{2l+1}{l(l+1)-E}\right)+\mathcal{O}(1)$$

for $E\in(l(l-1),l(l+1))$ and any positive integer l with the error term independent of l. Moreover, there is a $K>0$ such that $g(k)\geqslant K$ holds for all k large enough.

Proof: The error can be estimated explicitly; we shall show that

$$\left|g(k)-\frac{(-1)^l}{4\pi}\left(-\frac{2l-1}{l(l-1)-E}+\frac{2l+1}{l(l+1)-E}\right)\right|<\frac{1}{2\pi}. \tag{4.21}$$

To this end we have to find a bound to (4.18) on the interval $(l(l-1),l(l+1))$ with the two singular terms removed. The terms to the left and to the right of this pair form alternative sequences with the decreasing modulus, and as such each of them may be estimated by the (modulus of) the first term of such a sequence, i.e., by

$$\frac{1}{4\pi}\left|\frac{2l-3}{(l-1)(l-2)-E}\right| \quad \text{and} \quad \frac{1}{4\pi}\left|\frac{2l+3}{(l+1)(l+2)-E}\right|,$$

respectively. Taking the maxima of these expressions and summing them we arrive at (4.21). To get the second claim, we have have to compare this result with a lower bound to the modulus of the sum of the two singular terms. The minimum $\pi^{-1}+\mathcal{O}(l^{-1})$ of the latter is reached at $E=l^2-\frac{1}{4}+\mathcal{O}(l^{-2})$, so this part wins over the other one once the error terms become small enough. ■

Lemma IV.3: For a positive integer l and $E\in(l(l-1),l(l+1))$ we have

$$Z(k)=\frac{1}{4\pi}\left(\frac{2l-1}{l(l-1)-E}+\frac{2l+1}{l(l+1)-E}\right)-\frac{\ln l}{2\pi}+\mathcal{O}(1), \tag{4.22}$$

where the error term is independent of l.

Proof: We again split the two singular terms in (4.22) and write the rest as $Z_-(k,l)+Z_+(k,l)-(\ln\rho)2\pi+c(G)$, where

$$Z_-(k,l):=\frac{1}{4\pi}\sum_{j=1}^{l-2}\left(\frac{2j+1}{j(j+1)-E}-\sum_{n=0}^{2j}\frac{1}{j^2+n+1}\right),$$

$$Z_+(k,l):=\frac{1}{4\pi}\sum_{j=l+1}^{\infty}\left(\frac{2j+1}{j(j+1)-E}-\sum_{n=0}^{2j}\frac{1}{j^2+n+1}\right).$$

It is easy to see that

$$\sum_{n=0}^{2j}\frac{1}{j^2+n+1}=\frac{2}{j}+\mathcal{O}(j^{-2})$$

as $j\to\infty$, so the jth term in $Z_\pm(k,l)$ can be estimated from above by

$$\frac{1}{4\pi}\left(\frac{2j+1}{j(j+1)-l(l+1)}-\frac{2}{j}+\mathcal{O}(j^{-2})\right)$$

and from below by the same expression with $l(l+1)$ replaced by $l(l-1)$. Using the identity

$$\frac{2j+1}{j(j+1)-l(l+1)}=\frac{1}{j+l+1}-\frac{1}{l-j}$$

we find

$$4\pi Z_-(k,l)=\left(-\sum_{m=2}^{l-1}+\sum_{m=l+2}^{2l-1}-2\sum_{m=1}^{l-2}\right)\frac{1}{m}+\sum_{m=1}^{l-2}\mathcal{O}(m^{-2})=-3\ln l+\mathcal{O}(1),$$

$$\begin{aligned}4\pi Z_+(k,l)&=\lim_{n\to\infty}\left[\left(\sum_{m=1}^{n-l}+\sum_{m=2l+2}^{n+l+1}-2\sum_{m=l+1}^{n}\right)\frac{1}{m}+\sum_{m=l+1}^{n}\mathcal{O}(m^{-2})\right]\\&=\lim_{n\to\infty}\ln\frac{(n-l)((n+l+1)}{n^2}+\ln(l+1)+\mathcal{O}(1)=\ln l+\mathcal{O}(1).\end{aligned}$$

Summing the expressions we get the upper bound in (4.22); the lower one is obtained in the same way. ■

Lemma IV.4: For any l large enough the interval $(l(l-1),l(l+1))$ contains a point μ_l such that $\Delta(\sqrt{\mu_l})=0$. The number μ_l has the following properties:

(i) $l(l+1)-\mu_l=2l(\ln l)^{-1}(1+\mathcal{O}(1))$,

(ii) $\dfrac{2l+1}{l(l+1)-E}\leqslant\ln l+\mathcal{O}(1)$ *for* $E\leqslant\mu_l$,

(iii) $\dfrac{2l-1}{l(l-1)-E}=\mathcal{O}(1)$ *for* $E>\mu_l$, *and*

(iv) finally, $\dfrac{Z(\sqrt{\mu_l})}{|g(\sqrt{\mu_l})|}=-1+\mathcal{O}((\ln l)^{-1})$.

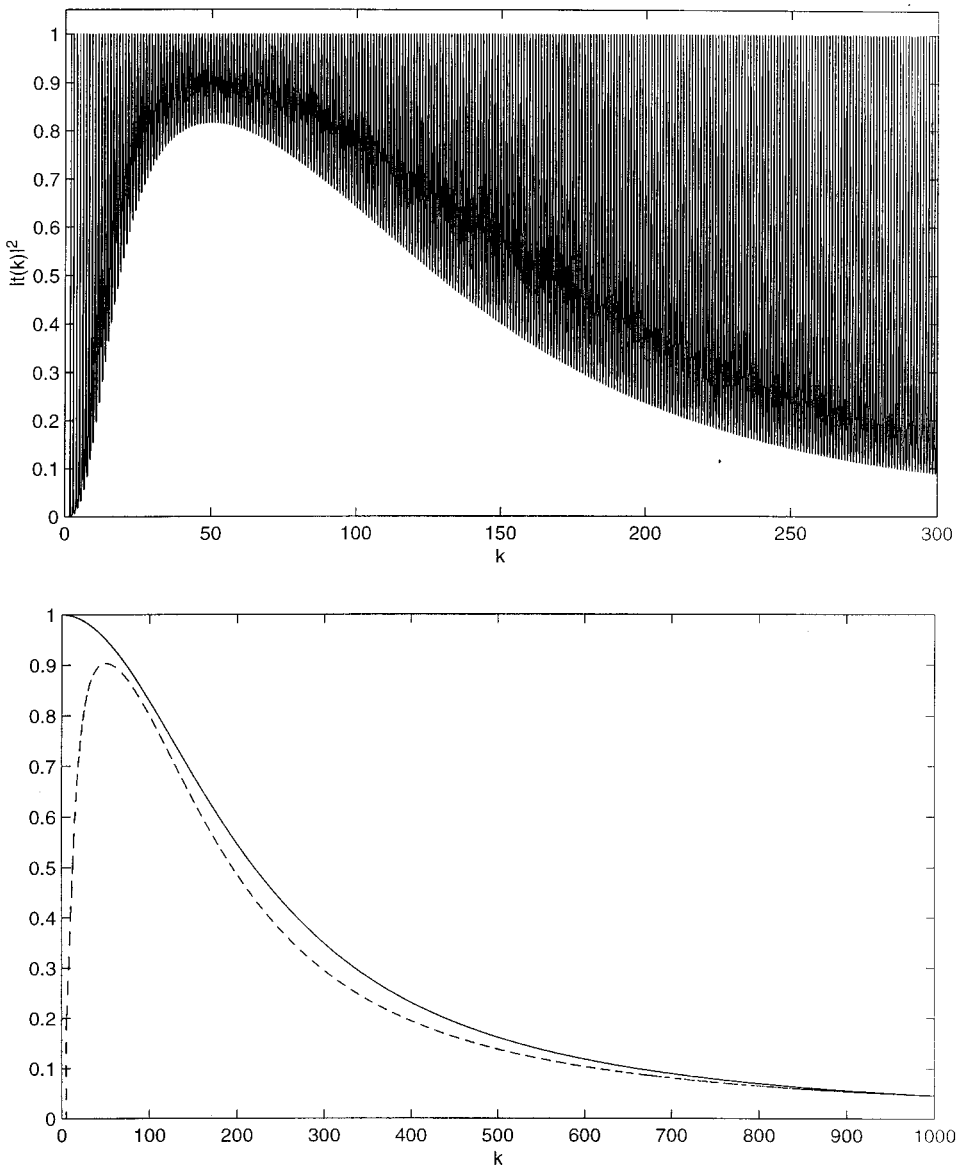

FIG. 7. The transition probability of a sphere of unit radius on a line ($\rho=0.01$). The lower graph compares the asymptotic behavior of $|t(k)|^2$ for δ'-interaction with suitably chosen strength and that of averaged transmission probability plotted in the upper graph. The averaging is done over ten neighboring peaks of each point.

Proof: Fix l. We have $Z(k)^2-g(k)^2=(Z(k)+(-1)^l g(k))(Z(k)-(-1)^l g(k))$, and by the preceding lemmas these expressions equal

$$\frac{1}{2\pi}\frac{2l\pm 1}{l(l\pm 1)-E}-\frac{1}{2\pi}\ln\rho+\mathcal{O}(1).$$

The term with the minus sign is negative in $(l(l-1),l(l+1))$ provided l is large enough. The other term is sign changing for large l so it has has a root. In view of Lemma 4.1 there is just one μ_l such that

$$\frac{2l+1}{l(l+1)-\mu_l}-\ln l+\mathcal{O}(1)=0\,; \tag{4.23}$$

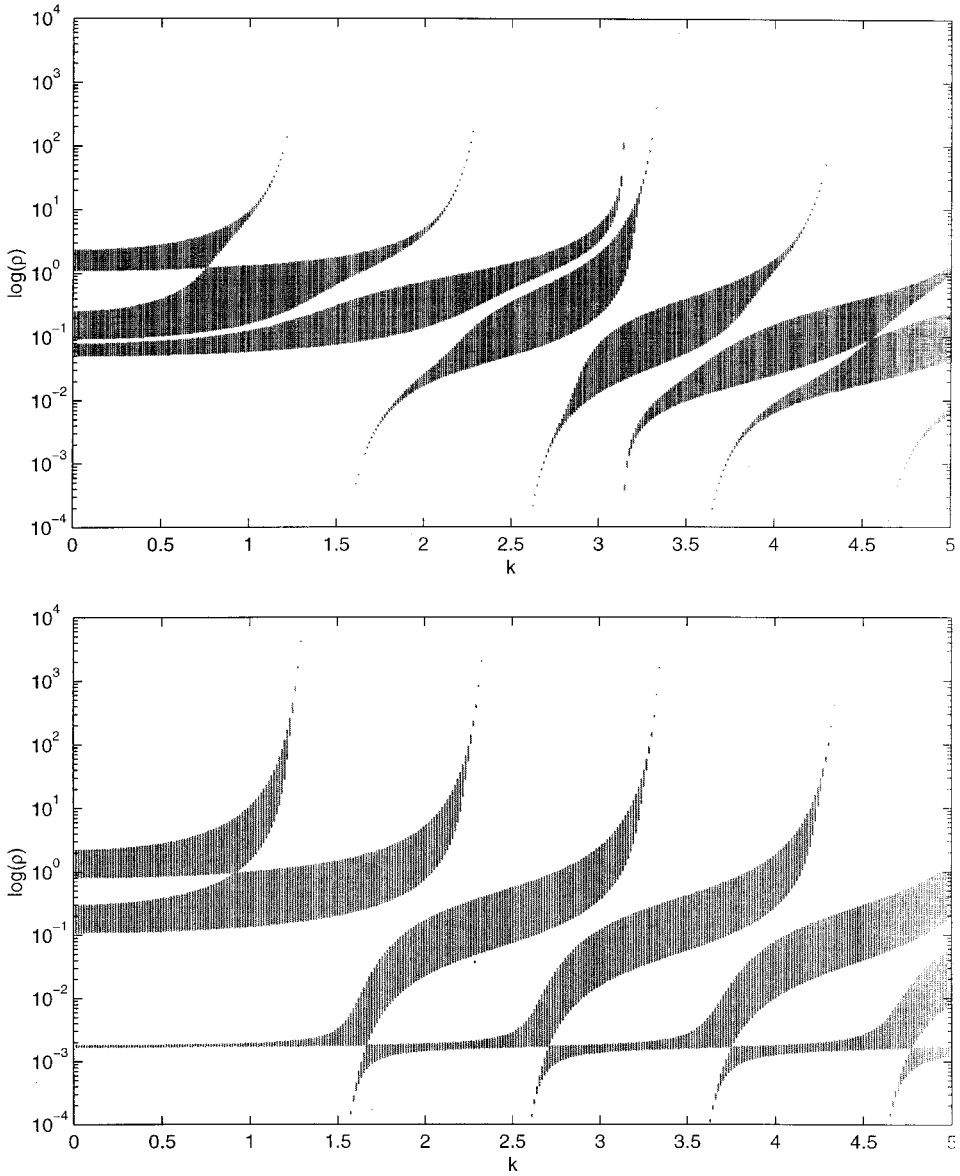

FIG. 8. Band spectrum of an infinite ''bubble'' array. The spheres are of unit radius, the spacing is $l=1$ (upper figure) and $l=0.01$ (lower figure), ρ is the contact radius.

this proves *(i)*. The relation (4.23) yields also the next two claims:

$$\frac{2l+1}{l(l+1)-E} \leqslant \frac{2l+1}{l(l+1)-\mu_l} = \ln l + \mathcal{O}(1) \tag{4.24}$$

and

$$\left|\frac{2l-1}{l(l-1)-E}\right| \leqslant \frac{2l-1}{\mu_l - l(l-1)} = \frac{2l-1}{2l(1-[1+\mathcal{O}(1)]/[\ln l])} = \mathcal{O}(1). \tag{4.25}$$

Finally, *(iv)* follows from *(ii)* and *(iii)* which yield

$$Z(\sqrt{\mu_l})=\frac{1}{4\pi}(\ln l+\mathcal{O}(1))-\frac{1}{2\pi}\ln l+\mathcal{O}(1)=-\frac{1}{4\pi}\ln l+\mathcal{O}(1)$$

and $|g(\sqrt{\mu_l})|=(1/4\pi)\ln l+\mathcal{O}(1)$. ■

Now we are in position to prove the main result of this subsection:

Theorem IV.5: Let $K_\varepsilon:=\mathbb{R}\setminus\cup_{l=2}^{\infty}(\mu_l-\varepsilon(l)(\ln l)^{-2},\mu_l+\varepsilon(l)(\ln l)^{-2})$, *where* $\varepsilon(\cdot)$ *is a positive strictly increasing function which tends to* ∞ *and obeys the inequality* $|\varepsilon(x)|\leqslant x\ln x$ *for* $x>1$. *Then there is a positive* c *such that the transmission probability satisfies the bound*

$$|t(k)|^2\leqslant c\varepsilon(l)^{-2} \tag{4.26}$$

for $k^2\in K_\varepsilon\cap(l(l-1),l(l+1))$ *and any* l *large enough. On the other hand, there are sharp resonance peaks localized on* K_ε,

$$|t(\sqrt{\mu_l})|^2=1+\mathcal{O}((\ln l)^{-1}) \tag{4.27}$$

as $l\to\infty$.

Proof: In the first part we are going to estimate the modulus of the numerator in (4.20) from below. The leading term at high energies is the one with $\Delta(k)$; we shall estimate it on the set K_ε; i.e., away of the zeros of the coefficient. Consider the neighborhood

$$I_l:=(\mu_l-2l(\ln l)^{-1},\mu_l+2l(\ln l)^{-1})$$

of μ_l on which the following estimates are valid:

$$\begin{aligned}\frac{1}{2k}(Z'(k)+(-1)^l g'(k))&=\sum_{m=0}^{\infty}\frac{2m+1}{m(m+1)-E}(1+(-1)^{l+m})\\&=\left(\sum_{m=0}^{l-2}+\sum_{m=l+1}^{\infty}\right)\frac{2m+1}{(m(m+1)-E)^2}(1+(-1)^{l+m})\\&\quad+\frac{2(2l+1)}{(l(l+1)-E)^2}\\&\geqslant\frac{2(2l+1)}{(l(l+1)-E)^2}\\&\geqslant\frac{2(2l+1)}{(l(l+1)-\mu_l+2l(\ln l)^{-1})^2}=\frac{2(2l+1)}{(2l(\ln l)^{-1}(2+\mathcal{O}(1))^2}\geqslant c_1\frac{(\ln l)^2}{l}\end{aligned}$$

for some $c_1>0$. Combining this result with Lemma 4.1 we are able to say how the factors constituting $\Delta(k)$ are separated from zero for $E\in(l(l-1),l(l+1))$, which does not belong to the interval $(\mu_l-\varepsilon(l)(\ln l)^{-2},(\mu_l+\varepsilon(l)(\ln l)^{-2})\subset I_l$:

$$|Z(k)+(-1)^l g(k)|\geqslant\varepsilon(l)(\ln l)^{-2}c_1 l^{-1}(\ln l)^2=c_1 l^{-1}\varepsilon(l). \tag{4.28}$$

Now we begin estimating the modulus of the transmission amplitude from below. In the following, c_j always means a positive constant. Using the expression (4.20) we get a simple lower bound,

$$|t(k)|\leqslant\frac{4\pi\rho}{|[1-2\pi Z(k)]/k|g(k)|-[\pi^2\Delta(k)/|g(k)|](k^{-1}-4k\rho^2)|}, \tag{4.29}$$

obtained by neglecting the imaginary part of the denominator. First we shall show that

$$\frac{1-2\pi Z(E)}{k|g(k)|}=\mathcal{O}(1) \tag{4.30}$$

as $l\to\infty$. Using Lemmas 4.2 and 4.3 we estimate this expression by

$$\frac{|\ln l+\mathcal{O}(1)|}{kK}+\frac{1}{2\pi k}\left|\frac{(2l+1)/[l(l+1)-E]+(2l-1)/[l(l-1)-E]}{(2l+1)/[l(l+1)-E]-(2l-1)/[l(l-1)-E]-2}\right|\leqslant c_2,$$

where in the second term we have used the explicit lower bound on $|g(k)|$, estimated the modulus of the fraction by $(2l+1)/(l-1)\leqslant 5$, and employed finally $k=\sqrt{E}=l+\mathcal{O}(1)$. For the second term in the denominator of (4.29) we shall show that

$$\frac{\pi^2\Delta(k)}{|g(k)|}(k^{-1}-4k\rho^2)\geqslant c_3\varepsilon(l) \tag{4.31}$$

holds for all $E\in(l(l-1),l(l+1))\setminus(\mu_l-\varepsilon(l)(\ln l)^{-2},\mu_l+\varepsilon(l)(\ln l)^{-2})$, which will give (4.26) with $c:=(c_3/4\pi\rho)^2$. Consider first the case $E\leqslant\mu_l$, when (4.28) together with Lemmas 4.4(ii) yields

$$\begin{aligned}
&\pi^2|k^{-1}-4k\rho^2|\,\frac{|Z(k)+(-1)^l g(k)||Z(k)-(-1)^l g(k)|}{|(1/4\pi)\,((2l+1)/[l(l+1)-E]-(2l-1)/[l(l-1)-E])+\mathcal{O}(1)|}\\
&\quad\geqslant 4\pi^2\rho^2k|1-(2\rho k)^{-2}|\,\frac{c_1 l^{-1}\varepsilon(l)\,(1/2\pi)\,|(2l-1)/[l(l-1)-E]-\ln l+\mathcal{O}(1)|}{|-(1/4\pi)(2l-1)/[l(l-1)-E]-(1/4\pi)\ln l+\mathcal{O}(1)|}\\
&\quad\geqslant c_4 k\,\frac{\varepsilon(l)}{l}\geqslant c_5\varepsilon(l),
\end{aligned}$$

where in the last step we used again $k=l+\mathcal{O}(1)$. Let further $E>\mu_l$. We divide the argument into two parts. First we suppose

$$\frac{2l+1}{l(l+1)-E}\leqslant 2\ln l;$$

then

$$\begin{aligned}
&\pi^2|k^{-1}-4k\rho^2|\,\frac{|Z(k)+(-1)^l g(k)||Z(k)-(-1)^l g(k)|}{|(1/4\pi)\,((2l+1)/[l(l+1)-E]-(2l-1)/[l(l-1)-E])+\mathcal{O}(1)|}\\
&\quad\geqslant 4\pi^2\rho^2k|1-(2\rho k)^{-2}|\,\frac{c_1 l^{-1}\varepsilon(l)|\ln l+\mathcal{O}(1)|}{|\ln l+\mathcal{O}(1)|}\geqslant c_6\varepsilon(l)
\end{aligned}$$

by (4.28) and Lemma 4.4(iii). On the other hand, if

$$\frac{2l+1}{l(l+1)-E}\geqslant 2\ln l, \tag{4.32}$$

the same expression is bounded from below by

$$\begin{aligned}
&4\pi^2\rho^2k|1-(2\rho k)^{-2}|\,\frac{|(1/4\pi)(2l+1)/[l(l+1)-E]+\mathcal{O}(1)||(1/2\pi)\ln l+\mathcal{O}(1)|}{|(1/4\pi)(2l+1)/[l(l+1)-E]+\mathcal{O}(1)|}\\
&\quad\geqslant c_7 k|1-(2\rho k)^{-2}|\ln l\geqslant c_8\varepsilon(l),
\end{aligned}$$

where the denominator and the first term in the numerator have been estimated by means of (4.23) and (4.32), in the second term we have neglected one of the two terms of the same sign, and the last inequality follows from the fact that $x \ln x \geqslant \varepsilon(x)$ by assumption. To conclude the proof of (4.26), it is sufficient to put $c_3 := \min\{c_5, c_6, c_8\}$ in (4.31).

The rest is easier; the existence of resonance peaks at which the sphere is almost transparent follows from the relations

$$
\begin{aligned}
|t(\mu_l)| &= \left| \frac{1}{4\pi\rho\sqrt{\mu_l}\, g(\sqrt{\mu_l})} - \frac{Z(\sqrt{\mu_l})}{g(\sqrt{\mu_l})} \left(i + \frac{1}{2\rho\sqrt{\mu_l}} \right) \right|^{-1} \\
&= \left| \left(i + \frac{1}{2\rho\sqrt{\mu_l}} \right) (1 + \mathcal{O}((\ln l)^{-1})) + \frac{1}{\rho\sqrt{\mu_l}} (\ln l + \mathcal{O}(1)) \right|^{-1} \\
&= |i + \mathcal{O}((\ln l)^{-1})|^{-1} = 1 + \mathcal{O}((\ln l)^{-1}),
\end{aligned}
$$

where we have used Lemma 4.4(iv). ■

The proved theorem can be illustrated by numerically evaluated transmission probability $|t(k)|^2$. The curve oscillates almost regularly, but with the amplitude spanning from small values to unity for sufficiently large k. The lower enveloping curve of $|t(k)|^2$ behaves as $(E \ln E)^{-1}$ as we proved earlier. The analogous conclusion for another (unphysical) coupling between the sphere and the leads were compared in Ref. 10 to scattering properties of the δ'-interaction, the transmission of which decays like E^{-1} as $E \to \infty$. We conjecture that the ''bubble'' has exactly this asymptotic if $|t(k)|^2$ is replaced by its ''smoothed,'' i.e., locally averaged version. The conjecture is supported by Fig. 7; it compares an averaged $|t(k)|^2$ of a ''bubble'' on the line and $|t(k)|^2$ of δ'-interaction. The averaging is done over ten neighboring peaks of a given point. The strength of the δ'-interaction is chosen so as to reach the same value of $|t(k)|^2$ at a distant k. These two curves seem to have the same asymptotic behavior.

Let us finally use the result to express scattering on an array of bubble scatterers and compare it with the band spectrum of the periodic system. This is done on Fig. 8 which shows the band spectrum of an infinite array of bubbles on the line. What is different from analogical spectra of loop or comb arrays is the concentration of bands to small values ρ (note the logarithmic scale).

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Folding in the Skyrme model

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There are only three stable singularities of a differentiable map between three-dimensional manifolds, namely folds, cusps and swallowtails. A Skyrme configuration is a map from space to SU_2, and its singularities correspond to the points where the baryon density vanishes. In this article we consider the singularity structure of Skyrme configurations. The Skyrme model can only be solved numerically. However, there are good analytic ansätze. The simplest of these, the rational map ansatz, has a nongeneric singularity structure. This leads us to introduce a nonholomorphic ansatz as a generalization. For baryon numbers 2, 3, and 4, the approximate solutions derived from this ansatz are closer in energy to the true solutions than any other ansatz solution. We find that there is a tiny amount of negative baryon density for baryon number 3, but none for 2 or 4. We comment briefly on the relationship to Bogomolny–Prasad–Sommerfield monopoles. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1388199]

I. INTRODUCTION

The Skyrme model is a nonlinear SU_2 field theory.[1] In addition to the fundamental excitations, the spectrum also includes topologically charged soliton solutions. The model was proposed by Skyrme as a theory of nuclear physics in which the fundamental excitations are pions and the solitons are nucleons. The Skyrme energy function is

$$E=\int\left\{-\frac{1}{2}\mathrm{Tr}\,(R_iR_i)-\frac{1}{16}\mathrm{Tr}([R_i,R_j][R_i,R_j])\right\}\mathrm{d}^3x, \tag{1}$$

where R_i is the su_2-valued current $R_i=(\partial_iU)U^{-1}$. The SU_2-valued field U is required to attain its vacuum value, the identity, at spatial infinity and, so, it is a map between topological three-spheres. This is the origin of the topological charge, B.

The one-Skyrmion is spherical and is given by the hedgehog ansatz

$$U_1(\mathbf{x})=\exp(if(r)\hat{\mathbf{n}}\cdot\boldsymbol{\sigma}), \tag{2}$$

where $\hat{\mathbf{n}}=\hat{\mathbf{x}}$ is the outward pointing unit normal and $\boldsymbol{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ are the Pauli matrices. $f(r)$ is a shape function and is usually determined numerically. It is very well approximated by the kink profile:[2] $f(r)=4\arctan(\exp(-r))$. The one-Skyrmion has six zero modes: three translational modes and three isospin modes corresponding to global SU_2 transformations.

Two well-separated Skyrmions attract or repel, depending upon their mutual isospin orientation. Two attracting one-Skyrmions will move towards each other and form a bound state whose

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energy is 0.95 times the energy of two one-Skyrmions. This two-Skyrmion is torus shaped[3,4] and is axially symmetric, in the sense that axial rotations in space are equivalent to isospin rotations, which are conjugations of U by a constant SU_2 matrix.

In the Skyrme model, the classical B-nucleon nucleus is a B-Skyrmion; that is, a minimum energy Skyrme field with topological charge B. For B from 3 to 22, the Skyrmion has been calculated numerically by evolving an attractive configuration.[5–7] All the known Skyrmions have the bulk of their energy density on a fullerene-like shell. A geometric interpretation of this shell-like structure was given in Ref. 8. Furthermore, Skyrmions often have a very symmetrical shape.

A. The rational map ansatz

The rational map ansatz introduced in Ref. 9 is a simple ansatz for Skyrmions. It is similar to the one-Skyrmion (2). The one-Skyrmion is a hedgehog map in which the outward pointing unit normal, $\hat{\mathbf{n}}$, maps a two-sphere identically to a two-sphere. In the ansatz, the hedgehog map is replaced by a more general holomorphic map, $\hat{\mathbf{n}}_R$, from Riemann sphere to Riemann sphere. The rational map ansatz is given by

$$U(r,z)=\exp(if(r)\hat{\mathbf{n}}_R\cdot\boldsymbol{\sigma}), \tag{3}$$

where

$$\hat{\mathbf{n}}_R=\frac{1}{1+|R|^2}(2\,\mathrm{Re}(R),2\,\mathrm{Im}(R),1-|R|^2) \tag{4}$$

and $R(z)$ is a holomorphic map in z. Here, z is related to the standard angular coordinates ϕ and θ by the stereographic projection $z=\tan(\theta/2)\exp(i\phi)$. R is also a stereographic coordinate on the Riemann sphere. In the ansatz, this Riemann sphere is a latitudinal two-sphere in $SU_2\cong S^3$.

The ansatz maps spheres around the origin in space to latitudinal two-spheres in SU_2. The shape function f is a function of r only, so each map between two-spheres is identical. The boundary conditions on f are $f(0)=\pi$ and $f(\infty)=0$. These conditions are determined by requiring that U is well defined at the origin and attains the vacuum value at infinity. In principle, we could have $f(0)=N_f\pi$ for any nonzero integer N_f, but solutions with $N_f>1$ have rather high energy and so we only consider $N_f=1$.

Thus, the ansatz depends on a holomorphic map between two-spheres. Any holomorphic map of finite topological charge can be written as a rational map

$$R(z)=\frac{p(z)}{q(z)}, \tag{5}$$

where p and q are polynomials in z. The topological charge, N_R, of the map is equal to the algebraic degree and this, in turn, is given by the maximal degree of the two polynomials.

The easiest way to calculate the energy of an ansatz field is to use the geometric formulation of the Skyrme model.[10] A Skyrme field is a map between three-manifolds with metrics and so there is a strain tensor. This is given by

$$D_{ij}=-\tfrac{1}{2}\mathrm{Tr}(R_iR_j). \tag{6}$$

The static energy, E, and the baryon number, B, of a Skyrme field can be written in terms of the eigenvalues, λ_1^2, λ_2^2, and λ_3^2, of this tensor:

$$E=\int(\lambda_1^2+\lambda_2^2+\lambda_3^2+\lambda_1^2\lambda_2^2+\lambda_2^2\lambda_3^2+\lambda_1^2\lambda_3^2), \tag{7}$$

$$B=\frac{1}{2\pi^2}\int \lambda_1\lambda_2\lambda_3 . \tag{8}$$

The strain tensor of the ansatz field (3) can be calculated to give

$$B=\frac{2}{\pi}\int (-f'\sin^2 f)\mathrm{d}r\,\frac{1}{4\pi}\int \left(\frac{1+|z|^2}{1+|R|^2}\left|\frac{\mathrm{d}R}{\mathrm{d}z}\right|\right)^2 \frac{2i\,\mathrm{d}z\,\mathrm{d}\bar{z}}{(1+|z|^2)^2}, \tag{9}$$

$$=N_R , \tag{10}$$

where N_R is the degree of the rational map.

Similarly, the energy E is given by

$$E=4\pi\int \left(f'^2 r^2+2N_R(f'^2+1)\sin^2 f+\mathcal{I}\,\frac{\sin^4 f}{r^2}\right)\mathrm{d}r, \tag{11}$$

where

$$\mathcal{I}=\frac{1}{4\pi}\int \left(\frac{1+|z|^2}{1+|R|^2}\left|\frac{\mathrm{d}R}{\mathrm{d}z}\right|\right)^4 \frac{2i\,\mathrm{d}z\,\mathrm{d}\bar{z}}{(1+|z|^2)^2}. \tag{12}$$

Thus, the minimum energy ansatz field is found by choosing polynomials p and q which minimize $\mathcal{I}$ and then calculating the shape function f numerically. These minimum energy ansatz fields have been calculated for all the known Skyrmions and are found to have energies that exceed the true, numerically determined, minima[7,9] by less than 3%.

B. The rational map ansatz and negative baryon density

The accuracy of the ansatz is established by observing how close in energy the minimum energy ansatz configurations are to the true minima. In other words, it is not known whether the ansatz fields resemble the true fields in regions where the energy density is low. In fact, for the approximate fields calculated within the ansatz, the region of zero baryon density has a rather special structure. There are $2B-2$ radial half-lines which meet at the origin and extend out to infinity. The zeros of the baryon density correspond to the folds in the Skyrme fields, considered as maps between three-spheres. Line-like zeros are not generic. It is possible that these nongeneric zeros are a natural consequence of minimizing the Skyrme energy.[11,12] However, it may be that this is a weakness of the rational map ansatz and Skyrmions have a more generic folding structure.

If it is a weakness, it is not a very serious one. Most current interest is in finding minimum energy Skyrme configurations. However, the issue of determining the structure of Skyrme fields in the regions where there is little energy may be of some practical importance, for example, in calculations in which the Skyrmion fields are used as backgrounds for fermion excitations modeling heavy flavors (see Ref. 13).

In this article, we consider the consequences of generalizing the rational map ansatz to include a larger class of maps. These maps permit a more natural, though not wholly generic, folding structure. This generalized ansatz is not as convenient as the original one. However, it does result in ansatz fields which are even closer to the true minima.

Our interest in this problem is partly motivated by BPS monopoles. There are many interesting similarities between Skyrmions and BPS monopoles. For example, there are two rational map descriptions of monopoles,[14,15] and it is widely believed that the space of attracting Skyrmions is related to the space of monopoles. It was discovered in Ref. 29 that the tetrahedral three-monopole has a negative multiplicity Higgs zero. Subsequent examination revealed that the octahedral five-monopole also has extra zeros but the cubic four-monopole does not.[17]

There is evidence that this pattern is mimicked by Skyrmions for $B=3$ and 4. These Skyrmions were studied in Ref. 18 using the Atiyah–Manton ansatz.[19] It was observed that there is no negative baryon density in the approximate four-Skyrmion, but there is in the approximate three-Skyrmion case. In the approximate three-Skyrmion there is a region of negative baryon density surrounding the origin. This extends out along four thin tubes which twice pinch to points and then widen at very large distance until they merge and form another region of negative baryon density at spatial infinity.

In this article, we generalize the rational map ansatz so that there can be negative baryon density. We calculate ansatz fields that approximate the true minima more closely than the original rational map ansatz. The ansatz for the three-Skyrmion has tubes of negative baryon density extending out from the origin; the ansatz for the four-Skyrmion does not. Furthermore, there is an octahedrally symmetric $B=5^*$ saddle-point configuration. The ansatz for this saddle point also has negative baryon density.

Thus, our investigation adds to the evidence that there may be regions of negative baryon density in certain Skyrmions. This occurs in those examples where the corresponding monopole has negative multiplicity Higgs zeros. Of course, our conclusions are based on an ansatz and the true solution does not necessarily possess the same singularity structure. Unfortunately, it is difficult to observe negative baryon density directly in the numerical solutions.

C. Singularities of differentiable maps

The theory of singularities deals with smooth maps between manifolds. One of its main aims is to classify the points where the Jacobian of a map does not have maximal rank. These are the singularities. Some singularities are unstable, in the sense that a small perturbation of the map can alter the nature of the singularity. For maps between low dimensional manifolds, there are only a small number of stable singularities. In this section, we describe the three stable singularities of smooth maps between three-dimensional manifolds. We will follow Ref. 20.

Let $f:M\to N$ be a map from a three-dimensional manifold M to a three-dimensional manifold N. Locally, there are coordinates $\{y_1,y_2,y_3\}$ on N and $\{x_1,x_2,x_3\}$ on M so that

$$\begin{aligned} y_1&=f_1(x_1,x_2,x_3),\\ y_2&=f_2(x_1,x_2,x_3),\\ y_3&=f_3(x_1,x_2,x_3). \end{aligned} \tag{13}$$

The matrix $J=(\partial f_i/\partial x_j)$ is the Jacobian matrix of the map. The singularities are the points where $\det J=0$. There are only three stable singularities: folds, cusps and swallowtails. These are described by giving their normal forms. The normal form is a standard choice of coordinates for the neighborhood of the singularity. Any stable singularity can be expressed locally in terms of the corresponding normal form by a smooth change of variables.

The simplest singularity is the fold, which can be visualized as the line along which a piece of paper has been folded. A fold has the normal form

$$\begin{aligned} y_1&=x_1^2,\\ y_2&=x_2,\\ y_3&=x_3. \end{aligned} \tag{14}$$

It is worth considering the number of preimages of the map. For points of N with $y_1>0$ there are two preimages, whereas for points with $y_1<0$ there are no preimages. The fold is located at $y_1=0$, which has one preimage. Restricted to the set of points $y_1=0$, f maps the x_2x_3-plane onto the y_2y_3-plane.

The Jacobian matrix of this map is

$$J=\begin{pmatrix} 2x_1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{15}$$

It is singular at $x_1=0$, which, of course, is the location of the fold. The rank of the Jacobian matrix at the fold is two. In fact, this is true of all three stable singularities. Any singularity with a rank one or rank zero Jacobian matrix is unstable.

Two folds can end on a cusp. This has the normal form:

$$\begin{aligned} y_1&=x_1^3+x_1x_2, \\ y_2&=x_2, \\ y_3&=x_3. \end{aligned} \tag{16}$$

In order to get a better understanding of this singularity, we calculate the Jacobian matrix:

$$J=\begin{pmatrix} 3x_1^2+x_2 & x_1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{17}$$

J does not have maximal rank for $x_1^2=-x_2/3$. This is a pair of folds. The cusp occurs at the line $(0,0,x_3)$ where the two folding surfaces $(\pm\sqrt{-x_2/3},x_2,x_3)$ meet.

The most complicated stable singularity is called the swallowtail and its normal form is

$$\begin{aligned} y_1&=x_1^4+x_1^2x_2+x_1x_3, \\ y_2&=x_2, \\ y_3&=x_3. \end{aligned} \tag{18}$$

In this case, the Jacobian matrix is given by

$$J=\begin{pmatrix} 4x_1^3+2x_1x_2+x_3 & x_1^2 & x_1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{19}$$

The points of the folds satisfy the equation $x_3=-4x_1^3-2x_1x_2$. The folds meet to form four cusp lines which meet at the origin. The origin is the swallowtail.

This classification is known as Whitney's theorem. This theorem states that a map of a three-dimensional manifold to a three-dimensional manifold is stable at a point if, and only if, the map can be described in local coordinates in one of the four forms: a regular point with $y_1=x_1$, $y_2=x_2$, and $y_3=x_3$ or one of the three singular forms given above. Furthermore, maps with stable singularities are dense in the space of all smooth maps: any map can be approximated arbitrarily closely by a map with stable singularities.

II. FOLDING AND RATIONAL MAPS

We begin this section by showing that the simplest singularity of the rational map ansatz is unstable. This will lead us to introduce the nonholomorphic rational map ansatz in the following section. Furthermore, we show that for $B>1$ there is an unstable singularity at the origin.

In the holomorphic rational map ansatz there is a map from $\mathbf{R}^3$ to S^3 which maps $(r,z,\overline{z})$ to $(f(r),R(z),\overline{R}(\overline{z}))$. Away from the origin, we can define local coordinates $\{\mathrm{Re}(z),\mathrm{Im}(z),x_3\}$ and $\{y_1,y_2,y_3\}$ such that

$$y_1=\mathrm{Re}(R),$$
$$y_2=\mathrm{Im}(R), \tag{20}$$
$$y_3=x_3.$$

The simplest rational map with a singularity is

$$R(z)=z^2, \tag{21}$$

which gives

$$y_1=x_1^2-x_2^2,$$
$$y_2=2x_1x_2, \tag{22}$$
$$y_3=x_3.$$

The Jacobian matrix has rank one for the line $(0, 0, x_3)$. This is not one of the stable singularities.

Let us consider small perturbations around (21). Adding terms proportional to z only shifts the singularity. Therefore, we consider the following map:

$$R(z,\overline{z})=z^2+2\epsilon\overline{z}. \tag{23}$$

Since multiplying ϵ by a phase $e^{i\phi}$ only rotates the singularities by ϕ, we can take ϵ to be real. Using real coordinates, the Jacobian matrix can be written as

$$J=\begin{pmatrix} 2x_1+2\epsilon & -2x_2 & 0 \\ 2x_2 & 2x_1-2\epsilon & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{24}$$

The Jacobian matrix is singular for $x_1^2+x_2^2=\epsilon^2$. Therefore, the singular points lie on a cylinder with radius ϵ. They can be parametrized by $x_1=\epsilon\cos\alpha$ and $x_2=\epsilon\sin\alpha$ for $\alpha\in[0,2\pi]$, x_3 is arbitrary. Restricting the map to the singular surface, labeled by α and x_3, we can calculate the cusp lines. The surface is singular where

$$\frac{dy_1}{d\alpha}=\frac{dy_2}{d\alpha}=\frac{dy_3}{d\alpha}=0, \tag{25}$$

therefore, the cusps form lines where α is zero, $2\pi/3$ or $4\pi/3$, and x_3 is arbitrary.

In Fig. 1, we show the image of a set of concentric circles of radius ρ in the x_1x_2-plane. By rescaling space and target space coordinates, the value of ϵ can be changed. For convenience, we set $\epsilon=1$ in the figure. For small radius, ρ, the $\overline{z}$ term is dominant and the image of the circle is a deformed circle. As the radius increases, the circle becomes more and more deformed. The $\rho=1$ circle maps to the singular curve. This curve has three spikes. The points of these spikes are the cusps and running between them are three folds. Above this value of ρ, the map folds back on itself. The points inside the fold have four preimages: a $\rho<1$ preimage with negative Jacobian and three $\rho>1$ preimages with positive Jacobians. Eventually, the image circle passes completely through the folding region: for $\rho>3$ the image is a trefoil shape. Every point outside the fold has just two preimages, each with positive Jacobian.

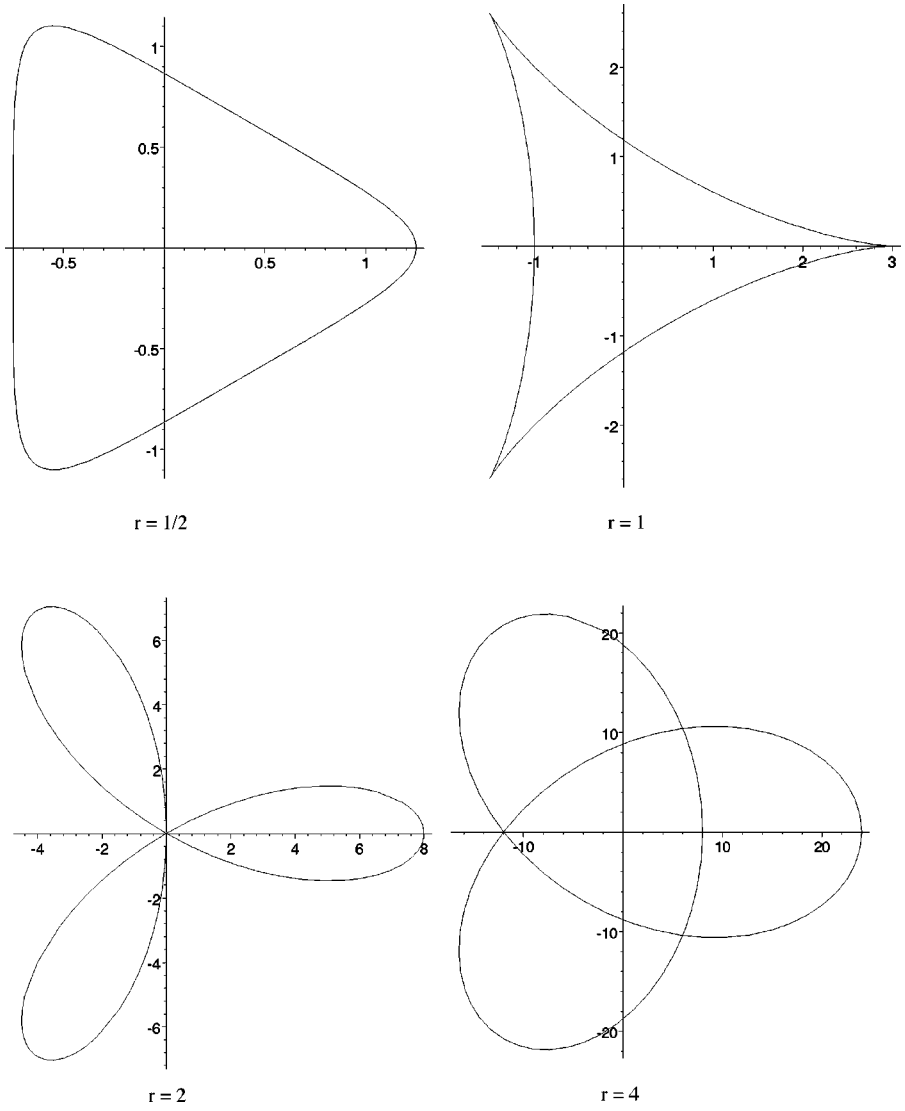

FIG. 1. The image of concentric circles $z=\rho e^{i\phi}$ of various radii ρ under $R(z,\bar{z})=z^2+2\bar{z}$. Note that the scale is different for each graph.

In general, the map $R(z)=z^n$ for $n\geqslant 2$ has an unstable singularity on the x_3-axis. This unstable singularity can be removed by adding an anti-holomorphic perturbation. The perturbed map $R(z)=z^n+n\epsilon\bar{z}$ has a folding surface at $z=\epsilon\exp(i\alpha)$. There are $n+1$ cusps which are located at $\alpha=2\pi k/(n+1)$ where $k=0,\ldots,n$. This map possesses a natural C_{n+1}-symmetry, which maps the cusps into each other.

It is worth noting that z^2 is a stable singularity within the set of holomorphic functions, whereas z^n for $n>2$ is unstable even as a holomorphic map. Therefore, we do not expect the latter singularities to occur for a generic holomorphic map.

Let us also consider the singularities of the rational map ansatz at the origin. Locally, the shape function can be written as

$$f(r)=\pi-Ar^{\nu}+O(r^{\nu+1}), \tag{26}$$

where A is an arbitrary positive constant and

$$\nu = -\tfrac{1}{2} + \tfrac{1}{2}\sqrt{8B+1}. \tag{27}$$

For $B=1$ this exponent is equal to one. This means that the Jacobian has full rank at the origin. However, for $B>1$ the exponent ν is greater than one. In this case the Jacobian of the rational map ansatz has rank zero. Moreover, the derivative $R_z(z)$ vanishes for certain values of z. Therefore, lines of degenerate singularities with rank one Jacobian matrices meet at the origin. Here they form an even more degenerate singularity with a rank zero Jacobian matrix. In Sec. III B, we argue that for $B=3$ there is a more likely singularity configuration close to the origin.

A. Nonholomorphic rational maps

The rational map ansatz restricts the ansatz fields in three different ways. It requires that concentric two-spheres around the origin in space are mapped to two-spheres in SU_2. It also requires that this map is the same for all concentric two-spheres, and it requires that the map between two-spheres is a holomorphic map. Our intention here is to relax the third of these conditions. We will consider a larger class of maps. The maps we will consider will be rational maps in the sense that they will have the form of a ratio between polynomials. However, the polynomials will depend on $\overline{z}$ as well as z, so they will not be holomorphic maps.

To begin with, we consider the ansatz

$$U(r,z,\overline{z}) = \exp(if(r)\hat{\mathbf{n}}_R\cdot\boldsymbol{\sigma}), \tag{28}$$

where, as before,

$$\hat{\mathbf{n}}_R = \frac{1}{1+|R|^2}(2\mathrm{Re}(R),2\mathrm{Im}(R),1-|R|^2) \tag{29}$$

but, without assuming R is holomorphic,

$$R = R(z,\overline{z}). \tag{30}$$

In order to derive the energy, E, we calculate the eigenvalues λ_1^2, λ_2^2 and λ_3^2 of the strain tensor (6). The strain tensor can be written as

$$(D_{ij}) = \begin{pmatrix} f'^2 & 0 & 0 \\ 0 & A(R_z+R_{\overline{z}})(\overline{R}_z+\overline{R}_{\overline{z}}) & iA(R_z\overline{R}_z-R_{\overline{z}}\overline{R}_{\overline{z}}) \\ 0 & iA(R_z\overline{R}_z-R_{\overline{z}}\overline{R}_{\overline{z}}) & -A(R_z-R_{\overline{z}})(\overline{R}_z-\overline{R}_{\overline{z}}) \end{pmatrix}, \tag{31}$$

where

$$A = \left(\frac{1+|z|^2}{1+|R|^2}\frac{\sin f}{r}\right)^2, \tag{32}$$

and has eigenvalues

$$\begin{aligned} \lambda_1^2 &= f'^2, \\ \lambda_2^2 &= \left(\frac{|R_z|+|R_{\overline{z}}|}{r}\frac{1+|z|^2}{1+|R|^2}\sin f\right)^2, \\ \lambda_3^2 &= \left(\frac{|R_z|-|R_{\overline{z}}|}{r}\frac{1+|z|^2}{1+|R|^2}\sin f\right)^2. \end{aligned} \tag{33}$$

Notice that λ_2^2 and λ_3^2 are only equal if $R_z^-=0$, or $R_z=0$. In the first case, the energy of the holomorphic rational map ansatz (11) is reproduced. The second case corresponds to a purely anti-holomorphic ansatz and is just the holomorphic ansatz composed with a reflection.

Using Eq. (7) the energy E can be rewritten as

$$E=4\pi\int\left(r^2f'^2+2\mathcal{J}(f'^2+1)\sin^2f+\mathcal{I}\frac{\sin^4f}{r^2}\right)\mathrm{d}r, \tag{34}$$

where $\mathcal{I}$ and $\mathcal{J}$ are given

$$\mathcal{J}=\frac{1}{4\pi}\int\left(\frac{(|R_z|^2+|R_z^-|^2)(1+|z|^2)^2}{(1+|R|^2)^2}\right)\frac{2i\ \mathrm{d}z\mathrm{d}\bar{z}}{(1+|z|^2)^2} \tag{35}$$

and

$$\mathcal{I}=\frac{1}{4\pi}\int\left(\frac{(|R_z|^2-|R_z^-|^2)(1+|z|^2)^2}{(1+|R|^2)^2}\right)^2\frac{2i\ \mathrm{d}z\mathrm{d}\bar{z}}{(1+|z|^2)^2}. \tag{36}$$

As in the holomorphic ansatz, $\mathcal{I}$ is essentially the integral of the square of the Jacobian. However, $\mathcal{J}$ is not the integral of the Jacobian of R.

There is a close relationship between this energy functional and the baby Skyrme model on a two-sphere. The baby Skyrme model[21,22] is a sigma-model in $(2+1)$ dimensions with a fourth order Skyrme-like interaction. The baby-Skyrme model on the two-sphere is of independent interest, primarily because there is a phase transition as the radius of the sphere is changed.[23,24]

On a unit two-sphere, the baby Skyrme fields map S^2 to S^2 and the energy functional is of the form $g_1\mathcal{J}+g_2\mathcal{I}$ where g_1 and g_2 are coupling constants. $\mathcal{J}$ is the sigma-model energy and $\mathcal{I}$ is the Skyrme energy. For a given shape function, f, the energy E in (34) is of this form with g_1 and g_2 calculated by integrating the shape function over r.

Obviously, it would be possible to regard the holomorphic maps between two-spheres as ansätze for baby Skyrme fields. For a holomorphic map, $\mathcal{J}$ is equal to the topological degree. Thus, the holomorphic map which minimizes $\mathcal{I}$ gives the best approximation to the energy minimizing baby Skyrme field. In other words, to find the baby Skyrme energy minimizing holomorphic map, the values of g_1 and g_2 need not be known. This is one of the reasons why the original rational map ansatz is so convenient to use: the rational map is found first and the shape function is then determined numerically.

For more general maps we need to employ an iterative algorithm. First, using the $\mathcal{I}$ minimizing holomorphic rational map, a shape function can be calculated numerically. This gives provisional values for the coupling constants g_1 and g_2. The next step is to minimize the baby-Skyrme energy with these values of g_1 and g_2. This determines a new map between the Riemann spheres. The original shape function is not optimized for this new map, so a new shape function must be calculated. A new profile function gives new coupling constants and so the whole procedure has to be iterated. In practice, this procedure is simplified by the fact that we only consider one-parameter families of nonholomorphic rational maps.

Another major advantage of using holomorphic maps is that there is only a finite-dimensional family of holomorphic maps of given topological degree. In contrast, the space of general maps between two-spheres of a given degree is infinite dimensional. One way to avoid this problem would be to minimize the baby Skyrme model numerically. However, our interest here is in the folding behavior of minimum energy Skyrmions and so we would prefer to find an approximate analytic solution whose folding behavior we can analyze. For this reason, we will restrict our attention to maps of the form

$$R(z,\overline{z})=\frac{p(z,\overline{z})}{q(z,\overline{z})}, \tag{37}$$

where p and q are polynomials in both z and $\overline{z}$. We will call the polynomial degree of this map (N_1,N_2), where N_1 is the maximal holomorphic degree of the polynomials p and q and N_2 is their maximal antiholomorphic degree. By counting the number of preimages of a given value of R and taking into account the sign of the Jacobian at each preimage, it follows that a general map of this form has topological degree N_1-N_2. Some maps will have a different degree because p and q may have a common factor. Maps of this type are called spurious.

According to formula (8), the baryon number is

$$B=\frac{2}{\pi}\int f'\sin^2 f\,\mathrm{d}r\,\frac{1}{4\pi}\int\frac{(|R_z|^2-|R_{\overline{z}}|^2)(1+|z|^2)^2}{(1+|R|^2)^2}\,\frac{2i\,\mathrm{d}z\mathrm{d}\overline{z}}{(1+|z|^2)^2}. \tag{38}$$

B is no longer an integral over squares, as it was for the holomorphic rational map ansatz. It is possible that the baryon density could be locally negative. We will find that this is what happens for certain values of B.

B. Symmetric nonholomorphic rational maps

The Skyrmions that we are interested in are symmetrical: the three-Skyrmion is tetrahedrally symmetric and the four-Skyrmion is octahedrally symmetric.[5] Rather than minimizing the ansatz energy over the whole space of maps, we restrict our attention to maps that have the same symmetry as the numerically determined minimum energy solution.

An SO_3 rotation g acts on the Riemann sphere z as a Möbius transformation

$$z\mapsto g(z)=\frac{\alpha z+\beta}{-\overline{\beta}z+\overline{\alpha}}, \tag{39}$$

where $|\alpha|^2+|\beta|^2=1$. There is also a Möbius action on the rational maps. A Möbius transformation of the rational map is equivalent to a global group transformation of the corresponding Skyrme fields. A Skyrme field is symmetric under a rotation, g, if the rotated fields are a global group transformation of the original fields. In the same way, the rational map $R(z,\overline{z})$ is symmetric under g if

$$R(g(z),\overline{g(z)})=\frac{\alpha' R(z,\overline{z})+\beta'}{-\overline{\beta}' R(z,\overline{z})+\overline{\alpha}'}, \tag{40}$$

where α' and β' are not necessarily the same as α and β.

Symmetric nonholomorphic rational maps can be calculated using elementary representation theory. In this subsection, we describe this construction. In the next section, we will derive nonholomorphic rational maps for various B.

The Riemann sphere is isomorphic to $\mathbf{CP}^1$, the one-dimensional complex projective space. $\mathbf{CP}^1$ can be labeled by a pair of complex numbers $[u,v]$, where the square bracket indicates the relation

$$[u,v]\cong[\lambda u,\lambda v] \tag{41}$$

with $\lambda\in\mathbf{C}^\times$. These homogeneous coordinates, u and v, are related to the inhomogeneous coordinate by $z=u/v$. The rotation group acts linearly on the homogenous coordinates and, so, it is easier to use these coordinates to describe the representation theory. However, we switch to

inhomogeneous coordinates whenever they are more convenient. Similarly, we can label the Riemann sphere by the complex conjugates of u and v, $[\overline{u},\overline{v}]$, also subject to relation (41). A nonholomorphic rational map takes the form

$$R(u,v,\overline{u},\overline{v})=[p(u,v,\overline{u},\overline{v}),q(u,v,\overline{u},\overline{v})]. \tag{42}$$

This rational map must be well-defined under the relation (41). Therefore, p and q have to be homogeneous: they are of the form

$$p(u,v,\overline{u},\overline{v})=\sum_{i=0}^{N_1}\sum_{j=0}^{N_2} a_{ij}u^i v^{N_1-i}\overline{u}^j\overline{v}^{N_2-j}, \tag{43}$$

$$q(u,v,\overline{u},\overline{v})=\sum_{i=0}^{N_1}\sum_{j=0}^{N_2} b_{ij}u^i v^{N_1-i}\overline{u}^j\overline{v}^{N_2-j}. \tag{44}$$

It should be noted that the topological degree does not depend on the value of N_1+N_2, it only depends on their difference. Choosing N_1 and N_2 corresponds to a truncation of the possible maps between Riemann spheres. This truncation is similar to truncating a Fourier expansion. In this article we will consider nonholomorphic maps with N_2 equal one or two.

Under an SO_3 rotation about the unit vector $\hat{\mathbf{n}}$ by an angle θ, the $[u,v]$ coordinates transform by an SU_2 transformation $\exp(i(\theta/2)\hat{\mathbf{n}}\cdot\boldsymbol{\sigma})$. The SO_3 action on the Riemann sphere $[u,v]$ can now be written as

$$\begin{aligned} u&\mapsto u'=(a_0+ia_3)u+(a_2+ia_1)v,\\ v&\mapsto v'=(-a_2+ia_1)u+(a_0-ia_3)v, \end{aligned} \tag{45}$$

where $a_i=n_i\sin(\theta/2)$ and $a_0=\cos(\theta/2)$. The coordinates $[\overline{u},\overline{v}]$ transform as the complex conjugate of (45). Let G be the double group of a finite subgroup of SO_3. The rational map $[p,q]$ is G invariant if an SU_2 transformation of $[u,v]$ and $[\overline{u},\overline{v}]$ is equivalent to an SU_2 transformation of $[p,q]$.

A homogeneous polynomial of degree N in z transforms as $\mathbf{N+1}$, the $(N+1)$-dimensional irreducible representation of SU_2. It follows that the homogeneous polynomial p of degree N_1 in z and degree N_2 in $\overline{z}$ transforms as $(\mathbf{N_1+1})\otimes(\mathbf{N_2+1})$. This representation can be decomposed into irreducible representations of some finite group G. These decompositions can be calculated using the characters. Tables of these decompositions can be found, for example, in Ref. 25.

By decomposing the $(\mathbf{N_1+1})\otimes(\mathbf{N_2+1})$ as a representation of G we can determine whether or not there is a G invariant degree (N_1,N_2) rational map. In fact, the rational map $[p,q]$ can be G-invariant in two different ways. One possibility is that

$$(\mathbf{N_1+1})\otimes(\mathbf{N_2+1})\big|_G=E\oplus \text{ other irreducible representations of } G, \tag{46}$$

and $\{p,q\}$ form a basis for the two-dimensional irreducible representation E. This means p and q are transformed into linear combinations of each other under Möbius transformations of z. Moreover, by a choice of basis, these combinations are unitary. This is always possible, because every representation of a finite group is equivalent to a unitary representation.[26] The second possibility is that

$$(\mathbf{N_1+1})\otimes(\mathbf{N_2+1})\big|_G=A_1\oplus A_2\oplus \text{other irreducible representations of } G, \tag{47}$$

and p is a basis for A_1, and q is a basis of A_2. Here, A_1 and A_2 are two different one-dimensional representations of G. In this case, there is a one-parameter family of G-symmetric rational maps: namely $R=[p,aq]$. The parameter a can be chosen to be real, because a Möbius transformation of R can change the phase of a.

Of course, there is also a one-parameter family when

$$(\mathbf{N_1+1})\otimes(\mathbf{N_2+1})\big|_G = 2E \oplus \text{other irreducible representations of } G \tag{48}$$

because, in this case, there is a one-parameter family of choices of an E inside $2E$. In order to construct a basis of this one-parameter family, we can construct a projector $P_{\alpha\beta}$. Given a representation ρ and a two-dimensional unitary representation $\rho^{(2)}_{\alpha\beta}$, the projector is given by

$$P_{\alpha\beta}=\frac{2}{|G|}\sum_{g\in G}\rho^{(2)}_{\alpha\beta}(g^{-1})\rho(g). \tag{49}$$

For details of this construction, see Refs. 9 and 27. It is not always necessary to construct projectors. In the $B=2$ case discussed later, the invariant map is calculated by direct calculation and in the $B=3$ case it is derived from other, previously known, examples.

III. SKYRMIONS FROM NONHOLOMORPHIC RATIONAL MAPS

In this section, we use nonholomorphic rational maps to approximate the Skyrmions with baryon numbers 2–4. In each of these cases, there is a one-parameter family of maps with the correct symmetry. Once the approximating map is found, we can discuss the folding structure. We also consider the $B=5^*$ octahedral saddle point which also has a one-parameter family of symmetric maps. It is more tractable than the five-Skyrmion, because the five-Skyrmion is not very symmetrical.

A. $B=2$: The torus

For $B=2$, the holomorphic rational map which minimizes $\mathcal{I}$ is

$$R(z)=z^2. \tag{50}$$

It has the same D_∞ symmetry as the true solution. There is an axial symmetry

$$R(e^{i\chi}z)=e^{2i\chi}R(z) \tag{51}$$

and a symmetry under rotation by π around an orthogonal axis

$$R\left(\frac{1}{z}\right)=\frac{1}{R(z)}. \tag{52}$$

The group theory methods discussed in the last section are not really needed here. The most general D_∞-symmetric map can be calculated by writing out the general (3,1) rational map and applying the symmetries (51) and (52). It is

$$R(z,\overline{z})=\frac{az^2(z\overline{z}+1)+bz^2(z\overline{z}-1)}{a(z\overline{z}+1)+b(-z\overline{z}+1)}. \tag{53}$$

The true solution also has a reflection symmetry. In the holomorphic case, that reflection symmetry is $R(\overline{z})=\overline{R(z)}$. If we impose the same symmetry for the nonholomorphic map, then the parameters a and b have to be real, up to a common phase. Moreover, since the pair (a,b) and $(\lambda a,\lambda b)$ gives rise to the same rational map for all $\lambda\in\mathbf{C}^\times$, we can set $a=\cos\theta$ and $b=\sin\theta$. The polynomials have been chosen such that the value $\theta=0$ corresponds to the holomorphic rational (2,0) map. θ is in the range $[-\pi/2,\pi/2]$, because under $\theta\mapsto\theta+\pi$ both $\sin\theta$ and $\cos\theta$ change sign.

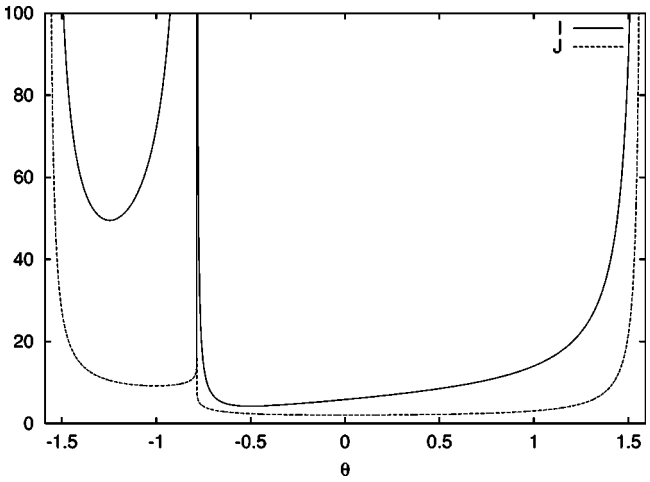

FIG. 2. $\mathcal{I}$ and $\mathcal{J}$ as a function of θ for $B=2$.

In Fig. 2, we show the value of $\mathcal{J}$ and $\mathcal{I}$ as a function of θ. There are two poles, one at $\theta=-\pi/4$ and another at $\theta=\pm\pi/2$. Both of these poles correspond to points where the maps are spurious. At $\theta=-\pi/4$, the cancellation of the common factor changes the topological degree,

$$R(z,\overline{z})|_{\theta=-\pi/4}=\frac{z}{z}, \tag{54}$$

whereas at $\theta=\pm\pi/2$ it does not:

$$R(z,\overline{z})|_{\theta=\pm\pi/2}=-z^2. \tag{55}$$

Thus, while the integrals are nonsingular at $\theta=\pm\pi/2$, they diverge as this value of θ is approached. These poles are considered in detail in Ref. 27. In Ref. 27, it is also shown that there is some negative baryon density only if $-\pi/2<\theta<-\pi/4$ or $\pi/4<\theta<\pi/2$.

To find the best approximation to the true minimum, we calculate the value of θ which minimizes the energy. The energy is a combination of $\mathcal{I}$ and $\mathcal{J}$. The optimal value for $\mathcal{J}$ is at the holomorphic rational map value $\theta=0$. However, $\mathcal{I}$ is minimal for $\theta\approx-0.503$. Minimizing energy (34) with respect to θ numerically, using the golden rule algorithm,[28] gives an optimal value of $\theta\approx-0.202$. The energy per Skyrmion calculated with this method is $E/B\approx1.191$. In contrast, for the holomorphic rational map $\theta=0$, we obtain $E/B\approx1.208$. The true value of the energy per Skyrmion is $E/B\approx1.1791$. For the energy minimizing value of θ, the baryon density is positive everywhere except at the origin. Thus, we find that there is no negative baryon density for $B=2$, even though there is a significant improvement in the energy. It seems that the axial symmetry stabilizes the unstable singularity.

B. $B=3$: The tetrahedron

The three-Skyrmion has tetrahedral symmetry T. The holomorphic rational map ansatz is

$$\begin{aligned} p_T(z)&=-i\sqrt{3}z^2+1,\\ q_T(z)&=z^3-i\sqrt{3}z, \end{aligned} \tag{56}$$

and $\{p_T,q_T\}$ is a basis for the E_2' in

$$\mathbf{4}|_T=E_2'\oplus E_3'. \tag{57}$$

TABLE I. The decomposition of irreducible representations of SU_2 as representations of T.

$\mathbf{1}\vert_T = A_1$
$\mathbf{2}\vert_T = E_1'$
$\mathbf{3}\vert_T = F$
$\mathbf{4}\vert_T = E_2' \oplus E_3'$
$\mathbf{5}\vert_T = A_2 \oplus A_3 \oplus F$
$\mathbf{6}\vert_T = E_1' \oplus E_2' \oplus E_3'$
$\mathbf{7}\vert_T = A_1 \oplus 2F$

The decompositions can be easily derived from the characters. Tables of these decompositions can also be found in, for example, Ref. 25. For convenience, a short table is given in Table I.

Here, we are interested in the nonholomorphic maps of degree (4,1). These correspond to the ten-dimensional representation $\mathbf{5}\otimes\mathbf{2}$ and can be decomposed into

$$\begin{aligned} \mathbf{5}\otimes\mathbf{2} &= \mathbf{6}\oplus\mathbf{4}, \\ (\mathbf{6}\oplus\mathbf{4})\vert_T &= E_1{}' \oplus 2E_2{}' \oplus 2E_3{}'. \end{aligned} \tag{58}$$

Both $\{1,z\}$ and $\{1,\overline{z}\}$ are a basis of the irreducible representation $E_1{}'$ of T. When they are multiplied, they decompose into $A_1 \oplus F$. For convenience, a multiplication table for the tetrahedral group is given in Table II.

A basis for this A_1 is

$$k = z\overline{z} + 1. \tag{59}$$

Furthermore, because $A_1 \otimes E_2' = E_2'$, $\{kp_T, kq_T\}$ is a basis for an E_2' inside $\mathbf{5}\otimes\mathbf{2}$. Explicitly, this basis is

$$\begin{aligned} p_1(z,\overline{z}) &= i\sqrt{3}z^3\overline{z} + i\sqrt{3}z^2 - z\overline{z} - 1, \\ q_1(z,\overline{z}) &= z^4\overline{z} + z^3 - i\sqrt{3}z^2\overline{z} - i\sqrt{3}z. \end{aligned} \tag{60}$$

The rational map for this basis is spurious: $[p_1,q_1] = [kp_T, kq_T] = [p_T, q_T]$. The common factor of k cancels. However, when we have a second independent basis, $\{p_2,q_2\}$, we will be able to form nonspurious linear combinations involving p_1 and q_1.

To find an independent pair of basis vectors in $2E_2'$, we use the A_2 in $\mathbf{5}\vert_T = A_2 + A_3 + F$. A basis for this A_2 is the Klein polynomial

$$k_f = z^4 - 2i\sqrt{3}z^2 + 1. \tag{61}$$

TABLE II. A multiplication table for the irreducible representations of T.

A_1	A_2	A_3	F	E_1'	E_2'	E_3'	$\otimes$
A_1	A_2	A_3	F	E_1'	E_2'	E_3'	A_1
	A_3	A_1	F	E_2'	E_3'	E_1'	A_2
		A_2	F	E_3'	E_1'	E_2'	A_3
			$A_1 \oplus A_2 \oplus A_3 \oplus 2F$	$E_1' \oplus E_2' \oplus E_3'$	$E_1' \oplus E_2' \oplus E_3'$	$E_1' \oplus E_2' \oplus E_3'$	F
				$A_1 \oplus F$	$A_2 \oplus F$	$A_3 \oplus F$	E_1'
					$A_3 \oplus F$	$A_1 \oplus F$	E_2'
						$A_2 \oplus F$	E_3'

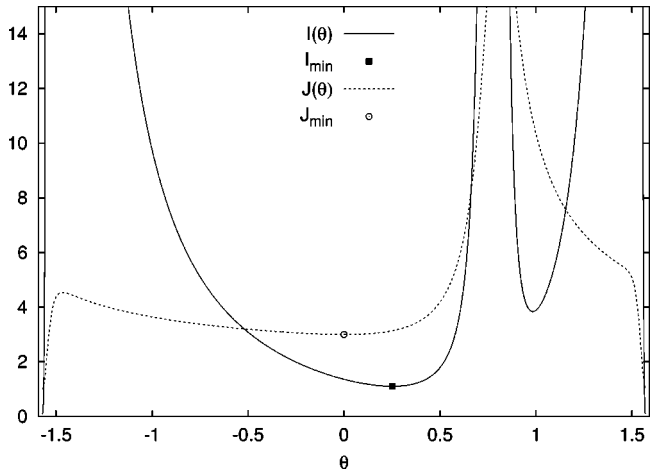

FIG. 3. $\mathcal{I}$ and $\mathcal{J}$ as a function of θ for $B=3$. Here $\mathcal{I}$ is rescaled by a factor of 10.

This is often called the face polynomial, because its zeros are the face points of a tetrahedron. Of course, the distinction between this and the vertex polynomial is a matter of convention. Now, $A_2\otimes E_1'=E_2'$ and so the required basis for E_2' can be found by multiplying k_f by $[1,-\overline{z}]$. Thus, a second basis is given by

$$\begin{aligned} p_2(z,\overline{z}) &= z^4-2i\sqrt{3}z^2+1, \\ q_2(z,\overline{z}) &= -z^4\overline{z}+2i\sqrt{3}z^2\overline{z}-\overline{z}. \end{aligned} \tag{62}$$

As with the other basis pair, the rational map for this basis is spurious: $[p_2,q_2]=[k_f,k_f\overline{z}]=[1,-\overline{z}]$.

A general T-symmetric nonholomorphic rational map of degree 3 is given by

$$R(z,\overline{z})=\frac{\cos\ \theta p_1+\sin\ \theta e^{i\phi}p_2}{\cos\ \theta q_1+\sin\ \theta e^{i\phi}q_2}. \tag{63}$$

The two angles θ and ϕ parametrize all maps. When $\theta=0$ this map is spurious and reduces to the tetrahedrally symmetric degree (3,0) rational map studied in Ref. 9. $\theta=\pm\pi/2$ is also spurious, here the map reduces to a degree (0,1) map. In this case, the cancellation changes the topological degree of the map. It is expected that $\mathcal{I}$ tends to infinity as this value of θ is approached.

For $\phi=0$, the map also has an additional reflection symmetry and the symmetry group becomes T_d. Since the numerically determined minimum seems to have this symmetry, it is expected that the best result from the rational map ansatz will come from $\phi=0$. We have confirmed this and will restrict our discussion to this case.

In Fig. 3, we display $\mathcal{I}$ and $\mathcal{J}$ as a function of the angle θ. The minimum of $\mathcal{J}$ is still at the rational map value $\theta=0$ with $\mathcal{J}=3$. However, the minimum of $\mathcal{I}$ is at $\theta\approx0.252$ with $\mathcal{I}\approx11.04$. The minimum of the energy can now be calculated by varying θ, using a simple minimization scheme in which the shape function is recalculate at each step. We obtain $E/B\approx1.160$ for $\theta\approx0.155$. The holomorphic rational map value is $E/B\approx1.184$, whereas the exact solution has $E/B\approx1.1462$. Therefore, the nonholomorphic rational map ansatz is a significant improvement.

Furthermore, there are regions of negative baryon density. In the holomorphic ansatz the singularities of the rational maps correspond to points on the face centers of a tetrahedron. Let us consider the baryon density near these points. The determinant of the Jacobian of the map R is proportional to the baryon density in (38):

$$B_R=\frac{(|R_z|^2-|R_{\bar{z}}|^2)(1+|z|^2)^2}{4\pi(1+|R|^2)^2}, \tag{64}$$

where we have integrated over r using the boundary conditions on f.

It is convenient to reorient the map (63) using the Möbius transformation

$$z\mapsto\frac{2z+(\sqrt{3}-1)(1+i)}{(1-\sqrt{3})(1-i)z+2}. \tag{65}$$

If the holomorphic map (56) is rotated in this way, it is singular at $z=0$, that is, B_R for the holomorphic map vanishes at $z=0$. If we rotate the nonholomorphic map (63) by the same Möbius transformation and expand B_R in terms of z and $\bar{z}$ we obtain

$$B_R\approx -0.17+10.8z\bar{z}, \tag{66}$$

where θ has been set to the energy minimizing value 0.155. For $z=0$ the baryon density is negative and, to lowest order in z and $\bar{z}$, the folds lie on a circle around the origin in the z-plane. Thus, the nonholomorphic rational map ansatz predicts tubes of negative baryon density. In fact, the total negative baryon density, B_-, can be calculated numerically. It is $B_-\approx 0.000\,089$.

Finally, we discuss the general singularity structure of the three-Skyrmion. All the singularities are of z^2 type and break up into three cusps connected by folds. This is compatible with the tetrahedral symmetry. Therefore, a three-Skyrmion consists of four tubes of folds, one through each of the faces of the tetrahedron. Each of these tubes contains three cusp lines. There are 12 cusp lines in total.

Unfortunately, it is difficult to directly examine the Skyrmion at the origin and at infinity using these methods. It is possible to speculate on what the singularity structure is, based on the assumption that the singularities are all generic.

From the discussion in Sec. I C we know that four cusp lines meet in a swallowtail. The cusp lines have to respect the tetrahedral symmetry. If the singularities are generic, they must meet in a swallowtail. Therefore, the 12 cusp lines cannot meet at the origin but have to split up earlier.

Considering only the cusp structure, one possible configuration would be that the three cusp lines of each fold tube meet in a swallowtail, resulting in one further cusp. The simplest tetrahedrally symmetric configuration would be that this cusp meets similar cusps of the remaining three fold tubes at the origin. However, we also know that the instanton approximation to the three-Skyrmion has negative baryon density at the origin,[18] whereas this possible configuration does not, because it has a singularity at the origin.

The following configuration is more likely. Each cusp of the fold splits up into three cusps at a swallowtail at some distance from the origin. Two of the cusp lines connect to the remaining two swallowtails of the fold tube. The last cusp line connects to the nearest swallowtail belonging to a different fold tube. This configuration is again tetrahedrally symmetric. Moreover, at the origin the baryon density is nonzero. We will call the cusp lines which follow the fold tubes *long cusp lines*, the cusp lines which connect swallowtails of the same fold tube *short cusp lines* and the cusp lines which connect swallowtails of different fold tubes *medium cusp lines*. In this configuration there are 12 long cusp lines, six medium cusp lines, and 12 short cusp lines. Note that the medium cusp lines lie on the edges of a tetrahedron.

In order to decide the sign of the baryon density at the origin, it is worth considering the folds of this configuration. Folds separate positive from negative baryon density. Moreover, precisely two folds end in one cusp. There are three folding surfaces in each fold tube. Each of these folding surfaces ends in two long cusp lines and one short cusp line. There are four additional folding surfaces, which can be visualized as the sides of a tetrahedron. Each of these folding surfaces ends

TABLE III. The decomposition of the irreducible representations of SU_2 as representations of O.

$\mathbf{1}\|_O = A_1$
$\mathbf{2}\|_O = E_1'$
$\mathbf{3}\|_O = F_1$
$\mathbf{4}\|_O = G'$
$\mathbf{5}\|_O = E \oplus F_2$
$\mathbf{6}\|_O = E_2' \oplus G'$
$\mathbf{7}\|_O = A_2 \oplus F_1 \oplus F_2$
$\mathbf{8}\|_O = E_1' \oplus E_2' \oplus G'$
$\mathbf{9}\|_O = A_1 \oplus E \oplus F_1 \oplus F_2$

in three medium cusp lines and three short cusp lines. These are all the folding surfaces because precisely two folding surfaces end in each of the cusps. Therefore, the baryon density at the origin has the same sign as the baryon density inside the fold tubes.

Thus, the baryon density at the origin is negative, as it is in the instanton ansatz.[18] In the instanton configuration the negative baryon density tubes pinch at two points. It is not possible to decide using our methods whether this is a peculiarity of the instanton ansatz or a feature of the three-Skyrmion.

C. $B=4$: The cube

The minimum energy $B=4$ configuration looks like a cube and has octahedral symmetry O. The corresponding invariant holomorphic map is

$$\begin{aligned} p_O(z) &= 2\sqrt{3}z^2, \\ q_O(z) &= z^4 + 1. \end{aligned} \tag{67}$$

These polynomials are a basis of the E in

$$\mathbf{5}\|_O = E \oplus F_2 . \tag{68}$$

As before, these decompositions can be easily calculated, but, for convenience, a table of them is given in Table III.

In the tetrahedral case, there was a unique invariant (3,0) map and a one-parameter family of (4,1) maps. The same thing does not happen here: if we consider (5,1) maps we obtain

$$\begin{aligned} \mathbf{6} \otimes \mathbf{2} &= \mathbf{7} \oplus \mathbf{5}, \\ (\mathbf{7} \oplus \mathbf{5})\|_O &= A_2 \oplus E \oplus F_1 \oplus 2F_2 , \end{aligned} \tag{69}$$

and the E is just the spurious map $[kp_O, kq_O] = [p_O, q_O]$. $k = 1 + z\bar{z}$ is the invariant polynomial discussed earlier. In other words, the only invariant (5,1) map reduces to the holomorphic map.

This means that, in order to derive a one-parameter family of invariant rational maps, we need to consider degree (6,2):

$$\begin{aligned} \mathbf{7} \otimes \mathbf{3} &= \mathbf{9} \oplus \mathbf{7} \oplus \mathbf{5}, \\ (\mathbf{9} \oplus \mathbf{7} \oplus \mathbf{5})\|_O &= A_1 \oplus A_2 \oplus 2E \oplus 2F_1 \oplus 3F_2 . \end{aligned} \tag{70}$$

Thus, there is a one-parameter family corresponding to the $2E$.

Since $\mathbf{3} \otimes \mathbf{3} = \mathbf{5} \oplus \mathbf{3} \oplus \mathbf{1}$ there is an essentially unique degree (2,2) SU_2 invariant. This is k^2 and so $(k^2 p_O, k^2 q_O)$ spans an E inside the $2E$. Explicitly this is

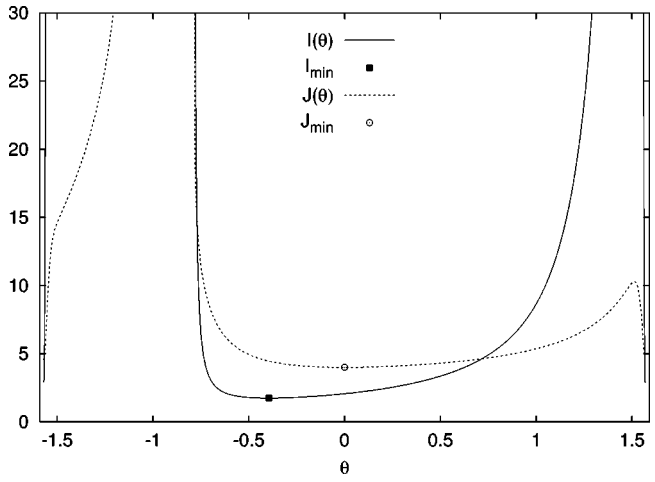

FIG. 4. $\mathcal{I}$ and $\mathcal{J}$ as a function of θ for $B=4$. Here $\mathcal{I}$ is rescaled by a factor of 10.

$$p_1(z,\overline{z})=2\sqrt{3}(z^4\overline{z^2}+2z^3\overline{z}+z^2),$$
$$q_1(z,\overline{z})=z^6\overline{z^2}+2z^5\overline{z}+z^4+z^2\overline{z^2}+2z\overline{z}+1. \tag{71}$$

By calculating the projection matrix we can derive another pair of basis vectors in $2E$:

$$p_2(z,\overline{z})=\sqrt{3}(-z^6+z^4\overline{z^2}-8z^3\overline{z}+z^2-\overline{z^2}),$$
$$q_2(z,\overline{z})=-z^6\overline{z^2}+4z^5\overline{z}-7z^4-7z^2\overline{z^2}+4z\overline{z}-1, \tag{72}$$

and the general invariant rational map has the same form as in the three-Skyrmion case, (63). As before, $\phi=0$ imposes the reflection symmetry of the true solution, and $\theta=0$ corresponds to the holomorphic map.

In Fig. 4 we show $\mathcal{I}$ and $\mathcal{J}$ as a function of the angle θ. At $\theta=0$ the graph of $\mathcal{J}$ has its global minimum. There is a local minimum at $\theta=\pm\pi/2$. The minimum value of $\mathcal{I}$ does not occur at the rational map value but at $\theta\approx-0.40$. Therefore, there is the possibility of deriving a lower energy. Indeed, minimizing the energy with respect to θ leads to $E=1.127$ for $\theta\approx-0.138$. This energy is only 0.6% above the true solution. By contrast the holomorphic rational map ansatz energy is 1.5% above the true solution.

As before, we can examine the baryon density in the neighborhood of a singularity of the holomorphic ansatz. In this case, the map is already oriented so that the holomorphic map has a singularity at $z=0$. Setting $\theta=-0.138$ and expanding the density, B_R, in powers of z and $\overline{z}$ we obtain

$$B_R\approx 2.54z\overline{z}. \tag{73}$$

Therefore, B_R vanishes at $z=0$, and there is no negative baryon density anywhere to lowest order.

D. $B=5^*$: The octahedron

The $B=5^*$ saddle point is octahedral in shape. The group theory involved in this example is very like the group theory required for $B=3$. There is a holomorphic map

$$p_O(z)=z^5-5z,$$
$$q_O(z)=-5z^4+1, \tag{74}$$

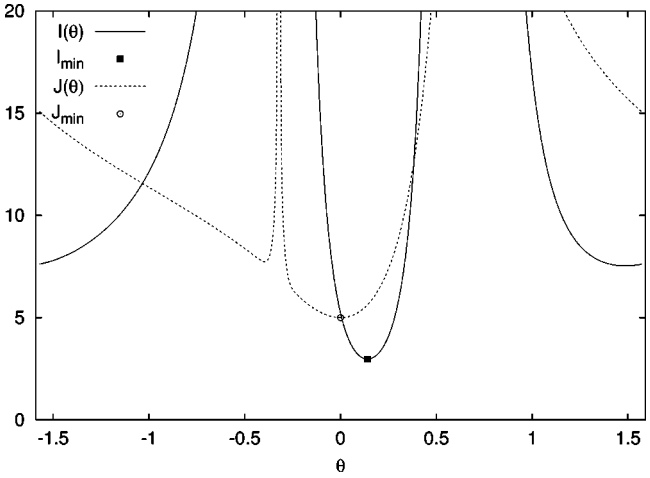

FIG. 5. $\mathcal{I}$ and $\mathcal{J}$ as a function of θ for $B=5^*$. Here $\mathcal{I}$ is rescaled by a factor of 10.

corresponding to the E_2' in

$$\mathbf{6}|_O = E_2' \oplus G'. \tag{75}$$

The generalization to (6,1) maps leads to a one-parameter family because

$$\mathbf{7} \otimes \mathbf{2} = \mathbf{8} \oplus \mathbf{6},$$

$$(\mathbf{8} \oplus \mathbf{6})|_O = E_1' \oplus 2E_2' \oplus 2G'. \tag{76}$$

Multiplying the holomorphic maps by the SU_2 invariant, $k = z\bar{z} + 1$, gives

$$\begin{aligned} p_1(z,\bar{z}) &= z^6\bar{z} + z^5 - 5z^2\bar{z} - 5z, \\ q_1(z,\bar{z}) &= -5z^5\bar{z} - 5z^4 + z\bar{z} + 1, \end{aligned} \tag{77}$$

and calculating the projection matrices gives

$$\begin{aligned} p_2(z,\bar{z}) &= 3z^6\bar{z} - 23z^5 - 15z^2\bar{z} + 11z, \\ q_2(z,\bar{z}) &= 11z^5\bar{z} - 15z^4 - 23z\bar{z} + 3. \end{aligned} \tag{78}$$

Thus, as before, a one-parameter family of invariant maps is given by (62) with $\phi = 0$. $\theta = 0$ gives the holomorphic map.

In Fig. 5 we display the graphs of $\mathcal{I}$ and $\mathcal{J}$ as a function of θ. There is a global minimum of $\mathcal{J}$ at the rational map value $\mathcal{J} = 5$. The graph of $\mathcal{I}$ has a minimum at $\theta \approx 0.141$. Minimizing the energy with respect to θ results in $E = 1.157$ for $\theta \approx 0.082$. This energy is only 1.7% above the true energy. In comparison, the energy of the holomorphic rational map ansatz is 8.3% above the true energy. This significant improvement gives an indication that negative baryon density plays an important role in this case. A local expansion shows that the nonholomorphic rational map has negative Jacobian determinant when z takes the values of the singularities of the holomorphic rational map. Finally, the integral of the negative baryon density is $B_- \approx 0.000\,97$, which is a factor of 10 larger than for $B = 3$.

IV. CONCLUSION

This article was motivated by the theory of singularities of differentiable maps and, in particular, by Whitney's theorem. This theorem states that there are only three types of stable singularities of maps between three-manifolds. We showed that the holomorphic rational map ansatz for Skyrmions[9] does not have a stable singularity structure: it does not even allow folding. We introduced a nonholomorphic rational map ansatz that allows folding. For baryon numbers 2, 3, and 4, the approximate solutions derived from this ansatz are closer in energy to the true Skyrmions than any other ansatz solution.

The key idea of the nonholomorphic rational map ansatz is to construct maps between Riemann spheres which are not holomorphic but have the same symmetry as the true solutions. We described this construction in detail and calculated the nonholomorphic rational maps for baryon numbers 2, 3, and 4, and for the octahedrally symmetric $B=5^*$ saddle point. Nonholomorphic rational maps can have folding and, therefore, negative baryon density. We found that there is negative baryon density for $B=3$ and $B=5^*$ but not for $B=2$ and $B=4$.

By decomposing group representations we showed that there is a one-parameter family of tetrahedrally symmetric (4,1) maps. These maps have topological degree three. The ansatz energy was minimized within this family to find the best approximation to the three-Skyrmion. The (4,1) maps have antiholomorphic degree one and so they are minimal generalizations of the original holomorphic map. For $B=5^*$ the situation is similar: there is a one-parameter family of octahedrally symmetric (6,1) maps. However, for $B=4$ the (5,1) maps do not contain a one-parameter family of octahedral maps, only the (6,2) maps do. The (5,1) maps can be thought of as the first order effect, and the (6,2) maps as a second order effect. In fact, for $B=4$, the holomorphic rational map is remarkably close to the true solution. The energy error is 1.5%. The holomorphic rational map approximation to the three-Skyrmion has an error of 3.3%. $B=7$ seems to be similar to $B=4$. The seven-Skyrmion is dodecahedral and it is easy to check that only the (10,3) maps contain a one-parameter family of icosahedrally symmetric maps. Again, the holomorphic rational map is extremely close to the true solution, with an error of only 1.1%. Therefore, we do not expect that negative baryon density occurs for $B=7$.

There is an icosahedrally-symmetric $B=11^*$ saddle point. The holomorphic rational map ansatz approximates it quite poorly. It predicts an energy which is far larger than 11 one-Skyrmions, whereas the true solution is a saddle-point solution with $E/B=1.158$. This can be viewed as an indication that negative baryon density plays a major role. The representation theory also suggests that there is negative baryon density because there is a one-parameter family of icosahedrally symmetric (12,1) maps.

It seems possible to decide heuristically whether or not a Skyrmion of a certain symmetry possesses negative baryon density. In Sec. I C we showed that a z^n singularity can be decomposed into folds which contain $n+1$ cusps and that there is a natural C_{n+1} symmetry which maps the cusps into each other. It seems likely that negative baryon density occurs if this C_{n+1} symmetry is compatible with the symmetry of the faces.

Direct computation shows that in the holomorphic rational map ansatz for $B=2$, 3, 4, 5^*, 7 and 11^* all the singularities are of z^2 type. Therefore, negative baryon density occurs, if the faces have a C_3 symmetry. The faces of the tetrahedron, the octahedron and the icosahedron are equilateral triangles. This is consistent with what we found: there is negative baryon density for $B=3$ and 5^*. It suggests that there is also negative baryon density for $B=11^*$. On the other hand, the faces of a torus are round, the faces of a cube are squares and the faces of a dodecahedron are pentagons. Correspondingly, we did not find any negative baryon density for $B=2$ and 4 and do not expect negative baryon density for $B=7$.

In the three-Skyrmion case we discussed the singularity structure at the origin. Assuming tetrahedral symmetry and generic singularities we conjectured a configuration with 16 folding surfaces, 30 cusp lines and 12 swallowtails. This is compatible with the instanton calculations in Ref. 18.

It appears that there are a large number of swallowtails, cusps and folds for both the three-Skyrmion and $B=5^*$ saddle point, but nongeneric singularities for the two- and four-Skyrmions.

TABLE IV. The numerical results.

	True[a]	Holomorphic[b]		Minimizing $\mathcal{I}$ [c]		Minimizing energy[d]			
B	E/B	$\mathcal{I}$	E/B	$\mathcal{I}$	E/B	$\mathcal{J}$	$\mathcal{I}$	B_-	E/B
1	1.2322	1	1.232	1	0	1	1	0	1.232
2	1.1791	5.81	1.208	4.20	0	2.04	4.98	0	1.191
3	1.1462	13.58	1.184	11.04	0.000 88	3.04	11.48	0.000 09	1.160
4	1.1201	20.65	1.137	17.50	0	4.04	18.95	0	1.127
5*	1.138	52.10	1.232	29.72	0.008 41	5.20	32.93	0.000 97	1.157

[a]These are the energies obtained in Ref. 7 by numerical minimization of the Skyrme energy.
[b]These are the values obtained in Ref. 9 using the holomorphic ansatz.
[c]$\mathcal{I}$ is minimized within the class of maps considered.
[d]These are the best results obtained with the nonholomorphic rational map ansatz.

Thus, while it may be that in nonextremal Skyrme configurations there are certain folding features associated with each interacting one-Skyrmion, this is not necessarily apparent in the extremal configurations.

It might be interesting to examine the number of antivacuum points, that is, the number of points where $U=-1$. A one-Skyrmion is centered around a single antivacuum point and, in a configuration of well-separated Skyrmions, the individual Skyrmions can be thought of as being positioned at the antivacuum points. However, as the Skyrmions approach each other, there may be more antivacuum points, some with positive Jacobian and some with negative. This is certainly what is implied by the folding seen in the three-Skyrmion and $B=5^*$ saddle point, and by the corresponding monopole configurations.

The topological charge of a BPS monopole is equal to the number of zeros of the Higgs field provided that the zeros are counted with their multiplicity. Furthermore, well-separated one-monopoles are centered around a zero of the Higgs field. However, the total number of zeros can exceed the topological charge. In Ref. 29, three-monopole fields were calculated using the mixture of analytic and numerical methods first described in Refs. 30 and 16. It was found that the number of zeros of the Higgs field can be as high as seven, with five zeros of positive winding number and two of negative winding number. In Ref. 17, the cubic four-monopole, octahedral five-monopole and dodecahedral seven-monopole calculated in Refs. 30, 16, and 31 were examined and it was found that zeros with negative winding number occur for the octahedral five-monopole but not for the cubic four-monopole and the dodecahedral seven-monopole. This pattern is mimicked by what we have found for Skyrmions. This possibility was discussed in Ref. 17.

It is also interesting that in monopole dynamics, as an individual monopole approaches other monopoles, its zero of the Higgs field often splits into three zeros, two with positive winding and one with negative winding.[29,17] Perhaps something similar happens in the case of Skyrmions.

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APPENDIX: NUMERICAL RESULTS

For convenience the main numerical results have been gathered together in Table IV. As discussed earlier, the table shows that the minima of $\mathcal{I}$ and $\mathcal{J}$ do not coincide and so the more general nonholomorphic rational map ansatz is closer to the true energy than the holomorphic ansatz. However, only for $B=3$ and $B=5^*$ are there regions of negative baryon density. These regions are quite small.

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The onset of superconductivity in a domain with a corner

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We study the variational problem related to the onset of superconductivity that identifies the transition from the normal state to the superconducting state of a sample in the presence of an applied magnetic field. Our concern is a thin sample whose 2-D cross-section has a corner. In particular, we focus on the quarter-plane. We show a first eigenfunction minimizing the associated Rayleigh quotient exists and decays away from the corner. We also give a rigorous upper bound for the eigenvalue which is related to the critical temperature at which superconductivity emerges. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1387466]

I. INTRODUCTION

Superconductivity is a phenomenon characterized by the loss of electric resistivity and the expulsion of magnetic fields attempting to penetrate a sample. The onset of superconductivity is observed when a sample is cooled below a certain critical temperature. When the material is subjected to an applied magnetic field, the value of this critical temperature is lowered even further. In particular, very large magnetic fields destroy superconductivity. In the absence of superconducting behavior, the sample is in the so-called normal state, where it retains normal conductivity and permeability to magnetic fields.

Ginzburg–Landau theory provides a good framework to understand some aspects of superconductivity.[1] When a 2-D cross-section Ω of a thin cylindrical sample is subjected to a perpendicular uniform applied magnetic field of magnitude h and the sample is surrounded by insulating media, the free energy is described by

$$G(\Psi,\mathbf{A})=\int_{\Omega}\frac{1}{2}|(i\nabla+\mathbf{A})\Psi|^2+\frac{\mu}{4}(|\Psi|^2-1)^2dxdy+\frac{\kappa^2}{2\mu}\int_{\mathbf{R}^2}|\nabla\times\mathbf{A}-h\hat{\mathbf{z}}|^2dxdy.$$

Here we have chosen a nondimensionalization with respect to a characteristic radius R of the cross-section.[2] The function $\Psi:\Omega\to\mathbf{C}^2$ is the order parameter whose modulus is the density of superconducting electrons. The vector field $\mathbf{A}:\mathbf{R}^2\to\mathbf{R}^2$ is the magnetic potential with $\nabla\times\mathbf{A}=(0,0,A_x^{(2)}-A_y^{(1)})$ being the induced magnetic field. The GL parameter κ is the ratio of two material characteristic lengths and μ is a temperature related parameter defined by

$$\mu=\frac{R^2(T_c-T)}{\xi_0^2T_c}.$$

Here T is the temperature, T_c is the critical temperature in the absence of the applied magnetic field and ξ_0 is the coherence length at zero temperature.

For the pair $(\Psi,\mathbf{A})$ to be achievable physical states, for a given temperature and applied magnetic field strength h, they should be stable critical points of the free energy G. In particular, as Giorgi and Phillips proved in Ref. 3, for very large values of h the only critical point is the normal state in which $\Psi\equiv0$ and $\mathbf{A}=h\mathbf{A_n}$ such that $\nabla\times\mathbf{A_n}=\hat{\mathbf{z}}$.

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Our interest lies in studying the onset of superconductivity as it bifurcates from the normal solution. This occurs as the temperature drops below the critical value and the normal state is no longer a stable physical state. We look at the second variation of G at $(0,h\mathbf{A_n})$ to detect such a change in behavior:

$$\delta^2 G((0,h\mathbf{A_n});\phi,\mathbf{B}) = \int_\Omega |(i\nabla + h\mathbf{A_n})\phi|^2 - \mu|\phi|^2 + \frac{\kappa^2}{\mu}|\nabla\times\mathbf{B}|^2 dxdy.$$

The second variation is positive for values of μ below the value determined by the minimization problem:

$$\lambda(h) = \inf_{\phi\in H^1(\Omega)} \frac{\int_\Omega |(i\nabla + h\mathbf{A_n})\phi|^2 dxdy}{\int_\Omega |\phi|^2 dxdy}. \tag{1.1}$$

Hence, the normal state is no longer stable for values of $\mu > \lambda(h)$.

A critical point of the variational problem (1.1) satisfies the linear elliptic eigenvalue problem:

$$(i\nabla + h\mathbf{A_n})^2\Psi = \lambda(h)\Psi \quad \text{in } \Omega, \tag{1.2}$$

$$(i\nabla + h\mathbf{A_n})\Psi\cdot\nu = 0 \quad \text{on } \partial\Omega, \tag{1.3}$$

where ν is the outer unit normal vector to $\partial\Omega$. Alternatively, this problem arises from linearizing the Euler–Lagrange system of the free energy $G(\Psi,\mathbf{A})$ about the normal state.

In an attempt to study the effect of the boundary on the onset of superconductivity, Saint James and de Gennes[4] considered the case in which Ω is the half-plane with applied magnetic field strength $h=1$. They found that the solution of the eigenvalue problem concentrates on the boundary and decays exponentially towards the interior. They approximate the minimum eigenvalue of the half-plane to be about 0.59. From now on we will denote this eigenvalue $\lambda(1)$ of the half-plane by $\lambda_{\mathbf{H}}$.

More recently, using a perturbation method for nonlinear bifurcation problems initiated by Millman and Keller,[5] Chapman[6] pursued a more complete formal analysis of the half-plane. Shifting the investigation to samples with bounded cross-section, Bauman Phillips and Tang[7] investigated stability issues in great detail via bifurcation theory with regard to the onset of superconductivity in a disc. They showed that the minimum eigenvalue for the disc is lower than that for the half-plane by a term proportional to the curvature of the disc. Along with that they showed that superconductivity emerges uniformly around the boundary of the disc with a big vortex at the core.

Bernoff and Sternberg[8] pursued the case of a general bounded domain with smooth boundary. Using formal asymptotics they found that the first eigenfunction would concentrate exponentially at the boundary point of maximum curvature. Again, they found that the minimum eigenvalue is less than that for the half-plane by a term proportional to the maximum curvature of the boundary. The expansion for $\lambda(h)$ on bounded smooth domains was found to take the form

$$\lambda(h) \sim \lambda_{\mathbf{H}} h - \frac{\kappa_{\max}}{3I_0} h^{1/2} \quad \text{for } h \gg 1, \tag{1.4}$$

where $\kappa_{\max}$ is the maximum curvature on the boundary of the domain and I_0 is a universal constant. A rigorous argument capturing the first term in this expansion can be found in Refs. 9 and 10. Note the implication here is that superconductivity is induced at a higher temperature in domains with a large maximum curvature.

Naturally this leads one to look at domains with corners where the curvature is infinite. In this article we will study domains with right angles. One might then expect that at the transition, the order parameter concentrates at the corner. By analogy with the case of smooth bounded domains, where the expansion of the minimum eigenvalue has the value for the half-plane at the leading

order [cf. (1.4)], one would expect for square domains that the leading order value would correspond to the quarter-plane. This yields our motivation in this article to study the problem on the quarter-plane.

A striking feature of the eigenvalue problem on the half-plane is the nonexistence of an L^2 eigenfunction. This can be understood intuitively when one recognizes that the boundary of this domain consists of an infinite straight line. As all points along the boundary look the same, one would not expect any decay along that direction. To make this nonexistence rigorous is nontrivial however (see Refs. 11 and 10). On the other hand, in this article we establish the existence and exponential decay of the minimizer for the quarter-plane, $\mathbf{Q}$. This is a major difference from the half-plane problem.

Theorem 1.1: *There exists a function $\Psi_\infty \in H^1(Q)$ that minimizes the energy*

$$\lambda_{\mathbf{Q}} \equiv \inf_{\Psi \in H^1(\mathbf{Q})} \frac{\int_{\mathbf{Q}} |(i\nabla + \mathbf{A})\Psi|^2 dxdy}{\int_{\mathbf{Q}} |\Psi|^2 dxdy}. \tag{1.5}$$

In particular, Ψ_∞ satisfies the problem

$$(i\nabla + \mathbf{A})^2 \Psi_\infty = \lambda_{\mathbf{Q}} \Psi_\infty \quad \text{in } \mathbf{Q}, \tag{1.6}$$

$$(i\nabla + \mathbf{A})\Psi_\infty \cdot \nu = 0 \quad \text{on } \partial\mathbf{Q}. \tag{1.7}$$

Moreover, for every multi-index α, there exist positive constants c_1^α and c_2^α such that

$$|D^\alpha \Psi_\infty(z)| \leqslant c_1^\alpha e^{-c_2^\alpha |z|} \quad \text{for all } z \in \mathbf{Q}. \tag{1.8}$$

By using similar methods we also show that the first eigenfunction in a square decays exponentially away from the four corners, cf. Theorem 3.2. The proof of Theorem 1.1 requires finding a minimizing sequence which we choose to be a sequence of minimizers of the variational problem on squares of increasing size so that they approach the quarter-plane in the limit. However, if we consider the variational problem as it is, the solution may concentrate at all four corners. As we expect a solution for the quarter-plane to concentrate at the one corner only and to decay exponentially towards the interior, we impose the Dirichlet boundary condition on the sides of the square that lie inside the quarter-plane in building our minimizing sequence.

The compactness of this sequence comes from uniform exponential estimates. For that purpose we down scale all the squares of increasing size to the unit square. With this rescaling, each function in the minimizing sequence is a minimizer on the unit square with increasing magnetic field strength. The method used in proving the exponential decay on the unit square is a blow-up argument used by del Pino, Felmer, and Sternberg[10] where they proved an exponential decay of the minimizer on the half-plane and for arbitrary bounded smooth domains away from the boundary.

On the experimental front, physicists are interested in the onset of superconductivity in many topologies including mesoscopic squares of size $2-4$ μm. In their experiments they study the temperature/field transition line (see, e.g., Refs. 12–14). In Ref. 15 we did numerical simulations using the linearized Ginzburg–Landau problem on the unit square. Our results were in good agreement with the experimental data for certain ranges for the field. Moreover, by an elementary rescaling along with the exponential decay for the eigenfunction for the problem on the quarter-plane, one can show that for large magnetic field strength the minimum eigenvalue for the unit square $\lambda(h) \sim \lambda_{\mathbf{Q}} h$, where $\lambda_{\mathbf{Q}}$ is the minimum eigenvalue for the quarter-plane. We found using finite element methods that $\lambda_{\mathbf{Q}}$ take the approximate value of 0.55. Note that the quarter-plane value is smaller than the value for the half-plane.

While in this article we address the case of a domain with a right angle corner, we intend to turn our attention next to study the nature of the dependence of the minimum eigenvalue (and

hence the temperature) on the angle in the corner. There are some numerical studies on wedges of differing angles suggesting that the eigenvalue is a monotone increasing function of the angle (see Refs. 16 and 17).

Simultaneous to our study, Almog[18] has been studying the problem on the half-infinite strip and in long rectangles of fixed width. Using Fourier transform techniques, he studies the decay of the order parameter and the location of the vortices. His approach is totally different from the one we are presenting here. We feel that our results complement his nicely, in that we are proving the *a priori* decay of the eigenfunction, thus extending the validity of Almog's use of Fourier transform techniques. He also constructs a test function which he uses to prove that the eigenvalue for the half-infinite strip is strictly less than that for the infinite strip. We will use a variant of his construction to prove a similar result comparing the smallest eigenvalue for the half-plane and the quarter-plane.

We organize the article as follows. In Section II we compare the eigenvalues of the problem on different domains and with different boundary conditions. In Sec. III we prove the exponential decay of the minimizer on the unit square for sufficiently large field strength h. We conclude in Sec. IV with the existence Theorem 1.1 in the quarter-plane.

II. EIGENVALUES: GAPS AND BOUNDS

In this section we discuss the minimum eigenvalue of the problem on different domains: the plane, the half-plane, the half-line and the quarter-plane with natural boundary conditions. In addition, we compare the minimum eigenvalue of the problem on the quarter-plane under different boundary conditions. We also discuss the relation between the eigenvalues of the quarter-plane and squares.

We denote the quarter-plane by $\mathbf{Q}=\{(x,y):x>0,y>0\}$, the half-plane by $\mathbf{H}=\{(x,y):x>0\}$ and the square of side ℓ by $Q_\ell=\{(x,y):0<x<\ell,0<y<\ell\}$.

For any domain Ω we define the h-dependent Rayleigh quotient related to (1.2) and (1.3):

$$R_\Omega(u,h)=\frac{\int_\Omega|(i\nabla+h\mathbf{A})u|^2dxdy}{\int_\Omega|u|^2dxdy},$$

and an h-independent Rayleigh quotient:

$$R_\Omega(u)=\frac{\int_\Omega|(i\nabla+\mathbf{A})u|^2dxdy}{\int_\Omega|u|^2dxdy}.$$

Here $\mathbf{A}$ is a vector field describing the normal state which satisfies

$$\nabla\times\mathbf{A}\equiv(0,0,A_x^{(2)}-A_y^{(1)})=(0,0,1). \tag{2.1}$$

We note that the infima of these Rayleigh quotients are independent of the particular choice of $\mathbf{A}$ in the light of the gauge invariance recorded in the following lemma:

Lemma 2.1: For $\psi\in H^1(\Omega,\mathbf{C})$, $\phi\in H^1(\Omega,\mathbf{R})$ *and* $\mathbf{A}\in C^1(\mathbf{R}^2,\mathbf{R}^2)$, *we have*

$$\int_\Omega|(i\nabla+\mathbf{A})\psi|^2dxdy=\int_\Omega|(i\nabla+\mathbf{A}+\nabla\phi)\psi e^{i\phi}|^2dxdy.$$

Moreover, if ψ *solves the equation*

$$(i\nabla+\mathbf{A})^2\psi=\lambda\psi \quad in \quad \Omega,$$

then $\tilde{\psi}=\psi e^{i\phi}$ *solves the equation*

$$(i\nabla+\mathbf{A}+\nabla\phi)^2\tilde{\psi}=\lambda\tilde{\psi} \quad in \quad \Omega.$$

We start with the following lemma concerning the minimization problem on the full-plane $\mathbf{R}^2$:

Lemma 2.2 (cf. Refs. 10 and 11). *For* $\mathbf{A}:\mathbf{R}^2\to\mathbf{R}^2$ *satisfying (2.1), we have*

$$\lambda_{\mathbf{R}^2}\equiv \inf_{\psi\in H^1(\mathbf{R}^2)} \frac{\int_{\mathbf{R}^2}|(i\nabla+\mathbf{A})\psi|^2 dxdy}{\int_{\mathbf{R}^2}|\psi|^2 dxdy}=1.$$

The proof uses the Gaussian as a test function and makes use of Fourier series techniques.

Now we consider the 2-D problem on the half-plane $\mathbf{H}$ which is connected to the 1-D problem on the half-line given by

$$-\psi''+(x-\beta)^2\psi=\lambda\psi \quad x\in(0,\infty), \tag{2.2}$$

$$\psi'(0)=0 \quad \psi(\infty)=0. \tag{2.3}$$

This connection comes up when one seeks a solution to (1.2) and (1.3) with $\mathbf{A}=(0,x)$ via separation of variables. Then one finds that Ψ has the form $\Psi(x,y)=\psi(x)e^{i\beta y}$ for any real number β. Recall that because of gauge invariance the choice of the vector field $\mathbf{A}$ leaves the modulus unchanged and the eigenvalue the same. For each $\beta\in\mathbf{R}$, the first eigenvalue $\lambda(\beta)$ can be captured by minimizing the associated Rayleigh quotient:

$$\lambda(\beta)=\inf_{\psi\in H^1((0,\infty))}\frac{\int_0^\infty(\psi')^2+(x-\beta)^2\psi^2 dx}{\int_0^\infty\psi^2 dx}. \tag{2.4}$$

Minimizing over β one finds the following.

Theorem 2.3: (cf. Refs. 19 and 20)

(i) There is a unique number $\beta^*\in\mathbf{R}$ *such that*

$$\lambda_1\equiv\lambda(\beta^*)=\inf_{\beta\in\mathbf{R}}\lambda(\beta), \quad \beta^*=\sqrt{\lambda_1}.$$

(ii) The corresponding first eigenfunction $\psi_1(x)$ *decays exponentially as* $x\to\infty$.

Proof: See Refs. 19 and 20.

We note that standard numerical schemes yield that $\lambda_1\approx 0.59$.

Proposition 2.4: The value λ_1, *defined in Theorem 2.3, is the same as the first eigenvalue for the half-plane. That is,*

$$\lambda_1=\lambda_{\mathbf{H}}\equiv \inf_{\phi\in H^1(\mathbf{H})} R_{\mathbf{H}}(\phi).$$

The proof involves straightforward use of the Fourier transform. See Ref. 11.

Next we turn to the eigenvalue problem on squares and their relation to the eigenvalue problem on the quarter-plane. We want to minimize the Rayleigh quotient on the unit square, among competitors that vanish on the sides of the square that lie inside the quarter-plane. We denote this portion of ∂Q_1 by $\Gamma_D^1=\{(x,y)\in\partial Q_1: x=1 \text{ or } y=1\}$. More precisely, we consider

$$\lambda(h)=\inf_{\substack{u\in H^1(Q_1)\\ u=0 \text{ on } \Gamma_D^1}} R_{Q_1}(u,h). \tag{2.5}$$

We will frequently invoke the transformation $\tilde{z}=\sqrt{h}\,z$, for $z\in Q_1$. This maps Q_1 onto $Q_{\sqrt{h}}$. As a result, this transformation allows us to rewrite the Rayleigh quotient on Q_1 as

$$R_{Q_1}(u,h)=hR_{Q_{\sqrt{h}}}(u).$$

This implies that

$$\frac{\lambda(h)}{h} = \inf_{\substack{u \in H^1(Q_{\sqrt{h}}) \\ u=0 \text{ on } \Gamma_D^{\sqrt{h}}}} R_{Q_{\sqrt{h}}}(u), \tag{2.6}$$

where obviously $\Gamma_D^{\sqrt{h}} = \{(x,y) \in \partial Q_{\sqrt{h}} : x = \sqrt{h} \text{ or } y = \sqrt{h}\}$.

We find out that these eigenvalues have the following property:

Lemma 2.5: The sequence $\{\lambda(h)/h\}_{h>0}$ *is a monotone decreasing sequence.*

Proof: First note that for any $h>0$ the minimizer to (2.6) exists by the direct method of the calculus of variations. Now suppose that $h_1 < h_2$. Let v_{h_1} be a minimizer of the problem on $Q_{\sqrt{h_1}}$. With v_{h_1} vanishing on $\Gamma_D^{\sqrt{h_1}}$ we may extend it to be zero on $\mathbf{Q} - Q_{\sqrt{h_1}}$. Hence v_{h_1} can be viewed as a competitor for the eigenvalue problem on $Q_{\sqrt{h_2}}$. Therefore,

$$\frac{\lambda(h_2)}{h_2} \leqslant R_{Q_{\sqrt{h_2}}}(v_{h_1}) = R_{Q_{\sqrt{h_1}}}(v_{h_1}) = \frac{\lambda(h_1)}{h_1}.$$

Thus $\{\lambda(h)/h\}_{h>0}$ is decreasing. ■

Remark 2.6: As a result of this lemma the sequence $\{\lambda(h)/h\}_{h>0}$ is bounded and $\lim_{h\to\infty} \lambda(h)/h$ exists. Furthermore, using a similar argument to the previous lemma one finds $\lambda_{\mathbf{Q}} \leqslant \lambda(h)/h$, for $h>0$. In fact, as a by-product of Theorem 4.1 we will find that $\lambda_{\mathbf{Q}} = \lim_{h\to\infty} \lambda(h)/h$.

In Ref. 18, Almog studies the related problem on the infinite strip and the half-infinite strip of a fixed width. In determining that the eigenvalues for the full strip and the semi-strip are separated, he provides a key test function that makes use of the first eigenfunction of the 1-D problem on a finite interval. By making an analogous construction in a quarter-plane we obtain the following result.

Theorem 2.7: (Cf. Ref. 18, Lemma 3.)

(i) For any vector fields $\mathbf{A}:\mathbf{R}^2 \to \mathbf{R}^2$ *and* $\mathbf{B}:\mathbf{R}^2 \to \mathbf{R}^2$ *with* $\nabla \times \mathbf{A} = \nabla \times \mathbf{B} = (0,0,1)$,

$$\lambda_{\mathbf{Q}} \equiv \inf_{\phi \in H^1(\mathbf{Q})} \frac{\int_{\mathbf{Q}} |(i\nabla + \mathbf{A})\phi|^2 dxdy}{\int_{\mathbf{Q}} |\phi|^2 dxdy} < \inf_{\eta \in H^1(\mathbf{H})} \frac{\int_{\mathbf{H}} |(i\nabla + \mathbf{B})\eta|^2 dxdy}{\int_{\mathbf{H}} |\eta|^2 dxdy} \equiv \lambda_{\mathbf{H}}.$$

(ii) One also has

$$\lim_{h\to\infty} \frac{\lambda(h)}{h} < \lambda_{\mathbf{H}}.$$

The proof follows by evaluating the Rayleigh quotient on the quarter-plane with $\mathbf{A} = (0, x)$ and

$$\phi(x,y) = C(\epsilon)\psi_1(x)e^{i\beta^* y}(e^{-\epsilon y} + i\epsilon^{1/2}(x-\beta^*)e^{-y}), \tag{2.7}$$

where $\epsilon>0$, $C(\epsilon)$ is a positive constant such that $\epsilon < C^2(\epsilon) < 2\epsilon$ and $\psi_1(x)$ is the first eigenfunction introduced in Theorem 2.3. This choice of the test function gives

$$\lambda_{\mathbf{Q}} \leqslant \lambda_1 - 2\epsilon^{3/2}C_1 + \epsilon^2 C_2,$$

where C_1 and C_2 are positive real numbers independent of ϵ. The conclusion *(i)* of the theorem is complete in light of Proposition 2.4.

As we mentioned in Remark 2.6 the limit in *(ii)* exists. Then for the minimization problem (2.6), we use a similar construction to (2.7) but replace $\psi_1(x)$ by $\psi_1(x)\rho_h(x,y)$ where $h\to\infty$ and ρ_h is a cutoff function that vanishes on $Q - Q_{\sqrt{h}}$, in particular it vanishes on $\Gamma_D^{\sqrt{h}}$. This makes the test function a valid competitor for the mixed Neumann Dirichlet problem on a square of side $\sqrt{h}$.

Since $\psi_1(x)$ decays exponentially, the error involved when taking the limit is exponentially small. Hence (ii) follows. ■

Remark 2.8: As we noted earlier, one can numerically approximate $\lambda_{\mathbf{H}} \approx 0.59$. However, a rigorous analyical estimate of $\lambda_{\mathbf{H}} < 1$ can be seen by making a construction similar to (2.7) but using the 2-D Gaussian which is the first eigenfunction associated with $\lambda_{\mathbf{R}^2}$, the first eigenvalue for the problem on the full plane $\mathbf{R}^2$. With $\mathbf{A} = \frac{1}{2}(-y,x)$ we use the test function:

$$\eta(x,y) = \tilde{C}(\epsilon) e^{-(x^2+y^2)/4}(1 + i\epsilon y),$$

where $1/2\pi \leqslant \tilde{C}(\epsilon) \leqslant 1/\pi$. Plugging the test function in the Rayliegh quotient we find that

$$\lambda_{\mathbf{H}} \leqslant 1 - \frac{\epsilon}{\sqrt{2\pi}} + 2\epsilon^2.$$

Now we introduce some related eigenvalue problems that will emerge in the next section. In all of these, **A** satisfies (2.1). We start with the Dirichlet problem,

$$\lambda_{HD} = \inf_{\substack{\phi \in H^1(\mathbf{H}) \\ \phi = 0 \text{ on } \partial\mathbf{H}}} \frac{\int_{\mathbf{H}} |(i\nabla + \mathbf{A})\phi|^2 dxdy}{\int_{\mathbf{H}} |\phi|^2 dxdy} \equiv \inf_{\substack{\phi \in H^1(\mathbf{H}) \\ \phi = 0 \text{ on } \partial\mathbf{H}}} R_{\mathbf{H}}(\phi), \tag{2.8}$$

and the associated problem,

$$(i\nabla + \mathbf{A})^2 \Psi = \lambda \Psi \quad \text{in } \mathbf{H}, \tag{2.9}$$

$$\Psi = 0 \quad \text{on } \partial\mathbf{H}. \tag{2.10}$$

Similarly we consider the Dirichlet problem in **Q**,

$$\lambda_{QD} = \inf_{\substack{\phi \in H^1(\mathbf{Q}) \\ \phi = 0 \text{ on } \partial\mathbf{Q}}} \frac{\int_{\mathbf{Q}} |(i\nabla + \mathbf{A})\phi|^2 dxdy}{\int_{\mathbf{Q}} |\phi|^2 dxdy} \equiv \inf_{\substack{\phi \in H^1(\mathbf{Q}) \\ \phi = 0 \text{ on } \partial\mathbf{Q}}} R_{\mathbf{Q}}(\phi), \tag{2.11}$$

and the associated problem

$$(i\nabla + \mathbf{A})^2 \Psi = \lambda \Psi \quad \text{in } \mathbf{Q}, \tag{2.12}$$

$$\Psi = 0 \quad \text{on } \partial\mathbf{Q}. \tag{2.13}$$

Finally we introduce the eigenvalue problem for mixed Neumann and Dirichlet boundary conditions in the quarter-plane:

$$\lambda_{QM} = \inf_{\substack{\phi \in H^1(\mathbf{Q}) \\ \phi = 0 \text{ on } \Gamma_D}} \frac{\int_{\mathbf{Q}} |(i\nabla + \mathbf{A})\phi|^2 dxdy}{\int_{\mathbf{Q}} |\phi|^2 dxdy} \equiv \inf_{\substack{\phi \in H^1(\mathbf{Q}) \\ \phi = 0 \text{ on } \Gamma_D}} R_{\mathbf{Q}}(\phi), \tag{2.14}$$

where $\Gamma_D = \{(x,y) \in \partial\mathbf{Q} : x = 0 \text{ and } y \geqslant 0\}$, and consider the associated problem:

$$(i\nabla + \mathbf{A})^2 \Psi = \lambda \Psi \quad \text{in } \mathbf{Q}, \tag{2.15}$$

$$(i\nabla + \mathbf{A})\Psi \cdot (0,-1) = 0 \quad \text{on } \Gamma_N, \tag{2.16}$$

$$\Psi = 0 \quad \text{on } \Gamma_D, \tag{2.17}$$

where $\Gamma_N = \{(x,y) \in \partial\mathbf{Q} : y = 0 \text{ and } x > 0\}$.

In the next lemma we compare these different eigenvalues.

Lemma 2.9:

(i) $\lambda_{\mathbf{H}} \leqslant \lambda_{QM} \leqslant \lambda_{QD}$.
(ii) $\lambda_{\mathbf{H}} \leqslant \lambda_{HD}$.

Proof: To prove $\lambda_H \leqslant \lambda_{QM}$, consider any competitor for the mixed boundary value problem on the quarter-plane (2.15)–(2.17), $\Psi \in H^1(\mathbf{Q})$, $\Psi \equiv 0$ on Γ_D. We define $\tilde{\Psi}$ on $\mathbf{H}$ by extending Ψ to be identically zero on the left quarter plane. Now $R_{\mathbf{H}}(\tilde{\Psi}) = R_{\mathbf{Q}}(\Psi)$ implies that $\lambda_{\mathbf{H}} \leqslant R_{\mathbf{Q}}(\Psi)$ for any $\Psi \in H^1(\mathbf{Q})$ with $\Psi \equiv 0$ on Γ_D, so we conclude that $\lambda_{\mathbf{H}} \leqslant \lambda_{QM}$. The inequality $\lambda_{QM} \leqslant \lambda_{QD}$ is trivial since a competitor for the Dirichlet problem is also a competitor for the variational problem with mixed boundary conditions. Similarly $\lambda_{\mathbf{H}} \leqslant \lambda_{HD}$. ■

The next lemma affirms the nonexistence of nontrivial bounded solutions for the boundary value problems (2.9) and (2.10), (2.12) and (2.13), and (2.15)–(2.17), where λ is below the associated first eigenvalues. By a solution we mean a classical solution to the partial differential equation (PDE), classically satisfying the boundary conditions away from the corner (for the case $\mathbf{Q}$) and lying in $H^2_{\mathrm{loc}}(\mathbf{Q})$ in this case.

Lemma 2.10:

(i) *If* $\lambda < \lambda_{\mathbf{R}^2}$, *then there are no nontrivial bounded solutions to the equation* $(i\nabla + \mathbf{A})^2 \Psi = \lambda \Psi$ *in* $\mathbf{R}^2$.
(ii) *If* $\lambda < \lambda_{\mathbf{H}}$, *then there are no nontrivial bounded solutions to the equation* $(i\nabla + \mathbf{A})^2 \Psi = \lambda \Psi$ *on* $\mathbf{H}$ *satisfying* $(i\nabla + \mathbf{A})\Psi \cdot (-1,0) = 0$ *on* $\partial \mathbf{H}$.
(iii) *If* $\lambda < \lambda_{HD}$, *then there are no nontrivial bounded solutions to (2.9) and (2.10).*
(iv) *If* $\lambda < \lambda_{QM}$, *then there are no nontrivial bounded solutions to (2.15)–(2.17).*
(v) *If* $\lambda < \lambda_{QD}$, *then there are no nontrivial bounded solutions to (2.12) and (2.13).*

Proof: Property (i) is proved in Ref. 11 (Prop. 2.3) and property *(ii)* is proved in Ref. 11 Lemma 5.1 Also, an alternative proof is given in Ref. 10, Theorem 3.2. Property *(iii)* is proved similar to (ii). To prove (iv), we follow the proof of Ref. 11, Lemma 5.1. The argument proceeds by contradiction. Assume that ψ is a nontrivial bounded solution of (2.15)–(2.17) for $\lambda < \lambda_{QM}$. For each positive integer k, let η_k be a non-negative smooth cut off function such that $\mathrm{spt}(\eta_k) \subset B(0,2k)$, $\eta_k \equiv 1$ on $B(0,k)$, $|\nabla \eta_k| < 2/k$. Multiplying the PDE (2.15) by the test function $\eta_k \overline{\Psi}$ and using that $\Psi \in H^2_{loc}(\mathbf{Q})$, we may carry out integration by parts. We find that the boundary terms vanish due to the boundary conditions (2.16) and (2.17) and η_k vanishing on the $\partial B(0,2k)$. So we obtain the integral equation:

$$\int_{\mathbf{Q}} |(i\nabla + \mathbf{A})(\eta_k \Psi)|^2 = \lambda \int_{\mathbf{Q}} |\Psi|^2 |\eta_k|^2 + \int_{\mathbf{Q}} |\nabla \eta_k|^2 |\Psi|^2. \tag{2.18}$$

Since $(\eta_k \Psi) \in H^1(\mathbf{Q})$ is a competitor of the minimization problem we find that

$$(\lambda_{QM} - \lambda) \int_{\mathbf{Q}} |\eta_k|^2 |\Psi|^2 < \int_{\mathbf{Q}} |\nabla \eta_k|^2 |\Psi|^2.$$

Since $\Psi \in L^\infty(\mathbf{Q})$ we find for every positive integer k

$$(\lambda_{QM} - \lambda) \int_{B(0,k)} |\Psi|^2 \leqslant 4\pi \|\Psi\|_{L^\infty(\mathbf{Q})}.$$

Hence $\Psi \in L^2(\mathbf{Q})$. Therefore,

$$(\lambda_{QM}-\lambda)\leqslant \frac{4}{k^2}\frac{\|\Psi\|^2_{L^2(\mathbf{Q})}}{\|\Psi\|^2_{L^2(B(0,k))}},$$

and as $k\to\infty$ we conclude that $\lambda_{QM}=\lambda$, a contradiction.

Property *(v)* is proved similarly. ■

A. An upper bound on $\lambda_{\mathbf{Q}}$

Recall from Theorem 2.7 that $\lambda_{\mathbf{Q}}<\lambda_{\mathbf{H}}$. However, this theorem does not provide a quantitative value for the gap between the two values. Applying any of the standard numerical schemes, one finds $\lambda_{\mathbf{H}}=\lambda_1\approx 0.59$. Using finite elements, on the other hand, we find that $\lambda_{\mathbf{Q}}\approx 0.55$ (see Ref. 15). We conclude this section with a rigorous upper bound on $\lambda_{\mathbf{Q}}$ using a specific test function. References 17 and 21 made attempts to provide an upper bound on wedges using a similar construction; however, theirs lack a term similar to $e^{i(1/3)r^3q(\theta)}$.

Proposition 2.11: The eigenvalue $\lambda_{\mathbf{Q}}$ for the quarter-plane satisfies the upper bound $\lambda_{\mathbf{Q}}\leqslant 0.5772$

Proof: We define a test function on the quarter-plane. To this end, we describe the quarter-plane in polar coordinates $\{(r,\theta): r>0 \text{ and } 0\leqslant\theta\leqslant\pi/2\}$. The test function for (1.5) that we propose is

$$u(r,\theta)=e^{-(r^2/2)s(\theta)}e^{i(rp(\theta)+(1/2)r^2g(\theta)+(1/3)r^3q(\theta))}, \tag{2.19}$$

where $s(\theta)=a_0(5+\sin^2(2\theta))$, $g(\theta)=\frac{1}{4}\sin(4\theta)$, $p(\theta)=a_1\cos(2\theta)$, $q(\theta)=a_2(\cos(6\theta)-1.7\cos(2\theta))$.

Here a_0, a_1, and a_2 are real numbers which will be determined by minimizing the functional with the restriction that a_0 be positive. It is clear that $u\in C^\infty(\mathbf{Q})\cap H^1(\mathbf{Q})$. Due to gauge invariance of the energy and the choice of polar coordinates of the test function, it is convenient to choose $\mathbf{A}=\frac{1}{2}r(-\sin\theta,\cos\theta)=\frac{1}{2}r\mathbf{e}_\theta$, where $\mathbf{e}_\theta$ is the unit tangent vector.

Via change of variable we have for any function v:

$$|(i\nabla+\mathbf{A})v|^2=\left\{\left|\frac{\partial v}{\partial r}\right|^2+\frac{1}{r^2}\left|\frac{\partial v}{\partial\theta}\right|^2+\frac{i}{2}\left(\overline{v}\frac{\partial v}{\partial\theta}-v\frac{\partial\overline{v}}{\partial\theta}\right)+\frac{r^2}{4}|v|^2\right\}\equiv F\left[v,\frac{\partial v}{\partial r},\frac{\partial v}{\partial\theta}\right].$$

The Rayleigh quotient $R_{\mathbf{Q}}(u)$ would appear in polar coordinates in the form

$$R_Q(u)=\frac{\int_0^{\pi/2}\int_0^\infty F[u,\partial u/\partial r,\partial u/\partial\theta]r\,dr\,d\theta}{\int_0^{\pi/2}\int_0^\infty |u|^2 r\,dr\,d\theta}.$$

In computing $R_{\mathbf{Q}}(u)$ we write $|\partial u/\partial r|^2$, $|\partial u/\partial\theta|^2$, $-\mathrm{Im}(\overline{u}\partial u/\partial\theta)\equiv(i/2)(\overline{u}\partial u/\partial\theta-u\,\partial\overline{u}/\partial\theta)$ and $|u|^2$ in terms of s,g,p and q:

$$\left|\frac{\partial u}{\partial r}\right|^2=[r^2s(\theta)^2+(rg(\theta)+p(\theta)+r^2q(\theta))^2]e^{-r^2s(\theta)},$$

$$\left|\frac{\partial u}{\partial\theta}\right|^2=\left[\left(-\frac{1}{2}r^2s'(\theta)\right)^2+\left(\frac{1}{2}r^2g'(\theta)+rp'(\theta)+\frac{1}{3}r^3q'(\theta)\right)^2\right]e^{-r^2s(\theta)},$$

$$-\mathrm{Im}\left(\overline{u}\frac{\partial u}{\partial\theta}\right)=\left(-\frac{1}{2}r^2g'(\theta)-rp'(\theta)-\frac{1}{3}r^3q'(\theta)\right)e^{-r^2s(\theta)},$$

$$|u|^2=e^{-r^2s(\theta)}.$$

Recall that the functions s, g, p and q depend on free values a_0, a_1 and a_2. Therefore we write the energy to indicate this dependence:

$$R_Q(u)=\tilde{R}_Q(a_0,a_1,a_2)=\frac{I_1+I_2+I_3+I_4}{I_5},$$

where

$$\begin{aligned}
I_1&=\int_0^{\pi/2}\int_0^{\infty}\left|\frac{\partial u}{\partial r}\right|^2 r\,dr\,d\theta\\
&=\int_0^{\pi/2}\frac{s^2(\theta)}{2s^2(\theta)}+\frac{g^2(\theta)}{2s^2(\theta)}+\frac{p^2(\theta)}{2s(\theta)}+\frac{q^2(\theta)}{s^3(\theta)}\\
&\quad+\frac{2\sqrt{\pi}g(\theta)p(\theta)}{4s(\theta)^{3/2}}+\frac{6\sqrt{\pi}g(\theta)q(\theta)}{8s(\theta)^{5/2}}+\frac{p(\theta)q(\theta)}{2s(\theta)^2}\,d\theta,\\
I_2&=\int_0^{\pi/2}\int_0^{\infty}\frac{1}{r^2}\left|\frac{\partial u}{\partial \theta}\right|^2 r\,dr\,d\theta\\
&=\int_0^{\pi/2}\frac{s'(\theta)}{8s(\theta)^2}+\frac{g'(\theta)^2}{8s(\theta)^2}+\frac{p'(\theta)^2}{2s(\theta)}+\frac{q'(\theta)^2}{9s(\theta)^3}\\
&\quad+\frac{g'(\theta)p'(\theta)\sqrt{\pi}}{4s(\theta)^{3/2}}+\frac{\sqrt{\pi}g'(\theta)q'(\theta)}{8s(\theta)^{5/2}}+\frac{p'(\theta)q'(\theta)}{3s(\theta)^2}\,d\theta,\\
I_3&=\int_0^{\pi/2}\int_0^{\infty}-\mathrm{Im}\left(\overline{u}\frac{\partial u}{\partial \theta}\right) r\,dr\,d\theta\\
&=\int_0^{\pi/2}-\frac{g'(\theta)}{2s(\theta)^2}-\frac{\sqrt{\pi}p'(\theta)}{4s(\theta)^{3/2}}-\frac{\sqrt{\pi}q'(\theta)}{8s(\theta)^{5/2}}\,d\theta,\\
I_4&=\int_0^{\pi/2}\int_0^{\infty}\frac{r^2}{4}|u|^2 r\,dr\,d\theta\\
&=\int_0^{\pi/2}\frac{1}{8s(\theta)^2}\,d\theta,\\
I_5&=\int_0^{\pi/2}\int_0^{\infty}|u|^2 r\,dr\,d\theta\\
&=\int_0^{\pi/2}\frac{1}{2s(\theta)}\,d\theta.
\end{aligned}$$

Through a laborious but straightforward use of elementary integration techniques, we find that each term above can be integrated in closed form. To give a feel for that process we include the ones appearing in I_1:

$$\int_0^{\pi/2}\frac{g(\theta)^2}{s(\theta)^2}\,d\theta=\frac{1}{a_0^2\,32}\left[-4\theta-\frac{11\arctan(\sqrt{(5/6)}\cot(2\theta))}{\sqrt{30}}-\frac{\sin(4\theta)}{2(5+\sin(2\theta)^2)}\right]_0^{\pi/2},$$

$$\int_0^{\pi/2} \frac{p(\theta)^2}{2s(\theta)}\,d\theta = \frac{a_1^2}{2\,a_0}\left[-\theta - \sqrt{\frac{3}{10}}\arctan\left(\sqrt{\frac{5}{6}}\cot(2\theta)\right)\right]_0^{\pi/2},$$

$$\int_0^{\pi/2} \frac{q(\theta)^2}{s(\theta)^3}\,d\theta = \frac{a_2^2}{8000\,a_0^3}\left[\frac{10\,523\,927\arctan(\sqrt{(5/6)}\cot(2\theta))}{30\sqrt{30}} - 1\,280\,000\theta + \frac{37249\sin(4\theta)}{(5+\sin(2\theta)^2)^2} - \frac{1368563\sin(4\theta)}{60(5+\sin(2\theta)^2)}\right]_0^{\pi/2},$$

$$\int_0^{\pi/2} \frac{\sqrt{\pi}g(\theta)p(\theta)}{2s(\theta)^{3/2}}\,d\theta = \frac{a_1\sqrt{\pi}}{8a_0^{3/2}}\left[-\frac{\cos(2\theta)}{\sqrt{5+\sin^2(2\theta)}} + \arctan\left(\frac{\cos(2\theta)}{\sqrt{5+\sin^2(2\theta)}}\right)\right]_0^{\pi/2},$$

$$\int_0^{\pi/2} \frac{3\sqrt{\pi}g(\theta)q(\theta)}{4s(\theta)^{5/2}}\,d\theta = \frac{3a_2\sqrt{\pi}}{16a_0^{5/2}}\left[\frac{-193\cos^3(2\theta)}{180(5+\sin^2(\theta))^{3/2}} + \frac{4\cos(2\theta)}{(5+\sin^2(2\theta))^{1/2}} - 4\arctan\left(\frac{\cos(2\theta)}{\sqrt{5+\sin^2(2\theta)}}\right)\right]_0^{\pi/2},$$

$$\int_0^{\pi/2} \frac{p(\theta)q(\theta)}{s(\theta)^2}\,d\theta = \frac{a_1a_2}{a_0^2}\left[4\theta + \frac{2207\arctan(\sqrt{5/6}\cot(2\theta))}{200\sqrt{30}} + \frac{193\sin(4\theta)}{400(5+\sin^2(2\theta))}\right]_0^{\pi/2}.$$

To find the desired minimum value, we feed the energy $\tilde{R}(a_0,a_1,a_2)$ into Mathematica and minimize over the parameters a_0, a_1 and a_2. The minimum is acheived at the values $a_0 = 0.051\,853$, $a_1 = -0.052\,868\,9$, and $a_2 = 0.031\,566$. Substituting these values into $\tilde{R}_Q(a_0,a_1,a_2)$, the value obtained is 0.577 23. ■

III. EXPONENTIAL DECAY

The main theorem of this section provides exponential decay for minimizers of the eigenvalue problem on the unit square in the regime $h \gg 1$. The argument is inspired by that used in the proof in Ref. 10, Theorems 3.1 and 4.3, and uses a blow-up argument. In Theorem 3.1 they prove that the minimizer decays exponentially away from the boundary of the half-plane, while in Theorem 4.3, they prove that a minimizer of the problem on any smooth bounded domain decays exponentially away from the boundary. Turning to the case of the unit square, however, we shall see that new issues emerge which lead us to confront the eigenvalue problems (2.9)–(2.17) introduced in the previous section. Recall that $\Gamma_D^1 = \{(x,y) \in \partial Q_1 : x = 1 \text{ or } y = 1\}$.

Theorem 3.1: *Let* $\{\Psi^h\}$ *be any sequence of eigenfunctions that minimize the energy*

$$\lambda(h) = \inf_{\substack{\Psi \in H^1(Q_1) \\ \Psi = 0 \text{ on } \Gamma_D^1}} \frac{\int_{Q_1} |(i\nabla + h\mathbf{A})\Psi|^2 dxdy}{\int_{Q_1} |\Psi|^2},$$

normalized so that $\|\Psi^h\|_{L^2(Q_1)} = 1$. *Then there exists a constant* $h_0 > 0$ *and for every multi-index* α, *there exist positive constants* c_1^α *and* c_2^α *independent of* h *such that*

$$|D^\alpha \Psi^h(z)| \leqslant (\sqrt{h})^{|\alpha|} c_1^\alpha e^{-c_2^\alpha \sqrt{h}|z|} \quad \text{for all} \quad z = (x,y) \in Q_1 \quad \text{and} \quad h \geqslant h_0.$$

Theorem 3.2: *Let* $\{\Psi^h\}$ *be any sequence of eigenfunctions that minimize the energy*

$$\lambda(h)=\inf_{\Psi\in H^1(Q_1)}\frac{\int_{Q_1}|(i\nabla+h\mathbf{A})\Psi|^2dxdy}{\int_{Q_1}|\Psi|^2},$$

normalized so that $\|\Psi^h\|_{L^2(Q_1)}=1$. *Then there exists a constant* $h_0>0$ *and for every multi-index* α, *there exist positive constants* c_1^α *and* c_2^α *independent of* h *such that*

$$|D^\alpha\Psi^h(z)|\leqslant(\sqrt{h})^{|\alpha|}c_1^\alpha e^{-c_2^\alpha\sqrt{h}\tilde{d}(z)}\quad \textit{for all}\quad z=(x,y)\in Q_1\quad \textit{and}\quad h\geqslant h_0,$$

where

$$\tilde{d}(z)=\min_{1\leqslant i\leqslant 4} dist(z,p_i)\quad \textit{and}\quad p_i\in\{(0,0),(1,0),(0,1),(1,1)\}.$$

Theorem 3.3: *Let* Ψ *be any bounded solution to* $(i\nabla+\mathbf{A})^2\Psi=\lambda\Psi$ *in the quarter-plane* $\mathbf{Q}$, *with* $(i\nabla+\mathbf{A})\Psi\cdot\nu=0$ *on* $\partial\mathbf{Q}$. *Then if* $\lambda<\lambda_{\mathbf{H}}$, *for every multi-index* α *there exist positive constants* c_1^α *and* c_2^α *such that*

$$|D^\alpha\Psi(z)|\leqslant c_1^\alpha e^{-c_2^\alpha|z|}\quad \textit{for all}\quad z\in\mathbf{Q}.$$

Proof of Theorem 3.1; Note that a minimizer on Q_1 is a weak solution of the Euler–Lagrange equation. By standard elliptic regularity, one finds Ψ^h is C^∞ in the interior of Q_1, and C^1 up to the boundary away from the corners. Furthermore, by an elementary reflection argument one can argue that $\Psi^h\in H^2(Q_1)$. Hence, Ψ^h is a bounded classical solution to the eigenvalue problem:

$$(i\nabla+h\mathbf{A})^2\Psi^h=\lambda(h)\Psi^h\quad \text{in}\quad Q_1, \tag{3.1}$$

$$(i\nabla+h\mathbf{A})\Psi^h\cdot\nu=0\quad \text{in}\quad \Gamma_N^1, \tag{3.2}$$

$$\Psi^h=0\quad \text{in}\quad \Gamma_D^1, \tag{3.3}$$

where $\Gamma_N^1=\{(x,y)\in\partial Q_1: x=0 \text{ or } y=0\}$, $\Gamma_D^1=\{(x,y)\in\partial Q_1: x=1 \text{ or } y=1\}$ and ν is the outer unit normal vector on Γ_N^1.

Since Ψ^h is bounded on $\overline{Q_1}$ we renormalize Ψ^h such that $\|\Psi^h\|_{L^\infty(Q_1)}=1$. Recall that by gauge invariance, choosing a different potential that satisfies (2.1) modifies Ψ^h by $e^{i\phi}$ for a suitable ϕ independent of h, hence the above exponential estimate is altered only by choosing different constants. Here it is convenient to choose $\mathbf{A}=(0,x)$.

Let $\Omega(k,h,R)=\{z\in Q_1:|z|\geqslant Rk/\sqrt{h}\}$ where k is a positive integer, $h>0$ and $R>0$. Of course for certain values of h,R and k $\Omega(k,h,R)$ will be empty. The exponential decay is equivalent to establishing the claim: There exist positive real numbers R_0 and h_0 such that

$$\|\Psi^h\|_{L^\infty(\Omega(k+1,h,R))}<\tfrac{1}{2}\|\Psi^h\|_{L^\infty(\Omega(k,h,R))} \tag{3.4}$$

for all $h\geqslant h_0$, all $R\geqslant R_0$ and all positive integers k such that $\Omega(k+1,h,R)$ is nonempty.

Proceeding by contradiction, we assume there exist sequences $R_j\to\infty$, $h_j\to\infty$ and a sequence of positive integers k_j such that $\Omega(k_j+1,h_j,R_j)$ is nonempty and

$$\|\Psi^{h_j}\|_{L^\infty(\Omega(k_j+1,h_j,R_j))}\geqslant\tfrac{1}{2}\|\Psi^{h_j}\|_{L^\infty(\Omega(k_j,h_j,R_j))}\equiv\tfrac{1}{2}m_j. \tag{3.5}$$

Define $\tilde{\Psi}^{h_j}$ by

$$\tilde{\Psi}^{h_j}(z)=\frac{\Psi^{h_j}}{m_j}.$$

Notice that for all j

$$\|\tilde{\Psi}^{h_j}\|_{L^\infty(\Omega(k_j,h_j,R_j))}=1 \tag{3.6}$$

and

$$\tfrac{1}{2}\leqslant\|\tilde{\Psi}^{h_j}\|_{L^\infty(\Omega(k_j+1,h_j,R_j))}\leqslant 1. \tag{3.7}$$

Now, (3.7) allows us to choose z_j in $\Omega(k_j+1,h_j,R_j)$ such that

$$|\tilde{\Psi}^{h_j}(z_j)|\geqslant\tfrac{1}{2}. \tag{3.8}$$

From this point we proceed to use $\tilde{\Psi}^{h_j}$ to define a sequence of uniformly bounded nonvanishing functions on bigger and bigger balls, half-balls and quarter-balls to cover $\mathbf{R}^2$, $\mathbf{H}$, and $\mathbf{Q}$, respectively. Eventually, we want to establish compactness of this sequence to obtain a limit function that leads to a contradiction of condition (3.5).

To ensure that the sequence is nonvanishing we want our blow-ups to include the points z_j, since $\tilde{\Psi}^{h_j}(z_j)$ is bounded away from zero by (3.8). Therefore we focus on the location of z_j inside Q_1, in particular its distance from the boundary of Q_1 and the corners on the boundary. By the definition of $\Omega(k_j,h_j,R_j)$, we find this situation is best described by the quantities $\sqrt{h_j}\,\mathrm{dist}(z_j,\partial Q_1)$ and $\sqrt{h_j}\,\mathrm{dist}(z_j,p)$ where p is a corner point on the boundary. Taking the limit of these quantities, there are only three possibilities:

(1) $\lim_{h_j\to\infty}\sqrt{h_j}\,\mathrm{dist}(z_j,\partial Q_1)=\infty$.
(2) There exists a positive constant C_1 such that $\mathrm{dist}(z_j,\partial Q)\leqslant C_1/\sqrt{h_j}$ and $\lim_{h_j\to\infty}\sqrt{h_j}\,\mathrm{dist}(z_j,p)=\infty$, where p is any of the corner points on ∂Q_1.
(3) There exists a positive constant C_2 and a corner point $p_0\in\{(1,0),(0,1),(1,1)\}$ such that $\mathrm{dist}(z_j,p_0)\leqslant C_2/\sqrt{h_j}$.

We attempt to draw balls, half-balls or quarter-balls containing z_j as each case above allows. We have two concerns; one is to ensure that the functions inherit uniform boundedness via (3.6). This is attained by making sure that these sets containing z_j are subsets of $\Omega(k_j,h_j,R_j)$. The other concern is that these sets, when blown-up, should increase in size in order to cover the unbounded set $\mathbf{R}^2$, $\mathbf{H}$, or $\mathbf{Q}$.

The case (1) is very similar to the case dealt with in Ref. 10, Theorem 4.3. We only describe the spirit of the argument and work out more detail in the case (2). The condition given in (1) implies that the sequence is away from the boundary or approaches the boundary slowly. Hence we can take a ball centered at z_j with radius $\tilde{R}_j/\sqrt{h_j}$ where $\tilde{R}_j=\min\{R_j,\sqrt{h_j}\mathrm{dist}(z_j,\partial Q_1)\}$. Note that as $j\to\infty$, the balls $B(0,\tilde{R}_j)$ cover $\mathbf{R}^2$.

We define the sequence functions $f_j:B(0,\tilde{R}_j)\to\mathbf{C}$ by

$$f_j(x,y)=\tilde{\Psi}_j\left(\frac{x}{\sqrt{h_j}}+x_j,\frac{y}{\sqrt{h_j}}+y_j\right)e^{-i\sqrt{h_j}\,x_j\,y},$$

where $z_j=(x_j,y_j)$. Notice that by (3.6) and (3.8)

$$|f_j(0,0)|=|\tilde{\Psi}_j(z_j)|\geqslant\tfrac{1}{2}\quad\text{and}\quad\|f_j\|_{B(0,\tilde{R}_j)}\leqslant 1.$$

Moreover, f_j solves the PDE:

$$(i\nabla+\mathbf{A})^2 f_j=\frac{\lambda(h_j)}{h_j}f_j\ \text{ in }\ B(0,\tilde{R}_j). \tag{3.9}$$

Using the PDE (3.9) and standard elliptic regularity estimates on any fixed ball $B(0,S)$, one finds the sequence is compact in $C^2(B(0,S))$. Hence through a diagonalization argument, one can extract a subsequence that converges in C^2 on compact subsets of $\mathbf{R}^2$ to a function f_∞ that solves the PDE:

$$(i\nabla+\mathbf{A})^2 f_\infty = \lim_{h_j\to\infty} \frac{\lambda(h_j)}{h_j} f_\infty \quad \text{in } \mathbf{R}^2.$$

In light of Lemma 2.2, Lemma 2.7(ii) and Remark 2.8, $\lim_{h_j\to\infty}\lambda(h_j)/h_j<1$. This contradicts Lemma 2.10(i) and hence contradicts the inequality in (3.5).

Moving on to the next scenario, condition (2), we see the sequence $\{z_j\}$ must have a limit point on either Γ_N^1 or Γ_D^1. We will treat the case when the sequence is approaching the side $\{(0,y):0<y\leqslant 1\}\subset\Gamma_N^1$ in detail. The other side of Γ_N^1 is treated similarly. Afterwards, we will briefly comment on the case when the sequence is approaching Γ_D^1.

Suppose $z_j=(x_j,y_j)$ is approaching the side $\Gamma^1_{N,\text{left}}=\{(0,y)\in\partial Q_1:0<y<1\}$ or perhaps the corner point (0,1). Condition (2) implies that for j sufficiently large

$$x_j=\text{dist}(z_j,\Gamma^1_{N,\text{left}})<\frac{C_1}{\sqrt{h_j}}<\min\left\{\frac{R_j}{2\sqrt{h_j}},1-y_j\right\}. \tag{3.10}$$

We draw half-balls centered at the point $(0,y_j)$ with a radius $\tilde{R}_j/\sqrt{h_j}$ where $\tilde{R}_j=\min\{R_j/2,\sqrt{h_j}(1-y_j)\}$. Again notice that $\tilde{R}_j\to\infty$ as $j\to\infty$ so that the half-balls when blown up will cover the half-plane $\mathbf{H}$ and that the half-balls are inside $\Omega(k_j,h_j,R_j)\subset Q_1$.

We use the conventional notation for a half-ball of radius r, $B^+(0,r)=\{(x,y)\in B(0,r):x\geqslant 0\}$.

Now we define $f_j:B^+(0,\tilde{R}_j)\to\mathbf{C}$ by

$$f_j(x,y)=\tilde{\Psi}_j\left(\frac{x}{\sqrt{h_j}},\frac{y}{\sqrt{h_j}}+y_j\right).$$

Note that $(\sqrt{h_j}x_j,0)\in B^+(0,C_1)$ by (3.10). As a consequence of this and of (3.8), $|f_j(\sqrt{h_j}x_j,0)|=|\tilde{\Psi}_j(z_j)|\geqslant\frac{1}{2}$. Hence,

$$\sup_{B^+(0,C_1)}|f_j|\geqslant\tfrac{1}{2}. \tag{3.11}$$

In addition (3.6) leads to a uniform bound on f_j:

$$\|f_j\|_{L^\infty(B^+(0,\tilde{R}_j))}\leqslant 1. \tag{3.12}$$

Furthermore, f_j satisfies the equation

$$(i\nabla+\mathbf{A})^2 f_j=\frac{\lambda(h_j)}{h_j}f_j \quad \text{on } B^+(0,\tilde{R}_j), \tag{3.13}$$

$$(i\nabla+\mathbf{A})f_j\cdot\nu=0 \quad \text{on } \Gamma_N^{B^+}, \tag{3.14}$$

where $\Gamma_N^{B^+}=\{(x,y)\in\partial B^+(0,\tilde{R}_j):x=0\}$.

Now our objective is to show that the sequence f_j is compact in order to extract a subsequence that converges uniformly on compact subsets of $\mathbf{H}$. To that end we fix a half-ball $B^+(0,S)$. Let χ be a smooth cutoff function such that $\chi\equiv 1$ on the ball $B(0,S-1)$, $\chi\equiv 0$ on $\mathbf{H}-B(0,S)$ and $|\nabla\chi|\leqslant 2$.

We suppress the j index, multiply the PDE (3.13) by $\chi^2\overline{f}$ (where $\overline{f}$ is the complex conjugate of f), and integrate by parts to obtain

$$\int_{B^+(0,S)}\chi^2|\nabla f|^2+2\overline{f}\chi\nabla\chi\cdot\nabla f+\chi^2(2ix\overline{f}f_y+x^2|f|^2)dxdy=\frac{\lambda(h)}{h}\int_{B^+(0,S)}\chi^2|f|^2dxdy. \tag{3.15}$$

In integrating by parts one makes use of the Neumann boundary condition on $\Gamma_N^{B^+}$ and that χ vanishes on the rounded part of $B^+(0,S)$. Using the Cauchy–Schwartz inequality, the uniform bound on f, the local boundedness of $\mathbf{A}$ and χ, and boundedness of $\lambda(h)/h$ (Remark 2.6), we find for some positive constants C_1 and C_2

$$\int_{B^+(0,S-1)}|\nabla f|^2dxdy\leqslant C_1(S)\left(\int_{B^+(0,S-1)}|\nabla f|^2dxdy\right)^{1/2}+C_2(S). \tag{3.16}$$

With this and (3.12) we conclude that there is a constant $C(S)$ that does not depend on h such that

$$\|f\|_{H^1(B^+(0,S-1))}<C(S). \tag{3.17}$$

Reverting back to the notation f_j, we write $f_j=u_j+iv_j$ and express the PDE (3.13) as a system:

$$-\Delta u_j=2\mathbf{A}\cdot\nabla v_j-|\mathbf{A}|^2u_j+\frac{\lambda(h_j)}{h_j}u_j, \tag{3.18}$$

$$-\Delta v_j=2\mathbf{A}\cdot\nabla u_j-|\mathbf{A}|^2v_j+\frac{\lambda(h_j)}{h_j}v_j. \tag{3.19}$$

Since u_j and v_j are in $H^1(B^+(0,S-1))$, then by standard interior elliptic estimates, bootstrapping and Sobolev embedding we conclude that $f_j\in C^{2,\alpha}(\tilde{B}^+(0,S-1))$, where

$$\tilde{B}^+(0,S-1)=B^+(0,S-1)-\left\{(x,y)\in B^+(0,S-1):x<\frac{1}{S}\right\}.$$

Moreover, using boundary regularity estimates (cf. Ref. 22), bootstrapping and Sobolev embedding we obtain an estimate on the $C^{1,\alpha}(\overline{B^+(0,S-1)})$ norm of u_j+iv_j, where the estimate is independent of j. With regularity and uniform boundedness (3.12) we find f_j is a compact sequence in $C^{2,\alpha}(\tilde{B}^+(0,S-1))\cap\ C^{1,\alpha}(\overline{B^+(0,S-1)})$.

Using a standard diagonalization argument one obtains a subsequence converging on compact subsets of $\mathbf{H}$ to a function $f_\infty\in C^{2,\alpha}(\mathbf{H})\cap C^1(\overline{\mathbf{H}})$. This limit function, f_∞ solves the problem

$$-\Delta f_\infty+2i\mathbf{A}\cdot\nabla f_\infty+|\mathbf{A}|^2f_\infty=\lim_{j\to\infty}\frac{\lambda(h_j)}{h_j}f_\infty\ \text{ in }\ \mathbf{H}, \tag{3.20}$$

$$(i\nabla+\mathbf{A})f_\infty\cdot\nu=0\quad\text{ on }\ \partial\mathbf{H}. \tag{3.21}$$

Moreover, (3.11) implies

$$\sup_{\mathbf{H}}|f_\infty|\geqslant\tfrac{1}{2}.$$

Thus, f_∞ is a bounded nontrivial classical solution of the eigenvalue problem (3.20) and (3.21). By Theorem 2.7 *(ii)*, $\lim_{j\to\infty}\lambda(h_j)/h_j<\lambda_H$. On the other hand, Lemma 2.10 *(ii)* asserts that there is no such nontrivial bounded solution for the problem (3.20) and (3.21) in $\mathbf{H}$. Hence condition (3.5) is again contradicted.

If the sequence $\{z_j\}$ is approaching Γ_D^1 on which the Dirichlet condition holds, we follow the same lines as above with a slight difference. We find f_∞ that solves the problem (2.9) and (2.10) with $\lambda=\lim_{h_j\to\infty}\lambda(h_j)/h_j$. We invoke Lemma 2.9 *(ii)* and Lemma 2.10 *(iii)* to get the contradiction in this case.

In the case condition (3) holds, we assume first that $p_0=(1,0)$. Here we will draw quarter-balls centered at p_0.

We denote a quarter-ball centered at the origin with radius r by $B^q(0,r)=B(0,r)\cap\{(x,y):x\leqslant 0,y\geqslant 0\}$.

We define $f_j:B^q(0,R_j)\to\mathbf{C}$ by

$$f_j(x,y)=\tilde{\Psi}_j\left(1+\frac{x}{\sqrt{h_j}},\frac{y}{\sqrt{h_j}}\right)e^{-i\sqrt{h_j}y}.$$

Note that condition (3) implies that $(\sqrt{h_j}(x_j-1),\sqrt{h_j}y_j)\in B^q(0,C_2)$. So at these points

$$|f_j(\sqrt{h_j}(x_j-1),\sqrt{h_j}y)|=|\tilde{\Psi}_j(z_j)|\geqslant\tfrac{1}{2}.$$

Hence,

$$\sup_{B^q(0,C_2)}|f_j|\geqslant\tfrac{1}{2}. \tag{3.22}$$

Moreover, the f_j's are uniformly bounded with

$$\|f_j\|_{L^\infty(B^q(0,R_j))}\leqslant 1. \tag{3.23}$$

In addition, f_j solves the problem

$$(i\nabla+\mathbf{A})^2 f_j=\frac{\lambda(h_j)}{h_j}f_j \text{ in } B^q(0,R_j), \tag{3.24}$$

$$(i\nabla+\mathbf{A})f_j\cdot\nu=0 \text{ on } \{(x,0):-R_j<x<0\}, \tag{3.25}$$

$$f_j=0 \text{ on } \{(0,y):0<y<R_j\}. \tag{3.26}$$

Again we wish to establish compactness of the sequence $\{f_j\}$. To reach this goal, we follow the same approach as in dealing with condition (2). We find that for any fixed quarter-ball $B^q(0,S)$

$$\|f_j\|_{H^1(B^q(0,S-1))}\leqslant C(S). \tag{3.27}$$

We once again apply interior and global elliptic regularity theory to the problem (3.24)–(3.26). One finds uniform bounds on $\{f_j\}$ in $C^{2,\alpha}(\tilde{B}^q(0,S))\cap C^{1,\alpha}\hat{B}^q(0,S))\cap H^2(B^q(0,S-1))$, where

$$\tilde{B}^q(0,S-1)=B^q(0,S-1)-\left\{(x,y):x<\frac{1}{S}\text{ or }y<\frac{1}{S}\right\}$$

and

$$\hat{B}^q(0,S-1)=B^q(0,S-1)-B^q\left(0,\frac{1}{S}\right).$$

Using a diagonalization argument on bigger and bigger quarter-balls one can find a subsequence that converges on compact subsets of the left quarter-plane to a function f_∞. Since the problem is invariant under a 270° counter-clockwise rotation, so that **A** still satisfies (2.1), we may replace the left quarter-plane with the right quarter-plane **Q**. Thus, f_∞ solves

$$(i\nabla+\mathbf{A})^2 f_\infty = \lim_{h_j\to\infty} \frac{\lambda(h_j)}{h_j} f_\infty \quad \text{in} \quad \mathbf{Q}, \tag{3.28}$$

$$(i\nabla+\mathbf{A}) f_\infty \cdot \nu = 0 \quad \text{on} \quad \Gamma_N, \tag{3.29}$$

$$f_\infty = 0 \quad \text{on} \quad \Gamma_D, \tag{3.30}$$

and in light of (3.22) and (3.23), f_∞ satisfies

$$\sup_{\mathbf{Q}} |f_\infty| \geqslant \tfrac{1}{2} \quad \text{while} \quad \|f_\infty\|_{L^\infty(\mathbf{Q})} \leqslant 1.$$

These make f_∞ a nontrivial bounded classical solution to the eigenvalue problem (2.15)–(2.17) with $\lambda = \lim_{h_j\to\infty} \lambda(h_j)/h_j$. This contradicts Lemma 2.10(iv) since by Theorem 2.7 and Lemma 2.9(i), $\lim_{h_j\to\infty} \lambda(h_j)/h_j < \lambda_{QM}$.

In case $p_0=(0,1)$ the argument is similar to the above case. On the other hand, when $p_0=(1,1)$, our treatment leads us to a limit function that solves the problem (2.12) and (2.13) with Dirichlet boundary conditions on both sides. In this case we invoke Lemma 2.9(i) and Lemma 2.10(v) to reach a contradiction to condition (3.5). Thus claim (3.4) is established.

By this we have completed the proof of the exponential decay estimate:

$$|\Psi^h(z)| \leqslant c_1 e^{c_2\sqrt{h}|z|} \quad \text{for all} \quad z \in Q_1 \tag{3.31}$$

for some positive constants c_1 and c_2.

To obtain exponential decay of higher derivatives using (3.31) one follows the method used in Ref. 10. ■

Proof of Theorem 3.2: The proof is similar to the one above. The minimizers Ψ^h solve the eigenvalue problem;

$$(i\nabla+h\mathbf{A})^2\Psi^h = \lambda(h)\Psi^h \quad \text{in} \quad Q_1, \tag{3.32}$$

$$(i\nabla+h\mathbf{A})\Psi\cdot\nu = 0 \quad \text{on} \quad \partial Q_1. \tag{3.33}$$

This results in replacing the $\Omega(k,h,R)$ by the sets $\tilde{\Omega}(k,h,R)=\{z\in Q_1 : \tilde{d}(z) < Rk/\sqrt{h}\}$. Notice that the argument in the proof of Theorem 3.1 follows as above in obtaining the sequence $\{z_j\}$. We find that among the three conditions listed when taking the limit of the quantity $\sqrt{h_j}\,\mathrm{dist}(z,\partial Q_1)$, we are only confronted with conditions (1) and (2). Since only the Neumann condition holds on the boundary, we need only invoke Theorem 2.7 and Lemma 2.10(i) and (ii) to get a contradiction of a condition equivalent to (3.5). ■

Proof of Theorem 3.3: This is again proved by the blow-up technique, but it is easier than the previous two results. See the proof of Ref. 10, Theorem 3.1 for a similar argument. ■

IV. EXISTENCE OF A MINIMIZER

Theorem 4.1: *There exists a function $\Psi_\infty \in H^1(\mathbf{Q})$ that minimizes the energy*

$$\lambda_{\mathbf{Q}} \equiv \inf_{\Psi\in H^1(\mathbf{Q})} \frac{\int_{\mathbf{Q}} |(i\nabla+\mathbf{A})\Psi|^2 dxdy}{\int_{\mathbf{Q}} |\Psi|^2 dxdy}.$$

In particular, Ψ_∞ satisfies the PDE and the boundary conditions:

$$(i\nabla+\mathbf{A})^2\Psi=\lambda_Q\Psi \quad \text{in } \mathbf{Q}, \tag{4.1}$$

$$(i\nabla+\mathbf{A})\Psi\cdot\nu=0 \quad \text{on } \partial\mathbf{Q}. \tag{4.2}$$

Moreover, for every multi-index α, there exist positive constants c_1^α and c_2^α such that

$$|D^\alpha\Psi(z)|\leqslant c_1^\alpha e^{-c_2^\alpha|z|} \quad \text{for all } z\in\mathbf{Q}.$$

Proof: We obtain a minimizing sequence by considering $\{\Psi^h\}$, the set of minimizers of the variational problem (2.6). These exist by the direct method of the calculus of variations. Each is a classical solution of the eigenvalue problem:

$$(i\nabla+\mathbf{A})^2\Psi^h=\frac{\lambda(h)}{h}\Psi^h \quad \text{in } Q_{\sqrt{h}},$$

$$(i\nabla+\mathbf{A})\Psi^h\cdot\nu=0 \quad \text{on } \Gamma_N^{\sqrt{h}}, \tag{4.3}$$

$$\Psi^h=0 \quad \text{on } \Gamma_D^{\sqrt{h}}.$$

Again, we find that Ψ^h is in C^∞ inside $Q_{\sqrt{h}}$, C^1 up to the boundary of $Q_{\sqrt{h}}$ away from the corners and in $H^2(Q_{\sqrt{h}})$, hence bounded on the closure of $Q_{\sqrt{h}}$. Thus, we can renormalize Ψ^h so that

$$\|\Psi^h\|_{L^\infty}=1. \tag{4.4}$$

In addition, through the rescaling $\tilde{z}=\sqrt{h}\,z$, one can define $\tilde{\Psi}^h:Q_1\to\mathbf{C}$ by $\tilde{\Psi}^h(z)=\Psi^h(\tilde{z})$. Then $\tilde{\Psi}^h$ minimizes the h-dependent Rayleigh quotient (2.5) on Q_1. By Theorem 3.1 $\tilde{\Psi}$ obeys the exponential decay estimate for an h-independent constants c_1^α and c_2^α:

$$|D^\alpha\tilde{\Psi}^h(z)|\leqslant c_1^\alpha e^{-c_2^\alpha\sqrt{h}|z|} \quad \forall z\in Q_1$$

for every multi-index α and sufficiently large h.

Via the chain rule we have

$$D_{\tilde{z}}^\alpha\Psi^h(\tilde{z})=D_z^\alpha\tilde{\Psi}^h(z)(\sqrt{h})^{|\alpha|}.$$

Hence we have the estimate for Ψ^h on $Q_{\sqrt{h}}$:

$$|D^\alpha\Psi^h(z)|\leqslant c_1^\alpha e^{-c_2^\alpha|z|} \quad \forall z\in Q_{\sqrt{h}}, \tag{4.5}$$

for h sufficiently large.

From (4.5) we see that a subsequence of $\{\Psi^h\}$ will converge in $C^{2,\alpha}$ on compact subsets of $\mathbf{Q}$. Denoting this limit by Ψ_∞, we see that Ψ_∞ is a classical solution of the problem

$$(i\nabla+\mathbf{A})^2\Psi_\infty=\lim_{h_j\to\infty}\frac{\lambda(h_j)}{h_j}\Psi_\infty \quad \text{in } \mathbf{Q}, \tag{4.6}$$

$$(i\nabla+\mathbf{A})\Psi_\infty\cdot\nu=0 \qquad \text{on } \partial\mathbf{Q}. \tag{4.7}$$

Furthermore, in light of the uniform convergence of the subsequence of $\{\Psi^h\}$ on compact subsets of $\mathbf{Q}$, along with the exponential decay estimate (4.5), one obtains the same exponential decay estimate on Ψ_∞:

$$|D^{\alpha}\Psi_{\infty}(z)| \leq c_1^{\alpha} e^{-c_2^{\alpha}|z|} \quad \forall z \in \mathbf{Q}. \tag{4.8}$$

In particular, this shows that $\Psi_{\infty} \in H^1(\mathbf{Q})$, hence it is a competitor for the Rayleigh quotient on $\mathbf{Q}$.

To complete the proof, it remains to show that Ψ_{∞} is a minimizer and therefore

$$\lambda_{\mathbf{Q}} = \lim_{h_j \to \infty} \frac{\lambda(h_j)}{h_j} \tag{4.9}$$

(cf. Remark 2.6). Recalling the notation

$$R_{\Omega}(\phi) = \frac{\int_{\Omega} |(i\nabla + \mathbf{A})\phi|^2 dxdy}{\int_{\Omega} |\phi|^2 dxdy},$$

note that Ψ_{∞} will minimize if

$$R_{\mathbf{Q}}(\Psi_{\infty}) = \inf_{\phi \in H^1(Q)} R_{\mathbf{Q}}(\phi). \tag{4.10}$$

Proceeding by contradiction to establish (4.10), fix $\epsilon_0 > 0$, and, using the density of $C_0^{\infty}(\mathbf{Q})$ in $H^1(\mathbf{Q})$, suppose there is an $\eta \in C_0^{\infty}(\mathbf{Q})$ such that

$$R_{\mathbf{Q}}(\Psi_{\infty}) = R_{\mathbf{Q}}(\eta) + \epsilon_0. \tag{4.11}$$

Then we choose h_1 sufficiently large such that

(1) $spt(\eta) \subset Q_{h_1}$,

(2) $|R_Q(\Psi_{\infty}) - R_{Q_{\sqrt{h_1}}}(\Psi_{\infty})| < \frac{1}{2}\epsilon_0$, and

(3) $\forall h > h_1$,

$$|R_{Q_{\sqrt{h}}}(\Psi^h) - R_{Q_{\sqrt{h_1}}}(\Psi^h)| < \tfrac{1}{4}\epsilon_0. \tag{4.12}$$

Note that conditions (2) and (3) follow from the exponential decay estimates.

Now $\Psi^{h_1} \in H^1(Q_{\sqrt{h_1}})$ and can be extended to be identically zero outside $Q_{\sqrt{h_1}}$. Therefore, Ψ^{h_1} can be seen as a competitor on $Q_{\sqrt{h}}$ for $h > h_1$. Moreover, recall that Ψ^h is a minimizer of the eigenvalue problem on $Q_{\sqrt{h}}$ for all $h > 0$. Hence,

$$R_{Q_{\sqrt{h}}}(\Psi^h) \leq R_{Q_{\sqrt{h}}}(\Psi^{h_1}) = R_{Q_{\sqrt{h_1}}}(\Psi^{h_1}). \tag{4.13}$$

Since η is a competitor and Ψ^{h_1} is a minimizer for the problem on $Q_{\sqrt{h_1}}$, we have

$$R_{Q_{\sqrt{h_1}}}(\Psi^{h_1}) \leq R_{Q_{\sqrt{h_1}}}(\eta) = R_Q(\eta), \tag{4.14}$$

where the last equality is due to our choice of η with $\mathrm{spt}(\eta) \subset Q_{\sqrt{h_1}}$. Then by (4.11) and condition (2) in the choice of h_1, we find

$$R_{Q_{\sqrt{h_1}}}(\Psi^{h_1}) \leq R_Q(\Psi_{\infty}) - \epsilon_0 \tag{4.15}$$

$$\leq R_{Q_{\sqrt{h_1}}}(\Psi_{\infty}) + \frac{\epsilon_0}{2} - \epsilon_0 \tag{4.16}$$

$$= R_{Q_{\sqrt{h_1}}}(\Psi_{\infty}) - \frac{\epsilon_0}{2}. \tag{4.17}$$

Now combining (4.13) and (4.17) along with (4.12) we have

$$R_{Q_{\sqrt{h_1}}}(\Psi^h) < R_{Q_{\sqrt{h_1}}}(\Psi_\infty) - \frac{\epsilon_0}{4} \quad \forall h > h_1. \tag{4.18}$$

Since $\Psi^h \to \Psi_\infty$ uniformly in $C^{2,\alpha}(Q_{\sqrt{h_1}})$ we have

$$R_{Q_{\sqrt{h_1}}}(\Psi^h) \to R_{Q_{\sqrt{h_1}}}(\Psi_\infty) \text{ as } h \to \infty.$$

Then, taking the limit in (4.18) we obtain

$$R_{Q_{\sqrt{h_1}}}(\Psi_\infty) < R_{Q_{\sqrt{h_1}}}(\Psi_\infty) - \frac{\epsilon_0}{4},$$

a contradiction. Therefore,

$$\lambda_{\mathbf{Q}} = \lim_{h_j \to \infty} \frac{\lambda(h_j)}{h_j} \quad \text{and} \quad R_{\mathbf{Q}}(\Psi_\infty) = \lambda_{\mathbf{Q}},$$

i.e., Ψ_∞ is a minimizer. ■

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Two- and three-dimensional Hamiltonians with shape invariance symmetry

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Via a special dimensional reduction, that is, Fourier transforming over one of the coordinates of Casimir operator of su(2) Lie algebra and 4-oscillator Hamiltonian, we have obtained two- and three-dimensional Hamiltonian with shape invariance symmetry. Using this symmetry we have obtained their eigenspectrum. In the mean time we show equivalence of shape invariance symmetry and Lie algebraic symmetry of these Hamiltonians. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Exactly solvable quantum Hamiltonians (ESQH) have always attracted a lot of interest in theoretical physics and mathematical physics. Hence, construction of exactly solvable models is of great interest.[1–6] Familiar solvable potentials (particularly one-dimensional potentials) have the property of shape invariance. For these potentials, eigenvalues and eigenvectors can be derived using well-known methods of supersymmetric quantum mechanics together with shape invariant factorization. The majority of potentials have also been shown to poses a Lie algebraic symmetry and hence are also solvable by group theoretical techniques. Actually one can establish a connection between ESQH with shape invariance symmetry and ESQH with Lie algebraic symmetry and one can show that they are indeed equivalent.[7,8] One of the authors could give some two- and three-dimensional shape invariant Hamiltonians.[9–11] In these papers they have shown that the shape invariance symmetry of these models is due to existence of some Lie algebraic symmetry. Hence in this paper we construct new two- and three-dimensional (EQSH) with shape invariance symmetry, where su(2) and Heisenberg algebra are responsible for the existence of shape invariance symmetry in them.

This paper is organized as follows: In Sec. II, using the left and right invariant vector fields of su(2) Lie algebra we first construct its Casimir operator. Then via Fourier transformation over one of the coordinates we construct the two-dimensional Hamiltonian $H_q(\theta,\psi)$ which poses shape invariance symmetry. Using this symmetry we obtain its eigenspectrum analytically. In Sec. III starting with a Hamiltonian of 4-oscillator and Fourier transforming over one of the coordinates we obtain a three-dimensional Hamiltonian corresponding to motion of a charged particle in the presence of an electric field. We show that this three-dimensional Hamiltonian poses a shape invariance symmetry and using this symmetry we obtain its eigenspectrum. What is so important in both models, is that both Hamiltonians factorize shape invariantly into product of second order differential operators. These second order operators themselves consist of the product of first order differential operators. The paper ends with a brief conclusion.

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II. TWO-DIMENSIONAL HAMILTONIAN OBTAINED FROM SU(2) MANIFOLD

A. Left and right invariant vector field of SU(2)

Considering the following parametrization of su(2) group manifold,[12]

$$\begin{aligned}\Lambda &= \exp(i\vec{\sigma}\cdot\vec{n}\psi)\\ &= A\begin{pmatrix}\exp(i\psi) & 0\\ 0 & \exp(-i\psi)\end{pmatrix}A^{-1}\\ &= \begin{pmatrix}\cos(\psi)-i\cos(\theta)\sin(\psi) & -i\sin(\theta)\sin(\psi)\exp(-i\phi)\\ -i\sin(\theta)\sin(\psi)\exp(i\phi) & \cos(\psi)+i\cos(\theta)\sin(\psi)\end{pmatrix},\end{aligned} \tag{2.1}$$

where σ_i, $i=1$, 2, and 3 are used Pauli matrices and $\vec{n}$ is unit vector defined as

$$\vec{n}=\sin(\theta)\cos(\phi)\vec{i}+\sin(\theta)\sin(\phi)\vec{j}+\cos(\theta)\vec{k}$$

and matrix A corresponds to coherent state representation of su(2) defined as[13]

$$A=\begin{pmatrix}1 & \tau\\ 0 & 1\end{pmatrix}\begin{pmatrix}\exp\left(\frac{\beta}{2}\right) & 0\\ 0 & \exp\left(\frac{-\beta}{2}\right)\end{pmatrix}\begin{pmatrix}1 & 0\\ -\tau^{\star} & 1\end{pmatrix},$$

with $\tau=\tan(\theta/2)\exp(-i\phi)$ and $\beta=\ln(1+\tau\tau^{\star})$.

In order to obtain the left and right invariant vector field su(2) manifold with the above parametrization, it is convenient first to calculate its left and right invariant one form defined as $\Lambda^{-1}d\Lambda$ and $d\Lambda\,\Lambda^{-1}$, respectively.[14]

As an example, writing left invariant one form

$$\Lambda^{-1}d\Lambda=e_{\alpha}^{a}\,d\xi^{\alpha}\,\sigma_a,$$

where e_{α}^{a} are 3-beins and $\xi^{\alpha}=(\theta,\phi,\psi)$ are coordinates of su(2) manifold. Defining the inverse of 3-bein $e_{a}^{\alpha}=g^{\alpha\beta}\delta_{ab}e_{\beta}^{b}$ with $g^{\alpha\beta}$ as inverse of metric $g_{\alpha\beta}$:

$$g_{\alpha,\beta}=\begin{pmatrix}1 & 0 & 0\\ 0 & \sin^2(\psi) & 0\\ 0 & 0 & \sin^2(\psi)\sin^2(\theta)\end{pmatrix},$$

then the left invariant vector fields are defined as

$$L_a=e_{a}^{\alpha}\frac{\partial}{\partial\xi^{\alpha}}.$$

Using the above prescription we obtain the following expression for left and right invariant vector fields of su(2), respectively:

$$L_{+}=\frac{i}{2}e^{i\phi}\left[\sin(\theta)\partial_{\psi}+(i+\cos(\theta)\cot(\psi))\partial_{\theta}+\left(-\cot(\theta)+i\frac{\cot(\psi)}{\sin(\theta)}\right)\partial_{\phi}\right], \tag{2.2}$$

$$L_{-}=\frac{i}{2}e^{-i\phi}\left[\sin(\theta)\partial_{\psi}+(-i+\cos(\theta)\cot(\psi))\partial_{\theta}+\left(-\cot(\theta)-i\frac{\cot(\psi)}{\sin(\theta)}\right)\partial_{\phi}\right], \tag{2.3}$$

$$L_3=\frac{i}{2}(-\cos(\theta)\partial_\psi+\sin(\theta)\cot(\psi)\partial_\theta-\partial_\phi), \tag{2.4}$$

$$R_+=\frac{i}{2}e^{i\phi}\left[\sin(\theta)\partial_\psi+(-i+\cos(\theta)\cot(\psi))\partial_\theta+\left(\cot(\theta)+i\frac{\cot(\psi)}{\sin(\theta)}\right)\partial_\phi\right], \tag{2.5}$$

$$R_-=\frac{i}{2}e^{-i\phi}\left[\sin(\theta)\partial_\psi+(i+\cos(\theta)\cot(\psi))\partial_\theta+\left(\cot(\theta)-i\frac{\cot(\psi)}{\sin(\theta)}\right)\partial_\phi\right], \tag{2.6}$$

$$R_3=\frac{i}{2}(-\cos(\theta)\partial_\psi+\sin(\theta)\cot(\psi)\partial_\theta+\partial_\phi), \tag{2.7}$$

where $L_\pm=L_1\pm iL_2$ and $R_\pm=R_1\pm iR_2$. It is straightforward to show that the left and right invariant vector fields fulfill the following su(2) Lie algebra:

$$[L_+,L_-]=2L_3,\quad [L_3,L_\pm]=\pm L_\pm, \tag{2.8}$$

$$[R_+,R_-]=-2R_3,\quad [R_3,R_\pm]=\mp R_\pm, \tag{2.9}$$

also, the left and right invariant generator commute with each other

$$[\vec{L},\vec{R}]=0. \tag{2.10}$$

Considering the Casimir operators of su(2) defined as

$$L^2=\tfrac{1}{2}(L_+L_-+L_-L_+)+L_3^2,$$

and ignoring the scale 1/4, we obtain

$$L^2=-\frac{1}{\sin^2(\psi)}\partial_\psi\sin^2(\psi)\partial_\psi-\frac{1}{\sin^2(\psi)}\left(\frac{1}{\sin(\theta)}\partial_\theta\sin(\theta)\partial_\theta+\frac{1}{\sin^2(\theta)}\partial_\phi^2\right), \tag{2.11}$$

in obtaining the above formula we have used the left invariant generators. It is straightforward to show that we can obtain the same result with right invariant generators, too, that is Casimir operator of left and right operators are the same.

B. $H_q(\theta,\psi)$ Hamiltonian

Here through dimensional reduction we show that the above Casimir operator reduces to a Hamiltonian of motion of a charged particle in the presence of electric field. Hence, first we make one-dimensional re'duction (eliminate the coordinate ϕ) through the usual Fourier transformation defined as

$$\tilde{f}(q)=\frac{1}{\sqrt{2\pi}}\int_0^{2\pi}f(\phi)\exp(-i\phi q)d\phi, \tag{2.12}$$

over an arbitrary function $f(\phi)$. Obviously the Casimir operator (2.11) reduces to the following operator:

$$L_q^2(\theta,\psi)=-\frac{1}{\sin^2(\psi)}\partial_\psi\sin^2(\psi)\partial_\psi-\frac{1}{\sin^2(\psi)}\left(\frac{1}{\sin(\theta)}\partial_\theta\sin(\theta)\partial_\theta-\frac{q^2}{\sin^2(\theta)}\right), \tag{2.13}$$

in the Hilbert space of Fourier transformed wave functions. In general, the nonrelativistic Hamiltonian of a charged particle over a two-dimensional with metric $g_{\mu\nu}$ in the presence of magnetostatic field $\vec{B}$ with vector potential $\vec{A}$ and electrostatic field $\vec{E}$ with scalar potential V can be written as[8,15]

$$H=-\frac{1}{\sqrt{g}}(\partial_\mu-iA_\mu)(\sqrt{g}g^{\mu\nu}(\partial_\nu-iA_\nu))+V, \tag{2.14}$$

where g is the determinant of metric $g_{\mu\nu}$. After similarity transformation of the Casimir operator (2.13) defined as

$$\tilde{L}_q^2(\theta,\psi)=\sin^{\frac{1}{2}}(\psi)L_q^2(\theta,\psi)\sin^{-\frac{1}{2}}(\psi),$$

we have

$$\tilde{L}_q^2(\theta,\psi)=-\frac{1}{\sin(\psi)}\partial_\psi\sin(\psi)\partial_\psi-\frac{1}{\sin^2(\psi)}\left(\frac{1}{\sin(\theta)}\partial_\theta\sin(\theta)\partial_\theta-\frac{q^2}{\sin^2(\theta)}\right)+\frac{1}{4}\cot^2(\psi)-\frac{1}{2}. \tag{2.15}$$

Comparing the operator (2.15) with the Hamiltonian (2.14) we obtain

$$g_{\psi\psi}=1,\quad g_{\theta\theta}=\sin^2(\psi),\quad g_{\psi\theta}=g_{\theta\psi}=0$$

and

$$A_\psi=0,\quad A_\theta=\frac{i}{2}\cot(\theta)=d\left(\frac{i}{2}\ln(\sin(\theta))\right). \tag{2.16}$$

It is trivial to see that the vector potential given in (2.16) corresponds to pure u(1) gauge field, hence it can eliminate the theory of the gauge transform $A\rightarrow A_\mu+\partial_\mu\chi$ with gauge function $\chi=(i/2)\ln(\sin(\theta))$. After the above gauge transformation the su(2) Casimir Hamiltonian reduces to

$$H_q(\theta,\psi)\equiv e^{-\chi}\tilde{L}_q^2(\theta,\psi)e^{\chi}=-\frac{1}{\sin(\psi)}\partial_\psi\sin(\psi)\partial_\psi-\frac{1}{\sin^2(\psi)}\partial_\theta^2+\frac{q^2-\frac{1}{4}}{\sin^2(\psi)\sin^2(\theta)}-\frac{3}{4}, \tag{2.17}$$

which can be interpreted as a nonrelativistic Hamiltonian of a point particle over two-dimensional sphere with metric

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

in the presence of electric field with scalar potential

$$V=\frac{q^2-\frac{1}{4}}{\sin^2(\psi)\sin^2(\theta)}-\frac{3}{4}.$$

Similarly, the left and right invariant vector fields given in (2.2)–(2.7) take the following form after the above given operations, that is, dimensional reduction, similarity transformation and gauge transformation:

$$\tilde{L}'_+(q)=\tilde{L}_+(q)+g(\theta,\psi,q),\quad \tilde{R}'_+(q)=\tilde{R}_+(q)-g^\star(\theta,\psi,q),$$

$$\tilde{L}'_-(q)=\tilde{L}_-(q)-g^\star(\theta,\psi,q),\quad \tilde{R}'_-(q)=\tilde{R}_-(q)+g(\theta,\psi,q),$$

$$\tilde{L}'_3(q)=\tilde{L}_3(q),\quad \tilde{R}'_3(q)=\tilde{R}_3(q),$$

where

$$\tilde{L}_+(q)=\frac{i}{2}\left(\sin(\theta)\partial_\psi+(i+\cos(\theta)\cot(\psi))\partial_\theta+i(q-1)\left(-\cot(\theta)+i\frac{\cot(\psi)}{\sin(\theta)}\right)\right)e^{-(\partial/\partial q)}, \tag{2.18}$$

$$\tilde{L}_-(q)=\frac{i}{2}\left(\sin(\theta)\partial_\psi+(-i+\cos(\theta)\cot(\psi))\partial_\theta+i(q+1)\left(-\cot(\theta)-i\frac{\cot(\psi)}{\sin(\theta)}\right)\right)e^{\partial/\partial q}, \tag{2.19}$$

$$\tilde{L}_3(q)=\frac{i}{2}(-\cos(\theta)\partial_\psi+\sin(\theta)\cot(\psi)\partial_\theta-iq), \tag{2.20}$$

$$\tilde{R}_+(q)=\frac{i}{2}\left(\sin(\theta)\partial_\psi+(-i+\cos(\theta)\cot(\psi))\partial_\theta+i(q-1)\left(\cot(\theta)+i\frac{\cot(\psi)}{\sin(\theta)}\right)\right)e^{-(\partial/\partial q)}, \tag{2.21}$$

$$\tilde{R}_-(q)=\frac{i}{2}\left(\sin(\theta)\partial_\psi+(i+\cos(\theta)\cot(\psi))\partial_\theta+i(q+1)\left(\cot(\theta)-i\frac{\cot(\psi)}{\sin(\theta)}\right)\right)e^{\partial/\partial q}, \tag{2.22}$$

$$\tilde{R}_3(q)=\frac{i}{2}(-\cos(\theta)\partial_\psi+\sin(\theta)\cot(\psi)\partial_\theta+iq) \tag{2.23}$$

with $g(\theta,\psi,q)$ is

$$g(\theta,\psi,q)=\frac{1}{4}\left(\cot(\theta)-i\frac{\cot(\psi)}{\sin(\theta)}\right)e^{\partial/\partial q},$$

where* means the usual complex conjugation. With some calculation one can show that the above algebra, that is, the commutation relations is unchanged under the above-mentioned transformation and the Hamiltonian $H_q(\theta,\psi)$ can be written in terms of generator (2.18)–(2.20) in the following form:

$$H_q(\theta,\psi)=\tfrac{1}{2}(\tilde{L}'_+(q)\tilde{L}'_-(q)+\tilde{L}'_-(q)\tilde{L}'_+(q))+\tilde{L}'_3(q)^2.$$

Hence, $H_q(\theta,\psi)$ is still Casimir operator su(2) Lie algebra with generator given in (2.18)–(2.23).

C. Algebraic solution of $H_q(\theta,\psi)$ Hamiltonian

In order to obtain eigenspectrum of Hamiltonian (2.17) by algebraic method, first we obtain eigenspectrum of the Casimir operator (2.11). Since this operator commutes with the left and right invariant generator given in (2.10), therefore, we can obtain representation of su(2) simply by finding simultaneous eigenfunctions of the set commuting operators (R_3,L_3,L^2). Denoting their simultaneous eigenfunction by $\chi^l_{m_L,m_R}(\theta,\psi,\phi)$, we can write

$$L^2\chi^l_{m_L,m_R}(\theta,\psi,\phi)=l(l+1)\chi^l_{m_L,m_R}(\theta,\psi,\phi), \tag{2.24}$$

$$L_3\chi^l_{m_L,m_R}(\theta,\psi,\phi)=m_L\chi^l_{m_L,m_R}(\theta,\psi,\phi), \tag{2.25}$$

$$R_3\chi^l_{m_L,m_R}(\theta,\psi,\phi)=m_R\chi^l_{m_L,m_R}(\theta,\psi,\phi). \tag{2.26}$$

Now solving the difference of the first order differential equations (2.25) and (2.26) we deduce that $\chi^l_{m_L,m_R}(\theta,\psi,\phi)$ is proportional to $e^{-i(m_R-m_L)\phi}$, hence we have $\chi^l_{m_L,m_R}(\theta,\psi,\phi)=e^{-i(m_R-m_L)\phi}f(\theta,\psi)$, where $f(\theta,\psi)$ can be determined from the solution of the sum of the equations (2.25) and (2.26), that is

$$-i\cos(\theta)\partial_\psi f(\theta,\psi)+i\sin(\theta)\cot(\psi)\partial_\theta f(\theta,\psi)=(m_L+m_R)f(\theta,\psi). \tag{2.27}$$

Now considering the highest weight defined by $m_L=-m_R=l$, that is the right-hand side of the Eq. (2.27) vanishes, hence it can be solved by characteristic method which leads to the following results:

$$\chi^l_{l,-l}(\theta,\psi,\phi)=\exp(2il\phi)f^{\max}(\sin(\psi)\sin(\theta)),$$

where $f^{\max}$ is an arbitrary function which can be determined by solving the first order differential equation:

$$R_+\chi^l_{l,-l}(\theta,\psi,\phi)=0,\quad L_+\chi^l_{l,-l}(\theta,\psi,\phi)=0.$$

Since the highest weight $\chi^l_{l,-l}$ belongs to the kernel of raising operators R_+ and L_+ therefore the sum of Eqs. (2.2) and (2.5) leads to

$$u\frac{df^{\max}(u)}{du}=2lf^{\max}(u),$$

where $u=\sin(\psi)\sin(\theta)$. Therefore solving the above equation we obtain $f^{\max}(u)=u^{2l}$, hence $\chi^l_{l,-l}(\theta,\psi,\phi)$ has the following form:

$$\chi^l_{l,-l}(\theta,\psi,\phi)=e^{2il\phi}(\sin(\psi)\sin(\theta))^{2l}. \tag{2.28}$$

The other eigenweights can be obtained through the operation of the lowering operator R_- and L_- over the highest eigenfunction, that is, we have

$$\chi^l_{m_L,m_R}(\theta,\psi,\phi)=(L_-)^{l-m_L}(R_-)^{l+m_R}(e^{2il\phi}(\sin(\psi)\sin(\theta))^{2l}). \tag{2.29}$$

In order to eliminate the coordinate ϕ, first we transfer the function $e^{2il\phi}$ to the left-hand side of the operators R_- and L_- in (2.29), then we get

$$\chi^l_{m_L,m_R}(\theta,\psi,\phi)=e^{i(m_L-m_R)\phi}L_-(m_L-m_R+1)L_-(m_L-m_R+2)$$
$$\cdots L_-(l-m_R)R_-(l-m_R+1)\cdots R_-(2l)(\sin(\psi)\sin(\theta))^{2l}, \tag{2.30}$$

where the operator $L_-(m)$ and $R_-(m)$ are defined as

$$L_-(m)=\frac{i}{2}\left(\sin(\theta)\partial_\psi+(-i+\cos(\theta)\cot(\psi))\partial_\theta+im\left(-\cot(\theta)-i\frac{\cot(\psi)}{\sin(\theta)}\right)\right), \tag{2.31}$$

$$R_-(m)=\frac{i}{2}\left(\sin(\theta)\partial_\psi+(i+\cos(\theta)\cot(\psi))\partial_\theta+im\left(\cot(\theta)-i\frac{\cot(\psi)}{\sin(\theta)}\right)\right). \tag{2.32}$$

Finally Fourier transformation of (2.30) leads to

$$\chi^{l}_{q,m}(\theta,\psi)=L_{-}(q+1)L_{-}(q+2)\cdots L_{-}\left(l+\frac{q-m}{2}\right)R_{-}\left(l+\frac{q-m}{2}+1\right)$$
$$\cdots R_{-}(2l)(\sin(\psi)\sin(\theta))^{2l}, \tag{2.33}$$

where $q=m_L-m_R$ and $m=m_L+m_R$.

Since the left and right invariant generator commute with each other, we can exchange these operators in (2.29) before Fourier transformation, but after Fourier transformation we can use only the relation $L_{-}(q)R_{-}(q-1)=R_{-}(q)L_{-}(q-1)$. Since the Hamiltonian $H_q(\theta,\psi)$ can be obtained from the relations (2.15) and (2.17) via similarity transform and gauge transform, that is, we have

$$H_q(\theta,\psi)=\exp(-\xi)L^2_q(\theta,\psi)\exp(\xi),\quad L^2_q(\theta,\psi)\chi^{l}_{q,m}(\theta,\psi)=l(l+1)\chi^{l}_{q,m}(\theta,\psi), \tag{2.34}$$

where $\xi=-\frac{1}{2}\ln(\sin(\psi)\sin(\theta))$. Hence the eigenfunction of Hamiltonian $H_q(\theta,\psi)$ can be written as

$$\tilde{\chi}^{l}_{q,m}(\theta,\psi)=\exp(-\xi)\chi^{l}_{q,m}(\theta,\psi). \tag{2.35}$$

D. Shape invariance symmetry of $H_q(\theta,\psi)$

Here in this section we show that the Hamiltonian $H_q(\theta,\psi)$ poses both degeneracy and shape invariance symmetry.[5,1,2] As it is shown in Sec. (II C), functions $\tilde{\chi}^{l}_{q,m}(\theta,\psi)=(\sin(\psi)\sin(\theta))^{\frac{1}{2}}\chi^{l}_{q,m}(\theta,\psi)$ are eigenfunctions of the Hamiltonian $H_q(\theta,\psi)$ with the corresponding eigenvalue $l(l+1)$. Since $|m_R|\leqslant l$ and $|m_L|\leqslant l$, therefore, $|q|\leqslant 2l$ and for a given value of q the parameter m can take the following values:

$$m=\begin{cases}0,\pm 2,\pm 4,\ldots,\pm(2l-|q|) & \text{for}\quad |q|=\text{even},\\ \pm 1,\pm 3,\ldots,\pm(2l-|q|) & \text{for}\quad |q|=\text{odd}.\end{cases} \tag{2.36}$$

Since the eigenvalue of Hamiltonian $H_q(\theta,\psi)$ is independent of m, therefore it has $(2l+1-|q|)$ degenerate states for a given l or given energy $l(l+1)$. To see the shape invariance symmetry of Hamiltonian $H_q(\theta,\psi)$, first we consider the Fourier transformed left and right invariant vector fields:

$$\tilde{L}_{+}(q)\equiv L_{+}(q-1)e^{-(\partial/\partial q)}$$
$$=\frac{i}{2}\left(\sin(\theta)\partial_{\psi}+(i+\cos(\theta)\cot(\psi))\partial_{\theta}+i(q-1)\left(-\cot(\theta)+i\frac{\cot(\psi)}{\sin(\theta)}\right)\right)e^{-(\partial/\partial q)}, \tag{2.37}$$

$$\tilde{L}_{-}(q)\equiv L_{-}(q+1)e^{\partial/\partial q}$$
$$=\frac{i}{2}\left(\sin(\theta)\partial_{\psi}+(-i+\cos(\theta)\cot(\psi))\partial_{\theta}+i(q+1)\left(-\cot(\theta)-i\frac{\cot(\psi)}{\sin(\theta)}\right)\right)e^{\partial/\partial q}, \tag{2.38}$$

$$\tilde{L}_3(q)\equiv L_3(q)=\frac{i}{2}(-\cos(\theta)\partial_{\psi}+\sin(\theta)\cot(\psi)\partial_{\theta}-iq), \tag{2.39}$$

and

$$\tilde{R}_{+}(q)\equiv R_{+}(q-1)e^{-(\partial/\partial q)}$$
$$=\frac{i}{2}\left(\sin(\theta)\partial_{\psi}+(-i+\cos(\theta)\cot(\psi))\partial_{\theta}+i(q-1)\left(\cot(\theta)+i\frac{\cot(\psi)}{\sin(\theta)}\right)\right)e^{-(\partial/\partial q)}, \tag{2.40}$$

$$\tilde{R}_-(q)\equiv R_-(q+1)e^{\partial/\partial q}$$

$$=\frac{i}{2}\left(\sin(\theta)\partial_\psi+(i+\cos(\theta)\cot(\psi))\partial_\theta+i(q+1)\left(\cot(\theta)-i\frac{\cot(\psi)}{\sin(\theta)}\right)\right)e^{\partial/\partial q}, \tag{2.41}$$

$$\tilde{R}_3(q)\equiv R_3(q)=\frac{i}{2}(-\cos(\theta)\partial_\psi+\sin(\theta)\cot(\psi)\partial_\theta+iq). \tag{2.42}$$

After some tedious algebraic calculation we can derive the following relation between the above operators:

$$L_3(q\pm1)L_\pm(q)-L_\pm(q)L_3(q)=\pm L_\pm(q), \tag{2.43}$$

$$R_3(q\pm1)R_\pm(q)-R_\pm(q)R_3(q)=\mp R_\pm(q), \tag{2.44}$$

the above relations indicate that Hamiltonian $H_q(\theta,\psi)$ poses shape invariance symmetry. Since by acting the operators $R_\pm(q)$ and $L_\pm(q)$ on both sides of eigenvalue equations:

$$L_q^2(\theta,\psi)\chi^l_{q,m}(\theta,\psi)=l(l+1)\chi^l_{q,m}(\theta,\psi),$$

$$R_3(q)\chi^l_{q,m}(\theta,\psi)=\frac{m-q}{2}\chi^l_{q,m}(\theta,\psi),$$

$$L_3(q)\chi^l_{q,m}(\theta,\psi)=\frac{m+q}{2}\chi^l_{q,m}(\theta,\psi),$$

we get

$$R_\pm(q)\chi^l_{q,m}(\theta,\psi)=A_\pm(q,m)\chi^l_{q\pm1,m\mp1}(\theta,\psi), \tag{2.45}$$

$$L_\pm(q)\chi^l_{q,m}(\theta,\psi)=B_\pm(q,m)\chi^l_{q\pm1,m\pm1}(\theta,\psi), \tag{2.46}$$

with

$$A_\pm(q,m)=\tfrac{1}{2}\sqrt{(2l\mp(m-q))(2l\pm(m-q)+2)}, \tag{2.47}$$

$$B_\pm(q,m)=\tfrac{1}{2}\sqrt{(2l\mp(m+q))(2l\pm(m+q)+2)}. \tag{2.48}$$

The above relations imply that the pair of operators (L_-,R_+) $[(L_+,R_-)]$ map degenerate eigenstates of Hamiltonian $H_q(\theta,\psi)$ for given value of q into each other, that is they decrease [increase] the quantum number m by 2 units as follows:

$$L_-(q+1)R_+(q)\chi^l_{q,m}(\theta,\psi)=A_+(q,m)B_-(q+1,m-1)\chi^l_{q,m-2}(\theta,\psi),$$

$$L_+(q-1)R_-(q)\chi^l_{q,m}(\theta,\psi)=A_-(q,m)B_+(q-1,m+1)\chi^l_{q,m+2}(\theta,\psi).$$

Now introducing the operator $Y_+(q):=L_+(q-1)R_-(q)$ and $Y_-(q):=L_-(q+1)R_+(q)$ as raising and lowering operators of degenerate states of Hamiltonian $H_q(\theta,\psi)$, then we have the following shape invariance like symmetry between the degenerate states of Hamiltonian $H_q(\theta,\psi)$:

$$Y_-(q)Y_+(q)\chi^l_{q,m}(\theta,\psi)=E(q,m)\chi^l_{q,m}(\theta,\psi),$$

$$Y_+(q)Y_-(q)\chi^l_{q,m+2}(\theta,\psi)=E(q,m)\chi^l_{q,m+2}(\theta,\psi),$$

where

$$E(q,m)=A_-(q,m)A_+(q,m+2)B_-(q+1,m+1)B_+(q-1,m+1).$$

Thus, for a given value of q, we can obtain eigenfunction of Hamiltonian $H_q(\theta,\psi)$ with eigenvalue $l(l+1)$, simply by acting the pairs of operators $(L_-,R_+)[(L_+,R_-)]$ over the highest weight [lowest weight], where here we have derived the eigenfunction $\chi^l_{q,m}(\theta,\psi)$ by acting the lowering operator over the highest eigenstate as follows:

$$\chi^l_{q,m}(\theta,\psi)=k^{-1}(Y_-(q))^{(2l-|q|-m)/2}\chi^l_{q,(2l-|q|)}(\theta,\psi), \tag{2.49}$$

where

$$k=B_-(q+1,m+1)B_-(q+1,m+3)$$
$$\times B_-(q+1,2l-|q|-1)A_+(q,m+2)A_+(q,m+4)\cdots A_+(q,2l-|q|),$$

using the relation (2.33) we can obtain the highest weight eigenstates for $q>0$ and $q<0$,

$$\chi^l_{q,(2l-|q|)}(\theta,\psi)=\begin{cases} L_-(q+1)L_-(q+2) & \\ \quad\times L_-(0)R_-(1)R_-(2)\ldots R_-(2l)(\sin(\theta)\sin(\psi))^{2l} & \text{for } q<0,\\ R_-(q+1)R_-(q+2)\ldots R_-(2l)(\sin(\theta)\sin(\psi))^{2l} & \text{for } q>0.\end{cases}$$

On the other hand, pair operators $(L_+,R_+)[(L_-,R_-)]$ leave the eigenvalue m and l unchanged while they increase [decrease] the parameter q by 2 units, that is they map eigenfunctions of the Hamiltonian corresponding to the same energy with different q into each other, that is they map isospectral Hamiltonians into each other with nothing but shape invariance, to show the shape invariance symmetry, we set the related operators over $\chi^l_{q,m}(\theta,\psi)$, we then obtain

$$L_+(q+1)R_+(q)\chi^l_{q,m}(\theta,\psi)=A_+(q,m)B_+(q+1,m-1)\chi^l_{q+2,m}(\theta,\psi),$$

$$L_-(q-1)R_-(q)\chi^l_{q,m}(\theta,\psi)=A_-(q,m)B_-(q-1,m+1)\chi^l_{q-2,m}(\theta,\psi).$$

Obviously, the combined actions of the above operators leave the eigenvalues m and l unchanged while changing the parameter q by 2 units. Hence we define the operator $X_+(q):=L_+(q+1)R_+(q)$ and $X_-(q):=L_-(q+1)R_-(q+2)$ as raising and lowering the operators of parameter q, then the shape invariance symmetry means

$$X_-(q)X_+(q)\chi^l_{q,m}(\theta,\psi)=N(q,m)\chi^l_{q,m}(\theta,\psi),$$

$$X_+(q)X_-(q)\chi^l_{q+2,m}(\theta,\psi)=N(q,m)\chi^l_{q+2,m}(\theta,\psi),$$

where

$$N(q,m)=A_+(q,m)A_-(q+2,m)B_+(q+1,m-1)B_-(q+1,m+1)$$

or

$$N(q,m)=\tfrac{1}{16}(2l-m-q)(2l+m+q+2)$$
$$\times\sqrt{(2l-m+q)(2l-m+q+4)(2l+m-q+2)(2l+m-q-2)}.$$

Since for fixed values of energy $l(l+1)$ and given values of m, the parameter q can take the following values:

$$q=(2l-|m|),(2l-|m|-2),\ldots,-(2l-|m|-2),-(2l-|m|).$$

Hence obtaining the highest eigenstates, by solving the following first order differential equation:

$$X_+(2l-|m|)\chi^l_{(2l-|m|),m}(\theta,\psi)=0,$$

where the integral leads to

$$\chi^l_{(2l-|m|),m}(\theta,\psi)=\begin{cases} L_-(2l-m+1)L_-(2l-m+2)\ldots L_-(2l)(\sin(\theta)\sin(\psi))^{2l} & \text{for } m<0,\\ R_-(2l-m+1)R_-(2l-m+2)\ldots R_-(2l)(\sin(\theta)\sin(\psi))^{2l} & \text{for } m>0.\end{cases}$$

Therefore using the shape invariance relation, we can obtain the eigenstates of Hamiltonian $H_q(\theta,\psi)$ by consecutive action of the q-lowering operator over the q-highest weight eigenstate,

$$\chi^l_{q,m}(\theta,\psi)=f^{-1}X_-(q)X_-(q+2)\cdots X_-(2l-|m|-4)X_-(2l-|m|-2)\chi^l_{(2l-|m|),m}(\theta,\psi)$$

$$f=A_(q+2,mA_(q+4,m\cdots A_-(2l-|m|,m)$$

$$\times B_-(q+1,m+1)B_-(q+3,m+1)\cdots B_-(2l-|m|-1,m+1).$$

III. THREE-DIMENSIONAL HAMILTONIAN OBTAINED FROM 4-OSCILLATORS

In this section using the su(2) parametrization of the preceding section, we obtain a special three-dimensional Hamiltonian from the Hamiltonian of 4-oscillator with the same frequency, where we obtain its spectrum via corresponding spectrum of 4-oscillator Hamiltonian. We show that thus obtained Hamiltonians poses shape invariance symmetry. The Hamiltonian of the 4-oscillator with the same frequency can be written as

$$H=-\frac{1}{2}\sum_{i=0}^{4}\left(P_i^2+\frac{1}{2}\omega^2x_i^2\right)$$

now making the following change of variable:

$$\begin{aligned} x_1&=-r\sin(\psi)\sin(\theta)\sin(\phi),\\ x_2&=r\sin(\psi)\sin(\theta)\cos(\phi),\\ x_3&=r\sin(\psi)\cos(\theta),\\ x_4&=r\cos(\psi),\end{aligned} \tag{3.1}$$

where ψ,θ,ϕ are the same coordinates used in the parametrization su(2) manifold, the Hamiltonian takes the following form:

$$H(r,\theta,\psi,\phi)=-\frac{1}{2}\left[\frac{1}{r^3}\partial_r r^3\partial_r + \frac{1}{r}\left(\partial_\psi^2+2\cot(\psi)\partial_\psi+\frac{1}{\sin^2(\psi)}\left(\partial_\theta^2+\cot(\theta)\partial_\theta+\frac{1}{\sin^2(\theta)}\partial_\phi^2\right)\right)\right]+\frac{1}{2}\omega^2r^2. \tag{3.2}$$

Since the angular part of the above Hamiltonian is the same as the one given in (2.11), therefore, its eigenspectrum can be obtained straightforwardly through routine separation of variables into radial and angular parts which we are not interested in here. Actually here we are concerned with the special Hamiltonian which can be obtained from this 4-oscillator Hamiltonian, that is, those Hamiltonians which pose shape invariance symmetry.

In order to achieve it, we write the above Hamiltonian in terms of raising and lowering operators defined in the usual way:

$$H=\omega(a_1^\dagger a_1+a_2^\dagger a_2+a_3^\dagger a_3+a_4^\dagger a_4+2), \tag{3.3}$$

where $a_i(a_i^\dagger)$ are defined as

$$a_i=\sqrt{\frac{\omega}{2}}\left(x_i+\frac{1}{\omega}\frac{d}{dx_i}\right),\quad a_i^\dagger=\sqrt{\frac{\omega}{2}}\left(x_i-\frac{1}{\omega}\frac{d}{dx_i}\right),$$

these operators have the following form in radial coordinate (3.1):

$$\begin{aligned}a_1(a_1^\dagger)=&\sqrt{\frac{\omega}{2}}\Bigg[-r\sin(\psi)\sin(\theta)\sin(\phi)+(-)\frac{1}{\omega}\Bigg(-\sin(\psi)\sin(\theta)\sin(\phi)\partial_r\\&-\frac{1}{r}\cos(\psi)\sin(\theta)\cos(\phi)\partial_\psi-\frac{1}{r}\frac{\cos(\theta)\sin(\phi)}{\sin(\psi)}\partial_\theta-\frac{1}{r}\frac{\cos(\phi)}{\sin(\psi)\sin(\theta)}\partial_\phi\Bigg)\Bigg],\end{aligned}$$

$$\begin{aligned}a_2(a_2^\dagger)=&\sqrt{\frac{\omega}{2}}\Bigg[r\sin(\psi)\sin(\theta)\cos(\phi)+(-)\frac{1}{\omega}\Bigg(\sin(\psi)\sin(\theta)\cos(\phi)\partial_r\\&+\frac{1}{r}\cos(\psi)\sin(\theta)\cos(\phi)\partial_\psi+\frac{1}{r}\frac{\cos(\theta)\cos(\phi)}{\sin(\psi)}\partial_\theta-\frac{1}{r}\frac{\sin(\phi)}{\sin(\psi)\sin(\theta)}\partial\phi\Bigg)\Bigg],\end{aligned}$$

$$\begin{aligned}a_3(a_3^\dagger)=&\sqrt{\frac{\omega}{2}}\Bigg[r\sin(\psi)\cos(\theta)+(-)\frac{1}{\Omega}\Bigg(\sin(\psi)\cos(\theta)\partial_r\\&+\frac{1}{r}\cos(\psi)\cos(\theta)\partial_\psi-\frac{1}{r}\frac{\sin(\theta)}{\sin(\psi)}\partial_\theta\Bigg)\Bigg],\end{aligned}$$

$$a_4(a_4^\dagger)=\sqrt{\frac{\omega}{2}}\left[r\cos(\psi)+(-)\frac{1}{\omega}\left(\cos(\psi)\partial_r-\frac{1}{r}\sin\psi\partial_\psi\right)\right].$$

Now defining the set of new operators $A_i(A_i^\dagger)$, $i=1, 2$ in terms of $a_i(a_i^\dagger)$:

$$A_1=\frac{1}{\sqrt{2}}(a_1+ia_2),\quad A_1^\dagger=\frac{1}{\sqrt{2}}(a_1^\dagger-ia_2^\dagger),$$

$$A_2=\frac{1}{\sqrt{2}}(a_1-ia_2),\quad A_2^\dagger=\frac{1}{\sqrt{2}}(a_1^\dagger+ia_2^\dagger),$$

where, these new operators have the following differential form in radial coordinates:

$$\begin{aligned}A_1=&\frac{i}{\sqrt{2}}\sqrt{\frac{\omega}{2}}e^{i\phi}\Bigg[r\sin(\psi)\sin(\theta)\\&+\frac{1}{\omega}\left(\sin(\psi)\sin(\theta)\partial_r-\frac{1}{r}\cos(\psi)\sin(\theta)\partial_\psi+\frac{1}{r}\frac{\cos(\theta)}{\sin(\psi)}\partial_\theta+\frac{1}{r}\frac{i}{\sin(\psi)\sin(\theta)}\partial\phi\right)\Bigg],\end{aligned}\tag{3.4}$$

$$A_1^\dagger=\frac{-i}{\sqrt{2}}\sqrt{\frac{\omega}{2}}e^{-i\phi}\Bigg[r\sin(\psi)\sin(\theta)+\frac{1}{\omega}\Bigg(\sin(\psi)\sin(\theta)\partial_r+\frac{1}{r}\cos(\psi)\sin(\theta)\partial_\psi+\frac{1}{r}\frac{\cos(\theta)}{\sin(\psi)}\partial_\theta-\frac{1}{r}\frac{i}{\sin(\psi)\sin(\theta)}\partial\phi\Bigg)\Bigg], \quad (3.5)$$

$$A_2=-\frac{i}{\sqrt{2}}\sqrt{\frac{\omega}{2}}e^{-i\phi}\Bigg[r\sin(\psi)\sin(\theta)+\frac{1}{\omega}\Bigg(\sin(\psi)\sin(\theta)\partial_r+\frac{1}{r}\cos(\psi)\sin(\theta)\partial_\psi+\frac{1}{r}\frac{\cos(\theta)}{\sin(\psi)}\partial_\theta-\frac{1}{r}\frac{i}{\sin(\psi)\sin(\theta)}\partial\phi\Bigg)\Bigg], \quad (3.6)$$

$$A_2^\dagger=\frac{i}{\sqrt{2}}\sqrt{\frac{\omega}{2}}e^{i\phi}\Bigg[r\sin(\psi)\sin(\theta)-\frac{1}{\omega}\Bigg(\sin(\psi)\sin(\theta)\partial_r+\frac{1}{r}\cos(\psi)\sin(\theta)\partial_\psi+\frac{1}{r}\frac{\cos(\theta)}{sin(\psi)}\partial_\theta+\frac{1}{r}\frac{i}{\sin(\psi)\sin(\theta)}\partial\phi\Bigg)\Bigg]. \quad (3.7)$$

It is also straightforward to show that they have the following commutator relations:

$$[A_i,A_j^\dagger]=\delta_{ij}, \quad [A_i,A_j]=[A_i^\dagger,A_j^\dagger]=0, \quad i,j=1,2,$$

the 4-oscillators Hamiltonian (3.3) can be written in terms of the new oscillators as follows:

$$H=\omega(A_1^\dagger A_1+A_2^\dagger A_2+a_3^\dagger a_3+a_4^\dagger a_4+2). \quad (3.8)$$

Now its eigenspectrum can be obtained by solving the following eigenvalue equation:

$$H\Psi_{(n_1,n_2,n_3,n_4)}(r,\theta,\phi,\psi)=E_{(n_1,n_2,n_3,n_4)}\Psi_{(n_1,n_2,n_3,n_4)}(r,\theta,\phi,\psi), \quad (3.9)$$

by the usual algebraic method, hence its eigenfunction can be written as

$$\Psi_{(n_1,n_2,n_3,n_4)}(r,\theta,\phi,\psi)=N(A_1^\dagger)^{n_1}(A_2^\dagger)^{n_2}(a_3^\dagger)^{n_3}(a_4^\dagger)^{n_4}\exp\left(-\frac{\omega}{2}r^2\right), \quad (3.10)$$

with $N=\omega/\pi\sqrt{n_1!n_2!n_3!n_4!}$ as normalization constant, and energy $E_{(n_1,n_2,n_3,n_4)}=(n_1+n_2+n_3+n_4+2)\omega$. Using the differential representation of the operator, the wave function (3.10) can be written in the following form:

$$\Psi_{(n_1,n_2,n_3,n_4)}(r,\theta,\phi,\psi)=N2^{(1/2)(n_1+n_2)}e^{i(n_2-n_1)\phi}e^{-(1/2)r^2}(r\sin(\psi)\sin(\theta))^{(n_1+n_2)}\times\mathcal{H}_{n_3}(r\sin(\psi)\cos(\theta))\mathcal{H}_{n_4}(r\cos(\psi))\sum_{i=0}^{n_1}(-1)^i i!\binom{n_1}{i}\binom{n_2}{i}\times(r\sin(\psi)\sin(\theta))^{2i}, \quad (3.11)$$

where $\mathcal{H}_n$ is Hermit polynomial of degree n and $\binom{n_1}{i}=n!/r!(n-r)!$. Now with the same prescription used in the preceding section, we can eliminate ϕ, by Fourier transforming over it, hence, Fourier transforming over ϕ, 4-oscillator Hamiltonian reduces to the following Hamiltonian:

$$H_m(r,\theta,\psi)=-\frac{1}{2}\left[\frac{1}{r^3}\partial_r r^3\partial_r + \frac{1}{r^2}\left(\partial_\psi^2+2\cot(\psi)\partial_\psi+\frac{1}{\sin^2(\psi)}\left(\partial_\theta^2+\cot(\theta)\partial_\theta-\frac{m^2}{\sin^2(\theta)}\right)\right)\right]+\frac{1}{2}\omega^2 r^2, \tag{3.12}$$

where after similarity transformation through function $r^{1/2}$, it reduces to

$$\begin{aligned}\tilde{H}_m(r,\theta,\psi)&=r^{1/2}H_m(r,\theta,\psi)r^{-1/2}\\&=-\frac{1}{2}\left[\frac{1}{r^2}\partial_r r^2\partial_r+\frac{1}{r^2}\left(\partial_\psi^2+2\cot(\psi)\partial_\psi+\frac{1}{\sin^2(\psi)}\left(\partial_\theta^2+\cot(\theta)\partial_\theta-\frac{m^2}{\sin^2(\theta)}\right)\right)\right]\\&\quad+\frac{1}{2}\omega^2 r^2+\frac{3}{8r^2}.\end{aligned} \tag{3.13}$$

On the other hand, the Hamiltonian $H_m(r,\theta,\psi)$ given by (3.12) can be written in the following form:

$$H_m(r,\theta,\psi)=\omega(A_1^\dagger(m+1)A_1(m)+A_2^\dagger(m-1)A_2(m)+a_3^\dagger a_3+a_4^\dagger a_4+2), \tag{3.14}$$

with

$$A_1(m)=\frac{i}{\sqrt{2}}\sqrt{\frac{\omega}{2}}\left[r\sin(\psi)\sin(\theta)+\frac{1}{\omega}\left(\sin(\psi)\sin(\theta)\partial_r-\frac{1}{r}\cos(\psi)\sin(\theta)\partial_\psi+\frac{1}{r}\frac{\cos(\theta)}{\sin(\psi)}\partial_\theta-\frac{1}{r}\frac{m}{\sin(\psi)\sin(\theta)}\right)\right], \tag{3.15}$$

$$A_1^\dagger(m)=-\frac{i}{\sqrt{2}}\sqrt{\frac{\omega}{2}}\left[r\sin(\psi)\sin(\theta)-\frac{1}{\omega}\left(\sin(\psi)\sin(\theta)\partial_r+\frac{1}{r}\cos(\psi)\sin(\theta)\partial_\psi+\frac{1}{r}\frac{\cos(\theta)}{\sin(\psi)}\partial_\theta+\frac{1}{r}\frac{m}{\sin(\psi)\sin(\theta)}\right)\right], \tag{3.16}$$

$$A_2(m)=-\frac{i}{\sqrt{2}}\sqrt{\frac{\omega}{2}}\left[r\sin(\psi)\sin(\theta)+\frac{1}{\omega}\left(\sin(\psi)\sin(\theta)\partial_r+\frac{1}{r}\cos(\psi)\sin(\theta)\partial_\psi+\frac{1}{r}\frac{\cos(\theta)}{\sin(\psi)}\partial_\theta+\frac{1}{r}\frac{m}{\sin(\psi)\sin(\theta)}\right)\right], \tag{3.17}$$

$$A_2^{\dagger}(m)=\frac{i}{\sqrt{2}}\sqrt{\frac{\omega}{2}}\Bigg[r\sin(\psi)\sin(\theta) - \frac{1}{\omega}\Bigg(\sin(\psi)\sin(\theta)\partial_r+\frac{1}{r}\cos(\psi)\sin(\theta)\partial_\psi+\frac{1}{r}\frac{\cos(\theta)}{sin(\psi)}\partial_\theta-\frac{1}{r}\frac{m}{\sin(\psi)\sin(\theta)}\Bigg)\Bigg]. \tag{3.18}$$

It is straightforward to derive the following relation between Hamiltonian (3.12) and operator $A_i(m)(A_i^{\dagger}(m))$, $i=1, 2$:

$$\begin{aligned} H(m-1)A_1^{\dagger}(m)-A_1^{\dagger}(m)H(m)&=\omega A_1^{\dagger}(m),\\ H(m+1)A_2^{\dagger}(m)-A_2^{\dagger}(m)H(m)&=\omega A_2^{\dagger}(m),\\ H(m+1)A_1(m)-A_1(m)H(m)&=-\omega A_1(m),\\ H(m-1)A_2(m)-A_2(m)H(m)&=-\omega A_2(m), \end{aligned} \tag{3.19}$$

where $H(m)\coloneqq H_m(r,\theta,\psi)$. The above relations indicate that the Hamiltonian (3.12) poses shape invariance symmetry, to see it, we consider the Fourier transformation of eigenvalue equation (3.9):

$$H(m)\Psi_{(n,m,n_3,n_4)}(r,\theta,\psi)=E_{(n,n_3,n_4)}\Psi_{(n,m,n_3,n_4)}(r,\theta,\psi), \tag{3.20}$$

where $n=n_1+n_2, m=n_2-n_1$, and $E_{(n,n_3,n_4)}=(n+n_3+n_4+2)\omega$. Since n_1 and n_2 are positive integer, therefore n is also a positive integer, but m is an integer. For a given value of m, the quantum number n can be either even integer or odd integer, since, quantum numbers n_1 and n_2 should vary by the same amount, so that m remains constant. Actually for given value of m, the quantum number n can take the following value:

$$n=|m|,|m|+2,|m|+4,\ldots,$$

on the other hand, for the value of n, the quantum number m can take the following values:

$$m=-n,-n+2,\ldots,n-2,n.$$

It is interesting to see that the energy of Hamiltonians $H_m(r,\theta,\psi)$ is independent of m, hence these Hamiltonians are isospectral which is due to existence of shape invariance symmetry as we show below.

Operating the operator $A_1^{\dagger}(m)$ on both sides of the eigenvalue relation (3.20) and using the relations (3.19), we get

$$H(m-1)(A_1^{\dagger}(m)\Psi_{n,m}(r,\theta,\psi))=(E_n+\omega)(A_1^{\dagger}(m)\Psi_{n,m}(r,\theta,\psi)),$$

therefore, $A_1^{\dagger}(m)\Psi_{n,m}(r,\theta,\psi))$ corresponds to the eigenfunction of $H(m-1)$ with corresponding eigenvalue E_{n+1}, that is

$$A_1^{\dagger}(m)\Psi_{n,m}(r,\theta,\psi)=\sqrt{\frac{n-m}{2}+1}\Psi_{n+1,m-1}(r,\theta,\psi),$$

where $\Psi_{n,m}(r,\theta,\psi)\coloneqq\Psi_{(n,m,n_3,n_4)}(r,\theta,\psi)$ and $E_n\coloneqq E_{(n,n_3,n_4)}$. Similarly operating operator $A_2^{\dagger}(m)$ on both sides of (3.20) and using (3.19) we get

$$H(m+1)(A_2^{\dagger}(m)\Psi_{n,m}(r,\theta,\psi))=(E_n+\omega)(A_2^{\dagger}(m)\Psi_{n,m}(r,\theta,\psi)),$$

which leads to

$$A_2^\dagger(m)\Psi_{n,m}(r,\theta,\psi)=\sqrt{\frac{n+m}{2}+1}\,\Psi_{n+1,m+1}(r,\theta,\psi).$$

Also by acting the operators $A_1(m)$ and $A_2(m)$ on the eigenvalue relation (3.20) and using the relations (3.19), we obtain

$$H(m+1)(A_1(m)\Psi_{n,m}(r,\theta,\psi))=(E_n-\omega)(A_1(m)\Psi_{n,m}(r,\theta,\psi)),$$

$$H(m-1)(A_2(m)\Psi_{n,m}(r,\theta,\psi))=(E_n-\omega)(A_2(m)\Psi_{n,m}(r,\theta,\psi)),$$

which imply the following relations:

$$A_1(m)\Psi_{n,m}(r,\theta,\psi)=\sqrt{\frac{n-m}{2}}\Psi_{n-1,m+1}(r,\theta,\psi),$$

$$A_2(m)\Psi_{n,m}(r,\theta,\psi)=\sqrt{\frac{n+m}{2}}\Psi_{n-1,m-1}(r,\theta,\psi).$$

From the above relations we conclude that the pair of operators $(A_2(m),A_1^\dagger(m))$ or $(A_2^\dagger(m),A_1(m))$ acting at eigenfunction $\Psi_{n,m}(r,\theta,\psi)$ of Hamiltonian $H(m)$, give the eigenfunction of the Hamiltonian $H(m\pm2)$ with the same energy as follows:

$$A_2(m-1)A_1^\dagger(m)\Psi_{n,m}(r,\theta,\psi)=\tfrac{1}{2}\sqrt{(n+m)(n-m+2)}\Psi_{n,m-2}(r,\theta,\psi),$$

$$A_2^\dagger(m+1)A_1(m)\Psi_{n,m}(r,\theta,\psi)=\tfrac{1}{2}\sqrt{(n-m)(n+m+2)}\Psi_{n,m-2}(r,\theta,\psi).$$

Now introducing the operators $A_-(m):=A_2(m-1)A_1^\dagger(m)$ and $A_+(m):=A_2^\dagger(m-1)A_1(m-2)$, we have

$$A_-(m)A_+(m)\Psi_{n,m-2}(r,\theta,\psi)=E(n,m)\Psi_{n,m-2}(r,\theta,\psi),$$

$$A_+(m)A_-(m)\Psi_{n,m}(r,\theta,\psi)=E(n,m)\Psi_{n,m}(r,\theta,\psi),$$

where

$$E(n,m)=\tfrac{1}{4}(n+m)(n-m+2).$$

The above relations show the existence of shape invariance symmetry between the Hamiltonian $H(m)$ and $H(m-2)$ with the same given eigenvalue E_n. Hence we can obtain the eigenfunction $\Psi_{n,m}(r,\theta,\psi)$ of Hamiltonian $H(m)$ by consecutive action of related raising operators over $\Psi_{n,n}(r,\theta,\psi)$:

$$\Psi_{n,m}(r,\theta,\psi)=c^{-1}A_-(m+2)A_-(m+4)\cdots A_-(n-2)A_-(n)\Psi_{n,n}(r,\theta,\psi),$$

where

$$c=\frac{1}{2^{(n-m)/2}}\sqrt{(n-m)!!2n(2n-2)\cdots(n+m+4)(n+m+2)}$$

and

$$(n-m)!!=(n-m)(n-m-2)\cdots4\times2,$$

$$\Psi_{n,n}(r,\theta,\psi)\equiv\Psi_{(n,n,n_3,n_4)}(r,\theta,\psi)=(a_3^\dagger)^{n_3}(a_4^\dagger)^{n_4}A_2^\dagger(n-1)A_2^\dagger(n-2)\cdots A_2^\dagger(1)A_2^\dagger(0)e^{-1/2\,\omega r^2}.$$

Of course we can obtain the eigenfunction $\Psi_{(n,m,n_3,n_4)}(r,\theta,\psi)$ by reduction of coordinate ϕ via Fourier transformation of (3.11), which have the following form:

$$\Psi_{(n,m,n_3,n_4)}(r,\theta,\psi)=N2^{n/2}e^{-(1/2)r^2}(r\sin(\psi)\sin(\theta))^n \times\mathcal{H}_{n_3}(\sin(\psi)\sin(\theta))\mathcal{H}_{n_4}(r\cos(\psi)) \times\sum_{i=0}^{(n-m)/2}(-1)^i i!\binom{\frac{n-m}{2}}{i}\binom{\frac{n+m}{2}}{i}(r\sin(\psi)\sin(\theta))^{2i}.$$

IV. CONCLUSION

In this work, Fourier transforming over three- and four-dimensional Hamiltonian associated with su(2) and Heisenberg Lie algebra we have been able to obtain two- and three-dimensional Hamiltonians with shape invariance symmetry. It would be interesting to obtain many-body Hamiltonians in one or higher dimension, which poses shape invariance symmetry by appropriate Fourier transformation over some coordinates of the Hamiltonian associated with higher ranks semisimple and nonsemisimple Lie algebra, which is under investigation.

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The Bargmann representation for the quantum mechanics on a sphere

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The Bargmann representation is constructed corresponding to the coherent states for a particle on a sphere introduced in Kowalski and Rembieliński, J. Phys. A: **33**, 6035 (2000). The connection is discussed between the introduced formalism and the standard approach based on the Hilbert space of square integrable functions on a sphere S^2. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1385376]

I. INTRODUCTION

In our recent paper[1] the coherent states for a particle on a sphere have been introduced. As with the standard coherent states[2] those states are labeled by points of the classical phase space, i.e., the cotangent bundle T^*S^2. It is worthwhile to recall that the celebrated spin coherent states[3] are not related to the phase space for a particle on the sphere S^2. One of the most characteristic properties of coherent states is the existence of the Bargmann representation. Such a representation is of importance not only from the mathematical point of view. An example of applications are the Husimi functions, i.e., the elements of the Bargmann space, in the theory of quantum chaos. In this work we introduce the Bargmann representation referring to the coherent states for a particle on a sphere mentioned above. It should be noted that, in opposition to the case of the standard coherent states, the construction of such a Bargmann representation is a highly nontrivial problem. The paper is organized as follows. In Sec. II we recall the basic properties of the coherent states for a particle on a sphere. Sections III–V are devoted to the construction of the Bargmann representation. In Sec. VI we discuss the connection of the introduced Bargmann representation and the standard coordinate representation for the quantum mechanics on a sphere.

II. COHERENT STATES FOR A PARTICLE ON A SPHERE

Our purpose in this section is to recall the basic properties of the coherent states for a particle on a sphere introduced in Ref. 1. Those states are related to the $e(3)$ algebra of the form

$$[J_i,J_j]=\mathrm{i}\epsilon_{ijk}J_k, \quad [J_i,X_j]=\mathrm{i}\epsilon_{ijk}X_k, \quad [X_i,X_j]=0, \quad i,j,k=1,2,3. \tag{2.1}$$

The Casimir operators are given in a unitary irreducible representation by

$$\mathbf{X}^2=r^2, \quad \mathbf{J}\cdot\mathbf{X}=\lambda, \tag{2.2}$$

where a dot designates the scalar product. In Ref. 1 we restricted to the special case $\lambda=0$, so

$$\mathbf{J}\cdot\mathbf{X}=0. \tag{2.3}$$

The irreducible representation of (2.1) under the choice (2.3) is spanned by the common eigenvectors $|j,m;r\rangle$ of the operators $\mathbf{J}^2$, $\mathbf{X}^2$ and $\mathbf{J}\cdot\mathbf{X}$. We have

$$\mathbf{J}^2|j,m;r\rangle=j(j+1)|j,m;r\rangle,\ J_3|j,m;r\rangle=m|j,m;r\rangle, \tag{2.4a}$$

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$$\mathbf{X}^2|j,m;r\rangle = r^2|j,m;r\rangle,\ (\mathbf{J}\cdot\mathbf{X}/r)|j,m;r\rangle = 0, \tag{2.4b}$$

where $-j \leqslant m \leqslant j$. The operators $J_\pm = J_1 \pm iJ_2$, $X_\pm = X_1 \pm iX_2$ and X_3 act on the vectors $|j,m;r\rangle$ as follows:

$$J_\pm|j,m;r\rangle = \sqrt{(j\mp m)(j\pm m+1)}\,|j,m\pm 1;r\rangle, \tag{2.5a}$$

$$X_\pm|j,m;r\rangle = \mp\frac{r\sqrt{(j\pm m+1)(j\pm m+2)}}{\sqrt{(2j+1)(2j+3)}}|j+1,m\pm 1;r\rangle \pm \frac{r\sqrt{(j\mp m-1)(j\mp m)}}{\sqrt{(2j-1)(2j+1)}}|j-1,m\pm 1;r\rangle, \tag{2.5b}$$

$$X_3|j,m;r\rangle = \frac{r\sqrt{(j-m+1)(j+m+1)}}{\sqrt{(2j+1)(2j+3)}}|j+1,m;r\rangle + \frac{r\sqrt{(j-m)(j+m)}}{\sqrt{(2j-1)(2j+1)}}|j-1,m;r\rangle. \tag{2.5c}$$

The orthogonality and completeness conditions satisfied by the vectors $|j,m;r\rangle$ can be written as

$$\langle j,m;r|j',m';r\rangle = \delta_{jj'}\delta_{mm'}, \tag{2.6}$$

$$\sum_{j=0}^{\infty}\sum_{m=-j}^{j}|j,m;r\rangle\langle j,m;r| = I, \tag{2.7}$$

where I is the identity operator.

We are now in a position to introduce the coherent states for a particle on a sphere. Namely, these states are defined as the solution of the eigenvalue equation of the form

$$\mathbf{Z}|\mathbf{z}\rangle = \mathbf{z}|\mathbf{z}\rangle, \tag{2.8}$$

where $\mathbf{Z}$ is given by

$$\mathbf{Z} = \left(\frac{e^{1/2}}{\sqrt{1+4\mathbf{J}^2}}\sinh\tfrac{1}{2}\sqrt{1+4\mathbf{J}^2} + e^{1/2}\cosh\tfrac{1}{2}\sqrt{1+4\mathbf{J}^2}\right)\frac{\mathbf{X}}{r} + i\left(\frac{2e^{1/2}}{\sqrt{1+4\mathbf{J}^2}}\sinh\tfrac{1}{2}\sqrt{1+4\mathbf{J}^2}\right)\mathbf{J}\times\frac{\mathbf{X}}{r}, \tag{2.9}$$

where the cross designates the vector product. The operator $\mathbf{Z}$ and $\mathbf{z}\in\mathbf{C}^3$ obey

$$\mathbf{Z}^2 = 1,\ \mathbf{z}^2 = 1. \tag{2.10}$$

We also write down the following matrix representation of the operator $\mathbf{Z}$ which is crucial for the algebraic analysis of the problem:

$$e^{-(\boldsymbol{\sigma}\cdot\mathbf{J}+1)}\boldsymbol{\sigma}\cdot\mathbf{X} = \boldsymbol{\sigma}\cdot\mathbf{Z}, \tag{2.11}$$

where σ_i, $i=1,2,3$, are the Pauli matrices.

As with the standard coherent states we can generate the coherent states from the "fiducial vector" $|\mathbf{n}_3\rangle$ such that

$$\mathbf{Z}|\mathbf{n}_3\rangle = \mathbf{n}_3|\mathbf{n}_3\rangle, \tag{2.12}$$

where $\mathbf{n}_3 = (0,0,1)$, and

$$|\mathbf{n}_3\rangle = \sum_{j=0}^{\infty} e^{-(1/2)j(j+1)}\sqrt{2j+1}\,|j,0;r\rangle. \tag{2.13}$$

Namely, the coherent states are given by

$$|\mathbf{z}\rangle = \exp\left[\frac{\operatorname{arccosh} z_3}{\sqrt{1-z_3^2}}(\mathbf{z}\times\mathbf{n}_3)\cdot\mathbf{J}\right]|\mathbf{n}_3\rangle. \tag{2.14}$$

The projection of the coherent states (2.14) on the discrete basis vectors $|j,m;r\rangle$ is

$$\langle j,m;r|\mathbf{z}\rangle = e^{-(1/2)j(j+1)}\sqrt{2j+1}\frac{(2|m|)!}{|m|!}\sqrt{\frac{(j-|m|)!}{(j+|m|)!}}\left(\frac{-\epsilon(m)z_1+\mathrm{i}z_2}{2}\right)^{|m|}C_{j-|m|}^{|m|+1/2}(z_3), \tag{2.15}$$

where $\epsilon(m)$ is the sign of m, and $C_n^{\alpha}(x)$ are the Gegenbauer polynomials expressed with the help of the hypergeometric function ${}_2F_1(a,b,c;z)$ by

$$C_n^{\alpha}(x) = \frac{\Gamma(n+2\alpha)}{\Gamma(n+1)\Gamma(2\alpha)}\,{}_2F_1(-n,n+2\alpha,\alpha+\tfrac{1}{2};\tfrac{1}{2}(1-x)). \tag{2.16}$$

As mentioned earlier the coherent states are labeled by points of the classical phase space T^*S^2. The most natural complex parametrization of the phase space discussed in Ref. 1 is of the form

$$\mathbf{z} = \cosh|\mathbf{l}|\,\frac{\mathbf{x}}{r} + \mathrm{i}\frac{\sinh|\mathbf{l}|}{|\mathbf{l}|}\mathbf{l}\times\frac{\mathbf{x}}{r}, \tag{2.17}$$

where the vectors $\mathbf{l}$, $\mathbf{x}\in\mathbf{R}^3$, fulfill $\mathbf{x}^2 = r^2$ and $\mathbf{l}\cdot\mathbf{x} = 0$, that is $\mathbf{l}$ is the classical angular momentum and $\mathbf{x}$ is the radius vector of a particle on a sphere. Clearly, the vector $\mathbf{z}$ satisfies the second equation of (2.10). We point out that due to the quantum fluctuations the practically exact coincidence of average values of $\mathbf{J}$ and $\mathbf{X}$ in the normalized coherent state $|\mathbf{z}\rangle/\sqrt{\langle\mathbf{z}|\mathbf{z}\rangle}$, where $\mathbf{z}$ is given by (2.17), with $\mathbf{l}$ and $\mathbf{x}$, respectively, takes place for $|\mathbf{l}|\geqslant 10$.[1]

III. SCALAR PRODUCT

In this section we identify the Bargmann space of analytic functions corresponding to the coherent states for a particle on a sphere described above. We now restrict, without loss of generality, to the case with the unit sphere. On introducing the spherical coordinates $\mathbf{x} = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$, and parametrizing the tangent vector $\mathbf{l}$ by its norm $|\mathbf{l}| \equiv l$ and the angle α between $\mathbf{l}$ and the meridian passing through the point with the radius vector $\mathbf{x}$, we obtain from (2.17) the following natural coordinates of the phase space compatible with the constraints:

$$\begin{aligned} z_1 &= \cosh l\,\sin\theta\cos\varphi + \mathrm{i}\sinh l(\sin\alpha\cos\varphi\cos\theta - \cos\alpha\sin\varphi),\\ z_2 &= \cosh l\,\sin\theta\sin\varphi + \mathrm{i}\sinh l(\sin\alpha\sin\varphi\cos\theta + \cos\alpha\cos\varphi),\\ z_3 &= \cosh l\cos\theta - \mathrm{i}\sinh l\sin\alpha\sin\theta. \end{aligned} \tag{3.1}$$

Taking into account the fact that $\mathbf{z}$ transforms as the vector we find that the Bargmann space should be specified by

$$\langle\phi|\psi\rangle = \frac{1}{8\pi^2}\int_0^{2\pi}d\varphi\int_0^{\pi}\sin\theta\,d\theta\int_0^{2\pi}d\alpha\int_0^{\infty}dl\,h(l)(\phi(\mathbf{z}^*(\theta,\varphi,\alpha,l)))^*\psi(\mathbf{z}^*(\theta,\varphi,\alpha,l)), \tag{3.2}$$

where $\phi(\mathbf{z}^*) = \langle\mathbf{z}|\phi\rangle$, $\mathbf{z}^* = (z_1^*, z_2^*, z_3^*)$, $h(l)$ is an unknown density and $\mathbf{z}(\theta,\varphi,\alpha,l)$ is expressed by (3.1). Clearly, the corresponding resolution of the identity can be written in the form

$$\frac{1}{8\pi^2}\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\alpha \int_0^{\infty} h(l)dl\, |\mathbf{z}(\theta,\varphi,\alpha,l)\rangle\langle \mathbf{z}(\theta,\varphi,\alpha,l)| = I. \tag{3.3}$$

In order to fix $h(l)$ consider the basis of the Bargmann space with the scalar product (3.2),

$$e_{jm}(\mathbf{z}(\theta,\varphi,\alpha,l)) = \langle j,m|\mathbf{z}\rangle, \tag{3.4}$$

where $|j,m\rangle \equiv |j,m;1\rangle$ and $\langle j,m;r|\mathbf{z}\rangle$ is given by (2.15) and (3.1). Using (3.2) and (3.4) we get after some calculation,

$$\begin{aligned}\langle j,m|j',m'\rangle &= \frac{1}{8\pi^2}\int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta\, d\theta \int_0^{2\pi} d\alpha \int_0^{\infty} dl\, h(l) \\ &\quad \times (e_{jm}(\mathbf{z}^*(\theta,\varphi,\alpha,l)))^* e_{j'm'}(\mathbf{z}^*(\theta,\varphi,\alpha,l)) \\ &= \delta_{jj'}\delta_{mm'} e^{-j(j+1)} \int_0^{\infty} dl\, h(l) P_j(\cosh 2l),\end{aligned} \tag{3.5}$$

where $P_n(z)$ are the Legendre polynomials such that

$$P_n(z) = \frac{1}{2^n n!}\frac{d^n}{dz^n}(z^2-1)^n. \tag{3.6}$$

Thus the normalization condition for the orthonormal basis $\{|j,m\rangle\}$ leads to the following equation on the density $h(l)$:

$$\int_0^{\infty} dl\, h(l) P_j(\cosh 2l) = e^{j(j+1)}. \tag{3.7}$$

We remark that the problem of the solution of this equation is highly nontrivial (see the Acknowledgements) and it is related to the so called problem of moments.[4] We now recall that the Legendre polynomials satisfy the differential equation

$$\left((z^2-1)\frac{d^2}{dz^2} + 2z\frac{d}{dz}\right) P_n(z) = n(n+1)P_n(z). \tag{3.8}$$

From (3.8) it follows easily that

$$\frac{1}{\sinh\rho}\,\frac{d}{d\rho}\sinh\rho\frac{d}{d\rho}P_n(\cosh\rho) = n(n+1)P_n(\cosh\rho). \tag{3.9}$$

We remark that the operator from the left hand side of (3.9) is simply the Laplacian for the two-dimensional hyperbolic space. Consider the heat kernel at the origin in hyperbolic space,[5] given by

$$k_{H^2}(\rho,t) = 2^{1/2}(4\pi t)^{-3/2} e^{-t/4} \int_{\rho}^{\infty} \frac{s e^{-s^2/4t}}{(\cosh s - \cosh\rho)^{1/2}} ds. \tag{3.10}$$

This heat kernel obeys the equation

$$\frac{\partial k_{H^2}}{\partial t} = \frac{1}{\sinh\rho}\,\frac{d}{d\rho}\sinh\rho\frac{d}{d\rho}k_{H^2}(\rho,t), \tag{3.11}$$

subject to the initial condition

$$2\pi \lim_{t\to 0} \int_0^\infty k_{H^2}(\rho,t) f(\rho) \sinh\rho \, d\rho = f(0), \tag{3.12}$$

where f is an arbitrary continuous function with at most exponential growth at infinity. Putting $f(\rho)=P_n(\cosh\rho)$, and making use of (3.11), (3.12) and the fact that $k_{H^2}(\rho,t)$ and $(d/d\rho)k_{H^2}(\rho,t)$ decay faster-than-exponentially, we get

$$2\pi \int_0^\infty k_{H^2}(\rho,t) P_n(\cosh\rho) \sinh\rho \, d\rho = e^{tn(n+1)}. \tag{3.13}$$

Hence, setting in (3.13) $\rho=2l$ and $t=1$, we finally find that the desired density $h(l)$ satisfying (3.7) is

$$h(l) = 4\pi k_{H^2}(2l,1) \sinh 2l \tag{3.14a}$$

$$= \frac{e^{-1/4} \sinh 2l}{\sqrt{2\pi}} \int_{2l}^\infty \frac{s e^{-s^2/4}}{(\cosh s - \cosh 2l)^{1/2}} ds. \tag{3.14a}$$

We have thus identified the Bargmann space for the quantum mechanics on a sphere specified by (3.2) and (3.14). Taking into account (3.1), (3.14a) and the relation which is an immediate consequence of (2.17) such that

$$\mathbf{z}\cdot\mathbf{z}^* = |\mathbf{z}|^2 = \cosh 2l, \tag{3.15}$$

the following form can be derived of the scalar product (3.2) written with the help of the complex variables $\mathbf{z}$ (3.1) analogous to the usual Bargmann representation[6] for the standard coherent states:

$$\langle \phi | \psi \rangle = \int_{\mathbf{z}^2=1} d\mu(\mathbf{z}) (\phi(\mathbf{z}^*))^* \psi(\mathbf{z}^*), \tag{3.16}$$

where

$$d\mu(\mathbf{z}) = \frac{1}{4\pi} k_{H^2}(\operatorname{arccosh}(\mathbf{z}\cdot\mathbf{z}^*),1) dz_1 \, dz_2 \, dz_3 \, dz_1^* \, dz_2^* dz_3^*, \tag{3.17}$$

and $\phi(\mathbf{z}^*)=\langle \mathbf{z}|\phi\rangle$. Evidently, the completeness of the coherent states can be written with the help of the measure $d\mu(\mathbf{z})$ as

$$\int_{\mathbf{z}^2=1} d\mu(\mathbf{z}) |\mathbf{z}\rangle\langle\mathbf{z}| = I. \tag{3.18}$$

IV. REPRODUCING KERNEL

As is well-known the existence of the reproducing kernel is one of the most characteristic properties of coherent states. In view of (3.18) the reproducing property can be written in the form

$$\phi(\mathbf{w}^*) = \int_{\mathbf{z}^2=1} d\mu(\mathbf{z}) \mathcal{K}(\mathbf{w}^*,\mathbf{z}) \phi(\mathbf{z}^*), \tag{4.1}$$

where $\phi(\mathbf{w}^*)=\langle \mathbf{w}|\phi\rangle$, and

$$\mathcal{K}(\mathbf{w}^*,\mathbf{z}) = \langle \mathbf{w}|\mathbf{z}\rangle. \tag{4.2}$$

It should be noted that the reproducing kernel $\mathcal{K}(\mathbf{w}^*,\mathbf{z})$ is the complex conjugate of the analytic function

$$\phi_{\mathbf{w}}(\mathbf{z}^*)=\langle \mathbf{z}|\mathbf{w}\rangle, \tag{4.3}$$

representing the abstract coherent state $|\mathbf{w}\rangle$ also called its symbol. The formula on the overlap $\langle \mathbf{z}|\mathbf{w}\rangle$ can be obtained from (2.14), (2.13) and (2.15). Namely, we have

$$\langle \mathbf{z}|\mathbf{w}\rangle=\sum_{j=0}^{\infty} e^{-j(j+1)}(2j+1)P_j(\mathbf{z}^*\cdot\mathbf{w}), \tag{4.4}$$

where $P_j(z)$ are the Legendre polynomials given by (3.6).

V. ACTION OF OPERATORS

We now discuss the action of operators in the Bargmann representation. We first observe that an immediate consequence of (2.8) is the following formula on the action of operators $\mathbf{Z}^\dagger$:

$$\mathbf{Z}^\dagger\phi(\mathbf{z}^*)=\mathbf{z}^*\phi(\mathbf{z}^*), \tag{5.1}$$

where $\phi(\mathbf{z}^*)=\langle \mathbf{z}|\phi\rangle$ and we recall that $\mathbf{z}^2=1$. Now consider the action of the operator $\mathbf{J}^2$. By (2.4a) the action of the operator $\mathbf{J}^2$ on the basis $e_{jm}(\mathbf{z}^*)=\langle \mathbf{z}|j,m\rangle$ of the Bargmann space is the following one:

$$\mathbf{J}^2 e_{jm}(\mathbf{z}^*)=j(j+1)e_{jm}(\mathbf{z}^*). \tag{5.2}$$

Using (2.15), the differential equation satisfied by the Gegenbauer polynomials of the form

$$\left((z^2-1)\frac{d^2}{dz^2}+(2\lambda+1)\frac{d}{dz}-n(2\lambda+n)\right)C_n^\lambda(z)=0, \tag{5.3}$$

and (5.2) we find that the operator $\mathbf{J}^2$ acts in the representation (3.16) as follows:

$$\mathbf{J}^2\phi(\mathbf{z}^*)=-\left(\mathbf{z}^*\times\frac{\partial}{\partial\mathbf{z}^*}\right)^2\phi(\mathbf{z}^*). \tag{5.4}$$

Taking into account (5.4) and (5.1) we obtain

$$\mathbf{J}\phi(\mathbf{z}^*)=-\mathrm{i}\left(\mathbf{z}^*\times\frac{\partial}{\partial\mathbf{z}^*}\right)\phi(\mathbf{z}^*). \tag{5.5}$$

The relation (5.5) can be easily checked on the basis $e_{jm}(\mathbf{z}^*)$ with the help of (2.15), (2.4a) and (2.5a). Further, using (2.5c), (2.15) and elementary properties of the Gegenbauer polynomials we get

$$X_3\phi(\mathbf{z}^*)=e^{-(1/2)\mathbf{J}^2}z_3^* e^{(1/2)\mathbf{J}^2}\phi(\mathbf{z}^*), \tag{5.6}$$

where the action of $\mathbf{J}^2$ is given by (5.4). The action of the remaining coordinates of the position operator $\mathbf{X}$ can be obtained by means of the following identity describing the complex rotation of $\mathbf{X}$:

$$e^{\mathbf{w}\cdot\mathbf{J}}\mathbf{X}e^{-\mathbf{w}\cdot\mathbf{J}}=\cosh\sqrt{\mathbf{w}^2}\,\mathbf{X}-\mathrm{i}\,\frac{\sinh\sqrt{\mathbf{w}^2}}{\sqrt{\mathbf{w}^2}}\mathbf{w}\times\mathbf{X}+\frac{1-\cosh\sqrt{\mathbf{w}^2}}{\mathbf{w}^2}\mathbf{w}(\mathbf{w}\cdot\mathbf{X}). \tag{5.7}$$

Namely, we have

$$X_1\phi(\mathbf{z}^*)=-\frac{\mathrm{i}}{\sinh 1}(e^{J_2-(1/2)\mathbf{J}^2}z_3^*e^{(1/2)\mathbf{J}^2-J_2}-\cosh 1\,e^{-(1/2)\mathbf{J}^2}z_3^*e^{(1/2)\mathbf{J}^2})\phi(\mathbf{z}^*), \tag{5.8a}$$

$$X_2\phi(\mathbf{z}^*)=\frac{\mathrm{i}}{\sinh 1}(e^{J_1-(1/2)\mathbf{J}^2}z_3^*e^{(1/2)\mathbf{J}^2-J_1}-\cosh 1\,e^{-(1/2)\mathbf{J}^2}z_3^*e^{(1/2)\mathbf{J}^2})\phi(\mathbf{z}^*), \tag{5.8b}$$

where the action of the operators J_i, $i=1,2$, and $\mathbf{J}^2$ is given by (5.5) and (5.4), respectively. Finally, taking into account the identity

$$\mathbf{Z}=e^{-(1/2)\mathbf{J}^2}\mathbf{X}e^{(1/2)\mathbf{J}^2}, \tag{5.9}$$

which is a straightforward consequence of (2.11) and the commutation relation

$$[\mathbf{J}^2,\boldsymbol{\sigma}\cdot\mathbf{X}]=-2(\boldsymbol{\sigma}\cdot\mathbf{J}+1)\boldsymbol{\sigma}\cdot\mathbf{X}, \tag{5.10}$$

following directly from (2.1) and (2.3), we obtain the action of the operator $\mathbf{Z}$. It follows that

$$Z_1\phi(\mathbf{z}^*)=-\frac{\mathrm{i}}{\sinh 1}(e^{J_2-\mathbf{J}^2}z_3^*e^{\mathbf{J}^2-J_2}-\cosh 1\,e^{-\mathbf{J}^2}z_3^*e^{\mathbf{J}^2})\phi(\mathbf{z}^*), \tag{5.11a}$$

$$Z_2\phi(\mathbf{z}^*)=\frac{\mathrm{i}}{\sinh 1}(e^{J_1-\mathbf{J}^2}z_3^*e^{\mathbf{J}^2-J_1}-\cosh 1\,e^{-\mathbf{J}^2}z_3^*e^{\mathbf{J}^2})\phi(\mathbf{z}^*), \tag{5.11b}$$

$$Z_3\phi(\mathbf{z}^*)=e^{-\mathbf{J}^2}z_3^*e^{\mathbf{J}^2}\phi(\mathbf{z}^*). \tag{5.11c}$$

VI. THE BARGMANN REPRESENTATION AND THE COORDINATE REPRESENTATION

In this section we discuss the relationship between the introduced Bargmann representation and the standard coordinate representation for the quantum mechanics on a sphere. We begin with recalling the basic facts about the coordinate representation. Consider the position operators $\mathbf{X}$ for a particle on a sphere satisfying the $e(3)$ algebra (2.1). Recall that we restrict to the irreducible representations which fulfil (2.3) and $\mathbf{X}^2=1$. The coordinate representation is spanned by the common eigenvectors $|\mathbf{x}\rangle$ of the position operators such that

$$\mathbf{X}|\mathbf{x}\rangle=\mathbf{x}|\mathbf{x}\rangle, \tag{6.1}$$

where $\mathbf{x}^2=1$. The resolution of the identity is of the form

$$\int_{\mathbf{x}^2=1}d\nu(\mathbf{x})|\mathbf{x}\rangle\langle\mathbf{x}|=I, \tag{6.2}$$

where $d\nu(\mathbf{x})=d\nu(\theta,\varphi)=\sin\theta\,d\varphi\,d\theta$, accordingly to the natural, i.e., spherical coordinates $\mathbf{x}=(\sin\theta\cos\varphi,\sin\theta\sin\varphi,\cos\theta)$ compatible with the constraint $\mathbf{x}^2=1$. The completeness gives rise to a functional representation of vectors such that

$$\langle\phi|\psi\rangle=\int_{\mathbf{x}^2=1}d\nu(\mathbf{x})\,\phi^*(\mathbf{x})\,\psi(\mathbf{x}), \tag{6.3}$$

where $\phi(\mathbf{x})=\langle\mathbf{x}|\phi\rangle$. Clearly, we can write the completeness condition (6.2) and the scalar product (6.3) as

$$\int_0^{2\pi}d\varphi\int_0^{\pi}\sin\theta\,d\theta|\theta,\varphi\rangle\langle\theta,\varphi|=I, \tag{6.4}$$

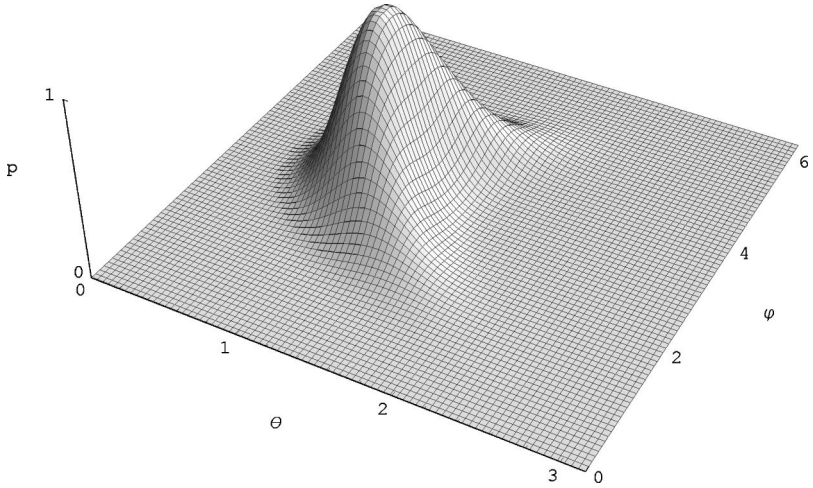

FIG. 1. The plot of the probability density given by (6.14) in the spherical coordinates $\mathbf{x}=(\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\cos\theta)$, where $\mathbf{z}=\cosh|\mathbf{l}|\overline{\mathbf{x}}+\mathrm{i}(\sinh|\mathbf{l}|/|\mathbf{l}|)\mathbf{l}\times\overline{\mathbf{x}}$ [see (2.17)] and $\overline{\mathbf{x}}=(\sin\overline{\theta}\cos\overline{\varphi},\sin\overline{\theta}\sin\overline{\varphi},\cos\overline{\theta})$ with $\overline{\theta}=\pi/3$ and $\overline{\varphi}=\pi$. The viewpoint slightly above the surface.

where $|\theta,\varphi\rangle\equiv|\mathbf{x}\rangle$, and

$$\langle\phi|\psi\rangle=\int_0^{2\pi}d\varphi\int_0^{\pi}\sin\theta\,d\theta\,\phi^*(\theta,\varphi)\psi(\theta,\varphi),\tag{6.5}$$

where $\phi(\theta,\varphi)=\langle\theta,\varphi|\phi\rangle$, respectively. The passage from the coordinate representation to the angular momentum representation generated by the vectors $|j,m\rangle$ satisfying (2.4) with $r=1$ is given by

$$\langle\theta,\varphi|j,m\rangle=Y_{jm}(\theta,\varphi)=(-1)^{(m-|m|)/2}\sqrt{\frac{(2j+1)(j-|m|)!}{4\pi(j+|m|)!}}P_j^{|m|}(\cos\theta)e^{\mathrm{i}m\varphi},\tag{6.6}$$

where $Y_{jm}(\theta,\varphi)$ are the spherical harmonics and $P_n^m(z)$ are the associated Legendre polynomials which can be defined by

$$P_n^m(z)=(-1)^m(1-z^2)^{m/2}\frac{d^m}{dz^m}P_n(z),\tag{6.7}$$

where $P_n(z)$ are the Legendre polynomials given by (3.6). Of course, $Y_{jm}(\theta,\varphi)$ form the orthonormal basis of the Hilbert space of the square integrable functions on a sphere S^2 specified by the scalar product (6.5). Taking into account (6.6) and the identity

$$C_{n-m}^{m+1/2}(z)=(-1)^m\frac{(1-z^2)^{-m/2}m!2^m}{(2m)!}P_n^m(z),\tag{6.8}$$

where $m+1$ is natural, we find that the kernel (6.6) can be written in the form analogous to (2.15) such that

$$\langle\mathbf{x}|j,m\rangle=\sqrt{\frac{2j+1}{4\pi}}\ \frac{(2|m|)!}{|m|!}\sqrt{\frac{(j-|m|)!}{(j+|m|)!}}\left(\frac{-\epsilon(m)x_1-\mathrm{i}x_2}{2}\right)^{|m|}C_{j-|m|}^{|m|+1/2}(x_3).\tag{6.9}$$

Now, let $|(\mathbf{x},\mathbf{l})\rangle$ designate the coherent state $|\mathbf{z}\rangle$ in accordance with the parametrization of the phase space given by (2.17). Equations (5.9), (2.15) and (6.9) taken together yield

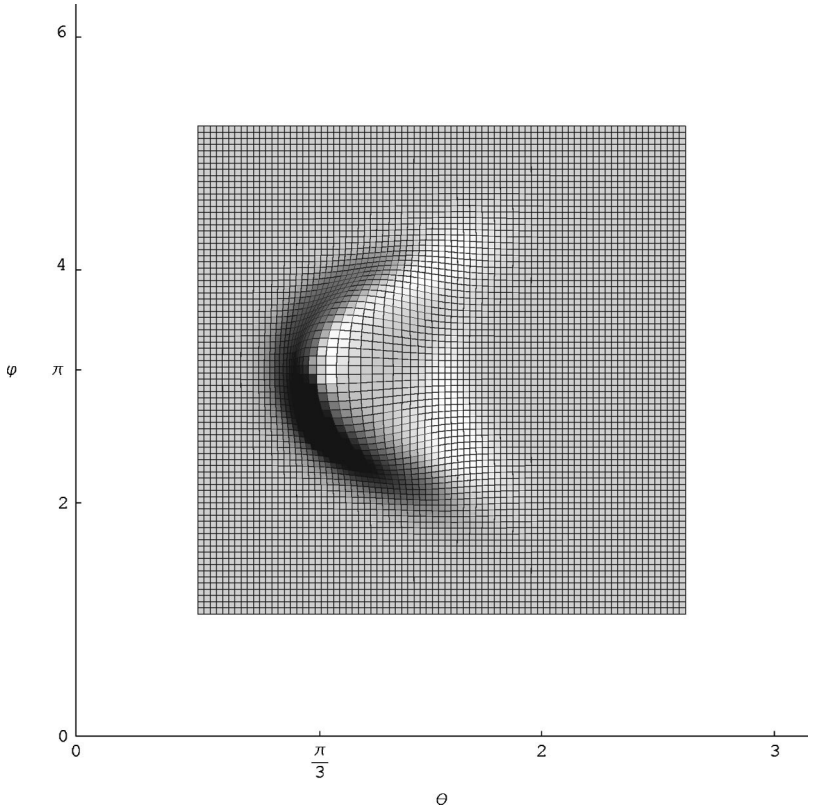

FIG. 2. The plot of the surface from Fig. 1 with the viewpoint directly above. The maximum of the probability density given by (6.14) at $\mathbf{x}=\overline{\mathbf{x}}$ is easily seen.

$$|(\mathbf{x},\mathbf{0})\rangle = \sqrt{4\pi}e^{-(1/2)\mathbf{J}^2}|\mathbf{x}\rangle. \tag{6.10}$$

Using (2.14), (6.10) and (2.13) and proceeding as with (4.4) we find that the passage from the coordinate representation to the coherent states representation is described by the matrix element

$$\langle \mathbf{x}|\mathbf{z}\rangle = \frac{1}{\sqrt{4\pi}} \sum_{j=0}^{\infty} e^{-(1/2)j(j+1)}(2j+1)P_j(\mathbf{x}\cdot\mathbf{z}). \tag{6.11}$$

Evidently, (6.11) defines a unitary map $U:\phi\rightarrow\tilde{\phi}$ from the standard Hilbert space of square integrable functions on the sphere S^2 with the scalar product (6.3) onto the Bargmann space of analytic functions specified by the scalar product (3.16), of the form

$$(U\phi)(\mathbf{z}^*) = \int_{\mathbf{x}^2=1} d\nu(\mathbf{x})k(\mathbf{x}\cdot\mathbf{z}^*)\phi(\mathbf{x}), \tag{6.12}$$

where $k(\mathbf{x}\cdot\mathbf{z})=\langle \mathbf{x}|\mathbf{z}\rangle$. The inverse operator U^{-1} is given by

$$(U^{-1}\tilde{\phi})(\mathbf{x}) = \int_{\mathbf{z}^2=1} d\mu(\mathbf{z})k(\mathbf{x}\cdot\mathbf{z})\tilde{\phi}(\mathbf{z}^*). \tag{6.13}$$

We finally discuss the probability density $p_{\mathbf{z}}(\mathbf{x})$ for the coordinates in the normalized coherent state $|\mathbf{z}\rangle/\sqrt{\langle \mathbf{z}|\mathbf{z}\rangle}$ such that

$$p_{\mathbf{z}}(\mathbf{x}) = \frac{|\langle \mathbf{x}|\mathbf{z}\rangle|^2}{\langle \mathbf{z}|\mathbf{z}\rangle}, \tag{6.14}$$

where $\langle \mathbf{x}|\mathbf{z}\rangle$ and $\langle \mathbf{z}|\mathbf{z}\rangle$ are given by (6.11) and (4.4), respectively. We recall that (6.14) is also called, especially in the context of the theory of quantum chaos the Husimi representation for the localized state on the sphere $|\mathbf{x}\rangle$. Let $\mathbf{z}=\cosh|\mathbf{l}|\overline{\mathbf{x}}+\mathrm{i}(\sinh|\mathbf{l}|/|\mathbf{l}|)\mathbf{l}\times\overline{\mathbf{x}}$ [see (2.17)], so $\overline{\mathbf{x}}$ corresponds to the position and $\mathbf{l}$ to the angular momentum of a particle on a sphere. From computer simmulations it follows that the function $p_{\mathbf{z}}(\mathbf{x})$ is peaked at $\mathbf{x}=\overline{\mathbf{x}}$ (see Figs. 1 and 2). Therefore the parameter $\mathbf{x}$ in the formula (2.17) can be really regarded as the classical position for a particle on a sphere.

VII. DISCUSSION

In this work we have introduced the Bargmann representation referring to the coherent states for a particle on a sphere. The very general construction of the Bargmann space, where the configuration space is a symmetric space, has been recently introduced by Stenzel.[7] As remarked by Hall[8] such construction generalizes the case discussed herein with the configuration space coinciding with the sphere S^2. Nevertheless, it is not formulated in terms of the usual scheme of construction of Bargmann spaces by means of the resolution of the identity for the corresponding coherent states. More precisely, the coherent states are not utilized at all in Ref. 7. The approach taken up in Ref. 7 is very general and as far as we are aware the observations of our work are one of the first concrete nontrivial examples of the general construction discussed in Ref. 7. On the other hand, the construction introduced by Stenzel shows that the formalism introduced in this paper has a deeper mathematical context. We finally point out that the results obtained herein seem to be of interest also in the theory of classical orthogonal polynomials in the complex domain as well as the theory of heat kernels.

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We would like to thank Brian Hall for invaluable comments, especially for pointing out the solution to Eq. (3.7) in terms of the heat kernel for the hyperbolic space. We are convinced that without the solution of (3.7) provided by Brian we could not write this paper. We are also greatful to the referee for helpful comments.

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Algorithms to solve the (quantum) Sutherland model

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We give a self-contained presentation and comparison of two different algorithms to explicitly solve quantum many body models of indistinguishable particles moving on a circle and interacting with two-body potentials of $1/\sin^2$-type. The first algorithm is due to Sutherland and well-known; the second one is a limiting case of a novel algorithm to solve the elliptic generalization of the Sutherland model. These two algorithms are different in several details. We show that they are equivalent, i.e., they yield the same solution and are equally simple. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1389472]

I. INTRODUCTION

We recently presented a novel algorithm to solve the elliptic version of the (quantum) Calogero–Sutherland system.[1,2] In the trigonometric limit, such an algorithm was discovered already about 30 years ago by Sutherland.[3,4] Somewhat surprisingly, the former algorithm in that limit reduces to one which is different from Sutherland's, even though it yields the same solution and is equally simple. The purpose of this article is to give a detailed and self-contained comparison of these two algorithms, including a proof of their equivalence.

The Sutherland model is defined by the differential operator

$$H=-\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2}+2\lambda(\lambda-1)\sum_{1\leqslant j<k\leqslant N}V(x_j-x_k) \tag{1}$$

with $-\pi\leqslant x_j\leqslant\pi$, $N=2,3,\ldots$, $\lambda>0$, and

$$V(r)=\frac{1}{4\sin^2(r/2)}. \tag{2}$$

[To ease notation, we set the length of space to 2π from the start. Of course, an arbitrary length $L>0$ can be easily introduced by rescaling $x_j\to(2\pi/L)x_j$, $H\to(2\pi/L)^2H$, etc.] This differential operator defines a self-adjoint operator on the Hilbert space of square integrable functions on $[-\pi,\pi]^N$, providing a quantum mechanical model for N indistinguishable particles moving on a circle of length 2π and interacting with a two body potential proportional to $V(r)$ where λ determines the coupling strength. (To be precise: This model corresponds to a particularly nice self-adjoint extension of this differential operator which, for $\lambda>1$, corresponds to the Friedrich's extension.[5]) To solve this model amounts to constructing a complete set of eigenfunctions and corresponding eigenvalues of this Hamiltonian.

The starting point for Sutherland's algorithm is the following.

Fact 1:[3] *The wave function*

$$\Psi_0(\mathbf{x})=\prod_{1\leqslant j<k\leqslant N}\psi(x_k-x_j)^{\lambda} \tag{3}$$

with

$$\psi(r)=\sin(r/2) \tag{4}$$

is the ground state of the Sutherland Hamiltonian, $H\Psi_0 = E_0\Psi_0$ with E_0 given in Eq. 9 below.

[To fix the phase of Ψ_0 above, one can interpret $\sin(r/2)^\lambda$ as $\lim_{\varepsilon\downarrow 0}\sin(r/2+\mathrm{i}\varepsilon)^\lambda$, for example. Anyway, the phase ambiguities associated with the exponentiated sines are irrelevant here. In Appendix B 1 we will have to be more careful about similar phase ambiguities in the functions $F(\mathbf{x};\mathbf{y})$ defined later.]

Exploiting this fact, Sutherland constructed all other eigenfunctions f using the following ansatz,

$$f(\mathbf{x}) = \Psi_0(\mathbf{x})\Phi(\mathbf{x}), \tag{5}$$

where Φ are symmetric polynomials (i.e., non-negative powers) in the variables $z_j = \exp(\mathrm{i}x_j)$.[4] The symmetric polynomials thus obtained are the so-called Jack polynomials which have been studied extensively in the mathematics literature, see, e.g., Refs. 6 and 7.

Our algorithm is based on the following.

Fact 2:[1] *The function*

$$F(\mathbf{x};\mathbf{y}) = \frac{\Pi_{1\leqslant j<k\leqslant N}\psi(x_k-x_j)^\lambda \Pi_{1\leqslant j<k\leqslant N}\psi(y_j-y_k)^\lambda}{\Pi_{j,k=1}^{N}\psi(x_j-y_k)^\lambda}, \tag{6}$$

$\psi(r)$ *as in Eq. (4), obeys the following identity,*

$$\sum_{j=1}^{N}\left(\frac{\partial^2}{\partial x_j^2}-\frac{\partial^2}{\partial y_j^2}\right)F(\mathbf{x};\mathbf{y}) = 2\lambda(\lambda-1)\sum_{1\leqslant j<k\leqslant N}(V(x_k-x_j)-V(y_j-y_k))F(\mathbf{x};\mathbf{y}) \tag{7}$$

with $V(r)$ *as in Eq. (2).*

Note that we can write this latter identity as

$$H(\mathbf{x})F(\mathbf{x};\mathbf{y}) = H(\mathbf{y})F(\mathbf{x};\mathbf{y}), \tag{8}$$

where H is the differential operator in Eq. (1) but acting on different arguments $\mathbf{x}$ and $\mathbf{y}$, as indicated. The idea of our algorithm is to take the Fourier transform of Eq. (8) with respect to the variables $\mathbf{y}$, and this yields an identity allowing us to construct eigenfunctions and the corresponding eigenvalues (Proposition 1).

It is interesting to note that Fact 2 holds true in the elliptic case as well [in this case, $\psi(r)$ is a Jacobi theta function $\vartheta_1(r/2)$ with *nome* $q=\exp(-\beta/2)$ and $V(r)$ is Weierstrass' elliptic function $\wp(r)$ with periods 2π and $\mathrm{i}\beta$],[1] in contrast to Fact 1.[8] For the convenience of the reader, an elementary proof of Fact 2 (in the trigonometric case) is given in Appendix A. (This proof uses Fact 1; a self-contained proof valid also in the elliptic case will be given in Ref. 3.)

The plan of the rest of this article is as follows. In Sec. II we review the Sutherland algorithm,[4] mainly to introduce our notation. Section III contains a detailed description of our algorithm. In the final section, Sec. IV, we give the arguments which prove that both algorithms are equivalent, despite various differences. Lengthy proofs are deferred to two Appendices.

II. SUTHERLAND'S ALGORITHM

We use $H\Psi_0 = E_0\Psi_0$ with[3]

$$E_0 = \tfrac{1}{12}\lambda^2 N(N^2-1) \tag{9}$$

and make the ansatz $f=\Phi\Psi_0$. With that the eigenvalue equation $Hf=Ef$ becomes $H'\Phi = E'\Phi$ with $E' = E-E_0$ and[4]

$$H' = -\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2} - \mathrm{i}\lambda\sum_{1\leqslant j<k\leqslant N}\left(\frac{\mathrm{e}^{\mathrm{i}x_j}+\mathrm{e}^{\mathrm{i}x_k}}{\mathrm{e}^{\mathrm{i}x_j}-\mathrm{e}^{\mathrm{i}x_k}}\right)\left(\frac{\partial}{\partial x_j}-\frac{\partial}{\partial x_k}\right). \tag{10}$$

One now determines the action of H' on symmetric polynomials

$$S_{\mathbf{n}}(\mathbf{x})=\sum_{P}\prod_{j=1}^{N}\mathrm{e}^{\mathrm{i}n_j x_{Pj}} \tag{11}$$

where (we note in passing that n_j in Ref. 4 corresponds to n_{N+1-j} below)

$$n_1\geqslant n_2\geqslant\cdots\geqslant n_N\geqslant 0 \tag{12}$$

and the sum is over all permutations P of $\{1,2,\ldots,N\}$. Using the identity[4]

$$(\mathrm{e}^{\mathrm{i}x}+\mathrm{e}^{\mathrm{i}y})\left(\frac{\mathrm{e}^{\mathrm{i}kx}-\mathrm{e}^{\mathrm{i}ky}}{\mathrm{e}^{\mathrm{i}x}-\mathrm{e}^{\mathrm{i}y}}\right)=\mathrm{e}^{\mathrm{i}kx}+\mathrm{e}^{\mathrm{i}ky}+2\sum_{\nu=1}^{k-1}\mathrm{e}^{\mathrm{i}[(k-\nu)x+\nu y]}$$

for $k>0$, one obtains

$$H'S_{\mathbf{n}}=E'_{\mathbf{n}}S_{\mathbf{n}}+\lambda\sum_{1\leqslant j<k\leqslant N}(n_j-n_k)\sum_{\nu=1}^{n_j-n_k-1}S_{\mathbf{n}-\nu\mathbf{E}_{jk}}, \tag{13}$$

where we introduced the notation

$$(\mathbf{E}_{jk})_l=\delta_{jl}-\delta_{kl},\quad j,k,l=1,2,\ldots,N, \tag{14}$$

and defined

$$E'_{\mathbf{n}}=\sum_{j=1}^{N}n_j^2+\lambda\sum_{1\leqslant j<k\leqslant N}(n_j-n_k)=\sum_{j=1}^{N}(n_j^2+\lambda[N+1-2j]n_j). \tag{15}$$

We now introduce the notation

$$\underline{\boldsymbol{\mu}}=\sum_{1\leqslant j<k\leqslant N}\mu_{jk}\mathbf{E}_{jk} \tag{16}$$

for non-negative integers $\boldsymbol{\mu}_{jk}$, and observe that there is a natural order on the set of all these $\underline{\boldsymbol{\mu}}$ (which we can identify with $\mathbb{N}_0^{N(N-1)/2}$),

$$\underline{\boldsymbol{\mu}}<\underline{\boldsymbol{\mu}}'\quad\text{if}\quad\mu_{jk}<\mu'_{jk}\ \text{ for all }\ j<k. \tag{17}$$

It is obvious that $H'S_{\mathbf{n}}$ is a finite linear combination of symmetrized plane waves $S_{\mathbf{n}-\underline{\boldsymbol{\mu}}}$ with $\underline{\boldsymbol{\mu}}\geqslant\underline{\mathbf{0}}$. We thus can make the following ansatz for the eigenfunctions of H',

$$\Phi_{\mathbf{n}}=\sum_{\underline{\boldsymbol{\mu}}\geqslant\underline{\mathbf{0}}}c_{\underline{\boldsymbol{\mu}}}S_{\mathbf{n}-\underline{\boldsymbol{\mu}}} \tag{18}$$

with

$$c_{\underline{\boldsymbol{\mu}}}=0\quad\text{if}\quad(\mathbf{n}-\underline{\boldsymbol{\mu}})_j<(\mathbf{n}-\underline{\boldsymbol{\mu}})_k\ \text{ for at least one }\ j<k. \tag{19}$$

The latter condition shows that there are only a finite number of non-zero $c_{\underline{\boldsymbol{\mu}}}$, i.e., the $\Phi_{\mathbf{n}}$ are polynomials. Then $H'\Phi_{\mathbf{n}}=E'\Phi_{\mathbf{n}}$ implies $E'=E'_{\mathbf{n}}$ and the following recursion relations for the coefficients $c_{\underline{\boldsymbol{\mu}}}$,

$$[E'_{\mathbf{n}}-E'_{\mathbf{n}-\underline{\boldsymbol{\mu}}}]c_{\underline{\boldsymbol{\mu}}}=\lambda\sum_{1\leqslant j<k\leqslant N}\sum_{\nu=1}^{n_j-n_k}[(\mathbf{n}-\underline{\boldsymbol{\mu}})_j-(\mathbf{n}-\underline{\boldsymbol{\mu}})_k+2\nu]c_{\underline{\boldsymbol{\mu}}-\nu\mathbf{E}_{jk}} \tag{20}$$

(we used the fact that the functions $S_{\mathbf{n}}$ are linearly independent). We can set $c_{\mathbf{0}}=1$ (this fixes the normalization of the eigenfunctions) and then determine the other $c_{\boldsymbol{\mu}}$ recursively, which is possible provided that there is no resonance, i.e., if $E'_{\mathbf{n}}-E'_{\mathbf{n}+\boldsymbol{\mu}}$ is nonzero. This is the case: we shall prove at the end of this section that

$$E'_{\mathbf{n}}-E'_{\mathbf{n}-\boldsymbol{\mu}}=\sum_{j<k}\mu_{jk}[(\mathbf{n}-\boldsymbol{\mu})_j-(\mathbf{n}-\boldsymbol{\mu})_k+(n_j-n_k)+2\lambda(k-j)], \tag{21}$$

which is manifestly positive and shows that resonances indeed do not occur. This completes the construction of eigenfunctions and eigenvalues of the Sutherland model: Note that the symmetrized plane waves $S_{\mathbf{n}}$ provide a complete orthonormal basis of the corresponding noninteracting Hamiltonian (obtained by setting $\lambda=0$), and we have constructed eigenfunctions $f_{\mathbf{n}}=\Phi_{\mathbf{n}}\Psi_0$ and corresponding eigenvalues $E_{\mathbf{n}}=E'_{\mathbf{n}}+E_0$ with E_0 in Eq. (9), which are one-to-one to this free solution which is known to provide a complete basis.

Remark 1: We can write [cf. Eq. (15)] $E'_{\mathbf{n}}=\Sigma_j[n_j+\frac{1}{2}\lambda(N+1-2j)]^2-E'_0$ with

$$E'_0=\sum_{j=1}^{N}\frac{1}{4}\lambda^2(N+1-2j)^2. \tag{22}$$

It is easy to show that $E'_0=E_0$ [cf. Eq. (9)], which is somewhat remarkable and implies the following simple form of the eigenvalues,

$$E_{\mathbf{n}}=\sum_{j=1}^{N}\left(n_j+\lambda\left[\frac{1}{2}(N+1)-j\right]\right)^2. \tag{23}$$

The novel algorithm in the next section will yield this simple form of the eigenvalues directly.

For the convenience of the reader, we conclude this section with a proof of Eq. (21).

Proof of Eq. (21): Equation (15) implies

$$E'_{\mathbf{n}}-E'_{\mathbf{n}-\boldsymbol{\mu}}=\sum_j\mu_j[-\mu_j+2n_j+\lambda(N+1-2j)]$$

with

$$\mu_j=(\boldsymbol{\mu})_j=\sum_{k>j}\mu_{jk}-\sum_{k<j}\mu_{kj}. \tag{24}$$

Using

$$\sum_j\mu_j a_j=\sum_{j<k}\mu_{jk}(a_j-a_k) \tag{25}$$

we get

$$E'_{\mathbf{n}}-E'_{\mathbf{n}-\boldsymbol{\mu}}=\sum_{j<k}\mu_{jk}[(\mu_k-\mu_j)+2(n_j-n_k)+2\lambda(k-j)],$$

which proves Eq. (21). □

III. THE NOVEL ALGORITHM

This algorithm is based on the following proposition which, roughly speaking, is obtained by taking the Fourier transform of the remarkable identity in Eq. (8) with respect to **y**.

Proposition 1: Let H be as in Eqs. (1) and (2). Then

$$H\hat{F}(\mathbf{x};\mathbf{n})=E_{\mathbf{n}}\hat{F}(\mathbf{x};\mathbf{n})-\gamma\sum_{1\leqslant j<k\leqslant N}\sum_{\nu=1}^{\infty}\nu\hat{F}(\mathbf{x};\mathbf{n}+\nu\mathbf{E}_{jk}),\tag{26}$$

where

$$\hat{F}(\mathbf{x};\mathbf{n})=\mathcal{P}_{\mathbf{n}}(\mathbf{x})\Psi_0(\mathbf{x}),\quad \mathbf{n}\in\mathbb{Z}^N\tag{27}$$

with Ψ_0 *as in Eqs. (3) and (4) and*

$$\mathcal{P}_{\mathbf{n}}(\mathbf{x})=\lim_{\varepsilon\downarrow 0}\int_{-\pi}^{\pi}\frac{dy_1}{(2\pi)}e^{in_1y_1}\cdots\int_{-\pi}^{\pi}\frac{dy_l}{(2\pi)}e^{in_Ny_N}\frac{\Pi_{1\leqslant j<k\leqslant N}(1-e^{i(y_j-y_k)-(k-j)\varepsilon})^{\lambda}}{\Pi_{j,k=1}^{N}(1-e^{i(x_k-y_j)-j\varepsilon})^{\lambda}},\tag{28}$$

$\mathbf{E}_{jk}$ *as in Eq. (14),* $E_{\mathbf{n}}$ *in Eq. (23), and*

$$\gamma=2\lambda(\lambda-1).\tag{29}$$

(Proof in Appendix B 1.)

Remark 2: To see that these functions $\mathcal{P}_{\mathbf{n}}$ are well-defined, we note that they can be written as

$$\mathcal{P}_{\mathbf{n}}(\mathbf{x})=\oint_{\mathcal{C}_1}\frac{d\xi_1}{2\pi i\xi_1}\xi_1^{n_1}\cdots\oint_{\mathcal{C}_N}\frac{d\xi_N}{2\pi i\xi_N}\xi_N^{n_N}\frac{\Pi_{j<k}(1-\xi_j/\xi_k)^{\lambda}}{\Pi_{j,k}(1-e^{ix_k}/\xi_j)^{\lambda}}$$

with integration paths $\mathcal{C}_j:\xi_j=e^{\varepsilon j}e^{iy_j}$, $-\pi\leqslant y_j\leqslant\pi$, where $\varepsilon>0$ is arbitrary.

We now show that this proposition provides a solution algorithm: Eq. (26) implies that the action of H on the functions $\hat{F}(\mathbf{x};\mathbf{n})$ is triangular, i.e., $H\hat{F}(\mathbf{x};\mathbf{n})$ is a linear combination of functions $F(\mathbf{x};\mathbf{n}+\boldsymbol{\mu})$ with $\boldsymbol{\mu}\geqslant\underline{\mathbf{0}}$. We thus can make the following ansatz for eigenfunctions,

$$f_{\mathbf{n}}(\mathbf{x})=\sum_{\boldsymbol{\mu}\geqslant\underline{\mathbf{0}}}a_{\boldsymbol{\mu}}F(\mathbf{x};\mathbf{n}+\boldsymbol{\mu}),\tag{30}$$

and then $Hf_{\mathbf{n}}=Ef_{\mathbf{n}}$ implies

$$\sum_{\boldsymbol{\mu}\geqslant\underline{\mathbf{0}}}F(\mathbf{x};\mathbf{n}+\boldsymbol{\mu})\left([E_{\mathbf{n}+\boldsymbol{\mu}}-E]a_{\boldsymbol{\mu}}-\gamma\sum_{1\leqslant j<k\leqslant N}\sum_{\nu=1}^{\mu_{jk}}\nu a_{\boldsymbol{\mu}-\nu\mathbf{E}_{jk}}\right)=0.$$

We thus see that how we get a solution of $Hf_{\mathbf{n}}=Ef_{\mathbf{n}}$ is we set $E=E_{\mathbf{n}}$ and determine the coefficients $a_{\boldsymbol{\mu}}$ by the following recursion relations,

$$[E_{\mathbf{n}+\boldsymbol{\mu}}-E_{\mathbf{n}}]a_{\boldsymbol{\mu}}=\gamma\sum_{1\leqslant j<k\leqslant N}\sum_{\nu=1}^{\mu_{jk}}\nu a_{\boldsymbol{\mu}-\nu\mathbf{E}_{jk}},\tag{31}$$

which has triangular structure: we can set $a_{\underline{\mathbf{0}}}=1$ (this fixes the normalization), and then the other $a_{\boldsymbol{\mu}}$ can be determined recursively in terms of the $a_{\boldsymbol{\mu}'}$ where $\boldsymbol{\mu}'<\boldsymbol{\mu}$, at least if there is no resonance, i.e., if $E_{\mathbf{n}+\boldsymbol{\mu}}-E_{\mathbf{n}}$ does not vanish. This is true due to the following.

Lemma 1:

$$E_{\mathbf{n}+\boldsymbol{\mu}}-E_{\mathbf{n}}=\sum_{j=1}^{N}\mu_j^2+\sum_{1\leqslant j<k\leqslant N}2\mu_{jk}[(n_j-n_k)+\lambda(k-j)]\tag{32}$$

with μ_j *in Eq. (24), which is manifestly positive provided that Eq. (12) holds true.*

(Proof in Appendix B 2.)

Moreover, the following lemma shows that the $f_{\mathbf{n}}$ are in fact symmetric polynomials, i.e., a finite linear combination of the functions $S_{\mathbf{n}}$ in Eq. (11).

Lemma 2: The functions $\mathcal{P}_{\mathbf{n}}$ in Eq. (28) all are symmetric polynomials in the variables $z_j = \exp(\mathrm{i}x_j)$ which are nonzero only if

$$n_j + n_{j+1} + \ldots + n_N \geqslant 0 \quad \forall j = 1,2,\ldots,N. \tag{33}$$

They can be written as

$$\mathcal{P}_{\mathbf{n}}(\mathbf{x}) = \sum_{\mathbf{m}} p_{\mathbf{n},\mathbf{m}} S_{\mathbf{m}}(\mathbf{x}) \tag{34}$$

with $S_{\mathbf{m}}(\mathbf{x})$ as in Eq. (11), and the coefficients are

$$p_{\mathbf{n},\mathbf{m}} = \Sigma'' \prod_{1 \leqslant j' < k' \leqslant N} \prod_{j,k=1}^{N} \binom{\lambda}{\mu_{j'k'}} \binom{-\lambda}{\nu_{jk}} (-1)^{\mu_{j'k'} + \nu_{jk}}, \tag{35}$$

where the sum Σ'' is over all non-negative integers μ_{jk}, ν_{jk} restricted by the following $2N$ equations,

$$n_j = \sum_{l=1}^{N} \nu_{lj} + \sum_{l=1}^{j-1} \mu_{lj} - \sum_{l=j+1}^{N} \mu_{jl}, \quad m_j = \sum_{l=1}^{N} \nu_{jl}, \tag{36}$$

and $m_1 \geqslant m_2 \geqslant \cdots \geqslant m_N \geqslant 0$, implying in particular that there are only terms such that

$$\sum_{j=1}^{N} m_j = \sum_{j=1}^{N} n_j. \tag{37}$$

(Proof in Appendix B 3.)

Indeed, this lemma implies the sum in Eq. (30) has only a finite number of nonzero terms [since there is only a finite number of $\boldsymbol{\mu}$ such that $\mathbf{n}' = \mathbf{n} + \boldsymbol{\mu}$ obeys all the conditions in Eq. (33)], and thus the $f_{\mathbf{n}}$ are a finite number of terms each of which is a finite linear combination of functions $S_{\mathbf{n}}$ in Eq. (11).

IV. CONCLUSIONS

We can summarize our discussion in the previous sections as follows.

Proposition 2: For each $\mathbf{n} \in \mathbb{Z}^N$ such that $n_1 \geqslant n_2 \geqslant \cdots \geqslant n_N \geqslant 0$, the standard algorithm reviewed in Sec. III and the novel one presented in Sec. IV both yield an eigenfunction $f_{\mathbf{n}}$ of the Sutherland Hamiltonian H in Eq. (1). In both cases, this eigenfunction is of the form

$$f_{\mathbf{n}}(\mathbf{x}) = \Phi_{\mathbf{n}}(\mathbf{x}) \Psi_0(\mathbf{x})$$

with Ψ_0 in Eqs. (3) and (4) and $\Phi_{\mathbf{n}}$ a symmetric polynomial in the variables $z_j = \exp(\mathrm{i}x_j)$, and the corresponding eigenvalues $E_{\mathbf{n}}$ are given in Eq. (23).

It thus follows from Theorem 3.1 in Ref. 7 that, for nondegenerate eigenvalues $E_{\mathbf{n}}$, the eigenfunctions $f_{\mathbf{n}}$ obtained with the two algorithms are equal (up to normalization), and the functions $\Phi_{\mathbf{n}}$ are proportional to the so-called Jack polynomials (see Sec. 2 in Ref. 9 for details; this latter reference actually seems to suggest that this is true even for nondegenerate eigenvalues). We feel that this is quite remarkable since, even though the two algorithms look somewhat similar and both yield the same solution, there are several differences in details:

(i) The building blocks of the eigenfunctions in the novel algorithm are the functions $\mathcal{P}_{\mathbf{n}}$ defined in Eq. (28) and not the plane waves $S_{\mathbf{n}}$ in Eq. (11).

(ii) With the standard algorithm, one obviously obtains eigenfunctions with polynomials $\Phi_{\mathbf{n}}$ which have the form

$$\Phi_{\mathbf{n}} = \sum_{\mathbf{m} \leqslant \mathbf{n}} v_{\mathbf{n},\mathbf{m}} S_{\mathbf{m}},$$

where the partial order here is defined as

$$\mathbf{m} \leqslant \mathbf{n} : \Leftrightarrow \sum_{j=1}^{k} m_j \leqslant \sum_{j=1}^{k} n_j \quad \forall k = 1,2,\ldots,N. \tag{38}$$

[This is called *dominance ordering* in Ref. 7; the latter fact follows from Eq. (18) and $\mathbf{n} \geqslant \mathbf{n} - \boldsymbol{\mu}$ for all $\boldsymbol{\mu} \geqslant \underline{\mathbf{0}}$]. This is not at all obvious for the eigenfunctions obtained with the novel algorithm [but of course should be true as well, at least for nondegenerate eigenfunctions.]

(iii) In both algorithms it is important to rule out the occurrence of resonances, but the reason for that is different [cf. Eq. (21) with Lemma 1 above, and observe the different sign of $\boldsymbol{\mu}$].

(iv) In the novel algorithm the restriction in Eq. (12) can be dropped, and in fact the solutions thus obtained are relevant in the elliptic case.[1] There seems no way to drop this restriction in the standard algorithm.

(v) From Sutherland's algorithm it seems somewhat surprising that the eigenvalues all can be written in the simple form $E_{\mathbf{n}} = \Sigma_j P_j^2$, but from the novel algorithm this is obvious.

(vi) As discussed in the Introduction, the novel algorithm can be generalized to the elliptic case.[1,2]

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APPENDIX A: PROOF OF FACT 2

We note that

$$F(\mathbf{x};\mathbf{y}) = \Psi_0(\mathbf{x})\Psi_0(\mathbf{y}) \frac{1}{\prod_{j,k=1}^{N} \psi(x_j - y_k)^{\lambda}}, \tag{A1}$$

with Ψ_0 in Eq. (3) and ψ in Eq. (4). Using $H\Psi_0 = E_0\Psi_0$ (Ref. 3) and the Leibniz rule of differentiation we obtain

$$H(\mathbf{x})F(\mathbf{x};\mathbf{y}) = \Bigg(E_0 + 2\lambda^2 \sum_{j,l} \sum_{k \neq j} \phi(x_j - x_k)\phi(x_j - y_l) + \sum_{j,k} \lambda \phi'(x_j - y_k) - \sum_{j,k,l} \lambda^2 \phi(x_j - y_k)\phi(x_j - y_l) \Bigg) F(\mathbf{x};\mathbf{y}),$$

where

$$\phi(r) = \psi'(r)/\psi(r) = \tfrac{1}{2}\cot(r/2) \tag{A2}$$

(the prime indicates differentiation). Thus

$$[H(\mathbf{x}) - H(\mathbf{y})]F(\mathbf{x};\mathbf{y}) = \lambda^2(\cdot)F(\mathbf{x};\mathbf{y})$$

with

$$(\cdot) \equiv \Bigg[\sum_{j,l} \sum_{k \neq j} 2\phi(x_j - x_k)\phi(x_j - y_l) - \sum_{j,k} \sum_{l \neq k} \phi(x_j - y_k)\phi(x_j - y_l) \Bigg] - [\mathbf{x} \leftrightarrow \mathbf{y}],$$

where "$[\mathbf{x}\leftrightarrow\mathbf{y}]$" means "the same terms but with $\mathbf{x}$ and $\mathbf{y}$ interchanged" (we used that all terms which are even under $[\mathbf{x}\leftrightarrow\mathbf{y}]$ cancel). Relabeling indices and using $\phi(-r)=-\phi(r)$ we rewrite

$$(\cdot)=\sum_{j,l}\sum_{k\neq j}[\phi(x_j-x_k)\phi(x_j-y_l)+\phi(x_k-x_j)\phi(x_k-y_l)-\phi(x_l-y_j)\phi(x_l-y_k)]-[\mathbf{x}\leftrightarrow\mathbf{y}]$$

$$=\sum_{j,l}\sum_{k\neq j}[\phi(x_j-x_k)\phi(x_j-y_l)+\phi(x_j-x_k)\phi(y_l-x_k)+\phi(y_l-x_j)\phi(y_l-x_k)]-[\mathbf{x}\leftrightarrow\mathbf{y}].$$

We now can use the trigonometric identity

$$\cot(x)\cot(y)+\cot(x)\cot(z)+\cot(y)\cot(z)=1 \quad \text{if } x+y+z=0, \tag{A3}$$

which shows that

$$\phi(x_j-x_k)\phi(x_j-y_l)+\phi(x_j-x_k)\phi(y_l-x_k)+\phi(y_l-x_j)\phi(y_l-x_k)=-\tfrac{1}{2}$$

and thus proves $(\cdot)=0$. □

APPENDIX B: OTHER PROOFS

1. Proof of Proposition 1

We first observe two simple but useful facts. First, the relation in Eq. (8) remains true if we replace $F(\mathbf{x};\mathbf{y})$ by

$$F'(\mathbf{x};\mathbf{y})=c\,\mathrm{e}^{\mathrm{i}P\sum_{j=1}^{N}(x_j-y_j)}F(\mathbf{x};\mathbf{y}) \tag{B1}$$

for arbitrary constants $P\in\mathbb{R}$ and $c\in\mathbb{C}$. [To see this, introduce center-of-mass coordinates $X=\sum_{j=1}^{N}x_j/N$ and $x_j'=(x_j-x_1)$ for $j=2,\ldots,N$, and similarly for y. Then $H(\mathbf{x})=-\partial^2/\partial X^2+H_c(\mathbf{x}')$, and similarly for $H(\mathbf{y})$. Invariance of Eq. (8) under $F\to\mathrm{e}^{-\mathrm{i}P(X-Y)N}F$ thus follows from $(\partial/\partial X+\partial/\partial Y)F(\mathbf{x};\mathbf{y})=0$, and the latter is implied by the obvious invariance of $F(\mathbf{x};\mathbf{y})$ under $x_j\to x_j+a$, $y_j\to y_j+a$, $a\in\mathbb{R}$. The invariance of Eq. (8) under $F\to cF$ is trivial, of course.] Second, the variables y_j in Eq. (8) need not be real but can be complex.

As mentioned, we intend to perform a Fourier transformation of the identity in Eq. (8), i.e., apply to it $(2\pi)^{-N}\int\mathrm{d}^N\mathbf{y}\,\mathrm{e}^{\mathrm{i}\mathbf{P}\cdot\mathbf{y}}$ with suitable momenta $\mathbf{P}$. We need to do this with care: first, the differential operator $H(\mathbf{y})$ has singularities at points $y_j=y_k$, and, second, the function $F(\mathbf{x};\mathbf{y})$ is not periodic in the variables y_j but changes by phase factors under $y_j\to y_j+2\pi$. We therefore need to specify suitable integration contours for the y_j's avoiding the singular points, and we need to choose the P_j so as to compensate the nonperiodicity. To do that, we replace the real coordinates y_j by

$$z_j=y_j-\mathrm{i}j\varepsilon \tag{B2}$$

with $\varepsilon>0$ a regularization parameter: as we will see, we can then integrate along the straight lines from $y_j=-\pi$ to π and after that perform the limit $\varepsilon\downarrow 0$. Since for all $j<k$, $z_j-z_k=y_j-y_k+\mathrm{i}\varepsilon_{kj}$ with $\varepsilon_{kj}=(k-j)\varepsilon>0$, we can use

$$\sin[(y+\mathrm{i}\varepsilon)/2]=\tfrac{1}{2}\,\mathrm{e}^{\mathrm{i}\pi/2}\mathrm{e}^{-\mathrm{i}y/2+\varepsilon/2}(1-\mathrm{e}^{\mathrm{i}y-\varepsilon}) \tag{B3}$$

for $\varepsilon>0$. Taking the log of this identity and differentiating we obtain $(1/2\cot[(y+\mathrm{i}\varepsilon)/2])=-\mathrm{i}/[1-\exp(\mathrm{i}y-\varepsilon)]$. Expanding the rhs in a geometric series and differentiating once more yields

$$\frac{1}{4\sin^2[(y+\mathrm{i}\varepsilon)/2]}=-\sum_{\nu=1}^{\infty}\nu\mathrm{e}^{\mathrm{i}\nu y-\nu\varepsilon}. \tag{B4}$$

This accounts for all singularities and branch cuts in a consistent way. To determine the suitable **P** use Eq. (B3) and compute

$$F(\mathbf{x};\mathbf{z})=(\cdots)\,\Psi_0(\mathbf{x})\check{\mathcal{P}}^{\varepsilon}(\mathbf{x};\mathbf{y})$$

with $\Psi_0(\mathbf{x})$ in Eqs. (3) and (4),

$$\check{\mathcal{P}}^{\varepsilon}(\mathbf{x};\mathbf{y})=\frac{\prod_{1\leqslant j<k\leqslant N}(1-e^{i(y_j-y_k)-(k-j)\varepsilon})^{\lambda}}{\prod_{j,k=1}^{N}(1-e^{i(x_j-y_k)-k\varepsilon})^{\lambda}} \tag{B5}$$

a function periodic in all the y_j, and

$$(\cdots)=\left(\frac{1}{2}e^{i\pi\lambda/2}\right)^{N(N-1)/2-N^2}\frac{\prod_{1\leqslant j<k\leqslant N}e^{-i\lambda(y_j-y_k)/2+\lambda(k-j)\varepsilon/2}}{\prod_{j,k=1}^{N}e^{-i\lambda(x_j-y_k)/2+\lambda k\varepsilon/2}}$$

$$=\text{const}\,e^{i\lambda N\Sigma_{j=1}^{N}(x_j-y_j)/2}e^{-i\lambda\Sigma_{j=1}^{N}(N+1-2j)y_j/2}$$

[we used $\Sigma_{j<k}(y_j-y_k)=\Sigma_j(N+1-2j)y_j$]. We thus see that we can choose P and c in Eq. (B1) such that

$$F'(\mathbf{x};\mathbf{z})=e^{-i\lambda\Sigma_{j=1}^{N}[(N+1)/2-j]y_j}\check{\mathcal{P}}^{\varepsilon}(\mathbf{x};\mathbf{y})\Psi_0(\mathbf{x}). \tag{B6}$$

We need to choose the Fourier variables $\mathbf{P}=(P_1,\ldots,P_N)$ such that $e^{i\mathbf{P}\cdot\mathbf{y}}F'(\mathbf{x};\mathbf{z})$ is periodic in all y_j, and this implies

$$P_j=n_j+\lambda[\tfrac{1}{2}(N+1)-j],\quad n_j\in\mathbb{Z}. \tag{B7}$$

We now can apply $(2\pi)^{-N}\int d^N\mathbf{y}\,e^{i\mathbf{P}\cdot\mathbf{y}}$ to the identity $H(\mathbf{x})F'(\mathbf{x};\mathbf{z})=H(\mathbf{z})F'(\mathbf{x};\mathbf{z})$. We recall

$$H(\mathbf{z})=-\sum_j\frac{\partial^2}{\partial y_j^2}+\gamma\sum_{j<k}\frac{1}{4\sin^2[(y_j-y_k+i(k-j)\varepsilon)/2]}$$

and use Eq. (B4). After taking the limit $\varepsilon\downarrow 0$ we obtain Eq. (26): the lhs is obvious (note that $\hat{F}$ is the Fourier transform of F'). The rhs has two terms. The first one is equal to $\Sigma_j P_j^2\hat{F}$ and comes from the derivative terms which we evaluated by partial integration. The second term is obtained from the $1/\sin^2$-terms in $H(\mathbf{z})F'$ which we computed using Eq. (B4). □

2. Proof of Lemma 1

We write $(\mathbf{n}+\boldsymbol{\mu})_j=n_j+\mu_j$ with μ_j in Eq. (16). Thus Eqs. (23) and (25) imply

$$E_{\mathbf{n}+\boldsymbol{\mu}}-E_{\mathbf{n}}=\sum_j\left(\mu_j^2+2\mu_j\left(n_j+\lambda\left[\frac{1}{2}(N+1)-j\right]\right)\right),$$

and with Eq. (25) we obtain Eq. (32). □

3. Proof of Lemma 2

It is straightforward to evaluate $\mathcal{P}_{\mathbf{n}}(\mathbf{x})$ in Eq. (28) by expanding all terms in Taylor series (using the binomial series) and then performing the y_j integrations which corresponds to a projection onto the y_j-independent terms. The result is

$$\mathcal{P}_{\mathbf{n}}(\mathbf{x})=\sum{}'\prod_{1\leqslant j'<k'\leqslant N}\prod_{j,k=1}^{N}\binom{\lambda}{\mu_{j'k'}}\binom{-\lambda}{\nu_{jk}}(-1)^{\mu_{j'k'}+\nu_{jk}}e^{i\nu_{jk}x_j} \tag{B8}$$

where the sum Σ' is over all non-negative integers $\mu_{kk'}$ and ν_{jl} such that

$$n_j - \sum_{l=1}^{N} \nu_{lj} - \sum_{l=1}^{j-1} \mu_{lj} + \sum_{l=j+1}^{N} \mu_{jl} = 0. \tag{B9}$$

Recalling the definition of $S_{\mathbf{n}}$ in Eq. (11) we obtain Eqs. (34)–(36).

We now argue that this latter system of equations can have solutions only if the conditions in Eq. (33) all hold, which implies that otherwise $\mathcal{P}_{\mathbf{n}}$ is zero. To see this we add up the last $N+1-k$ relation in Eq. (B9) ($k=N,N-1,\ldots,1$), and by a relabeling of indices we obtain

$$\sum_{j=k}^{N} n_j = \sum_{j=k}^{N} \sum_{l=1}^{N} \nu_{lj} + \sum_{l=1}^{k-1} \sum_{j=k}^{N} \mu_{lj}$$

where the rhs is always manifestly positive. This proves Eq. (33). Setting $k=1$ and comparing with Eq. (36) we obtain Eq. (37). Moreover, for fixed n_j, there are at most a finite number of different solutions of Eq. (B9), implying that $\mathcal{P}_{\mathbf{n}}$ is a polynomial. To see that we write Eq. (B9) as follows,

$$n_j + \sum_{l=j+1}^{N} \mu_{jl} = \sum_{l=1}^{N} \nu_{lj} + \sum_{l=1}^{j-1} \mu_{lj}, \tag{B10}$$

and determine possible solutions for decreasing values of j starting at $j=N$. It is easy to prove by induction that there is only a finite number of solutions

$$\{\nu_{lj}\}_{j,l=1}^{N}, \{\mu_{jl}\}_{1 \leqslant j < l \leqslant N} \in \mathbb{N}_0^{N^2 + N(N-1)/2}$$

of this system of equations: For $j=N$ we get

$$n_N = \sum_{l=1}^{N} \nu_{lN} + \sum_{l=1}^{N-1} \mu_{lN}$$

and there is obviously only a finite number of different solutions $\{\nu_{lN}\}_{l=1}^{N}, \{\mu_{lN}\}_{l=1}^{N-1}$ of that equation. If we consider Eq. (B10) for some $j=j_0<N$, the possible solutions for $\{\mu_{j_0,l}\}_{l>j_0}$ were already determined by the equations for $j>j_0$ and, by the induction hypothesis, there is only a finite number of them. One thus only has to consider a finite number of equations, and each of them obviously has only a finite number of solutions $\{\nu_{lj}\}_{l=1}^{N}, \{\mu_{lj}\}_{l=1}^{j-1}$. □

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Yang–Mills field quantization in the factor space

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The perturbation theory over inverse interaction constant $1/g$ is constructed for Yang–Mills theory. It is shown that the new perturbation theory is free from the gauge ghosts and Gribov's ambiguities, and each order over $1/g$ presents the gauge-invariant quantity. It is remarkable that offered perturbation theory did not contain divergences, at least in the vector fields sector, and no renormalization procedure is necessary for it. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The perturbation theory for $(3+1)$-dimensional Yang–Mills field theory in the vicinity of the extremum $u^a_\mu(x)$ of the action will be described.[1] It is our first publication in this field and it seems reasonable to define from the very beginning the level of its completeness. Namely, we would like to show that, contrary to the ordinary perturbative QCD (pQCD), the offered theory may be used at arbitrary distances. Accordingly, the theory is free from divergences at least in the vector fields sector. Besides the perturbation theory is operated with transparently gauge invariant quantities and no ghosts and Gribov ambiguities would hinder the computations.

We will realize the perturbation theory in the factor space $\mathcal{G}/\mathcal{H}$, where $\mathcal{G}$ is the symmetry group of theory and $\mathcal{H}$ is the symmetry of $u^a_\mu(x)$. Introductory notes for this formalism were given in Ref. 2.

The usefulness of such choice follows from homogeneity and isotropy of $\mathcal{G}/\mathcal{H}$ in the semi-classical approximation. The developed perturbation theory is formulated to describe the violation of these property quantum excitations. One may note that we offer the realization of perturbation theory in terms of the action-angle type variables. As an example one may have in mind the factor space[3]

$$W_G = O(4,2)\times G/O(4)\times O(2), \tag{1}$$

where G is the non-Abelian gauge group.

The formalism will be demonstrated for simplest quantity—the vacuum-into-vacuum transition amplitude

$$\mathcal{Z}(u) = \langle \mathrm{vac};u|\mathrm{vac};u\rangle,$$

along the path $u^a_\mu(x)$. Moreover, following the idea that the calculation should be adjusted to the experiment's ability,[2] we will restrict ourselves to calculating only the modulo squire

$$\mathcal{N}(u) = |\langle \mathrm{vac};u|\mathrm{vac};u\rangle|^2 = |\mathcal{Z}(u)|^2,$$

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since, being the unmeasurable quantity, the phase of $\mathcal{Z}(u)$ is not important from a physical point of view[4] (it is the principle of ''minimal necessity'' in our terminology).

This quantity $\mathcal{N}(u)$ would normalize the observables and is equal to squire of the volume of $\mathcal{G}/\mathcal{H}$, see Ref. 5. So, it defines a number of expected on the trajectory $u_{\mu a}(x)$ degrees of freedom, i.e. $(\ln \mathcal{N}(u))/2$ is proportional to the dimension of $\mathcal{G}/\mathcal{H}$. In the example (1):

$$\dim W_G = \dim G + 8 \tag{2}$$

since the $O(4)\times O(2)$-invariant solution $u_{\mu a}(x)$ breaks both the gauge and the spatial symmetries. Last one includes the translational and spatial conformal transformations.[3]

Having in consideration the probabilitylike quantity $\mathcal{N}(u)$, one can include into formalism the total probabilities conservation principle (see Ref. 2, where the role of unitarity condition in the formation of quantum dynamics is described in detail). So, one may prove that if we postulate the path-integral representation for $\mathcal{Z}(u)$, see (13) for the scalar field case, and take into account the S-matrix unitarity condition then, if the canonical perturbation series exist (at least in Borel sense), $\mathcal{N}$ has the following strict path-integral representation:

$$\mathcal{N} = e^{-i\mathcal{K}(je)} \int DM_j(A) e^{-2iU(A,e)}. \tag{3}$$

In this expression $\mathcal{K}(je)$ acts as the differential operator of the auxiliary variables $j_{a\mu}$ and $e_{a\mu}$ at $j_{a\mu} = e_{a\mu} = 0$, see (15) and (84), and the expansion of $\exp\{-i\mathcal{K}\}$ generates the perturbation series. The functional $U(A,e)$ defines interaction. It may be expressed through the input classical action, see (16) and (85). The main point of our consideration is the differential measure DM_j since it is δ-like:

$$DM_j(A) = \prod_{a,\mu} \prod_x \mathrm{d}A^{a\mu}(x)\, \delta\left(\frac{\delta S(A)}{\delta A^a_\mu(x)} + j^{a\mu}(x) \right), \tag{4}$$

where $S(A)$ is the classical Yang–Mills action. Notice that using the Fourier transform of functional δ-function in (4), one may easily find from (3) that $\mathcal{N}(u) = |\mathcal{Z}(u)|^2$.

The structure of representation (3) did not depend on the dimension of the system, concrete form of the Lagrangian, and other ''local'' properties of the theory. We will not repeat for this reason the derivation of (3) since it is the same as in Ref. 2 [and Ref. 6, where the $(1+1)$-dimensional exactly integrable field theory was considered].

Following the definitions of δ-function and operator $\mathcal{K}(je)$, one should start from the equation:

$$\frac{\delta S(A)}{\delta A^a_\mu(x)} = 0. \tag{5}$$

So, having a theory on the δ-like measure, we must consider[2] only the *strict* solution of Lagrange equation. Notice that Eq. (5) also has the ''trivial'' solution $A^a_\mu(x) = 0$, with the corresponding factor space W_0, $\dim W_0 = \dim G$, where G is the gauge group. The pQCD presents expansion around just this ''trivial'' solution.

Then, if the general position concerning initial data is analyzed, we should neglect this ''trivial'' solution since we will assume that our solution $u^a_\mu(x)$ is live in the factor space of $\dim(\mathcal{G}/\mathcal{H}) > \dim W_0$. This is a formal reason why the expansion in vicinity of $u_{\mu a}(x) \neq \mathrm{const}$ would be considered. Corresponding realization of the Yang–Mills theory would be the topological QCD (tQCD).

This selection rule[2] is our definition of the ground state. Its importance should be stressed. It says that first of all one should consider such solution of the Lagrange equation in the Minkowski space which is live in the factor space $\mathcal{G}/\mathcal{H}$ of highest dimension since, generally speaking, other orbits are realized on zero measure.[7]

The extraordinary role of the factor space has specific explanation. At first glance δ-likeness of measure (4) solves the problem of path integral calculation. But actually, to calculate the remaining integral in (3), measure (4) forces us to search new forms of perturbation theory. The formal reason is hidden in inhomogeneity of our Lagrange equation, see (4),[8]

$$-\frac{\delta S(A)}{\delta A^a_\mu(x)}=j^{a\mu}(x). \tag{6}$$

So, the exact solutions of this equation are unknown even in the expansion over $j^{a\mu}(x)$ form if the corresponding homogeneous equation (5) has nontrivial solution $u_{a\mu}(x)\neq\text{const}$.

Nevertheless one may try to solve this equation in the form of some perturbation series, expanding solution over $j^{a\mu}(x)$. This will lead to the theory which may have a near resemblance of the canonical one, see, e.g., Ref. 9, where the ''straight pass'' approximation was considered.

But the canonical perturbation theory for non-Abelian gauge theories have additional problems. First of all, the method of Faddeev–Popov,[10] introduced for separation of dynamical degrees of freedom from pure gauge ones, in most cases leads to the cumbersome perturbation theory with nonunitary ghost fields Lagrangian.[11] In the quantum gravity this, at first glance, technical complication, rises up to a fundamental one, see, e.g., Ref. 12.

Then, it was noted that it is impossible to fix the Coulomb gauge unambiguously for the Yang–Mills potentials of nontrivial topology.[13] Moreover, it was shown later that this conclusion did not depend on the chosen gauge, and is general for non-Abelian gauge theories[14] if the expansion is built around the nontrivial topology gauge orbits.[15]

We will realize another approach to the problem. Namely, we will consider the mapping into the corresponding to $u_{a\mu}=u_{a\mu}(x;\xi,\eta,\lambda_a)$ factor space. Formally the mapping can be performed since the δ-like measure (4) defines the necessary and sufficient set of contributions into the functional integral. We will find the explicit form of $\mathcal{K}$, U, and DM_j in the $\mathcal{G}/\mathcal{H}$ space. This is our first quantitative result.

Following the idea formulated in Ref. 2, we will formulate the transformation in such a way that $u_{a\mu}=u_{a\mu}(x;\xi,\eta,\lambda_a)$ would be the generator of transformation:

$$u_{a\mu}:A_{a\mu}(x)\to(\xi(t),\eta(t),\lambda_a(x)), \tag{7}$$

where the set $(\xi,\eta,\lambda_a)\in\mathcal{G}/\mathcal{H}$ will coincide at $j^{a\mu}(x)=0$ with integration parameters of Eq. (5), $\lambda_a(\mathbf{x})$ is the gauge phase and the variables ξ and η are the consequence of the spatial symmetry breaking. For example (1), $\dim(\xi+\eta)=8$. So, the combination of generators violated by $u_{a\mu}$ subgroup will be taken as the new quantum variables, instead of the Yang–Mills potentials $A_{\mu a}$. In other words, just the variables extracted by the Faddeev–Popov ansatz as the ''nonphysical'' ones would be the dynamical variables of the tQCD.

The problem of definition and farther quantization of the factor space was solved in Ref. 2. The method consists in formal mapping into the symplectic phase space W of the arbitrary high dimension, considering all dynamical variables of extended space as the q-numbers. It is the first step of calculations. Notice that the transformation always may be done canonically and the Jacobian of transformation would be equal to one. For this reason no ghost fields will appear.

Then the formalism allows to reduce W:

$$W=(\mathcal{G}/\mathcal{H})\times R^*. \tag{8}$$

This reduction of W up to $\mathcal{G}/\mathcal{H}$ is the second step of calculations. The realized transformation is singular since $\dim(\mathcal{G}/\mathcal{H})<\dim W$. Nevertheless we will be able to extract corresponding artifact infinity equal to the volume of R^* and cancel it by the normalization.

The proof that the set of q-numbers extracted this way is necessary and sufficient for quantization of the factor space $\mathcal{G}/\mathcal{H}$ will be crucial for our formalism. We will find that:

$$\mathcal{G}/\mathcal{H}=T^*V\times R, \tag{9}$$

where the quantum degrees of freedom only belong to the cotangent symplectic manifold T^*V[16] and R is the c-number parameter's subspace. The direct product (9) means that we will be able to isolate the quantum degrees of freedom from classical ones. So, it will be shown that $\lambda_a \in R$.

We will find that each order of the tQCD perturbation theory is transparently gauge invariant. This result seems natural since the gauge invariant quantity, the "probability" $\mathcal{N}(u)$, is calculated. Therefore, there will not be a necessity to fix the gauge and, therefore, no "copies" of Gribov[13] would arise. Moreover, it will be shown that no unphysical singularities connected to the Gribov's ambiguity[17] would occur in the formalism. This is our second quantitative result.

It is not hard to show, see also Ref. 2, that developed perturbation theory in the $\mathcal{G}/\mathcal{H}$ space presents expansion over $1/g$, where g is the interaction constant, and does not contain the terms $\sim g^n$, with $n>0$. Such type of perturbation theory, over $1/g$, presents a definite problem from ordinary renormalization procedures point of view.

Indeed, the ordinary quantum field theory scheme assumes the multiplicative renormalization of the interaction constant: the renormalized constant $g_R = Z^{1/2} g < \infty$ and the renormalization factor $Z = \infty$ because of the ultraviolet divergences. Then, having the expansion over $1/g$, we come to an evident contradiction: It is impossible to have the *infinite multiplicative* renormalizations in expansions over g and over $1/g$ simultaneously. For this reason this question would be considered in more detail in our approach. We will show that our perturbation theory would not contain the divergences and the problem with renormalization would not arise. This is our third result.

It should be noted here that these results have been proposed to be obtained in Ref. 18 to distinguish the quantization on the factor space, but now this is done for complete perturbation theory. However it is noteworthy that quantitative progress was achieved taking into account the unitarity condition.

It was mentioned in Ref. 2 that our perturbation theory, over $1/g$, is dual to ordinary one, over g.[19] So, we may realize the expansion over g, or over $1/g$, and the choice is defined only by convenience. If the states counted by the expansion over g and over $1/g$ belong to orthogonal Hilbert spaces[20] then there should not be any connection among terms of both expansions,[2] only the result of summation of series should coincide. For this reason our formalism did not hide the contradiction: The expansion over g may contain divergences and it needs the renormalization, but the expansion over $1/g$ may be divergence free and no renormalizations would be necessary in it.[21]

In the chosen way of calculations even the notion of *interacting* gluons in the Yang–Mills theory would disappear (as well as the pQCD Feynman diagrams). Yet, we cannot exclude the real (mass-shell) particle (gluon) emission[22] on the to-day level of understanding of abilities of our formalism and, therefore, we cannot prove that the states counted in the expansion over g and over $1/g$ belong to the orthogonal Hilbert space. So, we will leave unsolved the problem of colored quanta emission since the question of confinement demands more careful analysis.

The paper is organized as follows. Considering the solutions of Yang–Mills equation, one may use the *ansatz*:[23]

$$A^a_\mu(x) = \eta^a_{\mu\nu} \partial^\nu \ln \varphi(x), \tag{10}$$

where $\eta^a_{\mu\nu}$ are the real matrices. This ansatz reduces the Yang–Mills equation to the form:[3]

$$\partial^2 \varphi + \kappa \varphi^3 = 0, \tag{11}$$

where κ is the integration constant. So, in Sec. II we will formulate the ideology of mapping into the simpler factor space $W = O(4,2)/O(4) \times O(2)$ for scalar $O(4,2)$-invariant field theory with the action:

$$S(\varphi) = \int \mathrm{d}^4 x \left(\frac{1}{2} (\partial_\mu \varphi)^2 - \frac{\kappa}{4} \varphi^4 \right). \tag{12}$$

In Sec. III we will formulate the tQCD in the $\mathcal{G}/\mathcal{H}$ factor space.

II. SCALAR CONFORMALLY INVARIANT FIELD THEORY

A. Definitions

We concentrate our attention in the present section on the calculation of $|\mathcal{Z}(u)|^2$, where

$$\mathcal{Z}=\int D\varphi e^{iS(\varphi)} \tag{13}$$

and $S(\varphi)$ is the action defined in (12).

As was explained, the integral

$$\mathcal{N}\equiv|\mathcal{Z}|^2=e^{-i\mathcal{K}(je)}\int DM_j(\varphi,\pi)e^{-2iU(\varphi,e)} \tag{14}$$

will be analyzed instead of (13). Here

$$2\mathcal{K}(je)=\mathrm{Re}\int_{C_+}\mathrm{d}x\,\frac{\delta}{\delta j(x)}\,\frac{\delta}{\delta e(x)}\equiv\mathrm{Re}\int_{C_+}\mathrm{d}x\,\hat{j}(x)\hat{e}(x). \tag{15}$$

At the very end of calculations one should take the auxiliary variables j and e equal to zero. The interactions are introduced by the functional

$$-2U(\varphi,e)=S_{C_+}(\varphi+e)-S_{C_-}(\varphi-e)-2\,\mathrm{Re}\int_{C_+}\mathrm{d}^4x e\,\frac{\delta S(\varphi)}{\delta\varphi}$$

$$=2\kappa\,\mathrm{Re}\int_{C_+}\mathrm{d}x\,\varphi(x)e^3(x)+O(\epsilon). \tag{16}$$

The complex time formalism of Mills[24] was used and $S_{C_\pm}$ is the action defined on the complex time contour $C_\pm$. For sake of definiteness, we will use the complex time contours

$$C_\pm: t\to t\pm i\epsilon,\quad \epsilon\to+0,\quad |t|\leqslant\infty. \tag{17}$$

Let $\varphi_\pm$ be the fields on the $C_\pm$ branches of the Mills time contour and let $\partial C_\pm$ be the boundary of these branches. It was assumed the "periodic" (closed-path[6]) boundary condition:

$$\varphi_+(t\in\partial C_+)=\varphi_-(t\in\partial C_-), \tag{18}$$

when the representation (14) was derived. This boundary condition should be maintained in the factor space.

Notice that considering the theory with Lagrangian (12), one may write $U(\varphi,e)$ in the following equivalent form [with $O(\epsilon)$ accuracy]:

$$3!U(\varphi,e)=-\int\mathrm{d}^4xe(x)^3\frac{\delta^3}{\delta\varphi(x)^3}S(\varphi)=-\int\mathrm{d}^4x\left\{e(x)\frac{\delta}{\delta\varphi(x)}\right\}^3S(\varphi). \tag{19}$$

This representation is useful for investigation of the perturbation theory symmetry properties. The indication that the contribution belongs to the Mills time contour was not shown in (19) since it was assumed that, for instance,

$$\frac{\delta j(t\in C_a)}{\delta j(t'\in C_b)}=\delta_{ab}\delta(t-t'),\quad a,b=+,-. \tag{20}$$

For this reason it is sufficient to indicate the branch of the Mills contour only in the definition of the operator (15).

We will consider the ''phase space'' motion:

$$DM_j(\varphi,\pi)=\prod_x \mathrm{d}\varphi(x)\mathrm{d}\pi(x)\,\delta\left(\dot{\varphi}(x)-\frac{\delta H_j}{\delta\pi(x)}\right)\delta\left(\dot{\pi}(x)+\frac{\delta H_j}{\delta J(x)}\right). \tag{21}$$

It is important that the formalism involves the *total* Hamiltonian

$$H_j=\int \mathrm{d}^3x\left[\frac{1}{2}\pi^2+\frac{1}{2}(\nabla\varphi)^2+\frac{\kappa}{4}\varphi^4-j\varphi\right] \tag{22}$$

and the last term $\sim j\varphi$ may be interpreted as the time-dependent energy of random quantum excitations. It is evident that we may find the measure (9) if the first δ-function in (21) is used to calculate the integral over π. Thus, the representation (14), with the measure (21), may be considered as the ''first-order'' formalism.

This ends the definition of the field theory on the Dirac measure.

B. Mapping into the factor space

Having a theory defined on the δ-like measure, arbitrary transformations are easily available. We will start from the general situation introducing N fields $\{\xi(x),\eta(x)\}_N$, where N is arbitrary.

To perform the transformation:

$$(\varphi(x),\pi(x))\rightarrow\{\xi(x),\eta(x)\}_N \tag{23}$$

one should insert

$$1=\frac{1}{\Delta(\varphi,\pi)}\int D\xi D\eta\prod_x \delta(F_\xi(\varphi,\pi;\xi,\eta))\prod_x \delta(F_\eta(\varphi,\pi;\xi,\eta)) \tag{24}$$

into the integral (14). The functional δ-function $\Pi_x\delta$ has following properties:

$$\begin{gathered}\int DX\prod_x \delta(X(x))=1,\\ \int DX\prod_x \delta(\partial_\mu X(x))=\int\prod_x \mathrm{d}X(x)\,\delta(\partial_\mu X(x))=\int\prod_{x\neq x_\mu}\mathrm{d}X_{(\mu)}(x).\end{gathered} \tag{25}$$

Here $X_{(\mu)}(x)$ is the solution of equation $\partial_\mu X(x)=0$, i.e., is the arbitrary, including constant, x_μ independent function.

Having the measure (21) and inserting the unit (24) into (14) the integrals of type

$$\int D\xi D\eta D\varphi D\pi\Delta^{-1}(\varphi,\pi)\prod \delta(F_\xi(\varphi,\pi;\xi,\eta))\,\delta(F_\eta(\varphi,\pi;\xi,\eta))\,\delta\left(\dot{\varphi}-\frac{\delta H_j}{\delta\pi}\right)\delta\left(\dot{\pi}+\frac{\delta H_j}{\delta\varphi}\right) \tag{26}$$

would appear. Notice that the $(\dim\xi+\dim\eta)=N$ was chosen arbitrary.

It is important that both measures in (26), over (ξ,η) and over (φ,π), are δ-like. This allows one to change order of integration and integrate first over φ and π. It is natural, at first glance, to use for this purpose the last two δ-functions. Then the first ones will define the constraint. This scheme may restore the Wentzel–Kramers–Brillouin perturbation theory, if the unit (24) is reduced to the Faddeev–Popov *ansatz*.[2] But if the first two δ-functions of (26) are used to calculate the integrals over φ and π, we perform transformation to the new dynamical variables (ξ,η). Then the last two δ-functions will give the dynamical equations for (ξ,η). Both ways of computation would give the same result since one may use arbitrary δ-functions.

Thus, we wish to use the fact that the δ-like measure defines a complete set of contributions. Moreover, as follows from (14) and (15), the quantum perturbations, both in the $(\varphi,\pi)\in V$ and $(\xi,\eta)\in W$ spaces, would be generated by the same operator $\exp\{-i\mathcal{K}(je)\}$ and the interactions in both above-mentioned cases are described by the same functional $U(u,e)$. This circumstance allows one to describe the *quantum* dynamics in terms of new variables.

Then, if the ''phase space flow'' (u,p) belongs to the manifold $\mathcal{G}/\mathcal{H}$ completely, we should be able to ''restore'' it through the (u,p) flow. This is our key idea. We will see that this order of computation, inverse to the ordinary one,[25] is mostly natural for us since it allows one to start transformation from mostly general variables $(\xi,\eta)\in W$.

Following space–time local realization of the algebraic equations was offered in[2,6]

$$\begin{aligned} F_{\xi}(\varphi,\pi;\xi,\eta)&=\varphi(x)-u(x;\xi(x),\eta(x))=0,\\ F_{\eta}(\varphi,\pi;\xi,\eta)&=\pi(x)-p(x;\xi(x),\eta(x))=0, \end{aligned} \tag{27}$$

where $u=u(x;\xi(x),\eta(x))$, $p=p(x;\xi(x),\eta(x))$ are some *compound* functions. We will assume that this functions would be defined in accordance with our choice of $\mathcal{G}/\mathcal{H}$. The equalities (27) can be satisfied for arbitrary given $u(x;\xi(x),\eta(x)),p(x;\xi(x),\eta(x))$ and arbitrary N since integration over all $\varphi(x)$ and $\pi(x)$ is assumed.

Therefore, the integral in (24) is not equal to zero since, generally speaking, it always exist. The result of integration in (24) is denoted by $\Delta(\varphi,\ \pi)$ and in this sense the equality (24) is satisfied identically. The additional constraints for $u(x;\xi,\eta)$ and $p(x;\xi,\eta)$ will be offered later.

We will specify (27) adding the condition that the time dependence is hidden in $\xi(y,t)$ and $\eta(y,t)$, $x=(y,t)$, $\dim(y)=3$. Thus, we would use, instead of (27), the equations:

$$\varphi(y,t)=u(y;\xi(y,t),\eta(y,t)),\quad \pi(y,t)=p(y;\xi(y,t),\eta(y,t)). \tag{28}$$

In other aspects the functions $u(y;\xi,\eta),p(y;\xi,\eta)$ for the time being are arbitrary. Notice that the offered additional condition is evident since (u,p) would belong to $\mathcal{G}/\mathcal{H}$ completely. But, nevertheless, we will examine it.[26] Notice also the noncovariantness of equalities (28). This is a consequence of necessity of using the Hamiltonian formalism.[2]

The integration measures in (26) over $\xi(y,t)$ and $\eta(y,t)$ are defined on the total Mills time contour $C=C_{+}+C_{-}$:

$$\int_{C}\mathrm{d}t=\int_{C_{+}+C_{-}}\mathrm{d}t=\int_{C_{+}}\mathrm{d}t+\int_{C_{-}}\mathrm{d}t, \tag{29}$$

and the integration should be performed with boundary condition (18):

$$u(;\xi(,t\in\partial C_{+}),\eta(,t\in\partial C_{+}))=u(;\xi(,t\in\partial C_{-}),\eta(,t\in\partial C_{-})). \tag{30}$$

Depending on the topology of the trajectory $u(;\xi,\eta)$, this boundary condition may lead to nontrivial consequences.

The mapping (28) is generated by the function u:

$$u:(\varphi,\pi)\to(\xi,\eta) \tag{31}$$

since the ''first-order'' formalism is considered. It is important also to note that this transformation did not conserve the dimension:

$$\dim(\varphi,\pi)(y,t)\neq\dim(\xi,\eta)(y,t) \tag{32}$$

since $(\xi,\eta)\in\mathcal{G}/\mathcal{H}$ and $(\varphi,\pi)\in V$.

Proposition I: The Jacobian of transformation of the δ-like measure always can be done equal to one.

Using first two δ-functions in (26) to perform integration over $(\varphi,\ \pi)$ the Jacobian of the transformation (31) takes the form:

$$J=\frac{1}{\Delta(u,p)}\prod_{y,t}\ \delta\left(\dot{u}(y;\xi,\eta)-\frac{\delta H_j(u,p)}{\delta p(y;\xi,\eta)}\right)\delta\left(\dot{p}(y;\xi,\eta)+\frac{\delta H_j(u,p)}{\delta u(y;\xi,\eta)}\right), \tag{33}$$

where definitions (27) and (28) were used. Notice that $\Delta=\Delta(u,p)$, as a result of integration over φ and π.

We should diagonalize arguments of remaining δ-functions. For this purpose the following trick will be used.[2] So, for instance,

$$\delta\left(\dot{u}-\frac{\delta H_j}{\delta p}\right)=\delta\left(u_\xi\cdot\dot{\xi}+u_\eta\cdot\dot{\eta}-\frac{\delta H_j}{\delta p}\right)$$

$$=\delta\left(u_\xi\cdot\left\{\dot{\xi}-\frac{\delta h_j}{\delta\eta}\right\}+u_\eta\cdot\left\{\dot{\eta}+\frac{\delta h_j}{\delta\xi}\right\}+u_\xi\cdot\frac{\delta h_j}{\delta\eta}-u_\eta\cdot\frac{\delta h_j}{\delta\xi}-\frac{\delta H_j}{\delta p}\right),$$

where $u_X\equiv\partial u/\partial X$, $X=\xi,\ \eta$ and $h_j=h_j(\xi,\eta)$ is the auxiliary functional. Let us choose it by the equality:

$$u_\xi\cdot\frac{\delta h_j}{\delta\eta}-u_\eta\cdot\frac{\delta h_j}{\delta\xi}-\frac{\delta H_j}{\delta p}=\frac{\partial u}{\partial\xi}\cdot\frac{\delta h_j}{\delta\eta}-\frac{\partial u}{\partial\eta}\cdot\frac{\delta h_j}{\delta\xi}-\frac{\delta H_j}{\delta p}=\{u,h_j\}-\frac{\delta H_j}{\delta p}=0, \tag{34}$$

where $\{,\}$ is the Poisson bracket. The scalar product means that the sets $\{\xi\}$ and $\{\eta\}$ were ordered in such a way that the Poisson bracket would be well defined. This ordering is always possible iff W is the symplectic manifold.

Then, if (34) is satisfied,

$$\delta\left(\dot{u}-\frac{\delta H_j}{\delta p}\right)=\delta\left(u_\xi\left\{\dot{\xi}-\frac{\delta h_j}{\delta\eta}\right\}+u_\eta\left\{\dot{\eta}+\frac{\delta h_j}{\delta\xi}\right\}\right),$$

The analogous expression one may find for the second δ-function:

$$\delta\left(\dot{p}+\frac{\delta H_j}{\delta u}\right)=\delta\left(p_\xi\left\{\dot{\xi}-\frac{\delta h_j}{\delta\eta}\right\}+p_\eta\left\{\dot{\eta}+\frac{\delta h_j}{\delta\xi}\right\}\right),$$

and h_j and p should obey additional to (34) equality:

$$\{p,h_j\}+\frac{\delta H_j}{\delta u}=0. \tag{35}$$

On this stage two equalities (34) and (35) are the equations for functions $u(;\xi,\eta)$, $p(;\xi,\eta)$ and $h_j(\xi,\eta)$. Thus, being vague, this mechanism of mapping is able to endure more constraints.

Using the ordinary property of the δ-function:

$$\delta(a-b)=\int \mathrm{d}c\ \delta(c-a)\,\delta(c-b),$$

we can write that

$$J(\xi,\eta)=\frac{1}{\Delta(u,p)}\int D\xi' D\eta'\prod_x\ \delta(u_\xi\cdot\xi'+u_\eta\cdot\eta')\,\delta(p_\xi\cdot\xi'+p_\eta\cdot\eta')$$

$$\times\delta\left(\xi'-\left\{\dot{\xi}-\frac{\delta h_j}{\delta\eta}\right\}\right)\delta\left(\eta'-\left\{\dot{\eta}+\frac{\delta h_j}{\delta\xi}\right\}\right). \tag{36}$$

Let us assume that the functional integral $\Delta(u,p)$ may be written in the form:

$$\Delta(u,p)=\int D\xi' D\eta' \prod_{y,t} \delta(\varphi(y,t)-u(y;\xi+\xi',\eta+\eta'))\,\delta(\pi(y,t)-p(y;\xi+\xi',\eta+\eta'))$$

$$=\int D\xi' D\eta' \prod_{y,t} \delta(u_\xi \xi'+u_\eta \eta')\,\delta(p_\xi \xi'+p_\eta \eta')\neq 0. \tag{37}$$

This is possible since the functions $\varphi(y,t)$ and $\pi(y,t)$ were chosen in such a way that the equalities (27) are satisfied. The inequality (37) excludes the degeneracy. For this reason only $\xi'=\eta'=0$ are essential in the integral (37).

As a result the determinant $\Delta(u,p)$ is canceled identically:

$$DM_j(\xi,\eta)=\prod_{y,t} \mathrm{d}\xi(y,t)\,\eta(y,t)\,\delta\left(\dot{\xi}(y,t)-\frac{\delta h_j}{\delta\eta(y,t)}\right)\delta\left(\dot{\eta}(y,t)+\frac{\delta h_j}{\delta\xi(y,t)}\right) \tag{38}$$

since one may leave an arbitrary pair of δ functions in (36) and $\xi'=\eta'=0$ are essential. Therefore, because of cancellation of the functional determinants our perturbation theory would be free from the ghost fields. This considerably simplifies the described formalism. Notice that equalities (34), (35), and (37) should be satisfied to have this result.

The transformed measure (38) depends on the auxiliary functional $h_j=h_j(\xi,\eta)$, defined by equalities (34) and (35). So, choosing *arbitrary* $u(;\xi,\eta)$ and $p(;\xi,\eta)$ with the property (37), one may find h_j from (34) and (35), and then (38) would be the transformed measure.

Therefore, mapping (31) based on Eqs. (34) and (35) admits one more equation for $u(;\xi,\eta)$, $p(;\xi,\eta)$, and $h_j(\xi,\eta)$. We will consider the following example in the present paper. One may note from (38) that h_j has a meaning of transformed Hamiltonian of new equations:

$$\dot{\xi}(y,t)=\frac{\delta h_j(\xi,\eta)}{\delta\eta(y,t)},\quad \dot{\eta}(y,t)=-\frac{\delta h_j(\xi,\eta)}{\delta\xi(y,t)}. \tag{39}$$

Proposition II: If

$$h_j(\xi,\eta)=H_j(u,p). \tag{40}$$

then the Poisson equations (34), (35) would define the "phase space flow" (u,p).

Indeed, having in mind (28),

$$\dot{u}=u_\xi\dot{\xi}+u_\eta\dot{\eta}=u_\xi\frac{\delta h_j}{\delta\eta}-u_\eta\frac{\delta h_j}{\delta\xi}=\{u,h_j\}=\frac{\delta H_j}{\delta p}, \tag{41}$$

where (39) and then (34) were used. The same equation one may find for p:

$$\dot{p}=p_\xi\dot{\xi}+p_\eta\dot{\eta}=p_\xi\frac{\delta h_j}{\delta\eta}-p_\eta\frac{\delta h_j}{\delta\xi}=\{p,h_j\}=-\frac{\delta H_j}{\delta u}. \tag{42}$$

Therefore, having (40), Eqs. (34) and (35), simultaneously with (39), are equal to the Hamiltonian equations (41) and (42). Notice also that in this case the time dependence actually should be hidden into ξ and η.

It should be stressed also that as follows (41) and (42) fixed by (34), (35) and completed by (40) and (37) transformations are unique in those respects that other ''types'' of mapping would lead to ''unnatural,'' much more complicated, formalism.

Having (34), (35), (40) and taking into account (37), we get to the ''overdetermined'' system of constraints, which may be inconsistent. The Coulomb problem gives a quantum mechanical

example of such a system.[2] At all evidence, the $O(4)\times O(2)$-invariant solution did not also obey (37). On the other hand, if we reject (37) then the determinant $\Delta(u,p)$ is not canceled and the formalism would contain the ghosts.

C. Structure of dual perturbation theory

The problem of mapping for the degenerate case was solved in Ref. 2. It was assumed that one may ''softly'' take off the degeneracy, i.e., that there exist some parameter $\varepsilon\to 0$ which regulates the strength of degeneracy breaking and at $\varepsilon=0$ we have the degenerate limit.[27] The following proposition will be important in this connection.

Proposition III: The quantum perturbation conserves the topology of phase space flow.

Indeed, notice that Eqs. (34) and (35) should be satisfied for arbitrary $j(y,t)$. Let us consider the consequence of this proposition. Remembering (22), and using definition (40), we find that (34) at $j=0$ gives equality:

$$\{u_\xi p_\eta - u_\eta p_\xi - 1\}\frac{\delta H}{\delta p(y,t)} = \{u_\eta u_\xi - u_\xi u_\eta\}\frac{\partial H}{\partial u(y,t)}, \quad H = H_j|_{j=0}.$$

Here u and p are the compound functions of $\xi=\xi(y,t)$ and $\eta=\eta(y,t)$. This equality is identically satisfied if the space–time local Poisson brackets:

$$\{u(y,t),p(y,t)\}=1, \quad \{u(y,t),u(y,t)\}=0 \tag{43}$$

are satisfied. Equation (35) at $j=0$ adds the following conditions:

$$\{u(y,t),p(y,t)\}=1, \quad \{p(y,t),p(y,t)\}=0. \tag{44}$$

It is not hard to see that the higher orders over j did not give new conditions, i.e., the Poison algebra, completed by (40), is closed. In other words, the quantum perturbations conserve the topology[28] of the phase space flow.

Proposition III means that the quantum perturbations would not alter the structure of $u=u(;\xi,\eta)$ and $p=p(;\xi,\eta)$ and they are solutions of *classical* (homogeneous) equations:

$$\{u(y;\xi,\eta),h(\xi,\eta)\}=\frac{\delta H(u,p)}{\delta p(y;\xi,\eta)}, \quad \{p(y;\xi,\eta),h(\xi,\eta)\}=-\frac{\delta H(u,p)}{\delta u(y;\xi,\eta)}. \tag{45}$$

The j dependence is defined by Eq. (39) and is confined completely in ξ and η only.

So, we may start from a theory with generalized Hamiltonian:

$$h_j(\xi,\eta)=H_j(u,p)+\varepsilon\tilde{H}_j(u,p), \tag{46}$$

where the additive term $\sim\varepsilon\to 0$. This proposition means that the ''direct'' mechanism of degeneracy breaking is considered[27] and the Hamiltonian $h_j(\xi,\eta)$ may be chosen in such a way that some of the *derivatives* over auxiliary (artificial) fields ξ' and η' have a property:

$$u_{\xi'}\sim u_{\eta'}\sim p_{\xi'}\sim p_{\eta'}\sim\varepsilon\to 0, \quad (\xi',\eta')\in R^*. \tag{47}$$

This is enough to formulate conserving the phase space volume transformation of quantum theory.

Thus, we start from the variables $(\xi,\eta)\in W$ and scalar functions $u=u(y;\xi,\eta)$, $p=p(y;\xi,\eta)$. They should obey the inequality (37) and define the functional $h_j(\xi,\eta)$ through the equations (34) and (35). This allows one to cancel the determinant $\Delta(u,p)$. Then we extract the auxiliary variables ξ' and η' assuming (47). This will allow one to exclude the auxiliary variables and should reduce the system to a physical one. The physical content of this procedure was described in Ref. 2.

The following property of the perturbation theory in W space will be used to realize this program of reduction. As a result of our mapping the integral $\mathcal{N}$ takes the form:

$$\mathcal{N}(u)=e^{-i\mathcal{K}(je)}\int DM_j(\xi,\eta)e^{-2iU(u,e)}, \tag{48}$$

where $DM_j(\xi,\eta)$ is defined in (38). Notice that in this expression U depends on $u=u(y;\xi,\eta)$.

It was shown in Ref. 2 that the mapped representation (48) allows one to split the ''quantum force'' $j(y,t)$ and corresponding ''virtual field'' $e(y,t)$ on the projection on the axes of W. It is easy to find the result of this procedure:

$$2\mathcal{K}(je)=\mathrm{Re}\int_{C_+}\mathrm{d}^3x\,\mathrm{d}t\{\hat{j}_\xi(y,t)\cdot\hat{e}_\xi(y,t)+\hat{j}_\eta(y,t)\cdot e_\eta(y,t)\} \tag{49}$$

and

$$e=e_\xi\cdot\frac{\partial u}{\partial\eta}-e_\eta\cdot\frac{\partial u}{\partial\xi}. \tag{50}$$

The caret symbol in (49) means the derivative over the corresponding quantity. At the very end of the calculation one should take $j_X=e_X=0$, $X=(\xi,\eta)$. The scalar product means summation over all components of ξ and η.

Inserting (50) into (19) one can find that

$$\begin{aligned}-3!U(u,e)&=\int\mathrm{d}^3x\,\mathrm{d}t\left\{e_\xi\cdot\frac{\partial u}{\partial\eta}\frac{\delta}{\delta u}-e_\eta\cdot\frac{\partial u}{\partial\xi}\frac{\delta}{\delta u}\right\}^3S(u)\\&=\int\mathrm{d}^3x\,\mathrm{d}t\left\{e_\xi\cdot\frac{\partial u}{\partial\eta}\frac{\partial}{\partial u}-e_\eta\cdot\frac{\partial u}{\partial\xi}\frac{\partial}{\partial u}\right\}^3\mathcal{L}(u),\end{aligned} \tag{51}$$

where $\mathcal{L}(u)$ is the Lagrangian density. This shows that the interaction functional $U(u,e)$ has the symmetry properties of the Lagrangian density.

Formally the new perturbation generating operator (49) gives the same perturbation series, but with the rearranged sequence of terms, i.e., the splitting of j did not change the ''convergence'' of the perturbation series (over $1/\kappa$ since $u\sim1/\sqrt{k}$). At the same time, this splitting of the source j is useful since it allows one to analyze the excitation of each degree of freedom, i.e., of components of the phase space flow along the axis of W, independently.

Noting that e_X, $X=\xi,\eta$, is conjugate to j_X, it is easy to conclude that the action of the operator (49) leads to the operator

$$\left\{\frac{\delta}{\delta j_\xi}\cdot\frac{\partial u}{\partial\eta}\frac{\partial}{\partial u}-\frac{\delta}{\delta j_\eta}\cdot\frac{\partial u}{\partial\xi}\frac{\partial}{\partial u}\right\}\sim\{\hat{j}\wedge\hat{X}\}.$$

This operator is the invariant of canonical transformations. If by some reason $\mathrm{d}\omega_X^2=\hat{j}_X\wedge\hat{X}=0$, then the motion along the Xth axis will be classical. This is the mechanism of reduction of the quantum degrees of freedom. The important properties of our formalism were described in Ref. 2. We will continue this question in Sec. II D.

Proposition IV: New fields ξ and η cannot depend on the coordinate y if the scalar theory is considered, i.e.,

$$\xi=\xi(t),\quad \eta=\eta(t), \tag{52}$$

for scalar theory (12).

This conclusion follows from Proposition III. The reason is that the dynamical problem was divided into two parts. The first part of the problem consists in the solution of the *classical* equations (45). It defines a structure of the compound functions $u(y;\xi,\eta)$ and $p(y;\xi,\eta)$. The second part consists in the definition of the *time* dependence of (ξ,η) through Eqs. (39) and (40). Finally, if (ξ,η) in zero order over $j(y,t)$ are the y independent parameters, the quantum perturbations are unable to change this property.

It is noticeable that if $\xi=\xi(t)$ and $\eta=\eta(t)$ then we will find from (34) and (35), instead of (43) and (44), the *canonical* equal-time commutator relations:

$$\{u(y;\xi(t),\eta(t)),p(y';\xi(t),\eta(t))\}=\delta(y-y'). \tag{53}$$

Thus, our quantization scheme would restore the canonical one in the factor space W. In this sense the independence of ξ and η from y is natural.

Nevertheless it seems useful to demonstrate Proposition IV explicitly. The elements (49) and (38) are used in the Appendix to demonstrate the reduction:

$$(\xi,\eta)(y,t)\to(\xi,\eta)(t). \tag{54}$$

This involves reduction of the operators:

$$(\hat{j}_X,\hat{e}_X)(y,t)\to(\hat{j}_X,\hat{e}_X)(t),\quad X=\xi,\eta. \tag{55}$$

The structure of the corresponding perturbation theory is described in Sec. II D.

D. Reduction

Therefore, for considered scalar theory,

$$2\mathcal{K}(je)=\mathrm{Re}\int_{C_+}\mathrm{d}t\{\hat{j}_\xi(t)\cdot\hat{e}_\xi(t)+\hat{j}_\eta(t)\cdot e_\eta(t)\} \tag{56}$$

and

$$e(y;\xi(t),\eta(t))=e_\xi(t)\cdot\frac{\partial u(y;\xi(t),\eta(t))}{\partial\eta(t)}-e_\eta(t)\cdot\frac{\partial u(y;\xi(t),\eta(t))}{\partial\xi(t)}. \tag{57}$$

The result of the disappearance of y dependencies in ξ and η is a reduction of the field-theoretical problem to the quantum mechanical one. So, $L(u)=V(\xi,\eta)$ here play the role of the mechanical potential for a particle with the *phase space* coordinate (ξ,η).

The measure takes the form:

$$DM_j(\xi,\eta)=\prod_t\mathrm{d}\xi(t)\mathrm{d}\eta(t)\,\delta(\dot{\xi}(t)-\omega_\eta(\xi,\eta)-j_\xi(t))\,\delta(\dot{\eta}(t)+\omega_\xi(\xi,\eta)-j_\eta(t)), \tag{58}$$

where the "velocity"

$$\omega_X(\xi,\eta)=\frac{\partial h(\xi,\eta)}{\partial X}. \tag{59}$$

Let us remember now the definition (47):

$$u=u(y;\xi(t),\eta(t);\varepsilon\xi'(t),\varepsilon\eta'(t)),\quad \varepsilon\to0, \tag{60}$$

where

$$\dim\xi=n,\quad \dim\eta=m,\quad \dim(\xi+\xi')=\dim(\eta+\eta')=N. \tag{61}$$

Inserting (60) into Lagrangian, we find that

$$L(u)=\int \mathrm{d}^3x\mathcal{L}(u(y;\xi(t),\eta(t)))+O(\varepsilon). \tag{62}$$

We are now able to define the dimension of T^*V taking

$$N=\dim(\mathcal{G}/\mathcal{H}). \tag{63}$$

So, $N=8$ for example (1).

Proposition V: If we have (60) and (61) then

$$\dim T^*V=\min\{n,m\}. \tag{64}$$

Let us consider the following three possibilities to demonstrate this proposition.

(*a*) $n=m$, $N=2n$.

In this case the interaction functional $U(u,e)$ takes the form:

$$-3!U(u,e)=\int \mathrm{d}t\left\{\left(e_x\cdot\frac{\partial}{\partial\eta}-e_\eta\cdot\frac{\partial}{\partial\xi}\right)_n+\left(e_{x'}\cdot\frac{\partial}{\partial\eta'}-e_{\eta'}\cdot\frac{\partial}{\partial\xi'}\right)_{N-n}\right\}^3, \tag{65}$$

where (62) was used. The index n means that the scalar products include n terms, and N may be chosen equal to n. The measure

$$DM_j(\xi,\eta)=\prod_t \mathrm{d}^n\xi(t)\mathrm{d}^n\eta(t)\,\delta^{(n)}(\dot\xi-\omega_n-j_\xi)\,\delta^{(n)}(\dot\eta+\omega_\xi-j_\eta).$$

(*b*) $n>m$, $N=n+m$.

In this case

$$-3!U(u,e)=\int \mathrm{d}t\left\{\left(e_x\cdot\frac{\partial}{\partial\eta}-e_\eta\cdot\frac{\partial}{\partial\xi}\right)_m+\left(e'_\eta\cdot\frac{\partial}{\partial\xi}\right)_{(n-m)}\right\}^3 V(\xi,\eta), \tag{66}$$

since η' is absent in $V(\xi,\eta)$. Therefore, e'_η has only the $(n-m)$ components.

The measure takes the form:

$$DM_j(\xi,\eta)=\prod_t \mathrm{d}^n\xi(t)\mathrm{d}^m\eta(t)\mathrm{d}^{(n-m)}\eta'(t)\,\delta^{(m)}(\dot\xi-\omega_\eta-j_\xi)\,\delta^{(m)}(\dot\eta+\omega_\xi-j_\eta)$$
$$\times\,\delta^{(n-m)}(\dot\xi-j_\xi)\,\delta^{(n-m)}(\dot\eta'+\omega_\xi-j_{\eta'})$$

since $N=(n+m)$. Notice that η' is contained only in the argument of the last δ-function. For this reason we always can perform the shift: $\dot\eta'\to\dot\eta'-\omega_\xi+j_{\eta'}$. As a result:

$$DM_j(\xi,\eta)=\prod_t \mathrm{d}^m\xi(t)\,\eta^m(t)\,\delta^{(m)}(\dot\xi-\omega_\eta-j_\xi)\,\delta^{(m)}(\dot\eta+\omega_\xi-j_\eta)\,\delta^{(n-m)}(\dot\xi-j_\xi)\,\delta^{(n-m)}(\dot\eta')$$

and the $j_{\eta'}$ dependence disappears. For this reason the $\hat j_{\eta'}$ dependence in the operator $\mathcal{K}$ may be omitted. As a result,

$$2\mathcal{K}(je)=\mathrm{Re}\int_{C_+}\mathrm{d}t\{(\hat{j}_\xi\cdot\hat{e}_\xi)_m+(\hat{j}_\eta\cdot\hat{e}_\eta)_m+(\hat{j}_\xi\cdot\hat{e}_\xi)_{(n-m)}\}.$$

There is not an operator $\hat{e}'_\eta$ and, for this reason, one should take $e_{\eta'}$ equal to zero. Therefore,

$$-3!U(u,e)=\int\mathrm{d}t\left\{e_x\cdot\frac{\partial}{\partial\eta}-e_\eta\cdot\frac{\partial}{\partial\xi}\right\}_m^3 V(\xi,\eta) \tag{67}$$

and the $(n-m)$ components of e_ξ and j_ξ may be taken equal to zero everywhere:

$$2\mathcal{K}(je)=\mathrm{Re}\int_{C_+}\mathrm{d}t\{\hat{j}_\xi\cdot\hat{e}_\xi+\hat{j}_\eta\cdot\hat{e}_\eta\}_m. \tag{68}$$

Accordingly,

$$DM_j(\xi,\eta)=\mathrm{d}R\prod_t\mathrm{d}^m\xi(t)\mathrm{d}^m\eta(t)\,\delta^{(m)}(\dot{\xi}-\omega_\eta-j_\xi)\,\delta^{(m)}(\dot{\eta}+\omega_\xi-j_\eta), \tag{69}$$

where

$$\mathrm{d}R=d^{(N-2m)}\xi(0) \tag{70}$$

is the element of R. The trivial auxiliary elements were omitted.

The same analyses may be done for the case $n<m$.

As a result, assuming that η is the ''action'' variable,

$$\omega_\eta=\omega(\eta)\equiv\partial h(\eta)/\partial\eta,\quad \omega_\xi=0,$$

we can write:

$$DM_j(\xi,\eta)=\mathrm{d}R\prod_{i=1}^{\min\{m,n\}}\prod_t\mathrm{d}\xi_i(t)\,\eta_i(t)\,\delta(\dot{\xi}_i-\omega_i(\eta)-j_{i\xi})\,\delta(\dot{\eta}_i-j_{i\eta}). \tag{71}$$

Therefore,

$$W=T^*V\times R \tag{72}$$

and $\mathrm{d}R$ is the differential measure of the subspace R.

This ends the proof of Proposition V.

So, the equation for ξ and η take the form:

$$\dot{\xi}(t)=\omega(\eta)+j_\xi(t),\quad \dot{\eta}(t)=j_\eta(t). \tag{73}$$

The second equation is simply integrable:

$$\eta(t)=\eta_0+\int\mathrm{d}t'\,g(t-t')j_\eta(t')\equiv\eta_0+\eta_j(t). \tag{74}$$

Inserting this solution into the first equation in (73) one may find:

$$\xi(t)=\xi_0+\int\mathrm{d}t'\,g(t-t')\omega(\eta_0+\eta_j(t'))+\int\mathrm{d}t'\,g(t-t')j_\xi(t')\equiv\xi_0+\overline{\omega_j}(t)t+\xi_j(t), \tag{75}$$

where the abbreviation

$$\overline{\omega}(t)t=\int \mathrm{d}t'\, g(t-t')\omega(\eta_0+\eta_j(t')) \tag{76}$$

was used. The Green function $g(t-t')$ was defined in[2]

$$g(t-t')=\Theta(t-t'), \tag{77}$$

where $\Theta(t-t')$ is the step function with boundary property:

$$\Theta(0)=1. \tag{78}$$

As a result,

$$u=u(y;\xi_0+\overline{\omega}_j(t)t+\xi_j,\eta_0+\eta_j) \tag{79}$$

and the term

$$\sim\frac{1}{n!}\{-2iU(u,j)\}^n=O\left(\frac{1}{\kappa^n}\right)$$

gives the nth order of our perturbation theory over $1/\kappa$ since $u=O(1/\sqrt{\kappa})$.

III. NON-ABELIAN GAUGE FIELD THEORY

A. Yang–Mills theory on Dirac measure

The action of considered theory

$$S(A)=\frac{1}{2g}\int \mathrm{d}^4x F_{\mu\nu a}(A)F_a^{\mu\nu}(A) \tag{80}$$

is the $O(4,2)$ invariant and the Yang–Mills fields

$$F_{\mu\nu a}(A)=\partial_\mu A_{\nu a}-\partial_\nu A_{\mu a}-C_a^{bc}A_{\mu b}A_{\nu c} \tag{81}$$

are the covariant of non-Abelian gauge transformations. The gauge group will not be specified.

We will consider the integral

$$\mathcal{N}=e^{-i\mathcal{K}(je)}\int DM_j e^{-2iU(A,e)}, \tag{82}$$

where the measure

$$DM_j(A)=\prod_{\mu,a}\prod_x \mathrm{d}A_\mu^a(x,t)\,\delta(D_a^{\nu b}F_{\nu\mu b}-j_{\mu a}) \tag{83}$$

is manifestly conformal and gauge invariant if $j_{\mu a}=0$. The covariant derivative

$$D_a^{\mu b}=\partial^\mu\delta_a^b+C_a^{bc}A_c^\mu.$$

The perturbations generating operator

$$2\mathcal{K}(je)=\mathrm{Re}\int_{C_+}\mathrm{d}^4x\frac{\delta}{\delta j_a^\mu(x,t)}\frac{\delta}{\delta e_{\mu a}(x,t)}\equiv\mathrm{Re}\int_{C_+}\mathrm{d}^4x\hat{j}_{\mu a}(x,t)\hat{e}_a^\mu(x,t). \tag{84}$$

The auxiliary variables $j_{\mu a}$ and e_a^μ should be taken equal to zero at the very end of the calculations. The functional

$$-2U(A,e)=(S_{C_+}(A+e)-S_{C_-}(A-e))-2\,\mathrm{Re}\int_{C_+}\mathrm{d}^4x e_a^\mu(x)\frac{\delta S(A)}{\delta A_a^\mu}+O(\varepsilon) \tag{85}$$

describes interactions. All the above-mentioned quantities are defined on the Mills time contours

$$C_\pm : t\to t\pm i\epsilon,\quad \epsilon\to+0,\quad |t|\leqslant\infty. \tag{86}$$

This gives the rule as to avoid the light-cone singularities solving the equation:

$$D_a^{\nu b}F_{\mu\nu b}=j_{\mu a}. \tag{87}$$

One can omit in (85) terms $\sim\epsilon\to+0$. Therefore, $U(A,e)=O(e^3)$ and may contain only the odd powers of $e_{a\mu}$. This means that we may write $U(A,e)$ in the form:

$$U(A,e)=-\int\mathrm{d}^4x\left\{e_a^\mu(x)\frac{\delta}{\delta A_a^\mu(x)}\right\}^3 S(A), \tag{88}$$

see (19).

B. First-order formalism

The noncovariant first-order formulation in terms of the ''electric'' field

$$E_a^i=F_a^{i0}, \tag{89}$$

presents an introduction into the necessary for us Hamiltonian description. The action in this term has the form

$$S_{C_\pm}(A,F)=\frac{1}{g}\int_{C_\pm}\mathrm{d}^4x\left\{\dot{\mathbf{A}}_a\cdot\mathbf{E}_a+\frac{1}{2}(\mathbf{E}_a^2+\mathbf{B}_a^2(\mathbf{A}))-A_{0a}(\mathbf{D}\cdot\mathbf{E})_a\right\}, \tag{90}$$

where the ''magnetic'' field

$$B_{ia}(\mathbf{A})=(\mathrm{rot}\,\mathbf{A})_{ia}+\tfrac{1}{2}\epsilon_{ijk}[A_j,A_k]_a \tag{91}$$

is not the independent quantity and was introduced to shorten the formulas. Notice that A_{0a} did not contain the conjugate pair and the action S is linear over it.

The measure (83) may be written in the first-order formalism representation ($d\mathbf{A}_a=\prod_i \mathrm{d}A_{ia}$):

$$DM_j(\mathbf{A},\mathbf{P})=\prod_{a,i}\prod_x\mathrm{d}\mathbf{A}_{ai}(x)\mathrm{d}\mathbf{P}_{ai}(x)\,\delta(\mathbf{D}_a^b\cdot\mathbf{P}_b)\,\delta\left(\dot{\mathbf{P}}_a(x)+\frac{\delta H_j(\mathbf{A},\mathbf{P})}{\delta\mathbf{A}_a(x)}\right)\delta\left(\dot{\mathbf{A}}_a(x)-\frac{\delta H_j(\mathbf{A},\mathbf{P})}{\delta\mathbf{P}_a(x)}\right), \tag{92}$$

where $H_j(\mathbf{A},\mathbf{P})$ is the total Hamiltonian:

$$H_j=\frac{1}{2g}\int\mathrm{d}^3x(\mathbf{P}_a^2+\mathbf{B}_a^2(\mathbf{A}))+\int\mathrm{d}^3x\mathbf{j}_a\mathbf{A}_a, \tag{93}$$

$\mathbf{P}_a(x)\equiv\mathbf{E}_a(x)$ is the conjugate to $\mathbf{A}_a(x)$ momentum and $\mathbf{B}_a(\mathbf{A})$ was defined in (91). We may introduce into DM_j the additional δ-function:

$$\prod_a\prod_x\delta\left(\mathbf{B}_a^i-(\mathrm{rot}\,\mathbf{A})_a^i-\frac{1}{2}\varepsilon_{jk}^i[A^j,A^k]_a\right). \tag{94}$$

Then the Hamiltonian in (93) becomes symmetric over electric $\mathbf{E}_a$ and magnetic $\mathbf{B}_a$ fields.

Notice that the first δ-function in (92) is the consequence of linearity of the action over A_{0a}. The time component A_{0a} has the meaning of Lagrange multiplier for the Gauss law:

$$\mathbf{D}_a^b \cdot \mathbf{P}_b = 0. \tag{95}$$

It should be stressed that there is not an equation for the time component A_{0a}. Moreover, the A_{0a} dependence completely disappeared from formalism since the interaction functional $U(A,e)$ is defined by the third derivative over $A_{\mu a}$, see (88).

C. Mapping into the factor space

The measure (92) is not physical since it contains three (for given a) vector potentials $\mathbf{A}_a(x)$. To exclude the unphysical degree of freedom, the gauge fixing Faddeev–Popov *ansatz* is often used. But we will consider, as was described previously, another approach.

We will introduce the functional

$$\Delta(A,P) = \int D\xi D\eta \prod_a \delta(\mathbf{A}_a(x) - \mathbf{u}_a(x;\xi(x),\eta(x)))\,\delta(\mathbf{P}_a(x) - \mathbf{p}_a(x;\xi(x),\eta(x))) \tag{96}$$

to realize the transformation

$$u{:}(A,P)_a(x) \to (\xi,\eta)(x), \tag{97}$$

to the compound vector functions $(\mathbf{u},\mathbf{p})_a(x;\xi(x),\eta(x))$ of the space–time local parameters $(\xi,\eta)(x)$. It is assumed that $\Delta \neq 0$.

Performing transformation (97), we find:

$$DM_j(\xi,\eta) = \frac{1}{\Delta_c(u)} \prod_a \prod_x \mathrm{d}\xi \mathrm{d}\eta\, \mathrm{d}\lambda_a \mathrm{d}q_a\, \delta(\mathbf{D}_a^b \cdot \mathbf{p}_b)\, \delta\left(\dot{\mathbf{u}}_a(x) - \frac{\delta H_j}{\delta \mathbf{p}_a(x)}\right) \delta\left(\dot{\mathbf{p}}_a(x) + \frac{\delta H_j}{\delta \mathbf{u}_a(x)}\right). \tag{98}$$

Here the gauge phase λ_a and conjugate to it q_a was extracted from the set of variables ξ and η.

Using the result of Sec. III B, one may diagnolize arguments of δ-functions. As a results:

$$DM_j(\xi,\eta,\lambda,Q) = \prod_{x,t,a} \mathrm{d}\xi\, \mathrm{d}\eta\, \mathrm{d}\lambda\, \mathrm{d}q\, \delta(\mathbf{D}_a^b(\mathbf{u}) \cdot \mathbf{p}_b)\, \delta\left(\dot{\lambda}_a - \frac{\delta h_j}{\delta q_a}\right) \delta\left(\dot{q}_a + \frac{\delta h_j}{\delta \lambda_a}\right)$$
$$\times \delta\left(\dot{\xi} - \frac{\delta h_j}{\partial \eta}\right) \delta\left(\dot{\eta} + \frac{\partial h_j}{\partial \xi}\right). \tag{99}$$

Equality (99) holds iff h_j is defined by Poisson equations (for the three vectors given $\mathbf{u}_a$ and $\mathbf{p}_a$):

$$\{\mathbf{u}_a(x), h_j\} = \frac{\delta H_j}{\delta \mathbf{p}_a(x)}, \quad \{\mathbf{p}_a(x), h_j\} = -\frac{\delta H_j}{\delta \mathbf{u}_a(x)} \tag{100}$$

considering $(\xi,\ \eta)$ and (λ,q) in the Poisson brackets as the canonically conjugate pairs.

If we add to (100) one more equation:

$$h_j(\xi,\eta,\lambda,q) = H_j(\mathbf{u}_a,\mathbf{p}_a) \tag{101}$$

then, as was shown in Sec. III B, $\mathbf{u}_a$ and $\mathbf{p}_a$ should be solution of incident equations, assuming that (100) holds on the measure (99). Then

$$\mathbf{D}_a^b(u) \cdot \mathbf{p}_b \equiv 0 \tag{102}$$

since $\mathbf{p}_b$ is the solution of Eq. (100) at arbitrary $j_{\mu a}$. This remarkable result is the consequence of mapping into the invariant space $\mathcal{G}/\mathcal{H}$ to which the classical flow belongs completely. Therefore, the corresponding δ-function in (111) gives identically

$$\prod_x \delta(0).$$

This infinite factor should be canceled by normalization and will not be mentioned later. Note that the formalism contains one sources $\mathbf{j}_a$ conjugate to the coordinates $\mathbf{u}_a$ only, see (101) and (93).

So, the described mapping gives the measure:

$$DM_j(\xi,\eta,\lambda,Q)=\prod_{x,t;a} \mathrm{d}\lambda_a \mathrm{d}q_a \mathrm{d}\xi \mathrm{d}\eta\, \delta(\dot{\lambda}_a)\, \delta\left(\dot{q}_a+\frac{\delta h_j}{\delta \lambda_a}\right) \delta\left(\dot{\xi}-\frac{\partial h_j}{\partial \eta}\right) \delta\left(\dot{\eta}+\frac{\partial h_j}{\partial \xi}\right). \tag{103}$$

We have taken into account here that $(u,p)_a$ are q_a independent. The Hamiltonian h_j is defined by Eq. (101):

$$2gh_j=\int \mathrm{d}^3x(p_a^2+\mathbf{B}_a^2(u))+\int d^3x \mathbf{j}_a\mathbf{u}_a\equiv h+J, \tag{104}$$

where h is the unperturbated by $\mathbf{j}_a$ Hamiltonian.

Helping the Proposition V, we can exclude the q_a dependence:

$$DM_j(\xi,\eta,\lambda)=\mathrm{d}R\prod_{x;a} \mathrm{d}\lambda_a \mathrm{d}\xi \mathrm{d}\eta\, \delta(\dot{\lambda}_a)\, \delta(\dot{\xi}-\omega-j_\xi)\, \delta(\dot{\eta}-j_\eta), \tag{105}$$

where the ''velocity'' $\omega=\partial h/\partial\eta$. The perturbations generating operator takes the form:

$$2\mathcal{K}(je)=\int \mathrm{d}t\{\hat{j}_\xi \hat{e}_\xi+\hat{j}_\eta \hat{e}_\eta\}. \tag{106}$$

At the same time one should replace in (85) $\mathbf{e}_a$ on

$$\mathbf{e}_a(x)=e_\xi(t)\frac{\partial \mathbf{u}_a(x;\xi,\eta,\lambda)}{\partial\eta(t)}-e_\eta(t)\frac{\partial \mathbf{u}_a(x;\xi,\eta,\lambda)}{\partial\xi(t)}. \tag{107}$$

As follows from (105) we should consider the time independent gauge transformations:

$$\dot{\lambda}_a(x)=0. \tag{108}$$

To remove this constraint we should generalize Eq. (100). So, if we consider the equation:

$$\{\mathbf{u}_a(x;\xi,\eta,\lambda),h_j\}=\frac{\delta H_j}{\delta \mathbf{p}_a(x)}-\Omega_a(x)\frac{\partial \mathbf{u}(x;\xi,\eta,\lambda)}{\partial \lambda_a} \tag{109}$$

instead of the first equation in (100) then one should replace in (105)

$$\prod_{x,a} \mathrm{d}\lambda_a(x)\,\delta(\dot{\lambda}_a(x))\to\prod_{x;a} \mathrm{d}\lambda_a(x)\,\delta(\dot{\lambda}_a(x)-\Omega_a(x)), \tag{110}$$

where $\Omega_a(x)$ is the arbitrary function of y and t. This is the most general representation for gauge measure in our formalism.

As a result, the main elements of quantum Yang–Mills theory in the $\mathcal{G}/\mathcal{H}$ space looks as follows.

(i) The measure

$$DM_j(\xi,\eta,\lambda)=\mathrm{d}R\prod_{x;a}\mathrm{d}\lambda_a\mathrm{d}\xi\mathrm{d}\eta\,\delta(\dot\lambda_a(x)-\Omega_a(x))\,\delta(\dot\xi-\omega-j_\xi)\,\delta(\dot\eta-j_\eta). \tag{111}$$

Using definition (25), one may note that

$$\int\prod_{x,a}\mathrm{d}\lambda_a\,\delta(\dot\lambda_a(x)-\Omega_a(x))$$

means integration over all functions $\lambda_a(y,t)$ of the arbitrary given time dependence. At the same time

$$\frac{\int\Pi_{x;a}\mathrm{d}\lambda_a\,\delta(\dot\lambda_a(x)-\Omega_a(x))}{\int\Pi_{x;a}\mathrm{d}\lambda_a}\equiv 0. \tag{112}$$

Therefore our normalization on the gauge group volume differs from the ordinary one. But this will not affect the result since all contributions will be gauge invariant.

(ii) The quantum perturbation's generating operator

$$2\hat K(\mathbf{je})=\int dt\{\hat{\mathbf{j}}_\xi\cdot\hat{\mathbf{e}}_\xi+\hat{\mathbf{j}}_\eta\cdot\hat{\mathbf{e}}_\eta\}. \tag{113}$$

(iii) The interactions functional $U(\mathbf{u},\overline{e})$ depends on

$$\mathbf{e}_a=\mathbf{e}_\xi\cdot\frac{\partial\mathbf{u}_a}{\partial\eta}-\mathbf{e}_\eta\cdot\frac{\partial\mathbf{u}_a}{\partial\xi}. \tag{114}$$

Note the motion along λ orbits is exactly classical and the dependence of nondynamical variables has disappeared.

D. Gauge invariance

We wish to quantize the theory without gauge fixing *ansatz* and, therefore, the theory contains three *independent* potential $\mathbf{u_{ia}}$, $i=1,2,3$ for each color index a. We may avoid this problem with the unphysical degrees of freedom if the theory would depend only on the gauge-invariant observable quantities: the color electric, $\mathbf{E}_a$, and magnetic, $\mathbf{B}_a$, fields.

Proposition VI: Each order over $1/g$ *is explicitly gauge invariant.*

The interactions functional U has following explicit form:

$$-3!\,U(\mathbf{u},e)=\frac{1}{g}\int\mathrm{d}x\prod_{k=1}^{3}\left\{e_{a_k}\frac{\partial}{\partial u_{a_k}}\right\}F^{\mu\nu a}F_{\mu\nu a},$$

where e_a was defined in (114). Using this definition, we find:

$$-3!\,U(\mathbf{u},e)=\int\mathrm{d}x\prod_{k=1}^{3}\left\{\left[\mathbf{e}_\xi\cdot\frac{\partial\mathbf{u}_a}{\partial\eta}-\mathbf{e}_\eta\cdot\frac{\partial\mathbf{u}_a}{\partial\xi}\right]\frac{\partial}{\partial\mathbf{u}_{\mathbf{a}_k}}\right\}F^{\mu\nu a}F_{\mu\nu a}. \tag{115}$$

The summation over repeated indices is assumed.

The last expression is manifestly gauge invariant since the operator is singlet of gauge transformations and $F^{\mu\nu a}F_{\mu\nu a}$ is the gauge invariant quantity.

E. Divergences

Expression (115) may be written in the form:

$$-3!U(\mathbf{u},\overline{e})=\int \mathrm{d}t\prod_{k=1}^{3}\left\{\left[\mathbf{e}_{\xi}\cdot\frac{\partial\mathbf{u}_a}{\partial\eta}-\mathbf{e}_{\eta}\cdot\frac{\partial\mathbf{u}_a}{\partial\xi}\right]\frac{\partial}{\partial\mathbf{u}_{\mathbf{a_k}}}\right\}\mathcal{L}(u), \tag{116}$$

where

$$\mathcal{L}(u)=\int \mathrm{d}^3x F^{\mu\nu a}F_{\mu\nu a}$$

is the Yang–Mills Lagrangian.

Result of action of the perturbation generating operator gives the expression:

$$\mathcal{N}(u)=\int DM(\xi,\eta):e^{-2iU(u,e)}:, \tag{117}$$

where the operator

$$-3!(2i)^3\mathcal{U}(u,e)=\int \mathrm{d}t\prod_{k=1}^{3}\left\{\left[\frac{\delta}{\delta\mathbf{j}_{\xi}}\cdot\frac{\partial\mathbf{u}_a}{\partial\eta}-\frac{\delta}{\delta\mathbf{j}_{\eta}}\cdot\frac{\partial\mathbf{u}_a}{\partial\xi}\right]\frac{\partial}{\partial\mathbf{u}_a}\right\}\mathcal{L}(u), \tag{118}$$

where u_{ia} depends on the solution of equations:

$$\dot{\xi}-\omega(\eta)=j_{\xi},\quad \dot{\eta}=j_{\eta} \tag{119}$$

and the measure is j_X, $X=\xi,\eta$ independent:

$$DM=\mathrm{d}R\prod_a\prod_{y,t}D\lambda_a\delta(\dot{\lambda}_a-\Omega)\,\delta(\dot{\xi}-\omega(\eta))\,\delta(\dot{\eta}).$$

Such ''shift'' is possible since Eqs. (119) are linear over j_X.

We can conclude that if $u_{a\mu}$ is not singular,

$$|S(u)|<\infty, \tag{120}$$

then the theory did not contain divergences since the differential operator in (118) cannot change convergence of the time integrals. Notice that the $O(4)\times O(2)$ solution obeys this property.[3]

IV. CONCLUSION

It was shown that there exists such formulation of the quantum Yang–Mills theory which is (a) divergence free (at least in the vector fields sector), (b) did not contain the gauge ghosts, and (c) is sufficiently consistent, i.e., the quantization scheme is free from the Gribov ambiguities.

It was shown in Ref. 2 that if $\partial(\mathcal{G}/\mathcal{H})$ is the boundary then the quantum corrections are accumulated on this boundary, i.e., the intersection $\partial u_{a\mu}\cap\partial(\mathcal{G}/\mathcal{H})$, where $\partial u_{a\mu}$ is the flow in the $\mathcal{G}/\mathcal{H}$ coordinate system, defines the value of quantum corrections. If $\partial u_{a\mu}\cap\partial(\mathcal{G}/\mathcal{H})=0$ then the semiclassical approximation is exact. This is the crucial property of our topological QCD.

For this reason the tQCD seems attractive and the question of whether it takes the place of pQCD seems important. The experimentally examined consequences of the tQCD would be extremely interesting and they will be investigated in the first place.

Being convergent, the exactness of estimation of the measurables in tQCD should be higher then in the ''logarithmic'' pQCD. Moreover, the convergence means that the main contributions

are accumulated on the large distances. This property is typical for hadron physics. Therefore, the main point of our future publications would be the prediction of the small-scale effects, where we can compare our approach with pQCD.

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APPENDIX: REDUCTION OF THE SPACE DEGREES OF FREEDOM

Action of the operator $\exp\{-i\mathcal{K}\}$ leads to

$$\mathcal{N}(u)=\int DM_j(\xi,\eta):e^{-2i\mathcal{U}(u,j)}:, \tag{A1}$$

where

$$-3!(2i)^3\mathcal{U}(u,j)=\int \mathrm{d}^3x\,\mathrm{d}t\,\prod_{a,k}\left\{\left[\frac{\delta}{\delta\mathbf{j}_\xi}\cdot\frac{\partial\mathbf{u}_a}{\partial\eta}-\frac{\delta}{\delta\mathbf{j}_\eta}\cdot\frac{\partial\mathbf{u}_a}{\partial\xi}\right]\frac{\partial}{\partial\mathbf{u}_a}\right\}\mathcal{L}(u) \tag{A2}$$

and the colons in (A1) mean the ''normal product,'' when the variational derivatives over j_X in the expansion of $\exp\{-2i\mathcal{U}(u,j)\}$ stay to the left of all functions.

The measure

$$DM_j(\xi,\eta)=\prod_{y,t}\mathrm{d}\xi\mathrm{d}\eta\,\delta(\dot\xi-\omega_\eta-j_\xi)\,\delta(\dot\eta+\omega_\xi-j_\eta).$$

Then, to calculate the remaining integral in (A1), one should find solution of inhomogeneous equations:

$$\dot\xi(y,t)-\omega_\eta(y,t;\xi,\eta)=j_\xi(y,t),\quad \dot\eta(y,t)+\omega_\xi(y,t;\xi,\eta)=j_\eta(y,t), \tag{A3}$$

where

$$\omega_X(y,t;\xi,\eta)=\delta h(\xi,\eta)/\delta X(y,t).$$

As follows from (A2), if some operators $\hat j_{X'}$ over the ''auxiliary'' variable X' were not contain in $\mathcal{U}(u,j)$ then the auxiliary variables X' should obey the homogeneous, classical, equations, with $j_{X'}=0$ on the right-hand side.

The solutions of inhomogeneous equation (A3) will be searched expanding over j_X:

$$\begin{aligned}\xi(y,t)&=\xi^0(y,t)+\int \mathrm{d}^4x'\,\xi^1_\xi(y,t;y',t')j_\xi(y',t')+\int \mathrm{d}^4x'\,\xi^1_n(y,t;y',t')j_\eta(y',t')+\cdots,\\ \eta(y,t)&=\eta^0(y,t)+\int \mathrm{d}^4x'\,\eta^1_\eta(y,t;y',t')j_\eta(y',t')+\int \mathrm{d}^4x'\,\eta^1_\xi(y,t;y',t')j_\xi(y',t')+\cdots.\end{aligned} \tag{A4}$$

So, the equations:

$$\dot\xi^0(y,t)=\omega_\eta(y,t;\xi^0,\eta^0),\quad \dot\eta^0(y,t)=-\omega_\xi(y,t;\xi^0,\eta^0) \tag{A5}$$

should be solved in the lowest order over j_X. The function $u(y;\xi(y,t),\eta(y,t))$ should obey the ''boundary'' property:

$$u(y;\xi(y,t),\eta(y,t))|_{j=0}=u(y;\xi^0,\eta^0)=u(y,t;\xi_0,\eta_0), \tag{A6}$$

where ξ_0 and η_0 are the integration constants of the Lagrange equation (11). The equality (A6) defines the starting set of the necessary variables ξ and η. Notice that, as follows from Proposition III, the quantum perturbations should not change this set.

Let us distinguish the variables $\xi \in \mathcal{G}/\mathcal{H}$ by the equality:

$$\frac{\delta}{\delta\xi}h\bigg|_{j_x=0}=0. \tag{A7}$$

This assumes that the set η can be expressed through the set conserved generators. In example (1), they are the generators of translation and special conformal transformation. Notice that Proposition III means that the quantum perturbations did not alter this definition.

Inserting (A7) into (A5) we find at $j_X=0$ the equations:

$$\dot{\xi}^0(y,t)=\omega_\eta(\eta^0)\equiv\omega(\eta^0), \quad \dot{\eta}^0(y,t)=0. \tag{A8}$$

The functions with arbitrary y dependence may satisfy this equations. Using solution of this equation:

$$\xi^0(y,t)=\omega(\eta^0)t+\xi_0, \quad \eta^0(y,t)=\eta_0, \tag{A9}$$

where ξ_0 and η_0 are the integration constants, we will see that the dependence on y in (A6) did not play any role because of the degeneracy over y. For this reason we will put out the y dependence in ξ^0 and η^0.

It is not hard to show that the degeneracy over y will be conserved in arbitrary order over j_X. Indeed, inserting the expansions (A4) into Eq. (A3), we find in the first order over j_ξ:

$$\partial_t\xi^1_y(y,t;y',t')-\xi^1_\xi(y,t;y',t')\frac{\delta^2h(\xi,\eta)}{\delta\xi(y',t')\,\delta\xi(y,t)}\bigg|_{j=0}-\xi^1_\eta(y,t;y',t')\frac{\delta^2h(\xi,\eta)}{\delta\eta(y',t')\,\delta\xi(y,t)}\bigg|_{j=0}$$

$$=\delta(y-y')\,\delta(t-t').$$

Notice that

$$\frac{\delta h(\xi,\eta)}{\delta\xi(y,t)}\bigg|_{j=0}=\frac{\delta}{\delta\xi(y,t)}\{h(\xi,\eta)|_{j=0}\}=0,$$

where (A7) was used. Therefore, the equation for ξ^1_ξ has a structure:

$$\dot{\xi}^1_\xi(y,t;y',t')=\delta(y-y')\,\delta(t-t'), \tag{A10}$$

where the boundary conditions (A9) were applied. Notice that this equation is linear.

Inserting the solution of Eq. (A10):

$$\xi^1_\xi(y,t;y',t')=\delta(y-y')g(t-t'), \tag{A11}$$

where $g(t-t')$ is the Green function defined in Ref. 2, into (A4), we find the term

$$\sim\int \mathrm{d}t'\,g(t-t')j_\xi(y,t').$$

So, the y dependence is contained in the auxiliary source j_ξ only. For this reason it cannot play a dynamical role. The same phenomena one can observe considering other terms in the decomposition (A4).

Therefore, admitting that the quantum perturbations switched on adiabatically, i.e., may be taken into account perturbatively, and for this reason are unable to change the topology of the classical trajectory $u(y;\xi,\eta)$, Proposition III, one may conclude that it is enough to take $\xi=\xi(t)$ and $\eta=\eta(t)$ in the considered scalar theory.

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[16] This conclusion would be in accordance with the canonical formalism, where existence of the canonical commutator is the necessary and sufficient condition of quantization.
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[20] This property usually is postulated, see, e.g., R. Jackiw, Rev. Mod. Phys. **49**, 681 (1977), but it can be proved explicitly if the *topological* solitons are considered (Ref. 6).
[21] The intriguing question concerning ''asymptotic freedom'' in our perturbation theory will be considered in subsequent publications.
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[28] Indeed, let us remind that in the result of the canonical momentum mapping $J:(q,k)\to(Q,K)$ we find $q(Q,K)$ and $k(Q,K)$. This function completed by Hamiltonian equations for Q and K solves the dynamical problem. Therefore, the time dependence is contained only in Q and K. But, as was mentioned in Ref. 25, the structure of W is *ad hoc* unknown for the field theory case. For this reason we later check this assumption.

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Coherent states for SU(3)

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We define coherent states for SU(3) using six bosonic creation and annihilation operators. These coherent states are explicitly characterized by six complex numbers with constraints. For the completely symmetric representations $(n,0)$ and $(0,m)$, only three of the bosonic operators are required. For mixed representations (n,m), all six operators are required. The coherent states provide a resolution of identity, satisfy the continuity property, and possess a variety of group theoretic properties. We introduce an explicit parametrization of the group SU(3) and the corresponding integration measure. Finally, we discuss the path integral formalism for a problem in which the Hamiltonian is a function of SU(3) operators at each site. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1385563]

I. INTRODUCTION

Coherent states have been used for a long time in different areas of physics.[1,2] In the area of quantum optics, coherent states based on the Heisenberg–Weyl group (which are described later in this work) have been extensively used to study the interaction of a single mode of electromagnetic radiation with a two-level atomic system (for instance, the Jaynes–Cummings model).[3] Coherent states based on the noncompact Lie group SU(1,1) have also been used to study certain problems in quantum optics.[4] In condensed matter physics, coherent states for the Lie group SU(2) have been very useful for studying Heisenberg spin systems using the path integral formalism.[5–8] These studies have been generalized to systems with SU(N) symmetry, although such studies have usually been restricted to the completely symmetric representations.[6,9] However, there is a recent discussion of coherent states for arbitrary irreducible representations of SU(3) in Ref. 10. The purpose of our work is to discuss a coherent state formalism which is valid for all representations of SU(3), and to give an explicit characterization of them in terms of complex numbers and the states of some harmonic oscillators. (Our work differs in this respect from Ref. 10 which does not use harmonic oscillator operators to define the basis states.) As we will see, this way of characterization is very similar to those used for the Heisenberg–Weyl and SU(2) coherent states. But, there are certain additional features (such as tracelessness) which are redundant in the simpler case of SU(2).

One can imagine various possible applications of coherent states for SU(3). In quantum optics, coherent states for SU(3) may turn out to be useful for studying the interaction of a three-level atomic system with three modes of electromagnetic radiation (corresponding to the three possible energy differences of the atom). We should also mention that there have been many other studies of SU(3) in the recent mathematical physics literature, including the geometric phase for three-level systems[11] and the study of Clebsch–Gordon coefficients and the outer multiplicity problem.[12] These studies do not use coherent states; however, our work is likely to shed new light on some of these studies. For instance, we will use two triplets of complex numbers z and w which

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are similar to the ones used in Ref. 12, except that we will normalize the triplets to unity. Similarly, it is well known that the geometric phases in the different representations of SU(2) may be obtained by integrating around a closed loop the overlap of two coherent states which differ infinitesimally from each other.[7,8] In the same way, it should be possible to derive the geometric phases for SU(3) representations from the coherent states discussed below.

The organization of the article is as follows. Section II will motivate our ideas and techniques using two examples which are simpler than the SU(3) group. We start with the standard group theoretical definitions of the coherent states of the Heisenberg–Weyl and SU(2) groups. We then discuss another way of defining SU(2) coherent states using the Schwinger or Holstein–Primakoff representation of the Lie algebra of SU(2)[13] in terms of harmonic oscillator creation and annihilation operators. This definition is discussed in some detail as it can be extended to the SU(3) group. We then establish its equivalence with the standard group theoretical coherent state definition.[2] In Sec. III, we generalize the SU(2) Lie algebra in terms of harmonic oscillators to the SU(3) group, and construct the irreducible representations of SU(3). We describe the structure of SU(3) matrices in an explicit way, and provide an integration measure for this eight-dimensional manifold. In Sec. IV, we use this group structure to construct a set of SU(3) coherent states which are explicitly characterized by a set of complex numbers which are equivalent to eight real variables. We prove various identities expected for coherent states such as the resolution of identity and a transformation from a particular coherent state to the general coherent state. In Sec. V, we provide an alternative set of coherent states for SU(3) which require only five real variables; although these share some of the features of the coherent states defined in Sec. IV, they have a few limitations arising from the smaller number of variables used. In Sec. VI, we discuss how coherent states can be used to develop a path integral formalism for problems involving SU(3) variables.

II. HEISENBERG–WEYL AND SU(2) COHERENT STATES

There are many definitions of coherent states used in the literature. However, the most essential ingredients common in all these definitions are the continuity and completeness properties.[1]

(1) These are states in a Hilbert space $\mathcal{H}$ associated which are characterized by a set of continuous variables $\{\vec{z}\}$, and the coherent states $|\vec{z}\rangle$ are strongly continuous functions of the labels $\{\vec{z}\}$.
(2) There exists a positive measure $d\mu(\vec{z})$ such that the unit operator $\mathcal{I}$ admits the resolution of identity

$$\mathcal{I}=\int d\mu(\vec{z})|\vec{z}\rangle\langle\vec{z}|. \tag{1}$$

Given a group G, the coherent states in a given representation R are functions of q parameters denoted by $\{z_1,z_2,\ldots,z_q\}$, and are defined as

$$|\vec{z}\rangle\equiv T_R(g(\vec{z}))|0\rangle_R. \tag{2}$$

Here $T_R(g(\vec{z}))$ is a group element in the representation R, and $|0\rangle_R$ is a fixed vector belonging to R. In the simplest example of the Heisenberg–Weyl group, the Lie algebra contains three generators. It is defined in terms of creation annihilation operators $(a,a^\dagger)$ satisfying

$$[a,a^\dagger]=\mathcal{I},\quad [a,\mathcal{I}]=0,\quad [a^\dagger,\mathcal{I}]=0. \tag{3}$$

This algebra has only one infinite dimensional irreducible representation which can be characterized by occupation number states $|n\rangle\equiv(a^\dagger)^n/\sqrt{n!}\,|0\rangle$ with $n=0,1,2,\ldots$. A generic group element in (2) can be characterized by $T(g)=\exp(i\alpha\mathcal{I}+za^\dagger-\overline{z}a)$ with an angle α and a complex parameter z. Therefore,

$$|\alpha,z\rangle_\infty = \exp(i\alpha)|z\rangle, \quad |z\rangle = \exp(za^\dagger - \bar{z}a)|0\rangle = \sum_{n=0}^{\infty} F_n(z)|n\rangle, \tag{4}$$

where the sum runs over all the basis vectors of the infinite dimensional representation, and

$$F_n(z) = \frac{z^n}{\sqrt{n!}}\exp(-|z|^2/2) \tag{5}$$

are the coherent state expansion coefficients. This feature, i.e., an expansion of the coherent states in terms of basis vectors of a given representation with analytic functions of complex variables ($F_n(z)$) as coefficients, will also be present in the case of SU(2) and SU(3) groups. It is easy to see that Eq. (4) provides a resolution of identity as in (1) with the measure $d\mu(z) = dz d\bar{z}$.

We now briefly review the next simplest example, i.e., the coherent states associated with the SU(2) group. The SU(2) Lie algebra is given by a set of three angular momentum operators $\{\vec{J}\} \equiv \{J_1, J_2, J_3\}$ or equivalently by $\{J_+, J_-, J_3\}$, ($J_\pm \equiv J_1 \pm iJ_2$) satisfying

$$[J_3, J_\pm] = \pm J_\pm, \quad [J_+, J_-] = 2J_3. \tag{6}$$

The SU(2) group has a Casimir operator given by $\vec{J}\cdot\vec{J}$, and the different irreducible representations are characterized by its eigenvalues $j(j+1)$, where j is an integer or half-odd-integer. A given basis vector in representation j is labeled by the eigenvalue m of J_3 as $|j,m\rangle$. We characterize the SU(2) group elements U by the Euler angles, i.e., $U(\theta,\phi,\psi) \equiv \exp(i\phi J_3)\exp(i\theta J_2)\exp(i\psi J_3)$. The standard group theoretical definition (2) takes $|0\rangle_j$ in (2) to be the highest weight state $|j,j\rangle$ and is of the form

$$\begin{aligned} |\hat{n}(\theta,\phi)\rangle_j &= U(\theta,\phi,\psi)|j,j\rangle, \\ &= \sum_{m=-j}^{+j} C_m(\theta,\phi)|j,m\rangle, \end{aligned} \tag{7}$$

In (7), the coefficients $C_m(\theta,\phi)$ are given by

$$C_m(\theta,\phi) = e^{im\phi}\sqrt{\frac{(2j)!}{(j+m)!(j-m)!}}\left[\sin\frac{\theta}{2}\right]^{j-m}\left[\cos\frac{\theta}{2}\right]^{j+m}, \tag{8}$$

where we have ignored possible phase factors.

The algebra in Eq. (6) can be realized in terms of a doublet of harmonic oscillator creation and annihilation operators $\vec{a} \equiv (a_1, a_2)$ and $\vec{a}^\dagger \equiv (a_1^\dagger, a_2^\dagger)$, respectively.[13] They satisfy the simpler bosonic commutation relation $[a_i, a_j^\dagger] = \delta_{ij}$ with $i,j = 1,2$. The vacuum state is $|0,0\rangle$. In terms of these operators,

$$J^a \equiv \tfrac{1}{2}a_i^\dagger(\sigma^a)_{ij}a_j, \tag{9}$$

where σ^a denote the Pauli matrices. (We will generally use the convention that repeated indices are summed over). It is easy to check that the operators in (9) satisfy the SU(2) Lie algebra with the Casimir $\vec{J}\cdot\vec{J} \equiv \frac{1}{4}\vec{a}^\dagger\cdot\vec{a}(\vec{a}^\dagger\cdot\vec{a}+2)$. Thus the representations of SU(2) can be characterized by the eigenvalues of the occupation number operator; the spin value j is equal to $(N_1+N_2)/2$ where N_1 and N_2 are the eigenvalues of $a_1^\dagger a_1$ and $a_2^\dagger a_2$, respectively.

With these harmonic oscillator creation and annihilation operators, another definition of SU(2) coherent states is obtained by directly generalizing (4). We define a doublet of complex numbers (z_1, z_2) with the constraint $|z_1|^2 + |z_2|^2 = 1$; this gives three independent real parameters which define the sphere S^3. Let us parameterize

$$z_1 = \cos\chi e^{i\beta_1} \quad \text{and} \quad z_2 = \sin\chi e^{i\beta_2}, \tag{10}$$

where $0 \leqslant \chi \leqslant \pi/2$ and $0 \leqslant \beta_1, \beta_2 < 2\pi$. The integration measure on this space takes the form

$$d\Omega_{S^3} = \frac{1}{\pi^2} dz_1 d\bar{z_1} dz_2 d\bar{z_2} \delta(|z_1|^2 + |z_2|^2 - 1) = \frac{1}{2\pi^2} \cos\chi \sin\chi d\chi d\beta_1 d\beta_2, \tag{11}$$

where we have introduced a normalization factor so that $\int d\Omega_{S^3} = 1$. The SU(2) coherent state in the representation N is now defined as

$$|z_1, z_2\rangle_{N=2j} = \delta_{\vec{a}^\dagger \cdot \vec{a}, N} \sqrt{N!} \exp(\vec{z} \cdot \vec{a}^\dagger)|0,0\rangle = \sum_{N_1, N_2}{}' F_{N_1, N_2} |N_1, N_2\rangle_j . \tag{12}$$

In the second equation in (12), the Σ' implies that only the terms satisfying the constraint $a^\dagger \cdot a = N \equiv 2j$ are included or equivalently that

$$N_1 + N_2 = N. \tag{13}$$

With (13), the states $|N_1, N_2\rangle_j$ form a $(2j+1)$-dimensional representation of SU(2). The expansion coefficients $F_{N_1, N_2}(z_1, z_2)$ are analytic functions of (z_1, z_2) and are given by

$$F_{N_1, N_2} \equiv \left(\frac{N!}{N_1! N_2!} \right)^{1/2} z_1^{N_1} z_2^{N_2}. \tag{14}$$

Equations (12) and (14) are similar to (4) and (5), respectively. This will be generalized to the SU(3) case in Sec. III. It is easy to check that (12) provides the resolution of identity with the measure given in (11), namely,

$$\int d\Omega_{\mathrm{SU}(2)} |z_1, z_2\rangle_{jj} \langle z_1, z_2| = \frac{1}{2j+1} \sum_{m=-j}^{j} |j,m\rangle\langle j,m|. \tag{15}$$

Now we change variables from N_1 and $N_2 = 2j - N_1$ to $m = \frac{1}{2}(N_1 - N_2)$, and define

$$\omega \equiv \frac{z_1}{z_2} = e^{i\phi} \cot\frac{\theta}{2}. \tag{16}$$

These parameters are related to the ones given in (10) as $\theta = 2\chi$ and $\phi = \beta_1 - \beta_2$. We now consider an unit sphere S^2 with its south pole touching the point $\omega = 0$. The sphere is characterized by (θ, ϕ) where θ and ϕ are the polar and azimuthal angles, respectively. Using the stereographic projection, it is easy to verify that

$$|z_1, z_2\rangle_j = (z_1)^{2j} \sum_{m=-j}^{j} \sqrt{\frac{(2j)!}{(j+m)!(j-m)!}} (\omega)^{(m-j)} |j,m\rangle = |\hat{n}(\theta, \phi)\rangle_j , \tag{17}$$

where we have again ignored possible phase factors. Equation (17) can also be written as

$$|z_1, z_2\rangle_j = (z_1)^{2j} \exp\left(\frac{z_2}{z_1} J_- \right) |z_1 = 1,\, z_2 = 0\rangle_j , \tag{18}$$

where $|z_1 = 1,\, z_2 = 0\rangle_{N=2j} = |j,j\rangle$ and we have used the fact that $J_- = a_2^\dagger a_1$. Equations (17) and (18) establish the equivalence between the group theoretical theoretical definition (7) and the one using Schwinger bosons (12).

The stationary subgroup of a particular coherent state is defined as the subgroup H of the full group G which leaves that coherent state invariant up to a phase; the coherent states are functions

of the coset space G/H.[2] It is clear from the previous discussion that the stationary subgroup of the SU(2) coherent states is U(1); therefore the coherent states correspond to the coset space $\mathrm{SU}(2)/\mathrm{U}(1)=S^2$ which is parametrized by the angles (θ,ϕ).

III. SU(3) AND ITS REPRESENTATIONS

Let us first discuss a parametrization of SU(3) matrices, i.e., 3×3 unitary matrices with unit determinant. To motivate this, let us first consider a parametrization of SO(3) matrices. Consider a real vector of unit length of the form

$$\vec{p}=\begin{pmatrix}\sin\theta\cos\phi\\ \sin\theta\sin\phi\\ \cos\theta\end{pmatrix}. \tag{19}$$

The most general real vector q of unit length which is orthogonal to p is given by

$$\vec{q}=\begin{pmatrix}\cos\chi\cos\theta\cos\phi+\sin\chi\sin\phi\\ \cos\chi\cos\theta\sin\phi-\sin\chi\cos\phi\\ -\cos\chi\sin\theta\end{pmatrix}. \tag{20}$$

Finally, we define a third unit vector $\vec{r}=\vec{p}\times\vec{q}$, i.e., $r_1=p_2q_3-p_3q_2$, etc. Then a 3×3 matrix whose columns are given by the vectors p,q and r is an SO(3) matrix.

We will now generalize the previous construction to obtain an SU(3) matrix. A complex vector of unit norm is given by

$$\vec{z}=\begin{pmatrix}\sin\theta\cos\phi e^{i\alpha_1}\\ \sin\theta\sin\phi e^{i\alpha_2}\\ \cos\theta e^{i\alpha_3}\end{pmatrix}, \tag{21}$$

where $0\leqslant\theta,\phi\leqslant\pi/2$ and $0\leqslant\alpha_1,\alpha_2,\alpha_3<2\pi$. Then the integration measure for $\vec{z}$, which is equivalent to the sphere S^5, is given by

$$\begin{aligned}d\Omega_{S^5}&=\frac{2}{\pi^3}dz_1d\bar{z}_1dz_2d\bar{z}_2dz_3d\bar{z}_3\delta(|z_1|^2+|z_2|^2+|z_3|^2-1)\\ &=\frac{1}{\pi^3}\sin^3\theta\cos\theta\cos\phi\sin\phi d\theta d\phi d\alpha_1 d\alpha_2 d\alpha_3,\end{aligned} \tag{22}$$

which has been normalized to make $\int d\Omega_{S^5}=1$. The most general complex vector $\vec{w}$ of unit norm satisfying $\vec{z}\cdot\vec{w}=0$ is given by

$$\vec{w}=\begin{pmatrix}e^{i(\beta_1-\alpha_1)}\cos\chi\cos\theta\cos\phi+e^{i(\beta_2-\alpha_1)}\sin\chi\sin\phi\\ e^{i(\beta_1-\alpha_2)}\cos\chi\cos\theta\sin\phi-e^{i(\beta_2-\alpha_2)}\sin\chi\cos\phi\\ -e^{i(\beta_1-\alpha_3)}\cos\chi\sin\theta\end{pmatrix}, \tag{23}$$

where $0\leqslant\chi\leqslant\pi/2$ and $0\leqslant\beta_1,\beta_2<2\pi$ just as in the integration measure for S^3 in (11). We may now define a third complex vector of unit norm as $\vec{v}=\bar{\vec{z}}\times\vec{w}$, where $\bar{\vec{z}}\equiv\vec{z}^{\star}$. Then we can check that a 3×3 matrix whose columns are given by z, $\bar{w}$ and v, i.e.,

$$S=\begin{pmatrix} z_1 & \bar{w}_1 & \bar{z}_2 w_3-\bar{z}_3 w_2 \\ z_2 & \bar{w}_2 & \bar{z}_3 w_1-\bar{z}_1 w_3 \\ z_3 & \bar{w}_3 & \bar{z}_1 w_2-\bar{z}_2 w_1 \end{pmatrix} \tag{24}$$

is an SU(3) matrix.

The integration measure for the group SU(3) is given by a product of (22) and (11) as[14,15]

$$d\Omega_{\mathrm{SU}(3)}=\frac{1}{2\pi^5}\sin^3\theta\cos\theta\cos\phi\sin\phi\cos\chi\sin\chi d\theta d\phi d\chi d\alpha_1 d\alpha_2 d\alpha_3 d\beta_1 d\beta_2, \tag{25}$$

which is normalized so that $\int d\Omega_{\mathrm{SU}(3)}=1$. To prove Eq. (25), we note that the matrix in (24) can be written as a product of two SU(3) matrices, i.e., $S=A_3A_2$, where

$$A_3=\begin{pmatrix} \sin\theta\cos\phi e^{i\alpha_1} & \cos\theta\cos\phi e^{i\alpha_1} & -\sin\phi e^{-i\alpha_2-i\alpha_3} \\ \sin\theta\sin\phi e^{i\alpha_2} & \cos\theta\sin\phi e^{i\alpha_2} & \cos\phi e^{-i\alpha_1-i\alpha_2} \\ \cos\theta e^{i\alpha_3} & -\sin\theta e^{i\alpha_3} & 0 \end{pmatrix}, \tag{26}$$

and

$$A_2=\begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\chi e^{-i\beta_1} & \sin\chi e^{i\beta_2-i\alpha_1-i\alpha_2-i\alpha_3} \\ 0 & -\sin\chi e^{-i\beta_2+i\alpha_1+i\alpha_2+1\alpha_3} & \cos\chi e^{i\beta_1} \end{pmatrix}. \tag{27}$$

The structure of the matrix A_3 is determined entirely by the three-dimensional complex vector which forms its first column; hence the integration measure corresponding to it is given by (22). The matrix A_2 is determined by the two-dimensional complex vector which forms its second column; its contribution to the integration measure is therefore given by (11). Note that although the parameter appearing in A_2 is $\beta_2-\alpha_1-\alpha_2-\alpha_2$ instead of only β_2 as in (10), this makes no difference in the product measure given in (25) since the differentials $d\alpha_i$ already appear in the integration measure coming from A_3. Incidentally, this procedure generalizes to any SU(N); the integration measure is given by a product of measures for S^{2N-1}, S^{2N-3}, $\ldots$, S^3.[14]

In short, we have defined two complex vectors $\vec{z}=(z_1,z_2,z_3)$ and $\vec{w}=(w_1,w_2,w_3)$ in (21) and (23). These satisfy the constraints

$$\begin{aligned} \vec{\bar{z}}\cdot\vec{z}&=|z_1|^2+|z_2|^2+|z_3|^2=1, \\ \vec{\bar{w}}\cdot\vec{w}&=|w_1|^2+|w_2|^2+|w_3|^2=1, \end{aligned} \tag{28}$$

and

$$\vec{z}\cdot\vec{w}=z_1w_1+z_2w_2+z_3w_3=0. \tag{29}$$

These constraints leave eight real degrees of freedom as required for SU(3). We will take $\vec{z}$ and $\vec{w}$ to transform respectively as the 3 and $3^\star$ representation of SU(3). Thus an SU(3) transformation acts on the matrix S in Eq. (24) by multiplication from the left.

Let us now define two triplets of harmonic oscillator creation and annihilation operators (a_i,b_i), $i=1,2,3$, satisfying

$$\begin{aligned} [a_i,a_j^\dagger]&=\delta_{ij}, \quad [b_i,b_j^\dagger]=\delta_{ij}, \\ [a_i,b_j]&=0, \quad [a_i,b_j^\dagger]=0. \end{aligned} \tag{30}$$

We will often denote these two triplets by $(\vec{a},\vec{b})$ and the two number operators by $N_a(\equiv\vec{a}^\dagger\cdot\vec{a})$ and $N_b(\equiv\vec{b}^\dagger\cdot\vec{b})$. Similarly, their vacuum state is denoted by $|\vec{0}_a,\vec{0}_b\rangle$. Henceforth, we will ignore the subscripts a,b and will denote the vacuum state by $|\vec{0},\vec{0}\rangle$, and the eigenvalues of N_a, N_b by N and M, respectively.

Now let λ^a, $a=1,2,\ldots,8$ be the generators of SU(3) in the fundamental representation; they satisfy the SU(3) Lie algebra $[\lambda^a,\lambda^b]=if^{abc}\lambda^c$. Let us define the following operators

$$Q^a=a^\dagger\lambda^a a-b^\dagger\lambda^{*a}b, \tag{31}$$

where $a^\dagger\lambda^a a\equiv a_i^\dagger\lambda_{ij}^a a_j$, and $b^\dagger\lambda^{*a}b\equiv b_i^\dagger\lambda_{ij}^{*a}b_j$. To be explicit,

$$\begin{aligned}
Q^3&=\tfrac{1}{2}(a_1^\dagger a_1-a_2^\dagger a_2-b_1^\dagger b_1+b_2^\dagger b_2),\\
Q^8&=\frac{1}{2\sqrt{3}}(a_1^\dagger a_1+a_2^\dagger a_2-2a_3^\dagger a_3-b_1^\dagger b_1-b_2^\dagger b_2+2b_3^\dagger b_3),\\
Q^1&=\tfrac{1}{2}(a_1^\dagger a_2+a_2^\dagger a_1-b_1^\dagger b_2-b_2^\dagger b_1),\\
Q^2&=-\frac{i}{2}(a_1^\dagger a_2-a_2^\dagger a_1+b_1^\dagger b_2-b_2^\dagger b_1),\\
Q^4&=\tfrac{1}{2}(a_1^\dagger a_3+a_3^\dagger a_1-b_1^\dagger b_3-b_3^\dagger b_1),\\
Q^5&=-\frac{i}{2}(a_1^\dagger a_3-a_3^\dagger a_1+b_1^\dagger b_3-b_3^\dagger b_1),\\
Q^6&=\tfrac{1}{2}(a_2^\dagger a_3+a_3^\dagger a_2-b_2^\dagger b_3-b_3^\dagger b_2),\\
Q^7&=-\frac{i}{2}(a_2^\dagger a_3-a_3^\dagger a_2+b_2^\dagger b_3-b_3^\dagger b_2).
\end{aligned} \tag{32}$$

It can be checked that these operators satisfy the SU(3) algebra among themselves, i.e., $[Q^a,Q^b]=if^{abc}Q^c$. Further,

$$\begin{aligned}
&[Q^a,a_i^\dagger]=\lambda_{ji}^a a_j^\dagger,\quad [Q^a,b_i^\dagger]=-\lambda_{ji}^{*a}b_j^\dagger,\\
&[Q^a,a^\dagger\cdot a]=0,\quad [Q^a,b^\dagger\cdot b]=0,\\
&[Q^a,a^\dagger\cdot b^\dagger]=0,\quad [Q^a,a\cdot b]=0.
\end{aligned} \tag{33}$$

From Eqs. (33), it is clear that the three states $a_i^\dagger|\vec{0},\vec{0}\rangle$ with $(N=1,\ M=0)$ and $b_i^\dagger|\vec{0},\vec{0}\rangle$ with $(N=0,\ M=1)$ transform respectively as the fundamental representation (3) and its conjugate representation $(3^\star)$. By taking the direct product of N $\vec{a}^\dagger$'s and M $\vec{b}^\dagger$'s we can now form higher representations. We now define an operator

$$O^{i_1 i_2\cdots i_N}_{j_1 j_2\cdots j_M}\equiv a_{i_1}^\dagger a_{i_2}^\dagger\ldots a_{i_N}^\dagger b_{j_1}^\dagger b_{j_2}^\dagger\ldots b_{j_M}^\dagger. \tag{34}$$

Under SU(3) transformation the states defined as $|\tilde{\psi}\rangle_{(N,M)}\equiv O^{i_1 i_2\cdots i_N}_{j_1 j_2\cdots j_M}|\vec{0},\vec{0}\rangle$ will all have $N_a=N$ and $N_b=M$, and will transform among themselves. Further, $|\tilde{\psi}\rangle=N|\tilde{\psi}\rangle$ and $N_b|\tilde{\psi}\rangle=M|\tilde{\psi}\rangle$. However, these do not form an irreducible representation because $\vec{a}\cdot\vec{b}$ and $\vec{a}^\dagger\cdot\vec{b}^\dagger$ are

SU(3) invariant operators [see (33)]. A general basis vector in the irreducible representation (N,M) is obtained by subtracting the traces and completely symmetrizing in upper and lower indices.[16] More explicitly, a state in (N,M) representation is given by

$$
\begin{aligned}
|\psi\rangle^{i_1,i_2,\ldots i_N}_{j_1,j_2,\ldots,j_M} \equiv \Bigg[& O^{i_1 i_2 \cdots i_N}_{j_1 j_2 \cdots j_M} + L_1 \sum_{l_1=1}^{N} \sum_{k_1=1}^{M} \delta^{i_{l_1}}_{j_{k_1}} O^{i_1 i_2 .. i_{l_1-1} i_{l_1+1} .. i_N}_{j_1 j_2 .. j_{k_1-1} j_{k_1+1} \cdots j_M} \\
& + L_2 \sum_{l_1,l_2=1}^{N} \sum_{k_1,k_2=1}^{M} \delta^{i_{l_1}}_{j_{k_1}} \delta^{i_{l_2}}_{j_{k_2}} O^{i_1 i_2 .. i_{l_1-1} i_{l_1+1} .. i_{l_2-1} i_{l_2+1} .. i_N}_{j_1 j_2 .. j_{k_1-1} j_{k_1+1} .. j_{k_2-1} j_{k_2+1} \cdots j_M} \\
& + L_3 \sum_{l_1,l_2,l_3=1}^{N} \sum_{k_1,k_2,k_3=1}^{M} \delta^{i_{l_1}}_{j_{k_1}} \delta^{i_{l_2}}_{j_{k_2}} \delta^{i_{l_3}}_{j_{k_3}} O^{i_1 i_2 .. i_{l_1-1} i_{l_1+1} .. i_{l_2-1} i_{l_2+1} .. i_{l_3-1} i_{l_3+1} .. i_N}_{j_1 j_2 .. j_{k_1-1} j_{k_1+1} .. j_{k_2-1} j_{k_2+1} .. j_{k_3-1} j_{k_3+1} \cdots j_M} \\
& + \ldots + L_Q \sum_{l_1,l_2,l_3,..,l_Q=1}^{N} \sum_{k_1,k_2,k_3,..,k_Q=1}^{M} \delta^{i_{l_1}}_{j_{k_1}} \delta^{i_{l_2}}_{j_{k_2}} .. \delta^{i_{l_Q}}_{j_{k_Q}} \\
& \times O^{i_1 i_2 .. i_{l_1-1} i_{l_1+1} .. i_{l_2-1} i_{l_2+1} .. i_{l_Q-1} i_{l_Q+1} .. i_N}_{j_1 j_2 .. j_{k_1-1} j_{k_1+1} .. j_{k_2-1} j_{k_2+1} .. j_{k_Q-1} j_{k_Q+1} \cdots j_M} \Bigg] |\vec{0},\vec{0}\rangle, \qquad (35)
\end{aligned}
$$

where $Q = \mathrm{Min}(N,M)$,

$$
L_q \equiv \frac{(-1)^q (a^\dagger \cdot b^\dagger)^q}{q!(N+M+1)(N+M)(N+M-1)\cdots(N+M+2-q)}, \qquad (36)
$$

and all the sums in (35) are over different indices, i.e., $l_1 \neq l_2 \cdots \neq l_q$ and $k_1 \neq k_2 \neq \cdots \neq k_q$. The coefficients in Eq. (36) are chosen to satisfy the tracelessness condition

$$
\sum_{i_l,j_k=1}^{3} \delta^{i_l}_{j_k} |\psi\rangle^{i_1,i_2,\ldots i_N}_{j_1,j_2,\ldots,j_M} = 0, \quad \text{for all } l = 1,2,\ldots N, \quad \text{and } k = 1,2,\ldots M. \qquad (37)
$$

For future purposes, a more compact notation for describing all the states given above is to write

$$
O^{i_1 i_2 \cdots i_N}_{j_1 j_2 \cdots j_M} \equiv (a_1^\dagger)^{N_1} (a_2^\dagger)^{N_2} (a_3^\dagger)^{N_3} (b_1^\dagger)^{M_1} (b_2^\dagger)^{M_2} (b_3^\dagger)^{M_3}, \qquad (38)
$$

where (N_i, M_i) denote all the possible eigenvalues of the occupation number operators $(a_i^\dagger a_i, b_i^\dagger b_i)$ satisfying

$$
N_1 + N_2 + N_3 = N \quad \text{and} \quad M_1 + M_2 + M_3 = M. \qquad (39)
$$

The action of (38) on the vacuum is given by

$$
O^{N_1 N_2 N_3}_{M_1 M_2 M_3} |\vec{0},\vec{0}\rangle = (N_1! N_2! N_3! M_1! M_2! M_3!)^{1/2} |^{N_1 N_2 N_3}_{M_1 M_2 M_3}\rangle. \qquad (40)
$$

We can now write the basis vectors of the representation (N,M) as

$$
\begin{aligned}
|\psi\rangle^{i_1,i_2,\ldots i_N}_{j_1,j_2,\ldots,j_M} \equiv |\psi\rangle^{N_1 N_2 N_3}_{M_1 M_2 M_3} = & \left[O^{N_1 N_2 N_3}_{M_1 M_2 M_3} + \sum_{q=1}^{Q} L_q \sum_{[\vec{\alpha}]_q} \right] {}^{N_1}C_{\alpha_1}\, {}^{N_2}C_{\alpha_2}\, {}^{N_3}C_{\alpha_3}\, {}^{M_1}C_{\alpha_1}\, {}^{M_2}C_{\alpha_2} \\
& \times {}^{M_3}C_{\alpha_3}\, \alpha_1!\, \alpha_2!\, \alpha_3!\, O^{N_1-\alpha_1 N_2-\alpha_2 N_3-\alpha_3}_{M_1-\alpha_1 M_2-\alpha_2 M_3-\alpha_3} |\vec{0},\vec{0}\rangle. \qquad (41)
\end{aligned}
$$

In this equation, $[\vec{\alpha}]_q$ denotes the sets of three non-negative integers $(\alpha_1,\alpha_2,\alpha_3)$ satisfying $\alpha_1+\alpha_2+\alpha_3=q$, and $N_i-\alpha_i\geqslant 0$, $M_i-\alpha_i\geqslant 0$ for $i=1,2,3$. The $\Sigma_{[\vec{\alpha}]_q}$ denotes a summation over all sets of three such integers. In the notation of Eq. (41), the tracelessness condition (37) for the $(N+1, M+1)$ representation takes the form

$$\sum_{[\vec{\gamma}]_1} |\psi\rangle^{N_1+\gamma_1 N_2+\gamma_2 N_3+\gamma_3}_{M_1+\gamma_1 M_2+\gamma_2 M_3+\gamma_3}=0. \tag{42}$$

The definition in (41) satisfies the condition given in (42). This can be verified by using the identity

$$\begin{aligned}
&\sum_{[\vec{\gamma}]_1}\sum_{[\vec{\alpha}]_q} \alpha_1!\alpha_2!\alpha_3!{}^{N_1+\gamma_1}C_{\alpha_1}{}^{N_2+\gamma_2}C_{\alpha_2}{}^{N_3+\gamma_3}C_{\alpha_3}{}^{M_1+\gamma_1}C_{\alpha_1}{}^{M_2+\gamma_2}C_{\alpha_2}{}^{M_3+\gamma_3}C_{\alpha_3}\\
&\quad\times O^{N_1+\gamma_1-\alpha_1 N_2+\gamma_2-\alpha_2 N_3+\gamma_3-\alpha_3}_{M_1+\gamma_1-\alpha_1 M_2+\gamma_2-\alpha_2 M_3+\gamma_3-\alpha_3}\\
&\quad=\left[(N+M+2-q)\sum_{[\vec{\alpha}]_{q-1}}+(\vec{a}^\dagger\cdot\vec{b}^\dagger)\sum_{[\vec{\alpha}]_q}\right]\\
&\quad\times\alpha_1!\alpha_2!\alpha_3!{}^{N_1}C_{\alpha_1}{}^{N_2}C_{\alpha_2}{}^{N_3}C_{\alpha_3}{}^{M_1}C_{\alpha_1}{}^{M_2}C_{\alpha_2}{}^{M_3}C_{\alpha_3}O^{N_1-\alpha_1 N_2-\alpha_2 N_3-\alpha_3}_{M_1-\alpha_1 M_2-\alpha_2 M_3-\alpha_3}.
\end{aligned}\tag{43}$$

The dimension $D(N,M)$ of the representation (N,M) can be obtained as follows. For the $(N,0)$ representation, no tracelessness condition needs to be imposed, and the dimension is simply given by the number of states in Eq. (40) which satisfy $\Sigma_i N_i=N$ and $\Sigma_i M_i=0$. This gives $D(N,0)=(N+1)(N+2)/2$. Similarly, $D(0,M)=(M+1)(M+2)/2$. Now $D(N,M)$ is given by the number of states satisfying $\Sigma_i N_i=N$, $\Sigma_i M_i=M$, which is equal to the product $D(N,0)D(0,M)$, *minus* the number of states satisfying $\Sigma_i N_i=N-1$, $\Sigma_i M_i=M-1$, which is equal to $D(N-1,0)D(0,M-1)$; the subtraction is because of the tracelessness condition. This gives

$$D(N,M)=\tfrac{1}{2}(N+1)(M+1)(N+M+2). \tag{44}$$

IV. SU(3) COHERENT STATES

We now observe that the states in Eq. (35) can be extracted from the following generating function,

$$|\vec{z},\vec{w}\rangle_{(N,M)}\equiv\sqrt{N!M!}\,\exp(\vec{z}\cdot\vec{a}^\dagger+\vec{w}\cdot\vec{b}^\dagger)|\vec{0},\vec{0}\rangle, \tag{45}$$

where we have to project onto the subspace of states with $\vec{a}^\dagger\cdot\vec{a}=N$ and $\vec{b}^\dagger\cdot\vec{b}=M$ to obtain the representation (N,M). More explicitly,

$$|\vec{z},\vec{w}\rangle_{(N,M)}=\frac{(\vec{z}\cdot\vec{a}^\dagger)^N}{\sqrt{N!}}\frac{(\vec{w}\cdot\vec{b}^\dagger)^M}{\sqrt{M!}}|\vec{0},\vec{0}\rangle=\sum_{N_1,N_2,N_3}{}'\ \sum_{M_1,M_2,M_3}{}'\ F_{\vec{N},\vec{M}}(z_1,z_2,z_3;w_1,w_2,w_3)|^{N_1N_2N_3}_{M_1M_2M_3}\rangle. \tag{46}$$

In (46), Σ' implies that the occupation numbers (N_i,M_i) satisfy Eq. (39), and $F_{\vec{N},\vec{M}}(\vec{z},\vec{w})$ are given by

$$F_{\vec{N},\vec{M}}(\vec{z},\vec{w})=\left(\frac{N!M!}{N_1!N_2!N_3!M_1!M_2!M_3!}\right)^{1/2} z_1^{N_1}z_2^{N_2}z_3^{N_3}w_1^{M_1}w_2^{M_2}w_3^{M_3}. \tag{47}$$

On expanding the right hand side of (46), the coefficients of $z_1^{N_1}z_2^{N_2}z_3^{N_3}w_1^{M_1}w_2^{M_2}w_3^{M_3}$ give the basis vectors of SU(3) in the representation (N,M). It is important to note that the tracelessness conditions in Eq. (35) are *automatically* satisfied by the state in (46). This is because we can always replace $|^{N_1N_2N_3}_{M_1M_2M_3}\rangle$ by the SU(3) basis vectors $|\psi\rangle^{N_1N_2N_3}_{M_1M_2M_3}$ defined in (41).

It is instructive to consider a specific example here. The coherent state of the representation (1,1), i.e., the adjoint representation of SU(3), is given by

$$|\vec{z},\vec{w}\rangle_{(1,1)}=\sum_{i,j=1}^{3} z_i w_j a_i^\dagger b_j^\dagger|\vec{0},\vec{0}\rangle. \tag{48}$$

We then see that the sum of the coefficients of the three states $|^{100}_{100}\rangle$, $|^{010}_{010}\rangle$ and $|^{001}_{001}\rangle$ is zero due to the constraint in Eq. (29). Hence there are only eight linearly independent states on the right hand side of Eq. (48) as there should be; these eight states can be taken to be

$$\begin{gathered}|V_1\rangle=\frac{1}{\sqrt{2}}(|^{100}_{100}\rangle-|^{010}_{010}\rangle),\quad |V_2\rangle=\frac{1}{\sqrt{6}}(|^{100}_{100}\rangle+|^{010}_{010}\rangle-2|^{001}_{001}\rangle),\\ |V_3\rangle=|^{100}_{010}\rangle,\ |V_4\rangle=|^{010}_{100}\rangle,\\ |V_5\rangle=|^{100}_{001}\rangle,\ |V_6\rangle=|^{001}_{100}\rangle,\\ |V_7\rangle=|^{010}_{001}\rangle,\ |V_8\rangle=|^{001}_{010}\rangle.\end{gathered} \tag{49}$$

The states defined in Eq. (46) will be called the coherent state of the representation (N,M). Note that Eqs. (39), (46), and (47) are analogous to the corresponding SU(2) equations (13), (12), and (14) respectively. The SU(3) coherent states (46) are normalized to unity, i.e.,

$${}_{(N,M)}\langle\vec{z},\vec{w}|\vec{z},\vec{w}\rangle_{(N,M)}=1. \tag{50}$$

To prove this, we use the operator identities

$$e^Ae^B=e^Be^Ae^{[A,B]}\quad \text{and}\quad e^ABe^{-A}=B+[A,B], \tag{51}$$

which hold if $[A,B]$ commutes with both A and B. We find that

$$\langle\vec{0},\vec{0}|\exp[\bar{\vec{z}}\cdot\vec{a}+\bar{\vec{w}}\cdot\vec{b}]\exp[\vec{z}\cdot\vec{a}^\dagger+\vec{w}\cdot\vec{b}^\dagger]|\vec{0},\vec{0}\rangle=\exp[\bar{\vec{z}}\cdot\vec{z}+\bar{\vec{w}}\cdot\vec{w}]. \tag{52}$$

On comparing terms of order $(\bar{\vec{z}}\cdot\vec{z})^N(\bar{\vec{w}}\cdot\vec{w})^M$ on both sides of this equation and using the definition in (46), we obtain Eq. (50). In the same way, we can show that

$${}_{(N,M)}\langle\vec{z},\vec{w}|\vec{z}+d\vec{z},\vec{w}+d\vec{w}\rangle_{(N,M)}=1+N\sum_i \bar{z}_i dz_i+M\sum_i \bar{w}_i dw_i, \tag{53}$$

where $d\vec{z}$ and $d\vec{w}$ denote small deviations from $\vec{z}$ and $\vec{w}$. This equation will be used to derive the path integral formalism[6,7] in Sec. V, and it would also be useful for obtaining the geometric phase for systems with SU(3) symmetry.[11]

We can prove that the states defined in Eq. (46) satisfy the resolution of identity, i.e.,

$$\int d\Omega |\vec{z},\vec{w}\rangle_{(N,M)(N,M)}\langle\vec{z},\vec{w}| = \frac{1}{D(N,M)} \sum_{i=1}^{D(N,M)} |V_i\rangle\langle V_i|, \tag{54}$$

where V_i denotes a set of orthonormal basis vectors of (N,M). [See Eq. (49) for the explicit example of the representation (1,1).] To verify the normalization on the right-hand side of Eq. (54), it is convenient to look at a particular basis vector $|^{N00}_{0M0}\rangle$. [This has the maximum eigenvalue $(N+M)/2$ of the operator Q^3 given in Eq. (32).] From Eq. (46), the coefficient of this vector in the coherent state is given by $z_1^N w_2^M$. Integrating the modulus squared of this using Eqs. (21)–(25), we obtain the factor of $1/D(N,M)$ in Eq. (54). This is as it should be so that taking the trace of both sides of (54) gives unity.

A second property of coherent states is that they are overcomplete. This is clear for the states in (46) since they are continuous functions of the complex variables $(\vec{z},\vec{w})$, while the dimension of the representation (N,M) is finite.

The coherent states in (46) have a third property which is group theoretical, and is analogous to Eq. (18) for the SU(2) coherent states. Namely, we can go from a particular coherent state, say, $|z_1=1,w_2=1\rangle_{(N,M)}=|^{N00}_{0M0}\rangle$ to the general coherent state $|z,w\rangle_{(N,M)}$ by acting with an exponential of certain combinations of the SU(3) generators Q^a. First of all, we can check that

$$|z,w\rangle_{(N,M)} = z_1^N w_2^M \exp\left[\frac{z_2}{z_1}a_2^\dagger a_1 + \frac{z_3}{z_1}a_3^\dagger a_1 + \frac{w_1}{w_2}b_1^\dagger b_2 + \frac{w_3}{w_2}b_3^\dagger b_1\right]|z_1=1,w_2=1\rangle_{(N,M)}. \tag{55}$$

Then we can use Eq. (51) and the constraint (29) to rewrite this in the form[10]

$$|z,w\rangle_{(N,M)} = z_1^N w_2^M \exp\left[\frac{z_2}{z_1}(Q^1-iQ^2) + \frac{z_3}{z_1}(Q^4-iQ^5) - \frac{w_3}{w_2}(Q^6+iQ^7)\right]|z_1=1,w_2=1\rangle_{(N,M)}, \tag{56}$$

which is similar in structure to Eq. (18).

Another property of these coherent states which is important for their path integral applications is that the expectation value of the SU(3) operators (32) in a coherent state should be given by an SU(3) covariant function of $(\vec{z},\vec{w})$ and their complex conjugates. We find that

$${}_{(N,M)}\langle\vec{z},\vec{w}|Q^a|\vec{z},\vec{w}\rangle_{(N,M)} = N\overline{z_i}\lambda^a_{ij}z_j - M\overline{w_i}\lambda^{*a}_{ij}w_j. \tag{57}$$

This can be proved by using the identities in Eq. (51) to show that

$$\langle\vec{0},\vec{0}|\exp[\vec{\overline{z}}\cdot\vec{a}+\vec{\overline{w}}\cdot\vec{b}]a_i^\dagger a_j \exp[\vec{z}\cdot\vec{a}^\dagger+\vec{w}\cdot\vec{b}^\dagger]|\vec{0},\vec{0}\rangle = \overline{z_i}z_j \exp[\vec{\overline{z}}\cdot\vec{z}+\vec{\overline{w}}\cdot\vec{w}], \tag{58}$$

and a similar identity for the expectation value of $b_i^\dagger b_j$ in terms of $\overline{w_i}w_j$. Equation (57) can now be obtained by comparing terms of order $\overline{z}^N z^N \overline{w}^M w^M$ on the two sides of Eq. (58).

The stationary subgroup of the coherent states defined in this section is generally U(1)×U(1), corresponding to multiplying the vectors $\vec{z}$ and $\vec{w}$ by independent phase factors. These coherent states are therefore functions of the coset space SU(3)/U(1)×U(1).[10] However, for the completely symmetric representations $(N,0)$ and $(0,M)$, the coherent states use only three complex numbers ($\vec{z}$ or $\vec{w}$) which define the space $\mathrm{SU(3)/SU(2)}\sim S^5$; the stationary subgroup is then U(1) which corresponds to multiplying that complex vector by a phase factor. In those cases, the coherent states are functions of the coset space SU(3)/SU(2)×U(1).

V. AN ALTERNATIVE DEFINITION OF SU(3) COHERENT STATES

The SU(3) coherent states discussed in Sec. IV involve eight real parameters, and satisfy some simple group theoretic properties similar to the SU(2) coherent states of Sec. II. It is possible that there may be some applications of coherent states which do not require so many parameters. In

this section, we will discuss an alternative kind of coherent state which only requires five real parameters. We will see later that these coherent states suffer from some problems and they seem to lack some of the group theoretic properties precisely because they use fewer parameters.

We observe that the states in (35) can be extracted from the following generating function:

$$|\vec{z},\vec{\bar{z}}\rangle \equiv \exp(\vec{z}\cdot\vec{a}^\dagger)\exp(\vec{\bar{z}}\cdot\vec{b}^\dagger)\left[1+\sum_{q=1}^{Q} L_q\right]|\vec{0},\vec{0}\rangle, \tag{59}$$

and we have to project onto the subspace of states with $\vec{a}^\dagger\cdot\vec{a}=N$ and $\vec{b}^\dagger\cdot\vec{b}=M$ to obtain the representation (N,M). To be explicit,

$$|\vec{z},\vec{\bar{z}}\rangle_{(N,M)} = \left[\frac{(\vec{z}\cdot\vec{a}^\dagger)^N}{N!}\frac{(\vec{\bar{z}}\cdot\vec{b}^\dagger)^M}{M!}+\sum_{q=1}^{Q} L_q\frac{(\vec{z}\cdot\vec{a}^\dagger)^{N-q}}{(N-q)!}\frac{(\vec{\bar{z}}\cdot\vec{b}^\dagger)^{M-q}}{(M-q)!}\right]|\vec{0},\vec{0}\rangle. \tag{60}$$

On expanding the right hand side of (60), the coefficients of the tensors $z_{i_1}z_{i_2}\cdots z_{i_N}\bar{z}_{j_1}\bar{z}_{j_2}\cdots\bar{z}_{j_M}$ give the basis vectors of SU(3) in the representation (N,M).

The SU(3) coherent states in the representation (N,M) are defined as in Eq. (60),

$$\begin{aligned}|\vec{z},\vec{\bar{z}}\rangle_{(N,M)} &\equiv \frac{1}{N!M!}\sum_{i_1,i_2,\ldots}\sum_{j_1,j_2,\ldots} z_{i_1}z_{i_2}\cdots z_{i_N}\bar{z}_{j_1}\bar{z}_{j_2}\cdots\bar{z}_{j_M}|\psi\rangle^{i_1 i_2\cdots i_N}_{j_1 j_2\cdots j_M}\\ &= \sum_{N_1,N_2,N_3}\sum_{M_1,M_2,M_3}\frac{z_1^{N_1}z_2^{N_2}z_3^{N_3}\bar{z}_1^{M_1}\bar{z}_2^{M_2}\bar{z}_3^{M_3}}{N_1!N_2!N_3!M_1!M_2!M_3!}|\psi\rangle^{N_1N_2N_3}_{M_1M_2M_3}.\end{aligned} \tag{61}$$

To give a specific example, the coherent state of the representation (1,1) is given by

$$|\vec{z},\vec{\bar{z}}\rangle_{(1,1)} = \sum_{i,j=1}^{3} z_i\bar{z}_j a_i^\dagger b_j^\dagger|\vec{0},\vec{0}\rangle - \frac{1}{3}\sum_{i=1}^{3} a_i^\dagger b_i^\dagger|\vec{0},\vec{0}\rangle. \tag{62}$$

We will now prove that the states defined in (61) satisfy the resolution of identity,

$$\int d\Omega_{S^5}|\vec{z},\vec{\bar{z}}\rangle_{(N,M)(N,M)}\langle\vec{z},\vec{\bar{z}}| = 1. \tag{63}$$

To prove this, we use the definition (41) and the integration measure for $\vec{z}$ given in (22). We find that

$$\int d\Omega_{S^5}|z,\bar{z}\rangle\langle z,\bar{z}| = \mathcal{C}\sum_{N_i,M_i}\left(\sum_{\delta_i}\left(\prod_{i=1}^{3}\frac{(N_i+M_i+\delta_i)!}{(N_i+\delta_i)!(M_i+\delta_i)!}\right)|\psi\rangle^{N_1+\delta_1N_2+\delta_2N_3+\delta_3}_{M_1+\delta_1M_2+\delta_2M_3+\delta_3}\right)\ {}^{N_1N_2N_3}_{M_1M_2M_3}\langle\psi|, \tag{64}$$

where the δ_i are integers satisfying

$$\sum_{i=1}^{3}\delta_i = 0, \tag{65}$$

and the constant $\mathcal{C}$ is determined shortly. We now use the following property,

$$\sum_{\delta_i}\left(\prod_{i=1}^{3}\frac{(N_i+M_i+\delta_i)!}{(N_i+\delta_i)!(M_i+\delta_i)!}\right)|\psi\rangle^{N_1+\delta_1N_2+\delta_2N_3+\delta_3}_{M_1+\delta_1M_2+\delta_2M_3+\delta_3} = |\psi\rangle^{N_1N_2N_3}_{M_1M_2M_3}, \tag{66}$$

which is a consequence of Eq. (37) for the basis vectors of a representation of SU(3). Thus Eq. (64) can be simplified to

$$\int d\Omega_{S^5}|z,\overline{z}\rangle\langle z,\overline{z}| = \mathcal{C}\sum_{N_i,M_i} |\psi\rangle^{N_1N_2N_3}_{M_1M_2M_3}{}^{N_1N_2N_3}_{M_1M_2M_3}\langle\psi|. \tag{67}$$

The normalization constant $\mathcal{C}$ in Eq. (67) can be fixed by looking at one particular basis vector of the representation (N,M), say,

$$|\psi\rangle^{N00}_{0M0}. \tag{68}$$

From Eq. (61), the coefficient of this vector in the coherent state $|\vec{z},\vec{\overline{z}}\rangle$ is $z_1^N\overline{z_2}^M/(N!M!)$. Integrating this as in (22), we find that

$$\mathcal{C} = \frac{2}{N!M!(N+M+2)!}. \tag{69}$$

Finally, let us consider the analog of the property given in Eq. (57) for the (z,w) coherent states. We can prove that

$${}_{(N,M)}\langle\vec{z},\vec{\overline{z}}|Q^a|\vec{z},\vec{\overline{z}}\rangle_{(N,M)} = (N-M)\overline{z_i}\lambda^a_{ij}z_j. \tag{70}$$

To prove this, we use the identities in (51) to show that

$$\langle\vec{0},\vec{0}|\exp[\vec{\overline{z}}\cdot\vec{a}+\vec{z}\cdot\vec{b}]a_i^\dagger a_j\exp[\vec{z}\cdot\vec{a}^\dagger+\vec{\overline{z}}\cdot\vec{b}^\dagger]|\vec{0},\vec{0}\rangle = \overline{z_i}z_j\exp[2\vec{\overline{z}}\cdot\vec{z}]. \tag{71}$$

On expanding this equation and comparing terms which are of order N in both z_i and $\overline{z_i}$, we find that the expectation value of Q^a in the representation $(N,0)$ satisfies Eq. (70). In a similar way, we can prove Eq. (70) in the representation $(0,M)$. Finally, we can generalize the proof to the representation (N,M) by using Eq. (33); since Q^a commutes with $\vec{a}\cdot\vec{b}$ and $\vec{a}^\dagger\cdot\vec{b}^\dagger$, it commutes with the operators L_q which are require to enforce tracelessness in Eq. (35).

Note that (70) vanishes for the self-conjugate representations in which $N=M$. There is a similar problem for the differential change in overlap analogous to Eq. (53). We find that the coherent states defined in this section satisfy

$$\frac{\langle\vec{z},\vec{\overline{z}}|\vec{z}+d\vec{z},\vec{\overline{z}}+d\vec{\overline{z}}\rangle}{\langle\vec{z},\vec{\overline{z}}|\vec{z},\vec{\overline{z}}\rangle} = 1+N\sum_i \overline{z_i}dz_i + M\sum_i d\overline{z_i}z_i \tag{72}$$

in the representation (N,M). The left hand side of this equation is equal to 1 if $N=M$ due to the constraint $\Sigma_i\overline{z_i}z_i=1$. These two problems imply that the $(z,\overline{z})$ coherent states are unlikely to be useful for path integral applications in the representations with $N=M$.

For the $(z,\overline{z})$ coherent states, we have not yet found the construction of the group theoretical property analogous to (56) in the general representation (N,M). This would be an interesting topic for future studies.

The stationary subgroup of the coherent states defined in this section is $\mathrm{U}(1)=S^1$, corresponding to multiplying $\vec{z}$ by a phase factor. These coherent states are therefore functions of the manifold S^5/S^1.

VI. PATH INTEGRAL FORMALISM

We will now use the (z,w) coherent states presented in Sec. IV to derive the path integral for a problem which has SU(3) variables in some representation (N,M). (For convenience, we will drop the subscript (N,M) on the coherent states in this section.) We begin by discussing a problem

involving the Hamiltonian of a single site with a SU(3) variable. For any Hamiltonian which is a function of the SU(3) operators Q^a, we define its coherent state expectation value to be

$$E(z,\overline{z},w,\overline{w}) \equiv \langle z,w|\hat{H}|z,w\rangle. \tag{73}$$

If the Hamiltonian is linear in the SU(3) operators, i.e.,

$$\hat{H} = \sum_{a=1}^{8} c_a Q^a, \tag{74}$$

then Eq. (73) can be found using Eq. (57). But if the Hamiltonian is not linear in the SU(3) operators, then Eq. (73) has to be evaluated separately.

Let us now consider the propagator in imaginary time

$$G(z^{(F)},w^{(F)},z^{(I)},w^{(I)};T) = \langle z^{(F)},w^{(F)}|\exp(-T\hat{H})|z^{(I)},w^{(I)}\rangle, \tag{75}$$

where the superscripts I and F denote initial and final states, respectively, and we are suppressing the subscripts $i\,(=1,2,3)$ on z and w for the moment. We write the exponential in (75) as a product of $\mathcal{N}$ terms, and use the resolution of identity in (54) to insert a complete set of states between each pair of terms. A typical term looks like

$$\langle z^{(n+1)},w^{(n+1)}|\exp(-\epsilon\hat{H})|z^{(n)},w^{(n)}\rangle, \tag{76}$$

where $\epsilon = T/\mathcal{N}$. We are eventually interested in taking the limit $\mathcal{N}\to\infty$ holding T fixed. In that case, we may assume that $(z^{(n+1)},w^{(n+1)})$ is close to $(z^{(n)},w^{(n)})$ in (76), so that $dz_i^{(n)} = z_i^{(n+1)} - z_i^{(n)}$ and $dw_i^{(n)} = w_i^{(n+1)} - w_i^{(n)}$ are small. Using Eqs. (53) and (73), we can write (76) as

$$\begin{aligned}&\langle z^{(n+1)},w^{(n+1)}|\exp(-\epsilon\hat{H})|z^{(n)},w^{(n)}\rangle \\ &\quad = \exp\left[N\sum_i \overline{z}_i^{(n)} dz_i^{(n)} + M\sum_i \overline{w}_i^{(n)} dw_i^{(n)} - \epsilon E(z^{(n)},\overline{z^{(n)}},w^{(n)},\overline{w^{(n)}})\right]\end{aligned} \tag{77}$$

to first order in ϵ, $dz_i^{(n)}$ and $dw_i^{(n)}$. In the limit $\epsilon = d\tau \to 0$, we can write the propagator in (75) in the path integral form

$$G(z^{(F)},w^{(F)},z^{(I)},w^{(I)};T) = \int \mathcal{D}\Omega_{\mathrm{SU(3)}}(\tau)\exp(-S[z,w]),$$

where

$$S[z,w] = \int_0^T d\tau\left[-N\sum_i \overline{z}_i \frac{dz_i}{d\tau} - M\sum_i \overline{w}_i \frac{dw_i}{d\tau} + E(z,\overline{z},w,\overline{w})\right], \tag{78}$$

and

$$\mathcal{D}\Omega_{\mathrm{SU(3)}}(\tau) \equiv \prod_n d\Omega_{\mathrm{SU(3)}}(n),$$

and (z,w) are functions of τ which satisfy the boundary conditions $(z(0),w(0)) = (z^{(I)},w^{(I)})$ and $(z(T),w(T)) = (z^{(F)},w^{(F)})$. Note that we have written the functional integral measure in (78) in terms of the measure given in Eq. (25). Alternatively, we can write the functional integral measure in terms of $\mathcal{D}z\mathcal{D}\overline{z}\mathcal{D}w\mathcal{D}\overline{w}$ if we introduce appropriate Lagrange multiplier fields in the action S to enforce the constraints in Eqs. (28) and (29) at each time τ.

We can now generalize the above construction to a problem involving several sites which are labeled by a parameter x, provided that the Hamiltonian is linear in the SU(3) variables at *each* site. We introduce a coherent state at each site, and write the energy functional as

$$E[z,\bar{z},w,\bar{w}]=\langle z,w|\hat{H}|z,w\rangle, \quad \text{where } |z,w\rangle\equiv\prod_x |z(x),w(x)\rangle. \tag{79}$$

Then we can show that

$$\langle z^{(F)}(x),w^{(F)}(x)|\exp(-T\hat{H})|z^{(I)}(x),w^{(I)}(x)\rangle=\int \mathcal{D}\Omega_{\mathrm{SU(3)}}(x,\tau)\exp(-S[z,w]),$$

$$S[z,w]=\int_0^T d\tau\left[-\sum_x\left\{N\sum_i \bar{z}_i(x)\frac{dz_i(x)}{d\tau}-M\sum_i \bar{w}_i(x)\frac{dw_i(x)}{d\tau}\right\}+E[z,\bar{z},w,\bar{w}]\right], \tag{80}$$

$$\mathcal{D}\Omega_{\mathrm{SU(3)}}(x,\tau)\equiv\prod_{x,n} d\Omega_{\mathrm{SU(3)}}(x,n).$$

Note that the first two terms in the actions S given in Eqs. (78) and (80) are purely imaginary due to the constraints in (28). To show this explicitly, we can rewrite those terms as

$$\begin{aligned}\sum_i \bar{z}_i dz_i&=\frac{1}{2}\sum_i (\bar{z}_i dz_i-d\bar{z}_i z_i),\\ \sum_i \bar{w}_i dw_i&=\frac{1}{2}\sum_i (\bar{w}_i dw_i-d\bar{w}_i w_i).\end{aligned} \tag{81}$$

As an example of a problem to which this formalism can be applied, we can consider the SU(3) invariant Hamiltonian

$$\hat{H}=\sum_{x,y} J_{x,y}\sum_a Q^a(x)Q^a(y). \tag{82}$$

This is called the SU(3) Heisenberg model. It has been discussed extensively in the literature for the completely symmetric representations $(N,0)$;[6] for those representations, we can use the simpler measure $d\Omega_{S^5}$ given in Eq. (22) instead of $d\Omega_{\mathrm{SU(3)}}$. Our construction of coherent states now allows a study of the Heisenberg model in any representation (N,M).

VII. SUMMARY AND DISCUSSION

In this article we have exploited the representation of the SU(3) Lie algebra in terms of six harmonic oscillator creation and annihilation operators to generate all the representations of SU(3). This harmonic oscillator form of the algebra enables us to define the SU(3) coherent states in terms of two triplets of complex numbers. In this sense the SU(2) definition (12) and SU(3) definition (45) are analogous to that of the Heisenberg–Weyl coherent states (4). The SU(3) coherent states are characterized by two triplets of complex numbers with four real constraints. This explicit construction in terms of complex numbers can be used to derive the geometrical phase of SU(3). Further, the path integral formalism discussed in the previous section can be used to obtain the field theory for the SU(3) Heisenberg model and study its topological aspects as in the SU(2) case.[17] Work in this direction is in progress and will be reported elsewhere.

For any group G, we can use a certain number of harmonic oscillator operators to construct the group operators as in Eqs. (32) and (33). If we can find the appropriate set of complex numbers

which transform according to that group and satisfy the necessary constraints, we can use our method to provide an explicit complex number parametrization of the corresponding coherent states.

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Large-*N* theory from the axiomatic point of view

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The state space and observables for the leading order of the large-*N* theory are constructed. The obtained model (''theory of infinite number of fields'') is shown to obey Wightman-type axioms (including invariance under boost transformations). The considered class of exactly solvable relativistic quantum models involves good examples of theories containing such difficulties as volume divergences associated with the Haag theorem, Stueckelberg divergences, and infinite renormalization of the wave function. © *2001 American Institute of Physics.*
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I. INTRODUCTION

There are different approaches to quantum field theory (QFT). Some of them are based on calculations of average values like Green functions, *S* matrix; for these purposes, different techniques can be applied: one can use the functional integral approach, write down the *T* exponent of the integral of interaction Lagrangian, solve the Dyson–Schwinger equations or use the Bogoliubov axiomatic approach.[1,2]

There are also ways to construct QFT with the help of equations of motion: one finds the classical Hamiltonian of the theory, canonically quantizes it, and writes the Schrodinger equation.

All approaches to QFT are somehow equivalent. On the one hand, one can obtain the *S* matrix and the Green functions by formally integrating equations of motion. On the other hand, one can obtain Wightman functions by analytic continuation of the Euclidean Green functions[2] and then apply the Wightman theorem[3,4] and reconstruct state space, evolution, and boost operators of the theory.

However, there are QFT divergences, so that it is necessary to perform renormalization of the theory in each approach. Renormalization is much easier in the *S* matrix (or Green functions) approach since they are manifestly covariant, contrary to the Hamiltonian method.

The approach, based on the equations, of motion contains additional difficulties associated with the problem of Stueckelberg divergences[5] and Haag theorem (see, for example, Refs. 2 and 4). Although the vacuum divergences associated with the Haag theorem can be removed within the perturbation theory with the help of the Faddeev transformation,[6] while Stueckelberg divergences can be treated in the analogous way,[7] renormalization of equations of motion is a strongly nontrivial problem even within the perturbation framework.

Unfortunately, for general QFT models, renormalization was performed even for the *S* matrix approach within the perturbation theory only: the Bogoliubov–Parasiuk theorem was proven.[1] However, if the Green functions of the theory are constructed only perturbatively, the possible application of the Wightman reconstruction theorem at least requires additional investigations, so that the problem of constructing the state space seems to be interesting even in the perturbation theory.

Large-*N* expansion is another approximate scheme for QFT.[8–10] This approximation, widely used in QFT allows us to obtain nonperturbative results and investigate the behavior of the Green functions, the effective action, dynamical and spontaneous symmetry breaking.

The traditional approaches to the $1/N$ expansion enable us to evaluate different quantities just

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mentioned. However, some problems of the large-N theories remain to be understood. What are states and observables in the theory of infinite number of fields? Can one determine such a theory as a large-N limit?

From the axiomatic field theory point of view,[2–4] the relativistic QFT is constructed if:

(i) the Hilbert state space $\mathcal{H}$ is specified,
(ii) the operators $U_g:\mathcal{H}\to\mathcal{H}$ corresponding to the Poincare transformations g are specified; the group property $U_{g_1}U_{g_2}=U_{g_1g_2}$ is satisfied, and
(iii) the field operators are constructed.

The introduced objects should obey certain (Wightman-type) axioms.

It happens that the axiomatic formulation of the large-N QFT can be obtained within the third-quantized approach developed recently as discussed in Ref. 11. It allows us to construct not only known but also new formal asymptotic solutions to the large-N Schrodinger equation. The correspondence between third-quantized framework and standard large-N approaches is discussed in Ref. 11.

It is interesting that the large-N limit of QFT may be viewed as a theory of a variable number of fields. This is analogous to the statistical physics: the system of a large but fixed number of particles can be considered as a set of quasiparticles which can be created and annihilated. Analogously, the large-N field system can be treated from the ''quasifield'' point of view: there is an amplitude that there are no fields, that there is one field, two fields, etc. Thus, the large-N limit of QFT is *not* a field theory in the usual treatment since one can not define usual field operators. However, the property of the relativistic invariance remains. Moreover, we will introduce the analog of notion of field which is very useful for constructing boost transformations.

The models of an infinite number of fields constructed in this paper seem to be remarkable from the point of view of the constructive field theory.[12,13] The old problem of QFT is to construct the nontrivial model of field theory obeying all Wightman axioms. Such examples were constructed for the cases of two- and three-dimensional space–time. The models presented here are considered in higher dimensions.

The models considered in this paper are good examples of theories that contain such difficulties as Stueckelberg divergences[5] and volume divergences associated with the Haag theorem. There was a hypothesis[12] that the models with the Stueckelberg divergences can not be constructed with the help of the Hamiltonian methods. However, we show this hypothesis to be incorrect.

This paper is organized as follows. As an example, we consider the $\lambda(\varphi^a\varphi^a)^2$ model in $(d+1)$-dimensional space–time with the following Lagrangian:

$$\mathcal{L}=\frac{1}{2}\partial_\mu\varphi^a\partial_\mu\varphi^a-\frac{m^2}{2}\varphi^a\varphi^a-\frac{\lambda}{4N}(\varphi^a\varphi^a)^2,$$

we sum over repeated indices $a=1,\ldots,N$, and $\mu=0,\ldots,d$. In Sec. II, the $N=\infty$-limit of the model is heuristically constructed. The Hamiltonian, momentum, angular momentum, and boost generator are presented. It is heuristically shown that they formally obey usual commutation relations of the Poincare algebra. However, the divergences show us that the obtained expressions are not mathematically well-defined. Section III is devoted to the problem of renormalization of the Hamiltonian. The momentum and angular momentum are also investigated. The spectral and vacuum axioms are checked.

It is not easy to construct operators of boost transformation (Lorentz rotation) and check the group properties. It is convenient first to introduce the composed field being an analog of the large-N operator $\Sigma_{a=1}^N\varphi^a(x_1)\ldots\varphi^a(x_k)$. Such operators (multifields) being analogs of fields of ordinary QFT are constructed in Sec. IV. They are shown to be operator distributions. The cyclic property of the vacuum state is checked. The invariance of multifields under spatial rotations and space–time translations is checked. Section V deals with the construction of the operator of boost transformation. This allows us to construct the representation of the Poincare group and check the

relativistic invariance of the theory. The results of Sec. IV are essentially used. Section VI contains concluding remarks.

II. WHAT IS A THEORY OF INFINITE NUMBER OF FIELDS?

This section deals with investigation of the theory of N fields, $\varphi^1, \ldots, \varphi^N$ as $N \to \infty$. Such models were considered in context of calculations of physical quantities such as Green functions. It seems to be useful to formulate the $N=\infty$-theory: to determine the state space, Poincare transformations, field operators, etc.

A. Multifield canonical operator

In the functional Schrodinger representation, states of the N-field system at time t are specified by the functionals $\Psi_N^t[\varphi^1(\cdot), \ldots, \varphi^N(\cdot)]$ depending on the field configurations $\varphi^1(\mathbf{x}), \ldots, \varphi^N(\mathbf{x})$, and $\mathbf{x}=(x_1, \ldots, x_d)$. The inner product is formally written via the functional integral

$$(\Psi_N, \Psi_N) = \int D\varphi^1 \ldots D\varphi^N |\Psi_N[\varphi^1(\cdot), \ldots, \varphi^N(\cdot)]|^2.$$

The evolution equation has the form

$$i\frac{d}{dt}\Psi_N^t = \mathcal{H}_N \Psi_N^t, \tag{2.1}$$

with the Hamiltonian presented as a sum of the free Hamiltonian and interaction

$$\mathcal{H}_N = \int d\mathbf{x} \left[-\frac{1}{2}\frac{\delta^2}{\delta\varphi^a(\mathbf{x})\delta\varphi^a(\mathbf{x})} + \frac{1}{2}(\nabla\varphi^a)(\mathbf{x})(\nabla\varphi^a)(\mathbf{x}) + \frac{m^2}{2}\varphi^a(\mathbf{x})\varphi^a(\mathbf{x}) + \frac{\lambda}{4N}(\varphi^a(\mathbf{x})\varphi^a(\mathbf{x}))^2 \right]. \tag{2.2}$$

If one considers states of a few number of particles in comparison with N, one can suppose that almost all fields are in the vacuum state. This treatment leads us to the following structure of the wave functional Ψ_N^t. If all fields $\varphi^1, \ldots, \varphi^N$ are in the same (vacuum) state, the N-field state Ψ_N is

$$\Psi_N[\varphi^1(\cdot), \ldots, \varphi^N(\cdot)] = c\Phi_0[\varphi^1(\cdot)] \ldots \Phi_0[\varphi^N(\cdot)]. \tag{2.3}$$

If $(N-1)$ fields are in the state Φ_0, while 1 field is in the state f_1, the N-field state can be written as

$$\Psi_N[\varphi^1(\cdot), \ldots, \varphi^N(\cdot)] = \frac{1}{\sqrt{N}}\sum_{a=1}^{N} \Phi_0[\varphi^1(\cdot)] \ldots \Phi_0[\varphi^{a-1}(\cdot)] f_1[\varphi^a(\cdot)] \Phi_0 \times [\varphi^{a+1}(\cdot)] \ldots \Phi_0[\varphi^N(\cdot)]. \tag{2.4}$$

Without loss of generality, one can suppose that (Φ_0, and f_1)$=0$. Otherwise, one could decompose the functional f_1 into two parts, one of them being proportional to Φ_0, another being orthogonal to Φ_0. The case $f_1 = \text{const}\Phi_0$ does not lead to a new functional since expressions (2.3) and (2.4) coincide then.

Analogously, the state corresponding to $(N-k)$ fields in the vacuum state and k fields in the state $f_k(\varphi^1, \ldots, \varphi^k)$ being symmetric with respect to transpositions of $\varphi^1, \ldots, \varphi^k$ and satisfying the orthogonality condition

$$\int D\varphi_1 \Phi_0^*[\varphi^1(\cdot)] f_k[\varphi^1(\cdot), \ldots, \varphi^k(\cdot)] = 0 \tag{2.5}$$

has the form

$$\Psi_N[\varphi^1(\cdot), \ldots, \varphi^N(\cdot)] = \frac{1}{\sqrt{N^k k!}} \sum_{1 \leqslant a_1 \neq \ldots \neq a_k \leqslant N} f_k[\varphi^{a_1}(\cdot), \ldots, \varphi^{a_k}(\cdot)] \prod_{a \neq a_1 \ldots a_k} \Phi_0[\varphi^a(\cdot)]. \tag{2.6}$$

Finally, one can consider the superposition of states (2.6) with rapid decreasing at $k \to \infty$ set of norms $||f_k||$. This is the most general form of a state ''with a few number of particles,'' provided that one takes into account symmetric functionals Ψ only. Nonsymmetric functionals are investigated in Appendix B.

We see that symmetric states in the theory of a large number of fields occur to be specified by infinite sets

$$f = \begin{pmatrix} f_0 \\ f_1[\varphi^1(\cdot)] \\ \cdots \\ f_k[\varphi^1(\cdot), \ldots, \varphi^k(\cdot)] \\ \cdots \end{pmatrix} \tag{2.7}$$

where f_k are symmetric functionals satisfying Eq. (2.5). One can say that f_k is a probability amplitude that k fields are in the nonvacuum state. We see that the theory of a large number of fields is equivalent to the theory of a variable number of fields. This observation is analogous to the quasiparticle conception in statistical physics.

The mapping $K_N : f \mapsto \Psi_N$ of the form

$$(K_N f)[\varphi^1(\cdot), \ldots, \varphi^N(\cdot)] = \sum_{k=0}^{N} \frac{1}{\sqrt{N^k k!}} \sum_{1 \leqslant a_1 \neq \ldots \neq a_k \leqslant N} f_k[\varphi^{a_1}(\cdot), \ldots, \varphi^{a_k}(\cdot)] \prod_{a \neq a_1 \ldots a_k} \Phi_0[\varphi^a(\cdot)], \tag{2.8}$$

will be called as a multifield canonical operator analogous to the multiparticle canonical operator used in statistical physics.[11,14] The orthogonality condition (2.5) implies that

$$||K_N f||^2 = \sum_{k=0}^{N} \frac{N!}{N^k (N-k)!} ||f_k||^2 \to_{N \to \infty} \sum_{k=0}^{\infty} ||f_k||^2. \tag{2.9}$$

We see that sets (2.7) may be identified with states of the system of $N = \infty$ fields, while the relation (2.9) can be considered as an argument that the norm of a state should be chosen as

$$||f||^2 = \sum_{k=0}^{\infty} ||f_k||^2.$$

Thus, decomposition (2.8) gives us a relationship between the theory of a large number of fields and the theory of a variable number of fields.

B. Representation of operators

Let us write operators of physical quantities in the representation (2.7). It will be convenient to present them via the third-quantized creation and annihilation operators which can be

introduced as follows.[11] The creation operator $A^+[\varphi(\cdot)]$ increases the number of fields, i.e., transforms the set $f=(0,0,\ldots,0,f_{k-1},0,\ldots)$ into $(0,\ldots,0,(A^+[\varphi(\cdot)]f)_k,0,\ldots)$, The functional $(A^+[\varphi(\cdot)]f)_k[\varphi^1(\cdot),\ldots,\varphi^k(\cdot)]$ being the k-th component of the set $(A^+[\varphi(\cdot)]f)$ is expressed via the $(k-1)$-th component of f:

$$(A^+[\varphi(\cdot)]f)_k[\varphi^1(\cdot),\ldots,\varphi^k(\cdot)]$$
$$=\frac{1}{\sqrt{k}}\sum_{a=1}^{k}\delta(\varphi(\cdot)-\varphi^a(\cdot))f_{k-1}[\varphi^1(\cdot),\ldots,\varphi^{a-1}(\cdot),\varphi^{a+1}(\cdot),\ldots,\varphi^k(\cdot)]. \tag{2.10}$$

The annihilation operator $A^-[\varphi(\cdot)]$ is

$$(A^-[\varphi(\cdot)]f)_{k-1}[\varphi^1(\cdot),\ldots,\varphi^{k-1}(\cdot)]=\sqrt{k}f_k[\varphi(\cdot),\varphi^1(\cdot),\ldots,\varphi^{k-1}(\cdot)]. \tag{2.11}$$

The condition (2.5) is not invariant under transformations (2.10) and (2.11). Consider the modified creation and annihilation operators:

$$\tilde{A}^+[\varphi(\cdot)]=A^+[\varphi(\cdot)]-\Phi_0^*[\varphi(\cdot)]\int D\phi\Phi_0[\phi(\cdot)]A^+[\phi(\cdot)],$$

$$\tilde{A}^-[\varphi(\cdot)]=A^-[\varphi(\cdot)]-\Phi_0[\varphi(\cdot)]\int D\phi\Phi_0^*[\phi(\cdot)]A^-[\phi(\cdot)].$$

To write operators in the representation (3.7), consider the orthonormal basis $(\Phi_0,\Phi_1,\ldots)$ in the space of functionals,

$$\int D\varphi\Phi_i^*[\varphi(\cdot)]\Phi_j[\varphi(\cdot)]=\delta_{ij},$$

which contain the vacuum functional Φ_0 entering to expression (2.8). Investigate the following ''elementary'' operators

$$\mathcal{O}_N^{ij}\Psi[\varphi^1(\cdot),\ldots,\varphi^N(\cdot)]=\sum_{a=1}^{N}\Phi_i[\varphi^a(\cdot)]\int D\phi\Phi_j^*[\phi(\cdot)]\Psi$$
$$\times[\varphi^1(\cdot),\ldots,\varphi^{a-1}(\cdot),\phi(\cdot),\varphi^{a+1}(\cdot),\ldots,\varphi^N(\cdot)]. \tag{2.12}$$

Apply them to the expression (2.8). It is necessary to distinguish four cases.

(i) $i=j=0$.

Due to the condition (2.5), one has

$$(\mathcal{O}_N^{00}K_Nf)[\varphi^1(\cdot),\ldots,\varphi^N(\cdot)]$$
$$=\sum_{k=0}^{N}(N-k)\frac{1}{\sqrt{N^k k!}}\sum_{1\leqslant a_1\neq\ldots\neq a_k\leqslant N}f_k[\varphi^{a_1}(\cdot),\ldots,\varphi^{a_k}(\cdot)]\prod_{a\neq a_1\ldots a_k}\Phi_0[\varphi^a(\cdot)].$$

This means that the operator $\mathcal{O}_N^{00}$ acts in the space (3.7) as $N-\hat{n},$, i.e.,

$$\mathcal{O}_N^{00}K_Nf=K_N(N-\hat{n})f,$$

where $\hat{n}=\int D\varphi\tilde{A}^+[\varphi(\cdot)]\tilde{A}^-[\varphi(\cdot)]$ is the operator of number of fields,

$$(\hat{n}f)_k=kf_k.$$

(ii) $i=0, j\neq 0$.
It follows from the symmetry condition that

$$(\mathcal{O}_N^{0j}K_N f)[\varphi^1(\cdot),\ldots,\varphi^N(\cdot)]$$
$$=\sum_{k=0}^{N}\frac{1}{\sqrt{N^k k!}}\sum_{p=1}^{k}\frac{1}{\sqrt{k}}\sum_{1\leqslant a_1\neq\ldots\neq a_k\leqslant N}\Phi_0[\varphi^{a_p}(\cdot)]\left(\int D\phi\tilde{A}^-[\phi(\cdot)]\Phi_j^*[\phi(\cdot)]f\right)_{k-1}$$
$$\times[\varphi^{a_1}(\cdot),\ldots,\varphi^{a_{p-1}}(\cdot),\varphi^{a_{p+1}}(\cdot),\ldots,\varphi^{a_k}(\cdot)]\prod_{a\neq a_1\ldots a_k}\Phi_0[\varphi^a(\cdot)]. \tag{2.13}$$

After redefining $a_1=b_1,\ldots,a_{p-1}=b_{p-1}$, $a_{p+1}=b_p,\ldots,a_k=b_{k-1}$, and $a_k=b$, we obtain that the symbol Σ_k can be substituted by k, while Σ_j transforms to $(N-k+1)$. Thus, one obtains the following commutation rule:

$$\mathcal{O}_N^{0j}K_N f=K_N(N-\hat{n})\frac{1}{\sqrt{N}}\int D\phi\tilde{A}^-[\phi(\cdot)]\Phi_j^*[\phi(\cdot)]f.$$

(iii) $i\neq 0$, $j=0$.
Due to Eq. (2.5), we have

$$(\mathcal{O}_N^{i0}K_N f)[\varphi^1(\cdot),\ldots,\varphi^N(\cdot)]$$
$$=\sum_{k=0}^{N}\frac{1}{\sqrt{N^k k!}}\sum_{1\leqslant a_1\neq\ldots\neq a_k\leqslant N}f_k[\varphi^{i_1}(\cdot),\ldots,\varphi^{i_k}(\cdot)]$$
$$\sum_{a\neq a_1\ldots a_k}\Phi_i[\varphi^a(\cdot)]\prod_{b\neq a,a_1\ldots a_k}\Phi_0[\varphi^b(\cdot)]. \tag{2.14}$$

After symmetrization, the commutation rule takes the form

$$\mathcal{O}_N^{i0}K_N f=K_N\sqrt{N}\int D\phi\tilde{A}^+[\phi(\cdot)]\Phi_i[\phi(\cdot)]f.$$

(iv) $i\neq 0$, $j\neq 0$.
Analogously, we find that

$$\mathcal{O}_N^{ij}K_N f=K_N\int D\varphi\tilde{A}^+[\varphi(\cdot)]\Phi_i[\varphi(\cdot)]\int D\phi\tilde{A}^+[\phi(\cdot)]\Phi_j^*[\phi(\cdot)].$$

Any operator can be represented via elementary operators (2.12). Consider an example.
The operator $\Sigma_{a=1}^N\varphi^a(\mathbf{x})\varphi^a(\mathbf{x})$ is expressed as

$$\sum_{a=1}^{N}\varphi^a(\mathbf{x})\varphi^a(\mathbf{x})=\sum_{ij=0}^{\infty}\int D\phi\Phi_i^*[\phi(\cdot)]\phi(\mathbf{x})\phi(\mathbf{x})\Phi_j[\phi(\cdot)]\mathcal{O}_N^{ij}.$$

Therefore, the following commutation rule takes place:

$$\lambda\sum_{a=1}^{N}\varphi^a(\mathbf{x})\varphi^a(\mathbf{x})K_N=K_N\tilde{\mathcal{Q}}_N(\mathbf{x}),$$

where the operator $\tilde{\mathcal{Q}}_N(\mathbf{x})$ consists of the constant term of order $O(N)$, the linear in creation–annihilation operators term of order $O(\sqrt{N})$ and the regular as $N\to\infty$ term which is quadratic in creation and annihilation operators:

$$\tilde{\mathcal{Q}}_N(\mathbf{x})=\lambda(N-\hat{n})(\Phi_0,\phi(\mathbf{x})\phi(\mathbf{x})\Phi_0)+\lambda\sqrt{N}\int D\phi\tilde{A}^+[\phi(\cdot)]\phi(\mathbf{x})\phi(\mathbf{x})\Phi_0[\phi(\cdot)]$$
$$+\frac{\lambda}{\sqrt{N}}(N-\hat{n})\int D\phi\tilde{A}^-[\phi(\cdot)]\phi(\mathbf{x})\phi(\mathbf{x})\Phi_0^*[\phi(\cdot)]$$
$$+\lambda\int D\phi\tilde{A}^+[\phi(\cdot)]\phi(\mathbf{x})\phi(\mathbf{x})\tilde{A}^-[\phi(\cdot)]. \tag{2.15}$$

C. Evolution equation at $N=\infty$

Analogously to the previous Sec. II B, the operators $\Sigma_{a=1}^n(\nabla\varphi^a)^2(\mathbf{x})$ and $\Sigma_{a=1}^N(-\delta^2/\delta\varphi^a(\mathbf{x})\delta\varphi^a(\mathbf{x}))$ can be also written in the representation (2.7). Since the Hamiltonian (2.2) contains the considered operator expressions only, it can be also commuted with the multifield canonical operator,

$$\mathcal{H}_N K_N=K_N\tilde{\mathcal{H}}_N.$$

The transformed Hamiltonian $\tilde{\mathcal{H}}_N$ is

$$\tilde{\mathcal{H}}_N=\int d\mathbf{x}\Bigg[(N-\hat{n})(\Phi_0,\mathcal{E}_0(\mathbf{x})\Phi_0)+\sqrt{N}\int D\phi\tilde{A}^+[\phi(\cdot)]\mathcal{E}_0(\mathbf{x})\Phi_0[\phi(\cdot)]$$
$$+\frac{1}{\sqrt{N}}(N-\hat{n})\int D\phi\Phi_0^*[\phi(\cdot)]\mathcal{E}_0(\mathbf{x})\tilde{A}^-[\phi(\cdot)]$$
$$+\int D\phi\tilde{A}^+[\phi(\cdot)]\mathcal{E}_0(\mathbf{x})\tilde{A}^-[\phi(\cdot)]+\frac{1}{4N\lambda}\tilde{\mathcal{Q}}_N^2(\mathbf{x}),\Bigg] \tag{2.16}$$

where

$$\mathcal{E}_0(\mathbf{x})=-\frac{1}{2}\frac{\delta^2}{\delta\phi(\mathbf{x})\delta\phi(\mathbf{x})}+\frac{1}{2}(\nabla\phi)^2(\mathbf{x})+\frac{m^2}{2}\phi^2(\mathbf{x}).$$

Expression (2.16) contains the terms of order $O(N)$, $O(N^{1/2})$, and $O(1)$ and the terms damping as $N\to\infty$:

$$\tilde{\mathcal{H}}_N=N\tilde{\mathcal{H}}^0+N^{1/2}\tilde{\mathcal{H}}^1+\tilde{\mathcal{H}}^2+O(N^{-1/2}). \tag{2.17}$$

The operator $\tilde{\mathcal{H}}^0$ is a multiplication by the divergent c-number quantity

$$\tilde{\mathcal{H}}^0=\int d\mathbf{x}(\Phi_0,\mathcal{E}_0(\mathbf{x})\Phi_0)+\frac{\lambda}{4}\int d\mathbf{x}(\Phi_0,\phi(\mathbf{x})\phi(\mathbf{x})\Phi_0)^2.$$

As usual in QFT, the vacuum energy is set to zero by adding a constant to the Hamiltonian, so that the Hamiltonian is defined up to a constant, and the quantity $\tilde{\mathcal{H}}^0$ can be neglected.

The operator $\tilde{\mathcal{H}}^1$ is a linear combination of creation and annihilation operators:

$$\tilde{\mathcal{H}}^1=\int D\phi\tilde{A}^+[\phi(\cdot)]Z[\phi(\cdot)]+\int D\phi\tilde{A}^-[\phi(\cdot)]Z^*[\phi(\cdot)],$$

with

$$Z[\phi(\cdot)]=\int d\mathbf{x}\left[-\frac{1}{2}\frac{\delta^2}{\delta\phi(\mathbf{x})\delta\phi(\mathbf{x})}+\frac{1}{2}(\nabla\phi(\mathbf{x}))^2+\frac{m^2+\lambda(\Phi_0,\phi^2(\mathbf{x})\Phi_0)}{2}\phi^2(\mathbf{x})\right]\Phi_0[\phi(\cdot)].$$

The operator $\tilde{\mathcal{H}}^1$ vanishes if and only if

$$Z=\text{const}\,\Phi_0. \tag{2.18}$$

We choose the functional Φ_0 to be a vacuum state functional for the field of the mass μ,

$$\Phi_0[\phi(\cdot)]=\text{const}\exp\left[-\frac{1}{2}\int d\mathbf{x}\phi(\mathbf{x})\sqrt{-\Delta+\mu^2}\phi(\mathbf{x})\right], \tag{2.19}$$

so that Eq. (2.18) will take the form

$$\mu^2=m^2+\lambda(\Phi_0,\phi^2(\mathbf{x})\Phi_0). \tag{2.20}$$

This is a well-known equation in the $1/N$-expansion theory (see, for example, Ref. 9).

The remaining nonvanishing as $N\to\infty$ part of the Hamiltonian is quadratic in creation and annihilation operators,

$$\tilde{H}\equiv\tilde{\mathcal{H}}^2=\int D\phi\tilde{A}^+[\phi(\cdot)]:\int d\mathbf{x}\mathcal{E}(\mathbf{x}):\tilde{A}^-[\phi(\cdot)]+\frac{\lambda}{4}\int d\mathbf{x}Q_0^2(\mathbf{x}), \tag{2.21}$$

where: $\hat{O}:=\hat{O}-(\Phi_0,\hat{O}\Phi_0)$,

$$\mathcal{E}(\mathbf{x})=\left[-\frac{1}{2}\frac{\delta^2}{\delta\phi(\mathbf{x})\delta\phi(\mathbf{x})}+\frac{1}{2}(\nabla\phi(\mathbf{x}))^2+\frac{\mu^2}{2}\phi^2(\mathbf{x})\right],$$

$$Q_0(\mathbf{x})=\int D\phi(\tilde{A}^+[\phi(\cdot)]+\tilde{A}^-[\phi(\cdot)])\phi^2(\mathbf{x})\Phi_0[\phi(\cdot)].$$

Since the term (2.21) is the only term remaining as $N=\infty$, one can say that the theory of $N=\infty$ fields is as follows. States in this theory are sets (2.7) obeying Eq. (2.5). The Hamiltonian of the model has the form (2.21), the evolution equation is $i\dot{f}=\tilde{H}f$.

D. Representation of the Poincare algebra

We have specified the state space of the theory of $N=\infty$ fields and evolution operator. However, to construct the *relativistic* quantum theory, it is necessary to specify the operators $U_{\Lambda,a}$ corresponding to Poincare transformations

$$x'^{\mu}=\Lambda^{\mu}_{\nu}x^{\nu}+a^{\mu},\quad \mu,\nu=\overline{0,d},$$

where the matrix Λ of Lorentz transformation satisfies the property

$$\Lambda^T g\Lambda=g,$$

($g=\text{diag}\{1,-1,-1,\ldots\}$, Λ^T is the matrix transposed to Λ). The composition law of the Poincare transformations is

$$(\Lambda_1,a_1)(\Lambda_2,a_2)=(\Lambda_1\Lambda_2,a_1+\Lambda_1a_2),$$

so that any Poincare transformation can be presented as $(\Lambda,a)=(0,a)(\Lambda,0)$. Furthermore, one can introduce the local coordinates $\theta_{\lambda\mu}$ ($\lambda,\mu=\overline{1,d}$, $\theta_{\lambda\mu}=-\theta_{\mu\lambda}$) on the Lorentz group,[2] such that

$$\Lambda=\exp(\tfrac{1}{2}\theta_{\lambda\mu}l^{\lambda\mu}),$$

with

$$(l^{\lambda\mu})^{\alpha}_{\beta}=-g^{\lambda\alpha}\delta^{\mu}_{\beta}+g^{\mu\alpha}\delta^{\lambda}_{\beta}.$$

The operators $U_{\Lambda,a}$ are required to form the representation of the Poincare group, so that

$$U_{\Lambda_1,a_1}U_{\Lambda_2,a_2}=U_{(\Lambda_1,a_1)(\Lambda_2,a_2)}.$$

Making use of the theory of representations of the Lie groups, one finds[2]

$$U_{\Lambda,a}=\exp(i\tilde{P}^{\mu}a_{\mu})\exp\left(\frac{i}{2}\tilde{M}^{\lambda\mu}\theta_{\lambda\mu}\right),$$

for some operators $\tilde{P}^{\mu}$ and $\tilde{M}^{\lambda\mu}$ obeying the commutation relations of the Poincare algebra

$$[\tilde{P}^{\lambda},\tilde{P}^{\mu}]=0,\quad [\tilde{M}^{\lambda\mu},\tilde{P}^{\nu}]=i(g^{\mu\nu}\tilde{P}^{\lambda}-g^{\lambda\nu}\tilde{P}^{\mu}),$$

$$[\tilde{M}^{\lambda\mu},\tilde{M}^{\rho\sigma}]=-i(g^{\lambda\rho}\tilde{M}^{\mu\sigma}-g^{\mu\rho}\tilde{M}^{\lambda\sigma}+g^{\mu\sigma}\tilde{M}^{\lambda\rho}-g^{\lambda\sigma}\tilde{M}^{\mu\rho}). \tag{2.22}$$

Let us construct the operators $\tilde{P}^{\lambda}$ and $\tilde{M}^{\lambda\mu}$ for the $N=\infty$-theory. For the N-field theory, one has:[1]

$$\mathcal{P}^{\mu}_{N}=\int d\mathbf{x}\mathcal{T}^{\mu 0}_{N}(\mathbf{x}),\quad \mathcal{M}^{\mu\lambda}_{N}=\int d\mathbf{x}(x^{\mu}\mathcal{T}^{\lambda 0}_{N}(\mathbf{x})-x^{\lambda}\mathcal{T}^{\mu 0}_{N}(\mathbf{x})),$$

where we integrate over surface $x^0=0$, while

$$\mathcal{T}^{00}_{N}(\mathbf{x})=-\frac{1}{2}\frac{\delta^2}{\delta\varphi^a(\mathbf{x})\delta\varphi^a(\mathbf{x})}+\frac{1}{2}(\nabla\varphi^a)(\mathbf{x})(\nabla\varphi^a)(\mathbf{x})+\frac{m^2}{2}\varphi^a(\mathbf{x})\varphi^a(\mathbf{x})+\frac{\lambda}{4N}(\varphi^a(\mathbf{x})\varphi^a(\mathbf{x}))^2,$$

$$\mathcal{T}^{k0}_{N}(\mathbf{x})=\sum_{a=1}^{N}\left(\partial^k\varphi^a(\mathbf{x})\frac{1}{i}\frac{\delta}{\delta\varphi^a(\mathbf{x})}\right).$$

Let us commute these operators with the multifield canonical operator,

$$\mathcal{P}^{\mu}_{N}K_N=K_N\tilde{\mathcal{P}}^{\mu}_{N},\quad \mathcal{M}^{\mu\nu}_{N}K_N=K_N\tilde{\mathcal{M}}^{\mu\nu}_{N},$$

expand the result in $1/N$:

$$\tilde{\mathcal{P}}^{\mu}_{N}=N\tilde{\mathcal{P}}^{\mu,0}+N^{1/2}\tilde{\mathcal{P}}^{\mu,1}+\tilde{\mathcal{P}}^{\mu,2}+\ldots,\ \tilde{\mathcal{M}}^{\mu\nu}_{N}=N\tilde{\mathcal{M}}^{\mu\nu,0}+N^{1/2}\tilde{\mathcal{M}}^{\mu\nu,1}+\tilde{\mathcal{M}}^{\mu\nu,2}+\ldots.$$

It will be shown that the operators $\tilde{\mathcal{P}}^{\mu,0}$, $\tilde{\mathcal{P}}^{\mu,1}$, $\tilde{\mathcal{M}}^{\mu\nu,0}$, and $\tilde{\mathcal{M}}^{\mu\nu,1}$ vanish, so that the remaining nonvanishing at $N=\infty$ parts

$$\tilde{P}^{\mu}=\tilde{\mathcal{P}}^{\mu,2},\quad \tilde{M}^{\mu\nu}=\tilde{\mathcal{M}}^{\mu\nu,2},$$

should be viewed as generators of Poincare transformations in the $N=\infty$-theory.

Be mindful also that the operator $\tilde{\mathcal{P}}^{0}_{N}=\tilde{H}$ has been already constructed in Sec. II C.

Consider the operator

$$\mathcal{P}^{k}_{N}=\int d\mathbf{x}\sum_{a=1}^{N}\partial^k\varphi^a(\mathbf{x})\frac{1}{i}\frac{\delta}{\delta\varphi^a(\mathbf{x})}.$$

After commuting with multifield canonical operator, one has

$$\tilde{\mathcal{P}}^{k,0}=\left(\Phi_0,\int d\mathbf{x}\partial^k\phi(\mathbf{x})\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{x})}\Phi_0\right),$$

$$\tilde{\mathcal{P}}^{k,1}=\int D\phi(\tilde{A}^+[\phi(\cdot)]Z^k[\phi(\cdot)]+\tilde{A}^-[\phi(\cdot)]Z^{k*}[\phi(\cdot)]), \tag{2.23}$$

where

$$Z^k[\phi(\cdot)]=\int d\mathbf{x}\partial^k\phi(\mathbf{x})\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{x})}\Phi_0[\phi(\cdot)].$$

Since Φ_0 has been chosen to be a vacuum functional for the field of the mass μ, while the operator $\int d\mathbf{x}\partial^k\phi(\mathbf{x})\,1/i\,\delta/\delta\phi(\mathbf{x})$ is a momentum operator for the functional Schrodinger representation, one has $Z^k=0$, $\tilde{\mathcal{P}}^{k,0}=0$, and $\tilde{\mathcal{P}}^{k,1}=0$. Thus, the operator

$$\tilde{P}^k\equiv\tilde{\mathcal{P}}^{k,2}=\int D\phi\tilde{A}^+[\phi(\cdot)]:\int d\mathbf{x}\partial^k\phi(\mathbf{x})\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{x})}:\tilde{A}^+[\phi(\cdot)], \tag{2.24}$$

can be viewed as a momentum operator in the $N=\infty$ theory.

Analogously, we find that

$$\tilde{M}^{ml}=\tilde{\mathcal{M}}^{ml,2}=\int D\phi\tilde{A}^+[\phi(\cdot)]:\int d\mathbf{x}(x^m\partial^l\phi(\mathbf{x})-x^l\partial^m\phi(\mathbf{x}))\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{x})}:\tilde{A}^-[\phi(\cdot)]. \tag{2.25}$$

The boost operator presented as

$$\mathcal{M}^{k0}=\int d\mathbf{x}x^k\mathcal{T}^{00}(\mathbf{x}),$$

after commuting with the multiparticle canonical operator gives us:

$$\tilde{\mathcal{M}}^{k0,0}=\int d\mathbf{x}x^k(\Phi^0,\mathcal{E}_0(\mathbf{x})\Phi_0)+\frac{\lambda}{4}\int d\mathbf{x}x^k(\Phi_0,\phi(\mathbf{x})\phi(\mathbf{x})\Phi_0).$$

Since the integrand is an odd function with respect to x^m, it seems to be natural that $\tilde{\mathcal{M}}^{m0,0}=0$. The operator $\tilde{\mathcal{M}}^{k0,1}$ has the structure (2.23) with

$$Z^k[\phi(\cdot)]=\int d\mathbf{x}x^k\mathcal{E}(\mathbf{x})\Phi_0[\phi(\cdot)].$$

Since the vacuum state Φ_0 is invariant under boost transformations, while

$$\int d\mathbf{x}x^k\mathcal{E}(\mathbf{x}),$$

is a boost generator, one has $Z^k=0$ and $\tilde{\mathcal{M}}^{k0,1}=0$. The remaining term is

$$\tilde{M}^{k0}=\tilde{\mathcal{M}}^{k0,2}=\int D\phi\tilde{A}^+[\phi(\cdot)]\int d\mathbf{x}x^k:\mathcal{E}(\mathbf{x}):\tilde{A}^-[\phi(\cdot)]+\frac{\lambda}{4}\int d\mathbf{x}x^kQ_0^2(\mathbf{x}). \tag{2.26}$$

The commutation relations (2.22) are formally satisfied. Namely, the operators (2.21), (2.24), (2.25), and (2.26) can be presented as

$$\tilde{H}=\tilde{H}_0+\lambda\tilde{H}_1, \quad \tilde{P}^k=\tilde{P}^k_0,$$

$$\tilde{M}^{k0}=\tilde{M}^{k0}_0+\lambda\tilde{M}^{k0}_1, \quad \tilde{M}^{kl}=\tilde{M}^{kl}_0. \tag{2.27}$$

For $\lambda=0$-case, the check of relations (2.22) is identical to the standard check of the Poincare invariance of the free QFT. For the general case, it is sufficient to justify the following commutation relations:

$$[\tilde{H}_1,\tilde{P}^k_0]=0, \quad [\tilde{H}_1,\tilde{M}^{kl}_0]=0, \tag{2.28}$$

$$[\tilde{M}^{k0}_1,\tilde{P}^l_0]=-ig^{kl}\tilde{H}_1, \quad [\tilde{M}^{k0}_1,\tilde{M}^{mn}_0]=-i(g^{km}\tilde{M}^{0n}_1-g^{kn}\tilde{M}^{0m}_1). \tag{2.29}$$

$$[\tilde{M}^{k0}_1,\tilde{M}^{l0}_1]=0, \quad [\tilde{M}^{k0}_1,\tilde{H}_1]=0, \tag{2.30}$$

$$[\tilde{M}^{k0}_1,\tilde{H}_0]+[\tilde{M}^{k0}_0,\tilde{H}_1]=0, \quad [\tilde{M}^{k0}_1,\tilde{M}^{l0}_0]+[\tilde{M}^{k0}_0,\tilde{M}^{l0}_1]=0. \tag{2.31}$$

It is straightforward to check that

$$[\tilde{P}^l_0,Q_0(\mathbf{x})]=-i\partial^l Q_0(\mathbf{x}), \quad [\tilde{M}^{mn}_0,Q_0(\mathbf{x})]=-i(x^m\partial^n-x^n\partial^m)Q_0(\mathbf{x}).$$

We obtain relations (2.28) and (2.29) then. Equations (2.30) are corollaries of the property $[Q(\mathbf{x}),Q(\mathbf{y})]=0$. The relation $[\mathcal{E}(\mathbf{x}),Q_0(\mathbf{y})]\sim\delta(\mathbf{x}-\mathbf{y})$ imply Eq. (2.31). Thus, the formal Poincare invariance is checked. However, the divergences and renormalization have not been considered yet.

E. Mode decomposition

We have specified states of the $N=\infty$-theory as sets

$$f=\begin{pmatrix} f_0 \\ f_1[\varphi^1(\cdot)] \\ \cdots \\ f_k[\varphi^1(\cdot),\ldots,\varphi^k(\cdot)] \\ \cdots \end{pmatrix} \tag{2.32}$$

of symmetric functionals $f_k[\varphi^1,\ldots,\varphi^k]$ satisfying relation (2.5) such that

$$||f||^2=\sum_{k=0}^{\infty}\int D\varphi^1,\ldots,D\varphi^k|f[\varphi^1(\cdot),\ldots,\varphi^k(\cdot)]|^2<\infty.$$

However, this definition is ill defined since the measure of functional integration is not determined mathematically. Instead of constructing the measure, it is convenient to use another representation for the k-field functionals.

Consider the basis functionals

$$\Phi^{(n)}_{\mathbf{k}_1\ldots\mathbf{k}_n}[\varphi(\cdot)]=\frac{1}{\sqrt{n!}}a^+_{\mathbf{k}_1}\ldots a^+_{\mathbf{k}_n}\Phi_0[\varphi(\cdot)], \quad n=1,2,3,\ldots, \tag{2.33}$$

corresponding to n particles with momenta $\mathbf{k}_1,\ldots,\mathbf{k}_n$. The operators $a^+_{\mathbf{k}}$ are usual quantum field creation operators:

$$a^+_{\mathbf{k}}=\frac{1}{(2\pi)^{d/2}}\int d\mathbf{x}e^{i\mathbf{kx}}\left[\sqrt{\frac{\omega_{\mathbf{k}}}{2}}\varphi(\mathbf{x})-\frac{1}{\sqrt{2\omega_{\mathbf{k}}}}\frac{\delta}{\delta\varphi(\mathbf{x})}\right],$$

with $\omega_{\mathbf{k}}=\sqrt{\mathbf{k}^2+\mu^2}$. Integrating by parts and using the commutation relations between creation and annihilation operators, we find that the inner product (2.1) for the functionals (2.33) has the form

$$(\Phi^{(n)}_{\mathbf{k}_1\dots\mathbf{k}_n},\Phi^{(m)}_{\mathbf{p}_1\dots\mathbf{p}_m})=0,\quad m\neq n;$$

$$(\Phi^{(n)}_{\mathbf{k}_1\dots\mathbf{k}_n},\Phi^{(n)}_{\mathbf{p}_1\dots\mathbf{p}_n})=\frac{1}{n!}\sum_{\sigma}\ \delta(\mathbf{k}_1-\mathbf{p}_{\sigma_1})\dots\delta(\mathbf{k}_n-\mathbf{p}_{\sigma_n}),\tag{2.34}$$

the sum is taken over all transpositions of indices 1,...,n. Equations (2.34) can be viewed as a definition of the functional integral (2.1).

Decompose the functional f_k satisfying Eq. (2.5) as

$$\begin{aligned}&f_k(\varphi^1(\cdot),\dots,\varphi^k(\cdot))\\&\quad=\sum_{l_1\dots l_k=1}^{\infty}\int d\mathbf{p}^1_1\dots d\mathbf{p}^1_{l_1}\dots d\mathbf{p}^k_1\dots d\mathbf{p}^k_{l_k}f^k_{l_1;\mathbf{p}^1_1\dots\mathbf{p}^1_{l_1};\dots l_k,\mathbf{p}^k_1\dots\mathbf{p}^k_{l_k}}\Phi^{(l_1)}_{\mathbf{p}^1_1\dots\mathbf{p}^1_{l_1}}\\&\qquad[\phi^1(\cdot)]\dots\Phi^{(l_k)}_{\mathbf{p}^k_1\dots\mathbf{p}^k_{l_k}}[\phi^k(\cdot)].\end{aligned}$$

One can uniquely specify the set (2.32) of functionals by specifying the set of functionals

$$f^k_{l_1;\mathbf{p}^1_1\dots\mathbf{p}^1_{l_1};\dots l_k,\mathbf{p}^k_1\dots\mathbf{p}^k_{l_k}},\tag{2.35}$$

being symmetric under transpositions of $\mathbf{p}^m_i$ and $\mathbf{p}^m_j$, as well as under transpositions of sets $l_m,\mathbf{p}^m_1\dots\mathbf{p}^m_{l_m}$, and $l_s,\mathbf{p}^s_1\dots\mathbf{p}^s_{l_s}$. The quantity $||f||^2$ can be presented as

$$||f||^2=\sum_{k=0}^{\infty}\sum_{l_1\dots l_k=1}^{\infty}\int d\mathbf{p}^1_1\dots d\mathbf{p}^1_{l_1}\dots d\mathbf{p}^k_1\dots d\mathbf{p}^k_{l_k}|f^k_{l_1;\mathbf{p}^1_1\dots\mathbf{p}^1_{l_1};\dots l_k,\mathbf{p}^k_1\dots\mathbf{p}^k_{l_k}}|^2.$$

Creation and annihilation operators can be decomposed as

$$A^+[\varphi(\cdot)]=\sum_{n=0}^{\infty}\int d\mathbf{k}_1\dots d\mathbf{k}_n\Phi^{(n)*}_{\mathbf{k}_1\dots\mathbf{k}_n}[\varphi(\cdot)]A^{+(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}.$$

$$A^-[\varphi(\cdot)]=\sum_{n=0}^{\infty}\int d\mathbf{k}_1\dots d\mathbf{k}_n\Phi^{(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}[\varphi(\cdot)]A^{-(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}.\tag{2.36}$$

The operators $A^{\pm(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}$ defined as

$$A^{+(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}=\int D\phi A^+[\phi(\cdot)]\Phi^{(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}[\phi(\cdot)],\quad A^{-(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}=\int D\phi A^-[\phi(\cdot)]\Phi^{*(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}[\phi(\cdot)],$$

create (annihilate) the field in the n-particle state with momenta $\mathbf{k}_1,\dots,\mathbf{k}_n$. They are invariant under transpositions of momenta $\mathbf{k}_1,\dots,\mathbf{k}_n$ and obey the ordinary canonical commutation relations:

$$[A^{\pm(m)}_{\mathbf{k}_1\dots\mathbf{k}_m},A^{\pm(n)}_{\mathbf{p}_1\dots\mathbf{p}_n}]=0,\quad [A^{-(m)}_{\mathbf{k}_1\dots\mathbf{k}_m},A^{+(n)}_{\mathbf{p}_1\dots\mathbf{p}_n}]=0,m\neq n\tag{2.37}$$

$$[A^{-(m)}_{\mathbf{k}_1\dots\mathbf{k}_m}, A^{+(n)}_{\mathbf{p}_1\dots\mathbf{p}_n}] = \frac{1}{n!}\sum_{\sigma}\ \delta(\mathbf{k}_1-\mathbf{p}_{\sigma_1})\dots\delta(\mathbf{k}_n-\mathbf{p}_{\sigma_n}). \tag{2.38}$$

Any vector f can be written via creation operators and vacuum state

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \\ \cdots \\ 0 \\ \cdots \end{pmatrix} \tag{2.39}$$

as follows:

$$f = \sum_{k=0}^{\infty}\frac{1}{\sqrt{k!}}\sum_{l_1\dots l_k=1}^{\infty}\int d\mathbf{p}^1_1\dots d\mathbf{p}^1_{l_1}\dots d\mathbf{p}^k_1\dots d\mathbf{p}^k_{l_k}$$
$$f^k_{l_1;\mathbf{p}^1_1\dots\mathbf{p}^1_{l_1};\dots l_k,\mathbf{p}^k_1\dots\mathbf{p}^k_{l_k}} A^{+(l_1)}_{\mathbf{p}^1_1\dots\mathbf{p}^1_{l_1}}\dots A^{+(l_k)}_{\mathbf{p}^k_1\dots\mathbf{p}^k_{l_k}}|0\rangle.$$

Making use of the QFT formulas:

$$\int d\mathbf{x}\mathcal{E}(\mathbf{x}) := \int d\mathbf{k}\omega_{\mathbf{k}}a^+_{\mathbf{k}}a^-_{\mathbf{k}},$$

$$\phi^2(\mathbf{x})\Phi_0 = \frac{1}{(2\pi)^d}\int\frac{d\mathbf{k}}{\sqrt{2\omega_{\mathbf{k}}}}\frac{d\mathbf{p}}{\sqrt{2\omega_{\mathbf{p}}}}e^{-i(\mathbf{k}+\mathbf{p})\mathbf{x}}a^+_{\mathbf{k}}a^+_{\mathbf{p}}\Phi_0, \tag{2.40}$$

one transforms expression (2.21) to the following form:

$$\tilde{H} = \sum_{n=1}^{\infty}\int d\mathbf{k}_1\dots d\mathbf{k}_n A^{+(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}(\omega_{\mathbf{k}_1}+\dots+\omega_{\mathbf{k}_n})A^{-(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}$$
$$+\frac{\lambda}{4}\int d\mathbf{x}\left(\frac{\sqrt{2}}{(2\pi)^d}\int\frac{d\mathbf{k}_1}{\sqrt{2\omega_{\mathbf{k}_1}}}\frac{d\mathbf{k}_2}{\sqrt{2\omega_{\mathbf{k}_2}}}(A^{+(2)}_{\mathbf{k}_1\mathbf{k}_2}e^{-i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{x}}+A^{-(2)}_{\mathbf{k}_1\mathbf{k}_2}e^{i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{x}})\right)^2. \tag{2.41}$$

Analogously,

$$\tilde{P}^l = \sum_{n=1}^{\infty}\int d\mathbf{k}_1\dots d\mathbf{k}_n A^{+(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}(k^l_1+\dots+k^l_n)A^{-(n)}_{\mathbf{k}_1\dots\mathbf{k}_n},$$

$$\tilde{M}^{ml} = \sum_{n=1}^{\infty}\int d\mathbf{k}_1\dots d\mathbf{k}_n A^{+(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}\sum_{s=1}^{n}\left(k^l_s i\frac{\partial}{\partial k^m_s}-k^m_s i\frac{\partial}{\partial k^l_s}\right)A^{-(n)}_{\mathbf{k}_1\dots\mathbf{k}_n},$$

$$\tilde{M}^{l0} = \sum_{n=1}^{\infty}\int d\mathbf{k}_1\dots d\mathbf{k}_n A^{+(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}\sum_{s=1}^{n}\left(i\omega_{\mathbf{k}_s}\frac{\partial}{\partial k^l_s}+i\frac{k^l_s}{2\omega_{\mathbf{k}_s}}\right)A^{-(n)}_{\mathbf{k}_1\dots\mathbf{k}_n} \tag{2.42}$$
$$+\frac{\lambda}{4}\int d\mathbf{x}x^l\left(\frac{\sqrt{2}}{(2\pi)^d}\int\frac{d\mathbf{k}_1}{\sqrt{2\omega_{\mathbf{k}_1}}}\frac{d\mathbf{k}_2}{\sqrt{2\omega_{\mathbf{k}_2}}}(A^{+(2)}_{\mathbf{k}_1\mathbf{k}_2}e^{-i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{x}}+A^{-(2)}_{\mathbf{k}_1\mathbf{k}_2}e^{i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{x}})\right)^2.$$

F. Decomposition of the state space

We see that the Hilbert space of the $N=\infty$-theory can be presented as

$$\mathcal{F}(\oplus_{n=1}^{\infty}\mathcal{H}^{\vee n}) \tag{2.43}$$

(the notations of Appendix A are used), where $\mathcal{H}$ is a space of complex functions $f_{\mathbf{k}}$, $\mathbf{k}\in\mathbf{R}^d$ from $L^2(\mathbf{R}^d)$. Analogously to lemma A.8, the space (2.43) is isomorphic to

$$\mathcal{F}(\mathcal{H}^{\vee 2})\otimes\mathcal{F}(\mathcal{H}+\oplus_{n=3}^{\infty}\mathcal{H}^{\vee n})\equiv\mathcal{F}\otimes\check{\mathcal{F}}, \tag{2.44}$$

while the operators (2.41) and (2.42) can be viewed as the following operators in the space (2.44):

$$\tilde{H}=H\otimes 1+1\otimes\check{H},\quad \tilde{P}^k=P^k\otimes 1+1\otimes\check{P}^k,$$

$$\tilde{M}^{ml}=M^{ml}\otimes 1+1\otimes\check{M}^{ml},\quad \tilde{M}^{k0}=M^{k0}\otimes 1+1\otimes\check{M}^{k0}. \tag{2.45}$$

The operators $\check{H}$, $\check{P}^k$, $\check{M}^{kl}$, and $\check{M}^{k0}$ are the same as in the free theory:

$$\begin{aligned}
\check{H}&=\sum_{n=1,3,4,\dots}\int d\mathbf{k}_1\dots d\mathbf{k}_n A^{+(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}(\omega_{\mathbf{k}_1}+\dots+\omega_{\mathbf{k}_n})A^{-(n)}_{\mathbf{k}_1\dots\mathbf{k}_n},\\
\check{P}^l&=\sum_{n=1,3,4\dots}\int d\mathbf{k}_1\dots d\mathbf{k}_n A^{+(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}(k_1^l+\dots+k_n^l)A^{-(n)}_{\mathbf{k}_1\dots\mathbf{k}_n},\\
\check{M}^{ml}&=\sum_{n=1,3,4,\dots}\int d\mathbf{k}_1\dots d\mathbf{k}_n A^{+(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}\sum_{s=1}^{n}\left(k_s^l i\frac{\partial}{\partial k_s^m}-k_s^m i\frac{\partial}{\partial k_s^l}\right)A^{-(n)}_{\mathbf{k}_1\dots\mathbf{k}_n},\\
\tilde{M}^{l0}&=\sum_{n=1,3,4,\dots}\int d\mathbf{k}_1\dots d\mathbf{k}_n A^{+(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}\sum_{s=1}^{n}\left(i\omega_{\mathbf{k}_s}\frac{\partial}{\partial k_s^l}+i\frac{k_s^l}{2\omega_{\mathbf{k}_s}}\right)A^{-(n)}_{\mathbf{k}_1\dots\mathbf{k}_n}.
\end{aligned} \tag{2.46}$$

The only nontrivial part of operators (2.45) correspond to the space $\mathcal{F}(\mathcal{H}^{\vee 2})$:

$$\begin{aligned}
H&=\int d\mathbf{k}_1 d\mathbf{k}_2 A^{+(2)}_{\mathbf{k}_1\mathbf{k}_2}(\omega_{\mathbf{k}_1}+\omega_{\mathbf{k}_2})A^{-(2)}_{\mathbf{k}_1\mathbf{k}_2}+\frac{\lambda}{4}\int d\mathbf{x}\\
&\left(\frac{\sqrt{2}}{(2\pi)^d}\int\frac{d\mathbf{k}_1}{\sqrt{2\omega_{\mathbf{k}_1}}}\frac{d\mathbf{k}_2}{\sqrt{2\omega_{\mathbf{k}_2}}}(A^{+(2)}_{\mathbf{k}_1\mathbf{k}_2}e^{-i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{x}}+A^{-(2)}_{\mathbf{k}_1\mathbf{k}_2}e^{i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{x}})\right)^2.\\
\tilde{P}^l&=\int d\mathbf{k}_1 d\mathbf{k}_2 A^{+(2)}_{\mathbf{k}_1\mathbf{k}_2}(k_1^l+k_2^l)A^{-(2)}_{\mathbf{k}_1\mathbf{k}_2}\\
M^{ml}&=\int d\mathbf{k}_1 d\mathbf{k}_2 A^{+(2)}_{\mathbf{k}_1\mathbf{k}_2}\sum_{s=1}^{2}\left(k_s^l i\frac{\partial}{\partial k_s^m}-k_s^m i\frac{\partial}{\partial k_s^l}\right)A^{-(2)}_{\mathbf{k}_1\mathbf{k}_2}.
\end{aligned} \tag{2.47}$$

$$\begin{aligned}
M^{l0}&=\int d\mathbf{k}_1 d\mathbf{k}_2 A^{+(2)}_{\mathbf{k}_1\mathbf{k}_2}\sum_{s=1}^{2}\left(i\omega_{\mathbf{k}_s}\frac{\partial}{\partial k_s^l}+i\frac{k_s^l}{2\omega_{\mathbf{k}_s}}\right)A^{-(2)}_{\mathbf{k}_1\mathbf{k}_2}\\
&+\frac{\lambda}{4}\int d\mathbf{x}x^l\left(\frac{\sqrt{2}}{(2\pi)^d}\int\frac{d\mathbf{k}_1}{\sqrt{2\omega_{\mathbf{k}_1}}}\frac{d\mathbf{k}_2}{\sqrt{2\omega_{\mathbf{k}_2}}}(A^{+(2)}_{\mathbf{k}_1\mathbf{k}_2}e^{-i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{x}}+A^{-(2)}_{\mathbf{k}_1\mathbf{k}_2}e^{i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{x}})\right)^2.
\end{aligned}$$

The operators (2.45) correspond to the representation of the Poincare group in $\mathcal{F}\otimes\check{\mathcal{F}}$ of the form:

$$\tilde{U}_{\Lambda,a}=U_{\Lambda,a}\otimes\check{U}_{\Lambda,a},$$

with

$$U_{\Lambda,a}=\exp(iP_\mu a^\mu)\exp\left(\frac{i}{2}M^{\Lambda\mu}\theta_{\lambda\mu}\right),\quad \check{U}_{\Lambda,a}=\exp(i\check{P}_\mu a^\mu)\exp\left(\frac{i}{2}\check{M}^{\lambda\mu}\theta_{\lambda\mu}\right).$$

To express the operators $\check{U}_{\Lambda,a}$, it is convenient to introduce the operators $u_{\Lambda,a}$ of the unitary representation of the Poincare group in $\mathcal{H}$:

$$(u_{\Lambda,a}f)_{\mathbf{k}}=\exp(i\omega_{\mathbf{k}}a_0-i\mathbf{ka})\sqrt{\frac{(\Lambda^{-1})^0_n k^n+(\Lambda^{-1})^0_0\omega_{\mathbf{k}}}{\omega_{\mathbf{k}}}}f_{(\Lambda^{-1})^m_n k^n+(\Lambda^{-1})^m_0\omega_{\mathbf{k}}},\tag{2.48}$$

with generators

$$p^l=k^l,\quad p^0=\omega_{\mathbf{k}},\quad m^{l0}=i\left(\omega_{\mathbf{k}}\frac{\partial}{\partial k^l}+\frac{k^l}{2\omega_{\mathbf{k}}}\right),$$
$$m^{ln}=i\left(k^n\frac{\partial}{\partial k^l}-k^l\frac{\partial}{\partial k^n}\right).\tag{2.49}$$

By $\tilde{u}_{\Lambda,a}:\mathcal{H}\oplus\oplus_{n=3}^{\infty}\mathcal{H}^{\vee n}\to\mathcal{H}\oplus\oplus_{n=3}^{\infty}\mathcal{H}^{\vee n}$, we denote the operator

$$\tilde{u}_{\Lambda,a}(f_1,f_3,f_4,\dots)=(u_{\Lambda,a}f_1,u^{\otimes 3}_{\Lambda,a}f_3,u^{\otimes 4}_{\Lambda,a}f_4,\dots).$$

We can notice that

$$\check{U}_{\Lambda,a}=\mathcal{U}(\tilde{u}_{\Lambda,a})$$

(the notations of Appendix A are used).

Thus, the operators $\check{U}_{\Lambda,a}$ are constructed. The only nontrivial problem is to construct the representation of the Poincare group corresponding to the generators (2.47).

G. Problem of divergences

1. The Haag theorem and volume divergences

Apply the Hamiltonian (2.47) to the vacuum state. The result will be

$$H|0\rangle=\frac{\lambda}{4}\frac{2}{(2\pi)^d}\int\frac{d\mathbf{k}_1}{\sqrt{2\omega_{\mathbf{k}_1}}}\frac{d\mathbf{k}_2}{\sqrt{2\omega_{\mathbf{k}_2}}}\frac{d\mathbf{p}_1}{\sqrt{2\omega_{\mathbf{p}_1}}}\frac{d\mathbf{p}_1}{\sqrt{2\omega_{\mathbf{p}_2}}}A^+_{\mathbf{k}_1\mathbf{k}_2}A^+_{\mathbf{p}_1\mathbf{p}_2}\delta(\mathbf{k}_1+\mathbf{k}_2+\mathbf{p}_1+\mathbf{p}_2)|0\rangle,$$

where $A^+_{\mathbf{k}_1\mathbf{k}_2}\equiv A^{+(2)}_{\mathbf{k}_1\mathbf{k}_2}$. Because of the δ function, the quantity $||H\Phi^{(0)}||^2$ diverges. This is a volume divergence associated with the Haag theorem (see, for example, Ref. 2). An analogous infinite quantity appears when one applied the perturbation theory in λ for the evolution operator.

Within the perturbation theory, such difficulty can be resolved with the help of the Faddeev transformation.[6]

2. The Stueckelberg divergences

Even after removing the vacuum divergences, the problem is not completely resolved. If one considers the perturbation theory for the Schrodinger equation of motion, one finds that there are UV divergences even in the tree approximation. Namely, for the first order of the perturbation theory, one has

$$e^{iH_0t}\tilde{H}_1e^{-iH_0t}\equiv\tilde{H}_1(t)=\frac{1}{(2\pi)^d}\int\frac{d\mathbf{k}_1}{\sqrt{2\omega_{\mathbf{k}_1}}}\frac{d\mathbf{k}_2}{\sqrt{2\omega_{\mathbf{k}_2}}}\frac{d\mathbf{p}_1}{\sqrt{2\omega_{\mathbf{p}_1}}}\frac{d\mathbf{p}_1}{\sqrt{2\omega_{\mathbf{p}_2}}}$$
$$A^+_{\mathbf{k}_1\mathbf{k}_2}A^-_{\mathbf{p}_1\mathbf{p}_2}\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{p}_1-\mathbf{p}_2)e^{-it(\omega_{\mathbf{k}_1}\omega_{\mathbf{k}_2}+\omega_{\mathbf{p}_1}+\omega_{\mathbf{p}_2})}. \tag{2.50}$$

Applying the first-order evolution operator

$$U_t=-i\lambda\int_0^t d\tau\tilde{H}_1(\tau),$$

to the vector

$$\Phi^0=\int d\mathbf{p}_1d\mathbf{p}_2A^+_{\mathbf{p}_1\mathbf{p}_2}\Phi^0_{\mathbf{p}_1\mathbf{p}_2},$$

we find

$$U_t\Phi^0=\int d\mathbf{p}_1d\mathbf{p}_2A^+_{\mathbf{p}_1\mathbf{p}_2}\Phi^t_{\mathbf{p}_1\mathbf{p}_2},$$

with

$$\Phi^t_{\mathbf{k}_1\mathbf{k}_2}=\frac{1}{(2\pi)^d}\frac{1}{\sqrt{2\omega_{\mathbf{k}_1}}}\frac{1}{\sqrt{2\omega_{\mathbf{k}_2}}}\int\frac{1}{\sqrt{2\omega_{\mathbf{p}_1}}}\frac{1}{\sqrt{2\omega_{\mathbf{p}_2}}}\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{p}_1-\mathbf{p}_2)$$
$$\Phi^{(0)}_{\mathbf{p}_1\mathbf{p}_2}\frac{e^{-it(\omega_{\mathbf{k}_1}+\omega_{\mathbf{k}_2}-\omega_{\mathbf{p}_1}-\omega_{\mathbf{p}_2})}-1}{i(\omega_{\mathbf{k}_1}+\omega_{\mathbf{k}_2}-\omega_{\mathbf{p}_1}-\omega_{\mathbf{p}_2})}.$$

The integral

$$\int d\mathbf{k}_1d\mathbf{k}_2|\Phi^t_{\mathbf{k}_1\mathbf{k}_2}|^2,$$

diverges for $d\geqslant 4$. This is a Stueckelberg divergence.

III. CONSTRUCTION OF THE HAMILTONIAN

The purpose of this section is to define mathematically the operators in the Hilbert space that corresponds to the formal expression (2.47). For $d+1=4$ and 5, it is necessary to perform the infinite renormalization of the coupling constant, for $d+1\geqslant 6$, the model is nonrenormalizable. Sections II A–C deal with the heuristic construction of the Hamiltonian; in Sec. II D, representation for space–time translations and spatial rotations is constructed.

A. Diagonalization of the Hamiltonian

Since the Hamiltonian (2.47) is quadratic with respect to creation and annihilation operators, one can perform the canonical transformation of creation and annihilation operators in order to take the Hamiltonian to the canonical form.

It is convenient to introduce new variables,

$$Q_{\mathbf{Ps}}=\frac{1}{\sqrt{2\Omega_{\mathbf{Ps}}}}(A^{+}_{\mathbf{P}/2-\mathbf{s},\mathbf{P}/2+\mathbf{s}}+A^{-}_{-\mathbf{P}/2-\mathbf{s},-\mathbf{P}/2+\mathbf{s}}),$$
$$\Pi_{\mathbf{Ps}}=i\sqrt{\frac{\Omega_{\mathbf{Ps}}}{2}}(A^{+}_{\mathbf{P}/2-\mathbf{s},\mathbf{P}/2+\mathbf{s}}-A^{-}_{-\mathbf{P}/2-\mathbf{s},-\mathbf{P}/2+\mathbf{s}}). \tag{3.1}$$

Here,

$$\Omega_{\mathbf{Ps}}=\omega_{\mathbf{P}/2-\mathbf{s}}+\omega_{\mathbf{P}/2-\mathbf{s}}. \tag{3.2}$$

The operators (3.1) obey the properties:

$$Q_{\mathbf{Ps}}=Q_{\mathbf{P},-\mathbf{s}}=Q^{*}_{-\mathbf{P},\mathbf{s}},\Pi_{\mathbf{Ps}}=\Pi_{\mathbf{P},-\mathbf{s}}=\Pi^{*}_{-\mathbf{P},\mathbf{s}},$$

and canonical commutation relations:

$$[Q_{\mathbf{Ps}},Q_{\mathbf{P}'\mathbf{s}'}]=0,\quad [\Pi_{\mathbf{Ps}},\Pi_{\mathbf{P}'\mathbf{s}'}]=0,\quad [Q_{\mathbf{Ps}},\Pi_{\mathbf{P}'\mathbf{s}'}]=i\,\delta_{\mathbf{PP}'}\,\tfrac{1}{2}(\delta_{\mathbf{s}-\mathbf{s}'}+\delta_{\mathbf{s}+\mathbf{s}'}).$$

The Hamiltonian takes the following form up to an additive constant:

$$H=\frac{1}{2}\int d\mathbf{P}(\Pi_{\mathbf{P}},\Pi_{\mathbf{P}})+\frac{1}{2}\int d\mathbf{P}(Q_{\mathbf{P}},(M_P)^2\mathbf{Q}_{\mathbf{P}}). \tag{3.3}$$

Here $\Pi_{\mathbf{P}}$, $Q_{\mathbf{P}}$ are operator-valued even functions of the variable $\mathbf{s}$. The inner product (f,g) of two even functions $f_{\mathbf{s}}$ and $g_{\mathbf{s}}$ is, as usual, $\int d\mathbf{s} f^{*}_{\mathbf{s}} g_{\mathbf{s}}$. $(M_{\mathbf{P}})^2$ is the following operator in the space of even functions:

$$((M_{\mathbf{P}})^2\varphi)_{\mathbf{s}}=\Omega^2_{\mathbf{Ps}}\varphi_s+\frac{\lambda}{(2\pi)^d}\int d\mathbf{s}'\sqrt{\frac{2\Omega_{\mathbf{Ps}}}{2\omega_{\mathbf{P}/2+\mathbf{s}}2\omega_{\mathbf{P}/2-\mathbf{s}}}}\sqrt{\frac{2\Omega_{\mathbf{Ps}'}}{2\omega_{\mathbf{P}/2+\mathbf{s}'}2\omega_{\mathbf{P}/2-\mathbf{s}'}}}\varphi_{\mathbf{s}'}. \tag{3.4}$$

The operator (3.3) can be diagonalized by the following procedure:

$$Q_{\mathbf{P}}=\frac{1}{\sqrt{2M_{\mathbf{P}}}}(C^{+}_{\mathbf{P}}+C^{-}_{-\mathbf{P}}),$$
$$\Pi_{\mathbf{P}}=i\sqrt{\frac{M_{\mathbf{P}}}{2}}(C^{+}_{\mathbf{P}}-C^{-}_{-\mathbf{P}}), \tag{3.5}$$

where $C^{\pm}_{\mathbf{P}}$ are operator-valued functions $C^{\pm}_{\mathbf{Ps}}$ of the variable $\mathbf{s}$. They obey the usual canonical commutation relations:

$$[C^{-}_{\mathbf{Ps}},C^{+}_{\mathbf{Ps}}]=\delta_{\mathbf{PP}'}\,\tfrac{1}{2}(\delta_{\mathbf{s}-\mathbf{s}'}+\delta_{\mathbf{s}+\mathbf{s}'}),\quad [C^{\pm}_{\mathbf{Ps}},C^{\pm}_{\mathbf{Ps}}]=0.$$

The Hamiltonian takes the form:

$$H=\int d\mathbf{P}d\mathbf{s}d\mathbf{s}'C^{+}_{\mathbf{Ps}}(M_{\mathbf{P}})_{\mathbf{ss}'}C^{-}_{\mathbf{Ps}'}. \tag{3.6}$$

The $(M_{\mathbf{P}})_{\mathbf{ss}'}$ is a matrix element of the operator $M_{\mathbf{P}}$.

One should use then another, nonFock representation for the operators $A^{\pm}_{\mathbf{k}_1\mathbf{k}_2}$, which is a Fock representation for the transformed operators $C^{\pm}_{\mathbf{Ps}}$. The Hamiltonian (3.6) is then a self-adjoint operator if $M_{\mathbf{P}}$ is self-adjoint. The evolution operator is expressed via the unitary operator $e^{-iM_{\mathbf{P}}t}$. To construct $M_{\mathbf{P}}$, one should first check that $(M_{\mathbf{P}})^2$ is a positively definite self-adjoint operator

and define $M_{\mathbf{P}}\equiv\sqrt{(M_{\mathbf{P}})^2}$, making use of the functional calculus of self-adjoint operators. The operator $(M_{\mathbf{P}})^{1/2}$ entering to expression (3.5) can be constructed in analogous way.

B. Definition of the Hamiltonian and its properties

Formula (3.4) for the operator $(M_{\mathbf{P}})^2$ is not well defined since the vector

$$\sqrt{\frac{2\Omega_{\mathbf{Ps}}}{2\omega_{\mathbf{P}/2+\mathbf{s}'}2\omega_{\mathbf{P}/2-\mathbf{s}'}}},$$

considered as a function of $\mathbf{s}$ does not belong to L^2. The operator (3.4) is therefore analogous to the quantum mechanical Hamiltonian corresponding to the particle moving in the singular potential like δ function. The theory of singular potentials is developed in Ref. 15.

To construct mathematically the (unbounded) self-adjoint operator $(M_{\mathbf{P}})^2$, one may first construct the (bounded) operator $(M_{\mathbf{P}})^{-2}$, and prove that it is invertible and positively definite. Then, the operator $(M_{\mathbf{P}})^2$ is defined as $(M_{\mathbf{P}})^2\equiv((M_{\mathbf{P}})^{-2})^{-1}$.

To find the vector

$$\varphi=(M_{\mathbf{P}})^{-2}\psi,$$

one should solve the equation $\psi=(M_{\mathbf{P}})^2\varphi$. It has the following form:

$$\begin{aligned}\psi_{\mathbf{s}}&=\Omega_{\mathbf{Ps}}^2\varphi_{\mathbf{s}}+c\sqrt{\frac{2\Omega_{\mathbf{Ps}}}{2\omega_{\mathbf{P}/2+\mathbf{s}}2\omega_{\mathbf{P}/2-\mathbf{s}}}},\\ c&=\frac{\lambda}{(2\pi)^d}\int d\mathbf{s}\sqrt{\frac{2\Omega_{\mathbf{Ps}}}{2\omega_{\mathbf{P}/2+\mathbf{s}}2\omega_{\mathbf{P}/2-\mathbf{s}}}}\varphi_{\mathbf{s}}.\end{aligned}\tag{3.7}$$

Eqs. (3.7) imply that

$$c=\frac{\lambda_R^{\mathbf{P}}}{(2\pi)^d}\int d\mathbf{s}\sqrt{\frac{2\Omega_{\mathbf{Ps}}}{2\omega_{\mathbf{P}/2+\mathbf{s}}2\omega_{\mathbf{P}/2-\mathbf{s}}}}\frac{1}{\Omega_{\mathbf{Ps}}^2}\psi_{\mathbf{s}},\tag{3.8}$$

with the "renormalized" coupling constant $\lambda_R^{\mathbf{P}}$ expressed from the relation

$$\frac{1}{\lambda_R^{\mathbf{P}}}=\frac{1}{\lambda}+\frac{1}{(2\pi)^d}\int d\mathbf{s}\frac{2\Omega_{\mathbf{Ps}}}{2\omega_{\mathbf{P}/2+\mathbf{s}}2\omega_{\mathbf{P}/2-\mathbf{s}}}\frac{1}{\Omega_{\mathbf{Ps}}^2}.\tag{3.9}$$

The operator $(M_{\mathbf{P}})^{-2}$ has then the form

$$((M_{\mathbf{P}})^{-2}\psi)_{\mathbf{s}}=\frac{1}{\Omega_{\mathbf{Ps}}^2}\psi_{\mathbf{s}}-\frac{\lambda_R^{\mathbf{P}}}{(2\pi)^d}\chi_{\mathbf{Ps}}\int d\mathbf{s}'\,\chi_{\mathbf{Ps}'}\psi_{\mathbf{s}'},\tag{3.10}$$

with

$$\chi_{\mathbf{Ps}}=\frac{1}{\Omega_{\mathbf{Ps}}^2}\cdot\sqrt{\frac{2\Omega_{\mathbf{Ps}}}{2\omega_{\mathbf{P}/2+\mathbf{s}}2\omega_{\mathbf{P}/2-\mathbf{s}}}}.\tag{3.11}$$

The function (3.11) treated as a function of $\mathbf{s}$ belongs to L^2 for $d+1<6$. For these values of the space-time dimensionality, the operator $(M_{\mathbf{P}})^{-2}$ is bounded and self-adjoint, provided that the quantity $\lambda_R^{\mathbf{P}}$ is finite. Since the integral entering to the right-hand side of Eq. (3.9) diverges at d

$+1=4$ and 5, for these values of d it is necessary to perform infinite renormalization of the coupling constant. This means that λ should be chosen in such a way that $|\lambda_R^{\mathbf{P}}|<\infty$. The fact that λ is $\mathbf{P}$-independent means that

$$\frac{1}{\lambda_R^{\mathbf{P}_1}}-\frac{1}{\lambda_R^{\mathbf{P}_2}}=\frac{1}{(2\pi)^d}\int d\mathbf{s}\left[\frac{1}{2\Omega_{\mathbf{P}_1\mathbf{s}}\omega_{\mathbf{P}_1/2+\mathbf{s}}\omega_{\mathbf{P}_1/2-\mathbf{s}}}-\frac{1}{2\Omega_{\mathbf{P}_2\mathbf{s}}\omega_{\mathbf{P}_2/2+\mathbf{s}}\omega_{\mathbf{P}_2/2-\mathbf{s}}}\right]. \tag{3.12}$$

Note that the integral in the right-hand side of Eq. (4.12) is well defined at $d+1=4$ and 5, since

$$\frac{\partial}{\partial\mathbf{P}}\left(\frac{1}{2\Omega_{\mathbf{P}_2\mathbf{s}}\omega_{\mathbf{P}_2/2+\mathbf{s}}\omega_{\mathbf{P}_2/2-\mathbf{s}}}\right)=O(|\mathbf{s}|^{-5}),s\to\infty.$$

The fact that the operator (3.10) is invertible can be understood as follows. Suppose that $(M_{\mathbf{P}})^{-2}\psi=0$ for some ψ. This means that

$$\psi_{\mathbf{s}}=c\Omega_{\mathbf{P}\mathbf{s}}^2\chi_{\mathbf{P}\mathbf{s}}, \tag{3.13}$$

for some multiplier c. But the function (3.13) does not belong to L^2. Thus, the operator $(M_{\mathbf{P}})^{-2}$ is invertible.

To investigate the positive definiteness of the operator $(M_{\mathbf{P}})^{-2}$, calculate the integral

$$I(\mathbf{P},\epsilon)=\frac{1}{(2\pi)^d}\int\frac{d\mathbf{s}}{2\omega_{\mathbf{P}_2/2+\mathbf{s}}\omega_{\mathbf{P}_2/2-\mathbf{s}}}\frac{1}{\Omega_{\mathbf{P}_2\mathbf{s}}^2+\epsilon^2},$$

making use of the dimensional regularization. First of all, introduce new variables, $\mathbf{k}_1=\mathbf{P}/2+\mathbf{s}$, $\mathbf{k}_2=\mathbf{P}/2-\mathbf{s}$, so that $\int d\mathbf{s}\to\int d\mathbf{k}_1 d\mathbf{k}_2\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{P})$. Next, use the identity

$$\frac{\omega_1+\omega_2}{2\omega_1\omega_2(\epsilon^2+(\omega_1+\omega_2)^2)}=\frac{1}{2\pi}\int\frac{d\xi}{(\omega_1^2+\xi^2)(\omega_2^2+(\xi-\epsilon)^2)},$$

so that

$$I(\mathbf{P},\epsilon)=\frac{1}{(2\pi)^{d+1}}\int\frac{d\mathbf{k}_1 d\mathbf{k}_2 d\xi\,\delta(\mathbf{k}_1+\mathbf{k}_2-\mathbf{P})}{(\xi^2+\omega_{\mathbf{k}_1}^2)((\xi-\epsilon)^2+\omega_{\mathbf{k}_2}^2)}.$$

Introduce, as usual, the α representation: $a^{-1}=\int_0^\infty d\alpha e^{-\alpha a}$. We get

$$I(\mathbf{P},\epsilon)=\frac{1}{(2\pi)^{d+1}}\int_0^\infty d\alpha\int_0^\infty d\beta e^{-\mu^2(\alpha+\beta)}\left(\frac{\pi}{\alpha+\beta}\right)^{d+1/2}e^{-\alpha\beta/\alpha+\beta(\mathbf{P}^2+\epsilon^2)}. \tag{3.14}$$

Therefore,

$$\frac{1}{\lambda_R^{\mathbf{P}}}-\frac{1}{\lambda_R^0}=\frac{1}{(2\pi)^{d+1}}\int_0^\infty d\alpha\int_0^\infty d\beta e^{-\mu^2(\alpha+\beta)}\left(\frac{\pi}{\alpha+\beta}\right)^{d+1/2}(e^{-\alpha\beta/\alpha+\beta\,\mathbf{P}^2}-1)<0. \tag{3.15}$$

The requirement $(M_{\mathbf{P}})^{-2}\geqslant 0$ is a corollary of the condition $\lambda_R^{\mathbf{P}}<0$. Inequality (3.15) implies that it is sufficient to require $\lambda_R<0$. This is a well known condition of absence of tachyons[16–19] in the large-N theory. Thus, we have constructed the Hamiltonian.

Another way to define the Hamiltonian is the following.[15] One can use the theory of self-adjoint extensions.[20] Consider the operator $\Omega_{\mathbf{P}\mathbf{s}}^2$ defined on the domain consisting of such φ that

$$\int d\mathbf{s}\varphi_{\mathbf{s}}\sqrt{\frac{2\Omega_{\mathbf{Ps}}}{2\omega_{\mathbf{P}/2+\mathbf{s}}2\omega_{\mathbf{P}/2-\mathbf{s}}}}=0.$$

If $d+1\geqslant 6$, the operator is essentially self-adjoint. This corresponds to the ''triviality'' (or non-renormalizability) of the model. If $d+1<6$, there is a one-parametric family of self-adjoint extensions specified by the parameter $\lambda_R^{\mathbf{P}}$. However, the condition (3.12) can not be obtained by the self-adjoint extension method. One should use another argumentation like Poincare invariance.

C. Momentum and angular momentum

Let us express the momentum and angular momentum operators via new creation and annihilation operators $C_{\mathbf{Ps}}^{\pm}$. It follows from Eqs. (3.1) that operators (2.47) can be written as

$$P^l=\int d\mathbf{P}d\mathbf{s}Q_{\mathbf{Ps}}P^l i\Pi_{-\mathbf{Ps}},$$
$$M^{ml}=\int d\mathbf{P}d\mathbf{s}Q_{\mathbf{Ps}}\left(iP^l\frac{\partial}{\partial P^m}+is^l\frac{\partial}{\partial s^m}-iP^m\frac{\partial}{\partial P^l}-is^m\frac{\partial}{\partial s^l}\right)i\Pi_{-\mathbf{Ps}}. \tag{3.16}$$

Since the kernel of the operator $M_{\mathbf{P}}^{-2}$ (3.10) is invariant under spatial rotations

$$\mathbf{P}\to O\mathbf{P},\quad \mathbf{s}\to O\mathbf{s},\quad \mathbf{s}'\to O\mathbf{s}',$$

with orthogonal matrix O, it commutes with the rotation operator of the form $Of_{\mathbf{Ps}}=f_{O\mathbf{P},O\mathbf{s}}$. Analogously, any function of M obey this property. Since the operator

$$iP^l\frac{\partial}{\partial P^m}+is^l\frac{\partial}{\partial s^m}-iP^m\frac{\partial}{\partial P^l}-is^m\frac{\partial}{\partial s^l},$$

is a generator of a rotation, it commutes with any function of M. Making use of this property, we find

$$M^{ml}=\int d\mathbf{P}d\mathbf{s}C_{\mathbf{Ps}}^{+}\left(iP^l\frac{\partial}{\partial P^m}+is^l\frac{\partial}{\partial s^m}-iP^m\frac{\partial}{\partial P^l}-is^m\frac{\partial}{\partial s^l}\right)C_{\mathbf{Ps}}^{-}.$$

Analogously,

$$P^l=\int d\mathbf{P}d\mathbf{s}C_{\mathbf{Ps}}^{+}P^l C_{\mathbf{Ps}}^{-}.$$

D. Representation for space–time translations and space rotations

The problem of divergences made us change the representation for the operators $A_{\mathbf{k}_1\mathbf{k}_2}^{\pm(2)}$. We have considered the space $\mathcal{H}_2\subset L^2(\mathbf{R}^{2d})$ of functions $f_{\mathbf{Ps}}$ which obey the property $f_{\mathbf{P},-\mathbf{s}}=f_{\mathbf{P},\mathbf{s}}$. The space $\mathcal{F}(\mathcal{H}_2)$ has been considered instead of $\mathcal{F}(\mathcal{H}^{\vee 2})$. Therefore, the space (3.44) is substituted by $\mathcal{F}(\mathcal{H}_2)\otimes\check{\mathcal{F}}$. One should define then operators H, P^l, M^{ml}, M^{m0}, and $U_{\Lambda,a}$ in $\mathcal{F}(\mathcal{H}_2)$ that corresponds to formal expressions (2.47). The operators H, P^l, M^{ml} have just been considered.

Let λ_R^0 be a fixed negative quantity. Set $\mathbf{P}_2=0$, $\mathbf{P}_1=\mathbf{P}$ in Eq. (3.12) and define the quantity $\lambda_R^{\mathbf{P}}$. Consider the operator $M^{-2}:\mathcal{H}_2\to\mathcal{H}_2$ of the form

$$(M^{-2}\psi)_{\mathbf{Ps}}=\Omega_{\mathbf{Ps}}^{-2}\psi_{\mathbf{Ps}}-\frac{\lambda_R^{\mathbf{P}}}{(2\pi)^d}\chi_{\mathbf{Ps}}\int d\mathbf{s}'\chi_{\mathbf{Ps}'}\psi_{\mathbf{Ps}'},$$

where $\chi_{\mathbf{Ps}}$ has the form (3.11). Since the operator M^{-2} is positively definite and self-adjoint, the self-adjoint positive operator $M \equiv (M^{-2})^{-1/2}$ is uniquely defined. The Hamiltonian operator is

$$H = \mathcal{F}(M),$$

(the notations from Appendix A are used), while

$$e^{-iHt} = \mathcal{U}(e^{-iMt}).$$

Analogously,

$$P^l = \mathcal{F}(P^l),$$

$$M^{ml} = \mathcal{F}\left(iP^l \frac{\partial}{\partial P^m} + is^l \frac{\partial}{\partial s^m} - iP^m \frac{\partial}{\partial P^l} - is^m \frac{\partial}{\partial s^l} \right).$$

The space rotations being Lorentz transformations with

$$\Lambda_i^0 = 0, \quad \Lambda_0^i = 0, \quad \Lambda_0^0 = 1, \tag{3.17}$$

are represented by the operators $U_{\Lambda,0} = \mathcal{U}(u_{\Lambda,0})$ with

$$(u_{\Lambda,0} f)_{\mathbf{Ps}} = f_{\Lambda^{-1}\mathbf{P}, \Lambda^{-1}\mathbf{s}}. \tag{3.18}$$

For space–time translations, one has

$$U_{1,a} = e^{iHt} e^{-iP^l a^l} = \mathcal{U}(e^{iMt} e^{-i\mathbf{Pa}}). \tag{3.19}$$

Thus, we have constructed the operators $U_{\Lambda,a}$ corresponding to the Poincare transformations obeying Eq. (3.17): $U_{\Lambda,a} = U_{0,a} U_{\Lambda,0}$.

Lemma 3.1: The group property

$$U_{\Lambda_1,a_1} U_{\Lambda_2,a_2} = U_{\Lambda_1\Lambda_2, a_1 + \Lambda_1 a_2}$$

is satisfied for Poincare transformations obeying Eq. (3.17).

Proof: It is sufficient to show that

$$U_{\Lambda_1\Lambda_2,0} = U_{\Lambda_1,0} U_{\Lambda_2,0}, \tag{3.20}$$

$$U_{1,a_1} U_{1,a_2} = U_{1,a_1+a_2}, \tag{3.21}$$

$$U_{\Lambda,0} U_{1,a} U_{\Lambda,0}^{-1} = U_{1,\Lambda a}. \tag{3.22}$$

The property (3.20) is an obvious corollary of the definition (3.18). Relation (3.21) is a corollary of the Stone theorem and the property

$$[e^{iMt}, e^{-i\mathbf{Pa}}] = 0. \tag{3.23}$$

Definition (3.18) and commutation relation

$$[u_{\Lambda,0}, e^{iMt}] = 0, \tag{3.24}$$

imply property (3.22). Lemma 3.1 is proved.

Let us check now some axioms of quantum field theory.

Lemma 3.2: (Existence and uniqueness of a vacuum). *For vector* $\Phi \in \mathcal{F}(\mathcal{H}_2)$, *the following statements are equivalent:*

(i) invariance under space–time translations: for all a

$$U_{0,a}\Phi=\Phi, \quad \text{and}$$

(ii) $\Phi=c|0>$ *for some multiplier* $c\in\mathbf{C}$.

The proof is obvious. We now investigate now spectral properties.

Lemma 3.3: The spectrum of the operator P^μ *is a subset of a set* $\{0\}\cup\{(\epsilon,\mathbf{p})|\epsilon^2-\mathbf{p}^2>0$.

Proof: It is sufficient to prove that $\sigma(M_{\mathbf{p}}^2)\subset(\mathbf{P}^2,\infty)$. The property $\epsilon^2\in\sigma(M_{\mathbf{p}}^2)$ means that the operator $\epsilon^2-M_{\mathbf{p}}^2$ is not boundedly invertible. Since

$$((\epsilon^2-M_{\mathbf{p}}^2)^{-1}\psi)_{\mathbf{s}}=(\epsilon^2-\Omega_{\mathbf{Ps}}^2)^{-1}\psi_{\mathbf{s}}+\frac{(\Omega_{\mathbf{Ps}}^2-\epsilon^2)^{-1}\Omega_{\mathbf{Ps}}^2\chi_{\mathbf{Ps}}\int d\mathbf{s}'\,\chi_{\mathbf{Ps}'}\Omega_{\mathbf{Ps}'}^2(\Omega_{\mathbf{Ps}'}^2-\epsilon^2)^{-1}}{\frac{(2\pi)^d}{\lambda_R^{\mathbf{P}}}-\int d\mathbf{s}\chi_{\mathbf{Ps}}^2\Omega_{\mathbf{Ps}}^4(\Omega_{\mathbf{Ps}}^{-2}-(\Omega_{\mathbf{Ps}}^2-\epsilon^2)^{-1})},$$

$\epsilon^2\in\sigma(M_2)$ if and only if

$$\epsilon=\omega_{\mathbf{P}/2-\mathbf{s}}+\omega_{\mathbf{P}/2+\mathbf{s}}, \tag{3.25}$$

for some $\mathbf{s}$ or

$$\frac{(2\pi)^d}{\lambda_R^{\mathbf{P}}}-\int d\mathbf{s}\chi_{\mathbf{Ps}}^2\Omega_{\mathbf{Ps}}^4(\Omega_{\mathbf{Ps}}^{-2}-(\Omega_{\mathbf{Ps}}^2-\epsilon^2)^{-1})=0. \tag{3.26}$$

Since $\omega_{\mathbf{P}/2+\mathbf{s}}+\omega_{\mathbf{P}/2-\mathbf{s}}\geqslant 2\omega_{\mathbf{P}/2}=\sqrt{\mathbf{P}^2+4\mu^2}>|\mathbf{P}|$, these values of ϵ obey the property $\epsilon^2\in(\mathbf{P}^2$ and $\infty)$. It follows from Eq. (3.14) that Eq. (3.26) can be transformed to the form

$$\frac{1}{(2\pi)^{d+1}}\int_0^\infty d\alpha\int_0^\infty d\beta e^{-\mu^2(\alpha+\beta)}\left(\frac{\pi}{\alpha+\beta}\right)^{d+1/2}(e^{-\alpha\beta/\alpha+\beta(\mathbf{P}^2-\epsilon^2)}-1)=-\frac{1}{\lambda_R^0}. \tag{3.27}$$

Since $\lambda_R^0<0$, the left-hand side of Eq. (3.27) should be positive. This means $\epsilon^2>\mathbf{P}^2$. Lemma is proved.

IV. COMPOSED FIELD OPERATORS

In Sec. III, we have constructed the Hamiltonian of the theory of ''infinite number of fields'' which was shown to be a self-adjoint operator in the Hilbert space. However, it is also necessary to check the property of the Poincare invariance.

To simplify the investigation, it is convenient to introduce an analog of the notion of a field which is very useful in traditional QFT: the Wightman axiomatic approach allows us to reduce the problem of Poincare invariance of the theory to the problem of Poincare invariance of Wightman functions.

However, it is not easy to introduce the field $\varphi^a(x)$ since we have not considered the non-symmetric N-field states yet. However, one can investigate the properties of the ''multifield operators'':

$$\mathcal{W}_{N,k}(x_1,\ldots,x_k)=\frac{1}{N}\sum_{a=1}^{N}\varphi^a(x_1)\ldots\varphi^a(x_k). \tag{4.1}$$

Consider this operator at $x_1^0=\ldots=x_k^0=0$. The results of Sec. II imply that

$$\mathcal{W}_{N,k}(x_1,\ldots,x_k)K_Nf=K_N\tilde{\mathcal{W}}_{N,k}(x_1,\ldots,x_k)f, \tag{4.2}$$

with

$$\tilde{\mathcal{W}}_{N,k}(\mathbf{x}_1,\ldots,\mathbf{x}_k)=\int D\phi|\Phi_0[\phi(\cdot)]|^2\phi(\mathbf{x}_1)\ldots\phi(\mathbf{x}_k)+N^{-1/2}\tilde{W}_k(\mathbf{x}_1,\ldots\mathbf{x}_k)+O(N^{-1}). \tag{4.3}$$

The operator $\tilde{W}_k$ can be presented as

$$\begin{aligned}\tilde{W}_k(\mathbf{x}_1,\ldots,\mathbf{x}_k)&=\int D\phi(\tilde{A}^+[\phi(\cdot)]+\tilde{A}^-[\phi(\cdot)])\phi(\mathbf{x}_1)\ldots\phi(\mathbf{x}_k)\Phi_0[\phi(\cdot)]\\&=\sum_{n=1}^{\infty}\int d\mathbf{p}_1\ldots d\mathbf{p}_n[A^{(n)+}_{\mathbf{p}_1\ldots\mathbf{p}_n}(\Phi^{(n)}_{\mathbf{p}_1\ldots\mathbf{p}_n},\phi(\mathbf{x}_1)\ldots\phi(\mathbf{x}_k)\Phi_0)\\&\quad+A^{(n)-}_{\mathbf{p}_1\ldots\mathbf{p}_n}(\Phi^{(n)}_{\mathbf{p}_1\ldots\mathbf{p}_n},\phi(\mathbf{x}_1)\ldots\phi(\mathbf{x}_k)\Phi_0)^*].\end{aligned} \tag{4.4}$$

One can expect that Heisenberg operator will also obey the relation of the type (4.3):

$$\begin{aligned}\tilde{\mathcal{W}}_{N,k}(x_1,\ldots,x_k)&=(\Phi_0[\phi(\cdot)],\phi(x_1)\ldots\phi(x_k)\Phi_0[\phi(\cdot)])\\&\quad+N^{-1/2}\tilde{W}_k(x_1,\ldots x_k)+O(N^{-1}).\end{aligned} \tag{4.5}$$

Here $\phi(x)$ is a Heisenberg operator of the free field of the mass μ. The property (4.5) is to be checked in Appendix B.

The multifield operators $\tilde{W}_k(x_1,\ldots,x_k)$ being analogs of fields are to be investigated.

A. Multifield operators

In this subsection, we compute the explicit form of the operators $\tilde{W}_k(x_1,\ldots,x_k)$.

The "k-field" (4.1) satisfies the Heisenberg equation

$$\left(\frac{\partial}{\partial x^\mu_A}\frac{\partial}{\partial x_{A\mu}}+m^2+\frac{\lambda}{N}\sum_{b=1}^{N}\varphi^b(x_A)\varphi^b(x_A)\right)\mathcal{W}_{N,k}(x_1,\ldots,x_k)=0.$$

The property (4.2) implies that

$$\left(\frac{\partial}{\partial x^\mu_A}\frac{\partial}{\partial x_{A\mu}}+m^2+\lambda\tilde{\mathcal{W}}_{N,2}(x_A,x_A)\right)\tilde{\mathcal{W}}_{N,k}(x_1,\ldots,x_k)=0.$$

Use now the property (4.5). One can notice that $m^2+\lambda(\Phi_0,\phi(x_A)\phi(x_A)\Phi_0)=\mu^2$. Therefore,

$$\begin{aligned}&\left(\frac{\partial}{\partial x^\mu_A}\frac{\partial}{\partial x_{A\mu}}+\mu^2+\frac{\lambda}{\sqrt{N}}\tilde{W}_2(x_A,x_A)+O(N^{-1})\right)((\Phi_0,\phi(x_1)\ldots\phi(x_k)\Phi_0)\\&\quad+N^{-1/2}\tilde{W}_k(x_1,\ldots,x_k)+O(N^{-1}))=0.\end{aligned} \tag{4.6}$$

The terms of order $O(1)$ give us an equation on the vacuum average value. It has the form

$$\left(\frac{\partial}{\partial x^\mu_A}\frac{\partial}{\partial x_{A\mu}}+\mu^2\right)(\Phi_0,\phi(x_1)\ldots\phi(x_k)\Phi_0)=0.$$

This equation is automatically satisfied. The terms of order $O(N^{1/2})$ lead to the nontrivial equation:

$$\left(\frac{\partial}{\partial x_A^\mu}\frac{\partial}{\partial x_{A\mu}}+\mu^2\right)\tilde{W}_k(x_1,\ldots,x_k)+Q(x_A)(\Phi_0,\phi(x_1)\ldots\phi(x_k)\Phi_0)=0, \tag{4.7}$$

with

$$Q(x_A)=\lambda\tilde{W}_2(x_A,x_A). \tag{4.8}$$

To perform an investigation of Eq. (4.7), it is convenient to introduce the linear combinations of the multifields $\tilde{W}_k$. It follows from the Wick theorem that the operators (4.4) can be presented as

$$\tilde{W}_k(\mathbf{x}_1,\ldots,\mathbf{x}_k)=\sum\ (\Phi_0,\phi(\mathbf{x}_{l_1^1})\phi(\mathbf{x}_{l_1^2})\Phi_0)\ldots(\Phi_0,\phi(\mathbf{x}_{l_\nu^1})\phi(\mathbf{x}_{l_\nu^2})\Phi_0)\hat{W}_{k-2\nu}(\mathbf{x}_{m_1},\ldots,\mathbf{x}_{m_{k-2\nu}}). \tag{4.9}$$

Here, the summation is performed over all decompositions of the set

$$\{1,2,\ldots,k\}=\{l_1^1,l_1^2\}\cup\ldots\cup\{l_\nu^1,l_\nu^2\}\cup\{m_1,\ldots,m_{k-2\nu}\},$$

while

$$l_1^1<l_1^2,\quad l_\nu^1<l_\nu^2,\quad m_1<\ldots<m_{k-2\nu},\quad k-2\nu>0.$$

The operator $\hat{W}_s(\mathbf{x}_1,\ldots,\mathbf{x}_s)$ entering to the formula (5.9) has the form

$$\hat{W}_s(\mathbf{x}_1,\ldots,\mathbf{x}_s)=\int d\mathbf{p}_1\ldots d\mathbf{p}_s[A^{(s)+}_{\mathbf{p}_1\ldots\mathbf{p}_s}(\Phi^{(s)}_{\mathbf{p}_1\ldots\mathbf{p}_s},:\phi(\mathbf{x}_1)\ldots\phi(\mathbf{x}_s):\Phi_0) + A^{(s)-}_{\mathbf{p}_1\ldots\mathbf{p}_s}(\Phi^{(s)}_{\mathbf{p}_1\ldots\mathbf{p}_s},:\phi(\mathbf{x}_1)\ldots\phi(\mathbf{x}_s):\Phi_0)^*]. \tag{4.10}$$

The notation :: is used for the Wick ordering of combinations of fields

$$\phi(\mathbf{x})=\frac{1}{(2\pi)^{d/2}}\int\frac{d\mathbf{k}}{\sqrt{2\omega_\mathbf{k}}}[a^+_\mathbf{k}e^{-i\mathbf{kx}}+a^-_\mathbf{k}e^{i\mathbf{kx}}].$$

Analogously, we define the Heisenberg operators $\hat{W}_s(x_1,\ldots,x_s)$ from the recursive relations

$$\tilde{W}_k(x_1,\ldots,x_k)=\sum\ (\Phi_0,\phi(x_{l_1^1})\phi(x_{l_1^2})\Phi_0)\ldots(\Phi_0,\phi(x_{l_\nu^1})\phi(x_{l_\nu^2})\Phi_0)\hat{W}_{k-2\nu}(x_{m_1},\ldots,x_{m_{k-2\nu}}). \tag{4.11}$$

Applying the Wick theorem to the combinations of the field and momenta operators

$$\pi(\mathbf{x})=\frac{1}{i}\frac{\delta}{\delta\phi(\mathbf{x})}=\frac{1}{(2\pi)^{d/2}}\int\frac{d\mathbf{k}}{\sqrt{2}}i\sqrt{\omega_\mathbf{k}}[a^+_\mathbf{k}e^{-i\mathbf{kx}}+a^-_\mathbf{k}e^{i\mathbf{kx}}],$$

we obtain in an analogous way that

$$\frac{\partial}{\partial x^0_{i_1}}\ldots\frac{\partial}{\partial x^0_{i_l}}\hat{W}_s(x_1,\ldots,x_s)$$

$$=\int d\mathbf{p}_1\ldots d\mathbf{p}_s[A^{(s)+}_{\mathbf{p}_1\ldots\mathbf{p}_s}(\Phi^{(s)}_{\mathbf{p}_1\ldots\mathbf{p}_s},:\phi(\mathbf{x}_1)\ldots\pi_{i_1}(\mathbf{x}_{i_1})\ldots\pi_{i_l}(\mathbf{x}_{i_1})\ldots\phi(\mathbf{x}_s):\Phi_0)$$

$$+A^{(s)-}_{\mathbf{p}_1\ldots\mathbf{p}_s}(\Phi^{(s)}_{\mathbf{p}_1\ldots\mathbf{p}_s},:\phi(\mathbf{x}_1)\ldots\pi_{i_1}(\mathbf{x}_{i_1})\ldots\pi_{i_l}(\mathbf{x}_{i_1})\phi(\mathbf{x}_s):\Phi_0)^*], \tag{4.12}$$

for $i_1<\ldots<i_l$, $x^0_1=\ldots=x^0_s=0$.

Let us find an equation on the operator $\hat{W}_s$. For $k=2$ and $\tilde{W}_2=\hat{W}_2$, so that

$$\left(\frac{\partial}{\partial x^\mu_A}\frac{\partial}{\partial x_{A\mu}}+\mu^2\right)\hat{W}_2(x_1,x_2)+Q(x_A)(\Phi_0,\phi(x_1)\phi(x_2)\Phi_0)=0. \tag{4.13}$$

For odd values of k, one has $(\Phi_0,\phi(x_1)\ldots\phi(x_k)\Phi_0)=0$, so that

$$\left(\frac{\partial}{\partial x^\mu_A}\frac{\partial}{\partial x_{A\mu}}+\mu^2\right)\tilde{W}_k(x_1,\ldots,x_k)=0.$$

It follows from the recursive relations that

$$\left(\frac{\partial}{\partial x^\mu_A}\frac{\partial}{\partial x_{A\mu}}+\mu^2\right)\hat{W}_k(x_1,\ldots,x_k)=0. \tag{4.14}$$

Let us show that Eq. (4.14) is also satisfied for even values of $k\neq 2$. For definiteness, consider the case $A=1$. The general case can be investigated analogously. The quantity

$$\left(\frac{\partial}{\partial x^\mu_1}\frac{\partial}{\partial x_{1\mu}}+\mu^2\right)\tilde{W}_k(x_1,\ldots,x_k),$$

entering to the left-hand side of Eq. (4.7) can be decomposed into two parts. One of them ecorresponds to the case $k-2\nu=2$, another to $k-2\mu>2$. The first part is

$$\left(\frac{\partial}{\partial x^\mu_1}\frac{\partial}{\partial x_{1\mu}}+\mu^2\right)\sum(\Phi_0,\phi(x_{l^1_1})\phi(x_{l^2_1})\Phi_0)\ldots(\Phi_0,\phi(x_{l^1_\nu})\phi(x_{l^2_\nu})\Phi_0)\hat{W}_2(x_1,x_{m_2})$$

$$=-Q(x_1)\sum(\Phi_0,\phi(x_1)\phi(x_{m_2})\Phi_0)(\Phi_0,\phi(x_{l^1_1})\phi(x_{l^2_1})\Phi_0)\ldots(\Phi_0,\phi(x_{l^1_\nu})\phi(x_{l^2_\nu})\Phi_0)$$

$$=-Q(x_1)(\Phi_0,\phi(x_1)\ldots\phi(x_k)\Phi_0). \tag{4.15}$$

The second part reads

$$\left(\frac{\partial}{\partial x^\mu_1}\frac{\partial}{\partial x_{1\mu}}+\mu^2\right)$$

$$\times\sum_{k-2\nu>2}(\Phi_0,\phi(x_{l^1_1})\phi(x_{l^2_1})\Phi_0)\ldots(\Phi_0,\phi(x_{l^1_\nu})\phi(x_{l^2_\nu})\Phi_0)\hat{W}_{k-2\nu}(x_{m_1},\ldots,x_{m_{k-2\nu}}). \tag{4.16}$$

It follows from Eq. (4.7) then that the quantity (4.16) should vanish. We obtain by induction that the functions $\hat{W}_4$, $\hat{W}_6$, etc. obey Eq. (4.14).

To find an explicit form of $\hat{W}_k$, prove the following proposition.

Proposition 4.1: Let

$$\left(\frac{\partial}{\partial x_A^\mu}\frac{\partial}{\partial x_{A\mu}}+\mu^2\right)f_k(x_1,\ldots,x_k)=0, \quad A=\overline{1,k} \tag{4.17}$$

and

$$\frac{\partial}{\partial x_{i_1}^0}\ldots\frac{\partial}{\partial x_{i_l}^0}f_k(x_1,\ldots,x_k)=0, \quad i_1<\ldots<i_l, \quad x_1^0=\ldots=x_k^0=0.$$

Then $f_k=0$.

Proof: Consider the spatial Fourier transformation $\tilde{f}_k(\mathbf{p}_1,t_1;\ldots;\mathbf{p}_k,$ and $t_k)$ of the function f_k. It obeys the set of equations

$$\left(\frac{\partial}{\partial t_A}\frac{\partial}{\partial t_A}+\omega_{\mathbf{p}_A^2}\right)\tilde{f}_k(\mathbf{p}_1,t_1;\ldots;\mathbf{p}_k,t_k)=0, \quad A=\overline{1,k},$$

with $\omega_{\mathbf{p}}=\sqrt{\mathbf{p}^2+\mu^2}$. This implies that

$$\tilde{f}_k(\mathbf{p}_1,t_1;\ldots;\mathbf{p}_k,t_k)=\sum_{\sigma_1,\ldots,\sigma_k\in\{-1,1\}}\alpha_{\sigma_1\ldots\sigma_k}(\mathbf{p}_1,\ldots,\mathbf{p}_k)e^{i\sigma_1\omega_{\mathbf{p}_1}t_1+\ldots+i\sigma_k\omega_{\mathbf{p}_k}t_k}.$$

One can express the coefficients α as

$$\alpha_{\sigma_1\ldots\sigma_k}(\mathbf{p}_1,\ldots,\mathbf{p}_k)=\left(\frac{1}{2}-\frac{i\sigma_1}{2\omega_{\mathbf{p}_1}}\right)\ldots\left(\frac{1}{2}-\frac{i\sigma_k}{2\omega_{\mathbf{p}_k}}\right)\tilde{f}_k(\mathbf{p}_1,t_1,\ldots,\mathbf{p}_k,t_k).$$

Therefore, $\alpha_{\sigma_1\ldots\sigma_k}(\mathbf{p}_1,\ldots,\mathbf{p}_k)=0$. This implies $f_k=0$. Proposition is proved.

Denote

$$\begin{aligned}\hat{W}_s^0(x_1,..,x_s)=\int d\mathbf{p}_1\ldots d\mathbf{p}_s[&A^{(s)+}_{\mathbf{p}_1\ldots\mathbf{p}_s}(\Phi^{(s)}_{\mathbf{p}_1\ldots\mathbf{p}_s},:\phi(x_1)\ldots\phi(x_s):\Phi_0)\\&+A^{(s)-}_{\mathbf{p}_1\ldots\mathbf{p}_s}(\Phi^{(s)}_{\mathbf{p}_1\ldots\mathbf{p}_s},:\phi(x_1)\ldots\phi(x_s):\Phi_0)^*].\end{aligned} \tag{4.18}$$

Consider the operator distribution $f_s=\hat{W}_s-\hat{W}_s^0$ obeying the condition of proposition 4.1. This implies $f_k=0$, so that $\hat{W}_s=\hat{W}_s^0$. The explicit form of the operator $\hat{W}_s$ is

$$\begin{aligned}&\hat{W}_s(\mathbf{x}_1,t_1,\ldots,\mathbf{x}_s,t_s)\\&=\frac{1}{(2\pi)^{sd/2}}\int\frac{d\mathbf{p}_1}{\sqrt{2\omega_{\mathbf{p}_1}}}\ldots\frac{d\mathbf{p}_s}{\sqrt{2\omega_{\mathbf{p}_s}}}\sqrt{k!}(A^{+(s)}_{\mathbf{p}_1\ldots\mathbf{p}_s}e^{i\omega_{\mathbf{p}_1}t_1+\ldots+i\omega_{\mathbf{p}_s}t_s-i\mathbf{p}_1\mathbf{x}_1-\ldots-i\mathbf{p}_s\mathbf{x}_s}\\&+A^{-(s)}_{\mathbf{p}_1\ldots\mathbf{p}_s}e^{-i\omega_{\mathbf{p}_1}t_1-\ldots-i\omega_{\mathbf{p}_s}t_s+i\mathbf{p}_1\mathbf{x}_1+\ldots+i\mathbf{p}_s\mathbf{x}_s}).\end{aligned} \tag{4.19}$$

Let $f\in\mathcal{S}(\mathbf{R}^{ds})$. Consider the operators

$$\hat{W}_s[f]=\int dx_1\ldots dx_s\hat{W}_s(x_1,\ldots,x_s)f(x_1,\ldots,x_s).$$

They are defined on the set $\check{D}$ of all finite vectors of $\check{\mathcal{F}}$. The set $\check{D}$ is invariant under the operator $\hat{W}_s[f]$.

Proposition 4.2: (1) $\hat{W}_s(x_1,\ldots,x_s)$ $(s\neq 2)$ *is an operator distribution. (2) The set*

$$\hat{W}_{s_1}[f_1]\ldots\hat{W}_{s_k}[f_k]|0>, \quad f_j\in\mathcal{S}(\mathbf{R}^{dj})$$

is a total set in $\check{\mathcal{F}}$. *The first statement is obvious. The second statement is a corollary of lemma A14.*

Thus, we see that the k-field $3\tilde{W}_k$ has the form (4.11), the operators $\hat{W}_s$ having the form (4.18) are already found. The remaining problem is to find the explicit form of the bifield $\hat{W}_2(x_1,$ and $x_2)$. Since an equation for the bifield contains the operator $Q(x)$ being an analog of the composed $\lambda\varphi^a\varphi^a$ field, let us investigate first its properties.

B. The $\lambda\varphi^a\varphi^a$ composed field

The operator $Q(x)=Q(\mathbf{x},t)$ can be presented as

$$\begin{aligned}Q(\mathbf{x},t)&=e^{iHt}\lambda\hat{W}_2(\mathbf{x},0,\mathbf{x},0)e^{-iHt}\\&=\lambda\frac{\sqrt{2}}{(2\pi)^d}\int\frac{d\mathbf{k}_1}{\sqrt{2\omega_{\mathbf{k}_1}}}\frac{d\mathbf{k}_2}{\sqrt{2\omega_{\mathbf{k}_2}}}(A^+_{\mathbf{k}_1\mathbf{k}_2}(t)e^{-i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{x}}+A^-_{\mathbf{k}_1\mathbf{k}_2}(t)e^{i(\mathbf{k}_1+\mathbf{k}_2)\mathbf{x}}),\end{aligned}\tag{4.20}$$

where

$$A^{\pm}_{\mathbf{k}_1\mathbf{k}_2}(t)=e^{iHt}A^{\pm(2)}_{\mathbf{k}_1\mathbf{k}_2}e^{-iHt}.$$

After transformations (3.1) and (3.5), expression (4.20) takes the form

$$\begin{aligned}Q(\mathbf{x},t)&=\lambda\frac{\sqrt{2}}{(2\pi)^d}\int d\mathbf{P}d\mathbf{s}\sqrt{\frac{2\Omega_{\mathbf{Ps}}}{2\omega_{\mathbf{P}/2+\mathbf{s}}2\omega_{\mathbf{P}/2-\mathbf{s}}}}e^{-i\mathbf{Px}}Q_{\mathbf{Ps}}(t)\\&=\int d\mathbf{P}d\mathbf{s}(C^+_{\mathbf{Ps}}\gamma_{\mathbf{Ps}}(\mathbf{x},t)+C^-_{\mathbf{Ps}}\gamma^*_{\mathbf{Ps}}(\mathbf{x},t))\\&=C^+[\gamma(\mathbf{x},t)]+C^-[\gamma(\mathbf{x},t)],\end{aligned}$$

where

$$\gamma(\mathbf{x},t)=\frac{\sqrt{2}}{(2\pi)^d}e^{-i\mathbf{Px}}\frac{1}{\sqrt{2M}}e^{iMt}\lambda\Omega\chi.\tag{4.21}$$

Our purpose is to prove that $Q(x)$ is an operator distribution. Therefore, we should show that $(\chi(\mathbf{x},t))_{\mathbf{Ps}}$ can be viewed as a vector distribution. However, an infinite quantity λ^{-1} and function $\Omega^2\chi\notin L^2$ enter to Eq. (4.21). It is remarkable that these divergences can be eliminated: one can use the property:

$$M^{-2}\lambda\Omega^2\chi=\lambda_R\chi.$$

Here λ_R is an operator of multiplication by $\lambda^{\mathbf{P}}_R$. Thus, the vector function (4.21) can be written as

$$\gamma(\mathbf{x},t)=(2\pi)^{-d}e^{-i\mathbf{Px}}e^{iMt}M^{3/2}\lambda_R\chi.\tag{4.22}$$

One can present it as

$$\gamma(\mathbf{x},t)=(2\pi)^{-d}(-\Delta+1)^{m}\left(-\frac{\partial^2}{\partial t^2}\right)e^{-i\mathbf{P}\mathbf{x}}e^{iMt}M^{-1/2}(\mathbf{P}^2+1)^{-m}\lambda_R\chi.$$

Since $M^{-1/2}(\mathbf{P}^2+1)^{-m}\lambda_R\chi\in\mathcal{H}_2$ for sufficiently large m, the function $e^{-i\mathbf{P}\mathbf{x}}e^{iMt}M^{-1/2}(\mathbf{P}^2+1)^{-m}\lambda_R\chi$ is a bounded continuous vector function, we obtain from lemmas A.12 and A.13 that γ is a vector distribution. Lemma A.14 implies that $Q(\mathbf{x},t)$ is an operator distribution.

C. Canonical variables as operator distributions

The purpose of this subsection is to investigate the properties of the operators $Q_{\mathbf{Ps}}$ and $\Pi_{\mathbf{Ps}}$. These properties will be essentially used.

First of all, notice that

$$Q_{\mathbf{Ps}}=C^{+}[\xi_{\mathbf{Ps}}]+C^{-}[\xi_{-\mathbf{Ps}}],\quad \Pi_{\mathbf{Ps}}=C^{+}[\pi_{\mathbf{Ps}}]+C^{-}[\pi_{-\mathbf{Ps}}],$$

where $\xi_{\mathbf{Ps}}$ and $\pi_{\mathbf{Ps}}$ have the form

$$(\xi_{\mathbf{Ps}})_{\mathbf{P}'\mathbf{s}'}=\delta_{\mathbf{P}\mathbf{P}'}((2M_{\mathbf{P}}^{-1/2})_{\mathbf{s}\mathbf{s}'},\quad (\pi_{\mathbf{Ps}})_{\mathbf{P}'\mathbf{s}'}=i\delta_{\mathbf{P}\mathbf{P}'}((M_{\mathbf{P}}/2)^{-1/2})_{\mathbf{s}\mathbf{s}'}.$$

Consider the integrals

$$\int d\mathbf{P}d\mathbf{s}\varphi_{\mathbf{Ps}}\xi_{\mathbf{Ps}}=(2M)^{-1/2}\overline{\varphi},\tag{4.23}$$

$$\int d\mathbf{P}d\mathbf{s}\varphi_{\mathbf{Ps}}\pi_{\mathbf{Ps}}=i(M/2)^{1/2}\overline{\varphi},\tag{4.24}$$

where $\varphi_{\mathbf{Ps}}$ are complex functions from $\mathcal{S}(\mathbf{R}^{2d})$,

$$\overline{\varphi}_{\mathbf{Ps}}=\tfrac{1}{2}(\varphi_{\mathbf{Ps}}+\varphi_{\mathbf{P},-\mathbf{s}}).\tag{4.25}$$

Since $(2M)^{-1/2}$ is a bounded operator, the integral (4.23) is always defined. However, $(M/2)^{1/2}$ is not a bounded operator, so that quantity (4.24) may be not defined. We see that the expression for $\xi_{\mathbf{Ps}}$ defines a vector distribution, while $\pi_{\mathbf{Ps}}$ is not a vector distribution.

To consider objects like $\pi_{\mathbf{Ps}}$ as vector distributions, it is necessary to perform the renormalization procedure. Let

$$Q_{\mathbf{P}}(t)=\frac{1}{(2\pi)^d}\int d\mathbf{x}e^{i\mathbf{P}\mathbf{x}}Q(\mathbf{x},t)=-\ddot{R}_{\mathbf{P}}(t),$$

$$R_{\mathbf{P}}(t)=\frac{1}{(2\pi)^d}\int d\mathbf{x}e^{i\mathbf{P}\mathbf{x}}R(\mathbf{x},t)=C^{+}[r_{\mathbf{P}}(t)]+C^{-}[r_{-\mathbf{P}}(t)],$$

where

$$(r_{\mathbf{P}}(t))_{\mathbf{P}'\mathbf{s}'}=(2\pi)^{-d}\delta_{\mathbf{P}\mathbf{P}'}(e^{iMt}M^{-1/2}\lambda_R\chi)_{\mathbf{P}'\mathbf{s}'}$$

is a vector distribution.

Denote

$$\pi_{\mathbf{Ps}}^{ren}=\pi_{\mathbf{Ps}}-\frac{1}{\sqrt{2}}\Omega_{\mathbf{Ps}}^2\chi_{\mathbf{Ps}}\dot{r}_{\mathbf{P}}(0),\tag{4.26}$$

where $\chi_{\mathbf{Ps}}$ has the form (3.11). One has

$$\int d\mathbf{P}ds\pi^{ren}_{\mathbf{Ps}}\varphi_{\mathbf{Ps}}=i(M/2)^{1/2}\left[\overline{\varphi}-\frac{\lambda^R}{(2\pi)^d}\chi\int ds'\,\overline{\varphi}_{\mathbf{Ps}'}\Omega^2_{\mathbf{Ps}'}\chi_{\mathbf{Ps}'}\right]=i(M/2)^{1/2}M^{-2}\Omega^2\overline{\varphi}.$$

Since $\Omega^2\overline{\varphi}\in L^2$, while $M^{-3/2}$ is a bounded operator, $\pi^{ren}_{\mathbf{Ps}}$ is a vector distribution. We obtain from lemma A.14 the following proposition.

Proposition 4.5: $Q_{\mathbf{Ps}}$ and

$$\Pi^{ren}_{\mathbf{Ps}}=\Pi_{\mathbf{Ps}}-\frac{1}{\sqrt{2}}\Omega^2_{\mathbf{Ps}}\chi_{\mathbf{Ps}}\dot{R}_{\mathbf{P}}(0) \tag{4.27}$$

are operator distributions.

Investigate now the transformation properties of these distributions. Analogously to the previous subsection, we obtain

Proposition 4.6: For spatial rotations, the following properties are satisfied:

$$u_{\Lambda,0}\xi_{\mathbf{P},\mathbf{s}}=\xi_{\Lambda\mathbf{P},\Lambda\mathbf{s}},\quad u_{\Lambda,0}\pi^{ren}_{\mathbf{P},\mathbf{s}}=\pi^{ren}_{\Lambda\mathbf{P},\Lambda\mathbf{s}},\quad u_{\Lambda,0}r_{\mathbf{P}}(t)=r_{\Lambda\mathbf{P}}(t).$$

Corollary: Under conditions (3.17), the operators $Q_{\mathbf{Ps}}$, $\Pi^{ren}_{\mathbf{Ps}}$ obey the following transformation properties

$$U_{\Lambda,0}Q_{\mathbf{Ps}}U^{-1}_{\Lambda,0}=Q_{\Lambda\mathbf{P},\Lambda\mathbf{s}},\quad U_{\Lambda,0}\Pi^{ren}_{\mathbf{Ps}}U^{-1}_{\Lambda,0}=\Pi^{ren}_{\Lambda\mathbf{P},\Lambda\mathbf{s}},\quad U_{\Lambda,0}R_{\mathbf{P}}(t)U^{-1}_{\Lambda,0}=R_{\Lambda\mathbf{P}}(t),$$

$$U_{1,\mathbf{a}}Q_{\mathbf{Ps}}U^{-1}_{1,\mathbf{a}}=e^{-i\mathbf{Pa}}Q_{\mathbf{P},\mathbf{s}},\quad U_{1,\mathbf{a}}\Pi^{ren}_{\mathbf{Ps}}U^{-1}_{1,\mathbf{a}}=e^{-i\mathbf{Pa}}\Pi^{ren}_{\mathbf{P},\mathbf{s}},\quad U_{1,a}R_{\mathbf{P}}(t)U^{-1}_{1,a}=R_{\mathbf{P}}(t+a_0). \tag{4.28}$$

D. The bifield operator

In this section, we construct the bifield operator $\hat{W}_2(x_1, x_2)$ which obey Eq. (4.13) and initial conditions (4.12). We show it to be an operator distribution of $\mathbf{x}_1$ and $\mathbf{x}_2$ at fixed values of x^0_1, x^0_2. It can be also viewed as an operator distribution of x_1, and x_2.

First of all, consider the spatial Fourier transformation

$$\hat{W}_2(\mathbf{x},t_x;\mathbf{y},t_y)=\frac{1}{(2\pi)^d}\int d\mathbf{k}d\mathbf{p}w_2(\mathbf{k},t_x;\mathbf{p},t_y)e^{-i\mathbf{kx}-i\mathbf{py}}.$$

Initial conditions (4.12) can be presented in the following form

$$\begin{aligned}
w_2(\mathbf{k},0;\mathbf{p},0)&=\sqrt{\frac{\omega_{\mathbf{k}}+\omega_{\mathbf{p}}}{\omega_{\mathbf{k}}\omega_{\mathbf{p}}}}Q_{\mathbf{k}+\mathbf{p},\mathbf{k}-\mathbf{p}/2},\\
\frac{\partial}{\partial t_x}w_2(\mathbf{k},0;\mathbf{p},0)&=\sqrt{\frac{\omega_{\mathbf{k}}(\omega_{\mathbf{k}}+\omega_{\mathbf{p}})}{\omega_{\mathbf{p}}}}\Pi_{\mathbf{k}+\mathbf{p},\mathbf{k}-\mathbf{p}/2},\\
\frac{\partial}{\partial t_y}w_2(\mathbf{k},0;\mathbf{p},0)&=\sqrt{\frac{\omega_{\mathbf{p}}(\omega_{\mathbf{k}}+\omega_{\mathbf{p}})}{\omega_{\mathbf{k}}}}\Pi_{\mathbf{k}+\mathbf{p},\mathbf{k}-\mathbf{p}/2},\\
\frac{\partial}{\partial t_x}\frac{\partial}{\partial t_y}w_2(\mathbf{k},0;\mathbf{p},0)&=\sqrt{(\omega_{\mathbf{p}}(\omega_{\mathbf{k}}+\omega_{\mathbf{p}}))\omega_{\mathbf{k}}}Q_{\mathbf{k}+\mathbf{p},\mathbf{k}-\mathbf{p}/2}.
\end{aligned} \tag{4.29}$$

Eqs.(4.13) can be written as

$$\left(\frac{\partial^2}{\partial t_x \partial t_x}+\omega_{\mathbf{k}}^2\right) w_2(\mathbf{k},t_x;\mathbf{p},t_y)+\frac{1}{2\omega_{\mathbf{p}}} e^{-i\omega_{\mathbf{p}}(t_x-t_y)} Q_{\mathbf{k}+\mathbf{p}}(t_x)=0.$$
$$\left(\frac{\partial^2}{\partial t_y \partial t_y}+\omega_{\mathbf{p}}^2\right) w_2(\mathbf{k},t_x;\mathbf{p},t_y)+\frac{1}{2\omega_{\mathbf{k}}} e^{-i\omega_{\mathbf{k}}(t_x-t_y)} Q_{\mathbf{k}+\mathbf{p}}(t_y)=0. \tag{4.30}$$

These equations and initial conditions lead to the following formal solution

$$\begin{aligned} w_2(\mathbf{k},t_x;\mathbf{p},t_y)=&\sqrt{\frac{\omega_{\mathbf{k}}+\omega_{\mathbf{p}}}{\omega_{\mathbf{k}}\omega_{\mathbf{p}}}}\, Q_{\mathbf{k}+\mathbf{p},\mathbf{k}-\mathbf{p}/2}\cos(\omega_{\mathbf{k}}t_x+\omega_{\mathbf{p}}t_y)\\ &+\frac{1}{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{p}}(\omega_{\mathbf{k}}+\omega_{\mathbf{p}})}}\,\Pi_{\mathbf{k}+\mathbf{p},\mathbf{k}-\mathbf{p}/2}\sin(\omega_{\mathbf{k}}t_x+\omega_{\mathbf{p}}t_y)\\ &-\int_0^{t_x} d\tau \frac{\sin(\omega_{\mathbf{k}}(t_x-\tau))}{\omega_{\mathbf{k}}}\,\frac{1}{2\omega_{\mathbf{p}}} e^{-i\omega_{\mathbf{p}}(\tau-t_y)} Q_{\mathbf{k}+\mathbf{p}}(\tau)\\ &-\int_0^{t_y} d\tau \frac{\sin(\omega_{\mathbf{p}}(t_y-\tau))}{\omega_{\mathbf{p}}}\,\frac{1}{2\omega_{\mathbf{k}}} e^{-i\omega_{\mathbf{k}}(t_x-\tau)} Q_{\mathbf{k}+\mathbf{p}}(\tau). \end{aligned} \tag{4.31}$$

This form is not suitable for investigation since $\Pi_{\mathbf{Ps}}$ has been discovered not to be a distribution, while $Q_{\mathbf{ps}}$ is a distribution rather that ordinary function. However, we can use the relation $Q=-\ddot{R}$ and integrate by parts. We obtain:

$$\begin{aligned} w_2(\mathbf{k},t_x;\mathbf{p},t_y)=&\sqrt{\frac{\omega_{\mathbf{k}}+\omega_{\mathbf{p}}}{\omega_{\mathbf{k}}\omega_{\mathbf{p}}}} Q_{\mathbf{k}+\mathbf{p},\mathbf{k}-\mathbf{p}/2}\cos(\omega_{\mathbf{k}}t_x+\omega_{\mathbf{p}}t_y)+\frac{1}{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{p}}(\omega_{\mathbf{k}}+\omega_{\mathbf{p}})}}\,\Pi^{ren}_{\mathbf{k}+\mathbf{p},\mathbf{k}-\mathbf{p}/2}\\ &\times\sin(\omega_{\mathbf{k}}t_x+\omega_{\mathbf{p}}t_y)-\int_0^{t_x} d\tau \frac{\partial}{\partial\tau}\left(\frac{\sin(\omega_{\mathbf{k}}(t_x-\tau))}{\omega_{\mathbf{k}}}\,\frac{1}{2\omega_{\mathbf{p}}} e^{-i\omega_{\mathbf{p}}(\tau-t_y)}\right)\frac{\partial}{\partial\tau} R_{\mathbf{k}+\mathbf{p}}(\tau)\\ &-\int_0^{t_y} d\tau \frac{\partial}{\partial\tau}\left(\frac{\sin(\omega_{\mathbf{p}}(t_y-\tau))}{\omega_{\mathbf{p}}}\,\frac{1}{2\omega_{\mathbf{k}}} e^{-i\omega_{\mathbf{k}}(t_x-\tau)}\right)\frac{\partial}{\partial\tau} R_{\mathbf{k}+\mathbf{p}}(\tau). \end{aligned} \tag{4.32}$$

Since for any smooth function φ, the integral

$$\int_0^t d\tau \dot{R}_{\mathbf{P}}(\tau)\varphi(\tau)=R_{\mathbf{P}}(\tau)\varphi(\tau)\big|_0^t-\int_0^t d\tau \dot{\varphi}(\tau) R_{\mathbf{P}}(\tau)$$

is defined as an operator distribution of $\mathbf{P}$ ($R_{\mathbf{P}}(\tau)$ is a distribution of $\mathbf{P}$ at fixed τ), while $Q_{\mathbf{Ps}}$ and $\Pi^{ren}_{\mathbf{Ps}}$ are operator distributions, expression (4.32) gives us an operator distribution. Thus, we obtain the following proposition.

Proposition 4.7: $w_2(\mathbf{k},t_x;\mathbf{p},t_y)$ is:

(1) an operator distribution of $\mathbf{k}$ *and* $\mathbf{p}$ *at fixed* t_x, t_y, *and*

(2) an operator distribution of $\mathbf{k},t_x,\mathbf{p}$, *and* t_y.

Corollary of proposition 4.6 implies the following statement.

Proposition 4.8: The transformation properties of w_2 under spatial rotations and translations are:

$$U_{\Lambda,0} w_2(\mathbf{k},t_x,\mathbf{p},t_y)U^{-1}_{\Lambda,0}=w_2(\Lambda\mathbf{k},t_x,\Lambda\mathbf{p},t_y)$$
$$U_{1,a} w_2(\mathbf{k},t_x,\mathbf{p},t_y)U^{-1}_{1,a}=e^{-i(\mathbf{k}+\mathbf{p})\mathbf{a}} w_2(\mathbf{k},t_x;\mathbf{p},t_y). \tag{4.33}$$

Corollary: $\hat{W}(\mathbf{x},t_x;\mathbf{y},t_y)$ *is a* t_x*- and* t_y*-dependent operator distribution of* $\mathbf{x}$ *and* $\mathbf{y}$ *with the following transformation properties under spatial rotations and translations:*

$$U_{\Lambda,0}\hat{W}_2(\mathbf{x},t_x,\mathbf{y},t_y)U_{\Lambda,0}^{-1}=\hat{W}_2(\Lambda\mathbf{x},t_x,\Lambda\mathbf{y},t_y),$$
$$U_{1,a}\hat{W}_2(\mathbf{x},t_x,\mathbf{y},t_y)U_{1,a}^{-1}=\hat{W}_2(\mathbf{x}+\mathbf{a},t_x;\mathbf{y}+\mathbf{a},t_y). \tag{4.34}$$

$\hat{W}(x,y)$ *is also an operator distribution of* x *and* y.

Consider the operators

$$W_2[f,t_x,t_y]=\int d\mathbf{x}d\mathbf{y}\hat{W}_2(\mathbf{x},t_x;\mathbf{y},t_y)f(\mathbf{x},\mathbf{y}).$$

Proposition 4.9: The set of all finite linear combinations

$$\sum_n W_2[f_{n,1},t_{x,1}^n,t_{y,1}^n]\ldots W_2[f_{n,s_n},t_{x,s_n}^n,t_{y,s_n}^n]|0\rangle \tag{4.35}$$

is dense in $\mathcal{F}(\mathcal{H}_2)$.

To prove this proposition, it is sufficient to consider the case $t_{x,i}^n=t_{y,i}^n=0$ only and use lemma A.15.

One can also consider the operators

$$W_2[g]=\int dt_x dt_y d\mathbf{x}d\mathbf{y}W_2(\mathbf{x},t_x;\mathbf{y},t_y)g(\mathbf{x},t_x,\mathbf{y},t_y).$$

Proposition 4.10: The set of all finite linear combinations

$$\sum_n W_2[g_{n,1}]\ldots W_2[g_{n,s_n}]|0\rangle \tag{4.36}$$

is dense in $\mathcal{F}(\mathcal{H}_2)$.

To prove this proposition, it is sufficient to approximate the vector (4.35) by the vector (4.36) by choosing

$$g_{n,k}(\mathbf{x},t_x;\mathbf{y},t_y)=f_{n,k}(\mathbf{x},\mathbf{y})\frac{1}{\epsilon^2}\varphi(t_x/\epsilon,t_y/\epsilon)$$

for any smooth function $\varphi(\tau_x,\tau_y)$ with compact support such that $\int d\tau_x d\tau_y\varphi(\tau_x,\tau_y)=1$.

Thus, the cyclic property of the vacuum state is checked.

E. Invariance under time translations

The purpose of this subsection is to check the invariance property of the bifield under time translations:

$$U_{1,a}\hat{W}_2(\mathbf{x},t_x,\mathbf{y},t_y)U_{1,a}^{-1}=\hat{W}_2(\mathbf{x},t_x+t,\mathbf{y},t_y+t), \tag{4.37}$$

if $a^0=t$ and $\mathbf{a}=0$. Let us prove first the following proposition. Denote

$$Q_{\mathbf{Ps}}(T)=e^{iHT}Q_{\mathbf{Ps}}e^{-iHT},\quad \Pi_{\mathbf{Ps}}^{ren}(T)=e^{iHT}\Pi_{\mathbf{Ps}}^{ren}e^{-iHT}.$$

For smooth function $f(\tau)$, let

$$\int_0^T d\tau f(\tau)\frac{\partial}{\partial\tau}R_{\mathbf{P}}(\tau)\equiv f(\tau)R_{\mathbf{P}}(\tau)|_0^T-\int_0^T d\tau\frac{\partial f}{\partial\tau}R_{\mathbf{P}}(\tau).$$

Proposition 4.11: The following properties are satisfied:

$$\begin{aligned}
Q_{\mathbf{Ps}}(T)&=Q_{\mathbf{Ps}}\cos(\Omega_{\mathbf{Ps}}T)+\Pi_{\mathbf{Ps}}^{ren}\frac{sin(\Omega_{\mathbf{Ps}})T}{\Omega_{\mathbf{Ps}}}\\
&\quad-\int_0^T\frac{d\tau}{2\sqrt{\omega_{\mathbf{P}/2-\mathbf{s}}\omega_{\mathbf{P}/2+\mathbf{s}}\Omega_{\mathbf{Ps}}}}\frac{\partial}{\partial\tau}[\sin(\Omega_{\mathbf{Ps}}(T-\tau))]\frac{\partial}{\partial\tau}R_{\mathbf{P}}(\tau),\\
\Pi_{\mathbf{Ps}}^{ren}(T)&=\Pi_{\mathbf{Ps}}^{ren}\cos(\Omega_{\mathbf{Ps}}T)-Q_{\mathbf{Ps}}\Omega_{\mathbf{Ps}}\sin(\Omega_{\mathbf{Ps}}T)\\
&\quad-\int_0^T\frac{d\tau}{2}\sqrt{\frac{\Omega_{\mathbf{Ps}}}{\omega_{\mathbf{P}/2-\mathbf{s}}\omega_{\mathbf{P}/2+\mathbf{s}}}}\frac{\partial}{\partial\tau}[\cos(\Omega_{\mathbf{Ps}}(T-\tau))]\frac{\partial}{\partial\tau}R_{\mathbf{P}}(\tau).
\end{aligned}\tag{4.38}$$

Proof: First of all, notice that

$$\begin{aligned}
Q_{\mathbf{Ps}}(T)&=C^+[\xi_{\mathbf{Ps}}(T)]+C^-[\xi_{-\mathbf{Ps}}(T)],\\
\Pi_{\mathbf{Ps}}^{ren}(T)&=C^+[\pi_{\mathbf{Ps}}^{ren}(T)]+C^-[\pi_{-\mathbf{Ps}}^{ren}(T)],
\end{aligned}\tag{4.39}$$

where $\xi_{\mathbf{Ps}}(T)$ and $\pi_{\mathbf{Ps}}^{ren}(T)$ are the following vector distributions:

$$\begin{aligned}
(\xi_{\mathbf{Ps}}(T))_{\mathbf{P}'\mathbf{s}'}&=\delta_{\mathbf{PP}'}(e^{iM_{\mathbf{P}}T}(2M_{\mathbf{P}})^{-1/2})_{\mathbf{ss}'},\\
(\pi_{\mathbf{Ps}}^{ren}(T))_{\mathbf{P}'\mathbf{s}'}&=\delta_{\mathbf{PP}'}(i\Omega^2M_{\mathbf{P}}^{-2}(M_{\mathbf{P}}/2)^{1/2}e^{iM_{\mathbf{P}}T})_{\mathbf{ss}'}.
\end{aligned}\tag{4.40}$$

Formulas (4.38) mean that

$$\begin{aligned}
\xi_{\mathbf{Ps}}(T)&=\xi_{\mathbf{Ps}}\cos(\Omega_{\mathbf{Ps}}T)+\pi_{\mathbf{Ps}}^{ren}\frac{\sin(\Omega_{\mathbf{Ps}})T}{\Omega_{\mathbf{Ps}}}\\
&\quad-\int_0^T\frac{d\tau}{2\sqrt{\omega_{\mathbf{P}/2-\mathbf{s}}\omega_{\mathbf{P}/2+s}\Omega_{\mathbf{Ps}}}}\frac{\partial}{\partial\tau}[\sin(\Omega_{\mathbf{Ps}}(T-\tau))]\frac{\partial}{\partial\tau}r_{\mathbf{P}}(\tau),\\
\pi_{\mathbf{Ps}}^{ren}(T)&=\pi_{\mathbf{Ps}}^{ren}\cos(\Omega_{\mathbf{Ps}}T)-\xi_{\mathbf{Ps}}\Omega_{\mathbf{Ps}}\sin(\Omega_{\mathbf{Ps}}T)\\
&\quad-\int_0^T\frac{d\tau}{2}\sqrt{\frac{\Omega_{\mathbf{Ps}}}{\omega_{\mathbf{P}/2-\mathbf{s}}\omega_{\mathbf{P}/2+\mathbf{s}}}}\frac{\partial}{\partial\tau}[\cos(\Omega_{\mathbf{Ps}}(T-\tau))]\frac{\partial}{\partial\tau}r_{\mathbf{P}}(\tau).
\end{aligned}\tag{4.41}$$

Integrating relations (4.41) with the function $\varphi\in\mathcal{S}(\mathbf{R}^{2d})$ and applying the operator $(2M_P)^{1/2}$, we transform them to the form

$$e^{iMT}\overline{\varphi}=\cos(\Omega T)\overline{\varphi}+iM^{-1}\Omega\sin(\Omega T)\overline{\varphi}+\int_0^T d\tau(e^{iM\tau})^{\cdot}(\Omega^{-2}-M^{-2})\cos(\Omega(T-\tau))\Omega^2\overline{\varphi},\tag{4.42}$$

$$\begin{aligned}
ie^{iMT}M^{-1}\Omega^2\overline{\varphi}&=iM^{-1}\cos(\Omega T)\overline{\varphi}-\Omega\sin(\Omega T)\overline{\varphi}\\
&\quad-\int_0^T d\tau(e^{iMT})^{\cdot}(\Omega^{-2}-M^{-2})\Omega^3\sin(\Omega(T-\tau))\overline{\varphi}.
\end{aligned}\tag{4.43}$$

Here, Ω is the operator of multiplication by $\Omega_{\mathbf{p}_s}$. We have used the definition of the operator M^{-2}.

Relation (4.43) is a corollary of the relation (4.42) is sufficient to consider the time derivatives of Eq. (4.42). The simplest way to check Eq. (4.42) is to consider the Laplace transformations of the left-hand side

$$\int_0^\infty e^{iMT}e^{-\omega T}dT=\frac{1}{\omega-iM}, \tag{4.44}$$

and of the right-hand side:

$$\frac{\omega}{\omega^2+\Omega^2}+iM^{-1}\frac{\Omega^2}{\omega^2+\Omega^2}+\frac{iM}{\omega-iM}(\Omega^{-2}-M^{-2})\Omega^2\frac{\omega}{\omega^2+\Omega^2}. \tag{4.45}$$

Formulas (4.44) and (4.45) coincide. Thus, Eq. (4.42) is satisfied at $T>0$, the check procedure for $T<0$ is analogous. Proposition is proved.

Proposition 4.12: Relation (4.37) is satisfied.

Proof: One has

$$\begin{aligned}
e^{iHT}w_2(\mathbf{k},t_x;\mathbf{p},t_y)e^{-iHT}=&\sqrt{\frac{\omega_\mathbf{k}+\omega_\mathbf{p}}{\omega_\mathbf{k}\omega_\mathbf{p}}}Q_{\mathbf{k}+\mathbf{p};\mathbf{k}-\mathbf{p}/2}(T)\cos(\omega_\mathbf{k}t_x+\omega_\mathbf{p}t_y)\\
&+\frac{1}{\sqrt{\omega_\mathbf{k}\omega_\mathbf{p}(\omega_\mathbf{k}+\omega_\mathbf{p})}}\Pi_{\mathbf{k}+\mathbf{p};\mathbf{p}-\mathbf{k}/2}(T)\sin(\omega_\mathbf{k}t_x+\omega_\mathbf{p}t_y)\\
&-\int_0^{t_x}d\tau\frac{\sin(\omega_\mathbf{k}(t_x-\tau))}{2\omega_\mathbf{k}\omega_\mathbf{p}}e^{-i\omega_\mathbf{p}(\tau-t_y)}Q_{\mathbf{k}+\mathbf{p}}(\tau+T)\\
&-\int_0^{t_y}d\tau\frac{\sin(\omega_\mathbf{p}(t_y-\tau))}{2\omega_\mathbf{k}\omega_\mathbf{p}}e^{-i\omega_\mathbf{k}(t_x-\tau)}Q_{\mathbf{k}+\mathbf{p}}(\tau+T)
\end{aligned}$$

$$\begin{aligned}
w_2(\mathbf{k},t_x+T;\mathbf{p},t_y+T)=&\sqrt{\frac{\omega_\mathbf{k}+\omega_\mathbf{p}}{\omega_\mathbf{k}\omega_\mathbf{p}}}Q_{\mathbf{k}+\mathbf{p};\mathbf{k}-\mathbf{p}/2}\cos(\omega_\mathbf{k}(t_x+T)+\omega_\mathbf{p}(t_y+T))\\
&+\frac{1}{\sqrt{\omega_\mathbf{k}\omega_\mathbf{p}(\omega_\mathbf{k}+\omega_\mathbf{p})}}\Pi_{\mathbf{k}+\mathbf{p};\,\mathbf{p}-\mathbf{k}/2}\sin(\omega_\mathbf{k}(t_x+T)+\omega_\mathbf{p}(t_y+T))\\
&-\int_0^{t_x+T}d\tau\frac{\sin(\omega_\mathbf{k}(t_x+T-\tau))}{2\omega_\mathbf{k}\omega_\mathbf{p}}e^{-i\omega_\mathbf{p}(\tau-t_y-T)}Q_{\mathbf{k}+\mathbf{p}}(\tau)\\
&-\int_0^{t_y+T}d\tau\frac{\sin(\omega_\mathbf{p}(t_y+T-\tau))}{2\omega_\mathbf{k}\omega_\mathbf{p}}e^{-i\omega_\mathbf{k}(t_x+T-\tau)}Q_{\mathbf{k}+\mathbf{p}}(\tau).
\end{aligned} \tag{4.46}$$

It follows from proposition 4.11 that

$$e^{iHT}w_2(\mathbf{k},t_x;\mathbf{p},t_y)e^{-iHT}=w_2(\mathbf{k},t_x+T;\mathbf{p},t_y+T).$$

We obtain relation (4.37). Proposition is proved.

V. POINCARE INVARIANCE OF THE THEORY

The purpose of this section is to check the property of relativistic invariance of the theory which mean that: (a) the unitary representation of the Poincare group $(\Lambda,a)\mapsto\tilde{U}_{\Lambda,a}$ is constructed:

$$\widetilde{U}_{\Lambda_1,a_1}\widetilde{U}_{\Lambda_2,a_2}=\widetilde{U}_{(\Lambda_1,a_1)(\Lambda_2,a_2)}, \tag{5.1}$$

(b) the k-field operators $\widetilde{W}_k(x_1,\ldots,x_k)$ are Poincare invariant:

$$\widetilde{U}_{\Lambda,a}\widetilde{W}_k(x_1,\ldots,x_k)\widetilde{U}^{-1}_{\Lambda,a}=\widetilde{W}_k(\Lambda x_1+a,\ldots,\Lambda x_k+a), \tag{5.2}$$

and (c) the vacuum state is Poincare invariant:

$$\widetilde{U}_{\Lambda,a}|0\rangle=|0\rangle. \tag{5.3}$$

To simplify the problem, one should be mindful that the state space has been decomposed according to Eq. (2.44), while the operators $\widetilde{U}_{\Lambda,a}$ are looked for in the form $U_{\Lambda,a}\otimes\breve{U}_{\Lambda,a}$. The operators $\breve{U}_{\Lambda,a}$ have already been constructed in Sec. II F.

First of all, we investigate the property of invariance of the operators $\hat{W}_k(x_1,\ldots x_k)$ of the form (4.18) (at $k\neq 2$). These operators are of the form $1\otimes\hat{W}_k(x_1,\ldots x_k)$.

Lemma 5.1: (1) The vacuum state is invariant under action of operators $\breve{U}_{\Lambda,a}$ and (2) For $k\neq 2$, the operators $\hat{W}_k(x_1,\ldots,x_k)$ obey the property

$$\breve{U}_{\Lambda,a}\hat{W}_k(x_1,\ldots,x_k)\breve{U}^{-1}_{\Lambda,a}=\hat{W}_k(\Lambda x_1+a,\ldots,\Lambda x_k+a). \tag{5.4}$$

Proof: The first property is obvious. To prove the second property, it follows from Eq. (4.19), lemma A.11 and formula (2.48) imply that

$$\begin{aligned}\breve{U}_{\Lambda,a}\hat{W}_s(x_1,\ldots,x_s)\breve{U}^{-1}_{\Lambda,a}=\frac{\sqrt{s!}}{(2\pi)^{sd/2}}\int\frac{d\mathbf{p}_1}{\sqrt{2\omega_{\mathbf{p}_1}}}\ldots\frac{d\mathbf{p}_s}{\sqrt{2\omega_{\mathbf{p}_s}}}\\ \times(A^{+(s)}_{\mathbf{p}_1\ldots\mathbf{p}_s}e^{i(p_1+\ldots+p_s)a}e^{i(\Lambda^{-1}p_1\cdot x_1+\ldots+\Lambda^{-1}p_s\cdot x_s)}\\ +A^{-(s)}_{\mathbf{p}_1\ldots\mathbf{p}_s}e^{-i(p_1+\ldots+p_s)a}e^{-i(\Lambda^{-1}p_1\cdot x_1+\ldots+\Lambda^{-1}p_s\cdot x_s)}).\end{aligned} \tag{5.5}$$

Property $\Lambda^{-1}p\cdot x=p\cdot\Lambda x$ imply Eq. (5.4). Lemma is proved.

Lemma 5.2: Let $U_{\Lambda,a}$ be unitary operators in $\mathcal{F}$ such that (a) the group property

$$U_{\Lambda_1,a_1}U_{\Lambda_2,a_2}=U_{(\Lambda_1,a_1)(\Lambda_2,a_2)}, \tag{5.6}$$

is satisfied, (b) the bifield operator is invariant

$$U_{\Lambda,a}\hat{W}_2(x,y)U^{-1}_{\Lambda,a}=\hat{W}_2(\Lambda x+a,\Lambda y+a), \tag{5.7}$$

and (c) the vacuum state is invariant:

$$U_{\Lambda,a}|0\rangle=|0\rangle. \tag{5.8}$$

Then, the operators $\widetilde{U}_{\Lambda,a}=U_{\Lambda,a}\otimes\breve{U}_{\Lambda,a}$ obey properties (5.1)–(5.3).

This lemma is a direct corollary of lemma 5.1 and formula (4.9) for the operators $\widetilde{W}_k(x_1,\ldots,x_k)$.

The remaining problem is to construct operators $U_{\Lambda,a}$ satisfying relations (5.6)–(5.8). One possible way may be the following. The operators P^μ and M^{mn} in $\mathcal{F}$ have been already constructed. One should then try to construct the operator M^{0k} and check the commutation relations of the Poincare algebra.

However, the following problems arise in this approach. It is not easy to check the self-adjointness of the operator M^{0k} since it is an unbounded operator. Further, to construct the group representation from the algebra representation, one should check the conditions of the Nelson theorem[21] or investigate the properties of analytic vectors.[22–24]

Therefore, another approach will be used for constructing the operators $U_{\Lambda,a}$. First of all, we will check the invariance of the Wightman function

$$\langle 0|\hat{W}_2(x,y)\hat{W}_2(x',y')|0\rangle=\langle 0|\hat{W}_2(\Lambda x+a,\Lambda y+a)\hat{W}_2(\Lambda x'+a,\Lambda y'+a)|0\rangle. \tag{5.9}$$

Then, we will define the operator $U_{\Lambda,a}$ from the property

$$U_{\Lambda,a}\hat{W}_2(x_1,y_1)\ldots\hat{W}_2(x_k,y_k)|0\rangle=\hat{W}_2(\Lambda x_1+a,\Lambda y_1+a)\ldots\hat{W}_2(\Lambda x_k+a,\Lambda y_k+a)|0\rangle. \tag{5.10}$$

This definition will be shown to be correct if and only if the property (6.9) is satisfied. Let us investigate the properties of the Wightman functions.

A. The QQ propagator

First of all, we investigate the vacuum average value $\langle 0|Q(x)Q(y)|0\rangle$. It has the form

$$\langle 0|Q(x)Q(y)|0\rangle=\frac{1}{(2\pi)^{2d}}\int d\mathbf{P}(\lambda\Omega^2\chi,e^{i\mathbf{P}(\mathbf{x}-\mathbf{y})-iM(x^0-y^0)}M^{-1}\lambda\Omega^2\chi). \tag{5.11}$$

The vector $\lambda\Omega^2\chi$ is viewed as $\lambda_R M^2\chi$. To check the Poincare invariance of the average (5.11), present it as

$$\langle 0|Q(x)Q(y)|0\rangle=\frac{1}{(2\pi)^{d+1}}\int dPV(P)e^{-iP(x-y)},$$

with

$$V(P^0,\mathbf{P})=\frac{1}{(2\pi)^{d-1}}\int(\lambda\Omega^2\chi)_{\mathbf{Ps}}(\delta(M_{\mathbf{P}}-P^0)M_{\mathbf{P}}^{-1}\lambda\Omega^2\chi)_{\mathbf{Ps}}d\mathbf{s}. \tag{5.12}$$

Making use of the relations

$$\delta(M_{\mathbf{P}}-P^0)M_{\mathbf{P}}^{-1}=2\theta(P^0)\delta(M_{\mathbf{P}}^2-(P^0)^2),\quad 2\pi i\delta(x)=\frac{1}{x-i0}-\frac{1}{x+i0},$$

and

$$\int d\mathbf{s}(\lambda\Omega^2\chi)_{\mathbf{Ps}}\left(\frac{1}{M_{\mathbf{P}}^2+\epsilon^2}\lambda\Omega^2\chi\right)_{\mathbf{Ps}}=\lambda(2\pi)^d\left[1-\frac{1}{1+\lambda I(\mathbf{P},\epsilon)}\right],$$

we take the formula (5.12) to the form

$$V(P^0,\mathbf{P})=2i\theta(P^0)\left[\frac{\lambda}{1+\lambda I(\mathbf{P},i(P^0+i0))}-\frac{\lambda}{1+\lambda I(\mathbf{P},i(P^0-i0))}\right], \tag{5.13}$$

where I is of the form (3.14). We see that the function $\langle 0|Q(x)Q(y)|0\rangle$ is Poincare invariant.

It will be also necessary to calculate the propagator of the field Q. Formally, one has

$$\langle 0|TQ(x)Q(y)|0\rangle=\theta(x^0-y^0)\langle 0|Q(x)Q(y)|0\rangle-\theta(y^0-x^0)\langle 0|Q(y)Q(x)|0\rangle. \quad (5.14)$$

Equation (5.11) implies

$$\langle 0|TQ(x)Q(y)|0\rangle=\frac{1}{(2\pi)^{2d}}\int d\mathbf{P}(\lambda\Omega^2\chi,e^{i\mathbf{P}(\mathbf{x}-\mathbf{y})-iM|x^0-y^0|}M^{-1}\lambda\Omega^2\chi).$$

The Fourier transformation of the propagator which is defined from the relation

$$\langle 0|TQ(x)Q(y)|0\rangle=\frac{1}{(2\pi)^{d+1}}\int dPG_Q(P)e^{-iPx},$$

can be presented as

$$G_Q(P^0,\mathbf{P})=-2i\int d\mathbf{s}(\lambda\Omega^2\chi)_{\mathbf{Ps}}((M_{\mathbf{P}}^2-P_0^2-i0)^{-1}\lambda\Omega^2\chi)_{\mathbf{Ps}}=-2i\lambda+\frac{2i\lambda}{1+\lambda I(\mathbf{P},i(P^0+i0))}.$$

We see that formally calculated propagator consists of the singular part

$$\langle 0|TQ(x)Q(y)|0\rangle^{\text{sing}}=-2i\lambda\,\delta(x-y),$$

and of the regular (renormalized) part with the Fourier transformation

$$G_Q^{ren}(P^0,\mathbf{P})=\frac{2i\lambda}{1+\lambda I(\mathbf{P},i(P^0+i0))}. \quad (5.15)$$

However, this difficulty is usual: the T product is defined up to a quasilocal quantity being proportional to $\delta(x-y)$. Note also that the result (5.15) is in agreement with the approach based on the summation of Feynman graphs.[8]

Thus, we have obtained the following result.

Proposition 5.3: The average value $\langle 0|Q(x)Q(y)|0\rangle$ *is Poincare invariant. Its Fourier transformation has the form (5.13).*

B. The W_2Q average

The purpose of this subsection is to compute the average values

$$F_1(x,y,z)=\langle 0|\hat{W}_2(x,y)Q(z)|0\rangle,\quad F_2(x,y,z)=\langle 0|Q(z)\hat{W}_2(x,y)|0\rangle. \quad (5.16)$$

However, explicit formulas for the operators $\hat{W}_2$ are complicated, so that direct calculations are too difficult. Therefore, the indirect method will be used. First of all, these averages will be calculated at $x^0=y^0>z^0$ and $z^0>x^0=y^0$, correspondingly. Then, we will investigate the properties of the Fourier transformation of the averages. The equations on the averages will be obtained. Then, the solution of the equations will be found.

1. The $x^0=y^0$ case

Consider the average value $\langle 0|Tw_2(\mathbf{p},0;\mathbf{k},0)Q_{\mathbf{P}}(t)|0\rangle$. According to subsection IV. D

$$w_2(\mathbf{p},0;\mathbf{k},0)=\sqrt{\frac{\omega_{\mathbf{k}}+\omega_{\mathbf{p}}}{\omega_{\mathbf{k}}\omega_{\mathbf{p}}}}Q_{\mathbf{k}+\mathbf{p},\mathbf{k}-\mathbf{p}/2}. \quad (5.17)$$

Therefore,

$$\langle 0|Tw_2(\mathbf{p},0;\mathbf{k},0)Q_{\mathbf{p}}(t)|0\rangle = \frac{1}{(2\pi)^{2d}}\sqrt{\frac{\omega_{\mathbf{k}}+\omega_{\mathbf{p}}}{2\omega_{\mathbf{k}}\omega_{\mathbf{p}}}}\delta_{\mathbf{k}+\mathbf{p}+\mathbf{P},0}[\,\theta(-t)(e^{iMt}M^{-1}\lambda\Omega^2\chi)_{\mathbf{P},\mathbf{k}-\mathbf{p}/2}+\theta(t) \times(e^{-iMt}M^{-1}\lambda\Omega^2\chi)_{\mathbf{P},\mathbf{k}-\mathbf{p}/2}]. \tag{5.18}$$

Consider the Fourier transformation of the average (5.17) defined as

$$G(\mathbf{k},\mathbf{p},\epsilon)\,\delta_{\mathbf{k}+\mathbf{p},\mathbf{P}} = \int dt e^{-i\epsilon t}\langle 0|Tw_2(\mathbf{p},0;\mathbf{k},0)Q_{\mathbf{p}}(t)|0\rangle. \tag{5.19}$$

One has

$$G(\mathbf{k},\mathbf{p},\epsilon) = \frac{1}{(2\pi)^d}\sqrt{\frac{2(\omega_{\mathbf{k}}+\omega_{\mathbf{p}})}{\omega_{\mathbf{k}}\omega_{\mathbf{p}}}}\frac{1}{i}\left(\frac{1}{M^2_{\mathbf{k}+\mathbf{p}}-\epsilon^2-i0}\lambda\Omega^2\chi\right)_{\mathbf{k}+\mathbf{p},\mathbf{k}-\mathbf{p}/2}.$$

Making use of the definition of the operator $M^2_{\mathbf{p}}$, we obtain

$$G(\mathbf{k},\mathbf{p},\epsilon) = -\frac{1}{(2\pi)^d}\frac{2(\omega_{\mathbf{k}}+\omega_{\mathbf{p}})}{2\omega_{\mathbf{k}}2\omega_{\mathbf{p}}}\frac{1}{(\omega_{\mathbf{k}}+\omega_{\mathbf{p}})^2-\epsilon^2-i0}G^{ren}_Q(\epsilon,\mathbf{k}+\mathbf{p}).$$

Applying the Fourier transformation to Eq. (5.19), we obtain that

$$\langle 0|T\hat{W}_2(x,y)Q(z)|0\rangle = -i\int d\xi\langle 0|TQ(\xi)Q(z)|0\rangle^{ren}\langle 0|T\phi(x)\phi(y)|0\rangle\langle 0|T\phi(y)\phi(\xi)|0\rangle, \tag{5.20}$$

provided that $x=(\mathbf{x},0)$, $y=(\mathbf{y},0)$, and $z=(\mathbf{z},t)$, while $\langle 0|T\phi(x)\phi(y)|0\rangle$ is the usual propagator of the free scalar field

$$\langle 0|T\phi(x)\phi(y)|0\rangle = \frac{1}{(2\pi)^d}\int\frac{d\mathbf{k}}{2\omega_{\mathbf{k}}}e^{-i\mathbf{k}(\mathbf{x}-\mathbf{y})}e^{-i\omega_{\mathbf{k}}|x^0-y^0|}.$$

Formula (5.20) is valid not only at $x^0=y^0=0$ but also at $x^0=y^0\neq 0$ because of translation invariance properties (Sec. IV). Note also that formula (5.20) is in agreement with the approach based on the summation of Feynman graphs.[8]

Thus, the following result is obtained.

Proposition 5.4: The Green function $\langle 0|T\hat{W}_2(x,y)Q(z)|0\rangle$ *has the form (5.20), provided that* $x^0=y^0$.

2. Properties of the W_2 field

Consider the state $\hat{W}_2(x,y)|0\rangle$. Our purpose is to prove the following property.

Lemma 5.5: The Fourier transformation

$$\int dy\hat{W}_2(x,y)e^{-ipy}|0\rangle \tag{5.21}$$

vanishes at $p^0<0$.

Proof: Consider the vector

$$\int dt_y e^{i\epsilon t_y}w_2(\mathbf{k},t_x;\mathbf{p},t_y)|0\rangle, \tag{5.22}$$

provided that $\epsilon>0$. It is sufficient to show that it vanishes. The vector (5.22) can be presented as

$$C^+[\alpha(\mathbf{k},t_x;\mathbf{p},\boldsymbol{\epsilon})]|0\rangle,$$

with the following vector α:

$$(\alpha(\mathbf{k},t_x;\mathbf{p},\boldsymbol{\epsilon}))_{\mathbf{p}'\mathbf{s}'}=\frac{1}{2}e^{-i\omega_{\mathbf{k}}t_x}\delta_{\mathbf{k}+\mathbf{p},\mathbf{p}'}\Bigg[\sqrt{\frac{\omega_{\mathbf{k}}+\omega_{\mathbf{p}}}{\omega_{\mathbf{k}}\omega_{\mathbf{p}}}}(2M_{\mathbf{k}+\mathbf{p}})^{-1/2}_{\mathbf{k}-\mathbf{p}/2\,s'}$$
$$-\frac{1}{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{p}}(\omega_{\mathbf{k}}+\omega_{\mathbf{p}})}}(M_{\mathbf{k}+\mathbf{p}}/2)^{1/2}_{\mathbf{k}-\mathbf{p}/2s'}$$
$$+\frac{1}{(2\pi)^d}\frac{1}{2\omega_{\mathbf{k}}\omega_{\mathbf{p}}}\left(\frac{1}{\omega_{\mathbf{k}}+\omega_{\mathbf{p}}+M_{\mathbf{k}+\mathbf{p}}}M^{-1/2}_{\mathbf{k}+\mathbf{p}}\lambda\Omega^2\chi\right)_{P's'}\Bigg]. \tag{5.23}$$

It follows from the definition of the operator $M_{\mathbf{p}}$ that the quantity (5.23) vanishes. Lemma is proved.

Corollary: The Fourier transformations

$$\int F_1(x,y,z)e^{ipx}dp, \quad \int dy e^{-ipy}F_2(x,y,z) \tag{5.24}$$

vanish at $p^0<0$.

3. Equations for average values

Let us obtain equations for vacuum averages (5.16). It follows from definition (4.32) that

$$\left(\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\mu}+\mu^2\right)\hat{W}_2(x,y)+Q(x)\langle 0|\phi(x)\phi(y)|0\rangle=0.$$

$$\left(\frac{\partial}{\partial y^\mu}\frac{\partial}{\partial y^\mu}+\mu^2\right)\hat{W}_2(x,y)+Q(y)\langle 0|\phi(x)\phi(y)|0\rangle=0.$$

Here, $\langle 0|\phi(x)\phi(y)|0\rangle$ is the vacuum average for the free scalar field.

Thus, we obtain the following statement.

Proposition 5.6: The functions (5.16) obey the following equations:

$$\left(\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\mu}+\mu^2\right)F_1(x,y,z)+\langle 0|Q(x)Q(z)|0\rangle\langle 0|\phi(x)\phi(y)|0\rangle=0.$$

$$\left(\frac{\partial}{\partial y^\mu}\frac{\partial}{\partial y^\mu}+\mu^2\right)F_1(x,y,z)+\langle 0|Q(y)Q(z)|0\rangle\langle 0|\phi(x)\phi(y)|0\rangle=0.$$

$$\left(\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\mu}+\mu^2\right)F_2(x,y,z)+\langle 0|Q(z)Q(x)|0\rangle\langle 0|\phi(x)\phi(y)|0\rangle=0. \tag{5.25}$$

$$\left(\frac{\partial}{\partial y^\mu}\frac{\partial}{\partial y^\mu}+\mu^2\right)F_2(x,y,z)+\langle 0|Q(z)Q(y)|0\rangle\langle 0|\phi(x)\phi(y)|0\rangle=0.$$

Let us prove the following lemma.

Lemma 5.7: Let $F_1(x,y,z)$ *and* $F_2(x,y,x)$ *be distributions obeying the following properties.*

(a) For some distributions, Φ_1 *and* Φ_2

$$F_1(x,y,z)=\Phi_1(x-z,y-z),\quad F_2(x,y,z)=\Phi_2(x-z,y-z),$$

(b) the functions F_1 and F_2 obey Eqs. (5.25),

(c) the Fourier transformations (5.24) vanish at $p^0<0$, and

(d) $F_1(x,y,z)=\langle 0|T\hat{W}_2(x,y)Q(z)|0\rangle$ at $x^0=y^0>z^0$; $F_2(x,y,z)=\langle 0|T\hat{W}_2(x,y)Q(z)|0\rangle$ at $x^0=y^0<z^0$. Then,

$$F_1(x,y,z)=\langle 0|\hat{W}_2(x,y)Q(z)|0\rangle,\quad F_2(x,y,z)=\langle 0|Q(z)\hat{W}_2(x,y)|0\rangle.$$

Proof: Consider the functions

$$\tilde{F}_1(x,y,z)=F_1(x,y,z)-\langle 0|\hat{W}_2(x,y)Q(z)|0\rangle,\quad \tilde{F}_2(x,y,z)=F_2(x,y,z)-\langle 0|Q(z)\hat{W}_2(x,y)|0\rangle.$$

One has $\tilde{F}_{1,2}(x,y,z)=\tilde{\Phi}_{1,2}(x-z,y-z)$. The functions $\tilde{\Phi}_{1,2}$ obey the following properties:

(a)

$$\left(\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\mu}+\mu^2\right)\tilde{\Phi}_{1,2}(x,y)=0,\quad \left(\frac{\partial}{\partial y^\mu}\frac{\partial}{\partial y^\mu}+\mu^2\right)\tilde{\Phi}_{1,2}(x,y)=0,$$

(b) Fourier transformations $\int dx\tilde{\Phi}_1(x,y)e^{ipx}$ and $\int dy\tilde{\Phi}_1(x,y)e^{-ipy}$ vanish if $p^0<0$,

(c) $\tilde{\Phi}_1(x,y)=0$ at $x^0=y^0>0$, and $\tilde{\Phi}_2(x,y)=0$ at $x^0=y^0<0$.

Properties (a) and (b) mean that

$$\tilde{\Phi}_1(x,y)=\int d\mathbf{k}d\mathbf{p}[\alpha^+_{\mathbf{kp}}e^{-i\omega_{\mathbf{k}}x^0+i\omega_{\mathbf{p}}y^0}+\alpha^-_{\mathbf{kp}}e^{-i\omega_{\mathbf{k}}x^0-i\omega_{\mathbf{p}}y^0}]e^{-i\mathbf{kx}-i\mathbf{py}};$$

$$\tilde{\Phi}_2(x,y)=\int d\mathbf{k}d\mathbf{p}[\beta^+_{\mathbf{kp}}e^{i\omega_{\mathbf{k}}x^0+i\omega_{\mathbf{p}}y^0}+\beta^-_{\mathbf{kp}}e^{-i\omega_{\mathbf{k}}x^0+i\omega_{\mathbf{p}}y^0}]e^{-i\mathbf{kx}-i\mathbf{py}},$$

for some $\alpha^\pm_{\mathbf{kp}}$, $\beta^\pm_{\mathbf{kp}}$. Property (c) means that

$$\alpha^+_{\mathbf{kp}}e^{i\omega_{\mathbf{p}}x^0}+\alpha^-_{\mathbf{kp}}e^{-i\omega_{\mathbf{p}}x^0}=0,\quad x^0>0;$$

$$\beta^+_{\mathbf{kp}}e^{i\omega_{\mathbf{k}}x^0}+\beta^-_{\mathbf{kp}}e^{-i\omega_{\mathbf{k}}x^0}=0,\quad x^0<0.$$

We obtain that $\alpha^\pm_{\mathbf{kp}}=0$ and $\beta^\pm_{\mathbf{kp}}=0$. Therefore, $\tilde{\Phi}_1=0$ and $\tilde{\Phi}_2=0$. Lemma is proved.

Lemma 5.8: The average values have the form

$$\begin{aligned}
F_1(x,y,z)&=\langle 0|\hat{W}_2(x,y)Q(z)|0\rangle\\
&=\frac{1}{i}\int d\xi[(\langle 0|T\phi(x)\phi(\xi)|0\rangle-\langle 0|\phi(x)\phi(\xi)|0\rangle)\langle 0|Q(\xi)Q(z)|0\rangle\langle 0|\phi(\xi)\phi(y)|0\rangle\\
&\quad+\langle 0|T\phi(y)\phi(\xi)|0\rangle-\langle 0|\phi(y)\phi(\xi)|0\rangle)\langle 0|Q(\xi)Q(z)|0\rangle\langle 0|\phi(x)\phi(\xi)|0\rangle\\
&\quad+\langle 0|\phi(x)\phi(\xi)|0\rangle\langle 0|\phi(y)\phi(\xi)|0\rangle\langle 0|TQ(\xi)Q(z)|0\rangle^{ren}]\\
F_2(x,y,z)&=\langle 0|Q(z)\hat{W}_2(x,y)|0\rangle\\
&=\frac{1}{i}\int d\xi[(\langle 0|T\phi(x)\phi(\xi)|0\rangle-\langle 0|\phi(\xi)\phi(x)|0\rangle)\langle 0|Q(z)Q(\xi)|0\rangle\langle 0|\phi(\xi)\phi(y)|0\rangle\\
&\quad+(\langle 0|T\phi(y)\phi(\xi)|0\rangle-\langle 0|\phi(\xi)\phi(y)|0\rangle)\langle 0|Q(z)Q(\xi)|0\rangle\langle 0|\phi(x)\phi(\xi)|0\rangle\\
&\quad+\langle 0|\phi(\xi)\phi(x)|0\rangle\langle 0|\phi(\xi)\phi(y)|0\rangle\langle 0|TQ(z)Q(\xi)|0\rangle^{ren}].
\end{aligned}\tag{5.26}$$

Proof: It is sufficient to check the conditions of lemma 5.7. Condition (a) is obvious. Equations (5.25) are corollaries of the property

$$\left(\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\mu}+\mu^2\right)\langle 0|T\phi(x)\phi(y)|0\rangle=\frac{1}{i}\delta(x-y). \tag{5.27}$$

Let us check the condition (c). Note that the Fourier transformations

$$\int dxe^{ipx}\langle 0|\phi(x)\phi(\xi)|0\rangle, \quad \int dxe^{ipx}\langle 0|Q(x)Q(\xi)|0\rangle$$

vanish if $p^0<0$. The same property is also valid for the function

$$\int dxe^{ipx}\langle 0|\phi(x)\phi(\xi)|0\rangle\langle 0|Q(x)Q(\xi)|0\rangle.$$

Since the integral operator with the kernel $\langle 0|T\phi(x)\phi(\xi)|0\rangle$ multiplies the Fourier transformation by $(\mu^2-p^2-i0)^{-1}$, the quantity

$$\int dxe^{ipx}F_1(x,y,z)$$

vanishes if $p^0<0$. The analogous property for the function F_2 is checked in the same way. Property (c) is checked.

To check property (d), note that under condition $x^0=y^0>z^0$, the function F_1 can be presented as

$$\begin{aligned}\frac{1}{i}\Big[&\int d\xi\langle 0|T\phi(x)\phi(\xi)-\phi(x)\phi(\xi)|0\rangle\langle 0|TQ(\xi)Q(z)|0\rangle^{ren}\langle 0|T\phi(\xi)\phi(y)|0\rangle\\ &+\int d\xi\langle 0|T\phi(y)\phi(\xi)-\phi(y)\phi(\xi)|0\rangle\langle 0|TQ(\xi)Q(z)|0\rangle^{ren}\langle 0|T\phi(x)\phi(\xi)|0\rangle\\ &+\int d\xi\langle 0|\phi(x)\phi(\xi)|0\rangle\langle 0|\phi(y)\phi(\xi)|0\rangle\langle 0|TQ(\xi)Q(z)|0\rangle^{ren}\Big]\end{aligned} \tag{5.28}$$

since the first and second integrands may be nonzero only at $\xi^0>x^0=y^0>z^0$. The obtained expression coincides with (5.20). Thus, property (d) is checked for the function F_1. The check for the function F_2 is analogous. Conditions of lemma 5.7 are checked. This implies lemma 5.8.

C. The W_2W_2 averages

The purpose of this subsection is to find explicit forms of the average value

$$F(x,y:x',y')=\langle 0|\hat{W}_2(x,y)\hat{W}_2(x'.y')|0\rangle. \tag{5.29}$$

We consider first the $x^0=y^0>x^{0\prime}=y^{0\prime}$ case. Then, equations on the function F will be obtained. The solution of this equation will be found.

1. The equal-time case

Consider the Green function

$$\langle 0|Tw_2(\mathbf{p},t;\mathbf{k},t)w_2(\mathbf{p}',\tau;\mathbf{k}',\tau)|0\rangle = \sqrt{\frac{\omega_{\mathbf{k}}+\omega_{\mathbf{p}}}{\omega_{\mathbf{k}}\omega_{\mathbf{p}}}}\sqrt{\frac{\omega_{\mathbf{k}'}+\omega_{\mathbf{p}'}}{\omega_{\mathbf{k}'}\omega_{\mathbf{p}'}}}\delta_{\mathbf{k}+\mathbf{p};\mathbf{k}'+\mathbf{p}'} \times\left(\frac{1}{2M_{\mathbf{k}+\mathbf{p}}}e^{-iM_{\mathbf{k}+\mathbf{p}}|t-\tau|}\right)_{\mathbf{k}-\mathbf{p}/2;\mathbf{k}'-\mathbf{p}'/2},$$

and its Fourier transformation

$$\delta_{\mathbf{k}+\mathbf{p};\mathbf{k}'+\mathbf{p}'}G_2(\mathbf{p},\mathbf{k},\mathbf{p}',\mathbf{k}',\epsilon)=\int dte^{i\epsilon t}\langle 0|Tw_2(\mathbf{p},t;\mathbf{k},t)w_2(\mathbf{p}',0;\mathbf{k}',0)|0\rangle. \tag{5.30}$$

One has

$$G_2(\mathbf{p},\mathbf{k},\mathbf{p}',\mathbf{k}',\epsilon)=\sqrt{\frac{\omega_{\mathbf{k}}+\omega_{\mathbf{p}}}{\omega_{\mathbf{k}}\omega_{\mathbf{p}}}}\sqrt{\frac{\omega_{\mathbf{k}'}+\omega_{\mathbf{p}'}}{\omega_{\mathbf{k}'}\omega_{\mathbf{p}'}}}\frac{1}{i}\left(\frac{1}{M^2_{\mathbf{k}+\mathbf{p}}-\epsilon^2-i0}\right)_{\mathbf{k}-\mathbf{p}/2;\mathbf{k}'-\mathbf{p}'/2}.$$

Making use of the definition of the operator $M^2_{\mathbf{P}}$, we obtain:

$$\begin{aligned}G_2(\mathbf{p},\mathbf{k},\mathbf{p}',\mathbf{k}',\epsilon)=&\sqrt{\frac{\omega_{\mathbf{k}}+\omega_{\mathbf{p}}}{\omega_{\mathbf{k}}\omega_{\mathbf{p}}}}\sqrt{\frac{\omega_{\mathbf{k}'}+\omega_{\mathbf{p}'}}{\omega_{\mathbf{k}'}\omega_{\mathbf{p}'}}}\frac{1}{2i}\frac{1}{(\omega_{\mathbf{k}}+\omega_{\mathbf{p}})^2-\epsilon^2-i0}\\ &\times\left(\delta_{\mathbf{k}-\mathbf{p}/2,\,\mathbf{k}'-\mathbf{p}'/2}+\delta_{\mathbf{k}-\mathbf{p}/2,\,\mathbf{p}'-\mathbf{k}'/2}\right)+\frac{1}{(2\pi)^d}\frac{\omega_{\mathbf{k}}+\omega_{\mathbf{p}}}{2\omega_{\mathbf{k}}\omega_{\mathbf{p}}}\frac{\omega_{\mathbf{k}'}+\omega_{\mathbf{p}'}}{2\omega_{\mathbf{k}'}\omega_{\mathbf{p}'}}\\ &\times\frac{1}{(\omega_{\mathbf{k}}+\omega_{\mathbf{p}})^2-\epsilon^2-i0}\frac{1}{(\omega_{\mathbf{k}'}+\omega_{\mathbf{p}'})^2-\epsilon^2-i0}G_Q^{ren}(\epsilon,\mathbf{k}+\mathbf{p}).\end{aligned} \tag{5.31}$$

Applying the Fourier transformation to expression (5.30), we obtain that

$$\begin{aligned}\langle 0|T\hat{W}_2(x,y)\hat{W}_2(x',y')|0\rangle=&\langle 0|T\phi(x)\phi(x')|0\rangle\langle 0|T\phi(y)\phi(y')|0\rangle+\langle 0|T\phi(x)\phi(y')|0\rangle\\ &\times\langle 0|T\phi(y)\phi(x')|0\rangle-\int d\xi d\xi'\langle 0|TQ(\xi)Q(\xi)|0\rangle^{ren}\\ &\times\langle 0|T\phi(x)\phi(\xi)|0\rangle\langle 0|T\phi(y)\phi(\xi)|0\rangle\\ &\times\langle 0|T\phi(\xi')\phi(x')|0\rangle\langle 0|T\phi(\xi')\phi(y')|0\rangle\end{aligned} \tag{5.32}$$

provided that $x^0=y^0=t$, $x^{0\prime}=y^{0\prime}=\tau$. Equation (5.32) is in agreement with the approach based on summation of Feynman graphs. We have obtained the following statement.

Proposition 5.9: The Green function F has the form (5.32) at $x^0=y^0$ and $x^{0\prime}=y^{0\prime}$.

The following statements are analogs of proposition 5.6 and corollary of lemma 5.5.

Proposition 5.10: The function F (5.29) obeys the following equations

$$\left(\frac{\partial}{\partial x^\mu}\frac{\partial}{\partial x^\mu}+\mu^2\right)F(x,y,x',y')=-\langle 0|\phi(x)\phi(y)|0\rangle\langle 0|Q(x)\hat{W}_2(x',y')|0\rangle,$$

$$\left(\frac{\partial}{\partial y^\mu}\frac{\partial}{\partial y^\mu}+\mu^2\right)F(x,y,x',y')=-\langle 0|\phi(x)\phi(y)|0\rangle\langle 0|Q(y)\hat{W}_2(x',y')|0\rangle,$$

$$\left(\frac{\partial}{\partial x'^{\mu}}\frac{\partial}{\partial x'^{\mu}}+\mu^2\right)F(x,y,x',y')=-\langle 0|\phi(x')\phi(y')|0\rangle\langle 0|\hat{W}_2(x',y')Q(x')|0\rangle,$$

$$\left(\frac{\partial}{\partial y'^{\mu}}\frac{\partial}{\partial y'^{\mu}}+\mu^2\right)F(x,y,x',y')=-\langle 0|\phi(x')\phi(y')|0\rangle\langle 0|\hat{W}_2(x',y')Q(y')|0\rangle, \quad (5.33)$$

Proposition 5.11: The Fourier transformations

$$\int dx e^{ipx}F(x,y,x',y'), \quad \int dy' e^{-ipy'}F(x,y,x',y') \quad (5.34)$$

vanish at $p^0<0$.

Lemma 5.12: Let $F(x,y,x',y')$ *be a distribution obeying the following properties: (a) the function F obey Eq. (5.33), and (b) the Fourier transformations (5.34) vanish at* $p^0<0$, *and (c) at* $x^0=y^0>x^{0\prime}=y^{0\prime}$

$$F(x,y;x',y')=\langle 0|T\hat{W}_2(x,y)\hat{W}_2(x',y')|0\rangle.$$

Then,

$$F(x,y;x',y')=\langle 0|\hat{W}_2(x,y)\hat{W}_2(x',y')|0\rangle.$$

Proof: Consider the function

$$\tilde{F}(x,y;x',y')=F(x,y;x',y')-\langle 0|\hat{W}_2(x,y)\hat{W}_2(x',y')|0\rangle$$

obeying the properties:

(a)

$$\left(\frac{\partial}{\partial x^{\mu}}\frac{\partial}{\partial x^{\mu}}+\mu^2\right)\tilde{F}(x,y,x',y')=0, \quad \left(\frac{\partial}{\partial y^{\mu}}\frac{\partial}{\partial y^{\mu}}+\mu^2\right)\tilde{F}(x,y,x',y')=0,$$

$$\left(\frac{\partial}{\partial x^{\mu\prime}}\frac{\partial}{\partial x^{\mu\prime}}+\mu^2\right)\tilde{F}(x,y,x',y')=0, \quad \left(\frac{\partial}{\partial y^{\mu\prime}}\frac{\partial}{\partial y\mu\prime}+\mu^2\right)\tilde{F}(x,y,x',y')=0, \quad (5.35)$$

(b) the Fourier transformations

$$\int dx e^{ipx}\tilde{F}(x,y,x',y'), \quad \int dy' e^{-ipy'}\tilde{F}(x,y,x',y')$$

vanish at $p^0<0$. (c) $\tilde{F}(x,y;x',y')=0$ at $x^0=y^0>x^{0\prime}=y^{0\prime}$.

Therefore,

$$\begin{aligned}\tilde{F}(x,y;x',y')=\int d\mathbf{k}d\mathbf{p}d\mathbf{k}'d\mathbf{p}'[&\alpha^{++}_{\mathbf{kpk'p'}}e^{i\omega_{\mathbf{k}}x^0+i\omega_{\mathbf{p}}y^0+i\omega_{\mathbf{k}'}x^{0\prime}-i\omega_{\mathbf{p}'}y^{0\prime}}\\&+\alpha^{+-}_{\mathbf{kpk'p'}}e^{i\omega_{\mathbf{k}}x^0+i\omega_{\mathbf{p}}y^0-i\omega_{\mathbf{k}'}x^{0\prime}-i\omega_{\mathbf{p}'}y^{0\prime}}+\alpha^{-+}_{\mathbf{kpk'p'}}e^{i\omega_{\mathbf{k}}x^0-i\omega_{\mathbf{p}}y^0+i\omega_{\mathbf{k}'}x^{0\prime}-i\omega_{\mathbf{p}'}y^{0\prime}}\\&+\alpha^{--}_{\mathbf{kpk'p'}}e^{i\omega_{\mathbf{k}}x^0-i\omega_{\mathbf{p}}y^0-i\omega_{\mathbf{k}'}x^{0\prime}-i\omega_{\mathbf{p}'}y^{0\prime}}]e^{-i(\mathbf{kx}+\mathbf{py}+\mathbf{k}'\mathbf{x}'+\mathbf{p}'\mathbf{y}')}. \quad (5.36)\end{aligned}$$

Relation (c) implies that

$$\alpha^{++}_{\mathbf{kpk'p'}} e^{i\omega_{\mathbf{p}} y^0 + i\omega_{\mathbf{k'}} x^{0\prime}} + \alpha^{+-}_{\mathbf{kpk'p'}} e^{i\omega_{\mathbf{p}} y^0 - i\omega_{\mathbf{k'}} x^{0\prime}} + \alpha^{-+}_{\mathbf{kpk'p'}} e^{-i\omega_{\mathbf{p}} y^0 + i\omega_{\mathbf{k'}} x^{0\prime}} + \alpha^{--}_{\mathbf{kpk'p'}} e^{-i\omega_{\mathbf{p}} y^0 - i\omega_{\mathbf{k'}} x^{0\prime}} = 0$$

at $x^0 = y^0 > x^{0\prime} = y^{0\prime}$. Therefore, all α vanish, so that $\tilde{F} = 0$. Lemma 5.12 is proved.

3. Explicit form of average values

Lemma 5.13: The function F has the form

$$\begin{aligned} F(x,y;x',y') &= \langle 0|\phi(x)\phi(x')|0\rangle\langle 0|\phi(y)\phi(y')|0\rangle + \langle 0|\phi(x)\phi(y')|0\rangle\langle 0|\phi(y)\phi(x')|0\rangle \\ &- i\int d\xi \langle 0|\phi(x)\phi(\xi)|0\rangle\langle 0|\phi(y)\phi(\xi)|0\rangle\langle 0|TQ(\xi)\hat{W}_2(x',y')|0\rangle \\ &- i\int d\xi [\langle 0|T\phi(x)\phi(\xi) - \phi(x)\phi(\xi)|0\rangle\langle 0|\phi(\xi)\phi(y)|0\rangle + \langle 0|T\phi(y)\phi(\xi) \\ &- \phi(y)\phi(\xi)|0\rangle\langle 0|\phi(x)\phi(\xi)|0\rangle]\langle 0|Q(\xi)\hat{W}_2(x',y')|0\rangle \\ &+ \int d\xi d\xi' \langle 0|T\phi(x')\phi(\xi') - \phi(x')\phi(\xi')|0\rangle\langle 0|T\phi(\xi')\phi(y') - \phi(\xi')\phi(y')|0\rangle \\ &\times \langle 0|\phi(x)\phi(\xi)|0\rangle\langle 0|\phi(y)\phi(\xi)|0\rangle\langle 0|TQ(\xi)Q(\xi')|0\rangle, \end{aligned} \tag{5.37}$$

where $\langle 0|TQ(\xi)\hat{W}_2(x',y')|0\rangle$ *is the function of the form (5.20).*

Since the straightforward check of the conditions of lemma 5.12 is analogous to proof of lemma 5.8, proof of lemma 5.13 is obvious.

Corollary: The function F is Poincare invariant:

$$F(x,y;x',y') = F(\Lambda x + a, \Lambda y + a, \Lambda x' + a, \Lambda y' + a).$$

D. Check of Poincare invariance

First of all, note that all Wightman functions are Poincare invariant.

Lemma 5.14: The following property is satisfied:

$$\langle 0|\hat{W}_2(x_1,y_1)\ldots\hat{W}_2(x_n,y_n)|0\rangle = \langle 0|\hat{W}_2(\Lambda x_1 + a, \Lambda y_1 + a)\ldots\hat{W}_2(\Lambda x_n + a, \Lambda y_n + a)|0\rangle.$$

To prove this lemma, it is sufficient to notice that operators $\hat{W}_2(x,y)$ are linear combinations of creation and annihilation operators, so that the Wick theorem is applicable.

Lemma 5.15: 1. There exists a unique unitary operator $U_{\Lambda,a}$ *obeying the properties:* $U_{\Lambda,a}|0\rangle = |0\rangle$,

$$U_{\Lambda,a}\hat{W}_2(x_1,y_1)\ldots\hat{W}_2(x_n,y_n)|0\rangle = \hat{W}_2(\Lambda x_1 + a, \Lambda y_1 + a)\ldots\hat{W}_2(\Lambda x_n + a, \Lambda y_n + a)|0\rangle \tag{5.38}$$

2. The group property (5.6) is satisfied, and 3. The invariance property (5.7) is satisfied.

Proof: Let $W_2[f] = \int dxdy\hat{W}_2(x,y)f(x,y)$,

$$\Phi = c|0\rangle + \sum_{n=1}^{N} W_2[f_{n,1}]\ldots W_2[f_{n,i_n}]0\rangle. \tag{5.39}$$

Set

$$U_{\Lambda,a}\Phi = c|0\rangle + \sum_{n=1}^{N} W_2[u_{\Lambda,a}f_{n,1}]\ldots W_2[u_{\Lambda,a}f_{n,i_n}]0\rangle$$

with

$$(u_{\Lambda,a}f)(x,y)=f(\Lambda^{-1}(x-a),\Lambda^{-1}(y-a)).$$

It follows from lemma 5.14 that $(U_{\Lambda,a}\Phi,U_{\Lambda,a}\Phi)=(\Phi,\Phi)$. This means that $U_{\Lambda,a}\Phi=0$, provided that $\Phi=0$. Thus, the mapping $U_{\Lambda,a}:\mathcal{D}\to\mathcal{D}$ is defined (here $\mathcal{D}$ is a set of all vectors of the form (5.38)). This mapping is a linear isometric (and therefore bounded) operator, while $\mathcal{D}$ is a dense subset of $\mathcal{F}$. Therefore, the operator $U_{\Lambda,a}$ can be uniquely extended to the space $\mathcal{F}$. Thus, there exists a unique isometric operator $U_{\Lambda,a}$ obeying the property (5.38).

Check the group property. Consider the operator

$$V=U_{\Lambda_1,a_1}U_{\Lambda_2,a_2}U_{((\Lambda_1,a_1)(\Lambda_2a_2))^{-1}}.$$

It satisfies the property:

$$V\hat{W}_2(x_1,y_1)\ldots\hat{W}_2(x_n,y_n)|0\rangle=\hat{W}_2(x_1,y_1)\ldots\hat{W}_2(x_n,y_n)|0\rangle$$

Thus, $V=1$. The group property is checked. One analogously proves that $U^{-1}_{\Lambda,a}=U_{(\Lambda,a)^{-1}}$, so that the isometric operator $U_{\Lambda,a}$ is unitary.

One also has

$$U_{\Lambda,a}\hat{W}_2(x,y)U^{-1}_{\Lambda,a}\hat{W}_2(x_1,y_1)\ldots\hat{W}_2(x_n,y_n)|0\rangle$$
$$=\hat{W}(\Lambda x+a,\Lambda y+a)\hat{W}_2(x_1,y_1)\ldots\hat{W}_2(x_n,y_n)|0\rangle.$$

Thus, the property (5.7) is satisfied on the subspace $\mathcal{D}\subset\mathcal{F}$. Lemma 5.15 is proved.

Thus, we have checked the property of Poincare invariance of the theory.

VI. CONCLUSIONS

An old problem of axiomatic and constructive field theory is to construct a nontrivial model of relativistic QFT which obey Wightman axioms. The known models successfully constructed[13] in two- and three-dimensional space–time do not contain such difficulties as Stueckelberg divergences and infinite renormalization of the wave function.

A suitable language to describe the states and observables of the large-N theory in the leading order of $1/N$-expansion is the notion of third quantization introduced in quantum cosmology[25,26] in order to describe processes with variable number of universes.

The third-quantized model considered in this paper may be viewed as a large-N limit of the ordinary field theory. However, it can be also interpreted as an independent model of relativistic quantum theory. We have seen that such properties as renormalizability are satisfied in higher dimensions with respect to ordinary field theories (cf. Ref. 27): the model (2.47) is renormalized at $d+1\leqslant 5$, while the $(\varphi^a\varphi^a)^2$ model is renormalized at $d+1\leqslant 4$ only. Thus, usage of third-quantized models leads to new types of renormalizable theories in higher dimensions.

For the simplicity, we have considered the large-N approximation for the $(\varphi^a\varphi^a)^2$ model only. One can also consider the $\varphi^a\varphi^a\Phi$ model. For this case, the phenomenon of infinite renormalization of the wave function should be investigated: it happens that indefinite inner product should be introduced in the state space.[28] Investigation of the large-N QED (quantum electrodynamics) in the third-quantized formulation gives us a good example of renormalizable gauge theory beyond perturbation theory.

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APPENDIX A: SOME PROPERTIES OF THE FOCK SPACE

Let $\mathcal{H}$ be a Hilbert space. Denote by $\mathcal{H}^{\otimes n}=\mathcal{H}\otimes\ldots\otimes\mathcal{H}$ the n-th tensor degree of space $\mathcal{H}$. Let π be a transposition $(\pi_1,\ldots,\pi_n)$, $1\leqslant\pi_1\neq\ldots\neq\pi_n\leqslant n$ of numbers $(1,\ldots,n)$. Consider the operator $\hat{\pi}$ in $\mathcal{H}^{\otimes n}$ which is uniquely defined from the relation

$$\hat{\pi}(e_1\otimes\ldots\otimes e_n)=e_{\pi_1}\otimes\ldots\otimes e_{\pi_n},\quad e_1,\ldots,e_n\in\mathcal{H}.$$

By Sym, we denote the symmetrization operator

$$\mathrm{Sym}\,\Phi_n=\frac{1}{n!}\sum_{\pi}\hat{\pi}\Phi_n,\quad \Phi_n\in\mathcal{H}^{\otimes n},$$

which is a projector. Introduce the notation $\mathcal{H}^{\vee n}=\mathrm{Sym}\,\mathcal{H}^{\otimes n}$ for the symmetrized n-th tensor degree of $\mathcal{H}$. Denote also $\mathcal{H}^{\vee 0}=\mathbf{C}$.

Lemma A.1: The set $\{f^{\otimes n}\equiv f\otimes\ldots\otimes f|f\in\mathcal{H}\}$ *is a total set in* $\mathcal{H}^{\vee n}$.

Proof: Let $\Phi_n\in\mathcal{H}^{\vee n}$, $\Phi_n\perp f\otimes\ldots\otimes f$ for all $f\in\mathcal{H}$. It is necessary to prove that $\Phi_n=0$. For

$$f=\alpha_1e_1+\ldots+\alpha_ne_n,\quad \alpha_1,\ldots,\alpha_n\in\mathbf{C},\quad e_1,\ldots,e_n\in\mathcal{H}$$

one has

$$0=\sum_{i_1\ldots i_n=1}^{n}\alpha_{i_1}\ldots\alpha_{i_n}(\Phi_n,e_{i_1}\otimes\ldots\otimes e_{i_n}).$$

The right-hand side of this relation is a polynomial in $\alpha_1,\ldots,\alpha_n$. The coefficient of $\alpha_1\ldots\alpha_n$ should be equal to zero:

$$n!(\Phi_n,\mathrm{Sym}\,e_1\otimes\ldots\otimes e_n)=0. \tag{A1}$$

Relation (A1) is satisfied for all $e_1,\ldots,e_n\in\mathcal{H}$.

Let $f_1,f_2,\ldots$ be an orthonormal basis in $\mathcal{H}$. Then $\{f_{i_1}\otimes\ldots\otimes f_{i_n},i_1,\ldots,i_n=\overline{1,\infty}\}$ is an orthonormal basis in $\mathcal{H}^{\otimes n}$. The vector Φ_n can be presented as

$$\Phi_n=\sum_{i_1\ldots i_n=1}^{\infty}\Phi^n_{i_1\ldots i_n}f_{i_1}\otimes\ldots\otimes f_{i_n}.$$

Since

$$\mathrm{sym}\,\Phi_n=\sum_{i_1\ldots i_n=1}^{\infty}\frac{1}{n!}\sum_{\pi}\Phi^n_{i_{\pi_1}\ldots i_{\pi_n}}f_{i_1}\otimes\ldots\otimes f_{i_n},$$

$\Phi_n\in\mathcal{H}^{\vee n}$ if and only if $\Phi^n_{i_1\ldots i_n}$ is symmetric with respect to transpositions of $i_1,\ldots,i_n$.

For symmetric Φ^n one has

$$(\mathrm{Sym}\,f_{j_1}\otimes\ldots f_{j_n},\Phi_n)=\Phi^n_{j_1\ldots j_n}.$$

Thus, Eq. (A1) implies that $\Phi^n_{i_1\ldots i_n}=0$ and $\Phi_n=0$. Lemma is proved.

Definition A.1: The space

$$\mathcal{F}(\mathcal{H})=\oplus_{n=0}^{\infty}\mathcal{H}^{\vee n}$$

is a Fock space.

Let $f\in\mathcal{H}$. The creation and annihilation operators $A_n^+(f):\mathcal{H}^{\vee n-1}\to\mathcal{H}^{\vee n}$, $A_n^-(f):\mathcal{H}^{\vee n}\to\mathcal{H}^{\vee n-1}$ are defined from the relations:

$$A_n^+(f)e^{\otimes n-1}=\frac{1}{\sqrt{n}}\sum_{k=0}^{n-1} e^{\otimes k}\otimes f\otimes e^{\otimes(n-k-1)},$$
$$A_n^-(f)e^{\otimes n}=\sqrt{n}(f,e)e^{\otimes n-1}. \tag{A2}$$

Lemma A.2: The definition (A2) is correct. $A_n^\pm(f)$ are bounded operators and $||A_n^\pm(f)||\leqslant\sqrt{n}||f||$.

Proof: One has

$$||A_n^+(f)\sum_i e_i^{\otimes n-1}||\leqslant\frac{1}{\sqrt{n}}||\sum_i e_i^{\otimes k}\otimes f\otimes e_i^{\otimes(n-k-1)}||$$
$$=\frac{1}{\sqrt{n}}\sum_{k=0}^{n-1}||f||||\sum_i e_i^{\otimes n-1}||=\sqrt{n}||f||||\sum_i e_i^{\otimes n-1}||.$$

$$||A_n^-(f)\sum_i e_i^{\otimes n}||^2=||A_{n+1}^+(f)\sum_i e_i^{\otimes n}||^2-||f||^2||\sum_i e_i^{\otimes n}||^2\leqslant n||f||^2||\sum_i e_i^{\otimes n}||^2.$$

Lemma 2 is proved.

Definition A.2: The operators

$$A^+(f)(\Phi_0,\Phi_1,\Phi_2,\dots)=(0,A_1^+(f)\Phi_0,A_2^+(f)\Phi_1,\dots)$$

and

$$A^-(f)(\Phi_0,\Phi_1,\dots)=(A_1^-(f)\Phi_1,A_2^-(f)\Phi_2,\dots)$$

are called creation and annihilation operators in the Fock space. The finite vectors of the form $(\Phi_0,\dots,\Phi_n,0,0,\dots)$ belong to the domains of $A^\pm(f)$.

Definition A.3: The vector $|0\rangle=(1,0,0,\dots)$ is a vacuum vector.

Lemma A.3: The vector $f=(0,\dots,0,\mathrm{Sym}\,f_1\otimes\dots\otimes f_n,0,\dots)$ can be presented as

$$f=\frac{1}{\sqrt{n!}}A^+(f_1)\dots A^+(f_n)|0\rangle.$$

The proof is straightforward.

Lemma A.4: The following commutation relations take place:

$$[A^\pm(f_1),A^\pm(f_2)]=0 \text{ and } [A^-(f_1),A^+(f_2)]=(f_1,f_2).$$

The operators $A^+(f)$ and $A^-(f)$ are conjugated.

Definition A.4: A coherent state $C(f)$ is a vector $\Phi\in\mathcal{F}$ of the form $C(f)=\Phi=(\Phi_0,\Phi_1,\dots,\Phi_n,\dots)$ with $\Phi_n=1/\sqrt{n!}\,f^{\otimes n}$.

Lemma A.5: The following relations take place:

$$(C(f),C(f))=\exp(f,f), \quad \text{and } A^-(f)C(g)=(g,f)C(g).$$

Lemma A.6: Let $g\in\mathcal{H}$ and g_n, and $n=1,2,\dots$ be such a sequence of elements of $\mathcal{H}$ that $||g_n-g||\to_{n\to\infty}0$. Then $||C(g_n)-C(g)||\to_{n\to\infty}0$.

Proof: Let $\xi_n=g_n-g$. Then,

$$||C(g+\xi_n)-C(g)||^2=e^{(g,g)}[e^{(g,\xi_n)}e^{(\xi_n,g)}e^{(\xi_n,\xi_n)}-e^{(\xi_n,g)}-e^{(g,\xi_n)}+1]\to_{n\to\infty}0.$$

Lemma A.7: The set $\{C(f)|f\in\mathcal{H}\}$ *is a total set in* $\mathcal{F}(\mathcal{H})$.

Proof: Let $\Phi=(\Phi_0,\Phi_1,\ldots,\Phi_n,\ldots)\perp C(\alpha f)$ for all $\alpha\in\mathbf{C}$ and $f\in\mathcal{H}$. Therefore,

$$\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}(f^{\otimes n},\Phi_n)=0.$$

The series absolutely converges for all α because of the Cauchy–Bunyakovski inequality. Therefore, $(f^{\otimes n}$ and $\Phi_n)=0$ for all f, so that $\Phi_n=0$. Lemma is proved.

Lemma A.8: Let $\mathcal{H}=\mathcal{H}_1\oplus\mathcal{H}_2$. *Then, there exists a unique isomorphism* $I:\mathcal{F}(\mathcal{H}_1)\otimes\mathcal{F}(\mathcal{H}_2)\to\mathcal{F}(\mathcal{H})$ *such that*

$$I(C(f_1)\otimes C(f_2))=C(f_1\oplus f_2),\quad f_1\in\mathcal{H}_1,f_2\in\mathcal{H}_2. \tag{A3}$$

Proof: The mapping (A3) conserves the inner product. Therefore, formula (A3) uniquely defines an isometric operator. Lemma A.7 applied for the space $\mathcal{F}(\mathcal{H})$ implies that the set $I(C(f_1)\otimes C(f_2))$ is a total set in $\mathcal{F}(\mathcal{H})$, so that $I(\mathcal{F}(\mathcal{H}_1)\otimes\mathcal{F}(\mathcal{H}_2))=\mathcal{F}(\mathcal{H})$. Thus, I is an isomorphism. Lemma is proved.

Lemma A.9: Let $f=f_1+f_2$, $f_1\in\mathcal{H}_1$, $f_2\in\mathcal{H}_2$. *Then,*

$$I^{-1}A^{\pm}(f)I=A^{\pm}(f_1)\otimes 1+1\otimes A^{\pm}(f_2). \tag{A4}$$

Proof: It is sufficient to note that the matrix elements of the left-hand and right-hand sides of Eq. (A4) between $C(f_1)\otimes C(f_2)$ and $C(\tilde{f}_1)\otimes C(\tilde{f}_2)$ coincide.

Let U be a bounded operator in $\mathcal{H}$. By $\mathcal{U}(U)$, we denote the operator $\mathcal{U}(U):\mathcal{F}(\mathcal{H})\to\mathcal{F}(\mathcal{H})$ of the form

$$\mathcal{U}(U)(f_0,f_1,\ldots,f_n,\ldots)=(f_0,Uf_1,U\otimes Uf_2,\ldots,U^{\otimes n}f_n,\ldots).$$

Let $\mathcal{H}$ be a self-adjoint operator in $\mathcal{H}$. Consider the one-parametric group of unitary operators e^{-iHt}. The operator-valued mapping $t\mapsto\mathcal{U}(e^{-iHt})$ can be also viewed as a one-parametric group. According to the Stone theorem, it has the form

$$\mathcal{U}(e^{-iHt})=e^{-i\mathcal{F}(H)t},$$

for some self-adjoint operator $\mathcal{F}(H)$ in $\mathcal{F}(\mathcal{H})$. The explicit form of this operator is

$$(\mathcal{F}(H)f)_n=\sum_{k=0}^{n-1}1^{\otimes k}\otimes H\otimes 1^{\otimes(n-k-1)}f_n.$$

Let $\varphi_1,\varphi_2,\ldots$ be an orthonormal basis in $\mathcal{H}$. Let

$$Hf=\sum_{ij=1}^{\infty}H_{ij}\varphi_i(\varphi_j,f).$$

Proposition A.10:

$$\mathcal{F}(H)=\sum_{ij=1}^{\infty}H_{ij}A^{+}[\varphi_i]A^{-}[\varphi_j].$$

The proof is straightforward.

Lemma A.11: Let U *be an unitary operator in* $\mathcal{H}$, $f\in\mathcal{H}$. *Then,*

$$\mathcal{U}(U)A^{\pm}(f)\mathcal{U}(U)^{-1}=A^{\pm}(Uf). \tag{A5}$$

To prove the lemma, it is sufficient to consider the matrix elements of the sides of Eq. (A5) between coherent states.

Formulate now some results concerning vector and operator distributions. Let $\mathcal{S}(\mathbf{R}^n)$ be a space of complex smooth functions $u:\mathbf{R}^n\to\mathbf{C}$ such that

$$||u||_{l,m}=\max_{\alpha_1+\ldots+\alpha_n\leqslant l}\sup_{x\in\mathbf{R}^n}(1+|x|)^m\left|\frac{\partial^{\alpha_1+\ldots\alpha_n}u(x)}{\partial x_1^{\alpha_1}\ldots\partial x_n^{\alpha_n}}\right|\to_{k\to\infty}0.$$

We say that the sequence $\{u_k\}\in\mathcal{S}(\mathbf{R}^n),k=\overline{1,\infty}$ tends to zero if

$$||u_k||_{l,m}\to_{k\to\infty}0$$

for all l and m.

Definition A.5: Let $\mathcal{H}$ be a Hilbert space. A vector distribution f on $\mathbf{R}^n$ is a linear mapping $f:\mathcal{S}(\mathbf{R}^n)\to\mathcal{H}$ such that $||f(u_k)||\to_{k\to\infty}0$ if $u_k\to_{k\to\infty}0$.

Remark: We will write $f(\varphi)=\int dx f(x)\varphi(x)$ and say that $f(x)$ is a vector distribution of the argument $x\in\mathbf{R}^n$.

Lemma A.12: Let $f:\mathbf{R}^n\to\mathcal{H}$ be a strongly continuous bounded vector function. Then $f(\varphi)=\int dx f(x)\varphi(x)$ is a vector distribution.

Lemma A.13: Let f be a vector distribution. Then $\partial f/\partial x^{\alpha}$ is a vector distribution. The proof is straightforward.

Definition A.6: Let $\mathcal{D}\subset\mathcal{H}$ be a dense subset of $\mathcal{H}$. An operator distribution A is a linear mapping

$$\varphi\in\mathcal{S}(\mathbf{R}^n)\mapsto A(\varphi):\mathcal{D}\to\mathcal{D},$$

such that for all $\Phi\in\mathcal{D}$ the mapping $\varphi\mapsto A(\varphi)\Phi$ is a vector distribution.

Let $\mathcal{D}$ be a subset of the Fock space $\mathcal{F}(\mathcal{H})$ which consists of all finite vectors $(f_0,f_1,\ldots,f_k,0,\ldots)$.

Lemma A.14: Let f be a vector distribution. Then $A^{\pm}(f)$ is an operator distribution. Investigate now the cyclic property of the vacuum vector.

Let $\mathcal{G}\in\mathcal{H}\oplus\mathcal{H}$. Consider the operators

$$B(f,g)=A^{+}(f)+A^{-}(g),\quad \text{and}\,(f,g)\in\mathcal{G}.$$

By $I_1:\mathcal{H}\oplus\mathcal{H}\to\mathcal{H}$ we denote the operator $I_1(f,g)=f$.

Lemma A.15: Let $I_1\mathcal{G}$ be a dense subset of $\mathcal{H}$. Then the set of all linear combinations

$$\sum_n c_n B(f_{n,1},g_{n,1})\ldots B(f_{n,k_n},g_{n,k_n})|0\rangle,\quad (f_{i,k_i},g_{i,k_i})\in\mathcal{G} \tag{A6}$$

is dense in $\mathcal{F}(\mathcal{H})$.

Proof: Let $\Phi\in\mathcal{F}(\mathcal{H})$. One should prove that it can be approximated by the linear combination (A6). Lemma A.7 implies that it is sufficient to prove this statement for the coherent states $C(\varphi)$. Choose such a sequence $f_n\in I_1\mathcal{G}$ that $f_n\to\varphi$. Lemma A.6 implies that $C(\varphi)$ can be approximated by $C(f_n)$. Furthermore, the coherent state $C(f_n)$ can be approximated a by finite linear combination of vectors $(A^{+}(f_n))^m|0\rangle$. For some g_n one has $(f_n,g_n)\in\mathcal{G}$. The vector $(A^{+}(f_n))^m|0\rangle$ can be presented as a linear combination of vectors $(B(f_n,g_n))^k|0\rangle$, Lemma A.15 is proved.

APPENDIX B: WHAT IS FIELD?

In Sec. IV, we have investigated the commutation rule between operators $1/N\sum_{a=1}^{N}\varphi^a(x_1)\ldots\varphi^a(x_k)$ and multifield canonical operator

$$\frac{1}{N}\sum_{a=1}^{N}\varphi^a(x_1)\ldots\varphi^a(x_k)K_N=K_N[(\Phi_0,\phi(x_1)\ldots\phi(x_k)\Phi_0)+N^{-1/2}\tilde{W}_k(x_1,\ldots,x_k)+O(N^{-1})].$$

The operators $\tilde{W}_k(x_1,\ldots,x_k)$ acting in the space (2.43) of the theory of infinite number of fields were interpreted as multifield operators.

The purpose of this appendix is to construct analogs of the operators $\varphi^a(x)$ in the $N=\infty$-theory.

One can notice that conception of symmetric states only is not valid for this purpose. If the state $\Psi_N[\varphi^1,\ldots,\varphi^N]$ were symmetric with respect to transpositions of the fields $\varphi^1,\ldots,\varphi^N$, the state $\varphi^1(\mathbf{x})\Psi_N[\varphi^1,\ldots,\varphi^N]$ is not symmetric. Thus, it is necessary to consider the nonsymmetric solutions of Eq. (2.1).

Consider the states of large-N theory which are symmetric with respect to $N-s$ fields $\varphi^{s+1},\ldots,\varphi^N$ only, where s is a finite quantity. Analogously to Eq. (2.6), let Ψ_N be of the form

$$(K_N^s f)[\varphi^1,\ldots,\varphi^N]$$
$$=\sum_{k=0}^{N-s}\frac{\sqrt{k!}}{N^{k/2}}\sum_{s+1\leqslant a_1<\ldots<a_k\leqslant N} f_k[\varphi^1,\ldots,\varphi^s,\varphi^{a_1},\ldots,\varphi^{a_k}]\prod_{a>s,a\neq a_1\ldots a_k}\Phi_0[\varphi^a], \tag{B1}$$

where $f_k[\varphi^1,\ldots,\varphi^s,\phi^1,\ldots,\phi^k]$ are functionals being symmetric under transpositions of fields $\phi^1,\ldots,\phi^k$ and obeying the condition

$$\int D\phi_1\Phi_0^*[\phi_1]f_k[\varphi^1,\ldots,\varphi^s,\phi^1,\ldots,\phi^k]=0. \tag{B2}$$

We see that states under consideration are specified by infinite sets

$$\begin{pmatrix} f_0[\varphi^1,\ldots,\varphi^s] \\ f_1[\varphi^1,\ldots,\varphi^s,\phi^1] \\ \cdots \\ f_k[\varphi^1,\ldots,\varphi^s,\phi^1,\ldots,\phi^k] \\ \cdots \end{pmatrix}. \tag{B3}$$

The state space is then isomorphic to

$$\tilde{\mathcal{F}}_s=\mathcal{H}^{\otimes s}\otimes\mathcal{F}(\oplus_{n=1}^{\infty}\mathcal{H}^{\vee n}). \tag{B4}$$

Since the symmetric state can be viewed as a state of the form (B1), there should be exist an operator $I_s:\tilde{\mathcal{F}}_0\to\tilde{\mathcal{F}}_s$ such that

$$K_N^s I_s f=K_N f.$$

Let us present the explicit form of the operator I_1. One has

$$(K_N f)[\varphi^1,\ldots,\varphi^N]=\sum_{k=0}^{N}\frac{\sqrt{k!}}{N^{k/2}}\sum_{1\leqslant a_1<\ldots<a_k\leqslant N} f_k[\varphi^{a_1},\ldots,\varphi^{a_k}]\prod_{a\neq a_1\ldots a_k}\Phi_0[\varphi^a]$$
$$=\sum_{k=0}^{N}\frac{\sqrt{k!}}{N^{k/2}}\sum_{2\leqslant a_2<\ldots<a_k\leqslant N} f_k[\varphi^1,\varphi^{a_2},\ldots,\varphi^{a_k}]\prod_{a\neq 1,a_2,\ldots,a_k}\Phi_0[\varphi^a]$$
$$+\sum_{k=0}^{N}\frac{\sqrt{k!}}{N^{k/2}}\Phi_0[\varphi^1]\sum_{2\leqslant a_1<\ldots<a_k\leqslant N} f_k[\varphi^{a_1},\ldots,\varphi^{a_k}]\prod_{a\neq 1,a_2,\ldots,a_k}\Phi_0[\varphi^a]. \tag{B5}$$

We see that

$$(I_1 f)_k[\varphi^1,\phi^1,\ldots,\phi^k]=\Phi_0[\varphi^1]f_k[\phi^1,\ldots,\phi^k]+N^{-1/2}(\tilde{A}^-[\varphi^1]f)_k[\phi^1,\ldots,\phi^k]. \tag{B6}$$

One can also perform the symmetrization procedure for the vector (B1) and obtain the symmetric state. Therefore, there should exist an operator $S_s:\tilde{\mathcal{F}}_s\to\tilde{\mathcal{F}}_0$ such that

$$\mathrm{Sym}\,K_N^s f=K_N S_s f.$$

Construct the operator S_1. If

$$\int D\varphi^1 f_k[\varphi^1,\phi^1,\ldots,\phi^k]\Phi_0^*[\varphi^1]=0, \tag{B7}$$

one obtains from direct calculation that

$$(S_1 f)_k[\phi^1,\ldots,\phi^k]=N^{-1/2}\int D\varphi(\tilde{A}^+[\varphi]f)_k[\varphi,\phi^1,\ldots,\phi^k].$$

If

$$f_k[\varphi^1,\phi^1,\ldots,\phi^k]=\Phi_0[\varphi^1]g_k[\phi^1,\ldots,\phi^k], \tag{B8}$$

then

$$(S_1 f)_k[\phi^1,\ldots,\phi^k]=\frac{N-k}{N}g_k[\phi^1,\ldots,\phi^k].$$

Generally, f_k can be viewed as a superposition of vectors obeying conditions (B7) and (B8) correspondingly, so that

$$(S_1 f)_k[\phi^1,\ldots,\phi^k]=\left[1-\frac{\hat{n}}{N}\right]\int D\varphi\Phi_0^*[\varphi]f_k[\varphi,\phi^1,\ldots,\phi^k]$$
$$+N^{-1/2}\int D\varphi(\tilde{A}^+[\varphi]f)_k[\varphi,\phi^1,\ldots,\phi^k]. \tag{B9}$$

The Schrodinger field $\varphi^1(\mathbf{x})$ in $\tilde{\mathcal{F}}_1$ may be viewed as an operator of multiplication by $\varphi^1(\mathbf{x})$, since

$$\varphi^1(\mathbf{x})K_N^1=K_N^1\varphi^1(\mathbf{x}).$$

The multifield can be constructed from the field φ^1 as

$$\tilde{\mathcal{W}}_{N,k}(x_1,\ldots,x_k)=S_1\varphi^1(x_1)\ldots\varphi^1(x_k)I_1 \tag{B10}$$

since

$$\frac{1}{N}\sum_{a=1}^{N}\varphi^a(x_1)\ldots\varphi^a(x_k)=\mathrm{Sym}\,\varphi^1(x_1)\ldots\varphi^1(x_k).$$

One can notice from Eqs. (B6) and (B9), that formula (B10) is in agreement with the results of Sec. IV.

To construct the Heisenberg field operator $\varphi^1(x):\tilde{\mathcal{F}}_1\to\tilde{\mathcal{F}}_1$, it is necessary to commute the Hamiltonian operator $\mathcal{H}_N$ with the operator K_N^1. We obtain:

$$\mathcal{H}_N K_N^1=K_N^1\tilde{\mathcal{H}}_N^1, \tag{B11}$$

where

$$\tilde{\mathcal{H}}_N^1=\tilde{\mathcal{H}}_N+\int d\mathbf{x}\left[-\frac{1}{2}\frac{\delta^2}{\delta\varphi^1(\mathbf{x})\,\delta\varphi^1(\mathbf{x})}+\frac{1}{2}(\nabla\varphi^1)^2(\mathbf{x})+\frac{\mu^2}{2}(\varphi^1(\mathbf{x}))^2\right]+O(N^{-1/2}).$$

Therefore, the Heisenberg operator

$$\varphi^1(\mathbf{x},t)=e^{i\tilde{\mathcal{H}}_N^1 t}\varphi^1(\mathbf{x})e^{-i\tilde{\mathcal{H}}_N^1 t}$$

coincides with the operator of the free scalar field up to $O(N^{-1/2})$. Therefore, for operator $\tilde{\mathcal{W}}_{N,k}$ one has

$$\tilde{\mathcal{W}}_{N,k}(x_1,\ldots,x_k)=\int D\varphi^1\Phi_0^*[\varphi^1]\varphi^1(x_1)\ldots\varphi^1(x_k)\Phi_0[\varphi^1]+O(N^{-1/2}). \tag{B12}$$

This result confirms the hypothesis of Sec. IV.

In order to obtain the explicit form of the $O(N^{-1/2})$-term of formula (B12), it is necessary to compute the $O(N^{-1/2})$-term in Eq. (B11). The result is in agreement with Sec. IV.

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Exact solvability of superintegrable systems

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It is shown that all four superintegrable quantum systems on the Euclidean plane possess the same underlying hidden algebra $sl(3)$. The gauge-rotated Hamiltonians, as well as their integrals of motion, once rewritten in appropriate coordinates, preserve a flag of polynomials. This flag corresponds to highest-weight finite-dimensional representations of the $sl(3)$-algebra, realized by first-order differential operators. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The purpose of this article is to establish a relation between two different concepts in quantum mechanics: superintegrability and exact solvability. More specifically, we relate these two concepts in nonrelativistic quantum mechanics in two-dimensional Euclidean space E_2.

The notion of integrability in quantum mechanics[1] comes naturally as a generalization of a similar notion in classical mechanics (see, e.g., Ref. 2). A quantum mechanical system in E_n described by the stationary Schrödinger equation

$$H\Psi = E\Psi, \quad H = -\tfrac{1}{2}\Delta + V(x_1, \ldots, x_n), \tag{1}$$

is completely integrable if there exists a set of $(n-1)$ algebraically independent linear operators $X_a, a = 1,2, \ldots, n-1$ commuting with the Hamiltonian and among each other

$$[H, X_a] = 0, \quad [X_a, X_b] = 0. \tag{2}$$

The system is it superintegrable if there exist k additional operators, Y_b, $b = 1, \ldots, k$, where $0 < k \leqslant (n-1)$, commuting with the Hamiltonian. It is "maximally superintegrable" if $k = n-1$.

The operators X_a, Y_b are usually assumed to be polynomials in the momenta $\{p_1, \ldots, p_n\}$ with coordinate dependent coefficients. A systematic search for superintegrable systems in E_2 and E_3 was conducted some time ago.[3–5] A restriction was imposed, namely that the operators X_a and Y_b should be second-order polynomials in momenta. It turned out that the existence of such commuting operators leads to the separation of variables in the Schrödinger equation. Superintegrable systems are actually *superseparable*: they allow the separation of variables in at least two coordinate systems.

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A large body of literature exists on superintegrable systems in E_n.[3–17] In particular, it has been shown recently[17] that the superintegrable systems in E_2 are characterized by the existence of at least two generalized Lie symmetries.

Quantum mechanical problems which can be called it exactly solvable are defined quite differently. An exactly solvable quantum mechanical system can be characterized by the fact that in its solution space one can indicate explicitly an infinite flag of functional linear spaces, which is preserved by the Hamiltonian.[18] In general, the flag should be of such a type that a basis for the entire space of solutions is obtained as a union of bases for the invariant subspaces. In this paper the flag is constructed using polynomials in two variables that provide bases for finite-dimensional representations of $sl(3)$ (see the following). Therefore, the flag generates a dense subspace in the Hilbert space of the bound state eigenfunctions. We recall that a flag is formed by an infinite set of functional linear spaces which can be ordered in such a way that each of them properly contains the previous one as a subspace. One important particular example of these flags is given by finite-dimensional representation spaces of semi-simple Lie algebras of first order differential operators. In this case the Hamiltonian is an element of the universal enveloping algebra of a Lie algebra.

In order to clarify the situation let us consider as an example the case of one-dimensional (quasi)-exactly solvable problems.[19] Due to Sophus Lie it is known that the only Lie algebra of first-order differential operators which acts on the real line and possesses finite-dimensional representations is the $sl(2,\mathbb{R})$-algebra (for a discussion see, for example, e.g., Refs. 20 and 22), realized as

$$J_n^+ = x^2 d_x - nx, \quad J_n^0 = x d_x - \frac{n}{2}, \quad J_n^- = d_x. \tag{3}$$

For integer n the generators (3) possess a common invariant subspace $\mathcal{P}_n = \langle x^k | 0 \leqslant k \leqslant n \rangle$, which is the linear space of polynomials. It is evident that the spaces $\mathcal{P}_n$ as functions of the parameter n form a flag. This flag is preserved by any element of the universal enveloping algebra of the $sl(2,\mathbb{R})$ parabolic subalgebra J_n^0, J_n^- for any n. Therefore, an element of this enveloping algebra can be viewed as a Hamiltonian, which defines an exactly solvable system. In a similar manner one can introduce the notion of a quasi-exactly solvable problem for which the Hamiltonian possesses the invariant subspace $\mathcal{P}_n$. It can be proven[22] that a necessary and sufficient condition for a one-dimensional Hamiltonian to be quasi-exactly solvable is that it belongs to the universal enveloping algebra of the $sl(2,\mathbb{R})$-algebra taken in realization (3). (Up to change of variables and gauge transformation.)

For two-dimensional problems there exist four candidates for underlying hidden Lie algebra:[23,20,21,18] $sl(3,\mathbb{R})$, $sl(2,\mathbb{R}) \oplus sl(2,\mathbb{R}), o(3,1)$, a parametric family $gl(2,\mathbb{R}) \ltimes \mathbf{R}^{r+1}$ and some of their subalgebras. In particular, the algebra $gl(3,\mathbb{R}) \supset sl(3,\mathbb{R})$, realized as

$$\begin{gathered} J_1 = \partial_t, \quad J_2 = \partial_u, \\ J_3 = t\partial_t, \quad J_4 = u\partial_u, \quad J_5 = u\partial_t, \quad J_6 = t\partial_u, \\ J_7 = t^2\partial_t + tu\partial_u - nt, \quad J_8 = tu\partial_t + u^2\partial_u - nu, \\ X = n, \end{gathered} \tag{4}$$

will be used in this article as well as, more specifically the maximal parabolic subalgebra of $sl(3,\mathbb{R})$ formed by the generators $\{J_{1,\ldots,6}\}$.

For integer n the generators (4) possess a common invariant subspace $\mathcal{P}_n^{(2)} = \langle t^k u^m | 0 \leqslant k + m \leqslant n \rangle$, which is the linear space of polynomials. Similar to the case of $sl(2,\mathbb{R})$ the spaces $\mathcal{P}_n^{(2)}$ as functions of the parameter n form a flag. This flag is preserved by any element of the universal enveloping algebra of the parabolic subalgebra $\{J_{1,\ldots,6}\}$.[18] Therefore, an element of this enveloping algebra viewed as a Hamiltonian defines an *exactly solvable* system with the hidden algebra $sl(3,\mathbb{R})$.

Both superintegrable and exactly solvable systems have numerous applications in physics. Among the simplest superintegrable ones are the Coulomb system and the harmonic oscillator in spaces of any dimension. The celebrated many-body Calogero model is superintegrable as well as the Hartmann potential of quantum chemistry.[10,9]

II. HIDDEN ALGEBRA OF SUPERINTEGRABLE HAMILTONIANS

There exist precisely four quantum (and also classical) Hamiltonians defined on E_2, characterized by two integrals of motion, $[H,X_{1,2}]=0$, such that $X_{1,2}$ are quadratic in the momenta.[3,4,17] Thus, they are maximally superintegrable and for their classical counterparts all trajectories are closed. It was shown that these four Hamiltonians exhaust the list of two-dimensional Hamiltonians characterized by two integrals of motion in the form of second-order differential operators. They admit the separation of variables in two (or even more) different coordinate systems. We will show that all of them possess a hidden $sl(3,\mathbb{R})$ algebra. In particular, this implies that there exists a coordinate system where the Hamiltonian, as well as the integrals of motion, after a similarity transformation (gauge rotation) can be rewritten in terms of the generators of the maximal parabolic subalgebra of $sl(3,\mathbb{R})$. Furthermore, two of these Hamiltonians have a striking feature. For each of them, multiplied by a suitable factor f, there exists another set of two commuting operators, $[fH,Y_{1,2}]=0$. This can be considered as a generalization of the notion of integrability in quantum mechanics: commuting operators appear not for the Hamiltonian, but for the Hamiltonian multiplied by a factor.

Case I: The first Hamiltonian written in Cartesian coordinates is given by

$$H_{\mathrm{I}}\left(x,y;\frac{\omega^2}{2},\frac{A}{2},\frac{B}{2}\right)=-\frac{1}{2}(\partial_x^2+\partial_y^2)+\frac{\omega^2}{2}(x^2+y^2)+\frac{1}{2}\left(\frac{A}{x^2}+\frac{B}{y^2}\right), \tag{5}$$

where $A,B>-1/8$ are parameters. The corresponding Schrödinger equation separates in three different coordinate systems: Cartesian, polar, and elliptical. The eigenfunctions can be written in the form

$$\Psi_{n,m}(x,y)=x^{p_1}y^{p_2}L_n^{(-1/2+p_1)}(\omega x^2)L_m^{(-1/2+p_2)}(\omega y^2)\exp\left(-\frac{\omega x^2}{2}-\frac{\omega y^2}{2}\right), \tag{6}$$

where $L_k^{(\alpha)}(z)$ are Laguerre polynomials, $n,m=0,1,2,\ldots$ and the parameters $p_{1,2}$ are defined by $A=p_1(p_1-1),B=p_2(p_2-1)$. The degree of degeneracy of eigenstates is given by a number of partitions of an integer into the sum of two integers.

We perform a gauge rotation of $H_{\mathrm{I}}(x,y)$, using the ground state eigenfunction $\Psi_{0,0}(x,y)$ as a gauge factor and then a change of variables

$$\begin{aligned} h^I &\equiv \frac{1}{\omega}(\Psi_{0,0}(x,y))^{-1}H_I(x,y)\Psi_{0,0}(x,y)\big|_{t=\omega x^2,u=\omega y^2} \\ &=-2t\partial_t^2-2u\partial_u^2+2t\partial_t+2u\partial_u-(2p_1+1)\partial_t-(2p_2+1)\partial_u+1+p_1+p_2, \end{aligned} \tag{7}$$

with eigenvalues $E(n,m)=n+m,n,m=0,1,2,\ldots$.

It is easy to check that after a gauge rotation with the same gauge factor $\Psi_{0,0}(x,y)$ and a change of variables for the integrals of motion, we arrive at the operators

$$\hat{x}_C^{\mathrm{I}}=2t\partial_t^2-2u\partial_u^2-2t\partial_t+2u\partial_u+(2p_1+1)\partial_t-(2p_2+1)\partial_u-p_1+p_2, \tag{8}$$

$$\hat{x}_R^{\mathrm{I}}=4tu(\partial_t-\partial_u)^2+2[(2p_1+1)u-(2p_2+1)t](\partial_t-\partial_u)-(p_1+p_2)^2. \tag{9}$$

These three operators $h^{\mathrm{I}},\hat{x}_C^{\mathrm{I}},\hat{x}_R^{\mathrm{I}}$ obey the commutation relations

$$[h^{\mathrm{I}},\hat{x}_C^{\mathrm{I}}]=[h^{\mathrm{I}},\hat{x}_R^{\mathrm{I}}]=0,$$

and

$$[\hat{x}_C^{\mathrm{I}},\hat{x}_R^{\mathrm{I}}]=32tu\partial_{tuu}^3-32tu\partial_{ttu}^3-8t(2p_2+1-2u)\partial_{tt}^2+8u(2p_1+1-2t)\partial_{uu}^2+16[(2p_2+1)t-(2p_1+1)u]\partial_{tu}^2-4(2p_1+1)(2p_2+1-2u)\partial_t+4(2p_2+1)(2p_1+1-2t)\partial_u. \tag{10}$$

They generate an infinite-dimensional algebra.

The operators $h^{\mathrm{I}},\hat{x}_C^{\mathrm{I}},\hat{x}_R^{\mathrm{I}}$ as well as the commutator $[\hat{x}_C^{\mathrm{I}},\hat{x}_R^{\mathrm{I}}]$ can be immediately rewritten in terms of the generators $\{J_{1,\ldots,6}\}$ of the maximal parabolic subalgebra of $sl(3,\mathbb{R})$. They have the form

$$h^{\mathrm{I}}=-2J_3J_1-2J_4J_2+2J_3+2J_4-(2p_1+1)J_1-(2p_2+1)J_2, \tag{11}$$

$$\hat{x}_C^{\mathrm{I}}=2J_3J_1-2J_4J_2-2J_3+2J_4+(2p_1+1)J_1-(2p_2+1)J_2, \tag{12}$$

$$\hat{x}_R^{\mathrm{I}}=4J_3J_5+4J_4J_6-8J_3J_4+2(2p_1+1)J_5-2(2p_2+1)J_3-2(2p_1+1)J_4+2(2p_2+1)J_6. \tag{13}$$

The commutation relation (10) is rewritten as

$$[\hat{x}_C^{\mathrm{I}},\hat{x}_R^{I}]=32J_4J_3(J_2-J_1)-16J_4J_6+16J_3J_5+8(2p_1+1)J_4(J_2-2J_1)+8(2p_2+1)J_3(2J_2-J_1)+8(2p_1+1)J_5-8(2p_2+1)J_6+4(2p_1+1)(2p_2+1)(J_2-J_1). \tag{14}$$

Evidently, the operators (11)–(14) preserve a triangular flag of polynomials $\mathcal{P}^{(2)}$ in t,u:

$$h(t):\mathcal{P}_n(t,u)\mapsto\mathcal{P}_n(t,u),$$

where $\mathcal{P}_n(t,u)=\langle t^pu^q|0\leqslant p+q\leqslant n\rangle$. Hence, the operators $h^{\mathrm{I}},\hat{x}_C^{\mathrm{I}},\hat{x}_R^{\mathrm{I}}$ are characterized by infinitely many finite-dimensional invariant subspaces and thus possess infinitely many polynomial eigenfunctions.

Case II: The second superintegrable Hamiltonian can be separated in Cartesian and parabolic coordinates. In Cartesian coordinates it is given by

$$H_{\mathrm{II}}(x,y)=-\frac{1}{2}(\partial_x^2+\partial_y^2)+2\omega^2x^2+\frac{\omega^2}{2}y^2+\frac{B}{2y^2}, \tag{15}$$

where $B>-1/8$ is a parameter. The eigenfunctions and eigenvalues have the form

$$\Psi_{n,m}(x,y)=y^{p_2}H_n(\sqrt{2\omega}x)L_m^{(-1/2+p_2)}(\omega y^2)\exp\left(-\omega x^2-\frac{\omega y^2}{2}\right),$$

$$E_{n,m}=\omega\left[2(n+m)+p_2+\frac{3}{2}\right], \tag{16}$$

where $n,m=0,1,2,\ldots$; the parameter p_2 is defined by the relation $B=p_2(p_2-1)$. The degree of degeneracy is given by the number of partitions of a non-negative integer into the sum of two nonnegative integers.

We perform a gauge rotation of $H_{\rm II}(x,y)$ with the ground state eigenfunction (16), $\Psi_{0,0}(x,y)$ as a gauge factor and then a change of variables

$$h^{\rm II}\equiv\frac{1}{\omega}(\Psi_{0,0}(x,y))^{-1}H_{\rm II}(x,y)\Psi_{0,0}(x,y)\big|_{t=\sqrt{2\omega}x,u=\omega y^2}$$

$$=-\partial_t^2-2u\partial_u^2+2t\partial_t+(2u-1-2p_2)\partial_u+\frac{3}{2}+p_2. \tag{17}$$

It is easy to check that the operators

$$\hat{x}_C^{\rm II}=2\partial_t^2-4u\partial_u^2-4t\partial_t+2(2u-1-2p_2)\partial_u-1+2p_2, \tag{18}$$

$$\hat{x}_P^{\rm II}=-4tu\partial_u^2+4u\partial_{tu}^2-(2u-1-2p_2)\partial_t-2t(1+2p_2)\partial_u, \tag{19}$$

generate an infinite dimensional algebra. They obey the commutation relations

$$[h^{\rm II},\hat{x}_C^{\rm II}]=[h^{\rm II},\hat{x}_P^{\rm II}]=0,$$

and

$$[\hat{x}_C^{\rm II},\hat{x}_P^{\rm II}]=-32u\partial_{tuu}^3-16(1+2p_2-2u)\partial_{tu}^2+32tu\partial_{uu}^2$$
$$+8(1+2p_2-2u)\partial_t+16t(1+2p_2)\partial_u]. \tag{20}$$

The operators $h^{\rm II},\hat{x}_C^{\rm II},\hat{x}_P^{\rm II}$ as well as the commutator $[\hat{x}_C^{\rm II},\hat{x}_P^{\rm II}]$ can be immediately rewritten in terms of the generators (4) and have the form

$$h^{\rm II}=-J_1J_1-2J_4J_2+2J_3+2J_4-(1+2p_2)J_2+\tfrac{3}{2}+p_2, \tag{21}$$

$$\hat{x}_C^{\rm II}=2J_1J_1-4J_4J_2-4J_3+4J_4-2(1+2p_2)J_2-1+2p_2, \tag{22}$$

$$\hat{x}_P^{\rm II}=-4J_4J_6+4J_1J_4-2J_5+(1+2p_2)J_1-2(1+2p_2)J_6. \tag{23}$$

Evidently, operators (21)–(23) preserve the same triangular flag of polynomials as in case I but in variables x,u:

$$h(x,u):\mathcal{P}_n(x,u)\mapsto\mathcal{P}_n(x,u),$$

where $\mathcal{P}_n(x,u)=\langle x^pu^q|0\leqslant p+q\leqslant n\rangle$. Thus, the operators $h^{\rm II},\hat{x}_C^{\rm II},\hat{x}_P^{\rm II}$ have infinitely many finite dimensional invariant subspaces and infinitely many polynomial eigenfunctions.

Case III: The third superintegrable Hamiltonian

$$H_{\rm III}(x,y)=-\frac{1}{2}(\partial_x^2+\partial_y^2)+\frac{\alpha}{2r}+\frac{1}{4r^2}\left(\frac{\beta_1}{\cos^2\frac{\phi}{2}}+\frac{\beta_2}{\sin^2\frac{\phi}{2}}\right), \tag{24}$$

where $\beta_{1,2}>-1/8$ are parameters and $x=r\cos\phi,y=r\sin\phi$. It admits the separation of variables in polar and parabolic coordinates. In parabolic coordinates it has the form

$$H_{\rm III}(\xi,\eta)=-\frac{1}{2}\frac{1}{\xi^2+\eta^2}(\partial_\xi^2+\partial_\eta^2)+\frac{1}{\xi^2+\eta^2}\left(2\alpha+\frac{\beta_1}{\xi^2}+\frac{\beta_2}{\eta^2}\right), \tag{25}$$

with $x=\frac{1}{2}(\xi^2-\eta^2),y=\xi\eta$. The eigenfunctions corresponding to the energy E are

$$\Psi_{n,m}=\xi^{p_1}\eta^{p_2}L_n^{(-1/2+p_1)}(\sqrt{-2E}\,\xi^2)L_m^{(-1/2+p_2)}(\sqrt{-2E}\,\eta^2)e^{-\sqrt{-E/2}(\xi^2+\eta^2)}, \tag{26}$$

where $2\beta_1=p_1(p_1-1),2\beta_2=p_2(p_2-1)$. It is easy to see that the Schrödinger equation $H_{\rm III}\Psi=E\Psi$ can be transformed into

$$\left[-\frac{1}{2}(\partial_\xi^2+\partial_\eta^2)-E(\xi^2+\eta^2)+\frac{\beta_1}{\xi^2}+\frac{\beta_2}{\eta^2}\right]\Psi=-2\alpha\Psi. \tag{27}$$

We introduce the notation

$$Q_{\rm III}\equiv(\xi^2+\eta^2)(H_{\rm III}-E)-2\alpha. \tag{28}$$

Equation (27) can be written as

$$Q_{\rm III}\Psi=-2\alpha\Psi, \tag{29}$$

and $Q^{\rm III}$ can be related to $H^{\rm I}$,

$$Q_{\rm III}=H_{\rm I}(\xi,\eta;-E,\beta_1,\beta_2), \tag{30}$$

[cf. (5)]. We draw the striking conclusion that the Hamiltonian of the first problem (case I) written in Cartesian coordinates coincides with a modified third Hamiltonian $Q^{\rm III}$ written in parabolic coordinates (!). The parameter (-2α) plays the role of spectral parameter which is the energy in case I, $(-2\alpha)\leftrightarrow E^{\rm I}$. Thus, the analysis performed for case I can be repeated for this case.

We perform a gauge rotation of the operator $Q_{\rm III}$ with a gauge factor given by the multiplier figuring in Eq. (26),

$$M_{\rm III}=\xi^{p_1}\eta^{p_2}e^{-\sqrt{-E/2}(\xi^2+\eta^2)}. \tag{31}$$

Notice that in this case, contrary to those of $H_{\rm I}$ and $H_{\rm II}$, the gauge factor is not universal. It depends on the energy E. Thus E in the multiplier M is the considered energy, not the ground state one.

Thus we have

$$q^{\rm III}\equiv\frac{1}{\sqrt{-2E}}M_{\rm III}^{-1}Q_{\rm III}(x,y)M_{\rm III},$$

and with a change of coordinates $t=\sqrt{-2E}\,\xi^2,u=\sqrt{-2E}\,\eta^2$ we get

$$q^{\rm III}=-2t\partial_t^2-2u\partial_u^2+2t\partial_t+2u\partial_u-(2p_1+1)\partial_t-(2p_2+1)\partial_u+1+p_1+p_2. \tag{32}$$

This operator coincides *exactly* with the operator $h^{\rm I}$ (7). Its spectrum is equal to $-2\alpha/\sqrt{-E}=2(n+m)+1+p_1+p_2,n,m=0,1,2,\ldots$.

Thus, the operator $q^{\rm III}$ commutes with $\hat{x}_C^{\rm I},\hat{x}_R^{\rm I}$. We shall call these operators $\hat{x}_C^{\rm III},\hat{x}_R^{\rm III}$. The operator $q^{\rm III}$ can be rewritten in terms of the generators $\{J_{1,\ldots,6}\}$ of the maximal parabolic subalgebra of $sl(3,\mathbb{R})$ [see (4)] . We see that the Hamiltonian (24) is exactly solvable.

The above observation gives rise to an interesting question about the connection between the operators commuting with original Hamiltonian (24) and the operators $\hat{x}_C^{\rm III},\hat{x}_R^{\rm III}$.

The operators that commute with $Q_{\rm III}$ of Eq. (28) can be read off from those of case H_1. They are in parabolic coordinates

$$X_C^{\rm III}=-\frac{1}{2}(\partial_\xi^2-\partial_\eta^2)-E(\xi^2-\eta^2)+\frac{\beta_1}{\xi^2}-\frac{\beta_2}{\eta^2},$$
$$X_R^{\rm III}=(\xi\partial_\eta-\eta\partial_\xi)^2-2(\xi^2+\eta^2)\left(\frac{\beta_1}{\xi^2}+\frac{\beta_2}{\eta^2}\right). \tag{33}$$

The operators that commute with the original Hamiltonian $H_{\rm III}$ of Eq. (25), if written in parabolic coordinates, are[3,4,17]

$$X_P=\frac{1}{\xi^2+\eta^2}\left(\eta^2\partial_\xi^2-\xi^2\partial_\eta^2+2\alpha(\xi^2-\eta^2)-2\beta_1\frac{\eta^2}{\xi^2}+2\beta_2\frac{\xi^2}{\eta^2}\right),$$
$$X_R=(\xi\partial_\eta-\eta\partial_\xi)^2-2(\xi^2+\eta^2)\left(\frac{\beta_1}{\xi^2}+\frac{\beta_2}{\eta^2}\right). \tag{34}$$

Let us consider, quite generally, a Hamiltonian H and an operator Q, defined by

$$H=\frac{Q+K}{\xi^2+\eta^2}+E, \tag{35}$$

where K is a constant and E is the energy. Let X be an operator commuting with the Hamiltonian: $[H,X]=0$. The operator Q then satisfies

$$[Q,X]=(\xi^2+\eta^2)\left[X,\frac{1}{\xi^2+\eta^2}\right](\xi^2+\eta^2)(H-E). \tag{36}$$

Thus, if the operator X commutes with H (strongly, as an operator), it commutes weakly, on functions Ψ satisfying $(H-E)\Psi=0$, with Q. So, in order to relate operators that commute with H and those that commute with Q, we have to consider linear combinations of the type $AX_P+BX_R+f(\xi,\eta)\ (H-E)$. Here A and B are constants, but $f(\xi,\eta)$ can be any function, since $H-E$ vanishes on the ''energy shell.''

Let us return to the problem at hand, i.e., the system characterized by the Hamiltonian $H_{\rm III}$, or equivalently, by the operator $Q_{\rm III}$. We have the following simple relation between the original integrals X_P and X_R and the modified ones (33)

$$X_C^{\rm III}=-X_P+(\xi^2-\eta^2)(H-E),\quad X_R^{\rm III}=X_R. \tag{37}$$

Case IV: The fourth superintegrable Hamiltonian admits the separation of variables in two mutually perpendicular parabolic systems of coordinates. In the usual parabolic coordinates ξ,η it has the form

$$H_{\rm IV}(\xi,\eta)=-\frac{1}{2}\frac{1}{\xi^2+\eta^2}(\partial_\xi^2+\partial_\eta^2)+\frac{1}{\xi^2+\eta^2}(2\alpha+\beta\xi+\gamma\eta). \tag{38}$$

The eigenfunctions are products of Laguerre polynomials times an energy dependent multiplier, namely

$$M_{\rm IV}=(\xi-\beta/2E)^{p_1}(\eta-\gamma/2E)^{p_2}e^{-\sqrt{-E/2}[(\xi-\beta/2E)^2+(\eta-\gamma/2E)^2]}$$

with a condition $\alpha+\dfrac{\beta^2}{4E}+\dfrac{\gamma^2}{4E}+\sqrt{-2E}=0$ and $p_1,p_2=0,1$.

The corresponding Schrödinger equation $H_{\mathrm{IV}}\Psi=E\Psi$ can be rewritten as

$$\left[-\frac{1}{2}(\partial_\xi^2+\partial_\eta^2)-E\left(\xi-\frac{\beta}{2E}\right)^2-E\left(\eta-\frac{\gamma}{2E}\right)^2\right]\Psi=\left(-2\alpha-\frac{\beta^2+\gamma^2}{4E}\right)\Psi. \tag{39}$$

For the operator on the left-hand side we introduce the notation

$$Q_{\mathrm{IV}}\equiv(\xi^2+\eta^2)(H^{\mathrm{IV}}-E)-2\alpha-\frac{\beta^2+\gamma^2}{4E}.$$

Equation (39) can be written as

$$Q_{\mathrm{IV}}\Psi=\tilde{\alpha}\Psi,$$

with the new spectral parameter $\tilde{\alpha}=-2\alpha-(\beta^2+\gamma^2)/4E$.

The operator Q^{IV} can be related to H^{I},

$$Q_{\mathrm{IV}}=H_{\mathrm{I}}(\xi,\eta;-E,0,0), \tag{40}$$

[cf. (5) and (30)]. We see that similar to case III the Hamiltonian of case I written in Cartesian coordinates coincides with a modified fourth Hamiltonian Q_{IV} written in parabolic coordinates. The parameter $\tilde{\alpha}$ plays the role of a spectral parameter which was the energy in the first case, $\tilde{\alpha}\leftrightarrow E^{\mathrm{I}}$. Thus, the analysis performed for case I can be again repeated for this case.

Writing the gauge rotated operator Q_{IV} in new coordinates

$$t=\sqrt{-2E}(\xi-\beta/2E)^2,\quad u=\sqrt{-2E}(\eta-\gamma/2E)^2$$

we get

$$q^{\mathrm{IV}}\equiv\frac{1}{\sqrt{-2E}}M_{\mathrm{IV}}^{-1}Q_{\mathrm{IV}}(x,y)M_{\mathrm{IV}}$$

$$=-2t\partial_t^2-2u\partial_u^2+2t\partial_t+2u\partial_u-(2p_1+1)\partial_t-(2p_2+1)\partial_u+1+p_1+p_2.$$

This operator coincides *exactly* with the operator h^{I} (7) and q^{III} (32). Its spectrum is equal to $2(n+m)+1+p_1+p_2, n,m=0,1,2,\ldots$.

Thus, the operator q^{IV} commutes with $\hat{x}_C^{\mathrm{I}},\hat{x}_R^{\mathrm{I}}$. We shall call these operators $\hat{x}_C^{\mathrm{IV}},\hat{x}_R^{\mathrm{IV}}$. The operator q^{IV} (as well as $\hat{x}_C^{\mathrm{IV}},\hat{x}_R^{\mathrm{IV}}$) can be rewritten in terms of the generators $\{J_{1,\ldots,6}\}$ of the maximal parabolic subalgebra of $sl(3,\mathbb{R})$ [see (4)] and hence is exactly solvable.

As in case III one can give the connection between the operators commuting with original Hamiltonian (38) and the operators $\hat{x}_C^{\mathrm{IV}},\hat{x}_R^{\mathrm{IV}}$. The operators commuting with H_{IV} are[3,4,17]

$$X_1=\frac{1}{2(\xi^2+\eta^2)}\{\eta^2\partial_\xi^2-\xi^2\partial_\eta^2+2\alpha(\xi^2-\eta^2)+2\xi\eta(\gamma\xi-\beta\eta)\},$$

$$X_2=\frac{1}{(\xi^2+\eta^2)}\{\xi\eta(\partial_\xi^2+\partial_\eta^2)+(-\beta\eta+\gamma\xi)(\xi^2-\eta^2)-4\alpha\xi\eta\}-\partial_{\xi\eta}^2. \tag{41}$$

Two second order differential operators commuting with Q_{IV} of Eq. (40) can be related to (41) and are given by

$$Q^{(1)}=-2X_1+(\xi^2-\eta^2)(H_{\rm IV}-E)+\frac{\gamma^2-\beta^2}{4E}, \tag{42}$$

$$Q^{(2)}=X_2+2\xi\eta(H_{\rm IV}-E)-\frac{\beta\gamma}{2E}. \tag{43}$$

From this point of view the fourth superintegrable system is particularly simple. Explicitly, we have a new ''Hamiltonian''

$$Q_{\rm IV}=-\frac{1}{2}(\partial_\xi^2+\partial_\eta^2)-E\left[\left(\xi-\frac{\beta}{2E}\right)^2+\left(\eta-\frac{\gamma}{2E}\right)^2\right], \tag{44}$$

which corresponds to the harmonic oscillator, while one of the commuting operators satisfies

$$Q^{(1)}=X_C^{\rm I}, \tag{45}$$

where the integral $X_C^{\rm I}$ [see Eq. (8)] is written in the coordinates $(\xi-\beta/2E),(\eta-\gamma/2E)$.

In turn, the operator $\hat{X}_R^{\rm I}$ reduces to

$$\hat{X}_R^{\rm I}=\left[\left(\xi-\frac{\beta}{2E}\right)\partial_\eta-\left(\eta-\frac{\gamma}{2E}\right)\partial_\xi\right]^2\equiv L_z^2. \tag{46}$$

Thus, the superintegrable system characterized by the Hamiltonian $H_{\rm IV}(\xi,\eta)$ has been reduced to a harmonic oscillator with ''frequency'' $\omega=\sqrt{-E/2}$ and a displaced equilibrium point $\xi=\beta/2E$, $\eta=\gamma/2E$. It is well known that the harmonic oscillator is invariant under an SU(2) group. Indeed, we find that the ''Hamiltonian'' $Q_{\rm IV}$ commutes with $Q^{(1,2)}$ and L_z. The operators (42), (43), (44) and L_z form the basis of a $u(2)$ symmetry algebra with $Q_{\rm IV}$ as its center.

III. CONCLUSION

In general, integrability of a quantum system does not guarantee that spectrum and eigenfunctions can be found in sufficiently explicit form. The simplest example of this situation is given by one-dimensional quantum dynamics which is integrable for any potential. The main message of the present work is that the superintegrable systems on E_2 with the integrals given by second-order differential operators are exactly solvable as well. We conjecture that the property of exact solvability will remain valid for higher dimensional superintegrable systems of the above-mentioned type.

Note added in proof. Our conjecture on the exact solvability of general superintegrable systems has recently received further development. Indeed, all superintegrable systems with second order in momentum integrals of motion in a two-dimensional space of revolution with non-constant curvature were recently found (E. G. Kalnins, J. M. Kress, and P. Winternitz, Superintegrability in a two-dimensional space of nonconstant curvature, submitted for publication). All of them turned out to be exactly solvable.

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Geometric quantization on the super-disk

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In this article we discuss the geometric quantization on a certain type of infinite dimensional super-disk. Such systems are quite natural when we analyze coupled bosons and fermions. The large-N limit of a system like that corresponds to a certain super-homogeneous space. First, we define an example of a super-homogeneous manifold: a super-disk. We show that it has a natural symplectic form, and it can be used to introduce classical dynamics once a Hamiltonian is chosen. Existence of moment maps provide a Poisson realization of the underlying symmetry super-group. These are the natural operators to quantize via methods of geometric quantization, and we show that this can be done. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1387270]

I. INTRODUCTION

Geometric quantization is an interesting and useful program for quantizing systems whose phase spaces have a simple geometric description.[1] It is not always the case that the phase space has a nice geometric structure, and, even if it does, the result of quantizing via this method does not actually solve the problem, but in many cases just helps one to formulate it. The geometric approach to quantization goes back to works of Berezin[2–5] and at about the same time appeared in the mathematics literature as well.

In this work we will extend our previous analysis[6] to the context of super-geometry. This is interesting in two ways: one is purely mathematical, it gives a natural way to construct unitary representations of the underlying symmetry group. The other one is the possibility of understanding physical systems which have coupled bosons and fermions. Super-geometry sets the natural arena for formulating and studying these problems. Our approach originates from ideas of Rajeev on the large-N limit of field theories. Rajeev has shown that a proper large-N limit of quantum chromodynamics (QCD) in two dimensions has a natural phase space given by an infinite dimensional Grassmannian.[7] This general philosophy can be extended to other cases.[6,8] Whenever there is a mixture of fermions and bosons, the large-N phase space is expected to be a certain kind of super-homogeneous manifold. In gauge theory, we have shown that this space is given by a certain kind of super-Grassmannian.[8] If instead we are looking at a fermionic system which has only a finite number of degrees of freedom coupled to a bosonic field theory, its large-N limit can be formulated as a certain type of super-disk. This can be seen as follows: we get for such a system, in the language of creation and annihilation operators, bilinears of the form

$$N(p,q)=\frac{2}{N}:a^{\dagger\alpha}(p)a(q)_{\alpha}:,\quad M_{ij}=\frac{2}{N}\chi_i^{\dagger\alpha}\chi_{\alpha j},\quad Q_i(p)=\frac{2}{N}\chi_i^{\dagger\alpha}a_{\alpha}(p),\quad \overline{Q_i}(p)=\frac{2}{N}a^{\dagger\alpha}(p)\chi_{\alpha i}, \tag{1}$$

where we have a normal ordering : : for only the bosonic products and α denotes a ''color'' index. These operators are the natural ones for the large-N phase space of the theory. In general it may not be possible to express all the dynamical variables in terms of these bilinears, but if we restrict ourselves to the ''color invariant'' sector, these are the only ones we can compose. We note that

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this statement is strictly true when we look at a gauge theory in $1+1$ dimensions,[8] but for that we need infinite degrees of freedom for the fermions, and that requires an analog of the Grassmannian. In some other cases this is only an approximation to the full model, the validity of which has to be tested depending on the specifics. As an example we write down a nonrelativistic model, where a bosonic self-coupled field also couples with localized fermionic sources,

$$H=\int \left(:\nabla \phi^{\dagger\alpha}.\nabla \phi_\alpha + m^2 \phi^{\dagger\alpha}\phi_\alpha + \frac{\lambda^2}{2}(\phi^{\dagger\alpha}\phi_\alpha)^2: + g\sum_i \rho(x)(\phi_\alpha \chi_i^{\dagger\alpha}(t) + \phi^{\dagger\alpha}\chi_{\alpha i}(t)) \right). \quad (2)$$

These models may exhibit rather nontrivial dynamics, depending on the dimension we may need to renormalize the coupling constants. Our approach with Hilbert–Schmidt operators excludes cases which require renormalization, although a general super-disk is still present. The above operators actually provide a realization of the super-Lie algebra $U(\mathcal{H}^e_-, \mathcal{H}^e_+ | \mathcal{H}^o_+)$ as we will see. In fact, one can see that many super-Lie algebras have natural realizations by fermionic and bosonic operators.[9]

In this article we will only deal with the mathematical aspects of this problem and think of geometric quantization as a method for constructing the quantum Hilbert space where the dynamics takes place. Solving a specific model perhaps should be done first in the classical setting of the large-N limit.

II. THE SUPER-DISK

In this section we present a brief definition of the super-disk which we denote by D_1^I following Ref. 10; we mostly adopt their conventions. As we will see there is a small difference between our approach and this reference. In the same reference there is a nice discussion of other cases, which one can generalize in the same way, but we choose to look at the above simpler case for the sake of clarity. The previous paper by the same authors[11] give a more detailed discussion of the $U(1,1|1)$ case. Since the general case in Ref. 10 is treated in a sussinct manner, we prefer to give a detailed discussion and believe that some of the explicit formulas could be useful for the reader. The physically interesting case requires an additional complication compared to the one in Ref. 10: one should look at an infinite Grassmann algebra. We will briefly discuss this generalization, yet the results are not so simple and as rigorous as in the finite dimensional one. Some other useful sources are the lectures of Kostant[12] and the books by Berezin[13] and Manin.[14]

Let us consider two Hilbert spaces, $\mathcal{H}^e$ and $\mathcal{H}^o$, which correspond to the even and odd spaces, respectively. In physically interesting cases they are either both separable infinite dimensional, or the even one is separable infinite dimensional and the odd one is finite dimensional. To keep the rigor we will only deal with $\mathcal{H}^o_+$ finite dimensional, but arbitrarily large. Let us assume that its dimension is N; later on we will extend this to infinite dimensions. We will split the even space into positive and negative parts, each piece being infinite dimensional, $\mathcal{H}^e=\mathcal{H}^e_-\oplus\mathcal{H}^e_+$. We will really think of the odd part as the positive subspace and denote it as $\mathcal{H}^o_+$. This is just for convenience at the moment since we have not attached any physical significance to D_1^I.

We may denote the $\mathbf{Z}$ graded super-space as $\mathcal{H}$, which splits with respect to $\mathbf{Z}_2$ grading as $\mathcal{H}^e|\mathcal{H}^o$. It will be better to decompose this space as $\mathcal{H}=\mathcal{H}^e_-\oplus\mathcal{H}^e_+|\mathcal{H}^o_+$. Let us introduce the set of complex super matrices Z such that

$$Z=[w \quad \theta], \quad (3)$$

where $w:\mathcal{H}^e_+\to\mathcal{H}^e_-$ and $\theta:\mathcal{H}^o_+\to\mathcal{H}^e_-$. Furthermore, we require the following convergence conditions $w\in\mathcal{I}_2$ and $\theta\in\mathcal{I}_2$, where $\mathcal{I}_2$ denotes the Hilbert–Schmidt ideal in this context. A super space is given by the algebra of smooth functions living on it. In any given super-chart $\mathcal{U}$ we have $C^\infty(\mathcal{U})\approx C^\infty(U)\otimes\wedge(\mathbf{C}^s)$ for some s, and here U denotes the corresponding open set for the base manifold. [In Ref. 10 the underlying function algebra for the odd generators is chosen to be $\wedge(\mathbf{C}^{mq})$. We will instead take the set of generators as $\wedge(\mathbf{C}^n)$, and θ denotes the matrix of linear transformations from the super vector space $\mathcal{H}^o_+$ to $\mathcal{H}^e_-$.]

Let us explain the meaning of these convergence conditions: if we expand the matrix w into a series,

$$w = w_B + w_{a_1 a_2} \xi^{a_1} \xi^{a_2} + \cdots , \tag{4}$$

where ξ^a denotes half of the odd generators and this series terminates. There are also Hermitian conjugates, that is, we have a set of coordinates ξ^a and ξ^{*a}. (Since the base manifold is contractable, this expression is true; otherwise we need to assume it on any given chart.) Then, we assume that each one of these matrices is in the Hilbert–Schmidt class,[15] i.e., $w_B^\dagger w_B, w_{a_1 a_2}^\dagger w_{a_1 a_2}, \ldots, w_{12\ldots r}^\dagger w_{12\ldots r} \in \mathcal{I}_1$. Here we use $\mathcal{I}_1$ to denote trace class operators. This decomposition is basis dependent, but the condition is basis invariant. It is possible to see this by looking at a change of basis which is given by an invertible super-matrix (non-type changing one):

$$(SwS^{-1})_B = S_B w_B S_B^{-1} \cdots ,$$

$$(SwS^{-1})_{a_1 a_2 \cdots a_{2k}} = S_B w_{a_1 a_2 \cdots a_{2k}} S_B^{-1} + \cdots + S_{a_1 \cdots a_{2m}} w_{a_{2m+1} \cdots a_{2n}} S^{-1}_{a_{2n+1} \cdots a_{2k}} \cdots ,$$

etc., and we see that each component is replaced by a sum, each term of which is conjugated by some bounded operators. The conjugated elements themselves are of Hilbert–Schmidt class. From this we conclude that our condition is basis independent. We point out that some variants of this argument on the Hilbert–Schmidt condition will be used over and over again. We have the same for θ except that θ only has odd terms. Notice that the second of these conditions is automatically true since the odd space is finite dimensional. In a more general case we will mention later on, there will be extra convergence conditions on the odd generators. In this setting w is even and θ is odd. For computations it is sometimes better to decompose a given matrix into its ordinary part and its nilpotent part, just like a super number being decomposed into an ordinary complex number plus the rest. We use the terminology of deWitt[16] and call it body and soul decomposition. For example, $w = w_B + w_S$ and $\theta = \theta_S$. Let us define the restricted super-disk as the algebra of functions generated by the above set of super-operators Z with a further condition on w,

$$1 - w_B^\dagger w_B > 0. \tag{5}$$

Notice that we can interpret these to be the elements which generate the C^∞ functions on the super-disk. For later use we must give a meaning to $Z^\dagger Z$, so we define it to be the tensor product,

$$Z^\dagger Z = \begin{pmatrix} w^\dagger w & w^\dagger \theta \\ \theta^\dagger w & \theta^\dagger \theta \end{pmatrix}.$$

We do not demand any extra conditions on the θ variable. The inverse of $1 - Z^\dagger Z$ can be computed; we write

$$(1 - Z^\dagger Z)^{-1} = 1 + Z^\dagger (1 - ZZ^\dagger)^{-1} Z, \tag{6}$$

and similarly for w_B we have $(1 - w_B w_B^\dagger)^{-1} = 1 + w_B (1 - w_B^\dagger w_B)^{-1} w_B^\dagger$ and the operator on the right is well-defined due to positivity condition. This means that the inverse on the left also exists. Since we use a finite dimensional odd-space we can define

$$\begin{aligned} (1 - ZZ^\dagger)^{-1} &= (1 - w_B w_B^\dagger - w_B^\dagger w_S - w_S^\dagger w_B - w_S^\dagger w_S - \theta\theta^\dagger)^{-1} \\ &= [1 - (1 - w_B w_B^\dagger)^{-1} (w_B^\dagger w_S + w_S^\dagger w_B + w_S^\dagger w_S + \theta\theta^\dagger)]^{-1} (1 - w_B w_B^\dagger)^{-1}, \end{aligned}$$

the first inverse in the last term can be expressed via a terminating expansion,

$$[1-(1-w_Bw_B^\dagger)^{-1}(w_B^\dagger w_S+w_S^\dagger w_B+w_S^\dagger w_S+\theta\theta^\dagger)]^{-1}$$
$$=1+(1-w_Bw_B^\dagger)^{-1}(w_B^\dagger w_S+w_S^\dagger w_B+w_S^\dagger w_S+\theta\theta^\dagger)-\cdots$$
$$+(-1)^{s-1}[(1-w_Bw_B^\dagger)^{-1}(w_B^\dagger w_S+w_S^\dagger w_B+w_S^\dagger w_S+\theta\theta^\dagger)]^s,$$

where we assume that the degree of nilpotency of the supermatrix is $s+1$. We note that this is a general fact. If the body of a matrix is invertible, then the matrix is invertible. This series does not have to terminate in the infinite dimensional case, so one has to impose the invertibility condition separately, or assume that the infinite formal expansion can be given a meaning (see the book by deWitt[16]). The definition we propose later on may result in a deviation from the Kostant–Berezin–Leites definition.[12,13]

There is a natural super-operator on the space $\mathcal{H}$ given with respect to the above direct sum as

$$J=\begin{pmatrix}1&0&0\\0&-1&0\\0&0&-1\end{pmatrix}. \tag{7}$$

Similar to the finite dimensional case, we have an action of a certain super-pseudounitary group on the super-disk D_1^I. Let us define the set of superoperators $g:\mathcal{H}\to\mathcal{H}$ with a bounded inverse, such that they leave the operator J invariant:

$$gJg^\dagger=J. \tag{8}$$

Let us explicitly write this condition in a block decomposition:

$$g=\begin{pmatrix}A&B\\C&D\end{pmatrix}, \tag{9}$$

and here $A:\mathcal{H}_-^e\to\mathcal{H}_-^e$, $B:\mathcal{H}_+^e|\mathcal{H}_+^o\to\mathcal{H}_-^e$, $C:\mathcal{H}_-^e\to\mathcal{H}_+^e|\mathcal{H}_+^o$. Finally, $D:\mathcal{H}_+^e|\mathcal{H}_+^o\to\mathcal{H}_+^e|\mathcal{H}_+^o$. This representation is better suited for our needs. We have then

$$AA^\dagger-BB^\dagger=1,\quad CA^\dagger=DB^\dagger,\quad DD^\dagger-CC^\dagger=1. \tag{10}$$

Using the invertibility we see that $g^\dagger Jg=J$ is also true, hence we get

$$A^\dagger A-C^\dagger C=1,\quad A^\dagger B=C^\dagger D,\quad D^\dagger D-B^\dagger B=1. \tag{11}$$

The first one means, in terms of body and soul decomposition,

$$A_BA_B^\dagger-B_BB_B^\dagger=1,\quad A_S^\dagger A_B+A_B^\dagger A_S+A_S^\dagger A_S+C_B^\dagger C_S+C_S^\dagger C_B+C_S^\dagger C_S=0, \tag{12}$$

and similarly for the others. This means that the body parts of these matrices obey exactly the usual pseudounitary conditions, hence we can do everything in the same way like the non-super-case. Among these sets of operators we pick the ones which satisfy a convergence condition, written with respect to the direct sum decomposition $\mathcal{H}_-^e\oplus\mathcal{H}_+^e|\mathcal{H}_+^o$,

$$g=\begin{pmatrix}\mathcal{B}&\mathcal{I}_2&\mathcal{I}_2\\\mathcal{I}_2&\mathcal{B}&\mathcal{B}\\\mathcal{I}_2&\mathcal{B}&\mathcal{B}\end{pmatrix}, \tag{13}$$

and these conditions are imposed on the components of each term, i.e., if we expand the upper corner, $\beta=\beta_a\xi^a+\beta_{a_1a_2a_3}\xi^{a_1}\xi^{a_2}\xi^{a_3}+\cdots$, each term belongs to $\mathcal{I}_2$ and similarly for the other parts. We may also economically express these in the form $[J,g]\in\mathcal{I}_2$, with the above interpretation for the ideal. Therefore we can summarize the above set of operators in the form of a group:

$$U_1(\mathcal{H}^e_-,\mathcal{H}^e_+|\mathcal{H}^o_+)=\{g|g^{-1}\ \text{exists},\ [J,g]\in\mathcal{I}_2\quad\text{and}\ gJg^\dagger=J\},\tag{14}$$

where the ideal condition refers to our convention. The main point is to show that the convergence conditions hold after the multiplication. This follows the same line of arguments as before. If one writes explicitly the components, we see that each one is a finite sum of Hilbert–Schmidt operators. We leave it to the reader to check the details. This group is one possible super version of the pseudounitary group. We refer to this set as the restricted super-pseudounitary group.

Just like the classical case, the restricted super-pseudounitary group has an action on the super-disk D_1^I. This action is written in the super-operator language exactly as in the classical case:

$$Z\mapsto(AZ+B)(CZ+D)^{-1},\tag{15}$$

where we use

$$g=\begin{pmatrix}A & B\\ C & D\end{pmatrix}.\tag{16}$$

We need to clarify the action of C, if we denote C as $\binom{c}{\gamma}$,

$$CZ=C\otimes Z=\begin{pmatrix}cw & c\theta\\ \gamma w & \gamma\theta\end{pmatrix},\tag{17}$$

which shows that the action is well-defined and the resulting operator goes from $\mathcal{H}^e_+|\mathcal{H}^o_+$ to $\mathcal{H}^e_+|\mathcal{H}^o_+$, thus we can add D to this. Let us note that the inverse on the right exists. This is because the even part has an inverse and we can define the inverse by a terminating expansion. Just for an illustration we give the explicit version. The reader who is familiar with this kind of manipulations is advised to skip this part: We would like to show that $CZ+D$ has an inverse. We know that D^{-1} is well-defined, hence it is better to look at $D^{-1}CZ+1$. We use the following formula for the inverse of a super-matrix:

$$\begin{pmatrix}\tilde A & \tilde B\\ \tilde C & \tilde D\end{pmatrix}^{-1}=\begin{pmatrix}(\tilde A-\tilde B\tilde D^{-1}\tilde C)^{-1} & -\tilde A^{-1}\tilde B(\tilde D-\tilde C\tilde A^{-1}\tilde B)^{-1}\\ -\tilde D^{-1}\tilde C(\tilde A-\tilde B\tilde D^{-1}\tilde C)^{-1} & (\tilde D-\tilde C\tilde A^{-1}\tilde B)^{-1}\end{pmatrix}.\tag{18}$$

This can be written in the following form:

$$\begin{pmatrix}1+(d_{11}-\delta_{12}d_{22}^{-1}\delta_{21})^{-1}cw & ***\\ -d_{11}^{-1}\delta_{12}(d_{22}-\delta_{21}d_{11}^{-1}\delta_{12})^{-1}\gamma w & 1-d_{22}^{-1}\delta_{21}(d_{11}-\delta_{12}d_{22}^{-1}\delta_{21})^{-1}c\theta\\ *** & +(d_{22}-\delta_{21}d_{11}^{-1}\delta_{12})^{-1}\gamma\theta\end{pmatrix}.\tag{19}$$

To prove the invertibility, we do not need the explicit forms of the off-diagonal components. This is why they are not shown in the above matrix. The lower diagonal block is invertible, due to the nilpotency of the part added to 1. Hence we need to check only the upper diagonal block (actually, this is a general result). To do this we recall that the super-pseudounitarity means, $DD^\dagger=1+CC^\dagger$, written in terms of components. The upper block gives us $d_{11}d_{11}^\dagger=cc^\dagger+1-\delta_{12}\delta_{12}^\dagger$. This means that we can define an inverse square root of the above matrix; for this we use the following integral representation,

$$T^{-1/2}=\frac{1}{\pi}\int_0^\infty\frac{d\lambda}{\lambda^{1/2}}(T+\lambda I)^{-1}.\tag{20}$$

This formula is used for a positive operator and can be extended to the super case when the body of the super-matrix is positive. (This is the case for us as we will see shortly.) As a result we get

$$(d_{11}d_{11}^{\dagger})^{-1/2}=\frac{1}{\pi}\int_0^{\infty}\frac{d\lambda}{\lambda^{1/2}}[(c_Bc_B^{\dagger}+\lambda 1+1)^{-1}+(c_Bc_B^{\dagger}+\lambda 1+1)^{-1}f_S(c_Bc_B^{\dagger}+\lambda 1+1)^{-1}$$
$$+\cdots\ -(-1)^r((c_Bc_B^{\dagger}+\lambda 1+1)^{-1}f_S)^r(c_Bc_B^{\dagger}+\lambda 1+1)^{-1}].$$

Here we use $f_S=c_Bc_S^{\dagger}+c_Sc_B^{\dagger}+c_Sc_S^{\dagger}+\delta_{12}\delta_{12}^{\dagger}$, which is a nilpotent matrix, and we assumed that it has degree $r+1$. The first term is the usual term $(1+c_Bc_B^{\dagger})^{-1/2}$, the others are nilpotent contributions. Hence when we write this first diagonal block in this form,

$$1+u(1+c_Bc_B^{\dagger})^{-1/2}c_Bw_B+\text{nilpotent parts},\tag{21}$$

where u is a unitary piece that we cannot determine—stripped off from its possible nilpotent part. It is enough to show that this leading part is invertible, but that is the same as in the non-super case: $\|w_B^{\dagger}c_B^{\dagger}(1+c_Bc_B^{\dagger})^{-1/2}u^{\dagger}u(1+c_Bc_B^{\dagger})^{-1/2}c_Bw_B\|\leqslant\|w_B^{\dagger}w_B\|<1$. This implies that the series expansion will converge and we have an invertible element. This concludes our demonstration. Of course we have done more than just showing that the inverse is well-defined, we also got an expansion of the inverse, which is useful to show the convergence condition in the infinite dimensional case. There is a simpler way to show the invertibility, which we repeat here for clarity,

$$(CZ+D)=\begin{pmatrix} cw+d_{11} & c\theta+\delta_{12}\\ \gamma w+\delta_{21} & \gamma\theta+d_{22}\end{pmatrix},\tag{22}$$

and as we have observed for invertibility, it is enough to know the invertibility of the body parts. We have $d_{11}d_{11}^{\dagger}=cc^{\dagger}+1-\delta_{12}\delta_{12}^{\dagger}$, the body parts satisfy $(d_{11})_B(d_{11}^{\dagger})_B=1+c_Bc_B^{\dagger}$, and using the same argument as before this implies that the body is invertible (we already know d_{22} is invertible).

One can check that the resulting operator Z' is an element of the super-disk. We briefly indicate how this is done: The convergence conditions are easy since we have $Z\in\mathcal{I}_2$ and $B\in\mathcal{I}_2$. If we want to show that the resulting operator satisfies $1-w_B'^{\dagger}w_B'>0$, we look at $((AZ+B)(CZ+D)^{-1})_B$. This comes from w',

$$w'=(Aw+b)(cw+d_{11}-(c\theta+\delta_{12})(\gamma\theta+d_{22})^{-1}(\gamma w+\delta_{21}))^{-1},\tag{23}$$

which has body part

$$w_B'=(A_Bw_B+b_B)(c_Bw_B+(d_{11})_B)^{-1}.\tag{24}$$

We have from the pseudounitarity conditions $A_BA_B^{\dagger}-b_Bb_B^{\dagger}=1$, $c_BA_B^{\dagger}=(d_{11})_Bb_B^{\dagger}$, $(d_{11})_B(d_{11}^{\dagger})_B-c_Bc_B^{\dagger}=1$. But these are exactly the conditions for the ordinary pseudounitary group $U_1(\mathcal{H}_-^e,\mathcal{H}_+^e)$, hence the positivity condition follows as in the ordinary case. Of course the point is to show that the action is transitive, and hence to prove that the super-disk is a homogeneous manifold. Let us go over this point as well using similar techniques to the above proof. To prove this it is enough to show that the action is transitive over the generating set of elements for the $C^{\infty}(D_1^I)$ we introduced, $Z=[w\ \theta]$. (Notice that a super manifold is really defined through the algebra of functions living on it.) Let us show that we can obtain all the generators starting from $Z=0$ using the group action. Recall that the pseudounitarity imposes the following conditions,

$$AA^{\dagger}-BB^{\dagger}=1,\quad CA^{\dagger}=DB^{\dagger},\quad D^{\dagger}D-B^{\dagger}B=1.\tag{25}$$

The last one uses the opposite multiplication. For any $Z=BD^{-1}$, if we insert this into the last one we see that $D=(1-Z^{\dagger}Z)^{-1/2}U$, where U is an arbitrary super-unitary element acting on the same space, is a solution. Later on we will prove that this square root makes sense and the body belongs to the desired class, but first we will present the formal solution in the super-matrix form:

$$g=\begin{pmatrix} (1-ZZ^\dagger)^{-1/2}V & Z(1-Z^\dagger Z)^{-1/2}U \\ (1-Z^\dagger Z)^{-1}Z^\dagger(1-ZZ^\dagger)^{1/2}V & (1-Z^\dagger Z)^{-1/2}U \end{pmatrix}, \tag{26}$$

where $V\in U(\mathcal{H}^e_-)$ and $U\in U(\mathcal{H}^e_+|\mathcal{H}^o_+)$. In fact, this shows the ambiguity in the solution to be exactly the subset we mode out with. Let us prove the claim using the integral form of the square root of the matrix. We begin with A,

$$\begin{aligned}(1-ZZ^\dagger)^{-1/2}&=\frac{1}{\pi}\int_0^\infty \frac{d\lambda}{\lambda^{1/2}}(\lambda 1+1-ww^\dagger-\theta\theta^\dagger)^{-1}\\ &=(1-w_Bw_B^\dagger)^{-1/2}+\frac{1}{\pi}\int_0^\infty \frac{d\lambda}{\lambda^{1/2}}(\lambda 1+1-w_Bw_B^\dagger)^{-1}f_S(\lambda 1+1-w_Bw_B^\dagger)^{-1}\\ &\quad+\cdots-(-1)^r\frac{1}{\pi}\int_0^\infty \frac{d\lambda}{\lambda^{1/2}}(\lambda 1+1-w_Bw_B^\dagger)^{-1}[f_S(\lambda 1+1-w_Bw_B^\dagger)^{-1}]^r,\end{aligned}$$

where $f_S=w_Sw_B^\dagger+w_Bw_S^\dagger+w_Sw_S^\dagger+\theta\theta^\dagger$. All the terms are properly defined. Let us now indicate that D is well-defined. We do this for the upper corner only,

$$D=(1-Z^\dagger Z)^{-1/2}=\frac{1}{\pi}\int_0^\infty \frac{d\lambda}{\lambda^{1/2}}\begin{pmatrix} \lambda 1+1-w^\dagger w & -w^\dagger\theta \\ -\theta^\dagger w & \lambda 1+1-\theta^\dagger\theta \end{pmatrix}^{-1}. \tag{27}$$

[Just for fun, we suggest to the reader to show the following identity, which gives an alternative proof of the existence, $(1-Z^\dagger Z)^{-1/2}=1+Z^\dagger((1-ZZ^\dagger)^{-1/2}-\frac{1}{2}\int_0^1 dt(1-tZZ^\dagger)^{-1/2})Z$.] As a result of this expression we see that all the elements are well-defined and belong to the correct classes. In fact, we can write the expansion for d_{11},

$$\begin{aligned}d_{11}&=(1-w_B^\dagger w_B)^{-1/2}+\frac{1}{\pi}\int_0^\infty \frac{d\lambda}{\lambda^{1/2}}(\lambda 1+1-w_B^\dagger w_B)^{-1}\times(w_B^\dagger w_S+w_S^\dagger w_B+w_S^\dagger w_S\\ &\quad+w^\dagger\theta(\lambda 1+1-\theta^\dagger\theta)^{-1}\theta^\dagger w)(\lambda 1+1-w_B^\dagger w_B)^{-1}+\cdots,\end{aligned}$$

where the series terminates. One can see that the rest of it can be done in a simple way since the expressions for B, C have explicit multiplicative factors of Z, which is in the Hilbert–Schmidt class, so we skip the details for brevity. Let us also check again the stability subgroup of $Z=0$ is given by $U(\mathcal{H}^e_-)\times U(\mathcal{H}^e_+|\mathcal{H}^o_+)$. For $Z=0$, $Z'=BD^{-1}$; if we set this to zero, since D is invertible, we get $B=0$. From the invariance of J we get $AA^\dagger=1$ as well as $A^\dagger A=1$, and this together with $AC^\dagger-BD^\dagger=0$ implies $C=0$. The result of this is the diffeomorphim we are after:

$$D_1^I=U_1(\mathcal{H}^e_-,\mathcal{H}^e_+|\mathcal{H}^o_+)/U(\mathcal{H}^e_-)\times U(\mathcal{H}^e_+|\mathcal{H}^o_+). \tag{28}$$

We emphasize that the explicit coordinate Z shows that this is a super-complex manifold; the group action point of view instead shows that this space is a super-homogeneous space.

III. SUPER-SYMPLECTIC STRUCTURE

In this section we will discuss the classical mechanics on this super-disk. There is a natural super-symplectic structure, it is homogeneous and further more it is Kähler. This is a natural choice from the point of view of geometry and, as we will see, it also provides us a natural method of quantization, which is an extension of the Bargmann representation to this case.[6] The analysis of symmetric domains and the use of Toeplitz operators in the quantization problem is thoroughly discussed in the book by Upmeier.[17] We also recommend the articles by Borthwick *et al.*[18]

It will be simpler to use the following super-operator to show that the disk is a super-symplectic space,

$$\Phi=-1+2\begin{pmatrix}(1-ZZ^\dagger)^{-1} & -(1-ZZ^\dagger)^{-1}Z\\ Z^\dagger(1-ZZ^\dagger)^{-1} & -Z^\dagger(1-ZZ^\dagger)^{-1}Z\end{pmatrix}. \tag{29}$$

Notice that this operator is well-defined on $\mathcal{H}^e_-\oplus\mathcal{H}^e_+|\mathcal{H}^o_+$. The reader can check that

$$\Phi^2=1,\quad J\Phi^\dagger J=\Phi. \tag{30}$$

An important point is that the action of the group on Z becomes very simple on Φ, $Z\to g\circ Z$ induces $\Phi\to g\Phi g^{-1}$ (see the Appendix). $Z=0$ corresponds to $\Phi=J$, and we can check that $\Phi(Z)=g(Z)Jg(Z)^{-1}$ (see the Appendix). We may define a symplectic form on D_1^I using Φ; formally,

$$\Omega=\frac{i}{4}\mathrm{Str}\Phi d\Phi\wedge d\Phi. \tag{31}$$

What we mean by this two form is that if we take two vector fields V_u, V_v, which are generated by the action of the super-Lie group, we get a number:

$$\Omega(V_u,V_v)=\frac{i}{8}\mathrm{Str}J[[J,g^{-1}ug]_s,[J,g^{-1}vg]_s]_s. \tag{32}$$

Using the above formal expression, we see that Ω is closed and, furthermore, it is homogeneous. This easily follows from the transformation of Φ under the group action. One can actually see this by looking at its explicit form. The nondegeneracy and super-Kähler structures are best understood around J. Then we use the homogeneity to distribute this form over all the manifold. When we restrict ourselves to the point J:

$$\Omega|_{Z=0}=i\mathrm{Str}\begin{pmatrix}-dZ\wedge dZ^\dagger & 0\\ 0 & dZ^\dagger\wedge dZ\end{pmatrix}. \tag{33}$$

Here the two wedge products have different meanings: $dZ\wedge dZ^\dagger=dw\wedge dw^\dagger+d\theta\wedge d\theta$ and

$$dZ^\dagger\wedge dZ=\begin{pmatrix}dw^\dagger\wedge dw & dw^\dagger\wedge d\theta\\ d\theta^\dagger\wedge dw & d\theta^\dagger\wedge d\theta\end{pmatrix}. \tag{34}$$

Hence we can rewrite this expression as

$$\Omega|_{Z=0}=i\mathrm{Str}\begin{pmatrix}-dw\wedge dw^\dagger-d\theta\wedge d\theta^\dagger & 0\\ 0 & \begin{pmatrix}dw^\dagger\wedge dw & dw^\dagger\wedge d\theta\\ d\theta^\dagger\wedge dw & d\theta^\dagger\wedge d\theta\end{pmatrix}\end{pmatrix}. \tag{35}$$

By expanding the trace,

$$\begin{aligned}\Omega|_{Z=0}&=i\left[-\mathrm{Tr}dw\wedge dw^\dagger-\mathrm{Tr}d\theta\wedge d\theta^\dagger+\mathrm{Str}\begin{pmatrix}dw^\dagger\wedge dw & dw^\dagger\wedge d\theta\\ d\theta^\dagger\wedge dw & d\theta^\dagger\wedge d\theta\end{pmatrix}\right]\\ &=i[-\mathrm{Tr}dw\wedge dw^\dagger-\mathrm{Tr}d\theta\wedge d\theta^\dagger+\mathrm{Tr}dw^\dagger\wedge dw-\mathrm{Tr}d\theta^\dagger\wedge d\theta]\\ &=-2i\mathrm{Tr}dw\wedge dw^\dagger-2i\mathrm{Tr}d\theta\wedge d\theta^\dagger=-2i\mathrm{Tr}dZ\wedge dZ^\dagger.\end{aligned}$$

(This incidentally shows that the form is super-Kähler.[19,20,14]) By contracting this with two vector fields at the origin, we get

$$\Omega(V_u,V_v)|_{Z=0}=-2i[\mathrm{Tr}(b_1b_2^\dagger-b_2b_1^\dagger)+\mathrm{Tr}(\beta_1\beta_2^\dagger+\beta_2\beta_1^\dagger)]. \tag{36}$$

Notice that we use the vector $[b\ \beta]$ for the component u_{12} of the Lie algebra element (this could be somewhat confusing but we try to avoid the prolifiration of indices). Using the above form it is possible to prove the nondegeneracy; this is given in the Appendix. The symplectic form above provides us with a Poisson structure,

One can define classical dynamics on this super-space, given an even Hamiltonian, a physical observable, H. The time evolution of any observable O is given by

$$\frac{\partial O}{\partial t}=\{H,O\}_s. \tag{37}$$

One can naturally ask if there are moment maps which generate the goup action. It is not possible to use $F_u=(i/2)\mathrm{Str}\Phi u$ due to divergence of the trace, but it is possible to do a vacuum subtraction and get a convergent one. To prove this we use a rearrangement of the formula for Φ:

$$\Phi(Z)=J+\begin{pmatrix} 2Z(1-Z^\dagger Z)^{-1}Z^\dagger & -2(1-ZZ^\dagger)^{-1}Z \\ 2Z^\dagger(1-ZZ^\dagger)^{-1} & -2Z^\dagger(1-ZZ^\dagger)^{-1}Z \end{pmatrix}. \tag{38}$$

If we look at now the difference $\Phi(Z)-J$, the last part remains. The diagonal parts of this operator are better behaved than the off-diagonal parts, $Z(1-Z^\dagger Z)^{-1}Z^\dagger\in\mathcal{I}_1$, in our sense as one can see, and similarly for the other one. The off-diagonal parts are actually in $\mathcal{I}_2$. So when we look at $(\Phi(Z)-J)u$, we see that

$$\begin{pmatrix} \mathcal{I}_1 & \mathcal{I}_2 & \mathcal{I}_2 \\ \mathcal{I}_2 & \mathcal{I}_1 & \mathcal{I}_1 \\ \mathcal{I}_2 & \mathcal{I}_1 & \mathcal{I}_1 \end{pmatrix}\begin{pmatrix} \mathcal{B} & \mathcal{I}_2 & \mathcal{I}_2 \\ \mathcal{I}_2 & \mathcal{B} & \mathcal{B} \\ \mathcal{I}_2 & \mathcal{B} & \mathcal{B} \end{pmatrix}=\begin{pmatrix} \mathcal{I}_1 & \mathcal{I}_2 & \mathcal{I}_2 \\ \mathcal{I}_2 & \mathcal{I}_1 & \mathcal{I}_1 \\ \mathcal{I}_2 & \mathcal{I}_1 & \mathcal{I}_1 \end{pmatrix}. \tag{39}$$

Hence a conditional trace exists: if we throw away the nontrace parts, $\mathrm{Str}_J(\Phi(Z)-J)u=\frac{1}{2}\mathrm{Str}[(\Phi(Z)-J)u+J(\Phi(Z)-J)uJ]$ is actually convergent. We see that this is very similar to the ordinary disk case in Ref. 6.

A general discussion shows that we get a Poisson realization of the super-Lie algebra through the moment maps:

$$\{F_u,F_v\}_s=F_{[u,v]_s}+\Sigma_s(u,v). \tag{40}$$

It is possible to find this central term by evaluating everything at the origin, $\Phi=J$:

$$\Sigma_s(u,v)=\frac{i}{8}\mathrm{Str}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}\left[\left[\left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},u\right],\left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},v\right]\right]\right]_s$$

$$=\frac{i}{2}\mathrm{Str}_J[J,u]v.$$

It is interesting to write down the central term explicitly:

$$\Sigma_s(u,v)=-2i\mathrm{Str}\begin{pmatrix} b_1b_2^\dagger+\beta_1\beta_2^\dagger & * \\ * & \begin{pmatrix} b_1^\dagger b_2 & b_1^\dagger\beta_2 \\ \beta_1^\dagger b_2 & \beta_1^\dagger\beta_2 \end{pmatrix} \end{pmatrix}$$

$$=-2i(\mathrm{Tr}(b_1b_2^\dagger-b_2b_1^\dagger)+\mathrm{Tr}(\beta_1\beta_2^\dagger)-\mathrm{Tr}(\beta_1^\dagger\beta_2))$$

$$=-2i(\mathrm{Tr}(b_1b_2^\dagger-b_2b_1^\dagger)+\mathrm{Tr}(\beta_1\beta_2^\dagger+\beta_2\beta_1^\dagger)),$$

and we see that at each step the diagonals are in $\mathcal{I}_1$ and hence the traces are all well-defined. This is equal to the symplectic form at the origin we computed before using the explicit coordinate Z as it should be. This type of central term is expected when there are bosons and fermions mixed. An interesting discussion of such central extensions from the Fock space point of view is given in Ref. 21. In Ref. 22 $\mathbf{Z}_2$ graded Schwinger terms for neutral particles are worked out, and in Ref. 23 current super-algebras are studied providing a generalization of Mickelsson–Rajeev cocyle.[24] The use of pseudodifferential operators in this reference we believe is better motivated in these higher dimensional cases. There should be a similar extension of our results using this restricted class of operators.

We are therefore equipped with a powerful geometric setting to develop our geometric quantization program.

IV. GEOMETRIC QUANTIZATION

Our presentation here will be somewhat more concise; most of the computations can be done similar to our previous work, except one has to watch for the signs. The technical details and explanation of the main ideas are already given in Ref. 12. We recommend the examples in Refs. 19 and 20, and one can read a more general program in Ref. 25 (we believe it is interesting to follow the philosophy of the last reference).

We can follow exactly the same steps in Ref. 6 and introduce a prequantization line bundle (for ordinary geometric quantization we refer to Refs. 1 and 26–28), and we introduce a super-one form on this bundle:

$$\Theta_s=\frac{1}{\hbar}(\mathrm{Str}(1-Z^\dagger Z)^{-1}dZ^\dagger Z-\mathrm{Str}(1-Z^\dagger Z)^{-1}Z^\dagger dZ). \tag{41}$$

This is used to define the covariant derivate as in the nonsuper-case [strictly speaking in the model of super-sections this acts on the prolongation, $\Gamma(M,\wedge(\mathbf{C}^N)\otimes K)$ where K is a prequantum complex line bundle on the base M]:

$$\nabla_V=\mathcal{L}^s_V+\Theta_s(V), \tag{42}$$

where we used a superscript to denote the super-Lie derivative. For any given super-function, we have the vector field generated from the symplectic form,

$$\Omega(V_f,*)=-df. \tag{43}$$

Using this vector field a prequantization operator is obtained,

$$\tilde{f}=-i\hbar\nabla_{V_f}+f. \tag{44}$$

This gives us a representation of the Poisson brackets:

$$\widetilde{\{f,g\}}_s=-i\hbar[\tilde{f},\tilde{g}]_s. \tag{45}$$

As in the ordinary case, we need to restrict the prequantum Hilbert space, since the prequantization map does not lead to an irreducible representation. We will choose super-holomorphic functions,

$$\nabla_{Z^\dagger}\psi(Z,Z^\dagger)=0. \tag{46}$$

The super analysis is designed to provide a complete analogy to the usual analysis, hence most of what we said follows from routine yet long (and care required due to signs) computations.

We can solve for this holomorphicity condition as in the ordinary case:

$$\nabla_{Z^\dagger}\psi=0, \quad \psi(Z,Z^\dagger)=\mathrm{sdet}^{1/\hbar}(1-Z^\dagger Z)\Psi(Z), \tag{47}$$

where $\Psi(Z)$ denotes a super-holomorphic function on the disk. We define the super-determinant (or Berezinian) as

$$\mathrm{sdet}\begin{pmatrix}\tilde{A} & \tilde{B}\\ \tilde{C} & \tilde{D}\end{pmatrix}=\det(\tilde{A}-\tilde{B}\tilde{D}^{-1}\tilde{C})(\det\tilde{D})^{-1}, \tag{48}$$

where the operator is written according to the even and odd decomposition of the super Hilbert space. The infinite dimensionality of the underlying space requires the full operator to be of the form $1+\mathcal{I}_1$, otherwise one has to use a conditional determinant. The resulting operators for the moment maps acting on holomorphic sections will be exactly the same as in the ordinary case,

$$\hat{F}_u\Psi(Z)=-i\hbar\left[\mathcal{L}^S_{V_u}-\frac{1}{\hbar}\mathrm{Str}(u_{21}Z)\right]\Psi(Z), \tag{49}$$

where we have used the same letters to denote the components of the Lie algebra elements,

$$u=\begin{pmatrix}u_{11} & u_{12}\\ u_{21} & u_{22}\end{pmatrix},$$

not to bring new notation. Holomorphicity is clearly preserved and these are the correct operators to start a quantization program.

These moment maps can be integrated to a representation of a central extension of the super-pseudounitary group:

$$\rho(g^{-1})\Psi(Z)=\mathrm{sdet}^{-1/\hbar}(D^{-1}CZ+1)\Psi((AZ+B)(CZ+D)^{-1}). \tag{50}$$

This is a well-defined representation. Let us see that the determinant exits:

$$\begin{pmatrix}(d^{-1})_{11} & (\delta^{-1})_{12}\\ (\delta^{-1})_{21} & (d^{-1})_{22}\end{pmatrix}\begin{pmatrix}cw & c\theta\\ \gamma w & \gamma\theta\end{pmatrix}=\begin{pmatrix}\mathcal{B} & \mathcal{B}\\ \mathcal{B} & \mathcal{B}\end{pmatrix}\begin{pmatrix}\mathcal{I}_1 & \mathcal{I}_1\\ \mathcal{I}_1 & \mathcal{I}_1\end{pmatrix}=\begin{pmatrix}\mathcal{I}_1 & \mathcal{I}_1\\ \mathcal{I}_1 & \mathcal{I}_1\end{pmatrix}. \tag{51}$$

This shows that the determinant is absolutely convergent—independent of the basis chosen. The central term of the representation is given by

$$c_S(g_1,g_2)=\mathrm{sdet}^{1/\hbar}[(D_1D_2)^{-1}C_1B_2+1]. \tag{52}$$

Derivation of this super-central term does not present any more difficulties than the ordinary case (see the appendix of Ref. 29), the convergence issue follows the same lines as the above one and we leave the details to the reader.

V. INFINITE DIMENSIONAL CASE

We will propose a way of extending our results when $\mathcal{H}^o$ is infinite dimensional. In this section we will not repeat the previous arguments, since some of them are direct generalizations and some of them require a much deeper study. We plan to come back to those issues in another publication, so in this section we only give a sketch of ideas. While we were working on this problem, we became aware of a rather similar set of ideas by Schmidt in Ref. 30. Which set of ideas is more appropriate for our problem is not so clear to us at this moment, so we follow our point of view. We plan to take a more detailed study of all these issues in the future.

First we change our notion of a super-number:

$$z=z_B+\sum_{N=0}^{\infty}\sum_{a_1<a_2<\ldots<a_N} z_{a_1a_2\ldots a_N}\xi^{a_1}\xi^{a_2}\cdots\ \xi^{a_N}, \tag{53}$$

where we assume that the sums have square integrable coefficients $\Sigma_N^{\infty}\Sigma_{a_1<a_2<\ldots<a_N}|z_{a_1a_2\ldots a_N}|^2<\infty$. This makes the product of two super-numbers well-defined, hence it behaves much better than the formal sums and it is physically more transparent as well. The product becomes

$$(zt)_{a_1a_2\ldots a_N}=\sum_n z_{(a_1a_2\ldots a_n}t_{a_{n+1}\ldots a_N)}, \tag{54}$$

here $(\ldots)$ denotes an appropriate symmetrization of the indices, due to the ordering of the generators (keeping the previous ordering in mind). From a more abstract point of view, when we look at the algebra of smooth functions on this flat space we get $C^{\infty}(F)\approx\oplus_{l^2}\wedge^k\mathcal{H}$ and this is what defines the Cartesian product of super-numbers. We will naturally represent the right hand side as the naive Fock space of the Hilbert space: $\mathcal{F}(\mathcal{H})=\oplus_{l^2}\wedge^k\mathcal{H}$. (This is not the Fock space corresponding to the Dirac sea, it is the naive one.) We look at again the matrix algebra modeled on these super-numbers; they will be transformations from $Z:\mathcal{H}_+^e|\mathcal{H}_+^o\to\mathcal{H}_-^e$ written explicitly, $Z=Z_B+\Sigma_N\Sigma_{a_1<a_2<\ldots<a_N}Z_{a_1a_2\ldots a_N},\xi^{a_1}\xi^{a_2}\cdots\ \xi^{a_N}$, matrix coefficients satisfying

$$\sum_N\sum_{a_1<a_2<\ldots<a_N}\|Z_{a_1a_2\ldots a_N}\|_2^2<\infty, \tag{55}$$

where $\|*\|_2$ denotes the norm in the Hilbert–Schmidt ideal. This implies that we have a space of matrices which is modeled on $\mathcal{I}_2\otimes\mathcal{F}(\mathcal{H})$. We may use the above convergence condition to get an inner product:

$$\langle Z,W\rangle=\sum_N\sum_{a_1<a_2<\ldots<a_N}\mathrm{Tr}Z^{\dagger}_{a_1a_2\ldots a_N}W_{a_1\ldots a_N}. \tag{56}$$

We note that this abstract space is still a Hilbert space with the above inner product, and indeed that will equip us with all the luxuries of Hilbert spaces. We can prove by using standard techniques that the product of two such matrices, ZW, is still in the above class, i.e.,

$$\sum_N\sum_{a_1<a_2<\ldots<a_N}\|(ZW)_{a_1a_2\ldots a_N}\|_2^2=\sum_N\sum_{a_1<a_2<\ldots<a_N}\|\sum_n Z_{(a_1a_2\ldots a_n}W_{a_{n+1}\ldots a_N)}\|_2^2<\infty. \tag{57}$$

There is the same type of possible reorderings of the indices in this expression. The rest will follow exactly the same lines as before. The convergence conditions should be checked much more carefully this time.

The disk is defined as $1-w_B^{\dagger}w_B>0$, and $Z=[w\ \theta]$, where each one of these super-matrices satisfies the above condition for being in $\mathcal{I}_2$. We can define the same symplectic form,

$$\Omega(V_u,V_v)=\frac{i}{8}\mathrm{Str}J[[J,g^{-1}ug]_s,[J,g^{-1}vg]_s]_s; \tag{58}$$

here each term is in $\mathcal{I}_2$.

The rest of the arguments apart from the convergence issues are exactly the same, so we leave the details to a future work.

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APPENDIX: TRANSFORMATION RULE OF Φ

For completeness we define here A^α where $0<\alpha<1$ and the body of the super-operator is positive,

$$A^\alpha=\frac{\sin\pi\alpha}{\pi}\int_0^\infty \frac{d\lambda}{\lambda^{1-\alpha}}(\lambda 1+A)^{-1}. \tag{A1}$$

The advantage of this expression is that we may actually expand the inverse and obtain a series for the super operator. Note that there is no simple recursive process when α is not a rational number.

In this part we will give a proof of the following transformation rule: $Z\mapsto g\circ Z$ implies $\Phi\mapsto g\Phi g^{-1}$. First we note that when $Z\mapsto(AZ+B)(CZ+D)^{-1}$, we have $(1-Z^\dagger Z)^{-1}\mapsto(CZ+D)(1-Z^\dagger Z)^{-1}(CZ+D)^{-1}$. Next we rewrite $\Phi(Z)$:

$$\Phi=-1+2\begin{pmatrix} K^{-1} & -K^{-1}Z \\ Z^\dagger K^{-1} & -Z^\dagger K^{-1}Z\end{pmatrix}=1+2\begin{pmatrix} Z^\dagger S^{-1}Z & -ZS^{-1} \\ S^{-1}Z^\dagger & -S^{-1}\end{pmatrix}, \tag{A2}$$

where $K=(1-ZZ^\dagger)$ and $S=(1-Z^\dagger Z)$. Using the previous observation we see that

$$\Phi(g\circ Z)=1+2\begin{pmatrix} (AZ+B)S^{-1}(AZ+B)^\dagger & -(AZ+B)S^{-1}(CZ+D)^\dagger \\ (CZ+D)S^{-1}(AZ+B)^\dagger & -(CZ+D)S^{-1}(CZ+D)^\dagger\end{pmatrix}. \tag{A3}$$

One can see that the previous expression can be written as

$$\Phi(g\circ Z)=1+2\begin{pmatrix} A & B \\ C & D\end{pmatrix}\begin{pmatrix} Z^\dagger S^{-1}Z & -ZS^{-1} \\ S^{-1}Z^\dagger & -S^{-1}\end{pmatrix}\begin{pmatrix} A^\dagger & -C^\dagger \\ -B^\dagger & D^\dagger\end{pmatrix}, \tag{A4}$$

which is precisely what we claimed. The next point to check is $\Phi(Z)=g(Z)Jg(Z)^{-1}=g(Z)g(Z)^\dagger J$:

$$\begin{aligned} g(Z)g(Z)^\dagger&=\begin{pmatrix} K^{-1/2} & ZS^{-1/2} \\ S^{-1/2}Z^\dagger K^{1/2} & S^{-1/2}\end{pmatrix}\begin{pmatrix} K^{-1/2} & K^{1/2}ZS^{-1} \\ S^{-1/2}Z^\dagger & S^{-1/2}\end{pmatrix} \\ &=\begin{pmatrix} K^{-1}+ZS^{-1}Z^\dagger+1-1 & 2ZS^{-1} \\ 2S^{-1}Z^\dagger & S^{-1}Z^\dagger KZS^{-1}+S^{-1}\end{pmatrix}.\end{aligned}$$

Multiply this with $J=\left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$. Then in the last line use $-(S^{-1}Z^\dagger KZS^{-1}+S^{-1})=-(S^{-1}Z^\dagger KK^{-1}Z+S^{-1})$, which gives $-(S^{-1}Z^\dagger Z+S^{-1})=S^{-1}(1-Z^\dagger Z)-S^{-1}-S^{-1}$. This gives $1-2S^{-1}$, and the result follows.

We will prove the nondegeneracy of the super-two form:

$$\Omega(V_u,V_v)|_{Z=0}=-2i\mathrm{Tr}(b_1b_2^\dagger-b_2b_1^\dagger)-2i\mathrm{Tr}(\beta_1\beta_2^\dagger+\beta_2\beta_1^\dagger). \tag{A5}$$

Here we write $V_u(Z)=u_{11}Z-Zu_{22}-Zu_{21}Z+u_{21}$, and similarly for the $V_u(Z^\dagger)$. Furthermore, we write $u_{12}=[b\ \beta]$, hoping that the use of the same letters for the Lie algebra elements will not cause any confusion. Let us expand each term as a super-matrix (ignoring the multiplicative factor $-2i$),

$$\mathrm{Tr}((b_1)_B(b_2)_B^\dagger-(b_2)_B(b_1)_B^\dagger)=0,$$

$$\mathrm{Tr}((b_1)_{a_1a_2}(b_2)_B^\dagger-(b_2)_{a_1a_2}(b_1)_B^\dagger)\xi^{a_1}\xi^{a_2}=0,$$

$$\mathrm{Tr}((b_1)_B(b_2)_{a_1a_2}^\dagger-(b_2)_B(b_1)_{a_1a_2}^\dagger)\xi^{*a_1}\xi^{*a_2}=0,$$

$$\begin{aligned}&\mathrm{Tr}((b_1)_{a_1a_2a_3a_4}(b_2)_B^\dagger\xi^{a_1}\xi^{a_2}\xi^{a_3}\xi^{a_4}+(b_1)_{a_1a_2}(b_2)_{a_3a_4}^\dagger\xi^{a_1}\xi^{a_2}\xi^{*a_3}\xi^{*a_4}\\&\quad+(b_1)_B(b_2)_{a_1a_2a_3a_4}^\dagger\xi^{*a_1}\xi^{*a_2}\xi^{*a_3}\xi^{*a_4})\\&\quad-\mathrm{Tr}((b_2)_{a_1a_2}(b_1)_{a_3a_4}^\dagger\xi^{a_1}\xi^{a_2}\xi^{*a_3}\xi^{*a_4}+(b_2)_B(b_1)_{a_1a_2a_3a_4}^\dagger\xi^{*a_1}\xi^{*a_2}\xi^{*a_3}\xi^{*a_4}\\&\quad+(b_2)_{a_1a_2a_3a_4}(b_1)_B^\dagger\xi^{a_1}\xi^{a_2}\xi^{a_3}\xi^{a_4})=0,\end{aligned}$$

$$\ldots,$$

where the dots refer to the continuation of this expansion. From these relations we conclude that an iterative process gives us the required nondegeneracy.

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Cohomology of the infinite-order jet space and the inverse problem

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Cohomology of the bicomplex of exterior forms on the infinite-order jet space of a smooth fiber bundle of a field model is computed. This provides a solution of the global inverse problem of the calculus of variations in Lagrangian field theory and time-dependent mechanics. In the case of an affine fiber bundle, the outcomes to BRST theory are discussed. We show that there is no topological obstruction to constructing global descent equations in the even field sector of BRST theory. [DOI: 10.1063/1.1390328]

I. INTRODUCTION

Let $Y \to X$ be a smooth fiber bundle of a field model. We obtain cohomology of exterior forms on the infinite order jet space $J^\infty Y$ of $Y \to X$. The $J^\infty Y$ provides the most general framework for describing the dynamics of field systems on fiber bundles.[1] It consists of the equivalence classes of sections of $Y \to X$ identified by their Taylor series at points $x \in X$. The exterior differential d on $J^\infty Y$ splits into the sum of the vertical differential d_V and the horizontal (total) differential d_H. These differentials, together with the variational operator δ, constitute the variational bicomplex of exterior forms on $J^\infty Y$.

The following two differential algebras of exterior forms $\mathcal{O}^*_\infty$ and $\mathcal{T}^*_\infty$ are usually considered on $J^\infty Y$.

The first one is the direct limit of graded differential algebras of exterior forms on finite order jet manifolds. This algebra is most interesting for physical applications because it consists of exterior forms on finite order jet manifolds. Lagrangian field theory is phrased in terms of $\mathcal{O}^*_\infty$.[1] Extended to the jet space of ghosts and antifields, the algebra $\mathcal{O}^*_\infty$ is the main ingredient in the field-antifield BRST theory for studying BRST cohomology modulo d_H.[2–5] Passing to the direct limit of the de Rham complexes of exterior forms on finite order jet manifolds, de Rham cohomology of $\mathcal{O}^*_\infty$ has been found to coincide with de Rham cohomology of the fiber bundle Y.[6,7] However, this is not a way of studying other cohomology of the algebra $\mathcal{O}^*_\infty$.

To solve this problem, we enlarge $\mathcal{O}^*_\infty$ to the graded differential algebra $\mathcal{T}^*_\infty$ of exterior forms of locally finite order on $J^\infty Y$. This is the structure algebra of the sheaf of germs of exterior forms on finite order jet manifolds. The d_H and δ cohomology of $\mathcal{T}^*_\infty$ have been investigated in Refs. 8 and 9. Due to Lemma 2 below, we simplify this investigation and prove that the differential algebra $\mathcal{O}^*_\infty$ has the same d_H and δ cohomology as $\mathcal{T}^*_\infty$ (see Theorem 7). In particular, this provides a solution of the global inverse problem of the calculus of variations in Lagrangian field theory and time-dependent mechanics.

For applications to BRST theory, the case of an affine bundle $Y \to X$ is relevant. The BRST cohomology modulo d_H has been introduced in the case of a contractible fiber bundle $Y = \mathbb{R}^{n+m}$

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$\to\mathbb{R}^n$ when the horizontal differential d_H is exact. Its exactness is essential for constructing the (local) descent equations. Here, we show that, in the case of an arbitrary affine bundle $Y\to X$, there is no topological obstruction to constructing global descent equations in the even field sector of BRST theory. Note that affine bundles provide a standard framework in quantum field theory. If $Y\to X$ is an affine bundle, d_H cohomology of $\mathcal{O}^*_\infty$ coincides with de Rham cohomology of the base X. It follows that every d_H-closed element ϕ of $\mathcal{O}^*_\infty$ can be written in the form

$$\phi=\varphi+d_H\xi, \quad \xi\in\mathcal{O}^*_\infty,$$

where φ is a closed form on X. Consequently, the obstruction to the exactness of the horizontal differential d_H lies only in exterior forms on X. Since the BRST operator eliminates these forms, the global descent equations can be constructed though their right-hand side is not zero. We come to the same result for the differential algebra $\mathcal{P}$ of exterior forms which are polynomials in field variables and for its subalgebra $\overline{\mathcal{P}}$ of x-independent forms. These are algebras which one deals with in the even field sector of BRST theory.

The article is organized as follows. In Sec. II, the differential algebras $\mathcal{O}^*_\infty$ and $\mathcal{T}^*_\infty$ on $J^\infty Y$ are introduced in an algebraic way. In Sec. III, the variational complex on $J^\infty Y$ is set. Section IV is devoted to cohomology of the differential algebra $\mathcal{T}^*_\infty$. In Sec. V, the isomorphism of d_H and δ cohomology of $\mathcal{O}^*_\infty$ to that of $\mathcal{T}^*_\infty$ is proved. In Sec. VI, a solution of the inverse problem of the calculus in variations in different classes of exterior forms is provided. Section VII is devoted to the cohomology of $\mathcal{O}^*_\infty$ in the case of an affine bundle. In Sec. VIII, cohomology of the polynomial algebras $\mathcal{P}$ and $\overline{\mathcal{P}}$ is described.

II. THE DIFFERENTIAL CALCULUS ON $J^\infty Y$

Smooth manifolds throughout are assumed to be real, finite-dimensional, Hausdorff, paracompact, and connected. Put further $\dim X=n\geqslant 1$.

Recall that the infinite order jet space $J^\infty Y$ of a smooth fiber bundle $Y\to X$ is defined as a projective limit $(J^\infty Y,\pi^\infty_r)$ of the inverse system

$$X\overset{\pi}{\leftarrow}Y\overset{\pi^1_0}{\leftarrow}\cdots\leftarrow J^{r-1}Y\overset{\pi^r_{r-1}}{\leftarrow}J^rY\leftarrow\cdots \tag{1}$$

of finite order jet manifolds J^rY of $Y\to X$, where π^r_{r-1} are affine bundles (see Refs. 1 and 5 for a survey of the infinite order jet technique). Endowed with the projective limit topology, $J^\infty Y$ is a paracompact Fréchet manifold.[8] A bundle coordinate atlas $\{U_Y,(x^\lambda,y^i)\}$ of $Y\to X$ yields the manifold coordinate atlas

$$\{(\pi^\infty_0)^{-1}(U_Y),(x^\lambda,y^i_\Lambda)\}, \quad 0\leqslant|\Lambda|,$$

of $J^\infty Y$, together with the transition functions

$$y'^i_{\lambda+\Lambda}=\frac{\partial x^\mu}{\partial x'^\lambda}d_\mu y'^i_\Lambda, \tag{2}$$

where $\Lambda=(\lambda_k\cdots\lambda_1)$, $\lambda+\Lambda=(\lambda\lambda_k\cdots\lambda_1)$ are symmetric multi-indices and d_λ denotes the total derivative

$$d_\lambda=\partial_\lambda+\sum_{|\Lambda|\geqslant 0}y^i_{\lambda+\Lambda}\partial^\Lambda_i.$$

With the inverse system (1), one has the direct system

$$\mathcal{O}^*(X) \xrightarrow{\pi^*} \mathcal{O}_0^* \xrightarrow{\pi_0^{1*}} \mathcal{O}_1^* \xrightarrow{\pi_1^{2*}} \cdots \xrightarrow{\pi_{r-1}^{r*}} \mathcal{O}_r^* \to \cdots \tag{3}$$

of graded differential $\mathbb{R}$-algebras $\mathcal{O}_r^*$ of exterior forms on finite order jet manifolds J^rY, where π_{r-1}^{r*} are pull-back monomorphisms. Its direct limit is the above-mentioned graded differential $\mathbb{R}$-algebra $(\mathcal{O}_\infty^*, \pi_r^{\infty *})$ of exterior forms on finite order jet manifolds modulo the pull-back identification. The $\mathcal{O}_\infty^*$ is a differential calculus over the $\mathbb{R}$-ring $\mathcal{O}_\infty^0$ of continuous real functions on $J^\infty Y$ which are the pull-back of smooth real functions on finite order jet manifolds by surjections π_r^∞.

Let us enlarge $\mathcal{O}_\infty^0$ to the $\mathbb{R}$-ring $\mathcal{T}_\infty^0$ of continuous real functions on $J^\infty Y$ such that, given $f \in \mathcal{T}_\infty^0$ and any point $q \in J^\infty Y$, there exists a neighborhood of q where f coincides with the pull-back of a smooth function on some finite order jet manifold. The reason lies in the fact that the paracompact space $J^\infty Y$ admits a partition of unity by elements of the ring $\mathcal{T}_\infty^0$.[8] Therefore, sheaves of $\mathcal{T}_\infty^0$-modules on $J^\infty Y$ are fine and, consequently, acyclic. Then, the abstract de Rham theorem on cohomology of a sheaf resolution (Theorem 2.12.1 in Ref. 10) can be called into play.

Remark 1: Throughout, we follow the terminology of Ref. 10 where by a sheaf S over a topological space Z is meant a sheaf bundle $S \to Z$. Accordingly, $\Gamma(S)$ denotes the canonical presheaf of sections of the sheaf S, and $\Gamma(Z,S)$ is the group of global sections of S. All sheaves in the following are ringed spaces, but we omit this terminology if there is no danger of confusion.

Let us define a differential calculus over the ring $\mathcal{T}_\infty^0$. Let $\mathfrak{O}_r^*$ be a sheaf of germs of exterior forms on the r-order jet manifold J^rY and $\Gamma(\mathfrak{O}_r^*)$ its canonical presheaf. There is the direct system of canonical presheaves

$$\Gamma(\mathfrak{O}_X^*) \xrightarrow{\pi^*} \Gamma(\mathfrak{O}_0^*) \xrightarrow{\pi_0^{1*}} \Gamma(\mathfrak{O}_1^*) \xrightarrow{\pi_1^{2*}} \cdots \xrightarrow{\pi_{r-1}^{r*}} \Gamma(\mathfrak{O}_r^*) \to \cdots,$$

where π_{r-1}^{r*} are pull-back monomorphisms with respect to open surjections π_{r-1}^r. Its direct limit $\mathfrak{O}_\infty^*$ is a presheaf of graded differential $\mathbb{R}$-algebras on $J^\infty Y$. Let $\mathfrak{T}_\infty^*$ be a sheaf constructed from $\mathfrak{O}_\infty^*$ and $\Gamma(\mathfrak{T}_\infty^*)$ its canonical presheaf. The structure algebra $\mathcal{T}_\infty^* = \Gamma(J^\infty Y, \mathfrak{T}_\infty^*)$ of the sheaf $\mathfrak{T}_\infty^*$ is a desired differential calculus over the $\mathbb{R}$-ring $\mathcal{T}_\infty^0$. There are the $\mathbb{R}$-algebra monomorphisms $\mathfrak{O}_\infty^* \to \Gamma(\mathfrak{T}_\infty^*)$ and $\mathcal{O}_\infty^* \to \mathcal{T}_\infty^*$.

For short, we agree to call elements of $\mathcal{T}_\infty^*$ the exterior forms on $J^\infty Y$. Restricted to a coordinate chart $(\pi_0^\infty)^{-1}(U_Y)$ of $J^\infty Y$, they can be written in the familiar coordinate form, where horizontal forms $\{dx^\lambda\}$ and contact one-forms $\{\theta_\Lambda^i = dy_\Lambda^i - y_{\lambda+\Lambda}^i dx^\lambda\}$ constitute the set of generators of the algebra $\mathcal{T}_\infty^*$. There is the canonical decomposition

$$\mathcal{T}_\infty^* = \oplus_{k,s} \mathcal{T}_\infty^{k,s}, \quad 0 \leqslant k, \quad 0 \leqslant s \leqslant n,$$

of $\mathcal{T}_\infty^*$ into $\mathcal{T}_\infty^0$-modules $\mathcal{T}_\infty^{k,s}$ of k-contact and s-horizontal forms, together with the corresponding projections

$$h_k : \mathcal{T}_\infty^* \to \mathcal{T}_\infty^{k,*}, \quad 0 \leqslant k, \quad h^s : \mathcal{T}_\infty^* \to \mathcal{T}_\infty^{*,s}, \quad 0 \leqslant s \leqslant n.$$

Accordingly, the exterior differential on $\mathcal{T}_\infty^*$ is decomposed into the sum $d = d_H + d_V$ of horizontal and vertical differentials such that

$$d_H \circ h_k = h_k \circ d \circ h_k, \quad d_H(\phi) = dx^\lambda \wedge d_\lambda(\phi), \quad \phi \in \mathcal{T}_\infty^*,$$

$$d_V \circ h^s = h^s \circ d \circ h^s, \quad d_V(\phi) = \theta_\Lambda^i \wedge \partial_\Lambda^i \phi.$$

III. THE VARIATIONAL COMPLEX

Being nilpotent, the differentials d_V and d_H provide the natural bicomplex $\{\mathcal{T}_\infty^{k,m}\}$ of the graded differential algebra $\mathcal{T}_\infty^*$. Here, we restrict our consideration to its row

$$0 \longrightarrow \mathbb{R} \longrightarrow \mathcal{T}^0_\infty \xrightarrow{d_H} \mathcal{T}^{0,1}_\infty \xrightarrow{d_H} \cdots \xrightarrow{d_H} \mathcal{T}^{0,n}_\infty, \tag{4}$$

called the horizontal complex. To complete it to the variational complex, let us consider the variational operator $\delta=\tau\circ d$ on $\mathcal{T}^{*,n}_\infty$ where τ is the projection $\mathbb{R}$-module endomorphism

$$\tau=\sum_{k>0}\frac{1}{k}\overline{\tau}\circ h_k\circ h^n,$$

$$\overline{\tau}(\phi)=(-1)^{|\Lambda|}\theta^i\wedge[d_\Lambda(\partial^\Lambda_i\rfloor\phi)], \quad 0\leqslant|\Lambda|, \quad \phi\in\mathcal{T}^{>0,n}_\infty,$$

of $\mathcal{T}^*_\infty$ such that $\tau\circ d_H=0$ (see, e.g., Refs. 1, 6, and 11). The variational operator on $\mathcal{T}^{*,n}_\infty$ is nilpotent, and obeys the relation

$$\delta\circ\tau-\tau\circ d=0. \tag{5}$$

Put $\mathfrak{E}_k=\tau(\mathfrak{T}^{k,n}_\infty)$ and $E_k=\tau(\mathcal{T}^{k,n}_\infty)$, $k>0$. Since τ is a projection operator, there are the isomorphisms

$$\Gamma(\mathfrak{E}_k)=\tau(\Gamma(\mathfrak{T}^{k,n}_\infty)), \quad E_k=\Gamma(J^\infty Y,\mathfrak{E}_k).$$

Let $\mathbb{R}$ denote the constant sheaf on $J^\infty Y$. With operators d_H and δ, we have the variational complex

$$0 \longrightarrow \mathbb{R} \longrightarrow \mathfrak{T}^0_\infty \xrightarrow{d_H} \mathfrak{T}^{0,1}_\infty \xrightarrow{d_H} \cdots \xrightarrow{d_H} \mathfrak{T}^{0,n}_\infty \xrightarrow{\delta} \mathfrak{E}_1 \xrightarrow{\delta} \mathfrak{E}_2 \longrightarrow \cdots \tag{6}$$

of the sheaf $\mathfrak{T}^*_\infty$ and the variational complex

$$0 \longrightarrow \mathbb{R} \longrightarrow \mathcal{T}^0_\infty \xrightarrow{d_H} \mathcal{T}^{0,1}_\infty \xrightarrow{d_H} \cdots \xrightarrow{d_H} \mathcal{T}^{0,n}_\infty \xrightarrow{\delta} E_1 \xrightarrow{\delta} E_2 \longrightarrow \cdots \tag{7}$$

of its structure algebra $\mathcal{T}^*_\infty$. The similar variational complex $\{\mathcal{O}^*_\infty,\overline{E}_k\}$ of the graded differential algebra $\mathcal{O}^*_\infty$ takes place. There are the well-known statements summarized usually as the algebraic Poincaré lemma (see, e.g., Refs. 11 and 12).

Lemma 1: If Y is a contractible fiber bundle $\mathbb{R}^{n+p}\to\mathbb{R}^n$, the variational complex $\{\mathcal{O}^*_\infty,\overline{E}_k\}$ of the graded differential algebra $\mathcal{O}^*_\infty$ is exact.

It follows that the variational complex of sheaves (6) is exact for any smooth fiber bundle $Y\to X$. Moreover, the sheaves $\mathfrak{T}^{*,n}$ in this complex are fine, and so are the sheaves $\mathfrak{E}_k$ in accordance with the following lemma.

Lemma 2: Sheaves $\mathfrak{E}_k$, $k>0$, are fine.

Proof: Though $\mathbb{R}$-modules $E_{k>1}$ fail to be $\mathcal{T}^0_\infty$-modules,[11] one can use the fact that the sheaves $\mathfrak{E}_{k>0}$ are projections $\tau(\mathfrak{T}^{k,n}_\infty)$ of sheaves of $\mathcal{T}^0_\infty$-modules. Let $\mathfrak{U}=\{U_i\}_{i\in I}$ be a locally finite open covering of $J^\infty Y$ and $\{f_i\in\mathcal{T}^0_\infty\}$ the associated partition of unity. For any open subset $U\subset J^\infty Y$ and any section φ of the sheaf $\mathfrak{T}^{k,n}_\infty$ over U, let us put $h_i(\varphi)=f_i\varphi$. Then, $\{h_i\}$ provide a family of endomorphisms of the sheaf $\mathfrak{T}^{k,n}_\infty$, required for $\mathfrak{T}^{k,n}_\infty$ to be fine. Endomorphisms h_i of $\mathfrak{T}^{k,n}_\infty$ also yield the $\mathbb{R}$-module endomorphisms

$$\overline{h_i}=\tau\circ h_i:\mathfrak{E}_k\xrightarrow{in}\mathfrak{T}^{k,n}_\infty\xrightarrow{h_i}\mathfrak{T}^{k,n}_\infty\xrightarrow{\tau}\mathfrak{E}_k$$

of the sheaves $\mathfrak{E}_k$. They possess the properties required for $\mathfrak{E}_k$ to be a fine sheaf. Indeed, for each $i\in I$, there is a closed set $\operatorname{supp} f_i\subset U_i$ such that $\overline{h_i}$ is zero outside this set, while the sum $\Sigma_{i\in I}\overline{h_i}$ is the identity morphism.

Thus, the variational complex (6) is a resolution of the constant sheaf $\mathbb{R}$ on $J^\infty Y$. Therefore, the above-mentioned abstract de Rham theorem (see Appendix A) can be utilized in order to find cohomology of the the variational complex (7) of the differential algebra $\mathcal{T}^*_\infty$.

IV. COHOMOLOGY OF $\mathcal{T}^*_\infty$

We start from the following facts.

Lemma 3: There is an isomorphism

$$H^*(J^\infty Y,\mathbb{R})=H^*(Y,\mathbb{R})=H^*(Y) \tag{8}$$

between cohomology $H^*(J^\infty Y,\mathbb{R})$ of $J^\infty Y$ with coefficients in the constant sheaf $\mathbb{R}$, that $H^*(Y,\mathbb{R})$ of Y, and de Rham cohomology $H^*(Y)$ of Y.

Proof: Since Y is a strong deformation retract of $J^\infty Y$ (see Appendix B), the first isomorphism in (8) follows from the Vietoris–Begle theorem,[13] while the second one is a consequence of the well-known de Rham theorem.

Lemma 4: Let us consider the de Rham complex of sheaves

$$0\to\mathbb{R}\to\mathfrak{T}^0_\infty\overset{d}{\to}\mathfrak{T}^1_\infty\overset{d}{\to}\cdots \tag{9}$$

on $J^\infty Y$ and the corresponding de Rham complex of their structure algebras

$$0\to\mathbb{R}\to\mathcal{T}^0_\infty\overset{d}{\to}\mathcal{T}^1_\infty\overset{d}{\to}\cdots. \tag{10}$$

There is an isomorphism

$$H^*(\mathcal{T}^*_\infty)=H^*(Y)$$

of de Rham cohomology $H^*(\mathcal{T}^*_\infty)$ of the graded differential algebra $\mathcal{T}^*_\infty$ to that $H^*(Y)$ of the fiber bundle Y.

Proof: The proof is obvious. The complex (9) is exact due to the Poincaré lemma, and is a resolution of the constant sheaf $\mathbb{R}$ on $J^\infty Y$ since $\mathfrak{T}^*_\infty$ are sheaves of $\mathcal{T}^0_\infty$-modules. Then, the abstract de Rham theorem and Lemma 3 complete the proof.

It follows that every closed form $\phi\in\mathcal{T}^*_\infty$ splits into the sum

$$\phi=\varphi+d\xi,\quad \xi\in\mathcal{T}^*_\infty, \tag{11}$$

where φ is a closed form on the fiber bundle Y. This splitting plays an important role in the sequel.

Turn now to the variational complex (6). Bearing in mind Lemma 3 and by virtue of the abstract de Rham theorem, we obtain the following.

Proposition 5: There is an isomorphism

$$H^*_{\rm var}(\mathcal{T}^*_\infty)=H^*(Y) \tag{12}$$

between cohomology $H^*_{\rm var}(\mathcal{T}^*_\infty)$ of the variational complex (7) and de Rham cohomology of the fiber bundle Y, namely,

$$H^{k<n}_{\rm var}(\mathcal{T}^*_\infty)=H^{k<n}(d_H;\mathcal{T}^*_\infty)=H^{k<n}(Y),$$

$$H^{k\geqslant n}_{\rm var}(\mathcal{T}^*_\infty)=H^{k-n}(\delta;\mathcal{T}^*_\infty)=H^{k\geqslant n}(Y),$$

where $H^*(d_H;\mathcal{T}^*_\infty)$ and $H^*(\delta;\mathcal{T}^*_\infty)$ denote d_H and δ cohomology of the differential algebra $\mathcal{T}^*_\infty$.

The isomorphism (12) recovers the result of Ref. 8 for $H^*_{\rm var}(\mathcal{T}^*_\infty)$ and that of Ref. 9 for $H^0(\delta;\mathcal{T}^*_\infty)$ and $H^1(\delta;\mathcal{T}^*_\infty)$, but let us say something more. The relation (5) for τ and the relation

$h_0 d = d_H h_0$ for h_0 define homomorphisms of the de Rham complex (10) of the algebra $\mathcal{T}^*_\infty$ to the variational complex (7). The corresponding homomorphism of their cohomology groups is an isomorphism by virtue of Lemma 4 and Proposition 5. Then, the splitting (11) leads to the following decompositions.

Proposition 6: Any d_H-closed form $\sigma \in \mathcal{T}^{0,m}_\infty$, $0<m<n$, is represented by the sum

$$\sigma = h_0\varphi + d_H\xi, \quad \xi \in \mathcal{T}^{0,m-1}_\infty, \tag{13}$$

where φ is a closed m-form on Y. Any δ-closed form $\sigma_k \in \mathcal{T}^{k,n}_\infty$, $k \geqslant 0$, is represented by the sum

$$\sigma_{k=0} = h_0\varphi + d_H\xi, \quad \xi \in \mathcal{T}^{0,n-1}_\infty, \tag{14}$$

$$\sigma_{k>0} = \tau(\varphi) + \delta(\xi), \quad \xi \in E_{k-1}, \tag{15}$$

where φ is a closed $(n+k)$-form on Y.

V. COHOMOLOGY OF $\mathcal{O}^*_\infty$

The following theorem gives us d_H and δ cohomology of the differential algebra $\mathcal{O}^*_\infty$. As was mentioned previously, de Rham cohomology of $\mathcal{O}^*_\infty$ is equal to that of Y.

Theorem 7: The differential algebra $\mathcal{O}^*_\infty$ has the same d_H and δ cohomology as $\mathcal{T}^*_\infty$, i.e.,

$$H^*(d_H;\mathcal{O}^*_\infty) = H^*(d_H;\mathcal{T}^*_\infty), \quad H^*(\delta;\mathcal{O}^*_\infty) = H^*(\delta;\mathcal{T}^*_\infty).$$

Proof: Let the common symbol D stand for the coboundary operators d_H and δ of the variational bicomplex. Bearing in mind the decompositions (13)–(15), it suffices to show that, if an element $\phi \in \mathcal{O}^*_\infty$ is D-exact with respect to the algebra $\mathcal{T}^*_\infty$ (i.e., $\phi = D\varphi$, $\varphi \in \mathcal{T}^*_\infty$), then it is D-exact in the algebra $\mathcal{O}^*_\infty$ (i.e., $\phi = D\varphi'$, $\varphi' \in \mathcal{O}^*_\infty$). Lemma 1 states that, if Y is a contractible fiber bundle and a D-exact form ϕ on $J^\infty Y$ is of finite jet order $[\phi]$ (i.e., $\phi \in \mathcal{O}^*_\infty$), there exists an exterior form $\varphi \in \mathcal{O}^*_\infty$ on $J^\infty Y$ such that $\phi = D\varphi$. Moreover, a glance at the homotopy operators for d_H and δ in Ref. 12 shows that the jet order $[\varphi]$ of φ is bounded for all exterior forms ϕ of fixed jet order. Let us call this fact the finite exactness of the operator D. Given an arbitrary fiber bundle Y, the finite exactness takes place on $J^\infty Y|_U$ over any open subset U of Y which is homeomorphic to a convex open subset of $\mathbb{R}^{\dim Y}$. Now, we show the following.

(i) Suppose that the finite exactness of the operator D takes place on $J^\infty Y$ over open subsets U, V of Y and their nonempty overlap $U \cap V$. Then, it is also true on $J^\infty Y|_{U\cup V}$.

(ii) Given a family $\{U_\alpha\}$ of disjoint open subsets of Y, let us suppose that the finite exactness takes place on $J^\infty Y|_{U_\alpha}$ over every subset U_α from this family. Then, it is true on $J^\infty Y$ over the union $\cup_\alpha U_\alpha$ of these subsets.

If assertions (i) and (ii) hold, the finite exactness of D on $J^\infty Y$ takes place because one can construct the corresponding covering of the manifold Y (see Lemma 9.5 in Ref. 14).

Proof of (i): Let $\phi = D\varphi \in \mathcal{O}^*_\infty$ be a D-exact form on $J^\infty Y$. By assumption, it can be brought into the form $D\varphi_U$ on $(\pi^\infty_0)^{-1}(U)$ and $D\varphi_V$ on $(\pi^\infty_0)^{-1}(V)$, where φ_U and φ_V are exterior forms of finite jet order. Due to the decompositions (13)–(15), one can choose the forms φ_U, φ_V such that $\varphi - \varphi_U$ on $(\pi^\infty_0)^{-1}(U)$ and $\varphi - \varphi_V$ on $(\pi^\infty_0)^{-1}(V)$ are D-exact forms. Let us consider the difference $\varphi_U - \varphi_V$ on $(\pi^\infty_0)^{-1}(U\cap V)$. It is a D-exact form of finite jet order which, by assumption, can be written as $\varphi_U - \varphi_V = D\sigma$ where an exterior form σ is also of finite jet order. Lemma 8 shows that $\sigma = \sigma_U + \sigma_V$ where σ_U and σ_V are exterior forms of finite jet order on $(\pi^\infty_0)^{-1}(U)$ and $(\pi^\infty_0)^{-1}(V)$, respectively. Then, putting

$$\varphi'_U = \varphi_U - D\sigma_U, \quad \varphi'_V = \varphi_V + D\sigma_V,$$

we have the form ϕ equal to $D\varphi'_U$ on $(\pi_0^\infty)^{-1}(U)$ and $D\varphi'_V$ on $(\pi_0^\infty)^{-1}(V)$, respectively. Since the difference $\varphi'_U-\varphi'_V$ on $(\pi_0^\infty)^{-1}(U\cap V)$ vanishes, we obtain $\phi=D\varphi'$ on $(\pi_0^\infty)^{-1}(U\cup V)$ where

$$\varphi' \stackrel{\text{def}}{=} \begin{cases} \varphi'|_U=\varphi'_U, \\ \varphi'|_V=\varphi'_V \end{cases}$$

is of finite jet order.

Proof of (ii): Let $\phi\in\mathcal{O}^*_\infty$ be a D-exact form on $J^\infty Y$. The finite exactness on $(\pi_0^\infty)^{-1}(\cup U_\alpha)$ holds since $\phi=D\varphi_\alpha$ on every $(\pi_0^\infty)^{-1}(U_\alpha)$ and, as was mentioned previously, the jet order $[\varphi_\alpha]$ is bounded on the set of exterior forms $D\varphi_\alpha$ of fixed jet order $[\phi]$.

Lemma 8: Let U and V be open subsets of a fiber bundle Y and $\sigma\in\mathfrak{O}^*_\infty$ an exterior form of finite jet order on $(\pi_0^\infty)^{-1}(U\cap V)\subset J^\infty Y$. Then, σ splits into a sum $\sigma_U+\sigma_V$ of exterior forms σ_U and σ_V of finite jet order on $(\pi_0^\infty)^{-1}(U)$ and $(\pi_0^\infty)^{-1}(V)$, respectively.

Proof: By taking a smooth partition of unity on $U\cup V$ subordinate to the cover $\{U,V\}$ and passing to the function with support in V, one gets a smooth real function f on $U\cup V$ which is 0 on a neighborhood of $U-V$ and 1 on a neighborhood of $V-U$ in $U\cup V$. Let $(\pi_0^\infty)^*f$ be the pull-back of f onto $(\pi_0^\infty)^{-1}(U\cup V)$. The exterior form $((\pi_0^\infty)^*f)\sigma$ is zero on a neighborhood of $(\pi_0^\infty)^{-1}(U)$ and, therefore, can be extended by 0 to $(\pi_0^\infty)^{-1}(U)$. Let us denote it σ_U. Accordingly, the exterior form $(1-(\pi_0^\infty)^*f)\sigma$ has an extension σ_V by 0 to $(\pi_0^\infty)^{-1}(V)$. Then, $\sigma=\sigma_U+\sigma_V$ is a desired decomposition because σ_U and σ_V are of finite jet order which does not exceed that of σ.

VI. THE GLOBAL INVERSE PROBLEM

The variational complex (7) provides the algebraic approach to the calculus of variations on fiber bundles.[1,6,11] For instance, the variational operator δ acting on $\mathcal{T}^{0,n}_\infty$ is the Euler–Lagrange map, while δ acting on E_1 is the Helmholtz–Sonin map. Let us relate the cohomology isomorphism (12) to the global inverse problem of the calculus in variations. As a particular repetition of Proposition 6, we come to its following solution in the class of exterior forms of locally finite jet order.

Theorem 9: A Lagrangian $L\in\mathcal{T}^{0,n}_\infty$ is variationally trivial, i.e., $\delta(L)=0$ if and only if

$$L=h_0\varphi+d_H\xi, \quad \xi\in\mathcal{T}^{0,n-1}_\infty, \tag{16}$$

where φ is a closed n-form on Y [see expression (14)].

Theorem 10: An Euler–Lagrange-type operator $\mathcal{E}\in E_1$ satisfies the Helmholtz condition $\delta(\mathcal{E})=0$ if and only if

$$\mathcal{E}=\delta(L)+\tau(\phi), \quad L\in\mathcal{T}^{0,n}_\infty, \tag{17}$$

where ϕ is a closed $(n+1)$-form on Y [see expression (15)].

Theorem 10 recovers the result of Refs. 9 and 8.

Theorem 7 provides the similar solution of the global inverse problem in the class of exterior forms of finite jet order. This is the case of higher order Lagrangian field theory. Namely, the theses of Theorems 9 and 10 remain true if all exterior forms in expressions (16) and (17) belong to $\mathcal{O}^*_\infty$. In this case, Theorem 10 contains the well-known result of Ref. 15. Thus, the obstruction to the exactness of the finite order calculus of variations is the same as for exterior forms of locally finite order, without minimizing the order of Lagrangians. The main point for physical applications is that this obstruction is given by closed forms on the fiber bundle Y, and is of first order.

Remark: The local exactness of the calculus of variations has been proved in the class of exterior forms of finite order by use of homotopy operators which do not minimize the order of Lagrangians (see, e.g., Refs. 11 and 12). The infinite variational complex of such exterior forms on $J^\infty Y$ has been studied by many authors (see, e.g., Refs. 1, 6, 11, and 12). However, these forms on $J^\infty Y$ fail to constitute a sheaf. Therefore, the cohomology obstruction to the exactness of the

calculus of variations has been obtained in the class of exterior forms of locally finite jet order which make up the differential algebra $\mathcal{T}^*_\infty$.[8,9] Several statements without proof were announced in Ref. 7. A solution of the global inverse problem in the calculus of variations in the class of exterior forms of a fixed jet order has been suggested in Ref. 9 by a computation of cohomology of the fixed order variational sequence (see Refs. 16 and 17 for another variant of such a variational sequence). The key point of this computation lies in the local exactness of the finite order variational sequence which, however, requires rather sophisticated *ad hoc* technique in order to be reproduced (see also Ref. 18). Therefore, the results of Ref. 9 were not widely recognized. The first thesis of Ref. 9 agrees with Theorem 9 for finite order Lagrangians, but says that the jet order of the form ξ in expression (16) is $k-1$ if L is a k-order variationally trivial Lagrangian. The second one states that a $2k$-order Euler–Lagrange operator can always be associated with a k-order Lagrangian.

Theorems 9 and 10 for elements of $\mathcal{O}^*_\infty$ provide a solution of the global inverse problem in time-dependent mechanics treated as a particular field theory on smooth fiber bundles over $X=\mathbb{R}$.[19] Note that, in time-dependent mechanics, the inverse problem is more intricate than in field theory. Given a second-order dynamic equation, one studies the existence of an associated Newtonian system and its equivalence to a Lagrangian one.[19] Since a fiber bundle $Y\to\mathbb{R}$ is trivial, de Rham cohomology of Y is equal to that of its typical fiber M, and so is de Rham cohomology $H^*(J^\infty Y)$ of $J^\infty Y$. The variational complex (7) in time-dependent mechanics takes the form

$$0\to\mathbb{R}\to\mathcal{T}^0_\infty\xrightarrow{d_t}\mathcal{T}^{0,1}_\infty\xrightarrow{\delta}E_1\xrightarrow{\delta}E_2\to\cdots.$$

Its cohomology coincides with de Rham cohomology of M. In particular, Theorem 9 states that a Lagrangian L of time-dependent mechanics is variationally trivial if and only if it takes the form

$$L=(\varphi_t+\varphi_i y^i_t)\mathrm{d}t+d_t\xi,$$

where $\varphi=\varphi_t\,\mathrm{d}t+\varphi_i\,\mathrm{d}y^i$ is a closed one-form on Y (see also Ref. 7).

VII. THE CASE OF AN AFFINE BUNDLE

Let $Y\to X$ be an affine bundle. Since X is a strong deformation retract of Y, de Rham cohomology of Y and, consequently, $J^\infty Y$ is equal to that of X. An immediate consequence of this fact is the following cohomology isomorphisms:

$$H^{<n}(d_H;\mathcal{O}^*_\infty)=H^{<n}(X),\quad H^0(\delta;\mathcal{O}^*_\infty)=H^n(X),\quad H^k(\delta;\mathcal{O}^*_\infty)=0.$$

It follows that every d_H-closed form $\phi\in\mathcal{O}^{0,m<n}_\infty$ is represented by the sum

$$\phi=\varphi+d_H\xi,\quad \xi\in\mathcal{O}^{0,m-1}_\infty, \tag{18}$$

where φ is a closed form on X. Similarly, any variationally trivial Lagrangian takes the form

$$L=\varphi+d_H\xi,\quad \xi\in\mathcal{O}^{0,n-1}_\infty,$$

where φ is a closed n-form on X. The decomposition (18) shows that, since the BRST operator eliminates exterior forms on X, there is no topological obstruction to constructing global descent equations in the physical field sector of BRST theory.

For applications to BRST theory, we will restrict our consideration to the horizontal complex (4) and the similar complex of the differential algebra $\mathcal{O}^*_\infty$. In the case of an affine bundle $Y\to X$, we can lower this complex onto the base X as follows.

Let us consider the open surjection $\pi^\infty: J^\infty Y\to X$ and the direct image $\{\pi^\infty_*\mathfrak{T}^*_\infty\}$ on X of the sheaf $\mathfrak{T}^*_\infty$. Its stalk over a point $x\in X$ consists of the equivalence classes of sections of the sheaf

$\mathfrak{T}^*_\infty$ which coincide on the inverse images $(\pi^\infty)^{-1}(U_x)$ of neighborhoods U_x of x. Put further the notation $\mathfrak{TX}^*_\infty = \pi^\infty_* \mathfrak{T}^*_\infty$. Since $\pi^\infty_* \mathbb{R} = \mathbb{R}$, we have the following complex of sheaves on X:

$$0 \longrightarrow \mathbb{R} \longrightarrow \mathfrak{TX}^0_\infty \xrightarrow{d_H} \mathfrak{TX}^{0,1}_\infty \xrightarrow{d_H} \cdots \xrightarrow{d_H} \mathfrak{TX}^{0,n}_\infty . \tag{19}$$

Every point $x \in X$ has a base of open contractible neighborhoods $\{U_x\}$ such that the sheaves $\mathfrak{T}^{0,*}_\infty$ of $\mathcal{T}^*_\infty$-modules are acyclic on the inverse images $(\pi^\infty)^{-1}(U_x)$ of these neighborhoods. Then, in accordance with the Leray theorem,[20] cohomology of $J^\infty Y$ with coefficients in the sheaves $\mathfrak{T}^{0,*}_\infty$ are isomorphic to that of X with coefficients in their direct images $\mathfrak{TX}^{0,*}_\infty$, i.e., the sheaves $\mathfrak{TX}^{0,*}_\infty$ on X are acyclic. Furthermore, Lemma 1 also shows that the complexes of sections of sheaves $\mathfrak{T}^{0,*}_\infty$ over $(\pi^\infty_0)^{-1}(U_x)$ are exact. It follows that the horizontal complex (19) on X is exact, and is a resolution of the constant sheaf $\mathbb{R}$ on X. Due to the $\mathbb{R}$-algebra isomorphism $\mathcal{T}^*_\infty = \Gamma(X, \mathfrak{TX}^*_\infty)$, one can think of the horizontal complex (4) as being the complex of the structure algebras of the sheaves in the horizontal complex (19) on X.

VIII. COHOMOLOGY OF POLYNOMIAL ALGEBRAS

Given the sheaf $\mathfrak{TX}^*_\infty$ on X, let us consider its subsheaf $\mathfrak{P}^*_\infty$ of germs of exterior forms which are polynomials in the fiber coordinates y^i_Λ, $|\Lambda| \geqslant 0$, of the topological fiber bundle $J^\infty Y \to X$. This property is coordinate independent due to the transition functions (2). The $\mathfrak{P}^*_\infty$ is a sheaf of $C^\infty(X)$-modules. Its structure algebra $\mathcal{P}^*_\infty$ is a $C^\infty(X)$-subalgebra of $\mathcal{T}^*_\infty$. For shot, one can say that $\mathcal{P}^*_\infty$ consists of exterior forms on $J^\infty Y$ which are locally polynomials in fiber coordinates y^i_Λ.

We have the subcomplex

$$0 \longrightarrow \mathbb{R} \longrightarrow \mathfrak{P}^0_\infty \xrightarrow{d_H} \mathfrak{P}^{0,1}_\infty \xrightarrow{d_H} \cdots \xrightarrow{d_H} \mathfrak{P}^{0,n}_\infty \tag{20}$$

of the horizontal complex (19) on X. As a particular variant of the algebraic Poincaré lemma, the exactness of the complex (20) follows from the form of the homotopy operator for d_H or can be proved in a straightforward way (see, e.g., Ref. 4). Since the sheaves $\mathfrak{P}^{0,*}_\infty$ of $C^\infty(X)$-modules on X are acyclic, the complex (20) is a resolution of the constant sheaf $\mathbb{R}$ on X. Hence, cohomology of the complex

$$0 \longrightarrow \mathbb{R} \longrightarrow \mathcal{P}^0_\infty \xrightarrow{d_H} \mathcal{P}^{0,1}_\infty \xrightarrow{d_H} \cdots \xrightarrow{d_H} \mathcal{P}^{0,n}_\infty \tag{21}$$

of the structure algebras $\mathcal{P}^{0,<n}_\infty$ of sheaves $\mathfrak{P}^{0,<n}_\infty$ is equal to that of X. It follows that every d_H-closed polynomial form $\phi \in \mathcal{P}^{0,m<n}_\infty$ splits into the sum

$$\phi = \varphi + d_H \xi, \quad \xi \in \mathcal{P}^{0,m-1}_\infty , \tag{22}$$

where φ is a closed form on X.

Let P^*_∞ be $C^\infty(X)$-subalgebra of the polynomial algebra $\mathcal{P}^*_\infty$ which consists of exterior forms which are polynomials in the fiber coordinates y^i_Λ. Obviously, P^*_∞ is a subalgebra of $\mathcal{O}^*_\infty$. In BRST theory, P^*_∞ is an algebra of exterior forms of even fields and antifields. As a repetition of Theorem 7, one can show that P^*_∞ have the same cohomology as $\mathcal{P}^*_\infty$, i.e., if ϕ in the decomposition (22) is an element of $P^{0,*}_\infty$ then ξ is so. It follows that, in the case of the polynomial algebra P^*_∞, we also have no topological obstruction to constructing global descent equations in BRST theory.

Let us consider the subsheaf $\overline{\mathfrak{P}}^*_\infty$ of the sheaf $\mathfrak{P}^*_\infty$ which consists of germs of x-independent polynomial forms. Its structure algebra $\overline{P}^*_\infty$ is a subalgebra of the algebra P^*_∞. We have the complex of sheaves

$$0 \longrightarrow \mathbb{R} \longrightarrow \overline{\mathfrak{P}}^0_\infty \xrightarrow{d_H} \overline{\mathfrak{P}}^{0,1}_\infty \xrightarrow{d_H} \cdots \xrightarrow{d_H} \overline{\mathfrak{P}}^{0,n}_\infty,$$

which fails to be exact. The obstruction to its exactness at the term $\overline{\mathfrak{P}}^{0,k}_\infty$ is provided by the germs of k-forms on X with constant coefficients.[4] Let us denote the sheaf of such germs by S^k_X. For any $0<k<n$, we have the short exact sequence of sheaves

$$0 \to \operatorname{Im} d_H \to \operatorname{Ker} d_H \to S^k_X \to 0$$

and the sequence of their structure modules

$$0 \to \Gamma(X, \operatorname{Im} d_H) \to \Gamma(X, \operatorname{Ker} d_H) \to \Gamma(X, S^k_X) \to 0,$$

which is exact because S^k_X is a subsheaf of $\mathbb{R}$-modules of the sheaf $\operatorname{Ker} d_H$. Then, the k-cohomology group of the horizontal complex

$$0 \longrightarrow \mathbb{R} \longrightarrow \overline{P}^0_\infty \xrightarrow{d_H} \overline{P}^{0,1}_\infty \xrightarrow{d_H} \cdots \xrightarrow{d_H} \overline{P}^{0,n}_\infty$$

of the algebra $\overline{P}^*_\infty$ is isomorphic to the $\mathbb{R}$-module $\Gamma(X, S^k_X)$ of global constant k-forms on the manifold X. If a manifold X is not locally affine, the module $\Gamma(X, S^{0,k}_\infty)$ is empty and, consequently, the differential d_H is exact on the algebra $\overline{\mathcal{P}}^{0,<n}$. In this case, there is no obstruction to constructing global descent equations. If a manifold X is locally affine, e.g., parallelizable, any d_H-closed element $\phi \in \overline{P}^{0,k}_\infty$, $0<k<n$, splits into the sum

$$\phi = \varphi + d_H \xi, \quad \varphi \in \Gamma(X, S^k_X), \quad \xi \in \overline{P}^{0,k-1}_\infty.$$

Since the BRST operator eliminates exterior forms on X, elements $\varphi \in \Gamma(X, S^k_X)$ also do not provide an obstruction to the existence of global descent equations.

Thus, we observe that, in the sector of even fields and antifields of BRST theory, there is no topological obstruction to constructing global descent equations.

APPENDIX A

We quote the following variant of the abstract de Rham theorem.

Let

$$0 \longrightarrow S \xrightarrow{h} S_0 \xrightarrow{h^0} S_1 \xrightarrow{h^1} \cdots \xrightarrow{h^{p-1}} S_p \xrightarrow{h^p} S_{p+1}, \quad p>1 \tag{23}$$

be an exact sequence of sheaves on a paracompact topological space Z, where the sheaves S_p and S_{p+1} are not necessarily acyclic, and let

$$\begin{aligned} &0 \longrightarrow \Gamma(Z,S) \xrightarrow{h_*} \Gamma(Z,S_0) \xrightarrow{h^0_*} \Gamma(Z,S_1) \xrightarrow{h^1_*} \\ &\cdots \xrightarrow{h^{p-1}_*} \Gamma(Z,S_p) \xrightarrow{h^p_*} \Gamma(Z,S_{p+1}) \end{aligned} \tag{24}$$

be the corresponding cochain complex of structure groups of these sheaves.

Theorem 11: The q-cohomology groups of the cochain complex (24) for $0 \leqslant q \leqslant p$ are isomorphic to the cohomology groups $H^q(Z,S)$ of Z with coefficients in the sheaf S.

APPENDIX B

We construct a homotopy from $J^\infty Y$ to Y in an explicit form. Let $\gamma_{(k)}$, $k \leqslant 1$, be global sections of the affine jet bundles $J^k Y \to J^{k-1} Y$. Then, we have a global section

$$\gamma: Y \ni (x^\lambda, y^i) \to (x^\lambda, y^i, y^i_\Lambda = \gamma^i_{(|\Lambda|)\Lambda} \circ \gamma_{(|\Lambda|-1)} \circ \cdots \circ \gamma_{(1)}) \in J^\infty Y \tag{25}$$

of the open surjection $\pi^\infty_0 : J^\infty Y \to Y$. Let us consider the map

$$[0,1]\times J^\infty Y \ni (t; x^\lambda, y^i, y^i_\Lambda) \to (x^\lambda, y^i, y'^i_\Lambda) \in J^\infty Y, \quad 0 < |\Lambda|, \tag{26}$$

$$y'^i_\Lambda = f_k(t) y^i_\Lambda + (1 - f_k(t))\, \gamma_{(k)}{}^i_\Lambda(x^\lambda, y^i, y^i_\Sigma), \quad |\Sigma| < k = |\Lambda|,$$

where $f_k(t)$ is a continuous monotone real function on $[0,1]$ such that

$$f_k(t) = \begin{cases} 0, & t \leqslant 1 - 2^{-k} \\ 1, & t \geqslant 1 - 2^{-(k+1)}. \end{cases} \tag{27}$$

A glance at the transition functions (2) shows that, although written in a coordinate form, this map is globally defined. It is continuous because, given an open subset $U_k \subset J^k Y$, the inverse image of the open set $(\pi^\infty_k)^{-1}(U_k) \subset J^\infty Y$, is the open subset

$$(t_k,1]\times(\pi^\infty_k)^{-1}(U_k) \cup (t_{k-1},1]\times(\pi^\infty_{k-1})^{-1}(\pi^k_{k-1}[U_k \cap \gamma_{(k)}(J^{k-1}Y)])$$

$$\cup \cdots \cup [0,1]\times(\pi^\infty_0)^{-1}(\pi^k_0[U_k \cap \gamma_{(k)} \circ \cdots \circ \gamma_{(1)}(Y)])$$

of $[0,1]\times J^\infty Y$, where $[t_r,1] = \operatorname{supp} f_r$. Then, the map (26) is a desired homotopy from $J^\infty Y$ to Y which is identified with its image under the global section (25).

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A robust approach to protein foldability measures based on spin-glass models

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Spin-glass models and related methods have been applied to protein folding problems, often by assuming an underlying Gaussian distribution for the energy level distribution. In this paper, we derive robust foldability measures that relax the Gaussian distribution assumption implicit in current foldability and energy gap measures. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379746]

I. INTRODUCTION

Spin-glass models and their analogs have been applied to problems involving protein structures[1] and protein folding.[2–4] In particular, spin-glass models have been used to determine whether proteins can be characterized as to their foldability potential.[2] Spin glasses are magnetic systems whose periodicity (translational invariance) is broken by ''frozen randomness,'' characterized by metastable states with essentially indeterminate relaxation times to a stable phase. Spin glasses can be alloys of a nonmagnetic atom of a noble metal and a magnetic atom of a transition metal (like manganese or iron). Nonstoichiometric ternary alloys exhibiting a periodic crystalline structure, but with the magnetic atoms randomly scattered through the lattice sites are other types of spin glasses as are non-crystalline alloys of aluminum and gadolinium, where the atoms are in random spatial positions. Spin glasses all display similar thermodynamic behavior, notably, singularities at a critical temperature.[5]

II. SPIN-GLASS MODELS AND THE RANDOM ENERGY MODEL

The Sherrington–Kirkpatrick (SK) spin-glass model[6] is an Ising model in which spins are coupled by infinite-ranged random interactions. Their probability density is taken to be Gaussian in the conventional formulation. Following Petritis,[5] the SK model is of the mean-field type (the strength of the interactions between interacting magnetic atoms retains the same magnitude throughout the material) that is defined over sites $\Lambda_N=\{1,...,N\}$ with dual lattice Λ_N^* of Λ_N having a complete graph $K_N=\{\{i,j\}:i\in\Lambda_N, j\in\Lambda_N, i\neq j\}=\{\{i,j\}:i\in\Lambda_N, j\in\Lambda_N, i<j\}$ over N. Now consider a group of independent, centered, Gaussian random variables with variance $1:(J_{ij})_{\{i,j\}\in\Lambda_N^*}$ indexed by Λ_N^*. The interaction energy (Hamiltonian) of this model is

$$I_N(\sigma)=-\frac{1}{\sqrt{N}}\sum_{\{i,j\}\in\Lambda_N^*}J_{ij}\sigma_i\sigma_j. \tag{1}$$

The sum extends over $|\Lambda_N^*|=N(N-1)/2$ terms, and the normalization is in $\sqrt{N}$. The use of the normal distribution is for computational convenience, and the central limit theorem is far from being applicable in this case. Formulating (1) as a time-dependent stochastic process, we obtain the standard derivation:

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$$I_N(t,\sigma) := -\frac{1}{\sqrt{N}} \sum_{\{i,j\}\in\Lambda_N^*} B_{ij}(t)\sigma_i\sigma_j, \quad \sigma \in S_N := \{-1,+1\}^N, \tag{2}$$

where the $B_{i,j}$ are independent Brownian motions with variance $\mathbb{E}B_{i,j}^2 = t$ if $i<j$ and $\mathbb{E}B_{i,j}^2 = t/2$ if $i=j$. Let $E_\sigma(\cdot) = 2^{-N}\Sigma_{\sigma\in S_N}(\cdot)$ be the uniform probability on the configuration space S_N. The partition function with time dependence is then

$$Z_N(t) = E_\sigma \exp\{I_N(t,\sigma) - Nt/4\}, \tag{3}$$

which, apart from a minor term, defines the same Gibbs measure as (1) that we will denote $\rho_{N,t}$. Since $Z_N(t)$ is a positive martingale (a ''martingale'' represents a generalization of the concept of a sum of independent random variables) with mean 1, Z_N has stochastic differential $dZ_N(t)$ and log martingale M_N defined by the stochastic integral:

$$M_N(t) = \int_0^t Z_N(s)^{-1}\, dZ_N(s). \tag{4}$$

M_N is a centered martingale of the form

$$\langle M_N\rangle(t) = \int_0^t E^{\rho_{N,s}^{\otimes 2}}\left[\frac{1}{2}\left(\frac{\sigma.\sigma'}{\sqrt{N}}\right)^2\right] ds, \tag{5}$$

where $E^{\rho_{N,s}^{\otimes 2}}$ is the expectation over two independent replicas σ,σ' associated with the Gibbs measure $\rho_{N,s}$.

For the simplified (time-independent) Hamiltonian of (1), we can define a partition function as

$$Z_N = \sum_{\sigma\in\Sigma_N} \exp(-\beta I_N(\sigma)), \tag{6}$$

where β is the inverse temperature and is a random variable (for every fixed β). The quenched free energy is

$$F_N(\beta) = -\frac{1}{\beta}\log Z_N(\beta), \tag{7}$$

and the quenched specific free energy is defined by

$$f_N(\beta) = \frac{1}{|\Lambda_N|} F_N(\beta). \tag{8}$$

Due to computational difficulties involving the log term in (7), Edwards and Anderson[7] proposed the famous replica trick: instead of computing $\mathbb{E}\log Z_N$, they compute $\mathbb{E}Z_N^R$, where R is the number of replicas [independent copies of the model (in σ) all having the same random interactions J]. Thus, for positive R, one needs to compute the moments of the partition function. Parisi[8] and Mezard, Parisi, and Virasoro[9] observed that as a consequence of phase transition, there is a breaking of the symmetry group S_R over replicas, and that introducing infinite replica symmetry breaking, inducing an ultrametric structure to the space of states, provides a heuristic solution for the specific free energy that is in reasonable agreement with rigorous results. [Earlier, Mezard, Parisi, and Virasoro[10] discussed the fluctuations (of order $1/N$) of the free energy to define the pure state weights of the model. They explain how to obtain the replica symmetry-breaking solution of the SK model without introducing replicas.] Derrida[11,12] describes two simplified SK-based models, the random energy model (REM), and the generalized random energy model (GREM). In the

case of the REM model, the energy levels E_i form a system of independent, identically distributed variables, and the partition function is written as a sum over 2^N energy levels,

$$Z(\beta)=\sum_{i=1}^{2^N} \exp(-\beta E_i), \tag{9}$$

where β is the inverse temperature. For the GREM, correlations between the energy levels are introduced hierarchically. The energy levels are defined:

$$E_{k_1,\ldots,k_n}=\sqrt{N}\sum_{j=1}^{n} \sqrt{a_j}\epsilon^j_{k_1,\ldots,k_j}, \tag{10}$$

and the partition function is then

$$Z(\beta)=\sum_{k_1=1}^{\alpha_1^N} \cdots \sum_{k_n=1}^{\alpha_n^N} \exp\left(\beta\sqrt{N}\sum_{j=1}^{n} \sqrt{a_j}\epsilon^j_{k_1,\ldots,k_j}\right). \tag{11}$$

Spin-glass models have been used to describe protein folding, and to explain certain salient features such as abrupt transitions between folded and unfolded states; multiexponential kinetics; and misfolds, irreversible denaturation, and protein drift.[13]

III. FOLDABILITY AND ENERGY GAP

Briefly summarizing Buchler and Goldstein, the equilibrium glass transition temperature, T_g, or ''heteropolymer freezing'' temperature, is defined as the temperature where the protein chain entropy drops below zero and the chain attains one of its low-energy, metastable states. Using the REM (which does not incorporate conformation energy correlations), one can demonstrate that T_g demarcates the kinetic behavior into two classes. For $T>T_g$, the escape rate distribution from low-energy metastable states is lognormal, fast rates are much more likely than slow rates; for $T<T_g$, the kinetic distribution of rates becomes more uniform, so that both slow and fast escape rates become equally likely.[2] Using the REM (and setting k_B to one), one can determine that the equilibrium glass temperature is

$$T_g=\sqrt{\frac{\sigma^2}{2S_0}}, \tag{12}$$

where σ^2 is the variance or ''roughness'' (squared) of the REM energy distribution, and S_0 is the conformational entropy of the system. One can thus surmise that ''rougher'' energy landscapes lead to higher glass transition temperatures. The presence of protein drift, misfolds, irreversible denaturation, discrete intermediates, and multiexponential kinetics would indicate proteins with rougher energy landscapes than those that fold consistently and have single-exponential kinetics. Since the folded state must be thermodynamically preferable to other possible structures at equilibrium, it was postulated that optimal folding landscapes would tend to maximize folding temperature T_f, a measure of relative stability, and minimize T_g, that is, increase the ratio, T_f/T_g.[14–16] Using the REM, one can show that

$$\frac{T_f}{T_g}=\sqrt{\frac{\mathcal{F}^2}{2S_0}}+\sqrt{\frac{\mathcal{F}^2}{2S_0}-1},$$

where the foldability, $\mathcal{F}$, is

$$\mathcal{F}=\frac{\overline{E}-E_{\mathrm{ns}}}{\sigma} \tag{13}$$

where $\bar{E}$ is the average energy of the protein chain in all conformations, $E_{\rm ns}$ is the energy of the native structure, and σ is the ''roughness'' of the REM energy landscape. Monte Carlo kinetic and molecular dynamic simulations have shown that fast folding proteins had higher average foldabilities and larger T_f/T_g ratios.[15,16] The quantification of folding ability by $\mathcal{F}$ has contributed to further development of protein designability research.

An equivalent measure relating to folding kinetics is the energy gap, Δ_g, defined as

$$\Delta_g = E_g - E_{\rm ns}, \tag{14}$$

where E_g is the glass transition energy and $E_{\rm ns}$ is the native state energy.

For now, assume that the energy states are uncorrelated, using the REM model, one can show, in the limit of large proteins, that the energy distribution of compact states is of Gaussian form. The density of states of a REM heteropolymer sequence is denoted $\Omega(E) = n\rho_{\rm REM}(E)$, where n is the number of compact protein structures and $\rho_{\rm REM}(E)$ is a normalized Gaussian distribution:

$$\rho_{\rm REM}(E) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(E-\bar{E})^2/2\sigma^2}, \tag{15}$$

where $\bar{E}$ is the average energy of the compact states and σ is the roughness of the energy density landscape. If we consider deriving the foldability of the native state, $\mathcal{F}$, as a function of the number of compact protein structures n, the condition that the native state energy $E_{\rm ns}$ has the lowest value among all other $n-1$ energies follows from native state uniqueness and thermodynamic considerations. One can thus describe the native state energy distribution in the REM by

$$\rho(E_{\rm ns}|n) = \rho_{\rm REM}\mathcal{P}(E_{\rm ns} < n-1). \tag{16}$$

Using (15), and assuming independence of energies, we obtain

$$\rho_{\rm REM}(E_{\rm ns}) = \frac{1}{\sigma\sqrt{2\pi}} e^{-(E_{\rm ns}-\bar{E})^2/2\sigma^2}, \tag{17}$$

and

$$\mathcal{P}(E_{\rm ns} < n-1) = \left[\int_{E_{\rm ns}}^{\infty} \rho_{\rm REM}(E)\,\delta E \right]^{(n-1)}, \tag{18}$$

combining, and normalizing $\left(\int_{-\infty}^{+\infty} \rho(E_{\rm ns}|n)\,\delta E_{\rm ns} = 1\right)$ gives the density of native states energies as

$$\rho(E_{\rm ns}|n) = n\rho_{\rm REM}(E_{\rm ns}) \left[\int_{E_{\rm ns}}^{\infty} \rho_{\rm REM}(E)\,\delta E \right]^{(n-1)}, \tag{19}$$

substituting (17) and evaluating (18), one obtains

$$\rho(E_{\rm ns}|n) = \frac{n}{\sigma\sqrt{2\pi}} e^{-(E_{\rm ns}-\bar{E})^2/2\sigma^2} \left[\frac{1}{2}\left(1 - {\rm Erf}\left(\frac{E_{\rm ns}-\bar{E}}{\sigma\sqrt{2}} \right) \right) \right]^{(n-1)}, \tag{20}$$

which is of the form of an extreme value distribution. To convert to foldability, we use (13) to obtain

$$\rho(\mathcal{F}) = \frac{n}{\sqrt{2\pi}} e^{-\mathcal{F}^2/2} \left[\frac{1}{2}\left(1 + {\rm Erf}\left(\frac{\mathcal{F}}{\sqrt{2}} \right) \right) \right]^{(n-1)}. \tag{21}$$

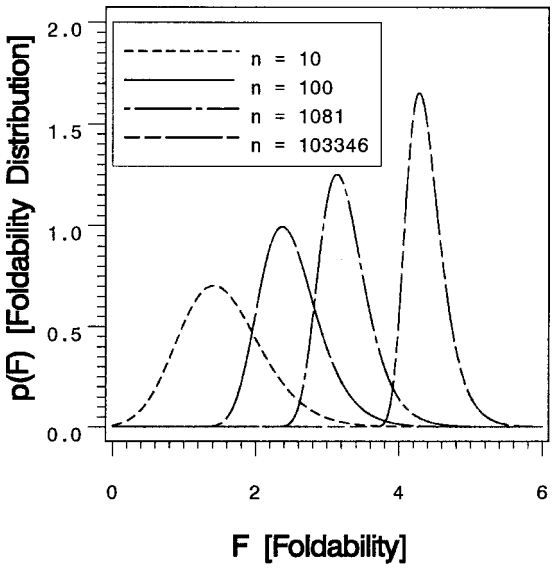

FIG. 1. Plot of the foldability distribution $\rho(\mathcal{F})$ for different numbers of compact energy states using the random energy model (based on Fig. 1 of Buchler and Goldstein).

Figure 1 displays foldability distribution curves for various values of n (this figure is based on Fig. 1 of Buchler and Goldstein). Having completed the summarization of the Buchler and Goldstein's derivation, we will now introduce the new methodology.

IV. ROBUST ESTIMATION

Though the assumption of a Gaussian distribution (from which the extreme value distribution shown above is derived) is conventional and definitely plausible, we need to be able to account for irregularities in the distribution, and keep in mind that ''large datasets of high quality show significant deviations from normality in cases which should be prime examples for the normal [Gaussian] law of errors....''.[17] To address this concern, we propose using a robust estimator, which is of an approximate parametric class. Robust methods allow us to retain the general parametric form of the model while compensating for deviations from the assumed distribution.[18,19] In statistical parlance ''robust'' methods are intermediate between the usual parametric (e.g., Gaussian assumption) techniques and nonparametric or distribution-free methods.

We can now derive a robust version of (21), by introducing the notion of the α-trimmed mean $(0<\alpha<\frac{1}{2})$, which is

$$T(F)=\int_{\alpha}^{1-\alpha} F^{-1}(t)dt/(1-2\alpha), \tag{22}$$

where $T(F)$ indicates a functional of the distribution of energies of compact states.[17] The trimmed mean is a robust estimator, and is intuitively appealing, since one removes the $[\alpha n]$ smallest and the $[\alpha n]$ largest energies (where $[\cdot]$ indicates the integer function), excluding E_{ns} from this operation, and then takes the mean of the remaining values. One can also replace σ with the standard deviation of this reduced set to produce a trimmed standard deviation, σ_t. Setting $\overline{E_t}=T(F)$, we now can define robust foldability as $\mathcal{F}_t=(\overline{E_t}-E_{\mathrm{ns}})/\sigma_t$, yielding

$$\rho(\mathcal{F}_t)=\frac{n-[2\alpha n]}{\sqrt{2\pi}}e^{-\mathcal{F}_t^2/2}\left[\frac{1}{2}\left(1+\mathrm{Erf}\left(\frac{\mathcal{F}_t}{\sqrt{2}}\right)\right)\right]^{(n-[2\alpha n]-1)}. \tag{23}$$

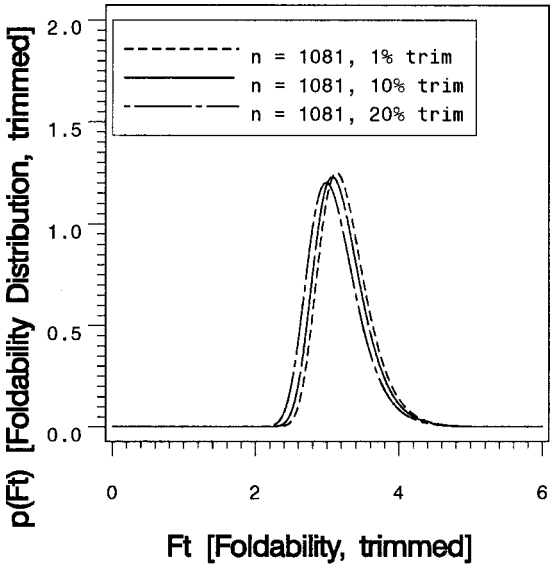

FIG. 2. Plot of the robust (trimmed) foldability distribution $\rho(\mathcal{F}_t)$ for various degrees of trimming for $n=1081$ compact energy states.

This relation is useful when the underlying energy distribution of compact states has a skewed, non-Gaussian character, or is predominantly Gaussian with outliers, and reduces to (21) when the underlying distribution is Gaussian or close to Gaussian, giving it wide applicability for the actual, nonidealized distributions one can see in practice. Figure 2 shows the trimmed foldability distributions for various levels of trimming when $n=1081$. Figure 3 plots the energy gap distributions for the same values of n that were used in Fig. 1 (this figure is based on Fig. 2 of Buchler and Goldstein, with the x-axis corrected). Note the small percentage of area under the curves in Fig. 3 for which $\Delta_g>0$, the weakest foldability criterion. Though foldability increases with n, only a small fraction of REM heteropolymer sequences tend to be foldable as protein size increases.

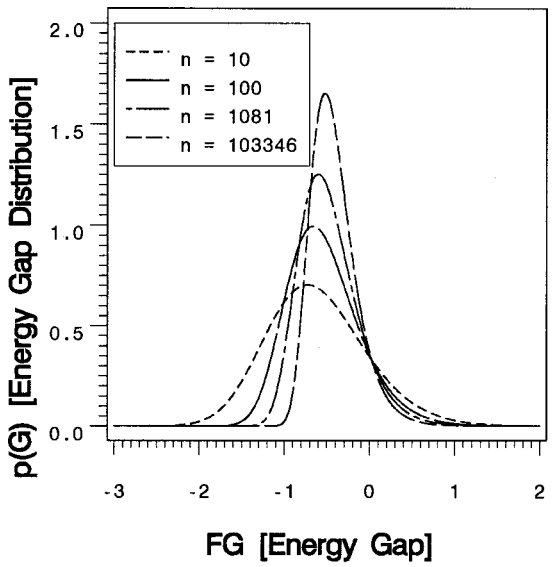

FIG. 3. Plot of the energy gap distribution $\rho(\Delta_g)$ for different numbers of compact energy states using the random energy model (based on Fig. 2 of Buchler and Goldstein with the x axis corrected).

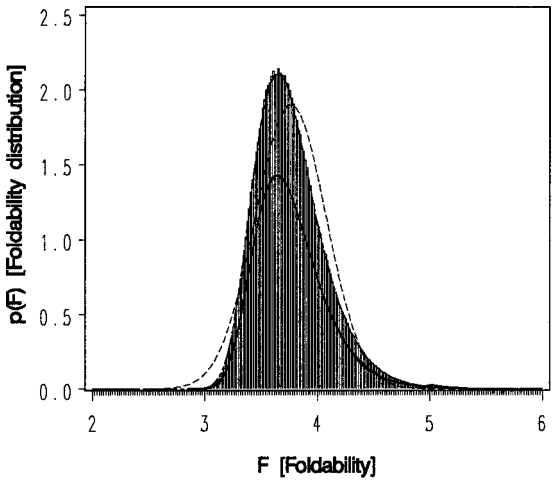

FIG. 4. Nonparametric kernel density (-------), normal (---), and $\rho(\mathcal{F})$ (—) fits to simulated noisy energy level data with outliers.

Using a similar argument as for foldability, we can obtain a robust version of the Buchler and Goldstein equation (13) for the energy gap distribution:

$$\rho(\Delta_{gt}) = \frac{n-[2\alpha n]}{\sqrt{2\pi}} e^{-(\sqrt{2\ln(n-[2\alpha n])}+\Delta_{gt})^2/2}\left[\frac{1}{2}\left(1+\mathrm{Erf}\left(\frac{\sqrt{2\ln(n-[2\alpha n])}+\Delta_{gt}}{\sqrt{2}}\right)\right)\right]^{(n-[2\alpha n]-1)}. \tag{24}$$

Note that $\rho(\Delta_{gt})$ is identical to $\rho(\mathcal{F}_t)$ except for the shifting factor $\sqrt{2\ln(n-[2\alpha n])}$.

An alternative method for deriving a robust estimator would be to find the trimming level and the value of m, in (25) below that causes the curve described by (25) to most closely approach the nonparametric kernel density estimation[20] fit (see Sec. V) to the energy levels histogram:

$$\rho(\mathcal{F}_p) = \frac{m}{\sqrt{2\pi}} e^{-(\mathcal{F}_p)^2/2}\left[\frac{1}{2}\left(1+\mathrm{Erf}\left(\frac{\mathcal{F}_p}{\sqrt{2}}\right)\right)\right]^{(m-1)}. \tag{25}$$

Here, $\mathcal{F}_p$ is based on the proportion of observations included to match the curves. More formally, consider a sequence of one-dimensional observations $X_1,\ldots,X_n$ that are independent and identically distributed. These observations belong to some sample space $\mathcal{S}$, which is a subset of the real line $\mathbb{R}$. As a measure of discrepancy, consider the Prokhorov distance[21] between two probability distributions $\mathcal{G}$ and $\mathcal{H}$ in $\mathcal{F}(\mathcal{S})$:

$$\pi(\mathcal{G},\mathcal{H})\inf\{\varepsilon;\mathcal{G}(A)\leqslant\mathcal{H}(A^{\varepsilon})+\varepsilon \quad \text{for all } A\}, \tag{26}$$

where A^{ε} is the set of all points with distance from A less than ε. Equation (25) results from matching (21) to the nonparametric kernel density curve with tolerance ε. Note that one could also use the Hellinger or Lévy distances or the bounded Lipschitz metric.[22]

V. EXAMPLE AND DISCUSSION

Figure 4 displays a foldability distribution that is somewhat irregular and has fairly long tails. This corresponds to an energy distribution of compact states that is moderately noisy with outliers. Superimposed on the histogram are three curves: the nonparametric kernel density fit, which can be made to fit any histogram to any degree of accuracy, and is used here as the reference curve, the best normal distribution fit, which is skewed to the right due to the long tail of the distribution, and the $\rho(\mathcal{F})$ fit to the distribution, which is more centered, but clearly is appreciably affected by the

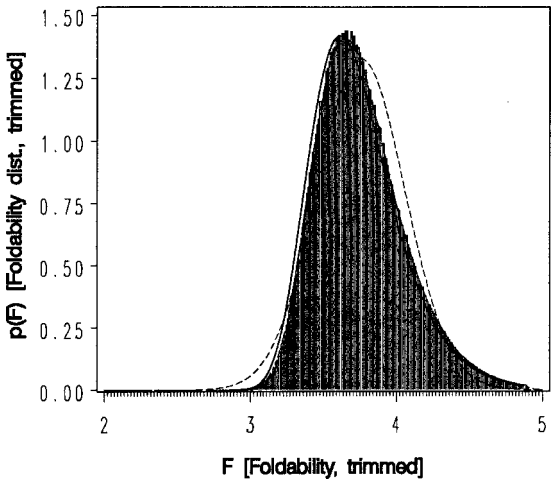

FIG. 5. Nonparametric kernel density (-———-), normal (---), and robust $\rho(\mathcal{F}_p)$ (—) fits to trimmed simulated noisy energy level data with outliers.

irregularities and long tails of the distribution. In Fig. 5, the trimmed foldability distribution is displayed. Note that the histogram bars appear slightly different from those of Fig. 4 due to recalculation after trimming. The best normal distribution fit is still somewhat skewed to the right, but the trimmed $\rho(\mathcal{F}_p)$ fit to the distribution nearly coincides with the reference curve, and is just slightly skewed left, since the left tail of the distribution is still a little long, though of low density. Thus, the robust trimmed estimator distinctly improves the fit to the distribution when noise and outliers are present.

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Translation-covariant Markovian master equation for a test particle in a quantum fluid

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A recently proposed master equation in the Lindblad form is studied with respect to covariance properties and existence of a stationary solution. The master equation describes the interaction of a test particle with a quantum fluid, the so-called Rayleigh gas, and is characterized by the appearance of a two-point correlation function known as the dynamic structure factor, which reflects symmetry and statistical mechanics properties of the fluid. In the case of a free gas, all relevant physical parameters such as fugacity, ratio between the masses, momentum transfer, and energy transfer are put into evidence, giving an exact expansion of the dynamic structure factor. The limit in which these quantities are small is then considered. In particular, in the Brownian limit a Fokker–Planck equation is obtained in which the corrections due to quantum statistics can be explicitly evaluated and are given in terms of the Bose function $g_0(z)$ and the Fermi function $f_0(z)$. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1386409]

I. INTRODUCTION

The study of dissipative systems in a quantum mechanical framework is a subject of major interest for many physical communities especially in connection with applications. Recently, however, the subject has gained new interest also for physicists concerned with foundations of quantum mechanics, due to the relevance of the notion of decoherence as a gateway between the classical and quantum worlds.[1] This interest is strongly supported and partially motivated by a spectacular improvement in many experimental techniques useful for handling with great precision single- or few-particle systems, checking for coherence properties in their dynamical evolution.[2] In this connection models for quantum dissipation determined by the symmetry properties of the microphysical interaction and by symmetry and statistical mechanics properties of the environment could be of interest for a large class of phenomena. In the Markovian limit quantum-dynamical semigroups[3] seem the most natural quantum mechanical framework for the description of dissipative systems[4] and a lot of work has been done in this direction, both at rigorous and formal levels, especially with reference to the structural result of Lindblad, which fixes the form of the generator of a completely positive quantum-dynamical semigroup in the case of norm continuity.[5] In this article we will study in detail some structural properties of a recently proposed Markovian master equation for the description of the dynamics of a test particle in a fluid,[6–9] the so-called Rayleigh gas.[4] This simple but realistic model is of particular interest in statistical mechanics, being a paradigmatic example which opens the way to the study of interacting truly many-body systems. In the quantum regime a feature of independent interest is the relevance of quantum statistics of particles making up the fluid, especially in connection with the recent experimental realization of almost noninteracting degenerate gas samples of both Bose and Fermi particles.[10] The considered master equation was derived by assuming a translationally invariant interaction between the test particle and a homogeneous fluid, and has the general structure of a generator of translation-covariant dynamical semigroups considered in Ref. 11. In this way a direct

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physical interpretation arises, at least in a particular case, of the general structure given in Ref. 11. Further symmetry or equilibrium properties, which are of fundamental relevance in order to determine the realm of validity of a given master equation,[9] are shown to be a direct consequence of particular physical features of the environment, embodied in a specific two-point correlation function, the so-called dynamic structure factor.[12]

The article is organized as follows: in Sec. II the master equation is introduced and the property of covariance with respect to translations and rotations is considered with reference to the corresponding symmetries of the environment embodied in its dynamic structure factor; moreover, the existence of a stationary solution is proved, provided the environment is in a β-KMS state.[13] In Sec. III the case of a free quantum gas is considered, the dynamic structure factor is explicitly calculated, its exact expansion with respect to the relevant physical parameters is obtained and in the limit of small fugacity z the expression for Maxwell–Boltzmann particles is recovered. In Sec. IV the Brownian limit in which the test particle is much heavier than the particles making up the gas is dealt with, together with the limit of small momentum transfer, leading from the master equation to a Fokker–Planck equation, strongly dependent on the statistics of the gas. In Sec. V the obtained results are briefly summarized and discussed.

II. GENERAL FEATURES OF THE MASTER EQUATION

Let us recall the general expression of the master equation proposed in Refs. 7 and 8 for the description of the motion of a test particle in a homogeneous fluid supposed to be at equilibrium, whose properties we are going to study. The obtained result is based on a scattering theory derivation, assuming a translationally invariant interaction in terms of two-particle collisions, and is expected to be valid on a time scale much longer than the relaxation time of the environment. In the Schrödinger picture the master equation is given by

$$\frac{d\hat{\varrho}}{dt}=\mathcal{M}[\hat{\varrho}]=-\frac{i}{\hbar}[\hat{H}_0,\hat{\varrho}]+\mathcal{L}[\hat{\varrho}], \tag{1}$$

where $\hat{H}_0=\hat{\boldsymbol{p}}^2/2M$ is the Hamiltonian of the free particle, M being the mass of the test particle, while the dissipative part is given by the following mapping with a Lindblad structure:

$$\mathcal{L}[\,\cdot\,]=\int_{\mathbf{R}^3}d\mu(\boldsymbol{q})\left[\hat{U}(\boldsymbol{q})\sqrt{S(\boldsymbol{q},\hat{\boldsymbol{p}})}\cdot\sqrt{S(\boldsymbol{q},\hat{\boldsymbol{p}})}\hat{U}^{\dagger}(\boldsymbol{q})-\frac{1}{2}\{S(\boldsymbol{q},\hat{\boldsymbol{p}}),\cdot\}\right], \tag{2}$$

where the integral is over the parameter space of the translation group in momentum space in three dimensions, the parameter $\boldsymbol{q}$ being the momentum transferred in a collision, $\{\hat{A},\hat{B}\}$ denotes the Jordan product $\hat{A}\circ\hat{B}=\hat{A}\hat{B}+\hat{B}\hat{A}$, and the operator $\hat{\boldsymbol{p}}$ is the generator of translations. The unitary operators $\hat{U}(\boldsymbol{q})=e^{(i/\hbar)\boldsymbol{q}\cdot\hat{\boldsymbol{x}}}$, $\boldsymbol{q}\in\mathbf{R}^3$, are the generators of translations in momentum space or boosts. The positive measure $d\mu(\boldsymbol{q})$ is given by

$$d\mu(\boldsymbol{q})=\frac{2\pi}{\hbar}(2\pi\hbar)^3 n|\tilde{t}(q)|^2 d^3\boldsymbol{q}, \tag{3}$$

thus being invariant under both rotations and translations. In fact n is the particle density in the macroscopic system, and the function $\tilde{t}(q)$, given by

$$\tilde{t}(q)=\int_{\mathbf{R}^3}d^3\boldsymbol{x}\frac{e^{(i/\hbar)\boldsymbol{q}\cdot\boldsymbol{x}}}{(2\pi\hbar)^3}t(x),$$

where $q=|\boldsymbol{q}|$ and $x=|\boldsymbol{x}|$, is the Fourier transform with respect to the transferred momentum $\boldsymbol{q}$ of the T matrix describing the translationally and rotationally invariant interaction between the test particle and the particles of the fluid, which is supposed to be energy independent. The function

$S(\boldsymbol{q},\boldsymbol{p})$, which appears operator-valued in (2), is a positive two-point correlation function known as the dynamic structure factor,[12] given by the Fourier transform with respect to energy transfer $E(\boldsymbol{q},\boldsymbol{p})$ and momentum transfer $\boldsymbol{q}$ of the time dependent pair correlation function of the fluid

$$S(\boldsymbol{q},\boldsymbol{p})=\frac{1}{2\pi\hbar}\int_{\mathbf{R}}dt\int_{\mathbf{R}^3}d^3\boldsymbol{x}\,e^{(i/\hbar)[E(\boldsymbol{q},\boldsymbol{p})t-\boldsymbol{q}\cdot\boldsymbol{x}]}G(\boldsymbol{x},t), \tag{4}$$

where $G(\boldsymbol{x},t)$ is the time dependent pair correlation function

$$G(\boldsymbol{x},t)=\frac{1}{N}\int_{\mathbf{R}^3}d^3\boldsymbol{y}\langle N(\boldsymbol{y})N(\boldsymbol{y}+\boldsymbol{x},t)\rangle, \tag{5}$$

$N(\boldsymbol{y})$ being the operator density of particles in the fluid and $\langle\cdots\rangle$ the ensemble average with respect to the state of the macroscopic system. The expression $E(\boldsymbol{q},\boldsymbol{p})$ gives the energy transfer in a collision where the test particle changes its momentum from $\boldsymbol{p}$ to $\boldsymbol{p}+\boldsymbol{q}$, so that

$$E(\boldsymbol{q},\boldsymbol{p})=E_{p+q}-E_p=\frac{q^2}{2M}+\frac{\boldsymbol{p}\cdot\boldsymbol{q}}{M}. \tag{6}$$

Note that in (4) we have used as variables momentum and energy transferred to the test particle. In the sequel we will use both the equivalent notations $S(\boldsymbol{q},\boldsymbol{p})$ and $S(\boldsymbol{q},E(\boldsymbol{q},\boldsymbol{p}))\equiv S(\boldsymbol{q},E)$, according to convenience. The dynamic structure factor is a very important physical quantity, giving the spectrum of spontaneous fluctuations of the system, and it is of direct experimental access: in fact, as first obtained by van Hove in a fundamental work,[14] it is directly related to the energy dependent differential cross-section per target particle describing scattering of a microscopic probe off a macroscopic sample through the formula

$$\frac{d^2\sigma}{d\Omega_{p'}dE_{p'}}=(2\pi\hbar)^6\left(\frac{M}{2\pi\hbar^2}\right)^2\frac{p'}{p}|\tilde{t}(q)|^2S(\boldsymbol{q},E), \tag{7}$$

referring to scattering of the microscopic probe from $\boldsymbol{p}$ to $\boldsymbol{p}'=\boldsymbol{p}+\boldsymbol{q}$. The dynamic structure factor is given in (7) as a function of momentum and energy transfer, which are the measured quantities in scattering experiments, the energy E being related to $\boldsymbol{q}$ and $\boldsymbol{p}$ through (6). The appearance of the dynamic structure factor in (7) gives the physical reason for its being positive definite for every system. The main point in (1) and (2) is the determination of the specific expressions for the measure $d\mu(\boldsymbol{q})$ given by (3), and of the operator valued function $S(\boldsymbol{q},\cdot)$, given by (4), which can only be obtained on the basis of a microphysical derivation of the equation, relying on some physical model. A general structure encompassing (2) has already been considered by Holevo in a purely mathematical context, studying the general structure of generators of translation-covariant dynamical semigroups.[11] In particular Holevo has proven that when the generator is bounded it must have a structure of the form (1) with $\mathcal{L}$ given by (2) provided all operators appearing in (1) and (2) are bounded[11] [see also Refs. 15 and 16, where further restrictions to the structure of (2) appear, to be discussed later on], and allowing, instead of the structure

$$\hat{U}(\boldsymbol{q})\sqrt{S(\boldsymbol{q},\hat{\boldsymbol{p}})}\cdot\sqrt{S(\boldsymbol{q},\hat{\boldsymbol{p}})}\hat{U}^\dagger(\boldsymbol{q})$$

appearing in (2), where $S(\boldsymbol{q},\hat{\boldsymbol{p}})$ is self-adjoint and positive, the more general structure

$$\hat{U}(\boldsymbol{q})L(\boldsymbol{q},\hat{\boldsymbol{p}})\cdot L^\dagger(\boldsymbol{q},\hat{\boldsymbol{p}})\hat{U}^\dagger(\boldsymbol{q}).$$

If the generator is unbounded also diffusion terms of the form considered in (37) may appear, and the operators appearing in (1) and (2) may be unbounded (see Ref. 11 for further details). In the

general model considered here the Hamiltonian is given by the unbounded operator $\hat{H}_0 = \hat{\boldsymbol{p}}^2/2M$, while the remaining part of the generator is determined by the explicit expression of the physical quantities $\tilde{t}(q)$ and $S(\boldsymbol{q},\boldsymbol{p})$, depending on the specific model for the fluid.

We now consider the behavior of (1) with respect to symmetry transformations. Let us consider a locally compact group G and a unitary representation $\hat{U}(g)$, with $g \in G$, on the Hilbert space of the system. Following Ref. 11 we say that a mapping $\mathcal{M}$ in the Schrödinger picture is G-covariant if it commutes with the mapping $\mathcal{U}_g[\,\cdot\,] = \hat{U}(g)\cdot\hat{U}^\dagger(g)$ for all $g \in G$:

$$\mathcal{M}[\mathcal{U}_g[\,\cdot\,]] = \mathcal{U}_g[\mathcal{M}[\,\cdot\,]]. \tag{8}$$

Let us first consider the case of spatial translations. Then the unitary operators are given by $\hat{U}(\boldsymbol{a}) = e^{-(i/\hbar)\boldsymbol{a}\cdot\hat{\boldsymbol{p}}}$ with $\boldsymbol{a} \in \mathbf{R}^3$ and exploiting

$$[\hat{U}(\boldsymbol{a}),\hat{H}_0] = 0,\ [\hat{U}(\boldsymbol{a}),S(\boldsymbol{q},\hat{\boldsymbol{p}})] = 0,$$

together with the Weyl CCR,

$$\hat{U}(\boldsymbol{q})\hat{U}(\boldsymbol{a}) = \hat{U}(\boldsymbol{a})\hat{U}(\boldsymbol{q})e^{(i/\hbar)\boldsymbol{a}\cdot\boldsymbol{q}},$$

one immediately has that the mapping $\mathcal{M}$ given by (1) is translation-covariant. This property goes back to homogeneity of the fluid and translational invariance of the interaction, as can be seen in the derivation of the master equation.[7,8] We then consider invariance under rotations, so that the relevant set of unitary operators takes the form $\hat{U}(R)$, with $R \in \mathbf{SO}(3)$. In this case exploiting $[\hat{U}(R),\hat{H}_0] = 0$ and the relations

$$\hat{U}^\dagger(R)\hat{U}(\boldsymbol{q})\hat{U}(R) = \hat{U}(R^{-1}\boldsymbol{q}),\ \hat{U}^\dagger(R)\hat{\boldsymbol{p}}\hat{U}(R) = R\hat{\boldsymbol{p}},$$

one has that $\mathcal{M}$ is rotation-covariant provided the dynamic structure factor satisfies for $R \in \mathbf{SO}(3)$

$$S(R\boldsymbol{q},R\boldsymbol{p}) = S(\boldsymbol{q},\boldsymbol{p}). \tag{9}$$

In fact, if (9) holds, one has

$$\begin{aligned}\mathcal{M}[\mathcal{U}_R[\,\cdot\,]] &= \int_{\mathbf{R}^3} d\mu(\boldsymbol{q})\ \hat{U}(R)\left[\hat{U}(R^{-1}\boldsymbol{q})\sqrt{S(\boldsymbol{q},R\hat{\boldsymbol{p}})}\cdot\sqrt{S(\boldsymbol{q},R\hat{\boldsymbol{p}})}\hat{U}^\dagger(R^{-1}\boldsymbol{q}) - \frac{1}{2}\{S(\boldsymbol{q},R\hat{\boldsymbol{p}}),\cdot\}\right]\hat{U}^\dagger(R)\\ &= \int_{\mathbf{R}^3} d\mu(\boldsymbol{q})\ \hat{U}(R)\left[\hat{U}(\boldsymbol{q})\sqrt{S(\boldsymbol{q},\hat{\boldsymbol{p}})}\cdot\sqrt{S(\boldsymbol{q},\hat{\boldsymbol{p}})}\hat{U}^\dagger(\boldsymbol{q}) - \frac{1}{2}\{S(\boldsymbol{q},\hat{\boldsymbol{p}}),\cdot\}\right]\hat{U}^\dagger(R)\\ &= \mathcal{U}_R[\mathcal{M}[\,\cdot\,]].\end{aligned}$$

On the other hand, (9) is directly linked to rotational invariance of the surrounding environment, as one can see observing that $E(\boldsymbol{q},\boldsymbol{p})$ as given by (6) satisfies

$$E(R\boldsymbol{q},R\boldsymbol{p}) = E(\boldsymbol{q},\boldsymbol{p}),$$

and considering the identity

$$\begin{aligned}S(R\boldsymbol{q},R\boldsymbol{p}) &= \frac{1}{2\pi\hbar}\int_{\mathbf{R}} dt \int_{\mathbf{R}^3} d^3\boldsymbol{x}\, e^{(i/\hbar)[E(R\boldsymbol{q},R\boldsymbol{p})t - R\boldsymbol{q}\cdot\boldsymbol{x}]}G(\boldsymbol{x},t)\\ &= \frac{1}{2\pi\hbar}\int_{\mathbf{R}} dt \int_{\mathbf{R}^3} d^3\boldsymbol{x} e^{(i/\hbar)[E(\boldsymbol{q},\boldsymbol{p})t - \boldsymbol{q}\cdot\boldsymbol{x}]}G(R\boldsymbol{x},t)\end{aligned}$$

so that (9) holds if and only if the pair correlation function is invariant under rotations,

$$G(R\boldsymbol{x},t)=G(\boldsymbol{x},t).$$

In order to proceed further and consider the existence of stationary solutions we make the natural assumption that the state of the macroscopic system, with respect to which the expectation value in (5) is calculated, is a β-KMS state, so that the relation

$$\langle \hat{A}(w)\hat{B}\rangle=\langle \hat{B}\hat{A}(w+i\hbar\beta)\rangle \tag{10}$$

holds. This in turn implies that the dynamic structure factor $S(\boldsymbol{q},\boldsymbol{p})$ satisfies an identity known as *detailed balance condition*,[12]

$$S(\boldsymbol{q},\boldsymbol{p})=e^{-\beta(q^2/2M+\boldsymbol{p}\cdot\boldsymbol{q}/M)}S(-\boldsymbol{q},\boldsymbol{p}+\boldsymbol{q}), \tag{11}$$

usually expressed in terms of the dependence on the transferred energy

$$S(\boldsymbol{q},E(\boldsymbol{q},\boldsymbol{p}))=e^{-\beta E(\boldsymbol{q},\boldsymbol{p})}S(-\boldsymbol{q},-E(\boldsymbol{q},\boldsymbol{p})), \tag{12}$$

the sign of the exponential being determined by the fact that we are considering momentum and energy transferred to the particle. It will prove useful for further considerations to introduce a symmetrized version of the dynamic structure factor, given by

$$\tilde{S}(\boldsymbol{q},E)=e^{(\beta/2)E}S(\boldsymbol{q},E) \tag{13}$$

or equivalently

$$\tilde{S}(\boldsymbol{q},\boldsymbol{p})=e^{(\beta/2)(q^2/2M+\boldsymbol{p}\cdot\boldsymbol{q}/M)}S(\boldsymbol{q},\boldsymbol{p}), \tag{14}$$

satisfying instead of (12) the more symmetric

$$\tilde{S}(\boldsymbol{q},E)=\tilde{S}(-\boldsymbol{q},-E),$$

so that (11) becomes

$$\tilde{S}(\boldsymbol{q},\boldsymbol{p})=\tilde{S}(-\boldsymbol{q},\boldsymbol{p}+\boldsymbol{q}). \tag{15}$$

We now look for a stationary solution of (1), given that the environment is in a β-KMS state, so that due to (10) the dynamic structure factor satisfies the detailed balance condition as in (11). According to translation covariance of the generators we look for a solution invariant under translation, of the form $\rho(\hat{\boldsymbol{p}})$. Since $[\hat{H}_0,\rho(\hat{\boldsymbol{p}})]=0$, $\rho(\hat{\boldsymbol{p}})$ will be a stationary solution of (1) provided

$$\begin{aligned}\mathcal{L}[\rho(\hat{\boldsymbol{p}})]&=\int_{\mathbf{R}^3}d\mu(\boldsymbol{q})\,[\hat{U}(\boldsymbol{q})S(\boldsymbol{q},\hat{\boldsymbol{p}})\rho(\hat{\boldsymbol{p}})\hat{U}^{\dagger}(\boldsymbol{q})-S(\boldsymbol{q},\hat{\boldsymbol{p}})\rho(\hat{\boldsymbol{p}})]\\&=\int_{\mathbf{R}^3}d\mu(\boldsymbol{q})\,[S(\boldsymbol{q},\hat{\boldsymbol{p}}-\boldsymbol{q})\rho(\hat{\boldsymbol{p}}-\boldsymbol{q})-S(\boldsymbol{q},\hat{\boldsymbol{p}})\rho(\hat{\boldsymbol{p}})]=0.\end{aligned} \tag{16}$$

Introducing the function

$$A(\boldsymbol{q},\boldsymbol{p})=S(\boldsymbol{q},\boldsymbol{p}-\boldsymbol{q})\rho(\boldsymbol{p}-\boldsymbol{q})-S(\boldsymbol{q},\boldsymbol{p})\rho(\boldsymbol{p}), \tag{17}$$

the requirement (16) becomes

$$\int_{\mathbf{R}^3} d\mu(\boldsymbol{q})\, A(\boldsymbol{q},\boldsymbol{p}) = 0. \tag{18}$$

A sufficient condition for (18) to be valid is that $A(\boldsymbol{q},\boldsymbol{p})$ be an odd function in $\boldsymbol{q}$, and we shall see that this is exactly the case if $\rho(\hat{\boldsymbol{p}})$ has the canonical structure $\rho_0(\hat{\boldsymbol{p}}) = e^{-\beta \hat{\boldsymbol{p}}^2/2M}$, with M the mass of the test particle and β the inverse temperature of the macroscopic system, as it is to be expected on physical grounds. Let $\rho_0(\hat{\boldsymbol{p}}) = e^{-\beta \hat{\boldsymbol{p}}^2/2M}$. Then

$$\rho_0(\boldsymbol{p}-\boldsymbol{q}) = \rho_0(\boldsymbol{p}) e^{-\beta(q^2/2M - \boldsymbol{p}\cdot\boldsymbol{q}/M)},$$

so that

$$A(\boldsymbol{q},\boldsymbol{p}) = \rho_0(\boldsymbol{p})[S(\boldsymbol{q},\boldsymbol{p}-\boldsymbol{q}) e^{-\beta(q^2/2M - \boldsymbol{p}\cdot\boldsymbol{q}/M)} - S(\boldsymbol{q},\boldsymbol{p})]$$

and exploiting (11)

$$A(\boldsymbol{q},\boldsymbol{p}) = \rho_0(\boldsymbol{p})[S(-\boldsymbol{q},\boldsymbol{p}) - S(\boldsymbol{q},\boldsymbol{p})],$$

which is manifestly odd in $\boldsymbol{q}$.

As mentioned earlier the structure given in (2) is a particular realization of the general expression considered in Ref. 11; however, it does not meet the more stringent requirements exhibited by the dissipative mapping considered in Ref. 16. According to Ref. 11 these requirements are unnecessary if one is looking for the most general translation-covariant generator and we shall show that in the present framework they would lead to unphysical results. In fact the structure proposed in Ref. 16 for the dissipative part would take in the Schrödinger picture the form

$$\mathcal{L}[\,\cdot\,] = \int_{\mathbf{R}^3} d\mu(\boldsymbol{q}) \left[P(\boldsymbol{q},\hat{\boldsymbol{p}}) \cdot P^{\dagger}(\boldsymbol{q},\hat{\boldsymbol{p}}) - \frac{1}{2}\{P^{\dagger}(\boldsymbol{q},\hat{\boldsymbol{p}}) P(\boldsymbol{q},\hat{\boldsymbol{p}}), \cdot\} \right], \tag{19}$$

with the further requirement

$$P^{\dagger}(\boldsymbol{q},\hat{\boldsymbol{p}}) = P(-\boldsymbol{q},\hat{\boldsymbol{p}}), \tag{20}$$

which in our case, since

$$P(\boldsymbol{q},\hat{\boldsymbol{p}}) = \hat{U}(\boldsymbol{q}) \sqrt{S(\boldsymbol{q},\hat{\boldsymbol{p}})} \tag{21}$$

is not satisfied, being equivalent to the requirement

$$\hat{U}(\boldsymbol{q}) \sqrt{S(\boldsymbol{q},\hat{\boldsymbol{p}})} = \hat{U}(\boldsymbol{q}) \sqrt{S(-\boldsymbol{q},\hat{\boldsymbol{p}}+\boldsymbol{q})},$$

which does not hold due to the presence of the factor $e^{-\beta(q^2/2M + \boldsymbol{p}\cdot\boldsymbol{q}/M)}$ in (11). If instead of the dynamic structure factor $S(\boldsymbol{q},\boldsymbol{p})$ one would consider the symmetrized dynamic structure factor $\tilde{S}(\boldsymbol{q},\boldsymbol{p})$ given by (14), so that $P(\boldsymbol{q},\boldsymbol{p})$ in (21) would be replaced by

$$\tilde{P}(\boldsymbol{q},\hat{\boldsymbol{p}}) = \hat{U}(\boldsymbol{q}) \sqrt{\tilde{S}(\boldsymbol{q},\hat{\boldsymbol{p}})},$$

then according to (15) the relation (20) would hold and the dissipative mapping $\mathcal{L}$ would conform to the structure proposed in Ref. 16. In this case, however, one would have the unphysical result that $\rho_0(\hat{\boldsymbol{p}}) = e^{-\beta \hat{\boldsymbol{p}}^2/2M}$ is no longer a stationary solution, because

$$\tilde{A}(\boldsymbol{q},\boldsymbol{p}) = \tilde{S}(\boldsymbol{q},\boldsymbol{p}-\boldsymbol{q})\rho_0(\boldsymbol{p}-\boldsymbol{q}) - \tilde{S}(\boldsymbol{q},\boldsymbol{p})\rho_0(\boldsymbol{p})$$

is no longer odd in $\boldsymbol{q}$. Other unphysical features linked to the further restriction (20) will be considered in Sec. IV. Note that these features can only be discovered with reference to a specific structure of a translation-covariant generator determined by starting from some microphysical model. In fact the restriction (20), though unnecessary from a mathematical standpoint, could have proven interesting as well from a physical point of view, thus suggesting the result of Ref. 16 as a useful starting point for phenomenological approaches. This does not seem to be the case, in fact the substitution $S(\boldsymbol{q},\boldsymbol{p})\to\widetilde{S}(\boldsymbol{q},\boldsymbol{p})$, natural in order to comply with Ref. 16, leads to unphysical results.

III. EXACT EXPRESSION FOR A FREE QUANTUM GAS

It is of course of interest to analyze the mapping $\mathcal{M}$ given in (1) for a model in which the dynamic structure factor of the fluid can be explicitly calculated: this is the case for an ideal quantum gas considered at finite temperature $T=1/\beta k$, where k is Boltzmann's constant, and obeying either Bose or Fermi statistics. Apart from simplicity, the case of a free gas can be of interest also in view of the recent experimental realization of dilute quantum samples of Bose or Fermi particles in the degenerate regime.[10] The dynamic structure factor for an ideal gas takes the form[12]

$$S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})=\frac{1}{n}\int_{\mathbf{R}^3}\frac{d^3\boldsymbol{k}}{(2\pi\hbar)^3}\,\langle n_k\rangle_{\mathrm{B/F}}(1\pm\langle n_{k-q}\rangle_{\mathrm{B/F}})\,\delta\left(\frac{(\boldsymbol{p}+\boldsymbol{q})^2}{2M}+\frac{(\boldsymbol{k}-\boldsymbol{q})^2}{2m}-\frac{\boldsymbol{p}^2}{2M}-\frac{\boldsymbol{k}^2}{2m}\right), \quad (22)$$

where the indexes B or F and signs $+$ or $-$ refer to Bose or Fermi statistics, respectively, M is the mass of the test particle, m is the mass of the particles making up the gas, n is the density of particles in the gas, and $\langle n_k\rangle_{\mathrm{B/F}}$ is

$$\langle n_k\rangle_{\mathrm{B/F}}=\frac{1}{z^{-1}e^{\beta\epsilon_k}\mp 1},\qquad \epsilon_k=\frac{\boldsymbol{k}^2}{2m},$$

where z is the fugacity of the gas, related to the chemical potential μ by $z=e^{\beta\mu}$. For a Bose gas at finite temperature $0\leqslant z<1$, while for a Fermi gas $z\geqslant 0$. The integral in (22) can be explicitly calculated both for bosons and fermions, giving the result (A6) obtained in Appendix A:

$$S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})=\mp\frac{1}{(2\pi\hbar)^3}\,\frac{2\pi m^2}{n\beta q}\,\frac{1}{1-e^{\beta E(\boldsymbol{q},\boldsymbol{p})}}\log\left[\frac{1\mp z\exp[-(\beta/8m)(2mE(\boldsymbol{q},\boldsymbol{p})+q^2)^2/q^2]}{1\mp z\exp[-(\beta/8m)(2mE(\boldsymbol{q},\boldsymbol{p})-q^2)^2/q^2]}\right], \quad (23)$$

with $q=|\boldsymbol{q}|$. In the same way one can consider the case of a free gas of particles satisfying Maxwell–Boltzmann statistics, thus having

$$S_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p})=\frac{1}{n}\int_{\mathbf{R}^3}\frac{d^3\boldsymbol{k}}{(2\pi\hbar)^3}\,\langle n_k\rangle_{\mathrm{MB}}\,\delta\left(\frac{(\boldsymbol{p}+\boldsymbol{q})^2}{2M}+\frac{(\boldsymbol{k}-\boldsymbol{q})^2}{2m}-\frac{\boldsymbol{p}^2}{2M}-\frac{\boldsymbol{k}^2}{2m}\right), \quad (24)$$

with

$$\langle n_k\rangle_{\mathrm{MB}}=ze^{-\beta\epsilon_k},$$

so that the integral in (24) can also be explicitly calculated giving the expression (A8):

$$S_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p})=\frac{1}{(2\pi\hbar)^3}\,\frac{2\pi m^2}{n\beta q}\,z\exp\left[-\frac{\beta}{8m}\,\frac{(2mE(\boldsymbol{q},\boldsymbol{p})+q^2)^2}{q^2}\right]. \quad (25)$$

A convenient way to write (23) and (25) for later expansions is in terms of the function

$$\sigma(\boldsymbol{q},\boldsymbol{p})=\frac{1}{2q}[q^2+2\alpha ME(\boldsymbol{q},\boldsymbol{p})], \tag{26}$$

where the ratio $\alpha=m/M$ between the masses of the particles of the gas and of the test particle has been put into evidence, thus obtaining, respectively,

$$S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})=\mp\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}\frac{1}{1-\exp[(\beta/2m)(2\sigma(\boldsymbol{q},\boldsymbol{p})q-q^2)]}\times\log\left[\frac{1\mp z\exp[-(\beta/2m)\sigma^2(\boldsymbol{q},\boldsymbol{p})]}{1\mp z\exp[-(\beta/2m)(\sigma(\boldsymbol{q},\boldsymbol{p})-q)^2]}\right] \tag{27}$$

and

$$S_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p})=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}z\exp\left[-\frac{\beta}{2m}\sigma^2(\boldsymbol{q},\boldsymbol{p})\right]. \tag{28}$$

We have thus put into evidence all the physical parameters which are of interest in specifying the physical model under consideration and its range of validity: $\boldsymbol{q}$, E, α, and z. In this perspective the expression for a gas of Maxwell–Boltzmann particles can also be obtained as expected from the dynamic structure factor for a Bose or Fermi gas in the limit of small fugacity z. In fact, starting from (27) and expanding the logarithm up to first order in z one has

$$\begin{aligned}S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p},z\ll 1)&=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}\frac{z}{1-\exp[(\beta/2m)(2\sigma(\boldsymbol{q},\boldsymbol{p})q-q^2)]}\\&\quad\times\left\{\exp\left[-\frac{\beta}{2m}\sigma^2(\boldsymbol{q},\boldsymbol{p})\right]-\exp\left[-\frac{\beta}{2m}(\sigma(\boldsymbol{q},\boldsymbol{p})-q)^2\right]\right\}\\&=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}z\exp\left[-\frac{\beta}{2m}\sigma^2(\boldsymbol{q},\boldsymbol{p})\right]=S_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p}).\end{aligned}$$

Both (23) and (25) or equivalently (27) and (28) are invariant under rotation, as one can see from the fact that they depend on $\boldsymbol{q}$ and $\boldsymbol{p}$ only through $E(\boldsymbol{q},\boldsymbol{p})$ and the modulus q of $\boldsymbol{q}$, so that

$$S_{\mathrm{B/F}}(R\boldsymbol{q},R\boldsymbol{p})=S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p}),\quad S_{\mathrm{MB}}(R\boldsymbol{q},R\boldsymbol{p})=S_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p}),$$

thus leading to a rotation-covariant mapping $\mathcal{M}$ when substituted in (1). In order to grant the existence of the stationary solution $\rho_0(\hat{\boldsymbol{p}})$ we have to check that the obtained expressions satisfy the principle of detailed balance. Starting from (23) we have, setting for simplicity $E(\boldsymbol{q},\boldsymbol{p})=E$ and inverting the argument of the logarithm,

$$\begin{aligned}e^{-\beta E}S_{\mathrm{B/F}}(-\boldsymbol{q},-E)&=\mp\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}\frac{e^{-\beta E}}{1-e^{-\beta E}}\log\left[\frac{1\mp z\exp[-(\beta/8m)(-2mE+q^2)^2/q^2]}{1\mp z\exp[-(\beta/8m)(-2mE-q^2)^2/q^2]}\right]\\&=\mp\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}\frac{1}{1-e^{\beta E}}\log\left[\frac{1\mp z\exp[-\beta/8m)(2mE+q^2)^2/q^2]}{1\mp z\exp[-(\beta/8m)(2mE-q^2)^2/q^2]}\right]\\&=S_{\mathrm{B/F}}(\boldsymbol{q},E),\end{aligned}$$

which proves (12). Similarly

$$e^{-\beta E}S_{\mathrm{MB}}(-\boldsymbol{q},-E)=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}z\exp[-\beta E]\exp\left[-\frac{\beta}{8m}\frac{(-2mE+q^2)^2}{q^2}\right]$$
$$=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}z\exp\left[-\frac{\beta}{8m}\frac{(2mE+q^2)^2}{q^2}\right]=S_{\mathrm{MB}}(\boldsymbol{q},E).$$

The master equation (1) for the Rayleigh gas in the case of a free gas of Bose or Fermi particles takes therefore the form

$$\frac{d\hat{\varrho}}{dt}=\mathcal{M}_{\mathrm{B/F}}[\hat{\varrho}]=-\frac{i}{\hbar}[\hat{H}_0,\hat{\varrho}]+\int_{\mathbf{R}^3}d\mu(\boldsymbol{q})$$
$$\times\left[\hat{U}(\boldsymbol{q})\sqrt{S_{\mathrm{B/F}}(\boldsymbol{q},\hat{\boldsymbol{p}})}\,\hat{\varrho}\,\sqrt{S_{\mathrm{B/F}}(\boldsymbol{q},\hat{\boldsymbol{p}})}\hat{U}^{\dagger}(\boldsymbol{q})-\frac{1}{2}\{S_{\mathrm{B/F}}(\boldsymbol{q},\hat{\boldsymbol{p}}),\hat{\varrho}\}\right],\qquad(29)$$

with $S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})$ given explicitly by (23), and a similar expression $\mathcal{M}_{\mathrm{MB}}$ can be considered for a free gas of Maxwell–Boltzmann particles. Both $\mathcal{M}_{\mathrm{B/F}}$ and $\mathcal{M}_{\mathrm{MB}}$ are translation- and rotation-covariant and admit the same stationary solution with the canonical structure $\rho_0(\hat{\boldsymbol{p}})$.

IV. BROWNIAN LIMIT

In the framework of an ideal gas considered in Sec. III, i.e., referring to $\mathcal{M}_{\mathrm{B/F}}$ and $\mathcal{M}_{\mathrm{MB}}$, we now want to consider the physically distinguished case in which the test particle is much heavier than the particles making up the gas, so that $\alpha=m/M$ is much smaller than one, the so-called Brownian limit. In order to do this we have to evaluate the dynamic structure factor for a free gas in the case $\alpha\ll 1$. The natural starting points are expressions (27) and (28) in which the factor α has been put into evidence through the function (26). In particular we have the relations

$$\frac{\beta}{2m}\sigma^2(\boldsymbol{q},\boldsymbol{p})=\frac{\beta}{8m}q^2+\frac{\beta}{2}\frac{1}{2M}[q^2+2\boldsymbol{p}\cdot\boldsymbol{q}]+\frac{\beta}{2}\frac{1}{q^2}\alpha\frac{1}{4M}[q^2+2\boldsymbol{p}\cdot\boldsymbol{q}]^2$$
$$=\frac{\beta}{8m}q^2+\frac{\beta}{2}E(\boldsymbol{q},\boldsymbol{p})+\frac{\beta}{2}\frac{m}{q^2}E^2(\boldsymbol{q},\boldsymbol{p}),$$

$$\frac{\beta}{2m}(\sigma(\boldsymbol{q},\boldsymbol{p})-q)^2=\frac{\beta}{8m}q^2-\frac{\beta}{2}\frac{1}{2M}[q^2+2\boldsymbol{p}\cdot\boldsymbol{q}]+\frac{\beta}{2}\frac{1}{q^2}\alpha\frac{1}{4M}[q^2+2\boldsymbol{p}\cdot\boldsymbol{q}]^2$$
$$=\frac{\beta}{8m}q^2-\frac{\beta}{2}E(\boldsymbol{q},\boldsymbol{p})+\frac{\beta}{2}\frac{m}{q^2}E^2(\boldsymbol{q},\boldsymbol{p}),\qquad(30)$$

$$\frac{\beta}{2m}(2\sigma(\boldsymbol{q},\boldsymbol{p})q-q^2)=\frac{\beta}{2M}[q^2+2\boldsymbol{p}\cdot\boldsymbol{q}]=\beta E(\boldsymbol{q},\boldsymbol{p}).$$

The Brownian limit can now be taken neglecting the terms of order α in (30) or equivalently considering small energy transfer, corresponding to a broader time scale, and keeping in (30) only the terms linear in E, disregarding higher powers of the energy transfer. The resulting dynamic structure factors, denoted by an index ∞, are given by

$$S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})=\mp\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}\frac{1}{1-e^{\beta[q^2/2M+\boldsymbol{q}\cdot\boldsymbol{p}/M]}}\log\left[\frac{1\mp ze^{-(\beta/8m)q^2}e^{-(\beta/2)[q^2/2M+\boldsymbol{q}\cdot\boldsymbol{p}/M]}}{1\mp ze^{-(\beta/8m)q^2}e^{+(\beta/2)[q^2/2M+\boldsymbol{q}\cdot\boldsymbol{p}/M]}}\right]\qquad(31)$$

and

$$S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p})=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}ze^{-(\beta/8m)q^2}e^{-(\beta/2)[q^2/2M+\boldsymbol{q}\cdot\boldsymbol{p}/M]}, \tag{32}$$

respectively. Considering the corresponding expressions in terms of $E(\boldsymbol{q},\boldsymbol{p})$,

$$S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},E(\boldsymbol{q},\boldsymbol{p}))=\mp\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}\frac{1}{1-e^{\beta E(\boldsymbol{q},\boldsymbol{p})}}\log\left[\frac{1\mp ze^{-(\beta/8m)q^2}e^{-(\beta/2)\,E(\boldsymbol{q},\boldsymbol{p})}}{1\mp ze^{-(\beta/8m)q^2}e^{+(\beta/2)\,E(\boldsymbol{q},\boldsymbol{p})}}\right] \tag{33}$$

and

$$S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E(\boldsymbol{q},\boldsymbol{p}))=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}ze^{-(\beta/8m)q^2}e^{-(\beta/2)\,E(\boldsymbol{q},\boldsymbol{p})}, \tag{34}$$

one immediately sees that rotational invariance is preserved in this approximation. One can check that also the detailed balance condition is not spoiled. In fact from (33) one has

$$\begin{aligned}e^{-\beta E}S^{\infty}_{\mathrm{B/F}}(-\boldsymbol{q},-E)&=\mp\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}\frac{e^{-\beta E}}{1-e^{-\beta E}}\log\left[\frac{1\mp ze^{-(\beta/8m)q^2}e^{+(\beta/2)\,E}}{1\mp ze^{-(\beta/8m)q^2}e^{-(\beta/2)\,E}}\right]\\&=\mp\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}\frac{1}{1-e^{\beta E}}\log\left[\frac{1\mp ze^{-(\beta/8m)q^2}e^{-(\beta/2)\,E}}{1\mp ze^{-(\beta/8m)q^2}e^{+(\beta/2)\,E}}\right]\\&=S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},E),\end{aligned}$$

and from (34)

$$e^{-\beta E}S^{\infty}_{\mathrm{MB}}(-\boldsymbol{q},-E)=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}ze^{-(\beta/8m)q^2}e^{-\beta E(\boldsymbol{q},\boldsymbol{p})}e^{(\beta/2)\,E(\boldsymbol{q},\boldsymbol{p})}=S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E).$$

As a result, in place of (29) we now consider the mapping $\mathcal{M}^{\infty}_{\mathrm{B/F}}$:

$$\begin{aligned}\frac{d\hat{\varrho}}{dt}=\mathcal{M}^{\infty}_{\mathrm{B/F}}[\hat{\varrho}]&=-\frac{i}{\hbar}[\hat{H}_0,\hat{\varrho}]+\int_{\mathbf{R}^3}d\mu(\boldsymbol{q})\\&\times\left[\hat{U}(\boldsymbol{q})\sqrt{S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},\hat{\boldsymbol{p}})}\,\hat{\varrho}\,\sqrt{S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},\hat{\boldsymbol{p}})}\hat{U}^{\dagger}(\boldsymbol{q})-\frac{1}{2}\{S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},\hat{\boldsymbol{p}}),\hat{\varrho}\}\right],\end{aligned} \tag{35}$$

and similarly $\mathcal{M}^{\infty}_{\mathrm{MB}}$ for Maxwell–Boltzmann statistics. $\mathcal{M}^{\infty}_{\mathrm{B/F}}$ and $\mathcal{M}^{\infty}_{\mathrm{MB}}$ are still translation- and rotation-covariant and admit the same stationary solution with the canonical structure $\rho_0(\hat{\boldsymbol{p}})$.

In the master equation (1), or according to the physical system under consideration (29) or (35), the quantum scattering rate or transition probability appears through the dynamic structure factor and the square modulus of the Fourier transform of the T matrix determining the integration measure (3), these quantities being connected to the differential scattering cross-section by (7). In order to pass from the master equation to the related Fokker–Planck equation through a Kramers–Moyal expansion, as stressed by van Kampen[17] we need to put into evidence a small parameter governing the size of the fluctuations in the macroscopic system. In our case this parameter is naturally given by the momentum transfer $\boldsymbol{q}$, which through the dynamic structure factor is directly linked to the equilibrium fluctuations of the macroscopic system. Small $\boldsymbol{q}$ means long-wavelength fluctuations, corresponding to the macroscopic, long range properties of the environment. It is physically meaningful to consider both approximations $|\boldsymbol{q}|\ll 1$ and $\alpha\ll 1$, or equivalently small energy transfer, together, so that starting from the Maxwell–Boltzmann case,

$$\mathcal{M}^{\infty}_{\mathrm{MB}}[\cdot]=-\frac{i}{\hbar}[\hat{H}_0,\cdot]+z\frac{4\pi^2m^2}{\beta\hbar}\int_{\mathbf{R}^3}d^3\boldsymbol{q}\frac{|\tilde{t}(q)|^2}{q}e^{-(\beta/8m)(1+2\alpha)q^2}$$
$$\times\left[e^{(i/\hbar)\boldsymbol{q}\cdot\hat{\boldsymbol{x}}}e^{-(\beta/4M)\boldsymbol{q}\cdot\hat{\boldsymbol{p}}}.e^{-(\beta/4M)\boldsymbol{q}\cdot\hat{\boldsymbol{p}}}e^{-(i/\hbar)\boldsymbol{q}\cdot\hat{\boldsymbol{x}}}-\frac{1}{2}\{e^{-(\beta/2M)\boldsymbol{q}\cdot\hat{\boldsymbol{p}}},\cdot\}\right]$$

we expand the dissipative part of the mapping in the small parameter $\boldsymbol{q}$. We will expand the operators depending on $\boldsymbol{q}$ up to second order, so as to have contributions at most bilinear in the operators $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{p}}$, position and momentum of the Brownian particle. We thus obtain a structure analogous to the classical Fokker–Planck equation, with a friction term linearly proportional to velocity: this class of models is known as quantum Brownian motion.[18–20] Recalling that $\alpha\ll 1$ and exploiting the symmetry properties of the integration measure the result for the dissipative part is[7]

$$-z\frac{2\pi^2m^2}{\beta\hbar}\int_{\mathbf{R}^3}d^3\boldsymbol{q}\frac{|\tilde{t}(q)|^2}{q}e^{-(\beta/8m)\,q^2}\sum_{i=1}^{3}\boldsymbol{q}_i^2$$
$$\times\left\{\frac{1}{\hbar^2}[\hat{\boldsymbol{x}}_i,[\hat{\boldsymbol{x}}_i,\cdot]]+\frac{\beta^2}{16M^2}[\hat{\boldsymbol{p}}_i,[\hat{\boldsymbol{p}}_i,\cdot]]+\frac{i}{\hbar}\frac{\beta}{2M}[\hat{\boldsymbol{x}}_i,\{\hat{\boldsymbol{p}}_i,\cdot\}]\right\},$$

where $i=1,2,3$ denotes Cartesian coordinates. Due to the isotropy of the environment we have $\boldsymbol{q}_i^2=\frac{1}{3}q^2$, so that we can define the coefficients

$$D_{pp}=\frac{2}{3}\frac{\pi^2m^2}{\beta\hbar}\int_{\mathbf{R}^3}d^3\boldsymbol{q}\,|\tilde{t}(q)|^2qe^{-(\beta/8m)\,q^2},$$

$$D_{xx}=\left(\frac{\beta\hbar}{4M}\right)^2D_{pp}, \tag{36}$$

$$\gamma=\left(\frac{\beta}{2M}\right)D_{pp},$$

and introduce the following mapping describing quantum dissipation:

$$\mathcal{L}_{\mathrm{QD}}[\cdot]=-\frac{D_{pp}}{\hbar^2}\sum_{i=1}^{3}[\hat{\boldsymbol{x}}_i,[\hat{\boldsymbol{x}}_i,\cdot]]-\frac{D_{xx}}{\hbar^2}\sum_{i=1}^{3}[\hat{\boldsymbol{p}}_i,[\hat{\boldsymbol{p}}_i,\cdot]]-\frac{i}{\hbar}\gamma\sum_{i=1}^{3}[\hat{\boldsymbol{x}}_i,\{\hat{\boldsymbol{p}}_i,\cdot\}], \tag{37}$$

thus coming to the Fokker–Planck equation

$$\frac{d\hat{\varrho}}{dt}=-\frac{i}{\hbar}[\hat{H}_0,\hat{\varrho}]+\mathcal{L}_{\mathrm{MB}}[\hat{\varrho}]=-\frac{i}{\hbar}[\hat{H}_0,\hat{\varrho}]+z\mathcal{L}_{\mathrm{QD}}[\hat{\varrho}]. \tag{38}$$

In view of the result (38) for the Fokker–Planck equation describing the motion of the Brownian particle in a gas obeying Maxwell–Boltzmann statistics, we now look for the corrections to (38) brought about by quantum statistics at finite temperature. As usual we will deal with both Bose and Fermi statistics, exploiting expression (B6) obtained in Appendix B by deriving an exact expansion for $S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},E)$:

$$S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},E)=S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E)\Bigg[\sum_{k=0}^{\infty}(\pm z)^k-\frac{\beta}{8m}q^2\sum_{k=1}^{\infty}(\pm)^k k z^k + \frac{1}{12}(\beta E)^2\sum_{k=1}^{\infty}(\pm)^k k z^k+\frac{1}{24}(\beta E)^2\sum_{k=1}^{\infty}(\pm)^k k^2 z^k+O(q^4)\Bigg], \tag{39}$$

where a suitable expansion in the small parameter $\boldsymbol{q}$ has already been performed. Let us first introduce the Bose–Einstein and the Fermi–Dirac functions,[21,22] given by

$$g_{\nu}(z)=\frac{1}{\Gamma(\nu)}\int_0^{+\infty}dx\,\frac{x^{\nu-1}}{z^{-1}e^x-1},\quad 0\leqslant z<1,\ \nu>0, \tag{40}$$

and

$$f_{\nu}(z)=\frac{1}{\Gamma(\nu)}\int_0^{+\infty}dx\,\frac{x^{\nu-1}}{z^{-1}e^x+1},\quad 0\leqslant z<\infty,\ \nu>0, \tag{41}$$

respectively, related for integer ν by $f_n(z)=-g_n(-z)$. These functions, typically appearing in the quantum statistical mechanics of Bose and Fermi systems, satisfy the recurrence relations

$$g_{\nu-1}(z)=z\frac{\partial}{\partial z}[g_{\nu}(z)],\quad f_{\nu-1}(z)=z\frac{\partial}{\partial z}[f_{\nu}(z)], \tag{42}$$

so that they can be defined also for $\nu\leqslant 0$. Starting from (42) and exploiting the following representations for $|z|<1$,

$$g_{\nu}(z)=\sum_{k=1}^{\infty}\frac{z^k}{k^{\nu}},\quad f_{\nu}(z)=\sum_{k=1}^{\infty}(-)^{k-1}\frac{z^k}{k^{\nu}},$$

one can write (39) in the Bose case as

$$S^{\infty}_{\mathrm{B}}(\boldsymbol{q},E)=S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E)\left[\frac{g_0(z)}{z}-\frac{\beta}{8m}q^2 g_{-1}(z)+\frac{1}{24}(\beta E)^2(g_{-2}(z)+2g_{-1}(z))+O(q^4)\right] \tag{43}$$

and in the Fermi case as

$$S^{\infty}_{\mathrm{F}}(\boldsymbol{q},E)=S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E)\left[\frac{f_0(z)}{z}+\frac{\beta}{8m}q^2 f_{-1}(z)-\frac{1}{24}(\beta E)^2(f_{-2}(z)+2f_{-1}(z))+O(q^4)\right], \tag{44}$$

where the functions appearing in (43) can be written for $0\leqslant z<1$ in closed form as

$$g_0(z)=\frac{z}{1-z},\qquad g_{-1}(z)=\frac{z}{(1-z)^2},\quad g_{-2}(z)=\frac{z+z^2}{(1-z)^3}, \tag{45}$$

while the functions appearing in (44) can be written for $0\leqslant z<\infty$ in closed form as

$$f_0(z)=\frac{z}{1+z}, \tag{46}$$

$$f_{-1}(z)=\frac{z}{(1+z)^2},\quad f_{-2}(z)=\frac{z-z^2}{(1+z)^3}.$$

To evaluate the corrections due to quantum statistics we note that when $S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E(\boldsymbol{q},\boldsymbol{p}))$ is substituted by an expression of the form

$$S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E(\boldsymbol{q},\boldsymbol{p}))A[1+2Bq^2+2C(\boldsymbol{p}\cdot\boldsymbol{q})^2],$$

so that keeping terms at most quadratic in $\boldsymbol{q}$ in the correction

$$\sqrt{S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E(\boldsymbol{q},\boldsymbol{p}))}\to\sqrt{S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E(\boldsymbol{q},\boldsymbol{p}))}\sqrt{A}[1+Bq^2+C(\boldsymbol{p}\cdot\boldsymbol{q})^2],$$

the mapping $\mathcal{M}^{\infty}_{\mathrm{MB}}$ always in the same approximation becomes

$$\begin{aligned}
&-\frac{i}{\hbar}[\hat{H}_0,\cdot]+A\int_{\mathbf{R}^3}d\mu(\boldsymbol{q})\left[\hat{U}(\boldsymbol{q})\sqrt{S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\hat{\boldsymbol{p}})}\cdot\sqrt{S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\hat{\boldsymbol{p}})}\hat{U}^{\dagger}(\boldsymbol{q})-\frac{1}{2}\{S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\hat{\boldsymbol{p}}),\cdot\}\right]\\
&\quad+2AB\int_{\mathbf{R}^3}d\mu(\boldsymbol{q})\,q^2\left[\hat{U}(\boldsymbol{q})\sqrt{S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\hat{\boldsymbol{p}})}\cdot\sqrt{S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\hat{\boldsymbol{p}})}\hat{U}^{\dagger}(\boldsymbol{q})-\frac{1}{2}\{S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\hat{\boldsymbol{p}}),\cdot\}\right]\\
&\quad+AC\int_{\mathbf{R}^3}d\mu(\boldsymbol{q})\,[\hat{U}(\boldsymbol{q})\sqrt{S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\hat{\boldsymbol{p}})}\{(\hat{\boldsymbol{p}}\cdot\boldsymbol{q})^2,\cdot\}\sqrt{S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\hat{\boldsymbol{p}})}\hat{U}^{\dagger}(\boldsymbol{q})-\{S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\hat{\boldsymbol{p}})(\hat{\boldsymbol{p}}\cdot\boldsymbol{q})^2,\cdot\}].
\end{aligned}\tag{47}$$

Looking at (47) one immediately sees that, keeping terms at most quadratic in $\boldsymbol{q}$, the last two terms are to be neglected, since the dynamic structure factor $S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\hat{\boldsymbol{p}})$ and the unitary operators $\hat{U}(\boldsymbol{q})$ can now only bring in a constant factor. The only change in the structure of the mapping is therefore given by the numerical factor A multiplying the dissipative part. This factor is actually given by $g_0(z)/z$ in the Bose case and by $f_0(z)/z$ in the Fermi case. The Fokker–Planck equation (38) in the case of Bose statistics of the gas therefore becomes

$$\frac{d\hat{\varrho}}{dt}=-\frac{i}{\hbar}[\hat{H}_0,\hat{\varrho}]+\mathcal{L}_{\mathrm{B}}[\hat{\varrho}]=-\frac{i}{\hbar}[\hat{H}_0,\hat{\varrho}]+g_0(z)\mathcal{L}_{\mathrm{QD}}[\hat{\varrho}],\tag{48}$$

while for Fermi particles one has

$$\frac{d\hat{\varrho}}{dt}=-\frac{i}{\hbar}[\hat{H}_0,\hat{\varrho}]+\mathcal{L}_{\mathrm{F}}[\hat{\varrho}]=-\frac{i}{\hbar}[\hat{H}_0,\hat{\varrho}]+f_0(z)\mathcal{L}_{\mathrm{QD}}[\hat{\varrho}],\tag{49}$$

and the following simple relations hold:

$$\begin{aligned}
&\mathcal{L}_{\mathrm{MB}}=z\mathcal{L}_{\mathrm{QD}},\\
&\mathcal{L}_{\mathrm{B}}=g_0(z)\mathcal{L}_{\mathrm{QD}}=\frac{z}{1-z}\mathcal{L}_{\mathrm{QD}}=\frac{1}{1-z}\mathcal{L}_{\mathrm{MB}},\\
&\mathcal{L}_{\mathrm{F}}=f_0(z)\mathcal{L}_{\mathrm{QD}}=\frac{z}{1+z}\mathcal{L}_{\mathrm{QD}}=\frac{1}{1+z}\mathcal{L}_{\mathrm{MB}}.
\end{aligned}\tag{50}$$

According to (50) and setting after (36)

$$\gamma_{\mathrm{MB}}=z\gamma=z\frac{\beta}{2M}D_{pp}=z\frac{1}{3}\frac{\pi^2m^2}{M\hbar}\int d^3\boldsymbol{q}\,|\tilde{t}(q)|^2qe^{-(\beta/8m)q^2},\tag{51}$$

one has the following very simple relation between the friction coefficients in (38) and (48) or (49):

$$\gamma_{\mathrm{B/F}}=\frac{\gamma_{\mathrm{MB}}}{1\mp z}. \tag{52}$$

The relationship between the Fokker–Planck equations for Maxwell–Boltzmann or Bose and Fermi statistics, as given, respectively, by (38), (48) and (49), is actually remarkably simple: they have the very same operator structure, apart from an overall coefficient depending on the fugacity of the gas, which determines the relative weight of the dissipative contribution to the dynamics. As it is to be expected, only the statistics of the reservoir is of relevance, since the test particle is a single particle. The Fokker–Planck equations obtained for the description of quantum dissipation may be compactly written:

$$\frac{d\hat{\varrho}}{dt}=-\frac{i}{\hbar}[\hat{H}_0,\hat{\varrho}]+\zeta(z)\mathcal{L}_{\mathrm{QD}}[\hat{\varrho}], \tag{53}$$

with $\zeta(z)$ defined as follows:

$$\zeta(z)=\begin{cases} z, & \text{Maxwell–Boltzmann,}\\ z/(1-z), & \text{Bose,}\\ z/(1+z) & \text{Fermi.}\end{cases} \tag{54}$$

We now briefly come back to the question dealt with at the end of Sec. II about the physical relevance of the structure of the translation-covariant master equation obtained in Ref. 16. As already stressed, the master equation (1), while having the general translation-covariant structure considered in Ref. 11, does not comply with the further restrictions given in Ref. 16, while this would be the case if instead of the dynamic structure factor $S(\boldsymbol{q},\boldsymbol{p})$ one would consider the symmetrized correlation function $\tilde{S}(\boldsymbol{q},\boldsymbol{p})$, which is an even function of $\boldsymbol{q}$ and $E(\boldsymbol{q},\boldsymbol{p})$. This could be considered a natural phenomenological ansatz in view of the result obtained in Ref. 16. In Sec. II we showed, however, that this substitution would spoil the existence of the expected stationary solution. More than this, if we now consider the Brownian limit, the symmetrized version of $S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\hat{\boldsymbol{p}})$, which can be immediately obtained from (34), reads

$$\tilde{S}^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E(\boldsymbol{q},\boldsymbol{p}))=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}ze^{-(\beta/8m)q^2},$$

so that the dependence on $\boldsymbol{p}$ is completely lost and the whole operator structure in (37) and (38) is washed out, apart from the double commutator with the position operators $\hat{\boldsymbol{x}}_i$. In particular the friction term is missing, so that, even though a Lindblad structure is retained, only a completely different physics can be described. In the same way, for the Bose or Fermi dynamic structure factor in the Brownian limit one has from (B6)

$$\tilde{S}^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},E)=\tilde{S}^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E)\Bigg[\sum_{k=0}^{\infty}(\pm z)^k-\frac{\beta}{8m}q^2\sum_{k=1}^{\infty}(\pm)^k kz^k + \frac{1}{12}(\beta E)^2\sum_{k=1}^{\infty}(\pm)^k kz^k+\frac{1}{24}(\beta E)^2\sum_{k=1}^{\infty}(\pm)^k k^2z^k+O(q^4)\Bigg],$$

and, once again, recalling (47) written in terms of $\tilde{S}^{\infty}_{\mathrm{MB}}$ rather than S^{∞}_{MB}, one sees that under the same approximations as before the operator structure in the dissipative part of both (48) and (49) is washed out apart from the contribution due to the double commutator in the position operators of the particle $\hat{\boldsymbol{x}}_i$.

We now consider some structural features of the mapping $\mathcal{L}_{\mathrm{QD}}$ given by (37) in terms of which the Fokker–Planck equation (53) encompassing all three statistics is given. G-covariance of $\mathcal{L}_{\mathrm{QD}}$ under translations and rotations immediately follows from its very structure and the transformation laws for the operators $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{p}}$:

$$\hat{U}^{\dagger}(\boldsymbol{a})\hat{\boldsymbol{x}}\hat{U}(\boldsymbol{a})=\hat{\boldsymbol{x}}+\boldsymbol{a},\quad \hat{U}^{\dagger}(\boldsymbol{a})\hat{\boldsymbol{p}}\hat{U}(\boldsymbol{a})=\hat{\boldsymbol{p}},\quad \hat{U}^{\dagger}(R)\hat{\boldsymbol{x}}\hat{U}(R)=R\hat{\boldsymbol{x}},\quad \hat{U}^{\dagger}(R)\hat{\boldsymbol{p}}\hat{U}(R)=R\hat{\boldsymbol{p}}.$$

One can also see that an operator with the expected canonical structure is a stationary solution of (53) in that

$$\mathcal{L}_{\mathrm{QD}}[\rho_0(\hat{\boldsymbol{p}})]=0,$$

due to the relationship

$$\frac{\gamma}{D_{pp}}=\frac{\beta}{2M} \tag{55}$$

obeyed by the coefficients defined in (36) and entering in (37). A few more remarks are in order. The typical structure of translation-covariant mappings describing quantum dissipation in analogy with the classical Fokker–Planck equation that one finds in the physical literature is given by[23]

$$\mathcal{L}^{\chi}_{\mathrm{FP}}[\,\cdot\,]=-\frac{i}{\hbar}\gamma\sum_{i=1}^{3}[\hat{\boldsymbol{x}}_i,\{\hat{\boldsymbol{p}}_i,\cdot\}]-\frac{1}{\hbar^2}\frac{2M\gamma}{\beta}\sum_{i=1}^{3}[\hat{\boldsymbol{x}}_i,[\hat{\boldsymbol{x}}_i,\cdot]]-\chi\frac{\beta\gamma}{M}\sum_{i=1}^{3}[\hat{\boldsymbol{p}}_i,[\hat{\boldsymbol{p}}_i,\cdot]], \tag{56}$$

where the ratio between the first two coefficients, given by $\beta/2M$ as in (55), is fixed by the requirement that $\rho_0(\hat{\boldsymbol{p}})$ be a stationary solution, i.e., $\mathcal{L}^{\chi}_{\mathrm{FP}}[\rho_0(\hat{\boldsymbol{p}})]=0$, and the only freedom left, apart from the overall multiplying coefficient γ, is given by the adimensional factor χ. If one further asks that (56) can be cast in Lindblad form, so that $\mathcal{L}^{\chi}_{\mathrm{FP}}$ is the generator of a completely positive dynamical semigroup,[19] one has the further simple requirement[18,24]

$$\chi\geqslant\tfrac{1}{8}. \tag{57}$$

In fact under this condition, observing that for the operators

$$\hat{\boldsymbol{B}}_{i\pm}=\hat{\boldsymbol{x}}_i\pm i\kappa\hat{\boldsymbol{p}}_i$$

we have the identity

$$\hat{\boldsymbol{B}}_{i\pm}\cdot\hat{\boldsymbol{B}}^{\dagger}_{i\pm}-\tfrac{1}{2}\{\hat{\boldsymbol{B}}^{\dagger}_{i\pm}\hat{\boldsymbol{B}}_{i\pm},\cdot\}=-\tfrac{1}{2}\{[\hat{\boldsymbol{x}}_i,[\hat{\boldsymbol{x}}_i,\cdot]]+\kappa^2[\hat{\boldsymbol{p}}_i,[\hat{\boldsymbol{p}}_i,\cdot]]\pm 2i\kappa[\hat{\boldsymbol{x}}_i,\{\hat{\boldsymbol{p}}_i,\cdot\}]\mp i\kappa[\{\hat{\boldsymbol{x}}_i,\hat{\boldsymbol{p}}_i\},\cdot]\},$$

we may write $\mathcal{L}^{\chi}_{\mathrm{FP}}$ in an explicit Lindblad form in terms of the two generators

$$\hat{\boldsymbol{L}}_{i+}=\hat{\boldsymbol{x}}_i+i\frac{\hbar\beta}{M}\sqrt{\frac{\chi}{2}}\,\hat{\boldsymbol{p}}_i,\quad \hat{\boldsymbol{L}}_{i-}=\hat{\boldsymbol{x}}_i-i\frac{\hbar\beta}{M}\sqrt{\frac{\chi}{2}}\,\hat{\boldsymbol{p}}_i$$

according to

$$\mathcal{L}^{\chi}_{\mathrm{FP}}[\cdot]=+\frac{2\gamma M}{\hbar^2\beta}\left(1+\sqrt{\frac{1}{8\chi}}\right)\sum_{i=1}^{3}\left[\hat{\boldsymbol{L}}_{i+}\cdot\hat{\boldsymbol{L}}^{\dagger}_{i+}-\frac{1}{2}\{\hat{\boldsymbol{L}}^{\dagger}_{i+}\hat{\boldsymbol{L}}_{i+},\cdot\}\right]$$

$$+\frac{2\gamma M}{\hbar^2\beta}\left(1-\sqrt{\frac{1}{8\chi}}\right)\sum_{i=1}^{3}\left[\hat{\boldsymbol{L}}_{i-}\cdot\hat{\boldsymbol{L}}^{\dagger}_{i-}-\frac{1}{2}\{\hat{\boldsymbol{L}}^{\dagger}_{i-}\hat{\boldsymbol{L}}_{i-},\cdot\}\right]-\frac{i}{\hbar}\frac{\gamma}{2}\sum_{i=1}^{3}[\{\hat{\boldsymbol{x}}_i,\hat{\boldsymbol{p}}_i\},\cdot]. \tag{58}$$

The Fokker–Planck structure $\mathcal{L}_{\mathrm{QD}}$ falls within this class, with the coefficient γ given by (36) in terms of a suitable integral of the Fourier transform of the T matrix describing collisions at microphysical level. Moreover, it corresponds to the value $\chi=\frac{1}{8}$ in (57), so that

$$\mathcal{L}_{\mathrm{QD}}=\mathcal{L}^{1/8}_{\mathrm{FP}}. \tag{59}$$

This in turn implies that $\mathcal{L}_{\mathrm{QD}}$ can be written in a manifest Lindblad form in terms of a single generator for each Cartesian direction. We make the choice[7,24]

$$\hat{\boldsymbol{a}}_i=\frac{\sqrt{2}}{\lambda_M}\left(\hat{\boldsymbol{x}}_i+\frac{i}{\hbar}\frac{\lambda_M^2}{4}\hat{\boldsymbol{p}}_i\right),$$

where $\lambda_M=\sqrt{\hbar^2\beta/M}$, the thermal wavelength associated to the Brownian particle, is put into evidence, so that one has the commutation relations

$$[\hat{\boldsymbol{a}}_i,\hat{\boldsymbol{a}}^{\dagger}_j]=\delta_{ij}.$$

In such a way we have the alternative expression

$$\mathcal{L}_{\mathrm{QD}}[\cdot]=-\frac{D_{pp}}{\hbar^2}\frac{\lambda_M^2}{4}\sum_{i=1}^{3}\frac{i}{\hbar}[\{\hat{\boldsymbol{x}}_i,\hat{\boldsymbol{p}}_i\},\cdot]+\frac{D_{pp}}{\hbar^2}\lambda_M^2\sum_{i=1}^{3}\left[\hat{\boldsymbol{a}}_i\cdot\hat{\boldsymbol{a}}^{\dagger}_i-\frac{1}{2}\{\hat{\boldsymbol{a}}^{\dagger}_i\hat{\boldsymbol{a}}_i,\cdot\}\right], \tag{60}$$

in which the single generator feature is put into evidence.

V. CONCLUSIONS AND REMARKS

In this article we have considered the behavior with respect to covariance under translations and rotations, and the existence of a stationary solution of a recently proposed master equation (1) for the description of the interaction of a test particle with a fluid, a physical model corresponding to the so-called Rayleigh gas. The key result in (1) is the appearance of a two-point correlation function known as dynamic structure factor and given by (4), the general structure conforming to results already obtained in the mathematical literature for the generator of a translation-covariant dynamical semigroup. This correlation function, depending on symmetry and statistical mechanics properties of the fluid, directly determines the behavior of the master equation with respect to covariance under translations and rotations, and existence of a stationary solution with the expected canonical form. Considering the specific case of a free gas, the dynamic structure factor has been explicitly evaluated for Bose, Fermi, and Maxwell–Boltzmann statistics, and the dependence on the physical parameters determining the peculiar features of the model under consideration has been put into evidence in an exact expansion of the dynamic structure function. These parameters are the fugacity of the gas z, the ratio between mass of the gas particles and of the test particle α, the transferred momentum $\boldsymbol{q}$, and the transferred energy $E(\boldsymbol{q},\boldsymbol{p})$. Stability of the covariance properties of the master equation and of the existence of a stationary solution is then considered in the limit in which these parameters are small, together with the different explicit expressions of the master equation. In particular, in the Brownian limit $\alpha\ll 1$ and considering small momentum transfer, corresponding through the physical interpretation of the dynamic structure factor to long-wavelength fluctuations, a Fokker–Planck equation with a Lindblad structure is obtained, given by (53), where the results corresponding to Bose, Fermi, and Maxwell–Boltzmann statistics

are jointly considered. The correction due to quantum statistics in the Fokker-Planck equation is simply expressed through the Bose and Fermi functions given by (45) and (46), respectively.

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APPENDIX A: DERIVATION OF EQ. (23) AND EQ. (25)

In this Appendix we want to explicitly calculate the expression of the dynamic structure factor for a free gas as a function of $\boldsymbol{q}$ and $\boldsymbol{p}$. Working at finite temperature we can carry out the calculation for both Bose and Fermi particles at the same time adopting the convention that the symbol $\pm$ means a $+$ sign for Bose particles and $-$ for Fermi particles. We start from the expression

$$S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})=\frac{1}{n}\int_{\mathbf{R}^3}\frac{d^3\boldsymbol{k}}{(2\pi\hbar)^3}\,\langle n_k\rangle_{\mathrm{B/F}}(1\pm\langle n_{k-q}\rangle_{\mathrm{B/F}})\,\delta\left(\frac{(\boldsymbol{p}+\boldsymbol{q})^2}{2M}+\frac{(\boldsymbol{k}-\boldsymbol{q})^2}{2m}-\frac{\boldsymbol{p}^2}{2M}-\frac{\boldsymbol{k}^2}{2m}\right)$$

with

$$\langle n_k\rangle_{\mathrm{B/F}}=\frac{1}{z^{-1}e^{\beta\epsilon_k}\mp 1},\qquad \epsilon_k=\frac{\boldsymbol{k}^2}{2m},$$

which can be found, for example, in Ref. 12 and corresponds to (4) for a free gas apart from a singular term proportional, in the continuum limit considered here, to $\delta^3(\boldsymbol{q})$, relevant only for $\boldsymbol{q}=0$ and not contributing to the master equation. In fact, in the derivation of the master equation the contributions for $\boldsymbol{q}=0$ exactly cancel out. This term according to (7) corresponds to forward scattering. We now have to evaluate the integral in $\boldsymbol{k}$. This is most easily done writing $S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})$ in the form

$$S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})=\frac{1}{n}\int_{\mathbf{R}^3}\frac{d^3\boldsymbol{k}}{(2\pi\hbar)^3}\,\langle n_k\rangle_{\mathrm{B/F}}(1\pm\langle n_{k-q}\rangle_{\mathrm{B/F}})\,\delta(E(\boldsymbol{q},\boldsymbol{p})+\epsilon_{k-q}-\epsilon_k)$$

and observing that

$$\langle n_k\rangle_{\mathrm{B/F}}(1\pm\langle n_{k-q}\rangle_{\mathrm{B/F}})=\frac{1}{1-e^{\beta(\epsilon_k-\epsilon_{k-q})}}(\langle n_k\rangle_{\mathrm{B/F}}-\langle n_{k-q}\rangle_{\mathrm{B/F}}),$$

so that one has

$$\begin{aligned}
S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})&=\frac{1}{n}\,\frac{1}{1-e^{\beta E(\boldsymbol{q},\boldsymbol{p})}}\int_{\mathbf{R}^3}\frac{d^3\boldsymbol{k}}{(2\pi\hbar)^3}\,(\langle n_k\rangle_{\mathrm{B/F}}-\langle n_{k-q}\rangle_{\mathrm{B/F}})\,\delta(E(\boldsymbol{q},\boldsymbol{p})+\epsilon_{k-q}-\epsilon_k)\\
&=\frac{1}{n}\,\frac{1}{1-e^{\beta E(\boldsymbol{q},\boldsymbol{p})}}\int_{\mathbf{R}^3}\frac{d^3\boldsymbol{k}}{(2\pi\hbar)^3}\,\{\langle n_k\rangle_{\mathrm{B/F}}\delta(E(\boldsymbol{q},\boldsymbol{p})+\epsilon_{k-q}-\epsilon_k)\\
&\quad-\langle n_k\rangle_{\mathrm{B/F}}\delta(E(\boldsymbol{q},\boldsymbol{p})+\epsilon_k-\epsilon_{k+q})\}\\
&=\frac{1}{n}\,\frac{2m}{1-e^{\beta E(\boldsymbol{q},\boldsymbol{p})}}\int_{\mathbf{R}^3}\frac{d^3\boldsymbol{k}}{(2\pi\hbar)^3}\,\langle n_k\rangle_{\mathrm{B/F}}\{\delta(2mE(\boldsymbol{q},\boldsymbol{p})+q^2-2\boldsymbol{k}\cdot\boldsymbol{q})\\
&\quad-\delta(2mE(\boldsymbol{q},\boldsymbol{p})-q^2-2\boldsymbol{k}\cdot\boldsymbol{q})\}.
\end{aligned}\tag{A1}$$

We are thus led to consider an integral of the form

$$\int_{\mathbf{R}^3} d^3\boldsymbol{k}\,\langle n_k\rangle_{\,\mathrm{B/F}}\,\delta(\,\eta-2\boldsymbol{k}\cdot\boldsymbol{q}) \tag{A2}$$

with η a real parameter. Denoting by ξ the cosine of the angle between $\boldsymbol{k}$ and $\boldsymbol{q}$ the integral in (A2) becomes

$$\begin{aligned} &2\pi\int_{-1}^{1} d\xi \int_0^{+\infty} dk\, k^2 \langle n_k\rangle_{\,\mathrm{B/F}}\,\delta(\,\eta-2\xi kq) \\ &\quad=\int_{-1}^{1} d\xi \int_0^{+\infty} dk\, k^2 \langle n_k\rangle_{\mathrm{B/F}} \int_{-\infty}^{+\infty} dp\, e^{ip(\,\eta-2\xi kq)} \\ &\quad=\int_{-\infty}^{+\infty} dk\, k\langle n_k\rangle_{\,\mathrm{B/F}} \int_{-\infty}^{+\infty} dp\, \frac{e^{ip(\,\eta+2kq)}}{i2pq}. \end{aligned} \tag{A3}$$

and, using the identity

$$k\langle n_k\rangle_{\,\mathrm{B/F}}=\pm\frac{m}{\beta}\frac{d}{dk}\log[1\mp ze^{-\epsilon_k}], \tag{A4}$$

we get, integrating by parts,

$$\begin{aligned} \int_{\mathbf{R}^3} d^3\boldsymbol{k}\,\langle n_k\rangle_{\,\mathrm{B/F}}\,\delta(\,\eta-2\boldsymbol{k}\cdot\boldsymbol{q}) &= \mp\frac{2\pi m}{\beta}\int_{-\infty}^{+\infty} dk\,\log[1\mp ze^{-\epsilon_k}]\int_{-\infty}^{+\infty}\frac{dp}{2\pi}\, e^{ip(\,\eta+2kq)} \\ &= \mp\frac{\pi m}{\beta q}\log\left\{1\mp z\exp\left[-\frac{\beta}{8m}\left(\frac{\eta}{q}\right)^2\right]\right\}. \end{aligned} \tag{A5}$$

Inserting the result (A5) in (A1) one immediately has

$$S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})=\mp\frac{1}{(2\pi\hbar)^3}\,\frac{2\pi m^2}{n\beta q}\,\frac{1}{1-e^{\beta E(\boldsymbol{q},\boldsymbol{p})}}\log\left[\frac{1\mp z\,\exp[-(\beta/8m)(2mE(\boldsymbol{q},\boldsymbol{p})+q^2)^2/q^2)]}{1\mp z\,\exp[-(\beta/8m)(2mE(\boldsymbol{q},\boldsymbol{p})-q^2)^2/q^2]}\right]. \tag{A6}$$

In a similar way, starting from the expression of a gas of Maxwell–Boltzmann particles

$$S_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p})=\frac{1}{n}\int_{\mathbf{R}^3}\frac{d^3\boldsymbol{k}}{(2\pi\hbar)^3}\,\langle n_k\rangle_{\mathrm{MB}}\,\delta\left(\frac{(\boldsymbol{p}+\boldsymbol{q})^2}{2M}+\frac{(\boldsymbol{k}-\boldsymbol{q})^2}{2m}-\frac{\boldsymbol{p}^2}{2M}-\frac{\boldsymbol{k}^2}{2m}\right),$$

with

$$\langle n_k\rangle_{\mathrm{MB}}=ze^{-\beta\epsilon_k},$$

we write it in the form

$$\begin{aligned} S_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p}) &= \frac{1}{n}\int_{\mathbf{R}^3}\frac{d^3\boldsymbol{k}}{(2\pi\hbar)^3}\,\langle n_k\rangle_{\mathrm{MB}}\,\delta(E(\boldsymbol{q},\boldsymbol{p})+\epsilon_{k-q}-\epsilon_k) \\ &= \frac{2m}{n}\int_{\mathbf{R}^3}\frac{d^3\boldsymbol{k}}{(2\pi\hbar)^3}\,\langle n_k\rangle_{\mathrm{MB}}\,\delta(2mE(\boldsymbol{q},\boldsymbol{p})+q^2-2\boldsymbol{k}\cdot\boldsymbol{q}). \end{aligned} \tag{A7}$$

Analogously to (A2) we have to consider

$$\int_{\mathbf{R}^3} d^3\boldsymbol{k}\,\langle n_k\rangle_{\mathrm{MB}}\,\delta(\eta-2\boldsymbol{k}\cdot\boldsymbol{q}),$$

which according to (A3) becomes

$$\int_{-\infty}^{+\infty} dk\,k\langle n_k\rangle_{\mathrm{MB}}\int_{-\infty}^{+\infty} dp\,\frac{e^{ip(\eta+2kq)}}{i2pq}.$$

Exploiting instead of (A4) the relation

$$k\langle n_k\rangle_{\mathrm{MB}}=-\frac{m}{\beta}\frac{d}{dk}ze^{-\epsilon_k}$$

we obtain

$$\int_{\mathbf{R}^3} d^3\boldsymbol{k}\,\langle n_k\rangle_{\mathrm{MB}}\,\delta(\eta-2\boldsymbol{k}\cdot\boldsymbol{q})=\frac{\pi m}{\beta q}z\exp\left[-\frac{\beta}{8m}\left(\frac{\eta}{q}\right)^2\right],$$

which has to be substituted in (A7) leading to

$$S_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p})=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}z\exp\left[-\frac{\beta}{8m}\frac{(2mE(\boldsymbol{q},\boldsymbol{p})+q^2)^2}{q^2}\right]. \tag{A8}$$

APPENDIX B: EXACT EXPANSION OF $S_{\mathrm{B/F}}$ AND DERIVATION OF EQ. (39)

We will now derive an expression for $S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})$ equivalent to (27), in which, however, a series expansion in powers of the fugacity z is put into evidence. The starting point is the Taylor expansion for the logarithm $\log(1+x)=\Sigma_{k=1}^{\infty}(-)^{k+1}x^k/k$, which leads us to write (27) in the form

$$S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})=\mp\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}\frac{1}{1-e^{(\beta/2m)(2\sigma(\boldsymbol{q},\boldsymbol{p})q-q^2)}}$$
$$\times\sum_{k=1}^{\infty}(-)^{k+1}\frac{(\mp z)^k}{k}e^{-(\beta/2m)\sigma^2(\boldsymbol{q},\boldsymbol{p})}[1-e^{k(\beta/2m)(2\sigma(\boldsymbol{q},\boldsymbol{p})q-q^2)}]. \tag{B1}$$

Considering now in (B1) a geometrical progression of reason $e^{(\beta/2m)(2\sigma(\boldsymbol{q},\boldsymbol{p})q-q^2)}$, according to the formula

$$1-x^k=(1-x)\sum_{n=0}^{k-1}x^n, \tag{B2}$$

Eq. (B1) becomes

$$S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})=\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}\sum_{k=1}^{\infty}(\pm)^{k+1}\frac{z^k}{k}e^{-k(\beta/2m)\sigma^2(\boldsymbol{q},\boldsymbol{p})}\sum_{n=0}^{k-1}e^{n(\beta/2m)(2\sigma(\boldsymbol{q},\boldsymbol{p})q-q^2)},$$

where it is to be noted that the sum over n is due to the presence of the statistical correction $1\pm\langle n_{k-q}\rangle_{\mathrm{B/F}}$ in (22) and disappears, being replaced by a factor of 1, if this correction is neglected. It is worthwhile to put into evidence a factor

$$\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}ze^{-(\beta/2m)\sigma^2(\boldsymbol{q},\boldsymbol{p})},$$

corresponding to the expression of the dynamic structure factor for a free gas of Maxwell–Boltzmann particles, thus obtaining

$$S_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})=S_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p})\left[1+\sum_{k=1}^{\infty}(\pm)^k\frac{z^k}{k+1}e^{-k(\beta/2m)\sigma^2(\boldsymbol{q},\boldsymbol{p})}\sum_{n=0}^{k}e^{n(\beta/2m)(2\sigma(\boldsymbol{q},\boldsymbol{p})q-q^2)}\right].$$

In the Brownian limit $\alpha\ll 1$ considered in Sec. IV, neglecting in (30) the contributions of order α, this expression goes simply over to

$$S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})=S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p})\left[1+\sum_{k=1}^{\infty}(\pm)^k\frac{z^k}{k+1}e^{-k(\beta/8m)q^2}e^{-k(\beta/2)[q^2/2M+\boldsymbol{q}\cdot\boldsymbol{p}/M]}\sum_{n=0}^{k}e^{n\beta[q^2/2M+\boldsymbol{q}\cdot\boldsymbol{p}/M]}\right], \tag{B3}$$

where $S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},\boldsymbol{p})$ and $S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},\boldsymbol{p})$ are given, respectively, by (31) and (32). In terms of $E(\boldsymbol{q},\boldsymbol{p})$ Eq. (B3) takes the remarkably compact form

$$S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},E)=S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E)\left[1+\sum_{k=1}^{\infty}(\pm)^k\frac{z^k}{k+1}e^{-k(\beta/8m)q^2}e^{-k(\beta/2)E}\sum_{n=0}^{k}e^{n\beta E}\right], \tag{B4}$$

where $S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},E)$ and $S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E)$ are given by (33) and (34). We now go one step further noting that the following identity holds:

$$e^{-k(\beta/2)E}\sum_{n=0}^{k}e^{n\beta E}=\frac{\sinh[(k+1)(\beta/2)E]}{\sinh((\beta/2)E)},$$

which can be easily obtained exploiting (B2), so that (B4) becomes

$$S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},E)=S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E)\sum_{k=0}^{\infty}(\pm)^k\frac{z^k}{k+1}e^{-k(\beta/8m)q^2}\frac{\sinh[(k+1)(\beta/2)E]}{\sinh((\beta/2)E)}. \tag{B5}$$

Equation (B5) is the most convenient expression in order to consider the limit of small momentum transfer. Exploiting the expansion

$$\frac{\sinh[\frac{1}{2}(k+1)\beta E]}{\sinh(\frac{1}{2}\beta E)}=(k+1)\left[1+\frac{1}{24}(\beta E)^2(k^2+2k)+O(E^4)\right]$$

and recalling that E is given by (6) we may write (B5) as

$$\begin{aligned}S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},E)=S^{\infty}_{\mathrm{MB}}(\boldsymbol{q},E)\Bigg[&\sum_{k=0}^{\infty}(\pm z)^k-\frac{\beta}{8m}q^2\sum_{k=1}^{\infty}(\pm)^k kz^k\\&+\frac{1}{12}(\beta E)^2\sum_{k=1}^{\infty}(\pm)^k kz^k+\frac{1}{24}(\beta E)^2\sum_{k=1}^{\infty}(\pm)^k k^2z^k+O(q^4)\Bigg].\end{aligned} \tag{B6}$$

Recalling (B5) and the explicit expression of S^{∞}_{MB} given by (22) one also has

$$S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},E)=\pm\frac{1}{(2\pi\hbar)^3}\frac{2\pi m^2}{n\beta q}\frac{e^{-(\beta/2)E}}{\sinh((\beta/2)E)}\sum_{k=1}^{\infty}(\pm)^k\frac{z^k}{k}e^{-k(\beta/8m)q^2}\sinh\left(k\frac{\beta}{2}E\right)$$

and, exploiting[22]

$$\sum_{k=1}^{\infty} \frac{p^k}{k} \sinh(kx) = \operatorname{arth}\left[\frac{p \sinh x}{1 - p \cosh x}\right],$$

we obtain the alternative expression

$$S^{\infty}_{\mathrm{B/F}}(\boldsymbol{q},E) = \pm \frac{1}{(2\pi\hbar)^3} \frac{2\pi m^2}{n\beta q} \frac{e^{-(\beta/2)E}}{\sinh((\beta/2)E)} \operatorname{arth}\left[\frac{\pm z e^{-(\beta/8m)q^2} \sinh((\beta/2)E)}{1 \mp z e^{-(\beta/8m)q^2} \cosh((\beta/2)E)}\right] \tag{B7}$$

equivalent to (31) as can also be directly checked starting from the identity

$$\operatorname{arth} x = \frac{1}{2} \log\left[\frac{1+x}{1-x}\right]. \tag{B8}$$

Note that (31) and (B7) in the Fermi case can also be written in the form

$$S^{\infty}_{\mathrm{F}}(\boldsymbol{q},E) = -\frac{1}{(2\pi\hbar)^3} \frac{\pi m^2}{n\beta q} \frac{e^{-(\beta/2)E}}{\sinh((\beta/2)E)} \log\left[\frac{1 - [z/(1+z)](1 - e^{-(\beta/8m)q^2} e^{-(\beta/2)E})}{1 - [z/(1+z)](1 - e^{-(\beta/8m)q^2} e^{+(\beta/2)E})}\right]$$

and

$$S^{\infty}_{\mathrm{F}}(\boldsymbol{q},E) = -\frac{1}{(2\pi\hbar)^3} \frac{2\pi m^2}{n\beta q} \frac{e^{-(\beta/2)E}}{\sinh((\beta/2)E)} \operatorname{arth}\left[\frac{[z/(1+z)] e^{-(\beta/8m)q^2} \sinh((\beta/2)E)}{[z/(1+z)](1 - e^{-(\beta/8m)q^2} \cosh((\beta/2)E)) - 1}\right],$$

respectively, which can be useful if one is interested in an expansion for large values of z. According to (B8), also for $S_{\mathrm{B/F}}(\boldsymbol{q},E)$ given by (23) one has the alternative expression

$$S_{\mathrm{B/F}}(\boldsymbol{q},E) = \pm \frac{1}{(2\pi\hbar)^3} \frac{2\pi m^2}{n\beta q} \frac{e^{-(\beta/2)E}}{\sinh((\beta/2)E)} \operatorname{arth}\left[\frac{\pm z e^{-(\beta/8m)q^2} e^{-(\beta/2)(m/q^2)E^2} \sinh((\beta/2)E)}{1 \mp z e^{-(\beta/8m)q^2} e^{-(\beta/2)(m/q^2)E^2} \cosh((\beta/2)E)}\right]. \tag{B9}$$

The validity of the detailed balance condition for (B9) according to (12) can immediately be checked observing that both $\sinh x$ and $\operatorname{arth} x$ are odd functions, while $\cosh x$ is an even function.

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A class of nonconservative Lagrangian systems on Riemannian manifolds

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We generalize results of Rauch-Wojciechowski, Marciniak and Lundmark, concerning a class of nonconservative Lagrangian systems, from the Euclidean to the Riemannian case. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In a number of recent publications,[1–4] Rauch-Wojciechowski, Marciniak, and Lundmark have discussed an interesting class of systems of second-order ordinary differential equations, whose members, when viewed as classical mechanical systems, are in a sense completely integrable. These systems originally generated interest because they are derived from the stationary flows of soliton-type evolution equations; but they have more recently been studied in their own right because they include well-known cases of integrable bi-Hamiltonian systems and cases where the Hamilton–Jacobi equation separates. Of these papers we will refer most often to Ref. 2, which contains the most general exposition of the theory which we seek to develop further. In particular, Ref. 2 deals with systems with n of degrees of freedom, and therefore subsumes (at least so far as the issues we intend to discuss are concerned) Ref. 4, which is largely restricted to systems with two degrees of freedom.

The systems of second-order equations under consideration take the general form of Lagrange's equations in mechanics:

$$\frac{d}{dt}\left(\frac{\partial T}{\partial \dot{q}^i}\right) - \frac{\partial T}{\partial q^i} = Q_i\,,$$

where T is the kinetic energy function and the ''generalized forces'' Q_i need not be derivable from a potential energy function. In all the publications mentioned above the kinetic energy is taken to have the Euclidean form, $T=\frac{1}{2}\Sigma(\dot{q}^i)^2$; we however will deal with the more general situation in which T is derived from a Riemannian metric, $T=\frac{1}{2}g_{ij}\dot{q}^i\dot{q}^j$. In addition, the systems are required to possess quadratic integrals of the motion, of a special kind, called by Lundmark integrals of cofactor type. Of particular interest are those systems which possess two independent quadratic integrals of cofactor type: such a system can be regarded as the restriction of a bi-Hamiltonian flow on a phase space of one more dimension, and has a further hierarchy of integrals in involution.

As we have just pointed out, the primary aim of our article is to derive in the Riemannian case results which parallel those that Lundmark *et al.* have obtained in the Euclidean one. In doing so we, of course, extend the range of application of their theory. However, in justifying our efforts we would put greater emphasis on the increased level of geometrical insight we have achieved into the results of the group in Linköping. In particular, we claim to have considerably clarified, by generalizing them;

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(1) the concept and properties of a cofactor system;
(2) the origin of the so-called ''fundamental equation'' involved in the definition of a cofactor pair system; and
(3) the construction of the bi-Hamiltonian structure associated with a cofactor pair system.

Several of the methods we use were developed in a recent paper on bi-Hamiltonian systems and conformal Killing tensors,[5] which was concerned with a certain class of conservative systems whose Hamilton–Jacobi equations separate; we will briefly indicate how such systems can be regarded as a subset of the cofactor pair systems discussed in this article.

The Linköping group refer to the differential equations they consider as ''Newton equations of quasi-Lagrangian type,'' because in the Euclidean case it turns out that when there is a quadratic first integral E the equations can formally be cast into the form $d/dt(\partial E/\partial \dot{q}^i)+\partial E/\partial q^i=0$, which resembles Lagrange's equations but has a wrong sign. This is, in our opinion, a complete artifact of the systems under consideration, which has nothing to do with the fundamental issues which are at stake. In fact, the more general systems on Riemannian spaces we will introduce simply do not have this very nonintrinsic property. We have therefore decided to describe them as ''nonconservative Lagrangian systems'' instead. In doing so we are conscious that our work, together with that of Rauch-Wojciechowski, Marciniak, Lundmark and others in this field, is closely connected with the researches of Bertrand and Darboux in the second half of the nineteenth century, which are summarized by Whittaker in articles 151 and 152 of Ref. 6.

The structure of this article is as follows. In Sec. II we recall some aspects of Poisson structures for later use. We concentrate in particular on the construction of a nonstandard Poisson structure on T^*Q out of the complete lift of a type $(1,1)$ tensor field on Q. In Sec. III, we take a non-conservative Lagrangian system as the starting point and investigate under what circumstances it has a quasi-Hamiltonian representation with respect to such a nonstandard Poisson structure. This leads us to an interesting class of special conformal Killing tensors J, which are discussed in more detail in Sec. IV. The main result in that section is that the cofactor tensor of such a J is a Killing tensor. Coming back then to the idea we started from, and inspired by the work of Lundmark[2] in the Euclidean case, we more formally introduce the notion of a cofactor system in Sec. V and complete the discussion of its quasi-Hamiltonian representation. In Sec. VI, we show how a cofactor system can also be given a Hamiltonian representation on an extended manifold. Section VII is about cofactor pair systems, that is, systems which have a double cofactor representation. We show how this leads to a gauged bidifferential calculus which provides an intrinsic generalization of the ''fundamental equations'' referred to above. We further establish complete integrability by exploiting the double Poisson structure on the extended space. Finally, we briefly explain the relation between this work and recent work on the separability of the Hamilton–Jacobi equation.

II. POISSON STRUCTURES

It will be convenient to recall some generalities here about Poisson structures, which will at the same time serve to fix the sign conventions which we will adopt.

A Poisson structure on a manifold M is a bivector field Π which satisfies $[\Pi,\Pi]=0$, where $[\cdot,\cdot]$ is the Schouten bracket. The associated Poisson bracket of functions f, g is given by $\{f,g\}=\Pi(df,dg)$; the vanishing of the Schouten bracket entails the Jacobi identity for the Poisson bracket. Also associated with such a bivector field is a map P of 1-forms to vector fields on M, given by $\langle P(\alpha),\beta\rangle=\Pi(\alpha,\beta)$ for any pair of 1-forms α, β. The vector field $P(dh)$ is the Hamiltonian vector field corresponding to the Hamiltonian function h. The Poisson structure is nonsingular if its Poisson map is.

Two Poisson structures Π_1, Π_2 are compatible if $[\Pi_1,\Pi_2]=0$. When this condition holds, $a_1\Pi_1+a_2\Pi_2$ is Poisson for any constants a_1 and a_2. The collection of Poisson bivectors $a_1\Pi_1+a_2\Pi_2$ is called a Poisson pencil.

Let $\phi:M\to M$ be a diffeomorphism. For any bivector field Π on M we can use ϕ^*, the map of forms induced by ϕ, to transform Π into a new bivector field Π_ϕ by

$$(\Pi_\phi)(\alpha,\beta)=\phi^{-1}{}^*\Pi(\phi^*\alpha,\phi^*\beta).$$

This is the natural extension to bivector fields of the map of vector fields induced by a diffeomorphism. The corresponding transform P_ϕ of the map P is given as a linear map $T_x^*M\to T_xM$, $x\in M$, by

$$P_\phi|_x=\phi_{*x}\circ P|_{\phi^{-1}(x)}\circ\phi_x^*.$$

There is no guarantee that Π_ϕ will be Poisson even when Π is: we will deal with a case in which it is below. For the present, merely note that if ϕ and ψ are two diffeomorphisms then $\Pi_{\phi\circ\psi}=(\Pi_\psi)_\phi$ and likewise $P_{\phi\circ\psi}=(P_\psi)_\phi$.

The cotangent bundle T^*Q of a manifold Q has a standard Poisson bivector Π_0 whose expression in terms of standard coordinates (q^i,p_i) is

$$\Pi_0=\frac{\partial}{\partial p_i}\wedge\frac{\partial}{\partial q^i}.$$

The corresponding Poisson map P_0 is given in terms of the canonical symplectic form ω by $P_0(\alpha)\lrcorner\omega=-\alpha$.

Let J be a nonsingular type (1,1) tensor field on Q. It defines a diffeomorphism $\hat{J}$ of T^*Q which is fiber preserving and linear on fibers, given by $\hat{J}(q^i,p_i)=(q^i,J_i^jp_j)$ (note that J acts here on covectors, that is to say, it is its adjoint that is involved). The bivector field $(\Pi_0)_{\hat{J}}=\Pi_J$ is a Poisson bivector if and only if the torsion, or Nijenhuis tensor, N_J of J is zero. When this is the case Π_J is compatible with Π_0, and we obtain an example of a Poisson–Nijenhuis structure. The corresponding Poisson map P_J is given by $P_J=\tilde{J}\circ P_0=P_0\circ\tilde{J}^*$, where $\tilde{J}$ is the complete lift of J, a type (1,1) tensor field on T^*Q, and $\tilde{J}^*$ is its adjoint (acting on 1-forms).

In the sequel we will carry out several coordinate calculations involving these constructs, in situations where we have a symmetric connection at our disposal. We therefore give coordinate representations of them using bases of local vector fields and 1-forms adapted to the connection, given by

$$\frac{\partial}{\partial q^i}+\Gamma_{ij}^k p_k\frac{\partial}{\partial p_j}=X_i,\quad \frac{\partial}{\partial p_i},$$

for vector fields, where $\Gamma_{ij}^k=\Gamma_{ji}^k$ are the connection coefficients, and

$$dq^i,\quad dp_i-\Gamma_{ij}^k p_k dq^j=\pi_i,$$

for 1-forms; these are dual bases. The indices i, j, k, etc., range over $1,2,\ldots,n=\dim M$, and the Einstein summation convention is in force. Then,

$$\tilde{J}=J_j^i\left(X_i\otimes dq^j+\frac{\partial}{\partial p_j}\otimes\pi_i\right)+(J_{i|j}^k-J_{j|i}^k)p_k\frac{\partial}{\partial p_i}\otimes dq^j.$$

The vertical bar divides off the differentiation index in a covariant differential from the other indices. The condition $N_J=0$ can be written:

$$J_l^k(J_{i|j}^l-J_{j|i}^l)=J_j^lJ_{i|l}^k-J_i^lJ_{j|l}^k.$$

In order to calculate Hamiltonian vector fields with respect to P_J it is enough to know $\tilde{J}$ since one can use either of the formulas $P_J=\tilde{J}\circ P_0$ and $P_J=P_0\circ\tilde{J}^*$; it is useful to remember that for a symmetric connection P_0 can be written

$$P_0=\frac{\partial}{\partial p_i}\wedge X_i\,.$$

However, to facilitate comparison with Refs. 2–4 we give the formula for P_J:

$$P_J=J^i_j\frac{\partial}{\partial p_j}\wedge X_i-\frac{1}{2}(J^k_{i|j}-J^k_{j|i})p_k\frac{\partial}{\partial p_i}\wedge\frac{\partial}{\partial p_j}.$$

Finally, we will have occasion to discuss situations where we have more than one type (1,1) tensor field at our disposal. In the first place, suppose that J has vanishing torsion, and that A is another type (1,1) tensor field such that JA also has vanishing torsion (where JA is the type (1,1) tensor field whose components are $J^i_kA^k_j$, that is, JA is the composition $J\circ A$ acting on vector fields). Then Π_{JA} is a Poisson bivector. It can be expressed in terms of Π_J by means of the formula $\Pi_{\phi\circ\psi}=(\Pi_\psi)_\phi$ with $\phi=\hat{A}$, $\psi=\hat{J}$: note that since A and J act on T^*Q by their adjoints, $\widehat{JA}=\hat{A}\circ\hat{J}$. Thus, $\Pi_{JA}=(\Pi_J)_{\hat{A}}$. It follows that for any Hamiltonian function H,

$$P_{JA}(d(\hat{A}^{-1}{}^*H))=\hat{A}_*P_J(dH).$$

Second, suppose that J and K both have vanishing torsion and that $[J,K]=0$ where $[\,\cdot\,,\cdot\,]$ here is the Nijenhuis bracket. Then $aJ+bK$ has vanishing torsion for all constants a and b, so that P_{aJ+bK} is a Poisson map for all a and b; and from the formula for P_J we see that $P_{aJ+bK}=aP_J+bP_K$. Thus, aP_J+bP_K is a Poisson pencil in this case.

III. NONCONSERVATIVE LAGRANGIAN SYSTEMS

A geometrical description of the kind of general Lagrange equations mentioned in the Introduction can be obtained as follows. Let S denote the canonical vertical endomorphism on a tangent bundle TQ and Γ a second-order differential equation field. As was described in Ref. 7, Γ represents a nonconservative Lagrangian system, if there exists a 1-form $\phi=dL-\mu$ on TQ, where L is a regular Lagrangian and μ is semibasic, such that $\mathcal{L}_\Gamma(S^*(\phi))=\phi$. It is easy to verify that, in coordinates (q^i,u^i) on TQ, this requirement means that

$$\Gamma\left(\frac{\partial L}{\partial u^i}\right)-\frac{\partial L}{\partial q^i}=-M_i\,,$$

where the M_i are the components of μ (the minus sign here is a matter of convention). We shall consider the particular case in which the nonconservative forces $-M_i$ do not depend on the velocities, so that μ is a 1-form on Q; and L is a pure kinetic energy Lagrangian. The latter means that the base manifold Q is assumed to be Riemannian (or pseudo-Riemannian) with metric tensor $g=(g_{ij})$, and that $L=T=\frac{1}{2}g_{ij}u^iu^j$. If Γ^i_{jk} are the Christoffel symbols for the corresponding Levi-Civita connection, and if we put $M^i=g^{ij}M_j$ as is usual, the resulting second-order differential equation field is of the form

$$\Gamma=u^i\frac{\partial}{\partial q^i}-(\Gamma^i_{jk}u^ju^k+M^i)\frac{\partial}{\partial u^i}.$$

Another way of characterizing such vector fields is to say that $\Gamma=\Gamma_0-M^V$, where Γ_0 is the geodesic field for the connection and M^V is the vertical lift of a vector field M on Q.

We will show that it is possible, in certain interesting cases, to find a quasi-Hamiltonian representation for such a system; that is to say, to represent it as a scalar multiple of a Hamiltonian vector field. However, we will not assume that the Poisson structure with respect to which this vector field is Hamiltonian is the standard one; instead, we will look for a suitable Poisson structure of the form Π_J defined by some type (1,1) tensor field J on Q whose torsion vanishes.

We use g to define a diffeomorphism $\hat{g}:TQ\to T^*Q$ by $p_i=g_{ij}u^j$. We will denote by $\hat{\Gamma}$ the transform of Γ by $\hat{g}$, that is, $\hat{\Gamma}=\hat{g}_*\Gamma$. We have

$$\hat{\Gamma}=g^{ij}p_jX_i-M_i\frac{\partial}{\partial p_i},$$

where the X_i are the vector fields on T^*Q adapted to the connection specified above.

Equip T^*Q with a Poisson structure Π_J and Poisson map P_J as described earlier. We wish to determine under what circumstances one can find a J with $N_J=0$ such that the given system satisfies $F\hat{\Gamma}=P_J(dH)$ for some functions F and H. We will now solve this problem under the assumption that H is quadratic in the momenta, so that $H=\frac{1}{2}A^{ij}p_ip_j+V$ for some symmetric tensor A and function V on Q; we will further assume that A is nonsingular.

For such H we find, after a little calculation, that

$$P_J(dH)=J^i_kA^{jk}p_jX_i-\left[\left(\frac{1}{2}J^l_iA^{jk}{}_{|l}-(J^j_{i|l}-J^j_{l|i})A^{kl}\right)p_jp_k+J^j_i\frac{\partial V}{\partial q^j}\right]\frac{\partial}{\partial p_i}.$$

For this to equal $F\hat{\Gamma}$ we must first have

$$J^i_kA^{jk}=Fg^{ij}.$$

Thus F must be a function on Q, so that the quadratic and zeroth-order terms in the other coefficients must be equated separately. As a result, we require that

$$J^l_iA^{jk}{}_{|l}=(J^j_{i|l}-J^j_{l|i})A^{kl}+(J^k_{i|l}-J^k_{l|i})A^{jl}$$

$$J^j_i\frac{\partial V}{\partial q^j}=FM_i.$$

On lowering the index i in the first condition we see that J_{ij} is a scalar multiple of the inverse of A^{ij}, and so is symmetric because A^{ij} is. By differentiating this equation and multiplying by J twice we obtain

$$J^m_jJ^n_kJ^l_iA^{jk}{}_{|l}=\frac{\partial F}{\partial q^l}J^{mn}J^l_i-FJ^l_iJ^{mn}{}_{|l}.$$

The second condition therefore can equivalently be replaced by

$$\frac{\partial F}{\partial q^l}J^{mn}J^l_i=F[J^l_iJ^{mn}{}_{|l}+g^{lm}J^n_k(J^k_{i|l}-J^k_{l|i})+g^{ln}J^m_k(J^k_{i|l}-J^k_{l|i})].$$

We now use the assumption that $N_J=0$ to rearrange the last four terms; when this is done, the first term on the right-hand side cancels, and after some indices have been lowered we obtain

$$\frac{\partial F}{\partial q^l}J_{jk}J^l_i=F(J^l_kJ_{ij|l}+J^l_jJ_{ik|l}-J^l_iJ_{jk|l}).$$

The part of this equation symmetric in i and j gives

$$J_{ij|k}=\tfrac{1}{2}(\alpha_ig_{jk}+\alpha_jg_{ik})$$

where we have written

$$\alpha_i = \frac{1}{F} J_i^j \frac{\partial F}{\partial q^j}.$$

The skew-symmetric part is then automatically satisfied. It further follows from the formula for $J_{ij|k}$ that $\alpha_k = (J_i^i)_{|k}$, or $\alpha = \alpha_i dq^i = d(\operatorname{tr} J)$. Hence, if $J_{ij|k}$ has the required structure, the α_i is actually determined, so that the relations $J_i^j \partial F/\partial q^j = F\alpha_i$ should be seen as equations for admissible functions F.

We next show that a particular solution for F is $\det J$. We have

$$\det J = \frac{1}{n!} \delta^{i_1 i_2 \cdots i_n}_{j_1 j_2 \cdots j_n} J^{j_1}_{i_1} J^{j_2}_{i_2} \cdots J^{j_n}_{i_n},$$

where $\delta^{i_1 i_2 \cdots i_n}_{j_1 j_2 \cdots j_n}$ is the generalized Kronecker delta (see, for example, Ref. 8). Thus

$$\frac{\partial}{\partial q^k} \det J = \frac{1}{(n-1)!} \delta^{i i_2 \cdots i_n}_{j j_2 \cdots j_n} J^j_{i|k} J^{j_2}_{i_2} \cdots J^{j_n}_{i_n}.$$

Now

$$\frac{1}{(n-1)!} \delta^{i i_2 \cdots i_n}_{j j_2 \cdots j_n} J^{j_2}_{i_2} \cdots J^{j_n}_{i_n} = C^i_j$$

is the cofactor tensor of J, which satisfies

$$J^i_k C^k_j = (\det J)\, \delta^i_j.$$

So, we may write

$$J^k_i \frac{\partial}{\partial q^k} \det J = J^k_i C^l_j J^j_{l|k} = \frac{1}{2} J^k_i C^l_j (\alpha_l \delta^j_k + \alpha^j g_{kl}) = \frac{1}{2} (J^j_i C^l_j \alpha_l + J^k_i C^l_k \alpha_l) = (\det J)\, \alpha_i,$$

where we have used the fact that C_{ij} is symmetric, which follows from the symmetry of J_{ij}.

Now suppose that F is any solution: we show that F is a constant multiple of $\det J$. We have

$$\frac{1}{F} J^j_i \frac{\partial F}{\partial q^j} = \alpha_i = \frac{1}{\det J} J^j_i \frac{\partial}{\partial q^j} \det J,$$

from which it follows that

$$J^j_i \frac{\partial}{\partial q^j} \left(\frac{F}{\det J} \right) = 0,$$

and so $F = k \det J$.

Once we have fixed a J in a quasi-Hamiltonian representation $F\hat{\Gamma} = P_J(dH)$ for the given system, multiplying F by a constant factor is a quite irrelevant degree of freedom, since it can be compensated for by adapting the Hamiltonian. So without loss of generality we can take $F = \det J$, when the first condition on J becomes $J^i_k A^{jk} = (\det J) g^{ij}$, and identifies A^i_j as the cofactor tensor of J^i_j. Finally, there is a restriction on the nonconservative forces, which must have the form

$$M_i = (\det J)^{-1} J_i^j \frac{\partial V}{\partial q^j}$$

for some function V on Q.

We shall return to the formulation of the conclusions of this analysis in Sec. V, after looking in more detail at the special kind of tensor fields J has revealed.

IV. SPECIAL CONFORMAL KILLING TENSORS

A tensor J which satisfies the condition $J_{ij|k} = \frac{1}{2}(\alpha_i g_{jk} + \alpha_j g_{ik})$ for some α_i has very interesting properties. In the first place, $J_{(ij|k)} = \alpha_{(i} g_{jk)}$ (brackets denote symmetrization), which says that J is a conformal Killing tensor of g; and furthermore $\alpha = \alpha_i dq^i$ is exact, so it is a conformal Killing tensor of gradient type. In the course of the argument in the previous section it was assumed that the torsion of J vanishes (this was necessary to ensure that Π_J is Poisson): but in fact the vanishing of the torsion is an easy consequence of the defining condition. Moreover, as we showed in Ref. 5, a conformal Killing tensor whose torsion vanishes and which has functionally independent eigenfunctions must necessarily satisfy this condition. A symmetric type (0,2) tensor J on Q such that

$$J_{ij|k} = \tfrac{1}{2}(\alpha_i g_{jk} + \alpha_j g_{ik}),$$

will therefore be called a *special conformal Killing tensor*. In the Euclidean case a tensor is a special conformal Killing tensor if and only if it is an elliptic coordinates matrix in Lundmark's terminology,[2] or a planar inertia tensor in Benenti's.[9]

We will deal only with special conformal Killing tensors which are nonsingular. The inverse of a type (1,1) tensor will be denoted by an overbar when we need to use indices.

The determinant of a type (1,1) tensor is a scalar (this is not so for a type (2,0) or (0,2) tensor), so whenever we use determinants it is to be assumed that the corresponding tensor is in type (1,1) form. This also applies to the formula $A = (\det J) J^{-1}$, which may be used to define the cofactor tensor of J when it is nonsingular. Elsewhere, the usual rules for raising and lowering indices apply. Thus, for example, $A_{ij} = (\det J)\overline{J}_{ij}$: it is symmetric if J is.

When J is special conformal Killing, by taking the covariant derivative of the equation $A_{ij} J_l^j = (\det J) g_{il}$ and using the defining condition one can deduce that

$$A_{ij|k} = (\det J)(\overline{J}_{ij}\overline{J}_{kl} - \tfrac{1}{2}\overline{J}_{ik}\overline{J}_{jl} - \tfrac{1}{2}\overline{J}_{il}\overline{J}_{jk})\alpha^l,$$

from which one easily derives the following remarkable property of any special conformal Killing tensor.

Proposition 1: The cofactor tensor of a nonsingular special conformal Killing tensor is a Killing tensor.

Proof: It follows immediately from the formula above that $A_{(ij|k)} = 0$. □

Note further that A has the same eigenvectors as J.

A special conformal Killing tensor J may be used to define a couple of differential operators with nice properties. In the first place, we can form the operator d_J in the sense of Frölicher–Nijenhuis theory:[10] this is the derivation of degree 1 of the exterior algebra $\wedge(Q)$ of forms on Q, over the algebra $C^\infty Q$ of real-valued C^∞ functions on Q, which anticommutes with the exterior derivative d (i.e., is a derivation of type d_*), and whose action on $C^\infty(Q)$ is given by $d_J f = J^*(df)$. Furthermore, d_J has the coboundary property $d_J{}^2 = 0$ because the torsion N_J is zero. What is more, since by assumption J is nonsingular, d_J satisfies a Poincaré lemma: that is to say, for a k-form θ, the condition $d_J\theta = 0$ is sufficient as well as necessary for the local existence of a $(k-1)$-form φ such that $\theta = d_J\varphi$. This result can be found in a paper by Willmore.[11]

In the previous section we came across an interesting property in which d_J is involved. We showed there that if J is a special conformal Killing tensor, $F=\det J$ satisfies $J_i^j\partial F/\partial q^j=F\alpha_i$ where $\alpha=d(\operatorname{tr}J)$. Hence,

$$d_J(\det J)=(\det J)\alpha=(\det J)d(\operatorname{tr}J).$$

(In fact this holds for any tensor J whose torsion vanishes.) By acting with d_J on both sides, it easily follows that $d_J\alpha=0$, that is, $d_Jd(\operatorname{tr}J)=0$. (In fact for any tensor J whose torsion vanishes, $d_J(\operatorname{tr}J)=\frac{1}{2}d(\operatorname{tr}J^2)$.)

These properties enable us to define the following differential operator D_J, which also acts on forms θ on Q; D_J will turn out to have an important role in relation to the fundamental equation mentioned in the Introduction.

$$D_J\theta=(\det J)^{-1}d_J((\det J)\theta)=d_J\theta+\alpha\wedge\theta.$$

Note that D_J is not a derivation (in the sense of Frölicher–Nijenhuis), but it is clear from the first expression that D_J satisfies $D_J{}^2=0$, so it is an example of a (scalar) gauged differential operator, in the terminology of Ref. 12. Moreover, we see that once again $D_J\theta=0$ is a sufficient condition for there to be a form φ (locally) such that $\theta=D_J\varphi$: we have $d_J((\det J)\theta)=0$, so there is a φ' such that $(\det J)\theta=d_J\varphi'$, when $\varphi=(\det J)^{-1}\varphi'$ satisfies $D_J\varphi=\theta$.

Note finally that the condition on the nonconservative forces derived in the previous section can now be written in coordinate-free form with the aid of the 1-form $\mu=M_idq^i$ of the beginning of that section. The condition reads

$$\mu=(\det J)^{-1}d_JV=D_J((\det J)^{-1}V).$$

Hence, in order for the nonconservative Lagrangian system Γ to have a quasi-Hamiltonian representation as described in the previous section, there must be a function $V'=(\det J)^{-1}V$ such that $\mu=D_JV'$. But so long as we are concerned only with local considerations, this is equivalent to the condition $D_J\mu=0$.

V. COFACTOR SYSTEMS

We can now describe explicitly the class of nonconservative Lagrangian systems Γ we are analyzing: they are those determined by a metric tensor g which admits a special conformal Killing tensor J, and a 1-form μ on the configuration manifold Q such that $D_J\mu=0$. Systems of this type, in the Euclidean case, are what Lundmark calls cofactor systems, though he does not define them in quite the same way; we will use the same terminology even though it does not really match our definition.

Definition: A nonconservative system Γ on TQ, generated by a metric tensor field g and a 1-form μ on Q, is said to be a *cofactor system*, if g admits a nonsingular special conformal Killing tensor J and μ satisfies $D_J\mu=0$.

The results of the preceding sections can now be summarized as follows.

Theorem 2: A nonconservative system Γ on TQ determined by the couple (g,μ) on Q, has a quasi-Hamiltonian representation $F\hat{\Gamma}=P_J(dH)$, where J is a type (1,1) tensor field on Q, and H is a function on T^*Q quadratic in momenta, if and only if it is a cofactor system.

Proof: The argument developed in Sec. III proves the following assertion: the condition $F\hat{\Gamma}=P_J(dH)$ with H quadratic, assuming $N_J=0$, is equivalent to the requirements for having a cofactor system. But as we observed in Sec. IV, a special conformal Killing tensor automatically has zero torsion. Therefore, conversely, every cofactor system has a quasi-Hamiltonian representation of the desired type. □

Notice that for a special conformal Killing tensor

$$P_J = J^i_j \frac{\partial}{\partial p_j} \wedge X_i - \frac{1}{4}(\alpha_i p_j - \alpha_j p_i) \frac{\partial}{\partial p_i} \wedge \frac{\partial}{\partial p_j}.$$

Lundmark *et al.* approach the analysis of nonconservative Lagrangian systems by discussing the conditions under which such a system has a quadratic first integral $E = \frac{1}{2}A_{ij}u^i u^j + V$. Any cofactor system has a quasi-Hamiltonian representation with a quadratic Hamiltonian, which then is necessarily conserved, but the cofactor systems are a subclass of the non-conservative Lagrangian systems with quadratic integrals. We will complete the picture by identifying exactly which of the properties or conditions we have encountered entail that the function $E = \frac{1}{2}A_{ij}u^i u^j + V$ is a constant of the motion. We have

$$\Gamma(E) = \frac{1}{2}A_{ij|k}u^i u^j u^k - \left(A_{ij}M^j - \frac{\partial V}{\partial q^i} \right) u^i.$$

Thus, in order that $\Gamma(E)$ be zero, A must satisfy $A_{(ij|k)} = 0$, which is to say that it must be a Killing tensor. Moreover, we must have $A^*\mu = dV$. As we have seen, the first condition is satisfied automatically when A is the cofactor tensor of a special conformal Killing tensor (but of course there may be Killing tensors which are not of this type), and the restriction on μ then takes the form $\mu = D_J((\det J)^{-1}V)$. These remarks are supposed to explain the origins of the ''cofactor system.''

We will also take this opportunity to comment on the use of the term ''quasi-Lagrangian'' to describe nonconservative Lagrangian systems with quadratic integrals in the Euclidean case. Note that the commutator of any second-order equation field $\Gamma = u^i \partial/\partial q^i + f^i \partial/\partial u^i$ on TQ with $\partial/\partial u^j$ is given by

$$\left[\Gamma, \frac{\partial}{\partial u^j} \right] = -\frac{\partial}{\partial q^j} - \frac{\partial f^i}{\partial q^j} \frac{\partial}{\partial u^i}.$$

It follows that for any first integral E of Γ we will have

$$\Gamma\left(\frac{\partial E}{\partial u^j} \right) + \frac{\partial E}{\partial q^j} = -\frac{\partial f^i}{\partial u^j} \frac{\partial E}{\partial u^i}.$$

Hence, if the right-hand sides of the given equations (i.e., the functions f^i) are velocity independent, it will trivially be the case that every first integral E leads to a relation which formally looks like Euler–Lagrange equations with the wrong sign. In the Euclidean case, in Cartesian coordinates, the right-hand sides are indeed velocity independent. However, if the space is not Euclidean the equations will certainly not have this feature; indeed, they will not even in the Euclidean case if curvilinear coordinates are used. On the other hand, as we have already seen and will see further in what follows, the systems we are considering do have all the intrinsic features which explain the essential properties of what were called quasi-Lagrangian systems in Refs. 2–4. It seems to us, therefore, that the fact that the systems considered there have quasi-Lagrangian representations is not significant.

Given the prominent role played by the function $\frac{1}{2}A_{ij}u^i u^j + V$ in the concept of a cofactor system, one might naturally ask why one should not, to obtain a quasi-Hamiltonian representation, map TQ to T^*Q by $u^i \mapsto A_{ij}u^j$ rather than $u^i \mapsto g_{ij}u^j$. To do so is equivalent to carrying out the map $\hat{A}$ on T^*Q. Note that since $JA = (\det J)I$, and the torsion of a multiple of the identity vanishes, P_{JA} is certainly a Poisson map. The dynamics is transformed to $\hat{A}_*\hat{\Gamma}$. In Sec. II we showed that $P_{JA}(d(\hat{A}^{-1}{}^*H)) = \hat{A}_* P_J(dH)$. It follows that

$$(\det J)\hat{A}_*\hat{\Gamma} = \hat{A}_* P_J(dH) = P_{JA}(d(\hat{A}^{-1}{}^*H)),$$

which is to say that $\hat{A}_*\hat{\Gamma}$ is quasi-Hamiltonian with respect to $P_{JA}=P_{(\det J)I}$, with Hamiltonian

$$\hat{A}^{-1}*H=(\det J)^{-1}\hat{J}^*H=(\det J)^{-1}(\tfrac{1}{2}A^{ij}J^k_iJ^l_jp_kp_l+V)=\tfrac{1}{2}J^{ij}p_ip_j+(\det J)^{-1}V.$$

This formulation, in the Euclidean case, is essentially that given by the second of the two non-standard Poisson structures in Ref. 3.

Once one has noticed this trick one realizes that there are other possible ways of obtaining a quasi-Hamiltonian representation of a cofactor system. Indeed, by applying the map $\hat{J}^{-1}$ one sees that there is a quasi-Hamiltonian representation with respect to the standard Poisson structure. However, when we come to discuss cofactor pair systems these alternatives will not do, because they will associate different vector fields on T^*Q with the original vector field Γ on TQ: it is far better to stick with the single vector field $\hat{\Gamma}=\hat{g}_*\Gamma$ on T^*Q and represent it in quasi-Hamiltonian form with respect to two Poisson structures.

VI. HAMILTONIAN STRUCTURE FOR A COFACTOR SYSTEM

We now show how to represent a cofactor system as a Hamiltonian vector field with respect to a Poisson structure defined on an extended manifold. This involves an application of what is in fact a general construction which applies to any quasi-Hamiltonian vector field. This construction is the subject of the following theorem.

Theorem 3: Let Π be a Poisson bivector on a manifold M, and Z a vector field on M with the property that there is a nowhere-vanishing function F such that FZ is a Hamiltonian vector field with respect to Π, with Hamiltonian function H. Then there is a Poisson bivector $\hat{\Pi}$ on $M\times\mathbb{R}$ which projects onto Π, and a vector field, Hamiltonian with respect to $\hat{\Pi}$, whose restriction to the zero section is Z. Furthermore, $H+zF$ is a Casimir of $\hat{\Pi}$ (where z is the coordinate on $\mathbb{R}$).

Proof: Let π denote the projection $\pi:M\times\mathbb{R}\to M$. We can extend Π to $M\times\mathbb{R}$ simply by ignoring z: that is, for 1-forms on M we put $\Pi(\pi^*\alpha,\pi^*\beta)=\Pi(\alpha,\beta)$, while $\Pi(dz,\cdot)=0$ (so that z is a Casimir for Π). We consider a bivector of the form

$$\hat{\Pi}=\Pi+(Z+zW)\wedge\frac{\partial}{\partial z},$$

where W is a vector field independent of z (that is, $\langle W,dz\rangle=0$ and $\mathcal{L}_{\partial/\partial z}W=0$), and seek a W for which $\hat{\Pi}$ is Poisson. If we find one, then the Hamiltonian vector field corresponding to $-z$ will be $Z+zW$, agreeing with Z on $z=0$; and the projection of $\hat{\Pi}$ to M will be Π (or in other words π will be a Poisson map). We require that $[\hat{\Pi},\hat{\Pi}]=0$. Now for any bivector field Ω and vector fields X, Y,

$$[\Omega+X\wedge Y,\Omega+X\wedge Y]=[\Omega,\Omega]+2(\mathcal{L}_X\Omega\wedge Y-X\wedge\mathcal{L}_Y\Omega-X\wedge Y\wedge[X,Y]),$$

so we require that

$$\mathcal{L}_{Z+zW}\Pi\wedge\frac{\partial}{\partial z}=(Z+zW)\wedge\frac{\partial}{\partial z}\wedge(-W)=Z\wedge W\wedge\frac{\partial}{\partial z}.$$

For any bivector field Ω, function f and vector field V,

$$\mathcal{L}_{fV}\Omega=f\mathcal{L}_V\Omega-V\wedge S(df),$$

where S is the map of 1-forms corresponding to Ω. So $[\hat{\Pi},\hat{\Pi}]=0$ is equivalent to

$$(\mathcal{L}_Z\Pi+z\mathcal{L}_W\Pi)\wedge\frac{\partial}{\partial z}=Z\wedge W\wedge\frac{\partial}{\partial z}.$$

The conditions for $\hat{\Pi}$ to be Poisson are

$$\mathcal{L}_Z\Pi = Z\wedge W,\ \mathcal{L}_W\Pi = 0.$$

Now $Z = F^{-1}P(dH)$, where P is the Poisson map corresponding to Π, so (since the Lie derivative of Π by a Hamiltonian vector field is zero)

$$\mathcal{L}_Z\Pi = -P(dH)\wedge P(dF^{-1}) = F^{-2}P(dH)\wedge P(dF),$$

so both requirements are satisfied if

$$W = F^{-1}P(dF).$$

That is to say,

$$\hat{\Pi} = \Pi + (Z + zF^{-1}P(dF))\wedge\frac{\partial}{\partial z} = \Pi + F^{-1}P(dH + z\,dF)\wedge\frac{\partial}{\partial z}$$

is a Poisson tensor on $M\times\mathbb{R}$.

It follows by a direct calculation that $H+zF$ is a Casimir of $\hat{\Pi}$. □

It is useful to note, for future reference, that in fact the bivector $\Pi + (kZ + zW)\wedge\partial/\partial z$ is Poisson for every constant k; or what amounts to the same thing, $\hat{\Pi}$ is compatible with the (highly degenerate) Poisson bivector $Z\wedge\partial/\partial z$. This is established by the following computation:

$$\begin{aligned}\left[\hat{\Pi}, Z\wedge\frac{\partial}{\partial z}\right] &= \mathcal{L}_Z\hat{\Pi}\wedge\frac{\partial}{\partial z} - Z\wedge\mathcal{L}_{\partial/\partial z}\hat{\Pi}\\ &= \left(\mathcal{L}_Z\Pi + z[Z,W]\wedge\frac{\partial}{\partial z}\right)\wedge\frac{\partial}{\partial z} - Z\wedge\left(\left[\frac{\partial}{\partial z}, Z + zW\right]\wedge\frac{\partial}{\partial z}\right)\\ &= (Z\wedge W)\wedge\frac{\partial}{\partial z} - Z\wedge\left(W\wedge\frac{\partial}{\partial z}\right) = 0.\end{aligned}$$

Of course the Hamiltonian vector field corresponding to $-z$ for this modified Poisson structure restricts on $z=0$ not to Z but to a constant multiple of it.

Returning to the case of a given cofactor system, we may use the construction in the theorem above to represent $\hat{\Gamma}$ as the restriction to $z=0$ of a Hamiltonian vector field on $T^*Q\times\mathbb{R}$. The function F in this case is $\det J$, which is a function on Q. The Hamiltonian vector field associated with $\det J$ by Π_J is $-(d_J(\det J))^V = -(\det J)\alpha^V$. Thus,

$$\hat{\Pi}_J = \Pi_J + (\hat{\Gamma} - z\alpha^V)\wedge\frac{\partial}{\partial z},$$

or in other words

$$\hat{P}_J = J^i_j\frac{\partial}{\partial p_j}\wedge X_i - \tfrac{1}{4}(\alpha_i p_j - \alpha_j p_i)\frac{\partial}{\partial p_i}\wedge\frac{\partial}{\partial p_j} + g^{ij}p_j X_i\wedge\frac{\partial}{\partial z} - (M_i + z\alpha_i)\frac{\partial}{\partial p_i}\wedge\frac{\partial}{\partial z}.$$

This agrees with the Poisson structure for a cofactor system in the n-dimensional Euclidean case given in Ref. 2 and in two dimensions in Ref. 4, and is the obvious generalization once one has realized that introducing the metric involves using the basis adapted to the connection.

Note that the Hamiltonian representation of the given cofactor system on $T^*Q\times\mathbb{R}$ is

$$\hat{\Gamma} - z\alpha^V = \hat{\Gamma}_0 - (\mu + z\alpha)^V,$$

so it is obtained by a kind of deformation of the nonconservative forces.

VII. COFACTOR PAIR SYSTEMS

We now consider nonconservative Lagrangian systems which are of cofactor type in two ways—what Lundmark calls cofactor pair systems.

Suppose that the metric g admits two independent special conformal Killing tensors J and K. The condition for a given system $\Gamma=\Gamma_0-M^V$ to be of cofactor type (at least locally) with respect to both J and K is that $D_J\mu=D_K\mu=0$. We must examine the relation between the operators D_J and D_K.

If J and K are two special conformal Killing tensors then clearly $aJ+bK$ is also a special conformal Killing tensor for any constants a, b, with corresponding 1-form $a\alpha+b\beta$, where $\alpha=d(\mathrm{tr}\,J)$, $\beta=d(\mathrm{tr}\,K)$. Using the representation $D_J\theta=d_J\theta+\alpha\wedge\theta$ we see that

$$D_{aJ+bK}=aD_J+bD_K,$$

since $D_J{}^2=D_K{}^2=D_{aJ+bK}{}^2=0$, it follows that

$$D_JD_K+D_KD_J=0.$$

It is worth pointing out that it also follows that the Nijenhuis bracket $[J,K]$ vanishes, and that $d_J\beta+d_K\alpha=0$. (Incidentally, for any pair of tensors such that $[J,K]=0$, $d_J(\mathrm{tr}\,K)+d_K(\mathrm{tr}\,J)=d(\mathrm{tr}\,JK)$.)

There are functions V' and W' so that $\mu=D_JV'=D_KW'$, where $V=(\det J)V'$ and $W=(\det K)W'$ are the ''potentials'' in the quadratic integrals of Γ. These functions satisfy

$$D_JD_KW'=0 \text{ and } D_KD_JV'=0,$$

since $D_JD_K+D_KD_J=0$, they are both solutions of the same equation:

$$D_JD_K\phi=0.$$

This is the generalization of the so-called ''fundamental equation'' of Refs. 1, 2, and 4. In view of the anticommutativity of the operators D_J and D_K, the 2-form $D_JD_K\phi$ is obviously skew symmetric in J and K. It is given in terms of the components of J and K by

$$D_JD_K\phi=(J_i^kK_j^l\phi_{|kl}+\tfrac{3}{2}(J_i^k\beta_j-K_i^k\alpha_j)\phi_{|k}+((J_i^k\beta_k)_{|j}+\alpha_i\beta_j))dq^i\wedge dq^j.$$

The term involving a covariant derivative of $J^*\beta$ may not seem to have the required skew-symmetry property at first sight, but is essentially $d_J\beta$, which is equal to $-d_K\alpha$.

We leave it to the reader to verify that this covariant fundamental equation reduces exactly to the one Lundmark put forward in coordinates for the Euclidean case. It suffices to take for the matrix J an expression of the form $J_{ij}=aq_iq_j+b_iq_j+b_jq_i+c_{ij}$ (the position of the indices is rather irrelevant in the Euclidean case, so we write them here as lower indices); accordingly, $\alpha_i=2(aq_i+b_i)$.

We now establish the complete integrability of a cofactor pair system. Since $D_{aJ+bK}\mu=aD_J\mu+bD_K\mu=0$, the vector field $\hat{\Gamma}$ corresponding to the given cofactor pair system is the restriction to $z=0$ of the Hamiltonian vector field of $-z$ for the Poisson structure

$$\hat{\Pi}(a,b)=\Pi_{aJ+bK}+(\hat{\Gamma}-z(a\alpha^V+b\beta^V))\wedge\frac{\partial}{\partial z}$$

for every a and b. Note that this is not the same as

$$a\left(\Pi_J+(\hat{\Gamma}-z\alpha^V)\wedge\frac{\partial}{\partial z}\right)+b\left(\Pi_K+(\hat{\Gamma}-z\beta^V)\wedge\frac{\partial}{\partial z}\right)$$

except when $a+b=1$, so this does not define a Poisson pencil as written. This is a minor difficulty, which can be dealt with by adding $(a+b-1)\hat{\Gamma}\wedge\partial/\partial z$ to $\hat{\Pi}(a,b)$, and using the standard results about Poisson pencils to prove complete integrability; however, it seems interesting, and more pleasing, to establish complete integrability directly.

We write $A(a,b)$ for the cofactor tensor of $aJ+bK$. It is a homogeneous polynomial of degree $n-1$ in a, b (where $n=\dim Q$). Let $V(a,b)$ be a solution of

$$D_{aJ+bK}((\det(aJ+bK)^{-1}V(a,b)))=\mu$$

or equivalently $dV(a,b)=A(a,b)^*\mu$; it is again a homogeneous polynomial in a and b of degree $n-1$. We set

$$A(a,b)=\sum_{m=1}^{n} A_{(m)}a^{n-m}b^{m-1}, \quad V(a,b)=\sum_{m=1}^{n} V_{(m)}a^{n-m}b^{m-1},$$

and thereby define n functions $H_{(m)}$ on T^*Q, $m=1,2,\ldots,n$ by

$$H_{(m)}=\tfrac{1}{2}A^{ij}_{(m)}p_ip_j+V_{(m)}.$$

Note that $H_{(1)}$ is the Hamiltonian function for $(\det J)\hat{\Gamma}$ with respect to Π_J, and $H_{(n)}$ the Hamiltonian function for $(\det K)\hat{\Gamma}$ with respect to Π_K.

Theorem 4: The functions $H_{(m)}$ are first integrals of $\hat{\Gamma}$ which are in involution with respect to the Poisson brackets associated with Π_J and Π_K.

Proof: We know that $C(a,b)=H(a,b)+z\det(aJ+bK)=\frac{1}{2}A(a,b)^{ij}p_ip_j+V(a,b)+z\det(aJ+bK)$ is a Casimir of $\hat{\Pi}(a,b)$, and $\hat{\Gamma}-z(a\alpha^V+b\beta^V)$ is a Hamiltonian vector field, for every a and b. So in particular $(\hat{\Gamma}-z(a\alpha^V+b\beta^V))C(a,b)\equiv 0$. Now $H(a,b)=\Sigma_{m=1}^{n}H_{(m)}$. On setting $z=0$ we find that $H_{(m)}$ is a first integral of $\hat{\Gamma}$ for $m=1,2,\ldots,n$. Now set

$$\det(aJ+bK)=\sum_{l=0}^{n}\Delta_{(l)}a^{n-l}b^{l}.$$

It then follows from the fact that $C(a,b)$ is a Casimir that (on T^*Q)

$$\{\cdot,H_{(m)}\}_J+\{\cdot,H_{(m-1)}\}_K=\Delta_{(m)}\hat{\Gamma}$$

for $2\leqslant m\leqslant n$, while $\{\cdot,H_{(1)}\}_J=(\det J)\hat{\Gamma}$ and $\{\cdot,H_{(n)}\}_K=(\det K)\hat{\Gamma}$ (which just confirms that $\hat{\Gamma}$ is Hamiltonian up to a scalar factor for the Poisson brackets determined by both J and K). It follows that

$$\{H_{(r)},H_{(s)}\}_J+\{H_{(r)},H_{(s-1)}\}_K=\Delta_{(m)}\hat{\Gamma}(H_{(r)})=0$$

for $1\leqslant r\leqslant n$ and $2\leqslant s\leqslant n$, from which the usual kind of induction argument leads to the $H_{(m)}$ being in involution with respect to both Poisson brackets. □

We make some final observations now, which will establish a link between our new results and related work in Hamilton–Jacobi theory. The cofactor tensor of $aJ+bK$ is a Killing tensor for every a, b (or at least those for which $aJ+bK$ is nonsingular). It follows that $A_{(m)}$ is a Killing tensor for each m. In particular, if $K=I$, and if J has functionally independent eigenfunctions, we generate from the one special conformal Killing tensor n independent Killing tensors, one of which is g and another of which is the cofactor tensor of J; and since the eigenvectors of $aJ+bI$ are the same as the eigenvectors of J, these Killing tensors have the same eigenvectors. Furthermore, they commute pairwise in the sense of their corresponding quadratic functions having vanishing Poisson bracket (in this case, $\{\cdot,\cdot\}_K$ is the standard Poisson bracket). It follows that these Killing tensors form a Stäckel system (for full details see, Ref. 13). Moreover, $\hat{\Gamma}$ is the

Hamiltonian flow of the Hamiltonian $\frac{1}{2}g^{ij}p_ip_j+V$, where $D_JdV=0$; it then follows by results of Refs. 5 and 14 that the Hamilton–Jacobi equation for this Hamiltonian is separable in orthogonal coordinates.

The fact that the existence of a special conformal Killing tensor leads to the orthogonal separability of the Hamilton–Jacobi equation for the geodesic flow was first pointed out by Benenti in Ref. 9. The more general case, in which there is a potential, has been discussed from points of view close to that of this article in Refs. 5 and 14. In Ref. 14 a bi-Hamiltonian structure was introduced, essentially equivalent to the Poisson pencil $\hat{\Pi}_{aJ+bI}$. In Ref. 5 the special nature of the conformal Killing tensor which plays such a central role in the theory was investigated.

VIII. CONCLUSIONS

As is often the case, the generalization of the results of Refs. 1–4 has led to the clarification of several of the concepts and methods used in these papers. In particular, the Poisson structures introduced there have been shown to be examples of two general constructions: first, the construction of a Poisson–Nijenhuis structure on a cotangent bundle via the complete lift of a type (1,1) tensor with vanishing torsion, which is well known; and second, the ''lifting'' of a Poisson structure and a quasi-Hamiltonian vector field to an extended space which is the subject of Theorem 3 above. This latter result appears to be new. It should be noted that it is not dependent on the existence of a bi-Hamiltonian or quasi-bi-Hamiltonian structure, but only on a single quasi-Hamiltonian vector field. Nevertheless, it clearly has potential application in the field of quasi-bi-Hamiltonian systems (as defined for example in Ref. 15), of which the case $K=I$ discussed at the end of the last section is an example. Indeed, the results obtained here for a particular class of what might be called bi-quasi-Hamiltonian systems should be capable of generalization to provide a theory of such systems. We are currently investigating this possibility. It is noteworthy that the differential operators D_J and D_K play an important role here, so that the theory of cofactor pairs provides an example of a gauged bidifferential calculus in the sense of Ref. 12; this seems to us to be likely to be a feature of the general theory of bi-quasi-Hamiltonian systems we have in mind. Finally, from the opposite point of view as one might say, the properties of cofactor tensors of special conformal Killing tensors have not been noticed before in published accounts of Benenti's theory of inertia tensors and the orthogonal separability of the Hamilton–Jacobi equation, so far as we are aware. An article on this subject (Ref. 13), has been submitted for publication. In Ref. 14, Ibort *et al.* speculate that there is ''a deep relation, still to be worked out, between the geometry of Killing tensors on a Riemannian manifold and the geometry of a particular class of Poisson manifolds.'' It seems to us that the remarkable properties of special conformal Killing tensors form part of this deep geometrical structure.

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A family of completely integrable multi-Hamiltonian systems explicitly related to some celebrated equations

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By introducing a spectral problem with an arbitrary parameter, we derive a Kaup–Newell-type hierarchy of nonlinear evolution equations, which is explicitly related to many important equations such as the Kundu equation, the Kaup–Newell (KN) equation, the Chen–Lee–Liu (CLL) equation, the Gerdjikov–Ivanov (GI) equation, the Burgers equation, the modified Korteweg-deVries (MKdV) equation and the Sharma–Tasso–Olver equation. It is shown that the hierarchy is integrable in Liouville's sense and possesses multi-Hamiltonian structure. Under the Bargann constraint between the potentials and the eigenfunctions, the spectral problem is nonlinearized as a finite-dimensional completely integrable Hamiltonian system. The involutive representation of the solutions for the Kaup–Newell-type hierarchy is also presented. In addition, an N-fold Darboux transformation of the Kundu equation is constructed with the help of its Lax pairs and a reduction technique. According to the Darboux transformation, the solutions of the Kundu equation is reduced to solving a linear algebraic system and two first-order ordinary differential equations. It is found that the KN, CLL, and GI equations can be described by a Kundu-type derivative nonlinear Schrödinger equation involving a parameter. And then, we can construct the Hamiltonian formulations, Lax pairs and N-fold Darboux transformations for the Kundu, KN, CLL, and GI equations in explicit and unified ways. [DOI: 10.1063/1.1389288]

I. INTRODUCTION

It is well-known that given a properly chosen spectral problem, one can relate it to a hierarchy of nonlinear evolution equations. A central and difficult topic in the study of integrable systems is to find new Lax or Liouville integrable systems such as those associating with certain nonlinear evolution equations of physical significance.[1–10] Among them, three typical examples are Ablowitz-Kaup-Newell-Segur (AKNS), Wadati-Konno-Ichikawa (WKI), and KN hierarchies which contain the well-known Schrödinger equation, Korteweg–de Vries (KdV) equation, MKdV equation, Burgers equation, and KN equation as their special reductions. Especially, this approach plays an important role in the study of integrablity, Lax pair, conserved law, Hamiltonian structure, and Darboux transformation of nonlinear evolution equations. The demonstration of a bi-Hamiltonian structure for nonlinear evolution equations is a direct and elegant method of proving its complete integrability.[11–15] If a set of nonlinear evolution equations can be formulated as a Hamiltonian system in two distinct but compatible ways, then, by a theorem of Magri,[11,12] they rise to an infinite sequence of conserved Hamiltonians which are in involution with respect to either one of these two symplectic structures. Recently two other effective approaches that produce infinite-dimensional and finite-dimensional integrable Hamiltonian systems, respectively, also have been developed. The first one is the trace identity,[9] which is powerful for constructing infinite-dimensional Liouville integrable Hamiltonian systems. Starting from a properly spectral problem, many integrable hierarchies and their Hamiltonian structure have been obtained by applying this method.[9,10] The second one is called a nonlinearization technique,[16,17] which is also

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proved to be a powerful tool for obtaining new finite-dimensional integrable Hamiltonian systems from various soliton hierarchies. Under the Bargmann or Neumann constraints between the potentials and the eigenvalues which play a central role in the process of nonlinearization, the eigenvalue problem is nonlinearized as a finite-dimensional completely integrable system. The list covered the eigenvalue problems associated the well-known soliton hierarchies such as the AKNS, Jaulent-Miodek, KN examples, etc.[17–20]

The Darboux transformation method based Lax pairs have been proven to be one of the most fruitful algorithmic procedures to get explicit solutions of nonlinear evolution equations.[3,21] The first and successive Darboux transformations of trivial solutions are called single solitons and multi-solitons, respectively. The key for constructing a Darboux transformation is to expose a kind of covariant property that corresponding spectral problems possess. There are many tricks for getting explicit solutions to various soliton equations, including the KdV, Davey–Stewartson, self-dual Yang–Mills equations, etc.[21–28] In Refs. 22 and 23, a systematic method is presented to directly construct an explicit formula for N-fold Darboux transformation of AKNS hierarchy. This N-fold Darboux transformation formula can be interpreted as a nonlinear superposition of a single Darboux transformation. Moreover, the solutions of any systems in AKNS hierarchy are reduced to solving a linear algebraic system, which is very suitable for generating multi-soliton solutions by symbolic computation on a computer.

The nonlinear Schrödinger equation is one of the most generic soliton equations. To study the effect of higher order perturbations, various modifications and generalizations of the Schrödinger equation have been proposed and studied for years. Among them, there are four celebrated derivative nonlinear Schrödinger equations, which are the KN equation[6]

$$iq_t+q_{xx}+i(|q|^2q)_x=0, \tag{1}$$

the CLL equation[29,30]

$$iq_t+q_{xx}+i|q|^2q_x=0, \tag{2}$$

the GI equation[31,32]

$$iq_t+q_{xx}-iq^2q_x^*+\tfrac{1}{2}|q|^4q=0, \tag{3}$$

and the Kundu equation[32–34]

$$iq_t+q_{xx}+2i(2\delta+\alpha)|q|^2q_x+i(4\delta+\alpha)q^2q_x^*+\delta(4\delta+\alpha)|q|^4q=0, \tag{4}$$

where q^* denotes the complex conjugate of q. It is found that they may be transformed into each other by a gauge transformation, and the method of gauge transformation also can be applied to some generalized cases.[32,34] In recent years, the spectral problem, Hamiltonian structure, Painlevé property, exact solutions and other properties associated with the Kaup–Newell equation have been investigated in detail.[6,9,34,35] But little work has been done on the CLL, GI, and Kundu equations (2)–(4), since the corresponding results for these three equations may be obtained from KN equation (1) by some gauge transformation in principle.[33,35–37] However, it seems difficult to obtain their explicit results in this way, because we must solve integrable equation like (6) in practice. The integration will become very complicated with the increase of iterative times, especially in multi-soliton solutions.

The purpose of this article is to present some new explicit results on Eqs. (1)–(4) with the help of a spectral problem

$$y_x=Uy=\begin{pmatrix} -i\lambda^2-i\beta qr & \lambda q \\ \lambda r & i\lambda^2+i\beta qr \end{pmatrix}y, \tag{5}$$

where q, r are two potentials, and β is an arbitrary parameter. In the fact, the spectral problem (5) is a similar extension of the Kaup–Newell spectral problem.[6] By setting

$$\tilde{y}=\begin{pmatrix} \exp\left(-i\beta\int qr\,dx\right) & 0 \\ 0 & \exp\left(i\beta\int qr\,dx\right) \end{pmatrix} y,$$
$$q=\tilde{q}\exp\left(-2i\beta\int \tilde{q}\tilde{r}dx\right), \quad r=\tilde{r}\exp\left(2i\beta\int \tilde{q}\tilde{r}\,dx\right), \tag{6}$$

and by simple calculation, we know that the spectral problem (5) is equivalent to the standard Kaup–Newell spectral problem

$$\tilde{y}_x=\begin{pmatrix} -i\lambda^2 & \lambda\tilde{q} \\ \lambda\tilde{r} & i\lambda^2 \end{pmatrix}\tilde{y}. \tag{7}$$

In Ref. 38, for the special case of the spectral problem (5) ($\beta=\frac{1}{2}$), we ever derived a GI hierarchy and constructed an explicit Darboux transformation of the GI equation (1) by using a systematic technique. Here we would like to generalize these results and give some new and more general results. First, it interests us that the hierarchy corresponding to the spectral problem (5) is explicitly related to many important equations such as the Kundu, KN, CLL, GI, Burgers, MKdV, and Sharma–Tasso–Olver (STO) equations.[39–41] To our knowledge, except for the KN equation, the other six equations are not explicitly found in the Kaup–Newell hierarchy.[6,9] And only the GI and MKdV equations belong to the GI hierarchy.[38] Second, by introducing a modified function, we develop a more general method than that used in Refs. 23 and 38 in order to construct the explicit N-fold Darboux transformation for the Kundu equation (4). Third, it is found that the KN, CLL, and GI equations can be described by a Kundu-type equation. In this way, their Lax pairs, Hamiltonian formulations, and Darboux transformation are all given in a unified and explicit way.

This article is organized as follows. In Sec. II, we first derive Kaup–Newell-type hierarchy equations corresponding to the spectral problem (5). It is shown that the hierarchy is integrable in Liouville's sense and possesses multi-Hamiltonian structure by means of trace identity.[9] Then we show that several kinds of important equations such as Kundu, KN, CLL, GI, Burgers, MKdV, and STO equations all belong to the hierarchy as special reductions in Sec. III. In Sec. IV, through the nonlinearization of the eigenvalue, a completely integrable Bargmann system is obtained under a constraint between the potential and eigenfunctions. Moreover, the involutive solutions for the Kaup–Newell-type hierarchy is further constructed in Sec. V. In Sec. VI, a systematic technique is further developed to construct an explicit N-fold Darboux transformation for the coupled Kundu system with help of its Lax pairs. In this way, the solutions of the coupled Kundu equations are reduced to solving two linear algebraic systems and two first-order ordinary differential equations. The Darboux transformation of the coupled Kundu system is further reduced to the Darboux transformation of the Kundu equation via the reduction technique in Sec. VII.

II. THE KAUP–NEWELL-TYPE HIERARCHY AND ITS MULTI-HAMILTONIAN FORMULATION

We first solve the adjoint representation of spectral problem (5),

$$V_x=[U,V]=UV-VU,$$

with

$$V=\begin{pmatrix} a & b \\ c & -a \end{pmatrix}=\sum_{j=0}^{\infty}\begin{pmatrix} a_j & b_j \\ c_j & -a_j \end{pmatrix}\lambda^{-j},$$

and obtain the following recursive formulas:

$$a_{2j+1}=b_{2j}=c_{2j}=0,$$

$$a_{2jx}=qc_{2j+1}-rb_{2j+1}=-\beta qr(qc_{2j-1}-rb_{2j-1})-\tfrac{1}{2}i(qc_{2j-1x}+rb_{2j-1x}),$$

$$b_{2j+1}=\tfrac{1}{2}ib_{2j-1x}+iqa_{2j}-\beta qrb_{2j-1},$$

$$c_{2j+1}=-\tfrac{1}{2}ic_{2j-1x}+ira_{2j}-\beta qrc_{2j-1}.$$

The above recursion equations can be solved successively to deduce that by using Mathematica

$$a_0=-2i,\quad b_1=2q,\quad c_1=2r,\quad a_2=-iqr,$$

$$b_3=iq_x-(2\beta-1)q^2r,\quad c_3=-ir_x-(2\beta-1)qr^2,$$

$$a_4=\tfrac{1}{4}[2(rq_x-qr_x)+i(8\beta-3)q^2r^2],$$

$$b_5=\tfrac{1}{4}[-2q_{xx}-6i(2\beta-1)qrq_x-4i\beta q^2r_x+(8\beta^2-12\beta+3)q^3r^2],$$

$$c_5=\tfrac{1}{4}[-2r_{xx}+6i(2\beta-1)qrr_x+4i\beta r^2q_x+(8\beta^2-12\beta+3)q^2r^3], \tag{8}$$

$$a_6=\tfrac{1}{8}[2i(qr_{xx}+rq_{xx})+6(2\beta-1)(q^2rr_x-qr^2q_x)-2iq_xr_x-i\beta(24\beta^2-24\beta+5)q^3r^3],$$

and

$$\begin{pmatrix}c_{2j+1}\\ b_{2j+1}\end{pmatrix}=L_1L_2\begin{pmatrix}c_{2j-1}\\ b_{2j-1}\end{pmatrix},\quad j=1,2,\ldots, \tag{9}$$

where

$$L_1=\frac{1}{2}\begin{pmatrix}r\partial^{-1}r & -i+r\partial^{-1}q\\ i+q\partial^{-1}r & q\partial^{-1}q\end{pmatrix},\quad L_2=\begin{pmatrix}0 & \partial+2i\beta qr\\ \partial-2i\beta qr & 0\end{pmatrix}$$

are two skew-symmetric operators, that is, $L_1^*=-L_1$, $L_2^*=-L_2$.

Consider the auxiliary spectral problem

$$y_t=V^{(m)}y, \tag{10}$$

where

$$V^{(m)}=\begin{pmatrix}\Delta_m & 0\\ 0 & -\Delta_m\end{pmatrix}+\sum_{j=0}^{m}\begin{pmatrix}a_{2j}\lambda^{2(m-j)+2} & b_{2j+1}\lambda^{2(m-j)+1}\\ c_{2j+1}\lambda^{2(m-j)+1} & -a_{2j}\lambda^{2(m-j)+2}\end{pmatrix}.$$

Then the compatibility condition between (5) and (10) leads to

$$-i\beta(qr)_t=-i\beta(q_tr+r_tq)=\Delta_{mx},$$

$$q_t=b_{2m+1x}+2i\beta qrb_{2m+1}+2q\Delta_m,$$

$$r_t=c_{2m+1x}-2i\beta qrc_{2m+1}-2r\Delta_m,$$

from which we obtain

$$\Delta_m=-i\beta\partial^{-1}(qc_{2m+1x}+rb_{2m+1x})-2\beta^2\partial^{-1}qr(qc_{2m+1}-rb_{2m+1})=2\beta a_{2(m+1)}$$

and

$$\begin{pmatrix} q_t \\ r_t \end{pmatrix} = L_3 L_2 \begin{pmatrix} c_{2m+1} \\ b_{2m+1} \end{pmatrix}, \tag{11}$$

where

$$L_3 = \begin{pmatrix} 1-2i\beta q\partial^{-1} r & -2i\beta q\partial^{-1} q \\ 2i\beta r\partial^{-1} r & 1+2i\beta r\partial^{-1} q \end{pmatrix}.$$

By using (9) and (11), the desired Kaup–Newell-type hierarchy associated with spectral problem (5) is obtained as follows:

$$\begin{pmatrix} q_t \\ r_t \end{pmatrix} = (L_3 L_2) \begin{pmatrix} c_{2m+1} \\ b_{2m+1} \end{pmatrix} = (L_3 L_2)(L_1 L_2) \begin{pmatrix} c_{2m-1} \\ b_{2m-1} \end{pmatrix}$$

$$= (L_3 L_2)(L_1 L_2)^m \begin{pmatrix} 2r \\ 2q \end{pmatrix}, \quad m = 1,2,\ldots . \tag{12}$$

In the following we will establish the multi-Hamiltonian structure for the hierarchy (12) and show it is integrable in Liouville's sense. In order to apply trace identity,[9,10] we need to rewrite (12) in another form. Let

$$G_{2j+1} = (c_{2j+1} - 2i\beta r a_{2j}, b_{2j+1} - 2i\beta q a_{2j})^T.$$

Noting that $a_{2j} = \partial^{-1}(q c_{2j+1} - r b_{2j+1})$, then we have

$$(c_{2j+1}, b_{2j+1})^T = L_3^* G_{2j+1}, \quad j \geqslant 0,$$

where L_3^* denotes the conjugation operator of L_3. In this way, the evolution hierarchy (12) is written in the form

$$u_t = J G_{2m+1} = J L G_{2m-1} = \cdots = J L^m G_1, \tag{13}$$

where $G_1 = (2(1-2\beta)r, 2(1-2\beta)q)^T$, $u = (q,r)^T$, $J = L_3 L_2 L_3^*$, $L = {L_3^*}^{-1} L_1 L_2 L_3^*$.

Proposition 1: All operators JL^k $(k = 0,1,2,\ldots,m)$ are skew-symmetric.

Proof: Since L_1 and L_2 are skew-symmetric, it is clear that $J = L_3 L_2 L_3^*$ and $JL = L_3 L_2 L_1 L_2 L_3^*$ are skew-symmetric. Suppose that JL^{k-1} is skew-symmetric. Then it holds that

$$(JL^k)^* = (JL^{k-1}L)^* = L^*(JL^{k-1})^* = -L^* J L^{k-1}$$

$$= L^* J^* L^{k-1} = -JLL^{k-1} = -JL^k,$$

which implies that JL^k is skew-symmetric. The proof is completed.

Following the notation used in Ref. 9, we take Killing–Cartan form $\langle A,B \rangle$ is $tr(AB)$. Then direct calculation gives

$$\left\langle V, \frac{\partial U}{\partial q} \right\rangle = c\lambda - 2i\beta r a, \quad \left\langle V, \frac{\partial U}{\partial r} \right\rangle = b\lambda - 2i\beta q a,$$

$$\left\langle V, \frac{\partial U}{\partial \lambda} \right\rangle = -4ia\lambda + rb + qc.$$

By using trace identity, we have

$$\frac{\delta}{\delta u}(-4ia\lambda + rb + qc) = \lambda^{-\gamma} \frac{\partial}{\partial \lambda}(\lambda^{\gamma}(c\lambda - ira, b\lambda - iqa)^T),$$

which is equivalent to

$$\frac{\delta}{\delta u}(-4ia_{2m+2}+rb_{2m+1}+qc_{2m+1})=(-2m+\gamma)G_{2m+1}. \tag{14}$$

To fix the γ in (14), we let $m=0$ and find $\gamma=0$. Therefore we conclude that

$$G_{2m+1}=\frac{\delta H_m}{\delta u}, \tag{15}$$

where

$$H_0=2qr, \quad H_m=\frac{4ia_{2m+2}-rb_{2m+1}-qc_{2m+1}}{2m}, \quad m\geqslant 1. \tag{16}$$

Combining (13) with (15) gives the desired multi-Hamiltonian formulation of the hierarchy (12)

$$u_t=J\frac{\delta H_m}{\delta u}=JL\frac{\delta H_{m-1}}{\delta u}=\cdots=JL^m\frac{\delta H_0}{\delta u}, \quad m=1,2,\ldots . \tag{17}$$

Finally, we discuss the integrablity of the hierarchy (12) or (17). It is crucial to show the existence of infinite involutive conserved densities. Usually the inner product between two functions f and g is defined by $(f,g)=\int f\cdot g\,dx$, and the Poisson bracket is defined by $\{f,g\}=(\delta f/\delta u, J\,\delta g/\delta u)$. In particular, f and g are called involutive if $\{f,g\}=0$.

Proposition 2: The Hamiltonian functions $\{H_m\}$ $(m=0,1,\ldots)$ defined by (16) constitute common conserved densities for the whole hierarchy (17).

Proof: By using Proposition 1, we find that

$$\{H_n,H_m\}=\left(\frac{\delta H_n}{\delta u},J\frac{\delta H_m}{\delta u}\right)=(L^nG_1,JL^mG_1)=(L^nG_1,L^*JL^{m-1}G_1)$$

$$=(L^{n+1}G_1,JL^{m-1}G_1)=\{H_{n+1},H_{m-1}\}.$$

Repeating the previous argument gives

$$\{H_n,H_m\}=\{H_m,H_n\}=\{H_{m+n},H_0\}. \tag{18}$$

On the other hand, we find

$$\{H_m,H_n\}=(L^mG_1,JL^nG_1)=(J^*L^mG_1,L^nG_1)=-\{H_n,H_m\}. \tag{19}$$

Then combining (18) with (19) leads to

$$\{H_m,H_n\}=0,$$

which implies that $\{H_m\}$ are in involution. Furthermore, we have

$$\left(\int H_m\,dx\right)_t=\left(\frac{\delta H_m}{\delta u},u_t\right)=\left(\frac{\delta H_m}{\delta u},J\frac{\delta H_n}{\delta u}\right)=\{H_m,H_n\}=0,$$

which shows that $\{H_m\}$ are also conserved densities. The proof is completed.

In summary, we arrive at the followings

Theorem 1: (i) The hierarchy (17) is an integrable Hamiltonian system in the Liouville sense. (ii) The Hamiltonain functions $\{H_m\}$ are conserved densities of whole hierarchy (17) and they are involutive in pairs.

III. A REDUCTION AND SOME IMPORTANT EQUATIONS FROM THE KAUP–NEWELL-TYPE HIERARCHY

To indicate the interest of our Kaup–Newell-type hierarchy (12), we provide a reduction and some important equations that contain in the hierarchy and give explicit expressions of Hamiltonian structure and Lax pairs for these equations.

Example 1: As $\beta=0$, the spectral problem (5) reduces to Kaup–Newell spectral problem (7), and the hierarchy (12) leads to the well-known Kaup–Newell hierarchy

$$u_t=JL^m\begin{pmatrix}2r\\2q\end{pmatrix},\quad m=1,2,\ldots, \tag{20}$$

where

$$J=L_3L_2L_3^*|_{\beta=0}=\begin{pmatrix}0&\partial\\\partial&0\end{pmatrix},$$

$$L=L_3L_2L_1L_2L_3^*|_{\beta=0}=\frac{1}{2}\begin{pmatrix}\partial q\partial^{-1}q\partial & i\partial^2+\partial q\partial^{-1}r\partial\\ -i\partial^2+\partial r\partial^{-1}q\partial & \partial r\partial^{-1}r\partial\end{pmatrix}.$$

Obviously J and L are two skew-symmetric operators. The Kaup–Newell hierarchy (20) can be cast in multi-Hamiltonian formulations

$$u_t=J\frac{\delta H_m}{\delta u}=JL\frac{\delta H_{m-1}}{\delta u}=\cdots=JL^m\frac{\delta H_0}{\delta u},\quad m=1,2,\ldots,$$

where H_m are determined by (16) with $\beta=0$.

Example 2: The first system of the hierarchy (12) ($m=1$) is the coupled Kundu system

$$\begin{aligned}&iq_t+q_{xx}+2i(2\beta-1)qrq_x+i(4\beta-1)q^2r_x+\beta(4\beta-1)q^3r^2=0,\\&ir_t-r_{xx}+2i(2\beta-1)qrr_x+i(4\beta-1)r^2q_x-\beta(4\beta-1)q^2r^3=0.\end{aligned} \tag{21}$$

It can be reduced to the Kundu-type equation as $r=-q^*$,

$$iq_t+q_{xx}-2i(2\beta-1)|q|^2q_x-i(4\beta-1)q^2q_x^*+\beta(4\beta-1)|q|^4q=0, \tag{22}$$

which is the same with the equation (4) for $\delta=-\beta$, $\alpha=1$. As $\beta=0$, $\beta=\frac{1}{4}$ and $\beta=\frac{1}{2}$, Eq. (22) is separately reduced to the KN, CLL, and GI equations (1)–(3). Setting $r=i$, $\beta=\frac{1}{4}$ in system (21), we get a new complex Burgers equation

$$iq_t+q_{xx}+qq_x=0,$$

which becomes a real version if we let $i\lambda\to\lambda$ in the spectral problem (5).

Now according to Theorem 1, we conclude that Kundu system (21) is Liouville integrable and possesses the bi-Hamiltonian structure

$$u_t=J\frac{\delta H_1}{\delta u}=JL\frac{\delta H_0}{\delta u},$$

where Hamiltonian functions H_0 and H_1 are

$$H_0=2qr, \quad H_1=\tfrac{1}{2}[i(rq_x-qr_x)-(4\beta-1)q^2r^2]. \tag{23}$$

The Lax pairs corresponding to the system (21) may be given by the spectral problem (5) and the auxiliary problem

$$y_t=V^{(1)}y, \quad V^{(1)}=\begin{pmatrix} v_{11}^{(1)} & v_{12}^{(1)} \\ v_{21}^{(1)} & -v_{11}^{(1)} \end{pmatrix}, \tag{24}$$

with

$$v_{11}^{(1)}=-2i\lambda^4-iqr\lambda^2+\beta(rq_x-qr_x)+\tfrac{1}{2}i\beta(8\beta-3)q^2r^2,$$

$$v_{12}^{(1)}=2q\lambda^3+[iq_x-(2\beta-1)q^2r]\lambda, \quad v_{21}^{(1)}=2r\lambda^3+[-ir_x-(2\beta-1)qr^2]\lambda.$$

Example 3: With the help of Mathematica, we easily find that the second system of the hierarchy (12) $(m=2)$ is

$$\begin{aligned} &q_t+\tfrac{1}{4}[2q_{xxx}+6i(2\beta-1)r(qq_x)_x+6i(4\beta-1)qq_xr_x-6(2\beta-1)(4\beta-1)q^3rr_x \\ &\quad -3(8\beta^2-12\beta+3)q^2r^2q_x+4i\beta(2\beta-1)(4\beta-1)q^4r^3]=0, \\ &r_t+\tfrac{1}{4}[2r_{xxx}-6i(2\beta-1)q(rr_x)_x-6i(4\beta-1)rq_xr_x-6(2\beta-1)(4\beta-1)r^3qq_x \\ &\quad -3(8\beta^2-12\beta+3)q^2r^2r_x-4i\beta(2\beta-1)(4\beta-1)q^3r^4]=0, \end{aligned} \tag{25}$$

which reduces to the MKdV equation for $r=2$, $\beta=\frac{1}{2}$,

$$q_t+\tfrac{1}{2}(q_{xxx}+6q^2q_x)=0,$$

and the complex STO equation for $r=2$, $\beta=\frac{1}{4}$,

$$q_t+\tfrac{1}{2}[q_{xxx}-3i(qq_x)_x-3q^2q_x]=0. \tag{26}$$

If we let $i\lambda\to\lambda$ in the spectral problem (5), then we will get the real version of the STO equation that was studied by Olver and Gudkov:[39,41]

$$q_t+\tfrac{1}{2}[q_{xxx}-3(qq_x)_x-3q^2q_x]=0.$$

The system (25) is Liouville integrable and possesses the tri-Hamiltonian structure

$$u_t=J\frac{\delta H_2}{\delta u}=JL\frac{\delta H_1}{\delta u}=JL^2\frac{\delta H_0}{\delta u},$$

where Hamiltonian functions H_0, H_1 are determined by (23), and

$$H_2=\tfrac{1}{4}(4ia_6-rb_5-qc_5),$$

with a_6, b_5 and c_5 given by (8).

The Lax pairs corresponding to the system (25) are given by the spectral problem (5) and an auxiliary problem

$$y_t=V^{(2)}y=\begin{pmatrix} v_{11}^{(2)} & v_{12}^{(2)} \\ v_{21}^{(2)} & -v_{11}^{(2)} \end{pmatrix}y,$$

with

$$v_{11}^{(2)}=-2i\lambda^6-iqr\lambda^4+\tfrac{1}{4}[2(qr_x-rq_x)+i(8\beta-3)q^2r^2]\lambda^2+2\beta a_6,$$

$$v_{12}^{(2)}=2q\lambda^5+[iq_x-(2\beta-1)q^2r]\lambda^3+b_5\lambda,$$

$$v_{21}^{(2)}=2r\lambda^5+[-ir_x-(2\beta-1)qr^2]\lambda^3+c_5\lambda.$$

IV. A COMPLETELY INTEGRABLE BARGMANN SYSTEM

Let $\lambda_j(j=1,\ldots,N)$ be different eigenvalues of Eq. (5), and (ψ_j,ϕ_j) be associated eigenfunctions. Then the functional gradient λ_j with respect to $u=(q,r)^T$ is

$$\frac{\delta\lambda_j}{\delta u}=\left(\frac{\delta\lambda_j}{\delta q},\frac{\delta\lambda_j}{\delta r}\right)^T=\gamma_j^{-1}(\lambda_j\phi_j^2-2i\beta r\psi_j\phi_j,-\lambda_j\psi_j^2-2i\beta q\psi_j\phi_j)^T,$$

where $\gamma_j=\int(q\phi_j^2-r\psi_j^2+4i\lambda_j\psi_j\phi_j)\,dx$.

Proposition 3: J and $K=JL$ are Lenard's pair of operators

$$K\frac{\delta\lambda_j}{\delta u}=\lambda_j^2J\frac{\delta\lambda_j}{\delta u}, \tag{27}$$

and $\{G_{2j+1}\}$ are Lenard's sequence

$$JG_{2j+3}=KG_{2j+1},\quad j=0,1,\ldots. \tag{28}$$

Proof: Making use of the spectral problem (5), direct verification indicates that

$$L_3^*\frac{\delta\lambda_j}{\delta u}=\lambda_j\begin{pmatrix}\phi_j^2\\-\psi_j^2\end{pmatrix}, \tag{29}$$

$$L_1L_2\begin{pmatrix}\phi_j^2\\-\psi_j^2\end{pmatrix}=\lambda_j^2\begin{pmatrix}\phi_j^2\\-\psi_j^2\end{pmatrix}. \tag{30}$$

Substituting (29) into (30) and multiplying L_3L_2 on both sides of it, then (27) is obtained. Obviously (28) holds according to (13).

Consider the Bargmann constraint

$$G_1=\sum_{j=1}^{N}\gamma_j\frac{\delta\lambda_j}{\delta u}, \tag{31}$$

or equivalently

$$q=-\frac{\langle\wedge\psi,\psi\rangle}{2(1-2\beta+i\beta\langle\psi,\phi\rangle)},\quad r=\frac{\langle\wedge\phi,\phi\rangle}{2(1-2\beta+i\beta\langle\psi,\phi\rangle)}, \tag{32}$$

where $\psi=(\psi_1,\ldots,\psi_N)^T,\phi=(\phi_1,\ldots,\phi_N)^T,\wedge=\mathrm{diag}(\lambda_1,\ldots,\lambda_N)$, and $\langle\cdot,\cdot\rangle$ is the standard inner product in R^N. Under the Bargmann constraint (32), Eq. (5) is nonlinearized into a finite-dimensional Hamiltonian system

$$\begin{aligned}\psi_x&=-i\wedge^2\psi+\frac{i\beta\psi\langle\wedge\psi,\psi\rangle\langle\wedge\phi,\phi\rangle}{4(1-2\beta+i\beta\langle\psi,\phi\rangle)^2}-\frac{\wedge\phi\langle\wedge\psi,\psi\rangle}{2(1-2\beta+i\beta\langle\psi,\phi\rangle)}=-\frac{\partial H}{\partial\phi},\\ \phi_x&=i\wedge^2\phi-\frac{i\beta\phi\langle\wedge\psi,\psi\rangle\langle\wedge\phi,\phi\rangle}{4(1-2\beta+i\beta\langle\psi,\phi\rangle)^2}+\frac{\wedge\psi\langle\wedge\phi,\phi\rangle}{2(1-2\beta+i\beta\langle\psi,\phi\rangle)}=\frac{\partial H}{\partial\psi},\end{aligned} \tag{33}$$

whose Hamiltonian function H is

$$H=\langle i\wedge^2\psi,\phi\rangle+\frac{\langle\wedge\psi,\psi\rangle\langle\wedge\phi,\phi\rangle}{2(1-2\beta+i\beta\langle\psi,\phi\rangle)}. \tag{34}$$

The Poisson bracket of two functions in sympletic space $(R^{2N},d\psi\wedge d\phi)$ is defined as

$$(F,G)=\sum_{j=1}^{N}\left(\frac{\partial F}{\partial\psi_j}\frac{\partial G}{\partial\phi_j}-\frac{\partial F}{\partial\phi_j}\frac{\partial G}{\partial\psi_j}\right)=\left\langle\frac{\partial F}{\partial\psi},\frac{\partial G}{\partial\phi}\right\rangle-\left\langle\frac{\partial F}{\partial\phi},\frac{\partial G}{\partial\psi}\right\rangle,$$

which is skew-symmetric, bilinear and satisfies the Jacobi identity. In particular, F and G are called in involution if $(F,G)=0$. Now we consider the function system

$$F_m=2(1-2\beta+i\beta\langle\psi,\phi\rangle)\langle\wedge^{2m+2}\psi,\phi\rangle+\frac{1}{2}\sum_{j=0}^{m}\begin{vmatrix}\langle\wedge^{2(m-j)+1}\psi,\psi\rangle & \langle\wedge^{2(m-j)+2}\psi,\phi\rangle\\ \langle\wedge^{2j}\psi,\phi\rangle & \langle\wedge^{2j+1}\phi,\phi\rangle\end{vmatrix},$$

$$m=0,1,\ldots. \tag{35}$$

Proposition 4: The inner product $\langle\partial F_m/\partial\psi,\partial F_n/\partial\phi\rangle$ is symmetrical about m and n, i.e.,

$$\left\langle\frac{\partial F_m}{\partial\psi},\frac{\partial F_n}{\partial\phi}\right\rangle=\left\langle\frac{\partial F_n}{\partial\psi},\frac{\partial F_m}{\partial\phi}\right\rangle. \tag{36}$$

Proof: Noticing that

$$\begin{aligned}\frac{\partial F_m}{\partial\psi}&=2i\beta\phi\langle\wedge^{2m+2}\psi,\phi\rangle+(2+i\langle\psi,\phi\rangle)\wedge^{2m+2}\phi+\sum_{j=1}^{m}(\langle\wedge^{2(m-j)+1}\phi,\phi\rangle\wedge^{2j+1}\psi\\&\quad-\langle\wedge^{2(m-j)+2}\psi,\phi\rangle\wedge^{2j}\phi),\\\frac{\partial F_n}{\partial\phi}&=2i\beta\psi\langle\wedge^{2n+2}\psi,\phi\rangle+(2+i\langle\psi,\phi\rangle)\wedge^{2n+2}\psi+\sum_{j=1}^{m}(\langle\wedge^{2(n-j)+1}\psi,\psi\rangle\wedge^{2j+1}\phi\\&\quad-\langle\wedge^{2(n-j)+2}\psi,\phi\rangle\wedge^{2j}\psi).\end{aligned} \tag{37}$$

Through a series of direct calculations, it is easy to see that $\langle\partial F_m/\partial\psi,\partial F_n/\partial\phi\rangle$ is the sum of the symmetrical items about m and n. So (36) is proved.

Proposition 5: The functions defined by (35) are in involution in pair

$$(F_m,F_n)=0.$$

Proof: By Proposition 4, we have

$$\begin{aligned}(F_m,F_n)&=\left\langle\frac{\partial F_m}{\partial\psi},\frac{\partial F_n}{\partial\phi}\right\rangle-\left\langle\frac{\partial F_m}{\partial\phi},\frac{\partial F_n}{\partial\psi}\right\rangle\\&=\left\langle\frac{\partial F_n}{\partial\psi},\frac{\partial F_m}{\partial\phi}\right\rangle-\left\langle\frac{\partial F_m}{\partial\phi},\frac{\partial F_n}{\partial\psi}\right\rangle=0.\end{aligned}$$

Proposition 6: $(H,F_m)=0$.

Proof: As we did before, making use of (34) and (37) and through direct calculation, we have

$$(H,F_m)=\left\langle\frac{\partial H}{\partial\psi},\frac{\partial F_m}{\partial\phi}\right\rangle-\left\langle\frac{\partial H}{\partial\phi},\frac{\partial F_m}{\partial\psi}\right\rangle=0.$$

In summary, we conclude the following.

Theorem 2: The Hamiltonian system defined by (33) is completely integrable in the Liouville sense in the symplectic manifold $(R^{2N}, d\psi \wedge d\phi)$.

Theorem 3: Let (ψ, ϕ) be a solution of Bargmann system (33). Then q and r defined by (32) satisfy a stationary Kaup–Newell-type equation

$$X_{2N+1} + c_1 X_{2N-1} + \cdots + c_N X_1 = 0, \tag{38}$$

where $X_{2j+1} = JG_{2j+1}$, $j = 0,1,\ldots,N$, and $c_1, c_2, \ldots, c_N$ are suitably chosen constants.

Proof: Operating with $(J^{-1}K)^k$ upon the expression of (31) and in virtue of (27) and (28), we have

$$G_{2k+1} + \beta_1 G_{2k-1} + \cdots + \beta_k G_1 + \beta_{k+1} G_{-1} = \sum_{j=1}^{N} \gamma \lambda_j^{2k} \gamma_j \frac{\delta \lambda_j}{\delta u}, \tag{39}$$

where $\beta_1, \beta_2, \ldots, \beta_{k+1}$ are arbitrary constants, $G_{-1} = (0,0)^T$, and $\partial^{-1} 0 = 1$. Consider the polynomial

$$P(\lambda) = \prod_{j=1}^{N} (\lambda - \lambda_j^2) = p_0 \lambda^N + \cdots + p_N, \quad p_0 = 1.$$

Acting with the operator $J\Sigma_{k=1}^{N} p_{N-k}$ on (39), we have (38), where $c_1, \ldots, c_N$ depend on $\beta_1, \ldots, \beta_{k+1}$ and $\lambda_1, \ldots, \lambda_N$.

V. INVOLUTIVE SOLUTIONS OF KAUP–NEWELL-TYPE HIERARCHY

The involutive solutions of Kaup–Newell-type hierarchy associated with Bargmann system (33) can be further given. Consider the canonical system of F_m-flow

$$(F_m): \quad \begin{pmatrix} \psi_{t_m} \\ \phi_{t_m} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial F_m}{\partial \psi} \\ \dfrac{\partial F_m}{\partial \phi} \end{pmatrix} = I \nabla F_m, \quad I = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix}, \tag{40}$$

where I_N is an $N \times N$ unit matrix. Let $g_m^{t_m}$ denote the solution operator of the initial value problem (40). Then the solutions of Eq. (40) are expressed as

$$\begin{pmatrix} \psi_{t_m} \\ \phi_{t_m} \end{pmatrix} = g_m^{t_m} \begin{pmatrix} \psi(0) \\ \phi(0) \end{pmatrix}.$$

Since any two F_k, F_l are in involution, we have[18,42] the following.

Proposition 7: (i) Any two canonical system (F_k), (F_l) are compatible. (ii) The Hamiltonian phase-flows $g_k^{t_m}$ and $g_m^{t_l}$ commute.

Denote the flow variables of (H) and (F_m) by $x = t_0$ and $t = t_m$, respectively. Then the involutive solution of the consistent (H) and (F_m),

$$\begin{pmatrix} \psi_{x,t_m} \\ \phi_{x,t_m} \end{pmatrix} = g_0^x g_m^{t_m} \begin{pmatrix} \psi(0,0) \\ \phi(0,0) \end{pmatrix},$$

is a smooth function of (x, t_m) in view of the commutativity of flow g_0^x and $g_m^{t_m}$.

Theorem 4: Let $(\psi(x,t_m), \phi(x,t_m))^T$ be an involutive solution of the consistent system (H), (F_m), and

$$q(x,t_m)=-\frac{\langle \wedge\psi,\psi\rangle}{2(1-2\beta+i\beta\langle\psi,\phi\rangle)},\quad r(x,t_m)=\frac{\langle \wedge\phi,\phi\rangle}{2(1-2\beta+i\beta\langle\psi,\phi\rangle)}.$$

Then we have (i) the equations (H), (F_m) are reduced to the spatial part and the time part, respectively, of Lax pairs for the high-order generalized Kaup–Newell equations

$$\begin{pmatrix}\psi_x\\ \phi_x\end{pmatrix}=\begin{pmatrix}-i\wedge^2-i\beta qr & \wedge q\\ \wedge r & i\wedge^2+i\beta qr\end{pmatrix}\begin{pmatrix}\psi\\ \phi\end{pmatrix},\tag{41}$$

$$\begin{pmatrix}\psi_{t_m}\\ \phi_{t_m}\end{pmatrix}=\sum_{j=0}^{m}c_jV_{\wedge}^{(m-j)}\begin{pmatrix}\psi\\ \phi\end{pmatrix},\tag{42}$$

where $V_{\wedge}^{(m-j)}$ is determined by (10) in which λ is replaced by $\wedge=\mathrm{diag}(\lambda_1,...,\lambda_N)$. (ii) $q(x,t_m)$ and $r(x,t_m)$ satisfy the high-order Kundu equation

$$(q_{t_m},r_{t_m})=X_{2m+1}+c_1X_{2m-1}+\cdots+c_mX_1.\tag{43}$$

Proof: Obviously (41) holds from (33) and (34). Making use of (28), (33) and (38), direct and tedious calculation leads to (42) and (43).

VI. DARBOUX TRANSFORMATION

In this section, we shall construct an N-fold Darboux transformation for the coupled Kundu system (21). The Darboux transformation is actually a special gauge transformation

$$\tilde{y}=Ty\tag{44}$$

of the solutions of the Lax pairs (5) and (24). It is required that $\tilde{y}$ also satisfies Lax pairs (5) and (24) with some $\tilde{U}$ and $\tilde{V}^{(1)}$, i.e.,

$$\tilde{y}_x=\tilde{U}\tilde{y},\quad \tilde{U}=(T_x+TU)T^{-1},\tag{45}$$

$$\tilde{y}_t=\tilde{V}^{(1)}\tilde{y},\quad \tilde{V}^{(1)}=(T_t+TV^{(1)})T^{-1}.\tag{46}$$

By cross differentiating (45) and (46), we get

$$\tilde{U}_t-\tilde{V}_x^{(1)}+[\tilde{U},\tilde{V}^{(1)}]=T(U_t-V_x^{(1)}+[U,V^{(1)}])T^{-1},\tag{47}$$

which implies that in order to make system (21) invariant under the gauge transformation (44), we should require $\tilde{U}$ and $\tilde{V}^{(1)}$, have the same forms as U and $V^{(1)}$, respectively. At the same time the old potentials q and r in U, $V^{(1)}$ will be mapped into new potentials $\tilde{q}$ and $\tilde{r}$ in $\tilde{U}$, $\tilde{V}^{(1)}$. This process can be done continually and usually it may yield a series of multi-soliton solutions. Based on the idea,[23,38] we can construct an N-fold Darboux transformation for coupled Kundu system (21) as follows:

Let $(\phi_1(x,t,\lambda),\phi_2(x,t,\lambda))^T$ and $(\psi_1(x,t,\lambda),\psi_2(x,t,\lambda))^T$ be two basic solutions of spectral problem (5) and (24), and use them to define two linear algebraic systems for A_k, B_k, C_k and D_k $(0\leqslant k\leqslant N-1)$:

$$\sum_{k=0}^{N-1}(A_k+\alpha_j\lambda_jB_k)\lambda_j^{2k}=-\lambda_j^{2N},\quad 1\leqslant j\leqslant 2N,\tag{48}$$

$$\sum_{k=0}^{N-1}(\lambda_jC_k+\alpha_jD_k)\lambda_j^{2k}=-\alpha_j\lambda_j^{2N},\quad 1\leqslant j\leqslant 2N,\tag{49}$$

with

$$\alpha_j=\frac{\phi_2(\lambda_j)-\gamma_j\psi_2(\lambda_j)}{\phi_1(\lambda_j)-\gamma_j\psi_1(\lambda_j)},\quad 1\leqslant j\leqslant 2N, \tag{50}$$

where λ_j and γ_j are some parameters suitably chosen, such that determinants of the coefficients for (48) and (49) are nonzero. Hence A_k, B_k, C_k, and D_k are uniquely determined by (48) and (49). Now we let

$$T=\begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda)\end{pmatrix}=Q\left(I\lambda^{2N}+\sum_{k=0}^{N-1}(Q_{2k}+\lambda Q_{2k+1})\lambda^{2k}\right), \tag{51}$$

which is a $(2N)$th order polynomial in λ with matrix coefficient, and

$$Q=\begin{pmatrix}\delta_N & 0\\ 0 & 1/\delta_N\end{pmatrix},\quad I=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},$$

$$Q_{2k}=\begin{pmatrix}A_k & 0\\ 0 & D_k\end{pmatrix},\quad Q_{2k+1}=\begin{pmatrix}0 & B_k\\ C_k & 0\end{pmatrix},\quad 0\leqslant k\leqslant N-1,$$

where $\delta_N=\delta_N(x,t)$ is a function to be determined later, which plays an important role in constructing an explicit Darboux transformation of system (21) in this article. As $\delta_N=1$ or $Q=I$, the form of matrix T in (51) is exactly the same as that in our previous paper,[38] where we constructed a Darboux transformation for GI equation (3). From (48), (49) and (51), it is easy to see that $\det T(\lambda)$ is $(4N)$th order polynomial of λ, and $\pm\lambda_j$ $(1\leqslant j\leqslant 2N)$ are all its roots. Therefore we have

$$\det T(\lambda)=\prod_{j=1}^{2N}(\lambda^2-\lambda_j^2). \tag{52}$$

Proposition 8: Let δ_N satisfy a first-order ordinary equation

$$\partial_x\ln\delta_N=(2\beta-1)(rB_{N-1}-qC_{N-1}-2iB_{N-1}C_{N-1}). \tag{53}$$

Then matrix $\tilde{U}$ determined by (44) has the same form as U, that is,

$$\tilde{U}=\begin{pmatrix}-i\lambda^2-i\beta\tilde{q}\tilde{r} & \lambda\tilde{q}\\ \lambda\tilde{r} & i\lambda^2+i\beta\tilde{q}\tilde{r}\end{pmatrix},$$

where the transformations between q, r and $\tilde{q}$, $\tilde{r}$ are given by

$$\tilde{q}=\delta_N^2(q+2iB_{N-1}),\quad \tilde{r}=\delta_N^{-2}(r-2iC_{N-1}). \tag{54}$$

The transformation (44) and (54): $(y,q,r)\to(\tilde{y},\tilde{q},\tilde{r})$ is a Darboux transformation of the spectral problem (5).

Proof: Let $T^{-1}=T^*/\det T$ and

$$(T_x+TU)T^*=\begin{pmatrix}f_{11}(\lambda) & f_{12}(\lambda)\\ f_{21}(\lambda) & f_{22}(\lambda)\end{pmatrix}. \tag{55}$$

It is easy to see that $f_{11}(\lambda)$ and $f_{22}(\lambda)$ are (4N+2)th order polynomials in λ, and $f_{12}(\lambda)$ and $f_{21}(\lambda)$ are (4N+1)th order polynomials in λ.

On the other hand, making use of (5) and (48)–(50), we find that

$$\alpha_{jx}=\lambda_j r-\lambda_j q\alpha_j^2+2i(\lambda_j^2+\beta qr)\alpha_j,$$

$$A(\pm\lambda_j)=\mp\alpha_j B(\pm\lambda_j),\quad C(\pm\lambda_j)=\mp\alpha_j D(\pm\lambda_j).$$

From the above equalities, it is easy to verify that all $\pm\lambda_j$ $(1\leqslant j\leqslant 2N)$ are roots of $f_{kj}(\lambda)$ $(k,j=1,2)$, which together with (52) implies that $f_{kj}(\lambda)$ may be divided by $\det T$, and thus $(T_x+TU)T^{-1}$ is a second order polynomial in λ with matrix coefficients, that is,

$$T_x+TU=(\tilde{U}_2\lambda^2+\tilde{U}_1\lambda+\tilde{U}_0)T, \tag{56}$$

where the matrices $\tilde{U}_2(x,t)$, $\tilde{U}_1(x,t)$ and $\tilde{U}_0(x,t)$ do not depend on λ.

We denote $U=U_2\lambda^2+U_1\lambda+U_0$, with

$$U_2=\begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix},\quad U_1=\begin{pmatrix}0 & q\\ r & 0\end{pmatrix},\quad U_0=\begin{pmatrix}-i\beta qr & 0\\ 0 & i\beta qr\end{pmatrix}.$$

Comparing the coefficients of λ^{2N+2}, λ^{2N+1}, and λ^{2N} in (56) yields

$$(2N+2)\text{th coeff.:}\ \ \tilde{U}_2=QU_2Q^{-1}=U_2,$$

$$(2N+1)\text{th coeff.:}\ \ \tilde{U}_1=(QU_1+[QQ_{2N-1},U_2])Q^{-1}=\begin{pmatrix}0 & \tilde{q}\\ \tilde{r} & 0\end{pmatrix},$$

$$(2N)\text{th coeff.:}$$

$$\tilde{U}_0=\partial_x\ln Q+(QU_0+QQ_{2N-1}U_1-\tilde{U}_1QQ_{2N-1}+[QQ_{2N-2},U_2])Q^{-1}=\begin{pmatrix}-i\beta\tilde{q}\tilde{r} & 0\\ 0 & i\beta\tilde{q}\tilde{r}\end{pmatrix},$$

where $\tilde{q}$ and $\tilde{r}$ are given by (54). The proof is completed.

Next we try to prove that $\tilde{V}^{(1)}$ in (46) has the same form as $V^{(1)}$ under the transformations (44) and (54).

Proposition 9: Suppose that δ_N satisfies another compatible first-order ordinary differential equation

$$\begin{aligned}\partial_t\ln\delta_N=&(2\beta-1)[i(qC_{N-1x}+rB_{N-1x})-i(q_xC_{N-1}+r_xB_{N-1})-2(B_{N-1}C_{N-1x}-B_{N-1x}C_{N-1})\\&-(4\beta-1)qr(rB_{N-1}-qC_{N-1})-i(r^2B_{N-1}^2+q^2C_{N-1}^2)-4(rB_{N-1}^2C_{N-1}\\&-qB_{N-1}C_{N-1}^2)+8i\beta qrB_{N-1}C_{N-1}+4iB_{N-1}^2C_{N-1}^2].\end{aligned} \tag{57}$$

Then matrix $\tilde{V}^{(1)}$ in (46) has the same form as $V^{(1)}$ under the same transformation (44) and (54).

Proof: In a way similar to Proposition 8, we can prove that $(T_t+TV^{(1)})T^{-1}$ is a fourth-order polynomial in λ with matrix coefficients, that is,

$$T_t+TV^{(1)}=(\tilde{V}_4\lambda^4+\tilde{V}_3\lambda^3+\tilde{V}_2\lambda^2+\tilde{V}_1\lambda+\tilde{V}_0)T. \tag{58}$$

We write $V^{(1)}$ in the form $V^{(1)}=V_4\lambda^4+V_3\lambda^3+V_2\lambda^2+V_1\lambda+V_0$, with

$$V_4=\begin{pmatrix}-2i & 0\\ 0 & 2i\end{pmatrix},\quad V_3=\begin{pmatrix}0 & 2q\\ 2r & 0\end{pmatrix},\quad V_2=\begin{pmatrix}-iqr & 0\\ 0 & iqr\end{pmatrix},$$

$$V_1=\begin{pmatrix}0 & iq_x-(2\beta-1)q^2r\\ -ir_x-(2\beta-1)qr^2 & 0\end{pmatrix},$$

$$V_0=\begin{pmatrix} \beta(rq_x-qr_x)+\frac{1}{2}i\beta(8\beta-3)q^2r^2 & 0 \\ 0 & -\beta(rq_x-qr_x)-\frac{1}{2}i\beta(8\beta-3)q^2r^2 \end{pmatrix}.$$

Comparing the coefficients of λ^{2N+j} $(j=0,1,2,3,4)$ yields

$$(2N+4)\text{th coeff.: } \tilde{V}_4=QV_4Q^{-1}=V_4,$$

$$(2N+3)\text{th coeff.: } \tilde{V}_3=(QV_3+[QQ_{2N-1},V_4])Q^{-1}=\begin{pmatrix} 0 & 2\tilde{q} \\ 2\tilde{r} & 0 \end{pmatrix},$$

$$\begin{aligned}(2N+2)\text{th coeff.: } \tilde{V}_2&=(QV_2+QQ_{2N-1}V_3-\tilde{V}_3QQ_{2N-1}+[QQ_{2N-2},V_4])Q^{-1}\\ &=\begin{pmatrix} -i\tilde{q}\tilde{r} & 0 \\ 0 & i\tilde{q}\tilde{r} \end{pmatrix},\end{aligned}$$

$$\begin{aligned}(2N+1)\text{th coeff.: } \tilde{V}_1&=(QV_1+QQ_{2N-1}V_2-\tilde{V}_2QQ_{2N-1})Q^{-1}\\ &\quad+(QQ_{2N-2}V_3-\tilde{V}_3QQ_{2N-2}+[QQ_{2N-3},V_4])Q^{-1},\end{aligned} \tag{59}$$

$(2N)$th coeff.:

$$\begin{aligned}\tilde{V}_0&=\partial_t\ln Q+(QV_0+QQ_{2N-1}V_1-\tilde{V}_1QQ_{2N-1}+QQ_{2N-2}V_2-\tilde{V}_2QQ_{2N-2}+QQ_{2N-3}V_3\\ &\quad-\tilde{V}_3QQ_{2N-3}+[QQ_{2N-4},V_4])Q^{-1}\\ &=\partial_t\delta_N+(QV_0+QQ_{2N-1}V_1-\tilde{V}_1QQ_{2N-1})Q^{-1}+\frac{1}{2}U_2\tilde{U}_1([QQ_{2N-3},V_4]+QQ_{2N-2}V_3\\ &\quad-\tilde{V}_3QQ_{2N-2})Q^{-1}-\frac{1}{2}([QQ_{2N-3},V_4]+Q_{2N-2}V_3-\tilde{V}_3Q_{2N-2})U_2U_1Q^{-1}.\end{aligned} \tag{60}$$

Again comparing the coefficient of λ^{2N-1} in (56) and noting that $V_4=2U_2$, $V_3=2U_1$, $\tilde{V}_3=2\tilde{U}_1$, $U_0=\beta V_2$, $\tilde{U}_0=\beta\tilde{V}_2$, we find that

$$\begin{aligned}&[QQ_{2N-3},V_4]+QQ_{2N-2}V_3-\tilde{V}_3QQ_{2N-2}\\ &\quad=-2Q_xQ_{2N-1}-2QQ_{2N-1x}+2\tilde{U}_0QQ_{2N-1}-2QQ_{2N-1}U_0.\end{aligned} \tag{61}$$

Substituting (61) into (59) and (60), direct calculation shows that $\tilde{V}_1$ and $\tilde{V}_0$ possess the same form as V_1 and V_0. By using (53), (54), and (57) and noting that q, r, $\tilde{q}$, $\tilde{r}$ satisfy the Kundu equation (21), in virtue of Mathematica direct and tedious verification shows that $\delta_{Nxt}=\delta_{Ntx}$, that is to say, Eqs. (53) and (57) are compatible. The theorem is completed.

Propositions 8 and 9 show that the transformations (44) and (54) change the Lax pairs (5) and (24) into other Lax pairs (45) and (46) of the same type. Therefore both of the Lax pairs lead to the same coupled Kundu system (21). We call the transformation $(y,q,r)\to(\tilde{y},\tilde{q},\tilde{r})$ a Darboux transformation of coupled Kundu system (21). In summary, we arrive at the following theorem.

Theorem 5: The solutions (q,r) of coupled Kundu system (21) are mapped into their new solution $(\tilde{q},\tilde{r})$ under Darboux transformation (44) and (54), where B_{N-1} and C_{N-1} are given by (48) and (49), and δ_N is determined by two first-order ordinary differential equations (53) and (57).

VII. REDUCTION OF DARBOUX AND ITS APPLICATION

In this section, the N-fold Darboux transformation of the Kundu equation (22) will be obtained from that of coupled Kundu system (21) by using a reduction technique. For this purpose we let $r=-q^*$, and choose two solutions of the Lax pairs (5) and (24) as

$$\phi(\lambda)=(\phi_1(\lambda),\phi_2(\lambda))^T,\quad \psi(\lambda)=(-\phi_2^*(\lambda^*),\phi_1^*(\lambda^*))^T,$$

and parameters

$$\lambda_{2j}=\lambda_{2j-1}^*,\quad \gamma_{2j}=-\gamma_{2j-1}^{*^{-1}},\quad 1\leqslant j\leqslant N.$$

Then it is easy to show that $\alpha_{2j}^{-1}=-\alpha_{2j-1}^*$, $D_k^*=A_k$, $C_k^*=-B_k$ $(0\leqslant k\leqslant N-1)$. In this way, the corresponding systems (48)–(50) are reduced to

$$\sum_{k=0}^{N-1}(A_k+\lambda_{2j-1}\alpha_{2j-1}B_k)\lambda_{2j-1}^{2k}=-\lambda_{2j-1}^{2N},\tag{62}$$

$$\sum_{k=0}^{N-1}(\alpha_{2j-1}^*A_k-\lambda_{2j-1}^*B_k)\lambda_{2j-1}^{*^{2k}}=-\alpha_{2j-1}^*\lambda_{2j-1}^{*^{2N}},\quad 1\leqslant j\leqslant N.\tag{63}$$

$$\alpha_{2j-1}=\frac{\phi_2(\lambda_{2j-1})-\gamma_{2j-1}\psi_2(\lambda_{2j-1})}{\phi_1(\lambda_{2j-1})-\gamma_{2j-1}\psi_1(\lambda_{2j-1})},\tag{64}$$

and Eqs. (53) and (57) are reduced to

$$\partial_x\delta_N=2(2\beta-1)[\mathrm{Im}(q^*B_{N-1})+i|B_{N-1}|^2],\tag{65}$$

$$\begin{aligned}\partial_t\delta_N=2(2\beta-1)[&-i\,\mathrm{Re}(q^*B_{N-1x}-q_x^*B_{N-1})-2\,\mathrm{Im}(B_{N-1}^*B_{N-1x})+(4\beta-1)|q|^2\,\mathrm{Im}(q^*B_{N-1})\\&-i\,\mathrm{Re}(q^{*^2}B_{N-1}^2)-4\,\mathrm{Im}(q^*|B_{N-1}|^2B_{N-1})+4i\beta|q|^2|B_{N-1}|^2+2i|B_{N-1}|^4].\end{aligned}\tag{66}$$

Based on these results we have the following theorem:

Theorem 6: Suppose that δ_N satisfies ordinary differential equations (65) and (66), and A_k, B_k are given by the linear algebraic system (62) and (63). Then solution q of Kundu equation (22) is mapped into its a new solution $\tilde{q}$ under the Darboux transformation

$$\tilde{q}=\delta_N^2(q+2iB_{N-1}).\tag{67}$$

In the following, we shall apply the Darboux transformation (67) to construct explicit solutions of Kundu equation (22). As usual, we make a Darboux transformation starting from a special solution of Eq. (21). Substituting $q=0$ $(q=r=0)$ into the Lax pairs (5) and (24), we find that two basic solutions can be chosen as

$$\phi(\lambda)=\begin{pmatrix}\exp(-i\lambda^2x-2i\lambda^4t)\\0\end{pmatrix},\quad \psi(\lambda)=\begin{pmatrix}0\\\exp(i\lambda^2x+2i\lambda^4t)\end{pmatrix}.$$

According to (64), we have

$$\alpha_{2j-1}=-\exp(2i\lambda_{2j-1}^2x+4i\lambda_{2j-1}^4t+\delta_j+i\mu_j),\quad 1\leqslant j\leqslant N,\tag{68}$$

where $\gamma_{2j-1}=\exp(\delta_j+i\mu_j)$. We shall discuss only the case $N=1$.

Let $\lambda_1=\xi_1+i\eta_1$ $(\xi_1\neq\eta_1)$. Then solving the linear algebraic system (62) and (63) yields

$$B_0=\frac{2i\xi_1\eta_1\exp(iY_1)}{\xi_1\cosh(X_1)+i\eta_1\sinh(X_1)}, \tag{69}$$

where

$$X_1=4\xi_1\eta_1x+16\xi_1\eta_1(\xi_1^2-\eta_1^2)t+\delta_1, \quad Y_1=-2(\xi_1^2-\eta_1^2)x+4(\xi_1^4-\eta_1^4-6\xi_1^2\eta_1^2)t+\mu_1. \tag{70}$$

By using (69), solving Eqs. (65) and (66) corresponding to $q=r=0$ by using Mathematica gives

$$\delta_1=\exp\{2(2\beta-1)[if(x,t)+(\xi_1^2+\eta_1^2)(\xi_1^2-\eta_1^2)^{-1}g(x,t)]\},$$

where

$$g(x,t)=\arctan[\xi_1^{-1}\eta_1\tanh(X_1)], \quad f(x,t)=-g(x,t)+\frac{\xi_1\eta_1(\xi_1^2+\eta_1^2)\sinh(2X_1)}{(\xi_1^2-\eta_1^2)^2+(\xi_1^4-\eta_1^4)\cosh(2X_1)}.$$

In this way, a one-soliton solution of the Kundu equation (21) is obtained with the help of the Darboux transformation (67):

$$\tilde{q}=2i\delta_1^2B_0.$$

The N-fold Darboux transformation (67) presented here has some merits. First, the solution $\tilde{q}$ in (67) is the N-fold Darboux transformation of the solution q. It can be interpreted as a nonlinear superposition of the initial solution q and N-soliton solution. It contains all pure N-soliton solutions of the Kundu equation in a unified form. Therefore, it provides unified and explicit N-soliton solutions for Kundu, KN, CLL, and GI equation. Second, the solutions of the Kundu equation are reduced to solving a linear algebraic system and two first-order ordinary differential equations. It is easy to produce its multi-soliton solutions by symbolic computation on a computer. At last, for the case $\beta=\frac{1}{2}$, all results obtained in this article can be reduced to the corresponding ones.[38]

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Binary symmetry constraints of $\mathcal{N}$-wave interaction equations in 1+1 and 2+1 dimensions

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Binary symmetry constraints of the $\mathcal{N}$-wave interaction equations in $1+1$ and $2+1$ dimensions are proposed to reduce the $\mathcal{N}$-wave interaction equations into finite-dimensional Liouville integrable systems. A new involutive and functionally independent system of polynomial functions is generated from an arbitrary order square matrix Lax operator and used to show the Liouville integrability of the constrained flows of the $\mathcal{N}$-wave interaction equations. The constraints on the potentials resulting from the symmetry constraints give rise to involutive solutions to the $\mathcal{N}$-wave interaction equations, and thus the integrability by quadratures are shown for the $\mathcal{N}$-wave interaction equations by the constrained flows. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1388898]

I. INTRODUCTION

It is a usual practice to utilize the idea of linearization in analyzing nonlinear differential or differential-difference equations (see, for example Refs. 1 and 2). The method of inverse scattering transform is an important application of such an idea to the theory of soliton equations,[3,4] which has been recognized as one of the most significant contributions in the field of applied mathematics in the second half of the last century. The general formulation of Lax pairs is a spectacular tool of realization of inverse scattering transform,[5] by which one can break a nonlinear problem into a couple of linear problems and then handle the resulting linear problems to solve the nonlinear problem.

Recently in the past decade, an unusual way of using the nonlinearization technique arose in the theory of soliton equations.[6–10] Although using the idea of nonlinearization is not normally considered to be a good direction in studying nonlinear equations, one gradually realizes that the nonlinearization technique provides a powerful approach for analyzing soliton equations, especially for showing the integrability by quadratures for soliton equations. The manipulation of nonlinearization not only leads to finite-dimensional Liouville integrable systems,[6–15] but also decomposes infinite-dimensional soliton equations, in whatever dimensions, into finite-dimensional Liouville integrable systems.[16–18] Moreover, it narrows the gap between infinite-dimensional soliton equations and finite-dimensional Liouville integrable systems,[11,16,18] and paves a method of separation of variables for soliton equations,[19,20] which can also be used to analyze the resulting finite-dimensional integrable systems.[21–23] Mathematically speaking, much excitement in the study of nonlinearization comes from a kind of specific symmetry constraints,[24–27] engendered from the variational derivative of the spectral parameter.[26,27] It is due to symmetry constraints that the nonlinearization technique is so powerful in showing the integrability by quadratures for soliton equations.[28,29] The study of symmetry constraints itself is an important part of the kernel of the mathematical theory of nonlinearization, which is also a common conceptional umbrella under which one can manipulate both mono-nonlinearization[6] and binary nonlinearization.[26]

However, all examples of application of the nonlinearization technique, discussed so far, are

related to lower-order matrix (here, and in what follows, a matrix is assumed to be square) spectral problems of soliton equations, most of which are only concerned with second-order traceless matrix spectral problems. On the one hand, there appears much difficulty in handling the Liouville integrability[30] of the so-called constrained flows generated from spectral problems, in the case of the third- and fourth-order matrix spectral problems.[28,31,32] It is a challenging task to extend the theory of nonlinearization to the case of higher-order matrix spectral problems. On the other hand, one also notices that mono-nonlinearization cannot be carried out in the cases of odd-order matrix spectral problems and even-order, including the simplest second-order, nontraceless matrix spectral problems. Even for even-order traceless matrix spectral problems, it is not clear how to determine pairs of canonical variables to obtain Hamiltonian structures of the constrained flows while doing mono-nonlinerization. Therefore, one has to take into account adjoint spectral problems and manipulate binary nonlinearization for the case of general matrix spectral problems. In the theory of binary nonlinearization,[33] there exists a natural way for determining symplectic structures to exhibit Hamiltonian forms of the constrained flows.

In this article, we would like to establish a concrete example to apply the nonlinearization technique to the case of higher-order matrix spectral problems, by manipulating binary nonlinearization for arbitrary-order matrix spectral problems associated with the $\mathcal{N}$-wave interaction equations in both $1+1$ and $2+1$ dimensions. The resulting theory will show a direct way for generating sufficiently many integrals of motion, and more importantly for proving the functional independence of the required integrals of motion, for the Liouville integrability of the constrained flows resulting from higher-order matrix spectral problems.

Let us recall some basic notation on binary nonlinearization (see, for example, Ref. 33 for a detailed description). Let us assume that we have a matrix spectral problem

$$\phi_x = U\phi = U(u,\lambda)\phi, \quad U=(U_{ij})_{r\times r}, \quad \phi=(\phi_1,\ldots,\phi_r)^T \tag{1.1}$$

with a spectral parameter λ and a potential $u=(u_1,\ldots,u_q)^T$. Suppose that the compatability conditions

$$U_{t_m} - V^{(m)}_x + [U,V^{(m)}] = 0, \quad m \geqslant 0,$$

of the spectral problem (1.1) and the associated spectral problems

$$\phi_{t_m} = V^{(m)}\phi = V^{(m)}(u,u_x,\ldots;\lambda)\phi, \quad V^{(m)}=(V^{(m)}_{ij})_{r\times r}, \quad m\geqslant 0, \tag{1.2}$$

determine an isospectral ($\lambda_{t_m}=0$) soliton hierarchy

$$u_{t_m} = X_m(u) = JG_m = J\frac{\delta \tilde{H}_m}{\delta u}, \quad m\geqslant 0, \tag{1.3}$$

where J is a Hamiltonian operator and $\tilde{H}_m$ are Hamiltonian functionals. Obviously, the compatability conditions of the adjoint spectral problem

$$\psi_x = -U^T(u,\lambda)\psi, \quad \psi=(\psi_1,\ldots,\psi_r)^T, \tag{1.4}$$

and the adjoint associated spectral problems

$$\psi_{t_m} = -V^{(m)T}\lambda = -V^{(m)T}(u,u_x,\ldots;\lambda)\psi \tag{1.5}$$

still give rise to the same hierarchy $u_{t_m}=X_m(u)$ defined by (1.3). It has been pointed out[16,26] that $J\delta\lambda/\delta u$ is a common symmetry of all equations in the hierarchy (1.3). Introducing N distinct eigenvalues $\lambda_1,\lambda_2,\ldots,\lambda_N$, we have

$$\phi^{(s)}_x = U(u,\lambda_s)\phi^{(s)}, \quad \psi^{(s)}_x = -U^T(u,\lambda_s)\psi^{(s)}, \quad 1\leqslant s\leqslant N, \tag{1.6}$$

and

$$\phi_{t_m}^{(s)}=V^{(m)}(u,u_x,\ldots;\lambda_s)\phi^{(s)},\quad \psi_{t_m}^{(s)}=-V^{(m)T}(u,u_x,\ldots;\lambda_s)\psi^{(s)},\quad 1\leqslant s\leqslant N, \tag{1.7}$$

where we set the corresponding eigenfunctions and adjoint eigenfunctions as $\phi^{(s)}$ and $\psi^{(s)}$, $1\leqslant s\leqslant N$. It is assumed that the conserved covariant G_{m_0} does not depend on any derivative of u with respect to x, and thus the so-called general binary Bargmann symmetry constraint reads as

$$X_{m_0}=\sum_{s=1}^{N} E_s\mu_s J\frac{\delta\lambda_s}{\delta u},\quad \text{i.e.,}\quad JG_{m_0}=J\sum_{s=1}^{N}\mu_s\psi^{(s)T}\frac{\partial U(u,\lambda_s)}{\partial u}\phi^{(s)}, \tag{1.8}$$

where μ_s, $1\leqslant s\leqslant N$, are arbitrary nonzero constants, and E_s, $1\leqslant s\leqslant N$, are normalized constants. The right-hand side of the symmetry constraint (1.8) is a linear combination of N symmetries

$$E_s J\frac{\delta\lambda_s}{\delta u}=J\psi^{(s)T}\frac{\partial U(u,\lambda_s)}{\partial u}\phi^{(s)},\quad 1\leqslant s\leqslant N.$$

Such symmetries are not Lie point, contact or Lie–Bäcklund symmetries, since $\phi^{(s)}$ and $\psi^{(s)}$ cannot be expressed in terms of x, u and derivatives of u with respect to x to some finite order. Suppose that (1.8) has an inverse function

$$u=\tilde{u}=\tilde{u}(\phi^{(1)},\ldots,\phi^{(N)};\psi^{(1)},\ldots,\psi^{(N)}). \tag{1.9}$$

Replacing u with $\tilde{u}$ in the system (1.6) or the system (1.7), we obtain the so-called spatial constrained flow:

$$\phi_x^{(s)}=U(\tilde{u},\lambda_s)\phi^{(s)},\quad \psi_x^{(s)}=-U^T(\tilde{u},\lambda_s)\psi^{(s)},\quad 1\leqslant s\leqslant N, \tag{1.10}$$

or the so-called temporal constrained flows:

$$\phi_{t_m}^{(s)}=V^{(m)}(\tilde{u},\tilde{u}_x,\ldots;\lambda_s)\phi^{(s)},\quad \psi_{t_m}^{(s)}=-V^{(m)T}(\tilde{u},\tilde{u}_x,\ldots;\lambda_s)\psi^{(s)},\quad 1\leqslant s\leqslant N. \tag{1.11}$$

The main problem of nonlinearization is to show that the spatial constrained flow (1.10) and the temporal constrained flows (1.11) under the control of (1.10) are Liouville integrable. Then if $\phi^{(s)}$ and $\psi^{(s)}$, $1\leqslant s\leqslant N$, solve two constrained flows (1.10) and (1.11) simultaneously, $u=\tilde{u}$ will give rise to a solution to the mth soliton equation $u_{t_m}=X_m(u)$. It also follows that the soliton equation $u_{t_m}=X_m(u)$ is decomposed into two finite-dimensional Liouville integrable systems, and $u=\tilde{u}$ presents a Bäcklund transformation between infinite-dimensional soliton equations and finite-dimensional Liouville integrable systems. More generally, if a soliton equation is associated with a set of spectral problems

$$\phi_{x_i}=U^{(i)}(u,\lambda)\phi,\quad 1\leqslant i\leqslant p,$$

then it will be decomposed into $p+1$ finite-dimensional Liouville integrable systems. The above whole process is called binary nonlinearization.[16,33]

This article is structured as follows. In Sec. II, we will present binary symmetry constraints of the $\mathcal{N}$-wave interaction equations in $1+1$ dimensions, and show Hamiltonian structures and Lax presentations of the corresponding constrained flows. In Sec. III, we consider the $2+1$ dimensional case. We will similarly construct binary symmetry constraints of the $\mathcal{N}$-wave interaction equations in $2+1$ dimensions, and discuss some properties of the corresponding constrained flows. In Sec. IV, we go on to propose an involutive system of functionally independent polynomial functions, generated from an arbitrary-order matrix Lax operator, along with an alternative involutive and functionally independent system. An **r**-matrix formulation will be established for

the Lax operator, and used to show the involutivity of the obtained system of polynomial functions, together with Newton's identities on elementary symmetric polynomials. A detailed proof will also be made for the functional independence of the system of polynomial functions by using the determinant property of the tensor product of matrices. In Sec. V, two applications of the involutive system engendered in Sec. IV will be given, which verify that all constrained flows associated with the $\mathcal{N}$-wave interaction equations in both $1+1$ and $2+1$ dimensions are Liouville integrable. Moreover, a kind of involutive solution of the $\mathcal{N}$-wave interaction equations in two cases will be depicted. These also show the integrability by quadratures for the $\mathcal{N}$-wave interaction equations. Finally, in Sec. VI, some concluding remarks will be given, together with conclusions.

II. BINARY SYMMETRY CONSTRAINTS IN 1+1 DIMENSIONS

A. $n\times n$ AKNS hierarchy and 1+1 dimensional $\mathcal{N}$-wave interaction equations

Let n be an arbitrary natural number strictly greater than 2. We begin with the $n\times n$ matrix AKNS spectral problem[34]

$$\phi_x = U\phi = U(u,\lambda)\phi, \quad U(u,\lambda) = \lambda U_0 + U_1(u), \quad \phi = (\phi_1,\ldots,\phi_n)^T, \tag{2.1}$$

with a spectral parameter λ and

$$U_0 = \mathrm{diag}(\alpha_1,\ldots,\alpha_n), \quad U_1(u) = (u_{ij})_{n\times n}, \tag{2.2}$$

where α_i, $1\leqslant i\leqslant n$, are distinct constants, and $u_{ii}=0$, $1\leqslant i\leqslant n$. The standard AKNS spectral problem, i.e., the spectral problem (2.1) with $n=2$, has been analyzed in Ref. 35, but it cannot generate any $\mathcal{N}$-wave interaction equations and thus it is not discussed here. In order to express related soliton equations in a compact form, we write down the potential u as

$$\begin{gathered} u=\rho(U), \quad \text{i.e., } u=(u_{21},u_{12},u_{13},u_{31},u_{23},u_{32})^T, \quad \text{when } n=3, \\ u=(u_{21},u_{12},u_{13},u_{31},u_{14},u_{41},u_{23},u_{32},\ldots,u_{n,n-1},u_{n-1,n})^T, \quad \text{when } n\geqslant 4, \end{gathered} \tag{2.3}$$

in which we arrange the exponents u_{ij} in a specific way, first from smaller to larger of the integers $k=i+j$ and then symmetrically for each set $\{u_{i,k-i}|1\leqslant i\leqslant k-1\}$.

Let us now consider the construction of the $1+1$ dimensional $\mathcal{N}$-wave interaction equations and its whole isospectral hierarchy associated with the spectral problem (2.1). We first solve the stationary zero-curvature equation for W:

$$W_x - [U,W] = 0, \quad W = (W_{ij})_{n\times n}, \tag{2.4}$$

which is equivalent to

$$\begin{gathered} W_{ij,x} + u_{ij}(W_{ii}-W_{jj}) + \sum_{\substack{k=1\\k\neq i,j}}^{n} (u_{kj}W_{ik} - u_{ik}W_{kj}) - \lambda(\alpha_i-\alpha_j)W_{ij} = 0, \quad i\neq j, \\ W_{ii,x} = \sum_{\substack{k=1\\k\neq i}}^{n} (u_{ik}W_{ki} - u_{ki}W_{ik}), \end{gathered} \tag{2.5}$$

where $1\leqslant i,j\leqslant n$. We look for a formal solution of the form

$$W = \sum_{l\geqslant 0} W_l \lambda^{-l}, \quad W_l = (W_{ij}^{(l)})_{n\times n}, \tag{2.6}$$

and thus (2.5) becomes the following recursion relation

$$W_{ii,x}^{(0)}=0, \quad W_{ij}^{(0)}=0, \quad i\neq j, \tag{2.7a}$$

$$W_{ij,x}^{(l)}+u_{ij}(W_{ii}^{(l)}-W_{jj}^{(l)})+\sum_{\substack{k=1\\k\neq i,j}}^{n}(u_{kj}W_{ik}^{(l)}-u_{ik}W_{kj}^{(l)})-(\alpha_i-\alpha_j)W_{ij}^{(l+1)}=0, \quad i\neq j, \tag{2.7b}$$

$$W_{ii,x}^{(l+1)}=\sum_{\substack{k=1\\k\neq i}}^{n}(u_{ik}W_{ki}^{(l+1)}-u_{ki}W_{ik}^{(l+1)}), \tag{2.7c}$$

where $1\leqslant i,j\leqslant n$ and $l\geqslant 0$. In particular, from the above recursion relation, we have that

$$W_{ii}^{(0)}=\beta_i=\text{const}, \quad W_{ij}^{(0)}=0, \quad 1\leqslant i\neq j\leqslant n, \tag{2.8}$$

and

$$W_{ii}^{(1)}=0, \quad W_{ij}^{(1)}=\frac{\beta_i-\beta_j}{\alpha_i-\alpha_j}u_{ij}, \quad 1\leqslant i\neq j\leqslant n. \tag{2.9}$$

We require that

$$W_{ij}^{(l)}|_{u=0}=0, \quad 1\leqslant i,j\leqslant n, \quad l\geqslant 1. \tag{2.10}$$

This condition (2.10) means to identify all constants of integration to be zero while using (2.7) to determine W, and thus all W_l, $l\geqslant 1$, will be uniquely determined. For example, we can obtain from (2.7) under (2.10) that

$$W_{ij}^{(2)}=\frac{\beta_i-\beta_j}{(\alpha_i-\alpha_j)^2}u_{ij,x}+\frac{1}{\alpha_i-\alpha_j}\sum_{\substack{k=1\\k\neq i,j}}^{n}\left(\frac{\beta_k-\beta_i}{\alpha_k-\alpha_i}-\frac{\beta_k-\beta_j}{\alpha_k-\alpha_j}\right)u_{ik}u_{kj}, \quad 1\leqslant i\neq j\leqslant n,$$
$$W_{ii}^{(2)}=\sum_{\substack{k=1\\k\neq i}}^{n}\frac{\beta_k-\beta_i}{(\alpha_k-\alpha_i)^2}u_{ik}u_{ki}, \quad 1\leqslant i\leqslant n. \tag{2.11}$$

It is easy to see that the recursion relation (2.7) can lead to

$$2u_{ij}\partial^{-1}u_{ij}W_{ji}^{(l)}+(\partial-2u_{ij}\partial^{-1}u_{ji})W_{ij}^{(l)}+\sum_{\substack{k=1\\k\neq i,j}}^{n}[u_{ij}\partial^{-1}u_{ik}W_{ki}^{(l)}+(u_{kj}-u_{ij}\partial^{-1}u_{ki})W_{ik}^{(l)}]$$
$$+\sum_{\substack{k=1\\k\neq i,j}}^{n}[u_{ij}\partial^{-1}u_{kj}W_{jk}^{(l)}-(u_{ik}+u_{ij}\partial^{-1}u_{jk})W_{kj}^{(l)}]=(\alpha_i-\alpha_j)W_{ij}^{(l+1)}, \quad i\neq j, \tag{2.12}$$

where $1\leqslant i,j\leqslant n$, $l\geqslant 1$, and ∂^{-1} is the inverse operator of $\partial=\partial/\partial x$. This can be written as the Lenard form

$$MG_{l-1}=JG_l, \quad l\geqslant 1, \tag{2.13}$$

where $G_l=\rho(W_{l+1})$ is generated from W_{l+1} in the same way as that for u, and J is a constant operator

$$\begin{cases} J=\mathrm{diag}((\alpha_1-\alpha_2)\sigma_0,(\alpha_1-\alpha_3)\sigma_0,(\alpha_2-\alpha_3)\sigma_0), & \text{when } n=3, \\ J=\mathrm{diag}(\underbrace{(\alpha_1-\alpha_2)\sigma_0,(\alpha_1-\alpha_3)\sigma_0,(\alpha_1-\alpha_4)\sigma_0,(\alpha_2-\alpha_3)\sigma_0,\ldots,(\alpha_{n-1}-\alpha_n)\sigma_0}_{n(n-1)/2}), & \\ & \text{when } n\geqslant 4, \end{cases} \tag{2.14}$$

with σ_0 being given by

$$\sigma_0=\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

For example, when $n\geqslant 4$, we have

$$G_{l-1}=(W_{21}^{(l)},W_{12}^{(l)},W_{31}^{(l)},W_{13}^{(l)},W_{41}^{(l)},W_{14}^{(l)},W_{32}^{(l)},W_{23}^{(l)},\ldots,W_{n,n-1}^{(l)},W_{n-1,n}^{(l)})^T, \quad l\geqslant 1, \tag{2.15}$$

the first of which reads as

$$\begin{aligned} G_0=\Big(& \frac{\beta_1-\beta_2}{\alpha_1-\alpha_2}u_{21},\frac{\beta_1-\beta_2}{\alpha_1-\alpha_2}u_{12},\frac{\beta_1-\beta_3}{\alpha_1-\alpha_3}u_{31},\frac{\beta_1-\beta_3}{\alpha_1-\alpha_3}u_{13},\frac{\beta_1-\beta_4}{\alpha_1-\alpha_4}u_{41}, \\ & \frac{\beta_1-\beta_4}{\alpha_1-\alpha_4}u_{14},\ldots,\frac{\beta_{n-1}-\beta_n}{\alpha_{n-1}-\alpha_n}u_{n,n-1},\frac{\beta_{n-1}-\beta_n}{\alpha_{n-1}-\alpha_n}u_{n-1,n}\Big)^T. \end{aligned} \tag{2.16}$$

The operators J and M are skew-symmetric and can be shown to be a Hamiltonian pair.[36,37]

We proceed to introduce the associated spectral problems with the spectral problem (2.1),

$$\phi_{t_m}=V^{(m)}\phi, \quad V^{(m)}=V^{(m)}(u,\lambda)=(\lambda^m W)_+, \quad m\geqslant 1, \tag{2.17}$$

where the symbol $+$ stands for the choice of the part of non-negative powers of λ. Note that we have

$$W_{lx}=[U_0,W_{l+1}]+[U_1,W_l], \quad l\geqslant 0,$$

and we can compute that

$$\begin{aligned} [U,V^{(m)}]&=\Big[\lambda U_0+U_1,\sum_{l=0}^{m}\lambda^{m-l}W_l\Big] \\ &=\sum_{l=0}^{m}[U_0,W_l]\lambda^{m+1-l}+\sum_{l=0}^{m}[U_1,W_l]\lambda^{m-l} \\ &=\sum_{l=0}^{m-1}[U_0,W_{l+1}]\lambda^{m-l}+\sum_{l=0}^{m}[U_1,W_l]\lambda^{m-l}, \end{aligned}$$

where we have used $[U_0,W_0]=0$. Therefore, under the isospectral conditions

$$\lambda_{t_m}=0, \quad m\geqslant 1, \tag{2.18}$$

the compatibility conditions of the spectral problem (2.1) and the associated spectral problems (2.17), i.e., the zero-curvature equations

$$U_{t_m}-V_x^{(m)}+[U,V^{(m)}]=0, \quad m\geqslant 1,$$

equivalently lead to

$$U_{1t_m}=W_{mx}-[U_1,W_m]=[U_0,W_{m+1}], \quad m\geqslant 1.$$

This gives rise to the so-called $n\times n$ AKNS soliton hierarchy

$$u_{t_m}=X_m:=JG_m, \quad m\geqslant 1, \tag{2.19}$$

where J and $G_m=\rho(W_{m+1})$ are determined by (2.14) and (2.13).

Applying the trace identity[38]

$$\frac{\delta}{\delta u}\int \mathrm{tr}\left(W\frac{\partial U}{\partial \lambda}\right)dx=\lambda^{-\gamma}\frac{\partial}{\partial\lambda}\lambda^{\gamma}\mathrm{tr}\left(W\frac{\partial U}{\partial u}\right),$$

where γ is a constant to be determined, we can obtain

$$\frac{\delta\tilde{H}_l}{\delta u_{ij}}=W_{ji}^{(l)}, \quad \tilde{H}_l:=-\frac{1}{l}\int(\alpha_1W_{11}^{(l+1)}+\alpha_2W_{22}^{(l+1)}+\ldots+\alpha_nW_{nn}^{(l+1)})\,dx, \quad l\geqslant 1, \tag{2.20}$$

in which $1\leqslant i\neq j\leqslant n$ and γ is determined to be zero. In this computation, we need to note that

$$\mathrm{tr}\left(W\frac{\partial U}{\partial\lambda}\right)=\mathrm{tr}(WU_0)=\sum_{l\geqslant 0}(\alpha_1W_{11}^{(l)}+\alpha_2W_{22}^{(l)}+\ldots+\alpha_nW_{nn}^{(l)})\lambda^{-l},$$

and

$$\mathrm{tr}\left(W\frac{\partial U}{\partial u_{ij}}\right)=\mathrm{tr}(WE_{ij})=W_{ji}=\sum_{l\geqslant 0}W_{ji}^{(l)}\lambda^{-l}, \quad 1\leqslant i\neq j\leqslant n,$$

where E_{ij} is an $n\times n$ matrix whose (i,j) entry is one but other entries are all zero. Therefore, the isospectral hierarchy (2.19) has a bi-Hamiltonian formulation

$$u_{t_m}=X_m=J\frac{\delta\tilde{H}_{m+1}}{\delta u}=M\frac{\delta\tilde{H}_m}{\delta u}, \quad m\geqslant 1. \tag{2.21}$$

The first nonlinear system in the hierarchy (2.19) is the $1+1$ dimensional $\mathcal{N}$-wave interaction equations[39]

$$u_{ij,t_1}=\frac{\beta_i-\beta_j}{\alpha_i-\alpha_j}u_{ij,x}+\sum_{\substack{k=1\\k\neq i,j}}^{n}\left(\frac{\beta_i-\beta_k}{\alpha_i-\alpha_k}-\frac{\beta_k-\beta_j}{\alpha_k-\alpha_j}\right)u_{ik}u_{kj}, \quad 1\leqslant i\neq j\leqslant n. \tag{2.22}$$

This system is actually equivalent to the following equation in the matrix form

$$U_{1t_1}=W_{1x}-[U_1,W_1], \tag{2.23}$$

which can be rewritten as

$$P_{t_1}=Q_x-[P,Q], \quad [U_0,Q]=[W_0,P], \tag{2.24}$$

where P and Q are assumed to be two off-diagonal potential matrices. Based on (2.23), a vector field $\rho(\delta P)$ is a symmetry of (2.22) if the matrix δP satisfies the linearized system of (2.22):

$$(\delta P)_{t_1}=(\delta Q)_x-[U_1,\delta Q]-[\delta P,W_1] \tag{2.25}$$

with δQ being determined by

$$[U_0,\delta Q]=[W_0,\delta P]. \tag{2.26}$$

The $\mathcal{N}$-wave interaction equations (2.22) contains a couple of physically important nonlinear models as special reductions,[40] for example, three-wave interaction equations arising in fluid dynamics and plasma physics,[41–43] with U being chosen to be an anti-Hermitian matrix. Its Darboux transformation has been established in Ref. 44, which allows one to construct soliton solutions in a purely algebraic way. The Darboux transformation has also been analyzed for the $\mathcal{N}$-wave interaction equations with additional linear terms.[45]

B. Binary symmetry constraints in 1+1 dimensional case

We would like to present binary symmetry constraints of the $1+1$ dimensional $\mathcal{N}$-wave interaction equations (2.22). To this end, we need to introduce the adjoint spectral problem of (2.1):

$$\psi_x=-U^T(u,\lambda)\psi, \quad \psi=(\psi_1,\ldots,\psi_n)^T, \tag{2.27}$$

and the adjoint associated spectral problem of (2.17):

$$\psi_{t_m}=-V^{(m)T}(u,\lambda)\psi, \tag{2.28}$$

where U and $V^{(m)}$ are given as in (2.1) and (2.17), respectively. The compatability condition of (2.27) and (2.28) still gives rise to $u_{t_m}=X_m$ defined by (2.19).

The variational derivative of the spectral parameter λ with respect to the potential u can be calculated by (see Refs. 26, 28, or 16 for a detailed deduction)

$$\frac{\delta\lambda}{\delta u}=E^{-1}\psi^T\frac{\partial U}{\partial u}\phi, \quad \text{i.e.,} \ \frac{\delta\lambda}{\delta u_{ij}}=E^{-1}\phi_i\psi_j, \quad 1\leqslant i\neq j\leqslant n, \tag{2.29}$$

where E is the normalized constant:

$$E=-\int_{-\infty}^{\infty}\psi^T\frac{\partial U}{\partial\lambda}\phi\,dx.$$

A direct calculation can show that the variational derivative satisfies the following equation:

$$M\frac{\delta\lambda}{\delta u}=\lambda J\frac{\delta\lambda}{\delta u}. \tag{2.30}$$

Since λ does not vary with respect to time, we have a specific common symmetry $J(\delta\lambda/\delta u)$ of the hierarchy (2.19). To carry out binary nonlinearization, we take a Lie point symmetry of the $\mathcal{N}$-wave interaction equations (2.22),

$$Y_0:=\rho([\Gamma,U_1]), \quad \Gamma=\mathrm{diag}(\gamma_1,\ldots,\gamma_n), \tag{2.31}$$

where $\gamma_1,\gamma_2,\ldots,\gamma_n$ are arbitrary distinct constants ($X_0=JG_0$ is an example with $\Gamma=W_0$). It can be easily checked that

$$(\delta P, \delta Q) = ([\Gamma, U_1], [\Gamma, W_1])$$

satisfies (2.25), and thus Y_0 is a symmetry of (2.22). Then, make the following binary Bargmann symmetry constraint

$$Y_0 = \mu E J \frac{\delta \lambda}{\delta u} = \mu J \psi^T \frac{\partial U}{\partial u} \phi, \tag{2.32}$$

where μ is an arbitrary nonzero constant, J is defined by (2.14), and ϕ and ψ are the eigenfunction and adjoint eigenfunction of (2.1) and (2.27), respectively. Upon introducing N distinct eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_N$, we obtain a general binary symmetry constraint

$$Y_0 = J \sum_{s=0}^{N} \mu_s \psi^{(s)T} \frac{\partial U(u, \lambda_s)}{\partial u} \phi^{(s)} := Z_0, \tag{2.33}$$

where μ_s, $1 \leqslant s \leqslant N$, are N nonzero constants, and $\phi^{(s)}$ and $\psi^{(s)}$, $1 \leqslant s \leqslant N$, are eigenfunctions and adjoint eigenfunctions defined by

$$\phi_x^{(s)} = U(u, \lambda_s)\phi^{(s)}, \quad \psi_x^{(s)} = -U^T(u, \lambda_s)\psi^{(s)}, \quad 1 \leqslant s \leqslant N, \tag{2.34}$$

and

$$\phi_{t_1}^{(s)} = V^{(1)}(u, \lambda_s)\phi^{(s)}, \quad \psi_{t_1}^{(s)} = -V^{(1)T}(u, \lambda_s)\psi^{(s)}, \quad 1 \leqslant s \leqslant N. \tag{2.35}$$

Let us rewrite the left-hand side of (2.33) as the matrix form

$$\delta P = \rho^{-1}(Z_0) = \left[U_0, \sum_{s=1}^{N} \mu_s \phi^{(s)} \psi^{(s)T} \right], \tag{2.36}$$

which allows us to prove, by a direct computation as in Ref. 46 but more conveniently, that the vector field $Z_0 = \rho(\delta P)$ is really a symmetry of the $\mathcal{N}$-wave interaction equations (2.22). Now the symmetry problem is equivalent to showing that

$$(\delta P, \delta Q) = \left(\left[U_0, \sum_{s=1}^{N} \mu_s \phi^{(s)} \psi^{(s)T} \right], \left[W_0, \sum_{s=1}^{N} \mu_s \phi^{(s)} \psi^{(s)T} \right] \right) \tag{2.37}$$

satisfies the linearized system (2.25), when $\phi^{(s)}$ and $\psi^{(s)}$, $1 \leqslant s \leqslant N$, satisfy (2.34) and (2.35). A detailed proof will be given in Appendix A.

Therefore, we have the following binary symmetry constraint:

$$Y_0 = J \sum_{s=0}^{N} \mu_s \psi^{(s)T} \frac{\partial U(u, \lambda_s)}{\partial u} \phi^{(s)}, \quad \text{i.e.,} \quad [\Gamma, U_1] = \left[U_0, \sum_{s=1}^{N} \mu_s \phi^{(s)} \psi^{(s)T} \right]. \tag{2.38}$$

When N and μ_s vary, (2.38) provides us with a set of binary symmetry constraints of the $\mathcal{N}$-wave interaction equations (2.22). Let us assume that

$$\phi^{(s)} = (\phi_{1s}, \phi_{2s}, \ldots, \phi_{ns})^T, \quad \psi^{(s)} = (\psi_{1s}, \psi_{2s}, \ldots, \psi_{ns})^T, \tag{2.39}$$

in order to get an explicit expression for u from the symmetry constraint (2.38), and introduce two diagonal matrices

$$A = \mathrm{diag}(\lambda_1, \ldots, \lambda_N), \quad B = \mathrm{diag}(\mu_1, \ldots, \mu_N), \tag{2.40}$$

which will be used throughout our discussion. Solving the Bargmann symmetry constraint (2.38) for u, we obtain

$$u_{ij}=\tilde{u}_{ij}:=\frac{\alpha_i-\alpha_j}{\gamma_i-\gamma_j}\langle\Phi_i,B\Psi_j\rangle,\quad 1\leqslant i\neq j\leqslant n, \tag{2.41}$$

where B is given by (2.40), and Φ_i and Ψ_i are defined by

$$\Phi_i=(\phi_{i1},\phi_{i2},\ldots,\phi_{iN})^T,\quad \Psi_i=(\psi_{i1},\psi_{i2},\ldots,\psi_{iN})^T,\quad 1\leqslant i\leqslant n, \tag{2.42}$$

and $\langle\cdot,\cdot\rangle$ denotes the standard inner-product of the Euclidean space $\mathbb{R}^N$.

Note that the compatability condition of (2.34) and (2.35) is still nothing but the $1+1$ dimensional $\mathcal{N}$-wave interaction equations (2.22). Now using (2.41), we nonlinearize the spatial part (2.34) and the temporal part (2.35) of spectral problems and adjoint spectral problems of the $\mathcal{N}$-wave interaction equations (2.22). Namely we replace u_{ij} with $\tilde{u}_{ij}$ in N replicas of the spectral problems and adjoint spectral problems (2.34) and N replicas of the associated spectral problems and adjoint associated spectral problems (2.35), and then obtain two constrained flows for the $\mathcal{N}$-wave interaction equations (2.22):

$$\phi_x^{(s)}=U(\tilde{u},\lambda_s)\phi^{(s)},\quad \psi_x^{(s)}=-U^T(\tilde{u},\lambda_s)\psi^{(s)},\quad 1\leqslant s\leqslant N, \tag{2.43}$$

and

$$\phi_{t_1}^{(s)}=V^{(1)}(\tilde{u},\lambda_s)\phi^{(s)},\quad \psi_{t_1}^{(s)}=-V^{(1)T}(\tilde{u},\lambda_s)\psi^{(s)},\quad 1\leqslant s\leqslant N, \tag{2.44}$$

where $\tilde{u}=\rho((\tilde{u}_{ij})_{n\times n})$ is defined like u. For example, when $n\geqslant 4$, we have

$$\tilde{u}=(\tilde{u}_{21},\tilde{u}_{12},\tilde{u}_{31},\tilde{u}_{13},\tilde{u}_{14},\tilde{u}_{41},\tilde{u}_{23},\tilde{u}_{32},\ldots,\tilde{u}_{n,n-1},\tilde{u}_{n-1,n})^T. \tag{2.45}$$

In order to analyze the Liouville integrability of the above two constrained flows, let us first introduce a symplectic structure

$$\omega^2=\sum_{i=1}^{n}Bd\Phi_i\wedge d\Psi_i=\sum_{i=1}^{n}\sum_{s=1}^{N}\mu_s d\phi_{is}\wedge d\psi_{is} \tag{2.46}$$

over $\mathbb{R}^{2nN}$, and then the corresponding Poisson bracket

$$\begin{aligned}\{f,g\}=\omega^2(Idg,Idf)&=\sum_{i=1}^{n}\left(\left\langle\frac{\partial f}{\partial\Psi_i},B^{-1}\frac{\partial g}{\partial\Phi_i}\right\rangle-\left\langle\frac{\partial f}{\partial\Phi_i},B^{-1}\frac{\partial g}{\partial\Psi_i}\right\rangle\right)\\&=\sum_{i=1}^{n}\sum_{s=1}^{N}\mu_s^{-1}\left(\frac{\partial f}{\partial\psi_{is}}\frac{\partial g}{\partial\phi_{is}}-\frac{\partial f}{\partial\phi_{is}}\frac{\partial g}{\partial\psi_{is}}\right),\quad f,g\in C^\infty(\mathbb{R}^{2nN}),\end{aligned} \tag{2.47}$$

where the vector field Idf is defined by

$$\omega^2(X,Idf)=df(X),\quad X\in T(\mathbb{R}^{2nN}).$$

A Hamiltonian system with a Hamiltonian H defined over the symplectic manifold $(\mathbb{R}^{2nN},\omega^2)$ is given by

$$\Phi_{it}=\{\Phi_i,H\}=-B^{-1}\frac{\partial H}{\partial\Psi_i},\quad \Psi_{it}=\{\Psi_i,H\}=B^{-1}\frac{\partial H}{\partial\Phi_i},\quad 1\leqslant i\leqslant n, \tag{2.48}$$

where t is assumed to be the evolution variable. Second, we need a matrix Lax operator

$$L^{(1)}(\lambda)=C_1+D_1(\lambda), \tag{2.49}$$

with C_1 and $D_1(\lambda)$ being defined by

$$C_1=\Gamma=\mathrm{diag}(\gamma_1,\ldots,\gamma_n),\quad D_1(\lambda)=(D_{ij}^{(1)}(\lambda))_{n\times n},\quad D_{ij}^{(1)}(\lambda)=\sum_{s=1}^{N}\frac{\mu_s}{\lambda-\lambda_s}\phi_{is}\psi_{js}, \tag{2.50}$$

where $1\leqslant i,\ j\leqslant n$. Note that upon taking binary nonlinearization, we obtain

$$U(\tilde{u},\lambda)=\lambda U_0+U_1(\tilde{u})=\lambda U_0+(\tilde{u}_{ij}),\ \ \tilde{u}_{ij}=\frac{\alpha_i-\alpha_j}{\gamma_i-\gamma_j}\langle\Phi_i,B\Psi_j\rangle, \tag{2.51}$$

$$V^{(1)}(\tilde{u},\lambda)=\lambda W_0+W_1(\tilde{u})=\lambda W_0+(\tilde{v}_{ij}),\ \ \tilde{v}_{ij}:=\frac{\beta_i-\beta_j}{\alpha_i-\alpha_j}\tilde{u}_{ij}=\frac{\beta_i-\beta_j}{\gamma_i-\gamma_j}\langle\Phi_i,B\Psi_j\rangle, \tag{2.52}$$

where $1\leqslant i,\ j\leqslant n$.

Theorem 2.1: *Under the symplectic structure (2.46), the spatial constrained flow (2.43) and the temporal constrained flow (2.44) for the 1+1 dimensional $\mathcal{N}$-wave interaction equations (2.22) are Hamiltonian systems with the evolution variables x and t_1, and the Hamiltonians*

$$H_1^x=-\sum_{k=1}^{n}\alpha_k\langle A\Phi_k,B\Psi_k\rangle-\sum_{1\leqslant k<l\leqslant n}\frac{\alpha_k-\alpha_l}{\gamma_k-\gamma_l}\langle\Phi_k,B\Psi_l\rangle\langle\Phi_l,B\Psi_k\rangle, \tag{2.53}$$

$$H_1^{t_1}=-\sum_{k=1}^{n}\beta_k\langle A\Phi_k,B\Psi_k\rangle-\sum_{1\leqslant k<l\leqslant n}\frac{\beta_k-\beta_l}{\gamma_k-\gamma_l}\langle\Phi_k,B\Psi_l\rangle\langle\Phi_l,B\Psi_k\rangle, \tag{2.54}$$

respectively, where A and B are defined by (2.40), and Φ_i and Ψ_i, $1\leqslant i\leqslant n$, are defined by (2.42). Moreover, they possess necessary Lax representations, i.e., we have

$$(L^{(1)}(\lambda))_x=[U(\tilde{u},\lambda),L^{(1)}(\lambda)],\quad (L^{(1)}(\lambda))_{t_1}=[V^{(1)}(\tilde{u},\lambda),L^{(1)}(\lambda)], \tag{2.55}$$

where $L^{(1)}(\lambda)$, U, and $V^{(1)}(\lambda)$ are given by (2.49)–(2.52), if (2.43) and (2.44) hold, respectively.

Proof: A direct calculation can show the Hamiltonian structures of the spatial constrained flow (2.43) and the temporal constrained flow (2.44) with H_1^x and H_1^t defined by (2.53) and (2.54). Let us then check the Lax representations. By using (2.43), we can compute that

$$\begin{aligned}
(L^{(1)}(\lambda))_x&=\sum_{s=1}^{N}\frac{\mu_s}{\lambda-\lambda_s}(\phi_x^{(s)}\psi^{(s)T}+\phi^{(s)}\psi_x^{(s)T})\\
&=\sum_{s=1}^{N}\frac{\mu_s}{\lambda-\lambda_s}(U(\tilde{u},\lambda_s)\phi^{(s)}\psi^{(s)T}-\phi^{(s)}\psi^{(s)T}U(\tilde{u},\lambda_s))\\
&=\sum_{s=1}^{N}\frac{\mu_s}{\lambda-\lambda_s}[U(\tilde{u},\lambda_s),\phi^{(s)}\psi^{(s)T}]\\
&=[U(\tilde{u},\lambda),L^{(1)}(\lambda)-C_1]-\left[U_0,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right]\\
&=[U(\tilde{u},\lambda),L^{(1)}(\lambda)]+[C_1,U(\tilde{u},\lambda)]-\left[U_0,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right]\\
&=[U(\tilde{u},\lambda),L^{(1)}(\lambda)]+[C_1,U_1(\tilde{u})]-\left[U_0,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right].
\end{aligned}$$

This implies that $(L^{(1)}(\lambda))_x=[U(\tilde{u},\lambda),L^{(1)}(\lambda)]$ if and only if

$$[C_1,U_1(\tilde{u})]=\left[U_0,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right].$$

The above equality equivalently requires the constraints on the potentials shown in (2.41). Therefore, the spatial constrained flow (2.43) has the necessary Lax representation defined as in (2.55). The proof of the other necessary Lax representation $(L^{(1)}(\lambda))_{t_1}=[V^{(1)}(\tilde{u},\lambda),L^{(1)}(\lambda)]$ is completely similar, and thus we omit it. The proof is finished. ■

We remark that the Lax representations (2.55) are not sufficient. Namely, we cannot obtain the spatial constrained flow (2.43) or the temporal constrained flow (2.44) from the corresponding Lax representation in (2.55). This can be easily observed by considering a special class of solutions of (2.55). For example, either any vector functions $\phi^{(s)}$ with $\psi^{(s)}=0$, $1\leqslant s\leqslant N$, or any vector functions $\psi^{(s)}$ with $\phi^{(s)}=0$, $1\leqslant s\leqslant N$, will solve (2.55), but it is easy to see that they do not always solve (2.43) [or (2.44)] since $\phi^{(s)}$ and $\psi^{(s)}$, $1\leqslant s\leqslant N$, have to solve some ordinary differential equations (ODEs) resulting from (2.43) [or (2.44)].

III. BINARY SYMMETRY CONSTRAINTS IN 2+1 DIMENSIONS

A. 2+1 dimensional $\mathcal{N}$-wave interaction equations

Let n be an arbitrary natural number strictly greater than 2. Similar to the case of the $1+1$ dimensional **N**-wave interaction equations, let us begin with the Lax system

$$F_y=JF_x+PF,\quad F_t=KF_x+QF,\quad F=(f_1,\ldots,f_n)^T \tag{3.1}$$

in $2+1$ dimensions. Here it is assumed that

$$J=\mathrm{diag}(J_1,\ldots,J_n),\quad K=\mathrm{diag}(K_1,\ldots,K_n),\quad J_i\neq J_j,\quad K_i\neq K_j,\quad 1\leqslant i\neq j\leqslant n, \tag{3.2}$$

are two constant diagonal matrices, and P and Q are two $n\times n$ off-diagonal potential matrices

$$P=P(x,y,t)=(p_{ij})_{n\times n},\quad Q=Q(x,y,t)=(q_{ij})_{n\times n}. \tag{3.3}$$

The compatability condition $F_{yt}=F_{ty}$ of the Lax system (3.1) reads as

$$[J,Q]=[K,P],\quad P_t-Q_y+[P,Q]+JQ_x-KP_x=0, \tag{3.4}$$

which is called the $2+1$ dimensional $\mathcal{N}$-wave interaction equations.[47] The equation $[J,Q]=[K,P]$ tells us that Q can be represented by P and vice versa, and so, practically, we have just one of two potential matrices to be solved. The adjoint system of the Lax system (3.1) is given by

$$G_y=JG_x-P^TG,\quad G_t=KG_x-Q^TG,\quad G=(g_1,\ldots,g_n)^T, \tag{3.5}$$

whose compatability condition $G_{yt}=G_{ty}$ still gives rise to the $2+1$ dimensional $\mathcal{N}$-wave interaction equations (3.4).

We first use a symmetry constraint of the $2+1$ dimensional $\mathcal{N}$-wave interaction equations (3.4) to change the above problem in $2+1$ dimensions to three problems in $1+1$ dimensions. As made in Refs. 48, and 49, we introduce the spectral problems

$$\phi_x=\Omega^x(F,G,\lambda)\phi=(\lambda\Omega_0^x+\Omega_1^x)\phi=\begin{pmatrix}\lambda I_n & F\\ G^T & 0\end{pmatrix}\phi, \tag{3.6a}$$

$$\phi_y=\Omega^y(P,F,G,\lambda)\phi=(\lambda\Omega_0^y+\Omega_1^y)\phi=\begin{pmatrix}\lambda J+P & JF\\ G^TJ & 0\end{pmatrix}\phi, \tag{3.6b}$$

$$\phi_t=\Omega^t(Q,F,G,\lambda)\phi=(\lambda\Omega_0^t+\Omega_1^t)\phi=\begin{pmatrix}\lambda K+Q & KF\\ G^TK & 0\end{pmatrix}\phi, \tag{3.6c}$$

where I_n is the nth-order identity matrix and $\phi=(\phi_1,\ldots,\phi_n,\phi_{n+1})^T$. The new extended potentials in the above spectral systems consist of not only the original potentials, P and Q, but also the solutions of the Lax system and the adjoint Lax system, F and G. The compatability conditions $\phi_{xy}=\phi_{yx}$, $\phi_{xt}=\phi_{tx}$, and $\phi_{yt}=\phi_{yt}$ give rise to the $2+1$ dimensional $\mathcal{N}$-wave interaction equations (3.4), the original Lax system (3.1) and its adjoint system (3.5), and the nonlinear symmetry constraint of (3.4):

$$P_x=[FG^T,J],\quad Q_x=[FG^T,K]. \tag{3.7}$$

It is easy to check that $(\delta P,\delta Q)=([FG^T,J],[FG^T,K])$ satisfies the linearized system of the $2+1$ dimensional $\mathcal{N}$-wave interaction equations (3.4):

$$[J,\delta Q]=[K,\delta P],\quad (\delta P)_t-(\delta Q)_y+[\delta P,Q]+[P,\delta Q]+J(\delta Q)_x-K(\delta P)_x=0, \tag{3.8}$$

when F and G solve the Lax system (3.1) and the adjoint Lax system (3.5), respectively. Therefore, (3.7) is really a symmetry constraint of the $2+1$ dimensional $\mathcal{N}$-wave interaction equations (3.4), since both sides of (3.7) are symmetries of (3.4). Now we see that the original problem in $2+1$ dimensions is transformed into three problems in $1+1$ dimensions. The spectral problems (3.6) are our starting point to make a link of the $2+1$ dimensional $\mathcal{N}$-wave interaction equations (3.4) to finite-dimensional integrable systems.

B. Binary symmetry constraints in 2+1 dimensional case

Let us start from the spectral problems in (3.6), which are similar to those for the $1+1$ dimensional $\mathcal{N}$-wave interaction equations (2.22). The main difference is that the coefficient matrix of λ in the x-part of the spectral problems (3.6) is

$$\Omega_0^x=\mathrm{diag}(\underbrace{1,\ldots,1}_{n},0), \tag{3.9}$$

whose diagonal entries are not distinct. However, the y-part of the spectral problems (3.6) has the same property as the spectral problem (2.1) in $1+1$ dimensions. Therefore, we use the y-part of the spectral problems (3.6) to compute the variational derivatives of λ:

$$\frac{\delta\lambda}{\delta p_{ij}}=E^{-1}\psi^T\frac{\partial\Omega^y}{\partial p_{ij}}\phi=E^{-1}\phi_i\psi_j,\quad \frac{\delta\lambda}{\delta q_{ij}}=E^{-1}\psi^T\frac{\partial\Omega^y}{\partial q_{ij}}\phi=E^{-1}\frac{J_i-J_j}{K_i-K_j}\phi_i\psi_j,\quad 1\leqslant i\neq j\leqslant n,$$

$$\frac{\delta\lambda}{\delta f_i}=E^{-1}\psi^T\frac{\partial\Omega^y}{\partial f_i}\phi=E^{-1}J_i\phi_{n+1}\psi_i,\quad \frac{\delta\lambda}{\delta g_i}=E^{-1}\psi^T\frac{\partial\Omega^y}{\partial g_i}\phi=E^{-1}J_i\phi_i\psi_{n+1},\quad 1\leqslant i\leqslant n,$$

where E is the normalized constant, and $\psi=(\psi_1,\ldots,\psi_n,\psi_{n+1})^T$ is an adjoint eigenfunction of the adjoint spectral problems

$$\psi_x=-(\Omega^x(F,G,\lambda))^T\psi=-(\lambda(\Omega_0^x)^T+(\Omega_1^x)^T)\psi=-\begin{pmatrix}\lambda I_n & G\\ F^T & 0\end{pmatrix}\psi, \tag{3.10a}$$

$$\psi_y=-(\Omega^y(P,F,G,\lambda))\psi=-(\lambda(\Omega_0^y)+(\Omega_1^y)^T)\psi=-\begin{pmatrix}\lambda J+P^T & JG\\ F^TJ & 0\end{pmatrix}\psi, \tag{3.10b}$$

$$\psi_t=-(\Omega^t(Q,F,G,\lambda))^T\psi=-(\lambda(\Omega_0^t)^T+(\Omega_1^t)^T)\psi=-\begin{pmatrix}\lambda K+Q^T & KG\\ F^TK & 0\end{pmatrix}\psi. \tag{3.10c}$$

These variational derivatives of λ give us a conserved covariant and also a clue to compute a required symmetry, expressed in terms of eigenfunctions and adjoint eigenfunctions.

As in the $1+1$ dimensional case, upon introducing N distinct eigenvalues $\lambda_1,\lambda_2,\ldots,\lambda_N$, we have

$$\phi_x^{(s)}=\Omega^x(u,\lambda_s)\phi^{(s)},\quad \phi_y^{(s)}=\Omega^y(u,\lambda_s)\phi^{(s)},\quad \phi_t^{(s)}=\Omega^t(u,\lambda_s)\phi^{(s)},\quad 1\leqslant s\leqslant N, \tag{3.11}$$

and

$$\psi_x^{(s)}=-(\Omega^x)^T(u,\lambda_s)\psi^{(s)},\quad \psi_y^{(s)}=-(\Omega^y)^T(u,\lambda_s)\psi^{(s)},\quad \psi_t^{(s)}=-(\Omega^t)^T(u,\lambda_s)\psi^{(s)},\quad 1\leqslant s\leqslant N, \tag{3.12}$$

where $\phi^{(s)}$ and $\psi^{(s)}$ are $n+1$ dimensional vector functions:

$$\phi^{(s)}=(\phi_{1s},\ldots,\phi_{ns},\phi_{n+1,s})^T,\quad \psi^{(s)}=(\psi_{1s},\ldots,\psi_{ns},\psi_{n+1,s})^T,\quad 1\leqslant s\leqslant N. \tag{3.13}$$

To carry out binary nonlinearization, we need to construct two special symmetries, one of which is a Lie point symmetry, and the other of which is not a Lie point, contact or Lie–Bäcklund symmetry, but generated from (3.11) and (3.12). Let us choose a set of $n+1$ arbitrary distinct constants $\delta_1,\ldots,\delta_n,\delta_{n+1}$, and set

$$\Delta=\mathrm{diag}(\delta_1,\ldots,\delta_n). \tag{3.14}$$

Similar to the $1+1$ dimensional case, it can be directly shown that

$$(\delta P,\delta Q,\delta F,\delta G)=([\Delta,P],[\Delta,Q],\Delta F-\delta_{n+1}F,\Delta G-\delta_{n+1}G) \tag{3.15}$$

and

$$\begin{gathered}\delta p_{ij}=(J_i-J_j)\langle\Phi_i,B\Psi_j\rangle,\quad \delta q_{ij}=(K_i-K_j)\langle\Phi_i,B\Psi_j\rangle,\quad 1\leqslant i\neq j\leqslant n,\\ \delta f_i=\langle\Phi_i,B\Psi_{n+1}\rangle,\quad \delta g_i=\langle\Phi_{n+1},B\Psi_i\rangle,\quad 1\leqslant i\leqslant n,\end{gathered} \tag{3.16}$$

are two symmetries of the equations (3.4), (3.1) and (3.5). That is to say, that they satisfy the linearized system of the equations (3.4), (3.1) and (3.5): the first subsystem (3.8) and the second subsystem

$$\begin{gathered}(\delta F)_y=J(\delta F)_x+(\delta P)F+P\,\delta F,\quad (\delta F)_t=K(\delta F)_x+(\delta Q)F+Q\,\delta F,\\ (\delta G)_y=J(\delta G)_x-(\delta P)^TG-P^T\delta G,\quad (\delta G)_t=K(\delta G)_x-(\delta Q)^TG-Q^T\delta G,\end{gathered} \tag{3.17}$$

for all solutions (P,Q,F,G) of (3.4), (3.1) and (3.5). Here we remind that

$$B=\mathrm{diag}(\mu_1,\ldots,\mu_N)^T$$

is defined by (2.40), $\langle\cdot,\cdot\rangle$ denotes the standard inner product of $\mathbb{R}^N$, and Φ_i and Ψ_i are similarly defined as

$$\Phi_i=(\phi_{i1},\phi_{i2},\ldots,\phi_{iN})^T,\quad \Psi_i=(\psi_{i1},\psi_{i2},\ldots,\psi_{iN})^T,\quad 1\leqslant i\leqslant n+1. \tag{3.18}$$

Now a binary Bargmann symmetry constraint of (3.4), (3.1) and (3.5) can be taken as

$$([\Delta,P])_{ij}=(J_i-J_j)\langle\Phi_i,B\Psi_j\rangle,\quad ([\Delta,Q])_{ij}=(K_i-K_j)\langle\Phi_i,B\Psi_j\rangle,\quad 1\leqslant i\neq j\leqslant n, \tag{3.19}$$

$$(\Delta F-\delta_{n+1}F)_i=\langle\Phi_i,B\Psi_{n+1}\rangle,\quad (\Delta G-\delta_{n+1}G)_i=\langle\Phi_{n+1},B\Psi_i\rangle,\quad 1\leqslant i\leqslant n. \tag{3.20}$$

This symmetry constraint gives us the following choice for the constraints on the extended potentials

$$p_{ij}=\tilde{p}_{ij}:=\frac{J_i-J_j}{\delta_i-\delta_j}\langle\Phi_i,B\Psi_j\rangle,\quad q_{ij}=\tilde{q}_{ij}:=\frac{K_i-K_j}{\delta_i-\delta_j}\langle\Phi_i,B\Psi_j\rangle,\quad 1\leqslant i\neq j\leqslant n, \tag{3.21}$$

$$f_i=\tilde{f}_i:=\frac{1}{\delta_i-\delta_{n+1}}\langle\Phi_i,B\Psi_{n+1}\rangle,\quad g_i=\tilde{g}_i:=\frac{1}{\delta_i-\delta_{n+1}}\langle\Phi_{n+1},B\Psi_i\rangle,\quad 1\leqslant i\leqslant n. \tag{3.22}$$

One can express the above symmetry constraint in another way. Actually, it can be proved that

$$(\delta P,\delta Q)=([\Delta,P],[\Delta,Q]),$$

and under the constraint (3.22),

$$\delta p_{ij}=(J_i-J_j)\langle\Phi_i,B\Psi_j\rangle,\quad \delta q_{ij}=(K_i-K_j)\langle\Phi_i,B\Psi_j\rangle,\quad 1\leqslant i\neq j\leqslant n,$$

are two symmetries of the $2+1$ dimensional $\mathcal{N}$-wave interaction equations (3.4).

Now plug the above expressions for the extended potentials, (3.21) and (3.22), into the spectral problems (3.6) and the adjoint spectral problems (3.10), and then we get the constrained flows

$$\phi_x^{(s)}=\Omega^x(\tilde{F},\tilde{G},\lambda_s)\phi^{(s)},\quad \psi_x^{(s)}=-(\Omega^x(\tilde{F},\tilde{G},\lambda_s))^T\psi^{(s)}, \tag{3.23}$$

$$\phi_y^{(s)}=\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda_s)\phi^{(s)},\quad \psi_y^{(s)}=-(\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda_s))^T\psi^{(s)}, \tag{3.24}$$

$$\phi_t^{(s)}=\Omega^t(\tilde{Q},\tilde{F},\tilde{G},\lambda_s)\phi^{(s)},\quad \psi_t^{(s)}=-(\Omega^t(\tilde{Q},\tilde{F},\tilde{G},\lambda_s))^T\psi^{(s)}, \tag{3.25}$$

where

$$\tilde{P}=(\tilde{p}_{ij})_{n\times n},\quad \tilde{Q}=(\tilde{q}_{ij})_{n\times n},\quad \tilde{F}=(\tilde{f}_1,\ldots,\tilde{f}_n)^T,\quad \tilde{G}=(\tilde{g}_1,\ldots,\tilde{g}_n)^T. \tag{3.26}$$

All these three constrained flows are systems of ordinary differential equations of ϕ_{is} and ψ_{is}, $1\leqslant i\leqslant n+1$, $1\leqslant s\leqslant N$.

We introduce the symplectic structure

$$\omega^2=\sum_{i=1}^{n+1}Bd\Phi_i\wedge d\Psi_i=\sum_{i=1}^{n+1}\sum_{s=1}^{N}\mu_s d\phi_{is}\wedge d\psi_{is} \tag{3.27}$$

over $\mathbb{R}^{2(n+1)N}$. The corresponding Poisson bracket and the corresponding Hamiltonian form with the Hamiltonian H and the evolution variable t are similarly taken as

$$\{f,g\}=\sum_{i=1}^{n+1}\left(\left\langle\frac{\partial f}{\partial\Psi_i},B^{-1}\frac{\partial g}{\partial\Phi_i}\right\rangle-\left\langle\frac{\partial f}{\partial\Phi_i},B^{-1}\frac{\partial g}{\partial\Psi_i}\right\rangle\right),\quad f,g\in C^\infty(\mathbb{R}^{2(n+1)N}), \tag{3.28}$$

$$\Phi_{it}=\{\Phi_i,H\}=-B^{-1}\frac{\partial H}{\partial\Psi_i},\quad \Psi_{it}=\{\Psi_i,H\}=B^{-1}\frac{\partial H}{\partial\Phi_i},\quad 1\leqslant i\leqslant n+1. \tag{3.29}$$

Similar to Theorem 2.1, we have the following.

Theorem 3.1: *Under the symplectic structure (3.27), three constrained flows (3.23), (3.24) and (3.25) are Hamiltonian systems with the evolution variables x, y and t, and the Hamiltonians*

$$H_2^x=-\sum_{k=1}^{n}\langle A\Phi_k,B\Psi_k\rangle-\sum_{k=1}^{n}\frac{1}{\delta_k-\delta_{n+1}}\langle\Phi_k,B\Psi_{n+1}\rangle\langle\Phi_{n+1},B\Psi_k\rangle, \tag{3.30}$$

$$H_2^y=-\sum_{k=1}^{n} J_k\langle A\Phi_k,B\Psi_k\rangle-\sum_{1\leqslant k<l\leqslant n}\frac{J_k-J_l}{\delta_k-\delta_l}\langle\Phi_k,B\Psi_l\rangle\langle\Phi_l,B\Psi_k\rangle$$
$$-\sum_{k=1}^{n}\frac{J_k}{\delta_k-\delta_{n+1}}\langle\Phi_k,B\Psi_{n+1}\rangle\langle\Phi_{n+1},B\Psi_k\rangle, \tag{3.31}$$

$$H_2^t=-\sum_{k=1}^{n} K_k\langle A\Phi_k,B\Psi_k\rangle-\sum_{1\leqslant k<l\leqslant n}\frac{K_k-K_l}{\delta_k-\delta_l}\langle\Phi_k,B\Psi_l\rangle\langle\Phi_l,B\Psi_k\rangle$$
$$-\sum_{k=1}^{n}\frac{K_k}{\delta_k-\delta_{n+1}}\langle\Phi_k,B\Psi_{n+1}\rangle\langle\Phi_{n+1},B\Psi_k\rangle, \tag{3.32}$$

respectively, where A and B are defined by (2.40), Φ_i *and* Ψ_i, $1\leqslant i\leqslant n+1$, *are defined by (3.18). Moreover, they possess the necessary Lax representations*

$$(L^{(2)}(\lambda))_x=[\Omega^x(\tilde{F},\tilde{G},\lambda),L^{(2)}(\lambda)], \tag{3.33}$$

$$(L^{(2)}(\lambda))_y=[\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda),L^{(2)}(\lambda)], \tag{3.34}$$

$$(L^{(2)}(\lambda))_t=[\Omega^t(\tilde{Q},\tilde{F},\tilde{G},\lambda),L^{(2)}(\lambda)], \tag{3.35}$$

respectively, where $\tilde{P}$, $\tilde{Q}$, $\tilde{F}$ *and* $\tilde{G}$ *are given by (3.26), (3.21) and (3.22), and* $L^{(2)}(\lambda)$ *is defined by*

$$L^{(2)}(\lambda)=C_2+D_2(\lambda),\quad C_2=\mathrm{diag}(\Delta,\delta_{n+1})=\mathrm{diag}(\delta_1,\ldots,\delta_n,\delta_{n+1}),$$
$$D_2=(D_{ij}^{(2)})_{n+1,n+1},\quad D_{ij}^{(2)}=\sum_{s=1}^{N}\frac{\mu_s}{\lambda-\lambda_s}\phi_{is}\psi_{js},\quad 1\leqslant i,j\leqslant n+1. \tag{3.36}$$

Proof: It can be verified by a direct calculation that all three constrained flows (3.23)–(3.25) have the Hamiltonian structures under the symplectic structure (3.27) with the Hamiltonian functions H_2^x, H_2^y and H_2^t shown in (3.30)–(3.32). Let us now check three Lax representations (3.33)–(3.35). Since the proofs are similar for all three cases, we just show the second case, i.e., the Lax representation of the constrained flow (3.24). By using (3.24), we can compute that

$$(L^{(2)}(\lambda))_y=\sum_{s=1}^{N}\frac{\mu_s}{\lambda-\lambda_s}(\phi_y^{(s)}\psi^{(s)T}+\phi^{(s)}\psi_y^{(s)T})$$
$$=\sum_{s=1}^{N}\frac{\mu_s}{\lambda-\lambda_s}(\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda_s)\phi^{(s)}\psi^{(s)T}-\phi^{(s)}\psi^{(s)T}\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda_s))$$
$$=\sum_{s=1}^{N}\frac{\mu_s}{\lambda-\lambda_s}[\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda_s),\phi^{(s)}\psi^{(s)T}]$$
$$=\sum_{s=1}^{N}\frac{\mu_s}{\lambda-\lambda_s}([\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda),\phi^{(s)}\psi^{(s)T}]-[\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda)$$
$$-\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda_s),\phi^{(s)}\psi^{(s)T}])$$
$$=[\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda),L^{(2)}(\lambda)-C_2]-\left[\Omega_0^y,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right]$$
$$=[\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda),L^{(2)}(\lambda)]-[\Omega_1^y(\tilde{P},\tilde{F},\tilde{G}),C_2]-\left[\Omega_0^y,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right].$$

Therefore, it follows that $(L^{(2)}(\lambda))_y=[\Omega^y(\tilde{P},\tilde{F},\tilde{G},\lambda),L^{(2)}(\lambda)]$ if and only if

$$[C_2,\Omega_1^y(\tilde{P},\tilde{F},\tilde{G})]=\left[\Omega_0^y,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right].$$

This equality equivalently requires the nonlinear constraints on the potentials defined by (3.21) and (3.22). Therefore, the constrained flow (3.24) has the necessary Lax representation shown in (3.34). The proof is finished. ■

We also remark that the Lax representations (3.33)–(3.35) are not sufficient to generate the corresponding constrained flows defined by (3.23)–(3.25), since the Gateaux derivative operators of the Lax operators Ω^x, Ω^y and Ω^t given in (3.23)–(3.25) are not injective. However, it will be shown that they are good enough in generating integrals of motion of the constrained flows.

IV. AN INVOLUTIVE AND FUNCTIONALLY INDEPENDENT SYSTEM OF POLYNOMIAL FUNCTIONS

Let m be an arbitrary natural number. We start from an mth-order matrix Lax operator

$$L(\lambda)=L(\lambda;c_1,\ldots,c_m)=C+D(\lambda), \tag{4.1}$$

with C and $D(\lambda)$ being defined by

$$C=\mathrm{diag}(c_1,\ldots,c_m),\quad D(\lambda)=(D_{ij}(\lambda))_{m\times m},\quad D_{ij}(\lambda)=\sum_{s=1}^{N}\frac{\mu_s}{\lambda-\lambda_s}\phi_{is}\psi_{js},\quad 1\leqslant i,j\leqslant m. \tag{4.2}$$

Here c_i, λ_s, and μ_s are arbitrary constants satisfying

$$\prod_{s=1}^{N}\mu_s\neq 0,\quad \lambda_i\neq\lambda_j,\quad 1\leqslant i\neq j\leqslant N, \tag{4.3}$$

and ϕ_{is} and ψ_{js} are pairs of canonical variables of the symplectic manifold $(\mathbb{R}^{2mN},\omega^2)$ with the symplectic structure

$$\omega^2=\sum_{i=1}^{m}\sum_{s=1}^{N}\mu_s d\phi_{is}\wedge d\psi_{is}. \tag{4.4}$$

The corresponding Poisson bracket reads as

$$\{f,g\}=\omega^2(Idg,Idf)=\sum_{i=1}^{m}\sum_{s=1}^{N}\mu_s^{-1}\left(\frac{\partial f}{\partial\psi_{is}}\frac{\partial g}{\partial\phi_{is}}-\frac{\partial f}{\partial\phi_{is}}\frac{\partial g}{\partial\psi_{is}}\right),\quad f,g\in C^\infty(\mathbb{R}^{2mN}). \tag{4.5}$$

A. r-matrix formulation

As usual, two special matrices defined by the tensor product of matrices are chosen as

$$L_1(\lambda)=L(\lambda)\otimes I_m,\quad L_2(\mu)=I_m\otimes L(\mu), \tag{4.6}$$

where I_m is the mth-order identity matrix, and

$$(A\otimes B)_{ij,kl}=a_{ik}b_{jl}\ \text{ if }\ A=(a_{ij})\ \text{ and }\ B=(b_{ij}). \tag{4.7}$$

We want to find an $m^2\times m^2$ matrix $\mathbf{r}=\mathbf{r}(\lambda,\mu)$ so that we have an $\mathbf{r}$-matrix formulation[50,51]

$$\{L(\lambda)\overset{\otimes}{,}L(\mu)\}=[\mathbf{r}(\lambda,\mu),L_1(\lambda)+L_2(\mu)], \tag{4.8}$$

with the Poisson bracket $\{L(\lambda)\overset{\otimes}{,}L(\mu)\}$ being defined by

$$(\{L(\lambda)\overset{\otimes}{,}L(\mu)\})_{ij,kl}=\{L_{ik}(\lambda),L_{jl}(\mu)\}=\omega^2(IdL_{jl}(\mu),IdL_{ik}(\lambda)),\quad 1\leqslant i,j,k,l\leqslant m, \tag{4.9}$$

where $L=(L_{ij})_{m\times m}$ is assumed. Let us first compute $\{L_{ij}(\lambda),L_{kl}(\mu)\}$. When $i\neq l$ and $j\neq k$, it is easy to obtain $\{L_{ij}(\lambda),L_{kl}(\mu)\}=0$. When $i\neq l$ and $j=k$, we have

$$\begin{aligned}\{L_{ij}(\lambda),L_{jl}(\mu)\}&=\sum_{s=1}^{N}\mu_s\frac{\phi_{is}}{\lambda-\lambda_s}\frac{\psi_{ls}}{\mu-\lambda_s}\\&=\sum_{s=1}^{N}\frac{1}{\mu-\lambda}\left(\frac{\mu_s}{\lambda-\lambda_s}-\frac{\mu_s}{\mu-\lambda_s}\right)\phi_{is}\psi_{ls}\\&=\frac{1}{\mu-\lambda}(L_{il}(\lambda)-L_{il}(\mu)).\end{aligned}$$

Similarly, when $i=l$ and $j\neq k$, we have

$$\{L_{ij}(\lambda),L_{ki}(\mu)\}=-\sum_{s=1}^{N}\mu_s\frac{\psi_{js}}{\lambda-\lambda_s}\frac{\phi_{ks}}{\mu-\lambda_s}=\frac{1}{\mu-\lambda}(L_{kj}(\mu)-L_{kj}(\lambda)),$$

and when $i=l$ and $j=k$, we have

$$\begin{aligned}\{L_{ij}(\lambda),L_{ji}(\mu)\}&=\sum_{s=1}^{N}\mu_s\frac{\phi_{is}}{\lambda-\lambda_s}\frac{\psi_{is}}{\mu-\lambda_s}-\sum_{s=1}^{N}\mu_s\frac{\psi_{js}}{\lambda-\lambda_s}\frac{\phi_{js}}{\mu-\lambda_s}\\&=\frac{1}{\mu-\lambda}[(L_{ii}(\lambda)-L_{ii}(\mu))-(L_{jj}(\lambda)-L_{jj}(\mu))].\end{aligned}$$

Therefore, we obtain

$$\{L_{ij}(\lambda),L_{kl}(\mu)\}=\begin{cases}0,\quad \text{when } i\neq l,\ j\neq k;\\ \dfrac{1}{\mu-\lambda}(L_{kj}(\mu)-L_{kj}(\lambda)),\quad \text{when } i=l,\ j\neq k;\\ \dfrac{1}{\mu-\lambda}(L_{il}(\lambda)-L_{il}(\mu)),\quad \text{when } i\neq l,\ j=k;\\ \dfrac{1}{\mu-\lambda}[(L_{ii}(\lambda)-L_{ii}(\mu))-(L_{jj}(\lambda)-L_{jj}(\mu))],\quad \text{when } i=l,\ j=k.\end{cases} \tag{4.10}$$

In view of this property, we claim that

$$\mathbf{r}(\lambda,\mu)=\frac{1}{\mu-\lambda}\mathcal{P},\quad \mathcal{P}=\sum_{p,q=1}^{m}E_{pq}\otimes E_{qp}, \tag{4.11}$$

where E_{pq} is an $m\times m$ matrix with the (p,q) entry being one but the others, zero. Let us second compute that

$$\left(\left[\frac{1}{\mu-\lambda}\mathcal{P},L_1(\lambda)+L_2(\mu)\right]\right)_{ij,kl}$$

$$=\frac{1}{\mu-\lambda}([\mathcal{P},L_1(\lambda)]+[\mathcal{P},L_2(\mu)])_{ij,kl}$$

$$=\frac{1}{\mu-\lambda}\sum_{p,q=1}^{m}([E_{pq},L(\lambda)]\otimes E_{qp}+E_{qp}\otimes[E_{pq},L(\mu)])_{ij,kl}$$

$$=\frac{1}{\mu-\lambda}\sum_{p,q=1}^{m}([E_{pq},L(\lambda)])_{ik}(E_{qp})_{jl}+(E_{qp})_{ik}[E_{pq},L(\mu)]_{jl}$$

$$=\frac{1}{\mu-\lambda}([E_{lj},L(\lambda)]_{ik}+[E_{ki},L(\mu))]_{jl},$$

where we have used $(A\otimes B)(A'\otimes B')=(AA')\otimes(BB')$. Further noting that

$$[E_{pq},L]=E_{pq}L-LE_{pq}=p\text{th}\begin{bmatrix} 0 & \cdots & \overset{q\text{th}}{-L_{1p}} & \cdots & 0 \\ \vdots & & \vdots & & \vdots \\ L_{q1} & \cdots & L_{qq}-L_{pp} & \cdots & L_{qm} \\ \vdots & & \vdots & & \vdots \\ 0 & \cdots & -L_{mp} & \cdots & 0 \end{bmatrix},$$

we have

$$\left(\left[\frac{1}{\mu-\lambda}\mathcal{P},L_1(\lambda)+L_2(\mu)\right]\right)_{ij,kl}$$

$$=\begin{cases} 0, & \text{when } i\neq l,\ j\neq k; \\ \dfrac{1}{\mu-\lambda}(L_{jk}(\lambda)-L_{jk}(\mu)), & \text{when } i=l,\ j\neq k; \\ \dfrac{1}{\mu-\lambda}(-L_{il}(\lambda)+L_{il}(\mu)), & \text{when } i\neq l,\ j=k; \\ \dfrac{1}{\mu-\lambda}[(L_{jj}(\lambda)-L_{ii}(\lambda))+(L_{ii}(\mu)-L_{jj}(\mu))], & \text{when } i=l,\ j=k. \end{cases} \tag{4.12}$$

Now (4.10) and (4.12) shed right on the following theorem.

Theorem 4.1: *If $L(\lambda)=L(\lambda;c_1,\ldots,c_m)$ is defined by (4.1) and (4.2), then the* **r***-matrix formulation*

$$\{L(\lambda)\overset{\otimes}{,}L(\mu)\}=[\mathbf{r}(\lambda,\mu),L(\lambda)\otimes I_m+I_m\otimes L(\mu)],\quad \mathbf{r}=\frac{1}{\mu-\lambda}\sum_{i,j=1}^{m}E_{ij}\otimes E_{ji} \tag{4.13}$$

holds for arbitrary constants $c_1,c_2,\ldots,c_m$.

It follows from (4.13) that

$$\{L^k(\lambda)\overset{\otimes}{,}L^l(\mu)\}=[\mathbf{r}^{k,l}(\lambda,\mu),L_1(\lambda)+L_2(\mu)],\quad k,l\geqslant 1, \tag{4.14}$$

where $\mathbf{r}^{k,l}(\lambda,\mu)$ is given by[52]

$$\mathbf{r}^{k,l}(\lambda,\mu)=\sum_{i=1}^{k}\sum_{j=1}^{l}L_1^{k-i}(\lambda)L_2^{l-j}(\mu)\mathbf{r}(\lambda,\mu)L_1^{i-1}(\lambda)L_2^{j-1}(\mu). \tag{4.15}$$

Since for $A=(a_{ij})_{m\times m}$ and $B=(b_{ij})_{m\times m}$ we have

$$\mathrm{tr}\{A\overset{\otimes}{,}B\}=\sum_{i,j=1}^{m}\{A\overset{\otimes}{,}B\}_{ij,ij}=\sum_{i,j=1}^{m}\{a_{ii},b_{jj}\}=\{\mathrm{tr}A,\mathrm{tr}B\}, \tag{4.16}$$

we can compute, based on (4.14), that

$$\begin{aligned}&\{\mathrm{tr}L^k(\lambda),\mathrm{tr}L^l(\mu)\}\\&=\mathrm{tr}\{L^k(\lambda)\overset{\otimes}{,}L^l(\mu)\}=\mathrm{tr}[\mathbf{r}^{k,l}(\lambda,\mu),L_1(\lambda)+L_2(\mu)]=0,\quad k,l\geqslant 1.\end{aligned} \tag{4.17}$$

This will be used to generate an involutive system of functions defined over the symplectic manifold $(\mathbb{R}^{2mN},\omega^2)$ for any natural number m.

B. An involutive and functionally independent system

Let us begin to construct an involutive system of polynomial functions by expanding

$$\det(\nu I_m-L(\lambda))=\nu^m-\mathcal{F}_\lambda^{(1)}\nu^{m-1}+\mathcal{F}_\lambda^{(2)}\nu^{m-2}+\cdots+(-1)^m\mathcal{F}_\lambda^{(m)},\quad \nu=\mathrm{const}, \tag{4.18}$$

where $\mathcal{F}_\lambda^{(k)}$, $1\leqslant k\leqslant m$, must read as

$$\mathcal{F}_\lambda^{(k)}=\mathcal{F}_\lambda^{(k)}(c_1,\ldots,c_m)=\sum_{1\leqslant j_1<j_2<\cdots<j_k\leqslant m}\begin{vmatrix}L_{j_1j_1}&L_{j_1j_2}&\cdots&L_{j_1j_k}\\L_{j_2j_1}&L_{j_2j_2}&\cdots&L_{j_2j_k}\\\vdots&\vdots&\ddots&\vdots\\L_{j_kj_1}&L_{j_kj_2}&\cdots&L_{j_kj_k}\end{vmatrix},\quad 1\leqslant k\leqslant m. \tag{4.19}$$

Here we mention once more that $L=(L_{ij})_{m\times m}$ is assumed. We define bilinear functions $\overset{ij}{Q}_\lambda$ on $\mathbb{R}^N$

$$\overset{ij}{Q}_\lambda=\sum_{s=1}^{N}\mu_s\frac{\phi_{is}\psi_{js}}{\lambda-\lambda_s}=\sum_{l\geqslant 0}\langle A^l\Phi_i,B\Psi_j\rangle\lambda^{-l-1},\quad 1\leqslant i,j\leqslant m, \tag{4.20}$$

where A and B are given by (2.40), and Φ_i and Ψ_i are defined as before,

$$\Phi_i=(\phi_{i1},\phi_{i2},\ldots,\phi_{iN})^T,\quad \Psi_i=(\psi_{i1},\psi_{i2},\ldots,\psi_{iN})^T,\quad 1\leqslant i\leqslant m. \tag{4.21}$$

Then we have

$$L_{ij}=\sum_{l\geqslant 0}\langle A^l\Phi_i,B\Psi_j\rangle\lambda^{-l-1}=\overset{ij}{Q}_\lambda,\quad 1\leqslant i\neq j\leqslant m,$$

$$L_{ii}=c_i+\sum_{l\geqslant 0}\langle A^l\Phi_i,B\Psi_i\rangle\lambda^{-l-1}=c_i+\overset{ii}{Q}_\lambda,\quad 1\leqslant i\leqslant m.$$

Therefore, the system of functions $\mathcal{F}_\lambda^{(k)}$ is transformed into

$$\mathcal{F}_\lambda^{(k)}=\sum_{1\leqslant j_1<j_2<\cdots<j_k\leqslant m}\begin{vmatrix} c_{j_1}+Q_\lambda^{j_1j_1} & Q_\lambda^{j_1j_2} & \cdots & Q_\lambda^{j_1j_k} \\ Q_\lambda^{j_2j_1} & c_{j_2}+Q_\lambda^{j_2j_2} & \cdots & Q_\lambda^{j_2j_k} \\ \vdots & \vdots & \ddots & \vdots \\ Q_\lambda^{j_kj_1} & Q_\lambda^{j_kj_2} & \cdots & c_{j_k}+Q_\lambda^{j_kj_k} \end{vmatrix}, \quad 1\leqslant k\leqslant m. \tag{4.22}$$

A set of more concrete formulas for computing $\mathcal{F}_\lambda^{(k)}$ will be given in Appendix B. Now we further expand $\mathcal{F}_\lambda^{(k)}$ as a power series of $1/\lambda$:

$$\mathcal{F}_\lambda^{(k)}=\mathcal{F}_\lambda^{(k)}(c_1,\ldots,c_m)=\sum_{l\geqslant 0}F_{kl}(c_1,\ldots,c_m)\lambda^{-l}, \quad 1\leqslant k\leqslant m. \tag{4.23}$$

Based on the formulas of $\mathcal{F}_\lambda^{(k)}$ in Appendix B, it is not difficult to find that

$$F_{k0}=F_{k0}(c_1,\ldots,c_m)=\sum_{1\leqslant j_1<j_2<\cdots<j_k\leqslant m}\prod_{p=1}^{k}c_{j_p},$$

$$\begin{aligned} F_{kl}&=F_{kl}(c_1,\ldots,c_m)\\ &=\sum_{1\leqslant j_1<j_2<\cdots<j_k\leqslant m}\sum_{r=1}^{\min(k,l)}\sum_{1\leqslant i_1<i_2<\cdots<i_r\leqslant k}\prod_{\substack{p=1\\ p\neq i_1,i_2,\cdots,i_r}}^{k}c_{j_p}\\ &\quad\times\sum_{\substack{p_1+p_2+\cdots+p_r=l-r\\ p_1,p_2,\cdots,p_r\geqslant 0}}\begin{vmatrix} \langle A^{p_1}\Phi_{j_{i_1}},B\Psi_{j_{i_1}}\rangle & \langle A^{p_2}\Phi_{j_{i_2}},B\Psi_{j_{i_1}}\rangle & \cdots & \langle A^{p_r}\Phi_{j_{i_r}},B\Psi_{j_{i_1}}\rangle \\ \langle A^{p_1}\Phi_{j_{i_1}},B\Psi_{j_{i_2}}\rangle & \langle A^{p_2}\Phi_{j_{i_2}},B\Psi_{j_{i_2}}\rangle & \cdots & \langle A^{p_r}\Phi_{j_{i_r}},B\Psi_{j_{i_2}}\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle A^{p_1}\Phi_{j_{i_1}},B\Psi_{j_{i_r}}\rangle & \langle A^{p_2}\Phi_{j_{i_2}},B\Psi_{j_{i_r}}\rangle & \cdots & \langle A^{p_r}\Phi_{j_{i_r}},B\Psi_{j_{i_r}}\rangle \end{vmatrix}, \quad l\geqslant 1, \end{aligned} \tag{4.24}$$

which are all polynomials in the canonical variables ϕ_{is} and ψ_{is}, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$.

Theorem 4.2: *For all constants $c_1,c_2,\ldots,c_m$, the polynomial functions in ϕ_{is} and ψ_{is}, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$: $F_{il}(c_1,\ldots,c_m)$, $1\leqslant i\leqslant m$, $l\geqslant 1$, defined by (4.24), are in involution in pair with respect to the Poisson bracket (4.5).*

Proof: On the one hand, by using Newton's identities on elementary symmetric polynomials[53]

$$\zeta_k(\lambda)-\mathcal{F}_\lambda^{(1)}\zeta_{k-1}(\lambda)+\mathcal{F}_\lambda^{(2)}\zeta_{k-2}(\lambda)+\cdots+(-1)^{k-1}\mathcal{F}_\lambda^{(k-1)}\zeta_1(\lambda)+(-1)^k k\mathcal{F}_\lambda^{(k)}=0,$$

where $1\leqslant k\leqslant m$ and

$$\zeta_i(\lambda)=\operatorname{tr}L^i(\lambda), \quad 1\leqslant i\leqslant m,$$

we can have

$$\mathcal{F}_\lambda^{(k)}=\mathcal{F}_\lambda^{(k)}(\zeta_1(\lambda),\zeta_2(\lambda),\ldots,\zeta_k(\lambda)), \quad 1\leqslant k\leqslant m. \tag{4.25}$$

Therefore, we can compute that

$$\{\mathcal{F}_\lambda^{(k)},\mathcal{F}_\mu^{(i)}\}=\{\mathcal{F}_\lambda^{(k)}(\zeta_1(\lambda),\zeta_2(\lambda),\ldots,\zeta_k(\lambda)),\mathcal{F}_\mu^{(i)}(\zeta_1(\mu),\zeta_2(\mu),\ldots,\zeta_i(\mu))\}$$

$$=\sum_{l=1}^{k}\sum_{j=1}^{i}\frac{\partial\mathcal{F}_\lambda^{(k)}}{\partial\zeta_l(\lambda)}\frac{\mathcal{F}_\mu^{(i)}}{\partial\zeta_j(\mu)}\{\mathrm{tr}L^l(\lambda),\mathrm{tr}\,L^j(\mu)\}=0,\quad 1\leqslant k,i\leqslant m.$$

The last equality is a consequence of the involutivity of $\zeta_i(\lambda)$, $1\leqslant i\leqslant m$, shown in (4.17). On the other hand, we have

$$\{\mathcal{F}_\lambda^{(k)},\mathcal{F}_\mu^{(i)}\}=\sum_{l,j\geqslant 0}\{F_{kl},F_{ij}\}\lambda^{-l}\mu^{-j}.$$

It follows that the polynomial functions $F_{il}=F_{il}(c_1,\ldots,c_m)$, $1\leqslant i\leqslant m$, $l\geqslant 1$, are in involution in pair with respect to the Poisson bracket (4.5). ■

Let us now go on to show the functional independence of the polynomial functions $F_{is}(c_1,\ldots,c_m)$, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$.

Theorem 4.3: *If all constants $c_1,c_2,\ldots,c_m$ are distinct, then the polynomial functions in ϕ_{is} and ψ_{is}, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$: $F_{is}(c_1,\ldots,c_m)$, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, defined by (4.24), are functionally independent over a dense open subset of $\mathbb{R}^{2mN}$.*

Proof: Let P_0 be a point of $\mathbb{R}^{2mN}$ satisfying

$$\phi_{is}=\varepsilon,\quad 1\leqslant i\leqslant m,\quad 1\leqslant s\leqslant N,$$

where ε is a small constant. Keep (4.24) in mind, and then at this point P_0, we obviously have

$$\frac{\partial F_{is_1}}{\partial\psi_{js_2}}=\frac{\partial}{\partial\psi_{js_2}}\sum_{1\leqslant j_1<j_2<\cdots<j_i\leqslant m}\sum_{q=1}^{i}\prod_{\substack{p=1\\p\neq q}}^{i}c_{j_p}\langle A^{s_1-1}\Phi_{j_q},B\Psi_{j_q}\rangle+\mathrm{O}(\varepsilon^2)$$

$$=\varepsilon\sum_{\substack{1\leqslant j_1<j_2<\cdots<j_{i-1}\leqslant m\\ j_1,j_2,\cdots,j_{i-1}\neq j}}c_{j_1}c_{j_2}\cdots c_{j_{i-1}}\lambda_{s_2}^{s_1-1}\mu_{s_2}+\mathrm{O}(\varepsilon^2),\tag{4.26}$$

where $1\leqslant i,j\leqslant m$, $1\leqslant s_1,s_2\leqslant N$. In the above computation, only the term with $r=1$ in the expression (4.24) of F_{is} contributes to the first-order term of ε. Let the matrix Θ_N be defined by

$$\Theta_N=(\Theta_{ij}^{(N)})_{N\times N},\quad \Theta_{ij}^{(N)}=\lambda_i^{j-1}\mu_i,\quad 1\leqslant i,j\leqslant N,$$

whose determinant is easily found to be

$$\det(\Theta_N)=\prod_{i=1}^{N}\mu_i\prod_{1\leqslant i<j\leqslant N}(\lambda_j-\lambda_i).$$

Then at the point P_0, the Jacobian of the functions F_{is_1} with respect to ψ_{js_2} can be computed as follows

$$\frac{\partial(F_{11},\cdots,F_{1N},F_{21},\cdots,F_{2N},\cdots,F_{m1},\cdots,F_{mN})}{\partial(\psi_{11},\cdots,\psi_{1N},\psi_{21},\cdots,\psi_{2N},\cdots,\psi_{m1},\cdots,\psi_{mN})}$$

$$= \varepsilon^{mN} \begin{vmatrix} \Theta_N & \sum_{i=2}^{m} c_i\Theta_N & \sum_{2\leqslant i<j\leqslant m} c_ic_j\Theta_N & \cdots & \prod_{i=2}^{m} c_i\Theta_N \\ \Theta_N & \sum_{\substack{i=1\\ i\neq 2}}^{m} c_i\Theta_N & \sum_{\substack{1\leqslant i<j\leqslant m\\ i,j\neq 2}} c_ic_j\Theta_N & \cdots & \prod_{\substack{i=1\\ i\neq 2}}^{m} c_i\Theta_N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \Theta_N & \sum_{i=1}^{m-1} c_i\Theta_N & \sum_{1\leqslant i<j\leqslant m-1} c_ic_j\Theta_N & \cdots & \prod_{i=1}^{m-1} c_i\Theta_N \end{vmatrix} + \mathrm{O}(\varepsilon^{mN+1})$$

$$= \varepsilon^{mN}\det(\Omega_m\otimes\Theta_N) + \mathrm{O}(\varepsilon^{mN+1})$$

$$= \varepsilon^{mN}(\det(\Omega_m))^N(\det(\Theta_N))^m + \mathrm{O}(\varepsilon^{mN+1})$$

$$= \varepsilon^{mN}\prod_{1\leqslant i<j\leqslant m}(c_i-c_j)^N\prod_{i=1}^{N}\mu_i\prod_{1\leqslant i<j\leqslant N}(\lambda_j-\lambda_i)^m + \mathrm{O}(\varepsilon^{mN+1}),$$

where we have used the determinant property of the tensor product of matrices and the determinant result of the matrix Ω_m in Appendix C. This allows us to conclude that if the constants $c_1,c_2,\ldots,c_m$ are distinct, the above Jacobian is not zero at P_0 when $\varepsilon\neq 0$ is small enough. Since the Jacobian is a polynomial function of ϕ_{is} and ψ_{is}, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, it is not zero over a dense open subset of $\mathbb{R}^{2mN}$. Therefore, the functions F_{is}, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, are functionally independent over that dense open subset of $\mathbb{R}^{2mN}$. The proof is completed. ■

C. An alternative involutive system to the F_{is}'s

We would like to express the involutive system of the polynomial functions F_{is} in another way, and so we introduce

$$s_0(v_1,\cdots,v_m)=1, \tag{4.27a}$$

$$s_k(v_1,\cdots,v_m)=\sum_{1\leqslant j_1<j_2<\cdots<j_k\leqslant m} v_{j_1}\cdots v_{j_k}, \quad 1\leqslant k\leqslant m, \tag{4.27b}$$

$$s_k(v_1,\cdots,v_m)=0, \quad \text{when } k\geqslant m+1 \text{ or } k\leqslant -1, \tag{4.27c}$$

where $v_1,v_2,\ldots,v_m$ are m numbers. Obviously, for $m\geqslant 2$, we have the following relation:

$$s_k(v_1,\ldots,v_m)=v_m s_{k-1}(v_1,\ldots,v_{m-1})+s_k(v_1,\ldots,v_{m-1}), \quad k\in\mathbb{Z}. \tag{4.28}$$

Let us now define

$$E_{1l}=F_{1l}, \quad E_{il}=(-1)^{i+1}F_{il}+\sum_{j=1}^{i-1}(-1)^{j+1}s_j(c_1,\ldots,c_m)E_{i-j,l}, \quad i\geqslant 2, \ l\geqslant 1. \tag{4.29}$$

From (4.29), we can have

$$F_{il}=\sum_{j=0}^{i-1}(-1)^{i-j+1}s_j(c_1,\ldots,c_m)E_{i-j,l}, \quad i,l\geqslant 1. \tag{4.30}$$

Therefore, by Proposition D.2 in Appendix D, we obtain

$$E_{il}=E_{il}(c_1,\ldots,c_m)$$
$$=\sum_{r=1}^{\min(i,l)}(-1)^{r+1}\sum_{1\leqslant j_1<j_2<\cdots<j_r\leqslant m}\ \sum_{\substack{l_1+l_2+\cdots+l_r=i-r\\ l_1,l_2,\cdots,l_r\geqslant 0}} c_{j_1}^{l_1}c_{j_2}^{l_2}\cdots c_{j_r}^{l_r}$$
$$\times\sum_{\substack{p_1+p_2+\cdots+p_r=l-r\\ p_1,p_2,\cdots,p_r\geqslant 0}}\begin{vmatrix}\langle A^{p_1}\Phi_{j_1},B\Psi_{j_1}\rangle & \langle A^{p_2}\Phi_{j_2},B\Psi_{j_1}\rangle & \cdots & \langle A^{p_r}\Phi_{j_r},B\Psi_{j_1}\rangle\\ \langle A^{p_1}\Phi_{j_1},B\Psi_{j_2}\rangle & \langle A^{p_2}\Phi_{j_2},B\Psi_{j_2}\rangle & \cdots & \langle A^{p_r}\Phi_{j_r},B\Psi_{j_2}\rangle\\ \vdots & \vdots & \ddots & \vdots\\ \langle A^{p_1}\Phi_{j_1},B\Psi_{j_r}\rangle & \langle A^{p_2}\Phi_{j_2},B\Psi_{j_r}\rangle & \cdots & \langle A^{p_r}\Phi_{j_r},B\Psi_{j_r}\rangle\end{vmatrix},\tag{4.31}$$

where $1\leqslant i\leqslant m$ and $l\geqslant 1$. Obviously, each E_{il} is a linear combination of the F_{il}'s, and hence $\{E_{ik},E_{jl}\}=0$ holds for all $1\leqslant i,j\leqslant m$ and $k,l\geqslant 1$. This means that the polynomial functions E_{is}, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, are also in involution in pair.

In order to show the functional independence of E_{is}, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, similar to the proof of Theorem 4.3, let P_0 be a point of $\mathbb{R}^{2mN}$ satisfying $\phi_{is}=\varepsilon$, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, where ε is a small constant. Then at this point P_0, we have

$$\frac{\partial E_{is_1}}{\partial\psi_{js_2}}=\varepsilon c_j^{i-1}\lambda_{s_2}^{s_1-1}\mu_{s_2}+\mathrm{O}(\varepsilon^2),\quad 1\leqslant i,j\leqslant m,\ \ 1\leqslant s_1,s_2\leqslant N.\tag{4.32}$$

Hence a direct argument can give rise to

$$\frac{\partial(E_{11},\cdots,E_{1N},E_{21},\cdots,E_{2N},\cdots,E_{m1},\cdots,E_{mN})}{\partial(\psi_{11},\cdots,\psi_{1N},\psi_{21},\cdots,\psi_{2N},\cdots,\psi_{m1},\cdots,\psi_{mN})}$$
$$=\varepsilon^{mN}\prod_{i=1}^{N}\mu_i\prod_{1\leqslant i<j\leqslant N}(\lambda_j-\lambda_i)^m\prod_{1\leqslant i<j\leqslant m}(c_j-c_i)^N+\mathrm{O}(\varepsilon^{mN+1}).\tag{4.33}$$

Therefore, if $c_1,c_2,\ldots,c_m$ are distinct, the above Jacobian is not zero at P_0 when $\varepsilon\neq 0$ is small enough. This implies that the functions E_{is}, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, are functionally independent over a dense open subset of $\mathbb{R}^{2mN}$.

Let us sum up these results in the following theorem.

Theorem 4.4: *All polynomial functions in ϕ_{is} and ψ_{is}, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$: $E_{il}(c_1,\ldots,c_m)$, $1\leqslant i\leqslant m$, $l\geqslant 1$, defined by (4.31), are in involution in pair with respect to the Poisson bracket (4.5) for all constants $c_1,c_2,\ldots,c_m$. Moreover, among them the polynomial functions $E_{is}(c_1,\ldots,c_m)$, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, are functionally independent over a dense open subset of $\mathbb{R}^{2mN}$ for distinct constants $c_1,c_2,\ldots,c_m$.*

Note that all polynomial functions F_{il} are also linear combinations of the E_{il}'s. The above theorem actually shows us an alternative to the involutive and functionally independent system of the polynomial functions F_{is}, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$. The E_{is}'s have the compact form for the constants $c_1,c_2,\ldots,c_m$, and thus it is more convenient to deal with them.

V. LIOUVILLE INTEGRABILITY AND INVOLUTIVE SOLUTIONS

Let us now turn to establish the Liouville integrability of the obtained constrained flows, and to present involutive solutions of the $\mathcal{N}$-wave interaction equations in both $1+1$ and $2+1$ dimensions. The involutive system of the polynomial functions

$$F_{is}=F_{is}(c_1,\ldots,c_m),\quad 1\leqslant i\leqslant m,\quad 1\leqslant s\leqslant N,$$

alternatively

$$E_{is}=E_{is}(c_1,\ldots,c_m),\quad 1\leqslant i\leqslant m,\quad 1\leqslant s\leqslant N,$$

will play an extremely important role in the following discussion.

A. Liouville integrability of the constrained flows

For the $1+1$ dimensional case, we have the matrix Lax operator as defined by (2.49) and (2.50), i.e.,

$$L^{(1)}(\lambda)=L^{(1)}(\lambda;\gamma_1,\ldots,\gamma_n)=C_1(\gamma_1,\ldots,\gamma_n)+D_1(\lambda),$$

where C_1 and $D_1(\lambda)$ are given by (2.50). Note that

$$\gamma_i\neq\gamma_j,\quad 1\leqslant i\neq j\leqslant n.$$

According to Theorems 4.2 and 4.3 for the case $m=n$ and $c_i=\gamma_i$, $1\leqslant i\leqslant n$, we know that $F_{is}(\gamma_1,\ldots,\gamma_n)$, $1\leqslant i\leqslant n$, $1\leqslant s\leqslant N$, defined by (4.24), are functionally independent over a dense open subset of $\mathbb{R}^{2nN}$ and in involution in pair with respect to the Poisson bracket (2.47), i.e.,

$$\{f,g\}=\sum_{i=1}^{n}\left(\left\langle\frac{\partial f}{\partial\Psi_i},B^{-1}\frac{\partial g}{\partial\Phi_i}\right\rangle-\left\langle\frac{\partial f}{\partial\Phi_i},B^{-1}\frac{\partial g}{\partial\Psi_i}\right\rangle\right),\quad f,g\in C^{\infty}(\mathbb{R}^{2nN}).$$

Theorem 5.1: *Let $\gamma_1,\gamma_2,\ldots,\gamma_n$ be n distinct numbers. Then the spatial constrained flow (2.43) and the temporal constrained flow (2.44) of the $1+1$ dimensional $\mathcal{N}$-wave interaction equations (2.22) are Liouville integrable Hamiltonian systems, which possess involutive and functionally independent integrals of motion*

$$F_{is}(\gamma_1,\ldots,\gamma_n),\quad 1\leqslant i\leqslant n,\quad 1\leqslant s\leqslant N,$$

defined by (4.24) in the case

$$m=n,\quad c_i=\gamma_i,\quad 1\leqslant i\leqslant n.$$

Proof: From the necessary Lax representations of the spatial constrained flow (2.43) and the temporal constrained flow (2.44),

$$(L^{(1)}(\lambda))_x=[U(\tilde{u},\lambda),L^{(1)}(\lambda)],\quad (L^{(1)}(\lambda))_{t_1}=[V^{(1)}(\tilde{u},\lambda),L^{(1)}(\lambda)],$$

which are shown in Theorem 2.1, we can obtain[26]

$$(L^{(1)}(\lambda))^i)_x=[U(\tilde{u},\lambda),(L^{(1)}(\lambda))^i],\quad (L^{(1)}(\lambda))^j)_{t_1}=[V^{(1)}(\tilde{u},\lambda),(L^{(1)}(\lambda))^j],\quad i,j\geqslant 1,$$

and thus we have

$$(\mathrm{tr}(L^{(1)}(\lambda))^i)_x=\mathrm{tr}((L^{(1)}(\lambda))^i)_x=\mathrm{tr}[U(\tilde{u},\lambda),(L^{(1)}(\lambda))^i]=0,\quad i\geqslant 1,$$

$$(\mathrm{tr}(L^{(1)}(\lambda))^j)_{t_1}=\mathrm{tr}((L^{(1)}(\lambda))^j)_{t_1}=\mathrm{tr}[V^{(1)}(\tilde{u},\lambda),(L^{(1)}(\lambda))^j]=0,\quad j\geqslant 1.$$

Therefore, $\mathcal{F}_{\lambda}^{(k)}(\gamma_1,\ldots,\gamma_n)$ are all generating functions of integrals of motion of (2.43) and (2.44) in the light of the expression (4.25) determined by Newton's identities. It follows that $F_{is}(\gamma_1,\ldots,\gamma_n)$, $1\leqslant i\leqslant n$, $1\leqslant s\leqslant N$, are all integrals of motion of the spatial constrained flow (2.43) and the temporal constrained flow (2.44). Note that all constants $\gamma_1,\gamma_2,\ldots,\gamma_n$ are distinct. Therefore, Theorems 4.2 and 4.3 in the case of $m=n$ and $c_i=\gamma_i$, $1\leqslant i\leqslant n$, together with Theorem 2.1, show that the spatial constrained flow (2.43) and the temporal constrained flow (2.44) are Liouville integrable Hamiltonian systems, which possess the involutive and functionally independent integrals of motion $F_{is}(\gamma_1,\ldots,\gamma_n)$, $1\leqslant i\leqslant n$, $1\leqslant s\leqslant N$. The proof is finished. ■

We remark that from the Lax representations shown in Theorem 2.1, we have

$$(\nu I_n - L^{(1)}(\lambda))_x = [U(\tilde{u},\lambda), \nu I_n - L^{(1)}(\lambda)],$$

$$(\nu I_n - L^{(1)}(\lambda))_{t_1} = [V^{(1)}(\tilde{u},\lambda), \nu I_n - L^{(1)}(\lambda)]$$

for any constant ν. It follows[54] that $\det(\nu I_n - L^{(1)}(\lambda))$ is a common generating function of integrals of motion of the constrained flows (2.43) and (2.44), and thus so are $\mathcal{F}_\lambda^{(k)}(\gamma_1,\ldots,\gamma_n)$, $1\leqslant k\leqslant n$. This is an alternative proof for showing that $\mathcal{F}_\lambda^{(k)}(\gamma_1,\ldots,\gamma_n)$, $1\leqslant k\leqslant n$, are the generating functions of integrals of motion of (2.43) and (2.44).

For the $2+1$ dimensional case, a completely similar argument can give rise to the following theorem on the Liouville integrability of the constrained flows (3.23)–(3.25) of the $2+1$ dimensional $\mathcal{N}$-wave interaction equations (3.4).

Theorem 5.2: *Let $\delta_1,\ldots,\delta_n,\delta_{n+1}$ be $n+1$ distinct numbers. Then all three constrained flows (3.23)–(3.25) of the $2+1$ dimensional $\mathcal{N}$-wave interaction equations (3.4) are Liouville integrable Hamiltonian systems, which possess the involutive and functionally independent integrals of motion*

$$F_{is}(\delta_1,\ldots,\delta_n,\delta_{n+1}), \quad 1\leqslant i\leqslant n+1, \quad 1\leqslant s\leqslant N,$$

defined by (4.24) in the case

$$m=n+1, \quad c_i=\delta_i, \quad 1\leqslant i\leqslant n+1.$$

B. Involutive solutions of the $\mathcal{N}$-wave interaction equations

We would like to show that the constrained flows provide involutive solutions to the $\mathcal{N}$-wave interaction equations in both $1+1$ and $2+1$ dimensions. For the $1+1$ dimensional case, we have the following result.

Theorem 5.3: *If $\phi_{is}(x,t_1)$ and $\psi_{is}(x,t_1)$, $1\leqslant i\leqslant n$, $1\leqslant s\leqslant N$, solve the spatial constrained flow (2.43) and the temporal constrained flow (2.44) simultaneously, then*

$$u_{ij}(x,t_1)=\frac{\alpha_i-\alpha_j}{\gamma_i-\gamma_j}\langle \Phi_i(x,t_1), B\Psi_j(x,t_1)\rangle, \quad 1\leqslant i\neq j\leqslant n, \tag{5.1}$$

with $\Phi_i(x,t_1)$ and $\Psi_i(x,t_1)$ being given by

$$\Phi_i(x,t_1)=(\phi_{i1}(x,t_1),\ldots,\phi_{iN}(x,t_1))^T, \quad \Psi_i(x,t_1)=(\psi_{i1}(x,t_1),\ldots,\psi_{iN}(x,t_1))^T, \quad 1\leqslant i\leqslant n,$$

solve the $1+1$ dimensional $\mathcal{N}$-wave interaction equations (2.22).

Proof: Note that the $1+1$ dimensional $\mathcal{N}$-wave interaction equations (2.22) is the compatability condition of the spectral problem (2.1) and the associated spectral problem (2.17) with $m=1$ or the adjoint spectral problem (2.27) and the adjoint associated spectral problem (2.28) with $m=1$ for whatever potential u. Therefore, the $1+1$ dimensional $\mathcal{N}$-wave interaction equations (2.22) are also the compatability condition of the spatial constrained flow (2.43) and the temporal constrained flow (2.44) under the constraint (2.41). Now $\phi_{is}(x,t_1)$ and $\psi_{is}(x,t_1)$, $1\leqslant i\leqslant n$, $1\leqslant s\leqslant N$, are assumed to solve (2.43) and (2.44) simultaneously, and thus the potential defined by (5.1) must satisfy the compatability condition of the spatial constrained flow (2.43) and the temporal constrained flow (2.44). This means that the potential defined by (5.1) must be a solution to the $1+1$ dimensional $\mathcal{N}$-wave interaction equations (2.22). The proof is finished. ■

We remark that a direct computation can also show the above theorem. For the $2+1$ dimensional case, a similar deduction can give rise to the following theorem.

Theorem 5.4: *If $\phi_{is}(x,t)$ and $\psi_{is}(x,t)$, $1\leqslant i\leqslant n+1$, $1\leqslant s\leqslant N$, solve the constrained flows (3.23)–(3.25) simultaneously, then*

$$p_{ij}(x,y,t)=\frac{J_i-J_j}{\delta_i-\delta_j}\langle\Phi_i(x,y,t),B\Psi_j(x,y,t)\rangle,\quad 1\leqslant i\neq j\leqslant n,$$
$$q_{ij}(x,y,t)=\frac{K_i-K_j}{\delta_i-\delta_j}\langle\Phi_i(x,y,t),B\Psi_j(x,y,t)\rangle,\quad 1\leqslant i\neq j\leqslant n, \tag{5.2}$$

with $\Phi_i(x,t)$ *and* $\Psi_i(x,t)$ *being given by*

$$\Phi_i(x,t)=(\phi_{i1}(x,t),\ldots,\phi_{iN}(x,t))^T,\quad \Psi_i(x,t)=(\psi_{i1}(x,t),\ldots,\psi_{iN}(x,t))^T,\quad 1\leqslant i\leqslant n+1,$$

solve the $2+1$ *dimensional* $\mathcal{N}$*-wave interaction equations (3.4).*

Also, one can find that

$$f_i=\frac{1}{\delta_i-\delta_{n+1}}\langle\Phi_i,B\Psi_{n+1}\rangle,\quad g_i=\frac{1}{\delta_i-\delta_{n+1}}\langle\Phi_{n+1},B\Psi_i\rangle,\quad 1\leqslant i\leqslant n \tag{5.3}$$

provide a solution to the Lax system (3.1) and the adjoint Lax system (3.5) with the potentials given by (5.2). What's more, (5.2) and (5.3) automatically satisfy our first symmetry constraint (3.7).

In the following theorem, the solutions given in Theorems 5.3 and 5.4 are shown to be involutive.

Theorem 5.5: *The Hamiltonians* H_1^x *and* $H_1^{t_1}$ *of the constrained flows in* $1+1$ *dimensions, defined by (2.53) and (2.54), are the second-order polynomial functions of* $E_{il}(\gamma_1,\ldots,\gamma_n)$, $1\leqslant i\leqslant n$, $l=1,2$, *and thus they commute, i.e.,*

$$\{H_1^x,H_1^{t_1}\}=0, \tag{5.4}$$

where the Poisson bracket $\{\cdot,\cdot\}$ *is defined by (2.47). The Hamiltonians* H_2^x, H_2^y *and* H_2^t *of the constrained flows in* $2+1$ *dimensions, defined by (3.30)–(3.32), are also the second-order polynomial functions of* $E_{il}(\delta_1,\ldots,\delta_n,\delta_{n+1})$, $1\leqslant i\leqslant n+1$, $l=1,2$, *and thus they commute with each other, i.e.,*

$$\{H_2^x,H_2^y\}=\{H_2^x,H_2^t\}=\{H_2^y,H_2^t\}=0, \tag{5.5}$$

where the Poisson bracket $\{\cdot,\cdot\}$ *is defined by* (3.28).

Proof: Directly from the explicit expression (4.31) of the E_{is}'s, we have

$$E_{i1}=\sum_{j=1}^{m}c_j^{i-1}\langle\Phi_j,B\Psi_j\rangle,\quad 1\leqslant i\leqslant m, \tag{5.6}$$

$$\begin{aligned}E_{i2}&=\sum_{j=1}^{m}c_j^{i-1}\langle A\Phi_j,B\Psi_j\rangle\\&\quad-\sum_{1\leqslant j<k\leqslant m}\frac{c_j^{i-1}-c_k^{i-1}}{c_j-c_k}(\langle\Phi_j,B\Psi_j\rangle\langle\Phi_k,B\Psi_k\rangle-\langle\Phi_j,B\Psi_k\rangle\langle\Phi_k,B\Psi_j\rangle)\\&=\sum_{j=1}^{m}c_j^{i-1}\mathcal{E}_j-\sum_{\substack{j,k=1\\j\neq k}}^{m}\frac{c_j^{i-1}}{c_j-c_k}\langle\Phi_j,B\Psi_j\rangle\langle\Phi_k,B\Psi_k\rangle,\quad 1\leqslant i\leqslant m,\end{aligned} \tag{5.7}$$

where the $\mathcal{E}_j$'s are defined as follows:

$$\mathcal{E}_j=\langle A\Phi_j,B\Psi_j\rangle+\sum_{\substack{k=1\\k\neq j}}^{m}\frac{1}{c_j-c_k}\langle\Phi_j,B\Psi_k\rangle\langle\Phi_k,B\Psi_j\rangle,\quad 1\leqslant j\leqslant m. \tag{5.8}$$

Now solving (5.6) for $\langle\Phi_i,B\Psi_i\rangle$, $1\leqslant i\leqslant m$, leads to

$$\langle\Phi_i,B\Psi_i\rangle=\left(\prod_{\substack{r=1\\r\neq i}}^{m}\frac{1}{c_i-c_r}\right)\sum_{j=1}^{m}(-1)^{m-j}s_{m-j}(c_1,\ldots,c_{i-1},\hat{c}_i,c_{i+1},\ldots,c_m)E_{j1},\quad 1\leqslant i\leqslant m, \tag{5.9}$$

where the s_j's are defined by (4.27) and $\hat{c}_i$ means that c_i does not appear. Therefore, each $\langle\Phi_i,B\Psi_i\rangle$ can be expressed as a linear combination of E_{i1}, $1\leqslant i\leqslant m$. Similarly, solving (5.7) for $\mathcal{E}_j$, $1\leqslant j\leqslant m$, leads to

$$\begin{aligned}\mathcal{E}_i=&\left(\prod_{\substack{r=1\\r\neq i}}^{m}\frac{1}{c_i-c_r}\right)\sum_{j=1}^{m}(-1)^{m-j}s_{m-j}(c_1,\ldots,c_{i-1},\hat{c}_i,c_{i+1},\ldots,c_m)\\&\times\left(E_{j2}+\sum_{\substack{k,l=1\\k\neq l}}^{m}\frac{c_k^{j-1}}{c_k-c_l}\langle\Phi_k,B\Psi_k\rangle\langle\Phi_l,B\Psi_l\rangle\right),\quad 1\leqslant i\leqslant m.\end{aligned} \tag{5.10}$$

This expression together with (5.9) implies that each $\mathcal{E}_j$ can be expressed as a linear combination of E_{i1} and E_{i2}, $1\leqslant i\leqslant m$.

In the $1+1$ dimensional case, we have $m=n$, $c_j=\gamma_j$, $1\leqslant j\leqslant n$. Hence

$$\mathcal{E}_j=\langle A\Phi_j,B\Psi_j\rangle+\sum_{\substack{k=1\\k\neq j}}^{n}\frac{1}{\gamma_j-\gamma_k}\langle\Phi_j,B\Psi_k\rangle\langle\Phi_k,B\Psi_j\rangle,\quad 1\leqslant j\leqslant n. \tag{5.11}$$

The Hamiltonians H_1^x and $H_1^{t_1}$ in Theorem 2.1 can be easily expressed as

$$H_1^x=-\sum_{k=1}^{n}\alpha_k\mathcal{E}_k,\quad H_1^{t_1}=-\sum_{k=1}^{n}\beta_k\mathcal{E}_k, \tag{5.12}$$

where the $\mathcal{E}_k$'s are defined by (5.11).

Likewise, in the $2+1$ dimensional case, we have $m=n+1$, $c_j=\delta_j$, $\quad 1\leqslant j\leqslant n+1$. Hence

$$\begin{aligned}\mathcal{E}_j=&\langle A\Phi_j,B\Psi_j\rangle+\sum_{\substack{k=1\\k\neq j}}^{n}\frac{1}{\delta_j-\delta_k}\langle\Phi_j,B\Psi_k\rangle\langle\Phi_k,B\Psi_j\rangle+\frac{1}{\delta_j-\delta_{n+1}}\langle\Phi_j,B\Psi_{n+1}\rangle\langle\Phi_{n+1},B\Psi_j\rangle,\\&1\leqslant j\leqslant n,\end{aligned} \tag{5.13}$$

$$\mathcal{E}_{n+1}=\langle A\Phi_{n+1},B\Psi_{n+1}\rangle+\sum_{k=1}^{n}\frac{1}{\delta_{n+1}-\delta_k}\langle\Phi_{n+1},B\Psi_k\rangle\langle\Phi_k,B\Psi_{n+1}\rangle. \tag{5.14}$$

The Hamiltonians H_2^x, H_2^y and H_2^t in Theorem 3.1 can be expressed as

$$H_2^x=-\sum_{k=1}^{n}\mathcal{E}_k,\quad H_2^y=-\sum_{k=1}^{n}J_k\mathcal{E}_k,\quad H_2^t=-\sum_{k=1}^{n}K_k\mathcal{E}_k, \tag{5.15}$$

where the $\mathcal{E}_k$'s are defined by (5.13).

Therefore, H_1^x and $H_1^{t_1}$ are linear combinations of $E_{il}(\gamma_1,\ldots,\gamma_n)$, $\quad 1\leqslant i\leqslant n$, $\quad l=1,2$, and H_2^x, H_2^y and H_2^t are linear combinations of $E_{il}(\delta_1,\ldots,\delta_n,\delta_{n+1})$, $\quad 1\leqslant i\leqslant n+1$, $\quad l=1,2$. It follows from Theorem 4.4 that H_1^x and $H_1^{t_1}$ are in involution, and H_2^x, H_2^y and H_2^t are in involution in pair, too. The proof is finished. ■

We remark that a direct computation can also give a proof for the involutive property of the Hamiltonians of the constrained flows in both $1+1$ and $2+1$ dimensions. Only a new set of equalities

$$\frac{a_j-a_i}{c_j-c_i}\frac{b_k-b_i}{c_k-c_i}-\frac{a_k-a_i}{c_k-c_i}\frac{b_j-b_i}{c_j-c_i}+\mathrm{cycle}(i,j,k)=0,\quad 1\leqslant i,j,k\leqslant n,$$

has to be utilized, where a_i, b_i, and c_i, $1\leqslant i\leqslant n$, are arbitrary constants. This just needs a direct check, too. However, the proof of Theorem 5.5 also gives rise to the explicit expressions for all Hamiltonians of the constrained flows in both $1+1$ and $2+1$ dimensions, in terms of the integrals of motion E_{is}.

Now if we denote the Hamiltonian flows of the spatial constrained flow (2.43) and the temporal constrained flow (2.44) by $g_x^{H_1^x}$ and $g_t^{H_1^{t_1}}$, respectively, then the above theorems present a kind of involutive solution to the $1+1$ dimensional $\mathcal{N}$-wave interaction equations (2.22):

$$\begin{aligned}u_{ij}(x,t_1)&=\frac{\alpha_i-\alpha_j}{\gamma_i-\gamma_j}\langle g_x^{H_1^x}g_t^{H_1^{t_1}}\Phi_{i0},g_x^{H_1^x}g_t^{H_1^{t_1}}B\Psi_{j0}\rangle\\&=\frac{\alpha_i-\alpha_j}{\gamma_i-\gamma_j}\langle g_t^{H_1^{t_1}}g_x^{H_1^x}\Phi_{i0},g_t^{H_1^{t_1}}g_x^{H_1^x}B\Psi_{j0}\rangle,\quad 1\leqslant i\neq j\leqslant n,\end{aligned}\tag{5.16}$$

where the initial values Φ_{i0} and Ψ_{i0} of Φ_i and Ψ_i can be taken to be any arbitrary constant vectors of the Euclidean space $\mathbb{R}^N$. Similarly, if we denote the Hamiltonian flows of the constrained flows (3.23)–(3.25) by $g_x^{H_2^x}$, $g_y^{H_2^y}$, and $g_t^{H_2^t}$, respectively, then the above theorems present a kind of involutive solutions to the $2+1$ dimensional $\mathcal{N}$-wave interaction equations (3.4):

$$\begin{aligned}p_{ij}(x,t)&=\frac{J_i-J_j}{\delta_i-\delta_j}\langle g_x^{H_2^x}g_y^{H_2^y}g_t^{H_2^t}\bar{\Phi}_{i0},g_x^{H_2^x}g_y^{H_2^y}g_t^{H_2^t}B\bar{\Psi}_{j0}\rangle\\&=\frac{J_i-J_j}{\delta_i-\delta_j}\langle g_y^{H_2^y}g_t^{H_2^t}g_x^{H_2^x}\bar{\Phi}_{i0},g_y^{H_2^y}g_t^{H_2^t}g_x^{H_2^x}B\bar{\Psi}_{j0}\rangle\\&=\frac{J_i-J_j}{\delta_i-\delta_j}\langle g_t^{H_2^t}g_x^{H_2^x}g_y^{H_2^y}\bar{\Phi}_{i0},g_t^{H_2^t}g_x^{H_2^x}g_y^{H_2^y}B\bar{\Psi}_{j0}\rangle\\&=\cdots,\quad 1\leqslant i\neq j\leqslant n,\end{aligned}\tag{5.17}$$

$$\begin{aligned}q_{ij}(x,t)&=\frac{K_i-K_j}{\delta_i-\delta_j}\langle g_x^{H_2^x}g_y^{H_2^y}g_t^{H_2^t}\bar{\Phi}_{i0},g_x^{H_2^x}g_y^{H_2^y}g_t^{H_2^t}B\bar{\Psi}_{j0}\rangle\\&=\frac{K_i-K_j}{\delta_i-\delta_j}\langle g_y^{H_2^y}g_t^{H_2^t}g_x^{H_2^x}\bar{\Phi}_{i0},g_y^{H_2^y}g_t^{H_2^t}g_x^{H_2^x}B\bar{\Psi}_{j0}\rangle\\&=\frac{K_i-K_j}{\delta_i-\delta_j}\langle g_t^{H_2^t}g_x^{H_2^x}g_y^{H_2^y}\bar{\Phi}_{i0},g_t^{H_2^t}g_x^{H_2^x}g_y^{H_2^y}B\bar{\Psi}_{j0}\rangle\\&=\cdots,\quad 1\leqslant i\neq j\leqslant n,\end{aligned}\tag{5.18}$$

where the initial values $\bar{\Phi}_{i0}$ and $\bar{\Psi}_{i0}$ of Φ_i and Ψ_i can also be taken to be any arbitrary constant vectors of the Euclidean space $\mathbb{R}^N$.

Note that all constrained flows in both $1+1$ and $2+1$ dimensions are Liouville integrable, and that the initial values of Φ_i and Ψ_i, $1\leqslant i\leqslant n$, can be arbitrarily chosen. Therefore, together with Theorems 5.1 and 5.2, the above involutive solutions also show us the richness of solutions and the integrability by quadratures for the $\mathcal{N}$-wave interaction equations in both $1+1$ and $2+1$ dimensions. Of importance is of course that binary symmetry constraints decompose the

$\mathcal{N}$-wave interaction equations in both $1+1$ and $2+1$ dimensions into finite-dimensional Liouville integrable Hamiltonian systems, and the resulting involutive solutions present the Bäcklund transformations between the $\mathcal{N}$-wave interaction equations in both $1+1$ and $2+1$ dimensions and these finite-dimensional Liouville integrable Hamiltonian systems.

VI. CONCLUSIONS AND REMARKS

We have introduced a class of special symmetry constraints, (2.38) in the $1+1$ dimensional case, and (3.19) and (3.20) in the $2+1$ dimensional case, for the $\mathcal{N}$-wave interaction equations in both $1+1$ and $2+1$ dimensions. These symmetry constraints nonlinearize the $n\times n$ spectral problem and adjoint spectral problem, (2.34) and (2.35), and the $(n+1)\times(n+1)$ spectral problem and adjoint spectral problem, (3.11) and (3.12), into finite-dimensional Liouville integrable Hamiltonian systems, and decompose the $\mathcal{N}$-wave interaction equations in both $1+1$ and $2+1$ dimensions into these finite-dimensional Liouville integrable Hamiltonian systems. A general involutive and functionally independent system of the polynomial functions $F_{is}(c_1,\ldots,c_m)$, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, or alternatively $E_{is}(c_1,\ldots,c_m)$, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, associated with an arbitrarily higher-order matrix Lax operator, was presented and used to show the Liouville integrability of the resulting constrained flows. The nonlinear constraints on the potentials, resulting from the symmetry constraints, also provide us with a class of Bäcklund transformations from the $\mathcal{N}$-wave interaction equations to the obtained finite-dimensional Liouville integrable systems. The involutive solutions to the $\mathcal{N}$-wave interaction equations are given through the constrained flows, and thus the integrability by quadratures has been exhibited for the $\mathcal{N}$-wave interaction equations. The special case with $\Gamma=W_0$, i.e., $\mathrm{diag}(\gamma_1,\ldots,\gamma_n)=\mathrm{diag}(\beta_1,\ldots,\beta_n)$ of two reductions of $n=3$ and $n=4$ in $1+1$ dimensions presents all results established in Refs. 31 and 32.

We point out that for a more general matrix Lax operator $L=C+D$ with any constant matrix $C=(c_{ij})_{m\times m}$ and the matrix D defined by (4.2), the **r**-matrix formulation (4.13) still holds. Therefore, an involutive system of polynomial functions can be generated, but we do not know what conditions on the matrix C can ensure the functional independence of that involutive system. We are also curious about other examples of higher-order matrix Lax operators which lead to involutive and functionally independent systems. Our crucial techniques to present the involutive and functionally independent system F_{is}, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, are the **r**-matrix formulation, Newton's identities on elementary symmetric polynomials, and the determinant property of tensor products of matrices; and the whole process of their applications provides an efficient way to show the involutive property and the functional independence.

Of course, one of the important results in binary nonlinearization is the integrability of soliton equations by quadratures, which implies that one can integrate soliton equations themselves by quadratures. However, the potentials obtained by symmetry constraints can be proved to belong to a kind of finite-gap-type solutions containing multi-soliton solutions, and thus they may not present solutions to given initial value and/or boundary problems of soliton equations. It is a challenging problem to establish a general theory of complete integrability for nonlinear differential and differential-difference equations, which should state what mathematical properties the equations must possess so that their solutions to initial value and/or boundary problems can also be determined by quadratures.

Symmetry constraints yield nonlinear constraints on potentials of soliton equations, and put linear spectral problems (linear with respect to eigenfunctions) into nonlinear constrained flows (nonlinear again with respect to eigenfunctions), which makes it more complicated to solve soliton equations. However, since spectral problems are overdetermined, one needs additional conditions (compatability conditions) to guarantee the existence of eigenfunctions of spectral problems. The symmetry property brings us the Liouville integrability for nonlinear constrained flows. Thus, symmetry constraints make up for the disadvantage of nonlinearization in manipulating binary nonlinearization. Of special interest in the study of symmetry constraints are creating new classical integrable systems,[55] which supplement the known class of integrable systems,[56] and exposing the integrability by quadratures for soliton equations by using constrained flows.[33]

The idea of binary nonlinearization is quite similar to that of using adjoint symmetries to generate conservation laws for differential equations, both Lagrangian and non-Lagrangian.[57] In binary nonlinearization, we adopt adjoint spectral problems to formulate Hamiltonian structures for constrained flows so that finite-dimensional Liouville integrable systems result. Note that there exist also some special symmetry constraints which do not yield Hamiltonian structures with constant coefficient symplectic forms, including both canonical and noncanonical ones, for constrained flows.[46] Therefore, it will be particularly interesting and important to classify symmetry constraints which exhibit Hamiltonian structures with constant and variable coefficient symplectic forms for constrained flows.

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APPENDIX A: NON-LIE SYMMETRIES

Proposition A.1: If $\phi^{(s)}$ *and* $\psi^{(s)}$, $1\leqslant s\leqslant N$, *satisfy (2.34) and (2.35), then the vector field*

$$Z_0=J\sum_{s=1}^{N}\mu_s\psi^{(s)T}\frac{\partial U(u,\lambda_s)}{\partial u}\phi^{(s)}=\rho\left(\left[U_0,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right]\right) \tag{A1}$$

is a symmetry of the $1+1$ *dimensional* $\mathcal{N}$*-wave interaction equations (2.22).*

Proof: It is required to show that

$$(\delta P,\delta Q)=\left(\left[U_0,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right],\left[W_0,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right]\right) \tag{A2}$$

satisfies the linearized system (2.25). By using (2.34) and (2.35), we can first compute that

$$\begin{aligned}\left(\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right)_{t_1}&=\sum_{s=1}^{N}\mu_s\phi^{(s)}_{t_1}\psi^{(s)T}+\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}_{t_1}\\&=\sum_{s=1}^{N}\mu_sV^{(1)}(u,\lambda_s)\phi^{(s)}\psi^{(s)T}-\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}V^{(1)}(u,\lambda_s)\\&=\sum_{s=1}^{N}\mu_s[V^{(1)}(u,\lambda_s),\phi^{(s)}\psi^{(s)T}]\\&=\sum_{s=1}^{N}\lambda_s\mu_s[W_0,\phi^{(s)}\psi^{(s)T}]+\left[W_1,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right],\end{aligned}$$

and, similarly, we can have

$$\left(\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right)_{x}=\sum_{s=1}^{N}\lambda_s\mu_s[U_0,\phi^{(s)}\psi^{(s)T}]+\left[U_1,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right].$$

Thus, noting the Jacobi identity, it follows that

$$
\begin{aligned}
(\delta P)_{t_1}-(\delta Q)_x &= \left[U_0,\left(\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right)_{t_1}\right]-\left[W_0,\left(\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right)_x\right]\\
&=\sum_{s=1}^{N}\lambda_s\mu_s([U_0,[W_0,\phi^{(s)}\psi^{(s)T}]]-[W_0,[U_0,\phi^{(s)}\psi^{(s)T}]])\\
&\quad+\left[U_0,\left[W_1,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right]\right]-\left[W_0,\left[U_1,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right]\right]\\
&=\left[U_0,\left[W_1,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right]\right]-\left[W_0,\left[U_1,\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T}\right]\right],
\end{aligned}
$$

where δP and δQ are defined by (A2). Then, again noting the Jacobi identity, we can have

$$
\begin{aligned}
&(\delta P)_{t_1}-(\delta Q)_x+[U_1,\delta Q]+[\delta P,W_1]\\
&\quad=\left[\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T},[U_0,W_1]\right]-\left[\sum_{s=1}^{N}\mu_s\phi^{(s)}\psi^{(s)T},[W_0,U_1]\right]=0,
\end{aligned}
$$

in the last step of which we have used $[U_0,W_1]=[W_0,U_1]$. The proof is finished. ■

All of the symmetries presented in this proposition are not Lie point, contact, or Bäcklund symmetries, since they cannot be written in terms of the potentials u_{ij} and their spatial derivatives.

APPENDIX B: FORMULAS FOR COMPUTING $\mathcal{F}_\lambda^{(k)}$

Immediately from the expressions of $\mathcal{F}_\lambda^{(k)}$ in (4.22), we can obtain the following more concrete formulas for computing $\mathcal{F}_\lambda^{(k)}$:

$$
\mathcal{F}_\lambda^{(1)}=\sum_{i=1}^{m}(c_i+\overset{ii}{Q}_\lambda),
$$

$$
\mathcal{F}_\lambda^{(2)}=\sum_{1\leqslant i<j\leqslant m}\left(c_ic_j+c_j\overset{ii}{Q}_\lambda+c_i\overset{jj}{Q}_\lambda+\begin{vmatrix}\overset{ii}{Q}_\lambda & \overset{ij}{Q}_\lambda\\ \overset{ji}{Q}_\lambda & \overset{jj}{Q}_\lambda\end{vmatrix}\right),
$$

$$
\begin{aligned}
\mathcal{F}_\lambda^{(3)}=&\sum_{1\leqslant i<j<k\leqslant m}(c_ic_jc_k+c_ic_k\overset{jj}{Q}_\lambda+c_jc_k\overset{ii}{Q}_\lambda+c_ic_j\overset{kk}{Q}_\lambda)\\
&+\sum_{1\leqslant i<j<k\leqslant m}\left(c_i\begin{vmatrix}\overset{jj}{Q}_\lambda & \overset{jk}{Q}_\lambda\\ \overset{kj}{Q}_\lambda & \overset{kk}{Q}_\lambda\end{vmatrix}+c_j\begin{vmatrix}\overset{ii}{Q}_\lambda & \overset{ik}{Q}_\lambda\\ \overset{ki}{Q}_\lambda & \overset{kk}{Q}_\lambda\end{vmatrix}+c_k\begin{vmatrix}\overset{ii}{Q}_\lambda & \overset{ij}{Q}_\lambda\\ \overset{ji}{Q}_\lambda & \overset{jj}{Q}_\lambda\end{vmatrix}+\begin{vmatrix}\overset{ii}{Q}_\lambda & \overset{ij}{Q}_\lambda & \overset{ik}{Q}_\lambda\\ \overset{ji}{Q}_\lambda & \overset{jj}{Q}_\lambda & \overset{jk}{Q}_\lambda\\ \overset{ki}{Q}_\lambda & \overset{kj}{Q}_\lambda & \overset{kk}{Q}_\lambda\end{vmatrix}\right),\\
&\cdots,\\
\mathcal{F}_\lambda^{(k)}=&\sum_{1\leqslant j_1<j_2<\ldots<j_k\leqslant m}\left(\prod_{p=1}^{k}c_{j_p}+\sum_{i=1}^{k}\prod_{\substack{p=1\\p\neq i}}^{k}c_{j_p}\overset{j_ij_i}{Q}_\lambda+\sum_{1\leqslant i_1<i_2\leqslant k}\prod_{\substack{p=1\\p\neq i_1,i_2}}^{k}c_{j_p}\begin{vmatrix}\overset{j_{i_1}j_{i_1}}{Q}_\lambda & \overset{j_{i_1}j_{i_2}}{Q}_\lambda\\ \overset{j_{i_2}j_{i_1}}{Q}_\lambda & \overset{j_{i_2}j_{i_2}}{Q}_\lambda\end{vmatrix}\right)
\end{aligned}
$$

$$+\sum_{1\leqslant j_1<j_2<\ldots<j_k\leqslant m}\ \sum_{1\leqslant i_1<i_2<i_3\leqslant k}\ \prod_{\substack{p=1\\ p\neq i_1,i_2,i_3}}^{k} c_{j_p}\begin{vmatrix} {}^{j_{i_1}j_{i_1}}Q_\lambda & {}^{j_{i_1}j_{i_2}}Q_\lambda & {}^{j_{i_1}j_{i_3}}Q_\lambda \\ {}^{j_{i_2}j_{i_1}}Q_\lambda & {}^{j_{i_2}j_{2}}Q_\lambda & {}^{j_{i_2}j_{i_3}}Q_\lambda \\ {}^{j_{i_3}j_{i_1}}Q_\lambda & {}^{j_{i_3}j_{i_2}}Q_\lambda & {}^{j_{i_3}j_{i_3}}Q_\lambda \end{vmatrix}+\ldots$$

$$+\sum_{1\leqslant j_1<j_2<\ldots<j_k\leqslant m}\begin{vmatrix} {}^{j_1j_1}Q_\lambda & {}^{j_1j_2}Q_\lambda & \cdots & {}^{j_1j_k}Q_\lambda \\ {}^{j_2j_1}Q_\lambda & {}^{j_2j_2}Q_\lambda & \cdots & {}^{j_2j_k}Q_\lambda \\ \vdots & \vdots & \ddots & \vdots \\ {}^{j_kj_1}Q_\lambda & {}^{j_kj_2}Q_\lambda & \cdots & {}^{j_kj_k}Q_\lambda \end{vmatrix},$$

$$\ldots,$$

$$\mathcal{F}_\lambda^{(m)}=\prod_{p=1}^{m} c_p+\sum_{i=1}^{m}\prod_{\substack{p=1\\ p\neq i}}^{m} c_p\,{}^{ii}Q_\lambda+\sum_{1\leqslant i<j\leqslant m}\prod_{\substack{p=1\\ p\neq i,j}}^{m} c_p\begin{vmatrix} {}^{ii}Q_\lambda & {}^{ij}Q_\lambda \\ {}^{ji}Q_\lambda & {}^{jj}Q_\lambda \end{vmatrix}$$

$$+\sum_{1\leqslant i<j<k\leqslant m}\ \prod_{\substack{p=1\\ p\neq i,j,k}}^{k} c_p\begin{vmatrix} {}^{ii}Q_\lambda & {}^{ij}Q_\lambda & {}^{ik}Q_\lambda \\ {}^{ji}Q_\lambda & {}^{jj}Q_\lambda & {}^{jk}Q_\lambda \\ {}^{ki}Q_\lambda & {}^{kj}Q_\lambda & {}^{kk}Q_\lambda \end{vmatrix}+\ldots+\begin{vmatrix} {}^{11}Q_\lambda & {}^{12}Q_\lambda & \cdots & {}^{1m}Q_\lambda \\ {}^{21}Q_\lambda & {}^{22}Q_\lambda & \cdots & {}^{2r}Q_\lambda \\ \vdots & \vdots & \ddots & \vdots \\ {}^{m1}Q_\lambda & {}^{r2}Q_\lambda & \cdots & {}^{mm}Q_\lambda \end{vmatrix}.$$

APPENDIX C: THE DETERMINANT OF Ω_m

The following proposition has been used while showing the functional independence of the polynomial functions $F_{is}(c_1,\ldots,c_m)$, $1\leqslant i\leqslant m$, $1\leqslant s\leqslant N$, which is of interest itself.

Proposition C.1: Let $m\geqslant 2$, and $c_1,c_2,\ldots,c_m$ be constants. Then

$$\det(\Omega_m)=\begin{vmatrix} 1 & \sum_{i=2}^{m} c_i & \sum_{2\leqslant i<j\leqslant m} c_ic_j & \sum_{2\leqslant i<j<k\leqslant m} c_ic_jc_k & \cdots & \prod_{i=2}^{m} c_i \\ 1 & \sum_{\substack{i=1\\ i\neq 2}}^{m} c_i & \sum_{\substack{1\leqslant i<j\leqslant m\\ i,j\neq 2}} c_ic_j & \sum_{\substack{1\leqslant i<j<k\leqslant m\\ i,j,k\neq 2}} c_ic_jc_k & \cdots & \prod_{\substack{i=1\\ i\neq 2}}^{m} c_i \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \sum_{i=1}^{m-1} c_i & \sum_{1\leqslant i<j\leqslant m-1} c_ic_j & \sum_{1\leqslant i<j<k\leqslant m-1} c_ic_jc_k & \cdots & \prod_{i=1}^{m-1} c_i \end{vmatrix}$$

$$=\prod_{1\leqslant i<j\leqslant m}(c_i-c_j). \tag{C1}$$

Proof: We prove this proposition by the principle of mathematical induction. It is obvious that (C1) is true when $m=2$. Suppose that (C1) is true when $m=l$. Let us verify that (C1) is also true when $m=l+1$. Note that

$$\sum_{\substack{1\leqslant i_1<i_2<\ldots<i_k\leqslant l+1\\ i_1,i_2,\ldots,i_k\neq j}} c_{i_1}c_{i_2}\ldots c_{i_k} - \sum_{\substack{1\leqslant i_1<i_2<\ldots<i_k\leqslant l+1\\ i_1,i_2,\ldots,i_k\neq i}} c_{i_1}c_{i_2}\ldots c_{i_k}$$

$$=(c_i-c_j)\sum_{\substack{1\leqslant i_1<i_2<\ldots<i_{k-1}\leqslant l+1\\ i_1,i_2,\ldots,i_{k-1}\neq i,j}} c_{i_1}c_{i_2}\ldots c_{i_{k-1}},$$

$$1\leqslant i,j\leqslant l+1, \quad 1\leqslant k\leqslant l.$$

For each $2\leqslant j\leqslant l+1$, we subtract

$$\sum_{2\leqslant i_1<i_2<\ldots<i_{j-1}\leqslant l+1}^{l+1} c_{i_1}c_{i_2}\ldots c_{i_{j-1}}\times \text{the first column of } \det(\Omega_{l+1})$$

from the jth column of $\det(\Omega_{l+1})$, and then we have

$$\det(\Omega_{l+1})$$

$$=\begin{vmatrix} 1 & 0 & 0 & 0 & \ldots & 0 \\ 1 & c_1-c_2 & (c_1-c_2)\sum_{i=3}^{l+1} c_i & (c_1-c_2)\sum_{3\leqslant i<j\leqslant l+1} c_ic_j & \ldots & (c_1-c_2)\prod_{i=3}^{l+1} c_i \\ 1 & c_1-c_3 & (c_1-c_3)\sum_{\substack{i=2\\ i\neq 3}}^{l+1} c_i & (c_1-c_3)\sum_{\substack{2\leqslant i<j\leqslant l+1\\ i,j\neq 3}} c_ic_j & \ldots & (c_1-c_3)\prod_{\substack{i=2\\ i\neq 3}}^{l+1} c_i \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & c_1-c_{l+1} & (c_1-c_{l+1})\sum_{i=2}^{l} c_i & (c_1-c_{l+1})\sum_{2\leqslant i<j\leqslant l} c_ic_j & \ldots & (c_1-c_{l+1})\prod_{i=2}^{l} c_i \end{vmatrix}$$

$$=\prod_{j=2}^{l+1}(c_1-c_j)\begin{vmatrix} 1 & \sum_{i=3}^{l+1} c_i & \sum_{3\leqslant i<j\leqslant l+1} c_ic_j & \ldots & \prod_{i=3}^{l+1} c_i \\ 1 & \sum_{\substack{i=2\\ i\neq 3}}^{l+1} c_i & \sum_{\substack{2\leqslant i<j\leqslant l+1\\ i,j\neq 3}} c_ic_j & \ldots & \prod_{\substack{i=2\\ i\neq 3}}^{l+1} c_i \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \sum_{i=2}^{l} c_i & \sum_{2\leqslant i<j\leqslant l} c_ic_j & \ldots & \prod_{i=2}^{l} c_i \end{vmatrix} = \prod_{1\leqslant i<j\leqslant l+1}(c_i-c_j),$$

in the last step of which we have used the inductive assumption. This means that (C1) is also true when $m=l+1$, i.e., the inductive step is satisfied. Therefore, the formula (C1) is always true by the principle of mathematical induction. The proof is finished. ■

APPENDIX D: TWO IDENTITIES ON SYMMETRIC POLYNOMIALS

Let the s_j's be symmetric polynomials defined by (4.27).

Proposition D.1: For any integers r and i with $i\geqslant r\geqslant 1$, and any numbers $c_1,\ldots,c_r$, we have

$$\sum_{j=0}^{i-r}(-1)^j s_j(c_1,\ldots,c_r)\sum_{\substack{l_1+\ldots+l_r=i-r-j\\ l_1,\ldots,l_r\geqslant 0}} c_1^{l_1}\ldots c_r^{l_r}=\begin{cases}1, & \text{if } i=r,\\ 0, & \text{if } i>r.\end{cases} \tag{D1}$$

Proof: Use the principle of mathematical induction on r. When $r=1$ and $i=1$, the left-hand side of (D1) is 1. When $r=1$ and $i>1$, the left-hand side of (D1) is 0. Hence (D1) holds when $r=1$.

Now suppose that (D1) holds when $r=k$, i.e.,

$$\sum_{j=0}^{i-k}(-1)^j s_j(c_1,\ldots,c_k)\sum_{\substack{l_1+\ldots+l_k=i-k-j\\ l_1,\ldots,l_k\geqslant 0}} c_1^{l_1}\ldots c_k^{l_k}=\begin{cases}1, & \text{if } i=k,\\ 0, & \text{if } i>k.\end{cases} \tag{D2}$$

Then, when $r=k+1$, the left-hand side of (D1) is

$$\sum_{j=0}^{i-k-1}(-1)^j s_j(c_1,\ldots,c_{k+1})\sum_{\substack{l_1+\cdots+l_{k+1}=i-k-j-1\\ l_1,\cdots,l_{k+1}\geqslant 0}} c_1^{l_1}\cdots c_{k+1}^{l_{k+1}}. \tag{D3}$$

By using (4.28), it equals

$$\begin{aligned}&\sum_{j=0}^{i-k-1}(-1)^j\sum_{l_{r+1}=0}^{i-k-j-1} c_{k+1}^{l_{k+1}+1}s_{j-1}(c_1,\ldots,c_k)\sum_{\substack{l_1+\cdots+l_k=i-k-j-1-l_{k+1}\\ l_1,\ldots,l_k\geqslant 0}} c_1^{l_1}\cdots c_k^{l_k}\\ &\quad+\sum_{j=0}^{i-k-1}(-1)^j\sum_{l_{r+1}=0}^{i-k-j-1} c_{k+1}^{l_{k+1}}s_j(c_1,\ldots,c_k)\sum_{\substack{l_1+\cdots+l_k=i-k-j-1-l_{k+1}\\ l_1,\cdots,l_k\geqslant 0}} c_1^{l_1}\cdots c_k^{l_k}\\ &=\sum_{l_{r+1}=0}^{i-k-1} c_{k+1}^{l_{k+1}+1}\sum_{j=0}^{i-k-l_{k+1}-2}(-1)^{j+1}s_j(c_1,\ldots,c_k)\sum_{\substack{l_1+\cdots+l_k=i-k-j-l_{k+1}-2\\ l_1,\cdots,l_k\geqslant 0}} c_1^{l_1}\cdots c_k^{l_k}\\ &\quad+\sum_{l_{r+1}=0}^{i-k-1} c_{k+1}^{l_{k+1}}\sum_{j=0}^{i-k-l_{k+1}-1}(-1)^j s_j(c_1,\ldots,c_k)\sum_{\substack{l_1+\cdots+l_k=i-k-j-l_{k+1}-1\\ l_1,\cdots,l_k\geqslant 0}} c_1^{l_1}\cdots c_k^{l_k},\end{aligned} \tag{D4}$$

where an empty sum is understood to be zero.

When $i=k+1$, it is easy to see that (D4) equals 1. If $i>k+1$, then by (D2), the first sum equals

$$-c_{k+1}^{l_{k+1}+1}\big|_{l_{k+1}=i-k-2}=-c_{k+1}^{i-k-1}, \tag{D5}$$

and again, by (D2), the second sum equals

$$c_{k+1}^{l_{k+1}}\big|_{l_{k+1}=i-k-1}=c_{k+1}^{i-k-1}. \tag{D6}$$

Hence (D4) equals 0 if $i>k+1$, which implies that (D1) holds when $r=k+1$. Therefore, (D1) always holds by the principle of mathematical induction. The proposition is proved. ■

Proposition D.2: For any integers m, r, i with $i\geqslant r+1\geqslant 2$, m numbers $c_1,\ldots,c_m$, and r integers $j_1,\ldots,j_r$ with $1\leqslant j_1<\ldots<j_r\leqslant m$, we have

$$\sum_{j=0}^{i-r}(-1)^{i-r-j}s_j(c_1,\ldots,c_m)\sum_{\substack{l_1+\cdots+l_r=i-r-j\\ l_1,\ldots,l_r\geqslant 0}}c_{j_1}^{l_1}\cdots c_{j_r}^{l_r}=\sum_{\substack{1\leqslant\rho_1<\cdots<\rho_{i-r}\leqslant m\\ \rho_\alpha\neq j_\beta \text{ for all } \alpha,\beta}}c_{\rho_1}\cdots c_{\rho_{i-r}}. \quad \text{(D7)}$$

Proof: Without loss of generality, suppose that $j_i=i$ when $i=1,\ldots,r$, since each $s_j(c_1,\ldots,c_m)$ is symmetric with respect to $c_1,\ldots,c_m$. Then, (D7) becomes

$$\sum_{j=0}^{i-r}(-1)^{i-r-j}s_j(c_1,\ldots,c_m)\sum_{\substack{l_1+\cdots+l_r=i-r-j\\ l_1,\cdots,l_r\geqslant 0}}c_1^{l_1}\cdots c_r^{l_r}=\sum_{r+1\leqslant\rho_1<\cdots<\rho_{i-r}\leqslant m}c_{\rho_1}\cdots c_{\rho_{i-r}}. \quad \text{(D8)}$$

Obviously, for any fixed j with $r+1\leqslant j\leqslant m$, both sides of (D8) are linear with respect to c_j.

We use the principle of mathematical induction on i to prove (D8). When $i=r+1$, both sides of (D8) equal $c_{r+1}+\cdots+c_m$.

Suppose that (D8) holds when $i=k$ $(k>r)$. Then, when $i=k+1$, the left-hand side of (D8) reads as

$$R:=\sum_{j=0}^{k+1-r}(-1)^{k+1-r-j}s_j(c_1,\ldots,c_m)\sum_{\substack{l_1+\cdots+l_r=k+1-r-j\\ l_1,\cdots,l_r\geqslant 0}}c_1^{l_1}\cdots c_r^{l_r}$$

$$=\sum_{j=-1}^{k-r}(-1)^{k-r-j}s_{j+1}(c_1,\ldots,c_m)\sum_{\substack{l_1+\cdots+l_r=k-r-j\\ l_1,\cdots,l_r\geqslant 0}}c_1^{l_1}\cdots c_r^{l_r}. \quad \text{(D9)}$$

Then by (4.28), we have

$$\frac{\partial R}{\partial c_m}=\sum_{j=0}^{k-r}(-1)^{k-r-j}s_j(c_1,\ldots,c_{m-1})\sum_{\substack{l_1+\cdots+l_r=k-r-j\\ l_1,\cdots,l_r\geqslant 0}}c_1^{l_1}\cdots c_r^{l_r}. \quad \text{(D10)}$$

By the inductive assumption, it becomes

$$\frac{\partial R}{\partial c_m}=\sum_{r+1\leqslant\rho_1<\ldots<\rho_{k-r}\leqslant m-1}c_{\rho_1}\cdots c_{\rho_{k-r}}. \quad \text{(D11)}$$

Hence we obtain

$$R=\sum_{r+1\leqslant\rho_1<\cdots<\rho_{k-r}\leqslant m-1}c_{\rho_1}\cdots c_{\rho_{k-r}}c_m+R_1(c_1,\ldots,c_{m-1}), \quad \text{(D12)}$$

where R_1 is a polynomial. Since R is symmetric with respect to $c_{r+1},\ldots,c_m$, we have

$$R=\sum_{r+1\leqslant\rho_1<\cdots<\rho_{k+1-r}\leqslant m}c_{\rho_1}\cdots c_{\rho_{k+1-r}}+R_0(c_1,\ldots,c_r), \quad \text{(D13)}$$

where by setting $c_{r+1}=\cdots=c_m=0$ in (D9), R_0 is determined to be

$$R_0(c_1,\ldots,c_r)=\sum_{j=0}^{k+1-r}(-1)^{k+1-r-j}s_j(c_1,\ldots,c_r)\sum_{\substack{l_1+\cdots+l_r=k+1-r-j\\ l_1,\ldots,l_r\geqslant 0}}c_1^{l_1}\cdots c_r^{l_r}. \quad \text{(D14)}$$

By Proposition D.1, $R_0=0$ since $k+1=i>r$. Hence

$$R=\sum_{r+1\leqslant\rho_1<\cdots<\rho_{k+1-r}\leqslant m} c_{\rho_1}\cdots c_{\rho_{k+1-r}}, \tag{D15}$$

which implies that (D8) holds when $i=k+1$. Therefore, (D8) holds for all $i>r$ by the principle of mathematical induction. The proof is completed. ■

The identity (D7) is needed in presenting an alternative involutive system E_{is}'s to the F_{is}'s in Sec. IV C.

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Degenerate dynamical systems

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Dynamical systems, whose symplectic structure degenerates, becoming noninvertible at some points along the orbits, are analyzed. It is shown that for systems with a finite number of degrees of freedom, like in classical mechanics, the degeneracy occurs on domain walls that divide phase space into nonoverlapping regions, each one describing a nondegenerate system, causally disconnected from each other. These surfaces are characterized by the sign of the Liouville flux density on them, behaving as sources or sinks of orbits. In this latter case, once the system reaches the domain wall, it acquires a new gauge invariance and one degree of freedom is dynamically frozen, while the remaining degrees of freedom evolve regularly thereafter. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1389088]

I. INTRODUCTION

A number of dynamical systems of physical interest possess field-dependent symplectic forms which degenerate, becoming noninvertible for some particular configurations. Systems as diverse as vortex interactions in fluids,[1] and gravitation theories in dimensions $d>4$ containing higher powers of curvature in the Lagrangian exhibit this feature (see, e.g., Ref. 2). Models of this kind naturally arise in different contexts of current high energy physics, ranging from cosmology and brane worlds[3,4] to strings and M-theory.[5–7]

The problem is how to describe the evolution of the system near a degenerate configuration and, if it could reach such a state, how it would evolve afterwards. The standard hypotheses in the treatment of dynamical systems, however, exclude the possibility that the symplectic form may have nonconstant rank throughout phase space, even in classical mechanics (see, e.g., Refs. 8, and 9).

As a first step towards understanding the general problem, here we analyze degenerate dynamical systems in classical mechanics. We show that it is possible to fully characterize the evolution of these systems.

It should be emphasized that this degeneracy is independent of Poincaré's classification of singularities. A Poincaré singularity occurs at critical points of the Hamiltonian, which are generically isolated, whereas the symplectic form degenerates on surfaces which are generically domain walls. This kind of surface cannot be understood as dense sets of Poincaré singularities. Roughly speaking, a symplectic degeneracy is the counterpart of a Poincaré singularity in that, in the latter the gradient of the Hamiltonian vanishes, whereas the former can be interpreted as an infinite gradient.

The previous point can be made more explicit by considering the simplest example of a degenerate system, whose phase flow satisfies

$$\begin{pmatrix} 0 & x_2 \\ -x_2 & 0 \end{pmatrix} \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} = \begin{pmatrix} E_1 \\ E_2 \end{pmatrix}, \tag{1}$$

with $E_1 E_2 \neq 0$, which degenerates at $x_2 = 0$. An equivalent formulation in the $x_2 \neq 0$ region is

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} = \frac{1}{x_2} \begin{pmatrix} -E_2 \\ E_1 \end{pmatrix}, \tag{2}$$

which can be viewed as a phase flow where the gradient of the Hamiltonian diverges as $x_2 \to 0$. The required symplectomorphism (canonical transformation) to obtain Eq. (2) from Eq. (1) is noninvertible throughout phase space, however.

II. FIRST-ORDER LAGRANGIANS AND THEIR SYMPLECTIC FORMS

Let us consider a system whose action is a one-form A, integrated over a $(0+1)$-dimensional worldline embedded in a $(2n+1)$-dimensional spacetime of signature $(-,+,\ldots,+)$,

$$S[z;1,2] = \int_1^2 A_\mu \dot{z}^\mu \, d\tau, \tag{3}$$

The field A_μ is a prescribed set of $2n+1$ functions of the embedding coordinates z^μ, which are the dynamical variables.[10] This action is manifestly invariant under reparametrizations of the worldline $\tau \to \tau'(\tau)$, and diffeomorphisms $z^\mu \to z'^\mu(z)$.[11] Identifying the affine parameter with the timelike embedding coordinate $z^0 := t$, so that $z^i = z^i(t)$, the action reads

$$S[z;1,2] = \int_{t_1}^{t_2} [A_i \dot{z}^i + A_0] \, dt. \tag{4}$$

The equations of motion are given by

$$F_{ij} \dot{z}^j + E_i = 0, \tag{5}$$

where we have defined $E_i \equiv \partial_i A_0 - \partial_0 A_i$ and $F_{ij} \equiv \partial_i A_j - \partial_j A_i$. In the following, we assume A_i and A_0 to be time-independent.

These dynamical systems are naturally classified according to the rank ρ of the symplectic form F_{ij}.[12] Thus, three cases are distinguished: (A) regular Hamiltonian systems, for which the symplectic form has constant maximal rank, $\rho(F_{ij}) = 2n$ throughout phase space Γ,[10] (B) singular or constrained Hamiltonian systems, which have a constant nonmaximal rank, $\rho(F_{ij}) = 2m < 2n$ throughout Γ,[9] and, (C) degenerate systems, which have nonconstant rank $\rho(F_{ij})$ throughout Γ.

III. DEGENERATE SYSTEMS

We will focus our discussion in the degenerate case (C), which has been traditionally left aside in the literature. We will assume that the zero-measure subset of Γ given by

$$\Sigma = \{ z \in \Gamma / F = 0 \}, \tag{6}$$

where $F := \det(F_{ij})$, is not dense. Thus, outside Σ, the symplectic form F_{ij} has a constant rank $2n$, and the dynamical structure there is described through case (A) above.[13]

Under these conditions, nothing prevents the system, starting from a generic state for which $F \neq 0$, from reaching a point on Σ after some finite time. Having this scenario in mind, we address the following points:

(i) the description of the locus of Σ,
(ii) classification of the phase flow near Σ, and
(iii) whether Σ can be reached and, in that case, the fate of the system thereafter.

A. Degeneracy surfaces Σ

As is well known, a skew-symmetric $2n \times 2n$ matrix $F_{ij}(z)$ can be brought into the block-diagonal form by an orthogonal transformation. Thus the two-form $\mathcal{F} = 1/2 F_{ij} dz^i \wedge dz^j$ can be block diagonalized in an open set, under a local $O(2n)$ coordinate transformation $z^i \to x^i(z)$,

$$\mathcal{F}=\sum_{r=1}^{n} f_r(z)dx^{2r-1}\wedge dx^{2r}. \tag{7}$$

However, *in open sets containing points of the degeneracy surfaces, the Darboux-like coordinates x^i cannot be brought into the standard canonical form, because at least one of the f_r's in (7) vanishes at* Σ. Hence, further (finite) rescalings cannot normalize the f_r's to 1. As a consequence, the set Σ is the union of the $(2n-1)$-dimensional surfaces

$$\Sigma_r=\{z\in\Gamma/f_r(z)=0\},$$

that is, $\Sigma=\cup_{r=1}^{n}\Sigma_r$.

Moreover, by virtue of the Bianchi identity $(d\mathcal{F}=0)$, it can be shown that $f_r(x)$ depends only on the pair of conjugate coordinates (x^{2r-1},x^{2r}). This means that the degeneracy surfaces are constant along the remaining coordinates.

We assume that the f_r's are smooth Morse functions on the corresponding $(x^{2r-1}-x^{2r})$ planes, which ensures that they possess only simple zeros except at isolated points; the cases where f_r has zeros of higher order can be thought of as the merging of simple zeros. Hence, the level curves $f_r(x^{2r-1},x^{2r})=0$ divide the $(x^{2r-1}-x^{2r})$-plane into nonoverlapping sets and therefore,

Lemma 1: The locus of the degeneracy surfaces Σ corresponds to a collection of domain walls, splitting the phase space Γ into a number of nonoverlapping regions.

B. Characterization of the phase flow near Σ

Generically, at a surface Σ_r the rank $\rho(F_{ij})$ is lowered by 2, and at points where k of these surfaces intersect, ρ is lowered by $2k$. In a sufficiently small neighborhood of the surface Σ_r, the behavior of the system is dominated by the dynamical variables $x^\alpha=(x^{2r-1}-x^{2r})$, whose corresponding equations of motion can be read from Eq. (5) as

$$\epsilon_{\alpha\beta}f(x)\dot{x}^\beta=-E_\alpha, \tag{8}$$

where for simplicity, we have set $r=1$, so that α and $\beta=1,2$ and $f:=f_1$. Near a degeneracy surface Σ_r, the remaining dynamical variables z^a $(a=3,\ldots,2n)$ behave like the phase space coordinates of a regular system.

Here it is assumed that E_α remains finite and does not vanish on Σ_1 (i.e., Poincaré singularities are assumed to be located outside Σ), therefore, Eq. (8) implies that the velocity becomes tangent to the (x^1-x^2) plane, because the components $\dot{x}^\alpha$ become unbounded as the orbit approaches Σ_1, while the other components $(\dot{z}^a)$ remain finite.

Due to the fact that f has a simple zero at Σ_1, $\dot{x}^\alpha$ reverses its sign across the degeneracy surface. Consequently, the phase flow evolves in opposite directions on each side of Σ. Thus, in a local neighborhood of Σ, one of the following three situations occur: (a) Orbits flow towards Σ and end there, (b) the orbits originate at the degeneracy surface and flow away from it, or (c) the orbits run parallel to Σ, but in opposite directions on each side.

Hence, the surfaces act as sinks or sources for the orbits in cases (a) and (b), respectively, which naturally suggests a classification of the local nature of Σ into $\Sigma^{(-)}$, $\Sigma^{(+)}$, and $\Sigma^{(0)}$ for the cases (a), (b) and (c), respectively (see Fig. 1).

In all three cases there is no flux across the degeneracy surface, and therefore, we have the following.

Lemma 2: The regions on either side of Σ are causally disconnected and dynamically independent from each other.

An immediate consequence of this is the violation of Liouville's theorem at the surfaces of degeneracy. In fact, outside the degeneracy surfaces, the Liouville current

$$j^i=\sqrt{F}\dot{z}^i \tag{9}$$

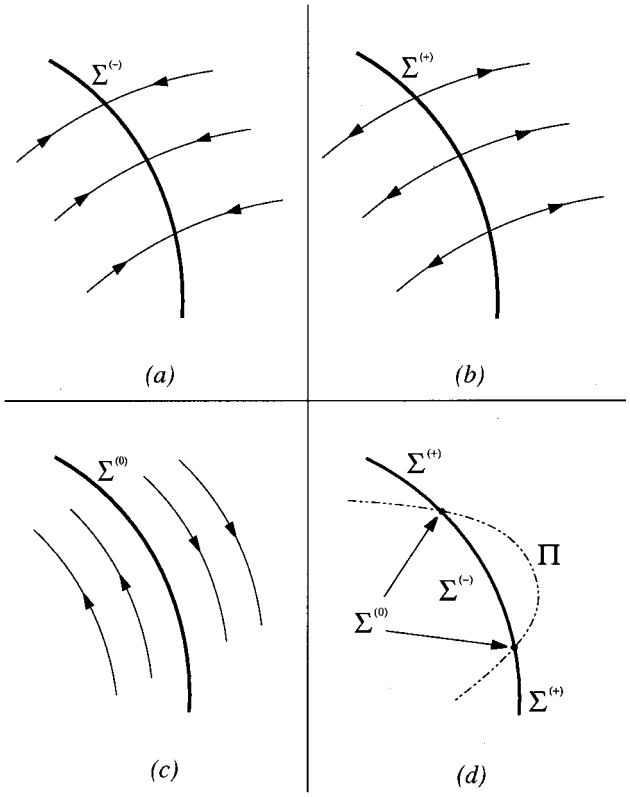

FIG. 1. (a), (b) and (c) show the qualitative local flow in the neighborhood of $\Sigma^{(+)}$, $\Sigma^{(-)}$ and $\Sigma^{(0)}$, respectively. The global structure of degeneracy surfaces is shown in (d).

is divergence-free ($\partial_i j^i = 0$) by virtue of the equations of motion and the identity $\partial_i(\sqrt{F}F^{ij}E_j) = 0$, with $F^{ij}F_{jk} = \delta^i_k$. This means that Liouville's theorem holds outside Σ, where the dynamical behavior is regular. Moreover, j^i has a finite limit as the system approaches a degeneracy surface, whose only nonvanishing components on each side of Σ are

$$j^\alpha = |f|\dot{x}^\alpha = sgn(f)\epsilon^{\alpha\beta}E_\beta . \tag{10}$$

The local character of the degeneracy surfaces Σ can be inferred from the flux of j^i across a pill box enclosing a portion of Σ. The flux density $\Phi = j^i n_i$ across the lids of the pill box is given by the projection of j^i along the normal to the surface $n_i = \partial_i F^{1/2}$, whose only nonvanishing components are $n_\alpha = \partial_\alpha |f|$, that is,

$$\Phi = -F^{1/2}F^{ij}E_j\partial_i F^{1/2} = \partial_\alpha f \epsilon^{\alpha\beta}E_\beta . \tag{11}$$

Note that Φ is not only finite, but continuous on Σ. Therefore, we have the following lemma.

Lemma 3: The local character of the degeneracy surfaces is given by $\Sigma^{(\eta)}$ with $\eta = sgn(\Phi)$. Furthermore, in general, Σ is globally piecewise attractive ($\Sigma^{(-)}$) or repulsive ($\Sigma^{(+)}$), and is of type $\Sigma^{(0)}$ at the intersections with the surfaces $\Pi = \{z \in \Gamma / \Phi(z) = 0\}$ [see Fig. 1.(d)].

Hence, $\Sigma^{(0)}$ generically corresponds to the boundaries between $\Sigma^{(-)}$ and $\Sigma^{(+)}$ (that is, $\Sigma^{(0)} = \partial\Sigma^{(-)}$) which is a subset of codimension 2 in phase space.

In the particular case, when both surfaces Σ and Π coincide on an open set, Σ is globally of type $\Sigma^{(0)}$. This occurs for example, if $E_i|_{\Sigma^{(0)}} = \partial_i(h(z^i)F^{1/2})$, whose only nonvanishing components are of the form $E_\alpha = \tilde{h}(z^a)\partial_\alpha f$ for some functions h and $\tilde{h} \neq 0$.[14]

C. Evolution towards $\Sigma^{(-)}$

The degeneracy surfaces $\Sigma^{(+)}$ and $\Sigma^{(-)}$ represent sets of initial and final states of the system, respectively. Configurations at a surface $\Sigma^{(+)}$ are unstable against small perturbations, and it seems unlikely that a system could be prepared there. On the other hand, if one considers the system at $\Sigma^{(-)}$, a small perturbation to move it away from the surface would require an infinite acceleration. In this sense, the surfaces $\Sigma^{(-)}$ represent stable final states for the evolution of the system, and any initial configuration sufficiently near the degeneracy surface is doomed to fall on it. Then, the question whether the system can be consistently defined on $\Sigma^{(-)}$ naturally arises.

For simplicity, let us consider a system possessing a single surface of degeneracy which is globally of type $\Sigma^{(-)}$. We will now show that when the system reaches $\Sigma^{(-)}$, two coordinates become nondynamical; the system acquires a new gauge symmetry on the degeneracy surface which corresponds to displacements along $\Sigma^{(-)}$, and one degree of freedom is lost.

Following Dirac's approach for constrained systems,[15] the action (4) possesses $2n$ primary constraints coming from the definition of the canonical momenta $p_i=\partial L/\partial \dot{z}^i$,

$$\phi_i(z,p)\equiv p_i-A_i(z,t)\approx 0, \tag{12}$$

whose Poisson brackets are $\{\phi_i,\phi_j\}=F_{ij}$. Outside $\Sigma^{(-)}$, the invertibility of F_{ij} implies that the constraints ϕ_i are second class. However, at the degeneracy surface, the rank of F_{ij} is reduced by two, thus, two of the ϕ's have vanishing Poisson brackets with the whole set of constraints.

Although the constraint structure changes abruptly at $\Sigma^{(-)}$, after the system reaches this surface, its evolution can be described by a standard constrained system, as can be seen through a suitable change of basis for the constraints ϕ_i.

Linear combinations of the form $\varphi_{(\alpha)}=e^i_{(\alpha)}\phi_i$ become first class provided $e^i_{(\alpha)}$ are null vectors of F_{ij}. This can only happen at the degeneracy surface, where there are two such vectors. They can be chosen so that one is tangent and the other is normal to the surfaces $F=\text{const}$, namely, $e^i_{(1)}F_{ij}=1/2\partial_j F$ and $e^i_{(2)}F_{ij}=F_{ij}\partial_i\sqrt{F}$. In Darboux-like coordinates, their only nonvanishing components are $e^\alpha_{(1)}=\epsilon^{\alpha\beta}\partial_\beta f$ and $e^\alpha_{(2)}=\delta^{\alpha\beta}\partial_\beta f$, with $\alpha=1,2$.

In the basis $\phi_i=\{\varphi_{(\alpha)};\phi_a\}$, with $a=3,\ldots,2n$, the constraint algebra reads

$$\begin{aligned}
&\{\varphi_{(\alpha)},\varphi_{(\beta)}\}\approx \tfrac{1}{4}\epsilon_{(\alpha)(\beta)}F^{-1/2}(\partial_i F)^2=f\epsilon_{(\alpha)(\beta)}|\partial f|^2,\\
&\{\varphi_{(\alpha)},\phi_b\}\approx e^i_{(\alpha)}F_{ib}=0,\\
&\{\phi_a,\phi_b\}=F_{ab}.
\end{aligned} \tag{13}$$

From this it is apparent that, on the surface $\Sigma^{(-)}$, the constraints $\varphi_{(\alpha)}$ have vanishing Poisson brackets, and are therefore candidates for first class constraints.

In order to examine whether $\varphi_{(\alpha)}$ are first or second class at the degeneracy surface ($f=0$), it is necessary to compute their Poisson brackets with f. The only nonvanishing bracket involving f is

$$\{f,\varphi_{(2)}\}=e^\alpha_{(2)}\partial_\alpha f=|\partial_\alpha f|^2, \tag{14}$$

which cannot vanish on Σ because, by hypothesis, f has a simple zeros there. This shows that $\varphi_{(1)}$ is first class, while $(f,\varphi_{(2)})$ form a conjugate pair of second class constraints.

The transformations generated by $\varphi_{(\alpha)}$ correspond to $\delta z^a=0$, and

$$\delta x^\alpha=\{x^\alpha,\xi^{(\beta)}\varphi_{(\beta)}\}=\xi^{(\beta)}e^\alpha_{(\beta)}=\xi^\alpha. \tag{15}$$

Thus, the constraints $\varphi_{(1)}$ and $\varphi_{(2)}$ generate tangent and normal displacements to $\Sigma^{(-)}$, respectively, as expected. Hence, $f\approx 0$ can be viewed as the gauge fixing condition associated with the "gauge generator" $\varphi_{(2)}$. This is summarized in the following.

Lemma 4: On the degeneracy surface $\Sigma^{(-)}$, the system acquires a new gauge invariance, because the second class constraint $\varphi_{(1)}$ becomes first class, while the number of second class constraints $(f,\varphi_{(2)},\phi_a)$ remains the same $(2n)$. Since each first class constraint eliminates one degree of freedom, we conclude that one degree of freedom is dynamically frozen on the degeneracy surface.

We illustrate these results in the following examples.

IV. EXAMPLES

A. Simplest degenerate system

The simplest case of a degenerate dynamical system is provided by the Lagrangian

$$L_D = A_\alpha \dot{x}^\alpha + A_0, \tag{16}$$

with $A_1=0$, $A_2=x_1x_2$, $A_0=-\nu x_1$. The symplectic form, $F_{\alpha\beta}=\epsilon_{\alpha\beta}x_2$, degenerates at the surface $x_2=0$, which is of type $\Sigma^{(\eta)}$, with $\eta=sgn(\nu)$. The orbits run perpendicular to $\Sigma^{(\eta)}$ and take a finite time to connect a point on the surface with a point outside.

This example captures the essence of the behavior of any degenerate system in a neighborhood of a degeneracy surface of type $\Sigma^{(+)}$ or $\Sigma^{(-)}$. In particular, the shock-wave solutions of Burgers' equation,

$$\partial_t u + u\partial_x u = \nu \partial_x^2 u, \tag{17}$$

which is relevant in the context of turbulence, exhibit this behavior. These solutions are of the form

$$u(x,t) = -2\nu \sum_{k=1}^{2n} (x - z_k(t))^{-1}, \tag{18}$$

where $z_k(t)$ are complex coordinates which come in conjugate pairs and satisfy a vortexlike equation.[16] The corresponding equations of motion for $z_k(t)$ can be obtained from an action of the form (4), which for $n=1$ and $z=x_1+ix_2$ reads

$$\begin{pmatrix} 0 & x_2 \\ -x_2 & 0 \end{pmatrix} \begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \end{pmatrix} = \begin{pmatrix} \nu \\ 0 \end{pmatrix}, \tag{19}$$

whose associated Lagrangian is precisely given by (16). This solution describes a one-dimensional shock wave centered at $x=x_1$, with peaks at $x=x_1\pm x_2(t)$ of height $\mp 2\nu/x_2(t)$, traveling outwards from x_1.

B. Coupling with a regular system

The next example examines explicitly the fate of a degenerate system when it reaches a surface of type $\Sigma^{(-)}$. A simple Lagrangian for which this occurs is of the form

$$L = L_D(x^\alpha) + L_R(z^a) - V_\lambda(x^\alpha, z^a). \tag{20}$$

Here,

$$L_D(x^\alpha) = A_\alpha \dot{x}^\alpha - H_D(x^\alpha), \tag{21}$$

with $\alpha=1,2$, is some two-dimensional degenerate system possessing a global surface of type $\Sigma^{(-)}$ at $f(x^\alpha)=0$; $L_R(z^a)$ is a regular system with Hamiltonian $H_R(z^a)$, and $V_\lambda(x^\alpha,z^a)$ is an interaction term of the form

$$V_\lambda = \lambda f(x^\alpha) H_R(z^a). \tag{22}$$

This coupling is chosen so that it vanishes on $\Sigma^{(-)}$ and does not change the flux density Φ there, so that the character of the degeneracy surface does not depend on the coupling constant λ. Note that this coupling would be trivial in the case of nondegenerate systems. Furthermore, the presence of H_R in the coupling implies that, besides the conservation of the total Hamiltonian $H=H_D+H_R+V_\lambda$, the equations of motion

$$\dot{z}^a=(1+\lambda f(x))F^{ab}\partial_b H_R \tag{23}$$

give rise to a separate conservation law for H_R, because $\dot{H}_R=\dot{z}^a\partial_a H_R=0$. In turn, this implies that the remaining equations of motion,

$$\epsilon_{\alpha\beta}f(x)\dot{x}^\beta=\partial_\alpha(H_D+\lambda f(x)H_R), \tag{24}$$

can be integrated as an autonomous two-dimensional subsystem. Once these equations have been solved, and their solutions substituted in (23), it is apparent that the solutions of Eq. (23) describe the same orbits as in the decoupled case ($\lambda=0$) but with a reparametrized time,

$$z^a(t)=z^a_{(\lambda=0)}(\tau),$$

with

$$\frac{d\tau}{dt}=1+\lambda f(x(t)).$$

Note that as the orbits approach the surface $\Sigma^{(-)}$, this time reparametrization remains finite.

Once the system reaches the degeneracy surface ($f(x)\to 0$), both time coordinates become identical and, *on* $\Sigma^{(-)}$, *all traces of the degenerate subsystem disappear, including the information about its initial conditions* $x^\alpha(t_0)$.

Thus from the moment the degeneracy surface is reached, the system becomes a regular one, described by $L_R(z^a)$, and the degrees of freedom of the degenerate system are forever lost.

In order to illustrate this point, consider the degenerate Lagrangian given by Eq. (16) with $\nu<0$, coupled with a one-dimensional harmonic oscillator in the form (22). In that case, the total energy is $\mathcal{E}=\mathcal{E}_R(1+\lambda x_2)+\nu x_1$, where $\mathcal{E}_R$ is the energy of the harmonic oscillator, which is separately conserved. Equation (24) is readily integrated as

$$x_2(t)=\pm\sqrt{2\nu t+(x_2(t_0))^2},$$

for $t<(x_2(t_0))^2/2\nu$, and $x_2(t)=0$ afterwards.

Hence, the harmonic oscillator coordinates $Z=z^1+iz^2$ evolve according to

$$Z(t)=Z_0\exp(i\tau),$$

with $|Z_0|^2=2\mathcal{E}_R$, where the reparametrized time is given by

$$\tau=t+\frac{\lambda}{3\nu}[2\nu t+(x_2(t_0))^2]^{3/2},$$

for $t<(x_2(t_0))^2/2\nu$, and $\tau=t$ afterwards.

V. DISCUSSION AND OVERVIEW

The degeneracy of the symplectic form opens up the possibility of a violation of Liouville's theorem. In fact, the divergence of the current $j^i=\sqrt{F}\dot{z}^i$ reads,

$$\partial_i j^i=-\partial_i[\sqrt{F}F^{ij}]\partial_j A_0-\sqrt{F}F^{ij}\partial_i\partial_j A_0.$$

If $A_0 = -H$ is continuous and differentiable, the second term in the R. H. S. vanishes identically. However, the first term can give rise to a non-zero contribution, responsible for the jump in the flow across Σ. In this sense, the problem we address here is the counterpart of Poincaré classical study of singularities in the phase flow. Both cases correspond to different classes of possible singularities in the phase flow, and, hence, the degeneracy surfaces cannot be understood as a dense set of Poincaré's singularities.

It is reasonable to expect that the extension of our analysis to field theory would lead to the possibility that the symplectic form degenerates for field configurations where some local degrees of freedom should freeze out and some field components become nondynamical. In the case of higher dimensional gravity, this means that as the system reaches a degeneracy surface, some dynamical components of the metric become redundant, which would correspond to a sort of dynamical dimensional reduction mechanism.

The quantum mechanical analysis of this kind of degenerate systems shows that there is no tunneling across a surface of degeneracy Σ, but there is a nonvanishing propagation amplitude between states in the bulk and on Σ.[17] These results would be relevant for the quantum Hall effect,[18] and also for strings propagating in a background possessing a nonconstant B-field.[19]

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Lorentzian regularization and the problem of point-like particles in general relativity

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The two purposes of the article are (1) to present a regularization of the self-field of point-like particles, based on Hadamard's concept of ''partie finie,'' that permits in principle to maintain the Lorentz covariance of a relativistic field theory, and (2) to use this regularization for defining a model of stress-energy tensor that describes point-particles in post-Newtonian expansions (e.g., 3PN) of general relativity. We consider specifically the case of a system of two point-particles. We first perform a Lorentz transformation of the system's variables which carries one of the particles to its rest frame, next implement the Hadamard regularization within that frame, and finally come back to the original variables with the help of the inverse Lorentz transformation. The Lorentzian regularization is defined in this way up to any order in the relativistic parameter $1/c^2$. Following a previous work of ours, we then construct the delta-pseudo-functions associated with this regularization. Using an action principle, we derive the stress-energy tensor, made of delta-pseudo-functions, of point-like particles. The equations of motion take the same form as the geodesic equations of test particles on a fixed background, but the role of the background is now played by the regularized metric. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1384864]

I. INTRODUCTION

In recent years, the problem of the dynamics of gravitationally interacting compact objects in general relativity has received a lot of attention. This is due in part to the interest of the theoretical problem in its own, and in part to the ongoing development of laser-interferometric detectors for observing gravitational radiation. In the absence of an exact solution of the problem, one has recourse to successive post-Newtonian approximations (formal expansions in powers of $1/c$). Within such approximations, it makes sense to model the compact objects with some ''point-like particles,'' exactly as we do in a standard way within the Newtonian theory. However, the self-field of point-particles is infinite at the very location of a particle, and thus must be somehow regularized. The regularization is quite straightforward in the Newtonian theory, but it becomes nontrivial when going to high post-Newtonian approximations. Dealing with this problem, the present authors[1] developed a method for regularizing the infinite self-field of point-particles, which is based on the concept of ''partie finie,'' in the sense of Hadamard,[2,3] of a singular function at the place of one of its singular points (see, e.g., Refs. 4–7 for entries to the mathematical literature). We know that the Hadamard regularization yields the correct result for the equations of motion of two particles up to the so-called second and half post-Newtonian (2.5PN) approximation, corresponding to the order $1/c^5$ beyond the Newtonian acceleration. Indeed, the problem has been completely solved at that order;[8–19] notably some derivations make use of this regularization (e.g., Refs. 12 and 19). In the present state of the art, we are concerned with the 3PN (or $1/c^6$)

approximation.[20–25] In fact, starting at this high post-Newtonian order, the regularization may become physically incomplete because of the appearance of an undetermined coefficient in the equations of motion.[20–25]

The Hadamard regularization, investigated in Ref. 1, is performed in a three-dimensional Euclidean space with generic point $\mathbf{x}\in\mathbb{R}^3$, which is viewed as the spatial hypersurface labeled by $t=\text{const}$ in a global coordinate system $\{t,\mathbf{x}\}$ covering the whole space–time. In particular, the regularization involves a spatial average, performed at $t=\text{const}$, over the direction of approach to the singularity. As such a regularization makes use of a preferred spatial hypersurface $t=\text{const}$, it is clearly incompatible with the framework of special or general relativity, which embodies a global Lorentz (or Poincaré) frame invariance. Notably, we expect that the post-Newtonian equations of motion of point-like particles in harmonic coordinates (which we recall preserve the global Lorentz invariance) should exhibit at some stage a violation of the Lorentz invariance due to the latter regularization. The fact is that the breakdown of the Lorentz invariance due to the regularization occurs only at the very high 3PN approximation. Until the 2.5PN order, it is sufficient to regularize within a preferred slice $t=\text{const}$ of the harmonic coordinate system to obtain some Lorentz-invariant equations of motion.[19]

The first purpose of this article is to define a regularization *à la* Hadamard[2,3] that is compatible with the Lorentz structure of a relativistic field theory. This completes the definition, proposed in Ref. 1, of a specific version of the Hadamard regularization (based notably on a particular class of pseudo-functions). To achieve this purpose, we shall simply perform the standard Hadamard regularization within the hypersurface that is geometrically orthogonal, in the sense of the Minkowski metric, to the four-velocity of the particle. In separate papers,[24,25] we apply the latter ''Lorentzian'' regularization (together with the distributional derivatives introduced in Ref. 1) to the computation of the binary equations of motion at the 3PN order in harmonic coordinates and find that, indeed, it permits the preserving of their Lorentz invariance (in some case at the price of adjusting some parameter). A different approach to the problem of incorporating the Lorentz invariance in the 3PN equations of motion consists of deriving a generic regularized dynamics, within the ADM-Hamiltonian formalism of general relativity, involving an arbitrary regularization parameter, and determining this parameter uniquely by requiring the Lorentz invariance.[23] (See Sec. 2 in Ref. 25 for a discussion on our point-mass regularization and its relation to Ref. 23.)

Throughout the article, we assume the existence of a preferred Minkowski metric, as selected for instance by the condition of harmonic coordinates in general relativity, with respect to which the trajectories of particles are represented by accelerated world lines like in special relativity. Most of our investigation is valid not only in the case of the gravitational field but also for any Lorentz-tensor field propagating on the Minkowski background. Furthermore, we shall define the Lorentzian regularization in a sense of formal expansion series in $1/c^2$, so that all the formulas in the article will be given by some infinite series of relativistic corrections when c tends toward infinity. This is all we need for the derivation of the equations of motion to the 3PN order.[24,25]

Since we are interested in the application to the motion of two particles, we shall define the regularization around one of the particles (say particle 1), and shall consider that its acceleration is purely due to particle 2. (However, our definitions could be generalized to a system of N particles.) Notice that particle 2 enters this regularization scheme through the Lorentz transformation of its own variables to the rest frame of particle 1, and the replacement of the acceleration of 1 in terms of the equations of the binary motion. In general, working at some given relativistic order, we shall need to know the equations of motion up to a lower order only, therefore giving us the possibility of an iterative process. In this article, we always assume that we know the relevant equations of motion at this order, and that these are Lorentz-invariant.

Our second purpose is to derive an expression, compatible with the latter regularization, for the stress-energy tensor of point-like particles in post-Newtonian expansions of general relativity. Thanks to this regularization, we are able to give a sense to the value of the metric coefficients at the very location of the particle. Our basic assumption is that the matter action is the same as for *test* particles moving on a prescribed background gravitational field, except that the metric at the location of the particles is replaced by its regularized value in the sense of the (Lorentzian)

regularization. From this assumption, we prove that the Dirac measure in the stress-energy tensor must be replaced by a certain generalized function defined by means of the Hadamard prescription. In the case of two particles (the generalization to N particles is immediate), we obtain

$$T^{\mu\nu}_{\text{particle}}=\frac{m_1 c v_1^\mu v_1^\nu}{\sqrt{-[g_{\rho\sigma}]_1 v_1^\rho v_1^\sigma}}\,\text{Pf}\left(\frac{\Delta(\mathbf{x}-\mathbf{y}_1)}{\sqrt{g(t,\mathbf{x})}}\right)+1\leftrightarrow 2, \tag{1.1}$$

where m_1 is the mass of the particle 1, and $v_1^\mu=(c,\mathbf{v}_1)$ its coordinate velocity, i.e., $\mathbf{v}_1=d\mathbf{y}_1/dt$, $\mathbf{y}_1=\mathbf{y}_1(t)$ being the trajectory parametrized by the coordinate time t (the symbol $1\leftrightarrow 2$ denotes the same expression but corresponding to the second particle). The notation $[g_{\rho\sigma}]_1$ means that the metric $g_{\rho\sigma}(t,\mathbf{x})$ is to be computed at the point $\mathbf{x}=\mathbf{y}_1(t)$ following the regularization (of course $[g_{\rho\sigma}]_1$ depends on the positions and velocities of both particles 1 and 2). Note that the first factor in (1.1) is a mere function of time t. The second factor $\text{Pf}(\Delta(\mathbf{x}-\mathbf{y}_1)/\sqrt{g})$ is made of a special type of partie finie delta-pseudo-function associated with the regularization (following the definition given in Ref. 1). It involves (minus) the determinant of the metric $g_{\rho\sigma}$, namely g, evaluated at the point $(t,\mathbf{x})$, and a generalization $\text{Pf}\Delta(\mathbf{x}-\mathbf{y}_1)$ of the Dirac function defined in such a way that its action on a singular function yields the value of the function at the singular point in the sense of the regularization. Among the rules for handling the delta-pseudo-functions, we are allowed to write $\text{Pf}(\Delta(\mathbf{x}-\mathbf{y}_1)/\sqrt{g})=(1/\sqrt{g})\text{Pf}\Delta(\mathbf{x}-\mathbf{y}_1)$, whereas it is strictly forbidden to replace the latter quantity by $[1/\sqrt{g}]_1\text{Pf}\Delta(\mathbf{x}-\mathbf{y}_1)$.

The stress-energy tensor (1.1) takes the same form as the one of test particles moving in a fixed background, but with the role of the background played by the regularized metric generated by the bodies. In particular, the equations of motion obtained from the covariant conservation of that tensor ($\nabla_\nu T^{\mu\nu}_{\text{particle}}=0$) take the same form as the ''geodesic equations'' when considered with respect to the regularized metric. Our definition of the stress-energy tensor (1.1) constitutes a proposal that we have found to be the most natural in the problem of the equations of binary motion at the 3PN order,[24,25] but that we have not proved to be generally valid to higher post-Newtonian orders (nor of course when considered outside a framework of post-Newtonian expansions). The tensor (1.1) appears to be a good candidate for the characterization of point-like particles in post-Newtonian expansions of general relativity.

The plan of this article is the following. In Sec. II, we recall from Ref. 1 the material needed in the subsequent parts concerning the Hadamard regularization and the associated pseudo-functions. In Sec. III, we investigate the formulas needed to regularize, for the Lorentz transformation of some field point as well as two source points, and we define the new regularization around one of the particles as taking place within the instantaneous spatial hypersurface of the particle. In Sec. IV, we give the formulas for this regularization at the level of the first relativistic correction $1/c^2$. Finally, in Sec. V, we derive from an action principle our model of stress-energy tensor of point-like particles; the covariant conservation of this tensor leads to the equations of motion.

II. HADAMARD REGULARIZATION

To make the present article self-contained, we shall review in this section the classic notions of the Hadamard regularization of singular functions and divergent integrals,[2,3] as well as the construction, by Blanchet and Faye,[1] of a set of pseudo-functions associated with it. We follow closely the investigation of our previous article[1] and employ most of its notation. A coordinate system $\{t,\mathbf{x}\}$ being given on space–time (for instance, the harmonic coordinates used in Sec. IV), we consider some functions $F(\mathbf{x})$ defined on the spatial slice $t=\text{const}$, where $\mathbf{x}\in\mathbb{R}^3$ denotes the position in the slice. We say that the function $F(\mathbf{x})$ belongs to the class $\mathcal{F}$ if and only if F is a smooth function on $\mathbb{R}^3$ except at two isolated points $\mathbf{y}_1$ and $\mathbf{y}_2$, and admits around each of these points the following power-like singular expansions. Denoting by $r_1=|\mathbf{x}-\mathbf{y}_1|$ the spatial distance to the point 1, and by $\mathbf{n}_1=(\mathbf{x}-\mathbf{y}_1)/r_1$ the spatial direction of approach to 1, we assume that, for any $N\in\mathbb{N}$,

$$F(\mathbf{x}) = \sum_{a_0 \leqslant a \leqslant N} r_1^a \, {}_1f_a(\mathbf{n}_1) + o(r_1^N). \tag{2.1}$$

The coefficients ${}_1f_a$ of the various powers of r_1 are smooth functions of the unit vector $\mathbf{n}_1$, and the remainder tends to zero strictly more rapidly than r_1^N when $r_1 \to 0$. The powers a of r_1 in that expansion are assumed to be real, $a \in \mathbb{R}$, to range in discrete steps, i.e., $a \in (a_i)_{i \in \mathbb{N}}$, and to be bounded from below, i.e., $a_0 \leqslant a$ for some $a_0 \in \mathbb{R}$. Similarly, we assume the same type of expansion around point 2,

$$\forall N \in \mathbb{N}, \quad F(\mathbf{x}) = \sum_{b_0 \leqslant b \leqslant N} r_2^b \, {}_2f_b(\mathbf{n}_2) + o(r_2^N), \tag{2.2}$$

where $r_2 = |\mathbf{x} - \mathbf{y}_2|$ and $\mathbf{n}_2 = (\mathbf{x} - \mathbf{y}_2)/r_2$. Thus, to each function F in the class $\mathcal{F}$ are associated two discrete families of indices a and b, and two corresponding families of coefficients ${}_1f_a(\mathbf{n}_1)$ and ${}_2f_b(\mathbf{n}_2)$, all of them depending on F. We shall refer to the coefficients ${}_1f_a$ for which $a < 0$ (and similarly to ${}_2f_b$ when $b < 0$) as the *singular* coefficients of F in the expansion when $r_1 \to 0$. Since $a \geqslant a_0(F)$ and $b \geqslant b_0(F)$, the number of singular coefficients of F is always finite.

The so-called "partie finie" in the sense of Hadamard[2,3] of the singular function F at the location of the singular point $\mathbf{y}_1$ is equal to the angular average, say ${}_1\hat{f}_0$, of the zeroth-order coefficient, ${}_1f_0(\mathbf{n}_1)$, in the expansion of the function when $r_1 \to 0$ we assumed in (2.1); namely

$$(F)_1 = \underset{1}{\hat{f}_0} \equiv \int \frac{d\Omega_1}{4\pi} \, {}_1f_0(\mathbf{n}_1), \tag{2.3}$$

where $d\Omega_1 = d\Omega(\mathbf{n}_1)$ denotes the solid angle element of origin $\mathbf{y}_1$ and direction $\mathbf{n}_1$. The latter angular integration is performed within the coordinate hypersurface $t = \text{const}$. A crucial property of the Hadamard partie finie is its "nondistributivity" with respect to the multiplication, in the sense that

$$(FG)_1 \neq (F)_1 (G)_1 \tag{2.4}$$

in general. When applied to the gradient $\partial_i F$ of a function $F \in \mathcal{F}$, the definition (2.3) yields a useful formula which permits one to compute rapidly the partie finie of complicated expressions involving gradients:

$$(\partial_i F)_1 = 3 \left(\frac{n_1^i}{r_1} F \right)_1. \tag{2.5}$$

Closely related to the concept of partie finie of a singular function is the definition of the partie finie (Pf) of the divergent integral $\int d^3\mathbf{x} F$. Throughout this article, we assume that the functions decrease fast enough at infinity (when $|\mathbf{x}| \to +\infty$) so that the possible divergencies of integrals come only from the bounds located at the two singular points 1 and 2. The "partie-finie integral" reads[2,3] as

$$\mathrm{Pf}_{s_1, s_2} \int d^3\mathbf{x} F = \lim_{s \to 0} \left\{ \int_{\mathbb{R}^3 \setminus B_1(s) \cup B_2(s)} d^3\mathbf{x} F + 4\pi \sum_{a+3<0} \frac{s^{a+3}}{a+3} \left(\frac{F}{r_1^a} \right)_1 + 4\pi \ln\left(\frac{s}{s_1} \right) (r_1^3 F)_1 + 1 \leftrightarrow 2 \right\}. \tag{2.6}$$

The integral on the right side extends over $\mathbb{R}^3$ deprived from two closed spherical balls $B_1(s)$ and $B_2(s)$ of radius s centered on the two singularities [thus $B_1(s)$ and $B_2(s)$ are defined by $r_1 \leqslant s$ and $r_2 \leqslant s$]. The other terms, which are defined by means of the partie finie in the sense of (2.3), are chosen in such a way that the limit $s \to 0$ exists. The notation $1 \leftrightarrow 2$ indicates the same terms as the

two previous ones but corresponding to the other point. The summation index a satisfies $a_0 \leqslant a < -3$ (in particular the sum is always finite). Notice the two arbitrary constants s_1 and s_2 which are introduced in order to adimensionalize the arguments of the logarithms in (2.6); the partie finie owns an ambiguity through these constants (hence the notation Pf_{s_1,s_2}). The close connection between the partie finie of a singular function (2.3) and that of a divergent integral (2.6) is most easily seen from the fact that[1]

$$\mathrm{Pf} \int d^3\mathbf{x} \partial_i F = -4\pi (n_1^i r_1^2 F)_1 + 1 \leftrightarrow 2 \ . \tag{2.7}$$

Unlike in the case of continuous functions, the (partie finie) integral of a gradient is nonzero in general, and equal to the sum of the parties finies, in the sense of (2.3), of the surface integrals surrounding the singularities, in the limit where the surface areas tend to zero. This fact motivated the introduction and study in Ref. 1 of a new derivative operator acting on $\mathcal{F}$, satisfying a property of ''integration by parts'' implying that the integral of any gradient is always zero. This operator generalizes for the class of functions $\mathcal{F}$ the standard distributional derivative of Schwartz.[3]

Let us associate to any $F \in \mathcal{F}$ a pseudo-function denoted PfF and defined to be the following linear form acting on the class $\mathcal{F}$:

$$\forall G \in \mathcal{F}, \quad \langle \mathrm{Pf}F, G \rangle = \mathrm{Pf} \int d^3\mathbf{x} F G, \tag{2.8}$$

where the right side is a partie-finie integral in the sense of (2.6); we use a duality bracket to denote the result of the action of the pseudo-function PfF on G. A fundamental definition adopted in Ref. 1, and motivated by the application to physics, concerns the product of two pseudo-functions, or of a function and a pseudo-function, which is the ''*ordinary*'' pointwise product in the sense that

$$\mathrm{Pf}F . \mathrm{Pf}G = F . \mathrm{Pf}G = G . \mathrm{Pf}F = \mathrm{Pf}(FG). \tag{2.9}$$

Thus, for instance,

$$\langle \mathrm{Pf}F . \mathrm{Pf}G, H \rangle = \mathrm{Pf} \int d^3\mathbf{x} FGH. \tag{2.10}$$

The product (2.9) chosen in Ref. 1 dictates most of the subsequent properties of the pseudo-functions, as well as their generalized distributional derivatives. (Refer to Refs. 26–28 for mathematical treatises on generalized functions and distributions.) In particular, the derivatives do not in general satisfy the Leibniz rule for the derivation of the product, although they satisfy it in an ''integrated sense,'' according to the rule of integration by parts.

The Riesz[29] delta-function, given for $\varepsilon > 0$ by ${}_\varepsilon\delta(\mathbf{x}) = [\varepsilon(1-\varepsilon)/4\pi] |\mathbf{x}|^{\varepsilon - 3}$, tends, in the usual sense of distribution theory, towards the Dirac measure when $\varepsilon \to 0$. When considered with respect to the singular point $\mathbf{y}_1$, the Riesz delta-function allows us to define a useful element of our class,

$${}_\varepsilon\delta_1(\mathbf{x}) \equiv {}_\varepsilon\delta(\mathbf{x} - \mathbf{y}_1) = \frac{\varepsilon(1-\varepsilon)}{4\pi} r_1^{\varepsilon - 3} \in \mathcal{F}. \tag{2.11}$$

Therefore it is possible to associate to ${}_\varepsilon\delta_1$ (for any $\varepsilon > 0$) the pseudo-function $\mathrm{Pf}_\varepsilon \delta_1$ following the prescription (2.8). Applying the limit $\varepsilon \to 0$, we obtain[1]

$$\lim_{\varepsilon \to 0} \langle \mathrm{Pf}_\varepsilon \delta_1, F \rangle \equiv \lim_{\varepsilon \to 0} \mathrm{Pf} \int d^3\mathbf{x}_\varepsilon \delta_1 F = (F)_1, \tag{2.12}$$

where the value of F at the point 1 on the right side is defined by the prescription (2.3). This motivates us for introducing a new pseudo-function, which we shall call the delta-pseudo-function $\mathrm{Pf}\delta_1$, as the formal limit of the pseudo-functions $\mathrm{Pf}_\varepsilon\delta_1$ when $\varepsilon\to 0$. By definition,

$$\forall F\in\mathcal{F},\quad \langle \mathrm{Pf}\delta_1,F\rangle=(F)_1. \tag{2.13}$$

Clearly, the delta-pseudo-function $\mathrm{Pf}\delta_1$ generalizes the notion of Dirac distribution $\delta_1\equiv\delta(\mathbf{x}-\mathbf{y}_1)$ to the case where the ''test'' functions are singular and belong to the class $\mathcal{F}$. Extending the definition of the product (2.9) to include the delta-pseudo-function we pose

$$\mathrm{Pf}F.\mathrm{Pf}\delta_1=F.\mathrm{Pf}\delta_1=\mathrm{Pf}(F\delta_1), \tag{2.14}$$

as well as, for instance,

$$\mathrm{Pf}(F\delta_1).\mathrm{Pf}G=\mathrm{Pf}(F\delta_1).G=\mathrm{Pf}(FG\delta_1). \tag{2.15}$$

The new object $\mathrm{Pf}(F\delta_1)$ in (2.14) and (2.15) has no equivalent in distribution theory; it satisfies

$$\forall G\in\mathcal{F},\quad \langle \mathrm{Pf}(F\delta_1),G\rangle=(FG)_1. \tag{2.16}$$

We notice for future reference that a consequence of the ''nondistributivity'' of the Hadamard partie finie [see (2.4)] is that

$$\mathrm{Pf}(F\delta_1)\neq(F)_1\mathrm{Pf}\delta_1. \tag{2.17}$$

We are not allowed to replace a singular function that appears in factor of the delta-pseudo-function at point 1 by its regularized value at that point.

The derivative of the delta-pseudo-function $\mathrm{Pf}\delta_1$ was constructed in Ref. 1. As it turns out, it takes the form of an ''ordinary'' derivative: $\partial_i(\mathrm{Pf}\delta_1)=\mathrm{Pf}(\partial_i\delta_1)$; due to the presence of the delta-pseudo-function, there are no distributional terms associated with it. We have simply (from the rule of integration by parts)

$$\forall F\in\mathcal{F},\quad \langle \partial_i(\mathrm{Pf}\delta_1),F\rangle=-\langle \mathrm{Pf}\delta_1,\partial_iF\rangle=-(\partial_iF)_1. \tag{2.18}$$

The differentiation of the more complicated object $\mathrm{Pf}(F\delta_1)$ proceeds in the same way:

$$\forall G\in\mathcal{F},\quad \langle \partial_i[\mathrm{Pf}(F\delta_1)],G\rangle=-\langle \mathrm{Pf}(F\delta_1),\partial_iG\rangle=-(F\partial_iG)_1. \tag{2.19}$$

Note that, as a consequence of the identity (2.5), we can write for the intrinsic form of this object

$$\partial_i[\mathrm{Pf}(F\delta_1)]=\mathrm{Pf}\left[r_1^3\partial_i\left(\frac{F}{r_1^3}\right)\delta_1\right]. \tag{2.20}$$

Because the derivative of the delta-pseudo-function is equal to the ordinary one, the Leibniz rule for the derivative of a product happens to still hold. For instance, in the case of the product of $\mathrm{Pf}(F\delta_1)$ with some pseudo-function $\mathrm{Pf}G$, we have

$$\partial_i[\mathrm{Pf}(F\delta_1).\mathrm{Pf}G]=\partial_i[\mathrm{Pf}(F\delta_1)].\mathrm{Pf}G+\mathrm{Pf}(F\delta_1).\partial_i(\mathrm{Pf}G). \tag{2.21}$$

The proof uses the combination of (2.15) and (2.19).

III. LORENTZIAN REGULARIZATION

To define a Lorentzian regularization *à la* Hadamard (based on the investigation of Ref. 1 and on Sec. II), we now need to specify in a precise way the dependence of a function $F(\mathbf{x})$ in the class $\mathcal{F}$ on the ''source'' variables at the coordinate time t of a global frame $\{\mathbf{x},t\}$. We assume (as everywhere else in this article) that we are working at some given finite order in a relativistic or

post-Newtonian approximation. Up to a given order, we can choose as the source variables the two trajectories $\mathbf{y}_1(t)$ and $\mathbf{y}_2(t)$ in the frame $\{\mathbf{x},t\}$, and the two coordinate velocities $\mathbf{v}_1(t)=d\mathbf{y}_1/dt$ and $\mathbf{v}_2(t)=d\mathbf{y}_2/dt$ (the trajectories of the particles are timelike world lines in Minkowski space–time). Indeed, it is legitimate to assume only the latter source variables because, up to a given post-Newtonian order, we can order-reduce the accelerations and all derivatives of accelerations by means of the equations of motion of the particles up to the appropriate accuracy (in general the precision of the equations of motion needed for this order-reduction is one order less than the given post-Newtonian order at which we are performing a calculation). Of course, we are assuming that these equations of motion are known (they are known presently to the 2.5PN order,[13,14,19] and the general motivation of this work is to get them up to the 3PN order[22,24,25]). Thus, we assume that the function $F\in\mathcal{F}$ really reads

$$F(\mathbf{x},t)=F[\mathbf{x};\mathbf{y}_1(t),\mathbf{y}_2(t);\mathbf{v}_1(t),\mathbf{v}_2(t)]. \tag{3.1}$$

We denote with the same letter F, by a slight abuse of notation, the function of the field point $(\mathbf{x},t)$ and the functional of the field point and source variables on the right-hand-side. For definiteness, we assume that the two trajectories are smooth functions of time, i.e., $\mathbf{y}_1$, $\mathbf{y}_2\in C^\infty(\mathbb{R}^3)$, and that F is a smooth functional of the two velocities $\mathbf{v}_1$, $\mathbf{v}_2$ (see also Sec. IX of Ref. 1 for details about our assumptions). By (3.1), we mean that the dependence of F on the coordinate time t is through (and only through) the two instantaneous trajectories $\mathbf{y}_1$, $\mathbf{y}_2$ and velocities $\mathbf{v}_1$, $\mathbf{v}_2$. Note also that it is implicitly assumed with our notation (3.1) that the function F depends *locally* on time t (no dependence over the trajectories and velocities at some time earlier than t for instance). Furthermore, very often in applications, we shall find that the dependence of F on the spatial position $\mathbf{x}$ appears only via the two spatial distances to the source points, $\mathbf{r}_1(t)=\mathbf{x}-\mathbf{y}_1(t)$ and $\mathbf{r}_2(t)=\mathbf{x}-\mathbf{y}_2(t)$. In this article, we shall generally suppose, in order to simplify the presentation, that this is the case; namely, the function F, as a functional of the source variables, is

$$F(\mathbf{x},t)=F[\mathbf{r}_1(t),\mathbf{r}_2(t);\mathbf{v}_1(t),\mathbf{v}_2(t)]. \tag{3.2}$$

The hypothesis (3.2) does not constitute a very severe restriction. The extension to the more general case (3.1) is generally straightforward; moreover, (3.2) is always verified in the problem of the post-Newtonian equations of motion of binary systems. In this section, we shall define the Lorentzian regularized value of the function F at the location of the singularity 1, in contrast to the non-invariant regularized value defined by (2.3) within the "global" coordinate hypersurface $t=\text{const}$. We shall denote by $[F]_1$ the new Lorentzian regularization of F at point 1, defined within the instantaneous rest frame of particle 1 at $t'=\text{const}$ [in contrast with the notation $(F)_1$ used in (2.3) for the old regularization]. In addition, we shall introduce a delta-pseudo-function denoted by $\mathrm{Pf}\Delta_1$ associated with the new regularization [similar to the delta-pseudo-function $\mathrm{Pf}\delta_1$ which was defined in (2.13) in the case of the old regularization].

A. Lorentz transformation of the source variables

In this article, it is sufficient to consider only those homogeneous proper Lorentz transformations which change the velocity of a global inertial frame $\{x^\mu\}=\{ct,\mathbf{x}\}$. More specifically, let us consider the Lorentz boost

$$x'^\mu=\Lambda^\mu{}_\nu(\mathbf{V})x^\nu, \tag{3.3}$$

where the Lorentz matrix $\Lambda^\mu{}_\nu(\mathbf{V})$, depending on the constant boost velocity $\mathbf{V}$, is given by

$$\Lambda^0{}_0(\mathbf{V})=\gamma, \tag{3.4a}$$

$$\Lambda^i{}_0(\mathbf{V})=-\gamma\frac{V^i}{c}, \tag{3.4b}$$

$$\Lambda^0{}_j(\mathbf{V}) = -\gamma \frac{V_j}{c}, \tag{3.4c}$$

$$\Lambda^i{}_j(\mathbf{V}) = \delta^i_j + \frac{\gamma^2}{\gamma+1}\frac{V^i V_j}{c^2}. \tag{3.4d}$$

We indifferently denote the components of the boost vector by $\mathbf{V}=(V^i)=(V_i)$ (spatial indices $i,j=1,2,3$). The Lorentz factor γ reads

$$\gamma = \frac{1}{\sqrt{1-\mathbf{V}^2/c^2}}, \tag{3.5}$$

with $\mathbf{V}^2=\delta_{ij}V^iV^j$ (of course $|\mathbf{V}|<c$). The inverse transformation is $x^\nu=\Lambda_\mu{}^\nu(\mathbf{V})x'^\mu$ where the components of $\Lambda_\mu{}^\nu(\mathbf{V})=\eta_{\mu\rho}\eta^{\nu\sigma}\Lambda^\rho{}_\sigma(\mathbf{V})$ are obtained directly from (3.3) by changing $\mathbf{V}\to -\mathbf{V}$. The choice of sign made in the $0i$ components of the boost (3.4) is such that a particle which has velocity $\mathbf{V}$ at time t in the frame $\{x^\mu\}$ is at rest in the frame $\{x'^\mu\}$ at time t'.

We introduce on one side the space–time event Q, which represents for us a ''field'' point located outside the two world lines of the particles, and on the other side the space–time events P_1, M_1 and P_2, M_2, which are ''source'' points, lying respectively on the world lines of particles 1 and 2 (see later in this work for their definition). The coordinates of the event Q are $(t,\mathbf{x})$ in the frame $\{x^\mu\}$ and $(t',\mathbf{x}')$ in the frame $\{x'^\mu\}$. Sorting out the spatial and temporal indices in (3.3), we have

$$ct' = c\Lambda^0{}_0 t + \Lambda^0{}_j x^j, \tag{3.6a}$$

$$x'^i = c\Lambda^i{}_0 t + \Lambda^i{}_j x^j. \tag{3.6b}$$

The points P_1 and P_2 are now defined as the two events that are located on the trajectories of the particles and are ''simultaneous'' with the event Q in the frame $\{x^\mu\}$, i.e., that belong to the same spatial slice $t=\text{const}$ as Q. The coordinates of P_1 and P_2 in $\{x^\mu\}$ are denoted by $(t,\mathbf{y}_1)$ and $(t,\mathbf{y}_2)$, respectively, the two trajectories $\mathbf{y}_1=\mathbf{y}_1(t)$ and $\mathbf{y}_2=\mathbf{y}_2(t)$ being parametrized by the coordinate time t in that frame. On the other hand, in the new frame $\{x'^\mu\}$, the coordinates of P_1 and P_2 are $(\tau_1',\mathbf{z}_1')$ and $(\tau_2',\mathbf{z}_2')$. Evidently, the primed coordinates are related to the unprimed ones by the Lorentz boost (3.3), so that

$$c\tau_1' = c\Lambda^0{}_0 t + \Lambda^0{}_j y_1^j, \tag{3.7a}$$

$$z_1'^i = c\Lambda^i{}_0 t + \Lambda^i{}_j y_1^j, \tag{3.7b}$$

in the case of the event P_1 [where $y_1^j=y_1^j(t)$, $y_2^j=y_2^j(t)$], and

$$c\tau_2' = c\Lambda^0{}_0 t + \Lambda^0{}_j y_2^j, \tag{3.8a}$$

$$z_2'^i = c\Lambda^i{}_0 t + \Lambda^i{}_j y_2^j, \tag{3.8b}$$

in the case of the event P_2. In the new frame $\{x'^\mu\}$, the source events that are simultaneous with Q are not P_1 and P_2, but some other events M_1 and M_2, whose coordinates in the primed frame are thus $(t',\mathbf{y}_1')$ and $(t',\mathbf{y}_2')$; the coordinate time t' is the same as that of Q in the primed frame, and the spatial coordinates are the trajectories of the particles $\mathbf{y}_1'=\mathbf{y}_1'(t')$ and $\mathbf{y}_2'=\mathbf{y}_2'(t')$ which are labeled by t' in the new frame. Let $(\tau_1,\mathbf{z}_1)$ and $(\tau_2,\mathbf{z}_2)$ be the coordinates of M_1 and M_2 in the original frame $\{x^\mu\}$. By definition,

$$ct' = c\Lambda^0{}_0 \tau_1 + \Lambda^0{}_j z_1^j, \tag{3.9a}$$

$$y_1'^i = c\Lambda^i{}_0\tau_1 + \Lambda^i{}_j z_1^j, \tag{3.9b}$$

$$ct' = c\Lambda^0{}_0\tau_2 + \Lambda^0{}_j z_2^j, \tag{3.9c}$$

$$y_2'^i = c\Lambda^i{}_0\tau_2 + \Lambda^i{}_j z_2^j, \tag{3.9d}$$

where $y_1'^i = y_1'^i(t')$ and $y_2'^i = y_2'^i(t')$. Beware of our notation, where τ_1' (for instance) is the time coordinate of P_1 in $\{x'^\mu\}$ while τ_1 is the time coordinate in $\{x^\mu\}$ of the *different* event M_1. Since the events M_1 and M_2 are located on the world lines of the particles parametrized by $\mathbf{y}_1(t)$ and $\mathbf{y}_2(t)$ in $\{x^\mu\}$, it is clear that at time τ_1 in that frame their coordinates are related to the trajectories by

$$\mathbf{z}_1 = \mathbf{y}_1(\tau_1), \tag{3.10a}$$

$$\mathbf{z}_2 = \mathbf{y}_2(\tau_2). \tag{3.10b}$$

Similarly, from the fact that P_1 and P_2 are also on the world lines, which write as $\mathbf{y}_1'(t')$ and $\mathbf{y}_2'(t')$ in the frame $\{x'^\mu\}$, we deduce that their coordinates in $\{x'^\mu\}$ satisfy

$$\mathbf{z}_1' = \mathbf{y}_1'(\tau_1'), \tag{3.11a}$$

$$\mathbf{z}_2' = \mathbf{y}_2'(\tau_2'). \tag{3.11b}$$

By eliminating t' from the equations (3.6a) and (3.9a) we immediately obtain

$$c\Lambda^0{}_0(\tau_1 - t) = \Lambda^0{}_i(x^i - z_1^i), \tag{3.12}$$

or, equivalently, taking also into account (3.4),

$$\tau_1 - t = -\frac{1}{c^2}\mathbf{V}.(\mathbf{x} - \mathbf{z}_1), \tag{3.13}$$

where the usual Euclidean scalar product between (boldface) vectors is denoted by a dot. With the help of the latter formula for expressing τ_1, we can restate the belonging of $\mathbf{z}_1$ to the particle world line at time τ_1 [see (3.10a)] as

$$\mathbf{z}_1 = \mathbf{y}_1\left(t - \frac{1}{c^2}\mathbf{V}.(\mathbf{x} - \mathbf{z}_1)\right). \tag{3.14}$$

Recall that $\mathbf{z}_1$ is the spatial coordinate in the old frame of the event M_1 which is simultaneous with the field point Q in the *new* frame. Clearly, the equation (3.14) determines the vector $\mathbf{z}_1$ as a function of the coordinates $(t,\mathbf{x})$ of the field-point event Q (see the Appendix). Here, let us view $\mathbf{z}_1$ as a "vector" field $\mathbf{z}_1(\mathbf{x})$, solution of (3.14), lying in the three-dimensional space $t = \text{const}$. It is evident from (3.14) that the function $\mathbf{z}_1(\mathbf{x})$ admits a fixed point at $\mathbf{y}_1 = \mathbf{y}_1(t)$, in the sense that

$$\mathbf{z}_1(\mathbf{y}_1) = \mathbf{y}_1. \tag{3.15}$$

Unless specified otherwise [like in (3.14)], the notation $\mathbf{y}_1$ always means $\mathbf{y}_1(t)$. The mathematical justification of (3.15) is the following. From the fact that the world line of the particle is timelike we can write, for any instants $\hat{t}$ and $\overline{t}$, the inequality $|\mathbf{y}_1(\hat{t}) - \mathbf{y}_1(\overline{t})| < c|\hat{t} - \overline{t}|$. Hence, applying the definition (3.14), we find that our function $\mathbf{z}_1(\mathbf{x})$ obeys, for any positions $\hat{\mathbf{x}}$ and $\overline{\mathbf{x}}$, the further inequalities $|\mathbf{z}_1(\hat{\mathbf{x}}) - \mathbf{z}_1(\overline{\mathbf{x}})| < (1/c)|\mathbf{V}.(\hat{\mathbf{x}} - \overline{\mathbf{x}})| \leqslant |\mathbf{V}|/c|\hat{\mathbf{x}} - \overline{\mathbf{x}}|$. Now recall that $|\mathbf{V}|/c < 1$, so the latter inequalities mean exactly that the function $\mathbf{x} \to \mathbf{z}_1(\mathbf{x})$ is a *contracting* application with respect

to the usual Euclidean norm (i.e., it satisfies the property of Lipschitz with a ratio $k=|\mathbf{V}|/c$ strictly less than one). Therefore, by the theorem of Picard, the function admits a unique fixed point, which of course is nothing but $\mathbf{y}_1$. (Besides, at the location of the fixed point, we have $\tau_1=t$.)

In this article, we establish the general solution of the equation (3.14) in the form of an infinite (post-Newtonian) power series in $1/c^2$. We shall not discuss the convergence properties of this series and simply employ it to define the regularization up to any relativistic order. This is sufficient for the application to the problem of the equations of motion of particles in the post-Newtonian approximation. The general solution of (3.14), as determined in the Appendix, reads

$$\mathbf{z}_1=\mathbf{y}_1+\sum_{n=1}^{+\infty}\frac{(-)^n}{c^{2n}n!}\left(\frac{\partial}{\partial t}\right)^{n-1}[(\mathbf{V}.\mathbf{r}_1)^n\mathbf{v}_1], \tag{3.16}$$

with shorthand notations $\mathbf{y}_1=\mathbf{y}_1(t)$, $\mathbf{r}_1=\mathbf{x}-\mathbf{y}_1(t)$, and $\mathbf{v}_1=\mathbf{v}_1(t)$. The many derivatives $\partial/\partial t$ on the right side are partial time derivatives with respect to the coordinate time t, the spatial coordinate $\mathbf{x}$ being held constant. They act on $\mathbf{r}_1$ through the trajectory $\mathbf{y}_1$: we have $\partial\mathbf{r}_1/\partial t=-\mathbf{v}_1$ or $\partial(\mathbf{V}.\mathbf{r}_1)/\partial t=-\mathbf{V}.\mathbf{v}_1$ for instance. On the other side, they act of course on velocities and (derivatives of) accelerations: thus $\partial\mathbf{v}_1/\partial t=\mathbf{a}_1$, $\partial\mathbf{a}_1/\partial t=\mathbf{b}_1$, $\partial\mathbf{b}_1/\partial t=\mathbf{c}_1$, and so on, where $\mathbf{a}_1$, $\mathbf{b}_1$, $\mathbf{c}_1$ represent the acceleration, and its first and second derivatives (in these cases the partial derivative is a total derivative, e.g., $d\mathbf{v}_1/dt=\mathbf{a}_1$). Thus, to high post-Newtonian order, (3.16) contains many accelerations and derivatives of accelerations, but it is understood that this formula is order-reduced, consistent with the post-Newtonian order; i.e., all accelerations and derivatives of accelerations are to be replaced by the functionals of the positions and velocities deduced from the equations of motion. Combining (3.13) and (3.16), we easily find the corresponding solution for the time coordinate τ_1,

$$\tau_1=t+\sum_{n=1}^{+\infty}\frac{(-)^n}{c^{2n}n!}\left(\frac{\partial}{\partial t}\right)^{n-1}[(\mathbf{V}.\mathbf{r}_1)^n]. \tag{3.17}$$

[Of course, since $\mathbf{V}$ is a constant vector, it could be as well put outside the partial time derivative operators in both (3.16) and (3.17).] Finally, Eqs. (3.16) and (3.17) determine completely the space–time event M_1. From them, we can recover directly the fact that when $\mathbf{x}=\mathbf{y}_1$ (at the fixed point) then $\mathbf{z}_1=\mathbf{y}_1$ and $\tau_1=t$: there are on the right sides of both relations $n-1$ partial time derivatives acting on a term that involves the nth power $(\mathbf{V}.\mathbf{r}_1)^n$, so that at least one of the scalar products $\mathbf{V}.\mathbf{r}_1$ is left undifferentiated, and makes the sums in (3.16) and (3.17) vanish when $\mathbf{r}_1=0$. Replacing both $\mathbf{z}_1$ and τ_1 as given by the infinite post-Newtonian series back into the relation (3.10a), expressing both sides of the resulting equation as the same type of post-Newtonian series with the help of a formal Taylor expansion when $c\to\infty$, and finally equating all the coefficients of these two series yields an interesting mathematical formula relating together some sums of products of derivatives. This formula is derived in the Appendix (where we also present a direct proof of it). Notice that the same reasoning as before can be done on the coordinates of the event P_1 in the new frame, which we find to be given by

$$\mathbf{z}_1'=\mathbf{y}_1'+\sum_{n=1}^{+\infty}\frac{1}{c^{2n}n!}\left(\frac{\partial}{\partial t'}\right)^{n-1}[(\mathbf{V}.\mathbf{r}_1')^n\mathbf{v}_1'], \tag{3.18a}$$

$$\tau_1'=t'+\sum_{n=1}^{+\infty}\frac{1}{c^{2n}n!}\left(\frac{\partial}{\partial t'}\right)^{n-1}[(\mathbf{V}.\mathbf{r}_1')^n], \tag{3.18b}$$

where $\mathbf{y}_1'=\mathbf{y}_1'(t')$, $\mathbf{r}_1'=\mathbf{x}'-\mathbf{y}_1'(t')$, and $\mathbf{v}_1'=\mathbf{v}_1'(t')$. Evidently, the result (3.18) can also be deduced directly from (3.16) and (3.17) by changing $\mathbf{V}$ into $-\mathbf{V}$ and replacing all the non-primed variables by the corresponding primed ones.

We are now able to give all the transformation laws of field and source variables between the frames $\{x^\mu\}$ and $\{x'^\mu\}$. Of course, from (3.6), the transformation of the field variables is the standard Lorentz one,

$$t' = \gamma\left(t - \frac{1}{c^2}(\mathbf{V}.\mathbf{x}) \right), \tag{3.19a}$$

$$\mathbf{x}' = \mathbf{x} - \gamma\mathbf{V}\left(t - \frac{1}{c^2}\frac{\gamma}{\gamma+1}(\mathbf{V}.\mathbf{x}) \right). \tag{3.19b}$$

Concerning the source variables, we are interested in the expressions of the new positions $\mathbf{y}'_1(t')$, $\mathbf{y}'_2(t')$ and velocities $\mathbf{v}'_1(t')$, $\mathbf{v}'_2(t')$ in the new frame at time t'. These are straightforwardly obtained from inserting the results (3.16) and (3.17) into the equations (3.9), as well as the similar results corresponding to point 2. We find, for trajectories,

$$\begin{aligned}\mathbf{y}'_1 = \mathbf{y}_1 &- \gamma\mathbf{V}\left(t - \frac{1}{c^2}\frac{\gamma}{\gamma+1}(\mathbf{V}.\mathbf{x}) \right) \\ &+ \sum_{n=1}^{+\infty} \frac{(-)^n}{c^{2n} n!}\left(\frac{\partial}{\partial t}\right)^{n-1}\left[(\mathbf{V}.\mathbf{r}_1)^n \left(\mathbf{v}_1 - \frac{\gamma}{\gamma+1}\mathbf{V} \right) \right],\end{aligned} \tag{3.20a}$$

$$\begin{aligned}\mathbf{y}'_2 = \mathbf{y}_2 &- \gamma\mathbf{V}\left(t - \frac{1}{c^2}\frac{\gamma}{\gamma+1}(\mathbf{V}.\mathbf{x}) \right) \\ &+ \sum_{n=1}^{+\infty} \frac{(-)^n}{c^{2n} n!}\left(\frac{\partial}{\partial t}\right)^{n-1}\left[(\mathbf{V}.\mathbf{r}_2)^n \left(\mathbf{v}_2 - \frac{\gamma}{\gamma+1}\mathbf{V} \right) \right].\end{aligned} \tag{3.20b}$$

By subtracting the latter equations (3.20) to $\mathbf{x}'$ as given by (3.19b) we obtain the spatial distances $\mathbf{r}'_1 = \mathbf{x}' - \mathbf{y}'_1(t')$ and $\mathbf{r}'_2 = \mathbf{x}' - \mathbf{y}'_2(t')$ as

$$\mathbf{r}'_1 = \mathbf{r}_1 - \sum_{n=1}^{+\infty} \frac{(-)^n}{c^{2n} n!}\left(\frac{\partial}{\partial t}\right)^{n-1}\left[(\mathbf{V}.\mathbf{r}_1)^n \left(\mathbf{v}_1 - \frac{\gamma}{\gamma+1}\mathbf{V} \right) \right], \tag{3.21a}$$

$$\mathbf{r}'_2 = \mathbf{r}_2 - \sum_{n=1}^{+\infty} \frac{(-)^n}{c^{2n} n!}\left(\frac{\partial}{\partial t}\right)^{n-1}\left[(\mathbf{V}.\mathbf{r}_2)^n \left(\mathbf{v}_2 - \frac{\gamma}{\gamma+1}\mathbf{V} \right) \right]. \tag{3.21b}$$

These relations will play the crucial role in the definition of our Lorentzian regularization. Of interest also is the expression of the relative distance between the two particles, i.e., $\mathbf{y}'_{12} = \mathbf{y}'_1 - \mathbf{y}'_2 = \mathbf{r}'_2 - \mathbf{r}'_1$ given by

$$\mathbf{y}'_{12} = \mathbf{y}_{12} + \sum_{n=1}^{+\infty} \frac{(-)^n}{c^{2n} n!}\left(\frac{\partial}{\partial t}\right)^{n-1}\left[(\mathbf{V}.\mathbf{r}_1)^n \left(\mathbf{v}_1 - \frac{\gamma}{\gamma+1}\mathbf{V} \right) - (\mathbf{V}.\mathbf{r}_2)^n \left(\mathbf{v}_2 - \frac{\gamma}{\gamma+1}\mathbf{V} \right) \right]. \tag{3.22}$$

Finally, we compute the expressions of the coordinate velocities $\mathbf{v}'_1(t') = d\mathbf{y}'_1/dt'$ and $\mathbf{v}'_2(t') = d\mathbf{y}'_2/dt'$ in the new frame. They follow immediately from the law of transformation of the time derivative, $\partial'_t = \gamma\partial_t + \gamma V^i \partial_i$, and we obtain

$$\mathbf{v}'_1 = \frac{1}{\gamma}\mathbf{v}_1 - \mathbf{V} + \frac{1}{\gamma}\sum_{n=1}^{+\infty} \frac{(-)^n}{c^{2n} n!}\left(\frac{\partial}{\partial t}\right)^{n}\left[(\mathbf{V}.\mathbf{r}_1)^n \left(\mathbf{v}_1 - \frac{\gamma}{\gamma+1}\mathbf{V} \right) \right], \tag{3.23a}$$

$$\mathbf{v}_2'=\frac{1}{\gamma}\mathbf{v}_2-\mathbf{V}+\frac{1}{\gamma}\sum_{n=1}^{+\infty}\frac{(-)^n}{c^{2n}n!}\left(\frac{\partial}{\partial t}\right)^n\left[(\mathbf{V}.\mathbf{r}_2)^n\left(\mathbf{v}_2-\frac{\gamma}{\gamma+1}\mathbf{V}\right)\right]. \tag{3.23b}$$

Notice that although the velocities $\mathbf{v}_1'(t')$ and $\mathbf{v}_2'(t')$ are some mere functions of the coordinate time t' in the new frame, they depend, when expressed in terms of quantities belonging to the old frame, on both time *and* space coordinates t and $\mathbf{x}$. This is obvious because by changing the space coordinate $\mathbf{x}$ of the field point Q while keeping $t=\text{const}$ we change the time coordinate t' of the source events M_1 and M_2 and therefore the values of their particle velocities (soon as the trajectories are accelerated). This fact is important and has to be taken correctly into account in the regularization process defined in the next subsection. The inverse formulas are obtained in the same way by substituting (3.18) into the inverse of (3.7). They correspond of course to changing $\mathbf{V}$ into $-\mathbf{V}$ and replacing everywhere the unprimed labels by primed ones. We find, for the spatial distances and velocities,

$$\mathbf{r}_1=\mathbf{r}_1'-\sum_{n=1}^{+\infty}\frac{1}{c^{2n}n!}\left(\frac{\partial}{\partial t'}\right)^{n-1}\left[(\mathbf{V}.\mathbf{r}_1')^n\left(\mathbf{v}_1'+\frac{\gamma}{\gamma+1}\mathbf{V}\right)\right], \tag{3.24a}$$

$$\mathbf{r}_2=\mathbf{r}_2'-\sum_{n=1}^{+\infty}\frac{1}{c^{2n}n!}\left(\frac{\partial}{\partial t'}\right)^{n-1}\left[(\mathbf{V}.\mathbf{r}_2')^n\left(\mathbf{v}_2'+\frac{\gamma}{\gamma+1}\mathbf{V}\right)\right], \tag{3.24b}$$

$$\mathbf{v}_1=\frac{1}{\gamma}\mathbf{v}_1'+\mathbf{V}+\frac{1}{\gamma}\sum_{n=1}^{+\infty}\frac{1}{c^{2n}n!}\left(\frac{\partial}{\partial t'}\right)^{n}\left[(\mathbf{V}.\mathbf{r}_1')^n\left(\mathbf{v}_1'+\frac{\gamma}{\gamma+1}\mathbf{V}\right)\right], \tag{3.24c}$$

$$\mathbf{v}_2=\frac{1}{\gamma}\mathbf{v}_2'+\mathbf{V}+\frac{1}{\gamma}\sum_{n=1}^{+\infty}\frac{1}{c^{2n}n!}\left(\frac{\partial}{\partial t'}\right)^{n}\left[(\mathbf{V}.\mathbf{r}_2')^n\left(\mathbf{v}_2'+\frac{\gamma}{\gamma+1}\mathbf{V}\right)\right]. \tag{3.24d}$$

B. Definition of the regularization

Let us consider a function F belonging to the class $\mathcal{F}$ and being at the same time a *scalar* under Lorentz transformations, i.e., $F(\mathbf{x},t)=F'(\mathbf{x}',t')$. More precisely, we restrict ourselves to the case of a dependence on $\mathbf{x}$ only via the distances $\mathbf{r}_1$ and $\mathbf{r}_2$ [cf. (3.2)]; this means

$$F[\mathbf{r}_1(t),\mathbf{r}_2(t);\mathbf{v}_1(t),\mathbf{v}_2(t)]=F'[\mathbf{r}_1'(t'),\mathbf{r}_2'(t');\mathbf{v}_1'(t'),\mathbf{v}_2'(t');\mathbf{V}], \tag{3.25}$$

where we use the same slightly abusive notation as in (3.2), with addition, on the right side, of the explicit mention of the dependence over the boost vector $\mathbf{V}$. All the variables in both frames $\{x^\mu\}$ and $\{x'^\mu\}$ are related to each other by the formulas developed in the previous subsection. The regularization process goes as follows.

(i) Starting from $F[\mathbf{r}_1,\mathbf{r}_2;\mathbf{v}_1,\mathbf{v}_2]$ defined in the frame $\{x^\mu\}$, we first determine the new functional $F'[\mathbf{r}_1',\mathbf{r}_2';\mathbf{v}_1',\mathbf{v}_2';\mathbf{V}]$ in the boosted frame $\{x'^\mu\}$. To do so, we replace all the variables $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{v}_1$, $\mathbf{v}_2$ by their expressions in terms of the new ones $\mathbf{r}_1'$, $\mathbf{r}_2'$, $\mathbf{v}_1'$, $\mathbf{v}_2'$ as given by the formulas (3.24), in which it is understood that all the accelerations are order-reduced up to some given specified post-Newtonian order. Performing all the necessary post-Newtonian reexpansions to that order, we indeed obtain in that way (since F is a Lorentz scalar) the new functional F' of the new distances $\mathbf{r}_1'$, $\mathbf{r}_2'$ and velocities $\mathbf{v}_1'$, $\mathbf{v}_2'$. In addition, F' depends as expected on the constant $\mathbf{V}$ which is yet unspecified at this stage.

(ii) We compute the Hadamard regularization of F' at point 1 following exactly the same rules as defined in (2.3), but in the boosted frame $\{x'^\mu\}$ (in particular, within the coordinate slice $t'=\text{const}$). In words, we perform the expansion of F' when the spatial distance r_1' tends to zero, and obtain the same type of power-law expansion as in (2.1) [since the form of the relations (3.24) shows that the structure of the expansions in both frames must be the same]. However, we get

some primed functional coefficients ${}_1f'_a$ that differ from the unprimed coefficients ${}_1f_a$ appearing in (2.1). The boost vector $\mathbf{V}$ is simply held constant in the process. Thus, $\forall N \in \mathbb{N}$,

$$F'[\mathbf{r}'_1,\mathbf{r}'_2;\mathbf{v}'_1,\mathbf{v}'_2;\mathbf{V}] = \sum_{a_0 \leqslant a \leqslant N} r'^a_1 {}_1f'_a(\mathbf{n}'_1;\mathbf{y}'_{12};\mathbf{v}'_1,\mathbf{v}'_2;\mathbf{V}) + o(r'^N_1), \tag{3.26}$$

with the notation $r'_1 = |\mathbf{x}' - \mathbf{y}'_1|$, $\mathbf{n}'_1 = (\mathbf{x}' - \mathbf{y}'_1)/r'_1$, and $\mathbf{y}'_{12} = \mathbf{y}'_1 - \mathbf{y}'_2$. (The fact that the coefficients ${}_1f'_a$ depend on $\mathbf{y}'_{12}$ instead of the two individual trajectories $\mathbf{y}'_1$, $\mathbf{y}'_2$ is due to our restriction that F' depends on $\mathbf{x}'$ via the distances $\mathbf{r}'_1$ and $\mathbf{r}'_2$; also, the accelerations depend on the relative distance $\mathbf{y}'_{12}$.) Now, like in (2.3), we pick up the zeroth-order coefficient in the r'_1-expansion (3.26) and average over the angles. This defines a certain functional of the separation vector $\mathbf{y}'_{12}$, the velocities $\mathbf{v}'_1$, $\mathbf{v}'_2$ and the boost velocity $\mathbf{V}$,

$$\hat{f}'_{0\,1}(\mathbf{y}'_{12};\mathbf{v}'_1,\mathbf{v}'_2;\mathbf{V}) = \int \frac{d\Omega'_1}{4\pi} f'_{0\,1}(\mathbf{n}'_1;\mathbf{y}'_{12};\mathbf{v}'_1,\mathbf{v}'_2;\mathbf{V}). \tag{3.27}$$

We insist that the angular average is performed *in the new frame*, within the spatial hypersurface $t' = \text{const}$; in particular, the solid angle element in (3.27) is the one associated with the unit direction $\mathbf{n}'_1$ in that hypersurface: $d\Omega'_1 = d\Omega(\mathbf{n}'_1)$. Here again, $\mathbf{V}$ is considered as a simple constant "spectator" vector during the average.

(iii) We impose that the new frame is actually the rest frame of particle 1 at the event P_1. Recalling that the Lorentz boost (3.4) brings a particle with velocity $\mathbf{V}$ in the frame $\{x^\mu\}$ at rest in the frame $\{x'^\mu\}$, we see that we must choose

$$\mathbf{V} = \mathbf{v}_1(t). \tag{3.28}$$

We come back to the original variables in the unprimed frame by using the transformation laws (3.22) and (3.23), in the limit where the field point $\mathbf{x}$ tends to the source point $\mathbf{y}_1(t)$ (because we are located at the event P_1), with $\mathbf{V} = \mathbf{v}_1$ according to (3.28). Note that, in this limit $\mathbf{r}_1 \to \mathbf{0}$, the coordinate time t' of the event Q in the primed frame is equal to the coordinate time τ'_1 of the event P_1. It is important to realize that both the computation of the limit when $\mathbf{r}_1 \to \mathbf{0}$ and the replacement of the vector $\mathbf{V}$ by (3.28) are to be done *after* performing the many partial time differentiations in (3.22) and (3.23). Consider first the primed variable $\mathbf{y}'_{12}$, which is given by (3.22) where we apply the replacement $\mathbf{r}_1 = \mathbf{0}$ (as well as $\mathbf{V} = \mathbf{v}_1$). In (3.22) the $n-1$ partial time derivatives acting on the term proportional to $(\mathbf{V}.\mathbf{r}_1)^n$ will clearly lead to zero in the limit $\mathbf{r}_1 = \mathbf{0}$; indeed, by an argument met previously, there are not "enough" derivatives to make a nonzero contribution. So the variable to be used when coming back to the original frame is

$$\mathbf{y}'_{12} = \left(\mathbf{y}_{12} - \sum_{n=1}^{+\infty} \frac{(-)^n}{c^{2n} n!} \left(\frac{\partial}{\partial t} \right)^{n-1} \left[(\mathbf{V}.\mathbf{r}_2)^n \left(\mathbf{v}_2 - \frac{\gamma}{\gamma+1} \mathbf{V} \right) \right] \right) \Bigg|_{\substack{\mathbf{r}_2 = \mathbf{y}_{12} \\ \mathbf{V} = \mathbf{v}_1}}. \tag{3.29}$$

As indicated by the notation one must implement the replacements of $\mathbf{r}_2$ by $\mathbf{y}_{12}$ (this is equivalent to $\mathbf{r}_1 = \mathbf{0}$) and of $\mathbf{V}$ by $\mathbf{v}_1$ *after* the $n-1$ time differentiations. In the case of the primed velocity of particle 2, given by (3.23b), we simply have

$$\mathbf{v}'_2 = \left(\frac{1}{\gamma} \mathbf{v}_2 - \mathbf{V} + \frac{1}{\gamma} \sum_{n=1}^{+\infty} \frac{(-)^n}{c^{2n} n!} \left(\frac{\partial}{\partial t} \right)^n \left[(\mathbf{V}.\mathbf{r}_2)^n \left(\mathbf{v}_2 - \frac{\gamma}{\gamma+1} \mathbf{V} \right) \right] \right) \Bigg|_{\substack{\mathbf{r}_2 = \mathbf{y}_{12} \\ \mathbf{V} = \mathbf{v}_1}}. \tag{3.30}$$

The formulas (3.29) and (3.30) define, after order-reduction of the accelerations, some functionals $\mathbf{y}'_{12}[\mathbf{y}_{12};\mathbf{v}_1,\mathbf{v}_2]$ and $\mathbf{v}'_2[\mathbf{y}_{12};\mathbf{v}_1,\mathbf{v}_2]$ that we use for coming back to the initial frame $\{x^\mu\}$. Clearly, the primed velocity $\mathbf{v}'_1$ of point 1, at which we perform the regularization, deserves a special treatment. From (3.23a) we obtain

$$\mathbf{v}'_1=\left(\frac{1}{\gamma}\mathbf{v}_1-\mathbf{V}+\frac{1}{\gamma}\sum_{n=1}^{+\infty}\frac{(-)^n}{c^{2n}n!}\left(\frac{\partial}{\partial t}\right)^n\left[(\mathbf{V}.\mathbf{r}_1)^n\left(\mathbf{v}_1-\frac{\gamma}{\gamma+1}\mathbf{V}\right)\right]\right)\Bigg|_{\substack{\mathbf{r}_1=\mathbf{0}\\ \mathbf{V}=\mathbf{v}_1}}. \tag{3.31}$$

Here, there are n time derivatives which is *a priori* enough to make a contribution. The only possibility is to differentiate successively each of the n factors $\mathbf{V}.\mathbf{r}_1$, yielding for each of the terms in the sum $n!$ identical contributions. Hence, we arrive at a much simpler series,

$$\mathbf{v}'_1=\left(\frac{1}{\gamma}\mathbf{v}_1-\mathbf{V}+\frac{1}{\gamma}\sum_{n=1}^{+\infty}\left(\frac{\mathbf{V}.\mathbf{v}_1}{c^2}\right)^n\left(\mathbf{v}_1-\frac{\gamma}{\gamma+1}\mathbf{V}\right)\right)\Bigg|_{\mathbf{V}=\mathbf{v}_1}, \tag{3.32}$$

which can now easily be summed up. The result is

$$\mathbf{v}'_1=\left(\frac{(1/\gamma)\mathbf{v}_1-\mathbf{V}+[\gamma/(\gamma+1)(\mathbf{V}.\mathbf{v}_1/c^2)]\mathbf{V}}{1-\mathbf{V}.\mathbf{v}_1/c^2}\right)\Bigg|_{\mathbf{V}=\mathbf{v}_1}, \tag{3.33}$$

from which we immediately deduce that the primed velocity of particle 1 must be zero,

$$\mathbf{v}'_1=\mathbf{0}. \tag{3.34}$$

This is of course the expected result because the boost velocity was chosen to be equal to the instantaneous velocity of particle 1 in the unprimed frame at the instant t; however, the details of the above proof constitute a necessary consistency check of the formulas.

(iv) The choice of boost vector $\mathbf{V}=\mathbf{v}_1$, together with the equivalent statement that $\mathbf{v}'_1=\mathbf{0}$, as well as the expressions (3.29) and (3.30) defining the two functionals $\mathbf{y}'_{12}[\mathbf{y}_{12};\mathbf{v}_1,\mathbf{v}_2]$ and $\mathbf{v}'_2[\mathbf{y}_{12};\mathbf{v}_1,\mathbf{v}_2]$, are put into (3.27), which gave the result ${}_1\hat{f}'_0$ of the spherical average in the Hadamard regularization performed in the primed frame. Therefore, the regularized value of F at point 1 is defined by

$$[F]_1=\underset{1}{\hat{f}'_0}(\mathbf{y}'_{12}[\mathbf{y}_{12};\mathbf{v}_1,\mathbf{v}_2];\mathbf{0},\mathbf{v}'_2[\mathbf{y}_{12};\mathbf{v}_1,\mathbf{v}_2];\mathbf{v}_1). \tag{3.35}$$

The new regularization $[F]_1$ acts, like the old one $(F)_1$, as a certain functional of the relative distance $\mathbf{y}_{12}$ and the velocities $\mathbf{v}_1$, $\mathbf{v}_2$. However, in generic cases, $[F]_1$ differs from $(F)_1$ by relativistic terms at least of the order $1/c^2$ (we investigate in Sec. IV the exact relation between both regularizations to the first relativistic order $1/c^2$). In the problem of the post-Newtonian equations of motion, we have found[22,24] that the new regularization $[F]_1$ adds some extra terms to the acceleration computed using the regularization $(F)_1$; these new terms are of order 3PN and manage to make the 3PN equations of motion invariant with respect to Lorentz transformations. Indeed, with the regularization $(F)_1$ the Lorentz invariance of the equations of motion would be broken at the 3PN order. Finally, let us introduce as we did in Ref. 1 (see also Sec. II) a delta-pseudo-function associated with the new regularization $[F]_1$. By definition, the "Lorentzian" delta-pseudo-function denoted $\mathrm{Pf}\Delta_1$ [to contrast with the noninvariant one $\mathrm{Pf}\delta_1$ defined by (2.13)] is such that

$$\forall F\in\mathcal{F},\quad \langle \mathrm{Pf}\Delta_1,F\rangle=[F]_1, \tag{3.36}$$

where the right side is given by the new regularization (3.35). By definition, we have in the case of the new regularization the same laws for the multiplication as in Sec. II, for instance

$$FG.\mathrm{Pf}\Delta_1=\mathrm{Pf}(F\Delta_1).G=\mathrm{Pf}(F\Delta_1).\mathrm{Pf}G=\mathrm{Pf}(FG\Delta_1), \tag{3.37}$$

where the pseudo-function $\mathrm{Pf}(F\Delta_1)$ is defined by

$$\forall G\in\mathcal{F},\quad \langle \mathrm{Pf}(F\Delta_1),G\rangle=[FG]_1. \tag{3.38}$$

This pseudo-function $\mathrm{Pf}(F\Delta_1)$ is at the basis of our proposal for the stress-energy tensor of point-particles in Sec. V. And, like in the case of $\mathrm{Pf}(F\delta_1)$, we are not allowed to replace this pseudo-function by the product of the regularized value of the function times the delta-pseudo-function, namely,

$$\mathrm{Pf}(F\Delta_1)\neq[F]_1\mathrm{Pf}\Delta_1. \tag{3.39}$$

The derivatives of $\mathrm{Pf}\Delta_1$ and $\mathrm{Pf}(F\Delta_1)$ are constructed in the same way as for the original regularization in Sec. II. Therefore,

$$\forall G\in\mathcal{F},\quad \langle \partial_i[\mathrm{Pf}(F\Delta_1)],G\rangle=-\langle \mathrm{Pf}(F\Delta_1),\partial_i G\rangle=-[F\partial_i G]_1. \tag{3.40}$$

However, the identity (2.5) is not valid in the case of the new regularization, so we do not have a result similar to (2.20) [see (4.13) for the equivalent of (2.5) at the first relativistic order]. For the product of $\mathrm{Pf}(F\delta_1)$ with some $\mathrm{Pf}G$, the Leibniz rule holds:

$$\partial_i[\mathrm{Pf}(F\Delta_1).\mathrm{Pf}G]=\partial_i[\mathrm{Pf}(F\Delta_1)].\mathrm{Pf}G+\mathrm{Pf}(F\Delta_1).\partial_i(\mathrm{Pf}G). \tag{3.41}$$

This is a consequence of the definition (3.40) and the law (3.37).

IV. THE REGULARIZATION AT THE FIRST RELATIVISTIC ORDER

At this point, it is instructive (and useful in practice) to present the complete formulas that define the Lorentzian regularization $[F]_1$ at the level of the first relativistic corrections $1/c^2$, i.e., neglecting all the terms of order $O(1/c^4)$. [Notice that, consistent with Sec. III, we must consider that the boost vector $\mathbf{V}$ itself is of order $O(1)$, so that, for instance, the factor $\mathbf{V}^2/c^2$ really represents a small relativistic correction of the order $O(1/c^2)$.] Furthermore, we shall obtain at this $1/c^2$ level a formula linking the new regularization $[F]_1$ to the old one $(F)_1$. Like in Sec. III, we assume that the function F depends on $\mathbf{x}$ through the two distances $\mathbf{r}_1(t)$ and $\mathbf{r}_2(t)$ only; this implies a relation between the partial derivatives:

$$\partial_i F+\frac{\partial F}{\partial y_1^i}+\frac{\partial F}{\partial y_2^i}=0 \tag{4.1}$$

(where $\partial_i=\partial/\partial x^i$). We suppose also that F is a Lorentz scalar, cf. (3.25).

We follow the general specification for the regularization in Sec. III. We first express the vectorial distances $\mathbf{r}_1$, $\mathbf{r}_2$ and velocities $\mathbf{v}_1$, $\mathbf{v}_2$ in the boosted frame $\{x'^\mu\}$ using the transformation formulas (3.24) restricted to the order $1/c^2$. For the distances, we get

$$\mathbf{r}_1=\mathbf{r}_1'-\frac{1}{c^2}(\mathbf{V}.\mathbf{r}_1')\left[\mathbf{v}_1'+\frac{1}{2}\mathbf{V}\right]+O\left(\frac{1}{c^4}\right), \tag{4.2a}$$

$$\mathbf{r}_2=\mathbf{r}_2'-\frac{1}{c^2}(\mathbf{V}.\mathbf{r}_2')\left[\mathbf{v}_2'+\frac{1}{2}\mathbf{V}\right]+O\left(\frac{1}{c^4}\right). \tag{4.2b}$$

The relative distance $\mathbf{y}_{12}=\mathbf{r}_2-\mathbf{r}_1$ reads as

$$\mathbf{y}_{12}=\mathbf{y}'_{12}+\frac{1}{c^2}[-\tfrac{1}{2}(\mathbf{V}.\mathbf{y}'_{12})\mathbf{V}+(\mathbf{V}.\mathbf{r}'_1)\mathbf{v}'_1-(\mathbf{V}.\mathbf{r}'_2)\mathbf{v}'_2]+O\left(\frac{1}{c^4}\right), \tag{4.3}$$

while, for instance, the relative separation $r_{12}=|\mathbf{y}_{12}|$ is

$$r_{12}=r'_{12}\left(1+\frac{1}{c^2}\left[-\tfrac{1}{2}(\mathbf{V}.\mathbf{n}'_{12})^2+\frac{r'_1}{r'_{12}}(\mathbf{V}.\mathbf{n}'_1)(\mathbf{v}'_1.\mathbf{n}'_{12})-\frac{r'_2}{r'_{12}}(\mathbf{V}.\mathbf{n}'_2)(\mathbf{v}'_2.\mathbf{n}'_{12})\right]\right)+O\left(\frac{1}{c^4}\right), \tag{4.4}$$

where $\mathbf{n}'_1=\mathbf{r}'_1/r'_1$, $\mathbf{n}'_2=\mathbf{r}'_2/r'_2$, and $\mathbf{n}'_{12}=\mathbf{y}'_{12}/r'_{12}$. For the two velocities, we find

$$\mathbf{v}_1=\mathbf{v}'_1+\mathbf{V}+\frac{1}{c^2}([-\tfrac{1}{2}\mathbf{V}^2-\mathbf{V}.\mathbf{v}'_1]\mathbf{v}'_1-\tfrac{1}{2}(\mathbf{V}.\mathbf{v}'_1)\mathbf{V}+(\mathbf{V}.\mathbf{r}'_1)\mathbf{a}'_1)+O\left(\frac{1}{c^4}\right), \tag{4.5a}$$

$$\mathbf{v}_2=\mathbf{v}'_2+\mathbf{V}+\frac{1}{c^2}([-\tfrac{1}{2}\mathbf{V}^2-\mathbf{V}.\mathbf{v}'_2]\mathbf{v}'_2-\tfrac{1}{2}(\mathbf{V}.\mathbf{v}'_2)\mathbf{V}+(\mathbf{V}.\mathbf{r}'_2)\mathbf{a}'_2)+O\left(\frac{1}{c^4}\right), \tag{4.5b}$$

where the two accelerations $\mathbf{a}'_1$ and $\mathbf{a}'_2$ are to be replaced, consistent with the approximation, by their Newtonian values: $\mathbf{a}'_1=-(Gm_2/r'^2_{12})\,\mathbf{n}'_{12}+O(1/c^2)$ and $\mathbf{a}'_2=(Gm_1/r'^2_{12})\mathbf{n}'_{12}+O(1/c^2)$. [Notice that in Sec. III the regularization has been defined regardless of the type of special-relativistic interaction involved; in the case of electromagnetism, for instance, we should simply replace the accelerations by their Coulombian values in (4.5).]

Next, we substitute the expressions (4.2) and (4.5) into the scalar function $F[\mathbf{r}_1,\mathbf{r}_2;\mathbf{v}_1,\mathbf{v}_2]$ and perform the expansion to the first order. The result is the scalar function $F'[\mathbf{r}'_1,\mathbf{r}'_2;\mathbf{v}'_1,\mathbf{v}'_2;\mathbf{V}]$ in the new frame; thus

$$\begin{aligned}F'[\mathbf{r}'_1,\mathbf{r}'_2;\mathbf{v}'_1,\mathbf{v}'_2;\mathbf{V}]=F[\mathbf{r}'_1,\mathbf{r}'_2;\mathbf{v}'_1+\mathbf{V},\mathbf{v}'_2+\mathbf{V}]&+\frac{1}{c^2}(\mathbf{V}.\mathbf{r}'_1)[v'^i_1+\tfrac{1}{2}V^i]\frac{\partial F}{\partial y^i_1}\\&+\frac{1}{c^2}(\mathbf{V}.\mathbf{r}'_2)\left[v'^i_2+\frac{1}{2}V^i\right]\frac{\partial F}{\partial y^i_2}+\frac{1}{c^2}\left(\left[-\frac{1}{2}\mathbf{V}^2-\mathbf{V}.\mathbf{v}'_1\right]v'^i_1\right.\\&\left.-\frac{1}{2}(\mathbf{V}.\mathbf{v}'_1)V^i+(\mathbf{V}.\mathbf{r}'_1)a'^i_1\right)\frac{\partial F}{\partial v^i_1}+\frac{1}{c^2}\left(\left[-\frac{1}{2}\mathbf{V}^2-\mathbf{V}.\mathbf{v}'_2\right]v'^i_2\right.\\&\left.-\frac{1}{2}(\mathbf{V}.\mathbf{v}'_2)V^i+(\mathbf{V}.\mathbf{r}'_2)a'^i_2\right)\frac{\partial F}{\partial v^i_2}+O\left(\frac{1}{c^4}\right),\end{aligned} \tag{4.6}$$

where we have used $\partial F/\partial r^i_1=-\partial F/\partial y^i_1$ and $\partial F/\partial r^i_2=-\partial F/\partial y^i_2$. Note that, to this order, the partial derivatives in (4.6) can be evaluated at the primed values $\mathbf{r}'_1$, $\mathbf{r}'_2$ and $\mathbf{v}'_1+\mathbf{V}$, $\mathbf{v}'_2+\mathbf{V}$, or equivalently at the nonprimed ones $\mathbf{r}_1$, $\mathbf{r}_2$ and $\mathbf{v}_1$, $\mathbf{v}_2$. Now we pick up in the new frame the term of zeroth order in the expansion when $r'_1\to 0$, and perform the angular average with respect to the direction $\mathbf{n}'_1$. This yields the functional of the variables $\mathbf{y}'_{12}$, $\mathbf{v}'_1$, $\mathbf{v}'_2$, and $\mathbf{V}$ which has been defined in (3.27). Since these operations of expanding and averaging represent nothing but the Hadamard regularization in the old sense of (2.3), we can denote them by using the parenthesis appropriate for this regularization. Therefore,

$$\hat{f}'_{0\,1}(\mathbf{y}'_{12};\mathbf{v}'_1,\mathbf{v}'_2;\mathbf{V}) = \Bigg(F[\mathbf{r}_1,\mathbf{r}_1+\mathbf{y}'_{12};\mathbf{v}'_1+\mathbf{V},\mathbf{v}'_2+\mathbf{V}] + \frac{1}{c^2}(\mathbf{V}.\mathbf{r}_1)\left[v'^{i}_1 + \frac{1}{2}V^i \right]\frac{\partial F}{\partial y^i_1}$$
$$+ \frac{1}{c^2}(\mathbf{V}.\mathbf{r}_1+\mathbf{V}.\mathbf{y}'_{12})\left[v'^{i}_2 + \frac{1}{2}V^i \right]\frac{\partial F}{\partial y^i_2}$$
$$+ \frac{1}{c^2}\left(\left[-\frac{1}{2}\mathbf{V}^2 - \mathbf{V}.\mathbf{v}'_1 \right] v'^{i}_1 - \frac{1}{2}(\mathbf{V}.\mathbf{v}'_1)V^i + (\mathbf{V}.\mathbf{r}_1)a'^{i}_1 \right)\frac{\partial F}{\partial v^i_1}$$
$$+ \frac{1}{c^2}\left(\left[-\frac{1}{2}\mathbf{V}^2 - \mathbf{V}.\mathbf{v}'_2 \right] v'^{i}_2 - \frac{1}{2}(\mathbf{V}.\mathbf{v}'_2)V^i + [\mathbf{V}.\mathbf{r}_1+\mathbf{V}.\mathbf{y}'_{12}]a'^{i}_2 \right)\frac{\partial F}{\partial v^i_2}\Bigg)_1$$
$$+ O\left(\frac{1}{c^4}\right). \tag{4.7}$$

We have replaced here the vectorial distance $\mathbf{r}'_1$ by the unprimed notation $\mathbf{r}_1$, noticing that $\mathbf{r}'_1$ is the dummy variable with respect to which the regularization proceeds (with this notation $\mathbf{r}'_2$ is replaced by $\mathbf{r}_1+\mathbf{y}'_{12}$). Following (3.35), the Lorentzian regularization $[F]_1$ is achieved by posing $\mathbf{V}=\mathbf{v}_1$ and $\mathbf{v}'_1=\mathbf{0}$, as well as $\mathbf{y}'_{12}=\mathbf{y}'_{12}[\mathbf{y}_{12};\mathbf{v}_1,\mathbf{v}_2]$ and $\mathbf{v}'_2=\mathbf{v}'_2[\mathbf{y}_{12};\mathbf{v}_1,\mathbf{v}_2]$, where the latter functionals are defined in the general case by (3.29) and (3.30). It is convenient to obtain first an intermediate formula by setting $\mathbf{V}=\mathbf{v}_1$ and $\mathbf{v}'_1=\mathbf{0}$ in (4.7), and by replacing into the terms that are already of order $1/c^2$ the primed variables $\mathbf{y}'_{12}$ and $\mathbf{a}'_1$, $\mathbf{a}'_2$ by the unprimed ones. Using also the identity (4.1), we arrive at

$$[F]_1 = \Bigg(F[\mathbf{r}_1,\mathbf{r}_1+\mathbf{y}'_{12};\mathbf{v}_1,\mathbf{v}_1+\mathbf{v}'_2] + \frac{1}{2c^2}(\mathbf{v}_1.\mathbf{r}_1)v^i_1\partial_i F$$
$$+ \frac{1}{c^2}(\mathbf{v}_1.\mathbf{r}_1)\left[v^i_1\frac{\partial F}{\partial y^i_1} + v^i_2\frac{\partial F}{\partial y^i_2} + a^i_1\frac{\partial F}{\partial v^i_1} + a^i_2\frac{\partial F}{\partial v^i_2} \right] + \frac{1}{c^2}\left(\frac{1}{2}(\mathbf{v}_1.\mathbf{v}_2)v^i_1 + \left[\frac{1}{2}\mathbf{v}_1^2 - \mathbf{v}_1.\mathbf{v}_2 \right]v^i_2 \right.$$
$$\left. + (\mathbf{v}_1.\mathbf{y}_{12})a^i_2 \right)\frac{\partial F}{\partial v^i_2} + \frac{1}{c^2}(\mathbf{v}_1.\mathbf{y}_{12})\left[-\frac{1}{2}v^i_1 + v^i_2 \right]\frac{\partial F}{\partial y^i_2}\Bigg)_1 + O\left(\frac{1}{c^4}\right), \tag{4.8}$$

where $\mathbf{y}'_{12}$ and $\mathbf{v}'_2$ in the first term of the right side are given functions of $\mathbf{y}_{12}$, $\mathbf{v}_1$ and $\mathbf{v}_2$ obtained by approximating (3.29) and (3.30) to the first order. We find

$$\mathbf{y}'_{12} = \mathbf{y}_{12} + \frac{1}{c^2}(\mathbf{v}_1.\mathbf{y}_{12})\left[-\frac{1}{2}\mathbf{v}_1 + \mathbf{v}_2 \right] + O\left(\frac{1}{c^4}\right), \tag{4.9a}$$

$$\mathbf{v}'_2 = -\mathbf{v}_1 + \mathbf{v}_2 + \frac{1}{c^2}\left(-\frac{1}{2}(\mathbf{v}_1.\mathbf{v}_2)\mathbf{v}_1 + \left[-\frac{1}{2}\mathbf{v}_1^2 + \mathbf{v}_1.\mathbf{v}_2 \right]\mathbf{v}_2 - (\mathbf{v}_1.\mathbf{y}_{12})\mathbf{a}_2 \right) + O\left(\frac{1}{c^4}\right) \tag{4.9b}$$

(where the acceleration is equal to its Newtonian value). By inserting (4.9) into (4.8) and expanding to order $1/c^2$, it is easily seen that we cancel out exactly the two last terms on the right-hand side of (4.8), so that the result simplifies appreciably:

$$[F]_1 = \left(F[\mathbf{r}_1,\mathbf{r}_2;\mathbf{v}_1,\mathbf{v}_2] + \frac{1}{2c^2}(\mathbf{v}_1.\mathbf{r}_1)v_1^i\partial_i F + \frac{1}{c^2}(\mathbf{v}_1.\mathbf{r}_1)\left[v_1^i\frac{\partial F}{\partial y_1^i} + v_2^i\frac{\partial F}{\partial y_2^i} + a_1^i\frac{\partial F}{\partial v_1^i} + a_2^i\frac{\partial F}{\partial v_2^i}\right]\right)_1 + O\left(\frac{1}{c^4}\right). \tag{4.10}$$

Finally, we recognize on the right side the partial time derivative,

$$\partial_t F = v_1^i\frac{\partial F}{\partial y_1^i} + v_2^i\frac{\partial F}{\partial y_2^i} + a_1^i\frac{\partial F}{\partial v_1^i} + a_2^i\frac{\partial F}{\partial v_2^i}, \tag{4.11}$$

so that our final result writes

$$[F]_1 = \left(F + \frac{1}{c^2}(\mathbf{r}_1.\mathbf{v}_1)\left[\partial_t F + \frac{1}{2}v_1^i\partial_i F\right]\right)_1 + O\left(\frac{1}{c^4}\right). \tag{4.12}$$

The result (4.12) displays the first relativistic corrections brought about by our Lorentzian regularization $[F]_1$. As a check of the formula, let us apply it to the case of the special combination $\partial_i F - 3(n_1^i/r_1)F$ which, as we know from (2.5), has no partie finie at the point 1 in the sense of the old regularization. This is no longer true in the sense of the new regularization. Using the equation (4.12) we find instead

$$[\partial_i F]_1 = \left[3\frac{n_1^i}{r_1}\left(1 - \frac{1}{c^2}(\mathbf{n}_1.\mathbf{v}_1)^2\right)F - \frac{1}{c^2}v_1^i\partial_t F\right]_1 + O\left(\frac{1}{c^4}\right). \tag{4.13}$$

The check consists of remarking that because of (2.5) we have $(\partial_i' F' - 3(n'^i_1/r_1')F')_1 = 0$ in the rest frame of particle 1, therefore the equation $[\partial_i' F' - 3(n'^i_1/r_1')F']_1 = 0$ must hold in any frame by definition of the new regularization. In the frame where the particle velocity is $\mathbf{v}_1$ we have $\mathbf{r}_1' = \mathbf{r}_1 + (1/2c^2)(\mathbf{v}_1.\mathbf{r}_1)\mathbf{v}_1 + O(1/c^4)$ and $\partial_i' = \partial_i + (1/c^2)v_1^i\partial_t + (1/2c^2)v_1^iv_1^j\partial_j + O(1/c^4)$. Inserting these relations into the previous equation, and using the fact that F is a scalar, we recover the formula (4.13) after a short computation.

V. THE STRESS-ENERGY TENSOR OF POINT-PARTICLES

With the Lorentzian regularization in hand, we make a proposal for the description of point-like particles in (post-Newtonian approximations of) general relativity. We recall first the general context of the problem. We want to solve the field equations of general relativity by means of analytic post-Newtonian series, with matter source describing appropriately defined point-particles. The stress-energy tensor of the matter source is supposed to be spatially isolated; we recall that, in this case, general relativity admits the Poincaré group as a global symmetry. We assume the existence and unity of a global harmonic coordinate system, defined by the gauge conditions

$$\partial_\nu h^{\mu\nu} = 0\ , \tag{5.1a}$$

$$h^{\mu\nu} = \sqrt{g}g^{\mu\nu} - \eta^{\mu\nu}, \tag{5.1b}$$

where $g^{\mu\nu}$ denotes the inverse of the covariant metric $g_{\mu\nu}$, and where g is the opposite of its determinant. The harmonic gauge conditions (5.1) introduce a preferred Minkowskian structure, with Minkowski metric given by $\eta^{\mu\nu} = \mathrm{diag}(-1,1,1,1) = \eta_{\mu\nu}$. Thus, the gravitational field can be described in harmonic coordinates by the Lorentzian tensor field $h^{\mu\nu}$ propagating on the

Minkowskian background $\eta^{\mu\nu}$. Similarly, one can think of the trajectories of the particles as accelerated world lines in Minkowski space–time. Subject to the conditions (5.1) the Einstein field equations take the form of wave equations on the flat background,

$$\Box h^{\mu\nu}=\frac{16\pi G}{c^4}gT^{\mu\nu}+\Lambda^{\mu\nu}[h,\partial h,\partial^2 h], \tag{5.2}$$

where the flat d'Alembertian operator is given by $\Box=\eta^{\mu\nu}\partial_\mu\partial_\nu$. The right-hand side is made of the sum of the matter source term, with spatially compact support, plus the gravitational source term $\Lambda^{\mu\nu}$, given by a certain functional of the field variables $h^{\rho\sigma}$ and its first and second space–time derivatives, and at least of second order in h. A consequence of the harmonicity conditions is that

$$\partial_\nu\left(gT^{\mu\nu}+\frac{c^4}{16\pi G}\Lambda^{\mu\nu}\right)=0\ , \tag{5.3}$$

which is equivalent (through the contracted Bianchi identity) to the covariant conservation of the matter stress-energy tensor $T^{\mu\nu}$,

$$\nabla_\nu T^{\mu\nu}=0\ , \tag{5.4}$$

the latter equation being in turn equivalent to

$$\partial_\nu(\sqrt{g}g_{\lambda\mu}T^{\mu\nu})=\tfrac{1}{2}\sqrt{g}\partial_\lambda g_{\mu\nu}T^{\mu\nu}. \tag{5.5}$$

In this section we regard the matter tensor $T^{\mu\nu}$ as a Lorentz tensor defined with respect to the Minkowski metric $\eta_{\mu\nu}$ singled out by our choice of harmonic coordinates.

To define a model for point-like particles, we follow essentially the derivation of the stress-energy tensor of *test* masses moving on a fixed *smooth* background (see, e.g., Ref. 30, p. 360). However, in the case of ''self-gravitating'' particles, we do not have a smooth background at our disposal, and the metric becomes singular at the location of the point-masses. Essentially, we shall propose the value of the (post-Newtonian) metric coefficients on each of the particles to be given by the Lorentzian regularization defined in Sec. III. This entails supposing that the metric coefficients belong to the class of functions $\mathcal{F}$. This is correct up to the 2PN order;[19] however, we know that the expansion of the metric coefficients (in harmonic coordinates) near the particles, instead of being of the type (2.1) and (2.2), involve some logarithms of the distance to the singularities starting at 3PN order. It was shown[22] that, at this order, the logarithms can be considered as some constants and included into the definition of the partie finie; moreover, they can be finally eliminated from the equations of motion by a change of coordinates. This suggests that we might consider more generally the logarithms as some constants, motivating our assumption that $g_{\mu\nu}\in\mathcal{F}$. On the other hand, it is known[22,24] that the constants s_1 and s_2 entering the partie finie integral (2.6) must be adjusted in order that the equations of motion can be deducible from a Lagrangian, and in particular admit a conserved energy. For these reasons (presence of logarithms, equations of motion not directly admitting an energy), the following derivation of the stress-energy tensor for particles cannot be considered to be a rigorous proof. However, as we shall see, it is nicely consistent with the regularization, and its result satisfying. Our basic assumption is that the dynamics of the particles follows from the variation, with respect to the metric, of the action

$$I_{\text{particle}}=-m_1c\int_{-\infty}^{+\infty}dt\sqrt{-[g_{\mu\nu}]_1v_1^\mu v_1^\nu}+1\leftrightarrow 2, \tag{5.6}$$

where $v_1^\mu=(c,d\mathbf{y}_1/dt)$ denotes the coordinate velocity of particle 1 (we consider a two-body system, but the generalization to N bodies is immediate). The crucial point is that the value of $g_{\mu\nu}$ at 1 is assumed to be given by the Lorentzian regularization defined in Sec. III. We vary the action

(5.6) with respect to the metric, i.e., we imagine that $g_{\mu\nu}\in\mathcal{F}$ is subject to an infinitesimal variation $g_{\mu\nu}\to g_{\mu\nu}+\delta g_{\mu\nu}$ and compute the corresponding change in the action. However, we want the variation of the metric to correspond to the same matter system with two singularities 1 and 2. The evident and most natural way to ensure this is to suppose that $\delta g_{\mu\nu}\in\mathcal{F}$. Under the latter variation the regularized value of the metric at the point 1 undergoes the infinitesimal change $[g_{\mu\nu}]_1 \to[g_{\mu\nu}]_1+[\delta g_{\mu\nu}]_1$. Therefore, the variation of the action (5.6) reads as

$$\delta I_{\text{particle}}=\frac{1}{2}m_1 c\int_{-\infty}^{+\infty}dt\,\frac{v_1^\mu v_1^\nu}{\sqrt{-[g_{\rho\sigma}]_1 v_1^\rho v_1^\sigma}}[\delta g_{\mu\nu}]_1+1\leftrightarrow 2. \tag{5.7}$$

From the defining property (3.36) of the delta-pseudo-function $\text{Pf}\Delta_1$, we can rewrite (5.7) in the equivalent form

$$\delta I_{\text{particle}}=\frac{1}{2}m_1 c\int_{-\infty}^{+\infty}dt\,\frac{v_1^\mu v_1^\nu}{\sqrt{-[g_{\rho\sigma}]_1 v_1^\rho v_1^\sigma}}\langle \text{Pf}\Delta_1,\delta g_{\mu\nu}\rangle+1\leftrightarrow 2. \tag{5.8}$$

Now, recall that the duality bracket is defined by the partie finie of the three-dimensional integral [cf. (2.8)], so the latter expression can be cast into the standard form appropriate to the definition of a stress-energy tensor $T^{\mu\nu}_{\text{particle}}$, namely,

$$\delta I_{\text{particle}}=\frac{1}{2}\int_{-\infty}^{+\infty}dt\langle\sqrt{g}T^{\mu\nu}_{\text{particle}},\delta g_{\mu\nu}\rangle. \tag{5.9}$$

The only difference with the standard definition is that the partie finie takes care of the divergencies at the positions of the particles. By comparing (5.8) and (5.9), we readily find that the corresponding stress-energy tensor density is given by

$$\sqrt{g}T^{\mu\nu}_{\text{particle}}=m_1 c\frac{v_1^\mu v_1^\nu}{\sqrt{-[g_{\rho\sigma}]_1 v_1^\rho v_1^\sigma}}\text{Pf}\,\Delta_1+1\leftrightarrow 2. \tag{5.10}$$

The stress-energy tensor itself comes immediately from the rule of multiplication of pseudo-functions (3.37):

$$T^{\mu\nu}_{\text{particle}}=m_1 c\frac{v_1^\mu v_1^\nu}{\sqrt{-[g_{\rho\sigma}]_1 v_1^\rho v_1^\sigma}}\text{Pf}\left(\frac{\Delta_1}{\sqrt{g}}\right)+1\leftrightarrow 2, \tag{5.11}$$

This tensor takes the same form as the stress-energy tensor of test particles moving on a smooth background, except that the role of the background field is now played by the metric generated by the particles, regularized following the prescription (3.35). Notice in particular that the factor $1/\sqrt{g}$ inside the partie finie sign Pf should not be replaced by its regularized value at 1 [see (3.39)]. We propose the tensor (5.11) as a model of particles in the post-Newtonian approximation. From the product rules for pseudo-functions, we get the matter source term on the right-hand side of (5.2) as

$$gT^{\mu\nu}_{\text{particle}}=m_1 c\frac{v_1^\mu v_1^\nu}{\sqrt{-[g_{\rho\sigma}]_1 v_1^\rho v_1^\sigma}}\text{Pf}\,(\sqrt{g}\Delta_1)+1\leftrightarrow 2. \tag{5.12}$$

The post-Newtonian iteration of the field equations in Refs. 22 and 24 is based on the latter expression of the matter source term.

We now derive the equations of motion of particle 1 from the covariant conservation of the stress-energy tensor (5.11):

$$\nabla_\nu T^{\mu\nu}_{\text{particle}} = 0 \ . \tag{5.13}$$

Notice that thanks to the presence of the delta-pseudo-function, we know that the derivative is "ordinary" and satisfies the Leibniz rule in the sense of (3.41). Thus, we can transform $\nabla_\nu T^{\mu\nu}_{\text{particle}}$ in the standard way and find that the equation (5.13) is equivalent, like in the case of continuous sources, to the alternative form

$$\partial_\nu(\sqrt{g} g_{\lambda\mu} T^{\mu\nu}_{\text{particle}}) = \frac{1}{2}\sqrt{g}\partial_\lambda g_{\mu\nu} T^{\mu\nu}_{\text{particle}}. \tag{5.14}$$

Then, we integrate (5.14) over a closed volume V_1 surrounding particle 1 exclusively. The role of the three-dimensional integral is played here by the duality bracket defined by (2.8). Let us denote by $\mathbf{1}_{\mathrm{V}_1}$ the characteristic function of the volume V_1, such that $\mathbf{1}_{\mathrm{V}_1}(\mathbf{x}) = 1$ if $\mathbf{x} \in \mathrm{V}_1$ and $\mathbf{1}_{\mathrm{V}_1}(\mathbf{x}) = 0$ otherwise [notably, $\mathbf{1}_{\mathrm{V}_1}(\mathbf{y}_2) = 0$]. Thus, we consider

$$\langle \partial_\nu(\sqrt{g} g_{\lambda\mu} T^{\mu\nu}_{\text{particle}}), \mathbf{1}_{\mathrm{V}_1} \rangle = \left\langle \frac{1}{2}\sqrt{g}\partial_\lambda g_{\mu\nu} T^{\mu\nu}_{\text{particle}}, \mathbf{1}_{\mathrm{V}_1} \right\rangle. \tag{5.15}$$

(Though $\mathbf{1}_{\mathrm{V}_1}$ does not belong to the class $\mathcal{F}$, it is locally integrable on $\mathbb{R}^3$ and we know that the duality bracket applies on such functions as well; see Ref. 1.) The partial derivative ∂_ν on the left-hand side is split into a time derivative and a space derivative. Following the rule (3.40), the spatial derivative ∂_i is shifted to the right side of the bracket, where it applies on the characteristic function $\mathbf{1}_{\mathrm{V}_1}$. Because of the presence of the delta-pseudo-function, the derivative of $\mathbf{1}_{\mathrm{V}_1}$ is to be taken in an ordinary sense and is zero. Following the rule (9.7) in Ref. 1, an analogous reasoning is valid for the time-derivative $\partial_0 = (1/c)\partial_t$ which can thus simply be put outside the bracket. Thus, we get

$$\frac{d}{cdt}\{\langle \sqrt{g} g_{\lambda\mu} T^{\mu 0}_{\text{particle}}, \mathbf{1}_{\mathrm{V}_1} \rangle\} = \left\langle \frac{1}{2}\sqrt{g}\partial_\lambda g_{\mu\nu} T^{\mu\nu}_{\text{particle}}, \mathbf{1}_{\mathrm{V}_1} \right\rangle. \tag{5.16}$$

Next, we insert into (5.16) the specific expression (5.10) of the stress-energy density of particles. Because of the presence of the function $\mathbf{1}_{\mathrm{V}_1}$ only the part corresponding to particle 1 contributes, and we obtain

$$\frac{d}{dt}\left\{ \frac{v_1^\mu}{\sqrt{-[g_{\rho\sigma}]_1 v_1^\rho v_1^\sigma}} \langle \mathrm{Pf}(g_{\lambda\mu}\Delta_1), \mathbf{1}_{\mathrm{V}_1} \rangle \right\} = \frac{1}{2} \frac{v_1^\mu v_1^\nu}{\sqrt{-[g_{\rho\sigma}]_1 v_1^\rho v_1^\sigma}} \langle \mathrm{Pf}(\partial_\lambda g_{\mu\nu}\Delta_1), \mathbf{1}_{\mathrm{V}_1} \rangle. \tag{5.17}$$

Finally, the effect of the brackets on both sides of the latter equation is to take the value at point 1 in the sense of the Lorentzian regularization (3.35). Thereby our final result reads as

$$\frac{d}{dt}\left(\frac{[g_{\lambda\mu}]_1 v_1^\mu}{\sqrt{-[g_{\rho\sigma}]_1 v_1^\rho v_1^\sigma}} \right) = \frac{1}{2} \frac{[\partial_\lambda g_{\mu\nu}]_1 v_1^\mu v_1^\nu}{\sqrt{-[g_{\rho\sigma}]_1 v_1^\rho v_1^\sigma}}. \tag{5.18}$$

The equations of motion of particle 1 have the same formal structure as the geodesic equations of a test particle. In separate papers[22,24,25] we use (5.18) to derive explicitly the equations of motion of the two particles at the 3PN approximation.

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APPENDIX: SOLUTION OF THE EQUATION (3.14)

We are looking for the vector $\mathbf{z}_1$ satisfying the equation

$$\mathbf{z}_1=\mathbf{y}_1\left(t-\frac{1}{c^2}\mathbf{V}.(\mathbf{x}-\mathbf{z}_1)\right), \tag{A1}$$

where $\mathbf{y}_1(t)$ represents a given smooth (C^∞) time-like trajectory and $\mathbf{V}$ a constant vector with norm $|\mathbf{V}|<c$. Clearly, for a given trajectory, the solution $\mathbf{z}_1$ depends on the field point $\mathbf{x}$ as well as on time t. It was shown in the text after (3.15) that the application $\mathbf{x}\to\mathbf{z}_1$ is contracting with fixed point $\mathbf{y}_1$. Here, let us look for the solution $\mathbf{z}_1$ in the form of a function of the coordinates,

$$\mathbf{z}_1=\mathbf{z}_1(\mathbf{x},t). \tag{A2}$$

From (A1) we compute the partial derivatives of $\mathbf{z}_1$ with respect to t and x^i, considered to be independent, and readily obtain

$$\frac{\partial\mathbf{z}_1}{\partial x^i}=-\frac{1}{c^2}\left[V_i-\mathbf{V}.\frac{\partial\mathbf{z}_1}{\partial x^i}\right]\mathbf{v}_1\left(t-\frac{1}{c^2}\mathbf{V}.(\mathbf{x}-\mathbf{z}_1)\right), \tag{A3a}$$

$$\frac{\partial\mathbf{z}_1}{\partial t}=\left[1+\frac{1}{c^2}\mathbf{V}.\frac{\partial\mathbf{z}_1}{\partial t}\right]\mathbf{v}_1\left(t-\frac{1}{c^2}\mathbf{V}.(\mathbf{x}-\mathbf{z}_1)\right). \tag{A3b}$$

Contracting these equations with the vector $\mathbf{V}$ we can obtain the scalar products $\mathbf{V}.\partial\mathbf{z}_1/\partial x^i$ and $\mathbf{V}.\partial\mathbf{z}_1/\partial t$, and use them back into (A3) with the result that

$$\frac{\partial\mathbf{z}_1}{\partial x^i}=-\frac{1}{c^2}V_i\frac{\mathbf{v}_1}{1-\mathbf{V}.\mathbf{v}_1/c^2}, \tag{A4a}$$

$$\frac{\partial\mathbf{z}_1}{\partial t}=\frac{\mathbf{v}_1}{1-\mathbf{V}.\mathbf{v}_1/c^2}, \tag{A4b}$$

where the velocity $\mathbf{v}_1$ is evaluated at the instant $t-(1/c^2)\mathbf{V}.(\mathbf{x}-\mathbf{z}_1)$. In particular, we find that $\mathbf{z}_1$ must be a solution of the following first-order differential equation:

$$\frac{\partial\mathbf{z}_1}{\partial x^i}=-\frac{1}{c^2}V_i\frac{\partial\mathbf{z}_1}{\partial t}. \tag{A5}$$

Conversely, let us prove that a vector $\mathbf{z}_1$ that (i) satisfies the differential equation (A5) and (ii) admits $\mathbf{y}_1(t)$ as a *fixed* point, i.e., is such that

$$\mathbf{z}_1(\mathbf{y}_1(t),t)=\mathbf{y}_1(t) \tag{A6}$$

necessarily satisfies the original equation (A1). Such a $\mathbf{z}_1(\mathbf{x},t)$ being given, we perform in the equation (A5) the change of variables $(x^i,t)\to(\rho_1^i,\tau_1)$ defined by

$$\rho_1^i=x^i-z_1^i(\mathbf{x},t), \tag{A7a}$$

$$\tau_1 = t - \frac{1}{c^2}\mathbf{V}.(\mathbf{x}-\mathbf{z}_1(\mathbf{x},t)). \tag{A7b}$$

Using (A5) it is easy to obtain the laws of transformation of the partial derivatives:

$$\frac{\partial}{\partial \rho_1^i} = \frac{\partial}{\partial x^i} + \frac{1}{c^2} V_i \frac{\partial}{\partial t}, \tag{A8a}$$

$$\frac{\partial}{\partial \tau_1} = \frac{\partial}{\partial t} + B_j^i \frac{\partial z_1^j}{\partial t} \frac{\partial}{\partial x^i}, \tag{A8b}$$

where B_j^i denotes the matrix inverse of $A_k^j = \delta_k^j + (1/c^2) V_k (\partial z_1^j / \partial t)$ (i.e., $A_j^i B_k^j = \delta_k^i$; in the case considered here where the velocities are strictly less than c the matrix A_j^i is a deformation of the unit matrix and thus admits an inverse). Now, under the change of variables (A7) the differential equation (A5) becomes simply

$$\frac{\partial \mathbf{z}_1}{\partial \rho_1^i} = \mathbf{0}, \tag{A9}$$

whose general solution is an arbitrary function of the time variable τ_1. Therefore, there must exists a trajectory $\mathbf{Y}_1$ such that

$$\mathbf{z}_1 = \mathbf{Y}_1(\tau_1) = \mathbf{Y}_1\left(t - \frac{1}{c^2}\mathbf{V}.(\mathbf{x}-\mathbf{z}_1) \right). \tag{A10}$$

Imposing now that $\mathbf{y}_1(t)$ is a fixed point for this solution $\mathbf{z}_1$ in the sense of (A6) leads immediately to

$$\mathbf{Y}_1(t) = \mathbf{y}_1(t), \tag{A11}$$

so the equation (A1) is recovered exactly. Thus, solving (A1) is equivalent to solving the differential equation (A5) supplemented by the condition (A6). Notice that from (A1) or equivalently from (A5) and (A6) we find that $\mathbf{z}_1$ tends to the fixed point in the ''nonrelativistic'' limit $c \to +\infty$, i.e.,

$$\lim_{c \to +\infty} \{\mathbf{z}_1(\mathbf{x},t)\} = \mathbf{y}_1(t). \tag{A12}$$

This suggests to look for the solution $\mathbf{z}_1$ in the form of an infinite series of relativistic corrections of successive orders $1/c^{2n}$ [from (A5) we know that $\mathbf{z}_1$ is a function of $1/c^2$]. Thus, taking also into account the limit (A12), we pose

$$\mathbf{z}_1(\mathbf{x},t) = \mathbf{y}_1(t) + \sum_{n=1}^{+\infty} \frac{1}{c^{2n}} \overset{n}{\mathbf{Z}}_1(\mathbf{x},t), \tag{A13}$$

and we look for each one of the unknown coefficients $\overset{n}{\mathbf{Z}}_1(\mathbf{x},t)$. By placing the series (A13) into both sides of the equation (A5) and identifying the factors of the powers of $1/c^2$ on each side we find, for any $n \geqslant 1$,

$$\frac{\partial \overset{n}{\mathbf{Z}}_1}{\partial x^i} = -V_i \frac{\partial \overset{n-1}{\mathbf{Z}}_1}{\partial t}, \tag{A14}$$

with the convention that $\overset{0}{\mathbf{Z}}_1 = \mathbf{y}_1(t)$. The equations (A14) are to be solved using the condition of fixed point $\mathbf{y}_1$ [cf. (A6)], which implies that, $\forall n \geqslant 1$,

$$\overset{n}{\mathbf{Z}}_1(\mathbf{y}_1(t),t) = \mathbf{0}. \tag{A15}$$

The solution of (A14) and (A15) is found by induction over n. As an induction hypothesis suppose that

$$\overset{n-1}{\mathbf{Z}}_1 = \frac{(-)^{n-1}}{(n-1)!}\left(\frac{\partial}{\partial t}\right)^{n-2}[(\mathbf{V}.\mathbf{r}_1)^{n-1}\mathbf{v}_1], \tag{A16}$$

where $\mathbf{r}_1 = \mathbf{x} - \mathbf{y}_1$, and where the partial time derivatives act on t keeping the space coordinate $\mathbf{x}$ fixed: for instance, $\partial \mathbf{r}_1 / \partial t = -\mathbf{v}_1$ and $\partial \mathbf{v}_1 / \partial t = d\mathbf{v}_1 / dt = \mathbf{a}_1$, where $\mathbf{a}_1$ is the acceleration. Notice that (A16) satisfies the condition (A15) because it involves $n-2$ partial time derivatives while there is a factor $(\mathbf{V}.\mathbf{r}_1)^{n-1}$ inside the brackets, so after differentiation there will remain at least one factor $\mathbf{V}.\mathbf{r}_1$ making the result be zero when $\mathbf{x} = \mathbf{y}_1$. Inserting (A16) into the right-hand side of (A14) we obtain the equation to be satisfied for the next-order coefficient,

$$\frac{\partial \overset{n}{\mathbf{Z}}_1}{\partial x^i} = V_i \frac{(-)^n}{(n-1)!}\left(\frac{\partial}{\partial t}\right)^{n-1}[(\mathbf{V}.\mathbf{r}_1)^{n-1}\mathbf{v}_1], \tag{A17}$$

which can be rewritten equivalently in the form

$$\frac{\partial \overset{n}{\mathbf{Z}}_1}{\partial x^i} = \frac{\partial}{\partial x^i}\left\{\frac{(-)^n}{n!}\left(\frac{\partial}{\partial t}\right)^{n-1}[(\mathbf{V}.\mathbf{r}_1)^{n}\mathbf{v}_1]\right\}, \tag{A18}$$

showing that the most general solution is necessarily of the type

$$\overset{n}{\mathbf{Z}}_1 = \frac{(-)^n}{n!}\left(\frac{\partial}{\partial t}\right)^{n-1}[(\mathbf{V}.\mathbf{r}_1)^{n}\mathbf{v}_1] + \mathbf{C}(t), \tag{A19}$$

where $\mathbf{C}(t)$ denotes an arbitrary vector depending only on time t. However, this vector must be zero on account of the fact that the result should be zero when $\mathbf{x} = \mathbf{y}_1$. Therefore we have proved by induction that

$$\overset{n}{\mathbf{Z}}_1 = \frac{(-)^n}{n!}\left(\frac{\partial}{\partial t}\right)^{n-1}[(\mathbf{V}.\mathbf{r}_1)^{n}\mathbf{v}_1], \tag{A20}$$

so the vector $\mathbf{z}_1$ solving at once (A5) and (A6), or equivalently (A1), takes the form of the rather interesting infinite series

$$\mathbf{z}_1 = \mathbf{y}_1 + \sum_{n=1}^{+\infty} \frac{(-)^n}{c^{2n} n!}\left(\frac{\partial}{\partial t}\right)^{n-1}[(\mathbf{V}.\mathbf{r}_1)^{n}\mathbf{v}_1], \tag{A21}$$

which constitutes the solution needed for our work in Sec. III. Furthermore, subtracting $\mathbf{x}$ from this solution and contracting with $\mathbf{V}$ we obtain after a short calculation the quantity τ_1 which was defined in (A7b):

$$\tau_1 = t + \sum_{n=1}^{+\infty} \frac{(-)^n}{c^{2n} n!} \left(\frac{\partial}{\partial t} \right)^{n-1} [(\mathbf{V}.\mathbf{r}_1)^n]. \tag{A22}$$

Now, recall that the latter quantity τ_1 is such that $\mathbf{z}_1 = \mathbf{y}_1(\tau_1)$. Therefore, we see that we can find an alternative expression of the vector $\mathbf{z}_1$ by inserting into $\mathbf{y}_1(\tau_1)$ the series expansion (A22) found for τ_1. Using an infinite Taylor expansion we are led to

$$\mathbf{z}_1 = \mathbf{y}_1 + \sum_{p=0}^{+\infty} \frac{1}{(p+1)!} \frac{d^p \mathbf{v}_1}{dt^p} \left(\sum_{n=1}^{+\infty} \frac{(-)^n}{c^{2n} n!} \left(\frac{\partial}{\partial t} \right)^{n-1} [(\mathbf{V}.\mathbf{r}_1)^n] \right)^{p+1}. \tag{A23}$$

Each of the terms is composed of $p+1$ sums; accordingly we introduce $p+1$ summation indices $n_1, \ldots, n_p, n_{p+1}$ so that

$$\mathbf{z}_1 = \mathbf{y}_1 + \sum_{p=0}^{+\infty} \frac{1}{(p+1)!} \frac{d^p \mathbf{v}_1}{dt^p} \sum_{n_1=1}^{+\infty} \cdots \sum_{n_p=1}^{+\infty} \sum_{n_{p+1}=1}^{+\infty} \frac{(-)^{n_1 + \ldots + n_{p+1}}}{c^{2(n_1 + \ldots + n_{p+1})}} \times \left(\frac{\partial}{\partial t} \right)^{n_1 - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_1}}{n_1!} \right] \cdots \left(\frac{\partial}{\partial t} \right)^{n_p - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_p}}{n_p!} \right] \left(\frac{\partial}{\partial t} \right)^{n_{p+1} - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_{p+1}}}{n_{p+1}!} \right]. \tag{A24}$$

Next we pose $k = n_1 + \cdots + n_p + n_{p+1}$, replace the index n_{p+1} by k, and operate $p+1$ commutations of summations to arrive at

$$\mathbf{z}_1 = \mathbf{y}_1 + \sum_{k=1}^{+\infty} \frac{(-)^k}{c^{2k}} \sum_{p=0}^{k-1} \frac{1}{(p+1)!} \frac{d^p \mathbf{v}_1}{dt^p} \sum_{n_1=1}^{q_1} \cdots \sum_{n_p=1}^{q_p} \times \left(\frac{\partial}{\partial t} \right)^{n_1 - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_1}}{n_1!} \right] \cdots \left(\frac{\partial}{\partial t} \right)^{n_p - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_p}}{n_p!} \right] \left(\frac{\partial}{\partial t} \right)^{n_{p+1} - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_{p+1}}}{n_{p+1}!} \right], \tag{A25}$$

in which $n_{p+1} = k - \Sigma_{i=1}^{p} n_i$ and $q_j = 1 + \Sigma_{i=j}^{p+1} (n_i - 1)$ (with $1 \leqslant j \leqslant p$). We must identify the latter complicated expression with the simpler form of the vector $\mathbf{z}_1$ given by (A21). From identifying the powers of $1/c^2$ in both expressions we immediately obtain

$$\left(\frac{\partial}{\partial t} \right)^{k-1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^k}{k!} \mathbf{v}_1 \right] = \sum_{p=0}^{k-1} \frac{1}{(p+1)!} \frac{d^p \mathbf{v}_1}{dt^p} \sum_{n_1=1}^{q_1} \cdots \sum_{n_p=1}^{q_p} \times \left(\frac{\partial}{\partial t} \right)^{n_1 - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_1}}{n_1!} \right] \cdots \left(\frac{\partial}{\partial t} \right)^{n_p - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_p}}{n_p!} \right] \left(\frac{\partial}{\partial t} \right)^{n_{p+1} - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_{p+1}}}{n_{p+1}!} \right]. \tag{A26}$$

Finally, from using the binomial formula for the derivative of a product, we can identify on each side of the latter equation the coefficients of each $d^p \mathbf{v}_1 / dt^p$, and we arrive at the relation, valid for any p and any $k \geqslant p+1$,

$$\sum_{n_1=1}^{q_1} \cdots \sum_{n_p=1}^{q_p} \left(\frac{\partial}{\partial t} \right)^{n_1 - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_1}}{n_1!} \right] \cdots \left(\frac{\partial}{\partial t} \right)^{n_p - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_p}}{n_p!} \right] \left(\frac{\partial}{\partial t} \right)^{n_{p+1} - 1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^{n_{p+1}}}{n_{p+1}!} \right] = \frac{(p+1)(k-1)!}{(k-1-p)!} \left(\frac{\partial}{\partial t} \right)^{k-p-1} \left[\frac{(\mathbf{V}.\mathbf{r}_1)^k}{k!} \right]. \tag{A27}$$

The latter relation actually represents a quite general mathematical formula because we have specified nothing about the scalar product $\mathbf{V}.\mathbf{r}_1$. Therefore, the relation (A27) holds in fact in the case of an arbitrary sufficiently differentiable function $f(t)$, so

$$\sum_{n_1=1}^{q_1}\cdots\sum_{n_p=1}^{q_p}\left(\frac{d}{dt}\right)^{n_1-1}\left[\frac{f^{n_1}}{n_1!}\right]\cdots\left(\frac{d}{dt}\right)^{n_p-1}\left[\frac{f^{n_p}}{n_p!}\right]\left(\frac{d}{dt}\right)^{n_{p+1}-1}\left[\frac{f^{n_{p+1}}}{n_{p+1}!}\right]$$
$$=\frac{(p+1)(k-1)!}{(k-1-p)!}\left(\frac{d}{dt}\right)^{k-p-1}\left[\frac{f^k}{k!}\right]. \tag{A28}$$

The equivalence obtained above between the formula (A1) and the differential equation (A5) together with the auxiliary condition (A6) shows *indirectly* that the mathematical formula (A28) is correct. However, a *direct* proof of this formula has been found by Tanaka, Sasaki, and Tagoshi (private communication). Here we reproduce their proof in the particular case where $p=1$, so that $q_1=k-1$ and $n_2=k-n$ (where $n\equiv n_1$), in which case the formula reads, for any $k\geqslant 2$,

$$\sum_{n=1}^{k-1}\left(\frac{d}{dt}\right)^{n-1}\left[\frac{f^n}{n!}\right]\left(\frac{d}{dt}\right)^{k-n-1}\left[\frac{f^{k-n}}{(k-n)!}\right]=2(k-1)\left(\frac{d}{dt}\right)^{k-2}\left[\frac{f^k}{k!}\right]. \tag{A29}$$

We replace $f(t)$ in (A29) by its Fourier transform, $f(t)=\int_{-\infty}^{+\infty}(d\omega/2\pi)e^{i\omega t}\tilde{f}(\omega)$, and readily find that in order to prove the formula (A29) it suffices to prove the statement that the equation

$$\sum_{n=1}^{k-1}\binom{k}{n}(\omega_{(1}+\omega_2+\cdots+\omega_n)^{n-1}(\omega_{n+1}+\cdots+\omega_{k)})^{k-n-1}=2(k-1)(\omega_1+\omega_2+\cdots+\omega_k)^{k-2} \tag{A30}$$

holds identically for any family of real frequencies $\omega_1,\ \ldots,\ \omega_k$. Most importantly, the parentheses around indices on the left side of (A30) indicate the complete symmetrization over the k frequencies $\omega_1,\ \ldots,\ \omega_k$ [in addition, $\binom{k}{n}$ denotes the binomial coefficient]. Let us single out one of the frequencies, for instance ω_k, and rewrite (A30) in a form involving an explicit symmetrization over the other $k-1$ frequencies, $\omega_1,\ \ldots,\ \omega_{k-1}$, only:

$$\sum_{n=1}^{k-1}\binom{k-1}{n}(\omega_{(1}+\cdots+\omega_n)^{n-1}(\omega_{n+1}+\cdots+\omega_{k-1)}+\omega_k)^{k-n-1}$$
$$=(k-1)(\omega_1+\omega_2+\cdots+\omega_k)^{k-2} \tag{A31}$$

(in which we have simplified a factor 2 on both sides of the equation). Furthermore, let us replace in the latter formula ω_k by some sum $\omega_k+\cdots+\omega_{k+s}$, and symmetrize over the whole set of frequencies $\omega_1,\ \ldots,\ \omega_{k+s}$. This yields, for any s,

$$\sum_{n=1}^{k-1}\binom{k-1}{n}(\omega_{(1}+\cdots+\omega_n)^{n-1}(\omega_{n+1}+\cdots+\omega_{k+s)})^{k-n-1}$$
$$=(k-1)(\omega_1+\omega_2+\cdots+\omega_{k+s})^{k-2}. \tag{A32}$$

Now we prove that the equation (A30), or equivalently (A31), is true by induction on the integer k. Therefore, our induction hypothesis is that (A31) is correct for *any* $k\leqslant K$, and from this we want to show that it is correct again for $k=K+1$. Note that from our induction hypothesis we know that (A32) is also correct for any $k\leqslant K$ and *any* s. Consider the sum defined by the left side of (A31) in the case where $k=K+1$, say

$$S_{K+1}=\sum_{n=1}^{K}\binom{K}{n}(\omega_{(1}+\cdots+\omega_{n})^{n-1}(\omega_{n+1}+\cdots+\omega_{K)}+\omega_{K+1})^{K-n}, \tag{A33}$$

where we recall that one of the frequencies, i.e., ω_{K+1}, is "artificially" singled out. However, S_{K+1} is also given by half the left-hand side of (A30) and is symmetric in $\omega_1, \ldots, \omega_{K+1}$. We want to show that S_{K+1} is equal to the right-hand side of (A31) with $k=K+1$. To this end, we transform S_{K+1} with the help of the binomial formula, and obtain after a short calculation

$$S_{K+1}=\sum_{l=0}^{K-1}\frac{\omega_{K+1}^{l}}{l!}\frac{K!}{(K-l)!}\sum_{n=1}^{K-l}\binom{K-l}{n}(\omega_{(1}+\cdots+\omega_{n})^{n-1}(\omega_{n+1}+\cdots+\omega_{K)})^{K-n-l}. \tag{A34}$$

Now we have two sums over l and n, and it is easy to recognize that the second sum, over n, can be simplified as soon as $l\geqslant 1$ by means of (A32) which is correct by induction under the condition that $k\leqslant K$ and for any s. Posing $K-l=k-1$ and $k+s=K$ we see that this condition is realized if and only if $l\geqslant 1$. After simplification we find

$$S_{K+1}=K(\omega_1+\cdots+\omega_{K+1})^{K-1}+\Psi_{K+1}(\omega_1,\ldots,\omega_K), \tag{A35}$$

where the first term is the result we want to obtain, and where the second term is a certain function of the frequencies $\omega_1, \ldots, \omega_K$ but which does *not* depend on ω_{K+1}. The expression of Ψ_{K+1} is given for completeness as

$$\Psi_{K+1}=\sum_{n=1}^{K}\binom{K}{n}(\omega_{(1}+\cdots+\omega_{n})^{n-1}(\omega_{n+1}+\cdots+\omega_{K)})^{K-n}-K(\omega_1+\cdots+\omega_K)^{K-1}. \tag{A36}$$

Now we use the fact that S_{K+1} is actually fully symmetric with respect to the $K+1$ frequencies $\omega_1, \ldots, \omega_{K+1}$. Therefore the function Ψ_{K+1} must be a pure constant, independent on any ω_n. Furthermore, we know also that S_{K+1} is a homogeneous polynomial of degree $K-1$ in all the $\omega_1, \ldots, \omega_{K+1}$, so this constant must in fact be zero: $\Psi_{K+1}=0$. Finally we are able to conclude on the desired result,

$$S_{K+1}=K(\omega_1+\cdots+\omega_{K+1})^{K-1}. \tag{A37}$$

Incidentally, notice that the equality $\Psi_{K+1}=0$ is itself a consequence of the same mathematical formula, since it follows from setting $k=K+1$ and posing $\omega_{K+1}=0$ in (A31).

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Nonlinear spinor in a Kerr–Schild background

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We study the nonlinear spinor field in a Kerr–Schild background by first looking for solitonic solutions in the absence of rotation, given that in the special relativistic limit there are solitonic solutions in this approximation. Since for the scalar field problem at least two independent radial functions are needed for the solitonic solutions to exist, we introduce a dilation field by deforming the Kerr–Schild metric by a Weyl factor. We find that for the parameter space studied there are no solitonic solutions in the spherically symmetric approximation. While in the present work we have studied the spinor field, we also had in mind a corresponding study of a scalar field in the same background where it may be of interest for describing a rotating stellar soliton. The proposed strategy in both cases begins by looking for solitonic solutions in the absence of rotation and then continues by perturbatively correcting for the rotation required by the angular dependence of the Kerr background. The strategy appears to be unsuccessful. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1388031]

I. INTRODUCTION

Elementary particle solitons have been extensively investigated at the level of special relativity first in the context of Abelian theories and later in non-Abelian theories. In the Abelian case the solitons are stabilized by the conservation of physical charges and in the non-Abelian theories by topological constraints.

At the general relativistic level less is known. In particular the influence of the gravitational field on the known special relativistic structures has not been extensively studied. There have been, however, many studies of boson stars, which present a similar formal problem, but concern stellar structure rather than elementary particles.

At the level of particle physics, one has an eigenvalue problem that attempts to model the elementary particles similar to the way that the Schrödinger equation models atoms and nuclei. In the $1/N$ limit of standard theory Witten and collaborators have described a solitonic model of baryons.[1]

In examining string and supergravity theories from this viewpoint one finds two kinds of solitons. In the first class are the black-hole solitons which concentrate mass within a lump but are not true solitons since they carry central singularities and horizons. Typical of the second class are the topological solitons discovered by Strominger: these are five-branes immersed in a ten-dimensional space. Since they are singularity free they resemble solitons but are more precisely described as instantons, since their metric is Euclidean. Although nontopological solitons have not been found in these theories it is natural to ask if they exist in these or in other string or supergravity theories or in other completions of Einstein theory.

The present paper, a continuation of earlier exploratory studies along these lines,[2] promotes the nonlinear spinor soliton to the general relativistic level. The original nonlinear spinor field,[3]

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characterized by a free spinor Lagrangian plus a quartic spinor interaction, was motivated by the then recently discovered universal Fermi interaction, and the conjecture that solitonic solutions of this equation might model the elementary particles. A current scenario might describe quarks and leptons while the quartic interaction would have to be mediated by heavy bosons. In the earlier model it turned out that this equation admitted only a small number of solitonic solutions in a way depending on the value of the ''Fermi constant,'' which could be tuned to allow, for example, only three generations. Here we take the step of adding gravitational couplings to the original picture; and although the coupled spinor-gravitational field does not fall out of any of the currently favored fundamental theories, the solitons so defined should be of interest because of the fundamental character of both the spinor and gravitational fields.

The organization of the paper is as follows. In Sec. II the Lagrangian of the nonlinear spinor in a gravitational field is introduced. Sections III, IV, and V describe various basic aspects of the Kerr–Schild background including the effects of the Weyl rescaling of the metric with a dilation field. Sections VI–IX, introduce the spin connection, present the spinor field field equations, and display the contribution of the spinor to the energy momentum tensor. Section X discusses the full set of Einstein equations for a spinor in a Weyl rescaled Kerr–Schild background. Before attempting the solution of the full set of equations, we consider the special relativistic limit in Secs. XI and XII. Finally in Sec. XIII we present the results of the numerical treatment of the full set of equations. We end with a discussion of the results.

II. FORMULATION

We shall investigate solitons formed by the interaction of a nonlinear spinor field with the Einstein gravitational field. These two fields are to be codetermined by the following action:

$$S=\int d^4x\sqrt{-g}(R-KL), \tag{2.1}$$

where

$$L=g^{\mu\lambda}{:}\overline{\psi}\gamma_\mu\nabla_\lambda\psi{:}-V(I). \tag{2.2}$$

Here

$$\nabla_\lambda=\partial_\lambda+\Gamma_\lambda, \tag{2.3}$$

where Γ_λ is the spin connection satisfying

$$\partial_\lambda\gamma_\mu-\Gamma^\sigma_{\lambda\mu}\gamma_\sigma+(\gamma_\mu,\Gamma_\lambda)=0 \tag{2.4}$$

in terms of the Christoffel connection $\Gamma^\sigma_{\lambda\mu}$. The notation: requires that the enclosed expression be symmetrized and Hermitized. The interaction $V(I)$, which may be rather general, may be chosen to generalize the universal Fermi interaction. For simplicity, however, we choose I to be the scalar $\overline{\psi}\psi$.

Then the energy momentum tensor is

$$\theta_{\mu\lambda}=\frac{\partial L}{\partial g^{\mu\lambda}}-\frac{1}{2}Lg_{\mu\lambda} \tag{2.5}$$

and the gravitational equations of motion are

$$R_{\mu\lambda}=K\Theta_{\mu\lambda}, \quad K=-8\pi\frac{k}{c^2}, \tag{2.6}$$

where K is Newton's constant and

$$\Theta_{\mu\lambda} = \theta_{\mu\lambda} - \tfrac{1}{2}\theta g_{\mu\lambda}. \tag{2.7}$$

By (2.2) one finds

$$\Theta_{\mu\lambda} := \overline{\psi}\gamma_\mu \nabla_\lambda \psi : - \tfrac{1}{2} V(I) g_{\mu\lambda}. \tag{2.8}$$

In addition to the gravitational field equation (2.6) one has the following spinor field equation:

$$g^{\mu\lambda}\gamma_\mu \nabla_\lambda \psi - \frac{\partial V}{\partial \overline{\psi}} = 0. \tag{2.9}$$

The coupled equations (2.6) and (2.9) determine the structure of the soliton.

III. KERR–SCHILD METRIC

Solutions of the Dirac equation in the presence of an assigned time independent gravitational field have been discussed. These include solutions in a gravitational background produced by a rotating source such as a rotating star.[4–6] For a rotating source the full Kerr–Schild background metric is required.

Here the role of the rotating source is played by the spinor field itself, since it necessarily carries angular momentum. The present problem is more difficult, however, than the problem of a rotating star since the spinor and gravitational fields are here codetermined while in the example of the star the gravitational field is a given background. On the other hand we know from the special relativistic problem[3] that there are solitonic eigenfunctions of a spinor field in the background described by a spherical potential.

We shall therefore assume a spherically symmetric degenerate form of the Kerr–Schild gravitational field with the understanding that it may be necessary to add more structure in order to obtain a more refined solution.

IV. THE STATIC KERR–SCHILD METRIC

Let us describe a gravitational field defined by the following Kerr–Schild metric:

$$g_{\alpha\beta} = \eta_{\alpha\beta} - 2m \ell_\alpha \ell_\beta. \tag{4.1}$$

Here $\eta_{\alpha\beta}$ is Minkowskian with the signature $(1, -1, -1, -1)$ and ℓ_α is a null static field:

$$\ell^\alpha \ell_\alpha = 0, \tag{4.2}$$

$$\frac{\partial \ell_\alpha}{\partial t} = 0. \tag{4.3}$$

For this metric

$$\det g = \det \eta = -1. \tag{4.4}$$

Set

$$\ell^\alpha = \ell^0 (1, \vec{\lambda}). \tag{4.5}$$

Then

$$\lambda_k \lambda_k = 1. \tag{4.6}$$

In the general case

$$\partial_i \lambda_j = \alpha P_{ij} + \beta \Lambda_{ji}, \tag{4.7}$$

where

$$P_{ij} = \delta_{ij} - \lambda_i \lambda_j, \tag{4.8}$$

$$\Lambda_{ij} = \epsilon_{ijk} \lambda_k. \tag{4.9}$$

Both α and β are harmonic functions. The function α may be regarded as a Newtonian potential in the presence of rotation, while β is the specific angular momentum of the source. In both the rotating and nonrotating cases the λ_i describe the paths followed by infalling particles. The divergence and curl of $\vec{\lambda}$ are determined by α and β, respectively.

At this point we leave the general formulation and focus in the spherically symmetric case. In this context λ_i is given by

$$\lambda_i = \frac{x_i}{r}, \quad r^2 = x_i x_i. \tag{4.10}$$

Then

$$\partial_i \lambda_j = \frac{1}{r}(\delta_{ij} - \lambda_i \lambda_j) \tag{4.11}$$

and α is exactly the Newtonian potential while β vanishes. Then also

$$\partial_i \lambda_i = \frac{2}{r}, \tag{4.12}$$

$$\partial_i \lambda_j - \partial_j \lambda_i = 0, \tag{4.13}$$

$$\lambda^i \partial_i \lambda_j = \lambda^i \partial_j \lambda_i = 0. \tag{4.14}$$

In the Newtonian case α is also ℓ_0^2. It is useful to introduce two scalar fields, C and D, by

$$C \ell_\alpha = -\ell^\mu \partial_\mu \ell_\alpha \tag{4.15}$$

and

$$D = \partial_\mu \ell^\mu. \tag{4.16}$$

Then

$$C = \lambda_k \partial_k \ell_0 = \frac{d\ell_0}{dr} = \ell_0' \tag{4.17}$$

$$D = \ell_0' + \frac{2}{r} \ell_0. \tag{4.18}$$

The Christoffel connection is a quadratic form in m:

$$\Gamma^\mu_{\alpha\beta} = \overset{1}{\Gamma}{}^\mu_{\alpha\beta} + \overset{2}{\Gamma}{}^\mu_{\alpha\beta}, \tag{4.19}$$

where

$$\overset{1}{\Gamma}{}^{\mu}_{\alpha\beta}=\tfrac{1}{2}\,\eta^{\mu\tau}(\partial_{\alpha}h_{\beta\tau}+\partial_{\beta}h_{\alpha\tau}-\partial_{\tau}h_{\alpha\beta}) \tag{4.20}$$

and

$$\overset{2}{\Gamma}{}^{\mu}_{\alpha\beta}=-4m^{2}C\not{\ell}^{\mu}\not{\ell}_{\alpha}\not{\ell}_{\beta}. \tag{4.21}$$

Here

$$h_{\alpha\beta}=g_{\alpha\beta}-\eta_{\alpha\beta}=-2m\not{\ell}_{\alpha}\not{\ell}_{\beta}. \tag{4.22}$$

Also

$$\Gamma^{\mu}_{\mu\alpha}=0, \tag{4.23}$$

$$\not{\ell}_{\mu}\Gamma^{\mu}_{\alpha\beta}=-2C\not{\ell}_{\alpha}\not{\ell}_{\beta}, \tag{4.24}$$

$$\not{\ell}^{\alpha}\Gamma^{\mu}_{\alpha\beta}=2C\not{\ell}^{\mu}\not{\ell}_{\beta}. \tag{4.25}$$

The Ricci tensor is

$$R_{00}=(2m^{2}\varphi-m)\nabla^{2}\varphi, \tag{4.26}$$

$$R_{0k}=2m^{2}(\varphi\nabla^{2}\varphi)\lambda_{k}, \tag{4.27}$$

$$R_{jk}=\delta_{jk}\frac{2m}{r}\left(\varphi'+\frac{2\varphi}{r}\right)+\lambda_{j}\lambda_{k}\left[m\left(\varphi''-\frac{4\varphi}{r^{2}}\right)+2m^{2}\varphi\nabla^{2}\varphi\right]. \tag{4.28}$$

Here $\varphi=\not{\ell}_{0}^{2}$. The gravitational field described by the special assumptions that we have made is now defined completely by the function $\varphi(r)$ which is exactly the Newtonian potential if there is no rotation.

V. THE RESCALED KERR–SCHILD METRIC

Because of the back action of the spinor field acting through its energy momentum tensor it is necessary to introduce a second gravitational potential. To do this we rescale the Kerr–Schild metric by introducing the dilaton field, $\sigma(r)$, as follows:

$$\overline{g}_{\alpha\beta}=e^{2\sigma(r)}g_{\alpha\beta}. \tag{5.1}$$

The rescaled connection is now

$$\overline{\Gamma}^{\mu}_{\alpha\beta}=\Gamma^{\mu}_{\alpha}+\delta^{\mu}_{\alpha}\partial_{\beta}\sigma+\delta^{\mu}_{\beta}\partial_{\alpha}\sigma-g_{\alpha\beta}g^{\mu\tau}\partial_{\tau}\sigma \tag{5.2}$$

and the Ricci tensor then becomes

$$R_{\alpha\beta}=\overset{0}{R}_{\alpha\beta}-2\sigma_{\alpha\beta}-[\Delta_{2}\sigma+2\Delta_{1}\sigma]g_{\alpha\beta}, \tag{5.3}$$

$$\Delta_{1}\sigma=g^{\mu\lambda}\partial_{\mu}\sigma\partial_{\lambda}\sigma, \tag{5.4}$$

$$\Delta_{2}\sigma=g^{\mu\lambda}\sigma_{,\mu\lambda}, \tag{5.5}$$

$$\sigma_{\mu\lambda}=\sigma_{,\mu\lambda}-\sigma_{,\mu}\sigma_{,\lambda} \tag{5.6}$$

or

$$R_{\mu\lambda}=\overset{0}{R}_{\mu\lambda}-\Delta_{\mu\lambda} \tag{5.7}$$

where

$$\Delta_{\mu\lambda}=2\sigma_{\mu\lambda}+g_{\mu\lambda}\Delta_c \tag{5.8}$$

and

$$\overset{0}{R}_{\mu\lambda}=R_{\mu\lambda}\quad(\sigma=0). \tag{5.9}$$

One finds

$$\Delta_{00}=2m(1-2m\varphi)\varphi'\sigma'+(1-2m\varphi)\Delta_c, \tag{5.10}$$

$$\Delta_{0k}=\{-4m^2\varphi\varphi'\sigma'-2m\varphi\Delta_c\}\lambda_k, \tag{5.11}$$

$$\Delta_{jk}=\left[2(1-2m\varphi)\frac{\varphi'}{r}-\Delta_c\right]\delta_{jk} +2\left[\sigma''-\frac{\sigma'}{r}-(\sigma')^2-m\left(\varphi'-\frac{2}{r}\varphi\right)\sigma'-2m^2\varphi\sigma'\varphi'-2m\varphi\Delta_c\right]\lambda_j\lambda_k, \tag{5.12}$$

and

$$\Delta_c=\Delta_2\sigma+2\Delta_1\sigma, \tag{5.13}$$

$$\Delta_2\sigma=-\nabla^2\sigma+2m\varphi\sigma''+2m\left(\varphi'+\frac{2}{r}\varphi\right)\sigma', \tag{5.14}$$

$$\Delta_1\sigma=(2m\varphi-1)(\sigma')^2. \tag{5.15}$$

The gravitational field is now defined by the two scalar functions $\varphi(r)$ and $\sigma(r)$. The Ricci tensor becomes

$$R_{00}=(\hat{\varphi}-1)[\tfrac{1}{2}\nabla^2\hat{\varphi}+\hat{\varphi}'\sigma'+\Delta_c], \tag{5.16}$$

$$R_{0k}=\hat{\varphi}[\tfrac{1}{2}\nabla^2\hat{\varphi}+\hat{\varphi}'\sigma'+\Delta_c]\lambda_k, \tag{5.17}$$

$$R_{jk}=R^a\eta_{jk}+R^b\lambda_j\lambda_k, \tag{5.18}$$

where

$$R^a=-\frac{1}{r}\left(\hat{\varphi}'+\frac{2}{r}\hat{\varphi}\right)-2(1-\hat{\varphi})\frac{\sigma'}{r}-\Delta_c, \tag{5.19}$$

$$R^b=\frac{1}{2}\hat{\varphi}''-\frac{1}{r^2}\hat{\varphi}+\frac{1}{2}\hat{\varphi}\nabla^2_{\hat{\varphi}}-2\left[\sigma''-\frac{\sigma'}{r}-(\sigma')^2-\left(\frac{\hat{\varphi}'}{2}-\frac{1}{r}\hat{\varphi}\right)\sigma'-\frac{1}{2}\hat{\varphi}\hat{\varphi}'\sigma'-\hat{\varphi}\Delta_c\right], \tag{5.20}$$

$$\hat{\varphi}=2m\varphi, \tag{5.21}$$

$$\Delta_c = -\nabla^2\sigma + \hat{\varphi}\sigma'' + \left(\hat{\varphi}' + \frac{2}{r}\hat{\varphi}\right)\sigma' + 2(\hat{\varphi}-1)(\sigma')^2. \tag{5.22}$$

VI. THE SPIN CONNECTION

The Dirac matrices corresponding to the Kerr–Schild metric (before rescaling) may be chosen as follows:[5]

$$\gamma_\alpha = \eta_\alpha - \sqrt{2m}\,\ell_\alpha \eta_5, \tag{6.1}$$

where

$$(\eta_\alpha, \eta_\beta)_+ = 2\eta_{\alpha\beta}, \tag{6.2}$$

$$\eta_5 = \eta_0\eta_1\eta_2\eta_3. \tag{6.3}$$

A choice more useful for computing the spin connection is[7]

$$\gamma_\alpha = \eta_\alpha - m\ell_\alpha\hat{\tau}, \tag{6.4}$$

where

$$\hat{\tau} = \ell^\mu \eta_\mu \tag{6.5}$$

or

$$\gamma_\alpha = e^\mu_\alpha \eta_\mu \tag{6.6}$$

with

$$e^\mu_\alpha = \delta^\mu_\alpha - m\ell_\alpha\ell^\mu. \tag{6.7}$$

If $g_{\mu\lambda}$ is rescaled, then γ_μ must also be rescaled and

$$\overline{\gamma}_\mu = \overline{e}^{\lambda}_{\mu}\eta_\lambda, \tag{6.8}$$

where

$$\overline{e}^{\lambda}_{\mu} = e^{\sigma(r)}e^\lambda_\mu \tag{6.9}$$

while the new spin connection $\overline{\Gamma}_\lambda$ must satisfy

$$\partial_\lambda\overline{\gamma}_\mu - \overline{\Gamma}^\alpha_{\mu\lambda}\overline{\gamma}_\alpha + (\overline{\gamma}_\mu, \overline{\Gamma}_\lambda) = 0. \tag{6.10}$$

Here the Cristoffel connection $\overline{\Gamma}^\alpha_{\mu\lambda}$ is given by (5.2).

Let us set

$$\Gamma_\lambda = g_{\lambda\alpha\beta}(\eta^\alpha, \eta^\beta) = 2g_{\lambda[\alpha\beta]}\eta^\alpha\eta^\beta, \tag{6.11}$$

$$\overline{\Gamma}_\lambda = \overline{g}_{\lambda\alpha\beta}(\overline{\eta}^\alpha, \overline{\eta}^\beta) = 2\overline{g}_{\lambda[\alpha\beta]}\overline{\eta}^\alpha\overline{\eta}^\beta. \tag{6.12}$$

Then (6.10) leads to the following relations:

$$-8\overline{g}_{\lambda[\beta\rho]} = (e^{-1})^\mu_\beta\overline{\Gamma}^\alpha_{\mu\lambda}e_{\alpha\rho} + (e^{-1})^\mu_\beta\partial_\lambda e_{\mu\rho} + \eta_{\rho\beta}\partial_\lambda\sigma. \tag{6.13}$$

Since the second and third terms are symmetric in β and ρ, they will cancel when multiplied by the commutator in (6.12) and therefore may be dropped. Then

$$-8\overline{g}_{\lambda[\beta\rho]}=(e^{-1})^{\mu}_{\beta}\overline{\Gamma}^{\alpha}_{\mu\lambda}e_{\alpha\rho}. \tag{6.14}$$

Set

$$\overline{\Gamma}^{\mu}_{\alpha\lambda}=\Gamma^{\mu}_{\alpha\lambda}+\Delta^{\mu}_{\alpha\lambda}, \tag{6.15}$$

$$\overline{g}_{\lambda[\beta\rho]}=g_{\lambda[\beta\rho]}+E_{\lambda[\beta\rho]}. \tag{6.16}$$

Then

$$-4E_{\lambda\beta\rho}=(e^{-1})^{\mu}_{\beta}\Delta^{\alpha}_{\mu\lambda}e_{\alpha\rho}+\eta_{\beta\rho}\partial_{\lambda}\sigma, \tag{6.17}$$

where

$$\Delta^{0}_{\mu\lambda}=\delta^{\alpha}_{\mu}\partial_{\lambda}\sigma+\delta^{\alpha}_{\lambda}\partial_{\mu}\sigma-g_{\mu\lambda}g^{\alpha\tau}\partial_{\tau}\sigma. \tag{6.18}$$

Since $E_{\lambda\beta\rho}$ is antisymmetric in β and ρ, we may drop the second term in (6.17). Reduction of (6.14) and (6.17) gives

$$g^{\alpha\beta}_{\mu}=-\frac{m}{4}\partial^{\alpha}(\not{\ell}_{\mu}\not{\ell}^{\beta}), \tag{6.19}$$

$$E^{\alpha\beta}_{\mu}=\tfrac{1}{4}[e^{\alpha}_{\mu}\partial^{\beta}\sigma-(\not{\ell}^{\mu}\partial_{\mu}\sigma)\not{\ell}^{\alpha}\delta^{\beta}_{\mu}], \tag{6.20}$$

$$\overline{\Gamma}_{\mu}=\tfrac{1}{4}[-m\partial^{\alpha}(\not{\ell}_{\mu}\not{\ell}^{\beta})+e^{\alpha}_{\mu}\partial^{\beta}\sigma-m\not{\ell}^{\alpha}\delta^{\beta}_{\mu}\nabla\sigma](\gamma_{\alpha},\gamma_{\beta}), \tag{6.21}$$

where

$$\nabla\sigma=\not{\ell}^{\alpha}\partial_{\alpha}\sigma. \tag{6.22}$$

VII. THE SPINOR FIELD EQUATIONS

In the rescaled Kerr–Schild metric Eq. (2.12) becomes

$$\overline{\gamma}^{\mu}(\partial_{\mu}+\overline{\Gamma}_{\mu})\psi-\frac{\partial V}{\partial\overline{\psi}}=0, \tag{7.1}$$

where $\overline{\Gamma}_{\mu}$ is the spin connection and $\partial V/\partial\psi$ represents all the nonlinear interactions. We shall assume a four-component spinor and adopt the following ansatz:

$$\psi=Z\Omega+W\beta\Omega \tag{7.2}$$

with

$$\Omega=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\\lambda_3\\\lambda_+\end{pmatrix},\quad \beta=\begin{pmatrix}I&0\\0&-I\end{pmatrix}, \tag{7.3}$$

when $\vec{\lambda}$ is the three-vector defined by (4.5) and $\lambda_+=\lambda_1+i\lambda_2$. If Z and W are complex conjugates so that

$$Z-\tfrac{1}{2}(F+iG),$$
$$W=\tfrac{1}{2}(F-iG), \tag{7.4}$$

then

$$\psi=\frac{1}{\sqrt{2}}e^{i\omega t}\begin{pmatrix} F \\ 0 \\ i\,G\lambda_3 \\ i\,G\lambda_+ \end{pmatrix}=\frac{1}{\sqrt{2}}e^{i\omega t}\begin{pmatrix} F \\ 0 \\ i\,G\cos\theta \\ i\,G\sin\theta e^{i\phi} \end{pmatrix}. \tag{7.5}$$

If the ambient space is flat and ψ is described by (7.5) then ψ is also an eigenfunction of the Dirac angular momentum with spin 1/2. Therefore in the limit of weak gravitational field we may require that ψ approach (7.5).[3]

By (6.5)

$$\hat{\tau}\Omega=0,$$
$$\hat{\tau}\beta\Omega=2\not{\ell}_0\Omega. \tag{7.6}$$

Define

$$\tau=\eta_k\lambda_k=-\eta^k\lambda_k, \tag{7.7}$$

then

$$\tau\Omega=\beta\Omega,$$
$$\tau\beta\Omega=-\Omega \tag{7.8}$$

also

$$\hat{\tau}^2=0, \quad \tau^2=-1, \tag{7.9}$$

$$\frac{d\tau}{dr}=0. \tag{7.10}$$

The following identity is also useful:

$$\eta_s\partial_s=\tau\left(\frac{d}{dr}+\frac{1}{r}\right)-\frac{1}{r}\tau\beta k, \tag{7.11}$$

where

$$k=\beta(\vec{\Sigma}\vec{L}+1), \quad \vec{L}=\vec{r}\times\vec{p}. \tag{7.12}$$

Here

$$\vec{\Sigma}=\begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}. \tag{7.13}$$

Note also

$$k\beta=\beta k, \tag{7.14}$$
$$k\Omega=\Omega. \tag{7.15}$$

To reduce (7.1) let us next compute

$$\gamma^\mu \partial_\mu \psi = \eta^\mu \partial_\mu \psi + m \hat{\tau}^{\not\mu} \partial_\mu \psi. \tag{7.16}$$

By (7.2) and (7.11) we find

$$\overline{\gamma}^\mu \partial_\mu \psi = e^\sigma \left[(1-2m\varphi) W' + i\omega(1+2m\varphi) W + (W-Z)\frac{1}{r} \right] \Omega$$
$$- e^\sigma \left[Z' - i\omega Z + (Z-W)\left(\frac{1}{r}\right) \right] \beta\Omega. \tag{7.17}$$

By (6.8) and (6.21) the spin connection gives the contribution

$$\overline{\gamma}^\mu \overline{\Gamma}_\mu \psi = (W f_2 \Omega + Z f_1 \beta\Omega) e^\sigma, \tag{7.18}$$

where

$$f_1 = \tfrac{3}{2}\sigma', \tag{7.19}$$

$$f_2 = 3m\sigma'\varphi - \frac{3}{2}\sigma' - m\left(\varphi' + \frac{2}{r}\varphi \right). \tag{7.20}$$

Let us choose the invariant nonlinear interaction to be a functional of

$$I = \tilde{\psi}\psi$$
$$= \overline{S}W + Z\overline{W}. \tag{7.21}$$

Then the nonlinear term in the equation of motion is

$$\frac{\partial V}{\partial \overline{\psi}} = \frac{dV}{dI}\frac{\partial I}{\partial \overline{\psi}} \tag{7.22}$$

$$= V' \psi. \tag{7.23}$$

For definiteness we take

$$V(I) = m_0 I + \frac{g}{2} I^2, \quad m_0 > 0, \ g < 0. \tag{7.24}$$

Then

$$\frac{\partial V}{\partial \overline{\psi}} = (m_0 + gI)\psi = [m_0 Z + g(\overline{Z}W + \overline{W}Z)Z]\Omega + [m_0 W + g(\overline{Z}W + \overline{W}Z)W]\beta\Omega \tag{7.25}$$

and the differential equation (7.1) becomes by (7.17) and (7.18)

$$\mathcal{Z}\Omega + \mathcal{W}(\beta\Omega) = 0, \tag{7.26}$$

where

$$\mathcal{Z}=(1-2m\varphi)W'+(W-Z)\frac{1}{r}+[i\omega(1+2m\varphi)+f_2]W-e^{-\sigma}[m_0+g(\bar{Z}W+\bar{W}Z)]Z \tag{7.27}$$

and

$$\mathcal{W}=-Z'+(i\omega+f_1)Z-(Z-W)\frac{1}{r}-e^{-\sigma}[m_0+g(\bar{Z}W+\bar{W}Z)]W. \tag{7.28}$$

The spinors Ω and $\beta\Omega$ are orthogonal:

$$\Omega^{+}(\beta\eta)=0. \tag{7.29}$$

Then by (7.26)

$$\mathcal{Z}=\mathcal{W}=0. \tag{7.30}$$

By (7.27) and (7.28) one sees that (7.30) implies two complex differential equations for z and w or four real equations for real components (Z_1,Z_2,W_1,W_2).

VIII. THE SOURCE OF THE GRAVITATIONAL FIELD

The source of the gravitational field, the energy-momentum tensor of the spinor field, is described by (2.8).

Let us consider

$$:\bar{\psi}\bar{\gamma}_\alpha\bar{\nabla}_\beta\psi: \tag{8.1}$$

where $\bar{\psi}$ is the usual Dirac adjoint and where

$$\nabla_\beta=\partial_\beta+\bar{\Gamma}_\beta. \tag{8.2}$$

Here $\bar{\Gamma}_\beta$ is the spin connection given by (6.21).

Let us decompose the bilinear part of the energy-momentum tensor as follows:

$$\overset{0}{\Theta}_{\alpha\beta}=:\bar{\psi}\bar{\gamma}_\alpha\partial_\beta\psi:, \tag{8.3}$$

$$\overset{1}{\Theta}_{\alpha\beta}=:\bar{\psi}\bar{\gamma}_\alpha\bar{\Gamma}_\beta\psi: \tag{8.4}$$

where ψ is given by (7.2).

It turns out that all the matrix elements of (8.3) and (8.4) are expressible in terms of λ_k and μ_k given by

$$\lambda_k=\Omega^{\dagger}\eta_k\beta\Omega \tag{8.5}$$

and

$$\mu_k=\Omega^{\dagger}\eta_k\Omega. \tag{8.6}$$

Here λ_k is the three-vector defined by (4.5) and alternatively expressed as

$$\lambda_k=(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta) \tag{8.7}$$

while $\vec{\mu}$ is an imaginary vector orthogonal to $\vec{\lambda}$ and given by

$$\mu_k = i\epsilon_{ks3}\lambda_s . \tag{8.8}$$

One finds that the gravitational equations are of the form

$$A\lambda_k + B\mu_k = 0 \tag{8.9}$$

and since $\vec{\lambda}$ and $\vec{\mu}$ are orthogonal

$$A = B = 0. \tag{8.10}$$

The corresponding gravitational equations then reduce to

$$B = \overline{W}Z - \overline{Z}W = 0 \tag{8.11}$$

becomes a constraint on the components of the spinor ψ.

Equation (8.11) implies

$$W = uZ, \tag{8.12}$$

where u is a real function. One finds for the complete energy-momentum tensor:

$$\Theta_{\alpha\beta} = \overset{0}{\Theta}_{\alpha\beta} + \overset{1}{\Theta}_{\alpha\beta} - \tfrac{1}{2}Vg_{\alpha\beta}, \tag{8.13}$$

$$\Theta_{00} = \frac{e^{\sigma}}{2}\left\{\left[\left(1 - \frac{3\hat{\varphi}}{2} + \varphi^2\right)\sigma' + \frac{(\hat{\varphi}-1)}{2}\,\frac{\hat{\varphi}'}{2}\right]\Delta + \left[\left(\frac{\hat{\varphi}}{2} - \frac{\hat{\sigma}^2}{2}\right)\sigma' - \frac{\hat{\varphi}\hat{\varphi}'}{4}\right]\Sigma\right\} - \frac{1}{2}(1-\hat{\varphi})e^{2\sigma}V, \tag{8.14}$$

$$\begin{aligned}\Theta_{0j} = \Bigg[\Bigg\{\Bigg[\frac{1}{2}\left(1 - \frac{\hat{\varphi}}{2}\right)\Sigma' + \frac{\hat{\varphi}}{2}\Delta'\Bigg] + \frac{\Delta}{4}\left[\frac{\hat{\varphi}'}{2}(\hat{\varphi}-1) + \sigma'\left(-3\,\frac{\hat{\varphi}}{2} + \hat{\varphi}^2\right)\right] \\ + \frac{\Sigma}{4}\left[-\frac{\hat{\varphi}'}{2}(\hat{\varphi}'+1) + \sigma'\left(1 - \frac{\hat{\varphi}}{2} - \hat{\varphi}^2\right)\right]\Bigg\}e^{\sigma} + \frac{1}{2}\,\hat{\varphi}Ve^{2\sigma}\Bigg]\lambda_j\end{aligned} \tag{8.15}$$

after having dropped the μ_j term

$$\begin{aligned}\Theta_{jk} = \Bigg[\Bigg\{\Bigg[\left(\frac{\hat{\varphi}}{2} - 1\right)\sigma' + \frac{1}{r}\,\frac{\hat{\varphi}}{2} - \frac{2}{r}\Bigg]\frac{\Delta}{2} + \left[\frac{\hat{\varphi}}{2}\sigma' + \frac{1}{r}\,\frac{\hat{\varphi}}{2}\right]\frac{\Sigma}{2}\Bigg\}e^{\sigma} - \frac{1}{2}Ve^{2\sigma}\Bigg]\eta_{jk} \\ + \Bigg[\Bigg\{\Bigg[-\frac{\hat{\varphi}}{2}\Sigma' + \left(1 + \frac{\hat{\varphi}}{2}\right)\Delta'\Bigg] + \left[\frac{\hat{\varphi}}{2r} - \frac{2}{r} + \frac{\hat{\varphi}\hat{\varphi}'}{4} + \left(-1 + \frac{\hat{\varphi}}{2} + \hat{\varphi}^2\right)\sigma'\right]\frac{\Delta}{2} \\ + \left[\frac{\hat{\varphi}}{2r} - \left(1 + \frac{\hat{\varphi}}{2}\right)\frac{\hat{\varphi}'}{2} - \left(\frac{\hat{\varphi}}{2} + \hat{\varphi}^2\right)\sigma'\right]\frac{\Sigma}{2}\Bigg\}e^{\sigma} + \frac{1}{2}\,\hat{\varphi}Ve^{2\sigma}\Bigg]\lambda_j\lambda_k .\end{aligned} \tag{8.16}$$

Here

$$\begin{aligned}\Sigma &= \overline{\psi}\eta_0\psi = |Z|^2 + |W|^2, \\ \Delta &= |Z|^2 - |W|^2.\end{aligned} \tag{8.17}$$

Let us also write

$$\Theta_{jk} = \Theta^a\eta_{jk} + \Theta^b\lambda_j\lambda_k .$$

IX. REDUCTION OF THE SPINOR EQUATION

Because of the constraint (8.12) ($W=uZ$) it is now possible to show that one may reduce the equations (7.30) from a system of four real equations with four real functions to two real equations with two real functions.

Set

$$\alpha=1-2m\varphi,$$
$$\beta=1+2m\varphi. \tag{9.1}$$

Then

$$\mathcal{Z}=\alpha W'+\frac{1}{r}(W-Z)+[i\beta\omega+f_2]W-e^{-\sigma}[m_0+g(\overline{Z}W+\overline{W}Z)]Z=0, \tag{9.2}$$

$$\mathcal{W}=Z'-(i\omega+f_1)Z-\frac{1}{r}(W-Z)+e^{-\sigma}[m_0+g(\overline{Z}W+\overline{W}Z)]W=0. \tag{9.3}$$

Equation (9.2) and (9.3) may be combined by eliminating Z'/Z. Then

$$\alpha u'+[\alpha u^2+(1-\alpha)u-1]\frac{1}{r}+i\omega(\alpha+1)u+(f_2+\alpha f_1)u$$
$$-e^{-\sigma}[m_0+g(\overline{Z}W+\overline{W}Z)](1+\alpha u^2)=0. \tag{9.4}$$

Since all terms in this equation are real except $2i\omega(\alpha+1)u$, it follows that $\omega=0$.

It then follows from (8.12) and (9.3) that Z'/Z is also real or that the argument of Z is constant and may be equated to zero. Then Z may be taken real, and we may therefore take both W and Z real in (9.2) and (9.3).

$$\alpha W'+(W-Z)\frac{1}{r}+f_2W-e^{-\sigma}[m_0+2gWZ]Z=0, \tag{9.5}$$

$$Z'-f_1Z-(W-Z)\frac{1}{r}+e^{-\sigma}[m_0+2gWZ]W=0. \tag{9.6}$$

X. GRAVITATIONAL FIELD EQUATIONS

The gravitational equations (2.6) may be reduced to the following four equations:

$$(1-\hat{\varphi})[-\tfrac{1}{2}\nabla^2\hat{\varphi}-\hat{\varphi}'\sigma'-\Delta_c]=K\Theta_{00}, \tag{10.1}$$

$$\hat{\varphi}\left[\frac{1}{2}\nabla^2\hat{\varphi}+\hat{\varphi}'\sigma'+\Delta_c\right]\lambda_k=K\Theta_{0k}, \tag{10.2}$$

$$\left[\frac{1}{r}\left(\hat{\varphi}'+\frac{2\hat{\varphi}}{r}\right)-2(1-\hat{\varphi})\frac{\sigma'}{r}+\Delta_c\right]=-K\Theta^a, \tag{10.3}$$

$$\frac{\hat{\varphi}''}{2}-\frac{2\hat{\varphi}}{r^2}+\frac{1}{2}\hat{\varphi}\nabla^2\hat{\varphi}-2\left[\sigma''-\frac{\sigma'}{r}-(\sigma')^2-\left(\frac{\hat{\varphi}'}{2}-\frac{1}{r}\hat{\varphi}\right)\sigma'-\frac{1}{2}\hat{\varphi}\hat{\varphi}'\sigma'-\hat{\varphi}\Delta_c\right]=K\Theta^b, \tag{10.4}$$

where $\hat{\varphi}=2m\varphi$,

$$\Theta_{jk}=\Theta^{a}\eta_{jk}+\Theta^{b}\lambda_{j}\lambda_{k}. \tag{10.5}$$

Δ_c is given by (5.13), Θ by (8.14)–(8.16). By (10.1) and (10.2)

$$\hat{\varphi}\Theta_{00}+(\Theta_{0k}\lambda_{k})(1-\hat{\varphi})=0. \tag{10.6}$$

To study these equations near the origin impose solitonic boundary conditions requiring that all fields be finite with flat tangents at the origin. Then

$$\hat{\varphi}'(0)=\sigma'(0)=Z'(0)=W'(0)=0, \tag{10.7}$$

$$\Delta_c(0)=[-\nabla^2\sigma+\hat{\varphi}\sigma'']_{r=0}. \tag{10.8}$$

From (8.17)

$$\Delta(0)=0, \quad \Sigma(0)=2Z^2. \tag{10.9}$$

By (8.14)–(8.17)

$$[\Theta_{00}]_{r=0}=\frac{e^{2\sigma}}{2}[\hat{\varphi}(0)-1]V[I(0)], \tag{10.10}$$

$$[\Theta_{0k}]_{r=0}=\frac{e^{2\sigma}}{2}V[I(0)]\hat{\varphi}(0)\lambda_{k}, \tag{10.11}$$

$$[\Theta^{a}_{jk}]_{r=0}=\left[\frac{\Sigma}{4}\left(\frac{\hat{\varphi}}{r}\right)e^{\sigma}-\frac{e^{2\sigma}}{2}V\right]_{r=0}\eta_{jk}, \tag{10.12}$$

$$[\Theta^{b}_{jk}]_{r=0}=\left[\frac{\Sigma}{4}\left(\frac{\hat{\varphi}}{r}\right)e^{\sigma}+\hat{\varphi}e^{2\sigma}\frac{V}{2}\right]_{r=0}\lambda_{j}\lambda_{k}. \tag{10.13}$$

By (10.3)

$$\lim_{r\to 0}\left\{2\hat{\varphi}(r)-2r^2\left[(1-\hat{\varphi}(r))\frac{\sigma'(r)}{r}-\frac{\hat{\varphi}}{2}\sigma''+\frac{\nabla^2\sigma}{2}\right]\right\}=\lim_{r\to 0}\frac{K}{2}r^2\left(\hat{\varphi}\frac{\Sigma}{r}-e^{2\sigma}V\right). \tag{10.14}$$

Therefore

$$\hat{\varphi}(0)=0. \tag{10.15}$$

The vanishing of $\hat{\varphi}(r)$ at the origin now implies the additional reduction of (10.1)

$$-\frac{1}{2}\hat{\varphi}''(0)+\sigma''(0)=-\frac{K}{2}e^{2\sigma(0)}V[I(0)]. \tag{10.1$'$}$$

XI. THE SPECIAL RELATIVISTIC EIGENVALUE PROBLEM

In a previous study of a nonlinear scalar field coupled to the gravitational field it was found that the eigensolutions of the complete set of differential equations is critically dependent on the behavior of the nonlinear component alone. By following the earlier argument we shall now find, however, that the pattern for the nonlinear spinor problem is quite different.

As before, we begin by associating an approximately conserved function with the nonlinear equations after they have been decoupled from the gravitational field. In this special relativistic limit where $(m=0,\ \sigma=0)$ we have $f_1=f_2=0$. After deletion of the mass and nonlinear coupling the two equations (9.5) and (9.6) become

$$W'-\frac{dV}{dI}Z+\frac{W-Z}{r}=0, \tag{11.1}$$

$$Z'+\frac{dV}{dI}W-\frac{W-Z}{r}=0. \tag{11.2}$$

We consider the auxiliary equations obtained by deleting the explicit dependence on r,

$$W'-\mathcal{V}Z=0, \tag{11.3}$$

$$Z'+\mathcal{V}W=0, \tag{11.4}$$

where

$$\mathcal{V}=\frac{dV}{dI}. \tag{11.5}$$

Any invariant function $(\mathcal{F})$ associated with these equations satisfies

$$\mathcal{F}'=\frac{\partial\mathcal{F}}{\partial W}W'+\frac{\partial\mathcal{F}}{\partial Z}Z'=0 \tag{11.6}$$

or

$$\mathcal{F}'=\mathcal{V}\left(W\frac{\partial}{\partial Z}-Z\frac{\partial}{\partial Z}\right)\mathcal{F}=0. \tag{11.7}$$

Hence if F is a functional of W^2+Z^2, it will be conserved for any solution of the set (11.3), (11.4).

For the complete equations (11.1) and (11.2) however, we have

$$\mathcal{F}'=\frac{\partial\mathcal{F}}{\partial W}\left(\mathcal{V}Z+\frac{Z-W}{r}\right)+\frac{\partial\mathcal{F}}{\partial Z}\left(-\mathcal{V}W-\frac{Z-W}{r}\right)=\left(\frac{\partial\mathcal{F}}{\partial W}-\frac{\partial\mathcal{F}}{\partial Z}\right)\frac{Z-W}{r} \tag{11.8}$$

$$=2(W-Z)\frac{\partial\mathcal{F}}{\partial\Sigma}\left(\frac{Z-W}{r}\right). \tag{11.9}$$

Then

$$\mathcal{F}'=-2\frac{\partial\mathcal{F}}{\partial\Sigma}(W-Z)^2. \tag{11.10}$$

In the simplest case

$$\mathcal{F}(\Sigma)=\Sigma. \tag{11.11}$$

Then

$$\mathcal{F}'=-\frac{2(W-Z)^2}{r}\leqslant 0. \tag{11.12}$$

According to (11.3) and (11.4) the representative point moves in the circle ($\Sigma = \text{const}$) in the $W-Z$ plane. According to (11.1) and (11.2) the motion of this point deviates from the circle to satisfy (11.12), which directs the motion always toward lower values of F, i.e., toward the origin. The representative point will therefore spiral into the origin.

If the corresponding curve in configuration space represents an eigensolution it must satisfy the following boundary conditions at the origin and at ∞:

At $r=0$,

$$W' = Z' = 0 \tag{11.13}$$

and at $r=\infty$,

$$W' = Z' = W = Z = 0. \tag{11.14}$$

To satisfy these boundary conditions on Eqs. (11.1) and (11.2) the eigensolution must begin at a point on the line $W=Z$ and it must end at the origin.

For the particular choice of (2.9) we have

$$I = 2ZW. \tag{11.15}$$

The $\mathcal{V}$ is constant on the hyperbolas

$$WZ = \text{constant} \tag{11.16}$$

and along the asymptote $\mathcal{V}$ is a function of Z^2.

In an earlier discussion of the special relativistic limit the Dirac spinor was taken to be (7.5). As long as there is no gravitational coupling there is no problem with this ansatz, and if one chooses V to be given by (7.25) one finds according to Eqs. (16a), (16b) of Ref. 3

$$F' + \mu G + 2\gamma(G^2 - F^2)G = 0, \tag{11.17}$$

$$G' + \mu F + \frac{2}{r}G + 2\gamma(G^2 - F^2)F = 0, \tag{11.18}$$

where we also set $\omega = 0$ and μ and γ are the. Here F and G are the large and small components of ψ as given by (7.5). The dissipative function $\bar{H}$ associated with these equations is

$$\bar{H} = \mu(G^2 - F^2) + \gamma(G^2 - F^2)^2 \tag{11.19}$$

leading to a phase portrait with two attractions.

To compare (11.18) and (11.19) with the present equations (11.1) and (11.2) set

$$f = W + Z, \tag{11.20}$$

$$g = W - Z. \tag{11.21}$$

Then (11.1) and (11.2) become

$$f' + \mathcal{V}g = 0, \tag{11.22}$$

$$g' - \mathcal{V}f + \frac{2g}{r} = 0, \tag{11.23}$$

where

$$\mathcal{V} = m_0 + \gamma I \tag{11.24}$$

and

$$I=2WZ+\tfrac{1}{2}(f^2-g^2). \tag{11.25}$$

Then

$$f'+m_0g+\frac{\gamma}{2}(f^2-g^2)g=0, \tag{11.26}$$

$$g'-m_0f+\frac{2g}{2}-\frac{\gamma}{2}(f^2-g^2)f=0. \tag{11.27}$$

Here f and g are large and small components in (11.26) and (11.27) just as F and G are large and small components in (11.17) and (11.18).

There is a term by term correspondence between the pair (11.26), (11.27) and the pair (11.17), (11.18) except for signs. The difference in signs, however, gives rise to a completely different phase portrait for the dissipative function in the two cases. In particular, there is only one attractor associated with (11.26) and (11.27) while there are two attractors in the other case.

The distinction between the two cases may be pushed a little further as follows.

The dissipative function for the (f, g) pair may be chosen as a function of (f^2+g^2) since

$$\frac{d}{dr}(f^2+g^2)=-\frac{4g^2}{r}\leqslant 0 \tag{11.28}$$

by (11.26) and (11.27). The corresponding argument for the (F, G) pair yields

$$\frac{d}{dr}(F^2-G^2)=-\frac{4G^2}{r}\leqslant 0. \tag{11.29}$$

Therefore one may choose a function of f^2+g^2 in one case and of F^2-G^2 in the other to qualify as a dissipative function. In the (F, G) case we chose the dissipative function to be the Hamiltonian of the associated mechanical problem (with the explicit r term deleted), i.e., the Hamiltonian equations corresponding to the Hamiltonian (11.19) are the differential equations (11.17) and (11.18) where G plays the role of the momentum. The corresponding step with the (f, g) pair is not possible because (11.26) and (11.27) are not derivable from a Hamiltonian as one may see as follows.

If a Hamiltonian did exist for this set then we would have

$$\begin{aligned}\frac{\partial^2 H}{\partial q\,\partial p}&=\frac{\partial \dot{q}}{\partial q}(q,p),\\ \frac{\partial^2 H}{\partial p\,\partial q}&=-\frac{\partial \dot{p}}{\partial p}(q,p),\end{aligned} \tag{11.30}$$

or

$$\frac{\partial \dot{q}(p,q)}{\partial q}=-\frac{\partial \dot{q}(q,p)}{\partial p}. \tag{11.31}$$

Since f and g play the roles of the generalized coordinate and momentum, respectively, and since r plays the role of the time, the condition (11.31) reads for the pair (f, g),

$$\frac{\partial f'(f,g)}{\partial f}=-\frac{\partial g'(f,g)}{\partial g}. \tag{11.32}$$

Since this relation is not satisfied for Eqs. (11.26) and (11.27), there is no corresponding Hamiltonian.

Additionally one cannot retain the (F,G) description with (8.11) since the pair (8.11), (7.4), implies

$$Z^2 = W^2 \tag{11.33}$$

and therefore either $F=0$ or $G=0$.

XII. BEHAVIOR AT LARGE r

At large r we require that all functions and their first and second derivatives vanish. We also drop all terms in $\Theta_{\mu\nu}$ of order $1/r$. Then by (10.1)–(10.4) in the limit

$$\Theta_{\mu\nu} = 0 \tag{12.1}$$

and by (8.15)–(8.17)

$$V(I) = 0. \tag{12.2}$$

By (7.25) and the preceding equation

$$I = 0, \quad \frac{2\mu}{\gamma}. \tag{12.3}$$

Let us choose $I=0$. Then

$$\lim_{r\to 0}(f^2 - g^2) = 0 \tag{12.4}$$

by (11.26).

In the limit (11.27) and (11.28) become

$$f' + \mu g = 0, \tag{12.5}$$

$$g' - \mu f + \frac{2g}{r} = 0, \tag{12.6}$$

or

$$g'' + \frac{2}{r}g' + \mu^2 g - \frac{2}{r^2}g = 0. \tag{12.7}$$

f and g are of opposite parity and since $f(0)\neq 0$ we take f even. Then to order $1/r$,

$$f = \frac{\sin \mu\nu}{r} \tag{12.8}$$

and

$$g = \frac{\cos \mu\nu}{r}. \tag{12.9}$$

In contrast to this behavior the (F,G) pair approach zero as $e^{\mu\nu}/r$.

XIII. SOLUTIONS OF THE GRAVITATIONAL FIELD EQUATIONS

First we consider the solutions to the gravitational field equations (10.1)–(10.5) when the matter fields are set to zero.

Equation (10.1) gives

$$\hat{\varphi}''-(1-2\hat{\varphi})\sigma''=-\frac{2}{r}\hat{\varphi}'-4\sigma'\hat{\varphi}'+\frac{2}{r}(1-2\hat{\varphi})\sigma'+2(1-2\hat{\varphi})(\sigma')^2. \tag{13.1}$$

Multiplying (10.5) by $\lambda^j\lambda^k$ and contracting we obtain

$$(1+2\hat{\varphi})\hat{\varphi}''-(3-4\hat{\varphi}^2)\sigma''=-\frac{2}{r}(1+2\hat{\varphi})\hat{\varphi}'-(4+8\hat{\varphi})\sigma'\hat{\varphi}'+\frac{1}{r}(2-8\hat{\varphi}^2)\sigma'-8\hat{\varphi}^2(\sigma')^2. \tag{13.2}$$

The preceding two equations can be combined to solve for $\hat{\varphi}''$ and σ'':

$$\sigma''=(\sigma')^2 \tag{13.3}$$

and

$$\hat{\varphi}''=-\frac{2}{r}\hat{\varphi}'-4\sigma'\hat{\varphi}'+\frac{2}{r}(1-2\hat{\varphi})\sigma'+3(1-2\hat{\varphi})(\sigma')^2. \tag{13.4}$$

Equation (13.3) gives a solution of the form

$$\sigma\sim-\log(r), \tag{13.5}$$

which when substituted into (13.4) leads to

$$\hat{\varphi}\sim\pm r^2. \tag{13.6}$$

It is apparent that the coupling of the dilaton field with the Kerr–Schild scalar does not give a finite theory. We have proceeded to study the full set of equations (10.1)–(10.5), including the matter fields, in order to find out if these fields provide the necessary attractive properties to yield finite soliton type solutions.

Once again we selected Eq. (10.1) and the contraction of Eq. (10.5) with $\lambda^j\lambda^k$,

$$\sigma''=(\sigma')^2-K\frac{e^{\sigma}}{4}\left[4Z'Z-4W'W(1+2\hat{\varphi})+Z^2\left(\sigma'-4\frac{\hat{\varphi}'\hat{\varphi}}{(1-2\hat{\varphi})}\right)+W^2\sigma'(1-2\hat{\varphi})\right], \tag{13.7}$$

$$\hat{\varphi}''=-\frac{2}{r}\hat{\varphi}'-4\sigma'\hat{\varphi}'+\frac{2}{r}(1-2\hat{\varphi})\sigma'+3(1-2\hat{\varphi})(\sigma')^2-K\frac{e^{\sigma}}{4}\left[Z^2\left[(3-2\hat{\varphi})\sigma'-4\frac{(1-\hat{\varphi})}{(1-2\hat{\varphi})}\hat{\varphi}'\right]\right.$$
$$\left.+W^2[(4\hat{\varphi}^2-1)\sigma'+2\hat{\varphi}']+2Z'Z(1-2\hat{\varphi})+2W'W(4\hat{\varphi}^2-1)-2e^{\sigma}V\right]. \tag{13.8}$$

To look for numerical solutions it is necessary to recast Eqs. (9.6), (9.7), (13.7), and (13.8) in dimensionless form. This was accomplished by introducing a fundamental length r_0 to rescale the variable r and a fundamental field strength ψ_0 to rescale the fermionic fields. The equations of interest depend on three parameters: $\beta=m_0r_0^2$, $\gamma=gr_0^2\psi_0^2/2$ and $\delta=K\psi_0^2$. To validate the numerical analysis we used two different methods: the MATLAB differential equation suite[8] and the subroutine SDRIV2 from the SLATE package.[9]

We explored a large portion of the three-dimensional parameter space looking for finite solutions for the fields σ, $\hat{\varphi}$, W, and Z. By systematically exploring the three-dimensional parameter

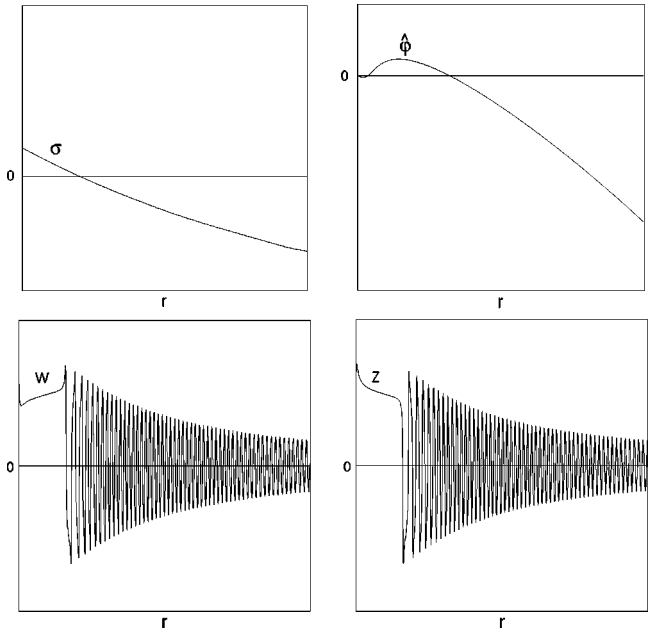

FIG. 1. Type A solution with nonsingular fields at finite r. The parameter values are: $\beta=0.044$, $\gamma=14.257$, and $\delta=-0.001$ (*since* K is negative).

space two types of solutions were encountered. The solutions of type A are shown in Fig. 1. While the fermion fields settle into the damped oscillations which characterize the special relativistic solutions, the fields σ and $\hat{\varphi}$, while finite at small r, tend to $-\infty$ for large values of r. These solutions are characterized by a strong coupling for the four fermion interaction (γ) in comparison to the mass (β) and the fermion field strength (δ). The values of the parameters for the solutions displayed in the figure are: $\beta=0.044$, $\gamma=14.257$, and $\delta=-0.001$ (since K is negative). We have not discovered a systematic relation between the values of the parameters that lead to a solution of type A. However the general pattern is $\delta \ll \beta \ll \gamma$. The other solution encountered, that we identify as type B, presents damped oscillations for the fermion fields while the σ and $\hat{\varphi}$ fields are positive and monotonically increasing. This solution becomes singular at finite r when the term $(2\hat{\varphi}-1)$, in Eqs. (9.5), (13.7) and (13.8), vanishes. We did not find any systematic relation between the relative values of the parameters that lead to the solution of type B. Since the equations are nonlinear, the solutions are very sensitive to the parameter values. A change in the fourth significant figure in one of the parameters can lead to a change in the output from a type A to a type B solution.

From the numerical analysis it appears that the gravitational sector dominates and the fields σ and $\hat{\varphi}$ follow the general trend of Eqs. (13.5) and (13.6) when there is no coupling to matter. While the numerical work performed does not constitute an exhaustive proof for the nonexistence of finite solutions as $r\to\infty$, it appears to be unlikely that there is a combination of parameters that would lead to such solutions.

XIV. DISCUSSION

It is known that at least two independent radial functions are needed for the solitonic solutions of the field equations that describe gravitational and scalar fields.[7] There are therefore two independent radial functions in our ansatz for the present problem in which the gravitational field is coupled to a Dirac field. In our case, however, the second (Weyl) field would be described as a dilaton if it were localized.

In the original special relativistic problem it was found that there were no solitons for arbitrary values of the ''Fermi coupling constant.'' In fact even when there were, there were only a few

eigensolutions of the nonlinear equation. Initially encouraged by this result we set to look for numerical solutions of the equations for the gravitational and fermion fields. We explored systematically a large portion of the three-dimensional parameter space and only encountered the singular solutions of type A and B described in sec. XIII. While the solutions of type B are very common, those of type A occur for a particular ordering of the relative strengths of the parameters. We found that a variation in the fourth significant figure in any of the parameters could lead to a ''jump'' from a type A to a type B solution. While this does not constitute a definite proof of the nonexistence of finite solutions we think that it is unlikely that any combination of parameters may yield a result different from the singular solutions of type A and B.

In light of our failure to find a localized soliton in an earlier study,[2] it may be further argued that the choice of a dilaton field for the second function makes a solution unlikely. In that work we proved that there are soliton solutions of the interacting gravitational, electromagnetic, scalar, and dilaton fields only if the dilaton field is excluded. Aside from the problem of the dilaton we have also shown (in Secs. XI and XII) that the non linear spinor field behaves quite differently in the special relativistic and general relativistic problems. For these reasons we now believe that the rescaled and spherically degenerate Kerr–Schild metric probably does not admit a spinor solution.

We have studied only the spherically problem. There is then the possibility that one would find a solitonic solution if the full angular dependence of the Kerr solution were restored. In fact the Kerr background was chosen in the first place to allow for the backaction on the gravitational field of the angular momentum carried by the spinor field.

Our original strategy was based on the expectation that there were solitons in the spherically symmetric background, as there are in the special relativistic problem, and that these solutions could then be improved by perturbatively taking into account the angular dependence of the Kerr geometry. In view of the present results this strategy no longer seems promising.

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Noncanonical quantization of gravity. II. Constraints and the physical Hilbert space

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The program of quantizing the gravitational field with the help of affine field variables is continued. For completeness, a review of the selection criteria that singles out the affine fields, the alternative treatment of constraints, and the choice of the initial (before imposition of the constraints) ultralocal representation of the field operators is initially presented. As analogous examples demonstrate, the introduction and enforcement of the gravitational constraints will cause sufficient changes in the operator representations so that all vestiges of the initial ultralocal field operator representation disappear. To achieve this introduction and enforcement of the constraints, a well characterized phase space functional integral representation for the reproducing kernel of a suitably regularized physical Hilbert space is developed and extensively analyzed. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1385375]

I. INTRODUCTION AND THE MAIN POINTS OF PAPER I

In a previous paper[1] (hereafter referred to as P-I) an introduction and outline of a program of noncanonical quantization of the gravitational field was presented. The key concepts in the present approach are (i) a careful selection of the basic kinematical variables, (ii) the use of a quantization procedure that treats all constraints alike, (iii) the use of ultralocal field operator representations prior to introducing constraints, and (iv) the imposition of the gravitational constraints, a process in which all traces of the temporary ultralocal representation characteristics are replaced with the physically relevant ones. In this section, we briefly review topics (i), (ii), and (iii) which have largely been discussed already in P-I.

A. Nature of the basic gravitational variables

One of the central requirements for the present program is the preservation, on quantization, of the positive–definite character of the spatial part of the classical metric $g_{ab}(x)$, $a,b\in\{1,2,3\}$ (or more generally $a,b\in\{1,\ldots,s\}$ in an s-dimensional space, $s\geqslant 1$). Insisting on this requirement leads us to adopt *affine commutation relations* (in contrast, for example, to canonical commutation relations) which are expressed in terms of the local metric field operators $\hat{g}_{ab}(x)$ $[=\hat{g}_{ba}(x)]$ [which were denoted by $\sigma_{ab}(x)$ in P-I] and suitable local ''scale'' field operators $\hat{\pi}^c_d(x)$ [which were denoted by $\kappa^c_d(x)$ in P-I]. The word ''local'' here is intended to mean that these expressions only become operators after smearing with suitable spatial test functions. In units where $\hbar=1$, which are commonly assumed throughout this paper, the basic set of affine commutation relations reads

$$
\begin{aligned}
&[\,\hat{\pi}^a_b(x),\,\hat{\pi}^c_d(y)\,]=\tfrac{1}{2}i[\,\delta^c_b\hat{\pi}^a_d(x)-\delta^a_d\hat{\pi}^c_b(x)\,]\,\delta(x,y),\\
&[\,\hat{g}_{ab}(x),\,\hat{\pi}^c_d(y)\,]=\tfrac{1}{2}i[\,\delta^c_a\hat{g}_{bd}(x)+\delta^c_b\hat{g}_{ad}(x)\,]\,\delta(x,y),\\
&[\,\hat{g}_{ab}(x),\,\hat{g}_{cd}(y)\,]=0.
\end{aligned}
\tag{1}
$$

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These commutation relations are translations of identical Poisson brackets (modulo $i\hbar$, of course) for corresponding classical fields, namely, the spatial metric $g_{ab}(x)$ and the mixed-valence ("scale") field $\pi^c_d(x) \equiv g_{bd}(x)\pi^{bc}(x)$, along with the usual Poisson brackets between the metric field $g_{ab}(x)$ and the canonical momentum field $\pi^{cd}(x)$. While *classically* there is essentially nothing to be gained by using the field $\pi^c_d(x)$ rather than $\pi^{cd}(x)$, *quantum mechanically* the situation changes completely. This change arises because the affine commutation relations—and *only* the affine commutation relations—admit local self-adjoint operator solutions for both $\hat{g}_{ab}(x)$ and $\hat{\pi}^c_d(x)$ which in addition have the property that $\hat{g}_{ab}(x) > 0$ for all x. This latter property means that for any nonvanishing set $\{u^a\}$ of real numbers and any nonvanishing, non-negative test function, $f(x) \geqslant 0$, that

$$\int f(x)u^a \hat{g}_{ab}(x)u^b \, d^3x > 0. \tag{2}$$

Other choices of basic variables fail this test. For example, self-adjoint canonical variables lead to metrics that have spectra unbounded below as well as above, while triad fields and their canonical partners lead to metrics that are non-negative, but not necessarily positive definite.

B. How quantum constraints are to be imposed

Since gravity is a reparametrization invariant theory, it follows that the dynamics—indeed, *the entire physical content of the gravitational field*—enters through imposition of the relevant constraints, specifically, the diffeomorphism and Hamiltonian constraints.[2,3] These constraints lead to an open set of *first-class* constraints in the classical theory, but on quantization and in virtue of an anomaly (or, alternatively, a factor ordering problem), they give rise to a set of operator constraints that, partially at least, are *second class* in nature. There exist several methods to deal with the quantum theory of second-class constraints in the literature, but generally such methods treat the first- and second-class constraints, and thereby the variables on which they depend, in fundamentally different ways.

An exception to the rule of a different operator treatment for first- and second-class constraints is offered by the *projection operator method* approach to the quantization of systems with constraints.[4–6] The projection operator method was already discussed in P-I, and that discussion also included several elementary applications of the technique to simple, few degree-of-freedom systems. We do not repeat that discussion here. Instead, we simply observe that, rather than impose the self-adjoint quantum constraints in the idealized (Dirac) form $\Phi_\alpha |\psi\rangle_{\text{phys}} = 0$, $\alpha \in \{1,\ldots,A\}$, on vectors $|\psi\rangle_{\text{phys}}$ in a putative physical Hilbert space, $|\psi\rangle_{\text{phys}} \in \mathfrak{H}_{\text{phys}}$, we define a (possibly regularized) $\mathfrak{H}_{\text{phys}} \equiv \mathbb{E}\mathfrak{H}$, in which $\mathbb{E}$ denotes a *projection operator* defined by

$$\mathbb{E} = \mathbb{E}(\Sigma_\alpha \Phi^2_\alpha \leqslant \delta(\hbar)^2), \tag{3}$$

where $\delta(\hbar)$ is a positive *regularization parameter* (not a δ-function!) and we have assumed that $\Sigma_\alpha \Phi^2_\alpha$ is self-adjoint. As a final step, the parameter $\delta(\hbar)$ is reduced as much as required, and, in particular, when some second-class constraints are involved, $\delta(\hbar)$ ultimately remains strictly positive. This general procedure treats all constraints simultaneously and treats them all on an equal basis.

C. Why ultralocal fields are relevant

In quantizing any theory with constraints, including reparametrization invariant theories, we invariably follow the rule: *Quantize first, reduce second*, also used by Dirac.[3]

Remark: Some other quantization procedures reduce (i.e., impose constraints) first and quantize second, a scheme that may lead to different and generally incorrect results, especially when the physical phase space (the quotient of the constraint surface by the gauge transformations) is non-Euclidean.[7] We do not comment further on these alternative procedures.

It must be strongly emphasized that in the initial quantization phase of this pair of operations, one must remain neutral toward, or even better, blind to any specifics of the constraints to be imposed. In particular, in the initial, quantization phase, reparametrization invariance requires that basic fields are statistically independent at any spatial separation; correlations between fields that are spatially separated, and which originate from the particular physics of the theory under discussion, will arise only after the relevant constraints are imposed. Before the constraints are ever discussed, the nature of the field operators is *ultralocal*, the name given to field-operator representations which are, in fact, statistically independent for all distinct spatial points. The primary representation already presented in P-I for the basic local affine quantum field operators, and before constraints have been introduced, is for this very reason ultralocal in character. In the present paper, we shall discuss the relevant constraints for gravity and argue, to the extent possible at present, that the imposition of the constraints leads to field operator representations that are no longer ultralocal in character. Indeed, we shall argue that all traces of an initial ultralocal representation disappear when the constraints are fully enforced.

Remark: As an illustration of these general procedures, it is important at this point to observe that a relativistic free field of mass m (and, in addition, well-defined interacting fields) can be quantized starting from a reparametrization invariant formulation and with an initial field operator representation that is ultralocal in nature.[8] After imposing the appropriate constraint, it may be shown, by a suitable modification of the reproducing kernel—see Sec. IV for a brief discussion—how the conventional and *non*ultralocal field operator representation for the relativistic free field of an *arbitrary* mass m emerges, as well as how the conventional propagator for such a system also arises.

D. Outline of remaining sections

In Sec. II, we discuss in some detail the formulation of the initial stage of quantization in the absence of the gravitational constraints. In Sec. III, the gravitational constraints are introduced, and a novel, but generally familiar, functional integral representation of the desired expressions is developed. Finally, in Sec. IV, and aided by the use of several analogies, we present a lengthy discussion of the virtues, as we see them, of the specific functional integral representation developed in this paper.

II. REPRODUCING KERNEL FOR THE ORIGINAL HILBERT SPACE, AND ITS FUNCTIONAL INTEGRAL REPRESENTATION

A. Basic field operator representation and the original Hilbert space

For reasons briefly sketched above, we adopt as basic local field operators the positive–definite, local self-adjoint metric operators $\hat{g}_{ab}(x)$, and the local self-adjoint ''scale'' operators $\hat{\pi}^c_d(x)$, which satisfy the affine commutation relations (1) in the ''original'' Hilbert space $\mathfrak{H}$. Here $x=\{x^a\}_{a=1}^3$ denotes the coordinates (each with the dimension of *length*) of a point in a classical topological space $\mathcal{S}$, which, for the sake of discussion, we may assume is topologically equivalent to $\mathbb{R}^3$. The term $\delta(x,y)$ which enters the affine commutation relations is a Dirac δ-function ''scalar density'' with dimensions $(\text{length})^{-3}$. Moreover, the affine commutation relations uniquely tell us that $\hat{\pi}^c_d(x)$ transforms as a mixed-valence tensor density of weight one and has the engineering dimensions of an *action* (due to $\hbar$) times $(\text{length})^{-3}$, i.e., $\mathsf{M/LT}$ in terms of mass (M), length (L), and time (T). We require that $\hat{g}_{ab}(x)$ transform as a covariant tensor of rank two, and that $\hat{g}_{ab}(x)$ is dimensionless.

1. An auxiliary, but temporary, structure

For purposes of the present section, we shall need to augment the classical topological space $\mathcal{S}$ with one additional structure, namely a volume form. Specifically, we adopt a real, positive scalar density of weight one, $b(x)$, $0<b(x)<\infty$, $x\in\mathcal{S}$, with which we may define, at each point, an invariant volume form $dV\equiv b(x)d^3x$. Additionally, in keeping with its transformation properties, we further insist that $b(x)$ has the dimensions of L^{-3}.

The introduction of the auxiliary structure represented by $b(x)$ is required *before the constraints are introduced, but whatever choice is made, it will* disappear completely *after the constraints are fully enforced.*

More explicitly, several arguments are offered below to justify the introduction of the auxiliary structure represented by the function $b(x)$, $x \in \mathcal{S}$, prior to the introduction of the constraints. In Secs. III and IV, we will observe that we expect all the irrelevant freedom present in $b(x)$ to be ''squeezed out'' by the constraints and replaced with another, *non*arbitrary structure with the same dimensions. This is exactly the process observed in other cases that have been explicitly dealt with, and the particular case of a reparametrization invariant relativistic free field will be summarized in Sec. IV.[8]

2. Original reproducing kernel

Dual to the local operators $\hat{g}_{ab}(x)$ and $\hat{\pi}^c_d(x)$, we next introduce two real, c-number functions $\pi^{ab}(x)$ $[=\pi^{ba}(x)]$ and $\gamma^d_c(x)$, which, initially, may be taken as smooth functions of compact support. Here π^{ab} transforms as a contravariant tensor density of rank two and has dimensions M/LT, while γ^d_c transforms as a mixed tensor and is dimensionless. With $|\eta\rangle$—called the *fiducial vector*—an as yet unspecified unit vector in $\mathfrak{H}$, we consider the set of unit vectors (in units where $\hbar = 1$) each of which is given by

$$|\pi,\gamma\rangle \equiv e^{i\int \pi^{ab}(x)\hat{g}_{ab}(x)d^3x}\, e^{-i\int \gamma^d_c(x)\hat{\pi}^c_d(x)d^3x}\,|\eta\rangle. \tag{4}$$

As π^{ab} and γ^d_c range over the space of smooth functions of compact support, such vectors form a set of *coherent states*.

The complex functional $\langle \pi'',\gamma''|\pi',\gamma'\rangle$ formed by the inner product of two such coherent states will be a functional of fundamental importance in the present study of gravity. In particular, the functional $\langle \pi'',\gamma''|\pi',\gamma'\rangle$, whatever form it takes, is manifestly a positive–definite functional that fulfills the defining condition that

$$\sum_{j,k=1}^{J} \alpha^*_j \alpha_k \langle \pi_j,\gamma_j|\pi_k,\gamma_k\rangle \geqslant 0 \tag{5}$$

for general sets $\{\alpha_j\}$ and $\{\pi_j,\gamma_j\}$ for any $J<\infty$. Furthermore, $\langle \pi'',\gamma''|\pi',\gamma'\rangle$ is always a continuous functional in some natural functional topology, e.g., a topology defined by the particular expression itself.[9] As a continuous, positive–definite functional, it follows that we may adopt the expression $\langle \pi'',\gamma''|\pi',\gamma'\rangle$ as a *reproducing kernel*, and use it to define an associated *reproducing kernel Hilbert space* $\mathcal{C}$.[10] Let two elements of a dense set of elements in $\mathcal{C}$ be given by

$$\begin{aligned} \psi(\pi,\gamma) &\equiv \sum_{j=1}^{J} \alpha_j \langle \pi,\gamma|\pi_j,\gamma_j\rangle, \quad J<\infty, \\ \phi(\pi,\gamma) &\equiv \sum_{k=1}^{K} \beta_k \langle \pi,\gamma|\overline{\pi}_k,\overline{\gamma}_k\rangle, \quad K<\infty, \end{aligned} \tag{6}$$

where $\{\overline{\pi}_k,\overline{\gamma}_k\}_{k=1}^K$ denotes another independent set of (real) fields. These are continuous functionals of the fields π and γ. As the inner product of these two elements we adopt

$$(\psi,\phi) \equiv \sum_{j=1}^{J}\sum_{k=1}^{K} \alpha^*_j \beta_k \langle \pi_j,\gamma_j|\overline{\pi}_k,\overline{\gamma}_k\rangle. \tag{7}$$

We complete the space of functions by including the limit point of all Cauchy sequences in the norm $\|\psi\| \equiv (\psi,\psi)^{1/2}$.

The result of the above construction is the (separable) reproducing kernel Hilbert space $\mathcal{C}$ composed of bounded, continuous functionals. Moreover, the Hilbert space $\mathcal{C}$ provides an especially useful functional representation of our original Hilbert space, which was referred to as the "primary container" in P-I.

B. Choice of the fiducial vector and explicit form of the reproducing kernel

As argued in Sec. I, the representation of the basic field operators $\hat{g}_{ab}$ and $\hat{\pi}_d^c$ must be ultralocal prior to the introduction of any constraints. To fulfill this requirement, it is necessary that

$$\langle \pi'', \gamma'' | \pi', \gamma' \rangle = \exp\left\{ - \int b(x) d^3x \, L[\pi''(x), \gamma''(x); \pi'(x), \gamma'(x)] \right\} \tag{8}$$

for some dimensionless scalar function L. This function is determined by the representation of the affine field operators and the fiducial vector $|\eta\rangle$, and as minimum conditions we require that

$$\langle \eta | \hat{g}_{ab}(x) | \eta \rangle \equiv \tilde{g}_{ab}(x), \tag{9}$$

$$\langle \eta | \hat{\pi}_d^c(x) | \eta \rangle \equiv 0. \tag{10}$$

Here, $\tilde{g}(x) \equiv \{\tilde{g}_{ab}(x)\}$ is a fixed, smooth, positive–definite metric function determined by the choice of $|\eta\rangle$ (see P-I). Whether $\mathcal{S}$ is compact or noncompact, the choice of $\tilde{g}(x)$ will determine the topology of the spacelike surfaces under consideration; if $\mathcal{S}$ is noncompact, then $\tilde{g}(x)$ also determines the asymptotic form of the spacelike surfaces under consideration.

For reasons to be offered below, we choose $|\eta\rangle$ so that the overlap function of two coherent states is given (when $\hbar = 1$) by

$$\langle \pi'', \gamma'' | \pi', \gamma' \rangle = \exp\left[-2 \int b(x) d^3x \times \ln\left(\frac{\det\{\frac{1}{2}[g''^{ab}(x) + g'^{ab}(x)] + \frac{1}{2} i b(x)^{-1} [\pi''^{ab}(x) - \pi'^{ab}(x)]\}}{\{\det[g''^{ab}(x)] \det[g'^{ab}(x)]\}^{1/2}} \right) \right]. \tag{11}$$

Several comments about this basic expression are in order.

Initially, regarding (11), we observe that γ'' and γ' do *not* appear in the explicit functional form given. In particular, the smooth matrix γ has been replaced by the smooth matrix g which is defined at every point by

$$g(x) \equiv e^{\gamma(x)/2} \tilde{g}(x) e^{\gamma(x)^T/2} \equiv \{g_{ab}(x)\}, \tag{12}$$

where $\gamma(x)^T$ denotes the transpose of the matrix $\gamma(x)$. Observe that the so-defined matrix $\{g_{ab}(x)\}$ is manifestly positive–definite for all x. The map $\gamma \to g$ is clearly many-to-one since γ has *nine* independent variables at each point while g, which is symmetric, has only *six*. In view of this functional dependence *we may denote the given functional in (11) by* $\langle \pi'', g'' | \pi', g' \rangle$, *and henceforth we shall adopt this notation exclusively*.

1. Single affine matrix degree of freedom

An elementary example of the notational change from γ to g may be seen quite directly in what occurs for a *single* affine matrix degree of freedom (in contrast to a field of such degrees of freedom). To that end, and following Ref. 11 closely, we introduce the Lie algebra for affine matrix self-adjoint operator degrees of freedom composed of the symmetric 3×3 matrix $\{\sigma_{ab}\}$ and the 3×3 matrix $\{\kappa_d^c\}$, which together obey the affine commutation relations [cf. (1)]

$$[\kappa_b^a,\kappa_d^c]=i\tfrac{1}{2}(\delta_b^c\kappa_d^a-\delta_d^a\kappa_b^c),$$

$$[\sigma_{ab},\kappa_d^c]=i\tfrac{1}{2}(\delta_a^c\sigma_{db}+\delta_b^c\sigma_{ad}), \tag{13}$$

$$[\sigma_{ab},\sigma_{cd}]=0.$$

We choose the faithful, irreducible representation for which the operator matrix $\{\sigma_{ab}\}$ is symmetric and positive definite, and which is unique up to unitary equivalence. Furthermore, we choose a representation which diagonalizes $\{\sigma_{ab}\}$ as $k\equiv\{k_{ab}\}$, which we refer to as the k-representation. In the associated L^2 representation space, and for arbitrary real matrices $F=\{F^{ab}\}$, $F^{ba}=F^{ab}$, and $B=\{B_d^c\}$, it follows that

$$U[F,B]\psi(k)\equiv e^{iF^{ab}\sigma_{ab}}e^{-iB_d^c\kappa_c^d}\psi(k)=(\det[S])^2e^{iF^{ab}k_{ab}}\psi(SkS^T), \tag{14}$$

where $S\equiv e^{-B/2}=\{S_b^a\}$ and $(SkS^T)_{ab}\equiv S_a^ck_{cd}S_b^d$. The given transformation is unitary within the inner product defined by

$$\int_+\psi(k)^*\psi(k)dk, \tag{15}$$

where $dk\equiv\Pi_{a\leqslant b}\,dk_{ab}$, and the "+" sign denotes an integration over only that part of the six-dimensional k-space where the elements form a symmetric, positive–definite matrix, $\{k_{ab}\}>0$. To define coherent states we choose an extremal weight vector,

$$\eta(k)\equiv C(\det[k])^{\beta-1}e^{-\beta\,\mathrm{tr}[\tilde{G}^{-1}k]}, \tag{16}$$

where $\beta>0$, $\tilde{G}=\{\tilde{G}_{ab}\}$ is a fixed positive–definite matrix, C is determined by normalization, and tr denotes the trace. This choice leads to the expectation values

$$\langle\eta|\sigma_{ab}|\eta\rangle=\int_+\eta(k)^*k_{ab}\eta(k)dk=\tilde{G}_{ab}, \tag{17}$$

$$\langle\eta|\kappa_d^c|\eta\rangle=\int_+\eta(k)^*\kappa_d^c\eta(k)dk=0. \tag{18}$$

In the k-representation, it follows that the affine matrix coherent states are given by

$$\langle k|F,B\rangle\equiv C(\det[S])^2(\det[SkS^T])^{\beta-1}\,e^{i\,\mathrm{tr}[Fk]}\,e^{-\beta\,\mathrm{tr}[\tilde{G}^{-1}SkS^T]}. \tag{19}$$

Observe that what really enters the functional argument is the positive–definite matrix $G^{-1}\equiv S^T\tilde{G}^{-1}S$ where we set $G\equiv\{G_{ab}\}$. Thus without loss of generality we can drop the label B (or equivalently S) and replace it with G. Hence the affine matrix coherent states become

$$\langle k|F,G\rangle\equiv C'(\det[G^{-1}])^{\beta}(\det[k])^{\beta-1}\,e^{i\,\mathrm{tr}[Fk]}\,e^{-\beta\,\mathrm{tr}[G^{-1}k]}, \tag{20}$$

where $C'=C(\det[\tilde{G}])^{\beta}$ is a new normalization constant. It is now straightforward to determine that

$$\begin{aligned}\langle F'',G''|F',G'\rangle&=\int_+\langle F'',G''|k\rangle\langle k|F',G'\rangle dk\\&=\left[\frac{\{\det[G''^{-1}]\det[G'^{-1}]\}^{1/2}}{\det\{\frac{1}{2}[(G''^{-1}+G'^{-1})+i\beta^{-1}(F''-F')]\}}\right]^{2\beta}.\end{aligned} \tag{21}$$

In arriving at this result, we have used normalization of the coherent states to eliminate the constant C'.

2. Lattice construction

Suppose now that we consider an independent lattice of such matrix degrees of freedom and build the corresponding coherent state overlap as the product of ones just like (21). Let $\mathbf{n}$ label a lattice site and let $\mathbf{n}\in\mathbf{N}$, which in turn is a finite subset of $\mathbb{Z}^3$. In that case the coherent state overlap is given by

$$\langle F'',G''|F',G'\rangle_{\mathbf{N}}=\prod_{\mathbf{n}\in\mathbf{N}}\left[\frac{\{\det[G''^{-1}_{[\mathbf{n}]}]\det[G'^{-1}_{[\mathbf{n}]}]\}^{1/2}}{\det\{\frac{1}{2}[(G''^{-1}_{[\mathbf{n}]}+G'^{-1}_{[\mathbf{n}]})+i\beta^{-1}_{[\mathbf{n}]}(F''_{[\mathbf{n}]}-F'_{[\mathbf{n}]})]\}}\right]^{2\beta_{[\mathbf{n}]}}. \tag{22}$$

As our next step we wish to take a limit in which the number of independent matrix degrees of freedom tends to infinity in such a way that not only does the lattice size diverge but also the lattice spacing tends to zero so that, loosely speaking, the lattice points approach the points of the space $\mathcal{S}$. In order for the limit to be nonzero, it is necessary that the exponent $\beta_{[\mathbf{n}]}\to 0$ in a suitable way. To that end we set

$$\beta_{[\mathbf{n}]}\equiv b_{[\mathbf{n}]}\Delta, \tag{23}$$

where Δ has the dimensions L^3, and thus $b_{[\mathbf{n}]}$ has the dimensions L^{-3}. In addition we need to let $F^{ab}_{[\mathbf{n}]}\equiv\pi^{ab}_{[\mathbf{n}]}\Delta$, and we rename $G_{ab[\mathbf{n}]}$ as $g_{ab[\mathbf{n}]}$ and call the matrix elements of $G^{-1}_{[\mathbf{n}]}$ by $g^{ab}_{[\mathbf{n}]}$. With these changes (22) becomes

$$\langle \pi'',g''|\pi',g'\rangle_{\mathbf{N}}\equiv\prod_{\mathbf{n}\in\mathbf{N}}\left[\frac{\{\det[g''^{ab}_{[\mathbf{n}]}]\det[g'^{ab}_{[\mathbf{n}]}]\}^{1/2}}{\det\{\frac{1}{2}[(g''^{ab}_{[\mathbf{n}]}+g'^{ab}_{[\mathbf{n}]})+ib^{-1}_{[\mathbf{n}]}(\pi''^{ab}_{[\mathbf{n}]}-\pi'^{ab}_{[\mathbf{n}]})]\}}\right]^{2b_{[\mathbf{n}]}\Delta}. \tag{24}$$

Finally, we take the limit as described above and the result is given by (11), namely,

$$\langle \pi'',g''|\pi',g'\rangle=\exp\left[-2\int b(x)d^3x \times\ln\left(\frac{\det\{\frac{1}{2}[g''^{ab}(x)+g'^{ab}(x)]+\frac{1}{2}ib(x)^{-1}[\pi''^{ab}(x)-\pi'^{ab}(x)]\}}{\{\det[g''^{ab}(x)]\det[g'^{ab}(x)]\}^{1/2}}\right)\right]. \tag{25}$$

In this way we see how the continuum result may be obtained as a limit starting from a collection of independent affine matrix degrees of freedom. The necessity of ending with an integral over the space $\mathcal{S}$ has directly led to the requirement that we introduce the scalar density $b(x)$.

C. Additional arguments favoring $b(x)$

As a further general comment about (11) or (25) we observe that $\langle \pi'',g''|\pi',g'\rangle$ is *invariant* under general (smooth, invertible) coordinate transformations $x\to\overline{x}=\overline{x}(x)$, and we say that the given expression characterizes a *diffeomorphism invariant realization* of the affine field operators. This property holds, in part, because $b(x)$ transforms as a scalar density in both places that it appears. Thus $b(x)$, which has the dimensions of L^{-3}, plays an essential dimensional and transformational role in each place that it appears. Note that if $\hbar$ is explicitly introduced into (25) or (11), it appears only in the change $[\pi''^{ab}(x)-\pi'^{ab}(x)]\to[\pi''^{ab}(x)-\pi'^{ab}(x)]/\hbar$. If one insisted on building an acceptable ultralocal positive–definite functional using only $\pi''^{ab}(x)$, $g''^{ab}(x)$, $\pi'^{ab}(x)$, $g'^{ab}(x)$, and $\hbar$, then that construction would not appear to be possible simply on dimensional grounds.

As another argument for the appearance of $b(x)$, we observe that (25) involves not only the c-number fields π and g (or γ), but the particular representation of the local operators $\hat{g}_{ab}$ and $\hat{\pi}^c_d$ as well as the choice of the fiducial vector $|\eta\rangle$. It is entirely natural that the function $b(x)$ may emerge as a needed functional parameter in defining the operator representation and/or the vector $|\eta\rangle$, and this property is explicitly illustrated in P-I.

As a final argument for the appearance of the scalar density $b(x)$, we briefly recall properties of the local operator product for ultralocal affine field operators.[1] In particular, the formal local product reads

$$\hat{g}_{ab}(x)\hat{g}_{cd}(x)=\delta(x,x)\hat{E}_{abcd}(x)+\text{l.s.t.} \tag{26}$$

Here $\hat{E}_{abcd}(x)$ is a local fourth-order covariant tensor density operator of weight -1, $\delta(x,x)$ is a divergent multiplier with dimensions L^{-3}, which arises when the ''scalar density'' delta function $\delta(x,y)$ is evaluated at coincident points, and l.s.t. denotes ''less singular terms.'' Before adopting the proper local operator product, we introduce a scalar density $b(x)$, $0<b(x)<\infty$, with dimensions L^{-3}, and consider

$$\hat{g}_{ab}(x)\hat{g}_{cd}(x)=b(x)[b(x)^{-1}\delta(x,x)]\hat{E}_{abcd}(x)+\text{l.s.t.} \tag{27}$$

Finally, we choose

$$[\hat{g}_{ab}(x)\hat{g}_{cd}(x)]_R\equiv b(x)\hat{E}_{abcd}(x)\quad(=\hat{g}_{ab}(x)\hat{g}_{cd}(x)/[b(x)^{-1}\delta(x,x)]) \tag{28}$$

as the proper renormalized (subscript R) local operator product. (Limits involving test function sequences offer a mathematically precise construction.) The given choice leads to a local operator that transforms as a tensor in the natural fashion and, moreover, carries the natural engineering dimensions. To achieve this desirable property in a local product *requires* the introduction of an auxiliary scalar density $b(x)$.

For additional properties regarding local products of the relevant affine field operators, see P-I. Essentially, all these properties are almost entirely based on the analysis of local operator products in scalar ultralocal field theories, an analysis which is described in detail, for example, in Ref. 12.

We have offered several reasons for the appearance of the scalar density $b(x)$ at the present stage of the analysis. However, we emphasize once again that $b(x)$ will disappear when the constraints are fully enforced, whatever choice was originally made. An example of the process by which this fundamental transformation takes place is presented in Sec. IV.

D. Functional integral representation for the coherent state overlap functional

For further analysis, especially when we take up the issue of introducing the constraints in Sec. III, it is useful to introduce an alternative representation of the functional expression (25). The alternative representation we have in mind is that of a specific functional integral, which, indeed, has already been introduced in P-I. That such a representation should exist is an immediate consequence of the fact that (25) fulfills a complex polarization condition, which then leads to (25) being annihilated by a negative, second-order functional derivative operator. Exponentiating this operator, times a parameter $\nu>0$, letting the resultant operator act on general functionals of π'' and g'', and including any necessary ν-dependent prefactor, will, in the limit $\nu\to\infty$, lead to a dense set of functions in the reproducing kernel Hilbert space $\mathcal{C}$. Alternatively, letting the same operator act on a suitable δ-functional will lead to the expression (25). The functional integral of interest arises in this last expression by introducing the analog of a Feynman–Kac–Stratonovich representation. The mathematics behind these foregoing several sentences is well illustrated in P-I for both a simple, single affine degree-of-freedom example as well as for the affine field theory.

The result of the operations outlined above leads to a functional integral representation for $\langle\pi'',g''|\pi',g'\rangle$ in (25), which is given (for $\hbar=1$) by

$$\langle \pi'', g'' | \pi', g' \rangle = \exp\Bigg[-2 \int b(x) d^3x \times \ln\Bigg(\frac{\det\{\frac{1}{2}[g''^{ab}(x) + g'^{ab}(x)] + \frac{1}{2} i b(x)^{-1} [\pi''^{ab}(x) - \pi'^{ab}(x)]\}}{\{\det[g''^{ab}(x)] \det[g'^{ab}(x)]\}^{1/2}} \Bigg) \Bigg]$$

$$= \lim_{\nu \to \infty} \overline{\mathcal{N}}_\nu \int \exp\Big[-i \int g_{ab} \dot{\pi}^{ab} \, d^3x \, dt \Big] \exp\Big\{ -(1/2\nu) \int [b(x)^{-1} g_{ab} g_{cd} \dot{\pi}^{bc} \dot{\pi}^{da} + b(x) g^{ab} g^{cd} \dot{g}_{bc} \dot{g}_{da}] d^3x \, dt \Big\} \prod_{x,t} \prod_{a \leqslant b} d\pi^{ab}(x,t) dg_{ab}(x,t). \tag{29}$$

Here, because of the way the new independent variable t appears on the right-hand side of this expression, it is natural to interpret t, $0 \leqslant t \leqslant T$, $T > 0$ as coordinate "time." The fields on the right-hand side all depend on space and time, i.e., $g_{ab} = g_{ab}(x,t)$, $\dot{g}_{ab} = \partial g_{ab}(x,t)/\partial t$, etc., and, importantly, the integration domain of the formal measure is strictly limited to the domain where $\{g_{ab}(x,t)\}$ is a positive–definite matrix for all x and t. For the boundary conditions, we have $\pi'^{ab}(x) \equiv \pi^{ab}(x,0)$, $g'_{ab}(x) \equiv g_{ab}(x,0)$, as well as $\pi''^{ab}(x) \equiv \pi^{ab}(x,T)$, $g''_{ab}(x) \equiv g_{ab}(x,T)$ for all x. Observe that the right-hand side holds for *any* T, $0 < T < \infty$, while the middle term is *independent of T altogether*.

Although the functional integral on the right-hand side is formal it nevertheless conveys a great deal of information. Let us first examine it from a dimensional and transformational standpoint. As presented, $\hbar = 1$; to see where $\hbar$ would appear we may simply replace each π^{ab} by $\pi^{ab}/\hbar$. With ν having the dimensions of T^{-1} and $\overline{\mathcal{N}}_\nu$ absorbing any remaining dimensions from the formal measure, then the right-hand side of (29) is dimensionally satisfactory. From the point of view of (formal) transformations under coordinate changes, it is clear, with $\overline{\mathcal{N}}_\nu$ transforming appropriately, that the right-hand side is formally invariant under coordinate transformations involving the spatial coordinates alone.

Remark: A discussion about transformations of the right-hand side under spatially dependent transformations of the time coordinate has been given in P-I and is not repeated here. It is clear that the result of the limit $\nu \to \infty$ on the right-hand side must be invariant under all such transformations simply because the middle term is independent of the time variable altogether.

As presented—and indeed as originally derived—the *result* of the functional integral (the middle term) came before the functional integral *representation* of that result (the right-hand side). However, we can also interpret (29) in the opposite order, that is, to presume that the functional integral (right-hand side) is primary and that the answer (the middle term) is the result of evaluating the functional integral. This perspective encourages us to examine the expression in the integrand of the functional integral somewhat more carefully from a traditional standpoint. We first observe that the formal, flat part of the measure has the expected appearance of the *canonical measure* for a conventional, canonical functional integral quantization of gravity. The phase factor contains an acceptable classical symplectic potential term in a formal functional integral for gravity in which the rest of the classical action—the terms involving the constraints—are absent.

Remark: This characterization is, of course, quite appropriate since we still are in the first phase of our dual approach: quantize first, reduce second. The patient reader will be rewarded with the addition of the expected constraints and Lagrange multiplier terms in the next section.

The second, ν-dependent factor in the integrand serves as a *regularizing factor* for the functional integral. Formally, as $\nu \to \infty$, such a factor disappears from the integrand leaving the expected (preconstraint) formal functional integral integrand, such as it is. However, the ν-dependent term plays a fundamentally important role within the integral itself since it *literally serves to define the functional integral*.

It is important to make this last point quite clear, and for that purpose we temporarily discuss the formal expression (with $\hbar=1$ again)

$$d\mu^{\nu}(\pi,g)=\mathcal{M}_{\nu}\exp\left\{-(1/2\nu)\int [b(x)^{-1}g_{ab}g_{cd}\dot{\pi}^{bc}\dot{\pi}^{da}+b(x)g^{ab}g^{cd}\dot{g}_{bc}\dot{g}_{da}]d^3x\,dt\right\}$$

$$\times\prod_{x,t}\prod_{a\leqslant b}d\pi^{ab}(x,t)dg_{ab}(x,t). \tag{30}$$

We assert that for fixed $b(x)$, $0<b(x)<\infty$ and fixed ν, $0<\nu<\infty$, this expression characterizes a *bona fide, countably additive, positive measure*, μ^{ν}, on the space of generalized functions $\pi^{ab}=\pi^{ab}(x,t)$ and $g_{ab}=g_{ab}(x,t)$, where for any nonvanishing u^a and any nonvanishing, nonnegative test function $f(x)\geqslant 0$, the positive–definite matrix condition $\int f(x)u^a g_{ab}(x,t)u^b\,d^3x>0$ holds for (almost) all t, $0<t<T$. The fields π^{ab} and g_{ab} satisfy the boundary conditions at $t=0$ and $t=T$ given previously. The factor $\mathcal{M}_{\nu}$ is adjusted so that the measures μ^{ν} form a semigroup with respect to combining time intervals, e.g., $0\to T$, $T>0$, and then $T\to T+T'$, $T'>0$, being equivalent to $0\to T+T'$. If $\{h_p(x)\}_{p=1}^{\infty}$ denotes an orthonormal set of test functions defined so that

$$\int h_p(x)h_q(x)b(x)d^3x=\delta_{pq}, \tag{31}$$

$$b(x)\sum_{p=1}^{\infty}h_p(x)h_p(y)=\delta(x,y), \tag{32}$$

then we assert that there exist finite, nonzero constants N_P^{ν} for all ν and all $P\in\{1,2,3,\ldots\}$ such that

$$N_P^{\nu}\int\exp\left[-i\sum_{p=1}^{P}\int g_{ab(p)}(t)\,\dot{\pi}^{ab}_{(p)}(t)dt\right]d\mu^{\nu}(\pi,g) \tag{33}$$

is well defined. In this expression,

$$g_{ab(p)}(t)\equiv\int h_p(x)g_{ab}(x,t)b(x)\,d^3x, \tag{34}$$

$$\dot{\pi}^{ab}_{(p)}(t)\equiv\int h_p(x)\,\dot{\pi}^{ab}(x,t)\,d^3x. \tag{35}$$

Moreover, the set of constants $\{N_P^{\nu}\}$ may be chosen so that

$$\langle\pi'',g''|\pi',g'\rangle\equiv\lim_{P\to\infty}\lim_{\nu\to\infty}N_P^{\nu}\int\exp\left[-i\sum_{p=1}^{P}\int g_{ab(p)}(t)\,\dot{\pi}^{ab}_{(p)}(t)\,dt\right]d\mu^{\nu}(\pi,g). \tag{36}$$

This is one of the ways that the formal functional integral (29) can be given a rigorous meaning.

There is another way to give rigorous meaning to (29) that we would also like to discuss. In this procedure we use a spatial lattice but keep the time variable t continuous. This regularization scheme takes us back to the lattice construction given earlier [cf. (24)], except now we add a phase-space path integral representation as well. For present purposes we again introduce the symbol Δ, with dimensions L^3, to denote a uniformly (coordinate) sized, small spatial cell. Then the lattice regularized path integral expression for $\langle\pi'',g''|\pi',g'\rangle_{\mathbf{N}}$ in (24) is given by[13]

$$\overline{\mathcal{N}}_\nu^{\mathbf{N}} \int e^{-i\Sigma_{\mathbf{n}} \int g_{ab[\mathbf{n}]} \dot{\pi}^{ab}_{[\mathbf{n}]} \Delta\, dt} \exp\Bigg\{ -\frac{1}{2\nu} \sum_{\mathbf{n}} \int [b^{-1}_{[\mathbf{n}]} g_{ab[\mathbf{n}]} g_{cd[\mathbf{n}]} \dot{\pi}^{bc}_{[\mathbf{n}]} \dot{\pi}^{da}_{[\mathbf{n}]} + b_{[\mathbf{n}]} g^{ab}_{[\mathbf{n}]} g^{cd}_{[\mathbf{n}]} \dot{g}_{bc[\mathbf{n}]} \dot{g}_{da[\mathbf{n}]}] \Delta\, dt \Bigg\} \prod_{\mathbf{n},t} \prod_{a \leqslant b} d\pi^{ab}_{[\mathbf{n}]}(t)\, dg_{ab[\mathbf{n}]}(t), \tag{37}$$

where $\mathbf{n} \in \mathbf{N}$, which itself is a finite subset of $\mathbb{Z}^3$. Here $\pi^{ab}_{[\mathbf{n}]}$, $g_{ab[\mathbf{n}]}$, and $b_{[\mathbf{n}]}$ represent average field values in the cell $\mathbf{n}$, and $b^{-1}_{[\mathbf{n}]} = 1/b_{[\mathbf{n}]}$. Next, we observe that there is a countably-additive, pinned, Brownian-motion measure formally defined by

$$d\mu^\nu_{\mathbf{N}}(\pi, g) \equiv \mathcal{N}_\nu^{\mathbf{N}} \exp\Bigg\{ -\frac{1}{2\nu} \sum_{\mathbf{n}} \int [b^{-1}_{[\mathbf{n}]} g_{ab[\mathbf{n}]} g_{cd[\mathbf{n}]} \dot{\pi}^{bc}_{[\mathbf{n}]} \dot{\pi}^{da}_{[\mathbf{n}]} + b_{[\mathbf{n}]} g^{ab}_{[\mathbf{n}]} g^{cd}_{[\mathbf{n}]} \dot{g}_{bc[\mathbf{n}]} \dot{g}_{da[\mathbf{n}]}] \Delta\, dt \Bigg\}$$
$$\times \prod_{\mathbf{n},t} \prod_{a \leqslant b} d\pi^{ab}_{[\mathbf{n}]}(t)\, dg_{ab[\mathbf{n}]}(t) \tag{38}$$

so that (37) becomes

$$\overline{N}_\nu^{\mathbf{N}} \int e^{-i\Sigma_{\mathbf{n}} \int g_{ab[\mathbf{n}]} \dot{\pi}^{ab}_{[\mathbf{n}]} \Delta\, dt}\, d\mu^\nu_{\mathbf{N}}(\pi, g), \tag{39}$$

where $\{\overline{N}_\nu^{\mathbf{N}}\}$ is a set of finite constants. Moreover, these constants may be chosen so that

$$\langle \pi'', g'' | \pi', g' \rangle = \lim_{\mathbf{N} \to \infty} \lim_{\nu \to \infty} \overline{N}_\nu^{\mathbf{N}} \int e^{-i\Sigma_{\mathbf{n}} \int g_{ab[\mathbf{n}]} \dot{\pi}^{ab}_{[\mathbf{n}]} \Delta\, dt}\, d\mu^\nu_{\mathbf{N}}(\pi, g). \tag{40}$$

Here, in the last step, the limit $\mathbf{N} \to \infty$ means that $\Delta \to 0$ and $\mathbf{N} \to \mathbb{Z}^3$ in such a way that all points $x \in \mathcal{S}$ are reached in a natural way. Observe that the presence of the continuous-time regularization factor in the formal functional integral for the entire space has controlled the spatial lattice regularization in a clear and natural fashion; although possible to introduce, no temporal lattice has been required to obtain a well-defined expression.

The present usage of well-defined, phase-space measures to define functional integrals in the limit that the "diffusion constant" parameter (ν) diverges is part of the general program of *continuous-time regularization*.[14] It is noteworthy that the use of a suitable *phase-space metric* to control the Brownian motion paths invariably leads to a coherent-state representation for the resultant quantum amplitude. These remarks conclude our brief excursion into a rigorous discussion of the functional integrals of present interest.

Another prospective regularization: Let us return to the formal functional integral (29) and examine that expression with regard to the scalar density $b(x)$. Superficially, in the limit $\nu \to \infty$ in which the regularizing term proportional to $(1/2\nu)$ in the exponent of the integrand formally vanishes, one might naively expect that the result of the integral would be independent of the function $b(x)$. But, no, that naive expectation is false since the result of that integral and subsequent limit, i.e., the middle term of (29), evidently depends importantly on $b(x)$. At first glance, that dependence seems highly unnatural. It may be thought—as the author did for a number of years[15]—that an alternative regularization expression may be more "natural" and would therefore be preferable. In particular, it was thought that the expression

$$\exp\Bigg\{ -(1/2\nu) \int [g^{-1/2} g_{ab} g_{cd} \dot{\pi}^{bc} \dot{\pi}^{da} + g^{1/2} g^{ab} g^{cd} \dot{g}_{bc} \dot{g}_{da}]\, d^3x\, dt \Bigg\}, \tag{41}$$

where $g = \det[g_{ab}]$, and which involves a different phase-space metric, was "better." However, in light of the discussion in the present paper, it is now evident that this expression is not even dimensionally consistent. This defect could be rectified by the introduction of a positive constant,

which we may call $\tilde{b}$, that stands in the place of the present b (next to $g^{1/2}$) and carries the dimensions L^{-3}. Indeed, we could also introduce in place of $\tilde{b}$ a positive scalar function $\tilde{b}(x)$ with dimensions L^{-3}. In any case, the failure of (41) purely on dimensional grounds, and the necessity thereby of introducing some sort of auxiliary dimensioned parameter (or function) surely renders (41) far less ''natural'' than had been previously assumed.

As another possible argument against (41), we note that if that form of a proposed regularization was used in an expression like (29) in place of the present form of regularization, there is absolutely no guarantee that the result will describe a reproducing kernel with other than a *one-dimensional reproducing kernel Hilbert space*, which is the general result for a ''random'' choice of phase-space metric. The fact that the present form of (29) generates a suitable, infinite-dimensional reproducing kernel Hilbert space is a fundamentally important feature, which, in our case, is a consequence of having started with an appropriate reproducing kernel to begin with.

Although the author has not foreclosed any possible interest in a $\tilde{b}$ modified version of the regularization (41), all present indications point to the version (30) that features the scalar density $b(x)$. This shift of allegiance has also been bolstered by the realization that the role of $b(x)$ is confined to the initial phase of quantization and that $b(x)$ will disappear entirely after the constraints are fully enforced. On the strength of this argument, it is the version based on (30) and not (41) that is analyzed in the remainder of the present paper.

III. INTRODUCTION OF THE GRAVITATIONAL CONSTRAINTS

A. Key principles in heuristic form

There are four gravitational constraint functions, the three diffeomorphism constraints

$$H_a(x) = -2\,\pi^b_{a|b}(x), \tag{42}$$

where ''|'' denotes covariant differentiation with respect to the spatial metric g_{ab}, and the Hamiltonian constraint, which, in suitable units (i.e., $c^3/G = 16\pi$), reads

$$H(x) = g(x)^{-1/2}[\,\pi^a_b(x)\,\pi^b_a(x) - \tfrac{1}{2}\pi^a_a(x)\,\pi^b_b(x)\,] + g(x)^{1/2}\,{}^{(3)}R(x), \tag{43}$$

where $g(x) \equiv \det[g_{ab}(x)]$ and ${}^{(3)}R(x)$ denotes the scalar curvature derived from the spatial metric.[16] Classically, these constraint functions vanish, and the region in phase space on which they vanish is called the *constraint hypersurface*.

It is instructive to evaluate the classical Poisson brackets between the constraint fields. For this purpose, we enlist only the basic nonvanishing Poisson bracket given by

$$\{g_{ab}(x), \pi^{cd}(y)\} = \tfrac{1}{2}(\,\delta^c_a\delta^d_b + \delta^c_b\delta^d_a)\,\delta(x,y). \tag{44}$$

It follows that

$$\{H_a(x), H_b(y)\} = \delta_{,a}(x,y)H_b(x) - \delta_{,b}(x,y)H_a(x), \tag{45}$$

$$\{H_a(x), H(y)\} = \delta_{,a}(x,y)H(x), \tag{46}$$

$$\{H(x), H(y)\} = \delta_{,a}(x,y)g^{ab}(x)H_b(x). \tag{47}$$

In these expressions, $\delta_{,a}(x,y) \equiv \partial\delta(x,y)/\partial x^a$, which transforms as a ''vector density.'' It is clear that the Poisson brackets of the constraints vanish on the constraint hypersurface because the right-hand sides of (45)–(47) all vanish there, i.e., when $H_a(x) = 0 = H(x)$ for all $x \in \mathcal{S}$. This vanishing property of the Poisson brackets is characteristic of *first-class constraints*. Often, the Poisson bracket structure of constraints is that of a Lie bracket in which case such constraints are referred to as closed first-class constraints. In order for the Poisson bracket structure to be that of a Lie bracket, it is necessary that the coefficients of the constraints on the right-hand side involve

no dynamical variables. Taken by themselves, we note from (45) that the three diffeomorphism constraint functions form a set of closed first-class constraints. However, because of the last equation (47), it is clear that the complete set of four gravitational constraint functions do *not* have a Poisson structure which is that of a Lie algebra, and consequently the gravitational constraints are said to form an open first-class system of constraints. Such a situation does not automatically imply trouble in the corresponding quantum theory, but significant difficulties do arise in a number of cases. Quantum gravity is one of those cases.

Let us proceed formally in order to see the essence of the problem. Suppose that $\mathcal{H}_a(x)$ and $\mathcal{H}(x)$ represent local self-adjoint constraint operators for the gravitational field. Standard calculations lead to the commutation relations (with $\hbar=1$)

$$[\mathcal{H}_a(x),\mathcal{H}_b(y)]=i[\,\delta_{,a}(x,y)\,\mathcal{H}_b(x)-\delta_{,b}(x,y)\,\mathcal{H}_a(x)], \tag{48}$$

$$[\mathcal{H}_a(x),\mathcal{H}(y)]=i\,\delta_{,a}(x,y)\,\mathcal{H}(x), \tag{49}$$

$$[\mathcal{H}(x),\mathcal{H}(y)]=i\tfrac{1}{2}\delta_{,a}(x,y)[\hat{g}^{ab}(x)\mathcal{H}_b(x)+\mathcal{H}_b(x)\hat{g}^{ab}(x)], \tag{50}$$

where to ensure the Hermitian character we have symmetrized the right-hand side of the last expression. In the usual Dirac approach to constraints alluded to in Sec. I, one asks that $\Phi_\alpha|\psi\rangle_{\rm phys}=0$ for all constraints. If we assert that $\mathcal{H}_a(x)|\psi\rangle_{\rm phys}=0$ and $\mathcal{H}(x)|\psi\rangle_{\rm phys}=0$, then consistency holds for the first two sets of constraint commutators, but not for the third commutator in virtue of the fact that it is almost surely the case that $\hat{g}^{ab}(x)\,|\psi\rangle_{\rm phys}\notin\mathfrak{H}_{\rm phys}$, even if it were smeared. The expected behavior is somewhat like that of the single degree-of-freedom example where $Q|\psi\rangle=0$ and $P|\psi\rangle=0$ imply for standard Heisenberg operators that $[Q,P]|\psi\rangle=i|\psi\rangle=0$, i.e., there are no nonvanishing solutions. This behavior is characteristic of second-class constraints, and as a consequence of our discussion we are led to conclude, from a quantum mechanical standpoint, that part of the gravitational constraints are *second-class constraints*.[17] For the projection operator method of constrained system quantization, however, second-class constraints cause no special difficulty and, in particular, they are treated in just the same way as first-class constraints, as already noted in Sec. I.

Remark: Some researchers prefer to modify the theory so as to eliminate the second-class nature of the gravitational constraints. Instead, we accept the second-class constraints for what they are.

Assuming that the constraint fields $\mathcal{H}_a(x)$ and $\mathcal{H}(x)$ are local self-adjoint operators, we could—as one of several different alternatives—proceed as follows. Initially, besides the real, orthonormal set of test functions $\{h_p(x)\}$ introduced in Sec. II, let us introduce an additional set of real test functions $\{f^a_{p\,A}(x)\}$, $A\in\{1,2,3\}$, with the following properties:

$$b(x)\sum_{p=1}^{\infty}\sum_{A=1}^{3} f^a_{p\,A}(x)f^b_{p\,A}(y)=\tilde{g}^{ab}(x)\,\delta(x,y), \tag{51}$$

$$\int f^a_{p\,A}(x)f_{q\,B\,a}(x)b(x)\,d^3x=\delta_{pq}\delta_{AB}\,, \tag{52}$$

where $f_{q\,B\,a}(x)\equiv\tilde{g}_{ab}(x)f^b_{q\,B}(x)$. Regarding the set of functions $\{f^a_{p\,A}(x)\}$, the index A is a dreibein index, while the index a is a three-space vector index. With the help of these sets of expansion functions, let us introduce

$$\mathcal{H}_{(p)\,A}\equiv\int f^a_{p\,A}(x)\mathcal{H}_a(x)\,d^3x, \tag{53}$$

$$\mathcal{H}_{(p)}\equiv\int h_p(x)\mathcal{H}(x)\,d^3x, \tag{54}$$

each for $1 \leqslant p < \infty$, and similarly for other vector and scalar functions. In this form as well, part of the constraint operators are second class. To accomodate all these constraints we introduce a set of projection operators defined for all $P \in \{1,2,3,\ldots\}$ and given by

$$\mathbb{E}_P \equiv \mathbb{E}(X_P^2 \leqslant \delta(\hbar)^2), \tag{55}$$

$$X_P^2 \equiv \sum_{p=1}^{P} 2^{-p} \left[\sum_{A=1}^{3} (\mathcal{H}_{(p)\,A})^2 + \mathcal{H}_{(p)}^2 \right]. \tag{56}$$

As defined, the projection operators $\mathbb{E}_P$ are regularized and they serve to define regularized physical Hilbert spaces $\mathfrak{H}_{\text{phys}} \equiv \mathbb{E}_P \mathfrak{H}$. These regularized physical Hilbert spaces may, in turn, be characterized by their own reproducing kernels

$$\langle \pi'', g'' | \mathbb{E}_P | \pi', g' \rangle, \tag{57}$$

and the regularized physical Hilbert spaces themselves may, therefore, be represented by the associated reproducing kernel Hilbert spaces.

The final step in the present construction procedure would involve suitable limits to remove the regularizations. More familiar procedures to enforce the constraints are discussed in Sec. IV.

B. Functional integral representation for the relevant projection operators

In an earlier work,[5] we have presented a very general procedure to construct the projection operator $\mathbb{E}(\Sigma_\alpha \Phi_\alpha^2 \leqslant \delta(\hbar)^2)$ by means of a universal functional integral procedure. In particular, it follows that

$$\mathbb{E}(\Sigma_\alpha \Phi_\alpha^2 \leqslant \delta(\hbar)^2) = \int \mathbf{T}\, e^{-i\int \lambda^\alpha(t)\Phi_\alpha\, dt}\, \mathcal{D}R(\lambda), \tag{58}$$

where $\mathbf{T}$ denotes the time-ordering operator, $\{\lambda^\alpha(t)\}_{\alpha=1}^{A}$, $0 \leqslant t < T$, denotes a set of c-number "Lagrange multiplier" functions, and $\mathcal{D}R(\lambda)$ denotes a formal measure on such functions. A suitable measure R may be determined as follows: First, introduce a Gaussian integral over the set $\{\lambda^\alpha(t)\}$ so that

$$\mathcal{N}_\gamma \int \mathbf{T}\, e^{-i\int \lambda^\alpha(t)\Phi_\alpha\, dt}\, e^{(i/4\gamma)\int \Sigma_\alpha \lambda^\alpha(t)^2\, dt}\, \mathcal{D}\lambda = e^{-i\gamma \Sigma_\alpha \Phi_\alpha^2}. \tag{59}$$

Second, and last, integrate over γ according to the rule

$$\lim_{\zeta \to 0^+} \lim_{L \to \infty} \int_{-L}^{L} \frac{\sin\{\gamma[\delta(\hbar)^2 + \zeta]\}}{\pi\gamma} e^{-i\gamma \Sigma_\alpha \Phi_\alpha^2}\, d\gamma = \mathbb{E}(\Sigma_\alpha \Phi_\alpha^2 \leqslant \delta(\hbar)^2). \tag{60}$$

The inclusion of the variable ζ and the limit $\zeta \to 0^+$ ensures that we include the equality sign in the argument of $\mathbb{E}$. Observe that this construction is entirely independent of the nature of the set of constraints $\{\Phi_\alpha\}$.

Next, we continue to proceed formally in order to envisage how the projection operator method may be used in the case of gravity. Adopting the foregoing analysis, we suggest that

$$\mathbb{E}_P = \mathbb{E}\left(\sum_{p=1}^{P} 2^{-p} \left[\sum_{A=1}^{3} (\mathcal{H}_{(p)\,A})^2 + \mathcal{H}_{(p)}^2 \right] \right) = \int \mathbf{T}\, e^{-i\Sigma_{p=1}^{P} \int [\Sigma_{A=1}^{3} N_{(p)\,A}\, \mathcal{H}_{(p)\,A} + N_{(p)} \mathcal{H}_{(p)}]\, dt}\, \mathcal{D}R(N^a, N) \tag{61}$$

for an appropriately defined formal measure R. Observe that the integral over the measure R may well integrate over degrees of freedom that are not present in the time-ordered product (such as for

$p>P$); however, there is no harm in doing so since R is already defined so that $\int \mathcal{D}R=1$. We may also go one step further and assert that as $P\to\infty$ we obtain the formal expression

$$\mathbb{E}=\int \mathbf{T}\, e^{-i\int [N^a\mathcal{H}_a+N\mathcal{H}]\, d^3x\, dt}\, \mathcal{D}R(N^a,N), \tag{62}$$

which, heuristically at least, realizes the projection operator that projects the original Hilbert space onto a correspondingly regularized physical Hilbert space.

C. Functional integral representation of the reproducing kernel for the physical Hilbert space

In Sec. II, we presented in (25) a continuous-time regularized functional integral representation of the reproducing kernel $\langle \pi'',g''|\pi',g'\rangle$ for the original Hilbert space. The reproducing kernel for the (regularized) physical Hilbert space is given, in turn, by the expression $\langle \pi'',g''|\mathbb{E}|\pi',g'\rangle$. In order to give this latter expression a functional integral representation we first regard

$$\int\, [N^a\mathcal{H}_a+N\mathcal{H}]\, d^3x \tag{63}$$

as a time-dependent ''Hamiltonian'' for some fictitious theory, in which case

$$\begin{aligned}
&\langle \pi'',g''|\mathbf{T}\, e^{-i\int [N^a\mathcal{H}_a+N\mathcal{H}]\, d^3x\, dt}|\pi',g'\rangle \\
&\quad=\lim_{\nu\to\infty}\overline{\mathcal{N}}_\nu\int\, \exp\left\{-i\int\, [g_{ab}\dot\pi^{ab}+N^aH_a+NH]d^3x\, dt\right\} \\
&\qquad\times\exp\left\{-(1/2\nu)\int\, [b(x)^{-1}g_{ab}g_{cd}\dot\pi^{bc}\dot\pi^{da}+b(x)g^{ab}g^{cd}\dot g_{bc}\dot g_{da}]\, d^3x\, dt\right\} \\
&\qquad\times\prod_{x,t}\prod_{a\leqslant b}\, d\pi^{ab}(x,t)\, dg_{ab}(x,t).
\end{aligned} \tag{64}$$

In this expression, there appear symbols $H_a(\pi,g)$ and $H(\pi,g)$ corresponding to the quantum operators $\mathcal{H}_a$ and $\mathcal{H}$. Superficially, these symbols may (formally) be identified with the classical diffeomorphism and Hamiltonian constraint functions, in which case the expression (64) contains in its phase, and up to a surface term, the full Einstein action. Thus (64) comes ever closer to looking like a more traditional functional integral for gravity.

However, before integrating over the functions N^a and N and completing the story, we need to caution the reader that $\hbar$ is not zero (but rather one) and therefore the symbols H_a and H may not coincide with their usual classical expressions. All we can say at present is that H_a is a symbol for the operator $\mathcal{H}_a$, $a=1,2,3$, and that H is a symbol for the operator $\mathcal{H}$. The connection between symbol and operator is implicitly contained in (64), and since, for the moment, the functions N_a and N are general functions within our control, we may use that fact to assert that

$$\begin{aligned}
&\langle \pi'',g''|\int\, [M^a(y)\mathcal{H}_a(y)+M(y)\mathcal{H}(y)]d^3y|\pi',g'\rangle \\
&\quad=\lim_{\nu\to\infty}\overline{\mathcal{N}}_\nu\int\, e^{-i\int g_{ab}\dot\pi^{ab}d^3x\, dt}\int\, [M^a(y)H_a(y,s)+M(y)H(y,s)]d^3y \\
&\qquad\times\exp\left\{-(1/2\nu)\int\, [b(x)^{-1}g_{ab}g_{cd}\dot\pi^{bc}\dot\pi^{da}+b(x)g^{ab}g^{cd}\dot g_{bc}\dot g_{da}]d^3x\, dt\right\} \\
&\qquad\times\prod_{x,t}\prod_{a\leqslant b}\, d\pi^{ab}(x,t)dg_{ab}(x,t)
\end{aligned} \tag{65}$$

for any smooth (test) functions M^a and M and for any time s, $0<s<T$. Equation (65) gives an implicit connection between symbol and operator for the present theory. We observe that the more traditional connection between symbol and operator that normally holds for Wiener-regularized coherent-state path integrals[14] is unavailable in the present case since we are dealing with so-called weak coherent states for which no resolution of unity exists; see Refs. 1 and 13.

In addition, thanks to analyticity in the present case, the diagonal matrix elements of an operator uniquely determine the operator, and so we can also assert the connection between symbol and operator (given by setting $\pi'',g''=\pi',g'$),

$$\begin{aligned}\int\ & [M^a(y)\langle \pi',g'|\mathcal{H}_a(y)|\pi',g'\rangle + M(y)\langle \pi',g'|\mathcal{H}(y)|\pi',g'\rangle]d^3y \\ &= \lim_{\nu\to\infty}\overline{\mathcal{N}}_\nu\int e^{-i\oint g_{ab}\dot{\pi}^{ab}\,d^3x\,dt}\int [M^a(y)H_a(y,s)+M(y)H(y,s)]d^3y \\ &\quad\times\exp\left\{-(1/2\nu)\int [b(x)^{-1}g_{ab}g_{cd}\dot{\pi}^{bc}\dot{\pi}^{da}+b(x)g^{ab}g^{cd}\dot{g}_{bc}\dot{g}_{da}]d^3x\,dt\right\} \\ &\quad\times\prod_{x,t}\prod_{a\leqslant b}d\pi^{ab}(x,t)dg_{ab}(x,t),\end{aligned} \tag{66}$$

again for smooth functions M^a and M and any s, $0<s<T$. We note that $\langle \pi',g'|\mathcal{H}_a(y)|\pi',g'\rangle$ and $\langle \pi',g'|\mathcal{H}(y)|\pi',g'\rangle$ denote still other symbols that are often associated with the local operators $\mathcal{H}_a(x)$ and $\mathcal{H}(x)$, respectively. In (66), the notation $\oint g_{ab}\dot{\pi}^{ab}\,d^3x\,dt$ means that only closed paths in phase space enter, i.e., just those paths for which the functions

$$\pi^{ab}(x,0)=\pi^{ab}(x,T)\equiv\pi'^{ab}(x), \tag{67}$$

$$g_{ab}(x,0)=g_{ab}(x,T)\equiv g'_{ab}(x) \tag{68}$$

for all $x\in\mathcal{S}$. Note that a *closed* line integral in phase space involves just the symplectic form, and the result of the integral $\oint g_{ab}\dot{\pi}^{ab}\,d^3x\,dt$ is *invariant* under any (smooth) change of canonical coordinates.

Reproducing kernel for the physical Hilbert space: We now complete the story by interpreting the otherwise arbitrary c-number functions N^a and N as Lagrange multiplier functions and integrating them out of (64). Since N^a and N are not dynamical variables that must enter the formal phase-space functional integral measure in a prescribed way (i.e., as "$dp\,dq$"), we are free to integrate them as we choose—and we choose to integrate them in such a way as to *enforce the quantum constraints*, at least in a regulated fashion. As explained above, one natural way to achieve our goal involves the formal integration measure $\mathcal{D}R(N^a,N)$.

Combining several steps previously described, we now assert that the reproducing kernel for the regularized physical Hilbert space has the phase-space functional integral representation given by

$$\begin{aligned}\langle \pi'',g''|\mathbb{E}|\pi',g'\rangle &= \int \langle \pi'',g''|\mathbf{T}e^{-i\int[N^a\mathcal{H}_a+N\mathcal{H}]d^3x\,dt}|\pi',g'\rangle\mathcal{D}R(N^a,N) \\ &= \lim_{\nu\to\infty}\overline{\mathcal{N}}_\nu\int e^{-i\int[g_{ab}\dot{\pi}^{ab}+N^aH_a+NH]d^3x\,dt} \\ &\quad\times\exp\left\{-(1/2\nu)\int [b(x)^{-1}g_{ab}g_{cd}\dot{\pi}^{bc}\dot{\pi}^{da}+b(x)g^{ab}g^{cd}\dot{g}_{bc}\dot{g}_{da}]d^3x\,dt\right\} \\ &\quad\times\left[\prod_{x,t}\prod_{a\leqslant b}d\pi^{ab}(x,t)dg_{ab}(x,t)\right]\mathcal{D}R(N^a,N).\end{aligned} \tag{69}$$

In this final expression we have reached our primary goal, at least from a formal perspective. Despite the general appearance of (69), we emphasize once again that this representation has been based on the affine commutation relations and *not* on any canonical commutation relations. Later, we shall discuss a more careful definition of this formal expression along lines introduced in Sec. II, but for now let us examine (69) for its own sake.

We first comment on the range of integration for the "lapse" variable $N(x,t)$, a subject of recurrent interest.[18] Our view is that the range $-\infty<N(x,t)<\infty$ is the proper range when quantizing the theory. After all, in the Hamiltonian viewpoint, *space–time is a derived structure* of the classical theory. In principle, the issue here is no more complicated than for the reparametrized one-dimensional free particle. For this example, the original classical action is $I=\int[p\dot{q}-\frac{1}{2}p^2]dt$, where $\dot{q}\equiv dq/dt$, and has solutions $p(t)=p_o$ and $q(t)=p_o t+q_o$. The reparametrized version is given by $I'=\int[pq^*+st^*-\lambda(s+\frac{1}{2}p^2)]d\tau$, where $q^*\equiv dq/d\tau$, $t^*\equiv dt/d\tau$, and has solutions $p(\tau)=p_o$, $s(\tau)=s_o=-\frac{1}{2}p_o^2$, $t(\tau)\equiv\int_0^\tau\lambda(\sigma)d\sigma$, and $q(\tau)=t(\tau)p_o+q_o$. The function $\lambda(\tau)$ is essentially arbitrary. If, for example, $\lambda(\tau)=3\tau^2-1$, i.e., $t(\tau)=\tau(\tau^2-1)$, the solution seems "to go backward in time," but that interpretation gives to the variable τ an unwarranted physical significance. The given solution is not wrong, it just repeats itself for a while. We can avoid a repeating behavior, e.g., by simply dropping the interval $-1\leqslant\tau<1$. No such issues occur if we require that $\lambda(\tau)>0$ for all τ, in which case τ does indeed merit the name of "reparametrized time." By analogy, the function $N(x,t)$—which we have loosely called the lapse function—only deserves that name when, in the classical solution space, we insist that $N(x,t)>0$; otherwise it is just another Lagrange multiplier function, no more and no less.

When one starts from a classical perspective, with its focus on physically relevant functions $N(x,t)$ which are strictly positive, it is a conceptual leap to change to functions $N(x,t)$ that can take on both signs.[18] However, when one starts from the quantum theory, as we have done, there is no such leap to make.

As a second topic regarding (69) we focus on its general structure. With H_a and H formally equal to the constraint functions of gravity (possibly up to terms in $\hbar$,) the action appearing in the phase factor is indeed appropriate to gravity.[18] Moreover, the domain of integration is restricted to positive-definite metrics $\{g_{ab}(x,t)\}>0$. Indeed, the particular ν-dependent regularizing phase-space metric in (69) *prevents the metric variable* $\{g_{ab}\}$ *from escaping the positive–definite domain.*

As a useful analogy, we note that the two-dimensional phase space metric

$$\beta^{-1}q^2\,dp^2+\beta q^{-2}\,dq^2 \tag{70}$$

is geodesically complete in the half-space $(p,q)\in\mathbb{R}\times\mathbb{R}^+$, and when it is part of a Brownian motion measure, as in the formal expression [cf., (38)]

$$\mathcal{N}e^{-(1/2\nu)\int[\beta^{-1}q^2\dot{p}^2+\beta q^{-2}\dot{q}^2]dt}\,\mathcal{D}p\,\mathcal{D}q, \tag{71}$$

it automatically restricts the Brownian motion trajectories to the half-space $\mathbb{R}\times\mathbb{R}^+$.

Last, we comment on the formal functional integration measure in (69), specifically for the Lagrange multiplier functions N^a and N. The formal measure $\mathcal{D}R$ has been defined earlier and is unlike conventional measures chosen for such variables. As emphasized here, and elsewhere,[5] the measure $\mathcal{D}R$ is *designed to implement the quantum constraints*—as befits a quantum theory—and it has *not* been selected to enforce the classical constraints. Observe well that we have not "blindly postulated" the functional integral (69), but instead it has been *derived* as a specific functional integral representation of the well-chosen quantum matrix elements on the left-hand side. Unfamiliar as the measure $\mathcal{D}R$ may appear, we maintain that $\mathcal{D}R$—or some other measure equivalent to it—is the proper measure to choose to achieve our goal. Whether different treatments of the Lagrange multiplier functions that have been adopted by other workers are indeed equivalent or not to the use of $\mathcal{D}R$ is an interesting question, but it is not one we pursue here.

IV. DISCUSSION

In the preceding analysis, we have been strongly guided by the operator structure of the assumed theory of affine quantum gravity, and this discussion has led us to the formal functional integral representation (69) for the desired matrix elements. As was previously the case [cf. (29)], we now wish to turn (69) around and adopt the formal functional integral as our starting point and, in effect, use that expression to *define* the reproducing kernel for the regularized physical Hilbert space. Specifically, for that purpose, let us focus on the formal expression

$$\lim_{\nu\to\infty}\overline{\mathcal{N}}_\nu\int e^{i\int[\pi^{ab}\dot{g}_{ab}-N^aH_a-NH]d^3x\,dt}\exp\Bigg\{-(1/2\nu)\int[b(x)^{-1}g_{ab}g_{cd}\dot{\pi}^{bc}\dot{\pi}^{da}$$

$$+b(x)g^{ab}g^{cd}\dot{g}_{bc}\dot{g}_{da}]d^3x\,dt\Bigg\}\mathcal{D}\pi\,\mathcal{D}g\,\mathcal{D}R(N^a,N). \tag{72}$$

Note the change of the kinematic term, which simply amounts to a phase factor in the definition of the coherent states. Also we have introduced the common shorthand $\mathcal{D}\pi\,\mathcal{D}g$ for the bracketed term in (69). For the sake of discussion, we shall refer to (72) as the ''nonstandard expression.'' Our goal in this section is to discuss the nonstandard expression and see what steps are necessary to give it a proper meaning. We shall do so in a three step procedure: First, we compare the ''standard'' (see below) and ''nonstandard'' expressions. Second, we discuss a regularization and its removal that ultimately involves the elimination of the scalar density $b(x)$. Third, we examine the aspect of the problem that normally accounts for the perturbative nonrenormalizability of the gravitational field.

A. First look at the nonstandard expression

It is interesting to compare (72) with what we refer to as the standard expression for a phase-space functional integral for gravity. By the ''standard expression'' we mean the formal functional integral

$$\mathcal{M}\int e^{i\int[\pi^{ab}\dot{g}_{ab}-N^aH_a-NH]d^3x\,dt}\mathcal{D}\pi\,\mathcal{D}g\,\mathcal{D}N, \tag{73}$$

where $\mathcal{D}N\equiv\Pi_{x,t}dN(x,t)\Pi_a\,dN^a(x,t)$. In several important ways, the standard expression is *very* different than the nonstandard expression. Let us first comment on some of those differences. Much as it would be nice to think otherwise, one must recognize that the standard expression (73) is *totally undefined* as it stands; it is little more than a fancy way of writing $0\times(\infty)$. It begs for a definition as the limit of meaningful expressions [much as $0\times(\infty)$ may, for example, be defined as $\lim_{x\to 0}x\times(7/x)=7$], but what set of meaningful expressions should be chosen in the gravitational case is far from clear. A lattice limit? But then, what form should the regularized lattice expressions take? Symmetry and covariance offer only limited guidance. In point of fact, this same question faces any standard phase-space path integral, even that for a single degree of freedom in which a conventional lattice definition—as originally envisaged by Tobocman[19]—makes certain assumptions about the nature of the phase-space coordinates which may or may not be true.

Remark: The skeptical reader is urged to propose a lattice prescription to quantize the nonrelativistic free particle of unit mass by a phase-space path integral whose Hamiltonian H is expressed in canonical coordinates p and q such that $H=\frac{1}{2}(p^2+q^2)$.

A further complication of the standard functional integral expression (73) arises from the *unbounded nature* of the formal integral $\int\cdots\mathcal{D}N$ over the Lagrange multiplier variables. This choice of integration measure, which is designed to enforce the classical constraints and thereby reduce the classical phase space before quantization, necessitates *gauge fixing* (to eliminate concomitant divergences) which reduces the classical phase space further to the physical phase space (at least locally) where each point labels a physically distinct state. Quantization on the reduced phase space is formally aided by the introduction of some additional factor (e.g., a Faddeev–

Popov determinant, or its analogue), which may well lead to significant (Gribov) ambiguities which require a substantial modification of the functional integral,[20,7] and give rise to serious problems (such as unitary violation) within a BRST formulation.[21]

Nonstandard expression: Let us raise similar issues regarding the nonstandard expression (72). Although (72) is formal as it stands, it can, to a considerable extent, already be regarded as ''nearly'' well defined. As noted in Sec. II, we can combine several factors together to make, for all finite ν, a positive, countably additive, pinned measure on generalized functions. What makes (72) not well defined is the fact that the formal integrand does not constitute an integrable function with respect to that measure. We have already encountered that problem in Sec. II before any constraints were introduced, and we found that we could overcome that problem by regularizing the integrand and removing that regularization as a final step. Superficially, the same property holds when the constraint functions are present (say for fixed Lagrange multiplier values), save for one very important distinction (involving the field operator representation) which we shall address in the second point of discussion below.

Regarding the integration over the Lagrange multiplier variables, we emphasize the vast difference afforded by the projection operator method. First and foremost is the fact that *no gauge fixing* is introduced, no ghosts are used, no Faddeev–Popov determinant (or its analogue) arises, and consequently, no Gribov ambiguities can exist. These properties arise, largely, because $\int \mathcal{D}R(N^a,N)=1$, while $\int \mathcal{D}N=\infty$. The difference here could not be greater, and it arises because in the former case one quantizes first and reduces second, while in the latter case one reduces first and quantizes second. Except in basically trivial cases, the second option is fraught with substantial obstacles.[7]

One of the most significant differences between the standard and the nonstandard expressions refers to the representation of the quantum mechanical amplitudes that is involved. For the standard expression, it is usually assumed that (73) leads to a representation in which the metric field operator $\hat{g}_{ab}(x)$ is diagonalized and thus is sharply represented. In combination with any needed auxiliary factor in the functional integral, diffeomorphism invariance suggests that (73) depends only on the ''geometry'' of the initial and final three surfaces, and not on the details of any specific metric expressions.[16,18] An analogous view is also prominent in the associated ''loop quantum gravity'' in which, e.g., bras and kets depend only on knot invariants as labels of ''physically'' distinguishable states.[22] In contrast, the representation afforded by the nonstandard expression (72) is that of a *coherent-state representation*, which depends on smooth metric g_{ab} and momentum π^{ab} fields, that represent not *sharp* operator (eigen)values but suitable *mean* values, e.g.,

$$\langle \pi,g|\hat{\pi}^{ab}(x)|\pi,g\rangle=\pi^{ab}(x), \tag{74}$$

$$\langle \pi,g|\hat{g}_{ab}(x)|\pi,g\rangle=g_{ab}(x), \tag{75}$$

$$\langle \pi,g|\hat{\pi}^{b}_{a}(x)|\pi,g\rangle=g_{ac}(x)\pi^{cb}(x). \tag{76}$$

Note well, that besides the local self-adjoint metric $\hat{g}_{ab}(x)$ and scale field $\hat{\pi}^{b}_{a}(x)$ operators, we have used the momentum *bilinear form* $\hat{\pi}^{ab}(x)$ (which is *not* a local operator) in the first of these expressions. These expectations are not gauge invariant, nor should they be, since they are taken in the ''original'' Hilbert space where the constraints are not fulfilled. The gauge invariant part of the metric field, for example, and in so far as the regularized physical Hilbert space is concerned, is determined by the matrix elements

$$\langle \pi'',g''|\mathbb{E}g_{ab}(x)\mathbb{E}|\pi',g'\rangle, \tag{77}$$

which is an expression that does not require restricting the functional dependence of the bras and kets.

B. Second look at the nonstandard expression

In interpreting (72) we have concluded above that we must first regularize the integrand in order to obtain an integrable function. For the kinematic term $\int \pi^{ab}\dot{g}_{ab}\, d^3x\, dt$—and even for the diffeomorphism constraint contribution $-\int N^a H_a\, d^3x\, dt$—any natural regularization, such as one based on the expansion functions $\{h_p(x)\}$ and $\{f^a_{pA}(x)\}$, or a lattice formulation as discussed in Sec. II, will be compatible regularizations. For these terms alone, the limit of the regularized functional integral as the regularization is removed will converge to the desired result. The implication of this fact is that these parts of the integrand are compatible with the initial (ultralocal) representation of the field operators; in fact, they are compatible with any diffeomorphism invariant realization. However, when it comes time to consider the Hamiltonian constraint, the behavior is quite different. While it is true that regularizing the Hamiltonian constraint will lead to a set of well-defined functional integrals, the limit of such regularized expressions will *not* converge to an acceptable result. There are two basic and important reasons for this unsatisfactory behavior, one of which (wrong field operator representation) we will deal with in this section, the other of which (perturbative nonrenormalizability of gravity) we will discuss in the next section.

The first reason for the lack of a suitable convergence of the regularized nonstandard functional integral relates to the fact that the representation of the field operators needed to satisfy the Hamiltonian constraint is unitarily inequivalent to the ultralocal representation imposed in the initial stage of the quantization procedure. It is at the present stage of the analysis that we finally encounter the fact that our initial choice of field operator representation is incompatible with making the Hamiltonian constraint operator $\mathcal{H}(x)$ into a densely defined local operator. Stated otherwise, using the ultralocal operator representation, the operator $\int N(x,t)\mathcal{H}(x)d^3x\, dt$, for any nonzero smooth function $N(x,t)$, has only the zero vector in its domain. This defect must be fixed before proceeding, and in so doing we will be explicitly led to a new representation of the field operators, one that is unitarily inequivalent to our starting (ultralocal) representation. In the process of effecting this change of representation, the scalar density $b(x)$ will disappear from the scene entirely.

1. Pedagogical example

It is pedagogically useful to outline an analogous story for a simpler and more familiar example. Consider general, locally self-adjoint field and momentum operators, $\hat{\phi}(x)$ and $\hat{\pi}(x)$, $x\in\mathbb{R}^3$, which satisfy the canonical commutation relations

$$[\hat{\phi}(x),\hat{\pi}(y)]=i\,\delta(x-y). \tag{78}$$

Build a set of coherent states

$$|\pi,\phi\rangle\equiv e^{i[\hat{\phi}(\pi)-\hat{\pi}(\phi)]}|\eta\rangle, \tag{79}$$

where $\hat{\phi}(\pi)\equiv\int\hat{\phi}(x)\pi(x)d^3x$ and $\hat{\pi}(\phi)\equiv\int\hat{\pi}(x)\phi(x)d^3x$, with π and ϕ real test functions, and $|\eta\rangle$ is a normalized but otherwise unspecified fiducial vector. Note well that the choice of $|\eta\rangle$ in effect determines the representation of the canonical field operators. We next present a portion of the story from Ref. 8.

We initially choose $|\eta\rangle$ to correspond to an ultralocal representation such that

$$\langle\pi'',\phi''|\pi',\phi'\rangle=\exp\left\{\frac{1}{2}i\int[\phi''(x)\pi'(x)-\pi''(x)\phi'(x)]d^3x\right\}$$
$$\times\exp\left(-\frac{1}{4}\int\{M(x)^{-1}[\pi''(x)-\pi'(x)]^2+M(x)[\phi''(x)-\phi'(x)]^2\}d^3x\right). \tag{80}$$

Here $M(x)$, $0<M(x)<\infty$, is an arbitrary (smooth) function of the ultralocal representation with the dimensions of M. The given ultralocal field operator representation is in fact unitarily inequivalent for each distinct function $M(x)$. [Note well that $M(x)$ here plays the role of $b(x)$ in the present paper.]

We wish to apply this formulation to describe the *relativistic free field of mass m* for which the Hamiltonian operator is formally given by

$$\mathcal{H}=\frac{1}{2}\int :\{\hat{\pi}(x)^2+[\nabla\hat{\phi}(x)]^2+m^2\hat{\phi}(x)^2\}:d^3x. \tag{81}$$

If we build this operator out of the field and momentum operators in the ultralocal representation, then no matter what vector is used to define : :, $\mathcal{H}$ will have only the zero vector in its domain. We need to change the field operator representation, which means we have to change the fiducial vector from $|\eta\rangle$ to $|0;m\rangle$, the true ground state of the proposed Hamiltonian operator $\mathcal{H}$.

Let us first regularize the formal Hamiltonian $\mathcal{H}$. To that end, let $\{u_n(x)\}$ denote a complete set of real, orthonormal functions on $\mathbb{R}^3$ and define the sequence of kernels, for all $N\in\{1,2,3,\ldots\}$, given by

$$K_N(x,y)\equiv\sum_{n=1}^{N} u_n(x)u_n(y), \tag{82}$$

which converges to $\delta(x-y)$ as a distribution when $N\to\infty$. Let

$$\hat{\phi}_N(x)\equiv\int K_N(x,y)\,\hat{\phi}(y)\,d^3y, \tag{83}$$

$$\hat{\pi}_N(x)\equiv\int K_N(x,y)\,\hat{\pi}(y)d^3y, \tag{84}$$

and with these operators build the sequence of regularized Hamiltonian operators

$$\mathcal{H}_N\equiv\frac{1}{2}\int :\{\hat{\pi}_N(x)^2+[\nabla\hat{\phi}_N(x)]^2+m^2\hat{\phi}_N(x)^2\}:d^3x \tag{85}$$

for all N, where : : denotes normal order with respect to the ground state $|0;m\rangle_N$ of $\mathcal{H}_N$.

We would like to have a constructive way to identify the ground state of $\mathcal{H}_N$. For this purpose consider the set

$$S_N\equiv\left\{\frac{\Sigma_{j,k=1}^{J}\,a_j^*a_k\langle\pi_j,\phi_j|e^{-\mathcal{H}_N^2}|\pi_k,\phi_k\rangle}{\Sigma_{j,k=1}^{J}\,a_j^*a_k\langle\pi_j,\phi_j|\pi_k,\phi_k\rangle}:J<\infty\right\} \tag{86}$$

for general sets $\{a_j\}$ (not all zero), $\{\pi_j\}$, and $\{\phi_j\}$. (How these expressions may be generated is discussed in Ref. 8.) As N grows, the general element in S_N becomes exponentially small, save for elements that correspond to vectors which well approximate the ground state $|0;m\rangle_N$. Suitable linear combinations can convert the original reproducing kernel $\langle\pi'',\phi''|\pi',\phi'\rangle$ to the reproducing kernel $\langle\pi'',\phi'';m|\pi',\phi';m\rangle_N$ which is based on a fiducial vector that has the form $|0;m\rangle_N$ for the first N degrees of freedom and is unchanged for the remaining degrees of freedom. Finally, we may take the limit $N\to\infty$ which then leads to

$$\langle \pi'', \phi''; m | \pi', \phi'; m \rangle = \exp\left\{ \frac{1}{2} i \int [\tilde{\phi}''^*(k)\tilde{\pi}'(k) - \tilde{\pi}''^*(k)\tilde{\phi}'(k)] d^3k \right\}$$
$$\times \exp\left(-\frac{1}{4} \int \{\omega(k)^{-1} |\tilde{\pi}''(k) - \tilde{\pi}'(k)|^2 + \omega(k) |\tilde{\phi}''(k) - \tilde{\phi}'(k)|^2\} d^3k \right), \tag{87}$$

where $\omega(k) \equiv \sqrt{k^2 + m^2}$ and $\tilde{\pi}(k) \equiv (2\pi)^{-3/2} \int e^{-ik\cdot x} \pi(x) d^3x$, etc. The procedure sketched above is referred to as *recentering the coherent states* or equivalently as *recentering the reproducing kernel*. This form of reproducing kernel is no longer ultralocal and contains no trace of the scalar function $M(x)$, whatever form it may have had. Moreover, and this is an important point, the new representation is fully compatible with the Hamiltonian $\mathcal{H}$ being a non-negative, self-adjoint operator. Indeed, the expression for the propagator is given by

$$\langle \pi'', \phi''; m | e^{-i\mathcal{H}T} | \pi', \phi'; m \rangle = L'' L' \exp\left[\int \tilde{\zeta}''^*(k) e^{-i\omega(k)T} \tilde{\zeta}'(k) d^3k \right], \tag{88}$$

where

$$\tilde{\zeta}(k) \equiv [\omega(k)^{1/2} \tilde{\phi}(k) + i\omega(k)^{-1/2} \tilde{\pi}(k)] / \sqrt{2}, \tag{89}$$

$$L \equiv \exp\left[-\frac{1}{2} \int |\tilde{\zeta}(k)|^2 d^3k \right]. \tag{90}$$

The definition offered by (88) is continuous in T, which is the principal guarantor that the expression

$$\mathcal{H} = \frac{1}{2} \int :\{\hat{\pi}(x)^2 + [\nabla \hat{\phi}(x)]^2 + m^2 \hat{\phi}(x)^2\}: d^3x, \tag{91}$$

where : : denotes normal ordering with respect to the ground state $|0; m\rangle$ of the operator $\mathcal{H}$, is a self-adjoint operator as desired.

Let us summarize the basic content of the present pedagogical example. Even though we started with a very general ultralocal representation, as characterized by the general function $M(x)$, we have forced a complete change of representation to one compatible with the Hamiltonian operator for a relativistic free field of arbitrary mass m. In so doing all trace of the initial arbitrary function $M(x)$ has disappeared, and in its place, effectively speaking, has appeared the pseudodifferential operator $\sqrt{-\nabla^2 + m^2}$ having only its dimension (mass) in common with the original function $M(x)$. The original ultralocal representation is completely gone. [Remark: A moments reflection should convince the reader that a comparable analysis can be made for either the interacting ϕ_2^4 or ϕ_3^4 model as well, both of which satisfy (78), showing that the general argument is not limited just to free theories; see Ref. 8.]

2. Strong coupling gravity

The discussion in the present paper has been predicated on the assumption that we are analyzing the gravitational field and therefore the classical Hamiltonian is that given in (43). However, it is pedagogically instructive if we briefly comment on an approximate theory—based on the so-called ''strong coupling approximation''[23]—where the Hamiltonian constraint (43) is replaced by the expression

$$H_{\mathrm{SCA}}(x) \equiv g(x)^{-1/2} [\pi_b^a(x) \pi_a^b(x) - \tfrac{1}{2} \pi_a^a(x) \pi_b^b(x)] + 2\Lambda g(x)^{1/2}, \tag{92}$$

in which the term proportional to ${}^{(3)}R(x)$ has been dropped, and where we have also introduced the cosmological constant Λ (with dimensions L^{-2}) and an associated auxiliary term in the Hamiltonian. The result is a model for which the new Hamiltonian constraint (92) is indeed compatible with some form of an ultralocal representation. The proper form of that ultralocal representation may be determined by a similar procedure, i.e., by studying an analogue of the set S_N, and by recentering the reproducing kernel based on ensuring that the quantum version of $H_{\rm SCA}(x)$ is a local self-adjoint operator. In so doing, we note that it may happen that not all arbitrariness of the original scalar density $b(x)$ is "squeezed out" by the recentering procedure described above. This situation occurs because a one-parameter arbitrariness generally remains for typical ultralocal models.[12] [Any remaining arbitrariness in the ultralocal case is in contrast with that of the true Hamiltonian constraint for gravity for which we expect no trace of the original function $b(x)$ to remain.] These remarks conclude our discussion of strong coupling gravity.

C. Third look at the nonstandard expression

The preceding discussion has been based on the assumption that some fiducial vector can be found compatible with the Hamiltonian operator constraint, or stated otherwise, that the Hamiltonian constraint can actually be realized as a local self-adjoint operator. This requirement is by no means obvious, and it is to this issue that we now turn our attention. The difficulty arises because the naive form of the Hamiltonian constraint operator almost surely needs some form of renormalization if it is going to be well defined. If perturbation theory is any guide, we not only expect that there will be renormalization counterterms, but because gravity is perturbatively nonrenormalizable, one may expect an infinite number of distinct counterterms. On the other hand, as we next argue, it is possible that perturbation theory is not a very reliable guide in the case of perturbatively nonrenormalizable theories.

1. Nonrenormalizable scalar fields

Consider the case of perturbatively nonrenormalizable quartic, self-interacting scalar fields, i.e., the so-called ϕ^4_n theories, where the space–time dimension $n \geqslant 5$. On the one hand, viewed perturbatively, such theories entail an infinite number of distinct counterterms. On the other hand, the continuum limit of a straightforward Euclidean lattice formulation leads to a quasifree theory—a genuinely *noninteracting* theory—whatever choice is made for the renormalized field strength, mass, and coupling constant.[24] In the author's view both of these results are unsatisfactory. Instead, it is possible that an *intermediate behavior* holds true, even though that cannot be proven yet. Let us illustrate an analogous but simpler situation where the conjectured intermediate behavior can be rigorously established.

Consider an ultralocal quartic interacting scalar field, which, viewed classically, is nothing but the relativistic ϕ^4_n model with all the spatial gradients in the usual free term dropped. As a mathematical model of quantum field theory, an ultralocal model is readily seen to be perturbatively nonrenormalizable, while the continuum limit of a straightforward lattice formulation becomes quasifree, basically because of the vise grip of the Central Limit Theorem. Perturbative nonrenormalizability and lattice-limit triviality is similar to the behavior for relativistic ϕ^4_n models, but for the simpler ultralocal model for which an intermediate approach can be rigorously proven to hold.[12] Roughly speaking, a characterization of this intermediate behavior is the following: From a functional integral standpoint, and for any positive value of the quartic coupling constant, the quartic interaction acts like a *hard-core* in history space projecting out certain contributions that would otherwise be allowed by the free theory alone. This phenomenon takes the form of a nonstandard, nonclassical counterterm in the Hamiltonian that does *not* vanish as the coupling constant of the quartic interaction vanishes. Specifically, for the model in question, the additional counterterm is *a counterterm for the kinetic energy* and is formally proportional to $\hbar^2/\phi(x)^2$, which in form is not unlike the centripetal potential that arises in spherical coordinates in three-dimensional quantum mechanics. In summary, inclusion of a formal additional interaction proportional to $\hbar^2/\phi(x)^2$ in the Hamiltonian density is sufficient to result in a well-defined and nontrivial

(i.e., non-Gaussian) quantum theory for interacting ultralocal scalar models. In addition, it may be shown[12] that the classical limit of such quantum theories reproduces the classical model with which one started.

The foregoing brief summary holds rigorously for the ultralocal scalar fields, and it is conjectured that a suitable counterterm would lead to an acceptable intermediate behavior for the relativistic models ϕ_n^4, $n \geqslant 5$. What form should the counterterm take in the case of the relativistic ϕ_n^4 models? We can make a plausible suggestion guided by the following general principle that holds in the ultralocal case: The counterterm should be an ultralocal (because the kinetic energy is ultralocal) potential term arising from the kinetic energy. For the relativistic field that argument suggests the counterterm should again be proportional to $\hbar^2/\phi(x)^2$. It is also part of this general conjecture that the same counterterm is not limited to ϕ_n^4 models, but should be effective for other nonrenormalizable interactions, e.g., such as ϕ_n^6, $n \geqslant 4$, etc. The full argument available at present to support this conjecture appears in Chap. 11 of Ref. 12. (It may even be possible to examine this proposal by means of suitable Monte Carlo studies, but so far this challenge has not been taken up.)

Note well that the hard-core picture of nonrenormalizable interactions leads to such interactions behaving as *discontinuous perturbations*: Once turned on, such interactions cannot be completely turned off. Stated otherwise, as the nonlinear coupling constant is reduced toward zero, the theory passes continuously to a ''pseudofree'' theory—different than the ''free'' theory—*which retains the effects of the hard core*. The interacting theory is *continuously connected* to the pseudofree theory, and may even possess some form of perturbation theory about the pseudofree theory. Evidently, the presence of the hard-core interaction makes any perturbation theory developed about the original unperturbed theory almost totally meaningless.

2. Nonrenormalizable gravity

Although the differences between gravity and nonrenormalizable scalar interaction are significant in their details, there are certain similarities we wish to draw on. Most importantly, one can argue[25] that the nonlinear contributions to gravity act as a hard-core interaction in a quantization scheme, and thus the general picture sketched above for nonrenormalizable scalar fields should apply to gravity as well. Assuming that the analogy holds further, there should be a nonstandard, nonclassical counterterm that incorporates the dominant, irremovable effects of the hard-core interaction. Accepting the principle that in such cases perturbation theory offers no clear hint as to what counterterms should be chosen, we appeal to the guide used in the scalar case. Thus, as our proposed counterterm, we look for an ultralocal potential arising from the kinetic energy that appears in the Hamiltonian constraint. In fact, the only ultralocal potential that has the right transformation properties is proportional to $\hbar^2 g(x)^{1/2}$. Thus we are led to conjecture that the ''nonstandard counterterm'' is none other than a term like the familiar cosmological constant contribution. Unlike the scalar field which required an unusual term proportional to $1/\phi(x)^2$, the gravitational case has resulted in suggesting a term proportional to an ''old friend,'' namely $g(x)^{1/2}$. At first glance, it seems absurd that such a harmless looking term could act to ''save'' the nonrenormalizability of gravity. In its favor we simply note that the analogy with how other nonrenormalizable theories are ''rescued'' is too strong to dismiss the present proposal out of hand—and of course one must resist any temptation ''to think perturbatively.'' Any attempt to consider this possibility must wait until another occasion; we hope to return to this subject elsewhere.

As one small aspect of this problem, let us briefly discuss how the factor $\hbar^2$ arises in the gravitational case. Merely from a *dimensional* point of view, we note that (the first term of) the local kinetic energy operator has a formal structure given by

$$-\frac{16\pi G}{c^3}\hbar^2\left(\frac{\delta}{\delta g_{cb}(x)}\, g_{ac}(x)\, g(x)^{-1/2}\, g_{bd}(x)\, \frac{\delta}{\delta g_{da}(x)} - \cdots\right), \tag{93}$$

where we have restored the factor $16\pi G/c^3$. Thus the anticipated counterterm is proportional to $(G\hbar^2/c^3)g(x)^{1/2}$. We next cast this term into the usual form for a contribution to the potential part of the Hamiltonian constraint, namely, in a form proportional to $(c^3/G)\Lambda g(x)^{1/2}$. Hence, to recast our anticipated counterterm into this form, we need a factor proportional to

$$\frac{G^2\hbar^2}{c^6} \equiv l^4_{\text{Planck}} \approx (10^{-33}\,\text{cm})^4. \tag{94}$$

In the classical symbol for the Hamiltonian constraint operator, this factor is multiplied by an expectation value with dimensions L^{-6} originating from the density nature of the two momentum factors and leading to an overall factor with the dimensions L^{-2} that is proportional to $\hbar^2$ as claimed. Let us call the resultant counterterm $\Lambda_C\, g(x)^{1/2}$. Since the sign of the DeWitt metric that governs the kinetic energy term is indefinite, it is not even possible to predict the sign of Λ_C. However, one thing appears certain. While the proposed counterterm $\Lambda_C\, g(x)^{1/2}$ is certainly not cosmological in origin, its influence may well be.

The foregoing scenario has assumed the hard-core model of nonrenormalizable interactions applies to the theory of gravity. However, that may well not be the case, and, instead, some other counterterm(s) may be required to cure the theory of gravity. Note well that the general structure of our approach to quantize gravity is largely insensitive to just what form of regularization and renormalization is required. In particular, the use of the affine field variables, the application of the projection operator method to impose constraints, and the development of the nonstandard phase-space functional integral representation for the reproducing kernel of the regularized physical Hilbert space all have validity quite independently of the form in which the Hamiltonian constraint is ultimately turned into a local self-adjoint operator. Although we have outlined one particular version in which the Hamiltonian constraint may possibly be made into a densely defined local operator, we are happy to keep an open mind about the procedure by which this ultimately may take place since many different ways in which this process can occur are fully compatible with the general principles of our proposed quantization scheme for the gravitational field.

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Analytic torsion of all vector bundles over an elliptic curve

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The spectrum of the Hodge–Laplace operator of all holomorphic vector bundles (with parallel curvature metrics) over a flat elliptic curve is shown to be the union of the spectra of some infinite set of (explicit) finite rank matrices. The analytic torsion is then deduced by direct computation. Another evaluation of the analytic torsion is then performed using Bismut, Gillet, and Soulé's comparison formula for short exact sequences of vector bundles. This is a test for this method which could be useful when direct calculation is hopeless. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1390329]

I. INTRODUCTION

Analytic torsion for holomorphic Hermitian vector bundles over complex manifolds was introduced by Ray and Singer in Ref. 1. In the case of a Riemann surface, it equals the determinant of some Laplacian, and is as such an important tool in string theory.[2] More recently, it appeared as a part of the direct image of vector bundles in Arakelov geometry.[3,4] Explicit computations have been performed in the case of line bundles over Riemann surfaces,[1,5–7] complex projective spaces,[8–11] complex tori,[1,12,13] Θ divisors on Abelian varieties,[14] certain quotients of $K3$ surfaces,[15] compact Lie groups[16] and for equivariant bundles on compact symmetric spaces,[17] locally symmetric spaces of noncompact type,[18] and complex homogeneous spaces.[19] The purpose here is to evaluate the analytic torsion of all vector bundles (of any rank) over a one-dimensional complex torus, i.e., an elliptic curve, by two different methods.

In Sec. II, I show that thanks to Atiyah's classification[20] the problem reduces to bundles of the type $F_r \otimes L$, where F_r is a particular rank r flat indecomposable vector bundle and L is a line bundle. Three cases are to be studied: L is either trivial, or flat and nontrivial or of positive degree: the results are then stated at the end of Sec. II (see theorem 4 below). The first method is performed in Sec. III: the spectrum of the Hodge–Laplace operator is shown to be the union of the spectra of some infinite set of explicit matrices; the analytic torsion is then obtained by direct application of the zeta-regularization procedure. The second method presented in Sec. IV uses Bismut, Gillet, and Soulé's formula (theorem 0.3 of Ref. 21) for short exact sequences of vector bundles. Although this method provides less information (on the spectrum) it has the advantage that the calculation of the Bott–Chern transgression form[22] entering in the formula is the same in the three cases, and that it could be useful in other contexts where direct information on the spectrum is not available. Methods of the same kind appear in Refs. 11 and 12 using different comparison formulas from the one used here.

II. CLASSIFICATION OF VECTOR BUNDLES AND ANALYTIC TORSION

A. Results from Atiyah's classification

Let E be any elliptic curve (i.e., a one-dimensional complex torus). Atiyah classified in Ref. 20 all indecomposable vector bundles over an elliptic curve, (see Refs. 23–26 for further developments). For any holomorphic vector bundle F on E, let $\Gamma(F)$ denote the space of global holomorphic sections of F.

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Proposition (Ref. 20 theorem 5 (i)): For any $r \geqslant 1$ there exists a unique (up to holomorphic isomorphism) indecomposable vector bundle F_r of rank *r and degree 0 for which*

$$\dim \Gamma(F_r) = 1.$$

Theorem 1: *(see Ref. 23 proposition 2.1 and remark page 63.) For any $r \in \mathbb{N}$ and $d \in \mathbb{Z}$ let $k = (d,r)$ be their greatest common divisor, then for any indecomposable vector bundle $V_{r,d}$ of rank r and degree d over E there exists an elliptic curve E', an isogeny $\iota : E' \to E$ of degree r/k, and a line bundle L' over E' of degree d/k such that*

$$V_{r,d} = \iota_*(L' \otimes F'_k).$$

[*F'_k stands for the unique rank k indecomposable flat vector bundle over E' such that* $\dim \Gamma(F'_k) = 1$.]

Proof: Let $\iota : E' \to E$ be any isogeny of degree r/k, because of the preceding proposition, one has $\iota^* F_k = F'_k$. Then for any bundle B on E',

$$\iota_*(B \otimes F'_k) = (\iota_* B) \otimes F_k .$$

Now if B is a line bundle, if $d/k = \deg B$ and r/k are coprime, $\iota_* B$ is indecomposable (cf. Ref. 23, proposition 2.1). Then $(\iota_* B) \otimes F_k$ is indecomposable too (cf. Ref. 20, lemma 2.3) and of desired rank and degree. Finally all indecomposable bundles on E of rank r and degree d are obtained by tensoring $(\iota_* B) \otimes F_k$ by some flat line bundle L on E [cf. Ref. 20, theorem 5 (ii)] then clearly $\iota^* L$ is a flat line bundle on E' and

$$(\iota_* B) \otimes F_k \otimes L = \iota_*(B \otimes \iota^* L) \otimes F_k = \iota_*(B \otimes \iota^* L \otimes F'_k)$$

one sets $L' = B \otimes \iota^* L$ and the theorem is proved. □

B. Semihomogeneity

Definition: A bundle G on E is said to be semihomogeneous if for any $z \in E$ there exists a flat line bundle L on E such that the translated bundle equals

$$t_z^* G = G \otimes L.$$

Theorem: *Any indecomposable bundle on E is semihomogeneous.*

Proof: It suffices to check it for bundles of the form $L \otimes F_r$ for any r and any line bundle L. Any F_r and any flat line bundle is easily seen to be translation invariant, and so is any bundle of the form $L \otimes F_r$ where L is a flat line bundle. If L is some nonzero degree line bundle, then $t_z^* L \otimes L^{-1}$ is clearly a flat line bundle so that L is semihomogeneous. The same holds then for $L \otimes F_r$. □

Proposition 2: Reciprocally, for any flat line bundle L and any nonzero degree indecomposable bundle G there exists some $z \in E$ (not necessarily unique) such that

$$G \otimes L \cong t_z^* G.$$

Proof: Of course it is enough to check it for $F_r \otimes B$ where B is a nonzero degree line bundle. F_r being translation invariant, only the case of B is relevant. But this is a consequence of Ref. 27, theorem 1 (p. 77) and proposition (p. 80). □

C. Reduction of the problem

Let F be any holomorphic vector bundle on E. Fix some translation invariant Kähler metric on E and choose some hermitian metric on F, consider the Cauchy–Riemann operator $\overline{\partial} : \Gamma^\infty(E,F) \to \Gamma^\infty(E, T^{*(0,1)}E \otimes F)$ and its adjoint $\overline{\partial}^* : \Gamma^\infty(E, T^{*(0,1)}E \otimes F) \to \Gamma^\infty(E,F)$ with respect

to L^2 metrics. (Here and throughout, Γ^∞ stands for the space of $\mathcal{C}^\infty$ sections of the indicated bundle on the indicated manifold). The Hodge–Laplace operator is then $\Delta^{0,0}=\overline{\partial}^*\overline{\partial}$ on $\Gamma^\infty(E,F)$ and $\Delta^{0,1}=\overline{\partial}\overline{\partial}^*$ on the space $\Gamma^\infty(E,T^{*(0,1)}E\otimes F)$ of forms of complex type (0,1) on E with values in F. The definition of the analytic torsion (Ref. 1, definition 1.2) reduces here to

$$\Theta(F)=\sqrt{\det{}'\,\Delta^{0,1}}=\sqrt{\det{}'\,\Delta^{0,0}},$$

$\det'$ being the ζ-regularized product of nonzero eigenvalues (the second equality follows from Hodge theory). More precisely, let P be the orthogonal projection on the orthocomplement of $\operatorname{Ker}\Delta^{(0,1)}$ in $\Gamma^\infty(E,T^{*(0,1)}E\otimes F)$, the function

$$\zeta_F(s)=\operatorname{Tr}(\Delta^{-s}P)=\frac{1}{\Gamma(s)}\int_0^{+\infty}t^{s-1}\operatorname{Tr}(P\exp(-t\Delta^{(0,1)}))dt \tag{1}$$

is holomorphic for $\operatorname{Re}(s)>1$, has a meromorphic continuation to $\mathbb{C}$, and one sets

$$\Theta(F)=\exp-\tfrac{1}{2}\zeta_F'(0).$$

Theorem: *If F is any vector bundle on E, if the metric on E is translation invariant, then the analytic torsions of F and its dual F^* (endowed with the dual metric) coincide. (In fact the spectra of the Hodge–Laplace operators coincide.)*

Proof: This result is due to Poincaré duality (it is valid for any complex manifold with parallel-metrized trivial canonical bundle): the obvious coupling

$$F\times(T^{*(0,1)}E\otimes F^*)\to T^{*(0,1)}E$$

with the fact that $T^{*(0,1)}E$ has a nonzero parallel section $d\overline{z}$ induces a duality

$$\Gamma^\infty(E,F)\tilde{\to}\Gamma^\infty(E,T^{*(0,1)}E\otimes F),$$

which commutes with the Hodge–Laplace operators. Of course the same result holds for $\Gamma^\infty(E,T^{*(0,1)}E\otimes F)\tilde{\to}\Gamma^\infty(E,F^*)$. By Hodge theory the positive eigenvalues on $\Gamma^\infty(E,F)$ and $\Gamma^\infty(E,T^{*(0,1)}E\otimes F)$ coincide (with multiplicity). So the analytic torsions coincide. □

Note that the analytic torsion (respectively, the spectrum) of a bundle of the form $F\oplus G$ is simply the product (respectively, the union) of the analytic torsions (respectively, of the spectra) of F and G provided the metric on $F\oplus G$ is the direct sum of metrics on F and G.

Now if $\iota:E'\to E$ is an isogeny and F a bundle on E', then the spectra of the Hodge–Laplace operators of F on E' and of ι_*F on E coincide, provided ι is isometric and the metric on ι_*F is the push-forward metric, so the analytic torsions also coincide (these two last arguments were used in Ref. 12, Sec. 4.2).

Moreover analytic torsions of F and its translate t_z^*F also coincide provided the metric on E is translation invariant and under obvious conditions on the metrics of F and t_z^*F.

For all these reasons, the problem is reduced to the calculation in the case of $L\otimes F_r$ for all line bundles L of non-negative degree; note that the result only depends on the degree of L if it is positive because of proposition 2. This of course does not hold if L is flat.

Remark: From the calculation for particular metrics [the metric on E will be taken translation invariant and the metrics on the bundles will be specified later—see (5) below], the general case can be deduced by using the anomaly formula of Ref. 28 (theorem 1.23) which relates analytic torsions for two different couples of metrics (on E and F) to the ratio of L^2 norms on harmonic forms (which in positive degree are holomorphic hence independent of the metrics) and an integral over E of explicitly computable quantities. The computation which is performed in Sec. IV is of the same sort.

D. Known results for line bundles

The case of nonflat line bundles over complex tori has been studied in Ref. 12, Sec. 4.2 and Ref. 13, yielding to the following result.

Theorem: *A line bundle L of degree $d>0$ endowed with its canonical translation invariant curvature metric over a flat elliptic curve of volume η has spectrum:*

$$\left\{\frac{2\pi nd}{\eta}, n\in\mathbb{N}\right\}$$

on sections with multiplicity d for any eigenvalue.

The spectrum on (0,1)-forms coincide by Hodge theory for positive eigenvalues, there is no zero eigenvalue on (0,1)-forms since $d>0$.

Proof: I recall the argument of Ref. 13: The Hodge–Laplace operator is explicitly calculated in some holomorphic trivialization of F to be

$$-2\frac{\partial^2}{\partial z\partial\overline{z}}+\frac{2\pi d}{\eta}\underline{z}\frac{\partial}{\partial\overline{z}}$$

on sections and

$$-2\frac{\partial^2}{\partial z\partial\overline{z}}+\frac{2\pi d}{\eta}\underline{z}\frac{\partial}{\partial\overline{z}}+\frac{2\pi d}{\eta}$$

on L-valued (0,1)-forms. On the one hand this shows that tensoring with the parallel form $d\overline{z}$ provides a bijection between the λ-eigenspace on sections and the $(\lambda+2\pi d/\eta)$-eigenspace on (0,1)-forms. On the other hand Hodge theory provides a bijection between eigenspaces on sections and on (0,1)-forms corresponding to the same positive eigenvalue. Harmonic forms are determined by cohomology, so there are none in degree (0,1) and the space of harmonic sections has dimension d, from which all the eigenspaces can be recovered by successive use of the two preceding bijections. The same trick applies for higher dimensional complex tori provided the line bundle has a nondegenerate (not necessarily positive) first Chern class (see Ref. 13). □

Note (for later use), that it follows that there exists a spectral orthonormal L^2-base $(\alpha_{j,k})_{\substack{j\in\mathbb{N}\\1\leq k\leq d}}$ of $\Gamma^\infty(E,A)$ which verifies for any j and k:

$$\overline{\partial}\alpha_{j,k}=\sqrt{\frac{\pi jd}{\eta}}\,\alpha_{j-1,k}d\overline{z}. \tag{2}$$

Explicit calculation then yields

Corollary: The analytic torsion of a line bundle L of degree $d>0$ endowed with its canonical translation invariant curvature metric over a flat elliptic curve of volume η equals

$$\Theta(L)=\left(\frac{d}{\eta}\right)^{-d/4}.$$

Now theorem 1 asserts that any indecomposable bundle F of coprime degree d and rank r over E is the direct image of some degree d line bundle L over another elliptic curve E' by a degree r isogeny $\iota:E'\to E$. Thus

Corollary: If an indecomposable bundle F of coprime degree $d\neq 0$ and rank r over E is endowed with the push-forward by the above isogeny of the canonical parallel-curvature metric of the line bundle L then its spectrum is given by

$$\left\{\frac{2\pi n|d|}{r\eta}, n\in\mathbb{N}\right\},$$

where all positive eigenvalues have multiplicity $|d|$ both on sections and on (0,1)-forms and the zero eigenvalue has multiplicity $|d|$ on sections if $d>0$, $|d|$ on (0,1)-forms if $d<0$ and 0 otherwise. Its analytic torsion is

$$\Theta(F)=\left(\frac{|d|}{r\eta}\right)^{-|d|/4}.$$

Note that from Ref. 24, Appendix A, the vector bundles referred to in this corollary are exactly the stable ones. The push-forward metric on them is in this case Hermite–Einstein.

I recall now some basic facts about flat line bundles: There exists some lattice Λ in $\mathbb{C}$ [endowed with its canonical metric $(z_1,z_2)\to z_1\overline{z_2}$] such that E is isomorphic and isometric to $\mathbb{C}/\Lambda$. (Any two flat metrics on E only differ from some multiplicative positive real factor.) Λ can be chosen to be generated by x and $x\tau$ where x is a positive real number and:

$$-\tfrac{1}{2}<\mathrm{Re}\,\tau\leqslant\tfrac{1}{2},\quad |\tau|>1$$

(τ is the modular invariant of E and of course $\eta=x^2\,\mathrm{Im}\,\tau$). Let Λ^* be the dual lattice to Λ:

$$\Lambda^*=\{\gamma\in\mathbb{C}/\mathrm{Im}(\gamma\overline{u})\in\mathbb{Z}\ \text{ for any }\ u\in\Lambda\}=\frac{1}{\eta}\Lambda.$$

Then it is a standard fact that the Hodge–Laplace operator on functions and (0,1)-forms (i.e., for the trivial line bundle) has spectrum

$$\{2\pi^2|\gamma|^2\ ,\gamma\in\Lambda^*\},$$

the eigenspaces being provided by Fourier decomposition. [The Hodge–Laplace operator is the half of the ''usual'' (Riemannian) Laplacian].

The flat line bundles are parametrized by the dual elliptic curve $\hat{E}=\mathbb{C}/\Lambda^*$, and in a canonical holomorphic trivialization, global $\mathcal{C}^\infty$ sections of the flat line bundle $L_{\hat{\alpha}}$ corresponding to $\hat{\alpha}\in\hat{E}$ are simply Λ-periodic multiples of the function $\exp(2\pi i\,\mathrm{Im}(\alpha\overline{z}))$ where $\alpha\in\mathbb{C}$ is any pre-image of $\hat{\alpha}\in\hat{E}$. The eigenspaces are then once more provided by Fourier decomposition, i.e., spanned by the

$$\varphi_{\alpha+\gamma}(z)=\frac{1}{\sqrt{\eta}}\exp(2\pi i\,\mathrm{Im}((\alpha+\gamma)\overline{z})) \tag{3}$$

for $\gamma\in\Lambda^*$ ($1/\sqrt{\eta}$ provides L^2-orthonormality), and the spectrum is given by

$$\{2\pi^2|\alpha+\gamma|^2,\gamma\in\Lambda^*\}.$$

In both cases the analytic torsion is given by Kronecker limit formulas:

Theorem 3: *The analytic torsion of $L_{\hat{\alpha}}$ for nonzero $\hat{\alpha}$ equals*

$$\Theta(L_{\hat{\alpha}})=e^{-\pi\,\mathrm{Im}\,\tau(b^2-b+1/6)}\prod_{k=-\infty}^{+\infty}|1-e^{2\pi i(|k|\tau+\varepsilon_k\sqrt{\eta\,\mathrm{Im}\,\tau}\alpha)}|$$

(cf. Ref. 1, theorem 4.1) where $\varepsilon_k=\mathrm{sign}(k+\frac{1}{2})$ and $b=\sqrt{\eta/\mathrm{Im}\,\tau}\,\mathrm{Im}\,\alpha$ is supposed to lie in $[0,1]$ (by choosing some suitable preimage of $\hat{\alpha}$ in $\mathbb{C}$). The analytic torsion of the trivial line bundle on E equals

$$\Theta(\mathcal{O})=\sqrt{2\,\eta\,\mathrm{Im}\,\tau}e^{-\pi\,\mathrm{Im}\,\tau/6}\prod_{k>0}|1-e^{2\pi ik\tau}|^2.$$

Note that here $\alpha=(\eta \operatorname{Im}\tau)^{-1/2}(a+b\tau)$, and the corresponding character verifies: $\chi_{\hat{\alpha}}(n+m\tau)=\exp 2\pi i(-am+bn)$. This explains little differences with Ref. 1.

E. Statement of the results

Proposition: F_r is given by the following automorphy factor:

$$\phi_u(V,z)=(M(u)V,z+u)$$

for $u\in\Lambda$ and $V\in\mathbb{C}^r$ with

$$M(u)=\begin{pmatrix} 1 & \overline{u} & \frac{\overline{u}^2}{2} & \cdots & \frac{\overline{u}^{r-1}}{(r-1)!} \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \frac{\overline{u}^2}{2} \\ \vdots & & \ddots & \ddots & \overline{u} \\ 0 & \cdots & \cdots & 0 & 1 \end{pmatrix}.$$

Proof: The proposed vector bundle on E is topologically trivial spanned by the following $\mathcal{C}^\infty$ sections:

$$\rho_{1,r}=\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \rho_{2,r}=\begin{pmatrix} \overline{z} \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad \cdots \quad \rho_{r,r}=\begin{pmatrix} \frac{\overline{z}^{r-1}}{(r-1)!} \\ \vdots \\ \overline{z} \\ 1 \end{pmatrix}, \tag{4}$$

which verify for any $2\leqslant q\leqslant r$:

$$\overline{\partial}\rho_{q,r}=\rho_{q-1,r}d\overline{z} \text{ and } \overline{\partial}\rho_{1,r}=0.$$

Thus $\rho_{1,r}$ spans $\Gamma(F_r)$ and $\rho_{r,r}d\overline{z}$ generates $H^1(F_r)$.

Now it follows from theorem 5 and corollary 2 of Ref. 20 that F_r is characterized by $\dim\Gamma(F_r)=1$ and the existence of nonsplit exact sequences for any r and s:

$$0\to F_s\to F_r\to F_{r-s}\to 0.$$

Here the exact sequence is obviously provided by the maps

$$\begin{pmatrix} \varsigma_1 \\ \vdots \\ \varsigma_s \end{pmatrix}\mapsto\begin{pmatrix} \varsigma_1 \\ \vdots \\ \varsigma_s \\ 0 \\ \vdots \\ 0 \end{pmatrix} \text{ and } \begin{pmatrix} \varsigma_1 \\ \vdots \\ \varsigma_s \\ \varsigma_{s+1} \\ \vdots \\ \varsigma_r \end{pmatrix}\mapsto\begin{pmatrix} \varsigma_{s+1} \\ \vdots \\ \varsigma_r \end{pmatrix}$$

and the morphism $\Gamma(F_{r-s})\to H^1(F_s)$ associated to it maps $\rho_{1,r-s}$ to the class of $\rho_{s,s}\,d\overline{z}$. □

The preceding sections $\rho_{q,r}$ will be taken pointwise orthogonal of constant norm ν_q. One considers then the $\sigma_q:=(1/\nu_q)\rho_{q,r}$ which give a pointwise orthonormal frame of F_r and verify:

$$\overline{\partial}\sigma_q=\frac{\nu_{q-1}}{\nu_q}\sigma_{q-1}d\overline{z}=:\lambda_q\sigma_{q-1}d\overline{z} \tag{5}$$

(of course λ_1 vanishes). (This metric on F_r is of course not Hermite–Einstein since F_r is not stable.)

The following sections are devoted to the proof of

Theorem 4: *(i) The analytic torsion of F_r equals*

$$\Theta(F_r)=\sqrt{\prod_{q=2}^{r}(2|\lambda_q|^2)}\exp\left(\frac{-\eta}{2\pi}\sum_{q=2}^{r}|\lambda_q|^2\right)(2\eta\,\mathrm{Im}\,\tau)^{r/2}e^{-r\pi\,\mathrm{Im}\,\tau/6}\prod_{k>0}|1-e^{2\pi ik\tau}|^{2r}.$$

(ii) If $L_{\hat{\alpha}}$ is a nontrivial flat line bundle on E, choose a preimage α of $\hat{\alpha}$ such that $b=\sqrt{\eta/\mathrm{Im}\,\tau}\,\mathrm{Im}\,\alpha$ lies in $[0,1]$, the analytic torsion of $F_r\otimes L_{\hat{\alpha}}$ equals

$$\Theta(F_r\otimes L_{\hat{\alpha}})=\exp\left(-\frac{\eta}{2\pi}\sum_{q=2}^{r}|\lambda_q|^2\right)e^{-r\pi\,\mathrm{Im}\,\tau(b^2-b+1/6)}\prod_{k=-\infty}^{+\infty}|1-e^{2\pi i(|k|\tau+\varepsilon_k\sqrt{\eta\,\mathrm{Im}\,\tau}\alpha)}|^r,$$

where (as before) $\varepsilon_k=\mathrm{sign}(k+\frac{1}{2})$.

(iii) If A is a degree d line bundle on E, the analytic torsion of $F_r\otimes A$ equals

$$\Theta(F_r\otimes A)=\left(\frac{d}{\eta}\right)^{-dr/4}\exp\left(-\frac{\eta}{2\pi}\sum_{q=2}^{r}|\lambda_q|^2\right)\prod_{\ell=2}^{r}\left(\sum_{j=0}^{\ell-1}\left(\frac{\pi d}{\eta}\right)^{-j}\frac{|\lambda_{\ell-j+1}|^2\cdots|\lambda_\ell|^2}{j!}\right)^{d/2}$$

(the $j=0$ term in the last sum is to be taken equal to 1).

(iv) An indecomposable vector bundle V on E of nonzero degree d and rank r with greatest common divisor $(d,r)=k$ is the direct image by an isogeny of degree r/k of $F_k\otimes A$ where A is a line bundle of degree d/k. Put on V the push-forward by this isogeny of the metric on $F_k\otimes A$ considered in (iii)

$$\Theta(V)=\left(\frac{|d|}{r\eta}\right)^{-|d|/4}\exp\left(-\frac{r\eta}{2k\pi}\sum_{q=2}^{k}|\lambda_q|^2\right)\prod_{\ell=2}^{k}\left(\sum_{j=0}^{\ell-1}\left(\frac{\pi|d|}{r\eta}\right)^{-j}\frac{|\lambda_{\ell-j+1}|^2\cdots|\lambda_\ell|^2}{j!}\right)^{|d|/2k}.$$

Note that part *(iv)* is a direct consequence of part *(iii)*.

III. DIRECT CALCULATION

A. The Hodge–Laplace operator in matricial form

Consider the L^2 normalized spectral base $(\varphi_{\alpha+\gamma})_{\gamma\in\Lambda^*}$ of $\Gamma^\infty(E,L_{\hat{\alpha}})$. The fact that the $(\sigma_q)_{1\leqslant q\leqslant r}$ provide a pointwise orthonormal base of F_r ensures that $(\sigma_q\otimes\varphi_{\alpha+\gamma})_{\gamma\in\Lambda^*}^{1\leqslant q\leqslant r}$ is a L^2 orthonormal base of $\Gamma^\infty(E,F_r\otimes L_{\hat{\alpha}})$. Previous calculations (5), (3) yield

$$\overline{\partial}(\sigma_q\otimes\varphi_{\alpha+\gamma})=\lambda_q\sigma_{q-1}\otimes\varphi_{\alpha+\gamma}d\overline{z}+\pi(\alpha+\gamma)\sigma_q\otimes\varphi_{\alpha+\gamma}d\overline{z}.$$

The adjoint $\overline{\partial}^*$ is then easily deduced:

$$\overline{\partial}^*(\sigma_q\otimes\varphi_{\alpha+\gamma}d\overline{z})=2\overline{\lambda}_{q+1}\sigma_{q+1}\otimes\varphi_{\alpha+\gamma}+2\pi(\overline{\alpha}+\overline{\gamma})\sigma_q\otimes\varphi_{\alpha+\gamma}.$$

The factor 2 is due to the fact that $\|d\overline{z}\|^2=2$. The Hodge–Laplace operator $\Delta=\overline{\partial}^*\overline{\partial}$ then reads:

$$\Delta(\sigma_q\otimes\varphi_{\alpha+\gamma})=(2\pi^2|\alpha+\gamma|^2+2|\lambda_q|^2)\sigma_q\otimes\varphi_{\alpha+\gamma}+2\pi(\overline{\alpha}+\overline{\gamma})\lambda_q\sigma_{q-1}\otimes\varphi_{\alpha+\gamma}$$
$$+2\pi(\alpha+\gamma)\overline{\lambda}_{q+1}\sigma_{q+1}\otimes\varphi_{\alpha+\gamma}.$$

Thus for any $\gamma\in\Lambda^*$, the matrix of Δ in the (invariant) subspace $\mathrm{Vect}\{\sigma_q\otimes\varphi_{\alpha+\gamma},1\leqslant q\leqslant r\}$ reads:

$$\mathcal{M}_{\alpha,\gamma,r}=\begin{pmatrix} 2\pi^2|\alpha+\gamma|^2 & 2\pi(\overline{\alpha}+\overline{\gamma})\lambda_2 & 0 & \dots & 0 \\ 2\pi(\alpha+\gamma)\overline{\lambda_2} & 2\pi^2|\alpha+\gamma|^2+2|\lambda_2|^2 & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 2\pi(\overline{\alpha}+\overline{\gamma})\lambda_r \\ 0 & \dots & 0 & 2\pi(\alpha+\gamma)\overline{\lambda_r} & 2\pi^2|\alpha+\gamma|^2+2|\lambda_r|^2 \end{pmatrix}.$$

The spectrum of Δ consists of the union of the spectra of the $\mathcal{M}_{\alpha,\gamma,r}$ when γ goes around Λ^*.

In the same vein consider the L^2 normalized spectral base $(\alpha_{j,k})_{\substack{j\in\mathbb{N}\\1\leqslant k\leqslant d}}$ of $\Gamma^\infty(E,A)$ [cf. (2)]. Then clearly $(\sigma_q\otimes\alpha_{j,k})_{1\leqslant q\leqslant r,1\leqslant k\leqslant d,j\in\mathbb{N}}$ is an L^2 orthonormal base of $\Gamma^\infty(E,F_r\otimes A)$ for which

$$\overline{\partial}(\sigma_q\otimes\alpha_{j,k})=\lambda_q\sigma_{q-1}\otimes\alpha_{j,k}d\overline{z}+\sqrt{\frac{\pi jd}{\eta}}\,\sigma_q\otimes\alpha_{j-1,k}d\overline{z},$$

$$\overline{\partial}^*(\sigma_q\otimes\alpha_{j,k}d\overline{z})=2\overline{\lambda}_{q+1}\sigma_{q+1}\otimes\alpha_{j,k}+2\sqrt{\frac{\pi(j+1)d}{\eta}}\,\sigma_q\otimes\alpha_{j+1,k}, \tag{6}$$

$$\begin{aligned}\Delta(\sigma_q\otimes\alpha_{j,k})=&\left(2|\lambda_q|^2+\frac{2\pi jd}{\eta}\right)\sigma_q\otimes\alpha_{j,k}+2\lambda_q\sqrt{\frac{\pi(j+1)d}{\eta}}\,\sigma_{q-1}\otimes\alpha_{j+1,k}\\&+2\overline{\lambda}_{q+1}\sqrt{\frac{\pi jd}{\eta}}\,\sigma_{q+1}\otimes\alpha_{j-1,k}.\end{aligned}$$

Thus if $\ell\geqslant r$, the subspaces $\mathcal{V}_{\ell,k}:=\mathrm{Vect}\{\sigma_q\otimes\alpha_{j,k},q+j=\ell\}$ have dimension r and are respected by Δ. The matrix of Δ in the base $(\sigma_q\otimes\alpha_{\ell-q,k})_{1\leqslant q\leqslant r}$ reads:

$$\mathcal{M}_{r,k,\ell}=\begin{pmatrix} \frac{2\pi(\ell-1)d}{\eta} & 2\lambda_2\sqrt{\frac{\pi(\ell-1)d}{\eta}} & 0 & \dots & 0 \\ 2\overline{\lambda}_2\sqrt{\frac{\pi(\ell-1)d}{\eta}} & 2|\lambda_2|^2+\frac{2\pi(\ell-2)d}{\eta} & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 2\lambda_r\sqrt{\frac{\pi(\ell-r+1)d}{\eta}} \\ 0 & \dots & 0 & 2\overline{\lambda}_r\sqrt{\frac{\pi(\ell-r+1)d}{\eta}} & 2|\lambda_r|^2+\frac{2\pi(\ell-r)d}{\eta} \end{pmatrix}$$

and it does not depend on k. But if $1\leqslant\ell\leqslant r-1$, then $\mathcal{V}_{\ell,k}:=\mathrm{Vect}\{\sigma_q\otimes\alpha_{j,k},q+j=\ell\}$ has dimension ℓ, it is respected by Δ whose matrix in the base $(\sigma_q\otimes\alpha_{\ell-q,k})_{1\leqslant q\leqslant\ell}$ reads (it remains independent of k):

$$\mathcal{M}_{r,k,\ell}=\begin{pmatrix} \frac{2\pi(\ell-1)d}{\eta} & 2\lambda_2\sqrt{\frac{\pi(\ell-1)d}{\eta}} & 0 & \cdots & 0 \\ 2\overline{\lambda_2}\sqrt{\frac{\pi(\ell-1)d}{\eta}} & 2|\lambda_2|^2+\frac{2\pi(\ell-2)d}{\eta} & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 2\lambda_\ell\sqrt{\frac{\pi d}{\eta}} \\ 0 & \cdots & 0 & 2\overline{\lambda_\ell}\sqrt{\frac{\pi d}{\eta}} & 2|\lambda_\ell|^2 \end{pmatrix}.$$

For $\ell\geqslant r+1$ the matrices $\mathcal{M}_{r,k,\ell}$ are invertible but for $\ell\leqslant r$ they all have a one-dimensional kernel spanned by

$$\left(\sum_{q=1}^{\ell}\frac{(-1)^q}{\sqrt{(\ell-q)!}}\lambda_{q+1}\lambda_{q+2}\cdots\lambda_\ell\left(\frac{\pi d}{\eta}\right)^{q/2}\sigma_q\otimes\alpha_{\ell-q,k}\right)$$

(the product $\lambda_{q+1}\lambda_{q+2}\cdots\lambda_\ell$ is to be taken equal to 1 in the $q=\ell$ term of the sum).

B. Calculation of the analytic torsion

1. The case of $F_r\otimes L_{\hat{\alpha}}$ for a nontrivial flat bundle $L_{\hat{\alpha}}$

The characteristic polynomials $P_{\alpha,\gamma,r}(X)=\det(\mathcal{M}_{\alpha,\gamma,r}-X\mathrm{Id})$ verify

$$P_{\alpha,\gamma,r}(X)=(2\pi^2|\alpha+\gamma|^2+2|\lambda_r|^2-X)P_{\alpha,\gamma,r-1}(X)-4\pi^2|\alpha+\gamma|^2|\lambda_r|^2P_{\alpha,\gamma,r-2}(X)$$

from which it is easily deduced that

$$\begin{aligned}P_{\alpha,\gamma,r}(X)=(-X)^r&+\left(2r\pi^2|\alpha+\gamma|^2+2\sum_{q=2}^{r}|\lambda_q|^2\right)(-X)^{r-1}\\&+\left[2r(r-1)\pi^4|\alpha+\gamma|^4+4(r-2)\pi^2|\alpha+\gamma|^2\sum_{q=2}^{r}|\lambda_q|^2+4\sum_{p<q}(|\lambda_p|^2|\lambda_q|^2)\right]\\&\times(-X)^{r-2}+\cdots+(2\pi^2|\alpha+\gamma|^2)^r.\end{aligned}$$

Thus the following symmetric functions of eigenvalues of $\mathcal{M}_{\alpha,\gamma,r}$ equal

$$\sum_{\mu\in\mathrm{Spec}\,\mathcal{M}_{\alpha,\gamma,r}}\mu^2=4r\pi^4|\alpha+\gamma|^4+16\pi^2|\alpha+\gamma|^2\sum_{q=2}^{r}|\lambda_q|^2+4\sum_{q=2}^{r}|\lambda_q|^4,$$

$$\sum_{\mu\in\mathrm{Spec}\,\mathcal{M}_{\alpha,\gamma,r}}(\mu-2\pi^2|\alpha+\gamma|^2)^2=8\pi^2|\alpha+\gamma|^2\sum_{q=2}^{r}|\lambda_q|^2+4\sum_{q=2}^{r}|\lambda_q|^4,$$

then if $\zeta_{\hat{\alpha},r}$ (respectively, $\zeta_{\hat{\alpha}}$) stands for the zeta function (1) of $F_r\otimes L_{\hat{\alpha}}$ (respectively of $L_{\hat{\alpha}}$)

$$\zeta_{\hat{\alpha},r}(s)=\sum_{\mu\in\operatorname{Spec}\Delta}\mu^{-s}$$

$$=\sum_{\gamma\in\Lambda^*}(2\pi^2|\alpha+\gamma|^2)^{-s}\sum_{\mu\in\operatorname{Spec}\mathcal{M}_{\alpha,\gamma,r}}\left[\left(\frac{\mu}{2\pi^2|\alpha+\gamma|^2}\right)^{-s}-1+1\right]$$

$$=r\sum_{\gamma\in\Lambda^*}(2\pi^2|\alpha+\gamma|^2)^{-s}+\sum_{\gamma\in\Lambda^*}(2\pi^2|\alpha+\gamma|^2)^{-s}$$

$$\times\sum_{\mu\in\operatorname{Spec}\mathcal{M}_{\alpha,\gamma,r}}\left[-s\log\frac{\mu}{2\pi^2|\alpha+\gamma|^2}+\frac{s^2}{2}\left(\log\frac{\mu}{2\pi^2|\alpha+\gamma|^2}\right)^2+s^3f(\alpha,\gamma,r,s)\right].$$

But $\det\mathcal{M}_{\alpha,\gamma,r}=(2\pi^2|\alpha+\gamma|^2)^r$ so that

$$\sum_{\mu\in\operatorname{Spec}\mathcal{M}_{\alpha,\gamma,r}}\log\frac{\mu}{2\pi^2|\alpha+\gamma|^2}$$

vanishes:

$$\zeta_{\hat{\alpha},r}(s)=r\zeta_{\hat{\alpha}}(s)+\frac{s^2}{2}\sum_{\gamma\in\Lambda^*}(2\pi^2|\alpha+\gamma|^2)^{-s}\left[\sum_{\mu\in\operatorname{Spec}\mathcal{M}_{\alpha,\gamma,r}}\left(\frac{\mu}{2\pi^2|\alpha+\gamma|^2}-1\right)^2+g(\alpha,\gamma,r,s)\right]$$

$$+s^3\sum_{\gamma\in\Lambda^*}(2\pi^2|\alpha+\gamma|^2)^{-s}f(\alpha,\gamma,r,s).$$

For any norm $\|\ \|$ on matrices there exists a positive constant c_r such that for any $\gamma\in\Lambda^*$,

$$\|\mathcal{M}_{\alpha,\gamma,r}-2\pi^2|\alpha+\gamma|^2\mathrm{Id}\|\leqslant c_r\sqrt{2\pi^2|\alpha+\gamma|^2}$$

so that there exist positive constants c_1 and c_2 which verify for any α and γ:

$$|g(\alpha,\gamma,r,s)|\leqslant c_1(2\pi^2|\alpha+\gamma|^2)^{-3/2},$$

$$|f(\alpha,\gamma,r,s)|\leqslant c_2(2\pi^2|\alpha+\gamma|^2)^{-3/2}.$$

These bounds on f and g ensure that the derivative at $s=0$ of the corresponding terms vanish (they are products of s^2 times functions which are holomorphic around 0). So

$$\zeta'_{\hat{\alpha},r}(0)=r\zeta'_{\hat{\alpha}}(0)+\left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0}\left[\frac{s^2}{2}\sum_{\gamma\in\Lambda^*}(2\pi^2|\alpha+\gamma|^2)^{-s-2}\times\left(8\pi^2|\alpha+\gamma|^2\sum_{q=2}^{r}|\lambda_q|^2+4\sum_{q=2}^{r}|\lambda_q|^4\right)\right]$$

$$=r\zeta'_{\hat{\alpha}}(0)+\left.\frac{\mathrm{d}}{\mathrm{d}s}\right|_{s=0}\left[\frac{s^2}{2}\left(4\zeta_{\hat{\alpha}}(s+1)\sum_{q=2}^{r}|\lambda_q|^2+4\zeta_{\hat{\alpha}}(s+2)\sum_{q=2}^{r}|\lambda_q|^4\right)\right].$$

Finally $\zeta_{\hat{\alpha}}$ is holomorphic around 0 and 2 and has a simple pole at $s=1$ which is easily calculated from the Minakshisundaram–Pleijel formula:

$$\operatorname{Tr}\exp -t\Delta_{\hat{\alpha}}=\frac{\eta}{2\pi t}+\mathcal{O}(t) \quad \text{as} \quad t\to 0,$$

$$\begin{aligned}\zeta_{\hat{\alpha}}(s)&=\frac{1}{\Gamma(s)}\int_0^\infty t^{s-1}\operatorname{Tr}(\exp -t\Delta_{\hat{\alpha}})\mathrm{d}t\\&=\frac{1}{\Gamma(s)}\int_0^1 t^{s-1}\left(\frac{\eta}{2\pi t}\right)\mathrm{d}t+\frac{1}{\Gamma(s)}\int_0^1 t^{s-1}\left(\operatorname{Tr}(\exp -t\Delta_{\hat{\alpha}})-\frac{\eta}{2\pi t}\right)\mathrm{d}t\\&\quad+\frac{1}{\Gamma(s)}\int_1^\infty t^{s-1}\operatorname{Tr}(\exp -t\Delta_{\hat{\alpha}})\mathrm{d}t\\&=\frac{\eta}{2\pi(s-1)\Gamma(s)}+\frac{1}{\Gamma(s)}\int_0^1 t^{s-1}\left(\operatorname{Tr}(\exp -t\Delta_{\hat{\alpha}})-\frac{\eta}{2\pi t}\right)\mathrm{d}t\\&\quad+\frac{1}{\Gamma(s)}\int_1^\infty t^{s-1}\operatorname{Tr}(\exp -t\Delta_{\hat{\alpha}})\mathrm{d}t\\&=\frac{\eta}{2\pi(s-1)}+\mathcal{O}(1) \quad \text{as} \quad s\to 1.\end{aligned}$$

(Here $\Delta_{\hat{\alpha}}$ is the Hodge–Laplace operator for $L_{\hat{\alpha}}$.) Thus

$$\zeta'_{\hat{\alpha},r}(0)=r\zeta'_{\hat{\alpha}}(0)+\frac{\eta}{\pi}\sum_{q=2}^{r}|\lambda_q|^2,$$

$$\log(\Theta(F_r\otimes L_{\hat{\alpha}}))=r\log(\Theta(L_{\hat{\alpha}}))-\frac{\eta}{2\pi}\sum_{q=2}^{r}|\lambda_q|^2,$$

$$\Theta(F_r\otimes L_{\hat{\alpha}})=\exp\left(-\frac{\eta}{2\pi}\sum_{q=2}^{r}|\lambda_q|^2\right)e^{-r\pi\,\mathrm{Im}\,\tau(b^2-b+1/6)}\prod_{k=-\infty}^{+\infty}|1-e^{2\pi i(|k|\tau+\varepsilon_k\sqrt{\eta\,\mathrm{Im}\,\tau}\alpha)}|^r$$

(with the notations of theorem 3). This proves part (*ii*) of theorem 4.

2. The case of F_r

The difference here is that $\mathcal{M}_{0,0,r}$ has kernel of rank one spanned by the section σ_1; it is then straightforward to calculate the product of nonvanishing eigenvalues of $\mathcal{M}_{0,0,r}$ (which is diagonal):

$$\det'(\mathcal{M}_{0,0,r})=2^{r-1}\left(\prod_{q=2}^{r}|\lambda_q|^2\right).$$

Then

$$\zeta_{F_r}(s)=\sum_{\mu\in\operatorname{Spec}\Delta_{F_r}\setminus\{0\}}\mu^{-s}=\sum_{\mu\in\operatorname{Spec}\mathcal{M}_{0,0,r}\setminus\{0\}}\mu^{-s}+\sum_{\gamma\in\Lambda^*\setminus\{0\}}\sum_{\mu\in\mathcal{M}_{0,\gamma,r}}\mu^{-s}.$$

The second term is treated exactly as before so that

$$\zeta'_{F_r}(0)=-\log\det'(\mathcal{M}_{0,0,r})+r\zeta'_{\mathcal{O}}(0)+\frac{\eta}{\pi}\sum_{q=2}^{r}|\lambda_q|^2,$$

$$\log\Theta(F_r)=\frac{1}{2}\sum_{q=2}^{r}\log(2|\lambda_q|^2)+r\log\Theta(\mathcal{O})-\frac{\eta}{2\pi}\sum_{q=2}^{r}|\lambda_q|^2,$$

$$\Theta(F_r)=\sqrt{\prod_{q=2}^{r}(2|\lambda_q|^2)}\exp\left(\frac{-\eta}{2\pi}\sum_{q=2}^{r}|\lambda_q|^2\right)(2\eta\,\mathrm{Im}\,\tau)^{r/2}e^{-r\pi\,\mathrm{Im}\,\tau/6}\prod_{k>0}|1-e^{2\pi ik\tau}|^{2r}$$

(with the notations of theorem 3). This proves part *(i)* of theorem 4.

3. The case of $F_r \otimes A$ where A is a line bundle of degree $d>0$

First of all, consider the matrices

$$\mathcal{M}^*_\ell = \begin{pmatrix} 2|\mu_\ell|^2 + \frac{2\pi(\ell-1)d}{\eta} & 2\mu_{\ell-1}\sqrt{\frac{\pi(\ell-1)d}{\eta}} & 0 & \dots & 0 \\ 2\overline{\mu}_{\ell-1}\sqrt{\frac{\pi(\ell-1)d}{\eta}} & 2|\mu_{\ell-1}|^2 + \frac{2\pi(\ell-2)d}{\eta} & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 2\mu_1\sqrt{\frac{\pi d}{\eta}} \\ 0 & \dots & 0 & 2\overline{\mu}_1\sqrt{\frac{\pi d}{\eta}} & 2|\mu_1|^2 \end{pmatrix}$$

then one directly obtains

$$\begin{aligned} \det \mathcal{M}^*_\ell &= \left(\frac{2\pi(\ell-1)d}{\eta} + 2|\mu_\ell|^2\right)\det \mathcal{M}^*_{\ell-1} - 4|\mu_{\ell-1}|^2 \frac{\pi(\ell-1)d}{\eta}\det \mathcal{M}^*_{\ell-2} \\ &= 2^\ell |\mu_1|^2|\mu_2|^2\cdots|\mu_\ell|^2. \end{aligned} \tag{7}$$

Now set

$$\mathcal{M}_\ell = \begin{pmatrix} \frac{2\pi(\ell-1)d}{\eta} & 2\mu_{\ell-1}\sqrt{\frac{\pi(\ell-1)d}{\eta}} & 0 & \dots & 0 \\ 2\overline{\mu}_{\ell-1}\sqrt{\frac{\pi(\ell-1)d}{\eta}} & 2|\mu_{\ell-1}|^2 + \frac{2\pi(\ell-2)d}{\eta} & \ddots & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 2\mu_1\sqrt{\frac{\pi d}{\eta}} \\ 0 & \dots & 0 & 2\overline{\mu}_1\sqrt{\frac{\pi d}{\eta}} & 2|\mu_1|^2 \end{pmatrix}$$

and consider the characteristic polynomials

$$P^*_\ell(X) = \det(\mathcal{M}^*_\ell - X\mathrm{Id}),$$

$$P_\ell(X) = \det(\mathcal{M}_\ell - X\mathrm{Id}) = (-X)^\ell + (-X)^{\ell-1}\mathrm{Tr}\,\mathcal{M}_\ell + \dots + (-X)\det{}'\,\mathcal{M}_\ell,$$

where $\det'\mathcal{M}_\ell$ is the product of nonzero eigenvalues of $\mathcal{M}_\ell$ [of course $\det\mathcal{M}_\ell$ vanishes from (7)]. The obvious relation

$$P^*_\ell(X) = P_\ell(X) + 2|\mu_\ell|^2 P^*_{\ell-1}(X)$$

yields

$$P_\ell(X)=\left(\frac{2\pi(\ell-1)d}{\eta}-X\right)P^*_{\ell-1}(X)-4|\mu_{\ell-1}|^2\frac{\pi(\ell-1)d}{\eta}P^*_{\ell-2}(X)$$
$$=\left(\frac{2\pi(\ell-1)d}{\eta}-X\right)P_{\ell-1}(X)-2|\mu_{\ell-1}|^2X\,P^*_{\ell-2}(X)$$

from which one successively deduces

$$\det'\,\mathcal{M}_\ell=\frac{2\pi(\ell-1)d}{\eta}\det'\,\mathcal{M}_{\ell-1}+2|\mu_{\ell-1}|^2\det\mathcal{M}^*_{\ell-2}$$
$$=2^{\ell-1}\sum_{j=0}^{\ell-1}\left(\frac{\pi d}{\eta}\right)^{\ell-1-j}(\ell-1)(\ell-2)\cdots(j+1)\prod_{i=1}^{j}|\mu_i|^2.$$

Thus changing μ_i by $\lambda_{\ell+1-i}$ yields for $\ell\leqslant r$,

$$\det'\,\mathcal{M}_{r,k,\ell}=\left(\frac{2\pi d}{\eta}\right)^{\ell-1}(\ell-1)!\sum_{j=0}^{\ell-1}\left(\frac{\pi d}{\eta}\right)^{-j}\frac{|\lambda_{\ell-j+1}|^2|\lambda_{\ell-j+2}|^2\cdots|\lambda_\ell|^2}{j!},$$

where the $j=0$ term of the sum is to be taken equal to 1.

The characteristic polynomials $P_{r,k,\ell}(X)=\det(\mathcal{M}_{r,k,\ell}-X\mathrm{Id})$ verify for $\ell\geqslant r$,

$$P_{r,k,\ell}(X)=\left(2|\lambda_r|^2+\frac{2\pi(\ell-r)d}{\eta}-X\right)P_{r-1,k,\ell}(X)-4|\lambda_r|^2\frac{\pi(\ell-r+1)d}{\eta}P_{r-2,k,\ell}(X)$$

from which one deduces:

$$P_{r,k,\ell}(X)=(-X)^r+(-X)^{r-1}\left[\frac{2\pi d}{\eta}\left(r\ell-\frac{r(r+1)}{2}\right)+2\sum_{q=2}^{r}|\lambda_q|^2\right]$$
$$+(-X)^{r-2}\left[4\sum_{p<q}(|\lambda_p|^2|\lambda_q|^2)\right.$$
$$\left.+\frac{4\pi d}{\eta}\left((r-2)\ell\sum_{q=2}^{r}|\lambda_q|^2+\sum_{q=2}^{r}|\lambda_q|^2\left[-\frac{(r-1)(r-2)}{2}-2(r-q)\right]\right)\right.$$
$$\left.+\frac{4\pi^2d^2}{\eta^2}r(r-1)\left(\frac{\ell^2}{2}-\frac{(r+1)\ell}{2}+\frac{(r+1)(3r+2)}{24}\right)\right]$$
$$+\cdots+\left(\frac{2\pi d}{\eta}\right)^r(\ell-1)(\ell-2)\cdots(\ell-r).$$

Thus one gets the following symmetric functions of the eigenvalues of $\mathcal{M}_{r,k,\ell}$:

$$\sum_{\mu\in\operatorname{Spec}\mathcal{M}_{r,k,\ell}}\mu^2=\frac{4\pi^2d^2r}{\eta^2}\ell^2+\ell\left[-\frac{4\pi^2d^2}{\eta^2}r(r+1)+\frac{16\pi d}{\eta}\sum_{q=2}^{r}|\lambda_q|^2\right]$$
$$+\frac{4\pi^2d^2}{\eta^2}\frac{r(r+1)(2r+1)}{3}+\frac{4\pi d}{\eta}\sum_{q=2}^{r}(-8r+4q+2)|\lambda_q|^2+4\sum_{q=2}^{r}|\lambda_q|^4,$$

$$\sum_{\mu\in\operatorname{Spec}\mathcal{M}_{r,k,\ell}}\left(\mu-\frac{2\pi\ell d}{\eta}\right)^2=\frac{2\pi^2d^2r(r+1)(2r+1)}{3\eta^2}+\frac{8\pi d(\ell+1)}{\eta}\sum_{q=2}^{r}|\lambda_q|^2$$
$$+\frac{16\pi d}{\eta}\sum_{q=2}^{r}q|\lambda_q|^2+4\sum_{q=2}^{r}|\lambda_q|^4$$

from which as before if $\zeta_{r,d}$ stands for the zeta function (1) of $F_r\otimes A$,

$$\zeta_{r,d}(s)=\sum_{\mu\in\operatorname{Spec}\Delta\setminus\{0\}}\mu^{-s}$$
$$=d\sum_{\ell\leqslant r}\sum_{\mu\in\operatorname{Spec}\mathcal{M}_{r,k,\ell}\setminus\{0\}}\mu^{-s}+d\sum_{\ell>r}\left(\frac{2\pi\ell d}{\eta}\right)^{-s}\sum_{\mu\in\operatorname{Spec}\mathcal{M}_{r,k,\ell}}\left[\left(\frac{\eta\mu}{2\pi\ell d}\right)^{-s}-1+1\right]$$
$$=d\sum_{\ell\leqslant r}\cdots+dr\sum_{\ell>r}\left(\frac{2\pi\ell d}{\eta}\right)^{-s}+d\sum_{\ell>r}\left(\frac{2\pi\ell d}{\eta}\right)^{-s}$$
$$\times\left[\sum_{\mu\in\operatorname{Spec}\mathcal{M}_{r,k,\ell}}-s\log\frac{\eta\mu}{2\pi\ell d}+\frac{s^2}{2}\left(\log\frac{\eta\mu}{2\pi\ell d}\right)^2+s^3f(r,\ell,s)\right]$$
$$=d\sum_{\ell\leqslant r}\cdots+dr\sum_{\ell>r}\left(\frac{2\pi\ell d}{\eta}\right)^{-s}-ds\sum_{\ell>r}\left(\frac{2\pi\ell d}{\eta}\right)^{-s}\log\frac{(\ell-1)(\ell-2)\cdots(\ell-r)}{\ell^r}$$
$$+\frac{ds^2}{2}\sum_{\ell>r}\left(\frac{2\pi\ell d}{\eta}\right)^{-s}\left(\sum_{\mu\in\operatorname{Spec}\mathcal{M}_{r,k,\ell}}\left(\frac{\eta\mu}{2\pi\ell d}-1\right)^2+g(r,\ell,s)+2sf(r,\ell,s)\right).$$

As before there exist constants c_f and c_g such that for any ℓ,

$$|f(r,\ell,s)|\leqslant c_f\left(\frac{2\pi\ell d}{\eta}\right)^{-3/2},$$

$$|g(r,\ell,s)|\leqslant c_g\left(\frac{2\pi\ell d}{\eta}\right)^{-3/2},$$

so that the corresponding terms do not contribute to $\zeta'_{r,d}(0)$. Thus

$$\zeta'_{r,d}(0)=-d\sum_{\ell=2}^{r}\log\det{}'\,\mathcal{M}_{r,k,\ell}+dr\,\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\left[\left(\frac{2\pi d}{\eta}\right)^{-s}\left(\zeta(s)-\sum_{\ell=1}^{r}\ell^{-s}\right)\right]$$
$$-d\,\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\left[s\sum_{\ell>r}\left(\frac{2\pi\ell d}{\eta}\right)^{-s}\sum_{m=1}^{r}\log\frac{\ell-m}{\ell}\right]$$
$$+d\,\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\left[\frac{s^2}{2}\sum_{\ell>r}\left(\frac{2\pi\ell d}{\eta}\right)^{-s-2}\left(\frac{2\pi^2d^2r(r+1)(2r+1)}{3\eta^2}\right.\right.$$
$$\left.\left.+\frac{8\pi d(\ell+1)}{\eta}\sum_{q=2}^{r}|\lambda_q|^2+\frac{16\pi d}{\eta}\sum_{q=2}^{r}q|\lambda_q|^2+4\sum_{q=2}^{r}|\lambda_q|^4\right)\right]$$

(where ζ stands for the Riemann zeta function).

Lemma:

$$r\,\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\left[\left(\frac{2\pi d}{\eta}\right)^{-s}\left(\zeta(s)-\sum_{\ell=1}^{r}\ell^{-s}\right)\right]-\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\left[s\sum_{\ell>r}\left(\frac{2\pi\ell d}{\eta}\right)^{-s}\sum_{m=1}^{r}\log\left(\frac{\ell-m}{\ell}\right)\right]$$
$$=\frac{r^2}{2}\log\left(\frac{2\pi d}{\eta}\right)-\frac{r}{2}\log(2\pi)+\sum_{j=1}^{r-1}\log(j!).$$

Thus, simplifying the last term as in the case of $F_r\otimes L_{\hat{\alpha}}$ one obtains:

$$\zeta'_{r,d}(0)=-d\sum_{\ell=2}^{r}\log\left(\left(\frac{2\pi d}{\eta}\right)^{\ell-1}(\ell-1)!\sum_{j=0}^{\ell-1}\left(\frac{\pi d}{\eta}\right)^{-j}\frac{|\lambda_{\ell-j+1}|^2\cdots|\lambda_\ell|^2}{j!}\right)+d\,\frac{r^2}{2}\log\left(\frac{2\pi d}{\eta}\right)$$
$$-\frac{dr}{2}\log(2\pi)+d\sum_{j=1}^{r-1}\log(j!)+d\left(\sum_{q=2}^{r}|\lambda_q|^2\right)\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\left[2s^2\sum_{\ell>r}\left(\frac{2\pi\ell d}{\eta}\right)^{-s-1}\right]$$
$$=-d\sum_{\ell=2}^{r}\log\left(\sum_{j=0}^{\ell-1}\left(\frac{\pi d}{\eta}\right)^{-j}\frac{|\lambda_{\ell-j+1}|^2\cdots|\lambda_\ell|^2}{j!}\right)$$
$$+\frac{dr}{2}\log\left(\frac{2\pi d}{\eta}\right)-\frac{dr}{2}\log(2\pi)+\frac{\eta}{\pi}\sum_{q=2}^{r}|\lambda_q|^2,$$

$$\log\Theta(F_r\otimes A)=\frac{d}{2}\sum_{\ell=2}^{r}\log\left(\sum_{j=0}^{\ell-1}\left(\frac{\pi d}{\eta}\right)^{-j}\frac{|\lambda_{\ell-j+1}|^2\cdots|\lambda_\ell|^2}{j!}\right)-\frac{dr}{4}\log\left(\frac{d}{\eta}\right)-\frac{\eta}{2\pi}\sum_{q=2}^{r}|\lambda_q|^2\,,$$

$$\Theta(F_r\otimes A)=\prod_{\ell=2}^{r}\left(\sum_{j=0}^{\ell-1}\left(\frac{\pi d}{\eta}\right)^{-j}\frac{|\lambda_{\ell-j+1}|^2\cdots|\lambda_\ell|^2}{j!}\right)^{d/2}\left(\frac{d}{\eta}\right)^{-dr/4}\exp\left(-\frac{\eta}{2\pi}\sum_{q=2}^{r}|\lambda_q|^2\right).$$

This proves part *(iii)* of theorem 4.

Proof (of the lemma): Let $\tilde{\gamma}$ be the Euler constant:

$$\tilde{\gamma}=\lim_{n\to\infty}\left(\sum_{k=1}^{n}\frac{1}{k}-\log n\right)=\lim_{s\to0}\left(\zeta(1+s)-\frac{1}{s}\right)$$

then for any $1\leqslant m\leqslant r$:

$$\sum_{\ell>r}\left(\log\frac{\ell-m}{\ell}+\frac{m}{\ell}\right)=m\tilde{\gamma}+\log\left(\frac{r!}{(r-m)!}\right)-\sum_{\ell=1}^{r}\frac{m}{\ell}.$$

The proposed quantity then equals

$$\begin{aligned}
&=-r\log\left(\frac{2\pi d}{\eta}\right)(\zeta(0)-r)+r\left(\zeta'(0)+\sum_{\ell=2}^{r}\log\ell\right)\\
&\quad-\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\left[s\left(\frac{2\pi d}{\eta}\right)^{-s}\sum_{\ell>r}\frac{-r(r+1)}{2}\ell^{-s-1}\right]\\
&\quad-\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\left[s\left(\frac{2\pi d}{\eta}\right)^{-s}\sum_{\ell>r}\ell^{-s}\sum_{m=1}^{r}\left(\log\frac{\ell-m}{\ell}+\frac{m}{\ell}\right)\right]\\
&=r\left(r+\frac{1}{2}\right)\log\left(\frac{2\pi d}{\eta}\right)-\frac{r}{2}\log(2\pi)+r\log(r!)+\frac{r(r+1)}{2}\\
&\quad\times\frac{\mathrm{d}}{\mathrm{d}s}\Big|_{s=0}\left[s\left(\frac{2\pi d}{\eta}\right)^{-s}\left(\zeta(s+1)-\sum_{\ell=1}^{r}\ell^{-s-1}\right)\right]-\sum_{\ell>r}\sum_{m=1}^{r}\left(\log\frac{\ell-m}{\ell}-\frac{\ell-m}{\ell}\right)\\
&=r\left(r+\frac{1}{2}\right)\log\left(\frac{2\pi d}{\eta}\right)-\frac{r}{2}\log(2\pi)+r\log(r!)-\frac{r(r+1)}{2}\log\left(\frac{2\pi d}{\eta}\right)\\
&\quad+\frac{r(r+1)}{2}\left(\tilde{\gamma}-\sum_{\ell=1}^{r}\frac{1}{\ell}\right)-\sum_{m=1}^{r}\left(m\tilde{\gamma}+\log\frac{r!}{(r-m)!}-\sum_{\ell=1}^{r}\frac{m}{\ell}\right)
\end{aligned}$$

from which the lemma immediately follows. □

IV. SECOND EVALUATION OF THE ANALYTIC TORSION

A. Bismut, Gillet, and Soulé's formula

Let ξ be any holomorphic Hermitian vector bundle over E. Let $H^1(\xi)$ denote the cohomology group $H^1(E,\mathcal{O}_E(\xi))$. The determinant of the cohomology of ξ is taken to be the complex line [cf. Ref. 28, (1.1)]

$$\delta(\xi)=(\det\Gamma(\xi))^{-1}\otimes\det H^1(\xi),$$

where for any vector space V, $\det V$ is the complex line $\wedge^{\dim V}V$, and for a complex line δ, δ^{-1} is its dual. Hodge theory provides an identification of the cohomology groups $\Gamma(\xi)$ and $H^1(\xi)$ with the space of harmonic sections and harmonic forms of type (0,1) with values in ξ. The L^2 inner product on $\Gamma^\infty(E,\xi)$ and $\Gamma^\infty(E,T^{*(0,1)}E\otimes\xi)$ restricted to harmonic forms gives Hermitian scalar products on $\Gamma(\xi)$ and $H^1(\xi)$.

Definition 5: The L^2 metric on $\delta(\xi)$ is the inner product associated with the Hermitian L^2 product on $\Gamma(\xi)$ *and $H^1(\xi)$. Its norm is denoted $|\ |_{L^2}$.*

The Quillen metric on $\delta(\xi)$ is the inner product whose associated norm is

$$\|\ \|_Q=|\ |_{L^2}\cdot\Theta(\xi)$$

where $\Theta(\xi)$ is the analytic torsion of ξ. (cf. Ref. 28, (1.34)).

This Quillen metric will be used in the following way: Let

$$(\Xi):\quad 0\to\xi'\to\xi\to\xi''\to 0$$

be an exact sequence of vector bundles over E. Then the ''long'' exact sequence in cohomology

$$0\to\Gamma(\xi')\to\Gamma(\xi)\to\Gamma(\xi'')\to H^1(\xi')\to H^1(\xi)\to H^1(\xi'')\to 0$$

provides an identification of complex lines:

$$\delta(\xi')\otimes\delta(\xi'')\cong\delta(\xi)$$

or equivalently a canonical element $\mathcal{T}\in\delta(\xi')\otimes\delta(\xi)^{-1}\otimes\delta(\xi'')$. On the other hand if ξ', ξ, and ξ'' are metrized, Chern–Weil theory provides explicit representatives $\mathrm{ch}(\xi')$, $\mathrm{ch}(\xi)$, and $\mathrm{ch}(\xi'')\in\Gamma^\infty(E,\wedge^{\mathrm{even}}T^*E)$ of Chern characters of ξ', ξ, and ξ'', and Bott and Chern constructed in Ref. 22 (see also Ref. 21, theorem 1.29) an explicit form $\widetilde{\mathrm{ch}}(\Xi)$ such that

$$-\frac{\overline{\partial}\partial}{2\pi i}\widetilde{\mathrm{ch}}(\Xi)=-\mathrm{ch}(\xi)+\mathrm{ch}(\xi')+\mathrm{ch}(\xi''),$$

E being endowed with a parallel (Kähler) metric, the Todd genus of E in Chern–Weil theory is simply 1 so that theorem 0.3 of Ref. 21 becomes here

Theorem 6:

$$\log\|\mathcal{T}\|_Q^2=-\int_E\widetilde{\mathrm{ch}}(\Xi),$$

where $\|\ \|_Q$ *is the metric on* $\delta(\xi')\otimes\delta(\xi)^{-1}\otimes\delta(\xi'')$ *associated with the Quillen metrics on* $\delta(\xi')$, $\delta(\xi)$ *and* $\delta(\xi'')$.

B. The transgression form

Let $\mathcal{O}$ denote the trivial line bundle on E. Recall the

Proposition: (Ref. 20, corollary 2) For any $r>0$ *there exists a short exact sequence of vector bundles on the elliptic curve* E:

$$(\Xi_r):\quad 0\to F_r\overset{v}{\to}F_{r+1}\overset{v}{\to}\mathcal{O}\to 0.$$

v maps the section $\rho_{r+1,r+1}$ of F_{r+1} to the global section 1 of $\mathcal{O}$. Consider the $\mathbb{Z}/2\mathbb{Z}$-graduated vector bundle $(F_r\oplus\mathcal{O})\oplus F_{r+1}$ with its Hermitian compatible connection ∇. Metrics on F_r and F_{r+1} are taken as in (5) so that the first map v of (Ξ_r) is an isometric immersion, the metric on $\mathcal{O}$ is supposed to be parallel and such that the global section 1 has (constant) local norm ν_{r+1}. The operator v of the exact sequence (Ξ_r) is seen as an odd endomorphism of $(F_r\oplus\mathcal{O})\oplus F_{r+1}$, let v^* be its adjoint: one then obtains an isometric immersion $v^*:\mathcal{O}\to F_{r+1}$. For any non-negative $t\in\mathbb{R}$, define the superconnection on $(F_r\oplus\mathcal{O})\oplus F_{r+1}$,

$$C_t=\nabla+\sqrt{t}(v+v^*).$$

Consider the endomorphism N_V of $(F_r\oplus\mathcal{O})\oplus F_{r+1}$ which multiplies by 0 (respectively 1, respectively, 2) the elements of F_r (respectively of F_{r+1}, respectively of $\mathcal{O}$) and Tr_s the supertrace (which is the trace on $F_r\oplus\mathcal{O}$ minus the trace on F_{r+1}). Let $\phi\in\mathrm{End}(\wedge^{\mathrm{even}}T^*E)$ be the operator which divides 2-forms on E by $2\pi i$ and leaves functions unchanged. Then from Ref. 21, definition 1.16, theorem 1.17, and corollary 1.30

$$\widetilde{\mathrm{ch}}(\Xi_r)=\phi R'(0),$$

where R is the meromorphic continuation to $\mathbb{C}$ of the holomorphic function (with values in $\Gamma^\infty(E,\wedge^{\mathrm{even}}T^*_{\mathbb{R}}E)$)

$$R(s)=\frac{-1}{\Gamma(s)}\int_0^{+\infty}t^{s-1}\,\mathrm{Tr}_s(N_V\exp-C_t^2)\mathrm{d}t.$$

If one trivializes F_r and F_{r+1} in the σ_q, one obtains from (5) that

$$\nabla\sigma_q = -\overline{\lambda}_{q+1}\sigma_{q+1}dz + \lambda_q\sigma_{q-1}d\overline{z}$$

Let ε be the endomorphism of $\wedge^\bullet T^*E$ which multiplies by $(-1)^k$ the forms of degree k. The matrix of C_t with respect to $F_r \oplus F_{r+1} \oplus \mathcal{O}$ then reads (F_r and F_{r+1} being trivialised in the σ_q and $\mathcal{O}$ in the global parallel unitary section $1/\nu_{r+1}$)

$$C_t = \begin{pmatrix}
d & \lambda_2 d\overline{z} & 0 & \cdots & 0 & \varepsilon\sqrt{t} & 0 & \cdots & \cdots & \cdots & 0 & 0 \\
-\overline{\lambda}_2 dz & d & \ddots & \ddots & \vdots & 0 & \varepsilon\sqrt{t} & \ddots & & & \vdots & \vdots \\
0 & \ddots & \ddots & \ddots & 0 & \vdots & \ddots & \ddots & \ddots & & \vdots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \lambda_r d\overline{z} & \vdots & & \ddots & \ddots & \ddots & \vdots & \vdots \\
0 & \cdots & 0 & -\overline{\lambda}_r dz & d & 0 & \cdots & \cdots & 0 & \varepsilon\sqrt{t} & 0 & 0 \\
\varepsilon\sqrt{t} & 0 & \cdots & \cdots & 0 & d & \lambda_2 d\overline{z} & 0 & \cdots & \cdots & 0 & 0 \\
0 & \ddots & \ddots & & \vdots & -\overline{\lambda}_2 dz & \ddots & \ddots & \ddots & & \vdots & \vdots \\
\vdots & \ddots & \ddots & \ddots & \vdots & 0 & \ddots & \ddots & \ddots & \ddots & \vdots & \vdots \\
\vdots & & \ddots & \ddots & 0 & \vdots & \ddots & \ddots & \ddots & \ddots & & \\
\vdots & & & \ddots & \varepsilon\sqrt{t} & \vdots & & \ddots & \ddots & \ddots & \lambda_{r+1} d\overline{z} & 0 \\
0 & \cdots & \cdots & \cdots & 0 & 0 & \cdots & \cdots & 0 & -\overline{\lambda}_{r+1} dz & d & \varepsilon\sqrt{t} \\
0 & \cdots & \cdots & \cdots & 0 & 0 & \cdots & \cdots & \cdots & 0 & \varepsilon\sqrt{t} & d
\end{pmatrix}.$$

Indeed, v (and v^*) act on a differential form with values in $(F_r \oplus \mathcal{O}) \oplus F_{r+1}$ as

$$v(\theta \otimes \varsigma) = \varepsilon\theta \otimes v(\varsigma)$$

[here θ is a local differential form and ς a local section of $(F_r \oplus \mathcal{O}) \oplus F_{r+1}$]; this is a consequence of the $\mathbb{Z}/2\mathbb{Z}$-grading of $\wedge^\bullet T^*E \hat{\otimes} ((F_r \oplus \mathcal{O}) \oplus F_{r+1})$ (cf. Ref. 21, p. 57, this property is essential in proving Ref. 21, proposition 1.6). Thus

$$C_t^2 = t\mathrm{Id} + M_1 \varepsilon dz + M_2 \varepsilon d\overline{z} + M_3 dz \wedge d\overline{z},$$

where M_3 is diagonal with entries

$$|\lambda_2|^2, |\lambda_3|^2 - |\lambda_2|^2, \cdots, |\lambda_r|^2 - |\lambda_{r-1}|^2, -|\lambda_r|^2,$$

$$|\lambda_2|^2, |\lambda_3|^2 - |\lambda_2|^2, \cdots, |\lambda_{r+1}|^2 - |\lambda_r|^2, -|\lambda_{r+1}|^2,$$

$$0$$

and M_2 is the conjugated transpose of

$$M_1=\begin{pmatrix} 0 & \cdots & \cdots & 0 & 0 & \cdots & \cdots & \cdots & 0 & 0 \\ \vdots & & & \vdots & \vdots & & & & \vdots & \vdots \\ \vdots & & & \vdots & \vdots & & & & \vdots & \vdots \\ 0 & \cdots & \cdots & 0 & 0 & \cdots & \cdots & \cdots & 0 & 0 \\ 0 & \cdots & \cdots & 0 & 0 & \cdots & \cdots & \cdots & 0 & 0 \\ 0 & \ddots & & \vdots & \vdots & & & & \vdots & \vdots \\ \vdots & \ddots & \ddots & \vdots & \vdots & & & & \vdots & \vdots \\ \vdots & & 0 & 0 & \vdots & & & & \vdots & \vdots \\ 0 & \cdots & 0 & \overline{\lambda}_{r+1}\sqrt{t} & 0 & \cdots & \cdots & \cdots & 0 & 0 \\ 0 & \cdots & \cdots & 0 & 0 & \cdots & 0 & -\overline{\lambda}_{r+1}\sqrt{t} & 0 & 0 \end{pmatrix}.$$

One deduces:

$$\exp -C_t^2=e^{-t}(\mathrm{Id}-M_1\varepsilon dz-M_2\varepsilon d\overline{z}-M_3dz\wedge d\overline{z}+\tfrac{1}{2}(M_2M_1-M_1M_2)dz\wedge d\overline{z})$$

with

$$M_2M_1-M_1M_2=|\lambda_{r+1}|^2t\begin{pmatrix} 0 & \cdots & \cdots & 0 & 0 & \cdots & \cdots & \cdots & 0 & 0 \\ \vdots & \ddots & & \vdots & \vdots & & & & \vdots & \vdots \\ \vdots & & 0 & 0 & \vdots & & & & \vdots & \vdots \\ 0 & \cdots & 0 & 1 & 0 & \cdots & \cdots & \cdots & 0 & 0 \\ 0 & \cdots & \cdots & 0 & 0 & \cdots & \cdots & \cdots & 0 & 0 \\ \vdots & & & \vdots & \vdots & \ddots & & & \vdots & \vdots \\ \vdots & & & \vdots & \vdots & & 0 & 0 & 0 & \vdots \\ \vdots & & & \vdots & \vdots & & 0 & 1 & 0 & \vdots \\ 0 & \cdots & \cdots & 0 & 0 & \cdots & 0 & 0 & -1 & 0 \\ 0 & \cdots & \cdots & 0 & 0 & \cdots & \cdots & \cdots & 0 & -1 \end{pmatrix}.$$

Now

$$\mathrm{Tr}_s(N_V\mathrm{Id})=-(r+1)+2,$$

$$\mathrm{Tr}_s(N_VM_1)=\mathrm{Tr}_s(N_VM_2)=\mathrm{Tr}_s(N_VM_3)=0,$$

$$\mathrm{Tr}_s[N_V(M_2M_1-M_1M_2)]=-2|\lambda_{r+1}|^2t,$$

$$\mathrm{Tr}_s(N_V\exp -C_t^2)=(1-r-t|\lambda_{r+1}|^2dz\wedge d\overline{z})e^{-t},$$

$$R(s)=\frac{r-1}{\Gamma(s)}\int_0^{+\infty}t^{s-1}e^{-t}\mathrm{d}t+\frac{|\lambda_{r+1}|^2}{\Gamma(s)}\left(\int_0^{+\infty}t^se^{-t}\,\mathrm{d}t\right)dz\wedge d\overline{z}$$

$$=r-1+|\lambda_{r+1}|^2\frac{\Gamma(s+1)}{\Gamma(s)}dz\wedge d\overline{z}=r-1+s|\lambda_{r+1}|^2dz\wedge d\overline{z}.$$

So that if $d\,\mathrm{Vol}\ (=(i/2)dz\wedge d\overline{z})$ denotes the volume form on E:

$$\widetilde{\mathrm{ch}}(\Xi_r)=\phi R'(0)=|\lambda_{r+1}|^2\frac{dz\wedge d\overline{z}}{2\pi i}=-|\lambda_{r+1}|^2\frac{d\,\mathrm{Vol}}{\pi}. \tag{8}$$

C. Second evaluation of the analytic torsion

1. The case of F_r

From definition 5, theorem 6, and formula (8) one obtains

$$\log(\Theta(F_r))=\log(\Theta(F_{r-1}))+\log(\Theta(\mathcal{O}))+\frac{1}{2}\log|\mathcal{T}|^2_{L^2}+\frac{1}{2}\int_E-|\lambda_r|^2\frac{d\,\mathrm{Vol}}{\pi}$$

where $\mathcal{T}$ is the canonical element of $\delta(\Xi_r):=\delta(F_{r-1})\otimes\delta(F_r)^{-1}\otimes\delta(\mathcal{O})$ associated with the exact sequence

$$0\overset{0}{\to}\Gamma(F_{r-1})\to\Gamma(F_r)\overset{0}{\to}\Gamma(\mathcal{O})\to H^1(F_{r-1})\overset{0}{\to}H^1(F_r)\to H^1(\mathcal{O})\overset{0}{\to}0.$$

The indicated maps are zero maps, the other ones are isomorphisms. The choice of metrics ensures that $\Gamma(F_{r-1})\to\Gamma(F_r)$ is an isometry; the isomorphism $H^1(F_r)\to H^1(\mathcal{O})$ maps $\sigma_r d\bar{z}$ [in the notation of (4)] to $(1/\nu_r)d\bar{z}$ so that its norm in 1 (because of the particular choice of metric on $\mathcal{O}$); the isomorphism $\Gamma(\mathcal{O})\to H^1(F_{r-1})$ maps the global trivial section 1 (which has local norm ν_r) to $\rho_{r-1,r-1}d\bar{z}$ so that its norm is

$$\sqrt{2}\left|\frac{\nu_{r-1}}{\nu_r}\right|.$$

From this one obtains

$$\log|\mathcal{T}|^2_{\delta(\Xi_r)}=\log(2|\lambda_r|^2)$$

($|\ |_{\delta(\Xi_r)}$ is the norm on $\delta(\Xi_r)$ associated to $|\ |_{L^2}$ on $\delta(F_r)$, $\delta(F_{r+1})$, and $\delta(\mathcal{O})$). Thus

$$\log(\Theta(F_r))=\log(\Theta(F_{r-1}))+\log(\Theta(\mathcal{O}))+\frac{1}{2}\log(2|\lambda_r|^2)-|\lambda_r|^2\frac{\eta}{2\pi}$$

$$=r\log(\Theta(\mathcal{O}))+\frac{1}{2}\sum_{q=2}^{r}\log(2|\lambda_q|^2)-\frac{\eta}{2\pi}\left(\sum_{q=2}^{r}|\lambda_q|^2\right)$$

as previously.

2. The case of $F_r\otimes L_{\hat{\alpha}}$ for a nontrivial line bundle $L_{\hat{\alpha}}$

Lemma. If

$$(\Xi):\quad 0\to\xi'\to\xi\to\xi''\to 0$$

is a metrised short exact sequence of vector bundles and β is a metrised vector bundle, then for the exact sequence:

$$(\Xi\otimes\beta):\quad 0\to\xi'\otimes\beta\to\xi\otimes\beta\to\xi''\otimes\beta\to 0$$

one has

$$\widetilde{\mathrm{ch}}(\Xi\otimes\beta)=\widetilde{\mathrm{ch}}(\Xi)\wedge\mathrm{ch}(\beta),$$

where $\mathrm{ch}(\beta)$ *is the Chern–Weil form obtained from* β*'s Hermitian compatible connection.*

Proof: This can be seen either from direct calculation from Ref. 21, definition 1.16 and the multiplicativity of the Chern character form, or using the axiomatic definition of Bott–Chern classes in Ref. 21, sec. 1.f) and the fact that the formula holds for a split exact sequence (Ξ) (where both sides of the equality vanish). □

One thus obtains

$$\widetilde{\mathrm{ch}}(\Xi_r\otimes L_{\hat{\alpha}})=\widetilde{\mathrm{ch}}(\Xi_r)=-|\lambda_r|^2\frac{d\,\mathrm{Vol}}{\pi}$$

(which remains true for any metric on $L_{\hat{\alpha}}$). Thus as before

$$\log(\Theta(F_r\otimes L_{\hat{\alpha}}))=\log(\Theta(F_{r-1}\otimes L_{\hat{\alpha}}))+\log(\Theta(L_{\hat{\alpha}}))-\frac{|\lambda_r|^2}{2}\int_E\frac{d\mathrm{Vol}}{\pi}$$

$$=r\log(\Theta(L_{\hat{\alpha}}))-\frac{\eta}{2\pi}\left(\sum_{q=2}^{r}|\lambda_q|^2\right)$$

(because $L_{\hat{\alpha}}$, $F_r\otimes L_{\hat{\alpha}}$ and $F_{r-1}\otimes L_{\hat{\alpha}}$ are acyclic so that here the L^2 norm of $\mathcal{T}$ is canonically equal to 1).

3. The case of $F_r\otimes A$ for a nonzero degree line bundle A

As before

$$\widetilde{\mathrm{ch}}(\Xi_r\otimes A)=\widetilde{\mathrm{ch}}(\Xi_r)=-|\lambda_r|^2\frac{d\,\mathrm{Vol}}{\pi}$$

so that

$$\log(\Theta(F_r\otimes A))=\log(\Theta(F_{r-1}\otimes A))+\log(\Theta(A))+\frac{1}{2}\log|\mathcal{T}|^2_{L^2}-\frac{|\lambda_r|^2}{2}\int_E\frac{d\,\mathrm{Vol}}{\pi}$$

$\mathcal{T}$ being the canonical element of

$$\delta(F_{r-1}\otimes A)\otimes\delta(F_r\otimes A)^{-1}\otimes\delta(A)$$

associated with the exact sequence

$$0\to\Gamma(F_{r-1}\otimes A)\to\Gamma(F_r\otimes A)\to\Gamma(A)\to H^1(F_{r-1}\otimes A)\to H^1(F_r\otimes A)\to H^1(A)\to 0.$$

All the H^1 vanish, the injection $\Gamma(F_{r-1}\otimes A)\to\Gamma(F_r\otimes A)$ is isometric with orthogonal complement in $\Gamma(F_r\otimes A)$ generated by the mutually orthogonal elements

$$\left(\sum_{j=1}^{r}\frac{(-1)^j}{\sqrt{(r-j)!}}\lambda_{j+1}\lambda_{j+2}\cdots\lambda_r\left(\frac{\pi d}{\eta}\right)^{j/2}\sigma_j\otimes\alpha_{r-j,k}\right)_{1\le k\le d}.$$

They are all of norm

$$\sqrt{\sum_{j=1}^{r}\frac{|\lambda_{j+1}|^2\ldots|\lambda_r|^2}{(r-j)!}\left(\frac{\pi d}{\eta}\right)^j}$$

and project to the

$$\left(\frac{(-1)^r}{\nu_r}\left(\frac{\pi d}{\eta}\right)^{r/2}\alpha_{0,k}\right)_{1\le k\le d},$$

which make an orthogonal base of $\Gamma(A)$. Thus

$$|\mathcal{T}|^2_{L^2}=\left(\sum_{j=1}^{r}\frac{|\lambda_{j+1}|^2\ldots|\lambda_r|^2}{(r-j)!}\left(\frac{\pi d}{\eta}\right)^{j-r}\right)^d$$

the term $j=r$ in this sum is to be taken equal to 1. (The $1/\nu_r$ are ''killed'' by the particular choice of metric on $\mathcal{O}$) then

$$\begin{aligned}\log(\Theta(F_r\otimes A))&=\log(\Theta(F_{r-1}\otimes A))+\log(\Theta(A))-|\lambda_r|^2\frac{\eta}{2\pi}\\&\quad+\frac{d}{2}\log\left(\sum_{j=1}^{r}\frac{|\lambda_{j+1}|^2\ldots|\lambda_r|^2}{(r-j)!}\left(\frac{\pi d}{\eta}\right)^{j-r}\right)\\&=r\log(\Theta(A))-\frac{\eta}{2\pi}\sum_{q=2}^{r}|\lambda_q|^2+\frac{d}{2}\sum_{k=2}^{r}\log\left(\sum_{j=1}^{k}\frac{|\lambda_{j+1}|^2\ldots|\lambda_k|^2}{(k-j)!}\left(\frac{\pi d}{\eta}\right)^{j-k}\right)\end{aligned}$$

as desired.

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Small time controllability of systems on compact Lie groups and spin angular momentum

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In this article, we develop some general results on the properties of the reachable sets for right invariant bilinear systems with state varying on compact Lie groups. The main results consist of a characterization of the set of states reachable in arbitrary time from the identity of the group. This, under suitable assumptions, is proved to be a Lie subgroup of the underlying Lie group. We apply these results to the analysis of the controllability of particles with spin. The results are motivated by and generalize the results in another work [D. D'Alessandro, Sys. Control Lett. **41**, 213–221 (2000)], where the specific model of a spin $\frac{1}{2}$ particle system in an electro-magnetic field was considered. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1388197]

I. INTRODUCTION

In recent years there has been a large amount of interest in the development and application of techniques from control theory for the manipulation of the state of quantum mechanical systems (see, e.g., Refs. 1–4). In typical laboratory experiments, an electro-magnetic field is used to drive the state of a quantum system to a desired value. The electro-magnetic field is seen as a control and classical issues of control theory such as analysis of controllability and development of methods for control have a natural physical interpretation in this setting. As an application of the results in this article, we will consider the simple but important example of a particle with spin angular momentum immersed in an electro-magnetic field and perform an analysis of the controllability of this system. No restriction will be placed on the value of the spin of the particle so that the systems considered include, for example, both Helium ^{3}He and ^{4}He molecules as well as an electron and a proton. In physical situations a time varying electro-magnetic field is used to induce a rotation and an analysis of the controllability for this kind of systems tells us what rotations can be achieved at a given time. This problem was dealt with in Ref. 5 for systems of spin $\frac{1}{2}$ particles and the research there was motivated by the problem of controlling the state of quantum bits in order to achieve prescribed logic operations in quantum computing.[6] For any system of this kind the describing model is given by Schrödinger equation with the control multiplying the state variable. This is a right invariant bilinear system whose state varies on a compact Lie group.

Controllability of systems on Lie groups was dealt with in Ref. 7 and in a number of following papers. References 8 and 9 give an up-to-date account of the main results and we refer to them for further references on this topic. It is a problem of great fundamental and practical importance to characterize the set of states that can be obtained in arbitrary small time. This set is, in general, not the whole Lie group even if the control is allowed to be a general Lebesgue measurable function (see Example 8.1 in Ref. 7). To the best of the author's knowledge, a systematic study of this set has not been carried out in the literature, although sufficient conditions are available for it to be the whole Lie group.[10] In the present article, we present a study of the set of states reachable from the identity of the group at any arbitrary time. We prove that this set is either empty or it is dense in a Lie subgroup of the underlying Lie group. If an additional regularity assumption is verified (small time local controllability of the identity of the group), then this set is, in fact, a connected

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Lie subgroup of the underlying group. The article is organized as follows. Sections II–IV are of general interest since they deal with controllability properties of general right invariant bilinear systems on compact Lie groups. In particular, in Sec. II we describe the mathematical model we want to study and give the basic definitions. We also prove a sufficient condition for the set of states reachable at any arbitrary time from the identity to be empty. This motivates the study of this set in the following two sections. In Sec. III, we prove that this set is either empty or is dense in a Lie subgroup of the underlying Lie group and in Sec. IV we relate the property of this set to be a connected Lie subgroup to the small time local controllability of the identity of the group. If this is verified, given the correspondence between connected Lie subgroups and Lie subalgebras, the problem of characterizing the set of states reachable from the identity at any arbitrary time can be approached studying the structure of the Lie algebra. Sections V and VI contain application of these results to the system of a particle with spin in an electro-magnetic field. In particular, in Sec. V the model for this system is described as a right invariant bilinear system on a compact Lie group and the controllability analysis for this system is presented in Sec. VI.

II. SYSTEMS ON COMPACT LIE GROUPS

In this section we study general systems of the form

$$\dot{X}=AX+\sum_{i=1}^{m} B_i X u_i . \tag{1}$$

The state X varies on a compact matrix Lie group G while the matrices A, B_i, $i=1,\ldots,m$, are constant matrices belonging to the corresponding Lie algebra $\mathcal{G}$. The restriction to *matrix* Lie groups is not necessary in the following and is considered here only for the sake of concreteness. The control functions u_i, $i=1,\ldots,m$, are piecewise continuous functions defined on some interval of $\mathbf{R}^+$. The matrices B_i, $i=1,\ldots,m$, are assumed to be linearly independent although this is done without loss of generality. In fact, it is always possible to reduce the analysis of the behavior of the system (1) to this case by opportunely redefining the control functions. System (1) is right invariant in that if $X(t)$ is a solution corresponding to the initial condition equal to the identity matrix, the solution corresponding to the initial condition F is given by $X(t)F$.

The following Lie algebras and Lie groups are associated to the system in (1):

(i) $\mathcal{L}$ is the Lie algebra generated by $\{A,B_1,\ldots,B_m\}$ and $e^{\mathcal{L}}$ is the corresponding connected Lie subgroup of G.
(ii) $\mathcal{L}_0$ is the ideal in $\mathcal{L}$ generated by $\{B_1,\ldots,B_m\}$ and $e^{\mathcal{L}_0}$ is the corresponding connected Lie subgroup of G.
(iii) $\mathcal{B}$ is the Lie algebra generated by $\{B_1,\ldots,B_m\}$ and $e^{\mathcal{B}}$ is the corresponding connected Lie subgroup of G.

Notice that $\mathcal{L}_0$ has co-dimension 0 or 1 in $\mathcal{L}$ according to whether A is or is not in $\mathcal{L}_0$.

The following sets of states reachable from the identity I are associated to the system (1).

(i) $R(T)$; the set of all the possible values for $X(T)$ [solution of (1) at time T with initial condition equal to the identity I] obtained by varying the controls $u_1,\ldots,u_m$, in the set of all the piecewise continuous functions defined in $[0,T]$. This is also expressed by saying that, for every $X_f \in R(T)$, there exists a piecewise continuous control function defined in $[0,T]$ which *drives* the state of the system from the identity to X_f.
(ii) $\mathcal{R}(\leqslant T) := \cup_{0\leqslant t\leqslant T} R(t)$.
(iii) $\mathcal{R} := \cup_{0\leqslant t<\infty} R(t)$.

We have $R(0)=\mathcal{R}(\leqslant 0)=\{I\}$, and, by right invariance, the set of states reachable *from* a point $X\in G$ are given by $R(T)X$, $\mathcal{R}(\leqslant T)X$ and $\mathcal{R}X$, respectively. Therefore, a study of the states reachable from the identity gives information on the states reachable from any other point. It will be useful sometimes to consider the sets $R^{-1}(T)$. These are the sets of all the matrices X in G for

which there exist control functions, $u_1,\ldots,u_m$, driving the solution of (1) from $X\in R^{-1}(T)$ to the identity I, in time T. This is sometimes called the set of states *controllable* to the identity. By the right invariance property, the set of all the states that can be driven to a state X in time T is given by $R^{-1}(T)X$. It also follows from the right invariance that $R^{-1}(T)=[R(T)]^{-1}$ and that if X is an interior point of $R(T)$, then X^{-1} is an interior point of $R^{-1}(T)$.

From the results of Ref. 7, we have that $\mathcal{R}=G$ if and only if $\mathcal{L}=\mathcal{G}$ and, more in general, $\mathcal{R}=e^{\mathcal{L}}$. Moreover, there exists a time T such that $\mathcal{R}(\leqslant T)=e^{\mathcal{L}}$. At every time t, $R(t)\subseteq e^{At}e^{\mathcal{L}_0}$, and the interior of $R(t)$ with respect to the topology of $e^{At}e^{\mathcal{L}_0}$ is not empty. It also follows from a result in Ref. 10 that, if $\mathcal{B}=\mathcal{L}$, then $R(t)=e^{\mathcal{L}}$, for every $t>0$. This is the case for homogeneous systems $(A=0)$.[11]

The main topic of the following two sections is the study of the set of states reachable at any arbitrary time in the cases where the above recalled condition of Ref. 10 does not guarantee that it is equal to $e^{\mathcal{L}}$. More specifically, we are interested in the study of the set

$$\mathcal{A}:=\cap_{t>0}R(t). \tag{2}$$

The examples in Refs. 5 and 7 show that the set $\mathcal{A}$ might not be the whole $e^{\mathcal{L}}$. In fact, it may be empty, as the following Proposition shows.

Proposition 2.1: If $\mathcal{L}_0$ has co-dimension 1 in $\mathcal{L}$, then $\mathcal{A}$ is empty.

Proof: It follows from the above recalled result in Ref. 7 that, for every $t>0$,

$$R(t)\subseteq e^{At}e^{\mathcal{L}_0}, \tag{3}$$

and therefore $\mathcal{A}\subseteq\cap_{t>0}e^{At}e^{\mathcal{L}_0}$. The right hand side of this inclusion is the empty set, if $A\notin\mathcal{L}_0$. In order to see this, assume $\cap_{t>0}e^{At}e^{\mathcal{L}_0}\neq\varnothing$ and pick $\tau_1,\tau_2>0$, with $\tau_2-\tau_1=t$, such that

$$e^{A\tau_1}F_1=e^{A\tau_2}F_2, \tag{4}$$

for some F_1 and F_2 in $e^{\mathcal{L}_0}$. From this, it follows that

$$e^{A\tau_1}F_1F_2^{-1}e^{-A\tau_1}=e^{At}\in e^{\mathcal{L}_0}, \tag{5}$$

since $e^{\mathcal{L}_0}$ is a normal subgroup (Ref. 12, p. 106 ff.). The fact that $e^{At}\in e^{\mathcal{L}_0}$, for all $t\in\mathbf{R}$, implies $A\in\mathcal{L}_0$, which we have excluded. □

In the following, we consider the system (1) as varying on $e^{\mathcal{L}}$ and the topology on $e^{\mathcal{L}}$ is the one induced by the one of G. Since we will be studying the set $\mathcal{A}$, we can assume, from the previous proposition, that $\mathcal{L}_0=\mathcal{L}$. Since the interior of $R(t)$ is not empty in $e^{At}e^{\mathcal{L}_0}$,[7] for every t, we have, in our case, that $R(t)$ has nonempty interior in $e^{\mathcal{L}}$ for every t.

III. SET OF STATES REACHABLE AT ANY ARBITRARY TIME

In the following three theorems, we assume that $\mathcal{A}$ is not empty. This can be checked, for example, by constructing a class of controls (for example, constant controls) steering to a fixed point in G (for example, the identity) in arbitrary time.

Theorem 3.1: *Assume $\mathcal{A}$ is not empty. Then it is a semigroup and $\overline{\mathcal{A}}$ is a Lie subgroup of G, in particular it contains the identity I.*

Proof: If $X_1\in R(t_1)$, and $X_2\in R(t_2)$, then, by right invariance $X_2X_1\in R(t_1+t_2)$. If X_1 and X_2 are in $\mathcal{A}$, t_1 and t_2 can be chosen positive but otherwise arbitrary, therefore t_2+t_1 is also arbitrary and $X_2X_1\in\mathcal{A}$. This shows that $\mathcal{A}$ is a semigroup. Since $\mathcal{A}$ is a semigroup, so is $\overline{\mathcal{A}}$. The previous argument also shows that if X is in $\mathcal{A}$, then X^n is in $\mathcal{A}$ for every positive integer n. At this point, we follow an idea of Ref. 7 (Thm. 6.5) to prove that X^{-1} is in $\overline{\mathcal{A}}$. Because of compactness, the sequence $\{X^n\}$ has a convergent subsequence $X^{n(k)}$. The sequence of elements in $\mathcal{A}$, $\{X^{n(k+1)-n(k)-1}\}$, converges, as k tends to infinity, to X^{-1} and therefore $X^{-1}\in\overline{\mathcal{A}}$. Since $\overline{\mathcal{A}}$ is a closed subgroup of the Lie group G it is a Lie subgroup of G (see, e.g., Ref. 13, p. 110). □

Theorem 3.2: *Assume $\mathcal{A}$ is not empty. If $t_1<t_2$, then $\overline{R}(t_1)\subseteq\overline{R}(t_2)$.*

Proof: We prove $R(t_1)\subseteq\overline{R}(t_2)$. Let X be an element of $R(t_1)$ and $\{X_n\}$ a sequence of elements in $\mathcal{A}$ converging to the identity which is in $\overline{\mathcal{A}}$ by the previous theorem. Since every X_n is in $R(t_2-t_1)$, all the elements of the sequence $\{XX_n\}$ are in $R(t_2)$ and since this sequence converges to X, $X\in\overline{R}(t_2)$. This also proves that $\overline{R}(t_1)\subseteq\overline{R}(t_2)$. Notice that we also have $intR(t_1)\subseteq intR(t_2)$. This follows immediately from the general property (see, e.g., Ref. 10) $intR(t)=int\overline{R}(t)$, for every $t>0$. □

Theorem 3.3: *Assume $\mathcal{A}$ is not empty. Then, $e^{\mathcal{B}}\subseteq\cap_{t>0}\overline{R}(t)$.*

Proof: Assume $X_f\in e^{\mathcal{B}}$, then there exists an integer $l>0$ and l real numbers $\alpha_1,\ldots,\alpha_l$ such that (see Lemma 6.2 in Ref. 7)

$$X_f=e^{\alpha_l B_{i_l}}e^{\alpha_{l-1}B_{i_{l-1}}}\cdots e^{\alpha_1 B_{i_1}}, \tag{6}$$

with $\{i_1,i_2,\ldots,i_l\}\in\{1,2,\ldots,m\}$. Then the piecewise constant control defined on the interval $[(j-1)/n, j/n)$, $j=1,\ldots,l$, as

$$\begin{aligned} u_{i_j}&=n\alpha_j,\\ u_k&=0,\quad k\neq i_j, \end{aligned} \tag{7}$$

gives for the state of system (1) at time $1/n$

$$X_n:=e^{(A+n\alpha_l B_{i_l})(1/n)}e^{(A+n\alpha_{l-1}B_{i_{l-1}})(1/n)}\cdots e^{(A+n\alpha_1 B_{i_1})(1/n)}. \tag{8}$$

We have that $X_n\in R(1/n)$ and

$$\lim_{n\to\infty}X_n=X_f. \tag{9}$$

Fix $t>0$. For every $n>1/t$, using Theorem 3.2, we have

$$X_n\in\overline{R}(t). \tag{10}$$

This implies $X_f\in\overline{R}(t)$, and since t is arbitrary, we have $X_f\in\cap_{t>0}\overline{R}(t)$. □

IV. CONSEQUENCES OF SMALL TIME LOCAL CONTROLLABILITY

The three theorems proved in the previous section can all be sharpened if we assume *small time local controllability* for the identity element I of the group ($STLCI$). $STLCI$ means that there exists a time $T>0$ such that the identity is in the interior of the reachable set $R(t)$ for every t, $0<t\leqslant T$. This is readily seen to imply that the identity is in the interior of the reachable set $R(t)$ for every $t>0$. This also implies that the identity is in the interior of $R^{-1}(t)$ and, by right invariance, that every point X is an interior point of the set of states controllable to X in time t, which is $R^{-1}(t)X$. The main result will be Theorem 4.3 which states that under this assumption the set $\mathcal{A}$ has the structure of a Lie group whose subalgebra contains $\mathcal{B}$. The following two lemmas contain generalizations of Theorems 3.1–3.3 when $STLCI$ is verified.

Lemma 4.1: $STLCI$ implies that $\mathcal{A}$ is not empty and it is a closed Lie subgroup of G.

Proof: It is obvious that $\mathcal{A}$ is not empty since it contains at least the identity. From Theorem 4.1, all we have to prove is that $\mathcal{A}$ is closed. To see this notice that if $I\in intR(t)$, then $I\in int[R(t)]^{-1}$, namely, I is in the interior of the set of states controllable to the identity in time t. This means, by right invariance, that every $X\in e^{\mathcal{L}}$ is in the interior of the set of states controllable to X in time t, which is $[intR(t)]^{-1}X$. Now, pick $X\in\overline{\mathcal{A}}$. There exists an element $Y\in\mathcal{A}\cap[intR(t)]^{-1}X$. The point Y can be reached from I in time t and X can be reached from Y in time t. Therefore $X\in R(2t)$, and since t is arbitrary, $X\in\mathcal{A}$. □

Lemma 4.2: Assume STLCI is verified. Then $t_1<t_2$ *implies that*

$$R(t_1)\subseteq R(t_2). \tag{11}$$

Moreover, $\cap_{t>0}\overline{R}(t)=\cap_{t>0}R(t):=\mathcal{A}$. *As a consequence,* $e^{\mathcal{B}}\subseteq\mathcal{A}$.

Proof: The proof of (11) follows immediately from the fact that $I\in R(t)$ for every t. As for the second statement, assume that $X_f\in\overline{R}(\tau)$, $\forall\tau>0$. Pick $\tau=t-\epsilon$, with $t>\epsilon>0$. *STLCI* implies that X_f is in $int(R^{-1}(\epsilon)X_f)$. From $X_f\in\overline{R}(t-\epsilon)$, we obtain that $R(t-\epsilon)\cap R^{-1}(\epsilon)X_f$ is not empty. If Y is a point in it, we can steer the state of the system from the identity to Y in time $t-\epsilon$ and from Y to X_f in time ϵ. Therefore, $X_f\in R(t)$ and since t is arbitrary $X_f\in\mathcal{A}$. The fact that $e^{\mathcal{B}}\subseteq\mathcal{A}$ is immediate from Theorem 3.3. □

Theorem 4.3: *If STLCI is verified, then* $\mathcal{A}$ *is a closed, connected Lie subgroup of G whose Lie algebra contains* $\mathcal{B}$.

Proof: The result is already contained in Lemmas 4.1 and 4.2, except for the fact that $\mathcal{A}$ is connected. However, since $R(t)$ is path-connected, for every $t>0$ (see Ref. 7, Lemma 4.4), so is $\overline{R}(t)$. From Lemma 4.2, $\mathcal{A}$ is the intersection of a decreasing sequence of continua [the compact and connected sets $\overline{R}(t)$] and therefore is itself a continuum (see Ref. 14, Theorem 7, p. 212) and in particular it is connected. The second statement follows from the one to one correspondence between subalgebras of $\mathcal{G}$ and connected Lie subgroups of G. □

From Theorem 4.3, it follows that, once *STLCI* is proved, one can approach the problem of characterizing $\mathcal{A}$ at the Lie algebra level. In fact $\mathcal{A}$ is a Lie group whose Lie algebra contains $\mathcal{B}$. One can consider all the Lie algebras containing $\mathcal{B}$. In some cases, as in the case of systems with spin angular momentum considered in the next section, the only Lie algebra containing $\mathcal{B}$ is $\mathcal{L}$, so that if one proves that not every state can be reached in arbitrary time, then it immediately follows that $\mathcal{A}=e^{\mathcal{B}}$.

There have been many studies concerning the property of small time local controllability for a given point in the state space of a nonlinear system. Many results (see, e.g., Ref. 8) deal with the case in which the point is an equilibrium point of the system when the control is set to zero. We give here a criterion, based on the maximum principle.[15,8] The proof is a generalization of the one used in Ref. 5 for the case of two-level quantum systems. We use the following notation: $ad_X^0Y:=Y, ad_X^kY=[X,ad_X^{k-1}Y]$.

Theorem 4.4: *Assume there exists a time T such that, for every* $\tau\leqslant T$, *there exists a piecewise constant control* u_τ *steering from the identity to the identity in time* τ. *Denote the values assumed by the function* u_τ *by* $\mathcal{U}_\tau:=\{u_1,u_2,\ldots,u_{k(\tau)}\}$. *For a value* u_j *define the matrix*

$$F_j:=A+\sum_{i=1}^{m}B_iu_{ij}, \tag{12}$$

where u_{ij}, $i=1,\ldots,m$, *are the components of* u_j. *Assume that, for every* τ, *there exists a* $u_j\in\mathcal{U}_\tau$ *such that*

$$ad_{F_j}^nB_i, \quad n=0,1,2,\ldots,k, \quad i=1,\ldots,m, \tag{13}$$

span the whole Lie Algebra $\mathcal{L}$. *Here k is the dimension of the Lie group. Then, the system has the STLCI property.*

Proof: We apply the maximum principle for systems on Lie groups[15] in the form that gives information on the structure of reachable sets.[8] We obtain that the identity is in the interior of the reachable set at time τ, $R(\tau)$, if the only matrix $M\in\mathcal{L}$ such that

$$\left\langle M,X^{-1}(t)\left(A+\sum_{i=1}^{m}B_iu_{ij}\right)X(t)\right\rangle=\min_{v_1,\ldots,v_m}\left\langle M,X^{-1}(t)\left(A+\sum_{i=1}^{m}B_iv_i\right)X(t)\right\rangle=\text{const} \tag{14}$$

is the zero matrix.[15] Since u_j is finite, (14) implies that

$$\langle M, X^{-1}(t)B_iX(t)\rangle \equiv 0, \quad i=1,\ldots,m, \tag{15}$$

in some interval of positive measure, $[t_1,t_2]\subseteq[0,\tau]$. Differentiating (15) n times at t_1, one obtains

$$\langle M, X^{-1}(t_1)ad_{F_j}^n B_iX(t_1)\rangle = 0, \quad n=1,2,\ldots, \tag{16}$$

and since $ad_{F_j}^n B_i$, $n=0,1,\ldots,k$, $i=1,2,\ldots,m$, span the whole Lie algebra $\mathcal{L}$, (16) and (15) with $t=t_1$ imply $M=0$. □

V. PARTICLES WITH SPIN IN AN ELECTRO-MAGNETIC FIELD

In this and the following section we apply the results obtained in the previous sections and perform the controllability analysis of a class of quantum systems. We consider a particle with spin and all the other degrees of freedom ignored under the action of an externally applied electro-magnetic field. We review the basic facts about the mathematical model in this section (see, e.g., Ref. 16) and perform the controllability analysis in the next section.

The (time varying) Hamiltonian describing the system is given by

$$H(t) := \gamma \mathbf{J}\cdot\mathbf{B} := \gamma(J_xB_x(t)+J_yB_y(t)+J_zB_z(t)). \tag{17}$$

In (17) γ is the *gyromagnetic ratio* of the particle, $J_{x,y,z}$ are the x,y,z components of the spin angular momentum operators and $B_{x,y,z}$ are the (time varying) components of the electro-magnetic field which play the role of control. $J_{x,y,z}$ are Hermitian operators on the underlying Hilbert space which satisfy the *fundamental commutation relations*

$$[J_x,J_y]=i\hbar J_z, \quad [J_y,J_z]=i\hbar J_x, \quad [J_z,J_x]=i\hbar J_y. \tag{18}$$

The theory of angular momentum in quantum mechanics originates from these relations (see, e.g., Ref. 16, Chap. 3). The evolution (rotation) operator X is obtained by solving Schrödinger equation

$$i\hbar\dot{X}(t)=H(t)X(t), \tag{19}$$

with initial condition $X(0)$ given by the identity operator. The Hamiltonian is given in (17), and we are interested here in a controllability analysis of this system, namely, we want to investigate what are the rotations that can be achieved in a particular configuration for system (19).

The spin of a particle may assume a value j which is either a positive integer or a positive half integer. For a particle with spin j the operators J_x, J_y, J_z can be represented by $2j+1\times 2j+1$ Hermitian matrices which we still denote by J_x, J_y, J_z. Defining $S_{x,y,z} := -iJ_{x,y,z}/\hbar$, we can write Schrödinger equations (19) and (17) for the evolution matrix as

$$\dot{X}(t)=\gamma(S_xB_x(t)+S_yB_y(t)+S_zB_z(t))X(t), \tag{20}$$

which has to be solved with $X(0)=I_{2j+1\times 2j+1}$. The matrices S_x, S_y, S_z satisfy the commutation relations corresponding to (18):

$$[S_x,S_y]=S_z, \quad [S_y,S_z]=S_x, \quad [S_z,S_x]=S_y. \tag{21}$$

They are skew-Hermitian and it follows immediately from (21) that they have zero trace. Therefore, they span a three-dimensional subalgebra of the Lie algebra su$(2j+1)$ of skew-Hermitian $2j+1\times 2j+1$ matrices with zero trace. We denote this three-dimensional Lie algebra by $\mathcal{G}_j$ and the corresponding connected Lie subgroup of SU$(2j+1)$ by G_j. An inner product $\langle\cdot,\cdot\rangle$ can be defined in $\mathcal{G}_j$ by

$$\langle A,B\rangle := \mathrm{Trace}(AB^*), \tag{22}$$

where B^* denotes the conjugate transpose of the matrix B. The Lie algebra $\mathcal{G}_j$ is semisimple (it is not Abelian and it has no Abelian ideal) and the Lie subgroup G_j is compact. The first statement can be verified by computing the Killing matrix $K_{ik}=\mathrm{Trace}(AdS_iAdS_k)$, $i,k=x,y,z$, and verifying that it is not degenerate (namely its determinant is different from zero). AdS_i is the matrix representation of the linear operator acting on $\mathcal{G}_j$ by $Y\to[S_i,Y]$. This is Cartan's criterion of semisimplicity (see, e.g., Ref. 17, p. 14). Compactness can be checked by applying Weyl's theorem (see, e.g., Ref. 17, p. 20), checking that the Killing matrix K_{ik} is negative definite. Both these results can also be obtained by noticing that for every j, the Lie algebra $\mathcal{G}_j$ is isomorphic to the Lie algebra su(2) [or so(3)], of skew-Hermitian 2×2 matrices with zero trace (antisymmetric real 3×3 matrices) and therefore the corresponding Lie group is isomorphic either to the Lie group of 2×2 special unitary matrices SU(2) or to the Lie group of 3×3 special orthogonal matrices SO(3), and therefore semisimplicity and compactness follow from known properties of the Lie algebras su(2) and so(3) and the corresponding Lie groups SU(2) and SO(3).

The above recalled result about the isomorphism between the Lie group G_j and SU(2) or SO(3) is crucial to the controllability analysis for spin angular momentum systems that will follow because it reduces the study to two cases: the Lie groups SU(2) and SO(3). This result appeared in a study by E. P. Wigner (Ref. 18, pp. 163–168). We state it in the following theorem.

Theorem 5.1: *G_j is isomorphic to* SO(3) *for j integer and isomorphic to* SU(2) *for j half-integer.*

VI. CONTROLLABILITY OF SPIN ANGULAR MOMENTUM

We refer to the system in the general form (1) that we repeat here,

$$\dot{X}=AX+\sum_{i=1}^{m} B_iXu_i, \tag{23}$$

where it is now understood that the matrices $A,B_1,\ldots,B_m$ are in the Lie algebras $\mathcal{G}_j$, as defined in the previous section. This general form includes all the possible geometric configurations that can be realized in a laboratory. For example, one could apply a constant electro-magnetic field and a time varying one at an angle of 30° in the $x-y$ plane so that both the components of the field in the x and y directions have a constant component (modeled by the matrix A) and a time varying component.

First notice that if two (or more) inputs are available, since we have assumed $B_1,\ldots,B_m$ linearly independent, $B_1,\ldots B_m$ generate the whole Lie algebra $\mathcal{G}_j$.[19] In this case, one can apply a result in Ref. 10 (Theorem 5.3) to conclude that $R(t)=G_j$ for every t. Therefore, the only nontrivial case is the single-input one. We also assume that A and B_1 are linearly independent in this case which, in physical terms, means that there are at least two nonparallel directions for the driving electro-magnetic field. If this is not the case, then the solution of (23) is just $X(t)=e^{\int_0^t A+B_1u(\tau)d\tau}$.

Consider now system (23) with a single input assuming the matrices A and B in su(2) [or so(3)] and the corresponding solution X in SU(2) [or SO(3)]. This is always possible because of the Lie group isomorphism of Theorem 5.1. Explicit expressions for this isomorphism are given, for example, in Ref. 20 (pp. 135–141). We write the system as

$$\dot{X}=AX+BXu. \tag{24}$$

Consider the constant input $u=-\langle A,B\rangle/\langle B,B\rangle+v$. The eigenvalues of the matrix $A+Bu$ are $0,\pm i\sqrt{v^2+p^2}$ in the so(3) case and $\pm i\sqrt{(\langle B,B\rangle/2)\,v^2+p^2}$, in the su(2) case. Here p is the magnitude of the purely imaginary conjugate eigenvalues of $A-\langle A,B\rangle/\langle B,B\rangle B$. These expressions show that the nonzero eigenvalues can be made arbitrarily large in magnitude by choosing v large, and therefore the corresponding solution of (24) returns to the identity in arbitrary small

time. This shows that the identity is in $R(t)$ for each t. Define $F:=A-\langle A,B\rangle/\langle B,B\rangle B+Bv$. Since A and B are assumed to be linearly independent so are B and F. Recalling that su(2) [and so(3)] have no two-dimensional subalgebras, it is easily seen that B, $ad_F B$ and $ad_F^2 B$ span the whole su(2) [or so(3)] so that we can apply Theorem 4.4 to conclude that the identity is in the interior of the reachable set $R(t)$ for every t. Using again the fact that su(2) [so(3)] does not have two dimensional subalgebras, we conclude from Theorem 4.3 that the set of states reachable in arbitrary time $\mathcal{A}$ for this system is either the whole group or the subgroup $e^{\mathcal{B}}$, where, in this case, $\mathcal{B}$ is the one dimensional subalgebra generated by B in (24). However, the set of states reachable in arbitrary time is not the whole group. An example of this phenomenon was given in Ref. 7 for SO(3) (Example 8.1 in Ref. 7) and, in fact, this example is somehow canonical since *every* system on SO(3) with one input has this property. In order to see this consider the system (24) and assume, without loss of generality, that A and B are orthogonal (we can always do this by shifting the input $u\rightarrow-\langle A,B\rangle/\langle B,B\rangle+v$). Moreover, by an appropriate change of coordinates and rescaling of time, we can always assume

$$A=\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad B=\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \tag{25}$$

which is the system considered in Ref. 7. The same steps can be carried on for systems varying on SU(2) with Eq.(24) and some algebraic manipulations show that not all the states can be obtained in arbitrary small time.[5] Alternatively one can use the two-to-one correspondence between SU(2) and SO(3) (Refs. 5 and 20, p. 124) and argue that, if all the states could be obtained in SU(2), in arbitrary time, the same would be true for SO(3). Applying the isomorphism of Theorem 5.1, we conclude with the following theorem.

Theorem 6.1: *Consider a system with spin under the action of an electro-magnetic field as described by Eq.* (24). *Then the set of rotations (states) that can be obtained in arbitrary time is given by the one dimensional Lie subgroup corresponding to the one dimensional Lie algebra generated by the matrix B*

During the revision of the present article the author learned about a recent article[21] where the model of spin systems is considered in the context of the theory of symmetric spaces. The result of Theorem 6.1 can also be obtained applying the results in Ref. 21. This can be done by noticing the isomorphism of $\mathcal{G}_j$ with su(2) and the fact that system (24) (with A and B orthogonal) is underlying a Cartan decomposition[17] of the Lie algebra su(2). If t_F denotes the infimum of the times $t\geqslant 0$ such that $X_f\in R(t)$, the only states X_f having $t_F=0$ are the ones in $e^{\mathcal{B}}$. Using the fact that $I\in R(t)$, $\forall t>0$, one can conclude that $e^{\mathcal{B}}=\mathcal{A}$ in this case. The analysis based on the results of Ref. 21 has the merit that can be easily generalized, to characterize, for a given time $T>0$, the set of states that can be reached in time $T+\Delta$, $\forall\Delta>0$. On the other hand, the derivation presented here, based on the general properties of the set $\mathcal{A}$ proved in the previous sections, gives further information concerning the *STLCI* property of the model.

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Exponentiation of the spinor representation of the Lorentz group

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An exact finite expression for the exponentiation of the (spin $\frac{1}{2}$) spinor representation of the Lorentz group is obtained. From this expression an exact finite expression for the exponentiation of the vector representation of the Lorentz group is derived. The two expressions are compared with the literature in the special cases of either spatial rotations or boosts, only. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1388899]

I. INTRODUCTION

The Lorentz group is a Lie group. This guarantees the existence of an exponential mapping from the Lie algebra of the Lorentz group to the Lorentz group itself. Formally, each element of the group is defined as an infinite power series. Obtaining an exact finite expression for this power series is a difficult issue as the Lorentz group is non-Abelian. Concerning this issue, the Baker–Campbell–Hausdorff formula[1] is of no use as it consists of an infinite series of commutator terms which cannot in general be summed explicitly. Therefore, usual treatments of the Lorentz group are almost exclusively concerned with infinitesimal transformations[2] where only the first terms of the power series need to be considered.

However, by focusing on specific representations of the Lorentz group the issue becomes more tractable because it then reduces to the exponentiation of noncommuting matrices, instead of noncommuting generators (operators). The representations of the Lorentz group are the (single-valued) tensor representations, corresponding to tensor fields (integral spin), and the (two-valued) spinor representations, corresponding to spinor fields (half-integral spin)[3].

Based on the Cayley–Hamilton theorem, Zeni and Rodrigues[4] obtained an exact finite expression for the exponentiation of the vector representation of the Lorentz group. Their work was generalized by Barut, Zeni, and Laufer[5] to include all orthogonal groups. Using the Cayley–Hamilton theorem, too, Shimabukuro and Rosa[6] treated the semi-simple Lie groups.

Other methods for obtaining exact finite expressions for the exponentiation of various representations of various Lie groups exist in the literature. Leite and Crouch[7] used the method of Putzer[8] which, analogous to methods based on the Cayley–Hamilton theorem, is based on the calculation of eigenvalues. In connection with the Lorentz group, Clifford algebras are used in a paper by Zeni and Rodrigues[9] and in a paper by Froelich and Salingaros.[2] The methods based on the calculation of eigenvalues have the drawback that the expressions obtained with them can become quite intricate. In this article none of the methods described hitherto will be deployed.

Any field can be written in terms of (spin $\frac{1}{2}$) spinor fields.[10,11] Therefore, an exact finite expression for the exponentiation of any representation of the Lorentz group can, in principle, be derived from an expression for the (spin $\frac{1}{2}$) spinor representation of the Lorentz group. The purpose of this article is to illustrate this line of thought. First, an expression for the (spin $\frac{1}{2}$) spinor representation is obtained. Then, from that expression an expression for the vector representation is derived. Finally, these two expressions are compared with the literature in the special cases of either spatial rotations or boosts, only.

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II. ALGEBRA

The Lorentz algebra is (using $\hbar=1$) given by

$$[S_i,S_j]=i\varepsilon_{ijk}S_k,$$

$$[S_i,K_j]=i\varepsilon_{ijk}K_k,$$

$$[K_i,K_j]=-i\varepsilon_{ijk}S_k,$$

where $\mathbf{S}=(S_1,S_2,S_3)$ and $\mathbf{K}=(K_1,K_2,K_3)$ are the (infinitesimal) generators of spatial rotations and boosts, respectively. (A sum over k is implicit.) In four-vector notation the Lorentz algebra takes the form

$$[M_{\alpha\beta},M_{\gamma\delta}]=i\eta_{\alpha\gamma}M_{\beta\delta}-i\eta_{\alpha\delta}M_{\beta\gamma}+i\eta_{\beta\delta}M_{\alpha\gamma}-i\eta_{\beta\gamma}M_{\alpha\delta},$$

where $\eta=\mathrm{diag}(-1,1,1,1)$ is the Minkowski metric and $M_{\alpha\beta}$ is defined by

$$M_{\alpha\beta}=\begin{pmatrix} 0 & K_1 & K_2 & K_3 \\ -K_1 & 0 & S_3 & -S_2 \\ -K_2 & -S_3 & 0 & S_1 \\ -K_3 & S_2 & -S_1 & 0 \end{pmatrix}. \tag{1}$$

The generators $\mathbf{A}=(A_1,A_2,A_3)$ and $\mathbf{B}=(B_1,B_2,B_3)$, defined by

$$\mathbf{A}=\tfrac{1}{2}(\mathbf{S}+i\mathbf{K}), \tag{2}$$

$$\mathbf{B}=\tfrac{1}{2}(\mathbf{S}-i\mathbf{K}), \tag{3}$$

obey the algebra

$$[A_i,A_j]=i\varepsilon_{ijk}A_k, \tag{4}$$

$$[B_i,B_j]=i\varepsilon_{ijk}B_k, \tag{5}$$

$$[A_i,B_j]=0. \tag{6}$$

III. SPINOR REPRESENTATION

The (spin $\frac{1}{2}$) spinor representation of the Lorentz group is given by

$$M_{\mu\nu}=\frac{1}{4i}[\gamma_\mu,\gamma_\nu], \tag{7}$$

where $\gamma_\mu=(\gamma_0,\boldsymbol{\gamma})=(\gamma_0,\gamma_1,\gamma_2,\gamma_3)$ are the Dirac matrices with (anticommutator) algebra

$$\{\gamma_\mu,\gamma_\nu\}=2\eta_{\mu\nu}.$$

A possible choice, to be used later in the article, for the Dirac matrices is

$$\gamma_0=i\begin{pmatrix} 1_2 & 0_2 \\ 0_2 & -1_2 \end{pmatrix},\quad \boldsymbol{\gamma}=\begin{pmatrix} 0_2 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0_2 \end{pmatrix}, \tag{8}$$

where $\boldsymbol{\sigma}=(\sigma_1,\sigma_2,\sigma_3)$ are the Pauli matrices, 1_2 is the 2×2 identity matrix, and 0_2 is the 2×2 matrix with zero entries only.

Using Eqs. (1) and (7) the matrices **S** and **K** can be written as

$$\mathbf{S}=\frac{1}{4i}\boldsymbol{\gamma}\times\boldsymbol{\gamma}=\frac{1}{2}\gamma_0\gamma_5\boldsymbol{\gamma}, \tag{9}$$

$$\mathbf{K}=\frac{1}{4i}[\gamma_0,\boldsymbol{\gamma}]=\frac{1}{2i}\gamma_0\boldsymbol{\gamma}, \tag{10}$$

where $\gamma_5\equiv i\gamma_0\gamma_1\gamma_2\gamma_3$. From these equations and the definitions of **A** and **B** it follows that

$$\mathbf{A}=\frac{1}{2}\gamma_0\frac{1_4+\gamma_5}{2}\boldsymbol{\gamma}=\frac{1}{2}\gamma_0 P_R\boldsymbol{\gamma}, \tag{11}$$

$$\mathbf{B}=-\frac{1}{2}\gamma_0\frac{1_4-\gamma_5}{2}\boldsymbol{\gamma}=-\frac{1}{2}\gamma_0 P_L\boldsymbol{\gamma}, \tag{12}$$

where the right and left (helicity) projection operators $P_R=(1_4+\gamma_5)/2$ and $P_L=(1_4-\gamma_5)/2$, respectively, have been introduced. The properties of the projection operators imply

$$(\boldsymbol{\chi}\cdot\mathbf{A})^2=(\tfrac{1}{2})^2\boldsymbol{\chi}^2P_L, \tag{13}$$

$$(\boldsymbol{\chi}\cdot\mathbf{B})^2=(\tfrac{1}{2})^2\boldsymbol{\chi}^2P_R, \tag{14}$$

for any (complex) vector $\boldsymbol{\chi}$.

IV. EXPONENTIATION OF THE SPINOR REPRESENTATION

The exponentiation of the (spin $\frac{1}{2}$) spinor representation is given by

$$\Lambda_S=\exp[-i(\boldsymbol{\omega}\cdot\mathbf{S}+\boldsymbol{\zeta}\cdot\mathbf{K})], \tag{15}$$

where $\boldsymbol{\omega}$ and $\boldsymbol{\zeta}$ are real vectors, and **S** and **K** are given by (9) and (10). According to Eqs. (2), (3), and (6), Λ_S can be factorized as

$$\Lambda_S=\exp(-i\boldsymbol{\chi}^*\cdot\mathbf{A})\exp(-i\boldsymbol{\chi}\cdot\mathbf{B}), \tag{16}$$

where the complex vector $\boldsymbol{\chi}$ is defined by

$$\boldsymbol{\chi}=\boldsymbol{\omega}+i\boldsymbol{\zeta}. \tag{17}$$

From Eqs. (13) and (14) and the Taylor expansion of the exponential function it follows that

$$\exp(-i\boldsymbol{\chi}\cdot\mathbf{A})=1_4+[(\Phi_0-1)1_4-i\gamma_0\boldsymbol{\Phi}\cdot\boldsymbol{\gamma}]P_L, \tag{18}$$

$$\exp(-i\boldsymbol{\chi}\cdot\mathbf{B})=1_4+[(\Phi_0-1)1_4+i\gamma_0\boldsymbol{\Phi}\cdot\boldsymbol{\gamma}]P_R, \tag{19}$$

where the functions Φ_0 and $\boldsymbol{\Phi}$ are defined by

$$\Phi_0(\boldsymbol{\chi})=\cos\left(\frac{\chi}{2}\right), \tag{20}$$

$$\boldsymbol{\Phi}(\boldsymbol{\chi})=\begin{cases}\dfrac{1}{\chi}\sin\left(\dfrac{\chi}{2}\right)\boldsymbol{\chi}, & \chi\neq 0,\\[2ex] \dfrac{1}{2}\boldsymbol{\chi}, & \chi=0,\end{cases} \tag{21}$$

with the complex scalar χ defined by

$$\chi^2=\boldsymbol{\chi}^2=\boldsymbol{\omega}^2-\boldsymbol{\zeta}^2+2i\,\boldsymbol{\omega}\cdot\boldsymbol{\zeta}.$$

(The sign ambiguity in the definition of χ does not matter for its usage in this article. The case $\chi=0$ corresponds to $\boldsymbol{\omega}^2=\boldsymbol{\zeta}^2\wedge\boldsymbol{\omega}\cdot\boldsymbol{\zeta}=0$.)

From Eqs. (16), (18), and (19) it follows that

$$\begin{aligned}\Lambda_S&=1_4+[(\Phi_0^*-1)1_4-i\,\gamma_0\boldsymbol{\Phi}^*\cdot\boldsymbol{\gamma}]P_L+[(\Phi_0-1)1_4+i\,\gamma_0\boldsymbol{\Phi}\cdot\boldsymbol{\gamma}]P_R\\&=[\mathrm{Re}(\Phi_0)1_4+i\,\mathrm{Im}(\Phi_0)\,\gamma_5]+[\mathrm{Re}(\boldsymbol{\Phi})1_4+i\,\mathrm{Im}(\boldsymbol{\Phi})\,\gamma_5]\cdot i\,\gamma_5\gamma_0\boldsymbol{\gamma},\end{aligned}\tag{22}$$

which make up an exact finite expression for the exponentiation of the (spin $\frac{1}{2}$) spinor representation of the Lorentz group.

The inverse transformation Λ_S^{-1} is given by $\Lambda_S^{-1}(\boldsymbol{\chi})=\Lambda_S(-\boldsymbol{\chi})$ or, according to Eqs. (20)–(22),

$$\Lambda_S^{-1}=[\mathrm{Re}(\Phi_0)1_4+i\,\mathrm{Im}(\Phi_0)\,\gamma_5]-[\mathrm{Re}(\boldsymbol{\Phi})1_4+i\,\mathrm{Im}(\boldsymbol{\Phi})\,\gamma_5]\cdot i\,\gamma_5\gamma_0\boldsymbol{\gamma}.\tag{23}$$

V. EXPONENTIATION OF THE VECTOR REPRESENTATION

Under Lorentz transformations the Dirac matrices γ_μ transform as a four-vector

$$\Lambda_S^{-1}\gamma^\mu\Lambda_S=(\Lambda_V)^\mu{}_\nu\gamma^\nu,$$

where $(\Lambda_V)^\mu{}_\nu$ are the components of the Lorentz transformation in the vector representation. The trace properties of the Dirac matrices imply

$$(\Lambda_V)^\mu{}_\nu=\tfrac{1}{4}\mathrm{Tr}(\Lambda_S^{-1}\gamma^\mu\Lambda_S\gamma_\nu)=\tfrac{1}{4}\,\eta^{\mu\sigma}\mathrm{Tr}(\Lambda_S^{-1}\gamma_\sigma\Lambda_S\gamma_\nu).\tag{24}$$

Straightforward, but tedious, calculations, inserting the expressions for Λ_S and Λ_S^{-1} in (24) and using the standard trace properties for the Dirac matrices (and the general cyclic property of the trace), give

$$(\Lambda_V)^\mu{}_\nu=\eta^{\mu\sigma}[\Lambda^{(1)}_{\sigma\nu}+\Lambda^{(2)}_{\sigma\nu}+\Lambda^{(3)}_{\sigma\nu}],\tag{25}$$

where

$$\Lambda^{(1)}_{\mu\nu}=[\mathrm{Re}(\Phi_0)^2+\mathrm{Im}(\Phi_0)^2]\,\eta_{\mu\nu},\tag{26}$$

$$\begin{aligned}\Lambda^{(2)}_{\mu\nu}=&-2[\mathrm{Re}(\Phi_0)\mathrm{Re}(\Phi_i)+\mathrm{Im}(\Phi_0)\mathrm{Im}(\Phi_i)]\cdot\varepsilon_{0i\mu\nu}\\&+2[\mathrm{Re}(\Phi_0)\mathrm{Im}(\Phi_i)-\mathrm{Im}(\Phi_0)\mathrm{Re}(\Phi_i)]\cdot(\eta_{i\mu}\eta_{0\nu}-\eta_{i\nu}\eta_{0\mu}),\end{aligned}\tag{27}$$

$$\begin{aligned}\Lambda^{(3)}_{\mu\nu}=&[\mathrm{Re}(\Phi_i)\mathrm{Re}(\Phi_j)+\mathrm{Im}(\Phi_i)\mathrm{Im}(\Phi_j)](\eta_{i\mu}\eta_{j\nu}+\eta_{i\nu}\eta_{j\mu}-\eta_{ij}\delta_{\mu\nu})\\&+[\mathrm{Re}(\Phi_i)\mathrm{Im}(\Phi_j)-\mathrm{Im}(\Phi_i)\mathrm{Re}(\Phi_j)](\varepsilon_{0ij\mu}\eta_{0\nu}+\varepsilon_{0ij\nu}\eta_{0\mu}).\end{aligned}\tag{28}$$

Notice that $\Lambda^{(1)}_{\mu\nu}$ and $\Lambda^{(3)}_{\mu\nu}$ are symmetric matrices whereas $\Lambda^{(2)}_{\mu\nu}$ is an antisymmetric matrix.

The inverse transformation Λ_V^{-1} is, analogous to the spinor case, given by $\Lambda_V^{-1}(\boldsymbol{\chi})=\Lambda_V(-\boldsymbol{\chi})$, which corresponds to the following substitutions:

$$\Lambda^{(1)}_{\mu\nu}\to\Lambda^{(1)}_{\mu\nu},$$

$$\Lambda^{(2)}_{\mu\nu}\to-\Lambda^{(2)}_{\mu\nu}=\Lambda^{(2)}_{\nu\mu},$$

$$\Lambda^{(3)}_{\mu\nu}\to\Lambda^{(3)}_{\mu\nu}.$$

VI. SPATIAL ROTATIONS

According to (17), the case of spatial rotations, only, is characterized by $\boldsymbol{\chi}=\boldsymbol{\omega}$ for which

$$\Phi_0=\cos\left(\frac{\omega}{2}\right), \tag{29}$$

$$\boldsymbol{\Phi}=\sin\left(\frac{\omega}{2}\right)\hat{\boldsymbol{\omega}}, \tag{30}$$

where $\hat{\boldsymbol{\omega}}=\boldsymbol{\omega}/\omega$ has been introduced.

A. Spinor representation

According to Eqs. (22), (29), and (30) the Lorentz transformation for spatial rotations, only, reduces to

$$\begin{aligned}\Lambda_S&=\mathrm{Re}(\Phi_0)1_4+\mathrm{Re}(\boldsymbol{\Phi})\cdot i\gamma_5\gamma_0\boldsymbol{\gamma}\\&=\cos\left(\frac{\omega}{2}\right)1_4+\sin\left(\frac{\omega}{2}\right)\hat{\boldsymbol{\omega}}\cdot i\gamma_5\gamma_0\boldsymbol{\gamma},\end{aligned}$$

or, using the choice of Dirac matrices in (8),

$$\Lambda_S=\cos\left(\frac{\omega}{2}\right)1_4-i\sin\left(\frac{\omega}{2}\right)\begin{pmatrix}\hat{\boldsymbol{\omega}}\cdot\boldsymbol{\sigma} & 0_2\\ 0_2 & \hat{\boldsymbol{\omega}}\cdot\boldsymbol{\sigma}\end{pmatrix}. \tag{31}$$

Equation (31) agrees with Eq. (3.2.44) of Sakurai[12] for the transformation of a two-component spinor.

B. Vector representation

According to Eqs. (25), (29), and (30) the Lorentz transformation for spatial rotations, only, reduces to

$$\Lambda_V=1_4+\sin(\omega)(\hat{\boldsymbol{\omega}}\cdot\mathbf{S})+[1-\cos(\omega)](\hat{\boldsymbol{\omega}}\cdot\mathbf{S})^2, \tag{32}$$

where the matrices $\mathbf{S}$ are defined as

$$(S_i)_{\mu\nu}=-\varepsilon_{0i\mu\nu}, \tag{33}$$

in accordance with Eq. (11.91) of Jackson.[13]

VII. BOOSTS

According to (17), the case of boosts, only, is characterized by $\boldsymbol{\chi}=i\boldsymbol{\zeta}$ for which

$$\Phi_0=\cosh\left(\frac{\zeta}{2}\right), \tag{34}$$

$$\boldsymbol{\Phi}=i\sinh\left(\frac{\zeta}{2}\right)\hat{\boldsymbol{\zeta}}, \tag{35}$$

where $\hat{\boldsymbol{\zeta}}=\boldsymbol{\zeta}/\zeta$ has been introduced.

A. Spinor representation

According to (22), (34), and (35) the Lorentz transformation for boosts, only, reduces to

$$\Lambda_S = \mathrm{Re}(\Phi_0)1_4 + i\,\mathrm{Im}(\boldsymbol{\Phi})\,\gamma_5 \cdot i\gamma_5\gamma_0\boldsymbol{\gamma}$$

$$= \cosh\left(\frac{\zeta}{2}\right)1_4 - \sinh\left(\frac{\zeta}{2}\right)\hat{\boldsymbol{\zeta}}\cdot\gamma_0\boldsymbol{\gamma},$$

or, using the choice of Dirac matrices in (8),

$$\Lambda_S = \cosh\left(\frac{\zeta}{2}\right)1_4 - i\sinh\left(\frac{\zeta}{2}\right)\begin{pmatrix} 0_2 & \hat{\boldsymbol{\zeta}}\cdot\boldsymbol{\sigma} \\ -\hat{\boldsymbol{\zeta}}\cdot\boldsymbol{\sigma} & 0_2 \end{pmatrix}. \tag{36}$$

B. Vector representation

According to (25), (34), and (35) the Lorentz transformation for boosts, only, reduces to

$$\Lambda_V = 1_4 - \sinh(\zeta)(\hat{\boldsymbol{\zeta}}\cdot\mathbf{K}) + [\cosh(\zeta) - 1](\hat{\boldsymbol{\zeta}}\cdot\mathbf{K})^2, \tag{37}$$

where the matrices **K** are defined as

$$(K_i)_{\mu\nu} = \delta_{i\mu}\delta_{0\nu} + \delta_{i\nu}\delta_{0\mu}, \tag{38}$$

in accordance with Eq. (11.91) of Jackson.[13] Equation (37) agrees with Eq. (11.98) of Jackson[13].

VIII. CONCLUSION

In this article an exact finite expression for the exponentiation of the (spin $\frac{1}{2}$) spinor representation of the Lorentz group has been obtained. From that expression an exact finite expression for the exponentiation of the vector representation of the Lorentz group has been derived. The two expressions have been compared with the literature in the special cases of either spatial rotations or boosts, only.

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Ruijsenaars' commuting difference operators and invariant subspace spanned by theta functions

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We study a family of mutually commutative difference operators introduced by Ruijsenaars. The conjugations of these operators with an appropriate function give the Hamiltonians of some relativistic quantum systems. These operators can be regarded as elliptic analogs of the Macdonald operators and their coefficients consist of the Jacobi theta functions. We show that these operators act on the space of meromorphic functions on the Cartan subalgebra of affine Lie algebras and that the space spanned by characters of a fixed positive level is invariant under the action of these operators. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In Ref. 1, Ruijsenaars introduced a family of mutually commutative operators, whose coefficients consist of theta functions, as a relativistic quantum many-body system, i.e., an elliptic difference analog of the Calogero–Moser model. Since then, these operators have been studied extensively from various points of view, in particular, by analogy with the Macdonald operators. The eigenvectors of the Macdonald operators are a two-parameter extension of the Schur functions or the characters of finite-dimensional simple Lie algebras. In the elliptic case, it was clarified in Refs. 2 and 3 that the elliptic analogs of type $A_l^{(1)}$ and $C_2^{(1)}$ have an invariant subspace in the meromorphic functions and that this space is actually spanned by the characters of the corresponding affine Lie algebra. These facts are found through studies of an extension of the Sklyanin algebra.[4] Independently, in Ref. 5, the Boltzmann weight of the matrix elements of Belavin's elliptic R-matrix was calculated using this fact implicitly.

In a series of Cherednik's papers,[6–8] it was clarified that the double affine Hecke algebra plays an essential role in Macdonald theory. There are some algebras that are considered as describing the structure of the elliptic analogs.[4,9–11] In this article, we employ yet another approach called the root algebra to these operators. Although this algebra was introduced by Cherednik, our construction is novel even in the trigonometric cases, due to the existence of spectral parameters. To be more precise, by setting these parameters appropriately, the difference operators automatically become invariant under the action of the Weyl group, while in the theory of the Hecke algebra, they are obtained through symmetrization. Following the previous works[12,13] we construct a family of mutually commuting difference operators associated with arbitrary affine root systems. These operators are shown to act on the vector space of the Weyl group invariant meromorphic functions and, furthermore, on the space spanned by the characters of a fixed positive level.

This article is organized as follows: In Sec. II, we present the notation and definitions used in this article. In Sec. III, we define the root algebras that were introduced by Cherednik in the development of the theory of affine Hecke algebras. In Sec. IV, we demonstrate some examples of the generators of a commutative subalgebra in the root algebras. In Sec. V, we give some representations of the root algebras with a spectral parameter, which consist of Jacobi's theta functions and act on the meromorphic functions on the Cartan subalgebra. We show that when we assign a

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special value to the spectral parameter, the difference operators preserve the Weyl group invariant subspace. By construction, they form a commutative family. In Sec. VI, we calculate the explicit forms of these operators at this spectral parameter and observe that they can be regarded as an elliptic analog of the Macdonald operators. In twisted cases, we have the difference and quantum version of the systems that is recently proposed and is dealt with in terms of the Lax formalism.[14] We also prove that the generators are algebraically independent and thus the commutative subalgebra is isomorphic to a polynomial ring. In Sec. VII, we show in our main theorem (Theorem VII.5) that they have a finite-dimensional invariant subspace of theta functions of positive level, where the key of the proof is due to Refs. 5 and 15. The last section is devoted to the concluding remarks.

To end this section, we present two elliptic difference operators which take the simplest form among the generators respectively in the root systems of type $A_{l-1}^{(1)}$ and $A_{2l}^{(2)}$:

$$\hat{Y}_{A_{l-1}^{(1)}}^{-\lambda_1}=\sum_{j=1}^{l}\prod_{\substack{k=1\\k\neq j}}^{l}\frac{\vartheta_1(x_j-x_k-\mu)}{\vartheta_1(x_j-x_k)}\tau_j(\kappa)\prod_{k=1}^{l}\tau_k(-\kappa/l), \tag{1.1}$$

$$\begin{aligned}\hat{Y}_{A_{2l}^{(2)}}^{-\lambda_1}=&\sum_{j=1}^{l}\left(\left(\prod_{\substack{k=1\\k\neq j}}^{l}\frac{\vartheta_1(x_j-x_k-\mu)}{\vartheta_1(x_j-x_k)}\frac{\vartheta_1(x_j+x_k-\mu)}{\vartheta_1(x_j+x_k)}\right)\left(\prod_{r=0}^{3}\frac{\vartheta_r(x_j-\mu_r)}{\vartheta_r(x_j)}\frac{\vartheta_r(x_j+\kappa/2-\mu_r')}{\vartheta_r(x_j+\kappa/2)}\right)\right)\tau_j(\kappa)\\&+\sum_{j=1}^{l}\left(\left(\prod_{\substack{k=1\\k\neq j}}^{l}\frac{\vartheta_1(-x_j-x_k-\mu)}{\vartheta_1(-x_j-x_k)}\frac{\vartheta_1(-x_j+x_k-\mu)}{\vartheta_1(-x_j+x_k)}\right)\right.\\&\left.\times\left(\prod_{r=0}^{3}\frac{\vartheta_r(-x_j-\mu_r)}{\vartheta_r(-x_j)}\frac{\vartheta_r(-x_j-\kappa/2-\mu_r')}{\vartheta_r(-x_j-\kappa/2)}\right)\right)\tau_j(-\kappa)\\&+\sum_{p=0}^{3}\left(\frac{\pi}{\vartheta_1'(0)}\right)^2\frac{2}{\vartheta_1(\mu)\vartheta_1(\kappa+\mu)}\left(\prod_{r=0}^{3}\vartheta_r(\mu_{\pi_p r}+\kappa/2)\vartheta_r(\mu'_{\pi_p r})\right)\\&\times\left(\prod_{j=1}^{l}\frac{\vartheta_p(x_j-\kappa/2-\mu)}{\vartheta_p(x_j-\kappa/2)}\frac{\vartheta_p(-x_j-\kappa/2-\mu)}{\vartheta_p(-x_j-\kappa/2)}\right),\end{aligned} \tag{1.2}$$

where we have omitted an irrelevant additive constant in the $A_{2l}^{(2)}$ system, and realized the root systems in $\mathbb{C}^l$ in the standard way; $\vartheta_j(x)=\vartheta_j(x;\tau)$ is the Jacobi theta function and $\tau_i(\kappa)$ is a translation of the variable x_i by κ. π_j $(j=0,1,2,3)$ denotes the permutation: $\pi_1=\mathrm{id}$, $\pi_2=(12)\times(03)$, $\pi_3=(13)(02)$, and $\pi_0=(01)(23)$. The parameters κ, μ, μ_r, and μ_r' $(r=0,1,2,3)$ are arbitrary constants. The operator (1.1) was introduced in Ref. 1 together with the whole family of commuting difference operators, while the operator (1.2) was conjectured to be a member of a commutative family in Refs. 16 and 17. The $A_{2l}^{(2)}$-type model was referred to as *D*-type or *BC*-type in previous papers.

If we set $\kappa=l\mu/k$ in the $A_{l-1}^{(1)}$ case and $\kappa=(\mu_{\alpha_0}+2\mu_\theta+2(l-1)\mu)/k$ in the $A_{2l}^{(2)}$ case, where $\mu_{\alpha_0}=\Sigma\mu_r'$ and $\mu_\theta=(\Sigma\mu_r)/2$, then these operators have an invariant subspace which consists of the characters of level k corresponding to each affine Lie algebra. When the parameters μ, μ_θ, and μ_{α_0} are set to be unity, we see that κ reduces to $h^\vee/k$, where $h^\vee$ is the dual Coxeter number. For the derivation of these facts in each case, see Refs. 2, 18 and 19.

II. AFFINE ROOT SYSTEMS

We give some well-known facts about affine root systems and affine Weyl groups,[20–22] which are standard tools in the theory of affine Hecke algebras. Some of the definitions are slightly changed and extended so that they include twisted affine root systems. The notation is mainly due to Ref. 23.

Let $\mathfrak{g}$ be the affine Lie algebra of type $X_N^{(r)}$, $\mathfrak{h}$ its Cartan subalgebra of dim $\mathfrak{h}=l+2$, $I=\{0,...,l\}$ a set of indices, $\Pi=\{\alpha_i|i\in I\}\subset\mathfrak{h}^*$ the set of simple roots, $\Pi^\vee=\{\alpha_i^\vee|i\in I\}\subset\mathfrak{h}$ the set of simple coroots, Δ the root system, Q and $Q^\vee$ the root and coroot lattices, and P and $P^\vee$ the weight and coweight lattices:

$$Q=\bigoplus_{i\in I}\mathbb{Z}\alpha_i\subset P=\bigoplus_{i\in I}\mathbb{Z}\Lambda_i\oplus\mathbb{C}\delta\subset\mathfrak{h}^*, \tag{2.1}$$

$$Q^\vee=\bigoplus_{i\in I}\mathbb{Z}\alpha_i^\vee\subset P^\vee=\bigoplus_{i\in I}\mathbb{Z}\Lambda_i^\vee\oplus\mathbb{C}K\subset\mathfrak{h}, \tag{2.2}$$

where $\langle\alpha_i,\Lambda_j^\vee\rangle=\delta_{ij}$, $\langle\Lambda_i,\alpha_j^\vee\rangle=\delta_{ij}$, and $d=\Lambda_0^\vee$. Since the normalized invariant form is nondegenerate on $\mathfrak{h}$, we have an isomorphism $\nu:\mathfrak{h}\to\mathfrak{h}^*$ defined by

$$\langle\nu(h),h_1\rangle=(h|h_1),\quad h,h_1\in\mathfrak{h}, \tag{2.3}$$

and the induced bilinear form $(\cdot|\cdot)$ on $\mathfrak{h}^*$. Let $\mathring{I}=\{1,...,l\}$, $\mathring{\Pi}=\{\alpha_i|i\in\mathring{I}\}$, and $\mathring{\Pi}^\vee=\{\alpha_i^\vee|i\in\mathring{I}\}$. Let $\mathring{\mathfrak{h}}^*$ be the subspace of $\mathfrak{h}^*$ spanned by $\mathring{\Pi}$ over $\mathbb{C}$. For $\lambda\in\mathfrak{h}^*$, denote by $\overline{\lambda}$ the orthogonal projection of λ on $\mathring{\mathfrak{h}}^*$. Let $\mathring{Q}$ be the sublattice of Q generated by $\mathring{\Pi}$ and $\mathring{P}$ the projection of P on $\mathring{\mathfrak{h}}^*$. The dual notions $\mathring{\mathfrak{h}}$, $\overline{h}$, $\mathring{Q}^\vee$ and $\mathring{P}^\vee$ are defined similarly:

$$\mathring{Q}=\bigoplus_{i\in\mathring{I}}\mathbb{Z}\alpha_i\subset\mathring{P}=\bigoplus_{i\in\mathring{I}}\mathbb{Z}\overline{\Lambda_i}\subset\mathring{\mathfrak{h}}^*, \tag{2.4}$$

$$\mathring{Q}^\vee=\bigoplus_{i\in\mathring{I}}\mathbb{Z}\alpha_i^\vee\subset\mathring{P}^\vee=\bigoplus_{i\in\mathring{I}}\mathbb{Z}\overline{\Lambda_i^\vee}\subset\mathring{\mathfrak{h}}. \tag{2.5}$$

Let $\mathfrak{h}_\mathbb{R}$ be the $\mathbb{R}$-span of $\{\alpha_i^\vee\}_{i\in I}\cup\{d\}$ and let $\mathring{\mathfrak{h}}_\mathbb{R}$ be the $\mathbb{R}$-span of $\{\alpha_i^\vee\}_{i\in\mathring{I}}$. Let Δ^{re}, Δ^{im}, Δ_+, and Δ_- be the set of real roots, imaginary roots, positive roots, and negative roots, respectively. Then one has the disjoint unions $\Delta=\Delta^{\mathrm{re}}\cup\Delta^{\mathrm{im}}=\Delta_+\cup\Delta_-$. Let Δ_l be the set of the longest real roots. For $\alpha\in\Delta^{\mathrm{re}}$, let $\gamma_\alpha:=r$ if $\alpha\in\Delta_l$ and $\gamma_\alpha:=1$ otherwise, where r is from the type $X_N^{(r)}$. Then the real roots are written as

$$\Delta^{\mathrm{re}}=\begin{cases}\{\alpha+n\gamma_\alpha\delta|\alpha\in\mathring{\Delta},n\in\mathbb{Z}\}, & \text{if } X_N^{(r)}\neq A_{2l}^{(2)},\\ \{\alpha+n\gamma_\alpha\delta|\alpha\in\mathring{\Delta},n\in\mathbb{Z}\}\cup\{\frac{1}{2}(\alpha+(2n-1)\delta)|\alpha\in\mathring{\Delta}_l,n\in\mathbb{Z}\}, & \text{if } X_N^{(r)}=A_{2l}^{(2)}.\end{cases} \tag{2.6}$$

For $\alpha\in\Delta^{\mathrm{re}}$, let s_α be a reflection defined by

$$s_\alpha(\lambda):=\lambda-\langle\lambda,\alpha^\vee\rangle\alpha,\quad\lambda\in\mathfrak{h}^*. \tag{2.7}$$

The Weyl group $\mathring{W}$ is generated by the fundamental reflections $\{s_i:=s_{\alpha_i}|i\in\mathring{I}\}$ on $\mathfrak{h}^*$ and the affine Weyl group W is generated by $\{s_i|i\in I\}$. The defining relations are given by $s_i^2=id$ and the Coxeter relations:

$$(s_is_j)^{m_{ij}}=id,\quad\text{for } i\neq j\in I, \tag{2.8}$$

where $m_{ij}=2$ if α_i and α_j are disconnected in the Dynkin diagram and $m_{ij}=3,4,6$ if 1, 2, 3 lines respectively connect α_i and α_j. We note that there is no Coxeter relation in the affine root systems of rank 2. For $\mu\in\mathring{\mathfrak{h}}^*$, we define endomorphisms τ_μ of the vector space $\mathfrak{h}^*$ by

$$\tau_\mu(\lambda):=\lambda+\langle\lambda,K\rangle\mu-((\lambda|\mu)+\tfrac{1}{2}|\mu|^2\langle\lambda,K\rangle)\delta, \tag{2.9}$$

where $|\mu|^2$ stands for $(\mu|\mu)$. The actions of s_α,τ_μ are naturally induced on $\mathfrak{h}$ via the form $\langle\cdot,\cdot\rangle$ as follows ($h\in\mathfrak{h}$):

$$s_\alpha(h)=h-\langle\alpha,h\rangle\alpha^\vee, \tag{2.10}$$

$$\tau_\mu(h)=h+\langle\delta,h\rangle\nu^{-1}(\mu)-(\langle\mu,h\rangle+\tfrac{1}{2}|\mu|^2\langle\delta,h\rangle)K. \tag{2.11}$$

Let a_i and $a_i^\vee$ be the labels of the Dynkin diagram from Table Aff in Ref. 23. Note that $a_0=2$ if $X_N^{(r)}\neq A_{2l}^{(2)}$ and $a_0=1$ otherwise, and that $a_0^{-1}\gamma_\theta=1$. Let $\theta:=\delta-a_0\alpha_0\in\mathring{\Delta}_+$, $M:=\nu(\mathbb{Z}(\mathring{W}\cdot\theta^\vee))\subset\mathring{\mathfrak{h}}^*$. For an arbitrary lattice L, we denote by T_L the corresponding group of translations of L.

Proposition II.1: The group W is the semidirect product $W=\mathring{W}\ltimes T_M$.

Let $\hat{M}:=\{\lambda\in\mathring{\mathfrak{h}}^*|\alpha\in\Delta^{\mathrm{re}},(\alpha|\lambda)\in\gamma_\alpha\mathbb{Z}\}$. Then we see that $\hat{M}\subset\mathring{P}$ and $T_{\hat{M}}$ is normalized by $\mathring{W}$.

Definition II.2: The extended affine Weyl group $\hat{W}$ is the semidirect product $\hat{W}:=\mathring{W}\ltimes T_{\hat{M}}$.

The lattice $\hat{M}$ is taken to be the finest so that $T_{\hat{M}}$ acts on Δ, and thus the extended affine Weyl group acts on Δ. Here are the explicit description of $\hat{M}$ and its canonical basis $\{\lambda_i|i\in\mathring{I}\}$:

$$\hat{M}=\begin{cases}\nu(\mathring{P}^\vee), & \text{if } r=1,\\ \mathring{P}, & \text{otherwise}\end{cases},\quad \lambda_i=\begin{cases}\nu(\overline{\Lambda_i^\vee}), & \text{if } r=1,\\ \overline{\Lambda_i}, & \text{otherwise.}\end{cases} \tag{2.12}$$

We also use $\hat{M}_-:=\oplus_{i\in\mathring{I}}\mathbb{Z}_{\leqslant 0}\lambda_i$.

We use another action of the affine Weyl group on $\mathfrak{h}$. Fix $\kappa\in\mathbb{C}$. Let $\mathfrak{h}_\kappa:=\{h\in\mathfrak{h}|\langle\delta,h\rangle=\kappa\}$. Since W acts on $\mathfrak{h}_\kappa$, W acts on the affine space $\mathfrak{h}_\kappa\mathrm{mod}\mathbb{C}K$. We identify $\mathfrak{h}_\kappa\mathrm{mod}\mathbb{C}K$ with $\mathring{\mathfrak{h}}$ by projection. By this identification, we obtain affine transformations from $\hat{W}$ and affine linear functionals from $\langle\alpha,\cdot\rangle$ for $\alpha\in\Delta$. We denote so-obtained maps by af, so that

$$\mathrm{af}(w)(\overline{h})=\overline{w(h)},\quad \mathrm{af}(\alpha)(\overline{h})=\langle\alpha,h\rangle, \tag{2.13}$$

for $h\in\mathfrak{h}_\kappa$. Explicitly we have for $h\in\mathring{\mathfrak{h}}$

$$\mathrm{af}(\mathring{w})(h)=\mathring{w}(h),\quad \mathrm{af}(\tau_\mu)(h)=h+\kappa\nu^{-1}(\mu), \tag{2.14}$$

$$\mathrm{af}(\mathring{\alpha}+n\delta)(h)=\langle\mathring{\alpha},h\rangle+\kappa n. \tag{2.15}$$

Note that

$$\mathrm{af}(\alpha)\circ\mathrm{af}(w)=\mathrm{af}(w^{-1}\alpha). \tag{2.16}$$

We define an action of the extended affine Weyl group on the space $\mathcal{M}$ of meromorphic functions on $\mathbb{H}:=\mathring{\mathfrak{h}}/\mathring{Q}^\vee$ by

$$(wf)(h):=f(\mathrm{af}(w^{-1})h). \tag{2.17}$$

Let Ω be the subgroup of $\hat{W}$ which stabilizes the affine Weyl chamber C.

Proposition II.3: The subgroup Ω is isomorphic to $\hat{W}/W\simeq T_{\hat{M}}/T_M$ and thus Abelian. The extended affine Weyl group $\hat{W}$ is isomorphic to the semidirect product $W\rtimes\Omega$.

Definition II.4: (1) The length $\ell(w)$ of $w\in W$ is the length ℓ of the reduced decomposition:

$$w = s_{i_1} \cdots s_{i_\ell}, \quad \text{for } i_k \in I, \tag{2.18}$$

$$\ell(id) = 0. \tag{2.19}$$

(2) The length $\ell(\hat{w})$ of $\hat{w} \in \hat{W}$ is the number of the negative roots made positive by $\hat{w}$:

$$\ell(\hat{w}) := |\Delta_{\hat{w}}|, \tag{2.20}$$

$$\Delta_{\hat{w}} := \{\alpha \in \Delta_+ \cap \hat{w}\Delta_-\}, \tag{2.21}$$

which is equivalent to the definition $\ell(w)$ for $w \in W$. The reduced decomposition of $\hat{w} \in \hat{W}$ is $\hat{w} = w\omega = s_{i_1} \cdots s_{i_\ell} \omega$, where $\omega \in \Omega$ and $\ell = \ell(\hat{w}) = \ell(w)$.

The set $\Delta_{\hat{w}}$ is explicitly described as $\Delta_{\hat{w}} = \{\alpha^{(1)} = \alpha_{i_1}, \alpha^{(2)} = s_{i_1}(\alpha_{i_2}), \ldots, \alpha^{(\ell)} = w s_{i_\ell}(\alpha_{i_\ell})\}$. By definition, $\Delta_{\hat{w}}$ is independent of reduced expressions. One sees that $\Omega = \{\omega \in \hat{W}, \ell(\omega) = 0\}$.

Definition II.5: A weight $\lambda \in \hat{M}$ is said to be minuscule if $\Delta_{\tau_{-\lambda}} \subset \mathring{\Delta}_+$.

We use the following useful formulas, which can be easily derived from the previous definitions:

$$\Delta_{\tau_{\lambda_-}} = \begin{cases} \left\{ \alpha - n\gamma_\alpha \delta \,\middle|\, \alpha \in \mathring{\Delta}_+, 0 \geqslant n > \dfrac{1}{\gamma_\alpha}(\lambda_- | \alpha) \right\}, & \text{if } X_N^{(r)} \neq A_{2l}^{(2)}, \\ \left\{ \alpha - n\gamma_\alpha \delta \,\middle|\, \alpha \in \mathring{\Delta}_+, 0 \geqslant n > \dfrac{1}{\gamma_\alpha}(\lambda_- | \alpha) \right\} \cup & \\ \quad \left\{ \dfrac{1}{2}(\alpha - (2n-1)\delta) \,\middle|\, \alpha \in (\mathring{\Delta}_+)_l, 0 \geqslant n > \dfrac{1}{2}(\lambda_- | \alpha) \right\}, & \text{if } X_N^{(r)} = A_{2l}^{(2)}, \end{cases} \tag{2.22a}$$

$$\ell(\tau_{\lambda_-}) = \begin{cases} \displaystyle\sum_{\alpha \in \mathring{\Delta}_+} \left| \frac{1}{\gamma_\alpha}(\alpha | \lambda_-) \right|, & \text{if } X_N^{(r)} \neq A_{2l}^{(2)}, \\ \displaystyle\sum_{\alpha \in \mathring{\Delta}_+} |(\alpha | \lambda_-)|, & \text{if } X_N^{(r)} = A_{2l}^{(2)}, \end{cases} \tag{2.22b}$$

$$\ell(s_j \tau_{-\lambda_i}) = \ell(\tau_{-\lambda_i}) + 1, \tag{2.22c}$$

$$\ell(s_i \tau_{-\lambda_i}) = \ell(\tau_{-\lambda_i}) - 1, \tag{2.22d}$$

$$\ell(\tau_{\lambda_-} w) = \ell(\tau_{\lambda_-}) + \ell(w), \tag{2.22e}$$

$$\ell(\tau_{\lambda_- + \lambda'_-}) = \ell(\tau_{\lambda_-}) + \ell(\tau_{\lambda'_-}), \tag{2.22f}$$

where $i \neq j \in \mathring{I}$, λ_-, $\lambda'_- \in \hat{M}_-$, $w \in \mathring{W}$.

Next we summarize the definitions and properties of theta functions associated with affine Lie algebras.[23,24] In this article, we fix the coefficient of K and d as 0 and $-\tau$, respectively. Thus for $\lambda = \overline{\lambda} + k\Lambda_0 + u\delta \in \mathfrak{h}^*$, we define a function $e^\lambda = e(\lambda)$ on $\mathbb{H}$ by $e^\lambda(h) = e(\lambda)(h) := e^{2\pi i(\langle \overline{\lambda}, h \rangle) - u\tau}$. Although $e^{k\Lambda_0}$ is always 1, we leave such terms in order to see the correspondence to the theta functions in Ref. 23.

Definition II.6: Fix a non-negative integer k. A theta function of level k is a holomorphic function F on $\mathbb{H}$ such that the following condition holds:

$$F(h - \tau\nu^{-1}(\lambda)) = e^{k\lambda + k|\lambda|^2 \delta/2} F(h), \quad \text{for } \lambda \in \hat{M}. \tag{2.23}$$

Let Th^k denote the vector space over $\mathbb{C}$ of the theta functions of level k. For $\lambda \in \mathfrak{h}^*$ such that level $(\lambda)=k>0$ and $\overline{\lambda} \in \mathring{P}$, we set

$$\Theta_\lambda := e^{-|\lambda|^2 \delta/2k} \sum_{\mu \in M} e^{\tau\mu(\lambda)}, \tag{2.24}$$

It is known that $\{\Theta_\lambda | \text{level}(\lambda)=k\}$ is a basis of Th^k.

We also use

$$A_\lambda := \sum_{w \in \mathring{W}} (-1)^{\ell(w)} \Theta_{w(\lambda)}. \tag{2.25}$$

We close this section by observation of the relation between the Jacobi theta function and the theta functions introduced earlier. Consider the root system of type $A_1^{(1)}$. Then $\Pi=\{\alpha_0,\alpha_1\}$, $M=\mathbb{Z}\alpha_1$ and $(\alpha_1|\alpha_1)=2$. We have four theta functions of level 2 for $k \in \mathbb{Z}/4\mathbb{Z}$,

$$\Theta_{2\Lambda_0+k\overline{\Lambda_1}} = e(2\Lambda_0) \sum_{n \in \mathbb{Z}} e\left(-\frac{1}{2}\left(2n+\frac{k}{2}\right)^2 \delta + \left(2n+\frac{k}{2}\right)\alpha_1\right). \tag{2.26}$$

We see that level$(\rho)=h^\vee=2$:

$$A_\rho = \Theta_{2\Lambda_0+(1/2)\alpha_1} - \Theta_{2\Lambda_0-(1/2)\alpha_1} = e\left(\rho - \frac{1}{8}\delta\right) \prod_{\alpha \in \Delta_+} (1-e(-\alpha)). \tag{2.27}$$

This function is related to the Jacobi theta function as

$$-i\,\vartheta_1(\langle \alpha_1, h\rangle;\tau) = A_\rho(h). \tag{2.28}$$

Generally, if $X_N^{(r)} \neq A_{2l}^{(2)}$,

$$A_\rho(h) = e(h^\vee \Lambda_0) f(\tau) (-i)^{|\mathring{\Delta}_+|} \prod_{\alpha \in \mathring{\Delta}_+} \vartheta_1(\langle \alpha, h\rangle; \gamma_\alpha \tau), \tag{2.29}$$

for some function $f(\tau)$ which depends only on τ.

III. ROOT ALGEBRAS

We shall define the root algebras after Cherednik.[22] Let $\mathcal{T}$ be the tensor algebra over $\mathbb{C}$ generated by independent variables $\{R_\alpha | \alpha \in \Delta^{\text{re}}\}$. Then the action of $\hat{w} \in \hat{W}$ on Δ^{re} induces an action on $\mathcal{T}$ by $^{\hat{w}}: R_\alpha \mapsto R_{\hat{w}(\alpha)}$.

Definition III.1: Let $\mathcal{I}$ be the two-sided ideal in $\mathcal{T}$ which is generated by all the elements of the form for $i \neq j \in I$, and $\hat{w} \in \hat{W}$:

$$\underbrace{{}^{\hat{w}}(R_{\alpha_i} \otimes R_{s_i\alpha_j} \otimes R_{s_i s_j \alpha_i} \otimes \cdots)}_{m_{ij} \text{ factors}} - \underbrace{{}^{\hat{w}}(R_{\alpha_j} \otimes R_{s_j\alpha_i} \otimes R_{s_j s_i \alpha_j} \otimes \cdots)}_{m_{ij} \text{ factors}}. \tag{3.1}$$

The root algebra $\tilde{\mathcal{R}}$ is $\mathcal{T}/\mathcal{I}$. $\{R_\alpha | \alpha \in \Delta^{\text{re}}\}$ are called the R-matrices.

Because of the $\hat{W}$-invariance of $\mathcal{I}$, the action of $\hat{W}$ is induced on $\tilde{\mathcal{R}}$. For simplicity, we write products in $\tilde{\mathcal{R}}$ in the usual way for associative algebras.

Theorem III.2 (Cherednik): *(1) There exists a unique set* $\{R_{\hat{w}} | \hat{w} \in \hat{W}\} \subset \tilde{\mathcal{R}}$ *satisfying the relations*

$$R_{vw} = R_v {}^v R_w, \quad R_{\tau_i} = R_{\alpha_i} (i \in I), \quad R_\omega = 1, \tag{3.2}$$

where $\omega\in\Omega$, v, $w\in\hat{W}$ *and* $\ell(vw)=\ell(v)+\ell(w)$.

(2) *We have the R-matrix for* $\hat{w}\in\hat{W}$ *and its arbitrary reduced decomposition* $\hat{w}=w\omega=s_{i_1}\ldots s_{i_\ell}\omega$ *as*

$$R_{\hat{w}}=R_{\alpha^{(1)}}\ldots R_{\alpha^{(\ell)}},$$
$$\alpha^{(1)}=\alpha_{i_1},\quad \alpha^{(2)}=s_{i_1}(\alpha_{i_2}),\quad \ldots,\quad \alpha^{(\ell)}=ws_{i_\ell}(\alpha_{i_\ell})\in\Delta_{\hat{w}}. \tag{3.3}$$

Proof: If $R_{\hat{w}}$ satisfies (3.2), then $R_{\hat{w}}$ must be of the form (3.3). Thus it is sufficient to show that (3.3) is well defined.

Let $\hat{w}=s_{i_1}s_{i_2}\cdots s_{i_\ell}\omega=s_{j_1}s_{j_2}\cdots s_{j_\ell}\omega$ be any two reduced expressions. By Matsumoto's lemma, we see that one can be obtained from the other only by a sequence of Coxeter relations,

$$\begin{aligned}\hat{w}&=s_{i_1}s_{i_2}\cdots s_{i_\ell}\omega\\ &=\underbrace{s_{i_1}s_{i_2}\cdots s_{i_k}}_{w_1}\underbrace{s_is_j\cdots}_{\substack{w_2\\ m_{ij}\ \text{times}}}\underbrace{s_{i_{k+m_{ij}+1}}\cdots s_{i_\ell}\omega}_{w_3} &\text{(3.4a)}\\ &=\underbrace{s_{i_1}s_{i_2}\cdots s_{i_k}}_{w_1}\underbrace{s_js_i\cdots}_{\substack{w_2\\ m_{ij}\ \text{times}}}\underbrace{s_{i_{k+m_{ij}+1}}\cdots s_{i_\ell}\omega}_{w_3} &\text{(3.4b)}\\ &\ \ \vdots\\ &=s_{j_1}s_{j_2}\cdots s_{j_\ell}\omega.\end{aligned}$$

From the expressions (3.4a) and (3.4b), we have the corresponding elements (3.3) in the root algebra,

$$R_{w_1}{}^{w_1}\underbrace{(R_{\alpha_i}R_{s_i\alpha_j}R_{s_is_j\alpha_i}\cdots)}_{m_{ij}\ \text{factors}}{}^{w_1w_2}(R_{w_3}), \tag{3.5a}$$

$$R_{w_1}{}^{w_1}\underbrace{(R_{\alpha_j}R_{s_j\alpha_i}R_{s_js_i\alpha_j}\cdots)}_{m_{ij}\ \text{factors}}{}^{w_1w_2}(R_{w_3}), \tag{3.5b}$$

which are equivalent due to Definition III.1. By applying this argument to each step in (3.4), we conclude that $R_{\hat{w}}$ is uniquely determined by $\hat{w}$. □

Instead of the original root algebra, we use the following extension, where $\tilde{\mathcal{R}}$ is combined with the translation group $T_{\hat{M}}$:

Definition III.3: $\mathcal{R}:=\tilde{\mathcal{R}}\rtimes T_{\hat{M}}$:

$$(R\tau_\lambda)(R'\tau_\mu)=R({}^{\tau_\lambda}R')\tau_{\lambda+\mu}, \tag{3.6}$$

where R, $R'\in\tilde{\mathcal{R}}$ and λ, $\mu\in\hat{M}$.

We see that $\mathcal{R}$ is generated by $\{\tau_{\lambda_i},R_\alpha|i\in\mathring{I},\alpha\in\mathring{\Delta}\}$ if $X_N^{(r)}\neq A_{2l}^{(2)}$ and $\{\tau_{\lambda_i},R_\alpha|i\in\mathring{I},\alpha\in\mathring{\Delta},2\alpha-\delta\in\mathring{\Delta}\}$ if $X_N^{(r)}=A_{2l}^{(2)}$.

Theorem III.4: *The subalgebra* $\mathcal{S}\subset\mathcal{R}$ *generated by* $\{Y^\lambda:=R_{\tau_\lambda}\tau_\lambda|\lambda\in\hat{M}_-\}$ *forms a commutative algebra and is generated by* $\{Y^{-\lambda_i}|i\in\mathring{I}\}$.

Proof: Let $\lambda,\ \mu\in\hat{M}_-$. Then we have $\ell(\tau_\lambda)+\ell(\tau_\mu)=\ell(\tau_{\lambda+\mu})$ by the formulas (2.22), which implies that $R_{\tau_{\lambda+\mu}}$ constructed from two reduced expressions $\tau_{\lambda+\mu}=\tau_\lambda\tau_\mu=\tau_\mu\tau_\lambda$ coincides due to Theorem III.2,

$$R_{\tau_{\lambda+\mu}}=R_{\tau_\lambda}({}^{\tau_\lambda}R_{\tau_\mu})=R_{\tau_\mu}({}^{\tau_\mu}R_{\tau_\lambda}). \tag{3.7}$$

By Definition III.3 and the definition of Y^ν, we have $Y^{\lambda+\mu}=Y^\lambda Y^\mu=Y^\mu Y^\lambda$. □

IV. AFFINE ROOT SYSTEMS OF RANK 3

We present some examples of the above construction. The rank of the lowest nontrivial affine root system is 3 and there are six types of affine root systems of rank 3. We denote $\alpha=\alpha_1$ and $\beta=\alpha_2$ where $|\alpha_1|\geqslant|\alpha_2|$, and $\lambda=\lambda_1$ and $\mu=\lambda_2$, respectively. We have the following systems that are mutually commutative by construction:

$A_2^{(1)}$
$$Y^{-\lambda}=R_\alpha R_{\alpha+\beta}\tau_{-\lambda}, \tag{4.1a}$$
$$Y^{-\mu}=R_\beta R_{\alpha+\beta}\tau_{-\mu}, \tag{4.1b}$$

$C_2^{(1)}$
$$Y^{-\lambda}=R_\alpha R_{\alpha+\beta}R_{\alpha+2\beta}\tau_{-\lambda}, \tag{4.2a}$$
$$Y^{-\mu}=R_\beta R_{\alpha+2\beta}R_{\alpha+\beta}R_{\alpha+2\beta+\delta}\tau_{-\mu}, \tag{4.2b}$$

$G_2^{(1)}$
$$Y^{-\lambda}=R_\alpha R_{\alpha+\beta}R_{2\alpha+3\beta}R_{\alpha+2\beta}R_{\alpha+3\beta}R_{2\alpha+3\beta+\delta}\tau_{-\lambda}, \tag{4.3a}$$
$$Y^{-\mu}=R_\beta R_{\alpha+3\beta}R_{\alpha+2\beta}R_{2\alpha+3\beta}R_{\alpha+\beta}R_{\alpha+3\beta+\delta}R_{2\alpha+3\beta+\delta} R_{\alpha+2\beta+\delta}R_{\alpha+3\beta+2\delta}R_{2\alpha+3\beta+2\delta}\tau_{-\mu}, \tag{4.3b}$$

$A_4^{(2)}$
$$Y^{-\lambda}=R_\alpha R_{\alpha+\beta}R_{\alpha+2\beta}R_{(1/2)\alpha+(1/2)\delta}R_{\alpha+\beta+\delta}R_{(1/2)\alpha+\beta+(1/2)\delta}\tau_{-\lambda}, \tag{4.4a}$$
$$Y^{-\mu}=R_\beta R_{\alpha+2\beta}R_{\alpha+\beta}R_{(1/2)\alpha+\beta+(1/2)\delta}\tau_{-\mu}, \tag{4.4b}$$

$D_3^{(2)}$
$$Y^{-\lambda}=R_\alpha R_{\alpha+\beta}R_{\alpha+2\beta}R_{\alpha+\beta+\delta}\tau_{-\lambda}, \tag{4.5a}$$
$$Y^{-\mu}=R_\beta R_{\alpha+2\beta}R_{\alpha+\beta}\tau_{-\mu}, \tag{4.5b}$$

$D_4^{(3)}$
$$Y^{-\lambda}=R_\alpha R_{\alpha+\beta}R_{2\alpha+3\beta}R_{\alpha+2\beta}R_{\alpha+3\beta}R_{\alpha+\beta+\delta}R_{\alpha+2\beta+\delta} R_{2\alpha+3\beta+3\delta}R_{\alpha+\beta+2\delta}R_{\alpha+2\beta+2\delta}\tau_{-\lambda}, \tag{4.6a}$$
$$Y^{-\mu}=R_\beta R_{\alpha+3\beta}R_{\alpha+2\beta}R_{2\alpha+3\beta}R_{\alpha+\beta}R_{\alpha+2\beta+\delta}\tau_{-\mu}. \tag{4.6b}$$

V. ELLIPTIC *R*-MATRICES

In this section, we give a class of the representation of the root algebra which describes Ruijsenaars' elliptic difference operators associated with affine root systems.

For $\alpha\in\Delta^{\mathrm{re}}$, let $\mu_\alpha\in\mathbb{C}$ be $\hat{W}$-invariant constants: $\mu_{\hat{w}(\alpha)}=\mu_\alpha$ for $\hat{w}\in\hat{W}$. Fix $\kappa\in\mathbb{C}$ and $\xi\in\mathring{\mathfrak{h}}^*$. We define $\hat{R}_\alpha\in\mathrm{End}_{\mathbb{C}}\mathcal{M}$ for $\alpha\in\Delta^{\mathrm{re}}$ by

$$\hat{R}_\alpha:=H_\alpha(\mu_\alpha)-H_\alpha(\langle\xi,\alpha^\vee\rangle)\circ s_\alpha, \tag{5.1}$$

where $H_\alpha(\eta)\in\mathcal{M}$ acts as a multiplication operator defined by

$$H_\alpha(\eta)(h) := \frac{\vartheta_1(-\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1(-\gamma_\alpha\eta;\gamma_\alpha\tau)} \frac{\vartheta_1(\mathrm{af}(\alpha)(h)-\gamma_\alpha\eta;\gamma_\alpha\tau)}{\vartheta_1(\mathrm{af}(\alpha)(h);\gamma_\alpha\tau)}. \tag{5.2}$$

Theorem V.1: *The map* $\pi: R_\alpha \mapsto \hat{R}_\alpha$, $\tau_\lambda \mapsto \tau_\lambda$ *induces a homomorphism from* $\mathcal{R}$ *to* $\mathrm{End}_{\mathbb{C}}\mathcal{M}$. *These R-matrices satisfy the unitarity*

$$\hat{R}_\alpha \hat{R}_{-\alpha} = \left(\frac{\vartheta_1(-\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1'(0;\gamma_\alpha\tau)}\right)^2 (\wp(\gamma_\alpha\mu_\alpha;1,\gamma_\alpha\tau)-\wp(\gamma_\alpha\langle\xi,\alpha^\vee\rangle;1,\gamma_\alpha))\mathrm{Id}_{\mathcal{M}}. \tag{5.3}$$

Besides the above representation, we have more general forms that depend on the relation among Q, $Q^\vee$, M. For $\alpha \in \Delta^{\mathrm{re}}$, let

$$N_\alpha := \left\{ (m_\alpha, n_\alpha) \in \mathbb{R}^2_{>0} \,\middle|\, \begin{array}{c} \overline{\alpha^\vee} \in m_\alpha \mathring{Q}^\vee, \quad m_\alpha\langle\alpha, \mathring{Q}^\vee\rangle \subset \mathbb{Z}, \\ n_\alpha\gamma_\alpha\overline{\alpha^\vee} \in m_\alpha M, m_\alpha(M|\alpha) \subset n_\alpha\gamma_\alpha\mathbb{Z} \end{array} \right\}. \tag{5.4}$$

This condition is required when the root algebra acts on the vector space spanned by theta functions (Proposition VII.1) and is an elliptic analog in the representation of the Hecke algebras.[25]

We enumerate the set N_α as

$X_N^{(r)}$	root	(m_α^1, n_α^1)	(m_α^2, n_α^2)	(m_α^3, n_α^3)	(m_α^4, n_α^4)
$C_l^{(1)}$	long	(1,1)	(1,2)	(1/2,1)	(1/2,1/2)
$A_{2l-1}^{(2)}$	long	(1,1)			(1/2,1/2)
$D_{l+1}^{(2)}$	short	(1,1)	(1,2)		
$A_{2l}^{(2)}$	short	(2,1)	(2,2)	(1,1)	(1,1/2)
$A_{2l}^{(2)}$	long	(1,1/2)	(1,1)	(1/2,1/2)	(1/2,1/4)
otherwise		(1,1)			

Here we have numbered the elements of N_α for later convenience. Let $g_\alpha^j \in \mathbb{C}$ for $1 \leqslant j \leqslant 4$ $\hat{W}$-invariant constants. If $(m_\alpha^j, n_\alpha^j) \notin N_\alpha$, set $g_\alpha^j = 0$. In place of (5.2), we define

$$H_\alpha(\eta)(h) := \sum_{(m_\alpha^j, n_\alpha^j) \in N_\alpha} g_\alpha^j \frac{\vartheta_1(-n_\alpha^j\gamma_\alpha\mu_\alpha/m_\alpha^j; n_\alpha^j\gamma_\alpha\tau)}{\vartheta_1(-n_\alpha^j\gamma_\alpha\eta/m_\alpha^j; n_\alpha^j\gamma_\alpha\tau)} \frac{\vartheta_1(m_\alpha^j\mathrm{af}(\alpha)(h)-n_\alpha^j\gamma_\alpha\eta/m_\alpha^j; n_\alpha^j\gamma_\alpha\tau)}{\vartheta_1(m_\alpha^j\mathrm{af}(\alpha)(h); n_\alpha^j\gamma_\alpha\tau)}. \tag{5.5}$$

Then we have a more general representation of $\mathcal{R}$ including Theorem V.1.

Theorem V.2: *The map* π *in Theorem V.1 with* (5.5) *induces a homomorphism from* $\mathcal{R}$ *to* $\mathrm{End}_{\mathbb{C}}\mathcal{M}$. *These R-matrices satisfy the unitarity*

$$\hat{R}_\alpha \hat{R}_{-\alpha} = u_\alpha(\tau)\mathrm{Id}_{\mathcal{M}}, \tag{5.6}$$

where $u_\alpha(\tau)$ *depends only on* τ *and vanishes if* $\langle\xi,\alpha^\vee\rangle = \pm\mu_\alpha$.

Proof: We can verify the relations (3.1) case-by-case, by a direct substitution of (5.5); for details, see Refs. 26 and 15. □

Remark V.3: The function $u_\alpha(\tau)$ is explicitly given by

$$u_\alpha(\tau) = ((p_1.g_\alpha)^2, (p_2.g_\alpha)^2, (p_3.g_\alpha)^2, (p_4.g_\alpha)^2).S.d_\alpha,$$

$$S=\frac{1}{4}\begin{pmatrix}1&0&0&0\\-1&0&0&1\\-1&4&0&0\\1&-4&4&-1\end{pmatrix},\quad g_\alpha=\begin{pmatrix}\tilde{g}_\alpha^1\\\tilde{g}_\alpha^2\\\tilde{g}_\alpha^3\\\tilde{g}_\alpha^4\end{pmatrix},\quad d_\alpha=\begin{pmatrix}d_\alpha^1\\d_\alpha^2\\d_\alpha^3\\d_\alpha^4\end{pmatrix},$$

$$p_1=(2,1,1,2),\quad p_2=(0,0,1,2),\quad p_3=(0,1,1,0),\quad p_4=(0,0,1,0),$$

$$\tilde{g}_\alpha^j=g_\alpha^j\frac{\vartheta_1(-n_\alpha^j\gamma_\alpha\mu_\alpha/m_\alpha^j;n_\alpha^j\gamma_\alpha\tau)}{\vartheta_1'(0;n_\alpha^j\gamma_\alpha\tau)},$$

$$d_\alpha^j=\wp(n_\alpha^j\gamma_\alpha\mu_\alpha/m_\alpha^j;1,n_\alpha^j\gamma_\alpha\tau)-\wp(n_\alpha^j\gamma_\alpha\langle\xi,\alpha^\vee\rangle/m_\alpha^j;1,n_\alpha^j\gamma_\alpha\tau). \tag{5.7}$$

We employ these operators even for the affine root systems of rank 2, though they do not have any Coxeter relations.

We shall clarify some properties of the operators $\hat{Y}^\lambda=\pi(Y^\lambda)$.

Lemma V.4: The R-matrices $\hat{R}$ satisfy the following relations:

$$\hat{R}_{-\alpha_j}\hat{R}_{\tau_{-\lambda_i}}={}^{s_j}\hat{R}_{\tau_{-\lambda_i}}\hat{R}_{-\alpha_j},\quad \textit{for}\ \ j\neq i, \tag{5.8}$$

$$\hat{R}_{\tau_{-\lambda_i}}=\hat{R}_{\alpha_i}\mathbf{R}, \tag{5.9}$$

where **R** *is a product of some R-matrices.*

Proof: Combining (2.22), the unitarity (5.6), and an equality $s_j\tau_{-\lambda_i}=\tau_{-\lambda_i}s_j$, we obtain (5.8) for generic ξ and thus for all $\xi\in\mathring{\mathfrak{h}}^*$. The form (5.9) is due to the fact that $\ell(s_i\tau_{-\lambda_i})=\ell(\tau_{-\lambda_i})-1$ implies the exchange condition,[20] $\tau_{-\lambda_i}=s_{i_1}\cdots s_{i_\ell}\omega=s_is_{i_1}\cdots s_{i_{m-1}}s_{i_{m+1}}\cdots s_{i_\ell}\omega$ for some m.□

If the parameter ξ satisfies $\langle\xi,\alpha_i^\vee\rangle=-\mu_{-\alpha_i}$, then the R-matrix $\hat{R}_{-\alpha_i}$ reduces to the form $\hat{R}_{-\alpha_i}=2H_{-\alpha}(\mu_{-\alpha})P_i^{(-)}$, where $P_i^{(-)}$ is the antisymmetric projection $1/2(1-s_i)$. Let

$$\mathring{\rho}_\mu:=\sum_{i\in\mathring{I}}\mu_{\alpha_i}\overline{\Lambda}_i=\frac{1}{2}\sum_{\alpha\in\mathring{\Delta}_+}\mu_\alpha\alpha. \tag{5.10}$$

From these properties, we have the following theorem:

Theorem V.5: *Let $\mathcal{V}:=\mathcal{M}^{\mathring{W}}$, the $\mathring{W}$-invariant subspace of $\mathcal{M}$ and let $\xi=-\mathring{\rho}_\mu$. Then $\hat{Y}^\lambda\in\mathrm{End}_{\mathbb{C}}\mathcal{V}$.*

Proof: It is sufficient to check it for the generators $\hat{Y}^{-\lambda_i}$. By Lemma V.4, we see that $\hat{R}_{-\alpha_j}\hat{Y}^{-\lambda_i}|_{\mathcal{V}}=0$, for $j\neq i$ by (5.8), and for $j=i$ by (5.9), noting that the unitarity (5.6) vanishes. Hence $\hat{Y}^{-\lambda_i}|_{\mathcal{V}}=s_j\hat{Y}^{-\lambda_i}|_{\mathcal{V}}$ for all $j\in\mathring{I}$.

Remark V.6: The symbol Y^λ is adopted since in a certain limit, it reduces to the same one up to a constant factor as in the affine Hecke algebras, where Y^λ is defined for all $\lambda\in\hat{M}$.

Remark V.7: $\hat{Y}^\lambda$ has its inverse in $\mathrm{End}_{\mathbb{C}}\mathcal{M}$ for generic $\xi\in\mathring{\mathfrak{h}}^*$, but loses its inverse when $\xi=-\mathring{\rho}_\mu$.

VI. ELLIPTIC DIFFERENCE OPERATORS

In this section, we calculate the explicit forms of the operators $\hat{Y}^\lambda$ for some λ on the space $\mathcal{V}=\mathcal{M}^{\mathring{W}}$. Throughout this section, we fix $\xi=-\mathring{\rho}_\mu$.

Lemma VI.1 (Ruijsenaars[27]): Let $D=\Sigma_\lambda V_\lambda\tau_\lambda$ (finite sum) where $V_\lambda\in\mathcal{M}$. If $Df=0$ for all $f\in\mathcal{V}$, then $V_\lambda=0$ for all λ.

Lemma VI.2: If $wD|_{\mathcal{V}}=D|_{\mathcal{V}}$ *for* $w\in\mathring{W}$, *then* $V_\lambda=V_{w\lambda}$.

Theorem VI.3: *Let* $(-\lambda)$ *be minuscule. Then we have*

$$\hat{Y}^\lambda|_{\mathcal{V}}=\frac{1}{|\mathring{W}_\lambda|}\sum_{w\in\mathring{W}} w\left(\prod_{\substack{\alpha\in\mathring{\Delta}_+\\(\lambda|\alpha)=-\gamma_\alpha}} H_\alpha(\mu_\alpha)\tau_\lambda\right)\Bigg|_{\mathcal{V}}, \tag{6.1}$$

where $\mathring{W}_\lambda$ *is the stabilizer of* λ *in* $\mathring{W}$.

Proof: Notice that R_{τ_λ} consists of nonaffine R-matrices, R_α for $\alpha\in\mathring{\Delta}_+$, because $(-\lambda)$ is minuscule. Substituting the R-matrices (5.1) into $\hat{Y}^\lambda$ and expanding them, we see that every term includes a translation operator of the form $\tau_{w(\lambda)}w$, where

$$w=s_{\alpha(p)}\cdots s_{\alpha(1)}\in\mathring{W}, \tag{6.2}$$

$$\alpha\{q\}:=\alpha^{(m_q)},\quad 1\leqslant m_p<m_{p-1}<\cdots<m_2<m_1\leqslant\ell(\tau_\lambda), \tag{6.3}$$

and $\Delta_{\tau_\lambda}=\{\alpha^{(1)}=\alpha_{i_1},\alpha^{(2)}=s_{i_1}(\alpha_{i_2}),\ldots,\alpha^{(\ell)}=s_{i_1}s_{i_2}\cdots s_{i_{\ell-1}}(\alpha_{i_\ell})\}$ for a reduced expression $\tau_\lambda=s_{i_1}s_{i_2}\cdots s_{i_\ell}\omega$. Let us show that $w(\lambda)=\lambda$ implies $w=id$. Suppose $w(\lambda)=\lambda$ and $w\neq id$. Then we have $\ell(w\tau_\lambda)=\ell(\tau_\lambda w)$. From (2.22), $\ell(\tau_\lambda w)=\ell(\tau_\lambda)+\ell(w)>\ell(\tau_\lambda)$ while $\ell(w\tau_\lambda)<\ell(\tau_\lambda)$ by a direct calculation, which leads to a contradiction. This implies that the term including $\tau_\lambda w, w\in\mathring{W}$, appears if and only if $w=id$. The coefficient of this term can be easily calculated,

$$\prod_{\substack{\alpha\in\mathring{\Delta}_+\\(\lambda|\alpha)=-\gamma_\alpha}} H_\alpha(\mu_\alpha). \tag{6.4}$$

The $\mathring{W}$-invariance of the operator $\hat{Y}^\lambda$ and Lemma VI.2 yields the form (6.1). □

It is worth noting that as in the trigonometric case,[28] we can rewrite $\hat{Y}^\lambda$ in a simply laced root system as follows:

$$\hat{Y}^\lambda|_{\mathcal{V}}=\frac{1}{|\mathring{W}_\lambda|}\sum_{w\in\mathring{W}}\frac{(\tau_{-\mu w\lambda/\kappa}A_\rho)}{A_\rho}\tau_{w\lambda}\Bigg|_{\mathcal{V}}, \tag{6.5}$$

where we have set $\mu=\mu_\alpha$ and $g_\alpha^1=1$.

In general, it is complicated and difficult to compute explicit forms of the operators when λ is not minuscule. It is the case even in the framework of the affine Hecke algebras. There is no minuscule weight available in the root systems of type $E_8^{(1)}$, $F_4^{(1)}$, $G_2^{(1)}$, $A_{2l}^{(2)}$, $E_6^{(2)}$ and $D_4^{(3)}$. However, every root system processes the "quasi-minuscule" weight $\nu(\theta^\vee)$ in the sense of the following properties:

Lemma VI.4:

(1) $\Delta_{\tau_{-\nu(\theta^\vee)}}=\Delta_{s_\theta}\cup\{a_0^{-1}(\delta+\theta)\}$.
(2) $(\nu(\theta^\vee)|\alpha)=0$ *or* γ_α *for* $\alpha\in\mathring{\Delta}_+$, $\alpha\neq\theta$, *and* $(\nu(\theta^\vee)|\theta)=2$.
(3) $\nu(\theta^\vee)=\lambda_i$ *where* α_i *is the unique vertex connected to* α_0 *if* $X_N^{(r)}\neq A_l^{(1)}$.

Proof: We see that $s_\theta\alpha_0=s_\theta(a_0^{-1}(\delta-\theta))=a_0^{-1}(\delta+\theta)\in\Delta_+^{\mathrm{re}}$, which implies the first statement due to the expression $s_\theta s_0=\tau_{-\nu(\theta^\vee)}$. The second statement is immediate from the first and (2.22). Since $\langle\underline{\nu}(\theta^\vee),\alpha_i^\vee\rangle=\langle a_0^{-1}\theta,\alpha_i^\vee\rangle=\langle a_0^{-1}\delta-\alpha_0,\alpha_i^\vee\rangle=-\langle\alpha_0,\alpha_i^\vee\rangle$, we have $\nu(\theta^\vee)=-\Sigma_{i\in\mathring{I}}\langle\alpha_0,\alpha_i^\vee\rangle\Lambda_i$. Then the last statement follows from the tables in Refs. 20 and 23. □

Since in the root system of type $A_l^{(1)}$, every λ_i is minuscule, we have the explicit form of $\hat{Y}^{-\nu(\theta^\vee)}$ by Theorem VI.3. So we concentrate on the other root systems. Fix i as in Lemma VI.4.

By the expression $\tau_{-\nu(\theta^\vee)}=s_\theta s_0$, we have $Y^{-\nu(\theta^\vee)}=R_{s_\theta}R_{a_0^{-1}(\theta+\delta)}\tau_{-\nu(\theta^\vee)}=R_{s_\theta}\tau_{-\nu(\theta^\vee)}R_{-\alpha_0}$. For the operator $\hat{Y}^{-\nu(\theta^\vee)}$, an analogous statement to Lemma V.4 holds.

Lemma VI.5: The R-matrices $\hat{R}$ satisfy the following relations:

$$\hat{R}_{-\alpha_j}\hat{R}_{s_\theta}={}^{s_j}\hat{R}_{s_\theta}\hat{R}_{-\alpha_j},\quad \textit{for}\ \ j\neq i, \tag{6.6}$$

$$\hat{R}_{s_\theta}=\hat{R}_{\alpha_i}\mathbf{R}, \tag{6.7}$$

where **R** *is a product of some R-matrices.*

Proof: We have $s_j\tau_{-\nu(\theta^\vee)}=\tau_{-\nu(\theta^\vee)}s_j$ and $s_js_0=s_0s_j$ for $j\neq i$, since α_i is the unique vertex connected to α_0. Then s_j and $s_\theta=\tau_{-\nu(\theta^\vee)}s_0$ commute, which implies $\ell(s_js_\theta)=\ell(s_\theta)+1$ and thus (6.6). The form (6.7) follows from the fact that $\ell(s_i\tau_{-\nu(\theta^\vee)})=\ell(\tau_{-\nu(\theta^\vee)})-1$ implies $\ell(s_is_\theta)=\ell(s_\theta)-1$ and the exchange condition. □

Let $\mathring{W}_i$ be the parabolic subgroup generated by $\{s_j|j\in\mathring{I},j\neq i\}$ and $\mathcal{V}_i$ be the $\mathring{W}_i$-invariant subspace of $\mathcal{M}$.

Lemma VI.6: The operator $\hat{R}_{s_\theta}\tau_{-\nu(\theta^\vee)}$ maps $\mathcal{V}_i$ to $\mathcal{V}$ and the operator $\hat{R}_{-\alpha_0}$ maps *$\mathcal{V}$ to $\mathcal{V}_i$.*

Proof: The former statement can be shown in the same way as Theorem V.5, and the latter, directly. □

Theorem VI.7:

$$\hat{Y}^{-\nu(\theta^\vee)}\Big|_{\mathcal{V}}=\frac{1}{|\mathring{W}_{\nu(\theta^\vee)}|}\sum_{w\in\mathring{W}}w\Bigg(\Bigg(\prod_{\substack{\alpha\in\mathring{\Delta}_+\\ \langle\alpha,\theta^\vee\rangle>0}}H_\alpha(\mu_\alpha)\Bigg)\times(H_{\alpha_0^{-1}(\theta+\delta)}(\mu_{\alpha_0})\tau_{-\nu(\theta^\vee)}-H_{a_0^{-1}(\theta+\delta)}(-(\mathring{\rho}_\mu|\theta)))\Bigg)\Bigg|_{\mathcal{V}}. \tag{6.8}$$

Proof: The explicit form of $\hat{R}_{s_\theta}\tau_{-\nu(\theta^\vee)}$ on $\mathcal{V}_i$ can be computed in a similar way to Theorem VI.3. Since $Y^{-\nu(\theta^\vee)}=R_{s_\theta}\tau_{-\nu(\theta^\vee)}R_{-\alpha_0}$, we obtain the form (6.8). □

The operator (1.2) is actually (6.8) of type $A_{2l}^{(2)}$, where the terms without translations are gathered by use of identities of the theta functions. In Refs. 18 and 19, we calculated the explicit forms of $\hat{Y}^{-\lambda_j}|_{\mathcal{V}}$ for all $j\in\mathring{I}$ in this root system. The operator (6.8) in the affine root systems of type $E_8^{(1)}$, $F_4^{(1)}$, $G_2^{(1)}$ and $A_{2l}^{(2)}$ should be compared to the Macdonald(–Koornwinder) operator $D_{\theta^\vee}$ of types E_8, F_4, G_2 and BC_l respectively, while the operator (6.1) in the rest root systems of type $X_l^{(1)}$ should be compared to $E_{\nu^{-1}(\lambda_i)}$ of type X_l.[29,30] See the Appendix for details.

In order to investigate a general $\hat{Y}^\lambda$, let us define a partial order in $\hat{M}_-$. We remark that this partial order is different from that in the affine Hecke algebras.

Definition VI.8: Let $\lambda,\lambda'\in\hat{M}_-$. We write $\lambda\geqslant\lambda'$ if $\ell(\tau_\lambda)>\ell(\tau_{\lambda'})$ or $\lambda=\lambda'$.

For an arbitrary weight $\lambda\in\hat{M}_-$, we have the "leading term" of $\hat{Y}^\lambda$ with respect to the order $>$.

Theorem VI.9: *Let $\lambda\in\hat{M}_-$. Then we have*

$$\hat{Y}^\lambda|_{\mathcal{V}}=\frac{1}{|\mathring{W}_\lambda|}\sum_{w\in\mathring{W}}w\Bigg(g_\lambda^\lambda\tau_\lambda+\sum_{\lambda>\lambda'}g_{\lambda'}^\lambda\tau_{\lambda'}\Bigg)\Bigg|_{\mathcal{V}}, \tag{6.9}$$

where $g_{\lambda'}^\lambda\in\mathcal{M}$. In particular, we have $g_\lambda^\lambda=\Pi_{\alpha\in\Delta_{\tau_\lambda}}H_\alpha(\mu_\alpha)$.

Proof: Because $\hat{Y}^{\lambda}$ is $\mathring{W}$-invariant, it is sufficient to calculate the coefficients of the translations of antidominant weights. A translation $\tau_{\lambda'}, \lambda' \in \hat{M}_-$ in the expansion of $\hat{Y}^{\lambda}$ appears as $w\tau_{\lambda} = \tau_{\lambda'}\mathring{w}$ where $\mathring{w} \in \mathring{W}$ and

$$w = s_{\alpha\{p\}} \cdots s_{\alpha\{1\}} \in W, \tag{6.10}$$

$$\alpha\{q\} = \alpha^{(m_q)}, \quad 1 \leqslant m_p < m_{p-1} < \cdots < m_2 < m_1 \leqslant \ell(\tau_{\lambda}). \tag{6.11}$$

Then $\ell(\tau_{\lambda}) \geqslant \ell(w\tau_{\lambda}) = \ell(\tau_{\lambda'}, \mathring{w}) = \ell(\tau_{\lambda'}) + \ell(\mathring{w})$, which implies $\ell(\tau_{\lambda}) > \ell(\tau_{\lambda'})$ if $w \neq id$. Hence the expression (6.9). □

Theorem VI.10: *$\{\hat{Y}^{-\lambda_i} | i \in \mathring{I}\}$ are algebraically independent on $\mathcal{V}$.*

Proof: Let $Y = \Sigma_{\lambda} a_{\lambda} Y^{\lambda} \in \mathcal{S}$ with $a_{\lambda} \in \mathbb{C}$. Let M_Y be the set of all the maximal antidominant weights in the expansion of $\hat{Y}$ on $\mathcal{V}$. Then we have

$$\hat{Y}|_{\mathcal{V}} = \sum_{\lambda \in M_Y} \sum_{w \in \mathring{W}} w(a_{\lambda} g_{\lambda}^{\lambda} \tau_{\lambda} + \text{lower terms } (\lambda' > \lambda))|_{\mathcal{V}}. \tag{6.12}$$

Fix $\lambda \in M_Y$. Suppose $\hat{Y} f = 0$ for all $f \in \mathcal{V}$. Then by Lemma VI.2 $a_{\lambda} = 0$ and hence the result. □

The following statement is immediate from this theorem.

Corollary VI.11: $\mathcal{S} \simeq \mathbb{C}[T_{\hat{M}_-}]$.

VII. ACTION ON THETA FUNCTIONS OF LEVEL *K*

The aim of this section is to show that the operators $\hat{Y}^{\lambda}$ in the previous sections act on $(Th^k)^{\mathring{W}}$, the $\mathring{W}$-invariant space of the theta functions of level k, or the space of the characters. To be more precise, we identify $\hat{Y}^{\lambda}$ with an operator on $(Th^k)^{\mathring{W}}$ by restricting the domain. The basic idea is from Refs. 5 and 15, where the matrix elements of Belavin's $\mathbb{Z}_k$-symmetric elliptic R-matrix and associated K-matrices are calculated. Now it turns out that they are the elliptic difference operators of type $A_1^{(1)}$ or $A_2^{(2)}$.

Let us outline our strategy. Since the representation π in Theorem V.2 does not preserve Th^k for general $\xi \in \mathring{\mathfrak{h}}^*$, we introduce another representation $\overline{\pi}$ which always preserve this space. The images of $\mathcal{S}$ by π and $\overline{\pi}$ coincide when we set $\xi = -\mathring{\rho}_{\mu}$. As was shown, $\pi(\mathcal{S})$ at this value preserves $\mathring{W}$-invariant subspace, and so does $\overline{\pi}(\mathcal{S})$. On the other hand, $\overline{\pi}(\mathcal{S})$ preserves Th^k by construction, and so does $\pi(\mathcal{S})$. Therefore we can deduce that $\pi(\mathcal{S}) = \overline{\pi}(\mathcal{S})$ acts on $(Th^k)^{\mathring{W}}$.

Let $h_{\mu}^{\vee} := (\mathring{\rho}_{\mu} | \theta) + \mu_{\alpha_0} = \Sigma_{i \in I} \mu_{\alpha_i} a_i^{\vee}$ and $\Xi := (\xi + \mathring{\rho}_{\mu})/h_{\mu}^{\vee}$. Throughout this section, we fix $\kappa = h_{\mu}^{\vee}/k$ though some of the following statements do not require this condition.

We extend the action of τ_{λ} on $\mathcal{M}$ for arbitrary $\lambda \in \mathring{\mathfrak{h}}^*$ by $(\tau_{\lambda} f)(h) := f(h - \kappa \nu^{-1}(\lambda))$. For $\alpha \in \Delta^{\mathrm{re}}$ such that $\overline{\alpha} \in \mathring{\Delta}$, let $\overline{R}_{\alpha}$ be defined by

$$\overline{R}_{\alpha} := \tau_{\epsilon_{\alpha}} \hat{R}_{\overline{\alpha}} \tau_{\phi_{\alpha}}, \tag{7.1}$$

where $\epsilon_{\alpha} := (1/h_{\mu}^{\vee})(-(1/2)\mu_{\alpha}\overline{\alpha} - \xi + \eta_{\alpha})$, $\phi_{\alpha} := (1/h_{\mu}^{\vee})(-(1/2)\mu_{\alpha}\overline{\alpha} + \xi - \eta_{\alpha})$, and $\eta_{\alpha} \in \mathring{\mathfrak{h}}^*$ is taken arbitrary such that $\langle \eta_{\alpha}, \overline{\alpha}^{\vee} \rangle = 0$. Then $\overline{R}_{\alpha}$ is well-defined since $\overline{R}_{\alpha}$ does not depend on the choice of η_{α} and it will be soon proved that $\overline{R}_{\alpha} \in \mathrm{End}_{\mathbb{C}} \mathcal{M}$. For α such that $\overline{\alpha} \notin \mathring{\Delta}$, i.e., $\alpha \in \hat{W}\alpha_0$ in the $A_{2l}^{(2)}$ system, we need another definition for $\hat{R}_{\overline{\alpha}}$ or $H_{\overline{\alpha}}$ which is straightforward.

According to our plan, we show that this operator acts on Th^k.

Proposition VII.1: For arbitrary $\xi \in \mathring{\mathfrak{h}}^*$, $\overline{R}_{\alpha} \in \mathrm{End}_{\mathbb{C}}(Th^k)$.

Proof: For $f \in Th^k$ we check the behavior of the function

$$(\overline{R}_\alpha f)(h)=H_{\overline{\alpha}}(\mu_\alpha)(\mathrm{af}(\tau_{-\epsilon_\alpha})(h))f(\mathrm{af}(\tau_{-\phi_\alpha-\epsilon_\alpha})(h))-H_{\overline{\alpha}}(\langle\xi,\overline{\alpha^\vee}\rangle)(\mathrm{af}(\tau_{-\epsilon_\alpha})\times(h))f(\mathrm{af}(\tau_{-\phi_\alpha-s_{\overline{\alpha}}(\epsilon_\alpha)}\circ s_{\overline{\alpha}})(h)) \tag{7.2}$$

under $h\to h+\mu(\mu\in\mathring{Q}^\vee)$ and $h\to h-\tau\nu^{-1}(\lambda)(\lambda\in\hat{M})$.

For $\mu\in\mathring{Q}^\vee$, we have $(\overline{R}_\alpha f)(h)=(\overline{R}_\alpha f)(h+\mu)$ since

$$H_{\overline{\alpha}}(\eta)(h+\mu)=H_{\overline{\alpha}}(\eta)(h), \tag{7.3}$$

$$f(h+\mu)=f(h), \tag{7.4}$$

$$\mathrm{af}(\tau_\epsilon)(h+\mu)=h+\mu+\kappa\nu^{-1}(\epsilon)=\mathrm{af}(\tau_\epsilon)(h)+\mu, \tag{7.5}$$

$$\mathrm{af}(\tau_\epsilon\circ s_{\overline{\alpha}})(h+\mu)=\mathrm{af}(\tau_\epsilon\circ s_{\overline{\alpha}})(h)+s_{\overline{\alpha}}(\mu). \tag{7.6}$$

For $\lambda\in\hat{M}$, we have $(\overline{R}_\alpha f)(h-\tau\nu^{-1}(\lambda))=e^{k\lambda+k|\lambda|^2\delta/2}(\overline{R}_\alpha f)(h)$ since

$$H_{\overline{\alpha}}(\eta)(h-\tau\nu^{-1}(\lambda))=e^{-2\pi i(\overline{\alpha}|\lambda)\eta}H_{\overline{\alpha}}(\eta)(h), \tag{7.7}$$

$$f(h-\tau\nu^{-1}(\lambda))=e^{k\lambda+k|\lambda|^2\delta/2}f(h), \tag{7.8}$$

$$\phi_\alpha+\epsilon_\alpha=-k\kappa\mu_\alpha\overline{\alpha}, \tag{7.9}$$

$$\phi_\alpha+s_{\overline{\alpha}}\epsilon_\alpha=k\kappa\langle\xi,\overline{\alpha^\vee}\rangle\overline{\alpha}. \tag{7.10}$$

The holomorphy of $\overline{R}_\alpha f$, which can be checked in each case, completes the proof. □

To show that the operators $\overline{R}_\alpha$ are a representation of the root algebra, we need some statements.

Lemma VII.2: Let $\hat{w}=w\omega=s_{i_1}\cdots s_{i_\ell}\omega\in\hat{W}$ *be a reduced expression. Let*

$$\eta_n:=-\mathring{\rho}_\mu+\sum_{m=1}^{n-1}\nu_m\overline{\alpha^{(m)}}+\frac{1}{2}\nu_n\overline{\alpha^{(n)}}, \tag{7.11}$$

where $\Delta_{\hat{w}}=\{\alpha^{(1)}=\alpha_{i_1},\alpha^{(2)}=s_{i_1}(\alpha_{i_2}),\ldots,\alpha^{(\ell)}=ws_{i_\ell}(\alpha_{i_\ell})\}$,

$$\nu_n:=\begin{cases}\mu_n, & \text{if } \alpha_{i_n}\neq\alpha_0,\\ -(\mathring{\rho}_\mu|\theta), & \text{if } \alpha_{i_n}=\alpha_0,\end{cases} \tag{7.12}$$

and $\mu_n:=\mu_{\alpha^{(n)}}$. *Then* $\langle\eta_n,\overline{(\alpha^{(n)})^\vee}\rangle=0$.

Proof: Observe that if $\alpha^{(n)}=s_{i_1}\cdots s_{i_{n-1}}\alpha_{i_n}$, then $\overline{\alpha^{(n)}}=\overline{s}_{i_1}\cdots\overline{s}_{i_{n-1}}\overline{\alpha_{i_n}}$ and $\overline{(\alpha^{(n)})^\vee}=\overline{s}_{i_1}\cdots\overline{s}_{i_{n-1}}\overline{\alpha_{i_n}^\vee}$, where $\overline{s}_i:=s_i$ for $i\neq0$ and $\overline{s}_0:=s_\theta$.

$$\begin{aligned}\langle-\mathring{\rho}_\mu,\overline{(\alpha^{(n)})^\vee}\rangle&=\langle-\mathring{\rho}_\mu,\overline{s}_{i_1}\cdots\overline{s}_{i_{n-1}}\overline{\alpha_{i_n}^\vee}\rangle\\&=\langle-\mathring{\rho}_\mu+\nu_1\overline{\alpha^{(1)}},\overline{s}_{i_2}\cdots\overline{s}_{i_{n-1}}\overline{\alpha_{i_n}^\vee}\rangle\\&=\langle-\mathring{\rho}_\mu,\overline{s}_{i_2}\ldots\overline{s}_{i_{n-1}}\overline{\alpha_{i_n}^\vee}\rangle-\nu_1\langle\overline{\alpha^{(1)}},\overline{(\alpha^{(n)})^\vee}\rangle\\&\ \ \vdots\\&=-\sum_{m=1}^{n-1}\nu_m\langle\overline{\alpha^{(m)}},\overline{(\alpha^{(n)})^\vee}\rangle-\nu_n.\end{aligned} \tag{7.13}$$

Then we have

$$\left\langle -\mathring{\rho}_\mu+\sum_{m=1}^{n-1}\nu_m\overline{\alpha^{(m)}}+\frac{1}{2}\nu_n\overline{\alpha^{(n)}},\overline{(\alpha^{(n)})^\vee}\right\rangle=0. \tag{7.14}$$

□

Proposition VII.3.: Let $\hat{w}=s_{i_1}\cdots s_{i_\ell}\omega\in\hat{W}$ *be a reduced expression. Then*

$$\overline{R}_{\alpha^{(1)}}\overline{R}_{\alpha^{(2)}}\cdots\overline{R}_{\alpha^{(\ell)}}=\tau_{-\Xi}\hat{R}_{\alpha^{(1)}}\hat{R}_{\alpha^{(2)}}\cdots\hat{R}_{\alpha^{(\ell)}}\tau_{\lambda_{\hat{w}}}\tau_\Xi, \tag{7.15}$$

where $\lambda_{\hat{w}}:=(1/h_\mu^\vee)\Sigma_{n=1}^{\ell}\mu_n\overline{\alpha^{(n)}}=-(1/h_\mu^\vee)\Sigma_{\alpha\in\Delta_{\hat{w}}}\mu_\alpha\overline{\alpha}$.

Proof: We set $\eta_{\alpha^{(n)}}=\eta_n$ obtained in Lemma VII.2 and set

$$\lambda:=-\frac{1}{h_\mu^\vee}\sum_{m=1}^{\ell}\nu_m\overline{\alpha^{(m)}}, \tag{7.16}$$

$$\epsilon_n:=\frac{1}{2h_\mu^\vee}(\nu_n-\mu_n)\overline{\alpha^{(n)}},\quad 1\leqslant n\leqslant\ell, \tag{7.17}$$

so that

$$\overline{R}_{\alpha^{(1)}}\overline{R}_{\alpha^{(2)}}\cdots\overline{R}_{\alpha^{(\ell)}}=\tau_{-\Xi}(\tau_{\epsilon_1}\hat{R}_{(\overline{\alpha^{(1)}})}\tau_{\epsilon_1})(\tau_{\epsilon_2}\hat{R}_{(\overline{\alpha^{(2)}})}\tau_{\epsilon_2})\cdots(\tau_{\epsilon_\ell}\hat{R}_{(\overline{\alpha^{(\ell)}})}\tau_{\epsilon_\ell})\tau_\lambda\tau_\Xi. \tag{7.18}$$

Let $\overline{w}_n=\overline{s}_{i_1}\cdots\overline{s}_{i_n}$. Then we have

$$\epsilon_n=\begin{cases}-\overline{\alpha^{(n)}}/2=\overline{w}_{n-1}\nu(\theta^\vee)/2, & \text{if } i_n=0,\\ 0, & \text{if } i_n\neq 0,\end{cases} \tag{7.19}$$

and

$$\tau_{\epsilon_n}\hat{R}_{(\overline{\alpha^{(n)}})}\tau_{\epsilon_n}=\begin{cases}\tau_{(-\overline{\alpha^{(n)}}/2)}\hat{R}_{(\overline{\alpha^{(n)}})}\tau_{(-\overline{\alpha^{(n)}}/2)}=\hat{R}_{(\overline{w}_{n-1}\alpha_0)}\tau_{(\overline{w}_{n-1}\nu(\theta^\vee))}, & \text{if } i_n=0,\\ \hat{R}_{(\overline{\alpha^{(n)}})}=\hat{R}_{(\overline{w}_{n-1}\alpha_{i_n})}, & \text{if } i_n\neq 0,\end{cases} \tag{7.20}$$

where we have used $\tau_{(-\overline{\alpha^{(n)}}/2)}(\overline{\alpha^{(n)}})=(\overline{\alpha^{(n)}})+a_0^{-1}\delta=\overline{w}_{n-1}\alpha_0$ if $i_n=0$. By using the identities

$$\alpha^{(n)}=s_{i_1}\cdots s_{i_{n-1}}\alpha_{i_n}=\left(\prod_{\substack{m<n\\ i_m=0}}\tau_{(\overline{w}_{m-1}\nu(\theta^\vee))}\right)\overline{w}_{n-1}\alpha_{i_n}, \tag{7.21}$$

and

$$\begin{aligned}\sum_{i_m=0}\overline{w}_{m-1}\nu(\theta^\vee)+\lambda&=-\sum_{i_m=0}\overline{\alpha^{(m)}}-\frac{1}{h_\mu^\vee}\sum_{m=1}^{\ell}\mu_m\overline{\alpha^{(m)}}+\frac{1}{h_\mu^\vee}\sum_{i_m=0}(\mu_m+(\mathring{\rho}_\mu|\theta))\overline{\alpha^{(m)}}\\&=-\frac{1}{h_\mu^\vee}\sum_{m=1}^{\ell}\mu_m\overline{\alpha^{(m)}}=\lambda_{\hat{w}},\end{aligned} \tag{7.22}$$

we arrive at (7.15). □

Apply this proposition to an element that has two reduced expressions of the form

$$\hat{w}=\underbrace{s_i s_j s_i \ldots}_{m_{ij}\ \text{factors}}=\underbrace{s_j s_i s_j \ldots}_{\mathrm{m}_{ij}\ \text{factors}}, \tag{7.23}$$

for $i\neq j\in I$. Then the relation

$$\overline{R}_{\alpha_i}\overline{R}_{s_i\alpha_j}\overline{R}_{s_is_j\alpha_i}\cdots=\overline{R}_{\alpha_j}\overline{R}_{s_j\alpha_i}\overline{R}_{s_js_i\alpha_j}\cdots \tag{7.24}$$

immediately follows. Regarding $w\Pi$ for $w\in\mathring{W}$ as a set of fundamental roots in Lemma VII.2 and Proposition VII.3, we have proved the following theorem:

Theorem VII.4: *The map* $\overline{\pi}:R_\alpha\mapsto\overline{R}_\alpha$, $\tau_\lambda\mapsto\mathrm{Id}_{\mathcal{M}}$ *induces a homomorphism from* $\mathcal{R}$ *to* $\mathrm{End}_{\mathbb{C}}(Th^k)$.

For $\lambda\in\hat{M}_-$, we set $\overline{Y^\lambda}:=\overline{\pi}(Y^\lambda)=\overline{R}_{\alpha^{(1)}}\overline{R}_{\alpha^{(2)}}\cdots\overline{R}_{\alpha^{(\ell)}}\in\mathrm{End}_{\mathbb{C}}(Th^k)$. Now we are in position to prove the main theorem as follows:

Theorem VII.5: *Let* $\kappa=h^\vee_\mu/k$ *and* $\xi=-\mathring{\rho}_\mu$. *Then* $\hat{Y}^\lambda=\overline{Y^\lambda}\in\mathrm{End}_{\mathbb{C}}((Th^k)^{\hat{W}})$.

By Proposition VII.3, we have already shown

$$\overline{Y^\lambda}=\tau_{-\Xi}\hat{R}_{\alpha^{(1)}}\cdots\hat{R}_{\alpha^{(\ell)}}\tau_{\lambda'}\tau_\Xi=\tau_{-\Xi}\hat{R}_{\tau_\lambda}\tau_{\lambda'}\tau_\Xi, \tag{7.25}$$

where $\lambda'=-(1/h^\vee_\mu)\Sigma_{n=1}^{\ell}\mu_n\overline{\alpha^{(n)}}=-(1/h^\vee_\mu)\Sigma_{\alpha\in\Delta_{\tau_\lambda}}\mu_\alpha\overline{\alpha}$. Since $\Xi=0$ if we set $\xi=-\mathring{\rho}_\mu$, we have only to show that $\lambda'=\lambda$.

Due to the formulas (2.22), we have another description of λ' which can be regarded as an image of λ by some linear map:

$$-\sum_{\alpha\in\Delta_{\tau_\lambda}}\mu_\alpha\overline{\alpha}=\begin{cases}\displaystyle\sum_{\alpha\in\mathring{\Delta}_+}\frac{1}{\gamma_\alpha}\mu_\alpha(\alpha|\lambda)\alpha, & \text{if } X_N^{(r)}\neq A_{2l}^{(2)},\\ \displaystyle\sum_{\alpha\in\mathring{\Delta}_+}\frac{1}{\gamma_\alpha}\mu_\alpha(\alpha|\lambda)\alpha+\frac{1}{4}\mu_{\alpha_0}\sum_{\alpha\in(\mathring{\Delta}_+)_l}(\alpha|\lambda)\alpha, & \text{if } X_N^{(r)}=A_{2l}^{(2)}.\end{cases} \tag{7.26}$$

Lemma VII.6: Let $L:\mathring{\mathfrak{h}}^*\to\mathring{\mathfrak{h}}^*$ *be a linear map defined by* $L:\lambda\mapsto\frac{1}{2}\Sigma_{\alpha\in\mathring{\Delta}}\nu_\alpha(\alpha|\lambda)\alpha$ *where* ν_α *is* $\mathring{W}$*-invariant constant. Then* $L=a\,\mathrm{Id}_{\mathring{\mathfrak{h}}^*}$ *for some* $a\in\mathbb{C}$.

Proof: We see $L\in\mathrm{End}_{\mathring{W}}(\mathring{\mathfrak{h}}^*)$. Since $\mathring{W}$ acts on $\mathring{\mathfrak{h}}^*$ irreducibly, the statement follows from Schur's lemma.

By Lemma VII.6, we see that $-\Sigma_{\alpha\in\Delta_{\tau_\lambda}}\mu_\alpha\overline{\alpha}=a\lambda$ for some $a\in\mathbb{C}$. The following proposition completes the proof of Theorem VII.5.

Proposition VII.7. $-\Sigma_{\alpha\in\Delta_{\tau_\lambda}}\mu_\alpha\overline{\alpha}=h^\vee_\mu\lambda$.

Proof: Let L be the linear map defined in the right-hand side of (7.26). Due to Lemma VII.6, we can evaluate the factor a at any element of $\mathring{\mathfrak{h}}^*$. Recall that every root system has the quasi-minuscule weight $\nu(\theta^\vee)$, whose properties we have already investigated.

(i) $X_N^{(r)}\neq A_{2l}^{(2)}$

$$L(\nu(\theta^\vee))=\sum_{\alpha\in\mathring{\Delta}_+}\frac{1}{\gamma_\alpha}\mu_\alpha\langle\alpha,\theta^\vee\rangle\alpha=\sum_{\substack{\alpha\in\mathring{\Delta}_+\\ \langle\alpha,\theta^\vee\rangle\neq0}}\mu_\alpha\alpha+\mu_\theta\theta=a\,\nu(\theta^\vee), \tag{7.27}$$

where we have used Lemma VI.4. By applying $(\cdot|\theta)$ in the last equality, we obtain

$$a=\frac{1}{2}\sum_{\alpha\in\mathring{\Delta}_+}\mu_\alpha(\alpha|\theta)+\mu_\theta=(\mathring{\rho}_\mu|\theta)+\mu_{\alpha_0}. \tag{7.28}$$

(ii) $X_N^{(r)}=A_{2l}^{(2)}$

In a similar manner, we have

$$L(\nu(\theta^\vee))=\sum_{\substack{\alpha\in\mathring{\Delta}_+\\ \langle\alpha,\theta^\vee\rangle\neq 0}}\mu_\alpha\alpha+\sum_{\substack{\alpha\in(\mathring{\Delta}_+)_l\\ \langle\alpha,\theta^\vee\rangle\neq 0}}\frac{1}{2}\mu_{\alpha_0}\alpha=a\,\nu(\theta^\vee), \tag{7.29}$$

and consequently

$$a=(\mathring{\rho}_\mu|\theta)+\tfrac{1}{4}\mu_{\alpha_0}(\rho_l|\theta)=(\mathring{\rho}_\mu|\theta)+\mu_{\alpha_0}, \tag{7.30}$$

where

$$\rho_l=\sum_{\alpha\in(\mathring{\Delta}_+)_l}\alpha.$$

In both cases, $L(\nu(\theta^\vee))=h_\mu^\vee\nu(\theta^\vee)$ and we have $-\Sigma_{\alpha\in\Delta_{\tau_\lambda}}\mu_\alpha\overline{\alpha}=L(\lambda)=h_\mu^\vee\lambda$, as required.

Remark VII.8: Note that we also showed that

$$\sum_{\alpha\in\mathring{\Delta}}(\lambda|\alpha)(\mu|\alpha)=2h^\vee(\lambda|\mu),\quad \text{for } \lambda,\mu\in\mathring{\mathfrak{h}}^*, \tag{7.31}$$

in the nontwisted root systems. See Corollary 8.7 of Ref. 23.

VIII. CONCLUDING REMARKS

We constructed mutually commuting difference operators by means of root algebras. Since the operator is represented in a single product of affine *R*-matrices, we had only to pursue the image of each *R*-matrix and therefore succeeded in proving that they act on the characters of the irreducible representations of affine Lie algebras. However, the simultaneous diagonability of the difference operators and the procedure of the diagonalization have yet to be solved in contrast with the trigonometric cases.[6–8,31]

Since this operator was originally introduced as a quantum many-body system, the self-adjointness on the space of square integrable functions should be an important problem. In the trigonometric case, we readily see that the Macdonald operators are essentially self-adjoint on the polynomials of exponential since the operators are diagonalized in terms of the Macdonald polynomials. In the elliptic case, however, this problem is less investigated. See, for example, Refs. 32 and 33, where the two-body system is extensively studied by constructing the explicit eigenvectors, or Ref. 34 where the extensibility to positive self-adjoint operators is shown by introducing a certain measure on a torus. These systems correspond to negative levels in terms of affine Lie algebras. This problem will be discussed elsewhere.

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APPENDIX: RELATION TO MACDONALD OPERATORS

Let $e^{\lambda}(h)=e^{2\pi i\langle\lambda,h\rangle}(\lambda\in\mathring{\mathfrak{h}})$ be a function on $\mathbb{H}$. We set $q=e^{2\pi i\kappa}$ and $t_{\alpha}=e^{-2\pi i\mu_{\alpha}\gamma_{\alpha}}$.

Theorem A.1: *In the limit $\tau\to i\infty$, $\hat{Y}^{\lambda}$ for a minuscule weight $-\lambda$ and $\hat{Y}^{-\theta}$ reduce respectively to M^{λ} and $M^{-\theta}+c'$ where*

$$M^{\lambda}:=c_{\lambda}\sum_{w\in\mathring{W}}w\left(\prod_{\substack{\alpha\in\mathring{\Delta}_{+}\\(\lambda|\alpha)=-\gamma_{\alpha}}}\frac{1-t_{\alpha}e^{\alpha}}{1-e^{\alpha}}\tau_{\lambda}\right),\tag{A1}$$

$$M^{-\theta}:=c_{-\theta}\sum_{w\in\mathring{W}}w\left(\left(\prod_{\substack{\alpha\in\mathring{\Delta}_{+}\\(\theta|\alpha)>0}}\frac{1-t_{\alpha}e^{\alpha}}{1-e^{\alpha}}\right)\left(\frac{1-t_{\theta}qe^{\theta}}{1-qe^{\theta}}\right)(\tau_{-\theta}-1)\right),\tag{A2}$$

and for $\lambda\in\mathring{\mathfrak{h}}$,

$$c_{\lambda}:=\frac{e^{-2\pi i(\lambda|\mathring{\rho}_{\mu})}}{|\mathring{W}_{\lambda}|}.\tag{A3}$$

The term c' is given by

$$c'=r\frac{r-t_{\theta}}{r-1}\sum_{w\in\mathring{W}^{\theta}}\prod_{\alpha\in\Delta w}t_{\alpha},\tag{A4}$$

where $r=e^{2\pi i(\mathring{\rho}_{\mu}|\theta)}$ and $\mathring{W}^{\theta}$ is the minimal coset representatives of $\mathring{W}_{\theta}$, or the set of elements of smallest length in each coset in $\mathring{W}/\mathring{W}_{\theta}$.

Proof: It is sufficient to show the equation (A4). A direct calculation shows that the term c' is given by

$$c'=c_{-\theta}\frac{r-t_{\theta}}{r-1}\sum_{w\in\mathring{W}}\prod_{\substack{\alpha\in\mathring{\Delta}_{+}\\(\theta|\alpha)>0}}\frac{1-t_{\alpha}e^{w\alpha}}{1-e^{w\alpha}},\tag{A5}$$

and we see that this term is independent of h, which is implied by the following lemma related to the Poincaré polynomials. □

Lemma A.2 (cf. Ref. 35): Let $\mathring{W}^{\theta}$ be the minimal coset representatives of $\mathring{W}_{\theta}$. Then we have

$$\sum_{w\in\mathring{W}}\prod_{\substack{\alpha\in\mathring{\Delta}_{+}\\(\theta|\alpha)>0}}\frac{1-t_{\alpha}e^{w\alpha}}{1-e^{w\alpha}}=|\mathring{W}_{\theta}|\left(\sum_{w\in\mathring{W}}\prod_{\alpha\in\Delta_{w}}t_{\alpha}\right)\Big/\left(\sum_{w\in\mathring{W}_{\theta}}\prod_{\alpha\in\Delta_{w}}t_{\alpha}\right)$$

$$=|\mathring{W}_{\theta}|\sum_{w\in\mathring{W}^{\theta}}\prod_{\alpha\in\Delta_{w}}t_{\alpha}.\tag{A6}$$

Proof: Let $\Delta_{\theta}:=\{\alpha\in\mathring{\Delta}|(\theta|\alpha)=0\}$. Then one sees that Δ_{θ} is a root system whose simple roots are $\Pi_{\theta}:=\{\alpha_i\in\mathring{\Pi}|(\theta|\alpha_i)=0\}$. The parabolic subgroup generated by the reflections of Π_{θ} coincides with $\mathring{W}_{\theta}$. Then we have

$$\sum_{w\in\mathring{W}_{\theta}}\prod_{\alpha\in(\Delta_{\theta})_{+}}\frac{1-t_{\alpha}e^{w\alpha}}{1-e^{w\alpha}}=\left(\sum_{w\in\mathring{W}_{\theta}}\prod_{\alpha\in\Delta_{w}}t_{\alpha}\right).\tag{A7}$$

Since the right-hand side is independent of h, we have for any $v\in\mathring{W}$

$$\sum_{w\in \mathring{W}_\theta} \prod_{\alpha\in(\mathring{\Delta}_\theta)_+} \frac{1-t_\alpha e^{v w\alpha}}{1-e^{v w\alpha}} = \sum_{w\in \mathring{W}_\theta} \prod_{\alpha\in \mathring{\Delta}_w} t_\alpha . \tag{A8}$$

The set $\Delta^\theta=\{\alpha\in \mathring{\Delta}_+ | (\theta|\alpha)>0\}$ is $\mathring{W}_\theta$-invariant,

$$\Delta^\theta = v\Delta^\theta, \quad \text{for } v\in \mathring{W}_\theta \tag{A9}$$

Thus we have

$$\prod_{\alpha\in\Delta^\theta} \frac{1-t_\alpha e^{wv\alpha}}{1-e^{wv\alpha}} = \prod_{\alpha\in\Delta^\theta} \frac{1-t_\alpha e^{w\alpha}}{1-e^{w\alpha}}. \tag{A10}$$

From (A8) and (A10),

$$\begin{aligned}
&\left(\sum_{w\in \mathring{W}} \sum_{\alpha\in\Delta^\theta} \frac{1-t_\alpha e^{w\alpha}}{1-e^{w\alpha}}\right)\left(\sum_{w\in \mathring{W}_\theta} \prod_{\alpha\in\mathring{\Delta}_w} t_\alpha\right)\\
&\quad = |\mathring{W}| \sum_{w\in \mathring{W}^\theta} \left(\prod_{\alpha\in\Delta^\theta} \frac{1-t_\alpha e^{w\alpha}}{1-e^{w\alpha}}\right)\left(\sum_{v\in \mathring{W}_\theta} \prod_{v\in(\mathring{\Delta}_\theta)_+} \frac{1-t_\alpha e^{wv\alpha}}{1-e^{wv\alpha}}\right)\\
&\quad = |\mathring{W}_\theta| \sum_{w\in \mathring{W}^\theta} \sum_{v\in \mathring{W}_\theta} \prod_{\alpha\in\mathring{\Delta}_+} \frac{1-t_\alpha e^{wv\alpha}}{1-e^{wv\alpha}}\\
&\quad = |\mathring{W}_\theta| \sum_{w\in \mathring{W}} \prod_{\alpha\in\mathring{\Delta}_+} \frac{1-t_\alpha e^{w\alpha}}{1-e^{w\alpha}}\\
&\quad = |\mathring{W}_\theta| \left(\sum_{w\in \mathring{W}} \prod_{\alpha\in\mathring{\Delta}_w} t_\alpha\right),
\end{aligned} \tag{A11}$$

which implies the first equality. The second equality is an immediate consequence of the relation $\Delta_{uv}=\Delta_u\cup u\Delta_v$ for $u\in \mathring{W}^\theta$ and $v\in \mathring{W}_\theta$.

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Essential self-adjointness of the elliptic Ruijsenaars models

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We study the elliptic Ruijsenaars models associated with arbitrary root systems, which are difference analogs of the Calogero–Moser model. We give a dense subspace in the space of square integrable functions invariant under the action of the Weyl group on a torus as a domain of its Hamiltonian and prove its essential self-adjointness by using perturbation theory. It is also clarified that these models consist of pure point spectrum. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The elliptic Ruijsenaars model was introduced as a relativistic analog of the Calogero–Moser system[1] and its Hamiltonian is a difference operator with elliptic function coefficients. We adopt a little different Hamiltonian from the original one in order to treat it from the viewpoint of affine root systems, which is given by

$$H_{A_{l-1}^{(1)}}=\sum_{j=1}^{l}\left(\prod_{\substack{k=1\\k\neq j}}^{l}\frac{\vartheta_1(x_j-x_k-\mu)}{\vartheta_1(x_j-x_k)}\right)^{1/2}\left(\tau_j(\kappa)\prod_{k=1}^{l}\tau_k(-\kappa/l)\right)\left(\prod_{\substack{k=1\\k\neq j}}^{l}\frac{\vartheta_1(x_j-x_k+\mu)}{\vartheta_1(x_j-x_k)}\right)^{1/2}, \tag{1.1}$$

where $\vartheta_j(x)=\vartheta_j(x;\tau)$ is the Jacobi theta function and $\tau_i(\kappa)$ is a translation of the variable x_i by κ. Besides this model, a BC-type analog was proposed by van Diejen,[2–5] whose Hamiltonian is given by

$$\begin{aligned}H_{A_{2l}^{(2)}}=&\sum_{j=1}^{l}\left(\left(\prod_{\substack{k=1\\k\neq j}}^{l}\frac{\vartheta_1(x_j-x_k-\mu)}{\vartheta_1(x_j-x_k)}\frac{\vartheta_1(x_j+x_k-\mu)}{\vartheta_1(x_j+x_k)}\right)\left(\prod_{r=0}^{3}\frac{\vartheta_r(x_j-\mu_r)}{\vartheta_r(x_j)}\frac{\vartheta_r(x_j+\kappa/2-\mu_r')}{\vartheta_r(x_j+\kappa/2)}\right)\right)^{1/2}\\&\times\tau_j(\kappa)\left(\left(\prod_{\substack{k=1\\k\neq j}}^{l}\frac{\vartheta_1(x_j-x_k+\mu)}{\vartheta_1(x_j-x_k)}\frac{\vartheta_1(x_j+x_k+\mu)}{\vartheta_1(x_j+x_k)}\right)\right.\\&\left.\times\left(\prod_{r=0}^{3}\frac{\vartheta_r(x_j+\mu_r)}{\vartheta_r(x_j)}\frac{\vartheta_r(x_j-\kappa/2+\mu_r')}{\vartheta_r(x_j-\kappa/2)}\right)\right)^{1/2}\\&+\sum_{j=1}^{l}\left(\left(\prod_{\substack{k=1\\k\neq j}}^{l}\frac{\vartheta_1(-x_j-x_k-\mu)}{\vartheta_1(-x_j-x_k)}\frac{\vartheta_1(-x_j+x_k-\mu)}{\vartheta_1(-x_j+x_k)}\right)\right.\\&\left.\times\left(\prod_{r=0}^{3}\frac{\vartheta_r(-x_j-\mu_r)}{\vartheta_r(-x_j)}\frac{\vartheta_r(-x_j-\kappa/2-\mu_r')}{\vartheta_r(-x_j-\kappa/2)}\right)\right)^{1/2}\end{aligned}$$

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$$\times\tau_j(-\kappa)\Bigg(\Bigg(\prod_{\substack{k=1\\k\neq j}}^{l}\frac{\vartheta_1(-x_j-x_k+\mu)}{\vartheta_1(-x_j-x_k)}\frac{\vartheta_1(-x_j+x_k+\mu)}{\vartheta_1(-x_j+x_k)}\Bigg)$$
$$\times\Bigg(\prod_{r=0}^{3}\frac{\vartheta_r(-x_j+\mu_r)}{\vartheta_r(-x_j)}\frac{\vartheta_r(-x_j+\kappa/2+\mu_r')}{\vartheta_r(-x_j+\kappa/2)}\Bigg)\Bigg)^{1/2}$$
$$+\sum_{p=0}^{3}\left(\frac{\pi}{\vartheta_1'(0)}\right)^2\frac{2}{\vartheta_1(\mu)\vartheta_1(\kappa+\mu)}\Bigg(\prod_{r=0}^{3}\vartheta_r(\mu_{\pi_p r}+\kappa/2)\vartheta_r(\mu'_{\pi_p r})\Bigg)$$
$$\times\Bigg(\prod_{j=1}^{l}\frac{\vartheta_p(x_j-\kappa/2-\mu)}{\vartheta_p(x_j-\kappa/2)}\frac{\vartheta_p(-x_j-\kappa/2-\mu)}{\vartheta_p(-x_j-\kappa/2)}\Bigg), \tag{1.2}$$

where we have omitted an irrelevant additive constant in $A_{2l}^{(2)}$ system and realized the root systems in $\mathbb{C}^l$ in the standard way. π_j $(j=0,1,2,3)$ denotes the permutation: $\pi_1=\mathrm{id}$, $\pi_2=(12)(03)$, $\pi_3=(13)(02)$, and $\pi_0=(01)(23)$. The parameters are $\kappa,\tau\in i\mathbb{R}_{>0}$, and $\mu,\mu_j,\mu_j'\in i\mathbb{R}$ $(j=0,1,2,3)$ in order to ensure the formal self-adjointness of the Hamiltonians. Generalizations to arbitrary affine root systems are considered in Refs. 6–8.

For these models, there are many papers which treat their Hamiltonians as operators on meromorphic functions and concern their algebraic aspects such as commutativity,[1–6] relations to elliptic quantum algebras[9,10] and actions on the space of characters.[7,8,11,12] However, the self-adjointness was rarely discussed. In the two-body case, elaborate works are done by Ruijsenaars,[13–15] where infinitely many numbers of the explicit eigenvectors are constructed in the space of square integrable functions without Weyl group invariance and the completeness is to be solved. Concerning self-adjointness, the hyperbolic case should also be remarkable.[16]

The main purpose of this article is to give an appropriate domain in the space of square integrable functions which makes the Hamiltonian essentially self-adjoint. We suppose that the system is on a torus and is Weyl-group invariant as in the trigonometric models. A difficulty in the choice of the domain arises from the fact that the Hamiltonian includes the shift operators in the pure imaginary direction where the functions are not defined. Thus as a domain of the Hamiltonian, we should choose such functions as can be extended naturally to a complex region. In other words, they should be sufficiently analytic for the Hamiltonian to make sense. In this article, we employ the well-developed perturbation theory for the purpose and show that the Kato–Rellich theorem works well in the difference cases as in the differential cases.

This article is organized as follows: in Sec. II, we give definitions and basic facts about affine root systems and affine Weyl groups used in this article. In Secs. III and IV, we introduce the root algebra due to Cherednik. This algebra plays the role of the affine Hecke algebra in the trigonometric cases, and contains a commutative subalgebra which comes from the translation subgroup in affine Weyl groups. We clarify that if we give some representation on the space of meromorphic functions, one of the generators of the commutative subalgebra coincides with the conjugated Hamiltonian of the elliptic Ruijsenaars model by some function. In Sec. V, we show the essential self-adjointness of the elliptic Ruijsenaars models not of type $A_{2l}^{(2)}$. First we show the essential self-adjointness of the conjugated Hamiltonian in the square integrable functions with a weight function and then those of the original Hamiltonian without a weight function. We introduce an appropriate subspace of meromorphic functions invariant under the action of the corresponding Weyl group and regard this space as a subspace of the space of square integrable functions. Then the conjugated Hamiltonians are symmetric and semi-bounded below on this domain and thus can be extended to self-adjoint operators. The technique of integration by parts in the differential cases is replaced by the Cauchy theorem in the difference cases. Furthermore, we show that these Hamiltonians with a special coupling constant are essentially self-adjoint, in fact, and consist of only point spectrum. Then we apply the perturbation theory to these operators. We show their essential self-adjointness with the coupling constants in a neighborhood of the special point by use

of the Kato–Rellich theorem. The compactness of resolvents is inherited. In Sec. VI, we study the $A_{2l}^{(2)}$-type case. Although this model has nine arbitrary parameters and is very complicated, the method in the previous section works well in this model.

In this article, we restrict our attention to the lowest order operator acting on Weyl group invariant subspace. Although the higher order operators commute with the Hamiltonian as operators acting on the space of meromorphic functions, the commutativity in the sense of quantum mechanics requires further investigation since their domains are unclear. We hope to remove these restrictions and recover Ruijsenaars' result in the near future.

II. AFFINE ROOT SYSTEMS

We give some well-known facts about affine root systems and affine Weyl groups,[17–19] which are standard tools in the theory of affine Hecke algebras. Some of the definitions are slightly changed and extended so that they include twisted affine root systems. The notation is mainly due to Ref. 20.

Let $\mathfrak{g}$ be the affine Lie algebra of type $X_N^{(r)}$, $\mathfrak{h}$ its Cartan subalgebra of $\dim \mathfrak{h}=l+2$, $I=\{0,\ldots,l\}$ a set of indices, $\Pi=\{\alpha_i|i\in I\}\subset\mathfrak{h}^*$ the set of simple roots, $\Pi^\vee=\{\alpha_i^\vee|i\in I\}\subset\mathfrak{h}$ the set of simple coroots, Δ the root system, Q and $Q^\vee$ the root and coroot lattices, P and $P^\vee$ the weight and coweight lattices:

$$Q=\bigoplus_{i\in I}\mathbb{Z}\,\alpha_i\subset P=\bigoplus_{i\in I}\mathbb{Z}\,\Lambda_i\oplus\mathbb{C}\delta\subset\mathfrak{h}^*, \tag{2.1}$$

$$Q^\vee=\bigoplus_{i\in I}\mathbb{Z}\,\alpha_i^\vee\subset P^\vee=\bigoplus_{i\in I}\mathbb{Z}\,\Lambda_i^\vee\oplus\mathbb{C}K\subset\mathfrak{h}, \tag{2.2}$$

where $\langle\alpha_i,\Lambda_j^\vee\rangle=\delta_{ij}$, $\langle\Lambda_i,\alpha_j^\vee\rangle=\delta_{ij}$, $d=\Lambda_0^\vee$. Since the normalized invariant form is nondegenerate on $\mathfrak{h}$, we have an isomorphism $\nu:\mathfrak{h}\to\mathfrak{h}^*$ defined by

$$\langle\nu(h),h_1\rangle=(h|h_1),\quad h,h_1\in\mathfrak{h}, \tag{2.3}$$

and the induced bilinear form $(\cdot|\cdot)$ on $\mathfrak{h}^*$. Let $\mathring{I}=\{1,\ldots,l\}$, $\mathring{\Pi}=\{\alpha_i|i\in\mathring{I}\}$ and $\mathring{\Pi}^\vee=\{\alpha_i^\vee|i\in\mathring{I}\}$. Let $\mathring{\mathfrak{h}}^*$ be the subspace of $\mathfrak{h}^*$ spanned by $\mathring{\Pi}$ over $\mathbb{C}$. For $\lambda\in\mathfrak{h}^*$, denote by $\overline{\lambda}$ the orthogonal projection of λ on $\mathring{\mathfrak{h}}^*$. Let $\mathring{Q}$ be the sublattice of Q generated by $\mathring{\Pi}$ and $\mathring{P}$ the projection of P on $\mathring{\mathfrak{h}}^*$. The dual notions $\mathring{\mathfrak{h}}$, $\overline{h}$, $\mathring{Q}^\vee$ and $\mathring{P}^\vee$ are defined similarly:

$$\mathring{Q}=\bigoplus_{i\in\mathring{I}}\mathbb{Z}\,\alpha_i\subset\mathring{P}=\bigoplus_{i\in\mathring{I}}\mathbb{Z}\,\overline{\Lambda_i}\subset\mathring{\mathfrak{h}}^*, \tag{2.4}$$

$$\mathring{Q}^\vee=\bigoplus_{i\in\mathring{I}}\mathbb{Z}\,\alpha_i^\vee\subset\mathring{P}^\vee=\bigoplus_{i\in\mathring{I}}\mathbb{Z}\,\overline{\Lambda_i^\vee}\subset\mathring{\mathfrak{h}}. \tag{2.5}$$

Let $\mathfrak{h}_\mathbb{R}$ be the $\mathbb{R}$-span of $\{\alpha_i^\vee\}_{i\in I}\cup\{d\}$ and let $\mathring{\mathfrak{h}}_\mathbb{R}$ be the $\mathbb{R}$-span of $\{\alpha_i^\vee\}_{i\in\mathring{I}}$. Let Δ^{re}, Δ^{im}, Δ_+ and Δ_- be the set of real roots, imaginary roots, positive roots and negative roots, respectively. Then one has the disjoint unions $\Delta=\Delta^{\mathrm{re}}\cup\Delta^{\mathrm{im}}=\Delta_+\cup\Delta_-$. Let Δ_l be the set of the longest real roots. For $\alpha\in\Delta^{\mathrm{re}}$, let $\gamma_\alpha:=r$ if $\alpha\in\Delta_l$ and $\gamma_\alpha:=1$ otherwise, where r is from the type $X_N^{(r)}$. Then the real roots are written as

$$\Delta^{\mathrm{re}}=\begin{cases}\{\alpha+n\gamma_\alpha\delta|\alpha\in\mathring{\Delta},n\in\mathbb{Z}\}, & \text{if } X_N^{(r)}\neq A_{2l}^{(2)},\\ \{\alpha+n\gamma_\alpha\delta|\alpha\in\mathring{\Delta},n\in\mathbb{Z}\}\cup\{\frac{1}{2}(\alpha+(2n-1)\delta)|\alpha\in\mathring{\Delta}_l,n\in\mathbb{Z}\}, & \text{if } X_N^{(r)}=A_{2l}^{(2)}.\end{cases} \tag{2.6}$$

For $\alpha\in\Delta^{\mathrm{re}}$, let s_α be a reflection defined by

$$s_\alpha(\lambda) := \lambda - \langle \lambda, \alpha^\vee \rangle \alpha, \quad \lambda \in \mathfrak{h}^*. \tag{2.7}$$

The Weyl group $\mathring{W}$ is generated by the fundamental reflections $\{s_i := s_{\alpha_i} | i \in \mathring{I}\}$ on $\mathfrak{h}^*$ and the affine Weyl group W is generated by $\{s_i | i \in I\}$. The defining relations are given by $s_i^2 = id$ and the Coxeter relations:

$$(s_i s_j)^{m_{ij}} = id, \quad \text{for } i \neq j \in I, \tag{2.8}$$

where $m_{ij} = 2$ if α_i and α_j are disconnected in the Dynkin diagram and $m_{ij} = 3,4,6$ if 1,2,3 lines, respectively, connect α_i and α_j. We note that there is no Coxeter relation in the affine root systems of rank 2. For $\mu \in \mathring{\mathfrak{h}}^*$, we define endomorphisms τ_μ of the vector space $\mathfrak{h}^*$ by

$$\tau_\mu(\lambda) := \lambda + \langle \lambda, K \rangle \mu - ((\lambda|\mu) + \tfrac{1}{2}|\mu|^2 \langle \lambda, K \rangle)\delta, \tag{2.9}$$

where $|\mu|^2$ stands for $(\mu|\mu)$. The actions of s_α, τ_μ are naturally induced on $\mathfrak{h}$ via the form $\langle \cdot, \cdot \rangle$ as follows ($h \in \mathfrak{h}$):

$$s_\alpha(h) = h - \langle \alpha, h \rangle \alpha^\vee, \tag{2.10}$$

$$\tau_\mu(h) = h + \langle \delta, h \rangle \nu^{-1}(\mu) - (\langle \mu, h \rangle + \tfrac{1}{2}|\mu|^2 \langle \delta, h \rangle) K. \tag{2.11}$$

Let a_i and $a_i^\vee$ be the labels of the Dynkin diagram from Table Aff in Ref. 20. Note that $a_0 = 2$ if $X_N^{(r)} = A_{2l}^{(2)}$ and $a_0 = 1$ otherwise. Let $\theta := \delta - a_0 \alpha_0 \in \mathring{\Delta}_+$. Then $a_0^{-1} \gamma_\theta = 1$ and $\nu^{-1}(\theta) = a_0 \theta^\vee$. Let $M := \nu(\mathbb{Z}(\mathring{W} \cdot \theta^\vee)) \subset \mathring{\mathfrak{h}}^*$. For an arbitrary lattice L, we denote by T_L the corresponding group of translations of L.

Proposition II.1: The group W is the semidirect product $W = \mathring{W} \ltimes T_M$.

Let $\hat{M} := \{\lambda \in \mathring{\mathfrak{h}}^* | \alpha \in \Delta^{\mathrm{re}}, (\alpha|\lambda) \in \gamma_\alpha \mathbb{Z}\}$. Then we see that $\hat{M} \subset \mathring{P}$ and $T_{\hat{M}}$ is normalized by $\mathring{W}$.

Definition II.2: The extended affine Weyl group $\hat{W}$ is the semidirect product $\hat{W} := \mathring{W} \ltimes T_{\hat{M}}$.

The lattice $\hat{M}$ is taken to be the finest so that $T_{\hat{M}}$ acts on Δ, and thus the extended affine Weyl group acts on Δ. Here are the explicit description of $\hat{M}$ and its canonical basis $\{\lambda_i | i \in \mathring{I}\}$:

$$\hat{M} = \begin{cases} \nu(\mathring{P}^\vee), & \text{if } r = 1, \\ \mathring{P}, & \text{otherwise,} \end{cases} \qquad \lambda_i = \begin{cases} \nu(\overline{\Lambda_i^\vee}), & \text{if } r = 1, \\ \overline{\Lambda_i}, & \text{otherwise.} \end{cases} \tag{2.12}$$

We also use $\hat{M}_- := \oplus_{i \in \mathring{I}} \mathbb{Z}_{\leqslant 0} \lambda_i$.

Fix $\kappa \in \mathbb{C}$. Let $\mathfrak{h}_\kappa := \{h \in \mathfrak{h} | \langle \delta, h \rangle = \kappa\}$. Since W acts on $\mathfrak{h}_\kappa$, W acts on the affine space $\mathfrak{h}_\kappa \bmod \mathbb{C}K$. We identify $\mathfrak{h}_\kappa \bmod \mathbb{C}K$ with $\mathring{\mathfrak{h}}$ by projection. By this identification, we obtain affine transformations from $\hat{W}$ and affine linear functionals from $\langle \alpha, \cdot \rangle$ for $\alpha \in \Delta$. We denote so obtained maps by af, so that

$$\mathrm{af}(w)(\overline{h}) = \overline{w(h)}, \quad \mathrm{af}(\alpha)(\overline{h}) = \langle \alpha, h \rangle, \tag{2.13}$$

for $h \in \mathfrak{h}_\kappa$. Explicitly we have for $h \in \mathring{\mathfrak{h}}$

$$\mathrm{af}(\mathring{w})(h) = \mathring{w}(h), \quad \mathrm{af}(\tau_\mu)(h) = h + \kappa \nu^{-1}(\mu), \tag{2.14}$$

$$\mathrm{af}(\mathring{\alpha} + n\delta)(h) = \langle \mathring{\alpha}, h \rangle + \kappa n. \tag{2.15}$$

Note that

$$\mathrm{af}(\alpha) \circ \mathrm{af}(w) = \mathrm{af}(w^{-1}\alpha). \tag{2.16}$$

We define an action of the extended affine Weyl group on the space $\mathcal{M}$ of meromorphic functions on $\mathbb{H}:=\mathring{\mathfrak{h}}/\mathring{Q}^\vee$ by

$$(wf)(h):=f(\mathrm{af}(w^{-1})h). \tag{2.17}$$

Let Ω be the subgroup of $\hat{W}$ which stabilizes the affine Weyl chamber C.

Proposition II.3: The subgroup Ω is isomorphic to $\hat{W}/W\simeq T_{\hat{M}}/T_M$, thus Abelian. The extended affine Weyl group $\hat{W}$ is isomorphic to the semidirect product $W\rtimes\Omega$.

Definition II.4:

(1) The length $\ell(w)$ of $w\in W$ is the length ℓ of the reduced decomposition:

$$w=s_{i_1}\cdots s_{i_\ell},\quad \text{for } i_k\in I, \tag{2.18}$$

$$\ell(id)=0. \tag{2.19}$$

(2) The length $\ell(\hat{w})$ of $\hat{w}\in\hat{W}$ is the number of the negative roots made positive by $\hat{w}$:

$$\ell(\hat{w}):=|\Delta_{\hat{w}}|, \tag{2.20}$$

$$\Delta_{\hat{w}}:=\{\alpha\in\Delta_+\cap\hat{w}\Delta_-\}, \tag{2.21}$$

which is equivalent to the definition $\ell(w)$ for $w\in W$. The reduced decomposition of $\hat{w}\in\hat{W}$ is $\hat{w}=w\omega=s_{i_1}\cdots s_{i_\ell}\omega$, where $\omega\in\Omega$ and $\ell=\ell(\hat{w})=\ell(w)$.

The set $\Delta_{\hat{w}}$ is explicitly described as $\Delta_{\hat{w}}=\{\alpha^{(1)}=\alpha_{i_1},\alpha^{(2)}=s_{i_1}(\alpha_{i_2}),\cdots,\alpha^{(\ell)}=ws_{i_\ell}(\alpha_{i_\ell})\}$. By definition, $\Delta_{\hat{w}}$ is independent of reduced expressions. One sees that $\Omega=\{\omega\in\hat{W},\ell(\omega)=0\}$.

Definition II.5: A weight $\lambda\in\hat{M}$ is said to be minuscule if $\Delta_{\tau_{-\lambda}}\subset\mathring{\Delta}_+$.

The weight $\nu^{-1}(\theta^\vee)$ is called the quasi-minuscule weight due to the following properties:

$$\langle\alpha,\theta^\vee\rangle=0\ \text{ or }\ \gamma_\alpha,\quad \text{for } \alpha(\neq\theta)\in\mathring{\Delta}_+,\quad \langle\theta,\theta^\vee\rangle=2. \tag{2.22}$$

The quasi-minuscule weight just fails to be minuscule:

$$\Delta_{\tau_{-\nu^{-1}(\theta^\vee)}}=\Delta_{s_\theta}\cup\{a_0^{-1}(\theta+\delta)\}. \tag{2.23}$$

We give the definitions of the Jacobi theta functions. For $\Im\tau>0$, the Jacobi theta functions are defined by

$$\vartheta_1(x;\tau):=-i\sum_{n\in\mathbb{Z}}\exp\left(i\pi\left(n+\frac{1}{2}\right)^2\tau+2\pi i\left(n+\frac{1}{2}\right)x+i\pi n\right), \tag{2.24a}$$

$$\vartheta_2(x;\tau):=\sum_{n\in\mathbb{Z}}\exp\left(i\pi\left(n+\frac{1}{2}\right)^2\tau+2\pi i\left(n+\frac{1}{2}\right)x\right), \tag{2.24b}$$

$$\vartheta_3(x;\tau):=\sum_{n\in\mathbb{Z}}\exp(i\pi n^2\tau+2\pi inx), \tag{2.24c}$$

$$\vartheta_0(x;\tau):=\sum_{n\in\mathbb{Z}}\exp(i\pi n^2\tau+2\pi inx+i\pi n). \tag{2.24d}$$

These functions are expressed by infinite products:

$$\vartheta_1(x;\tau)=ip^{1/8}z^{-1/2}(p;p)_\infty(z;p)_\infty(pz^{-1};p)_\infty, \tag{2.25a}$$

$$\vartheta_2(x;\tau)=p^{1/8}z^{-1/2}(p;p)_\infty(-z;p)_\infty(-pz^{-1};p)_\infty, \tag{2.25b}$$

$$\vartheta_3(x;\tau)=(p;p)_\infty(-p^{1/2}z;p)_\infty(-p^{1/2}z^{-1};p)_\infty, \tag{2.25c}$$

$$\vartheta_0(x;\tau)=(p;p)_\infty(p^{1/2}z;p)_\infty(p^{1/2}z^{-1};p)_\infty, \tag{2.25d}$$

where $p=e^{2\pi i\tau}$, $z=e^{2\pi ix}$ and

$$(z;q_1,\cdots,q_m)_\infty:=\prod_{n_1,\cdots,n_m\in\mathbb{Z}_{\geqslant 0}}(1-q_1^{n_1}\cdots q_m^{n_m}z). \tag{2.26}$$

Define constants a_j and b_j for $j=0,1,2,3$ as

$$a_1=0,\quad b_1=0, \tag{2.27a}$$

$$a_2=1,\quad b_2=0, \tag{2.27b}$$

$$a_3=1,\quad b_3=1, \tag{2.27c}$$

$$a_0=0,\quad b_0=1. \tag{2.27d}$$

Then the zeroes of $\vartheta_j(x;\tau)$ are expressed as $\mathbb{Z}+a_j/2+(\mathbb{Z}+b_j/2)\tau$.

III. ROOT ALGEBRAS

We shall define the root algebras after Cherednik.[19] See Refs. 6–8 for the details of the proofs.

Let $\mathcal{T}$ be the tensor algebra over $\mathbb{C}$ generated by independent variables $\{R_\alpha|\alpha\in\Delta^{\mathrm{re}}\}$. Then the action of $\hat{w}\in\hat{W}$ on Δ^{re} induces an action on $\mathcal{T}$ by ${}^{\hat{w}}\!:R_\alpha\mapsto R_{\hat{w}(\alpha)}$.

Definition III.1: Let $\mathcal{I}$ be the two-sided ideal in $\mathcal{T}$ which is generated by all the elements of the form for $i\neq j\in I$, and $\hat{w}\in\hat{W}$:

$$\underbrace{{}^{\hat{w}}(R_{\alpha_i}\otimes R_{s_i\alpha_j}\otimes R_{s_is_j\alpha_i}\otimes\cdots)}_{m_{ij}\ \text{factors}}-\underbrace{{}^{\hat{w}}(R_{\alpha_j}\otimes R_{s_j\alpha_i}\otimes R_{s_js_i\alpha_j}\otimes\cdots)}_{m_{ij}\ \text{factors}}. \tag{3.1}$$

The root algebra $\tilde{\mathcal{R}}$ is $\mathcal{T}/\mathcal{I}.\{R_\alpha|\alpha\in\Delta^{\mathrm{re}}\}$ are called the R-matrices.

Because of the $\hat{W}$-invariance of $\mathcal{I}$, the action of $\hat{W}$ is induced on $\tilde{\mathcal{R}}$. For simplicity, we write products in $\tilde{\mathcal{R}}$ in the usual way for associative algebras.

Theorem III.2 (Cherednik):

(1) There exists a unique set $\{R_{\hat{w}}|\hat{w}\in\hat{W}\}\subset\tilde{\mathcal{R}}$ *satisfying the relations*

$$R_{v\,w}=R_v{}^vR_w,\quad R_{s_i}=R_{\alpha_i}\quad(i\in I),\quad R_\omega=1, \tag{3.2}$$

where $\omega\in\Omega$, $v,w\in\hat{W}$ *and* $\ell(v\,w)=\ell(v)+\ell(w)$.

(2) We have the R-matrix for $\hat{w}\in\hat{W}$ *and its arbitrary reduced decomposition* $\hat{w}=w\omega=s_{i_1}\ldots s_{i_\ell}\omega$ *as*

$$\begin{gathered}R_{\hat{w}}=R_{\alpha^{(1)}}\ldots R_{\alpha^{(\ell)}},\\ \alpha^{(1)}=\alpha_{i_1},\quad \alpha^{(2)}=s_{i_1}(\alpha_{i_2}),\quad\ldots,\quad \alpha^{(\ell)}=ws_{i_\ell}(\alpha_{i_\ell})\in\Delta_{\hat{w}}.\end{gathered} \tag{3.3}$$

Instead of the original root algebra, we work with the following extension, where $\tilde{\mathcal{R}}$ is combined with the translation group $T_{\hat{M}}$:

Definition III.3: $\mathcal{R}:=\tilde{\mathcal{R}}\rtimes T_{\hat{M}}$:

$$(R\,\tau_\lambda)(R'\,\tau_\mu)=R\,({}^{\tau_\lambda}R')\,\tau_{\lambda+\mu}, \tag{3.4}$$

where $R,R'\in\tilde{\mathcal{R}}$ and $\lambda,\mu\in\hat{M}$.

Theorem III.4: *The subalgebra $\mathcal{S}\subset\mathcal{R}$ generated by $\{Y^\lambda:=R_{\tau_\lambda}\,\tau_\lambda|\lambda\in\hat{M}_-\}$ forms a commutative algebra and is generated by $\{Y^{-\lambda_i}|i\in\mathring{I}\}$.*

IV. DIFFERENCE OPERATORS WITH ELLIPTIC FUNCTION COEFFICIENTS

In this section, we give a class of the representation of the root algebra and construct the conjugated Hamiltonians of the elliptic Ruijsenaars models associated with affine root systems.

Let $\kappa,\tau\in\mathbb{C}$ and $\Im\tau>0$. For $\alpha\in\Delta^{\mathrm{re}}$, let $\mu_\alpha\in\mathbb{C}$ be $\hat{W}$-invariant constants: $\mu_{\hat{w}(\alpha)}=\mu_\alpha$ for $\hat{w}\in\hat{W}$, such that $\langle\mathring{\rho}_\mu,\alpha^\vee\rangle\neq\mathbb{Z}/\gamma_\alpha+\tau\mathbb{Z}$, where

$$\mathring{\rho}_\mu:=\sum_{i\in\mathring{I}}\mu_{\alpha_i}\overline{\Lambda}_i=\frac{1}{2}\sum_{\alpha\in\mathring{\Delta}_+}\mu_\alpha\alpha. \tag{4.1}$$

Fix $\xi\in\mathring{\mathfrak{h}}^*$ such that $\langle\xi,\alpha^\vee\rangle\neq\mathbb{Z}/\gamma_\alpha+\tau\mathbb{Z}$ for all $\alpha\in\Delta^{\mathrm{re}}$. We define $\hat{R}_\alpha\in\mathrm{End}_{\mathbb{C}}\mathcal{M}$ for $\alpha\in\Delta^{\mathrm{re}}$ by

$$\hat{R}_\alpha:=H_\alpha(\mu_\alpha)-H_\alpha(\langle\xi,\alpha^\vee\rangle)\circ s_\alpha, \tag{4.2}$$

where $H_\alpha(\eta)$ is a multiplication operator with the following function on $\mathbb{H}$:

$$H_\alpha(\eta)(h):=\frac{\vartheta_1(-\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1(-\gamma_\alpha\eta;\gamma_\alpha\tau)}\,\frac{\vartheta_1(\mathrm{af}(\alpha)(h)-\gamma_\alpha\eta;\gamma_\alpha\tau)}{\vartheta_1(\mathrm{af}(\alpha)(h);\gamma_\alpha\tau)}. \tag{4.3}$$

By the property (2.16), one sees that $wH_\alpha(\eta)(h)=H_{w\alpha}(\eta)(h)$ and, in particular, $\tau_\lambda\hat{R}_\alpha\tau_{-\lambda}=\hat{R}_{\tau_\lambda\alpha}={}^{\tau_\lambda}\hat{R}_\alpha$.

Theorem IV.1 (Refs. 7 and 8): *The map $\pi:R_\alpha\mapsto\hat{R}_\alpha$, $\tau_\lambda\mapsto\tau_\lambda$ induces a homomorphism from $\mathcal{R}$ to $\mathrm{End}_{\mathbb{C}}\mathcal{M}$. These R-matrices satisfy the unitarity*

$$\hat{R}_\alpha\hat{R}_{-\alpha}=\left(\frac{\vartheta_1(-\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1'(0;\gamma_\alpha\tau)}\right)^2(\wp(\gamma_\alpha\mu_\alpha;1,\gamma_\alpha\tau)-\wp(\gamma_\alpha\langle\xi,\alpha^\vee\rangle;1,\gamma_\alpha\tau))\mathrm{Id}_{\mathcal{M}}. \tag{4.4}$$

We employ these operators even for the affine root systems of rank 2, though they do not have any Coxeter relations.

Besides the representation above, we have more general forms that depend on the relation among $Q,Q^\vee,M$.[7,8] We classified them from the viewpoint of characters of integrable highest weight modules with positive levels. In particular, the operators of type $A_{2l}^{(2)}$ include nine parameters. In the rest of this section and the next section, we study the representation in Theorem IV.1 for the type $X_N^{(r)}\neq A_{2l}^{(2)}$ and we will deal with the type $A_{2l}^{(2)}$ in Sec. VI independently. In the case $X_N^{(r)}\neq A_{2l}^{(2)}$, we have

$$a_0=1,\quad \nu^{-1}(\theta)=\theta^\vee,\quad \mu_{\alpha_0}=\mu_\theta. \tag{4.5}$$

We shall clarify some properties of the operators $\hat{Y}^\lambda=\pi(Y^\lambda)$ for minuscule weights and the quasi-minuscule weight. Let $\mathbb{T}$ be the torus $\mathring{\mathfrak{h}}_{\mathbb{R}}/\mathring{Q}^\vee\subset\mathbb{H}$. Let $\mathcal{M}^{\mathring{W}}$ be the $\mathring{W}$-invariant subspace of $\mathcal{M}$. Let $\mathcal{M}_\lambda:=\{f|f\in\mathcal{M},f$ is holomorphic in a neighborhood of $\cup_{0\leqslant a\leqslant 1}(\mathrm{af}(\tau_{-a\lambda})\mathbb{T})\}$. □

Lemma IV.2: $\hat{R}_\alpha\in\mathrm{End}_{\mathbb{C}}(\mathcal{M}_0)$ $(\alpha\in\mathring{\Delta})$. *If $\kappa\notin\mathbb{Z}/\gamma_\alpha+\mathbb{Z}\tau$, then $\hat{R}_{\theta+\delta}\in\mathrm{End}_{\mathbb{C}}(\mathcal{M}_\theta,\mathcal{M}_0)$.*

Proof: Let $\alpha\in\mathring{\Delta}$ and $f\in\mathcal{M}_0$. Then a possible pole of $\hat{R}_\alpha f$ on $\mathbb{T}$ is h_0 such that $\mathrm{af}(\alpha)(h_0)=\langle\alpha,h_0\rangle\in\mathbb{Z}$ and vanishes since

$$f(h_0)-f(\mathrm{af}(s_\alpha)(h_0))=0, \tag{4.6}$$

by $\mathrm{af}(s_\alpha)(h_0)=h_0-\langle\alpha,h_0\rangle\alpha^\vee\equiv h_0(\mathrm{mod}\,\mathring{Q}^\vee)$.

The latter statement is implied by the fact that if $\kappa\notin\mathbb{Z}/\gamma_\alpha+\mathbb{Z}\tau$ and $f\in\mathcal{M}_\theta$, the functions $H_{\theta+\delta}(\eta)(h)$ in $\hat{R}_{\theta+\delta}$, $f(h)$ and $f(h-(\langle\theta,h\rangle+\kappa)\theta^\vee)$ are holomorphic in the neighborhood of $\mathbb{T}$. □

Theorem IV.3: *Let* $\xi=-\mathring{\rho}_\mu$. *Then* $\hat{Y}^\lambda\in\mathrm{End}_{\mathbb{C}}(\mathcal{M}_\lambda^{\mathring{W}},\mathcal{M}_0^{\mathring{W}})$ *for a minuscule weight* $-\lambda$. *In addition, if* $\kappa\notin\mathbb{Z}/\gamma_\alpha+\mathbb{Z}\tau$, *then* $\hat{Y}^{-\theta}\in\mathrm{End}_{\mathbb{C}}(\mathcal{M}_{-\theta}^{\mathring{W}},\mathcal{M}_0^{\mathring{W}})$.

Proof: It is obvious that $\tau_\lambda\in\mathrm{End}_{\mathbb{C}}(\mathcal{M}_\lambda,\mathcal{M}_{-\lambda})$. By construction, $\hat{Y}^\lambda$ takes the form of $\hat{R}_\alpha\hat{R}_\beta\cdots\hat{R}_\gamma\tau_\lambda$. For a minuscule weight, we see that from Theorem III.2, $\hat{Y}^\lambda$ consists of only non affine R-matrices, thus by Lemma IV.2 and $\mathcal{M}_{-\lambda}\subset\mathcal{M}_0$, we have

$$\mathcal{M}_\lambda\xrightarrow{\tau_\lambda}\mathcal{M}_{-\lambda}\subset\mathcal{M}_0\xrightarrow{\hat{R}_\gamma}\cdots\xrightarrow{\hat{R}_\alpha}\mathcal{M}_0, \tag{4.7}$$

and $\hat{Y}^\lambda\in\mathrm{End}_{\mathbb{C}}(\mathcal{M}_\lambda,\mathcal{M}_0)$. For the quasi-minuscule weight, the rightmost R-matrix in $\hat{Y}^{-\theta}$ is $\hat{R}_{\theta+\delta}$ and the others are nonaffine R-matrices.[7,8] By Lemma IV.2, we have

$$\mathcal{M}_{-\theta}\xrightarrow{\tau_{-\theta}}\mathcal{M}_\theta\xrightarrow{\hat{R}_{\theta+\delta}}\mathcal{M}_0\xrightarrow{\hat{R}_\gamma}\cdots\xrightarrow{\hat{R}_\alpha}\mathcal{M}_0, \tag{4.8}$$

and $\hat{Y}^{-\theta}\in\mathrm{End}_{\mathbb{C}}(\mathcal{M}_{-\theta},\mathcal{M}_0)$. In Refs. 7 and 8, we have shown that if $\xi=-\mathring{\rho}_\mu$, $\hat{Y}^\lambda\in\mathrm{End}_{\mathbb{C}}(\mathcal{M}^{\mathring{W}})$, which completes the proof.

For minuscule weights $-\lambda$ and the quasi-minuscule weight θ, we have the explicit forms of the operators on the space $\mathcal{M}^{\mathring{W}}$. In the following, we fix $\xi=-\mathring{\rho}_\mu$.

Theorem IV.4 (Refs. 7 and 8): *We have*

$$\hat{Y}^\lambda|_{\mathcal{M}^{\mathring{W}}}=\frac{1}{|\mathring{W}_\lambda|}\sum_{w\in\mathring{W}}w\left(\prod_{\substack{\alpha\in\mathring{\Delta}_+\\(\lambda|\alpha)=-\gamma_\alpha}}\frac{\vartheta_1(\langle\alpha,h\rangle-\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1(\langle\alpha,h\rangle;\gamma_\alpha\tau)}\tau_\lambda\right)\Bigg|_{\mathcal{M}^{\mathring{W}}}, \tag{4.9}$$

$$\begin{aligned}\hat{Y}^{-\theta}|_{\mathcal{M}^{\mathring{W}}}=\frac{1}{|\mathring{W}_\theta|}\sum_{w\in\mathring{W}}w\Bigg(&\left(\prod_{\substack{\alpha\in\mathring{\Delta}_+\\(\theta|\alpha)>0}}\frac{\vartheta_1(\langle\alpha,h\rangle-\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1(\langle\alpha,h\rangle;\gamma_\alpha\tau)}\right)\\&\times\left(\frac{\vartheta_1(\langle\theta,h\rangle+\kappa-\mu_\theta;\tau)}{\vartheta_1(\langle\theta,h\rangle+\kappa;\tau)}\tau_{-\theta}-\frac{\vartheta_1(-\mu_\theta;\tau)}{\vartheta_1((\mathring{\rho}_\mu|\theta);\tau)}\frac{\vartheta_1(\langle\theta,h\rangle+\kappa+(\mathring{\rho}_\mu|\theta);\tau)}{\vartheta_1(\langle\theta,h\rangle+\kappa;\tau)}\right)\Bigg)\Bigg|_{\mathcal{M}^{\mathring{W}}},\end{aligned} \tag{4.10}$$

where $\mathring{W}_\lambda$ *is the stabilizer of* λ *in* $\mathring{W}$.

Remark IV.5: The number of the minuscule weights is the same as the order of Ω. There is no minuscule weight available in the root systems of type $E_8^{(1)}$, $F_4^{(1)}$, $G_2^{(1)}$, $A_{2l}^{(2)}$, $E_6^{(2)}$ and $D_4^{(3)}$ since their Dynkin diagrams have no automorphism. However, every root system possesses the quasi-minuscule weight $\nu(\theta^\vee)$.

The following lemma is needed in the proof of the essential self-adjointness, which indicates that the term without shift operators in $\hat{Y}^{-\theta}$ is a bounded self-adjoint operator.

Lemma IV.6: The function

$$\hat{Y}_1^{-\theta}(h) := \frac{\vartheta_1(\mu_\theta;\tau)}{\vartheta_1((\mathring{\rho}_\mu|\theta);\tau)} \frac{1}{|\mathring{W}_\theta|} \sum_{w\in\mathring{W}} \left(w\left(\prod_{\substack{\alpha\in\mathring{\Delta}_+ \\ (\theta|\alpha)>0}} \frac{\vartheta_1(\langle\alpha,h\rangle-\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1(\langle\alpha,h\rangle;\gamma_\alpha\tau)} \right) \times\left(\frac{\vartheta_1(\langle\theta,h\rangle+\kappa+(\mathring{\rho}_\mu|\theta);\tau)}{\vartheta_1(\langle\theta,h\rangle+\kappa;\tau)} \right) \right) \tag{4.11}$$

is a function on $\mathring{\mathfrak{h}}/(\mathring{Q}^\vee+\tau\nu^{-1}(\hat{M}))$. *Moreover, if* $\tau\in i\mathbb{R}_{>0}$, $\kappa,\mu_\alpha\in i\mathbb{R}$ *and* $\kappa\notin\mathbb{Z}\tau$, *then* $\hat{Y}_1^{-\theta}(h)$ *is real-valued and continuous on* $\mathbb{T}$ *and thus has bounds*

$$-\infty<m_Y\leqslant\hat{Y}_1^{-\theta}(h)\leqslant M_Y<\infty,\quad h\in\mathbb{T}. \tag{4.12}$$

Proof: First we check that the function can be regarded as a function on $\mathring{\mathfrak{h}}/(\mathring{Q}^\vee+\tau\nu^{-1}(\hat{M}))$. For $h\to h+\beta^\vee$, the multiplicity is 1. For $h\to h+\tau\lambda(\lambda\in\nu^{-1}(\hat{M}))$, the multiplicity is

$$\exp 2\pi i\left(\sum_{\substack{\alpha\in\mathring{\Delta}_+ \\ (\theta|\alpha)>0}} \mu_\alpha\langle\alpha,\lambda\rangle-\langle\theta,\lambda\rangle(\mathring{\rho}_\mu|\theta) \right) = \exp 2\pi i\left(\sum_{\alpha\in\mathring{\Delta}_+} \frac{\mu_\alpha}{\gamma_\alpha}\langle\alpha,\theta^\vee\rangle\langle\alpha,\lambda\rangle-\mu_\theta\langle\theta,\lambda\rangle-(\mathring{\rho}_\mu|\theta)\langle\theta,\lambda\rangle \right), \tag{4.13}$$

where we have used the properties of θ (2.22). For the moment, we admit that

$$\sum_{\alpha\in\mathring{\Delta}_+} \frac{\mu_\alpha}{\gamma_\alpha}\langle\alpha,\theta^\vee\rangle\langle\alpha,\lambda\rangle=((\mathring{\rho}_\mu|\theta)+\mu_\theta)\langle\theta,\lambda\rangle, \tag{4.14}$$

then the multiplicity is 1 and the former statement follows.

Next we verify that all the poles on $\mathring{\mathfrak{h}}_\mathbb{R}$ vanish. Take $\beta\in\mathring{\Delta}$ and $h_0\in\mathring{\mathfrak{h}}_\mathbb{R}$ such that $\langle\beta,h_0\rangle\in\mathbb{Z}$ and $\langle\alpha,h_0\rangle\notin\mathbb{Z}$ for $\alpha(\neq\beta)\in\mathring{\Delta}$. Let $F(x,y;\gamma):=\vartheta_1(x+y;\gamma\tau)/\vartheta_1(x;\gamma\tau)$. Note that $F(x+1,y,\gamma)=F(x,y,\gamma)$. Then the residue at $c=0$ in the coordinate $h=h_0+c\beta^\vee/2$ is

$$\vartheta_1(-\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)\left(\sum_{\substack{w\in\mathring{W} \\ \beta\in w\Delta^\theta}} \left(\prod_{\substack{\alpha\in\Delta^\theta \\ w\alpha\neq\beta}} F(\langle w\alpha,h_0\rangle,-\gamma_\alpha\mu_\alpha;\gamma_\alpha) \right)(F(\langle w\theta,h_0\rangle+\kappa,(\mathring{\rho}_\mu|\theta);1)) \right.$$

$$\left. -\sum_{\substack{w\in\mathring{W} \\ -\beta\in w\Delta^\theta}} \left(\prod_{\substack{\alpha\in\Delta^\theta \\ w\alpha\neq-\beta}} F(\langle w\alpha,h_0\rangle,-\gamma_\alpha\mu_\alpha;\gamma_\alpha) \right)(F(\langle w\theta,h_0\rangle+\kappa,(\mathring{\rho}_\mu|\theta);1)) \right), \tag{4.15}$$

where $\Delta^\theta:=\{\alpha\in\mathring{\Delta}_+|\langle\alpha,\theta^\vee\rangle>0\}$. By replacing $w\to s_\beta w$ in the second term, we see that this residue vanishes since $\langle\beta,h_0\rangle=n\in\mathbb{Z}$ implies $s_\beta(h_0)=h_0-n\beta^\vee$ and $\langle\mathring{\Delta},\beta^\vee\rangle\in\mathbb{Z}$. By the Riemann theorem, the function is holomorphic in a neighborhood of h_0. The function $\hat{Y}_1^{-\theta}$ is real-valued on $\mathbb{T}$ because for $a\in\mathbb{R}$, $\overline{\vartheta_1(\langle\alpha,h\rangle+ia;\gamma_\alpha\tau)}=\vartheta_1(-\langle\alpha,h\rangle+ia;\gamma_\alpha\tau)$ and there exists $w_0\in\mathring{W}$ such that $w_0\mathring{\Delta}_+=\mathring{\Delta}_-$ and $w_0\theta=-\theta$.

Lemma IV.7: Let $L:\mathring{\mathfrak{h}}\to\mathring{\mathfrak{h}}$ *be a linear operator defined by*

$$L:h\mapsto\sum_{\alpha\in\mathring{\Delta}_+}\frac{\mu_\alpha}{\gamma_\alpha}\nu^{-1}(\alpha)\langle\alpha,h\rangle. \tag{4.16}$$

Then $L(h)=((\mathring{\rho}_\mu|\theta)+\mu_\theta)h$. *In particular,*

$$(\theta^\vee|L(\lambda))=\sum_{\alpha\in\mathring{\Delta}_+}\frac{\mu_\alpha}{\gamma_\alpha}\langle\alpha,\theta^\vee\rangle\langle\alpha,\lambda\rangle=((\mathring{\rho}_\mu|\theta)+\mu_\theta)\langle\theta,\lambda\rangle. \tag{4.17}$$

Proof: We see $L\in\mathrm{End}_{\mathring{W}}(\mathring{\mathfrak{h}})$. Since $\mathring{W}$ acts on $\mathring{\mathfrak{h}}^*$ irreducibly, Schur's lemma implies that $L(h)=a\,h$ for some $a\in\mathbb{C}$. We calculate this factor a. We have

$$L(\theta^\vee)=\sum_{\alpha\in\mathring{\Delta}_+}\frac{\mu_\alpha}{\gamma_\alpha}\nu^{-1}(\alpha)\langle\alpha,\theta^\vee\rangle=\sum_{\substack{\alpha\in\mathring{\Delta}_+\\ \langle\alpha,\theta^\vee\rangle\neq 0}}\mu_\alpha\nu^{-1}(\alpha)+\mu_\theta\theta^\vee=a\,\theta^\vee. \tag{4.18}$$

Applying $\langle\theta,\cdot\rangle$, we have

$$2a=\sum_{\substack{\alpha\in\mathring{\Delta}_+\\ (\alpha|\theta)\neq 0}}\mu_\alpha(\alpha|\theta)+2\mu_\theta=2(\mathring{\rho}_\mu|\theta)+2\mu_\theta, \tag{4.19}$$

thus $a=(\mathring{\rho}_\mu|\theta)+\mu_\theta$. □

V. ESSENTIAL SELF-ADJOINTNESS OF TYPE $X_N^{(r)}\neq A_{2l}^{(2)}$

A. Essential self-adjointness of elliptic Calogero–moser models

In the differential limit, the models are called the elliptic Calogero–Moser models. Because the Hamiltonians of these models are typical Schrödinger operators, we can establish the self-adjointness by use of well-developed perturbation theory.[21] First we briefly observe this fact.

The Hamiltonians of the Calogero–Sutherland models and the elliptic Calogero–Moser models are respectively given by

$$H_{\mathrm{T}}:=-\Delta+\sum_{\alpha\in\mathring{\Delta}_+}g_\alpha\frac{1}{\sin^2(2\pi\langle\alpha,h\rangle)}, \tag{5.1}$$

$$H_{\mathrm{E}}:=-\Delta+\sum_{\alpha\in\mathring{\Delta}_+}g_\alpha\wp(\langle\alpha,h\rangle;1,\gamma_\alpha\tau), \tag{5.2}$$

where the coupling constant g_α is a real number and invariant under the action of the Weyl group $\mathring{W}$ as $g_\alpha=g_{w\alpha}$. Δ is the Laplacian on $\mathbb{T}$. Let $L^2(\mathbb{T},d\mu)^{\mathring{W}}$ be the Hilbert space of $\mathring{W}$-invariant square integrable functions on $\mathbb{T}$ equipped with the inner product

$$(f,g):=\int_{\mathbb{T}}\overline{f}\cdot g\,d\mu, \tag{5.3}$$

where μ is the normalized Haar measure. We denote by $\|\cdot\|:=(\cdot,\cdot)^{1/2}$ the norm in $L^2(\mathbb{T},d\mu)^{\mathring{W}}$.

In the trigonometric case, if we adopt an appropriate domain $\mathcal{C}$ to the Hamiltonian (5.1), we can show its essential self-adjointness. Admitting this fact, we show that the elliptic models is essentially self-adjoint with the same domain.

Theorem V.1: *The Hamiltonian* (5.2) *is essentially self-adjoint on* $\mathcal{C}$.

Proof: We rewrite $H_{\mathrm{E}}=A+H_{\mathrm{T}}$, where $A=(H_{\mathrm{E}}-H_{\mathrm{T}})$. We see that

$$\|Au\| = \left(\int_{\mathbb{T}} \left| \sum_{\alpha \in \mathring{\Delta}_+} g_\alpha \left(\wp(\langle \alpha, h \rangle; 1, \gamma_\alpha \tau) - \frac{1}{\sin^2(2\pi \langle \alpha, h \rangle)} \right) u(h) \right|^2 d\mu \right)^{1/2}$$
$$\leqslant c\|u\|, \tag{5.4}$$

for a constant c, since the integrand is a continuous function on $\mathbb{T}$. This implies that A is bounded. The symmetry of the operator A is trivial. Then we deduce that $A + H_{\mathrm{T}}$ is essentially self-adjoint on $\mathcal{C}$. □

As is seen above, in the differential cases the essential self-adjointness of the elliptic models can be easily shown since they are relatively bounded to the trigonometric models with the relative bound 0 from the viewpoint of the Kato–Rellich theorem. We show that this theorem works well even in the difference cases, where we apply perturbation method to free particle systems instead of the corresponding trigonometric models.

B. Symmetry

Let $\tau \in i\mathbb{R}_{>0}$ and $\kappa, \mu_\alpha \in i\mathbb{R}$. Hereafter we fix $\xi = -\mathring{\rho}_\mu$ and restrict the domain of $\hat{Y}^\lambda$ to $\mathring{W}$-invariant functions. We treat μ_α as parameters of perturbation and suppose μ_α moves on pure imaginary numbers. Let n_0 be the number of the orbits of the roots and let $P_{\boldsymbol{\mu}} := i\mathbb{R}^{n_0}$. The topology on the space $P_{\boldsymbol{\mu}}$ of parameters $\boldsymbol{\mu} = (\mu_\alpha)$ is given by

$$d(\boldsymbol{\mu}, \boldsymbol{\mu}') := \max_{|\alpha|} \gamma_\alpha |\mu_\alpha - \mu'_\alpha|. \tag{5.5}$$

We denote $\boldsymbol{\mu}_0 = (\mu_\alpha = -\kappa) \in P_{\boldsymbol{\mu}}$ which is the start point of the perturbation.

Let $w_0 \in \mathring{W}$ such that $w_0 \mathring{\Delta}_+ = \mathring{\Delta}_-$. Then $w_0 \theta = -\theta$ and if $-\lambda$ is minuscule, $w_0 \lambda$ is also minuscule. Due to this observation, we see that the operator $\hat{Y}^\lambda$ for a minuscule weight or the quasi-minuscule weight coincides with $\hat{Y}^{-w_0\lambda}$ whose parameters κ and μ_α are replaced by $-\kappa$ and $-\mu_\alpha$, respectively. So we assume $\Im \kappa > 0$ without loss of generality. We set

$$p = e^{2\pi i \tau}, \quad q = e^{2\pi i \kappa}, \quad t_\alpha = e^{-2\pi i \mu_\alpha \gamma_\alpha}, \tag{5.6}$$

and define the meromorphic functions $m_\pm$ on $\mathbb{H}$ by

$$m_\pm(\mathbf{t} = (t_\alpha)) := e^{\pm \mathring{\rho}_\mu / \kappa} \prod_{\alpha \in \mathring{\Delta}_\pm} \frac{(e^\alpha; p^{\gamma_\alpha}, q^{\gamma_\alpha})_\infty}{(t_\alpha e^\alpha; p^{\gamma_\alpha}, q^{\gamma_\alpha})_\infty} \frac{(p^{\gamma_\alpha} q^{\gamma_\alpha} t_\alpha^{-1} e^{-\alpha}; p^{\gamma_\alpha}, q^{\gamma_\alpha})_\infty}{(p^{\gamma_\alpha} q^{\gamma_\alpha} e^{-\alpha}; p^{\gamma_\alpha}, q^{\gamma_\alpha})_\infty}. \tag{5.7}$$

We note that this function is a generalization of one introduced in Refs. 11 and 22. For the moment, we work with the variables p, q and t_α instead of τ, κ and μ_α. Let $P_{\mathbf{t}} := (0, \infty)^{n_0}$. Then t_α moves on $P_{\mathbf{t}}$. The start point $\boldsymbol{\mu}_0$ of the perturbation is $\mathbf{t}_0 = (t_\alpha = q^{\gamma_\alpha}) \in P_{\mathbf{t}}$ in this variable. The topology is induced on the space $P_{\mathbf{t}}$ by (5.6). We often write $\hat{Y}^\lambda = \hat{Y}^\lambda(\mathbf{t})$ in order to stress the dependency of $\mathbf{t}$. Let $m := m_+ m_-$ be a $\mathring{W}$-invariant function. On $\mathbb{T}$, we have $m_-(h) = m_+(-h) = \overline{m_+(h)}$ and $m(h) = (wm)(h) = (wm_+)(h)(wm_+)(-h)$ for $w \in \mathring{W}$, and in particular, $m(h)$ is an almost everywhere positive continuous function, $0 \leqslant m(\mathbf{t})(h) \leqslant M_{\mathbf{t}}$ and $\mu\{m(\mathbf{t})(h) = 0\} = 0$. Define the complex conjugate of $h = h_0 + ih_1 \in \mathbb{H}$ by $h^* = h_0 - ih_1$, where $h_0 \in \mathbb{T}$ and $h_1 \in \mathring{\mathfrak{h}}_{\mathbb{R}}$. Let $L^2(\mathbb{T}, m(\mathbf{t}) d\mu)^{\mathring{W}}$ be the Hilbert space equipped with the inner product

$$(f, g)_{\mathbf{t}} := \int_{\mathbb{T}} \overline{f(h)} g(h) m(\mathbf{t})(h). \tag{5.8}$$

For arbitrary $\lambda \in \mathring{\mathfrak{h}}^*_{\mathbb{R}}$, we see that $f \in \mathcal{M}_\lambda^{\mathring{W}}$ is continuous on $\mathbb{T}$, thus $f|_{\mathbb{T}} \in L^2(\mathbb{T}, m(\mathbf{t})d\mu)^{\mathring{W}}$. On the other hand, if $f \in L^2(\mathbb{T}, m(\mathbf{t})d\mu)^{\mathring{W}}$ almost everywhere coincides with $g \in \mathcal{M}_\lambda^{\mathring{W}}$ on $\mathbb{T}$, then it is unique. Hence we can embed $\mathcal{M}_\lambda^{\mathring{W}} \subset L^2(\mathbb{T}, m(\mathbf{t})d\mu)^{\mathring{W}}$ by restricting its domain to $\mathbb{T}$.

The function m_+ is related to $\hat{Y}^\lambda$ for minuscule weights $(-\lambda)$ and $\hat{Y}^{-\theta}$ as follows:

Proposition V.2: We have

$$\hat{Y}^\lambda(\mathbf{t}) = \frac{1}{|\mathring{W}_\lambda|} \sum_{w \in \mathring{W}} w\left(\frac{\tau_\lambda m_+(\mathbf{t})}{m_+(\mathbf{t})} \tau_\lambda \right), \tag{5.9}$$

$$\hat{Y}^{-\theta}(\mathbf{t}) = \frac{1}{|\mathring{W}_\theta|} \sum_{w \in \mathring{W}} w\left(\frac{\tau_{-\theta} m_+(\mathbf{t})}{m_+(\mathbf{t})} \tau_{-\theta} \right) + \hat{Y}_1^{-\theta}(\mathbf{t}). \tag{5.10}$$

Proof: It follows from the definition of the function m_+ (5.7) and the infinite product form of the Jacobi theta functions (2.25). □

We define the ''leading term'' of the operators $\hat{Y}^\lambda(\mathbf{t})$ which coincides with that defined in Refs. 7 and 8 in terms of a partial order in $\hat{M}_-$. For $\lambda \in \hat{M}_-$, let

$$\hat{Y}_0^\lambda(\mathbf{t}) := \frac{1}{|\mathring{W}_\lambda|} \sum_{w \in \mathring{W}} w\left(\frac{\tau_\lambda m_+(\mathbf{t})}{m_+(\mathbf{t})} \tau_\lambda \right). \tag{5.11}$$

Lemma V.3: Assume $p^n \neq q$ for $n \in \mathbb{Z}_{\geqslant 1}$. Then $\hat{Y}_0^{-\theta}(\mathbf{t}) \in \mathrm{End}_{\mathbb{C}}(\mathcal{M}_{-\theta}^{\mathring{W}}, \mathcal{M}_0^{\mathring{W}})$.

Proof: By Theorem IV.3 and Lemma IV.6, We have $\hat{Y}^{-\theta}(\mathbf{t})$, $\hat{Y}_1^{-\theta}(\mathbf{t}) \in \mathrm{End}_{\mathbb{C}}(\mathcal{M}_{-\theta}^{\mathring{W}}, \mathcal{M}_0^{\mathring{W}})$. Thus $\hat{Y}_0^{-\theta}(\mathbf{t}) = \hat{Y}^{-\theta}(\mathbf{t}) - \hat{Y}_1^{-\theta}(\mathbf{t}) \in \mathrm{End}_{\mathbb{C}}(\mathcal{M}_{-\theta}^{\mathring{W}}, \mathcal{M}_0^{\mathring{W}})$.

Lemma V.4: Let $\lambda \in \mathring{\mathfrak{h}}^*_{\mathbb{R}}$. Then $\mathcal{M}_\lambda^{\mathring{W}}$ is dense in $L^2(\mathbb{T}, m(\mathbf{t})d\mu)^{\mathring{W}}$.

Since a similar statement will be shown later, we give the proof as a remark after Proposition V.9 and proceed to the next step. The following theorem is shown similarly to the trigonometric cases[23,24] and a partial result is obtained in Ref. 25.

Theorem V.5: *Let $P_{\mathbf{t}}^{\mathrm{sym}} := (0,1)^{n_0} \subset P_{\mathbf{t}}$ and suppose $\mathbf{t} \in P_{\mathbf{t}}^{\mathrm{sym}}$. Then on $\mathcal{M}_\lambda^{\mathring{W}}$ and with respect to $(\cdot,\cdot)_{\mathbf{t}}$,*

(1) $\hat{Y}^\lambda$ for a minuscule weight is symmetric, and

(2) $\hat{Y}^{-\theta}$ is symmetric if $p < q$.

They are semi-bounded below and thus admit a self-adjoint extension.

Proof: We show that $(\hat{Y}^\lambda f, g)_{\mathbf{t}} = (f, \hat{Y}^\lambda g)_{\mathbf{t}}$ for $f, g \in \mathcal{M}_\lambda^{\mathring{W}}$.

First we prove the statement for a minuscule weight $(-\lambda)$ with the expression (5.9):

$$\begin{aligned}
(\hat{Y}^\lambda f, g)_{\mathbf{t}} &= \frac{1}{|\mathring{W}_\lambda|} \int_{\mathbb{T}} \sum_{w \in \mathring{W}} \overline{\frac{w(\tau_\lambda(m_+ f))(h)}{(w m_+)(h)}} \cdot g(h) m(h) \\
&= \frac{1}{|\mathring{W}_\lambda|} \int_{\mathbb{T}} \sum_{w \in \mathring{W}} \overline{\frac{w(\tau_\lambda(m_+ f))(h)}{(w m_+)(h)}} \cdot (w(m_+ g))(h)(w m_+)(-h) \\
&= \frac{1}{|\mathring{W}_\lambda|} \int_{\mathbb{T}} \sum_{w \in \mathring{W}} w(\overline{(\tau_\lambda(m_+ f))(h)} \cdot m_+ g(h)) \\
&= \frac{1}{|\mathring{W}_\lambda|} \int_{\mathbb{T}} \sum_{w \in \mathring{W}} w((\tau_{-\lambda}(m_- f^*))(h) \cdot m_+ g(h)),
\end{aligned} \tag{5.12}$$

where $f^*(h) := \overline{f(h^*)} \in \mathcal{M}^{\mathring{W}}_{-\lambda}$. Each term in the integrand has no poles on $\mathbb{T}$ due to the assumption $\mathbf{t} \in P^{\mathrm{sym}}_{\mathbf{t}}$ and the definition of $\mathcal{M}^{\mathring{W}}_{\lambda}$, then we can examine it separately. We have by the Cauchy theorem

$$\begin{aligned}
&\frac{1}{|\mathring{W}_\lambda|}\int_{\mathbb{T}} \sum_{w\in\mathring{W}} w((\tau_{-\lambda}(m_- f^*))(h)\cdot m_+ g(h)) \\
&\quad = \frac{|\mathring{W}|}{|\mathring{W}_\lambda|}\int_{\mathbb{T}} (\tau_{-\lambda}(m_- f^*))(h)\cdot m_+ g(h) \\
&\quad = \frac{|\mathring{W}|}{|\mathring{W}_\lambda|}\int_{\mathbb{T}} (m_- f^*)(h)\cdot (\tau_{\lambda}(m_+ g))(h) \\
&\quad = \frac{1}{|\mathring{W}_\lambda|}\int_{\mathbb{T}} \sum_{w\in\mathring{W}} w(\overline{(m_+ f)(h)}\cdot (\tau_{\lambda}(m_+ g))(h)) \\
&\quad = (f, \hat{Y}^\lambda g)_{\mathbf{t}}. \qquad (5.13)
\end{aligned}$$

For positivity, we have

$$\begin{aligned}
(\hat{Y}^\lambda f, f)_{\mathbf{t}} &= \frac{|\mathring{W}|}{|\mathring{W}_\lambda|}\int_{\mathbb{T}} (\tau_{-\lambda}(m_- f^*))(h)\cdot m_+ f(h) \\
&= \frac{|\mathring{W}|}{|\mathring{W}_\lambda|}\int_{\mathbb{T}} (\tau_{-\lambda/2}(m_- f^*))(h)\cdot (\tau_{\lambda/2}(m_+ f))(h) \\
&= \frac{|\mathring{W}|}{|\mathring{W}_\lambda|}\int_{\mathbb{T}} |(\tau_{\lambda/2}(m_+ f))(h)|^2 \\
&\geqslant 0. \qquad (5.14)
\end{aligned}$$

Next we prove the symmetry for the quasi-minuscule weight θ. Set $\lambda = -\theta$. A similar calculation for the case for a minuscule weight yields

$$\begin{aligned}
(\hat{Y}^\lambda f, g)_{\mathbf{t}} &= (\hat{Y}^\lambda_0 f, g)_{\mathbf{t}} + (\hat{Y}^\lambda_1 f, g)_{\mathbf{t}} \\
&= \frac{1}{|\mathring{W}_\lambda|}\int_{\mathbb{T}} \sum_{w\in\mathring{W}} w(\overline{(\tau_\lambda(m_+ f))(h)}\cdot m_+ g(h)) + \int_{\mathbb{T}} \overline{(\hat{Y}^\lambda_1 f)(h)}\cdot g(h) m(h) \\
&= \frac{|\mathring{W}|}{|\mathring{W}_\lambda|}\int_{\mathbb{T}} (\tau_{-\lambda}(m_- f^*))(h)\cdot m_+ g(h) + \int_{\mathbb{T}} \overline{(\hat{Y}^\lambda_1 f)(h)}\cdot g(h) m(h), \qquad (5.15)
\end{aligned}$$

where we have used Lemma V.3 to calculate the integrals above independently. It is sufficient to show that

$$\int_{\mathbb{T}} (\tau_{-\lambda}(m_- f^*))(h)\cdot m_+ g(h) = \int_{\mathbb{T}} (m_- f^*)(h)\cdot (\tau_{\lambda} m_+ g)(h) \qquad (5.16)$$

and

$$\int_{\mathrm{T}} \overline{(\hat{Y}_1^{\lambda} f)(h)} \cdot g(h) m(h) = \int_{\mathrm{T}} \overline{f(h)} \cdot (\hat{Y}_1^{\lambda} g)(h) m(h). \tag{5.17}$$

The first identity is implied by the Cauchy theorem due to $\mathbf{t} \in P_{\mathbf{t}}^{\mathrm{sym}}$, and $p<q$. The second identity follows from $\overline{\hat{Y}_1^{\lambda}(h)} = \hat{Y}_1^{\lambda}(h)$ by Lemma IV.6, which shows the symmetry. Again by Lemma IV.6,

$$(\hat{Y}^{\lambda} f, f)_{\mathbf{t}} = \frac{|\mathring{W}|}{|\mathring{W}_{\lambda}|} \int_{\mathrm{T}} |(\tau_{\lambda/2}(m_+ f))(h)|^2 + m_Y \|f\|_{\mathbf{t}}^2 \geqslant m_Y \|f\|_{\mathbf{t}}^2. \tag{5.18}$$

In both cases, the operator $\hat{Y}^{\lambda}$ is semi-bounded below. Thus they admit a self-adjoint extension by the Friedrichs–Freudenthal theorem.[26] □

C. Essential self-adjointness of unperturbed Hamiltonians

The essential self-adjointness of the unperturbed operator $\hat{Y}^{\lambda}(\mathbf{t}_0)$ on $\mathcal{M}_{\lambda}^{\mathring{W}}$ is shown directly by constructing all the eigenvectors of the leading term.

Theorem V.6: *Let* $(-\lambda)$ *be a minuscule weight or the quasi-minuscule weight* θ. *Assume*

$$\begin{aligned} &p<q, \quad \text{if } \lambda \text{ is a minuscule weight,} \\ &p<q^2, \quad \text{otherwise.} \end{aligned} \tag{5.19}$$

Then $\hat{Y}^{\lambda}(\mathbf{t}_0)$ *is essentially self-adjoint on* $\mathcal{M}_{\lambda}^{\mathring{W}}$ *and semi-bounded below with respect to* $(\cdot,\cdot)_{\mathbf{t}_0}$.

To prove Theorem V.6, we introduce the Schur functions, the characters of finite dimensional representations of simple Lie algebras. In terms of skew-symmetric functions

$$a_{\mu} := \sum_{w \in \mathring{W}} (-1)^{\ell(w)} e^{w\mu}, \tag{5.20}$$

the Schur functions are defined for $\mu \in \mathring{P}_+$ as

$$s_{\mu} := \frac{a_{\mu+\mathring{\rho}}}{a_{\mathring{\rho}}}. \tag{5.21}$$

It is well known that the Schur functions form a basis of $\mathbb{C}[\mathring{P}]^{\mathring{W}}$. Define

$$D := \prod_{\alpha \in \mathring{\Delta}} (p^{\gamma_\alpha} e^{\alpha}; p^{\gamma_\alpha})_{\infty}, \quad S_{\mu} := \frac{1}{|\mathring{W}|^{1/2}} \frac{s_{\mu}}{D}, \tag{5.22}$$

$$\mathcal{D} := \frac{1}{D} \mathbb{C}[\mathring{P}]^{\mathring{W}}. \tag{5.23}$$

Then due to the condition (5.19), one sees that $\mathcal{D} \subset \mathcal{M}_{\lambda}^{\mathring{W}}$. The functions $a_{\mathring{\rho}}$, D have the following properties:

$$w a_{\mathring{\rho}} = (-1)^{\ell(w)} a_{\mathring{\rho}}, \tag{5.24}$$

$$wD = D, \tag{5.25}$$

$$m_+(\mathbf{t}_0)=(-1)^{|\mathring{\Delta}_+|}a_{\mathring{\rho}}D, \tag{5.26}$$

$$m(\mathbf{t}_0)=a_{\mathring{\rho}}D\overline{a_{\mathring{\rho}}D}, \tag{5.27}$$

where $w\in\mathring{W}$.

Lemma V.7: $\mathbb{C}[\mathring{P}]$ *is dense in the space* $C(\mathbb{T})$ *of continuous functions on* $\mathbb{T}$ *equipped with the max norm* $\|\cdot\|_{\max}$.

Proof: $1,e^{\lambda}e^{\mu}=e^{\lambda+\mu},\overline{e^{\lambda}}=e^{-\lambda}\in\mathbb{C}[\mathring{P}]$, and for arbitrary $h,h'\in\mathbb{T}$, there exists $\lambda\in\mathring{P}$ such that $e^{\lambda}(h-h')\neq 1$. Then the statement is due to the Stone–Weierstrass theorem.

Lemma V.8: $L^2(\mathbb{T},d\mu)^{\mathring{W}}\subset L^2(\mathbb{T},m(\mathbf{t})d\mu)^{\mathring{W}}$.

Proof: The proof is implied by the inequality on $\mathbb{T}$:

$$|m(\mathbf{t})(h)|\leqslant M_{\mathbf{t}}<\infty. \tag{5.28}$$

Proposition V.9: $\mathcal{D}$ *is dense in* $L^2(\mathbb{T},m(\mathbf{t})d\mu)^{\mathring{W}}$.

Proof: Suppose $f\in L^2(\mathbb{T},m(\mathbf{t})d\mu)^{\mathring{W}}$. One sees that the measure $m(\mathbf{t})d\mu$ is regular. Hence for an arbitrary $\epsilon>0$, there exists a continuous function $\hat{f}_c$ such that $\|f-\hat{f}_c\|_{\mathbf{t}}<\epsilon/2$. Put $f_c=(\Sigma_{w\in\mathring{W}}w\hat{f}_c)/|\mathring{W}|$. Then

$$\|f-f_c\|_{\mathbf{t}}=\frac{1}{|\mathring{W}|}\left\|\sum_{w\in\mathring{W}}w(f-\hat{f}_c)\right\|_{\mathbf{t}}\leqslant\|f-\hat{f}_c\|_{\mathbf{t}}<\epsilon/2. \tag{5.29}$$

Since on $\mathbb{T}$, D is continuous and $0<m_D<|D(h)|<M_D<\infty$ and $f_c\in C(\mathbb{T})^{\mathring{W}}$, we can choose $f_p\in\mathbb{C}[\mathring{P}]^{\mathring{W}}$ such that $\|f_cD-f_p\|_{\max}<\epsilon m_D^{1/2}/(2M_{\mathbf{t}}^{1/2})$ thus $\|f_c-f_p/D\|<\epsilon/(2M_{\mathbf{t}}^{1/2})$, where we have used $\mu(\mathbb{T})=1$. Hence

$$\|f-f_p/D\|_{\mathbf{t}}\leqslant\|f-f_c\|_{\mathbf{t}}+M_{\mathbf{t}}^{1/2}\|f_c-f_p/D\|<\epsilon. \tag{5.30}$$

□

Remark V.10: As in the proof of Proposition V.9, one can show that $\mathbb{C}[\mathring{P}]^{\mathring{W}}$ is dense in $L^2(\mathbb{T},m(\mathbf{t})d\mu)^{\mathring{W}}$. Since $\mathbb{C}[\mathring{P}]^{\mathring{W}}\subset\mathcal{M}_{\lambda}^{\mathring{W}}$ for $\lambda\in\mathring{\mathfrak{h}}_{\mathbb{R}}^*$, we have the proof of Lemma V.4.

Propositon V.11: $\{S_\mu\}$ *forms a complete orthonormal system in* $L^2(\mathbb{T},m(\mathbf{t}_0)d\mu)^{\mathring{W}}$.

Proof: By Proposition V.9 and the fact that $\{S_\mu\}$ spans $\mathcal{D}$, it is sufficient to show that $(S_\mu,S_\nu)_{\mathbf{t}_0}=\delta_{\mu\nu}$. A direct calculation shows

$$\begin{aligned}(S_\mu,S_\nu)_{\mathbf{t}_0}&=\int_{\mathbb{T}}\overline{S_\mu}S_\nu m(\mathbf{t}_0)\\&=\frac{1}{|\mathring{W}|}\int_{\mathbb{T}}\left(\overline{\frac{a_{\mu+\mathring{\rho}}}{a_{\mathring{\rho}}D}}\right)\frac{a_{\nu+\mathring{\rho}}}{a_{\mathring{\rho}}D}a_{\mathring{\rho}}D\overline{a_{\mathring{\rho}}D}\\&=\frac{1}{|\mathring{W}|}\int_{\mathbb{T}}(\overline{a_{\mu+\mathring{\rho}}})a_{\nu+\mathring{\rho}}\\&=\frac{1}{|\mathring{W}|}\sum_{v,w\in\mathring{W}}(-1)^{\ell(wv)}\delta_{w(\mu+\mathring{\rho}),v(\nu+\mathring{\rho})}\\&=\delta_{\mu\nu},\end{aligned} \tag{5.31}$$

where we have used the fact that $w(\mu+\mathring{\rho})=v(\nu+\mathring{\rho})$ is equivalent to $v=w$ and $\mu=\nu$ since for $\mu\in\mathring{P}_+$, the $\mathring{W}$-orbit of $\mu+\mathring{\rho}$ meets the fundamental domain once and uniquely. □

Proposition V.12: Let $\lambda\in\hat{M}_-$. *Then*

$$\hat{Y}_0^{\lambda}(\mathbf{t}_0)S_\mu=E_\mu^{\lambda}S_\mu, \tag{5.32}$$

where

$$E_\mu^{\lambda}=\frac{1}{|\mathring{W}_\lambda|}\sum_{w\in\mathring{W}} q^{(\lambda|w(\mu+\mathring{\rho}))}\in\mathbb{R}_{>0}. \tag{5.33}$$

Proof:

$$\begin{aligned}
&\frac{1}{|\mathring{W}_\lambda|}\sum_{w\in\mathring{W}} w\left(\frac{\tau_\lambda m_+(\mathbf{t}_0)}{m_+(\mathbf{t}_0)}\tau_\lambda\right)S_\mu\\
&\quad=\frac{1}{|\mathring{W}_\lambda|}\frac{1}{|\mathring{W}|^{1/2}}\sum_{w\in\mathring{W}} w\left(\frac{\tau_\lambda a_{\mathring{\rho}}D}{a_{\mathring{\rho}}D}\tau_\lambda\left(\frac{a_{\mu+\mathring{\rho}}}{a_{\mathring{\rho}}D}\right)\right)\\
&\quad=\frac{1}{|\mathring{W}_\lambda|}\frac{1}{|\mathring{W}|^{1/2}}\sum_{w\in\mathring{W}} w\left(\frac{\tau_\lambda a_{\mu+\mathring{\rho}}}{a_{\mathring{\rho}}D}\right)\\
&\quad=\frac{1}{|\mathring{W}_\lambda|}\frac{1}{|\mathring{W}|^{1/2}}\frac{1}{a_{\mathring{\rho}}D}\sum_{w\in\mathring{W}}(-1)^{\ell(w)}w\left(\tau_\lambda\sum_{v\in\mathring{W}}(-1)^{\ell(v)}e^{v(\mu+\mathring{\rho})}\right)\\
&\quad=\frac{1}{|\mathring{W}_\lambda|}\frac{1}{|\mathring{W}|^{1/2}}\frac{1}{a_{\mathring{\rho}}D}\sum_{v,w\in\mathring{W}}(-1)^{\ell(wv)}q^{(\lambda|v(\mu+\mathring{\rho}))}e^{wv(\mu+\mathring{\rho})}\\
&\quad=\frac{1}{|\mathring{W}_\lambda|}\left(\sum_{w\in\mathring{W}} q^{(\lambda|w(\mu+\mathring{\rho}))}\right)S_\mu.
\end{aligned}\tag{5.34}$$

□

Proof of Theorem V.6: First we show that the leading term of $\hat{Y}^{\lambda}(\mathbf{t}_0)$ is essentially self-adjoint. It is sufficient to show that the range of $\hat{Y}_0^{\lambda}(\mathbf{t}_0)\pm i$ is dense in $L^2(\mathbb{T},m(\mathbf{t}_0)d\mu)^{\mathring{W}}$.[27,28] By Propositions V.11 and V.12, we have $(\hat{Y}_0^{\lambda}(\mathbf{t}_0)\pm i)S_\mu=(E_\mu^{\lambda}\pm i)S_\mu$ and deduce that its range is dense.

For a minuscule weight $(-\lambda)$, the leading term $\hat{Y}_0^{\lambda}(\mathbf{t}_0)$ coincides with the operator $\hat{Y}^{\lambda}(\mathbf{t}_0)$ itself, i.e., $\hat{Y}^{\lambda}(\mathbf{t}_0)=\hat{Y}_0^{\lambda}(\mathbf{t}_0)$. Hence the essential self-adjointness of $\hat{Y}^{\lambda}(\mathbf{t}_0)$ follows.

For the quasi-minuscule weight $-\lambda=\theta$, by Lemma IV.6, one sees that the operator $\hat{Y}_1^{\lambda}(\mathbf{t}_0)=\hat{Y}^{\lambda}(\mathbf{t}_0)-\hat{Y}_0^{\lambda}(\mathbf{t}_0)$ is a real bounded operator, which implies $\hat{Y}^{\lambda}(\mathbf{t}_0)=\hat{Y}_0^{\lambda}(\mathbf{t}_0)+\hat{Y}_1^{\lambda}(\mathbf{t}_0)$ is essentially self-adjoint.

The semi-boundedness follows from Theorem V.5 or is directly shown by $E_\mu^{\lambda}>0$ and $(\hat{Y}_1^{\lambda}(\mathbf{t}_0))(h)\geqslant m_Y$ on $\mathbb{T}$.

D. Essential self-adjointness

Now we are in position to discuss the essential self-adjointness of $\hat{Y}^{\lambda}(\mathbf{t})$.

Theorem V.13. (cf. Kato–Rellich): *Let V be a Hilbert space equipped with two equivalent inner products $(\cdot,\cdot)_1$, $(\cdot,\cdot)_2$. Suppose that T_1 and T_2 are linear operators defined on a dense subspace* D *and that T_1 is symmetric with respect to $(\cdot,\cdot)_1$ and T_2 is essentially self-adjoint with respect to $(\cdot,\cdot)_2$. If there exists $a\geqslant 0$ and $0\leqslant b<1$ such that*

$$\|(T_2-T_1)u\|_2 \leqslant a\|u\|_2+b\|T_2u\|_2, \quad u\in \mathsf{D}, \tag{5.35}$$

then T_1 *is essentially self-adjoint on* D *with respect to* $(\cdot,\cdot)_1$.

Proof: The proof is essentially due to Ref. 21. We may assume without loss of generality that there exists $a'>0$ and $0<b'<1$ such that

$$\|(T_2-T_1)u\|_2 < \|(b'T_2 \pm ia')u\|_2, \quad u\in \mathsf{D}. \tag{5.36}$$

Since T_2 is essentially self-adjoint, $(T_2\pm ic')$ has a dense range R in V and a bounded inverse. With $(T_2\pm ic')u=v$, this gives

$$\|(T_2-T_1)R(\mp ic',T_2)v\|_2 \leqslant b'\|v\|_2, \quad c'=a'/b', \quad v\in \mathsf{R}, \tag{5.37}$$

where $R(\zeta,T):=(T-\zeta)^{-1}$ denotes the resolvent of the operator T. $B_\pm := (T_2-T_1)R(\mp ic',T_2)$ is a bounded operator defined on the dense subspace R. Since $b'<1$, the Neumann series implies that the bounded inverse of the closure $1-\widetilde{B}_\pm=(1-B_\pm)^{\sim}$ exists, so that the range of $1-B_\pm$ is dense. On the other hand,

$$\begin{aligned} 1-B_\pm &= 1-((T_2\pm ic')-(T_1\pm ic'))R(\mp ic',T_2) \\ &= (T_1\pm ic')R(\mp ic',T_2), \end{aligned} \tag{5.38}$$

which shows that the range of $T_1\pm ic'$ is dense. Since $\|\cdot\|_1$ and $\|\cdot\|_2$ define the same topology on V, the range of $T_1\pm ic'$ is also dense with respect to the norm $\|\cdot\|_1$. The symmetry of T_1 completes the proof. □

Remark V.14: For Theorem V.13 it is sufficient that the topology defined by $\|\cdot\|_2$ is stronger than that defined by $\|\cdot\|_1$, i.e., $\|\cdot\|_1 \leqslant c\|\cdot\|_2$ for some $c>0$.

Proposition V.15: Let

$$P_{\mathbf{t}}^{\mathrm{iso}} := \{\mathbf{t}\in P_{\mathbf{t}} \,|\, p^{\gamma_\alpha n}q^{\gamma_\alpha m}\neq t_\alpha, n,m\in \mathbb{Z}_{\geqslant 1}\}, \tag{5.39}$$

and $\mathbf{t},\mathbf{t}'\in P_{\mathbf{t}}^{\mathrm{iso}}$. *Then* $L^2(\mathbb{T},m(\mathbf{t})d\mu)^{\mathring{W}}=L^2(\mathbb{T},m(\mathbf{t}')d\mu)^{\mathring{W}}$ *as a set. Furthermore, the identity map* $\iota: f\mapsto f$ *gives an isomorphism as a Banach space.*

Proof: The inequality on $\mathbb{T}$,

$$0<m_{\mathbf{t},\mathbf{t}'}\leqslant \frac{m(\mathbf{t})}{m(\mathbf{t}')}(h)\leqslant M_{\mathbf{t},\mathbf{t}'}<\infty, \tag{5.40}$$

leads to $L^2(\mathbb{T},m(\mathbf{t})d\mu)^{\mathring{W}}=L^2(\mathbb{T},m(\mathbf{t}')d\mu)^{\mathring{W}}$ as a set and

$$m_{\mathbf{t},\mathbf{t}'}^{1/2}\|\cdot\|_{\mathbf{t}'}\leqslant\|\cdot\|_{\mathbf{t}}\leqslant M_{\mathbf{t},\mathbf{t}'}^{1/2}\|\cdot\|_{\mathbf{t}'}. \tag{5.41}$$

□

Notice that $\mathbf{t}_0\in P_{\mathbf{t}}^{\mathrm{iso}}$ and that if $\mathbf{t}\notin P_{\mathbf{t}}^{\mathrm{iso}}$, then $L^2(\mathbb{T},m(\mathbf{t}_0)d\mu)^{\mathring{W}}\neq L^2(\mathbb{T},m(\mathbf{t})d\mu)^{\mathring{W}}$ as a set. Thus we can not apply Theorem V.13 in this case. We temporally set $\mathbf{t}\in P_{\mathbf{t}}^{\mathrm{iso}}$ for simplicity and remedy it later.

Theorem V.16: *Let* $(-\lambda)$ *be a minuscule weight or the quasi-minuscule weight* θ. *Assume* p, q *satisfy* (5.19) *and* $\mathbf{t}=(t_\alpha)\in P_{\mathbf{t}}^{\mathrm{iso}}\cap P_{\mathbf{t}}^{\mathrm{sym}}$. *If* $d(\mathbf{t},\mathbf{t}_0)<\epsilon$ *for sufficiently small* $\epsilon>0$, *then* $\hat{Y}^\lambda(\mathbf{t})$ *is essentially self-adjoint on* $\mathcal{M}_\lambda^{\mathring{W}}$ *and semi-bounded below with respect to* $(\cdot,\cdot)_{\mathbf{t}}$.

Proof: We have shown that $\hat{Y}^{\lambda}(\mathbf{t})$ is symmetric and semi-bounded below on $L^2(\mathbb{T}, m(\mathbf{t})d\mu)^{\mathring{W}}$ with domain $\mathcal{M}_{\lambda}^{\mathring{W}}$. First we show the statement for a minuscule weight. It is sufficient to prove that if $d(\mathbf{t},\mathbf{t}_0)<\epsilon$ for sufficiently small $\epsilon>0$, then there exists $0<b<1$ such that

$$\|(\hat{Y}^{\lambda}(\mathbf{t}_0)-\hat{Y}^{\lambda}(\mathbf{t}))f\|_{\mathbf{t}_0}\leqslant b\|\hat{Y}^{\lambda}(\mathbf{t}_0)f\|_{\mathbf{t}_0}, \quad f\in\mathcal{D}. \tag{5.42}$$

We estimate the left hand side of (5.42):

$$\begin{aligned}\hat{Y}^{\lambda}(\mathbf{t}_0)-\hat{Y}^{\lambda}(\mathbf{t}) &= \frac{1}{|\mathring{W}_{\lambda}|}\sum_{w\in\mathring{W}} w\left(\left(\frac{\tau_{\lambda}m_+(\mathbf{t}_0)}{m_+(\mathbf{t}_0)}-\frac{\tau_{\lambda}m_+(\mathbf{t})}{m_+(\mathbf{t})}\right)\tau_{\lambda}\right)\\ &= \frac{1}{|\mathring{W}_{\lambda}|}\sum_{w\in\mathring{W}} w\left(\delta(\mathbf{t})\frac{\tau_{\lambda}m_+(\mathbf{t}_0)}{m_+(\mathbf{t}_0)}\tau_{\lambda}\right),\end{aligned} \tag{5.43}$$

where $\delta(\mathbf{t})\in C(\mathbb{T})$ is given by

$$\delta(\mathbf{t}):=1-\left(\tau_{\lambda}\frac{m_+(\mathbf{t})}{m_+(\mathbf{t}_0)}\right)\left(\frac{m_+(\mathbf{t}_0)}{m_+(\mathbf{t})}\right). \tag{5.44}$$

Let $f\in\mathcal{D}$:

$$\begin{aligned}\|(\hat{Y}^{\lambda}(\mathbf{t}_0)-\hat{Y}^{\lambda}(\mathbf{t}))f\|_{\mathbf{t}_0}^2 &= \left\|\frac{1}{|\mathring{W}_{\lambda}|}\sum_{w\in\mathring{W}} w\left(\delta(\mathbf{t})\frac{\tau_{\lambda}m_+(\mathbf{t}_0)}{m_+(\mathbf{t}_0)}\tau_{\lambda}\right)f\right\|_{\mathbf{t}_0}^2\\ &= \frac{1}{|\mathring{W}_{\lambda}|^2}\int_{\mathbb{T}}\left|\sum_{w\in\mathring{W}} w\left(\delta(\mathbf{t})\frac{\tau_{\lambda}m_+(\mathbf{t}_0)}{m_+(\mathbf{t}_0)}\tau_{\lambda}f\right)\right|^2 m(\mathbf{t}_0)\\ &\leqslant \frac{|\mathring{W}|}{|\mathring{W}_{\lambda}|^2}\int_{\mathbb{T}}\sum_{w\in\mathring{W}}|w\delta(\mathbf{t})|^2\left|w\left(\frac{\tau_{\lambda}m_+(\mathbf{t}_0)}{m_+(\mathbf{t}_0)}\tau_{\lambda}f\right)\right|^2|wm_+(\mathbf{t}_0)|^2\\ &= \frac{|\mathring{W}|}{|\mathring{W}_{\lambda}|^2}\sum_{w\in\mathring{W}}\int_{\mathbb{T}}|w\delta(\mathbf{t})|^2|w\tau_{\lambda}(m_+(\mathbf{t}_0)f)|^2\\ &\leqslant \frac{|\mathring{W}|^2}{|\mathring{W}_{\lambda}|^2}\|\delta(\mathbf{t})\|_{\max}^2\int_{\mathbb{T}}|\tau_{\lambda}(m_+(\mathbf{t}_0)f)|^2\\ &= c(\mathbf{t})\int_{\mathbb{T}}|\tau_{\lambda}(m_+(\mathbf{t}_0)f)|^2\\ &= c(\mathbf{t})\|\tau_{\lambda}(m_+(\mathbf{t}_0)f)\|^2,\end{aligned} \tag{5.45}$$

where

$$c(\mathbf{t}):=(|\mathring{W}/\mathring{W}_{\lambda}|\|\delta(\mathbf{t})\|_{\max})^2. \tag{5.46}$$

By substituting $f=\Sigma_{\mu}b_{\mu}S_{\mu}$, $b_{\mu}\in\mathbb{C}$, we evaluate the norm as follows:

$$\int_{\mathbb{T}} |\tau_\lambda(m_+(\mathbf{t}_0)f)|^2 = \frac{1}{|\mathring{W}|}\int_{\mathbb{T}} \left| \sum_\mu b_\mu \tau_\lambda\left(a_{\mathring{\rho}} D\left(\frac{a_{\mu+\mathring{\rho}}}{a_{\mathring{\rho}} D} \right) \right) \right|^2$$

$$= \frac{1}{|\mathring{W}|}\int_{\mathbb{T}} \left| \sum_\mu b_\mu \tau_\lambda(a_{\mu+\mathring{\rho}}) \right|^2$$

$$= \frac{1}{|\mathring{W}|}\int_{\mathbb{T}} \left| \sum_\mu b_\mu \left(\sum_{v\in \mathring{W}} (-1)^{\ell(v)} q^{(\lambda|v(\mu+\mathring{\rho}))} e^{v(\mu+\mathring{\rho})} \right) \right|^2$$

$$= \frac{1}{|\mathring{W}|}\sum_\mu |b_\mu|^2 \left(\sum_{v\in \mathring{W}} q^{2(\lambda|v(\mu+\mathring{\rho}))} \right). \tag{5.47}$$

Finally we have

$$\|(\hat{Y}^\lambda(\mathbf{t}_0) - \hat{Y}^\lambda(\mathbf{t}))f\|_{\mathbf{t}_0}^2 \leqslant \frac{c(\mathbf{t})}{|\mathring{W}|}\sum_\mu |b_\mu|^2 \left(\sum_{v\in \mathring{W}} q^{2(\lambda|v(\mu+\mathring{\rho}))} \right). \tag{5.48}$$

Then we compute the right hand side of (5.42). By Proposition V.11,

$$\|\hat{Y}^\lambda(\mathbf{t}_0)f\|_{\mathbf{t}_0}^2 = \left\| \sum_\mu b_\mu \frac{1}{|\mathring{W}_\lambda|}\left(\sum_{w\in \mathring{W}} q^{(\lambda|w(\mu+\mathring{\rho}))} \right) S_\mu \right\|_{\mathbf{t}_0}^2$$

$$= \sum_\mu |b_\mu|^2 \frac{1}{|\mathring{W}_\lambda|^2}\left(\sum_{w\in \mathring{W}} q^{(\lambda|w(\mu+\mathring{\rho}))} \right)^2. \tag{5.49}$$

Since

$$\sum_{w\in \mathring{W}} q^{2(\lambda|w(\mu+\mathring{\rho}))} < \left(\sum_{w\in \mathring{W}} q^{(\lambda|w(\mu+\mathring{\rho}))} \right)^2, \tag{5.50}$$

we arrive at

$$\|(\hat{Y}^\lambda(\mathbf{t}_0) - \hat{Y}^\lambda(\mathbf{t}))f\|_{\mathbf{t}_0} < (|\mathring{W}|^{1/2}\|\delta(\mathbf{t})\|_{\max})\|\hat{Y}^\lambda(\mathbf{t}_0)f\|_{\mathbf{t}_0}. \tag{5.51}$$

We can show that $\delta(\mathbf{t})\to 0$ in $C(\mathbb{T})$, when $\mathbf{t}\to\mathbf{t}_0$ in $P_{\mathbf{t}}$. Equivalently, for $\mathbf{t}$ such that $d(\mathbf{t},\mathbf{t}_0)<\epsilon$ for sufficiently small $\epsilon>0$,

$$(|\mathring{W}|^{1/2}\|\delta(\mathbf{t})\|_{\max}) \leqslant 1, \tag{5.52}$$

which shows the essentially self-adjointness of $\hat{Y}^\lambda(\mathbf{t})$ with Proposition V.15 and Theorem V.13. See the Appendix for detail about (5.52).

For the quasi-minuscule weight $-\lambda=\theta$, we perform a perturbation from an essentially self-adjoint operator $\hat{Y}_0^\lambda(\mathbf{t}_0)$ instead of $\hat{Y}^\lambda(\mathbf{t}_0)$, i.e., we show there exist $a\geqslant 0$ and $0<b<1$ such that

$$\|(\hat{Y}_0^\lambda(\mathbf{t}_0) - \hat{Y}^\lambda(\mathbf{t}))f\|_{\mathbf{t}_0} \leqslant a\|f\|_{\mathbf{t}_0} + b\|\hat{Y}_0^\lambda(\mathbf{t}_0)f\|_{\mathbf{t}_0}, \quad f\in\mathcal{D}. \tag{5.53}$$

A similar calculation yields

$$\|(\hat{Y}_0^\lambda(\mathbf{t}_0) - \hat{Y}^\lambda(\mathbf{t}))f\|_{\mathbf{t}_0} \leqslant M_Y\|f\|_{\mathbf{t}_0} + (|\mathring{W}|^{1/2}\|\delta(\mathbf{t})\|_{\max})\|\hat{Y}_0^\lambda(\mathbf{t}_0)f\|_{\mathbf{t}_0}, \quad f\in\mathcal{D}, \tag{5.54}$$

where M_Y is an upper bound of $\hat{Y}_1^{\lambda}(\mathbf{t})$ in Lemma IV.6. □

Corollary V.17: Under the same condition in Theorem V.16, $\hat{Y}^{\lambda}(\mathbf{t})$ consists of pure point spectrum.

Proof: By the proof of Theorem V.13

$$R(ic',\hat{Y}^{\lambda}(\mathbf{t})^{\sim})=R(ic',\hat{Y}_0^{\lambda}(\mathbf{t}_0)^{\sim})(1-\widetilde{B}_-)^{-1}. \tag{5.55}$$

Since $\hat{Y}_0^{\lambda}(\mathbf{t}_0)^{\sim}$ consists of only point spectrum, its resolvent is a compact operator. Combining the fact that compact operators form an ideal in bounded operators, we deduce that the resolvent $R(ic',\hat{Y}^{\lambda}(\mathbf{t})^{\sim})$ is compact and thus $\hat{Y}^{\lambda}(\mathbf{t})$ consists of pure point spectrum. □

Remark V.18: In Theorem V.5, we have roughly estimated a lower bound of the operator $\hat{Y}^{\lambda}(\mathbf{t})$. We can estimate it more accurately. A lower bound of the operator $\hat{Y}_0^{\lambda}(\mathbf{t}_0)$ is obtained as

$$\begin{aligned}\frac{1}{|\mathring{W}_{\lambda}|}\sum_{w\in\mathring{W}} q^{(\lambda|w(\mu+\mathring{\rho}))} &\geqslant \frac{|\mathring{W}|}{|\mathring{W}_{\lambda}|}\left(\prod_{w\in\mathring{W}} q^{(\lambda|w(\mu+\mathring{\rho}))}\right)^{1/|\mathring{W}|}\\ &=|\mathring{W}/\mathring{W}_{\lambda}|, \quad \text{for all } \mu\in\mathring{P}_+.\end{aligned} \tag{5.56}$$

Thus for a minuscule weight, from (5.14),

$$\begin{aligned}(\hat{Y}^{\lambda}(\mathbf{t})f,f)_{\mathbf{t}} &= \frac{|\mathring{W}|}{|\mathring{W}_{\lambda}|}\int_{\mathrm{T}}|(\tau_{\lambda/2}(m_+(\mathbf{t})f))(h)|^2\\ &\geqslant b_{\lambda}\frac{|\mathring{W}|}{|\mathring{W}_{\lambda}|}\int_{\mathrm{T}}|(\tau_{\lambda/2}(m_+(\mathbf{t}_0)f))(h)|^2\\ &\geqslant \frac{b_{\lambda}}{|\mathring{W}_{\lambda}|}(\hat{Y}^{\lambda}(\mathbf{t}_0)f,f)_{\mathbf{t}_0}\\ &\geqslant \frac{b_{\lambda}}{|\mathring{W}_{\lambda}|}|\mathring{W}/\mathring{W}_{\lambda}|(f,f)_{\mathbf{t}_0}\\ &\geqslant \frac{b_{\lambda}m_{\mathbf{t}_0,\mathbf{t}}}{|\mathring{W}_{\lambda}|}|\mathring{W}/\mathring{W}_{\lambda}|(f,f)_{\mathbf{t}},\end{aligned} \tag{5.57}$$

where

$$b_{\lambda}=\min_{T}\left|\tau_{\lambda/2}\frac{m_+(\mathbf{t})}{m_+(\mathbf{t}_0)}\right|^2\geqslant 0. \tag{5.58}$$

If t_{α} satisfies

$$p^{\gamma_{\alpha}n}q^{\gamma_{\alpha}m/2}\neq t_{\alpha}, \quad n,m\in\mathbb{Z}_{\geqslant 1}, \tag{5.59}$$

then b_{λ} is positive and $\hat{Y}^{\lambda}(\mathbf{t})$ is positive definite. As for the quasi-minuscule weight, from (5.18),

$$
\begin{aligned}
(\hat{Y}^{\lambda}(\mathbf{t})f,f)_{\mathbf{t}} &= \frac{|\mathring{W}|}{|\mathring{W}_{\lambda}|}\int_{\mathbb{T}}|(\tau_{\lambda/2}(m_{+}(\mathbf{t})f))(h)|^2 + m_Y\|f\|_{\mathbf{t}}^2 \\
&\geqslant b_{\lambda}\frac{|\mathring{W}|}{|\mathring{W}_{\lambda}|}\int_{\mathbb{T}}|(\tau_{\lambda/2}(m_{+}(\mathbf{t}_0)f))(h)|^2 + m_Y\|f\|_{\mathbf{t}}^2 \\
&= \frac{b_{\lambda}}{|\mathring{W}_{\lambda}|}(\hat{Y}_0^{\lambda}(\mathbf{t}_0)f,f)_{\mathbf{t}_0} + m_Y\|f\|_{\mathbf{t}}^2 \\
&\geqslant \frac{1}{|\mathring{W}_{\lambda}|}(b_{\lambda}m_{\mathbf{t}_0,\mathbf{t}}|\mathring{W}/\mathring{W}_{\lambda}| + m_Y|\mathring{W}_{\lambda}|)(f,f)_{\mathbf{t}}. \qquad (5.60)
\end{aligned}
$$

We have postponed the case $\mathbf{t}\notin P_{\mathbf{t}}^{\mathrm{iso}}$. In this case, $L^2(\mathbb{T},m(\mathbf{t}_0)d\mu)^{\mathring{W}} \neq L^2(\mathbb{T},m(\mathbf{t})d\mu)^{\mathring{W}}$ as a set. In fact, the identity map $\iota: f\mapsto f$ is bounded and injective. The boundedness follows from the inequality $\|\cdot\|_{\mathbf{t}}\leqslant M_{\mathbf{t},\mathbf{t}_0}^{1/2}\|\cdot\|_{\mathbf{t}_0}$ where the constant $M_{\mathbf{t},\mathbf{t}_0}$ is from (5.40), and the injectivity follows from the fact that the measures of the zeroes of the functions $m(\mathbf{t}_0)$ and $m(\mathbf{t})$ are 0 with respect to μ. Moreover, we see that the range of ι is dense in $L^2(\mathbb{T},m(\mathbf{t})d\mu)^{\mathring{W}}$. Motivated by this observation, we need the following theorem which is a generalization of Theorem V.13.

Theorem V.19: *Let V_1 and V_2 be Hilbert spaces respectively equipped with inner products $(\cdot,\cdot)_1$ and $(\cdot,\cdot)_2$. Let $\iota: V_2\to V_1$ be a bounded and injective linear operator such that the range of ι is dense in V_1. Suppose that T_1 and T_2 are linear operators in V_2 defined on a dense subspace D and that $\iota\circ T_1\circ\iota^{-1}|_{\iota(\mathsf{D})}$ is symmetric in V_1 with respect to $(\cdot,\cdot)_1$ and T_2 is essentially self-adjoint in V_2 with respect to $(\cdot,\cdot)_2$. If there exist $a\geqslant 0$ and $0\leqslant b<1$ such that*

$$
\|(T_2-T_1)u\|_2 \leqslant a\|u\|_2 + b\|T_2u\|_2, \quad u\in\mathsf{D}, \qquad (5.61)
$$

then $\iota\circ T_1\circ\iota^{-1}|_{\iota(\mathsf{D})}$ is essentially self-adjoint on $\iota(\mathsf{D})$ with respect to $(\cdot,\cdot)_1$.

Proof: First we notice that the image by ι of a dense subspace W in V_2 is dense in V_1, which is shown as follows. Take arbitrary $u_1\in V_1$ and $\epsilon>0$. Then there exists $u_2\in V_2$ such that $\|u_1-\iota(u_2)\|_1<\epsilon/2$. For this u_2, there exists $u_2'\in W$ such that $\|u_2-u_2'\|_2<\epsilon/(2\|\iota\|)$. Hence we have

$$
\begin{aligned}
\|u_1-\iota(u_2')\|_1 &\leqslant \|u_1-\iota(u_2)\|_1 + \|\iota(u_2)-\iota(u_2')\|_1 \\
&\leqslant \|u_1-\iota(u_2)\|_1 + \|\iota\|\|u_2-u_2'\|_2 \\
&< \epsilon. \qquad (5.62)
\end{aligned}
$$

By the proof of Theorem V.13 and Remark V.14, we see that the range of $T_1\pm ic'$ is dense in V_2. Because $\iota\circ T_1\circ\iota^{-1}\pm ic'\,\mathrm{Id}_{V_1}|_{\iota(\mathsf{D})} = \iota\circ(T_1\pm ic'\,\mathrm{Id}_{V_2})\circ\iota^{-1}|_{\iota(\mathsf{D})}$, the assertion is proved. □

By Theorem V.19, we have removed the condition $\mathbf{t}\in P_{\mathbf{t}}^{\mathrm{iso}}$ in Theorem V.16 and Corollary V.17. We summarize the result obtained in this section.

Theorem V.20: *Let $(-\lambda)$ be a minuscule weight or the quasi-minuscule weight θ. Assume*

$$
\begin{cases} p<q, & \text{if } \lambda \text{ is a minuscule weight,} \\ p<q^2, & \text{otherwise} \end{cases} \qquad (5.63)
$$

and $\mathbf{t}=(t_\alpha)\in P_{\mathbf{t}}^{\mathrm{sym}}$. If $d(\mathbf{t},\mathbf{t}_0)<\epsilon$ for sufficiently small $\epsilon>0$, then $\hat{Y}^{\lambda}(\mathbf{t})$ is essentially self-adjoint on $\mathcal{M}_{\lambda}^{\mathring{W}}$ and semi-bounded below with respect to $(\cdot,\cdot)_{\mathbf{t}}$. $\hat{Y}^{\lambda}(\mathbf{t})$ consists of pure point spectrum.

So far, we have discussed the self-adjointness of the operators obtained from the formal Hamiltonians by gauge-transformation. We give the definitions of the Hamiltonians of the elliptic Ruijsenaars models by removing the weight functions. We define multiplication operators:

$$m^{-1/2}:L^2(\mathbb{T},d\mu)^{\mathring{W}}\to L^2(\mathbb{T},md\mu)^{\mathring{W}},\qquad f\mapsto fm^{-1/2},\tag{5.64}$$

$$m^{1/2}:L^2(\mathbb{T},md\mu)^{\mathring{W}}\to L^2(\mathbb{T},d\mu)^{\mathring{W}},\qquad f\mapsto fm^{1/2}.\tag{5.65}$$

These operators are bounded with norms $\|m^{-1/2}\|=\|m^{1/2}\|=1$ since

$$\|fm^{-1/2}\|_{\mathbf{t}}=\|f\|,\quad f\in L^2(\mathbb{T},d\mu)^{\mathring{W}},\tag{5.66}$$

$$\|fm^{1/2}\|=\|f\|_{\mathbf{t}},\quad f\in L^2(\mathbb{T},md\mu)^{\mathring{W}},\tag{5.67}$$

where we have used $\mu\{m=0\}=0$ for (5.66). In fact, $m^{-1/2}$ and $m^{1/2}$ are unitary operators and $(m^{1/2})^*=m^{-1/2}$. Then the composite $H^\lambda:=m^{1/2}\circ\hat{Y}^\lambda\circ m^{-1/2}$ is a densely defined linear operator with domain $\mathcal{M}^{\mathring{W}}_\lambda m^{1/2}$ on $L^2(\mathbb{T},d\mu)^{\mathring{W}}$.

Definition V.21: Fix an affine root system $X_N^{(r)}\neq A_{2l}^{(2)}$. Let $\kappa,\tau\in i\mathbb{R}_{>0}$. For $\alpha\in\Delta^{\mathrm{re}}$, let $\mu_\alpha\in i\mathbb{R}$ be $\hat{W}$-invariant constants such that $\langle\mathring{\rho}_\mu,\alpha^\vee\rangle\neq\mathbb{Z}/\gamma_\alpha+\tau\mathbb{Z}$. The elliptic Ruijsenaars model associated with affine root system $X_N^{(r)}$ is a quantum many-body system on $\mathbb{T}=\mathring{\mathfrak{h}}_{\mathbb{R}}/\mathring{Q}^\vee$, and its Hamiltonian is given by $H^\lambda=m^{1/2}\circ\hat{Y}^\lambda\circ m^{-1/2}$ and is expressed as

$$H^\lambda=\frac{1}{|\mathring{W}_\lambda|}\sum_{w\in\mathring{W}}w\left(\prod_{\substack{\alpha\in\mathring{\Delta}_+\\(\lambda|\alpha)=-\gamma_\alpha}}\frac{\vartheta_1(\langle\alpha,h\rangle-\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1(\langle\alpha,h\rangle;\gamma_\alpha\tau)}\right)^{1/2}\times\tau_\lambda\left(\prod_{\substack{\alpha\in\mathring{\Delta}_+\\(\lambda|\alpha)=-\gamma_\alpha}}\frac{\vartheta_1(\langle\alpha,h\rangle+\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1(\langle\alpha,h\rangle;\gamma_\alpha\tau)}\right)^{1/2},\tag{5.68a}$$

for a minuscule weight λ in $X_N^{(r)}\neq E_8^{(1)}$, $F_4^{(1)}$, $G_2^{(1)}$, $E_6^{(2)}$ or $D_4^{(3)}$, and

$$\begin{aligned}H^{-\theta}=&\frac{1}{|\mathring{W}_\theta|}\sum_{w\in\mathring{W}}w\left(\left(\prod_{\substack{\alpha\in\mathring{\Delta}_+\\(\theta|\alpha)>0}}\frac{\vartheta_1(\langle\alpha,h\rangle-\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1(\langle\alpha,h\rangle;\gamma_\alpha\tau)}\right)\left(\frac{\vartheta_1(\langle\theta,h\rangle+\kappa-\mu_\theta;\tau)}{\vartheta_1(\langle\theta,h\rangle+\kappa;\tau)}\right)\right)^{1/2}\\&\times\tau_{-\theta}\left(\left(\prod_{\substack{\alpha\in\mathring{\Delta}_+\\(\theta|\alpha)>0}}\frac{\vartheta_1(\langle\alpha,h\rangle+\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1(\langle\alpha,h\rangle;\gamma_\alpha\tau)}\right)\left(\frac{\vartheta_1(\langle\theta,h\rangle-\kappa+\mu_\theta;\tau)}{\vartheta_1(\langle\theta,h\rangle-\kappa;\tau)}\right)\right)^{1/2}\\&-\frac{\vartheta_1(-\mu_\theta;\tau)}{\vartheta_1((\mathring{\rho}_\mu|\theta);\tau)}\sum_{w\in\mathring{W}}w\left(\left(\prod_{\substack{\alpha\in\mathring{\Delta}_+\\(\theta|\alpha)>0}}\frac{\vartheta_1(\langle\alpha,h\rangle-\gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1(\langle\alpha,h\rangle;\gamma_\alpha\tau)}\right)\right.\\&\left.\times\left(\frac{\vartheta_1(\langle\theta,h\rangle+\kappa+(\mathring{\rho}_\mu|\theta);\tau)}{\vartheta_1(\langle\theta,h\rangle+\kappa;\tau)}\right)\right)\end{aligned}\tag{5.68b}$$

for the quasi-minuscule weight θ in $X_N^{(r)}=E_8^{(1)}$, $F_4^{(1)}$, $G_2^{(1)}$, $E_6^{(2)}$ or $D_4^{(3)}$.

We return to the original variables τ,κ,μ_α and rewrite Theorem V.20 by using the unitarity of $m^{-1/2}$ and $m^{1/2}$.

Theorem V.22: *Let*

$$P_{\boldsymbol{\mu}}^{\mathrm{sym}}:=\{\boldsymbol{\mu}=(\mu_\alpha)\mid \mu_\alpha\in i\mathbb{R}_{<0}\}, \tag{5.69}$$

and λ *be minuscule or quasi-minuscule. If*

$$\begin{gathered} 2|\kappa|<|\tau|, \quad X_N^{(r)}=E_8^{(1)},\ F_4^{(1)},\ G_2^{(1)},\ E_6^{(2)}\ \ or\ \ D_4^{(3)}, \\ |\kappa|<|\tau|, \quad otherwise, \end{gathered} \tag{5.70}$$

and $\boldsymbol{\mu}\in P_{\boldsymbol{\mu}}^{\mathrm{sym}}$ *satisfies* $|\mu_\alpha+\kappa|<\epsilon$ *for sufficiently small* $\epsilon>0$, *then the Hamiltonian* H^λ *(5.68) is essentially self-adjoint and semi-bounded below with domain* $\mathcal{M}_\lambda^{\mathring{W}}m^{1/2}$ *on* $L^2(\mathbb{T},d\mu)^{\mathring{W}}$ *and consists of pure point spectrum.*

We summarize the constraints of parameters τ,κ,μ_α that appeared above.

(1) $\kappa,\tau\in i\mathbb{R}_{>0}$, $\mu_\alpha\in i\mathbb{R}$ $(\alpha\in\Delta^{\mathrm{re}})$,

(2) $\langle\mathring{\rho}_\mu,\alpha^\vee\rangle\neq\mathbb{Z}/\gamma_\alpha+\tau\mathbb{Z}$,

(3) $\mu_\alpha\in i\mathbb{R}_{<0}$,

$|\kappa|<|\tau|$, if $X_N^{(r)}=E_8^{(1)},\ F_4^{(1)},\ G_2^{(1)},\ E_6^{(2)}$ or $D_4^{(3)}$,

(4) $2|\kappa|<|\tau|$, if $X_N^{(r)}=E_8^{(1)},\ F_4^{(1)},\ G_2^{(1)},\ E_6^{(2)}$ or $D_4^{(3)}$,

$|\kappa|<|\tau|$, otherwise,

(5) $|\mu_\alpha+\kappa|<\epsilon$ for sufficiently small $\epsilon>0$. More precisely, $\boldsymbol{\mu}$ is sufficient to satisfy $(|\mathring{W}|^{1/2}\|\delta(\mathbf{t})\|_{\max})\leqslant 1$.

In these conditions, conditions 1 and 2 are necessary. Condition 1 is required for the Hamiltonian to be a formally self-adjoint, or Hermite. By condition 2, the Hamiltonian for the quasi-minuscule weight is well-defined since the operator includes $(\mathring{\rho}_\mu|\theta)$ in the denominator. Condition 3 is essential if we choose the domain $\mathcal{M}_\lambda^{\mathring{W}}m^{1/2}$ since this condition is necessary for the Hamiltonian to be symmetric. Condition 4 enables us to construct a complete set of eigenfunctions of $\hat{Y}^\lambda(\mathbf{t}_0)$ in $\mathcal{M}_\lambda^{\mathring{W}}m^{1/2}$. Conditions 5 is set by a technical reason, i.e., depends on the perturbation. Condition 5 comes from the existence of the Neumann series in the perturbation. We may have a chance to remove conditions 3 and 4 by introducing a proper domain, and condition 5 by use of another way such as a perturbation from the trigonometric operators, i.e., the Macdonald operators.

VI. ESSENTIAL SELF-ADJOINTNESS OF TYPE $X_N^{(r)}=A_{2l}^{(2)}$

In this section, we show the essential self-adjointness of the elliptic Ruijsenaars model of type $A_{2l}^{(2)}$. For most part, we omit proofs, since they are complicated but essentially the same as in the previous sections. Sometimes we provide proofs or remarks. Throughout this section we fix the root system to $A_{2l}^{(2)}$. Here are some data concerning to this root system:

$$a_0=2, \quad \nu^{-1}(\theta)=2\theta^\vee, \quad \theta\in 2\mathring{P}, \quad \alpha_0=\tfrac{1}{2}(\delta-\theta), \quad \alpha_0^\vee=K-2\theta^\vee. \tag{6.1}$$

We begin with a general representation including Theorem IV.1. Let $\kappa,\tau\in i\mathbb{R}_{>0}$. Let $\mu_\alpha\in i\mathbb{R}$ be $\hat{W}$-invariant constants: $\mu_{\hat{w}(\alpha)}=\mu_\alpha$ for $\hat{w}\in\hat{W}$ such that $\langle\mathring{\rho}_\mu,\alpha^\vee\rangle\neq(\mathbb{Z}+\tau\mathbb{Z})/\gamma_\alpha$, where

$$\mathring{\rho}_\mu := \sum_{i\in I}^{\circ} \mu_{\alpha_i} \overline{\Lambda}_i = \frac{1}{2} \sum_{\alpha\in \mathring{\Delta}_+} \mu_\alpha \alpha. \tag{6.2}$$

Let $g_j, g_j' \in \mathbb{R}$ for $j=0,1,2,3$. Fix $\xi \in \mathring{\mathfrak{h}}^*$ such that $\langle \xi, \alpha^\vee \rangle \neq (\mathbb{Z}+\tau\mathbb{Z})/\gamma_\alpha$ for all $\alpha \in \Delta^{\mathrm{re}}$. We define $\hat{R}_\alpha \in \mathrm{End}_{\mathbb{C}}\mathcal{M}$ for $\alpha \in \Delta^{\mathrm{re}}$ by the same form as (4.2),

$$\hat{R}_\alpha := H_\alpha(\mu_\alpha) - H_\alpha(\langle \xi, \alpha^\vee \rangle) \circ s_\alpha, \tag{6.3}$$

where $H_\alpha(\eta)$ is a multiplication operator with the following function on $\mathbb{H}$:

$$H_\alpha(\eta)(h) := \begin{cases} \dfrac{\vartheta_1(-\mu_\alpha;\tau)}{\vartheta_1(-\eta;\tau)} \dfrac{\vartheta_1(\mathrm{af}(\alpha)(h)-\eta;\tau)}{\vartheta_1(\mathrm{af}(\alpha)(h);\tau)}, & \alpha \in \Delta_m, \\ \dfrac{\vartheta_1(-\mu_\alpha;\tau)}{\vartheta_1(-\eta;\tau)} \left(\displaystyle\sum_{j=0}^{3} g_j \frac{\vartheta_j(\mathrm{af}(\alpha)(h)-\eta;\tau)}{\vartheta_j(\mathrm{af}(\alpha)(h);\tau)} \right), & \alpha \in \Delta_s, \\ \dfrac{\vartheta_1(-2\mu_\alpha;\tau)}{\vartheta_1(-2\eta;\tau)} \left(\displaystyle\sum_{j=0}^{3} g_j' \frac{\vartheta_j(\mathrm{af}(\alpha)(h)/2-2\eta;\tau)}{\vartheta_j(\mathrm{af}(\alpha)(h)/2;\tau)} \right), & \alpha \in \Delta_l. \end{cases} \tag{6.4}$$

Theorem VI.1: *The map* $\pi: R_\alpha \mapsto \hat{R}_\alpha, \tau_\lambda \mapsto \tau_\lambda$ *induces a homomorphism from* $\mathcal{R}$ *to* $\mathrm{End}_{\mathbb{C}}\mathcal{M}$. *These R-matrices satisfy the unitarity*

$$\hat{R}_\alpha \hat{R}_{-\alpha} = u(\tau)\mathrm{Id}_{\mathcal{M}}, \tag{6.5}$$

where $u(\tau)$ *is independent of* $h \in \mathbb{H}$.

Analogous statements to Lemmas IV.2 and IV.6, and Theorems IV.3 and IV.4 hold for this representation.

Lemma VI.2: $\hat{R}_\alpha \in \mathrm{End}_{\mathbb{C}}(\mathcal{M}_0)$ $(\alpha \in \mathring{\Delta})$. *If* $\kappa \notin \mathbb{Z}_{\geqslant 1}\tau$, then $\hat{R}_{(\theta+\delta)/2} \in \mathrm{End}_{\mathbb{C}}(\mathcal{M}_{\theta/2}, \mathcal{M}_0)$.

Proof: From Lemma IV.2, $\hat{R}_\alpha \in \mathrm{End}_{\mathbb{C}}\mathcal{M}_0$ for $\alpha \in \mathring{\Delta}_m$. Thus it is sufficient to investigate long roots $\alpha \in \mathring{\Delta}_l$. Note that only the terms for $j=1,2$ have poles on $\mathbb{T}$. Let $f \in \mathcal{M}_0$. Then a possible pole h_0 on $\mathbb{T}$ is such that $\mathrm{af}(\alpha)(h_0) \in 2\mathbb{Z}$ for $j=1$ and $\mathrm{af}(\alpha)(h_0) \in 2\mathbb{Z}+1$ for $j=2$. By the property (6.1) $\mathrm{af}(s_\alpha)(h_0) = h_0 - \mathrm{af}(\alpha)(h_0)\alpha^\vee \equiv h_0 (\mathrm{mod}\, \mathring{Q}^\vee)$, and thus the pole on $\mathbb{T}$ vanishes.

We show the latter part. If $\kappa \notin \mathbb{Z}_{\geqslant 1}\tau$ and $f \in \mathcal{M}_\theta$, the functions $H_{(\theta+\delta)/2}(\eta)(h)$ in $\hat{R}_{(\theta+\delta)/2}$, $f(h)$ and $f(h-(\langle \theta, h\rangle + \kappa)\theta^\vee)$ are holomorphic in the neighborhood of $\mathbb{T}$. □

Theorem VI.3: *Let* $\xi = -\mathring{\rho}_\mu$. *If* $\kappa \notin \mathbb{Z}_{\geqslant 1}\tau$, *then* $\hat{Y}^{-\theta/2} \in \mathrm{End}_{\mathbb{C}}(\mathcal{M}^{\overset{\circ}{W}}_{-\theta/2}, \mathcal{M}^{\overset{\circ}{W}}_{0})$.

In the following, we fix $\xi = -\mathring{\rho}_\mu$.

Theorem VI.4:

$$\begin{aligned} \hat{Y}^{-\theta/2} = \frac{1}{|\mathring{W}_\theta|} \sum_{w\in \mathring{W}}^{\circ} w \Bigg(& \left(\prod_{\substack{\alpha \in (\mathring{\Delta}_m)_+ \\ (\theta|\alpha)>0}} \frac{\vartheta_1(\langle \alpha, h\rangle - \mu_\alpha;\tau)}{\vartheta_1(\langle \alpha, h\rangle;\tau)} \right) \left(\sum_{j=0}^{3} g_j' \frac{\vartheta_j(\langle \theta, h\rangle/2 - 2\mu_\theta;\tau)}{\vartheta_j(\langle \theta, h\rangle/2;\tau)} \right) \\ & \times \Bigg(\sum_{j=0}^{3} g_j \Bigg(\frac{\vartheta_j(\langle \theta, h\rangle/2 + \kappa/2 - \mu_{\alpha_0};\tau)}{\vartheta_j(\langle \theta, h\rangle/2 + \kappa/2;\tau)} \tau_{-\theta/2} \\ & - \frac{\vartheta_1(-\mu_{\alpha_0};\tau)}{\vartheta_1((\mathring{\rho}_\mu|\theta);\tau)} \frac{\vartheta_j(\langle \theta, h\rangle/2 + \kappa/2 + (\mathring{\rho}_\mu|\theta);\tau)}{\vartheta_j(\langle \theta, h\rangle/2 + \kappa/2;\tau)} \Bigg) \Bigg) \Bigg). \end{aligned} \tag{6.6}$$

In $A_{2l}^{(2)}$ case, we can calculate the explicit form of the second term of $\hat{Y}^{-\theta/2}$ up to a constant term.

Lemma VI.5: Set $\mu=\mu_\alpha$, $\alpha\in\Delta_m$. *The function*

$$\begin{aligned}\hat{Y}_1^{-\theta/2}(h):=&\frac{\vartheta_1(\mu_{\alpha_0};\tau)}{\vartheta_1((\mathring{\rho}_\mu|\theta);\tau)}\frac{1}{|\mathring{W}_\theta|}\sum_{w\in\mathring{W}}w\Bigg(\Bigg(\prod_{\substack{\alpha\in(\mathring{\Delta}_m)_+\\(\theta|\alpha)>0}}\frac{\vartheta_1(\langle\alpha,h\rangle-\mu;\tau)}{\vartheta_1(\langle\alpha,h\rangle;\tau)}\Bigg)\\&\times\Bigg(\sum_{j=0}^3 g'_j\frac{\vartheta_j(\langle\theta,h\rangle/2-2\mu_\theta;\tau)}{\vartheta_j(\langle\theta,h\rangle/2;\tau)}\Bigg)\Bigg(\sum_{j=0}^3 g_j\frac{\vartheta_j(\langle\theta,h\rangle/2+\kappa/2+(\mathring{\rho}_\mu|\theta);\tau)}{\vartheta_j(\langle\theta,h\rangle/2+\kappa/2;\tau)}\Bigg)\Bigg)\\=&\frac{\vartheta_1(\mu_{\alpha_0};\tau)\vartheta_1(\kappa;\tau)}{\vartheta_1(\mu;\tau)\vartheta_1(\kappa+\mu;\tau)}\sum_{j=0}^3 g_j\Bigg(\Bigg(\sum_{k=0}^3 g'_{\pi_j k}\frac{\vartheta_k(\kappa/2+2\mu_\theta;\tau)}{\vartheta_k(\kappa/2;\tau)}\Bigg)\\&\times\Bigg(\prod_{\alpha\in\mathring{\Delta}_l}\frac{\vartheta_j(\langle\alpha,h\rangle/2-\kappa/2-\mu;\tau)}{\vartheta_j(\langle\alpha,h\rangle/2-\kappa/2;\tau)}\frac{\vartheta_j(-\langle\alpha,h\rangle/2-\kappa/2-\mu;\tau)}{\vartheta_j(-\langle\alpha,h\rangle/2-\kappa/2;\tau)}\Bigg)\Bigg)\\&+F(\kappa,\mu,\mu_\theta,\mu_{\alpha_0}),\end{aligned}\tag{6.7}$$

where $F(\kappa,\mu,\mu_\theta,\mu_{\alpha_0})$ *is independent of* h, *and* π_j *are the elements of* $\mathfrak{S}_4$ *defined by* $\pi_1=id$, $\pi_2=(12)(03)$, $\pi_3=(13)(02)$, *and* $\pi_0=(01)(23)$, *is a function on* $\mathring{\mathfrak{h}}/(\mathring{Q}^\vee+\tau\nu^{-1}(\mathring{P}))$. *Moreover, if* $\kappa\notin\mathbb{Z}_{\geqslant 1}\tau$, *then* $\hat{Y}_1^{-\theta/2}(h)$ *is real-valued and continuous on* $\mathbb{T}$ *and thus has bounds*

$$-\infty<m_Y\leqslant\hat{Y}_1^{-\theta/2}(h)\leqslant M_Y<\infty,\quad h\in\mathbb{T}.\tag{6.8}$$

Proof: The proof is similar to that of Lemma IV.6. We show the equation (6.7). It is easy to see that the right hand side is periodic with respect to $\mathring{Q}^\vee+\tau\nu^{-1}(\mathring{P})$. The multiplicities of the left hand side are

$$\begin{aligned}&1,\quad h\to h+\beta^\vee\ (\beta^\vee\in\mathring{Q}^\vee),\\&\exp 2\pi i\Bigg(\sum_{\alpha\in\mathring{\Delta}_+}\frac{\mu_\alpha}{\gamma_\alpha}\langle\alpha,\theta^\vee\rangle\langle\alpha,\lambda\rangle-\langle\mathring{\rho}_\mu,\theta^\vee\rangle\langle\theta,\lambda\rangle\Bigg)=1,\quad h\to h+\tau\lambda\quad(\lambda\in\nu^{-1}(\mathring{P})),\end{aligned}\tag{6.9}$$

where we have used the properties of θ (6.1) and

$$\sum_{\alpha\in\mathring{\Delta}_+}\frac{\mu_\alpha}{\gamma_\alpha}\langle\alpha,\theta^\vee\rangle\langle\alpha,\lambda\rangle=\langle\mathring{\rho}_\mu,\theta^\vee\rangle\langle\theta,\lambda\rangle,\tag{6.10}$$

which will be implied by Lemma VI.6. By using $\{\alpha\in\mathring{\Delta}_m\,|\,(\alpha|\theta)>0\}=\{(\alpha+\theta)/2\,|\,\alpha\in\mathring{\Delta}_l,\alpha\neq\pm\theta\}$ and comparing the poles on both sides, we deduce the equality.

The latter part of the statement is clear from the right hand side. □

Lemma VI.6: Let $L:\mathring{\mathfrak{h}}\to\mathring{\mathfrak{h}}$ *be a linear operator defined by*

$$L:h\mapsto\sum_{\alpha\in\mathring{\Delta}_+}\frac{\mu_\alpha}{\gamma_\alpha}\nu^{-1}(\alpha)\langle\alpha,h\rangle.\tag{6.11}$$

Then $L(h)=(\mathring{\rho}_\mu|\theta)h$. *In particular,*

$$(\theta^\vee|L(\lambda))=\sum_{\alpha\in\mathring{\Delta}_+}\frac{\mu_\alpha}{\gamma_\alpha}\langle\alpha,\theta^\vee\rangle\langle\alpha,\lambda\rangle=\langle\mathring{\rho}_\mu,\theta^\vee\rangle\langle\theta,\lambda\rangle.\tag{6.12}$$

Remark VI.7: In Lemmas IV.7 and VI.6 the difference of the existence of the term μ_θ comes from $\gamma_\theta=2$ in $A_{2l}^{(2)}$.

Remark VI.8: The explicit form of $\hat{Y}_1^{\lambda}$ can be calculated due to the properties particular to $A_{2l}^{(2)}$, such as $\{\alpha\in\mathring{\Delta}_m \mid (\alpha|\theta)>0\}=\{(\alpha+\theta)/2 \mid \alpha\in\mathring{\Delta}_l, \alpha\neq\pm\theta\}$.

Lemma VI.9: Let $\nu_j\in\mathbb{C}$, $(j=0,1,2,3)$. *Set*

$$\nu=\sum_{j=0}^{3}\nu_j, \tag{6.13}$$

$$f_j=\frac{\vartheta_1(\nu_j;\tau)}{\vartheta_1(\nu;\tau)}\prod_{\substack{k=0\\k\neq j}}^{3}\frac{\vartheta_{\pi_j k}(\nu_k;\tau)}{\vartheta_{\pi_j k}(0;\tau)}=\frac{\vartheta_1(\nu_j;\tau)}{\vartheta_1(\nu;\tau)}\frac{\pi}{\vartheta_1'(0;\tau)}\prod_{\substack{k=0\\k\neq j}}^{3}\vartheta_{\pi_j k}(\nu_k;\tau). \tag{6.14}$$

Then the following identity holds:

$$\sum_{j=0}^{3}f_j\frac{\vartheta_j(x-\nu;\tau)}{\vartheta_j(x;\tau)}=\prod_{j=0}^{3}\frac{\vartheta_j(x-\nu_j;\tau)}{\vartheta_j(x;\tau)}. \tag{6.15}$$

Unfortunately, we do not have a weight function for the operator $\hat{Y}^{-\theta/2}$ due to the term including a sum. However, if we employ the product form obtained in Lemma VI.9, we can construct a weight function. Let $p=e^{2\pi i\tau}$, $q=e^{2\pi i\kappa}$, $t=e^{-2\pi i\mu}$ for $\alpha\in\Delta_m$, $t_j=e^{-2\pi i\mu_j}$ for $\alpha\in\Delta_s$, and $t_j'=e^{-2\pi i\mu_j'}$ for $\alpha\in\Delta_l$ and apply Lemma VI.9 so that $2\mu_\theta=\Sigma\mu_j$ and $\mu_{\alpha_0}=\Sigma\mu_j'$.

The parameters $\boldsymbol{\mu}=(\mu,\mu_0,\mu_1,\mu_2,\mu_3,\mu_0',\mu_1',\mu_2',\mu_3')$ and $\mathbf{t}=(t,t_0,t_1,t_2,t_3,t_0',t_1',t_2',t_3')$ are supposed to move on $P_{\boldsymbol{\mu}}:=i(-\infty,\infty)^9$ and $P_{\mathbf{t}}:=(0,\infty)^9$, respectively. Let $m_\pm$ be meromorphic functions on $\mathbb{H}$ defined by

$$\begin{aligned}m_\pm(\mathbf{t}):=e^{\pm\mathring{\rho}_\mu'/\kappa}&\prod_{\alpha\in(\mathring{\Delta}_m)_\pm}\frac{(e^\alpha;p,q)_\infty}{(te^\alpha;p,q)_\infty}\frac{(pqt^{-1}e^{-\alpha};p,q)_\infty}{(pqe^{-\alpha};p,q)_\infty}\\&\times\prod_{\alpha\in(\mathring{\Delta}_l)_\pm}\left(\left(\prod_{j=0}^{3}\frac{((-1)^{a_j}p^{b_j/2}e^{\alpha/2};p,q)_\infty}{((-1)^{a_j}p^{b_j/2}t_je^{\alpha/2};p,q)_\infty}\frac{((-1)^{a_j}p^{1-b_j/2}qt_j^{-1}e^{-\alpha/2};p,q)_\infty}{((-1)^{a_j}p^{1-b_j/2}qe^{-\alpha/2};p,q)_\infty}\right)\right.\\&\left.\times\left(\prod_{j=0}^{3}\frac{((-1)^{a_j}p^{b_j/2}q^{1/2}e^{\alpha/2};p,q)_\infty}{((-1)^{a_j}p^{b_j/2}q^{1/2}t_j'e^{\alpha/2};p,q)_\infty}\frac{((-1)^{a_j}p^{1-b_j/2}q^{1/2}t_j'^{-1}e^{-\alpha/2};p,q)_\infty}{((-1)^{a_j}p^{1-b_j/2}q^{1/2}e^{-\alpha/2};p,q)_\infty}\right)\right),\end{aligned} \tag{6.16}$$

where

$$\mathring{\rho}_\mu':=\frac{1}{2}\left(\sum_{\alpha\in\mathring{\Delta}_m}\mu\alpha+\sum_{\alpha\in\mathring{\Delta}_l}\frac{\mu_1+\mu_2+\mu_1'+\mu_2'}{2}\alpha\right), \tag{6.17}$$

and the constants a_j and b_j are defined in (2.27).

Proposition VI.10: We have

$$\hat{Y}^{-\theta/2}(\mathbf{t})=\hat{Y}_0^{-\theta/2}(\mathbf{t})+\hat{Y}_1^{-\theta/2}(\mathbf{t}), \tag{6.18}$$

$$\hat{Y}_0^{-\theta/2}(\mathbf{t}):=\sum_{w\in\mathring{W}}w\left(\frac{\tau_{-\theta/2}m_+(\mathbf{t})}{m_+(\mathbf{t})}\tau_{-\theta/2}\right). \tag{6.19}$$

Lemma VI.11: Assume $p^n\neq q$ *for* $n\in\mathbb{Z}_{\geqslant 1}$. *Then* $\hat{Y}_0^{-\theta/2}(\mathbf{t})\in\mathrm{End}_{\mathbb{C}}(\mathcal{M}_{-\theta/2}^{\mathring{W}},\mathcal{M}_0^{\mathring{W}})$.

Theorem VI.12: *Let* $P_{\mathbf{t}}^{\mathrm{sym}} := \{t \in P_{\mathbf{t}} \mid 0<t<1, 0<t_j<p^{-b_j/2}, 0<t_j'<p^{-b_j/2}q^{-1/2}\} \subset P_{\mathbf{t}}$ *and suppose* $\mathbf{t} \in P_{\mathbf{t}}^{\mathrm{sym}}$. *If* $p<q$, *then* $\hat{Y}^{-\theta/2}$ *is symmetric and semi-bounded below on* $\mathcal{M}^{\mathring{W}}_{-\theta/2}$ *with respect to* $(\cdot,\cdot)_{\mathbf{t}}$, *and thus admits a self-adjoint extension.*

In contrast to the other root systems, we can choose several start points of the perturbation. The essential self-adjointness of $\hat{Y}^{-\theta/2}(\mathbf{t}_n)$ on $\mathcal{M}^{\mathring{W}}_{-\theta/2}$ is shown directly in the case

$$0<p<q^{c_n}, \tag{6.20}$$

where

$$\mathbf{t}_0 := (q,1,1,1,1,1,q,q,1), \quad c_0 := 1, \tag{6.21a}$$

$$\mathbf{t}_1 := (q,1,1,1,1,q,q,q,1), \quad c_1 := 2, \tag{6.21b}$$

$$\mathbf{t}_2 := (q,1,1,1,1,1,q,q,q), \quad c_2 := 2, \tag{6.21c}$$

$$\mathbf{t}_3 := (q,1,1,1,1,q,q,q,q), \quad c_3 := 2. \tag{6.21d}$$

We define

$$D_n := \prod_{\alpha \in \mathring{\Delta}} (p^{\gamma_\alpha} e^{\alpha}; p^{\gamma_\alpha})_\infty \times \begin{cases} 1, & \text{if } n=0, \\ \displaystyle\prod_{\alpha \in \Delta_l} (p^{1/2} e^{\alpha/2}; p)_\infty, & \text{if } n=1, \\ \displaystyle\prod_{\alpha \in \Delta_l} (-p^{1/2} e^{\alpha/2}; p)_\infty, & \text{if } n=2, \\ \displaystyle\prod_{\alpha \in \Delta_l} (p e^{\alpha}; p^2)_\infty, & \text{if } n=3, \end{cases} \tag{6.22}$$

and

$$S_{\mu,n} := \frac{1}{|\mathring{W}|^{1/2}} \frac{s_\mu}{D_n}, \quad \mathcal{D}_n := \frac{1}{D_n} \mathbb{C}[\mathring{P}]^{\mathring{W}}, \tag{6.23}$$

where s_μ is the same as in the previous section. Then, due to the condition (6.20), one sees that $\mathcal{D}_n \subset \mathcal{M}^{\mathring{W}}_{-\theta/2}$.

Proposition VI.13: $\mathcal{D}_n$ *is dense in* $L^2(\mathbb{T}, m(\mathbf{t})d\mu)^{\mathring{W}}$. $\{S_{\mu,n}\} \subset \mathcal{D}_n$ *form a complete orthonormal system in* $L^2(\mathbb{T}, m(\mathbf{t}_n)d\mu)^{\mathring{W}}$ *and are the eigenvectors of the leading term* $\hat{Y}_0^\lambda(\mathbf{t}_n)$ *for* $\lambda \in \mathring{P}_-$:

$$\hat{Y}_0^\lambda(\mathbf{t}_n) S_{\mu,n} = E_\mu^\lambda S_{\mu,n}, \tag{6.24}$$

where

$$E_\mu^\lambda = \frac{1}{|\mathring{W}_\lambda|} \sum_{w \in \mathring{W}} q^{(\lambda | w(\mu+\mathring{\rho}))} \in \mathbb{R}_{>0}. \tag{6.25}$$

Theorem VI.14: *Assume* $p<q^{c_n}$. *Then* $\hat{Y}^{-\theta/2}(\mathbf{t}_n)$ *is essentially self-adjoint on* $\mathcal{M}^{\mathring{W}}_{-\theta/2}$ *and semi-bounded below with respect to* $(\cdot,\cdot)_{\mathbf{t}_n}$.

Theorem VI.15: *Assume* $p<q^{c_n}$ *and* $\mathbf{t}\in P_{\mathbf{t}}^{\mathrm{sym}}$. *If* $d(\mathbf{t},\mathbf{t}_n)<\epsilon$ *for sufficiently small* $\epsilon>0$, *then* $\hat{Y}^{\lambda}(\mathbf{t})$ *is essentially self-adjoint on* $\mathcal{M}_{\lambda}^{\mathring{W}}$, *semi-bounded below with respect to* $(\cdot,\cdot)_{\mathbf{t}}$ *and consists of pure point spectrum*.

Using Lemma VI.9, the expression of $\hat{Y}_1^{-\theta/2}$ in (6.7) and the identity

$$2\prod_{j=0}^{3}\vartheta_j(x)=\vartheta_1(2x)\frac{\vartheta_1'(0)}{\pi}, \tag{6.26}$$

we have the following.

Defintion VI.16: Fix the affine root system $X_N^{(r)}=A_{2l}^{(2)}$. Let $\kappa,\tau\in i\mathbb{R}_{>0}$. Let $\mu,\mu_j,\mu_j'\in i\mathbb{R},(j=0,1,2,3)$ and

$$\mu_\alpha=\begin{cases}\mu, & \text{if } \alpha\in\Delta_m,\\ \displaystyle\sum_{j=0}^{3}\mu_j', & \text{if } \alpha\in\Delta_s,\\ \displaystyle\sum_{j=0}^{3}\mu_j/2, & \text{if } \alpha\in\Delta_l,\end{cases} \tag{6.27}$$

so that $\langle\mathring{\rho}_\mu,\alpha^\vee\rangle\neq(\mathbb{Z}+\tau\mathbb{Z})/\gamma_\alpha$. The elliptic Ruijsenaars model associated with affine root system $A_{2l}^{(2)}$ is a quantum many-body system on $\mathbb{T}=\mathring{\mathfrak{h}}_{\mathbb{R}}/\mathring{Q}^\vee$, and its Hamiltonian is given by $H^{-\theta/2}=m^{1/2}\circ\hat{Y}^{-\theta/2}\circ m^{-1/2}$ and is expressed as

$$H^{-\theta/2}=\frac{1}{|\mathring{W}_\theta|}\sum_{w\in\mathring{W}}w(U_0(\boldsymbol{\mu})^{1/2}\circ\tau_{-\theta/2}\circ U_0(-\boldsymbol{\mu})^{1/2})+U_1(\boldsymbol{\mu})+U_2(\boldsymbol{\mu}), \tag{6.28}$$

where

$$U_0(\boldsymbol{\mu})(h):=\left(\prod_{\substack{\alpha\in(\mathring{\Delta}_m)_+\\(\theta|\alpha)>0}}\frac{\vartheta_1(\langle\alpha,h\rangle-\mu;\tau)}{\vartheta_1(\langle\alpha,h\rangle;\tau)}\right)\left(\prod_{j=0}^{3}\frac{\vartheta_j(\langle\theta,h\rangle/2-\mu_j;\tau)}{\vartheta_j(\langle\theta,h\rangle/2;\tau)}\,\frac{\vartheta_j(\langle\theta,h\rangle/2+\kappa/2-\mu_j';\tau)}{\vartheta_j(\langle\theta,h\rangle/2+\kappa/2;\tau)}\right), \tag{6.29}$$

$$\begin{aligned}U_1(\boldsymbol{\mu})(h):=\sum_{j=0}^{3}&\left(\frac{\pi}{\vartheta_1'(0;\tau)}\right)^2\frac{2}{\vartheta_1(\mu;\tau)\vartheta_1(\kappa+\mu;\tau)}\left(\prod_{k=0}^{3}\vartheta_k(\mu_{\pi_j k}+\kappa/2;\tau)\vartheta_k(\mu'_{\pi_j k};\tau)\right)\\&\times\left(\prod_{\alpha\in\mathring{\Delta}_l}\frac{\vartheta_j(\langle\alpha,h\rangle/2-\kappa/2-\mu;\tau)}{\vartheta_j(\langle\alpha,h\rangle/2-\kappa/2;\tau)}\,\frac{\vartheta_j(-\langle\alpha,h\rangle/2-\kappa/2-\mu;\tau)}{\vartheta_j(-\langle\alpha,h\rangle/2-\kappa/2;\tau)}\right),\end{aligned} \tag{6.30}$$

and $U_2(\boldsymbol{\mu}):=F(\kappa,\mu,\mu_\theta,\mu_{\alpha_0})$ is a constant.

Theorem VI.17: *Let*

$$P_{\boldsymbol{\mu}}^{\mathrm{sym}}:=\{\boldsymbol{\mu}=(\mu,\{\mu_j\},\{\mu_j'\})\,|\,\mu\in i\mathbb{R}_{<0},\quad \mu_j'\in i\mathbb{R}_{<b_j\Im\tau/2},\quad \mu_j\in i\mathbb{R}_{<b_j\Im\tau/2+\Im\kappa/2}\}, \tag{6.31}$$

and

$$\boldsymbol{\mu}_0:=-(\kappa,0,0,0,0,0,\kappa,\kappa,0),\quad c_0=1, \tag{6.32a}$$

$$\boldsymbol{\mu}_1:=-(\kappa,0,0,0,0,\kappa,\kappa,\kappa,0),\quad c_1=2, \tag{6.32b}$$

$$\boldsymbol{\mu}_2:=-(\kappa,0,0,0,0,0,\kappa,\kappa,\kappa),\quad c_2=2, \tag{6.32c}$$

$$\boldsymbol{\mu}_3 := -(\kappa,0,0,0,0,\kappa,\kappa,\kappa,\kappa), \quad c_3 = 2. \tag{6.32d}$$

If $c_n|\kappa| < |\tau|$ *and* $\boldsymbol{\mu} \in P_{\boldsymbol{\mu}}^{\mathrm{sym}}$ *satisfies* $d(\boldsymbol{\mu},\boldsymbol{\mu}_n) < \epsilon$ *for some* $n \in \{0,1,2,3\}$ *and sufficiently small* $\epsilon > 0$, *then the Hamiltonian* $H^{-\theta/2}$ (6.28) *is essentially self-adjoint and semi-bounded below with domain* $\mathcal{M}^{\mathring{W}}_{-\theta/2} m^{1/2}$ *on* $L^2(\mathbb{T}, d\mu)^{\mathring{W}}$ *and consists of pure point spectrum.*

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APPENDIX A: Equation (5.52)

Lemma A.1: Let $x \in \mathbb{C}$ *and* $\mu \in i\mathbb{R}$. *Then*

$$|\vartheta_1(x+\mu;\tau) - \vartheta_1(x;\tau)| \leqslant |\phi(\Im x,\mu;\tau)|, \tag{A1}$$

$$|\vartheta_1(x+\mu;\tau)| \leqslant |\varphi(\Im x,\mu;\tau)|, \tag{A2}$$

where

$$\phi(y,z;\tau) := 4\sum_{n\in\mathbb{Z}} \exp\left(i\pi\left(n-\frac{1}{2}\right)^2\tau\right)\cosh((2n-1)\pi y)\sin((2n-1)\pi z), \tag{A3}$$

$$\varphi(y,z;\tau) := 4\sum_{n\in\mathbb{Z}} \exp\left(i\pi\left(n-\frac{1}{2}\right)^2\tau\right)\cosh((2n-1)\pi y)\cos((2n-1)\pi z) \tag{A4}$$

are holomorphic functions on $\mathbb{C}^2$.

Proof: For $a \in \mathbb{C}$ and $b \in \mathbb{R}$, we have

$$\begin{aligned}|\sin(a+bi) - \sin a| &= |\sin a(\cosh b - 1) + i\cos a \sinh b| \\ &\leqslant (|\sin a| + |\cos a|)|\sinh b| \\ &\leqslant 2\cosh(\Im a)|\sinh b|. \end{aligned} \tag{A5}$$

Set $p = \exp(2\pi i\tau)$. By using (2.24),

$$\begin{aligned}|\vartheta_1(x+\mu;\tau) - \vartheta_1(x;\tau)| &= \left|2\sum_{n\in\mathbb{Z}} p^{(n-1/2)^2/2}(\sin(2n-1)\pi(x+\mu) - \sin(2n-1)\pi\mu)\right| \\ &\leqslant 4\sum_{n\in\mathbb{Z}} p^{(n-1/2)^2/2}\cosh((2n-1)\pi\Im x)|\sinh((2n-1)\pi\Im\mu)| \\ &= |\phi(\Im x,\mu;\tau)|. \end{aligned} \tag{A6}$$

The series converges uniformly absolutely on any compacts on $\mathbb{C}^2$. The latter part can be shown similarly. □

Lemma A.2: Let $a,b \in \mathbb{R}$ *and* $\tau \in i\mathbb{R}$. *Then* $|\vartheta_1(a+ib;\tau)| \geqslant |\vartheta_1(ib;\tau)|$.

Proof: We can assume $b \geqslant 0$ without loss of generality. Let $z = e^{2\pi i(a+ib)}$ and $p = e^{2\pi i\tau}$. Then $|z| \leqslant 1$, $0 < p < 1$ and $|1 - p^n z| \geqslant 1 - p^n|z| \geqslant 0$ for $n \geqslant 0$ and, by using the product form, we have

$$|\vartheta_1(a+ib;\tau)| \geqslant p^{1/8}|z|^{-1/2}(p;p)_\infty(|z|;p)_\infty(p|z|;p)_\infty = |\vartheta_1(ib;\tau)|. \tag{A7}$$

□

Lemma A.3: Let $a_i, b_i \in \mathbb{C}$ *for* $1 \leqslant i \leqslant n$. *Then*

$$\left|\prod_{i=1}^{n} a_i - \prod_{i=1}^{n} b_i\right| \leqslant n\Big(\max_{1\leqslant i\leqslant n}|a_i-b_i|\Big)\Big(\max_{1\leqslant i\leqslant n}\{|a_i|,|b_i|\}\Big)^{n-1}. \tag{A8}$$

Proof: The statement is implied by the following equality:

$$\prod_{i=1}^{n} a_i - \prod_{i=1}^{n} b_i = \sum_{j=1}^{n}\left(\prod_{i=1}^{j-1} a_i\right)(a_j-b_j)\left(\prod_{i=j+1}^{n} b_i\right). \tag{A9}$$

□

Proposition A.4: $\delta(\mathbf{t}) \to 0$ *in* $C(\mathbb{T})$ *as* $\mathbf{t} \to \mathbf{t}_0$ *in* $P_{\mathbf{t}}$.

Proof: First we show the cases for minuscule weights. Let $\Delta_\lambda := \{\alpha \in \mathring{\Delta}_+ | (\lambda|\alpha) = -\gamma_\alpha\}$. Recall that

$$\delta(\mathbf{t}) = 1 - \prod_{\alpha\in\Delta_\lambda} \frac{\vartheta_1(\langle\alpha,h\rangle - \gamma_\alpha\mu_\alpha;\gamma_\alpha\tau)}{\vartheta_1(\langle\alpha,h\rangle + \gamma_\alpha\kappa;\gamma_\alpha\tau)}. \tag{A10}$$

By applying Lemmas A.1, A.3, and A2 we have

$$\|\delta(\mathbf{t})\|_{\max} \leqslant \frac{|\Delta_\lambda||\phi(r\Im\kappa, d(\boldsymbol{\mu},\boldsymbol{\mu}_0);\tau)||\varphi(r\Im\kappa, d(\boldsymbol{\mu},\boldsymbol{\mu}_0);\tau)|^{|\Delta_\lambda|-1}}{\Pi_{\alpha\in\Delta_\lambda}|\vartheta_1(\gamma_\alpha\kappa;\gamma_\alpha\tau)|}, \tag{A11}$$

where r is from $X_N^{(r)}$ and we have used the monotonicity of ϕ and φ. Since $|\phi(a,0;\tau)| = 0$ and $|\varphi(a,\cdot;\tau)|$ is bounded in the neighborhood of the origin, it follows that $\|\delta(\mathbf{t})\|_{\max} \to 0$ as $d(\mathbf{t},\mathbf{t}_0) \to 0$.

The case for the quasi-minuscule weight is similarly shown. □

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Supergeneralization of Duffin–Kemmer–Petiau Algebra and Lie superalgebra osp(N,M)

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We will consider a supergeneralization of the Duffin–Kemmer–Petiau algebra. It has been shown to be intimately related to the Lie super algebra osp(N,M). We will also discuss its representations. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1386928]

The Duffin–Kemmer–Petiau algebra (hereafter referred to as DKP algebra) in the N-dimensional carrier space is defined by the relation

$$\beta_\mu\beta_\nu\beta_\lambda+\beta_\lambda\beta_\nu\beta_\mu=\delta_{\mu\nu}\beta_\lambda+\delta_{\nu\lambda}\beta_\mu \tag{1}$$

for $\mu,\nu,\lambda=1,2,\ldots,N$. For the case of $N=4$, it is well known (see, e.g., the article[1] by Krajcik and Nieto for an interesting historical account of the subject) that dimensions of its irreducible representations are restricted to one, five, and ten, and that the associated linear equation

$$\left(\sum_{\mu=1}^{4}\beta_\mu\frac{\partial}{\partial x_\mu}-m\right)\psi=0$$

specifies the spin 0 and 1 Klein–Gordon equations, respectively, for cases of five- and ten-dimensional realizations.

Fishbach *et al.*[2] have classified representations of the DKP algebra by reducing the problem to that of the Lie algebra so($N+1$) as follows. They first note that Eq. (1) implies the validity of

$$[[\beta_\mu,\beta_\nu],\beta_\lambda]=\delta_{\nu\lambda}\beta_\mu-\delta_{\mu\lambda}\beta_\nu \tag{2}$$

as well as

$$(\beta_\mu)^3=\beta_\mu. \tag{3}$$

Conversely, they show that Eqs. (2) and (3) lead to Eq. (1). Next, setting

$$J_{\mu\nu}=[\beta_\mu,\beta_\nu], \tag{4a}$$

$$J_{0\mu}=-J_{\mu0}=\beta_\mu, \tag{4b}$$

$$J_{00}=0, \tag{4c}$$

for $\mu,\nu,\lambda=1,2,\ldots,N$, it is easy to prove that Eq. (2) gives the so($N+1$) Lie algebra of

$$J_{AB}=-J_{BA}, \tag{5a}$$

$$[J_{AB},J_{CD}]=g_{BC}J_{AD}+g_{AD}J_{BC}-g_{AC}J_{BD}-g_{BD}J_{AC}, \tag{5b}$$

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now for values of A,B,C,D being $0,1,2,\ldots,N$. Here, we have set

$$g_{AB}=\begin{cases}\delta_{AB} & \text{if } A,B\neq 0\\ -1 & \text{if } A=B=0\\ 0 & \text{otherwise .}\end{cases} \tag{6}$$

Moreover, the constraint relation (3) is rewritten as

$$(J_{0\mu})^3=J_{0\mu}, \tag{7}$$

which restricts possible representations of the so$(N+1)$. Fishbach *et al.*[2] succeeded to specify all irreducible representations of the DKP algebra in terms of those of the corresponding so$(N+1)$ Lie algebra. Their results then can be more explicitly restated as follows. Let $T_{a_1a_2\ldots a_m}$ for a non-negative integer m to be a completely antisymmetric tensor for values of $a_1,a_2,\ldots,a_m$ to be $0,1,2,\ldots,N$. Then, the action of J_{AB} to the tensor is assumed to be given by

$$J_{AB}T_{a_1a_2\ldots a_m}=\sum_{j=1}^{m}\{g_{Ba_j}T_{a_1\ldots a_{j-1}Aa_{j+1}\ldots a_m}-g_{Aa_j}T_{a_1\ldots a_{j-1}Ba_{j+1}\ldots a_m}\}. \tag{8}$$

Moreover, if N is odd and $N+1=2m$, then the tensor must be chosen[3] to be either self-conjugate or anti-self-conjugate for the representation to remain irreducible. In other words, we can impose the condition

$$T_{a_1a_2\ldots a_m}=\pm\frac{1}{m!}\sum_{b_1,b_2,\ldots,b_m=1}^{2m}\epsilon_{a_1\ldots a_mb_1\ldots b_m}T_{b_1b_2\ldots b_m} \tag{9}$$

for the Levi-Civita symbol $\epsilon_{a_1\ldots a_mb_1\ldots b_m}$ in $2m$ dimension. Similarly, we can restrict the values of m to be $0\leqslant m\leqslant\frac{1}{2}(N+1)$ for the general tensor, since the other cases of $m>\frac{1}{2}(N+1)$ can be reduced[3] to the former by the use of the Levi–Civita symbol in a similar way.

In order to see more explicitly that this gives the realizations of the original DKP algebra, we introduce two completely antisymmetric tensors of rank n and $n+1$, respectively, for $m=n+1$ by

$$\phi^{(n+1)}_{\mu_1\ldots\mu_{n+1}}=T_{\mu_1\mu_2\ldots\mu_{n+1}}, \tag{10a}$$

$$\psi^{(n)}_{\mu_1\ldots\mu_n}=T_{0\mu_1\mu_2\ldots\mu_n} \tag{10b}$$

for values of $\mu_1,\mu_2,\ldots,\mu_{n+1}$ to range now to be $1,2,\ldots,N$. The possible values of n which specify the irreducible representations of the DKP algebra may be restricted to

$$0\leqslant n\leqslant\tfrac{1}{2}(N-1). \tag{10c}$$

Then, from Eqs. (4b) and (8), the action of β_μ's to those tensors are given by

$$\beta_\lambda\psi^{(n)}_{\mu_1\ldots\mu_n}=\phi^{(n+1)}_{\lambda\mu_1\ldots\mu_n}, \tag{11a}$$

$$\beta_\lambda\phi^{(n+1)}_{\mu_1\mu_2\ldots\mu_{n+1}}=\sum_{j=1}^{n+1}(-1)^{j-1}\delta_{\lambda\mu_j}\psi^{(n)}_{\mu_1\ldots\mu_{j-1}\mu_{j+1}\ldots\mu_{n+1}}. \tag{11b}$$

We can readily verify that these relations are consistent with the validity of Eq. (1). Moreover, for the case of $N=2n+1$ being odd, Eq. (11) can be replaced by a single relation of

$$\beta_\lambda \psi^{(n)}_{\mu_1 \ldots \mu_n} = \pm \frac{1}{n!} \sum_{\nu_1 \nu_2, \ldots, \nu_n = 1}^{N} \epsilon_{\lambda \mu_1 \ldots \mu_n \nu_1 \ldots \nu_n} \psi^{(n)}_{\nu_1 \ldots \nu_n} \tag{12}$$

in view of Eq. (9) now for $2n+1$ dimensional Levi-Civita symbol $\epsilon_{\lambda \mu_1 \ldots \nu_n}$. For $N=4$, these give the five-dimensional representation space consisting of ψ_0 and ϕ_μ for $n=0$, and ten-dimensional space spanned by ψ_μ and $\phi_{\mu\nu}$ with $\phi_{\mu\nu} = -\phi_{\nu\mu}$ for $n=1$, reproducing the well known fact of Ref. 1.

We have digressed into the representation theory of the DKP algebra in detail for the following reason. Let

$$\epsilon_{\mu\nu} = -\epsilon_{\nu\mu} \tag{13}$$

be a constant symplectic tensor, and consider now

$$\beta_\mu \beta_\nu \beta_\lambda - \beta_\lambda \beta_\nu \beta_\mu = \epsilon_{\mu\nu} \beta_\lambda - \epsilon_{\lambda\nu} \beta_\mu \tag{14}$$

for $\mu, \nu, \lambda = 1,2, \ldots, M$. Here we used the letter M instead of N for a reason which will become clear soon. We may call the algebra generated by β_μ's satisfying Eq. (14) a para-Duffin–Kemmer–Petiau algebra (hereafter referred to as PDKP algebra). In contrast to the DKP algebra, the new PDKP is now infinite dimensional. In particular, we will not have a simple polynomial constraint such as Eq. (3). Nevertheless, the analysis of the PDKP algebra will proceed analogously to the DKP case, except for the fact that the role of the Lie algebra so$(N+1)$ is now replaced by the Lie superalgebra osp$(1,M)$.[4,5]

First we note that Eq. (14) gives

$$[\{\beta_\mu, \beta_\nu\}, \beta_\lambda] = \epsilon_{\nu\lambda} \beta_\mu + \epsilon_{\mu\lambda} \beta_\nu \tag{15}$$

instead of Eq. (2), where $\{\beta_\mu, \beta_\nu\}$ is the anticommutator, i.e.,

$$\{\beta_\mu, \beta_\nu\} = \beta_\mu \beta_\nu + \beta_\nu \beta_\mu . \tag{16}$$

We now introduce J_{AB} by

$$J_{\mu\nu} = \{\beta_\mu, \beta_\nu\}, \tag{17a}$$

$$J_{0\mu} = -J_{\mu 0} = \beta_\mu , \tag{17b}$$

$$J_{00} = 0, \tag{17c}$$

together with g_{AB} for $A,B = 0,1,2 \ldots, M$ by

$$g_{AB} = \begin{cases} \epsilon_{AB} & \text{if } A,B = 1,2, \ldots, M \\ -1 & \text{if } A = B = 0 \\ 0 & \text{otherwise .} \end{cases} \tag{18}$$

We next define

$$[J_{AB}, J_{CD}\} = J_{AB} J_{CD} - (-1)^{(\sigma(A)+\sigma(B))(\sigma(C)+\sigma(D))} J_{CD} J_{AB} \tag{19}$$

as usual, where $\sigma(A)$ is the grade (or parity) given by

$$\sigma(A) = \begin{cases} 0 & \text{if } A = 0 \\ 1 & \text{if } A = 1,2, \ldots, M. \end{cases} \tag{20}$$

From Eq. (15), we can then verify the fact that J_{AB}'s now give the Lie super algebra osp(1,M), i.e.,

$$\text{(i)}\quad J_{AB}=-(-1)^{\sigma(A)\sigma(B)}J_{BA}, \tag{21a}$$

$$\text{(ii)}\quad [J_{AB},J_{CD}\}=g_{BC}J_{AD}-(-1)^{\sigma(A)\sigma(B)}g_{AC}J_{BD}-(-1)^{\sigma(C)\sigma(D)}g_{BD}J_{AC}+(-1)^{\sigma(A)\sigma(B)+\sigma(C)\sigma(D)}g_{AD}J_{BC}, \tag{21b}$$

$$\text{(iii)}\quad g_{AB}=(-1)^{\sigma(A)\sigma(B)}g_{BA}, \tag{21c}$$

$$\text{(iv)}\quad g_{AB}=0 \quad \text{if} \quad \sigma(A)\neq\sigma(B). \tag{21d}$$

Before going into further details, it may be worthwhile to emphasize the fact[4] that osp(1,M) is the only simple Lie superalgebra possessing the nice property that any of its finite dimensional representation is always fully reducible. We also note that a representation of the PDKP algebra is irreducible, if and only if the corresponding one of osp(1,N) is irreducible. Analogous to the DKP case, we now consider the completely superantisymmetric tensor $T_{a_1a_2\ldots a_m}$, which satisfies

$$T_{a_1\ldots a_ja_{j+1}\ldots a_m}=-(-1)^{\sigma(a_j)\sigma(a_{j+1})}T_{a_1\ldots a_{j+1}a_j\ldots a_m} \tag{22}$$

for the interchange of two adjacent indices a_j and a_{j+1} for $a_1,a_2,\ldots,a_m=0,1,2,\ldots,M$. The action of J_{AB} to this tensor is given by

$$J_{AB}T_{a_1a_2\ldots a_m}=\sum_{j=1}^{m}(-1)^{\Sigma_j(A,B)}\{g_{Ba_j}T_{a_1\ldots a_{j-1}Aa_{j+1}\ldots a_m}-(-1)^{\sigma(A)\sigma(B)}g_{Aa_j}T_{a_1\ldots a_{j-1}Ba_{j+1}\ldots a_m}\} \tag{23a}$$

where we have set for simplicity

$$\Sigma_j(A,B)=(\sigma(A)+\sigma(B))(\sigma(a_1)+\sigma(a_2)+\cdots+\sigma(a_{j-1})). \tag{23b}$$

Equations (23a) and (23b) are the analogs of Eq. (8) of the DKP case. We have to verify the fact that the tensor $T_{a_1\ldots a_m}$ supplies the representation space not only of the osp(1,M) but also of the PDKP algebra. For this, we first note that $T_{a_1a_2\ldots a_m}$ contain the zero index at most once in view of Eq. (22). We then introduce two tensors $\phi^{(n+1)}_{\mu_1\ldots\mu_{n+1}}$ and $\psi^{(n)}_{\mu_1\ldots\mu_n}$ again by Eqs. (10a) and (10b). However, in contrast to the DKP case, they are now completely symmetric in $\mu_1,\mu_2,\ldots,\mu_{n+1}$ instead of being completely antisymmetric because of Eq. (22). Then, Eqs. (17b) and (23a) lead to

$$\beta_\lambda\psi^{(n)}_{\mu_1\ldots\mu_n}=\phi^{(n+1)}_{\lambda\mu_1\ldots\mu_n}, \tag{24a}$$

$$\beta_\lambda\phi^{(n+1)}_{\mu_1\ldots\mu_{n+1}}=\sum_{j=1}^{n+1}\epsilon_{\lambda\mu_j}\psi^{(n)}_{\mu_1\ldots\mu_{j-1}\mu_{j+1}\ldots\mu_{n+1}}, \tag{24b}$$

which replace Eq. (11). We can explicitly verify now that Eqs. (24a) and (24b) are consistent with the PDKP relation of Eq. (14), i.e., they offer the desired irreducible realizations of the algebra. Since both tensors $\phi^{(n+1)}_{\mu_1\ldots\mu_{n+1}}$ and $\psi^{(n)}_{\mu_1\ldots\mu_n}$ are completely symmetric, there is no restriction such as in Eq. (10c) to the values of n. In particular, the PDKP algebra has an infinite number of finite dimensional irreducible representations in contrast to the case of the DKP algebra, reflecting the fact that the former is infinite dimensional. We also note that Rittenberg and Scheunert[6] have given a correspondence between representations of osp(1,2N) and so($2N+1$).

We must yet prove that the PDKP algebra has no finite dimensional irreducible representation other than those given by Eqs. (24a) and (24b) except for the trivial one of $\beta_\mu = 0$. Since there is no analog of the relation such as Eq. (3), this is more difficult to do. However, we could achieve it by studying the representations of osp$(1,M)$ corresponding to general tensors, and then by showing its incompatibility with Eq. (14) except for the case of the completely superantisymmertric realization. We will not go into details, however, since the demonstration is quite cumbersome.

At this point, we may speculate what will happen, if we consider the relation

$$\beta_\mu \beta_\nu \beta_\lambda - \beta_\lambda \beta_\nu \beta_\mu = \delta_{\mu\nu}\beta_\lambda - \delta_{\lambda\nu}\beta_\mu \tag{25}$$

for $\mu, \nu, \lambda = 1,2,\ldots,M$ instead of Eq. (14). At first glance, Eq. (25) would appear to be a more natural choice as the counterpart of the DKP algebra. We shall, however, prove in the following that Eq. (25) will admit only the trivial solution $\beta_\mu = 0$ identically, unless $M = 1$. Supose $M \geqslant 2$. Then for any two index μ, and λ satisfying $\mu \neq \lambda$, we choose $\mu = \nu \neq \lambda$, so that Eq. (25) gives

$$\beta_\mu^2 \beta_\lambda - \beta_\lambda \beta_\mu^2 = \beta_\lambda \quad \text{if} \quad \mu \neq \lambda. \tag{26}$$

We will prove that the validity of Eq. (26) implies $\beta_\mu = 0$ as follows. We multiply β_λ to both sides of Eq. (26) from the left- and right-hand sides to find

$$\beta_\mu^2 \beta_\lambda^2 - \beta_\lambda \beta_\mu^2 \beta_\lambda = \beta_\lambda^2,$$

$$\beta_\lambda \beta_\mu^2 \beta_\lambda - \beta_\lambda^2 \beta_\mu^2 = \beta_\lambda^2.$$

Adding both, this gives

$$\beta_\mu^2 \beta_\lambda^2 - \beta_\lambda^2 \beta_\mu^2 = 2\beta_\lambda^2 \quad \text{if} \quad \mu \neq \lambda. \tag{27}$$

Interchanging the role of μ and λ, Eq. (27) leads then to

$$\beta_\lambda^2 = -\beta_\mu^2 \quad \text{if} \quad \mu \neq \lambda.$$

In that case, the left-hand side of Eq. (26) is calculated to be

$$\beta_\mu^2 \beta_\lambda - \beta_\lambda \beta_\mu^2 = (-\beta_\lambda^2)\beta_\lambda - \beta_\lambda(-\beta_\lambda^2) = 0$$

and hence Eq. (26) requires the validity of $\beta_\lambda = 0$ identically.

We next show that both DKP and PDKP algebras are special cases of a larger supergeneralization of the DKP algebra. Let us consider $M+N$ indices $1,2,\ldots,M+N$ and divide them into two sets of

$$V_0 = \{1,2,\ldots,N\}, \tag{28a}$$

$$V_1 = \{N+1, N+2, \ldots, N+M\} \tag{28b}$$

and assign

$$\sigma(a) = \begin{cases} 0 & \text{if } a \in V_0 \\ 1 & \text{if } a \in V_1 \end{cases} \tag{29}$$

so that V_0 and V_1 correspond, respectively, to bosonic and fermionic indices. Similarly, we introduce g_{ab} for $a, b = 1,2,\ldots,M+N$ by

$$g_{ab}=\begin{cases}\delta_{\mu\nu} & \text{if } a=\mu,\ \ b=\nu\epsilon V_0\\ \epsilon_{\mu\nu} & \text{if } a=\mu,\ \ b=\nu\epsilon V_1\\ 0 & \text{otherwise,}\end{cases} \tag{30}$$

which satisfies

$$\text{(i)}\ \ g_{ba}=(-1)^{\sigma(a)\sigma(b)}g_{ab}, \tag{31a}$$

$$\text{(ii)}\ \ g_{ab}=0 \quad \text{if} \quad \sigma(a)\neq\sigma(b). \tag{31b}$$

Suppose that β_a for $a=1,2,\ldots,M+N$ now satisfy

$$\beta_a\beta_b\beta_c+(-1)^{\Sigma(a,b,c)}\beta_c\beta_b\beta_a=g_{ab}\beta_c+g_{bc}\beta_a, \tag{32a}$$

where for simplicity we have set

$$\Sigma(a,b,c)=\sigma(a)\sigma(b)+\sigma(b)\sigma(c)+\sigma(c)\sigma(a). \tag{32b}$$

We note that Eq. (32a) remains invariant under $a\leftrightarrow c$, if we note the validity of

$$g_{ba}=(-1)^{\Sigma(a,b,c)}g_{ab} \tag{33}$$

by Eqs. (31a) and (31b). For special cases of $V_1=0$ (or $M=0$) and $V_0=0$ (or $N=0$), Eqs. (32a) and (32b) reproduce Eqs. (1) and (14), respectively. We may call the algebra generated by β_a's satisfying Eqs. (32a) and (32b) the super DKP algebra or DKP superalgebra. We also note that Eq. (32a) is invariant under $\beta_a\rightarrow-\beta_a$ and $\beta_a\rightarrow(-1)^{\sigma(a)}\beta_a$.

Setting

$$J_{ab}=\beta_a\beta_b-(-1)^{\sigma(a)\sigma(b)}\beta_b\beta_a \tag{34}$$

and introducing the general commutator again by

$$[J_{ab},\beta_c\}=J_{ab}\beta_c-(-1)^{(\sigma(a)+\sigma(b))\sigma(c)}\beta_cJ_{ab}, \tag{35}$$

Eqs. (32a) and (32b) give

$$[J_{ab},\beta_c\}=g_{bc}\beta_a-(-1)^{\sigma(a)\sigma(b)}g_{ac}\beta_b. \tag{36}$$

We can now construct the Lie super algebra osp$(N+1,M)$ as follows. We set

$$\beta_a=J_{0a}=-J_{a0}, \tag{37a}$$

$$J_{00}=0, \tag{37b}$$

as well as

$$g_{0a}=g_{a0}=0, \quad g_{00}=-1, \quad \sigma(0)=0 \tag{37c}$$

for $a=1,2,\ldots,M+N$. We note that the new index zero is a bosonic one and can be incorporated into V_0. The enlarged algebra for J_{AB} with $A,B=0,1,2,\ldots,M+N$ satisfies Eq. (21). Therefore, it realizes the Lie superalgebra osp$(N+1,M)$. The special cases of $M=0$ and $N=0$ will reproduce the Lie algebra so$(N+1)$ and osp$(1,M)$, respectively, of the DKP and PDKP algebras.

The realization of the super DKP algebra is again related to the completely superantisymmetric tensor representation. However, we will not go into details, since we will present another and more direct way to construct it, shortly.

We remark that the Lie super algebra osp$(N+1,M)$ based upon a similar construction has also appeared in a study[7] of para-statistics in which bosons and fermions no longer commute with each other. A simpler osp(1,2) algebra occurs[8] as the Clebsch–Gordan algebra of combined spin $\frac{1}{2}$ and 1 representations of the angular momentum algebra so(3).

Finally, we can construct the direct realization of the DKP superalgebra without recourse to osp$(N+1,M)$ as follows. Let g_{ab} be a constant tensor again satisfying the condition

$$\text{(i)} \quad g_{ba}=(-1)^{\sigma(a)\sigma(b)}g_{ab}, \tag{38a}$$

$$\text{(ii)} \quad g_{ab}=0 \quad \text{if} \quad \sigma(a)\neq\sigma(b). \tag{38b}$$

Suppose that a set of operators Q_a and $\overline{Q}_a$ satisfy

$$Q_a\overline{Q}_bQ_c+(-1)^{\Sigma(a,b,c)}Q_c\overline{Q}_bQ_a=g_{ab}Q_c+g_{bc}Q_a, \tag{39a}$$

$$\overline{Q}_aQ_b\overline{Q}_c+(-1)^{\Sigma(a,b,c)}\overline{Q}_cQ_b\overline{Q}_a=g_{ab}\overline{Q}_c+g_{bc}\overline{Q}_a. \tag{39b}$$

If we introduce 2×2 matrices β_a by

$$\beta_a=\begin{pmatrix} 0 & Q_a \\ \overline{Q}_a & 0 \end{pmatrix}, \tag{40}$$

it is easy to see that they define the DKP superalgebra, i.e.,

$$\beta_a\beta_b\beta_c+(-1)^{\Sigma(a,b,c)}\beta_c\beta_b\beta_a=g_{ab}\beta_c+g_{bc}\beta_a. \tag{41}$$

We can find a realization of operators Q_a and $\overline{Q}_a$ satisfying Eqs. (39a) and (39b) as generalized annihilation and creation operators by

$$Q_a\overline{Q}_b+(-1)^{\sigma(a)\sigma(b)}\overline{Q}_bQ_a=g_{ab}, \tag{42a}$$

$$Q_aQ_b+(-1)^{\sigma(a)\sigma(b)}Q_bQ_a=0, \tag{42b}$$

$$\overline{Q}_a\,\overline{Q}_b+(-1)^{\sigma(a)\sigma(b)}\overline{Q}_b\,\overline{Q}_a=0. \tag{42c}$$

Setting

$$V_o=\{a|\sigma(a)=0\}, \tag{43a}$$

$$V_1=\{a|\sigma(a)=1\}, \tag{43b}$$

Q_a and $\overline{Q}_b$ for $a,b\epsilon V_0$ with $g_{ab}=\delta_{ab}$ then form the usual annihilation and creation operators of fermions, while those for $a,b\epsilon V_1$ with $g_{ab}=\epsilon_{ab}$ correspond to quasibosonic system. However, we note that bosonic operators now anticommute with fermionic ones.

In order to construct representations of the super DKP algebra, we introduce the Fock space by

$$Q_a|0\rangle=0, \tag{44a}$$

$$\overline{Q}_{a_1}\,\overline{Q}_{a_2}\ldots\overline{Q}_{a_m}|0\rangle=|a_1,a_2,\ldots,a_m\rangle \tag{44b}$$

from the vacuum state $|0\rangle$. We then calculate

$$\beta_c\begin{pmatrix} |a_1a_2\ldots a_m\rangle \\ |b_1b_2\ldots b_n> \end{pmatrix}=\begin{pmatrix} Q_c|b_1b_2\ldots b_n\rangle \\ |ca_1a_2\ldots a_m> \end{pmatrix}. \tag{45}$$

Moreover, we note

$$Q_c|b_1b_2\ldots b_n\rangle=\sum_{j=1}^{n}(-1)^{\Sigma_j}g_{cb_j}|b_1\ldots b_{j-1}b_{j+1}\ldots b_n\rangle, \tag{46a}$$

$$\Sigma_j\equiv j-1+\sigma(c)(\sigma(b_1)+\sigma(b_2)+\cdots+\sigma(b_{j-1})). \tag{46b}$$

We see that a set consisting of such two-component state vectors with $m=n+1$ for a fixed value of n forms a representation space of the

DKP superalgebra. If we identify

$$\psi^{(n)}_{a_1a_2\ldots a_n}=\begin{pmatrix} 0 \\ |a_1a_2\ldots a_n\rangle \end{pmatrix}, \tag{47a}$$

$$\phi^{(n+1)}_{a_1\ldots a_{n+1}}=\begin{pmatrix} |a_1a_2\ldots a_{n+1}\rangle \\ 0 \end{pmatrix}, \tag{47b}$$

then Eqs. (45) and (46) lead to

$$\beta_c\psi^{(n)}_{a_1a_2\ldots a_n}=\phi^{(n+1)}_{ca_1a_2\ldots a_n}, \tag{48a}$$

$$\beta_c\phi^{(n+1)}_{a_1a_2\ldots a_{n+1}}=\sum_{j=1}^{n+1}(-1)^{\Sigma_j}g_{ca_j}\psi^{(n)}_{a_1\ldots a_{j-1}a_{j+1}\ldots a_{n+1}} \tag{48b}$$

The special cases of $M=0$ and $N=0$ will then reproduce Eqs. (11) and (24), respectively. However, the above-given representation may not be irreducible for some cases because of the self-conjugate condition like Eq. (12) for antisymmetric tensor indices. The problem is somewhat involved and will be discussed elsewhere.

Returning to Eq. (45), consider now the case of $m\neq n+1$. We must then double the number of states by adding another two-component vectors now with $m\leftrightarrow n+1$. However, this leads in general to reducible representations.

There exists another realization of Eq. (39) in terms of the Cuntz algebra[9] generated by a single relation of

$$Q_a\overline{Q_b=}g_{ab}. \tag{49}$$

In this case, Eq. (45) is now rewritten as

$$\beta_c\begin{pmatrix} |a_1\ldots a_m\rangle \\ |b_1\ldots b_n \end{pmatrix}=\begin{pmatrix} g_{cb_1}|b_2\ldots b_n\rangle \\ |ca_1a_2\ldots a_m\rangle \end{pmatrix}. \tag{50}$$

This gives, however, reducible representations even for the case of $m=n+1$.

In ending this note, consider an $M+N$ dimensional supermanifold with N bosonic coordinate $x_1,x_2,\ldots,x_N$ and M fermionic Grassmann coordinate $z_1,z_2,\ldots,z_M$. We set $z_j=x_{j+N}$ for $j=1,2,\ldots,M$, and consider the wave equation

$$\left(\sum_{a=1}^{N+M} \beta_a \frac{\partial}{\partial x_a} - m \right) \xi = 0. \tag{51}$$

Then, Eq. (41) will lead to the generalized Klein–Gordon equation

$$\left(\sum_{\mu=1}^{N} \frac{\partial^2}{\partial x_\mu \partial x_\mu} + \sum_{j,k=1}^{M} \epsilon_{jk} \frac{\partial^2}{\partial z_j \partial z_k} \right) \xi = m^2 \xi \tag{52}$$

assuming $m \neq 0$.

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On the correlation functions of the vector bundle generalization of the *bc*-system

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It is shown that the determinants of the correlation functions of the generalized bc-system introduced recently are given as pullbacks of the non-Abelian theta divisor. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1388198]

I. INTRODUCTION

The usual bc-system appearing in bosonic string theory[1,2] is very well understood[1–4] and has also been considered in a rigorous algebro-geometric way by Raina.[5,6] Assuming some natural physical axioms, Raina showed the existence and uniqueness of the correlation functions and was able to rederive the explicit expressions using the geometry of the theta divisor. It is important to note that one considers in this approach not the quantum fields b,c themselves (which should be ''operator valued sections'' of certain line bundles), but their correlation functions inheriting the symmetries of the operators. A closely related cousin of the bc-sytem based on a Hermitian vector bundle of rank r was introduced in Ref. 7 and the existence and uniqueness of correlation functions was established for a particular class of bundles. The hope was that the correlation functions of this bc_r-system are determined completely by the geometry of the non-Abelian theta divisor, in complete analogy to the usual rank one case. Since at the time of writing the necessary formulas were lacking, this remained a hope, but in the meantime Ref. 8 appeared, providing some useful results. Unfortunately, only the determinants of the correlation functions can be described with the help of the results of Ref. 8, so there is still much to be done to realize this hope and it is unclear whether one will be able to do so along the lines pursued here.

In the second section we briefly recall the geometry of the system of rank one before we consider the higher rank case in the third section. Some of the difficulties concerning the current and the energy-momentum tensor are indicated. For the convenience of the reader we have stated the required result of Ref. 8 in an appendix. In the following Σ_g will be a Riemann surface of genus $g \geqslant 2$ with canonical bundle $K \equiv K_{\Sigma_g}$. The group of (isomorphism classes of) line bundles of degree d will be denoted by $Pic^d(\Sigma_g)$ and there is the canonical theta divisor $\Theta := \{L \in Pic^{g-1}(\Sigma_g) \mid h^0(\Sigma_g, L) \neq 0\} \subset Pic^{g-1}(\Sigma_g)$. We will denote by α^{-1} the inverse of the line bundle α and by $E^\vee$ the dual of the vector bundle E.

II. THE *bc*-SYSTEM REVISITED

Let $\alpha \in Pic^{g-1}(\Sigma_g) \backslash \Theta$, i.e., α is a line bundle of degree $g-1$ and satisfies $h^0(\Sigma_g, \alpha) = 0$. In the associated bc-system—given by an action $S \sim \int b \bar{\partial} c$—the field c (respectively, b) is a section of α (respectively, $K \otimes \alpha^{-1}$); note that there will be zero modes of neither b nor c due to our assumption on α. The propagator $\langle b(z)c(w) \rangle$ is then a meromorphic section of the line bundle $(K \otimes \alpha^{-1}) \boxtimes \alpha := \pi_1^*(K \otimes \alpha^{-1}) \otimes \pi_2^*(\alpha)$ over $\Sigma_g \times \Sigma_g$ having a simple pole on the diagonal $\Delta \subset \Sigma_g \times \Sigma_g$; here $\pi_i : \Sigma_g \times \Sigma_g \to \Sigma_g$, for $i = 1,2$, is the canonical projection onto the ith factor. Using the map $\phi_\alpha : \Sigma_g \times \Sigma_g \to Pic^{g-1}(\Sigma_g)$, given by $\phi_\alpha((z,w)) := \mathcal{O}(z-w) \otimes \alpha$, we pull back the theta divisor from $Pic^{g-1}(\Sigma_g)$ to obtain[5]

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$$\phi_\alpha^*(\mathcal{O}(\Theta)) \simeq (K\otimes\alpha^{-1})\boxtimes\alpha\otimes\mathcal{O}(\Delta). \tag{1}$$

Thus, the propagator is a meromorphic section of $\phi_\alpha^*(\mathcal{O}(\Theta))\otimes\mathcal{O}(-\Delta)$. Since the normalized section of $\phi_\alpha^*(\mathcal{O}(\Theta))$ is given by the (uniquely determined) theta function with characteristic α, i.e., by $\vartheta[\alpha](z-w)/\vartheta[\alpha](0)$, and the normalized section of $\mathcal{O}(\Delta)$ is given by the prime form $E(z,w)$, we get the desired result:

$$\langle b(z)c(w)\rangle = \frac{\vartheta[\alpha](z-w)}{\vartheta[\alpha](0)E(z,w)} \equiv S_\alpha(z,w). \tag{2}$$

In the case that α is an even theta characteristic, i.e., $\alpha^2=K$, the Szegö-kernel S_α—consequently the propagator also—is antisymmetric in its arguments.

In an analogous fashion one has maps $\phi_\alpha^n:(\Sigma_g\times\Sigma_g)^n\to Pic^{g-1}(\Sigma_g)$, given by

$$\phi_\alpha^n((z_1,w_1),\ldots,(z_n,w_n)) := \mathcal{O}\left(\sum_{i=1}^n z_i - \sum_{i=1}^n w_i\right)\otimes\alpha; \tag{3}$$

note that $\phi_\alpha^1=\phi_\alpha$ from above. The pullback of Θ under ϕ_α^n is given by[5,6]

$$(\phi_\alpha^n)^*(\mathcal{O}(\Theta))r \simeq (K\otimes\alpha^{-1})\boxtimes\alpha\boxtimes\cdots\boxtimes(K\otimes\alpha^{-1})\boxtimes\alpha\otimes\mathcal{O}(D_n), \tag{4}$$

where D_n is the divisor of poles and zeros

$$D_n := \sum_{1\le i<j\le 2n}(-1)^{i+j+1}\Delta_{ij} \tag{5}$$

and Δ_{ij} is the divisor where the ith and jth coordinates coincide. Hence, the $2n$-point function $\langle b(z_1)\cdots c(w_n)\rangle$ is given as the normalized section of $(\phi_\alpha^n)^*(\mathcal{O}(\Theta))\otimes\mathcal{O}(-D_n)$. Since the first factor leads to a theta function and the second to a product of prime forms, we obtain an explicit expression for the $2n$-point functions. Comparing the expression for the four-point function with the determinant of propagators (the bc-system is free, so the two expressions should coincide according to Wick's rule), we obtain the trisecant identity of Fay.[5,9] Now, let us turn to the higher rank case.

III. THE bc_r-SYSTEM

Let us denote by $\mathcal{U}_g(r,d)$ the moduli space of stable vector bundles of rank r and degree d on Σ_g; note that $\mathcal{U}_g(1,d)=Pic^d(\Sigma_g)$. In the case of higher rank we also have a natural "non-Abelian" theta divisor $\Theta_r := \{F\in\mathcal{U}_g(r,r(g-1)) \mid h^0(\Sigma_g,F)\neq 0\}\subset\mathcal{U}_g(r,r(g-1))$; for this see, e.g., Ref. 7 and the references given therein. The simplest bc_r-system is the one where no zero modes occur. For this to happen we have to choose $E\in\mathcal{U}_g(r,r(g-1))\backslash\Theta_r$. Then the field c (respectively, b) is a section of E (respectively, $K\otimes E^\vee$) and the action is given by $S\sim\int b\bar{\partial}_E c$, where a Hermitian metric on E is used to yield a good integrand. Consequently, the propagator $\langle b(z)c(w)\rangle$ is a meromorphic section of $(K\otimes E^\vee)\boxtimes E$ over $\Sigma_g\times\Sigma_g$ having a simple pole on the diagonal Δ. It is given[7] by the non-Abelian Szegö-kernel $S_E(z,w)$ as defined by Fay,[10] but explicit expressions are very difficult to obtain. In the following we will denote the highest nonvanishing exterior power of a vector bundle F by $\det(F)$. The determinant of the propagator is a section of $\det((K\otimes E^\vee)\boxtimes E)=\det(K\otimes E^\vee)\boxtimes\det(E)$. Since K is a line bundle and $E^\vee$ has rank r, we have

$$\det(K\otimes E^\vee) = K^{\otimes r}\otimes\det(E^\vee), \tag{6}$$

so that the determinant of the propagator is a meromorphic section of

$$(K^{\otimes r}\otimes\det(E^\vee))\boxtimes\det(E). \tag{7}$$

Now we need the geometric ingredients which are analogous to those used in the rank one case above. For $E \in \mathcal{U}_g(r, r(g-1))$ there is a map

$$\phi_E : \Sigma_g \times \Sigma_g \to \mathcal{U}_g(r, r(g-1)), \tag{8}$$

defined by $\phi_E((z,w)) := \mathcal{O}(z-w) \otimes E$. Since tensoring with a line bundle preserves stability and since $\deg(L \otimes E) = r\deg(L) + \deg(E)$ for any line bundle L, the map ϕ_E is indeed well defined. According to Ref. 8, the pullback of the non-Abelian theta divisor is given in complete analogy to (1) by

$$\phi_E^*(\mathcal{O}(\Theta_r)) \simeq (K^{\otimes r} \otimes \det(E^\vee)) \boxtimes \det(E) \otimes \mathcal{O}(\Delta)^{\otimes r}$$

[see Eq. (A2) in the Appendix]. Since we observed above (7) that the determinant of the propagator is a section of the line bundle $(K^{\otimes r} \otimes \det(E^\vee)) \boxtimes \det(E) = \phi_E^*(\mathcal{O}(\Theta_r)) \otimes \mathcal{O}(-\Delta)^{\otimes r}$, we can summarize these observations as follows.

Proposition 1: Let $E \in \mathcal{U}_g(r, r(g-1)) \backslash \Theta_r$ and ϕ_E as in (8). *Then the determinant of the propagator $\langle b(z)c(w) \rangle$ of the associated bc_r-system is a meromorphic section of the line bundle $\phi_E^*(\mathcal{O}(\Theta_r)) \otimes \mathcal{O}(-\Delta)^{\otimes r}$. In particular, one has for $z \sim w$ the expected singularity* $\det\langle b(z)c(w) \rangle \sim (z-w)^{-r}$.

Note that the above method gives only the determinant of the propagator. The propagator is given by $\langle b(z)c(w) \rangle = S_E(z,w)$, so that we identify the determinant of the non-Abelian Szegö-kernel as a pullback of the non-Abelian theta divisor:

$$\det(S_E(z,w)) \text{ is the meromorphic section of } \phi_E^*(\mathcal{O}(\Theta_r)) \otimes \mathcal{O}(-\Delta)^{\otimes r}.$$

In the rank one case we could use the fact that a section of $\phi_\alpha^*(\mathcal{O}(\Theta))$ is given by a theta function to obtain explicit expressions. The one-dimensionality of the space of theta functions (of level one) is expressed by $h^0(Pic^{g-1}(\Sigma_g), \mathcal{O}(\Theta)) = 1$. It is a fundamental result of Ref. 11 (and was essential for the mathematical proofs of the Verlinde formula, cf. Ref. 12) that this can be generalized to "non-Abelian theta functions," i.e., we have $h^0(\mathcal{U}_g(r, r(g-1)), \mathcal{O}(\Theta_r)) = 1$. This may be used to give an alternative proof of the existence and uniqueness of the propagator (and the higher correlation functions). On the other hand, it is well known[12] that this space of non-Abelian theta functions is very closely related to the space of conformal blocks of the Wess–Zumino–Witten (WZW) model on Σ_g with $\mathfrak{g} = \mathfrak{sl}(r, \mathbb{C})$ and level $k = 1$. Thus, there is indeed a geometrical connection between the bc_r-system and the above-mentioned WZW-model, as conjectured in Ref. 7.

In the usual bc-system the $U(1)$-current j_α is defined[3] by $j_\alpha(z) = -:b(z)c(z):$, where the dots indicate a regularization, which consists of subtracting the singularity in the operator product expansion of $b(z)c(w)$ before taking the limit $w \to z$. Thus, the one-point function of the current is given by

$$\langle j_\alpha(z) \rangle := -\lim_{w \to z} \left(\langle b(z)c(w) \rangle - \frac{1}{z-w} \right) = -a_0(z;\alpha), \tag{9}$$

where we have used (2) and the expansion of the Szegö-kernel, $S_\alpha(z,w) = 1/(z-w) + a_0(w;\alpha) + a_1(w;\alpha)(z-w) + \cdots$. Inserting the explicit expression for a_0 given in Ref. 10, one recovers the usual result.[13] In the bc_r-system associated to E the field b (respectively, c) is a section of $K \otimes E^\vee$ (respectively, E), so we expect that the regularized product $b(z)c(w)$ yields on the diagonal a section of $K \otimes \mathrm{End}(E)$. Defining the current J_E as above,

$$\langle J_E(z) \rangle := -\lim_{w \to z} \left(\langle b(z)c(w) \rangle - \frac{I}{z-w} \right) = -\lim_{w \to z} \left(S_E(z,w) - \frac{I}{z-w} \right),$$

we can now use the expansion of Fay's non-Abelian Szegö-kernel, $S_E(z,w) = I/(z-w) + a_0(w;E) + a_1(w;E)(z-w) + \cdots$, to obtain

$$\langle J_E(z)\rangle = -a_0(z;E),$$

in complete analogy to the rank one case above. According to p. 29 in Ref. 10, $a_0(z;E)$ is indeed a section of $K\otimes \mathrm{End}(E)$, as expected. In contrast to the rank one case, explicit expressions for the coefficients $a_i(z;E)$ are lacking. According to Raina[14,15] the geometric interpretation of this subtraction process requires that one considers the occuring bundles not on the diagonal $\Delta \simeq \Sigma_g \subset \Sigma_g \times \Sigma_g$, but on the first infinitesimal neighborhood of Δ. Following this approach he was able to give a complete treatment of the current j_α of the usual bc-system and rederive the explicit expressions known in the physical literature. It would be very beautiful if one had an analogous treatment of the current J_E of the bc_r-system.

Let us now consider the $2n$-point function $\langle b(z_1)c(w_1)\cdots b(z_n)c(w_n)\rangle$, which is a meromorphic section of the vector bundle $(K\otimes E^\vee)\boxtimes E\boxtimes\cdots\boxtimes(K\otimes E^\vee)\boxtimes E$ having simple poles (respectively, zeros) whenever two arguments of different (respectively, same) type coincide. In close analogy to the rank one case (3) we define a map

$$\phi_E^n : (\Sigma_g\times\Sigma_g)^n \to \mathcal{U}_g(r, r(g-1)),$$

$$((z_1,w_1),\ldots,(z_n,w_n)) \mapsto \mathcal{O}\left(\sum_{i=1}^n z_i - \sum_{i=1}^n w_i\right)\otimes E;$$

note that again $\phi_E^1 = \phi_E$. According to Ref. 8, the pullback of the non-Abelian theta divisor is then given in analogy to (4) by

$$(\phi_E^n)^*(\mathcal{O}(\Theta_r)) \simeq (K^{\otimes r}\otimes \det(E^\vee))\boxtimes\det(E)\boxtimes\cdots\boxtimes(K^{\otimes r}\otimes\det(E^\vee))\boxtimes\det(E)\otimes\mathcal{O}(D_n)^{\otimes r},$$

where D_n is the divisor defined in (5) [see Eq. (A1) in the Appendix]. Thus, using (6), we see that the (appropriately interpreted) determinant of the $2n$-point function is a section of $(\phi_E^n)^*(\mathcal{O}(\Theta_r))\otimes\mathcal{O}(-D_n)^{\otimes r}$. We collect these observations in the following proposition.

Proposition 2: Let $E\in\mathcal{U}_g(r,r(g-1))\backslash\Theta_r$ and $\phi_E^n:(\Sigma_g\times\Sigma_g)^n\to\mathcal{U}_g(r,r(g-1))$ be the map defined above. Then the determinant of the $2n$-point function $\langle b(z_1)\cdots c(w_n)\rangle$ of the associated bc_r-system is a meromorphic section of the line bundle $(\phi_E^n)^*(\mathcal{O}(\Theta_r))\otimes\mathcal{O}(-D_n)^{\otimes r}$.

Note that Proposition 2 reduces to Proposition 1 for $n=1$, since $D_1=\Delta_{12}\equiv\Delta$. As mentioned at the end of the last section, Raina was able to deduce the Fay identity from a comparison of two different representations of the four-point functions.[5,6] Since the bc_r-system is a free system, it was conjectured in Ref. 7 that a similar procedure should lead to a "non-Abelian Fay identity." The above results are by far too weak to establish such an identity, but nevertheless might provide a nontrivial check. A very promising result into the desired direction is contained in Ref. 8; a closely related result from a different point of view can be found in Ref. 16.

In the usual bc-system the four-point function $\langle b(z_1)c(w_1)b(z_2)c(w_2)\rangle$ is very important, since considering the limits $w_1\to z_1$, $w_2\to z_2$ of its regularized explicit form yields the two-point function $\langle j_\alpha(z_1)j_\alpha(z_2)\rangle$ of the current.[13] Considering, furthermore, the regularized limit $z_2\to z_1$, one obtains the one-point function of the energy-momentum tensor T_α:

$$\langle T_\alpha(z)\rangle := \frac{1}{2}\lim_{w\to z}\left(\langle j_\alpha(z)j_\alpha(w)\rangle - \frac{1}{(z-w)^2}\right) = a_1(z;\alpha) - \frac{1}{2}\partial_z a_0(z;\alpha); \tag{10}$$

in the second equation we have used again the coefficients a_i of the Szegö-kernel S_α. Inserting the explicit expressions for the a_i given in Ref. 10 yields the result of the physical literature.[4,17,18] Raina and Biswas have managed to give an algebro-geometric description of the energy-momentum tensor, this time using the second infinitesimal neighborhood of the diagonal.[15,19] In the bc_r-system the associated energy-momentum tensor T_E should be given as the limit of the regularized two-point function of the current J_E, i.e., $T_E(z)\sim :J_E(z)\otimes J_E(z):$. Local computations for the operator product expansion of $J_E(z)\otimes J_E(w)$ suggest, that—due to the non-Abelian struc-

ture coming from the higher rank—additional terms with a simple pole will appear and have to be subtracted, too. The main problem is that one does not have an explicit expression for the four-point function. In particular, there seems to be no straightforward generalization of Wick's rule, meaning here that one could calculate the four-point function as some kind of determinant of propagators. One expects that a relation similar to (10)—involving this time $a_0(z;E), a_1(z;E)$ and $\partial_z a_0(z;E)$—holds also in the higher rank case, where the additional tensor product structure will be involved. The naive expectation is that $\langle T_E(z)\rangle$ is a section of $K^{\otimes 2}\otimes \mathrm{End}(E)^{\otimes 2}$, but this is already false in the rank one case. Due to the regularization procedure the conformal symmetry is lost,[20] so that $12\langle T_\alpha(z)\rangle$ is a projective connection,[21] transforming as some kind of "perturbed" quadratic differential. One may wonder whether there is an analogous geometric structure lurking behind $\langle T_E(z)\rangle$.

IV. DISCUSSION

We have seen that the determinants of the correlation functions of the bc_r-system can be written as pullbacks of the non-Abelian theta divisor. It is not clear whether one can describe the correlation functions themselves within the approach pursued here. The current J_E was defined by $J_E(z)\sim :b(z)c(z):$, which can be written locally [where we write the field c as $c=(c_1,\ldots,c_r)^t$ and similarly for b] as $J_{E,ij}(z)\sim :b^j(z)c^i(z):$. Locally one can also define currents $J^a_{ij}\sim :b^j(T^a c)^i:$ for a simple Lie algebra $\mathfrak{g}$ with generators $\{T^a\}$. It is well known that the traces of J^a, i.e., $j^a:=\mathrm{Tr}(J^a)\sim :b^i T^a_{ij} c^j:$, give rise to a current algebra, thus to representations of the affine Lie algebra $\hat{\mathfrak{g}}$, (see p. 646 in Ref. 22). These affine Lie algebras correspond to WZW models, so that one expects that a geometric definition of the currents J^a [together with the $U(1)$-current J_E] should give a geometric interpretation of the non-Abelian bosonization.[23]

We hope that a further examination of the bc_r-system will uncover more interesting connections to the geometry of the non-Abelian theta divisor as well as to the corresponding WZW model. As should be clear from the above remarks and the discussion in Ref. 7, the main obstacle for further progress is that a suitably generalized Wick's rule lacks. If one had some kind of suitably generalized determinant DET for these matrices with matrix-valued entries, Wick's rule for the four-point function would mean that $\langle b(z_1)c(w_1)b(z_2)c(w_2)\rangle=\mathrm{DET}(\langle b(z_i)c(w_j)\rangle)$ and that one could use the right-hand side for all the computations indicated above, in particular for the energy-momentum tensor.

APPENDIX: A RESULT OF GÓMEZ GONZÁLES AND PLAZA MARTÍN

Here we state a recent result of Gómez Gonzáles and Plaza Martín concerning the pullback of the non-Abelian theta divisor Θ_r under the "addition morphism"; this is Theorem 3.1 in Ref. 8. From our point of view they are working not with a single system, but with a family parametrized by some scheme S. Their setup is as follows (we have slightly changed their notation to be consistent with the one used above). Let S be a scheme and Σ_g an irreducible proper smooth algebraic curve of genus $g\geqslant 2$ over $\mathbb{C}$ (i.e., a Riemann surface). We denote by $\mathcal{U}_g^{ss}(r,d)$ the moduli space of (equivalence classes of) semistable vector bundles of rank r and degree d on Σ_g; Seshadri proved that $\mathcal{U}_g^{ss}(r,d)$ is the natural compactification of $\mathcal{U}_g(r,d)$ from above.[24] The closure of Θ_r from above in $\mathcal{U}_g^{ss}(r,r(g-1))$ is again a divisor, which we also denote by Θ_r. Let $\mathcal{E}$ be a semistable bundle of rank r and degree $r(g-1)$ on $\Sigma_g\times S$; we interpret this as a family $\{\mathcal{E}_s\}_{s\in S}$ (with $\mathcal{E}_s\equiv\mathcal{E}_{|\Sigma_g\times\{s\}}$) of semistable bundles $\mathcal{E}_s\in\mathcal{U}_g^{ss}(r,r(g-1))$ on $\Sigma_g\times\{s\}\simeq\Sigma_g$. Let us furthermore introduce a map $\psi_{\mathcal{E}}:S\to\mathcal{U}_g^{ss}(r,r(g-1))$ by associating to $s\in S$ the restriction of $\mathcal{E}$ to $\Sigma_g\times\{s\}\simeq\Sigma_g$, i.e., $\psi_{\mathcal{E}}(s)=\mathcal{E}_s$. For each $n\in\mathbb{N}$ we now introduce the relative version of the generalization of (3), namely,

$$\phi^n_{\mathcal{E};S}:(\Sigma_g\times\Sigma_g)^n\times S\to\mathcal{U}_g^{ss}(r,r(g-1)),$$

$$((z_1,w_1),\ldots,(z_n,w_n),s)\mapsto\mathcal{O}\left(\sum_{i=1}^n z_i-\sum_{i=1}^n w_i\right)\otimes\mathcal{E}_s.$$

For $1\leqslant i\leqslant 2n$ there are natural projections p_i (respectively, π_i) from $(\Sigma_g\times\Sigma_g)^n\times S$ onto Σ_g (respectively, $\Sigma_g\times S$), where in both cases the image Σ_g is the ith component of $(\Sigma_g\times\Sigma_g)^n$. Let us denote the highest exterior product of a bundle F by $\det(F)$.

Theorem (Gómez Gonzáles, Plaza Martín): *Let $\mathcal{E}$ be a semistable vector bundle on $\Sigma_g\times S$ of rank r and degree $r(g-1)$. Then there is an isomorphism of line bundles on $(\Sigma_g\times\Sigma_g)^n\times S$:*

$$(\phi^n_{\mathcal{E};S})^*(\mathcal{O}(\Theta_r))\simeq\mathcal{O}(D_n)^{\otimes r}\otimes\left\{\bigoplus_{i=1}^{n}\left[\pi^*_{2i-1}(\det(\mathcal{E}^\vee))\otimes p^*_{2i-1}(K^{\otimes r})\otimes\pi^*_{2i}(\det(\mathcal{E}))\right]\right\}\otimes\psi^*_{\mathcal{E}}(\mathcal{O}(\Theta_r)),$$

where D_n is given in (5).

We will use this result in the very special case of a trivial family, i.e., we choose S to be a point $\{s_0\}$. We identify π_i and p_i and neglect the trivial map $\psi_{\mathcal{E}}$. Furthermore, the "family" $\mathcal{E}=\{\mathcal{E}_s\}_{s\in\{s_0\}}$ parametrized by one point is just one bundle $\mathcal{E}_{s_0}=\mathcal{E}_{|\Sigma_g\times\{s_0\}}$, which we denote by E. Then the formula of the theorem reduces to

$$\begin{aligned}(\phi^n_E)^*(\mathcal{O}(\Theta_r))&\simeq\mathcal{O}(D_n)^{\otimes r}\otimes\bigoplus_{i=1}^{n}\{p^*_{2i-1}(\det(E^\vee)\otimes K^{\otimes r})\otimes p^*_{2i}(\det(E))\}\\&\simeq\mathcal{O}(D_n)^{\otimes r}\otimes(K^{\otimes r}\otimes\det(E^\vee))\boxtimes\det(E)\boxtimes\cdots\boxtimes(K^{\otimes r}\otimes\det(E^\vee))\boxtimes\det(E),\end{aligned}\tag{A1}$$

where we have written $\phi^n_E:=\phi^n_{E;\{s_0\}}$. In particular, choosing $n=1$ one obtains with $D_1=\Delta_{12}\equiv\Delta$ and the abbreviation $\phi_E:=\phi^1_E$ the result

$$\phi^*_E(\mathcal{O}(\Theta_r))\simeq\mathcal{O}(\Delta)^{\otimes r}\otimes(K^{\otimes r}\otimes\det(E^\vee))\boxtimes\det(E).\tag{A2}$$

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Quasigraded Lie algebras on hyperelliptic curves and classical integrable systems

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A new family of infinite-dimensional Lie algebras on hyperelliptic curves is constructed. We show them to be quasigraded and explicitly find their central extensions. We also show, that constructed algebras in the case of zero central charge possess infinite number of invariant functions. Besides, they admit a decomposition into the direct sum of two subalgebras. These two facts together enables one to use them to construct new integrable systems. In such a way we find new integrable Hamiltonian systems, which are direct higher rank generalizations of the integrable systems of Steklov–Liapunov, associated with the e(3) algebra and Steklov–Veselov associated with the so(4) algebra. Besides we give hyperelliptic Lax representation for the generalized Euler tops. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1379066]

I. INTRODUCTION

The main purpose of the present paper is to introduce new integrable systems of Euler–Arnold-type on the finite-dimensional Lie algebras. It is known, that such systems admit Lax-pair representations (see Ref. 1),

$$\frac{dL(t)}{dt}=[L(t),M(t)], \tag{1}$$

where L and M are some matrix depending on the dynamical variables.

Almost in all cases the Lax operator depends also on an additional parameter, the so-called "spectral parameter," w: $L=L(w)$. This dependence permits to construct large number of integrals of motion via the expansion of functions $I^k(w)=\mathrm{Tr}\,L(w)^k$ in the series of the powers of the spectral parameter. Usually dependence of the Lax operator on w is rational or elliptic.

The natural approach to construction of new types of integrable systems is the search for the solutions of Lax equations with other (more complicated) dependence on the spectral parameter. We will solve this problem for the case of $L(w)$ with the hyperelliptic dependence on the spectral parameter.

Our approach is based on the usage of infinite-dimensional Lie algebras. It is known (see Refs. 2–4) that a group theoretical explanation of the integrability of Lax equations on finite-dimensional Lie algebras with the rational spectral parameters is based on the loop algebras, i.e., algebras of the form $\mathfrak{g}\otimes P(\lambda,\lambda^{-1})$. In the works (Refs. 5–7) it was shown, that the Lax equation with the elliptic spectral parameters on the algebra so(3) and some of its extensions could be obtained from the infinite-dimensional Lie algebras of the elliptic functions with the values in so(3) via the Kostant–Adler scheme (Refs. 8 and 9, see also Refs. 2–4).

We generalize construction of Ref. 6 on the case of classical matrix algebras of higher rank and investigate corresponding finite-dimensional integrable systems. Growth of the rank of algebra requires automatic growth of the genus of the curve. As a result we obtain algebras of gl(n)-, so(n)-, and sp(n)-valued functions on the hyperelliptic curves of genus $\mathfrak{g}$, where $n=2g+2$ or

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$n=2g+1$, or, to be more precise, on its double covering. Obtained algebras have many nice properties. They are quasigraded. They possess infinite number of invariant functions. They possess central extensions. In the rational degeneration of the curve they coincides with the ordinary loop algebras. So they could be viewed as ''hyperelliptic'' generalizations of the loop algebras.

There exists other higher genus generalization of the loop algebras, the so-called Krichiver–Novikov algebras (Ref. 10) of the matrix-valued holomorphic functions on the Riemanian surfaces with two punctured points. But Krichiver–Novikov algebras do not admit Kostant–Adler scheme compatible with quasigrading (see Ref. 11). Hence this generalization can not be used for producing new integrable systems with the spectral parameter on the higher genus curves.

Contrary to the Krichiver–Novikov algebras our algebras admit the Kostant–Adler scheme, and hence, could be used for constructing integrable systems.

Using our algebra as hidden symmetry algebra we obtain new integrable systems on $\mathfrak{g}\oplus\mathfrak{g}$ that describe two interacting generalized rigid bodies. This system is a direct higher rank generalization of the integrable case of Steklov and Veselov (see Ref. 12) on $so(4)=so(3)\oplus so(3)$. We also obtain new integrable systems on the semidirect sum $\mathfrak{g}+\mathfrak{g}$, that generalize the integrable case of Steklov–Liapunov on e(3) (see Ref. 13). Both systems possess natural hyperelliptic Lax representations. Besides, we find hyperelliptic Lax representation for the generalized Euler tops.

The structure of the discovered algebras provides the possibility of giving a two-dimensional generalization of the constructed integrable systems via the finite-gap extension method (see Refs. 5–7). We will return to this problem in our subsequent publications.

II. QUASIGRADED ALGEBRAS ON HYPERELLIPTIC CURVES

A. Hyperelliptic curve embedded in $\mathbb{C}^n$

Let us consider in the space $\mathbb{C}^n$ with the coordinates $w_1,w_2,\ldots,w_n$ the following system of quadrics:

$$w_i^2-w_j^2=a_j-a_i, \quad i,j=1,n, \tag{2}$$

where a_i are arbitrary complex numbers. Rank of this system is $n-1$, so substitution

$$w_i^2=w-a_i,$$

solves these equations. Moreover if we put $y=\prod_{i=1}^{n} w_i$ we obtain the equation of the hyperelliptic curve $\mathcal{H}$,

$$y^2=\prod_{i=1}^{n}(w-a_i). \tag{3}$$

Hence Eqs. (2) define embedding of the hyperelliptic curve $\mathcal{H}$ into the linear space C^n. Variable w is a local parameter on the curve and a_i its branching points.

Example 1: In the $n=3$ case all of these objects have a well-known analytical description. Indeed in this case curve under the consideration is elliptic. Its uniformization is made by the Weierstrass $\mathfrak{p}$-function and its derivative: $w=\mathfrak{p}(u)$, $y=1/2\mathfrak{p}'(u)$. Functions w_i are expressed via Jacobi elliptic functions (see Ref. 14), $w_1=1/\mathrm{sn}(u)$, $w_2=\mathrm{dn}(u)/\mathrm{sn}(u)$, $w_3=\mathrm{cn}(u)/\mathrm{sn}(u)$.

B. Classical Lie algebras

Let $\mathfrak{g}$ denote one of the classical matrix Lie algebras $\mathrm{gl}(n)$, $\mathrm{so}(n)$, and $\mathrm{sp}(n)$ over the field of the complex numbers. For the subsequent we will need a special form of their bases. Let us explicitly construct them. Let $I_{ij}\in \mathrm{Mat}(n,\mathbb{C})$ be a matrix defined as follows:

$$(I_{ij})_{ab}=\delta_{ia}\delta_{jb}.$$

Evidently, a basis in the algebra gl(n) could be built from the matrices $X_{ij}\equiv I_{ij}, i,j\in 1,...,n$. The commutation relations in gl(n) will have the following standard form:

$$[X_{ij},X_{kl}]=\delta_{kj}X_{il}-\delta_{il}X_{kj}.$$

The basis in the algebra so(n) could be chosen as $X_{ij}\equiv I_{ij}-I_{ji}$, $i,j\in 1,...,n$, with the following commutation relations:

$$[X_{ij},X_{kl}]=\delta_{kj}X_{il}-\delta_{il}X_{kj}+\delta_{jl}X_{ki}-\delta_{ki}X_{jl},$$

and "skew-symmetry" property $X_{ij}=-X_{ji}$.

The basis in the algebra sp(n) consists of the matrices $X_{ij}=I_{ij}-\epsilon_i\epsilon_j I_{-i-j}$, $i,j\in -n,\ldots,-1,1,...,n$, with the commutation relations

$$[X_{ij},X_{kl}]=\delta_{kj}X_{il}-\delta_{il}X_{kj}+\epsilon_i\epsilon_j(\delta_{j-l}X_{k-i}-\delta_{k-i}X_{-jl}),$$

and additional property $X_{ij}=-\epsilon_i\epsilon_j X_{-j-i}$, where $\epsilon_j=\operatorname{sign} j$.

C. Algebras on the curve

For the basic elements X_{ij} of all three algebras gl(n), so(n), and sp(n) we introduce the following algebra-valued functions on the curve $\mathcal{H}$, or to be more precise on its double covering,

$$X_{ij}^{+}(w)=X_{ij}\otimes w_i w_j,\quad X_{ij}^{-}(w)=X_{ij}\otimes w^{-1}w_i w_j. \tag{4}$$

Here we put $w_{-i}\equiv w_i$ in the case of sp(n). We will need the following definition (Ref. 10):

Definition 1: Infinite-dimensional Lie algebra $\tilde{\mathfrak{g}}$ is called $\mathbb{Z}$ quasigraded if there exists such $p,q\in\mathbb{Z}_+$ that

$$\tilde{\mathfrak{g}}=\sum_{j\in\mathbb{Z}}\tilde{\mathfrak{g}}_j,\quad \text{such that}\quad [\tilde{\mathfrak{g}}_i,\tilde{\mathfrak{g}}_j]\subset\sum_{k=-p}^{q}\tilde{\mathfrak{g}}_{i+j+k}. \tag{5}$$

The following theorem holds true:

Theorem 1: *(i) Functions $X_{ij}^{+}(w)$ and $X_{ij}^{-}(w)$ generate infinite-dimensional $\mathbb{Z}$ quasigraded Lie algebra $\tilde{\mathfrak{g}}_{\mathcal{H}}$.*
(ii) There exists a decomposition: $\tilde{\mathfrak{g}}_{\mathcal{H}}=\tilde{\mathfrak{g}}_{\mathcal{H}}^{+}+\tilde{\mathfrak{g}}_{\mathcal{H}}^{-}$, *where $\tilde{\mathfrak{g}}_{\mathcal{H}}^{+}$ and $\tilde{\mathfrak{g}}_{\mathcal{H}}^{-}$ are generated by $X_{ij}^{+}(w)$ and $X_{ij}^{-}(w)$, correspondingly.*

Proof: Let us introduce the following algebra-valued functions on the double covering of the curve $\mathcal{H}$:

$$X_{ij}^{n}=X_{ij}\otimes w^n w_i w_j.$$

To prove the theorem we will need the explicit form of their commutation relations:

Proposition 1: Elements X_{ij}^{n} form closed algebra with the following commutation relations:

$$(1)\quad [X_{ij}^{n},X_{ij}^{m}]=\delta_{kj}X_{il}^{n+m+1}-\delta_{il}X_{kj}^{n+m+1}+a_i\delta_{il}X_{kj}^{n+m}-a_j\delta_{kj}X_{il}^{n+m}\quad \text{for the gl}(n), \tag{6a}$$

$$(2)\quad [X_{ij}^{n},X_{ij}^{m}]=\delta_{kj}X_{il}^{n+m+1}-\delta_{il}X_{kj}^{n+m+1}+\delta_{jl}X_{ki}^{n+m+1}-\delta_{ik}X_{jl}^{n+m+1}+a_i\delta_{il}X_{kj}^{n+m}-a_j\delta_{kj}X_{il}^{n+m}$$
$$+a_i\delta_{ik}X_{jl}^{n+m}-a_j\delta_{jl}X_{ki}^{n+m}\quad \text{for the so}(n), \tag{6b}$$

$$(3)\quad [X_{ij}^{n},X_{ij}^{m}]=\delta_{kj}X_{il}^{n+m+1}-\delta_{il}X_{kj}^{n+m+1}+\epsilon_i\epsilon_j(\delta_{j-l}X_{k-i}^{n+m+1}-\delta_{i-k}X_{j-l}^{n+m+1})+a_i\delta_{il}X_{kj}^{n+m}$$
$$-a_j\delta_{kj}X_{il}^{n+m}+a_i\epsilon_i\epsilon_j(a_i\delta_{i-k}X_{j-l}^{n+m}-a_j\delta_{j-l}X_{k-i}^{n+m})\quad \text{for the sp}(n). \tag{6c}$$

Let us put

$$\tilde{\mathfrak{g}}_{\mathcal{H}} = \mathrm{Span}_{\mathbb{C}}\{X_{ij}^{m},\ m \in \mathbb{Z}\}.$$

From Proposition 1 follows that $\tilde{\mathfrak{g}}_{\mathcal{H}}$ is quasigraded. Besides, let us define the following subspaces:

$$\tilde{\mathfrak{g}}_{\mathcal{H}}^{+} = \mathrm{Span}_{\mathbb{C}}\{X_{ij}^{m}, m \geqslant 0\}, \tilde{\mathfrak{g}}_{\mathcal{H}}^{-} = \mathrm{Span}_{\mathbb{C}}\{X_{ij}^{-m}, m > 0\}.$$

From Proposition 1 follows that they are subalgebras. Taking into account that $X_{ij}^{+}(w) = X_{ij}^{0}$, $X_{ij}^{-}(w) = X_{ij}^{-1}$ and Proposition 1, it is easy to see that elements $X_{ij}^{+}(w)$ generate subalgebra $\tilde{\mathfrak{g}}_{\mathcal{H}}^{+}$ and elements $X_{ij}^{-}(w)$ generate subalgebra $\tilde{\mathfrak{g}}_{\mathcal{H}}^{-}$. Hence $X_{ij}^{+}(w)$ and $X_{ij}^{-}(w)$ generate $\tilde{\mathfrak{g}}_{\mathcal{H}}$. Theorem is proved.

Example 2: Let $\mathfrak{g} = \mathrm{so}(3)$. In this case the constructed algebra will coincide with the ''even'' subalgebra of the algebra of hidden symmetry of Landau–Lifschits equations (Ref. 5). Indeed, putting $X_k \equiv \epsilon_{ijk} X_{ij}$, we obtain the following commutation relations (Ref. 6):

$$[X_i^n, X_j^m] = \epsilon_{ijk} X_k^{n+m+1} + \epsilon_{ijk} a_k X_k^{n+m}.$$

Remark 1: From Proposition 1 follows, that in the rational degeneration of $\mathcal{H}$,

$$y^2 = w^n,$$

i.e., when $a_i = 0$, we obtain, that $w_i = \sqrt{w}$ and, hence, $\tilde{\mathfrak{g}}_{\mathcal{H}} = \tilde{\mathfrak{g}}$, where $\tilde{\mathfrak{g}}$ is a loop algebra.

Remark 2: Although algebra $\tilde{\mathfrak{g}}_{\mathcal{H}}$ was defined over the field of complex numbers, analogous construction, evidently, is also valid in the case when main field is $\mathbb{R}$. We have only to require in this case that $a_i \in \mathbb{R}$.

III. CENTRAL EXTENSION

To have the full analogy with the loop algebra, and keeping in mind possible application to quantum integrable systems, in this subsection we define central extensions of the algebras $\tilde{\mathfrak{g}}_{\mathcal{H}}$. First we are reminded of the following definition (see Ref. 10):

Definition 2: Cocycle χ on the quasigraded algebra is called local if

$$\chi(X_{ij}^{m}, X_{kl}^{n}) = 0, \quad \text{for all } |n+m| > K \text{ and for some } K \in \mathbb{Z}_{+}.$$

Let $(X|Y) = c_n \,\mathrm{tr}\, XY$, where $c_n = 2n$ for $\mathrm{gl}(n)$, $c_n = (n-2)$ for $\mathrm{so}(n)$, $c_n = (2n+2)$ for $\mathrm{sp}(n)$, be a standard invariant form on the classical Lie algebras $\mathrm{gl}(n)$, $\mathrm{so}(n)$ or $\mathrm{sp}(n)$. Let us define on $\tilde{\mathfrak{g}}_{\mathcal{H}}$ the following bilinear form:

$$\chi(X(w), Y(w)) = \oint \left(X(w) \middle| \frac{dY(w)}{dw} \right) dw, \tag{7}$$

where 1-cycle γ in the complex plane of variable w encircles point $w = 0$. The following theorem holds true:

Theorem 2: *(i) Bilinear form χ is skew-symmetric and satisfies the properties of the cocycle, and hence, determines a central extension of $\tilde{\mathfrak{g}}_{\mathcal{H}}$: $\hat{\mathfrak{g}}_{\mathcal{H}} = \tilde{\mathfrak{g}}_{\mathcal{H}} + \mathbb{C}c$ by the following formula:*

$$[X(w) + \alpha c, Y(w) + \beta c]' = [X(w), Y(w)] + \chi(X(w), Y(w))c.$$

(ii) Cocycle χ is local and its values on the bases elements are calculated by the following formulas:

$$\chi(X_{ij}^{m}, X_{kl}^{n}) = \chi^{mn}(a_i, a_j)(X_{ij}|X_{kl}), \tag{8}$$

where

$$\chi^{mn}(a_i, a_j) = (n+1)\delta_{n+m+2,0} - (n+1/2)(a_i + a_j)\delta_{n+m+1,0} + n a_i a_j \delta_{n+m,o}. \tag{9}$$

Proof: Skew symmetry of χ follows from the symmetry of $(\,|\,)$ and skew symmetry of the operator of differentiation. The skew symmetry of the differentiation operator is easy to prove by partial integration. We need only to prove, that integrated function is one-valued. Indeed, under the arbitrary values of the indices *i,j,k,l,* it is not true because it will contain square roots of the type, $w_i=\pm\sqrt{w-a_i}$. But direct calculation of the values of the invariant form $(\,|\,)$ on the bases vectors X_{ij} shows that expression (8) is not zero if and only if $i=l$, $j=k$ or $i=\pm k$, $j=\pm l$. Indeed: $(X_{ij}|X_{kl})=2n\delta_{il}\delta_{jk}$ for gl(n), $(X_{ij}|X_{kl})=(n-2)(\delta_{il}\delta_{jk}-\delta_{ik}\delta_{jl})$ for so(n), $(X_{ij}|X_{kl})=(2n+2)\times(\delta_{il}\delta_{jk}-\epsilon_i\epsilon_j\delta_{i-k}\delta_{j-l})$ for sp(n). Taking this into account we obtain

$$\begin{aligned}\chi(X^m_{ij},X^n_{kl})&=(X_{ij}|X_{kl})\left(\oint_\gamma w^m w_i w_j d(w^n w_k w_l)\right)\\&=(X_{ij}|X_{kl})\left(\oint_\gamma d(w^{n+m}w_i w_j w_k w_l)-\oint_\gamma w^n w_k w_l d(w^m w_i w_j)\right)\\&=-(X_{kl}|X_{ij})\left(\oint_\gamma w^n w_k w_l d(w^m w_i w_j)\right)\\&=-\chi(X^n_{kl},X^m_{ij}).\end{aligned}$$

This proves skew symmetry of the differentiation operation under the integral on the basic vectors and, hence on all algebras $\tilde{\mathfrak{g}}_{\mathcal{H}}$. Let us prove the cocycle property,

$$\chi([X(w),Y(w)],Z(w)])+\chi([Z(w),X(w)],Y(w)])+\chi([Y(w),Z(w)],X(w)])=0.$$

It is enough to consider the case when elements $X(w),Y(w),Z(w)$ coincide with the basis vectors. Let

$$F(X^p_{ij},X^s_{kl},X^t_{mn})\equiv\chi([X^p_{ij},X^s_{kl}],X^t_{mn})])+\chi([X^t_{mn},X^p_{ij}],X^s_{kl}])+\chi([X^s_{kl},X^t_{mn}],X^p_{ij}]).$$

Then taking into account the symmetry and Ad_G-invariance of $(\,|\,)$, we obtain

$$F(X^p_{ij},X^s_{kl},X^t_{mn})=([X_{ij},X_{kl}]|X_{mn})\oint_\gamma d(w^{p+s+t}w_i w_j w_k w_l w_m w_n).$$

Taking into account the explicit form of the commutation relation and invariant form, we see that function under the integration is one-valued. Hence, the correspondent integral is identically equal to zero. Part (i) is proved. Formula (8) follows from the arguments used in proof of part (i). Explicitly,

$$\chi^{mn}(a_i,a_j)=\left(\oint_\gamma w^m w_i w_j d(w^n w_i w_j)\right)=n\oint_\gamma w_i^2 w_j^2 w^{n+m-1}dw+1/2\oint_\gamma(w_i^2+w_j^2)w^{m+n}dw.$$

Taking into account that $w_i^2=w-a_i$ we obtain formula (9). Locality of cocycle follows from its explicit form. Theorem is proved.

Example 3: In the case of rational degeneration $a_i=0$ we obtain the following cocycle on the loop algebra:

$$\chi(X^m_{ij},X^n_{kl})=(n+1)\,\delta_{n+m+2,0}(X_{ij}|X_{kl}).$$

It passes to the standard one after passing to the standard basis by renaming the indices $m\to m-1$, $n\to n-1$.

IV. COADJOINT REPRESENTATION AND ITS INVARIANTS

To define the coadjoint representation we have to define $\tilde{\mathfrak{g}}^*_{\mathcal{H}}$. We assume that $\tilde{\mathfrak{g}}^*_{\mathcal{H}} \subset \mathfrak{g} \otimes A$, where A is an algebra of function on the double covering of the curve $\mathcal{H}$. Let us define the invariant pairing between $L(w) \in \tilde{\mathfrak{g}}^*_{\mathcal{H}}$ and $X(w) \in \tilde{\mathfrak{g}}_{\mathcal{H}}$ in the following way:

$$\langle X(w), L(w) \rangle_f = c_r \operatorname{res}_{w=0} f^{-1}(w) y^{-1}(w) (X(w) | Y(w)), \tag{10}$$

where $f(w)$ is arbitrary function on the curve $\mathcal{H}$. It is easy to show that element dual to X^{-m}_{ij} with respect to this pairing is $Y^m_{ij} \equiv (X^{-m}_{ij})^* = [w^{m-1} f(w) y(w) / w_i w_j] X^*_{ij}$. Hence the general element of the dual space has the following form:

$$L(w) = \sum_{m \in Z} \sum_{i,j=1}^{n} l^m_{ij} \frac{w^{m-1} f(w) y(w)}{w_i w_j} X^*_{ij}. \tag{11}$$

Coadjoint action of algebra $\tilde{\mathfrak{g}}_{\mathcal{H}}$ on its dual space $\tilde{\mathfrak{g}}^*_{\mathcal{H}}$ coincides with commutator,

$$\mathrm{ad}^*_{X(w)} L(w) = [L(w), X(w)]. \tag{12}$$

Explicitly co-adjoint action of the algebra has the following form:

$$(1)\ [X^n_{ij}, Y^m_{kl}] = \delta_{kj} Y^{n+m+1}_{il} - \delta_{il} Y^{n+m+1}_{kj} + a_j \delta_{il} Y^{n+m}_{kj} - a_i \delta_{kj} Y^{n+m}_{il} \quad \text{for the } \mathrm{gl}(n),$$

$$(2)\ [X^n_{ij}, Y^m_{kl}] = \delta_{kj} Y^{n+m+1}_{il} - \delta_{il} Y^{n+m+1}_{kj} + \delta_{jl} Y^{n+m+1}_{ki} - \delta_{ik} Y^{n+m+1}_{il} + a_j \delta_{il} Y^{n+m}_{kj} - a_i \delta_{kj} Y^{n+m}_{il} + a_j \delta_{ik} Y^{n+m}_{jl} - a_i \delta_{jl} Y^{n+m}_{ki} \quad \text{for the } \mathrm{so}(n),$$

$$(3)\ [X^n_{ij}, Y^m_{kl}] = \delta_{kj} Y^{n+m+1}_{il} - \delta_{il} Y^{n+m+1}_{kj} + \epsilon_i \epsilon_j (\delta_{j-l} Y^{n+m+1}_{k-i} - \delta_{i-k} Y^{n+m+1}_{j-l}) + a_j \delta_{il} Y^{n+m}_{kj} - a_i \delta_{kj} Y^{n+m}_{il} + \epsilon_i \epsilon_j (a_j \delta_{i-k} Y^{n+m}_{j-l} - a_i \delta_{j-l} Y^{n+m}_{k-i}) \quad \text{for the } \mathrm{sp}(n).$$

It is evident from the above formulas, that $\tilde{\mathfrak{g}}^*_{\mathcal{H}}$ is a quasigraded $\tilde{\mathfrak{g}}_{\mathcal{H}}$-module,

$$\tilde{\mathfrak{g}}^*_{\mathcal{H}} = \sum_{m \in \mathbb{Z}} (\tilde{\mathfrak{g}}^*_{\mathcal{H}})_m,$$

where $(\tilde{\mathfrak{g}}^*_{\mathcal{H}})_m = \mathrm{Span}_C \{ Y^m_{ij} | i,j = 1,...,n \}$.

Remark 3: Putting $f(w) = y(w)$ in the definition of the elements of dual space we obtain, $\tilde{\mathfrak{g}}^*_{\mathcal{H}} = \tilde{\mathfrak{g}}_{\mathcal{H}}$, i.e., dual element to each element of $\tilde{\mathfrak{g}}_{\mathcal{H}}$ belongs to $\tilde{\mathfrak{g}}_{\mathcal{H}}$. If $f(w) \neq y(w)$, then generally speaking, spaces $\tilde{\mathfrak{g}}^*_{\mathcal{H}}$ and $\tilde{\mathfrak{g}}_{\mathcal{H}}$, considering as subspaces in the algebra of functions on the double covering of the curve $\mathcal{H}$, do not coincide.

Remark 4: If $f = 1$ and $\mathfrak{g} = \mathrm{so}(n)$ elements of $\tilde{\mathfrak{g}}_{\mathcal{H}} + \tilde{\mathfrak{g}}^*_{\mathcal{H}}$ form a closed algebra. This will be an analog of the algebra of hidden symmetry of Landau–Lifschits equations (see Ref. 5). Unfortunately, for $n > 4$ it does not admit a Kostant–Adler scheme and cannot be used for the construction of integrable systems. That is why we will not consider it here.

From the explicit form of coadjoint action (12) follows the next statement:

Proposition 2: Functions $I^k_m(L(w)) = r \epsilon s_{w=0} w^{-m-1} Tr\, L(w)^k$, *where* $m \in \mathbb{Z}$, *are invariants of a coadjoint representation.*

Hence constructed Lie algebras not only admit decomposition into a direct sum of two subalgebras but also possess an infinite number of invariant functions. This permits us to use them in construction of integrable systems.

V. INTEGRABLE SYSTEMS FROM HYPERELLIPTIC ALGEBRAS

A. First Lie–Poisson structure

In the space $\tilde{\mathfrak{g}}^*_{\mathcal{H}}$ it is possible to define many Lie–Poisson structures using different pairings. We will use the pairing (10) with $f(w)=w$,

$$\langle X(w),L(w)\rangle_{-1}=c_n \operatorname{res}_{w=0} w^{-1}y^{-1}(w)(X(w)|Y(w)). \tag{13}$$

It defines brackets on $P(\tilde{\mathfrak{g}}^*_{\mathcal{H}})$ in the following way:

$$\{F(L),G(L)\}=\sum_{l,m\in Z}\sum_{i,j,p,s=1}^{n}\langle L(w),[X^{-l}_{ij},X^{-m}_{ps}]\rangle_{-1}\frac{\partial G}{\partial l^l_{ij}}\frac{\partial F}{\partial l^m_{ps}}. \tag{14}$$

From Proposition 2 follows the next statement:

Proposition 3: Functions $I^k_m(L(w))$ are central for brackets $\{\ ,\ \}$.

Taking into account that $l^m_{ij}=\langle L(w),X^{-m}_{ij}\rangle_{-1}$ it is easy to show that for the coordinate functions l^m_{ij} brackets (14) will have the following form:

$$(1)\ \{l^n_{ij},l^m_{ij}\}=\delta_{kj}l^{n+m-1}_{il}-\delta_{il}l^{n+m-1}_{kj}+a_i\delta_{il}l^{n+m}_{kj}-a_j\delta_{kj}l^{n+m}_{il}\quad \text{for the } \mathrm{gl}(n), \tag{15a}$$

$$\begin{aligned}(2)\ \{l^n_{ij},l^m_{ij}\}&=\delta_{kj}l^{n+m-1}_{il}-\delta_{il}l^{n+m-1}_{kj}+\delta_{jl}l^{n+m-1}_{ki}-\delta_{ik}l^{n+m-1}_{il}+a_i\delta_{il}l^{n+m}_{kj}-a_j\delta_{kj}l^{n+m}_{il}\\&\quad+a_i\delta_{ik}l^{n+m}_{jl}-a_j\delta_{jl}l^{n+m}_{ki}\quad \text{for the } \mathrm{so}(n),\end{aligned} \tag{15b}$$

$$\begin{aligned}(3)\ \{l^n_{ij},l^m_{ij}\}&=\delta_{kj}l^{n+m-1}_{il}-\delta_{il}l^{n+m-1}_{kj}+\epsilon_i\epsilon_j(\delta_{j-l}l^{n+m-1}_{k-i}-\delta_{i-k}l^{n+m-1}_{j-l})+a_i\delta_{il}l^{n+m}_{kj}\\&\quad-a_j\delta_{kj}l^{n+m}_{il}+a_i\epsilon_i\epsilon_j(a_i\delta_{i-k}l^{n+m}_{j-l}-a_j\delta_{j-l}l^{n+m}_{k-i})\quad \text{for the } \mathrm{sp}(n).\end{aligned} \tag{15c}$$

From the explicit form of the Poisson brackets follows that Lie–Poisson brackets in the subspaces $(\tilde{\mathfrak{g}}^*_{\mathcal{H}})_-=\Sigma^{\infty}_{m=0}(\tilde{\mathfrak{g}}^*_{\mathcal{H}})_{-m}$ and $(\tilde{\mathfrak{g}}^*_{\mathcal{H}})_+=\Sigma^{\infty}_{m=1}(\tilde{\mathfrak{g}}^*_{\mathcal{H}})_m$, up to the reverse of the sign of the upper indices, repeat commutation relations of the algebras $\tilde{\mathfrak{g}}^+_{\mathcal{H}}$ and $\tilde{\mathfrak{g}}^-_{\mathcal{H}}$, correspondingly. This, evidently, is the result of the following duality, $(\tilde{\mathfrak{g}}^+_{\mathcal{H}})^*=(\tilde{\mathfrak{g}}^*_{\mathcal{H}})_-$, $(\tilde{\mathfrak{g}}^-_{\mathcal{H}})^*=(\tilde{\mathfrak{g}}^*_{\mathcal{H}})_+$.

B. Second Lie–Poisson structure and Poisson subspaces

Let us introduce into the space $\tilde{\mathfrak{g}}^*_{\mathcal{H}}$ a new Poisson brackets $\{,\}_0$, which are a Lie–Poisson brackets for the algebra $\tilde{\mathfrak{g}}^0_{\mathcal{H}}$, where $\tilde{\mathfrak{g}}^0_{\mathcal{H}}=\tilde{\mathfrak{g}}^-_{\mathcal{H}}\oplus\tilde{\mathfrak{g}}^+_{\mathcal{H}}$. Explicitly, the brackets have the following form:

$$\{l^n_{ij},l^m_{kl}\}_0=-\{l^n_{ij},l^m_{kl}\},\quad n,m>0,\quad \{l^n_{ij},l^m_{kl}\}_0=\{l^n_{ij},l^m_{kl}\},\quad n,m\leqslant 0,$$

$$\{l^n_{ij},l^m_{kl}\}_0=0,\quad m\leqslant 0,\quad n>0\quad \text{or}\quad n\leqslant 0,\quad m>0.$$

Let subspace $\mathcal{M}_{s,p}\subset\tilde{\mathfrak{g}}^*_{\mathcal{H}}$ be defined as follows:

$$\mathcal{M}_{s,p}=\sum_{m=-s+1}^{p}(\tilde{g}^*_{\mathcal{H}})_m.$$

Brackets $\{,\}_0$ could be correctly restricted to $\mathcal{M}_{s,p}$. It follows from the next Proposition:

Proposition 4: Subspaces $\mathcal{J}_{p,s}=\Sigma^{-p-1}_{m=-\infty}(\tilde{\mathfrak{g}}_{\mathcal{H}})_m+\Sigma^{\infty}_{m=s}(\tilde{\mathfrak{g}}_{\mathcal{H}})_m$ are ideals in $\tilde{\mathfrak{g}}^0_{\mathcal{H}}$.

Proof follows from the explicit form of commutation relations in $\tilde{\mathfrak{g}}^0_{\mathcal{H}}$.

Now we are ready to prove the following important theorem:

Theorem 3: *Functions $\{I^k_m(L)\}$ commutes with respect to the restriction of the brackets $\{,\}_0$ on $\mathcal{M}_{s,p}$.*

Proof: It follows from the combination of Kostant–Adler scheme and previous Proposition. Indeed, due to the fact that $\{I^k_m(L)\}$ are Casimir functions on $\tilde{\mathfrak{g}}^*_{\mathcal{H}}$ they form a commutative

subalgebra with respect to the brackets $\{,\}_0$ (see Ref. 4). Hence they will stay commutative after the restriction to $\mathcal{M}_{s,p}=(\tilde{\mathfrak{g}}^0_{\mathcal{H}}/\mathcal{J}_{p,s})^*$, due to the fact, that projection onto quotient algebra is a canonical homomorphism. That proves the theorem.

C. Hamiltonian systems

We will consider Hamiltonian systems on $\mathcal{M}_{s,p}$ of the following form:

$$\frac{dl^k_{ij}}{dt}=\{l^k_{ij},H(l^m_{kl})\}_0, \tag{16}$$

where the Hamiltonian H is one of the functions I^k_m or their linear combination. These equations could be written in the Lax pair form (Ref. 4),

$$\frac{dL(w)}{dt}=[L(w),M(w)], \tag{17}$$

where $L(w)\in\mathcal{M}_{s,p}$, and the second operator is defined as follows: $M(w)=(P_- - P_+)\nabla H(L(w))$. Here $P_\pm$ are projection operators on the subalgebra $\tilde{\mathfrak{g}}^\pm_{\mathcal{H}}$,

$$\nabla H(L(w))=\sum_{k=-p}^{s-1}\sum_{ij=1}^{n}\frac{\partial H}{\partial l^k_{ij}}X^{-k}_{ij} \tag{18}$$

is an algebra-valued gradient of H.

Thus we have achieved our initial goal of constructing Hamiltonian systems admitting the Lax pair representation with the hyperelliptic spectral parameter and possessing a large number of mutually commuting (see Theorem 3) integrals of motion. In the next section we will consider several important examples.

VI. INTEGRABLE SYSTEMS IN FINITE-DIMENSIONAL QUOTIENTS

The most interesting examples from the physical point of view usually arises in the spaces $\mathcal{M}_{s,p}$ with small s and p. We will consider the case $|s+p|\leqslant 2$. We will assume that curve $\mathcal{H}$ is nondegenerated, i.e., $a_i\neq a_j$ for $i\neq j$. This requirement is necessary for completeness of the family of constructed commuting functions.

The basic algebra in all examples will be $\mathfrak{g}=\mathrm{so}(n)$, but analogous results are valid for $\mathfrak{g}=\mathrm{gl}(n)$ and $\mathfrak{g}=\mathrm{sp}(n)$. We chose for all examples the $\mathrm{so}(n)$ algebra because correspondent integrable systems are the most direct generalizations of classical integrable systems connected with so(3), so(4), and e(3).

A. Hyperelliptic Lax representation for the generalized Euler tops

Let us consider subspace $\mathcal{M}_{0,1}$. It is evident that $\mathcal{M}_{0,1}=(\tilde{\mathfrak{g}}^+_{\mathcal{H}}/\mathcal{J}_{1,0})^*=\mathfrak{g}^*$. The corresponding Lax operator $L(w)\in\mathcal{M}_{0,1}$ has the following form:

$$L(w)=w\sum_{i,j=1,n}l^{(1)}_{ij}\frac{y(w)}{w_iw_j}X^*_{ij}.$$

Let us consider the most interesting case $\mathfrak{g}=\mathrm{so}(n)$. In this case we have, $X^*_{ij}=X_{ij}$, $l^{(1)}_{ji}=-l^{(1)}_{ij}$. Lie–Poisson brackets between the coordinate functions $l^{(1)}_{ij}$ have the standard form,

$$\{l^{(1)}_{ij},l^{(1)}_{kl}\}=\delta_{kj}l^{(1)}_{il}-\delta_{il}l^{(1)}_{kj}+\delta_{jl}l^{(1)}_{ki}-\delta_{ki}l^{(1)}_{jl}.$$

Commuting integrals are constructed using expansions in the powers of w of the functions, $I_k(w)=\mathrm{Tr}(L(w))^k$. We are especially interested in the quadratic Hamiltonians. Let

$$h(w)\equiv I_2(w)=\sum_{s=2}^{n} h_s(l_{ij}^{(1)})w^s=w^2\sum_{ij}\left(\prod_{k\neq i,j}(w-a_k)\right)(l_{ij}^{(1)})^2.$$

We obtain

$$h_2=\left(\prod_k a_k\right)\sum_{i,j=1}^{n}\frac{(l_{ij}^1)^2}{a_ia_j},$$

$$\cdots$$

$$h_{n-1}=\sum_{i,j=1}^{n}\left(\sum_{k=1}^{n} a_k-(a_i+a_j)\right)(l_{ij}^{(1)})^2,$$

$$h_n=\sum_{i,j=1}^{n}(l_{ij}^{(1)})^2.$$

The last function in this set is a Casimir function, previously $n-1$ defined the nontrivial flows on each coadjoint orbit in $\mathfrak{g}^*$. For the Hamiltonian of the generalized rigid body we take $H(l_{ij}^{(1)})\equiv 1/2h_{n-1}(l_{ij}^{(1)})$. Equations of motion are

$$\frac{dL(w)}{dt}=[L(w),M(w)],$$

where the M operator has the following form:

$$M(w)=\sum_{ij}\left(\sum_{k=1}^{n} a_k-(a_i+a_j)\right)l_{ij}^{(1)}w^{-1}w_iw_jX_{ij}.$$

To show explicitly, that this is indeed a generalization of the ordinary rigid body case, and we will consider the standard so(3) case:

Example 4: Let $n=3$, i.e., $\mathfrak{g}=\mathrm{so}(3)$ and corresponding curve $\mathcal{H}$ is elliptic. Let us pass to the variables $l_k=\epsilon_{ijk}l_{ij}^{(1)}$ which are dual to the standard basis $X_k=\epsilon_{ijk}X_{ij}$ in the algebra so(3) and obtain the standard Lie brackets for coordinates of the momentum vector. In this case we have two independent integrals—Casimir function and Hamiltonian,

$$h_3=\sum_{i,j=1}^{3}(l_{ij}^{(1)})^2=\sum_{k=1}^{3}l_k^2,\quad h_2=\sum_{i,j=1}^{3}(a_1+a_2+a_3-(a_i+a_j))(l_{ij}^{(1)})^2=\sum_{k=1}^{3}a_kl_k^2.$$

It is evident that h_2 coincides with the standard rigid body (Euler top) Hamiltonian, where $a_k=I_k^{-1}$. Direct calculations give the following elliptic $L-M$ pair for Euler top:

$$L(w)=w\sum_{k=1}^{3}l_kw_kX_k,\quad M(w)=w^{-1}\sum_{k=1}^{3}a_kl_k\frac{y(w)X_k}{w_k}.$$

Correspondent Lax equations coincide with the equations of movement of the rigid body.

B. Generalized interacting tops

Let us consider subspace $\mathcal{M}_{1,1}$. In the case $a_i\neq 0$, as it follows from the arguments below, $(\tilde{\mathfrak{g}}_{\mathcal{H}}^{+}/\mathcal{J}_{1,1})\approx\mathfrak{g}\oplus\mathfrak{g}$. Hence $\mathcal{M}_{1,1}=(\mathfrak{g}\oplus\mathfrak{g})^*$. The corresponding Lax operator $L(w)\in\mathcal{M}_{1,1}$ has the following form:

$$L(w)=\sum_{i,j=1}^{n}(l_{ij}^{(0)}+wl_{ij}^{(1)})\frac{y(w)}{w_iw_j}X_{ij}^{*}.$$

Let us again consider the so(n) case and put $X_{ij}^{*}=X_{ij}$. Lie–Poisson brackets between the coordinate functions $l_{ij}^{(0)}$, $l_{ij}^{(1)}$, where $l_{ji}^{(k)}=-l_{ij}^{(k)}$, $k=0,1$, have the following form:

$$\{l_{ij}^{(0)},l_{kl}^{(0)}\}=-a_i\delta_{il}l_{kj}^{(0)}+a_j\delta_{kj}l_{il}^{(0)}-a_i\delta_{ik}l_{jl}^{(0)}+a_j\delta_{jl}l_{ki}^{(0)},$$

$$\{l_{il}^{(1)},l_{kl}^{(1)}\}=\delta_{kj}l_{il}^{(1)}-\delta_{il}l_{kj}^{(1)}+\delta_{jl}l_{ki}^{(1)}-\delta_{ki}l_{jl}^{(1)},$$

$$\{l_{ij}^{(0)},l_{kl}^{(1)}\}=0.$$

Putting $b_i=a_i^{1/2}$ and making the change of variables, $l_{ij}=l_{ij}^{(1)}$, $m_{ij}=l_{ij}^{(0)}/b_ib_j$, we obtain canonical coordinates of the direct sum of two algebras so(n),

$$\{m_{ij},m_{kl}\}=\delta_{kj}m_{il}-\delta_{il}m_{kj}+\delta_{jl}m_{ki}-\delta_{ki}m_{jl},$$

$$\{l_{ij},l_{kl}\}=\delta_{ki}l_{il}-\delta_{il}l_{kj}+\delta_{jl}l_{ki}-\delta_{ki}l_{jl},$$

$$\{l_{ij},m_{kl}\}=0.$$

Commuting integrals are constructed using expansions in the powers of w of the functions, $I_k(w)=\mathrm{Tr}(L(w))^k$. As in the previous example, we are mainly interested in the quadratic integrals. Let

$$h(w)\equiv I_2(w)=\sum_{s=0}^{n}h_s(l_{ij}^{(0)},l_{ij}^{(1)})w^s=\sum_{ij}\left(\prod_{k\neq i,j}(w-a_k)\right)(l_{ij}^{(0)}+wl_{ij}^{(1)})^2.$$

By straightforward calculations, making the described above replacement of variables we obtain

$$h_0=(-1)^{n-2}(b_1^2b_2^2\cdots b_n^2)\sum_{i,j=1}^{n}m_{ij}^2$$

$$h_1=(-1)^{n-1}\sum_{i,j=1}^{n}\left(\sum_{k\neq i,j}\frac{b_1^2b_2^2\cdots b_n^2}{b_k^2}\right)(m_{ij})^2-2\frac{b_1^2b_2^2\cdots b_n^2}{b_ib_j}m_{ij}l_{ij}$$

$$\cdots$$

$$h_{n-1}=-\sum_{i,j=1}^{n}\left(\sum_{k=1}^{n}b_k^2-(b_i^2+b_j^2)\right)l_{ij}^2-2b_ib_jm_{ij}l_{ij}$$

$$h_n=\sum_{i,j=1}^{n}(l_{ij})^2.$$

It is evident, that functions h_0 and h_n are invariants. Functions $h_1,\ldots,h_{n-1}$ generate nontrivial Hamiltonian flows. For the Hamiltonian of the generalized interacting rigid bodies we can take either h_{n-1} or h_1. Correspondent M-operator and Lax equations are calculated straightforwardly.

Example 5: Let $n=3$. In this case, making standard replacement of variables $l_i=\epsilon_{ijk}l_{ij}$, $m_i=\epsilon_{ijk}m_{ij}$ we obtain the following set of commuting functions:

$$h_0=\sum_{k=1}^{n}m_k^2,\quad h_1\left(\sum_{k=1}^{n}\left(\frac{b_1b_2b_3}{b_k^2}\right)(m_k)^2-2b_km_kl_k\right),$$

$$h_2=\sum_{i,j=1}^{n}\left(b_k^2 l_k^2-2\frac{b_1b_2b_3}{b_k}m_k l_k\right),\quad h_3=\sum_{k=1}^{n} l_k^2.$$

Here h_0, h_3, invariant functions and h_1, h_2 are two independent integrals discovered by Veselov (Ref. 12). Commutation relations between coordinates l_k and m_k of so(4) are standard,

$$\{l_i,l_j\}=\epsilon_{ijk}l_k,\ \{m_i,m_j\}=\epsilon_{ijk}m_k,\quad \{m_i l_j\}=0.$$

C. Generalized Steklov–Liapunov system

The last class of integrable systems we wish to consider here will be integrable systems that generalize classical integrable system of Steklov–Liapunov on $e(3)=so(3)+R^3$. Let us consider subspace $\mathcal{M}_{0,2}=(\tilde{\mathfrak{g}}^{+}_{\mathcal{H}}/\mathcal{J}_{2,0})^*$. It is easy to show that $\mathcal{M}_{0,2}=(\mathfrak{g}+\mathfrak{g})^*$. Corresponding Lax operator $L(w)\in\mathcal{M}_{0,2}$ has the following form:

$$L(w)=w\left(\sum_{i,j=1}^{n}(l_{ij}^{(1)}+wl_{ij}^{(2)})\frac{y(w)}{w_i w_j}X_{ij}^{*}\right).$$

We will again be concentrating on the $\mathfrak{g}=so(n)$ case and put $X_{ij}^{*}=X_{ij}$. Lie–Poisson brackets between coordinate functions $l_{ji}^{(1)}$, $l_{ji}^{(2)}$, where $l_{ji}^{(k)}=-l_{ij}^{(k)}$, $k=1,2$, are the following:

$$\{l_{ij}^{(1)},l_{ij}^{(1)}\}=\delta_{kj}l_{il}^{(1)}-\delta_{il}l_{kj}^{(1)}+\delta_{jl}l_{ki}^{(1)}-\delta_{ik}l_{jl}^{(1)}+a_i\delta_{il}l_{kj}^{(2)}-a_j\delta_{kj}l_{il}^{(2)}+a_i\delta_{ik}l_{jl}^{(2)}-a_j\delta_{jl}l_{ki}^{(2)},$$

$$\{l_{ij}^{(1)},l_{ij}^{(2)}\}=\delta_{kj}l_{il}^{(2)}-\delta_{il}l_{kj}^{(2)}+\delta_{jl}l_{ki}^{(2)}-\delta_{ik}l_{jl}^{(2)},$$

$$\{l_{ij}^{(2)},l_{ij}^{(2)}\}=0.$$

Commuting integrals are constructed using expansion in the powers of w of the functions, $I_k(w)=\mathrm{Tr}(L(w))^k$. We are again interested mainly in quadratic integrals. Let

$$h(w)\equiv I_2(w)=w^2\sum_{s=0}^{n}h_{s+2}(l_{ij}^{(1)},l_{ij}^{(2)})w^s=w^2\sum_{ij}\left(\prod_{k\neq i,j}(w-a_k)\right)(l_{ij}^{(1)}+wl_{ij}^{(2)})^2.$$

Direct calculations give

$$h_2=(-1)^{n-2}\sum_{i,j=1}^{n}\frac{a_1a_2\cdots a_n}{a_ia_j}(l_{ij}^{(1)})^2$$

$$\cdots$$

$$h_{n+1}=(-1)\left(\sum_{i,j=1}^{n}\left(\sum_{k=1}^{n}a_k-(a_i+a_j)\right)(l_{ij}^{(2)})^2-2l_{ij}^{(1)}l_{ij}^{(2)}\right),$$

$$h_{n+2}=\sum_{i,j=1}^{n}(l_{ij}^{(2)})^2.$$

Change of variables, $l_{ij}^{(1)}=l_{ij}-1/2(a_i+a_j)p_{ij}$, $l_{ij}^{(2)}=p_{ij}$ transform described above brackets to the canonical brackets on the half-direct sum $so(n)+so(n)$,

$$\{l_{ij},l_{kl}\}=\delta_{kj}l_{il}-\delta_{il}l_{kj}+\delta_{jl}l_{ki}-\delta_{ik}l_{jl},$$

$$\{l_{ij},p_{kl}\}=\delta_{kj}p_{il}-\delta_{il}p_{kj}+\delta_{jl}p_{ki}-\delta_{ik}p_{jl},$$

$$\{p_{ij},p_{kl}\}=0.$$

After such transformation we obtain the following set of Hamiltonians:

$$h_2=(-1)^{n-2}\sum_{i,j=1}^{n}\frac{a_1a_2\cdots a_n}{a_ia_j}(l_{ij}-1/2(a_i+a_j)p_{ij})^2$$

$$\cdots$$

$$h_{n+1}=(-1)\left(\sum_{k=1}^{n}a_k\right)\left(\sum_{i,j=1}^{n}p_{ij}^2\right)-2\left(\sum_{i,j=1}^{n}l_{ij}p_{ij}\right),$$

$$h_{n+2}=\sum_{i,j=1}^{n}p_{ij}^2.$$

Last two functions are invariant functions. First $n-1$ gives nontrivial flows on $\mathfrak{g}^*$. We will choose the function $H=h_2$ for the Hamiltonian function. The correspondent M operator is

$$M(w)=2\sum_{i,j=1}^{n}\frac{a_1a_2\cdots a_n}{a_ia_j}(l_{ij}-1/2(a_i+a_j)p_{ij})w^{-1}w_iw_jX_{ij}.$$

The Lax equation has the standard form (1).

Example 6: Let $n=3$. In this case, after the replacement of variables: $l_k=\epsilon_{ijk}l_{ij}$, $p_k=\epsilon_{ijk}p_{ij}$ we obtain the standard Lie–Poisson brackets on $\epsilon(3)^*$,

$$\{l_i,l_i\}=\epsilon_{ijk}l_k,\ \{l_i,p_j\}=\epsilon_{ijk}p_k,\ \{p_i,p_j\}=0,$$

and the following Hamiltonian:

$$H=(-1)^{n-2}\sum_{k=1}^{n}a_k(l_k-1/2(a_1+a_2+a_3-a_k)p_k)^2.$$

Up to the rescaling of momenta $p_i:p_i\to 2\sigma p_i$ Hamiltonian H coincides with the Hamiltonian of the Steklov–Liapunov system in the form of Kotter (Ref. 15).

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Lie algebras associated with the exponential solutions of nonautonomous linear differential equations

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A new free Lie algebra structure generated by a continuous set of operators is introduced. The Friedrichs' criterion, which is known for a finite (countable) number of generators, is extended to the continuous case. Based on Friedrichs' criterion, we obtain an explicit expression for the coefficients of the Magnus expansion, which is central for one to get approximately the exponential solutions of nonautonomous linear differential equations. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1383558]

I. INTRODUCTION

Consider the solution to the equation

$$\frac{\mathrm{d}U}{\mathrm{d}t}=H(t)u(t) \tag{1}$$

in the form

$$U(t)=\exp\Omega(t), \tag{2}$$

where $U(t)$, $H(t)$ are operators and $U(0)=I$ is the identity. The problem underlying this paper is to obtain $\Omega(t)$ in terms of the operator $H(t)$. Magnus[1] found the solution to (1) and (2) using a recursive method to express $\Omega(t)$ in the form of a series of multiple commutators[2]

$$\begin{aligned}\Omega(t)=&\int_0^t H(t_1)\mathrm{d}t_1+\frac{1}{2}\int_0^t\int_0^{t_1}[H(t_1),H(t_2)]\mathrm{d}t_1\,\mathrm{d}t_2\\&+\frac{1}{6}\int_0^t\int_0^{t_1}\int_0^{t_2}[[H(t_1),H(t_2)],H(t_3)]\mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3\\&+\frac{1}{6}\int_0^t\int_0^{t_1}\int_0^{t_2}[H(t_1),[H(t_2),H(t_3)]]\mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3+\cdots,\end{aligned} \tag{3}$$

where $[H_1,H_2]=H_1H_2-H_2H_1$ and the omitted terms are multiple integrals of the multiple commutators of H, of increasing orders. This expression is called the *Magnus expansion*. Several methods have been derived from the Magnus expansion which proved to be powerful tools for solving time-dependent problems. Those methods have been successfully applied to different fields of mathematics and physics.[2–5] Therefore, it is important to count with formulas (or efficient algorithms) to obtain the coefficients of the expansion (3). Motivated by this reason, recursive expressions for the n-order terms of the series were obtained[5–7] using different techniques. In

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particular, there are explicit formulas for the *fourth*,[5] *fifth*,[8] and sixth[9] order terms. As far as we know the only explicit formula of all orders has been given by Mielnik and Plebañski.[10] One of the objectives of this paper is to present a new formula (36)[11] for the coefficients of the Magnus expansion which results to be equivalent to the formula of Mielnik and Plebañski.

On the other hand, the Magnus expansion is the continuous analog to the *Baker–Campbell–Hausdorff formula*[12–14]

$$z=x+y+\tfrac{1}{2}[x,y]+\tfrac{1}{12}([[x,y],y]+[[y,x],x])+\cdots. \tag{4}$$

This formula is derived by writing $e^z=e^xe^y$, where x,y are elements of a noncommutative algebra. Friedrichs[15] proved that z is an element of the free Lie algebra generated by $\{x,y\}$. An interesting problem is to prove an analogous result for $\Omega(t)$, that means, is $\Omega(t)$ an element of a Lie algebra generated by $\{H(t):t\in\mathbb{R}\}$? In this paper we introduce certain algebraic structures which are useful to extend to the continuous case the most important results of the discrete case.[16] The relation between both problems is based on the following heuristic approach to the solution to problem (1) using formula (4):

Let $0=s_0<s_1<\ldots<s_n=t$ be a partition of the interval $[0,t]$. If we consider $H(t)$ constant and equal to $H(s_i)$ in the interval $[s_{i-1},s_i]$ and we define the operators

$$U_n(t)=\exp(H(s_n)\Delta s_n)\exp(H(s_{n-1})\Delta s_{n-1})\ldots\exp(H(s_1)\Delta s_1), \tag{5}$$

where $\Delta s_i=s_i-s_{i-1}$, it follows that $U_n(t)\to U(t)$ if $\max \Delta s_i\to 0$. Now, if we denote z of (4) by $x\#y$ and we use operation # in (5), we obtain that

$$U_n(t)=\exp(H(s_n)\Delta s_n\#H(s_{n-1})\Delta s_{n-1}\#\cdots\#H(s_1)\Delta s_1).$$

Observe that $\Omega_n(t)=H(s_n)\Delta s_n\#H(s_{n-1})\Delta s_{n-1}\#\cdots\#H(s_1)\Delta s_1$ is contained in the Lie algebra generated by $\{H(s_1),H(s_2),\ldots,H(s_n)\}$. Considering the limit when $n\to\infty$ or $\Delta s_i\to 0$, we have that $U(t)=\exp\Omega(t)$, where

$$\Omega(t)=\lim_{\max \Delta s_1\to 0}(H(s_n)\Delta s_n\#H(s_{n-1})\Delta s_{n-1}\#\ldots\#H(s_1)\Delta s_1).$$

Based on this heuristic idea,[10] we introduce here an adequate mathematical framework that puts the work of Magnus[1] in a precise form. To this end we extend the following results.[16] First we prove the continuous analog to *Friedrichs' criterion*. This criterion is the simplest way to decide when an element of an algebra is a *Lie element*. Once one knows that an element is a Lie element, it is easier to determine it explicitly. By the use of Friedrichs' criterion, we prove the Magnus' theorem and propose a formula (proved in Saenz and Suárez[11]) for the coefficients of the expansion (the *Magnus formula*). In this paper we concentrate on algebraic problems, however, a simple proof of the convergence of the Magnus' expansion for a sufficiently small t, provided that $H(t)$ is a local integrable and bounded operator, is included. The local convergence issue of the Magnus expansion has been treated in several papers.[4,6,17] Very few attempts have been made with respect to the global convergence problem.[1,18–21]

There are several other works where the mathematical formalization of the Magnus expansion has been addressed by considering different frameworks. Chen[22] proposed a generalization of the path integral. In particular, he proves that if a function $u(t)$ is a Lie element for every $t\in[a,b]$, then both

$$\int_a^b u(t)dt,\quad \frac{\mathrm{d}u(t)}{\mathrm{d}t}$$

are also Lie elements. However, the proof of Magnus' theorem, for that kind of path integration, is not constructive. In Huillet *et al.*[23] the authors use *grupoids* to simplify notation, but Magnus' theorem was not proved. Formula (3) was taken from Magnus,[1] since the paper is more in the direction of considering the nonstationary evolution equations as a canonical factorization into an infinite product of exponentials.[20] On the other hand, Strichartz[24] is closely related to our work. It involves an extension to the definitions considered in Jacobson[16] for the discrete case. The problem is that the obtained explicit formula is very complicated. Searching for a less computationally involved formulation, Duleba[25] introduced a method based on Hall basis. In our paper, the difference is the introduction of the ''algebras of coefficients'' (Volterra series) which give us at least two advantages: Local convergence of (3), implied by local integrability and boundedness of $H(t)$ (instead of the analyticity required in Strichartz[24]), and second, the calculation of the expansion coefficients is straightforward. We choose, as was proposed in Mielnik and Plebañski,[10] the use of ''algebras of coefficients'' instead of ''multiple commutators,'' in order to express $\Omega(t)$ as a series whose *n*-order term is given by only one multiple integral. By this way, the problem is transferred to the calculation of the series coefficients. It is worth mentioning that the *n*-order coefficient can be calculated [see formula (36)] without knowing the lower order coefficients.[10] In the other mentioned methods the terms of the expansion were calculated by a recursive algorithm.

A new and very interesting use of the Magnus expansion, initiated in Iserles and Nørsett,[6] is the solution of linear differential equations in Lie groups and homogeneous spaces. It concerns the retention of the Lie group structure by the truncated approximations of (3). For instance to solve dynamical systems which stay on a prescribed manifold or classical Hamiltonian systems.[26–28] Related to this idea, in the last few years, there has been an increasing interest in the design of efficient numerical integration techniques which preserve important qualitative properties of differential equations. It has been shown that a numerical method, based on Magnus expansions,[9,26,29–31] performs consistently better than the classical Runge–Kutta methods, especially for systems with high oscillations or complicated asymptotic behavior.[27,32,33]

As was previously mentioned, formulas (3) and (4) have been applied to different fields of mathematics and physics. For example in the theory of groups,[34–37] control theory,[23,38,39] partial differential equations,[40] nonlinear ordinary differential equations,[3,32,41] Lie groups,[6,30,42] and differential geometry.[22] In physics, they have been used in quantum mechanics, semiclassical atomic collisions theory, neutron transport, laser physics, multiphoton excitation of molecules, pulsed magnetic resonance spectra, magnetic lenses, optical lenses, plasma physics, the solar neutrino problem, high-resolution nuclear magnetic resonance spectroscopy, and Hamiltonian systems (celestial mechanics). There is an extensive list of references of applications to physics.[2–5]

The rest of the paper is organized as follows. Section II contains the preliminary definitions. In Sec. III we introduce the algebras and ordered linear spaces, which extend the definitions contained in Jacobson,[16] in order to characterize in an algebraic way the sets to which $\Omega(t)$ belongs. Section IV provides Friedrichs' criterion. In Sec. V we prove the Magnus expansion using Friedrichs' criterion, and present an application of this formula to the determination of the uniform exponential stability of a nonautonomous linear systems. Finally, Appendices A and B include the proofs of the main results.

II. PRELIMINARIES

Let F be the field of real or complex numbers ($\mathbb{R}$ or $\mathbb{C}$, respectively) and S_n be the group of permutations of order n.

Definition 1: The algebra of permutations of n elements, FS_n, *is the set of formal sums of the form:*

$$\sum_{i=1}^{n!} r_i \sigma_i ,$$

where $r_i \in F$, $\sigma_i \in S_n$, *and* $\sigma_j \neq \sigma_k$ *if* $j \neq k$.

The operations of addition, product, and multiplication by a scalar give to FS_n the structure of an associative algebra with unit over F. The identity of FS_n is the identity permutation of S_n which we denote by 1.

Now, let X be a linear space over F, and let $t>0$ and $n\in\mathbb{N}$. We denote by $\mathfrak{F}(T^n,X)$ the linear space of integrable functions a: $T^n\subset\mathbb{R}^n\to X$, where $T=[0,t]$. Each permutation $\sigma\in S_n$ can be identified with the following linear operator over $\mathfrak{F}(T^n,X)$:

$$\sigma a(t_1,\ldots,t_n)=a(t_{\sigma(1)},\ldots,t_{\sigma(n)}). \tag{6}$$

Defining $(\sigma_1\sigma_2)a=\sigma_1(\sigma_2 a)$, the rule (6) agrees with the evaluation of the product of two permutations from right to left. The rule (6) extends to the elements of FS_n linearly in the following way: If $a\in\mathfrak{F}(T^n,X)$, then

$$\left(\sum_{i=1}^{n!} r_i\sigma_i\right)a=\sum_{i=1}^{n!} r_i\sigma_i a.$$

Let us define two special elements D_n and E_n of FS_n:

$$D_n=\frac{1}{n}(1-C_{1,2})(1-C_{1,3})\ldots(1-C_{1,n}) \tag{7}$$

and

$$E_n=\frac{1}{n}(1-C_{1,n}^{-1})(1-C_{1,n-1}^{-1})\ldots(1-C_{1,2}^{-1}), \tag{8}$$

where 1 denotes the identity permutation and $C_{1,k}$ is the following cyclic permutation in S_n:

$$C_{1,k}=\begin{pmatrix}1 & 2 & \ldots & k-1 & k\\ k & 1 & \ldots & k-2 & k-1\end{pmatrix}. \tag{9}$$

In particular, if B is an associative algebra over F, with $\mathcal{H}\in\mathfrak{F}(T^n,B)$ and $\mathcal{H}(t_1,\ldots,t_n)=H(t_1)\ldots H(t_n)$, we have that D_n corresponds to the next Lie array:[10]

$$D_n(\mathcal{H}(t_1,\ldots,t_n))=D_n(H(t_1)\ldots H(t_n))=\frac{1}{n}[\ldots[[H(t_1),H(t_2)],H(t_3)],\ldots,H(t_n)], \tag{10}$$

where $[H_1,H_2]=H_1H_2-H_2H_1$. As we can see, nD_n corresponds to the linear transformation $\mathcal{O}$ given in Jacobson[16] for the discrete case. The most important property of the objects D_n and E_n is that they are idempotent, that is,

$$D_n^2=D_n \tag{11}$$

and

$$E_n^2=E_n. \tag{12}$$

A proof for (11) is outlined in Magnus *et al.*[43]

Let $N_n(t)$ be the commutative algebra over F of the functions of $\mathfrak{F}(T^n,F)$ which are zero almost everywhere in $T^n=[0,t]^n$. It is easy to prove that

$$FS_n(N_n(t))=N_n(t).$$

In particular

$$E_n(N_n(t))\subset N_n(t). \tag{13}$$

III. ALGEBRAS AND ORDERED LINEAR SPACES OF CONTINUOUS RANGE

Definition 2: Let $A_n(t)$ be a linear subspace of the Banach space $\mathcal{L}_p$ of functions defined in $T^n=[0,t]^n$ with values in F. For $n=0$, $A_0(t)=F$. The set of infinite sequences

$$A(t)=\prod_{n=0}^{\infty} A_n(t)=\{\{a_n\}_{n=0}^{\infty}:a_n\in A_n(t)\}$$

is called an algebra of coefficients *if it satisfies.*

(1) For every $\sigma\in S_n$ and $a\in A_n(t)$, we have that $\sigma a\in A_n(t)$.

(2) Given $a\in A_k(t)$ and $b\in A_m(t)$, the function $a\circ b$ is an element of $A_{k+m}(t)$, where

$$(a\circ b)(t_1,\ldots,t_{k+m})=a(t_1,\ldots,t_k)b(t_{k+1},\ldots,t_{k+m}). \tag{14}$$

The algebraic operations in $A(t)$ are defined in the following way: Let, $a,b\in A(t)$, $a=\{a_n\}_{n=0}^{\infty}$, $b=\{b_n\}_{n=0}^{\infty}$, with a_n, $b_n\in A_n(t)$, and $\alpha\in F$, then

$$a+b=\{a_n+b_n\}_{n=0}^{\infty},$$

$$\alpha a=\{\alpha a_n\}_{n=0}^{\infty},$$

$$ab=\{c_n\}_{n=0}^{\infty},$$

where $c_n=\Sigma_{k=0}^{n} a_k\circ b_{n-k}$. As it is easy to prove, the defined operations are closed in $A(t)$.

Proposition 3: $A(t)$ is an associative algebra with unit over F.

Since $A_n(t)\subset\mathcal{L}_p$, we understand that equality (14) is considered among elements in $\mathcal{L}_p$, that is, (14) is verified almost everywhere in T^n. This convention will follow from now on.

Example 4: If $A_n(t)$ is the linear space of continuous real functions of n variables, then $A(t)=\Pi_{n=0}^{\infty}A_n(t)$ satisfies conditions 1 and 2 of definition 2, thus it is an algebra of coefficients. The concept of algebra of coefficients is used in the definition of Volterra series which are frequently applied to the solution of Control problems.[44]

The next definition is motivated by (13).

Definition 5: Let $n\geqslant 2$. An element $a\in A_n(t)$ is called an ordered coefficient of degree *n if*

$$E_n a=a, \tag{15}$$

where E_n is given by (8).

In the finite case, as a consequence of the Dynkin–Specht–Wever's theorem,[16] Eq. (15) is satisfied by any Lie element.

Example 6: If $a(t_1,t_2)=t_1-t_2\in A_2(t)$, then $a(t_1,t_2)$ is an ordered coefficient of degree two:

$$E_2(a(t_1,t_2))=(\tfrac{1}{2}(1-C_{1,2}^{-1}))a(t_1,t_2)=\tfrac{1}{2}(a(t_1,t_2)-a(t_2,t_1))$$
$$=\tfrac{1}{2}(t_1-t_2-(t_2-t_1))=t_1-t_2=a(t_1,t_2).$$

But not necessarily every element of $A_2(t)$ *must be an ordered coefficient, for example,* $b(t_1,t_2)=t_1+t_2\in A_2(t)$ *is not an ordered coefficient of degree two:*

$$E_2(b(t_1,t_2))=(\tfrac{1}{2}(1-C_{1,2}^{-1}))b(t_1,t_2)=\tfrac{1}{2}b((t_1,t_2)-b(t_2,t_1))=\tfrac{1}{2}(t_1+t_2-(t_2+t_1))=0.$$

Denote by $\Lambda_n(t)$ the set of ordered coefficients of degree n in $A_n(t)$ for $n\geqslant 2$. Note that $\Lambda_n(t)$ is a linear subspace of $A_n(t)$. This is deduced from the fact that $E_n^2=E_n$ by (12), and therefore $\Lambda_n(t)=E_n(A_n(t))$.

Definition 7: The ordered linear space $\Lambda(t)$ *is the set of infinite sequences* $\Pi_{n=0}^{\infty}\Lambda_n(t)$, *with* $\Lambda_0(t)=\{0\}$ *and* $\Lambda_1(t)=A_1(t)$. *Every element of* $\Lambda(t)$ *is called a* sequence of ordered coefficients.

Observe that $\Lambda(t)$ is a linear subspace of $A(t)$. Now, let us define the operator $E:A(t)\rightarrow A(t)$ as the linear transformation such that, if $a=\{a_n\}_{n=0}^{\infty}$, we have that

$$E(a)=\{b_n\}_{n=0}^{\infty}, \tag{16}$$

where $b_0=0$, $b_1=a_1$, and $b_n(t_1,\ldots,t_n)=E_n(a_n(t_1,\ldots,t_n))$ for $n\geqslant 2$.

By the definition of a sequence of ordered coefficients and the fact that $E_n^2=E_n$ we obtain the next Proposition.

Proposition 8: The operator E is a projection, that is $E^2=E$, *and the range of E is equal to* $\Lambda(t)$.

The operator E is an *ordering operator*; this means that E forces the elements of the algebra $A(t)$ to acquire the structure of a sequence of ordered coefficients. The concept of ordering operator, as well as the analysis of other examples, can be found in Mielnik and Plebañski.[10]

Let G be a Hilbert space over the field F and A be the algebra of continuous operators over G, that is, A is the algebra of continuous linear transformations from the linear space G into itself. Following Jacobson,[16] let us define the free algebra $\mathcal{A}=F\oplus A\oplus(A\otimes A)\oplus\ldots$ and its extension to the formal series $\overline{\mathcal{A}}$, where $\oplus$ denotes the direct sum of linear spaces. The algebras $\mathcal{A}$ and $\overline{\mathcal{A}}$ are associative algebras with unit. To avoid any confusion between the usual product of operators defined in A with the free product given in the last two algebras we denote this last product by $\odot$. The problem of convergence of series in $\overline{\mathcal{A}}$ can be addressed using valuations.[16] Since G is a Hilbert space, it has a norm associated with its inner product. On the other hand, this norm allows us to define a standard norm in the algebra of operators A. This norm induces, in the natural way, a norm in the homogeneous spaces[45] $A\otimes\ldots\otimes A$. Let then $H:\mathbb{R}\rightarrow A$ be a continuous function which becomes zero only in a finite set of points of the interval $T=[0,t]$. It follows that every product of the form $H(t_1)\odot\ldots\odot H(t_n)$ is a continuous function of n variables. If we take $a_n\in A_n(t)$, we obtain that the function of n real variables $a_n(t_1,\ldots,t_n)H(t_1)\odot\ldots\odot H(t_n)$ is integrable over $T^n=[0,t]^n$. Therefore the integral

$$\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n \tag{17}$$

is defined and it is a homogeneous element of degree n in $\overline{\mathcal{A}}$.

With all these considerations we formulate the following

Definition 9: The algebra of continuous range $\mathcal{A}(t)$ *is the subset of* $\overline{\mathcal{A}}$ *whose elements can be given in the form*

$$a_0+\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n, \tag{18}$$

where $\{a_n\}_{n=0}^{\infty}\in A(t)$.

It is not difficult to see that $\mathcal{A}(t)$ is a subalgebra of $\overline{\mathcal{A}}$. In particular, the multiplication, defined by (14), is closed in $\mathcal{A}(t)$.

Let us define the function $\Phi: A(t) \to \mathcal{A}(t)$, for $a = \{a_n\}_{n=0}^{\infty} \in A(t)$, by

$$\Phi(a) = a_0 + \sum_{n=1}^{\infty} \int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) H(t_1) \odot \ldots \odot H(t_n) \mathrm{d}t_1 \ldots \mathrm{d}t_n . \tag{19}$$

Φ is an epimorphism between associative algebras with unit.

Note that, since H is continuous and null only on a finite set of points of $[0,t]$ then, if for every $s \in (0,t]$ it occurs that

$$\int_0^s \cdots \int_0^s a_n(t_1,\ldots,t_n) H(t_1) \odot \ldots \odot H(t_n) \mathrm{d}t_1 \ldots \mathrm{d}t_n = 0,$$

necessarily $a_n = 0$ (in $\mathcal{L}_p$). Hence, every element of $\mathcal{A}(t)$ is uniquely determined by the series (18). As Φ is an epimorphism between $A(t)$ and $\mathcal{A}(t)$, we have the following Proposition.

Proposition 10: $A(t)$ and $\mathcal{A}(t)$ are isomorphic as associative algebras with unit. The isomorphism is given by Φ.

Definition 11: The ordered linear space of continuous range $\Gamma(t)$ *is the subset of elements of $\mathcal{A}(t)$ written in the form*

$$\sum_{n=1}^{\infty} \int_0^t \cdots \int_0^t u_n(t_1,\ldots,t_n) H(t_1) \odot \ldots \odot H(t_n) \mathrm{d}t_1 \ldots \mathrm{d}t_n ,$$

where $\{u_n\}_{n=0}^{\infty} \in \Lambda(t)$ (note that $u_0 = 0$). Every element of $\Gamma(t)$ is called an ordered element.

Since $\Gamma(t) = \Phi(\Lambda(t))$, $\Gamma(t)$ is a linear subspace of $\mathcal{A}(t)$.

Remark 1: Every ordered element can be rewritten in the following way:

$$\int_0^t u_1(t_1) H(t_1) \mathrm{d}t_1 + \sum_{n=2}^{\infty} \frac{1}{n} \int_0^t \cdots \int_0^t u_n(t_1,\ldots,t_n) [\ldots[H(t_1),H(t_2)],\ldots,H(t_n)] \mathrm{d}t_1 \ldots \mathrm{d}t_n$$

(the Lie product $[\cdot]$ is defined with respect to the free product $\odot$). This is a consequence of the next equation that is satisfied by any ordered coefficient a_n,

$$\int_0^t \cdots \int_0^T a_n(t_1,\ldots,t_n) H(t_1) \odot \ldots \odot H(t_n) \mathrm{d}t_1 \ldots \mathrm{d}t_n = \frac{1}{n} \int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) \times [\ldots[[H(t_1),H(t_2)],H(t_3)],\ldots,H(t_n)] \mathrm{d}t_1 . \tag{20}$$

The proof of Eq. (20) follows by reordering the indexes of a_n, using the *Fubini's Theorem*, and transferring the permutations to the products of the operator H in the following way

$$\int_0^t \cdots \int_0^t a_n(t_1,\ldots t_n) H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n$$

$$= \int_0^t \cdots \int_0^t E_n(a_n(t_1,\ldots,t_n)) H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n$$

$$= \frac{1}{n}\int_0^t \cdots \int_0^t \left(\left(\prod_{k=2}^{n} (1-C_{1,n-k+2}^{-1}) \right)(a_n(t_1,\ldots,t_n)) \right) H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n$$

$$= \frac{1}{n}\int_0^t \cdots \int_0^t \left(\left(1+\sum_{i=2}^{n} (-1)^{i-1} \sum_{n\geqslant j_{i-1}>\ldots>j_1\geqslant 2} C_{1,j_{i-1}}^{-1}\ldots C_{1,j_1}^{-1} \right)(a_n(t_1,\ldots,t_n)) \right)$$
$$\times H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n$$

$$= \frac{1}{n}\int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n$$
$$+ \frac{1}{n}\sum_{i=2}^{n} (-1)^{i-1} \sum_{n\geqslant j_{i-1}>\ldots>j_1\geqslant 2} \int_0^t \cdots \int_0^t (C_{1,j_{i-1}}^{-1}\cdots C_{1,j_1}^{-1}(a_n(t_1,\ldots,t_n)))$$
$$\times H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n.$$

$$= \frac{1}{n}\int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n$$
$$+ \frac{1}{n}\sum_{i=2}^{n} (-1)^{i-1} \sum_{n\geqslant j_{i-1}>\ldots>j_1\geqslant 2} \int_0^t \cdots \int_0^t C_{1,j_1}\ldots C_{1,j_{i-1}}((C_{1,j_{i-1}}^{-1}\ldots C_{1,j_1}^{-1}(a_n(t_1,\ldots,t_n)))$$
$$\times H(t_1)\odot\ldots\odot H(t_n))\mathrm{d}t_1\ldots\mathrm{d}t_n$$

$$= \frac{1}{n}\int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n$$
$$+ \frac{1}{n}\sum_{i=2}^{n} (-1)^{i-1} \sum_{2\leqslant j_1<\ldots<j_{i-1}\leqslant n} \int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n)$$
$$\times (C_{1,j_1}\ldots C_{1,j_{i-1}}(H(t_1)\odot\ldots\odot H(t_n)))\mathrm{d}t_1\ldots\mathrm{d}t_n$$

$$= \int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) \left(\frac{1}{n} \left(1+\sum_{i=2}^{n} (-1)^{i-1} \sum_{2\leqslant j_1<\ldots<j_{i-1}\leqslant n} C_{1,j_1}\ldots C_{1,j_{i-1}} \right) \right.$$
$$\left. \times (H(t_1)\odot\ldots\odot H(t_n)) \right) \mathrm{d}t_1\ldots\mathrm{d}t_n$$

$$= \int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) \left(\left(\frac{1}{n}\prod_{k=2}^{n} (1-C_{1,k}) \right)(H(t_1)\odot\ldots\odot H(t_n)) \right) \mathrm{d}t_1\ldots\mathrm{d}t_n$$

$$= \frac{1}{n}\int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n)[\ldots[[H(t_1),H(t_2)],H(t_3)],\ldots,H(t_n)]\mathrm{d}t_1\ldots\mathrm{d}t_n. \qquad \square$$

Finally we consider convergence problems in the algebra of operators A. We propose the following definitions.

Definition 12: The algebra of convergent coefficients $\mathfrak{A}(t)$ *is the set of elements* $a=\{a_n\}_{n=0}^{\infty}\in A(t)$ *such that the series*

$$a_0 I+\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)H(t_1)\ldots H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n \tag{21}$$

converges absolutely in A, where I is the identity operator.

$\mathfrak{A}(t)$ is a subalgebra of $A(t)$. The Cauchy product of two series provides the closure of the product in $\mathfrak{A}(t)$.

Let us consider now the function $\Xi:\mathfrak{A}(t)\to A$, defined for $a=\{a_n\}_{n=0}^{\infty}\in\mathfrak{A}(t)$, by

$$\Xi(a)=a_0 I+\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)H(t_1)\ldots H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n\,. \tag{22}$$

Definition 13: The linear space of convergent ordered coefficients $\mathfrak{L}(t)$ *is defined as* $\mathfrak{L}(t)=\Lambda(t)\cap\mathfrak{A}(t)$; *that is, the sequences of ordered coefficients such that the series* (21) *converges absolutely in A. Every element of* $\mathfrak{L}(t)$ *is called a* sequence of convergent ordered coefficients.

As an example of a coefficients algebra we introduce the finite dimensional coefficients algebra which will be used in order to obtain a formula for the coefficients of the Magnus expansion.

Let us define the step function

$$\overline{\theta}(\tau)=\begin{cases}1 & \text{if } \tau>0\\ 0 & \text{if } \tau\leqslant 0\end{cases}$$

and the functions of n variables

$$\theta_{i,j}(t_1,\ldots,t_n)=\overline{\theta}(t_i-t_j), \tag{23}$$

for $1\leqslant i,j\leqslant n$, with $i\neq j$. Notice that $\theta_{i,j}=1-\theta_{j,i}$ almost everywhere in $\mathbb{R}^n$. Establish the functions

$$\theta^n_{\mathbf{i},\mathbf{j}}(t_1,\ldots,t_n)=\theta_{i_1,j_1}\ldots\theta_{i_k,j_k},$$

where $\mathbf{i}=(i_1,\ldots,i_k)$ and $\mathbf{j}=(j_1,\ldots,j_k)$, with $1\leqslant k\leqslant n-1$, and the indexes (i_p,j_p) are ordered in the lexicographic sense. Also, let $\Theta^n_1(t_1,\ldots,t_n)=1$. Define $A^f_n(t)$ as the linear subspace of the linear space $\mathcal{L}_p$ over $\mathbb{R}$ generated by the restrictions of Θ^n_1 and $\theta^n_{\mathbf{i},\mathbf{j}}$ to T^n. The multiplication between elements of $A^f_n(t)$ and $A^f_m(t)$ is defined in the same way as in (14), that is, it is defined for $\theta^n_{\mathbf{i},\mathbf{j}}\in A^f_n(t)$ and $\theta^m_{\mathbf{i}',\mathbf{j}'}\in A^f_m(t)$ as

$$\theta^n_{\mathbf{i},\mathbf{j}}\circ\theta^m_{\mathbf{i}',\mathbf{j}'}=\theta^{n+m}_{\mathbf{i}'',\mathbf{j}''}\,,$$

where $\mathbf{i}''=(i_1,\ldots,i_k,n+i'_1,\ldots,n+i'_r)$ and $\mathbf{j}''=(j_1,\ldots,j_k,n+j'_1,\ldots,n+j'_r)$. Now, the product extends linearly.

Note that $A^f_n(t)$ is a finite dimensional linear space. The coefficients algebra $\Pi_{n=0}^{\infty}A^f_n(t)$ is called the *finite dimensional coefficients algebra* and it is denoted by $A^f(t)$. Associated with this coefficients algebra we denote by $\Lambda^f_n(t)$, $\Lambda^f(t)$, $\mathcal{A}^f(t)$, $\Gamma^f(t)$, $\mathfrak{A}^f(t)$, and $\mathfrak{L}^f(t)$ the remainder linear spaces. Since $\Lambda^f_n(t)\subset A^f_n(t)$, then $\Lambda^f_n(t)$ is finite dimensional.

IV. FRIEDRICHS' CRITERION

Following Jacobson (Ref. 16), let us take the tensor product of the algebra $\mathcal{A}$ with itself, that is, $\mathcal{A}\otimes\mathcal{A}$ and its associated formal algebra $\overline{\mathcal{A}\otimes\mathcal{A}}$. The elements of $\overline{\mathcal{A}\otimes\mathcal{A}}$ are of the form

$$\sum_{n=0}^{\infty}\sum_{m=0}^{\infty} d_{m,n-m}, \tag{24}$$

where $d_{m,m-n}=c_{n,m}(a_m\otimes b_{n-m})$, with $c_{n,m}\in F$, and a_m, b_{n-m} are homogeneous elements of $\mathcal{A}$ of degrees m and $n-m$, respectively. If the element $d_{i,j}$ is not null, we call it a *homogeneous element of degree* (i,j). It follows immediately that every element of $\overline{\mathcal{A}\otimes\mathcal{A}}$ can be written, in a unique form, as a series (24) of homogeneous elements of different degrees (i,j). The free product given in $\overline{\mathcal{A}}$ will be related to the new product given in $\overline{\mathcal{A}\otimes\mathcal{A}}$ in the usual way, that is, if $\alpha,\beta,\gamma,\delta$ are in $\overline{\mathcal{A}}$ one obtains

$$(\alpha\odot\beta)\otimes(\gamma\odot\delta)=(\alpha\otimes\gamma)\odot(\beta\otimes\delta).$$

Remark 2: Taking advantage of the tensor notation let us consider the subalgebra $\mathcal{A}(t)\otimes\mathcal{A}(t)$ *of* $\overline{\mathcal{A}\otimes\mathcal{A}}$ *as the algebra whose elements can be written in the following form*:

$$\begin{aligned}
&a_{0,0}(1\otimes 1)+\int_0^t a_{1,0}(t_1)(H(t_1)\otimes 1)\mathrm{d}t_1+\int_0^t a_{0,1}(t_1)(1\otimes H(t_1))\mathrm{d}t_1)\\
&\quad+\sum_{n=2}^{\infty}\Bigg(\int_0^t\cdots\int_0^t a_{n,0}(t_1,\ldots,t_n)((H(t_1)\odot\ldots\odot H(t_n))\otimes 1)\mathrm{d}t_1\ldots\mathrm{d}t_n\\
&\quad+\sum_{m=1}^{n-1}\int_0^t\cdots\int_0^t a_{n,m}(t_1,\ldots,t_n)(H(t_1)\odot\ldots\odot H(t_{n-m}))\otimes(H(t_{n-m+1})\odot\ldots\odot H(t_n))\mathrm{d}t_1\ldots\mathrm{d}t_n\\
&\quad+\int_0^t\cdots\int_0^t a_{n,n}(t_1,\ldots,t_n)(1\otimes(H(t_1)\odot\ldots\odot H(t_n)))\mathrm{d}t_1\ldots\mathrm{d}t_n\Bigg),
\end{aligned}\tag{25}$$

with $a_{n,m}\in A_n(t)$. *Note that every integral of* (25) *is a homogeneous element of degree* $(n-m,m)$. □

For $a=\{a_n\}_{n=0}^{\infty}$ in $A(t)$ let the function $\Phi':A(t)\to\mathcal{A}(t)\otimes\mathcal{A}(t)$ be defined by

$$\begin{aligned}
\Phi'(a)=a_0(1\otimes 1)+\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)(H(t_1)\otimes 1+1\otimes H(t_1))\odot\ldots\odot(H(t_n\otimes 1+1\\
\otimes H(t_n))\mathrm{d}t_1\ldots\mathrm{d}t_n.
\end{aligned}$$

It is easy to prove that Φ' is a homomorphism between associative algebras with unit.

Finally, we define $\Delta:\mathcal{A}(t)\to\mathcal{A}(t)\otimes\mathcal{A}(t)$ as the homomorphism that makes the following chart commutative:

$$\begin{array}{ccc}
A(t) & \overset{\Phi^{-1}}{\underset{\Phi}{\leftrightarrows}} & \mathcal{A}(t)\\
& \searrow_{\Phi'} & \vdots\Delta\\
& & \mathcal{A}(t)\otimes\mathcal{A}(t).
\end{array}$$

Another way to define Δ is $\Delta=\Phi'\circ\Phi^{-1}$ ($\circ$ denotes composition). Even more concretely,

$$\Delta\left(a_0+\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n\right)$$

$$=a_0(1\otimes 1)+\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)(H(t_1)\otimes 1+1\otimes H(t_1))$$

$$\odot\ldots\odot(H(t_n)\otimes 1+1\otimes H(t_n))\mathrm{d}t_1\ldots\mathrm{d}t_n. \tag{26}$$

Observe that Δ is a homomorphism between associative algebras with unit, because it is the composition of Φ' and Φ^{-1}. On the other hand, Δ is the continuous analog to the *diagonal map* defined in Ref. 16.

We finish this section by presenting Friedrichs' criterion, which is the continuous extension to Friedrichs' theorem.[16]

Theorem 14: *(Friedrichs' criterion). An element α of $\mathcal{A}(t)$ is in $\Gamma(t)$, that is, α is an ordered element, if and only if $\Delta\alpha=\alpha\otimes 1+1\otimes\alpha$.*

See the proof in Appendix B.

V. MAGNUS EXPANSION

Let us define, given an element x of $\overline{\mathcal{A}}$ or $\overline{\mathcal{A}\otimes\mathcal{A}}$, the series

$$\exp x=e+x+\frac{x^2}{2!}+\cdots+\frac{x^n}{n!}+\cdots$$

and

$$\log(e+x)=x-\frac{x^2}{2}+\frac{x^3}{3}-\cdots+(-1)^{n+1}\frac{x^n}{n}+\cdots, \tag{27}$$

where e represents the identity element. Remember that if x is in the bilateral ideal $\overline{\mathcal{A}^{(1)}}=\overline{A\oplus(A\otimes A)\oplus\ldots}$, then $\exp x$ and $\log(1+x)$ converge, that is, they are elements of $\overline{\mathcal{A}}$. For convergent cases we have the identities $\exp(\log(1+x))=1+x$ and $\log(\exp x)=x$; furthermore, if $x\odot y=y\odot x$, then $\exp x\odot\exp y=\exp(x+y)$ and $\log((1+x)\odot(1+y))=\log(1+x)+\log(1+y)$.

In the following we are interested primarily in the log series. In order to apply the identities presented before, we will consider only convergent series. For the elements of $\mathcal{A}(t)$, written of the form $1+\beta$ with β in $\mathcal{A}(t)^{(1)}=\mathcal{A}(t)\cap\overline{\mathcal{A}^{(1)}}$, it gives a very important case of convergence in $\mathcal{A}(t)$ under the series log which will be examined in the sequel.

Proposition 15: For every α in $\mathcal{A}(t)$ given in the form

$$\alpha=1+\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n,$$

we have that $\log\alpha$ *is an element of* $\mathcal{A}(t)$.

Proof: Denote $\beta=\alpha-1$ by

$$\beta=\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t b_{1,n}(t_1,\ldots,t_n)H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n,$$

where $b_{1,n}=a_n$ for every $n\geqslant 1$. The successive powers of β are given by the following expression:

$$\beta^m=\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t b_{m,n}(t_1,\ldots,t_n)H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n.$$

Thus β^m are elements of $\mathcal{A}(t)$. Note that the homogeneous component of lowest degree in β^m must be at least of degree m. Therefore, by (27), we have that $\log \alpha$ is given by

$$\log \alpha = \sum_{n=1}^{\infty} \int_0^t \cdots \int_0^t \left(\sum_{m=1}^{n} \frac{(-1)^{m+1}}{m} b_{m,n}(t_1,\ldots,t_n) \right) H(t_1) \odot \ldots \odot H(t_n) \mathrm{d}t_1 \ldots \mathrm{d}t_n ,$$

which is an element of $\mathcal{A}(t)$ as we wanted to prove. ■

Since Δ is a homomorphism between associative algebras with unit, we have that, if $\log \alpha \in \mathcal{A}(t)$, then

$$\Delta(\log \alpha) = \log(\Delta \alpha). \tag{28}$$

Until now we have considered t fixed. Nevertheless, it is useful to consider the elements of $\mathcal{A}(t)$ and $\mathcal{A}(t) \otimes \mathcal{A}(t)$ as functions of t. Hence, we define the derivative with respect to t of α, $\mathrm{d}\alpha/\mathrm{d}t$, as the derivative of each element. This derivative is not necessarily an element of $\mathcal{A}(t)$ or $\mathcal{A}(t) \otimes \mathcal{A}(t)$, but certainly it is in $\overline{\mathcal{A}}$ or in $\overline{\mathcal{A} \otimes \mathcal{A}}$, respectively. Finally, the derivative of the tensor product of two elements $\alpha(t)$ and $\beta(t)$ of $\mathcal{A}(t)$ is given by the rule

$$\frac{\mathrm{d}}{\mathrm{d}t}(\alpha(t) \otimes \beta(t)) = \frac{\mathrm{d}}{\mathrm{d}t} \alpha(t) \otimes \beta(t) + \alpha(t) \otimes \frac{\mathrm{d}}{\mathrm{d}t} \beta(t). \tag{29}$$

The following is the Magnus theorem[1] which is the continuous analog of the Baker–Campbell–Hausdorff's theorem.[16]

Theorem 16: *Let $H(t)$ be a continuous function from $\mathbb{R}$ to the linear space of bounded operators over a Hilbert space G that is null only on a finite set of points. Let $U(t)$ be the solution of*

$$\frac{\mathrm{d}U}{\mathrm{d}t} = H(t)U(t), \quad U(0) = I, \tag{30}$$

where I denotes the identity operator. Then, if $U(t)$ has a logarithm $\Omega(t)$ given by the series (27) (*putting I instead of e*) *and this series converges absolutely in A, there exists an element $\psi(t)$ of $\mathcal{L}^f(t)$ (that is, a sequence of finite dimensional convergent ordered coefficients) such that $\Omega(t) = \Xi(\psi(t))$.*

Proof: The solution $U(t)$ to (28) is given by the series

$$U(t) = I + \int_0^t H(t_1)\mathrm{d}t_1 + \int_0^t \int_0^{t_1} H(t_1)H(t_2)\mathrm{d}t_1\,\mathrm{d}t_2 + \int_0^t \int_0^{t_1} \int_0^{t_2} H(t_1)H(t_2)H(t_3)\mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3 + \cdots . \tag{31}$$

Let us examine the "differential" equation in $\overline{\mathcal{A}}$ associated with (30):

$$\frac{\mathrm{d}}{\mathrm{d}t} \alpha(t) = H(t) \odot \alpha(t), \quad \alpha(0) = 1. \tag{32}$$

The solution to (32) is similar to (31) and it is given by

$$\alpha(t) = 1 + \int_0^t H(t_1)\mathrm{d}t_1 + \int_0^t \int_0^{t_1} H(t_1) \odot H(t_2)\mathrm{d}t_1\,\mathrm{d}t_2 + \int_0^t \int_0^{t_1} \int_0^{t_2} H(t_1) \odot H(t_2) \odot H(t_3)\mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3 + \cdots . \tag{33}$$

This can be proved by derivating component to component. Rewriting (33) in the following way (see (23)):

$$\alpha(t)=1+\int_0^t H(t_1)\mathrm{d}t_1+\sum_{n=2}^{\infty}\int_0^t\cdots\int_0^t \theta_{1,2}\ldots\theta_{n-1,n}H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n, \tag{34}$$

it becomes clear that $\alpha(t)$ is contained in $\mathcal{A}^f(t)$. By Proposition 15 we have that $\log\alpha(t)\in\mathcal{A}^f(t)$. By (29):

$$\frac{\mathrm{d}}{\mathrm{d}t}(\alpha(t)\otimes\alpha(t))=\frac{\mathrm{d}}{\mathrm{d}t}\alpha(t)\otimes\alpha(t)+\alpha(t)\otimes\frac{\mathrm{d}}{\mathrm{d}t}\alpha(t),$$

and from (32) we have

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(\alpha(t)\otimes\alpha(t))&=(H(t)\odot\alpha(t))\otimes\alpha(t)+\alpha(t)\otimes(H(t)\odot\alpha(t))\\&=(H(t)\otimes 1+1\otimes H(t))\odot(\alpha(t)\otimes\alpha(t)).\end{aligned}$$

Therefore, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}(\alpha(t)\otimes\alpha(t))=(H(t)\otimes 1+1\otimes H(t))\odot(\alpha(t)\otimes\alpha(t)),$$

with $\alpha(0)\otimes\alpha(0)=1\otimes 1$, which compared to (32) and taking into account (34) implies directly

$$\Delta(\alpha(t))=\alpha(t)\otimes\alpha(t). \tag{35}$$

So then, if $\omega(t)=\log\alpha(t)$, applying successively (28) and (35) we obtain

$$\begin{aligned}\Delta(\omega(t))=\Delta(\log\alpha(t))=\log(\Delta(\alpha(t)))&=\log(\alpha(t)\otimes\alpha(t))\\&=\log((\alpha(t)\otimes 1)\odot(1\otimes\alpha(t)))\\&=\log(\alpha(t)\otimes 1)+\log(1\otimes\alpha(t))\\&=(\log\alpha(t))\otimes 1+1\otimes\log\alpha(t)=\omega(t)\otimes 1+1\otimes\omega(t).\end{aligned}$$

It follows, by Friedrichs' criterion, that $\omega(t)=\log\alpha(t)$ is an element contained in $\Gamma^f(t)$. Consequently, $\psi(t)=\Phi^{-1}(\omega(t))$ is an element of $\Lambda^f(t)$. Finally, since it holds that $\Xi(\psi(t))=\Omega(t)=\log U(t)$, $\psi(t)$ is an element of $\mathfrak{A}^f(t)$, from where, we conclude that $\psi(t)\in\mathcal{L}^f(t)$ and $\Xi(\psi(t))=\Omega(t)$. ■

If $H(t)$ and $U(t)$ fulfill the conditions of Theorem 16 it is easy to get an expression for $\Omega(t)$ in terms of $H(t)$. Remember that $U(t)$ is given by

$$U(t)=I+\int_0^t H(t_1)\mathrm{d}t_1+\sum_{n=2}^{\infty}\int_0^t\cdots\int_0^t \theta_{1,2}\ldots\theta_{n-1,n}H(t_1)\ldots H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n.$$

Hence, applying the log series to $U(t)$ and calculating up to the third term, we have that $\Omega(t)$ is as follows:

$$\begin{aligned}\Omega(t)=&\int_0^t H(t_1)\mathrm{d}t_1+\int_0^t\int_0^t\left(\theta_{1,2}-\frac{1}{2}\right)H(t_1)H(t_2)\mathrm{d}t_1\,\mathrm{d}t_2\\&+\int_0^t\int_0^t\int_0^t\left(\theta_{1,2}\theta_{2,3}-\frac{1}{2}\theta_{1,2}-\frac{1}{2}\theta_{2,3}+\frac{1}{3}\right)\times H(t_1)H(t_2)H(t_3)\mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3+\cdots.\end{aligned}$$

Since the coefficients associated with $\Omega(t)$ are ordered, by (20) this allows one to rewrite the previous series in the following way:

$$\Omega(t)=\int_0^t H(t_1)\mathrm{d}t_1+\frac{1}{2}\int_0^t\int_0^t\left(\theta_{1,2}-\frac{1}{2}\right)[H(t_1),H(t_2)]\mathrm{d}t_1\,\mathrm{d}t_2$$
$$+\frac{1}{3}\int_0^t\int_0^t\int_0^t\left(\theta_{1,2}\theta_{2,3}-\frac{1}{2}\theta_{1,2}-\frac{1}{2}\theta_{2,3}+\frac{1}{3}\right)\times[[H(t_1),H(t_2)],H(t_3)]\mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3+\cdots.$$

Finally, integrating we obtain the *Magnus expansion:*

$$\Omega(t)=\int_0^t H(t_1)\mathrm{d}t_1+\frac{1}{2}\int_0^t\int_0^{t_1}[H(t_1),H(t_2)]\mathrm{d}t_1\,\mathrm{d}t_2$$
$$+\frac{1}{6}\int_0^t\int_0^{t_1}\int_0^{t_2}[[H(t_1),H(t_2)],H(t_3)]\mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3$$
$$+\frac{1}{6}\int_0^t\int_0^{t_1}\int_0^{t_2}[H(t_1),[H(t_2),H(t_3)]]\mathrm{d}t_1\,\mathrm{d}t_2\,\mathrm{d}t_3+\cdots.$$

Remark 3: From the fact that $\omega(t)$ is a Lie-element (Theorem 16) one can obtain an explicit expression for the coefficients of the Magnus expansion $\Omega(t)$, which we call the Magnus formula:[11]

$$\Omega(t)=\int_0^t H(t_1)\mathrm{d}t_1+\sum_{n=2}^{\infty}\frac{1}{n}\int_0^t\cdots\int_0^t L_n[\ldots[H(t_1),H(t_2)],\ldots,H(t_n)]\mathrm{d}t_1\,\mathrm{d}t_2\ldots\mathrm{d}t_n, \qquad (36)$$

where

$$L_n=\sum_{i=1}^{n}\frac{(-1)^{i+1}}{i}\sum_{j_1<j_2<\ldots<j_{n-i}<n}\prod_{m=1}^{n-i}\theta_{j_m j_m+1}.$$

□

As a corollary of (36) we get the local convergence of the Magnus formula (see also Refs. 6 and 17):

Proposition 17: Let $H(t)$ be a continuous function from $\mathbb{R}$ to the linear space of bounded operators over a Hilbert space G that is null only on a finite set of points. Let M be a positive real number such that $\|H(t)\|\leqslant M$ for all t. Then, the Magnus expansion converges for all $t\in[0,1/(2M))$.

Proof: It is easy to see that the coefficient L_n provides 2^{n-1} multiple integrals. Hence, we have that

$$\|\Omega(t)\|\leqslant\sum_{n=1}^{\infty}2^{n-1}M^n t^n.$$

Applying the division criterion, we obtain that $\Omega(t)$ converges if

$$t\leqslant\frac{1}{2M}.$$

□

As an example of a global result which follows immediately from the Magnus expansion, we will present a simple proof of a well-known result for the stability of triangular systems.

Consider the following triangular system:

$$\begin{cases} \dot{x}_1 = a_{11}(t)x_1 + & a_{12}(t)x_2 + \ldots + & a_{1n}(t)x_n \\ \dot{x}_2 = & a_{22}(t)x_2 + \ldots + & a_{2n}(t)x_n \\ \vdots & & \vdots \\ \dot{x}_n = & & a_{nn}(t)x_n \end{cases} . \tag{37}$$

Let us represent (37) in the following way:

$$\dot{U}(t) = H(t)U(t),$$

where

$$U(t) = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad H(t) = \begin{pmatrix} a_{11}(t) & a_{12}(t) & \ldots & a_{1n}(t) \\ 0 & a_{22}(t) & \ldots & a_{2n}(t) \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \ldots & a_{nn}(t) \end{pmatrix}.$$

The triangular matrix $H(t)$ can be represented as the sum $H(t) = D(t) + N(t)$, where $D(t)$ is the principal diagonal matrix and $N(t)$ is the nilpotent superior triangular matrix. In order to obtain an exponential solution, we apply the Magnus expansion (36). Thus we have

$$\Omega(t) = \int_0^t H(t_1)\mathrm{d}t_1 + \frac{1}{2}\int_0^t \int_0^{t_1} [H(t_1), H(t_2)]\mathrm{d}t_1\,\mathrm{d}t_2 + \ldots$$

$$= \begin{pmatrix} \int_0^t a_{11}(t_1)\mathrm{d}t_1 & & & 0 \\ & \int_0^t a_{22}(t_1)\mathrm{d}t_1 & & \\ & & \ddots & \\ 0 & & & \int_0^t a_{nn}(t_1)\mathrm{d}t_1 \end{pmatrix} + \hat{N}(t),$$

where $\hat{N}(t)$ is a nilpotent superior triangular matrix. Therefore the matrix $(1/t)\Omega(t)$ is given in the next form

$$(1/t)\Omega(t) = \begin{pmatrix} \frac{1}{t}\int_0^t a_{11}(t_1)\mathrm{d}t_1 & & & * \\ & \frac{1}{t}\int_0^t a_{22}(t_1)\mathrm{d}t_1 & & \\ & & \ddots & \\ 0 & & & \frac{1}{t}\int_0^t a_{nn}(t_1)\mathrm{d}t_1 \end{pmatrix}. \tag{38}$$

Since the eigenvalues of matrix (38) are the Lyapunov exponents

$$\lambda_i = \frac{1}{t}\int_0^t a_{ii}(t_1)\mathrm{d}t_1 \quad \text{for } i = 1,\ldots,n,$$

then, we have the following result:

Proposition 18: System (37) *is uniformly exponentially stable if there exist positive numbers* τ, ν *such that, for all* $t>\tau$, $(1/t)\int_0^t a_{ii}(t_1)\mathrm{d}t_1 \leqslant -\nu$ *for* $i=1,...,n$.

The proof follows from the next criterion on the uniform exponential stability of a nonautonomous linear system:[46]

Proposition 19: A sufficient condition for a linear system to be uniformly exponentially stable is that the eigenvalues of the $n\times n$ *matrix* $(1/t)\Omega(t)$ *be bounded as functions of* t *and have real parts* $\leqslant -\nu$ *for all* $t>\tau$ *for some positive numbers* ν *and* τ.

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APPENDIX A: THE ALGEBRA OF PERMUTATIONS

In this Appendix we prove the properties of the permutations $C_{1,k}$ which are relevant in the proof of the main results of this paper.

Proposition 20: Let $m>0$ *and* $i_1<\ldots<i_m$ *be any* m *positive integers. Now let us take the* (i_m-m) *positive integers smaller than* i_m *and different from the previous ones and let us call them* $i_{m+1}<\ldots<i_{i_m}$. *Then*

$$C_{1,i_1}\ldots C_{1,i_m}=\begin{pmatrix} 1 & 2 & \ldots & m & m+1 & \ldots & i_m \\ i_m & i_{m-1} & \ldots & i_1 & i_{m+1} & \ldots & i_{i_m} \end{pmatrix}. \tag{A1}$$

Proof: The proof follows by induction over m, assuming that $i_1\geqslant 2$. The case $i_1=1$ follows immediately from the fact $C_{1,1}=1$.

For $m=1$ the equality holds (A1) since from (7):

$$C_{1,i_1}=\begin{pmatrix} 1 & 2 & \ldots & i_1 \\ i_1 & 1 & \ldots & i_1-1 \end{pmatrix}.$$

Suppose that (A1) holds for $m=k$. We will prove it for $m=k+1$.

Let $i_1<\ldots<i_{k+1}$ with $i_{k+2}<\ldots<i_{i_{k+1}}$ be the first i_{k+1} positive integers. By the induction hypothesis,

$$C_{1,i_1}\ldots C_{1,i_k}=\begin{pmatrix} 1 & 2 & \ldots & k & k+1 & \ldots & i_k \\ i_k & i_{k-1} & \ldots & i_1 & i_{k+2} & \ldots & i_{i_k+1} \end{pmatrix}.$$

Note that $i_{i_{k+1}}<i_k<i_{k+1}$. Hence

$$C_{1,i_1}\ldots C_{1,i_k}C_{1,i_{k+1}}=\begin{pmatrix} 1 & 2 & \ldots & k & k+1 & \ldots & i_k \\ i_k & i_{k-1} & \ldots & i_1 & i_{k+2} & \ldots & i_{i_k+1} \end{pmatrix}C_{1,i_{k+1}},$$

From (7):

$$\begin{aligned}&\begin{pmatrix} 1 & 2 & \ldots & k & k+1 & \ldots & i_k \\ i_k & i_{k-1} & \ldots & i_1 & i_{k+2} & \ldots & i_{i_k+1} \end{pmatrix}C_{1,i_{k+1}} \\ &\quad=\begin{pmatrix} 1 & 2 & \ldots & k & k+1 & \ldots & i_k \\ i_k & i_{k-1} & \ldots & i_1 & i_{k+2} & \ldots & i_{i_k+1} \end{pmatrix}\begin{pmatrix} 1 & 2 & \ldots & i_{k+1} \\ i_{k+1} & 1 & \ldots & i_{k+1}-1 \end{pmatrix} \\ &\quad=\begin{pmatrix} 1 & 2 & \ldots & k+1 & k+2 & \ldots & i_{k+1} \\ i_{k+1} & i_k & \ldots & i_1 & i_{k+2} & \ldots & i_{i_{k+1}} \end{pmatrix}.\end{aligned}$$

■

Corollary 21:

$$C_{1,2}\ldots C_{1,n}=\begin{pmatrix}1 & 2 & \ldots & n-1 & n\\ n & n-1 & \ldots & 2 & 1\end{pmatrix}.$$

Corollary 22: Let $n\geqslant m>0$ and let $i_1<\ldots<i_m$ be m positive integers less or equal to n. Take now the $n-m$ positive integers less or equal to n that are different from the previous ones and let us call them $i_{m+1}<\ldots<i_n$. Then

$$C_{1,i_1}\ldots C_{1,i_m}=\begin{pmatrix}1 & 2 & \ldots & m & m+1 & \ldots & n\\ i_m & i_{m-1} & \ldots & i_1 & i_{m+1} & \ldots & i_n\end{pmatrix}.$$

Proof: It follows from Proposition 20 noting that $i_k=k$ for $k\geqslant i_m+1$. ■

From the above-given corollary one obtains the following results:

Corollary 23:

$$C_{1,i_1}\ldots C_{1,i_m}C_{1,2}\ldots C_{1,m}=\begin{pmatrix}1 & \ldots & m & m+1 & \ldots & n\\ i_1 & \ldots & i_m & i_{m+1} & \ldots & i_n\end{pmatrix}.$$

Corollary 24: $C^{-1}_{1,n}\ldots C^{-1}_{1,2}C^{-1}_{1,i_m}\ldots C^{-1}_{1,i_1}=C^{-1}_{1,i_n}\ldots C^{-1}_{1,i_{m+1}}$.

Corollary 25: $(C_{1,n})^m C^{-1}_{1,m}\ldots C^{-1}_{1,2}\ C^{-1}_{1,i_m}\ldots\ C^{-1}_{1,i_1}=C^{-1}_{1,n-m}\ldots C^{-1}_{1,2}C^{-1}_{1,i_n}\ldots C^{-1}_{1,i_{m+1}}$.

The next Lemma is used in the proof of Friedrichs' criterion.

Lemma 26: For n odd:

$$nE_n-n=\sum_{i=1}^{[[n/2]]}\left[(-1)^i(n-i)\prod_{k=2}^{i}C^{-1}_{1,i-k+2}+(-1)^{n-i}i\prod_{k=i+1}^{n}C^{-1}_{1,n-k+i+1}\right]\sigma_{n,n-1},$$

where E_n is given by (8), *$[[\cdot]]$ is the "largest-integer-less-or-equal-than" function, and*

$$\sigma_{n,m}=\left(\prod_{k=2}^{n-m}C^{-1}_{1,n-m-k+2}\right)\rho_{n,m},$$

with

$$\rho_{n,m}=\sum_{n\geqslant i_{n-m}>\ldots>i_1\geqslant 1}C^{-1}_{1,i_{n-m}}\ldots C^{-1}_{1,i_1}.$$

Proof: First, notice that given $C_{1,1}=1$ we can rewrite $\rho_{n,m}$ in a way more useful to our purposes:

$$\rho_{n,m}=\sum_{n\geqslant j_{n-m-1}>\ldots>j_1\geqslant 2}C^{-1}_{1,j_{n-m-1}}\ldots C^{-1}_{i,j_1}+\sum_{n\geqslant l_{n-m}>\ldots>l_1\geqslant 2}C^{-1}_{1,l_{n-m}}\ldots C^{-1}_{1,l_1}$$

(for $m=n-1$ the first summation is reduced to be equal to 1),

$$\begin{aligned}\rho_{n,m}&=\sum_{i=1}^{[[n/2]]}\left[(-1)^i(n-i)\prod_{k=2}^{i}C^{-1}_{1,i-k+2}+(-1)^{n-i}i\prod_{k=i+1}^{n}C^{-1}_{1,n-k+i+1}\right]\sigma_{n,n-1}\\ &=\sum_{i=1}^{[[n/2]]}\left[(-1)^i(n-i)\prod_{k=2}^{i}C^{-1}_{1,i-k+2}+(-1)^{n-i}i\prod_{k=i+1}^{n}C^{-1}_{1,n-k+i+1}\right]\left(\prod_{k=2}^{i}C^{-1}_{1,i-k+2}\right)\rho_{n,n-1}.\end{aligned}$$

As a consequence of Corollary 21 we have that $(\Pi_{k=2}^{i}C^{-1}_{1,i-k+2})^2=1$. Moreover,

$$\prod_{k=i+1}^{n} C^{-1}_{1,n-k+i+1} \prod_{k=2}^{i} C^{-1}_{1,i-k+2} = \prod_{k=2}^{n} C^{-1}_{1,n-k+2}.$$

Hence

$$\rho_{n,m} = \sum_{i=1}^{[[n/2]]} \left[(-1)^i (n-i) + (-1)^{n-i} i \prod_{k=2}^{n} C^{-1}_{1,n-k+2} \right] \rho_{n,n-1}$$
$$= \sum_{i=1}^{[[n/2]]} (-1)^i (n-i) \rho_{n,n-1} + \sum_{i=1}^{[[n/2]]} (-1)^{n-i} i \prod_{k=2}^{n} C^{-1}_{1,n-k+2} \rho_{n,n-1}.$$

Replacing in the second summation the index i by $n-i$ we obtain

$$\rho_{n,m} = \sum_{i=1}^{[[n/2]]} (-1)^i (n-i) \rho_{n,n-1} + \sum_{i=[[n/2]]+1}^{n-1} (-i)^i (n-i) \prod_{k=2}^{n} C^{-1}_{1,n-k+2} \rho_{n,i}.$$

Now, as a consequence of Corollary 24, we have that $\Pi_{k=2}^{n} C^{-1}_{1,n-k+2} \rho_{n,i} = \rho_{n,n-i}$. Hence

$$\rho_{n,m} = \sum_{i=1}^{[[n/2]]} (-1)^i (n-i) \rho_{n,n-1} + \sum_{i=[[n/2]]+1}^{n-1} (-i)^i (n-i) \rho_{n,n-i}$$

$$= \sum_{i=1}^{n-1} (-1)^i (n-i) \rho_{n,n-i}$$

$$= \sum_{i=1}^{n-1} (-1)^i (n-i) \left(\sum_{n \geqslant j_{i-1} > \ldots > j_i \geqslant 2} C^{-1}_{1,j_{i-1}} \ldots C^{-1}_{i,j_1} \right.$$
$$\left. + \sum_{n \geqslant l_i > \ldots > l_1 \geqslant 2} C^{-1}_{1,l_i} \ldots C^{-1}_{1,l_1} \right)$$

$$= \sum_{i=1}^{n-1} (-1)^i (n-i) \sum_{n \geqslant j_{i-1} > \ldots > j_1 \geqslant 2} C^{-1}_{i,j_{i-1}} \ldots C^{-1}_{1,j_1}$$
$$+ \sum_{i=1}^{n-1} (-1)^i (n-i) \sum_{n \geqslant l_i > \ldots > l_1 \geqslant 2} C^{-1}_{i,l_1} \ldots C^{-1}_{1,l_1}.$$

Replacing in the second double summation the index i by $i-1$ we obtain

$$\rho_{n,m} = \sum_{i=1}^{n-1} (-1)^i (n-i) \sum_{n \geqslant j_{i-1} > \ldots > j_i \geqslant 2} C^{-1}_{1,j_{i-1}} \ldots C^{-1}_{i,j_1}$$
$$+ \sum_{i=2}^{n} (-1)^{i-1} (n-i+1) \sum_{n \geqslant l_{i-1} > \ldots > l_1 \geqslant 2} C^{-1}_{1,l_{i-1}} \ldots C^{-1}_{1,l_1}.$$

Changing now the indexes l_k by j_k we have

$$\rho_{n,m}=\sum_{i=1}^{n-1}(-1)^i(n-i)\sum_{n\geqslant j_{i-1}>\ldots>j_i\geqslant 2}C^{-1}_{1,j_{i-1}}\ldots C^{-1}_{i,j_1}$$
$$+\sum_{i=2}^{n}(-1)^{i-1}(n-i+1)\sum_{n\geqslant j_{i-1}>\ldots>j_i\geqslant 2}C^{-1}_{1,j_{i-1}}\ldots C^{-1}_{1,j_1}$$
$$=-(n-1)+\sum_{i=2}^{n-1}(-1)^i(n-i)\sum_{n\geqslant j_{i-1}>\ldots>j_1\geqslant 2}C^{-1}_{1,j_{i-1}}\ldots C^{-1}_{1,j_1}$$
$$+\sum_{i=2}^{n-1}(-1)^{i-1}(n-i+1)\sum_{n\geqslant j_{i-1}>\ldots>j_1\geqslant 2}C^{-1}_{1,j_{i-1}}\ldots C^{-1}_{1,j_1}+(-1)^{n-1}\prod_{k=2}^{n}C^{-1}_{1,n-k+2}$$
$$=-(n-1)+\sum_{i=2}^{n-1}((-1)^i(n-i)+(-1)^{i-1}(n-i+1))\sum_{n\geqslant j_{i-1}>\ldots>j_1\geqslant 2}C^{-1}_{1,j_{i-1}}\ldots C^{-1}_{1,j_1}$$
$$+(-1)^{n-1}\prod_{k=2}^{n}C^{-1}_{1,n-k+2}$$
$$=-(n-1)+\sum_{i=2}^{n-1}(-1)^{i-1}(-n+i+n-i+1)\sum_{n\geqslant j_{i-1}>\ldots>j_1\geqslant 2}C^{-1}_{1,j_{i-1}}\ldots C^{-1}_{1,j_1}$$
$$+(-1)^{n-1}\prod_{k=2}^{n}C^{-1}_{1,n-k+2}$$
$$=-(n-1)+\sum_{i=2}^{n-1}(-1)^{i-1}\sum_{n\geqslant j_{i-1}>\ldots>j_1\geqslant 2}C^{-1}_{1,j_{i-1}}\ldots C^{-1}_{1,j_1}+(-1)^{n-1}\prod_{k=2}^{n}C^{-1}_{1,n-k+2}$$
$$=-(n-1)+\sum_{i=2}^{n}(-1)^{i-1}\sum_{n\geqslant j_{i-1}>\ldots>j_1\geqslant 2}C^{-1}_{1,j_{i-1}}\ldots C^{-1}_{1,j_1}$$
$$=nE_n-n.$$

■

APPENDIX B: PROOF OF FRIEDRICHS' CRITERION

($\Rightarrow$)
If $\alpha\in\Gamma(t)$ then there exists $a=\{a_n\}_{n=0}^{\infty}\in\Lambda(t)$ such that $\alpha=\Phi(a)$. Since a is in $\Lambda(t)$ we have that $a=E(a)$. This, by (16), implies that $a_0=0$ and $a_n=E_n(a_n)$, for $n\geqslant 2$. Therefore,

$$\alpha=\Phi(a)=\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n$$
$$=\int_0^t a_1(t_1)H(t_1)\mathrm{d}t_1+\sum_{n=2}^{\infty}\int_0^t\cdots\int_0^t E_n(a_n(t_1,\ldots,t_n))H(t_1)$$
$$\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n. \tag{B1}$$

Applying Δ [given by (26)] to (B1) we obtain

$$\Delta\alpha=\int_0^t a_1(t_1)(H(t_1)\otimes 1+1\otimes H(t_1))\mathrm{d}t_1+\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t E_n(a_n(t_1,\ldots,t_n))(H(t_1)\otimes 1+1\otimes H(t_1))\odot\ldots\odot(H(t_n)\otimes 1+\otimes H(t_n))\mathrm{d}t_1\ldots\mathrm{d}t_n.$$

By (20), every multiple integral can be reordered in the following way:

$$\Delta\alpha=\int_0^t a_1(t_1)(H(t_1)\otimes 1+1\otimes H(t_1))\mathrm{d}t_1+\sum_{n=2}^{\infty}\frac{1}{n}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)[\ldots[H(t_1)\otimes 1+1\otimes H(t_1),\ H(t_2)\otimes 1+1\otimes H(t_2)],\ldots,H(t_n)\otimes 1+1\otimes H(t_n)]\mathrm{d}t_1\ldots\mathrm{d}t_n. \tag{B2}$$

The Lie product $[\cdot]$ is defined with respect to the free product $\odot$. By induction one can prove that

$$[\ldots[H(t_1)\otimes 1+1\otimes H(t_1),H(t_2)\otimes 1+1\otimes H(t_2)],\ldots,H(t_n)\otimes 1+1\otimes H(t_n)]=[\ldots[H(t_1),H(t_2)],\ldots,H(t_n)]\otimes 1+1\otimes[\ldots[H(t_1),H(t_2)],\ldots,H(t_n)].$$

Applying this property to (B2), one obtains

$$\begin{aligned}\Delta\alpha=&\int_0^t a_1(t_1)(H(t_1)\otimes 1+1\otimes H(t_1))\mathrm{d}t_1+\sum_{n=2}^{\infty}\frac{1}{n}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)\\&\times([\ldots[H(t_1),H(t_2)],\ldots,H(t_n)]\otimes 1+1\otimes[\ldots[H(t_1),H(t_2)],\ldots,H(t_n)])\mathrm{d}t_1\ldots\mathrm{d}t_n\\=&\left(\int_0^t a_1(t_1)H(t_1)\mathrm{d}t_1+\sum_{n=2}^{\infty}\frac{1}{n}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)[\ldots[H(t_1),H(t_2)],\ldots,H(t_n)]\mathrm{d}t_1\ldots\mathrm{d}t_n\right)\\&\otimes 1+1\otimes\left(\int_0^t a_1(t_1)H(t_1)\mathrm{d}t_1+\sum_{n=2}^{\infty}\frac{1}{n}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)\right.\\&\left.\times\ [\ldots[H(t_1),H(t_2)],\ldots,H(t_n)]\mathrm{d}t_1\ldots\mathrm{d}t_n\right).\end{aligned}$$

Finally, using (20) it holds:

$$\begin{aligned}\Delta\alpha=&\left(\int_0^t a_1(t_1)H(t_1)\mathrm{d}t_1+\sum_{n=2}^{\infty}\int_0^t\cdots\int_0^t E_n(a_n(t_1,\ldots,t_n))H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n\right)\\&\otimes 1+1\otimes\left(\int_0^t a_1(t_1)H(t_1)\mathrm{d}t_1+\sum_{n=2}^{\infty}\int_0^t\cdots\int_0^t E_n(a_n(t_1,\ldots,t_n))H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n\right)\\=&\left(\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n\right)\\&\otimes 1+1\otimes\sum_{n=1}^{\infty}\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)H(t_1)\odot\ldots\odot H(t_n)\mathrm{d}t_1\ldots\mathrm{d}t_n=\alpha\otimes 1+1\otimes\alpha.\end{aligned}$$

($\Leftarrow$)
Let $\alpha=\Phi(a)$, $a=\{a_n\}_{n=0}^{\infty}\in A(t)$, as usual. Calculating $\Delta\alpha$ we find that:

$$\Delta\alpha = a_0(1\otimes 1) + \sum_{n=1}^{\infty} \int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) \prod_{m=1}^{n} \odot (H(t_m)\otimes 1 + 1\otimes H(t_m))\,\mathrm{d}t_1 \ldots \mathrm{d}t_n$$

$$= a_0(1\otimes 1) + \int_0^t a_1(t_1)(H(t_1)\otimes 1 + 1\otimes H(t_1))\,\mathrm{d}t_1$$

$$+ \sum_{n=2}^{\infty} \int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) \Bigg(\Bigg(\prod_{m=1}^{n} \odot H(t_m) \Bigg) \otimes 1$$

$$+ \sum_{m=1}^{n-1} \sum_{\substack{S_j \subset J_n \\ \#S_j = m}} \Bigg(\Bigg(\prod_{p\in J_n\setminus S_j} \odot H(t_p) \Bigg) \otimes \Bigg(\prod_{q\in S_j} \odot H(t_q) \Bigg) \Bigg) + 1 \otimes \prod_{m=1}^{n} \odot H(t_m) \Bigg)$$

$$\times \mathrm{d}t_1 \ldots \mathrm{d}t_n,$$

where $J_n = \{1,\ldots,n\}$, S_j and $J_n \setminus S_j$ are ordered sets. Taking into account that $a_0(1\otimes 1) = a_0 \otimes 1 = 1 \otimes a_0$, integrating separately, and reordering it results

$$\Delta\alpha = \alpha\otimes 1 + 1\otimes\alpha - a_0(1\otimes 1) + \sum_{n=2}^{\infty} \int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) \Bigg(\sum_{m=1}^{n-1} \sum_{\substack{S_j \subset J_n \\ \#S_j = m}} \Bigg(\Bigg(\prod_{p\in J_n\setminus S_j} \odot H(t_p) \Bigg)$$

$$\otimes \Bigg(\prod_{q\in S_j} \odot H(t_q) \Bigg) \Bigg) \Bigg) \mathrm{d}t_1 \ldots \mathrm{d}t_n.$$

By hypothesis, $\Delta\alpha = \alpha\otimes 1 + 1\otimes\alpha$. Then, we obtain

$$-a_0(1\otimes 1) + \sum_{n=2}^{\infty} \sum_{m=1}^{n-1} \int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) \times \sum_{\substack{S_j \subset J_n \\ \#S_j = m}} \Bigg(\Bigg(\prod_{p\in J_n\setminus S_j} \odot H(t_p) \Bigg)$$

$$\otimes \Bigg(\prod_{q\in S_j} \odot H(t_q) \Bigg) \Bigg) \mathrm{d}t_1 \ldots \mathrm{d}t_n = 0. \tag{B3}$$

First, this implies that $a_0 = 0$. On the other hand, it can be noted that every multiple integral of the previous expression represents a homogeneous element of different degree (i, j) in $\overline{\mathcal{A}\otimes\mathcal{A}}$. Therefore the equality (B3) holds if and only if every multiple integral is null. Hence,

$$\int_0^t \cdots \int_0^t a_n(t_1,\ldots,t_n) \sum_{\substack{S_j \subset J_n \\ \#S_j = m}} \Bigg(\Bigg(\prod_{p\in J_n\setminus S_j} \odot H(t_p) \Bigg) \otimes \Bigg(\prod_{q\in S_j} \odot H(t_q) \Bigg) \Bigg) \mathrm{d}t_1 \ldots \mathrm{d}t_n = 0 \tag{B4}$$

for $n \geqslant 2$ and for m between 1 and $n-1$. We are interested now in the summation that is behind the integral sign. First, we have that for every S_j, $J_n \setminus S_j = \{i_1,\ldots,i_{n-m}\}$ and $S_j = \{i_{n-m+1},\ldots,i_n\}$; more precisely, $i_1 < \ldots < i_{n-m}$ and $i_{n-m+1} < \ldots < i_n$, are all of them different, and together are J_n. Hence, using permutations and, from Corollary 23 in Appendix A:

$$\sum_{\substack{S_j\subset J_n\\ \#S_j=m}}\left(\left(\prod_{p\in J_n S_j}\odot H(t_p)\right)\otimes\left(\prod_{q\in S_j}\odot H(t_q)\right)\right)$$

$$=\sum_{\substack{i_1<\ldots<i_{n-m}\\ i_{n-m+1}<\ldots<i_n}}\begin{pmatrix}1 & \ldots & n-m & n-m+1 & \ldots & n\\ i_1 & \ldots & i_{n-m} & i_{n-m+1} & \ldots & i_n\end{pmatrix}$$

$$\times\left(\left(\prod_{p=1}^{n-m}\odot H(t_p)\right)\otimes\left(\prod_{q=n-m+1}^{n}\odot H(t_q)\right)\right)$$

$$=\sum_{1\leqslant i_1<\ldots<i_{n-m}\leqslant n}C_{1,i_1}\ldots C_{1,i_{n-m}}C_{1,2}\ldots C_{1,n-m}\left(\left(\prod_{p=1}^{n-m}\odot H(t_p)\right)\otimes\left(\prod_{q=n-m+1}^{n}\odot H(t_q)\right)\right).$$

Substituting this in (B4) we obtain

$$\int_0^t\cdots\int_0^t a_n(t_1,\ldots,t_n)\sum_{1\leqslant i_1<\ldots<i_{n-m}\leqslant n}C_{1,i_1}\ldots C_{1,i_{n-m}}C_{1,2}\ldots C_{1,n-m}\left(\left(\prod_{p=1}^{n-m}\odot H(t_p)\right)\right.$$
$$\left.\otimes\left(\prod_{q=n-m+1}^{n}\odot H(t_q)\right)\right)\mathrm{d}t_1\ldots\mathrm{d}t_n=0.$$

Applying (20) to the previous integral, and ordering the indexes in the product of $H(t)$ we get:

$$\int_0^t\cdots\int_0^t\left(\sum_{n\geqslant i_{n-m}>\ldots>i_1\geqslant 1}C^{-1}_{1,n-m}\ldots C^{-1}_{1,2}C^{-1}_{1,i_{n-m}}\ldots C^{-1}_{1,i_1}(a_n(t_1,\ldots,t_n))\right)\left(\prod_{p=1}^{n-m}\odot H(t_p)\right)$$
$$\otimes\left(\prod_{q=n-m+1}^{n}\odot H(t_q)\right)\mathrm{d}t_1\ldots\mathrm{d}t_n=0.$$

Conveying that $\Pi_{k=2}^{1}C^{-1}_{1,1-k+2}=1$, another way to represent the previous equation is

$$\int_0^t\cdots\int_0^t\left(\prod_{k=2}^{n-m}C^{-1}_{1,n-m-k+2}\sum_{n\geqslant i_{n-m}>\ldots>i_1\geqslant 1}C^{-1}_{1,i_{n-m}}\ldots C^{-1}_{1,i_1}(a_n(t_1,\ldots,t_n))\right)\left(\prod_{p=1}^{n-m}\odot H(t_p)\right)$$
$$\otimes\left(\prod_{q=n-m+1}^{n}\odot H(t_q)\right)\mathrm{d}t_1\ldots\mathrm{d}t_n=0.$$

Denoting by

$$\rho_{n,m}=\sum_{n\geqslant i_{n-m}>\ldots>i_1\geqslant 1}C^{-1}_{1,i_{n-m}}\ldots C^{-1}_{1,i_1}$$

and

$$\sigma_{n,m}=\left(\prod_{k=2}^{n-m}C^{-1}_{1,n-m-k+2}\right)\rho_{n,m},$$

we arrive at the fact that the previous integral vanishes if any only if $\sigma_{n,m}(a_n)=0$. Since this must be satisfied for each integral, we obtain the following infinite system of equations:

$$\sigma_{n,m}(a_n)=0\quad\text{for } n\geqslant 2\ \text{ and }\ 1\leqslant m\leqslant n-1.$$

These equations are not independent among themselves. To reduce them, applying Corollary 25 it results that

$$\sigma_{n,i}=(C_{1,n}^{m})\sigma_{n,n-i}.$$

Therefore, the reduced system, denoting by $[[\cdot]]$ the "largest-integer-less-or-equal-than" function, is given by:

$$\sigma_{n,m}(a_n)=0, \text{ for } n\geqslant 2 \text{ and } m \text{ between } \left[\left[\frac{n+1}{2}\right]\right] \text{ and } n-1. \tag{B5}$$

From this it will infer that $E_n(a_n)=a_n$ for $n\geqslant 2$, or equivalently $(nE_n-n)a_n=0$ for $n\geqslant 2$.

Recall that

$$nE_n=\prod_{k=2}^{n}(1-C_{1,n-k+2}^{-1})=1+\sum_{i=2}^{n}(-1)^{i-1}\sum_{n\geqslant j_{i-1}>\ldots>j_1\geqslant 2}C_{1,j_{i-1}}^{-1}\ldots C_{1,j_1}^{-1}$$

or equivalently

$$nE-n=-(n-1)+\sum_{i=2}^{n}(-1)^{i-1}\sum_{n\geqslant j_{i-1}>\ldots>j_1\geqslant 2}C_{1,j_{i-1}}^{-1}\ldots C_{1,j_1}^{-1}.$$

For n odd it yields:

$$nE_n-n=\sum_{i=1}^{[[n/2]]}\left[(-1)^i(n-i)\prod_{k=2}^{i}C_{1,i-k+2}^{-1}+(-1)^{n-i}i\prod_{k=i+1}^{n}C_{1,n-k+i+1}^{-1}\right]\sigma_{n,n-1}.$$

The proof that $(nE_n-n)a_n=0$ for the odd case, considering the system of Eqs. (B5), is given in Lemma 26 in Appendix A.

For n even we have:

$$nE_n-n=\sum_{i=1}^{n/2-1}\left[(-1)^i(n-i)\prod_{k=2}^{i}C_{1,i-k+2}^{-1}+(-1)^{n-i}i\prod_{k=i+1}^{n}C_{1,n-k+i+1}^{-1}\right]\sigma_{n,n-1}$$
$$+(-1)^{n/2}\frac{n}{2}\left(\prod_{k=2}^{n/2}C_{1,n/2-k+2}^{-1}\right)\sigma_{n,n/2}.$$

The proof that $(nE_n-n)a_n=0$ for the even case is similar to the odd case, thus, it will be omitted. Hence we conclude $\alpha\in\Gamma(t)$, and the proof of Friedrichs' criterion is complete. ■

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Discontinuities in Dirac eigenfunction expansions

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An expansion, over a finite interval, of a two-component function in a basis of eigenfunctions of a one-dimensional regular Dirac differential operator with separated homogeneous boundary conditions imposed at ends of the interval is considered. It is shown that at the ends of the domain the expansion does not converge to the expanded function unless the latter obeys at these points the same homogeneous boundary conditions as the basis eigenfunctions. General results obtained in the work are illustrated by an analytically solvable example. The problem is related to the R-matrix theory for Dirac particles. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1389471]

I. INTRODUCTION

In theoretical physics one frequently encounters the situation that a given function, defined over some domain, is expanded in a functional basis. Among a variety of bases used in such expansions, those generated by differential eigenvalue problems are of major importance. Properties of expansions in series of eigenfunctions of differential operators were extensively investigated by generations of mathematicians and mathematical physicists and their results are contained in a vast literature of the subject (cf. Refs. 1–6 and references therein).

Expansions, over a finite interval, of a given two-component function in a basis of eigenfunctions of a one-dimensional regular Dirac differential operator with separated homogeneous boundary conditions were studied, for instance, in Refs. 5 and 6. However, in these monographs only a particular case, when at ends of an interval an expanded function obeys the same boundary conditions as basis eigenfunctions, was considered. One may imagine expansion problems in which at end points a two-component function to be expanded is admitted to satisfy boundary conditions that differ from those obeyed by basis eigenfunctions. Problems of that kind are not of purely academic interest and are met in applications of relativistic quantum mechanics (e.g., in the R-matrix theory for Dirac particles[7–9]). It is also very likely that they may be encountered in a mathematical modeling of one-dimensional magnetohydrodynamical phenomena where differential operators of the Dirac type occur.[10,11] We have not found any mathematical study of such problems in available literature and it is a purpose of this work to fill in this gap to some extent. We concentrate on the interesting and important question concerning convergence of an eigenfunction expansion at ends of a domain. We prove that at these points the expansion does not converge to the expanded function unless the latter obeys there the same homogeneous boundary conditions as the basis functions. (That result is by no means obvious since in an analogous problem concerning expansions of one-component functions in bases generated by second-order Sturm–Liouville eigensystems the expansions do converge at the end points except the very special case when basis eigenfunctions are forced to vanish at these points!) Still we show that magnitudes of jumps in both components of the expansion may be precisely determined and we provide relevant expressions. These general results are illustrated by an analytically solvable example.

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II. THE PROBLEM

Consider the eigenproblem consisting of the Dirac differential system

$$\begin{pmatrix} p(x)-\lambda_n\rho(x) & -d/dx+t(x) \\ d/dx+t(x) & q(x)-\lambda_n\rho(x) \end{pmatrix}\begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix}=0 \quad (x_1\leqslant x\leqslant x_2) \tag{2.1}$$

augmented by the separated boundary conditions

$$f_n(x_i)\cos\alpha_i+g_n(x_i)\sin\alpha_i=0 \quad (i=1,2). \tag{2.2}$$

It is assumed that the interval $[x_1,x_2]\subset\mathbb{R}$ is finite, that $p(x)$, $q(x)$, $t(x)$, and $\rho(x)$ are real, bounded and continuous functions of the variable $x\in[x_1,x_2]$, with the additional constraint $\rho(x)>0$, and that α_1 and α_2 are real parameters. Under these assumptions the eigensystem (2.1) and (2.2) has an infinite number of discrete nondegenerate real eigenvalues λ_n.[5,6] The associated eigenfunctions are orthogonal in the sense of

$$\int_{x_1}^{x_2}dx\rho(x)[f_n(x)f_{n'}(x)+g_n(x)g_{n'}(x)]=0 \quad (\lambda_n\neq\lambda_{n'}). \tag{2.3}$$

If they are chosen to be real and normalized so that

$$\int_{x_1}^{x_2}dx\rho(x)[f_n(x)f_{n'}(x)+g_n(x)g_{n'}(x)]=\delta_{nn'}, \tag{2.4}$$

they obey the closure relation

$$\sum_{n=-\infty}^{\infty}\begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix}(f_n(x') \;\; g_n(x'))=\frac{\delta(x-x')}{\sqrt{\rho(x)\rho(x')}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (x_1<x,x'<x_2), \tag{2.5}$$

where $\delta(x-x')$ is the Dirac delta function defined so that[12–14]

$$\int_a^b dx'\,\delta(x-x')\phi(x')=\begin{cases} 0 & \text{for } x<a<b \text{ or } a<b<x, \\ \phi(x) & \text{for } a<x<b, \\ \dfrac{1}{2}\phi(x) & \text{for } a=x<b \text{ or } a<x=b \end{cases} \tag{2.6}$$

for any interval $[a,b]\subset\mathbb{R}$ and any sufficiently regular function $\phi(x)$ defined on $[a,b]$.

Let $(F(x)\;G(x))^{\mathrm{T}}$ be an arbitrary two-component function with continuous components of bounded variation in $[x_1,x_2]$. Its expansion in the set of eigenfunctions of the problem (2.1) and (2.2) is defined as

$$\begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix}=\sum_{n=-\infty}^{\infty}C_n\begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix} \quad (x_1\leqslant x\leqslant x_2) \tag{2.7}$$

with the coefficients

$$C_n=\int_{x_1}^{x_2}dx\rho(x)[f_n(x)F(x)+g_n(x)G(x)]. \tag{2.8}$$

The closure relation (2.5) implies that

$$\begin{pmatrix} F(x) \\ G(x) \end{pmatrix} = \begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix} \quad (x_1 < x < x_2). \tag{2.9}$$

The validity of Eqs. (2.5) and (2.9) is restricted to the *open* interval (x_1, x_2). Since both functions $(F(x) \quad G(x))^{\mathrm{T}}$ and $(\overline{F}(x) \quad \overline{G}(x))^{\mathrm{T}}$ are defined in the *closed* interval $[x_1, x_2]$, we ask the question: how are these functions related at the end points x_1 and x_2?

III. THE SOLUTION

To answer the question posed above, we have to consider an extension of the closure relation (2.5) to the case when one of the variables is fixed at x_i. In analogy with (2.5), we postulate

$$\sum_{n=-\infty}^{\infty} \begin{pmatrix} f_n(x_i) \\ g_n(x_i) \end{pmatrix} (f_n(x) \quad g_n(x)) = \frac{\delta(x-x_i)}{\rho(x_i)} \begin{pmatrix} I_i & J_i \\ K_i & L_i \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2), \tag{3.1}$$

where I_i, J_i, K_i, and L_i are yet unknown constants. Notice that, because of the boundary conditions (2.2), these constants are not independent but are related through

$$J_i = K_i = -I_i \cot \alpha_i, \quad L_i = I_i \cot^2 \alpha_i. \tag{3.2}$$

Hence, it follows that Eq. (3.1) may be rewritten in the form

$$\sum_{n=-\infty}^{\infty} \begin{pmatrix} f_n(x_i) \\ g_n(x_i) \end{pmatrix} (f_n(x) \quad g_n(x)) = \frac{I_i \delta(x-x_i)}{\rho(x_i)} \begin{pmatrix} 1 & -\cot \alpha_i \\ -\cot \alpha_i & \cot^2 \alpha_i \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2). \tag{3.3}$$

From Eqs. (2.7) and (2.8) we have

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \int_{x_1}^{x_2} dx \rho(x) \sum_{n=-\infty}^{\infty} \begin{pmatrix} f_n(x_i) \\ g_n(x_i) \end{pmatrix} (f_n(x) \quad g_n(x)) \begin{pmatrix} F(x) \\ G(x) \end{pmatrix}, \tag{3.4}$$

and, on substituting here Eq. (3.3) and performing integration, we obtain

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} \frac{1}{2} I_i F(x_i) - \frac{1}{2} I_i G(x_i) \cot \alpha_i \\ \frac{1}{2} I_i G(x_i) \cot^2 \alpha_i - \frac{1}{2} I_i F(x_i) \cot \alpha_i \end{pmatrix}. \tag{3.5}$$

Equation (3.5) implies

$$\overline{F}(x_i) \cos \alpha_i + \overline{G}(x_i) \sin \alpha_i = 0, \tag{3.6}$$

which might be also inferred from Eqs. (2.7) and (2.2).

To answer completely the question raised at the end of Sec. II, we have to determine the constants I_1 and I_2. To this end, let us choose

$$\begin{pmatrix} F(x) \\ G(x) \end{pmatrix} = \begin{pmatrix} f_k(x) \\ g_k(x) \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2), \tag{3.7}$$

where the function on the right is an eigenfunction of the system (2.1) and (2.2). Because of the orthonormality relation (2.4), in this particular case from Eq. (2.8) we infer

$$C_n = \delta_{nk} \tag{3.8}$$

and thus

$$\begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix} = \begin{pmatrix} f_k(x) \\ g_k(x) \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2). \tag{3.9}$$

Utilizing Eqs. (3.7) and (3.9) in Eq. (3.5), we arrive at the homogeneous algebraic system

$$\begin{pmatrix} \frac{1}{2}I_i - 1 & -\frac{1}{2}I_i \cot\alpha_i \\ -\frac{1}{2}I_i \cot\alpha_i & \frac{1}{2}I_i \cot^2\alpha_i - 1 \end{pmatrix} \begin{pmatrix} f_k(x_i) \\ g_k(x_i) \end{pmatrix} = 0. \tag{3.10}$$

Since $f_k(x_i)$ and $g_k(x_i)$ do not vanish simultaneously, one has

$$\det \begin{pmatrix} \frac{1}{2}I_i - 1 & -\frac{1}{2}I_i \cot\alpha_i \\ -\frac{1}{2}I_i \cot\alpha_i & \frac{1}{2}I_i \cot^2\alpha_i - 1 \end{pmatrix} = 0, \tag{3.11}$$

hence, it follows that

$$I_i = 2\sin^2\alpha_i . \tag{3.12}$$

In Appendix A we present an alternative derivation of that result.

Having determined the constants I_i, from Eqs. (3.3), (3.5), and (3.12) we deduce

$$\sum_{n=-\infty}^{\infty} \begin{pmatrix} f_n(x_i) \\ g_n(x_i) \end{pmatrix} (f_n(x) \quad g_n(x)) = \frac{\delta(x-x_i)}{\rho(x_i)} \begin{pmatrix} 2\sin^2\alpha_i & -\sin 2\alpha_i \\ -\sin 2\alpha_i & 2\cos^2\alpha_i \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2) \tag{3.13}$$

and

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} F(x_i)\sin^2\alpha_i - \frac{1}{2}G(x_i)\sin 2\alpha_i \\ G(x_i)\cos^2\alpha_i - \frac{1}{2}F(x_i)\sin 2\alpha_i \end{pmatrix}. \tag{3.14}$$

These two equations constitute the main result of this article.

If Eq. (3.14) is rewritten in the form

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} F(x_i) - [F(x_i)\cos\alpha_i + G(x_i)\sin\alpha_i]\cos\alpha_i \\ G(x_i) - [F(x_i)\cos\alpha_i + G(x_i)\sin\alpha_i]\sin\alpha_i \end{pmatrix}, \tag{3.15}$$

it is immediately seen that, since the sine and the cosine never vanish simultaneously, at the end point $x = x_i$ one has

$$\begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} F(x_i) \\ G(x_i) \end{pmatrix} \tag{3.16}$$

if and only if

$$F(x_i)\cos\alpha_i + G(x_i)\sin\alpha_i = 0, \tag{3.17}$$

i.e., if and only if the function to be expanded obeys at $x = x_i$ the same homogeneous boundary condition as the basis eigenfunctions. If the boundary condition (3.17) is not satisfied, Eqs. (2.9) and (3.15) imply that at $x = x_i$ the eigenfunction expansion (2.7) has a discontinuity

$$\lim_{x \to x_i} \begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix} - \begin{pmatrix} \overline{F}(x_i) \\ \overline{G}(x_i) \end{pmatrix} = \begin{pmatrix} F(x_i)\cos^2\alpha_i + \frac{1}{2}G(x_i)\sin 2\alpha_i \\ \frac{1}{2}F(x_i)\sin 2\alpha_i + G(x_i)\sin^2\alpha_i \end{pmatrix}. \tag{3.18}$$

This fact was not realized in early formulations of the R-matrix theory for Dirac particles[7,8] which resulted in errors corrected by Szmytkowski and Hinze.[15,16]

It should be emphasized that the previous results are specific for bases generated by Dirac differential eigenproblems; the reader is asked to consult Appendix B on the analogous problem for second-order Sturm–Liouville eigensystems.

It is interesting to consider Eqs. (3.13) and (3.14) in two particular cases. The first case is

$$\cos\alpha_i=0\Rightarrow\sin\alpha_i=\pm 1. \tag{3.19}$$

Then Eqs. (3.13) and (3.14) become, respectively,

$$\sum_{n=-\infty}^{\infty}\begin{pmatrix} f_n(x_i)\\ g_n(x_i)\end{pmatrix}(f_n(x)\quad g_n(x))=\frac{\delta(x-x_i)}{\rho(x_i)}\begin{pmatrix}2&0\\0&0\end{pmatrix}\quad (x_1\leqslant x\leqslant x_2), \tag{3.20}$$

$$\begin{pmatrix}\overline{F}(x_i)\\ \overline{G}(x_i)\end{pmatrix}=\begin{pmatrix}F(x_i)\\0\end{pmatrix}. \tag{3.21}$$

It is seen that in this case the expansion converges at $x=x_i$ in the upper component but fails to converge in the lower one unless $G(x_i)=0$. The second case to be considered is

$$\sin\alpha_i=0\Rightarrow\cos\alpha_i=\pm 1. \tag{3.22}$$

Then

$$\sum_{n=-\infty}^{\infty}\begin{pmatrix} f_n(x_i)\\ g_n(x_i)\end{pmatrix}(f_n(x)\quad g_n(x))=\frac{\delta(x-x_i)}{\rho(x_i)}\begin{pmatrix}0&0\\0&2\end{pmatrix}\quad (x_1\leqslant x\leqslant x_2) \tag{3.23}$$

and

$$\begin{pmatrix}\overline{F}(x_i)\\ \overline{G}(x_i)\end{pmatrix}=\begin{pmatrix}0\\G(x_i)\end{pmatrix}, \tag{3.24}$$

i.e., at $x=x_i$ the expansion converges in the lower component but fails to converge in the upper one unless $F(x_i)=0$.

IV. AN ILLUSTRATIVE EXAMPLE

As an example illustrating the general results obtained earlier, in this section we discuss the particular case when the Dirac eigenvalue problem (2.1) and (2.2) is

$$\begin{pmatrix}-\lambda_n & -d/dx\\ d/dx & -\lambda_n\end{pmatrix}\begin{pmatrix}f_n(x)\\ g_n(x)\end{pmatrix}=0\quad (0\leqslant x\leqslant b), \tag{4.1}$$

$$f_n(0)=0,\quad f_n(b)\cos\beta+g_n(b)\sin\beta=0. \tag{4.2}$$

Comparing Eqs. (4.1) and (4.2) with (2.1) and (2.2), one identifies

$$\rho(x)\equiv 1,\quad x_1=0,\quad x_2=b,\quad \alpha_1=0,\quad \alpha_2=\beta. \tag{4.3}$$

Solving the system (4.1) and (4.2), one finds that its eigenvalues are

$$\lambda_n=\frac{\pi n-\beta}{b},\quad n=0,\pm 1,\pm 2,\ldots, \tag{4.4}$$

while corresponding eigenfunctions, normalized according to

$$\int_0^b dx[f_n(x)f_{n'}(x)+g_n(x)g_{n'}(x)]=\delta_{nn'}, \tag{4.5}$$

are

$$\begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix}=\frac{1}{\sqrt{b}}\begin{pmatrix} \sin\lambda_n x \\ \cos\lambda_n x \end{pmatrix} \quad (0\leqslant x\leqslant b). \tag{4.6}$$

A. The closure relation and its extension

To verify that eigensolutions to the system (4.1) and (4.2) do obey Eqs. (2.5) and (3.13), we should investigate the series

$$\sum_{n=-\infty}^{\infty}\begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix}(f_n(x') \quad g_n(x'))=\begin{pmatrix} I(x,x') & J(x,x') \\ K(x,x') & L(x,x') \end{pmatrix} \tag{4.7}$$

in the domain $0\leqslant x,x'\leqslant b$. We begin with considering the series

$$I(x,x')=\sum_{n=-\infty}^{\infty} f_n(x)f_n(x') \tag{4.8}$$

in the extended domain $-\infty<x,x'<\infty$. To sum it, we construct a sequence of finite sums

$$I_N(x,x')=\sum_{n=-N}^{N} f_n(x)f_n(x')=\frac{1}{b}\sum_{n=-N}^{N}\sin[(\pi n-\beta)x/b]\sin[(\pi n-\beta)x'/b]. \tag{4.9}$$

Obviously, one has

$$I(x,x')=\lim_{N\to\infty} I_N(x,x'). \tag{4.10}$$

The sum in Eq. (4.9) is easily found to be

$$\begin{aligned} I_N(x,x')=&\frac{\sin[\pi(2N+1)(x-x')/2b]}{2b\sin[\pi(x-x')/2b]}\cos[\beta(x-x')/b] \\ &-\frac{\sin[\pi(2N+1)(x+x')/2b]}{2b\sin[\pi(x+x')/2b]}\cos[\beta(x+x')/b]. \end{aligned} \tag{4.11}$$

With the aid of the formula

$$\lim_{N\to\infty}\frac{\sin(2N+1)\pi x}{\sin\pi x}=\sum_{n=-\infty}^{\infty}\delta(x-n) \quad (N\in\mathbb{N}), \tag{4.12}$$

which is well known in the theory of Fourier series,[17] from Eqs. (4.10) and (4.11) we infer

$$I(x,x')=\sum_{n=-\infty}^{\infty}[\delta(x-x'-2nb)-\delta(x+x'-2nb)]\cos 2n\beta. \tag{4.13}$$

Let us now restrict to the case when $0<x,x'<b$. Then

$$-b<x-x'<b, \quad 0<x+x'<2b. \tag{4.14}$$

It is evident that under the constraints (4.14) the argument of the first delta in the summand in Eq. (4.13) may vanish if and only if $n=0$, while the argument of the second delta never vanishes. Consequently, in this case all but one term on the right side of Eq. (4.13) are effectively zero and the latter equation reduces to

$$I(x,x')=\delta(x-x') \quad (0<x,x'<b), \tag{4.15}$$

in agreement with the result that may be inferred from Eqs. (2.5) and (4.3).

Next we concentrate on the case $0\leqslant x\leqslant b$ and $x'=0$. This case is the simplest one since then Eq. (4.13) becomes

$$I(x,0)=\sum_{n=-\infty}^{\infty}[\delta(x-2nb)-\delta(x-2nb)]\cos 2n\beta=0 \quad (0\leqslant x\leqslant b), \tag{4.16}$$

which agrees with the result that may be obtained from Eqs. (4.3) and (3.13).

Finally, we consider the most interesting case $x'=b$. Then

$$\begin{aligned} I(x,b)&=\sum_{n=-\infty}^{\infty}[\delta(x-(2n+1)b)-\delta(x-(2n-1)b)]\cos 2n\beta \\ &=2\sin\beta\sum_{n=-\infty}^{\infty}\delta(x-(2n+1)b)\sin[(2n+1)\beta] \quad (-\infty<x<\infty). \end{aligned} \tag{4.17}$$

If $0\leqslant x\leqslant b$, the argument of the delta may vanish if and only if $n=0$; the remaining terms in the series are effectively zero and Eq. (4.17) reduces to

$$I(x,b)=2\sin^2\beta\,\delta(x-b) \quad (0\leqslant x\leqslant b), \tag{4.18}$$

which again agrees with the result that may be deduced from Eqs. (4.3) and (3.13).

The reader will find no difficulty in verifying that in the domain $0\leqslant x,x'\leqslant b$ the remaining three matrix elements on the right side of Eq. (4.7) are identical with those deduced from Eqs. (2.5), (4.3), and (3.13).

B. The expansion problem

Consider now the expansion of the two-component function

$$\begin{pmatrix} F(x) \\ G(x) \end{pmatrix}=\frac{1}{\sqrt{b}}\begin{pmatrix} \sin\lambda x \\ \cos\lambda x \end{pmatrix} \quad (0\leqslant x\leqslant b), \tag{4.19}$$

where λ is a real parameter, in the basis (4.6). The expansion is

$$\begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix}=\sum_{n=-\infty}^{\infty}\frac{C_n}{\sqrt{b}}\begin{pmatrix} \sin\lambda_n x \\ \cos\lambda_n x \end{pmatrix} \quad (0\leqslant x\leqslant b) \tag{4.20}$$

with the expansion coefficients given by

$$C_n=\frac{1}{b}\int_0^b dx[\sin\lambda_n x\sin\lambda x+\cos\lambda_n x\cos\lambda x]=\frac{\sin(\lambda_n-\lambda)b}{(\lambda_n-\lambda)b}. \tag{4.21}$$

On utilizing the relationship

$$\sin(\lambda_n-\lambda)b=\frac{\sin(\lambda b+\beta)\sin\lambda_n b}{\sin\beta}, \tag{4.22}$$

which stems from elementary trigonometry and from the boundary condition (4.2), the expansion (4.20) becomes

$$\begin{pmatrix} \overline{F}(x) \\ \overline{G}(x) \end{pmatrix} = \frac{\sin(\lambda b+\beta)}{\sqrt{b}\sin\beta} \sum_{n=-\infty}^{\infty} \frac{\sin\lambda_n b}{(\lambda_n-\lambda)b} \begin{pmatrix} \sin\lambda_n x \\ \cos\lambda_n x \end{pmatrix} \quad (0\leqslant x\leqslant b). \tag{4.23}$$

Below we shall attempt to sum the series on the right side of Eq. (4.23) at the end points $x=0$ and $x=b$.

Let us begin with the end point $x=0$. Then the expansion (4.23) becomes

$$\begin{pmatrix} \overline{F}(0) \\ \overline{G}(0) \end{pmatrix} = \frac{\sin(\lambda b+\beta)}{\sqrt{b}\sin\beta} \sum_{n=-\infty}^{\infty} \frac{\sin\lambda_n b}{(\lambda_n-\lambda)b} \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{4.24}$$

It is obvious that $\overline{F}(0)=0$ while evaluation of $\overline{G}(0)$ requires summation of the series

$$S_1 = \sum_{n=-\infty}^{\infty} \frac{\sin\lambda_n b}{(\lambda_n-\lambda)b}. \tag{4.25}$$

To perform the summation, we rewrite S_1 as follows:

$$S_1 = \sum_{n=-\infty}^{\infty} \frac{(-)^{n+1}\sin\beta}{\pi n-(\lambda b+\beta)} = \sin\beta\left[\frac{1}{\lambda b+\beta} + \sum_{n=1}^{\infty}(-)^n \frac{2(\lambda b+\beta)}{(\lambda b+\beta)^2-(\pi n)^2}\right]. \tag{4.26}$$

On making use of the known[18] partial fraction expansion of $1/\sin z$,

$$\frac{1}{\sin z} = \frac{1}{z} + \sum_{n=1}^{\infty}(-)^n \frac{2z}{z^2-(\pi n)^2}, \tag{4.27}$$

we obtain

$$S_1 = \frac{\sin\beta}{\sin(\lambda b+\beta)}, \tag{4.28}$$

hence, it follows that

$$\begin{pmatrix} \overline{F}(0) \\ \overline{G}(0) \end{pmatrix} = \frac{1}{\sqrt{b}} \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{4.29}$$

The same result may be inferred from Eqs. (3.14), (4.3), and (4.19).

Next we turn to the case of the end point $x=b$. Then the object of our interest is the series

$$\begin{pmatrix} \overline{F}(b) \\ \overline{G}(b) \end{pmatrix} = \frac{\sin(\lambda b+\beta)}{\sqrt{b}\sin\beta} \sum_{n=-\infty}^{\infty} \frac{\sin\lambda_n b}{(\lambda_n-\lambda)b} \begin{pmatrix} \sin\lambda_n b \\ \cos\lambda_n b \end{pmatrix}. \tag{4.30}$$

To sum it, we have to consider the series

$$S_2 = \sum_{n=-\infty}^{\infty} \frac{\sin^2\lambda_n b}{(\lambda_n-\lambda)b}, \tag{4.31}$$

$$S_3 = \sum_{n=-\infty}^{\infty} \frac{\sin\lambda_n b\cos\lambda_n b}{(\lambda_n-\lambda)b}. \tag{4.32}$$

Of these, only S_2 has to be investigated since, because of Eqs. (4.2) and (4.6), we have

$$S_3 = -S_2 \cot\beta. \tag{4.33}$$

To deal with the series S_2, we rewrite it in the following way:

$$S_2 = \sum_{n=-\infty}^{\infty} \frac{\sin^2\beta}{\pi n - (\lambda b + \beta)} = -\sin^2\beta \left[\frac{1}{\lambda b + \beta} + \sum_{n=1}^{\infty} \frac{2(\lambda b + \beta)}{(\lambda b + \beta)^2 - (\pi n)^2} \right]. \tag{4.34}$$

Hence, because of the known[18] partial fraction expansion of $\cot z$,

$$\cot z = \frac{1}{z} + \sum_{n=1}^{\infty} \frac{2z}{z^2 - (\pi n)^2}, \tag{4.35}$$

we find

$$S_2 = -\sin^2\beta \cot(\lambda b + \beta). \tag{4.36}$$

Consequently, Eq. (4.30) becomes

$$\begin{pmatrix} \overline{F}(b) \\ \overline{G}(b) \end{pmatrix} = \frac{1}{\sqrt{b}} \begin{pmatrix} -\sin\beta \cos(\lambda b + \beta) \\ \cos\beta \cos(\lambda b + \beta) \end{pmatrix}. \tag{4.37}$$

The same result may be inferred from Eqs. (3.14), (4.3), and (4.19).

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APPENDIX A: AN ALTERNATIVE DERIVATION OF EQ. (3.12)

Consider an auxiliary inhomogeneous boundary value problem

$$\begin{pmatrix} p(x) - \lambda\rho(x) & -d/dx + t(x) \\ d/dx + t(x) & q(x) - \lambda\rho(x) \end{pmatrix} \begin{pmatrix} f(x) \\ g(x) \end{pmatrix} = 0 \quad (x_1 \leqslant x \leqslant x_2), \tag{A1}$$

$$f(x_i)\cos\alpha_i + g(x_i)\sin\alpha_i = A_i \quad (i = 1,2), \tag{A2}$$

where the functions $p(x)$, $q(x)$, $t(x)$ and $\rho(x)$ are the same that appear in Eq. (2.1), $\lambda \in \mathbb{R}$, $\lambda \neq \lambda_n$, $A_i \in \mathbb{R}$, and $A_1^2 + A_2^2 \neq 0$. We construct the series

$$\begin{pmatrix} \overline{f}(x) \\ \overline{g}(x) \end{pmatrix} = \sum_{n=-\infty}^{\infty} c_n \begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2) \tag{A3}$$

with the coefficients defined by

$$c_n = \int_{x_1}^{x_2} dx \rho(x) [f_n(x) f(x) + g_n(x) g(x)]. \tag{A4}$$

It is obvious that, because of regularity of $(f(x) \quad g(x))^{\mathrm{T}}$ [implied by Eq. (A1)], one has

$$\begin{pmatrix} \overline{f}(x) \\ \overline{g}(x) \end{pmatrix} = \begin{pmatrix} f(x) \\ g(x) \end{pmatrix} \quad (x_1 < x < x_2) \tag{A5}$$

[cf. Eq. (2.9)] but, because of Eq. (2.2) and the definition (A3),

$$\overline{f}(x_i)\cos\alpha_i + \overline{g}(x_i)\sin\alpha_i = 0. \tag{A6}$$

To find a convenient expression for the coefficients (A4), we premultiply Eq. (2.1) by $(f(x) \quad g(x))^{\mathrm{T}}$, Eq. (A1) by $(f_n(x) \quad g_n(x))^{\mathrm{T}}$, subtract and integrate the result over the interval $[x_1, x_2]$. This yields

$$(\lambda_n - \lambda)\int_{x_1}^{x_2} dx\,\rho(x)[f_n(x)f(x) + g_n(x)g(x)] = [f_n(x)g(x) - f(x)g_n(x)]\Big|_{x_1}^{x_2}, \tag{A7}$$

hence, on making use of the boundary conditions (2.2) and (A2) and the definition (A4), it follows

$$c_n = \frac{A_2 f_n(x_2)}{(\lambda_n - \lambda)\sin\alpha_2} - \frac{A_1 f_n(x_1)}{(\lambda_n - \lambda)\sin\alpha_1}. \tag{A8}$$

Next, let us operate from the left on both sides of Eq. (A9) with the differential operator appearing in Eq. (A1). Because of Eq. (2.1), this gives

$$\begin{pmatrix} p(x) - \lambda\rho(x) & -d/dx + t(x) \\ d/dx + t(x) & q(x) - \lambda\rho(x) \end{pmatrix} \begin{pmatrix} \overline{f}(x) \\ \overline{g}(x) \end{pmatrix} = \rho(x) \sum_{n=-\infty}^{\infty} c_n(\lambda_n - \lambda) \begin{pmatrix} f_n(x) \\ g_n(x) \end{pmatrix} \quad (x_1 \leqslant x \leqslant x_2) \tag{A9}$$

or, after utilizing the result (A8),

$$\left[\frac{d}{dx} + t(x)\right]\overline{f}(x) + [q(x) - \lambda\rho(x)]\overline{g}(x) = \frac{A_2}{\sin\alpha_2}\rho(x)\sum_{n=-\infty}^{\infty} f_n(x_2)g_n(x) - \frac{A_1}{\sin\alpha_1}\rho(x)\sum_{n=-\infty}^{\infty} f_n(x_1)g_n(x) \quad (x_1 \leqslant x \leqslant x_2) \tag{A10}$$

and

$$\left[-\frac{d}{dx} + t(x)\right]\overline{g}(x) + [p(x) - \lambda\rho(x)]\overline{f}(x) = \frac{A_2}{\sin\alpha_2}\rho(x)\sum_{n=-\infty}^{\infty} f_n(x_2)f_n(x) - \frac{A_1}{\sin\alpha_1}\rho(x)\sum_{n=-\infty}^{\infty} f_n(x_1)f_n(x) \quad (x_1 \leqslant x \leqslant x_2). \tag{A11}$$

Right sides of Eqs. (A10) and (A11) may be transformed if one makes use of Eq. (3.3). This results in

$$\left[\frac{d}{dx} + t(x)\right]\overline{f}(x) + [q(x) - \lambda\rho(x)]\overline{g}(x) = -\frac{A_2 I_2 \cot\alpha_2}{\sin\alpha_2}\delta(x - x_2) + \frac{A_1 I_1 \cot\alpha_1}{\sin\alpha_1}\delta(x - x_1) \quad (x_1 \leqslant x \leqslant x_2), \tag{A12}$$

$$\left[-\frac{d}{dx}+t(x)\right]\overline{g}(x)+[p(x)-\lambda\rho(x)]\overline{f}(x)=\frac{A_2I_2}{\sin\alpha_2}\delta(x-x_2)-\frac{A_1I_1}{\sin\alpha_1}\delta(x-x_1)$$
$$(x_1\leqslant x\leqslant x_2). \tag{A13}$$

In the following step, we integrate Eqs. (A12) and (A13) either from x_1 to $x<x_2$, passing then to the limit $x\downarrow x_1$, or from $x>x_1$ to x_2, passing then to the limit $x\uparrow x_2$. The results may be compactly written as

$$f(x_i)-\overline{f}(x_i)=\frac{A_iI_i\cot\alpha_i}{2\sin\alpha_i}, \tag{A14}$$

$$g(x_i)-\overline{g}(x_i)=\frac{A_iI_i}{2\sin\alpha_i}. \tag{A15}$$

After supplementing Eqs. (A14) and (A15) by the boundary condition (A6), we obtain a set of three linear algebraic equations for three unknowns I_i, $\overline{f}(x_i)$ and $\overline{g}(x_i)$. Solving this set for I_i, one obtains

$$I_i=2\sin^2\alpha_i, \tag{A16}$$

which coincides with Eq. (3.12).

APPENDIX B: EXPANSIONS IN EIGENFUNCTIONS OF SECOND-ORDER STURM–LIOUVILLE SYSTEMS

Consider the second-order Sturm–Liouville eigensystem

$$\frac{d}{dx}\left(p(x)\frac{df_n(x)}{dx}\right)+q(x)f_n(x)-\lambda_n\rho(x)f_n(x)=0 \quad (x_1\leqslant x\leqslant x_2), \tag{B1}$$

$$f_n(x_i)\cos\alpha_i+p(x_i)f_n'(x_i)\sin\alpha_i=0 \quad (i=1,2) \tag{B2}$$

on the finite interval $[x_1,x_2]\subset\mathbb{R}$. Here $p(x)$, $q(x)$, and $\rho(x)$ are real, bounded and continuous functions of the variable $x\in[x_1,x_2]$, with the additional constraints $\rho(x)>0$, $p(x)\in C^1([x_1,x_2])$, and $p(x)\neq 0$, while α_1 and α_2 are real constants. Provided the eigenfunctions to the system (B1) and (B2) have been normalized according to

$$\int_{x_1}^{x_2}dx\rho(x)f_n(x)f_{n'}(x)=\delta_{nn'}, \tag{B3}$$

it holds

$$\sum_{n=0}^{\infty}f_n(x)f_n(x')=\frac{\delta(x-x')}{\sqrt{\rho(x)\rho(x')}} \quad (x_1<x,x'<x_2) \tag{B4}$$

and

$$\sum_{n=0}^{\infty}f_n(x_i)f_n(x)=\frac{I_i\delta(x-x_i)}{\rho(x_i)} \quad (x_1\leqslant x\leqslant x_2), \tag{B5}$$

where

$$I_i=\begin{cases}2 & \text{for } \sin\alpha_i\neq 0\\ 0 & \text{for } \sin\alpha_i=0.\end{cases} \tag{B6}$$

Equations (B5) and (B6) may be obtained in a way similar to that in which Eq. (3.13) has been derived.

Let $F(x)$ be any continuous function of bounded variation in $[x_1,x_2]$. Then, it follows from Eqs. (B4)–(B6) that its eigenfunction expansion, defined as

$$\overline{F}(x)=\sum_{n=0}^{\infty} f_n(x)\int_{x_1}^{x_2} dx'\rho(x')f_n(x')F(x') \quad (x_1\leqslant x\leqslant x_2), \tag{B7}$$

has the following properties:

$$\overline{F}(x)=F(x) \quad (x_1<x<x_2), \tag{B8}$$

$$\overline{F}(x_i)=\begin{cases}F(x_i) & \text{for } \sin\alpha_i\neq 0,\\ 0 & \text{for } \sin\alpha_i=0.\end{cases} \tag{B9}$$

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[12] In some cases it is convenient to define the Dirac delta function in the following way (Ref. 13):
$$\int_a^b dx'\,\delta(x-x')\phi(x')=\begin{cases}0 & \text{for } x<a<b \text{ or } a<b<x\\ \phi(x) & \text{for } a\leqslant x\leqslant b\end{cases},$$
for any interval $[a,b]\subset\mathbb{R}$ and any function $\phi(x)$ that is sufficiently regular in $[a,b]$. This definition, which differs from the one used in the present work, is usually adopted in the R-matrix theory when a Bloch operator is employed (Ref. 14). Either definition of the delta is correct as long as it is used consistently.
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Comment on "Exact constructions of square-root Helmholtz operator symbols: The focusing quadratic profile" [J. Math. Phys. 41, 4881 (2000)]

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In a recent article, Fishman *et al.*[1] gave the exact, standard and Weyl symbol constructions for both the inverse square root and the square-root Helmholtz operators for a position-dependent refractive index field of the form

$$K^2(z)=K_0^2-\omega^2 z^2, \tag{1}$$

where $K(\cdot)$ denotes the refractive index field, K_0, ω are positive constants, and the z axis is perpendicular to the propagation direction, which is along the x axis. The form of K given in Eq. (1) is known as the focusing quadratic profile.[1]

In Ref. 1, an extensive, in-depth analytical study is carried out and numerical results are presented in the form of two-dimensional graphs illustrating cross sections of the real and imaginary parts of the operator symbol surfaces over the pq plane. Unfortunately, a subsequent reexamination of the numerical results given in Ref. 1 has revealed that the computer program used to generate the first five of the six figures corresponding to the standard operator symbol (Ref. 1, Figs. 7–11), $h^s_{\mathbf{B}}(p,q)$, contained erroneous code.[2] Of the five figures in question, however, it is only in the first three (Ref. 1, Figs. 7–9) that the effects of the flawed computer code are immediately apparent. [As we will see, the last two of these five figures (Ref. 1, Figs. 10 and 11) appear to be virtually identical to their correct counterparts.]

The purpose of the present communication is to point out these erroneous figures and to give their corrected versions for the record. To this end, we return to Ref. 1, Eq. (III.40) and evaluate the contour integral appearing in that expression along the path $\mathcal{L}=\mathcal{C}''=\Gamma_1''+\Gamma_2''+\Gamma_3''$ in the complex τ plane in the indicated direction (see Ref. 1, Fig. 6). After simplifying, we find that the standard operator symbol corresponding to Eq. (1) is

$$h^s_{\mathbf{B}}(p,q)=h^s_{\mathbf{B},1}(p,q)+h^s_{\mathbf{B},2}(p,q)+h^s_{\mathbf{B},3}(p,q) \quad (Y\neq 0,1,2,3,\ldots), \tag{2}$$

where $\tau=x+\mathrm{i}y$, $Y=K_0^2(\bar{k}/\omega)$, p is the Fourier parameter, q replaces z as the transverse coordinate, and

$$h^s_{\mathbf{B},1}(p,q)=-\mathrm{i}(\omega/(\bar{k}\pi))^{1/2}\int_0^{1/Y}\mathrm{d}x\,\exp[Yx-(\chi/2)\tanh[2x]+\mathrm{i}Z(\operatorname{sech}[2x]-1)]\sqrt{\operatorname{sech}[2x]}$$
$$\times\{Y-\chi\operatorname{sech}^2[2x]-2\mathrm{i}Z\operatorname{sech}[2x]\tanh[2x]-\tanh[2x]\}\,x^{-1/2}, \tag{3}$$

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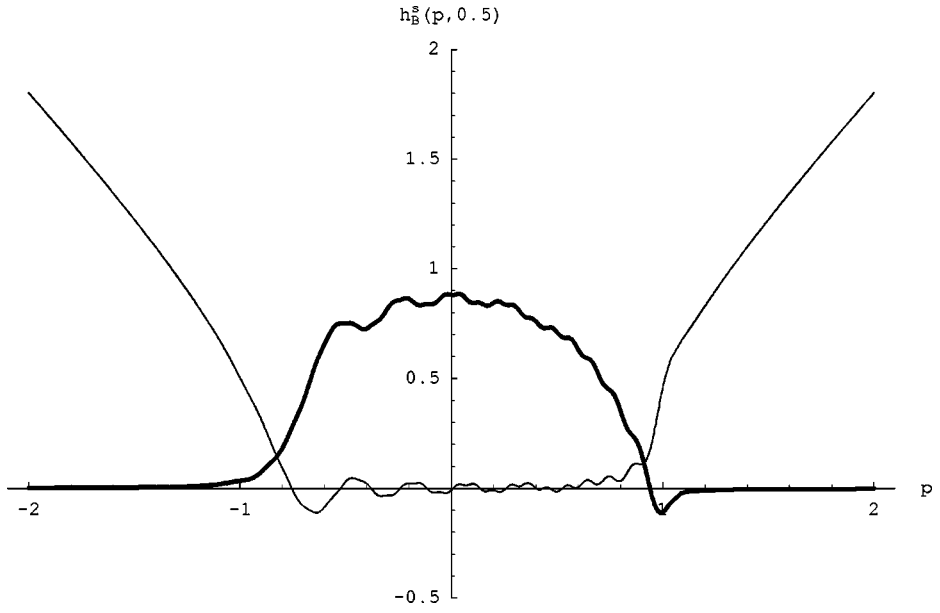

FIG. 1. (corrected form of Ref. 1, Fig. 7). $h^s_{\mathbf{B}}(p,q)$ vs p for $K^2(q)=K_0^2-\omega^2q^2$ with $K_0=\omega=1$, $q=0.5$, and $\overline{k}=50.5$. Bold line: Re$[h^s_{\mathbf{B}}(p,0.5)]$. Thin line: Im$[h^s_{\mathbf{B}}(p,0.5)]$.

$$h^s_{\mathbf{B},2}(p,q)=(2\omega/(\overline{k}\pi))^{1/2}\int_0^{2\pi}\mathrm{d}y\,\exp[Y(1/Y+\mathrm{i}y)-(\chi/2)\tanh[2(1/Y+\mathrm{i}y)]$$
$$+\mathrm{i}Z(\mathrm{sech}[2(1/Y+\mathrm{i}y)]-1)]$$
$$\times\exp[-(1/Y+\mathrm{i}y)]_2F_1[1/2,1;1;-\exp[-4(1/Y+\mathrm{i}y)]]$$
$$\times\{Y-\chi\,\mathrm{sech}^2[2(1/Y+\mathrm{i}y)]$$
$$-2\mathrm{i}Z\,\mathrm{sech}[2(1/Y+\mathrm{i}y)]\tanh[2(1/Y+\mathrm{i}y)]-\tanh[2(1/Y+\mathrm{i}y)]\}(1/Y+\mathrm{i}y)^{-1/2},\quad(4)$$

$$h^s_{\mathbf{B},3}(p,q)=-\pi^{-1}(\omega/\overline{k})^{1/2}\exp[\mathrm{i}\pi(2Y+3/4)]\int_0^{2\pi}\mathrm{d}y\,\Phi[\exp[2\mathrm{i}\pi Y],1/2,1-\mathrm{i}(1/Y+\mathrm{i}y)/(2\pi)]$$
$$\times\exp[-(1/Y+\mathrm{i}y)]_2F_1[1/2,1;1;-\exp[-4(1/Y+\mathrm{i}y)]]$$
$$\times\exp[Y(1/Y+\mathrm{i}y)-(\chi/2)\tanh[2(1/Y+\mathrm{i}y)]+\mathrm{i}Z(\mathrm{sech}[2(1/Y+\mathrm{i}y)]-1)]$$
$$\times\{Y-\chi\,\mathrm{sech}^2[2(1/Y+\mathrm{i}y)]-2\mathrm{i}Z\,\mathrm{sech}[2(1/Y+\mathrm{i}y)]\tanh[2(1/Y+\mathrm{i}y)]$$
$$-\tanh[2(1/Y+\mathrm{i}y)]\},\quad(5)$$

and where $\overline{k}(>0)$ is a reference wave number, $\chi=\overline{k}(p^2+\omega^2q^2)/\omega$, $Z=\overline{k}pq$, $\Phi[\xi,\sigma,\Delta]=\Sigma_{n=0}^{\infty}\xi^n/(\Delta+n)^{\sigma}$ is the Lerch transcendent,[3,4] ${}_2F_1[a,b;c;\xi]$ is the hypergeometric function defined in terms of the Gauss series,[3,5] and we have taken $\mathrm{R}=1/Y$ (see Ref. 1, Fig. 6 and p. 4921). In the expression for $h^s_{\mathbf{B}}(p,q)$ [i.e., Eq. (2)], $h^s_{\mathbf{B},1}(p,q)$ denotes the contribution arising from $\Gamma_1''+\Gamma_3''$, which was combined and simplified using the identity given in [Ref. 1, Eq. (III. 20)] with $m=1$, while the sum $h^s_{\mathbf{B},2}(p,q)+h^s_{\mathbf{B},3}(p,q)$ represents the contribution from the single line segment Γ_2'' (see Ref. 1, Fig. 6).

Having expressed $h^s_{\mathbf{B}}(p,q)$ as the sum of three, one-dimensional definite integrals, we are now in a position to numerically evaluate these integrals and plot the corrected figures. To accomplish this, MATHEMATICA 4.0 (see Ref. 3) was employed. This particular software package was chosen

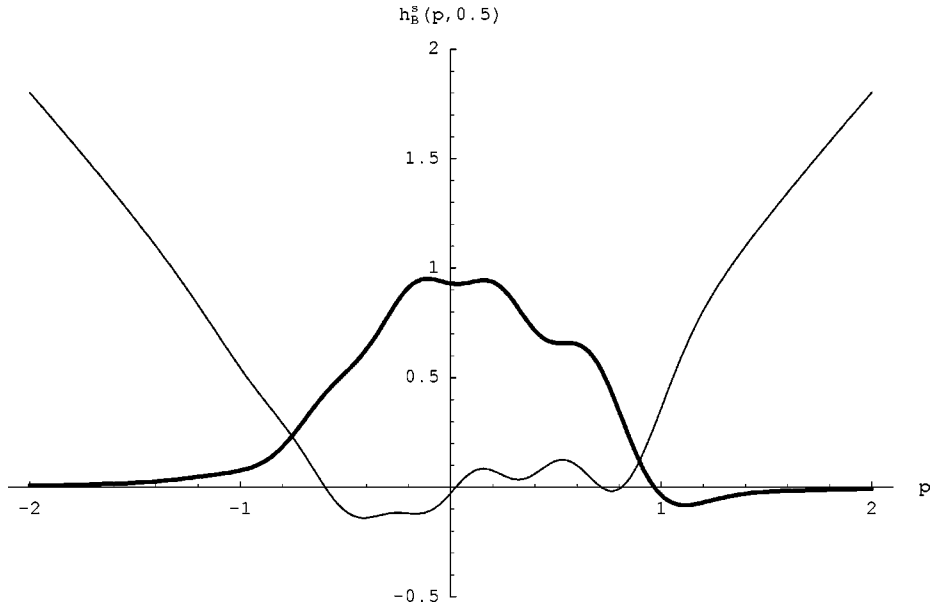

FIG. 2. (corrected form of Ref. 1, Fig. 8). $h^s_{\mathbf{B}}(p,q)$ vs p for $K^2(q)=K_0^2-\omega^2q^2$ with $K_0=\omega=1$, $q=0.5$, and $\overline{k}=10.5$. Bold line: Re$[h^s_{\mathbf{B}}(p,0.5)]$. Thin line: Im$[h^s_{\mathbf{B}}(p,0.5)]$.

because of its robust, adaptive numerical integration routines, it offers the Lerch transcendent and the ${}_2F_1$ hypergeometric as built-in functions that are tabulated for complex values of their arguments, and it is equipped with flexible graphics capabilities.

Obviously, for $q=0.5$ and $\overline{k}=50.5$, 10.5 the differences between the correct figures, Figs. 1 and 2, and the erroneous figures (Ref. 1, Figs. 7 and 8, respectively) are very pronounced, especially in terms of their oscillatory behavior. Note, however, that as the value of $\overline{k}$ is reduced, the

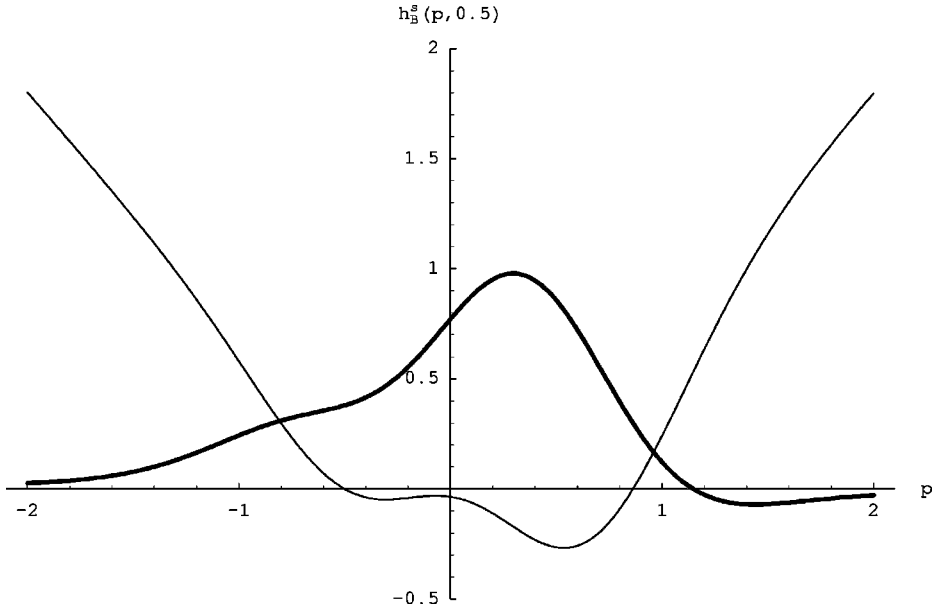

FIG. 3. (corrected form of Ref. 1, Fig. 9). $h^s_{\mathbf{B}}(p,q)$ vs p for $K^2(q)=K_0^2-\omega^2q^2$ with $K_0=\omega=1$, $q=0.5$, and $\overline{k}=3.5$. Bold line: Re$[h^s_{\mathbf{B}}(p,0.5)]$. Thin line: Im$[h^s_{\mathbf{B}}(p,0.5)]$.

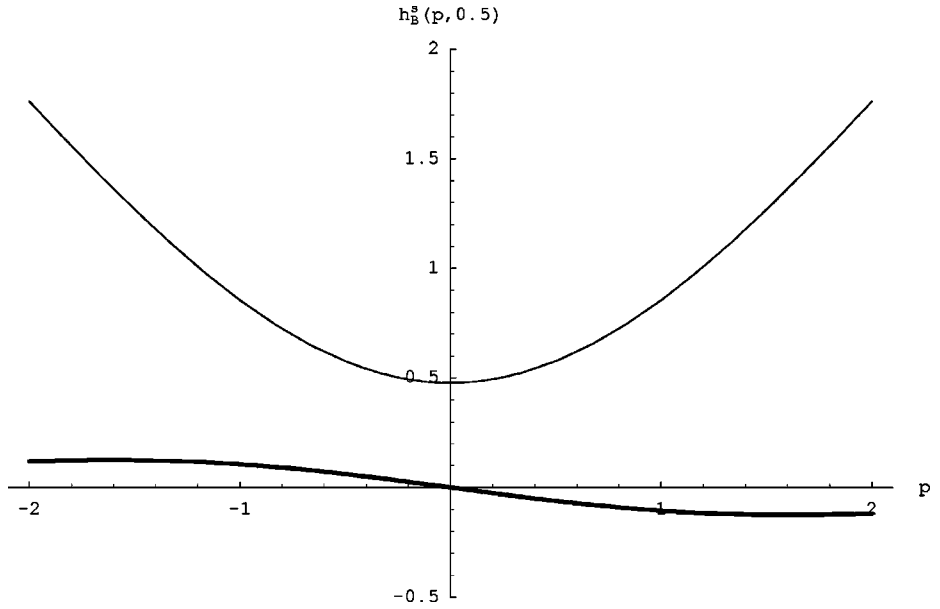

FIG. 4. (corrected form of Ref. 1, Fig. 10). $h^s_{\mathbf{B}}(p,q)$ vs p for $K^2(q)=K_0^2-\omega^2q^2$ with $K_0=\omega=1$, $q=0.5$, and $\overline{k}=0.5$. Bold line: Re$[h^s_{\mathbf{B}}(p,0.5)]$. Thin line: Im$[h^s_{\mathbf{B}}(p,0.5)]$.

last two erroneous figures corresponding to $q=0.5$ (Ref. 1, Figs. 9 and 10) approach their correct counterparts, Figs. 3 and 4, respectively. In fact, for $q=\overline{k}=0.5$ the correct and erroneous figures, that is, Fig. 4 and Ref. 1, Fig. 10, respectively, are virtually indistinguishable. Moreover, Figs. 1–4, all of which were plotted for $q=0.5$, exemplify the behavior of $h^s_{\mathbf{B}}(p,q)$ for the same value of q within the profile's well. Consider now Ref. 1, Fig. 11 and its correct counterpart Fig. 5, which were plotted for $q=1.5$ and therefore represent $h^s_{\mathbf{B}}(p,q)$ outside the well. Interestingly,

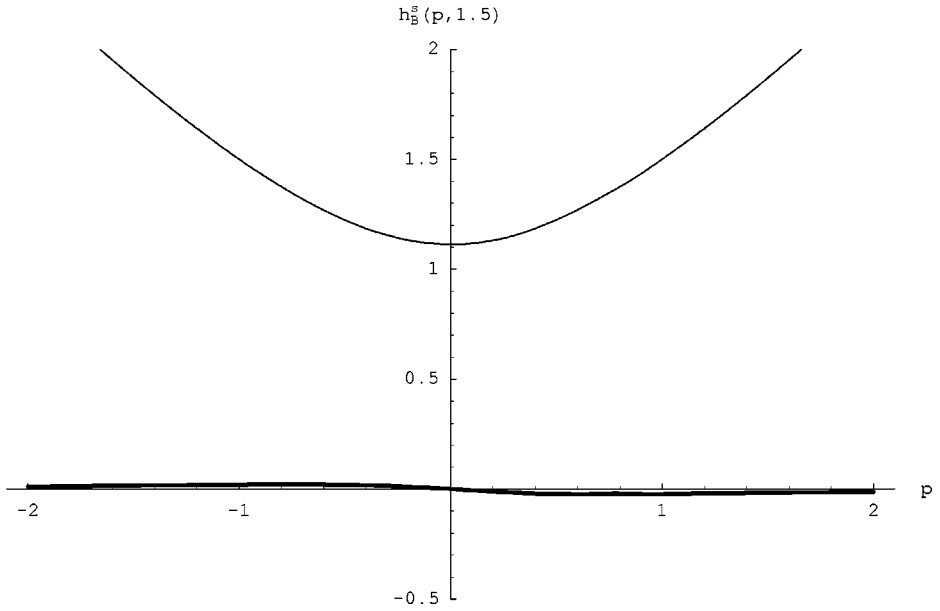

FIG. 5. (corrected form of Ref. 1, Fig. 11). $h^s_{\mathbf{B}}(p,q)$ vs p for $K^2(q)=K_0^2-\omega^2q^2$ with $K_0=\omega=1$, $q=1.5$, and $\overline{k}=10.5$. Bold line: Re$[h^s_{\mathbf{B}}(p,1.5)]$. Thin line: Im$[h^s_{\mathbf{B}}(p,1.5)]$.

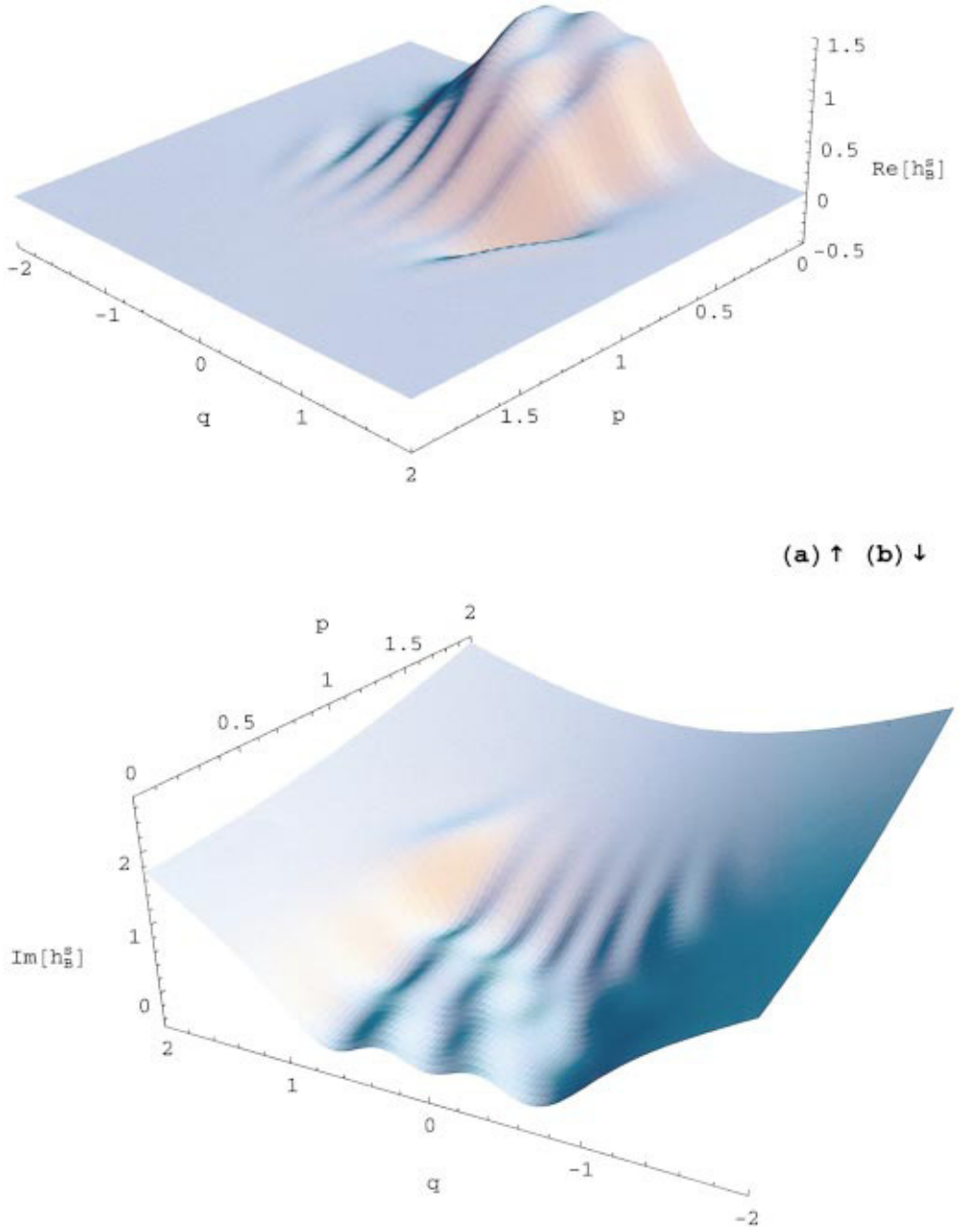

FIG. 6. (Color.) $h^s_{\mathbf{B}}(p,q)$ vs p and q for $K^2(q)=K_0^2-\omega^2q^2$ with $K_0=\omega=1$ and $\overline{k}=10.5$. (a) Re$[h^s_{\mathbf{B}}(p,q)]$. (b) Im$[h^s_{\mathbf{B}}(p,q)]$.

considering the relatively large value of $\overline{k}(=10.5)$ used, a comparison of these two figures reveals that they too are almost identical.

Finally, so as to give the reader a more complete picture, portions of the real and imaginary parts of the operator symbol surface corresponding to $h^s_{\mathbf{B}}(p,q)$ with $\overline{k}=10.5$ are given in Figs. 6(a) and 6(b), respectively. As mentioned earlier, Figs. 2 and 5 depict cross sections of the surfaces shown in Fig. 6 for fixed values of $q(=0.5,1.5)$ while Ref. 1, Fig. 12 does the same (correctly) for fixed $p(=0)$. When these cross sections are compared with the actual surfaces, however, it quickly becomes evident that the former provides very limited insight into the nature of the latter. Indeed, it appears quite difficult to grasp the intricate oscillatory structure exhibited by these

surfaces by simply viewing a collection of various cross sections. The reader is referred to Ref. 1, pp. 4922–4924 for details on the analytical properties of the surfaces appearing in Fig. 6.

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Small-energy asymptotics of the scattering matrix for the matrix Schrödinger equation on the line

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The one-dimensional matrix Schrödinger equation is considered when the matrix potential is self-adjoint with entries that are integrable and have finite first moments. The small-energy asymptotics of the scattering coefficients are derived, and the continuity of the scattering coefficients at zero energy is established. When the entries of the potential have also finite second moments, some more detailed asymptotic expansions are presented. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1398059]

I. INTRODUCTION

Consider the matrix Schrödinger equation

$$\psi''(k,x)+k^2\psi(k,x)=Q(x)\psi(k,x), \quad x\in\mathbf{R}, \tag{1.1}$$

where $x\in\mathbf{R}$ is the spatial coordinate, the prime denotes the derivative with respect to x, k^2 is the energy, $Q(x)$ is an $n\times n$ self-adjoint matrix potential, i.e., $Q(x)^\dagger=Q(x)$ with the dagger standing for the matrix conjugate transpose, and $\psi(k,x)$ is either an $n\times 1$ or an $n\times n$ matrix function. We use $\|\cdot\|$ to denote the (Euclidean) norm of a vector or the operator norm of a matrix. Let $L^1_m(\mathbf{R};\mathbf{C}^{n\times n})$ with $m\geqslant 0$ denote the Banach space of all measurable $n\times n$ matrix functions f for which $(1+|x|)^m\|f(x)\|$ is integrable on $\mathbf{R}$. If $n=1$, we denote this space by $L^1_m(\mathbf{R})$. In this paper we always assume that Q is self-adjoint and belongs to $L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$. Certain results will be obtained under the assumption that $Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$, but we will clearly indicate when this stronger assumption is needed. We use $\mathbf{C}^+$ to denote the upper-half complex plane and write $\overline{\mathbf{C}^+}$ for $\mathbf{C}^+\cup\mathbf{R}$.

Among the $n\times n$ solutions of (1.1) are the so-called Jost solution from the left, $f_l(k,x)$, and the Jost solution from the right, $f_r(k,x)$, satisfying the asymptotic boundary conditions

$$e^{-ikx}f_l(k,x)=I_n+o(1) \text{ and } e^{-ikx}f_l'(k,x)=ikI_n+o(1), \quad x\to+\infty, \tag{1.2}$$

$$e^{ikx}f_r(k,x)=I_n+o(1) \text{ and } e^{ikx}f_r'(k,x)=-ikI_n+o(1), \quad x\to-\infty, \tag{1.3}$$

where I_n denotes the identity matrix of order n. The existence of the Jost solutions can be established as in the scalar ($n=1$) case[1,2] by using the appropriate integral equations[3,4] [cf. (2.2), (2.3), and Theorem 2.1 in our paper].

For each $k\in\mathbf{R}\backslash\{0\}$ we have

$$f_l(k,x)=a_l(k)e^{ikx}+b_l(k)e^{-ikx}+o(1), \quad x\to-\infty, \tag{1.4}$$

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$$f_{\rm r}(k,x)=a_{\rm r}(k)e^{-ikx}+b_{\rm r}(k)e^{ikx}+o(1), \quad x\to+\infty, \tag{1.5}$$

where $a_{\rm l}(k)$, $b_{\rm l}(k)$, $a_{\rm r}(k)$, and $b_{\rm r}(k)$ are some $n\times n$ matrix functions of k. These matrix functions enter the scattering matrix $\mathbf{S}(k)$ defined in (2.22), and our primary aim is the analysis of the small-k behavior of $\mathbf{S}(k)$.

The motivation for this paper comes from our interest in the inverse scattering problem for (1.1), namely the recovery of Q from an appropriate set of data involving the scattering matrix. As is known from the scalar case, it is important to have detailed information about the behavior of $\mathbf{S}(k)$ for small k. For example,[1,2] this information is used to characterize the scattering data, so as to ensure that the potential Q constructed from the data at hand belongs to a certain class of functions such as $L^1_1(\mathbf{R})$ or $L^1_2(\mathbf{R})$. The inverse scattering problem for (1.1) when $n>1$ has been considered by several authors,[4–10] but we are not aware of any in-depth study of the small-k behavior of $\mathbf{S}(k)$. Not even the continuity of the scattering matrix at $k=0$ seems to have been established when $Q\in L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$; for example, in Ref. 6 (p. 294), the continuity at $k=0$ of the transmission coefficients is *assumed*. In the scalar case it is well known[1,2,11,12] that the continuity of $\mathbf{S}(k)$ at $k=0$ is easy to establish if $Q\in L^1_2(\mathbf{R})$, but not if only $Q\in L^1_1(\mathbf{R})$. In the matrix case, the situation is somewhat different. The decay of $Q(x)$ as $x\to\pm\infty$ plays an important role, but there are further complications due to the particular structure of the solution space of (1.1) at $k=0$. From the scalar case it is known[1,2,11] that the behavior of the solutions of (1.1) at $k=0$ makes it necessary to distinguish between two cases, the *generic case* and the *exceptional case*, and that the small-k behavior of $\mathbf{S}(k)$ is different in each case. If $n>1$, the situation is more complicated because the exceptional case gives rise to a variety of possibilities depending on the Jordan structure of a certain matrix associated with the solution space of (1.1) at $k=0$. In this paper we clarify the connection between the solutions of (1.1) at $k=0$ and the behavior of $\mathbf{S}(k)$ near $k=0$. As a result, we are able to prove the continuity of the scattering matrix at $k=0$ when $Q\in L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$ and to obtain more detailed asymptotic expansions when $Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$. The inverse problem is not considered here; we may report on it elsewhere.

This paper is organized as follows. In Sec. II we establish our notations and review some basic known results on the solutions of (1.1). Since this material is standard, we refer the reader to the literature for proofs and more details. In Sec. II we also give various characterizations of the generic and exceptional cases. In Sec. III we prove the continuity of the scattering matrix at $k=0$ in the generic case, and we obtain some more detailed asymptotic results when $Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$. The exceptional case is treated in Sec. IV; the main results are contained in Theorem 4.6 when $Q\in L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$ and in Theorem 4.7 when $Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$, where we prove the continuity and differentiability of $\mathbf{S}(k)$ at $k=0$, respectively. In Sec. V we discuss some special cases that illustrate the results of Sec. IV. Finally, the Appendix contains the proof of Proposition 4.2, which is a key result needed to establish Theorems 4.6 and 4.7.

II. SCATTERING COEFFICIENTS AND A CASE DISTINCTION

In this section we review some basic results about those solutions of (1.1) that are relevant to scattering theory, and we define the scattering coefficients and some related quantities. We also elaborate on the distinction between the generic case and the exceptional case which will play an important role in the subsequent sections.

We define the Faddeev functions $m_{\rm l}(k,x)$ and $m_{\rm r}(k,x)$ by

$$m_{\rm l}(k,x)=e^{-ikx}f_{\rm l}(k,x), \quad m_{\rm r}(k,x)=e^{ikx}f_{\rm r}(k,x). \tag{2.1}$$

From (1.2), (1.3), and (2.1) it follows that

$$m_{\rm l}(k,x)=I_n+\frac{1}{2ik}\int_x^\infty dy\,[e^{2ik(y-x)}-1]Q(y)m_{\rm l}(k,y), \tag{2.2}$$

$$m_{\rm r}(k,x)=I_n+\frac{1}{2ik}\int_{-\infty}^{x}dy\,[e^{2ik(x-y)}-1]Q(y)m_{\rm r}(k,y). \tag{2.3}$$

Some properties of the matrix functions $m_{\rm l}(k,x)$ and $m_{\rm r}(k,x)$ are summarized in the next theorem and its corollary. The proofs of these results can be obtained as in the scalar case and we refer the reader to the literature;[2–4,11] in particular, see Theorem 1.4.1 in Ref. 3 and Theorem 1 in Ref. 4. We denote differentiation with respect to k by an overdot and use C for suitable constants that do not depend on x or k.

Theorem 2.1: *If $Q\in L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$, then, for each $x\in\mathbf{R}$, the functions $m_{\rm l}(k,x)$, $m_{\rm r}(k,x)$, $m'_{\rm l}(k,x)$, and $m'_{\rm r}(k,x)$ are analytic in $k\in\mathbf{C}^+$* and *continuous in $k\in\overline{\mathbf{C}^+}$; moreover*

$$m_{\rm l}(k,x)=I_n+o(1),\quad m'_1(k,x)=o(1/x),\quad x\to+\infty, \tag{2.4}$$

$$m_{\rm r}(k,x)=I_n+o(1),\quad m'_{\rm r}(k,x)=o(1/x),\quad x\to-\infty,$$

$$\|m_{\rm l}(k,x)\|\leq C[1+\max\{0,-x\}],\quad \|m_{\rm r}(k,x)\|\leq C[1+\max\{0,x\}],\quad k\in\overline{\mathbf{C}^+}. \tag{2.5}$$

In addition, if $Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$, then $\dot m_{\rm l}(k,x)$ and $\dot m_{\rm r}(k,x)$ exist, are analytic in $\mathbf{C}^+$, continuous in $\overline{\mathbf{C}^+}$, and satisfy the estimates

$$\|\dot m_{\rm l}(k,x)\|\leq C(1+x^2),\quad \|\dot m_{\rm r}(k,x)\|\leq C(1+x^2),\quad k\in\overline{\mathbf{C}^+}.$$

In the following an asterisk will be used to denote complex conjugation. From (2.1) and Theorem 2.1 we get the following.

Corollary 2.2: Assume $Q\in L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$. Then, for each fixed $x\in\mathbf{R}$, the four matrix functions $f_{\rm l}(-k^*,x)^\dagger$, $f_{\rm r}(-k^*,x)^\dagger$, $f'_1(-k^*,x)^\dagger$, and $f'_{\rm r}(-k^*,x)^\dagger$ are analytic in $k\in\mathbf{C}^+$ and continuous in $\overline{\mathbf{C}^+}$. Moreover, if $Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$, then these functions are differentiable with respect to $k\in\overline{\mathbf{C}^+}$.

The scattering coefficients will be defined in terms of certain Wronskians involving the Jost solutions. We first state a standard result about such Wronskians, which is a consequence of the selfadjointness of Q. Let $[F;G]=FG'-F'G$ denote the Wronskian of two square matrix functions $F(x)$ and $G(x)$.

Proposition 2.3: For $k\in\mathbf{C}$, let $\phi(k,x)$ be any $n\times p$ solution and $\psi(k,x)$ any $n\times q$ solution of (1.1). Then the $p\times q$ Wronskian matrix $[\phi(\pm k^*,x)^\dagger;\psi(k,x)]$ is independent of x.

As a result of Proposition 2.3 the matrices $a_{\rm l}(k)$, $b_{\rm l}(k)$, $a_{\rm r}(k)$, and $b_{\rm r}(k)$ appearing in (1.4) and (1.5) can be expressed in terms of certain Wronskians of the Jost solutions as follows:

$$a_{\rm l}(k)=\frac{1}{2ik}[f_{\rm r}(-k^*,x)^\dagger;f_{\rm l}(k,x)],\quad k\in\overline{\mathbf{C}^+}\backslash\{0\}, \tag{2.6}$$

$$a_{\rm r}(k)=-\frac{1}{2ik}[f_1(-k^*,x)^\dagger;f_{\rm r}(k,x)],\quad k\in\overline{\mathbf{C}^+}\backslash\{0\}, \tag{2.7}$$

$$b_{\rm l}(k)=-\frac{1}{2ik}[f_{\rm r}(k,x)^\dagger;f_{\rm l}(k,x)],\quad k\in\mathbf{R}\backslash\{0\}, \tag{2.8}$$

$$b_{\rm r}(k)=\frac{1}{2ik}[f_1(k,x)^\dagger;f_{\rm r}(k,x)],\quad k\in\mathbf{R}\backslash\{0\}. \tag{2.9}$$

Alternatively, it is sometimes convenient to use the integral representations

$$a_{\rm l}(k)=I_n-\frac{1}{2ik}\int_{-\infty}^{\infty}dx\,Q(x)m_{\rm l}(k,x), \tag{2.10}$$

$$a_{\rm r}(k)=I_n-\frac{1}{2ik}\int_{-\infty}^{\infty}dx\,Q(x)m_{\rm r}(k,x), \tag{2.11}$$

$$b_{\rm l}(k)=\frac{1}{2ik}\int_{-\infty}^{\infty}dx\,e^{2ikx}\,Q(x)m_1(k,x), \tag{2.12}$$

$$b_{\rm r}(k)=\frac{1}{2ik}\int_{-\infty}^{\infty}dx\,e^{-2ikx}\,Q(x)m_{\rm r}(k,x), \tag{2.13}$$

which follow from (1.4), (1.5), and (2.1)–(2.5). Also, with the help of (1.2)–(1.5) and (2.6)–(2.9), we obtain

$$a_{\rm r}(-k^*)^\dagger=a_{\rm l}(k),\quad k\in\overline{\mathbf{C}^+}\backslash\{0\}, \tag{2.14}$$

$$b_{\rm r}(k)=-b_{\rm l}(k)^\dagger,\quad k\in\mathbf{R}\backslash\{0\}, \tag{2.15}$$

$$a_{\rm l}(k)^\dagger a_{\rm l}(k)=b_{\rm l}(k)^\dagger b_{\rm l}(k)+I_n,\quad k\in\mathbf{R}\backslash\{0\}, \tag{2.16}$$

$$a_{\rm r}(k)^\dagger a_{\rm r}(k)=b_{\rm r}(k)^\dagger b_{\rm r}(k)+I_n,\quad k\in\mathbf{R}\backslash\{0\}, \tag{2.17}$$

$$a_{\rm l}(-k)^\dagger b_{\rm l}(k)=b_{\rm l}(-k)^\dagger a_{\rm l}(k),\quad k\in\mathbf{R}\backslash\{0\}, \tag{2.18}$$

$$a_{\rm r}(-k)^\dagger b_{\rm r}(k)=b_{\rm r}(-k)^\dagger a_{\rm r}(k),\quad k\in\mathbf{R}\backslash\{0\}. \tag{2.19}$$

We define the transmission coefficient from the left, $T_{\rm l}(k)$, and the transmission coefficient from the right, $T_{\rm r}(k)$, by

$$T_{\rm l}(k)=a_{\rm l}(k)^{-1},\quad T_{\rm r}(k)=a_{\rm r}(k)^{-1}, \tag{2.20}$$

provided the inverses on the right-hand sides exist, and we define the reflection coefficient from the left, $L(k)$, and the reflection coefficient from the right, $R(k)$, by

$$L(k)=b_{\rm l}(k)a_{\rm l}(k)^{-1},\quad R(k)=b_{\rm r}(k)a_{\rm r}(k)^{-1}. \tag{2.21}$$

From (2.16) and (2.17) we see that $a_{\rm l}(k)$ and $a_{\rm r}(k)$ are nonsingular for $k\in\mathbf{R}\backslash\{0\}$. In $\mathbf{C}^+$, $a_{\rm l}(k)$ and $a_{\rm r}(k)$ are nonsingular except possibly at a finite number of points on the positive imaginary axis where[4] both $\det a_{\rm l}(k)=0$ and $\det a_{\rm r}(k)=0$; at these points, $T_{\rm l}(k)$ and $T_{\rm r}(k)$ have simple poles[8] corresponding to the bound states of (1.1). For $Q\in L_2^1(\mathbf{R};\mathbf{C}^{n\times n})$ the finiteness of the number of bound states has already been established in Refs. 4 and 13. We note that even if $Q\notin L_2^1(\mathbf{R};\mathbf{C}^{n\times n})$ but $Q\in L_1^1(\mathbf{R};\mathbf{C}^{n\times n})$, the finiteness follows from the (operator) inequality $Q(x)\geqslant-\|Q(x)\|I_n$ and the fact that in one dimension a scalar potential in $L_1^1(\mathbf{R})$ can support at most a finite number of bound states. Alternatively, the finiteness of the number of bound states will follow from the results of this paper (cf. Theorems 3.1 and 4.6), which show that $k=0$ cannot be an accumulation point for poles of either $T_{\rm l}(k)$ or $T_{\rm r}(k)$. Because of this latter property we will study the asymptotic behavior of the transmission coefficients as $k\to0$ through values in $\overline{\mathbf{C}^+}$. The reflection coefficients, on the other hand, in general do not have analytic extensions off the real axis, so their asymptotics will be studied for real k only. The $n\times n$ matrix functions $T_{\rm l}(k)$, $T_{\rm r}(k)$, $R(k)$, and $L(k)$ are referred to as scattering coefficients, and the $2n\times2n$ matrix

$$\mathbf{S}(k)=\begin{bmatrix}T_{\rm l}(k) & R(k)\\ L(k) & T_{\rm r}(k)\end{bmatrix}, \tag{2.22}$$

is called the scattering matrix.

From (2.15)–(2.17), we get

$$T_{\rm l}(k)^{\dagger}R(k)+L(k)^{\dagger}T_{\rm r}(k)=0, \quad k\in\mathbf{R}\backslash\{0\},$$

$$T_{\rm l}(k)^{\dagger}T_{\rm l}(k)+L(k)^{\dagger}L(k)=I_n, \quad k\in\mathbf{R}\backslash\{0\}, \tag{2.23}$$

$$T_{\rm r}(k)^{\dagger}T_{\rm r}(k)+R(k)^{\dagger}R(k)=I_n, \quad k\in\mathbf{R}\backslash\{0\}, \tag{2.24}$$

and hence, for $k\in\mathbf{R}\backslash\{0\}$, $\mathbf{S}(k)$ is unitary. Using (2.14) we obtain

$$T_{\rm r}(k)=T_{\rm l}(-k^*)^{\dagger}, \quad k\in\overline{\mathbf{C}^+}\backslash\{0\}, \tag{2.25}$$

whenever $a_{\rm r}(k)$ is nonsingular, and from (2.18) and (2.19) we get

$$L(-k)^{\dagger}=L(k), \quad R(-k)^{\dagger}=R(k), \quad k\in\mathbf{R}\backslash\{0\}.$$

In order to study $\mathbf{S}(k)$ in the small-energy limit, we need to make an important case distinction which involves the solutions to (1.1) with $k=0$, i.e., the solutions to

$$\phi''(x)=Q(x)\phi(x), \quad x\in\mathbf{R}. \tag{2.26}$$

We already know from (2.1) and Theorem 2.1 that $f_{\rm l}(0,x)$ is a solution of (2.26) satisfying $f_{\rm l}(0,x)=I_n+o(1)$ and $f_{\rm l}'(0,x)=o(1/x)$ as $x\to+\infty$. According to basic asymptotic results for systems of linear differential equations (Theorem 1.5.1 of Ref. 3), (2.26) also has an $n\times n$ matrix solution, $\phi_{\rm l}(x)$, satisfying

$$\phi_{\rm l}(x)=xI_n+o(x), \quad \phi_{\rm l}'(x)=I_n+o(1), \quad x\to+\infty.$$

Thus the columns of $f_{\rm l}(0,x)$ together with the columns of $\phi_{\rm l}(x)$ form a fundamental set of $2n$ vector solutions for (2.26). Any vector solution $\phi(x)$ of (2.26) can be written as

$$\phi(x)=f_{\rm l}(0,x)\,\eta_1+\phi_{\rm l}(x)\,\eta_2, \tag{2.27}$$

where $\eta_1,\eta_2\in\mathbf{C}^n$ are uniquely determined by $\phi(x)$. It follows from (2.27) that a vector solution of (2.26) is bounded as $x\to+\infty$ if and only if $\eta_2=0$, i.e., if and only if $\phi(x)=f_{\rm l}(0,x)\,\eta_1$ for some $\eta_1\in\mathbf{C}^n$. Moreover, in this case $\lim_{x\to+\infty}\phi(x)=\eta_1$ exists. This means that if a solution is bounded at $+\infty$, then it also has a limit as $x\to+\infty$. Also, (2.27) implies that any solution of (2.26) that is $o(x)$ as $x\to+\infty$ is necessarily bounded at $x=+\infty$ and any solution that is $o(1)$ as $x\to+\infty$ must be the zero solution. Similar results hold at $x=-\infty$; in particular, any solution of (2.26) that is $o(x)$ as $x\to-\infty$ is necessarily bounded at $x=-\infty$ and has a limit as $x\to-\infty$, and any solution that is $o(1)$ as $x\to-\infty$ must be the zero solution.

From (2.1)–(2.3) we see that $f_{\rm l}(0,x)$ and $f_{\rm r}(0,x)$ obey the integral equations

$$f_{\rm l}(0,x)=I_n+\int_x^{\infty}dy\,(y-x)Q(y)f_{\rm l}(0,y), \tag{2.28}$$

$$f_{\rm r}(0,x)=I_n-\int_{-\infty}^{x}dy\,(y-x)Q(y)f_{\rm r}(0,y). \tag{2.29}$$

In the subsequent analysis the two Wronskian matrices

$$\Delta_{\rm l}=[f_{\rm r}(0,x)^{\dagger};f_{\rm l}(0,x)], \quad \Delta_{\rm r}=-[f_{\rm l}(0,x)^{\dagger};f_{\rm r}(0,x)], \tag{2.30}$$

will play a key role. By Proposition 2.3, $\Delta_{\rm l}$ and $\Delta_{\rm r}$ are independent of x, and from (2.30) it follows that

$$\Delta_{\rm l}=\Delta_{\rm r}^{\dagger}. \tag{2.31}$$

The importance of these Wronskians lies in the fact that they are related to the transmission coefficients via (2.20) and

$$\Delta_{\rm l}=\lim_{k\to 0} 2ika_{\rm l}(k), \quad \Delta_{\rm r}=\lim_{k\to 0} 2ika_{\rm r}(k), \tag{2.32}$$

where the limits are taken from within $\overline{\mathbf{C}^+}$; (2.32) follows from (2.6), (2.7), and Corollary 2.2.

Evaluating the first Wronskian in (2.30) as $x\to-\infty$ and using (2.28) we obtain

$$\Delta_{\rm l}=\lim_{x\to-\infty} f_{\rm l}'(0,x)=-\int_{-\infty}^{\infty} dy\, Q(y) f_{\rm l}(0,y). \tag{2.33}$$

Similarly, from (2.29) and (2.30), letting $x\to+\infty$, we get

$$\Delta_{\rm r}=-\lim_{x\to+\infty} f_{\rm r}'(0,x)=-\int_{-\infty}^{\infty} dy\, Q(y) f_{\rm r}(0,y). \tag{2.34}$$

From (2.28) and (2.29) we also infer that

$$f_{\rm l}(0,x)=x\Delta_{\rm l}+o(x), \quad x\to-\infty,$$

$$f_{\rm r}(0,x)=-x\Delta_{\rm r}+o(x), \quad x\to+\infty. \tag{2.35}$$

Now we are ready to introduce the distinction between the exceptional case and the generic case. Let

$$\mathcal{N}=\{\xi\in\mathbf{C}^n: f_{\rm l}(0,x)\xi \text{ is bounded on } \mathbf{R}\}. \tag{2.36}$$

Then we say that the generic case occurs if $\mathcal{N}=\{0\}$ and we say that the exceptional case occurs if $\mathcal{N}\neq\{0\}$. These two cases can be characterized in other ways. We choose the above definition as our starting point and will arrive at some other characterizations as we go along.

We observe that the generic case occurs if and only if (2.26) has no bounded nontrivial solution. The exceptional case occurs if and only if there exists at least one nontrivial bounded solution. As the next theorem shows, we can alternatively characterize the two cases by means of the subspace

$$\mathcal{M}=\{\chi\in\mathbf{C}^n: f_{\rm r}(0,x)\chi \text{ is bounded on } \mathbf{R}\}. \tag{2.37}$$

Then the generic (exceptional) case occurs if and only if $\mathcal{M}=\{0\}$ ($\mathcal{M}\neq\{0\}$).

We mention that when $n=1$ the exceptional case occurs if and only if $f_{\rm l}(0,x)$ and $f_{\rm r}(0,x)$ are linearly dependent, i.e., the Wronskian $[f_{\rm r}(0,x);f_{\rm l}(0,x)]$ is zero. In our paper we generalize this characterization to the matrix case. In the scalar case it is also known that the generic (exceptional) case occurs if $T_{\rm l}(0)=0$ ($T_{\rm l}(0)\neq 0$). This will also turn out be true in the matrix case, but we do not use this property as our primary characterization because it is implicitly based on the assumption that $T_{\rm l}(k)$ is continuous at $k=0$, something we first need to prove.

The next theorem further clarifies the relations among the two cases, the Wronskians in (2.31), and the subspaces $\mathcal{N}$ and $\mathcal{M}$.

Theorem 2.4: *Assume* $Q\in L_1^1(\mathbf{R};\mathbf{C}^{n\times n})$. *Then we have*

(i) *The generic case occurs if and only if* $\Delta_{\rm l}$, *or equivalently* $\Delta_{\rm r}$, *is nonsingular.*
(ii) $\mathcal{N}=\text{Ker } \Delta_{\rm l}$ *and* $\mathcal{M}=\text{Ker } \Delta_{\rm r}$.
(iii) $\dim \mathcal{N}=\dim \mathcal{M}$.

Proof: If $\Delta_{\rm l}$ is nonsingular, then (2.35) implies that every solution of (2.26) of the form $f_{\rm l}(0,x)\eta$, with some nonzero vector $\eta\in\mathbf{C}^n$, becomes unbounded as $x\to-\infty$. Hence, if $\Delta_{\rm l}$ is nonsingular, then (2.26) has no bounded nontrivial solutions; so the generic case occurs. Con-

versely, suppose the generic case (i.e., $\mathcal{N}=\{0\}$) occurs and Δ_l is singular. Then, by (2.35), for any nonzero $\xi\in\mathrm{Ker}\ \Delta_l$, we have $f_l(0,x)\xi=o(x)$ as $x\to-\infty$. Hence, by the remarks following (2.26) and (2.27), $f_l(0,x)\xi$ is bounded, i.e., $\xi\in\mathcal{N}$ and thus $\mathcal{N}\neq\{0\}$. This is a contradiction. Therefore, in the generic case, Δ_l cannot be singular. This proves (i) for Δ_l. In view of (2.31), the assertion also holds if Δ_l is replaced by Δ_r. To prove (ii), suppose that $\xi\in\mathrm{Ker}\ \Delta_l$. Then, by (2.35), $f_l(0,x)\xi=o(x)$ as $x\to-\infty$. Hence $f_l(0,x)\xi$ is bounded and so $\xi\in\mathcal{N}$. Conversely, if $\xi\in\mathcal{N}$, then $f_l(0,x)\xi$ is bounded and, therefore, again by (2.35), $\Delta_l\xi=0$. This proves the first equality in (ii). The second equality is proved similarly. Finally, (iii) follows immediately from (2.31). ■

III. SMALL-*k* BEHAVIOR IN THE GENERIC CASE

In this section we analyze the behavior of the scattering coefficients near $k=0$ in the generic case. In order to state the next theorem, which is the main result of this section, we introduce the matrices

$$E_l=\int_{-\infty}^{\infty}dx\,xQ(x)m_l(0,x),\quad E_r=\int_{-\infty}^{\infty}dx\,xQ(x)m_r(0,x),\tag{3.1}$$

$$G_l=\int_{-\infty}^{\infty}dx\,Q(x)\dot{m}_l(0,x),\quad G_r=\int_{-\infty}^{\infty}dx\,Q(x)\dot{m}_r(0,x).$$

The quantities E_l and E_r will also play a role in Sec. IV.

Theorem 3.1: *Assume Q is a generic potential in $L^1_m(\mathbf{R};\mathbf{C}^{n\times n})$ for $m=1$ or 2. Then the scattering coefficients satisfy the following:*

(i) *If $m=1$, then*

$$T_l(k)=2ik\Delta_l^{-1}+o(k),\quad T_r(k)=2ik\Delta_r^{-1}+o(k),\quad k\to0\ \text{ in }\ \overline{\mathbf{C}^+},$$
$$R(k)=-I_n+o(1),\quad L(k)=-I_n+o(1),\quad k\to0\ \text{ in }\ \mathbf{R}.$$

(ii) *If $m=2$, then*

$$T_l(k)=2ik\Delta_l^{-1}+k^2\Delta_l^{-1}[4I_n+2iG_l]\Delta_l^{-1}+o(k^2),\quad k\to0\ \text{ in }\ \overline{\mathbf{C}^+},$$
$$T_r(k)=2ik\Delta_r^{-1}+k^2\Delta_r^{-1}[4I_n+2iG_r]\Delta_r^{-1}+o(k^2),\quad k\to0\ \text{ in }\ \overline{\mathbf{C}^+},$$
$$L(k)=-I_n+2ik[I_n+E_l]\Delta_l^{-1}+o(k),\quad k\to0\ \text{ in }\ \mathbf{R},$$
$$R(k)=-I_n+2ik[I_n-E_r]\Delta_r^{-1}+o(k),\quad k\to0\ \text{ in }\ \mathbf{R}.$$

Proof: Using the fact that in the generic case Δ_l and Δ_r are invertible, (i) is a consequence of (2.6)–(2.9), (2.20), (2.21), (2.32), and Corollary 2.2. When $Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$, expanding the integrals in (2.10)–(2.13) as

$$a_l(k)=\frac{1}{2ik}\Delta_l+I_n+\frac{i}{2}G_l+o(1),\quad k\to0\ \text{ in }\ \overline{\mathbf{C}^+},\tag{3.2}$$

$$b_l(k)=-\frac{1}{2ik}\Delta_l+E_l-\frac{i}{2}G_l+o(1),\quad k\to0\ \text{ in }\ \mathbf{R},\tag{3.3}$$

$$a_r(k)=\frac{1}{2ik}\Delta_r+I_n+\frac{i}{2}G_r+o(1),\quad k\to0\ \text{ in }\ \overline{\mathbf{C}^+},\tag{3.4}$$

$$b_r(k)=-\frac{1}{2ik}\Delta_r-E_r-\frac{i}{2}G_r+o(1),\quad k\to0\ \text{ in }\ \mathbf{R},\tag{3.5}$$

and using (2.20) and (2.21) we obtain (ii). ■

For later use we remark that when $Q \in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$, E_l and E_r can be expressed in terms of certain Wronskians, namely

$$I_n + E_l = i[\dot{f}_r(0,x)^\dagger; f_l(0,x)], \quad I_n - E_r = -i[\dot{f}_l(0,x)^\dagger; f_r(0,x)]. \tag{3.6}$$

Note that the Wronskians in (3.6) are independent of x because $\dot{f}_l(0,x)$ and $\dot{f}_r(0,x)$ are also solutions of (2.26). The expressions in (3.6) follow easily from (2.28), (2.29), and the corresponding integral equations for $\dot{f}_l(0,x)$ and $\dot{f}_r(0,x)$ [cf. (A.20)]. Moreover, we have $G_r = -G_l^\dagger$ and $E_r = E_l^\dagger + iG_l^\dagger$, as can be seen by using (2.14), (2.15), and (3.2)–(3.5).

Theorem 3.1 shows that if the generic case occurs, then $T_l(0) = 0$. In the next section we will see that the converse is also true.

IV. SMALL-*k* BEHAVIOR IN THE EXCEPTIONAL CASE

Recall that in the exceptional case (2.26) has at least one bounded nontrivial solution. In this section we analyze how this affects the small-k properties of $\mathbf{S}(k)$, and we prove in the exceptional case the continuity of $\mathbf{S}(k)$ at $k=0$ when $Q \in L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$ and its differentiability when $Q \in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$. It turns out that when $Q \in L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$ the exceptional case gives rise to certain technical complications that necessitate a careful study of certain asymptotic expansions. Since the proof of one result, namely Proposition 4.2, is especially long, that proof is given in the Appendix.

Recall the definitions of the subspaces $\mathcal{N}$ and $\mathcal{M}$ given in (2.36) and (2.37), respectively. There is a natural mapping from $\mathcal{N}$ to $\mathcal{M}$, which we denote by Γ, defined as follows. For every $\xi \in \mathcal{N}$, let

$$\chi = \lim_{x\to-\infty} f_l(0,x)\xi, \tag{4.1}$$

and put

$$\chi = \Gamma\xi. \tag{4.2}$$

Note that, by (2.36), $f_l(0,x)\xi$ is bounded and hence, by the discussion below (2.27), the limit in (4.1) exists. To see that Γ maps $\mathcal{N}$ into $\mathcal{M}$, we note that (4.1) implies

$$\lim_{x\to-\infty} [f_l(0,x)\xi - f_r(0,x)\chi] = 0.$$

Hence $f_l(0,x)\xi - f_r(0,x)\chi$ is a solution of (2.26) which approaches zero as $x\to-\infty$; therefore, it must be identically zero and we have

$$f_l(0,x)\xi = f_r(0,x)\chi, \quad x \in \mathbf{R}. \tag{4.3}$$

Hence $f_r(0,x)\chi$ is bounded, which implies $\chi \in \mathcal{M}$.

Proposition 4.1: Assume $Q \in L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$. Then Γ is a bijection between $\mathcal{N}$ and $\mathcal{M}$.

Proof: We have already seen that Γ maps $\mathcal{N}$ into $\mathcal{M}$. The map Γ is injective, for if $\Gamma\xi = 0$, then, by (4.2) and (4.3), $f_l(0,x)\xi = 0$ for all $x \in \mathbf{R}$ and hence $\xi = 0$. It is also onto, because for every $\chi \in \mathcal{M}$, $\lim_{x\to+\infty} f_r(0,x)\chi = \xi$ exists, and hence (4.3) holds; thus $\chi = \Gamma\xi$. ∎

The mapping Γ will make its appearance as a restriction to $\mathcal{N}$ of certain linear transformations defined on all of $\mathbf{C}^n$. One such representation immediately follows from (4.3). We can pick any x_0 for which $f_r(0,x_0)$ is invertible and write

$$\Gamma = [f_r(0,x_0)^{-1} f_l(0,x_0)]|_{\mathcal{N}}, \tag{4.4}$$

where the symbol $|_{\mathcal{N}}$ denotes the restriction to the subspace $\mathcal{N}$. Recall that when $n=1$, Γ becomes a constant, so that (4.4) expresses the fact that, in the exceptional case, the two Jost solutions at

k$k=0$ are linearly dependent. Clearly, (4.4) is valid whenever $Q\in L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$. Another representation of Γ that will play a role in this section is only valid when $Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$. It follows from (2.28) which, for any $\xi\in\mathcal{N}$, implies

$$\chi=\lim_{x\to-\infty} f_{\rm l}(0,x)\xi=\xi+\int_{-\infty}^{\infty} dy\, yQ(y)[f_{\rm l}(0,y)\xi], \tag{4.5}$$

where we have also used (2.33) and the fact that $\Delta_{\rm l}\xi=0$. Note that the integral on the right-hand side of (4.5) exists when $Q\in L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$ because $f_{\rm l}(0,y)\xi$ is bounded. However, without the vector ξ in the integrand, the integral in general does not exist as a matrix-valued integral, because some column vectors of the matrix $f_{\rm l}(0,y)$ may grow linearly as $y\to-\infty$. In fact, according to (2.35), this is always the case unless $\Delta_{\rm l}=0$. On the other hand, if $Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$, then the integral in (4.5) without the vector ξ in it exists as a matrix-valued integral and, in view of (3.1), we can write $\chi=(I_n+E_{\rm l})\xi$. In other words, we have

$$\Gamma=(I_n+E_{\rm l})|_{\mathcal{N}} \text{ provided } Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n}). \tag{4.6}$$

We will also need representations for Γ^{-1}. To this end we assume, without loss of generality, that $f_{\rm l}(0,0)$ is invertible. If not, we can perform a shift of the origin and use the fact that $f_{\rm l}(0,x)$ is invertible for x sufficiently large. We define

$$\mathcal{R}=f_{\rm l}(0,0)^{-1}f_{\rm r}(0,0), \tag{4.7}$$

and note that, by (4.3),

$$\mathcal{R}|_{\mathcal{M}}=\Gamma^{-1}. \tag{4.8}$$

Another representation for Γ^{-1} is obtained by using the integral relation for $f_{\rm r}(0,x)$ given in (2.29). If $Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$, then, for any $\chi\in\mathcal{M}$, by using (2.29), (2.34), and the fact that $\Delta_{\rm r}\chi=0$, we obtain

$$\xi=\lim_{x\to+\infty} f_{\rm r}(0,x)\chi=\chi-\left[\int_{-\infty}^{\infty} dy\, yQ(y)f_{\rm r}(0,y)\right]\chi,$$

and thus, by (3.1), $\xi=(I_n-E_{\rm r})\chi$. Therefore,

$$\Gamma^{-1}=(I_n-E_{\rm r})|_{\mathcal{M}} \text{ provided } Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n}).$$

After these preparations we are ready to begin the analysis of the small-k asymptotics of $\mathbf{S}(k)$ in the exceptional case. We first consider the Wronskian

$$W(k)=[f_{\rm r}(-k^*,x)^\dagger;f_{\rm l}(k,x)],\quad k\in\overline{\mathbf{C}^+},$$

which appears in (2.6) and, as seen from (2.20), is related to the transmission coefficient $T_{\rm l}(k)$ by

$$T_{\rm l}(k)=2ikW(k)^{-1}. \tag{4.9}$$

The method employed here to study $W(k)$ is patterned after that used in Ref. 12 in the scalar case. Unless otherwise stated, we will assume that k is real. This suffices for all the auxiliary results leading up to our main result given in Theorem 4.6. There we will extend the asymptotics from the real axis to $\mathbf{C}^+$ with the help of a Phragmén–Lindelöf theorem.

Using $[f_{\rm l}(0,x)^\dagger;f_{\rm l}(0,x)]=0$ we first write $W(k)$ in the form

$$W(k)=f_{\rm r}(-k,0)^\dagger[f_{\rm l}(0,0)^\dagger]^{-1}\Omega_1+\Omega_2 f_{\rm l}(0,0)^{-1}f_{\rm l}(k,0),$$

where we have defined

$$\Omega_1 = f_l(0,0)^\dagger f_l'(k,0) - f_l'(0,0)^\dagger f_l(k,0),$$

$$\Omega_2 = f_r(-k,0)^\dagger f_l'(0,0) - f_r'(-k,0)^\dagger f_1(0,0).$$

The quantities Ω_1 and Ω_2 can be written as Wronskians by means of a new solution, $\varphi(k,x)$, of (1.1), which is defined by the initial conditions

$$\varphi(k,0) = f_1(0,0), \quad \varphi'(k,0) = f_l'(0,0), \tag{4.10}$$

so that

$$\varphi(0,x) = f_1(0,x). \tag{4.11}$$

Then we have

$$W(k) = f_r(-k,0)^\dagger [f_l(0,0)^\dagger]^{-1} [\varphi(k,x)^\dagger; f_l(k,x)] + [f_r(-k,x)^\dagger; \varphi(k,x)] f_l(0,0)^{-1} f_l(k,0). \tag{4.12}$$

We mention that the particular choice of the solution $\varphi(k,x)$ is motivated by the fact that there is a crucial estimate, namely (A8) of the Appendix, for the difference $[\varphi(k,x) - \varphi(0,x)]\xi$ with $\xi \in \mathcal{N}$, which plays a key role in the proof of the next proposition. Since the proof of this proposition is lengthy, it is given in the Appendix.

Proposition 4.2: Assume $Q \in L^1_m(\mathbf{R}; \mathbf{C}^{n\times n})$ for $m = 1$ or 2. Then, as $k \to 0$ in $\mathbf{R}$ we have

$$[\varphi(k,x)^\dagger; f_l(k,x)] = \sum_{j=1}^{m} k^j Y_j + o(k^m), \tag{4.13}$$

where

$$Y_1 = iI_n, \quad Y_2 = \int_0^\infty dz\, [f_l(0,z)^\dagger f_l(0,z) - I_n],$$

and

$$[f_r(-k,x)^\dagger; \varphi(k,x)] = \sum_{j=0}^{m-1} k^j X_j + o(k^{m-1}), \tag{4.14}$$

with

$$X_0 = \Delta_1, \quad X_1 = i[I_n + E_1].$$

For $\xi \in \mathcal{N}$ we have

$$[f_r(-k,x)^\dagger; \varphi(k,x)]\xi = \sum_{j=1}^{m} k^j \check{X}_j \xi + o(k^m), \tag{4.15}$$

$$\check{X}_1 = i\Gamma, \quad \check{X}_2 = \int_{-\infty}^0 dz\, [f_r(0,z)^\dagger f_r(0,z) - I_n]\Gamma.$$

The notational differences between (4.14) and (4.15) are justified by the fact that in (4.15) the coefficient $\check{X}_1$ is used when $m = 1$, while in (4.14) the corresponding coefficient X_1 is used only when $m = 2$. Of course, if $m = 2$, then $\check{X}_1 = X_1|_{\mathcal{N}}$, by (4.6).

Our first goal is to find the leading terms in the asymptotics of $W(k)^{-1}$ as $k \to 0$. For this purpose it is convenient to temporarily replace the factors multiplying the Wronskians in (4.12) by their limits as $k \to 0$. That is, we consider the simpler expression

$$Z(k)=\mathcal{R}^{\dagger}[\varphi(k,x)^{\dagger};f_{\rm l}(k,x)]+[f_{\rm r}(-k,x)^{\dagger};\varphi(k,x)], \tag{4.16}$$

where we have used (4.7) via its adjoint. In order to further motivate the use of $Z(k)$, we note that on account of (4.12) and (4.16) we can write

$$W(k)^{-1}=f_{\rm l}(k,0)^{-1}f_{\rm l}(0,0)[Z(k)+\Theta_1(k)+\Theta_2(k)]^{-1}, \tag{4.17}$$

where

$$\Theta_1(k)=\mathcal{R}^{\dagger}[\varphi(k,x)^{\dagger};f_{\rm l}(k,x)][f_{\rm l}(k,0)^{-1}f_{\rm l}(0,0)-I_n], \tag{4.18}$$

$$\Theta_2(k)=\{f_{\rm r}(-k,0)^{\dagger}[f_{\rm l}(0,0)^{\dagger}]^{-1}-\mathcal{R}^{\dagger}\}[\varphi(k,x)^{\dagger};f_{\rm l}(k,x)]f_{\rm l}(k,0)^{-1}f_{\rm l}(0,0), \tag{4.19}$$

provided the second inverse on the right-hand side of (4.17) exists. The existence of this inverse will be established below, where we show that $Z(k)^{-1}$ exists for sufficiently small k and satisfies $Z(k)^{-1}=O(1/k)$ as $k\to 0$. This, together with the fact that, in view of (4.13) and Corollary 2.2, $\Theta_1(k)$ and $\Theta_2(k)$ are both $o(k)$ as $k\to 0$, implies

$$W(k)^{-1}=f_{\rm l}(k,0)^{-1}f_{\rm l}(0,0)Z(k)^{-1}\{I_n+[\Theta_1(k)+\Theta_2(k)]Z(k)^{-1}\}^{-1}, \tag{4.20}$$

where the inverse of the matrix inside the braces exists provided k is sufficiently small. This explains why we focus on $Z(k)$ in the next result, which is an immediate consequence of (4.16) and Proposition 4.2.

Corollary 4.3: Suppose that $Q\in L^1_m(\mathbf{R};\mathbf{C}^{n\times n})$ *for* $m=1$ *or* 2. *Then, as* $k\to 0$ *in* $\mathbf{R}$

$$Z(k)=\sum_{j=0}^{m-1}k^jV_j+o(k^{m-1}), \tag{4.21}$$

$$V_0=\Delta_1,\quad V_1=i[I_n+E_1+\mathcal{R}^{\dagger}].$$

Moreover, for $\xi\in\mathcal{N}$, *we have*

$$Z(k)\xi=\sum_{j=1}^{m}k^j\check{V}_j\xi+o(k^m), \tag{4.22}$$

$$\check{V}_1=i[\Gamma+\mathcal{R}^{\dagger}],$$

$$\check{V}_2=\mathcal{R}^{\dagger}\int_0^{\infty}dz\,[f_{\rm l}(0,z)^{\dagger}f_{\rm l}(0,z)-I_n]+\int_{-\infty}^{0}dz\,[f_{\rm r}(0,z)^{\dagger}f_{\rm r}(0,z)-I_n]\Gamma.$$

Now our task is to identify those matrix elements of $Z(k)^{-1}$ that dominate as $k\to 0$. To do this we choose a Jordan basis for Δ_1 as follows. We assume that there are κ Jordan chains indexed by α for $\alpha=1,...,\kappa$, each consisting of n_α vectors $u_{\alpha j}$, with $j=1,...,n_\alpha$, satisfying the relations

$$\begin{cases}(\Delta_1-\lambda_\alpha)u_{\alpha 1}=0,\\ (\Delta_1-\lambda_\alpha)u_{\alpha j}=u_{\alpha(j-1)},\quad j=2,...,n_\alpha.\end{cases} \tag{4.23}$$

Here λ_α is an eigenvalue of Δ_1, $u_{\alpha 1}$ is the corresponding eigenvector belonging to the αth chain, and the vectors $u_{\alpha j}$ with $j\neq 1$ are the generalized eigenvectors. We assume that the eigenvalue 0 of Δ_1 has geometric multiplicity μ and algebraic multiplicity ν; thus $\Sigma_{\alpha=1}^{\mu}n_\alpha=\nu$ and $\mu=\dim\ \mathcal{N}\geqslant 1$. We arrange the vectors of the Jordan basis in a list which is ordered according to the rule that $u_{\alpha j}$ comes before $u_{\beta s}$ if and only if $\alpha<\beta$ or $\alpha=\beta$ and $j<s$. In other words, this is the ''dictionary order'' of the two two-letter words αj and βs. It is necessary to specify an order on the Jordan basis because later we will have to perform certain permutations on these basis vectors.

We further assume that the first μ Jordan chains belong to the eigenvalue 0 of Δ_1 so that $\{u_{11},u_{21},\ldots,u_{\mu 1}\}$ forms a basis for the kernel of Δ_1. We will also need the adjoint Jordan basis $\{w_{\alpha j}\}$ whose vectors, for $\alpha=1,\ldots,\kappa$, satisfy $w_{\alpha j}^{\dagger}u_{\rho t}=\delta_{\alpha\rho}\delta_{jt}$, where $\delta_{\alpha\beta}$ denotes the Kronecker delta, and

$$\begin{cases}(\Delta_{\mathrm{r}}-\lambda_{\alpha}^{*})w_{\alpha n_{\alpha}}=0,\\ (\Delta_{\mathrm{r}}-\lambda_{\alpha}^{*})w_{\alpha j}=w_{\alpha(j+1),}\quad j=1,\ldots,n_{\alpha}-1.\end{cases}$$

Thus the set $\{w_{1n_1},\ldots,w_{\mu n_{\mu}}\}$ forms a basis for the kernel of Δ_{r}. The transition matrix from the standard basis to the Jordan basis will be denoted by $\mathcal{S}$. Given any $n\times n$ matrix M in the standard basis, we use $\tilde{M}$, where $\tilde{M}=\mathcal{S}^{-1}M\mathcal{S}$, to denote the matrix representation of M in the Jordan basis $\{u_{\alpha j}\}$. Then from (4.23) it follows that $\tilde{\Delta}_1$ has the appearance

$$\tilde{\Delta}_1=\bigoplus_{\alpha=1}^{\kappa}J_{n_{\alpha}}(\lambda_{\alpha}),\tag{4.24}$$

where $J_{n_{\alpha}}(\lambda_{\alpha})$ is the Jordan block with λ_{α} appearing on the diagonal and 1 on the first superdiagonal.

In the notation introduced above we can view the pair αj as a ''block index'' in the sense that α indicates the Jordan block (resp. the Jordan chain) to which the vector $u_{\alpha j}$ belongs, and j indicates the position within that block. Generalizing this notation, we will sometimes use block indices to designate the matrix elements of matrices represented in the Jordan basis $\{u_{\alpha j}\}$. Then the matrix elements of $\tilde{M}=\mathcal{S}^{-1}M\mathcal{S}$ in block index notation are given by

$$\tilde{M}_{\beta s;\alpha j}=w_{\beta s}^{\dagger}Mu_{\alpha j}.\tag{4.25}$$

An important observation about $\tilde{Z}(k)$ is that it has μ columns, namely those with ''addresses'' $\alpha 1$ for $\alpha=1,\ldots,\mu$ which are $O(k)$, and these are the only columns with this property. Any other column contains at least one element that tends to a nonzero limit as $k\to 0$. Now, as we shall see below, the entries of $\tilde{Z}(k)$ which determine the leading asymptotic behavior of $\tilde{Z}(k)^{-1}$ as $k\to 0$ form a submatrix of $\tilde{Z}(k)$ consisting of columns $\alpha 1$ and rows βn_{β}, where α and β both belong to $\{1,\ldots,\mu\}$. It is, therefore, convenient to perform suitable permutations of the columns and rows of $\tilde{Z}(k)$ in order to collect these particular matrix elements in a $\mu\times\mu$ diagonal block of a new matrix, called $\mathcal{Z}(k)$. The formal definition of these permutations and their implementation are as follows. Let π_1 be the permutation

$$\pi_1:(1,\ldots,\nu)\mapsto(q_1,\ldots,q_{\nu}),$$

where

$$q_{\tau}=\begin{cases}n_1+\cdots+n_{\tau-1}+1, & \tau=1,\ldots,\mu,\\ \tau-\mu+\alpha, & \tau=\mu+1,\ldots,\nu,\end{cases}\tag{4.26}$$

and $\alpha\in\{1,\ldots,\mu\}$ is the unique integer such that, for given τ and μ,

$$n_1+n_2+\cdots+n_{\alpha-1}-\alpha+j=\tau-\mu,$$

for some $j\in\{2,\ldots,n_{\alpha}\}$. Note that, since $n_{\alpha}\geqslant 1$, the quantity $n_1+n_2+\cdots+n_{\alpha-1}-\alpha$ is a nondecreasing function of α. Similarly, let π_2 be the permutation

$$\pi_2:(1,\ldots,\nu)\mapsto(\sigma_1,\ldots,\sigma_{\nu}),$$

where

$$\sigma_\alpha = \begin{cases} n_1 + \cdots + n_\alpha, & \alpha = 1,...,\mu, \\ \alpha - \mu + \rho - 1, & \alpha = \mu+1,...,\nu, \end{cases} \tag{4.27}$$

and $\rho \in \{1,...,\mu\}$ is the unique integer such that, for given α and μ

$$n_1 + n_2 + \cdots + n_{\rho-1} - \rho + s = \alpha - \mu,$$

for some $s \in \{2,...,n_\rho\}$. To implement these permutations we let $\hat{e}_j$ for $j = 1,...,\nu$ denote the column vectors of the standard basis in $\mathbf{C}^\nu$ and let Π_1 be the $\nu \times \nu$ permutation matrix whose jth column vector is $\hat{e}_{q_j}$, and let Π_2 be the $\nu \times \nu$ permutation matrix whose kth row vector is $\hat{e}^\dagger_{\sigma_k}$. Now observe that, if M is any $\nu \times \nu$ matrix, then the matrix $\Pi_2 M \Pi_1$ can be thought of as being obtained from M by a permutation of the columns according to π_1 and a permutation of the rows according to π_2. In order to apply these operations to $\tilde{Z}(k)$ we define

$$P_1 = \mathrm{diag}\{\Pi_1, I_{n-\nu}\}, \quad P_2 = \mathrm{diag}\{\Pi_2, I_{n-\nu}\},$$

$$\mathcal{Z}(k) = P_2 \tilde{Z}(k) P_1 = P_2 \mathcal{S}^{-1} Z(k) \mathcal{S} P_1, \tag{4.28}$$

and we partition $\mathcal{Z}(k)$ as

$$\mathcal{Z}(k) = \begin{bmatrix} \mathcal{A}(k) & \mathcal{B}(k) \\ \mathcal{C}(k) & \mathcal{D}(k) \end{bmatrix}, \tag{4.29}$$

where $\mathcal{A}(k)$ has size $\mu \times \mu$ and, consequently, $\mathcal{D}(k)$ has size $(n-\mu)\times(n-\mu)$. Then $\mathcal{A}(k)$ coincides with the submatrix of $\tilde{Z}(k)$ consisting of the elements in columns $\alpha 1$ and rows sn_s, where $1 \leqslant \alpha \leqslant \mu$ and $1 \leqslant s \leqslant \mu$. As we have already indicated above, the matrix $\mathcal{A}(k)$ determines the leading asymptotic behavior of $\mathcal{Z}(k)^{-1}$ as $k \to 0$. The next two propositions provide the necessary information about the behavior of the four matrix blocks in (4.29).

Proposition 4.4: Assume $Q \in L^1_m(\mathbf{R}; \mathbf{C}^{n\times n})$ for $m = 1$ or 2. Then the matrices $\mathcal{A}(k)$, $\mathcal{B}(k)$, $\mathcal{C}(k)$, and $\mathcal{D}(k)$ appearing in (4.29) behave near $k = 0$, with $k \in \mathbf{R}$, as

$$\mathcal{A}(k) = \sum_{j=1}^{m} k^j \mathcal{A}_j + o(k^m), \quad \mathcal{B}(k) = \sum_{j=1}^{m-1} k^j \mathcal{B}_j + o(k^{m-1}), \tag{4.30}$$

$$\mathcal{C}(k) = \sum_{j=1}^{m} k^j \mathcal{C}_j + o(k^m), \quad \mathcal{D}(k) = \sum_{j=0}^{m-1} k^j \mathcal{D}_j + o(k^{m-1}), \tag{4.31}$$

where in the expansion for $\mathcal{B}(k)$ the sum is absent when $m = 1$. Moreover, $\mathcal{A}_1$ and $\mathcal{D}_0$ are invertible.

Proof: We give the proof only for $\mathcal{B}(k)$; the proofs for the other matrices are similar. Let e_j for $j = 1,...,n$ denote the standard basis vectors in $\mathbf{C}^n$. Let $s \in \{1,...,\mu\}$ and first suppose that $p \in \{1,...,\nu-\mu\}$. Then we have

$$\mathcal{B}(k)_{sp} = e_s^\dagger \mathcal{Z}(k) e_{\mu+p} = e_s^\dagger P_2 \tilde{Z}(k) P_1 e_{\mu+p} = [\hat{e}^\dagger_{\sigma_s} \ 0] \tilde{Z}(k) \begin{bmatrix} \hat{e}_{q_{\mu+p}} \\ 0 \end{bmatrix}$$

$$= e^\dagger_{\sigma_s} \tilde{Z}(k) e_{q_{\mu+p}} = \tilde{Z}(k)_{\sigma_s q_{\mu+p}} = \tilde{Z}(k)_{sn_s;\alpha j},$$

where α and j are determined by (4.26) with $\tau = \mu + p \leqslant \nu$; hence $2 \leqslant j \leqslant n_\alpha$ and $1 \leqslant \alpha \leqslant \mu$. Thus it follows from (4.25) and Corollary 4.3 that $\mathcal{B}(k)_{sp} = o(1)$ if $m = 1$ and $\mathcal{B}(k)_{sp} = k\mathcal{B}_{1,sp} + o(k)$ if

$m=2$. Specifically, we have $\mathcal{B}_{1,sp}=w^{\dagger}_{sn_s}V_1u_{\alpha j}$, where V_1 is given in (4.21). It remains to consider the matrix elements with $p\in\{n-\nu+1,...,\nu-\mu\}$. Since $P_1e_{\mu+p}=e_{\mu+p}$, we obtain

$$\mathcal{B}(k)_{sp}=\tilde{Z}(k)_{\sigma_s(\mu+p)}=\tilde{Z}(k)_{sn_s;\alpha j}=w^{\dagger}_{sn_s}Z(k)u_{\alpha j},$$

where α and j are determined by the equation $n_1+\cdots+n_{\alpha-1}+j=\mu+p$; note that $\mu+p>\nu$ and thus $\alpha\geqslant\mu+1$. Since $s\leqslant\mu$, by using Corollary 4.3, we conclude that $\mathcal{B}(k)_{sp}=o(1)$ if $m=1$, and $\mathcal{B}(k)_{sp}=k\mathcal{B}_{1,sp}+o(k)$ with $\mathcal{B}_{1,sp}=w^{\dagger}_{sn_s}V_1u_{\alpha j}$ if $m=2$.

To prove that $\mathcal{A}_1$ is invertible we first note that for s and $j\in\{1,...,\mu\}$, we have

$$\mathcal{A}(k)_{sj}=\tilde{Z}(k)_{\sigma_s q_j}=\tilde{Z}(k)_{sn_s;j1}=w^{\dagger}_{sn_s}Z(k)u_{j1},$$

and thus, by (4.21)

$$\mathcal{A}_{1,sj}=w^{\dagger}_{sn_s}V_1u_{j1}=iw^{\dagger}_{sn_s}[\Gamma+\mathcal{R}^{\dagger}]u_{j1}. \tag{4.32}$$

We show that the kernel of the transformation $\mathcal{A}_1:\mathbf{C}^{\mu}\mapsto\mathbf{C}^{\mu}$ is trivial. Suppose there is a vector $(c_1,\ldots,c_{\mu})$ such that $\Sigma_{j=1}^{\mu}\mathcal{A}_{1,sj}c_j=0$ for $s=1,...,\mu$. Let $\xi=\Sigma_{j=1}^{\mu}c_ju_{j1}$ and $\chi=\Gamma\xi$ [cf. (4.2)]. Since $\chi\in\mathcal{M}$, it is a linear combination of the vectors $w_{1n_1},\ldots,w_{\mu n_{\mu}}$ and hence $\chi^{\dagger}V_1\xi=0$. On the other hand, by using (4.7), we obtain

$$\chi^{\dagger}V_1\xi=i\chi^{\dagger}[\Gamma+\mathcal{R}^{\dagger}]\xi=i(\|\chi\|^2+\|\xi\|^2),$$

which is nonzero unless $c_1=\cdots=c_{\mu}=0$. Hence $\mathcal{A}_1$ is invertible. Finally, from (4.28), (4.29), and Corollary 4.3, we get

$$\mathcal{D}_0=\mathrm{diag}\{I_{\nu-\mu},J_{n_{\mu+1}},\ldots,J_{n_{\kappa}}\}, \tag{4.33}$$

where $J_{n_{\alpha}}$ are the matrices appearing in (4.24). Clearly, $\mathcal{D}_0$ is invertible. ■

Next we study the behavior of the inverse of the matrix defined in (4.29) near $k=0$.

Proposition 4.5: Assume $Q\in L^1_m(\mathbf{R};\mathbf{C}^{n\times n})$ for $m=1$ or 2. Then as $k\to0$ in $\mathbf{R}$ we have the following:

(i) *If $m=1$, then*

$$\mathcal{Z}(k)^{-1}=\begin{bmatrix}(1/k)\mathcal{A}_1^{-1}+o(1/k) & o(1/k)\\ -\mathcal{D}_0^{-1}\mathcal{C}_1\mathcal{A}_1^{-1}+o(1) & \mathcal{D}_0^{-1}+o(1)\end{bmatrix}. \tag{4.34}$$

(ii) *If $m=2$, then*

$$\mathcal{Z}(k)^{-1}=\frac{1}{k}\mathcal{Z}_{-1}+\mathcal{Z}_0+o(1), \tag{4.35}$$

where

$$\mathcal{Z}_{-1}=\mathrm{diag}\{\mathcal{A}_1^{-1},0\}, \tag{4.36}$$

$$\mathcal{Z}_0=\begin{bmatrix}-\mathcal{A}_1^{-1}\mathcal{A}_2\mathcal{A}_1^{-1}+\mathcal{A}_1^{-1}\mathcal{B}_1\mathcal{D}_0^{-1}\mathcal{C}_1\mathcal{A}_1^{-1} & -\mathcal{A}_1^{-1}\mathcal{B}_1\mathcal{D}_0^{-1}\\ -\mathcal{D}_0^{-1}\mathcal{C}_1\mathcal{A}_1^{-1} & \mathcal{D}_0^{-1}\end{bmatrix}. \tag{4.37}$$

Proof: We exploit the fact that

$$\begin{bmatrix}I_{\mu} & -\mathcal{B}(k)\mathcal{D}(k)^{-1}\\ 0 & I_{n-\mu}\end{bmatrix}\mathcal{Z}(k)\begin{bmatrix}I_{\mu} & 0\\ -\mathcal{D}(k)^{-1}\mathcal{C}(k) & I_{n-\mu}\end{bmatrix}=\mathrm{diag}\{\mathcal{U}(k),\mathcal{D}(k)\}, \tag{4.38}$$

where

$$\mathcal{U}(k)=\mathcal{A}(k)-\mathcal{B}(k)\mathcal{D}(k)^{-1}\mathcal{C}(k).$$

By (4.30), (4.31), and Proposition 4.4, we have

$$\mathcal{B}(k)\mathcal{D}(k)^{-1}\mathcal{C}(k)=o(k),\quad \mathcal{A}(k)=k\mathcal{A}_1+o(k),$$

with $\det \mathcal{A}_1\neq 0$, and hence we conclude that, for small enough nonzero k, $\mathcal{U}(k)$ is invertible and

$$\mathcal{U}(k)^{-1}=\begin{cases}(1/k)\mathcal{A}_1^{-1}+o(1/k), & m=1,\\ (1/k)\mathcal{A}_1^{-1}-\mathcal{A}_1^{-1}\mathcal{A}_2\mathcal{A}_1^{-1}+\mathcal{A}_1^{-1}\mathcal{B}_1\mathcal{D}_0^{-1}\mathcal{C}_1\mathcal{A}_1^{-1}+o(1), & m=2.\end{cases} \tag{4.39}$$

As a result, from (4.38) we obtain

$$\mathcal{Z}(k)^{-1}=\begin{bmatrix}\mathcal{U}(k)^{-1} & -\mathcal{U}(k)^{-1}\mathcal{B}(k)\mathcal{D}(k)^{-1}\\ -\mathcal{D}(k)^{-1}\mathcal{C}(k)\mathcal{U}(k)^{-1} & \mathcal{D}(k)^{-1}\mathcal{C}(k)\mathcal{U}(k)^{-1}\mathcal{B}(k)\mathcal{D}(k)^{-1}+\mathcal{D}(k)^{-1}\end{bmatrix},$$

and hence (4.34)–(4.37) follow by using (4.30), (4.31), and (4.39). ■

The primary conclusion of Proposition 4.5 is that $\mathcal{Z}(k)^{-1}$ has a $1/k$-singularity at $k=0$ if $\dim \mathcal{N}\geqslant 1$. Therefore, $\tilde{Z}(k)^{-1}$ and $Z(k)^{-1}$ have a similar behavior. Indeed, from (4.28) and (4.35) we infer that

$$Z(k)^{-1}=\sum_{j=0}^{m-1} k^{j-1}Z_{j-1}+o(k^{m-2}),\quad k\to 0 \ \text{ in } \mathbf{R}, \tag{4.40}$$

where

$$Z_{-1}=\mathcal{S}P_1\mathcal{Z}_{-1}P_2\mathcal{S}^{-1},\quad Z_0=\mathcal{S}P_1\mathcal{Z}_0P_2\mathcal{S}^{-1}. \tag{4.41}$$

This leads us to the main result of this section. We will lift the restriction that k be real and allow $k\in\overline{\mathbf{C}^+}$ in the asymptotics of the transmission coefficients.

Theorem 4.6: *Assume* $Q\in L^1_1(\mathbf{R};\mathbf{C}^{n\times n})$ *and* $\dim \mathcal{N}\geqslant 1$. *Then the scattering coefficients are continuous at* $k=0$, *and we have*

$$T_{\mathrm{l}}(k)=2iZ_{-1}+o(1),\quad T_{\mathrm{r}}(k)=-2iZ_{-1}^{\dagger}+o(1),\quad k\to 0 \ \text{ in } \overline{\mathbf{C}^+}, \tag{4.42}$$

$$\operatorname{Im} T_{\mathrm{l}}(0)=\operatorname{Ker}\ \Delta_1,\quad \operatorname{Ker}\ T_{\mathrm{l}}(0)=\operatorname{Im}\Delta_1, \tag{4.43}$$

$$\operatorname{Im} T_{\mathrm{r}}(0)=\operatorname{Ker}\ \Delta_{\mathrm{r}},\quad \operatorname{Ker}\ T_{\mathrm{r}}(0)=\operatorname{Im}\Delta_{\mathrm{r}}, \tag{4.44}$$

$$L(k)=-I_n+\Gamma T_{\mathrm{l}}(0)+o(1),\quad R(k)=-I_n+\Gamma^{-1}T_{\mathrm{l}}(0)^{\dagger}+o(1),\quad k\to 0 \ \text{ in } \mathbf{R}, \tag{4.45}$$

$$\operatorname{Ker}\{I_n+L(0)\}=\operatorname{Ker}\ T_{\mathrm{l}}(0),\quad \operatorname{Ker}\ T_{\mathrm{r}}(0)=\operatorname{Ker}\{I_n+R(0)\}, \tag{4.46}$$

$$\operatorname{Im}\{I_n+L(0)\}=\operatorname{Im} T_{\mathrm{r}}(0),\quad \operatorname{Im}\{I_n+R(0)\}=\operatorname{Im} T_{\mathrm{l}}(0). \tag{4.47}$$

Proof: For $k\in\mathbf{R}$, the continuity of the transmission coefficients and (4.42) follow immediately from (2.25), (4.9), (4.20), (4.40), and (4.41). To extend the asymptotic formulas in (4.42) from $k\in\mathbf{R}$ to $k\in\overline{\mathbf{C}^+}$ we first note that

$$\det W(k)=[\det Z(k)][1+o(1)]=[\det \mathcal{Z}(k)][1+o(1)]=C_0k^{\mu}[1+o(1)],\quad k\to 0 \ \text{ in } \mathbf{R},$$

where $C_0=(-1)^{\nu-\mu}(\det \mathcal{A}_1)(\det\ \mathcal{D}_0)\neq 0$. This follows from (4.20), (4.28), (4.30), (4.36), (4.38), Proposition 4.4, and the fact that $(\det P_1)(\det P_2)=(-1)^{\nu-\mu}$. It follows that $k^{-\mu}\det W(k)\to C_0$ as

$k\to 0$ along the real axis. Since $\det W(k)$ extends as an analytic function to $\mathbf{C}^+$, there is a constant C such that $|k^{-\mu}\det W(k)|\leq C|k|^{-\mu}$ for k near 0 in $\overline{\mathbf{C}^+}$. Appealing to some theorems of Phragmén–Lindelöf (e.g., Theorems 1.4.1–1.4.4 in Ref. 14) we conclude that $k^{-\mu}\det W(k)\to C_0$ as $k\to 0$ in $\overline{\mathbf{C}^+}$. Thus there is a set $\Sigma_\epsilon=\{k\in\overline{\mathbf{C}^+}: 0<|k|<\epsilon\}$, with ϵ sufficiently small, on which $|\det W(k)|\geq C_1|k|^{\mu}$ for some constant C_1. Recalling the cofactor representation of the inverse of a matrix we conclude that

$$\|W(k)^{-1}\|\leq C_2|k|^{-\mu},\quad k\in\Sigma_\epsilon,$$

for some constant C_2. Since $T_l(k)\to T_l(0)$ as $k\to 0$ along the real axis, we can apply a Phragmén–Lindelöf theorem to $2ikW(k)^{-1}$ and conclude that, by (4.9), $T_l(k)\to T_l(0)$ as $k\to 0$ in $\overline{\mathbf{C}^+}$. This, together with (2.25), completes the proof of (4.42).

To prove (4.43) we note that (4.24) and (4.26) imply Ker $\tilde{\Delta}_l=\mathrm{Span}\{e_{q_1},\ldots,e_{q_\mu}\}$. Thus, in view of the form of $\mathcal{Z}_{-1}$ given in (4.36), we have

$$\mathrm{Im}\{P_1\mathcal{Z}_{-1}P_2\}=P_1\left\{\begin{bmatrix}u\\0\end{bmatrix}: u\in\mathbf{C}^\mu\right\}=P_1\mathrm{Span}\{e_1,\ldots,e_\mu\}=\mathrm{Ker}\ \tilde{\Delta}_l.$$

Since $\Delta_l=\mathcal{S}\tilde{\Delta}_l\mathcal{S}^{-1}$, the first equality in (4.43) follows from (4.41) and (4.42). To prove the second equality we note that

$$\mathrm{Im}\,\tilde{\Delta}_l=\mathrm{Span}\{e_k:\ k\notin\{\sigma_1,\ldots,\sigma_\mu\}\},$$

which follows from (4.24) and (4.25). Therefore,

$$\begin{aligned}\mathrm{Ker}\{\mathcal{Z}_{-1}P_2\}&=\left\{w\in\mathbf{C}^n: P_2w=\begin{bmatrix}0\\v\end{bmatrix},\quad v\in\mathbf{C}^{n-\mu}\right\}\\&=\{w\in\mathbf{C}^n: e_k^\dagger P_2w=0,\quad k=1,...,\mu\}\\&=\{w\in\mathbf{C}^n: e_{\sigma_k}^\dagger w=0,\quad k=1,...,\mu\}\\&=\mathrm{Im}\,\tilde{\Delta}_l.\end{aligned}$$

This implies Ker $T_l(0)=\mathrm{Im}\,\Delta_l$ and thus the second equality in (4.43) is proved. The equalities in (4.44) follow from (4.43) by taking adjoints and using the fact that $(\mathrm{Ker}\ M)^\perp=\mathrm{Im}\,M^\dagger$ for any $n\times n$ matrix M.

To prove the remaining assertions we use

$$f_l(k,x)T_l(k)=f_r(-k,x)+f_r(k,x)L(k),\quad k\in\mathbf{R}\backslash\{0\},\tag{4.48}$$

$$f_r(k,x)T_r(k)=f_l(-k,x)+f_l(k,x)R(k),\quad k\in\mathbf{R}\backslash\{0\},\tag{4.49}$$

which can be derived with the help of (1.4) and (1.5). From (4.48) and the continuity of $T_l(k)$ it immediately follows that $L(k)$ is continuous at $k=0$ and we have

$$f_r(0,x)[I_n+L(0)]=f_l(0,x)T_l(0).\tag{4.50}$$

Now choose x such that $f_r(0,x)$ is invertible and multiply (4.50) from the left by $f_r(0,x)^{-1}$. Owing to (4.4) and the first equation in (4.43), we can replace $f_r(0,x)^{-1}f_l(0,x)$ by Γ. Hence the first relation in (4.45) follows. Similarly, the second relation in (4.45) is obtained from (4.49). The two equalities in (4.46) are immediate consequences of (4.45). Finally, (4.47) follows from (4.43), (4.45), and Proposition 4.1. ■

From (4.43), (4.44), Proposition 2.4(i), and Theorem 3.1 we infer that the exceptional case occurs if and only if $T_l(0)\neq 0$. Moreover, (4.43), (4.46), and Theorem 3.1 show that $L(0)$ and $R(0)$ each have eigenvalue -1 if and only if $\Delta_l\neq 0$. In view of (2.23) and (2.24) we also have $\|L(0)\|=\|R(0)\|=1$ if and only if $\Delta_l\neq 0$. The case $\Delta_l=0$ can be called the purely exceptional case because then we have $\mathcal{N}=\mathcal{M}=\mathbf{C}^n$. This case is further analyzed in Example 5.4 of the next section.

Theorem 4.7: *Assume* $Q\in L^1_2(\mathbf{R};\mathbf{C}^{n\times n})$ *and* $\dim\mathcal{N}\geqslant 1$. *Then the scattering coefficients are differentiable at* $k=0$ *and*

$$T_l(k)=T_l(0)+k\dot{T}_l(0)+o(k),\quad k\to 0\ \text{ in }\ \overline{\mathbf{C}^+},\tag{4.51}$$

with

$$\dot{T}_l(0)=2i[Z_0-f_l^{-1}(0,0)\dot{f}_l(0,0)Z_{-1}+iH_1+iH_2],\tag{4.52}$$

where Z_{-1} *and* Z_0 *are given in (4.41) and*

$$H_1=Z_{-1}\mathcal{R}^\dagger f_l^{-1}(0,0)\dot{f}_l(0,0)Z_{-1},\quad H_2=Z_{-1}\dot{f}_r(0,0)^\dagger[f_l(0,0)^\dagger]^{-1}Z_{-1}.$$

Moreover,

$$T_r(k)=T_l(0)^\dagger-k^*\dot{T}_l(0)^\dagger+o(k),\quad k\to 0\ \text{ in }\ \overline{\mathbf{C}^+},$$

$$L(k)=-I_n+(I_n+E_l)T_l(0)+k\dot{L}(0)+o(k),\quad k\to 0\ \text{ in }\ \mathbf{R},$$

$$R(k)=-I_n+(I_n-E_r)T_r(0)+k\dot{R}(0)+o(k),\quad k\to 0\ \text{ in }\ \mathbf{R},$$

where E_l *and* E_r *are as in (3.1) and*

$$\dot{L}(0)=[I_n+E_l]\dot{T}_l(0)+i[\dot{f}_r(0,x)^\dagger;\dot{f}_l(0,x)]T_l(0),$$

$$\dot{R}(0)=[I_n-E_r]\dot{T}_r(0)-i[\dot{f}_l(0,x)^\dagger;\dot{f}_r(0,x)]T_r(0).$$

Proof: To prove (4.51) and (4.52) for $k\to 0$ in $\mathbf{R}$, we first note the expansions

$$f_l(k,0)^{-1}f_l(0,0)=I_n-kf_l(0,0)^{-1}\dot{f}_l(0,0)+o(k),$$

$$f_r(-k,0)^\dagger[f_l(0,0)^\dagger]^{-1}=\mathcal{R}^\dagger-k\dot{f}_r(0,0)^\dagger[f_l(0,0)^\dagger]^{-1}+o(k),$$

$$\Theta_1(k)=-ik^2\mathcal{R}^\dagger f_l(0,0)^{-1}\dot{f}_l(0,0)+o(k^2),$$

$$\Theta_2(k)=-ik^2\dot{f}_r(0,0)^\dagger[f_l(0,0)^\dagger]^{-1}+o(k^2),$$

which follow from (4.18), (4.19), together with (4.7) and Proposition 4.2. Inserting these expansions in (4.20) and using (4.9) we obtain (4.51) and (4.52). As with (4.42) we can use a Phragmén–Lindelöf argument to extend the result to $\overline{\mathbf{C}^+}$. To find the expansions for $L(k)$ and $R(k)$ we first note that the existence of $\dot{T}_l(0)$, together with (4.48) and (4.49), implies the existence of $\dot{L}(0)$ and $\dot{R}(0)$. Differentiating (4.48) with respect to k and taking the Wronskian with $\dot{f}_r(0,x)^\dagger$, we obtain

$$[\dot{f}_r(0,x)^\dagger;f_r(0,x)]\dot{L}(0)=[\dot{f}_r(0,x)^\dagger;\dot{f}_l(0,x)]T_l(0)+[\dot{f}_r(0,x)^\dagger;f_l(0,x)]\dot{T}_l(0),\tag{4.53}$$

where we have used $[\dot{f}_{\rm r}(0,x)^\dagger;\dot{f}_{\rm r}(0,x)]=0$. Using the integral relation (2.29) and that for $\dot{f}_{\rm r}(0,x)$ [cf. (A.20)] we obtain $[\dot{f}_{\rm r}(0,x)^\dagger;f_{\rm r}(0,x)]=-iI_{\rm n}$. Inserting this together with (3.6) in (4.53) and using (4.47) we get the expansion for $L(k)$. The proof of the expansion for $R(k)$ is similar. ■

V. EXAMPLES

In this section we consider some special cases that illustrate various details of the analysis in Sec. IV. With the exception of Example 5.4 we only consider $T_{\rm l}(k)$.

Example 5.1: Let $n=1$ with $Q\in L_2^1(\mathbf{R})$ and assume the exceptional case occurs. Then $Z(k)=\tilde{Z}(k)=\mathcal{Z}(k)=\mathcal{A}(k)$, and these are all scalar functions. We choose $\xi=1=w$ and put $\gamma=\Gamma=f_{\rm l}(0,0)/f_{\rm r}(0,0)$, where now γ is a real nonzero constant. Since $T_{\rm l}(k)=T_{\rm r}(k)$, we denote the transmission coefficient by $T(k)$. By (4.32) we have $\mathcal{A}_1=i(\gamma^2+1)/\gamma$,

$$\mathcal{A}_2=\gamma^{-1}\int_0^\infty dz\,[f_{\rm l}(0,z)^\dagger f_{\rm l}(0,z)-I_n]+\gamma\int_{-\infty}^0 dz\,[f_{\rm r}(0,z)^\dagger f_{\rm r}(0,z)-I_n],$$

so that

$$T(k)=\frac{2\gamma}{\gamma^2+1}+\frac{2ik\gamma\Xi}{(\gamma^2+1)^2}+o(k),\quad k\to 0\ \text{ in }\ \overline{\mathbf{C}^+},\tag{5.1}$$

where we have defined

$$\Xi=\gamma[\dot{f}_{\rm r}(0,x);\dot{f}_{\rm l}(0,x)]+\int_0^\infty dz\,[f_{\rm l}(0,z)^2-1]+\gamma^2\int_{-\infty}^0 dz\,[f_{\rm r}(0,z)^2-1].$$

In deriving (5.1) we have used the identity

$$\frac{\dot{f}_{\rm l}(0,x)}{f_{\rm r}(0,x)}+\frac{\dot{f}_{\rm r}(0,x)}{f_{\rm l}(0,x)}=-i[\dot{f}_{\rm r}(0,x);\dot{f}_{\rm l}(0,x)],\tag{5.2}$$

which can be verified as follows. Since $f_{\rm r}(0,x)$ and $\dot{f}_{\rm r}(0,x)$ are linearly independent solutions of (2.26), we can write

$$\dot{f}_{\rm l}(0,x)=c_1 f_{\rm r}(0,x)+c_2\dot{f}_{\rm r}(0,x),$$

and evaluate c_1 and c_2 as

$$c_1=-i[\dot{f}_{\rm r}(0,0);\dot{f}_{\rm l}(0,0)],\quad c_2=-\frac{1}{\gamma},$$

so that (5.2) follows. It seems that the expansion (5.1) is new under the assumption $Q\in L_2^1(\mathbf{R})$.

Example 5.2: Assume $Q\in L_1^1(\mathbf{R};\mathbf{C}^{n\times n})$ and suppose that $\tilde{\Delta}_1$ consists of one single Jordan block of size $n\geqslant 2$ associated with the eigenvalue 0. Thus $\kappa=1$, $\mu=1$, and $n=n_1=\nu$.

In this case we can simplify the notation by setting $u_{1j}=u_j$, for $j=1,...,n$. Then u_1 is the eigenvector for the eigenvalue 0 of Δ_1, that is $\mathcal{N}=\text{Span}\{u_1\}$. The adjoint basis is $\{w_1,\ldots,w_n\}$ and we have $\mathcal{M}=\text{Span}\{w_n\}$. The mapping Γ maps u_1 to a multiple of w_n, i.e., $\Gamma_{u1}=c_3 w_n$ for some $c_3\neq 0$. Moreover, $\mathcal{A}(k)$ is a scalar function and from (4.32) we obtain

$$\mathcal{A}_1=\frac{i}{c_3^*}(|c_3|^2\|w_n\|^2+\|u_1\|^2),$$

where we have used (4.7) via $\mathcal{R}w_n=(1/c_3)u_1$. The permutation matrices appearing in (4.28) are given by

$$P_1=I_n, \quad P_2=\begin{bmatrix} 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 1 & 0 \end{bmatrix}.$$

Using (4.41) and (4.42) we obtain

$$\tilde{T}_1(0)=\begin{bmatrix} 0 & 0 & \dots & 0 & 2/c_4 \\ 0 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & \dots & 0 & 0 \end{bmatrix},$$

where

$$c_4=\frac{1}{c_3^*}(|c_3|^2\|w_n\|^2+\|u_1\|^2), \quad \tilde{T}_1(0)=\mathcal{S}^{-1}T_1(0)\mathcal{S}.$$

Example 5.3: This example illustrates the situation where $\tilde{\Delta}_1$ in (4.24) consists of two Jordan blocks. We assume $Q\in L_1^1(\mathbf{R};\mathbf{C}^{n\times n})$ and let $n=3$, $\mu=2$, $n_1=1$, $n_2=2$, $\nu=3$, and $\kappa=2$, so that Δ_1 has the Jordan form

$$\tilde{\Delta}_1=\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}.$$

The Jordan basis is $\{u_{11},u_{21},u_{22}\}$, where $\{u_{11},u_{21}\}$ is a basis for $\mathcal{N}$, and the adjoint basis is $\{w_{11},w_{21},w_{22}\}$, where $\{w_{11},w_{22}\}$ is a basis for $\mathcal{M}$. In this case the rows of $\tilde{Z}(k)$ need to be permuted according to $\pi_2\colon(1,2,3)\mapsto(1,3,2)$, whereas no permutation of the columns is required. Thus we have

$$P_1=I_3, \quad P_2=\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}.$$

Then $\mathcal{A}(k)$ is a 2×2 matrix and

$$\mathcal{A}_1=\begin{bmatrix} w_{11}^\dagger V_1 u_{11} & w_{11}^\dagger V_1 u_{21} \\ w_{22}^\dagger V_1 u_{11} & w_{22}^\dagger V_1 u_{21} \end{bmatrix},$$

where V_1 is given in (4.21). Hence we obtain

$$\tilde{T}_1(0)=\frac{1}{\det \mathcal{A}_1}\begin{bmatrix} w_{22}^\dagger V_1 u_{21} & 0 & -w_{11}^\dagger V_1 u_{21} \\ -w_{22}^\dagger V_1 u_{11} & 0 & w_{11}^\dagger V_1 u_{11} \\ 0 & 0 & 0 \end{bmatrix}.$$

Example 5.4: This is the purely exceptional case mentioned above Theorem 4.7. We assume $Q \in L_1^1(\mathbf{R};\mathbf{C}^{n\times n})$ with $n>1$. We have $\Delta_1=0$, which implies $\mu=\nu=\kappa=n$. Then $\mathcal{N}=\mathcal{M}=\mathbf{C}^n$, and thus no restrictions are necessary in (4.4) and (4.8); that is, we have $\mathcal{R}=\Gamma^{-1}$. Moreover, $P_1=P_2=I_n$. It follows that

$$\mathcal{A}_1=i\mathcal{S}^{-1}[\Gamma+(\Gamma^{-1})^\dagger]\mathcal{S},$$

and thus, since $\mathcal{Z}_{-1}=\mathcal{A}_1^{-1}$, we obtain

$$T_l(0)=2i\mathcal{S}(\mathcal{S}\mathcal{A}_1)^{-1}=2\Gamma^\dagger(\Gamma\Gamma^\dagger+I_n)^{-1}.$$

For the reflection coefficients, after some straightforward manipulations, we find

$$L(0)=(\Gamma\Gamma^\dagger-I_n)(\Gamma\Gamma^\dagger+I_n)^{-1},\quad R(0)=(I_n-\Gamma^\dagger\Gamma)(\Gamma^\dagger\Gamma+I_n)^{-1}.$$

Example 5.5: Suppose $Q(x)$ is even and belongs to $L_1^1(\mathbf{R};\mathbf{C}^{n\times n})$. This implies that $f_r(0,x)=f_l(0,-x)$ and from (2.31), (2.33), and (2.34) we conclude that Δ_1 is self-adjoint. Hence Δ_1 is diagonalizable and there are no Jordan chains of length greater than 1. We have $\mu=\nu$, $n_\alpha=1$ for $1\leqslant\alpha\leqslant\kappa$, and $\kappa=n$. We also have $P_1=P_2=I_n$. It is possible that Δ_1 has some nonzero eigenvalues, so $\mu<n$ in general. If $\xi\in\mathcal{N}$, then

$$f_l(0,x)\xi=f_r(0,-x)\xi,$$

which implies that $f_r(0,x)\xi$ is bounded. This means $\xi\in\mathcal{M}$ and hence $\mathcal{N}=\mathcal{M}$. Furthermore, using (4.2) and (4.3) we conclude that

$$f_l(0,x)\chi=f_r(0,-x)\chi=f_l(0,-x)\xi, \tag{5.3}$$

where $\xi\in\mathcal{N}$ and $\chi=\Gamma\xi$. Letting $x\to-\infty$, we see that $\Gamma\chi=\xi$, that is

$$\Gamma^2=I_\mu. \tag{5.4}$$

It follows that Γ is diagonalizable because $(I_\mu\pm\Gamma)^p=2^{p-1}(I_\mu\pm\Gamma)$ for $p\geqslant1$ and has eigenvalues ±1. Let $\epsilon_\pm$ denote the corresponding multiplicities ($\epsilon_++\epsilon_-=\mu$). Since $n_\alpha=1$, we put $u_{\alpha1}=u_\alpha$ for the vectors of the Jordan basis for Δ_1 and assume that they are normalized and arranged such that

$$\Gamma u_\alpha=u_\alpha,\quad \alpha=1,...,\epsilon_+,$$

$$\Gamma u_\alpha=-u_\alpha,\quad \alpha=\epsilon_++1,...,\mu.$$

We also set $w_{sn_s}=w_s$, so that $w_s^\dagger u_\alpha=\delta_{s\alpha}$ for $s=1,...,n$ and $\alpha=1,...,n$. Note that as a consequence of (5.3), $\epsilon_+(\epsilon_-)$ is the number of linearly independent bounded even (odd) solutions of (2.26). Then from (4.8) and (5.4) we conclude that

$$w_s^\dagger\mathcal{R}^\dagger u_\alpha=(\Gamma^{-1}w_s)^\dagger u_\alpha=(\Gamma w_s)^\dagger u_\alpha=w_s^\dagger\Gamma^\dagger u_\alpha, \tag{5.5}$$

where $\Gamma^\dagger$ is the adjoint of Γ as a mapping from $\mathcal{N}$ to itself. Using (5.5) in (4.32) we obtain $\mathcal{A}_{1,sj}=iw_s^\dagger[\Gamma+\Gamma^\dagger]u_j$, and therefore

$$(\mathcal{A}_1^{-1})_{sj}=-iw_s^\dagger[\Gamma+\Gamma^\dagger]^{-1}u_j.$$

As a result, from (4.36), (4.41), and (4.42) we deduce that

$$T_l(0)=[2(\Gamma+\Gamma^\dagger)^{-1}]\oplus0,$$

where the direct sum refers to the direct decomposition $\mathbf{C}^n=\mathcal{N}\oplus\mathcal{N}'$ with

$$\mathcal{N}' = \mathrm{Span}\{u_{\mu+1},\ldots,u_n\}.$$

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APPENDIX: PROOF OF PROPOSITION 4.2

Proof: Since the assertions of Proposition 4.2 concern the small-k asymptotics, we assume that k lies in a fixed interval $[-\delta, \delta]$ with $\delta > 0$. In the following C is used to denote various constants that may depend on the choice of δ but not on k or x.

The solution $\varphi(k,x)$ of (1.1) defined by the initial conditions (4.10) satisfies the integral equation

$$\varphi(k,x) = f_1(0,0)\cos kx + f_1'(0,0)\left(\frac{\sin kx}{k}\right) + \frac{1}{k}\int_0^x dy\, \sin[k(x-y)]Q(y)\varphi(k,y), \tag{A1}$$

which can be solved by iteration. A standard Gronwall inequality shows that

$$\|\varphi(k,x)\| \leqslant C(1+|x|), \quad x \in \mathbf{R}. \tag{A2}$$

Therefore, by using (A1) and (A2), it follows that for each $k \in \mathbf{R}\backslash\{0\}$ we have

$$\varphi(k,x) = \alpha_\pm(k)e^{ikx} + \beta_\pm(k)e^{-ikx} + \epsilon_\pm(k,x), \tag{A3}$$

where $\epsilon_\pm(k,x)$ and $\epsilon_\pm'(k,x)$ are both $o(1)$ as $x \to \pm\infty$, and where

$$\alpha_\pm(k) = \frac{1}{2}f_1(0,0) + \frac{1}{2ik}f_1'(0,0) + \frac{1}{2ik}\int_0^{\pm\infty} dy\, e^{-iky}Q(y)\varphi(k,y), \tag{A4}$$

$$\beta_\pm(k) = \frac{1}{2}f_1(0,0) - \frac{1}{2ik}f_1'(0,0) - \frac{1}{2ik}\int_0^{\pm\infty} dy\, e^{iky}Q(y)\varphi(k,y).$$

From (A3) and (A4), together with (1.2) and (1.3), it follows that:

$$[\varphi(k,x)^\dagger; f_1(k,x)] = 2ik\alpha_+(k)^\dagger = ikf_1(0,0)^\dagger - f_1'(0,0)^\dagger - \int_0^\infty dz\, e^{ikz}\varphi(k,z)^\dagger Q(z), \tag{A5}$$

$$[f_r(-k,x)^\dagger; \varphi(k,x)] = 2ik\alpha_-(k) = ikf_1(0,0) + f_1'(0,0) - \int_{-\infty}^0 dz\, e^{-ikz}Q(z)\varphi(k,z). \tag{A6}$$

In order to control the remainder terms in the subsequent asymptotic expansions, we will need the estimates

$$\|\varphi(k,x) - \varphi(0,x)\| \leqslant C(1+\max\{0,-x\})\left(\frac{kx}{1+|k||x|}\right)^2, \tag{A7}$$

$$\|[\varphi(k,x) - \varphi(0,x)]\xi\| \leqslant C\left(\frac{kx}{1+|k||x|}\right)^2\|\xi\|, \quad \xi \in \mathcal{N}. \tag{A8}$$

The term $\max\{0,-x\}$ in (A7) accounts for the fact that $\varphi(0,x)$ is in general unbounded and $O(x)$ as $x \to -\infty$. In (A8), this term is absent because $\varphi(0,x)\xi$ is bounded when $\xi \in \mathcal{N}$. We omit the

proofs of (A7) and (A8) here because (A7) follows from (A1) by some standard estimates and (A8) can be proved by mimicking the proof in the scalar case (see Lemma 2.2 in Ref. 12).

Now consider the integral on the right-hand side of (A5) and write it as

$$\int_0^\infty dz\, e^{ikz}\varphi(k,z)^\dagger Q(z)=A_1(k)+A_2(k), \tag{A9}$$

where

$$A_1(k)=\int_0^\infty dz\, e^{ikz}\varphi(0,z)^\dagger Q(z), \tag{A10}$$

$$A_2(k)=\int_0^\infty dz\, e^{ikz}[\varphi(k,z)^\dagger-\varphi(0,z)^\dagger]Q(z). \tag{A11}$$

When $m=1$, from (A.10) we get

$$\begin{cases} A_1(k)=\displaystyle\int_0^\infty dz\,\varphi(0,z)^\dagger Q(z)+ik\int_0^\infty dz\, z\varphi(0,z)^\dagger Q(z)+\mathcal{F}(k), \\ \qquad =-f_1'(0,0)^\dagger+ik[f_1(0,0)^\dagger-I_n]+\mathcal{F}(k), \end{cases} \tag{A12}$$

where

$$\mathcal{F}(k)=\int_0^\infty dz\,(e^{ikz}-1-ikz)\varphi(0,z)^\dagger Q(z). \tag{A13}$$

Note that $\mathcal{F}(k)$ is $o(k)$ by (4.11), the boundedness of $f_1(0,z)$ on $[0,+\infty)$, and the estimate

$$|e^{ikz}-1-ikz|\leqslant\frac{Cz^2}{1+z},\quad z\geqslant 0.$$

In deriving (A12) we have also used the relations

$$\begin{cases} \displaystyle\int_0^\infty dz\,\varphi(0,z)^\dagger Q(z)=-f_1'(0,0)^\dagger, \\ \displaystyle\int_0^\infty dz\, z\varphi(0,z)^\dagger Q(z)=f_1(0,0)^\dagger-I_n, \end{cases} \tag{A14}$$

which follow from (2.28). Using (A7) in (A11) we see that

$$A_2(k)=o(k). \tag{A15}$$

Combining (A5), (A9), (A12), and (A15) we obtain

$$[\varphi(k,x)^\dagger;f_1(k,x)]=ikI_n+o(k),$$

which agrees with (4.13) for $m=1$.

Now consider (A5) for $m=2$, that is, $Q\in L_2^1(\mathbf{R};\mathbf{C}^{n\times n})$. In this case we can expand the remainder $\mathcal{F}(k)$ in (A12) as

$$\mathcal{F}(k)=\int_0^\infty dz\,\frac{(ikz)^2}{2}\varphi(0,z)^\dagger Q(z)+o(k^2), \tag{A16}$$

where we have used (A7), (A13), and the estimate

$$\left| e^{ikz} - 1 - ikz + \frac{k^2 z^2}{2} \right| \leqslant \frac{C(|k|z)^3}{1+|k|z}, \quad z \geqslant 0.$$

The integral in (A16) can be expressed in a form that does not involve Q explicitly. To see this, substitute $\varphi''(0,z)^\dagger$ for $\varphi(0,z)^\dagger Q(z)$ and replace the upper limit of integration by N. Then integrate by parts twice and let $N \to +\infty$. This gives

$$-\frac{k^2}{2}\left[\int_0^\infty dz\, z^2 \varphi''(0,z) \right]^\dagger = -\frac{k^2}{2} \lim_{N\to+\infty} \mathcal{G}_N^\dagger = -k^2 \int_0^\infty dz\, [f_1(0,z)^\dagger - I_n],$$

where we have defined

$$\mathcal{G}_N = N^2 \varphi'(0,N) - 2N[\varphi(0,N) - I_n] + 2\int_0^N dz\, [\varphi(0,z) - I_n].$$

Thus

$$\mathcal{F}(k) = -k^2 \int_0^\infty dz\, [f_1(0,z)^\dagger - I_n] + o(k^2). \tag{A17}$$

In the derivation of (A17) we have also used

$$\varphi'(0,N) = o(1/N^2), \quad \varphi(0,N) - I_n = o(1/N), \quad \varphi(0,N) - I_n \in L^1(\mathbf{R}^+; \mathbf{C}^{n\times n}). \tag{A18}$$

These properties follow directly from (2.28) and (4.11). The expression (A17) for $\mathcal{F}(k)$ has the advantage that it allows us to combine $\mathcal{F}(k)$ with another term that arises from the expansion of $A_2(k)$. To see this we return to (A11). In order to expand the difference $\varphi(k,x) - \varphi(0,x)$, we use the variation of parameters formula in the form

$$\varphi(k,x) = \varphi(0,x) + ik^2 f_1(0,x) \int_0^x dz\, \dot{f}_1(0,z)^\dagger \varphi(k,z) + ik^2 \dot{f}_1(0,x) \int_0^x dz\, f_1(0,z)^\dagger \varphi(k,z). \tag{A19}$$

We briefly mention some details of the derivation of (A19) because there is a useful identity that falls out in the process. We write (2.26) as a first-order system with $2n$ components and note that a fundamental matrix $\Psi(x)$ for this system and its inverse $\Psi(x)^{-1}$ are given by

$$\Psi(x) = \begin{bmatrix} f_1(0,x) & \dot{f}_1(0,x) \\ f_1'(0,x) & \dot{f}_1'(0,x) \end{bmatrix}, \quad \Psi(x)^{-1} = i \begin{bmatrix} \dot{f}_1'(0,x)^\dagger & -\dot{f}_1(0,x)^\dagger \\ f_1'(0,x)^\dagger & -f_1(0,x)^\dagger \end{bmatrix}.$$

By taking $x \to +\infty$ and using (2.4), one can prove that $\det \Psi(x) = i$. For this and also later we need to use certain asymptotic information about the functions $\dot{f}_1(0,x)$ and $\dot{f}_1'(0,x)$. It suffices to mention that $\dot{f}_1(0,x)$ is the unique solution of the integral equation

$$\dot{f}_1(0,x) = ixI_n + \int_x^\infty dy\, (y-x) Q(y) \dot{f}_1(0,y), \tag{A20}$$

which, incidentally, shows that $\dot{f}_1(0,x)$ is also a matrix solution of (2.26). Moreover, a Gronwall inequality gives

$$\|\dot{f}_1(0,x)\| \leqslant C(1+|x|), \quad x \in \mathbf{R}. \tag{A21}$$

The identity $\Psi(x)^{-1}\Psi(x) = I_{2n}$ is easily verified by using the Wronskian relations

$$[f_1(0,x)^\dagger; f_1(0,x)] = [\dot{f}_1(0,x)^\dagger; \dot{f}_1(0,x)] = 0,$$

$$[f_1(0,x)^\dagger; \dot{f}_1(0,x)] = [\dot{f}_1(0,x)^\dagger; f_1(0,x)] = iI_n,$$

which follow from (2.28), (A20), and the first formula in (A18) which indicates that $f_1'(0,x) = o(1/x^2)$ as $x \to +\infty$. Then (A19) is an easy consequence of the variation of parameters formula for first-order systems. The useful identity alluded to above appears when we write out the identity $\Psi(x)\Psi(x)^{-1} = I_{2n}$ (in this order!) in terms of the entries of the matrices involved. Among the resulting identities we find

$$f_1'(0,x)\dot{f}_1(0,x)^\dagger + \dot{f}_1'(0,x) f_1(0,x)^\dagger = iI_n,$$

which will be useful later.

By iterating (A19) once and using (4.11) we obtain

$$\varphi(k,x) = \varphi(0,x) + ik^2 f_1(0,x) \int_0^x dz\, \dot{f}_1(0,z)^\dagger f_1(0,z) + ik^2 \dot{f}_1(0,x) \int_0^x dz\, f_1(0,z)^\dagger f_1(0,z) + \rho(k,x), \tag{A22}$$

where $\rho(k,x)$ obeys

$$\|\rho(k,x)\| \leq Ck^2(1+|x|)^2 \left(\frac{kx}{1+|k|x|} \right)^2. \tag{A23}$$

This estimate follows by using (A7) and (A21). Taking the adjoint of $A_2(k)$ given in (A11) and expanding the exponential function there we get

$$A_2(k)^\dagger = \int_0^\infty dz\, Q(z)[\varphi(k,z) - \varphi(0,z)] + o(k^2), \tag{A24}$$

where we have used (A7) to determine the order of the error term. Now we insert (A22) into (A24) and proceed as in the derivation of (A17), using $\dot{f}_1''(0,x) = Q(x)\dot{f}_1(0,x)$ and two integrations by parts. We also use (A21), (A23), and the property $\dot{f}_1'(0,N) - iI_n = o(1/N)$ as $N \to +\infty$, which follows from (A20). The result is

$$\int_0^\infty dz\, Q(z)[\varphi(k,z) - \varphi(0,z)] = k^2 \int_0^\infty dz\, [f_1(0,z) - I_n] - k^2 \int_0^\infty dz\, [f_1(0,z)^\dagger f_1(0,z) - I_n] + o(k^2). \tag{A25}$$

Combining (A9), (A12), (A17), (A24), and (A25) we obtain

$$[\varphi(k,x)^\dagger; f_1(k,x)] = ikI_n + k^2 \int_0^\infty dz\, [f_1(0,z)^\dagger f_1(0,z) - I_n] + o(k^2),$$

which is the desired result in (4.13) for $m = 2$.

To prove (4.14) we return to the Wronskian in (A6). If $m = 1$, we have

$$\begin{cases} \displaystyle\int_{-\infty}^0 dz\, e^{-ikz} Q(z)\varphi(k,z) = \int_{-\infty}^0 dz\, Q(z)\varphi(0,z) + o(1), \\ \qquad\qquad = -\Delta_1 + f_1'(0,0) + o(1), \end{cases} \tag{A26}$$

where we have used (2.28) and (A14). The order of the error term is again a consequence of (A7). Substituting (A26) in (A6) we get (4.14) for $m = 1$. If $m = 2$, we have

$$\int_{-\infty}^{0} dz\, e^{-ikz} Q(z)\varphi(k,z) = -\Delta_1 + f_1'(0,0) - ik\int_{-\infty}^{0} dz\, zQ(z)\varphi(0,z) + o(k), \tag{A27}$$

and, using (3.1), (A14), and (A27) we obtain

$$\int_{-\infty}^{0} dz\, zQ(z)\varphi(0,z) = I_n + E_1 - f_1(0,0). \tag{A28}$$

Substituting this in (A6) we get

$$[f_r(-k,x)^\dagger; \varphi(k,x)] = \Delta_1 + ik(I_n + E_1) + o(k),$$

proving (4.14) when $m=2$.

It remains to prove (4.15). So pick $\xi \in \mathcal{N}$ and assume $m=1$. Then $\varphi(0,x)\xi$ stays bounded as $x \to -\infty$, which has the same effect on the integral in (A6), when it acts on ξ, as if m were 2. In particular, (A28) now becomes

$$\int_{-\infty}^{0} dz\, zQ(z)[\varphi(0,z)\xi] = \Gamma\xi - f_1(0,0)\xi,$$

where we have used (2.28) and (4.5). Since $\Delta_1\xi = 0$, from (A27) we obtain

$$\int_{-\infty}^{0} dz\, e^{-ikz} Q(z)[\varphi(k,z)\xi] = f_1'(0,0)\xi - ik\Gamma\xi + ikf_1(0,0)\xi + o(k).$$

Substituting this expression in (A6) we get

$$[f_r(-k,x)^\dagger; \varphi(k,x)]\xi = ik\Gamma\xi + o(k),$$

which agrees with (4.15) for $m=1$. If $m=2$ and $\xi \in \mathcal{N}$, then we can carry the expansion in (A27) further as in the case of (A9) and (A11). To obtain the corresponding coefficients in the expansion we could proceed by using variation of parameters in terms of the solutions $f_r(0,x)$ and $\dot{f}_l(0,x)$. However, there is a simpler approach that exploits the connection between the left and right Jost solutions for (1.1) under the substitution $x \mapsto -x$, that is, under the transformation $Q(x) \mapsto Q^\#(x)$, where $Q^\#(x) = Q(-x)$. We use the superscript # to indicate that a given quantity pertains to (1.1) with potential $Q^\#$. It is straightforward to show that

$$f_r(k,x) = f_l^\#(k,-x), \quad f_l(k,x) = f_r^\#(k,-x). \tag{A29}$$

We now introduce a solution $\omega(k,x)$ of (1.1) satisfying the initial conditions

$$\omega(k,0) = f_r(0,0), \quad \omega'(k,0) = f_r'(0,0).$$

Then it follows from (4.3) and (4.10) that for $\xi \in \mathcal{N}$ we have

$$\varphi(k,x)\xi = \omega(k,x)\chi, \tag{A30}$$

where $\chi = \Gamma\xi$. Since, by (4.10) and (A29)

$$\varphi^\#(k,0) = f_1^\#(k,0) = f_r(k,0), \quad \varphi^{\#\prime}(k,0) = f_1^{\#\prime}(k,0) = -f_r'(k,0),$$

we get $\varphi^\#(k,x) = \omega(k,-x)$, which, together with (A30), yields $\varphi^\#(k,-x)\chi = \varphi(k,x)\xi$. In the following argument we use the more elaborate notation. $[G(k,x); H(k,x)]_{(x_0)}$ to denote the Wronskian of two matrix functions $G(k,x)$ and $H(k,x)$ evaluated at $x = x_0$. Then we have

$$\begin{cases} [f_{\rm r}(-k,x)^{\dagger};\varphi(k,x)]_{(x)}\xi=[f_1^{\#}(-k,-x)^{\dagger};\varphi^{\#}(k,-x)]_{(x)}\chi \\ \qquad\qquad\qquad\qquad =-[f_1^{\#}(-k,x)^{\dagger};\varphi^{\#}(k,x)]_{(-x)}\chi \\ \qquad\qquad\qquad\qquad =[\varphi^{\#}(k,x)^{\dagger};f_1^{\#}(-k,x)]_{(-x)}^{\dagger}\chi \\ \qquad\qquad\qquad\qquad =[\varphi^{\#}(-k,x)^{\dagger};f_1^{\#}(-k,x)]_{(x)}^{\dagger}\chi, \end{cases} \tag{A31}$$

where in the the last step we have used the fact that the Wronskian is constant and that $\varphi(k,x)$ is an even function of k. The latter follows from the fact that the initial conditions in (4.10) are independent of k. Now the Wronskian on the right-hand side of (A31) is of the same form as that in (4.13). We can, therefore, apply the expansion given there. Then the integrand of Y_2 involves $f_1^{\#}(0,z)$ which can be rewritten in terms of $f_{\rm r}(0,z)$ by means of (A29). Using also (4.2), we obtain (4.15). The proof of Proposition 4.2 is now complete. ■

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Continuum quantum systems as limits of discrete quantum systems. III. Operators

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Convergence of a ''discrete'' operator to a ''continuum'' operator is defined. As examples, the circular rotor, the one-dimensional box, the harmonic oscillator, and the fractional Fourier transform are realized as limits of finite-dimensional quantum systems. Limits, thus defined, preserve algebraic structure. The results prepare for a sequel in which some affine canonical transforms will be ''discretized.'' © *2001 American Institute of Physics.* [DOI: 10.1063/1.1398582]

I. INTRODUCTION

The continuum fractional Fourier transform of Namias[1] is the limit of two discrete fractional Fourier transforms, namely, the Kravchuk function FRFT and the Harper function FRFT (see Refs. 2 and 3). Some very straightforward continuum quantum systems, such as the circular rotor, the one-dimensional box and the harmonic oscillator, can easily be realized as limits of equally straightforward finite-dimensional systems whose Hamiltonians are difference operators. For many purposes, the above assertions are clear enough without ''limit'' being understood to have any abstract meaning; nevertheless, the goal of this article is to assign an appropriate general meaning to ''limit,'' to state the above assertions precisely, and to prove them. It is not that we object to the usual common sense techniques—on the contrary, we shall validate them—but subsequently, in a sequel,[4] some ideas pioneered by Atakishiyev–Chumakov–Wolf[5] will be developed: continuum affine canonical transforms and continuum complex-order Fourier transforms will be realized as limits of analogous finite-dimensional transforms. In that application, common sense would not suffice.

Consider a Hilbert space $\mathcal{L}_\infty$, and Hilbert spaces $\mathcal{L}_n$, where the index n runs over some infinite set of positive integers. In Sec. II, we shall interface $\mathcal{L}_\infty$ with the spaces $\mathcal{L}_n$, and we shall assign a meaning to equations of the form

$$\hat{K}_\infty = \lim_n \hat{K}_n,$$

where $\hat{K}_\infty$ is a bounded operator on $\mathcal{L}_\infty$, and each $\hat{K}_n$ is a bounded operator on $\mathcal{L}_n$. In Sec. III, we shall assign a meaning to equations of the form

$$\mathcal{K}_\infty = \lim_n \mathcal{K}_n,$$

where $\mathcal{K}_\infty$ and $\mathcal{K}_n$ are quantum systems on $\mathcal{L}_\infty$ and $\mathcal{L}_n$, respectively. Convergence of vectors has already been discussed in two prequels to the present article. The first prequel[6] explains how $\mathcal{L}_\infty$ is to be interfaced with the spaces $\mathcal{L}_n$, and gives meaning to equations of the form

$$\psi_\infty = \lim_n \psi_n,$$

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where $\psi_\infty \in \mathcal{L}_\infty$ and $\psi_n \in \mathcal{L}_n$. Some of the main definitions and results from Ref. 6 are briefly recalled later in Sec. II. The second prequel[7] shows that widely used limiting techniques are in accordance with the definition of convergence.

With a view to applications, we might think of $\mathcal{L}_\infty$ as a ''continuum'' space, perhaps the Hilbert space formed from the space of square-integrable functions on a differentiable manifold. We might think of each space $\mathcal{L}_n$ as a ''discrete'' space, perhaps a Hilbert space with a coordinate system such that the coefficients of a vector may be interpreted as sample-point values of a function on the manifold. In the case where the manifold is $\mathbb{R}$, Digernes–Varadarájan–Varadhan[8] established a continuum-discrete correspondence—characterized in terms of limits—by embedding each $\mathcal{L}_n$ in $\mathcal{L}_\infty$. Our approach is more concerned with preservation of algebraic structure (linearity, inner products, composition, tensor products). We interface $\mathcal{L}_\infty$ with the spaces $\mathcal{L}_n$ by realizing the sequence $(\mathcal{L}_n)_n$ as an inductive resolution of $\mathcal{L}_\infty$. The definition of an inductive resolution (recalled in Sec. II) is entirely algebraic, and, by this virtue, it relieves us of any need to assign any abstract meaning to the jargon ''continuum'' and ''discrete.'' (As every physicist knows, these two terms often refer to different sides of the same coin.)

The preservation of algebraic structure will be crucial in Ref. 4, where we shall be considering some Lie groups with several degrees of freedom. In subsequent work, we shall present a more systematic study of a way in which ''continuum'' (usually infinite-dimensional) representations of Lie groups may be realized as limits of ''discrete'' (usually finite-dimensional) representations. (Part of the motive for this is to seek criteria for a system of numerically calculated transforms to respect ''continuum'' composition laws.) The results we give later, in Sec. III, and the applications we note in Sec. IV, all concern the special case of one-parameter groups. This special case is helpful as a stepping-stone because some of the concerns that arise in the general case reduce to trivialities here.

However, one-parameter systems are of interest in their own right, and can naturally be regarded as quantum dynamical systems, or, to use the language of Parthasarathy,[9] quantum stochastic processes. (Let us not quibble about the flexible definitions of these terms.) Thus, we are led back to a question addressed by Digernes–Varadarájan–Varadhan.[8] To what extent are spectra in the ''continuum'' scenario related to spectra in the ''discrete'' scenario? This question is explored in Sec. V. The author would like to thank the referee for some useful suggestions concerning Sec. V. Although the material there is still only an initial foray into the matter, it was absent from the previous version of this article.

General motives for a continuum-discrete correspondence—characterized in terms of limits, and preserving algebraic structure—are noted in the prequels, Refs. 6 and 7. Some more extensive references for applications may be found in those two papers. The *Gedankenexperiment* in Ref. 7, Sec. 2, gives a heuristic introduction to our line of approach.

II. INDUCTION OF BOUNDED OPERATORS

By an **operator** on a Hilbert space $\mathcal{L}$, we mean a linear map $\mathcal{D}\to\mathcal{L}$, where the domain $\mathcal{D}$ is a dense subspace of $\mathcal{L}$. Every bounded operator on $\mathcal{L}$ extends uniquely to a bounded operator on $\mathcal{L}$ with domain $\mathcal{L}$. Henceforth, all our bounded operators on a Hilbert space $\mathcal{L}$ shall be deemed to have domain $\mathcal{L}$. We write $U(\mathcal{L})$ for the group of unitary operators on $\mathcal{L}$.

We must briefly review some of the definitions and results of Ref. 6. Consider a Hilbert space $\mathcal{L}_\infty$, a dense subspace $\mathcal{S}$ of $\mathcal{L}_\infty$, an infinite set of positive integers $\mathcal{N}$, Hilbert spaces $\mathcal{L}_n$ for each $n \in \mathcal{N}$, and linear maps $\mathrm{res}_n : \mathcal{S} \to \mathcal{L}_n$. (The results below may easily be extended to the case where $\mathcal{N}$ is any directed set, as in Ref. 6.)

The linear maps res_n, called the **restriction maps**, are required to satisfy the reciprocity condition

$$\langle \phi | \chi \rangle = \lim_{n \in \mathcal{N}} \langle \mathrm{res}_n(\phi) | \mathrm{res}_n(\chi) \rangle$$

for all $\phi,\chi\in\mathcal{S}$. The sequence $(\mathcal{L}_n)_n$, equipped with the sequence $(\mathrm{res}_n)_n$, is called an **inductive resolution** of $\mathcal{L}_\infty$.

Given a vector $\psi\in\mathcal{L}_\infty$, and vectors $\psi_n\in\mathcal{L}_n$ for sufficiently large $n\in\mathcal{N}$ (not necessarily for all $n\in\mathcal{N}$), we say that the sequence $(\psi_n)_n$ **converges** to ψ_∞ provided the norms $\|\psi_n\|$ are bounded and

$$\langle\phi|\psi_\infty\rangle=\lim_{n\in\mathcal{N}}\langle\mathrm{res}_n(\phi)|\psi_n\rangle$$

for all $\phi\in\mathcal{S}$. The Riesz representation theorem guarantees that $(\psi_n)_n$ converges to at most one vector in $\mathcal{L}_\infty$. When $(\psi_n)_n$ converges to ψ_∞, we call ψ_∞ the **limit** of $(\psi_n)_n$, and we write $\psi_\infty=\lim_{n\in\mathcal{N}}\psi_n$. Note that $\phi=\lim_{n\in\mathcal{N}}\mathrm{res}_n(\phi)$ for all $\phi\in\mathcal{S}$.

Let us recall some results that we shall need from Ref. 6.

Theorem 2.1: (Ref. 6, Theorem 2.4) *Any vector $\psi_\infty\in\mathcal{L}_\infty$ is the limit of some sequence $(\psi_n)_n$, and, furthermore, the vectors $\psi_n\in\mathcal{L}_n$ may be chosen such that $\|\psi_\infty\|=\|\psi_n\|$ for all n.*

Let $\mathcal{B}_\infty=\{\beta_{j,\infty}:j\in J_\infty\}$ be any enumerated orthonormal basis for $\mathcal{L}_\infty$. Here, $J_\infty=\mathbb{N}$ if $\mathcal{L}_\infty$ is infinite-dimensional, while $J_\infty=\{0,1,\ldots,d-1\}$ if $\mathcal{L}_\infty$ has finite dimension d. By Ref. 6, Theorem 3.1, there exist $\mathcal{B}_n$, indexed by $n\in\mathcal{N}$, where each $\mathcal{B}_n$ is an enumerated orthonormal set $\mathcal{B}_n=\{\beta_{j,n}:j\in J_n\}$ in $\mathcal{L}_n$, and

$$\beta_{j,\infty}=\lim_{n\in\mathcal{N}}\beta_{j,n}$$

for all $j\in J_\infty$. Note that, for each basis vector $\beta_{j,\infty}$ in $\mathcal{L}_\infty$, a corresponding basis vector $\beta_{j,n}$ in $\mathcal{L}_n$ need not exist for all n, but the $\beta_{j,n}$ must exist for sufficiently large n.

As explained in Ref. 6, Sec. 3, the $\mathcal{B}_n$ cannot always be chosen such that each $\mathcal{B}_n$ is a basis. (In all our applications in Sec. IV, each of our chosen $\mathcal{B}_n$ is a basis. We also mention that, in all these applications, $\mathcal{L}_\infty$ is infinite-dimensional, $\mathcal{N}$ is a set of positive integers, and each $\mathcal{L}_n$ has finite dimension n.) We let $\mathcal{L}_n^\perp$ denote the subspace of $\mathcal{L}_n$ orthogonally complementary to the span of $\mathcal{B}_n$. Given a vector $\psi_\infty\in\mathcal{L}_\infty$, we write

$$\psi_\infty=\sum_{j=0}^{\infty}c_{j,\infty}\beta_{j,\infty}$$

with the understanding that $c_{j,n}=0$ for all $j\in\mathbb{N}-J_\infty$. Given $\psi_n\in\mathcal{L}_n$, we write

$$\psi_n=\psi_n^\perp+\sum_{j=0}^{\infty}c_{j,n}\beta_{j,n}$$

where $\psi_n^\perp\in\mathcal{L}_n^\perp$, and $c_{j,n}=0$ for all $j\in\mathbb{N}-J_n$. (Of course, if $\mathcal{B}_n$ is a basis, then $\psi_n^\perp=0$.) For later convenience, we define $\beta_{j,\infty}:=0$ when $j\in\mathbb{N}-J_\infty$, and $\beta_{j,n}:=0$ when $j\in\mathbb{N}-J_n$. Thus $c_{j,\infty}=\langle\beta_{j,\infty}|\psi_\infty\rangle$ and $c_{j,n}=\langle\beta_{j,n}|\psi_n\rangle$ for all $j\in\mathbb{N}$.

Theorem 2.2: (Ref. 6, Theorem 3.4) *Using the notation above, $\psi_\infty=\lim_{n\in\mathcal{N}}\psi_n$ if and only if the norms $\|\psi_n\|$ are bounded, and $c_{j,\infty}=\lim_{n\in\mathcal{N}}c_{j,n}$ for all $j\in J_\infty$.*

We can now turn to convergence of operators. Let $\hat{K}_\infty$ be a bounded operator on $\mathcal{L}_\infty$, and for sufficiently large $n\in\mathcal{N}$, let $\hat{K}_n$ be a bounded operator $\mathcal{L}_n$. We say that the sequence $(\hat{K}_n)_n$ **converges** to $\hat{K}_\infty$ provided the norms $\|\hat{K}_n\|$ are bounded, and for all $\psi_\infty\in\mathcal{L}_\infty$, and all sequences $(\psi_n)_n$ with $\psi_n\in\mathcal{L}_n$ and $\psi_\infty=\lim_{n\in\mathcal{N}}(\psi_n)$, we have

$$\hat{K}_\infty\psi_\infty=\lim_{n\in\mathcal{N}}(\hat{K}_n\psi_n).$$

Theorem 2.1 ensures that the sequence $(\hat{K}_n)_n$ converges to at most one bounded operator on $\mathcal{L}_\infty$. When $(\hat{K}_n)_n$ converges to $\hat{K}_\infty$, we call $\hat{K}_\infty$ the **limit** of $(\hat{K}_n)_n$, and we write $\hat{K}_\infty=\lim_{n\in\mathcal{N}}\hat{K}_n$.

Remark 2.3: Given bounded operators $\hat{K}_\infty = \lim_{n\in\mathcal{N}} \hat{K}_n$ *and* $\hat{K}'_\infty = \lim_{n\in\mathcal{N}} \hat{K}'_n$, *and given* $\lambda,\lambda' \in \mathbb{C}$, *then* $\lambda\hat{K}_\infty + \lambda'\hat{K}'_\infty = \lim_{n\in\mathcal{N}}(\lambda\hat{K}_n + \lambda'\hat{K}'_n)$ *and* $\hat{K}_\infty\hat{K}'_\infty = \lim_{n\in\mathcal{N}} \hat{K}_n\hat{K}'_n$.

Proof: This is obvious. □

Theorem 2.4: *Given any bounded* $\hat{K}_\infty$ *on* $\mathcal{L}_\infty$, *then there exist bounded operators* $\hat{K}_n$ *on each* $\mathcal{L}_n$ *such that* $\hat{K}_\infty = \lim_{n\in\mathcal{N}} \hat{K}_n$ *and* $\|\hat{K}_n\| = \|\hat{K}_\infty\|$ *for all* $n \in \mathcal{N}$.

Proof: Let $\mathcal{B}_\infty$ and $\mathcal{B}_n$ be as above. We define

$$K_{j,k} = \langle \beta_{j,\infty} | \hat{K}_\infty \beta_{k,\infty} \rangle$$

for all $j,k \in \mathbb{N}$. (Note that $K_{j,k} = 0$ unless j and k both belong to J_∞.) On each space $\mathcal{L}_n$, we define an operator $\hat{K}'_n$ annihilating $\mathcal{L}_n^\perp$ and such that

$$K_{j,k} = \langle \beta_{j,n} | \hat{K}'_n \beta_{k,n} \rangle$$

for all $j,k \in J_n$. Consider vectors $\psi_\infty \in \mathcal{L}_\infty$ and $\psi_n \in \mathcal{L}_n$ such that $\psi_\infty = \lim_n \psi_n$. Let the coefficients $c_{j,\infty}$ and $c_{j,n}$ be as above. Then

$$\|\hat{K}'_n \psi_n\|^2 = \sum_{j=0}^{\infty} \left| \sum_{k=0}^{\infty} K_{j,k} c_{k,n} \right|^2 \leqslant \|\hat{K}_\infty\|^2 \|\psi_n\|^2.$$

So the norms $\|\hat{K}'_n\|$ are bounded by $\|\hat{K}_\infty\|$. Given $\epsilon > 0$, then there exists a positive integer N and complex numbers $c_0, \ldots, c_{N-1}$ such that

$$\sum_{j=0}^{N-1} \left| \sum_{k=0}^{N-1} K_{j,k} c_k \right|^2 \geqslant (\|\hat{K}_\infty\| - \epsilon)^2 \sum_{j=0}^{N-1} |c_j|^2.$$

For sufficiently large $n \in \mathcal{N}$, we have $\{0,\ldots,N-1\} \cap J_\infty \subseteq J_n$, whereupon $\|\hat{K}'_n\| \geqslant \|\hat{K}_\infty\| - \epsilon$. Therefore, $\|\hat{K}_\infty\| = \lim_{n\in\mathcal{N}} \|\hat{K}'_n\|$.

We claim that $\hat{K}_\infty = \lim_n \hat{K}'_n$. Let $\phi \in \mathcal{S}$. For each n, let $\phi_n := \mathrm{res}_n(\phi)$. To prove the claim, it suffices to show that

$$\langle \phi | \hat{K}_\infty \psi_\infty \rangle = \lim_n \langle \phi_n | \hat{K}'_n \psi_n \rangle.$$

For each $j \in \mathbb{N}$, let $a_{j,\infty} := \langle \beta_{j,\infty} | \phi \rangle$ and $a_{j,n} := \langle \beta_{j,n} | \phi_n \rangle$. Thus

$$\phi = \sum_{j=0}^{\infty} a_{j,\infty} \beta_{j,\infty} \quad \text{and} \quad \phi_n = \phi_n^\perp + \sum_{j=0}^{\infty} a_{j,n} \beta_{j,n},$$

where $\psi_n^\perp \in \mathcal{L}_n^\perp$. We have

$$\langle \phi_n | \hat{K}'_n \psi_n \rangle = \sum_{j,k=0}^{\infty} \overline{a}_{j,n} K_{j,k} c_{k,n}$$

and a similar equation holds for $\langle \phi | \hat{K}_\infty \psi_n \rangle$. (By absolute convergence properties, all the sums we consider can be rearranged.) We have

$$|\langle \phi | \hat{K}_\infty \psi_\infty \rangle - \langle \phi_n | \hat{K}'_n \psi_n \rangle| \leqslant \left| \sum_{j,k=0}^{\infty} \overline{a}_{j,\infty} K_{j,k} (c_{k,\infty} - c_{k,n}) \right| + \left| \sum_{j,k=0}^{\infty} (\overline{a}_{j,\infty} - \overline{a}_{j,n}) K_{j,k} c_{k,n} \right|.$$

(Using the boundedness of $\hat{K}_\infty$, it is easy to check that these sums are absolutely convergent.) Letting C be an upper bound for the norms $\|\psi_n\|$, then

$$\sum_{j=0}^{\infty}\left|\sum_{k=0}^{\infty}K_{j,k}c_{k,n}\right|^2\leqslant C^2\|\hat{K}_\infty\|^2$$

for sufficiently large n. Part of Ref. 6, Lemma 3.3, says that $\Sigma_{j=0}^{\infty}|a_{j,\infty}-a_{j,n}|^2\leqslant\epsilon^2$ for sufficiently large n. Hence

$$\left|\sum_{j,k=0}^{\infty}(\overline{a}_{j,\infty}-\overline{a}_{j,n})\hat{K}_{j,k}c_{k,n}\right|\leqslant\epsilon C\|\hat{K}_\infty\|.$$

We may insist that $C\geqslant\|\psi_\infty\|$. Thereupon,

$$\sum_{j=0}^{\infty}\left|\sum_{k=0}^{\infty}K_{j,k}(c_{k,\infty}-c_{k,n})\right|^2\leqslant 4C^2\|\hat{K}_\infty\|^2$$

for sufficiently large n. The series $\Sigma_{j=0}^{\infty}|a_{j,\infty}|^2$ converges (to $\|\phi\|^2$), so there exists a positive integer M such that $\Sigma_{j=M}^{\infty}|a_{j,\infty}|^2\leqslant\epsilon^2$. We have

$$\left|\sum_{j=M}^{\infty}\sum_{k=0}^{\infty}\overline{a}_{j,\infty}K_{j,k}(c_{k,\infty}-c_{k,n})\right|\leqslant 2\epsilon C\|\hat{K}_\infty\|$$

for large n. To prove the claim, it now suffices to show that

$$\left|\sum_{j=0}^{M-1}\sum_{k=0}^{\infty}\overline{a}_{j,\infty}K_{j,k}(c_{k,\infty}-c_{k,n})\right|=O(\epsilon).$$

Let $j\in\mathbb{N}$. Suppose there exists some $\delta>0$ such that, for every positive integer L, there exist complex numbers $c_L,c_{L+1},\ldots$ satisfying

$$\sum_{k=L}^{\infty}|c_k|^2\leqslant 1\quad\text{and}\quad\left|\sum_{k=L}^{\infty}K_{j,k}c_k\right|>\delta.$$

Then there exist complex numbers $c_0,c_1,\ldots$ and integers $0=L_0<L_1<\cdots$ such that each $K_{j,k}c_k$ is a non-negative real, and

$$\sum_{k=L_{r-1}}^{L_r-1}|c_k|^2\leqslant\frac{1}{n^2}\ \text{and}\ \sum_{k=L_{r-1}}^{L_r-1}K_{j,k}c_k>\frac{\delta}{2n}$$

for all positive integers r. The series $\Sigma_{k=0}^{\infty}|c_k|^2$ converges while the series $\Sigma_{k=0}^{\infty}K_{j,k}c_k$ diverges. This contradicts the boundedness of $\hat{K}_\infty$. We deduce that, for any positive real B, there exists a positive integer L such that, for all complex numbers $c_L,c_{L+1},\ldots$ satisfying $\Sigma_{k=L}^{\infty}|c_k|^2\leqslant B$, we have $|\Sigma_{k=L}^{\infty}K_{j,k}c_k|\leqslant\epsilon/M$. For large n, we have $\Sigma_{k=0}^{\infty}|c_{k,\infty}-c_{k,n}|^2\leqslant 4C^2$. So there exists a positive integer L such that, for large n, and for all $j<M$, we have

$$\left|\sum_{k=L}^{\infty}K_{j,k}(c_{k,\infty}-c_{k,n})\right|\leqslant\epsilon/M.$$

Each $|a_{j,\infty}|\leqslant\|\phi\|$, so

$$\left|\sum_{j=0}^{M-1}\sum_{k=L}^{\infty}\overline{a}_{j,\infty}K_{j,k}(c_{k,\infty}-c_{k,n})\right|\leqslant\epsilon\|\phi\|$$

for large n. The claim will follow when we have shown that

$$\left| \sum_{j=0}^{M-1} \sum_{k=0}^{L-1} \overline{a}_{j,\infty} K_{j,k} (c_{k,\infty} - c_{k,n}) \right| = O(\epsilon)$$

for large n. By Theorem 2.2, $c_{k,\infty} = \lim_{n \in \mathcal{N}} c_{k,n}$. The claim is established.

To finish the argument, we must replace the operators $\hat{K}'_n$ with operators $\hat{K}_n$ on $\mathcal{L}_n$ such that $\|\hat{K}_n\| = \|\hat{K}_\infty\|$ for all $n \in \mathcal{N}$. We may assume that $\|\hat{K}_\infty\| = 1$. From the first paragraph of the argument, $\|\hat{K}'_n\|$ converges to 1. So $\hat{K}_n \neq 0$ for large n. When $\hat{K}'_n \neq 0$, we put $\hat{K}_n = \hat{K}'_n / \|\hat{K}'_n\|$, otherwise we put $\hat{K}_n = \hat{1}$. Then each $\|\hat{K}_n\| = 1$, and $\|\hat{K}_n - \hat{K}'_n\| \to 0$. Since the norms $\|\psi_n\|$ are bounded, $\|\hat{K}_n \psi_n - \hat{K}'_n \psi_n\| \to 0$. It was shown in Ref. 6, Remark 2.3, that, for $\theta_\infty \in \mathcal{L}_\infty$ and $\theta_n, \chi_n \in \mathcal{L}_n$ satisfying $\theta_\infty = \lim_{n \in \mathcal{N}} \theta_n$ and $\lim_{n \in \mathcal{N}} \|\theta_n - \chi_n\| = 0$, we have $\theta_\infty = \lim_{n \in \mathcal{N}} \chi_n$. Therefore, $\hat{K}_\infty \psi_\infty = \lim_{n \in \mathcal{N}} \hat{K}_n \psi_n$. □

Corollary 2.5: Given any bounded Hermitian operator $\hat{H}_\infty$ on $\mathcal{L}_\infty$, then there exist bounded Hermitian operators $\hat{H}_n$ on each $\mathcal{L}_n$ such that $\hat{H}_\infty = \lim_{n \in \mathcal{N}} \hat{H}_n$ and $\|\hat{H}_n\| = \|\hat{H}_\infty\|$ for each $n \in \mathcal{N}$.

Proof: In the proof of Theorem 2.4, if $\hat{K}_\infty$ is Hermitian, then so is each $\hat{K}_n$. □

In order to accommodate the possibility of working with a compound of several quantum stochastic processes (for example, a quantum system with several particles), we must discuss tensor products of inductive resolutions, and we must show how the limits of vectors and operators are compatible with the tensor product. Let $\mathcal{L}'_\infty$ be a Hilbert space, and let $\mathcal{S}'$ be a dense subspace of $\mathcal{L}'_\infty$. For each $n \in \mathcal{N}$, let $\mathcal{L}'_n$ be a Hilbert space, and let $\mathrm{res}'_n : \mathcal{S}' \to \mathcal{L}_n$ be restriction maps. Then $\mathcal{L}_\infty \otimes \mathcal{L}'_\infty$ has an inductive resolution with restriction maps $\mathrm{res}_n \otimes \mathrm{res}'_n : \mathcal{S} \otimes \mathcal{S}' \to \mathcal{L}_n \otimes \mathcal{L}'_n$. Given limits of vectors $\psi_\infty = \lim_n \psi_n$ and $\psi'_\infty = \lim_n \psi'_n$ in $\mathcal{L}_\infty$ and $\mathcal{L}'_\infty$, respectively, it is clear that we have a limit of vectors $\psi_\infty \otimes \psi'_\infty = \lim_n \psi_n \otimes \psi'_n$. By considering orthonormal coordinates and applying Ref. 6, Theorem 3.4, it is easy to check that limits of bounded operators preserve tensor products in the same way. (Warning: we are not invoking Ref. 6, Theorem 3.4, gratuitously. Not every sequence in $\mathcal{L}_n \otimes \mathcal{L}'_n$ converging to $\psi_\infty \otimes \psi'_\infty$ has terms of the form $\psi_n \otimes \psi'_n$.) These (rather trivial) remarks show that the limits behave well in the (rather banal) case of a fixed finite number of noninteracting processes. Presumably, they also behave well with respect to symmetric and antisymmetric tensor products, and with respect to the construction of free, symmetric, and antisymmetric Fock spaces (see Ref. 9, Chap. II). We leave that matter for further research.

III. CONVERGENCE OF QUANTUM SYSTEMS

Recall that a family $\{\hat{K}(t) : t \in \mathbb{R}\}$ of operators on a Hilbert space $\mathcal{L}$ is said to be **strongly continuous** provided each $\hat{K}(t)$ has domain $\mathcal{L}$ and, for all $\psi \in \mathcal{L}$, the function $\mathbb{R} \to \mathcal{L}$ given by $t \mapsto \hat{K}(t)\psi$ is continuous. If, furthermore, $\hat{K}(0) = \hat{1}$ and each $\hat{K}(t)$ is bounded, then we call $\{\hat{K}(t) : t \in \mathbb{R}\}$ a **quantum system** on $\mathcal{L}$. In that case, we sometimes consider a family of vectors $\{\psi(t) : t \in \mathbb{R}\}$ such that

$$\psi(t) = \hat{K}(t)\psi(0).$$

A quantum system $\mathcal{U} = \{\hat{U}(t) : t \in \mathbb{R}\}$ on $\mathcal{L}$ is said to be **unitary** provided each operator $\hat{U}(t)$ is unitary. If, furthermore,

$$\hat{U}(t)\hat{U}(t') = \hat{U}(t + t')$$

for all $t, t' \in \mathbb{R}$, then we say that $\mathcal{U}$ is **conservative**.

The boundedness condition in our general definition of a quantum system is somewhat artificial, but convenient for our purposes. Our main concern is with conservative systems, and these have been thoroughly studied in various contexts and from various perspectives. For a detailed

introduction to conservative systems as quantum stochastic systems, see Ref. 9, Chap. 1. Let us recall some well-known properties of conservative systems (introducing some notation that will be convenient in the proof of Theorem 3.5).

Suppose that $\mathcal{U}$ is conservative. Stone's theorem asserts that there exists a unique Hermitian operator $\hat{H}$ on $\mathcal{L}$ such that

$$U(t)=\exp(-i\hat{H}t).$$

We call $\hat{H}$ the **Hamiltonian** for $\mathcal{U}$. Conversely, every Hermitian operator on $\mathcal{L}$ is the Hamiltonian of a conservative quantum system. The bijective correspondence $\hat{H}\leftrightarrow\mathcal{U}$ allows us to characterize conservative quantum systems by the Schrödinger equation

$$i\frac{d}{dt}\psi(t)=\hat{H}\psi(t).$$

For the sake of rigor, we must mention that, as a definition,

$$\exp(-i\hat{H}t):=\int_{-\infty}^{\infty}e^{-its}dE(s),$$

where E is the spectral family for $\hat{H}$. The notation on the right-hand side is as in Ref. 10, Chap. 7. It may be worth explaining what this equation tells us. Introducing some notation that will be of use in the proof of Theorem 3.5, let us consider an integer m, and write $\hat{E}_m$ for the orthogonal projection on $\mathcal{L}$ associated with E and the half-open interval $[m,m+1)$. [Intuitively, we might think of $\hat{E}_m$ as the projection to the subspace $\hat{E}_m\mathcal{L}$ of $\mathcal{L}$ spanned by those ''eigenvectors'' whose ''eigenvalues'' are at least m and less than $m+1$. The operator $\hat{H}$ restricts to an operator on each subspace $\hat{E}_m\mathcal{L}$. Vaguely, we might think of $\hat{E}_m$ as a kind of ''eigenspace,'' whose associated ''eigenvalue'' is spread across the interval $[m,m+1)$.] Any vector in $\mathcal{L}$ is a sum of vectors belonging to the spaces $\hat{E}_m\mathcal{L}$, so the unitary operator $\exp(-i\hat{H}t)$ is determined by the condition that it restricts to an operator on $\hat{E}_m\mathcal{L}$ given by

$$\exp(-i\hat{H}t)\psi=\sum_{l=0}^{\infty}\frac{(-i\hat{H}t)^l}{l!}\psi$$

for all $\psi\in\hat{E}_m\mathcal{L}$. (The series converges because $\hat{H}$ restricts to a bounded operator on $\hat{E}_m\mathcal{L}$.)

Stone's theorem may be found in Ref. 10, Theorem 7.38. The bijectivity of the correspondence $\hat{H}\leftrightarrow\mathcal{U}$ is given in Ref. 15, Theorem 7.37. See also Ref. 9, Theorem 13.1.

Given a quantum system $\mathcal{K}_\infty=\{\hat{K}_\infty(t):t\in\mathbb{R}\}$ on $\mathcal{L}_\infty$, and quantum systems $\mathcal{K}_n=\{\hat{K}_n(t):t\in\mathbb{R}\}$ on $\mathcal{L}_n$ for sufficiently large $n\in\mathcal{N}$, we say that $(\mathcal{K}_n)_n$ **converges** to $\mathcal{K}_\infty$ provided

$$\hat{K}_\infty(t)=\lim_{n\in\mathcal{N}}\hat{K}_n(t)$$

for all $t\in\mathbb{R}$. Obviously, $(\mathcal{K}_n)_n$ converges to at most one quantum system on $\mathcal{L}_\infty$. When $(\mathcal{K}_n)_n$ converges to $\mathcal{K}_\infty$, we call $\mathcal{K}_\infty$ the **limit** of $(\mathcal{K}_n)_n$, and we write $\mathcal{K}_\infty=\lim_{n\in\mathcal{N}}\mathcal{K}_n$.

Remark 3.1: Let $\mathcal{K}_\infty=\{\hat{K}_\infty(t):t\in\mathbb{R}\}$ and $\mathcal{K}_n=\{\hat{K}_n(t):t\in\mathbb{R}\}$, respectively, be quantum systems on $\mathcal{L}_\infty$ and on each $\mathcal{L}_n$. Write $\psi_\infty(t)=\hat{K}_\infty(t)\psi_\infty(0)$ and $\psi_n(t)=\hat{K}_n(t)\psi_n(0)$. Then we have a limit of quantum systems $\mathcal{K}_\infty=\lim_{n\in\mathcal{N}}\mathcal{K}_n$ if and only if, given any initial state vectors $\psi_\infty(0)$ in $\mathcal{L}_\infty$ and $\psi_n(0)$ in each $\mathcal{L}_n$ with $\psi_\infty(0)=\lim_{n\in\mathcal{N}}(\psi_n(0))$, and writing $\psi_\infty(t)=\hat{K}_\infty(t)\psi_\infty(0)$ and $\psi_n(t)=\hat{K}_n(t)\psi_n(0)$, we have $\psi_\infty(t)=\lim_{n\in\mathcal{N}}\psi_n(t)$ for all $t\in\mathbb{R}$.

Proof: This is obvious. □

In particular, Remark 3.1 tells us that if the limit holds for the quantum systems and for the initial vectors, then the limit holds for all the time-evolved vectors. In case this seems counter-intuitive, we point out that, if $\psi_n(t)$ is to be a "good approximation" to $\psi_\infty(t)$, one should first fix t, and then choose n.

Theorem 3.2: *Any quantum system on $\mathcal{L}_\infty$ is the limit of a sequence of quantum systems on the spaces $\mathcal{L}_n$.*

Proof: Let $\mathcal{K}_\infty=\{\hat{K}_\infty(t):t\in\mathbb{R}\}$ be a quantum system on $\mathcal{L}_\infty$. For each $t\in\mathbb{R}$, and $j,k\in\mathbb{N}$, we define

$$K_{j,k}(t):=\langle\beta_{j,\infty}|\hat{K}_\infty(t)\beta_{k,\infty}\rangle.$$

Let $\hat{K}_n(t)$ be the operator in $\mathcal{L}_n$ constructed from the matrix entries $K_{j,k}(t)$ as in the proof of Theorem 2.4. Let $\mathcal{K}_n=\{\hat{K}_n(t):t\in\mathbb{R}\}$. Using the condition that $\mathcal{K}_\infty$ is strongly continuous, it is easy to check that each $\mathcal{K}_n$ is strongly continuous. □

Proposition 3.3: *Let $\hat{H}_\infty$ and each $\hat{H}_n$ be bounded Hermitian operators on $\mathcal{L}_\infty$ and $\mathcal{L}_n$, respectively, and suppose that the norms $\|\hat{H}_n\|$ are bounded. Let $\mathcal{U}_\infty$ and each $\mathcal{U}_n$ be the conservative systems with Hamiltonians $\hat{H}_\infty$ and $\hat{H}_n$, respectively. Then $\mathcal{U}_\infty=\lim_{n\in\mathcal{N}}\mathcal{U}_n$ if and only if $\hat{H}_\infty=\lim_{n\in\mathcal{N}}\hat{H}_n$.*

Proof: Write $\mathcal{U}_\infty=\{\hat{U}_\infty(t):t\in\mathbb{R}\}$ and $\mathcal{U}_n=\{\hat{U}_n(t):t\in\mathbb{R}\}$. For $m\in\mathbb{N}$, let

$$\hat{K}_{m,\infty}(t):=\sum_{k=0}^{m}\frac{(-i\hat{H}_\infty t)^k}{k!}\quad\text{and}\quad\hat{K}_{m,n}(t):=\sum_{k=0}^{m}\frac{(-i\hat{H}_n t)^k}{k!}.$$

Then $\hat{U}_\infty(t)=\lim_{m\to\infty}\hat{K}_{m,\infty}(t)$ and $\hat{U}_n(t)=\lim_{m\to\infty}\hat{K}_{m,n}(t)$.

Let $\epsilon>0$. Consider vectors $\phi\in\mathcal{S}$ and $\psi_\infty\in\mathcal{L}_\infty$ and $\psi_n\in\mathcal{L}_n$ such that $\psi_\infty=\lim_n\psi_n$. Write $\phi_n=\mathrm{res}_n(\phi)$. Let A be an upper bound for $\|\phi\|$ and $\|\phi_n\|$. Let B be an upper bound for $\|\hat{H}_\infty\|$ and $\|\hat{H}_n\|$. Let C be an upper bound for $\|\psi_\infty\|$ and $\|\psi_n\|$. Choose m such that

$$2AC\sum_{k=m}^{\infty}|Bt|^k/k!\leqslant\epsilon.$$

Then $\|\hat{U}_\infty(t)-K_{m,\infty}(t)\|\leqslant\epsilon/2AC\geqslant\|\hat{U}_n(t)-K_{m,n}(t)\|$ for sufficiently large n. Hence

$$|\langle\phi|\hat{U}_\infty(t)-\hat{K}_{m,\infty}(t)|\psi_\infty\rangle-\langle\phi_n|\hat{U}_n-\hat{K}_{m,n}(t)|\psi_n\rangle|\leqslant\epsilon.$$

If $\hat{H}_\infty=\lim_n\hat{H}_n$, then, by Remark 2.3, $\hat{K}_{m,\infty}=\lim_n\hat{K}_{m,n}$, hence $\hat{U}_\infty(t)\psi_\infty=\lim_{n\in\mathcal{N}}\hat{U}_n(t)\psi_n$.

Conversely, suppose that $\hat{U}_\infty(t)\psi_\infty=\lim_{n\in\mathcal{N}}\hat{U}_n(t)\psi_n$. Given t, we can put $\epsilon=t^2/2$ (and then choose m), where

$$|\langle\phi|\hat{K}_{m,\infty}(t)\psi_\infty\rangle-\langle\phi_n|\hat{K}_{m,n}(t)\psi_n\rangle|=O(t^2)$$

for sufficiently large n. Equating coefficients of t (the sums $\Sigma_{k=0}^{m}|\hat{H}_n t|^k/k!$ and the similar sum for $\hat{H}_\infty$ are bounded by $e^{B|t|}$), we obtain $\hat{H}_\infty\psi_\infty=\lim_n\hat{H}_n\psi_n$. □

Corollary 3.4: Let $\mathcal{U}_\infty$ be a conservative system on $\mathcal{L}_\infty$ with bounded Hamiltonian $\hat{H}_\infty$. Then there exist conservative systems $\mathcal{U}_n$ on $\mathcal{L}_n$ with bounded Hamiltonians $\hat{H}_n$ such that $\mathcal{U}_\infty=\lim_{n\in\mathcal{N}}\mathcal{U}_n$ and $\hat{H}_\infty=\lim_{n\in\mathcal{N}}\hat{H}_n$.

Proof: This is immediate from Corollary 2.5 and Proposition 3.3. □

Theorem 3.5: *Any conservative system on $\mathcal{L}_\infty$ is the limit of a sequence of conservative systems on the spaces $\mathcal{L}_n$.*

Proof: Let $\mathcal{U}_\infty=\{\hat{U}_\infty(t):t\in\mathbb{R}\}$ be a conservative system on $\mathcal{L}_\infty$, let $\hat{H}_\infty$ be the Hamiltonian for $\mathcal{U}_\infty$, and let E be the spectral family for $\hat{H}_\infty$. For each $m\in\mathbb{Z}$, let $\hat{E}_m$ be the orthogonal projection as above, and let $\mathcal{L}_{m,\infty}=\hat{E}_m\mathcal{L}_\infty$. The Hermitian operator $\hat{H}_\infty$ restricts to a Hermitian operator $\hat{H}_{m,\infty}$ on $\mathcal{L}_{m,\infty}$. Let $\mathcal{U}_{m,\infty}=\{\hat{U}_{m,\infty}(t):t\in\mathbb{R}\}$ be the conservative system on $\mathcal{L}_{m,\infty}$ with Hamiltonian $\hat{H}_{m,\infty}$. Any vector $\psi_\infty\in\mathcal{L}_\infty$ has a unique decomposition as a sum

$$\psi_\infty=\sum_{m\in\mathbb{Z}}\psi_{m,\infty}$$

where each $\psi_{m,\infty}\in\mathcal{L}_{m,\infty}$. We have $\hat{H}_\infty\psi_{m,\infty}=\hat{H}_{m,\infty}\psi_{m,\infty}$ and

$$\hat{U}_\infty(t)\psi_\infty=\sum_{m\in\mathbb{Z}}\hat{U}_{m,\infty}(t)\psi_{m,\infty}.$$

It is easy to see that there exists an enumerated orthonormal basis $\mathcal{B}_\infty=\{\beta_{j,\infty}:j\in J_\infty\}$ such that each $\beta_{j,\infty}$ belongs to one of the subspaces $\mathcal{L}_{m,\infty}$. The enumerated orthonormal sets $\mathcal{B}_n$, as in Sec. II, may be chosen such that each $J_n\subseteq J_\infty$. For each $m\in\mathbb{Z}$, let

$$J_\infty(m):=\{j\in J_\infty:\beta_{j,\infty}\in\mathcal{L}_{m,\infty}\}\quad\text{and}\quad J_n(m):=J_n\cap J_\infty(m).$$

Let $\mathcal{L}_{m,n}$ be the subspace of $\mathcal{L}_n$ spanned by the vectors $\beta_{j,n}$ such that $j\in J_n(m)$. Any vector $\chi_n\in\mathcal{L}_n$ has a unique decomposition as a sum

$$\chi_n=\chi_n^\perp+\sum_{m\in\mathbb{Z}}\chi_{m,n},$$

where $\chi_n^\perp\in\mathcal{L}_n^\perp$, and each $\chi_{m,n}\in\mathcal{L}_{m,n}$. For $j,k\in J_\infty$, let

$$H_{j,k}=\langle\beta_{j,\infty}|\hat{H}_\infty\beta_{k,\infty}\rangle.$$

Note that $H_{j,k}=\overline{H_{k,j}}$, and $H_{j,k}=0$ unless $j,k\in J_\infty(m)$ for some $m\in\mathbb{Z}$. Let $\hat{H}_{m,n}$ be the Hermitian operator on $\mathcal{L}_{m,n}$ such that

$$H_{j,k}=\langle\beta_{j,n}|\hat{H}_{m,n}\beta_{k,n}\rangle$$

for $j,k\in J_n(m)$. Let $\mathcal{U}_{m,n}=\{\hat{U}_{m,n}(t):t\in\mathbb{R}\}$ be the conservative system on $\mathcal{L}_{m,n}$ with Hamiltonian $\hat{H}_{m,n}$. Let $\hat{H}_n$ be the Hermitian operator on $\mathcal{L}_n$ such that $\hat{H}_n\chi_n^\perp=0$ and $\hat{H}_n\chi_{m,n}=\hat{H}_{m,n}\chi_{m,n}$. Let $\mathcal{U}_n=\{\hat{U}_n(t):t\in\mathbb{R}\}$ be the conservative system on $\mathcal{L}_n$ with Hamiltonian $\hat{H}_n$. Then

$$\hat{U}_n(t)\chi_n=\chi_n^\perp+\sum_{m\in\mathbb{Z}}\hat{U}_{m,n}(t)\chi_{m,n}.$$

We are to show that $\hat{U}_\infty(t)=\lim_{n\in\mathcal{N}}\hat{U}_n(t)$ for all $t\in\mathbb{R}$.

For each $n\in\mathcal{N}$, let $\psi_n\in\mathcal{L}_n$, and suppose that $\psi_\infty=\lim_{n\in\mathcal{N}}\psi_n$. Write

$$\psi_\infty=\sum_{j=0}^{\infty}c_{j,\infty}\beta_{j,\infty}\quad\text{and}\quad\psi_n=\psi_n^\perp+\sum_{j=0}^{\infty}c_{j,n}\beta_{j,n}$$

as in Sec. II. Fix $t\in\mathbb{R}$, and let $\theta_\infty=\hat{U}_\infty(t)\psi_\infty$ and $\theta_n=\hat{U}_n\psi_n$. We are to show that $\theta_\infty=\lim_n\theta_n$. Write

$$\theta_\infty = \sum_{j=0}^{\infty} d_{j,\infty}\beta_{j,\infty} \quad \text{and} \quad \theta_n = \theta_n^\perp + \sum_{j=0}^{\infty} d_{j,n}\beta_{j,n}$$

as we did for ψ_∞ and ψ_n. The norms $\|\theta_n\| = \|\psi_n\|$ are bounded. So, by Theorem 2.2, we are to show that $d_{j,\infty} = \lim_n d_{j,n}$ for all $j \in J_\infty$. Fix $j \in J_\infty$, and let m be such that $j \in J_\infty(m)$. We have

$$d_{j,\infty} = \sum_{k \in J_\infty(m)} \langle \beta_{j,\infty} | \hat{U}_{m,\infty}(t) \beta_{k,\infty} \rangle c_{k,\infty}.$$

The equation still holds with the symbol n instead of the symbol ∞. Replacing $\hat{H}_\infty$ with the Hermitian operator $\hat{E}_m \hat{H}_\infty = \hat{H}_\infty \hat{E}_m$ does not change $\hat{H}_{m,\infty}$ or $\hat{H}_{m,n}$, so it does not change $\hat{U}_{m,\infty}$ or $\hat{U}_{n,m}$. So it does not change $d_{j,\infty}$ or $d_{j,n}$. Therefore, we may assume that $\hat{H}_{m',\infty} = 0$ for all integers $m' \neq m$. Hence $\hat{H}_{m',n} = 0$ for all $m' \neq m$ and all $n \in \mathcal{N}$. But now $\hat{H}_\infty$ is bounded, indeed $\|\hat{H}_\infty\| \leqslant |m| + 1$. Furthermore, the operators $\hat{H}_n$ are constructed from $\hat{H}_\infty$ just as the operators $\hat{K}'_n$ were constructed from $\hat{K}_\infty$ in the proof of Theorem 2.4. So $\hat{H}_\infty = \lim_{n \in \mathcal{N}} \hat{H}_n$. Thanks to Proposition 3.3, the argument is now complete. □

Corollary 3.6: Any unitary operator on $\mathcal{L}_\infty$ is the limit of a sequence of unitary operators on the spaces $\mathcal{L}_n$.

Proof: Given a unitary operator $\hat{U}_\infty$ on $\mathcal{L}_\infty$, then by Ref. 10 Exercise 7.50, there exists a conservative system $\{\hat{U}_\infty(t) : t \in \mathbb{R}\}$ such that $\hat{U}_\infty = \hat{U}_\infty(1)$. Theorem 3.5 now gives the assertion. □

A more direct way to demonstrate Corollary 3.6 is to adapt the proof of Theorem 2.4, using the Gram–Schmidt process to modify the columns of the matrices $(K_{j,k})_{j,k \in J_n}$. The argument is fairly routine, although it is complicated by the need to make some arbitrary choices when the Gram–Schmidt process terminates prematurely.

The existence results above can be interpreted as saying that, in principle, any ''continuum'' system (of a particular kind) is the limit of a sequence of ''discrete'' systems (of the same kind). The next result provides one way of actually recognizing that a given ''continuum'' system is the limit of a given sequence of ''discrete'' systems.

Proposition 3.7: Let $\mathcal{U}_\infty = \{\hat{U}_\infty(t) : t \in \mathbb{R}\}$ be a conservative system on $\mathcal{L}_\infty$, and for each $n \in \mathcal{N}$, let $\mathcal{U}_n = \{\hat{U}_n(t) : t \in \mathbb{R}\}$ be a conservative system on $\mathcal{L}_n$. Let $\hat{H}_\infty$ and $\hat{H}_n$, respectively, be the Hamiltonians. Let $\mathcal{B}_\infty$ and $\mathcal{B}_n$ be as in Sec. II. Suppose that, for each $j \in J_\infty$, there exists a real $\lambda_{j,\infty}$ such that

$$\hat{H}_\infty \beta_{j,\infty} = \lambda_{j,\infty} \beta_{j,\infty}.$$

Suppose also that, for sufficiently large n, there exist reals $\lambda_{j,n}$ such that

$$\hat{H}_n \beta_{j,n} = \lambda_{j,n} \beta_{j,n}.$$

Then $\mathcal{U}_\infty = \lim_{n \in \mathcal{N}} \mathcal{U}_n$ if and only if $\lambda_{j,\infty} = \lim_{n \in \mathcal{N}} \lambda_{j,n}$ for all $j \in J_\infty$.

Proof: This follows quickly from Theorem 2.2. □

Proposition 3.7 yields an alternative (and very easy) proof of Theorem 3.5 in the special case of a conservative system on $\mathcal{L}_\infty$ with a diagonalizable Hamiltonian.

IV. SOME EXAMPLES OF CONTINUUM LIMITS OF DISCRETE SYSTEMS

In all the examples to follow, we shall apply Proposition 3.7 to show that the given ''continuum'' system is the limit of the given sequence of ''discrete'' systems. Each of the inductive resolutions is a sample-point inductive resolution, as in Ref. 6, Examples 2.A–2.F. Sample-point inductive resolutions are examined also in Ref. 7.

Example 4.A: The circular rotor. The rotor, in one dimension, is a model for a particle moving freely on a circle. Classically, the energy is proportional to the square of the angular momentum.

Let $\mathcal{S}$ be the space of smooth functions $\phi:\mathbb{R}\to\mathbb{C}$ such that ϕ has period unity and ϕ is square-integrable on a bounded domain. The inner product on $\mathcal{S}$ is given by integration over an interval of length unity. Making a suitable choice of units, the Hamiltonian $\hat{H}_\infty$ of the rotor has domain $\mathcal{S}$ and satisfies

$$\hat{H}_\infty\phi(x)=-d^2\phi(x)/dx^2$$

for $\phi\in\mathcal{S}$ and $x\in\mathbb{R}$. The completion $\mathcal{L}_\infty$ of $\mathcal{S}$ has an orthonormal basis $\mathcal{B}_\infty=\{\beta_{j,\infty}:j\in\mathbb{N}\}$ given by

$$\beta_{j,\infty}(x)=\begin{cases}\sqrt{2}\cos(\pi jx) & \text{if } j \text{ is even,}\\ \sqrt{2}\sin(\pi(j+1)x) & \text{if } j \text{ is odd.}\end{cases}$$

It is easy to check that $\mathcal{B}_\infty$ diagonalizes $\mathcal{H}_\infty$, indeed, $\hat{H}_\infty\beta_{j,\infty}=\lambda_{j,\infty}\beta_{j,\infty}$, where

$$\lambda_{j,\infty}=\begin{cases}\pi^2j^2 & \text{if } j \text{ is even,}\\ \pi^2(j+1)^2 & \text{if } j \text{ is odd.}\end{cases}$$

Let $\mathcal{N}$ be the set of positive odd integers. For each $n\in\mathcal{N}$, let $\mathcal{L}_n$ be the n-dimensional inner product space consisting of the functions $\mathbb{Z}\to\mathbb{C}$ with period n. The inner product on $\mathcal{L}_n$ is given by summation over n consecutive integers. We replace the differential operator $-d^2/dx^2$ with a difference operator $\hat{H}_n$ where

$$\hat{H}_n\psi(X)=n^2(-\psi(X-1)+2\psi(X)-\psi(X+1))$$

for $\psi\in\mathcal{L}_n$ and $X\in\mathbb{Z}$. Given an integer j with $0\leqslant j\leqslant n-1$, we put

$$\beta_{j,n}(X)=\begin{cases}\sqrt{2/n}\cos(\pi jX/n) & \text{if } j \text{ is even,}\\ \sqrt{2/n}\sin(\pi(j+1)X/n) & \text{if } j \text{ is odd.}\end{cases}$$

It is easy to check that $\{\beta_{j,n}:0\leqslant j\leqslant n-1\}$ is an orthonormal basis for $\mathcal{L}_n$ diagonalizing $\hat{H}_n$. Writing $\hat{H}_n\beta_{j,n}=\lambda_{j,n}\beta_{j,n}$, then

$$\lambda_{j,n}=\begin{cases}2n^2(1-\cos(2\pi jX/n)) & \text{if } j \text{ is even,}\\ 2n^2(1-\cos(2\pi(j+1)X/n)) & \text{if } j \text{ is odd.}\end{cases}$$

Let $\mathcal{U}_\infty$ be the conservative system on $\mathcal{L}_\infty$ with Hamiltonian $\hat{H}_\infty$. For each $n\in\mathcal{N}$, let $\mathcal{U}_n$ be the conservative system on $\mathcal{L}_n$ with Hamiltonian $\hat{H}_n$. Of course, it is heuristically ''obvious'' that $\mathcal{U}_\infty$ is some kind of ''limit'' of $\mathcal{U}_n$, but in order to formulate this observation mathematically, we must realize $(\mathcal{L}_n)_n$ as an inductive resolution of $\mathcal{L}_\infty$. We define $\mathrm{res}_n:\mathcal{S}\to\mathcal{L}_n$ such that

$$\mathrm{res}_n(\phi)(X)=\phi(X/n)/\sqrt{n}$$

for $\phi\in\mathcal{S}$ and $X\in\mathbb{Z}$ with $-n/2<X<n/2$. It is easy to check that the sequence $(\mathcal{L}_n)_n$, equipped with the sequence $(\mathrm{res}_n)_n$, is indeed an inductive resolution of $\mathcal{L}_\infty$. (In fact, this is the precisely the one-dimensional case of Ref. 6, Example 2.F.) Given $j\in\mathbb{N}$, then, for all $n>j$, we have $\beta_{j,n}=\mathrm{res}_n(\beta_{j,\infty})$. Therefore, $\beta_{j,\infty}=\lim_{n\in\mathcal{N}}\beta_{j,n}$. Since $\lambda_{n,\infty}=\lim_{n\in\mathcal{N}}\lambda_{j,n}$, Proposition 3.7 tells us that

$$\mathcal{U}_\infty=\lim_{n\in\mathcal{N}}\mathcal{U}_n.$$

Example 4.B: The one-dimensional box. For each $j\in\mathbb{N}$ and $x\in[-\frac{1}{2},\frac{1}{2}]$, we write

$$\beta_{j,\infty}(x)=\begin{cases}\sqrt{2}\cos(\pi(j+1)x) & \text{if } j \text{ is even,}\\ \sqrt{2}\sin(\pi(j+1)x) & \text{if } j \text{ is odd.}\end{cases}$$

Let $\mathcal{L}_\infty$ be the Hilbert space with orthonormal basis $\{\beta_{j,\infty}: j\in\mathbb{N}\}$. Let $\mathcal{S}$ be the dense subspace of $\mathcal{L}_\infty$ consisting of the smooth functions $[-\frac{1}{2},\frac{1}{2}]\to\mathbb{C}$. The box, in one dimension, is the conservative system $\mathcal{U}_\infty$ whose Hamiltonian $\hat{H}_\infty$ has domain $\mathcal{S}$ and is given by

$$\hat{H}_\infty\phi(x)=-d^2\phi(x)/dx^2$$

for $\phi\in\mathcal{S}$. Evidently $\hat{H}_\infty\beta_{j,\infty}=\lambda_{j,\infty}\beta_{j,\infty}$ where $\lambda_{j,\infty}=\pi^2(j+1)^2$.

Again, let $\mathcal{N}$ be the set of positive odd integers. Let $\mathcal{L}_n$ be the n-dimensional inner product space consisting of the complex-valued functions on the integers X lying in the interval $-n/2<X<n/2$. As in the previous example, we replace the differential operator $-d^2/dx^2$ with a difference operator $\hat{H}_n$, but this time the sample-points indexed by $(1-n)/2$ and $(n-1)/2$ are to be interpreted as end-points (they are no longer interpreted as being adjacent). Writing $n=2l+1$, we put

$$\hat{H}_n\psi(X)=\begin{cases}n^2(2\psi(-l)-\psi(1-l)) & \text{if } X=-l,\\ n^2(-\psi(X-1)+2\psi(X)-\psi(X+1)) & \text{if } -l<X<l,\\ n^2(-\psi(l-1)+2\psi(l)) & \text{if } X=l.\end{cases}$$

The operator $\hat{H}_n$ is diagonalized by the orthonormal basis $\mathcal{B}_n=\{\beta_{j,n}: 0\leqslant j\leqslant n-1\}$ of $\mathcal{L}_n$, where

$$\beta_{j,n}(X)=\begin{cases}\sqrt{\dfrac{2}{n-1}}\cos\left(\dfrac{\pi(j+1)X}{n+1}\right) & \text{if } j \text{ is even,}\\ \sqrt{\dfrac{2}{n+1}}\sin\left(\dfrac{\pi(j+1)X}{n+1}\right) & \text{if } j \text{ is odd.}\end{cases}$$

In fact, $\hat{H}_n\beta_{j,n}=\lambda_{j,n}\beta_{j,n}$ where $\lambda_{j,n}=2(1-\cos(\pi(j+1)/(n+1)))$.

We realize $(\mathcal{L}_n)_n$ as an inductive resolution of $\mathcal{L}_\infty$ by defining $\mathrm{res}_n:\mathcal{S}\to\mathcal{L}_n$ by the same formula as in Example 4.A. A straightforward calculation yields, for all $j\in\mathbb{N}$, all $x\in[-\frac{1}{2},\frac{1}{2}]$ and all sequences $(X_n)_n$ of integers such that $x=\lim_{n\in\mathcal{N}}X_n/\sqrt{n}$, the point-wise convergence condition

$$\beta_{j,\infty}(x)=\lim_{n\in\mathcal{N}}\sqrt{n}\beta_{j,n}(X_n/n).$$

The norms $\|\beta_{j,n}\|$ are all unity, and, in particular, they are bounded. In Ref. 7, Theorem 3.1, it was proved that point-wise convergence of vectors with bounded norms implies convergence; in particular,

$$\beta_{j,\infty}=\lim_{n\in\mathcal{N}}\beta_{j,n}.$$

Observing that each $\lambda_{j,\infty}=\lim_{n\in\mathcal{N}}\lambda_{j,n}$, we again conclude from Proposition 3.7 that

$$\mathcal{U}_\infty=\lim_{n\in\mathcal{N}}\mathcal{U}_n.$$

Example 4.C: The Harper function harmonic oscillator. In this example and the next, we review some results from Refs. 11 and 12, and we show how that material can be streamlined using Proposition 3.7. Recall that $L^2(\mathbb{R})$ has an orthonormal basis $\{h_{j,\infty}: j\in\mathbb{N}\}$ consisting of the functions $h_{j,\infty}:\mathbb{R}\to\mathbb{C}$, called the **Hermite–Gaussians**, which are given by

$$h_{j,\infty}(x) = C_j e^{-x^2/2} H_j(x),$$

where H_j is the Hermite polynomial of degree j, and C_j is a positive real normalization constant. The **continuum harmonic oscillator** is defined to be the conservative system $\mathcal{U}_\infty = \{\hat{U}_\infty(t) : t \in \mathbb{R}\}$ whose Hamiltonian $\hat{H}_\infty$ is given by $\hat{H}_\infty \psi(x) = (-d^2/dx^2 + x^2)\psi(x)$, or equivalently, $\hat{H}_\infty h_{j,\infty} = (2k+1) h_{j,\infty}$. Thus

$$\hat{U}_\infty(t) h_{j,\infty} = e^{-(2j+1)it} h_{j,\infty}.$$

Let $\mathcal{N}$ be an infinite set of positive integers such that $\sqrt{n_2/n_1} \in \mathbb{Z}$ for all $n_1, n_2 \in \mathcal{N}$ with $n_1 \leqslant n_2$. (At one point in the discussion, we shall make use of this peculiar hypothesis on $\mathcal{N}$, but the assertions probably hold for any infinite set $\mathcal{N}$ of positive integers.) Given an element $n \in \mathcal{N}$, let $\mathcal{L}_n$ be the n-dimensional inner product space consisting of the functions $\mathbb{Z} \to \mathbb{C}$ with period n. We realize $(\mathcal{L}_n)_n$ as an inductive resolution of $L^2(\mathbb{R})$ by defining restriction maps $\mathrm{res}_n : \mathcal{S}(\mathbb{R}) \to \mathcal{L}_n$ such that

$$\mathrm{res}_n(\phi)(X) = (n/2\pi)^{-1/4} \phi((n/2\pi)^{-1/2} X)$$

for $\phi \in \mathcal{S}(\mathbb{R})$ and $X \in \mathbb{Z}$. After Harper,[13] Namias,[1] Pei–Yeh[3] and others, we define the **Harper function harmonic oscillator** to be the conservative system $\mathcal{U}_n$ on $\mathcal{L}_n$ with Hamiltonian $\hat{H}_n$ such that

$$\hat{H}_n \psi(X) = \frac{n}{2\pi}(-\psi(X-1) + (4 - 2\cos(2\pi i X/n))\psi(X) - \psi(X+1))$$

for $\psi \in \mathcal{L}_n$ and $X \in \mathbb{Z}$. The definition and enumeration of the Harper functions $\beta_{0,n}, \beta_{1,n}, \ldots$ may be found in Ref. 3; see also Refs. 11 and 12. The Harper functions comprise an orthonormal basis for $\mathcal{L}_n$, they are eigenvectors of $\hat{H}_n$, and by Ref. 12, Theorem 2.5,

$$h_{j,\infty} = \lim_{n \in \mathcal{N}} \beta_{j,n}$$

for all $j \in \mathcal{N}$. (It is here that the peculiar hypothesis on $\mathcal{N}$ is used.) Combining this result with Ref. 12, Lemmas 3.1 and 3.9, it is easy to show that the eigenvalue $\lambda_{j,n}$ of $\hat{H}_n$ associated with $\beta_{j,n}$ satisfies

$$2j+1 = \lim_{n \in \mathcal{N}} \lambda_{j,n}.$$

Proposition 3.7 now yields

$$\mathcal{U}_\infty = \lim_{n \in \mathcal{N}} \mathcal{U}_n.$$

As suggested in Ref. 7, Sec. 3, the peculiar hypothesis on $\mathcal{N}$ can perhaps be relaxed using results that were not available when Ref. 12 was written.

Example 4.D: The Harper function fractional Fourier transform. We continue to use the notation from Example 4.C. After Namias, the **continuum FRFT** is defined to be the conservative system $\mathcal{F}_\infty = \{\hat{F}^t_\infty : t \in \mathbb{R}\}$ such that

$$\hat{F}^t_\infty h_{j,\infty} = e^{2\pi i j t} h_{j,\infty}.$$

As Namias observed, the continuum FRFT and the continuum harmonic oscillator are related by the equality

$$\hat{U}_\infty(t)=e^{-it}\hat{F}_\infty^{-t/\pi}.$$

Note that $\hat{F}^{1/4}$ is the usual Fourier transform. The **Harper function FRFT** comes in two versions, the **import** version $\mathcal{I}_n=\{\hat{I}_n^t:t\in\mathbb{R}\}$ and the **domestic** version $\mathcal{D}_n=\{\hat{D}_n^t:t\in\mathbb{R}\}$. The import version, defined by

$$\hat{I}_n^t\beta_{j,n}=e^{2\pi ijt}\beta_{j,n},$$

is perhaps rather artificial (its eigenvalues being ''imported'' from the continuum FRFT), but it has the virtue that $\hat{F}_n^{1/4}$ is the usual discrete Fourier transform. The domestic version, defined by

$$\hat{U}_n(t)=e^{-it}\hat{D}_n^{-t/\pi},$$

has the virtue that it has an explicit Hamiltonian, namely $(\hat{H}_n-1)/2$. By Proposition 3.7,

$$\mathcal{F}_\infty=\lim_{n\in\mathcal{N}}\mathcal{I}_n=\lim_{n\in\mathcal{N}}\mathcal{D}_n.$$

Example 4.E: The Kravchuk function harmonic oscillator. We retain the notation from Examples 4.C and 4.D, except that we now let $\mathcal{N}$ be any set of positive integers. Given $n\in\mathcal{N}$, let us write $n=2l+1$, and let $\mathcal{X}_n$ be the set consisting of the X such that $l+X$ and $l-X$ are both natural numbers. We write $L(\mathcal{X}_n)$ to denote the n-dimensional inner product space consisting of the complex-valued functions on $\mathcal{X}_n$. As in Ref. 7, Secs. 4 and 5, we realize $(L(\mathcal{X}_n))_n$ as an inductive resolution of $L^2(\mathbb{R})$ by defining $\mathrm{res}_n:\mathcal{S}(\mathbb{R})\to L(\mathcal{X}_n)$ such that

$$\mathrm{res}_n(\phi)(X)=l^{-1/4}\phi(l^{-1/2}X)$$

for $\phi\in\mathcal{S}(\mathbb{R})$ and $X\in\mathcal{X}_n$. Recall (or see Ref. 7, Sec. 5) that the Kravchuk functions $h_{j,n}$ comprise an orthonormal basis $\{h_{j,n}:0\leqslant j\leqslant n-1\}$ for $L(\mathcal{X}_n)$. The Kravchuk functions are discrete analog of the Hermite–Gaussians, and arise from a binomial weight function in place of a Gaussian weight function. By Ref. 7, Theorem 5.1,

$$h_{j,\infty}=\lim_{n\in\mathcal{N}}h_{j,n}$$

for all $j\in\mathbb{N}$. After Ref. 14, the **Kravchuk function harmonic oscillator** is defined to be the conservative system $\hat{K}_n=\{\hat{K}_n(t):t\in\mathbb{R}\}$ on $\mathcal{L}_n$ such that

$$\hat{H}_n(t)h_{j,n}=e^{-(2j+1)it}h_{j,n}.$$

By Proposition 3.7,

$$\mathcal{U}_\infty=\lim_{n\in\mathcal{N}}\mathcal{K}_n.$$

Example 4.F: The Kravchuk function fractional Fourier transform. We retain the notation from the previous three examples, $\mathcal{N}$ being any infinite set of positive integers. After Ref. 2, the **Kravchuk function FRFT** is defined to be the conservative system $\mathcal{F}_n=\{\hat{F}_n^t:t\in\mathbb{R}\}$ such that

$$\hat{F}_n^t h_{j,n}=e^{2\pi ijt}h_{j,n}.$$

Equivalently, $\mathcal{F}_n$ may be defined by

$$\hat{K}_n(t)=e^{-it}\hat{F}_n^{-t/\pi}.$$

By Proposition 3.7,

$$\mathcal{F}_\infty = \lim_{n \in \mathcal{N}} \mathcal{F}_n .$$

Comment: Advantages of the Kravchuk function FRFT over the Harper function FRFT. In applications of the Harper function FRFT, one must select either the import version, whose eigenvalues are integer powers of $e^{2\pi i t}$, but whose Hamiltonian is not known explicitly, or else one must select the domestic version, whose Hamiltonian is $(\hat{H}_n - 1)/2$, but whose eigenvalues are not known explicitly. Either way, the eigenvectors—the Harper functions—lack a known explicit formula, and have to be calculated numerically. The eigenvectors of the Kravchuk function FRFT $\mathcal{F}_n$ are integer powers of $e^{2\pi i t}$. As can be gleaned from Refs. 2 and 5, the Hamiltonian for $\mathcal{F}_n$ has a very simple description in terms of the n-dimensional irreducible representation of the Lie algebra su(2) (see also Ref. 4). The eigenvectors of $\mathcal{F}_n$—the Kravchuk functions—are given by a complicated but explicit formula.

V. SOME QUESTIONS AND REMARKS ON CONVERGENCE OF SPECTRA

An alternative description of a conservative system is provided by the spectral measure associated with the Hamiltonian. Throughout this section, we consider conservative systems $\mathcal{U}_\infty = \{\hat{U}_\infty(t) : t \in \mathbb{R}\}$ on $\mathcal{L}_\infty$ and $\mathcal{U}_n = \{\hat{U}_n(t) : t \in \mathbb{R}\}$ on each $\mathcal{L}_n$. Let $\hat{H}_\infty$ and $\hat{H}_n$ be the Hamiltonians for $\mathcal{U}_\infty$ and $\hat{U}_n$, respectively. If $\mathcal{U}_\infty = \lim_{n \in \mathcal{N}} \mathcal{U}_n$, how is the spectral measure for the Hermitian operator $\mathcal{H}_\infty$ related to the spectral measure for the operators $\mathcal{H}_n$? Or, more simply, how is the spectrum $\sigma(\hat{H}_\infty)$ (or the essential or residual spectrum) related to the spectra $\sigma(\hat{H}_n)$?

On the one hand, it would be desirable to have techniques for investigating the spectrum (or spectral measure) of an infinite-dimensional system by examining limiting properties of the spectra of finite-dimensional approximations. On the other hand, finite-dimensional systems are themselves of interest. (As a vague principle, any closed system of finite extent in space can have only finitely many independent nondecaying states.) Finite-dimensional systems are not always more amenable than infinite-dimensional systems (difference equations often have richer solutions than their analogous differential equations.) In connection with example 4.E, it is worth remembering that De Moivre, having established the correspondence between the Gaussian distribution and the binomial distribution, then employed the Gaussian as an approximation to the binomial. Continuum approximation to discrete phenomena has pervaded statistical techniques ever since. It is to be expected that results relating $\sigma(\hat{H}_\infty)$ and $\sigma(\hat{H}_n)$ could be usefully applied in either direction.

As regards practical methods for relating the spectra of discrete and continuum systems, the results in this article are simply not in competition with those in Ref. 8. We do not know whether or not their results can be extended to our more general context. (It should be mentioned that the examples considered in Sec. 4 are all, essentially, in the situation they considered.) The following result indictates that the questions above do have answers, and that our approach can be developed to yield alternative and more general methods.

Proposition 5.1: Suppose that $\mathcal{U}_\infty = \lim_n \mathcal{U}_n$. Suppose also that $\hat{H}_\infty$ and each $\hat{H}_n$ are bounded, and that the norms $\|\hat{H}_n\|$ are bounded. Then every point $\lambda \in \sigma(\hat{H}_n)$ is the limit $\lambda = \lim_n \lambda_n$ of points $\lambda_n \in \sigma(\hat{H}_n)$.

Proof: The condition $\lambda \in \sigma(\hat{H}_\infty)$ is equivalent to the condition that there exists a sequence $(\phi_m)_m$ of vectors in $\mathcal{L}_\infty$ such that $\|\phi_m\| = 1$ and $\|(\hat{H}_\infty - \lambda)\phi_m\| \to 0$ as $m \to \infty$ (see, for instance, Ref. 15, Theorem 5.10). Since $\mathcal{S}$ is dense in $\mathcal{L}_\infty$, we may insist that each $\phi_m \in \mathcal{S}$. Let $\epsilon > 0$, and fix m such that $\|(\hat{H}_\infty - \lambda)\phi_m\| \leqslant \epsilon/2$. By Proposition 3.3, the convergence hypothesis on $\mathcal{U}_\infty$ is equivalent to the condition that $\hat{H}_\infty = \lim_n \hat{H}_n$. Noting that $\lim_n \|\mathrm{res}_n(\phi_m)\| = 1$, and putting $\psi_n = \mathrm{res}_n(\phi_m)/\|\mathrm{res}_n(\phi_m)\|$, we have $\|(\hat{H}_n - \lambda)\psi_n\| \leqslant \epsilon$ for sufficiently large n. By a well-known criterion for existence of spectral points in an interval (see Ref. 12, Theorem 5.9), $\sigma(\hat{H}_n) \cap [\lambda - \epsilon, \lambda + \epsilon] \neq \varnothing$. □

Corollary 5.2: In the situation of Proposition 5.1, suppose that the limits $\lim_n \mu_n$ *of points* $\mu_n \in \sigma(\hat{H}_n)$ *comprise a discrete subset of* $\mathbb{R}$. *Then* $\hat{H}_n$ *is diagonalizable.* □

It seems probable that the boundedness condition in Proposition 5.1 can be removed by using a refinement of the argument (and the rider to Stone's theorem as recorded in Ref. 9, Theorem 13.1). A more systematic option would be to wait for that to become a corollary of a result expressing the condition $\mathcal{U}_\infty = \lim_n \mathcal{U}_n$ in terms of the spectral measures. We end with a few comments in this direction. Consider an interval I in $\mathbb{R}$. Write $\overline{I}$ and I° for the closure and the interior. Let $E_{I,\infty}$ and $E_{I,n}$ be the corresponding projections to $\mathcal{L}_\infty$ and $\mathcal{L}_n$ associated with $\hat{H}_\infty$ and $\mathcal{H}_n$. To see that convergence of the sequence $(\hat{H}_n)_n$ does not imply convergence of the sequence $(E_{I,n})_n$, let a be an end-point of I, and let $\hat{H}_n = (a + (-2)^n)\hat{1}$.

Question 5.A: Are the following conditions equivalent?

(1) $\mathcal{U}_\infty = \lim_n \mathcal{U}_n$.
(2) *If* $\psi_\infty = \lim_n \psi_n$ *with* $\psi_n \in E_{I,n}\mathcal{L}_n$, *then* $\psi_\infty \in E_{\overline{I},n}\mathcal{L}_\infty$.
(3) *If* $\psi_\infty = \lim_n \psi_n$ *with* $\psi_\infty \in E_{I^\circ,n}\mathcal{L}_\infty$ *and* $\|\psi_\infty\| = \lim_n \|\psi_n\|$, *then* $\lim_n \|(\hat{1} - \hat{E}_{I,n})\psi_n\| = 0$.

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Instantons in four-dimensional gauged O(5) Skyrme models

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We consider a family of four-dimensional nonlinear sigma models based on an O(5) symmetric group, whose fields take their values on the 4-sphere S^4. An SO(4)-subgroup of the model is gauged. The solutions of the model are characterized by two distinct topological charges, the Chern–Pontryagin charge of the gauge field and the degree of the map, i.e., the winding number, of the S^4 field. The one-dimensional equations arising from the variation of the action density subjected to spherical symmetry are integrated numerically. Several properties of the solutions thus constructed are pointed out. The only solution with *unit* Chern–Pontryagin charge are the usual BPST instantons with zero S^4 winding number, while solutions with *unit* S^4 winding number have zero Chern–Pontryagin charge.
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I. INTRODUCTION

The model considered in this work is described by the Lagrangian on $\mathbb{R}^4$

$$\mathcal{L}=\frac{\lambda_0}{24}|F_{\mu\nu}^{[\alpha\beta]}|^2+\frac{\lambda_1}{2}|D_\mu\phi^a|^2+\frac{\lambda_2}{24}|D_\mu\phi^a\times D_\nu\phi^b|^2$$

$$+\frac{\lambda_3}{72}|D_\mu\phi^a\times D_\nu\phi^b\times D_\rho\phi^c|^2+V(\phi^5,\cos\omega), \tag{1}$$

in terms of the S^4 valued fields $\phi^a=(\phi^\alpha,\phi^5)$ $(\alpha=1,2,3,4)$ satisfying the constraint

$$\phi^a\phi^a=1,$$

and the SO(4) gauge connection $A_\mu^{[\alpha\beta]}$ with curvature $F_{\mu\nu}^{[\alpha\beta]}$. The covariant derivatives in (1) are defined by

$$D_\mu\phi^\alpha=\partial_\mu\phi^\alpha+A_\mu^{[\alpha\beta]}\phi^\beta,\quad D_\mu\phi^5=\partial_\mu\phi^5. \tag{2}$$

(The brackets $[\cdots]$ imply antisymmetrization of indices throughout.)

The Lagrangian (1) differs from that of the various models considered in Ref. 1, in the physically important respect that the kinetic term *quadratic* in the S^4 field ϕ^a, which was absent

there,[1] is present here. Without a *quadratic* kinetic term, it is not possible to infer from *finite action conditions*, that that the matter field (in this case the S^4 valued field) becomes asymptotically a constant and hence consistent with *vacuum* field. It would then be impossible to interpret the resulting topologically stable finite action solution as an instanton. As a result of the Derrick scaling requirement, the system (1) features also a kinetic term *sextic* in the S^4 valued field. (1) differs from that in Ref. 1 also in the presence of the generic potential $V(\phi^5,\cos\omega)$

$$V(\phi^5,\omega)=\lambda(\cos\omega-\phi^5)^n, \quad 0\leqslant\omega\leqslant\pi, \quad n=\text{integer}, \tag{3}$$

whose role it is to fix the asymptotic value of the field ϕ^a, rather like the pion-mass potential in the usual three-dimensional O(4) Skyrme[2] model. Like in that case,[2] this term serves only the purpose of fixing the asymptotics, and will be considered only in this limited context. Moreover, anticipating our conclusions in Sec. II A, namely that only for $\omega=0$ is it possible to construct finite action solutions, the relevant $V(\phi^5,\omega=0)$ is

$$V(\phi^5,\omega=0)=\lambda(1-\phi^5), \tag{4}$$

in analogy with the pion-mass[2] potential. Notwithstanding, in Sec. II B we have described a model differing from (1) and characterized by nonzero ω (in particular $\omega=\pi/2$), which can support topologically stable finite action solutions. As will be seen there, the Lagrangian of such a model does not feature the usual YM term and is therefore not studied further here.

Our topologically stable finite action solutions are interpreted as instantons, although the latter are not always characterized by the second Chern–Pontryagin density, but also by the $S^4\to S^4$ degree of the S^4 valued field (which may or may not be integer).

By adapting the methods formulated in Ref. 3 used in establishing the topological lower bounds given by the degree of the map $S^4\to S^4$, a suitable such lower bound can be established for the action (1), for all positive values of λ_1, λ_2, λ_3, and λ_0. This will be established in Sec. II. In Sec. III, the system (1) will be subjected to spherical symmetry, and thenceforth we will restrict to the study of the ensuing one-dimensional equations numerically. The results of our numerical work is presented in Sec. IV, and Sec. V is devoted to the summary and discussion of our results.

In the work of Ref. 1, which employs the above model (1) with $\lambda_1=\lambda_3=0$, it was found that the action of the main SO(4) gauged O(5) model decreased with the Skyrme coupling λ_2 and exhibited a bifurcation at a value very close to and above the action of the (pure) Yang–Mills (YM) instanton.[4] Thus beyond a critical value of the coupling λ_2, the system did not support a finite action solution, and more importantly the action could be made smaller by decreasing λ_2. Our main aim in the present work is the verification of these two properties of the solutions when $\lambda_1>0$ and $\lambda_3>0$. We have found that these properties of the solution persist, namely that instantons can be constructed for values of λ_2 (holding λ_3 constant) up to some value λ_2^{cr}, and for values of λ_3 (holding λ_2 constant) up to some value λ_3^{cr}. Also, the actions of these instantons decrease with λ_2 and λ_3, respectively, consistently with the Derrick scaling requirement. We find surprisingly that the action at $\lambda_2=0$ is nonzero, inspite of the vanishing of the topological lower bound at that point. We defer discussion of the possible physical significance of these properties to Sec. V.

Another objective here is to probe the nature of the topological lower bounds. In Ref. 1, we were exclusively concerned with lower bounds stated in terms of the degree of the map of the S^4 valued field, such that the corresponding solutions supported *vanishing* Chern–Pontryagin charge. Here we attempt to construct numerically, instantons with *nonzero* Pontryagin charge when the S^4 field is nontrivial. We do not find such solutions and offer an analytic argument to support their nonexistence.

The boundary conditions employed for the S^4 valued field are

$$\lim_{r\to 0}\phi^5=-1, \quad \lim_{r\to\infty}\phi^5=\cos\omega, \tag{5}$$

but we will be restricting our numerical investigations to the $\omega=0$ case. For the gauge field we will adopt the vacuum behaviors

$$\lim_{r\to 0} A_\mu = 0, \quad \lim_{r\to\infty} A_\mu = qg\,\partial_\mu g^{-1}. \tag{6}$$

$q=0$ leads to zero Pontryagin charge. Pure-gauge $q=1$, and half-pure-gauge $q=\frac{1}{2}$, both lead to nonzero Pontryagin charges. The half-pure-gauge case $q=\frac{1}{2}$ pertains to $\omega\neq 0$, which we do not study numerically. The pure-gauge cases $q=0$ and $q=1$ both pertain to $\omega=0$, and are studied numerically. It turns out that instantons with nontrivial (S^4 valued) matter field can only be constructed for the $q=0$ case.

II. LOWER BOUNDS

The work in this section follows very closely that in Ref. 3 and that in Sec. II of Ref. 1. The analysis in Refs. 3 and 1 was adapted to the definition of topological charges presenting lower bounds on the actions, of systems supporting asymptotics with $\omega=0$ in (5). Here, we extend this analysis to include values of $0\leqslant\omega\leqslant\pi$. In the generic case therefore, we would expect solutions with a *fractional* analogue of the Baryon number in three dimensions,[5] while in the limiting case[1,3] $\omega=0$ this will be the degree of the map of the S^5 valued field taking an *integer* value.

We start with the definition of the winding number density

$$\varrho_0 = \frac{1}{64\pi^2}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{abcde}\partial_\mu\phi^a\partial_\nu\phi^b\partial_\rho\phi^c\partial_\sigma\phi^d\phi^e, \tag{7}$$

which is inadequate for our purposes here since it is *gauge variant*, and its *gauge invariant* version

$$\varrho_G = \frac{1}{64\pi^2}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{abcde}D_\mu\phi^a\,D_\nu\phi^b\,D_\rho\phi^c\,D_\sigma\phi^d\,\phi^e, \tag{8}$$

whose volume integral cannot be evaluated by stating the asymptotic conditions, i.e., it is not useful as a topological charge density.

The volume integral of (7) can indeed be evaluated by stating the asymptotic conditions (5), such that for $\omega=0$ the value of this integral is integer, and is fractional for $\omega\neq 0$. The normalization ensures that in the spherically symmetric case this is the unit charge, or winding number. The task is to define a suitable density which is (a) gauge invariant, and (b) its volume integral equals the volume integral of the density ϱ_0 (7).

To this end we find the relation between the two densities (7) and (8), in suitable form, such that *all gauge-variant terms appear as total divergences*. Thus,

$$\begin{aligned}\varrho_G = \varrho_0 + \partial_\mu(\phi^5\partial_\nu\Omega_{\nu\mu} + \tilde{\Omega}_\mu) + \frac{3}{64\pi^2}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta} \\ \times[\phi^\alpha D_\nu\phi^\beta D_\mu\phi^5 F^{\gamma\delta}_{\rho\sigma} - \tfrac{1}{8}\phi^5(1-\tfrac{1}{3}(\phi)^2)F^{\alpha\beta}_{\mu\nu}F^{\gamma\delta}_{\rho\sigma}],\end{aligned} \tag{9}$$

where

$$\Omega_{\nu\mu} = \frac{3}{64\pi^2}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}A_\sigma\phi^\alpha(2\partial_\rho\phi^\beta + (A_\rho\phi)^\beta), \tag{10}$$

$$\tilde{\Omega}_\mu = \frac{3}{128\pi^2}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}\left\{\phi^5\left(1-\frac{1}{3}(\phi)^2\right)A^{\gamma\delta}_\nu\left[\partial_\rho A^{\alpha\beta}_\sigma - \frac{2}{3}(A_\rho A_\sigma)^{\alpha\beta}\right]\right\}. \tag{11}$$

The volume integral of the (gauge-variant) total divergence terms in (9) can, after conversion to two surface integrals, be evaluated using the asymptotic values (5) and (6). If these surface

integrals vanished, then the volume integral of the remaining gauge-invariant terms could be expressed in terms of the volume integral of ϱ_0, namely the (integral or fractional) winding number, leading to the definition of a gauge-invariant topological charge density.

This can be checked by substituting the spherically symmetric Ansatz (31) and (32) in (10) and (11). One then sees immediately that the density (10) vanishes asymptotically by symmetry, while the density (11) yields a nonvanishing contribution to the corresponding surface integral, which depends on the asymptotic parameter ω. Thus the definition of the charge density to be given below is ω-dependent.

Making use of the relation

$$\tfrac{1}{4}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}F^{\alpha\beta}_{\mu\nu}F^{\gamma\delta}_{\rho\sigma}=\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}\partial_\mu\{A^{\gamma\delta}_\nu[\partial_\rho A^{\alpha\beta}_\sigma-\tfrac{2}{3}(A_\rho A_\sigma)^{\alpha\beta}]\} \tag{12}$$

one can add and subtract the gauge-invariant density

$$\cos\omega(\cos\omega-\tfrac{1}{3}\cos^2\omega)\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}F^{\alpha\beta}_{\mu\nu}F^{\gamma\delta}_{\rho\sigma}$$

to (9), such that the nonvanishing surface contribution of $\tilde{\Omega}_\mu$ is cancelled. After some rearrangement, the natural definition for the charge density ϱ pertaining to a system characterized by the asymptotic parameter ω is

$$\varrho=\varrho_G-\frac{3}{64\pi^2}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}\Big\{\phi^\alpha D_\nu\phi^\beta D_\mu\phi^5 F^{\gamma\delta}_{\rho\sigma}-\frac{1}{8}\Big[\phi^5\Big(1-\frac{1}{3}(\phi)^2\Big)-\cos\omega\Big(\cos\omega-\frac{1}{3}\cos^2\omega\Big)\Big]F^{\alpha\beta}_{\mu\nu}F^{\gamma\delta}_{\rho\sigma}\Big\}, \tag{13}$$

which is the manifestly gauge-invariant definition that is employed in establishing (Bogomol'nyi type) lower bounds, and which is equivalent to the definition

$$\varrho=\varrho_0+\partial_\mu(\phi^5\partial_\nu\Omega_{\nu\mu}+\hat{\Omega}_\mu), \tag{14}$$

in which $\Omega_{\nu\mu}$ is defined by (10) while $\hat{\Omega}_\mu$ is

$$\hat{\Omega}_\mu=\frac{3}{128\pi^2}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}\Big\{\Big[\phi^5\Big(1-\frac{1}{3}(\phi)^2\Big)-\cos\omega\Big(\cos\omega-\frac{1}{3}\cos^2\omega\Big)\Big]\times A^{\gamma\delta}_\nu\Big[\partial_\rho A^{\alpha\beta}_\sigma-\frac{2}{3}(A_\rho A_\sigma)^{\alpha\beta}\Big]\Big\}. \tag{15}$$

For the spherically symmetric fields (31) and (32), $x_\mu\hat{\Omega}_\mu$ vanishes asymptotically, and since we already know that $\Omega_{\nu\mu}$ vanishes asymptotically, we see that the volume integral of (14) equals the (generic fractional) winding number. The (topological charge) density is gauge-invariant, and its volume integral is just the winding number of the S^4 valued field.

Not surprisingly the definition (13) for the two most prominent cases $\varrho(\omega=0)$ and $\varrho(\omega=\pi/2)$, simplifies somewhat. After some manipulations one has

$$\varrho(0)=\varrho_G+\frac{3}{64\pi^2}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}\Big[\phi^5 D_\mu\phi^\alpha D_\nu\phi^\beta F^{\gamma\delta}_{\rho\sigma}+\frac{1}{12}((\phi^5)^3-1)F^{\alpha\beta}_{\mu\nu}F^{\gamma\delta}_{\rho\sigma}\Big], \tag{16}$$

$$\varrho\Big(\frac{\pi}{2}\Big)=\varrho_G+\frac{3}{64\pi^2}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}\phi^5\Big[D_\mu\phi^\alpha D_\nu\phi^\beta F^{\gamma\delta}_{\rho\sigma}+\frac{1}{12}(\phi^5)^2F^{\alpha\beta}_{\mu\nu}F^{\gamma\delta}_{\rho\sigma}\Big]. \tag{17}$$

In Secs. II A and II B we shall analyze models whose actions are bounded from below by the topological charges corresponding to (16), pertaining to $\omega=0$, and (17), pertaining to $\omega=\pi/2$.

A. Model with $\omega=0$

The relevant gauge-invariant charge density in this case is (16). The first term, ϱ_G can be reproduced as a consequence of the inequality

$$\left|\kappa_1 D_\mu\phi^a-\frac{\kappa_3^3}{3!}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{abcde}D_{[\nu}\phi^b D_{[\rho}\phi^c D_{\sigma]]}\phi^d\phi^e\right|^2\geqslant 0,$$

leading to

$$\kappa_1^2|D_\mu\phi^a|^2+\kappa_3^6|D_{[\nu}\phi^b D_{[\rho}\phi^c D_{\sigma]]}\phi^d|^2\geqslant\kappa_1\kappa_3^3\varrho_G, \tag{18}$$

where κ_1 and κ_3 are constants with the dimension of length. The next term in (16),

$$\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}\phi^5 D_\mu\phi^\alpha D_\nu^\beta F_{\rho\sigma}^{\gamma\delta},$$

is reproduced by the inequality

$$\left|\kappa_0^2 F_{\mu\nu}^{\alpha\beta}-\frac{\kappa_2^2}{2!^2}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}\phi^5 D_{[\rho}\phi^\gamma D_{\sigma]}\phi^\delta\right|^2\geqslant 0,$$

expanding which and adding the appropriate positive terms to the left-hand side yields

$$\kappa_0^4|F_{\mu\nu}^{\alpha\beta}|^2+\kappa_2^4|D_{[\mu}\phi^a D_{\nu]}\phi^b|^2\geqslant\kappa_0^2\kappa_2^2\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}\phi^5 D_\rho\phi^\gamma D_\sigma\phi^\delta F_{\mu\nu}^{\alpha\beta}. \tag{19}$$

Finally the last term in (16) can be reproduced by adding the two inequalities

$$(\phi^5)^2\left|\phi^5 F_{\mu\nu}^{\alpha\beta}-\frac{1}{2!^2}F_{\rho\sigma}^{\gamma\delta}\right|^2\geqslant 0,$$

$$\left|F_{\mu\nu}^{\alpha\beta}+\frac{1}{2!^2}F_{\rho\sigma}^{\gamma\delta}\right|^2\geqslant 0,$$

and then adding suitable positive quantities to the right-hand side to yield

$$\overline{\kappa}_4^4|F_{\mu\nu}^{\alpha\beta}|^2\geqslant\frac{1}{3!}\overline{\kappa}_4^4\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}[(\phi^5)^2-1]F_{\mu\nu}^{\alpha\beta}F_{\rho\sigma}^{\gamma\delta}. \tag{20}$$

The constants κ_0, in κ_1, κ_3, and $\overline{\kappa}_0$ in (18), (19), and (20), all have the dimension of length.

Adding (18), (19), and (20), we end up with an inequality whose left-hand side, up to some redefinitions, is precisely the system (1), without the potential term V. This Lagrangian is bounded from below by the right-hand side, which will be a topological bound if the latter coincides with the topological charge density (16) (up to a constant multiple). This turns out to be the case, provided that the constants κ_0, in κ_1, κ_3, and $\overline{\kappa}_0$ satisfy the following constraints:

$$\kappa_0^2\kappa_2^2=3\kappa_1\kappa_3^3,\quad 2\overline{\kappa}_0^4=3\kappa_1\kappa_3^3, \tag{21}$$

with the constant multiplying ϱ (16), equal to $\kappa_1\kappa_3^3$. Thus the action (before redefining the constants) is bounded from below as

$$S\geqslant\kappa_1\kappa_3^3 N, \tag{22}$$

where N is the winding number. The action S is the four-volume integral of the Lagrange density

$$\hat{\mathcal{L}}=(\kappa_0^4+\overline{\kappa}_0^4)|F_{\mu\nu}^{[\alpha\beta]}|^2+\kappa_1^2|D_\mu\phi^a|^2+\kappa_2^4|D_\mu\phi^a\times D_\nu\phi^b|^2+\kappa_3^6|D_\mu\phi^a\times D_\nu\phi^b\times D_\rho\phi^c|^2, \tag{23}$$

subject to the restrictions (21), which is up to some redefinitions coincides with (1) without the potential term V.

It is seen from (22) that the condition that this lower bound be nontrivial is that neither one of κ_1 and κ_3 should vanish. It could be thought that this means κ_2 can be set equal to zero without violating this bound, but from the first member of the constraint equations (21) we see that this is impossible. We conclude therefore that the lower bound remains valid only as long as all the constants $(\kappa_0,\kappa_1,\kappa_2,\kappa_3,)$, and hence also the couplings $(\lambda_0,\lambda_1,\lambda_2,\lambda_3,)$, remain positive and nonzero.

As will be shown in Sec. III, the constants λ_0 and λ_1 can be scaled away leaving only two independent coupling constants λ_2 and λ_3, both of which have to be positive and greater than zero if the lower bound (22) is to be preserved.

Before proceeding to the next section, we note that the Lagrangian (1) is not unique in being bounded from below by the topological charge density (16). Rather, it is the simplest system motivated by the requirements that it features the YM term and the *quadratic* kinetic term of the scalar field. An inspection of the spherically symmetric restriction of the YM term, Eq. (33) below, implies the finite action condition on the gauge field function $a(r)$

$$\lim_{r\to\infty} a(r)=\pm 1,$$

which in the language of the asymptotic conditions (6) means that $q=0$ and $q=1$, respectively. In the first case, the Pontryagin charge vanishes, while in the second case it is equal to 1.

B. Model with $\omega=\pi/2$

The relevant gauge-invariant charge density in this case is (17). Unlike in the previous section however, here we do not proceed straightforwardly to construct the simplest density which is bounded from below by (17).

The reason is that when $\omega\neq 0$ (as in the case case at hand with $\omega=\pi/2$) the gauge group SO(4) breaks down to SO(3) at infinity. This can easily be seen by rotating the asymptotic field ϕ^α $(\alpha=1,2,3,4)$ of length $|\phi^\alpha(\infty)|=\sin\omega$, to the constant vector field along the x_4 axis, by means of an appropriate SO(4) gauge transformation. The effect of this transformation on the so(4) gauge connection is, that it develops a line singularity along the x_4 axis, and its nonvanishing components then take their values in the residual so(3). We do not give the details of the passage to this Dirac gauge here, because this has been given in detail previously in Refs. 6 and 7, in the context of the SO(4)×U(1) gauged Higgs model. The analysis here is identical to that in Refs. 6 and 7, with the 4 component field ϕ^α here replacing the Higgs field $\Phi=\gamma_5\gamma_\mu\hat{x}_\mu$ of Refs. 6 and 7. Indeed this is the case for all d-dimensional $(d\geqslant 3)$SO(d) Higgs models with d-vector Higgs fields,[8] of which the most familiar is the Wu–Yang monopole in $d=3$.

The relevant information that follows from the preceding discussion is, that the asymptotic connection field $\tilde{A}^{ab}_\mu=(\tilde{A}^{ab}_i,\tilde{A}^{ab}_4)$, $(a=\alpha,5)$ in the Dirac gauge decays exactly as $1/r$, and its only nonvanishing component is

$$\tilde{A}^{[\alpha\beta]}_i=\frac{1}{r(1-\hat{x}_4)}(\delta^\alpha_i\hat{x}^\beta-\delta^\beta_j\hat{x}^\alpha), \tag{24}$$

which takes its values in so(3).

It follows that the corresponding asymptotic curvature field has the Coulomb decay $1/r^2$, and as a consequence the integral of the YM action density will diverge logarithmically in four dimensions. This simple fact can also be seen by inspecting the spherically symmetric YM action density in (33). Thus, in constructing the density bounded from below by the topological charge density (17), it is not legitimate to employ the usual YM action density.

The remedy is to use instead the YM density constructed from the antisymmetrized product of two curvature two-forms, namely,

$$|F^{abcd}_{\mu\nu\rho\sigma}|^2=|(F^{\alpha[\beta}_{\mu[\nu}F^{\gamma\delta]}_{\rho\sigma]}+F^{[\delta\gamma}_{\mu[\nu}F^{\beta]\alpha}_{\rho\sigma]})|^2.$$

This term arises naturally in reproducing the last term in the charge density (17). To reproduce the second term in the charge density, it is not legitimate to make use of inequality (19) since the latter features the usual YM density. Given that for the instanton (vacuum) interpretation of the solution we need to have the quadratic kinetic term of the scalar field, this necessitates the appearance of the term

$$|F^{\alpha\beta}_{[\mu\nu}D_{\lambda]}\phi^{\gamma}|^2.$$

Finally, to reproduce the first term, ϱ_G, in (17), the most economical option is to adopt the inequality (18). (This avoids the introduction of the additional and unnecessary term $|D_{[\mu}\phi^a D_{\nu]}\phi^b|^2$ in the Lagrangian.)

Following the above arguments, we write down the three topological inequalities corresponding to (18), (19), (20) for the present case with $\omega=\pi/2$. With (18) unchanged, we just give the second two

$$\overline{\kappa}_1^2|D_{[\mu}\phi^a|^2+\overline{\kappa}_3^6|F^{\alpha\beta}_{[\mu\nu}D_{\lambda]}\phi^{\gamma}|^2\geqslant 3\overline{\kappa}_1\overline{\kappa}_3^3\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}\phi^5 D_{\rho}\phi^{\gamma}D_{\sigma}\phi^{\delta}F^{\alpha\beta}_{\mu\nu}, \tag{25}$$

$$\overline{\kappa}_4^8|F^{abcd}_{\mu\nu\rho\sigma}|^2+\tau^2(\phi^5)^6\geqslant\tau\overline{\kappa}_4^{\frac{4}{2}\frac{3}{2}}\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\beta\gamma\delta}(\phi^5)^3F^{\alpha\beta}_{\mu\nu}F^{\gamma\delta}_{\rho\sigma}, \tag{26}$$

where the constants $\overline{\kappa}_1$, $\overline{\kappa}_3$, and $\overline{\kappa}_4$ all have the dimension of length, while τ is dimensionless.

Adding (18), (25), and (26) results in an inequality whose right-hand side can be identified (up to a numerical factor) with the topological charge density (17), provided that

$$\overline{\kappa}_1\overline{\kappa}_3^3=3\kappa_1\kappa_3^3, \quad 6\tau\overline{\kappa}_4^4=\kappa_1\kappa_3^3. \tag{27}$$

The resulting topological inequality bounding the action from below, analogous to (22), is

$$\tilde{S}\geqslant\kappa_1\kappa_3^3N, \tag{28}$$

in which the action $\tilde{S}$ is the four-volume integral of

$$\begin{aligned}\tilde{\mathcal{L}}=&\overline{\kappa}_4^8|F^{abcd}_{\mu\nu\rho\sigma}|^2+\overline{\kappa}_3^6|F^{ab}_{[\mu\nu}D_{\lambda]}\phi^c|^2+\kappa_3^6|D_{\mu}\phi^a\times D_{\nu}\phi^b\times D_{\rho}\phi^c|^2\\&+(\kappa_1^2+\overline{\kappa}_1^2)|D_{\mu}\phi^a|^2+\tau^2(\phi^5)^6,\end{aligned} \tag{29}$$

subject to the constraints (27). Note that the potential (3) with $\omega=0$ and $n=6$ appears quite naturally in (29), and in this case its presence is mandatory if the lower bound on the action is to be preserved.

Because (29) does not feature the usual YM term besides the F^4 term, it is not likely to be of any physical interest. Hence we do not analyze it numerically. We note that in the case of the SO(4)×U(1) Higgs model,[6,7] which also features the F^4 YM term to the exclusion of the usual F^2, it could be argued that at high energies that system reduced to a conventional SO(4)×U(1) Higgs system

$$\mathrm{Tr}(\lambda_2F^2_{\mu\nu}+\lambda_1D_{\mu}\Phi^2+\lambda_0(\Phi^2+\eta^2)^2), \tag{30}$$

where the constant η is the VEV of the Higgs field, and all fields are anti-Hermitian. In other words, the SO(4)×U(1) Higgs model was interpreted as the low energy effective action of (30). Unfortunately, we do not have such an interpretation for the system (29).

III. SPHERICAL SYMMETRY

The spherically symmetric Ansatz employed is

$$A_\mu^{[\alpha\beta]}=\frac{a(r)-1}{r}(\delta_\mu^\alpha\hat{x}^\beta-\delta_\mu^\beta\hat{x}^\alpha), \tag{31}$$

$$\phi^\alpha=\sin f(r)\hat{x}^\alpha, \quad \phi^5=\cos f(r). \tag{32}$$

As explained in Sec. II B, we will restrict our numerical analysis to the case of $\omega=0$, and hence give the spherically symmetric reduction only of the terms in the system (1), or (23), pertaining to $\omega=0$.

Substituting (31) and (32) into the component terms of (1) we have, for each term

$$|F_{\mu\nu}^{\alpha\beta}|^2=12\left[\left(\frac{a'}{r}\right)^2+\left(\frac{a^2-1}{r^2}\right)^2\right], \tag{33}$$

$$|D_\mu\phi^a|^2=f'^2+3\left(\frac{a^2\sin^2 f}{r^2}\right), \tag{34}$$

$$|D_\mu\phi^a\times D_\nu\phi^b|^2=12\left(\frac{a^2\sin^2 f}{r^2}\right)\left[f'^2+\left(\frac{a^2\sin^2 f}{r^2}\right)\right], \tag{35}$$

$$|D_\mu\phi^a\times D_\nu\phi^b\times D_\rho\phi^c|^2=36\left(\frac{a^2\sin^2 f}{r^2}\right)^2\left[3f'^2+\left(\frac{a^2\sin^2 f}{r^2}\right)\right]. \tag{36}$$

In the following we will study the classical solutions of the model (1) and characterize them by the classical action S defined by means of

$$S=\frac{1}{8\pi^2}\int d^4x\,\mathcal{L}. \tag{37}$$

The reduced one-dimensional Lagrangian is r^3 times the sum, with the appropriate numerical coefficients in (1), of all the above four terms. We do not display this one-dimensional Lagrangian, nor the ordinary differential equations that follow.

The asymptotic values of the function $f(r)$ corresponding to (5) translate to

$$\lim_{r\to 0} f(r)=\pi, \quad \lim_{r\to\infty} f(r)=\omega, \tag{38}$$

with $\omega=0$, while the asymptotic values of the function $a(r)$ for the cases $q=0$ and $q=1$ translate respectively, to

$$\lim_{r\to 0} a(r)=1, \quad \lim_{r\to\infty} a(r)=1, \tag{39}$$

$$\lim_{r\to 0} a(r)=1, \quad \lim_{r\to\infty} a(r)=-1. \tag{40}$$

Let us first point out that the embedded charge-one-BPST-instanton solutions[4]

$$a_{\mathrm{BPST}}(r)=\frac{k^2-r^2}{k^2+r^2}, \quad f(r)=n\pi \text{ (everywhere)} \tag{41}$$

(k is a real constant, n is an integer) exist irrespectively of the values of $\lambda_{1,2,3}$ and leads to $S_{\mathrm{BPST}}=\frac{4}{3}$, corresponding to the action of the charge-one-instanton solution of the Yang–Mills theory.[4] Here we are interested in classical solutions with nonconstant $f(r)$.

The number of four coupling constants can be reduced to two by using the following scaling argument. Transforming $r\to\sigma r$, we have

$$S(\lambda_1,\lambda_2,\lambda_3,\lambda_0)=S(\lambda_1\sigma^2,\lambda_2,\lambda_3\sigma^{-2},\lambda_0)=\lambda_1\sigma^2 S\left(1,\frac{\lambda_2}{\lambda_1\sigma^2},\frac{\lambda_3}{\lambda_1\sigma^4},\frac{\lambda_0}{\lambda_1\sigma^2}\right). \tag{42}$$

Choosing $\sigma^2=\lambda_0/\lambda_1$ this gives

$$S(\lambda_1,\lambda_2,\lambda_3,\lambda_0)=\lambda_0 S\left(1,\frac{\lambda_2}{\lambda_0},\frac{\lambda_3\lambda_1}{\lambda_0^2},1\right). \tag{43}$$

In the following we will make use of the above scaling property and set $\lambda_1=\lambda_0=1$.

IV. NUMERICAL RESULTS

We have studied numerically the solutions of the classical equations associated with (1) for the $\omega=0$ model, restricting to the one-dimensional spherically symmetric fields given by (33)–(36). Most of the work is carried out with the potential (4) decoupled, i.e., with $\lambda=0$.

In Ref. 1 the above equations have been studied in detail in the case $\lambda_1=\lambda_3=0$. Here we want to study the classical solutions for nonvanishing $\lambda_1,\lambda_2,\lambda_3$. Using the standard Derrick scaling argument, it is easily seen that regular classical solutions will exist only if the coupling constants λ_1,λ_3 are both nonzero. On the other hand, the topological lower bound (22) derived in the preceding section states that in addition to λ_1 and λ_0 (which we have already set to $\lambda_0=\lambda_1=1$ by scaling), both λ_2 and λ_3 must be positive and nonzero. On the basis of the last statement, there is no guarantee that the solution persists when λ_2 vanishes, even though this is consistent with the Derrick scaling requirement.

As a result of our numerical studies, we have learned that with the asymptotics (39), the solution persists when λ_2 vanishes. In this case there remains only one coupling constant to vary, λ_3, which is a simpler case to study and this is presented in Sec. IV A. In Sec. IV B, again with the asymptotics (39), we study the cases where λ_2 is varied for fixed nonzero value of λ_3, and also where λ_3 is varied for fixed nonzero value of λ_2. These families of solutions all have Pontryagin charge equal to zero. In Sec. (IV C), we present the results of our numerical search for solutions with *unit* Pontryagin charge and nontrivial scalar field, with asymptotics (40). The result is negative, and we have supplied an analytic construction in support of the nonexistence of such instantons.

A. Solutions with $a(0)=a(\infty)=1$ and $\lambda_2=0$

With these boundary conditions, the Chern–Pontryagin charge would be zero and the topological lower bound would be stated in terms of the degree of the map only.

Integrating the equations for small values of λ_3 we were able to construct solutions with

$$a(0)=1,\quad a(\infty)=1,\quad f(0)=\pi,\quad f(\infty)=0. \tag{44}$$

The profiles of the functions a,f of this solution are presented in Fig. 1 for $\lambda_3=0.425$ by the solid lines. In the limit $\lambda_3=0$ the classical action tends to zero and the function $a(r)$ tends to a constant : $a(r)=1$. When λ_3 increases, the function $a(r)$ develops a local minimum (at $r=r_m$) which becomes progressively deeper as indicated in Fig. 2. The general dependence of r_m on λ_3 is also reported on Fig. 2. At the same time the classical action of the solution increases with λ_3, and this is illustrated in Fig. 3.

This situation persists up to a critical value of λ_3, say λ_3^c, and numerically we found

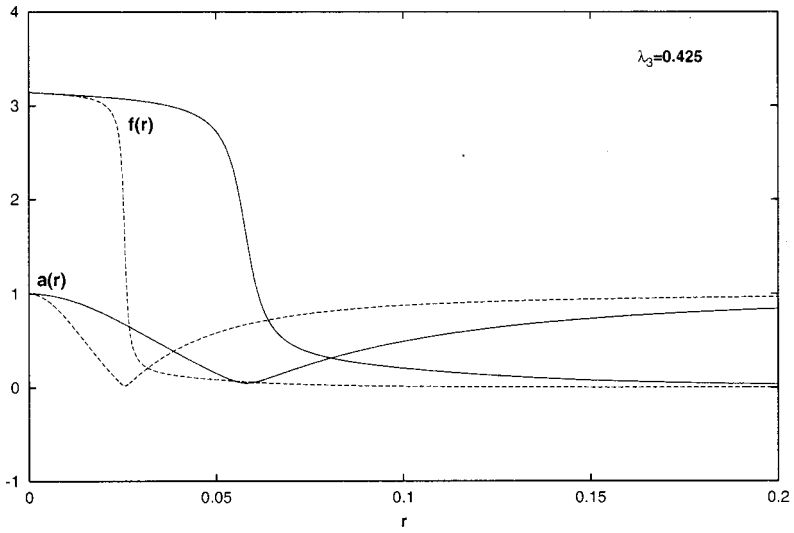

FIG. 1. The profiles of two solutions $a(r)$ and $f(r)$ as functions of r for $\lambda_2=0$ and $\lambda_3=0.425$ for the first branch (solid line) and the second branch (dotted line).

$$\lambda_3^c \approx 0.426\,61. \tag{45}$$

Corresponding to this critical value, we find $r_m \approx 0.041$, $a(r_m) \approx 0.034$, and $S \approx 1.3345$. In particular the value of the action is slightly higher than the value 4/3 corresponding to the action of the instanton solution of the Yang–Mills theory.[4]

In fact, a large part of this action comes from the Yang–Mills part of the Lagrangian and the contribution due to the S^4 valued matter field is rather tiny (less than one percent) because, as indicated by Fig. 1, the function $f(r)$ becomes very steep in the region where the function $a(r)$ has its minimum.

We found no solutions for $\lambda_3 > \lambda_3^c$; however, a careful analysis of the equations strongly suggests that a second branch of solution exists, as illustrated on Fig. 2. As far as the classical

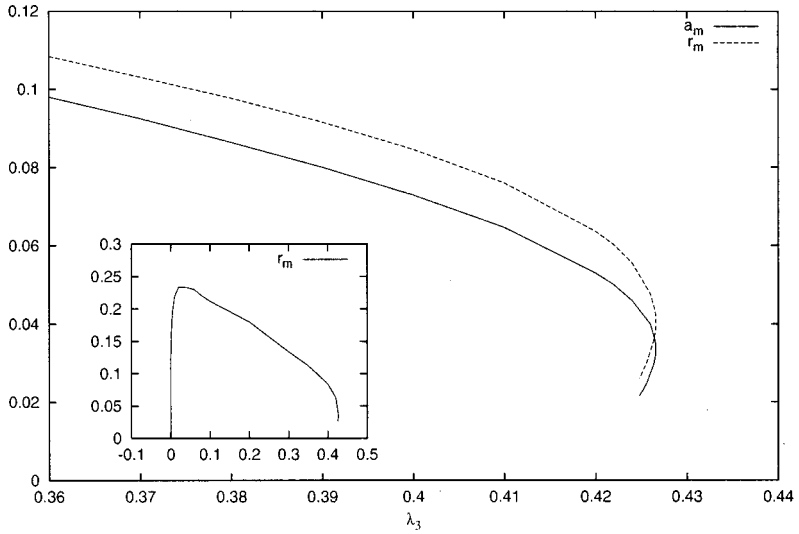

FIG. 2. λ_3 dependence of r_m and $a(r_m)$ for the two branches near the critical value of λ_3 when $\lambda_2=0.1$. The global dependence on r_m is displayed in the window.

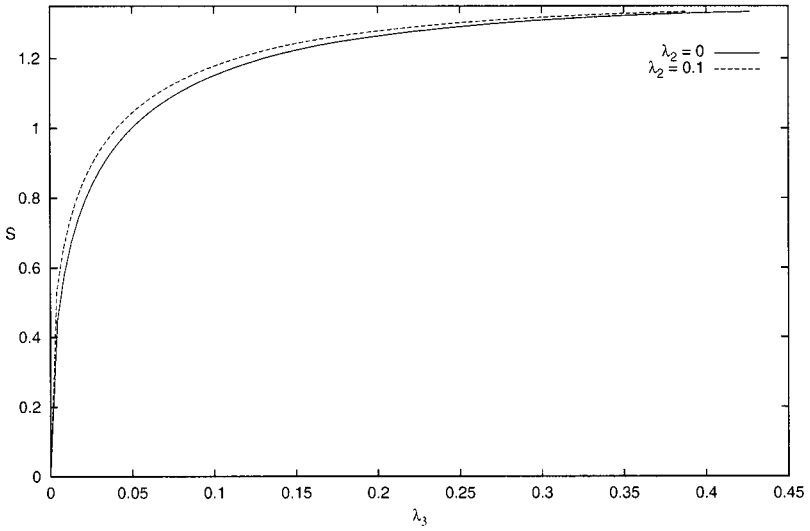

FIG. 3. λ_3 dependence of the action for $\lambda_2=0$ (solid line) and $\lambda_2=0.1$ (dotted line).

action of the two branches is concerned they terminate into a cusp at $\lambda_3=\lambda_3^c$, in a way very similar to Fig. 9 of Ref. 1.

As suggested by Fig. 2, it is very likely that when λ_3 decreases to below λ_3^c on the second branch, the minimum $a(r_m)$ has a tendency to approach zero while the derivative $f'(r_m)$ of the function $f(r)$ becomes infinite. For that reasons, the construction of the classical solution along this branch is numerically difficult and we we had to stop it at $\lambda_3\approx 0.4248$.

Nevertheless, it seems that the profile $a(r)$ of the solution on the second branch is such that

$$\lim_{\lambda_3\to\lambda_3^*} a(r)=|a_{\mathrm{BPST}}(r)|. \tag{46}$$

a_{BPST} being the profile of the charge-1 instanton (41) for an appropriate value of the scaling constant k. The numerical difficulties prevented the evaluation of λ_3^* but, according to Fig. 2, one can expect $\lambda_3^*\approx 0.42$.

The solutions were constructed with the subroutine COLSYS[9] (see Appendix of Ref. 10 for a short description) and with a high degree of accuracy: typically with an error less than 10^{-8}.

To finish this section we mention that the pattern of solutions presented above for $\lambda_2=0$ seems to persist for $\lambda_2>0$. For instance, for $\lambda_2=1$ we find $\lambda_3^c\approx 0.14$, i.e., a much lower value than in the case $\lambda_2=0$. More details are given in the next section.

B. Solutions with $a(1)=a(\infty)=1$ with $\lambda_2>0$, $\lambda_3>0$

In this section we present numerical results for solutions with the same asymptotics as in Sec. IV A, but (a) holding λ_2 fixed at $\lambda_2=0.1$ and varying λ_3, and (b) holding λ_3 fixed at $\lambda_3=0.1$ and varying λ_2.

As in Sec. IV A, the solutions do not appear to persist for arbitrarily large λ_3 (when $\lambda_2=0.1$), and arbitrarily large λ_2 (when $\lambda_3=0.1$). Unlike in Sec. IV A however, we have not endeavoured to find accurate critical values for the λ_2 and λ_3, respectively. The general features of the solutions remain unchanged whether or not λ_2 vanishes.

The action versus λ_3 (with $\lambda_2=0.1$) is plotted in Fig. 3. The action versus λ_2 (with $\lambda_3=0.1$) is plotted in Fig. 4. In both cases we note the remarkable feature that the action rises to just above the BPST instanton action $\frac{4}{3}$. This feature is shared with the restricted model with $\lambda_1=\lambda_3=0$ model studied in Ref. 1.

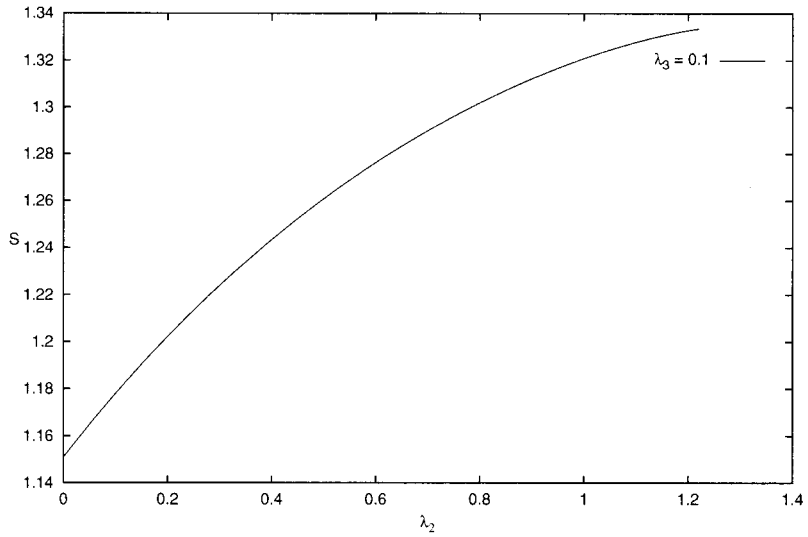

FIG. 4. λ_2 dependence of the action for $\lambda_2 = 0.1$.

Figure 5 is the analogue of Fig. 2, where the progress of $r_{\min}$ and $a_{\min}$, the position of the minimum and the value of the minimum of the function $a(r)$, are plotted against increasing λ_2 (with $\lambda_3 = 0.1$ fixed). Figures 2 (respectively, Fig. 5) describes the manner in which the solutions disappear as the value of the λ_3 (respectively, λ_2) approaches a critical value. (The analysis confirming the existence of two distinct branches is given only in Fig. 2.)

In addition to the above results, we have made a study of the generic system (1) with the potential (4) included. It turns out that decoupling the potential (4) results in no appreciable qualitative changes in the values of the action, for all values of the coupling constants λ_2 and λ_3. This property of the present model is shared by the usual (ungauged) Skyrme model.[2]

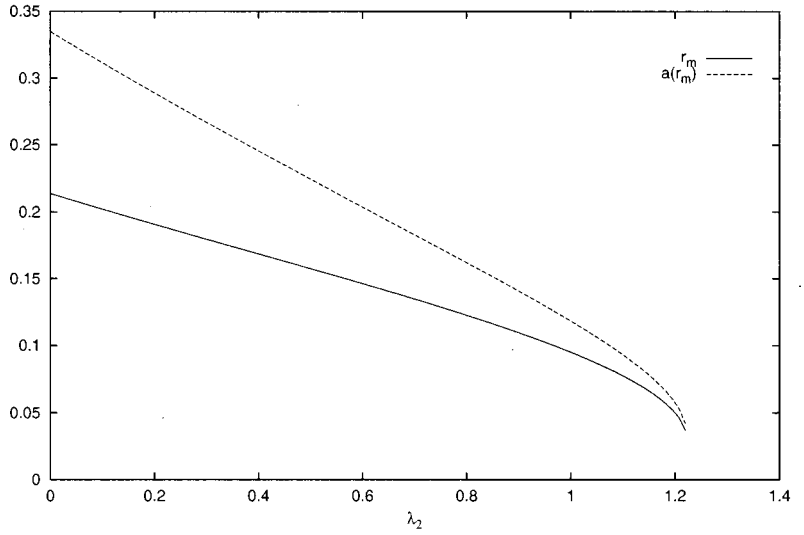

FIG. 5. λ_2 dependence of r_m and a_m for $\lambda_3 = 0.1$.

C. Solutions with $a(0)=-a(\infty)=1$

Should solutions of this type exist, their Chern–Pontryagin charge would be nonzero. As we shall see below, the only such solutions are those with trivial S^4 valued field, i.e., only the pure YM^4 instantons.

The set of boundary conditions

$$a(0)=1, \quad a(\infty)=-1, \quad f(0)=\pi, \quad f(\infty)=0, \tag{47}$$

pertain to *unit* Chern–Pontryagin charge for the spherically symmetric configuration at hand, and provide a natural alternative to the solution discussed above.

Although we could numerically exhibit regular configurations obeying these conditions and with an action slightly higher than 4/3, we have not succeeded in constructing a solution of the equations with these conditions. We used both COLSYS and a relaxation method to find solutions satisfying the boundary conditions (47) and all the numerical results accumulated leads us to the formulation of the following statement: the solutions of the equations of motion obeying (47) are constituted by the functions

$$a(r)=\frac{k^2-r^2}{k^2+r^2}, \quad k\in\mathbb{R}, \quad f(0)=0, \quad f(r)=\pi, \quad r>0 \tag{48}$$

considered in the limit $k\to 0$. The limiting configuration, which is determined in terms of step functions, has action $S=4/3$.

We now give an analytic construction to show that no such smooth solutions exist. To do this we will consider a suitably chosen one parameter family of field configurations and show that in the limit where the parameter vanishes, the field f becomes a step function shrunk near the origin and that the action reduces to the action of the instanton.

First of all let us write the expression for the action after performing the scaling $r=\sigma x$,

$$\begin{aligned} S=\frac{1}{2}\int \Bigg\{ & \lambda_0\left(\left(\frac{a_x}{x}\right)^2+\left(\frac{a^2-1}{x^2}\right)^2\right)+\sigma^2\lambda_1\left(f_x^2+3\left(\frac{a^2\sin^2 f}{x^2}\right)\right) \\ & +\lambda_2\frac{a^2\sin^2 f}{x^2}\left(f_x^2+\frac{a^2\sin^2 f}{x^2}\right)+\frac{\lambda_3}{\sigma^2}\left(\frac{a^2\sin^2 f}{x^2}\right)^2\left(3f_x^2+\frac{a^2\sin^2 f}{x^2}\right)\Bigg\}x^3\,dx. \end{aligned} \tag{49}$$

We then consider the following configuration: for a we take the usual instanton solution and we call x_0 the point where $a(x_0)=0$. For f we take

$$f=\pi \quad \text{if} \quad x\leqslant x_0-\frac{\epsilon}{2}, \tag{50}$$

$$f=\left(x_0+\frac{\epsilon}{2}-x\right)\frac{\pi}{\epsilon} \quad \text{if} \quad x_0-\frac{\epsilon}{2}\leqslant x\leqslant x_0+\frac{\epsilon}{2}, \tag{51}$$

$$f=0 \quad \text{if} \quad x\geqslant x_0+\frac{\epsilon}{2}. \tag{52}$$

We then notice that the support of the action density for the first three terms is the interval $[x_0-\epsilon/2, x_0+\epsilon/2]$. Moreover in that interval we can write

$$a=K(x-x_0)+O((x-x_0)^2), \tag{53}$$

where K is a constant. Defining

$$S_a = \int \frac{\lambda_0}{2}\left(\left(\frac{a_x}{x}\right)^2 + \left(\frac{a^2-1}{x^2}\right)^2\right) r^3\, dr \tag{54}$$

we can write

$$\begin{aligned} S = S_a + \frac{1}{2}\int_{x_0-\epsilon/2}^{x_0+\epsilon/2} \Bigg\{ & \sigma^2 \lambda_1 x^3 \left(\frac{\pi^2}{\epsilon^2} + \frac{3}{x^2}K^2 (x-x_0)^2 \sin^2 f\right) \\ & + \lambda_2 x^3 \left(\frac{K^2}{x^2}(x-x_0)^2 \sin^2 f \left(\frac{\pi^2}{\epsilon^2} + \frac{K^2}{x^2}(x-x_0)^2 \sin^2 f\right)\right) \\ & + \frac{\lambda_3}{\sigma^2} x^3 \left(\frac{K}{x}(x-x_0)\right)^2 \left(\frac{3}{\epsilon^2}\pi^2 + \frac{K^2}{x^2}(x-x_0)^2 \sin^2 f\right) \Bigg\} dx. \end{aligned} \tag{55}$$

We can the replace $\sin f$ by 1 and perform each of the integrals to the lowest order in ϵ which gives

$$\begin{aligned} S \leqslant S_a + \sigma^2 \frac{\lambda_1}{2}\left(\frac{1}{\epsilon} x_0 \pi^2 + K^2 x_0 \epsilon^3\right) + \lambda_1 \sigma^2 O(\epsilon) + \frac{\lambda_2}{2} K^2 \left(\frac{x_0}{3}\pi^2 \epsilon + \frac{K^2 \epsilon^5}{5(x_0+\epsilon/2)}\right) + \lambda_2 O(\epsilon^3) \\ + \frac{\lambda_3}{2\sigma^2} K^4 \left(\frac{3}{(x_0+\epsilon/2)^5}\epsilon^3 + \frac{K^2}{7(x_0+\epsilon/2)^3}\epsilon^7\right) + \frac{\lambda_3}{\sigma^2} O(\epsilon^5) \end{aligned} \tag{56}$$

choosing $\sigma = \epsilon$ we have

$$\lim_{\epsilon \to 0} S = S_a \tag{57}$$

and in that limit the field f becomes singular, showing that there are no regular solutions with this boundary conditions. This is indeed what we observed when we tried to compute such solution numerically.

V. SUMMARY AND DISCUSSION

The coupling of nonlinear sigma models to gauge fields often leads to sets of classical equations whose solutions obey various types of critical phenomena like bifurcations and/or pairs of solutions terminating into a cusp. The classical equations associated with the Lagrangian (1), in the spherically symmetric Ansatz, are of this type. These solutions seem to follow the same pattern, irrespectively of the different Skyrme terms added, i.e., these patterns seem to be independent of the dynamical details.

In this paper, we have studied the classical solutions ensuing from the Lagrangian (1) for three different sets of the two independent coupling constants (λ_2, λ_3). In spite of the fact that our analysis in Sec. II (specifically in Sec. II A) leads to the establishment of a topological lower bound on the action provided that both λ_2 and λ_3 be positive, we have found that in fact solutions persist at $\lambda_2 = 0$. A similar situation arises in the three-dimensional Skyrme model augmented by a sextic Skyrme term. In that case too, when the usual (quartic) Skyrme term is decoupled, thus invalidating the topological lower bound, the solution persists[11] notwithstanding. This most probably means that our (Bogomol'nyi type) analysis in Sec. II is not far reaching enough for the model at hand. For example, in the case of Hopf solitons, there exists no Bogomol'nyi type lower bound on the energy, but instead one finds that a bound nevertheless can be established in terms of Sobolev type inequalities.[12] We have not carried out the appropriate analysis here, but expect that this can be done. Accordingly we have treated the simplified model (1) with $\lambda_2 = 0$ as legitimate and have carried out the detailed analysis of exhibiting the cusp structure alluded to in the previous paragraph, for that model in Sec. IV A, which we summarize in the next paragraphs.

For the $\lambda_2 = 0$ model, clearly the two branches of solutions (the ones with nontrivial S^4 valued matter field) terminate into a cusp at $\lambda_3 = \lambda_3^c$. This is a typical situation met in catastrophe theory.

The spherically symmetric (BPST) instanton of the pure Yang–Mills theory[4] plays a major role and behaves as an attractor (at least when one of the coupling constants approaches a certain value) of the solution which excites both the matter and the gauge fields. It is very likely that the second branch of solutions bifurcates from the BPST branch at the critical value $\lambda_3=\lambda_3^*<\lambda_3^c$. However, due to the absolute value in the limit (46), the bifurcating solution does not occur in a standard, i.e. continuous way.

The qualitative features of the instanton of the $\lambda_2=0$ model just described were confirmed also in the generic model with nonvanishing λ_2 and λ_3, in Sec. IV B, where the cusp resulting from the existence of two distinct branches was not explicitly constructed.

In Sec. IV C, we verified that there existed no instantons with *unit* Pontryagin charge in this model, irrespective of the value of $S^4\to S^4$ winding number. This is important since it tells us that the zero Pontryagin charge instantons of this model are not the analogues of the triangle anomaly, and hence that the nonperturbative quasiclassical effects they describe must be given a new physical interpretation. (We return to this in the last paragraph.)

Before alluding to the possible physical relevance of the model, we note that nonvanishing Pontryagin charge instantons can readily be constructed by changing the model to feature a symmetry breaking potential (3) as opposed to (4). We have presented the simplest such model in Sec. II B, but did not carry out a numerical study in that case because the model involved was rather remote from known physically relevant models.

In short, we have seen that the system consisting of the interacting YM and O(5) sigma models supports instantons with vanishing Pontryagin charge, which do not describe quasiclassical effects analogous to the triangle anomaly, but which have the $S^4\to S^4$ winding number as the topological charge. Besides, the gauge group for this model is not that of the standard model. On the other hand, it is quite straightforward to construct an O(5) model interacting with the SO(3)×SO(2) YM system that supports such instantons, by adapting the analysis of Sec. II to that case. (That remains a future project.) Moreover, the number of independent S^4 valued fields is equal to four, just as the number of the Higgs doublet in the standard model, thus an SO(3)×SO(2) gauged O(5) model added to the standard model, could be regarded as a complicated low energy version of the latter, whose (axially symmetric) instantons can describe new nonperturbative effects. In this sense, the SO(4) gauged O(5) model studied here can be regarded as a prototype of a physically more relevant model.

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Algebraic treatment of super-integrable potentials

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The so(2,1) Lie algebra is applied to three classes of two- and three-dimensional Smorodinsky–Winternitz super-integrable potentials for which the path integral discussion has been recently presented in the literature. We have constructed the Green's functions for two important super-integrable potentials in R^2. Among the super-integrable potentials in R^3, we have considered two examples, one is maximally super-integrable and another one minimally super-integrable. The discussion is made in various coordinate systems. The energy spectrum and the suitably normalized wave functions of bound and continuous states are then deduced. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1396635]

I. INTRODUCTION

Ever since the success of the algebraic approach based on the noncompact groups in calculating the wave functions and the transition amplitudes for the hydrogen atom by Kleinert,[1] a renewed interest for this method has been emerging. Hence a large amount of physical problems for which the Schrödinger equation reduces to the confluent hypergeometric equation have been treated in the framework of this approach. In particular, the radial harmonic oscillator, the radial Coulomb and Morse oscillator potentials and the Natanzon confluent potentials,[2] which generalize the latter, have been discussed in a variety of SO(2,1) realizations.[3–9]

The above so(2,1) algebraic approach has also been applied to noncentral potentials such as the ring-shaped potential[10] introduced by Hartmann[11] to describe the molecular interaction of cyclic polyenes and the so-called double ring-shaped oscillator[12] which is the Quesne ring-shaped oscillator[13] plus an $r^{-2}\sec^2\theta$ term.

The (MS) variant of the algebraic method summarized in Sec. II has been developed by Milshtein and Strakhovenko[14] to construct the Green's function associated with the problem of Dirac electron in a static Coulomb field. The straightforward algebraic calculation of the Green's function for a given potential represents an undeniable advantage which allowed this variant to be given a great deal of attention, in recent years, following the development of path integration techniques. Hence a remarkable set of potentials has been studied in this algebraic approach. Among them, we can quote potentials of practical interest, such as Morse's,[15] the radial harmonic oscillator and the radial Coulomb potentials. The Hartmann ring-shaped potential,[16] the compound Coulomb plus Aharonov–Bohm potential[17] and two highly singular nonisotropic potentials associated to a highly distorted spherical Coulomb field with an additional double ring well and a highly distorted cylindrical Coulomb field have also been studied in parabolic coordinate systems.[18] Within the framework of the R^4 to R^3 non-bijective Kustaanheimo–Stiefel mapping, the Kaluza–Klein monopole system[19] and a noncentral potential[20] which generalizes the Coulomb potential and the Hartmann ring-shaped potential and also, due to its close link with the latter, the compound Coulomb plus Aharonov–Bohm potential have been treated by means of the same algebraic approach as Milshtein and Strakhovenko. Cylindrical parabolic coordinates have also been used in discussion for the so(2,1) algebraic method of another type of noncentral

potentials.[21,22] All these potentials discussed with the help of the (MS) variant appear in the general classification of potentials in two and three dimensions possessing dynamical invariance groups initiated about 30 years ago by Smorodinsky and co-workers,[23] continued by Kibler and Winternitz,[24] and revived, in recent years, by Evans.[25,26] This classification was established according to the number of degrees of freedom, quadratic integrals of motion in the momenta and coordinate systems in which the potential allows the separation of variables. The Hamiltonian systems with these potentials are called super-integrable. Generally, in n dimensions, a system is called ''minimally'' super-integrable if it has $(2n-2)$ constants or integrals of motion (including energy), and it is called ''maximally'' super-integrable if it has $(2n-1)$ integrals of motion.[27] A list of minimally super-integrable and maximally super-integrable potentials with the corresponding constants of motion in the classical form and all separating coordinate systems has been established by Evans.[28] On the basis of this classification, Grosche *et al.*[29] have recently presented a detailed path integral discussion of the so-called Smorodinsky–Winternitz super-integrable potentials in many coordinate systems. It is to be noted that almost all the potentials contained in this classification involve centrifugal or angular barriers which possess point singularities. Consequently, following Kleinert[30] the time sliced path integral for these potentials does not exist in any coordinate system. So, it is necessary to regularize the system in question by an appropriate set of new coordinates in order to find a path integral expression without collapse. This problem does not occur in the framework of the (MS) variant of the so(2,1) algebraic approach owing to its local (differential) character. This constitutes a great advantage in studying the problem of the Smorodinsky–Winternitz potentials in this framework.

The plan of this article is as follows. We briefly review the so(2,1) Lie algebra and its use in calculating Green's functions in Sec. II. We study a set of two potentials in two dimensions, algebraically obtain the Green's function in the various separating coordinate systems and deduce the energy spectrum as well as the corresponding normalized wave functions in Sec. III. Sections IV and V deal with two examples of three-dimensional potentials. The construction of the Green's functions is made in different coordinate systems. The energy spectrum and the normalized wave functions are evaluated. Section VI will be a conclusion.

II. GREEN'S FUNCTION AND so(2,1) LIE ALGEBRA

Let's briefly review the main features of so(2,1) Lie algebra and its use in the calculation of the Green's functions to make this paper self-contained. A set of three operators $\{T_1,T_2,T_3\}$ characterized by the commutation relations[31] define it:

$$[T_1,T_2]=-iT_1,\quad [T_2,T_3]=-iT_3,\quad [T_1,T_3]=-iT_2. \tag{1}$$

Because of the type of potentials we shall deal with in this paper, we have to use the following differential realization of the operators:

$$T_1(x)=-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial x^2}-\frac{\mu(\mu-1)}{x^2}\right),\quad T_2(x)=-\frac{i}{2}\left(x\frac{\partial}{\partial x}+\frac{1}{2}\right),\quad T_3(x)=\frac{M}{4\hbar^2}x^2, \tag{2}$$

with $0<x<\infty$.

By using Schwinger's integral representation,[32] the Green's function associated to a potential $V(x)$ with the SO(2,1) group symmetry is given by

$$G(x,x';E)=\int_0^\infty dS\,\exp\left[\frac{iS}{\hbar}(E+i0)\right]K(x,x';S), \tag{3}$$

where

$$K(x,x';S)=\exp\left\{-\frac{iS}{\hbar}\left[-\frac{\hbar^2}{2M}\nabla_x^2+V(x)\right]\right\}\delta(x-x')$$
$$=\exp\left\{-\frac{iS}{\hbar}[T_1(x)+2\hbar^2\omega^2T_3(x)]\right\}\delta(x-x'). \tag{4}$$

The calculation of this kernel is based upon the use of two Baker–Campbell–Hausdorff formulas[33]

$$\exp\left\{-\frac{iS}{\hbar}[T_1+2\hbar^2\omega^2T_3]\right\}=\exp(-iaT_3)\exp(-ibT_2)\exp(-icT_1), \tag{5}$$

where

$$a=2\hbar\omega\tan(\omega S),\quad b=2Ln[\cos(\omega S)],\quad c=\frac{1}{\hbar\omega}\tan(\omega S), \tag{6}$$

and

$$\exp(-i\alpha T_3)\exp(-i\beta T_2)\exp(-i\gamma T_1)=\exp(-icT_1)\exp(\tau T_3), \tag{7}$$

with

$$\alpha=\frac{i\tau}{1-i\tau c/2},\quad \beta=2Ln\left(1-\frac{i\tau c}{2}\right),\quad \gamma=\frac{c}{1-i\tau c/2}. \tag{8}$$

Here, we also have to use the Laplace transform of the Dirac distribution

$$\delta(x-x')=\frac{M}{2\hbar^2}\frac{x^\mu x'^{1-\mu}}{2i\pi}\int_{-i\infty+\delta}^{i\infty+\delta}d\tau\exp\left[\frac{M}{4\hbar^2}(x^2-x'^2)\tau\right],\quad \delta<0, \tag{9}$$

in order to obtain a manageable result as follows:

$$\exp(-i\gamma T_1)x^\mu=\left[1-i\gamma T_1+\frac{1}{2!}(-i\gamma T_1)^2+\cdots\right]x^\mu=x^\mu. \tag{10}$$

Using relations (9), (5) and (7), the kernel (4) can now be written

$$K(x,x';S)=\frac{M}{2\hbar^2}x'^{1-\mu}\exp(-iaT_3)\exp(-ibT_2)x^\mu\exp\left(\frac{iMx^2}{2\hbar^2c}\right)$$
$$\times\int_{-i\infty+\delta}^{i\infty+\delta}d\tau\frac{\exp\left(-\frac{Mx'^2}{4\hbar^2}\tau\right)\exp\left(\frac{Mx^2}{\hbar^2c^2}\frac{1}{\tau+2i/c}\right)}{\left(1-\frac{i\tau c}{2}\right)^{\mu+1/2}}, \tag{11}$$

where the well-known formula

$$\exp(-i\beta T_2)f(x)=\exp\left(-\frac{\beta}{4}\right)f\left(e^{-\beta/2}x\right) \tag{12}$$

has also been used.

The integral can be calculated thanks to the residue theorem after the $\exp((Mx^2/\hbar^2c^2)[1/(\tau+2i/c)])$ series has been effected. Hence, we obtain

$$K(x,x';S)=\frac{M\omega}{i\hbar\sin(\omega S)}\sqrt{xx'}\exp\left[\frac{iM\omega}{2\hbar}(x^2+x'^2)\cot(\omega S)\right]\times I_\lambda\left(\frac{M\omega xx'}{i\hbar\sin(\omega S)}\right), \tag{13}$$

where $\lambda=\mu-\frac{1}{2}$ and $I_\lambda(x)$ is the modified Bessel function.

We can now use (13) for any coordinate in a multi-dimensional system, provided that the $(H-E)^{-1}$ inverse resolvent operator can be transformed into a linear combination of the above mentioned $T_i\,(i=1,2,3)$ operators.

III. TWO-DIMENSIONAL MAXIMALLY SUPER-INTEGRABLE POTENTIALS

We shall study here a set of two important potentials belonging to a class of two-dimensional Smorodinsky–Winternitz potentials. They are characterized by the existence of three functionally independent integrals of motion, which means that there is a pair of quadratic operators corresponding to these integrals of motion which commute with the system's Hamiltonian. The number of such integrals being superior to that of degrees of liberty, they are thus called maximally super-integrable potentials.

A. Let us study the potential

$$V_1(\vec{\rho})=-\frac{\alpha_0}{\sqrt{x_1^2+x_2^2}}+\frac{\hbar^2}{4M}\frac{1}{\sqrt{x_1^2+x_2^2}}\left(\frac{k_1^2-\frac{1}{4}}{\sqrt{x_1^2+x_2^2}+x_1}+\frac{k_2^2-\frac{1}{4}}{\sqrt{x_1^2+x_2^2}-x_1}\right), \tag{14}$$

with positive α_0, k_1 and k_2 constants. It admits the following three functionally independent integrals of motion:

$$\begin{aligned} H_1&=\frac{P^2}{2M}+V_1(\vec{\rho}),\quad I_1=\frac{L_3^2}{2M}+\frac{\hbar^2\rho^2}{8M}\left(\frac{k_1^2-\frac{1}{4}}{x_1^2}+\frac{k_2^2-\frac{1}{4}}{x_2^2}\right),\\ I_2&=\frac{\{L_3,P_2\}}{4M}+\frac{\alpha(\eta-\xi)}{\xi\eta}-\frac{2(k_1^2-\frac{1}{4})}{\xi^2}+\frac{2(k_2^2-\frac{1}{4})}{\eta^2}. \end{aligned} \tag{15}$$

This potential is exactly solvable in two coordinate systems, namely parabolic and polar. For $k_1=k_2=\frac{1}{2}$, Eq. (14) can be reduced to the Coulomb potential treated with a path integral approach.[34,35] The algebraic solution to this potential via the (MS) variant is easier to establish using the parabolic coordinates or even the Levi-Cevita variables[36] defined by $x_1=u_1^2-u_2^2$, $x_2=2u_1u_2$ $(-\infty<u_1,u_2<+\infty)$. The Green's function $G(\vec{\rho},\vec{\rho'};E)$ associated to the potential (14), in Schwinger's integral representation, is given by

$$\begin{aligned} G(\vec{\rho},\vec{\rho'};E)=&\int_0^\infty\frac{dS}{4\rho}\exp\left\{-\frac{iS}{\hbar}\left[\frac{1}{4\rho}\sum_{j=1}^{2}\left(-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial u_j^2}-\frac{k_j^2-\frac{1}{4}}{u_j^2}\right)\right)-\frac{\alpha_0}{\rho}-E-i0\right]\right\}\\ &\times\prod_{j=1}^{2}\delta(u_j-u_j'). \end{aligned} \tag{16}$$

By applying the time transformation $S\to\tau$ defined by $\tau=S/4\rho$, the Green's function (16) can be written

$$G(\vec{\rho},\vec{\rho'};E)=\int_0^\infty d\tau\exp\left[\frac{i}{\hbar}(4\alpha_0+i0)\tau\right]\prod_{j=1}^{2}K(u_j,u_j';\tau), \tag{17}$$

where

$$K(u_j,u_j';\tau)=\exp\left\{-\frac{i\tau}{\hbar}[T_1(u_j)+2\hbar^2\omega^2T_3(u_j)]\right\}\delta(u_j-u_j'), \tag{18}$$

with $\mu_j=\frac{1}{2}\pm k_j$ and $\omega=\sqrt{-8E/M}$.

Using the Eq. (13), we can write the propagators (18) as follows:

$$K(u_j,u_j';\tau)=\frac{M\omega\sqrt{u_ju_j'}}{i\hbar\sin(\omega\tau)}\exp\left[\frac{iM\omega}{2\hbar}(u_j^2+u_j'^2)\cot(\omega\tau)\right]I_{\pm k_j}\left(\frac{M\omega u_ju_j'}{i\hbar\sin(\omega\tau)}\right). \tag{19}$$

1. Parabolic coordinates

In the parabolic coordinates $\xi=\sqrt{2}u_1$, $\eta=\sqrt{2}u_2$ and after changing $\omega\to 2\omega$ and $\tau\to\tau/2$ and by taking into account (19), the Green's function (17) becomes

$$G(\vec{\rho},\vec{\rho'};E)=\int_0^\infty d\tau\exp\left[\frac{i}{\hbar}(2\alpha_0+i0)\tau\right]K(\xi,\eta,\xi',\eta';\tau), \tag{20}$$

where

$$K(\xi,\eta,\xi',\eta';\tau)=\left(\frac{M\omega}{i\hbar\sin(\omega\tau)}\right)^2\sqrt{\xi\xi'\eta\eta'}\exp\left[\frac{iM\omega}{2\hbar}(\xi^2+\eta^2+\xi'^2+\eta'^2)\cot(\omega\tau)\right]$$
$$\times I_{\pm k_1}\left(\frac{M\omega\xi\xi'}{i\hbar\sin(\omega\tau)}\right)I_{\pm k_2}\left(\frac{M\omega\eta\eta'}{i\hbar\sin(\omega\tau)}\right), \tag{21}$$

with

$$\omega=\sqrt{-\frac{2E}{M}}. \tag{22}$$

To find the energy spectrum and the normalized wave functions of the bound states, we make use of the Hille and Hardy formula[37]

$$\frac{1}{1-z}\exp\left[-z\frac{x+y}{1-z}\right]I_\alpha\left(\frac{2\sqrt{xyz}}{1-z}\right)=(xyz)^{\alpha/2}\sum_{n=0}^\infty\frac{n!}{\Gamma(n+\alpha+1)}L_n^\alpha(x)L_n^\alpha(y)z^n,\quad |z|<1, \tag{23}$$

where the $L_n^\alpha(x)$ are the Laguerre polynomials, and the integration over S yields the quantization condition

$$n_1+n_2\pm\frac{k_1}{2}\pm\frac{k_2}{2}+p=0, \tag{24}$$

where $p=-\alpha_0/\hbar\omega$. Therefore, the Green's function (20) can be written as

$$G(\vec{\rho},\vec{\rho'};E)=i\hbar\sum_{n_1,n_2=0}^\infty\frac{\Psi_{n_1,n_2}(\xi_1,\eta_2)\Psi^*_{n_1,n_2}(\xi_1',\eta_2')}{E+i0-E_{n_1,n_2}}, \tag{25}$$

with the normalized wave functions ($a=\hbar^2/M\alpha_0$ is the Bohr radius)

$$\Psi_{n_1,n_2}(\xi,\eta)=\left[\frac{2}{a^2N^3}\frac{n_1!n_2!}{\Gamma(n_1\pm k_1+1)\Gamma(n_2\pm k_2+1)}\right]^{1/2}\left(\frac{\xi^2}{aN}\right)^{1/4\pm(k_1/2)}\left(\frac{\eta^2}{aN}\right)^{1/4\pm(k_2/2)}$$
$$\times\exp\left[-\frac{\xi^2+\eta^2}{2aN}\right]L_{n_1}^{\pm k_1}\left(\frac{\xi^2}{aN}\right)L_{n_2}^{\pm k_2}\left(\frac{\eta^2}{aN}\right), \tag{26}$$

and the discrete energy spectrum given by

$$E_{n_1,n_2}=-\frac{M\alpha_0^2}{2\hbar^2N^2},\quad N=n_1+n_2\pm\frac{k_1}{2}\pm\frac{k_2}{2}+1. \tag{27}$$

To determine the energy spectrum and the wave functions of the continuous states, let's go back to the expression (21) and use the dispersion formula[38]

$$\frac{2\pi\sqrt{xy}}{\sin\alpha}\exp[-(x+y)\cot\alpha]I_{2\mu}\left(\frac{2\sqrt{xy}}{\sin\alpha}\right)=\int_R dp\,\frac{\Gamma(\frac{1}{2}+\mu+ip)\Gamma(\frac{1}{2}+\mu-ip)}{\Gamma^2(2\mu+1)}M_{ip,\mu}\times(-2ix)M_{-ip,\mu}(2iy). \tag{28}$$

Given $x=(M\omega/2i\hbar)\,\xi'^2$, $y=(M\omega/2i\hbar)\,\xi^2$ and $\alpha=\omega\tau$, we obtain

$$\begin{aligned}K(\xi,\eta,\xi',\eta';\tau)=&\frac{1}{\sqrt{\xi\xi'\eta\eta'}\,\pi^2\Gamma^2(1\pm k_1)\Gamma^2(1\pm k_2)}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dp_\xi\,dp_\eta\\&\times\Gamma\left(\frac{1}{2}\pm\frac{k_1}{2}+ip_\xi\right)\Gamma\left(\frac{1}{2}\pm\frac{k_1}{2}-ip_\xi\right)\Gamma\left(\frac{1}{2}\pm\frac{k_2}{2}+ip_\eta\right)\Gamma\left(\frac{1}{2}\pm\frac{k_2}{2}-ip_\eta\right)\\&\times e^{(\pi-2\omega\tau)(p_\xi+p_\eta)}M_{-ip_\xi,\pm(k_1/2)}\left(\frac{M\omega}{\hbar}\xi^2\right)M_{ip_\xi,\pm(k_1/2)}\left(\frac{M\omega}{\hbar}\xi'^2\right)\\&\times M_{-ip_\eta,\pm(k_2/2)}\left(\frac{M\omega}{\hbar}\eta^2\right)M_{ip_\eta,\pm(k_2/2)}\left(\frac{M\omega}{\hbar}\eta'^2\right).\end{aligned} \tag{29}$$

If we now transfer (29) into (20), we shall obtain the poles of the continuous state Green's function by integration on the τ variable. They will be defined by

$$\omega(p_\xi+p_\eta)-\frac{i\alpha_0}{\hbar}=0. \tag{30}$$

If we convert this into energy via (22), the values of the energy will be

$$E_p=\frac{\hbar^2p^2}{2M}\quad\text{with}\quad p=\frac{1}{a(p_\xi+p_\eta)}. \tag{31}$$

Let's now change the variables defined by

$$p_\xi=\frac{1}{2p}\left(\frac{1}{a}+\varsigma\right)\quad\text{and}\quad p_\eta=\frac{1}{2p}\left(\frac{1}{a}-\varsigma\right). \tag{32}$$

In this case, we can write the Green's function as follows:

$$G^c(\xi,\eta,\xi',\eta';E)=i\hbar\int_0^\infty dp\int_{-\infty}^{\infty}d\varsigma\,\frac{\Psi_{p,\varsigma}(\xi,\eta)\Psi^*_{p,\varsigma}(\xi',\eta')}{E+i0-E_p}, \tag{33}$$

with the wave functions given by

$$\begin{aligned}\Psi_{p,\varsigma}(\xi,\eta)=&\frac{\left|\Gamma\left(\frac{1}{2}\pm\frac{k_1}{2}+\frac{i}{2p}\left(\frac{1}{a}+\varsigma\right)\right)\Gamma\left(\frac{1}{2}\pm\frac{k_2}{2}+\frac{i}{2p}\left(\frac{1}{a}-\varsigma\right)\right)\right|}{2\pi\Gamma(1\pm k_1)\Gamma(1\pm k_2)\sqrt{\xi\eta}}\,\frac{e^{\pi/2ap}}{\sqrt{p}}\,M_{-(i/2p)(1/a+\varsigma),\pm(k_1/2)}\\&\times(-ip\xi^2)M_{-(i/2p)(1/a-\varsigma),\pm(k_2/2)}(-ip\eta^2).\end{aligned} \tag{34}$$

2. Polar coordinates

Let's use the (ρ, ϕ) polar coordinates defined by

$$\xi=\sqrt{2}u_1=\sqrt{2\rho}\cos\frac{\phi}{2}, \quad \eta=\sqrt{2}u_2=\sqrt{2\rho}\sin\frac{\phi}{2}, \tag{35}$$

and the addition theorem formula[39]

$$\begin{aligned}\frac{z}{2}I_\nu(z\sin\alpha\sin\beta)I_\mu(z\cos\alpha\cos\beta)&\\ =(\sin\alpha\sin\beta)^\nu(\cos\alpha\cos\beta)^\mu\sum_{n=0}^{\infty}(\nu+\mu+2n+1)&\\ \times\frac{n!}{\Gamma(\nu+n+1)}\frac{\Gamma(\nu+\mu+n+1)}{\Gamma(\mu+n+1)}&\\ \times I_{\mu+\nu+2n+1}(z)P_n^{(\nu,\mu)}(\cos(2\alpha))P_n^{(\nu,\mu)}(\cos(2\beta)).&\end{aligned} \tag{36}$$

This will give us the following form of the Green's function (20):

$$G(\vec{\rho},\vec{\rho'};E)=\sum_{n=0}^{\infty}G_n(\rho,\rho';E)\Phi_n^{(\pm k_2,\pm k_1)}\left(\frac{\phi}{2}\right)\Phi_n^{(\pm k_2,\pm k_1)}\left(\frac{\phi'}{2}\right), \tag{37}$$

where the angular wave functions are those defined in function of the $P_n^{(\pm k_2,\pm k_1)}(\cos\phi)$ Jacobi polynomials by

$$\begin{aligned}\Phi_n^{(\pm k_2,\pm k_1)}(\phi)=&\left[2(2n\pm k_1\pm k_2+1)\frac{n!\Gamma(n\pm k_1\pm k_2+1)}{\Gamma(n\pm k_1+1)\Gamma(n\pm k_2+1)}\right]^{1/2}\\ &\times(\sin\phi)^{1/2\pm k_2}(\cos\phi)^{1/2\pm k_1}P_n^{(\pm k_2,\pm k_1)}(\cos(2\phi)).\end{aligned} \tag{38}$$

The radial Green's function $G_n(\rho,\rho';E)$ included in (37) is defined by

$$\begin{aligned}G_n(\rho,\rho';E)=&\frac{M\omega}{i\hbar}\int_0^\infty\frac{d\tau}{\sin(\omega\tau)}\exp\left[\frac{i}{\hbar}(2\alpha_0+i0)\tau\right]\\ &\times\exp\left[\frac{iM\omega}{2\hbar}(\rho+\rho')\cot(\omega\tau)\right]I_{2\lambda}\left(\frac{2M\omega\sqrt{\rho\rho'}}{i\hbar\sin(\omega\tau)}\right),\end{aligned} \tag{39}$$

with $\lambda=n+\frac{1}{2}(1\pm k_1\pm k_2)$.

Then, thanks to the formula[40]

$$\int_0^\infty dq\,\frac{e^{-2pq}}{\sinh q}\exp\left[-\frac{1}{2}(x+y)\coth q\right]I_{2\gamma}\left(\frac{\sqrt{xy}}{\sinh q}\right)=\frac{\Gamma(p+\gamma+\frac{1}{2})}{\Gamma(2\gamma+1)\sqrt{xy}}M_{-p,\gamma}(x)W_{-p,\gamma}(y), \tag{40}$$

valid for $\mathrm{Re}(p+\gamma+\frac{1}{2})>0$, $\mathrm{Re}(\gamma)>0$, and $y>x$, where $M_{-p,\gamma}(x)$ and $W_{-p,\gamma}(y)$ are the Whittaker functions, we can write (39) as follows:

$$G_n(\rho,\rho';E)=\frac{\Gamma(p+\lambda+\frac{1}{2})}{2i\omega\Gamma(2\lambda+1)\sqrt{\rho\rho'}}M_{-p,\lambda}\left(\frac{2M\omega}{\hbar}\rho'\right)W_{-p,\lambda}\left(\frac{2M\omega}{\hbar}\rho\right), \tag{41}$$

with $p=-\alpha_0/\hbar\omega$, $\omega=\sqrt{-2E/M}$, and $\rho>\rho'$.

From (41) and (37), we can deduce that the complete Green's function is given by

$$G(\vec{\rho},\vec{\rho'};E)=\sum_{n=0}^{\infty}\Phi_n^{(\pm k_2,\pm k_1)}\left(\frac{\phi}{2}\right)\Phi_n^{(\pm k_2,\pm k_1)}\left(\frac{\phi'}{2}\right)\frac{\Gamma(p+\lambda+\frac{1}{2})}{2i\omega\Gamma(2\lambda+1)\sqrt{\rho\rho'}}$$
$$\times M_{-p,\lambda}\left(\frac{2M\omega}{\hbar}\rho'\right)W_{-p,\lambda}\left(\frac{2M\omega}{\hbar}\rho\right). \tag{42}$$

The normalized wave functions and the energy spectrum of the bound states are given by expression (23) applied to $G_n(\rho,\rho';E)$ as defined in (39) provided we make the adequate change of variables and thus obtain:

$$\Psi_{m,n}(\rho,\phi)=\left[\frac{m!}{a^2(m+\lambda+\frac{1}{2})^3\Gamma(m+2\lambda+1)}\right]^{1/2}\left(\frac{2\rho}{a(m+\lambda+\frac{1}{2})}\right)^{\lambda}$$
$$\times\exp\left(-\frac{\rho}{a(m+\lambda+\frac{1}{2})}\right)L_m^{2\lambda}\left(\frac{2\rho}{a(m+\lambda+\frac{1}{2})}\right)\Phi_n^{(\pm k_2,\pm k_1)}\left(\frac{\phi}{2}\right), \tag{43}$$

$$E_{m,n}=-\frac{M\alpha_0^2}{2\hbar^2(m+\lambda+\frac{1}{2})^2}. \tag{44}$$

In order to evaluate the contribution of the continuous spectrum to the Green's function, let's write (41) as follows:

$$G_n(\rho,\rho';E)=\frac{i\hbar}{4\pi\Gamma(2\lambda+1)\sqrt{\rho\rho'}}\oint_C\frac{dz}{E+i0-\frac{\hbar^2z^2}{2M}}\Gamma(p+\lambda+\tfrac{1}{2})$$
$$\times M_{-p,\lambda}\left(\frac{2M\omega}{\hbar}\rho'\right)W_{-p,\lambda}\left(\frac{2M\omega}{\hbar}\rho\right), \tag{45}$$

where C is the closed contour,

$$C:\begin{cases}z=k;\quad k\in[-R,R],\\ z=\mathrm{Re}^{i\phi},\quad \phi\in(\pi,2\pi).\end{cases} \tag{46}$$

At the $R\to\infty$ limit, taking the asymptotic behavior of the Whittaker functions[41] into account, it is easy to demonstrate that the integral over the semicircle vanishes, which leads to

$$G_n(\rho,\rho';E)=\frac{i\hbar}{4\pi\Gamma(2\lambda+1)\sqrt{\rho\rho'}}\int_{-\infty}^{\infty}\frac{dk}{E+i0-\frac{\hbar^2k^2}{2M}}\Gamma(p+\lambda+\tfrac{1}{2})$$
$$\times M_{-p,\lambda}(-2ik\rho')W_{-p,\lambda}(-2ik\rho). \tag{47}$$

By using the following formulas[42]

$$M_{\lambda,\mu}(z)=e^{-i\pi(\mu+\frac{1}{2})}M_{-\lambda,\mu}(-z),\quad \text{with}\quad 2\mu\neq-1,-2,-3,\ldots, \tag{48}$$

and

$$M_{\lambda,\mu}(z)=\Gamma(2\mu+1)e^{i\pi\lambda}\left[\frac{W_{-\lambda,\mu}(-z)}{\Gamma(\mu-\lambda+\frac{1}{2})}+e^{-i\pi(\mu+\frac{1}{2})}\frac{W_{\lambda,\mu}(z)}{\Gamma(\mu+\lambda+\frac{1}{2})}\right], \tag{49}$$

valid for $\arg z\in]-3\pi/2,\pi/2[$, and $2\mu\neq -1,-2,-3,\ldots$, the expression (45) can be written

$$G_n(\rho,\rho';E)=\frac{i\hbar}{4\pi\Gamma^2(2\lambda+1)\sqrt{\rho\rho'}}\int_0^\infty dE_k\frac{\Psi_{k,n}(\rho)\Psi^*_{k,n}(\rho')}{E+i0-E_k} \tag{50}$$

where $E_k=\hbar^2k^2/2M$ and the radial wave functions given by

$$\Psi_{k,n}(\rho)=\left(\frac{M}{4\pi\hbar^2k}\right)^{1/2}\frac{|\Gamma(p+\lambda+\frac{1}{2})|}{\Gamma(2\lambda+1)}\frac{e^{i\pi p/2}}{\sqrt{\rho}}M_{-p,\lambda}(-2ik\rho), \tag{51}$$

with $p=-i/ak$.

B. Let us now study the potential

Let us now study the potential

$$V_2(\vec{\rho})=-\frac{\alpha_0}{\sqrt{x_1^2+x_2^2}}+\frac{\beta_1\sqrt{\sqrt{x_1^2+x_2^2}+x_1}+\beta_2\sqrt{\sqrt{x_1^2+x_2^2}-x_1}}{\sqrt{x_1^2+x_2^2}}, \tag{52}$$

with real β_1 and β_2 constants. This potential has the following three functionally independent integrals of motion:

$$\begin{aligned}H_2&=\frac{P^2}{2M}+V_2(\vec{\rho}),\quad I_1=\frac{\{L_3,P_1\}}{4M}-\frac{\alpha(\xi-\eta)+\beta_1\eta\sqrt{\xi/2}-\beta_2\xi\sqrt{\eta/2}}{\xi+\eta},\\ I_2&=\frac{\{L_3,P_1\}}{4M}-\frac{\alpha(\xi-\eta)+(\beta_1+\beta_2)(\eta\sqrt{\xi/2}-\xi\sqrt{\eta/2})}{\xi+\eta}.\end{aligned} \tag{53}$$

For given parabolic coordinates $x_1=\frac{1}{2}(\xi^2-\eta^2)$, $x_2=\xi\eta$, ($\xi>0$ and $\eta\in R$), in the Schwinger's integral representation, the Green's function associated to this potential can be expressed

$$G(\vec{\rho},\vec{\rho'};E)=\int_0^\infty dS\exp\left[\frac{iS}{\hbar}(E+i0)\right]\exp\left[-\frac{iS}{\hbar}H_2(\xi,\eta)\right]\frac{\delta(\xi-\xi')\delta(\eta-\eta')}{2\rho}, \tag{54}$$

where

$$H_2(\xi,\eta)=-\frac{\hbar^2}{2M}\frac{1}{2\rho}\left(\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}\right)-\frac{\alpha_0}{\rho}+\frac{1}{\rho}(\beta_1\xi+\beta_2\eta), \tag{55}$$

with $\rho=\frac{1}{2}(\xi^2+\eta^2)$.

If we now perform the time transformation defined by $\sigma=S/2\rho=S/(\xi^2+\eta^2)$ to separate the ξ and η variables and use the mutually orthogonal parabolic coordinates $(\tilde{\xi},\tilde{\eta})\rightarrow(\xi-(\beta_1/E),\eta-(\beta_2/E))$, we arrive at

$$G(\vec{\rho},\vec{\rho'};E)=\int_0^\infty d\sigma\exp\left[\frac{i\sigma}{\hbar}\left(2\alpha_0-\frac{\beta_1^2+\beta_2^2}{E}+i0\right)\right]K(\tilde{\xi},\tilde{\xi}';\sigma)K(\tilde{\eta},\tilde{\eta}';\sigma), \tag{56}$$

where each of kernels $K(\tilde{\xi},\tilde{\xi}';\sigma)$ and $K(\tilde{\eta},\tilde{\eta}';\sigma)$ can be treated with the so(2,1) Lie algebra and we have

$$K(x,x';\sigma)=\frac{1}{2}\sum_{\mu=0}^{1}\exp\left\{-\frac{i\sigma}{\hbar}[T_1(x)+2\hbar^2\omega^2T_3(x)]\right\}\delta(x-x')$$

$$=\sqrt{\frac{M\omega}{2i\pi\hbar\sin(\omega\sigma)}}\exp\left\{\frac{iM\omega}{2\hbar}\left[(x^2+x'^2)\cot(\omega\sigma)-\frac{2xx'}{\sin(\omega\sigma)}\right]\right\}, \tag{57}$$

with $x\equiv(\tilde{\xi}\text{ or }\tilde{\eta})$ and $\omega=\sqrt{-2E/M}$.

Substituting (57) into (56), we obtain

$$G(\vec{\rho},\vec{\rho'};E)=\frac{M\omega}{2i\pi\hbar}\int_0^\infty\frac{d\sigma}{\sin(\omega\sigma)}\exp\left[\frac{i\sigma}{\hbar}\left(2\alpha_0-\frac{\beta_1^2+\beta_2^2}{E}+i0\right)\right]$$

$$\times\exp\left\{\frac{iM\omega}{2\hbar}\left[(\tilde{\xi}^2+\tilde{\eta}^2+\tilde{\xi}'^2+\eta'^2)\cot(\omega\sigma)-\frac{2(\tilde{\xi}\tilde{\xi}'+\tilde{\eta}\tilde{\eta}')}{\sin(\omega\sigma)}\right]\right\}. \tag{58}$$

In order to determine the energy spectrum and the normalized wave functions of the bound states of the physical system, let's apply the Mehler formula[43]

$$\frac{1}{\sqrt{1-a^2}}\exp\left\{-\frac{1}{2(1-a^2)}[(x^2+x'^2)(1+a^2)-4xx'a]\right\}$$

$$=\exp\left[-\frac{1}{2}(x^2+x'^2)\right]\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{a}{2}\right)^nH_n(x)H_n(x'). \tag{59}$$

With the help of an adequate change of variables, the poles of the Green's function (58) will be obtained thanks to an integration over σ; the discrete energy spectrum is found by solving the equation

$$\omega^3-\frac{2\alpha_0}{N\hbar}\omega^2-2\frac{\beta_1^2+\beta_2^2}{NM\hbar}=0,\quad\text{or as well}\quad E_N=-\frac{M\omega_N^2}{2}, \tag{60}$$

with $N=n_1+n_2+1$. α_0 being positive, then this cubic equation has one real root:

$$\omega_N=\frac{2\alpha_0}{3N\hbar}+\lambda_1+\lambda_2, \tag{61}$$

where

$$\lambda_j=\left[\left(\frac{2\alpha_0}{3N\hbar}\right)^3+\frac{\beta_1^2+\beta_2^2}{NM\hbar}+(-1)^j\sqrt{\frac{\beta_1^2+\beta_2^2}{NM\hbar}\left(\frac{\beta_1^2+\beta_2^2}{NM\hbar}+2\left(\frac{2\alpha_0}{3N\hbar}\right)^3\right)}\right]^{1/3}; \tag{62}$$

with $(j=1,2)$.

We may obtain the normalized wave functions of the bound states from the residues of the integrated expression of the Green's function (58),

$$\Psi_{n_1,n_2}(\xi,\eta)=\frac{M}{\hbar}\left(\frac{1}{2^Nn_1!n_2!N\pi}\lim_{\omega\to\omega_N}\frac{\omega^3(\omega^2-\omega_N^2)}{\omega^3-\frac{2\alpha_0}{N\hbar}\omega^2-2\frac{\beta_1^2+\beta_2^2}{NM\hbar}}\right)^{1/2}$$

$$\times\exp\left[-\frac{M\omega_N}{2\hbar}(\tilde{\xi}^2+\tilde{\eta}^2)\right]H_{n_1}\left(\sqrt{\frac{M\omega_N}{\hbar}}\tilde{\xi}\right)H_{n_2}\left(\sqrt{\frac{M\omega_N}{\hbar}}\tilde{\eta}\right). \tag{63}$$

Here, it is obvious that only states with an even total number of oscillator quanta contribute.

To find the wave functions of the continuous states, let's go back to the Green's function (58) and make use of the following relation:

$$\frac{1}{\sqrt{2\pi\sin\alpha}}\exp(-(x+y)\cot\alpha)\exp\left(\frac{2\sqrt{xy}}{\sin\alpha}\right)$$
$$=\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty}dp\,e^{(\pi-2\alpha)p}\Bigg[\left|\Gamma\left(\frac{1}{4}+ip\right)\right|^2 E^{(0)}_{-\frac{1}{2}+2ip}$$
$$\times(e^{-i\pi/4}2\sqrt{x})E^{(0)}_{-\frac{1}{2}-2ip}(e^{i\pi/4}2\sqrt{y})+\left|\Gamma\left(\frac{3}{4}+ip\right)\right|^2 E^{(1)}_{-\frac{1}{2}+2ip}$$
$$\times(e^{-i\pi/4}2\sqrt{x})E^{(1)}_{-\frac{1}{2}-2ip}(e^{i\pi/4}2\sqrt{y})\Bigg], \tag{64}$$

which is established from the dispersion formula (28). The $E^{(0)}_{\nu}(z)$ and $E^{(1)}_{\nu}(z)$ are even and odd parabolic cylinder functions with respect to the variable z, respectively.[44] The poles of the continuous state Green's function will be obtained by integration on the τ variable. They will be given by

$$\omega(p_\xi+p_\eta)-\frac{i}{\hbar}\left(\alpha_0-\frac{\beta_1^2+\beta_2^2}{E}\right)=0. \tag{65}$$

Then, by performing the change of variables $(p_\xi,p_\eta)\rightarrow[(1/2p)((1/\tilde{a})+\varsigma),(1/2p)((1/\tilde{a})-\varsigma)]$ where $\tilde{a}=\hbar^2/M(\alpha_0-M(\beta_1^2+\beta_2^2)/\hbar^2p^2)$, it is possible to write the contribution of the continuous part to the Green's function as

$$G^c(\xi,\eta,\xi',\eta';E)=i\hbar\int_{-\infty}^{\infty}dp\int_{-\infty}^{\infty}d\varsigma\,\frac{\Psi^*_{p,\varsigma}(\xi',\eta')\Psi_{p,\varsigma}(\xi,\eta)}{E+i0-E_p}, \tag{66}$$

where $E_p=-(M\omega^2/2)=(\hbar^2p^2/2M)$, and the continuous functions $\Psi_{p,\varsigma}(\xi,\eta)$ have the form

$$\Psi_{p,\varsigma}(\xi,\eta)=\frac{e^{\pi/2\tilde{a}p}}{4\pi\sqrt{2}}\begin{pmatrix}\Gamma\left(\frac{1}{4}+\frac{i}{2p}\left(\frac{1}{\tilde{a}}+\varsigma\right)\right)E^{(0)}_{-1/2+i/p(1/\tilde{a}+\varsigma)}(e^{-i\pi/4}\sqrt{2p}\tilde{\xi})\\ \Gamma\left(\frac{3}{4}+\frac{i}{2p}\left(\frac{1}{\tilde{a}}+\varsigma\right)\right)E^{(1)}_{-1/2+i/p(1/\tilde{a}+\varsigma)}(e^{-i\pi/4}\sqrt{2p}\tilde{\xi})\end{pmatrix}$$
$$\times\begin{pmatrix}\Gamma\left(\frac{1}{4}+\frac{i}{2p}\left(\frac{1}{\tilde{a}}-\varsigma\right)\right)E^{(0)}_{-1/2+i/p(1/\tilde{a}-\varsigma)}(e^{-i\pi/4}\sqrt{2p}\tilde{\eta})\\ \Gamma\left(\frac{3}{4}+\frac{i}{2p}\left(\frac{1}{\tilde{a}}-\varsigma\right)\right)E^{(1)}_{-1/2+i/p(1/\tilde{a}-\varsigma)}(e^{-i\pi/4}\sqrt{2p}\tilde{\eta})\end{pmatrix}. \tag{67}$$

IV. THREE-DIMENSIONAL MAXIMALLY SUPER-INTEGRABLE POTENTIALS

In three-dimensional Euclidean space, Smorodinsky and co-workers have found a set of five potentials which have five functionally independent integrals of motion. These three-dimensional potentials are called maximally super-integrable potentials. At least, each potential of the so-called class of Smorodinsky–Winternitz potentials can be treated in two coordinate systems through the so(2,1) Lie algebraic approach. Here, we shall restrict ourselves to study the potential

$$V_3(\vec{r}) = -\frac{\alpha_0}{r} + \frac{\hbar^2}{2M}\left(\frac{k_1^2-\frac{1}{4}}{x_1^2} + \frac{k_2^2-\frac{1}{4}}{x_2^2}\right). \tag{68}$$

The integrals of motion are

$$H_3 = \frac{p^2}{2M} + V_3(\vec{r}), \quad I_1 = \frac{L_3^2}{2M} + \frac{\hbar^2}{2M}\left(\frac{k_1^2-\frac{1}{4}}{\cos^2\phi} + \frac{k_2^2-\frac{1}{4}}{\sin^2\phi}\right),$$

$$I_2 = \frac{L_2^2}{2M} + \frac{\hbar^2}{2M}\frac{k_1^2-\frac{1}{4}}{\tan^2\theta\cos^2\phi}, \quad I_3 = \frac{\vec{L}^2}{2M} + \frac{\hbar^2}{2M\sin^2\theta}\left(\frac{k_1^2-\frac{1}{4}}{\cos^2\phi} + \frac{k_2^2-\frac{1}{4}}{\sin^2\phi}\right), \tag{69}$$

$$I_4 = \frac{1}{4M}(I_{x_1x_2} + I_{x_2x_1}) - (\xi-\eta)\left[\frac{\alpha}{\xi+\eta} - \frac{\hbar^2}{2M\xi\eta}\left(\frac{k_1^2-\frac{1}{4}}{\cos^2\phi} + \frac{k_2^2-\frac{1}{4}}{\sin^2\phi}\right)\right],$$

where $I_{ij} = \{L_i, P_j\} = L_iP_j + P_jL_i$ with $(i,j) \equiv (x_1, x_2, x_3)$.

This potential is a generalization of the Coulomb potential analyzed by various authors in the path integral[45–56] and algebraic approach[57,58] contexts. As it features singularities for $x_1 = 0$ and $x_2 = 0$, all we need is to discuss it in the $0 < x_1,\ x_2 < \infty$ and $x_3 \in R$ area. It is possible to evaluate the Green's function

$$G(\vec{r},\vec{r'};E) = \int_0^\infty dS \exp\left[-\frac{iS}{\hbar}(H_3 - E - i0)\right]\delta(\vec{r}-\vec{r'}) \tag{70}$$

in parabolic and spherical coordinates.

A. Parabolic coordinates

For given parabolic coordinates $x_1 = \xi\eta\cos\phi$, $x_2 = \xi\eta\sin\phi$, $x_3 = \frac{1}{2}(\xi^2 - \eta^2)$, $\xi, \eta > 0$ and $0 \leqslant \phi < 2\pi$, the Green's function (70) can be written

$$G(\vec{r},\vec{r'};E) = \int_0^\infty dS \exp\left[-\frac{iS}{\hbar}(\tilde{H}_3 - E - i0)\right]\frac{\delta(\xi-\xi')\delta(\eta-\eta')\delta(\phi-\phi')}{\xi\eta(\xi^2+\eta^2)}, \tag{71}$$

with

$$\tilde{H}_3 = -\frac{\hbar^2}{2M}\left[\frac{1}{\xi^2+\eta^2}\left(\frac{\partial^2}{\partial\xi^2} + \frac{1}{\xi}\frac{\partial}{\partial\xi} + \frac{\partial^2}{\partial\eta^2} + \frac{1}{\eta}\frac{\partial}{\partial\eta}\right) + \frac{1}{\xi^2\eta^2}\frac{\partial^2}{\partial\phi^2}\right] - \frac{2\alpha_0}{\xi^2+\eta^2}$$
$$+ \frac{\hbar^2}{2M}\frac{1}{\xi^2\eta^2}\left(\frac{k_1^2-\frac{1}{4}}{\cos^2\phi} + \frac{k_2^2-\frac{1}{4}}{\sin^2\phi}\right). \tag{72}$$

Separating the angular part of the expression (71) by a time transformation defined by $\tau = S/\xi^2\eta^2$, we can deduce that

$$G(\vec{r},\vec{r'},E) = \int_0^\infty d\tau K(\xi,\eta,\xi',\eta';\tau)K(\phi,\phi';\tau), \tag{73}$$

where

$$K(\xi,\eta,\xi',\eta';\tau) = \exp\left\{-\frac{i\tau}{\hbar}[H_3(\xi,\eta) - E\xi^2\eta^2 - i0]\right\}\frac{\xi\eta}{\xi^2+\eta^2}\delta(\xi-\xi')\delta(\eta-\eta'), \tag{74}$$

and

$$K(\phi,\phi';\tau)=\exp\left\{-\frac{i\tau}{\hbar}\frac{\hbar^2}{2M}\left(-\frac{\partial^2}{\partial\phi^2}+\frac{k_1^2-\frac{1}{4}}{\cos^2\phi}+\frac{k_2^2-\frac{1}{4}}{\sin^2\phi}\right)\right\}\delta(\phi-\phi')$$
$$=\sum_{n=0}^{\infty}\Phi_n^{(\pm k_2,\pm k_1)}(\phi)\Phi_n^{(\pm k_2,\pm k_1)}(\phi')\exp\left(-\frac{i}{\hbar}\frac{\hbar^2\lambda_1^2}{2M}\tau\right), \tag{75}$$

with $\lambda_1=2n\pm k_1\pm k_2+1$.

It is to be noted that the explicit construction of the kernel $K(\phi,\phi';\tau)$ thanks to the (MS) variant of the algebraic technique is being investigated and will be the subject of our forthcoming publication.

Introducing (75) into (73) and applying the $\tau\rightarrow S$ inverse time transformation will allow us to write (73) as follows:

$$G(\vec{r},\vec{r'};E)=\sum_{n=0}^{\infty}\Phi_n^{(\pm k_2,\pm k_1)}(\phi)\Phi_n^{(\pm k_2,\pm k_1)}(\phi')\int_0^{\infty}dS\exp\left[\frac{iS}{\hbar}(E-i0)\right]$$
$$\times\exp\left\{-\frac{iS}{\hbar}[\tilde{H}_3(\xi,\eta)]\right\}\frac{\delta(\xi-\xi')\delta(\eta-\eta')}{\xi\eta(\xi^2+\eta^2)}, \tag{76}$$

where

$$\tilde{H}_3(\xi,\eta)=-\frac{\hbar^2}{2M}\frac{1}{\xi^2+\eta^2}\left(\frac{\partial^2}{\partial\xi^2}+\frac{1}{\xi}\frac{\partial}{\partial\xi}+\frac{\partial^2}{\partial\eta^2}+\frac{1}{\eta}\frac{\partial}{\partial\eta}\right)-\frac{2\alpha_0}{\xi^2+\eta^2}+\frac{\hbar^2\lambda_1^2}{2M\xi^2\eta^2}. \tag{77}$$

If we now eliminate the $(1/\xi)(\partial/\partial\xi)$ and $(1/\eta)(\partial/\partial\eta)$ operators by applying $(\partial^2/\partial\xi^2)+(1/\xi)(\partial/\partial\xi)$ and $(\partial^2/\partial\eta^2)+(1/\eta)(\partial/\partial\eta)$ on $\delta(\xi-\xi')/\sqrt{\xi\xi'}$ and $\delta(\eta-\eta')/\sqrt{\eta\eta'}$, respectively, we can then proceed with a new $S\rightarrow\sigma$ time transformation defined by $\sigma=S/(\xi^2+\eta^2)$, which will allow us to write

$$G(\vec{r},\vec{r'};E)=\sum_{n=0}^{\infty}\Phi_n^{(\pm k_2,\pm k_1)}(\phi)\Phi_n^{(\pm k_2,\pm k_1)}(\phi')\int_0^{\infty}d\sigma\exp\left[\frac{i}{\hbar}(2\alpha_0+i0)\sigma\right]$$
$$\times K_n(\xi,\xi';\sigma)K_n(\eta,\eta';\sigma), \tag{78}$$

with

$$K_n(u,u';\sigma)=\frac{1}{\sqrt{uu'}}\exp\left\{-\frac{i\sigma}{\hbar}\left[-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial u^2}-\frac{\lambda_1^2-\frac{1}{4}}{u^2}\right)-Eu^2\right]\right\}\delta(u-u'), \tag{79}$$

where $u\equiv(\xi$ or $\eta)$.

So, it is possible to give the kernel (79) in function of the so(2,1) Lie algebra operators. Indeed, by following the equations (2) and (13), we obtain

$$K_n(u,u';\sigma)=\frac{1}{\sqrt{uu'}}\exp\left\{-\frac{i\sigma}{\hbar}[T_1(u)+2\hbar^2\omega^2T_3(u)]\right\}\delta(u-u')$$
$$=\frac{M\omega}{i\hbar\sin(\omega\sigma)}\exp\left[\frac{iM\omega}{2\hbar}(u^2+u'^2)\cot(\omega\sigma)\right]I_{\lambda_1}\left(\frac{M\omega uu'}{i\hbar\sin(\omega\sigma)}\right), \tag{80}$$

with $\omega=\sqrt{-2E/M}$. The Green's function (78) can now be written

$$G(\vec{r},\vec{r'};E)=\sum_{n=0}^{\infty}\Phi_n^{(\pm k_2,\pm k_1)}(\phi)\Phi_n^{(\pm k_2,\pm k_1)}(\phi')G_n(\xi,\eta,\xi',\eta';E), \tag{81}$$

with

$$\begin{aligned}G_n(\xi,\eta,\xi',\eta';E)=&\left(\frac{M\omega}{i\hbar}\right)^2\int_0^{\infty}\frac{d\sigma}{\sin^2(\omega\sigma)}\exp\left[\frac{i}{\hbar}(2\alpha_0+i0)\sigma\right]\\&\times\exp\left[\frac{iM\omega}{2\hbar}(\xi^2+\eta^2+\xi'^2+\eta'^2)\cot(\omega\sigma)\right]\\&\times I_{\lambda_1}\left(\frac{M\omega\xi\xi'}{i\hbar\sin(\omega\sigma)}\right)I_{\lambda_1}\left(\frac{M\omega\eta\eta'}{i\hbar\sin(\omega\sigma)}\right).\end{aligned} \tag{82}$$

Thanks to the Hille and Hardy formula (23) for the discrete part and thanks to the scattering relation (28) for the continuous part, the Green's function (81) can be developed into partial waves as follows:

$$\begin{aligned}G(\vec{r},\vec{r'};E)=i\hbar\sum_{n=0}^{\infty}\Bigg\{&\sum_{n_1,n_2=0}^{\infty}\frac{\Psi_{n_1n_2,n}(\xi,\eta,\phi)\Psi^*_{n_1,n_2,n}(\xi',\eta',\phi')}{E+i0-E_N}\\&+\int_0^{\infty}dp\int_{-\infty}^{\infty}d\kappa\,\frac{\Psi_{p,\kappa,n}(\xi,\eta,\phi)\Psi^*_{p,\kappa,n}(\xi',\eta',\phi')}{E+i0-E_p}\Bigg\}.\end{aligned} \tag{83}$$

Hence, for bound states, the normalized wave functions and energy spectrum will be

$$\begin{aligned}\Psi_{n_1,n_2,n}(\xi,\eta,\phi)=&\left[\frac{2}{a^3N^4}\frac{n_1!n_2!}{\Gamma(n_1+\lambda_1+1)\Gamma(n_2+\lambda_2+1)}\right]^{1/2}\left(\frac{\xi\eta}{aN}\right)^{\lambda_1}\\&\times\exp\left(-\frac{\xi^2+\eta^2}{2aN}\right)L_{n_1}^{\lambda_1}\left(\frac{\xi^2}{aN}\right)L_{n_2}^{\lambda_1}\left(\frac{\eta^2}{aN}\right)\Phi_n^{(\pm k_2,\pm k_1)}(\phi),\end{aligned} \tag{84}$$

$$E_N=-\frac{M\alpha_0^2}{2\hbar^2N^2},\quad N=n_1+n_2+\lambda_1+1, \tag{85}$$

and, for the continuous states, the normalized wave functions and the energy spectrum will be

$$\begin{aligned}\Psi_{p,\kappa,n}(\xi,\eta,\phi)=&\frac{\left|\Gamma\left(\frac{1}{2}+\frac{\lambda_1}{2}+\frac{i}{2p}\left(\frac{1}{a}+\kappa\right)\right)\Gamma\left(\frac{1}{2}+\frac{\lambda_1}{2}+\frac{i}{2p}\left(\frac{1}{a}-\kappa\right)\right)\right|}{2\pi\Gamma^2(\lambda_1+1)\xi\eta}\\&\times\frac{e^{\pi/2ap}}{\sqrt{p}}M_{-i/2p[(1/a)+\kappa],(\lambda_1/2)}(-ip\xi^2)M_{-i/2p[(1/a)-\kappa],\lambda_1/2}(-ip\eta^2)\\&\times\Phi_n^{(\pm k_2,\pm k_1)}(\phi),\end{aligned} \tag{86}$$

$$E_p=\frac{\hbar^2p^2}{2M}. \tag{87}$$

B. Spherical coordinates

To study the problem in this coordinate system, we shall use the expression of the partial Green's function (82) and use the following change of variables:

$$(\xi,\eta)\to\left(\sqrt{2r}\cos\frac{\theta}{2},\sqrt{2r}\sin\frac{\theta}{2}\right). \tag{88}$$

The partial Green's function (86) then can be written

$$\begin{aligned}G_n(r,\theta,r',\theta';E)=&\sum_{m=0}^{\infty}(m+\lambda_1+\tfrac{1}{2})\frac{\Gamma(m+2\lambda_1+1)}{m!}P_{m+\lambda_1}^{-\lambda_1}(\cos\theta)\\&\times P_{m+\lambda_1}^{-\lambda_1}(\cos\theta')\int_0^{\infty}\frac{d\sigma}{\sin(\omega\sigma)}\exp\left[\frac{i}{\hbar}(2\alpha+i0)\sigma\right]\\&\times\exp\left[\frac{iM\omega}{\hbar}(r+r')\cot(\omega\sigma)\right]I_{2m+2\lambda_1+1}\left(\frac{2M\omega\sqrt{rr'}}{i\hbar\sin(\omega\sigma)}\right).\end{aligned} \tag{89}$$

We have used here the addition theorem (36), the connection between hypergeometric functions and the Jacobi polynomials[59]

$${}_2F_1\left(l+\alpha+\beta+1,-l;1+\alpha;\frac{1-t}{2}\right)=\frac{l!\Gamma(\alpha+1)}{\Gamma(l+\alpha+1)}P_l^{(\alpha,\beta)}(t), \tag{90}$$

as well as the relation between the hypergeometric functions and the Legendre polynomials,[60] and eventually the link between $P_\nu^{-m}(x)$ and $P_\nu^m(x)$ (Ref. 61).

In order to perform the integration on the σ time variable, we shall use the formula (40). Consequently, the final expression of the Green's function in spherical coordinates will be

$$\begin{aligned}G(\vec{r},\vec{r'};E)=&\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\left(m+\lambda_1+\frac{1}{2}\right)\frac{\Gamma(m+\lambda_1+1)}{m!}\frac{\Gamma(p+m+\lambda_1+1)}{\Gamma(2m+2\lambda_1+2)}\\&\times\frac{1}{i\omega rr'}M_{-p,m+\lambda_1+\frac{1}{2}}\left(\frac{2M\omega}{\hbar}r'\right)W_{-p,m+\lambda_1+\frac{1}{2}}\left(\frac{2M\omega}{\hbar}r\right)\\&\times P_{m+\lambda_1}^{-\lambda_1}(\cos\theta)P_{m+\lambda_1}^{-\lambda_1}(\cos\theta')\Phi_n^{(\pm k_2,\pm k_1)}(\phi)\Phi_n^{(\pm k_2,\pm k_1)}(\phi'),\end{aligned} \tag{91}$$

where $r>r'$ and $p=-\alpha_0/\hbar\omega$.

The Hille and Hardy formula (23) and an analytic proceeding consisting in using the Sommerfeld-Watson transformation[62] will help us to write the Green's function (91) in the form of a partial wave development consisting of two contributions of a discrete and a continuous part:

$$\begin{aligned}G(\vec{r},\vec{r'};E)=i\hbar\sum_{n,m=0}^{\infty}\Bigg\{&\sum_{l=0}^{\infty}\frac{\Psi_{l,m,n}(r,\theta,\phi)\Psi_{l,m,n}^*(r',\theta',\phi')}{E+i0-E_N}\\&+\int_0^{\infty}dk\frac{\Psi_{k,m,n}(r,\theta,\phi)\Psi_{k,m,n}^*(r',\theta',\phi')}{E+i0-\dfrac{\hbar^2k^2}{2M}}\Bigg\},\end{aligned} \tag{92}$$

with, for bound states, the poles located around the values of E and the normalized wave functions, respectively, given by

$$E_N=-\frac{M\alpha_0^2}{2\hbar^2N^2},\quad N=l+m+\lambda_1+1, \tag{93}$$

$$\Psi_{l,m,n}(r,\theta,\phi)=\left[\frac{(m+\lambda_1+\frac{1}{2})l!\Gamma(m+\lambda_1+1)}{a^3(l+\lambda_2+\frac{1}{2})^4 m!\Gamma(l+2\lambda_2+1)}\right]^{1/2}\left(\frac{2r}{a(l+\lambda_2+\frac{1}{2})}\right)^{\lambda_2-\frac{1}{2}}$$
$$\times\exp\left(-\frac{r}{a(l+\lambda_2+\frac{1}{2})}\right)L_l^{2\lambda_2}\left(\frac{2r}{a(l+\lambda_2+\frac{1}{2})}\right)$$
$$\times P_{m+\lambda_1}^{-\lambda_1}(\cos\theta)\Phi_n^{(\pm k_2,\pm k_1)}(\phi). \tag{94}$$

For continuous states, the normalized wave functions and energy spectrum are, respectively, given by

$$\Psi_{k,m,n}(r,\theta,\phi)=\frac{1}{\sqrt{2\pi}}\left[\left(m+\lambda_1+\frac{1}{2}\right)\frac{\Gamma(m+\lambda_1+1)}{m!}\right]^{1/2}\frac{\left|\Gamma\left(\frac{1}{2}+\lambda_2-\frac{i}{ak}\right)\right|}{\Gamma(2\lambda_2+1)}$$
$$\times\frac{e^{\pi/2ak}}{r}M_{(i/ak),\lambda_2}(-2ikr)P_{m+\lambda_1}^{-\lambda_1}(\cos\theta)\Phi_n^{(\pm k_2,\pm k_1)}(\phi). \tag{95}$$

V. THREE-DIMENSIONAL MINIMALLY SUPER-INTEGRABLE POTENTIALS

There are nine three-dimensional potentials which belong to the class of minimally super-integrable Smorodinsky–Winternitz potentials, that is to say three-dimensional potentials characterized by the existence of four functionally independent integrals of motion. Among them are seven potentials which have SO(2,1) as a dynamical group and thus their exact solution can be given via the (MS) variant of the algebraic approach in different coordinate systems. As an example, we shall discuss the potential

$$V_4(\vec{r})=-\frac{\alpha_0}{r}+\frac{\hbar^2}{2M(x_1^2+x_2^2)}\left(\frac{k_1^2x_3}{r}+F\left(\frac{x_2}{x_1}\right)\right), \tag{96}$$

with k_1 a positive constant. The corresponding observables have the form

$$H_4=\frac{\vec{P}^2}{2M}+V_4(\vec{r}),\quad I_1=\frac{L_z^2}{2M}+F(\tan\phi),\quad I_2=\frac{P_z^2}{2M}+\frac{\hbar^2}{2M}\frac{k_1^2\cos\theta+F(\tan\phi)}{\sin^2\theta},$$
$$I_3=\frac{1}{4M}(I_{x_1x_2}+I_{x_2x_1})-\alpha_0\frac{\xi-\eta}{\xi+\eta}+\frac{\hbar^2}{2M}\left(\frac{1}{\eta}-\frac{1}{\xi}\right)(k_1^2+F(\tan\phi)), \tag{97}$$

where $I_{ij}=\{L_i,P_j\}=L_iP_j+P_jL_i$ with $(i,j)\equiv(x_1,x_2,x_3)$.

The Green's function for this potential can be explicitly evaluated in the parabolic and spherical coordinate systems. For $F(y/x)=\gamma^2$ and γ a real constant, this potential reduces to the ring-shaped potential proposed by Hartmann as a model for the ring-shaped molecules. It has been analyzed by many authors in the framework of path integrals[63–67] and through the algebraic approach.[68–75] We can also notice the close link of the latter with the Coulomb potential plus the barrier created by the solenoid of Aharonov–Bohm[76] treated with the path integrals[77–79] and via the algebraic technique[80]. To give the solution for the potential (96) via the (MS) variant of the so(2,1) algebraic approach, we will use the Kustaanheimo–Stiefel transformation[81] $\{x_1,x_2,x_3\}\rightarrow\{u_j,j\in[1,4]\}$ corresponding to the surjection $R^4\rightarrow R^3$, which can be defined as

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = (A) \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix}, \quad (A) = \begin{pmatrix} u_3 & u_4 & u_1 & u_2 \\ -u_4 & u_3 & u_2 & -u_1 \\ -u_1 & -u_2 & u_3 & u_4 \\ -u_2 & u_1 & -u_4 & u_3 \end{pmatrix} \tag{98}$$

with the constraint

$$dx_4 = 2(-u_2\,du_1 + u_1\,du_2 - u_4\,du_3 + u_3\,du_4) = 0, \tag{99}$$

allowing to define a fourth coordinate

$$x_4 = 2\int^s (-u_2\dot{u}_1 + u_1\dot{u}_2 - u_4\dot{u}_3 + u_3\dot{u}_4)ds. \tag{100}$$

Moreover, we can show that

$$\begin{pmatrix} \dfrac{\partial}{\partial x_1} \\ \dfrac{\partial}{\partial x_2} \\ \dfrac{\partial}{\partial x_3} \\ \dfrac{1}{2r}\dfrac{\partial}{\partial x_4} \end{pmatrix} = \frac{1}{2r}(A) \begin{pmatrix} \dfrac{\partial}{\partial u_1} \\ \dfrac{\partial}{\partial u_2} \\ \dfrac{\partial}{\partial u_3} \\ \dfrac{\partial}{\partial u_4} \end{pmatrix}. \tag{101}$$

The (KS) transformation allows us to write the Laplacian $\vec{\nabla}^2$ in R^3 in terms of the Laplacian $\Box^2$ in R^4 as

$$\vec{\nabla}^2 = \frac{1}{4r}\Box^2 - \frac{1}{4r^2}\frac{\partial^2}{\partial x_4^2}, \quad \Box^2 = \sum_{j=1}^{4} \frac{\partial^2}{\partial u_j^2}, \tag{102}$$

where $r = (x_1^2 + x_2^2 + x_3^2)^{\frac{1}{2}} = u_1^2 + u_2^2 + u_3^2 + u_4^2$.

Using the Schwinger's integral representation, the Green's function relative to the potential $V_4(\vec{r})$ is written

$$G(\vec{r},\vec{r'};E) = \int_0^\infty dS \exp\left\{ -\frac{iS}{\hbar}\left[-\frac{\hbar^2}{2M}\vec{\nabla}^2 + V_4(\vec{r}) - E - i0 \right] \right\} \delta(\vec{r} - \vec{r'}). \tag{103}$$

It is possible to introduce an additional variable x_4 by means of the well-known identity

$$\int_{-\infty}^{\infty} \exp\left[\frac{i}{\hbar}\left(\frac{\hbar^2 S}{8Mr^2}\frac{\partial^2}{\partial x_4^2} \right) \right] \delta(x_4)\,dx_4 = 1, \tag{104}$$

and to show that expression (103) can be written as

$$G(\vec{r},\vec{r'};E) = \int_{-\infty}^{\infty} dx_4\, G(\vec{r},x_4,\vec{r'},0;E), \tag{105}$$

where

$$G(\vec{r},x_4,\vec{r'},0;E)=4r\int_0^\infty dS\,\exp\left\{-\frac{iS}{\hbar}[H_T-E-i0]\right\}\delta(\vec{r}-\vec{r'})\,\delta(x_4), \tag{106}$$

with

$$H_T=-\frac{\hbar^2}{2M}\left(\vec{\nabla}^2+\frac{1}{2r^2}\frac{\partial^2}{\partial x_4^2}\right)+V_4(\vec{r}). \tag{107}$$

Using (102) and (98), the Jacobian of this transformation given by $\partial(x_1,x_2,x_3,x_4)/\partial(u_1,u_2,u_3,u_4)=16r^2$, and the time transformation $\tau=S/4r$, the Green's function (106) can be set in the form

$$G(\vec{r},x_4,\vec{r'},0;E)=\frac{1}{4r}\int_0^\infty d\tau\,\exp\left[\frac{i}{\hbar}(4\alpha_0+i0)\tau\right]\exp\left\{-\frac{i\tau}{\hbar}\left[-\frac{\hbar^2}{2M}\Box^2+V(u)\right]\right\}\prod_{j=1}^{4}\delta(u_j-u_j'), \tag{108}$$

where

$$V(u)=\frac{\hbar^2k_1^2}{2M}\left(\frac{1}{u_1^2+u_2^2}-\frac{1}{u_3^2+u_4^2}\right)+\frac{\hbar^2}{2M}\left(\frac{1}{u_1^2+u_2^2}+\frac{1}{u_3^2+u_4^2}\right)F\left(\frac{u_2u_3-u_1u_4}{u_1u_3+u_2u_4}\right)-4Er. \tag{109}$$

The evaluation of this expression is possible in two coordinate systems.

A. Parabolic coordinates

Going on to the double polar coordinates

$$\begin{aligned}(u_1,u_2)\to(\eta,\phi_1):u_1&=\frac{\eta}{\sqrt{2}}\cos\phi_1,\quad u_2=\frac{\eta}{\sqrt{2}}\sin\phi_1,\\ (u_3,u_4)\to(\xi,\phi_2):u_3&=\frac{\xi}{\sqrt{2}}\cos\phi_2,\quad u_4=\frac{\xi}{\sqrt{2}}\sin\phi_2,\end{aligned} \tag{110}$$

the Green's function (108) becomes

$$\begin{aligned}G(\vec{r},x_4,\vec{r'},0;E)=\frac{1}{2r}\int_0^\infty d\tau\,\exp\left[\frac{i}{\hbar}(2\alpha_0+i0)\tau\right]\exp\left[-\frac{i\tau}{\hbar}H_p\right]\\ \times\frac{\delta(\xi-\xi')\delta(\eta-\eta')}{\sqrt{\xi\xi'\eta\eta'}}\,\delta(\phi_1-\phi_1')\delta(\phi_2-\phi_2'),\end{aligned} \tag{111}$$

where

$$H_p=-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}+\frac{1}{\xi}\frac{\partial}{\partial\xi}+\frac{1}{\eta}\frac{\partial}{\partial\eta}+\frac{1}{\xi^2}\frac{\partial^2}{\partial\phi_1^2}+\frac{1}{\eta^2}\frac{\partial^2}{\partial\phi_2^2}\right)+V_p, \tag{112}$$

with

$$V_p=-\frac{\hbar^2k_1^2}{2M}\left(\frac{1}{\xi^2}-\frac{1}{\eta^2}\right)+\frac{\hbar^2}{2M}\left(\frac{1}{\xi^2}+\frac{1}{\eta^2}\right)F(\tan(\phi_1-\phi_2)-E(\xi^2+\eta^2). \tag{113}$$

Here we have applied the rescaling of 2τ to τ.

At this point, we notice that the separation of variables is not possible. To achieve it, it is necessary to perform the integration on the variable x_4 by using the Euler's angles $\phi_1=(\alpha+\phi)/2$, $\phi_2=(\alpha-\phi)/2$, $(0\leqslant\phi<2\pi, 0\leqslant\alpha<4\pi)$.

Then, it is easy to see that $dx_4=r\,d\alpha$ and that by integration over α we are led to $4\pi\delta_{\nu,0}$. It follows that the Green's function (103) can be written

$$G(\vec{r},\vec{r'};E)=\int_0^\infty d\tau\exp\left[\frac{i}{\hbar}(2\alpha_0+i0)\tau\right]K_{\xi\eta}(\phi,\phi';\tau)K(\xi,\eta,\xi',\eta';\tau), \tag{114}$$

where

$$K_{\xi\eta}(\phi,\phi';\tau)=\exp\left\{-\frac{i\tau}{\hbar}\frac{\hbar^2}{2M}\left(\frac{1}{\xi^2}+\frac{1}{\eta^2}\right)\left[-\frac{\partial^2}{\partial\phi^2}+F(\tan\phi)\right]\right\}\delta(\phi-\phi') \tag{115}$$

and

$$K(\xi,\eta,\xi',\eta';\tau)=\frac{1}{\sqrt{\xi\xi'\eta\eta'}}\exp\left[-\frac{i\tau}{\hbar}H(\xi,\eta)\right]\delta(\xi-\xi')\delta(\eta-\eta'), \tag{116}$$

with

$$H(\xi,\eta)=-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial\xi^2}+\frac{\partial^2}{\partial\eta^2}\right)-\frac{\hbar^2}{2M}\left(k_1^2-\frac{1}{4}\right)\left(\frac{1}{\xi^2}-\frac{1}{\eta^2}\right)-4E(\xi^2+\eta^2). \tag{117}$$

In order to bring to a constant the mass appearing in the Hamiltonian contained the kernel to expression (115) let's perform the time transformation $\tau\rightarrow\sigma$ defined by $\sigma=\tau[(1/\xi^2)+(1/\eta^2)]$. Then, it follows that

$$\begin{aligned}K_{\xi\eta}(\phi,\phi';\tau)&=\exp\left\{-\frac{i\sigma}{\hbar}\frac{\hbar^2}{2M}\left[-\frac{\partial^2}{\partial\phi^2}+F(\tan\phi)\right]\right\}\delta(\phi-\phi')\\&=\int dE_{\lambda_\phi}\exp\left[-\frac{i}{\hbar}\left(\frac{1}{\xi^2}+\frac{1}{\eta^2}\right)E_{\lambda_\phi}\tau\right]\Psi_{\lambda_\phi}(\phi)\Psi^*_{\lambda_\phi}(\phi'),\end{aligned} \tag{118}$$

with $E_{\lambda_\phi}=\hbar^2\lambda_\phi^2/2M$. Here, we have assumed that the propagator associated with the potential $F(\tan\phi)$ is known.

Let's now insert (118) and (116) in the expression (114), we obtain

$$\begin{aligned}G(\vec{r},\vec{r'};E)=&\int dE_{\lambda_\phi}\Psi_{\lambda_\phi}(\phi)\Psi^*_{\lambda_\phi}(\phi')\frac{1}{\sqrt{\xi\eta\xi'\eta'}}\int_0^\infty d\tau\exp\left[\frac{i}{\hbar}(2\alpha_0+i0)\tau\right]\\&\times K(\xi,\xi';\tau)K(\eta,\eta';\tau),\end{aligned} \tag{119}$$

where

$$\begin{aligned}K(u,u';\tau)&=\exp\left\{-\frac{i\tau}{\hbar}\left[-\frac{\hbar^2}{2M}\left(\frac{\partial^2}{\partial u^2}-\frac{\lambda_\phi^2\mp k_1^2-\frac{1}{4}}{u^2}\right)-Eu^2\right]\right\}\delta(u-u')\\&=\exp\left\{-\frac{i\tau}{\hbar}[T_1(u)+2\hbar^2\omega^2T_3(u)]\right\}\delta(u-u');(u\equiv\xi,\eta),\end{aligned} \tag{120}$$

with $\omega=\sqrt{-2E/M}$.

Following formula (13), the kernels (120) are written

$$K(u,u';\tau)=\frac{M\omega}{i\hbar\sin(\omega\tau)}\exp\left[\frac{iM\omega}{2\hbar}(u^2+u'^2)\cot(\omega\tau)\right]I_{\lambda_{\mp}}\left(\frac{M\omega uu'}{i\hbar\sin(\omega\tau)}\right), \tag{121}$$

with $\lambda_{\mp}=\sqrt{\lambda_{\phi}^2\mp k_1^2}$.

Inserting (121) into (114) and by a procedure similar to that which has led to result (83), we obtain

$$G(\vec{r},\vec{r'};E)=i\hbar\int dE_{\lambda_\phi}\left\{\sum_{n_1,n_2=0}^{\infty}\frac{\Psi_{n_1,n_2,\lambda_\phi}(\xi,\eta,\phi)\Psi^*_{n_1,n_2,\lambda_\phi}(\xi',\eta',\phi')}{E+i0-E_N}\right.$$
$$\left.+\int_0^\infty dp\int_{-\infty}^{\infty}d\varsigma\frac{\Psi_{p,\varsigma,\lambda_\phi}(\xi,\eta,\phi)\Psi^*_{p,\varsigma,\lambda_\phi}(\xi',\eta',\phi')}{E+i0-E_p}\right\}, \tag{122}$$

with the normalized wave functions and the energy spectrum for the bound states,

$$\Psi_{n_1,n_2,\lambda_\phi}(\xi,\eta,\phi)=\left[\frac{2}{a^3N^4}\frac{n_1!n_2!}{\Gamma(n_1+\lambda_-+1)\Gamma(n_2+\lambda_++1)}\right]^{1/2}\left(\frac{\xi}{aN}\right)^{\lambda_-/2}\left(\frac{\eta}{aN}\right)^{\lambda_+/2}$$
$$\times\exp\left(-\frac{\xi^2+\eta^2}{2aN}\right)L_{n_1}^{\lambda_-}\left(\frac{\xi^2}{aN}\right)L_{n_2}^{\lambda_+}\left(\frac{\eta^2}{aN}\right)\Psi_{\lambda_\phi}(\phi), \tag{123}$$

$$E_N=-\frac{M\alpha_0^2}{2\hbar^2N^2},\quad N=n_1+n_2+\tfrac{1}{2}(\lambda_-+\lambda_+)+1, \tag{124}$$

for the continuous states,

$$\Psi_{p,\varsigma,\lambda_\phi}(\xi,\eta,\phi)=\frac{\left|\Gamma\left(\frac{1}{2}(1+\lambda_+)+\frac{i}{2p}\left(\frac{1}{a}+\varsigma\right)\right)\Gamma\left(\frac{1}{2}(1+\lambda_-)+\frac{i}{2p}\left(\frac{1}{a}-\varsigma\right)\right)\right|}{2\pi\Gamma(1+\lambda_+)\Gamma(1+\lambda_-)}$$
$$\times\frac{e^{\pi/2ap}}{\sqrt{p}\xi\eta}M_{-(i/2p)[(1/a)+\varsigma],(\lambda_-/2)}(-ip\xi^2)$$
$$\times M_{-(i/2p)[(1/a)-\varsigma],(\lambda_+/2)}(-ip\eta^2)\times\Psi_{\lambda_\phi}(\phi), \tag{125}$$

$$E_p=\frac{\hbar^2p^2}{2M}. \tag{126}$$

B. Spherical coordinates

With the help of the change of variables defined by

$$(\xi,\eta)\rightarrow\left(\sqrt{2r}\cos\frac{\theta}{2},\sqrt{2r}\sin\frac{\theta}{2}\right), \tag{127}$$

and by applying the Bateman's expansion formula (26), expression (119) is rewritten

$$G(\vec{r},\vec{r'};E)=\int dE_{\lambda_\phi}\Psi_{\lambda_\phi}(\phi)\Psi^{*}_{\lambda_\phi}(\phi')\sum_{n=0}^{\infty}\Phi_n^{(\lambda_+,\lambda_-)}\left(\frac{\theta}{2}\right)$$
$$\times\Phi_n^{(\lambda_+,\lambda_-)}\left(\frac{\theta'}{2}\right)\frac{1}{\sqrt{\sin\theta\sin\theta'}}\int_0^{\infty}d\tau\frac{M\omega}{i\hbar\sin(\omega\tau)}\exp\left[\frac{i}{\hbar}(2\alpha_0+i0)\tau\right]$$
$$\times\exp\left[\frac{iM\omega}{\hbar}(r+r')\cot(\omega\tau)\right]I_{2n+\lambda_++\lambda_-+1}\left(\frac{2M\omega\sqrt{rr'}}{i\hbar\sin(\omega\tau)}\right). \tag{128}$$

Performing the integration over the time variable τ with the help of formula (30), we obtain the following final form:

$$G(\vec{r},\vec{r'};E)=\int dE_{\lambda_\phi}\Psi_{\lambda_\phi}(\phi)\Psi^{*}_{\lambda_\phi}(\phi')\sum_{n=0}^{\infty}\frac{1}{\sqrt{\sin\theta\sin\theta'}}\Phi_n^{(\lambda_+,\lambda_-)}\left(\frac{\theta}{2}\right)$$
$$\times\Phi_n^{(\lambda_+,\lambda_-)}\left(\frac{\theta'}{2}\right)\frac{1}{2i\omega rr'}\frac{\Gamma(p+n+\frac{1}{2}(\lambda_++\lambda_-)+1)}{\Gamma(2n+\lambda_++\lambda_-+2)}$$
$$\times M_{-p,n+\frac{1}{2}(\lambda_++\lambda_-+1)}\left(\frac{2M\omega}{\hbar}r'\right)W_{-p,n+\frac{1}{2}(\lambda_++\lambda_-+1)}\left(\frac{2M\omega}{\hbar}r\right), \tag{129}$$

where $r>r'$ and $p=-\alpha_0/\hbar\omega$.

Following the calculation procedure in Sec. IV B, one shows that

$$G(\vec{r},\vec{r'};E)=i\hbar\int dE_{\lambda_\phi}\sum_{n=0}^{\infty}\left\{\sum_{l=0}^{\infty}\frac{\Psi_{l,n,\lambda_\phi}(r,\theta,\phi)\Psi^{*}_{l,n,\lambda_\phi}(r',\theta',\phi')}{E+i0-E_N}\right.$$
$$\left.+\int_0^{\infty}dk\frac{\Psi_{k,n,\lambda_\phi}(r,\theta,\phi)\Psi^{*}_{k,n,\lambda_\phi}(r',\theta',\phi')}{E+i0-\frac{\hbar^2k^2}{2M}}\right\}, \tag{130}$$

where the normalized wave functions and the energy spectrum are given by

$$\Psi_{l,n,\lambda_\phi}(\vec{r})=\frac{1}{a(l+\lambda_1+\frac{1}{2})^2}\left[\frac{2l!}{a\Gamma(l+2\lambda_1+1)}\right]^{1/2}\left(\frac{2r}{a(l+\lambda_1+\frac{1}{2})}\right)^{\lambda_1-1/2}$$
$$\times\exp\left(-\frac{r}{a(l+\lambda_1+\frac{1}{2})}\right)L_l^{2\lambda_1}\left(\frac{2r}{a(l+\lambda_1+\frac{1}{2})}\right)\sqrt{\frac{2}{\sin\theta}}\,\Phi_n^{(\lambda_+,\lambda_-)}\left(\frac{\theta}{2}\right)\Psi_{\lambda_\phi}(\phi), \tag{131}$$

$$E_N=-\frac{M\alpha_0^2}{2\hbar^2N^2},\quad N=l+\lambda_1+\tfrac{1}{2},\quad\text{and}\quad\lambda_1=n+\tfrac{1}{2}(\lambda_++\lambda_-+1), \tag{132}$$

for the bound states and

$$\Psi_{k,n,\lambda_\phi}(\vec{r})=\frac{\left|\Gamma\left(\frac{1}{2}+\lambda_1-\frac{i}{ak}\right)\right|}{\Gamma(2\lambda_1+1)}\frac{e^{\pi/2ak}}{r}M_{-(i/ak),\lambda_1}(-2ikr)\frac{1}{\sqrt{2\sin\theta}}\Phi_n^{(\lambda_+,\lambda_-)}\left(\frac{\theta}{2}\right)\Psi_{\lambda_\phi}(\phi), \tag{133}$$

$$E_k = \frac{\hbar^2 k^2}{2M}, \tag{134}$$

for the continuous states.

VI. CONCLUSION

In this paper, we have analyzed through the Milshtein and Strakhovenko variant of the so(2,1) Lie algebra a set of potentials belonging to three different classes of Smorodinsky–Winternitz potentials. The use of the second order differential operators of this algebra allows to write the Hamiltonian of these physical systems in form of a linear combination of the latter. Using the Schwinger's integral representation and with the help of two Baker–Campbell–Hausdorff formulas allowing the separation of the T_i operators and thus simplifying their action on a Laplace transform of a well chosen Dirac distribution, we have shown that we can construct the Green's functions in compact form in different coordinate systems. This method can be compared to the approach of the Schrödinger equation and to the Feynman's path integral technique. It gives a local view of the problem under consideration like the Schrödinger approach, but its advantage is in the computation of the explicit and compact form of the Green's function from which the energy spectrum and the suitably normalized wave functions are simultaneously extracted for the bound states and for the continuous states if they exist at one and the same time.

The advantage of the path integral approach in comparison with the algebraic method is that it provides a global view of the dynamics of the physical system, but a problem of singularity is often to be found at the origin of coordinates, and it requires a regularization which is rather complicated to perform. From this point of view, we can assert that this algebraic method has the advantage of not presenting this problem owing to the fact that it is local.

The method of Milshtein and Strakhovenko could become a powerful alternative approach to the path integral technique if we manage to extend its use to the treatment of the Pöschl–Teller potential class.

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Avoided crossings in mesoscopic systems: Electron propagation on a nonuniform magnetic cylinder

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We consider an electron constrained to move on a surface with revolution symmetry in the presence of a constant magnetic field B parallel to the surface axis. Depending on B and the surface geometry the transverse part of the spectrum typically exhibits many crossings which change to avoided crossings if a weak symmetry breaking interaction is introduced. We study the effect of such perturbations on the quantum propagation. This problem admits a natural reformulation to which tools from molecular dynamics can be applied. In turn, this leads to the study of a perturbation theory for the time dependent Born–Oppenheimer approximation.
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I. INTRODUCTION

Recent advances in experimental physics have made it possible to produce two-dimensional conducting surfaces of mesoscopic size. In such devices, the mean free path often exceeds the system size so the electron motion is ballistic and quantum coherence effects play a crucial role. This gives a motivation to strive for a complete understanding of the quantum mechanics of corresponding processes. In particular, conducting carbon ''nanotubes'' which are more or less uniform cylinders, belong to the family of surfaces that are nowadays experimentally within reach.[1] Since their discovery, lots of studies have been devoted to the elucidation of the spectral and transport properties of such devices, in a variety of situations and approximations, see, e.g., Refs. 2, 3, 4, and references therein. Nanotubes of different types can be combined, and also coupled to other carbon structures such as fullerene molecules,[5] producing a variety of cylindrical surfaces.

In this paper we study quantum propagation in an ''imperfect nanotube'' subject to a constant magnetic field parallel to the tube axis within a simple model. Our model assumes that a single electron is confined to a surface of revolution with slow variation of the radius along the revolution axis. Moreover, we assume that the rotational symmetry is weakly violated, either by an impurity or by an external field. In other words, the used idealization amounts to neglecting the atomic structure of the tube as well as the interaction between the electrons, but taking into account the gross shape of the device. Our aim is to study the propagation of the electron along such an imperfect nanotube in a homogenous magnetic field by means of the time-dependent Schrödinger equation, starting with an initially localized wave packet, and paying a particular attention to the transitions between angular levels caused by the symmetry breaking perturbation.

To understand the peculiarities of this quantum mechanical problem, it is useful to review briefly its classical counterpart; this is done in Sec. II. The first question in the quantum case is the meaning of the fact that the electron is confined to a surface. The most natural approach, in our opinion, is to consider the surface as a limiting situation of a thin hard-wall layer. This idea goes

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back to Refs. 6–8 and requires a renormalization in which the transverse contribution to the energy—blowing-up in the limit—is removed. One gets in this way an additional curvature-dependent term, in general attractive, to the potential. For the sake of completeness recall that there has been other recent works treating particle motion on revolution surfaces, see Refs. 9, 10, 11, and references therein. The last two papers aim at solvable models of compact surfaces (neglecting the curvature-dependent term), while Ref. 9 treats the Schrödinger and wave equations on noncompact cylindrical surfaces without a magnetic field from the PDE point of view.

Having thus found the Hamiltonian of our quantum system, we can analyze its spectral properties. When the rotational symmetry is preserved, we can perform (using a suitable gauge) the partial-wave decomposition. We can compute the angular part of the spectrum which depends on the actual cylinder radius varying along the tube axis. This brings to mind analogy with the molecular dynamics in which each angular state corresponds to an ''electronic'' level and the longitudinal coordinate measured along the axis corresponds to the one-dimensional ''nuclear'' configuration coordinate. Furthermore, when the rotational symmetry is broken by a perturbation, the above analogy remains valid and we may invoke the time-dependent Born–Oppenheimer approximation to describe the propagation along coupled angular levels according to Refs. 12–14. Recall that the theory in molecular systems involves a small parameter which is given by the mass ratio between ''electrons'' and ''nuclei.'' In our mesoscopic system, it is replaced by the parameter ϵ defined as the inverse of the length scale over which the variation of the radius of the nanotube takes place. Note, however, that we cannot directly apply the theory of Refs. 12–14 in our perturbative context and a modification is needed as we shall explain in Sec. IV.

The result of the analysis presented below gives a complete and rigorous description to the leading order of the wave function when the dynamics makes the electron go through a region where a perturbation couples angular levels. The basic picture is as follows. As long as the perturbed angular levels along the trajectory remain well isolated, the components of the wave function referring to the corresponding eigenstates are unchanged, to leading order. When the unperturbed angular levels display a crossing or an avoided crossing, transitions between the perturbed angular eigenstates may become non-negligible as in the mentioned molecular analogy, according to the well known mechanism of Landau–Zener transitions, see Ref. 13. At a heuristic level, when the electron meets an avoided crossing, we may replace the quantum mechanical degree of freedom x by a classical trajectory of the type $x \mapsto x_0 + tv$, where v is a velocity which can be considered as constant. This approximation leads to an effective time-dependent two-level system governing the transitions between the considered levels. The choice of a suitable time scale making the classical kinetic energy $mv^2/2$ constant and nonzero as the inverse length scale $\epsilon \to 0$ corresponds to the adiabatic limit $\epsilon \to 0$ in the above mentioned effective two-level Hamiltonian. Therefore, the transition probability $\mathcal{P}$ is then given by the Landau–Zener formula $\mathcal{P} \simeq e^{-c\delta^2/\epsilon}$, where δ is the minimum gap and the constant c is explicit.

We are going to consider precisely the situation where the transition amplitudes are of order one, under perturbations of order $\sqrt{\epsilon}$. In such cases, an initial wave function having a nonzero component in a single angular eigenspace before the (avoided) crossing splits in a nontrivial way between the corresponding angular eigenstates according to the Landau–Zener formula, again to leading order.

Let us note here that since the considered perturbations can arise from deformations and/or external fields, both allowed to vary over a wide range of values, situations where the typical size of the perturbation scales like the square root of the inverse length scale are certainly realistic. We choose to focus on these situations because they cause the most dramatic effects on the propagation. Indeed, we get from the Landau–Zener formula that other scaling laws make the avoided crossing either similar to a true crossing ($\mathcal{P} \simeq 1$) or to a set of well separated levels ($\mathcal{P} \simeq 0$).

We have already mentioned that despite being based on the paper,[13] our description is not a direct application of the molecular time-dependent Born–Oppenheimer approximation. Indeed, in the rigorous derivations of this approximation, the ''electronic'' spectrum and the eigenstates, i.e., the spectrum at fixed coordinate along the rotation axis in our setting, are taken as given data, and the approximate solution to the molecular Schrödinger equation is constructed from this informa-

tion, see Refs. 12–14. In our situation, by hypothesis, we only have access to that spectrum in a perturbative sense, and thus we need to develop a perturbative version of the time-dependent Born–Oppenheimer approximation that only requires knowledge of the leading terms of the Rayleigh–Schrödinger perturbation series. This is done in Sec. V, where the main technical result of the paper is stated in Theorem V.7. We believe that it is of an independent interest.

Precise statements of our results require a certain amount of notation and are therefore given below in Proposition IV.2 and Theorem V.7.

II. CLASSICAL MECHANICS

Let us start by describing the classical dynamics of the system. We consider a particle of mass m and charge e constrained to move on a smooth surface S with revolution symmetry around the axis OX in a homogeneous magnetic field $\mathbf{B}=Be_x$, $B\geqslant 0$, parallel to this axis.

Using cylindrical coordinates, the surface is characterized by the smooth positive real valued function $\mathbb{R}\ni x\mapsto R(x)\in\mathbb{R}_+^*$ such that

$$\begin{aligned} x&=x\\ y&=R(x)\cos(\theta),\\ z&=R(x)\sin(\theta) \end{aligned} \tag{2.1}$$

where $(x,\theta)\in\mathbb{R}\times S^1$. The squared length element on S is $ds^2=(1+R'(x)^2)dx^2+R(x)^2d\theta^2$, so the corresponding metric tensor $g_{ij}(x,\theta)$ is given by

$$g_{ij}(x,\theta)=\begin{pmatrix} 1+R'(x)^2 & 0\\ 0 & R^2(x)\end{pmatrix}. \tag{2.2}$$

Using the circular gauge, we express the vector potential at the surface as

$$\mathbf{A(r)}=\tfrac{1}{2}\mathbf{B}\wedge\mathbf{r}=\frac{R(x)B}{2}\begin{pmatrix}0\\ -\sin(\theta)\\ \cos(\theta)\end{pmatrix}. \tag{2.3}$$

This makes it possible to compute the Lagrangian function of the system,

$$\begin{aligned} L(\mathbf{r},\dot{\mathbf{r}})&=\tfrac{1}{2}m\dot{\mathbf{r}}^2+e\dot{\mathbf{r}}\mathbf{A(r)}\\ &=\frac{1}{2}m(\dot{x}^2(1+R'(x)^2)+R^2(x)\,\dot{\theta}^2)+\frac{eBR^2(x)\,\dot{\theta}}{2}. \end{aligned} \tag{2.4}$$

The system is integrable; we find that the momentum $p_\theta=(\partial L/\partial\dot{\theta})$ and the kinetic energy T are two constants of motion,

$$p_\theta=mR^2(x)\,\dot{\theta}+\frac{eBR^2(x)}{2}, \tag{2.5}$$

$$T=\tfrac{1}{2}m(\dot{x}^2(1+R'(x)^2)+R^2(x)\,\dot{\theta}^2). \tag{2.6}$$

Using (2.5) to express $\dot{\theta}$ as a function of x in (2.6), we deduce

$$T=\frac{1}{2}m\dot{x}^2(1+R'(x)^2)+\frac{1}{2m}\left(\frac{p_\theta^2}{R^2(x)}-p_\theta eB+\frac{e^2B^2}{4}R^2(x)\right)$$
$$=\frac{1}{2}m\dot{x}^2(1+R'(x)^2)+V(R(x)). \tag{27}$$

The effective potential $\mathbb{R}_+^* \ni R \mapsto V(R) \in \mathbb{R}_+$ admits a unique minimum at R_0 such that

$$R_0=\sqrt{\frac{2|p_\theta|}{|e|B}} \quad \text{and} \quad V(R_0)=\begin{cases} 0 & \text{if} \quad ep_\theta \geqslant 0 \\ \dfrac{|ep_\theta|B}{m} & \text{if} \quad ep_\theta<0 \end{cases}. \tag{2.8}$$

Note that if $p_\theta=0$, the potential $V(R)$ is harmonic on $\mathbb{R}_+^*$. From these considerations we deduce easily, in particular, that motions characterized by $\dot{x}(t)=0$ correspond either to $(x(t),\theta(t))=(x_0,\theta_0)$ for any initial conditions (x_0,θ_0), or to $(x(t),\theta(t))=(x_0,\theta_0-(eB/m)t)$, where $|e|B/m=:\omega_c$ is the cyclotronic frequency, for any initial conditions (x_0,θ_0), or finally to $(x(t),\theta(t))=(x_0,\theta_0+\omega t)$, where ω is any constant, for initial conditions (x_0,θ_0) such that $R'(x_0)=0$. In case $R'(x_0)\neq 0$, the first two motions are stable, whereas in the last one the stability depends on the local properties of R around x_0. In a similar way one can treat the general case with $\dot{x}(t)\neq 0$. The motion is governed by the effective potential determined by the shape of S, and the potential minima correspond to the points where the angular motion has the cyclotronic frequency.

Furthermore, notice that the addition of a supplementary exterior potential W, depending on x only, does not effect the functional dependence of p_θ and its value remains independent of time. It is just the second constant of motion which is changed in the sense that the total energy $E=T+W$ is now constant.

Finally, let us also give the corresponding Hamiltonian function of the system for future purposes. With $p_x=\partial L/\partial\dot{x}$ we compute

$$H(x,\theta,p_x,p_\theta)=\left(\frac{p_x^2}{2m(1+R'(x)^2)}+\frac{1}{2mR^2(x)}\left(p_\theta-\frac{eBR^2(x)}{2}\right)^2\right). \tag{2.9}$$

In the sequel we shall consider our charged particle to be an electron, $e=-|e|<0$, and use the rational units in which $|e|=m=1$ as well as $\hbar=c=1$.

III. QUANTUM MECHANICS

Consider now the same system in the framework of quantum mechanics. For the purpose of this section, the function $R:\mathbb{R}\to\mathbb{R}_+$ defining the surface S is supposed to be strictly positive and C^3; later we shall impose stronger requirements.

The Hilbert space of such a system is thus $L^2(S)$. To construct the Hamiltonian, however, it is not sufficient to replace the classical variables in (2.9) by the corresponding canonical operators. The most natural quantization consists in taking a particle confined to a cylindrical layer built over S and squeezing its thickness to zero, c.f. Refs. 6–8. One has of course to renormalize the energy in the limit, by subtracting the blowing-up part corresponding to the transverse motion.

In the absence of magnetic field, one arrives in this way to the Hamiltonian which is equal to the sum of the respective Laplace-Beltrami operator (times 1/2 in our units) and the curvature-induced potential $V(x)=-\frac{1}{8}(\varrho_1(x)^{-1}-\varrho_2(x)^{-1})^2$, where $\varrho_j(x)$, $j=1,2$, are the principal curvature radii at the given point. The second part is of a purely quantum nature and has no classical counterpart. In the present case the locally elliptical intersection of S with the normal plane has the radius $\varrho_1(x)=R(x)$, while for the intersection with the axial plane we find

$$\varrho_2(x)=-\frac{(1+R'(x)^2)^{3/2}}{R''(x)}; \tag{3.1}$$

the signs of ϱ_1, ϱ_2 coincide if both the osculation radii point the same side of the surface. Consequently, the curvature-induced potential equals

$$V(x) = -\frac{1}{8R(x)^2}\left(1+\frac{R(x)R''(x)}{(1+R'(x)^2)^{3/2}}\right)^2. \tag{3.2}$$

To express the kinetic (Laplace–Beltrami) part, $-\frac{1}{2}|g|^{-1/2}\partial_i|g|^{1/2}g^{ij}\partial_j$, we use (2.2) and the corresponding contravariant tensor on S,

$$g^{ij}(x) = \begin{pmatrix} (1+R'(x)^2)^{-1} & 0 \\ 0 & R(x)^{-2} \end{pmatrix}. \tag{3.3}$$

The Hamiltonian in the presence of magnetic field is then obtained by replacing the angular momentum operator $p_\theta = -i\partial_\theta$ by $p_\theta - A(x)R(x)$, where $A(x) := A_\theta(\mathbf{r})$; it acts as

$$\begin{aligned} H = &-\frac{1}{2R(x)\sqrt{1+R'(x)^2}}\partial_x\frac{R(x)}{\sqrt{1+R'(x)^2}}\partial_x + \frac{1}{2R(x)^2}\left(-i\partial_\theta + \frac{BR(x)^2}{2}\right)^2 \\ &-\frac{1}{8R(x)^2}\left(1+\frac{R(x)R''(x)}{(1+R'(x)^2)^{3/2}}\right)^2 \end{aligned} \tag{3.4}$$

on an appropriate domain in $L^2(\mathbb{R}\times S^1, R(x)\sqrt{1+R'(x)^2}\,dx\,d\theta)$. Due to the rotational symmetry it has a simple partial-wave decomposition; its H_m component is obtained replacing $-i\partial_\theta$ by its eigenvalue m. In this way the spectral analysis of H is reduced to a family of one-dimensional Sturm–Liouville problems. The magnetic term also has a natural meaning; we have

$$A(x)R(x) = \frac{BR(x)^2}{2} = \frac{\Phi(x)}{2\pi} = \phi(x), \tag{3.5}$$

where ϕ is the magnetic flux value measured in the standard units $(2\pi)^{-1}$, or the number of flux quanta passing through the cross section of the cylinder.

It may be convenient to get rid of the weight factor replacing the operator H above by an operator $\tilde{H}$ on $L^2(\mathbb{R})\otimes L^2(S^1)$. This is achieved by the unitary transformation $\psi \mapsto R^{1/2}(1+R'^2)^{1/4}\psi$. The only term in (3.4) which changes is the first one: by a straightforward computation we find

$$\tilde{H} = -\partial_x\frac{1}{2(1+R'(x)^2)}\partial_x + \frac{1}{2R(x)^2}\left(-i\partial_\theta + \frac{BR(x)^2}{2}\right)^2 + V_{21}(x) + V_{22}(x) \tag{3.6}$$

with

$$V_{21}(x) = -\frac{1}{8R(x)^2}\left(1+\frac{R(x)R''(x)}{(1+R'(x)^2)^{3/2}}\right)^2 \tag{3.7}$$

and

$$V_{22}(x) = \left(-\frac{R'^2}{8R^2(1+R'^2)} - \frac{7}{8}\frac{R'^2R''^2}{(1+R'^2)^3} + \frac{R''+R(R'R'''+R''^2)}{4R(1+R'^2)^2}\right)(x). \tag{3.8}$$

Spectral properties of the Hamiltonian are influenced by the geometry of S. Suppose, e.g., that the latter has asymptotically constant radius, $\lim_{|x|\to\infty} R(x) = R_0$. In the absence of magnetic field the problem is similar to that of a locally deformed Dirichlet strip[15,16] (it is simpler, however, unless a mode-coupling perturbation is introduced). In the s-wave part the effective potential V_{21}

creates a potential well when S is locally squeezed and a barrier in case of a protrusion. For higher partial waves and nonzero magnetic field, of course, the effective potential consists of several competing contributions.

IV. QUANTUM PROPAGATION

Our main interest in this paper is not so much the spectrum of the Hamiltonian (3.4) than the way in which an electron propagates over the surface of the cylinder. We will be particularly interested in the limiting situation when the radius modulation is gentle. This is conventionally described by means of the scaling transformation $x \mapsto \epsilon x$ which turns $\tilde{H}$ into $H(\epsilon)$ and by considering the asymptotic behavior as $\epsilon \to 0$. This can be considered as a semiclassical limit since as $\epsilon \to 0$ the wave packet size becomes ultimately much smaller than the length scale of the radius variations.

It is clear from the preceding section that the effective potential $V_2 = V_{21} + V_{22}$ is then dominated by the first term. Moreover, the operators (3.4) and (3.6) coincide to leading order, which will be the object of the following investigation. We write the action of $H(\epsilon)$ as

$$H(\epsilon) = -\frac{\epsilon^2}{2}\partial_x \frac{1}{1+\epsilon^2 V_1(x)}\partial_x + V_2(x,\epsilon) + \frac{1}{2R^2(x)}\left(-i\partial_\theta + \frac{BR^2(x)}{2}\right)^2 \tag{4.1}$$

on a suitable domain of $L^2(\mathbb{R}) \otimes L^2(S^1)$, where $R(x)$, $V_1(x) = R'(x)^2$ are smooth on $\mathbb{R}$ and $V_2(x,\epsilon)$ is smooth on $\mathbb{R} \times [-\epsilon_0, \epsilon_0]$, for some $\epsilon_0 > 0$. Introducing an R-dependent operator $h(R)$ for $R \in \mathbb{R}_+^*$ by

$$h(R) = \frac{1}{2R^2}\left(-i\partial_\theta + \frac{BR^2}{2}\right)^2 \tag{4.2}$$

on a suitable domain of $L^2(S^1)$, we can regard $H(\epsilon)$ as an operator on $L^2(\mathbb{R}, L^2(S^1))$ which we write as

$$H(\epsilon) = -\frac{\epsilon^2}{2}\partial_x \frac{1}{1+\epsilon^2 V_1(x)}\partial_x + V_2(x,\epsilon) + h(R(x)). \tag{4.3}$$

The spectral analysis of $h(R)$ is straightforward and yields a family of simple eigenvalues,

$$\sigma(h(R)) = \{\lambda_n(R), n \in \mathbb{Z}\} = \left\{\frac{1}{2R^2}\left(n + \frac{BR^2}{2}\right)^2, n \in \mathbb{Z}\right\}, \tag{4.4}$$

with the corresponding eigenvectors,

$$\varphi_n(\theta) = \exp(in\theta)/\sqrt{2\pi}, \quad n \in \mathbb{Z}. \tag{4.5}$$

Note that the eigenvalues $\lambda_n(R)$ correspond to the classical effective potential $V(R)$ in (2.7) with $n \in \mathbb{Z}$ in place of p_θ. For $n \neq m$ we have

$$\lambda_n(R) - \lambda_m(R) = \frac{(n-m)}{2}\left(\frac{(n+m)}{R^2} + B\right) \tag{4.6}$$

so that

$$\lambda_n(R) = \lambda_m(R) \Leftrightarrow n + m < 0 \quad \text{and} \quad R = R_{n,m} = \sqrt{\frac{-(n+m)}{B}}. \tag{4.7}$$

Moreover,

$$\lambda_n(R_{n,m}) = -\frac{B}{2}\frac{(n-m)^2}{(n+m)} > 0. \tag{4.8}$$

Hence any pair of levels $(\lambda_n(R),\lambda_m(R))$ with $n+m<0$ exhibits one and only one crossing as R varies, whereas other pairs never cross. The crossing points are well separated,

$$\{R_{n,m}:\ (n,m)\in\mathbb{N}^2,\ \ n+m<0\} = \left\{\ \sqrt{\frac{k}{B}} : k\in\mathbb{N}^*\right\}, \tag{4.9}$$

with $\sqrt{k/B} = R_{n,-(k+n)}$, $n\in\mathbb{N}$, and the values of the different pairs of levels crossing at $\sqrt{k/B}$, for k fixed, are also well separated since

$$\lambda_n(R_{n,-(k+n)}) = \frac{B}{2}\frac{(2n+k)}{k}. \tag{4.10}$$

We note also that $\lambda_n(R)-\lambda_{-n}(R) = Bn$.

Thus, depending on our choice of the function $R(x)$, the spectrum of $h(R(x))$ may display real or avoided crossings of an arbitrary width. Our aim is to adapt the techniques developed in Ref. 13 to describe the propagation of Gaussian wave packets (in the variable x) through these (avoided) crossings and, in particular, the splitting of the solution among the different angular levels $\lambda_n(R(x))$ involved. In particular, we can also suppose that the shape of the tube is gently changing in the way described above with the parameter ϵ entering in the definition of R; in any case, it will then turn out that the natural scale for the phenomena we want to describe is $\delta = \sqrt{\epsilon}$. We henceforth adopt δ as our small parameter and consider smooth functions $R(x,\delta)$ defined on $\mathbb{R}\times[-\delta_0,\delta_0]$. This means, in particular, that both the function V_1 and the operator h will depend on both x and δ in a smooth fashion.

However, the model discussed so far cannot exhibit transitions because of the rotational invariance which forbids passages between different levels λ_n. To get a nontrivial result, we perturb our system by introducing a real valued potential $\delta W(x,\theta,\delta)$, which is smooth on $\mathbb{R}\times S^1\times[-\delta_0,\delta_0]$ and violates the symmetry. For example, we can add a constant electric field in the direction $\mathbf{d} = \sin(\alpha)\mathbf{e}_z + \cos(\alpha)\mathbf{e}_x$, where $\alpha\notin\mathbb{Z}\pi$. As a consequence, we lose integrability of the system on the classical level, whereas in the quantum setting transitions between the different perturbed eigenstates become possible. By assumption, when considered as a (bounded) operator on $L^2(S^1)$ for (x,δ) fixed, the operator $\delta W(x,\theta,\delta)$ does not commute with $h(R(x,\delta))$, and therefore it perturbs the spectrum $\sigma(h(R(x,\delta))$. Note that for (x,δ) fixed, the above mentioned electric field gives rise to a bounded operator on $L^2(S^1)$. For the time being, let us keep the general form $\delta W(x,\theta,\delta)$ for the perturbation and describe the differences and similarities of the present case with respect to the paper.[13]

We introduce the operator g on (a suitable domain of) $L^2(\mathbb{R},L^2(S^1))$ by

$$g(x,\delta) = h(R(x,\delta)) + V_2(x,\delta) + \delta W(x,\theta,\delta) \tag{4.11}$$

so that the perturbed full Hamiltonian reads (with a slight abuse of notation)

$$H(\delta) = -\frac{\delta^4}{2}\partial_x\frac{1}{1+\delta^4 V_1(x,\delta)}\partial_x + g(x,\delta). \tag{4.12}$$

Without loss of generality, we can assume that $\int_{S^1} W(x,\theta,\delta)\,d\theta = 0$ by modifying $V_2(x,\delta)$ if necessary. We require the different potentials introduced so far to be smooth so that the following regularity hypothesis is fulfilled.

H0: *The operator g is strongly C^∞ in (x,δ) in $\mathbb{R}\times[-\delta_0,\delta_0]$.*

We want to approximate the solutions to the Schrödinger equation in a suitable time scale,

$$i\delta^2\frac{\partial\psi}{\partial t}=H(\delta)\psi, \tag{4.13}$$

for t in a finite time interval, as $\delta\to 0$, for initial conditions of a ''coherent state'' type, which we shall describe in detail below.

The first difference in comparison with Ref. 13 comes from the fact that the kinetic term gives rise to a perturbed Laplacian,

$$-\frac{\delta^4}{2}\partial_x\frac{1}{1+\delta^4V_1(x,\delta)}\partial_x=-\frac{\delta^4}{2}\partial_x^2+\frac{\delta^8}{2}\partial_x\frac{V_1(x,\delta)}{1+\delta^4V_1(x,\delta)}\partial_x$$

$$\equiv-\frac{\delta^4}{2}\partial_x^2+Y(x,\partial_x,\delta), \tag{4.14}$$

where

$$Y(x,\partial_x,\delta)=-\delta^4\frac{V_1(x,\delta)}{1+\delta^4V_1(x,\delta)}\frac{(-i\delta^2\partial_x)^2}{2}-\frac{\delta^4}{2}\left(-i\delta^2\partial_x\frac{V_1(x,\delta)}{1+\delta^4V_1(x,\delta)}\right)(-i\delta^2\partial_x). \tag{4.15}$$

We assume
H1:

$$\sup_{x\in\mathbb{R},|\delta|\leqslant\delta_0}|V_1^{(k)}(x,\delta)|<\infty,\quad k=0,1. \tag{4.16}$$

The factor δ^8 in front of the operator Y makes it possible to show that the influence of this term is negligible on the propagation of Gaussian states, so that the approximation given in Ref. 13 remains valid. This claim is the main result of this section and will be made precise in Proposition IV.2 below.

The second difference in comparison with Ref. 13 is that unless we have an explicitly solvable situation—and such situations are rare—in general we do not know the exact eigenvalues and eigenstates of the operator $g(x,\delta)$. However, the approximation derived in Ref. 13 is constructed on the basis of this exact knowledge. A way out is to use an incomplete information coming from the perturbation theory. Our second result, Theorem V.7, stated in Sec. V says that it is enough to know the first few terms in the perturbation series in order to construct an approximation that describes the propagation, even in the presence of avoided crossings, and that the result is as good as the one derived in Ref. 13.

The rest of this section is organized as follows. We proceed with the description of the ingredients needed for our approximation, in analogy with Ref. 13, assuming that we know the exact diagonal form of $g(x,\delta)$. Then we prove that the perturbation of the Laplacian by the operator Y does not effect the validity of this approximation. The next section will be devoted to the perturbative aspects mentioned above.

We will denote by $\mu_n(x,\delta)$ the eigenvalue of $g(x,\delta)$ such that $\mu_n(x,\delta)-\lambda_n(R(x,\delta))\to 0$ as $\delta\to 0$, for x such that $R(x,\delta)$ is far from $R_{n,m}$. The corresponding eigenvector will be denoted by $\Phi_n(x,\delta)$. If $R(x,\delta)$ lies in a neighborhood of $R_{n,m}$, we will denote by $\mu_{\mathcal{A}}(x,\delta)\geqslant\mu_{\mathcal{B}}(x,\delta)$ the almost degenerate perturbed eigenvalues with the corresponding eigenvectors $\Phi_{\mathcal{A}}(x,\delta)$ and $\Phi_{\mathcal{B}}(x,\delta)$. The reason for such a convention is that the unperturbed eigenvalues $\lambda_n(R(x,\delta)$ may or may not cross, are therefore the labeling of the μ's in terms of the indices n and m is not straightforward. Let $Q_n(x,\delta)$ be the one-dimensional spectral projection of $g(x,\delta)$ corresponding to $\mu_n(x,\delta)$ in the first case and $P(x,\delta)$ be the two-dimensional spectral projection of $g(x,\delta)$ corresponding to $\mu_{\mathcal{A}}(x,\delta)\geqslant\mu_{\mathcal{B}}(x,\delta)$ in the second case.

The situation we will study is that of avoided crossings of minimum width of order δ. Without loss of generality, we can assume the avoided crossing takes place in a neighborhood of $x=0$.

More precisely we suppose that:
H2: *The eigenvalues* $\mu_{\mathcal{A}}(x,\delta)$ *and* $\mu_{\mathcal{B}}(x,\delta)$ *are such that* $(\mu_{\mathcal{A}}-\mu_{\mathcal{B}})^{(-1)}\{0\}=(0,0)$ *in a neighborhood of* (0,0) *and* $\inf_{x\in I}(\mu_{\mathcal{A}}(x,\delta)-\mu_{\mathcal{B}}(x,\delta))=c|\delta|>0$ *for* $\delta\neq 0$, *where* c *is a constant and* I *is a small interval containing* 0.
We also set

$$g_{\parallel}(x,\delta)=g(x,\delta)P(x,\delta), \tag{4.17}$$

$$g_{\perp}(x,\delta)=g(x,\delta)(\mathbb{I}-P(x,\delta)). \tag{4.18}$$

We know from Ref. 17 that locally around (0,0) there exists an orthonormal basis, denoted by $\{\psi_1(x,\delta),\psi_2(x,\delta)\}$, of $P(x,\delta)L^2(S^1)$, which is regular in (x,δ) around (0,0). It is constructed in the standard Gram–Schmidt way: we choose an orthonormal basis $\{\psi_1,\psi_2\}$ of $P(0,0)L^2(S^1)$ and set

$$\phi_1(x,\delta)=\frac{P(x,\delta)\psi_1}{\|P(x,\delta)\psi_1\|}, \tag{4.19}$$

$$\phi_2(x,\delta)=\frac{(\mathbb{I}-|\phi_1(x,\delta)\rangle\langle\phi_1(x,\delta)|)P(x,\delta)\psi_2}{\|(\mathbb{I}-|\phi_1(x,\delta)\rangle\langle\phi_1(x,\delta)|)P(x,\delta)\psi_2\|}. \tag{4.20}$$

Moreover, there exists a (x,δ) independent unitary transform U such that in the orthonormal basis,

$$\psi_j(x,\delta)=U\phi_j(x,\delta),\quad j=1,2, \tag{4.21}$$

the matrix $g_{\parallel}(x,\delta)$ takes the form

$$\begin{aligned} g_{\parallel}(x,\delta)&=g_1(x,\delta)+\overline{V}(x,\delta)\\ &=\begin{pmatrix}\beta(x,\delta) & \gamma(x,\delta)+i\sigma(x,\delta)\\ \gamma(x,\delta)-i\sigma(x,\delta) & -\beta(x,\delta)\end{pmatrix}+\overline{V}(x,\delta), \end{aligned} \tag{4.22}$$

where $\overline{V}(x,\delta)=\mathrm{trace}(g(x,\delta)P(x,\delta))/2$ is a regular function of (x,δ) around the origin and

$$\begin{aligned} \beta(x,\delta)&=b_1x+b_2\delta+\mathcal{O}(2),\\ \gamma(x,\delta)&=c_2\delta+\mathcal{O}(2),\\ \sigma(x,\delta)&=\mathcal{O}(2),\\ \overline{V}(x,\delta)&=\mathcal{O}(0), \end{aligned} \tag{4.23}$$

where $b_1>0, c_2>0, b_2\in\mathbb{R}$, and the following notation is used for the sake of brevity:

$$\mathcal{O}(m)=\mathcal{O}((x^2+\delta^2)^{m/2}). \tag{4.24}$$

In order to get rid of the δ-dependence in the leading order of $\beta(x,\delta)$ in (4.22), we introduce new variables,

$$x'=b_1x+b_2\delta,\quad \delta'=c_2\delta,\quad t'=b_1^2/c_2^2t. \tag{4.25}$$

In terms of these variables, the Schrödinger Eq. (4.13) for

$$\phi(x',t')=\psi(x(x',\delta'),t(t')) \tag{4.26}$$

becomes

$$i\delta'^2\frac{\partial}{\partial t'}\phi(x',t')=-\frac{\delta'^4}{2}\partial_{x'}\frac{1}{1+\delta'^4V_1'(x',\delta')}\partial_{x'}\phi(x',t')+\frac{c_2^4}{b_1^2}g(x(x',\delta'),\delta(\delta'))\phi(x',t') \tag{4.27}$$

in the limit $\delta'\to 0$, with

$$V_1'(x',\delta')=V_1(x(x',\delta'),\delta(\delta'))/c_2^4, \tag{4.28}$$

$$g_{\|}(x(x',\delta'),\delta(\delta'))=\begin{pmatrix} x_1' & \delta' \\ \delta' & -x_1' \end{pmatrix}+\mathcal{O}(2)+\overline{V}(x(x',\delta'),\delta(\delta')), \tag{4.29}$$

where $\overline{V}(x(x',\delta'),\delta(\delta'))$ and $V_1'(x',\delta')$ are regular in (x',δ') around (0,0) and $\mathcal{O}(2)$ refers to x' and δ'. We introduce the fixed parameter $r=c_2^4/b_1^2>0$ and *henceforth drop the primes on the new variables*. We assume that $g_1(x,\delta)$ has the form (4.22) with the following local behavior around $x=0$ and $\delta=0$:

$$\begin{aligned} \beta(x,\delta)&=rx+\mathcal{O}(2),\\ \gamma(x,\delta)&=r\delta+\mathcal{O}(2),\\ \sigma(x,\delta)&=\mathcal{O}(2),\\ \overline{V}(x,\delta)&=\mathcal{O}(0) \end{aligned} \tag{4.30}$$

with $r>0$.

Let us next describe the building blocks of our Born–Oppenheimer states.

We begin with the definition of the semiclassical ''nuclear'' wave packets denoted as $\varphi_j(A,B,\hbar,a,\eta,x)$. This definition comes from Ref. 18; we have specified it to our setting where $x\in\mathbb{R}$. Since Ref. 18 provides a detailed discussion of these wave packets, we refrain from proving all their properties here.

We assume $a\in\mathbb{R}$, $\eta\in\mathbb{R}$ and $\hbar=\delta^2>0$. Let us stress that while the last symbol is useful when adapting the results of Ref. 18, it has nothing to do with the Planck's constant. We also assume that A and B are nonzero complex numbers that satisfy

$$\mathrm{Re}\,\overline{A}B=1. \tag{4.31}$$

This condition guarantees that $\mathrm{Re}\,BA^{-1}$ is positive, since $(\mathrm{Re}\,BA^{-1})^{-1}=|A|^2$.

Our definition of $\varphi_j(A,B,\hbar,a,\eta,x)$ is based on the following raising operator:

$$\mathcal{A}(A,B,\hbar,a,\eta)^*=\frac{1}{\sqrt{2\hbar}}\left[\overline{B}(x-a)-\overline{A}\left(-i\hbar\frac{\partial}{\partial x}-\eta\right)\right]. \tag{4.32}$$

Definition: For the index $j=0$, we define the normalized complex Gaussian wave packet (modulo the sign of the square root) by

$$\varphi_0(A,B,\hbar,a,\eta,x)=\pi^{-1/4}\hbar^{-1/4}A^{-1/2}\times\exp\{-BA^{-1}(x-a)^2/(2\hbar)+i\eta(x-a)/\hbar\}. \tag{4.33}$$

Then for any positive integer j we define

$$\varphi_j(A,B,\hbar,a,\eta,\cdot)=\frac{1}{\sqrt{j!}}(\mathcal{A}(A,B,\hbar,a,\eta)^*)^j\varphi_0(A,B,\hbar,a,\eta,\cdot). \tag{4.34}$$

Remarks:

(1) For $A=B=1$, $\hbar=1$, and $a=\eta=0$, the $\varphi_j(A, B, \hbar, a, \eta, \cdot)$ are just the standard harmonic-oscillator eigenstates with energies $j+1/2$;
(2) For each A, B, $\hbar$, a, and η, the set $\{\varphi_j(A, B, \hbar, a, \eta, \cdot)\}$ is an orthonormal basis for $L^2(\mathbb{R})$;
(3) The position and momentum uncertainties of the $\varphi_j(A, B, \hbar, a, \eta, \cdot)$ are $\sqrt{(j+1/2)\hbar}\,|A|$ and $\sqrt{(j+1/2)\hbar}|B|$, respectively;
(4) When we solve approximately the Schrödinger equation, the choice of the sign of the square root in the definition of $\varphi_0(A, B, \hbar, a, \eta, \cdot)$ is determined by continuity in t after an arbitrary initial choice;
(5) Defining the scaled Fourier transform to be

$$[\mathcal{F}_\hbar \Psi\,](\xi)=(2\pi\hbar)^{-1/2}\int_{\mathbb{R}}\Psi(x)e^{-i\xi x/\hbar}dx, \tag{4.35}$$

then

$$[\mathcal{F}_\hbar \varphi_l(A,B,\hbar,a,\eta,\cdot)](\xi)=(-i)^l\, e^{-i\eta a/\hbar}\varphi_l(B,A,\hbar,\eta,-a,\xi). \tag{4.36}$$

We also define

$$V^{\mathcal{A}}_{\mathcal{B}}(x,\delta)=\overline{V}(x,\delta)\pm\sqrt{\beta^2(x,\delta)+\gamma^2(x,\delta)+\sigma^2(x,\delta)}, \tag{4.37}$$

where $x\in\mathbb{R}$, $\delta>0$. Let $a^{\mathcal{C}}(t)$ and $\eta^{\mathcal{C}}(t)$ be the solutions of the classical equations of motion,

$$\frac{d}{dt}a^{\mathcal{C}}(t)=\eta^{\mathcal{C}}(t), \tag{4.38}$$

$$\begin{aligned}\frac{d}{dt}\eta^{\mathcal{C}}(t)&=-\nabla V^{\mathcal{C}}(a^{\mathcal{C}}(t),\delta), \quad \mathcal{C}=\mathcal{A},\mathcal{B},\\ \frac{d}{dt}S^{\mathcal{C}}(t)&=\eta^{\mathcal{C}}(t)^2/2-V^{\mathcal{C}}(a^{\mathcal{C}}(t),\delta),\end{aligned} \tag{4.39}$$

with the initial conditions

$$\begin{aligned}a^{\mathcal{C}}(0)&=0,\\ \eta^{\mathcal{C}}(0)&=\eta^0(\delta),\end{aligned} \tag{4.40}$$

where

$$\begin{aligned}\eta^0(\delta)&=\eta^0+\mathcal{O}(\delta), \quad \eta^0>0,\\ S^{\mathcal{C}}(0)&=0.\end{aligned} \tag{4.41}$$

The error term $\mathcal{O}(\delta)$ depends here on whether $\mathcal{C}$ is $\mathcal{A}$ or $\mathcal{B}$. In case of an isolated eigenvalue μ_n, $V^{\mathcal{C}}=V^n=\mu_n$.

We further introduce complex numbers which are defined by means of classical quantities. Let $A^{\mathcal{C}}(t)$ and $B^{\mathcal{C}}(t)$ be the solutions of the linear system,

$$\frac{d}{dt}A^{\mathcal{C}}(t)=iB^{\mathcal{C}}(t),$$
$$\frac{d}{dt}B^{\mathcal{C}}(t)=iV^{\mathcal{C}(2)}(a^{\mathcal{C}}(t),\delta)A^{\mathcal{C}}(t), \tag{4.42}$$

where $a^{\mathcal{C}}(t)$ is the solution of (4.38) and (4.40), with the initial conditions

$$A^{\mathcal{C}}(0)=A_0,$$
$$B^{\mathcal{C}}(0)=B_0, \tag{4.43}$$

and $V^{\mathcal{C}(2)}$ denotes the Hessian matrix of $V^{\mathcal{C}}$. It is easy to see that these quantities actually describe the linearized classical flow around the trajectory $(a^{\mathcal{C}}(t),\eta^{\mathcal{C}}(t))$. The above convention regarding $\mathcal{C}$ applies if μ_n is isolated in the spectrum. The asymptotics of these classical quantities for small t and δ are described in detail in Sec. II of Ref. 13.

The determination of the ''electronic'' part of the Born–Oppenheimer wave packet (B–O state, for short) is as follows. Although the ''electronic'' Hamiltonian is independent of time, it is convenient, since we deal with the time dependent Schrödinger equation, to choose specific time dependent ''electronic'' eigenvectors. Since they may become singular when the corresponding eigenvalues are degenerate, or almost degenerate, we shall define them for t in the outer regime, that is when $a(t)$ is far enough from 0. This outer regime is characterized by times t such that (see Ref. 13),

$$\delta^{1-\xi}\leqslant|t|\leqslant T,\quad \xi<1/3. \tag{4.44}$$

We shall have two sets of eigenvectors, denoted by $\Phi^{\pm}_{\mathcal{C}}(x,t,\delta)$, where the label $\pm$ refers to positive and negative times. Of course, this distinction is irrelevant if we consider an isolated eigenvalue μ.

Let $\eta^{\mathcal{C}}(t)$ be the momentum solution of the classical equations of motion (4.38) and (4.40). The normalized eigenvectors $\Phi^{\pm}_{\mathcal{C}}(x,t,\delta)$ are the solutions of

$$\langle\Phi^{\pm}_{\mathcal{C}}(x,t,\delta)|(\partial/\partial t+\eta^{\mathcal{C}}(t)\partial_x)\Phi^{\pm}_{\mathcal{C}}(x,t,\delta)\rangle\equiv 0 \tag{4.45}$$

for $\mathcal{C}=\mathcal{A},\mathcal{B}$ and $t\gtrless 0$. Since the eigenvalues $\mu_{\mathcal{A}}(x,\delta)$ and $\mu_{\mathcal{B}}(x,\delta)$ are nondegenerate for any time t small enough, such vectors exist, are unique up to an overall time independent phase factors, and are eigenvectors of $g_1(x,\delta)$ associated with $E_{\mathcal{C}}(x,\delta)$ for any time. More precisely, we define the angles $\varphi(x,\delta)$ and $\theta(x,\delta)$ by

$$\beta(x,\delta)=\sqrt{\beta^2(x,\delta)+\gamma^2(x,\delta)+\sigma^2(x,\delta)}\cos(\theta(x,\delta)), \tag{4.46}$$
$$\gamma(x,\delta)=\sqrt{\beta^2(x,\delta)+\gamma^2(x,\delta)+\sigma^2(x,\delta)}\sin(\theta(x,\delta))\cos(\varphi(x,\delta)), \tag{4.47}$$
$$\sigma(x,\delta)=\sqrt{\beta^2(x,\delta)+\gamma^2(x,\delta)+\sigma^2(x,\delta)}\sin(\theta(x,\delta))\sin(\varphi(x,\delta)), \tag{4.48}$$

and construct static eigenvectors. Let

$$\Phi^{-}_{\mathcal{A}}(x,\delta)=e^{i\varphi(x,\delta)}\cos(\theta(x,\delta)/2)\psi_1(x,\delta)+\sin(\theta(x,\delta)/2)\psi_2(x,\delta), \tag{4.49}$$
$$\Phi^{-}_{\mathcal{B}}(x,\delta)=e^{-i\varphi(x,\delta)}\cos(\theta(x,\delta)/2)\psi_2(x,\delta)-\sin(\theta(x,\delta)/2)\psi_1(x,\delta), \tag{4.50}$$

be the eigenvectors of $g_1(x,\delta)$ associated with $\mu_{\mathcal{C}}(x,\delta)$, $\mathcal{C}=\mathcal{A},\mathcal{B}$, for $\pi/2<\theta(x,\delta)\leqslant\pi$, and

$$\Phi^{+}_{\mathcal{A}}(x,\delta)=\cos(\theta(x,\delta)/2)\psi_1(x,\delta)+e^{-i\varphi(x,\delta)}\sin(\theta(x,\delta)/2)\psi_2(x,\delta), \tag{4.51}$$
$$\Phi^{+}_{\mathcal{B}}(x,\delta)=\cos(\theta(x,\delta)/2)\psi_2(x,\delta)-e^{i\varphi(x,\delta)}\sin(\theta(x,\delta)/2)\psi_1(x,\delta) \tag{4.52}$$

be the eigenvectors of $g_1(x,\delta)$ for $0\leqslant\theta(x,\delta)<\pi/2$. The solutions of (4.45) are of the form

$$\Phi_{\mathcal{C}}^{\pm}(x,t,\delta)=\Phi_{\mathcal{C}}^{\pm}(x,\delta)\mathrm{e}^{i\lambda_{\mathcal{C}}^{\pm}(x,t,\delta)},\quad \begin{cases} t>0 \\ t<0 \end{cases}, \tag{4.53}$$

where $\lambda_{\mathcal{C}}^{\pm}(x,t,\delta)$ is a real valued function satisfying the equation,

$$i\frac{\partial}{\partial t}\lambda_{\mathcal{C}}^{\pm}(x,t,\delta)+i\,\eta^{\mathcal{C}}(t)\partial_x\lambda_{\mathcal{C}}^{\pm}(x,t,\delta)+\langle\Phi_{\mathcal{C}}(x,\delta)|\,\eta^{\mathcal{C}}(t)\partial_x\Phi_{\mathcal{C}}(x,\delta)\rangle=0. \tag{4.54}$$

We can get an expression for $\lambda_{\mathcal{C}}^{\pm}$ and its derivatives as follows. We fix values of the indices and drop them in the notation. We introduce the new variable

$$\omega\equiv x-a(t) \tag{4.55}$$

and the notation

$$\lambda_r(\omega,t,\delta)\equiv\lambda(\omega+a(t),t,\delta), \tag{4.56}$$

$$\Phi_r(\omega,t,\delta)\equiv\Phi(\omega+a(t),\delta). \tag{4.57}$$

In terms of these new variables, Eq. (4.54) for λ_r reads

$$i\frac{\partial}{\partial t}\lambda_r(\omega,t,\delta)=-\langle\Phi_r(\omega,t,\delta)|\frac{\partial}{\partial t}|\,\Phi_r(\omega,t,\delta)\rangle \tag{4.58}$$

with

$$\frac{\partial}{\partial t}\Phi_r(\omega,t,\delta)=\eta(t)\partial_x\Phi(\omega+a(t),\delta). \tag{4.59}$$

By integration we get

$$\lambda_r(\omega,t,\delta)=-\int^t\eta(t')\langle\Phi(\omega+a(t'),\delta)|\partial_x\Phi(\omega+a(t'),\delta)\rangle dt'+\lambda_{r0}(\omega,\delta), \tag{4.60}$$

where we are free to set the integration constant $\lambda_{r0}(\omega,\delta)\equiv0$.

The ''nuclear'' wave function is localized around the classical trajectory in the semiclassical regime. In view of the genericity condition $\eta^0>0$, in the outer temporal region, the major part of the ''nuclear'' wave function will be supported away from the neighborhood where the levels almost cross. Hence we can introduce a cutoff function which does not significantly alter the solution and forces the support of the wave function to be away of this neighborhood. Let F be a C^∞ cutoff function,

$$F:\mathbb{R}^+\to\mathbb{R}, \tag{4.61}$$

such that

$$\begin{array}{lll} F(r)=1 & \ldots & 0\leqslant r\leqslant 1 \\ F(r)=0 & \ldots & r\geqslant 2 \end{array}. \tag{4.62}$$

The wave functions we construct below in the outer regime will be multiplied by the regularizing factor,

$$F(\|x-a^{\mathcal{C}}(t)\|/\delta^{1-\delta'}), \tag{4.63}$$

where $0<\delta'<\xi$, for $\mathcal{C}=\mathcal{A},\mathcal{B}$.

Remark: On the support of F the relation,

$$x=\eta^0(\delta)t+\mathcal{O}(\delta^{1-\delta'}+t^2) \tag{4.64}$$

holds true, and since $\eta^0(\delta)=\eta^0+\mathcal{O}(\delta)$, where $\eta^0>0$, we find that

$$|x|>c|t|, \tag{4.65}$$

uniformly in δ.

A Born–Oppenheimer state $\psi_j^{\mathcal{C}\pm}(x,\delta,t)$ is defined by

$$\psi_j^{\mathcal{C}\pm}(x,\delta,t)$$

$$=F(\|x-a^{\mathcal{C}}(t)\|/\delta^{1-\delta'})\varphi_j(A^{\mathcal{C}}(t),B^{\mathcal{C}}(t),\delta^2,a^{\mathcal{C}}(t),\eta^{\mathcal{C}}(t),x)\mathrm{e}^{iS^{\mathcal{C}}(t)/\delta^2}\Phi_{\mathcal{C}}^{\pm}(x,t,\delta). \tag{4.66}$$

It is a good approximation to the solution of the Schrödinger equation (4.13) as $\delta\to 0$ far enough of the crossing region, i.e., in the outer time regime (4.44), and when the operator Y defined in (4.15) is absent, as shown in Ref. 13 Proposition IV.2 below shows this is still true when Y is present.

In the inner time regime, characterized by the inequality (see Ref. 13),

$$-\delta^{1-\xi}\leqslant t\leqslant\delta^{1-\xi},\quad \xi<1/3, \tag{4.67}$$

we look for an approximation constructed by means of the classical quantities associated with the potential $\overline{V}(x,\delta)$, the average of $\mu^{\mathcal{A}}(x,\delta)$ and $\mu^{\mathcal{B}}(x,\delta)$. Let $a(t)$ and $S(t)$ be the corresponding classical quantities satisfying the initial conditions

$$\begin{aligned} a(0)&=0,\\ \eta(0)&=\eta^0,\\ S(0)&=0. \end{aligned} \tag{4.68}$$

It is suitable to use the rescaled variables

$$\begin{aligned} y&=(x-a(t))/\delta\\ s&=t/\delta. \end{aligned} \tag{4.69}$$

It is shown in Ref. 13 that a good approximation ψ_I of solutions to (4.13) in that regime, when Y is absent, is given by

$$\psi_I(y,s,\delta)=F(\|y\|\delta^{\delta'})\exp\left(i\frac{S(\delta s)}{\delta^2}+i\frac{\eta(\delta s)y}{\delta}\right)\chi(y,s,\delta), \tag{4.70}$$

with

$$\chi(y,s,\delta)=f_0(y,s)\psi_1(a(\delta s)+\delta y,\delta)+g_0(y,s)\psi_2(a(\delta s)+\delta y,\delta), \tag{4.71}$$

where f_0,g_0 are complex-valued functions solutions to

$$i\frac{\partial}{\partial s}\begin{pmatrix} f_0(y,s)\\ g_0(y,s)\end{pmatrix}=r\begin{pmatrix} \eta^0 s+y & 1\\ 1 & -(\eta^0 s+y)\end{pmatrix}\begin{pmatrix} f_0(y,s)\\ g_0(y,s)\end{pmatrix}. \tag{4.72}$$

The general solution to this equation is

$$\begin{pmatrix} f_0(y,s) \\ g_0(y,s) \end{pmatrix} = C_1(y) \begin{pmatrix} \dfrac{(1-i)}{2}\sqrt{\dfrac{r}{\eta^0}} D_{ir/2\eta^0-1}\left((-1+i)\sqrt{\dfrac{r}{\eta^0}}(\eta^0 s+y)\right) \\ D_{ir/2\eta^0}\left((-1+i)\sqrt{\dfrac{r}{\eta^0}}(\eta^0 s+y)\right) \end{pmatrix} + C_2(y) \times \begin{pmatrix} D_{-ir/2\eta^0}\left(-(1+i)\sqrt{\dfrac{r}{\eta^0}}(\eta^0 s+y)\right) \\ -\dfrac{(1+i)}{2}\sqrt{\dfrac{r}{\eta^0}} D_{-ir/2\eta^0-1}\left(-(1+i)\sqrt{\dfrac{r}{\eta^0}}(\eta^0 s+y)\right) \end{pmatrix}, \tag{4.73}$$

where the D_ν are parabolic cylinder functions. The coefficients $C_1(y)$ and $C_2(y)$ have to be determined by matching with the incoming solutions of the B–O type at the border of the inner and outer time regimes.

In particular, assuming for definiteness that the incoming B–O state ψ_{OI} is associated with the index l for the "nuclear" component and the $\mathcal{B}$ level with the initial momentum $\eta^{\mathcal{B}}(0)=\eta^0$, i.e., that

$$\psi_{\mathrm{OI}}(x,t,\delta)=\psi_l^{\mathcal{B}-}(x,t,\delta), \quad -T\leqslant t\leqslant -\delta^{1-\xi}, \tag{4.74}$$

we have

$$C_1(y)\equiv 0 \tag{4.75}$$

and

$$C_2(y)=-\delta^{-1/2}\varphi_l(A_0,B_0-irA_0/\eta^0,1,0,0,y)\mathrm{e}^{-(\pi r/8\eta_1^0)}\exp\left(\frac{ir}{2\eta^0}(y^2-2y)\right) \times\exp\left(i\frac{S_0^{\mathcal{B}}(\delta,-)}{\delta^2}+\frac{ir}{4\eta^0}(1+3\ln(2\eta^0)+\ln r-4\ln\delta)\right), \tag{4.76}$$

where $S_0^{\mathcal{B}}(\delta,-)$ is real and can be computed explicitly, see Ref. 13.

The analysis of Ref. 13 shows that in this situation, we get an outgoing solution given by a linear combination of B–O states, with explicit coefficients, associated with the same index l for the "nuclear" component but with both levels. The initial momentum is chosen as $\eta^{\mathcal{A}}(0)=\eta^0-2r\delta/\eta^0$ for the $\mathcal{A}$ level and the outgoing solution ψ_{OO} is of the form,

$$\psi_{\mathrm{OO}}(x,t,\delta)=-\mathrm{e}^{-\pi r/2\eta_1^0}\psi_l^{\mathcal{A}+}(x,\delta,t)+\mathrm{e}^{-\pi r/4\eta^0}\sqrt{\frac{\pi r}{\eta^0}}\frac{\mathrm{e}^{i\lambda(\delta)}}{\Gamma\left(1+\dfrac{ir}{2\eta^0}\right)}\psi_l^{\mathcal{B}+}(x,\delta,t) \tag{4.77}$$

provided $\delta^{1-\xi}\leqslant t\leqslant T$, where

$$\lambda(\delta)=\pi/4+S_0^{\mathcal{A}}(-,\delta)/\delta^2+\frac{r}{2\eta^0}(1+3\ln(2\eta^0)+\ln r-4\ln\delta). \tag{4.78}$$

Here again, $S_0^{\mathcal{A}}(\delta,-)$ is real and can be computed explicitly from Ref. 13.

Moreover, the function obtained by pasting the approximations constructed in the outer and inner temporal regions is an approximate solution to the Schrödinger equation when the perturbation Y of the Laplacian is absent [see (4.14)]. Similar explicit formulas are valid if the ingoing state is associated with the $\mathcal{A}$ level. Hence, the propagation through avoided crossings can be iterated.

We are going to show that the perturbation of the Laplacian in (4.14) does not affect the propagation of B–O states. The general strategy is simple: we write

$$H(\delta) = -\frac{\delta^4}{2}\Delta_x + g(x,\delta) + Y(x,\partial_x,\delta)$$

$$\equiv H_0(\delta) + Y(x,\partial_x,\delta) \tag{4.79}$$

and denote by $\Psi_l(x,t,\delta)$ the approximation given by $\psi_{\mathrm{OI}}, \psi_1, \psi_{\mathrm{OO}}$ in their respective time domains constructed in Ref. 13,

$$\Psi_l(x,t,\delta) = \begin{cases} \psi_{\mathrm{OI}}(x,t,\delta) & \cdots \quad -T \leqslant t \leqslant -\delta^{1-\xi} \\ \psi_1(x,t,\delta) & \cdots \quad -\delta^{1-\xi} \leqslant t \leqslant \delta^{1-\xi} \\ \psi_{\mathrm{OO}}(x,t,\delta) & \cdots \quad \delta^{1-\xi} \leqslant t \leqslant T \end{cases}. \tag{4.80}$$

We define ζ_l by

$$\begin{aligned} \xi_l(x,t,\delta) &= i\delta^2\partial_t\Psi_l(x,t,\delta) - H(\delta)\Psi_l(x,t,\delta) \\ &= i\delta^2\partial_t\Psi_l(x,t,\delta) - H_0(\delta)\Psi_l(x,t,\delta) - Y(x,\partial_x,\delta)\Psi_l(x,t,\delta) \\ &= \zeta_l^0(x,t,\delta) + \zeta_l^1(x,t,\delta), \end{aligned} \tag{4.81}$$

where ζ_l^0 is the error term controlled in Ref. 13 by means of the following abstract lemma.

Lemma IV.1: Suppose $H(\hbar)$ is a family of self-adjoint operators labeled by $\hbar > 0$. Suppose that $\psi(t,\hbar)$ belongs to the domain of $H(\hbar)$, is continuously differentiable in t, and solves approximately the Schrödinger equation in the sense that

$$i\hbar\frac{\partial\psi}{\partial t}(t,\hbar) = H(\hbar)\,\psi(t,\hbar) + \zeta(t,\hbar), \tag{4.82}$$

where $\zeta(t,\hbar)$, satisfies

$$\|\zeta(t,\hbar)\| \leqslant \mu(t,\hbar). \tag{4.83}$$

Then,

$$\|\mathrm{e}^{-itH(\hbar)/\hbar}\,\psi(0,\hbar) - \psi(t,\hbar)\| \leqslant \hbar^{-1}\int_0^t \mu(s,\hbar)\,ds \tag{4.84}$$

holds true for $t > 0$ and the analogous statement is valid for $t < 0$.

Using the same lemma to estimate the norm of ζ_l^1, we get

Proposition IV.2: Under the hypotheses (H0)–(H2), the function $\Psi_l(x,t,\delta)$ defined by (4.80) *is for any $T > 0$ an approximation to the solution $\psi(x,t,\delta)$ of the Schrödinger equation (4.13) such that*

$$\psi(x,t,\delta) = \Psi_l(x,t,\delta) + \mathcal{O}(\delta^p) \tag{4.85}$$

holds in the $L^2(\mathbb{R})$ sense for some $p > 0$ and all $t \in [-T,T]$.

The proof of this technical proposition is given in the Appendix.

V. PROPAGATION OF PERTURBED B–O STATES

Let us now turn to the second indicated step and replace the above B–O approximation by a construction making use of a perturbative knowledge of the exact eigenvectors and eigenvalues of

the operator $g_\parallel$ defined by (4.22). In particular, this needs to be done for the quantities appearing in (4.38), (4.42) determined by means of a classical potential given by an approximation of the spectrum of $g_\parallel$. We will show that it is enough to know the second order perturbation expansion in order to construct an approximation of the solution that is a perturbed version of our initial B–O states and still describes accurately the transitions between the ''electronic'' levels.

In order to make some explicit formulas simpler and to stress the effect of the perturbation, we will assume in this section that both the operators h and W are δ independent, i.e., we shall consider

$$g(x,\delta)=h(R(x))+V_2(x)+\delta W(x,\theta), \tag{5.1}$$

where V_2 commutes with h whereas W does not. This means that $h(x)$ is assumed to have a degeneracy at $x=0$ in the considered part of its spectrum that is lifted by W to leading order in δ. This is the generic situation we set out to investigate when the avoided crossing results from a weak symmetry-breaking violation of a true eigenvalue crossing. Note, however, that we are able to accommodate the general situation considered so far, at the cost of more complicated perturbation formulas.

Let us state a simple lemma which is at the basis of our constructions and which says that an approximation of an approximate solution is an approximate solution.

Lemma V.1: Let $H(\delta)$ be for all $\delta\in(0,\delta_0)$ a self-adjoint operator densely defined in a Hilbert space $\mathcal{H}$, and let $\psi_a(t,\delta)\in\mathcal{H}$, $\varphi_a(t,\delta)\in\mathcal{H}$ be time dependent vectors with the following property; there exists $c,p_1,p_2>0$ such that the relations

$$\|\mathrm{e}^{-iH(\delta)t/\delta^2}\psi_a(0,\delta)-\psi_a(t,\delta)\|\leqslant c\,\delta^{p_1} \tag{5.2}$$

and

$$\|\varphi_a(t,\delta)-\psi_a(t,\delta)\|\leqslant c\,\delta^{p_2} \tag{5.3}$$

hold for all t from an interval $I\subset\mathbb{R}$ and $0<\delta<\delta_0$. Then,

$$\|\mathrm{e}^{-iH(\delta)t/\delta^2}\varphi_a(0,\delta)-\varphi_a(t,\delta)\|\leqslant 3c\,\delta^{\min(p_1,p_2)},$$

$$\|\mathrm{e}^{-iH(\delta)t/\delta^2}\psi_a(0,\delta)-\varphi_a(t,\delta)\|\leqslant 3c\,\delta^{\min(p_1,p_2)}. \tag{5.4}$$

Proof: uses just the unitarity of the evolution group and the Cauchy–Schwarz inequality. □

Our approximate B–O states will require classical quantities defined by means of an approximation $\tilde{V}^{\mathcal{C}}$ of the potential $V^{\mathcal{C}}$ used in (4.38), (4.42). We have to estimate the error induced by this approximation. In order to do that, we make use of Gronwall's lemma (see e.g., Ref. 19) that we recall below.

Lemma V.2: Let E be a Banach space, $U\subset E$ be open, I be an interval of $\mathbb{R}$, and $f\in C^1(I\times U;E)$ be such that there exists $K>O$ with $\sup_{(t,x)\in I\times U}\|D_2f(t,x)\|_{\mathcal{L}(E)}\leqslant K$. Let $g:I\times U\to E$ be continuous and such that there exists $G>0$ with

$$\sup_{(t,x)\in I\times U}\|g(t,x)\|\leqslant G. \tag{5.5}$$

If α and β are C^1 maps from $J\to U$ (where $J\subseteq I$) satisfying for $t\in J$,

$$\alpha'(t)=f(t,\alpha(t)), \tag{5.6}$$

$$\beta'(t)=f(t,\beta(t))+\epsilon g(t,\beta(t)), \tag{5.7}$$

then

$$\|\alpha(t)-\beta(t)\| \leqslant \|\alpha(t_0)-\beta(t_0)\| e^{K|t-t_0|} + \epsilon G(e^{K|t-t_0|}-1)/K. \tag{5.8}$$

For convenience let us recall here our definition (4.66) of a Born–Oppenheimer state $\psi_j^{\mathcal{C}}(x,\delta,t)$ in the exterior regime,

$$\psi_j^{\mathcal{C}}(x,\delta,t) = F(\|x-a^{\mathcal{C}}(t)\|/\delta^{1-\delta'})\varphi_j(A^{\mathcal{C}}(t), B^{\mathcal{C}}(t), \delta^2, a^{\mathcal{C}}(t), \eta^{\mathcal{C}}(t), x) e^{iS^{\mathcal{C}}(t)/\delta^2}\Phi_{\mathcal{C}}^{\pm}(x,t,\delta). \tag{5.9}$$

We want to compare $\psi_j^{\mathcal{C}}(x,\delta,t)$ with an altered but similar definition based on approximate quantum and classical quantities for $\tilde{\psi}_j^{\mathcal{C}}(x,\delta,t)$,

$$\tilde{\psi}_j^{\mathcal{C}}(x,\delta,t) = F(\|x-\tilde{a}^{\mathcal{C}}(t)\|/\delta^{1-\delta'})\varphi_j(\tilde{A}^{\mathcal{C}}(t), \tilde{B}^{\mathcal{C}}(t), \delta^2, \tilde{a}^{\mathcal{C}}(t), \tilde{\eta}^{\mathcal{C}}(t), x) e^{i\tilde{S}^{\mathcal{C}}(t)/\delta^2}\tilde{\Phi}_{\mathcal{C}}^{\pm}(x,t,\delta). \tag{5.10}$$

All "tilded" classical quantities are generated by Eqs. (4.38), (4.42) with an approximate potential $\tilde{V}^{\mathcal{C}}(x,\delta)$ in place of $V^{\mathcal{C}}(x,\delta)$. The vector

$$\tilde{\Phi}_{\mathcal{C}}^{\pm}(x,t,\delta) = \tilde{\Phi}_{\mathcal{C}}^{\pm}(x,\delta) e^{i\tilde{\lambda}_{\mathcal{C}}^{\pm}(x,t,\delta)} \tag{5.11}$$

depends on the approximate classical quantities through the phase $\tilde{\lambda}_{\mathcal{C}}^{\pm}$ and on an approximate normalized quantum eigenstate $\tilde{\Phi}_{\mathcal{C}}^{\pm}(x,\delta)$. Note that we keep the same Gaussian function φ_j to construct the "nuclear" wave packet.

Our next goal is to apply Lemma V.1 to estimate the errors in terms of the difference between $\tilde{V}^{\mathcal{C}}$ and $V^{\mathcal{C}}$.

Lemma V.3: The following inequality holds in the outer time regime for the $L^2(\mathbb{R})$ norm:

$$\begin{aligned}
&\|\psi_j^{\mathcal{C}^{\pm}}(x,\delta,t) - \tilde{\psi}_j{}^{\mathcal{C}^{\pm}}(x,\delta,t)\| \\
&\leqslant c\Bigg(|\tilde{A}(t)-A(t)| + |\tilde{B}(t)-B(t)| + |\tilde{a}(t)-a(t)|/\delta^2 \\
&\quad + |\tilde{\eta}(t)-\eta(t)|/\delta^2 + \frac{|t|}{\delta^2}\sup_{s\in[0,t]}\left(|\tilde{\eta}(s)-\eta(s)| + |\tilde{V}(a(s))-V(a(s))|\right. \\
&\quad + \sup_{x\in[\tilde{a}(s),a(s)]}|\partial_x\tilde{V}(x)||\tilde{a}(s)-a(s)|) + \sup_{(x,t,\delta)}|F(\|x-\tilde{a}(t)\|/\delta^{1-\delta'})\tilde{\Phi}_{\mathcal{C}}^{\pm}(x,t,\delta) \\
&\quad \left. - F(\|x-a(t)\|/\delta^{1-\delta'})\Phi_{\mathcal{C}}^{\pm}(x,t,\delta)|.\right)
\end{aligned} \tag{5.12}$$

with some constant c.

Proof: The index $\mathcal{C}$ being fixed in this context, it will now be omitted. Other irrelevant parameters will also be dropped in the arguments. Note that since the function F is smooth, we can write

$$F(\|x-\tilde{a}(t)\|/\delta^{1-\delta'}) = F(\|x-a(t)\|/\delta^{1-\delta'}) + \mathcal{O}((\tilde{a}(t)-a(t))/\delta^{1-\delta'}) \tag{5.13}$$

and that the $L^2(S^1)$-norm of the vectors $\Phi_{\mathcal{C}}^{\pm}(x,t,\delta)$ equals one. Since

$$\tilde{V}(\tilde{a}) - V(a) = \tilde{V}(\tilde{a}) - \tilde{V}(a) + \tilde{V}(a) - V(a) \tag{5.14}$$

and η and $\tilde{\eta}$ are uniformly bounded, we infer

$$\tilde{S}(t)=\int_0^t(\tilde{\eta}^2(s)/2-\tilde{V}(\tilde{a}(s))ds)$$

$$=S(t)+\mathcal{O}\Big(|t|\sup_{s\in[0,t]}\Big(|\tilde{\eta}(s)-\eta(s)|+|\tilde{V}(a(s))-V(a(s))|$$

$$+\sup_{x\in[\tilde{a}(s),a(s)]}|\partial_x\tilde{V}(x)||\tilde{a}(s)-a(s)|\Big)\Big). \tag{5.15}$$

Then we compute

$$\varphi_l(\tilde{A},\tilde{B},\delta^2,\tilde{a},\tilde{\eta},x)-\varphi_l(A,B,\delta^2,a,\eta,x)$$

$$=e^{i\tilde{\eta}(x-\tilde{a})/\delta^2}(\varphi_l(\tilde{A},\tilde{B},\delta^2,\tilde{a},0,x)-\varphi_l(A,B,\delta^2,a,0,x))$$

$$+\varphi_l(A,B,\delta^2,a,0,x)(e^{i\tilde{\eta}((a-\tilde{a})/\delta^2)}-e^{i(\eta-\tilde{\eta})(x-a)/\delta^2})e^{i\tilde{\eta}(x-a)/\delta^2}. \tag{5.16}$$

From Lemma 3.1 in Ref. 13 we learn that as $\tilde{A}\to A$ and $\tilde{B}\to B$,

$$\varphi_l(\tilde{A},\tilde{B},\delta^2,\tilde{a},0,x)=\varphi_l(A,B,\delta^2,a,0,x)+\mathcal{O}(|\tilde{A}-A|+|\tilde{B}-B|+|\tilde{a}-a|/\delta)$$

holds in the $L^2(\mathbb{R})$ sense, which takes care of the first term. Then we note that the L^2 norm of the remaining term is equal to

$$\|\varphi_l(A,B,\delta^2,a,0,x)e^{i\tilde{\eta}((a-\tilde{a})/\delta^2)}-\varphi_l(A,B,\delta^2,a,\eta-\tilde{\eta},x)\|$$

$$=\|\varphi_l(B,A,\delta^2,0,-a,x)e^{i\tilde{\eta}(a-\tilde{a})/\delta^2}-e^{-i(\eta-\tilde{\eta})a/\delta^2}\varphi_l(B,A,\delta^2,\eta-\tilde{\eta},-a,x)\|$$

$$=\mathcal{O}((\tilde{a}-a)/\delta^2+(\tilde{\eta}-\eta)/\delta^2) \tag{5.17}$$

by using the Plancherel formula, the properties of the φ_j under Fourier transform, $\|\varphi_j\|=1$ and the above lemma again. Then, gathering these estimates and using the facts that $A(t)$ and $B(t)$ are uniformly bounded, we get the result. □

In order to use this lemma, we see that it is necessary to approximate $V^{\mathcal{C}}$ to an error of order $o(\delta^2)$ and to show that this induces errors of the same order in the classical trajectory $(\tilde{a}^{\mathcal{C}},\tilde{\eta}^{\mathcal{C}})$ and errors of order $o(1)$ in the linearized classical flow $(\tilde{A}^{\mathcal{C}},\tilde{B}^{\mathcal{C}})$. Moreover, the corresponding eigenstates $\tilde{\Phi}^{\pm}_{\mathcal{C}}$ should be at most at a distance $o(1)$ from $\Phi^{\pm}_{\mathcal{C}}$.

When we consider times away of the matching regime, i.e., $\tau\leqslant|t|\leqslant T$, where τ is independent of δ, it is easy to show the following result, just by using Gronwall's lemma and regular perturbation theory. We thus omit the proof.

Lemma V.4: Let the time interval (τ,T) be such that the solutions to (4.38), (4.40) satisfy the condition,

$$0\notin\{a^{\mathcal{C}}(t)\,|\,\tau\leqslant t\leqslant T,\quad 0<\delta<\delta_0\}\equiv P, \tag{5.18}$$

where the corresponding potential,

$$V^{\mathcal{C}}(x,\delta)=\mu^{\mathcal{C}}(x,\delta),\quad x\in P, \tag{5.19}$$

is the nondegenerate eigenvalue of $g(x,\delta)$ corresponding to $\Phi_{\mathcal{C}}(x,\delta)$. Let

$$\tilde{V}^{\mathcal{C}}(x,\delta)=\mu_0^{\mathcal{C}}(x)+\delta\mu_1^{\mathcal{C}}(x)+\delta^2\mu_2^{\mathcal{C}}(x),\quad x\in P, \tag{5.20}$$

be the second-order perturbation expansion for $\mu^{\mathcal{C}}(x,\delta)$. *We define* $\tilde{a}^{\mathcal{C}},\tilde{\eta}^{\mathcal{C}},\tilde{A}^{\mathcal{C}},\tilde{B}^{\mathcal{C}},\tilde{S}^{\mathcal{C}}$ *as above with the conditions,*

$$\tilde{a}^{\mathcal{C}}(\tau)=a^{\mathcal{C}}(\tau)+o(\delta^2),\quad \tilde{\eta}^{\mathcal{C}}(\tau)=\eta^{\mathcal{C}}(\tau)+o(\delta^2), \tag{5.21}$$

$$\tilde{A}^{\mathcal{C}}(\tau)=A^{\mathcal{C}}(\tau)+o(1),\quad \tilde{B}^{\mathcal{C}}(\tau)=B^{\mathcal{C}}(\tau)+o(1), \tag{5.22}$$

$$\tilde{S}^{\mathcal{C}}(\tau)=S^{\mathcal{C}}(\tau)+o(\delta^2), \tag{5.23}$$

and

$$\tilde{\Phi}_{\mathcal{C}}(x,t,\delta)=\Phi_{\mathcal{C}}(x,0)\mathrm{e}^{i\tilde{\lambda}_{\mathcal{C}}(x,t,\delta)}, \tag{5.24}$$

where $\tilde{\lambda}_{\mathcal{C}}(x,t,\delta)$ *is given by (4.54) with* $\Phi_{\mathcal{C}}(x,0)$ *in place of* $\Phi_{\mathcal{C}}(x,\delta)$ *and*

$$\tilde{\lambda}_{\mathcal{C}}(x,\tau,\delta)=\lambda_{\mathcal{C}}(x,\tau,\delta)+o(1). \tag{5.25}$$

Then there exists a solution $\psi(x,t,\delta)$ *to Eq. (4.13) such that*

$$\psi(x,t,\delta)=F(\|x-\tilde{a}^{\mathcal{C}}(t)\|/\delta^{1-\delta'})\varphi_j(\tilde{A}^{\mathcal{C}}(t),\tilde{B}^{\mathcal{C}}(t),\delta^2,\tilde{a}^{\mathcal{C}}(t),\tilde{\eta}^{\mathcal{C}}(t),x)\mathrm{e}^{i\tilde{S}^{\mathcal{C}}(t)/\delta^2}\tilde{\Phi}_{\mathcal{C}}(x,t,\delta)+o(1) \tag{5.26}$$

holds true in the L^2*-sense and for all* $\tau\leqslant t\leqslant T$.

Remark: We have the familiar explicit formulas,

$$\mu_0^{\mathcal{C}}(x)=\mu^{\mathcal{C}}(x,0), \tag{5.27}$$

$$\mu_1^{\mathcal{C}}(x)=\langle\Phi_{\mathcal{C}}(x,0)|W(x)\Phi_{\mathcal{C}}(x,0)\rangle, \tag{5.28}$$

$$\mu_2^{\mathcal{C}}(x)=-\langle\Phi_{\mathcal{C}}(x,0)|W(x)(h(x)-\mu^{\mathcal{C}}(x,0))_r^{-1}W(x)\Phi_{\mathcal{C}}(x,0)\rangle, \tag{5.29}$$

where the reduced resolvent is given by

$$(h(x)-\mu^{\mathcal{C}}(x,0))_r^{-1}=\sum_{j\neq\mathcal{C}}\frac{|\Phi_j(x,0)\rangle\langle\Phi_j(x,0)|}{(\mu^j(x,0)-\mu^{\mathcal{C}}(x,0))}. \tag{5.30}$$

The above result has to be modified for times close to the matching regime, since in that case degenerate perturbation theory is required to define the potential. Indeed, the approximate potential chosen in the lemma diverges as $x\to 0$, so that Gronwall's lemma cannot be used as it stands. Let us find the modified potential from perturbation theory.

The two eigenvalues of $g(x,\delta)$ which are of interest to us, $\mu_{\mathcal{A}}(x,\delta)$ and $\mu_{\mathcal{B}}(x,\delta)$, are given by the spectrum of $P(x,\delta)(h(x)+\delta W(x)+V_2(x))$. This operator is represented in the smooth orthonormal eigenbasis (4.21) by the matrix (4.22), which we can expand to second order in δ for any x in a neighborhood of the origin, since the projection $P(x,\delta)$ entering the definition of the basis (4.21) is regular. Hence we can write

$$g_{\|}(x,\delta)=\begin{pmatrix}\beta(x,\delta) & \gamma(x,\delta)+i\sigma(x,\delta)\\ \gamma(x,\delta)-i\sigma(x,\delta) & -\beta(x,\delta)\end{pmatrix}+\overline{V}(x,\delta), \tag{5.31}$$

where

$$\beta(x,\delta)=\beta_0(x)+\delta\beta_1(x)+\delta^2\beta_2(x)+\mathcal{O}(\delta^3)\equiv B_3(x,\delta)+\mathcal{O}(\delta^3), \tag{5.32}$$

$$\gamma(x,\delta)=\gamma_0(x)+\delta\gamma_1(x)+\delta^2\gamma_2(x)+\mathcal{O}(\delta^3)\equiv G_3(x,\delta)+\mathcal{O}(\delta^3), \tag{5.33}$$

$$\sigma(x,\delta)=\sigma_0(x)+\delta\sigma_1(x)+\delta^2\sigma_2(x)+\mathcal{O}(\delta^3)\equiv S_3(x,\delta)+\mathcal{O}(\delta^3), \tag{5.34}$$

$$\overline{V}(x,\delta)=\overline{V}_0(x)+\delta\overline{V}_1(x)+\delta^2\overline{V}_2(x)+\mathcal{O}(\delta^3)\equiv V_3(x,\delta)+\mathcal{O}(\delta^3), \tag{5.35}$$

with the error $\mathcal{O}(\delta^3)$ being C^∞ in x, and [see (4.30)],

$$\beta_0(x)=rx+\mathcal{O}(x^2),\quad \beta_1(x)=\mathcal{O}(x), \tag{5.36}$$

$$\gamma_0(x)=\mathcal{O}(x^2),\quad \gamma_1(x)=r+\mathcal{O}(x), \tag{5.37}$$

$$\sigma_0(x)=\mathcal{O}(x^2),\quad \sigma_1(x)=\mathcal{O}(x). \tag{5.38}$$

Let us set

$$s(x,\delta)=\sqrt{(B_3(x,\delta))^2+(G_3(x,\delta))^2+(S_3(x,\delta))^2} \tag{5.39}$$

and define our (explicit) modified potential by

$$\tilde{V}^{\mathcal{C}}(x,\delta)=\pm s(x,\delta)+V_3(x,\delta), \tag{5.40}$$

where the sign is chosen according to the value of $\mathcal{C}$. It is easy to check that by construction,

$$V^{\mathcal{C}}(x,\delta)-\tilde{V}^{\mathcal{C}}(x,\delta)=\mathcal{O}(\delta^3) \tag{5.41}$$

as $x\to 0$. As above, we employ tilde to mark the values generated by the modified potential. We only consider the dynamics for positive times, the other case being similar.

To define the perturbed classical trajectory, we will start integrating Newton's equations from a positive $t_0(\delta)=\delta^\kappa$, for some $2/3<\kappa<1$, using as initial condition the explicit asymptotic expansion given in Corollary 2.1 of Ref. 13,

Corollary V.5: In the outer regime $\delta\to 0$, $t\to 0$, $|t|/\delta\to\infty$ and $t^3/\delta^2\to 0$, we have

$$\begin{aligned} a^{\mathcal{A}}_{\mathcal{B}}(t)=&-\partial_x\overline{V}_3(0,\delta)\frac{t^2}{2}+\eta^0(\delta)t\pm\frac{r}{\eta^0(\delta)}\delta t\\ &\mp r\left[\frac{t^2}{2}+\frac{\delta^2\ln|t|}{2(\eta^0(\delta))^2}+\frac{\delta^2}{4(\eta^0(\delta))^2}(1+2\ln(2\eta^0(\delta)))-\frac{\delta^2\ln\delta}{2(\eta^0(\delta))^2}\right]\\ &+\mathcal{O}(t^3)+\mathcal{O}(\delta^4/t^2). \end{aligned}$$

The asymptotics for $\eta^{\mathcal{C}}(t)$ in the same regime is obtained by termwise differentiation of the above formulas up to errors $\mathcal{O}(t^2)+\mathcal{O}(\delta^4/t^3)$.

The choice of $t_0(\delta)$ ensures that

$$\tilde{a}(t_0)=a(t_0)+o(\delta^2), \tag{5.42}$$

$$\tilde{\eta}(t_0)=\eta(t_0)+o(\delta). \tag{5.43}$$

Whereas the error is small enough for the position, it is not the case for the momentum. Hence we resort to energy conservation in order to determine the momentum with sufficient accuracy.

Let us first note that due to the uniform boundedness of the force induced by the potentials $V^{\mathcal{C}}$ and $\tilde{V}^{\mathcal{C}}$, there exists $\tau>0$, small but independent of δ, and constants $0<C_1<C_2<\infty$, such that as long as $t\in[-\tau,\tau]$,

$$C_1<\eta^{\mathcal{C}}(t)<C_2, \tag{5.44}$$

and similarly for $\tilde{\eta}^{\mathcal{C}}$.

The unperturbed energy is given by

$$E^{\mathcal{C}}(\delta)=(\eta^{\mathcal{C}}(t))^2/2+V^{\mathcal{C}}(a^{\mathcal{C}}(t),\delta)=(\eta_0^{\mathcal{C}}(\delta))^2/2+V^{\mathcal{C}}(0,\delta)$$

$$\equiv\tilde{E}^{\mathcal{C}}(\delta)+V^{\mathcal{C}}(0,\delta)-\tilde{V}^{\mathcal{C}}(0,\delta), \tag{5.45}$$

where the perturbed energy $\tilde{E}^{\mathcal{C}}(\delta)$ is explicit. Hence

$$\eta^{\mathcal{C}}(t)=\sqrt{2(E^{\mathcal{C}}(\delta)-V^{\mathcal{C}}(a^{\mathcal{C}}(t),\delta))}>0 \tag{5.46}$$

holds for $t\in[-\tau,\tau]$, and we can define $\tilde{\eta}^{\mathcal{C}}(t)$ by energy conservation so that

$$\tilde{\eta}^{\mathcal{C}}(t):=\sqrt{2(\tilde{E}^{\mathcal{C}}(\delta)-\tilde{V}^{\mathcal{C}}(\tilde{a}^{\mathcal{C}}(t),\delta))}$$

$$=\eta^{\mathcal{C}}(t)+\mathcal{O}(\tilde{V}^{\mathcal{C}}(\tilde{a}^{\mathcal{C}}(t),\delta)-V^{\mathcal{C}}(a^{\mathcal{C}}(t),\delta))+\mathcal{O}(\tilde{V}^{\mathcal{C}}(0,\delta)-V^{\mathcal{C}}(0,\delta))$$

$$=\eta^{\mathcal{C}}(t)+\mathcal{O}\left(\sup_{x\to 0}|\tilde{V}^{\mathcal{C}}(x,\delta)-V^{\mathcal{C}}(x,\delta)|+\tilde{a}^{\mathcal{C}}(t)-a^{\mathcal{C}}(t)\right). \tag{5.47}$$

Thus using formula (5.47), we make an error in $\eta^{\mathcal{C}}$ of the same order as the error we make in $a^{\mathcal{C}}$ and $V^{\mathcal{C}}$.

Next we turn to the approximations $\tilde{A}^{\mathcal{C}}(t)$ and $\tilde{B}^{\mathcal{C}}(t)$. They are defined as solutions to the system (4.42) with $\tilde{V}^{\mathcal{C}}$ in place of $V^{\mathcal{C}}$ and initial conditions at $t=\pm t_0$, given by

$$\begin{pmatrix}\tilde{A}^{\mathcal{A}}_{\mathcal{B}}(t)\\ \tilde{B}^{\mathcal{A}}_{\mathcal{B}}(t)\end{pmatrix}=\begin{pmatrix}A(0)\\ B(0)\mp\mathrm{sign}(t)irA(0)/(\eta_0(\delta))\end{pmatrix}. \tag{5.48}$$

It remains finally to consider the perturbed eigenvectors $\tilde{\Phi}_{\mathcal{C}}(x,t,\delta)$ (where we dropped the index referring to the sign of t). The restrictions to the support of F mentioned in lemma V.3 and the estimate (5.44) imply that if we impose the condition

$$1-\delta'-\kappa>0, \tag{5.49}$$

we can write

$$x=a(t)+\mathcal{O}(\delta^{1-\delta'})\geqslant ct(1+\mathcal{O}(\delta^{1-\delta'-\kappa})\geqslant c\,\delta^{\kappa} \tag{5.50}$$

for some positive constant c, and the same estimate is true with a replaced by $\tilde{a}$.

Hence in the considered regime the eigenvalues $\mu^{\mathcal{C}}(x,0)$ of $P(x,0)(h(x)+V_2(x))$ display a gap that is at least of order $x=\mathcal{O}(\delta^{\kappa})$—see the behavior (4.30)—and we call the corresponding eigenvectors $\chi_{\mathcal{C}}(x)$. We define our perturbed static eigenvectors by

$$\tilde{\Phi}_{\mathcal{C}}(x,\delta)=\chi_{\mathcal{C}}(x) \tag{5.51}$$

and similarly, the phase corresponding to time dependent perturbed eigenvectors $\tilde{\Phi}_{\mathcal{C}}(x,t,\delta)$—in view (5.11)—by

$$\tilde{\lambda}_{\mathcal{C}r}(\omega,t,\delta)=i\int_{t_0(\delta)}^{t}ds\,\tilde{\eta}(s)\langle\tilde{\Phi}_{\mathcal{C}}(\omega+\tilde{a}(s),\delta)|\partial_x\tilde{\Phi}_{\mathcal{C}}(\omega+\tilde{a}(s),\delta)\rangle, \tag{5.52}$$

where we used the new variables (4.56) and (4.60).

The next lemma tells us that our definitions of $(\tilde{a}^{\mathcal{C}}(t),\tilde{\eta}^{\mathcal{C}}(t))$, $(\tilde{A}^{\mathcal{C}}(t),\tilde{B}^{\mathcal{C}}(t))$, and $\tilde{\Phi}_{\mathcal{C}}(x,\delta,t)$ are accurate enough for our purpose. The proof can be found in the Appendix.

Lemma V.6: With the definitions above, there exists a positive τ such that for all $t\in[t_0(\delta),\tau]$ we have

$$\tilde{a}^{\mathcal{C}}(t)=a^{\mathcal{C}}(t)+o(\delta^2), \tag{5.53}$$

$$\tilde{\eta}^{\mathcal{C}}(t)=\eta^{\mathcal{C}}(t)+o(\delta^2), \tag{5.54}$$

$$\tilde{A}^{\mathcal{C}}(t)=A^{\mathcal{C}}(t)+o(1), \tag{5.55}$$

$$\tilde{B}^{\mathcal{C}}(t)=B^{\mathcal{C}}(t)+o(1), \tag{5.56}$$

$$\tilde{\Phi}(x,t,\delta)=\Phi(x,t,\delta)+o(1). \tag{5.57}$$

Hence, with the definitions made above, we have a perturbed B–O state given by (5.10) that is explicitly expressed by means of perturbation theory in δ (modulo finding the solution of the classical equations of motion, of course) and which yields an approximation of the solution to the Schrödinger equation (4.13) for finite time intervals as $\delta\to 0$. In particular, putting together our results, we get the following statement:

Theorem V.7: *Adopt the hypotheses (H1) and (H2) and assume the behaviors (4.30). Suppose that* $2/3<\kappa<1$ *and* τ *is as in the above lemma. Let* $\tilde{\psi}_j^{\mathcal{C}\pm}(x,\delta,t)$ *with* $|t|\geqslant\delta^\kappa$ *be a perturbed B–O state according to (5.10) constructed by means of the approximate quantities considered in lemma V.4 if* $|t|\geqslant\tau$ *and in lemma V.6 if* $\delta^\kappa<|t|<\tau$*, subject to the condition that all classical quantities agree at the instants* $t=\pm\tau$*. Let* $\psi(x,\delta,t)$ *be a solution to Eq. (4.13) with* $\psi(x,\delta,-T)=\tilde{\psi}_j^{\mathcal{B}-}(x,\delta,-T)$*. Then,*

$$\psi(x,\delta,t)=\tilde{\psi}_j^{\mathcal{B}-}(x,\delta,t)+o(1), \tag{5.58}$$

holds as $\delta\to 0$ *for all* $-T\leqslant t\leqslant-\delta^\kappa$*, while*

$$\psi(x,\delta,t)=-\mathrm{e}^{-\pi r/2\eta^0}\tilde{\psi}_j^{\mathcal{A}+}(x,\delta,t)+\mathrm{e}^{-\pi r/4\eta^0}\sqrt{\frac{\pi r}{\eta^0}}\frac{\mathrm{e}^{i\lambda(\delta)}}{\Gamma\left(1+\dfrac{ir}{2\eta^0}\right)}\tilde{\psi}_j^{\mathcal{B}+}(x,\delta,t)+o(1) \tag{5.59}$$

holds for all $\delta^\kappa\leqslant t\leqslant T$*, with* $\lambda(\delta)$ *given by (4.78).*

Remarks:

(1) As a direct corollary, we get that to leading order, the transition probability $\mathcal{P}$ from the initial level $\mathcal{B}$ to the level $\mathcal{A}$ is given by the Landau–Zener formula,

$$\mathcal{P}=\mathrm{e}^{-\pi r/\eta^0}+o(1) \tag{5.60}$$

as $\delta\to 0$, where r is defined by the behavior (4.30) of the ''molecular'' Hamiltonian around the avoided crossing and η^0 is the initial classical momentum, see (4.40).

(2) It is possible also to give an explicit approximation of the wave function in the inner time regime, $-\delta^\kappa\leqslant t\leqslant\delta^\kappa$, in terms of quantities coming from perturbation theory. However, this temporal region being so short, it is not crucial for most applications to have a detailed approximation there.

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APPENDIX

Proof of Proposition IV.2: It is enough to show that the norm of ζ_l^1 in (4.81) is small and to apply to Lemma IV.1. Expression (4.15) together with (H1) show that we only need to control the effect of $p=-i\delta^2\partial_x$ and $p^2=(-i\delta^2\partial_x)^2$ on $\Psi_l(x,t,\delta)$, since for any ψ we have

$$\|Y(x,\partial_x,\delta)\psi\|\leqslant C(\delta^4\|p^2\psi\|+\delta^6\|p\psi\|). \tag{A1}$$

First consider the outer temporal region and the form (4.66). We know from the computations in Ref. 18 that

$$\|(p-\eta)\varphi_l(A,B,\delta^2,a,\eta,\cdot)\|=|B|\delta\sqrt{l+1/2}, \tag{A2}$$

$$\|(p-\eta)^2\varphi_l(A,B,\delta^2,a,\eta,\cdot)\|=|B|^2\delta^2\sqrt{(6l^2+6l+3)/4}. \tag{A3}$$

Moreover, we estimate

$$|pF(\|x-a^{\mathcal{C}}(t)\|/\delta^{1-\delta'})|\leqslant c_1\delta^{1+\delta'}, \tag{A4}$$

$$|p^2F(\|x-a^{\mathcal{C}}(t)\|/\delta^{1-\delta'})|\leqslant c_2\delta^{2(1+\delta')}, \tag{A5}$$

where the constants c_1,c_2 depend on F only. Away from the crossing region, the "electronic" eigenvectors are well defined and smooth in (x,δ). Hence we only need to consider what is going on in the neighborhood of $x=0$ to get an upper bound on the effect of p and p^2 on the eigenvectors $\Phi_{\mathcal{C}}^{\pm}(x,t,\delta)$ given by (4.53). We drop the indices and consider

$$\Phi(x,t,\delta)=\mathrm{e}^{i\lambda(x,t,\delta)}\Phi(x,\delta), \tag{A6}$$

where $\Phi(x,\delta)$ denote some static eigenvectors and $\lambda(x,\delta,t)$ the corresponding real valued function defined by (4.54). We compute

$$\partial_x\Phi(x,t,\delta)=\mathrm{e}^{i\lambda(x,t,\delta)}[\partial_x\Phi(x,\delta)+(i\partial_x\lambda(x,t,\delta))\Phi(x,\delta)], \tag{A7}$$

$$\begin{aligned}\partial_x^2\Phi(x,t,\delta)=\mathrm{e}^{i\lambda(x,t,\delta)}[&\partial_x^2\Phi(x,\delta)+2(i\partial_x\lambda(x,t,\delta))\partial_x\Phi(x,\delta)\{i\partial_x^2\lambda(x,t,\delta)\\&-(\partial_x\lambda(x,t,\delta))^2\}\Phi(x,\delta)].\end{aligned} \tag{A8}$$

As $\eta,\psi_j,\partial_x\psi_j,\partial_x^2\psi_j,\partial_x^3\psi_j$ are all $\mathcal{O}(0)$ as $(x,t)\to(0,0)$ in the support of F, we have

$$\partial_x\Phi(x,\delta)=\mathcal{O}(\partial_x\theta(x)+\partial_x\varphi(x))+\mathcal{O}(0), \tag{A9}$$

$$\partial_x^2\Phi(x,\delta)=\mathcal{O}((\partial_x\theta(x))^2+(\partial_x\varphi(x))^2+\partial_x^2\theta(x)+\partial_x^2\varphi(x))+\mathcal{O}(0) \tag{A10}$$

in the norm of the "electronic" Hilbert space. In expression (4.60) for λ, we first check by inspection that in all cases,

$$\langle\Phi|\partial_x\Phi\rangle=\mathcal{O}(\partial_x\varphi)+\mathcal{O}(0) \tag{A11}$$

(see, e.g., (3.50) in Ref. 13) since all functions of θ and ϕ are uniformly bounded and, moreover, the factor of $\partial_x\varphi$ is a function of θ only. Hence, by further differentiation we get

$$\partial_x\langle\Phi|\partial_x\Phi\rangle=\mathcal{O}(\partial_x^2\varphi+\partial_x\varphi+\partial_x\varphi\partial_x\theta+\partial_x\theta)+\mathcal{O}(0), \tag{A12}$$

$$\begin{aligned}\partial_x^2\langle\Phi|\partial_x\Phi\rangle=\mathcal{O}(&\partial_x^3\varphi+\partial_x^2\varphi\partial_x\theta+\partial_x\varphi\partial_x^2\theta+(\partial_x\varphi)^2\\&+\partial_x^2\varphi\partial_x\varphi\partial_x\theta+\partial_x^2\theta+(\partial_x\theta)^2+\partial_x\theta+\partial_x\varphi)+\mathcal{O}(0).\end{aligned} \tag{A13}$$

It remains to estimate $\partial_x\varphi$ and $\partial_x\theta$. We have

$$\varphi(x,\delta)=\arctan(\sigma(x,\delta)/\gamma(x,\delta)) \tag{A14}$$

provided $\gamma(x,\delta)$ is different from zero. Hence using (4.30) we get

$$\partial_x\varphi(x,\delta)=\frac{\gamma(x,\delta)\partial_x\sigma(x,\delta)-\sigma(x,\delta)\partial_x\gamma(x,\delta)}{\gamma^2(x,\delta)+\sigma^2(x,\delta)}, \tag{A15}$$

so that with the help of estimates of the type $|\gamma|/\sqrt{\gamma^2+\sigma^2}\leqslant 1$ we arrive at

$$\partial_x\varphi=\mathcal{O}\left(\frac{\partial_x\gamma+\partial_x\sigma}{\sqrt{\gamma^2+\sigma^2}}\right). \tag{A16}$$

By similar operations we eventually obtain

$$\partial_x^2\varphi=\mathcal{O}\left(\frac{\partial_x^2\gamma+\partial_x^2\sigma}{\sqrt{\gamma^2+\sigma^2}}\right)+\mathcal{O}\left(\frac{(\partial_x\gamma)^2+(\partial_x\sigma)^2+\partial_x\gamma\partial_x\sigma}{\gamma^2+\sigma^2}\right) \tag{A17}$$

and

$$\partial_x^3\varphi=\mathcal{O}\left(\frac{\partial_x^3\gamma+\partial_x^3\sigma}{\sqrt{\gamma^2+\sigma^2}}\right)+\mathcal{O}\left(\frac{\partial_x^2\gamma\partial_x\sigma+\partial_x^2\sigma\partial_x\gamma+\partial_x^2\gamma\partial_x\gamma+\partial_x^2\sigma\partial_x\sigma}{\gamma^2+\sigma^2}\right)$$
$$+\mathcal{O}\left(\frac{(\partial_x\gamma)^2\partial_x\sigma+(\partial_x\sigma)^2\partial_x\gamma+(\partial_x\gamma)^3+(\partial_x\sigma)^3}{\sqrt{\gamma^2+\sigma^2}^3}\right). \tag{A18}$$

Assuming further that

$$\|x\|=\mathcal{O}(\delta^\kappa),\quad \xi<2/3<\kappa<1-\xi<1, \tag{A19}$$

we get from the behavior (4.30) in this region

$$\partial_x\varphi=\mathcal{O}\left(\frac{1}{\delta^{1-\kappa}}\right), \tag{A20}$$

$$\partial_x^2\varphi=\mathcal{O}\left(\frac{1}{\delta}\right), \tag{A21}$$

$$\partial_x^3\varphi=\mathcal{O}\left(\frac{1}{\delta^{2-\kappa}}\right). \tag{A22}$$

Then we consider

$$\theta(x,\delta)=\arccos\left(\frac{\beta(x,\delta)}{\sqrt{\beta^2(x,\delta)+\gamma^2(x,\delta)+\sigma^2(x,\delta)}}\right). \tag{A23}$$

By computing derivatives and estimating as above, we easily get

$$\partial_x\theta=\mathcal{O}\left(\frac{\partial_x\beta}{\beta^2+\gamma^2+\sigma^2}\right)+\mathcal{O}\left(\frac{\partial_x\gamma+\partial_x\sigma}{\sqrt{(\beta^2+\gamma^2+\sigma^2)(\gamma^2+\sigma^2)}}\right), \tag{A24}$$

$$\partial_x^2\theta=\mathcal{O}\left(\frac{\partial_x^2\beta}{\beta^2+\gamma^2+\sigma^2}\right)+\mathcal{O}\left(\frac{\partial_x^2\gamma+\partial_x^2\sigma}{\sqrt{(\beta^2+\gamma^2+\sigma^2)(\gamma^2+\sigma^2)}}\right)+\mathcal{O}\left(\frac{\partial_x\beta(\partial_x\gamma+\partial_x\sigma)}{(\beta^2+\gamma^2+\sigma^2)\sqrt{(\gamma^2+\sigma^2)}}\right)$$
$$+\mathcal{O}\left(\frac{(\partial_x\gamma)^2+(\partial_x\sigma)^2+\partial_x\gamma\partial_x\sigma}{\sqrt{(\beta^2+\gamma^2+\sigma^2)}(\gamma^2+\sigma^2)}\right)+\mathcal{O}\left(\frac{(\partial_x\beta)^2}{\sqrt{\beta^2+\gamma^2+\sigma^{23}}}\right). \tag{A25}$$

Using (4.65), $\delta^\kappa C\geqslant|t|\geqslant\delta^{1-\xi}$, and (A19), we thus find

$$\partial_x\theta=\mathcal{O}\left(\frac{1}{\delta^{2(1-\xi)}}\right), \tag{A26}$$

$$\partial_x^2\theta=\mathcal{O}\left(\frac{1}{\delta^{3(1-\xi)}}\right). \tag{A27}$$

Gathering the different pieces, we obtain for the derivatives of λ in the regime just described

$$\lambda(x,t,\delta)=\mathcal{O}(t/\delta^{1-\kappa})=\mathcal{O}(1/\delta^{1-2\kappa}), \tag{A28}$$

$$\partial_x\lambda(x,t,\delta)=\mathcal{O}(1/\delta^{3-2\xi-2\kappa}), \tag{A29}$$

$$\partial_x^2\lambda(x,t,\delta)=\mathcal{O}(1/\delta^{4-4\xi-\kappa}), \tag{A30}$$

so that we obtain the following estimates for the derivatives of the vector $\Phi(x,t,\delta)$:

$$\partial_x\Phi(x,t,\delta)=\mathcal{O}(1/\delta^{2-2\xi}), \tag{A31}$$

$$\partial_x^2\Phi(x,t,\delta)=\mathcal{O}(1/\delta^{4-4\xi}). \tag{A32}$$

We are now in a position to estimate the effect of p and p^2 on the B–O states in the outer time regime,

$$\|p\psi_l^{\mathcal{C}}\|=\|(pF)\varphi_l\Phi^{\mathcal{C}}+F(p\varphi_l)\Phi^{\mathcal{C}}+F\varphi_l(p\Phi^{\mathcal{C}})\|$$
$$\leqslant c(\delta^{1+\delta'}+\|(p-\eta^{\mathcal{C}})\varphi_l\|+|\eta^{\mathcal{C}}|+\delta^2|\partial_x\Phi^{\mathcal{C}}|)$$
$$\leqslant c(l)(\delta^{1+\delta'}+\delta B^{\mathcal{C}}+|\eta^{\mathcal{C}}|+\delta^{2\xi}). \tag{A33}$$

We have already used above the fact that $|\eta^{\mathcal{C}}|$ is uniformly bounded as δ and t go to zero, and the same is true for $B^{\mathcal{C}}$—see Lemma 2.1 and Proposition 2.2 in Ref. 13. Finally we get in the outer temporal regime,

$$\|p\psi_l^{\mathcal{C}}\|\leqslant c(l) \tag{A34}$$

as $\delta\to0$, where $c(l)$ is some constant independent of time. By similar manipulations we also get in the same regime

$$\|p^2\psi_l^{\mathcal{C}}\|\leqslant c(l). \tag{A35}$$

Note that the nonvanishing term comes only from the action of p on the Gaussian state φ_l, which yields essentially $\eta^{\mathcal{C}}$ as expected, whereas the contribution from the derivatives of the ''electronic'' eigenvectors and cutoff function vanish. From the definition of Y we get a supplementary δ^4 which more than compensates for the denominator δ^2 appearing in (4.84),

$$\frac{1}{\delta^2}\int_{\delta^{1-\xi}}^{T}\|Y(x,\partial_x,\delta)\psi_I^{\mathcal{C}}(x,t,\delta)\|dt\leqslant c(l)\,\delta^4. \tag{A36}$$

We now need to perform the same type of analysis on the approximate wave function $\psi_I(y,s,\delta)$ given by (4.70) adopted in the inner temporal region. There we use the variables (4.69) so that the relations

$$\partial_y=\delta\partial_x \quad \text{and} \quad p=-i\,\delta\partial_y \tag{A37}$$

have to be employed to compute the derivatives of the different pieces in the definition of $\psi_I(y,s,\delta)$. In this case we need to show that

$$\begin{aligned}
&\frac{1}{\delta^2}\int_{-\delta^{1-\xi}}^{\delta^{1-\xi}}\|Y(x,\partial_x,\delta)\psi_I(y(x,t),s(t),\delta)\|dt\\
&\quad=\frac{1}{\delta}\int_{-\delta^{-\xi}}^{\delta^{-\xi}}\left\{\int|Y(\delta y+a(s\delta),\delta\partial_y,\delta)\psi_I(y,s,\delta)|^2\,\delta dy\right\}^{1/2}ds\\
&\quad\leqslant\frac{2}{\delta^{1+\xi}}\sup_{-\delta^{-\xi}\leqslant s\leqslant\delta^{-\xi}}\left\{\int|Y(\delta y+a(s\delta),\delta\partial_y,\delta)\psi_I(y,s,\delta)|^2\,\delta dy\right\}^{1/2}
\end{aligned} \tag{A38}$$

is of order δ^p for some positive p as $\delta\to 0$. As above, we denoted at that the norm in the ''electronic'' Hilbert space by a modulus. The estimates (A4), (A5) remain valid and we have

$$|p\,e^{i\eta(s\delta)y/\delta}|=|\eta(s\delta)|\leqslant C, \tag{A39}$$

$$|p^2e^{i\eta(s\delta)y/\delta}|=|\eta^2(s\delta)|\leqslant C, \tag{A40}$$

since $\eta(t)$ is uniformly bounded in the inner temporal regime. Noting that $x=a(\delta s)+\delta y=\mathcal{O}(\delta^{1-\xi})$, we also get from the regularity of the orthonormal basis $\{\psi_1(x,\delta),\psi_2(x,\delta)\}$ around (0,0) that

$$|p\,\psi_j(a(\delta s)+\delta y,\delta)|=\mathcal{O}(\delta^2), \tag{A41}$$

$$|p^2\psi_j(a(\delta s)+\delta y,\delta)|=\mathcal{O}(\delta^4) \tag{A42}$$

for $j=1,2$. Finally, the functions $f_0(y,s)$ and $g_0(y,s)$ determined in (4.73)–(4.76) and their derivatives can be estimated using the following remark. Up to phases, these functions are given as products of a Gaussian, a polynomial in y, a parabolic cylinder function, and a factor $1/\delta^{1/2}$ coming from the normalization of the function φ_l. Asymptotically, these parabolic cylinder functions, their first and second derivatives are of order $\mathcal{O}((s+\|y\|)^0)$, $\mathcal{O}((s+\|y\|))$, and $\mathcal{O}((s+\|y\|)^2)$, respectively, where $s=\mathcal{O}(\delta^{-\xi})$. Hence we can write

$$|f_0(y,s)|\leqslant P_1(y)e^{-y^2/2|A_0|^2}\delta^{-1/2}, \tag{A43}$$

$$|pf_0(y,s)|\leqslant P_2(y)e^{-y^2/2|A_0|^2}\delta^{-1/2+1-\xi}, \tag{A44}$$

$$|p^2f_0(y,s)|\leqslant P_3(y)e^{-y^2/2|A_0|^2}\delta^{-1/2+2-2\xi}, \tag{A45}$$

where A_0 is the initial condition (4.43) and P_j, $j=1,2,3$, are polynomials in y, the coefficients of which are independent of δ. They depend on l, the index of the chosen B–O state. Similar estimates are valid for g_0 in place of f_0. Having

$$p\psi_I = e^{iS(\delta s)/\delta^2} e^{i\eta(s\delta)y/\delta}[(pF + F\eta)(f_0\psi_1 + g_0\psi_2) + F((pf_0)\psi_1 + (pg_0)\psi_2 f_0(p\psi_1) + g_0(p\psi_2))] \tag{A46}$$

and the above estimates, we can write

$$|p\psi_I(y,s,\delta)| \leqslant P_4(y) e^{-y^2/2|A_0|^2} \delta^{-1/2}(\delta^{1+\delta'} + 1 + \delta^2 + \delta^{1-\xi}) \tag{A47}$$

with another polynomial P_4. Hence the right hand-side of (6.38) can be further estimated to give

$$\frac{1}{\delta^{1+\xi}} \sup_{-\delta^{-\xi} \leqslant s \leqslant \delta^{-\xi}} \left\{ \int |p\psi_I(y,s,\delta)|^2 \delta dy \right\}^{1/2} \leqslant c(l)/\delta^{1+\xi}. \tag{A48}$$

By similar manipulations we also get

$$\frac{1}{\delta^{1+\xi}} \sup_{-\delta^{-\xi} \leqslant s \leqslant \delta^{-\xi}} \left\{ \int |p^2\psi_I(y,s,\delta)|^2 \delta dy \right\}^{1/2} \leqslant c(l)/\delta^{1+\xi}. \tag{A49}$$

We note that here the leading order contribution comes from the action of p on the phase $e^{i\eta y/\delta}$ which gives η. The supplementary factor δ^4 in (6.1) yields the final estimate

$$\frac{1}{\delta^2} \int_{-\delta^{1-\xi}}^{\delta^{1-\xi}} \| Y(x, \partial_x, \delta)\psi_I(y(x,t), s(t), \delta) \| dt \leqslant c(l)\delta^{3-\xi}. \tag{A50}$$

Hence the proposition holds with $p = 3 - \xi$. □

Proof of Lemma V.6: As noted above, we cannot directly use Gronwall's lemma as stated in the text. Hence we need to prove that the two evolutions stay close enough to each other between times $t_0(\delta)$ and τ, where τ will be small but independent of δ by a more refined analysis. We consider the index $\mathcal{A}$ and drop it in the notation.

First, it is easy to check the following asymptotic properties as $(x,\delta) \to (0,0)$,

$$s(x,\delta) - \sqrt{\beta^2(x,\delta) + \gamma^2(x,\delta) + \sigma^2(x,\delta)} = \mathcal{O}(\delta^3), \tag{A51}$$

$$\partial_x s(x,\delta) - \partial_x \sqrt{\beta^2(x,\delta) + \gamma^2(x,\delta) + \sigma^2(x,\delta)} = \mathcal{O}\left(\frac{\delta^3}{\sqrt{x^2+\delta^2}} \right), \tag{A52}$$

$$s(x,\delta) = r\sqrt{x^2+\delta^2}\,(1 + \mathcal{O}(x+\delta)), \tag{A53}$$

$$\partial_x s(x,\delta) = \mathcal{O}(1), \tag{A54}$$

$$\partial_x^2 s(x,\delta) = \frac{r\delta^2}{(x^2+\delta^2)^{3/2}} + \mathcal{O}(1). \tag{A55}$$

We collect some preliminary observations on the solution $\tilde{a}(t)$ to the equation,

$$\ddot{\tilde{a}}(t) = -\partial_x \tilde{V}(\tilde{a}(t), \delta) \tag{A56}$$

for $t \in [t_0, \tau]$ with initial condition satisfying (5.42). We can choose $\tau > 0$ independent of δ, such that

$$a(t) - a(t_0(\delta)) \geqslant c_0(t - t_0(\delta)), \tag{A57}$$

for some $c_0 > 0$ and all $t \in [t_0(\delta), \tau]$. This implies easily by means of (5.42) that

$$\tilde{a}(t)-\tilde{a}(t_0(\delta))\geqslant c_1(t-t_0(\delta)) \tag{A58}$$

for all $t\in[t_0(\delta),\tau]$ with a uniform constant. Hence we can write

$$x^2+\delta^2|_{\theta_t}\geqslant c_3(\delta^\kappa+(t-t_0(\delta)))^2, \quad \forall\,\theta_t\in[\tilde{a}(t),a(t)]. \tag{A59}$$

Consider now the identities (dropping the δ dependence in the arguments),

$$\begin{aligned}\ddot{\tilde{a}}(t)-\ddot{a}(t)&=\partial_x V(a(t))-\partial_x\tilde{V}(\tilde{a}(t))\\ &=\partial_x\sqrt{\beta^2+\gamma^2+\sigma^2}(a(t))+\partial_x\overline{V}(a(t))-\partial_x s(\tilde{a}(t))-\partial_x V_3(\tilde{a}(t))\\ &=\partial_x(\sqrt{\beta^2+\gamma^2+\sigma^2}(a(t))-s(a(t)))+\partial_x(\overline{V}(a(t))-V_3(a(t)))\\ &\quad-\partial_x^2 s(\theta_t)(\tilde{a}(t)-a(t))+\partial_x^2 V_3(\theta_t)(\tilde{a}(t)-a(t)),\end{aligned} \tag{A60}$$

where $\theta_t\in(\tilde{a}(t),a(t))$. Now the first order derivatives are of order $\delta^3/(\delta^\kappa+(t-t_0(\delta))$, whereas the second order ones are of order $\delta^3/(\delta^\kappa+(t-t_0))^3$—see (A55) and (A59).

Hence introducing $d(t)=\tilde{a}(t)-a(t)$ we get an ODE of the form

$$\ddot{d}(t)=f(d(t),t)d(t)+g(d(t),t), \tag{A61}$$

where we have the *a priori* bounds,

$$\int_{t_0}^{t}|f(d(s),s)|ds\leqslant c\,\delta^2\int_{t_0}^{t}1/(\delta^\kappa+(s-t_0))^3 ds\leqslant c\,\delta^{2(1-\kappa)}, \tag{A62}$$

and since we can assume without loss that $\delta^k+(t-t_0(\delta))<1$,

$$\begin{aligned}\int_{t_0}^{t}|g(d(s),s)|&\leqslant\int_{t_0}^{t}\frac{c\,\delta^3}{(\delta^\kappa+(s-t_0))^3}ds\leqslant c\,\delta^3(|\ln(\delta^\kappa)|+|\ln(\delta^\kappa+(t-t_0)|)\\ &=\mathcal{O}(\delta^3\ln(\delta)).\end{aligned} \tag{A63}$$

Equation (A61) is equivalent to

$$d(t)=d(t_0)+(t-t_0)\dot{d}(t_0)+\int_{t_0}^{t}ds\int_{t_0}^{s}du(f(d(u),u)d(u)+g(d(u),u)). \tag{A64}$$

Let us denote

$$D(t)=\sup_{s\in[t_0,t]}|d(s)|. \tag{A65}$$

We deduce from the above bounds

$$\begin{aligned}|d(t)|&\leqslant|d(t_0)|+(t-t_0)|\dot{d}(t_0)|+c\int_{t_0}^{t}dsD(s)\,\delta^{2(1-\kappa)}+c\,\delta^3|\ln(\delta)|\\ &\leqslant c\left(|d(t_0)|+|\dot{d}(t_0)|+\delta^3|\ln(\delta)|+\int_{t_0}^{t}dsD(s)\,\delta^{2(1-\kappa)}\right)\end{aligned} \tag{A66}$$

and, as D is not decreasing,

$$D(t)\leqslant c\left(|d(t_0)|+|\dot{d}(t_0)|+\delta^3|\ln(\delta)|+\int_{t_0}^{t}dsD(s)\,\delta^{2(1-\kappa)}\right)$$

$$\leqslant c(|d(t_0)|+|\dot{d}(t_0)|+\delta^3|\ln(\delta)|+D(t)\,\delta^{2(1-\kappa)}). \tag{A67}$$

Since $\delta^{2(1-\kappa)}\to 0$, we find that

$$D(t)\leqslant c(|d(t_0)|+|\dot{d}(t_0)|+\delta^3|\ln(\delta)|). \tag{A68}$$

Plugging this into (A64) finally yields

$$d(t)=d(t_0)+(t-t_0)\dot{d}(t_0)+\mathcal{O}(\delta^{2(1-\kappa)}(|d(t_0)|+|\dot{d}(t_0)|)+\delta^3|\ln(\delta)|). \tag{A69}$$

As an immediate consequence of this result and (5.47) we have for any $t\in[t_0(\delta),\tau]$ with our choice of $t_0(\delta)$ and initial conditions (5.42),

$$\tilde{a}(t)-a(t)=o(\delta^2), \tag{A70}$$

$$\tilde{\eta}(t)-\eta(t)=o(\delta^2). \tag{A71}$$

Turning to $(A(t),B(t))$ and their approximations, we first note that by Ref. 13, p. 102, we have with our choice of $t_0(\delta)$,

$$\begin{pmatrix}\tilde{A}(t_0)\\ \tilde{B}(t_0)\end{pmatrix}-\begin{pmatrix}A(t_0)\\ B(t_0)\end{pmatrix}=o(1). \tag{A72}$$

Then we consider the equation [equivalent to (4.42) and (4.43)],

$$\begin{pmatrix}A(t)\\ B(t)\end{pmatrix}=\begin{pmatrix}A(t_0)\\ B(t_0)\end{pmatrix}+\int_{t_0}^{t}\begin{pmatrix}O & i\\ i\partial_x^2V(a(t)) & 0\end{pmatrix}\begin{pmatrix}A(s)\\ B(s)\end{pmatrix} \tag{A73}$$

and a similar one for the approximations with the tilded symbols everywhere. Introducing

$$\Delta(t)=\begin{pmatrix}\tilde{A}(t)\\ \tilde{B}(t)\end{pmatrix}-\begin{pmatrix}A(t)\\ B(t)\end{pmatrix},$$

we compute

$$\Delta(t)=\Delta(t_0)+\int_{t_0}^{t}\begin{pmatrix}0 & 0\\ i\partial_x^2\tilde{V}(\tilde{a}(s))-\partial_x^2V(a(s)) & 0\end{pmatrix}\begin{pmatrix}\tilde{A}(s)\\ \tilde{B}(s)\end{pmatrix}ds+\int_{t_0}^{t}\begin{pmatrix}0 & i\\ i\partial_x^2V(a(s)) & 0\end{pmatrix}\Delta(s)ds. \tag{A74}$$

But $\|\left(\begin{smallmatrix}\tilde{A}(t)\\ \tilde{B}(t)\end{smallmatrix}\right)\|=\mathcal{O}(1)$ by Ref. 13, $\int_{t_0}^{t}\partial_x^2\tilde{V}(\tilde{a}(s))ds=\mathcal{O}(\delta^{2(1-\kappa)})$ and similarly for the untilded quantities. Hence using the same type of manipulations as above, we deduce

$$\|\Delta(t)\|\leqslant c(\delta^{2(1-\kappa)}+\|\Delta(t_0)\|). \tag{A75}$$

It follows that

$$\begin{pmatrix}\tilde{A}(t)\\ \tilde{B}(t)\end{pmatrix}-\begin{pmatrix}A(t)\\ B(t)\end{pmatrix}=o(1) \tag{A76}$$

holds for any $t\in[t_0(\delta),\tau]$.

In order to deal with the ''electronic'' eigenvectors we consider the perturbation series for the resolvent $(h(x)+V_2(x)+\delta W(x)-z)^{-1}$ when the argument z runs through the circle of radius $|\mu^{\mathcal{A}}(x,0)-\mu^{\mathcal{B}}(x,0)|/4$ centered at any of the eigenvalue $\mu^{C}(x,0)$. Integration on this circle yields the eigenprojector $Q_j(x,\delta)$, $j=\mathcal{A},\mathcal{B}$, and the estimates

$$Q_j(x,\delta)=Q_j(x,0)+\mathcal{O}(\delta W(x)/|\mu^{\mathcal{A}}(x,0)-\mu^{\mathcal{B}}(x,0)|)=Q_j(x,0)+\mathcal{O}(\delta/x), \tag{A77}$$

$$\partial_x Q_j(x,\delta)=\partial_x Q_j(x,0)+\mathcal{O}(\delta/|\mu^{\mathcal{A}}(x,0)-\mu^{\mathcal{B}}(x,0)|^2)=\partial_x P_j(x,0)+\mathcal{O}(\delta/x^2). \tag{A78}$$

This, in turn, yields the following estimates on the eigenvectors $\Phi_j(x,\delta)$ of the perturbed operator $h(x)+\delta W(x)$:

$$\Phi_j(x,\delta)=\chi_j(x)+\mathcal{O}(\delta/x), \tag{A79}$$

$$\partial_x\Phi_j(x,\delta)=\partial_x\chi_j(x)+\mathcal{O}(\delta/x^2). \tag{A80}$$

Now we consider one eigenvector $\chi_j(x)$ and drop the index j. We note here that Eq. (3.58) in Ref. 13 shows that

$$\lambda_r(\omega,t,\delta)=\mathcal{O}(t/\delta^{1-\kappa}), \tag{A81}$$

so that $\lambda_r(\omega,t_0(\delta),\delta)=\mathcal{O}(\delta^{2\kappa-1})\to 0$ with δ. On the other hand, using the fact that $\chi(x)$ is smooth and that $\tilde{\eta}(t)$ is uniformly bounded on $[t_0(\delta),T]$ we find

$$\begin{aligned}
&\int_{t_0(\delta)}^{t} ids\,\eta(s)\langle\Phi(\omega,s,\delta)|\partial_x\Phi(\omega+a(s),\delta)\rangle\\
&\quad=\int_{t_0(\delta)}^{t} ids(\tilde{\eta}(s)+o(\delta^2))\times\langle(\tilde{\Phi}(\omega,s,\delta)\\
&\qquad+\mathcal{O}(\delta/(a(t)+\omega)))|(\partial_x\tilde{\Phi}(\omega+\tilde{a}(s),\delta)+\mathcal{O}(\delta/(a(s)+\omega)^2)))\rangle\\
&\quad=\int_{t_0(\delta)}^{t} ids\,\tilde{\eta}(s)\langle\tilde{\Phi}(\omega,s,\delta)|\partial_x\tilde{\Phi}(\omega+\tilde{a}(s),\delta)\rangle+o(1)\\
&\qquad+0(\delta\ln((t+\omega)/(t_0+\omega)))+\mathcal{O}(\delta(1/(t_0(\delta)+\omega)-1/(t+\omega))).
\end{aligned} \tag{A82}$$

Having $\omega=\mathcal{O}(\delta^{1-\delta'})$ and (5.49), the error terms above can be estimated by

$$o(1)+\mathcal{O}(\delta\ln(\delta)+\delta^{1-\kappa}) \tag{A83}$$

which goes to zero as $\delta\to 0$. It follows then that

$$\tilde{\lambda}(x,t,\delta)-\lambda(x,t,\delta)=o(1) \tag{A84}$$

and in turn we get

$$\tilde{\Phi}(x,t,\delta)-\Phi(x,t,\delta)=o(1), \tag{A85}$$

which concludes the proof. □

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Perturbation theory free from secular terms for the equations of motion of anharmonic oscillators

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We develop a time–independent perturbation theory in operator form for the equations of motion of classical and quantum-mechanical anharmonic oscillators. The method focuses on the frequency of the motion in the former case and in a frequency operator in the latter, producing a power series in a small coupling constant. The resulting expressions are free from secular instabilities that commonly appear in perturbation treatments of nonlinear problems. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1402175]

I. INTRODUCTION

Straightforward application of perturbation theory to classical equations of motion commonly produces secular terms that are unbounded even for periodic motion. For that reason, researchers have developed several alternative approaches that correct or completely overcome this failure of perturbation theory at large time. For example, methods like Lindstedt–Poincaré, renormalization, and multiple scales have been known for a long ago.[1–3] There has recently been great interest in similar approaches for quantum mechanics; the method of multiple scales[4,5] and the construction of minimal normal forms by means of near identity transformations[6] prove suitable for simple models such as anharmonic oscillators.

At first sight those approaches seem to become rather cumbersome even at moderately great orders of perturbation theory. For this reason, here we propose an alternative procedure that in our opinion is more straightforward, and at the same time provides a more systematic treatment of classical and quantum-mechanical perturbation theory. It is based on a recent discussion of the structure of the eigenvalues of nonlinear oscillators.[7] In Sec. II we consider classical anharmonic oscillators in one dimension, and in Sec. III we show that the method also applies to quantum-mechanical models almost without modification.

II. CLASSICAL MECHANICS

In order to simplify the discussion we restrict ourselves to one-dimensional models and use the following notation to indicate dependence of a dynamical variable F on time: $F(t)=F(q(t),p(t))$, $F(0)=F(q(0),p(0))=F(q,p)$, where $q(t)$ and $p(t)$ are the instantaneous values of the coordinate and momentum, respectively, and q and p are their initial values at $t=0$.

We believe that rewriting classical equations of motion in terms of operators facilitates the following discussion. For a given function $F(q,p)$ we construct the differential operator

$$\hat{F}=\frac{\partial F}{\partial q}\frac{\partial}{\partial p}-\frac{\partial F}{\partial p}\frac{\partial}{\partial q} \tag{1}$$

so that $\hat{F}G$ is the well-known Poisson bracket $\{F,G\}$.[3,8] If the Hamiltonian $H(q,p)$ does not depend explicitly on time we solve the time-evolution equation

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$$\frac{\mathrm{d}}{\mathrm{d}t}F(t)=-\hat{H}F(t) \tag{2}$$

formally as[3,8]

$$F(t)=\exp(-t\hat{H})F(0). \tag{3}$$

The present method is based on the assumption that it is possible to obtain a nonzero dynamical variable $A(q,p)$ that satisfies

$$\hat{H}A=i\Omega A, \tag{4}$$

where $\Omega=\Omega(q,p)$ is a constant of the motion:

$$\hat{H}\Omega=0. \tag{5}$$

Notice that for periodic motion Ω is real and therefore A is complex. Taking into account that $\hat{H}A^*=-i\Omega A^*$ one easily proves that $|A|^2$ is a constant of the motion. Moreover, the time evolution of A,

$$A(t)=\exp(-it\Omega)A(0), \tag{6}$$

clearly exhibits the dependence of the period of the motion $\tau=2\pi/\Omega$ on the values of q and p. One easily verifies that if A is a solution of Eq. (4), then $K(H)A$ will also be a solution for any arbitrary function K of H with exactly the same value of Ω. In order to determine A uniquely we add an arbitrary (and convenient) normalization condition. Notice that Ω (as any other property of the system) is independent of normalization.

For example, for the well-known harmonic oscillator

$$H=\frac{p^2}{2m}+\frac{m\omega^2q^2}{2} \tag{7}$$

we have[3]

$$A=\sqrt{\frac{m\omega}{2}}\left(q+\frac{ip}{m\omega}\right), \quad \Omega=\omega, \tag{8}$$

where we see that the period is independent of q and p. In this case we have arbitrarily normalized the function A in such a way that $\{A,A^*\}=-i$.

Except for a few trivial models, one cannot solve Eqs. (4) and (5) exactly, and therefore one resorts to approximate methods like perturbation theory. If we can write

$$H=H_0+\lambda H', \tag{9}$$

where $\lambda H'$ is a small perturbation to the exactly solvable Hamiltonian H_0, then it is reasonable to look for approximate solutions in the form of Taylor series

$$A=\sum_{j=0}^{\infty}A_j\lambda^j, \quad \Omega=\sum_{j=0}^{\infty}\Omega_j\lambda^j. \tag{10}$$

It follows from Eqs. (4) and (5) that the coefficients of the series (10) satisfy

$$\hat{H}_0\Omega_j=-\hat{H}'\Omega_{j-1}, \tag{11}$$

$$(\hat{H}_0 - i\Omega_0)A_j = i\sum_{k=1}^{j} \Omega_k A_{j-k} - \hat{H}' A_{j-1}. \tag{12}$$

As already noted, we assume that we can exactly solve the unperturbed equations

$$\hat{H}_0\Omega_0 = 0, \quad (\hat{H}_0 - i\Omega_0)A_0 = 0. \tag{13}$$

From now on we call zero eigenspace of an operator $\hat{G}$ the set of all functions $Z(q,p)$ that satisfy $\hat{G}Z=0$. If there are no elements of the zero eigenspaces of $\hat{H}_0$ and $\hat{H}_0 - i\Omega_0$ on the right-hand side of Eqs. (11) and (12), respectively, we can solve them formally as

$$\Omega_j = -\hat{H}_0^{-1}\hat{H}'\Omega_{j-1} + g_j, \tag{14}$$

$$A_j = (\hat{H}_0 - i\Omega_0)^{-1}\left(i\sum_{k=1}^{j} \Omega_k A_{j-k} - \hat{H}' A_{j-1} \right) + h_j, \tag{15}$$

where $g_j(q,p)$ and $h_j(q,p)$ are arbitrary elements of the zero eigenspaces of $\hat{H}_0$ and $\hat{H}_0 - i\Omega_0$, respectively. Because $g_j A_0$ belongs to the zero eigenspace of $\hat{H}_0 - i\Omega_0$, we can choose g_j in order to remove all elements of the zero eigenspace of $\hat{H}_0 - i\Omega_0$ from the right-hand side of Eq. (12); and therefore Eq. (15) makes sense. On the other hand, h_j enables us to select an appropriate normalization condition for the dynamical variable $A(q,p)$ (such as, for example, $\{A,A^*\} = -i$).

If $\exp(t\hat{G})q$ and $\exp(t\hat{G})p$ are bounded for all t, then we can invert the operator $\hat{G}$ [e.g., $\hat{G} = \hat{H}_0$ and $\hat{G} = \hat{H}_0 - i\Omega_0$ in Eqs. (11) and (12), respectively] as follows:

$$\begin{aligned} (\hat{G}+\alpha)^{-1} &= \int_{-\infty}^{0} \exp[(\hat{G}+\alpha)t]\,dt, \quad \alpha > 0, \\ \hat{G}^{-1} &= \lim_{\alpha\to 0} (\hat{G}+\alpha)^{-1}. \end{aligned} \tag{16}$$

Taking into account that

$$\lim_{\alpha\to 0} \alpha(\hat{G}+\alpha)^{-1} Z = Z \tag{17}$$

for any element $Z(q,p)$ of the zero eigenspace of $\hat{G}$, we realize that

$$\lim_{\alpha\to 0} \alpha(\hat{G}+\alpha)^{-1} U \tag{18}$$

extracts elements of the zero eigenspace of $\hat{G}$ from $U(q,p)$. We apply this recipe to Eq. (15) in order to determine the appropriate g_j. This approach requires suitable expressions for $\exp(t\hat{H}_0)q$ and $\exp(t\hat{H}_0)p$, which we easily obtain as follows:

$$\begin{aligned} \exp(t\hat{H}_0)q &= q\cos(\omega t) - \frac{p\sin(\omega t)}{m\omega}, \\ \exp(t\hat{H}_0)p &= p\cos(\omega t) + m\omega q \sin(\omega t). \end{aligned} \tag{19}$$

Moreover, for any function $U(q,p)$ we have $\exp(t\hat{H}_0)U(q,p) = U(e^{t\hat{H}_0}q, e^{t\hat{H}_0}p)$. In order to illustrate the application of Eq. (18), we choose the following simple example: $\hat{G} = \hat{H}_0$, and $U = q^2$. It is not difficult to verify that

$$\int_{-\infty}^{0} \exp[t(\hat{H}+\alpha)]q^2\,\mathrm{d}t = \frac{m^2\alpha^2q^2+2m^2\omega^2q^2+2m\alpha qp+2p^2}{m^2(\alpha^2+4\omega^2)\alpha},$$

$$\lim_{\alpha\to 0}\alpha\int_{-\infty}^{0} \exp[t(\hat{H}+\alpha)]q^2\,\mathrm{d}t = \frac{m^2\omega^2q^2+p^2}{2m^2\omega^2}. \tag{20}$$

Notice that the right-hand side of Eq. (20) is the part of q^2 that commutes with H_0 as stated previously, and it is therefore an element of the zero eigenspace of the operator $\hat{H}_0$.

Once we solve Eqs. (14) and (15) for $j=1,2,\ldots$, we easily obtain the period of the motion as a λ-power series

$$\begin{aligned}\tau &= \frac{2\pi}{\Omega_0+\Omega_1\lambda+\Omega_2\lambda^2+\Omega_3\lambda^3+\cdots}\\ &= 2\frac{\pi}{\Omega_0}\left(1-\frac{\Omega_1}{\Omega_0}\lambda-\frac{(\Omega_2\Omega_0-\Omega_1^2)}{\Omega_0^2}\lambda^2-\frac{(\Omega_3\Omega_0^2-2\Omega_1\Omega_2\Omega_0+\Omega_1^3)}{\Omega_0^3}\lambda^3+\cdots\right).\end{aligned} \tag{21}$$

As a simple illustrative example we consider the anharmonic oscillator given by

$$H_0=\frac{p^2}{2m}+\frac{m\omega^2q^2}{2}, \quad H'=q^4. \tag{22}$$

Notice that Eq. (8) gives us A_0 and Ω_0 for this choice of H_0. The calculation is straightforward but tedious; fortunately available software for symbolic computation, like MAPLE,[9] greatly facilitates the process. Notice that Eqs. (14) and (15) are suitable for programming according to Eqs. (16)–(18). (MAPLE worksheets and programs are available upon request.) For the anharmonic oscillator (22) we easily obtain the following expressions for the frequency coefficients in terms of the initial coordinate and momentum:

$$\begin{aligned}\Omega_1 &= \frac{3}{2}\frac{(m^2\omega^2q^2+p^2)}{m^3\omega^3},\\ \Omega_2 &= -\frac{3}{16}\frac{46m^2\omega^2p^2q^2+23p^4+7m^4\omega^4q^4}{m^6\omega^7},\\ \Omega_3 &= \frac{3}{32}\frac{449m^4\omega^4q^4p^2+633p^4m^2\omega^2q^2+27m^6\omega^6q^6+211p^6}{m^9\omega^{11}}.\end{aligned} \tag{23}$$

Notice that we can rewrite Ω_1 as a function of H_0,

$$\Omega_1=3\frac{H_0}{m^2\omega^3}, \tag{24}$$

because $\{H_0,\Omega_1\}=0$, but we cannot do the same with the coefficients Ω_j for $j>1$.

Choosing for simplicity the arbitrary zero-eigenspace elements $h_j(q,p)$ equal to zero we obtain

$$A_1=\frac{\sqrt{2}\sqrt{m\,\omega}[9m\omega qp^2+5m^3\omega^3q^3-3i(p^3+5m^2\omega^2q^2p)]}{16m^4\omega^5}, \tag{25}$$

$$A_2 = -\frac{\sqrt{2}}{32(m^6\omega^8\sqrt{m\omega})}[122m^3\omega^3p^2q^3 + 65m\omega p^4q + 13m^5\omega^5q^5 - i(13p^5 + 86m^2\omega^2q^2p^3 + 101m^4\omega^4pq^4)].$$

In order to verify the above-mentioned results we apply them to Duffing's equation[1,2]

$$\ddot{u}(t) + u(t) + 4\lambda u(t)^3 = 0. \tag{26}$$

Choosing the initial conditions $u(0) = x_0$, $v(0) = \dot{u}(0) = 0$, and expanding the exact period[1] in powers of λ, we obtain

$$\tau = 2\pi - 3\pi x_0^2\lambda + \frac{57\pi x_0^4\lambda^2}{8} - \frac{315\pi x_0^6\lambda^3}{16} + \cdots. \tag{27}$$

On the other hand, if we substitute $m = \omega = 1$, $p = 0$, and $q = x_0$ into Eq. (23), then Eq. (21) gives exactly Eq. (27) as one easily verifies.

III. QUANTUM MECHANICS

The method outlined previously for classical mechanics applies to quantum mechanics almost without modification. In this case the dynamical variables are linear operators $\{\hat{A}, \hat{B}, \hat{C}, \ldots\}$. For every linear operator $\hat{F}$ we define a superoperator $\hat{\hat{F}}$ that acts on the vector space of linear operators as follows: $\hat{\hat{F}}\hat{C} = [\hat{F}, \hat{C}] = \hat{F}\hat{C} - \hat{C}\hat{F}$.[3,10] If the Hamiltonian operator $\hat{H}$ is independent of time we solve the time-evolution equation

$$\frac{d\hat{P}(t)}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{P}(t)] = \frac{i}{\hbar}\hat{\hat{H}}\hat{P}(t), \tag{28}$$

formally as follows:[3,10]

$$\hat{P}(t) = \exp\left(\frac{it\hat{H}}{\hbar}\right)\hat{P}\exp\left(-\frac{it\hat{H}}{\hbar}\right) = \exp\left(\frac{it\hat{\hat{H}}}{\hbar}\right)\hat{P}, \tag{29}$$

where we write $\hat{P}(0) = \hat{P}$.

For simplicity and concreteness we consider the dimensionless Hamiltonian operator $\hat{H}(\hat{a}, \hat{a}^\dagger)$ for a one-dimensional anharmonic oscillator in terms of the annihilation $\hat{a}$ and creation $\hat{a}^\dagger$ operators that satisfy the bosonic commutation relation $[\hat{a}, \hat{a}^\dagger] = \hat{1}$. From now on we set $\hbar = 1$ in order to have dimensionless equations of motion, and omit the identity operator $\hat{1}$. As in the classical counterpart discussed previously, the key of the approach is to construct an operator $\hat{b}(\hat{a}, \hat{a}^\dagger)$ such that

$$\hat{\hat{H}}\hat{b} = -\hat{\Omega}\hat{b}, \tag{30}$$

where $\hat{\Omega}$ is a constant of the motion

$$\hat{\hat{H}}\hat{\Omega} = 0. \tag{31}$$

In the case of bounded motion the frequency operator $\hat{\Omega}$ is Hermitian ($\hat{\Omega}^\dagger = \hat{\Omega}$) and $\hat{b}^\dagger\hat{b}$ results in a constant of the motion. Moreover, the operator $\hat{b}$ changes in time according to

$$\hat{b}(t) = \exp(-it\hat{\Omega})\hat{b}. \tag{32}$$

Exactly as in classical mechanics, Eq. (30) does not determine $\hat{b}$ completely, and we require a normalization condition. The operator $\hat{\Omega}$ is independent of the normalization condition chosen and can therefore be considered to be a property of the system. The quantum-mechanical version of present method is exactly the one developed recently for the discussion of the structure of eigenvalues of nonlinear oscillators;[7] the main difference is that here we concentrate on perturbation theory instead of on the semiclassical limit. Moreover, we compare several normalization conditions for $\hat{b}$.

As in the classical case, it is not possible to solve Eqs. (30) and (31) exactly except for some simple models such as the harmonic oscillator. In nontrivial cases we resort to approximate methods; here we choose perturbation theory and write

$$\hat{H}=\hat{H}_0+\lambda\hat{H}' \tag{33}$$

provided that we can solve

$$\hat{\hat{H}}_0\hat{b}_0=-\hat{\Omega}_0\hat{b}_0,\hat{\hat{H}}_0\hat{\Omega}_0=0 \tag{34}$$

exactly. If we expand the solutions to Eqs. (30) and (31) in Taylor series of the perturbation parameter λ:

$$\hat{b}=\sum_{j=0}^{\infty}\hat{b}_j(\hat{a},\hat{a}^\dagger)\lambda^j,\quad \hat{\Omega}=\sum_{j=0}^{\infty}\hat{\Omega}_j(\hat{a},\hat{a}^\dagger)\lambda^j, \tag{35}$$

we easily obtain

$$(\hat{\hat{H}}_0+\hat{\Omega}_0)\hat{b}_j=-\hat{\hat{H}}'\hat{b}_{j-1}-\sum_{m=1}^{j}\hat{\Omega}_m\hat{b}_{j-m}, \tag{36}$$

$$\hat{\hat{H}}_0\hat{\Omega}_j+\hat{\hat{H}}'\hat{\Omega}_{j-1}=0. \tag{37}$$

We formally solve Eqs. (36) and (37) as follows (we write them in the order they should be solved):

$$\hat{\Omega}_j=\hat{\hat{H}}_0^{-1}[\hat{\Omega}_{j-1},\hat{H}']+\hat{N}_j, \tag{38}$$

$$\hat{b}_j=(\hat{\hat{H}}_0+\hat{\Omega}_0)^{-1}\left([\hat{b}_{j-1},\hat{H}']+\sum_{m=1}^{j}\hat{\Omega}_m\hat{b}_{j-m}\right)+\hat{N}_j', \tag{39}$$

where $\hat{N}_j$ and $\hat{N}_j'$ are zero-eigenspace elements that satisfy $\hat{\hat{H}}_0\hat{N}_j=0$ and $(\hat{\hat{H}}_0+\hat{\Omega}_0)\hat{N}_j'=0$ respectively. At every perturbation order j we choose $\hat{\Omega}_j$ to remove all elements of the zero eigenspace of $\hat{\hat{H}}_0+\hat{\Omega}_0$ from the right-hand side of Eq. (36) before we apply the superoperator $(\hat{\hat{H}}_0+\hat{\Omega}_0)^{-1}$.

For the particular case that

$$\hat{H}_0=\hat{a}^\dagger\hat{a}+\tfrac{1}{2}, \tag{40}$$

we have

$$\hat{b}_0=a,\quad \hat{\Omega}_0=1, \tag{41}$$

and

$$\hat{N}_j=\hat{g}_j(\hat{a}^\dagger\hat{a}),\quad \hat{N}_j'=f_j(\hat{a}^\dagger\hat{a})\hat{a}^\dagger, \tag{42}$$

where $\hat{g}_j(\hat{a}^\dagger\hat{a})$ and $\hat{f}_j(\hat{a}^\dagger\hat{a})$ are arbitrary functions of the number operator $\hat{a}^\dagger\hat{a}$. As indicated previously we choose $\hat{g}_j$ in order to remove all zero-eigenspace elements from the right-hand side of Eq. (36). On the other hand, $\hat{f}_j$ is determined by a normalization condition on the operator $\hat{b}$. We discuss some examples in the following.

The application of Eqs. (38) and (39) is straightforward when $\hat{H}_0$ is given by Eq. (40), and the perturbation is a polynomial function of the boson operators. In principle, we may apply a method similar to the one outlined in Eqs. (16)–(18). However, in what follows we proceed in a different way, and take into account that $F(\hat{\hat{H}}_0)\hat{a}^{\dagger m}\hat{a}^n=F(m-n)\hat{a}^{\dagger m}\hat{a}^n$ for any function $F(x)$ in order to systematically solve Eqs. (38) and (39), where we have $F(x)=x^{-1}$ and $F(x)=(x+1)^{-1}$, respectively. We have performed this calculation by hand, because we found it difficult to implement the necessary operator equations in MAPLE.

It is always instructive to study exactly solvable models; for that reason, in what follows we choose the case in which $\hat{H}_0$ is given by Eq. (40) and the perturbation is quadratic: $\hat{H}'=\frac{1}{2}(\hat{a}^2+\hat{a}^{\dagger 2})$. We easily obtain

$$\begin{aligned}\hat{\Omega}&=\Omega=\sqrt{1-\lambda^2},\\ \hat{b}&=\frac{\lambda}{\sqrt{2\sqrt{1-\lambda^2}(1-\sqrt{1-\lambda^2})}}\left(\hat{a}+\frac{1-\sqrt{1-\lambda^2}}{\lambda}\hat{a}^\dagger\right),\end{aligned} \tag{43}$$

provided that the normalization condition is $[\hat{b},\hat{b}^\dagger]=1$.

It is not difficult to verify that the above-outlined perturbation method exactly gives the Taylor expansions for Ω and $\hat{b}$ that converge for all $|\lambda|<1$. In this case the constant of the motion $\hat{b}^\dagger\hat{b}$ is a linear function of $\hat{H}$:

$$\hat{b}^\dagger\hat{b}=\frac{1}{\sqrt{1-\lambda^2}}\left(\hat{H}-\frac{\sqrt{1-\lambda^2}}{2}\right), \tag{44}$$

and the time evolution of $\hat{b}$ is remarkably simple:

$$\hat{b}(t)=\exp(-i\Omega t)\hat{b}. \tag{45}$$

In principle, we can improve the convergence properties of the perturbation series by an appropriate choice of $\hat{H}_0$.[3] Consider, for example, the operator

$$\hat{H}=\hat{a}^\dagger\hat{a}+\frac{1}{2}+\frac{\lambda}{2}(\hat{a}+\hat{a}^\dagger)^2. \tag{46}$$

The radius of convergence of the λ-power series for

$$\hat{\Omega}=\Omega=\sqrt{1+2\lambda} \tag{47}$$

is determined by a square-root branch point at $\lambda=-\frac{1}{2}$.

If, on the other hand, we split $\hat{H}$ as

$$\hat{H}=(1+\lambda)\left(\hat{a}^\dagger\hat{a}+\frac{1}{2}\right)+\frac{\beta\lambda}{2}(\hat{a}^2+\hat{a}^{\dagger 2}), \tag{48}$$

then the Taylor series about $\beta=0$ converges for all

$$\beta^2 < \frac{(1+\lambda)^2}{\lambda^2}.$$

Choosing $\beta = 1$ in order to recover the original operator (46), we conclude that this alternative approach converges for all $\lambda > -\frac{1}{2}$, which is certainly better than the condition $|\lambda| < \frac{1}{2}$ that follows from the straightforward expansion about $\lambda = 0$ discussed previously. We see that the present approach facilitates the discussion of the convergence properties of the normal forms.

As a nontrivial example we choose one of the anharmonic oscillators discussed by other authors:[6] $\hat{H}_0$ given by Eq. (40) and

$$\hat{H}' = \tfrac{1}{16}(\hat{a}+\hat{a}^\dagger)^4. \tag{49}$$

We believe it worthwhile to compare different normalization conditions for the operator $\hat{b}$. In the first place we choose $[\hat{b},\hat{b}^\dagger]=1$, so that the coefficients $\hat{b}_j$ and $\hat{b}_j^\dagger$ satisfy

$$\sum_{m=0}^{j} [\hat{b}_m, \hat{b}_{j-m}^\dagger] = \delta_{j0}. \tag{50}$$

This condition, which makes the transformation $\{\hat{a},\hat{a}^\dagger\} \to \{\hat{b},\hat{b}^\dagger\}$ canonical, is different from the ones chosen recently by other authors.[6,7]

Solving the perturbation equations of first and second order we easily obtain

$$\begin{aligned} \hat{\Omega}_1 &= \hat{g}_1 = \tfrac{3}{4}(\hat{a}^\dagger\hat{a}+1), \\ \hat{b}_1 &= \tfrac{1}{4}(\tfrac{1}{4}\hat{a}^{\dagger 3} + \tfrac{3}{2}\hat{a}^{\dagger 2}\hat{a} + \tfrac{3}{2}\hat{a}^\dagger - \tfrac{1}{2}\hat{a}^3), \\ \hat{f}_1 &= 0, \end{aligned} \tag{51}$$

and

$$\begin{aligned} \hat{\Omega}_2 &= \tfrac{3}{16}(\tfrac{1}{4}\hat{a}^{\dagger 4} + \hat{a}^{\dagger 3}\hat{a} + \tfrac{3}{2}\hat{a}^{\dagger 2} + \hat{a}^\dagger\hat{a}^3 + \tfrac{1}{4}\hat{a}^4 + \tfrac{3}{2}\hat{a}^2) + \hat{g}_2, \\ \hat{g}_2 &= -\tfrac{3}{64}(17\hat{a}^{\dagger 2}\hat{a}^2 + 51\hat{a}^\dagger\hat{a} + 24), \\ \hat{b}_2 &= \tfrac{3}{64}(\tfrac{1}{6}\hat{a}^{\dagger 5} - \tfrac{3}{4}\hat{a}^{\dagger 4}\hat{a} - \tfrac{21}{2}\hat{a}^{\dagger 3}\hat{a}^2 - \tfrac{3}{2}\hat{a}^{\dagger 3} - \tfrac{63}{2}\hat{a}^{\dagger 2}\hat{a} + 6\hat{a}^\dagger\hat{a}^4 - \tfrac{27}{2}\hat{a}^\dagger + \tfrac{3}{4}\hat{a}^5 + 12\hat{a}^3) + \hat{f}_2\hat{a}, \\ \hat{f}_2 &= \tfrac{27}{512}(\hat{a}^\dagger\hat{a})^2 + \tfrac{27}{256}\hat{a}^\dagger\hat{a} + \tfrac{9}{256}, \end{aligned} \tag{52}$$

respectively. By means of Eq. (51) and the properties of the boson operators we easily derive one of the results of Kahn and Zarni:[6]

$$\hat{b}(t)|0\rangle = \lambda e^{-it}\left[\frac{3}{8}\exp\left(-\frac{3\lambda i t}{2}\right)|1\rangle + \frac{\sqrt{6}}{16}\exp(-3\lambda i t)|3\rangle\right] + \mathcal{O}(\lambda^2), \tag{53}$$

where $|n\rangle, n = 0,1,\ldots$, are the eigenvectors of the number operator $\hat{a}^\dagger\hat{a}$. The difference in the sign of the exponents is due to the fact that Kahn and Zarni chose an uncommon equation of motion for the creation and annihilation operators: $d\hat{a}(t)/dt = i\hat{a} + \cdots$.[6] Notice that if we add corrections of second order to $\hat{b}(t)$, then it is not that easy to obtain a simple expression for $\hat{b}(t)|n\rangle$ because the operators $\hat{\Omega}_1$ and $\hat{\Omega}_2$ that appear in the exponent do not commute. This was presumably the reason why Kahn and Zarmi[6] (as well as other authors[4,5]) did not include such terms in their calculations.

For the second normalization condition we follow Kahn and Zarmi[6] and require that

$$\hat{\Omega} = \alpha \hat{b}^\dagger \hat{b} + \beta, \tag{54}$$

where

$$\alpha = \sum_{j=0}^{\infty} \alpha_j \lambda^j, \quad \beta = \sum_{j=0}^{\infty} \beta_j \lambda^j. \tag{55}$$

On expanding Eq. (54) in a Taylor series about $\lambda = 0$ we obtain

$$\hat{\Omega}_j = \sum_{m=0}^{j} \sum_{k=0}^{m} \alpha_{j-m} \hat{b}_k^\dagger \hat{b}_{m-k} + \beta_j . \tag{56}$$

Taking into account the above-mentioned results for $\hat{\Omega}_0$ and $\hat{\Omega}_1$ we easily obtain $\alpha_0 = 0$, $\beta_0 = 1$, $\alpha_1 = \beta_1 = \frac{3}{4}$. At this point f_1 is still undetermined. From Eq. (56) for $j = 2$ we obtain $\hat{g}_2$ in terms of α_2, β_2, $\hat{f}_1$ and the boson operators. Setting $\hat{f}_1$ in order to remove zero-space elements from the right-hand side of Eq. (36) for $j = 2$ we obtain

$$\begin{gathered} \hat{f}_1 = -\tfrac{17}{32} \hat{a}^\dagger \hat{a}, \\ \alpha_2 = -\tfrac{153}{64}, \quad \beta_2 = -\tfrac{9}{8}, \end{gathered} \tag{57}$$

and exactly the above-given expression for $\hat{g}_2$.

In principle, this variant of the near-identity transformation should be identical to the one of Kahn and Zarmi;[6] however, our expressions

$$\hat{\Omega} = (\tfrac{3}{4}\lambda - \tfrac{153}{64}\lambda^2 + \cdots) \hat{b}^\dagger \hat{b} + 1 + \tfrac{3}{4}\lambda - \tfrac{9}{8}\lambda^2 + \cdots, \tag{58}$$

$$[\hat{b}, \hat{b}^\dagger] = 1 - \frac{17\lambda}{8} \hat{a}^\dagger \hat{a} + \cdots, \tag{59}$$

do not exactly agree with theirs, presumably because of the previously-mentioned sign difference. We believe that our equations are correct as they have passed all the consistency tests; that is to say, they satisfy Eqs. (36), (37), and (56).

In order to stress the flexibility of present approach still further, we try other normalization conditions. For example, it is possible to set the operators $\hat{f}_j$ so that $[\hat{b}, \hat{b}^\dagger] = \hat{\Omega}$; that is to say:

$$\sum_{m=0}^{j} [\hat{b}_m^\dagger, \hat{b}_{j-m}] = \hat{\Omega}_j . \tag{60}$$

In this case we obtain $\hat{g}_1$ and $\hat{g}_2$ as before, and

$$\begin{gathered} \hat{f}_1 = \tfrac{3}{16}(\hat{a}^\dagger \hat{a} + 2), \\ \hat{f}_2 = -\tfrac{1}{256}(25 \hat{a}^{\dagger 2} \hat{a}^2 + 135 \hat{a}^\dagger \hat{a} + 153). \end{gathered} \tag{61}$$

It is not difficult to verify that the normalization condition $[\hat{b}, \hat{b}^\dagger] = \hat{\Omega}$ just discussed is equivalent to the one chosen by Speliotopoulos:[7] $\hat{H} = \hat{b}^\dagger \hat{b} + e$, where e is a real number. Taking into account the operator coefficients $\hat{b}_j$, and $\hat{b}_j^\dagger$, derived previously, one easily obtains the coefficients of

$$e = \sum_{j=0}^{\infty} e_j \lambda^j; \tag{62}$$

the first ones are:

$$e_0=\tfrac{1}{2}, \quad e_1=\tfrac{3}{16}, \quad e_2=-\tfrac{21}{128}. \tag{63}$$

IV. CONCLUSIONS

We have discussed a simple time-independent perturbation theory that leads to perturbation series for time-dependent dynamical variables in classical and quantum mechanics that are free from secular terms. The approach focuses on the frequency of the motion in the former case and on a frequency operator in the latter. We believe that our method is sufficiently clear, straightforward, and systematic, and that it is a useful complement to other procedures proposed earlier for the same purpose.[4–6] The approach is suitable for symbolic programming[9] through Eqs. (16)–(18), and remarkably flexible as it allows one to easily choose the most convenient normalization condition to completely determine the solutions. A noticeable advantage of the present method is that it is based on time-independent equations, which not only facilitate the calculation of perturbation corrections, but also the analysis of convergence of the series. We have also discussed problems that may hinder the application of nonsecular perturbation methods at perturbation orders greater than unity. The present method resembles the multiple-scale approach in that similar equations apply to classical and quantum mechanics,[4,5] but in our opinion the equations in our method are considerably simpler.

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The disorder deviation in the deconfined phase

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A systematic study of the strongly interacting matter under extreme conditions via the form of the thermal ratio of the disorder deviation is presented. The evolution of Fermi and Bose particles (quarks and gluons) is studied in the framework of multiparticle correlation and distribution functions to predict the size of the finite-temperature deconfined phase. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The existence of a deconfined phase of gluons and quarks has been predicted by quantum chromodynamics (QCD).[1] Aspects of QCD at finite density are very important as well as instructive in the sense of the observation of quark-gluon plasma (QGP), especially from the heavy vector meson (HVM) suppression, strangeness enhancement, hadron yield distributions versus temperature and dilepton excess. There is large amount of consistency among the different signatures of deconfined phase transition to a new excited state of matter. In the case of HVM suppression (e.g., $c\bar{c}$ bound state suppression), the CERN-SPS experiments clearly show that it is visible in high energy nuclear collisions starting from a definite value of the energy density in the right range. Enhanced strange particle production in high energy nuclear collisions offers another indication for the phase transition: in the deconfined phase strange quarks are more easily produced. The threshold for producing strange quarks is much lower than that for strange hadrons. In addition, the mass of the strange quark goes down in the case of the restoration of the chiral symmetry. Hence, the observation of large ratios for strange particles is considered as a remnant of the unconfined phase. The dilepton abundance, while well explained by ordinary sources in all other cases, for Pb–Pb collisions is instead observed as a neat excess.

There is a very popular point of view in literature that a deconfinement phase transition is predicted to occur at the typical energy scale involved, $T_c \simeq \Lambda_{\mathrm{QCL}} \simeq m_\pi \simeq m_s \simeq 140-200$ MeV, where T_c, Λ_{QCD}, m_π, and m_s are the critical temperature, the scale of QCD, the pion mass and a mass of the strange quark, respectively. Putting all above-mentioned indications together, the case of a high density state of matter onsetting at a critical temperature around 170 MeV is reasonably suitable.

Among the issues related to QGP, we attract attention to the problem of deconfined phase through the calculation of correlation and distribution functions[2] in the thermal theory of quantized fields. We consider the semiphenomenological model for the deconfinement existence within the framework of the Langevine-type equation. To do this, we follow the standard theory of quantized fields, replacing

(1) the asymptotic field operators and
(2) the vacuum expectation values

by

(1) the thermal field operators and
(2) the thermal statistical averages,

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respectively, in order to formulate correlation and distribution functions of produced particles.

The method of the Langevine equation and its extensions to the quantal case have been suggested and considered in Refs. 3–5 and 6–8, respectively. We propose that real physical processes that happen in the finite-temperature QCD should be replaced by a one-constituent (e.g., gluon or quark) propagation provided by a special kernel operator (in the master evolution equation) to be considered as an input of the model and disturbed by the random force F. We assume F to be the external source proposed as both a c-number function and an operator. The master equation is an operator one, so that there appear new additional issues about the commutation relations and the ordering of operators, which do not exist in the classical case.[8]

Based on the thermal operator-field technique, we introduce a thermal ratio of the disorder deviation (TRDD), reflecting the degree of deviation, from unity, of the ratio of the two-particle thermal momentum-dependent distribution to two one-particle thermal distribution functions of produced particles, gluons and/or quarks (g/q) in a partly deconfined phase state. We study the four-momentum correlations of identical particles which can be both useful and instructive to infer the shape of the particle emitter-source. We estimate the sensitivity of the TRDD functions to the size of the emitter. Within these features, the canonical formalism in a stationary state in the thermal equilibrium (SSTE) is formulated, and a closed structural resemblance between the SSTE and standard quantum field theory is revealed.

To clarify the internal structure of the disordering of particles, we use the consistent approach based on the evolution of dynamical variables as well as the extension to different modes provided by virtual transitions.

II. DISTRIBUTION FUNCTIONS. EVOLUTION EQUATION

Let us consider a hypothetical system of the quark-gluon excited local thermal phase in QCD where a canonical operator a and its Hermitian conjugate a^+ occur. We formulate the distribution functions (DF) of produced particles (gluons and quarks) in terms of point-to-point equal time temperature-dependent thermal correlation functions (CFs) of two operators

$$w(\vec{k},\vec{k}',t;T)=\langle a^+(\vec{k},t)a(\vec{k}',t)\rangle$$

$$=Tr[a^+(\vec{k},t)a(\vec{k}',t)e^{-H\beta}]/Tr(e^{-H\beta}).$$

Here, $\langle \ldots \rangle$ means the procedure of thermal statistical averaging; $\vec{k}$ and t are, respectively, momentum and time variables, $e^{-\mathrm{H}\beta}/Tr(e^{-\mathrm{H}\beta})$ stands for the standard density operator in the equilibrium and the Hamiltonian H is given by the squared form of the annihilation a_p and creation a_p^+ operators for Bose and Fermi particles, $\mathrm{H}=\Sigma_p \epsilon_p a_p^+ a_p$ (the energy ϵ_p and operators a_p, a_p^+ carry some index p,[9] where $p_\alpha=2\pi n_\alpha/L, n_\alpha=0,\pm 1,\pm 2,\ldots; V=L^3$ is the volume of the system considered); β is the inverse temperature of the environment, and $\beta=1/T$. The standard canonical commutation relation

$$[a(\vec{k},t),a^+(\vec{k}',t)]_\pm=\delta^3(\vec{k}-\vec{k}')$$

at every time t is used as usual for Bose $(-)$ and Fermi $(+)$ operators.

The probability to find two particles, gluons or quarks, with momenta $\vec{k}$ and $\vec{k}'$ in the same event at the time t normalized to the single spectrum of these particles is

$$R(\vec{k},\vec{k}',t)=W(\vec{k},\vec{k}',t)/[W(\vec{k},t)\cdot W(\vec{k}',t)].$$

Here, the one-particle thermal DF is defined as

$$W(\vec{k},t)=\langle b^+(\vec{k},t)b(\vec{k},t)\rangle,$$

where

$$b(\vec{k},t)=a(\vec{k},t)+\phi(\vec{k},t)$$

under an assumption of occurrence of the random source-function $\phi(\vec{k},t)$ being an operator, in general. The two-particle DF $W(\vec{k},\vec{k}',t)$ looks like

$$W(\vec{k},\vec{k}',t)=\langle b^+(\vec{k},t)b^+(\vec{k}',t)b(\vec{k},t)b(\vec{k}',t)\rangle.$$

The evolution properties of propagating particles in a randomly distributed environment come from the evolution equations

$$i\partial_t b(\vec{k},t)+A(\vec{k},t)=F(\vec{k},t)+P, \tag{1}$$

$$-i\partial_t b^+(\vec{k},t)+A^*(\vec{k},t)=F^+(\vec{k},t)+P, \tag{2}$$

where both b and b^+ are the special mode operators of the quark and gluon fields,[10] and P and $F(\vec{k},t)$ stand for the stationary external force and the random one, respectively, both acting from the environment. The only operator F has a zeroth value of the statistical average, $\langle F\rangle=0$. The interaction of the particles considered with the surrounding ones as well as providing the propagation is given by the operator $A(\vec{k},t)$, which can be defined as the one closely related to the dissipation force:

$$A(\vec{k},t)=\int_{-\infty}^{+\infty}K(\vec{k},t-\tau)b(\vec{k},\tau)d\tau. \tag{3}$$

An interplay of quarks and gluons with surrounding particles is embedded into the interaction complex kernel $K(\vec{k},t)$, while the real physical transitions are provided by the random source operator $F(\vec{k},t)$ [see Eqs. (1) and (2)]. The random evolution field operator $K(\vec{k},t)$ in (3) stands for the random noise and it is assumed to vary stochastically with a δ-like equal time correlation function[10]

$$\langle K^+(\vec{k},\tau)K(\vec{k}',\tau)\rangle=2(\pi\rho)^{1/2}\kappa\delta(\vec{k}-\vec{k}'),$$

where both the strength of the noise κ and the positive constant $\rho\to\infty$ define the effect of the Gaussian noise on the evolution of quarks and gluons in the thermalized environment.

The formal solution of (1) in the operator form in $S(\mathfrak{R}_4)$ $[k^\mu=(\omega=k^0,k_j)]$ is

$$\tilde{b}(k_\mu)=\tilde{a}(k_\mu)+\tilde{\phi}(k_\mu),$$

where the operator $\tilde{a}(k_\mu)$ is expressed via the Fourier transformed operator $\tilde{F}(k_\mu)$ and the Fourier transformed kernel function $\tilde{K}(k_\mu)$ [coming from (3)] as

$$\tilde{a}(k_\mu)=\tilde{F}(k_\mu)\cdot[\tilde{K}(k_\mu)-\omega]^{-1},$$

while the function $\tilde{\phi}(k_\mu)\sim P\cdot[\tilde{K}(k_\mu)-\omega]^{-1}$. The random force operator $F(\vec{k},t)$ can be expanded by using the Fourier integral

$$F(\vec{k},t)=\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\psi(k_\mu)\hat{c}(k_\mu)e^{-i\omega t}, \tag{4}$$

where the form $\psi(k_\mu)\cdot\hat{c}(k_\mu)$ is just the Fourier operator $\tilde{F}(k_\mu)=\psi(k_\mu)\cdot\hat{c}(k_\mu)$ and the canonical operator $\hat{c}(k_\mu)$ obeys the commutation relation

$$[\hat{c}(k_\mu),\hat{c}^+(k'_\mu)]_\pm=\delta^4(k_\mu-k'_\mu).$$

The function $\psi(k_\mu)$ in (4) is determined by the condition[10]

$$\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\left[\frac{\psi(k_\mu)}{\tilde{K}(k_\mu)-\omega}\right]^2=1.$$

III. TRDD AND THE SPACE–TIME SIZE

The enhanced probability for emission of two identical particles is given by the ratio R of DF in $S(\mathfrak{R}_4)$ as follows:

$$R_{b/f}(k_\mu,k'_\mu;T)=\frac{\tilde{W}(k_\mu,k'_\mu;T)}{\tilde{W}(k_\mu)\cdot\tilde{W}(k'_\mu)}, \tag{5}$$

where $\tilde{W}(k_\mu,k'_\mu;T)=\langle\tilde{b}^+(k_\mu)\tilde{b}^+(k'_\mu)\tilde{b}(k_\mu)\tilde{b}(k'_\mu)\rangle$ and $\tilde{W}(k_\mu)=\langle\tilde{b}^+(k_\mu)\tilde{b}(k_\mu)\rangle$. Using the Fourier solution of Eq. (1) in $S(\mathfrak{R}_4)$, one can get R-ratios for DF obeying Bose particles

$$R_b(k_\mu,k'_\mu;T)=1+D_b(k_\mu,k'_\mu;T) \tag{6}$$

and Fermi particles

$$R_f(k_\mu,k'_\mu;T)=R_b(k_\mu,k'_\mu;T)-2\frac{\Xi(k_\mu)\cdot\Xi(k'_\mu)}{\tilde{W}(k_\mu)\cdot\tilde{W}(k'_\mu)}, \tag{7}$$

where

$$D_b(k_\mu,k'_\mu)=\frac{\Xi(k_\mu,k'_\mu)[\Xi(k'_\mu,k_\mu)+\tilde{\phi}^+(k'_\mu)\tilde{\phi}(k_\mu)]+\Xi(k'_\mu,k_\mu)\tilde{\phi}^+(k_\mu)\tilde{\phi}(k'_\mu)}{\tilde{W}(k_\mu)\cdot\tilde{W}(k'_\mu)} \tag{8}$$

and the two-particle CF $\Xi(k_\mu,k'_\mu)$ looks like

$$\Xi(k_\mu,k'_\mu)=\langle\tilde{a}^+(k_\mu)\tilde{a}(k'_\mu)\rangle$$

$$=\frac{\psi^*(k_\mu)\cdot\psi(k'_\mu)}{[\tilde{K}^*(k_\mu)-\omega]\cdot[\tilde{K}(k'_\mu)-\omega']}\cdot\langle\hat{c}^+(k_\mu)\hat{c}(k'_\mu)\rangle. \tag{9}$$

Using the Kubo–Martin–Schwinger condition (μ is the chemical potential)

$$\langle a(\vec{k}',t')a^+(\vec{k},t)\rangle=\langle a^+(\vec{k},t)a(\vec{k}',t-i\beta)\rangle\cdot\exp(-\beta\mu),$$

the thermal statistical averages for the $\hat{c}(k_\mu)$-operator should be presented in the following form:

$$\langle\hat{c}^+(k_\mu)\hat{c}(k'_\mu)\rangle=\delta^4(k_\mu-k'_\mu)\cdot n(\omega,T),$$

$$\langle\hat{c}(k_\mu)\hat{c}^+(k'_\mu)\rangle=\delta^4(k_\mu-k'_\mu)\cdot[1\pm n(\omega,T)]$$

for Bose $(+)$ and Fermi $(-)$ statistics, where $n(\omega,T)=\{\exp[(\omega-\mu)\beta]\pm1\}^{-1}$. Inserting CF (9) into (8) and taking into account that the $\delta^4(k_\mu-k'_\mu)$-function should be changed by the smooth sharp function $\Omega(r)\cdot\exp(-q^2/2)$, one can get the following expression for the D_b-function:

$$D_b(k_\mu,k'_\mu;T)=\lambda(k_\mu,k'_\mu;T)\exp(-q^2/2)$$
$$\times[n(\bar{\omega},T)\Omega(r)\exp(-q^2/2)+\tilde{\phi}^*(k'_\mu)\tilde{\phi}(k_\mu)+\tilde{\phi}^*(k_\mu)\tilde{\phi}(k'_\mu)], \qquad (10)$$

where

$$\lambda(k_\mu,k'_\mu;T)=\frac{\Omega(r)}{\tilde{W}(k_\mu)\cdot\tilde{W}(k'_\mu)}\cdot n(\bar{\omega},T), \quad \bar{\omega}=\frac{1}{2}(\omega+\omega').$$

The function $\Omega(r)\cdot n(\omega;T)\cdot\exp(-q^2/2)$ describes the space–time size of the QGP fireball. Choosing the z-axis along the two-heavy-ion collision axis, one can put

$$q^2=(r_0\cdot Q_0)^2+(r_z\cdot Q_z)^2+(r_t\cdot Q_t)^2,$$

$$Q_\mu=(k-k')_\mu, \quad Q_0=\epsilon_{\vec{k}}-\epsilon_{\vec{k}'}, \quad Q_z=k_z-k'_z, \quad Q_t=[(k_x-k'_x)^2+(k_y-k'_y)^2]^{1/2},$$

$$\Omega(r)\sim r_0\cdot r_z\cdot r_t^2,$$

where r_0, r_z and r_t are timelike, longitudinal and transverse ''size'' components of the QGP fireball. Formally, the function D_b (10) is the positive one ranging from 0 to 1. The quantitative information (longitudinal r_z and transverse r_t components of the QGP spherical volume, the temperature T of the environment) could be extracted by fitting the theoretical formula (10) to the measured TRDD function and estimating the errors of the fit parameters. Formula (10) indicates that a chaotic g/q source emanating from the thermalized g/q fireball exists. Hence, the measurement of the space–time evolution of the g/q source would provide information of the g/q emission process and the general reaction mechanism. In formula (10) for the D_b-function, the temperature of the environment enters through the two-particle CF $\Xi(k_\mu,k'_\mu;T)$. If T is unstable, the $R_{b/f}$-functions (5) will change due to a change of DF $\tilde{W}$ which, in fact, can be considered as an effective density of the g/q source. Formula (6) looks like the following expresion for the experimental R-ratio using a source parametrization:

$$R_T(r)=1+\lambda_T(r)\cdot\exp(-r_t^2\cdot Q_t^2/2-r_z^2\cdot Q_z^2/2),$$

where $r_t(r_z)$ is the transverse (longitudinal) radius parameter of the source with respect to the beam axis and λ_T stands for the effective intercept parameter (chaoticity parameter) which has a general dependence of the mean momentum of the observed particle pair. Here, the dependence on the source lifetime is omitted. Since $0<\lambda_T<1$, one can conclude that the effective function λ_T can be interpreted as a function of the core particles to all particles produced. The chaocity parameter λ_T is the temperature-dependent and the positive one defined by

$$\lambda_T(r)=\frac{|\Omega(r)n(\bar{\omega};T)|^2}{\tilde{W}(k_\mu)\cdot\tilde{W}(k'_\mu)}.$$

Comparing (8) and (10) one can identify

$$\Xi(k_\mu,k'_\mu)=\Omega(r)\cdot n(\bar{\omega};T)\cdot\exp(-q^2/2).$$

There is no satisfactory tool to derive the precise analytical form of the random source function $\tilde{\phi}(k_\mu)$ in (8), but one can put [see (9) and taking into account $\tilde{\phi}(k_\mu)\sim P\cdot[\tilde{K}(k_\mu)-\omega]^{-1}$] (Refs. 11 and 10)

$$\tilde{\phi}(k_\mu)=[\alpha\cdot\Xi(k_\mu)]^{1/2},$$

where α is of the order $O(P^2/n(\omega,T)\cdot|\psi(k_\mu)|^2)$. Thus,

$$D_b(q^2;T)=\frac{\tilde{\lambda}^{1/2}(\bar{\omega};T)}{(1+\alpha)(1+\alpha')}e^{-q^2/2}[\tilde{\lambda}^{1/2}(\bar{\omega};T)e^{-q^2/2}+2(\alpha\alpha')^{1/2}]. \tag{11}$$

It is easy to see that in the vicinity of $q^2\approx 0$ one can get the full correlation if $\alpha=\alpha'=0$ and $\tilde{\lambda}(\bar{\omega};T)=1$. Putting $\alpha=\alpha'$ in (11) we find the formal lower bound on the space–time dimensionless size of the fireball for the Bose system:

$$q_b^2\geqslant\ln\frac{\tilde{\lambda}(\bar{\omega};T)}{[\sqrt{(\alpha+1)^2+\alpha^2}-\alpha]^2}.$$

In the case of Fermi particles, the following restriction on q_f^2 is valid [see (7)]:

$$\ln\frac{\tilde{\lambda}(\bar{\omega};T)}{[\sqrt{2\alpha(\alpha+1)+3}-\alpha]^2}\leqslant q_f^2\leqslant\ln\frac{\tilde{\lambda}(\bar{\omega};T)}{[\sqrt{\alpha^2+2}-\alpha]^2}.$$

In fact, the function $D_b(k_\mu,k'_\mu;T)$ in (10) could not be observed because of some model uncertainties. In the standard consideration, the TRDD function has to contain a background contribution as well as other physical particles (resonances) which have not been included in the calculation of the D_b-function. In order to be close to the experimental data, one has to expand the D_b-function as projected on some well-defined function [in $S(\Re_4)$] of the relative momentum of two particles produced in heavy-ion collisions $D_b(k_\mu,k'_\mu;T)\to D_b(Q_\mu^2;T)$. Thus, it will be very instructive to use the polynomial expansion which is suitable to avoid any uncertainties as well as characterize the degree of deviation from the Gaussian distribution, for example. In $(-\infty,+\infty)$, a complete orthogonal set of functions can be obtained with the help of the Hermite polynomials in the Hilbert space of the square integrable functions with the measure $d\mu(z)=\exp(-z^2/2)dz$. The function D_b corresponds to this class if

$$\int_{-\infty}^{+\infty}dq\,\exp(-q^2/2)|D_b(q)|^n<\infty,\quad n=0,1,2,\ldots.$$

The expansion in terms of the Hermite polynomials $H_n(q)$,

$$D_b(q)=\lambda\sum_n c_n\cdot H_n(q)\cdot\exp(-q^2/2), \tag{12}$$

is well suited for the study of possible deviation from both the experimental shape and the exact theoretical form of the TRDD function D_b in (10). The coefficients c_n in (12) are defined via the integrals over the expanded functions D_b because of the orthogonality condition

$$\int_{-\infty}^{+\infty}H_n(x)H_m(x)\exp(-x^2/2)dx=\delta_{n,m}.$$

Thus, the observation of the two-particle correlation (both for Bose and Fermi symmetrization) enable us to extract the properties of the structure of q^2, i.e., the space–time size of QGP formation.

In order to be close to an experiment one has to replace $R_{b,f}$ functions (6) and (7) with respect to the cylindrical symmetry angles θ and ϕ which are nonobservable ones at fixed Q_t:

$$R_{b,f}(k_\mu,k'_\mu;T)\to\bar{R}_{b,f}(Q_t;T)=N^{-1}\int dq_t dQ_z d\theta d\phi\,\tilde{W}(k_\mu,k'_\mu;T),$$

where

$$N=\int dq_t\, dQ_z d\theta d\phi \tilde{W}(k_\mu)\, \tilde{W}(k'_\mu),$$

$$q_t=\frac{1}{\cos\theta+\sin\theta}\left\{k_x+k_y\mp\frac{1}{2}Q_t[\cos(\theta+\phi)+\sin(\theta+\phi)]\right\}.$$

Then, $\overline{R}_{b,f}(Q_t;T)=1+\overline{D}_{b,f}(Q_t;T)$ with

$$\overline{D}_b(Q_t;T)=\frac{\overline{N}^{-1}(T)}{(1+\alpha)(1+\alpha')}\exp[-(r_tQ_t)^2]\,F_b(Q_t;T),$$

$$\overline{D}_f(Q_t;T)=\frac{1}{(1+\alpha)(1+\alpha')}\{\overline{N}^{-1}(T)\exp[-(r_tQ_t)^2]\,F_b(Q_t;T)-2\},$$

$$F_b(Q_t;T)=\int dq_t\, dQ_z\, d\theta\, d\phi\, n^2(\overline{\omega};T)\, e^{-\beta_{0Z}}[1+2\sqrt{\alpha\alpha'\tilde{\lambda}^{-1}(\overline{\omega};T)}\, e^{q^2/2}],$$

$$\beta_{0Z}\equiv(r_0Q_0)^2+(r_zQ_z)^2,$$

$$\overline{N}(T)=\int dq_t\, dQ_z\, d\theta\, d\phi\, n(\omega;T)\, n(\omega';T).$$

To avoid the trivial result, one should restrict the α-parameter as

$$\alpha\geqslant\tilde{\lambda}^{-1/2}(\overline{\omega};T)e^{q^2/2}-\tfrac{1}{2}\tilde{\lambda}^{1/2}(\overline{\omega};T)\, e^{-q^2/2}.$$

In conclusion of this section, the experimental data are quite desired to make the analysis of the particle fluctuation via TRDD.

IV. CONCLUSION

(1) We investigated the finite temperature DF (of produced identical particles, gluons and quarks) which can be both useful and instructive to infer the shape of the gluon/quark source-emitter. In fact, we have presented the method of extracting the intercept and source parameters from the shape of the TRDD function.
(2) The relations between the CF $\Xi(k_\mu,k'_\mu)$ (9) and the full R-functions for Bose (6) and Fermi (7) particles at the stage of the freeze-out are obtained. We have shown the sensitivity of the correlation functions to the space–time geometry of the source-emitter (10). The TRDD function D_b describes the size and shape of the space–time domain where the secondary observed particles are generated.
(3) One can conclude that, formally, the deconfined phase size scale can be determined by the evolution behavior of the field operators and the critical temperature $T=T_c$ [see formula (10)].
(4) Since, the TRDD function D_b is the positive one and restricted by 1, we expect that the R-ratio at too small values of Q_μ starts from the fixed point $R(Q_\mu\to 0)=2-\epsilon$ $(\epsilon\to+0)$ and then falls down (with the Gaussian shape) up to unity over some momentum scale interval of an order of the inverse source size.

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Creation operators and Bethe vectors of the osp(1|2) Gaudin model

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A Gaudin model based on the orthosymplectic Lie superalgebra osp(1|2) is studied. The eigenvectors of the osp(1|2) invariant Gaudin Hamiltonians are constructed by algebraic Bethe ansatz. Corresponding creation operators are defined by a recurrence relation. Furthermore, explicit solution to this recurrence relation is found. The action of the creation operators on the lowest spin vector yields Bethe vectors of the model. The relation between the Bethe vectors and solutions to the Knizhnik–Zamolodchikov equation of the corresponding super-conformal field theory is established. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Classifying integrable systems solvable in the framework of the quantum inverse scattering method[1,2] by underlying dynamical symmetry algebras, one could say that the Gaudin models are the simplest ones being related to loop algebras and classical *r*-matrices. More sophisticated solvable models correspond to Yangians, quantum affine algebras, elliptic quantum groups, etc.

Gaudin models[3,4] are related to classical *r*-matrices, and the density of Gaudin Hamiltonians

$$H^{(a)}=\sum_{b\neq a} r_{ab}(z_a-z_b) \tag{1.1}$$

coincides with the *r*-matrix. Condition of their commutativity $[H^{(a)},H^{(b)}]=0$ is nothing else but the classical Yang–Baxter equation (YBE).

The Gaudin models (GM) associated to classical *r*-matrices of simple Lie algebras were studied in many papers (see Refs. 4–11 and references therein). The spectrum and eigenfunctions were found using different methods (coordinate and algebraic Bethe ansatz,[4,5] separated variables,[6] etc.). A relation to the Knizhnik–Zamolodchikov equation of conformal field theory was established.[8–10]

There are additional peculiarities of Gaudin models related to classical *r*-matrices based on Lie superalgebras due to Z_2-grading of representation spaces and operators. The study of the osp(1|2) invariant Gaudin model corresponding to the simplest nontrivial super-case of the osp(1|2) invariant *r*-matrix[12] started in Ref. 13. The spectrum of the osp(1|2) invariant Gaudin Hamiltonians $H^{(a)}$ was given, the antisymmetry property of their eigenstates was claimed, and a two site model was connected with some physically interesting one (a Dicke model).

The creation operators used in the sl(2) Gaudin model coincide with one of the *L*-matrix entry.[4,5] However, in the osp(1|2) case, as we will show, the creation operators are complicated polynomials of the two generators $X^+(\lambda)$ and $v^+(\mu)$ of the loop superalgebra. We introduce *B*-operators belonging to the Borel subalgebra of the loop superalgebra $\mathcal{L}(\mathrm{osp}(1|2))$ by a recurrence relation. Acting on the lowest spin vector (bare vacuum) the *B*-operators generate exact

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eigenstates of the Gaudin Hamiltonians $H^{(a)}$, provided Bethe equations are imposed on parameters of the states. For this reason the *B*-operators are sometimes refereed to as the creation operators and the eigenstates as the Bethe vectors, or simply *B*-vectors. Furthermore, the recurrence relation is solved explicitly and the commutation relations between the *B*-operators and the generators of the loop superalgebra $\mathcal{L}(\mathrm{osp}(1|2))$ as well as the generators of the global superalgebra $\mathrm{osp}(1|2)\subset\mathcal{L}(\mathrm{osp}(1|2))$ are calculated. We prove that the constructed states are lowest spin vectors of the global finite dimensional superalgebra osp(1|2), as it is the case for many invariant quantum integrable models.[14] Moreover, a striking coincidence between the spectrum of the osp(1|2) invariant Gaudin Hamiltonians of spin s and the spectrum of the Hamiltonians of the sl(2) Gaudin model of the integer spin $2s$ is found.

A connection between the *B*-states, when the Bethe equations are not imposed on their parameters, of the Gaudin models for simple Lie algebras to the solutions to the Knizhnik–Zamolodchikov equation was established in Refs. 8 and 9. An explanation of this connection based on Wakimoto modules at critical level of the underlying affine algebra was given in Ref. 9. An explicit form of the Bethe vectors in the coordinate representation was given in both papers.[8,9] The coordinate Bethe ansatz for the *B*-states of the osp(1|2) Gaudin model is obtained in our article as well. Using commutation relations between the *B*-operators and the transfer matrix $t(\lambda)$, as well as the Hamiltonians $H^{(a)}$, we give an algebraic proof of the fact that explicitly constructed *B*-states yield a solution to the Knizhnik–Zamolodchikov equation corresponding to a super-conformal field theory. This connection permits us to calculate the norm of the eigenstates of the Gaudin Hamiltonians. An analogous connection is expected between the quantum osp(1|2) spin system related to the graded Yang–Baxter equation[12,15,16] and the quantum Knizhnik–Zamolodchikov equation following the lines of Ref. 17. We point out possible modifications of the Gaudin Hamiltonians and corresponding modifications of the Knizhnik–Zamolodchikov equation, similar to the case of the sl(2) Gaudin model which was interpreted in Refs. 18 and 19 as a quantization of the Schlesinger system.

The norm and correlation functions of the sl(2) invariant Gaudin model were evaluated in Ref. 6 using Gauss factorization of a group element and the Riemann–Hilbert problem. The study of this problem for the Gaudin model based on the osp(1|2) Lie superalgebra is in progress. However, we propose a formula for the scalar products of the Bethe states which is analogous to the sl(2) case.

The article is organized as follows. In Sec. II we recall the main data of the quantum osp(1|2) spin system: the osp(1|2) invariant solution to the graded Yang–Baxter equation (*R*-matrix), monodromy matrix $T(\lambda)$, the transfer matrix $t(\lambda)=1/2\,str\,T(\lambda)$, its eigenvalues and the Bethe equations. However, the eigenvectors of this quantum integrable spin system can be constructed only by a complicated recurrence procedure[20] which is not given here. Nevertheless, it is useful to recall the main data of the quantum integrable spin system because some characteristics of the corresponding Gaudin model can be obtained easily as a quasi-classical limit of these data. The osp(1|2) Gaudin model and its creation operators B_M are discussed thoroughly in Sec. III. Some of the most important properties of these operators are formulated and demonstrated: antisymmetry with respect to their arguments, commutation relations with the loop superalgebra generators, commutation relations with the generating function $t(\lambda)$ of the Gaudin Hamiltonians, a differential identity, valid in the case of the Gaudin realization of the loop superalgebra. Using these properties of the *B*-operators we prove in Sec. IV that, acting on the lowest spin vector Ω_-, these operators generate eigenvectors of the generating function of integrals of motion, provided the Bethe equations are imposed on the arguments of the *B*-operators. Possible modifications of the Gaudin Hamiltonians are pointed out also. An algebraic proof is given in Sec. V that constructed Bethe vectors are entering into solutions of the Knizhnik–Zamolodchikov equation of super-conformal field theory. A quasi-classical asymptotic with respect to a parameter of the Knizhnik–Zamolodchikov equation permits us to calculate the norm of the eigenstates of the Gaudin Hamiltonian. Further development on possible evaluation of correlation functions is discussed in the conclusion.

II. OSp(1|2)-INVARIANT *R*-MATRIX

Many properties of the Gaudin models can be obtained as a quasi-classical limit of the corresponding quantum spin systems related to solutions to the Yang–Baxter equation

$$R_{12}(\lambda-\mu)R_{13}(\lambda-\nu)R_{23}(\mu-\nu)=R_{23}(\mu-\nu)R_{13}(\lambda-\nu)R_{12}(\lambda-\mu). \tag{2.1}$$

Here the standard notation of the quantum inverse scattering method[1,2] is used to denote spaces $V_j, j=1,2,3$, on which corresponding R-matrices $R_{ij}, ij=12,13,23$, act nontrivially. In the quasi-classical limit $\eta\to 0$

$$R(\lambda;\eta)=I+\eta r(\lambda)+\mathcal{O}(\eta^2),$$

some relations simplify and therefore can be solved explicitly, providing more detailed results for the Gaudin model.

The graded Yang–Baxter equation[2,12] differs from the usual Yang–Baxter equation (2.1) by some sign factors due to the embedding of R-matrix into the space of matrices acting on the Z_2-graded tensor product $V_1\otimes V_2\otimes V_3$. At this point our aim is to reach a fundamental osp(1|2) invariant solution. The rank of the orthosymplectic Lie algebra osp(1|2) is one and its dimension is five. The three even generators are h, X^+, X^- and the two odd generators are v^+, v^-.[21] The (graded) commutation relations between the generators are

$$\begin{gathered}[h,X^\pm]=\pm 2X^\pm, \quad [h,v^\pm]=\pm v^\pm,\\ [X^+,X^-]=h, \quad [v^+,v^-]_+=-h,\\ [X^\mp,v^\pm]=v^\mp, \quad [v^\pm,v^\pm]_+=\pm 2X^\pm,\end{gathered} \tag{2.2}$$

together with $[X^\pm,v^\pm]=0$. Notice that the generators h and $v^\pm$ considered here in (2.2) differ by a factor of 2 from the ones used in Refs. 21 and 12. Thus the Casimir element is

$$c_2=h^2+2(X^+X^-+X^-X^+)+(v^+v^--v^-v^+)=h^2-h+4X^+X^-+2v^+v^-. \tag{2.3}$$

For further comparison with the sl(2) Gaudin model[4,5] and due to the chosen set of generators (2.2) we parametrize the finite dimensional irreducible representations $V^{(l)}$ of the osp(1|2) Lie superalgebra by an integer l, so that their dimensions $2l+1$ and the values of the Casimir element (2.3) $c_2=l(l+1)$ coincide with the same characteristics of the integer spin l irreducible representations of sl(2).

We proceed to write down the osp(1|2) invariant solution of the graded Yang–Baxter equation and the main data of the corresponding quantum spin system: the L-operator, the transfer matrix $t(\lambda)$, the eigenvalue of the generating function of the integrals of motion $t(\lambda)$ and the Bethe equations.

The fundamental irreducible representation V of osp(1|2) is three dimensional. We choose a gradation (parity) of the basis vectors $e_j;\ j=1,2,3$ to be (0,1,0).

The invariant R-matrix is a linear combination,[12]

$$R=\lambda\left(\lambda+\frac{3\eta}{2}\right)I+\eta\left(\lambda+\frac{3\eta}{2}\right)\mathcal{P}-\eta\lambda K, \tag{2.4}$$

of the three OSp(1|2) group invariant operators

$$[g\otimes g,X]=0, \quad g\in \mathrm{OSp}(1|2), \quad X\in \mathrm{End}(V\otimes V), \tag{2.5}$$

acting on $V\otimes V$: the identity I, the permutation $\mathcal{P}$ and a rank one projector K. In the equation (2.4) λ is the spectral parameter, and η is a quasi-classical parameter.

Using the projectors on the irreducible representation components in the Clebsch–Gordan decomposition $V\otimes V=V^{(2)}\otimes V^{(1)}\otimes V^{(0)}$,

$$P_2=\tfrac{1}{2}(I+\mathcal{P}),\quad P_1=\tfrac{1}{2}(I-\mathcal{P}-2K),\quad P_0=K, \tag{2.6}$$

one can represent the R-matrix (2.4) in the form

$$R(\lambda,\eta)=(\lambda+\eta)\left(\lambda+\frac{3\eta}{2}\right)\left(P_2+\frac{\lambda-\eta}{\lambda+\eta}P_1+\frac{\lambda-3\eta/2}{\lambda+3\eta/2}P_0\right). \tag{2.7}$$

Deforming these projectors to the quantum superalgebra $\mathrm{osp}_q(1|2)$ projectors[22,23] $P_i\to P_i(q)$ and substituting rational functions by trigonometric ones $[(\lambda\pm\eta)\to\sinh(\lambda\pm\eta)]$, one arrives at a trigonometric solution to the graded Yang–Baxter equation, in the braid group form, and corresponding anisotropic models.[23,24]

The L-operator of the quantum spin system on a one-dimensional lattice with N sites coincides with R-matrix acting in a tensor product $V_0\otimes V_a$ of auxiliary space V_0 and the space of states at site $a=1,2,\ldots,N$,

$$L_{0a}(\lambda-z_a)=R_{0a}(\lambda-z_a), \tag{2.8}$$

where z_a is a parameter of inhomogeneity (site dependence).[1,2] Corresponding monodromy matrix T is an ordered product of the L-operators

$$T(\lambda;\{z_a\}_1^N)=L_{0N}(\lambda-z_N)\cdots L_{01}(\lambda-z_1)=\prod_{\substack{a=1\\ \leftarrow}}^{N} L_{0a}(\lambda-z_a). \tag{2.9}$$

The commutation relations of the T-matrix entries follow from the FRT relation[1]

$$R_{12}(\lambda-\mu)T_1(\lambda)T_2(\mu)=T_2(\mu)T_1(\lambda)R_{12}(\lambda-\mu). \tag{2.10}$$

Multiplying (2.10) by R_{12}^{-1} and taking the super-trace over $V_1\otimes V_2$, one gets commutativity of the transfer matrix

$$t(\lambda)=\sum_j (-1)^{j+1}T_{jj}(\lambda;\{z_a\}_1^N)=T_{11}-T_{22}+T_{33} \tag{2.11}$$

for different values of the spectral parameter $t(\lambda)t(\mu)=t(\mu)t(\lambda)$.

The choice of the L-operators (2.8) corresponds to the following space of states of the osp(1|2)-spin system,

$$\mathcal{H}=\bigotimes_{a=1}^{N} V_a.$$

The eigenvalue of the transfer matrix $t(\lambda)$ in this space is[12]

$$\Lambda(\lambda;\{\mu_j\}_1^M)=\alpha_1^{(N)}(\lambda;\{z_a\}_1^N)\prod_{j=1}^{M} S_1(\lambda-\mu_j)-\alpha_2^{(N)}(\lambda;\{z_a\}_1^N)\prod_{j=1}^{M} S_1\left(\lambda-\mu_j+\frac{\eta}{2}\right)$$
$$S_{-1}(\lambda-\mu_j+\eta)+\alpha_3^{(N)}(\lambda;\{z_a\}_1^N)\prod_{j=1}^{M} S_{-1}\left(\lambda-\mu_j+\frac{3\eta}{2}\right), \tag{2.12}$$

where

$$\alpha_j^{(N)}(\lambda;\{z_a\}_1^N)=\prod_{b=1}^{N}\alpha_j(\lambda-z_b),\quad j=1,2,3,$$

$$\alpha_1(\lambda)=(\lambda+\eta)^N(\lambda+3\eta/2)^N,\quad \alpha_2(\lambda)=\lambda^N(\lambda+3\eta/2)^N, \tag{2.13}$$

$$\alpha_3(\lambda)=\lambda^N(\lambda+\eta/2)^N,\quad S_n(\mu)=\frac{\mu-n\eta/2}{\mu+n\eta/2}.$$

Although according to (2.12) the eigenvalue has formally two sets of poles at $\lambda=\mu_j-\eta/2$ and $\lambda=\mu_j-\eta$, the corresponding residues are zero due to the Bethe equations[12]

$$\prod_{a=1}^{N}\left(\frac{\mu_j-z_a+\eta/2}{\mu_j-z_a-\eta/2}\right)=\prod_{k=1}^{M}S_1(\mu_j-\mu_k)S_{-2}(\mu_j-\mu_k). \tag{2.14}$$

If we take different spins l_a at different sites of the lattice and the following space of states

$$\mathcal{H}=\bigotimes_{a=1}^{N}V_a^{(l_a)},$$

then the factors on the left hand side of (2.14) will be spin dependent too:

$$\frac{\mu_j-z_a+\eta l_a/2}{\mu_j-z_a-\eta l_a/2}.$$

The osp(1|2) invariant R-matrix (2.4) has more complicated structure than the sl(2) invariant R-matrix of C. N. Yang, $R=\lambda I+\eta\mathcal{P}$. As a consequence the commutation relations of the entries $T_{ij}(\lambda)$ of the T-matrix (2.9) are more complicated and construction of the eigenstates of the transfer matrix $t(\lambda)$ by the algebraic Bethe ansatz can be done only using a complicated recurrence relation expressed in terms of $T_{ij}(\mu_k)$ [Ref. 20; see also Ref. 15 for the case of osp(1|2)]. It will be shown later that, due to a simplification of this relation in the quasi-classical limit $\eta\to 0$, one can solve it and find the creation operators for the osp(1|2) Gaudin model explicitly. Furthermore, the commutation relations between the creation operators and the generators of the loop superalgebra as well as the generating function $t(\lambda)$ of the Gaudin Hamiltonians will be given explicitly.

III. OSp(1|2) GAUDIN MODEL AND CORRESPONDING CREATION OPERATORS

As in the case of any simple Lie algebra, the classical r-matrix of the orthosymplectic Lie algebra osp(1|2) can be expressed in a pure algebraic form using a (reduced) Casimir element in the tensor product osp(1|2)⊗osp(1|2):[12]

$$\hat{r}(\lambda)=\frac{1}{\lambda}c_2^{\otimes},$$
$$c_2^{\otimes}=h\otimes h+2(X^+\otimes X^-+X^-\otimes X^+)+(v^+\otimes v^--v^-\otimes v^+). \tag{3.1}$$

The matrix form of the Casimir element $\hat{r}$ in the fundamental representation π of osp(1|2) follows from (3.1) by substituting appropriate 3×3 matrices instead of the osp(1|2) generators (2.2)[21] and taking into account the Z_2-graded tensor product of even and odd matrices.[12] Alternatively, the same matrix form of $\hat{r}$ can be obtained as a term linear in η in the quasi-classical expansion of (2.4) and (2.7),

$$r(\lambda)=\frac{1}{\lambda}(\mathcal{P}-K),$$

where $\mathcal{P}$ is a graded permutation matrix and K is a rank one projector. Let us write explicitly the matrix form of $r_0=\mathcal{P}-K$ in the basis $e_1\otimes e_1, e_1\otimes e_2, e_1\otimes e_3, \ldots, e_3\otimes e_3$ of the tensor product of two copies of the fundamental representation $V\otimes V$:

$$r_0=\lambda r(\lambda)=\mathcal{P}-K=\begin{pmatrix} 1 & & & & & & & & \\ & 0 & & 1 & & & & & \\ & & -1 & & -1 & & 2 & & \\ & 1 & & 0 & & & & & \\ & & 1 & & 0 & & -1 & & \\ & & & & & 0 & & 1 & \\ & & 2 & & 1 & & -1 & & \\ & & & & & 1 & & 0 & \\ & & & & & & & & 1 \end{pmatrix} \tag{3.2}$$

with all the other entries of this 9×9 matrix being identically equal to zero.

A quasi-classical limit $\eta\to 0$ of the FRT-relations (2.10) results in a matrix form of the loop superalgebra relation ($T(\lambda;\eta)=I+\eta L(\lambda)+\mathcal{O}(\eta^2)$):

$$[\underset{1}{L}(\lambda),\underset{2}{L}(\mu)]=-[r_{12}(\lambda-\mu),\underset{1}{L}(\lambda)+\underset{2}{L}(\mu)]. \tag{3.3}$$

Both sides of this relation have the usual commutators of even 9×9 matrices $L_1(\lambda)=L(\lambda)\otimes I_3$, $L_2(\mu)=I_3\otimes L(\mu)$ and $r_{12}(\lambda-\mu)$, where I_3 is 3×3 unit matrix and $L(\lambda)$ has loop superalgebra valued entries:

$$L(\lambda)=\begin{pmatrix} h(\lambda) & -v^-(\lambda) & 2X^-(\lambda) \\ v^+(\lambda) & 0 & v^-(\lambda) \\ 2X^+(\lambda) & v^+(\lambda) & -h(\lambda) \end{pmatrix}. \tag{3.4}$$

The relation (3.3) is a compact matrix form of the following commutation relations between the generators $h(\lambda), v^{\pm}(\mu), X^{\pm}(\nu)$ of the loop superalgebra under consideration,

$$[h(\lambda),X^{\pm}(\mu)]=\mp 2\frac{X^{\pm}(\lambda)-X^{\pm}(\mu)}{\lambda-\mu},\quad [h(\lambda),v^{\pm}(\mu)]=\mp\frac{v^{\pm}(\lambda)-v^{\pm}(\mu)}{\lambda-\mu},$$

$$[X^+(\lambda),X^-(\mu)]=-\frac{h(\lambda)-h(\mu)}{\lambda-\mu},\quad [X^{\pm}(\lambda),v^{\mp}(\mu)]=-\frac{v^{\pm}(\lambda)-v^{\pm}(\mu)}{\lambda-\mu}, \tag{3.5}$$

$$[v^+(\lambda),v^-(\mu)]_+=\frac{h(\lambda)-h(\mu)}{\lambda-\mu},\quad [v^{\pm}(\lambda),v^{\pm}(\mu)]_+=\mp 2\frac{X^{\pm}(\lambda)-X^{\pm}(\mu)}{\lambda-\mu},$$

together with $[X^{\pm}(\lambda),v^{\pm}(\mu)]=0$.

Actually these commutation relations (3.5) define the positive part $\mathcal{L}_+(\mathrm{osp}(1|2))$ of the loop superalgebra. The usual generators Y_n of a loop algebra parametrized by a non-negative integer are obtained from the expansion of $Y(\lambda)$,

$$Y(\lambda)=\sum_{n\geqslant 0}\frac{Y_n}{\lambda^{n+1}}.$$

In particular, taking all $Y_n=0$ for $n>0$, one gets an L-operator $L(\lambda)=L_0/\lambda$, where L_0 is an osp(1|2)-valued matrix. This L_0 similar to r_0 satisfies a cubic characteristic equation with the osp(1|2) Casimir element (2.3) as coefficient:

$$L_0^3+2L_0^2-(c_2-1)L_0-c_2I=0. \tag{3.6}$$

A Gaudin realization of the loop algebra (3.5) can be defined through the generators $Y=(h,v^{\pm},X^{\pm})$,

$$Y(\lambda)=\sum_{a=1}^{N}\frac{Y_a}{\lambda-z_a},\quad Y_a\in\mathrm{End}(V_a), \tag{3.7}$$

where Y_a are osp(1|2) generators in an irreducible representation $V_a^{(l_a)}$ of the lowest spin $-l_a$ associated with each site a.[4,5] Then the L-operator (3.4) has the form

$$L(\lambda;\{z_a\}_1^N)=\sum_{a=1}^{N}\frac{L_a}{\lambda-z_a}. \tag{3.8}$$

Here $\{z_a\}_1^N$ are parameters of the model [cf. (2.8) and (2.9)]. It follows from the relation (3.8) that the first term in the asymptotic expansion near $\lambda=\infty$ defines generators of the global $\mathrm{osp}(1|2)\subset\mathcal{L}_+(\mathrm{osp}(1|2))$,

$$L_{gl}=\lim_{\lambda\to\infty}\lambda L(\lambda)=\sum_{a=1}^{N}L_a, \tag{3.9}$$

where

$$L_{gl}=\begin{pmatrix} h_{gl} & -v_{gl}^- & 2X_{gl}^- \\ v_{gl}^+ & 0 & v_{gl}^- \\ 2X_{gl}^+ & v_{gl}^+ & -h_{gl}\end{pmatrix}. \tag{3.10}$$

Moreover, from the equation (3.3) we get

$$\left[\underset{1}{L_{gl}},\underset{2}{L(\mu)}\right]=-\left[\underset{2}{r_0},\underset{2}{L(\mu)}\right], \tag{3.11}$$

here $\underset{1}{L_{gl}}=L_{gl}\otimes I_3$, e.g., $[h_{gl},v^+(\mu)]=v^+(\mu)$.

Let us consider the loop superalgebra $\mathcal{L}_+(\mathrm{osp}(1|2))$ as the dynamical symmetry algebra, i.e., as the algebra of observables. In order to define a dynamical system besides the algebra of observables we need to specify a Hamiltonian. It is a well-known fact that due to the r-matrix relation (3.3), the so-called Sklyanin linear brackets, the elements

$$\begin{aligned} t(\lambda)&=\tfrac{1}{2}\mathrm{str}L^2(\lambda)=h^2(\lambda)+2[X^+(\lambda),X^-(\lambda)]_+ +[v^+(\lambda),v^-(\lambda)]_- \\ &=h^2(\lambda)+h'(\lambda)+4X^+(\lambda)X^-(\lambda)+2v^+(\lambda)v^-(\lambda)\end{aligned} \tag{3.12}$$

commute for different values of the spectral parameter $t(\lambda)t(\mu)=t(\mu)t(\lambda)$. Thus, $t(\lambda)$ can be considered as a generating function of integrals of motion.

It is straightforward to calculate the commutation relations between the operator $t(\lambda)$ and the generators of the loop algebra $X^+(\mu)$ and $v^+(\mu)$:

$$[t(\lambda),X^+(\mu)]=4\frac{X^+(\mu)h(\lambda)-X^+(\lambda)h(\mu)}{\lambda-\mu}-\frac{v^+(\lambda)v^+(\mu)-v^+(\mu)v^+(\lambda)}{\lambda-\mu}, \tag{3.13}$$

$$[t(\lambda),v^+(\mu)]=2\frac{v^+(\mu)h(\lambda)-v^+(\lambda)h(\mu)}{\lambda-\mu}-4\frac{X^+(\mu)v^-(\lambda)-X^+(\lambda)v^-(\mu)}{\lambda-\mu}. \tag{3.14}$$

These relations will be important for the proof of Lemma 3.6 as well as the proof of the main theorem.

A direct consequence of the equation (3.11) is an invariance of the generating function of integrals of motion $t(\lambda)$ under the action of the global osp(1|2):

$$[t(\lambda),L_{gl}]=0. \tag{3.15}$$

Preserving some generality we can consider the representation space $\mathcal{H}_{ph}$ of the dynamical algebra to be a lowest spin $\rho(\lambda)$ representation of the loop superalgebra with the lowest spin vector Ω_-,

$$h(\lambda)\Omega_-=\rho(\lambda)\Omega_-, \quad v^-(\lambda)\Omega_-=0. \tag{3.16}$$

In particular, a representation of the Gaudin realization (3.8) can be obtained by considering irreducible representations $V_a^{(l_a)}$ of the Lie superalgebra osp(1|2) defined by a spin $-l_a$ and a lowest spin vector ω_a such that $v_a^-\omega_a=0$ and $h_a\omega_a=-l_a\omega_a$. Thus,

$$\Omega_-=\bigotimes_{a=1}^{N}\omega_a \quad \text{and} \quad \rho(\lambda)=\sum_{a=1}^{N}\frac{-l_a}{\lambda-z_a}. \tag{3.17}$$

It is a well-known fact in the theory of Gaudin models[4,5] that the Gaudin Hamiltonians

$$H^{(a)}=\sum_{b\neq a}\frac{c_2^{\otimes}(a,b)}{z_a-z_b}=\sum_{b\neq a}\frac{1}{z_a-z_b}(h_ah_b+2(X_a^+X_b^-+X_a^-X_b^+)+(v_a^+v_b^--v_a^-v_b^+)) \tag{3.18}$$

can be obtained as the residue of the operator $t(\lambda)$ at the point $\lambda=z_a$ using the expansion

$$t(\lambda)=\sum_{a=1}^{N}\left(\frac{l_a(l_a+1)}{(\lambda-z_a)^2}+2\frac{H^{(a)}}{\lambda-z_a}\right). \tag{3.19}$$

To construct the set of eigenstates of the generating function of integrals of motion $t(\lambda)$ we have to define appropriate creation operators. The creation operators used in the sl(2) Gaudin model coincide with one of the L-matrix entry.[4,5] However, in the osp(1|2) case the creation operators are complicated functions of the two generators of the loop superalgebra $X^+(\lambda)$ and $v^+(\mu)$.

Definition 3.1: Let $B_M(\mu_1,\ldots,\mu_M)$ *belong to the Borel subalgebra* $\mathcal{B}$ *of the* osp(1|2) *loop algebra* $\mathcal{L}_+(\text{osp}(1|2))$ *such that*

$$B_M(\mu_1,\ldots,\mu_M)=v^+(\mu_1)B_{M-1}(\mu_2,\ldots,\mu_M)+2X^+(\mu_1)\sum_{j=2}^{M}\frac{(-1)^j}{\mu_1-\mu_j}B_{M-2}^{(j)}(\mu_2,\ldots,\mu_M), \tag{3.20}$$

with $B_0=1$, $B_1(\mu)=v^+(\mu)$ *and* $B_M=0$ *for* $M<0$. *The notation adopted here is that upper index of* $B_{M-2}^{(j)}(\mu_2,\ldots,\mu_M)$ *means that the argument* μ_j *is omitted.*

Remark 3.1: It may be useful to write down the explicit expressions for the first few creation operators

$$B_0=1,\quad B_1(\mu)=v^+(\mu),\ B_2(\mu_1,\mu_2)=v^+(\mu_1)v^+(\mu_2)+2\frac{X^+(\mu_1)}{\mu_1-\mu_2},$$

$$B_3(\mu_1,\mu_2,\mu_3)=v^+(\mu_1)B_2(\mu_2,\mu_3)+2X^+(\mu_1)\left(\frac{v^+(\mu_3)}{\mu_1-\mu_2}-\frac{v^+(\mu_2)}{\mu_1-\mu_3}\right), \tag{3.21}$$

$$B_4(\mu_1,\mu_2,\mu_3,\mu_4)=v^+(\mu_1)B_3(\mu_2,\mu_3,\mu_4)+2X^+(\mu_1)\times\left(\frac{B_2(\mu_3,\mu_4)}{\mu_1-\mu_2}-\frac{B_2(\mu_2,\mu_4)}{\mu_1-\mu_3}+\frac{B_2(\mu_2,\mu_3)}{\mu_1-\mu_4}\right).$$

The creation operators $B_M(\mu_1,\ldots,\mu_M)$ together with $h(\nu)$ generate the Borel subalgebra $\mathcal{B}\subset\mathcal{L}_+$. As we will show later, the B-operators are such that the Bethe vectors are generated by their action on the lowest spin vector Ω_- (3.16). To prove this result we will need some important properties of the B-operators which are summarized in the following seven lemmas.

Lemma 3.1: The creation operators $B_M(\mu_1,\ldots,\mu_M)$ are antisymmetric functions of their arguments

$$B_M(\mu_1,\ldots,\mu_k,\mu_{k+1},\ldots,\mu_M)=-B_M(\mu_1,\ldots,\mu_{k+1},\mu_k,\ldots,\mu_M), \tag{3.22}$$

here $1\leqslant k<M$ and $M\geqslant 2$.

Sometimes an alternative formulation of the recurrence relation (3.20) can be useful.

Lemma 3.2: Alternatively, the recurrence relation (3.20) can be written in the following form,

$$B_M(\mu_1,\ldots,\mu_M)=B_{M-1}(\mu_1,\ldots,\mu_{M-1})v^+(\mu_M)+2\sum_{j=1}^{M-1}(-1)^{M-j-1}\times\frac{X^+(\mu_j)}{\mu_j-\mu_M}B^{(j)}_{M-2}(\mu_1,\ldots,\mu_{M-1}), \tag{3.23}$$

with $B_0=1$, $B_1(\mu)=v^+(\mu)$ and $B_N=0$, for $N<0$.

In the subsequent lemmas we will calculate the commutation relations between the generators of the loop superalgebra $\mathcal{L}(\mathrm{osp}(1|2))$ and the B-operators. In order to simplify the formulas we will omit the arguments and denote the creation operator $B_M(\mu_1,\ldots,\mu_M)$ by B_M. We suppose that it will not be difficult to restore the appropriate set of arguments.

Lemma 3.3: The commutation relations between the generator $v^+(\lambda)$ of the loop superalgebra and the creation operator B_M are given by

$$v^+(\lambda)B_M=(-1)^M B_M v^+(\lambda)+2\sum_{j=1}^{M}(-1)^j\frac{X^+(\lambda)-X^+(\mu_j)}{\lambda-\mu_j}B^{(j)}_{M-1}. \tag{3.24}$$

Here as in the previous lemma the upper index of $B^{(j)}_{M-1}$ means that the argument μ_j is omitted.

Lemma 3.4: The generator $h(\nu)$ has the following commutation relation with the B_M elements

$$h(\lambda)B_M=B_M\left(h(\lambda)+\sum_{i=1}^{M}\frac{1}{\lambda-\mu_i}\right)+\sum_{i=1}^{M}\frac{(-1)^i}{\lambda-\mu_i}\left(v^+(\lambda)B^{(i)}_{M-1}+2X^+(\lambda)\sum_{\substack{j=1\\ j\neq 1}}^{M}\frac{(-1)^{j+\Theta(i-j)}}{\mu_i-\mu_j}B^{(i,j)}_{M-2}\right). \tag{3.25}$$

Here $\Theta(j)$ is the Heaviside function,

$$\Theta(j)=\begin{cases}1 & if\ \ j>0,\\ 0 & if\ \ j\leqslant 0,\end{cases}$$

and the meaning of the upper indices of $B^{(i,j)}_{M-2}$ *is that the parameters* μ_i,μ_j *are omitted.*

Lemma 3.5: The generator $v^-(\lambda)$ *of the loop superalgebra has the following commutation relation with the B-operators:*

$$v^-(\lambda)B_M=(-1)^M B_M v^-(\lambda)+\sum_{j=1}^{M}(-1)^{j-1}B^{(j)}_{M-1}\left(\frac{h(\lambda)-h(\mu_j)}{\lambda-\mu_j}+\sum_{\substack{k=1\\k\neq j}}^{M}\frac{1}{(\lambda-\mu_k)(\mu_k-\mu_j)}\right)$$
$$+v^+(\lambda)\sum_{\substack{i,j=1\\i<j}}^{M}(-1)^{i-j-1}\frac{B^{(i,j)}_{M-2}}{\mu_i-\mu_j}\left(\frac{1}{\lambda-\mu_i}+\frac{1}{\lambda-\mu_j}\right). \tag{3.26}$$

Already at this point we can make some useful observations.

Remark 3.2: The commutation relations between the generators of the global osp(1|2) (3.10) *and the* B_M *elements follow from Lemmas 3.3–3.5. To see this we multiply (3.24)–(3.26) by* λ *and then take the limit* $\lambda\to\infty$. *In this way we obtain*

$$v^+_{gl}B_M=(-1)^M B_M v^+_{gl}-2\sum_{j=1}^{M}(-1)^j X^+(\mu_j)B^{(j)}_{M-1}, \tag{3.27}$$

$$h_{gl}B_M=B_M(h_{gl}+M), \tag{3.28}$$

$$v^-_{gl}B_M=(-1)^M B_M v^-_{gl}+\sum_{j=1}^{M}(-1)^j B^{(j)}_{M-1}\left(h(\mu_j)+\sum_{k\neq j}^{M}\frac{1}{\mu_j-\mu_k}\right). \tag{3.29}$$

The subsequent lemma is one of the most important results. The proof of the main theorem is based on the following.

Lemma 3.6: The generating function of integrals of motion $t(\lambda)$ *(3.12) has the following commutation relation with the creation operator* $B_M(\mu_1,\ldots,\mu_M)$*:*

$$t(\lambda)B_M=B_M t(\lambda)+2B_M\left(h(\lambda)\sum_{i=1}^{M}\frac{1}{\lambda-\mu_i}+\sum_{\substack{i,j=1\\i<j}}^{M}\frac{1}{(\lambda-\mu_i)(\lambda-\mu_j)}\right)$$
$$+2\sum_{i=1}^{M}\frac{(-1)^i}{\lambda-\mu_i}\left(v^+(\lambda)B^{(i)}_{M-1}+2X^+(\lambda)\sum_{\substack{j=1\\j\neq i}}^{M}\frac{(-1)^{j+\Theta(i-j)}}{\mu_i-\mu_j}B^{(i,j)}_{M-2}\right)\hat{\beta}_M(\mu_i)$$
$$+4\sum_{i=1}^{M}\frac{(-1)^i}{\lambda-\mu_i}B^{(i)}_{M-1}(X^+(\lambda)v^-(\mu_i)-X^+(\mu_i)v^-(\lambda)). \tag{3.30}$$

Here we use the following notation for the operator:

$$\hat{\beta}_M(\mu_i)=h(\mu_i)+\sum_{\substack{j=1\\j\neq i}}^{M}\frac{1}{\mu_i-\mu_j}.$$

In the Gaudin realization (3.7) the creation operators $B_M(\mu_1,\ldots,\mu_M)$ have some specific analytical properties.

Lemma 3.7: The B-operators in the Gaudin realization (3.7) satisfy an important differential identity,

$$\frac{\partial}{\partial z_a}B_M=\sum_{j=1}^{M}\frac{\partial}{\partial\mu_j}\left(\frac{(-1)^j}{\mu_j-z_a}\left(v_a^+B_{M-1}^{(j)}+2X_a^+\sum_{k\neq j}^{M}\frac{(-1)^{k+\Theta(j-k)}}{\mu_j-\mu_k}B_{M-2}^{(j,k)}\right)\right). \tag{3.31}$$

This identity will be a fundamental step in establishing a connection between the Bethe vectors and the Knizhnik–Zamolodchikov equation.

The proofs of the lemmas are based on the induction method. As illustrations, we prove explicitly lemmas 3.1 and 3.3.

Proof of Lemma 3.1: We prove Lemma 3.1 by induction. Consider $M=2$:

$$B_2(\mu_1,\mu_2)=v^+(\mu_1)v^+(\mu_2)+2\frac{X^+(\mu_1)}{\mu_1-\mu_2}.$$

Using the commutation relations (3.5) it is straightforward to check that $B_2(\mu_1,\mu_2)$ is antisymmetric:

$$B_2(\mu_1,\mu_2)=-B_2(\mu_2,\mu_1).$$

Assume $B_N(\mu_1,\ldots,\mu_N)$ is antisymmetric for $M>N\geqslant 2$. We have to prove that $B_M(\mu_1,\ldots,\mu_M)$ is antisymmetric also.

Consider $j\geqslant 2$. The antisymmetry of $B_M(\mu_1,\ldots,\mu_M)$ with respect to μ_j and μ_{j+1} follows directly from the recurrence relation (3.20) and our assumption. Namely, the terms $B_{M-2}^{(j)}\times(\mu_2,\ldots,\mu_M)/(\mu_1-\mu_j)$ and $B_{M-2}^{(j+1)}(\mu_2,\ldots,\mu_M)/(\mu_1-\mu_{j+1})$ enter with the opposite sign.

Therefore we only have to show the antisymmetry of $B_M(\mu_1,\ldots,\mu_M)$ with respect to the interchange of μ_1 and μ_2. To see this we have to iterate the recurrence relation (3.20) twice and combine the appropriate terms

$$\begin{aligned}B_M(\mu_1,\ldots,\mu_M)=&\left(v^+(\mu_1)v^+(\mu_2)+2\frac{X^+(\mu_1)}{\mu_1-\mu_2}\right)B_{M-2}(\mu_3,\ldots,\mu_M)\\&+2v^+(\mu_1)X^+(\mu_2)\sum_{j=3}^{M}\frac{(-1)^{j+1}}{\mu_2-\mu_j}B_{M-3}^{(j)}(\mu_3,\ldots,\mu_M)\\&+2v^+(\mu_2)X^+(\mu_1)\sum_{j=3}^{M}\frac{(-1)^{j}}{\mu_1-\mu_j}B_{M-3}^{(j)}(\mu_3,\ldots,\mu_M)\\&+4X^+(\mu_1)X^+(\mu_2)\sum_{j=3}^{M}\frac{(-1)^{j}}{\mu_1-\mu_j}\sum_{k=3}^{M}\frac{(-1)^{k+\Theta(j-k)}}{\mu_2-\mu_k}B_{M-4}^{(j,k)}(\mu_3,\ldots,\mu_M),\end{aligned} \tag{3.32}$$

where $B_{M-4}^{(j,k)}(\mu_3,\ldots,\mu_M)$ means that the arguments μ_j and μ_k are omitted. Since $v^+(\mu)$ commutes with $X^+(\nu)$, the antisymmetry of the right hand side of (3.32) with respect to μ_1 and μ_2 follows. Hence we have demonstrated the lemma. □

We proceed now to prove Lemma 3.3.

Proof of Lemma 3.3: In particular, when $M=1$ the expression (3.24) is just the anticommutator between $v^+(\lambda)$ and $v^+(\mu)$. Using the recurrence relations (3.20) it is straightforward to check that the formula (3.24) holds for $M=2$:

$$\begin{aligned}v^+(\lambda)B_2(\mu_1,\mu_2)=&B_2(\mu_1,\mu_2)v^+(\lambda)-2\frac{X^+(\lambda)-X^+(\mu_1)}{\lambda-\mu_1}v^+(\mu_2)\\&+2\frac{X^+(\lambda)-X^+(\mu_2)}{\lambda-\mu_2}v^+(\mu_1).\end{aligned} \tag{3.33}$$

Therefore we can proceed to demonstrate Lemma 3.3 by induction. Assume that the relation (3.24) holds for B_N, $M \geqslant N \geqslant 2$. Then we have to show the formula (3.24) is valid for $M+1$. We use the recurrence relations (3.20) to write

$$\begin{aligned} v^+(\lambda)B_{M+1} &= v^+(\lambda)\left(v^+(\mu_1)B_M + 2X^+(\mu_1)\sum_{j=2}^{M+1}\frac{(-1)^j}{\mu_1-\mu_j}B_{M-1}^{(j)}\right) \\ &= -v^+(\mu_1)v^+(\lambda)B_M - 2\frac{X^+(\lambda)-X^+(\mu_1)}{\lambda-\mu_1}B_M \\ &\quad + 2X^+(\mu_1)\sum_{j=2}^{M+1}\frac{(-1)^j}{\mu_1-\mu_j}v^+(\lambda)B_{M-1}^{(j)}. \end{aligned} \tag{3.34}$$

Now we can substitute the expressions for $v^+(\lambda)B_M$ and $v^+(\lambda)B_{M-1}^{(j)}$. After rearranging the terms in an appropriate way we have

$$v^+(\lambda)B_{M+1} = (-1)^{M+1}B_{M+1}v^+(\lambda) + 2\sum_{j=1}^{M+1}(-1)^j\frac{X^+(\lambda)-X^+(\mu_j)}{\lambda-\mu_j}B_M^{(j)}. \tag{3.35}$$

This completes the proof of the lemma. □

Subsequently we demonstrate Lemma 3.2.

Proof of Lemma 3.2: The first step in this proof is to use the antisymmetry property Lemma 3.1. The second step is to use the defining recurrence relations. Then we use Lemma 3.3 and finally after some cancellations we get the right hand side of the equation (3.23):

$$\begin{aligned} B_M(\mu_1,\ldots,\mu_M) &\overset{(3.22)}{=} (-1)^{M-1}B_M(\mu_M,\mu_1,\ldots,\mu_{M-1}) \\ &\overset{(3.20)}{=} (-1)^{M-1}v^+(\mu_M)B_{M-1}(\mu_1,\ldots,\mu_{M-1}) \\ &\quad + (-1)^{M-1}2X^+(\mu_M)\sum_{j=1}^{M-1}\frac{(-1)^{j-1}}{\mu_M-\mu_j}B_{M-2}^{(j)}(\mu_1,\ldots,\mu_{M-1}) \\ &\overset{(3.24)}{=} B_{M-1}(\mu_1,\ldots,\mu_{M-1})v^+(\mu_M) \\ &\quad + (-1)^{M-1}2\sum_{j=1}^{M-1}(-1)^j\frac{X^+(\mu_M)-X^+(\mu_j)}{\mu_M-\mu_j} \\ &\quad \times B_{M-2}^{(j)}(\mu_1,\ldots,\mu_{M-1}) + (-1)^{M-1}2X^+(\mu_M)\sum_{j=1}^{M-1}\frac{(-1)^{j-1}}{\mu_M-\mu_j} \\ &\quad \times B_{M-2}^{(j)}(\mu_1,\ldots,\mu_{M-1}) \\ &= B_{M-1}(\mu_1,\ldots,\mu_{M-1})v^+(\mu_M) + 2\sum_{j=1}^{M-1}(-1)^{M-j-1}\frac{X^+(\mu_j)}{\mu_j-\mu_M}B_{M-2}^{(j)} \\ &\quad \times(\mu_1,\ldots,\mu_{M-1}). \end{aligned}$$

□

The proofs of the other lemmas are analogous to the proofs of Lemmas 3.1 and 3.3. Since these proofs do not contain illuminating insights and are considerably longer than the two we have seen we will omit them.

The recurrence relation (3.20) can be solved explicitly. To be able to express the solution of the recurrence relation in a compact form it is useful to introduce a contraction operator d.

Definition 3.2: Let d be a contraction operator whose action on an ordered product $\prod_{j=1}^{M}{}_{\rightarrow} v^+(\mu_j)$, $M \geqslant 2$, is given by

$$d(v^+(\mu_1)v^+(\mu_2)\ldots v^+(\mu_M)) = 2\sum_{j=1}^{M-1} X^+(\mu_j) \sum_{k=j+1}^{M} \frac{(-1)^{\sigma(jk)}}{\mu_j-\mu_k} \prod_{m\neq j,k}^{M}{}_{\rightarrow} v^+(\mu_m), \quad (3.36)$$

where $\sigma(jk)$ is the parity of the permutation

$$\sigma:(1,2,...,j,j+1,...,k,\ldots,M)\rightarrow(1,2,...,j,k,j+1,...,M).$$

The d operator can be applied on an ordered product $\prod_{j=1}^{M}{}_{\rightarrow} v^+(\mu_j)$ consecutively several times. As an illustration, we explicitly apply the contraction operator d two times in the case when $M=4$:

$$\begin{aligned}
&d^2(v^+(\mu_1)v^+(\mu_2)v^+(\mu_3)v^+(\mu_4))\\
&\quad = d(d(v^+(\mu_1)v^+(\mu_2)v^+(\mu_3)v^+(\mu_4)))\\
&\quad = 2X^+(\mu_1)\left(\frac{d(v^+(\mu_3)v^+(\mu_4))}{\mu_1-\mu_2} - \frac{d(v^+(\mu_2)v^+(\mu_4))}{\mu_1-\mu_3} + \frac{d(v^+(\mu_2)v^+(\mu_3))}{\mu_1-\mu_4}\right)\\
&\qquad + 2X^+(\mu_2)\left(\frac{d(v^+(\mu_1)v^+(\mu_4))}{\mu_2-\mu_3} - \frac{d(v^+(\mu_1)v^+(\mu_2))}{\mu_2-\mu_4}\right) + 2X^+(\mu_3)\frac{d(v^+(\mu_1)v^+(\mu_2))}{\mu_3-\mu_4}\\
&\quad = 8X^+(\mu_1)\left(\frac{X^+(\mu_3)}{(\mu_1-\mu_2)(\mu_3-\mu_4)} - \frac{X^+(\mu_2)}{(\mu_1-\mu_3)(\mu_2-\mu_4)} + \frac{X^+(\mu_2)}{(\mu_1-\mu_3)(\mu_2-\mu_4)}\right).
\end{aligned}$$

It follows that the contraction operator d can be applied on an ordered product $\prod_{j=1}^{M}{}_{\rightarrow} v^+(\mu_j)$ up to $[M/2]$ times consecutively. The symbol $[M/2]$ denotes the integer part of $M/2$.

Theorem 3.1: Explicit solution to the recurrence relation (3.20) is given by

$$B_M(\mu_1,\ldots,\mu_M) = \prod_{j=1}^{M}{}_{\rightarrow} v^+(\mu_j) + \sum_{m=1}^{[M/2]} \frac{1}{m!} d^m \prod_{j=1}^{M}{}_{\rightarrow} v^+(\mu_j). \quad (3.37)$$

Here d is the contraction operator defined above (3.36).

The properties of the creation operators B_M studied in this section will be fundamental tools in determining some of the most important characteristics of the osp(1|2) Gaudin model. Our primary interest is to obtain the spectrum and the eigenvectors of the generating function of integrals of motion $t(\lambda)$ (3.12).

IV. SPECTRUM OF THE OSp(1|2) GAUDIN MODEL AND ITS MODIFICATIONS

With the help of the creation operators B_M it is possible to obtain the eigenvectors as well as the corresponding eigenvalues of the Gaudin Hamiltonians. This result is a direct consequence of the following theorem.

Theorem 4.1: *The lowest spin vector Ω_-* (3.16) *is an eigenvector of the generating function of integrals of motion* t(λ) *(3.12) with the corresponding eigenvalue $\Lambda_0(\lambda)$:*

$$t(\lambda)\Omega_- = \Lambda_0(\lambda)\Omega_-, \quad \Lambda_0(\lambda) = \rho^2(\lambda) + \rho'(\lambda). \tag{4.1}$$

Furthermore, the action of the B-operators on the lowest spin vector Ω_- yields the eigenvectors

$$\Psi(\mu_1,\ldots,\mu_M) = B_M(\mu_1,\ldots,\mu_M)\Omega_- \tag{4.2}$$

of the $t(\lambda)$ operator

$$t(\lambda)\Psi(\mu_1,\ldots,\mu_M) = \Lambda(\lambda;\{\mu_j\}_{j=1}^M)\Psi(\mu_1,\ldots,\mu_M), \tag{4.3}$$

with the eigenvalues

$$\Lambda(\lambda;\{\mu_j\}_{j=1}^M) = \Lambda_0(\lambda) + 2\rho(\lambda)\sum_{k=1}^M \frac{1}{\lambda-\mu_k} + 2\sum_{k<l}\frac{1}{(\lambda-\mu_k)(\lambda-\mu_l)}, \tag{4.4}$$

provided that the Bethe equations are imposed on the parameters $\{\mu_j\}_{j=1}^M$:

$$\beta_M(\mu_j) = \rho(\mu_j) + \sum_{k\neq j}^M \frac{1}{\mu_j-\mu_k} = 0. \tag{4.5}$$

Proof: The equation (4.1) can be checked by a direct substitution of the definitions of the operator $t(\lambda)$ and the lowest spin vector Ω_-, the equations (3.12) and (3.16), respectively.

To show the second part of the theorem, we use the equation (4.2) to express the Bethe vectors $\Psi(\mu_1,\ldots,\mu_M)$

$$t(\lambda)\Psi(\mu_1,\ldots,\mu_M) = t(\lambda)B_M(\mu_1,\ldots,\mu_M)\Omega_-. \tag{4.6}$$

Our next step is to use Lemma 3.6 and the definition of the lowest spin vector Ω_-, the equation (3.16), in order to calculate the action of the operator $t(\lambda)$ on the Bethe vectors when the Bethe equations (4.5) are imposed:

$$t(\lambda)B_M\Omega_- = B_M t(\lambda)\Omega_- + 2\left(\rho(\lambda)\sum_{i=1}^M\frac{1}{\lambda-\mu_i} + \sum_{i<j}^M\frac{1}{(\lambda-\mu_i)(\lambda-\mu_j)}\right)B_M\Omega_-. \tag{4.7}$$

We can express the first term on the right hand side since we know how the operator $t(\lambda)$ acts on the vector Ω_-, the equation (4.1),

$$t(\lambda)B_M\Omega_- = \left(\Lambda_0(\lambda) + 2\left(\rho(\lambda)\sum_{i=1}^M\frac{1}{\lambda-\mu_i} + \sum_{i<j}^M\frac{1}{(\lambda-\mu_i)(\lambda-\mu_j)}\right)\right)B_M\Omega_-. \tag{4.8}$$

The eigenvalue equation (4.3) as well as the expression for the eigenvalues (4.4) follow from the equation (4.8). □

Corollary 4.1: *In the Gaudin realization of the loop superalgebra given by the equations (3.7) and (3.17) the Bethe vectors $\Psi(\mu_1,\ldots,\mu_M)$ (4.2) are the eigenvectors of the Gaudin Hamiltonians (3.18),*

$$H^{(a)}\Psi(\mu_1,\ldots,\mu_M) = E_M^{(a)}\Psi(\mu_1,\ldots,\mu_M), \tag{4.9}$$

with the eigenvalues

$$E_M^{(a)} = \sum_{\substack{b=1\\ b\neq a}}^N \frac{l_a l_b}{z_a - z_b} + \sum_{j=1}^M \frac{l_a}{\mu_j - z_a}, \tag{4.10}$$

when the Bethe equations are imposed:

$$\beta_M(\mu_j)=\rho(\mu_j)+\sum_{k\neq j}^{M}\frac{1}{\mu_j-\mu_k}=\sum_{a=1}^{N}\frac{-l_a}{\mu_j-z_a}+\sum_{k\neq j}^{M}\frac{1}{\mu_j-\mu_k}=0. \tag{4.11}$$

Proof: The statement of the corollary follows from residue of the equation (4.3) at the point $\lambda=z_a$. The residue can be determined using (3.19), (4.4) and (4.1). □

The eigenvalue (4.4) of the operator $t(\lambda)$ and the Bethe equations (4.5) can be obtained also as the appropriate terms in the quasi-classical limit $\eta\to 0$ of the expressions (2.12) and (2.14).

Comparing the eigenvalues $E_M^{(a)}$ (4.10) of the Gaudin Hamiltonians and the Bethe equations (4.11) with the corresponding quantities of the sl(2) Gaudin model[4,5] we arrive to an interesting observation.

Remark 4.1: The spectrum of the osp(1|2) *Gaudin model with the spins l_a coincides with the spectrum of the* sl(2) *Gaudin system for the integer spins (cf. an analogous observation for partition functions of corresponding anisotropic vertex models in Ref. 23).*

Remark 4.2: The Bethe vectors are eigenstates of the global generator h_{gl},

$$h_{gl}\Psi(\mu_1,\ldots,\mu_M)=\left(-\sum_{a=1}^{N}l_a+M\right)\Psi(\mu_1,\ldots,\mu_M). \tag{4.12}$$

Moreover, these Bethe vectors are the lowest spin vectors of the global osp(1|2) *since they are annihilated by the generator v_{gl}^{-}*

$$v_{gl}^{-}\Psi(\mu_1,\ldots,\mu_M)=0, \tag{4.13}$$

once the Bethe equations are imposed (4.11). These conclusions follow from Remark 3.2*, the equations (3.28) and (3.29) and the definition of the Bethe vectors (4.2).*

Hence, action of the global generator v_{gl}^{+} on the lowest spin vectors $\Psi(\mu_1,\ldots,\mu_M)$ generates a multiplet of eigenvectors of the operator $t(\lambda)$:

$$(v_{gl}^{+})^m\Psi(\mu_1,\ldots,\mu_M),\quad m=1,2,\ldots,2\left(\sum_{a=1}^{N}l_a-M\right). \tag{4.14}$$

One can repeat the arguments of Refs. 14 and 1 to demonstrate combinatorially completeness of the constructed states.

As was pointed out already in Ref. 4 for the sl(2) case, there are several modifications of the Hamiltonians (3.18). One of them is the Richardson's pairing-force Hamiltonian.[25] These modifications can be formulated in the framework of universal L-operator and r-matrix formalism (3.3).[5]

Due to invariance of the r-matrix (3.1),

$$[r(\lambda),Y\otimes I+I\otimes Y]=0,\quad Y\in\mathrm{osp}(1|2), \tag{4.15}$$

one can add to the L-operator any element of osp(1|2),

$$L(\lambda)\to\tilde{L}(\lambda)=gY+L(\lambda), \tag{4.16}$$

preserving commutation relations (3.3). If we choose $Y=h$, then

$$\tilde{t}(\lambda)=\tfrac{1}{2}\,\mathrm{str}\tilde{L}^2(\lambda)=t(\lambda)+2gh(\lambda)+g^2 \tag{4.17}$$

will have the commutativity property, i.e., $\tilde{t}(\lambda)\tilde{t}(\mu)=\tilde{t}(\mu)\tilde{t}(\lambda)$. Hence we can take $\tilde{t}(\lambda)$ to be the generating function of the (modified) integrals of motion:

$$\tilde{t}(\lambda)=\sum_{a=1}^{N}\left(\frac{c_2(a)}{(\lambda-z_a)^2}+2\,\frac{\tilde{H}^{(a)}}{\lambda-z_a}\right)+g^2, \tag{4.18}$$

$$\tilde{H}^{(a)}=gh_a+\sum_{b\neq a}\frac{c_2^{\otimes}(a,b)}{z_a-z_b}. \tag{4.19}$$

Notice that the global osp(1|2) symmetry is now broken down to global $u(1)$:

$$[\tilde{t}(\lambda),h_{gl}]=\left[\tilde{t}(\lambda),\sum_{a=1}^{N}h_a\right]=0. \tag{4.20}$$

In this case the eigenstates Ψ_M are generated by the same B-operators. However, corresponding eigenvalues and Bethe equations are now given by

$$\tilde{\Lambda}(\lambda;\{\mu_j\}_{j=1}^{M})=\Lambda(\lambda;\{\mu_j\}_{j=1}^{M})+2g\rho(\lambda)+2g\sum_{j=1}^{M}\frac{1}{\lambda-\mu_j}+g^2, \tag{4.21}$$

$$\tilde{E}_M^{(a)}=E_M^{(a)}+g(-l_a), \tag{4.22}$$

$$-g+\sum_{a=1}^{N}\frac{l_a}{\mu_j-z_a}=\sum_{k\neq j}^{M}\frac{1}{\mu_j-\mu_k}. \tag{4.23}$$

The crucial step in the proof of these equations is the observation that the commutation relations between the operator $\tilde{t}(\lambda)$ (4.17) and the creation operators B_M are equal to the commutation relations (3.30) but with modified operator $\hat{\beta}_M(\mu_j)\to\hat{\beta}_M(\mu_j)+g$. To see this, notice the similarity between the terms with $v^+(\lambda)B_{M-1}^{(i)}$ operators and with $X^+(\lambda)B_{M-2}^{(i,j)}$ operators in Lemma 3.4, the equation (3.25), and in Lemma 3.6, the equation (3.30).

A Richardson-like Hamiltonian[25] can be obtained as a coefficient in the $\lambda\to\infty$ expansion

$$\tilde{t}(\lambda)=g^2+\frac{2g}{\lambda}\sum_{a=1}^{N}h_a+\frac{1}{\lambda^2}\left(2g\sum_{a=1}^{N}z_ah_a+c_2(gl)\right)+O\left(\frac{1}{\lambda^3}\right). \tag{4.24}$$

The first coefficient in this expansion is h_{gl}, global $u(1)$ symmetry generator (4.20). Let us denote the second coefficient by $2H_g$. Using the global osp(1|2) algebra generators one can write this Hamiltonian in the form

$$H_g=g\sum_{a=1}^{N}z_ah_a+2X_{gl}^{+}X_{gl}^{-}+v_{gl}^{+}v_{gl}^{-}, \tag{4.25}$$

where we have omitted the term $h_{gl}(h_{gl}-1)$. The eigenvalues of the Hamiltonian H_g are given by

$$H_g\Psi_M(\mu_1,\ldots,\mu_M)=E_g\Psi_M(\mu_1,\ldots,\mu_M),\quad E_g=\sum_{j=1}^{M}\mu_j-\sum_{a=1}^{N}l_az_a. \tag{4.26}$$

A realization of the generators in terms of fermionic oscillators in the sl(2) case yields a Richardson Hamiltonian.[25] In the osp(1|2) case, which we consider here, there are extra fermionic degrees of freedom due to the term $v_{gl}^{+}v_{gl}^{-}$ and constraints $(v_{gl}^{\pm})^2=X^{\pm}$.

One can realize Sklyanin bracket (3.3) using an L-operator with bosonic and fermionic oscillator entries,

$$L_{\mathrm{osc}}(\lambda)=\begin{pmatrix}\lambda & -\gamma & 2b\\ \gamma^{+} & 0 & \lambda\\ 2b^{+} & \gamma^{+} & -\lambda\end{pmatrix}, \tag{4.27}$$

where

$$[b,b^+]=1, \quad [\gamma,\gamma^+]_+=1, \quad \gamma^2=(\gamma^+)^2=0. \tag{4.28}$$

It is straightforward to see that the corresponding realization of the loop superalgebra will have only two nonzero commutators. Hence, one can consider a combination of Gaudin and oscillator realizations:

$$\widetilde{L}(\lambda)=L_{\mathrm{osc}}(\lambda)+L(\lambda). \tag{4.29}$$

Intergals of motion can be obtained using

$$\begin{aligned}\widetilde{t}(\lambda)&=\tfrac{1}{2}\,\mathrm{str}(L^2_{\mathrm{osc}}(\lambda)+2L_{\mathrm{osc}}(\lambda)L(\lambda)+L^2(\lambda))\\ &=t(\lambda)+\lambda^2+2(bb^++b^+b)+(\gamma^+\gamma-\gamma\gamma^+)+2(\lambda h(\lambda)+2(bX^+(\lambda)+b^+X^-(\lambda))\\ &\quad+(\gamma^+v^-(\lambda)-\gamma v^+(\lambda))).\end{aligned} \tag{4.30}$$

Corresponding *B*-operators can be constructed using

$$\widetilde{v}^+(\lambda)=\gamma^++v^+(\lambda), \quad \widetilde{X}^+(\lambda)=b^++X^+(\lambda). \tag{4.31}$$

Finally, the eigenvalues $\widetilde{\Lambda}$ and the Bethe equations are given by

$$\widetilde{\Lambda}(\lambda;\{\mu_j\}_{j=1}^M)=\Lambda(\lambda;\{\mu_j\}_{j=1}^M)+2(\lambda\rho(\lambda)+1)+\sum_{j=1}^M\frac{2\lambda}{\lambda-\mu_j}+\lambda^2, \tag{4.32}$$

$$-\mu_j+\sum_{a=1}^N\frac{l_a}{\mu_j-z_a}=\sum_{k\neq j}^M\frac{1}{\mu_j-\mu_k}. \tag{4.33}$$

Further modifications can be obtained considering the quasi-classical limit of the quantum spin system with nonperiodic boundary conditions and corresponding reflection equation.

The expression of the eigenvector of a solvable model in terms of local variables parametrized by sites of the chain or by space coordinates is known as coordinate Bethe ansatz.[4] The coordinate representation of the Bethe vectors gives explicitly analytical dependence on the parameters $\{\mu_i\}_1^M$ and $\{z_a\}_1^N$ useful in a relation to the Knizhnik–Zamolodchikov equation (Sec. V). Using the Gaudin realization (3.7) of the generators

$$v^+(\mu)=\sum_{a=1}^N\frac{v_a^+}{\mu-z_a}, \quad X^+(\mu)=\sum_{a=1}^N\frac{X_a^+}{\mu-z_a},$$

and the definition of the creation operators (3.37), one can get the coordinate representation of the *B*-operators:

$$B_M(\mu_1,\mu_2,\ldots,\mu_M)=\sum_\pi\,(v^+_{a_1}\cdots v^+_{a_M})_\pi\prod_{a=1}^N\,\varphi(\{\mu_m^{(a)}\}_1^{|\mathcal{K}_a|};z_a), \tag{4.34}$$

where the first sum is taken over ordered partitions π of the set $(1,2,\ldots,M)$ into subsets $\mathcal{K}_a$, $a=1,2,\ldots,N$, including empty subsets with the constraints

$$\bigcup_a\mathcal{K}_a=(1,2,\ldots,M), \quad \mathcal{K}_a\cap\mathcal{K}_b=\varnothing \ \text{ for } \ a\neq b.$$

The corresponding subset of quasi-momenta is

$$(\mu_1^{(a)}=\mu_{j_1},\mu_2^{(a)}=\mu_{j_2},\ldots\mu_{|\mathcal{K}_a|}^{(a)}=\mu_{j|\mathcal{K}_a|};j_m\in\mathcal{K}_a),$$

where $|\mathcal{K}_a|$ is the cardinality of the subset $\mathcal{K}_a$, and $j_k<j_{k+1}$, entering into the coordinate wave function

$$\varphi(\{\nu_m\}_1^{|\mathcal{K}|};z)=\sum_{\sigma\in\mathcal{S}_{|\mathcal{K}|}}(-1)^{p(\sigma)}((\nu_{\sigma(1)}-\nu_{\sigma(2)})(\nu_{\sigma(2)}-\nu_{\sigma(3)})\cdots(\nu_{|\mathcal{K}|}-z))^{-1}.$$

Due to the alternative sum over permutations $\sigma\in\mathcal{S}_{|\mathcal{K}|}$, this function is antisymmetric with respect to the quasi-momenta. Finally, the first factor in (4.34),

$$(v_{a_1}^+\cdots v_{a_M}^+)_\pi,$$

means that for $j_m\in\mathcal{K}_a$ corresponding indices of $v_{a_{jm}}^+$ are equal to a so that $v_{a_{jm}}^+=v_a^+$. One can collect these operators into product $\Pi_{a=1}^N(v_a^+)^{|\mathcal{K}_a|}$; consequently we have an extra sign factor $(-1)^{p(\pi)}$.

This coordinate representation is similar to the representations obtained in Refs. 8–10 for the Gaudin models related to the simple Lie algebras (see also Ref. 26). The Z_2-grading results in extra signs, while the complicated structure of the B_M-operators [for the sl(2)-GM they are just products of B_1-operators $B_1(\mu_j)=X^+(\mu_j)$] is connected with the fact that $(v_j^+)^2=X_j^+\neq 0$, while for $j\neq k$ v_j^+ and v_k^+ anticommute.

V. SOLUTIONS TO THE KNIZHNIK–ZAMOLODCHIKOV EQUATION

Correlation functions $\psi(z_1,\ldots,z_n)$ of the two dimensional conformal field theory satisfy the Knizhnik–Zamolodchikov equation[27]

$$\kappa\frac{\partial}{\partial z_a}\psi(z_1,\ldots,z_n)=\left(\sum_{b\neq a}\frac{Y_a^\alpha\otimes Y_b^\alpha}{z_a-z_b}\right)\psi(z_1,\ldots,z_n),\tag{5.1}$$

where Y_a^α are generators of an orthonormal basis of a simple Lie algebra in a finite dimensional irreducible representation V_a and $\psi(z_1,\ldots,z_n)$ is a function of N complex variables taking values in a tensor product $\otimes_{a=1}^N V_a$. The first term on the right hand side of (5.1) is a Gaudin Hamiltonian (1.1).

A relation between the Bethe vectors of the Gaudin model related to simple Lie algebras and the solutions to the Knizhnik–Zamolodchikov equation is well known for sometime.[8,9] The approach used here to obtain solutions to the Knizhnik–Zamolodchikov equation corresponding to superconformal field theory and Lie superalgebra osp(1|2) starting from *B*-vectors (4.2) is based on Ref. 8.

A solution in question is represented as a contour integral over the variables $\mu_1,\ldots,\mu_M$,

$$\psi(z_1,\ldots,z_N)=\oint\cdots\oint\phi(\vec{\mu}|\vec{z})\Psi(\vec{\mu}|\vec{z})d\mu_1\cdots d\mu_M,\tag{5.2}$$

where an integrating factor $\phi(\vec{\mu}|\vec{z})$ is a scalar function

$$\phi(\vec{\mu}|\vec{z})=\prod_{i<j}^M(\mu_i-\mu_j)^{1/\kappa}\prod_{a<b}^N(z_a-z_b)^{l_al_b/\kappa}\left(\prod_{k=1}^M\prod_{c=1}^N(\mu_k-z_c)^{-l_c/\kappa}\right),\tag{5.3}$$

and $\Psi(\vec{\mu}|\vec{z})$ is a Bethe vector (4.2) where the corresponding Bethe equations are not imposed.

As a first step in the proof that $\psi(z_1,\ldots,z_N)$ given by (5.2) is a solution of (5.1) we differentiate the product $\phi\Psi$ with respect to z_a and obtain

$$\partial_{z_a}(\phi\Psi)=\partial_{z_a}(\phi)\Psi+\phi\partial_{z_a}(\Psi). \tag{5.4}$$

Using (5.3) the first term on the right hand side can be calculated explicitly:

$$\kappa\partial_{z_a}\phi=\left(\sum_{\substack{b=1\\b\neq a}}^{N}\frac{l_a l_b}{z_a-z_b}-\sum_{j=1}^{M}\frac{l_a}{z_a-\mu_j}\right)\phi=E_M^{(a)}\phi. \tag{5.5}$$

Furthermore, taking a residue of (3.30) at $\lambda=z_a$ we have

$$H^{(a)}\Psi=E_M^{(a)}\Psi+\sum_{j=1}^{M}\frac{(-1)^j}{z_a-\mu_j}\beta_M(\mu_j)\tilde{\Psi}^{(j,a)}, \tag{5.6}$$

where

$$\tilde{\Psi}^{(j,a)}=\left(v_a^+B_{M-1}^{(j)}+2X_a^+\sum_{k\neq j}^{M}\frac{(-1)^{k+\Theta(j-k)}}{\mu_j-\mu_k}B_{M-2}^{(j,k)}\right)\Omega_-. \tag{5.7}$$

Hence (5.4) can be written as

$$\kappa\partial_{z_a}(\phi\Psi)=H^{(a)}(\phi\Psi)+\phi\sum_{j=1}^{M}\frac{(-1)^j}{\mu_j-z_a}\beta_M(\mu_j)\tilde{\Psi}^{(j,a)}+\kappa\phi\partial_{z_a}(\Psi). \tag{5.8}$$

Moreover, from (5.3) we also have

$$\kappa\partial_{\mu_j}\phi=\left(\sum_{a=1}^{N}\frac{-l_a}{\mu_j-z_a}+\sum_{\substack{j=1\\j\neq k}}^{M}\frac{1}{\mu_j-\mu_k}\right)\phi=\beta_M(\mu_j)\phi, \tag{5.9}$$

and from Lemma 3.7 follows

$$\partial_{z_a}\Psi=\sum_{j=1}^{M}(-1)^j\partial_{\mu_j}\left(\frac{\tilde{\Psi}^{(j,a)}}{\mu_j-z_a}\right). \tag{5.10}$$

Thus, using (5.9) and (5.10),

$$\kappa\partial_{z_a}(\phi\Psi)=H^{(a)}(\phi\Psi)+\kappa\sum_{j=1}^{M}\partial_{\mu_j}\left(\frac{(-1)^j}{\mu_j-z_a}\phi\tilde{\Psi}^{(j,a)}\right). \tag{5.11}$$

A closed contour integration of $\phi\Psi$ with respect to $\mu_1,\ldots,\mu_M$ will cancel the contribution from the terms under the sum in (5.11) and therefore $\psi(z_1,\ldots,z_N)$ given by (5.2) satisfies the Knizhnik–Zamolodchikov equation.

Conjugated Bethe vectors $(B_M\Omega_-)^*$ are entering into the solution $\tilde{\psi}(z_1,\ldots,z_N)$ of the dual Knizhnik–Zamolodchikov equation,

$$-\kappa\frac{\partial}{\partial z_a}\tilde{\psi}(z_1,\ldots,z_N)=\tilde{\psi}(z_1,\ldots,z_N)H^{(a)}. \tag{5.12}$$

The scalar product $(\tilde{\psi}(z_1,\ldots,z_N),\psi(z_1,\ldots,z_N))$ does not depend on $\{z_j\}_1^N$ and its quasi-classical limit $\kappa\to 0$ gives the norm of the Bethe vectors due to the fact that the stationary points of the contour integrals for $\kappa\to 0$ are solutions to the Bethe equations:[10]

$$\frac{\partial S}{\partial \mu_j}=\sum_{a=1}^{N}\frac{-l_a}{\mu_j-z_a}+\sum_{\substack{j=1\\ j\neq k}}^{M}\frac{1}{\mu_j-\mu_k}=0, \tag{5.13}$$

$$S(\vec{\mu}|\vec{z})=\kappa\ln\phi=\sum_{a<b}^{N} l_a l_b\ln(z_a-z_b)+\sum_{i<j}^{M}\ln(\mu_i-\mu_j)-\sum_{a=1}^{N}\sum_{j=1}^{M} l_a\ln(z_a-\mu_j). \tag{5.14}$$

According to the remark at the end of Sec. IV, analytical properties of the Bethe vectors of the osp(1|2) Gaudin model coincide with the analytical properties of the sl(2) Gaudin model. Thus, the expression for the norm of the Bethe vectors Ψ in (4.2) obtained as the first term in the asymptotic expansion $\kappa\to 0$ coincides also

$$(\Psi,\Psi)=\det\left(\frac{\partial^2 S}{\partial\mu_j\partial\mu_k}\right), \tag{5.15}$$

$$\frac{\partial^2 S}{\partial\mu_j^2}=\sum_{a=1}^{N}\frac{l_a}{(\mu_j-z_a)^2}-\sum_{k\neq j}^{M}\frac{1}{(\mu_j-\mu_k)^2},\quad \frac{\partial^2 S}{\partial\mu_j\partial\mu_k}=\frac{1}{(\mu_j-\mu_k)^2},\quad \text{for}\quad j\neq k. \tag{5.16}$$

Finally we notice that the modification of the Gaudin Hamiltonians we discussed at the end of the previous section can be easily transferred to the corresponding modification of the Knizhnik–Zamolodchikov equations. The modification (4.16) for the sl(2) Gaudin model was studied in Ref. 19 as a quantization of the Schlesinger system (see also Ref. 18). Both modifications are related with extra factors in the integrating scalar function (5.3),

$$\phi_j=\exp\left(\frac{S_j}{\kappa}\right),\quad j=0,1,2, \tag{5.17}$$

where $S_0=S$ in (5.14) and

$$S_1=S_0+g\sum_{j=1}^{M}\mu_j-g\sum_{a=1}^{N} l_a z_a, \tag{5.18}$$

$$S_2=S_0+\frac{1}{2}\sum_{j=1}^{M}\mu_j^2-\frac{1}{2}\sum_{a=1}^{N} l_a z_a^2, \tag{5.19}$$

correspond to the first (4.16) and second (4.29) modification, respectively.

VI. CONCLUSION

The Gaudin model corresponding to the simplest nontrivial Lie superalgebra osp(1|2) was studied. A striking similarity between some of the most fundamental characteristics of this system and the sl(2) Gaudin model was found. Although explicitly constructed creation operators B_M in (3.37) of the Bethe vectors are complicated polynomials of the L-operator entries $v^+(\lambda)$ and $X^+(\lambda)$, the coordinate form of the eigenfunctions defers only in signs from the corresponding states in the case of sl(2) model. Moreover, the eigenvalues and the Bethe equations coincide, provided that the sl(2) Gaudin model with integer spins is considered.

Let us point out that by the method proposed in this article one can construct explicitly creation operators of the Gaudin models related to trigonometric Izergin–Korepin r-matrix[20] and trigonometric osp(1|2) r-matrix[24] which have the same matrix structure as (3.2). Similarly to the simple Lie algebra case, solutions to the Knizhnik–Zamolodchikov equation were constructed from the Bethe vectors using algebraic properties of the creation operators B_M and the Gaudin

realization of the loop superalgebra $\mathcal{L}_+(\mathrm{osp}(1|2))$. This interplay between the Gaudin model and the Knizhnik–Zamolodchikov equation enabled us to determine the norm of eigenfunctions of the Gaudin Hamiltonians

$$\|\Psi(\mu_1,\ldots,\mu_M;\{z_a\}_1^N)\|^2=\det\left(\frac{\partial^2 S}{\partial\mu_j\partial\mu_k}\right).$$

The difficult problem of correlation function calculation for general Bethe vectors

$$\mathcal{C}(\{\nu_j\}_1^M;\{\mu_i\}_1^M;\{\lambda_k\}_1^K)=\left(\Omega_-,B_M^*(\nu_1,\ldots,\nu_M)\prod_{k=1}^K h(\lambda_k)B_M(\mu_1,\ldots,\mu_M)\Omega_-\right)$$

was solved nicely for the sl(2) Gaudin model in Ref. 6 using the Gauss factorization of the loop algebra group element and the appropriate Riemann–Hilbert problem. Although the corresponding factorization is known even for the quantum superalgebra $\mathrm{osp}_q(1|2)$,[28] the final expression of the correlation functions is difficult to obtain due to the complicated structure of the creation operators $B_M(\mu_1,\ldots,\mu_M)=\mathrm{Poly}(v^+,X^+)$ in (3.37). The study of this problem is in progress and the following expression for the scalar product of the Bethe states is conjectured (cf. Ref. 6):

$$(\Omega_-,B_M^*(\nu_1,\ldots,\nu_M)B_M(\mu_1,\ldots,\mu_M)\Omega_-)=\sum_{\sigma\in S_M}(-1)^{p(\sigma)}\det\mathcal{M}^\sigma,$$

where the sum is over symmetric group $\mathcal{S}_M$ and $M\times M$ matrix $\mathcal{M}^\sigma$ is given by

$$\mathcal{M}^\sigma_{jj}=\frac{\rho(\mu_j)-\rho(\nu_{\sigma(j)})}{\mu_j-\nu_{\sigma(j)}}-\sum_{k\neq j}^M\frac{1}{(\mu_j-\mu_k)(\nu_{\sigma(j)}-\nu_{\sigma(k)})},$$

$$\mathcal{M}^\sigma_{jk}=\frac{1}{(\mu_j-\mu_k)(\nu_{\sigma(j)}-\nu_{\sigma(k)})},\quad \text{for}\quad j,k=1,2,\ldots,M.$$

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Anomalies and Schwinger terms in NCG field theory models

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We study the quantization of chiral fermions coupled to generalized Dirac operators arising in NCG Yang–Mills theory. The cocycles describing chiral symmetry breaking are calculated. In particular, we introduce a generalized locality principle for the cocycles. Local cocycles are by definition expressions which can be written as generalized traces of operator commutators. In the case of pseudodifferential operators, these traces lead in fact to integrals of ordinary local de Rham forms. As an application of the general ideas we discuss the case of noncommutative tori. We also develop a gerbe theoretic approach to the chiral anomaly in the Hamiltonian quantization of NCG field theory. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The non-Abelian chiral anomaly appears in two different (but related) ways. First, it modifies the structure of current algebra. Historically, this was the way quantum mechanical symmetry breaking was first observed,[1] but it took some time before a clear mathematical formulation of this phenomenon was obtained.[2] On the other hand, the anomaly appears in the path integral formulation as a lack of gauge invariance of the effective action.[3] In either way, the anomaly can be thought of as an element of an appropriate group (or Lie algebra) cohomology group.

The non-Abelian gauge anomaly arises from a left–right nonsymmetric coupling of vector potentials to a Dirac fermion field. This process can be generalized in a straight-forward way in noncommutative geometry models. Instead of a standard Dirac operator one considers self-adjoint (invertible) unbounded operators D with the property that $1/|D|^p$ is "almost" trace-class for a given real number $p \geqslant 1$. "Almost" means that the spectral integral $\int_0^\Lambda (|\lambda|^p+\epsilon)^{-1} d\mu(\lambda)$ is at most logarithmically divergent at $\Lambda \to \infty$, for any positive number ϵ. After fixing such an operator we study generalized Dirac operators $D_A = D + A$ where A is any Hermitian bounded perturbation.

We stress that our considerations are very general: The family of Dirac operators could for example arise from a coupling of vector potentials through a star product (generalized Moyal brackets). All that is needed is that the L_p estimate mentioned above is valid. This has been proven to hold in a class of star product quantizations[4] defined by a constant antisymmetric θ matrix. We shall study some consequences of this in Sec. VII.

Our starting point for a construction of a NCG field theory model is a triple $(D, \int, \mathcal{B})$, where D is the Dirac operator acting in a Hilbert space H, $\mathcal{B}$ is an associative algebra of operators in H such that $[D, b]$ is bounded for all $b \in \mathcal{B}$. In addition, there is an "integration," or a generalized trace map, from operators ("p-forms") of the type $\omega = b_0[\epsilon, b_1][\epsilon, b_2]\cdots[\epsilon, b_p]$, or alternatively $|D|^{-p} b_0[D, b_1]\cdots[D, b_p]$, to complex numbers;[5] see also the discussion around Definition 10.8 in Ref. 6 for more details. Here $\epsilon = D/|D|$ is the sign of the Dirac operator. In some cases (but not always) one can prove an equality between the integrals of the two alternative expressions.[5] The generalized vector potentials are then linear combinations of 1-forms $A = b_0[D, b_1]$, or sometimes $a = b_0[\epsilon, b_1]$.

We study the BRST double complex based on de Rham forms on the space of vector poten-

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tials A with values in the space of the above operator p-forms ω, with $p=0,1,2,\ldots$. The NCG BSRT complex has been previously studied from different points of view in Ref. 7 and more recently in Ref. 8.

One of the central results in the present paper concerns the question of locality of the BRST cocycles. In abstract NCG models it is not *a priori* clear what this could mean because in the operator approach there is in general no space–time manifold to define local fields. However, in the ordinary space–time geometric setup many of the basic quantities can be written as ''traces'' of commutators of pseudodifferential operators. For example, this holds for non-Abelian Schwinger terms[9] and the gauge anomaly in the path integral formulation.[10] It turns out that these traces are in fact integrals of local differential forms. We adopt this as our starting point: We prove that in the NCG field theory models there is a ''local'' anomaly formula expressing the BRST cocycles as traces of commutators of nontrace-class operators.

The second main result concerns the description of the Hamiltonian anomaly in gerbe theoretic terms in which the basic object is a 3-cohomology class, the Dixmier–Douady class. The results are largely generalizations of the corresponding considerations for the standard coupling of local vector potentials to chiral fermions.[11] However, there is one important technicality which makes a difference between the ''classical'' and the NCG case. In the classical case the Dixmier–Douady class defines a de Rham form on the space of gauge orbits $\mathcal{A}/\mathcal{G}$. This is a smooth manifold when one restricts to the case of so-called based gauge transformations $\mathcal{G}_0$. In the NCG models the concept of based gauge transformations is not well-defined and the space of gauge orbits has singularities.

In order to avoid these singularities we realize the space of NCG gauge potentials for the Schatten index p as loops in gauge potentials for index $p-1$. Correspondingly, the group of gauge transformations for index p is the group of smooth loops in the gauge group for the case of index $p-1$ which allows us to define based gauge transformations in the usual way as loops through the neutral element at a fixed value of the argument. This leads then to a construction of a gerbe and its Dixmier–Douady class as a de Rham form in a standard way.

We want to thank Göran Lindblad for drawing to our attention to Ref. 12.

II. THE GENERAL SETUP FOR NCG DESCENT EQUATIONS AND ANOMALIES

Let D_0 be an unbounded self-adjoint operator in a complex Hilbert space H such that $|D_0|^{-1}\in L_{p+}$, that is, $|D_0|^{-p}\in L_{1+}$ for some $p\geqslant 1$. Here L_{1+} is the Dixmier ideal in the algebra of bounded operators in H. A positive operator T is in L_{1+} if it is compact and

$$\frac{1}{\log N}\sum_{k=1}^{N}\lambda_k$$

has a finite limit, where $\lambda_1\geqslant\lambda_2\geqslant\cdots$ are the eigenvalues of T. We also assume for simplicity that D_0 is invertible. However, the following discussion can be easily generalized to the case when D_0 is a finite rank perturbation of an invertible operator.

We shall work with bounded perturbations of the ''free Dirac operator'' D_0, denote $D_A=D_0+A$ where A is a bounded self-adjoint operator in H such that $[|D_0|,A]$ is bounded. We shall denote F_A a smoothed sign operator associated to D_A. The technical complication is that the map $A\mapsto D_A/|D_A|$ is not continuous when D_A has zero modes. Instead, we can take a smooth function f: $\mathbb{R}\to\mathbb{R}_+$ such that $f(x)-|x|$ approaches zero faster than any power of x as $|x|\mapsto\infty$ and $f(x)\geqslant m$ for some positive constant, and we define $F_A=D_A/f(D_A)$. For example, take $f(x)=+\sqrt{x^2+e^{-x^2}}$. Then $A\mapsto F_A$ is norm continuous. If D_A is the classical Dirac operator associated to a vector potential A on a compact manifold then the difference $D_A/|D_A|-F_A$ is an infinitely smoothing pseudodifferential operator and in particular a trace class operator.

The sign operator $D_A/|D_A|$ defines a Fock space representation of the canonical anticommutation relations algebra CAR. The generators in the CAR algebra are denoted by $a(v)$, $a^*(v)$, where $v\in H$. The algebra is defined by the basic relations

$$a(u)a(v)+a(v)a(u)=0=a^*(u)a^*(v)+a^*(v)a^*(u),$$
$$a^*(u)a(v)+a(v)a^*(u)=\langle v,u\rangle, \tag{2.1}$$

where the Hilbert space inner product $\langle\cdot,\cdot\rangle$ is antilinear in the first argument. The Dirac representation is then fixed by the requirement that there is a *vacuum vector* $|A\rangle\in\mathcal{F}_A$ such that

$$a^*(u)|A\rangle=0=a(v)|A\rangle, \text{ for } u\in H_-(A) \text{ and } v\in H_+(A), \tag{2.2}$$

where $H=H_+(A)\oplus H_-(A)$ is the polarization to the spectral subspaces $D_A\geqslant 0$, $D_A<0$, respectively.

Because of the potential zero modes of the Dirac operator the Dirac vacuum cannot in general be defined as a continuous function of A. Instead, we must be content with a choice of a polarization $H=W(A)\oplus W(A)^\perp$ such that $W(A)\sim H_+(A)$, where the equivalence is defined by the condition that the projection operators to the given subspaces differ only by Hilbert–Schmidt operators. The Hilbert–Schmidt condition comes from the requirement that the CAR representations defined by the two polarizations should be equivalent; for a review on CAR representations see Ref. 13. Let $\epsilon_W=\pi_W-\pi_{W^\perp}$ be the grading operator defined by the orthogonal projection $\pi_W: H\to W$. Then $\epsilon_{W(A)}-\epsilon_{H_+(A)}$ is Hilbert–Schmidt and $\epsilon_{H_+(A)}-F_A$ is trace-class and so F_A is an approximation of $\epsilon_{W(A)}$ modulo Hilbert–Schmidt operators. The advantage of working with F_A is that it is easier to produce explicit formulas (as we saw above), compared with the grading operators $\epsilon_{W(A)}$.

As an operator function $D_A/f(D_A)$ of D_A, the operator F_A satisfies $g^{-1}F_Ag=F_{A^g}$, with $A^g=g^{-1}Ag+g^{-1}[D_0,g]$ for a unitary transformation g such that $[D_0,g]$ is bounded. Denote by $\mathcal{B}$ the algebra of bounded operators b in H such that $[D_0,b]$ and $[|D_0|,b]$ are bounded. Then all the operators $A=b_0[D_0,b_1]$, for $b_i\in\mathcal{B}$, satisfy the condition $[|D_0|,A]$ is bounded. We denote by U_{p+} the group of unitary elements in $\mathcal{B}$. Any element $g\in U_{p+}$ satisfies $[\epsilon,g]\in L_{p+}$ where $\epsilon=D_0/|D_0|$.

Lemma 2.3: $F_A-\epsilon\in L_{p+}$ for any bounded operator A such that $[|D_0|,A]$ is bounded.

Proof: (1) We first prove that $|D_0+A|-|D_0|$ is bounded. We have assumed that D_0 is invertible, so $|D_0|\geqslant\mu$ for some positive constant μ. We use the norm estimate $\||X|-|Y|\|\leqslant\||X^*X-Y^*Y|^{1/2}\|$; see for example [Ref. 12, Sec. X.2]. Set $G=D_0A+AD_0$ and split $G=G_++G_-$ where G_+ commutes with ϵ and G_- anticommutes with ϵ. The linear equation,

$$G=|D_0|Z+Z|D_0|,$$

can be solved as $Z=Z_++Z_-$, with $Z_+=A_+\epsilon$ and

$$Z_-=\int_0^\infty e^{-t|D_0|}[|D_0|,\epsilon A_-]^{-t|D_0|}\,dt,$$

and thus Z is bounded, since $\|e^{-t|D_0|}\|\leqslant e^{-t\mu}$ and since $[|D_0|,\epsilon A_-]=\epsilon[|D_0|,A_-]$ is bounded by assumption. Setting $X=D_0A$ and $Y=|D_0|+Z$ in the above norm estimate we observe that $|D_0+A|-|\,|D_0|+Z|$ is bounded. In the case when $\|Z\|\leqslant\mu$ the operator $|D_0|+Z$ is positive and so $\||D_0|+Z|=|D_0|+Z$ and it follows that $|D_0+A|-|D_0|=(|D_0+A|-|\,|D_0|+Z|)+(|\,|D_0|+Z|-|D_0|)$ is bounded. In the general case, replace $D_0\mapsto D'=D_0+i\alpha$ for a real number α. Clearly $|D+i\alpha|-|D_0|$ and $|D_0+A+i\alpha|-|D_0+A|$ are bounded, so the question of whether $|D_0+A|-|D_0|$ is bounded is equivalent to whether $|D'+A|-|D'|$ is bounded. Now $|D'|\geqslant|\alpha|$ and so we have $\|Z\|\geqslant|D'|$ when we choose α large enough and the proof reduces to the special case above.

(2) We may assume without essential restriction that D_0+A is invertible so we can select $f(x)=|x|$ and

$$\begin{aligned} F_A-\epsilon &= (D_0+A)^{-1}|D_0+A|-D_0^{-1}|D_0| \\ &= (1+D_0^{-1}A)^{-1}D_0^{-1}|D_0+A|-D_0^{-1}|D_0| \\ &= \{(1+D_0^{-1}A)^{-1}-1\}\epsilon+(1+D_0^{-1}A)^{-1}D_0^{-1}T, \end{aligned}$$

for some bounded operator T. The second term on the right is then in L_{p+} since $D_0^{-1}\in L_{p+}$ and the first term is of the form $((1+S)^{-1}-1)\epsilon$ with $S\in L_{p+}$ and thus it belongs also to L_{p+}. □

The following discussion is based on a parametrization of the fermionic Fock space by the operator $a=F_A-\epsilon$. Thus the Dirac vacuum for the vector potential A is given by any grading operator ϵ_a which differs from $\epsilon+a$ by a Hilbert–Schmidt operator. Geometrically, this leads to the construction of a smooth infinite-dimensional vector bundle $\mathcal{F}$ over the parameter space $\mathcal{A}$ of generalized vector potentials. The fiber $\mathcal{F}_a$ is the Fock space defined by the grading operator ϵ_a. The quantized Dirac operator $\hat{D}_A$ acts as an unbounded positive operator in the fiber.

The group U_{p+} acts in the base space of the bundle. The problem arises as to whether the action can be lifted to the total space such that $g^{-1}\hat{D}_A g=\hat{D}_{A^g}$. In case of smooth vector potentials, $A=\gamma^k A_k$, and a massless Dirac operator it is known that the answer is negative. Instead, there is an extension $\hat{\mathcal{G}}$ of the group of gauge transformations $\mathcal{G}$ which acts in the total space. The obstruction to the $\mathcal{G}$ action is the extension term in the commutation relations of the Lie algebra Lie($\mathcal{G}$). This extension (Schwinger term) is a 2-cocycle $c_{n,2}$ of Lie($\mathcal{G}$) in the module of complex functions of the variable A. In the case of one space dimension, $n=1$, the cocycle does not depend on A and one may restrict to the module of constant functions.

There is an equivalent alternative way to view the obstruction. The standard construction in canonical quantization leads naturally to a bundle $P\mathcal{F}$ of *projective Fock spaces* which do not depend on any choices of the grading operator ϵ_a. The existence of a Fock bundle which gives $P\mathcal{F}$ as its projectivization is then related to triviality of a *Dixmier–Douady* class in $H^3(\mathcal{A}/\mathcal{G},\mathbb{Z})$.[11]

The main content of the present article is to explain how the local formulas for gauge anomalies, Schwinger terms, the Dixmier–Douady class, and all the cocycles related to these through the standard BRST descent equations extend to certain cocycles on the space of bounded operators A and the Lie algebra Lie(U_{p+}) such that a restriction to the classical case gives standard local formulas. A central ingredient is to use (noncyclic) extensions of the trace functional to nontrace-class operators.

The "infinitesimal version" of the gauge transformation $A\mapsto A^g$ in terms of the parameter a is

$$\delta_X a=[a,X]+[\epsilon,X], \quad \text{for } X\in\mathbf{u}_p=\mathrm{Lie}(U_{p+}). \tag{2.4}$$

Let us recall the basic definitions in NCG differential calculus for Fredholm modules.[5] The differentials of order n are linear combinations of operators of the type $b_0[\epsilon,b_1]\cdots[\epsilon,b_n]$ where $b_i\in\mathcal{B}$. One denotes $db=[\epsilon,b]$ for $b\in\mathcal{B}$. If $\phi\in\Omega^n$ is a differential of order n then $d\phi=\epsilon\phi+(-1)^{n+1}\phi\epsilon$. This gives a map $d:\Omega^n\to\Omega^{n+1}$ with $d^2=0$. The cohomology of this complex is trivial.

The coboundary operator associated to infinitesimal gauge transformations is denoted by δ. We work with cochains of order k, $\tau\in\Omega_k$, consisting of functions $\tau(a;X_1,\ldots,X_k)$ of $a\in\Omega^1$ and of Lie algebra elements $X_i\in\mathbf{u}_p$, linear in each X_i and totally antisymmetric in the arguments X_i. The standard Lie algebra coboundary operator is defined by

$$\begin{aligned} (\delta\tau_n)(a;X_1,\ldots,X_{n+1}) &= \sum_i (-1)^{i-1}\delta_{X_i}\tau(a;X_1,\ldots,\hat{X}_i,\ldots,X_{n+1}) \\ &\quad +\sum_{i<j}(-1)^{i+j}\tau(a;[X_i,X_j],..,\hat{X}_i,\ldots,\hat{X}_j,\ldots,X_{n+1}), \end{aligned} \tag{2.5}$$

where the hat means that the corresponding argument is deleted and δ_{X_i} is the Lie derivative acting on functions of a, the action on the argument being given by (2.4). We remind that the multilinear forms τ on a Lie algebra can be interpreted as left invariant differential forms on the corresponding Lie group (and *vice versa*) through the standard identification of a Lie algebra as left invariant vector fields.

We shall also work with a (d,δ) double complex consisting of δ forms taking values in the d complex Ω^*, using the standard BRST sign convention. The BRST ghost v can be interpreted as the Maurer–Cartan 1-form on the gauge group, that is, at the identity element it is the the tautological 1-form sending a Lie algebra element onto itself, $v=g^{-1}\,\delta g$. The sign conventions are encoded into the algebraic rules,

$$\begin{gathered} d^2=\delta^2=\delta d+d\,\delta=0, \\ \delta(v)=-v^2=\delta v+v\,\delta, \\ \delta(a)=-[a,v]_+-v^2=\delta a+a\,\delta, \\ d(v)=[\epsilon,v]_+=dv+vd, \\ d(a)=[\epsilon,a]_+=da+ad. \end{gathered} \tag{2.6}$$

We denote $[a,b]_+=ab+ba$.

Here a remark on notation is in order. We want to treat at the same time both the even and odd Fredholm modules (related to odd/even k.) To obtain the correct signs in (2.6), we need to make a reinterpretation of $x=v$, δ, ϵ and a.

Even Fredholm module. In this case we have, by definition, a Hermitian operator Γ in H with $\Gamma^2=1$ which anticommutes with ϵ and α, and the correct signs are accounted for if we interpret the ghost as Γv. To be precise, one should distinguish between v, δ, ϵ and a and

$$\begin{gathered} s(v)=\Gamma v,\ \ s(\delta)=\Gamma\delta, \\ s(\epsilon)=\epsilon,\ \ s(a)=a. \end{gathered} \tag{2.7}$$

Odd Fredholm module. We do not have a Γ at hand but we introduce it by doubling the original Hilbert space, $H\mapsto H\otimes\mathbb{C}^2$, and introducing the usual Pauli sigma matrices σ_3 and σ_1 acting on the second factor. We can then define

$$\begin{gathered} s(v)=v\otimes\sigma_1,\ \ s(\delta)=\delta\otimes\sigma_1, \\ s(\epsilon)=\epsilon\otimes\sigma_3,\ \ s(a)=a\otimes\sigma_3. \end{gathered} \tag{2.8}$$

In particular, the formulas $d(v)=[\epsilon,v]_+$ and $d(a)=[\epsilon,a]_+$ mean

$$d(s(v))=[s(\epsilon),s(v)]_+=[\epsilon,v]\otimes\sigma_3\sigma_1,$$

$$d(s(a))=[s(\epsilon),s(a)]_+=[\epsilon,a]_+\otimes\sigma_3^2=[\epsilon,a]_+\otimes 1,$$

where the sigma matrices account for the correct signs. We stress that the auxiliary space is just a tool to keep track of the signs (the even and odd case could actually be handled in a unified manner, but we choose to utilize Γ in the even case).

In both cases, the symbols $x=v$, δ, ϵ and a in (2.6) should actually be interpreted as $s(x)$ as specified above, and only for simplicity of the notation we write x instead of $s(x)$. We will sometimes also use this simplified notation below, in particular in the Appendix, but we will always clearly point this out.

In the standard discussion of anomalies in quantum field theory one constructs cocycles $c_{n,k}$ in the (Ω_*,δ) complex by integrating de Rham forms $\omega_{n,k}$ in Ω^n_* over a compact manifold of dimension n. In the NCG setting integration of forms is replaced by applying an appropriate trace functional to the operator valued forms. In fact, in the case of an odd Fredholm module the

integral is normally defined as the trace $\mathrm{tr}_C\,\phi$ where the conditional trace is defined as $\mathrm{tr}_C(X)=\frac{1}{2}\mathrm{tr}(X+\epsilon X\epsilon)$. However, in our notation we have to take the trace also in the auxiliary space $\mathbb{C}^2$, and the correct definition is

$$\int \phi=\frac{1}{2}\mathrm{tr}_C\sigma_3\phi. \tag{2.9}$$

In the case of an even Fredholm module the standard definition of the integral is $\mathrm{tr}_C(\Gamma\phi)$ whereas with our conventions the operator expression ϕ is already equipped (for odd k) with the Γ factor and we set

$$\int \phi=\mathrm{tr}_C\,\phi. \tag{2.10}$$

In the case of even k (in an even module) the integral vanishes.

The translation from the classical to NCG setting is straight-forward. The de Rham exterior derivation is replaced by the operation d described above (to the forms after the symbol "$\int$"). All the formal manipulations are done exactly in the same way as in the classical BRST complex. Of course, the nontriviality of the cohomology classes depends on what is meant by the trace [and the definition of the trace is intertwined by the choice of $(H,D_0,\mathcal{B})$].

The construction of a family of cocycles $c_{j,k}$ over a Fredholm module starts from the (NCG) operator valued Chern class F^n, where $F=d(a)+a^2\in\Omega^2$ is the curvature. The Chern–Simons form is defined by

$$c_{2n-1,0}(a)=\int n\int_0^1 dt\, a[td(a)+t^2a^2]^{n-1},$$

where $td(a)+t^2a^2=F(t)$ is the curvature associated with ta (a path connecting a and 0). The other terms in the complex (starting from the Chern class) are given by similar formulas where one has the curvature associated with $d+\delta$ and a path of vector potentials connecting $a+v$ and 0,

$$c_{2n-k-1,k}=\int n\int_0^1 dt(a[td(a)+t^2a^2+(1-t)d(v)]^{n-1})|_{[k]},\quad k=0,\ldots,n-1,$$

where now the curvature in the square brackets is obtained starting from the vector potential $ta+v$, and $(\cdots)|_{[k]}$ means the projection onto those terms which are of degree k in the "ghost" v, and similarly,

$$c_{2n-k-1,k}=\int n\int_0^1 dt(v[td(v)+(t^2-t)v^2]^{n-1})|_{[k]},\quad k=n,\ldots,2n,$$

where now the curvature is associated with tv. We stress that in the previous formulas for $c_{2n-k-1,k}$, we use the simplified notation where $x=v,a$ is short for $s(x)$ as discussed above. (We also recall that one can obtain different but equivalent formulas for $c_{2n-k-1,k}$ depending on the choice of path $a+v\to 0$, and we find it convenient to use the path consisting of two straight lines $a+v\to v$ and $v\to 0$ leading to cocycles with lowest possible powers of a.)[14]

The crucial property are the cocycle relations $\delta c_{j,k}=0$ for all j and k. In the standard case these are a consequence of the fact that the cocycles are integrals of traces of matrix valued de Rham forms, $c_{j,k}=\int_M \mathrm{tr}\omega_{j,k}$, which are linked by the so-called descent equations. These equations start with a relations connecting the Chern class and the Chern–Simons form, $F^n=d\omega_{2n-1,0}+(\cdots)$, and then continue,

$$\delta(\omega_{2n-1-k,k})+d(\omega_{2n-1,k+1})=(\cdots),\quad k=0,\ldots,2n-1,$$

where $(\cdots)$ are terms which have zero trace; they are explicitly commutators of matrix forms. Since all but the first term on the l.h.s. in these latter equations vanish under the combined trace and integral (the second term on the l.h.s. vanishes due to Stokes theorem) and $\delta\int=\int\delta$, one obtains the cocyle relations. In fact, in the standard case one usually applies to these descent equations the matrix trace, and therefore the terms $(\cdots)$ on the r.h.s. become zero. In the NCG generalizations, an analog of the separate matrix trace is usually not available (the matrix trace and the ordinary integration are combined in the abstract integral), and it is therefore natural to also keep the terms $(\cdots)$.[7] In fact, as we will show, the terms $(\cdots)$ contain interesting information: in case of the double complex based in a spectral triple they allow us to connect the forms $\omega_{j,k}$ and $\omega_{j+2,k}$ in different dimensions (d degree) but identical form degree, which, for example, provides an important link of the Schwinger terms in different dimensions (Theorem A4) and, in general, will allow us to obtain local forms of the NCG cocyles (Theorem 3.1).

As an example, the second Chern form is in the classical case the matrix trace of F^2, where $F=d(A)+A^2$ is the curvature form associated to a connection $A=A^\mu\,dx_\mu$. In general, one then can check by straightforward algebraic manipulations,

$$F^2=d(\omega_{3,0})+[a,\tilde{\omega}_{3,0}]_+,$$

where $\omega_{3,0}=\frac{1}{2}[d(a),a]_+ +\frac{2}{3}a^3$ is the three-dimensional Chern–Simons form (before applying the trace functional) and $\tilde{\omega}_{3,0}=\frac{1}{3}[d(a),a]_+ +\frac{1}{2}a^3$ is another 3-form. Note that for standard de Rham forms, the second term vanishes under the matrix trace. If we apply this relation in the Fredholm module setting we use $\int F^2=\mathrm{tr}_C(\Gamma F^2)$, and since $\Gamma[a,\tilde{\omega}]_+=[\Gamma a,\tilde{\omega}]$ the second term becomes a trace of a commutator which vanishes for appropriate p. Of course, in the classical case also the integral of the first term is zero in the case of a manifold without boundary. The other descent equations are, in the simplified notation where $x=a,v,\omega_{3-k,k}$, etc. is short for $s(x)$ as in Eqs. (2.7)–(2.8),

$$\delta(\omega_{3,0})+d(\omega_{2,1})=-\tfrac{1}{3}[a,\omega_{2,1}]_+-[v,\omega_{3,0}]_+,$$

$$\delta(\omega_{2,1})+d(\omega_{1,2})=-\tfrac{2}{3}[a,\omega_{1,2}]_+-[v,\omega_{2,1}]_+,$$

$$\delta(\omega_{1,2})+d(\omega_{0,3})=-[v,\omega_{1,2}]_+,$$

$$\delta(\omega_{0,3})=-\tfrac{1}{2}[v,\omega_{0,3}]_+,$$

where

$$\omega_{2,1}=\tfrac{1}{2}[a,d(v)]_+,\quad \omega_{1,2}=\tfrac{1}{2}[d(v),v]_+,\quad \omega_{0,3}=-\tfrac{1}{3}v^3,$$

all of them can be checked by straight-forward algebraic manipulations. As we have already said, the BRST ghost v can be interpreted as the Maurer–Cartan form on a group manifold, and thus are to be evaluated along tangent vectors X_j at the neutral element (i.e., Lie algebra elements). Moreover, in the end we are interested in integrals of the operator forms and we need to treat the cases of odd or even Fredholm modules separately, as discussed above.

For example, the form $\omega_{1,2}$ when evaluated for Lie algebra elements X, Y and integrated in an odd module of appropriate Schatten index p, gives

$$\int \omega_{1,2}(X,Y)=\tfrac{1}{2}\mathrm{tr}_C([d(X),Y]_+-[d(Y),X]_+),$$

where $d(X)=[\epsilon,X]$, and $\omega_{0,3}$ leads to

$$\int \omega_{0,3}(X,Y,Z)=-\mathrm{tr}_C[[X,Y],Z]_+,$$

and $\omega_{2,1}$ in an even module (appropriate p) leads to

$$\int \omega_{2,1}(X) = -\frac{1}{2}\mathrm{tr}_C[a,\Gamma d(X)]_+ = \frac{1}{2}\mathrm{tr}_C\,\Gamma[a,d(X)].$$

III. "LOCAL" NCG ANOMALIES AND SCHWINGER TERMS

In the case of the classical BRST complex all the cocycles $c_{j,k}$ are given in terms of differential forms which are differential polynomials in variables a,v. The Fredholm module cocycles involve terms like $[\epsilon,v],\epsilon a+a\epsilon$, and therefore are nonlocal in nature; when evaluated using the symbol calculus of pseudodifferential operators they contain terms of arbitrary high order in the partial derivatives.

However, even in the case of the Fredholm module cocycles (for classical vector potentials and gauge transformations) the locality is preserved in a certain sense. Namely, it turns out that the cocycles $c_{j,k}$ are equivalent (in the BRST cohomology) to cocycles $c'_{j,k}$ which can be written as renormalized traces of commutators of PSDO's. In the case of Schwinger terms this was observed in Ref. 9 and the same principle was applied to the calculation of the gauge anomaly for the chiral Dirac determinant in Ref. 10. The trace of a commutator depends only on the term in the asymptotic expansion of a PSDO which has order equal to $-\dim M$, and for this reason one needs to take into account only a finite number of derivatives of the symbols (since each differentiation in a homogeneous term decreases the order by one). In this sense the trace of a commutator is a local expression. In a more general setup, beyond the PSDO calculus, we take this as a *definition* of locality: cocycles which are traces of commutators in the algebra are called local.

We set up the following assumptions. There is a complex linear functional TR on the algebra generated by D_0, $|D_0|$ and $\mathcal{B}$ such that (1) it is equal to the ordinary trace for trace class operators, (2) it has the property that $\mathrm{TR}[A,B]=0$ when $AB,BA\in L_{1+}$ and (3) $\mathrm{TR}[\epsilon,W]=0$ (odd case), $\mathrm{TR}[\Gamma\epsilon,W]=0$ (even case), for bounded operators W, with $\epsilon=D_0/|D_0|$.

Example 1: Set $p=1$ and consider the cocycle $c(X,Y)=\mathrm{tr}_C X[\epsilon,Y]$, for $X,Y\in\mathcal{B}$. Here everything is defined in the original Hilbert space H and not in $H\otimes\mathbb{C}^2$. We can write

$$c_{1,2}(X,Y)=\tfrac{1}{4}\mathrm{tr}\epsilon[\epsilon,X][\epsilon,Y]=\mathrm{tr}_C X[\epsilon,Y]=\tfrac{1}{2}\mathrm{TR}\;\; X[\epsilon,Y]=\tfrac{1}{2}\mathrm{TR}[X\epsilon,Y]-\tfrac{1}{2}\mathrm{TR}\epsilon[X,Y].$$

The last term is the coboundary of the cochain $\theta(X)=\frac{1}{2}\mathrm{TR}\epsilon X$ and therefore the class of $c_{1,2}$ is given by

$$c_{\mathrm{loc}}(X,Y)=\tfrac{1}{2}\mathrm{TR}[X\epsilon,Y].$$

One can also check by a direct computation that c_{loc} is a cocycle:

$$\begin{aligned}2(\delta c_{\mathrm{loc}})(X,Y,Z)&=\mathrm{TR}\{[[X,Y]\epsilon,Z]+\mathrm{cycl.}\}\\&=\mathrm{TR}\{[[X,Y],[\epsilon,Z]]+\mathrm{cycl.}\}\\&=\mathrm{TR}[\epsilon,[[X,Y],Z]]+\mathrm{TR}[Y,[[\epsilon,X],Z]]-\mathrm{TR}[X,[[\epsilon,Y],Z]]+\mathrm{cycl.}\end{aligned}$$

By (3) the first term on the right vanishes and by (2) the second and third terms vanish. In the case when X, Y are multiplication operators, by smooth functions, on the circle S^1 the local cocycle becomes the central term in an affine Lie algebra,

$$c_{\mathrm{loc}}(X,Y)=\frac{1}{2\pi i}\int_{S^1}\mathrm{tr}X\,dY,$$

where the trace under the integral sign is a finite-dimensional matrix trace for the matrix valued functions X, Y.

The cocycle $c_{1,2}$ (or c_{loc}) arises in canonical quantization in the following way. To each pair of basis vectors e_i, e_j in H there corresponds an operator $\hat{e}_{ij}=a^*(e_i)a(e_j)$ in the Fock representation. We may label the basis vectors such that $e_i\in H_+$ for $i=0,1,2,...$, and $e_i\in H_-$ for $i=-1,-2,...$, where $H_\pm=\frac{1}{2}(1\pm\epsilon)H$. Then a matrix (α_{ij}) in this basis has the canonical quantization as the operator $\hat{\alpha}=\Sigma\alpha_{ij}\hat{e}_{ij}$. For infinite matrices this might diverge. Actually, that happens already when α is the unit matrix. To circumvent this one introduces the normal ordering $\hat{e}_{ij}\mapsto\hat{e}_{ij}-\delta_{ij}\theta(-i)$ with $\theta(x)=x$ for $x\geqslant 0$ and $\theta(x)=0$ for $x<0$. With these new operators $\hat{e}_{ij}$ the operator $\hat{\alpha}$ is defined in a dense domain for any bounded operator α such that $[\epsilon,\alpha]$ is Hilbert–Schmidt and the commutation relations are given by

$$[\hat{\alpha},\hat{\beta}]=\widehat{[\alpha,\beta]}+c_{1,2}(\alpha,\beta)$$

(Ref. 15).

Example 2: Here we consider the problem arising from quantization of gauge currents in three space dimensions. Typically, $[\epsilon,X]$ is not Hilbert–Schmidt but it belongs to the ideal $L_{3+}\subset L_4$. For this reason the expression for the 2-cocycle in the previous example does not converge for 3-dimensional gauge currents. Instead, one has to introduce a renormalization of the 2-cocycle,

$$c_{3,2}(a;X,Y)=\tfrac{1}{8}\mathrm{tr}_C a[[\epsilon,X],[\epsilon,Y]],$$

with $a=F_A-\epsilon$. One can check by a direct calculation that this is a cocycle in the sense that

$$c_{3,2}(a;[X,Y],Z)+\delta_X c_{3,2}(a;Y,Z)+\text{cyclic perm. of } X,Y,Z=0.$$

Let next $\eta(a;X)=\frac{1}{8}\mathrm{TR}\epsilon a[\epsilon,X]$. By a direct calculation one can check that $c_{3,2}=\delta\eta+c_{\mathrm{loc}}$ where now

$$8c_{\mathrm{loc}}(a;X,Y)=\mathrm{TR}[Y,\epsilon a[\epsilon,X]]-\mathrm{TR}[X,\epsilon a[\epsilon,Y]]+2\,\mathrm{TR}[X\epsilon,Y]-2\,\mathrm{TR}[Y\epsilon,X]$$

is explicitly a generalized trace of a sum of commutators. Using the "bare" BRST notation (without the auxiliary space $\mathbb{C}^2$) we can write $c_{\mathrm{loc}}=\frac{1}{4}\mathrm{TR}[v\epsilon,v]-\frac{1}{8}\mathrm{TR}[v,\epsilon a[\epsilon,v]]$.

In this example the canonical quantization of gauge currents is ill-defined even after normal ordering, precisely because $[\epsilon,X]$ is not Hilbert–Schmidt. However, there is an operator theoretic interpretation for second quantized $\hat{X},\hat{Y}$. These are now generators for unitary transformations between Fock spaces carrying inequivalent representations of the CAR algebra. Geometrically, there is a bundle of Fock spaces parametrized by the external field a and the gauge transformations act as unitary maps between the fibers.[16]

Example 3: As a final example we discuss the gauge anomaly in two space–time dimensions. Here we are in the even case and we have $\Gamma\epsilon=-\epsilon\Gamma$ and we consider gauge transformations X which commute with Γ. Then $c_{2,1}(a;X)=\mathrm{tr}_C\Gamma a[\epsilon,X]$ is a cocycle,

$$\delta_X c_{2,1}(a;Y)-\delta_Y c_{2,1}(a;X)-c_{2,1}(a;[X,Y])=0,$$

using the fact that $\mathrm{tr}_C[\epsilon,\cdot]=0$. In this case,

$$c_{2,1}(a;X)=\mathrm{TR}[\Gamma a\epsilon,X]+(\delta\eta)(a),$$

where $\eta(a)=\mathrm{TR}\ \Gamma a\epsilon$. In BRST notation, for an even module, $c_{\mathrm{loc}}=\mathrm{TR}[a\epsilon,s(v)]$. We leave it as an exercise for the reader to show that when inserting $\epsilon=D_0/|D_0|$, $D_0=-i\Sigma_{k=1}^2\gamma^k\partial_k$, $D_A=D_0+\Sigma\gamma^k A_k(x)$ and $a=D_A/|D_A|-\epsilon$ one obtains the standard formula for the non-Abelian gauge anomaly in two space–time dimensions,

$$c_{\mathrm{loc}}=\frac{1}{4\pi}\int \mathrm{tr}(A_1\,\partial_2 X-A_2\,\partial_1 X),$$

for a smooth infinitesimal gauge transformation X of compact support.

In the general case we have the following result

Theorem 3.1: *Let $n=1,2,...$, and $k=0,1,2,...$, and let the cocycle $c_{2n-1-k,k}$ be computed from the descent equations in Sec. II. Then for even k the cohomology class $[c_{2n-1-k,k}]$ is represented by a cocycle $c^{loc}_{2n-1-k,k}$ which is a generalized trace of a sum of commutators; each commutator is a polynomial in the operators a, ϵ and X_j (the latter operators correspond to the tangent vectors at which the ghosts were evaluated). In the case of odd k one has to add a term proportional to a generalized trace of $\omega_{0,k}$.*

This theorem is a reformulation of Theorems A4 and A5 in the Appendix, which also gives more explicit formulas.

IV. A MODEL FOR $\mathcal{A}/\mathcal{G}$

When $\mathcal{A}$ is the space of classical smooth vector potentials on a compact manifold M and $\mathcal{G}_0$ is the group of based smooth gauge transformations [based means that $g(p)=1$ at some given point $p\in M$] then the quotient $X=\mathcal{A}/\mathcal{G}_0$ is a smooth infinite-dimensional Banach manifold. If one tries to generalize this to the NCG setting, by replacing $\mathcal{A}$ by all bounded perturbations of the free Dirac operator and taking $\mathcal{G}$ as the group of unitaries in the algebra $\mathcal{B}$, one encounters the problem that there is no natural way to define what is meant by based gauge transformations; this leads to the difficulty that X is not a manifold, it has a lot of singularities since at a generic point in $\mathcal{A}$ the action of $\mathcal{G}$ is not free. Here we shall construct a model for $\mathcal{A}$ and $\mathcal{G}$ such that the quotient will be free of singularities.

Our construction is essentially based on Bott periodicity. Recall that the inductive limit $U(\infty)$ of the group $SU(N)$ as $N\mapsto\infty$ has an odd homotopy type: All its homotopy groups $\pi_{2k+1}U(\infty)$ are isomorphic to $\mathbb{Z}$ whereas the even homotopy groups are trivial. For this reason the group of based gauge transformations $f:M\to U(N)$, in the limit $N\mapsto\infty$, for $M=S^{2n}$ is homotopic to $U(\infty)$. In the odd-dimensional case, $M=S^{2n+1}$, the group of gauge transformations has an even homotopy type: All the even homotopy groups are isomorphic to $\mathbb{Z}$ and the odd homotopy groups are trivial. Denoting the gauge group in the even case by G [which has the homotopy type of $U(\infty)$] then the group of gauge transformations in the odd case is the group of based loops ΩG. This later group has the homotopy type of U'_p for any $p\geqslant 1$ where U'_p is defined in the following way: Let ϵ be a grading operator (it could be the sign of a Dirac operator) in a Hilbert space, with eigenvalues ± 1, both eigenspaces infinite dimensional. Set $U'_p(H)=\{g\in U(H)|[\epsilon,g]\in L_p\}$. Here $U(H)$ is the (contractible) group of all unitaries in the Hilbert space H. Recall that $U_{p+}(H)$ is the group of unitary elements in the algebra $\mathcal{B}$. All elements g in $U_{p+}(H)$ satisfy $[\epsilon,g]\in L_{p+}$.

Let now D_p, p an even integer, be a Hermitian operator in H such that $1/|D_p|\in L_{p+}$ and let Γ be a Hermitian operator in H such that $\Gamma^2=1$ and $\Gamma D_p=-D_p\Gamma$. Let $D_{p+1}=i\Gamma(d/dt)+D_p$. This operator is self-adjoint in an appropriate dense domain in the Hilbert space $\mathcal{H}=L^2(S^1,H)$ and has the property $1/|D_{p+1}|\in L_{(p+1)+}$.

A generalized vector potential is defined as a Hermitian time dependent bounded operator $A(t)$ in H. The ''Dirac operator'' coupled to $A(t)$ is then $D_{p+1}+A(t)$. The vector potential can be split as $A=A_0+A_1$, where A_0 commutes with Γ (the ''time component'' of A) and A_1 anticommutes with Γ (this is the ''space component'' of A). The time dependent gauge transformations are smooth functions $g(t)$ with values in the group $U_{p+}(H,\Gamma)$ of unitary operators $g\in U_{p+}(H)$ such that $[\Gamma,g]=0$. We can split $H=H_1\oplus H_2$ to eigenspaces of Γ corresponding to eigenvalues ± 1. Since $g\in U_{p+}(H,\Gamma)$ commutes with Γ we can write g as a direct sum of linear operators $g_i:H_i\to H_i$, $i=1,2$.

The group $U_{p+}(H,\Gamma)$ is a subgroup of the group $U'_{p+}(H,\Gamma)$ which consists of unitary operators g such that $[\epsilon,g]\in L_{p+}$ and $\Gamma g=g\Gamma$. These conditions mean that $g=g_1\oplus g_2$ with $g_2-\epsilon g_1\epsilon\in L_{p+}$. Thus the group U'_{p+} is parametrized by pairs of unitary operators (g_2,h) with g_2 an arbitrary unitary operator in H_2 and $h=g_2^{-1}\epsilon g_1\epsilon$ an unitary operator in H_2 such that $h-1\in L_{p+}$; we denote the group of these elements by $U^{p+}(H_2)$. Thus by Kuiper's theorem $U'_{p+}(H,\Gamma)$ is homotopy equivalent to $U^{p+}(H_2)$. A similar result holds for the subgroup

$U_{p+} \subset U'_{p+}$. In this case one chooses as parameters g_2 and $\tilde{h} = g_2^{-1} D_+^{-1} g_1 D_+$ and the conditions are as before. Here $D_+ : H_2 \to H_1$ is the restriction of D_p to H_2. [If D_+ has zero modes, replace D_+^{-1} by $D_-/(D_- D_+ + 1)$.]

For each time dependent perturbation there is a unique (nonperiodic) gauge transformation $g(t)$ such that $g(0) = 1$ and $A'(t) = g^{-1} A g + g^{-1}[D_p, g] + i g^{-1} \partial_t g$ is in the generalized temporal gauge, i.e., the even component $A'_0 = 0$. It follows that the quotient $\mathcal{A}/\mathcal{G}_0$, where $\mathcal{G}_0$ is the group of periodic gauge transformations $g(t)$ with $g(0) = 1$, is equal to the product $\mathcal{A}_1 \times U_{p+}(H, \Gamma)$. Here $\mathcal{A}_1$ is the space of bounded operators A in H such that $\Gamma A = -\Gamma A$ and the coordinate $g \in U_{p+}(H, \Gamma)$ comes from the holonomy $g = g(2\pi)$ around the circle.

Since $\mathcal{A}_1$ is an affine space, $\mathcal{A}/\mathcal{G}_0$ is homotopy equivalent to $U_{p+}(H, \Gamma)$.

We end this section by a remark on the homotopy type of the various groups involved. When the condition $[\epsilon, g] \in L_{p+}$ is replaced by $[\epsilon, g] \in L_p$ we obtain the group $U'_p(H, \Gamma) \subset U'_{p+}(H, \Gamma)$. Note that also $U_{p+} \subset U'_{p+\alpha}$ for any $\alpha > 0$. Similarly one can define U^p with $U^p \subset U^{p+} \subset U^{p+\alpha}$. According to Palais,[17] the groups U^p for all $p \geqslant 1$ are homotopy equivalent with $U(\infty)$. Similarly $U'_p(H)$ is homotopy equivalent to the group $U'_0(H)$ of unitary operators g such that $[\epsilon, g]$ is of finite rank. It is plausible that the same holds for the groups U_{p+} and U^{p+}, but the proof in Ref. 17 cannot directly be applied to these cases. The topology of these groups is determined by a norm topology on the operator ideals L_{p+}.

The natural norm on L_{p+} for $p > 1$ is given as

$$\|T\|_{p+} = \sup_{N \geqslant 1} N^{1/p-1} \sigma_N(T),$$

where $\sigma_N(T)$ is the sum of the N largest eigenvalues of $|T|$. In the case $p = 1$ the factor $N^{1/p-1}$ is replaced by $(\log N)^{-1}$.

V. THE GERBE OVER $\mathcal{A}/\mathcal{G}_0$

Each $A \in \mathcal{A}$ and $\lambda \notin \mathrm{Spec}(D_A)$ defines a fermionic Fock space $\mathcal{F}_{A,\lambda}$ with a Dirac vacuum $|A, \lambda\rangle$. To begin with, we have the polarization $\mathcal{H} = \mathcal{H}_+(A, \lambda) \oplus \mathcal{H}_-(A, \lambda)$ to a pair of infinite-dimensional subspaces, defined by the spectral projections $D_A > \lambda$ and $D_A < \lambda$. Then the Fock space $\mathcal{F}_{A,\lambda}$ is generated by the algebra of creation and annihilation operators $a^*(u), a(u)$ with the relations (2.1) and the characterization of the vacuum $|A, \lambda\rangle$ as in (2.2).

The Fock spaces depend on the choice of the vacuum level λ. However, for λ, $\mu \notin \mathrm{Spec}(D_A)$ there is a natural projective isomorphism $\mathcal{F}_{A,\lambda} \equiv \mathcal{F}_{A,\mu}$. This construction is equivariant with respect to the gauge group action, leading to a projective bundle $P\mathcal{F}$ over $\mathcal{A}/\mathcal{G}_0$. The question is whether there exists a true vector bundle $\mathcal{F}$ over $X = \mathcal{A}/\mathcal{G}_0$ such that $P\mathcal{F}$ is the projectivization of $\mathcal{F}$.

In general, there is an obstruction to the existence of $\mathcal{F}$. The obstruction can be described in terms of an element ω in $H^3(\mathcal{A}/\mathcal{G}_0, \mathbb{Z})$. This may or may not correspond to a nontrivial de Rham cohomology class. However, in the present setting there is a nontrivial obstruction as a de Rham form.

A more geometric way to describe the obstruction problem is to construct a family of local complex line bundles $\mathrm{DET}_{\lambda\lambda'}$ over $\mathcal{U}_{\lambda\lambda'} = \mathcal{U}_\lambda \cap \mathcal{U}_{\lambda'}$ with $\mathcal{U}_\lambda = \{A \in \mathcal{A}/\mathcal{G}_0 | \lambda \notin \mathrm{Spec}(D_A)\}$. Here $\mathrm{DET}_{\lambda\lambda'}$ is the top exterior power of the (finite-dimensional) spectral subspace of D_A corresponding to the open interval (λ, λ') (with $\lambda < \lambda'$). These line bundles have a set of natural isomorphisms,

$$\mathrm{DET}_{\lambda\lambda'} \otimes \mathrm{DET}_{\lambda'\lambda''} = \mathrm{DET}_{\lambda\lambda''},$$

which give the relations needed to define *a gerbe* over $\mathcal{A}/\mathcal{G}_0$. The gerbe is trivial if there is a family of local line bundles DET_λ over the open sets $\mathcal{U}_\lambda$ such that $\mathrm{DET}_{\lambda\lambda'} = \mathrm{DET}_\lambda^{-1} \otimes \mathrm{DET}_{\lambda'}$. Physically, these latter bundles are the local fermionic vacuum bundles. The nontriviality of the gerbe is measured by the nontriviality of the *Dixmier–Douady class* ω.[18]

The nontriviality of the obstruction as a de Rham form follows from the considerations in Refs. 11 and 19. The setting in the latter paper was similar to the present case except that a smaller base space, G_1 of unitaries which differ from the identity by a trace class operator, was considered instead of $U_{p+}(H,\Gamma)$.

On the group G_1 the obstruction form is particularly simple. It is given as the left invariant form

$$\omega(X,Y,Z)=\frac{i}{8\pi^2}\,\mathrm{tr}X[Y,Z],$$

where $X,Y,Z\in\mathrm{Lie}(G_1)$. This is normalized such that its integral over a fundamental 3-cycle in $U^3(H)\simeq U_3'(H,\Gamma)$ is equal to one. As it stands, ω does not extend to $U_p'(H,\Gamma)$ for $p>3$. Instead, we have to construct another representative for the cohomology class which extends to $U_p'(H,\Gamma)$, and actually also to the larger group $U_{p+}(H,\Gamma)$. Since $U_{q+}(H,\Gamma)\subset U_p'(H,\Gamma)$ for $q<p$, we get a normalized representative for the cohomology class also in the former group.

We shall treat both the even and odd cases at the same time and U_p' stands for $U_p'(H,\Gamma)$ in the case of an even Fredholm module and $U_p'=U_p'(H)$ in the odd case. In both cases we denote the left invariant Maurer–Cartan 1-form on the group by $g^{-1}\,\delta g$.

Next we consider the (d,δ) BRST bicomplex on the group manifold U_p'. As before, δ is the exterior differentiation on the group manifold with a choice of signs when acting on d forms such that $d\delta+\delta d=0$. We set $\Delta=d+\delta$, so $g^{-1}\,\Delta g=g^{-1}[\epsilon,g]+g^{-1}\,\delta g$ and the second component is the Maurer–Cartan 1-form on the group, i.e., the BRST ghost v.

The form

$$\theta_{k-j,j}=\int\,(g^{-1}\,\Delta g)^k|_{[j]}$$

is closed in the δ cohomology complex for any $k=0,1,2,\ldots$. Here $(\cdots)|_{[j]}$ denotes the component of δ degree (=ghost degree) j. In order that the integral is defined as a (graded) trace we have to assume that $k-j\geqslant p$.

Actually $\theta_{k-j,j}=0$ for all even k's. This follows from the anticommutator relations for d, δ and from the cyclic properties of the integral. The closedness for odd k follows from

$$\delta\theta=\int\,\delta(g^{-1}\,\Delta g)^k=\int\,\Delta(g^{-1}\,\Delta g)^k=-\int\,(g^{-1}\,\Delta g)^{k+1}=0,$$

since $k+1$ is even.

For $j=k$ and with a proper normalization $\theta_{k,j}$ is the generator of $H^k(U_p',\mathbb{Z})$ whereas for $j=0$ the integral gives the Fredholm index of P_+gP_+, where $P_+=\frac{1}{2}(1+\epsilon)$.

The case $j=3$ is of interest to us. In this case $k-j=2n$ is even, so $\theta_{2n,3}$ is an integral of an even d-form. We check that this is a nontrivial cohomology class. For that purpose, choose H as the Hilbert space of square integrable sections in a tensor product of a Dirac spinor bundle over the torus $T^{2n}=(S^1)^{2n}$ and a trivial $\mathbb{C}^N$ bundle with the natural $U(N)$ action in the fibers. The gauge transformations $g:T^{2n}\to U(N)$ act as multiplication operators on the spinor fields. Choosing D_0 as the Dirac operator defined by the metric on the torus and the trivial vector potential $A=0$ in the $\mathbb{C}^N$ bundle, one has,[5,20]

$$\mathrm{tr}_C\Gamma a_0[\epsilon,a_1]\cdots[\epsilon,a_{2n}]=\frac{1}{n!(2\pi i)^n}\int_{T^{2n}}\mathrm{tr}a_0\,da_1\cdots da_{2n},$$

for smooth functions $a_j:T^{2n}\to\mathbf{g}$, where $\mathbf{g}$ is the Lie algebra of $U(N)$ in its fundamental representation and 'd' on the right means the de Rham exterior derivative. It follows that, for any map $g(\cdot):S^3\to\mathrm{Map}(T^{2n},U(N))$, we have

$$\int_{S^3}\theta_{2n,3}=\frac{1}{n!(2\pi i)^n}\int_{S^3\times T^{2n}}\mathrm{tr}(g^{-1}\,dg)^{2n+3},$$

where g is thought of as a $U(N)$ valued function on $S^3\times T^{2n}$. In particular, for large N, this integral is equal to $24\pi^2\times$ a nonzero integer when g represents a nontrivial homotopy class in $\pi_{3+2n}(U(N))\simeq\mathbb{Z}$. Since $\theta_{2n,3}$ is nontrivial on the subgroup of smooth gauge transformations in $U_{2n+}(H,\Gamma)$ it must represent a nonzero cohomology class of the latter group and therefore also in the moduli space $X=\mathcal{A}/\mathcal{G}_0$.

Specializing from the result of Theorem 3.1 (cf. Lemma A3 in the Appendix) to the flat case $a=g^{-1}[\epsilon,g]$ we observe that the forms $\theta_{2n,3}$ can be written as sums of generalized traces of commutators plus a properly normalized 3-form $\mathrm{TR}(g^{-1}\,\delta g)^3$, modulo exact forms.

VI. SCHWINGER TERMS FROM THE DIXMIER–DOUADY CLASS

In this section we shall work with the Fredholm modules based on the ideals L_p instead of L_{p+}, and likewise with the groups of the type U_p'. This is because we want to use available information (based on results in Ref. 17) on the homotopy type of the infinite-dimensional groups.

Let θ_3 be a closed integral 3-form on $X=\mathcal{A}/\mathcal{G}_0$. The pull back $\pi^*\theta_3=\psi_3$ with respect to the canonical projection is a closed 3-form on the contractible space $\mathcal{A}$ and therefore $\psi_3=d\psi_2$ for some 2-form ψ_2. (In this section d means always the de Rham exterior derivative.)

Let $\mathcal{U}_\alpha$ be an open contractible subset of X and write $\theta_3=d\theta_{2,\alpha}$ on $\mathcal{U}_\alpha$. We define

$$\eta_\alpha=\psi_2-\pi^*\theta_{2,\alpha}$$

on $\pi^{-1}(\mathcal{U}_\alpha)$. Now $d\eta_\alpha=\psi_3-d\pi^*\theta_{2,\alpha}=\psi_3-\pi^*\,d\theta_{2\alpha}=\psi_3-\pi^*\theta_3=0$.

If $\mathcal{U}_\beta$ is another open subset of X then on $\mathcal{U}_\alpha\cap\mathcal{U}_\beta$ we have $\eta_\alpha-\eta_\beta=\pi^*(\theta_{2,\alpha}-\theta_{2,\beta})$. From this it follows, by the definition of the pull back map, that η_α and η_β agree *when evaluated along gauge orbits*. Thus there is a vertical 2-form η on $\mathcal{A}$, defined everywhere on $\mathcal{A}$, but which is closed only along gauge directions.

The vertical form η defines an extension of the Lie algebra of $\mathcal{G}$ by the Abelian Lie algebra **a** consisting of functions $f:\mathcal{A}\to\mathbb{C}$. The commutators are defined by

$$[(X,f),(Y,g)]=(\,[X,Y],\delta_X g-\delta_Y f+\eta(X,Y)).$$

On the right the Lie algebra elements X,Y are interpreted as vertical vector fields on $\mathcal{A}$. The Jacobi identity is precisely the condition that η is closed along vertical directions.

We can compute η more explicitly. Let $\mathcal{P}G$ denote the group of smooth paths in a group G originating from the identity in G. The product is defined as a pointwise multiplication along paths. Any $A\in\mathcal{A}$ splits uniquely as $A=A_0+A_1$ to even and odd components with respect to Γ. The even component A_0 is equal to $ig(t)^{-1}\partial_t g(t)$ for a uniquely defined smooth function $g:[0,1]\to U_p'(\Gamma,H)$ with $g(0)=1$. As in Sec. IV, we can write $\mathcal{A}=\mathcal{A}_1\times\mathcal{P}U_p'(\Gamma,H)$ and $\mathcal{A}/\mathcal{G}_0=\mathcal{A}_1\times U_p'(\Gamma,H)$.

Since $\mathcal{A}_1$ is a vector space, any closed form on $\mathcal{A}_1$ is exact and we may assume without loss of generality that θ_3 is a pull back of a form on $U_p'(\Gamma,H)$ with respect to the projection on the second factor.

By a direct calculation one can check that $d\psi_2=\pi^*\theta_3$ when ψ_2 is defined as

$$\psi_2(u,v)=\int_0^1\theta_3(g^{-1}\,\partial_t g,u_0(t),v_0(t))dt,$$

where the components u_0,v_0 of the tangent vectors $u,v\in\mathcal{A}$ are given as paths in the Lie algebra of $U_p'(\Gamma,H)$. Along vertical directions η is equal to ψ_2 and thus

$$\eta(g;X,Y)=\int_0^1 \theta_3(g^{-1}\partial_t g,X(t),Y(t))dt,$$

for periodic functions $X(t),Y(t)$ with values in Lie $(U_p'(\Gamma,H))$.

Since $\pi_2(U_p'(\Gamma,H))=0$, the group $\mathcal{G}_0$ of (based) loops in $U_p'(\Gamma,H)$ is simply connected. On the other hand, $\pi_2(\mathcal{L}_k U_p'(\Gamma,H))=\pi_3(U_p'(\Gamma,H))=\mathbb{Z}$ for any of the connected components $\mathcal{L}_k$ of the group $\mathcal{L}U_p'$ of smooth loops in U_p'. By Hurewicz' theorem, $H^2(\mathcal{L}_k U_p'(\Gamma,H),\mathbb{Z})=\mathbb{Z}$. In fact, the 2-form η restricted to a gauge orbit gives a representative for the basic class in $H^2(\mathcal{L}_k U_p',\mathbb{Z})$.

We shall work only in the connected component of identity $\mathcal{L}_0 U_p'$. The group extension of $\mathcal{L}_0 U_p'(\Gamma,H)$ corresponding to the Lie algebra extension above can be explicitly constructed in the same way as was done in Ref. 21 in the case of groups of classical gauge transformations.

The construction starts from the Cartesian product $\mathcal{P}(\mathcal{L}_0 U_p')\times \mathrm{Map}(\mathcal{A},S^1)$. The product is defined as

$$(f_1,\alpha_1)(f_2,\alpha_2)=\left(f_1 f_2,\alpha_1\alpha_2^{f_1}\exp\left(2\pi i\int_K \eta\right)\right),$$

where $f_1 f_2$ is just the point-wise product in the path group, α^f is the function obtained form α by gauge transforming (using the right action) the argument by $f(1)\in\mathcal{L}_0 U_p'$. The phase is evaluated by integrating the vertical 2-form η over a 2-surface K in the fiber at $A\in\mathcal{A}$. The surface is chosen such that its boundary consists of the paths $A\cdot f_1(t)$, $A\cdot f_1(1)f_2(t)$ and $A\cdot f_1(t)f_2(t)$. The value of the phase factor does not depend on the choice of K since the difference in the exponent is $2\pi i$ times an integral of the integral 3-form ω_3 over a closed 3-surface in U_p' and this is an integer.

The extension $\widehat{\mathcal{L}_0 U_p'}$ is now defined as

$$\mathcal{P}(\mathcal{L}_0 U_p')\times \mathrm{Map}(\mathcal{A},S^1)/\mathcal{Q},$$

where $\mathcal{Q}$ is the group of based loops (at the identity) in $\mathcal{L}_0 U_p'$ and the right action of $\mathcal{Q}$ is defined as the point-wise right action on $\mathcal{P}(\mathcal{L}_0 U_p')$ and as the simultaneous phase shift $\alpha\to\alpha'$,

$$\alpha'(A)=\alpha(A)\exp\left(2\pi i\int_\Sigma \eta\right),$$

where Σ is the 2-surface in the fiber through A, bounded by the loop $A\cdot g(t), g\in\mathcal{Q}$.

VII. THE CASE OF A NONCOMMUTATIVE TORUS

In this section we want to apply the general results for computing cocycles on a noncommutative torus. We start by recalling the basic definitions.[22]

Consider an algebra consisting of finite linear combinations of "noncommutative Fourier modes" u^r, where $r=(r_1,\ldots,r_n)$ is a vector of integers,

$$u^r=e^{\pi i\Sigma_{j<k}\theta_{jk}r_j r_k}u_1^{r_1}\cdots u_n^{r_n}$$

and the relations in the algebra are given as

$$u_i u_j=e^{-2\pi i\theta_{ij}}u_j u_i, \tag{7.1}$$

where θ is a real antisymmetric matrix. These relations lead to the multiplication formula

$$u^r\cdot u^{r'}=\lambda(r,r')u^{r+r'}, \tag{7.2}$$

with $\lambda(r,r')=\exp(-\pi i\Sigma r_j\theta_{jk}r_k')$.

There is an antilinear conjugation defined by $(u^r)^*=u^{-r}$ and a trace τ such that $\tau(u^r)=0$ if $r\neq 0$ and $\tau(u^0)=\tau(1)=1$. We define a Hilbert space H by tensoring the above algebra with the spinor and internal symmetry space $V=\mathbb{C}^{[(n+1)/2]}\otimes\mathbb{C}^N$ and completing with respect to the inner product defined by $\langle u^r,u^{r'}\rangle=\tau((u^r)^*u^{r'})=\delta_{rr'}$. Here $[a]$ is the integer part of a real number a. The trace is extended to the tensor product of the torus algebra and of End V by the matrix trace on End V. The adjoint of a multiplication operator by the element u^r is $(u^r)^*=u^{-r}$.

There is a commutative family of derivations δ_j $(j=1,2,...,n)$ defined by $\delta_j(u^r)=r_ju^r$. These derivations are represented by unbounded operators P_j in the Hilbert space H through $P_ju^r=r_ju^r$ which means that $[P_j,u^r]=r_ju^r$ for the corresponding multiplication operators u^r (we use the same notation for elements in the noncommutative torus algebra and vectors in the Hilbert space).

The (free) Dirac operator is defined by

$$D_0=\sum_k \gamma^k\delta_k,$$

where the gamma matrix algebra is defined using the standard Euclidean metric, $\gamma_i\gamma_j+\gamma_j\gamma_i=2\delta_{i,j}$.

As in the case of pseudodifferential operators on an ordinary torus we can introduce a symbol calculus. Consider first classical PSDO symbols $f=f(p)$ which are functions of the momenta p_j only and which have an asymptotic expansion $f\sim f_N+f_{N-1}+\cdots$ as a series of homogeneous symbols f_j of order j in the momenta, i.e., $f_j(\lambda p)=\lambda^j f(p)$ for $\lambda>1$ and for large momenta. Each such symbol defines an (in general unbounded) operator in H through $fu^r=f(r)u^r$. More generally, we consider operators

$$f=\sum_r u^r f^{(r)},$$

where each $f^{(r)}$ is a classical symbol of the above type tensored with a matrix operating in V. The definition makes sense even for infinite linear combinations assuming that the sequence $|f^{(r)}(p)|$ is rapidly decreasing as $|r|\to\infty$ for all values of p. From the definitions it follows that

$$u^{-r}f(p)u^r=f(p+r), \tag{7.3}$$

and therefore the product of a pair f,g of operators is defined by the "star product"

$$(f*g)^{(r)}(p)=\sum_s f^{(r-s)}(p)g^{(s)}(p+s)\lambda(r-s,s). \tag{7.4}$$

The only difference as compared to the commutative torus is the appearance of complex phases λ on the right hand side. The trace of the operator f (when it is defined) is given by

$$\mathrm{tr}\, f=\sum_{p\in\mathbb{Z}^n}\mathrm{tr}\, f^{(0)}(p),$$

where the trace on the right is the ordinary matrix trace in V. As usual, f is trace-class if and only if $\mathrm{ord}(f)<-n$. The borderline case $\mathrm{ord}(f)=-n$ is of special interest to us.

For complex numbers z with an enough large real part one can define

$$\zeta(z;f)=\mathrm{tr}\,(|P|+1)^{-z}f. \tag{7.5}$$

If f is trace-class then ζ is holomorphic at $z=0$ and $\mathrm{tr}\, f=\zeta(0;f)$. If $\mathrm{ord}(f)\geqslant -n$, the function ζ has in general a pole at $z=0$. The pole depends only on the component f_{-n}. The proof of this

statement follows from the corresponding result for PSDO's on the commutative torus since the spectrum of $f^{(0)}$ is exactly the same as in the commutative case. For the same reason the residue at $z=0$ can be calculated as a momentum space integral,

$$\mathrm{Res}(f)=\mathrm{res}_{z=0}\zeta(z;f)=\int_{|p|=1}\mathrm{tr}\, f^{(0)}_{-n}(p)dp. \tag{7.6}$$

For classical PSDO's on a compact manifold there is a useful formula relating the renormalized (noncyclic) trace of a commutator to an operator residue. This formula was used for the calculation of Schwinger terms in Refs. 9 and 23 and later generalized in Ref. 24 to a wider class of operators. First one defines a renormalized trace for nontraceclass PSDO's by

$$\mathrm{TR}\,A=\lim_{z\to 0}\left(\mathrm{tr}\,A|D|^{-z}-\frac{1}{z}\mathrm{Res}\,A\right). \tag{7.7}$$

The lack of cyclicity of TR is given by

$$\mathrm{TR}[A,B]=\mathrm{Res}\,A[l,B], \tag{7.8}$$

where $l=\log|D_0|=\log|P|$. We check that the same formula holds in the case of a noncommutative torus. By linearity, it is sufficient to prove the formula for each Fourier mode separately. So we take $A=u^r f(p)$ and $B=u^s g(p)$. By the definition of the trace, TR AB is nonzero only when $s=-r$, so we assume this. But now $\mathrm{TR}\,AB=\mathrm{TR}\,\lambda(r,s)\tilde{f}g$, where $\tilde{f}(p)=f(p-r)$. Since $\lambda(r,s)=1$ when $s=-r$, the trace formula for NC torus reduces to the formula on commutative torus and thus (7.8) holds.

Let us look closer at the case $n=3$. We have seen that the Schwinger term in three dimensions is equivalent (modulo coboundaries) to the "local" expression

$$8\omega_{3,2}=\mathrm{TR}\{[X,\epsilon a[\epsilon,Y]]-[Y,\epsilon a[\epsilon,X]]-2[X\epsilon,Y]+2[Y\epsilon,X]\}.$$

We now apply the residue formula in the case of noncommutative multiplication operators X,Y and we obtain

$$8\omega_{3,2}=-\mathrm{Res}\,\epsilon a[\epsilon,Y][l,X]+\mathrm{Res}\,\epsilon a[\epsilon,X][l,Y]. \tag{7.9}$$

Taking $a=F-\epsilon$ and $F=(D_0+A)|D_0+A|^{-1}$, the sign of a Dirac operator defined by a potential $A=\sigma^k A_k$ on the noncommutative torus, a straight-forward computation gives

$$\omega_{3,2}=\frac{i\pi}{6}\tau(A[[D_0,X],[D_0,Y]])=\frac{i\pi}{3}\epsilon^{ijk}\tau(A_i(\delta_j(X)\delta_k(Y)-\delta_j(Y)\delta_k(X))). \tag{7.10}$$

We have used the expansion

$$F=\epsilon+A/|P|-\epsilon A^k P_k/|P|^2+O(1/|P|^2)$$

and the formulas

$$\begin{aligned}[\epsilon,u^{(r)}]&=u^{(r)}(u^{(-r)}\epsilon u^{(r)}-\epsilon)\\&=u^{(r)}\left(\frac{(P_k+r_k)\sigma^k}{|P+r|}-\frac{P_k\sigma^k}{|P|}\right)\\&=u^{(r)}(r_k\sigma^k/|P|-\epsilon P_k r^k/|P|^2+O(1/|P|^2)),\end{aligned}$$

and similarly

$$[l,u^{(r)}]=u^{(r)}P_k r^k/|P|^2+O(1/|P|^2).$$

The derivation of (7.10) is then completed by taking into account

$$\mathrm{tr}\,\sigma_i\sigma_j\sigma_k=2i\epsilon_{ijk}\ \text{ and }\ \mathrm{Res}\frac{p_ip_j}{|p|^5}=\frac{4\pi}{3}\delta_{i,j}.$$

APPENDIX: NONCOMMUTATIVE DESCENT EQUATIONS

We assume linear operators d and δ acting on polynomials generated by a, v, $d(a)$, $d(v)$, $\delta(a)$ and $\delta(v)$, such that $d^2=0=\delta^2=d\delta+\delta d$. These operations are then uniquely fixed by the additional rules in (2.6) together with $\epsilon^2=I$. As mentioned in the text, we will use the simplified notation $x=a$, ϵ, v and δ short for $s(x)$ defined in (2.7), resp. (2.8), for even, resp. odd, Fredholm modules throughout this Appendix except in the Remark at the end.

We now state and give a proof of the noncommutative descent equations. We define

$$F(t)=td(a)+t^2a^2+(1-t)d(v),$$

$$F'(t)=(t^2-t)v^2+td(v)$$

and

$$\omega_{2n-1}=\int_0^1 dt\Psi_{2n-1}(t),\quad \tilde{\omega}_{2n-1}=\int_0^1 dt\ \ t\Psi_{2n-1}(t),$$

and similarly for ω'_{2n-1} and $\tilde{\omega}'_{2n-1}$, where

$$\Psi_{2n-1}(t)=\sum_{\nu=0}^{n-1}F(t)^{n-1-\nu}aF(t)^{\nu},$$

$$\Psi'_{2n-1}(t)=\sum_{\nu=0}^{n-1}F'(t)^{n-1-\nu}vF'(t)^{\nu}.$$

The noncommutative descent equations can be summarized by the following algebraic identities.

Lemma A1:

$$\begin{aligned}\delta(\omega_{2n-1})+d(\omega_{2n-1})&=-[v,\omega_{2n-1}]_+-[a,\tilde{\omega}_{2n-1}]_++F^n-(d(v))^n,\\ \delta(\omega'_{2n-1})+d(\omega'_{2n-1})&=-[v,\tilde{\omega}'_{2n-1}]_++(d(v))^n,\end{aligned}\tag{A2}$$

where $F=d(a)+a^2$.

Comparing equal powers of v we obtain from (A2),

$$\begin{aligned}d(\omega_{2n-1,0})&=-[a,\tilde{\omega}_{2n-1,0}]_++F^n,\\ \delta(\omega_{2n-k,k-1})+d(\omega_{2n-1-k,k})&=-[v,\omega_{2n-k,k-1}]_+-[a,\tilde{\omega}_{2n-k-1,k}]_+,\\ &\qquad k=1,\ldots,n-1,\\ \delta(\omega_{n,n-1})+d(\omega_{n-1,n})&=-[v,\omega_{n,n-1}]_+,\\ \delta(\omega_{2n-k,k-1})+d(\omega_{2n-k-1,k})&=-[v,\tilde{\omega}_{2n-k,k-1}]_+,\\ &\qquad k=n+1,\ldots,2n-1,\end{aligned}\tag{A3}$$

$$\delta(\omega_{0,2n-1}) = -[v, \tilde{\omega}_{0,2n-1}]_+ ,$$

where the k in $\omega_{2n-k-1,k}$ is the ghost degree, i.e., power in v, and

$$\omega_{2n-1} = \omega_{2n-1,0} + \omega_{2n-2,1} + \cdots + \omega_{n,n-1} + \cdots ,$$

$$\omega'_{2n-1} = \omega_{n-1,n} + \omega_{n-2,n+1} + \cdots + \omega_{0,2n-1} + \cdots$$

[note that the equation for $k=n$ is obtained by combining the two equations

$$\delta(\omega_{n,n-1}) = -[v, \omega_{n,n-1}]_+ - (d(v))^n,$$

$$d(\omega_{n-1,n}) = (d(v))^n,$$

obtained from the first and the second relation in Eq. (A2), respectively].

Proof of Lemma A1: (A2): We observe that

$$F(t) = (\epsilon + \delta + ta + v)^2 - I,$$

implying $\partial_t(F(t)) = [\epsilon + \delta + ta + v, a]_+$, and therefore

$$\begin{aligned} F^n - (d(v))^n &= \int_0^1 dt \partial_t (F(t))^n \\ &= \int_0^1 dt \sum_{\nu=0}^{n-1} F(t)^{n-1-\nu} [\epsilon + \delta + ta + v, a]_+ F(t)^\nu \\ &= \int_0^1 dt [\epsilon + \delta + ta + v, \Psi_{2n-1}]_+ \end{aligned}$$

[we used that $\epsilon + \delta + ta + v$ commutes with $F(t)$], implying the first identity in Eq. (A2). In a similar manner,

$$F'(t) = (\epsilon + \delta + tv)^2 - I,$$

implies $\partial_t(F'(t)) = [\epsilon + \delta + tv, v]_+$ and thus

$$\begin{aligned} (d(v))^n &= \int_0^1 dt\, \partial_t (F'(t))^n \\ &= \int_0^1 dt \sum_{\nu=0}^{n-1} F'(t)^{n-1-\nu} [\epsilon + \delta + tv, v]_+ F'(t)^\nu \\ &= \int_0^1 dt [\epsilon + \delta + tv, \Psi'_{2n-1}]_+ , \end{aligned}$$

yielding the second identity in Eq. (A2). □

Some applications: A simple special case of Eqs. (A3) is the following result. We point out that here, $x = a$ and ϵ *need not* to be interpreted as $s(x)$ but can be taken directly as operators in H.

Lemma A2: For flat a, i.e., $a = g^{-1}[\epsilon, g] = [g^{-1}\epsilon, g]$ for some invertible operator g, the following holds true:

$$a^{2n+1} = 4a^{2n-1} + 2[\epsilon, a^{2n-1}\epsilon] - [a, \epsilon a^{2n-1}], \tag{A4}$$

for all positive integers n.

Proof: For flat a we have $F=d(a)+a^2=0$, and thus the first equation in (A3) implies $[\epsilon,\omega_{2n-1,0}]_+=-[a,\tilde{\omega}_{2n-1,0}]_+$ where $\omega_{2n-1,0}$ is obtained from ω_{2n-1} above by substituting $F(t)=(t^2-t)a^2$, i.e., $\omega_{2n-1,0}=\int_0^1 dtn(t^2-t)^{n-1}a^{2n-1}\equiv c_n a^{2n-1}$, and similarly $\tilde{\omega}_{2n-1,0}=\int_0^1 dt\, tn(t^2-t)^{n-1}a^{2n-1}\equiv\tilde{c}_n a^{2n-1}$. Note that

$$2\tilde{c}_n-c_n=\int_0^1 dt\ \ n(2t-1)(t^2-t)^{n-1}=0,$$

implying

$$2[\epsilon,a^{2n-1}]_+=-[a,a^{2n-1}]_+ .$$

Multiplying this identity by ϵ we obtain

$$2\epsilon[\epsilon,a^{2n-1}]_+=4a^{2n-1}+2[\epsilon,a^{2n-1}\epsilon]=-\epsilon[a,a^{2n-1}]_+=-[\epsilon,a]_+a^{2n-1}+[a,\epsilon a^{2n-1}].$$

Inserting $[\epsilon,a]_+=d(a)=-a^2$ we obtain Eq. (A4). □

Note that the lemma gives as a byproduct a simple proof of the known index formula for the Fredholm index $\mathrm{ind}\,P_+gP_+$, where $g\in U_p'(H_+\oplus H_-)$ and P_+ is the projection to H_+. Namely, since according to Ref. 17 the connected components of U_p' are labeled by the Fredholm index of P_+gP_+, the index is a homotopy invariant, and the multiplication operator by the function $f(x)=e^{inx}$ on the unit circle $0\leqslant x\leqslant 2\pi$ has index $\mathrm{ind}\,P_+fP_+=n$ (by a simple exercise in Fourier analysis), it is sufficient to check that

$$n=\tfrac{1}{2}\,\mathrm{tr}\,f^{-1}[\epsilon,f],$$

and the general formula

$$\mathrm{ind}\,P_+gP_+=2^{-p}\,\mathrm{tr}(g^{-1}[\epsilon,g])^p$$

follows for odd positive integers p.

Local cocyles: The basic result implying the existence of the local cocycles is the following.

Lemma A3: The forms defined above obey

$$\begin{aligned}\epsilon[v,\omega_{2n-k,k-1}]_+ + \epsilon[a,\tilde{\omega}_{2n-k-1,k}]_+ &\simeq c_{n,k}\omega_{2n-k+1,k},\quad k=1,...,n-1,\\ \epsilon[v,\omega_{n,n-1}]_+ &\simeq c_{n,n}\omega_{n+1,n},\\ \epsilon[v,\tilde{\omega}_{2n-k,k-1}]_+ &\simeq c_{n,k}\omega_{2n-k+1,k},\quad k=n+1,...,2n,\end{aligned}\tag{A5}$$

where

$$c_{n,k}=\frac{2n+1-k}{n+1},$$

and "≃" means "equal up to commutator terms."

Proof: To prove the first relation in Eq. (A5) we observe

$$\begin{aligned}\epsilon[v,\omega_{2n-k,k-1}]_+ + \epsilon[a,\tilde{\omega}_{2n-k-1,k}]_+ &= [\epsilon,v]_+\omega_{2n-k,k-1}+[\epsilon,a]_+\tilde{\omega}_{2n-k-1,k}+[\epsilon\omega_{2n-k,k-1},v]\\ &\quad +[\epsilon\tilde{\omega}_{2n-k-1,k},a]\simeq d(v)\omega_{2n-k,k-1}+d(a)\tilde{\omega}_{2n-k-1,k},\end{aligned}$$

and thus what we actually need to prove is

$$d(v)\omega_{2n-k,k-1}+d(a)\tilde{\omega}_{2n-k-1,k}\simeq\frac{2n+1-k}{n+1}\omega_{2n-k+1,k}. \tag{A6}$$

For that it is convenient to define an ordering symbol $\{\ \ \}$ so that

$$\sum_{N=0}^{\infty}(a_1+a_2+\cdots a_k)^N:=\sum_{m_1,m_2,\ldots,m_k=0}^{\infty}\{a_1^{m_1},a_2^{m_2},\ldots,a_k^{m_k}\},$$

for all operators a_j (we regard this as generating function defining all possible $\{a_1^{m_1},a_2^{m_2},\ldots,a_k^{m_k}\}$). We observe that this definition implies

$$a_1\{a_1^{m_1},a_2^{m_2},\ldots,a_k^{m_k}\}\simeq\frac{m_1+1}{m_1+m_2+\cdots+m_k+1}\{a_1^{m_1+1},a_2^{m_2},\ldots,a_k^{m_k}\}.$$

We can thus write $\omega_{2n-k-1,k}=\int_0^1 dt\Omega_{2n-k-1,k}$ and $\tilde{\omega}_{2n-k-1,k}=\int_0^1 dt\, t\Omega_{2n-k-1,k}$, where

$$\Omega_{2n-k-1,k}=\{u^k,(p+q)^{n-k-1},a\}=\sum_{l=0}^{n-k-1}\{u^k,p^{n-k-l-1},q^l,a\},$$

with $u\equiv(1-t)d(v)$, $p\equiv td(a)$ and $q\equiv t^2a^2$. To prove Eq. (A6) we thus need to show that

$$\frac{2n+1-k}{n+1}\int_0^1 dt\{u^k,p^{n-k-l},q^l,a\}\simeq\int_0^1 dt\left(\frac{u}{1-t}\{u^{k-1},p^{n-k-l},q^l,a\}+p\{u^k,p^{n-k-l-1},q^l,a\}\right),$$

which follows from

$$\int_0^1 dt\left(\frac{2n+1-k}{n+1}-\frac{k}{(n+1)(1-t)}-\frac{n-k-l}{n+1}\right)t^{n-k-l}t^{2l}(1-t)^k$$
$$=\frac{1}{n+1}\int_0^1 dt\,\partial_t(t^{n+1-k+l}(1-t)^k)=0.$$

The proof of the second and third relations in Eq. (A5) is similar but simpler: Recalling $u=(1-t)d(v)$ we get

$$\epsilon[v,\omega_{n,n-1}]_+\simeq d(v)\omega_{n,n-1}=\int_0^1 dt\frac{1}{1-t}u[u^{n-1},a]_+$$
$$=\int_0^1 dt\frac{1}{1-t}\frac{n}{n+1}[u^n,a]_+$$
$$=\int_0^1 dt[u^n,a]_+=c_{n,n}\omega_{n+1,n},$$

since

$$\frac{n}{n+1}\int_0^1 dt(1-t)^{n-1}=\int_0^1 dt(1-t)^n,$$

and finally, with $r\equiv td(v)$ and $s\equiv(t^2-t)v^2$,

$$\epsilon[v,\tilde{\omega}_{2n-k,k-1}]_+ \simeq d(v)\tilde{\omega}_{2n-k,k-1}$$
$$= \int_0^1 dt \;\; r\{r^{2n-k}, s^{k-1-n}, v\}$$
$$\simeq \int_0^1 dt \, \frac{2n+1-k}{n+1} \{r^{2n+1-k}, s^{k-1-n}, v\} = c_{n,k}\omega_{2n-k+1,k}.$$

□

We obtain a generalization of Lemma A2.

Theorem A4: *Let*

$$\omega'_{2n-1-k,k} = C_{n,k}\omega_{2n-1-k,k}, \quad \text{where} \quad C_{n,k} = (-1)^n \frac{(2n-1-k)!!}{2^n n!}.$$

Then

$$\omega'_{2n+1-k,k} \simeq \omega'_{2n-1-k,k} - \frac{C_{n,k}}{2C_{n,k-1}} \delta(\epsilon\omega'_{2n-k,k-1}). \tag{A7}$$

Proof: Using the lemmas above, we observe that

$$-\delta(\epsilon\omega_{2n-k,k-1}) + 2\omega_{2n-1-k,k} \simeq -c_{n,k}\omega_{2n+1-k,k}, \quad k = 1,2,...,2n-1, \tag{A8}$$

where we have used that $\epsilon d(\omega) = \epsilon[\epsilon,\omega]_+ \simeq 2\omega$. By multiplying this with $(1/2)C_{n,k}$ and using the recursion relation

$$-\tfrac{1}{2}c_{n,k}C_{n,k} = C_{n+1,k},$$

we get Eq. (A7). □

Theorem A5: *For even k the k-cocyle,*

$$\omega^{\mathrm{loc}}_{2n+1-k,k} = \omega_{2n+1-k,k} + \delta B_{2n-k,k-1},$$

is local for some cochain $B_{2n-k,k-1}$, i.e., a sum of commutator terms. In the case when k is odd one has to add a term proportional to $\omega_{0,k}$ to the right hand side of the equation.

Proof: Equation (A8) implies

$$\omega_{2n+1-k,k} \simeq -\frac{2}{c_{n,k}}\omega_{2n-1-k,k} - \frac{1}{c_{n,k}}\delta(\omega_{2n-k,k-1})$$
$$\simeq \sum_{l'=0}^{l} (-1)^{l'+1} \frac{2^{l'}}{c_{n,k}c_{n-1,k}\cdots c_{n-l',k}} \delta(\omega_{2n-2l'-k,k-1})$$
$$+ (-1)^{l+1} \frac{2^l}{c_{n,k}c_{n-1,k}\cdots c_{n-l,k}} \omega_{2n-1-2l-k,k}.$$

In particular,

$$\omega_{2n+1-2k,2k} \simeq \sum_{l'=0}^{n-k} (-1)^{l'+1} \frac{1}{2} \frac{(n+1)!(n-2k-l')!}{(n-l')!(n-2k)!} \delta(\omega_{2n-2l'-2k,2k-1})$$

and

$$\omega_{2n-2k,2k+1} \simeq \sum_{l'=0}^{n-k-1} (-1)^{l'+1} \frac{1}{2} \frac{(n+1)!(n-2k-l'-1)!}{(n-l')!(n-2k-1)!} \delta(\omega_{2n-2l'-2k-1,2k}) + (-1)^{n-k} \frac{1}{2} \binom{n+1}{k} \omega_{0,2k+1},$$

which also gives an explicit formula for $B_{2n-k,k-1}$. □

Remark: Theorem A5 does not yet imply Theorem 3.1: we recall that we worked on an abstract BRST level here and $x=a$, ϵ, v and δ, etc. was short for $s(x)$ as in Eq. (2.7), resp. (2.8). As discussed in the text, to obtain forms $\omega_{2n-1-k,k}(a;X_1,\ldots,X_k)$ one has to evaluate the ghosts v at tangent vectors X_j and, in the case of an odd Fredholm module, take the trace in the auxiliary space with the Pauli matrix σ_3. To complete the proof of Theorem 3.1 one needs to check that the commutators mentioned in Theorem A5—which are on the abstract BRST level—turn into the commutators on the operator level mentioned in Theorem 3.1. We now show that this is indeed the case. For that we need to distinguish $s(x)$ from x. The commutators referred to in Theorem A5 are then of the form $[s(\alpha),s(\beta)]$ where $s(\alpha)$ and $s(\beta)$ are monomials in $s(v)$, $s(a)$ and $s(\epsilon)$.

In the case of an even Fredholm module, there is no extra auxiliary space [cf. (2.7)], and the BRST commutators $[s(\alpha),s(\beta)]$ immediately become operator commutator after the evaluation of the ghosts at the tangent vectors.

We thus can concentrate on odd Fredholm modules. Let n_α be the ghost degree of α [the number of $s(v)$] and d_α the sum of the numbers of $s(\epsilon)$ and $s(a)$ (which is of course only defined modulo 2), and similarly for β. Then $s(\alpha)=\pm\alpha\otimes\sigma_3^{d_\alpha}\sigma_1^{n_\alpha}$ and similarly for β, and thus

$$[s(\alpha),s(\beta)] = \pm((-1)^{n_\alpha d_\beta}\alpha\beta - (-1)^{d_\alpha n_\beta}\beta\alpha)\otimes\sigma_3^{d_\alpha+d_\beta}\sigma_1^{n_\alpha+n_\beta}.$$

In the odd case the ghost degree $k=n_\alpha+n_\beta$ is even and $d_\alpha+d_\beta$ is odd. Evaluating $[s(\alpha),s(\beta)]$ for Lie algebra elements X_j, we obtain (up to an irrelevant overall factor)

$$\sum_{P\in S_k} \mathrm{sign}_P(\alpha(X_{P(1)},\ldots,X_{P(n_\alpha)})\beta(X_{P(n_\alpha+1)},\ldots,X_{P(k)}) - (-1)^{n_\alpha n_\beta}(-1)^{n_\alpha d_\beta + d_\alpha n_\beta}\beta(X_{P(n_\alpha+1)},\ldots,X_{P(k)})\alpha(X_{P(1)},\ldots,X_{P(n_\alpha)})),$$

where S_k is the permutation group of k elements and sign_P gives the parity of a permutation P. One now needs to show that this always corresponds to a sum of commutators. For that we need only to check that the exponent $n_\alpha n_\beta + n_\alpha d_\beta + n_\beta d_\alpha$ is always even. But this follows from the fact that here $n_\alpha+n_\beta$ is even and $d_\alpha+d_\beta$ is odd.

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SUSY transformations for quasinormal modes of open systems

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Supersymmetry (SUSY) in quantum mechanics is extended from square-integrable states to those satisfying the outgoing-wave boundary condition, in a Klein–Gordon formulation. This boundary condition allows both the usual normal modes and quasinormal modes with complex eigenvalues ω. The simple generalization leads to three features: The counting of eigenstates under SUSY becomes more systematic; the linear-space structure of outgoing waves (nontrivially different from the usual Hilbert space of square-integrable states) is preserved by SUSY; and multiple states at the same frequency (not allowed for normal modes) are also preserved. The existence or otherwise of SUSY partners is furthermore relevant to the question of inversion: Are open systems uniquely determined by their complex outgoing-wave spectra? © *2001 American Institute of Physics.*
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I. INTRODUCTION

A. Outline

Supersymmetry (SUSY) in quantum field theory[1,2] relates bosons to fermions. Its analog in quantum mechanics[3,4] is interesting in its own right, and relates two (typically one-dimensional) Hamiltonians H and $\tilde{H}$ with the same spectrum of normal modes (NMs), or the same spectrum apart from one state. The classical limit[5] relates a one-parameter family of Hamiltonians $H(\xi)$. Although interest in SUSY quantum mechanics has in recent years been prompted by the analogous and important developments in field theory, the method is essentially the theory of Darboux transformations for second-order linear differential equations[6] and is also closely related to the factorization method.[7]

This paper generalizes SUSY in quantum mechanics to open systems and in particular to their quasinormal modes (QNMs), which are eigenfunctions satisfying the outgoing-wave condition (OWC) at infinity. The generalization itself is straightforward, and we focus on the novel features that ensue. After a brief introduction to open systems and QNMs in the rest of this section, this paper presents three main results.

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First, in the conventional discussion for the Schrödinger equation, spectrum preservation can be conveniently expressed in terms of the number of NMs $n(E)$ for H and $\tilde{n}(E)$ for $\tilde{H}$ at the same energy E, namely, that $n(E)=\tilde{n}(E)$ for all real E except a privileged value E_0 (usually chosen to be $E_0=0$). At this value, the difference is given by the Witten index[3]

$$\Delta(E_0)=n(E_0)-\tilde{n}(E_0), \tag{1.1}$$

which can be $+1$, 0, or -1. For open systems with the OWC, time-reversal invariance is broken, and it is appropriate to consider a Klein–Gordon equation (KGE) instead—in effect replacing $\partial_t \mapsto \partial_t^2$ or $E \mapsto \omega^2$ in the time-independent equation, and distinguishing $+\omega$ from $-\omega$ (since reversing the two converts an outgoing to an incoming wave).[8] Section II shows that the equality of spectrum for the KGE extends to the complex ω-plane except at the two privileged frequencies $\pm\Omega=\pm\sqrt{E_0}$, namely,

$$n(\omega)=\tilde{n}(\omega), \quad \omega \neq \pm\Omega. \tag{1.2}$$

At $\pm\Omega$, one needs to consider

$$\Delta(\pm\Omega)=n(\pm\Omega)-\tilde{n}(\pm\Omega). \tag{1.3}$$

These are again $+1$, 0, or -1, but with $\Delta(\Omega)=-\Delta(-\Omega)$ determined by the asymptotic behavior of the SUSY generator, to be defined below. In other words, under $H \mapsto \tilde{H}$, if a state is removed (added) at Ω, then a state is added (removed) at $-\Omega$. This relationship, which also applies to conservative systems and NMs provided we take the KGE point of view, sharpens the information provided by (1.1).

Secondly, SUSY preserves norms and inner products. However, for outgoing waves the usual norms and inner products are not useful. For example, an outgoing wave of frequency ω goes as $\exp[i\omega(|x|-t)]$ at spatial infinity. With $\mathrm{Im}\,\omega<0$ for QNMs (see Sec. I B), the exponential growth in $|x|$ renders the wave function not normalizable in the usual sense. A generalized norm for QNMs was first introduced by Zeldovich[9] many years ago, and shown to be useful for time-independent perturbation theory (of the *complex* eigenvalues).[10] An associated generalized inner product can also be defined.[11] The time-evolution operator turns out to be symmetric under this product (the analog of self-adjoint). Section III shows that SUSY preserves these generalized norms and inner products—a pleasant surprise, since their construction is totally unrelated to SUSY.

Thirdly, for non-conservative systems, there is no guarantee that the Hamiltonian can be completely diagonalized; in general the best that one can do is to decompose it into Jordan blocks (JBs).[12] Each block j, say of size $M_j \times M_j$, is associated with an eigenfrequency ω_j, with $M_j=1$ being the usual case of a QNM. Section IV shows that SUSY preserves the JB structure: except for $\omega_j=\pm\Omega$, a block of size M_j maps to a block also of size M_j at the same frequency ω_j. In fact, if we generalize the definition of $n(\omega_j)$ to be the order M_j of the block, then the relationship between $n(\omega)$ and $\tilde{n}(\omega)$ [cf. (1.2) and (1.3)] remains valid even for $n,\tilde{n}>1$.

Examples are given in Sec. V and a discussion is presented in Sec. VI, including a sketch of some issues for potentials with tails—which can lead to situations with *negative* n and $\tilde{n}$ that are nevertheless accommodated in the same formalism.

B. Quasinormal modes

In open systems, waves are not confined, but can escape: acoustic waves from a musical instrument, electromagnetic waves from a laser, and linearized gravitational waves from a Schwarzschild background (to infinity and into the horizon). These systems are often described (e.g., in the case of gravitational waves[13]) by the KGE

$$[\partial_t^2-\partial_x^2+V(x)]\phi(x,t)=0, \tag{1.4}$$

or (e.g., in the case of optics[14]) by the closely related[11] wave equation

$$[\rho(x)\partial_t^2 - \partial_x^2]\phi(x,t) = 0. \tag{1.5}$$

This paper deals only with the KGE, both because it is readily related to the Schrödinger equation in terms of which SUSY is usually formulated,[3,4] and also because it (unlike the wave equation) admits NMs which are interesting in the present discussion.

Except for Sec. VI D, we shall assume that $V(x)$ [or $\rho(x)-1$ in the case of the wave equation (1.5)] has finite support on the interval $I=[-a,a]$, which is natural for describing a system of limited extent, surrounded by a trivial medium such as vacuum.

We assume that the loss is only due to the boundary conditions. In particular, the potential V is real. Absorption may be described by a complex V, but causality then requires dispersion; the necessary generalization[15] will not be discussed here.

Among the solutions of (1.4), we consider the space Γ of states satisfying the OWC. We leave the time-domain definition to Sec. III; in the frequency domain, a function is in Γ if

$$\phi(x) \sim e^{+i\omega|x|}, \quad |x| \to \infty. \tag{1.6}$$

Because V is trivial outside I, the asymptotic conditions (1.6) can be stated at $x=\pm a$ instead:

$$\frac{\phi'(x)}{\phi(x)} = \pm i\omega, \quad x = \pm a. \tag{1.7}$$

The imposition of two boundary conditions in (1.7) forces the eigenvalues to be discrete, and these fall into two classes. First, there could be bound states or NMs;[16] these must (from the Schrödinger point of view) have $E=\omega^2<0$, and hence ω is purely imaginary. Since bound-state wave functions vanish at infinity, (1.6) dictates that $\mathrm{Im}\,\omega>0$. Second, there could be QNMs with complex eigenvalues ω^2. Because these waves escape, ϕ decreases, so $\mathrm{Im}\,\omega<0$.[17] Provided $\mathrm{Re}\,\omega\neq 0$, they occur in pairs: $\omega_{-j}=-\omega_j^*$, as is readily shown by conjugating the defining equation and boundary conditions. Those with $\mathrm{Re}\,\omega=0$ need not be paired; these *zero modes*[18] will be of particular importance below. Consider the potential shown by the broken line in Fig. 1(a); its NMs and QNMs are shown in Fig. 1(b). In this example, there is one NM (triangle) and a sequence of QNMs (crosses), including a zero mode. In contrast to the Schrödinger formulation, the use of the KGE and the introduction of Γ allows NMs and QNMs to be discussed together—and at least in this example the latter manifestly carry much richer information.

Even though QNM eigenfunctions are not square-integrable and do not form a conventional Hilbert space, they are useful for analyzing outgoing waves. Importantly, the complex QNM frequencies are often directly observable: e.g., the central frequency and width of an optical line observed from a laser cavity, or the rates of repetition and decay of a gravitational-wave signal that may within the next decade be detected by instruments such as LIGO.[19] In fact, the spectrum is often so rich that, under some broad conditions, namely, that $V(x)$ vanishes outside $[-a,a]$ and has singularities at $x=\pm a$, the eigenstates ϕ_j of Γ are *complete* for $x\in I$,[20] so that for $t\geqslant 0$ the observed wave signal can be represented as[21]

$$\phi(x,t) = \sum_{j\in\Gamma} a_j \phi_j(x) e^{-i\omega_j t}. \tag{1.8}$$

In cases where the ϕ_j's are not complete, it may still be possible to characterize the remainder, which could be, for example, a power law in t for long times.[22,23] Moreover, when the eigenstates are complete, one can set up a formalism that closely parallels the conservative case (see Refs. 11 and 24 and Sec. III B). One can even second-quantize using these eigenstates as a basis (e.g., to discuss thermal effects and atom–field interactions in an optical cavity).[25] These developments have been reviewed.[26] We shall see that much of the mathematical structure is preserved under SUSY.

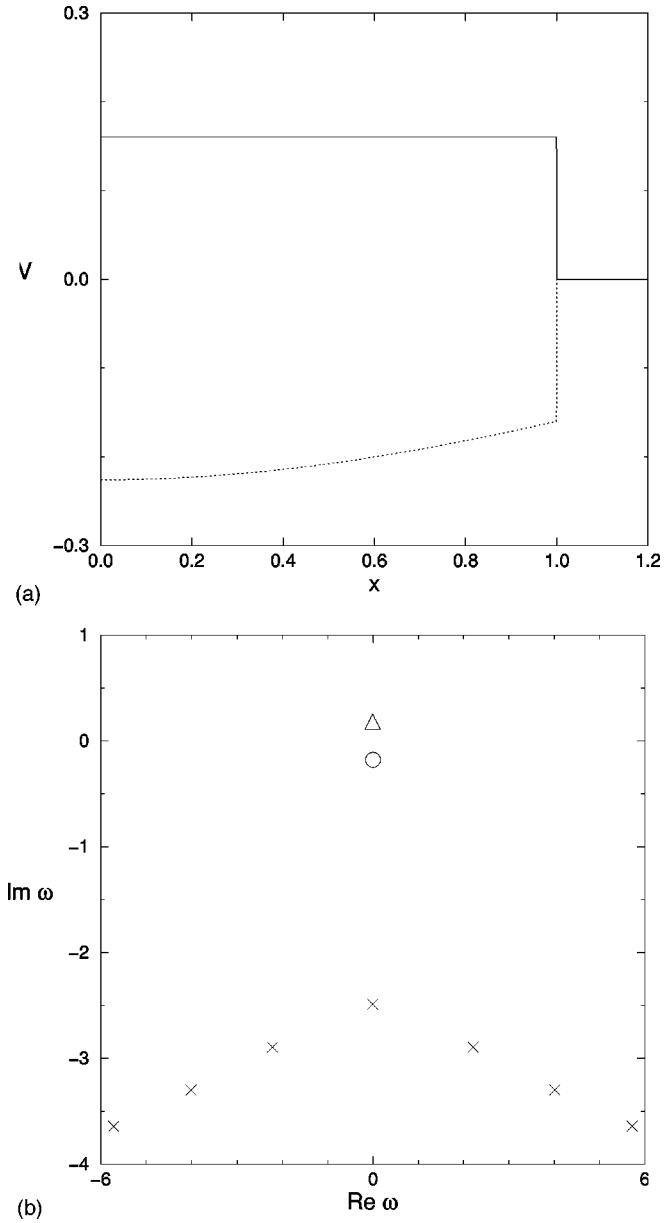

FIG. 1. (a) A square-barrier potential V (solid line) and its SUSY partner potential $\tilde{V}$ (broken line). Both potentials are symmetric and only the $x>0$ part is shown. The SUSY transformation is constructed by using the state at $\Omega=\omega_1=-0.181i$ [circle in (b)] as the generator. (b) The complex ω-plane showing the QNMs common to both potentials (crosses); the mode present only in V (circle), which corresponds to the generator Φ; and the mode present only in $\tilde{V}$ (triangle), which corresponds to $\tilde{\Phi}=\Phi^{-1}$.

II. FORMALISM

A. Supersymmetric quantum mechanics

In this paper we consider SUSY in the one-dimensional KGE (1.4), and especially in the corresponding eigenvalue problem

$$H\phi_j(x)=\omega_j^2\phi_j(x), \tag{2.1}$$

where

$$H = -\partial_x^2 + V(x). \tag{2.2}$$

The boundary conditions will be specified later. Insofar as the interest centers on the time-independent problem (2.1) and the spectrum, the Schrödinger equation, to which reference is usually made,[3,4] is included if we simply relabel $\omega^2 \mapsto E$.

If there exists another system

$$\tilde{H} = -\partial_x^2 + \tilde{V}(x), \tag{2.3}$$

with the same spectrum (or the same spectrum apart from one state), and moreover if the states in the two systems are related by

$$\tilde{\phi}(x) = A\phi(x), \tag{2.4}$$

where

$$\begin{aligned} A &= \partial_x + W(x), \\ -A^\dagger &= \partial_x - W(x), \end{aligned} \tag{2.5}$$

then the two systems are said to be SUSY partners. In particular, if $\phi_j(x)$ is an eigenfunction of H, then $\tilde{\phi}_j(x)$ (provided it does not vanish) is an eigenfunction of $\tilde{H}$ with the same eigenvalue. Normalization is deferred to Sec. III.

In order for (2.4) to preserve the spectrum, one needs

$$AH = \tilde{H}A, \tag{2.6}$$

from which it follows that:

$$\begin{aligned} V(x) &= W(x)^2 - W'(x) + \Omega^2, \\ \tilde{V}(x) &= W(x)^2 + W'(x) + \Omega^2, \end{aligned} \tag{2.7}$$

with $W(x)$ (called the SUSY potential) as in (2.5) and for some constant Ω^2. Since both V and $\tilde{V}$ have to be real, W and Ω^2 are also real. Moreover, the Hamiltonians can be represented as

$$\begin{aligned} H &= A^\dagger A + \Omega^2, \\ \tilde{H} &= AA^\dagger + \Omega^2. \end{aligned} \tag{2.8}$$

The two partner systems can be put into one linear space by introducing Pauli spinors, with the SUSY Hamiltonian $H_S = (-\partial_x^2 + W^2) \otimes \mathbb{1} - W' \otimes \sigma_z = \mathrm{diag}(H - \Omega^2, \tilde{H} - \Omega^2)$ and the supercharges $Q = A\sigma_-$, $Q^\dagger = A^\dagger \sigma_+$ satisfying the commutation and anticommutation relations: $\{Q, Q^\dagger\} = H_S$ and $\{Q, Q\} = \{Q^\dagger, Q^\dagger\} = [Q, H_S] = [Q^\dagger, H_S] = 0$.

Upon reversing the sign of W, (a) $V \leftrightarrow \tilde{V}$ [cf. (2.7)], and (b) $A \leftrightarrow -A^\dagger$ [cf. (2.5)]; thus the mapping from $\tilde{H}$ back to H is (up to a sign) achieved by $A^\dagger$. Note however that the mapping is the "inverse" only in a loose sense: $A^\dagger A$ is not the identity but $H - \Omega^2$ [cf. (2.8)].

We may regard (2.7) as a Riccati equation for W in terms of the given V. For $|x| > a$, both V and $\tilde{V}$ vanish, so $W^2 = -\Omega^2$. The first-order Riccati equation for W can satisfy two boundary conditions (at $x = \pm a$) only at special values of Ω^2; this condition becomes familiar if we define a generator $\Phi(x)$ by

$$W(x) = -\frac{\Phi'(x)}{\Phi(x)}. \tag{2.9}$$

Then (2.7) implies

$$H\Phi(x) = \Omega^2\Phi(x). \tag{2.10}$$

B. Boundary conditions

All the above may be regarded as a review of the familiar SUSY formalism for the Schrödinger equation[3,4] if we put $E=\omega^2$, $E_0=\Omega^2$ and in particular shift $V(x)$ so that $E_0=0$. Conventionally the discussion refers to wave functions which vanish at infinity (or, more precisely, are square-integrable). Here we consider *all* eigenfunctions in Γ, including both NMs and QNMs, with the former in the upper and the latter in the lower half of the frequency plane.

We should check immediately that $\phi\in\Gamma$ implies $\tilde{\phi}\in\Gamma$. For $x>a$, if $\phi(x)=Ce^{i\omega x}$ then $\tilde{\phi}(x)=A\phi(x)=(i\omega+W_+)Ce^{i\omega x}$, where

$$W(x=\pm a)=W_\pm \tag{2.11}$$

are the constant values for $x>a$ and $x<-a$, respectively. Thus ϕ and $\tilde{\phi}$ always satisfy the same type of boundary conditions, and the number of eigenstates in Γ is preserved under SUSY: $n(\omega)=\tilde{n}(\omega)$ [cf. (1.2)]—except when A or $A^\dagger$ destroys a state, to be discussed below.

C. Generator

The various SUSY transformations are related, in a one-to-one manner, to solutions of (2.10) for the generator Φ. First, suppose $\Omega^2>0$, so that Ω is real. Then outside I, Φ is oscillatory: either complex (e.g., $e^{i\Omega x}$), inadmissible since it leads to a complex W; or real (e.g., $\sin\Omega x$), inadmissible since its nodes lead to singularities in W. Thus, $\Omega^2<0$, and we denote $K\equiv|\Omega|$.

At each spatial extreme ($|x|>a$), Φ is in general a sum of increasing and decreasing functions, i.e.,

$$\Phi(x)=ce^{K|x|}+de^{-K|x|}. \tag{2.12}$$

If both $c,d\neq 0$ (to be called the mixed type), then the logarithmic derivative is (e.g., for $x>a$)

$$W(x)=-K+\frac{2dK}{c}e^{-2Kx}+\cdots, \tag{2.13}$$

so that $\tilde{V}=V+2W'$ acquires an exponential tail. (In the special case $\Omega=0$, the tail is not exponential but asymptotically inverse-square.) Thus, if we insist that $\tilde{V}$ also has finite support, the mixed type is not allowed and at each extreme Φ must be either purely decreasing ($\Phi\propto e^{-K|x|}$, denoted as D) or purely increasing ($\Phi\propto e^{K|x|}$, denoted as I). Outside I, the logarithmic derivative is then exactly $\pm K$, so $W'=0$, implying $\tilde{V}=0$. When both extremes are considered together, Φ must be one of three types, conveniently labeled with the parameter

$$\chi=\tfrac{1}{2}[\mathrm{sign}(W_+)-\mathrm{sign}(W_-)], \tag{2.14}$$

where $\chi=+1$, -1, and 0, respectively, for the DD, II, and DI/ID cases (in obvious notation). In the DI/ID case, the generator is purely incoming from one extreme and purely outgoing to the other, hence is a total-transmission mode (TTM). The relaxation to allow exponential tails for V and/or $\tilde{V}$ will be briefly mentioned in Sec. VI D.

The generator is annihilated by SUSY: $A\Phi=0$, trivially from (2.5) and (2.9). Furthermore, since reversing the sign of W interchanges the partners [cf. below (2.8)], in view of (2.9) the

transformation from $\tilde{H}$ back to H is generated by $\tilde{\Phi}=\Phi^{-1}$; this is guaranteed to be an eigenfunction of $\tilde{H}$, also with eigenvalue Ω^2. (Despite the notation, $\tilde{\Phi}$ is not the SUSY partner of Φ: $\tilde{\Phi} \neq A\Phi$.) The boundary conditions for $\tilde{\Phi}=\Phi^{-1}$ interchange D and I, so the reverse transformation is characterized by $\tilde{\chi}=-\chi$.

These observations allow a simple statement of the changes in the number of states when $H \mapsto \tilde{H}$. If $\chi=1$ [cf. below (2.14)], an NM Φ is destroyed at $\Omega=iK$ [$\Delta(iK)=1$] and a QNM $\tilde{\Phi}$ is created at $-\Omega=-iK$ [$\Delta(-iK)=-1$]. If $\chi=-1$, a QNM Φ is destroyed at $\Omega=-iK$ [$\Delta(-iK)=1$] and an NM $\tilde{\Phi}$ is created at $-\Omega=iK$ [$\Delta(iK)=-1$]. If $\chi=0$, no eigenstates of Γ are created or destroyed [$\Delta(iK)=\Delta(-iK)=0$], since Φ and $\tilde{\Phi}$ are TTMs rather than NMs or QNMs. Thus, all three cases satisfy

$$\Delta(iK)=-\Delta(-iK)=\chi, \tag{2.15}$$

where we emphasize the convention $\Omega=\pm iK$ with $K>0$. The cases $\chi=\pm 1$ lead to Hamiltonians whose spectra in Γ differ by one state (said to be essentially isospectral), whereas the case $\chi=0$ leads to Hamiltonians whose spectra in Γ are identical (said to be strictly isospectral).

These remarks provide a more complete picture of the mapping of eigenstates in Γ under SUSY: States do not simply appear or disappear, but are mapped to the mirror point in the complex plane.

Not all NMs, QNMs, or TTMs are eligible as the generator. First, Ω^2 must be real, which restricts QNMs to zero modes. Second, Φ cannot have nodes, or else W would acquire singularities. In the case of NMs, this restricts Φ to the ground state. For QNMs, nodes are not required by general theorems. At least for repulsive potentials, each eigenfunction can have *at most* one node or antinode; thus, for a symmetric repulsive V, even-parity eigenfunctions can have no nodes. There is consequently much more freedom in choosing a QNM (as opposed to an NM) as the generator. Some general statements concerning nodes in QNMs are given in the Appendix.

III. ORTHONORMALITY

A. Orthonormality for NMs

For conservative systems, SUSY preserves orthonormality. There are two issues: Orthogonality is preserved because the transformed NMs are eigenvectors of the self-adjoint operator $\tilde{H}$; and normalization is preserved if the transformation is changed to

$$\phi_j \mapsto \underline{\tilde{\phi}}_j = N_j \tilde{\phi}_j = N_j A \phi_j, \tag{3.1}$$

with

$$N_j^{-2}=\frac{\langle \tilde{\phi}_j | \tilde{\phi}_j \rangle}{\langle \phi_j | \phi_j \rangle}. \tag{3.2}$$

Equation (3.1) applies to each eigenstate j other than the generator Φ itself, namely, the ground state. It is readily shown that $N_j^{-2}=\omega_j^2-\Omega^2$, a result that can also be read off as a special case of the derivation below for states in Γ. Since $\omega_j^2-\Omega^2$ is the eigenvalue of $A^\dagger A$ [see (2.8)], (3.1) can be written in the operator form

$$\phi \mapsto \underline{\tilde{\phi}} = A(A^\dagger A)^{-1/2}\phi, \tag{3.3}$$

valid for any state ϕ, not just frequency eigenfunctions. (This and similar formulas below are restricted to the subspace orthogonal to Φ.) This makes it formally easy to verify the preservation of inner products:

$$\langle \underset{\sim}{\psi} | \underset{\sim}{\phi} \rangle = \langle \psi | (A^\dagger A)^{-1/2} A^\dagger A \, (A^\dagger A)^{-1/2} | \phi \rangle = \langle \psi | \phi \rangle. \tag{3.4}$$

However, when operating on a general wave function ϕ, the factor $(A^\dagger A)^{-1/2}$ can only be evaluated by projecting ϕ onto the eigenfunctions, and scaling each component by N_j. Thus, in practice, the significant result is the evaluation of this factor. We now generalize these concepts to states in Γ, in particular QNMs.

B. Normalization and inner product for QNMs

It is necessary to digress and review the concepts of orthogonality and normalization for QNMs. The central issue is that with the OWC, H is *not* self-adjoint in the usual sense, and different QNMs are *not* orthogonal under the usual inner product. Likewise, the norm $\int |\phi_j|^2 dx$ is divergent, since the wave function grows exponentially at infinity.

An appropriate normalizing factor for QNMs was first introduced by Zeldovich,[9] and later generalized and applied to other situations,[10] including models of linearized waves propagating on a Schwarzschild background:[27]

$$(\phi_j, \phi_j) = 2\omega_j \int_{-a}^{a} \phi_j(x)^2 \, dx + i[\phi_j(-a)^2 + \phi_j(a)^2]. \tag{3.5}$$

This expression goes as ϕ_j^2 rather than $|\phi_j|^2$, and is in general not real. The limits of the integral and the surface terms can be shifted from $\pm a$ to any $b_\pm$, where $\pm b_\pm > a$, without affecting the value of (3.5). This definition also applies to NMs: The surface terms vanish if we take $b_\pm \to \pm\infty$, recovering the conventional norm apart from a factor of $2\omega_j$. In the QNM case, (3.5) is the correct normalizing factor in the sense that, e.g., under a perturbation $V \mapsto V + \Delta V$, the complex QNM eigenvalues change by

$$\Delta(\omega_j^2) = \frac{\int \phi_j(x)^2 \Delta V(x) dx}{(\phi_j, \phi_j)}. \tag{3.6}$$

Since one no longer has positivity, there is the possibility that $(\phi_j, \phi_j) = 0$. This exceptional case can be separately taken care of,[28] and some interesting aspects are dealt with in Sec. IV.

To go beyond the normalizing factor and discuss an analog of orthogonality, one has to first regard each state as a two-component vector $\boldsymbol{\psi} = (\psi^1, \psi^2)^{\mathrm{T}} \equiv (\psi, \partial_t \psi)^{\mathrm{T}}$, which is most easily motivated by noticing that the dynamics requires two sets of initial data. The space Γ is then defined as all $\boldsymbol{\psi}$ satisfying

$$\psi^2(\pm a) = \mp \partial_x \psi^1(\pm a). \tag{3.7}$$

For an eigenstate, $\boldsymbol{\phi}_j = (\phi_j, -i\omega_j \phi_j)^{\mathrm{T}}$, and (1.7) would follow from (3.7).

In terms of the two-component vector, one can define a bilinear map[11,26]

$$(\boldsymbol{\psi}, \boldsymbol{\phi}) = i\left\{ \int_{-a}^{a} [\psi^1(x)\phi^2(x) + \psi^2(x)\phi^1(x)] dx + [\psi^1(-a)\phi^1(-a) + \psi^1(a)\phi^1(a)] \right\}, \tag{3.8}$$

to take the place of the usual inner product. For an eigenfunction, $(\boldsymbol{\phi}_j, \boldsymbol{\phi}_j)$ agrees with (3.5). The dynamics can be written in the first-order form $i\partial_t \boldsymbol{\phi} = \mathcal{H}\boldsymbol{\phi}$, with

$$\mathcal{H} = i \begin{pmatrix} 0 & 1 \\ \partial_x^2 - V & 0 \end{pmatrix}. \tag{3.9}$$

Importantly, $\mathcal{H}$ is symmetric:

$$(\mathcal{H}\boldsymbol{\psi},\boldsymbol{\phi})=(\boldsymbol{\psi},\mathcal{H}\boldsymbol{\phi}), \tag{3.10}$$

in the proof of which the surface terms generated upon integration by parts exactly cancel against those in (3.8). The relation (3.10) is the analog of self-adjointness, and leads to the usual proof that for two eigenvectors,

$$(\boldsymbol{\phi}_k,\boldsymbol{\phi}_j)=0 \tag{3.11}$$

whenever $\omega_k\neq\omega_j$. Provided that $(\boldsymbol{\phi}_j,\boldsymbol{\phi}_j)\neq 0$,[28] one can normalize these eigenfunctions in the usual way, i.e., by requiring (3.11) to be $2\omega_k\delta_{kj}$ in general [cf. (3.5) for this factor]. We henceforth refer to this property as orthonormality [and to (3.11) alone as orthogonality]. It also follows trivially that, provided this orthonormal system is complete (which is the case under fairly broad assumptions; see Sec. I B), time evolution is given by

$$\boldsymbol{\phi}(t)=\sum_j a_j\boldsymbol{\phi}_j e^{-i\omega_j t}, \tag{3.12}$$

generalizing (1.8) to two components, and

$$a_j=\frac{(\boldsymbol{\phi}_j,\boldsymbol{\phi}(t=0))}{(\boldsymbol{\phi}_j,\boldsymbol{\phi}_j)}. \tag{3.13}$$

The preservation of orthonormality under SUSY should therefore be sought in terms of the bilinear map (3.8).

C. Normalized SUSY transformation for QNMs

We first present a derivation of orthonormality that does not explicitly require the two-component formalism. With orthogonality already guaranteed by (3.11), it remains to compute the normalizing factor

$$(\tilde{\phi}_j,\tilde{\phi}_j)=2\omega_j\int_{-a}^{a}[(\partial_x+W)\phi_j]^2dx+i[\tilde{\phi}_j(-a)^2+\tilde{\phi}_j(a)^2]. \tag{3.14}$$

Integrate by parts to convert $(\partial_x\phi)^2$ to $-(\partial_x^2\phi)\phi$ plus a surface term, express the second derivative in terms of $V-\omega_j^2$ by means of the eigenvalue equation, and write the potential as $V=W^2-W'+\Omega^2$. Then, apart from a term $\propto\omega_j^2-\Omega^2$, the integrand becomes a total derivative $\partial_x(W\phi^2)$. Using $W(\pm a)^2=-\Omega^2$ and $\partial_x\phi_j(\pm a)=\pm i\omega_j\phi_j(\pm a)$ then leads to

$$\frac{(\tilde{\phi}_j,\tilde{\phi}_j)}{(\phi_j,\phi_j)}=\omega_j^2-\Omega^2. \tag{3.15}$$

Incidentally, the conservative case (nodal conditions at the ends of the interval[16]) is recovered by simply dropping all surface terms.

Since the ratio (3.15) is the eigenvalue of $A^\dagger A$, we can again write the normalized transformation for each eigenfunction as (3.3).

D. SUSY for two-component form

For eigenstates, the two components are trivially related, but in order to perform SUSY transformations on general wave functions in Γ (e.g., given a time-dependent state, to find its partner at all times), the second component must be considered explicitly.

Since SUSY must commute with time evolution and $\phi^2=\partial_t\phi^1$, both components must transform in the same way. Thus, the (unnormalized) SUSY transformation on two-component vectors is $\mathcal{A}=\mathrm{diag}(A,A)$, which satisfies

$$(\mathcal{A}\boldsymbol{\psi},\boldsymbol{\phi})=(\boldsymbol{\psi},\mathcal{A}^\dagger\boldsymbol{\phi}), \tag{3.16}$$

where $\mathcal{A}^\dagger\equiv\mathrm{diag}(A^\dagger,A^\dagger)$. In deriving (3.16), one has to integrate by parts: ∂_x changes sign so that $\mathcal{A}$ turns into $\mathcal{A}^\dagger$. The surface terms are seen to work out by using, e.g., $\phi^2(a)=\partial_t\phi^1(a)=-\partial_x\phi^1(a)$, and the known values of $W_\pm$. Note that $\mathcal{A}^\dagger\mathcal{A}=(H-\Omega^2)\otimes\mathbb{1}$, $\mathcal{A}\mathcal{A}^\dagger=(\tilde{H}-\Omega^2)\otimes\mathbb{1}$, i.e., the products do not relate to the two-component $\mathcal{H}$.

With (3.16), it is straightforward to show that the normalized SUSY transformation

$$\boldsymbol{\phi}\mapsto\tilde{\boldsymbol{\phi}}=\mathcal{A}(\mathcal{A}^\dagger\mathcal{A})^{-1/2}\boldsymbol{\phi}, \tag{3.17}$$

defined on the subspace orthogonal to $\boldsymbol{\Phi}$, preserves the bilinear map, in a manner that exactly parallels (3.4). In the exceptional case of SUSYs that generate a doubled state (see Sec. IV), the subspace has to exclude the *two* states on which $H-\Omega^2$ vanishes.

The linear-space structure for open systems (e.g., the replacement of inner products by bilinear maps) has an intrinsic geometric meaning for all outgoing states, not just QNMs.[29] It is therefore pleasing that this structure is preserved by SUSY, a superficially unrelated concept.

IV. JORDAN BLOCKS

A key concept in SUSY is the preservation of the spectrum. However, dissipative systems (such as waves satisfying the OWC) admit a spectral property not found for conservative systems. In terms of the Wronskian $J(\omega)$ to be defined below, this is exhibited as an Mth-order zero ($M>1$). Such a multiple zero emerges naturally when M QNM eigenvalues coalesce as system parameters are tuned, so that $M-1$ eigenvectors are "lost"[30] and must be replaced by other degrees of freedom. Thus, the Hamiltonian cannot be written as a diagonal matrix in the (biorthogonal) basis of eigenstates, but can only be decomposed into (Jordan) blocks[12] of size $M\times M$. When this happens, $(\boldsymbol{\phi}_j,\boldsymbol{\phi}_j)$ will vanish for some j, invalidating the formalism in Sec. III [see, e.g., (3.6) and (3.13)]. These issues have been discussed in detail with reference to waves in open systems.[28]

The simplest example of a JB (with $M=2$) is a harmonic oscillator going through critical damping. The eigenvalues $\omega_\pm=\pm\omega_\mathrm{R}-i\gamma$ coalesce when $\omega_\mathrm{R}\to0$. With one eigenvalue lost, the dynamics is not given by a sum of eigenfunctions with time dependence $\exp(-i\omega_\pm t)$, but by only *one* such eigenfunction, plus another term whose time dependence carries a prefactor t.

Our purpose in this Section is to establish that SUSY maps a JB in H into a JB in $\tilde{H}$, preserving the order M except when the eigenvalue coincides with $\pm\Omega$.

A. Wronskian

In this subsection we introduce the Wronskian $J(\omega)$, define JBs in terms of its multiple zeros, and describe the mapping of JBs under SUSY by a relation between $J(\omega)$ and its counterpart $\tilde{J}(\omega)$.

In the original system H, define solutions of the wave equation $f(\omega,x)$ and $g(\omega,x)$ satisfying the boundary conditions $f(\omega,-a)=1$, $f'(\omega,-a)=-i\omega$, $g(\omega,a)=1$, $g'(\omega,a)=i\omega$, where $'=\partial_x$. The function values are arbitrary normalizations, while the derivatives impose the OWC on the left and right, respectively. An eigenstate $\boldsymbol{\phi}_j$ in Γ satisfies the boundary condition on *both* the left (as for f) and the right (as for g): $\boldsymbol{\phi}_j\propto f(\omega_j,x)\propto g(\omega_j,x)$. Thus, the zeros of the (position-independent) Wronskian

$$J(\omega)=f'(\omega,x)g(\omega,x)-f(\omega,x)g'(\omega,x) \tag{4.1}$$

identify the eigenvalues in Γ. It can be shown [see (4.7) below] that $(\boldsymbol{\phi}_j,\boldsymbol{\phi}_j)\propto dJ(\omega_j)/d\omega$, so an Mth-order zero of $J(M>1)$ corresponds to the generalized norm being zero, and is precisely the JB phenomenon that we wish to investigate.

It is natural to generalize the definition of $n(\omega)$ to be the order of the zero, viz.,

$$n(\omega)=\frac{1}{2\pi i}\oint\frac{dJ(\omega')/d\omega'}{J(\omega')}d\omega', \tag{4.2}$$

on a contour of winding number $+1$ enclosing ω. This definition makes it clear that the total number of states (but *not* necessarily of eigenstates) within a contour is preserved under continuous changes of the system parameters. We note for future reference (see Sec. VI D) that poles of J (which can only occur if V does not have finite support) count as negative values of n.

Now consider the analogous construction in the partner system $\tilde{H}$, obtained, for example, by using an NM Φ of H as the generator, i.e., for $\chi=1$. By our convention, Φ is associated with a frequency $\Omega=iK$, and $W_{\pm}=\mp i\Omega$. The SUSY transformation gives[31]

$$\begin{aligned}\tilde{f}(\omega,x)&=(\partial_x+W)f(\omega,x)\\ \tilde{g}(\omega,x)&=(\partial_x+W)g(\omega,x),\end{aligned} \tag{4.3}$$

leading to the Wronskian

$$\tilde{J}^{\mathrm{u}}(\omega)=\tilde{f}'(\omega,x)\tilde{g}(\omega,x)-\tilde{f}(\omega,x)\tilde{g}'(\omega,x). \tag{4.4}$$

When (4.4) is written out using (4.3), some terms cancel by using $J'=0$, the second derivatives can be eliminated by the defining equation, and V is expressed in terms of W and Ω^2. Some arithmetic then leads to

$$\tilde{J}^{\mathrm{u}}(\omega)=(\omega^2-\Omega^2)\,J(\omega). \tag{4.5}$$

This Wronskian is however unnormalized (as indicated by the superscript), since only $C\tilde{f}$ and $D\tilde{g}$ satisfy the normalization conventions at $-a$ and $+a$, respectively, where $C=-D=i(\omega-\Omega)^{-1}$. Thus the normalized Wronskian $\tilde{J}(\omega)=CD\tilde{J}^{\mathrm{u}}(\omega)$ is

$$\tilde{J}(\omega)=\frac{\omega+\Omega}{\omega-\Omega}J(\omega). \tag{4.6}$$

The central result (4.6) neatly summarizes the correspondence between the two spectra for $\chi=1$. [Similar formulas for the other cases can all be consolidated by changing $\Omega\mapsto i\chi K$ in (4.6), and will not be separately discussed.] (a) For $\omega\neq\pm\Omega$, the spectra of H and $\tilde{H}$ are the same: A JB of order M in H maps to a JB also of order M in $\tilde{H}$ at the same frequency. This should be no surprise since up to the point of coalescence (for $M\geqslant 2$), the eigenvalues of the two systems are guaranteed (cf. Sec. II) to be in one-to-one correspondence; in a sense, the result here merely demonstrates that the limit is not singular. (b) Moreover, *at* the special frequencies $\pm\Omega$, M states at Ω (of which only *one* is an eigenstate) are mapped into $M-1$ states at Ω plus one state at $-\Omega$. In other words, we recover (2.15) even for JBs, i.e., even when $n,\tilde{n}>1$. Anticipating the possibility of poles in J (cf. Sec. VI D), we note that (4.6) implies that such poles are also preserved under SUSY, and would be accommodated by (1.2), (1.3), and (2.15) with negative n, $\tilde{n}$.

Incidentally, (3.15) on the change in normalization under SUSY follows simply from (4.5), since the bilinear map is related to the Wronskian by[26,32]

$$(f(\omega_j),g(\omega_j))=-\left[\frac{dJ(\omega)}{d\omega}\right]_{\omega_j}. \tag{4.7}$$

B. Doubling of states by SUSY

We have seen that (say for $\chi=1$) one has $\tilde{n}(-iK)-n(-iK)=1$. Where this increases from 0 to 1, the situation is straightforward—a QNM is created. When the increase is from 1 to 2, the situation is more subtle and merits a detailed examination. [The general case where this increases from M to $M+1$ ($M\geqslant 1$) will not be shown.]

Consider a system H with an NM Φ at $\Omega=iK$ and accidentally also a QNM Ψ_j at $-\Omega'\approx-\Omega$. If $\Omega'\neq\Omega$, there are *two* corresponding QNMs in the $\tilde{H}$-system, namely, $\tilde{\Phi}=\Phi^{-1}$ at $-\Omega$ and $\tilde{\Psi}_j=A\Psi_j$ at $-\Omega'$. Now tune the parameters of H so that $\Omega'\to\Omega$; in the limit we must have $\tilde{\Psi}_j\propto\tilde{\Phi}$,[28,30] as is readily verified. The proportionality constant can be evaluated by

$$\frac{\tilde{\Psi}_j}{\tilde{\Phi}}=\frac{\tilde{\Psi}_j(-a)}{\tilde{\Phi}(-a)}=2i\Omega\Psi_j(-a)\Phi(-a)$$

$$=\frac{\tilde{\Psi}_j(a)}{\tilde{\Phi}(a)}=-2i\Omega\Psi_j(a)\Phi(a). \tag{4.8}$$

The agreement of these two expressions can also be seen without invoking SUSY. One notes that $\mathbf{\Phi}$ and $\mathbf{\Psi}_j$, being eigenfunctions of $\mathcal{H}$ with distinct eigenvalues, are orthogonal. In the bilinear map, the integral term vanishes because the frequencies are opposite, leaving only the surface terms. Thus one finds $0=(\mathbf{\Psi}_j,\mathbf{\Phi})=i[\Psi_j(-a)\Phi(-a)+\Psi_j(a)\Phi(a)]$.

Now the frequency $-\Omega$ in $\tilde{H}$ must be associated with a doubled state. This can be seen in two ways: (a) Until the limit $\Omega'=\Omega$, there are two distinct states; (b) from the key relation (4.6), $\tilde{J}$ has a second-order zero. With the two QNMs collapsed into one, there has to be another basis vector, to which we now turn.

Using the normalization of f, one has $\Psi_j(x)=\Psi_j(-a)f(-\Omega,x)$, implying $\tilde{\Psi}_j(x)=\Psi_j(-a)\tilde{f}(-\Omega,x)$. [Analogous formulas for Φ and $\tilde{\Phi}$ follow from (4.8).] The double zero of $\tilde{J}(\omega)$ at $\omega=-\Omega$ means that $\tilde{f}(\omega,x)$ satisfies the OWC at $x=a$ not only *at* $\omega=-\Omega$, but also to first order away from the zero. This makes it plausible that, in the QNM expansion, $\partial_\omega\tilde{f}(\omega,x)|_{-\Omega}$ takes the place of the ''missing'' eigenfunction when $\tilde{\Phi}$ and $\tilde{\Psi}_j$ coincide, which has been confirmed in detail.[28] One thus defines, for an arbitrary α, a pair of functions $\tilde{\Psi}_{j,n}$, where $n=0,1$ is an intra-block index:

$$\tilde{\Psi}_{j,0}(x)=\tilde{\Psi}_j(x),$$

$$\tilde{\Psi}_{j,1}(x)=\Psi_j(-a)\partial_\omega\tilde{f}(\omega,x)|_{-\Omega}+\alpha\tilde{\Psi}_j(x), \tag{4.9}$$

and the second function satisfies

$$(\tilde{H}-\Omega^2)\tilde{\Psi}_{j,1}=-2\Omega\tilde{\Psi}_{j,0}. \tag{4.10}$$

Using this, one verifies that an outgoing solution is given by $\tilde{\Psi}_{j,1}(t)\equiv(\tilde{\Psi}_{j,1}-it\tilde{\Psi}_{j,0})e^{i\Omega t}$. This time dependence shows that the associated second component should be $\tilde{\Psi}^2_{j,1}=-i(-\Omega\tilde{\Psi}_{j,1}+\tilde{\Psi}_{j,0})$. The prefactor t and its counterpart if any in the H-system will be further explored below.

Next consider the bilinear map and normalization for these functions. For a double zero one always has $(\tilde{\mathbf{\Psi}}_{j,0},\tilde{\mathbf{\Psi}}_{j,0})=0$; cf. (4.7) [a choice of α in (4.9) such that also $(\tilde{\mathbf{\Psi}}_{j,1},\tilde{\mathbf{\Psi}}_{j,1})=0$ would be useful in wave function expansions]. The JB is normalized by one overall factor, the bilinear map between the two basis states[28]

$$\frac{(\tilde{\mathbf{\Psi}}_{j,1},\tilde{\mathbf{\Psi}}_{j,0})}{(\mathbf{\Psi}_j,\mathbf{\Psi}_j)}=\left[\frac{-\frac{1}{2}d^2\tilde{J}^{\mathrm{u}}(\omega)/d\omega^2}{-dJ(\omega)/d\omega}\right]_{-\Omega}=-2\Omega, \tag{4.11}$$

where in the numerator we have used the result analogous to (4.7) for a double zero.

Finally the reverse transform[33] generated by $-A^\dagger$ satisfies the following properties. (a) $A^\dagger\tilde{\Psi}_{j,0}\propto A^\dagger\tilde{\Phi}=0$. (b) Hence in $A^\dagger\tilde{\Psi}_{j,1}(t)$, the term $\propto te^{i\Omega t}$ is annihilated. (c) The remaining term in $A^\dagger\tilde{\Psi}_{j,1}$ is $c\Psi_j$, readily seen by observing that

$$(H-\Omega^2)(A^\dagger\tilde{\Psi}_{j,1})=A^\dagger(\tilde{H}-\Omega^2)\tilde{\Psi}_{j,1}=A^\dagger(-2\Omega\tilde{\Psi}_{j,0})=0, \tag{4.12}$$

so that $A^\dagger\tilde{\Psi}_{j,1}$ is an eigenfunction of H with eigenvalue Ω^2. In particular, the time dependence is $e^{i\Omega t}$ without any prefactor t. A straightforward computation shows that $c=-2\Omega$.

Since $A^\dagger A$ is not the identity, two different states in the H-system can be associated with $\tilde{\Psi}_{j,1}$. The first is $A^\dagger\tilde{\Psi}_{j,1}$ as discussed above. The second is the SUSY pre-image of $\tilde{\Psi}_{j,1}$ under A, which is readily found by noticing that[34]

$$\tilde{\Psi}_{j,1}(x)=\Psi_j(-a)\times\partial_\omega[(\partial_x+W)f(\omega,x)]_{-\Omega}=A\,\Psi_j(-a)\partial_\omega f(\omega,x)|_{-\Omega}. \tag{4.13}$$

However, $\Psi_j(-a)\partial_\omega f(\omega,x)|_{-\Omega}$ is *not* outgoing to $+\infty$, since $J(\omega)$ only has a first-order zero at $-\Omega$, and consequently $f(\omega,x)$ satisfies the OWC at $x=+a$ only *at* $-\Omega$, but not to first order away from it.

These remarks completely resolve the puzzle related to the prefactor t in the time evolution in the $\tilde{H}$-system. Namely, of the two corresponding wave functions of H, one has an exponential time dependence, while the other is not in Γ.

V. EXAMPLES

The formalism developed in this paper is general, in that given $V(x)$ with finite support, SUSY partners can be constructed whenever there are nodeless generator candidates. Nevertheless, some simple examples will suffice for an illustration.

Let V be a square barrier of height V_0 on I; without loss of generality henceforth $a=1$. In the even sector there are two zero modes for small values of V_0; e.g., for $V_0=0.16$ they occur at $\omega_1=-0.181i$, $\omega_2=-2.500i$. The wave functions are $\phi_j(x)=\cosh\alpha_j x$ within I (with $\alpha_1=0.242$, $\alpha_2=2.506$), and a real exponential for $|x|>a$; clearly each ϕ_j has no nodes.

This example already illustrates, as unexceptional, the existence of several nodeless zero modes—any one of which can be used as the generator Φ. We choose the state at $\Omega=\omega_1$; since Φ is purely increasing at both extremes, $\chi=-1$. Figure 1(a) shows V (solid line) and $\tilde{V}$ (dotted line). Figure 1(b) shows the spectra in the complex ω-plane: Most eigenvalues are common (crosses); one QNM exists only in H (circle), while one NM exists only in $\tilde{H}$ (triangle)—the two systems are essentially isospectral. Another essentially isospectral partner can be constructed using the state at ω_2 as the generator. The reverse transformations are characterized by $\tilde{\chi}=1$.

As V_0 increases, the two zero modes move closer together and merge at $V_0=0.291$, forming a JB in H (with $M=2$). This example illustrates the general results of Sec. IV (with H and $\tilde{H}$ interchanged).

As another example, consider a symmetric multi-step square barrier, with $V(x)$ being -10 for $|x|<0.1$, 1 for $0.1<|x|<1$ and zero for $|x|>1$ [solid line in Fig. 2(a)]. In this example, there is a TTM at $\Omega=-0.990i$ [square in Fig. 2(b)]—in fact a parity doublet with one propagating from the left ($\mathrm{TTM_L}$) and one propagating from the right ($\mathrm{TTM_R}$). We choose the former as the generator for a $\chi=0$ transformation. The partner potential $\tilde{V}$ is shown by the broken line in Fig. 2(a). Since

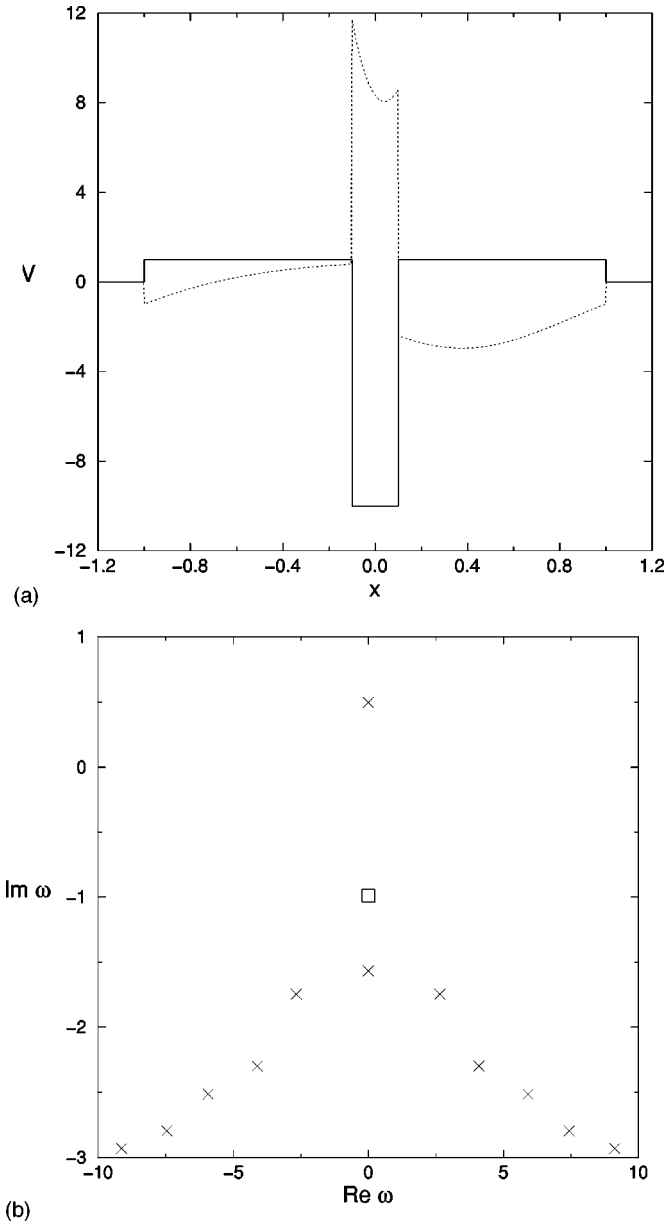

FIG. 2. (a) A multi-step potential V (solid line) and its SUSY partner potential $\tilde{V}$ (broken line). The SUSY transformation is constructed by using the $\mathrm{TTM_L}$ at $\Omega=-0.990i$ [square in (b)] as the generator. (b) The complex ω-plane showing the NM and QNMs common to both potentials (crosses). The square indicates a $\mathrm{TTM_L}$ and a $\mathrm{TTM_R}$ in V, and a doubled $\mathrm{TTM_R}$ in $\tilde{V}$.

the generator is not symmetric, neither is $\tilde{V}$. The states in Γ are exactly preserved [crosses in Fig. 2(b)].

In this example it is interesting to consider not just the states in Γ, but also TTMs (see also Sec. VI C). By arguments similar to those in Sec. II, one $\mathrm{TTM_L}$ Φ is destroyed and one $\mathrm{TTM_R}$ $\tilde{\Phi}=\Phi^{-1}$ is created at the same frequency Ω [square in Fig. 2(b)]. However, in this example, because V is symmetric, there is also a $\mathrm{TTM_R}$ $\Psi(x)=\Phi(-x)$ at Ω, and its partner $\tilde{\Psi}=A\Psi$ is again a $\mathrm{TTM_R}$ in the $\tilde{H}$-system. Thus, in the $\tilde{H}$-system, there is a *doubled* $\mathrm{TTM_R}$ state at Ω. The situation can again be analyzed in terms of the double zero of a Wronskian $\tilde{J}_{\mathrm{R}}(\omega)$, but in this case

J_R and $\tilde{J}_R$ refer to TTM_R's. For example, J_R is now defined in terms of a function f satisfying the outgoing-wave condition at $x=-a$ and a function g satisfying the incoming-wave condition at $x=a$. The obvious adaptation of the discussion in Sec. IV will not be given.

VI. DISCUSSION

A. Summary

In this paper, we have extended the usual discussion of SUSY as a relation between NMs of partner systems to include the QNMs as well. By viewing all these together in the space Γ, a more complete picture emerges. For example, in the usual discussion for NMs only, essentially isospectral transformations are said to lose or gain one state; now we see that (for $\chi=\pm 1$) when an NM appears (disappears), a corresponding QNM disappears (appears).

Furthermore, we have shown that the nontrivial linear-space structure for QNMs and any possible JBs are preserved by SUSY—the latter being a feature not found in conservative systems.

QNMs differ from NMs in two further regards. First, they have complex frequencies; nevertheless, even with twice as many constraints, matching the spectra turns out to be not any more difficult. Second, QNMs need not have an increasing number of nodes, and it is often possible to find several nodeless QNMs which generate distinct SUSY transformations—whereas the analogous operation for NMs would restrict the generator to the nodeless ground state.

These wider perspectives are gained only because attention is paid to the Klein–Gordon rather than the Schrödinger equation, since the concept of outgoing waves has no meaning in an equation that is first order in time.

Two further important properties are also preserved. (a) If V has a singularity say at $x=\pm a$ (e.g., a step), then $\tilde{V}$ will have the same type of singularity, but with the opposite sign, as can be seen from (2.7) by noticing that the most singular part is W'. (b) If V has finite support, then provided Φ is not of the mixed type, $\tilde{V}$ would likewise have no tail. These two properties are precisely the conditions for the eigenstates in Γ to be complete.[26] Thus, SUSY maps a complete basis to a complete basis (if, for the $\chi=\pm 1$ cases, $\Phi \mapsto \tilde{\Phi}$ is included as well).

B. Inversion

This work partially answers the question of QNM *inversion*. It is well known[35] that on a finite interval, *two* sets of real NM frequencies uniquely determine the potential V. Does *one* set of *complex* eigenfrequencies in Γ also uniquely determine V? The answer is negative: There can be strictly isospectral potentials if a TTM with purely imaginary frequency exists and can be used as a $\chi=0$ generator; Fig. 2 provides one such example. However, the following scenario is not yet ruled out. If we consider a half-line problem $0<x<\infty$ (say corresponding to the radial variable in a three-dimensonal system), imposing a nodal condition at $x=0$ and the OWC for $x>a$, can one set of QNM frequencies uniquely determine the potential? SUSY transformations (2.4) do not directly resolve this possibility—for which there is some numerical evidence[36]—since these one-sided systems do not feature an analog of TTMs with which one could construct strictly isospectral partners. Moreover, by (2.7) and (2.9) the nodal condition maps a regular V to $\tilde{V}\sim 2/x^2$ for $x\to 0^+$ (generalizing the well-known result that SUSY increases the angular momentum by one unit in the hydrogen atom). It would, therefore, be interesting to see if an enlarged class of transformations can address this question.

C. Total-transmission modes

The present paper refers in the main to states in Γ, i.e., states that satisfy the OWC at both extremes. One could develop the same formalism for TTMs; see, e.g., the end of Sec. V. Note that we here consider TTMs as states on which SUSY acts, rather than as ($\chi=0$) generators. To be more specific, the SUSY transformation acts on the space Γ_L of TTM_L's

$$\phi(x)\sim e^{i\omega x}, \quad |x|\to\infty, \tag{6.1}$$

or (equivalently, under $\omega \mapsto -\omega$) the space Γ_R of $\mathrm{TTM_R}$'s

$$\phi(x) \sim e^{-i\omega x}, \quad |x| \to \infty. \tag{6.2}$$

One significant difference is that a $\chi = \pm 1$ transformation preserves the eigenvalues in these spaces, whereas a $\chi = 0$ transformation may shift one state.

D. Tails

So far we have only considered potentials with finite support. We end with an outline of some issues that arise for long-range potentials.

The most obvious difference is that if V and/or $\tilde{V}$ are allowed to have tails that decay exponentially or slower in $|x|$, then the mixed-type SUSY transformation is allowed, and there is a *continuous* choice of generators.

However, there are a range of more subtle issues. First, the very definition of an outgoing wave requires care. At the numerical level, special treatment is needed to ensure convergence,[37] but there are matters of principle as well when the OWC $\phi(\omega,x) \sim e^{+i\omega|x|}$ is imposed only as $|x| \to \infty$. In that limit, the condition as stated becomes vacuous for $\mathrm{Im}\,\omega < 0$, since admixture of an (exponentially smaller) incoming solution would not alter this behavior. Rather, it is necessary to define the OWC in the upper half-plane in ω and analytically continue to the lower half-plane. A wave $\phi(\omega,x)$ is incoming if $\phi(-\omega,x)$ is outgoing;[8] this is equivalent to saying that incoming waves are defined first in the lower and continued to the upper half-plane. The necessity for these procedures makes it possible that (at certain singular points ω) a wave function can be *both* incoming and outgoing.

Singularities in the one-sided functions[38] can only occur because of the need to integrate the defining equation over an infinite range. Those values of ω for which these functions (say the left function f) are singular are said to be *anomalous*; if the potential is not oscillating, anomalous points can only occur on the imaginary axis—precisely where possible SUSY generators are to be found. The case of an exponential tail $V(x) \sim V_1 e^{-\lambda|x|}$ is of particular interest because the anomalous points (at $\omega_m = -im\lambda/2$, $m = 1,2,\ldots$) can be studied by the Born approximation, which in this case is equivalent to a power-series expansion in $z = e^{-\lambda|x|}$. More generally, if

$$V(x) = \sum_{k=1}^{\infty} V_k e^{-k\lambda|x|}, \tag{6.3}$$

then for particular choices of the coefficients V_k, one (or more) of the generically anomalous points ω_m may turn out to be regular—a situation we refer to as *miraculous*. The anomalous and miraculous properties for the one-sided functions f and g are inherited by their Wronskian J, which is central to the formalism. These concepts have been discussed in relation to a particular application.[39]

As far as SUSY is concerned, we only make one remark: Such singularities lead to poles in $J(\omega)$, thus are associated with negative values of $n(\omega)$, and are related in SUSY partners by (2.15). The Pöschl–Teller potential[40] $V(x) = \mathcal{V}\,\mathrm{sech}^2(x/b)$ illustrates many interesting features, including the existence of double poles of $J(\omega)$ which can merge with two zeros and lead to "nothing"—a potential that has total transmission at *all* energies.[41]

Anomalous points are exceptional (in the case of exponential tails being a discrete set of measure zero in the ω-plane) and miraculous cancellation of singularities doubly exceptional. One might therefore think that these are not important. Surprisingly however, the problem of linearized gravitational waves propagating on a black-hole background[42] is precisely miraculous in this sense, at the so-called algebraically special frequency Ω.[43] A generator at Ω leads to a SUSY transformation that exactly relates the axial and polar sectors, which are, therefore, isospectral in Γ. Among the more intriguing results is the following:[39] At Ω, there is a mode in the polar sector that is simultaneously a QNM *and* a TTM (i.e., at radial infinity it is purely outgoing but into the event horizon it is both outgoing and incoming), while no modes exist in the axial sector.

The subtle and perhaps counter-intuitive nature of these concepts demands a separate and rigorous examination, to which the foregoing is meant only as a preview—and as further illustration of the utility of SUSY in dealing with waves in open systems.

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APPENDIX: NODES IN QNM WAVE FUNCTIONS

Nodeless eigenstates play a special role in SUSY: They are candidates for the generator Φ. It is, therefore, useful to highlight the differences between NMs and QNMs in this regard, especially to contrast with the well-known property that there can be *only one* nodeless NM.

First of all, we show that for QNMs with $\mathrm{Re}\,\omega\neq 0$, there can be at most one node or antinode. This is not surprising: Since the eigenvalue is complex, the wave function has a changing phase, and it would be ''unlikely'' that the real and imaginary parts (or their derivatives) would vanish together. To prove this formally, take the Schrödinger point of view, so that the eigenvalue is $E=\omega^2$ with a nonzero imaginary part. Now consider a time-dependent QNM and suppose that it has nodes or antinodes at two points x_1, x_2. At these two points, the current

$$\mathcal{J}=i[\phi^*(\partial_x\phi)-(\partial_x\phi^*)\phi] \tag{A1}$$

vanishes. Then, flux conservation implies that the total probability in the interval $[x_1,x_2]$ is constant in time. Yet the wave function is either growing or decaying, since $\mathrm{Im}\,E\neq 0$, which is, therefore, a contradiction.

From the perspective of SUSY it is unfortunate that the above proof excludes the crucial imaginary axis. However, on that axis the statement remains valid for repulsive potentials, or more generally for potentials which are so weakly attractive that $V-\omega^2$ is positive definite.[44] Namely, let ϕ be a solution with two (anti)nodes. By taking the real or imaginary part, we may assume ϕ to be real. Now between two nodes ϕ would have an extremum, i.e., $\phi''\phi<0$ which is incompatible with the KGE. Similarly, an antinode can only be a global maximum or minimum, precluding the presence of any other nodes or antinodes.

Thus, except for the imaginary axis in the case of attractive potentials, QNMs can have at most one node or antinode. For symmetric potentials, in the even sector $x=0$ is already an antinode, so there can be no nodes anywhere.

For zero modes, i.e., QNMs with $\mathrm{Re}\,\omega=0$, nodes are more ''likely'': The eigenvalue is real and the wave function has a constant phase (say purely real), so a node requires only *one* condition, rather than two. Nevertheless, in contrast to the conservative case, the proof that there can be only one nodeless eigenstate can be bypassed.

The interlacing nodal structure of NM eigenfunctions follows from well-established Sturm–Liouville theory. For the present purpose, we do not need the full apparatus. Consider, for simplicity, a finite interval $[-a,a]$ and suppose there are two distinct nodeless eigenfunctions ϕ_1,ϕ_2, both real. Then they can both be chosen to be positive, which violates the orthogonality condition for NMs

$$\int_{-a}^{a}\phi_1(x)\,\phi_2(x)\,dx=0. \tag{A2}$$

We can attempt to transplant the argument to QNMs. For zero modes, the wave functions can again be chosen to be real, and if they are nodeless, positive definite. However, the analog of (A2) for two eigenfunctions with eigenvalues $\omega_j=-i\gamma_j$ is

$$-(\gamma_1+\gamma_2)\int_{-a}^{a}\phi_1(x)\phi_2(x)\,dx+[\phi_1(-a)\phi_2(-a)+\phi_1(a)\phi_2(a)]=0. \tag{A3}$$

Note in particular the signs of the two terms. With $\gamma_j>0$, this condition does *not* preclude both eigenfunctions from being positive definite.

Thus, we can make three remarks. (a) For NMs, there can be *only one* nodeless state. (b) For QNMs with $\mathrm{Re}\,\omega=0$, there *could be* more than one state with no node. (c) For QNMs with $\mathrm{Re}\,\omega\neq 0$, or with $\mathrm{Re}\,\omega=0$ but $V-\omega^2$ positive definite, each eigenfunction can have at most one node or antinode, and for symmetric potentials, *every* even eigenfunction is nodeless.

Case (b) in particular opens up the possibility of multiple SUSY transformations.

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The sufficient conditions under which the S-matrix orthogonal part is real and even

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The sufficient conditions under which the S-matrix orthogonal part $U(k)$ is real and even are proved. These conditions are required for generalization of the projection matrices method in the $N\times N$ Riemann–Hilbert boundary value problem, $N=2,3,...,N<+\infty$. The dependence of the analytical properties of the orthogonal matrix $U(k)$ on the S-matrix diagonal part is thoroughly considered. The examples in which the sufficient conditions are not realized and $\mathrm{Re}\,U(k)\neq 0$, $U(-k)=-U(k)$ are demonstrated. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The S-matrix belongs to a unitary matrix class and it is widely applied in the scattering theory and the inverse problem Refs. 1–3. As any unitary matrix, the S-matrix can be diagonalized by orthogonal matrix $U(k)$ on the real k axis. However, on the basis of this fact, it is impossible to tell more about analytical properties of $U(k)$.

There is a wide variety of different applications in which it is assumed that the equalities:

$$U^*(k)=U(k), \quad \mathrm{Im}\,k=0, \tag{1}$$

$$U(-k)=U(k), \quad \mathrm{Im}\,k=0, \tag{2}$$

are true; in this case the proof is not considered. As a rule, the reason is that the equalities (1) and (2) can easily be verified by calculations.

However, this approach is not adequate for generalization of fundamental mathematical methods as the mathematical generality of methods can be lost. Moreover, the amount of soluble problems can be decreased too.

Properties (1) and (2) play a really significant part in solving Riemann–Hilbert matrix boundary value problem by projection matrices method Refs. 4–7. This method allows solving the boundary value problem without using the system of the singular integral equations. Conditions (1) and (2) form the basis for the construction procedure of the projection matrices. Nevertheless, the individual proof of these equalities had never been carried out. It was because the equalities automatically resulted from the special assumptions for the S-matrix form and dimension.

For the above mentioned reasons generalization of the projection matrices method is impossible without detailed research of sufficient conditions under which the matrix $U(k)$ is real and even in case of $N\times N$ dimension, $N=2,3,...,N<+\infty$. For the projection matrices method to be promising, these conditions must define rather a wide unitary matrix class. Furthermore, the S-matrix is the fundamental object in the scattering theory and inverse problem. For these reasons the dependence of the analytical properties of the orthogonal matrix $U(k)$ on the S-matrix diagonal part is of great interest and it should be treated as a separate problem.

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The conditions under which the S-matrix orthogonal part is real are considered in Sec. II. The conditions under which the matrix $U(k)$ is even are proved in Sec. III. To illustrate the achieved results, at the end of Secs. II and III we consider the examples in which the sufficient conditions are not realized and $\mathrm{Re}\, U(k)\neq 0$, $U(-k)=-U(k)$.

II. THE SUFFICIENT CONDITION AT WHICH THE MATRIX $U(k)$ IS REAL

Let us consider the unitary matrix $S(k)$ on the real k axis at $k\in(-R,R), R>0$, i.e.

$$(S^*(k))^T=S^{-1}(k),\quad k\in(-R,R). \tag{3}$$

Let us assume that the matrix $S(k)$ has the form

$$S(k)=U(k)S^{(0)}(k)U^T(k),\quad k\in(-R,R), \tag{4}$$

where

$$U^{-1}(k)=U^T(k),\quad k\in(-R,R), \tag{5}$$

$$[S^{(0)}(k)]_{\alpha\beta}=\delta_{\alpha\beta}\exp(i2\,\delta_\alpha(k)),\quad \alpha,\beta=1,2,...,N,\quad k\in(-R,R), \tag{6}$$

$$\mathrm{Im}\,\delta_\alpha(k)=0,\quad \delta_\alpha(-k)=-\delta_\alpha(k),\quad \alpha=1,2,...,N,\quad k\in(-R,R), \tag{7}$$

$$\delta_{\alpha\beta}=\begin{cases}1, & \alpha=\beta,\\ 0, & \alpha\neq\beta,\end{cases}\quad \alpha,\beta=1,2,...,N.$$

Here the symbol $\delta_\alpha(k)$ designates some scalar function and $\delta_{\alpha\beta}$ is Kronecker delta.

Lemma 1. If conditions (3)–(7) are true and

$$\forall\,\alpha\neq\beta,\ \exists k_0,\ \delta_a(k_0)-\delta_\beta(k_0)\neq\pm\pi l,\quad l=0,1,2,...,\ l<+\infty,\quad k_0\in(-R,R), \tag{8}$$

then

$$U^*(k)=U(k),\quad k\in(-R,R). \tag{9}$$

Let us prove property (9). Using conditions (3)–(7) we can write

$$S(k)(S^*(k))^T=S(k)S^*(k)=E,\quad k\in(-R,R), \tag{10}$$

where E is the matrix unit. Let us designate as $C(k)$ the following matrix combination:

$$C(k)=U^T(k)U^*(k),\quad k\in(-R,R). \tag{11}$$

From formula (10) we easily obtain the following equality:

$$S^{(0)}(k)C(k)(S^{(0)}(k))^*=C(k),\quad k\in(-R,R). \tag{12}$$

Using formulas (6) and (7) we can rewrite (12) in the following form:

$$[C(k)]_{\alpha\beta}\exp(i2\,\delta_\alpha(k)-i2\,\delta_\beta(k))=[C(k)]_{\alpha\beta},\quad \alpha,\beta=1,2,...,N,\quad k\in(-R,R). \tag{13}$$

Let us discuss Eq. (13) in detail.

If $\alpha=\beta$ then (13) is true. Let us consider the case when $\alpha\neq\beta$. On the strength of condition (8) we can conclude that Eq. (13) will be true in the only case when

$$[C(k)]_{\alpha\beta}=0,\quad \alpha\neq\beta,\quad \alpha,\beta=1,2,...,N,\quad k\in(-R,R). \tag{14}$$

Let us calculate the value of the matrix element $[C(k)]_{\alpha\alpha}$, $\alpha=1,2,...,N$. Formulas (5) and (11) show us that the matrix $C(k)$ is orthogonal at $k\in(-R,R)$, i.e.,

$$\sum_{\gamma=1}^{N}[C(k)]_{\alpha\gamma}[C^T(k)]_{\gamma\beta}=\sum_{\gamma=1}^{N}[C(k)]_{\alpha\gamma}[C(k)]_{\beta\gamma}=\delta_{\alpha\beta},\quad \alpha,\beta=1,2,...,N,\quad k\in(-R,R). \tag{15}$$

Then from Eqs. (14) and (15) we can conclude that:

$$([C(k)]_{\alpha\alpha})^2=1,\quad \alpha=1,2,...N,\quad k\in(-R,R).$$

Thus

$$[C(k)]_{\alpha\alpha}=\pm 1,\quad \alpha=1,2,...,N,\quad k\in(-R,R). \tag{16}$$

Using formula (11) let us rewrite the left part of Eq. (16) in detail. We obtain the following results:

$$[C(k)]_{\alpha\alpha}=\sum_{\gamma=1}^{N}[U^T(k)]_{\alpha\gamma}[U^*(k)]_{\gamma\alpha}=\sum_{\gamma=1}^{N}[U(k)]_{\gamma\alpha}[U^*(k)]_{\gamma\alpha},\quad k\in(-R,R). \tag{17}$$

Since

$$[U(k)]_{\gamma\alpha}[U^*(k)]_{\gamma\alpha}=|[U(k)]_{\gamma\alpha}|^2\geqslant 0,\quad \alpha,\gamma=1,2,...,N,\quad k\in(-R,R),$$

then from (17) it follows that:

$$[C(k)]_{\alpha\alpha}\geqslant 0,\quad \alpha=1,2,...,N,\quad k\in(-R,R). \tag{18}$$

Taking into account formula (14) and comparing conditions (16) and (18) we can conclude that:

$$[C(k)]_{\alpha\beta}=\delta_{\alpha\beta},\quad \alpha,\beta=1,2,...,N,\quad k\in(-R,R).$$

Then formula (11) has the form

$$E=U^T(k)U^*(k),\quad k\in(-R,R). \tag{19}$$

On the whole property (9) results from (19), i.e., the lemma is proved now. It is evident that property (1) can be obtained from (9) at $R\to+\infty$. Thus, the sufficient conditions at which the S-matrix orthogonal part is real are proved.

Let us consider the simple example when condition (8) is not realized. Let us assume that the S-matrix orthogonal part has the form:

$$S^{(0)}(k)=\begin{pmatrix}\exp(i2\delta_1(k)) & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix},\quad k\in(-R,R),$$

i.e., condition (8) is not realized for the matrix elements $[S^{(0)}(k)]_{22}$,$[S^{(0)}(k)]_{33}$. It allows constructing the orthogonal matrix $U(k)$ that is not real

$$U(k)=\frac{1}{\sqrt{k^2-b^2}}\begin{pmatrix}1 & 0 & 0\\ 0 & k & ib\\ 0 & -ib & k\end{pmatrix},\quad k\in(-R,R),\quad b>0.$$

Here we can use any sheet of Riemann surface for $\sqrt{k^2-b^2}$ because it is unimportant in this case. Although, properties (3)–(7) of the S-matrix are true, the matrix $U(k)$ is not real and it can be singular at $k_1=b,\ k_2=-b,\ b<R$ now.

III. THE SUFFICIENT CONDITIONS AT WHICH THE MATRIX $U(k)$ IS EVEN

Let us designate as $A_{(-R,R)}$ the class of continuous matrix at $k\in(-R,R)$ (i.e., the matrix elements are continuous functions).

Lemma 2. If conditions (3)–(8) are true and

$$S(-k)=S^{-1}(k),\quad k\in(-R,R), \tag{20}$$

$$U(k)\in A_{(-R,R)},\quad k\in(-R,R), \tag{21}$$

then

$$U(-k)=U(k),\quad k\in(-R,R). \tag{22}$$

Let us prove property (22). Using the matrix $S(-k)$ instead of the matrix $S^*(k)$ and the matrix:

$$C(k,-k)=U^T(k)U(-k),\quad k\in(-R,R), \tag{23}$$

instead of $C(k)$ in the formulas (10), (12), (13), and (15), we can obtain the following results:

$$[C(k,-k)]_{\alpha\beta}=0,\quad \alpha\neq\beta,\ \alpha,\beta=1,2,...,N,\quad k\in(-R,R), \tag{24}$$

$$[C(k,-k)]_{\alpha\alpha}=\pm 1,\quad \alpha=1,2,...,N,\quad k\in(-R,R). \tag{25}$$

The formulas (24) and (25) are analogous in derivation to (14) and (16), respectively.

Taking into account Eq. (23) let us rewrite the left part of (25) in detail

$$[C(k,-k)]_{\alpha\alpha}=\sum_{\gamma=1}^{N}[U^T(k)]_{\alpha\gamma}[U(-k)]_{\gamma\alpha}=\sum_{\gamma=1}^{N}[U(k)]_{\gamma\alpha}[U(-k)]_{\gamma\alpha},$$
$$\alpha=1,2,...,N,\quad k\in(-R,R). \tag{26}$$

Let us assume that $k=0$ in the Eq. (26). According to lemma conditions, the matrix elements of $U(k)$ are the continuous functions at $k\in(-R,R)$ [see formula (21)]. It means that: $U(+0)=U(-0)$. Thus, Eq. (26) has the form

$$[C(0,0)]_{\alpha\alpha}=\sum_{\gamma=1}^{N}([U(0)]_{\gamma\alpha})^2,\quad \alpha=1,2,...,N, \tag{27}$$

now. Moreover, lemma conditions show us that (9) is true. Consequently, we can write

$$([U(0)]_{\gamma\alpha})^2\geqslant 0,\quad \alpha,\gamma=1,2,...,N. \tag{28}$$

Then from (27) and (28) it follows that:

$$[C(0,0)]_{\alpha\alpha}\geqslant 0,\quad \alpha=1,2,...,N. \tag{29}$$

Let us return to Eq. (25) now. On the strength of Eqs. (21) and (23) we can conclude that matrix elements of $C(k,-k)$ are continuous functions at $k\in(-R,R)$, i.e., $C(k,-k)\in A_{(-R,R)}$. Consequently, from two equalities

$$[C(k,-k)]_{\alpha\alpha}=1,\quad \alpha=1,2,...,N,\quad k\in(-R,R), \tag{30}$$

$$[C(k,-k)]_{\alpha\alpha}=-1, \quad \alpha=1,2,...,N, \quad k\in(-R,R), \tag{31}$$

only one must be true. Taking into account (29) we can conclude that Eq. (30) is true and Eq. (31) is false. Thus, on the basis of Eqs. (24) and (30) we can write

$$[C(k,-k)]_{\alpha\beta}=\delta_{\alpha\beta}, \quad \alpha,\beta=1,2,...,N, \quad k\in(-R,R).$$

Then formula (23) has the following form:

$$E=U^T(k)U(-k), \quad k\in(-R,R). \tag{32}$$

On the whole property (22) results from Eq. (32). It is evident that property (2) can be obtained from (22) at $R\to+\infty$. Thus, the sufficient conditions at which the S-matrix orthogonal part is even are proved.

In order to demonstrate the significance of condition (21) we shall consider the following example. Let us assume that the matrix $U(k)$ has the form:

$$U(k)=\frac{1}{\sqrt{k^2+\sqrt[3]{k^2}}}\begin{pmatrix} k & \sqrt[3]{k} \\ -\sqrt[3]{k} & k \end{pmatrix}, \quad k\in(-R,R), \tag{33}$$

and S-matrix diagonal part satisfies the conditions (6) and (7). Neither (9) nor (21) is true for the matrix $U(k)$ [see formula (33)] in general case. This is because the matrix elements of $U(k)$ are combinations of the 2-sheet and 3-sheet functions. However, using special conditions for the sheets of Riemann surface we can satisfy condition of (9). Since

$$\sqrt[3]{k}=|\sqrt[3]{k}|\exp\left[\frac{i}{3}(\arg k+2\pi l)\right], \quad k\in(-R,R), \quad l=0,1,2,$$

then we can fix the sheets of Riemann surface in the following way:

$$\sqrt[3]{k}=|\sqrt[3]{k}|, \quad k\in(0,R), \quad \arg k=0, \quad l=0, \tag{34}$$

$$\sqrt[3]{k}=-|\sqrt[3]{k}|, \quad k\in(-R,0), \quad \arg k=\pi, \quad l=1. \tag{35}$$

In this case the matrix $U(k)$ satisfies condition (9).

Let us prove that:

$$[U(+0)]_{12}\neq[U(-0)]_{12}. \tag{36}$$

In order to do this we calculate $[U(k)]_{12}$ at $k\in(0,R)$ in detail. On the basis of Eqs. (33) and (34) we can write

$$[U(k)]_{12}=\frac{\sqrt[3]{k}}{\sqrt{k^2+\sqrt[3]{k^2}}}=\frac{|\sqrt[3]{k}|}{\sqrt{|k|^2+|\sqrt[3]{k}|^2}}=\frac{|\sqrt[3]{k}|}{\sqrt{|\sqrt[3]{k}|^2}\sqrt{|k^{2/3}|^2+1}}, \quad k\in(0,R). \tag{37}$$

In this case we can use any sheet of Riemann surface for the function $\sqrt{|\sqrt[3]{k}|^2}$. Let us assume that

$$\sqrt{|\sqrt[3]{k}|^2}=|\sqrt[3]{k}|, \quad k\in(-R,R), \tag{38}$$

then

$$[U(k)]_{12}=\frac{|\sqrt[3]{k}|}{|\sqrt[3]{k}|\sqrt{|k^{2/3}|^2+1}}=\frac{1}{\sqrt{|k^{2/3}|^2+1}}, \quad k\in(0,R). \tag{39}$$

Using (35) and (38) it is easy to demonstrate that

$$[U(k)]_{12}=\frac{-|\sqrt[3]{k}|}{|\sqrt[3]{k}|\sqrt{|k^{2/3}|^2+1}}=\frac{-1}{\sqrt{|k^{2/3}|^2+1}},\quad k\in(-R,0). \tag{40}$$

Let us assume that $k\to+0$ in Eq. (39) and $k\to-0$ in Eq. (40). Thus

$$[U(+0)]_{12}=1,\quad [U(-0)]_{12}=-1,$$

whence follows the proof of Eq. (36).

We can obtain the analogous result for $[U(k)]_{21}$, i.e.,

$$[U(+0)]_{21}=-1,\quad [U(-0)]_{21}=1.$$

Using (34), (35), and (38) we can conclude that

$$[U(+0)]_{11}=[U(-0)]_{11}=0,\quad [U(+0)]_{22}=[U(-0)]_{22}=0.$$

The above introduced considerations show that conditions (3)–(8), and (20) are true. However, the condition (21) is not realized at $k=0$. On the basis of the Eqs. (33)–(35) we can see that

$$U(-k)=-U(k),\quad k\in(-R,R),$$

i.e., the matrix $U(k)$ is odd.

IV. THE CONCLUSION

To prove the conditions under which the matrix $U(k)$ is real we have done the following. One additional condition (8) has been added to the standard properties of the S-matrix (3)–(7) (at $R\to+\infty$). From the physical standpoint it means that processes described by the functions $\delta_\alpha(k)$, $\delta_\beta(k)$ α, $\beta=1,2,...,N$ are not identical.

In addition to formulas (3)–(7), three complementary conditions (8), (20), and (21) have been required to prove property (22). The essence of (8) has been discussed above. Formula (20) describes the standard property of the S-matrix for the elastic scattering at $R\to+\infty$. As for condition (21), it has been introduced for mathematical reasons. However, there are many applications where this condition is realized automatically.

Thus, conditions (3)–(8), (20), and (21) define rather a wide class of the unitary matrix which can be used in applications and in generalization of projection matrices method. Besides, they reflect dependence of analytical properties of the orthogonal matrix $U(k)$ on the S-matrix diagonal part.

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n-symplectic algebra of observables in covariant Lagrangian field theory

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n-symplectic geometry on the adapted frame bundle $\lambda:L_\pi E\to E$ of an $n=(m+k)$-dimensional fiber bundle $\pi:E\to M$ is used to set up an algebra of observables for covariant Lagrangian field theories. Using the principle bundle $\rho:L_\pi E\to J^1\pi$ we lift a Lagrangian $\mathcal{L}:J^1\pi\to\mathbb{R}$ to a Lagrangian $L:=\rho^*(\mathcal{L}):L_\pi E\to\mathbb{R}$, and then use L to define a "modified n-symplectic potential" $\hat{\theta}_L$ on $L_\pi E$, the Cartan–Hamilton–Poincaré (CHP) $\mathbb{R}^n$-valued 1-form. If the lifted Lagrangian is nonzero, then $(L_\pi E, d\hat{\theta}_L)$ is an n-symplectic manifold. To characterize the observables we define a lifted Legendre transformation ϕ_L from $L_\pi E$ into LE. The image $Q_L:=\phi_L(L_\pi E)$ is a submanifold of LE, and $(Q_L, d(\hat{\theta}|_{Q_L}))$ is shown to be an n-symplectic manifold. We prove the theorem that $\hat{\theta}_L=\phi_L^*(\theta|_{Q_L})$, and pull back the reduced canonical n-symplectic geometry on Q_L to $L_\pi E$ to define the algebras of observables on the n-symplectic manifold $(L_\pi E, d\hat{\theta}_L)$. To find the reduced n-symplectic algebra on Q_L we set up the equations of n-symplectic reduction, and apply the general theory to the model of a k-tuple of massless scalar fields on Minkowski space–time. The formalism set forth in this paper lays the ground work for a geometric quantization theory of fields. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1396835]

I. INTRODUCTION

In order to set up a quantization scheme for Lagrangian field theories modeled on the Kostant–Souriau theory of geometric quantization[1,2] one needs to find an analog of the algebra of observables $C^\infty(M,\mathbb{R})$ under the Poisson bracket and the isomorphic algebra of connection preserving vector fields on a line bundle $L^\times\to M$ over a symplectic manifold (M,ω). In this paper we construct an algebra of observables for covariant Lagrangian field theories using the n-symplectic theory[3–9] as the engine for the construction. In a companion paper[10] the algebra constructed here is used as the basis for setting up a Kostant–Souriau geometric quantization scheme for covariant Lagrangian field theories. For other geometric approaches to quantization of fields see the work of Kanatchikov[11] who bases his work on the polysymplectic geometry of Günther,[12] and also Hrabak,[13] whose work is based on the multisymplectic geometry of Gotay *et al.*[14]

Let $\mathcal{L}:J^1\pi\to\mathbb{R}$ be a field Lagrangian for a section of an $n=m+k$ dimensional fiber bundle $\pi:E\to M$ over the m dimensional manifold M. To use the n-symplectic theory to construct an algebra of observables we lift the Lagrangian on $J^1\pi$ to the bundle of adapted linear frames $L_\pi E$, the subbundle of LE that arises[15,8,9] due to the fiber structure of $E\to M$. (Throughout the paper we use the index range convention $i,j=1,2,\ldots,m$, $A,B=m+1,m+2,\ldots,m+k$, and $\alpha,\beta=1,2,\ldots,m+k$.) A point in $L_\pi E$ is a triple (e,e_i,e_A), where $e\in E$ and (e_i,e_A) is a linear frame for the tangent space to E at e in which the last k vectors (e_A) are vertical on $\pi:E\to M$. The lifting of $\mathcal{L}:J^1\pi\to\mathbb{R}$ to $L_\pi E$ is natural since $L_\pi E$ is known[9] to be an $H=\mathrm{GL}(m)\times\mathrm{GL}(k)$ principal fiber bundle over $J^1\pi$. If $\rho:L_\pi E\to J^1\pi$ then we put $L:=\rho^*(\mathcal{L})$. Using a lifted Legendre transformation we construct the Cartan–Hamilton–Poincaré (CHP) 1-forms $\hat{\theta}_L$ first introduced in

Ref. 9, and prove the theorem that $(L_\pi E, d\hat{\theta}_L)$ is an n-symplectic manifold provided the Lagrangian is nonzero. The observables of the theory are then the $\otimes^p\mathbb{R}^n$-valued functions $\hat{f}$ on $L_\pi E$ that satisfy the n-symplectic structure equation,

$$d\hat{f} = -p!\, X_{\hat{f}} \lrcorner d\hat{\theta}_L \tag{1.1}$$

for some $\otimes^{p-1}\mathbb{R}^n$-valued vector field $\hat{X}_{\hat{f}}$. (Here $\lrcorner$ denotes a tensor product in the range and interior product in the domain.) We will show that the set of allowable observables carries a natural graded Poisson algebra structure, and that the set of all corresponding vector-valued Hamiltonian vector fields $\hat{X}_{\hat{f}}$ has a natural Lie algebra structure as well.

The plan of the paper is the following. In Sec. II we develop the algebraic structure that is defined by an n-symplectic structure on an N-dimensional manifold P. Such a structure is defined by an $\mathbb{R}^n$-valued 2-form $\hat{\omega}$ that is both closed and nondegenerate. We will refer to $(P,\hat{\omega})$ as an n-symplectic manifold. To illustrate the theory we will carry along the canonical example of the bundle of linear frames $P=LE$ (Refs. 3, 4, 5 6) and its canonically defined n-symplectic structure $\hat{\omega}=d\hat{\theta}$, where $\hat{\theta}$ is the $\mathbb{R}^n$-valued soldering 1-form. In the general case we show that $\hat{\omega}$ defines a Poisson algebra SHF of $\otimes^p_{(\mathrm{sym})}\mathbb{R}^n$-valued functions on P, the observables of the theory, together with a Lie algebra of vector-valued Hamiltonian vector fields. When $P=LE$ and $\hat{\omega}=d\hat{\theta}$ the observables are symmetric polynomials in the $\mathbb{R}^n$-valued momenta $\hat{\pi}_\alpha$ with coefficients that are constant on the fibers of $\lambda: LE\to E$. The homogeneous polynomial observables in this case correspond uniquely to symmmetric contravariant tensor fields on E, and the Poisson bracket of two such observables on $L_\pi E$ corresponds[6] to the Schouten–Nijenhuis bracket[16,17] of the corresponding tensor fields on E. There is a corresponding development for $\otimes^p_{(\mathrm{skew})}\mathbb{R}^n$-valued functions on P, which turns out to be a graded Poisson algebra. The direct sum of these two algebras is then a graded Poisson algebra.

In Sec. III we present the relevant details of the canonical n-symplectic geometry on LE, and the reduced subbundle of adapted linear frames $L_\pi E$. In Sec. IV we recall the bundle structure $\rho: L_\pi E\to J^1\pi$ and the definition[9] of the modified soldering 1-forms on $L_\pi E$, which we refer to as the Cartan–Hamilton–Poincaré (CHP) $\mathbb{R}^n$-value 1-form. The CHP 1-form is defined herein as the pull-back, under a lifted Legendre transformation, of the canonical $\mathbb{R}^n$-valued soldering 1-form on LE to $L_\pi E$. We then prove the theorem that $(L_\pi E, d\hat{\theta}_L)$ is an n-symplectic manifold provided that L is nonzero. The algebra of observables defined by a Lagrangian is then the graded Poisson algebra defined by this n-symplectic structure.

In order to find the observables defined by a specific Lagrangian we consider in Sec. V the image $Q_L\subset LE$ of $L_\pi E$ under the lifted Legendre transformation. To characterize the n-symplectic observables on $(Q_L, d\hat{\theta})$ we carry out a reduction of the canonical n-symplectic geometry on LE to Q_L. Our method leads to a system of PDE's that characterize those n-symplectic observables on $(LE, d\hat{\theta})$ that restrict the observables on $(Q_L, d(\hat{\theta}|_{Q_L}))$. In Sec. VI we apply the theory to the massless n-tuple of scalar fields on Minkowski space–time. Section VII contains a brief summary of our results and some ideas for future work.

II. *n*-SYMPLECTIC GEOMETRY

Let P be an N-dimensional manifold, and let $(\hat{r}_\alpha)$ denote the standard basis of $\mathbb{R}^n$, with $1\leqslant n\leqslant N$. We suppose there exists on P an n-**symplectic structure**, namely, an $\mathbb{R}^n$-valued 2-form $\hat{\omega}=\omega^\alpha\otimes\hat{r}_\alpha$ that satisfies the following two conditions:

$$(C-1)\quad d\omega^\alpha=0\quad \forall\,\alpha=1,2,\ldots,n, \tag{2.1}$$

$$(C-2)\quad X\lrcorner\hat{\omega}=0\Leftrightarrow X=0. \tag{2.2}$$

Definition II.1: The pair $(P,\hat{\omega})$ *is an n-symplectic manifold.*

Remark: In Refs. 3–9,15 the term *n*-symplectic structure refers to the two-form that is the exterior derivative of the $\mathbb{R}^n$-valued soldering 1-form on frame bundles or subbundles of frame bundles. Günther[12] was perhaps the first to consider a manifold with a nondegenerate $\mathbb{R}^n$-valued 2-form, and he used the terms *polysymplectic structure* and *polysymplectic manifold* for the nondengenerate 2-form and manifold, respectively. In addition, when one adds a few extra conditions to conditions C-1 and C-2 one arrives at a *k-symplectic manifold*. Specifically, if P is required to support an np-dimensional distribution V such that

$$(C-3) \quad N=p(n+1),$$

$$(C-4) \quad \hat{\omega}|_{V\times V}=0,$$

then P is a *k-symplectic manifold* as defined by both de Léon *et al.*[19] and also by Awane.[18] To make this identification one needs to make the notational changes $n\to k$ and $p\to n$ in the above discussion. Thus all *k*-symplectic manifolds are *n*-symplectic, but not conversely. The canonical frame bundle example $(LE,d\hat{\theta})$ of an *n*-symplectic manifold introduced in the next paragraph is also a *k*-symplectic manifold. On the other hand the important example of the adapted frame bundle $L_\pi E$ that is central to this paper is *n*-symplectic, but not *k*-symplectic. The problem is that the *k*-symplectic dimensional requirement $N=p(n+1)$ cannot be satisifed on $L_\pi E$.

We will continue to use the name *n*-symplectic geometry for the structure in definition II in order to emphasize the geometrical and algebraic developments that our approach provides.

Remark: In this section we will carry along the canonical example $P=LE$, where LE is the (n^2+n)-dimensional bundle of linear frames of the n-dimensional manifold E. The bundle of frames LE supports a canonically defined *n*-symplectic form $\hat{\omega}=d\hat{\theta}$, where $\hat{\theta}$ is the $\mathbb{R}^n$-valued soldering 1-form, and is defined as follows. If X is a tangent vector to LE at $u=(e,e_\alpha)$, then

$$\hat{\theta}_u(X)=e^\alpha(\lambda_*(X))\hat{r}_\alpha, \tag{2.3}$$

where (e^α) denotes the coframe dual to the frame (e_α). The soldering form is evidently the frame bundle counterpart of the canonical 1-form θ on T^*E. It has been shown[4] that much of the canonical symplectic geometry on T^*E can be derived from the *n*-symplectic geometry on LE.

A. Canonical coordinates

Awane[18] has proved a generalized Darboux theorem for *k*-symplectic geometry. Thus in the neighborhood of each point $u\in P$ one can find canonical (or Darboux) coordinates (π_a^α,z^b), $\alpha,\beta=1,2,\ldots,k$ and $a,b=1,2,\ldots,n$. With respect to such canonical coordinates $\hat{\omega}$ takes the form

$$\hat{\omega}=(d\pi_a^\alpha\wedge dz^a)\otimes\hat{r}_\alpha. \tag{2.4}$$

Hence we have the following locally defined equations:

$$d\pi_a^\alpha=-\frac{\partial}{\partial z^a}\lrcorner\omega^\alpha, \quad dz^a=\frac{\partial}{\partial\pi_a^\alpha}\lrcorner\omega^\alpha, \quad (\mathfrak{X}_\alpha). \tag{2.5}$$

Remark: The approach used here to characterize algebras of observables requires the existence of such canonical coordinates. From the results in Ref. 3 we know that not all functions are *allowable n-symplectic* observables, even in the canonical case of frame bundles. Thus, for example, whether or not there exist pairs $(\hat{f}^{\alpha_1\alpha_2\cdots\alpha_p},\hat{X}_f^{\alpha_1\alpha_2\cdots\alpha_{p-1}})$, $p=1,2,\ldots$ that satisfy Eq. (2.8) below for a general *n*-symplectic manifold is an existence question, and must be demonstrated for each *n*-symplectic manifold. The formulas (2.5) will provide local examples of rank 1 solutions of the *n*-symplectic structure equations (2.8) when either the geometry is specialized to $k=n$-symplectic geometry where a Darboux theorem holds, or when canonical coordinates are simply known to exist. Fortunately in the cases we will consider later in this paper, and in particular on the adapted frame bundle $L_\pi E$, canonical coordinates are known to exist.

Example: On the bundle of linear frames $\lambda: LE \to E$ one can introduce canonical coordinates in the following way. Let (z^α) be a local chart on $U \subset E$. Then on $\tilde{U} = \lambda^{-1}(U)$ define coordinate functions $(\pi^\alpha_\beta, \tilde{z}^\mu)$ by

$$\pi^\alpha_\beta(u) := e^\alpha \left(\left. \frac{\partial}{\partial z^\beta} \right|_{\lambda(u)} \right) \forall u = (e, e_\alpha) \in \tilde{U},$$

$$\tilde{z}^\alpha(u) := z^\alpha(\lambda(u)) \forall u \in \tilde{U}. \tag{2.6}$$

Following standard notational conventions we will drop the ''over tilde'' on the lifted coordinates $\tilde{z}^\alpha$ and write simply z^α for both sets of coordinates. With respect to such a coordinate system on LE the soldering 1-form $\hat{\theta}$ has the local coordinate expression,

$$\hat{\theta} = (\pi^\alpha_\beta dz^\beta) \otimes \hat{r}_\alpha. \tag{2.7}$$

The n-symplectic 2-form $d\hat{\theta}$ clearly has the canonical form (2.4) in such a coordinate system.

B. The symmetric Poisson algebra defined by $\hat{\omega}$

Throughout this section we let $(P, \hat{\omega})$ be an n-symplectic manifold as defined above. It is convenient to introduce the multi-index notation,

$$\hat{r}_{\alpha_1 \alpha_2 \cdots \alpha_{n-\mu}} = \hat{r}_{\alpha_1} \otimes_s \hat{r}_{\alpha_2} \otimes_s \cdots \otimes_s \hat{r}_{\alpha_{n-\mu}}, \quad 0 \leqslant \mu \leqslant n-1.$$

In addition round brackets around indices $(\alpha\beta\gamma)$ denotes symmetrization over the enclosed indices.

Definition II.2: For each $p \geqslant 1$, let SHF^p denote the set of all $(\otimes_s)^p \mathbb{R}^n$-valued functions $\hat{f} = (\hat{f}^{\alpha_1 \alpha_2 \cdots \alpha_p}) = (\hat{f}^{(\alpha_1 \alpha_2 \cdots \alpha_p)})$ on P that satisfy the equations

$$d\hat{f}^{\alpha_1 \alpha_2 \cdots \alpha_p} = -p! X^{(\alpha_1 \alpha_2 \cdots \alpha_{p-1}}_{\hat{f}} \lrcorner \omega^{\alpha_p)} \tag{2.8}$$

for some set of vector fields $(X^{\alpha_1 \alpha_2 \cdots \alpha_{p-1}}_{\hat{f}})$. We then set

$$SHF = \oplus_{p \geqslant 1} SHF^p. \tag{2.9}$$

$\hat{f} \in SHF^p$ will be referred to as a symmetric Hamiltonian function of rank p.

Example: The locally defined functions $\hat{f}$ that satisfy (2.8) for the canonical n-symplectic manifold $(LE, d\hat{\theta})$ were given in Ref. 3. In particular, contrary to the situation in symplectic geometry, not all $(\otimes_s)^p \mathbb{R}^n$-valued functions on LE are compatible with Eq. (2.8). The $p = 1,2$ cases will clarify the structure. Let $ST^p(LE)$ denote the vector space of symmetric $(\otimes_s)^p \mathbb{R}^n$-valued GL($n$)-tensorial functions on LE that correspond uniquely to symmetric rank p contravariant tensor fields on E. Similarly let $C^\infty(E, (\otimes_s)^p \mathbb{R}^n)$ denote the set of smooth $(\otimes_s)^p \mathbb{R}^n$-valued functions on LE that are constant on fibers of LE. Then,

$$SHF^1 = T^1(LE) + C^\infty(E, \mathbb{R}^n), \tag{2.10}$$

$$SHF^2 = ST^2(LE) + T^1(LE) \otimes_s C^\infty(E, \mathbb{R}^n) + C^\infty(E, \mathbb{R}^n \otimes_s \mathbb{R}^n). \tag{2.11}$$

For example, if $\hat{f} = (\hat{f}^\alpha) \in SHF^1$ and $\hat{f} = (\hat{f}^{\alpha\beta}) \in SHF^2$, then in canonical coordinates $(\pi^\alpha_\beta, z^\gamma)$ the functions $\hat{f}^\alpha$ and $\hat{f}^{\alpha\beta}$ have the general forms

$$\hat{f}^\alpha = A^a \pi^\alpha_a + B^\alpha, \quad \hat{f}^{\alpha\beta} = A^{\mu\nu} \pi^\alpha_\mu \pi^\beta_\nu + B^{\mu(\alpha} \pi^{\beta)}_\mu + C^{\alpha\beta}, \tag{2.12}$$

where A^a, B^α, $A^{\mu\nu}=A^{(\mu\nu)}$, $B^{\mu\nu}$ and $C^{\mu\nu}=C^{(\mu\nu)}$ are all constant on the fibers of $\lambda:LE\to E$ and hence are pull-ups of functions defined on E.

Remark: The analogous results for the n-symplectic form given in (2.4) above are straightforward to work out in canonical coordinates. For the $p=1$ and $p=2$ symmetric cases, one finds

$$\hat{f}^\alpha=\mathcal{A}^a\pi_a^\alpha+\mathcal{B}^\alpha,\quad \hat{f}^{\alpha\beta}=\mathcal{A}^{ab}\pi_a^\alpha\pi_b^\beta+\mathcal{B}^{a(\alpha}\pi_a^{\beta)}+\mathcal{C}^{\alpha\beta}, \tag{2.13}$$

where now all coefficients are functions of the coordinates z^a.

Remark: Although $\hat{\omega}$ is nondegenerate in the sense given in Eq. (2.2) above, because of the symmetrization on the right-hand side in (2.8) the relationship between $\hat{f}$ and $(X_{\hat{f}}^{\alpha_1\alpha_2\cdots\ \alpha_{p-1}})$ is not unique unless $p=1$. Given a pair $(\hat{f}^{\alpha_1\alpha_2\cdots\ \alpha_p},X_{\hat{f}}^{\alpha_1\alpha_2\cdots\ \alpha_{p-1}})$ that satisfies (2.8) one can always add to $X_{\hat{f}}^{\alpha_1\alpha_2\cdots\ \alpha_{p-1}}$ vector fields $Y^{\alpha_1\alpha_2\cdots\ \alpha_{p-1}}$ that satisfy the kernel equation

$$Y^{(\alpha_1\alpha_2\cdots\ \alpha_{p-1}}\lrcorner\hat{\omega}^{\alpha_p)}=0 \tag{2.14}$$

to obtain a new pair $(\hat{f}^{\alpha_1\alpha_2\cdots\ \alpha_p},\overline{X}_{\hat{f}}^{\alpha_1\alpha_2\cdots\ \alpha_{p-1}})$ that also satisfies (2.8), where

$$\overline{X}_{\hat{f}}^{\alpha_1\alpha_2\cdots\ \alpha_{p-1}}=X_{\hat{f}}^{\alpha_1\alpha_2\cdots\ \alpha_{p-1}}+Y^{\alpha_1\alpha_2\cdots\ \alpha_{p-1}}.$$

Hence we associate with $\hat{f}\in SHF^p$ an equivalence class of $(\otimes_s)^{p-1}\mathbb{R}^k$-valued vector fields, which we denote by $[\![\hat{X}_{\hat{f}}]\!]=[\![X_{\hat{f}}^{\alpha_1\alpha_2\cdots\ \alpha_{p-1}}\hat{r}_{\alpha_1\alpha_2\cdots\ \alpha_{p-1}}]\!]$. We will see below that even though we obtain equivalence classes of Hamiltonian vector fields rather than vector fields, the geometry still carries natural algebraic structures.

Definition II.3: For each $p\geqslant 1$ let SHV^p denote the vector space of all equivalence classes of $(\otimes_s)^{p-1}\mathbb{R}^k$-valued vector fields $[\![\hat{X}_{\hat{f}}]\!]=[\![X_{\hat{f}}^{\alpha_1\alpha_2\cdots\ \alpha_{p-1}}\hat{r}_{\alpha_1\alpha_2\cdots\ \alpha_{p-1}}]\!]$ on P that satisfy Eqs. (2.8) for some $\hat{f}=\hat{f}^{\alpha_1\alpha_2\cdots\ \alpha_p}\hat{r}_{\alpha_1\alpha_2\cdots\ \alpha_p}\in SHF^p$. We then set

$$SHV=\oplus_{p\geqslant 1}SHV^p. \tag{2.15}$$

$[\![\hat{X}_{\hat{f}}]\!]$ will be referred to as the generalized rank p Hamiltonian vector field defined by $\hat{f}$.

Example: The Hamiltonian vector field $\hat{X}_{\hat{f}}$ for the rank 1 element in (2.12) is unique, and has the form

$$\hat{X}_{\hat{f}}=A^\alpha\frac{\partial}{\partial z^\alpha}-\left(\frac{\partial A^\beta}{\partial z^\gamma}\pi_\beta^\alpha+\frac{\partial B^\alpha}{\partial z^\gamma}\right)\frac{\partial}{\partial\pi_\gamma^\alpha}. \tag{2.16}$$

The equivalence class of $\mathbb{R}^n$-valued Hamiltonian vector fields corresponding to the rank 2 element in (2.12) on LE has representatives of the form,

$$\hat{X}_{\hat{f}}^\alpha=(A^{\mu\nu}\pi_\mu^\alpha+B^{\nu\alpha})\frac{\partial}{\partial z^\nu}-\frac{1}{2}\left(\frac{\partial A^{\mu\beta}}{\partial z^\gamma}\pi_\mu^\alpha\pi_\beta^\nu+\frac{\partial B^{\mu(\alpha}}{\partial z^\gamma}\pi_\mu^{\nu)}+\frac{\partial C^{\alpha\nu}}{\partial z^\gamma}\right)\frac{\partial}{\partial\pi_\gamma^\nu}+Y_\gamma^{\alpha\nu}\frac{\partial}{\partial\pi_\gamma^\nu}, \tag{2.17}$$

where $Y_\gamma^{\alpha\beta}$ are functions subject to the constraint

$$Y_\gamma^{(\alpha\beta)}=0,$$

but are otherwise completely arbitrary. The fact that $Y^\alpha=Y_\nu^{\alpha\mu}(\partial/\partial\pi_\nu^\mu)$ is purely vertical on $\lambda:LE\to E$ follows from (2.14).

Remark: For the n-symplectic rank 2 symmetric observable given above in (2.13), one can check easily that the local coordinate form of a representative $X_{\hat{f}}^\alpha$ of the equivalence class of Hamiltonian vector fields $[\![\hat{X}_{\hat{f}}]\!]^\alpha$ that satisfies (2.8) has the form,

$$X^\alpha=(\mathcal{A}^{ab}\pi_a^\alpha+\mathcal{B}^{b\alpha})\frac{\partial}{\partial z^b}-\frac{1}{2}\left(\frac{\partial\mathcal{A}^{ab}}{\partial z^d}\pi_a^\alpha\pi_b^\sigma+\frac{\partial\mathcal{B}^{a(\alpha}}{\partial z^d}\pi_a^{\sigma)}+\frac{\partial\mathcal{C}^{\alpha\sigma}}{\partial z^d}\right)\frac{\partial}{\partial\pi_d^\sigma}+Y^\alpha. \tag{2.18}$$

Poisson brackets:

Definition II.4: For $p,q\geqslant 1$ define a map $\{,\}:SHF^p\times SHF^q\to SHF^{p+q-1}$ as follows. For $\hat f=f^{\alpha_1\alpha_2\cdots\alpha_p}\hat r_{\alpha_1\alpha_2\cdots\alpha_p}\in SHF^p$ and $\hat g=g^{\beta_1\beta_2\cdots\beta_q}\hat r_{\beta_1\beta_2\cdots\beta_q}\in SHF^q$,

$$\{\hat f,\hat g\}^{\alpha_1\alpha_2\cdots\alpha_{p+q-1}}:=p!X_{\hat f}^{(\alpha_1\alpha_2\cdots\alpha_{p-1}}(\hat g^{\alpha_p\alpha_{p+1}\cdots\alpha_{p+q-1})}), \tag{2.19}$$

where $\hat X_{\hat f}^{\alpha_1\alpha_2\cdots\alpha_{p-1}}$ is any set of representatives of the equivalence class $[\![\hat X_{\hat f}]\!]$.

We need to make certain that $\{\hat f,\hat g\}$ is well-defined. Suppose we have two representatives $X_{\hat f}^{\alpha_1\alpha_2\cdots\alpha_{p-1}}$ and $\overline{X}_{\hat f}^{\alpha_1\alpha_2\cdots\alpha_{p-1}}=X_{\hat f}^{\alpha_1\alpha_2\cdots\alpha_{p-1}}+Y^{\alpha_1\alpha_2\cdots\alpha_{p-1}}$ of $[\![\hat X_{\hat f}]\!]$. Then it follows easily from (2.14) that

$$\overline{X}_{\hat f}^{(\alpha_1\alpha_2\cdots\alpha_{p-1}}(\hat g^{\alpha_p\alpha_{p+1}\cdots\alpha_{p+q-1})})=\hat X_{\hat f}^{(\alpha_1\alpha_2\cdots\alpha_{p-1}}(\hat g^{\alpha_p\alpha_{p+1}\cdots\alpha_{p+q-1})}).$$

Hence the bracket is independent of choice of representatives. That $\{\hat f,\hat g\}$ actually is in SHF^{p+q-1} will follow from corollary (2.6) below.

Definition II.5: Let $[\![\hat X_{\hat f}]\!]=[\![X_{\hat f}^{\alpha_1\alpha_2\cdots\alpha_{p-1}}\hat r_{\alpha_1\alpha_2\cdots\alpha_{p-1}}]\!]$ and $[\![\hat X_{\hat g}]\!]=[\![X_{\hat g}^{\alpha_1\alpha_2\cdots\alpha_{p-1}}\hat r_{\alpha_1\alpha_2\cdots\alpha_{p-1}}]\!]$ denote the equivalence classes of vector-valued vector fields determined by $\hat f\in SHF^p$ and $\hat g\in SHF^q$, respectively. Define a bracket $[\![,]\!]:SHV^p\times SHV^q\to SHV^{p+q-1}$ by

$$[\![[\![\hat X_{\hat f}]\!],[\![\hat X_{\hat g}]\!]]\!]=[\![[\hat X_{\hat f}^{(\alpha_1\alpha_2\cdots\alpha_{p-1}},\hat X_{\hat g}^{\alpha_p\alpha_{p+1}\cdots\alpha_{p+q-2})}]\hat r_{\alpha_1\alpha_2\cdots\alpha_{p+q-2}}]\!], \tag{2.20}$$

where the "inside" bracket on the right-hand side is the ordinary Lie bracket of vector fields calculated using arbitrary representatives. (Notice the symmetrization over all the upper indices in this equation.)

We again need to show that this bracket is well-defined. This is shown in the following lemma, in which we will need the formula

$$L_{X^{(J}}\omega^{\alpha)}=0 \tag{2.21}$$

which follows easily from (2.8) and the formula $L_X\omega=X\lrcorner d\omega+d(X\lrcorner\omega)$. In (2.21) J denotes the multiindex $\alpha_1\alpha_2\cdots\alpha_{p-1}$, and X^J denotes a representative of a rank p Hamiltonian vector field satisfying Eq. (2.8). The next lemma shows that the bracket defined in (2.20) is (i) independent of choice of representatives, and (ii) closes on the set of equivalence classes of vector-valued Hamiltonian vector fields.

Lemma II.6: Let $[\![\hat X_{\hat f}]\!]$ and $[\![\hat X_{\hat g}]\!]$ denote the equivalence classes of vector-valued vector fields determined by $\hat f\in SHF^p$ and $\hat g\in SHF^q$, respectively. Then

$$[\![[\![\hat X_{\hat f}]\!],[\![\hat X_{\hat g}]\!]]\!]=\frac{(p+q-1)!}{p!q!}[\![\hat X_{\{\hat f,\hat g\}}]\!] \tag{2.22}$$

Proof: We introduce the multiindex notation $I=\alpha_1\alpha_2\cdots\alpha_{p-1}$ and $J=\beta_1\beta_2\cdots\beta_{q-1}$, so that we may use the shorthand notation $X_{\hat f}^{\alpha_1\alpha_2\cdots\alpha_{p-1}}=X_{\hat f}^I$ and $X_{\hat g}^{\beta_1\beta_2\cdots\beta_{q-1}}=X_{\hat g}^J$. Then using the identity $L_X(Y\lrcorner\omega)=X\lrcorner(L_Y\omega)+[X,Y]\lrcorner\omega$ for any vector fields X,Y and any 2-form ω, we find

$$
\begin{aligned}
[\hat{X}_{\hat{f}}^{(I},\hat{X}_{\hat{g}}^{J}]\lrcorner\omega^{\alpha)} &= L_{\hat{X}_{\hat{f}}^{(I}}(\hat{X}_{\hat{g}}^{J}\lrcorner\omega^{\alpha)}) - \hat{X}_{\hat{f}}^{(I}\lrcorner(L_{\hat{X}_{\hat{g}}^{J}}\omega^{\alpha)}) \\
&= L_{\hat{X}_{\hat{f}}^{(I}}(\hat{X}_{\hat{g}}^{J}\lrcorner\omega^{\alpha)}) \quad [\text{by formula (2.21)}] \\
&= \hat{X}_{\hat{f}}^{(I}\lrcorner d(\hat{X}_{\hat{g}}^{J}\lrcorner\omega^{\alpha)}) + d(\hat{X}_{\hat{f}}^{(I}\lrcorner\hat{X}_{\hat{g}}^{J}\lrcorner\omega^{\alpha)}) \\
&= d(\hat{X}_{\hat{f}}^{(I}\lrcorner\hat{X}_{\hat{g}}^{J}\lrcorner\omega^{\alpha)}) \quad (\text{since } d(\hat{X}_{\hat{g}}^{(J}\lrcorner\omega^{\alpha)}) = d^2\hat{g}^{J\alpha} = 0) \\
&= -\frac{1}{q!}d(\hat{X}_{\hat{f}}^{(I}\lrcorner d\hat{g}^{J\alpha)}) \quad [\text{by (2.8)}] \\
&= -\frac{1}{p!q!}d(\{\hat{f},\hat{g}\}^{IJ\alpha}) \quad [\text{by (2.8)}].
\end{aligned}
$$

Hence we have shown that for arbitrary representatives of $[\![\hat{X}_{\hat{f}}]\!]$ and $[\![\hat{X}_{\hat{g}}]\!]$,

$$
d(\{\hat{f},\hat{g}\}^{IJ\alpha}) = -(p!q!)[\hat{X}_{\hat{f}}^{(I},\hat{X}_{\hat{g}}^{J}]\lrcorner\omega^{\alpha)}. \tag{2.23}
$$

Comparing this result with (2.8) we see that

$$
\frac{p!q!}{(p+q-1)!}[\hat{X}_{\hat{f}}^{(I},\hat{X}_{\hat{g}}^{J)}]\hat{r}_{IJ} \in [\![\hat{X}_{\{\hat{f},\hat{g}\}}]\!] \tag{2.24}
$$

holds for arbitrary representatives. The lemma follows. ■

Corollary II.7:

$$
\{\hat{f},\hat{g}\} \in SHF^{p+q-1}.
$$

Proof: The corollary follows from (2.23). ■

Theorem II.8: $(SHV,[\![,]\!])$ *is a Lie Algebra*.

Proof: The bracket defined in (2.20) is clearly antisymmetric. To check the Jacobi identity we note that we only need check it for arbitrary representatives, and we may use the very definition (2.20) for the calculation. Since the bracket on the right-hand side in (2.20) is the ordinary Lie bracket for vector fields, we see that the bracket defined in (2.20) also must obey the identity of Jacobi. ■

We can now show that SHF is a Poisson algebra under the bracket defined in (2.19).

Theorem II.9: $(SHF,\{,\})$ *is a Poisson algebra over the commutative algebra* $(SHF,\otimes_s)$.

Proof: The bracket defined in (2.19) is evidently antisymmetric. To check the Jacobi identity one proceeds exactly as in Ref. 3, which used a generalization of a proof given in Ref. 20. The proof of the Jacobi identity is given in the Appendix.

Now the symmetrized tensor product $\otimes_s$ makes SHF into a commutative algebra. If we now consider again elements $\hat{f}\in SHF^p$, $\hat{g}\in SHF^q$, and $\hat{h}\in SHF^r$, then by using definition (2.19) one may show that

$$
\{\hat{f},\hat{g}\otimes_s\hat{h}\} = \{\hat{f},\hat{g}\}\otimes_s\hat{h} + \hat{g}\otimes_s\{\hat{f},h\}. \tag{2.25}
$$

Thus the bracket defined in (2.19) acts as a derivation on the commutative algebra. ■

Example: In the canonical case $P=LE$ the brackets just defined have a well-known interpretation. As mentioned above the homogeneous elements in SHF^p make up the space $ST^p(LE)$, the symmetric rank p GL(n)-tensorial functions that correspond to symmetric rank p contravariant

tensor fields on E. Then $ST=\oplus_{p\geq 1}ST^p\subset SHF$, and the bracket $\{,\}:ST^p\times ST^q\to ST^{p+q-1}$ has been shown[6] to be the frame bundle version of the Schouten–Nijenhuis bracket[16,17] of the corresponding symmetric tensor fields on E.

Remark: There is also a Schouten–Nijenhuis bracket for antisymmetric contravariant tensor fields on E, and as one might expect this bracket also extends to LE. This leads to a graded n-symplectic Poisson algebra of tensor-valued functions on LE.[5]

III. THE CANONICAL n-SYMPLECTIC STRUCTURE ON $L_\pi E$

In this section we present a few additional details about canonical n-symplectic geometry on frame bundles that will be needed later. An adapted frame at $e\in E$ is a frame where the last k basis vectors are vertical. Note that coordinate frames that come from adapted coordinates are adapted frames. The adapted frame bundle of π, denoted $L_\pi E$, consists of all adapted frames for E,

$$L_\pi E=\{(e,\{e_i,e_A\}):e\in E,\{e_i,e_A\} \text{ is a basis for } T_eE, \text{ and } d_u\pi(e_A)=0\}.$$

We will use the same notation $\lambda:L_\pi E\to E$ to denote the restriction of the projection from LE to $L_\pi E$.

$L_\pi E$ is a reduced subbundle of LE,[15] the frame bundle of E. As such it is a principal fiber bundle over E. Its structure group is G_v, the nonsingular block lower triangular matrices,

$$G_v=\left\{\begin{pmatrix} A & 0\\ C & B\end{pmatrix}:A\in \mathrm{GL}(m),B\in \mathrm{GL}(k),C\in \mathbb{R}^{km}\right\}.$$

G_v acts on $L_\pi E$ on the right by

$$(e,\{e_i,e_A\})\cdot\begin{pmatrix} A & 0\\ C & B\end{pmatrix}=\{(e,\{e_iA^i_j+e_AC^A_j,e_AB^A_B\}).$$

Coordinates on $L_\pi E$:

If $(z^\alpha)=(x^i,y^A)$ are adapted coordinates on an open set $U\subseteq E$, then one may induce several different coordinates on $\lambda^{-1}(U)$. Coframe or n-symplectic momentum coordinates $(z^\alpha,\pi^i_j,\pi^A_j,\pi^A_B)$ on $\lambda^{-1}(U)$ are defined as follows. Let $u=(e,\{e_i,e_A\})$ denote a general point in $L_\pi E$. Then

$$z^\alpha(u)=z^\alpha(e),\quad \pi^i_j(u)=e^i\left(\frac{\partial}{\partial x^j}\right),\quad \pi^A_B(u)=e^A\left(\frac{\partial}{\partial y^B}\right),\quad \pi^A_j(u)=e^A\left(\frac{\partial}{\partial x^j}\right). \tag{3.1}$$

Here (e^i,e^A) is the coframe dual to (e_i,e_A), and as is customary we have retained the same symbols z^α for the induced horizontal coordinates. Note that the remaining coordinate functions $\pi^i_A(u)=e^i(\partial/\partial y^A)$ are identically zero on $L_\pi E$.

Frame or n-symplectic velocity coordinates $(z^\alpha,v^i_j,v^A_j,v^A_B)$ on $\lambda^{-1}(U)$ are defined by

$$z^\alpha(u)=z^\alpha(e),\ v^i_j(u)=e_j(x^i),\ v^A_B(u)=e_B(y^A),\ v^A_j(u)=e_j(y^A). \tag{3.2}$$

The v coordinates, viewed together as a block triangular matrix, form the inverse of the π coordinates above. The blocks have the following relations:

$$v^i_j\pi^j_k=\delta^i_k,\quad v^A_j\pi^j_k+v^A_B\pi^B_k=0,\quad v^A_B\pi^B_C=\delta^A_C.$$

Finally we define Lagrangian coordinates, which are constructed from the previous two coordinate systems,

$$z^\alpha(u)=z^\alpha(e),\quad u^i_j=\pi^i_j,\quad u^A_B=\pi^A_B,\quad u^A_j=v^A_i\pi^i_j=-v^A_B\pi^B_j. \tag{3.3}$$

The name Lagrangian coordinates refers to the fact, shown in Ref. 9, that the u^A_j coordinates are pull-ups, under the projection ρ defined in the next setion, of the standard jet coordinates on $J^1\pi$.

Later in the paper we will need the following formulas for the fundamental vertical vector fields $E^{*\alpha}_\beta$ on $L_\pi E$ in Lagrangian coordinates,

$$E^{*i}_j = -u^i_k \frac{\partial}{\partial u^j_k}, \quad E^{*A}_B = -u^A_C \frac{\partial}{\partial u^B_C}, \quad E^{*i}_A = u^i_k v^B_A \frac{\partial}{\partial u^B_k}. \tag{3.4}$$

IV. THE MODIFIED *n*-SYMPLECTIC STRUCTURE DEFINED BY A LAGRANGIAN *L*

To bring the Lagrangian into the n-symplectic picture, McLean and Norris[9] showed that $L_\pi E$ is a principal $H=\mathrm{GL}(m)\times\mathrm{GL}(k)$ bundle over the bundle $J^1\pi$ of 1-jets of sections of π. Letting $\rho: L_\pi E \to J^1\pi$ denote the projection, McLean and Norris then defined the CHP 1-forms θ^α_L on $L_\pi E$ as follows. If $\mathcal{L}$ is a Lagrangian on $J^1\pi$, the lifted Lagrangian is $\mathrm{L}=\rho^*(\mathcal{L})$. Define θ^α_L by

$$\theta^i_L := \tau \mathrm{L}\, \theta^i + E^{*i}_A(\mathrm{L})\, \theta^A, \tag{4.1}$$

$$\theta^A_L := \theta^A, \tag{4.2}$$

where $\tau=\tau(m)$ is a positive constant depending only on the dimension m of the base manifold M, and E^{*i}_A denotes the fundamental vertical vector field on $L_\pi E$ [see (3.4) above] corresponding to the element E^i_A in the standard basis (E^α_β) of $\mathrm{gl}(n)$. The quantities $E^{*i}_A(\mathrm{L})$, referred to as the "covariant canonical momenta" in Ref. 9, are globally defined on $L_\pi E$. In local canonical coordinates (z^α, π^μ_ν), these quantities have the local expressions,

$$E^{*i}_A(\mathrm{L}) = \pi^i_j p^j_B v^B_A, \quad p^j_B = \frac{\partial \mathrm{L}}{\partial u^B_j}, \tag{4.3}$$

and clearly are the frame components of the "canonical field momenta" $p^j_B = \partial \mathrm{L}/\partial u^B_j$. For different values of τ one can obtain the de Donder–Weyl theory[21,22] and the Caratheodory theory[23,22] as special cases of the formalism presented in Ref. 9. The significance of these CHP 1-forms as regards other geometrical theories was also considered by MacLean and Norris. In Ref. 9 it was shown that one may construct the CHP m-form on $J^1\pi$ from the CHP 1-forms on $L_\pi E$. In this regard see also Refs. 5, 8, 15.

It is clear from the definitions (4.1) and (4.2) that the CHP 1-forms have the property that

$$X \lrcorner \theta^\alpha_{\mathrm{L}} = 0 \,\forall\, \alpha = 1,2,\ldots,n \Leftrightarrow d\lambda(X) = 0.$$

Because of this property we can think of the CHP 1-forms as "modified soldering 1-forms," although the θ^α_L may not have the same transformation property under right translation as do the θ^α because of the presence of the Lagrangian L. However, by restricting attention to the H bundle $\rho: L_\pi E \to J^1\pi$, we can show that the θ^α_L are tensorial with respect to H transformations.

Lemma IV.1: For all $h \in H$ the CHP 1-forms θ^α_L satisfy the tensorial transformation law,

$$R^*_h(\theta^\alpha_L) = (h^{-1})^\alpha_\beta \theta^\beta_L. \tag{4.4}$$

Proof: The CHP 1-forms given in (4.1) and (4.2) can be expressed, using the Lagrangian coordinates defined in (3.3) above, in the form,

$$\theta^i = u^i_j(-\mathcal{H}^j_k dx^k + p^j_B dy^B), \tag{4.5}$$

$$\theta^A = u^A_B(-u^A_k dx^k + dy^B), \tag{4.6}$$

where we have introduced the definitions,

$$\mathcal{H}^i_j := p^i_A u^A_j - \tau \mathrm{L}\,\delta^i_j, \quad p^i_A := \frac{\partial \mathrm{L}}{\partial u^A_i}. \tag{4.7}$$

Using the additional definitions

$$(h^\alpha_\beta) = \begin{pmatrix} -\mathcal{H}^k_j & p^k_A \\ -u^E_j & \delta^E_A \end{pmatrix}, \quad ((\Delta u)^\alpha_\beta) = \begin{pmatrix} u^k_j & 0 \\ 0 & u^E_A \end{pmatrix}, \tag{4.8}$$

Eqs. (4.5) and (4.6) can be written in the following compact form:

$$\theta^\alpha_L = ((\Delta u)^\alpha_\beta) h^\beta_\gamma dz^\gamma. \tag{4.9}$$

The matrix $((\Delta u)^\alpha_\beta)$ in (4.9) transforms under the group H of the bundle $\rho: L_\pi E \to J^1\pi$ while the second factor (h^α_β) is H-invariant. In particular, $R^*_h((\Delta u)^\alpha_\mu) = (h^{-1})^\alpha_\beta (\Delta u)^\beta_\mu$. The lemma follows. ■

The lemma shows that the CHP 1-forms do behave like modified soldering 1-forms with respect to the bundle $\rho: L_\pi E \to J^1\pi$. The geometrical significance of the lemma is that the CHP-forms define a set of type 1–1 tensor fields on the jet bundle $J^1\pi$. To see this we recall that the canonical soldering 1-forms θ^α define the type 1–1 *identity tensor field* on E. The construction is as follows. Let $u = (e, e_\beta) \in LE$ be an arbitrary point in the bundle of frames of E. The coframe to (e_β) may be written as $(e^\beta = \pi^\beta_\alpha(u) dz^\alpha)$. Then $\hat{\theta} = (\theta^\alpha)$ defines the identity type 1–1 tensor field on E as follows:

$$\hat{\theta}(u) = (\pi^\alpha_\beta dz^\beta)(u) \otimes r_\alpha \to \pi^\alpha_\beta(u) dz^\beta \otimes e_\beta = e^\beta \otimes e_\beta = I_e. \tag{4.10}$$

The tensorial transformation property of $\hat{\theta}$ on LE or any of its subbundles guarantees that the 1–1 tensor field defined in (4.10) is well-defined. We can use a similar construction to define a 1–1 tensor field on $J^1\pi$ based on the CHP 1-forms.

Let $u = (e, e_\beta) \in L_\pi E$ be an arbitrary point in the bundle of adapted linear frames of E, and let $v = \rho(u) \in J^1\pi$ be the projection to $J^1\pi$. Then we define a 1–1 tensor field T on $J^1\pi$ as follows:

$$\begin{aligned} \hat{\theta}_L(u) \to T(v) &= \theta^i_L(u) \otimes e_i + \tau L(u)\, \theta^A_L \otimes e_A \\ &= ((\Delta u)^i_\beta)(u) h^\beta_\gamma(u) dz^\gamma \otimes e_i + \tau L(u) ((\Delta u)^A_\beta)(u) h^\beta_\gamma(u) dz^\gamma \otimes e_A. \end{aligned} \tag{4.11}$$

Notice the inclusion of the H-invariant factor $\tau L(u)$ in the definition.

It is easy to show from the definitions that $((\Delta u)^i_\beta)(u) e_i = \delta^i_\beta((\partial/\partial x^i) + u^A_i(v)\,(\partial/\partial y^A))$ and $((\Delta u)^A_\beta)(u) e_A = \delta^A_\beta(\partial/\partial y^A)$. Using these results together with the definition (4.7) in the last equation we can rewrite it as

$$T(v) = (-\mathcal{H}^i_j) dx^k \otimes \frac{\partial}{\partial x^i} - (u^B_k p^j_B u^A_j) dx^k \otimes \frac{\partial}{\partial y^A} + (p^j_A) dy^A \otimes \frac{\partial}{\partial x^j} + (p^j_B u^A_j + \tau L\, \delta^A_B) dy^B \otimes \frac{\partial}{\partial y^A}. \tag{4.12}$$

T is well-defined since the right-hand side of the definition of $T(v)$ is H-invariant. Hence the CHP 1-forms define a type 1–1 tensor field on $J^1\pi$, whose independent components with respect to any canonical chart on $L_\pi E$ are, after omitting minus signs:

$$\text{(a)} \quad (\mathcal{H}^i_j) dx^k \otimes \frac{\partial}{\partial x^i} \quad \text{the energy-momentum tensor of the field,} \tag{4.13}$$

$$\text{(b)} \quad (p^j_A) dy^A \otimes \frac{\partial}{\partial x^j} \quad \text{the canonical field momentum,} \tag{4.14}$$

$$\text{(c)} \quad (u_k^B p_B^j u_j^A) dx^k \otimes \frac{\partial}{\partial y^A} \quad \text{the canonical field momentum summed with field velocities} \tag{4.15}$$

$$\text{(d)} \quad (p_B^j u_j^A + \tau \mathrm{L} \delta_B^A) dy^B \otimes \frac{\partial}{\partial y^A} \quad \text{a new energy-momentum-type field.}$$

These tensor fields will be of importance in the application presented in Sec. VI.

The Legendre transformation: One can define the CHP 1-forms using a frame bundle version of the Legendre transformation. Given a Lagrangian $L: L_\pi E \to \mathbb{R}$ we obtain a mapping $\phi_L : L_\pi E \to LE$ given by

$$\phi_L(u) = \phi_L(e, e_i, e_A) = \left(e, \frac{1}{\tau L(u)} e_i, e_A - \frac{1}{\tau L(u)} E_A^{*a}(L)(u) e_a \right). \tag{4.16}$$

The condition that this mapping end up in LE is that the Lagrangian be **nonzero**, and *for the rest of this paper we will assume this condition*. We will refer to this mapping as the *n-symplectic Legendre transformation*. Our goal is to prove Theorem (IV.6), namely, that $\hat{\theta}_L = \phi_L^*(\hat{\theta})$, where $\hat{\theta}$ is the canonical soldering 1-form on the image of ϕ_L. This will follow easily once we exhibit the manifold structure of Q_L.

Lemma IV.2: If the lifted Lagrangian is nonzero, then the Legendre transformation (4.16) *is one-one.*

Proof: If $\phi_L(u) = \phi_L(\overline{u})$ then the two adapted frames must project to the same point in E. Equating vectors in the frame we find $[1/\tau \mathrm{L}(\overline{u})]\overline{e_i} = [1/\tau \mathrm{L}(u)] e_i$ and $\overline{e_A} - [1/\tau \mathrm{L}(\overline{u})] E_A^{*a}(\mathrm{L}) \times (\overline{u}) \overline{e_a} = e_A - [1/\tau \mathrm{L}(u)] E_A^{*a}(\mathrm{L})(u) e_a$. Using the first of these relations in the second and rearranging we obtain

$$\overline{e_A} - e_A = (E_A^{*a}(L)(\overline{u}) - E_A^{*a}(L)(u)) \frac{1}{\tau L(u)} e_i .$$

Since both $\overline{e_A}$ and e_A are vertical on E this implies that $(E_A^{*a}(L)(\overline{u}) - E_A^{*a}(L)(u)) = 0$. Hence $\overline{e_A} = e_A$ and $[1/\tau \mathrm{L}(\overline{u})]\overline{e_i} = [1/\tau \mathrm{L}(u)] e_i$. This implies that $\overline{u} = u \cdot h$ for $h \in H \subset G_V$. But since the Lagrangian L is lifted, it is H invariant and so $L(\overline{u}) = L(u)$, which implies that $\overline{u} = u$. ■

To clarify the meaning of the Legendre transformation (4.16) we introduce a new manifold $\tilde{P}$ as follows. Let J denote the subgroup of $\mathrm{GL}(n)$ consisting of matrices of the form,

$$\begin{pmatrix} I & \xi \\ 0 & I \end{pmatrix} \quad \xi \in \mathbb{R}^{m \times k}.$$

Define $\tilde{P}$ by

$$\tilde{P} = L_\pi E \cdot J = \{ (e_i, e_A + \xi_A^j e_j) \,|\, (e_i, e_A) \in L_\pi E, \xi \in \mathbb{R}^{m \times k} \}. \tag{4.17}$$

Lemma IV.3: $\tilde{P}$ is a open dense submanifold of the bundle of frames LE of E.

Proof: Private communication from Mike McLean. ■

Lemma IV.4: There is a canonical diffeomorphism from $\tilde{P}$ to the product manifold $L_\pi E \times \mathbb{R}^{m \times k}$.

Proof: If (e, e_i, e_A) is a point in $L_\pi E$, then we let $\tilde{e}_i = \pi_*(e_i)$. From the structure of $L_\pi E$ it is clear that $(\tilde{e}_i)$ is a linear frame for the tangent space to M at $\pi(e)$. Let $(\tilde{e}^i)$ denote the coframe dual to $(\tilde{e}_i)$. Now suppose $\overline{u} = (\overline{e_i}, \overline{e_A}) = (e_i, e_A + \xi_A^j e_j)$ is an arbitrary point in $\tilde{P}$. Then we have $\pi_*(\overline{e_i}) = \tilde{e}_i$. Using the fact that each e_A is vertical we have $\pi_*(\overline{e_A}) = \xi_A^i \tilde{e}_i$. Hence,

$$\xi_A^i = \tilde{e}^i(\pi_*(\overline{e_A})). \tag{4.18}$$

Define a mapping from $\tilde{P}$ to $L_\pi E \times \mathbb{R}^{m\times k}$ by

$$\overline{u} = (\overline{e_i}, \overline{e_A}) \to ((e_i, e_A), \xi_A^i) = ((\overline{e_i}, \overline{e_A} - \tilde{e}^j(\pi_*(\overline{e_A}))\overline{e_j}), \tilde{e}^i(\pi_*(\overline{e_A}))). \tag{4.19}$$

The mapping (4.19) is easily shown to be 1–1, and it is clearly smooth. The inverse mapping is the multiplication mapping $\mu: L_\pi E \times \mathbb{R}^{m\times k} \to \tilde{P}$ defined by

$$\mu((e_i, e_A), \xi_B^j) = (e_i, e_A + \xi_A^j e_j). \tag{4.20}$$

This inverse is evidently smooth. ■

Remark: The coordinate expression for this mapping is

$$\overline{u} = (\overline{e_i}, \overline{e_A}) \to ((e_i, e_A), \xi_A^i) = ((\overline{e_i}, \overline{e_B} - \overline{\pi}_A^j(\overline{u})\overline{V}_B^A(\overline{u})\overline{e_j}), -\overline{\pi}_A^j(\overline{u})\overline{V}_B^A(\overline{u})), \tag{4.21}$$

where $\overline{V}_B^A(\overline{u}) = v_B^A(u)$ are the components of the matrix inverse of the matrix $(\overline{\pi}_B^A(\overline{u})) = (\pi_B^A(u))$, which must necessarily be nonsingular because of the structure of $L_\pi E$. In the following we let $\overline{\rho}: L_\pi E \times \mathbb{R}^{m\times k} \to L_\pi E$ be the natural projection.

Suppose we are given a Lagrangian L on $L_\pi E$. Then it is easy to see that the Legendre transformation (4.16) can be expressed as the composition $\phi_L = \mu \circ \phi_2 \circ \phi_1$, where μ is the multiplication map defined in (4.20) above, ϕ_1 is the bundle automorphism

$$\phi_1: L_\pi E \to L_\pi E, \quad \phi_1(e_i, e_A) = \left(\frac{1}{\tau \mathrm{L}(u)} e_i, e_A\right), \tag{4.22}$$

and the mapping ϕ_2 is the global section of $\overline{\rho}$ given by

$$\phi_2(u) = \phi_2(e_i, e_B) = \left((e_i, e_B), -\frac{E_A^{*j}(L)(u)}{\tau L(u)}\right). \tag{4.23}$$

The mapping ϕ_1 is 1–1 since the Lagrangian L is invariant under the subgroup H, and $\overline{u} = \phi_1(u) = u \cdot h$ for

$$h = \begin{pmatrix} \tau \mathrm{L}(u) I & 0 \\ 0 & I \end{pmatrix}.$$

Q_L is then the image of $L_\pi E$ in $\tilde{P}$ under the C^∞ Legendre transformation. In particular, Q_L is the smooth image under the multiplication map of the global section $\phi_2(L_\pi E)$ of $\overline{\rho}: L_\pi E \times \mathbb{R}^{m\times k} \to L_\pi E$, and hence is a smooth manifold. The inverse of the Legendre transformation is then the composition $\phi_L^{-1} = \phi_1^{-1} \circ \phi_2^{-1} \circ \mu^{-1}$, where ϕ_2^{-1} is the projection $\overline{\rho}$ restricted to $\mu^{-1}(Q_L,)$ and $\phi_1^{-1}(\overline{u}) = \phi_1^{-1}(\overline{e_i}, \overline{e_A}) = (\mathrm{L}(\overline{u})\overline{e_i}, \overline{e_A})$. The inverse is thus also C^∞, and we have:

Lemma IV.5: If the Lagrangian L is nonzero, then the Legendre transformation $\phi_L: L_\pi E \to Q_L$ is a diffeomorphism.

Theorem IV.6: *Let L be the pull-up of a nonzero Lagrangian $\mathcal{L}$ on $J^1\pi$, and let ϕ_L denote the Legendre transformation defined above in* (4.16). *Then,*

$$\hat{\theta}_L = \phi_L^*(\hat{\theta}). \tag{4.24}$$

Proof: A straightforward calculation.

Remark: This theorem has an obvious analog in symplectic mechanics, where the symplectic form on the velocity phase space TE is, for a regular Lagrangian, the pull back under the Legendre

transformation of the canonical 1-form on T^*M. There is also a similar theorem in multisymplectic geometry where the CHP m- form on $J^1\pi$ is known[14] to be the pull back of the canonical multisymplectic m-form on $J^{1*}\pi$.

Now Q_L, being a submanifold of LE, supports the restriction $\hat{\theta}|_{Q_L}$ of the $\mathbb{R}^n$-valued soldering 1-form $\hat{\theta}$. It is easy to verify that the closed $\mathbb{R}^n$-valued 2-form $d\hat{\theta}|_{Q_L}$ is also nondegenerate, and hence $(Q_L, d(\hat{\theta}|_{Q_L}))$ is an n-symplectic manifold. Using the fact that Q_L and $L_\pi E$ are diffeomorphic under the Legendre transformation, we obtain the following corollary to Theorem IV.6.

Corollary IV.7: $(L_\pi E, d\hat{\theta}_L)$ *is an n-symplectic manifold.*

Remark: It is also not difficult to show by direct calculation that $d\hat{\theta}_L$ is nondegenerate.

We would now like to be able to find the n-symplectic observables defined by the n-symplectic structure $d\hat{\theta}_L$ on $L_\pi E$. However, since the new n-symplectic structure is not in canonical form in standard canonical coordinates (z^α, π^μ_ν), it is rather difficult to find the observables. This fact can be clarified as follows.

The local forms given above in (2.12) of the canonical n-symplectic algebras on LE were given in Ref. 3, and were found by solving the equations

$$L_{X^{(I}_{\hat{f}}} d\theta^{\alpha)} = 0 \tag{4.25}$$

for the locally n-symplectic Hamiltonian vector fields. Lawson[15] used the same technique to characterize the reduced algebra on $L_\pi E$ by solving the equations

$$L_{X^{(I}_{\hat{f}}} d(\theta|_{L_\pi E})^{\alpha)} = 0. \tag{4.26}$$

In both cases the equations were tractable because the n-symplectic forms could be written in canonical coordinates. On the other hand the equations $L_{X^{(I}_{\hat{f}}} d\theta^{\alpha)}_{\mathrm{L}} = 0$ are very complicated and are not easily solved. To get around this problem we will use Corollary (IV.7). If we identify the n-symplectic algebra on the n-symplectic manifold $(Q_L, d(\hat{\theta}|_{Q_L}))$, then we can use the Legendre transformation to transform back to $L_\pi E$. In particular, if $\hat{f}$ and $\hat{X}_{\hat{f}}$ satisfy the equation

$$d\hat{f} = -\hat{X}_{\hat{f}} \lrcorner d(\hat{\theta}) \tag{4.27}$$

on Q_{L}, then $\phi_L^*(\hat{f})$ and $\phi_{L*}^{-1}(\hat{X}_{\hat{f}})$ satisfy the equation

$$d(\phi_L^*(\hat{f})) = -\phi_{L*}^{-1}(\hat{X}_{\hat{f}}) \lrcorner d(\phi_L^*(\hat{\theta})) \tag{4.28}$$

on $L_\pi E$.

V. *n*-SYMPLECTIC REDUCTION

In order to characterize the n-symplectic observables on $(Q_L, d(\hat{\theta}|_{Q_L}))$ we will find a reduction of the n-symplectic geometry of $(\tilde{P}, d\hat{\theta})$ to $(Q_L, d(\hat{\theta}|_{Q_L}))$. Let $i: Q_L \to \tilde{P}$ be the inclusion mapping, and let $\hat{f}: \tilde{P} \to \mathbb{R}^n$ be an $\mathbb{R}^n$-valued observable for the canonical n-symplectic geometry on $(\tilde{P}, d\hat{\theta})$ such that its Hamiltonian vector field $\hat{X}_{\hat{f}}$ is tangent to Q_L at points of Q_L. Then on Q_L we have

$$d(i^*\hat{f}) = -\hat{X}_{\hat{f}} \lrcorner d(i^*\hat{\theta}). \tag{5.1}$$

This follows from the fact that $i_*(i_*^{-1}(\hat{X}_{\hat{f}})) = \hat{X}_{\hat{f}}$ at points of Q_L when $\hat{X}_{\hat{f}}$ is tangent to Q_L. Let $SHF|_{Q_L}$ be the restriction to Q_L of the subset of SHF on $\tilde{P}$ such that the corresponding Hamil-

tonian vector fields are tangent to Q_L at points of Q_L. The set $SHF|_{Q_L}$ will be the reduced symmetric n-symplectic algebra defined by the Lagrangian L. To find the reduced algebra we will derive the equations that $\hat{X}_{\hat{f}}$ must satisfy in order to be tangent to Q_L.

Define new coordinates on Q_L using the Legendre transformation to pull back the Lagrangian coordinates $(z^\alpha, u^i_j, u^A_k, u^A_B)$ define in (3.3) above. We let

$$\tilde{u}^\alpha = z^\alpha \circ \phi_L^{-1}, \quad \tilde{u}^i_j = u^i_j \circ \phi_L^{-1}, \quad \tilde{u}^A_B = u^A_B \circ \phi_L^{-1}, \quad \tilde{u}^A_j = u^A_j \circ \phi_L^{-1}. \tag{5.2}$$

Then the local vector fields

$$\frac{\partial}{\partial \tilde{u}^\alpha}, \quad \frac{\partial}{\partial \tilde{u}^i_j}, \quad \frac{\partial}{\partial \tilde{u}^A_j}, \quad \frac{\partial}{\partial \tilde{u}^A_B} \tag{5.3}$$

form a local basis of the tangent spaces of Q_L. Any vector field that is tangent to Q_L can be expressed locally in terms of this local basis. We first consider a rank 1 Hamiltonian vector field on $\tilde{P}$ given by [see (2.16)]

$$\hat{X}_{\hat{f}} = f^\alpha \frac{\partial}{\partial \overline{z}^\alpha} - \left(\frac{\partial f^\beta}{\partial \overline{z}^\gamma} \overline{\pi}^\alpha_\beta \right) \frac{\partial}{\partial \overline{\pi}^\alpha_\gamma} \tag{5.4}$$

corresponding to the observable $\hat{f}^\alpha = f^\beta(e)\,\overline{\pi}^\alpha_\beta$. We suppose that this vector field can be expanded in the basis 5.3 and write

$$\hat{X}_{\hat{f}} = X^\alpha \frac{\partial}{\partial \tilde{u}^\alpha} + X^i_j \frac{\partial}{\partial \tilde{u}^i_j} + X^A_B \frac{\partial}{\partial \tilde{u}^A_B} + X^A_j \frac{\partial}{\partial \tilde{u}^A_j}. \tag{5.5}$$

Equating these two forms for $\hat{X}_{\hat{f}}$ and using the fact [see (4.9)] that $\overline{\pi}^\alpha_\beta \circ \phi_L = (\Delta u)^\alpha_\sigma h^\sigma_\beta$ we find $X^\alpha = f^\alpha$ and

$$-\frac{\partial f^\sigma}{\partial \overline{z}^\beta} \overline{\pi}^\alpha_\sigma = X^\sigma \widetilde{\frac{\partial h^\kappa_\beta}{\partial z^\sigma}} (\Delta \tilde{u})^\alpha_\kappa + X^i_j \delta^\alpha_i \widetilde{h^j_\beta} + X^A_B \delta^\alpha_A \widetilde{h^B_\beta} + X^A_k (\Delta \tilde{u})^\alpha_\kappa \widetilde{\frac{\partial h^\kappa_\beta}{\partial u^A_k}}, \tag{5.6}$$

where the ''over tildes'' indicate that the term is to be evaluated in the new coordinates (5.2). These equations can be solved for the coefficients X^i_j, X^A_B, and X^A_k in terms of the components of $\partial h^\kappa_\beta / \partial u^A_k$, plus the following constraint equation:

$$-\frac{df^\sigma}{d\overline{z}^B} \tilde{h}^b_\sigma = f^\sigma \widetilde{\frac{\partial p^b_B}{\partial z^\sigma}} - \frac{df^b}{d\overline{z}^I} \tilde{p}^i_B - \frac{1}{\tau L} \left(f^\sigma \widetilde{\frac{\partial L}{\partial z^\sigma}} + \frac{df^\sigma}{\overline{z}^k} \tilde{p}^i_A \tilde{h}^A_\sigma \right) \tilde{p}^b_B + \frac{df^\sigma}{d\overline{z}^k} \tilde{h}^A_\sigma \widetilde{\frac{\partial p^b_B}{\partial u^A_k}}. \tag{5.7}$$

We next consider a rank 1 Hamiltonian vector field on P given by [see (2.16)]

$$\hat{X}_{\hat{f}} = \frac{\partial \xi^\alpha}{\partial \overline{z}^\gamma} \frac{\partial}{\partial \overline{\pi}^\alpha_\gamma} \tag{5.8}$$

corresponding to the observable $\hat{f}^\alpha = \xi^\alpha(e)$. Carrying out the same calculuation that we did for $\hat{f}^\alpha = f^\beta(e)\,\overline{\pi}^\alpha_\beta$ above we find the constraint equation

$$-\tau L \frac{\partial \xi^a}{\partial \overline{z}^b} = \tilde{p}^e_D \left(-\frac{d\xi^a}{d\overline{z}^e} + \tilde{u}^a_b \frac{d\xi^E}{d\overline{z}^k} \tilde{v}^A_E (-\tilde{p}^k_A \delta^b_e + \tilde{p}^b_A \delta^k_e) \right) + \tau \mathrm{L} \frac{d\xi^E}{d\overline{z}^k} \tilde{v}^A_E \tilde{u}^a_b \widetilde{\frac{\partial p^b_D}{\partial u^A_k}}. \tag{5.9}$$

An n-symplectic observable $\hat{f} = (f^\beta \overline{\pi}^\alpha_\beta + \xi^\alpha) r_\alpha$ on $\tilde{P}$ will be in $SHF|_{Q_L}$ if and only if it satisfies the two constraint Eqs. (5.7) and (5.9).

VI. APPLICATION: *k*-TUPLE OF MASSLESS SCALAR FIELDS ON FLAT SPACE–TIME

As an application of the general theory we will study the rank-1 n-symplectic subalgebra of observables that is defined by the simple model of a k-tuple of massless scalar fields on Minkowski space–time. Analysis of the more complicated higher rank portions of the algebra will be left for future work. For the k-tuple of massless scalar fields the bundle $\pi:E\to M$ over Minkowski space–time M is a trivial vector bundle with standard fiber $\mathbb{R}^k$. Such a system has a lifted Lagrangian of the form $L=\frac{1}{2}g^{ab}\delta_{AB}u_a^A u_b^B$, where g^{ab} are the contravariant components of the Minkowski metric tensor in arbitrary coordinates on the space–time manifold and δ_{AB} are the components of the Euclidean metic tensor for the internal space $\mathbb{R}^k$. Since global inertial coordinates exist on Minkowshi space–time, we will for the calculations restrict attention to canonical coordinates on LE that are induced by such inertial coordinates on space–time. Then the components of the metric tensor field will take the constant Minkowski form $(\eta^{ab})=\mathrm{diag}(-1,1,1,1)$, and the Lagrangian will be

$$\mathrm{L}=\tfrac{1}{2}\eta^{ab}\delta_{AB}u_a^A u_b^B. \tag{6.1}$$

Using this Lagrangian for the k-tuple of scalar fields on Minkowski space–time we find the standard result

$$p_A^i=\eta^{ij}\delta_{AB}u_j^B. \tag{6.2}$$

We observe that for this Lagrangian Eqs. (5.7) and (5.9) are satisfied by $f^\alpha=C^\alpha=$constant and $\xi^\alpha=K^\alpha=$constant.

Theorem VI.1: *The rank-1 n-symplectic Hamiltonian vector field (2.16) for the n-symplectic manifold* $(\tilde{P},d\hat{\theta})$ *will satisfy the reduction Eqs. (5.7) and (5.9) for the Lagrangian of the k-tuple of massless scalar fields on Minkowski space–time if*

$$f^\alpha=C^\alpha=\text{constant},\xi^\alpha=K^\alpha=\text{constant}. \tag{6.3}$$

Remark: We recall from Eq. (2.10) that the rank-1 algebra $HF^1=T^1(LE)\oplus C^\infty(E,\mathbb{R}^{m+k})$ is the direct sum of the rank-1 tensorial functions $T^1(LE)$ on LE that correspond uniquely to vector fields on E, with the $\mathbb{R}^{m+k}$-valued functions $C^\infty(LE,\mathbb{R}^{m+k})$ that are constant on fibers of LE, i.e., $C^\infty(E,\mathbb{R}^{m+k})$. The above theorem tells us that the subalgebra corresponding to the tensorial functions is a copy of the translation symmetry group $\mathbb{R}^{m+k}$ of the base manifold $E=\mathbb{R}^{m+k}$. Hence we may interpret the tensorial part of the rank-1 subalgebra corresponding to $f^\alpha=C^\alpha=$constant as the space of translational Killing vectors for the metrics η on M and δ on the fibers of E. The other part of the algebra, characterized by $\xi^\alpha=K^\alpha=$constant, can be identified also with $\mathbb{R}^{m+k}$. The part of the rank-1 algebra $SHF^1|_{Q_L}$ on Q_L determined by the theorem is therefore

$$\mathcal{G}=\mathbb{R}^{m+k}\oplus\mathbb{R}^{m+k}. \tag{6.4}$$

There is an alternative interpretation of the tensorial part of the rank-1 subalgebra in terms of "n-symplectic momentum mapping." In Ref. 5 it was pointed out that the translation group $\mathbb{R}^{m+k}$ lifts from $E=\mathbb{R}^{m+k}$ to LE to define an n-symplectic momentum mapping, and that for each $(\zeta^\alpha)\in\mathbb{R}^n$ the corresponding "momentum" is $\zeta^\alpha\pi_\alpha^\beta\hat{r}_\beta$. Notice that $\zeta^\alpha\pi_\alpha^\beta\hat{r}_\beta$ is precisely $\hat{\zeta}$, i.e., it is the tensorial function corresponding to the vector field $\zeta^\alpha(\partial/\partial z^\alpha)$ on E. Hence the tensorial part of the rank-1 subalgebra can also be thought of as the "set of all momenta" that arise from the n-symplectic momentum map defined by the lift of $\mathbb{R}^{m+k}$ to LE.

The algebra of observables on $L_\pi E$:

To obtain the n-symplectic algebra on $L_\pi E$ we must pull-back the observables $\hat{f}$ and use the inverse Legendre transformation to map the corresponding Hamiltonian vector fields $\hat{X}_{\hat{f}}$ to $L_\pi E$. Letting C^α and K^α denote constants, we have found rank 1 observables on $L_\pi E$ of the form,

$$\hat{F} := \phi_L^*(C^\alpha \overline{\pi}_\alpha^\beta + K^\alpha) r_\alpha = (C^\alpha \phi_L^*(\overline{\pi}_\alpha^\beta) + K^\alpha) r_\alpha .$$

From (4.9) and (4.24) one can infer that $\phi_L^*(\overline{\pi}_\beta^\alpha) = (\Delta u)_\sigma^\alpha h_\beta^\sigma$. Hence the rank 1 observables on $L_\pi E$ have the form,

$$\hat{F} = ((C^\beta (\Delta u)_\sigma^\alpha h_\beta^\sigma) + K^\alpha) r_\alpha . \tag{6.5}$$

Mapping the Hamitonian vector field $\hat{X}_{\hat{f}} = C^\alpha (\partial/\partial \overline{z}^\alpha)$ corresponding to $(C^\alpha \overline{\pi}_\alpha^\beta + K^\alpha) r_\alpha$ to $L_\pi E$ using $(\phi_L^{-1})_*$ one finds in this special case the simple result

$$(\phi_L^{-1})_* \left(C^\alpha \frac{\partial}{\partial \overline{z}^\alpha} \right) = C^\alpha \frac{\partial}{\partial z^\alpha} . \tag{6.6}$$

Hence for fixed values of C^α and K^α we have the n-symplectic rank 1 equation on $(L_\pi E, d\hat{\theta}_L)$,

$$d(C^\beta (\Delta u)_\sigma^\alpha h_\beta^\sigma) + K^\alpha) = -\left(C^\beta \frac{\partial}{\partial z^\beta} \right) \lrcorner d\theta_L^\alpha . \tag{6.7}$$

Because K^α are constants, this equation can be rewritten as

$$C^\beta d((\Delta u)_\sigma^\alpha h_\beta^\sigma)) = -\left(C^\beta \frac{\partial}{\partial z^\beta} \right) \lrcorner d\theta_L^\alpha . \tag{6.8}$$

We recall that in Sec. IV we observed that the CHP 1-forms $\theta_L^\alpha = (\Delta u)_\sigma^\alpha h_\beta^\sigma dz^\beta$ define the physical type 1–1 tensor fields on $J^1\pi$ given in Eq. (4.13)–(4.16). The part $\hat{F} = ((C^\beta (\Delta u)_\sigma^\alpha h_\beta^\sigma))\, r_\alpha$ of the rank 1 observable (6.5) will thus correspond to linear combinations of these type 1–1 tensor fields on $J^1\pi$; that is, linear combinations of field velocities, momentum, and energy-momentum tensors.

Remark: Notice that on Q_L the Hamiltonian vector field for the observable $\hat{f} = (C^\alpha \pi_\alpha^\beta + K^\beta)\hat{r}_\beta$ is $C^\alpha (\partial/\partial \overline{z}^\alpha)$, independent of the constants K^α. In fact the kernel of the mapping $HF^1 \to HV^1$ is the set of observables $K^\alpha \hat{r}_\alpha$, where K^α are all constants. Thus the mapping from the Lie algebra of rank-1 observables to the Lie algebra of rank-1 Hamiltonian vector fields is not an isomorphism. In Ref. 5 it was shown that this kernel for rank 1 observables can be removed by lifting the theory to the bundle of affine frames of E, thereby obtaining the desired isomorphism from observables to the vector fields that will serve as the Hamiltonian operators in a geometric quantization theory.

VII. CONCLUSIONS

The formulation of an n-symplectic algebra of observables for a covariant Lagrangian field theory set forth in this paper lays the foundations for a Kostant–Souriau geometric quantization theory of fields. The paper has three main parts. Part one is Sec. II of this paper, in which we developed the n-symplectic Poisson and graded Poisson algebras of observables defined on an abritrary n-symplectic manifold. These algebras paralleled the algebras presented in Ref. 3 for the special case of the bundle of linear frames of an n-dimensional manifold. In part two of the paper, consisting of Secs. III–IV, we set up the n-symplectic covariant field theory on $L_\pi E$ for a Lagrangian field theory. The theory includes the definition of an n-symplectic Legendre transformation, and the subsequent definition of the CHP 1-forms θ_L^α as the pull-back, under the Legendre transformation, of the canonical soldering 1-forms on LE. We then showed that $(L_\pi E, d\hat{\theta}_L)$ is an n-symplectic manifold, and set up the equations of n-symplectic reduction on $(Q_L, d(\hat{\theta}|_{Q_L})$ in order to identify the observables on $L_\pi E$. The third part of the paper, Sec. VI, presents a simple application of the theory to the model of a k-tuple of massless scalar fields on Minkowski space–time. We found that the rank 1 observables contain the translational Killing vectors of the

Minkowski space–time and the Euclidean fibers. When pulled back to $L_\pi E$ these observables correspond to linear combinations of the field velocities, momentum and energy-momentum tensors on $J^1\pi$.

We have pointed out that in the general theory on $L_\pi E$ the mapping from the Lie algebra of observables to the Lie algebra of Hamiltonian vector fields is not an isomorphism, the kernel of the mapping being the set of all constant $\mathbb{R}^n$-valued functions on $L_\pi E$. This is the analog of what occurs on a symplectic manifold. In a geometric quantization theory one needs an isomorphism in order to geometrize the Dirac quantization rules. In the present case one can establish such an isomorphism by lifting the theory to an appropriate affine frame bundle using the results in Ref. 5, where it was shown how to establish this isomorphism for the rank-1 n-symplectic algebras. This result was extended by Cartin to all n-symplectic observables in Ref. 24. We have therefore arrived at the frontiers of a geometric quantization theory of fields based on n-symplectic geometry.

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APPENDIX: PROOF OF THE JACOBI IDENTITY FOR THEOREM 2.9

Let $\hat{X}^I_{\hat{f}}$, $\hat{X}^J_{\hat{g}}$ and $\hat{X}^K_{\hat{h}}$ denote arbitrary sets of representatives of the equivalence classes of Hamiltonian vector fields determined by $\hat{f}\in SHF^p$, $\hat{g}\in SHF^q$, and $\hat{h}\in SHF^r$, respectively, where I,J,K denote the multi-indices $I=\alpha_2\alpha_3\cdots\alpha_p$, $J=\alpha_{p+1}\alpha_{p+2}\cdots\alpha_{p+q-1}$, and $K=\alpha_{p+q}\alpha_{p+q+1}\cdots\alpha_{p+q+r-2}$. Then by using $d\hat{\omega}=0$ and the standard identity for evaluating $d\omega(X,Y,Z)$ for ω a 2-form we obtain

$$\begin{aligned}0&=3d\omega^{(\alpha}(\hat{X}^I_{\hat{f}},\hat{X}^J_{\hat{g}},\hat{X}^{K)}_{\hat{h}})\\&=\hat{X}^{(I}_{\hat{f}}\omega^{\alpha}(\hat{X}^J_{\hat{g}},\hat{X}^{K)}_{\hat{h}})+\hat{X}^{(J}_{\hat{g}}\omega^{\alpha}(\hat{X}^K_{\hat{h}},\hat{X}^{I)}_{\hat{f}})+\hat{X}^{(K}_{\hat{h}}\omega^{\alpha}(\hat{X}^I_{\hat{f}},\hat{X}^{J)}_{\hat{g}})\\&\quad-\omega^{(\alpha}([\hat{X}^I_{\hat{f}},\hat{X}^J_{\hat{g}}],\hat{X}^{K)}_{\hat{h}})-\omega^{(\alpha}([\hat{X}^K_{\hat{h}},\hat{X}^I_{\hat{f}}],\hat{X}^{J)}_{\hat{g}})\\&\quad-\omega^{(\alpha}([\hat{X}^J_{\hat{g}},\hat{X}^K_{\hat{h}}],\hat{X}^{I)}_{\hat{f}}).\end{aligned}\tag{A1}$$

Equations (2.8) and (2.19) can be combined to yield the identity,

$$\omega^{(\alpha}(\hat{X}^I_{\hat{f}},\hat{X}^{J)}_{\hat{g}})=\frac{1}{2p!q!}\{\hat{f},\hat{g}\}^{\alpha IJ}.\tag{A2}$$

Using this formula and formula (2.21) in (A1) we obtain

$$\begin{aligned}0&=\hat{X}^{(I}_{\hat{f}}\left(\frac{1}{2q!r!}\{\hat{g},\hat{h}\}^{JK\alpha)}\right)+\hat{X}^{(J}_{\hat{h}}\left(\frac{1}{2p!q!}\{\hat{f},\hat{g}\}^{IJ\alpha)}\right)+\hat{X}^{(K}_{\hat{g}}\left(\frac{1}{2p!r!}\{\hat{h},\hat{f}\}^{KI\alpha)}\right)\\&\quad-\frac{(p+q-1)!}{p!q!}\omega^{(\alpha}(X^{IJ}_{\{\hat{f},\hat{g}\}},\hat{X}^{K)}_{\hat{h}})-\frac{(p+r-1)!}{p!r!}\omega^{(\alpha}(X^{KI}_{\{\hat{h},\hat{f}\}},\hat{X}^{J)}_{\hat{g}})-\frac{(q+r-1)!}{q!r!}\omega^{(\alpha}(X^{JK}_{\{\hat{g},\hat{h}\}},\hat{X}^{I)}_{\hat{f}}).\end{aligned}$$

Next we use the definition (2.19) in the first three terms and formula (A2) in the last three terms to obtain

$$
\begin{aligned}
0=&\frac{1}{2p!q!r!}\{\hat{f},\{\hat{g},\hat{h}\}\}^L+\frac{1}{2p!q!r!}\{\hat{h},\{\hat{f},\hat{g}\}\}^L+\frac{1}{2p!q!r!}\{\hat{g},\{\hat{h},\hat{f}\}\}^L\\
&-\frac{(p+q-1)!}{p!q!}\left(\frac{1}{2(p+q-1)!r!}\{\{\hat{f},\hat{g}\},\hat{h}\}^L\right)\\
&-\frac{(p+r-1)!}{p!r!}\left(\frac{1}{2(p+r-1)!q!}\{\{\hat{h},\hat{f}\},\hat{g}\}^L\right)\\
&-\frac{(q+r-1)!}{q!r!}\left(\frac{1}{2(q+r-1)!p!}\{\{\hat{g},\hat{h}\},\hat{f}\}^L\right),
\end{aligned}
$$

where the multi-index L denotes (αIJK). Cancelling the common factor $1/p!q!r!$ we obtain

$$
\begin{aligned}
0=&\tfrac{1}{2}\{\hat{f},\{\hat{g},\hat{h}\}\}^L+\tfrac{1}{2}\{\hat{h},\{\hat{f},\hat{g}\}\}^L+\tfrac{1}{2}\{\hat{g},\{\hat{h},\hat{f}\}\}^L-\tfrac{1}{2}\{\{\hat{f},\hat{g}\},\hat{h}\}^L-\tfrac{1}{2}\{\{\hat{h},\hat{f}\},\hat{g}\}^L-\tfrac{1}{2}\{\{\hat{g},\hat{h}\},\hat{f}\}^L\\
=&\{\hat{f},\{\hat{g},\hat{h}\}\}^L+\{\hat{h},\{\hat{f},\hat{g}\}\}^L+\{\hat{g},\{\hat{h},\hat{f}\}\}^L.
\end{aligned}
$$

Hence the n-symplectic bracket defined in (2.19) obeys the identity of Jacobi. ■

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On the stochastic mechanics of the free relativistic particle

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Given a positive energy solution of the Klein–Gordon equation, the motion of the free, spinless, relativistic particle is described in a fixed Lorentz frame by a Markov diffusion process with nonconstant diffusion coefficient. Proper time is an increasing stochastic process and we derive a probabilistic generalization of the equation $(d\tau)^2=-(1/c^2)\mathrm{d}X_\nu \mathrm{d}X_\nu$. A random time-change transformation provides the bridge between the t and the τ domain. In the τ domain, we obtain an $\mathbb{M}^4$-valued Markov process with singular and constant diffusion coefficient. The square modulus of the Klein–Gordon solution is an invariant, nonintegrable density for this Markov process. It satisfies a relativistically covariant continuity equation. [DOI: 10.1063/1.1401135]

I. INTRODUCTION

The purpose of this paper is to discuss a possible scenario for the free, spinless, relativistic particle, extending on Nelson's stochastic mechanics. This challenging problem has generated considerable interest in the past twenty years, see Refs. 1–10, and references therein. As is well known, the main difficulty in this generalization stems from the nonexistence of nontrivial Markov diffusion processes possessing the required relativistic covariance.[11,12] A number of attempts have been made to circumvent this problem, for instance by considering different classes of stochastic processes, see, e.g., Refs. 2, 3, 5, 10.

In this paper we propose a new approach. Corresponding to a positive energy solution of the Klein–Gordon equation, motion of the particle is described in a fixed Lorentz frame by an $\mathbb{R}^3$-valued Markov diffusion process with *nonconstant diffusion coefficient* (local covariance matrix). The role of *proper time* is played here by an increasing stochastic process, namely a *quadratic variation* process. We also derive a natural probabilistic generalization of the equation $(\mathrm{d}\tau)^2=-(1/c^2)\mathrm{d}X_\nu \mathrm{d}X_\nu$. A *random time-change transformation* provides the bridge between the t and the τ domain. In the τ domain, we obtain an $\mathbb{M}^4$-valued Markov process with singular and constant diffusion coefficient. The fourth component is proportional to a stopping time. The square modulus of the Klein–Gordon solution is an invariant, nonintegrable density for this Markov process. It satisfies a relativistically covariant continuity equation.

II. BACKGROUND ON DIFFUSION PROCESSES

In this section, we review some essential concepts and results of the kinematics of stochastic mechanics. We refer to Refs. 13–16 for a thorough account. In order to avoid any confusion, stochastic processes will be denoted by capital letters, as is customary in probability. Let $(\Omega,\mathcal{E},\mathbf{P})$ be a probability space. A stochastic process $\{X(t);t_0\leqslant t\leqslant t_1\}$ mapping $[t_0,t_1]$ into $L_n^2(\Omega,\mathcal{E},\mathbf{P})$ is called a *finite-energy diffusion* with constant diffusion coefficient $I_n\sigma^2$ if the path $X(\omega)$ belongs a.s. to $C([t_0,t_1];\mathbb{R}^n)$ (n-dimensional continuous functions) and

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$$X(t)-X(s)=\int_s^t \beta(\tau)\mathrm{d}\tau+\sigma[W_+(t)-W_+(s)],\quad t_0\leqslant s<t\leqslant t_1, \tag{2.1}$$

where the *forward drift* $\beta(t)$ is at each time t a measurable function of the past $\{X(\tau);0\leqslant\tau\leqslant t\}$, and $W_+(\cdot)$ is a standard, n-dimensional *Wiener process* with the property that $W_+(t)-W_+(s)$ is independent of $\{X(\tau);0\leqslant\tau\leqslant s\}$. Moreover, β must satisfy the finite-energy condition

$$E\left\{\int_{t_0}^{t_1}\beta(t)\cdot\beta(t)\mathrm{d}t\right\}<\infty. \tag{2.2}$$

In Ref. 17, Föllmer has shown that a finite-energy diffusion also admits a reverse-time differential. Namely, there exists a measurable function $\gamma(t)$ of the future $\{X(\tau);t\leqslant\tau\leqslant t_1\}$ called *backward drift*, and another Wiener process W_- such that

$$X(t)-X(s)=\int_s^t \gamma(\tau)\mathrm{d}\tau+\sigma[W_-(t)-W_-(s)],\quad t_0\leqslant s<t\leqslant t_1. \tag{2.3}$$

Moreover, γ satisfies

$$E\left\{\int_{t_0}^{t_1}\gamma(t)\cdot\gamma(t)\mathrm{d}t\right\}<\infty, \tag{2.4}$$

and $W_-(t)-W_-(s)$ is independent of $\{X(\tau);t\leqslant\tau\leqslant t_1\}$. Let us agree that $\mathrm{d}t$ always indicates a strictly positive variable. For any function f defined on $[t_0,t_1]$, let

$$d_+f(t):=f(t+\mathrm{d}t)-f(t)$$

be the *forward increment* at time t, and

$$d_-f(t)=f(t)-f(t-\mathrm{d}t)$$

be the *backward increment* at time t. For a finite-energy diffusion, Föllmer has also shown in Ref. 17 that the forward and backward drifts may be obtained as Nelson's conditional derivatives, namely

$$\beta(t)=\lim_{\mathrm{d}t\searrow 0}E\left\{\frac{d_+X(t)}{dt}\middle| X(\tau),t_0\leqslant\tau\leqslant t\right\}, \tag{2.5}$$

and

$$\gamma(t)=\lim_{\mathrm{d}t\searrow 0}E\left\{\frac{d_-X(t)}{dt}\middle| X(\tau),t\leqslant\tau\leqslant t_1\right\}, \tag{2.6}$$

the limits being taken in $L^2_n(\Omega,\mathcal{B},P)$. It was finally shown in Ref. 17 that the one-time probability density $\rho(\cdot,t)$ of $X(t)$ (which exists for every $t>t_0$) is absolutely continuous on $\mathbb{R}^n$ and the following relation holds $\forall t>0$:

$$E\{\beta(t)-\gamma(t)|X(t)\}=\sigma^2\nabla\log\rho(X(t),t). \tag{2.7}$$

Let us introduce the *current drift* $v(t):=(\beta(t)+\gamma(t))/2$ and the *osmotic drift* $u(t):=(\beta(t)-\gamma(t))/2$. Notice that, when σ tends to zero, v tends to $\dot{X}$, and u tends to zero. The finite-energy diffusion $X(\cdot)$ is called *Markovian* if there exist two measurable functions $b_+(\cdot,\cdot)$ and $b_-(\cdot,\cdot)$ such that $\beta(t)=b_+(X(t),t)$ a.s. and $\gamma(t)=b_-(X(t),t)$ a.s., for all t in $[t_0,t_1]$. The duality relation (2.7) now reads

$$b_+(X(t),t)-b_-(X(t),t)=\sigma^2\nabla\log\rho(X(t),t). \tag{2.8}$$

This immediately gives the *osmotic equation*

$$u(x,t)=\frac{\sigma^2}{2}\nabla\log\rho(x,t), \tag{2.9}$$

where $u(x,t):=(b_+(x,t)-b_-(x,t))/2$. The probability density $\rho(\cdot,\cdot)$ of $X(t)$ satisfies (at least weakly) the *Fokker–Planck equation*

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(b_+\rho)=\frac{\sigma^2}{2}\Delta\rho.$$

The latter can also rewritten, in view of (2.8), as the *equation of continuity* of hydrodynamics

$$\frac{\partial\rho}{\partial t}+\nabla\cdot(v\rho)=0, \tag{2.10}$$

where $v(x,t):=(b_+(x,t)+b_-(x,t))/2$.

Nelson's stochastic mechanics[13,16,14,18] is a quantization procedure for classical dynamical systems based on diffusion processes. Given a quantum evolution $\{\psi(x,t);t_0\leqslant t\leqslant t_1\}$, namely a solution of the Schrödinger equation

$$\frac{\partial\psi}{\partial t}=\frac{i\hbar}{2m}\Delta\psi-\frac{i}{\hbar}V(x)\psi, \tag{2.11}$$

satisfying Carlen's *finite action condition*

$$\|\nabla\psi\|_2^2\in L^1_{\mathrm{loc}}[(t_0,+\infty)], \tag{2.12}$$

it is possible to construct a measure on path-space under which the canonical coordinate process X is a finite-energy Markov diffusion process. Writing $\psi(x,t)=\exp R(x,t)+(i/\hbar)S(x,t)$, we have that the process X has current and osmotic drift fields given, respectively, by $v(x,t)=(1/m)\nabla S(x,t)$, and $u(x,t)=(\hbar/m)\nabla R(x,t)$. In particular, the (forward) Ito differential of X is given by

$$dX(t)=\left[\frac{\hbar}{m}\nabla(\Re\log\psi(X(t),t)+\Im\log\psi(X(t),t))\right]\mathrm{d}t+\sqrt{\frac{\hbar}{m}}dW_+(t), \tag{2.13}$$

see Ref. 19 and Ref. 18, Chap. IV, and references therein. Moreover, the probability density $\rho(\cdot,t)$ of $x(t)$ satisfies

$$\rho(x,t)=|\psi(x,t)|^2,\quad \forall t\in[t_0,t_1]. \tag{2.14}$$

We now need to recall the generalization to Markov processes with diffusion coefficient of the form $I_n\sigma(x,t)^2$, with $\sigma(x,t)\in\mathbb{R}$, the above-mentioned kinematics, see, e.g., Refs. 20–23. Let $\{X(t);t_0\leqslant t\leqslant t_1\}$ be an n-dimensional Markov diffusion process whose increments admit the two representations

$$d_+X(t)=b_+(X(t),t)\mathrm{d}t+\sigma_+(X(t),t)d_+W_+(t), \tag{2.15}$$

$$d_-X(t)=b_-(X(t),t)\mathrm{d}t+\sigma_-(X(t),t)d_-W_-(t), \tag{2.16}$$

where the drifts and diffusion coefficients are sufficiently regular. Here, W_+ and W_- are standard, n-dimensional Wiener processes adapted to the past and the future, respectively, of the process X. Then, the following relations hold:

$$\sigma_+(x,t)=\sigma_-(x,t)=\sigma(x,t), \tag{2.17}$$

$$b_+(x,t)-b_-(x,t)=\frac{1}{\rho}\nabla(\sigma(x,t)^2\rho(x,t)). \tag{2.18}$$

Letting, as usual, $v:=(b_++b_-)/2$ denote the current drift, we have, as before, that the Fokker–Planck equation can be rewritten as the continuity equation (2.10). Let $R(x,t):=\frac{1}{2}\log(\sigma(x,t)^2\rho(x,t))$. Then, observing that (2.18) can be rewritten as

$$b_+(x,t)-b_-(x,t)=\sigma(x,t)^2\nabla\log(\sigma(x,t)^2\rho(x,t)),$$

we get the following expression for the osmotic drift u:

$$u(x,t)=\sigma(x,t)^2\nabla R(x,t). \tag{2.19}$$

III. DESCRIPTION IN A FIXED INERTIAL FRAME

For the definitions and results about continuous martingales that occur in this section, we refer the reader to the Appendix and, for a thorough treatment, to Refs. 24 and 25. Let $\varphi:=\exp[R+(i/\hbar)S]$ be a solution of the Klein–Gordon equation

$$\Delta\varphi-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\varphi=\frac{m^2c^2}{\hbar^2}\varphi \tag{3.1}$$

on $[0,\infty)$, such that S satisfies on the same time interval

$$\frac{\partial S}{\partial t}+c\sqrt{m^2c^2+\nabla S\cdot\nabla S}=0. \tag{3.2}$$

This is precisely the family of solutions that was considered in Ref. 8. Indeed, let

$$\rho(x,t)=\frac{i\hbar}{2mc^2}\left(\overline{\varphi}\frac{\partial\varphi}{\partial t}-\varphi\frac{\partial\overline{\varphi}}{\partial t}\right)(x,t)=|\varphi(x,t)|^2\times\left(-\frac{1}{mc^2}\frac{\partial S}{\partial t}(x,t)\right), \tag{3.3}$$

$$\mathbf{j}(x,t)=\frac{\hbar}{2mi}(\overline{\varphi}\nabla\varphi-\varphi\nabla\overline{\varphi})(x,t)=|\varphi(x,t)|^2\times\left(\frac{1}{m}\nabla S(x,t)\right). \tag{3.4}$$

First of all, observe that because of (3.1), the pair $(\rho,\mathbf{j})$ satisfies a continuity-type equation

$$\frac{\partial\rho}{\partial t}+\nabla\cdot\mathbf{j}=0.$$

Moreover, from (3.2) it also follows that

$$\rho\geqslant 0, \tag{3.5}$$

$$\mathbf{j}\cdot\mathbf{j}-c^2\rho^2=-c^2|\varphi|^4. \tag{3.6}$$

The latter two conditions are equivalent to (5.10) in Ref. 8 (p. 4705). This class of solutions is nonempty. It contains at least all positive-frequency plane-wave solutions, namely solutions of the form

$$\varphi(x,t)=\exp[(i/\hbar)(\mathbf{p}\cdot x-p^0 t)],$$

where

$$p^0=+c\sqrt{\mathbf{p}\cdot\mathbf{p}+m^2c^2}.$$

Let

$$\rho_0(x):=\frac{i\hbar}{2mc^2}\left(\overline{\varphi}\frac{\partial\varphi}{\partial t}-\varphi\frac{\partial\overline{\varphi}}{\partial t}\right)(x,0)=|\varphi(x,0)|^2\times\left(-\frac{1}{mc^2}\frac{\partial S}{\partial t}(x,0)\right).$$

It follows from (3.2) that $\rho_0(x)\geqslant 0$. Let us suppose that ρ_0 integrates to one. Suppose that $\{X(t);t\geqslant 0\}$ is a Markov diffusion process such that $X(0)$ is distributed according to ρ_0, and having forward differential

$$d_+X(t)=\begin{pmatrix}\frac{1}{m}\nabla S+\frac{\hbar}{m}\nabla R\\ -\frac{1}{mc^2}\frac{\partial S}{\partial t}\end{pmatrix}(X(t),t)\,dt+\sqrt{\frac{\hbar}{m}}\frac{1}{\sqrt{-\frac{1}{mc^2}\frac{\partial S}{\partial t}(X(t),t)}}d_+W_+(t),\qquad(3.7)$$

where $W_+(\cdot)$ is a standard, three-dimensional Wiener process. In the previous notation, we have

$$\sigma^2(x,t):=\frac{\hbar}{-\frac{1}{c^2}\frac{\partial S}{\partial t}(x,t)}.$$

A standard calculation[26] shows that $\rho(x,t)$ in (3.3) satisfies the Fokker–Planck equation corresponding to (3.7). Hence, $\rho(x,t)$ is the probability density of $X(t)$. Moreover, the current drift of X is

$$v(X(t),t):=\begin{pmatrix}\frac{1}{m}\nabla S\\ -\frac{1}{mc^2}\frac{\partial S}{\partial t}\end{pmatrix}(X(t),t),\qquad(3.8)$$

and the osmotic drift is given by

$$u(X(t),t)=\begin{pmatrix}\frac{\hbar}{m}\nabla R\\ -\frac{1}{mc^2}\frac{\partial S}{\partial t}\end{pmatrix}(X(t),t).\qquad(3.9)$$

Let us define

$$M^i(t):=\int_0^t\frac{1}{\sqrt{-\frac{1}{mc^2}\frac{\partial S}{\partial s}(X(s),s)}}d_+W_+^i(s),\quad t\geqslant 0,\quad i=1,2,3.\qquad(3.10)$$

The stochastic processes $\{M^i(t);t\geqslant 0\}$ are continuous *local martingales*[24,25] with the same *quadratic variation*

$$\langle M\rangle(t)=\langle M^i\rangle(t):=\int_0^t \frac{1}{-\frac{1}{mc^2}\frac{\partial S}{\partial s}(X(s),s)}\,\mathrm{d}s. \tag{3.11}$$

Moreover, their *cross variations* satisfy

$$\langle M^i,M^j\rangle(t)=0,\quad 1\leqslant i\neq j\leqslant 3,\quad \forall t\geqslant 0. \tag{3.12}$$

Observe that $\langle M\rangle(t)$ is a strictly increasing process with differentiable sample paths. It satisfies, in view of (3.2) and (3.8),

$$\begin{aligned} d\langle M\rangle(t)&=\frac{1}{-\frac{1}{mc^2}\frac{\partial S}{\partial t}(X(t),t)}\,\mathrm{d}t\\ &=\sqrt{\frac{m^2c^2}{m^2c^2+\nabla S(X(t),t)\cdot\nabla S(X(t),t)}}\,\mathrm{d}t\\ &=\sqrt{1-\frac{\nabla S(X(t),t)\cdot\nabla S(X(t),t)}{m^2c^2+\nabla S(X(t),t)\cdot\nabla S(X(t),t)}}\,\mathrm{d}t\\ &=\sqrt{1-\frac{v(X(t),t)\cdot v(X(t),t)}{c^2}}\,\mathrm{d}t. \end{aligned} \tag{3.13}$$

If for some t and ω we have $v(X(t,\omega),t)=0$, then $d\langle M\rangle(t)=\mathrm{d}t$. We can therefore think of $d\langle M\rangle(t)$ as of an increment of the particle *random proper time*. Notice that (3.13) implies

$$\frac{d\langle M\rangle(t)}{\mathrm{d}t}\leqslant 1,\quad a.s.$$

Hence,

$$\langle M\rangle(t)\leqslant t,\ \ a.s.,\ \ \forall t\geqslant 0. \tag{3.14}$$

Furthermore, we have the following property of $d\langle M\rangle(t)$. Let us first recall that, in view of (2.5) and (2.6), we have

$$v(X(t),t)=\lim_{\mathrm{d}t\searrow 0} E\left\{\frac{d_sX(t)}{\mathrm{d}t}\middle| X(t)\right\}, \tag{3.15}$$

where the *symmetric increment* of X at time t is defined by

$$d_sX(t):=\frac{d_+X(t)+d_-X(t)}{2}=\frac{X(t+\mathrm{d}t)-X(t-\mathrm{d}t)}{2}.$$

We can therefore rewrite (3.13) as follows:

$$
\begin{aligned}
c^2[d\langle M\rangle(t)]^2 &= -[(ic)^2 + v(X(t),t)\cdot v(X(t),t)](\mathrm{d}t)^2 \\
&= -\left[\left(\frac{d(ict)}{\mathrm{d}t}\right)^2 + v(X(t),t)\cdot v(X(t),t)\right](\mathrm{d}t)^2 \\
&= -[(d(ict))^2 + E\{d_sX(t)|X(t)\}\cdot E\{d_sX(t)|X(t)\} + o((\mathrm{d}t)^2)].
\end{aligned}
\tag{3.16}
$$

Let us introduce

$$
X_\nu(t) = \begin{pmatrix} X(t) \\ ict \end{pmatrix}.
$$

Then (3.16) can be written as follows:

$$
[d\langle M\rangle(t)]^2 = -\frac{1}{c^2}E\{d_sX_\nu(t)|X_\nu(t)\}\cdot E\{d_sX_\nu(t)|X_\nu(t)\} + o((\mathrm{d}t)^2), \tag{3.17}
$$

generalizing the relation $(\mathrm{d}\tau)^2 = -(1/c^2)\mathrm{d}X_\nu \mathrm{d}X_\nu$ of classical relativistic mechanics.

IV. FROM THE t TO THE τ FORMULATION: A RANDOM TIME CHANGE

An important consequence of Levy's characterization of the Wiener process, see, e.g., Ref. 25, p. 82, is that any continuous local martingale may be viewed as a time-changed Wiener process, cf. Theorem A.2 in the Appendix. For $\tau \geqslant 0$, let us introduce the *stopping time*

$$
T(\tau) := \inf\{\sigma \geqslant 0 : \langle M\rangle(\sigma) \geqslant \tau\}.
$$

[In the case when the probability of the event $\{\omega : \lim_{t\to\infty}\langle M\rangle(t,\omega) = \infty\}$ is strictly less than one, the stopping time $T(\tau)$ has to be suitably modified, see Ref. 24, pp. 174–175.] Notice that

$$
\langle M\rangle(T(\tau)) = \tau, \quad T(\langle M\rangle(t)) = t. \tag{4.1}
$$

Then, the processes

$$
\tilde{W}^i_+(\tau) := M^i_{T(\tau)}, \quad i = 1,2,3,
$$

are standard, one-dimensional Wiener processes. Moreover, in view of property (3.12), we can apply a theorem of Knight (see Theorem A.3 in the Appendix), and conclude that the processes $\tilde{W}^i_+(\tau)$ are pairwise independent, and can, consequently, be viewed as the components of a standard, three-dimensional Wiener process $\tilde{W}_+(\tau)$. Let us introduce the stochastic process

$$
\tilde{X}(\tau) := X(T(\tau)), \quad \tau \geqslant 0.
$$

In view of (3.7), (3.11), and (4.1), the forward differential of $\tilde{X}$ is given by

$$
d_+\tilde{X}(\tau) = \left(\frac{1}{m}\nabla S + \frac{\hbar}{m}\nabla R\right)(\tilde{X}(\tau), T(\tau))\mathrm{d}\tau + \sqrt{\frac{\hbar}{m}}d_+\tilde{W}_+(\tau). \tag{4.2}
$$

Notice that $\tilde{X}(\tau)$ is a non-Markovian $\mathbb{R}^3$-valued diffusion process with constant diffusion coefficient $(\hbar/m)I_3$. The Markov property has therefore been destroyed by the random time change. From the first relation in (4.1), we get

$$\frac{\mathrm{d}T(\tau)}{\mathrm{d}\tau}=\left[\frac{d\langle M\rangle}{\mathrm{d}t}(T(\tau))\right]^{-1}.$$

In view of (3.11), we then get

$$\frac{\mathrm{d}T(\tau)}{\mathrm{d}\tau}=-\frac{1}{mc^2}\frac{\partial S}{\partial t}(\tilde{X}(\tau),T(\tau)). \tag{4.3}$$

Let us now define $\tilde{X}^4(\tau):=icT(\tau)$, $\tilde{S}(x_\nu)=\tilde{S}(x,x^4):=S(x,t)$, and $\tilde{R}(x_\nu)=\tilde{R}(x,x^4):=R(x,t)$. Equations (4.2) and (4.3) can now be rewritten as

$$d_+\tilde{X}(\tau)=\left(\frac{1}{m}\nabla\tilde{S}+\frac{\hbar}{m}\nabla\tilde{R}\right)(\tilde{X}(\tau),\tilde{X}^4(\tau))\mathrm{d}\tau+\sqrt{\frac{\hbar}{m}}d_+\tilde{W}_+(\tau), \tag{4.4}$$

$$d_+\tilde{X}^4(\tau)=\frac{1}{m}\frac{\partial\tilde{S}}{\partial x^4}(\tilde{X}(\tau),\tilde{X}^4(\tau))\mathrm{d}\tau. \tag{4.5}$$

Notice that $\tilde{X}_\nu(\tau)$ defined by

$$\tilde{X}_\nu(\tau)=\begin{pmatrix}\tilde{X}(\tau)\\ \tilde{X}_4(\tau)\end{pmatrix}$$

is an $\mathbb{M}^4$-valued *Markovian* stochastic process with marginal density at $\tau=0$ given by $\rho_0(x)\cdot\delta(x^4)$ since $T(0)=0$ a.s. Let us introduce the diffusion matrix

$$\Sigma^2:=\begin{pmatrix}\frac{\hbar}{m}I_3 & 0\\ 0 & 0\end{pmatrix}.$$

Then (4.4) and (4.5) can be rewritten in the form

$$d_+\tilde{X}_\nu(\tau)=\left(\frac{1}{m}\nabla_\nu\tilde{S}+\Sigma^2\nabla_\nu\tilde{R}\right)(\tilde{X}_\nu(\tau))\mathrm{d}\tau+\Sigma d_+\tilde{W}_\nu(\tau), \tag{4.6}$$

where $\tilde{W}_\nu$ is any standard, four-dimensional Wiener process whose first three components form $\tilde{W}_+$. The Fokker–Plank equation is then

$$\frac{\partial\rho_\nu}{\partial\tau}+\nabla_\nu\cdot\left[\left(\frac{1}{m}\nabla_\nu\tilde{S}+\Sigma^2\nabla_\nu\tilde{R}\right)\rho_\nu\right]=\frac{1}{2}\Sigma^2\Delta_\nu\rho_\nu. \tag{4.7}$$

Because of (3.1), $\varphi(x_\nu):=\exp[\tilde{R}(x_\nu)+(i/\hbar)\tilde{S}(x_\nu)]$ satisfies

$$\nabla_\nu\cdot\nabla_\nu\varphi=\frac{m^2c^2}{\hbar^2}\varphi.$$

The latter is equivalent to the system of p.d.e.s

$$-\frac{1}{2m}\nabla_\nu\tilde{S}\cdot\nabla_\nu\tilde{S}+\frac{\hbar^2}{2m}[\nabla_\nu\tilde{R}\cdot\nabla_\nu\tilde{R}+\nabla_\nu\cdot\nabla_\nu\tilde{R}]=\frac{mc^2}{2}, \tag{4.8}$$

$$\frac{1}{m}\nabla_\nu\tilde{S}\cdot\nabla_\nu\tilde{R}+\frac{1}{2m}\nabla_\nu\cdot\nabla_\nu\tilde{S}=0. \tag{4.9}$$

Let

$$\tilde{\rho}(x_\nu)=|\varphi(x_\nu)|^2.$$

From (4.9), we get that $\tilde{\rho}(x_\nu)$ satisfies (4.7). Thus, $\mu(\mathrm{d}x_\nu):=\tilde{\rho}(x_\nu)\mathrm{d}x_\nu$ is an *invariant* (σ-*finite*) *measure* for (4.4) and (4.5). Notice that $\tilde{\rho}(x_\nu)$ also satisfies the manifestly convariant equation

$$\nabla_\nu\cdot\left(\tilde{\rho}\frac{1}{m}\nabla_\nu\tilde{S}\right)=0.$$

If we give $\mu(\mathrm{d}x_\nu):=\tilde{\rho}(x_\nu)\mathrm{d}x_\nu$ as initial measure to (4.6), the probabilistic picture is lost. Nevertheless, it is possible to make sense of the time-reversed diffusion along the lines of Ref. 18 (pp. 44 and 45). Moreover, consider the *generator* of $\tilde{X}_\nu$ acting on smooth functions with compact support

$$\left(\frac{1}{m}\nabla_\nu\tilde{S}+\Sigma^2\nabla_\nu\tilde{R}\right)\cdot\nabla_\nu+\frac{1}{2}\Sigma^2\Delta_\nu.$$

The adjoint of this operator with respect to the measure $\mu(\mathrm{d}x_\nu)$ (Ref. 13, p. 104) is given by

$$\left(\frac{1}{m}\nabla_\nu\tilde{S}-\Sigma^2\nabla_\nu\tilde{R}\right)\cdot\nabla_\nu-\frac{1}{2}\Sigma^2\Delta_\nu.$$

Hence, in spite of the lack of a probabilistic picture we can still think of $(1/m)\nabla_\nu\tilde{S}$ as a bilateral velocity field associated with the equilibrium measure $\mu(x_\nu)$. Then, recalling that (3.2) implies

$$\nabla_\nu\tilde{S}(x_\nu)\cdot\nabla_\nu\tilde{S}(x_\nu)=-m^2c^2,$$

we get a τ-domain counterpart of relation (3.17).

V. CONCLUSION AND OUTLOOK

Although the process (4.4)–(4.5) is not relativistically covariant, our description does not appear to be in conflict with classical relativistic mechanics nor with Nelson's nonrelativistic theory. Indeed, in the case when we let the noise intensity in (3.7) tend to zero, we recover the equations of classical special relativity. In particular, the quadratic variation $\langle M\rangle$ defined by (3.11) tends to proper time τ and $T(\tau)$ tends to $t(\tau)$. On the other hand, when $v\cdot v\ll c^2$, motion of the particle in a fixed inertial frame is described by a Markov diffusion process with diffusion coefficient nearly equal to $\hbar/m$. The Schrödinger equation is then recovered through some appropriate procedure neglecting terms multiplied by $\hbar^2/c$, cf. Ref. 8, p. 4708.

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APPENDIX: CONTINUOUS MARTINGALES

We collect in this Appendix a few basic facts about continuous martingales. We refer the reader to Refs. 24 and 25 for the proofs and more information. Let $(\Omega,\mathcal{A},\mathbf{P})$ be a probability space, and let $\mathcal{F}:=(\mathcal{F}_t),t\in[t_0,t_1]$, be a nondecreasing family of sub σ-algebras of $\mathcal{A}$. It will be always assumed that $\mathcal{F}_{t_0}$ contains all the zero-probability sets in $\mathcal{A}$, and that the filtration is right-continuous, namely $\{\cap\mathcal{F}_t,t>s\}=\mathcal{F}_s$, for every s. A stochastic process $X:=\{X(t);t\in[t_0,t_1]\}$ is said to be *continuous* if it has continuous trajectories $X(t,\omega),t\in[t_0,t_1]$, with probability one. It is called $\mathcal{F}$-*adapted* if, for every t in $[t_0,t_1]$, $X(t)$ is $\mathcal{F}_t$-measurable. In that case, it

is customary to write $X=(X(t),\mathcal{F}_t)_{t\in[t_0,t_1]}$. The stochastic process $M=(M(t),\mathcal{F}_t)_{t\in[t_0,t_1]}$ is called a *martingale* (with respect to the *filtration* $\mathcal{F}_t, t\in[t_0,t_1]$) if it satisfies the two following conditions:

(1) $E\{|M(t)|\}<\infty, \quad \forall t,$
(2) $E\{M(t)|\mathcal{F}_s\}=M(s), \quad t\geqslant s.$

The continuous martingale $X=(X(t),\mathcal{F}_t)_{t\in[t_0,t_1]}$ is called *square-integrable* if $E\{X(t)^2\}<\infty$, $\forall t$ in $[t_0,t_1]$. Let $X=(X(t),\mathcal{F}_t)_{t\in[t_0,t_1]}$ be a continuous, square-integrable martingale with $X(t_0)=0$ with probability one. Then, the celebrated Doob–Meyer decomposition theorem implies that there exists a unique representation for $X(t)^2$,

$$X(t)^2=\langle X\rangle(t)+M(t), \quad t\in[t_0,t_1],$$

where $\langle X\rangle$ is an adapted, continuous, increasing process with $\langle X\rangle(t_0)=0$, and M is a continuous martingale with $M(t_0)=0$. The process $\langle X\rangle(\cdot)$ is called the *quadratic variation* of $X(\cdot)$. Consider now two continuous, square-integrable martingales $X=(X(t),\mathcal{F}_t)_{t\in[t_0,t_1]}$ and $Y=(Y(t),\mathcal{F}_t)_{t\in[t_0,t_1]}$. Their *cross-variation process* $\langle X,Y\rangle$ is defined for $t\in[t_0,t_1]$ by

$$\langle X,Y\rangle(t):=\tfrac{1}{4}[\langle X+Y\rangle(t)-\langle X-Y\rangle(t)].$$

The cross variation of X and Y is characterized by the fact that $XY-\langle X,Y\rangle$ is a continuous martingale.

A non-negative random variable $T(\omega)$ is called a *Markov time* or a *stopping time* (relative to the *filtration* $\mathcal{F}_t, t\in[t_0,t_1]$) if, for all t in $[t_0,t_1]$,

$$\{\omega: T(\omega)\leqslant t\}\in\mathcal{F}_t.$$

Let T be a stopping time relative to $\mathcal{F}_t, t\in[t_0,t_1]$. Then, the σ-field $\mathcal{F}_T$ *of events determined prior to the stopping time* T consists of those events $A\in\mathcal{A}$ for which $[A\cap\{\omega: T(\omega)\leqslant t\}]\in\mathcal{F}_t$, for every t in $[t_0,t_1]$.

The stochastic process $M=(M(t),\mathcal{F}_t)_{t\geqslant 0}$, is called a *local martingale* if there exists an increasing sequence of stopping times (with respect to $\mathcal{F}$) $\{T_n\}$, $n=1,2,...$ such that

(1) $\mathbf{P}(\lim T_n=\infty)=1;$
(2) for any n, the "stopped process" $(M(t\wedge T_n),t\geqslant 0$, is a martingale.

The decomposition result for the product of two square-integrable martingale extends to local martingales as follows. Let $X=(X(t),\mathcal{F}_t)_{t\in[t_0,t_1]}$ and $Y=(Y(t),\mathcal{F}_t)_{t\in[t_0,t_1]}$ be two continuous, local martingales. Then there is a unique adapted process $\langle X,Y\rangle$ such that $XY-\langle X,Y\rangle$ is a continuous local martingale. We write $\langle X\rangle$ instead of $\langle X,X\rangle$. We can now state Levy's martingale characterization of the Wiener process.

Theorem A.1: *Let $M=(M(t),\mathcal{F}_t)_{t\geqslant 0}$ be a continuous local martingale with $M(0)=0$ a.s. and quadratic variation $\langle M\rangle(t)=t$. Then M is a standard Wiener process.*

As a corollary to this theorem, we have the following result showing that continuous local martingales can be viewed as time-changed Wiener processes.

Theorem A.2: *Let $M=(M(t),\mathcal{F}_t)_{t\geqslant 0}$ be a continuous local martingale with $M(0)=0$ a.s. Suppose that $\lim_{t\to\infty}\langle M\rangle(t)=\infty$ with probability one. Define, for $\tau\geqslant 0$, the stopping time $T(\tau):=\inf\{t\geqslant 0:\langle M\rangle(t)>\tau\}$. Then the time-changed process $W=\{W(\tau):=(M(T(\tau)),\mathcal{G}_\tau:=\mathcal{F}_{T(\tau)})_{\tau\geqslant 0}\}$ is a standard Wiener process and we have, with probability one,*

$$M(t)=W(\langle M\rangle(t)), \quad t\geqslant 0.$$

The multivariate extension of this theorem is due to Knight (Ref. 24, p. 179).

Theorem A.3: *Let* $M=\{M(t)=(M^1(t),\dots,M^n(t)),\mathcal{F}_t)_{t\geq 0}\}$ *be a continuous process with* $M(0)=0$ *a.s. Suppose that the components* M^i *are local martingales satisfying the two following conditions:*

(1) $\lim_{t\to\infty}\langle M^i\rangle(t)=\infty, \quad i=1,...,n$ *a.s.*;
(2) $\langle M^i,M^j\rangle(t)=0, \quad i\neq j, t\geq 0.$

Let $T_i(\tau):=\inf\{t\geq 0:\langle M^i\rangle(t)>\tau\}, t\geq 0, i=1,...,n$. *Then the* $W^i(\tau):=M^i(T_i(\tau)), \tau\geq 0, i=1,...,n$ *are independent, standard Wiener processes.*

The nontrivial content of this theorem is that, although the M^i are not independent, applying first the appropriate time changes, and then forgetting the time changes, we get independent Wiener processes. Forgetting the time changes consists in replacing the filtrations $\{\mathcal{G}_\tau^i\}$ with the poorer filtrations $\{\mathcal{F}_\tau^{W^i}\}$.

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Stationary quantum source coding

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In this article the quantum version of the source coding theorem is obtained for a completely ergodic source. This result extends Schumacher's quantum noiseless coding theorem for memoryless sources. The control of the memory effects requires some earlier results of Hiai and Petz on high probability subspaces. Our result is equivalently considered as a compression theorem for noiseless stationary channels. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1398335]

I. INTRODUCTION

Although it is difficult to define a discipline, to give some idea we can say that the objective of quantum information theory is the transmission and manipulation of information stored in systems obeying quantum mechanics. A quantum channel has a source that emits systems in quantum states to the channel. For example, the source could be a laser that emits individual monochromatic photons and the channel could be an optical fiber. The noisy signal output of the channel arrives at the receiver. In principle, there are two very different problems about quantum channels. The sender has a quantum system in an unknown state and wants to have the receiver end up with a similar system in the same state. In this case we speak of a pure quantum channel which has a quantum mechanical input and output. On the other hand, one might want to use quantum states to carry classical information, roughly speaking, a sequence of zeros and ones. Now both the input and the output are classical; however, there is a quantum mechanical section in between. The classical information is encoded into a quantum state and this is sent down the channel. The higher the channel noise is, the more redundant the encoding must be in order to restore the original signal at the receiver, where the quantum signal is converted into classical information. In this article we do not deal with the problem of how such a scheme can be realistically implemented; practical quantum encoding and decoding requires a sophisticated ability to manipulate quantum states. However, we are interested in the amount of classical information getting through the channel which is assumed to be noiseless. It was emphasized already by Shannon that a computer memory is a communication channel. (Quantum or classical depends on the type of computer.) In an optimal situation the computer memory is free of any noise and this is the case we are concentrating on in the present work. We want to consider rather general noiseless quantum channels (with possibly memory effects but strong ergodic properties), and our aim is to discuss the quantum source coding theorem. As a general reference on quantum information theory we suggest Ref. 1, but the really necessary definitions are given here.

To each classical input message x_i there corresponds a signal state φ_i of the quantum communication system. The quantum states φ_i are functioning as code words of the messages. The signal states φ_i could be pure and orthogonal in the sense of quantum mechanics, but, for example, in quantum cryptography nonorthogonal states are used intentionally in order to avoid eavesdropping. At the moment we do not impose any condition on the signal states; they could be arbitrary pure or mixed states. In the stochastic model of communication, one assumes that each input message x_i appears with certain probability. Let p_{ji} be the probability that the message x_i is sent and y_j is received. The joint distribution p_{ji} yields marginal probability distributions p_i and q_j on

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the set of input and output messages. According to Shannon the mutual information

$$I=\sum_{i,j} p_{ji}\log\frac{p_{ji}}{p_i q_j}$$

measures the amount of information going through the channel from Alice to Bob. Of course, the relation of I to the quantum encoding and decoding should be made clear. This comes next.

The message x_i has *a priori* probability p_i and the mixed quantum state of the channel is

$$\varphi=\sum_i p_i\varphi_i .$$

This might be considered as the statistical operator of the *message ensemble*; for example, when φ_i is a pure state $|i\rangle\langle i|$, then $\varphi=\Sigma_i p_i|i\rangle\langle i|$ acts on the input Hilbert space $\mathcal{H}$. The distribution of the output is determined by a measurement, which is nothing else but a physical word for decoding. To each output message there corresponds an observable A_j on the output Hilbert space $\mathcal{K}$. It is customary to assume that $0\leqslant A_j$, $\Sigma_j A_j=\mathrm{id}$ (id stands for the identity operator) and $p_{ji}=p_i\varphi_i(A_j)$. The so-called *Kholevo bound*[2] provides an upper bound on the amount of information accessible to Bob in terms of von Neumann entropies:

$$I\leqslant S(\varphi)-\sum_i p_i S(\varphi_i).$$

[When $\lambda_1,\lambda_2,\ldots$ are the eigenvalues of the statistical operator of a quantum state ψ, then $S(\psi)=-\Sigma_k\lambda_k\log(\lambda_k)$.] In particular, if all signal states φ_i are pure, then $S(\varphi_i)=0$ and we have $I\leqslant S(\varphi)$. In this way the von Neumann entropy gets an information theoretical interpretation. Kholevo's bound is actually not very strong; it is attained only in trivial situations.[3]

The basic problem of communication theory is to maximize the amount of information received by Bob from Alice. However, up to now this problem is not well posed in our discussion yet. Let us deal with messages of length n; they are n-term-sequences of 0 and 1. (So, the size of this message set is 2^n.) For each message length n we carry out the above procedure of coding and decoding and the amount of information going through the channel is I_n. Since I_n is presumably proportional to n, the good information quantity is I_n/n, that is, the transmitted information per letter. Since Shannon's theory is not only stochastic but asymptotic as well, we are going to let n to ∞. In this way we need to repeat the above information transmission scheme for each n. The message set, the input Hilbert space $\mathcal{H}^{(n)}$, our coding, the channel state $\varphi^{(n)}$, the output Hilbert space $\mathcal{K}^{(n)}$, and the observables applied in the measurement are all depending on the parameter n.

The subject of the present article is faithful signal transmission, which bears the name noiseless channel. In place of faithful transmission, one can think of information storage. In this case the aim is to use the least possible number of Hilbert space dimensions per signal for coding. The new feature of the noiseless channel we are studying is the memory effect. Mathematically this means that the channel state (of the n-fold channel) is not of product type, but we assume stationarity and good ergodic properties. In Sec. II we use the standard formalism of statistical mechanics to describe such a channel. It turns out that the mean von Neumann entropy, familiar also from statistical mechanics, gives the optimal coding rate. The proof of our main result, Theorems 1 and 2, is similar to the proof presented in Ref. 4 for Schumacher's coding theorem. However, instead of typical sequences we use the high-probability subspace of strongly ergodic stationary states, a subject studied by Hiai and Petz in Ref. 5. We note for the interested reader that most of the concepts used in the present article are treated in detail in Ref. 6.

II. AN INFINITE SYSTEM SETTING OF THE SOURCE

If $\mathcal{H}$ is a finite-dimensional Hilbert space, then $(A,B)\mapsto\mathrm{Tr}(A^*B)$ defines an inner product on $\mathcal{B}(\mathcal{H})$, so for every linear functional φ on $\mathcal{B}(\mathcal{H})$ there exists a unique $D_\varphi\in\mathcal{B}(\mathcal{H})$ with the property

$\varphi(A)=\mathrm{Tr}(D_\varphi A)$. When φ is a state, then D_φ is the corresponding density matrix. Let X^n denote the set of all messages of length n. If $x^n\in X^n$ is a message, then a quantum state $\varphi(x^n)$ of the n-fold quantum system corresponds with it. The Hilbert space of the n-fold system is the n-fold tensor product $\mathcal{H}^{\otimes n}$ and $\varphi(x^n)$ has a statistical operator $D(x^n)$. If messages of length n are to be transmitted, then our quantum source should be put in the state $\varphi_n=\Sigma_{x^n}p(x^n)\varphi(x^n)$ with statistical operator $D_n=\Sigma_{x^n}p(x^n)D(x^n)$, where $p(x^n)$ is the probability of the message x^n. Since we want to let $n\to\infty$, it is reasonable to view all the n-fold systems as subsystems of an infinite one. In this way we can conveniently use a formalism standard in statistical physics (see Chap. 15 of Ref. 6).

Let an infinitely extended system be considered over the lattice $\mathbb{Z}$ of integers. The observable confined to a lattice site $k\in\mathbb{Z}$ form the self-adjoint part of a finite-dimensional matrix algebra $\mathcal{A}_k$, that is, the set of all operators acting on the finite-dimensional space $\mathcal{H}$. It is assumed that the local observables in any finite subset $\Lambda\subset\mathbb{Z}$ are those of the finite quantum system

$$\mathcal{A}_\Lambda=\bigotimes_{k\in\Lambda}\mathcal{A}k\,.$$

The quasilocal algebra $\mathcal{A}$ is the norm completion of the normed algebra $\mathcal{A}_\infty=\cup_\Lambda\mathcal{A}_\Lambda$, the union of all local algebras $\mathcal{A}_\Lambda$ associated with finite intervals $\Lambda\subset\mathbb{Z}$.

A state φ of the infinite system is a positive normalized functional $\mathcal{A}\to\mathbb{C}$. It does not make sense to associate a statistical operator to a state of the infinite system in general. However, φ restricted to a finite-dimensional local algebra $\mathcal{A}_\Lambda$ admits a density matrix D_Λ. We regard the algebra $\mathcal{A}_{[1,n]}$ as the set of all operators acting on the n-fold tensor product space $\mathcal{H}^{\otimes n}$. Moreover, we assume that the density D_n from the first part of this section is identical with $D_{[1,n]}$. Under this assumptions we call the state φ the state of the (infinite) channel. Roughly speaking, all the states used in the transmission of messages of length n are marginals of this φ. Coding, transmission, and decoding could be well formulated using the states $\varphi_n\equiv\varphi_{[1,n]}$. However, it is more convenient to formulate our setting in the form of an infinite system, particularly because we do not want to assume that the channel state φ is a product type. This corresponds to the possibility that our quantum source has a memory effect.

The right shift on the set $\mathbb{Z}$ induces a transformation γ on $\mathcal{A}$. A state φ is called *stationary* if $\varphi\circ\gamma=\varphi$. The state φ is called *ergodic* if it is an extremal point in the set of stationary states. Moreover, φ is *completely ergodic* when it is an extreme point for every $m\in\mathbb{N}$ in the convex set of all states ψ such that $\psi\circ\gamma^m=\psi$. By a *completely ergodic stationary quantum source* we simply mean a completely ergodic stationary state φ of the infinite system $\mathcal{A}$. Of course, a stationary product state, corresponding to a memoryless channel, is completely ergodic. The emphasis is put on other states here.

Next we show an example of a completely ergodic stationary quantum source from the context of algebraic states. For the details, see Ref. 7.

Example 1: Let $\mathcal{A}:=M_3(\mathbb{C})$, $\mathcal{B}:=M_2(\mathbb{C})$, *moreover let* $\{E_{ij}\}_{i,j=1}^e$ *be the usual matrix units of* $M_3(\mathbb{C})$. *Set*

$$V_1:=\begin{bmatrix}\frac{1}{\sqrt{2}} & 0\\ 0 & 0\end{bmatrix},\quad V_2:=\begin{bmatrix}0 & 0\\ \frac{1}{\sqrt{2}} & 0\end{bmatrix},\quad V_3:=\begin{bmatrix}0 & 1\\ 0 & 0\end{bmatrix}.$$

Then $\Sigma_{i=1}^3V_i^*V_i=I_\mathcal{B}$.

Let ρ *be a state on* $\mathcal{B}$ *with density matrix*

$$\begin{bmatrix}\frac{2}{3} & 0\\ 0 & \frac{1}{3}\end{bmatrix}.$$

Define $\Sigma:\mathcal{A}\otimes\mathcal{B}\to\mathcal{B}$ *by* $\Sigma(E_{ij}\otimes x):=V_i^*xV_j$. *It is easy to check that* Σ *is a completely positive unital map and* $\rho(\Sigma(I_{\mathcal{A}}\otimes x))=\rho(x), x\in\mathcal{B}$.

Then the algebraic state φ *generated by* $(\mathcal{B}, \Sigma, \rho)$ *is given by*

$$\varphi(E_{i_1j_1}\otimes\cdots\otimes E_{i_nj_n})=\rho(V_{i_1}^*\cdots V_{i_n}^*V_{j_n}\cdots V_{j_1}).$$

It is shown in Ref. 7 that φ *is completely ergodic. Of course, it is not a product state.*

It is well known in quantum statistical mechanics that, due to the subadditivity of the von Neumann entropy (proven first in Ref. 8 by Lieb and Ruskai), the limit

$$\lim_{n\to+\infty}\frac{1}{n}S(\varphi_n)=\inf\frac{1}{n}S(\varphi_n):=h$$

exists for any stationary state and this quantity is called the *mean entropy* of φ. (See Ref. 6 for a textbook treatment of the subject or Ref. 9 for some related properties of the mean entropy.)

III. SOURCE CODING

For a while we fix a message length n and we denote by d the dimension of the Hilbert space $\mathcal{H}$. Assume that our n-fold composite quantum system is operating as a quantum source and emits the quantum states $D^{(1)},D^{(2)},\ldots,D^{(m)}$ with *a priori* probabilities $p_1,p_2,\ldots,p_m$. (Therefore the state of the system is $D_n=\Sigma_i p_iD^{(i)}$.) By source coding we mean an association

$$D^{(i)}\mapsto\tilde{D}^{(i)},$$

where $\tilde{D}^{(i)}$ is some other statistical operator on the Hilbert space $\mathcal{H}^{\otimes n}$. (This definition allows $D^{(i)}=D^{(j)}$ but $\tilde{D}^{(i)}\neq\tilde{D}^{(j)}$. However, in the coding constructed in the proof of Theorem 1 this cannot happen.)

We denote by $\mathcal{K}_n$ the subspace spanned by the eigenvectors corresponding to all nonzero eigenvalues of all statistical operators $\tilde{D}^{(i)}, 1\leqslant i\leqslant m$. The goal of source coding is to keep the dimension of $\mathcal{K}_n$ to be small and to fulfill some fidelity criterium. (A mathematically demanding survey about quantum coding is Ref. 10.) The *source coding rate*

$$\limsup_{n\to\infty}\frac{\log\dim(\mathcal{K}_n)}{n}$$

expresses the resolution of the encoder in qubits per input symbol. (It is actually more precise to speak about ''qunats'' per input symbol, but the difference is only a constant factor.)

The distortion measure is a number which allows us to compare the goodness or badness of communication systems. The *fidelity* of the coding scheme was introduced by Schumacher:[11]

$$F:=\sum_i p_i\mathrm{Tr}D^{(i)}\tilde{D}^{(i)},$$

where p_i is a probability distribution on the input and $\tilde{D}^{(i)}$ is the density used to encode the density $D^{(i)}$. Note that $0\leqslant F\leqslant 1$ and $F=1$ if and only if $D^{(i)}=\tilde{D}^{(i)}$ are pure states.

First we present our positive source coding theorem for a completely ergodic source. The result says that the source coding rate may approach the mean entropy while we can keep the fidelity arbitrarily good.

Theorem 1: *Let* $\mathcal{H}$ *be a finite-dimensional Hilbert space, and* φ *be a completely ergodic state on* $B(\mathcal{H})^{\otimes\infty}$. *Then for every* $\varepsilon,\delta>0$ *there exists* $n_{\varepsilon,\delta}\in\mathbb{N}$ *such that for* $n\geqslant n_{\varepsilon,\delta}$ *there is a subspace* $\mathcal{K}_n(\varepsilon,\delta)$ *of* $\mathcal{H}^{\otimes n}$ *such that*

(i) $\log\dim\mathcal{K}_n(\varepsilon,\delta)<n(h+\delta)$ *and*

(ii) *for every extremal decomposition* $D_n=\Sigma_{i=1}^m p_i D^{(i)}$ *one can find an encoding* $D^{(i)}\mapsto\tilde{D}^{(i)}$ *with density matrices* $\tilde{D}^{(i)}$ *supported in* $\mathcal{K}_n(\varepsilon,\delta)$ *such that the fidelity* $F:=\Sigma_{i=1}^m p_i \mathrm{Tr} D^{(i)}\tilde{D}^{(i)}$ *exceeds* $1-\varepsilon$.

The negative part of the coding theorem tells that the source coding rate cannot exceed the mean entropy when the fidelity is good.

Theorem 2: *Let* $\mathcal{H}$ *be a finite-dimensional Hilbert space, and* φ *be a completely ergodic state on* $B(\mathcal{H})^{\otimes\infty}$. *Then for every* $\delta>0$ *there exist* $0<\eta<1$ *and* $n_\delta\in\mathbb{N}$ *such that for* $n\geqslant n_\delta$

(i) *for all subspaces* $\mathcal{K}_n$ *of* $\mathcal{H}^{\otimes n}$ *with the property* $\log\dim\mathcal{K}_n\leqslant n(h-\delta)$ *and*

(ii) *for every decomposition* $D_n=\Sigma_{i=1}^m p_i D^{(i)}$ *and for every encoding* $D^{(i)}\mapsto\tilde{D}^{(i)}$ *with density matrices* $\tilde{D}^{(i)}$ *supported in* $\mathcal{K}_n$, *the fidelity* $F:=\Sigma_{i=1}^m p_i \mathrm{Tr} D^{(i)}\tilde{D}^{(i)}$ *is smaller than* η.

The detailed proofs are given in the next section. Now we make some comments on the fidelity F. It is possible that $F<1$ although $D^{(i)}=\tilde{D}^{(i)}$. This fact might suggest to use another concept of fidelity. Since $D^{1/2}\geqslant D$ holds for a density matrix, we have

$$\mathrm{Tr}\ D_1^{1/2}D_2^{1/2}=\mathrm{TR}\ D_1^{1/4}D_2^{1/2}D_1^{1/4}\geqslant\mathrm{Tr}\ D_1^{1/4}D_2D_1^{1/4}=\mathrm{Tr}\ D_2^{1/2}D_1^{1/2}D_2^{1/2}$$
$$\geqslant\mathrm{Tr}\ D_2^{1/2}D_1D_2^{1/2}=\mathrm{Tr}\ D_1D_2.$$

This implies that

$$F':=\sum_i p_i \mathrm{Tr}[D^{(i)}]^{1/2}[\tilde{D}^{(i)}]^{1/2}\geqslant F.$$

Both our positive and negative source coding theorems hold if F is replaced by F'. (In the case of Theorem 1, this follows from the inequality $F'\geqslant F$ and, in the proof of Theorem 2, we will show $F'\leqslant\eta$.)

IV. HIGH-PROBABILITY SUBSPACE

The proof of Shannon's original source coding theorem is based on the typical sequences (Ref. 12, Chap. 1). The quantum extension of this result obtained by Schumacher still benefits from the classical result. When the channel state is a product, the densities D_n commute and simultaneous diagonalization is possible. If the memory effects are present, then these densities do not commute and in some sense we are in a really quantum mechanical noncommutative situation. Nevertheless, the high-probability subspace can be used, but new techniques are required.

Let $\mathcal{K}$ be a Hilbert space and D be a density matrix on $\mathcal{K}$. D has a Schatten decomposition $D=\Sigma_i\lambda_i|f_i\rangle\langle f_i|$, where $|f_i\rangle$'s are eigenvectors and the eigenvalues λ_i are numbered decreasingly: $\lambda_1\geqslant\lambda_2\geqslant\cdots$. Choose and fix $0<\varepsilon<1$. Let $n(\varepsilon)$ be the smallest integer such that

$$\sum_{i=1}^{n(\varepsilon)}\lambda_i\geqslant 1-\varepsilon.$$

The subspace $\mathrm{HP}(D,\varepsilon)$ spanned by the eigenvectors $|f_1\rangle,\ldots,|f_{n(\varepsilon)}\rangle$ is called the *high-probability subspace* corresponding to the level ε. Note that $\mathrm{HP}(D,\varepsilon)$ is not completely well defined. If there are multiplicities in the spectrum of D, then the Schatten decomposition is not unique. However, the dimension $n(\varepsilon)$ of $\mathrm{HP}(D,\varepsilon)$ is determined. The term "high-probability subspace" is borrowed from Ref. 13 and its role in macroscopic uniformity was discussed in Ref. 14.

In the following, φ will be a completely ergodic state on $\mathcal{A}^{\otimes\infty}$. For $\varepsilon\in(0,1)$ let

$$\beta_{\varepsilon,n}:=\inf\{\log\mathrm{Tr}_n(q)):q\in\mathbb{P}(\mathcal{A}^{\otimes n}),\varphi_n(q)\geqslant 1-\varepsilon\},$$

where $\mathbb{P}(\mathcal{A}^{\otimes n})$ denotes the set of projections of $\mathcal{A}^{\otimes n}$. ($\exp \beta_{\varepsilon,n}$ is the dimension of the high-probability subspace.) It was shown in Ref. 5 (and formulated in terms of relative entropy) that

$$\limsup_{n\to+\infty} \frac{1}{n}\beta_{\varepsilon,n} \geqslant h, \tag{1}$$

$$\liminf_{n\to+\infty} \frac{1}{n}\beta_{\varepsilon,n} \geqslant \frac{1}{1-\varepsilon}h - \frac{\varepsilon}{1-\varepsilon}\log d. \tag{2}$$

From this one can deduce the following.

Proposition: For every positive δ

(i) and for every positive ε *there exists* $N_{\varepsilon,\delta}\in\mathbb{N}$ *such that for every* $n>N_{\varepsilon,\delta}$ *there exists a projection* $q_n(\varepsilon,\delta)$ *in* $\mathcal{A}^{\otimes n}$ *such that*

$$\log(\mathrm{Tr}_n(q_n(\varepsilon,\delta)))<n(h+\delta) \quad \text{and} \quad \varphi_n(q)\geqslant 1-\varepsilon,$$

(ii) and there exists $1>\eta>0$ *and* $N_\delta\in\mathbb{N}$ *such that for every* $n>N_\delta$ *and for every projection* q *in* $\mathcal{A}^{\otimes n}$

$$\log(\mathrm{Tr}_n(q))\leqslant n(h-\delta)$$

implies $\varphi_n(q)\leqslant\eta$.

Part (i) of the proposition is a plain reformulation of (1). In order to see (ii) we first note that

$$\frac{1}{\eta}h - \frac{1-\eta}{\eta}\log d \to h \quad \text{as} \quad \eta\to 1.$$

Hence given $\delta>0$ we choose $0<\eta<1$ such that

$$\frac{1}{\eta}h - \frac{1-\eta}{\eta}\log d > h-\delta.$$

Next we replace ε by $1-\delta$ in (2):

$$\liminf_{n\to+\infty} \frac{1}{n}\inf\{\log \mathrm{Tr}_n(q)) : q\in\mathbb{P}(\mathcal{A}^{\otimes n}), \varphi_n(q)\geqslant 1-\eta\} \geqslant \frac{1}{\eta}h - \frac{1-\eta}{\eta}\log d > h-\delta. \tag{3}$$

In this way we arrived at (*ii*).

Next we prove the source coding theorem.

Proof of Theorem 1: Use part (*i*) of the proposition and set $q_n := q_n(\varepsilon/2,\delta)$, $\mathcal{K}_n(\varepsilon,\delta) := \mathrm{Ran} q_n$, where $n>n(\varepsilon,\delta):=N_{\varepsilon/2,\delta}$. Given an external decomposition $D_n=\Sigma_{i=1}^k p_i D^{(i)}$, that is, $D^{(i)}=|x_i\rangle\langle x_i|$ for some vectors x_i, we construct the coding densities $\tilde{D}^{(i)}$. Let

$$\tilde{x}_i := \frac{q_n x_i}{\|q_n x_i\|}, \quad \alpha_i := \|q_n x_i\|, \quad \beta_i := \|(I-q_n)x_i\|,$$

and let x be any unit vector such that $q_n x = x$. Then we set

$$\tilde{D}^{(i)} := \alpha_i^2 |\tilde{x}_i\rangle\langle\tilde{x}_i| + \beta_i^2 |x\rangle\langle x|.$$

Since $\tilde{x}_i, x\in\mathcal{K}_n(\varepsilon,\delta)$, we have supp $\tilde{D}^{(i)}\subset\mathcal{K}_n(\varepsilon,\delta)$. Furthermore,

$$\begin{aligned}\mathrm{Tr}\ D^{(i)}\tilde{D}^{(i)} &= \langle x_i, \tilde{D}^{(i)} x_i\rangle = \alpha_i^2 |\langle x_i|\tilde{x}_i\rangle|^2 + \beta_i^2 |\langle x_i, x\rangle|^2 \\ &\geqslant \alpha_i^2 |\langle x_i|\tilde{x}_i\rangle|^2 = \alpha_i^4 \geqslant 2\alpha_i^2 - 1 \\ &= 2\ \mathrm{Tr}\, q_n D^{(i)} - 1.\end{aligned}$$

We need to sum over i:

$$\sum_i\ p_i \mathrm{Tr}\, D^{(i)}\tilde{D}^{(i)} \geqslant \sum_i\ p_i(2\,\mathrm{Tr} q_n D^{(i)} - 1) = 2\,\mathrm{TR} D_n q_n - 1 = 2\varphi_n(q_n) - 1 \geqslant 1 - \varepsilon.$$

Proof of Theorem 2: For the given δ we choose η and $n(\delta)$ according to the proposition. Let q be the projection onto the subspace $\mathcal{K}_n$. We want to use the Schwarz inequality in the form

$$\left|\sum_i\ p_i \mathrm{Tr} x_i y_i\right| \leqslant \left[\sum_i\ p_i \mathrm{TR} x_i^* x_i\right]^{1/2}\left[\sum_i\ p_i \mathrm{TR} y_i^* y_i\right]^{1/2}$$

for $x_i = [D^{(i)}]^{1/2} q$ and $y_i = [\tilde{D}^{(i)}]^{1/2}$. Since $[\tilde{D}^{(i)}]^{1/2} = q[\tilde{D}^{(i)}]^{1/2}$ follows from the hypothesis, we have

$$\begin{aligned}F' = \sum_{i=1}^m\ p_i\, \mathrm{Tr}[D^{(i)}]^{1/2}[\tilde{D}^{(i)}]^{1/2} &= \sum_{i=1}^m\ p_i\, \mathrm{Tr}[D^{(i)}]^{1/2} q [\tilde{D}^{(i)}]^{1/2} \\ &\geqslant \left[\sum_{i=1}^m\ p_i\, \mathrm{Tr} D^{(i)} q\right]^{1/2}\left[\sum_{i=1}^m\ p_i\, \mathrm{Tr} D^{(i)}\right]^{1/2} \\ &= \varphi_n(q)^{1/2} \leqslant \sqrt{\eta}.\end{aligned}$$

This estimate completes the proof.

It was also shown in Ref. 7 that for strongly mixing algebraic states (especially for product states)

$$\lim_{n\to+\infty} \frac{1}{n}\beta_{\varepsilon,n} = h,$$

and, in this case, the negative part of the coding theorem holds in a stronger form: For every ε, $\delta > 0$ there exists $n_{\varepsilon,\delta} \in \mathbb{N}$ such that for $n \geqslant n_{\varepsilon,\delta}$ for all subspaces $\mathcal{K}_n$ of $\mathcal{H}^{\otimes n}$ with the property $\log \dim \mathcal{K}_n < n(h-\delta)$ and for every decomposition $D_n = \Sigma_{i=1}^m p_i D^{(i)}$ and for every encoding $D^{(i)} \leftrightarrow \tilde{D}^{(i)}$ with density matrices $\tilde{D}^{(i)}$ supported in $\mathcal{K}_n(\varepsilon,\delta)$, the fidelity $F := \Sigma_{i=1}^m p_i \mathrm{Tr} D^{(i)}\tilde{D}^{(i)}$ is smaller than ε.

There is a seemingly slight difference between the two theorems. The statistical operator D_n has an external decomposition in the first one and arbitrary decomposition in the second. The difference between the pure and mixed message ensembles is discussed in Ref. 15.

V. DISCUSSION

In this article a theory of quantum source coding subject to a fidelity criterion or quantum data compression is presented. The minimum of the source coding rate is studied under the conditions that Schumacher's fidelity must exceed $1-\varepsilon$ and the quantum mechanical state of the channel has a strong ergodic property. This latter condition allows many states with memory effect. For the mathematical model and in the proof of the main result techniques of quantum statistical mechanics are used. We prove that the minimal source coding rate is the mean entropy of the channel state, and, to some extent, it is independent of the message ensemble.

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Symmetries in the Hubbard model with *n*-fold orbital degeneracy

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The present paper studies the symmetries of the Hubbard model of electrons with generally n-fold orbital degeneracy. It is shown that $SU_d(2n)$ and $SU_c(2n)$ symmetries hold, respectively, for the model with completely repulsive or attractive on-site interaction and that with partly attractive interactions. An extended Lieb–Mattis transformation is given to map these two symmetries into each other. The subsymmetry $SU_d^{(e)}(n)\otimes SU_d^{(o)}(n)$ is found to be shared by the two models with arbitrary chemical potential μ. By assuming at most two electrons on each site it is found that $SU_d(2n)_{\mathcal{P}}$ and $SU_c(2n)_{\mathcal{P}}$ both exist in each kind of the two models and consequently lead to a larger symmetry $SU_d(2n)_{\mathcal{P}}\times SU_c(2n)_{\mathcal{P}}$. Another underlying symmetry $(SU_c^{(e)}(2)_{\mathcal{P}}\times\cdots\times SU_c^{(e)}(2)_{\mathcal{P}})\otimes(SU_c^{(o)}(2)_{\mathcal{P}}\times\cdots\times SU_c^{(o)}(2)_{\mathcal{P}})$ is also revealed for the unified U model under the excluding. The symmetry is valid for the partially attractive model with chemical potential $\mu=-U$. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1402956]

I. INTRODUCTION

Recently, considerable attention has been directed to studies on correlated electrons in the presence of orbital degrees of freedom, which is relevant to transitional-metal oxides,[1–5] C_{60} materials,[6] and artificial quantum dot arrays.[7] Apart from the numerical[8] and perturbative[9] works, theories based on symmetries were presented for one-dimensional models of these systems. An $SU(4)$ theory describing spin systems with orbital degeneracy was proposed[10,11] for a theoretical understanding of the observed unusual properties. The ground-state phase diagrams for the system with a symmetry breaking of $SU(4)\rightarrow SU(2)\times SU(2)$ were discussed in Refs. 9 and 12. For the two-fold orbital degenerate Hubbard model a recent paper[13] presented the $SU(4)$ theory and showed the underlying $SU_d(4)$ symmetry of spin-orbital double and a charge $SU_c(4)$ symmetry with an extended Lieb–Mattis transformation mapping those two $SU(4)$ generators into each other. On the basis of elementary degenerate perturbative theory, it was also shown that the effective Hamiltonian is equivalent to the $SO(6)$ and $SU(4)$ Heisenberg models, respectively, at half-filling and quarter-filling with strong coupling. In Ref. 14, the one-dimensional $SU(4)$ Hubbard model is extensively studied on the basis of Bethe ansatz solution. As for the symmetry theory of the one-dimensional Hubbard model without orbital degeneracy, it has been well investigated. Yang introduced the pairing operators and so constructed the symmetry $SU(2)\times SU(2)$.[15] Based on the symmetry Eßler *et al.*[16] discussed the completeness of the Bethe ansatz

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solutions, Pernici[17] showed the off-diagonal long-range order, Uglov and Korepin presented the Yangian symmetry $Y(sl(2))\oplus Y(sl(2))$,[18] and Eßler and Frahm considered the density correlations.[19] And it has been argued that the two-dimensional single-band Hubbard model has approximate $SO(5)$ symmetry.[20] But research on the Hubbard model with orbital degeneracy is still being accumulated. In the present paper we study the symmetries of the Hubbard model of electrons with generally n-fold orbital degeneracy. We show and clarify that the $SU_d(2n)$ and $SU_c(2n)$ symmetries hold, respectively, unlike in the simple Hubbard model for which both of the symmetries are valid, for the model with unified on-site interaction and that with partly attractive interactions. But the subsymmetry $SU_d^{(e)}(n)\otimes SU_d^{(o)}(n)$ is found to be valid for the two models and for arbitrary chemical potential μ. An extended Lieb–Mattis transformation as in Ref. 13 is given to map these two symmetries into each other. By assuming at most two electrons on each site, we find that the $SU_d(2n)_{\mathcal{P}}$ and $SU_c(2n)_{\mathcal{P}}$ symmetries both exist in each kind of the two models so we have a larger symmetry $SU_d(2n)_{\mathcal{P}}\times SU_c(2n)_{\mathcal{P}}$. Under the exclusion another underlying symmetry $(SU_c^{(e)}(2)_{\mathcal{P}}\times\cdots\times SU_c^{(e)}(2)_{\mathcal{P}})\otimes(SU_c^{(o)}(2)_{\mathcal{P}}\times\cdots\times SU_c^{(o)}(2)_{\mathcal{P}})$, which is not included in the $SU_d(2n)_{\mathcal{P}}\times SU_c(2n)_{\mathcal{P}}$, is also revealed for the unified U model with $\mu=U$ so that the model totally possesses the symmetry $SU_d(2n)_{\mathcal{P}}\times SU_c(2n)_{\mathcal{P}}\times[(SU_c^{(e)}(2)_{\mathcal{P}}\times\cdots\times SU_c^{(e)}(2)_{\mathcal{P}})\otimes(SU_c^{(o)}(2)_{\mathcal{P}}\times\cdots\times SU_c^{(o)}(2)_{\mathcal{P}})]$. The underlying symmetry is also valid for the partially attractive model with $\mu=-U$.

Consider the n-fold orbital degenerate electrons with states

$$|1\rangle=|1,\uparrow\rangle,\quad |2\rangle=|1,\downarrow\rangle,$$

$$\cdots,$$

$$|2n-1\rangle=|n,\uparrow\rangle,\quad |2n\rangle=|n,\downarrow\rangle, \tag{1}$$

where in a state $|l,\sigma\rangle$ l denotes the lth orbital component and $\sigma=\uparrow,\downarrow$ label the spin components. We start with a general Hamiltonian with n-fold orbital degeneracy expressed by

$$H=-\sum_{x,x'}\sum_{a}(t_{xx'}C_a^{+}(x)C_a(x')+t_{xx'}^{*}C_a^{+}(x')C_a(x))+\sum_{x}\sum_{a\neq a'}U_{aa'}n_a(x)n_{a'}(x)-\mu\sum_{x,a}n_a(x), \tag{2}$$

where $C_a^{+}(x)$ creates a fermion of state $|a\rangle$ at site x and $n_a(x)$ is the corresponding particle number operator. The notation of site is not restricted to one-dimensional case.

II. $SU_D(2n)$ AND $SU_C(2N)$ SYMMETRIES

Besides the $U(1)$ symmetry there exist two kinds of $SU(2n)$ symmetries for the orbital degenerate Hubbard model. We define

$$E_{ss'}=\sum_{x}C_s^{+}(x)C_{s'}(x),$$

$$D_m=N_m-N_{m+1},\quad N_m=\sum_{x}C_m^{+}(x)C_m(x), \tag{3}$$

they fulfill the commutation relations

$$[E_{ss'},E_{tt'}]=\delta_{s',t}E_{st'}-\delta_{s,t'}E_{ts'},$$

$$[D_m,E_{ss'}]=(\delta_{m,s}-\delta_{m,s'}-\delta_{m+1,s}+\delta_{m+1,s'})E_{ss'}. \tag{4}$$

These operators can construct an $SU(2n)$ Lie algebra

$$SU_d(2n):\{D_m,E_{ss'}|m=1,\ldots,2n-1;1\leqslant s\neq s'\leqslant 2n\}, \tag{5}$$

with $n(2n-1)$ of $E_{ss'}$ and there are totally $(2n)^2-1$ of generators. $\{D_m\}$ forms the commuting Cardan subalgebra of rank $2n-1$. The $E_{s(s+1)}$'s are the generators related to the simple roots. For any of $t_{xx'}$ and μ, all generators of $SU_d(2n)$ commute with the Hamiltonian (2) with unified on-site interaction $U_{aa'}=U$, so we have $SU_d(2n)$ symmetry of spin-orbital double in this case.

Let us define another set of operators

$$F_{\alpha_{2k-1}}=\sum_x f(x)C^+_{2k-1}(x)C^+_{2k}(x),$$

$$F_{\alpha_{2k}}=\sum_x f(x)C_{2k}(x)C_{2k+1}(x), \tag{6}$$

$$Q_m=\frac{1}{2}\sum_x [C^+_m(x)C_m(x)+C^+_{m+1}(x)C_{m+1}(x)-1],$$

where $k=1,\ldots,n$, $m=1,\ldots,2n-1$, $f(x)^2=1$, and $f(x+\delta)=-f(x)$ for any site x and nearest-neighbor $x+\delta$. The above-mentioned operators can realize another $SU(2n)$ Lie algebra which we shall denote by $SU_c(2n)$:

$$\{Q_m,F_\alpha,F_{-\alpha}\}. \tag{7}$$

$\{Q_m\}$ is the Cardan subalgebra. The $F_{\alpha_{2k-1}}$ and $F_{\alpha_{2k}}$ are the generators related to the simple roots, other generators relating to positive roots can be obtained by $F_{\alpha_i+\alpha_j}=[F_{\alpha_i},F_{\alpha_j}]$, the generators with negative roots will be $F_{-\alpha}=(F_\alpha)^\dagger$. If we assume that the on-site coupling $U_{aa'}=U$ for the states labeled by a,a' with different spin components while $U_{aa'}=-U$ for states with the same spin components

$$\begin{aligned} U_{aa'}&=U \text{ for odd even pair } a,a',\\ U_{aa'}&=-U \text{ for odd–odd or even–even pair } a,a', \end{aligned} \tag{8}$$

and the amplitudes $t_{xx'}$ of odd-neighbor hopping are real and those of even-neighbor hopping are imaginary

$$\begin{aligned} t^*_{xx'}&=t_{xx'} \text{ when } x\text{-}x' \text{ is odd neighbor},\\ t^*_{xx'}&=-t_{xx'} \text{ when } x\text{-}x' \text{ is even neighbor}, \end{aligned} \tag{9}$$

we will have the following relations:

$$[H,F_{\alpha_{2k}}]=2(\mu-U)F_{\alpha_{2k}},\quad [H,F_{\alpha_{2k-1}}]=-2(\mu-U)F_{\alpha_{2k-1}}. \tag{10}$$

If the chemical potential $\mu=U$, the Hamiltonian will commute with all the generators of $SU_c(2n)$ so the model has the charge $SU_c(2n)$ symmetry. In terms of the partially attractive (8), it can be easily proved that such a Hamiltonian with $\mu=U$ has the half-filled form

$$H=-\sum_{x,x'}\sum_a (t_{xx'}C^+_a(x)C_a(x')+t^*_{xx'}C^+_a(x')C_a(x))+\sum_x\sum_{a\neq a'} U_{aa'}\left(n_a(x)-\frac{1}{2}\right)\left(n_{a'}(x)-\frac{1}{2}\right). \tag{11}$$

The usual Hubbard model with the nearest-neighbor hopping is included in the class of (9). Whether $f(x)$ can be well defined depends on the lattice structures, if in a lattice any sum of the nearest-neighbor pair $\delta+\delta'$ is not a nearest neighbor and there are even sites on every perpendicular direction, $f(x)$ can be well defined as

$$f(x)=\exp(i\pi\cdot\mathbf{x}),\quad \pi=(\pi,\pi,\ldots),\quad \mathbf{x}=(x_1,x_2,\ldots). \tag{12}$$

x_i is the ith components of the site coordinate in the lattice basis. Such lattices (bipartite lattice) can be simple squared, centered squared in two-dimension; simple cubic and body-centered cubic in three-dimension. For the one-dimensional case and even total sites, $f(x)=\exp(i\pi x)$.

According to (10) for $\mu\neq U$, $F_{\alpha_{2k}}$ and $F_{\alpha_{2k-1}}$ are energy-shifting operators

$$\begin{aligned} H(F_{\alpha_{2k}}\psi_E)&=[E+2(\mu-U)](F_{\alpha_{2k}}\psi_E),\\ H(F_{\alpha_{2k-1}}\psi_E)&=[E-2(\mu-U)](F_{\alpha_{2k-1}}\psi_E), \end{aligned} \tag{13}$$

where ψ_E is the eigenstate of the partially attractive Hamiltonian: $H\psi_E=E\psi_E$.

It should be noted that the $SU_d(2n)$ does not commute with the partially attractive Hamiltonian which has only the $SU_c(2n)$ symmetry, neither does $SU_c(2n)$ with the unified U model which possesses the $SU_d(2n)$ symmetry. The two kinds of symmetries can be mapped into each other by an extended Lieb–Mattis transformation

$$\begin{aligned} C_a(x)&\mapsto\exp(i\pi\cdot\mathbf{x})C_a^+(x)\ \text{ for even }\ a,\\ C_a(x)&\mapsto C_a(x)\ \text{ for odd }\ a. \end{aligned} \tag{14}$$

The transformation leaves the hopping term (9) invariant and changes the sign of $U_{aa'}$ with odd–even pair a,a' in (11) so maps the model (11) into the unified $U_{aa'}=-U$ model.

The particle number of each state and the total spin can be expressed by

$$\begin{aligned} N_{2n}&=\left(N_e-\sum_{m=1}^{2n-1}mD_m\right)/2n,\\ N_j&=\sum_{m=j}^{2n-1}D_m+\left(N_e-\sum_{m=1}^{2n-1}mD_m\right)/2n,\quad j<2n, \end{aligned} \tag{15}$$

$$S_{\text{total}}=\sum_{m=1}^{n}D_{2m-1}/2, \tag{16}$$

where N_e is the number of total electrons.

III. $SU_D^{(E)}(N)\otimes SU_D^{(O)}(N)$ SYMMETRY

Unlike in the traditional Hubbard model for which both of the two symmetries are valid for on-site attractive and repulsive interactions, as we can see in Sec. II, for the orbital-degenerate Hubbard model the $SU_d(2n)$ symmetry of spin-orbital double only holds for the unified U Hubbard model with arbitrary chemical potential μ whereas the charge $SU_c(2n)$ symmetry merely exists in the other partly attractive half-filled model of which the chemical potential is $\mu=U$. But considering that $SU_d(2n)$ and $SU_c(2n)$ share some common generators $E_{2\nu,2\nu'}$ and $E_{2\nu-1,2\nu'-1}$, we will find the shared subsymmetry $SU_d^{(e)}(n)\otimes SU_d^{(o)}(n)$ yields for the two models with

$$SU_d^{(e)}(n):\{D_{2\nu,2\nu+2},E_{2\nu',2\nu''}|\,\nu\leqslant n-1,1\leqslant\nu'\neq\nu''\leqslant n\},$$
$$SU_d^{(o)}(n):\{D_{2\nu-1,2\nu+1},E_{2\nu'-1,2\nu''-1},|\,\nu\leqslant n-1,1\leqslant\nu'\neq\nu''\leqslant n\},\tag{17}$$

where $D_{m,m+2}=N_m-N_{m+2}$. In particular, we shall illustrate that the symmetry is valid for the partially attractive model with arbitrary chemical potential μ.

As the hopping term in the Hamiltonian and the chemical potential term $\mu\Sigma_{x,a}\,n_a(x)$ are $SU_d(2n)$ invariant, whether the Hubbard model possesses $SU_d(2n)$ symmetry depends on the commutation relation of the on-site interacting term and the $SU_d(2n)$ generators:

$$\left[E_m^k,\sum_{a\neq a'}U_{aa'}n_a(x)n_{a'}(x)\right]=C_m^+(x)C_{m+k}(x)\left(\sum_{a'\neq m+k}n_{a'}(x)U_{m+k,a'}-\sum_{a'\neq m}n_{a'}(x)U_{m,a'}\right)$$
$$+\left(\sum_{a\neq m+k}n_a(x)U_{a,m+k}-\sum_{a\neq m}n_a(x)U_{a,m}\right)C_m^+(x)C_{m+k}(x),\tag{18}$$

where

$$E_m^k=\sum_x\,C_m^+(x)C_{m+k}(x).$$

Surely for the case of unified $U_{aa'}=U$ we easily find that the above-mentioned commutation vanishes so that we have the $SU_d(2n)$ symmetry in this case, as obtained in the Sec. II. Although for the partially attractive model the above-mentioned commutator does not go null for all $k's$ and consequently we do not have $SU_d(2n)$ symmetry, the case with even k will be an exception. From the partially attractive (8) we find for even k's

$$U_{a,m+k}=U_{a,m}=-U,$$
$$\left(\sum_{a\neq m+k}n_a(x)U_{a,m+k}-\sum_{a\neq m}n_a(x)U_{a,m}\right)=n_m(x)U_{m,m+k}-n_{m+k}(x)U_{m+k,m}$$
$$=(n_m(x)-n_{m+k}(x))(-U).$$

Then Eq. (18) becomes

$$\left[E_m^k,\sum_{a\neq a'}U_{aa'}n_a(x)n_{a'}(x)\right]=C_m^+(x)C_{m+k}(x)(n_m(x)-n_{m+k}(x))(-U)+(n_m(x)$$
$$-n_{m+k}(x))C_m^+(x)C_{m+k}(x)(-U)$$
$$=(-C_m^+(x)C_{m+k}(x)+C_m^+(x)C_{m+k}(x))(-U)=0,$$

where we have used the following relations: $n_mC_m=C_m^+n_m=0$, $n_mC_m^+=C_m^+$, $C_mn_m=C_m$. E_m^k with even k's and odd (or even) m's corresponding to the $SU_d^{(o)}(n)$ (or $SU_d^{(e)}(n)$) generators. As a result, the $SU_d^{(e)}(n)\otimes SU_d^{(o)}(n)$ generators in (17) commute with the Hamiltonian of the partially attractive model for any chemical potential μ. Therefore the $SU_d^{(e)}(n)\otimes SU_d^{(o)}(n)$ symmetry is shared by the two models both for arbitrary μ.

IV. AT MOST TWO ELECTRONS ON EACH SITE

The application of Bethe ansatz method to the one-dimensional degenerate Hubbard model is based on such an assumption that prevents scattering process involving three or more electrons on

one site.[14,21,22] For the traditional Hubbard model the configurations of more than two electrons on one site are excluded automatically by the Pauli principle. In the continuum limit and for small densities or $U \gg t$ in the lattice model, the unwanted configurations in degenerate Hubbard model become negligible, so the Hamiltonian with three-electron configurations excluded will describe the system well. If we exclude more than two electrons on each site, we will find that the Hamiltonian has both $SU_d(2n)_{\mathcal{P}}$ and $SU_c(2n)_{\mathcal{P}}$ symmetries and furthermore a larger symmetry $SU_d(2n)_{\mathcal{P}} \times SU_c(2n)_{\mathcal{P}}$. In addition, we will find an underlying symmetry $(SU_c^{(e)}(2)_{\mathcal{P}} \times \cdots \times SU_c^{(e)}(2)_{\mathcal{P}}) \otimes (SU_c^{(o)}(2)_{\mathcal{P}} \times \cdots \times SU_c^{(o)}(2)_{\mathcal{P}})$.

Consider $U_{aa'} = U$ case, the Hamiltonian reads

$$\mathcal{H} = -t \sum_{\langle x,x' \rangle} \sum_{a} \mathcal{P} C_a^+(x) C_a(x') \mathcal{P} + U \sum_{x} \sum_{a \neq a'} n_a(x) n_{a'}(x) - \mu \sum_{x,a} n_a(x), \tag{19}$$

where $\langle x,x' \rangle$ represents the nearest-neighbor sites and let us define

$$\mathcal{F}_{\alpha_{2k-1}} = \sum_{x} \exp(i\boldsymbol{\pi} \cdot \mathbf{x}) \mathcal{P} C_{2k-1}^+(x) C_{2k}^+(x) \mathcal{P}, \tag{20}$$

$$\mathcal{F}_{\alpha_{2k}} = \sum_{x} \exp(i\boldsymbol{\pi} \cdot \mathbf{x}) \mathcal{P} C_{2k}(x) C_{2k+1}(x) \mathcal{P}, \tag{21}$$

where the operator $\mathcal{P}$ projects onto the subspace of states having at most two electrons on each site.[22] Other generators are also modified from the $SU_c(2n)$ in Sec. II. The $\mathcal{P}$ operator excludes such terms as $n_s C_{s'}^+ C_{s''}^+$, $C_s C_{s'} n_{s''}$ with three different s, s', and s'' so that

$$\left[\mathcal{P} C_s^+(x) C_{s'}^+(x) \mathcal{P}, \sum_{x'} \sum_{a \neq a'} n_a(x') n_{a'}(x') \right] = -2 \mathcal{P} C_s^+(x) C_{s'}^+(x) \mathcal{P}, \tag{22}$$

thus we have the relations similar to (10)

$$[\mathcal{H}, \mathcal{F}_{\alpha_{2k}}] = 2(\mu - U) \mathcal{F}_{\alpha_{2k}}, \quad [\mathcal{H}, \mathcal{F}_{\alpha_{2k-1}}] = -2(\mu - U) \mathcal{F}_{\alpha_{2k-1}}. \tag{23}$$

For $\mu \neq U$, $\mathcal{F}_{\alpha_{2k}}$ and $\mathcal{F}_{\alpha_{2k-1}}$ are energy-shifting operators for $\mathcal{H}$ as in (13). Set $\mu = U$ and the $\mathcal{F}_{\alpha_{2k-1}}$ and $\mathcal{F}_{\alpha_{2k}}$ will commute with the $\mathcal{H}$. $\mathcal{F}_{\alpha_{2k-1}}$, $\mathcal{F}_{\alpha_{2k}}$, and $N_s - N_{s'}$ can generate the $SU_c(2n)_{\mathcal{P}}$ symmetry so that $\mathcal{H}$ has both $SU_d(2n)_{\mathcal{P}}$ and $SU_c(2n)_{\mathcal{P}}$ symmetries,

$$SU_c(2n)_{\mathcal{P}} : \{\mathcal{Q}_m, \mathcal{F}_\alpha\}, \tag{24}$$

$$SU_d(2n)_{\mathcal{P}} : \{\mathcal{D}_m, \mathcal{E}_{ss'}\}, \tag{25}$$

where $\mathcal{Q}_m = \mathcal{P} Q_m \mathcal{P}$ and the $SU_d(2n)$ generators are correspondingly revised to be

$$\mathcal{E}_{ss'} = \mathcal{P} E_{ss'} \mathcal{P}, \quad \mathcal{D}_m = \mathcal{P} D_m \mathcal{P}. \tag{26}$$

The commutation relations are also modified, $\mathcal{E}_{ss'}$ and $\mathcal{E}_{tt'}$ commute except for the case of $s = t'$ and $s' = t$, other commutations remain the same. And it is similar for $\mathcal{F}_\alpha$. The two modified symmetries are not $SU(2n)$, their subsymmetries involving only two states are $SU(2)$.

It also can be similarly shown that both of the symmetries hold for the $\mathcal{P}$-modified model with partially attractive $U_{aa'} = U, -U$. As the two symmetries both hold for each of the models we can construct the larger symmetry $SU_d(2n)_{\mathcal{P}} \times SU_c(2n)_{\mathcal{P}}$ for each of them. If we do not exclude more than two electrons on each site, these two symmetries, respectively, belong to different models.

Besides $SU_d(2n)_{\mathcal{P}} \times SU_c(2n)_{\mathcal{P}}$ there exist some less obvious symmetries. Define

$$\mathcal{F}^{(+)}_{2k,2k'}=\sum_x \exp(i\pi\cdot\mathbf{x})\mathcal{P}C^+_{2k}(x)C^+_{2k'}(x)\mathcal{P},\quad \mathcal{F}^{(-)}_{2k,2k'}=(\mathcal{F}^{(+)}_{2k,2k'})^\dagger, \tag{27}$$

$$\mathcal{F}^{(+)}_{2k-1,2k'-1}=\sum_x \exp(i\pi\cdot\mathbf{x})\mathcal{P}C^+_{2k-1}(x)C^+_{2k'-1}(x)\mathcal{P},\quad \mathcal{F}^{(-)}_{2k-1,2k'-1}=(\mathcal{F}^{(+)}_{2k-1,2k'-1})^\dagger, \tag{28}$$

such generators are not included in (24) which contains pairing operators $\mathcal{F}^{(\pm)}_{ss'}$ only with odd–even pair ss'. It can be easily verified that these operators also commute with the unified U model (19) with $\mu=U$ so we find an underlying symmetry $(SU^{(e)}_c(2)_\mathcal{P}\times\cdots\times SU^{(e)}_c(2)_\mathcal{P})\otimes(SU^{(o)}_c(2)_\mathcal{P}\times\cdots\times SU^{(o)}_c(2)_\mathcal{P})$ with

$$SU^{(e)}_c(2)_\mathcal{P}:\{\mathcal{Q}_{2k,2k'},\quad \mathcal{F}^{(+)}_{2k,2k'},\quad \mathcal{F}^{(-)}_{2k,2k'}\},\quad k\neq k',\quad k,k'=1,\ldots,n, \tag{29}$$

$$SU^{(o)}_c(2)_\mathcal{P}:\{\mathcal{Q}_{2k-1,2k'-1},\quad \mathcal{F}^{(+)}_{2k-1,2k'-1},\quad \mathcal{F}^{(-)}_{2k-1,2k'-1}\},\quad k\neq k',\quad k,k'=1,\ldots,n. \tag{30}$$

There are, respectively, $C^2_n=n(n-1)/2$ of the $SU^{(e)}_c(2)_\mathcal{P}$ and $SU^{(o)}_c(2)_\mathcal{P}$ symmetries, and they are all SU(2). The extended Lieb–Mattis transformation (14) maps the above-mentioned symmetry into itself. A revised Lieb–Mattis transformation mapping into the corresponding $SU^{(e)}_d(2)_\mathcal{P}$ and $SU^{(o)}_d(2)_\mathcal{P}$ will involve a third kind of Hamiltonians with partially attractive $U_{aa'}$, which differs from what we discussed before. So finally we have the symmetry $SU_d(2n)_\mathcal{P}\times SU_c(2n)_\mathcal{P}\times[(SU^{(e)}_c(2)_\mathcal{P}\times\cdots\times SU^{(e)}_c(2)_\mathcal{P})\otimes(SU^{(o)}_c(2)_\mathcal{P}\times\cdots\times SU^{(o)}_c(2)_\mathcal{P})]$ for (19) with $\mu=U$. But for $U_{aa'}=U,-U$ case the underlying symmetry is valid for another chemical potential. The Hamiltonian under that exclusion is

$$\mathcal{H}'=-\sum_{\langle x,x'\rangle}\sum_a t\mathcal{P}C^+_a(x)C_a(x')\mathcal{P}+\sum_x\sum_{a\neq a'}U_{aa'}n_a(x)n_{a'}(x)-\mu\sum_{x,a}n_a(x), \tag{31}$$

where the partially attractive interaction $U_{aa'}$ is also defined by (8). Compared with (10) the commutation relations are different

$$[\mathcal{H}',\mathcal{F}^{(+)}_{2k,2k'}]=-2(\mu+U)\mathcal{F}^{(+)}_{2k,2k'}, \tag{32}$$

$$[\mathcal{H}',\mathcal{F}^{(-)}_{2k,2k'}]=2(\mu+U)\mathcal{F}^{(-)}_{2k,2k'}. \tag{33}$$

The different sign of U comes from $U_{2k,2k'}=-U$ while in Eq. (10) it is $U_{2k,2k\pm1}=U$. Therefore the symmetry $(SU^{(e)}_c(2)_\mathcal{P}\times\cdots\times SU^{(e)}_c(2)_\mathcal{P})\otimes(SU^{(o)}_c(2)_\mathcal{P}\times\cdots\times SU^{(o)}_c(2)_\mathcal{P})$ holds for $\mu=-U$.

It should be noted the underlying symmetry is valid under the exclusion, without the $\mathcal{P}$-exclusion its generators will commute with neither of the two kinds of models. And unlike $SU^{(o)}_d(n)\otimes SU^{(e)}_d(n)\subset SU_d(2n)$ in Sec. III, none of the $SU^{(o)}_c(2)_\mathcal{P}$ or $SU^{(e)}_c(2)_\mathcal{P}$ is any subsymmetry of $SU_c(2n)_\mathcal{P}$. Without the $\mathcal{P}$-exclusion, the $SU^{(e)}_c(2)$ and $SU^{(o)}_c(2)$ are subgroups of $SU_d(2n)\times SU_c(2n)$, since the generators of $SU^{(e)}_c(2)$ and $SU^{(o)}_c(2)$ can be obtained by the commutation product of F_α and $E_{ss'}$. But $SU^{(o)}_c(2)_\mathcal{P}$ or $SU^{(e)}_c(2)_\mathcal{P}$ cannot be generated by the commutations of $\mathcal{F}_\alpha$ and $\mathcal{E}_{ss'}$ which commute with each other under the $\mathcal{P}$-exclusion, so none of the underlying $SU^{(o)}_c(2)_\mathcal{P}$ or $SU^{(e)}_c(2)_\mathcal{P}$ is the subsymmetry of $SU_d(2n)_\mathcal{P}\times SU_c(2n)_\mathcal{P}$. Owing to the noncommuting relations as

$$[\mathcal{Q}_m,\mathcal{E}_{ss'}]=\tfrac{1}{2}\mathcal{E}_{ss'},$$

where $m=s$ but $m+1\neq s'$, the enlarged symmetry still cannot be written in a direct product $SU_d(2n)_\mathcal{P}\otimes SU_c(2n)_\mathcal{P}$ but $SU_d(2n)_\mathcal{P}\times SU_c(2n)_\mathcal{P}$. This is also a difference from the single-band Hubbard model, the symmetry for the single-band case in our notation is a direct product of the two $SU(2)$'s: i.e., $SO(4)\simeq SU_d(2)\otimes SU_c(2)$ on which the discussion on the completeness of the Bethe ansatz solution and the off-diagonal long-range order is based.[16,17]

V. BRIEF SUMMARY

In summary, we studied the symmetries of the Hubbard model of n-fold orbital degenerate electrons. We show and clarify that the $SU_d(2n)$ and $SU_c(2n)$ symmetries hold, respectively, for the model with unified on-site interaction and that with partly attractive interactions. An extended Lieb–Mattis transformation is given to map these two symmetries into each other. But the sub-symmetry $SU_d^{(e)}(n)\otimes SU_d^{(o)}(n)$ is found to be possessed by the two models and both for arbitrary chemical potential μ. By excluding more than two electrons on the same sites we find the $SU_d(2n)_{\mathcal{P}}$ and $SU_c(2n)_{\mathcal{P}}$ symmetries both exist in each kind of the two models, so we have an enlarged symmetry $SU_d(2n)_{\mathcal{P}}\times SU_c(2n)_{\mathcal{P}}$. Under this exclusion, another underlying symmetry $(SU_c^{(e)}(2)_{\mathcal{P}}\times\cdots\times SU_c^{(e)}(2)_{\mathcal{P}})\otimes(SU_c^{(o)}(2)_{\mathcal{P}}\times\cdots\times SU_c^{(o)}(2)_{\mathcal{P}})$ is also found for the unified U model with chemical potential $\mu=U$, and consequently this model has the symmetry $SU_d(2n)_{\mathcal{P}}\times SU_c(2n)_{\mathcal{P}}\times[(SU_c^{(e)}(2)_{\mathcal{P}}\times\cdots\times SU_c^{(e)}(2)_{\mathcal{P}})\otimes(SU_c^{(o)}(2)_{\mathcal{P}}\times\cdots\times SU_c^{(o)}(2)_{\mathcal{P}})]$. The underlying symmetry is valid for the partially attractive model with chemical potential $\mu=-U$.

ACKNOWLEDGMENTS

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Proof of a conjecture on the conductivity of checkerboards

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In 1985 Mortola and Steffé conjectured a formula for the effective conductivity tensor of a checkerboard structure where the unit cell of periodicity is square and subdivided into four equal squares each having a different conductivity. In this article their conjecture is proven. The key idea is to superimpose suitably reflected potentials to obtain the solution to the dual problem. This is then related back to the original problem using a well known theorem of Keller, thereby proving the conjecture. The analysis also yields formulas relating the potentials in the four squares. Independently, Craster and Obnosov have obtained a completely different proof of the conjecture. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1385564]

I. INTRODUCTION

There are relatively few microstructures which yield explicit formulas for their effective electrical conductivity. Such formulas are useful as benchmarks for testing numerical codes and as examples for illustrating more general theoretical results. One family of microstructures which has received considerable attention in this regard are checkerboards. Dykhne[1], using a duality argument, found that the effective conductivity σ_* of the standard checkerboard with squares of conductivity σ_1 and σ_2 is simply

$$\sigma_* = \sqrt{\sigma_1 \sigma_2}. \tag{1}$$

This solution was subsequently used[2,3] to show that the effective conductivity of a three-dimensional checkerboard (i.e., a face centered cubic arrangement of touching cubes) is $2\sqrt{\sigma_1\sigma_2}$ in the asymptotic limit when the ratio σ_1/σ_2 of the conductivity of the two phases is large. The result provided a crucial test showing the current limitations of a numerical method[4] based on fast Fourier transforms. Asymptotic and numerical results[3,5–7] for the effective conductivity of rectangular and parallelogram checkerboards were also obtained. The geometry consisting of a square array of squares oriented at 45° to the unit cell, which becomes a checkerboard when the squares touch, has become a test case for checking numerical methods.[8–12]

The explicit solution for the electric potential solving the conductivity equations in the standard two-dimensional checkerboard was obtained by Berdichevskii.[13] Subsequently, Mityushev and Zhorovina[14] and Obnosov[15,16] obtained explicit solutions for rectangular and triangular checkerboards.

Random checkerboards with the phases having a large contrast in their conductivities were studied by Sheng and Kohn,[17] Kozlov,[18] Berlyand and Golden[19] and Golden and Kozlov.[20] Miller,[21,22] Beran and Silnutzer[23] and Silnutzer[24] obtained bounds on the effective conductivity and bulk modulus for a class of materials called cell materials, where space is divided into cells and each cell is assigned randomly as phase 1 or phase 2, weighted according to what volume fraction one desires to achieve. The bounds depend on a certain parameter (denoted as G' in two dimensions and G in three dimensions). This parameter has been evaluated for square cells[25] and cubic cells,[26] thereby providing bounds on the effective conductivity and bulk modulus two- and three-dimensional random checkerboards. Numerical results for the conductivity of random square and hexagonal checkerboards were obtained by Torquato, Kim and Cule[27] and Suquet and Moulinec.[28]

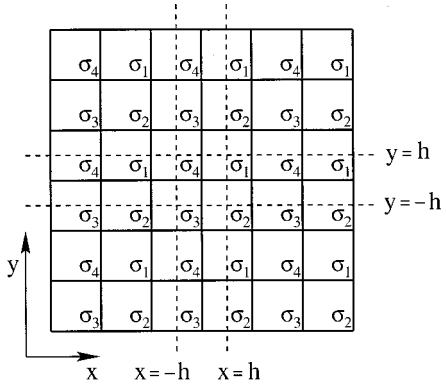

FIG. 1. The two-dimensional checkerboard structure. When the average electric field is applied in the x direction the electric potential is constant along the lines $x=h$ and $x=-h$, while the lines $y=h$ and $y=-h$ are lines of current flow.

Berdichevskii[29] applied a duality result to show that the two effective shear moduli $\mu_*^{(1)}$ and $\mu_*^{(2)}$ (corresponding to shears at 45° to each other) of a periodic checkerboard of two incompressible isotropic phases have the same product as the product of the two shear moduli μ_1 and μ_2 of the two isotropic phases. When both phases share the same two-dimensional bulk modulus κ it follows[30–32] that

$$(1/\mu_*^{(1)}+1/\kappa)(1/\mu_*^{(2)}+1/\kappa)=(1/\mu_1+1/\kappa)(1/\mu_2+1/\kappa). \tag{2}$$

Berlyand and Kozlov[33] obtained asymptotic solutions for the effective elastic moduli of checkerboards in the limit where there is a large contrast in the stiffnesses of the two phases. Interestingly, they found that such checkerboards would have an effective Poisson's ratio close to zero when stretched in a diagonal direction.

Over 15 years ago an interesting conjecture regarding the conductivity of four phase checkerboards was made by Mortola and Steffé.[34] The checkerboard they studied is periodic with a square unit cell of periodicity of side length $4h$. The unit cell is subdivided into four equal subsquares of side length $2h$ each filled with a different phase. These phases are numbered 1, 2, 3 and 4 going clockwise around the unit cell. The resulting checkerboard structure is illustrated in Fig. 1.

The equation of electrical conductivity takes the form

$$\nabla\cdot\sigma(x,y)\nabla\phi(x,y)=0, \tag{3}$$

where $\phi(x,y)$ is the electric potential and $\sigma(x,y)$ is the locally isotropic conductivity field taking the value σ_j in phase $j=1,2,3,4$. Alternatively, one can work with the system of equations

$$\nabla\cdot\mathbf{j}=0,\ \ \mathbf{j}(x,y)=\sigma(x,y)\mathbf{e}(x,y),\quad \mathbf{e}=\left(-\frac{\partial\phi}{\partial x},-\frac{\partial\phi}{\partial y}\right), \tag{4}$$

where $\mathbf{j}(x,j)$ is the current field and $\mathbf{e}(x,y)$ is the electric field. By finding periodic fields $\mathbf{j}$ and $\mathbf{e}$ which solve the equations (4) one can determine the effective conductivity tensor $\boldsymbol{\sigma}_*$ through the relation between the average current and average electric field which is governed by the effective constitutive law,

$$\langle\mathbf{j}\rangle=\boldsymbol{\sigma}_*\langle\mathbf{e}\rangle, \tag{5}$$

where the angular brackets denote averages over the unit cell of periodicity. Now when the average electric field is applied in the x direction, symmetry considerations imply that the lines $x=h$ and $x=-h$ in Fig. 1 are lines of constant electric potential, while the lines $y=h$ and $y=$

$-h$ are lines of current flow. Similarly when the average electric field is applied in the y direction, the lines $x=h$ and $x=-h$ are lines of current flow, while the lines $y=h$ and $y=-h$ are lines of constant electric potential. As observed by Mortola and Steffé[34] these considerations imply that the effective tensor is diagonal

$$\boldsymbol{\sigma}_* = \begin{pmatrix} \sigma_{*x} & 0 \\ 0 & \sigma_{*y} \end{pmatrix}. \tag{6}$$

Mortola and Steffé obtained upper and lower bounds on both σ_{*x} and σ_{*y} and they conjectured that the exact values would be given by the square root of the product of their upper and lower bounds, resulting in the formulas

$$\sigma_{*x} = \sqrt{\frac{\sigma_1\sigma_2\sigma_3\sigma_4(1/\sigma_1+1/\sigma_2+1/\sigma_3+1/\sigma_4)(\sigma_1+\sigma_2)(\sigma_3+\sigma_4)}{(\sigma_1+\sigma_2+\sigma_3+\sigma_4)(\sigma_1+\sigma_4)(\sigma_2+\sigma_3)}}, \tag{7}$$

$$\sigma_{*y} = \sqrt{\frac{\sigma_1\sigma_2\sigma_3\sigma_4(1/\sigma_1+1/\sigma_2+1/\sigma_3+1/\sigma_4)(\sigma_1+\sigma_4)(\sigma_2+\sigma_3)}{(\sigma_1+\sigma_2+\sigma_3+\sigma_4)(\sigma_1+\sigma_2)(\sigma_3+\sigma_4)}}. \tag{8}$$

They showed that these formulas were consistent with many analytical results. For example, when $\sigma_1\sigma_3=\sigma_2\sigma_4$ the formulas agree with an exact result of Marino and Spagnolo[35] for the effective conductivity tensor, and when $\sigma_3=\sigma_1$ and $\sigma_4=\sigma_2$ the formulas reduce to Dykhne's result (1) for the effective conductivity of a two-phase checkerboard. Mortola and Steffé also provided numerical calculations in support of the conjecture in the special case when

$$\sigma_1=\sigma_2=\sigma_3=1, \quad \sigma_4=\delta, \tag{9}$$

corresponding to a two-phase composite comprised of a square array of squares of conductivity δ occupying a volume fraction of $\frac{1}{4}$ in a matrix of conductivity 1. In this case, the effective conductivity tensor is isotropic and their conjecture implies

$$\sigma_{*x}=\sigma_{*y}=\sqrt{(1+3\delta)/(3+\delta)}. \tag{10}$$

This result was proved by Obnosov,[16] who also found explicit formulas for the potentials which solve the conductivity equations, and generalized the result to rectangular arrays of rectangles. When $\delta=100$ the formula (10) gives $\sigma_*=1.709\,482\,406\,194\,2$. Johan Helsing (private communication), using formulas (7) and (8) of Ref. 36, has numerically calculated the result to be $\sigma_*=1.709\,482\,406\,1(8)$ (digit within parenthesis not converged). So the agreement between theory and numerical calculations is outstanding. It should be added that Helsing's computations typically have this accuracy no matter what the geometry of the two-phase two-dimensional composite. Clearly such high accuracy results reduce the need for exact solutions. For the square array of squares at other volume fractions Cole, Li and Bak[37] obtained experimental results, Perrins,[38] Meidell,[39] and Lukkassen[40] obtained numerical results, and Kozlov and Vucans[41] have obtained an implicit formula for σ_* when $\sigma_1=0$.

In this paper I prove that the conjectured formulas (7) and (8) are indeed correct. Craster and Obnosov,[42] whose work I found about after my proof was complete, have also proved the conjecture. Our proofs are quite different. They apply conformal transformations to the solution of a basic problem involving four joined quarter planes, each with a different conductivity. This allows them to also solve the problem of a four-phase rectangular checkerboard. My solution is not so explicit, but on the other hand only involves linear algebra, and the idea of superimposing suitably reflected potentials.

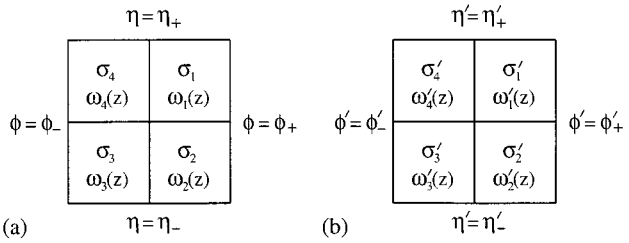

FIG. 2. (a) The region $\mathcal{R}$ bounded by the four lines $x=\pm h$ and $y=\pm h$, showing the complex potentials and conductivities within each phase, and the boundary conditions along each edge of $\mathcal{R}$. (b) By taking new potentials in each quadrant which are linear combinations of the old potential in that quadrant and the old potentials in the three other quadrants, suitably reflected, one obtains another solution to the problem but with new complex potentials and conductivities in the four squares and new boundary conditions along the edges of $\mathcal{R}$.

II. PROOF OF THE CONJECTURE

It suffices to prove the formula (7) for σ_{*x} since the formula (8) for σ_{*y} follows from it, by interchanging the roles of phases 2 and 4. Therefore we will assume that the applied electric field is in the x direction. We let ϕ_+ and ϕ_- denote the constant values that the electric potential takes along the lines $x=h$ and $x=-h$, respectively. The lines $y=h$ and $y=-h$ are lines of current flow. Due to symmetry it suffices to consider the equations in the square region $\mathcal{R}$ bounded by these four lines, as illustrated in Fig. 2(a).

We begin with some standard analysis. Since the field $\mathbf{j}$ is divergence free we can express it in terms of a current potential η:

$$\mathbf{j}=\left(-\frac{\partial \eta}{\partial y},\frac{\partial \eta}{\partial x}\right). \tag{11}$$

The continuity of η ensures continuity of the normal component of the current across each interface. Indeed, if $\mathbf{n}$ is the normal to the interface, then the current flux $\mathbf{j}\cdot\mathbf{n}$ is equal to the gradient of η in the direction tangential to the interface, which will be continuous across the interface. Rather than keeping track of the condition of continuity of the current flux across each interface, it is much simpler to keep track of the condition of continuity of the potential η across each interface. Also the fact that the lines $y=h$ and $y=-h$ are lines of current flow implies that the current potential is constant along these lines, taking values η_+ and η_-, respectively. It is convenient to introduce $z=x+iy$ and the complex potential

$$\omega=\phi+i\psi \quad \text{where} \quad \psi=\eta/\sigma. \tag{12}$$

The constitutive law $\mathbf{j}=\sigma\mathbf{e}$ implies that ϕ and ψ satisfy the Cauchy–Riemann equations, and consequently ω is an analytic function of z within each of the four phases. We let $\omega_j(z)=\phi_i(z)+i\psi_i(z)$ denote its value within phase j.

At the interfaces between the phases the continuity of the potentials ϕ and $\eta=\sigma\psi$ imposes the constraints

$$\begin{aligned}
&\phi_1=\phi_2, \quad \sigma_1\psi_1=\sigma_2\psi_2, \quad \text{when} \quad y=0, \quad 0\leqslant x\leqslant h,\\
&\phi_2=\phi_3, \quad \sigma_2\psi_2=\sigma_3\psi_3, \quad \text{when} \quad x=0, \quad 0\geqslant y\geqslant -h,\\
&\phi_3=\phi_4, \quad \sigma_3\psi_3=\sigma_4\psi_4, \quad \text{when} \quad y=0, \quad 0\geqslant x\geqslant -h,\\
&\phi_4=\phi_1, \quad \sigma_3\psi_3=\sigma_1\psi_1, \quad \text{when} \quad x=0, \quad 0\leqslant y\leqslant h.
\end{aligned} \tag{13}$$

Also the fact that $x=h$ and $x=-h$ are lines of constant electrical potential ϕ implies that

$$\begin{gathered}\phi_1=\phi_+,\ \text{when}\ x=h,\ 0\leqslant y\leqslant h,\\ \phi_2=\phi_+,\ \text{when}\ x=h,\ 0\geqslant y\geqslant -h,\\ \phi_3=\phi_-,\ \text{when}\ x=-h,\ 0\geqslant y\geqslant -h,\\ \phi_4=\phi_-,\ \text{when}\ x=-h,\ 0\leqslant y\leqslant h,\end{gathered}\tag{14}$$

while the fact that $y=h$ and $y=-h$ are lines of constant current potential η implies that

$$\begin{gathered}\sigma_1\psi_1=\eta_+,\ \text{when}\ y=h,\ 0\leqslant x\leqslant h,\\ \sigma_2\psi_2=\eta_-,\ \text{when}\ y=-h,\ 0\leqslant x\leqslant h,\\ \sigma_3\psi_3=\eta_-,\ \text{when}\ y=-h,\ 0\geqslant x\geqslant -h,\\ \sigma_4\psi_4=\eta_+,\ \text{when}\ y=h,\ 0\geqslant x\geqslant -h.\end{gathered}\tag{15}$$

Now the potentials $\phi-(\phi_+-\phi_-)x/(2h)$ and $\eta-(\eta_+-\eta_-)y/(2h)$ are periodic and since the gradient of a periodic potential has average value zero it follows that

$$\langle\mathbf{e}\rangle=(-(\phi_+-\phi_-)/(2h),0),\quad \langle\mathbf{j}\rangle=(-(\eta_+-\eta_-)/(2h),0).\tag{16}$$

Consequently it is the ratio of the two potential drops which determines the effective conductivity in the x direction:

$$\sigma_{*x}=\frac{\eta_+-\eta_-}{\phi_+-\phi_-}.\tag{17}$$

The key idea behind the present proof of the formula (7) for σ_{*x} is to consider new potentials in each quadrant which are linear combinations of the old potential in that quadrant and the old potentials in the three other quadrants, suitably reflected. With appropriate choices of the linear combinations, we will see that these new potentials solve a conductivity problem of the same type but with different conductivities σ_1', σ_2', σ_3', and σ_4' in the four squares, as illustrated in Fig. 2(b). Accordingly, let us introduce new complex potentials,

$$\begin{aligned}\omega_1'(z)&=\phi_1'(z)+i\psi_1'(z)=a_{11}\omega_1(z)+a_{12}\overline{\omega_2(\overline{z})}+a_{13}\omega_3(-z)+a_{14}\overline{\omega_4(-\overline{z})},\\ \omega_2'(z)&=\phi_2'(z)+i\psi_2'(z)=a_{21}\overline{\omega_1(\overline{z})}+a_{22}\omega_2(z)+a_{23}\overline{\omega_3(-\overline{z})}+a_{24}\omega_4(-z),\\ \omega_3'(z)&=\phi_3'(z)+i\psi_3'(z)=a_{31}\omega_1(-z)+a_{32}\overline{\omega_2(-\overline{z})}+a_{33}\omega_3(-z)+a_{34}\overline{\omega_4(\overline{z})},\\ \omega_4'(z)&=\phi_4'(z)+i\psi_4'(z)=a_{41}\overline{\omega_1(-\overline{z})}+a_{42}\omega_2(-z)+a_{43}\overline{\omega_3(\overline{z})}+a_{44}\omega_4(z),\end{aligned}\tag{18}$$

which are analytic functions of z, each defined within that subsquare of $\mathcal{R}$ containing phase 1, 2, 3, or 4, respectively.

We want to ensure that the new electrical potential ϕ' and the new current potential $\eta'=\sigma'\psi'$ are continuous across the interfaces between phases. In particular, the continuity of these potentials across the interface between phases 1 and 2 requires that

$$\begin{aligned}a_{11}\phi_1+a_{12}\phi_2+a_{13}\phi_3+a_{14}\phi_4&=a_{21}\phi_1+a_{22}\phi_2+a_{23}\phi_3+a_{24}\phi_4,\\ \sigma_1'(a_{11}\psi_1-a_{12}\psi_2+a_{13}\psi_3-a_{14}\psi_4)&=\sigma_2'(-a_{21}\psi_1+a_{22}\psi_2-a_{23}\psi_3+a_{24}\psi_4),\end{aligned}\tag{19}$$

when $y=0$ and $0\leqslant x\leqslant h$, where the minus signs in the latter equation arise because of the appearance of complex conjugates in (18). In view of the continuity conditions (13) on the potentials ϕ and $\sigma\psi$ across the interface these constraints reduce to

$$\begin{aligned}&(a_{11}+a_{12}-a_{21}-a_{22})\phi_1+(a_{13}+a_{14}-a_{23}-a_{24})\phi_3=0,\\&(\sigma_1'\sigma_2a_{11}-\sigma_1'\sigma_1a_{12}+\sigma_2'\sigma_2a_{21}-\sigma_2'\sigma_1a_{22})\psi_1/\sigma_2+(\sigma_1'\sigma_4a_{13}-\sigma_1'\sigma_3a_{14}+\sigma_2'\sigma_4a_{23}\\&\quad-\sigma_2'\sigma_3a_{24})\psi_3/\sigma_4=0,\end{aligned}\tag{20}$$

and will be satisfied provided the coefficients in brackets vanish. By similar considerations applied to the remaining interfaces between phases we arrive at the set of equations

$$\begin{aligned}&a_{11}+a_{12}-a_{21}-a_{22}=0,\quad a_{13}+a_{14}-a_{23}-a_{24}=0,\\&a_{31}+a_{32}-a_{41}-a_{42}=0,\quad a_{33}+a_{34}-a_{43}-a_{44}=0,\\&a_{21}+a_{24}-a_{31}-a_{34}=0,\quad a_{22}+a_{23}-a_{32}-a_{33}=0,\\&a_{11}+a_{14}-a_{41}-a_{44}=0,\quad a_{12}+a_{13}-a_{42}-a_{43}=0,\end{aligned}\tag{21}$$

which ensure continuity of the electrical potential ϕ', and at the set of equations

$$\begin{aligned}&\sigma_1'\sigma_2a_{11}-\sigma_1'\sigma_1a_{12}+\sigma_2'\sigma_2a_{21}-\sigma_2'\sigma_1a_{22}=0,\quad \sigma_1'\sigma_4a_{13}-\sigma_1'\sigma_3a_{14}+\sigma_2'\sigma_4a_{23}-\sigma_2'\sigma_3a_{24}=0,\\&\sigma_3'\sigma_2a_{31}-\sigma_3'\sigma_1a_{32}+\sigma_4'\sigma_2a_{41}-\sigma_4'\sigma_1a_{42}=0,\quad \sigma_3'\sigma_4a_{33}-\sigma_3'\sigma_3a_{34}+\sigma_4'\sigma_4a_{43}-\sigma_4'\sigma_3a_{44}=0,\\&-\sigma_2'\sigma_4a_{21}+\sigma_2'\sigma_1a_{24}-\sigma_3'\sigma_4a_{31}+\sigma_3'\sigma_1a_{34}=0,\quad \sigma_2'\sigma_3a_{22}-\sigma_2'\sigma_2a_{23}+\sigma_3'\sigma_3a_{32}-\sigma_3'\sigma_2a_{33}=0,\\&\sigma_1'\sigma_4a_{11}-\sigma_1'\sigma_1a_{14}+\sigma_4'\sigma_4a_{41}-\sigma_4'\sigma_1a_{44}=0,\quad -\sigma_1'\sigma_3a_{12}+\sigma_1'\sigma_2a_{13}-\sigma_4'\sigma_3a_{42}+\sigma_4'\sigma_2a_{43}=0,\end{aligned}\tag{22}$$

which ensure continuity of the current potential $\eta'=\sigma'\psi'$.

It is easy to check that when (21) and (22) are satisfied, then the new electrical potential ϕ' is constant along the lines $x=h$ and $x=-h$, while the new current potential η' is constant along the lines $y=h$ and $y=-h$. Specifically, as illustrated in Fig. 2(b), we have

$$\begin{aligned}&\phi=\phi_+'\ \text{ when }\ x=h,\ \ \phi'=\phi_-'\ \text{ when }\ x=-h,\\&\eta'=\eta_+'\ \text{ when }\ y=h,\ \ \eta'=\eta_-'\ \text{ when }\ y=-h,\end{aligned}\tag{23}$$

where

$$\begin{aligned}\phi_+'&=(a_{11}+a_{12})\phi_++(a_{13}+a_{14})\phi_-,\\\phi_-'&=(a_{31}+a_{32})\phi_++(a_{33}+a_{34})\phi_-,\end{aligned}\tag{24}$$

and

$$\begin{aligned}\eta_+'&=[(a_{11}/\sigma_1-a_{14}/\sigma_4)\eta_++(-a_{12}/\sigma_2+a_{13}/\sigma_3)\eta_-)]\sigma_1',\\\eta_-'&=[(-a_{21}/\sigma_1+a_{24}/\sigma_4)\eta_++(a_{22}/\sigma_2-a_{23}/\sigma_3)\eta_-)]\sigma_2'.\end{aligned}\tag{25}$$

Provided we can find a solution to the 16 equations (21) and (22) with a nonzero value of the potential drop $\phi'_+ - \phi'_-$ the new material with conductivities σ'_1, σ'_2, σ'_3, and σ'_4 must have effective conductivity

$$\sigma'_{*x} = \frac{\eta'_+ - \eta'_-}{\phi'_+ - \phi'_-} \tag{26}$$

in the x direction. If we consider the 16 coefficients a_{ij} and the four conductivities σ'_1, σ'_2, σ'_3, and σ'_4 to be unknowns, then there are more unknowns than equations and so we certainly expect many solutions. This is the basic idea. Finding an appropriate solution is the only difficulty.

Let us set

$$\sigma'_1 = 1/\sigma_2, \quad \sigma'_2 = 1/\sigma_3, \quad \sigma'_3 = 1/\sigma_4, \quad \sigma'_4 = 1/\sigma_1. \tag{27}$$

Then the new material corresponds to taking the original material, replacing all conductivities by their reciprocals, and then rotating the entire structure anticlockwise by 90°. Due to a theorem of Keller[43] (see also Refs. 44, 1, and 45) this new dual material has effective conductivity

$$\sigma'_{*x} = 1/\sigma_{*x} \tag{28}$$

in the x direction. We will see that this equation in conjunction with (26) provides the desired formula for σ_{*x}.

Making the substitutions (27) and using an algebraic manipulator, such as Maple, one solution to the equations is found to be

$$\begin{aligned}
a_{11} &= (\sigma_1+\sigma_3)(\sigma_4+\sigma_1)(\sigma_3+\sigma_4)(\sigma_1+\sigma_2)\sigma_2,\\
a_{12} &= 0,\\
a_{13} &= 0,\\
a_{14} &= (\sigma_4+\sigma_1)(\sigma_3+\sigma_4)(\sigma_4\sigma_1-\sigma_3\sigma_2)\sigma_2,\\
a_{21} &= \sigma_2(\sigma_1-\sigma_3)(\sigma_1+\sigma_3)(\sigma_4+\sigma_1)(\sigma_3+\sigma_4),\\
a_{22} &= (\sigma_1+\sigma_3)(\sigma_4+\sigma_1)(\sigma_3+\sigma_4)(\sigma_2+\sigma_3)\sigma_2,\\
a_{23} &= (\sigma_2+\sigma_3)(\sigma_4+\sigma_1)(\sigma_4\sigma_1-\sigma_3\sigma_2)\sigma_3,\\
a_{24} &= (\sigma_4+\sigma_1)(\sigma_4\sigma_2-\sigma_3^2)(\sigma_4\sigma_1-\sigma_3\sigma_2),\\
a_{31} &= (\sigma_1^2-\sigma_4\sigma_2)(\sigma_3+\sigma_4)(\sigma_1\sigma_2-\sigma_4\sigma_3),\\
a_{32} &= (\sigma_3+\sigma_4)(\sigma_1\sigma_2-\sigma_4\sigma_3)\sigma_2(\sigma_4+\sigma_1),\\
a_{33} &= \sigma_3(\sigma_4+\sigma_1)(\sigma_3\sigma_2\sigma_1+\sigma_3\sigma_1\sigma_4+2\sigma_4\sigma_1\sigma_2+2\sigma_3\sigma_4\sigma_2+\sigma_4\sigma_2^2+\sigma_4^2\sigma_2),\\
a_{34} &= \sigma_4(\sigma_1-\sigma_3)(\sigma_3\sigma_2\sigma_1+\sigma_3\sigma_1\sigma_4+2\sigma_4\sigma_1\sigma_2+2\sigma_3\sigma_4\sigma_2+\sigma_4\sigma_2^2+\sigma_4^2\sigma_2),\\
a_{41} &= \sigma_1(\sigma_1+\sigma_2)(\sigma_3+\sigma_4)(\sigma_1\sigma_2-\sigma_4\sigma_3),\\
a_{42} &= 0,\\
a_{43} &= 0,
\end{aligned} \tag{29}$$

$$a_{44}=(\sigma_3+\sigma_4)\sigma_1(\sigma_3\sigma_2\sigma_1+\sigma_3\sigma_1\sigma_4+2\sigma_4\sigma_1\sigma_2+2\sigma_3\sigma_4\sigma_2+\sigma_4\sigma_2^2+\sigma_4^2\sigma_2).$$

There are other solutions to the equations, but they all lead to the same result provided $\phi'_+ - \phi'_-$ is nonzero. This solution was picked because of its relative simplicity. By inserting the solution (29) in (24) and (25) one finds that the associated potential drops are

$$\begin{gathered}\phi'_+ - \phi'_- = \sigma_1\sigma_2\sigma_3\sigma_4(1/\sigma_1+1/\sigma_2+1/\sigma_3+1/\sigma_4)(\sigma_1+\sigma_2)(\sigma_3+\sigma_4)(\phi_+ - \phi_-),\\ \eta'_+ - \eta'_- = (\sigma_1+\sigma_2+\sigma_3+\sigma_4)(\sigma_1+\sigma_4)(\sigma_2+\sigma_3)(\eta_+ - \eta_-).\end{gathered} \tag{30}$$

Substituting these back in (26) and using (17) yields the desired relation between the effective conductivities σ'_{*x} and σ_{*x},

$$\sigma'_{*x}=\frac{(\sigma_1+\sigma_2+\sigma_3+\sigma_4)(\sigma_1+\sigma_4)(\sigma_2+\sigma_3)}{\sigma_1\sigma_2\sigma_3\sigma_4(1/\sigma_1+1/\sigma_2+1/\sigma_3+1/\sigma_4)(\sigma_1+\sigma_2)(\sigma_3+\sigma_4)}\sigma_{*x}, \tag{31}$$

which in conjunction with (28) proves that σ_{*x} is given by (7).

III. RELATIONS BETWEEN THE POTENTIALS AND EQUIVALENT CHECKERBOARDS

Some conclusions about the potentials in the four phases also follow from this analysis. Let $\mathbf{M}(\sigma_1,\sigma_2,\sigma_3,\sigma_4,\sigma'_1,\sigma'_2,\sigma'_3,\sigma'_4)$ denote the 16 by 16 matrix associated with the homogeneous system of equations (21) and (22). Using Maple one can readily verify that

$$\text{rank}[\mathbf{M}(\sigma_1,\sigma_2,\sigma_3,\sigma_4,\sigma'_1,\sigma'_2,\sigma'_3,\sigma'_4)]\leqslant 14. \tag{32}$$

In other words, the homogeneous system of equations (21) and (22) has a nonzero solution for the set of coefficients a_{ij} for any choice of the new conductivities σ'_1, σ'_2, σ'_3, and σ'_4. However, unless the new conductivities satisfy the condition that

$$\text{rank}[\mathbf{M}(\sigma_1,\sigma_2,\sigma_3,\sigma_4,\sigma'_1,\sigma'_2,\sigma'_3,\sigma'_4)]\leqslant 13, \tag{33}$$

the resulting potential drops $\phi'_+ - \phi'_-$ and $\eta'_+ - \eta'_-$ both turn out to be zero, and the potentials ϕ' and η' must therefore be constant everywhere, that is, one has obtained trivial potentials that solve the conductivity equations in the second checkerboard problem. By adding suitable constants to the original potentials ϕ and η one can ensure that the resulting potentials ϕ' and η' are both zero, implying certain linear relations among the four complex potentials $\omega_1(z)$, $\overline{\omega_2(\overline{z})}$, $\omega_3(-z)$ and $\overline{\omega_4(-\overline{z})}$ that hold for all z. Such relations can be used to reduce the equations (21) and (22) to a system of eight equations with eight unknowns, if desired. When the condition (33) is satisfied we will say that the two materials with conductivities $\sigma(x,y)$ and $\sigma'(x,y)$ are equivalent checkerboards. The equivalence holds in the sense that the potentials solving one checkerboard problem provide through (18) a nontrivial solution for the potentials in the other checkerboard problem.

To see how this works in a particular case, let us consider the special situation solved by Obnosov[16] where $\sigma_1=\sigma_2=\sigma_3=1$ and $\sigma_4=\delta$, as in (9). Then for any choice of the conductivities σ'_1, σ'_2, σ'_3, and σ'_4 the equations (21) and (22) are solved with

$$\begin{gathered}a_{11}=a_{13}=c_1+c_2/\sigma'_1,\quad a_{12}=c_1-c_2/\sigma'_1,\quad a_{14}=c_1\delta-c_2/\sigma'_1,\\ a_{21}=a_{23}=c_1-c_2/\sigma'_2,\quad a_{22}=c_1+c_2/\sigma'_2,\quad a_{24}=c_1\delta+c_2/\sigma'_4,\\ a_{31}=a_{33}=c_1+c_2/\sigma'_3,\quad a_{32}=c_1-c_2/\sigma'_3,\quad a_{34}=c_1\delta-c_2/\sigma'_3,\\ a_{41}=a_{43}=c_1-c_2/\sigma'_4,\quad a_{42}=c_1+c_2/\sigma'_4,\quad a_{42}=c_1\delta+c_2/\sigma'_4.\end{gathered} \tag{34}$$

where c_1 and c_2 are arbitrary constants. By substituting these formulas back in (24) and (25) one finds that

$$\phi'_- = \phi'_+ = c_1[2\phi_+ + (1+\delta)\phi_-], \quad \eta'_- = \eta'_+ = c_2[(1+1/\delta)\eta_+ + 2\eta_-]. \tag{35}$$

So the associated potential drops are zero.

Now, by adding appropriate constants to the electrical potential and conjugate electrical potential we can assume, without loss of generality, that

$$\phi_+ = -(1+\delta)\phi_-/2, \quad \eta_+ = -2\eta_-/(1+1/\delta). \tag{36}$$

Then the resulting potentials ϕ'_-, ϕ'_+, η'_-, and η'_+ given by (35) are zero. Consequently, the potentials $\omega'_1(z)$, $\omega'_2(z)$, $\omega'_3(z)$ and $\omega'_4(z)$ are zero for all z, and by substituting (34) back in (18) we obtain the relations

$$\begin{aligned} \omega_1(z) + \overline{\omega_2(\overline{z})} + \omega_3(-z) + \delta\overline{\omega_4(-\overline{z})} = 0, \\ \omega_1(z) - \overline{\omega_2(\overline{z})} + \omega_3(-z) - \overline{\omega_4(-\overline{z})} = 0. \end{aligned} \tag{37}$$

These identities allow us to express ω_2 and ω_4 in terms of ω_1 and ω_3:

$$\begin{aligned} \omega_2(z) = -(1+\delta)(\overline{\omega_1(\overline{z})} + \overline{\omega_3(-\overline{z})})/(1-\delta), \\ \omega_4(z) = 2(\overline{\omega_1(-\overline{z})} + \overline{\omega_3(\overline{z})})/(1-\delta) = -2\omega_2(-z)/(1+\delta). \end{aligned} \tag{38}$$

Thus there are some very simple relations among the potentials in the four subsquares.

Using Maple one can check that the condition (33) for equivalence will be satisfied if

$$\delta = f(\sigma'_1,\sigma'_2,\sigma'_3,\sigma'_4) \equiv \frac{b+5a+c}{b-3a}, \quad \text{or} \quad \delta = 1/f(\sigma'_1,\sigma'_2,\sigma'_3,\sigma'_4) = \frac{b+5a-c}{b-3a}, \tag{39}$$

where

$$\begin{aligned} a &= \sigma'_1\sigma'_3/(\sigma'_2\sigma'_4) + \sigma'_2\sigma'_4/(\sigma'_1\sigma'_3) - 2, \\ b &= (\sigma'_1+\sigma'_2+\sigma'_3+\sigma'_4)(1/\sigma'_1+1/\sigma'_2+1/\sigma'_3+1/\sigma'_4), \\ c &= 4\left|1/(\sigma'_1\sigma'_3) - 1/(\sigma'_2\sigma'_4)\right| \sqrt{(\sigma'_1+\sigma'_2)(\sigma'_2+\sigma'_3)(\sigma'_3+\sigma'_4)(\sigma'_4+\sigma'_1)}, \end{aligned} \tag{40}$$

The two values of δ given by (39) are reciprocals of each other. Thus any given checkerboard (with arbitrary positive conductivities σ'_1, σ'_2, σ'_3, and σ'_4) is equivalent to a square array of squares at a volume fraction of $\frac{1}{4}$ [with conductivities $\sigma_1=\sigma_2=\sigma_3=1$, and $\sigma_4=\delta$ where δ is given by (39)]. In other words, Obnosov's solution[16] for the square array of squares could be used to generate the solution for the potentials in the given checkerboard, using (18), where the set of coefficients a_{ij} is any solution to the equations (21) and (22) that is independent of the solutions (34). Such a solution can be easily found using Maple, but the expressions are not sufficiently concise to justify their reproduction here, especially in view of the explicit solution obtained by Craster and Obnosov.[42]

More generally, a checkerboard with four arbitrary conductivities σ_1, σ_2, σ_3, and σ_4 is equivalent to a checkerboard with conductivities σ'_1, σ'_2, σ'_3, and σ'_4 [in the sense that (33) is satisfied] if and only if they are each equivalent to a checkerboard with conductivities 1,1,1 and δ for some choice of δ, i.e., if and only if

$$f(\sigma_1,\sigma_2,\sigma_3,\sigma_4) = f(\sigma'_1,\sigma'_2,\sigma'_3,\sigma'_4). \tag{41}$$

The conductivities (27) satisfy this criterion of equivalence, which is what makes this proof of Mortola and Steffé's conjecture possible.

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Graphical representation of the partition function of a one-dimensional δ-function Bose gas

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The one-dimensional repulsive δ-function bose system is studied. By only using the Bethe ansatz equation, n-particle partition functions are exactly calculated. From this expression for the n-particle partition function, the n-particle cluster integral is derived. The results completely agree with those of the thermal Bethe ansatz (TBA). This directly proves the validity of the TBA. The theory of partitions and graphs is used to simplify the discussion. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1396836]

I. INTRODUCTION

We study statistical mechanics of a one-dimensional gas of Bose particles interacting through a repulsive delta function potential. The Hamiltonian for the system with n particles reads

$$H_n = -\sum_{i=1}^{n} \frac{\partial^2}{\partial x_i^2} + 2c \sum_{i>j} \delta(x_i - x_j). \tag{1.1}$$

Throughout the paper, we set $\hbar = 1$, $2m = 1$ and assume the potential is repulsive, $c > 0$.

The eigenvalues and the eigenstates are obtained by the Bethe ansatz (BA) method,[1,2] and the quantum inverse scattering method (QISM).[3–8] As a periodic boundary condition, the Bethe ansatz (BA) equation is derived. Using the BA equation, thermodynamic quantities are calculated by the thermal Bethe ansatz (TBA).[9,10] In the TBA, an ''interpretation'' of the particle density and the state density enables us to define the entropy of n-particle system in the thermodynamic limit.

With the quantum Gelfand–Levitan equation,[3,7] the field operator is expressed as a series of the terms each of which is a product of creation and annihilation operators in the scattering data space. The grand partition function is written as a field operator.[5] Creamer, Thacker, and Wilkinson[4] calculated the grand partition function using creation and annihilation operators of this system, but the analysis involves a delicate regularization that $2\pi\delta(0)$ is replaced by the volume L.

To be rigorous, it is desirable to examine these results by a different approach. In this paper, we present a method to calculate the thermodynamical quantities only by use of the BA equation which is derived exactly as a periodic boundary condition from both QISM and BA method. We calculate the n-particle partition function and evaluate the n-particle cluster integral.

The paper is organized as follows: The n-particle partition function and the n-particle cluster integral are derived with a method, which we call a direct method, in Sec. II. This method is shown explicitly for $n = 3$. In Sec. III, we consider the n-particle case, and reformulate the results in graphical expressions. The last section is devoted to concluding remarks and discussions. To avoid complexities, the details of a mathematical proof are summarized in Appendix A.

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II. DIRECT METHOD

We assume a finite system size L and the periodic boundary condition. It is known that the total energy E and the wave numbers k_j of the system (1.1) are determined by the following relations:

$$E=\sum_{j=1}^{n} k_j^2, \tag{2.1}$$

$$k_jL=2\pi m_j+\sum_{j'\neq j}\Delta(k_{j'}-k_j), \tag{2.2}$$

where m_j are integers or half-integers, and $\Delta(k)$ is the phase shift of two-particle scattering,

$$m_j\in\begin{cases}\mathbb{Z} & \text{if } N=\text{odd}\\ \mathbb{Z}+\frac{1}{2} & \text{if } N=\text{even},\end{cases} \tag{2.3}$$

$$m_j<m_{j+1}, \tag{2.4}$$

$$\Delta(k)=2\arctan\left(\frac{k}{c}\right), \tag{2.5}$$

$$-\pi<\Delta(k)<\pi.$$

Equation (2.2) is called the Bethe ansatz (BA) equation. Main objects to be calculated are the n-particle partition function Z_n,

$$Z_n=\mathrm{Tr}\,e^{-\beta H_n},\quad \beta=1/k_BT, \tag{2.6}$$

and the n-particle cluster integral b_n,

$$\sum_{n\geqslant 1} b_nz^n=\log\left(\sum_{n\geqslant 0} Z_nz^n\right), \tag{2.7}$$

where $z=e^{\beta\mu}$ with the chemical potential μ. By definition, $Z_0=1$ and we simply have

$$b_1=L^{-1}Z_1=\int\frac{dk}{2\pi}e^{-\beta k^2}. \tag{2.8}$$

We explain a direct method to evaluate the partition function for 3-particle case. To be explicit, the total energy is

$$E=k_1^2+k_2^2+k_3^2, \tag{2.9}$$

and the BA equation is

$$\begin{aligned}k_1L&=2\pi m_1+\Delta(k_2-k_1)+\Delta(k_3-k_1),\\ k_2L&=2\pi m_2+\Delta(k_1-k_2)+\Delta(k_3-k_2),\\ k_3L&=2\pi m_3+\Delta(k_1-k_3)+\Delta(k_2-k_3),\end{aligned} \tag{2.10}$$

$$m_1<m_2<m_3\in\mathbb{Z}. \tag{2.11}$$

By use of these relations (2.9)–(2.11), we can calculate the partition function Z_3 as follows:

$$
\begin{aligned}
Z_3 &= \sum_{m_1<m_2<m_3} e^{-\beta(k_1^2+k_2^2+k_3^2)} = \frac{1}{6}\sum_{m_1,m_2,m_3} e^{-\beta(k_1^2+k_2^2+k_3^2)} - \frac{1}{2}\sum_{m_1,m_2=m_3} e^{-\beta(k_1^2+k_2^2+k_3^2)} \\
&\quad + \frac{1}{3}\sum_{m_1=m_2=m_3} e^{-\beta(k_1^2+k_2^2+k_3^2)} \\
&= \frac{1}{6}\sum_{\tilde{m}_1,\tilde{m}_2,\tilde{m}_3} \int dm_1 dm_2 dm_3 e^{-\beta(k_1^2+k_2^2+k_3^2)+2\pi i(m_1\tilde{m}_1+m_2\tilde{m}_2+m_3\tilde{m}_3)} \\
&\quad - \frac{1}{2}\sum_{\tilde{m}_1',\tilde{m}_2'} \int dm_1', dm_2' e^{-\beta(2k_1'^2+k_2'^2)+2\pi i(m_1'\tilde{m}_1'+m_2'\tilde{m}_2')} + \frac{1}{3}\sum_{\tilde{m}''} \int dm'' e^{-\beta(3k^2)+2\pi i m''\tilde{m}''} \\
&= \frac{1}{6}\sum_{\tilde{m}_1,\tilde{m}_2,\tilde{m}_3} \int dk_1 dk_2 dk_3 \left|\frac{\partial m}{\partial k}\right| e^{-\beta(k_1^2+k_2^2+k_3^2)+iL(k_1\tilde{m}_1+k_2\tilde{m}_2+k_3\tilde{m}_3)} \\
&\quad \times \left(\frac{k_1-k_2+ic}{k_1-k_2-ic}\right)^{\tilde{m}_2-\tilde{m}_1}\left(\frac{k_2-k_3+ic}{k_2-k_3-ic}\right)^{\tilde{m}_3-\tilde{m}_2}\left(\frac{k_3-k_1+ic}{k_3-k_1-ic}\right)^{\tilde{m}_1-\tilde{m}_3} \\
&\quad - \frac{1}{2}\sum_{\tilde{m}_1',\tilde{m}_2'} \int dk_1', dk_2' \left|\frac{\partial m'}{\partial k'}\right| e^{-\beta(2k_1'^2+k_2'^2)+iL(k_1'\tilde{m}_1'+k_2'\tilde{m}_2')}\left(\frac{k_1'-k_2'+ic}{k_1'-k_2'-ic}\right)^{\tilde{m}_2-2\tilde{m}_1} \\
&\quad + \frac{1}{3}\sum_{\tilde{m}''} \int dk'' \frac{\partial m''}{\partial k''} e^{-\beta(3k^2)+iLk''\tilde{m}''},
\end{aligned}
\tag{2.12}
$$

where $|\partial m/\partial k|$, $|\partial m'/\partial k'|$, and $\partial m''/\partial k''$ are the Jacobians to be explained shortly. We have written explicitly all the steps of calculations which are common to those for general n.[11–13] In the second equality, we use a symmetry of the BA equation with respect to the exchange $m_i, k_i \leftrightarrow m_{i'}, k_{i'}$, in the third equality, we apply the Poisson's summation formula, and in the last equality, we change variables of integration from m to k.

The relation between k and m is defined by the BA equation. In (2.12), k', m', k'', and m'' are related as follows:

$$
\begin{aligned}
k_1'L &= 2\pi m_1' + 2\Delta(k_2'-k_1'), \\
k_2'L &= 2\pi m_2' + \Delta(k_1'-k_2'),
\end{aligned}
\tag{2.13}
$$

$$
k''L = 2\pi m''. \tag{2.14}
$$

Thus, the Jacobians, $|\partial m/\partial k|$, $|\partial m'/\partial k'|$, and $\partial m''/\partial k''$, are given by

$$
\begin{aligned}
(2\pi)^3\left|\frac{\partial m}{\partial k}\right| &= L^3 + 2L^2K(k_1-k_2) + 2L^2K(k_2-k_3) + 2L^2K(k_3-k_1) + 3LK(k_2-k_1)K(k_3-k_1) \\
&\quad + 3LK(k_1-k_2)K(k_3-k_2) + 3LK(k_1-k_3)K(k_2-k_3),
\end{aligned}
\tag{2.15}
$$

$$
(2\pi)^2\left|\frac{\partial m'}{\partial k'}\right| = L^2 + 3LK(k_1-k_2), \tag{2.16}
$$

$$
\frac{\partial m''}{\partial k''} = \frac{1}{2\pi}L, \tag{2.17}
$$

where

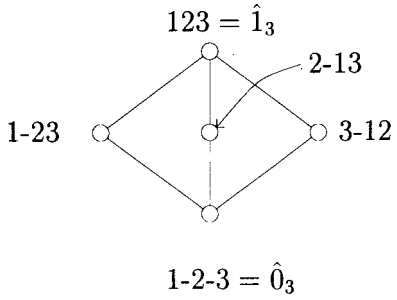


FIG. 1. Vertices of this graph are the elements of Π_3, and if $x<y$ then y is drawn "above" x (i.e., with a higher vertical coordinate). It is called the *Hasse diagram* (Ref. 14) of Π_3.

$$K(k)\equiv\frac{d\Delta(k)}{dk}=\frac{2c}{k^2+c^2}. \tag{2.18}$$

It is readily shown that all terms except $\tilde{m}_i=0$, $\tilde{m}_i'=0$ and $\tilde{m}''=0$ in (2.12) exponentially decay as L gets large. Although the discussion may include these decaying terms, we hereafter consider the expressions in the thermodynamic limit. Then, Z_3 becomes

$$\begin{aligned}Z_3=&\frac{1}{6}\int\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}\frac{dk_3}{2\pi}(L^3+6L^2K(k_1-k_2)+9LK(k_2-k_1)K(k_3-k_1))e^{-\beta(k_1^2+k_2^2+k_3^2)}\\&-\frac{1}{2}\int\frac{dk_1'}{2\pi}\frac{dk_2'}{2\pi}(L^2+3LK(k_1-k_2))e^{-\beta(2k_1'^2+k_3'^2)}+\frac{1}{3}\int\frac{dk''}{2\pi}Le^{-\beta(3k^2)}.\end{aligned} \tag{2.19}$$

It is much easier to show

$$Z_2=\frac{1}{2}\int\frac{dk_1'}{2\pi}\frac{dk_2'}{2\pi}(L^2+2LK(k_1-k_2))e^{-\beta(k_1'^2+k_3'^2)}-\frac{1}{2}\int\frac{dk''}{2\pi}Le^{-\beta(2k''^2)}. \tag{2.20}$$

From (2.8), (2.19), and (2.20), the cluster integral b_3 is given by

$$\begin{aligned}b_3=&\frac{1}{L}\left(Z_3-Z_2Z_1+\frac{1}{3}Z_1^3\right)=\frac{3}{2}\int\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}\frac{dk_3}{2\pi}K(k_2-k_1)K(k_3-k_1)e^{-\beta(k_1^2+k_2^2+k_3^2)}\\&-\frac{3}{2}\int\frac{dk_1'}{2\pi}\frac{dk_2'}{2\pi}K(k_1-k_2)e^{-\beta(2k_1'^2+k_3'^2)}+\frac{1}{3}\int\frac{dk''}{2\pi}e^{-\beta(3k^2)}.\end{aligned} \tag{2.21}$$

Thanks to the effective interaction $K(k)$, b_3 consists of only 3 terms. In the next section, we show that Z_n and b_n can be calculated in the same way.

III. PARTITION FUNCTION AND GRAPHS

A. Partition function

In order to present a general structure of the partition function, we need to explain some terminology in the theory of partition;[14] the partially ordered set (poset, for short).

Let $\Pi(S)$ denote a set of all partitions of a finite set S. In what follows, $[n]$ means a set $\{1,2,\ldots,n\}$, and write Π_n for $\Pi([n])$. We define partially order in $\Pi(S)$ by *refinement*, that is, define $x\leqslant y\in\Pi(S)$ if every block of x is contained in a block of y. For example, if $x\in\Pi_9$ has blocks 137-2-46-58-9 and $y\in\Pi_9$ has blocks 13467-2589, then $x\leqslant y$. Special elements in $\Pi(S)$ are $\hat{0}_S$ and $\hat{1}_S$ such that $x\geqslant\hat{0}_S$ and $x\leqslant\hat{1}_S$ for all $x\in\Pi(S)$. We write $\hat{0}_n$ and $\hat{1}_n$ for $\hat{0}_{[n]}$ and $\hat{1}_{[n]}$. Figure 1 shows the partially ordered elements in Π_3, that is, 1-2-3$<$1-23, 2-13, 3-12$<$123. In

addition, we define Möbius function of $\Pi(S)$ inductively as follows:

$$\mu(x,x)=1 \quad \text{for all } x\in\Pi(S),$$

$$\mu(x,y)=-\sum_{x\leqslant z<y}\mu(x,z) \quad \text{for all } x<y \text{ in } \Pi(S). \tag{3.1}$$

By use of those definitions, we can show some useful relations. For brevity, $\mathbb{N}$ and $\mathbb{C}$ stand, respectively, non-negative integers and complex numbers. (1) Let $\hat{f},\hat{g}:\Pi(S)\to\mathbb{C}$, then,

$$\hat{g}(x)=\sum_{y\geqslant x}\hat{f}(y), \quad \text{for all } x\in\Pi(S),$$

if and only if

$$\hat{f}(x)=\sum_{y\geqslant x}\mu(x,y)\hat{g}(y), \quad \text{for all } x\in\Pi(S). \tag{3.2}$$

This is called the Möbius inversion formula. (2) Let $\hat{g},\hat{J}:\Pi(S)\to\mathbb{C}$ and $f,h:\mathbb{N}\to\mathbb{C}$. If

$$\sum_{n\geqslant 0}h(n)\frac{u^n}{n!}=\exp\left(\sum_{n\geqslant 1}f(n)\frac{u^n}{n!}\right), \tag{3.3}$$

$$h(N_S)=\sum_{x\in\Pi(S)}\mu(\hat{0}_S,x)\hat{g}(x), \tag{3.4}$$

$$\hat{g}(x)=\sum_{\xi\in\Pi(x)}\prod_{y\in\xi}\hat{J}(y), \tag{3.5}$$

then

$$f(n)=\sum_{x\in\Pi_n}\mu(\hat{0}_n,x)\hat{J}(x). \tag{3.6}$$

We prove this relation in the Appendix.

With these two relations, we can derive the partition function Z_n and the cluster integral b_n in a compact way. First we define $f,h:\mathbb{N}\to\mathbb{C}$ and $\hat{h},\hat{g}:\Pi(S)\to\mathbb{C}$,

$$f(n)\equiv n!Lb_n, \tag{3.7}$$

$$h(n)\equiv n!Z_n, \tag{3.8}$$

$$\hat{h}(x)\equiv\sum_{m_1'\neq\cdots\neq m_l'}e^{-\beta(k_1^2+\cdots+k_n^2)}, \tag{3.9}$$

$$\hat{g}(x)\equiv\sum_{m_1',\cdots,m_l'}e^{-\beta(k_1^2+\cdots+k_n^2)}, \tag{3.10}$$

where

$$x\in\Pi(S), \quad \sigma_i\ni s_j\Rightarrow m_i'=m_j, \quad x=\{\sigma_1,\ldots,\sigma_l\}, \quad S=\{s_1,\ldots,s_n\}. \tag{3.11}$$

Recall that m and k are related by the BA equation. We see that Eq. (3.3) holds from the definition of cluster integral b_n, Eq. (2.7). From the definition (3.8)–(3.10), it is easy to show that

$$\hat{g}(x)=\sum_{y\geqslant x}\hat{h}(y), \tag{3.12}$$

$$\hat{h}(\hat{0}_n)=h(n). \tag{3.13}$$

Due to the Möbius inversion formula (3.2), (3.12) is equivalent to

$$\hat{h}(x)=\sum_{y\geqslant x}\mu(x,y)\hat{g}(y). \tag{3.14}$$

Substituting $\hat{0}_n$ for x in this equation, we obtain

$$h(n)=\sum_{y\in\Pi_n}\mu(\hat{0}_n,y)\hat{g}(y). \tag{3.15}$$

This is nothing but condition (3.4).

As we have mentioned in the previous section, we do not include exponentially decaying terms. Then, (3.10) is written as

$$\hat{g}(x)=\int\prod_{\sigma\in x}dm'_\sigma e^{-\beta(k_1^2+k_2^2+\cdots+k_n^2)} \tag{3.16}$$

$$=\int\prod_{\sigma\in x}dk'_\sigma\left|\frac{\partial m'}{\partial k'}\right|e^{-\beta(\Sigma_{\sigma\in x}N_\sigma k'^2_\sigma)}. \tag{3.17}$$

The transformation matrix and the Jacobian are given as follows:

$$\frac{\partial m'_\sigma}{\partial k'_{\sigma'}}=\frac{1}{2\pi}\times\begin{cases}L+\displaystyle\sum_{\sigma''\neq\sigma}N_{\sigma''}K(k'_{\sigma''}-k'_\sigma) & \text{if } \sigma=\sigma'\\ -N_{\sigma'}K(k'_{\sigma'}-k'_\sigma) & \text{if } \sigma\neq\sigma'\end{cases} \tag{3.18}$$

$$\sigma,\sigma',\sigma''\in x$$

$$\left|\frac{\partial m'}{\partial k'}\right|=\sum_{\xi\in\Pi(x)}\prod_{y\in\xi}\frac{L}{(2\pi)^{N_y}}\left(\sum_{\sigma\in y}N_\sigma\right)\sum_{t\in\mathcal{V}(y)}\left(\prod_{\sigma\in y}N_\sigma^{n(\sigma,t)-1}\right)$$

$$\times\left(\prod_{b\in\Xi(t)}K(k'_{\sigma_1(b)}-k'_{\sigma_2(b)})\right). \tag{3.19}$$

We explain the notations in (3.18) and (3.19). The number of elements in a set σ is denoted by N_σ. $\mathcal{V}(S)$ denotes a set of all undirected *trees* with a *vertex* set S. For instance, all the elements in $\mathcal{V}(\{\sigma_1,\sigma_2,\sigma_3\})$ are depicted in Fig. 2. We call a connection of two vertices a *branch.* $\Xi(t)$ denotes a set of all branches contained in a tree t. $n(\sigma,t)$ is the number of branches with which the vertex σ are connected in the tree t. $\sigma_1(b)$ and $\sigma_2(b)$ denote two end-vertices connected by a branch b.

A remaining task is a consistency with (3.5). We define a function $\hat{J}:\Pi(S)\to\mathbb{C}$ by

$$\hat{J}(x)\equiv\int\prod_{\sigma\in x}dk'_\sigma\left|\frac{\partial m'}{\partial k'}\right|_c e^{-\beta(\Sigma_{\sigma\in x}N_\sigma k'^2_\sigma)}, \tag{3.20}$$

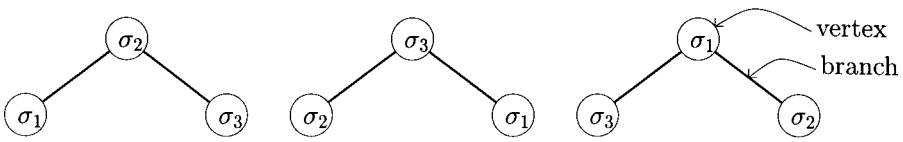


FIG. 2. A set of undirected trees, $\mathcal{V}(\{\sigma_1,\sigma_2,\sigma_3\})$, contains three elements.

where

$$\left|\frac{\partial m'}{\partial k'}\right|_c \equiv \frac{L}{(2\pi)^{N_x}}\left(\sum_{\sigma\in x} N_\sigma\right)\sum_{t\in\mathcal{V}(x)}\left(\prod_{\sigma\in x} N_\sigma^{n(\sigma,t)-1}\right)\left(\prod_{b\in\Xi(t)} K(k'_{\sigma_1(b)}-k'_{\sigma_2(b)})\right). \tag{3.21}$$

We can change the expression of the Jacobian $|\partial m'/\partial k'|$ from (3.19) into a sum of forests, that is, sets of trees. On the other hand, the right-hand side of (3.21) is a sum of connected forests, that is, trees. Therefore, we put a subscript c as $|\partial m'/\partial k'|_c$. With this definition, we see that the condition (3.5) follows from (3.17).

In this way, three conditions (3.3)–(3.5) are shown to be satisfied, which indicates that Eq. (3.6) holds. We write Eq. (3.6) explicitly,

$$b_n=\frac{1}{n!L}\sum_{x\in\Pi_n}\mu(\hat{0}_n,x)\int\prod_{\sigma\in x}dk'_\sigma\left|\frac{\partial m'}{\partial k'}\right|_c e^{-\beta(\Sigma_{\sigma\in x}N_\sigma k'^2_\sigma)}. \tag{3.22}$$

In fact, (3.15) is equivalent to

$$Z_n=\frac{1}{n!}\sum_{x\in\Pi_n}\mu(\hat{0}_n,x)\int\prod_{\sigma\in x}dk'_\sigma\left|\frac{\partial m'}{\partial k'}\right| e^{-\beta(\Sigma_{\sigma\in x}N_\sigma k'^2_\sigma)}. \tag{3.23}$$

The Jacobians in (3.22) and (3.23) are, respectively, (3.21) and (3.19). The explicit form of $\mu(\hat{0}_n,x)$ can be derived from (3.1),

$$\mu(\hat{0}_n,x)=\prod_{\sigma\in x}(-1)^{N_\sigma-1}(N_\sigma-1)! \tag{3.24}$$

It is easily shown[12,13] that the cluster integrals b_n agree with those derived from the thermal Bethe ansatz (TBA). It is also possible to derive the integral equation in TBA from (3.22).[13]

We give two remarks here. First, the Jacobian $|\partial m'/\partial k'|$ is essentially the inner product of the Bethe wave functions.[8] Second, the cluster integrals consist of only a finite number of terms.

B. Graph representation

We further develop a graphical representation of the cluster integral and the partition function. We draw an l times rolled coil for a Boltzmann weight $e^{-\beta l k^2}$ (Fig. 3). We call it l-toron following Montroll and Ward.[15,16] The *tree* consists of a toron or torons connected by branches. The *forest* consists of the trees. We denote by $\mathcal{V}_n$ a set of all the trees which satisfy the following two conditions: (1) all the vertices of the tree are made of torons, and (2) the sum of rolled number of

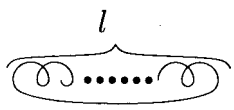


FIG. 3. l-toron.

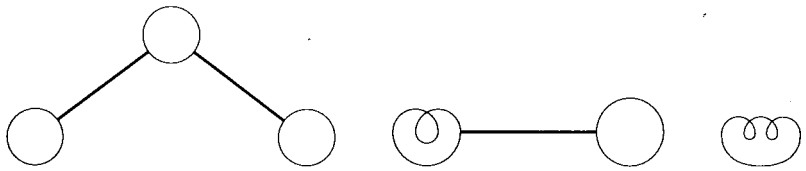


FIG. 4. A set of the trees, $\mathcal{V}_3$, contains three elements.

torons composing the tree is n. Figure 4 shows all the elements in $\mathcal{V}_3$. $\mathcal{W}_n$ is a set of all the forests which satisfy the following two conditions: (1) all the vertices of the forest are made of torons, and (2) the sum of rolled number of torons composing the forest is n. Simply, $\mathcal{V}_n$ is a subset of $\mathcal{W}_n$. Figure 5 exhibits all the elements in $\mathcal{W}_3$.

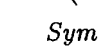
In terms of these terminologies, we may rewrite (3.23) and (3.22) as

$$Z_n = \sum_{f \in \mathcal{W}_n} \frac{Sym(f)}{n!} \prod_{t \text{ in the forest } f} \mathcal{S}(t), \tag{3.25}$$

$$b_n = \sum_{t \in \mathcal{V}_n} \frac{Sym(t)}{n!L} \mathcal{S}(t). \tag{3.26}$$

Here, $Sym(t)$ and $Sym(f)$ indicate symmetrical factors of graphs. In the case $t \in \mathcal{V}_n$ or $f \in \mathcal{W}_n$, $Sym(t)$ or $Sym(f)$ means the number of different ways in which a set $\{1,\ldots,n\}$ can be distributed to all the vertices of t or f at a time, on the condition that l elements are placed in a vertex made of l-toron. For example,

$$Sym\left(\text{  }\right) = 12, \tag{3.27}$$

$$Sym\left(\text{  }\right) = 3, \tag{3.28}$$

$$Sym\left(\text{  }\right) = 1. \tag{3.29}$$

From (3.22) and (3.23), we can show that $\mathcal{S}(t)$ in (3.25) and (3.26) is given as follows:

$$\mathcal{S}(t) \equiv L \sum_{\omega} N_\omega \left(\prod_{\omega} (-1)^{N_\omega - 1} (N_\omega - 1)! N_\omega^{n(\omega,t)-1} \right) \times \int \prod_{\omega} \frac{dk_\omega}{2\pi} \left(\prod_{b \in \Xi(t)} K(k_{\sigma_1(b)} - k_{\sigma_2(b)}) \right) e^{-\beta(\Sigma_\omega N_\omega k_\omega)}, \tag{3.30}$$

where N_ω denotes the rolled number of toron ω, and Σ_ω (or Π_ω) denotes a sum (or a product) with respect to all the toron ω in the tree t. For example,

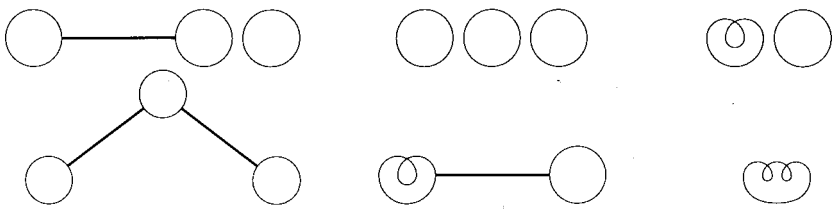


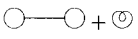
FIG. 5. A set of the forests, $\mathcal{W}_3$. Three graphs in the first line are not trees because the vertices are not connected on partially connected by branch(es).

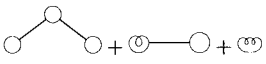
$$\mathcal{S}\left(\circledcirc\!\!-\!\!\circ\right) = L\times(2+1)\times\left((-1)^1\,1!2^0\times(-1)^0\,0!1^0\right) \times\int\frac{dk_{\omega_1}}{2\pi}\frac{dk_{\omega_2}}{2\pi}\left(K\left(k_{\omega_1}-k_{\omega_2}\right)\right)e^{-\beta\left(2k_{\omega_1}+k_{\omega_2}\right)}. \tag{3.31}$$

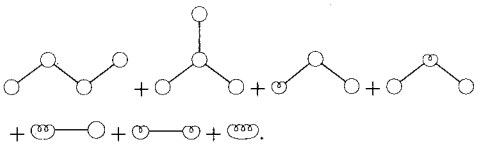
Substitution of (3.28) and (3.31) gives the second term in (2.21).

As examples, we list a graphical representation of the cluster integrals $b_1\sim b_4$,

$b_1 =$  (3.32)

$b_2 =$  (3.33)

$b_3 =$  (3.34)

$b_4 =$  (3.35)

IV. CONCLUDING REMARKS AND DISCUSSIONS

In this paper, we have studied a one-dimensional δ-function bose gas, (1.1), and have derived directly the partition function and the cluster integral, (3.23) and (3.22), from the Bethe ansatz equation, (2.2). This should be regarded as a proof of the thermal Bethe ansatz (TBA). The derivation is simplified by use of the partially ordered set in the theory of partition.

This direct method has some advantages. First, the method is rigorous. In the quantum field theoretic method, calculation is done at the infinite volume, therefore an interpretation of $2\pi\delta(0)$ as the volume is unavoidable. In the TBA, it is necessary to define the n-particle entropy. This procedure is based on an interpretation of the particle and state densities. In this sense, both field theoretic method and TBA remained to be proved. On the other hand, the direct method is free from such interpretations, and all calculations are traceable step by step.

Second, the method has a wide applicability. It should be remarked that in the direct method all the dependencies on the systems come only from the BA equation. In other words, the direct method may have the generality at least as well as TBA.

We conclude that the direct method will be useful and important in calculating the thermodynamic quantities in various integrable systems.

APPENDIX: A PROOF OF (3.6)

We use the same notation as in Sec. III A. It can be shown that, on condition that $h,f:\mathbb{N}\to\mathbb{C}$, we have

$$\sum_{n\geqslant 0}h(n)\frac{u^n}{n!}=\exp\left(\sum_{n\geqslant 1}f(n)\frac{u^n}{n!}\right) \tag{A1}$$

if and only if

$$h(n)=\sum_{x\in\Pi_n}\prod_{\sigma\in x}f(N_\sigma), \tag{A2}$$

$$h(0)=1. \tag{A3}$$

This is known as the cumulant expansion formula. Equation (A2) is equivalent to

$$\prod_{\sigma\in x}h(N_\sigma)=\sum_{y\leqslant x}\prod_{\sigma\in y}f(N_\sigma). \tag{A4}$$

For $\hat{H},\hat{F}:\Pi(S)\to\mathbb{C}$, the following relation holds:

$$\hat{H}(x)=\sum_{y\leqslant x}\hat{F}(y)\Leftrightarrow\hat{F}(x)=\sum_{y\leqslant x}\mu(x,y)\hat{H}(y). \tag{A5}$$

This is the Möbius inversion formula, which is a dual form of (3.2). With this formula, Eq. (A4) becomes

$$\prod_{\sigma\in x}f(N_\sigma)=\sum_{y\leqslant x}\mu(y,x)\prod_{\sigma\in y}h(N_\sigma). \tag{A6}$$

Substitution of $\hat{1}_n$ for x in (A6) yields

$$f(n)=\sum_{x\leqslant\hat{1}_n}\mu(y,\hat{1}_n)\prod_{\sigma\in y}h(N_\sigma). \tag{A7}$$

We suppose the existence of $\hat{g}:\Pi(S)\to\mathbb{C}$ which satisfies

$$h(N_S)=\sum_{x\in\Pi(S)}\mu(\hat{0}_S,x)\hat{g}(x). \tag{A8}$$

Using this relation, Eq. (A6) is written as

$$f(n)=\sum_{x\in\Pi_n}\mu(x,\hat{1}_n)\prod_{\sigma\in x}\sum_{y\in\Pi(\sigma)}\mu(\hat{0}_\sigma,y)\hat{g}(y)=\sum_{x\in\Pi_n}\mu(\hat{0}_n,x)\sum_{\xi\in\Pi(x)}\mu(\xi,\hat{1}_x)\prod_{y\in\xi}\hat{g}(y). \tag{A9}$$

In the second equality, we have used the following two relations:

$$\sum_{x\in\Pi_n}F(N_x)\prod_{\sigma\in x}\sum_{y\in\Pi(\sigma)}\hat{G}(y)=\sum_{x\in\Pi_n}\sum_{\xi\in\Pi(x)}F(N_\xi)\prod_{y\in\xi}\hat{G}(y), \tag{A10}$$

for $F:\mathbb{N}\to\mathbb{C}$, $\hat{G}:\Pi(S)\to\mathbb{C}$, and

$$\mu(\hat{0}_n,x)=\prod_{\sigma\in x}\mu(\hat{0}_{N_\sigma},\hat{1}_{N_\sigma}), \tag{A11}$$

for $x\in\Pi_n$. And, we suppose the existence of a map $\hat{J}:\Pi(S)\to\mathbb{C}$ which satisfies

$$\hat{g}(x)=\sum_{\xi\in\Pi(x)}\prod_{y\in\xi}\hat{J}(y). \tag{A12}$$

Then, a main part of the right-hand side of Eq. (A9) becomes

$$\begin{aligned}\sum_{\xi\in\Pi(x)}\mu(\xi,\hat{1}_x)\prod_{y\in\xi}\hat{g}(y)&=\sum_{\xi\in\Pi(x)}\mu(\xi,\hat{1}_x)\prod_{y\in\xi}\sum_{\zeta\in\Pi(y)}\prod_{z\in\zeta}\hat{J}(z)\\&=\sum_{\zeta\in\Pi(x)}\left(\sum_{\lambda\in\Pi(\zeta)}\mu(\lambda,\hat{1}_\zeta)\right)\prod_{z\in\zeta}\hat{J}(z)=\hat{J}(x).\end{aligned} \tag{A13}$$

The third equality is due to the following relation:

$$\sum_{x \in \Pi(S)} \mu(x, \hat{1}_S) = \delta(1, N_S). \tag{A14}$$

By use of relation (A13), (A9) becomes

$$f(n) = \sum_{x \in \Pi_n} \mu(\hat{0}_n, x) \hat{J}(x), \tag{A15}$$

which is (3.6). To summarize, using (A1), (A8), and (A12), we have proved (3.6).

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The Lax pairs for elliptic C_n and BC_n Ruijsenaars–Schneider models and their spectral curves

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We study the elliptic C_n and BC_n Ruijsenaars–Schneider models which are elliptic generalization of systems given in previous paper by the present authors [Chen *et al.*, J. Math. Phys. **41**, 8132 (2000)]. The Lax pairs for these models are constructed by Hamiltonian reduction technology. We show that the spectral curves can be parametrized by the involutive integrals of motion for these models. Taking nonrelativistic limit and scaling limit, we verify that they lead to the systems corresponding to Calogero–Moser and Toda types. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1389091]

I. INTRODUCTION

The Ruijsenaars–Schneider (RS) and Calogero–Moser (CM) models, as integrable many-body models, recently have attracted remarkable attention and have been extensively studied. They describe one-dimensional N-particle systems with pairwise interaction. Their importance lies in various fields ranging from lattice models in statistics physics,[1,2] to the field theory and gauge theory,[3,4] to the Seiberg–Witten theory,[5] etc. In particular, the study of the RS model is of great importance since it is the integrable relativistic generalization of the corresponding CM model.[6,7]

The Lax pairs for the CM models in various root systems have been constructed by Olshanetsky, and Perelomov[8] using reduction on symmetric space, and are further given by Inozemtsev in Ref. 9 without spectral parameter. It was almost 20 years until D'Hoker and Phong[10] constructed the Lax pairs with a spectral parameter for each of the finite dimensional Lie algebras, and the untwisted and twisted Calogero–Moser systems were introduced. Subsequently, Bordner *et al.*[11–13] succeeded in giving two types of Lax pairs associated to all of the Lie algebra: the root type and the minimal type, with and without spectral parameters. Even for all of the Coxeter group, the construction has been obtained in Ref. 14. In Ref. 15, Hurtubise and Markman utilized a so-called ''structure group,'' which combines a semisimple group and Weyl group, to construct CM systems associated with the Hitchin system, which in some degree generalizes the result of Refs. 10–14. Furthermore, the quantum version of the generalization has been developed in Refs. 16 and 17 at least for degenerate potentials of trigonometry after the works of Olshanetsky and Perelomov.[18]

So far as for the RS model, only the Lax pair of the A_{N-1} type RS model was obtained[6,2,19–22] and succeeded in recovering it by applying the Hamiltonian reduction procedure on a two-dimensional current group.[23] Although the commutative operators for the RS model based on various type Lie algebras have been given by Komori and co-workers,[24,25] Diejen,[26,27] and Hasegawa *et al.*,[1,28] the Lax integrability (or Lax pair representation) of the other type of RS model is still an open problem[5] except for a few degenerate cases.[27,30]

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In Refs. 29 and 30, we succeeded in constructing the Lax pair for C_n and BC_n RS systems only with the degenerate case (without spectral parameters). The r-matrix structure for them have been derived by Avan *et al.*[31] In this paper, we study the Lax pair for the most general C_n and BC_n RS models—the elliptic C_n and BC_n RS models. We shall give the explicit forms of Lax pairs for these systems by Hamiltonian reduction. We calculate the spectral curves for these systems, which are shown to be parametrized by a set of involutive integrals of motion. In particular, taking their nonrelativistic limit and scaling limit, we shall recover the systems of corresponding CM and Toda types, respectively. The other various degenerate cases are also be discussed and the connection between the Lax pair with a spectral parameter and the one without the spectral parameter is commented on.

The paper is organized as follows. The basic materials of the A_{N-1} RS model are reviewed in Sec. II, where we propose a Lax pair associating with the Hamiltonian which has a reflection symmetry with respect to the particles in the origin. This includes construction of a Lax pair for the A_{N-1} RS system together with its symmetry analysis. The main results are shown in Secs. III and IV. In Sec. III, we present the Lax pairs for the elliptic C_n and BC_n RS models by reducing the A_{N-1} RS model. The explicit forms for the Lax pairs are given in Sec. IV. Section V is devoted to deriving the spectral curves for these systems and their nonrelativistic counterpart, the Calogero–Moser model and scaling limit of the Toda model. Section VI shows the various degenerate limits: the trigonometric, hyperbolic, and rational cases. The last section is a brief summary and discussion.

II. THE A_{N-1}-TYPE RUIJSENAARS–SCHNEIDER MODEL

As a relativistic-invariant generalization of the A_{N-1}-type nonrelativistic Calogero–Moser model, the A_{N-1}-type Ruijsenaars–Schneider systems are completely integrable. The system's integrability was first shownd by Ruijsenaars.[6,7] The Lax pair for this model has been constructed in Refs. 6, 2, 19–22. Recent progress has shown that the compactification of higher dimension SUSY Yang–Mills theory and Seiberg–Witten theory can be described by this model.[5] Instanton correction of the prepotential associated with the sl_2 RS system has been calculated in Ref. 32.

A. Model and equations of motion

Let us briefly give the basics of this model. In terms of the canonical variables p_i, $x_i (i,j=1,\ldots,N)$ enjoying the canonical Poisson bracket

$$\{p_i,p_j\}=\{x_i,x_j\}=0, \quad \{x_i,p_j\}=\delta_{ij}, \tag{II.1}$$

the Hamiltonian of the A_{N-1} RS system reads

$$\mathcal{H}_{A_{N-1}}=\sum_{i=1}^{N}\left(e^{p_i}\prod_{k\neq i} f(x_i-x_k)+e^{-p_i}\prod_{k\neq i} g(x_i-x_k)\right), \tag{II.2}$$

where

$$\begin{aligned} f(x)&:=\frac{\sigma(x-\gamma)}{\sigma(x)},\\ g(x)&:=f(x)\big|_{\gamma\to-\gamma}, \quad x_{ik}:=x_i-x_k, \end{aligned} \tag{II.3}$$

and γ denotes the coupling constant. Here, $\sigma(x)$ is the Weierstrass σ function which is an entire, odd and quasiperiodic function with a fixed pair of the primitive quasiperiods $2\omega_1$ and $2\omega_3$. It can be defined as the infinite product

$$\sigma(x)=x\prod_{w\in\Gamma\setminus\{0\}}\left(1-\frac{x}{w}\right)\exp\left[\frac{x}{w}+\frac{1}{2}\left(\frac{x}{w}\right)^2\right],$$

where $\Gamma=2\omega_1\mathbb{Z}+2\omega_3\mathbb{Z}$ is the corresponding period lattice. Defining a third dependent quasiperiod $2\omega_2=-2\omega_1-2\omega_3$, one has

$$\sigma(x+2\omega_k)=-\sigma(x)e^{2\eta_k(x+\omega_k)},\quad \zeta(x+2\omega_k)=\zeta(x)+2\,\eta_k,\quad k=1,2,3,$$

where

$$\zeta(x)=\frac{\sigma'(x)}{\sigma(x)},\quad \wp(x)=-\zeta'(x),$$

and $\eta_k=\zeta(\omega_k)$ satisfy $\eta_1\omega_3-\eta_3\omega_1=\pi i/2$.

Notice that in Ref. 6 Ruijsenaars used another "gauge" of the momenta such that two are connected by the following canonical transformation:

$$x_i\to x_i,\quad p_i\to p_i+\frac{1}{2}\ln\prod_{j\neq i}^{N}\frac{f(x_{ij})}{g(x_{ij})}. \tag{II.4}$$

The Lax matrix for this model has the form(for the general elliptic case)

$$L(\lambda)=\sum_{i,j=1}^{N}\frac{\Phi(x_i-x_j+\gamma,\lambda)}{\Phi(\gamma,\lambda)}\exp(p_j)b_jE_{ij}, \tag{II.5}$$

where

$$\Phi(x,\lambda):=\frac{\sigma(x+\lambda)}{\sigma(x)\sigma(\lambda)},\quad b_j:=\prod_{k\neq j}f(x_j-x_k),\quad (E_{ij})_{kl}=\delta_{ik}\delta_{jl} \tag{II.6}$$

and λ is the spectral parameter. It is shown in Refs. 21, 33, 34 that the Lax operator satisfies the quadratic fundamental Poisson bracket

$$\{L_1,L_2\}=L_1L_2a_1-a_2L_1L_2+L_2s_1L_1-L_1s_2L_2, \tag{II.7}$$

where $L_1=L_{A_{N-1}}\otimes Id, L_2=Id\otimes L_{A_{N-1}}$ and the four matrices read

$$\begin{aligned} &a_1=a+w,\quad s_1=s-w,\\ &a_2=a+s-s^*-w,\quad s_2=s^*+w. \end{aligned} \tag{II.8}$$

The forms of a,s,w are

$$\begin{aligned} a(\lambda,\mu)&=-\zeta(\lambda-\mu)\sum_{k=1}^{N}E_{kk}\otimes E_{kk}-\sum_{k\neq j}\Phi(x_j-x_k,\lambda-\mu)E_{jk}\otimes E_{kj},\\ s(\lambda)&=\zeta(\lambda)\sum_{k=1}^{N}E_{kk}\otimes E_{kk}+\sum_{k\neq j}\Phi(x_j-x_k,\lambda)E_{jk}\otimes E_{kk},\\ w&=\sum_{k\neq j}\zeta(x_k-x_j)E_{kk}\otimes E_{jj}. \end{aligned} \tag{II.9}$$

The asterisk means

$$r^*=\Pi r\Pi\ \text{ with }\ \Pi=\sum_{k,j=1}^{N}E_{kj}\otimes E_{jk}. \tag{II.10}$$

Noticing that

$$L(\lambda)^{-1}{}_{ij}=\frac{\sigma(\gamma+\lambda)\sigma(\lambda+(N-1)\gamma)}{\sigma(\lambda)\sigma(\lambda+N\gamma)}\times\sum_{i,j=1}^{N}\frac{\Phi(x_i-x_j-\gamma,\lambda+N\gamma)}{\Phi(-\gamma,\lambda+N\gamma)}\exp(-p_i)b_j'E_{ij}, \tag{II.11}$$

$$b_j':=\prod_{k\neq j}g(x_j-x_k) \tag{II.12}$$

(the proof of the above-given identity is sketched in the Appendix) one can get the characteristic polynomials of $L_{A_{N-1}}$ (Refs. 35 and 34),

$$\det(L(\lambda)-v\cdot Id)=\sum_{j=0}^{N}\Phi(\gamma,\lambda)^{-j}(-v)^{N-j}\frac{\mathcal{H}_j^+}{\sigma^j(\gamma)}\times\frac{\sigma(\lambda+j\gamma)}{\sigma(\lambda)}, \tag{II.13}$$

and that of $L^{-1}_{A_{N-1}}$ by using formula given in Eq. (A8),

$$\begin{aligned}&\det\left(\frac{\sigma(\lambda)\sigma(\lambda-N\gamma)}{\sigma(\lambda-\gamma)\sigma(\lambda-(N-1)\gamma)}\times L(\lambda-N\gamma)^{-1}-v\cdot Id\right)\\&\quad=\sum_{j=0}^{N}\Phi(-\gamma,\lambda)^{-j}(-v)^{N-j}\times\frac{(\mathcal{H}_j^-)}{\sigma^j(-\gamma)}\frac{\sigma(\lambda-j\gamma)}{\sigma(\lambda)},\end{aligned} \tag{II.14}$$

where $(\mathcal{H}_0^{\pm})_{A_{N-1}}=(\mathcal{H}_N^{\pm})_{A_{N-1}}=1$, and

$$(\mathcal{H}_i^+)_{A_{N-1}}=\sum_{\substack{J\subset\{1,\ldots,N\}\\|J|=i}}\exp\left(\sum_{j\in J}p_j\right)\prod_{\substack{j\in J\\k\in\{1,\ldots,N\}\setminus J}}f(x_j-x_k), \tag{II.15}$$

$$(\mathcal{H}_i^-)_{A_{N-1}}=\sum_{\substack{J\subset\{1,\ldots,N\}\\|J|=i}}\exp\left(\sum_{j\in J}-p_j\right)\prod_{\substack{j\in J\\k\in\{1,\ldots,N\}\setminus J}}g(x_j-x_k). \tag{II.16}$$

Defining

$$(\mathcal{H}_i)_{A_{N-1}}=(\mathcal{H}_i^+)_{A_{N-1}}+(\mathcal{H}_i^-)_{A_{N-1}}, \tag{II.17}$$

from the fundamental Poisson bracket Eq. (II.7), we can verify that

$$\{(\mathcal{H}_i)_{A_{N-1}},(\mathcal{H}_j)_{A_{N-1}}\}=\{(\mathcal{H}_i^{\varepsilon})_{A_{N-1}},(\mathcal{H}_j^{\varepsilon'})_{A_{N-1}}\}=0,\quad \varepsilon,\varepsilon'=\pm,\quad i,j=1,\ldots,N. \tag{II.18}$$

In particular, the Hamiltonian Eq. (II.2) can be rewritten as

$$\begin{aligned}\mathcal{H}_{A_{N-1}}\equiv\mathcal{H}_1&=(\mathcal{H}_1^+)_{A_{N-1}}+(\mathcal{H}_1^-)_{A_{N-1}}\\&=\sum_{j=1}^{N}(e^{p_j}b_j+e^{-p_j}b_j')\\&=\mathrm{Tr}\left(L(\lambda)+\frac{\sigma(\lambda)\sigma(\lambda+N\gamma)}{\sigma(\gamma+\lambda)\,\sigma(\lambda+(N-1)\gamma)}L(\lambda)^{-1}\right).\end{aligned} \tag{II.19}$$

It should be remarked that the set of integrals of motion Eq. (II.17) has a reflection symmetry which is the key property for the later reduction to C_n and BC_n cases, i.e., if we set

$$p_i \leftrightarrow -p_i, \quad x_i \leftrightarrow -x_i, \tag{II.20}$$

then the Hamiltonians flows $(\mathcal{H}_i)_{A_{N-1}}$ are invariant with respect to this symmetry.

The canonical equations of motion associated with the Hamiltonian flows $\mathcal{H}_1^+$ in its generic (elliptic) form read

$$\ddot{x}_i = \sum_{j \neq i} \dot{x}_i \dot{x}_j (V(x_{ij}) - V(x_{ji})), \quad i = 1, \ldots, N, \tag{II.21}$$

where the potential $V(x)$ is given by

$$V(x) = \zeta(x) - \zeta(x+\lambda), \tag{II.22}$$

in which $\zeta(x) = \sigma'(x)/\sigma(x)$. Here, $x_i = x_i(t)$, $p_i = p_i(t)$, and the superimposed dot denotes t differentiation.

B. The construction of Lax pair for the A_{N-1} RS model

As for the A_{N-1} RS model, a generalized Lax pair has been given in Refs. 6, 2, and 19–22. But there is a common character that the time evolution of the Lax matrix $L_{A_{N-1}}$ is associated with the Hamiltonian $(\mathcal{H}_1^+)_{A_{N-1}}$. We will see in Sec. III that the Lax pair cannot reduce from that kind of forms directly. Instead, we give a new Lax pair in which the evolution of $L_{A_{N-1}}$ is associated with the Hamiltonian $\mathcal{H}_{A_{N-1}}$,

$$\dot{L}_{A_{N-1}} = \{L_{A_{N-1}}, \mathcal{H}_{A_{N-1}}\} = [M_{A_{N-1}}, L_{A_{N-1}}], \tag{II.23}$$

where $M_{A_{N-1}}$ can be constructed with the help of (r,s) matrices as follows:

$$M_{A_{N-1}} = \mathrm{Tr}_2\left((s_1 - a_2)\left(1 \otimes \left(L(\lambda) - \frac{\sigma(\lambda)\sigma(\lambda + N\gamma)}{\sigma(\gamma+\lambda)\,\sigma(\lambda+(N-1)\gamma)} L(\lambda)^{-1} \right) \right) \right). \tag{II.24}$$

The explicit expression of entries for $M_{A_{N-1}}$ is

$$M_{ij} = \Phi(x_{ij}, \lambda) e^{p_j} b_j - \Phi(x_{ij}, \lambda + N\gamma) e^{-p_i} b_j', \quad i \neq j, \tag{II.25}$$

$$M_{ii} = (\zeta(\lambda) + \zeta(\gamma)) e^{p_i} b_i - (\zeta(\lambda+\gamma) - \zeta(\gamma)) e^{-p_i} b_i' \tag{II.26}$$

$$+ \sum_{j \neq i} \left((\zeta(x_{ij} + \gamma) - \zeta(x_{ij})) e^{p_j} b_j \right.$$

$$\left. + \frac{\Phi(x_{ji} + \gamma, \lambda)}{\Phi(\gamma, \lambda)} \Phi(x_{ij}, \lambda + N\gamma) e^{-p_i} b_j' \right). \tag{II.27}$$

III. HAMILTONIAN REDUCTION OF C_n AND BC_n RS MODELS FROM A_{N-1}-TYPE MODELS

Let us first mention some results about the integrability of Hamiltonian (II.2). In Ref. 7 Ruijsenaars demonstrated that the symplectic structure of the C_n- and BC_n-types of RS systems can be proved integrable by embedding their phase space to a submanifold of the A_{2n-1} and A_{2n} type RS ones, respectively, while in Refs. 26, 27, and 25, Diejen and Komori, respectively, gave a series of commuting difference operators which led to their quantum integrability. However, there are not any results about their Lax representations so far except for the special degenerate case.[29,30] In this section, we concentrate our treatment on the exhibition of the explicit forms for general C_n and BC_n RS systems.

For the convenience of analysis of symmetry, let us first give vector representation of A_{N-1} Lie algebra. Introducing an N-dimensional orthonormal basis of $\mathbb{R}^N$,

$$e_j \cdot e_k = \delta_{j,k}, \quad j,k=1,\ldots,N. \tag{III.1}$$

Then the sets of roots and vector weights of A_{N-1} type are,

$$\Delta = \{e_j - e_k : j,k=1,\ldots,N\}, \tag{III.2}$$

$$\Lambda = \{e_j : j=1,\ldots,N\}. \tag{III.3}$$

The dynamical variables are canonical coordinates $\{x_j\}$ and their canonical conjugate momenta $\{p_j\}$ with the Poisson brackets of Eq. (II.1). In a general sense, we denote them by N-dimensional vectors x and p,

$$x=(x_1,\ldots,x_N)\in\mathbb{R}^N, \quad p=(p_1,\ldots,p_N)\in\mathbb{R}^N,$$

so that the scalar products of x and p with the roots $\alpha\cdot x$, $p\cdot\beta$, etc., can be defined. The Hamiltonian of Eq. (II.2) can be rewritten as

$$\mathcal{H}_{A_{N-1}} = \sum_{\mu\in\Lambda}\left(\exp(\mu\cdot p)\prod_{\Delta\ni\beta=\mu-\nu} f(\beta\cdot x)+\exp(-\mu\cdot p)\prod_{\Delta\ni\beta=-\mu+\nu} g(\beta\cdot x)\right). \tag{III.4}$$

Here, the condition $\Delta\ni\beta=\mu-\nu$ means that the summation is over roots β such that for $\exists\,\nu\in\Lambda$,

$$\mu-\nu=\beta\in\Delta. \tag{III.5}$$

So does for $\Delta\ni\beta=-\mu+\nu$.

A. The C_n model

The set of C_n roots consists of two parts, long roots and short roots:

$$\Delta_{C_n}=\Delta_L\cup\Delta_S, \tag{III.6}$$

in which the roots are conveniently expressed in terms of an orthonormal basis of $\mathbb{R}^n$:

$$\begin{aligned}\Delta_L&=\{\pm 2e_j: \quad j=1,\ldots,n\},\\ \Delta_S&=\{\pm e_j\pm e_k,: \quad j,k=1,\ldots,n\}.\end{aligned} \tag{III.7}$$

In the vector representation, vector weights Λ are

$$\Lambda_{C_n}=\{e_j,-e_j: \quad j=1,\ldots,n\}. \tag{III.8}$$

The Hamiltonian of the C_n model is given by

$$\mathcal{H}_{C_n}=\frac{1}{2}\sum_{\mu\in\Lambda_{C_n}}\left(\exp(\mu\cdot p)\prod_{\Delta_{C_n}\ni\beta=\mu-\nu} f(\beta\cdot x)+\exp(-\mu\cdot p)\prod_{\Delta_{C_n}\ni\beta=-\mu+\nu} g(\beta\cdot x)\right). \tag{III.9}$$

From the above-mentioned data, we notice that either for A_{N-1} or C_n Lie algebra, any root $\alpha\in\Delta$ can be constructed in terms with vector weights as $\alpha=\mu-\nu$ where $\mu,\nu\in\Lambda$. By simple comparison of representation between A_{N-1} and C_n, one can find that if replacing e_{j+n} with $-e_j$

in the vector weights of A_{2n-1} algebra, we can obtain the vector weights of C_n algebra. This also holds for the corresponding roots. This gives us a hint that it is possible to get the C_n model by this kind of reduction.

For the A_{2n-1} model let us set restrictions on the vector weights with

$$e_{j+n}+e_j=0, \quad \text{for } j=1,\ldots,n, \tag{III.10}$$

which correspond to the following constraints on the phase space of the A_{2n-1}-type RS model with

$$\begin{aligned} G_i &\equiv (e_{i+n}+e_i)\cdot x = x_i + x_{i+n} = 0, \\ G_{i+n} &\equiv (e_{i+n}+e_i)\cdot p = p_i + p_{i+n} = 0, \quad i=1,\ldots,n. \end{aligned} \tag{III.11}$$

Following Dirac's method,[36] we can show

$$\{G_i, \mathcal{H}_{A_{2n-1}}\} \simeq 0, \quad \text{for } \forall i \in \{1,\ldots,2n\}, \tag{III.12}$$

i.e., $\mathcal{H}_{A_{2n-1}}$ is the first class Hamiltonian corresponding to the constraints in Eq. (III.11). Here the "weak equal" symbol $\simeq$ represents that only after calculating the result of the left-hand side of the identity could we use the conditions of constraints. It should be pointed out that the most necessary condition ensuring Eq. (III.12) is the symmetry property of formula (II.20) for the Hamiltonian Eq. (II.2). So for an arbitrary dynamical variable A, we have

$$\begin{aligned} \dot{A} &= \{A, \mathcal{H}_{A_{2n-1}}\}_D = \{A, \mathcal{H}_{A_{2n-1}}\} - \{A, G_i\}\Delta_{ij}^{-1}\{G_j, \mathcal{H}_{A_{2n-1}}\} \\ &\simeq \{A, \mathcal{H}_{A_{2n-1}}\}, \quad i,j=1,\ldots,2n, \end{aligned} \tag{III.13}$$

where

$$\Delta_{ij} = \{G_i, G_j\} = 2\begin{pmatrix} 0 & Id \\ -Id & 0 \end{pmatrix}, \tag{III.14}$$

and $\{,\}_D$ denotes the Dirac bracket. By straightforward calculation, we have the nonzero Dirac brackets of

$$\begin{aligned} \{x_i, p_j\}_D &= \{x_{i+n}, p_{j+n}\}_D = \tfrac{1}{2}\delta_{i,j}, \\ \{x_i, p_{j+n}\}_D &= \{x_{i+n}, p_j\}_D = -\tfrac{1}{2}\delta_{i,j}. \end{aligned} \tag{III.15}$$

Using the above-mentioned data together with the fact that $\mathcal{H}_{A_{N-1}}$ is the first class Hamiltonian-[see Eq. (III.12)], we can directly obtain a Lax representation of the C_n RS model by imposing constraints G_k on Eq. (II.23),

$$\begin{aligned} \{L_{A_{2n-1}}, \mathcal{H}_{A_{2n-1}}\}_D &= \{L_{A_{2n-1}}, \mathcal{H}_{A_{2n-1}}\}|_{G_k, k=1,\ldots,2n}, \\ &= [M_{A_{2n-1}}, L_{A_{2n-1}}]|_{G_k, k=1,\ldots,2n} = [M_{C_n}, L_{C_n}], \end{aligned} \tag{III.16}$$

$$\{L_{A_{2n-1}}, \mathcal{H}_{A_{2n-1}}\}_D = \{L_{C_n}, \mathcal{H}_{C_n}\}, \tag{III.17}$$

where

$$\mathcal{H}_{C_n} = \tfrac{1}{2}\mathcal{H}_{A_{2n-1}}|_{G_k, k=1,\ldots,2n},$$

$$L_{C_n}=L_{A_{2n-1}}|_{G_k,k=1,\ldots,2n},$$
$$M_{C_n}=M_{A_{2n-1}}|_{G_k,k=1,\ldots,2n}, \tag{III.18}$$

so that

$$\dot{L}_{C_n}=\{L_{C_n},\mathcal{H}_{C_n}\}=[M_{C_n},L_{C_n}]. \tag{III.19}$$

Nevertheless, the $(\mathcal{H}_1^+)_{A_{N-1}}$ is not the first class Hamiltonian, so the Lax pair given by many authors previously cannot reduce to the C_n case directly in this way.

B. The BC_n model

The BC_n root system consists of three parts: long, middle, and short roots:

$$\Delta_{BC_n}=\Delta_L\cup\Delta\cup\Delta_S, \tag{III.20}$$

in which the roots are conveniently expressed in terms of an orthonormal basis of $\mathbb{R}^n$:

$$\begin{aligned}\Delta_L&=\{\pm 2e_j:\quad j=1,\ldots,n\},\\ \Delta&=\{\pm e_j\pm e_k:\quad j,k=1,\ldots,n\},\\ \Delta_S&=\{\pm e_j:\quad j=1,\ldots,n\}.\end{aligned} \tag{III.21}$$

In the vector representation, vector weights Λ can be

$$\Lambda_{BC_n}=\{e_j,-e_j,0:\quad j=1,\ldots,n\}. \tag{III.22}$$

The Hamiltonian of the BC_n model is given by

$$\mathcal{H}_{BC_n}=\frac{1}{2}\sum_{\mu\in\Lambda_{BC_n}}\left(\exp(\mu\cdot p)\prod_{\Delta_{BC_n}\ni\beta=\mu-\nu}f(\beta\cdot x)+\exp(-\mu\cdot p)\prod_{\Delta_{BC_n}\ni\beta=-\mu+\nu}g(\beta\cdot x)\right). \tag{III.23}$$

By similar comparison of representations between A_{N-1} and BC_n, one can find that if replacing e_{j+n} with $-e_j$ and e_{2n+1} with 0 in the vector weights of the A_{2n} Lie algebra, we can obtain the vector weights of the BC_n one. The same holds for the corresponding roots. So by the same procedure as the C_n model, we could get the Lax representation of the BC_n model.

For the A_{2n} model, we set restrictions on the vector weights with

$$\begin{aligned}e_{j+n}+e_j&=0\quad\text{for}\quad j=1,\ldots,n,\\ e_{2n+1}&=0,\end{aligned} \tag{III.24}$$

which correspond to the following constraints on the phase space of the A_{2n}-type RS model with

$$\begin{aligned}G_i'&\equiv(e_{i+n}+e_i)\cdot x=x_i+x_{i+n}=0,\\ G_{i+n}'&\equiv(e_{i+n}+e_i)\cdot p=p_i+p_{i+n}=0,\quad i=1,\ldots,n,\\ G_{2n+1}'&\equiv e_{2n+1}\cdot x=x_{2n+1}=0,\\ G_{2n+2}'&\equiv e_{2n+1}\cdot p=p_{2n+1}=0.\end{aligned} \tag{III.25}$$

Similarly, we can show

$$\{G_i, \mathcal{H}_{A_{2n}}\} \simeq 0, \quad \text{for} \quad \forall i \in \{1,\ldots,2n+1,2n+2\}, \tag{III.26}$$

i.e., $\mathcal{H}_{A_{2n}}$ is the first class Hamiltonian corresponding to the above-mentioned constraints Eq. (III.25). So L_{BC_n} and M_{BC_n} can be constructed as follows:

$$\begin{aligned} L_{BC_n} &= L_{A_{2n}}|_{G'_k, k=1,\ldots,2n+2}, \\ M_{BC_n} &= M_{A_{2n}}|_{G'_k, k=1,\ldots,2n+2}, \end{aligned} \tag{III.27}$$

while $\mathcal{H}_{BC_n}$ is

$$\mathcal{H}_{BC_n} = \tfrac{1}{2}\mathcal{H}_{A_{2n}}|_{G_k, k=1,\ldots,2n+2}, \tag{III.28}$$

due to the similar derivation of Eqs. (III.13)–(III.19).

IV. LAX REPRESENTATIONS OF THE C_n AND BC_n RS MODELS

A. The C_n model

The Hamiltonian of the C_n RS system is Eq. (III.9), so the canonical equations of motion are

$$\dot{x}_i = \{x_i, \mathcal{H}\} = e^{p_i} b_i - e^{-p_i} b'_i, \tag{IV.1}$$

$$\begin{aligned} \dot{p}_i = \{p_i, \mathcal{H}\} = &\sum_{j\neq i}^{n} \left(e^{p_j} b_j (h(x_{ji}) - h(x_j + x_i)) + e^{-p_j} b'_j (\hat{h}(x_{ji}) - \hat{h}(x_j + x_i))\right) \\ &- e^{p_i} b_i \left(2h(2x_i) + \sum_{j\neq i}^{n} (h(x_{ij}) + h(x_i + x_j))\right) \\ &- e^{-p_i} b'_i \left(2\hat{h}(2x_i) + \sum_{j\neq i}^{n} (\hat{h}(x_{ij}) + \hat{h}(x_i + x_j))\right), \end{aligned} \tag{IV.2}$$

where

$$h(x) := \frac{d \ln f(x)}{dx}, \quad \hat{h}(x) := \frac{d \ln g(x)}{dx},$$

$$b_i = f(2x_i) \prod_{k\neq i}^{n} (f(x_i - x_k) f(x_i + x_k)), \tag{IV.3}$$

$$b'_i = g(2x_i) \prod_{k\neq i}^{n} (g(x_i - x_k) g(x_i + x_k)).$$

The Lax matrix for the C_n RS model can be written in the following form:

$$(L_{C_n})_{\mu\nu} = e^{\nu\cdot p} b_\nu \frac{\Phi((\mu - \nu)\cdot x + \gamma, \lambda)}{\Phi(\gamma, \lambda)}, \tag{IV.4}$$

which is a $2n \times 2n$ matrix whose indices are labeled by the vector weights, denoted by $\mu, \nu \in \Lambda_{C_n}$, M_{C_n} can be written as

$$M_{C_n}=D+Y, \tag{IV.5}$$

where D denotes the diagonal part and Y denotes the off-diagonal part

$$Y_{\mu\nu}=e^{\nu\cdot p}b_\nu\Phi(x_{\mu\nu},\lambda)+e^{-\mu\cdot p}b'_\nu\Phi(x_{\mu\nu},\lambda+N\gamma), \tag{IV.6}$$

$$\begin{aligned}D_{\mu\mu}=&(\zeta(\lambda)+\zeta(\gamma))e^{\mu\cdot p}b_\mu-(\zeta(\lambda+\gamma)-\zeta(\gamma))e^{-\mu\cdot p}b'_\mu\\&+\sum_{\nu\neq\mu}\left((\zeta(x_{\mu\nu}+\gamma)-\zeta(x_{\mu\nu}))e^{\nu\cdot p}b_\nu+\frac{\Phi(x_{\nu\mu}+\gamma,\lambda)}{\Phi(\gamma,\lambda)}\Phi(x_{\mu\nu},\lambda+N\gamma)e^{-\mu\cdot p}b'_\nu\right)\end{aligned} \tag{IV.7}$$

and

$$\begin{aligned}b_\mu&=\prod_{\Delta_{C_n}\ni\beta=\mu-\nu}f(\beta\cdot x),\\ b'_\mu&=\prod_{\Delta_{C_n}\ni\beta=\mu-\nu}g(\beta\cdot x),\\ x_{\mu\nu}&:=(\mu-\nu)\cdot x.\end{aligned} \tag{IV.8}$$

The L_{C_n},M_{C_n} satisfies the Lax equation

$$\dot{L}_{C_n}=\{L_{C_n},\mathcal{H}_{C_n}\}=[M_{C_n},L_{C_n}], \tag{IV.9}$$

which is equivalent to the equations of motion (IV.1) and (IV.2). The Hamiltonian $\mathcal{H}_{C_n}$ can be rewritten as the trace of L_{C_n},

$$\mathcal{H}_{C_n}=\operatorname{tr}L_{C_n}=\frac{1}{2}\sum_{\mu\in\Lambda_{C_n}}(e^{\mu\cdot p}b_\mu+e^{-\mu\cdot p}b'_\mu). \tag{IV.10}$$

B. The BC_n model

The Hamiltonian of the BC_n model is expressed in Eq. (III.23), so the canonical equations of motion are

$$\dot{x}_i=\{x_i,\mathcal{H}\}=e^{p_i}b_i-e^{-p_i}b'_i, \tag{IV.11}$$

$$\begin{aligned}\dot{p}_i=\{p_i,\mathcal{H}\}=&\sum_{j\neq i}^{n}(e^{p_j}b_j(h(x_{ji})-h(x_j+x_i))+e^{-p_j}b'_j(\hat{h}(x_{ji})-\hat{h}(x_j+x_i)))\\&-e^{p_i}b_i\left(h(x_i)+2h(2x_i)+\sum_{j\neq i}^{n}(h(x_{ij})+h(x_i+x_j))\right)\\&-e^{-p_i}b'_i\left(\hat{h}(x_i)+2\hat{h}(2x_i)+\sum_{j\neq i}^{n}(\hat{h}(x_{ij})+\hat{h}(x_i+x_j))\right)-b_0(h(x_i)+\hat{h}(x_i)),\end{aligned} \tag{IV.12}$$

where

$$b_i = f(x_i) f(2x_i) \prod_{k \neq i}^{n} (f(x_i - x_k) f(x_i + x_k)),$$

$$b_i' g(x_i) g(2x_i) \prod_{k \neq i}^{n} (g(x_i - x_k) g(x_i + x_k)), \tag{IV.13}$$

$$b_0 = \prod_{i=1}^{n} f(x_i) g(x_i).$$

The Lax pair for the BC_n RS model can be constructed as the form of Eqs. (IV.4)–(IV.8) where one should replace the matrices labels with $\mu, \nu \in \Lambda_{BC_n}$, and roots with $\beta \in \Delta_{BC_n}$.

The Hamiltonian $\mathcal{H}_{BC_n}$ can also be rewritten as the trace of L_{BC_n},

$$\mathcal{H}_{BC_n} = \mathrm{tr}\, L_{BC_n} = \frac{1}{2} \sum_{\mu \in \Lambda_{BC_n}} (e^{\mu \cdot p} b_\mu + e^{-\mu \cdot p} b_\mu'). \tag{IV.14}$$

V. SPECTRAL CURVES OF THE C_n AND BC_n RS SYSTEMS

It has recently been pointed out in Refs. 4, 5, 37 and 38, that the SU(N) RS model is related to five-dimensional gauge theories. In the context of Seiberg–Witten theory, the elliptic RS integrable system can be linked with the relevant low energy effective action when a compactification from five dimension to four dimension is imposed with all of the fields belonging to the adjoint representation of the SU(N) gauge group.[5] More evidence for this correspondence between the SYM and RS models is depicted by calculating instanton correction of prepotential for SU(2) Seiberg-Witten theory in Ref. 32.

As for the spectral curve and its relation to the Seiberg–Witten spectral curve, much progress has been made in the correspondence of ''Calogero-Moser integrable theories and gauge theories.'' See the recent reviews in Refs. 39 and 40, and references therein. In the following we will give the spectral curves for C_n and BC_n systems, which are shown to be parametrized by the integrals of motion of the corresponding system. We will also see that the elliptic Calogero–Moser, Toda (affine and nonaffine) ones are particular limits of these systems.

A. Spectral curve of the C_n RS system

Given the Lax operator with spectral parameter for the Calogero–Moser system and of the RS system associated with Lie algebras $\mathcal{G}$, the spectral curve for the given system is defined as

$$\Gamma: R(v, \lambda) = \det(L(\lambda) - v \cdot Id) \equiv 0. \tag{V.1}$$

It is natural that the function $R(v,z)$ is invariant under time evolution,

$$\frac{\mathrm{d}}{\mathrm{d}t} R(v, \lambda) = \{\mathcal{H}, R(v, \lambda)\} = 0. \tag{V.2}$$

Thus, $R(v,\lambda)$ must be a function of only the n independent integrals of motion, which in super-Yang–Mills theory play the role of *moduli*, parametrizing the supersymmetric vacua of the gauge theory. This has been confirmed in the case of the elliptic Calogero–Moser system for general Lie algebra in Refs. 41 and 42 and in the case of the elliptic SU(N) RS system for the perturbative limit and some nonperturbative special point.[5]

As for the C_n RS system, the spectral curve can be generated by the Lax matrix $L(\lambda)_{C_n}$ as follows:

$$\det(L(\lambda)_{C_n}-v\cdot Id)=\sum_{j=0}^{2n}\frac{(\sigma(\lambda))^{(j-1)}\sigma(\lambda+j\gamma)}{(\sigma(\gamma+\lambda))^{j}}(-v)^{2n-j}(H_j)_{C_n}=0, \tag{V.3}$$

where $(\mathcal{H}_0)_{C_n}=(\mathcal{H}_{2n})_{C_n}=1$ and $(\mathcal{H}_i)_{C_n}=(\mathcal{H}_{2n-i})_{C_n}$ who Poisson commute

$$\{(\mathcal{H}_i)_{C_n},(\mathcal{H}_j)_{C_n}\}=0,\quad i,j=1,\ldots,n. \tag{V.4}$$

This can be deduced by verbose but straightforward calculation to verify that the $(\mathcal{H}_i)_{A_{2n-1}}$, $i=1,\ldots,2n$ is the first class Hamiltonian with respect to the constraints (III.11), using Eqs. (II.18), (III.13) and the first formula of Eq. (III.18).

The explicit form of $(\mathcal{H}_l)_{C_n}$ is

$$(\mathcal{H}_l)_{C_n}=\sum_{\substack{J\subset\{1,\ldots,n\},\ |J|\leqslant l\\ \varepsilon_j=\pm 1, j\in J}}\exp(p_{\varepsilon J})\,F_{\varepsilon J;J^c}\,U_{J^c,l-|J|},\quad l=1,\ldots,n \tag{V.5}$$

with

$$p_{\varepsilon J}=\sum_{j\in J}\varepsilon_j p_j,$$

$$F_{\varepsilon J;\,K}=\prod_{\substack{j,j'\in J\\ j<j'}}f^2(\varepsilon_j x_j+\varepsilon_{j'}x_{j'})\prod_{j\in J k\in K}f(\varepsilon_j x_j+x_k)f(\varepsilon_j x_j-x_k)\prod_{j\in J}f(2\varepsilon_j x_j), \tag{V.6}$$

$$U_{I,p}=\sum_{\substack{I'\subset I\\ |I'|=[p/2]}}\prod_{\substack{j\in I'\\ k\in I\setminus I'}}f(x_{jk})f(x_j+x_k)g(x_{jk})g(x_j+x_k)\begin{cases}0, & (p\ \text{odd})\\ 1, & (p\ \text{even})\end{cases}.$$

Here, $[p/2]$ denotes the integer part of $p/2$. As an example, for the C_2 RS model, the independent Hamiltonian flows $(\mathcal{H}_1)_{C_2}$ and $(\mathcal{H}_2)_{C_2}$ generated by the Lax matrix L_{C_2} are[29]

$$\begin{aligned}(\mathcal{H}_1)_{C_2}=\mathcal{H}_{C_2}=&e^{p_1}f(2x_1)\,f(x_{12})f(x_1+x_2)+e^{-p_1}g(2x_1)\,g(x_{12})g(x_1+x_2)\\ &+e^{p_2}f(2x_2)\,f(x_{21})f(x_2+x_1)+e^{-p_2}g(2x_2)\,g(x_{21})g(x_2+x_1),\end{aligned} \tag{V.7}$$

$$\begin{aligned}(\mathcal{H}_2)_{C_2}=&e^{p_1+p_2}f(2x_1)\,(f(x_1+x_2))^2f(2x_2)+e^{-p_1-p_2}g(2x_1)\,(g(x_1+x_2))^2g(2x_2)\\ &+e^{p_1-p_2}f(2x_1)\,(f(x_{12}))^2f(-2x_2)+e^{p_2-p_1}g(2x_1)\,(g(x_{12}))^2g(-2x_2)\\ &+2f(x_{12})\,g(x_{12})\,f(x_1+x_2)g(x_1+x_2).\end{aligned} \tag{V.8}$$

Similar to the form of ''gauge'' transformation of Eq. (II.4), we can check that the involutive Hamiltonians of Eq. (V.5) are identical to the one given by Diejen in Ref. 26 with the following transformation

$$x_i\to x_i,\quad p_i\to p_i+\frac{1}{2}\ln\left(\frac{f(2x_i)}{g(2x_i)}\prod_{j\neq i}^{n}\frac{f(x_{ij})f(x_i+x_j)}{g(x_{ij})g(x_i+x_j)}\right). \tag{V.9}$$

B. Spectral curve of the BC_n model

Similar to the calculation of the C_n case, the spectral curve of the BC_n RS system can be generated by Lax matrix $L(\lambda)_{BC_n}$ as follows

$$\det(L(\lambda)_{BC_n}-v\cdot Id)=0. \tag{V.10}$$

The explicit form of the spectral curve is

$$\det(L(\lambda)_{BC_n}-v\cdot Id)=\sum_{j=0}^{2n+1}\frac{(\sigma(\lambda))^{(j-1)}\sigma(\lambda+j\gamma)}{(\sigma(\gamma+\lambda))^{j}}(-v)^{2n+1-j}(\mathcal{H}_j)_{BC_n}=0, \tag{V.11}$$

where $(\mathcal{H}_0)_{BC_n}=(\mathcal{H}_{2n})_{BC_n}=1$ and $(\mathcal{H}_i)_{BC_n}=(\mathcal{H}_{2n+1-i})_{BC_n}$ Poisson commute

$$\{(\mathcal{H}_i)_{BC_n},(\mathcal{H}_j)_{BC_n}\}=0,\quad \forall i,j\in\{1,\ldots,n\}. \tag{V.12}$$

This can be deduced similarly to the C_n case to verify that $(\mathcal{H}_i)_{A_{2n}}$, $i=1,\ldots,2n$ is the first class Hamiltonian with respect to the constraints (III.25).

The explicit forms of $(\mathcal{H}_l)_{BC_n}$ are

$$(\mathcal{H}_l)_{BC_n}=\sum_{\substack{J\subset\{1,\ldots,n\},\ |J|\leqslant l\\ \varepsilon_j=\pm 1,\ j\in J}}\exp(p_{\varepsilon J})\,F_{\varepsilon J;J^c}U_{J^c,l-|J|},\quad l=1,\ldots,n \tag{V.13}$$

with

$$p_{\varepsilon J}=\sum_{j\in J}\varepsilon_j p_j,$$

$$F_{\varepsilon J;K}=\prod_{\substack{j,j'\in J\\ j<j'}}f^2(\varepsilon_j x_j+\varepsilon_j,x_{j'})\prod_{\substack{j\in J\\ k\in K}}f(\varepsilon_j x_j+x_k)f(\varepsilon_j x_j-x_k)\prod_{j\in J}f(2\varepsilon_j x_j)\prod_{j\in J}f(\varepsilon_j x_j), \tag{V.14}$$

$$U_{I,p}=\sum_{\substack{I'\subset I\\ |I'|=[p/2]}}\prod_{\substack{j\in I'\\ k\in I\setminus I'}}f(x_{jk})f(x_j+x_k)g(x_{jk})g(x_j+x_k)\begin{cases}\displaystyle\prod_{i\in I\setminus I'}f(x_i)g(x_i), & (p\ \text{odd})\\ \displaystyle\prod_{i\in I}f(x_i)g(x_i), & (p\ \text{even})\end{cases}.$$

It is similar to the C_n case for the relation between $(\mathcal{H}_l)_{BC_n}$ with the one given in Ref. 26:

$$x_i\to x_i,\quad p_i\to p_i+\tfrac{1}{2}\ln\left(\frac{f(x_i)}{g(x_i)}\frac{f(2x_i)}{g(2x_i)}\prod_{j\neq i}^{n}\frac{f(x_{ij})f(x_i+x_j)}{g(x_{ij})g(x_i+x_j)}\right). \tag{V.15}$$

Remarks: So far we have Lax matrices with the spectral parameter of Eq. (IV.4) for the C_n and BC_n RS models, and the corresponding spectral curve equation of Eqs. (V.3) and (V.11). It is expected that they will be useful to study the relation between the $5d$ SUSY gauge theory and these integrable models which have been pointed out in Ref. 5. More exactly, it is expected that these spectral curves would be identical to the complex curve in the context of SUSY gauge theory associated with the corresponding gauge group. On the other hand, these nonsimple laced models may be potential candidates which are connected with orientifold in brane theory, corresponding to the fact that the A_{n-1} RS model is connected with orbifold. This exact correspondence in these directions is missed and certainly desires further investigation.

C. Limit to the Calogero–Moser system and Toda system

The Calogero–Moser system can be achieved by taking the so-called ''nonrelativistic limit.'' The procedure is by rescaling $p_\mu \mapsto \beta p_\mu$, $\gamma \mapsto \beta\gamma$ and letting $\beta \mapsto 0$, followed by making a canonical transformation

$$p_\mu \mapsto p_\mu + \gamma \sum_{\Delta \ni \eta = \mu - \nu} \zeta(\eta \cdot x). \tag{V.16}$$

Here $p_\mu = \mu \cdot p$, such that

$$L \mapsto Id + \beta L_{\mathrm{CM}} + O(\beta^2), \tag{V.17}$$

and

$$\mathcal{H} \mapsto N + 2\beta^2 \mathcal{H}_{\mathrm{CM}} + O(\beta^2), \tag{V.18}$$

where $N = 2n$ for the C_n model and $N = 2n+1$ for BC_n model.

L_{CM} can be expressed as

$$L_{\mathrm{CM}} = p \cdot H + X, \tag{V.19}$$

where

$$H_{\mu\nu} = \mu \delta_{\mu\nu}, \quad X_{\mu\nu} = \gamma \Phi(x_{\mu\nu}, \lambda)(1 - \delta_{\mu\nu}). \tag{V.20}$$

The Hamiltonian $\mathcal{H}_{\mathrm{CM}}$ of the CM model can be given by

$$\mathcal{H}_{\mathrm{CM}} = \frac{1}{2} p^2 - \frac{\gamma^2}{2} \sum_{\alpha \in \Delta} \wp(\alpha \cdot x) = \frac{1}{4} \mathrm{tr}\, L^2 + \mathrm{const}, \tag{V.21}$$

where

$$\mathrm{const} = -\frac{N(N-1)\gamma^2}{4} \wp(\lambda).$$

All of the above-mentioned results are identified with the results of Refs. 8, 10, 12–15 up to a suitable choice of coupling parameters. Now the degenerate RS spectral curve reduces to

$$\Gamma: \; R(v, \lambda) = \det(L(\lambda)_{\mathrm{CM}} - v \cdot Id) \equiv 0, \tag{V.22}$$

which is exactly identified with the spectral curve analyzed in Refs. 39 and 41.

Starting from the CM system to the Toda system is more directly due to the progress that the limit to Toda for the general Lie algebra has been studied extensively in Refs. 43–45. The main idea is making a suitable scaling limit with the following parametrization:

$$\omega_1 = -i\pi, \quad \omega_3 \in \mathbf{R}_+, \quad \tau \equiv \frac{\omega_3}{\omega_1} = i\omega_3/\pi, \tag{V.23}$$

and shifting the dynamical variable x,

$$\begin{aligned} &x \to Q - 2\omega_3 \delta \rho^\vee, \quad p \to P, \\ &\lambda \to \log Z - \omega_3, \quad Z \in \mathbf{R}_+, \end{aligned} \tag{V.24}$$

TABLE I. Root system of A_{n-1}, C_n and BC_n types.

$\mathcal{G}$	All roots	Simple roots Π	$h_{\mathcal{G}}$	Dual Weyl vector $\rho^\vee$	Vector weights
A_{n-1}	$\pm e_i \pm e_j$, $1\leqslant i,\ j\leqslant n$, $i\neq j$	$e_i - e_{i+1}$, $i=1,\ldots,n-1$	n	$\Sigma_{j=1}^{n}(n-j)e_j$	e_i, $i=1,\ldots,n$
C_n	$\pm e_i \pm e_j, \pm 2e_i$, $1\leqslant i,\ j\leqslant n$, $i\neq j$	$e_i - e_{i+1}, 2e_n$, $i=1,\ldots,n-1$	$2n$	$\Sigma_{j=1}^{n}(n+\frac{1}{2}-j)e_j$	$e_i, -e_i$, $i=1,\ldots,n$
BC_n	$\pm e_i \pm e_j, \pm 2e_i, \pm e_i$ $1\leqslant i,\ j\leqslant n$, $i\neq j$	$e_i - e_{i+1}, e_n$, $i=1,\ldots,n-1$	$2n+1$	$\Sigma_{j=1}^{n}(n+1-j)e_j$ (define)	$e_i, -e_i, 0$, $i=1,\ldots,n$

in which $h_{\mathcal{G}}$ is the Coxeter number for the corresponding root system $\mathcal{G}$, $\rho^\vee$ the dual of the Weyl vector defined as $\rho^\vee = \frac{1}{2}\Sigma_{\alpha\in\Delta_+} 2\alpha/\alpha^2$, and δ satisfies $\delta \leqslant 1/h_{\mathcal{G}}$.

For convenience, we give the basics of these root systems as shown in Table I.

As for the C_n model, selecting $\rho^\vee = \rho^\vee_{C_n}$, $\gamma = im\, e^{\omega_3 \delta}$, one has the nonaffine C_n Toda model from the Hamiltonian of the CM model Eq. (V.21),

$$\mathcal{H}^{\text{Toda}}_{C_n} = \frac{1}{2}P^2 + m^2 \sum_{j=1}^{n-1} e^{Q_j - Q_{j+1}} + m^2\, e^{2Q_n}, \tag{V.25}$$

for $\delta < 1/h_{C_n}$ and $C_n^{(1)}$ Toda model

$$\mathcal{H}^{\text{Toda}}_{C_n^{(1)}} = \frac{1}{2}P^2 + m^2 e^{-2Q_1} + m^2 \sum_{j=1}^{n-1} e^{Q_j - Q_{j+1}} + m^2 e^{2Q_n} \tag{V.26}$$

for $\delta = 1/h_{C_n}$.

The same holds for the BC_n model. Selecting $\rho^\vee = \rho^\vee_{BC_n}$, $\gamma = im\, e^{\omega_3 \delta}$, one has the nonaffine B_n Toda model from the Hamiltonian of the CM model Eq. (V.21),

$$\mathcal{H}^{\text{Toda}}_{B_n} = \frac{1}{2}P^2 + m^2 \sum_{j=1}^{n-1} e^{Q_j - Q_{j+1}} + m^2\, e^{Q_n} \tag{V.27}$$

for $\delta < 1/h_{BC_n}$ and BC_n Toda model

$$\mathcal{H}^{\text{Toda}}_{BC_n} = \frac{1}{2}P^2 + m^2 e^{-2Q_1} + m^2 \sum_{j=1}^{n-1} e^{Q_j - Q_{j+1}} + m^2 e^{Q_n} \tag{V.28}$$

for $\delta = 1/h_{BC_n}$.

If we use the following gauge for $\Phi(x,\lambda)$:[46]

$$\Phi(x,\lambda) \to \frac{\sigma(x+\lambda)}{\sigma(\lambda)\sigma(x)} \exp(\zeta(\lambda)x), \tag{V.29}$$

it does not destroy the validity[45] for the Lax pair, We have the following limit for $\gamma\Phi(\alpha\cdot x,\lambda)$:

$$\gamma\Phi(\alpha\cdot x,\lambda)\to -m\exp\left(\frac{\alpha\cdot Q}{2}\right)\quad \text{for}\quad \alpha\in\Pi\quad (\delta\leqslant 1/h_{\mathcal{G}})$$

$$\to mZ\exp\left(-\frac{\alpha\cdot Q}{2}\right)\quad \text{for}\quad \alpha=\alpha_h\quad (\delta=1/h_{\mathcal{G}})$$

$$\to 0\quad \text{otherwise},$$

$$\gamma\Phi(-\alpha\cdot x,\lambda)\to m\exp\left(\frac{\alpha\cdot Q}{2}\right)\quad \text{for}\quad \alpha\in\Pi(\delta\leqslant 1/h_{\mathcal{G}})$$

$$\to -\frac{m}{Z}\exp\left(-\frac{\alpha\cdot Q}{2}\right),\quad \text{for}\quad \alpha=\alpha_h(\delta=1/h_{\mathcal{G}})$$

$$\to 0\quad \text{otherwise}. \tag{V.30}$$

So the Lax operator now reads

$$L_{\text{Toda}}=P\cdot H-im\sum_{\alpha\in\Pi}\exp\left(\frac{\alpha\cdot Q}{2}\right)[E(\alpha)-E(-\alpha)]+im\exp\left(\frac{\alpha_0\cdot Q}{2}\right)[ZE(-\alpha_0)-Z^{-1}E(\alpha_0)], \tag{V.31}$$

where $E(\alpha)_{\mu\nu}=\delta_{\mu-\nu,\alpha}$. This Lax operator holds for all the root systems of $A_{n-1}(A_{n-1}^{(1)})$, $C_n(C_n^{(1)})$, $B_n(BC_n)$ and coincides with the standard form given in Ref. 8. It is not difficult to find that the parameter Z now plays the role of a spectral parameter for the affine Toda model based on $\mathcal{G}^{(1)}$. When we refer to the Toda models based on a finite Lie algebra $\mathcal{G}$, we should only drop the terms containing the affine root α_0.

So the degenerate spectral curve for the Toda $A_{n-1}^{(1)}$, $C_n^{(1)}$, and $BC_n(A_{2n}^{(2)})$ systems can be defined

$$\Gamma: R(v,\lambda)=\det(L(\lambda)_{\text{Toda}}-v\cdot Id)\equiv 0, \tag{V.32}$$

which is identical to the one given in Refs. 47 and 48.

VI. DEGENERATE CASES

Let us now consider the other various special degenerate cases. As is well known, if one or both of the periods of the Weierstrass sigma function $\sigma(x)$ become infinite, there will occur three degenerate cases associated with trigonometric, hyperbolic, and rational systems. The degenerate limits of the functions $\Phi(x,\lambda)$, $\sigma(x)$, and $\zeta(x)$ will give corresponding Lax pairs which include spectral parameter. Moreover, when the spectral parameter value is on a certain limit, the Lax pairs without spectral parameter will be derived.

A. Trigonometric limit

The limit can be obtained by sending ω_3 to $i\infty$ with $\omega_1=\pi/2$, so that

$$\sigma(x)\to e^{(1/6)x^2}\sin x,$$
$$\zeta(x)\to\cot x+\tfrac{1}{3}x, \tag{VI.1}$$

and the function

$$\Phi(x,\lambda)\equiv\frac{\sigma(x+\lambda)}{\sigma(x)\sigma(\lambda)}$$

reduces to

$$\Phi(x,\lambda)\rightarrow(\cot\lambda-\cot x)e^{(1/3)xu}. \tag{VI.2}$$

By replacing the corresponding functions $\Phi(x,\lambda)$, $\sigma(x)$, and $\zeta(x)$ with the above-given form for the Lax pairs, we will get the corresponding spectral parameter dependent Lax pairs. For simplicity, we notice that the exponential part of the above-mentioned functions can be removed by applying suitable ''gauge'' transformation of the Lax matrix on which condition the functions can be valued as follows:

$$\begin{aligned}\sigma(x)&\rightarrow\sin x,\\ \zeta(x)&\rightarrow\cot x,\\ \Phi(x,\lambda)&\rightarrow(\cot\lambda-\cot x).\end{aligned} \tag{VI.3}$$

As for the spectral parameter independent Lax pair, furthermore, we can take the limit $\lambda\rightarrow i\infty$, so the function

$$\Phi(x,\lambda)\rightarrow\frac{1}{\sin x}, \tag{VI.4}$$

while the corresponding Lax matrix becomes

$$L_{\mu\nu}=e^{\nu\cdot p}b_{\nu}\frac{\sin\gamma}{\sin((\mu-\nu)\cdot x+\gamma)}, \tag{VI.5}$$

which is exactly the same as the spectral parameter independent Lax matrix given in Ref. 30.

B. Hyperbolic limit

In this case, the periods can be chosen by sending ω_1 to $i\infty$ with $\omega_3=\pi/2$, so following all the procedures in achieving the result of the trigonometric case, we can find the hyperbolic Lax pairs by simple replacement of the functions appearing in the trigonometric Lax pair as follows:

$$\begin{aligned}\sin x&\rightarrow\sinh x,\\ \cos x&\rightarrow\cosh x,\\ \cot x&\rightarrow\coth x.\end{aligned} \tag{VI.6}$$

The same as for the trigonometric case, we can get the Lax pairs with and without spectral parameter.

C. Rational limit

As far as the form of the Lax pair for the rational-type system is concerned, we can achieve it by making the following substitutions:

$$\begin{aligned}\sigma(x)&\rightarrow x,\\ \zeta(x)&\rightarrow\frac{1}{x},\\ \Phi(x,\lambda)&\rightarrow\frac{1}{x}+\frac{1}{\lambda}\end{aligned} \tag{VI.7}$$

for the spectral parameter dependent Lax pair, while furthermore, taking the limit $\lambda \to i\infty$, we can obtain the spectral parameter independent Lax pair. The explicit form of Lax matrix without spectral parameter is

$$L_{\mu\nu} = e^{\nu\cdot p} b_\nu \frac{\gamma}{(\mu-\nu)\cdot x+\gamma}. \tag{VI.8}$$

which completely coincides with the spectral parameter independent Lax matrix given in Ref. 30.

Remark: As for the various degenerate cases for the CM and Toda systems, one can follow the same procedure as for the RS model [please refer to Eqs. (VI.1)–(VI.8)].

VII. CONCLUDING REMARKS

In this paper, we have proposed the Lax pairs for elliptic C_n and BC_n RS models. The spectral parameter dependent and independent Lax pairs for the trigonometric, hyperbolic, and rational systems can be derived as the degenerate limits of the elliptic potential case. The spectral curves of these systems are given and shown depicted by the complete sets of involutive constant integrals of motion. They are expected be related to the five-dimensional gauge theory[4,5] and even to brane theory, which desires further study. In the nonrelativistic limit(scaling limit), these systems lead to CM(Toda) systems associated with the root systems of C_n and BC_n. There are still many open problems. For example, it seems to be a challenging subject to carry out a Lax pair with as many independent coupling constants as independent Weyl orbits in the set of roots, as done for the Calogero–Moser systems(see Refs. 8, 11–15). What is also interesting is to generalize the results obtained in this paper to the systems associated with all other Lie Algebras even to those associated with all the finite reflection groups.[14] Moreover, the issue of getting the r-matrix structure for these systems is deserved due to the success of calculating for the trigonometric BC_n RS system by Avan *et al.* in Ref. 31.

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APPENDIX

In this appendix we prove the identity equation (II.11) and then derive the relation between the Lax operator $L(\lambda)$ and its inverse of $L(\lambda)^{-1}$.

Using the result given in Ref. 6 of Eq. (B5), we have the following conclusion:

Let

$$C_{ij} = \frac{\sigma(q_i - r_j + \lambda)}{\sigma(q_i - r_j + \mu)}, \quad i,j = 1,\ldots,N, \tag{A1}$$

then one has

$$\det(C) = \sigma(\lambda-\mu)^{N-1}\sigma(\lambda+(N-1)\mu+\Sigma)\times\prod_{i<j}\sigma(q_i-q_j)\sigma(r_j-r_i)\prod_{i,j}\frac{1}{\sigma(q_i-r_j+\mu)}, \tag{A2}$$

where

$$\Sigma = \sum_{i=1}^{N}(q_i - r_j). \tag{A3}$$

So it is straightforward to compute the inverse of matrix C,

$$\begin{aligned}(C^{-1})_{ij} &= \text{the cofactor of } C \text{ with respect to } C_{ji}\\ &= \frac{\sigma(\lambda+(N-2)\mu+q_i-q_j)}{\sigma(\lambda-\mu)\sigma(\lambda+(N-1)\mu)\sigma(q_i-q_j-\mu)}\\ &\quad\times\frac{\Pi_l\sigma(q_j-q_l+\mu)\Pi_l\sigma(q_i-q_l-\mu)}{\Pi_{k\neq i}\sigma(q_i-q_k)\Pi_{k\neq j}\sigma(q_j-q_k)}.\end{aligned} \tag{A4}$$

From Eq. (II.5), we have

$$\begin{aligned}L(\lambda) &= \sum_{i,j=1}^{N}\frac{\Phi(x_{ij}+\gamma,\lambda)}{\Phi(\gamma,\lambda)}\exp(p_j)b_jE_{ij}\\ &= \frac{1}{\Phi(\gamma,\lambda)}\sum_{i,j=1}^{N}\frac{\sigma(x_{ij}+\gamma+\lambda)}{\sigma(x_{ij}+\gamma)\sigma(\lambda)}\exp(p_j)b_j\\ &= \frac{1}{\Phi(\gamma,\lambda)}\sum_{i,j=1}^{N}G_{ij}\exp(p_j)b_j,\end{aligned} \tag{A5}$$

where

$$G_{ij}:=\Phi(x_{ij}+\gamma,\lambda)=\frac{\sigma(x_{ij}+\gamma+\lambda)}{\sigma(x_{ij}+\gamma)\sigma(\lambda)},$$

with the help of Eq. (A4), one has

$$(G^{-1})_{ij}=\frac{\sigma(\lambda+(N-1)\gamma+x_{ij})}{\sigma(\lambda+N\gamma)\sigma(x_{ij}-\gamma)}\times\frac{\Pi_k\sigma(x_{jk}+\gamma)\Pi_k\sigma(x_{ik}-\gamma)}{\Pi_{k\neq i}\sigma(x_{ik})\Pi_{k\neq j}\sigma(x_{jk})}, \tag{A6}$$

so that

$$\begin{aligned}L(\lambda)^{-1}{}_{ij} &= \Phi(\gamma,\lambda)(G^{-1})_{ij}b_j^{-1}\exp(-p_i))E_{ij}\\ &= \frac{-\sigma(\gamma)^2\,\sigma(\lambda+\gamma)\sigma(\lambda+(N-1)\gamma+x_{ij})}{\sigma(\lambda)\sigma(\gamma)\sigma(\lambda+N\gamma)\sigma(x_{ij}-\gamma)}\times\exp(-p_i)\prod_{k\neq j}\frac{\sigma(x_{jk}+\gamma)}{\sigma(x_{jk})}\\ &= \frac{\sigma(\gamma+\lambda)\,\sigma(\lambda+(N-1)\gamma)}{\sigma(\lambda)\sigma(\lambda+N\gamma)}\times\frac{\Phi(x_{ij}-\gamma,\lambda+N\gamma)}{\Phi(-\gamma,\lambda+N\gamma)}\exp(-p_i)b_j'E_{ij}.\end{aligned} \tag{A7}$$

By comparing the forms of $L(\lambda)$ and $L(\lambda)^{-1}{}_{ij}$, we find $L(\lambda)^{-1}{}_{ij}$ can be expressed with $L(\lambda)$ as

$$L(\lambda)^{-1}{}_{ij}=L(\lambda)_{ij}\big|_{\gamma\to-\gamma,\lambda\to\lambda+N\gamma}\times\frac{\sigma(\gamma+\lambda)\,\sigma(\lambda+(N-1)\gamma)}{\sigma(\lambda)\sigma(\lambda+N\gamma)}\exp(-p_i-p_j). \tag{A8}$$

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Phase diagram for Abrikosov lattice

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Working in the framework of Abrikosov's theory, we propose a mathematical definition of the phase diagram and prove mathematically the validity of what is usually drawn in the physical literature. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In 1953 V. Ginzburg and L. Landau proposed a modelization for describing the states of a superconducting material. They introduced a functional depending on a wave function ϕ and a magnetic potential vector $\mathbf{A}$ whose local minima will describe the properties of the material, $|\phi|^2$ representing the local density of superconducting electrons. Abrikosov[1] has introduced a special modelization which predicts the periodic structure for the zeros of ϕ which was subsequently observed in some experiments. Our aim is to give a mathematical analysis of some aspects of his theory. For simplicity we restrict ourselves to the two-dimensional case and consider a case when the material is submitted to a constant external magnetic field H_{ext} which will be identified to a function. Then if $(\phi,\mathbf{A})$ is in the Sobolev space $H^1_{\text{loc}}(\mathbb{R}^2;\mathbb{C})\times H^1_{\text{loc}}(\mathbb{R}^2;\mathbb{R}^2)$ the density of the Ginzburg–Landau functional is

$$\tfrac{1}{2}\|ik^{-1}\nabla\phi+\mathbf{A}\phi\|^2+\tfrac{1}{4}(1-|\phi|^2)^2+\tfrac{1}{2}(\text{curl}\ \ \mathbf{A}-H_{\text{ext}})^2 \tag{1}$$

and is in $L^1_{\text{loc}}(\mathbb{R}^2)$; the constant k is called the Ginzburg–Landau parameter ($k>0$). Furthermore, this density is invariant under the gauge transform $(\phi',\mathbf{A}')=(\phi e^{ikg},\mathbf{A}+\nabla_g)$ with $g\in H^2_{\text{loc}}(\mathbb{R}^2)$. All other physically significant quantities like the density $|\phi|^2$ and the field curl $\mathbf{A}$ are left invariant by these gauge transforms.

We take $\mathcal{L}_1$ a two-dimensional lattice of $\mathbb{R}^2$ with fundamental domain Ω_1 of area 1. We consider the dilated lattice: $\mathcal{L}_\lambda=\sqrt{\lambda}\mathcal{L}_1$ with fundamental domain $\Omega_\lambda=\sqrt{\lambda}\Omega_1$. Following Abrikosov, we choose λ in $\mathbb{R}_+$ and restrict the variational space to the space $\mathcal{V}_\lambda$ of pairs $(\phi,\mathbf{A})$ which are gauge periodic with respect to $\mathcal{L}_\lambda$.[1] This means that, for all $v\in\mathcal{L}_\lambda$, there exists $g^v\in H^2_{\text{loc}}(\mathbb{R}^2)$ such that

$$\begin{aligned}\phi(z+v)&=e^{ikg^v(z)}\phi(z),\\ \mathbf{A}(z+v)&=\mathbf{A}(z)+\nabla g^v(z).\end{aligned} \tag{2}$$

Consequently, all the considered physical quantities are $\mathcal{L}_\lambda$-periodic. We denote by $|\Omega_\lambda|$ the area of Ω_λ which is actually equal to λ.

It is then a classical consequence of (2) that there exist $d\in\mathbb{Z}$ such that

$$2\pi d=k\int_{\Omega_\lambda}\text{curl}\ \ \mathbf{A}. \tag{3}$$

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Then we will analyze the problem obtained by fixing some quantization $d \in \mathbb{Z}$ and assuming that (3) is satisfied. This defines a smaller variational space $\mathcal{V}_{\lambda,d}$. The Ginzburg–Landau functional is obtained by integration of the local density over the fundamental domain Ω_λ and division by $|\Omega_\lambda|$. This gives

$$F(\phi,\mathbf{A}) = \frac{1}{|\Omega_\lambda|}\int_{\Omega_\lambda}\left[\frac{1}{2}\|ik^{-1}\nabla\phi+\mathbf{A}\phi\|^2+\frac{1}{4}(1-|\phi|^2)^2+\frac{1}{2}(\text{curl }\mathbf{A}-H_{\text{ext}})^2\right]dx. \tag{4}$$

This should consequently be understood as a mean energy. The analysis for fixed λ of the minima of the functional when $d=0$ is simple and one finds that the infimum of the functional is obtained for the so-called pure state $\phi=1$ and $\mathbf{A}=0$. This energy, which is independent of λ, is called the pure state energy and will be denoted by $E_{\mathcal{P}}$. We have

$$E_{\mathcal{P}} = \frac{H_{\text{ext}}^2}{2}. \tag{5}$$

The case $d=0$ is worthless for explaining the appearance of zeros for some value of (k,H_{ext}) and this leads us to the consideration of the case $d\neq 0$. From now on we assume $H_{\text{ext}}>0$ and $d \in \mathbb{N}^*$ (one can indeed show that the case $d<0$ is not energetically interesting). Let us define

$$\mathcal{E}_{k,H_{\text{ext}}} = \inf_{\lambda>0}\ \inf_{(\phi,\mathbf{A})\in\mathcal{V}_{\lambda,d}} F(\phi,\mathbf{A}). \tag{6}$$

We emphasize that the infimum is also taken with respect to λ, that is that we also minimize on the size of the domain. Let us now compute the energy of the so-called normal state corresponding to $\phi=0$ and curl $\mathbf{A}=H_{\text{ext}}$. An explicit solution is given by

$$\mathbf{A} = \frac{H_{\text{ext}}}{2}\begin{pmatrix}-y\\ x\end{pmatrix}, \tag{7}$$

and we observe that condition (3) imposes that this state belongs to $\mathcal{V}_{\lambda,d}$ with $\lambda = 2\pi d/kH_{\text{ext}}$. The corresponding energy will be called the normal energy and is equal to

$$E_{\mathcal{N}} = \tfrac{1}{4}. \tag{8}$$

This leads immediately to the following inequality:

$$\mathcal{E}_{k,H_{\text{ext}}} \leqslant E_{\mathcal{N}}. \tag{9}$$

We come back to the comparison with the pure energy $E_{\mathcal{P}}$. We will show in Corollary II.2 that, although the pure state is not in the variational space $\mathcal{V}_{\lambda,d}$ when $d\neq 0$, we still have

$$\mathcal{E}_{k,H_{\text{ext}}} \leqslant E_{\mathcal{P}}. \tag{10}$$

For a given $(k,H_{\text{ext}}) \in \mathbb{R}_+^*\times\mathbb{R}_+^*$, the questions are as follows.

(i) What is the infimum $\mathcal{E}_{k,H_{\text{ext}}}$ over $\lambda,\phi,\mathbf{A}$ of the functional?
(ii) Is this infimum attained?
(iii) In this last case, what are the properties of the minimizers?

This leads us to introduce three sets in $\mathbb{R}_+^*\times\mathbb{R}_+^*$:

$$\mathcal{N} = \{(k,H_{\text{ext}}) \in \mathbb{R}_+^*\times\mathbb{R}_+^* \text{ s.t. } \mathcal{E}_{k,H_{\text{ext}}} = E_{\mathcal{N}}\},$$

$$\mathcal{P} = \{(k,H_{\text{ext}}) \in \mathbb{R}_+^*\times\mathbb{R}_+^* \text{ s.t. } \mathcal{E}_{k,H_{\text{ext}}} = E_{\mathcal{P}}\}, \tag{11}$$

$$\mathcal{M}=\{(k,H_{\text{ext}})\in\mathbb{R}_+^*\times\mathbb{R}_+^* \text{ s.t. } \mathcal{E}_{k,H_{\text{ext}}}<\inf(E_{\mathcal{P}},E_{\mathcal{N}})\}.$$

The set $\mathcal{M}$ is the complementary of $\mathcal{P}\cup\mathcal{N}$ in $\mathbb{R}_+^*\times\mathbb{R}_+^*$. In the last case one can show that the infimum is attained for some triplet $(\lambda,\phi,\mathbf{A})$. In this case, $(\phi,\mathbf{A})$ is neither a pure state nor a normal state and is usually called a mixed state. The phase diagram is the picture corresponding to the description of $\mathcal{N}$, $\mathcal{P}$, and $\mathcal{M}$. Our main theorem gives a precise description of the boundaries of $\mathcal{N}$, $\mathcal{P}$, and $\mathcal{M}$.

Theorem I.1: *There exist two continuous functions* $k\mapsto H_{c1}(k)$ *and* $k\mapsto H_{c2}(k)$ on $\mathbb{R}_+$ *satisfying*

(1) $\forall k\leqslant 1/\sqrt{2}$ *we have* $H_{c1}(k)=1/\sqrt{2}$,
(2) $k\mapsto H_{c1}(k)$ *is decreasing and* $\lim_{k\to\infty}H_{c1}(k)=0$,
(3) $H_{c2}(k)=\max(k,1/\sqrt{2})$.

Then

$$\mathcal{N}=\{(k,H_{\text{ext}}),\ s.t.\ H_{\text{ext}}\geqslant H_{c2}(k)\},$$

$$\mathcal{P}=\{(k,H_{\text{ext}}),\ s.t.\ H_{\text{ext}}\leqslant H_{c1}(k)\},\tag{12}$$

$$\mathcal{M}=\{(k,H_{\text{ext}}),\ s.t.\ H_{c1}(k)<H_{\text{ext}}<H_{c2}(k)\}.$$

Let us remark that if $k\leqslant 1/\sqrt{2}$, we have $H_{c1}(k)=H_{c2}(k)=1/\sqrt{2}$, which is called the thermodynamic field. Our article is organized as follows: In the next section we make a change of variable and of unknowns which make the whole problem more easily tractable.

In Sec. III, we write the Bochner–Kodaira–Nakano formula for the rescaled functional which leads to a lower bound of the energy and we analyze the critical points. Then in Sec. IV we prove the monotonicity theorems which play an important role for analyzing the structure of $\mathcal{N}$, $\mathcal{P}$, and $\mathcal{M}$. In Sec. V, we give the qualitative form of the phase diagram.

II. RENORMALIZATION OF THE PROBLEM

We denote by $H_{\text{int}}=(1/\lambda)\int_{\Omega_\lambda}$ curl $\mathbf{A}$ the mean internal magnetic field induced by $\mathbf{A}$. The quantization relation (3) rewrites as

$$2\pi d=k\lambda H_{\text{int}}.\tag{13}$$

It is also a classical result (see Ref. 2 or 3 or Ref. 4, p. 21–29) that we can associate to the pair $(\phi,\mathbf{A})$, another pair $(\phi',\mathbf{A}')$ with the same Ginzburg–Landau energy but satisfying

$$\forall v\in\mathcal{L}_\lambda,\ \begin{cases}\phi'(z+v)=e^{ikg^v(z)}\phi'(z)\\ \mathbf{A}'(z+v)=\mathbf{A}'(z)+\nabla g^v(z)\end{cases}\ \text{with}\ g^v(x,y)=\frac{H_{\text{int}}}{2}(v_x y-v_y x)\tag{14}$$

and $\operatorname{div}\mathbf{A}'=0$. This reduction is rather involved and is performed by a suitable gauge transform and a translation in x. This is actually linked to the classification of complex line bundles over the torus. We will work with the vector bundle $E_{\lambda,d}$ whose C^∞ sections are described by

$$C^\infty(E_{\lambda,d})=\{\phi:\mathbb{R}^2\to\mathbb{C} \text{ s.t. } \forall(x,y)\in\mathbb{R}^2,\forall v=(v_x,v_y)\in\mathcal{L}_\lambda,$$
$$\phi((x,y)+v)=e^{i(\pi d/\lambda)(v_x y-v_y x)}\phi(x,y)\}.\tag{15}$$

In order to respect (13) we introduce

$$\mathcal{B}_d = \begin{cases} (\phi, \mathbf{A}) \in H^1_{\mathrm{loc}}(E_{\lambda,d}) \times H^1_{\mathrm{loc}}(\mathbb{R}^2, \mathbb{R}^2) \ \text{ s.t. } \exists H_{\mathrm{int}} > 0 \\ \text{with } \ 2\pi d = k\lambda H_{\mathrm{int}}, \ \ \mathbf{A} = \dfrac{H_{\mathrm{int}}}{2\pi}\mathbf{A}_0 + \mathbf{P} \\ \text{with } \ \mathbf{P} \ \ \mathcal{L}_\lambda\text{-periodic}, \ \ \mathrm{div}\,\mathbf{P} = 0 \ \ \text{and} \ \ \displaystyle\int_{\Omega_\lambda} \mathbf{P} = 0 \end{cases} \tag{16}$$

with $\mathbf{A}_0 = \pi\binom{-y}{x}$ and analyze the problem restricted to $\mathcal{B}_d$.

Let us start to compute $F(\phi, \mathbf{A})$. With the expression $\mathbf{A} = (H_{\mathrm{int}}/2\pi)\mathbf{A}_0 + \mathbf{P}$, we easily get:

$$\frac{1}{|\Omega_\lambda|}\int_{\Omega_\lambda} \frac{1}{2}(\mathrm{curl}\ \ \mathbf{A} - H_{\mathrm{ext}})^2 = \frac{1}{|\Omega_\lambda|}\int_{\Omega_\lambda} \frac{1}{2}(\mathrm{curl}\ \ \mathbf{P})^2 + \frac{1}{2}(H_{\mathrm{int}} - H_{\mathrm{ext}})^2. \tag{17}$$

This leads to the simple expression

$$F(\phi, \mathbf{A}) = F^{\mathrm{int}}(\phi, \mathbf{P}) + \tfrac{1}{2}(H_{\mathrm{int}} - H_{\mathrm{ext}})^2 \tag{18}$$

with

$$F^{\mathrm{int}}(\phi, \mathbf{P}) = \frac{1}{|\Omega_\lambda|}\int_{\Omega_\lambda} \frac{1}{2}\left\| ik^{-1}\nabla\phi + \left(\frac{H_{\mathrm{int}}}{2\pi}\mathbf{A}_0 + \mathbf{P}\right)\phi \right\|^2 + \frac{1}{4}(1 - |\phi|^2)^2 + \frac{1}{2}(\mathrm{curl}\ \ \mathbf{P})^2. \tag{19}$$

The functional F^{int} is called internal energy and depends only on H_{int}, k, ϕ, and $\mathbf{P}$. The second term on the rhs of (17) is a very simple magnetic energy: $1/2(H_{\mathrm{int}} - H_{\mathrm{ext}})^2$.

We want to analyze the properties of the minimizers in function of two parameters k and H_{ext} as explained in the Introduction and we recall that H_{int} and λ are linked by (13). We first start with a change of variables and of functions:

$$u(x) = \phi\left(x\sqrt{\frac{2\pi}{kH_{\mathrm{int}}}}\right)$$
$$\mathbf{a}(x) = \sqrt{\frac{2\pi k}{H_{\mathrm{int}}}}\left[\mathbf{A} - \frac{H_{\mathrm{int}}}{2\pi}\mathbf{A}_0\right]\left(x\sqrt{\frac{2\pi}{kH_{\mathrm{int}}}}\right) = \sqrt{\frac{2\pi k}{H_{\mathrm{int}}}}\mathbf{A}\left(x\sqrt{\frac{2\pi}{kH_{\mathrm{int}}}}\right) - \mathbf{A}_0(x) \ \ \text{and} \ \ \mu = \frac{H_{\mathrm{int}}}{2\pi k}. \tag{20}$$

In this change, the lattice $\mathcal{L}_\lambda$ becomes $\mathcal{L}_d = \sqrt{d}\mathcal{L}_1$ with fundamental domain $\Omega_d = \sqrt{d}\Omega_1$ of area d. The energy will obviously depend on the geometry of the lattice $\mathcal{L}_1$. It is a physical conjecture supported by many numerical results[5,6] that the minimal energy is attained when varying the geometry by the hexagonal lattice. Note that this remains a mathematical conjecture!

The C^∞ sections u of the new vector bundle E_d satisfy

$$\forall (x,y) \in \mathbb{R}^2, \forall v \in \mathcal{L}_d, \quad u((x,y) + v) = e^{i\pi(v_x y - v_y x)}u(x,y), \tag{21}$$

and the potential vector $\mathbf{a}$ belongs to the space

$$\left\{ \mathbf{a} \in H^1_{\mathrm{loc}}(\mathbb{R}^2; \mathbb{R}^2) \ \text{ such that } \ \mathrm{div}\,\mathbf{a} = 0, \ \ \mathbf{a} \ \text{ is } \ \mathcal{L}_d\text{-periodic and } \ \int_{\Omega_d} \mathbf{a} = 0 \right\}. \tag{22}$$

We denote by $\mathcal{A}_d$ the space of all pairs $(u, \mathbf{a})$ with u being a H^1_{loc} section of E_d (21) and $\mathbf{a}$ belonging to the space (22).

Let us define the functional $E_{H_{\mathrm{int}},k}$ over $\mathcal{A}_d$ by

$$E_{H_{\rm int},k}(u,\mathbf{a})=\frac{1}{d}\int_{\Omega_d}\frac{H_{\rm int}}{4\pi k}\|i\nabla u+(\mathbf{A}_0+\mathbf{a})u\|^2+\frac{1}{4}(1-|u|^2)^2+\frac{H_{\rm int}^2}{2(2\pi)^2}|\text{curl}\ \ \mathbf{a}|^2$$

$$=\frac{1}{d}\int_{\Omega_d}\frac{\mu}{2}\|i\nabla u+(\mathbf{A}_0+\mathbf{a})u\|^2+\frac{1}{4}(1-|u|^2)^2+\frac{\mu^2k^2}{2}|\text{curl}\ \ \mathbf{a}|^2. \tag{23}$$

After the change introduced in (20), the GL functional becomes

$$F(\phi,\mathbf{A})=E_{k,H_{\rm ext}}(H_{\rm int},u,\mathbf{a})=E_{H_{{\rm int},k}}(u,\mathbf{a})+\tfrac{1}{2}(H_{\rm int}-H_{\rm ext})^2. \tag{24}$$

The problem of minimizing the Ginzburg–Landau functional F is then split into two minimizing problems, one for $E_{H_{\rm int},k}$ over $\mathcal{A}_d$ and another one for the functional

$$\mathbb{R}_+\to\mathbb{R},$$

$$H_{\rm int}\mapsto m_E(H_{\rm int},k)+\tfrac{1}{2}(H_{\rm int}-H_{\rm ext})^2, \tag{25}$$

with

$$m_E(H_{\rm int},k)=\inf_{(u,\mathbf{a})\in\mathcal{A}_d}E_{H_{\rm int},k}(u,\mathbf{a}). \tag{26}$$

The quantization relation has disappeared and is now encoded in the functional space $\mathcal{A}_d$ [defined in (21) and (22)].

The function $H_{\rm int}\mapsto m_E(H_{\rm int},k)$ is increasing. We also observe that $\mathcal{E}_{k,H_{\rm ext}}$ introduced in (6) satisfies

$$\mathcal{E}_{k,H_{\rm ext}}=\inf_{H_{\rm int}\in\mathbb{R}_+^*}m_E(H_{\rm int},k)+\tfrac{1}{2}(H_{\rm int}-H_{\rm ext})^2. \tag{27}$$

The infimum of the Ginzburg–Landau functional is also obtained by taking the infimum of the map

$$(H_{\rm int},u,\mathbf{a})\mapsto E_{k,H_{\rm ext}}(H_{\rm int},u,\mathbf{a})=E_{H_{\rm int},k}(u,\mathbf{a})+\tfrac{1}{2}(H_{\rm int}-H_{\rm ext})^2 \tag{28}$$

over $\mathbb{R}_+^*\times\mathcal{A}_d$. Using the fact that $E_{H_{\rm int},k}$ is increasing with $H_{\rm int}$, one can show that

$$\mathcal{E}_{k,H_{\rm ext}}=\inf_{H_{\rm int}\in\,]0,H_{\rm ext}]}m_E(H_{\rm int},k)+\tfrac{1}{2}(H_{\rm int}-H_{\rm ext})^2=\inf_{H_{\rm int}\in\,]0,H_{\rm ext}],(u,\mathbf{a})\in\mathcal{A}_d}E_{k,H_{\rm ext}}(H_{\rm int},u,\mathbf{a}). \tag{29}$$

With the above renormalization we can prove that $E_{\mathcal{P}}$ is effectively obtained. We first show the following.

Proposition II.1: We have $\lim_{H_{\rm int}\to 0}m_E(H_{\rm int},k)=0$.

Proof: We have

$$E_{H_{\rm int},k}(u,0)=\frac{1}{d}\int_{\Omega_d}\frac{H_{\rm int}}{4\pi k}\|i\nabla u+\mathbf{A}_0u\|^2+\frac{1}{4}(1-|u|^2)^2. \tag{30}$$

Let $\epsilon>0$. Starting from $u=1$ in Ω_d, it is easy to find a function u_ϵ with compact support in Ω_d which satisfies

$$\int_{\Omega_d}(1-|u_\epsilon|^2)^2<2d\epsilon. \tag{31}$$

This u_ϵ can be extended to $\mathbb{R}^2$ by using the property (21).

Then we can find $\eta>0$ s.t., $\forall H_{\text{int}} \in]0,\eta]$,

$$\frac{1}{d}\int_{\Omega_d} \frac{H_{\text{int}}}{4\pi k} \| i\nabla u_\epsilon + \mathbf{A}_0 u_\epsilon \|^2 \leqslant \frac{\epsilon}{2}, \tag{32}$$

and we have obtained $E_{H_{\text{int}},k}(u_\epsilon,0)<\epsilon$ for $H_{\text{int}} \in]0,\eta]$. The proposition is then proved. **QED**

Coming back to the original problem and using (28), we obtain the following.

Corollary II.2: There exists a sequence ϕ_{λ_n} of sections of $C^\infty(E_{\lambda_n,d})$ with $\lambda_n \to \infty$ such that $\lim_{n\to\infty} F(\phi_{\lambda_n}, (2\pi d/k\lambda_n^2)\mathbf{A}_0) = H_{\text{ext}}^2/2$.

III. THE FUNCTIONAL $E_{H_{\text{int}},k}$

Let us now analyze the functional introduced in (23). We have the basic property.

Proposition III.1: If $(u,\mathbf{a}) \in \mathcal{A}_d$, then $E_{H_{\text{int}},k}(u,\mathbf{a})<\infty$.

Proof: The basic Sobolev imbeddings give us

$$(u,\mathbf{a}) \in L^p_{\text{loc}}(\mathbb{R}^2;\mathbb{C}) \times L^p_{\text{loc}}(\mathbb{R}^2;\mathbb{R}^2) \quad \text{if} \quad p<\infty. \tag{33}$$

So, the conclusion is obtained using standard Hölder estimates.[7] **QED**

Let us observe that, using the same estimates, one can in fact show that $E_{H_{\text{int}},k}$ is Fréchet differentiable. There is a Bochner–Kodaira–Nakano formula for $E_{H_{\text{int}},k}$ (see Refs. 8–10 for related formulas and results). We set $\mathbf{C}=\mathbf{A}_0+\mathbf{a}$ and we have

$$C_x = -\pi y + a_x, \quad C_y = \pi x + a_y \quad \text{and} \quad \text{curl } \mathbf{C} = 2\pi + \text{curl } \mathbf{a}. \tag{34}$$

Let us define A_+ by

$$A_+(u,\mathbf{a}) = \frac{1}{d}\int_{\Omega_d} \frac{\mu}{2} |D_+ u|^2 + \frac{1}{4} |\mu \text{ curl } \mathbf{C} - (1-|u|^2)|^2, \tag{35}$$

where

$$\mu = \frac{H_{\text{int}}}{2\pi k} \tag{36}$$

and

$$D_+ = \frac{\partial}{\partial x} + i\frac{\partial}{\partial y} + C_y - iC_x. \tag{37}$$

Theorem III.2 (Bochner–Kodaira–Nakano): *If $k=1/\sqrt{2}$ then, for all $(u,\mathbf{a}) \in \mathcal{A}_d$, we have*

$$E_{H_{\text{int},1/\sqrt{2}}}(u,\mathbf{a}) = \mu\pi - (\mu\pi)^2 + A_+(u,\mathbf{a}). \tag{38}$$

Proof: We perform computations with smooth functions and then extend by density:

$$
\begin{aligned}
2d(A_+(u,\mathbf{a})-E_{H_{\mathrm{int},1/\sqrt{2}}}(u,\mathbf{a}))&=\int_{\Omega_d}\mu\left[\left(\frac{\partial u}{\partial x}-iC_xu\right)\overline{\left(i\frac{\partial u}{\partial y}+C_yu\right)}+\overline{\left(\frac{\partial u}{\partial x}-iC_xu\right)}\left(i\frac{\partial u}{\partial y}+C_yu\right)\right.\\
&\quad\left.-(\mathrm{curl}\ \mathbf{C})(1-|u|^2)\right]+\frac{\mu^2}{2}\int_{\Omega_d}\{|\mathrm{curl}\ \mathbf{C}|^2-|\mathrm{curl}\ \mathbf{a}|^2\}\\
&=\mu\int_{\Omega_d}\frac{\partial}{\partial x}\left\{\overline{u}\left(i\frac{\partial u}{\partial y}+C_yu\right)\right\}-\frac{\partial}{\partial y}\left\{\overline{u}\left(i\frac{\partial u}{\partial x}+C_xu\right)\right\}\\
&\quad-\int_{\Omega_d}\mu(\mathrm{curl}\ \mathbf{C})+\frac{\mu^2}{2}\int_{\Omega_d}\{|\mathrm{curl}\ \mathbf{C}|^2-|\mathrm{curl}\ \mathbf{a}|^2\}\\
&=\mu\int_{\Omega_d}\mathrm{div}\,\mathbf{W}+2(\mu\pi)^2-2\mu\pi. \qquad (39)
\end{aligned}
$$

The vector field $\mathbf{W}$ appearing in (39) is defined by

$$
\mathbf{W}=\begin{pmatrix}\overline{u}\left(i\dfrac{\partial u}{\partial y}+C_yu\right)\\ -\overline{u}\left(i\dfrac{\partial u}{\partial x}+C_xu\right)\end{pmatrix} \qquad (40)
$$

and is $\mathcal{L}_d$-periodic on $\mathbb{R}^2$. This implies that $\int_{\Omega_d}\mathrm{div}\,\mathbf{W}=0$ and we immediately obtain (38).

QED

Let us observe as a consequence of (38) that

$$
m_E\left(H_{\mathrm{int}},\frac{1}{\sqrt{2}}\right)\geqslant\mu\pi-(\mu\pi)^2=\frac{H_{\mathrm{int}}}{\sqrt{2}}-\left(\frac{H_{\mathrm{int}}}{\sqrt{2}}\right)^2. \qquad (41)
$$

In fact it is possible to compute $m_E(H_{\mathrm{int}},1/\sqrt{2})$ (see Ref. 4, p. 127).

The spectral theory of $H=[i\nabla+\mathbf{A}_0]^2$ is especially important (see, for example, Ref. 11 or Ref. 4, p. 48). His spectrum $sp(H)$ is discrete and $sp(H)=2\pi+4\pi\mathbb{N}$. The multiplicity of 2π is equal to d.

We are interested in the minima of $E_{H_{\mathrm{int}},k}$ and we would also like to study the local stability of the pair (0, 0).

Proposition III.3: The pair (0, 0) *is a critical point for the functional* $E_{H_{\mathrm{int}},k}$.

The quadratic form $D^2_{(0,0)}E_{H_{\mathrm{int}},k}(\delta u,\delta\mathbf{a})$ *is positive definite if and only if* $k<H_{\mathrm{int}}$.

Proof: The first differential at $(u,\mathbf{a})$ is the linear form

$$
\begin{aligned}
D_{(u,\mathbf{a})}E_{H_{\mathrm{int}},k}(u',\mathbf{a}')&=\frac{1}{d}\int_{\Omega_d}\mathrm{Re}[\overline{u}'\{\mu[i\nabla+(\mathbf{A}_0+\mathbf{a})]^2u-(1-|u|^2)u\}]\\
&\quad+\frac{1}{d}\int_{\Omega_d}\mathbf{a}'\{\mu\,\mathrm{Re}[\overline{u}(i\nabla u+(\mathbf{A}_0+\mathbf{a})u)]+k^2\mu^2\mathrm{curl}^*\mathrm{curl}\ \mathbf{a}\}. \qquad (42)
\end{aligned}
$$

We easily get $D_{(0,0)}E_{H_{\mathrm{int}},k}=0$.

The second differential at $(u,\mathbf{a})$ is the bilinear form defined on $\mathcal{A}_d\times\mathcal{A}_d$ by

$$(u_1,\mathbf{a}_1),(u_2,\mathbf{a}_2)\mapsto \frac{1}{d}\int_{\Omega_d}\mathrm{Re}\{\mu\overline{u_1}[i\boldsymbol{\nabla}+\mathbf{A}]^2u_2\}+2\,\frac{1}{d}\int_{\Omega_d}\mathrm{Re}\left[\mu\int_{\Omega_d}[\mathbf{a}_2\overline{u_1}+\mathbf{a}_1\overline{u_2}]\cdot(i\boldsymbol{\nabla}u+\mathbf{C}u)\right]$$
$$+\frac{1}{d}\int_{\Omega_d}-(1-|u|^2)\mathrm{Re}\,\overline{u_1}u_2+2\,\mathrm{Re}(\overline{u}u_2)\mathrm{Re}(\overline{u}u_1)$$
$$+\frac{1}{d}\int_{\Omega_d}\mu\mathbf{a}_1\cdot\mathbf{a}_2|u|^2+\mu^2k^2\mathrm{curl}\ \ \mathbf{a}_1\cdot\mathrm{curl}\ \ \mathbf{a}_2, \tag{43}$$

with $\mathbf{C}=\mathbf{A}_0+\mathbf{a}$.

We get at (0, 0) the bilinear form

$$D^2_{(0,0)}E_{H_{\mathrm{int}},k}:\mathcal{A}_d\times\mathcal{A}_d\to\mathbb{R}, \tag{44}$$

$$(u_1,\mathbf{a}_1),(u_2,\mathbf{a}_2)\to\frac{1}{d}\int\Omega_d\,\mathrm{Re}\{\overline{u_1}(\mu[i\boldsymbol{\nabla}+\mathbf{A}_0]^2-1)u_2\}+\frac{1}{d}\int_{\Omega_d}\mu^2k^2\,\mathrm{curl}\ \ \mathbf{a}_1\,\mathrm{curl}\ \ \mathbf{a}_2.$$

The associated quadratic form is

$$D^2_{(0,0)}E_{H_{\mathrm{int}},k}(u',\mathbf{a}')=\frac{1}{d}\int_{\Omega_d}\overline{u'}(\mu[i\boldsymbol{\nabla}+\mathbf{A}_0]^2-1)u'+\mu^2k^2|\mathrm{curl}\ \ \mathbf{a}'|^2. \tag{45}$$

The term $\int_{\Omega_d}|\mathrm{curl}\ \ \mathbf{a}'|^2$ is positive definite as one can show using the definition of $\mathcal{A}_d$.
The operator $\mu[i\boldsymbol{\nabla}+\mathbf{A}_0]^2-1$ is positive definite if and only if $2\mu\pi-1>0$, i.e., if and only if $k<H_{\mathrm{int}}$. **QED**

IV. THE MONOTONICITY THEOREMS

Theorem IV.1: *If $(k,H_{\mathrm{ext}})\in\mathcal{P}$, then if $k'\leqslant k$ and $H'_{\mathrm{ext}}\leqslant H_{\mathrm{ext}}$, one has $(k',H'_{\mathrm{ext}})\in\mathcal{P}$.*

Proof: Let $(k,H_{\mathrm{ext}})\in\mathcal{P}$. We have $\mathcal{E}_{k,H_{\mathrm{ext}}}=H^2_{\mathrm{ext}}/2$. By definition (6) and (27) of $\mathcal{E}_{k,H_{\mathrm{ext}}}$, we have

$$\forall H_{\mathrm{int}}>0,\forall(u,\mathbf{a})\in\mathcal{A}_d,\quad E_{H_{\mathrm{int}},k}(u,\mathbf{a})+\frac{1}{2}(H_{\mathrm{int}}-H_{\mathrm{ext}})^2\geqslant\frac{H^2_{\mathrm{ext}}}{2}. \tag{46}$$

The inequality (46) is equivalent to $\forall H_{\mathrm{int}}>0$, $\forall(u,\mathbf{a})\in\mathcal{A}_d$,

$$\left\{\frac{1}{d}\int_{\Omega_d}\frac{H_{\mathrm{int}}}{4\pi k}\|i\boldsymbol{\nabla}u+(\mathbf{A}_0+\mathbf{a})u\|^2+\frac{1}{4}(1-|u|^2)^2+\frac{H^2_{\mathrm{int}}}{2(2\pi)^2}|\mathrm{curl}\ \ \mathbf{a}|^2\right\}+\frac{H^2_{\mathrm{int}}-2H_{\mathrm{int}}H_{\mathrm{ext}}}{2}\geqslant 0. \tag{47}$$

If k is decreasing, then $1/k$ is increasing; the integrals being positive, the left-hand side of (47) is increasing. If H_{ext} is decreasing, then the quantity $-2H_{\mathrm{int}}H_{\mathrm{ext}}$ is increasing and so the left-hand side is increasing again. Consequently, if $k'\leqslant k$ and $H'_{\mathrm{ext}}\leqslant H_{\mathrm{ext}}$, we get the inequality $E_{k',H'_{\mathrm{ext}}}(H_{\mathrm{int}},u,\mathbf{a})\geqslant H'^2_{\mathrm{ext}}/2$, $\forall(u,\mathbf{a})\in\mathcal{A}_d$ and, taking the infimum, $\mathcal{E}_{k',H'_{\mathrm{ext}}}\geqslant H'^2_{\mathrm{ext}}/2$. **QED**

Theorem IV.2: *If $(k,H_{\mathrm{ext}})\in\mathcal{N}$ and $k'\geqslant k$, then $(k',(k'/k)H_{\mathrm{ext}})\in\mathcal{N}$.*

Proof: Let $(k,H_{\mathrm{ext}})\in\mathcal{N}$. We have $\mathcal{E}_{k,H_{\mathrm{ext}}}=1/4$. Let us denote by $H'_{\mathrm{ext}}=(k'/k)H_{\mathrm{ext}}$ the new magnetic field. By definition of the set $\mathcal{N}$ and of $E_{k,H_{\mathrm{ext}}}$ [see (11) and (23)], we obtain

$$\forall H_{\mathrm{int}}>0,\forall(u,\mathbf{a})\in\mathcal{A}_d,$$
$$\left\{\frac{1}{d}\int_{\Omega_d}\frac{H_{\mathrm{int}}}{4\pi k}\|i\boldsymbol{\nabla}u+(\mathbf{A}_0+\mathbf{a})u\|^2+\frac{1}{4}(1-|u|^2)^2+\frac{H^2_{\mathrm{int}}}{8\pi^2}|\mathrm{curl}\ \ \mathbf{a}|^2\right\}+\frac{1}{2}(H_{\mathrm{int}}-H_{\mathrm{ext}})^2\geqslant\frac{1}{4}. \tag{48}$$

The inequality we wish to prove is

$$\forall H'_{\text{int}}>0,\ \forall (u,\mathbf{a})\in\mathcal{A}_d,$$
$$\left\{\frac{1}{d}\int_{\Omega_d}\frac{H'_{\text{int}}}{4\pi k'}\|i\nabla u+(\mathbf{A}_0+\mathbf{a})u\|^2+\frac{1}{4}(1-|u|^2)^2+\frac{H'^2_{\text{int}}}{8\pi^2}|\text{curl}\ \ \mathbf{a}|^2\right\}+\frac{1}{2}(H'_{\text{int}}-H'_{\text{ext}})^2\geqslant\frac{1}{4}. \tag{49}$$

We write in analogy with H'_{ext}, $H'_{\text{int}}=(k'/k)H_{\text{int}}$ and we obtain

$$\frac{H_{\text{int}}}{k}=\frac{H'_{\text{int}}}{k'}. \tag{50}$$

It is enough to show

$$\forall H_{\text{int}}>0,\ \forall (u,\mathbf{a})\in\mathcal{A}_d,$$
$$\left\{\frac{1}{d}\int_{\Omega_d}\frac{H_{\text{int}}}{4\pi k}\|i\nabla u+(\mathbf{A}_0+\mathbf{a})u\|^2+\frac{1}{4}(1-|u|^2)^2+\left(\frac{k'}{k}\right)^2\frac{H^2_{\text{int}}}{8\pi^2}|\text{curl}\ \ \mathbf{a}|^2\right\}+\left(\frac{k'}{k}\right)^2\frac{1}{2}(H_{\text{int}}-H_{\text{ext}})^2$$
$$\geqslant\frac{1}{4}. \tag{51}$$

This inequality is implied by (48) since $k'\geqslant k$. **QED**

Theorem IV.3: *If $(k,H_{\text{ext}})\in\mathcal{N}$, then if $H'_{\text{ext}}\geqslant H_{\text{ext}}$ we have $(k,H'_{\text{ext}})\in\mathcal{N}$.*

Proof: Let $(k,H_{\text{ext}})\in\mathcal{N}$. By definitions (11) and (27) of $\mathcal{E}_{k,H_{\text{ext}}}$, we have

$$\forall H_{\text{int}}>0, m_E(H_{\text{int}},k)+\tfrac{1}{2}(H_{\text{int}}-H_{\text{ext}})^2\geqslant E_{\mathcal{N}}. \tag{52}$$

At $H_{\text{int}}=H_{\text{ext}}$ this inequality implies

$$m_E(H_{\text{ext}},k)\geqslant E_{\mathcal{N}}. \tag{53}$$

We have to show inequality (52) with H_{ext} replaced by H'_{ext}. If $H_{\text{int}}\leqslant H_{\text{ext}}$, we trivially obtain

$$(H_{\text{int}}-H_{\text{ext}})^2\leqslant(H_{\text{int}}-H'_{\text{ext}})^2. \tag{54}$$

Then inequality (52) is shown with $H_{\text{int}}\in\,]0,H_{\text{ext}}]$ and H_{ext} replaced by H'_{ext}.
If $H_{\text{int}}>H_{\text{ext}}$, then we get from (53) and by monotonicity of m_E

$$m_E(H_{\text{int}},k)\geqslant m_E(H_{\text{ext}},k)\geqslant E_{\mathcal{N}}. \tag{55}$$

Consequently, inequality (52) is shown with $H_{\text{int}}\in\,]H_{\text{ext}},\infty[$ and H_{ext} replaced by H'_{ext}. **QED**

Let us consider the special case when $k=H_{\text{ext}}=1/\sqrt{2}$. We have the following lemma:

Lemma IV.4: The value of $\mathcal{E}_{1/\sqrt{2},1/\sqrt{2}}$ is 1/4 and $(1/\sqrt{2},1/\sqrt{2})\in\mathcal{P}\cap\mathcal{N}$.

Proof: We set $k=1/\sqrt{2}$. By the equality (29), it is sufficient to show

$$\forall H_{\text{int}}\in\left]0,\frac{1}{\sqrt{2}}\right],m_E(H_{\text{int}},k)+\frac{1}{2}\left(H_{\text{int}}-\frac{1}{\sqrt{2}}\right)^2\geqslant\frac{1}{4}. \tag{56}$$

Using (41) we remark that inequality (56) is implied by the inequality

$$\forall H_{\text{int}}\leqslant\frac{1}{\sqrt{2}},\ \left[\frac{H_{\text{int}}}{2k}-\left(\frac{H_{\text{int}}}{2k}\right)^2\right]+\frac{1}{2}\left(H_{\text{int}}-\frac{1}{\sqrt{2}}\right)^2\geqslant\frac{1}{4}. \tag{57}$$

But this inequality is in fact an equality and we get the claim.

The energy of normal state is $E_{\mathcal{N}}=1/4$. The energy of the pure state is $E_{\mathcal{P}}=1/2(1/\sqrt{2})^2=1/4$. **QED**

Theorem IV.5 (Type I superconductors): *If* $k\leqslant 1/\sqrt{2}$, *then*

$$\mathcal{E}_{k,H_{\text{ext}}}=\begin{cases} E_{\mathcal{P}} & \text{if } H_{\text{ext}}\leqslant \dfrac{1}{\sqrt{2}}, \\ E_{\mathcal{N}} & \text{if } H_{\text{ext}}\geqslant \dfrac{1}{\sqrt{2}}. \end{cases} \tag{58}$$

Proof: Lemma IV.4 combined with Theorem IV.1 gives the result in the case $H_{\text{ext}}\leqslant 1/\sqrt{2}$. In particular, if $k\leqslant 1/\sqrt{2}$, we have $(k,1/\sqrt{2})\in\mathcal{P}$ and so $\mathcal{E}_{k,1/\sqrt{2}}=E_{\mathcal{P}}=1/2(1/\sqrt{2})^2=1/4$. This is the energy $E_{\mathcal{N}}$. Then Theorem IV.3 gives the conclusion in the case $H_{\text{ext}}\geqslant 1/\sqrt{2}$. **QED**

Theorem IV.6 (Type II superconductors): *If* $H_{\text{ext}}\geqslant k\geqslant 1/\sqrt{2}$, *then*

$$\mathcal{E}_{k,H_{\text{ext}}}=E_{\mathcal{N}}. \tag{59}$$

In this case the infimum of the functional is attained by the normal state. In the case $k\geqslant 1/\sqrt{2}$ *and* $H_{\text{ext}}<k$ *we have* $(k,H_{\text{ext}})\notin\mathcal{N}$.

Proof: Lemma IV.4 combined with Theorems IV.2 and IV.3 gives the first result.

We have the functional equality

$$E_{k,H_{\text{ext}}}(H_{\text{ext}},u,\mathbf{a})=E_{H_{\text{ext}},k}(u,\mathbf{a}) \tag{60}$$

with $k<H_{\text{ext}}=H_{\text{int}}$. So the state $u=0$, $\mathbf{a}=0$ is not a local minimum of the functional by Proposition III.3 and so the normal state is not minimizing. **QED**

V. PHASE DIAGRAM

We define the following pure and normal sets $\mathcal{P}_k$ and $\mathcal{N}_k$ using the definition of pure and normal states (11):

$$\begin{aligned} \mathcal{P}_k&=\{H_{\text{ext}}\in\mathbb{R}_+^* \text{ s.t. } \mathcal{E}_{k,H_{\text{ext}}}=E_{\mathcal{P}}\}, \\ \mathcal{N}_k&=\{H_{\text{ext}}\in\mathbb{R}_+^* \text{ s.t. } \mathcal{E}_{k,H_{\text{ext}}}=E_{\mathcal{N}}\}. \end{aligned} \tag{61}$$

By Theorems IV.5 and IV.6, we know that $\mathcal{N}_k=[\sup(k,1/\sqrt{2}),+\infty[$. So it remains to determine $\mathcal{P}_k$. Here our results are not complete. However, we can show the following properties.

Theorem V.1: *The set* $\mathcal{P}_k$ *is of the form* $]0,H_{c1}(k)]$ *where* $H_{c1}(k)$ *is a continuous decreasing function of k and*

$$\inf\left(\frac{1}{2k},\frac{1}{\sqrt{2}}\right)\leqslant H_{c1}(k)\leqslant\frac{1}{\sqrt{2}}. \tag{62}$$

Proof:

Step 1: By Theorem IV.5 we know that in the case $k\leqslant 1/\sqrt{2}$, we have $]0,1/\sqrt{2}]=\mathcal{P}_k$.

Step 2: We suppose $k\geqslant 1/\sqrt{2}$. By the preceding definitions (61), we have

$$\begin{aligned} H_{\text{ext}}\in\mathcal{P}_k\Leftrightarrow\forall H_{\text{int}},u,\mathbf{a},&E_{H_{\text{int}},k}(u,\mathbf{a})+\frac{1}{2}(H_{\text{int}}-H_{\text{ext}})^2 \\ &\geqslant\frac{H_{\text{ext}}^2}{2} \end{aligned}$$

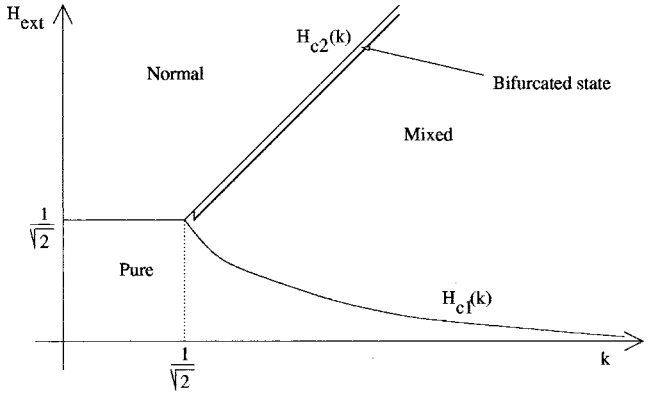

FIG. 1.

$$\Leftrightarrow \forall H_{\text{int}}, u, \mathbf{a}, \frac{1}{H_{\text{int}}} E_{H_{\text{int}},k}(u,\mathbf{a}) + \frac{H_{\text{int}}}{2} \geqslant H_{\text{ext}}$$

$$\Leftrightarrow \begin{cases} \forall H_{\text{int}} > 0, \forall (u,\mathbf{a}) \in \mathcal{A}_d \\ \dfrac{H_{\text{int}}}{2} + \dfrac{1}{4\pi dk} \displaystyle\int_{\Omega_d} \| i\nabla u + (\mathbf{A}_0 + \mathbf{a})u \|^2 \\ + \dfrac{1}{4dH_{\text{int}}} \displaystyle\int_{\Omega_d} (1-|u|^2)^2 + \dfrac{H_{\text{int}}}{2d(2\pi)^2} \int_{\Omega_d} |\text{curl } \mathbf{a}|^2 \geqslant H_{\text{ext}}. \end{cases} \tag{63}$$

But the function defined for $a, b > 0$,

$$\begin{aligned} \mathbb{R}_+^* &\to \mathbb{R}, \\ t &\mapsto at + \frac{b}{t}, \end{aligned} \tag{64}$$

has a minimum of $2\sqrt{ab}$. So we obtain

$$H_{\text{ext}} \in \mathcal{P}_k \Leftrightarrow H_{\text{ext}} \leqslant \inf_{(u,\mathbf{a}) \in \mathcal{A}_d} \left\{ \frac{1}{4\pi dk} \int_{\Omega_d} \| i\nabla u + (\mathbf{A}_0 + \mathbf{a})u \|^2 + \sqrt{\left[\frac{1}{2} + \frac{1}{2d(2\pi)^2} \int_{\Omega_d} |\text{curl } \mathbf{a}|^2 \right] \left[\frac{1}{d} \int_{\Omega_d} (1-|u|^2)^2 \right]} \right\}, \tag{65}$$

and so $\mathcal{P}_k =]0, H_{c1}(k)]$ with

$$H_{c1}(k) = \inf_{(u,\mathbf{a}) \in \mathcal{A}_d} \left\{ \frac{1}{4\pi dk} \int_{\Omega_d} \| i\nabla u + (\mathbf{A}_0 + \mathbf{a})u \|^2 + \sqrt{\left[\frac{1}{2} + \frac{1}{2d(2\pi)^2} \int_{\Omega_d} |\text{curl } \mathbf{a}|^2 \right] \left[\frac{1}{d} \int_{\Omega_d} (1-|u|^2)^2 \right]} \right\}. \tag{66}$$

Step 3: From the expression (66) it follows that $H_{c1}(k)$ is a decreasing function and $kH_{c1}(k)$ is an increasing function. From the first step we know that $H_{c1}(1/\sqrt{2}) = 1/\sqrt{2}$. Then $\forall k \geqslant 1/\sqrt{2}$ we have

$$H_{c1}(k) \leqslant \frac{1}{\sqrt{2}} \text{ and } kH_{c1}(k) \geqslant \frac{1}{2}. \tag{67}$$

The inequalities (62) are then proved.

Step 4: H_{c1} is a decreasing function of k so the limits

$$l_- = \lim_{k \to k_0, k<k_0} H_{c1}(k) \text{ and } l_+ = \lim_{k \to k_0, k>k_0} H_{c1}(k) \tag{68}$$

exist and satisfy $l_+ \leqslant l_-$. The function $kH_{c1}(k)$ is increasing so $k_0 l_- \leqslant k_0 l_+$ and we conclude that H_{c1} is continuous. **QED**

The proof that $H_{c1}(k) \to 0$ as $k \to \infty$ is contained in Ref. 4, p. 143. The exact value of $H_{c1}(k)$ seems impossible to compute; nevertheless, an analysis near $k = 1/2$ of the phase diagram will appear in a subsequent paper.

The phase diagram is a picture in the plane $(k, H_{\text{ext}}) \in \mathbb{R}_+^* \times \mathbb{R}_+^*$ on which all the three preceding states are drawn. We have proved that its qualitative shape is that in Fig. 1, which depends on the number d introduced in (3). This is the diagram encountered in the physical literature.[12–15]

In Ref. 4 there is a more precise analysis of the special case $d = 1$. Among other things there is a bifurcation analysis in the limit H_{ext} near k (Ref. 4, p. 79).[5,16–18] An asymptotic estimate of the energy gap between normal and mixed state extending results from Ref. 19 is available in (Ref. 4 p. 130), using these bifurcated states.

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Calogero–Moser systems with periodic and doubly periodic interaction potentials and loop algebras

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For a finite number of particles on the line pairwise interacting with $1/r^2$ potential, the positions are given by the eigenvalues of some time-dependent matrix. Infinite periodic or doubly periodic replication of the particles yields Calogero–Moser systems with periodic or doubly periodic interaction potential. We are thus led to consider matrices of infinite order, which are identified with Fourier series with matrix coefficients, depending on an additional parameter. These distributional loops of matrices (tori of matrices in the doubly periodic case) are shown to obey simple (partial) differential equations, which allow us to determine them explicitly. Thus we obtain the already known solution of the Calogero–Moser system on the circle, and provide a new insight for the system on the torus. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1401136]

I. INTRODUCTION

Calogero–Moser systems were introduced long ago and were proven to be completely integrable by Lax pairs technics, see Ref. 1. The systems with $1/r^2$ and $1/\sin^2 r$ interaction potentials received in Ref. 2 an enlightening geometric interpretation through Marsden–Weinstein reduction of geodesic flows on Lie algebras or Lie groups. However, the system with a Weierstrass $\mathcal{P}$ function interaction potential remains less understood. The two-particle system has been solved in Ref. 3, and the only known integration scheme in the general case was provided by Krichever in Ref. 4, through the solitonic solutions of the Kadomtsev–Patviashvili (KP) equation.

The present work starts from the solution of the system with $1/r^2$ interaction potential and proceeds by infinite replication. Calogero and Françoise had previously used a duplication scheme to produce new integrable systems and their solutions from the system on the line in Ref. 5. Here we have in mind the Eulerian development of $1/\sin^2$ and proceed by infinite replication by translations of the system on the line. The corresponding matrices are infinite dimensional and are interpreted as distributional elements of some loop algebra. The striking fact is that these distributions are just elementary differential operators. This allows us to give a new proof of the solution of the system with $1/\sin^2 r$ interaction potential.

Then, we apply a doubly infinite replication to investigate the system with Weierstrass $\mathcal{P}$ function interaction potential, which leads us to a partial differential operator on the space of doubly periodic functions with values in $\mathbb{C}^n$. Though this operator is very simple looking and very similar to the preceding one, it is indeed much more involved to determine its spectrum and this is beyond the author's reach. We connect this problem to some finite difference equation in a space of simply periodic analytic functions.

II. INFINITE REPLICATION

It is known that the Calogero–Moser system on the real line with $1/r^2$ pairwise interaction potential can be integrated in the following way.[2]

Let $x_1, x_2, \ldots, x_n$ denote the initial positions of the particles, and $y_1, \ldots, y_n$ their initial velocities,

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$$A=\begin{pmatrix} ix_1 & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & ix_n \end{pmatrix},$$

$$B=\begin{pmatrix} iy_1 & \dfrac{1}{x_2-x_1} & \dots & \dfrac{1}{x_n-x_1} \\ \dfrac{1}{x_1-x_2} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \dfrac{1}{x_n-x_{n-1}} \\ \dfrac{1}{x_1-x_n} & \dots & \dfrac{1}{x_{n-1}-x_n} & iy_n \end{pmatrix},$$

so that

$$[A,B]=M=\begin{pmatrix} 0 & -i & \dots & -i \\ -i & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -i \\ -i & \dots & -i & 0 \end{pmatrix}.$$

The position of particles at time t are then the eigenvalues of $A+tB$, divided by i.

We also recall that the positions at time t of the Calogero–Moser system on the circle with pairwise interaction potential $1/\sin^2(r/2)$ (also called the Sutherland system) are the arguments of the eigenvalues of the matrix $\exp(A)\cdot\exp(tC)$, where $C=(c_{k,l})$ with $c_{k,l}=i/e^{i(x_l-x_k)}-1$ for $k\neq l$ and $c_{k,k}=iy_k$,

Our first aim is to show that the solution of the system on the circle can be deduced from a system on the line with infinitely many particles.

Let us recall the Eulerian expansion:

$$\frac{1}{\sin^2 r}=\sum_{k\in\mathbb{Z}}\frac{1}{(r-k\pi)^2}.$$

According to this formula, one can write the Hamiltonian

$$H=\frac{1}{2}\sum_i y_i^2+\frac{1}{2}\sum_{i\neq j}\frac{1}{4\sin^2\dfrac{x_j-x_i}{2}}$$

in the form

$$\begin{aligned} H&=\frac{1}{2}\sum_i y_i^2+\frac{1}{2}\sum_{i\neq j}\sum_{k\in\mathbb{Z}}\frac{1}{(x_j-x_i-2k\pi)^2} \\ &=\frac{1}{2}\sum_i y_i^2+\frac{1}{2}\sum_{i\neq j}\lim_{N\to+\infty}\frac{1}{2N}\sum_{k,l\in[-N,N]}\frac{1}{[(x_j+2k\pi)-(x_i+2l\pi)]^2}. \end{aligned}$$

For all $i\in\mathbb{Z}$, let us write $i=kn+r$ with $1\leqslant r\leqslant n$ and set $x_i=x_r+2k\pi$ and $y_i=y_r$. The Hamiltonian takes thus the form

$$H=\lim_{N\to+\infty}\frac{1}{2N}\left[\frac{1}{2}\sum_{-nN\leqslant i\leqslant nN}y_i^2+\frac{1}{2}\sum_{\substack{-nN\leqslant i,j\leqslant nN\\ i\not\equiv j[n]}}\frac{1}{(x_j-x_i)^2}\right].$$

Therefore, the n-body Sutherland system on the circle is analogous to the infinitely many-body system on the line obtained by associating to each particle on the circle infinitely many particles on the line, 2π-distant of each other and animated with the same velocity.

We thus form the infinite dimensional matrices $\tilde{A}$, $\tilde{M}$, and $\tilde{B}$ indexed by $\mathbb{Z}\times\mathbb{Z}$ where

$$\tilde{A}=\begin{pmatrix}\ddots & & & & \\ & A-2i\pi I & 0 & 0 & \\ & 0 & A & 0 & \\ & 0 & 0 & A+2i\pi I & \\ & & & & \ddots\end{pmatrix},$$

$$\tilde{B}=\begin{pmatrix}\ddots & & & & \\ & P_0 & P_{-1} & P_{-2} & \\ & P_1 & P_0 & P_{-1} & \\ & P_2 & P_1 & P_0 & \\ & & & & \ddots\end{pmatrix},\quad \tilde{M}=\begin{pmatrix}\ddots & & & & \\ & M & M & M & \\ & M & M & M & \\ & M & M & M & \\ & & & & \ddots\end{pmatrix},$$

where

$$P_k=\begin{pmatrix} iy_1\delta_{k,0} & \dfrac{1}{x_2-x_1+2k\pi} & \cdots & \dfrac{1}{x_n-x_1+2k\pi}\\ \dfrac{1}{x_1-x_2+2k\pi} & \ddots & \ddots & \vdots\\ \vdots & \ddots & \ddots & \dfrac{1}{x_n-x_{n-1}+2k\pi}\\ \dfrac{1}{x_1-x_n+2k\pi} & \cdots & \dfrac{1}{x_{n-1}-x_n+2k\pi} & iy_n\delta_{k,0}\end{pmatrix}$$

so that $[\tilde{A},\tilde{B}]=\tilde{M}$.

III. LOOP ALGEBRAIC INTERPRETATION

The matrices $\tilde{A}$ and $\tilde{B}$ will be considered as linear operators on the space of one-periodic $\mathbb{C}^n$-valued functions $f:\theta\mapsto\Sigma_{k\in\mathbb{Z}}f_ke^{2ik\pi\theta}$.

Writing f as

$$f=\begin{pmatrix}\vdots\\ f_{-1}\\ f_0\\ f_1\\ \vdots\end{pmatrix},$$

one gets

$$\tilde{A}f=\begin{pmatrix} \vdots \\ -2i\pi f_{-1}+Af_{-1} \\ Af_0 \\ 2i\pi f_1+Af_1 \\ \vdots \end{pmatrix}=f'+Af,$$

where the prime designates derivation with respect to the variable θ, and

$$\tilde{B}f=\begin{pmatrix} \vdots \\ \cdots+P_0f_{-1}+P_{-1}f_0+P_{-2}f_1+\cdots \\ \cdots+P_1f_{-1}+P_0f_0+P_{-1}f_1+\cdots \\ \cdots+P_2f_{-1}+P_1f_0+P_0f_1+\cdots \\ \vdots \end{pmatrix}=\Lambda f,$$

where $\Lambda(\theta)=\cdots+P_{-1}e^{-2i\pi\theta}+P_0+P_1e^{2i\pi\theta}+\cdots$.

We now proceed to the computation of Λ.

The equation $[\tilde{A},\tilde{B}]=\tilde{M}$ can be rewritten in the following way: $\forall k\in\mathbb{Z}\ AP_k-P_k(A-2ik\pi I)=M$.

Multiplying each member by $e^{2ik\pi\theta}$, we get after summation:

$$A\sum_{k\in\mathbb{Z}}P_ke^{2ik\pi\theta}-\sum_{k\in\mathbb{Z}}P_ke^{2ik\pi\theta}A+\sum_{k\in\mathbb{Z}}2ik\pi P_ke^{2ik\pi\theta}=M\sum_{k\in\mathbb{Z}}e^{2ik\pi\theta}.$$

Thus $[A,\Lambda(\theta)]+\Lambda'(\theta)=M\delta_0$.

In order to solve this equation on the circle, we first solve the associated equation on the line: $[A,\Lambda(\theta)]+\Lambda'(\theta)=M\Sigma_{k\in\mathbb{Z}}\delta_k$ (cf. Poisson summation formula)
and we will retain the one-periodic solutions.

The associated homogeneous equation is

$$\Lambda'(\theta)=-[A,\Lambda(\theta)],$$

the general solution of which is $\Lambda(\theta)=e^{-\theta A}Ke^{\theta A}$ (K constant matrix).

The solution of the complete equation is obtained by varying the constant K, which satisfies the equation $e^{-\theta A}K'e^{\theta A}=M\Sigma_{k\in\mathbb{Z}}\delta_k$.

Therefore, K is constant on each interval $]k,k+1[$ $(k\in\mathbb{Z})$ and has Heaviside singularities at integer points. All that we need is the value of K on $]0,1[$. In order to get this value, we just write

$$B=P_0=\int_0^1\Lambda(\theta)\mathrm{d}\theta=\int_0^1e^{-\theta A}Ke^{\theta A}\,\mathrm{d}\theta.$$

Writing $K=(K_{k,l})_{1\leqslant k,l\leqslant n}$, we get

$$e^{-\theta A}Ke^{\theta A}=(e^{i\theta(x_l-x_k)}K_{kl})_{1\leqslant k,l\leqslant n}$$

and thus $iy_k=B_{k,k}=K_{k,k}$ and for $k\neq l$,

$$\frac{1}{x_l-x_k}=B_{k,l}=\frac{e^{i(x_l-x_k)}-1}{i(x_l-x_k)}K_{k,l},$$

which yields $K_{k,l}=i/e^{i(x_l-x_k)}-1$.

Thus K is the matrix C of the Kazdhan–Kostant–Sternberg theory[2] and $\Lambda(\theta)=e^{-\theta A}Ce^{\theta A}$.

Recall that the positions of the particle at time t are, in the finite case, the eigenvalues of $A+tB$ divided by i. We conjecture that in the case at hand, they are the eigenvalues of $\mathrm{d}/\mathrm{d}\theta+(A+t\Lambda(\theta))id$ (divided by i), acting on the space of one-periodic functions.

Since Λ is continuous except at integer points where it has Heaviside singularities, we look for the one-periodic, differentiable except at integer points, but everywhere continuous solutions of this equation.

On $]0, 1[$, this equation reads

$$f' + (A + e^{-\theta A} C e^{\theta A}) f = \lambda f.$$

Set $f(\theta) = e^{\lambda\theta} e^{-\theta A} g(\theta)$. The preceding differential equation is equivalent to

$$g'(\theta) + tCg(\theta) = 0$$

or

$$f(\theta) = e^{\lambda\theta} e^{-\theta A} e^{-t\theta C} f_0$$

with constant f_0.

This equation is satisfied by a nonzero, one-periodic and continuous function if only if $e^{-\lambda}$ is an eigenvalue of $e^{-A} e^{-tC}$

Thus, the eigenvalues of $\tilde{A} + t\tilde{B}$ are the (pure imaginary) complex numbers the exponentials of which are eigenvalues of $e^{tC} e^{A}$, which are the same as the eigenvalues of $e^{A} e^{tC}$.

This agrees with the solution given in Ref. 2.

IV. DOUBLY PERIODIC POTENTIAL

A. The operator

We apply the same scheme when the pairwise interaction potential is the Weierstrass $\mathcal{P}$ function,

$$\mathcal{P}(z) = \frac{1}{z^2} + \sum_{(k,l)\neq(0,0)} \left(\frac{1}{(z - 2k\pi - 2il\omega\pi)^2} - \frac{1}{(2k\pi + 2il\omega\pi)^2} \right).$$

We will use for this purpose matrices of infinite order indexed by $(\mathbb{Z}\times\mathbb{Z})^2$ instead of $\mathbb{Z}^2$, and the underlying Lie algebra will be the complexification of $u(n)$, that is $gl_n(\mathbb{C})$.

Vectors of $\mathbb{C}^{\mathbb{Z}\times\mathbb{Z}}$ will be identified with $\mathbb{C}^n$-valued doubly periodic functions (with periods 1 and $1/\omega$ with respect to variables θ and ϕ),

$$f(\theta, \phi) = \sum_{k,l} \xi_{k,l} e^{2ik\pi\theta} e^{2il\pi\omega\phi}.$$

The matrix $\tilde{A}$ now has the block decomposition

$$\tilde{A} = (A_{klk'l'})_{k,l,k',l' \in \mathbb{Z}}$$

with $A_{klk'l'} = A + (2ik\pi + 2l\omega\pi) I$ if $k = k'$ and $l = l'$ and $A_{k,l,k',l'} = 0$ otherwise. It is identified with the operator

$$(\tilde{A}f)(\theta, \phi) = Af(\theta, \phi) + \sum_{k,l} \xi_{k,l} (2ik\pi - 2l\omega\pi) e^{2ik\pi\theta} e^{2il\pi\omega\phi}$$

$$= Af(\theta, \phi) + \frac{\partial f}{\partial \theta} - \frac{1}{i} \frac{\partial f}{\partial \phi}$$

$$= Af(z) + 2 \frac{\partial f}{\partial \bar{z}}$$

(by writing $z=\theta+i\phi$).

In the same way, we identify $\tilde{B}$ with the multiplication operator $f\mapsto\Lambda f$ where Λ is a doubly periodic $gl_n(\mathbb{C})$-valued function.

With M having the same meaning as before, Λ satisfies the partial differential equation

$$[A,\Lambda]+2\frac{\partial\Lambda}{\partial\bar{z}}=M\delta_O$$

where O denotes the origin of the torus.

As before, we start by solving the equation on $\mathbb{C}$,

$$[A,\Lambda]+2\frac{\partial\Lambda}{\partial\bar{z}}=M\sum_{k,l}\ \delta_{k+il}/\omega,$$

rather than the equation on the torus, and then we will go back to the initial equation.

The solution of the homogeneous equation are the functions of the form

$$z\mapsto e^{-\bar{z}A/2}Ke^{\bar{z}A/2},$$

where K is any holomorphic matrix valued entire function.

We solve the complete equation by varying the ''constant'' K, which satisfies

$$2e^{-\bar{z}A/2}\frac{\partial K}{\partial\bar{z}}e^{\bar{z}A/2}=M\sum_{k,l}\ \delta_{k+il/\omega},$$

$$\frac{\partial K}{\partial\bar{z}}=\frac{1}{2}\sum_{\Omega\in\mathcal{R}}\ \delta_\Omega e^{\bar{\Omega}A/2}Me^{-\bar{\Omega}A/2},$$

where

$$\mathcal{R}=\mathbb{Z}+\frac{i}{\omega}\mathbb{Z}.$$

The solutions of this equation are the meromorphic functions whose poles are simple and are the points of the network $\mathcal{R}$, the residue at Ω being $(1/2\pi)e^{\bar{\Omega}A/2}Me^{-\bar{\Omega}A/2}$.

But Λ is also doubly periodic, and therefore

$$\forall\Omega\in\mathcal{R}\ \ e^{-(\bar{z}+\bar{\Omega})A/2}K(z+\Omega)e^{(\bar{z}+\bar{\Omega})A/2}=e^{-\bar{z}A/2}K(z)e^{\bar{z}A/2},$$

$$K(z+\Omega)=e^{\bar{\Omega}A/2}K(z)e^{-\bar{\Omega}A/2}.$$

Therefore, the diagonal coefficients of K are pole free (because the diagonal coefficients of M are null) elliptic functions, and thus they are constant. In the same way as mentioned earlier, writing $B=\int\int_{[0,1]^2}\Lambda$, we get $K_{k,k}=iy_k$; and the off-diagonal coefficients $K_{k,l}$ of K are meromorphic functions which satisfy

$$K_{k,l}(z+\Omega)=e^{\bar{\Omega}i(x_k-x_l)/2}K_{k,l}(z)$$

and with simple poles $\Omega\in\mathcal{R}$ and residues $(1/2i\pi)e^{\bar{\Omega}i(x_k-x_l)}$.

As we prefer to deal with (simply) periodic functions, we set

$$P(z)=e^{-zA/2}K(z)e^{zA/2}.$$

One has for all $\Omega\in\mathcal{R}$,

$$P(z+\Omega)=e^{-(z+\Omega)A/2}e^{\bar{\Omega}A/2}K(z)e^{-\bar{\Omega}A/2}e^{(z+\Omega)A/2}$$

$$=e^{-(\Omega-\bar{\Omega})A/2}P(z)e^{(\Omega-\bar{\Omega})A/2}.$$

Thus P is periodic with period 1 and

$$P(z+i/\omega)=e^{-i/\omega A}P(z)e^{i/\omega A}.$$

The diagonal coefficients of P are those of K. They are constants: $P_{k,k}=iy_k$.

The off-diagonal coefficients of P are meromorphic with simple poles on the network and residue at zero: $1/2i\pi$.

They satisfy

$$P_{k,l}(z+1)=P_{k,l}(z) \quad P_{k,l}(z+i/\omega)=e^{(x_k-x_l)/\omega}P_{k,l}(z). \tag{1}$$

Let us recall the definition of Riemann's theta functions (see for instance Ref. 6)

$$\vartheta\begin{bmatrix}a\\b\end{bmatrix}(z)=\sum_{m\in\mathbb{Z}}e^{i\pi[\tau(m-a)^2+2(m-a)(z-b)]},$$

where $\mathrm{Im}(\tau)>0$ and $a,b\in\mathbb{C}$. This defines an entire function which satisfies the fundamental relation

$$\vartheta\begin{bmatrix}a\\b\end{bmatrix}(z+p\tau+q)=e^{i\pi(-2pz-p^2\tau+2pb-2aq)}\vartheta\begin{bmatrix}a\\b\end{bmatrix}(z),$$

$\forall p,q\in\mathbb{Z}$ and the zeros of $\vartheta[{}^a_b]$ are simple and located at the $(a-\frac{1}{2})\tau+b-\frac{1}{2}+\tau b+q, p,q\in\mathbb{Z}$.

Set $\tau=i/\omega$. The function

$$Q=\frac{\vartheta\begin{bmatrix}a\\b\end{bmatrix}}{\vartheta\begin{bmatrix}a'\\b'\end{bmatrix}}$$

satisfies

$$Q\left(z+\frac{i}{\omega}p+q\right)=e^{i\pi(2(p/\omega)(b-b')-2(a-a')q)}Q(z).$$

This matches with (1) if we choose a,b,a',b' such that

$$a-a'=0, \quad b-b'=-i\frac{x_k-x_l}{2\pi\omega}$$

and the location of poles matches if $a'=b'=\frac{1}{2}$.

Then $P_{k,l}/Q$ is an elliptic function with at most one simple pole in the fundamental cell (since theta functions have just one simple zero in the fundamental cell), thus it is constant and equal to its value at zero.

Hence,

$$P_{k,l}(z)=\frac{1}{2i\pi}\times\frac{\vartheta'\begin{bmatrix}1/2\\1/2\end{bmatrix}(0)}{\vartheta\begin{bmatrix}1/2\\\frac{1}{2}-i\frac{x_k-x_l}{2\pi\omega}\end{bmatrix}(0)}\times\frac{\vartheta\begin{bmatrix}1/2\\\frac{1}{2}-i\frac{x_k-x_l}{2\pi\omega}\end{bmatrix}(z)}{\vartheta\begin{bmatrix}1/2\\1/2\end{bmatrix}(z)}$$

$$=\frac{1}{2i\pi}\times\frac{\vartheta_1'(0)}{\vartheta_1\left(i\frac{x_k-x_l}{2\pi\omega}\right)}\times\frac{\vartheta_1\left(z+i\frac{x_k-x_l}{2\pi\omega}\right)}{\vartheta_1(z)},$$

where we have set

$$\vartheta_1=\vartheta\begin{bmatrix}1/2\\1/2\end{bmatrix}$$

(Jacobi's notation).

We have another way for expressing the off-diagonal coefficients of P.

Let $\delta\in]0,2\pi[$. Consider the series

$$f(z)=\sum_{j\in\mathbb{Z}}\frac{e^{-j\delta}}{1-e^{-2j\pi/\omega}e^{2i\pi z}}.$$

This series converges normally on all compact of $\mathbb{C}\backslash\mathcal{R}$ and defines a meromorphic function with period 1 that verifies $f(z+i/\omega)=e^{\delta}f(z)$. Its only poles are simple and are the points of $\mathcal{R}$. Its residue at 0 is $1/-2i\pi$.

In the same way, for $\delta\in]-2\pi,0[$, the series

$$f(z)=\sum_{j\in\mathbb{Z}}\frac{e^{-j\delta}}{1-e^{2j\pi/\omega}e^{-2i\pi z}}$$

defines a meromorphic function with period 1 that verifies $f(z+(i/\omega))=e^{\delta}f(z)$. Its residue at 0 is $1/2i\pi$.

Suppose that $x_1<x_2<\cdots<x_n<x_1+2\pi$. Then one can write

$$\text{if } k<l \quad P_{k,l}(z)=\sum_{j\in\mathbb{Z}}\frac{e^{-j(x_k-x_l)/\omega}}{1-e^{2j\pi/\omega}e^{-2i\pi z}},$$

$$\text{if } k>l \quad P_{k,l}(z)=-\sum_{j\in\mathbb{Z}}\frac{e^{-j(x_k-x_l)/\omega}}{1-e^{-2j\pi/\omega}e^{2i\pi z}}.$$

B. The spectrum

We conjecture that the positions of the particles at time t are the eigenvalues of the operator

$$A+2\frac{\partial}{\partial\bar{z}}+t\Lambda(z)$$

acting on the space of doubly periodic functions (with periods 1 and i/ω).

Let λ be some (pure imaginary) complex number and f some doubly periodic function satisfying

$$Af+2\frac{\partial f}{\partial \bar{z}}+t\Lambda f=\lambda f.$$

Set $f(z)=e^{\lambda \bar{z}/2}e^{-\bar{z}A/2}g(z)$

The preceding equation becomes

$$2e^{\lambda \bar{z}/2}e^{-\bar{z}A/2}\frac{\partial g}{\partial \bar{z}}+te^{-\bar{z}A/2}K(z)e^{\bar{z}A/2}e^{\lambda \bar{z}/2}e^{-\bar{z}A/2}g(z)=0,$$

which amounts to

$$2\frac{\partial g}{\partial \bar{z}}+tK(z)g(z)=0.$$

Recall that K is holomorphic except at the points of the network $\mathcal{R}$. Set $g(z)=e^{-tz\bar{K}(z)/2}h(z)$.

The preceding equation amounts to $\partial h/\partial \bar{z}=0$, except at the points of the network. Therefore, except at these points, f takes the form

$$f(z)=e^{\lambda \bar{z}/2}e^{-\bar{z}A/2}e^{-tz\bar{K}(z)/2}h(z),$$

where h is holomorphic.

The function f is doubly periodic. This means that for all Ω in the network,

$$f(z+\Omega)=f(z).$$

Since

$$\begin{aligned}f(z+\Omega)&=e^{\lambda(\bar{z}+\bar{\Omega})/2}e^{-\bar{z}A/2}e^{-\bar{\Omega}A/2}e^{-t(\bar{z}+\bar{\Omega})K(z+\Omega)/2}h(z+\Omega)\\&=e^{\lambda(\bar{z}+\bar{\Omega})/2}e^{-\bar{z}A/2}e^{-t(\bar{z}+\bar{\Omega})K(z)/2}e^{-\bar{\Omega}A/2}h(z+\Omega),\end{aligned}$$

we get

$$h(z+\Omega)=e^{-\lambda\bar{\Omega}2}e^{\bar{\Omega}A/2}e^{t\bar{\Omega}K(z)/2}h(z).$$

Set then $h(z)=e^{tzK(z)/2}k(z)$ and recall that $K(z+\Omega)=e^{\bar{\Omega}A/2}K(z)e^{-\bar{\Omega}/2}$.

The preceding condition reads

$$e^{\bar{\Omega}A/2}e^{t(z+\Omega)K(z)/2}e^{-\bar{\Omega}A/2}k(z+\Omega)=e^{-\lambda\bar{\Omega}/2}e^{\bar{\Omega}A/2}e^{t\bar{\Omega}L(z)/2}e^{tK(z)/2}k(z),$$

which simplifies to

$$k(z+\Omega)=e^{-\lambda\bar{\Omega}/2}e^{\bar{\Omega}A/2}e^{t(\bar{\Omega}-\Omega)K(z)/2}k(z).$$

Then set $k(z)=e^{-\lambda z/2}e^{zA/2}\phi(z)$. The preceding condition reads thus

$$e^{-\lambda(z+\Omega)/2}e^{(z+\Omega)A/2}\phi(z+\Omega)=e^{-\lambda\bar{\Omega}/2}e^{\bar{\Omega}A/2}e^{t(\bar{\Omega}-\Omega)K(z)/2}e^{-\lambda z/2}e^{zA/2}\phi(z),$$

which simplifies to

$$\phi(z+\Omega)=e^{\lambda(\Omega-\bar{\Omega})/2}e^{-(z+\Omega-\bar{\Omega})A/2}e^{t(\bar{\Omega}-\Omega)K(z)/2}e^{zA/2}\phi(z).$$

Therefore we look for analytic functions on $\mathbb{C}\backslash\mathcal{R}$ satisfying ϕ is periodic with period 1 and

$$\phi(z+i/\omega)=e^{i\lambda/\omega}e^{-(z+2i/\omega)A/2}e^{-it/\omega K(z)}e^{zA/2}\phi(z)=e^{i\lambda/\omega}L(z)\phi(z), \tag{2}$$

where

$$L(z)=e^{-(z+2i/\omega)A/2}e^{-it/\omega K(z)}e^{zA/2}=e^{-i/\omega A}e^{-it/\omega P(z)}.$$

We conjecture that the correct condition is that ϕ, which coincides with f on the real axis, should have no singularity there.

Since ϕ is then holomorphic on the domain $|\mathrm{Im}(z)|<1$, we can write $\phi(z)=\Sigma_{j\in\mathbb{Z}}\phi_j e^{2i\pi jz}$, this expansion being valid in the same domain.

Since $L(x-i/2)$ is a smooth one-periodic function of the real variable x, we can write $L(x-(i/2))=\Sigma_{j\in\mathbb{Z}}L_j e^{2i\pi jx}$.

Condition (2) is satisfied if and only if it is satisfied on the line $\mathbb{R}-i/2$ (because only analytic functions are involved), and this reads:

$$\forall j\in\mathbb{Z}\ e^{-\pi j}\phi_j=e^{i\lambda}\sum_{k\in\mathbb{Z}}L_{j-k}e^{\pi k}\phi_k,$$

that is $e^{-i\lambda}=e^x$ is an eigenvalue of the infinite matrix $T=(T_{j,k})$ (block decomposition) with $T_{j,k}=e^{\pi(j+k)}L_{j-k}$.

Our problem is to express the Fourier expansion of $x\mapsto L(x-i/2)$, which is beyond our reach in the general case. However, some remarks can be made.

ϑ_1 is odd, therefore

$$P_{k,l}(-z)=-P_{l,k}(z)\quad \text{if}\ \ k\neq l.$$

The series expansion of P yields also

$$P_{k,l}(\overline{z})=-\overline{P_{l,k}(z)}.$$

For $x\in\mathbb{R}$, we have for $k\neq l$: $\overline{P_{k,l}(x-i/2)}=-P_{l,k}\overline{(x-i/2)}=-P_{l,k}(x+i/2)=-e^{x_l-x_k}P_{l,k}(x-i/2)$ and this holds also for $k=l$ since $P_{k,k}$ is a pure imaginary number.

Therefore, $e^{-iA/\omega}P(x-i/2)$ is skew-Hermitian, and thus, $-itP/\omega$ is Hermitian with respect to the Hermitian form with matrix e^{-iA}. Thus so is $e^{-itP/\omega}$ and thus $L=e^{-iA/\omega}e^{-itP/\omega}$ is Hermitian (at $x-i/2$ for real x).

Therefore for all integer j,

$$L_j=\int_0^1 e^{-2i\pi jx}L\left(x-\frac{i}{2}\right)\mathrm{d}x=\int_0^1 e^{-2i\pi jx}\left[\overline{L}\left(x-\frac{i}{2}\right)\right]^{\dagger}\mathrm{d}x$$

$$=\left[\overline{\int_0^1 e^{2i\pi jx}L\left(x-\frac{i}{2}\right)\mathrm{d}x}\right]^{\dagger}=[\overline{L}_{-j}]^{\dagger},$$

where the dagger denotes transposition, and thus the infinite matrix T is Hermitian.

Numerical-simulations confirm our conjectures. Quite surprisingly, finite submatrices of small order of the infinite matrix T give very accurate results. Using a submatrix of order 14, in the two-particle case at time 1, we obtained four digit agreement with the positions given by Runge–Kutta integration.

V. CONCLUSION

Our infinite replication scheme has succeeded in reinvestigating the Calogero–Moser system with $1/\sin^2 r$ potential, but made the system with elliptic potential more mysterious than ever by connecting it to a new finite difference equation. Many questions remain open. Does this problem

have a close form solution? How is it connected with the solution given by Krichever[4] through the KP equation? And is there a geometric interpretation of the system analogous to the one given by Kazdhan, Kostant, and Sternberg[5] for $1/\sin^2 r$ potential?

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Relation between the solitons of Yang–Mills–Higgs fields in 2+1 dimensional Minkowski space–time and anti-de Sitter space–time

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The Yang–Mills–Higgs–Bogomolny equations in both $2+1$ dimensional Minkowski space–time and $2+1$ dimensional anti-de Sitter space–time are known to be integrable and their soliton solutions have already been obtained. In this article, we show that there is a natural relation between the Lax pairs and soliton solutions in these two space–times when the curvature changes from 0 to -1. The changes of the asymptotic behaviors of the solitons are also discussed. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1398585]

I. INTRODUCTION

The Yang–Mills–Higgs–Bogomolny equations in both $2+1$ dimensional Minkowski space–time and $2+1$ dimensional anti-de Sitter space–time are known to be integrable.[1–4] There are several ways to solve them explicitly. The Darboux transformation method is one of them, which gives an easy way to obtain explicit soliton solutions.[5,6] Since the Lax pairs in both Minkowski and anti-de Sitter cases are known, the Darboux transformations can be constructed separately in these two cases.

The standard anti-de Sitter space–time has curvature -1. Naturally we can consider the anti-de Sitter space–time with constant curvature $-1/\rho^2(\rho>0)$. When $\rho\to+\infty$, the space–time tends to the Minkowski space–time. In this article, we consider the following problem: When ρ changes from 1 to $+\infty$, do the solitons in the anti-de Sitter space–time change to solitons in the Minkowski space–time?

In Sec. II, the Yang–Mills–Higgs–Bogomolny equations and their Lax pairs for general ρ are considered. When $\rho=1$ and $\rho\to+\infty$, they become the known equations and their Lax pairs for the Minkowski and anti-de Sitter cases. In Sec. III, the Darboux transformation is discussed. Using the Darboux transformation, we construct solitons in the SU(2) case in Sec. IV and give some examples. When ρ changes from 1 to $+\infty$, the shape of the solitons changes a lot. However, when the coordinates of the space–time depend on ρ suitably, the position of the solitons keeps in a finite region and the solitons in part of the anti-de Sitter space–time change to the solitons in the Minkowski space–time.

II. YANG–MILLS–HIGGS–BOGOMOLNY EQUATIONS AND THEIR LAX PAIRS

Let M be a three dimensional Lorentz manifold with metric $g=(g_{\mu\nu})$. $\{A_\mu \mid \mu=1,2,3\}$ is a gauge potential and Φ is a (scalar) Higgs field, both of which are valued in the Lie algebra of an $N\times N$ matrix Lie group G.

The Yang–Mills–Higgs–Bogomolny equation[1,7] is

$$D\Phi=*F, \tag{2.1}$$

or, written in terms of the components,

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$$D_\mu\Phi=\frac{1}{2\sqrt{|g|}}g_{\mu\nu}\epsilon^{\nu\alpha\beta}F_{\alpha\beta}, \tag{2.2}$$

where the action of the covariant derivative $D_\mu=\partial_\mu+A_\mu$ on Φ is $D_\mu\Phi=\partial_\mu\Phi+[A_\mu,\Phi]$, $\partial_\mu=\partial/\partial x^\mu$. $\{F_{\mu\nu}\}$ is the curvature corresponding to $\{A_\mu\}$, hence $F_{\mu\nu}=[D_\mu,D_\nu]$.

The $2+1$ dimensional anti-de Sitter space–time of constant curvature $-1/\rho^2$ $(\rho>0)$ is the hyperboloid $U^2+V^2-X^2-Y^2=\rho^2$ in $\mathbf{R}^{2,2}$ with the metric

$$ds^2=-dU^2-dV^2+dX^2+dY^2. \tag{2.3}$$

By defining

$$r=\frac{\rho}{U+X}-\rho+1,\quad x=\frac{Y}{U+X},\quad t=-\frac{V}{U+X}, \tag{2.4}$$

a part of the $2+1$ dimensional anti-de Sitter space–time with $U+X>0$ is represented by the Poincaré coordinates (r,x,t) with $r>-\rho+1$ and the metric is

$$ds^2=\frac{\rho^2}{(r+\rho-1)^2}(-dt^2+dr^2+dx^2)=\frac{\rho^2}{(r+\rho-1)^2}(dr^2+du\,dv), \tag{2.5}$$

where $u=x+t$ and $v=x-t$. Clearly, when $\rho\to+\infty$, the metric on this part of the $2+1$ dimensional anti-de Sitter space–time tends to the flat Minkowski metric on the whole $\mathbf{R}^{2,1}$. In order to consider the change of the solitons with respect to ρ, we only need to consider the solutions in this part.

With the metric (2.5) and the orientation (v,u,r), (2.2) becomes

$$D_u\Phi=\frac{r+\rho-1}{\rho}F_{ur},\quad D_v\Phi=-\frac{r+\rho-1}{\rho}F_{vr},\quad D_r\Phi=-\frac{2(r+\rho-1)}{\rho}F_{uv}. \tag{2.6}$$

When $\rho=1$, it is reduced to

$$D_u\Phi=rF_{ur},\quad D_v\Phi=-rF_{vr},\quad D_r\Phi=-2rF_{uv}. \tag{2.7}$$

Reference 4 showed that it had a Lax pair

$$(rD_r+\Phi-2(\zeta-u)D_u)\psi=0,\quad \left(2D_v+\frac{\zeta-u}{r}D_r-\frac{\zeta-u}{r^2}\Phi\right)\psi=0, \tag{2.8}$$

where $D_\mu\psi=\partial_\mu\psi+A_\mu\psi$ and ζ is a complex spectral parameter. That is, (2.7) is the integrability condition of the overdetermined system (2.8).

When $\rho>0$, the Yang–Mills–Higgs–Bogomolny equation (2.6) can be derived from (2.7) by substituting $r\to r+\rho-1$ and $\Phi\to\rho\Phi$. Moreover, since ζ is a constant in (2.8), we can replace ζ by $\rho\zeta$. After the substitution

$$r\to r+\rho-1,\quad \Phi\to\rho\Phi,\quad \zeta\to\rho\zeta, \tag{2.9}$$

(2.8) leads to the Lax pair of (2.6):

$$\begin{gathered}((r+\rho-1)D_r+\rho\Phi-2(\rho\zeta-u)D_u)\psi=0,\\ \left(2D_v+\frac{\rho\zeta-u}{r+\rho-1}D_r-\frac{\rho(\rho\zeta-u)}{(r+\rho-1)^2}\Phi\right)\psi=0.\end{gathered} \tag{2.10}$$

It is easy to check directly that the integrability condition of (2.10) is the Yang–Mills–Higgs–Bogomolny equation (2.6).

When $\rho\to+\infty$, the metric (2.5) becomes the standard Minkowski metric

$$ds^2=-dt^2+dr^2+dx^2=dr^2+du\,dv, \tag{2.11}$$

the Yang–Mills–Higgs–Bogomolny equation (2.6) becomes

$$D_u\Phi=F_{ur},\quad D_v\Phi=-F_{vr},\quad D_r\Phi=-2F_{uv}, \tag{2.12}$$

and the Lax pair (2.10) becomes

$$\begin{aligned}&(D_r+\Phi-2\zeta D_u)\psi=0,\\ &(2D_v+\zeta D_r-\zeta\Phi)\psi=0.\end{aligned} \tag{2.13}$$

Remark 1: If we substitute

$$r\to x,\quad \zeta\to\frac{1}{\lambda},\quad u\to y+t,\quad v\to y-t, \tag{2.14}$$

then (2.13) is changed to

$$(\lambda D_x-D_t-D_y+\lambda\Phi)\psi=0,\quad (\lambda D_t-\lambda D_y-D_x+\Phi)\psi=0, \tag{2.15}$$

which is just the Lax pair given by Ref. 2.

III. DARBOUX TRANSFORMATIONS

For $\rho\to+\infty$ and $\rho=1$, Refs. 5 and 6 gave the construction of the Darboux matrix separately based on a general method.[8] Here we show that these are the two special cases for general ρ.

For $\rho=1$, the Darboux transformation is given as follows.[6] Let $Z=\mathrm{diag}(\zeta_1,...,\zeta_N)$ be a diagonal matrix that satisfies

$$\partial_rZ-\frac{2(Z-u)}{r}(\partial_uZ)=0,\quad \partial_vZ+\frac{Z-u}{2r}(\partial_rZ)=0, \tag{3.1}$$

$H=(h_1,\ldots,h_N)$ where h_j is a solution of (2.8) with $\zeta=\zeta_j$. Then $G=\zeta-HZH^{-1}$ is a Darboux matrix for (2.8). That is, for any solution ψ of the Lax pair (2.8), $\tilde{\psi}=G\psi$ satisfies

$$(r\tilde{D}_r+\tilde{\Phi}-2(\zeta-u)\tilde{D}_u)\tilde{\psi}=0,\quad \left(2\tilde{D}_v+\frac{\zeta-u}{r}\tilde{D}_r-\frac{\zeta-u}{r^2}\tilde{\Phi}\right)\tilde{\psi}=0, \tag{3.2}$$

where $\tilde{D}_\mu=\partial_\mu+\tilde{A}_\mu$ and $\tilde{\Phi},\tilde{A}_\mu$ are other functions in the Lie algebra of G.

When $\rho>1$, a similar conclusion is obtained by the substitution (2.9) and $Z\to\rho Z$. Hence the Darboux matrix is given by

$$G(r,u,v,\zeta)=\zeta-\frac{u}{\rho}-S(r,u,v),\quad S(r,u,v)=H\left(Z-\frac{u}{\rho}\right)H^{-1}, \tag{3.3}$$

where $Z=\mathrm{diag}(\zeta_1,...,\zeta_N)$ satisfies

$$\partial_rZ-\frac{2(\rho Z-u)}{r+\rho-1}\partial_uZ=0,\quad \partial_vZ+\frac{\rho Z-u}{2(r+\rho-1)}\partial_rZ=0, \tag{3.4}$$

$H=(h_1,\ldots,h_N)$ and h_j is a solution of (2.10) with $\zeta=\zeta_j$. It can be checked that S satisfies

$$
\begin{aligned}
&(r+\rho-1)(\partial_r S+[A_r,S])-2\rho(\partial_u S+[A_u,S])S+\rho[\Phi,S]-2S=0,\\
&2(\partial_v S+[A_v,S])+\frac{\rho}{r+\rho-1}(\partial_r S+[A_r,S])S-\frac{\rho^2}{(r+\rho-1)^2}[\Phi,S]S=0.
\end{aligned}
\tag{3.5}
$$

By direct computation, we know that for any solution ψ of (2.10), $\tilde{\psi}=G\psi$ satisfies

$$
\begin{aligned}
&((r+\rho-1)\tilde{D}_r+\rho\tilde{\Phi}-2(\rho\zeta-u)\tilde{D}_u)\tilde{\psi}=0,\\
&\left(2\tilde{D}_v+\frac{\rho\zeta-u}{r+\rho-1}\tilde{D}_r-\frac{\rho(\rho\zeta-u)}{(r+\rho-1)^2}\tilde{\Phi}\right)\tilde{\psi}=0
\end{aligned}
\tag{3.6}
$$

with $\tilde{D}_\mu=\partial_\mu+\tilde{A}_\mu$ $(\mu=u,v,r)$,

$$
\begin{aligned}
&\tilde{A}_u=A_u,\\
&\tilde{A}_v=A_v+\frac{\rho}{2(r+\rho-1)}(\partial_r S+[A_r,S])-\frac{\rho^2}{2(r+\rho-1)^2}[\Phi,S],\\
&\tilde{A}_r=A_r-\frac{1+\rho(\partial_u S+[A_u,S])}{r+\rho-1},\\
&\tilde{\Phi}=\Phi-\frac{1+\rho(\partial_u S+[A_u,S])}{\rho}.
\end{aligned}
\tag{3.7}
$$

Hence G is really a Darboux matrix for (2.10).

According to (3.4), each $\zeta_j(j=1,\ldots,N)$ is a constant or a nonconstant solution of

$$
\partial_r\zeta-\frac{2(\rho\zeta-u)}{r+\rho-1}\partial_u\zeta=0,\quad \partial_v\zeta+\frac{\rho\zeta-u}{2(r+\rho-1)}\partial_r\zeta=0. \tag{3.8}
$$

The general nonconstant solution is given implicitly by

$$
v-\frac{(r+\rho-1)^2}{\rho\zeta-u}=C_1(\zeta,\rho), \tag{3.9}
$$

where C_1 is an arbitrary function, which is meromorphic to ζ and smooth to $\rho\in(0,+\infty)$.

In order to consider the limit for $\rho\to+\infty$, we rewrite (3.9) as

$$
v-\frac{(r+\rho-1)^2}{\rho\zeta-u}+\frac{\rho-1}{\zeta}=C(\zeta,\rho). \tag{3.10}
$$

Here $C(\zeta,\rho)$ is also an arbitrary function, which is holomorphic to ζ and smooth to ρ. Moreover, suppose that $\lim_{\rho\to+\infty}C(\zeta,\rho)$ exists.

When $\rho=1$, (3.10) becomes

$$
v-\frac{r^2}{\zeta-u}=C(\zeta,1), \tag{3.11}
$$

which is given by Ref. 6. When $\rho\to+\infty$, (3.10) becomes

$$
v-\frac{u}{\zeta^2}-\frac{2r}{\zeta}=C(\zeta,+\infty)-\frac{1}{\zeta}. \tag{3.12}
$$

When the group $G=U(N)$, there should be more constraints on ζ_j's and h_j's in the construction of the Darboux matrix. They are

$$\begin{gathered}\zeta_j=\zeta_0 \quad \text{or} \quad \overline{\zeta_0} \text{ for certain fixed } \zeta_0,\\ h_j^* h_k=0 \quad \text{if} \quad \zeta_j\neq\zeta_k,\end{gathered} \tag{3.13}$$

as mentioned in Refs. 5 and 6. If so, after the Darboux transformation, $\tilde{\Phi}\in u(N)$, $\tilde{A}_\mu\in u(N)$ provided that $\Phi\in u(N)$, $A_\mu\in u(N)$.

IV. SOLITON SOLUTIONS IN SU(2) CASE

Single soliton solutions are given by Darboux transformations from the trivial seed solution $\Phi=0$, $A_u=A_v=A_r=0$. In the construction of $S=H(Z-u/\rho)H^{-1}$, $Z=\mathrm{diag}(\zeta_1,\ldots,\zeta_N)$, where ζ_j is a constant or a nonconstant solution of (3.8), h_j is a column solution of (2.10) with $\zeta=\zeta_j$.

With the action of the Darboux matrix $G=\zeta-u/\rho-S$, (3.7) gives

$$\tilde{A}_u=0, \quad \tilde{A}_v=\frac{\rho\partial_r S}{2(r+\rho-1)}, \quad \tilde{A}_r=-\frac{1+\rho\partial_u S}{r+\rho-1}, \quad \tilde{\Phi}=-\frac{1+\rho\partial_u S}{\rho}. \tag{4.1}$$

Here we only consider the case where all ζ_j's are constants. When ζ_j's are nonconstant solutions of (3.8), we can obtain solutions in similar ways. However, in the latter case, solutions may only be defined when t is larger than some constant.[6] Now h_j satisfies

$$\partial_r h_j-\frac{2(\rho\zeta_j-u)}{r+\rho-1}\partial_u h_j=0, \quad \partial_v h_j+\frac{\rho\zeta_j-u}{2(r+\rho-1)}\partial_r h_j=0. \tag{4.2}$$

The general solution is

$$h_j=\omega(\zeta_j), \tag{4.3}$$

where

$$\omega(\zeta)=v-\frac{(r+\rho-1)^2}{\rho\zeta-u}+\frac{\rho-1}{\zeta}. \tag{4.4}$$

When $\rho=1$,

$$\omega(\zeta)=v-\frac{r^2}{\zeta-u}, \tag{4.5}$$

which is the same as the result in Ref. 6. When $\rho\to+\infty$,

$$\omega(\zeta)\to v-\frac{u}{\zeta^2}-\frac{2r}{\zeta}+\frac{1}{\zeta}. \tag{4.6}$$

With the substitution (2.14),

$$\omega(\lambda^{-1})\to(1-\lambda^2)y-(1+\lambda^2)t-2\lambda x+\lambda. \tag{4.7}$$

This coincides with Ref. 5.

When $G=\mathrm{SU}(2)$, the conditions (3.13) should be satisfied. Hence we want $\zeta_1=\zeta_0$, $\zeta_2=\overline{\zeta_0}$ for some $\zeta_0\in\mathbf{C}$ and

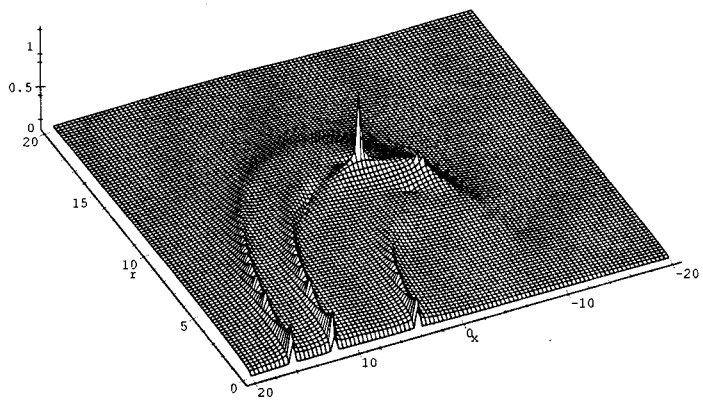

FIG. 1. $\rho=1$.

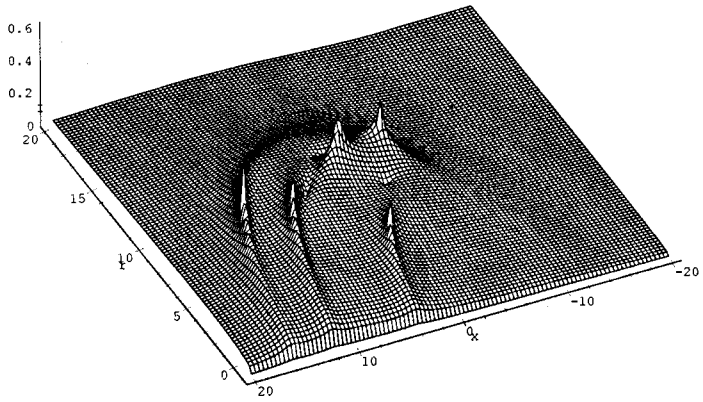

FIG. 2. $\rho=2$.

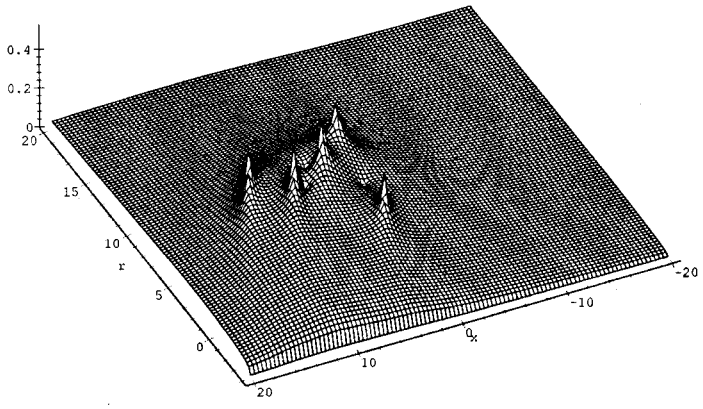

FIG. 3. $\rho=5$.

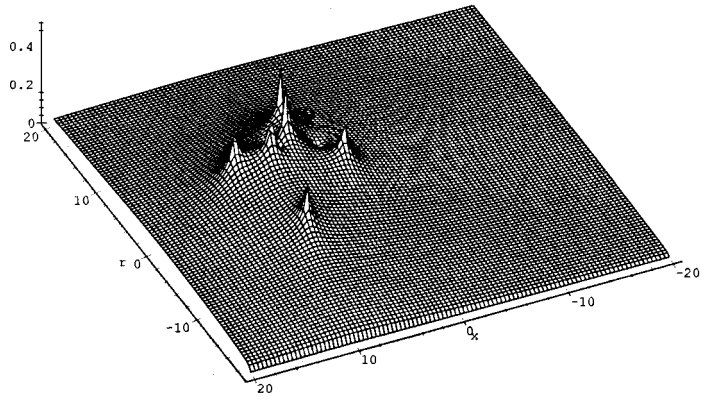

FIG. 4. $\rho=20$.

$$H=\begin{pmatrix} \alpha(\tau) & -\overline{\beta(\tau)} \\ \beta(\tau) & \overline{\alpha(\tau)} \end{pmatrix}, \tag{4.8}$$

where α, β are two holomorphic functions of $\tau=\omega(\zeta_0)$. Let $\sigma(\tau)=\beta(\tau)/\alpha(\tau)$. Then

$$S=\frac{\zeta_0-\overline{\zeta_0}}{1+|\sigma|^2}\begin{pmatrix} 1 & \overline{\sigma} \\ \sigma & |\sigma|^2 \end{pmatrix}+\overline{\zeta_0}-\frac{u}{\rho}, \tag{4.9}$$

$$\tilde{\Phi}=-\partial_u S-\frac{1}{\rho}=\frac{\zeta_0-\overline{\zeta_0}}{(1+|\sigma|^2)^2}\begin{pmatrix} (|\sigma|^2)_u & \overline{\sigma}^2\sigma_u-\overline{\sigma}_u \\ \sigma^2\overline{\sigma}_u-\sigma_u & -(|\sigma|^2)_u \end{pmatrix} \tag{4.10}$$

and

$$-\mathrm{tr}\tilde{\Phi}^2=\frac{8(\mathrm{Im}\,\zeta_0)^2}{(1+|\sigma|^2)^2}|\partial_u\sigma|^2. \tag{4.11}$$

When $\sigma(z)$ is a given meromorphic function of z which is independent of ρ, then by (4.6) and (4.5),

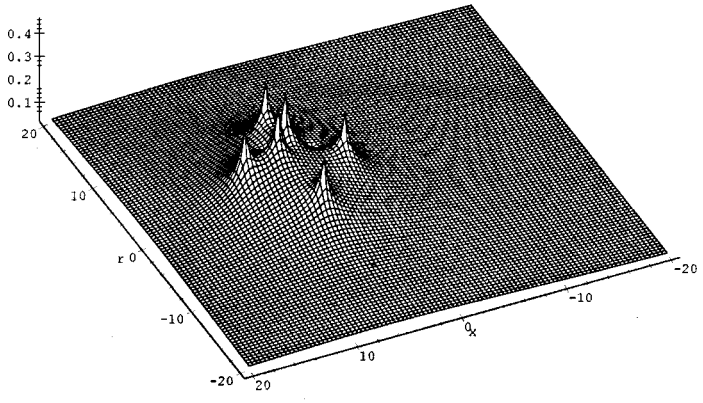

FIG. 5. $\rho=+\infty$.

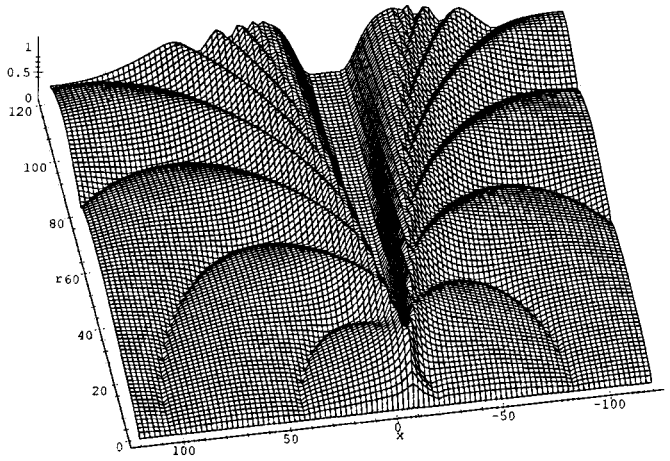

FIG. 6. $\rho=1$.

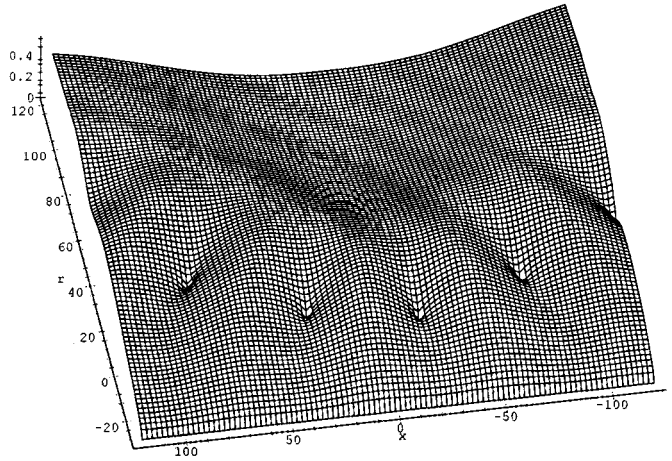

FIG. 7. $\rho=30$.

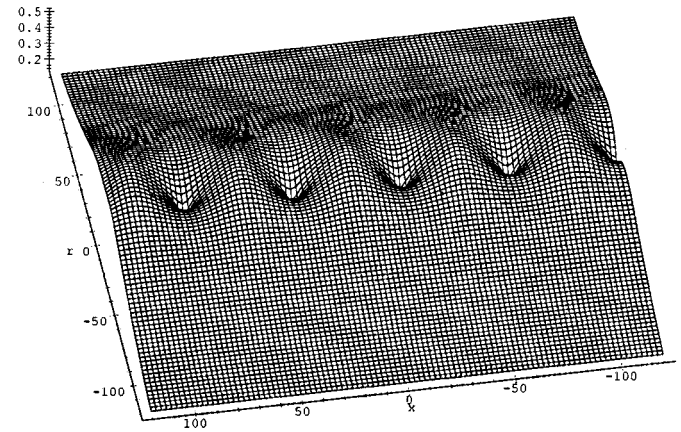

FIG. 8. $\rho=+\infty$.

$$\sigma(\tau)|_{\rho\to+\infty}=\sigma\left(v-\frac{u}{\zeta_0^2}-\frac{2r}{\zeta_0}+\frac{1}{\zeta_0}\right),\quad \sigma(\tau)|_{\rho=1}=\sigma\left(v-\frac{r^2}{\zeta_0-u}\right). \tag{4.12}$$

Hence when $\rho\to+\infty$ and $\rho=1$, the solutions tend to the soliton solutions in the Minkowski and anti-de Sitter space–time, respectively.

These are single soliton solutions. Each solution depends on a complex constant ζ_0 and a meromorphic function σ. Multi-soliton solutions can be constructed by successive Darboux transformations.[5,6] For simplicity, here we only consider the change of single soliton solutions with respect to ρ.

Example 1: $\sigma(\tau)$ is a polynomial of τ without multiple zero. In this case, the solutions are always localized. When $\rho=1$, the behavior of the asymptotic solution as $t\to\infty$ varies according to the roots of $\sigma(\tau)$.[6] Suppose τ_0 is a root of $\sigma(\tau)$. Then (1) if $|\mathrm{Im}\,\tau_0|\ll 1$, it corresponds to a ridge in the graph of $-\mathrm{tr}\tilde{\Phi}^2$; (2) if $\mathrm{Im}\,\tau_0\gg 1$, it corresponds to a peak; (3) if $\mathrm{Im}\,\tau_0\ll -1$, it corresponds to nothing. However, when $\rho\to+\infty$, each root of $\sigma(\tau)$ corresponds to a peak.[5] Figures 1–5 show the change of the solution with respect to ρ for fixed $t=10$, where $\zeta_0=2i$,

$$\sigma(\tau)=(\tau-2)(\tau-6)(\tau+6)(\tau-2i)(\tau-6i)(\tau+6i). \tag{4.13}$$

In these figures the vertical axis is $(-\mathrm{tr}\tilde{\Phi}^2)^{1/16}$.

Example 2: $\sigma(\tau)=\sin(\tau/20)$. For both finite and infinite ρ, the solution is always nonlocalized. For finite ρ, it behaves in a very complicated manner. However, for infinite ρ, (4.12) shows that the solution is invariant if (x,r) is changed to (x',r') with $\mathrm{Re}[(1-\zeta_0^{-2})(x'-x)-2\zeta_0^{-1}(r'-r)]=40\pi k$ (k is an arbitrary integer). Hence the solution is periodic in one direction. Figures 6–8 show this solution for $\rho=1,30,+\infty$ with $t=10$, $\zeta_0=2i$. In these figures the vertical axis is $(-\mathrm{tr}\tilde{\Phi}^2)^{1/8}$.

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The classification of plane symmetric spacetimes by isometries

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A complete classification of plane symmetric Lorentzian manifolds according to their additional isometries and metrics (or classes of metrics) is obtained by solving the Killing equations. We obtain all metrics (or classes of metrics), that admit the group of motions G_r (where $r=3,4,5,6,7$ and 10) containing $SO(2)\circledS\mathbb{R}^2$, the minimal symmetry inherited by the plane symmetric manifolds. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1385175]

A plane symmetric spacetime is a Lorentzian manifold possessing a physical stress–energy tensor and admitting $SO(2)\circledS\mathbb{R}^2$, which we shall henceforth denote by G_3, as the minimal isometry group in such a way that the group orbits are spacelike surfaces of constant curvature. The symmetry assumptions reduce the general metric of a Lorentzian manifold to the form[1]

$$ds^2=e^{2\nu(t,x)}\,dt^2-e^{2\lambda(t,x)}\,dx^2-e^{2\mu(t,x)}(dy^2+dz^2). \tag{1}$$

Our aim is to further classify this metric according to the additional isometries it admits. This can be achieved by following the methods developed in Ref. 2 with the modification introduced in Ref. 3. The procedure is to solve the Killing equations (KEs),

$$g_{ab,c}k^c+g_{ac}k^c_{,b}+g_{bc}k^c_{,a}=0 \quad (a,b,c,\ldots=0,1,2,3), \tag{2}$$

where "$_{,a}$" denotes partial derivatives with respect to the variables $x^a=(x^0=t,x^1=x,x^2=y,x^3=z)$. The metric coefficients, g_{ab}, are as given in Eq. (1) and the Killing vector (KV) field, $\mathbf{K}=k^a\partial/\partial x^a$, is arbitrary. This amounts to solving a system of 10 quasi-linear partial differential equations in seven unknown functions: the four functions of four variables, $k^a(a=0,1,2,3)$; and the three functions of two variables $\nu(t,x),\lambda(t,x)$ and $\mu(t,x)$.

For the metric (1), Eqs. (2) can be integrated to give $\mathbf{K}$ in terms of y and z explicitly. The expressions k^a depend upon three arbitrary constants, corresponding to the minimal isometries inherent in (1), and five arbitrary functions of integration depending upon t and x apart from the three functions $\nu(t,x),\lambda(t,x)$ and $\mu(t,x)$. A complete solution of these equations is given, providing all possible metrics admitting higher symmetries than the minimal G_3, along with the generators of KVs, $\mathbf{K}$.

It turns out that all metrics with $\dot{\mu}=0\neq\mu'$ admitting higher than the minimal symmetry group are plane symmetric metrics given (below) by the Eqs. (3), (5), (13), (17), (20), (22). All these metrics, except the metric given by Eq. (17), admit a timelike KV, $\partial/\partial t$.[4,5] The metrics with $\dot{\mu}\neq0=\mu'$ admitting higher (than the minimal) symmetry groups are given by Eqs. (4), (6), (14), (18), (21), (23). These metrics except the metric given by the Eq. (18) admit a spacelike KV, $\partial/\partial x$. The metrics with $\dot{\mu}=0=\mu'$, admitting higher symmetries are all Bertotti–Robinson type metrics given by Eqs. (7), (8), (9), (10), (11), (12).[4,5] The metrics with $\dot{\mu}\neq0\neq\mu'$ admitting higher symmetries are given by Eqs. (15), (16), (19), (24).

A complete list of metrics along with their KVs, corresponding Lie algebras and symmetry groups are provided here for the sake of completeness. All metrics other than those given below,

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admit only the symmetry group G_3. For example the plane-fronted gravitational waves solution is one of these infinitely many metrics admitting only the minimal symmetry.

The plane symmetric Lorentzian manifolds admitting G_{10} as the maximal isometry group, other than the Minkowski metric, are: (Ia) the anti-deSitter spacetime,

$$ds^2=e^{2x/a}(dt^2-dy^2-dz^2)-dx^2 \quad (a=\text{const}\neq 0), \tag{3}$$

with generators of the Lie algebra admitted by the metric (3),

$$X_0=\partial/\partial t, \quad X_1=\partial/\partial y, \quad X_2=\partial/\partial z, \quad X_3=z\partial/\partial y-y\partial/\partial z,$$

$$X_4=tz\partial/\partial t-az\partial/\partial x+yz\partial/\partial y+\tfrac{1}{2}(z^2-y^2+t^2-a^2e^{-2x/a})\partial/\partial z,$$

$$X_5=-ty\partial/\partial t+ay\partial/\partial x+\tfrac{1}{2}(z^2-y^2-t^2+a^2e^{-2x/a})\partial/\partial y-yz\partial/\partial z,$$

$$X_6=z\partial/\partial t+t\partial/\partial z, \quad X_7=y\partial/\partial t+t\partial/\partial y,$$

$$X_8=-\frac{1}{2a}(z^2+y^2+t^2+a^2e^{-2x/a})\partial/\partial t+t\partial/\partial x-\frac{ty}{a}\partial/\partial y-\frac{tz}{a}\partial/\partial z,$$

$$X_9=-\frac{t}{a}\partial/\partial t+\partial/\partial x-\frac{y}{a}\partial/\partial y-\frac{z}{a}\partial/\partial z,$$

satisfying the $SO(2,3)$ Lie algebra

$$[X_0,X_4]=X_6, \quad [X_0,X_5]=-X_7, \quad [X_0,X_6]=X_2, \quad [X_0,X_7]=X_1,$$

$$[X_0,X_8]=X_9, \quad [X_0,X_9]=-\frac{1}{a}X_0, \quad [X_1,X_3]=-X_2, \quad [X_1,X_4]=X_3,$$

$$[X_1,X_5]=aX_9, \quad [X_1,X_7]=X_0, \quad [X_1,X_8]=-\frac{1}{a}X_7, \quad [X_1,X_9]=-\frac{1}{a}X_1,$$

$$[X_2,X_3]=X_1, \quad [X_2,X_4]=-aX_9, \quad [X_2,X_5]=X_3, \quad [X_2,X_6]=X_0,$$

$$[X_2,X_8]=-\frac{1}{a}X_6, \quad [X_2,X_9]=-\frac{1}{a}X_2, \quad [X_3,X_4]=X_5, \quad [X_3,X_5]=-X_4,$$

$$[X_3,X_6]=-X_7, \quad [X_3,X_7]=X_6, \quad [X_4,X_6]=aX_8, \quad [X_4,X_9]=\frac{1}{a}X_4,$$

$$[X_5,X_7]=-aX_8, \quad [X_5,X_9]=\frac{1}{a}X_5, \quad [X_6,X_7]=X_3, \quad [X_6,X_8]=-\frac{1}{a}X_4,$$

$$[X_7,X_8]=\frac{1}{a}X_5, \quad [X_8,X_9]=\frac{1}{a}X_8, \quad [X_i,X_k]=0 \quad (\text{otherwise});$$

and (Ib) the deSitter spacetime,

$$ds^2=dt^2-e^{2t/a}(dx^2+dy^2+dz^2) \quad (a\neq 0), \tag{4}$$

with the generators

$$X_0=\partial/\partial x,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\partial/\partial y-y\partial/\partial z,$$

$$X_4=-az\partial/\partial t+xz\partial/\partial x+yz\partial/\partial y+\tfrac{1}{2}(z^2-y^2-x^2+a^2e^{-2t/a})\partial/\partial z,$$

$$X_5=ay\partial/\partial t-xy\partial/\partial x+\tfrac{1}{2}(z^2-y^2+x^2-a^2e^{-2t/a})\partial/\partial y-yz\partial/\partial z,$$

$$X_6=-z\partial/\partial x+x\partial/\partial z,\quad X_7=-y\partial/\partial x+x\partial/\partial y,$$

$$X_8=x\partial/\partial t+\frac{1}{2a}(z^2+y^2-x^2-a^2e^{-2t/a})\partial/\partial x-\frac{xy}{a}\partial/\partial y-\frac{xz}{a}\partial/\partial z,$$

$$X_9=\partial/\partial t-\frac{x}{a}\partial/\partial x-\frac{y}{a}\partial/\partial y-\frac{z}{a}\partial/\partial z,$$

satisfying the $SO(1,4)$ Lie algebra

$$[X_0,X_4]=-X_6,\quad [X_0,X_5]=X_7,\quad [X_0,X_6]=X_2,\quad [X_0,X_7]=X_1,$$

$$[X_0,X_8]=X_9,\quad [X_0,X_9]=-\frac{1}{a}X_0,\quad [X_1,X_3]=-X_2,\quad [X_1,X_4]=X_3,$$

$$[X_1,X_5]=aX_9,\quad [X_1,X_7]=-X_0,\quad [X_1,X_8]=-\frac{1}{a}X_7,\quad [X_1,X_9]=-\frac{1}{a}X_0,$$

$$[X_2,X_3]=X_1,\quad [X_2,X_4]=-aX_9,\quad [X_2,X_5]=X_3,\quad [X_2,X_6]=-X_0,$$

$$[X_2,X_8]=-\frac{1}{a}X_6,\quad [X_2,X_9]=-\frac{1}{a}X_2,\quad [X_3,X_4]=X_5,\quad [X_3,X_5]=-X_4,$$

$$[X_3,X_6]=-X_7,\quad [X_3,X_7]=X_6,\quad [X_4,X_6]=aX_8,\quad [X_4,X_9]=aX_4,$$

$$[X_5,X_7]=-aX_8,\quad [X_5,X_9]=\frac{1}{a}X_5,\quad [X_6,X_7]=-X_3,\quad [X_6,X_8]=\frac{1}{a}X_4,$$

$$[X_7,X_8]=-\frac{1}{a}X_5,\quad [X_8,X_9]=\frac{1}{a}X_8,\quad [X_i,X_k]=0\quad \text{(otherwise)}.$$

Both the metrics given by Eqs. (3) and (4) are Einstein spaces ($R_{ab}\propto g_{ab}$) with constant curvature.[2]

There do not exist Lorentzian metrics admitting G_9 and G_8 as the maximal isometry groups.[6,7]

The metrics admitting G_7 as the maximal group of motions are: (IIa) the anti-Einstein metric,

$$ds^2=dt^2-dx^2-e^{2x/a}(dy^2+dz^2)\quad (a\neq 0), \tag{5}$$

$$X_0=\partial/\partial t,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\partial/\partial y-y\partial/\partial z,$$

$$X_4=ay\partial/\partial x+\tfrac{1}{2}(z^2-y^2+a^2e^{-2x/a})\partial/\partial y-yz\partial/\partial z,$$

$$X_5=-az\partial/\partial x+yz\partial/\partial y+\tfrac{1}{2}(z^2-y^2-a^2e^{-2x/a})\partial/\partial z,$$

$$X_6=a\partial/\partial x-y\partial/\partial y-z\partial/\partial z,$$

$$[X_1,X_3]=-X_2,\quad [X_1,X_4]=X_6,\quad [X_1,X_5]=X_3,\quad [X_1,X_6]=-X_1,$$

$$[X_2,X_3]=X_1,\quad [X_2,X_4]=X_3,\quad [X_2,X_5]=-X_6,\quad [X_2,X_6]=-X_2,$$

$$[X_3,X_4]=-X_5,\quad [X_3,X_5]=X_4,\quad [X_4,X_6]=X_4,\quad [X_5,X_6]=X_5,$$

$$[X_i,X_k]=0\quad \text{(otherwise)},$$

with symmetry structure $SO(1,3)\otimes\mathbb{R}$; (IIb) the metric,

$$ds^2=dt^2-dx^2-e^{2t/a}(dy^2+dz^2)\quad (a\neq 0), \tag{6}$$

$$X_0=\partial/\partial x,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\partial/\partial y-y\partial/\partial z,$$

$$X_4=ay\partial/\partial t+\tfrac{1}{2}(z^2-y^2-a^2e^{-2t/a})\partial/\partial y-yz\partial/\partial z,$$

$$X_5=-az\partial/\partial t+yz\partial/\partial y+\tfrac{1}{2}(z^2-y^2+a^2e^{-2t/a})\partial/\partial z,$$

$$X_6=\partial/\partial t-\frac{y}{a}\partial/\partial y-\frac{z}{a}\partial/\partial z,$$

with the same Lie algebra.

The metrics admitting G_6 as the maximal isometry group are: (IIIa),

$$ds^2=\cosh^2\frac{x}{a}dt^2-dx^2-dy^2-dz^2\quad (a\neq 0), \tag{7}$$

$$X_0=\partial/\partial t,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\partial/\partial y-y\partial/\partial z,$$

$$X_4=-\tanh\frac{x}{a}\sin\frac{t}{a}\partial/\partial t+\cos\frac{t}{a}\partial/\partial x,$$

$$X_5=\tanh\frac{x}{a}\cos\frac{t}{a}\partial/\partial t+\sin\frac{t}{a}\partial/\partial x,$$

$$[X_0,X_4]=-\frac{1}{a}X_5,\quad [X_0,X_5]=\frac{1}{a}X_4,\quad [X_1,X_3]=-X_2,\quad [X_2,X_3]=X_1,$$

$$[X_4,X_5]=\frac{1}{a}X_0,\quad [X_i,X_k]=0\quad \text{(otherwise)},$$

and isometry group $G_3\otimes SO(1,2)$; (IIIb),

$$ds^2=\cos^2\frac{x}{a}dt^2-dx^2-dy^2-dz^2\quad (a\neq 0), \tag{8}$$

$$X_0=\partial/\partial t,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\partial/\partial y-y\partial/\partial z,$$

$$X_4=\tan\frac{x}{a}\sinh\frac{t}{a}\partial/\partial t+\cosh\frac{t}{a}\partial/\partial x,$$

$$X_5=\tan\frac{x}{a}\cosh\frac{t}{a}\,\partial/\partial t+\sinh\frac{t}{a}\,\partial/\partial x,$$

$$[X_0,X_4]=\frac{1}{a}X_5,\quad [X_0,X_5]=\frac{1}{a}X_4,\quad [X_1,X_3]=-X_2,\quad [X_2,X_3]=X_1,$$

$$[X_4,X_5]=\frac{1}{a}X_0,\quad [X_i,X_k]=0\quad \text{(otherwise)},$$

with isometry group $G_3\otimes SO(2,1)$; (IIIc),

$$ds^2=e^{2x/a}\,dt^2-dx^2-dy^2-dz^2\quad (a\neq 0), \tag{9}$$

$$X_0=\partial/\partial t,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\,\partial/\partial y-y\,\partial/\partial z,$$

$$X_4=-\frac{1}{2a}(t^2+a^2e^{-2x/a})\,\partial/\partial t+t\,\partial/\partial x,\quad X_5=-\frac{t}{a}\,\partial/\partial t+\partial/\partial x,$$

$$[X_0,X_4]=X_5,\quad [X_0,X_5]=-\frac{1}{a}X_0,\quad [X_1,X_3]=-X_2,\quad [X_2,X_3]=X_1,$$

$$[X_4,X_5]=\frac{1}{a}X_4,\quad [X_i,X_k]=0\quad \text{(otherwise)},$$

isometry group $G_3\otimes SO(1,2)$; (IIId),

$$ds^2=dt^2-\cosh^2\frac{t}{a}dx^2-dy^2-dz^2\quad (a\neq 0), \tag{10}$$

$$X_0=\partial/\partial x,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\,\partial/\partial y-y\,\partial/\partial z,$$

$$X_4=\cos\frac{x}{a}\,\partial/\partial t-\tanh\frac{t}{a}\sin\frac{x}{a}\,\partial/\partial x,$$

$$X_5=\sin\frac{x}{a}\,\partial/\partial t+\tanh\frac{t}{a}\cos\frac{x}{a}\,\partial/\partial x,$$

$$[X_0,X_4]=-\frac{1}{a}X_5,\quad [X_0,X_5]=\frac{1}{a}X_4,\quad [X_1,X_3]=-X_2,\quad [X_2,X_3]=X_1,$$

$$[X_4,X_5]=\frac{1}{a}X_0,\quad [X_i,X_k]=0\quad \text{(otherwise)},$$

isometry group $G_3\otimes SO(1,2)$; (IIIe),

$$ds^2=dt^2-\cos^2\frac{t}{a}dx^2-dy^2-dz^2\quad (a\neq 0), \tag{11}$$

$$X_0=\partial/\partial x,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\,\partial/\partial y-y\,\partial/\partial z,$$

$$X_4=\cosh\frac{x}{a}\,\partial/\partial t+\tan\frac{t}{a}\sinh\frac{x}{a}\,\partial/\partial x,$$

$$X_5=\sinh\frac{x}{a}\,\partial/\partial t+\tan\frac{t}{a}\cosh\frac{x}{a}\,\partial/\partial x,$$

with a Lie algebra identical to that of the metric (8) and the isometry group is $G_3\otimes SO(2,1)$; (IIIf),

$$ds^2=dt^2-e^{2t/a}\,dx^2-dy^2-dz^2 \quad (a\neq 0), \tag{12}$$

$$X_0=\partial/\partial x, \quad X_1=\partial/\partial y, \quad X_2=\partial/\partial z, \quad X_3=z\,\partial/\partial y-y\,\partial/\partial z,$$

$$X_4=x\,\partial/\partial t-\frac{1}{2a}(x^2+a^2e^{-2t/a})\,\partial/\partial x, \quad X_5=\partial/\partial t-\frac{x}{a}\,\partial/\partial x,$$

$$[X_0,X_4]=X_5, \quad [X_0,X_5]=-\frac{1}{a}X_0, \quad [X_1,X_3]=-X_2, \quad [X_2,X_3]=X_1,$$

$$[X_4,X_5]=\frac{1}{a}X_4, \quad [X_i,X_k]=0 \quad \text{(otherwise)},$$

isometry group $G_3\otimes SO(1,2)$; (IIIg),

$$ds^2=e^{2\nu(x)}(dt^2-dy^2-dz^2)-dx^2, \tag{13}$$

$$X_0=\partial/\partial t, \quad X_1=\partial/\partial y, \quad X_2=\partial/\partial z, \quad X_3=z\,\partial/\partial y-y\,\partial/\partial z,$$

$$X_4=z\,\partial/\partial t+t\,\partial/\partial z, \quad X_5=y\,\partial/\partial t+t\,\partial/\partial y,$$

$$[X_0,X_4]=X_0, \quad [X_0,X_5]=X_1, \quad [X_2,X_3]=X_1, \quad [X_1,X_3]=-X_2,$$

$$[X_3,X_4]=-X_5, \quad [X_1,X_5]=X_0, \quad [X_2,X_4]=X_0, \quad [X_4,X_5]=X_3,$$

$$[X_i,X_k]=0 \quad \text{(otherwise)};$$

(IIIh),

$$ds^2=dt^2-e^{2\lambda(t)}(dx^2+dy^2+dz^2), \tag{14}$$

$$X_0=\partial/\partial x, \quad X_1=\partial/\partial y, \quad X_2=\partial/\partial z, \quad X_3=z\,\partial/\partial y-y\,\partial/\partial z,$$

$$X_4=-z\,\partial/\partial x+x\,\partial/\partial z, \quad X_5=-y\,\partial/\partial x+x\,\partial/\partial y,$$

$$[X_0,X_4]=X_2, \quad [X_0,X_5]=X_1, \quad [X_1,X_3]=-X_2, \quad [X_1,X_5]=-X_0,$$

$$[X_2,X_3]=X_1, \quad [X_2,X_4]=-X_0, \quad [X_3,X_4]=-X_5, \quad [X_3,X_5]=X_4,$$

$$[X_i,X_k]=0 \quad \text{(otherwise)};$$

(IIIi),

$$ds^2=e^{2f(x)}[dt^2-e^{2t/a}(dy^2+dz^2)]-dx^2 \quad (a\neq 0), \tag{15}$$

$$X_0=-a\,\partial/\partial t+y\,\partial/\partial y+z\,\partial/\partial z, \quad X_1=\partial/\partial y, \quad X_2=\partial/\partial z, \quad X_3=z\,\partial/\partial y-y\,\partial/\partial z,$$

$$X_4=-az\,\partial/\partial t+yz\,\partial/\partial y+\tfrac{1}{2}(z^2-y^2+a^2e^{-2t/a})\,\partial/\partial z,$$

$$X_5=ay\,\partial/\partial t+\tfrac{1}{2}(z^2-y^2-a^2e^{-2t/a})\,\partial/\partial y-yz\,\partial/\partial z,$$

$$[X_0,X_1]=-X_1,\quad [X_0,X_2]=-X_2,\quad [X_0,X_4]=X_4,\quad [X_0,X_5]=X_5,$$

$$[X_1,X_3]=-X_2,\quad [X_1,X_4]=X_3,\quad [X_1,X_5]=-X_0,\quad [X_2,X_3]=X_1,$$

$$[X_2,X_4]=X_0,\quad [X_2,X_5]=X_3,\quad [X_3,X_4]=X_5,\quad [X_3,X_5]=-X_4,$$

$$[X_i,X_k]=0\quad \text{(otherwise)};$$

(IIIj),

$$ds^2=dt^2-e^{2f(t)}[dx^2+e^{2x/a}(dy^2+dz^2)]\quad (a\neq 0), \tag{16}$$

$$X_0=-a\partial/\partial x+y\partial/\partial y+z\partial/\partial z,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\partial/\partial y-y\partial/\partial z,$$

$$X_4=-az\partial/\partial x+yz\partial/\partial y+\tfrac{1}{2}(z^2-y^2-a^2e^{-2x/a})\partial/\partial z,$$

$$X_5=ay\partial/\partial x+\tfrac{1}{2}(z^2-y^2+a^2e^{-2x/a})\partial/\partial y-yz\partial/\partial z,$$

with a Lie algebra identical to that of the metric (15); (IIIk),

$$ds^2=e^{2\nu(t+x)}\,dt^2-e^{2\lambda(t+x)}\,dx^2-e^{2x/a}(dy^2+dz^2)\quad (a\neq 0), \tag{17}$$

subject to the constraint

$$e^{2(\lambda-x/a)}=e^{2(\nu-x/a)}-\left(\frac{2}{a}\right)\int e^{2(\nu-x/a)}dt,$$

$$X_0=\partial/\partial t-\partial/\partial x+\frac{y}{a}\partial/\partial y+\frac{z}{a}\partial/\partial z,\quad X_1=\partial/\partial y,$$

$$X_2=\partial/\partial z,\quad X_3=z\partial/\partial y-y\partial/\partial z,$$

$$X_4=-y\partial/\partial t+y\partial/\partial x+\left[\frac{1}{2a}(z^2-y^2)+\frac{a}{2}e^{2(\lambda-x/a)}-\frac{a}{2}e^{2(\nu-x/a)}\right]\partial/\partial y-\frac{yz}{a}\partial/\partial z,$$

$$X_5=z\partial/\partial t-z\partial/\partial x+\frac{yz}{a}\partial/\partial y+\left[\frac{1}{2a}(z^2-y^2)-\frac{a}{2}e^{2(\lambda-x/a)}+\frac{a}{2}e^{2(\nu-x/a)}\right]\partial/\partial z,$$

$$[X_0,X_1]=-\frac{1}{a}X_1,\quad [X_0,X_2]=-\frac{1}{a}X_2,\quad [X_0,X_4]=\frac{1}{a}X_4,\quad [X_0,X_5]=\frac{1}{a}X_5,$$

$$[X_1,X_3]=-X_2,\quad [X_1,X_4]=-X_0,\quad [X_1,X_5]=\frac{1}{a}X_3,\quad [X_2,X_3]=X_1,$$

$$[X_2,X_4]=\frac{1}{a}X_3,\quad [X_2,X_5]=X_0,\quad [X_3,X_4]=X_4,\quad [X_3,X_5]=-X_5,$$

$$[X_i,X_j]=0\quad \text{(otherwise)};$$

(IIIl),

$$ds^2=e^{2\nu(t+x)}\,dt^2-e^{2\lambda(t+x)}\,dx^2-e^{-2t/a}(dy^2+dz^2)\quad (a\neq 0), \tag{18}$$

subject to the constraint

$$e^{2(\lambda+t/a)}=e^{2(\nu+t/a)}-\left(\frac{2}{a}\right)\int e^{2(\nu+t/a)}dt,$$

$$X_0=\partial/\partial t-\partial/\partial x+\frac{y}{a}\partial/\partial y+\frac{z}{a}\partial/\partial z,\quad X_1=\partial/\partial y,$$

$$X_2=\partial/\partial z,\quad X_3=z\partial/\partial y-y\partial/\partial z,$$

$$X_4=-y\partial/\partial t+y\partial/\partial x+\left[\frac{1}{2a}(z^2-y^2)+\frac{a}{2}e^{2(\lambda+t/a)}-\frac{a}{2}e^{2(\nu+t/a)}\right]\partial/\partial y-\frac{yz}{a}\partial/\partial z,$$

$$X_5=z\partial/\partial t-z\partial/\partial x+\frac{yz}{a}\partial/\partial y+\left[\frac{1}{2a}(z^2-y^2)-\frac{a}{2}e^{2(\lambda+t/a)}+\frac{a}{2}e^{2(\nu+t/a)}\right]\partial/\partial z,$$

and a Lie algebra identical to that of the metric (17); (IIIm),

$$ds^2=e^{2\nu(t+x)}dt^2-e^{2\lambda(t+x)}dx^2-e^{-[(t-x)/a]}(dy^2+dz^2)\quad(a\neq 0),\tag{19}$$

subject to the constraint

$$e^{2[\lambda+(t-x)/2a]}=e^{2[\nu+(t-x)/2a]}-\left(\frac{2}{a}\right)\int e^{2[\nu+(t-x)/2a]}dt,$$

$$X_0=\partial/\partial t-\partial/\partial x+\frac{y}{a}\partial/\partial y+\frac{z}{a}\partial/\partial z,\quad X_1=\partial/\partial y,$$

$$X_2=\partial/\partial z,\quad X_3=z\partial/\partial y-y\partial/\partial z,$$

$$X_4=-y\partial/\partial t+y\partial/\partial x+\left[\frac{1}{2a}(z^2-y^2)-\frac{a}{2}e^{2[\nu+(t-x)/2a]}+\frac{a}{2}e^{2[\lambda+(t-x)/2a]}\right]\partial/\partial y-\frac{yz}{a}\partial/\partial z,$$

$$X_5=z\partial/\partial t-z\partial/\partial x+\frac{yz}{a}\partial/\partial y+\left[\frac{1}{2a}(z^2-y^2)+\frac{a}{2}e^{2[\nu+(t-x)/2a]}-\frac{a}{2}e^{2[\lambda+(t-x)/2a]}\right]\partial/\partial z,$$

with a Lie algebra identical to that of the metric (17).

The metrics admitting G_5 as the maximal isometry group are: (IVa),

$$ds^2=e^{2x/a}dt^2-dx^2-e^{2x/b}(dy^2+dz^2)\quad(a\neq 0\neq b\neq a),\tag{20}$$

$$X_0=\partial/\partial t,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\partial/\partial y-y\partial/\partial z,$$

$$X_4=-\frac{t}{a}\partial/\partial t+\partial/\partial x-\frac{y}{b}\partial/\partial y-\frac{z}{b}\partial/\partial z,$$

$$[X_0,X_4]=-\frac{1}{a}X_0,\quad [X_1,X_3]=-X_2,\quad [X_1,X_4]=-\frac{1}{b}X_1,\ [X_2,X_3]=X_1,$$

$$[X_2,X_4]=-\frac{1}{b}X_2,\quad [X_i,X_k]=0\quad(\text{otherwise}),$$

and isometry group $G_3\otimes\mathbb{R}^2$; and (IVb),

$$ds^2=dt^2-e^{2t/a}\,dx^2-e^{2t/b}(dy^2+dz^2)\quad (a\neq 0\neq b\neq a), \tag{21}$$

$$X_0=\partial/\partial x,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\,\partial/\partial y-y\,\partial/\partial z,$$

$$X_4=\partial/\partial t-\frac{x}{a}\,\partial/\partial x-\frac{y}{b}\,\partial/\partial y-\frac{z}{b}\,\partial/\partial z,$$

with a Lie algebra identical to that of the metric (20).

The metrics admitting G_4 as the maximal isometry group are: (Va),

$$ds^2=e^{2\nu(x)}\,dt^2-dx^2-e^{2\mu(x)}(dy^2+dz^2), \tag{22}$$

$$X_0=\partial/\partial t,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\,\partial/\partial y-y\,\partial/\partial z,$$

$$[X_1,X_3]=-X_2,\quad [X_2,X_3]=X_1,\quad [X_i,X_k]=0\quad (\text{otherwise}),$$

admitting $G_3\otimes\mathbb{R}$ with a timelike $\mathbb{R}$; (Vb),

$$ds^2=dt^2-e^{2\lambda(t)}\,dx^2-e^{2\mu(t)}(dy^2+dz^2), \tag{23}$$

$$X_0=\partial/\partial x,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\,\partial/\partial y-y\,\partial/\partial z,$$

with the same Lie algebra and a spacelike $\mathbb{R}$; (Vc),

$$ds^2=dt^2-dx^2-e^{2\mu(t\pm x)}(dy^2+dz^2), \tag{24}$$

$$X_0=\partial/\partial t\pm\partial/\partial x,\quad X_1=\partial/\partial y,\quad X_2=\partial/\partial z,\quad X_3=z\,\partial/\partial y-y\,\partial/\partial z,$$

with the same Lie algebra and a null $\mathbb{R}$.

This completes the classification of plane symmetric Lorentzian manifolds according to their isometries and metrics.

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On the gravitomagnetic effects in cylindrically symmetric space–times

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Using gyroscopes we generalize results, obtained for the gravitomagnetic clock effect in the particular case when the exterior space–time is produced by a rotating dust cylinder, to the case when the vacuum space–time is described by the general cylindrically symmetric Lewis space–time. Results are contrasted with those obtained for the Kerr space–time. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Recently Bonnor and Steadman[1] calculated and analyzed the gravitomagnetic clock effect, which is the difference in periods of a test particle moving in prograde and retrogade circular geodesic orbits around the axis of a rotating body. They applied their results to a cylindrically symmetric system produced by van Stockum metric[2] describing a rotating dust cylinder. The exterior space–time, containing two parameters, is a particular case of the general vacuum stationary cylindrically symmetric Lewis metric[2–4] containing four parameters. We extend some of their results to the general Lewis space–time by using the results obtained by us[5] for the gyroscope precession in cylindrically symmetric space–times. The clock effect and the gyroscope precession amount to similar physical processes. However, as it will be seen, using gyroscopes allows for a wider class of possible ''gedanken'' experiments. Indeed, we have to face two different effects: one is the influence of the rotation of the source on the gravitational field where the gyroscope is placed (the gravitomagnetic effect), which of course is absent in Newtonian theory; the other is related to the fact that the frame of the gyroscope may be rotating, producing a precession in the gyroscope (Thomas-like precession).

II. PRECESSION OF A GYROSCOPE MOVING IN A CIRCLE AROUND THE AXIS OF SYMMETRY

The Lewis metric can be written as

$$ds^2 = -f dt^2 + 2k dt d\phi + e^{\mu}(dr^2 + dz^2) + l d\phi^2, \tag{1}$$

where

$$f = a r^{1-n} - \frac{c^2 r^{1+n}}{n^2 a}, \tag{2}$$

$$k = -Af, \tag{3}$$

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$$l=\frac{r^2}{f}-A^2 f, \tag{4}$$

$$e^{\mu}=r^{(n^2-1)/2}, \tag{5}$$

with

$$A=\frac{cr^{1+n}}{naf}+b. \tag{6}$$

The parameters n, a, b, and c can be either real or complex, and the corresponding solutions belong to the Weyl or Lewis class, respectively. Here we restrict our study to the Weyl class (not to confound with Weyl metrics representing static and axially symmetric space–times).

The parameters n and a are proportional to the Newtonian energy per unit length and the topological defect, respectively, while b and c describe the stationarity of the source and are proportional to the angular momentum of the source producing a topological defect and the vorticity of the source, respectively.

Now it is important to stress that the transformations[6]

$$d\tau=\sqrt{a}(dt+bd\phi), \tag{7}$$

$$d\overline{\phi}=\frac{1}{n}[-cdt+(n-bc)d\phi] \tag{8}$$

cast the Weyl class of the Lewis metric into the Levi-Civita cylindrical metric (static). However, the transformations in (7) and (8) are not valid globally, and therefore both metrics are equivalent only locally, a fact that can be verified by calculating the corresponding Cartan scalars.[7] In order to globally transform the Weyl class of the Lewis metric into the static Levi-Civita metric, we have to make $b=0$. Indeed, if $b=0$ and c is different from zero, (7) gives an admissible transformation for the time coordinate and (8) represents the transformation to a rotating frame [implying thereby that the frame of (1) is itself rotating]. In other words, if $b=0$, (1) is just the exterior line element of a static cylinder, as seen by a rotating observer. However, since rotating frames (as in special relativity) are not expected to cover the whole space–time, and, furthermore, since the new angle coordinate ranges from $-\infty$ to ∞, it has been argued in the past[7] that both b and c have to vanish for (7) and (8) to be globally valid. This point of view is also reinforced by the fact that, assuming that only b has to vanish in order to globally cast (1) into Levi-Civita, we are lead to the intriguing result that there is no dragging outside rotating cylinders. We shall recall this question later.

The rotation Ω of the compass of inertia, or the gyroscope, with respect to a rotating frame with angular velocity ω moving around the axis of symmetry given by metric (1) can be easily calculated by using the Rindler–Perlick method.[8]

This consists in transforming the angular coordinate ϕ by

$$\phi=\phi'+\omega t, \tag{9}$$

where ω is a constant [observe that (8), with $b=0$, defines a rotation in the sense opposite to that in (9)]. Then the transformed metric is written in a canonical form

$$ds^2=-e^{2\Psi}(dt-\omega_i dx^i)^2+h_{ij}dx^i dx^j, \tag{10}$$

with Latin indexes running from 1 to 3 and Ψ, ω_i, and h_{ij} depend on the spatial coordinate x^i only (we are omitting primes). Then, it may be shown that the four-acceleration A_μ and the rotation three-vector Ω^i of the congruence of world lines $x^i=\text{const}$ are given by

$$A_\mu=(0,\Psi_{,i}), \tag{11}$$

$$\Omega^i=\tfrac{1}{2}e^{\Psi}(\det h_{mn})^{-1/2}\epsilon^{ijk}\omega_{k,j}, \tag{12}$$

where the comma denotes partial derivative. It is clear from the above that if $\Psi_{,i}=0$, then particles at rest in the rotating frame follow circular geodesics. On the other hand, since Ω^i describes the rate of rotation with respect to the proper time at any point at rest in the rotating frame, relative to the local compass of inertia, then $-\Omega^i$ describes the rotation of the compass of inertia (the *gyroscope*) with respect to the rotating frame. Applying (9) to the original frame of (1), with $t=t'$, $r=r'$, and $z=z'$, we cast (1) into the canonical form (10), and obtain [see (43) in Ref. 5]

$$\Omega=MNr^{(1-n^2)/4}\left(M^2ar^{1-n}-\frac{N^2r^{1+n}}{n^2a}\right)^{-1}, \tag{13}$$

where

$$M=1+b\omega, \quad N=n\omega-c(1+b\omega). \tag{14}$$

From (13) we can ask if there are ω's for which the gyroscope precession is null.

We see from (13) that the gyroscope does not precess if $M=0$ or $N=0$, thus producing $\Omega=0$ and implying respectively for the angular velocity of the frame

$$\omega_M=-\frac{1}{b}, \quad \omega_N=\frac{c}{n-bc}. \tag{15}$$

The physical meaning of this result will be discussed later. A similar result has been obtained in Ref. 1, but in the particular context of van Stockum solution, while our result is general and independent of the source.

The tangential velocity W of the gyroscope moving around the axis of symmetry for metric (1) is given by [see (53) in Ref. 9]

$$W=\frac{\omega(fl+k^2)^{1/2}}{f-\omega k}. \tag{16}$$

Substituting (2)–(5) into (16), we obtain

$$W=\frac{n\omega\chi}{(1+b\omega)(1-c^2\chi^2)+nc\omega\chi^2}, \tag{17}$$

where

$$\chi=\frac{r^n}{na}. \tag{18}$$

The angular velocities (15) give, respectively, from (17), the tangential velocities

$$W_M=\frac{1}{c\chi}, \quad W_N=c\chi, \tag{19}$$

and we observe that these velocities do not depend upon b in spite of the corresponding angular velocities depend upon b.

The Newtonian energy per unit length σ is given, in terms of n, by

$$\sigma=\tfrac{1}{4}(1-n), \tag{20}$$

and we consider the range $1>n>-1$ or $0<\sigma<\frac{1}{2}$. This range produces physically reasonable cylindrically symmetric sources.[7] However, no circular timelike geodesics exist for $n<0$, and, furthermore, it is not clear that $n<0$ represent cylinders.[10]

From (19) we see that as $r\to 0$, for $1>n>0$, $W_{M+}\to\infty$ and $W_{N+}\to 0$; while for $0>n>-1$, $W_{M-}\to 0$ and $W_{N-}\to-\infty$. We discard W_{M+} and W_{N-} as being unphysical.

Now, let us suppose that $1>n>0$. Then Ω vanishes for $\omega=\omega_N$. If, furthermore, $b=0$, then it follows at once from (8), that transformation (9) brings the system back to the nonrotating frame (the frame in which the line element is static), thereby explaining the vanishing of the precession. The remarkable fact, however, is that Ω vanishes for ω_N, even if b is different from zero. As for ω_M, we do not have a reasonable interpretation, unless we accept that (1) describes a cylinder only if $1>n>0$.

Now we study the case of infinite precession, $\Omega\to\infty$, for the gyroscope moving around the axis of symmetry. From (13) we have then

$$r^n=\frac{Mna}{N}, \tag{21}$$

and, considering (14), we can rewrite (21) for the angular velocity of the rotating frame,

$$\omega=\frac{1+c\chi}{n\chi-b(1+c\chi)}. \tag{22}$$

The corresponding tangential speed of the gyroscope becomes, using (16), (17), and (22),

$$W=1, \tag{23}$$

which means that the gyroscope attains infinite precession when its tangential velocity around the axis becomes the light velocity.

III. PRECESSION OF A GYROSCOPE AT REST

If the gyroscope is at rest in the original lattice, then we have [see (32) in Ref. 5]

$$\Omega=\frac{cr^{(1-n)(n-3)/4}}{a(1-c^2\chi^2)}. \tag{24}$$

Observe that it is the absolute value of Ω what appears in (31)–(34) in Ref. 5. We see that the precession is infinite if $c\chi=1$. It is remarkable that $c\chi=1$, if the gyroscope is moving around the axis of symmetry, produces a tangential speed of light (19), $W_{N+}=1$, with null precession; on the other hand, in this same case $c\chi=1$, while at rest its precession becomes infinite.

On the other hand, when $b=0$ and $c=0$, i.e., when the Weyl class of Lewis metric becomes the static Levi-Civita cylindrical space–time, the precession of a gyroscope moving around the axis of symmetry results in

$$\Omega=\frac{n\omega r^{(1-n)(n-3)/4}}{a(1-n^2\omega^2\chi^2)}, \tag{25}$$

with a tangential velocity obtained from (17),

$$W=n\omega\chi. \tag{26}$$

We observe that the gyroscope precession is the same in both cases, (24) and (25), if the angular velocity of the gyroscope, in the Levi-Civita space–time, is related to the vorticity of Lewis space–time by

$$\omega=\frac{c}{n}. \tag{27}$$

These two equal precessions, (24) and (25), suggest that (if $b=0$) it is equivalent to measure the precession of a gyroscope at rest with respect to the rotating Lewis source or moving around the corresponding static source. This situation, in turn, is a reminiscense of the non-Machian behavior of Newtonian gravity, where gravitomagnetic effects are absent.

IV. PRECESSION OF A GYROSCOPE IN A LOCALLY NONROTATING FRAME

Using the transformation

$$d\phi=d\bar{\phi}+\omega dt, \tag{28}$$

where ω is

$$\omega=-\frac{k}{l}, \tag{29}$$

the Lewis metric (1) transforms into a diagonal form near $r=r_0$. This frame is called locally nonrotating.[11,12] From (28) for the Lewis metric (1) we have

$$\omega=\frac{n^3a^2c-2n^2a^2bc^2+(bc-n)c^3r_0^{2n}+n^4a^4br_0^{-2n}}{n^4a^2-2n^3a^2bc+2n^2a^2b^2c^2-(n-bc)c^2r_0^{2n}-n^4a^4b^2r_0^{-2n}}, \tag{30}$$

which can be rewritten with (18),

$$\omega=\frac{(n-bc)c\chi_0^2+b}{(n-bc)^2\chi_0^2-b^2}, \tag{31}$$

where $\chi_0=\chi(r_0)$. The tangential velocity (17) with (31) becomes

$$W=\frac{(n-bc)c\chi_0^2+b}{n\chi_0}, \tag{32}$$

and the precession (13) with (31) becomes

$$\Omega=\frac{b(n-bc)r_0^{(1-n)(n-3)/4}}{a[(n-bc)^2\chi_0^2-b^2]}. \tag{33}$$

From (31) we see that there are two cases where ω does not depend upon a particular radius r_0 and produces no precession according to (33). These cases are, for $b=0$,

$$\omega=\frac{c}{n}, \quad W=c\chi_0; \tag{34}$$

and, for $bc=n$,

$$\omega=-\frac{1}{b}, \quad W=\frac{1}{c\chi_0}, \tag{35}$$

where we have included, from (32), the corresponding tangential velocities. We see from (34) that the result corresponds to what we obtained for ω_N in (15) and agrees with the analysis of the gyroscope at rest (24) compared to the precession in Levi-Civita's space–time (25). However, the

case (35), while producing a similar result compared to ω_M in (15), imposes the relation $b=n/c$. When $b\neq 0$ and $b\neq n/c$ the locally nonrotating frame produces non-null precession.

V. THE KERR SPACE–TIME

It is instructive to compare the situation described previously with that in the Kerr space.

In Boyer–Lindquist coordinates with $\theta=\pi/2$, the Kerr metric has the form (the Kerr parameter a, describing angular momentum per unit mass, not to be confounded with the parameter a of the Lewis metric)

$$ds^2=-\left(1-\frac{2m}{r}\right)dt^2-\frac{4am}{r}dtd\phi+\frac{1}{\Pi}dr^2+\left(r^2+a^2+\frac{2a^2m}{r}\right)d\phi^2, \tag{36}$$

where

$$\Pi=1-\frac{2m}{r}+\frac{a^2}{r^2}. \tag{37}$$

Then, applying the Rindler–Perlick method, one obtains after some lengthy calculations

$$e^{2\Psi}=\Lambda, \tag{38}$$

$$\omega_i=(0,0,\omega_\phi), \tag{39}$$

$$\omega_\phi=\frac{1}{\Lambda}\left[\omega(r^2+a^2)-\frac{2am}{r}(1-a\omega)\right], \tag{40}$$

$$h_{rr}=\frac{1}{\Pi}, \tag{41}$$

$$h_{\phi\phi}=\frac{\Pi}{\Lambda}r^2, \tag{42}$$

with

$$\Lambda=1-\omega^2(r^2+a^2)-\frac{2m}{r}(1-a\omega)^2. \tag{43}$$

Substituting (38)–(42) into (12) we obtain

$$\Omega=\frac{2}{\Lambda}\left[\omega-\frac{3m}{r}\omega(1-a\omega)+\frac{am}{r^3}(1-a\omega)^2\right]. \tag{44}$$

The value of the angular velocity ω for which there is no precession ($\Omega=0$) is easily obtained from (44) to be

$$\omega=-\frac{r^2(r-3m)-2ma^2-\sqrt{r^4(r-3m)^2-4ma^2r^3}}{2ma(3r^2+a^2)}; \tag{45}$$

this is the same value for which prograde and retrograde circular geodesics have the same period,[13] and which leads to the condition of no clock effect in Ref. 1, after replacing ω by its expression for a circular geodesic. This result was obtained before[14] and (together with other properties) led some authors to suggest that natural nonrotating observers are those moving with angular velocity (45) (see Ref. 13 and references therein). This identification, however, is not

necessarily correct. In fact, observe that a gyroscope at rest in the frame of (36) ($\omega=0$) will precess unless $a=0$, reflecting the well-known fact that the original frame of (36) is itself rotating with respect to a compass of inertia.[8] Therefore, the vanishing of Ω for observers rotating with angular velocity (45) only shows that the gravitational dragging effect of the source exactly cancels the Thomas-like precession due to the rotation of the frame where the gyroscope is placed: a frame which, as shown in Ref. 1, rotates relative to distant stars. Under these circumstances it becomes difficult to accept that those observers represent ''the most natural standard of non-rotation.''

VI. CONCLUSION

We have seen that a gyroscope at rest in the frame of (1) will precess independently of b, and in a similar way as a gyroscope moving around a static source with angular velocity given by (27). This result, together with the fact that transformations (7) and (8) cast (1) into a static cylindrical Levi-Civita line element if $b=0$, would indicate that the rotation of the source does not affect the gyroscope. However, for the gyroscope moving around the source, there exist two possible angular velocities for which there is no precession. The physical meaning of one of them (ω_M) is not understood by the authors, unless the range of n is restricted to $1>n>0$, in which case it is discarded. The situation with ω_N is clear if $b=0$, in which case (9) is just a transformation to the nonrotating frame if $\omega=\omega_N$. However, if b is not vanishing, then the reasons for the vanishing of Ω are obscure. Finally, if we define a locally nonrotating frame according to (28) and (29), then we see that a gyroscope at rest in such a frame will precess according to (33). The origin of this precession is rather surprising if we note that it appears even if $n=a=1$ (Minkowski) and $c=0$. But under these conditions (1) is not the Minkowskian line element corresponding to a rotating frame. So the question here is, what is the nature of b that makes the gyroscope precess?

In the Kerr case we have seen that the frame in which $\Omega=0$ can hardly be called nonrotating. The difference with the Lewis case (with $b=0$) becomes intelligible, if we note that the frame of (36) with $m=0$ does not represent a rotating Minkowskian observer, a conclusion confirmed by the fact that (44) with $m=\omega=0$ yields $\Omega=0$. However, as mentioned before, the frame of (36) is rotating with respect to a compass of inertia if $m\neq 0$ (yielding $\Omega\neq 0$). This is in contrast with the Lewis case, where Ω is not vanishing for the gyroscope at rest in (1) in the case $n=1$ (Minkowski). This conspicuous difference in the relation between the source of the field and the rotation, in both cases, seems to suggest, loosely speaking, that the behavior of the Kerr metric is more ''Machian'' than that of Lewis.

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Radiating sources in higher-dimensional gravity

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We study a time-dependent five-dimensional (5D) metric which contains a static four-dimensional (4D) sub-metric whose three-dimensional (3D) part is spherically symmetric. An expansion in the metric coefficient allow us to obtain close-to Schwarzschild approximation to a class of spherically symmetric solutions. Using Campbell's embedding theorem and the induced-matter formalism we obtain two 4D solutions. One describes a source with the stiff equation of state believed to be applicable to dense astrophysical objects, and the other describes a spherical source with a radial heat flow. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Campbell showed the theorem that any solution of the Einstein equations in N dimensions can be locally embedded in a Ricci-flat manifold of $(N+1)$ dimensions whose field equations in terms of the Ricci tensor are $R_{AB}=0$ $(A,B=0,1,...,N)$.[1] Tavakol and co-workers have recently noted the relevance of this to the embedding of lower-dimensional (possibly quantizeable) gravity in 4D Einstein gravity,[2] and the technique is clearly applicable to the recovery of solutions of 4D general relativity from 10D superstrings, 11D supergravity and M-theory.[3–6] A major application of Campbell's theorem is to induced-matter theory, wherein solutions of the 4D Einstein equations with matter are recovered from the 5D Kaluza–Klein equations in apparent vacuum.[7] This approach has been applied to cosmology,[8] clusters of galaxies[9] and the solar system,[10,11] where there is agreement with observational data. It is valuable in application to general relativity, since solutions of the Kaluza–Klein equations can yield new solutions of the Einstein equations. With regard to the latter, spherically symmetric sources such as stars can be modeled in the simplest way by the interior and exterior Schwarzschild solutions. But to include the radiation outside a star, more complicated solutions are required.[12] These include the Vaidya metric which uses a retarded time coordinate to describe a radiating atmosphere,[13] the metrics of Herrera and co-workers wherein spheres of matter are matched to exterior space–times,[14–16] and the metrics of Glass and Krisch which extend the Vaidya solution to include both a radiation field and a string fluid.[17] However, despite extensive work on starlike solutions of the 4D equations and the existence of Campbell's theorem which shows that such can be embedded in the ND equations, not much work has been done on spherically symmetric solutions of the 5D equations. Notable exceptions are solutions which have an isothermal equation of state in 4D[9] and ones which are flat in 5D but curved in 4D.[18] We will, therefore, present an analysis of a class of 5D metrics, and illustrate their relevance by isolating two 4D solutions. One describes a source with the stiff equation of state believed to be applicable to dense astrophysical objects, and the other describes a spherical source with radiation.

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II. 5D METRICS WITH 4D SPHERICAL SOURCES

In this section we let upper-case Latin indices run 0–4 and lower-case Greek indices run 0–3. We absorb the speed of light and the gravitational constant through the choices of units $c=1$, $8\pi G=1$. The coordinates are $x^A=t,\ r,\ \theta,\ \phi,\ y$ with $d\Omega^2\equiv d\theta^2+\sin^2\theta d\phi^2$ with (3D) spherical symmetry.

Consider the 5D line element with interval

$$dS^2=g_{AB}dx^Adx^B=\Phi^2ds^2-\Phi^{-4}dy^2, \tag{1}$$

$$ds^2=g_{\alpha\beta}dx^\alpha dx^\beta, \tag{2}$$

where $g_{\alpha\beta}=g_{\alpha\beta}(x^\mu)$ and $\Phi=\Phi(x^\mu)$. This metric is broad in scope and has been used in other contexts.[19] It also has the advantage that the 5D field equations $R_{AB}=0$ break down neatly into a set involving the 4D Ricci tensor and a conservation-type equation for the scalar field ($g_{44}=-\Phi^{-4}$)

$$R_{\alpha\beta}=6\Phi^{-2}\Phi_\alpha\Phi_\beta, \tag{3}$$

$$\Phi\Phi^\alpha_{;\alpha}-\Phi^\alpha\Phi_\alpha=0. \tag{4}$$

Here $\Phi^\alpha=g^{\alpha\beta}\Phi_\beta$, $\Phi^\alpha_{;\alpha}=g^{\alpha\beta}\Phi_{\alpha;\beta}$ and $R_{\alpha\beta}$ in (3) is made of $g_{\alpha\beta}$. Equations (3) and (4) admit many different types of solution, but here we choose a time-dependent scalar field and a static 4D geometry

$$\Phi=\Phi(t), \tag{5}$$

$$ds^2=B(r)dt^2-A(r)dr^2-r^2d\Omega^2. \tag{6}$$

These require that the left-hand side (lhs) of (3) should be independent of t and the rhs of (3) should be independent of r. Therefore both sides should equal to a constant, say, $6\lambda^2$. So we must have

$$\Phi=e^{\lambda t}. \tag{7}$$

Substituting this into Eq. (4), we find that (4) is satisfied. Using (6) and (7) in (3) gives the nonvanishing components

$$R_{00}=\frac{B''}{2A}-\frac{B'}{4A}\left(\frac{A'}{A}+\frac{B'}{B}\right)+\frac{1}{r}\frac{B'}{A}=6\lambda^2, \tag{8}$$

$$R_{11}=-\frac{B''}{2B}+\frac{B'}{4B}\left(\frac{A'}{A}+\frac{B'}{B}\right)+\frac{1}{r}\frac{A'}{A}=0, \tag{9}$$

$$R_{22}=\sin^{-2}\theta R_{33}=1-\frac{1}{A}+\frac{r}{2A}\left(\frac{A'}{A}-\frac{B'}{B}\right)=0, \tag{10}$$

with $A'\equiv dA/dr$. These are three equations in two unknowns, and determine a class of solutions which is time-dependent in 5D via (7) but static in 4D and spherically symmetric in 3D.

Let us manipulate (8)–(10). The sum of $AB^{-1}R_{00}$ of (8) and R_{11} of (9) gives

$$\frac{A'}{A}+\frac{B'}{B}=6\lambda^2r\frac{A}{B}. \tag{11}$$

And we can rewrite (10) as

$$\frac{A'}{A}-\frac{B'}{B}=-\frac{2}{r}(A-1). \tag{12}$$

Using (11) and (12), we verify that (8) and (9) are satisfied. Therefore, we need to solve (11) and (12) for A and B. Now (12) can be written as $(d/dr)\ln(A/B)=-2(A-1)/r$. Integrating this we get

$$B=A\exp\left[2\int_{r_0}^{r}\frac{A-1}{r}dr\right]. \tag{13}$$

Substituting this into (11), we obtain

$$\frac{A'}{A}+\frac{A-1}{r}=3\lambda^2 r\exp\left[-2\int_{r_0}^{r}\frac{A-1}{r}dr\right]. \tag{14}$$

Without loss of generality, let us introduce a mass function[20,21] via

$$A=\left(1-\frac{2\mu(r)}{r}\right)^{-1}. \tag{15}$$

Then (14) becomes

$$\mu'=\frac{3}{2}\lambda^2 r(r-2\mu)\exp\left[2\int_{r_0}^{r}\left(\frac{1}{r}-\frac{1}{r-2\mu}\right)dr\right]. \tag{16}$$

Here r_0 is a fiducial radius that can be chosen as appropriate to a physical situation. Thus if $r_0\to\infty$ we expect to recover the Schwarzschild case. The latter is indeed recovered for $\lambda=0$, when $\mu=M=$constant and (13) reads

$$B=A\exp\left[2\int_{\infty}^{r}\frac{A-1}{r}dr\right]=1-\frac{2M}{r}. \tag{17}$$

That is, $\lambda=0$ specifies the Schwarzschild limit of a class of solutions determined by (16) and one or the other of (11) and (12).

III. CLOSE-TO-SCHWARZSCHILD APPROXIMATION

We can study close-to-Schwarzschild approximation by expanding the mass function $\mu(r)$ of (15) for $|\lambda|$ small (i.e., $|\lambda|^{-1}\gg M$). Thus we write

$$\mu(r)=\sum_{n=0}^{\infty}\mu_n(r), \tag{18}$$

with $\mu_0=M$. Here μ_0 is the zero-order approximation of μ, $(\mu_0+\mu_1)$ is the first-order approximation, and so on. To obtain μ_1 we substitute μ_0 for μ in the rhs of (16) to obtain μ_1'. Integrating μ_1' gives μ_1. Then we substitute $(\mu_0+\mu_1)$ for μ in the rhs of (16) to obtain μ_2'. In this way we obtain the following recursion formulas for evaluating $\mu_n(r)$

$$\mu_0'=0,$$

$$\mu_1'=-\mu_0'+\frac{3}{2}\lambda^2 r(r-2M)\exp\left[2\int_{r_0}^{r}\left(\frac{1}{r}-\frac{1}{r-2M}\right)dr\right],$$

$$\mu_n'=-\sum_{m=0}^{n-1}\mu_m'+\frac{3}{2}\lambda^2 r\left(r-2\sum_{m=0}^{n-1}\mu_m\right)\exp\left\{2\int_{r_0}^{r}\left[\frac{1}{r}-\left(r-2\sum_{m=0}^{n-1}\mu_m\right)^{-1}\right]dr\right\}. \tag{19}$$

From this we find

$$\mu_1'=\frac{3}{2}\lambda^2\left(1-\frac{2M}{r_0}\right)^2\frac{r^3}{r-2M}, \tag{20}$$

and so

$$\mu_1=\frac{3}{2}\lambda^2\left(1-\frac{2M}{r_0}\right)^2\int_{r_0}^{r}\frac{r^3dr}{r-2M}. \tag{21}$$

In the region $r\gg 2M$ and $r_0\gg 2M$, we find

$$\mu_1\approx\tfrac{1}{2}\lambda^2 r^3, \tag{22}$$

where we have absorbed a constant term in μ_0 without loss of generality, so the first-order approximation of $A(r)$ in (15) is

$$A\approx\left(1-\frac{2M}{r}-\lambda^2 r^2\right)^{-1}. \tag{23}$$

Substituting this equation into (13), keeping only terms up to first order in λ^2 as well as in M, and neglecting a constant factor in B, we find

$$B\approx 1-\frac{2M}{r}+2\lambda^2 r^2. \tag{24}$$

From this coefficient and that of (23) we obtain the first order close-to-Schwarzschild approximation of the 5D solution as

$$dS^2\approx e^{2\lambda t}\left[\left(1-\frac{2M}{r}+2\lambda^2 r^2\right)dt^2-\left(1-\frac{2M}{r}-\lambda^2 r^2\right)^{-1}dr^2-r^2d\Omega^2\right]-e^{-4\lambda t}dy^2. \tag{25}$$

This metric is time-dependent. When $\lambda\to 0$, it tends to the 5D Schwarzschild solution. So we call (25) the close-to-Schwarzschild approximation for small $|\lambda|$, implying that the time-variation of the field should be very slow. We also find that the solution (25) belongs to the Type D class of the general time-dependent 5D metrics.[22] As regards the 4D part inside the square bracket in (25), it is interesting to note that it does *not* define the 4D Schwarzschild–de Sitter solution. In the latter, A and B both contain a term $\Lambda r^2/3$ where Λ is the cosmological constant. By contrast, whereas λ^2 has the same physical dimensions as Λ (namely *time*$^{-2}$ or *length*$^{-2}$), A and B in (23) and (24) contain terms with different signs and different sizes. This situation is analogous to another in Kaluza–Klein theory, where the exact solution of the 5D field equations for a charged point mass

does not exactly reproduce the 4D Reissner–Nordstrom solution.[23] Since the 5D equations are richer than the 4D ones, such situations may be expected; but even so, (25) defines a new solution.

IV. TWO EXACT 4D SOLUTIONS

There are, of course, many other solutions than those which are close to Schwarzschild. In general, we have a class of solutions of $R_{AB}=0$ with a metric

$$dS^2=e^{2\lambda t}[Bdt^2-Adr^2-r^2d\Omega^2]-e^{-4\lambda t}dy^2, \tag{26}$$

whose space–time potentials A, B are determined by (11) and (12). Alternatively, they are determined by (16) and one or the other of (11) and (12). We should recall, however, that while (8), (9), and (10) are 4D relations and can be used as such, the class of metrics (26) is 5D in nature. This means that we can use Campbell's theorem[1] and the induced-matter formalism[7] to generate 4D solutions of Einstein's equations with their appropriate matter. We now proceed to show how the 5D metric (26) produces two exact 4D solutions.

A. Solution with a stiff fluid

The first is obtained by splitting off the part inside square brackets in (26). The 4D metric is then

$$ds^2=g_{\alpha\beta}dx^\alpha dx^\beta=Bdt^2-Adr^2-r^2d\Omega^2, \tag{27}$$

and is static. We, therefore, expect that the source necessary to balance Einstein's equations will also be static. As mentioned above, the Kaluza–Klein equations $R_{AB}=0$ $(A,B=0,123,4)$ contain as a subset the Einstein equations $R_{\alpha\beta}-Rg_{\alpha\beta}/2=T_{\alpha\beta}$ $(\alpha,\beta=0,123)$. Here $T_{\alpha\beta}$ is the 4D energy-momentum tensor, which can always be constructed from the 5D geometry[1,2] and whose form is now well known.[7–9] For the present case, $R_{\alpha\beta}$ is given by (3), so the induced energy-momentum tensor is

$$T_{\alpha\beta}=R_{\alpha\beta}-\tfrac{1}{2}g_{\alpha\beta}R=6\Phi^{-2}(\Phi_\alpha\Phi_\beta-\tfrac{1}{2}g_{\alpha\beta}\Phi^\mu\Phi_\mu). \tag{28}$$

Using (7) and (27), we find that the nonvanishing components of this in mixed form are

$$T^0_0=-T^1_1=-T^2_2=-T^3_3=3\lambda^2B^{-1}. \tag{29}$$

This as expected represents a static source, which we can model as a perfect fluid with

$$T_{\alpha\beta}=(\rho+p)u_\alpha u_\beta-pg_{\alpha\beta}. \tag{30}$$

Here ρ is the density, p is the pressure and the 4-velocity is $u^\alpha=(u^0,0,0,0)$. Combining (29) and (30), we see that the source has

$$\rho=p=3\lambda^2B^{-1}. \tag{31}$$

This is the stiff equation of state in which the speed of sound waves approaches the speed of light, and has been applied in previous studies[14,16,21] to astrophysical situations such as collapsed stars and proto-galactic fluctuations.

B. Two-fluid solution with radiation and heat flow

The second solution we look at is obtained by splitting off the whole of the first part of (26). The 4D metric is then

$$d\tilde{s}^2=\tilde{g}_{\alpha\beta}dx^\alpha dx^\beta=e^{2\lambda t}[Bdt^2-Adr^2-r^2d\Omega^2], \tag{32}$$

and is time dependent. We, therefore, expect that the source necessary to balance Einstein's equations will also be time dependent. It should be noted that this property cannot in general be removed by a coordinate transformation based on Birkhoff's theorem, because the 4D metric (32) will have a source constructed from the 5D geometry that will in general not be vacuum; and because the 4D metric (32) is part of a 5D metric (26) and it is known that Birkhoff's theorem in its standard form breaks down in the transition from 4D to 5D,[24,25] as evidenced by the existence of both static and time-dependent soliton solutions.[24,26] To investigate the time-dependence of (32), let us make the coordinate transformation

$$e^{\lambda t}=1-\lambda\tilde{t}. \tag{33}$$

This brings (32) into the form

$$d\tilde{s}^2=\tilde{g}_{\alpha\beta}d\tilde{x}^{\alpha}d\tilde{x}^{\beta}=Bd\tilde{t}^2-(1-\lambda\tilde{t})^2(Adr^2+r^2d\Omega^2). \tag{34}$$

We can use this with $\phi\equiv\Phi^{-2}=e^{-2\lambda t}=(1-\lambda\tilde{t})^{-2}$ to evaluate the induced matter properties using the standard technique.[7–9] We note that

$$\tilde{R}_{\alpha\beta}=\phi^{-1}\widetilde{\phi_{\alpha;\beta}}, \tag{35}$$

$$\tilde{R}=\phi^{-1}\widetilde{\phi^{\alpha}_{;\alpha}}=0, \tag{36}$$

which can be used to form the induced energy-momentum tensor

$$\tilde{T}_{\alpha\beta}=\tilde{R}_{\alpha\beta}-\tfrac{1}{2}\tilde{g}_{\alpha\beta}\tilde{R}=\phi^{-1}\widetilde{\phi_{\alpha;\beta}}. \tag{37}$$

The nonvanishing components of this in mixed form are

$$\tilde{T}^0_0=6\lambda^2B^{-1}(1-\lambda\tilde{t})^{-2}, \tag{38}$$

$$\tilde{T}^1_1=\tilde{T}^2_2=\tilde{T}^3_3=-2\lambda^2B^{-1}(1-\lambda\tilde{t})^{-2}, \tag{39}$$

$$\tilde{T}^1_0=g_{00}g^{11}\tilde{T}^0_1=\lambda A^{-1}B^{-1}B'(1-\lambda\tilde{t})^{-3}. \tag{40}$$

We see from (38) that the density is inhomogeneous via $B=B(r)$ and is time dependent, as is the pressure by (39) though the latter is isotropic. We also see from (40) that there is an off-diagonal component. The latter can be accommodated by introducing a two-fluid model

$$\tilde{T}_{\alpha\beta}=\tilde{T}^{(1)}_{\alpha\beta}+\tilde{T}^{(2)}_{\alpha\beta}, \tag{41}$$

which as in other work[12,16] we take to be the sum of a perfect fluid and a radial heat flow

$$\tilde{T}^{(1)}_{\alpha\beta}(\tilde{\rho}+\tilde{p})u_{\alpha}u_{\beta}-\tilde{p}\tilde{g}_{\alpha\beta}, \tag{42}$$

$$\tilde{T}^{(2)}_{\alpha\beta}=q_{\alpha}u_{\beta}+u_{\alpha}q_{\beta}. \tag{43}$$

The heat-flux vector and the 4-velocity must obey the orthogonality condition

$$q_{\alpha}u^{\alpha}=0. \tag{44}$$

This we satisfy by taking

$$u^{\alpha}=(u^0,0,0,0), \quad u^0=B^{-1/2}, \tag{45}$$

$$q^{\alpha}=(0,q^{1},0,0), \tag{46}$$

where in (45) we have used the facts that r is a comoving coordinate and that the 4-velocities are normalized via $g_{\alpha\beta}u^{\alpha}u^{\beta}=Bu^{0}u^{0}=1$. Substituting (45) and (46) into (42) and (43) and these into (41) gives the nonvanishing components of the last in mixed form

$$\tilde{T}^{0}_{0}=\tilde{\rho}, \tag{47}$$

$$\tilde{T}^{1}_{1}=\tilde{T}^{2}_{2}=\tilde{T}^{3}_{3}=-\tilde{p}, \tag{48}$$

$$\tilde{T}^{1}_{0}=B^{1/2}q^{1}. \tag{49}$$

Comparing these with (38), (39), and (40) gives us the density, pressure and heat flow in explicit form

$$\tilde{\rho}=3\tilde{p}=6\lambda^{2}B^{-1}(1-\lambda\tilde{t})^{-2}, \tag{50}$$

$$q^{1}=\lambda A^{-1}B^{-3/2}B'(1-\lambda\tilde{t})^{-3}. \tag{51}$$

The equation of state is that of radiation or ultra-relativistic matter, and has been applied in previous studies[16,27] to astrophysical situations such as fermion soliton stars and the early universe.

V. DISCUSSION AND CONCLUSION

We have taken a 5D metric (1) which contains a 4D sub-metric (6) whose 3D part is spherically symmetric. An expansion in the metric coefficient allows us to recover the Schwarzschild case of general relativity in (17) as the zeroth approximation and a close-to-Schwarzschild case in (25) as the first order approximation to a class of spherically symmetric solutions. Any solution of the 5D Kaluza–Klein equations in apparent vacuum can be written as a solution of the 4D Einstein equations with matter. Two solutions have then been shown, with matter properties corresponding to those of a stiff fluid (31), and radiation or ultra relativistic particles with heat flow (50) and (51). These solutions can be applied to astrophysics, but are merely illustrative examples.

In the wider scheme, it is clear that (local) embedding theorems are powerful tools, whether applied to $N<4$ (possibly quantizeable) gravity,[2] 4D Einstein theory,[12] 5D Kaluza–Klein theory,[28] or 10D superstrings, 11D supergravity and M-theory.[3–6] Campbell's theorem ensures that any solution in ND can be embedded in a Ricci-flat solution in $(N+1)D$.[1] The Schwarzschild solution in 4D can of course be embedded in a flat space of $N\geqslant 6$.[29] And any solution in 4D can be embedded in a flat space of $N\geqslant 10$.[30] The implications of embedding theorems are diverse. If the aim is to find new solutions of general relativity, the higher-dimensional field equations are often surprisingly tractable, and the method of reduction to 4D is straightforward.[2] If the aim is to give meaning to higher-dimensional theories, the same method of reduction will inform about physicality in the 4D world. We should recall that field equations like those of Einstein or Kaluza–Klein allow the dimensionality to be freely chosen, which should be done partly with a view to what physics it is desired to describe and partly with a view to what technical constraints are involved. In the latter regard, it is well known that $N<4$ theories run into problems of formulation which are connected with the degenerate nature of lower-dimensional Riemannian spaces. For $N>4$ theories, problems arise with the physics if the spaces are subject to arbitrary technical constraints.[7,31,32] Our opinion, therefore, is that future work should be focused on higher-dimensional, fully covariant theory.

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The hyperbolic–hypergeometric functions

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In this work we present a new function to represent the approximate solution of a system of three charged particles. This function is based on an extension to two variables of the confluent hypergeometric function ${}_1F_1$ of Kummer and can be obtained using a method similar to that used by Appell and Kampé de Fériet. We analyze the general properties of the function such as integral representations, series expansions, and asymptotic limits. We also show that the proposed functions verify a relation similar to that satisfied by the exponential and trigonometric–hyperbolic ones. A generalization to *n*-dimension is also presented. The mathematical properties of the functions indicate that they are suitable to be included in computation of electronic emission in collision processes. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1396634]

I. INTRODUCTION

Many functions, very common in the solution of wave equations of various kinds, are special cases of the hypergeometric functions (Whittaker and Watson,[1] Sneddon[2]) or its close relative the confluent hypergeometric function. A few examples are the Bessel functions, the Laguerre functions, and the Airy functions. In particular, the solution for one of the most important problems in physics, the two-body Coulomb problem, comes in terms of hypergeometric functions.[3,4] The dynamics of the problem in the different regions of the coordinates space can be analyzed through the different properties of the Kummer functions.[3–5] On the other hand, different approximated solutions for the three-body Coulomb problem are written in terms of hypergeometric functions.[6–9] The approximate solution known as C3 is given by the product of three two-body Coulomb problems and in this way its dynamical properties depend on the Kummer function properties. Recently, the authors and co-workers introduced a new approximate solution for the three-body problem that can be written in terms of the degenerate Appell functions called Φ_2 by Horn.[10,11] The function Φ_2 can be obtained by a confluence process starting from the Appell hypergeometric function F_1 or F_2 (Ref. 12) and in this way is a confluent hypergeometric function in two variables that can be interpreted as the two-variables generalization of the Kummer function.

From the mathematical point of view, Erdélyi performed a detailed study of the Φ_2 hypergeometric function given different integral representations and asymptotic forms.[13] In 1941, Burchnall and Chaundy presented a method to express different hypergeometric functions as expansions in terms of Kummer functions.[14]

Based on the works of Appell and Kampé de Fériet,[10] Erdélyi,[13] and Burchnall and Chaundy,[14] it is possible to perform a carefull study of the dynamical properties of the three-body Coulomb problem modeled by the Φ_2 approach.[9,15] This function fulfills the Redmond asymptotic conditions for Coulomb potentials. The reduction to the two-body Coulomb problem is also verified when each of the charges are switched off. Nevertheless this function does not completely fulfill the Kato cusp's conditions that relate the wave function and its derivatives when one of the coordinates goes to zero.[16] The Φ_2 state is regular at the origin of coordinates, but does not verify these conditions on the derivatives.

In this work we propose a new hyperbolic–hypergeometric function based on physical arguments which retains the mentioned properties and improves the model including the Kato cusp's conditions in both the coordinate and momentum space. The new hyperbolic–hypergeometric function (called Φ_c) gives rise to other three related functions ($\Phi_s, \Phi^{\pm}$). We present a brief statement of the problem in Sec. I. In Sec. II we obtain the Φ_c function and show the relations with the Φ_2 function of two variables. We describe different properties of the new functions, with particular emphasis in the asymptotic behavior of Φ_c. Also we derive different integral representations and series expansions. In Sec. III the functions Φ_s, Φ^+, and Φ^- are obtained from the analysis Φ_c. In Sec. IV the derivatives of the functions Φ_c, Φ_s, Φ^+, and Φ^- and the connection between them and the hyperbolic–trigonometric functions is presented. Finally we outlook further extensions and applications of this set of functions. The appendix outlines the method to generalize these functions to more variables.

II. STATEMENT OF THE PROBLEM

Let us consider a system of three charged particles in the continuum, labeled by $i=1,2,3$. The relative coordinate $\mathbf{r}_i$ represents the distance between the particles j and k. The exact wave function describing the evolution of this system $\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ is not known in the general case and some physically based approximations are needed. Furthermore, all the approximate states obtained should verify the correct boundary conditions of the Coulomb potential. When all particles are far from each other, the wave function must satisfy the Redmond's conditions.[17] In the case of outgoing waves, we have

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=\prod_{j=1}^{3} \exp(i\alpha_j \ln(k_j r_j-\mathbf{k}_j\cdot\mathbf{r}_j)). \tag{1}$$

On the other hand, the wave function should be regular at the origin of coordinates $\mathbf{r}_j=0$. In 1951, Kato showed that there exists a solution of the Schrödinger equation for a system of charged particles. This equation presents as many singular points as particles involved in the system. These points corresponds to the conditions $|\mathbf{r}_j|=0$, $j=1$, 2 or 3. Besides the solutions $\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ should be regular in the coordinate space, that is to say,

$$\Psi(r_i=0)=C,$$

where C is a finite number. A second condition related with the momenta of the particles in the singular points can be stated as

$$\left.\frac{\partial\overline{\Psi}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)}{\partial r_i}\right]_{r_i=0} = Z_i\Psi(\mathbf{r}_i=0),$$

where $\overline{\Psi}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)$ represents the wave function averaged over a small sphere of radius $r\ll 1$ centered at the singular point $|\mathbf{r}_j|=0$:

$$\overline{\Psi}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=\frac{1}{2}\int \Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)dS\Big]_{r_i\to 0}.$$

There are only a few approximate solutions of the Schrödinger equation for the three-body Coulomb problem. The first proposal relies on a completely separable approximation of the wave equation written in parabolic coordinates. The solution is simply a product of three two-body Coulomb functions for each pair of particles.[4,18]

The Φ_2 approach can be considered as the next step in the approximated solution of the wave equation for a two heavy and one light particles system. In this solution the motion of the heavy partners is described by a two-body function, while the electron–ions interactions are described in a correlated way through the Erdélyi Φ_2 hypergeometric function.[8,13] This function has been successfully included in undistorted and distorted wave treatments of the ion–atom collision process.[4,19] The only drawback of this function is that it does not verify the Kato cusps condition already mentioned. The introduction of the correlation between the motions of the particles implies the generalization of the simple two-body solution given by the Kummer function.

The simplest way to perform this is to include more parameters, giving rise to the ${}_pF_q$ generalized functions. These functions are well documented in the literature.[20] On the other hand, we can generalize the Kummer functions by increasing the number of variables. Starting by the series expansion[21]

$$ {}_1F_1(b,c,x)=\sum_{m=0}^{\infty}\frac{(b)_m}{(c)_m}\frac{x^m}{m!} $$

we can write the product of ${}_1F_1(b,c,x)$ times ${}_1F_1(b',c',y)$ as follows:

$$ {}_1F_1(\beta,\gamma,x){}_1F_1(\beta',\gamma',y)=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{(\beta)_m(\beta')_n}{(\gamma)_m(\gamma')_n}\frac{x^m}{m!}\frac{y^n}{n!}, \tag{2} $$

where $(\beta)_m$ is the Pochhammer symbol given by $\beta(\beta+1)\cdots(\beta+m-1)$.

This series does not give us anything new since it is simply the product of two Kummer functions. However, if one or more of the two pairs of products

$$ (\beta)_m(\beta')_n \quad (\gamma)_m(\gamma')_n $$

are replaced by a composed product of the general type

$$ (\gamma)_{m+n} \tag{3} $$

we are lead to some entirely new functions. This procedure has been followed by Appell and Horn to derive the complete set of second order two-variables hypergeometric functions.[11] If we replace (3) in (2) we get the confluent hypergeometric function called Φ_2 by Horn:[11]

$$ \Phi_2(\beta,\beta',\gamma,x,y)=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}A_{m,n}\frac{x^m}{m!}\frac{y^n}{n!} \tag{4} $$

with

$$ A_{m,n}=\frac{(\beta)_m(\beta')_n}{(\gamma)_{m+n}}. $$

Other confluent hypergeometric function can be obtained using (2) or the product of confluent and Gauss functions and replacing appropriately different pairs of pochhammers.

Burchnall and Chaundy[14] using an operational technic gave a set of 26 expansions of hypergeometric functions, with some of them of confluent type. They showed that the Φ_2 power series (4) can be rewritten as follows in terms of Kummer functions:

$$\Phi_2(\beta,\beta',\gamma,x,y)=\sum_{m=0}^{\infty} A_m(-xy)^m\,{}_1F_1(\beta+m,\gamma+2m,x)\,{}_1F_1(\beta'+m,\gamma+2m,y), \tag{5}$$

where

$$A_m(\beta,\beta',\gamma)=\frac{(\beta)_m(\beta')_m}{m!(\gamma-1+m)_m(\gamma)_{2m}}.$$

This function has been used several times in physical problems. Olsson applied it in nuclear physics.[22] Recently, the author and co-workers made use of the $\Phi_2(\beta,\beta',\gamma,x,y)$ as a partially separable approximated solution for the three-body Coulomb problem (called the Φ_2 model).[8,9] The study of the physical properties of the Φ_2 model has shown that the Kato's cusp conditions are partially satisfied. The condition imposed by Kato over the first order derivative of the wave function means that the coefficient in the power expansion (4) should satisfy the following relation:

$$A_{1n}=\beta' A_{0n}, \quad A_{m1}=\beta A_{m0}$$

which is not satisfied by the Φ_2 function.

To obtain a function with correct Kato conditions, we introduce a new kind of generalization, similar to the one discussed before. Replacing the product of Kummer functions in the series (5) by its generalized form Φ_2 in the following form:

$$(-1)^m\,{}_1F_1[\beta+m,\gamma+2m,x]_1F_1[\beta'+m,\gamma+2m,y]\rightarrow\Phi_2(\beta+m,\beta'+m,\gamma+2m,x,y), \tag{6}$$

where the $(-1)^m$ is included to solve the problem with the Kato condition, we get a new kind of hypergeometric function:

$$\Phi_c(\beta,\beta',\gamma,x,y)=\sum_{m=0}^{\infty} A_m(xy)^m\Phi_2(\beta+m,\beta'+m,\gamma+2m,x,y) \tag{7}$$

which we will call $\Phi_c(\beta,\beta',\gamma,x,y)$. We should note that by the same method we can introduce a complete set of hypergeometric functions starting by the set given by Burchnall and Chaundy.[14]

III. PROPERTIES OF THE Φ_c FUNCTION

Some simple properties of the Φ_c function when the parameters or the variables are zero can be obtained using the reduction properties of the Φ_2 one:

$$\Phi_c(\beta=0)=\Phi_2(0,\beta',\gamma,x,y)={}_1F_1(\beta',\gamma,y),$$

$$\Phi_c(\beta'=0)=\Phi_2(\beta,0,\gamma,x,y)={}_1F_1(\beta,\gamma,y),$$

$$\Phi_c(x=y=0)=\Phi_2(\beta,\beta',\gamma,0,0)=1,$$

$$\Phi_c(x=0)=\Phi_2(\beta,\beta',\gamma,0,y)={}_1F_1(\beta',\gamma,y),$$

$$\Phi_c(y=0)=\Phi_2(\beta,\beta',\gamma,x,0)={}_1F_1(\beta,\gamma,x).$$

Introducing a useful relation satisfied by the Φ_2 function

$$\Phi_2(\beta,\beta',\gamma,x,x)={}_1F_1(\beta+\beta',\gamma,x)$$

we get the following series expansion in the case in which the variables satisfy the condition $x=y$:

$$\Phi_c(x=y)=\sum_{m=0}^{\infty} A_m x^{2m}\,{}_1F_1(\beta+\beta'+2m,\gamma+2m,x).$$

A. Asymptotic expansion

In this section we introduce expressions for the different asymptotic regions. First we analyze the asymptotic form of Φ_c for large values of $|x|$, $|y|$, and $|x-y|$. Then, we present expressions for the situation in which $|y|\to\infty$ and x remains small.

1. Large arguments

To analyze these regions we use the asymptotic form of the function $\Phi_2(\beta,\beta',\gamma,x,y)$ for large arguments, that is to say $|x|$, $|y|$ and $|x-y|\to\infty$. Following Erdélyi,[13] we write the asymptotic form of $\Phi_c(\beta,\beta',\gamma,x,y)$ in terms of Whittaker-type functions $\overline{z_4},\overline{z_5},\overline{z_6}$.

Using the asymptotic expression of the Φ_2 and replacing it in (7) we get

$$\Phi_c(\beta,\beta',\gamma,x,y)=\frac{\Gamma(\gamma)}{\Gamma(\gamma-\beta-\beta')}e^{i\pi(\beta+\beta')}\overline{z_4}+\frac{\Gamma(\gamma)}{\Gamma(\beta)}e^{i\pi(\beta+2\beta'-\gamma)}\overline{z_5}+\frac{\Gamma(\gamma)}{\Gamma(\beta')}e^{i\pi(\beta'-\gamma)}\overline{z_6}, \tag{8}$$

where

$$\overline{z_4}=x^{-\beta}y^{-\beta'}F_4(\beta,\beta',\gamma,x,y),$$

$$\overline{z_5}=(-x)^{\beta+\beta'-\gamma}(y-x)^{-\beta'}e^{x}F_5(\beta,\beta',\gamma,x,y),$$

$$\overline{z_6}=(x-y)^{-\beta}(-y)^{\beta+\beta'-\gamma}e^{y}F_6(\beta,\beta',\gamma,x,y),$$

with

$$F_4(\beta,\beta',\gamma,x,y)=\sum_{m=0}^{\infty}A_m(\gamma)_m\Phi_4\left(\beta+\beta'-\gamma+1,\beta+m,\beta'+M,-\frac{1}{x},-\frac{1}{y}\right),$$

$$F_5(\beta,\beta',\gamma,x,y)=\sum_{m=0}^{\infty}\frac{A_m(\gamma)_m}{(\beta)_m}\left(\frac{xy}{y-x}\right)^m\Phi_4\left(1-\beta-m,\gamma-\beta-\beta',\beta'+m,\frac{1}{x},\frac{1}{x-y}\right),$$

$$F_6(\beta,\beta',\gamma,x,y)=\sum_{m=0}^{\infty}\frac{A_m(\gamma)_m}{(\beta')_m}\left(\frac{xy}{x-y}\right)^m\Phi_4\left(1-\beta'-m,\beta+m,\gamma-\beta-\beta',\frac{1}{y-x},\frac{1}{y}\right),$$

the functions $\overline{z_4},\overline{z_5},\overline{z_6}$ are similar to those ones used by Erdélyi, replacing the functions Φ_i by the generalized F_i with $i=4$, 5 or 6. From the asymptotic limit (8) it can be easily verified that the Φ_c function satisfies the Redmond asymptotic conditions[17] since the leading order for x, $y\to\infty$ is

$$\Phi_c(\beta,\beta',\gamma,x,y)\to x^{-\beta}y^{-\beta'}$$

which is equivalent to (1).

2. Small $x,y\to\infty$

From Eq. (7) and using the asymptotic form of the Φ_2 in the case in which $y\to\infty$ and x^5 remains small

$$\Phi_2(\beta,\beta',\gamma,x,y)=\frac{\Gamma(\gamma)e^{i\pi\beta'}}{\Gamma(\gamma-\beta')}z_7+\frac{\Gamma(\gamma)e^{i\pi(\beta'-\gamma)}}{\Gamma(\beta')}z_6,$$

where

$$z_6=(x-y)^{-\beta}(-y)^{\beta+\beta'-\gamma}e^{y}\Phi_4\left(1-\beta',\beta,\gamma-\beta-\beta',\frac{1}{y-x},\frac{1}{y}\right),$$

$$z_7=y^{-\beta'}\Phi_5\left(\beta,\beta',\gamma-\beta',x,\frac{1}{y}\right).$$

Taking into account Eq. (7) we get

$$\Phi_c(\beta,\beta',\gamma,x,y)=\frac{\Gamma(\gamma)}{\Gamma(\gamma-\beta')}e^{i\pi\beta'}\overline{z_7}+\frac{\Gamma(\gamma)}{\Gamma(\beta')}e^{i\pi(\beta'-\gamma)}\overline{z_6},$$

where

$$\overline{z_7}(\beta,\beta',\gamma,x,y)=y^{-\beta'}G_5(\beta,\beta',\gamma,x,y),$$

with

$$G_5=\sum\frac{(-1)^m(\gamma)_m}{(\gamma-\beta')_m}A_m x^m\Phi_5\left(\beta+m,\beta'+m,\gamma-\beta'+m,x,\frac{1}{y}\right).$$

A similar expression for small $|y|$ and large $|x|$ can be obtained.

B. Integral representation

In this section we analyze two kinds of integral representations based on the two given for the Φ_2 hypergeometric function. This integral representations can be used to obtain analytical transition matrices for a variety of collision processes in atomic physics.

1. Single integral

We start rewriting $\Phi_c(\beta,\beta',\gamma,x,y)$ using the following integral representation for the $\Phi_2(\beta,\beta',\gamma,x,y)$ function:

$$\Phi_2(\beta,\beta',\gamma,x,y)=\frac{\Gamma(\gamma)}{2\pi i}\int e^{s}s^{-\gamma}F_1\left[\gamma,\beta,\beta',\gamma,\frac{x}{s},\frac{y}{s}\right]ds,$$

where

$$F_1\left[\gamma,\beta+m,\beta'+m,\gamma,\frac{x}{s},\frac{y}{s}\right]=\left(1-\frac{x}{s}\right)^{-\beta-m}\left(1-\frac{y}{s}\right)^{-\beta'-m}$$

represent the Appell[10] function for a special case of the parameters. Replacing this expression in (7) we obtain

$$\Phi_c=\frac{\Gamma(\gamma)}{2\pi i}\int ds\,e^{s}s^{-\gamma}\sum_{m=0}^{\infty}(\gamma)_{2m}A_m\left(\frac{x}{s}\right)^m\left(\frac{y}{s}\right)^m F_1\left[\gamma+2m,\beta+m,\beta'+m,\gamma+2m,\frac{x}{s},\frac{y}{s}\right].$$

Defining the new function

$$F_N(\alpha,\beta,\beta',\gamma,x,y)=\sum\ (\alpha)_{2m}A_m x^m y^m F_1(\alpha+2m,\beta+m,\beta'+m,\gamma+2m,x,y)$$

$$=\sum\ (\alpha)_{2m}A_m x^m y^m {}_2F_1(\alpha+2m,\beta+m,\gamma+2m,x)$$

$$\times {}_2F_1(\alpha+2m,\beta'+m,\gamma+2m,y),$$

we can rewrite

$$\Phi_c=\frac{\Gamma(\gamma)}{2\pi i}\int e^s s^{-\gamma} F_N\left(\gamma,\beta,\beta',\gamma,\frac{x}{s},\frac{y}{s}\right)ds.$$

The function ${}_2F_1(a,b,c,x)$ represents the Gauss function,[21] and the function $F_N(\alpha,\beta,\beta',\gamma,x,y)$ can be obtained from

$$F_1(\alpha,\beta,\beta',\gamma,x,y)=\sum\ \frac{(-1)^m(\alpha)_{2m}(\beta)_m(\beta')_m}{m!(\gamma-1+m)_m(\gamma)_{2m}}x^m y^m$$

$$\times F_2(\alpha+2m,\beta+m,\beta'+m,\gamma+2m,\gamma+2m,x,y) \tag{9}$$

by the substitutions

$$F_1(\alpha,\beta,\beta',\gamma,x,y)\to F_N(\alpha,\beta,\beta',\gamma,x,y),$$

$$F_2(\alpha+2m,\beta+m,\beta'+m,\gamma+2m,\gamma+2m,x,y)$$

$$\to(-1)^m F_1(\alpha+2m,\beta+m,\beta'+m,\gamma+2m,\gamma+2m,x,y)$$

on the left-hand and right-hand sides of Eq. (9). The symbol $F_2(\alpha,\beta,\beta',\gamma,\gamma',x,y)$ represents the other four Appell[10] functions.

2. Double integral

Starting from the integral representation of the Φ_2 function

$$\Phi_2=U(\beta,\beta',\gamma)\int_0^1 du\int_0^1 dv\ e^{ux+vy}K(\beta,\beta',\gamma,u,v),$$

where

$$U(\beta,\beta',\gamma)=\frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\beta')\Gamma(\gamma-\beta-\beta')},$$

$$K(\beta,\beta',\gamma,u,v)=u^{\beta-1}v^{\beta'-1}(1-u-v)^{\gamma-\beta-\beta'-1},$$

and replacing it in Φ_c [Eq. (7)], we get

$$\Phi_c=U(\beta,\beta',\gamma)\int_0^1 du\int_0^1 dv\ e^{ux+vy}K(\beta,\beta',\gamma,u,v)\sum\ \frac{1}{m!(\gamma-1+m)_m}(xyuv)^m.$$

The series which appear in the last equation can be added, giving the following result:

$$\sum_{m=0}^{\infty}\frac{(xyuv)^m}{m!(\gamma-1+m)_m}=\begin{cases}\dfrac{1}{\gamma-1}\,{}_1F_2\left(\gamma-1,\dfrac{1}{2}(\gamma-1),\dfrac{\gamma}{2},\dfrac{uvxy}{4}\right), & \gamma\neq 1,2,\\ \cosh(\sqrt{uvxy}), & \gamma=1,2.\end{cases} \tag{10}$$

In case $\gamma=1$ and 2 we can finally write

$$\Phi_c(\beta,\beta',\gamma,x,y)=U(\beta,\beta',\gamma)\int_0^1 du\int_0^1 dv\, e^{ux+vy}\cosh(\sqrt{uvxy})K(\beta,\beta',\gamma,u,v). \tag{11}$$

IV. THE HYPERBOLIC–HYPERGEOMETRIC FUNCTIONS

In this section we study the function (11) obtained in the last section corresponding to $\gamma=1$ and 2. It is possible to verify that the function ${}_1F_2(\gamma-1,\frac{1}{2}(\gamma-1),\gamma/2,uvxy/4)$ can be written in terms of the functions $\cosh(\sqrt{uvxy})$ and $\sinh(\sqrt{uvxy})$. Thus, the function Φ_c given for $\gamma>2$ can be rewritten in terms of the Φ_c function for γ equal to 1 and 2. That is to say, it is possible to obtain continuity relations similar to the ones obtained for the hypergeometric function Φ_2 and use them to write the function Φ_c as a sum of functions corresponding to $\gamma=1$ and 2.

Using the relation between exponential and hyperbolic–trigonometric functions it is possible to rewrite (11) as follows:

$$\Phi_c(\beta,\beta',\gamma,x,y)=\tfrac{1}{2}[\Phi^+(\beta,\beta',\gamma,x,y)+\Phi^-(\beta,\phi',\gamma,x,y)], \tag{12}$$

where

$$\Phi^\pm(\beta,\beta',\gamma,x,y)=U\int_0^1\int_0^1 du\,dv\, e^{ux+vy}e^{\pm\sqrt{uvxy}}K(\beta,\beta',\gamma,u,v). \tag{13}$$

From this equation we can define the function

$$\begin{aligned}\Phi_s(\beta,\beta',\gamma,x,y)&=\tfrac{1}{2}[\Phi^+(\beta,\beta',\gamma,x,y)-\Phi^-(\beta,\beta',\gamma,x,y)]\\&=U\int_0^1\int_0^1 du\,dv\, e^{ux+vy}\sinh(\sqrt{uvxy})K(\beta,\beta',\gamma,u,v)\\&\qquad\text{for}\quad \gamma=1,2\end{aligned} \tag{14}$$

that is similar to the starting point of this work.

The hypergeometric functions $\Phi_s,\Phi_c,\Phi^\pm$ constitute a set similar to the corresponding to the exponential and trigonometric–hyperbolic functions:

$$\Phi^\pm(\beta,\beta',\gamma,x,y)=\Phi_c(\beta,\beta',\gamma,x,y)\pm\Phi_s(\beta,\beta',\gamma,x,y).$$

Using the series expansion for the exponential function in the definitions for Φ^+ and Φ^- we can write

$$\Phi^\pm(\beta,\beta',\gamma,x,y)=U\sum_{m=0}^{\infty}\frac{(\pm1)^m}{m!}(xy)^{m/2}\int_0^1\int_0^1 du\,dv\, e^{ux+vy}(uv)^{m/2}K(\beta,\beta',\gamma,u,v).$$

Using now the relations

$$(uv)^{m/2}K(\beta,\beta',\gamma,u,v)=K\left(\beta+\frac{m}{2},\beta'+\frac{m}{2},\gamma+m,u,v\right)$$

and

$$\int_0^1\int_0^1 du\,dv\;\phi K\left(\beta+\frac{m}{2},\beta'+\frac{m}{2},\gamma+m,u,v\right)$$
$$=U\left(\beta+\frac{m}{2},\beta'+\frac{m}{2},\gamma+m\right)\Phi_2\left(\beta+\frac{m}{2},\beta'+\frac{m}{2},\gamma+m,x,y\right),$$

we get

$$\Phi^{\pm}(\beta,\beta',\gamma,x,y)=\sum_{m=0}^{\infty}(\pm 1)^m\frac{(\beta)_{m/2}(\beta')_{m/2}}{m!(\gamma)_m}(xy)^{m/2}\Phi_2\left(\beta+\frac{m}{2},\beta'+\frac{m}{2},\gamma+m,x,y\right),$$

which are the series expansions for the functions $\Phi^{\pm}(\beta,\beta',\gamma,x,y)$ in terms of the hypergeometric function $\Phi_2(\beta,\beta',\gamma,x,y)$. Furthermore, using the series expansion for the hyperbolic function[21] it is possible to write (14)

$$\Phi_s(\beta,\beta',\gamma,x,y)=\sum_{m=0}^{\infty}\frac{(\beta)_{m+1/2}(\beta')_{m+1/2}}{(2m+1)!(\gamma)_{2m+1}}(xy)^{m+1/2}$$
$$\times\Phi_2\left(\beta+m+\frac{1}{2},\beta'+m+\frac{1}{2},\gamma+2m+1,x,y\right).$$

A. Derivatives of $\Phi^{\pm}$ and $\Phi_{c,s}$ functions

In this section we will write the derivatives of $\Phi^{\pm}$ for the case in which $\gamma=1,2$. Denoting

$$\chi^{\pm}=e^{ux+vy\pm\sqrt{uvxy}},$$

the derivative of the function Φ^{+} is given by

$$\frac{d\Phi^{\pm}}{dx}=U\left[\int_0^1\int_0^1 du\,dv\left(u\pm\frac{uvy}{2\sqrt{uvxy}}\right)\chi^{\pm}K(\beta,\beta',\gamma,u,v)\right]$$

and, using

$$uK(\beta,\beta',\gamma,u,v)=K(\beta+1,\beta',\gamma+1,u,v),$$
$$(uv)^{1/2}K(\beta,\beta',\gamma,u,v)=K(\beta+\tfrac{1}{2},\beta'+\tfrac{1}{2},\gamma+1,u,v),$$

we can write

$$\frac{d\Phi^{\pm}}{dx}=U\int_0^1\int_0^1 du\,dv\;\chi^{\pm}K(\beta+1,\beta',\gamma+1,u,v)$$
$$\pm\frac{1}{2}U\sqrt{\frac{y}{x}}\int_0^1\int_0^1 du\,dv\;\chi^{\pm}K\left(\beta+\frac{1}{2},\beta'+\frac{1}{2},\gamma+1,u,v\right).$$

Then

$$\frac{d\Phi^{\pm}}{dx}=\frac{(\beta)_1}{(\gamma)_1}\Phi^{\pm}(\beta+1,\beta',\gamma+1,x,y)\pm\frac{1}{2}\sqrt{\frac{y}{x}}\frac{(\beta)_{1/2}(\beta')_{1/2}}{(\gamma)_1}\Phi^{\pm}\left(\beta+\frac{1}{2},\beta'+\frac{1}{2},\gamma+1,x,y\right).$$

With these expressions we can write the derivative of $\Phi_c(\beta,\beta',\gamma,x,y)$:

$$\frac{d\Phi_c}{dx}=\frac{1}{2}\frac{(\beta)_1}{(\gamma)_1}\Phi_c(\beta+1,\beta',\gamma+1,x,y)+\frac{1}{4}\sqrt{\frac{y}{x}}\frac{(\beta)_{1/2}(\beta')_{1/2}}{(\gamma)_1}\Phi_s\left(\beta+\frac{1}{2},\beta'+\frac{1}{2},\gamma+1,x,y\right).$$

In a similar way, for the $\Phi_s(\beta,\beta',\gamma,x,y)$ we can get

$$\frac{d\Phi_s}{dx}=\frac{1}{2}\frac{(\beta)_1}{(\gamma)_1}\Phi_s(\beta+1,\beta',\gamma+1,x,y)+\frac{1}{4}\sqrt{\frac{y}{x}}\frac{(\beta)_{1/2}(\beta')_{1/2}}{(\gamma)_1}\Phi_c\left(\beta+\frac{1}{2},\beta'+\frac{1}{2},\gamma+1,x,y\right).$$

We can see through the obtained expressions, that the derivatives of Φ_s and Φ_c satisfy relations which mix the trigonometric and the hypergeometric ones. For example, the derivative of Φ_s is written in terms of the same hypergeometric but with the parameters added in one, and besides depend on the Φ_c. The first term is a typical form for the derivative of a hypergeometric function; the second a typical trigonometric relation.

B. Expansion in terms of Kummer functions

In this section we will introduce a series expansion for the function $\Phi_c(\beta,\beta',\gamma,x,y)$ in terms of the Kummer function. Starting from (7) and using (5) we obtain

$$\Phi_c=\sum_n^\infty\sum_k^\infty(-1)^k A_n(\beta,\beta',\gamma)A_k(\beta+n,\beta'+n,\gamma+2n)$$
$$\times(xy)^{n+k}\,{}_1F_1[\beta+n+k,\gamma+2(n+k),x]\,{}_1F_1[\beta'+n+k,\gamma+2(n+k),y].$$

Now, applying the general relation:[12]

$$\sum_n^\infty\sum_k^\infty C_{k,n}=\sum_n^\infty\sum_k^n C_{k,n-k}$$

to our particular case we get for $\Phi_c(\beta,\beta',\gamma,x,y)$,

$$\Phi_c=\sum_n^\infty B_n(xy)^n\,{}_1F_1[\beta+n,\gamma+2n,x]\,{}_1F_1[\beta'+n,\gamma+2n,y], \tag{15}$$

where

$$B_n=\sum_{k=0}^n(-1)^k A_{n-k}(\beta,\beta',\gamma)A_k(\beta+n-k,\beta'+n-k,\gamma+2(n-k)). \tag{16}$$

The obtained expansion in terms of Kummer functions has some advantages in comparison with the power series one. The convergence is fast and only a few terms are necessary for most of the physical interest. By the other side, the representation (15) allows us to compute transition matrices for ion–atom collision by using the same procedure used in previous works.[15,19] In Fig. 1 we show the calculation of the double differential cross section for the ionization of helium by proton impact. The energy of the incoming proton is 1.5 MeV. We plot the energy of the ionized electrons as a function of its energy and for two different angles of emission. We compare the result obtained by using the continuum correlated wave model based in the Φ_c wave function[19] plotted with full line with the well-known continuum distorted wave–eikonal initial state (CDW)[23] with broken line. We see that some differences around the electron capture to the continuum peak but we are not sure if this effect is due to the inclusion of the Kato cusp conditions or due to the correlation introduced in the wave function. In the autoionization of atoms excited by ion impact

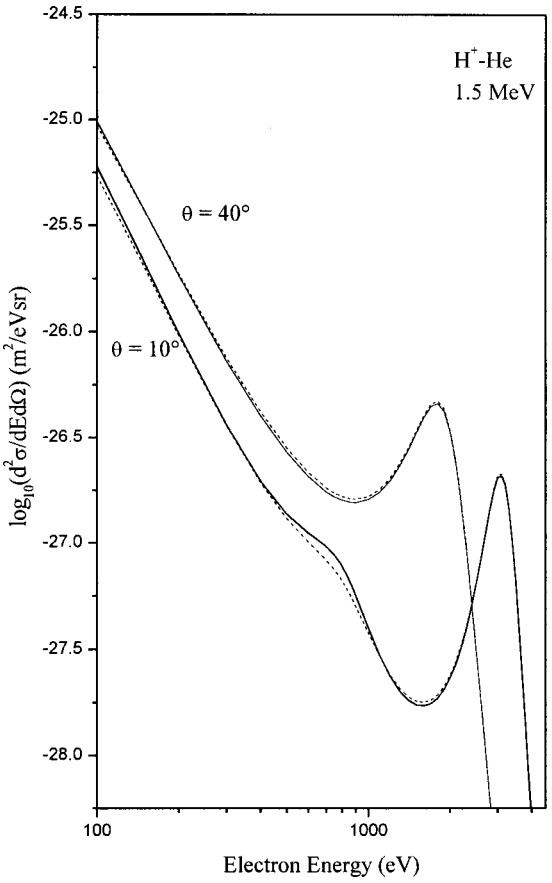

FIG. 1. DDCS for the collision 1.5 MeV $H^+ \rightarrow He$ where angle of the ionized electrons is 10 and 40 degres. Full line, CCWEIS model based in the Φ_c wave function (Ref. 19); broken line, CDWEIS model.

process the Kato cusp conditions are more relevant than in ionization itself, so we are working on that process to perform in future works a comparative analysis between the CDW, the Φ_2 model and the Φ_c one.

V. SUMMARY

In this work we have introduced a new set of functions through a substitution method similar to the used by Appell and Lauricella.[10] The function Φ_c is well founded on physical grounds. The other three Φ_s and $\Phi^{\pm}$, were introduced resulting from the study of the Φ_c one.

We have analyzed different properties like reduction in terms of coefficients and variables. We have introduced different integral representation and series expansion, and the derivatives of all the functions were showed as well as the connection between them.

These functions verify the required physical conditions of a Coulomb many-particle system as can be derived from their mathematical properties. In particular, they fullfil the Kato cusp conditions that were not satisfied by previous generalizations of the Kummer function. Besides of the Redmond asymptotic behavior and the reduction to a two-body Coulomb problem when each of the charges are fixed equal to zero.

We have applied this wave function calculating the double differential cross section for single ionization of He by proton impact. Furthermore, we have contrasted our results with the well-known CDW–EIS theory.

Following a similar method to that given in the present work, it would be possible to generate a complete set of hypergeometric function starting from the list given by Burchnall and Chaundy.[14]

APPENDIX

A possible generalization of the functions Φ_c, Φ_s, Φ^+, and Φ^- to the case of three and more variables can be done using the bounded integral representation. For example, the generalization of the Φ_c to three variables is

$$\phi_c^{(3)} = U^{(3)} \int_0^1 \int_0^1 \int_0^1 du\, dv\, dw\, e^{ux+vy+wz} \cosh(\sqrt{uvwxyz}) K(\beta,\beta',\beta',\gamma,u,v,w),$$

where we define

$$K(\beta_1,\beta_2,\ldots,\beta_n,\gamma,u_1,u_2,\ldots,u_n) = \left(1-\sum_{i=1}^{n} u_i\right)^{\gamma-\Sigma_{i=1}^{n}\beta_i-1} \prod_{i=1}^{n} u_i^{\beta_i-1}$$

and

$$U^{(n)} = \frac{\Gamma(\gamma)}{\Gamma(\gamma-\Sigma_{i=1}^{n}\beta_i)\Pi_{i=1}^{n}\Gamma(\beta_i)}.$$

Using the power series for the cosh (x), we get

$$\Phi_c^{(3)} = U^{(3)} \sum_{m=0}^{\infty} \frac{1}{(2m)!} (xyz)^m \int_0^1 \int_0^1 du\, dv\, e^{ux+vy+wz} K(\beta+m,\beta'+m,\beta'+m,\gamma+3m,u,v,w).$$

Replacing the integral representation of $\Phi_2^{(3)}(\beta,\beta',\beta',\gamma,x,y,z)$:[5]

$$\Phi_2^{(3)}(\beta,\beta',\beta'',\gamma,x,y,z) = U^{(3)} \int_0^1 \int_0^1 du\, dv\, e^{ux+vy+wz} K(\beta,\beta',\beta',\gamma,u,v,w),$$

we obtain the three-dimensional series expansion in terms of $\Phi_2^{(3)}(\beta,\beta',\beta',\gamma,x,y,z)$ for the function $\Phi_c^{(3)}(\beta,\beta',\beta',\gamma,x,y,z)$:

$$\Phi_c^{(3)}(\beta,\beta',\beta'',\gamma,x,y,z) = \sum_{m=0}^{\infty} \frac{(\beta)_m(\beta')_m(\beta')_m}{(2m)!(\gamma)_{3m}} (xyz)^m \times \Phi_2^{(3)}(\beta+m,\beta'+m,\beta'+m,\gamma+3m,x,y,z)$$

or alternatively, using (10) results in

$$\Phi_c^{(3)}(\beta,\beta',\beta'',\gamma,x,y,z) = \sum_{m=0}^{\infty} \frac{(\beta)_m(\beta')_m(\beta'')_m}{m!(\gamma-1+m)_m(\gamma)_{3m}} (xyz)^m \times \Phi_2^{(3)}(\beta+m,\beta'+m,\beta''+m,\gamma+3m,x,y,z)$$

for $\gamma=1,2$. General expressions for arbitrary γ result by the same method using (10).

The three-dimensional integral form Φ_s, Φ^+, and Φ^- are

$$\Phi_s^{(3)}(\beta,\beta',\beta'',\gamma,x,y,z)=U^{(3)}\int_0^1\int_0^1\int_0^1 du\,dv\,dw\,e^{ux+vy+wz}\sinh(\sqrt{uvwxyz})$$
$$\times K(\beta,\beta',\beta'',\gamma,u,v,w),$$

$$\Phi_{(3)}^{\pm}(\beta,\beta',\beta'',\gamma,x,y,z)=U^{(3)}\int_0^1\int_0^1 du\,dv\,e^{ux+vy+wz\pm\sqrt{uvwxyz}}K(\beta,\beta',\beta'',\gamma,u,v,w).$$

On the other hand, the n-dimensional form for $\Phi_c^{(n)}$ is

$$\Phi_c^{(n)}(\beta_1,\beta_2,\ldots,\beta_n,\gamma,x_1,x_2,\ldots,x_n)=U^{(n)}\int_0^1\int_0^1\cdots\int_0^1 du_1\,du_2\cdots du_n\,e^{\sum_{i=1}^n u_i x_i}$$
$$\times\cosh\left(\sqrt{\prod_{i=1}^n u_i x_i}\right)K(\beta_1,\beta_2,\ldots,\beta_n,\gamma,u_1,u_2,\ldots,u_n).$$

Similar expressions can be written for $\Phi_s^{(n)}$, $\Phi_{(n)}^{+}$, and $\Phi_{(n)}^{-}$.

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New solutions of the Jacobi equations for three-dimensional Poisson structures

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A systematic investigation of the skew-symmetric solutions of the three-dimensional Jacobi equations is presented. As a result, three disjoint and complementary new families of solutions are characterized. Such families are very general, thus unifying many different and well-known Poisson structures seemingly unrelated which now appear embraced as particular cases of a more general solution. This unification is not only conceptual but allows the development of algorithms for the explicit determination of important properties such as the symplectic structure, the Casimir invariants and the Darboux canonical form, which are known only for a limited sample of Poisson structures. These common procedures are thus simultaneously valid for all the particular cases which can now be analyzed in a unified and more economic framework, instead of using a case-by-case approach. In addition, the methods developed are valid globally in phase space, thus ameliorating the usual scope of Darboux' reduction which is only of local nature. Finally, the families of solutions found present some new nonlinear superposition principles which are characterized. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Poisson structures[1,2] have an important presence in all fields of Mathematical Physics.[1–35] A Poisson description of a given system is often the basis for the obtainment of fruitful insight and information through the use of a plethora of well-known adapted tools.[1,2,7,9,17,34,36–42]

The present work is devoted to finite-dimensional Poisson structures. These, when expressed in terms of a system of local coordinates on an n-dimensional manifold, take the form

$$\dot{x}_i = \sum_{j=1}^{n} J_{ij}\partial_j H, \quad i=1,\ldots,n. \tag{1}$$

Here and in what is to follow ∂_j means $\partial/\partial x_j$. The C^1 and real-valued function $H(x)$ in (1) is a constant of motion of the system, which plays the role of Hamiltonian. The $J_{ij}(x)$, called structure functions, are also C^1 and real-valued and constitute the entries of a $n\times n$ structure matrix $\mathcal{J}$. The $J_{ij}(x)$ have the property of being solutions of the Jacobi equations

$$\sum_{l=1}^{n} (J_{li}\partial_l J_{jk} + J_{lj}\partial_l J_{ki} + J_{lk}\partial_l J_{ij}) = 0. \tag{2}$$

In (2) indices i,j,k run from 1 to n. The structure functions also verify the additional condition of being skew-symmetric

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TABLE I. Some Poisson structures reported in the literature which are particular cases of solution (14). The original notations have been maintained for the parameters.

System	Reference(s)	$\psi_i(x_i)$	$\phi_i(x_i)$	$\eta(x)$
Euler top	[2, pp. 397–398]	1	x_i	1
Kermack–McKendrick	[10, J_1 in Eq. (177)]; [23, Eq. (5)]	1	1	rx_1x_2
Lorenz (1)	[9, Table III]	1	$\phi_1=(r/\sigma)x_1e^{(1-\sigma)t}$ $\phi_2=-x_2e^{(\sigma-1)t}$ $\phi_3=x_3e^{(1-3\sigma)t}$	1/2
Lotka–Volterra	[10, J_1 in Eq. (87)]; [22, Eq. (18)]	x_i	$\phi_1=-1$ $\phi_2=-bc$ $\phi_3=c$	1
Lotka–Volterra	[10, J_2 in Eq. (87)]; [22, Eq. (19)]	$\psi_1=cx_1$ $\psi_2=x_2$ $\psi_3=x_3$	$\phi_1=x_1$ $\phi_2=-(x_2+\nu)$ $\phi_3=ax_3+\mu$	1
Lotka–Volterra and Generalized Lotka–Volterra	[13, Eq. (11)]; [26, Eq. (10)]	x_i	$\phi_1=K_{23}$ $\phi_2=K_{31}$ $\phi_3=K_{12}$	1
Maxwell–Bloch	[7, Case 3]	1	$\phi_1=\nu x_1$ $\phi_2=\mu x_2$ $\phi_3=\nu+\mu x_3$	1
Ravinovich (1)	[9, Table III]	1	$\phi_1=-x_1/4$ $\phi_2=x_2/4$ $\phi_3=(x_3/2)e^{-2\nu t}$	1
Ravinovich (2)	[9, Table III]	1	$\phi_1=(x_1/4)e^{-\nu t}$ $\phi_2=(x_2/4)e^{-\nu t}$ $\phi_3=-h/2$	1
Ravinovich (4)	[9, Table III]	1	$\phi_1=-(x_1/2)e^{-\nu t}$ $\phi_2=-(x_2/2)e^{\nu_1 t}$ $\phi_3=he^{\nu_1 t}$	1
Ravinovich (5)	[9, Table III]	1	$\phi_1=(x_1/2)e^{\nu_2 t}$ $\phi_2=(x_2/2)e^{-\nu_2 t}$ $\phi_3=-he^{\nu_2 t}$	1
RTW interaction (1)	[9, Table III]	1	$\phi_1=x_1$ $\phi_2=x_2$ $\phi_3=(1/2)e^{-2t}$	1
RTW interaction (3)	[9, Table III]	1	$\phi_1=2x_1e^{-t}$ $\phi_2=2x_2e^{-t}$ $\phi_3=e^{-t}$	1
RTW interaction (4)	[9, Table III]	1	$\phi_1=2x_1e^{\gamma t}$ $\phi_2=2x_2e^{\gamma t}$ $\phi_3=e^{-(2+\gamma)t}$	1
RTW interaction (5)	[9, Table III]	1	$\phi_1=\delta x_1e^{-2t}$ $\phi_2=\delta x_2e^{-2t}$ $\phi_3=\delta/2$	1
Spin system	[19, Eq. (14)]	1	x_i	1

$$J_{ij}=-J_{ji} \quad \text{for all} \quad i,j. \tag{3}$$

One of the reasons justifying the importance of the Poisson representation is the local equivalence between Poisson systems and classical Hamiltonian systems, as stated by Darboux Theorem.[1]

Theorem 1.1 (Darboux): Consider an n-dimensional Poisson manifold for which the rank of the Poisson structure has constant value $2r$ everywhere. Then at each point of the manifold there exist local coordinates $(p_1,\ldots,p_r,q_1,\ldots,q_r,z_1,\ldots,z_{n-2r})$ in terms of which the equations of motion become

TABLE II. Some Poisson structures reported in the literature which are particular cases of solution (20). The original notations have been maintained for the parameters.

System	Reference	$\xi(x_1,x_2)=w(x)/v(x)$	$\eta(x)=v(x)$
Circle maps	[10, J_1 in Eq. (120)]	$-(x_2/x_1)^2$	$(x_1x_3)^2$
May–Leonard	[10, J_1 in Eq. (152)]	$(x_2/x_1)^{\alpha}$	$(\alpha-1)^{-1}x_2^{-\alpha}$
Ravinovich (6)	[9, Table III]	$(x_1/x_2)e^{2(\nu_2-\nu_1)t}$	$-(x_2/2)e^{(\nu_1-2\nu_2)t}$
Ravinovich (7)	[9, Table III]	$(x_1/x_2)e^{2(\nu_2-\nu_3)t}$	$(x_2/2)e^{-\nu_2 t}$
3D with a known first integral	[12, Eq. (18)]	$-f_2(x_1,x_2,t)/f_1(x_1,x_2,t)$	$-f_1(x_1,x_2,t)$

$$\dot{q}_i=\frac{\partial H}{\partial p_i},\quad \dot{p}_i=-\frac{\partial H}{\partial q_i},\quad i=1,\ldots,r,$$

$$\dot{z}_j=0,\quad j=1,\ldots,n-2r.$$

An interesting consequence of Darboux Theorem which will be reconsidered later is that two Poisson structures of the same dimension and rank can be transformed locally into each other by a suitable change of coordinates.[1] Both the Darboux Theorem and the previous remark are important for what follows.

The possibility of describing a given vector field not explicitly written in the form (1) in terms of a Poisson structure is an obvious question of fundamental importance in this context to which important efforts have been devoted in past years in a variety of approaches.[5–17,19,21–28] This explains, together with the intrinsic mathematical interest of the problem, the permanent attention deserved in the literature by the obtainment and classification of skew-symmetric solutions of the Jacobi equations,[3–18,20–24,26,27,29] both in the case of n-dimensional solutions[3,4,13,14,18,20,26,29] as well as in the important and better understood situation of dimension three.[7–12,17,22,23,27] In the three-dimensional case the strategy for finding suitable skew-symmetric solutions of the Jacobi equations makes use of very diverse—often problem-dependent—methods, and the state of affairs is certainly more elaborate than the one existing in general dimension n. Moreover, it is worth recalling that the three-dimensional scenario is particularly relevant for several reasons: First, a large number of three-dimensional systems arising in very diverse fields have a Poisson structure (see Tables I–IV for a sample). Therefore, three-dimensional Poisson structures are the natural framework for their analysis. Second, dimension three corresponds to the first nontrivial case where Poisson structure does not imply symplectic structure, i.e., it is the simplest meaningful kind of Poisson structures which is not symplectic. And third, three is the lowest dimension for which the Jacobi identities are not always identically verified. Since the complexity of equations (2) and (3) is increasing with the dimension n, the three-dimensional case is the simplest nontrivial one as well as a natural first approach to the full problem of analyzing systems (2) and (3).

In this work a systematic investigation of the skew-symmetric solutions of the three-dimensional Jacobi Eqs. (2) and (3) is presented. As we shall see, three disjoint categories of

TABLE III. Some Poisson structures reported in the literature which are particular cases of solution (21). The original notations have been maintained for the parameters.

System	Reference(s)	$\zeta(x_1,x_3)=u(x)/w(x)$	$\eta(x)=w(x)$
Kermack–McKendrick	[10, J_2 in Eq. (177)]; [23, Eq. (6)]	rx_1/a	$-ax_2$
Lorenz	[10, J_1 in Eq. (139)]	$-(2x_1)^{-1}$	$-x_1/2$
Lorenz (3)	[9, Table III]	$-(\sigma/x_1)e^{(2\sigma-1)t}$	$-(x_1/2)e^{-\sigma t}$
Lorenz (5)	[9, Table III]	$-x_1^{-1}e^{t}$	$-(x_1/2)e^{-t}$
Maxwell–Bloch	[7, Case 1]	x_1^{-1}	νx_1
Maxwell–Bloch	[10, J_2 in Eq. (159)]	$(k/2g)x_1^{1-2g}x_3^{2k-1}$	$k^{-1}x_1^{g}x_2^{1-g}x_3^{1-2k}$
Two-level	[10, Eq. (165)]	x_1/x_3	$x_3/(2x_1)$

TABLE IV. Some Poisson structures reported in the literature which are particular cases of solution (22). The original notations have been maintained for the parameters.

System	Reference	$\chi(x_2,x_3)=v(x)/u(x)$	$\eta(x)=u(x)$
Circle maps	[10, J_2 in Eq. (120)]	$-(x_3/x_2)^2$	$(x_1x_2)^2$
Lorenz	[10, J_2 in Eq. (139)]	x_2/x_3	$-x_3/2$
Maxwell–Bloch	[7, Case 2]	x_2/x_3	μx_3
May–Leonard	[10, J_2 in Eq. (152)]	$(x_3/x_2)^\alpha$	$(\alpha-1)^{-1}x_3^{-\alpha}$
Ravinovich (3)	[9, Table III]	$(x_2/x_3)e^{2(\nu_3-\nu)t}$	$(x_3/2)e^{-\nu_3 t}$

solutions of the problem appear naturally. For each of them, a new family of solutions is found. Such families are extremely general. This explains that many well-known three-dimensional Poisson structures and dynamical systems now happen to appear embraced as particular cases of a wider family, as we shall see in detail. Therefore, a first outcome is that of the unification of many different Poisson structures seemingly unrelated. Moreover, this unification is not only conceptual. In fact, the new families are amenable to explicit and detailed analysis, in spite of their generality. In particular, it is possible to develop algorithms for the determination of important properties such as the symplectic structure and the Darboux canonical form. The advantage of these common strategies is that they are simultaneously valid for all the particular cases which can now be analyzed in a unified and very economic way, instead of using a case-by-case approach. In addition, the methods developed are valid globally in phase space, thus ameliorating the usual scope of Darboux' theorem which does only guarantee, in principle, a local reduction.[1] The possibility of constructing the Darboux canonical form is also remarkable in view that the practical determination of Darboux' coordinates is a complicated task in general, which has been carried out only for a very limited sample of systems.[2,6,13,14,19] Finally, the families of solutions found have unexpected properties, such as the presence of simple nonlinear superposition principles which will be characterized.

For the sake of conciseness, in what follows we shall use the following notation for the entries of the three-dimensional structure matrix:

$$u(x):=J_{12}(x), \quad v(x):=J_{31}(x), \quad w(x):=J_{23}(x). \tag{4}$$

Now, if in the case $n=3$ we simplify the Jacobi identities (2) with the help of (3) and substitute also definition (4) the joint systems (2) and (3) take the form

$$u\partial_1 v - v\partial_1 u + w\partial_2 u - u\partial_2 w + v\partial_3 w - w\partial_3 v = 0. \tag{5}$$

The three-dimensional version of systems (2) and (3) shall be written in the compact form (5) in the rest of this work.

The structure of the article is as follows. In Secs. II–IV, respectively, three different, disjoint and complementary families of solutions are developed including their derivation and properties as well as examples. To conclude, Sec. V contains some final remarks.

II. FIRST FAMILY OF SOLUTIONS

For the characterization of the first family of solutions, it is convenient to begin with the establishment of an important general property of Eq. (5).

Theorem 2.1: Let $\{u(x),v(x),w(x)\}$ be a set of $C^1(\Omega)$ functions solution of Eq. (5) in an open domain $\Omega\subset\mathbb{R}^3$, and let $\mu(x):\Omega\to\mathbb{R}$ be an arbitrary $C^1(\Omega)$ function. Then $\{u^*(x),v^*(x),w^*(x)\}=\{\mu(x)u(x),\mu(x)v(x),\mu(x)w(x)\}$ is also a solution of Eq. (5).

Proof: It can be verified after direct substitution of $\{\mu(x)u(x),\mu(x)v(x),\mu(x)w(x)\}$ into Eq. (5). Q.E.D.

It is important to stress that this theorem is not valid in general in dimensions higher than three, as it can be easily verified. In order to physically interpret the result contained in Theorem 2.1 it is necessary to first formalize the concept of time reparametrization:[6]

Definition 2.2: Let $\Omega\subset\mathbb{R}^3$ be an open subset. A reparametrization of time is defined as a transformation of the form

$$\mathrm{d}\tau=\frac{1}{\mu(x)}\,\mathrm{d}t, \tag{6}$$

where t is the initial time variable, τ is the new time and $\mu(x):\Omega\to\mathbb{R}$ is a $C^1(\Omega)$ function which does not vanish in Ω.

In addition, let

$$\frac{\mathrm{d}x}{\mathrm{d}t}=\mathcal{J}\cdot\nabla H \tag{7}$$

be an arbitrary three-dimensional Poisson structure defined in an open domain $\Omega\subset\mathbb{R}^3$. Then, every reparametrization of time of the form (6) leads from (7) to the differential system:

$$\frac{\mathrm{d}x}{\mathrm{d}\tau}=\mu\mathcal{J}\cdot\nabla H. \tag{8}$$

Consequently, in the three-dimensional case reparametrizations (6) preserve the existence of a Poisson structure in the system, this time with structure matrix $\mu\mathcal{J}$ in (8). On the contrary, such transformations in general destroy the Poisson structure in higher dimensions because for a given $\mathcal{J}$ which is a structure matrix, $\mu\mathcal{J}$ is not necessarily a solution of (2) and (3).

We proceed now to characterize a first family of solutions of Eq. (5). For this, we shall assume that none of the solution functions $\{u(x),v(x),w(x)\}$ is identically zero (the relaxation of this condition will lead to the other two families of solutions, as we shall see in Sec. III and IV).

Definition 2.3: For every open domain $\Omega\subset\mathbb{R}^3$, we shall denote by $\Gamma_{[u,v,w]}(\Omega)$ the set of solutions of Eq. (5) defined in Ω which are of the form $\{u(x),v(x),w(x)\}$, with $u(x)$, $v(x)$ and $w(x)$ nonvanishing in Ω and $C^1(\Omega)$.

We have the following result:

Theorem 2.4: Consider the family of functions of the form

$$\begin{cases} u(x) &= \eta(x)\psi_1(x_1)\psi_2(x_2)\phi_3(x_3)\\ v(x) &= \eta(x)\psi_1(x_1)\phi_2(x_2)\psi_3(x_3),\\ w(x) &= \eta(x)\phi_1(x_1)\psi_2(x_2)\psi_3(x_3)\end{cases} \tag{9}$$

defined in an open set $\Omega\subset\mathbb{R}^3$, where $\{\eta,\psi_i,\phi_i\}$, $i=1,2,3$, are arbitrary $C^1(\Omega)$ functions of their respective arguments which do not vanish in Ω. Then the family of functions (9) belongs to $\Gamma_{[u,v,w]}(\Omega)$.

Proof: For solutions belonging to $\Gamma_{[u,v,w]}(\Omega)$, we can equivalently write (5) as

$$u^2\partial_1\left(\frac{v}{u}\right)+w^2\partial_2\left(\frac{u}{w}\right)+v^2\partial_3\left(\frac{w}{v}\right)=0. \tag{10}$$

From (10) it is clear that $\{u(x),v(x),w(x)\}$ are solutions if

$$\frac{v}{u}=\alpha(x_2,x_3)\Rightarrow\begin{cases} u &= u_1(x_2,x_3)\psi_1(x)\\ v &= v_1(x_2,x_3)\psi_1(x)\end{cases}, \tag{11}$$

$$\frac{u}{w}=\beta(x_1,x_3)\Rightarrow\begin{cases} u &= u_2(x_1,x_3)\psi_2(x) \\ w &= w_2(x_1,x_3)\psi_2(x) \end{cases}, \tag{12}$$

$$\frac{w}{v}=\gamma(x_1,x_2)\Rightarrow\begin{cases} v &= v_3(x_1,x_2)\psi_3(x) \\ w &= w_3(x_1,x_2)\psi_3(x) \end{cases}. \tag{13}$$

In (11)–(13) the functions $\{\alpha,\beta,\gamma,u_i,v_i,w_i,\psi_j\}$, with $i\in\{1,2,3\}$ and $j=1,2,3$, are $C^1(\Omega)$ and nonvanishing arbitrary functions of their respective arguments. A family of solutions of Eqs. (11)–(13) is found if we assume that $\psi_j(x)\equiv\psi_j(x_j)$ for all $j=1,2,3$. Then, taking also into account Theorem 2.1 and Definition 2.3 we arrive to result (9). Q.E.D.

Corollary 2.5: For every open domain $\Omega\subset\mathbb{R}^3$, solution (9) can be written as

$$J_{ij}(x)=\eta(x)\psi_i(x_i)\psi_j(x_j)\sum_{k=1}^{3}\epsilon_{ijk}\phi_k(x_k), \tag{14}$$

where indexes i,j run from 1 to 3, $\{\eta,\psi_i,\phi_i\}$ are arbitrary $C^1(\Omega)$ functions of their respective arguments which do not vanish in Ω and ϵ is the Levi-Civita symbol.

Definition 2.6: For every open domain $\Omega\subset\mathbb{R}^3$, the subset of $\Gamma_{[u,v,w]}(\Omega)$ composed of those solutions of Eq. (5) characterized by Theorem 2.4 will be denoted $\Delta(\Omega)$.

The family of solutions $\Delta(\Omega)$ is very general, therefore, containing numerous previously known structure matrices of very diverse three-dimensional systems as particular cases, as it can be seen in detail in Table I. Of special relevance are the Lie–Poisson structure matrix associated to the Lie algebra so(3) [for which $\psi_i(x_i)=1$, $\phi_i(x_i)=x_i$ and $\eta=1$] as well as the separable matrices[14] [$\phi_i(x_i)=$constant, $\eta=1$]. It is worth recalling that the time dependence of some of the structure matrices enumerated in Table I is immaterial in this context, since the Jacobi equations are time-independent and therefore time plays the only role of a parameter in the solutions.

As anticipated in Sec. I, the generality of solutions (14) is not an obstacle in what regards the characterization of their main properties. We begin by the symplectic structure and the Casimir invariant.

Proposition 2.7: For every open subset $\Omega\subset\mathbb{R}^3$, the rank of the Poisson structures belonging to $\Delta(\Omega)$ is constant in Ω and equal to 2, and a Casimir function of the family of solutions (14) forming $\Delta(\Omega)$ is

$$C(x)=\sum_{i=1}^{3}\int\frac{\phi_i(x_i)}{\psi_i(x_i)}\mathrm{d}x_i\,. \tag{15}$$

Moreover, the Casimir invariant (15) is globally defined in Ω and $C^2(\Omega)$.

Proof: The rank is constant in Ω and has value 2 as a consequence of the nonvanishing properties of functions $\{\eta,\psi_i,\phi_i\}$. In addition, according to the Pfaffian method,[41] which is the simplest in this case, the Casimir function is found to be the solution of the system

$$\sum_{i=1}^{3}\frac{\phi_i(x_i)}{\psi_i(x_i)}\mathrm{d}x_i=0.$$

The integration is immediate and leads to (15). The remaining properties of the Casimir invariant also arise from those of functions ϕ_i and ψ_i. Q.E.D.

It is interesting to notice that $\eta(x)$ does not affect neither the symplectic structure nor the form of the Casimir invariant. This is to be expected from the fact that it is a common factor of the structure functions.

We proceed now to construct globally the Darboux canonical form.

Theorem 2.8: For every three-dimensional Poisson system

$$\frac{\mathrm{d}x}{\mathrm{d}t}=\mathcal{J}\cdot\nabla H,$$

defined in an open domain $\Omega\subset\mathbb{R}^3$ and such that $\mathcal{J}\in\Delta(\Omega)$, the Darboux canonical form is accomplished globally in Ω in the new coordinate system $\{z_1,z_2,z_3\}$ and the new time τ, where $\{z_1,z_2,z_3\}$ is related to $\{x_1,x_2,x_3\}$ by the diffeomorphism globally defined in Ω

$$z_1(x_1)=\int\frac{\phi_1(x_1)}{\psi_1(x_1)}\mathrm{d}x_1,\quad z_2(x_2)=\int\frac{\phi_2(x_2)}{\psi_2(x_2)}\mathrm{d}x_2,\quad z_3(x)=\sum_{i=1}^{3}\int\frac{\phi_i(x_i)}{\psi_i(x_i)}\mathrm{d}x_i,$$

and the new time τ is given by the time reparametrization of the form (6)

$$\mathrm{d}\tau=\eta(x(z))\phi_1(x_1(z))\phi_2(x_2(z))\phi_3(x_3(z))\mathrm{d}t.$$

Proof: We begin by noticing that the Darboux theorem is applicable to family (14) because its members have constant rank 2 everywhere in Ω, as seen in Proposition 2.7. This is a key necessary condition[2] which is verified in the case of $\Delta(\Omega)$. Recall also that, after a general diffeomorphism $y=y(x)$, a given structure matrix $\mathcal{J}(x)$ is transformed into another one $\mathcal{J}'(y)$ according to the tensor rule

$$J'_{ij}(y)=\sum_{k,l=1}^{n}\frac{\partial y_i}{\partial x_k}J_{kl}(x)\frac{\partial y_j}{\partial x_l}. \tag{16}$$

The reduction can be carried out in three steps:

(i) Step 1: We perform a first change of variables, which is globally diffeomorphic in Ω

$$y_i(x_i)=\int\frac{\phi_i(x_i)}{\psi_i(x_i)}\mathrm{d}x_i,\quad i=1,2,3.$$

According to (16) we arrive to:

$$\mathcal{J}'(y)=\tilde{\eta}(y)\begin{pmatrix}0&1&-1\\-1&0&1\\1&-1&0\end{pmatrix}, \tag{17}$$

where $\tilde{\eta}(y)=\eta(x(y))\phi_1(x_1(y_1))\phi_2(x_2(y_2))\phi_3(x_3(y_3))$;

(ii) Step 2: we can make use of the Casimir $C=y_1+y_2+y_3$ of $\mathcal{J}'$ in (17) and perform a second change of variables globally diffeomorphic in $\mathbb{R}^3\supset\Omega'=y(\Omega)$:

$$z_1=y_1,\quad z_2=y_2,\quad z_3=y_1+y_2+y_3.$$

The new structure matrix can be found by means of (16)

$$\mathcal{J}''(z)=\hat{\eta}(z)\begin{pmatrix}0&1&0\\-1&0&0\\0&0&0\end{pmatrix},$$

where $\hat{\eta}(z)=\tilde{\eta}(y(z))$;

(iii) Step 3: Finally, we can make a reparametrization of time of the form (6), namely $\mathrm{d}\tau=\hat{\eta}(z)\mathrm{d}t$, where τ is the new time and $\hat{\eta}(z)$ is easily seen to be nonvanishing in $\Omega''=z(y(\Omega))$ and $C^1(\Omega'')$. The result is, according to Theorem 2.1 and (7) and (8), a new Poisson system with matrix

$$\mathcal{J}_D(z)=\begin{pmatrix}0&1&0\\-1&0&0\\0&0&0\end{pmatrix}, \tag{18}$$

and time τ. Consequently, the structure matrix $\mathcal{J}_D$ in (18) is already the one corresponding to the Darboux canonical form. The reduction is thus globally completed. Q.E.D.

According to the remarks made in the Introduction in connection with Darboux Theorem, it is worth noting an interesting corollary of Theorem 2.8, namely that all the diverse structures shown in Table I can actually be seen[1] as the global representation of the same basic Poisson structure (namely the Darboux one) in different systems of coordinates. This is obviously a consequence of the tensor transformation rule (16). However, in the case of Theorem 2.8 this equivalence is demonstrated globally in Ω, thus exceeding the usual scope of Darboux theorem. Notice also how this is founded on the fact that the rank of the structure matrix remains constant in Ω, which is ensured by the nonvanishing conditions verified by the solutions. Consideration of a possible variability in the value of the rank would lead to additional geometric issues[1] not regarded in this work for the sake of conciseness.

We conclude the exposition of the properties of the family of solutions (14) with a brief discussion of its associated nonlinear superposition principles. We have the starting result:

Proposition 2.9: For every open domain $\Omega\subset\mathbb{R}^3$, let $\{u,v,w\}$ and $\{u^*,v^*,w^*\}$ be two elements of $\Delta(\Omega)$. Then the set $\Delta(\Omega)$ has the structure of abelian group with respect to the operation of inner sum $\oplus$ given by

$$\oplus: \qquad \Delta(\Omega)\times\Delta(\Omega)\to\Delta(\Omega)$$

$$(\{u,v,w\},\{u^*,v^*,w^*\})\to\{u,v,w\}\oplus\{u^*,v^*,w^*\}=\{uu^*,vv^*,ww^*\}. \tag{19}$$

Proof: It is a consequence of the factorized form of the solutions (14). Q.E.D.

In what follows it will become evident why in this context the natural definition for operation (19) is that of a sum. For this, we need a previous definition:

Definition 2.10: For every open domain $\Omega\subset\mathbb{R}^3$, the subset of $\Delta(\Omega)$ composed of solutions $\{u,v,w\}$ such that $u(x)>0$, $v(x)>0$ and $w(x)>0$ for all $x\in\Omega$ will be denoted $\Delta^+(\Omega)$.

Notice that due to the nonvanishing character of the solutions forming $\Delta(\Omega)$, the definition of $\Delta^+(\Omega)$ is not very restrictive. In fact, most examples of Table I belong to $\Delta^+(\Omega)$ or do have admissible ranges of the system parameters or variables for which the Poisson structure is in $\Delta^+(\Omega)$. It is now possible to establish the following:

Theorem 2.11: For every open domain $\Omega\subset\mathbb{R}^3$, let $\{u,v,w\}$ and $\{u^*,v^*,w^*\}$ be two elements of $\Delta^+(\Omega)$ and let a be a real number. Then the set $\Delta^+(\Omega)$ has the structure of real vector space with respect to the two operations of inner sum $\oplus$ given by

$$\oplus: \qquad \Delta^+(\Omega)\times\Delta^+(\Omega)\to\Delta^+(\Omega)$$

$$(\{u,v,w\},\{u^*,v^*,w^*\})\to\{u,v,w\}\oplus\{u^*,v^*,w^*\}=\{uu^*,vv^*,ww^*\}$$

and product $\otimes$ by scalars

$$\otimes: \qquad \mathbb{R}\times\Delta^+(\Omega)\to\Delta^+(\Omega)$$

$$(a,\{u,v,w\})\to a\otimes\{u,v,w\}=\{u^a,v^a,w^a\}.$$

Proof: It is an extension of the proof of Proposition 2.9. Q.E.D.

Notice the interest of the fact that the results of the operations $\oplus$ and $\otimes$ belong to $\Delta^+(\Omega)$: According to Definition 2.10 this means that the results of those operations are also solutions—of the same kind $\Delta^+(\Omega)$—of Eq. (5). It is also remarkable that the nonlinear superposition principle just described has such a general linear algebraic structure. This is certainly infrequent in the domain of nonlinear PDEs.

The description of the first family of solutions is thus completed. We now proceed to examine a second, complementary case.

III. SECOND FAMILY OF SOLUTIONS

The second family of solutions arises when we consider the case in which one of the solution functions $\{u,v,w\}$ is identically zero, while the remaining two are not.

Definition 3.1: For every open domain $\Omega\subset\mathbb{R}^3$, we shall denote by $\Gamma_{[v,w]}(\Omega)$, $\Gamma_{[u,w]}(\Omega)$ and $\Gamma_{[u,v]}(\Omega)$ the sets of solutions $\{u,v,w\}$ of Eq. (5) defined in Ω which are of the forms $\{0,v(x),w(x)\}$, $\{u(x),0,w(x)\}$ and $\{u(x),v(x),0\}$, respectively, where $u(x)$, $v(x)$, and $w(x)$ are, when present, $C^1(\Omega)$ and nonvanishing in Ω.

Theorem 3.2: For every open subset $\Omega\subset\mathbb{R}^3$, the general solutions of Eq. (5) corresponding to $\Gamma_{[v,w]}(\Omega)$, $\Gamma_{[u,w]}(\Omega)$ and $\Gamma_{[u,v]}(\Omega)$ are, respectively,

$$\Gamma_{[v,w]}(\Omega)\Rightarrow\{u=0,v=\eta(x),w=\eta(x)\xi(x_1,x_2)\}, \tag{20}$$

$$\Gamma_{[u,w]}(\Omega)\Rightarrow\{v=0,w=\eta(x),u=\eta(x)\zeta(x_1,x_3)\}, \tag{21}$$

$$\Gamma_{[u,v]}(\Omega)\Rightarrow\{w=0,u=\eta(x),v=\eta(x)\chi(x_2,x_3)\}, \tag{22}$$

where functions $\{\eta,\xi,\zeta,\chi\}$ appearing in (20)–(22) are arbitrary, $C^1(\Omega)$ with regard to their respective arguments and nonvanishing in Ω.

Proof: It is immediate from Eq. (5). Q.E.D.

Accordingly, for example in the case $u=0$ we have found structure matrices of the form

$$\mathcal{J}=\eta(x)\begin{pmatrix}0 & 0 & -1\\ 0 & 0 & \xi(x_1,x_2)\\ 1 & -\xi(x_1,x_2) & 0\end{pmatrix}, \tag{23}$$

where η and ξ are $C^1(\Omega)$ and nonvanishing in Ω. As it can be seen, the overall factor considered in Theorem 2.1 already appears explicitly in (23) and needs not be added *a posteriori*.

Again, numerous well-known systems from diverse fields have Poisson structures which are particular cases of (20), (21), or (22), as it is displayed in Table II for $\Gamma_{[v,w]}(\Omega)$, in Table III for $\Gamma_{[u,w]}(\Omega)$ and in Table IV for $\Gamma_{[u,v]}(\Omega)$.

Following the same scheme than in the previous section, we now proceed to develop the main properties of the solutions just found. For the sake of conciseness this shall be done only for the case $\Gamma_{[v,w]}(\Omega)$, given that all the corresponding algorithms and results are entirely analogous for $\Gamma_{[u,w]}(\Omega)$ and $\Gamma_{[u,v]}(\Omega)$.

We shall begin with the symplectic structure and Casimir invariants. Again, the Pfaffian method[41] seems to be the simplest one in order to characterize these properties. From (23) the Pfaffian system to be solved is easily seen to be $\xi(x_1,x_2)\mathrm{d}x_1+\mathrm{d}x_2=0$. Clearly, this system cannot be solved without some additional information because it is very generic. In order to circumvent this difficulty, it is worth introducing a definition:

Definition 3.3: Let $\Omega\subset\mathbb{R}^2$ be an open domain and let $\xi:\Omega\rightarrow\mathbb{R}$ be a $C^1(\Omega)$ function which does not vanish in Ω. We shall say that $\xi(x_1,x_2)$ is separable in Ω if it can be written in the form

$$\xi(x_1,x_2)=\frac{\xi_1(x_1)}{\xi_2(x_2)}, \tag{24}$$

for all $(x_1,x_2)\in\Omega$, where $\xi_1(x_1)$ and $\xi_2(x_2)$ are $C^1(\Omega)$ and do not vanish in Ω.

Now note that all specific systems found in practice (see Table II) verify the property that $\xi(x_1,x_2)$ is separable [notice that the only exception is the last item of Table II, but this is not a specific system but a generic situation which does not correspond to any particular vector field, and therefore it does not affect the generality of (24)]. An analogous property is verified for all entries of Tables III and IV. Consequently, it seems well justified to conclude that, typically, ξ will be separable in the form indicated in Definition 3.3.

Proposition 3.4: For every open domain $\Omega\subset\mathbb{R}^3$, if a solution of the form (20) belonging to $\Gamma_{[v,w]}(\Omega)$ has a $\xi(x_1,x_2)$ which is separable in Ω according to (24), then the rank of such Poisson structure is constant in Ω and has value 2, and a Casimir function of the structure is

$$C(x_1,x_2)=\int \xi_1(x_1)\mathrm{d}x_1+\int \xi_2(x_2)\mathrm{d}x_2. \tag{25}$$

In addition, the Casimir invariant (25) is globally defined in Ω and $C^2(\Omega)$.

Proof: The rank is constant and of value 2 in Ω due to the nonvanishing properties of η, ξ_1 and ξ_2. Additionally, taking (24) into account the Pfaffian system to be solved[41] becomes $\xi_1(x_1)\mathrm{d}x_1+\xi_2(x_2)\mathrm{d}x_2=0$. This leads to the Casimir function immediately. The remaining properties of the Casimir invariant are a consequence of those of ξ_1 and ξ_2. Q.E.D.

The Darboux canonical form can also be computed under similar assumptions:

Theorem 3.5: For every three-dimensional Poisson system

$$\frac{\mathrm{d}x}{\mathrm{d}t}=\mathcal{J}\cdot\nabla H,$$

defined in an open subset $\Omega\subset\mathbb{R}^3$ and such that $\mathcal{J}\in\Gamma_{[v,w]}(\Omega)$ is given by (20) and $\xi(x_1,x_2)$ in (20) is separable in Ω according to (24), the Darboux canonical form is accomplished globally in Ω in the new coordinate system $\{y_1,y_2,y_3\}$ and the new time τ, where $\{y_1,y_2,y_3\}$ is related to $\{x_1,x_2,x_3\}$ by the diffeomorphism globally defined in Ω

$$y_1=\int \xi_1(x_1)\mathrm{d}x_1+\int \xi_2(x_2)\mathrm{d}x_2,\quad y_2=x_2,\quad y_3=x_3, \tag{26}$$

and the new time τ is given by the time reparametrization of the form (6)

$$\mathrm{d}\tau=\eta(x(y))\frac{\xi_1(x_1(y))}{\xi_2(y_2)}\mathrm{d}t.$$

Proof: Notice first that the Darboux theorem is applicable in this case[2] because solutions of $\Gamma_{[v,w]}(\Omega)$ of the forms (23) and (24) have constant rank 2 everywhere in Ω, as anticipated in Proposition 3.4. The reduction can be carried out in two steps:

(i) Step 1: The change of variables (26), which is globally diffeomorphic in Ω, is introduced. Notice that (26) is not the only possibility but it would be similar, for instance, to choose $\{y_1=x_1,y_2=C(x_1,x_2),y_3=x_3\}$. From (16), (23), (24), and (26) we are led to:

$$\mathcal{J}'(y)=\tilde{\eta}(y)\begin{pmatrix}0&0&0\\0&0&1\\0&-1&0\end{pmatrix},$$

where $\tilde{\eta}(y)=\eta(x(y))\xi(x(y))=\eta(x(y))\xi_1(x_1(y))/\xi_2(y_2)$.

(ii) Step 2: A reparametrization of time of the kind (6), i.e., $\mathrm{d}\tau=\tilde{\eta}(y)\mathrm{d}t$, where τ is the new time and $\tilde{\eta}(y)$ is clearly nonvanishing in $\Omega'=y(\Omega)$ and $C^1(\Omega')$. The resulting structure matrix is

$$\mathcal{J}_D(y)=\begin{pmatrix}0&0&0\\0&0&1\\0&-1&0\end{pmatrix}. \tag{27}$$

Since $\mathcal{J}_D$ in (27) corresponds to the Darboux canonical form, the reduction has been accomplished globally. Q.E.D.

To complete this section, we now consider the issue of nonlinear superposition principles. We have the following first result:

Proposition 3.6: For every open domain $\Omega\subset\mathbb{R}^3$, let $\{0,v,w\}$ and $\{0,v^*,w^*\}$ be two elements of $\Gamma_{[v,w]}(\Omega)$. Then the set $\Gamma_{[v,w]}(\Omega)$ has the structure of Abelian group with respect to the operation of inner sum $\oplus$ given by

$$\oplus: \quad \Gamma_{[v,w]}(\Omega)\times\Gamma_{[v,w]}(\Omega)\to\Gamma_{[v,w]}(\Omega)$$

$$(\{0,v,w\},\{0,v^*,w^*\})\to\{0,v,w\}\oplus\{0,v^*,w^*\}=\{0,vv^*,ww^*\}.$$

Proof: It is similar to that of Proposition 2.9. Q.E.D.

The corresponding results for $\Gamma_{[u,w]}(\Omega)$ and $\Gamma_{[u,v]}(\Omega)$ are completely analogous. An additional definition is required at this stage:

Definition 3.7: For every open domain $\Omega\subset\mathbb{R}^3$, the subset of $\Gamma_{[v,w]}(\Omega)$ composed of solutions $\{0,v,w\}$ such that $v(x)>0$ and $w(x)>0$ for all $x\in\Omega$ will be denoted $\Gamma^+_{[v,w]}(\Omega)$.

Of course, Definition 3.7 can be extended straightforwardly to characterize the sets $\Gamma^+_{[u,w]}(\Omega)$ and $\Gamma^+_{[u,v]}(\Omega)$. This is omitted for the sake of brevity, as usual. As it was done in the previous section, it is worth noting that the nonvanishing character of the functions constituting $\Gamma_{[v,w]}(\Omega)$, $\Gamma_{[u,w]}(\Omega)$, and $\Gamma_{[u,v]}(\Omega)$ implies that the definitions of $\Gamma^+_{[v,w]}(\Omega)$, $\Gamma^+_{[u,w]}(\Omega)$, and $\Gamma^+_{[u,v]}(\Omega)$ are not very restrictive in practice, as it can be verified in the examples lists provided in Tables II–IV, respectively. It is now possible to establish the main result:

Theorem 3.8: For every open domain $\Omega\subset\mathbb{R}^3$, let $\{0,v,w\}$ and $\{0,v^*,w^*\}$ be two elements of $\Gamma^+_{[v,w]}(\Omega)$ and let a be a real number. Then the set $\Gamma^+_{[v,w]}(\Omega)$ has the structure of real vector space with respect to the two operations of inner sum $\oplus$ given by

$$\oplus: \quad \Gamma^+_{[v,w]}(\Omega)\times\Gamma^+_{[v,w]}(\Omega)\to\Gamma^+_{[v,w]}(\Omega)$$

$$(\{0,v,w\},\{0,v^*,w^*\})\to\{0,v,w\}\oplus\{0,v^*,w^*\}=\{0,vv^*,ww^*\},$$

and product $\otimes$ by scalars

$$\otimes: \quad \mathbb{R}\times\Gamma^+_{[v,w]}(\Omega)\to\Gamma^+_{[v,w]}(\Omega)(a,\{0,v,w\})$$

$$\to a\otimes\{0,v,w\}=\{0,v^a,w^a\}.$$

Proof: It is formally analogous to that of Theorem 2.11. Q.E.D.

Notice that statements similar to Theorem 3.8 can be developed in parallel for $\Gamma^+_{[u,w]}(\Omega)$ and $\Gamma^+_{[u,v]}(\Omega)$. Such results are obviously in correspondence with those established in Theorem 2.11 of Sec. II for the nonlinear superposition principles in $\Delta^+(\Omega)$. Most observations made there are translatable into the present context in a straightforward way and are therefore disregarded.

Our analysis of the solutions of (5) can now be completed. This is the aim of the next section.

IV. THIRD FAMILY OF SOLUTIONS

Following the previous considerations, the last possibility is to look for solutions of (5) such that two of the three functions $\{u,v,w\}$ are identically zero, while the remaining one is not.

Definition 4.1: The sets of solutions $\{u,v,w\}$ of Eq. (5) defined in an open domain $\Omega\subset\mathbb{R}^3$ which are of the forms $\{u(x),0,0\}$, $\{0,v(x),0\}$ and $\{0,0,w(x)\}$, where $u(x)$, $v(x)$ and $w(x)$ are $C^1(\Omega)$ and nonvanishing in Ω, will be denoted $\Gamma_{[u]}(\Omega)$, $\Gamma_{[v]}(\Omega)$, and $\Gamma_{[w]}(\Omega)$, respectively.

Since all the results which are going to be examined are completely analogous for $\Gamma_{[u]}(\Omega)$, $\Gamma_{[v]}(\Omega)$ and $\Gamma_{[w]}(\Omega)$, we shall concentrate without lack of generality on the analysis of $\Gamma_{[w]}(\Omega)$.

Theorem 4.2: For every open domain $\Omega\subset\mathbb{R}^3$, the general solution of Eq. (5) corresponding to $\Gamma_{[w]}(\Omega)$ consists of the sets of functions of the form $\{u=0,v=0,w(x)\}$, where $w(x)$ is an arbitrary function belonging to $C^1(\Omega)$ and nonvanishing in Ω. Analogous results hold for $\Gamma_{[u]}(\Omega)$ and $\Gamma_{[v]}(\Omega)$.

Proof: It is immediate from Eq. (5). Q.E.D.

Accordingly, for example in the case of $\Gamma_{[w]}(\Omega)$ we have arrived to solutions of the form

$$\mathcal{J}(x)=\eta(x)\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & 1\\ 0 & -1 & 0\end{pmatrix}, \tag{28}$$

with $\eta(x)$ a function $C^1(\Omega)$ and nonvanishing in Ω. Notice that the multiplication by a global factor considered in Theorem 2.1 needs not be taken into account here, since it is already explicit in (28). Note also that solutions described by Theorem 4.2 correspond to structure matrices which are just time reparametrizations of the Darboux canonical form. Consequently, this kind of solutions is very simple and is only considered here for the sake of completeness: The analysis of properties such as the Casimir invariants, the Darboux canonical form or the existence of superposition principles becomes a straightforward version of those considered in Secs. II and III, and can, therefore, be omitted. In spite of such simplicity, examples of Poisson structures belonging to $\Gamma_{[u]}(\Omega)$, $\Gamma_{[v]}(\Omega)$, or $\Gamma_{[w]}(\Omega)$ are not uncommon in the literature.[7] In addition, it is worth mentioning that there is an important category of particular cases of (28) which are present in diverse systems, namely the structure matrices associated to the Lie algebra so(3) when expressed in certain noncartesian coordinates. The simplest possibility is probably that of spherical coordinates:[2]

$$\mathcal{J}_{\mathrm{so}(3)}(\rho,\theta,\varphi)=-\frac{1}{\rho\sin\varphi}\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & 1\\ 0 & -1 & 0\end{pmatrix}.$$

Additional instances of (28) arising from the Lie algebra so(3) for other choices of the coordinate system are also of customary use.[19]

V. FINAL REMARKS

Some new families of skew-symmetric solutions of the three-dimensional Jacobi equations have been presented. They have been developed according to a systematic plan consisting in examining solutions of Eq. (5) such that (i) none of the functions $\{u,v,w\}$ is identically zero (Sec. II); (ii) one of them is identically zero (Sec. III); (iii) two of them are identically zero (Sec. IV). This structuration of the solutions naturally embraces all nontrivial possibilities. The three resulting families have some remarkable properties already anticipated:

(i) They generalize many already known Poisson structures from well-known systems, which now become particular cases. Therefore the new solutions unify in a common framework those structures, which seemed to be unrelated. Several lists of such systems are provided in Tables I–IV;

(ii) This unification allows the development of simultaneous methods of analysis valid for every particular system, thus avoiding a case-by-case strategy. Specifically, it has been shown how to construct explicitly the Casimir invariant and the Darboux canonical form. This is interesting, as far as the determination of the Darboux coordinates is a nontrivial task only known for a limited sample of systems. Moreover, in this work such coordinates have been charazerized globally in phase space, therefore beyond the usual scope of Darboux' theorem, which only ensures a local reduction;

(iii) This unifying approach has uncovered the existence of nonlinear superposition principles within the families of solutions of (5). Such principles obey well defined linear algebraic structures, which is a uncommon property in the framework of nonlinear PDEs.

These results seem to indicate that the direct search of solutions of the Jacobi equations is a sensible line of research not only from a purely theoretical or a classification perspective, but also from the point of view of the analysis of Poisson structures, as well as mathematically interesting as an example of nonlinear system of PDEs. Of course, the three-dimensional scenario is probably

the simplest nontrivial representative case in all those senses, but it is worth recalling that a similar strategy has already produced some novel results in the most general n-dimensional situation.[14] Therefore, it seems justified to conclude that this philosophy will be a source of further advances in the understanding of finite-dimensional Poisson structures.

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Representations of $U_\epsilon^{\mathrm{res}}(sl_2)$ via restricted q-Fock spaces

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Two restricted $C[q,q^{-1}]$-forms of the well known q-boson algebra are introduced and the corresponding restricted q-Fock spaces defined. All of the irreducible highest weight representations, including the infinite dimensional ones, of $U_\epsilon^{\mathrm{res}}(sl_2)$ of type 1 are constructed through the restricted q-Fock spaces. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1389089]

I. INTRODUCTION AND NOTATIONS

In this article we take q and q^{-1} to be two indeterminates. We denote by $C(q)$ the field of rational functions of the indeterminate q and denote by $C[q,q^{-1}]$ the ring of Laurent polynomials in the indeterminates q and q^{-1}. As usual, the integer and non-negative integer sets are denoted by Z and Z^+, respectively, while the positive integer set, or the natural number set, is denoted by N. For $n\in Z, m\in N$ we use the following notations

$$[n]_q=\frac{q^n-q^{-n}}{q-q^{-1}},\quad [m]_q!=[m]_q[m-1]_q\cdots[1]_q,$$

$$\begin{bmatrix} n \\ m \end{bmatrix}_q=\frac{[n]_q[n-1]_q\cdots[n-m+1]_q}{[m]_q!}.$$

For an integer m that is not in N, we adopt the convention

$$\begin{bmatrix} n \\ m \end{bmatrix}_q=0.$$

For $\epsilon\in C$, $\left[\begin{smallmatrix} n \\ m \end{smallmatrix}\right]_\epsilon$ denotes the complex number obtained from $\left[\begin{smallmatrix} n \\ m \end{smallmatrix}\right]_q$ by substituting $q=\epsilon$ into the expression, as the symbol suggests.

Let U_q be an associative algebra over $C(q)$. Naively, it is natural to think of U_q as a family of algebras depending on a "parameter" q. Mathematically, this can be made precise as follows. If $\epsilon\in C$ is transcendental, one can specialize the indeterminate q to ϵ by defining $U_\epsilon=U_q\otimes_{C(q)}C$, via the algebra homomorphism $C(q)\to C$ that takes q to ϵ. When ϵ is algebraic the above homomorphism from $C(q)$ to C is not available and this direct specialization of U_q might not make sense. Nevertheless, one can proceed by first constructing a $C[q,q^{-1}]$-form, or integral form, of U_q, namely, a $C[q,q^{-1}]$-subalgebra $\tilde{U}_q$ of U_q such that $U_q=\tilde{U}_q\otimes_{C[q,q^{-1}]}C(q)$. Then one defines the specialization U_ϵ of U_q as $\tilde{U}_q\otimes_{C[q,q^{-1}]}C$, via the algebra homomorphism $C[q,q^{-1}]\to C$ that takes q to ϵ.

The quantum algebra $U_q(g)$ associated to a Kac–Moody algebra g is an associative algebra over $C(q)$. When ϵ is not a root of unity the representation theory of $U_\epsilon(g)$ has been well

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established.[1] To deal with the case where ϵ is a root of unity two $C[q,q^{-1}]$-forms of $U_q(g)$, namely, the "nonrestricted" form and the "restricted" form, have been introduced. In the "nonrestricted" form, one takes $\tilde{U}_q(g)$ to be the $C[q,q^{-1}]$-subalgebra of $U_q(g)$ generated by the Chevalley generators e_i, f_i and some other elements of $U_q(g)$. In this case, the finite dimensional representations of $U_\epsilon(g)$ have been studied by De Concini, Kac and Procesi, when g is finite dimensional, and by Beck and Kac, when g is untwisted affine.[2,3] The restricted $C[q,q^{-1}]$-form $U_q^{\mathrm{res}}(g)$ of $U_q(g)$ is introduced by Lusztig.[4] The study of representation theory of $U_\epsilon^{\mathrm{res}}(g)$ is pioneered also by Lusztig and developed by Chari and Pressley.[5–7]

The q-boson realization method has been widely used to construct representations of quantum algebras in both the generic case and the root of unity case.[8–16] Especially, cyclic q-boson algebra has been introduced to obtain the so called cyclic representations of $U_\epsilon(g)$ associated with the nonrestricted $C[q,q^{-1}]$-form of $U_q(g)$.[15,16] In this article, we will introduce two restricted $C[q,q^{-1}]$-forms of the well known q-boson algebra and define the restricted q-Fock spaces correspondingly. Then we will construct all irreducible highest weight representations of $U_\epsilon(sl_2)$ of type 1 on the restricted q-Fock spaces.

II. SOME BASIC FACTS ABOUT $U_\epsilon^{\mathrm{res}}(sl_2)$

Let us recall some definitions and basic facts. For details we refer readers to Ref. 1. Throughout this article we use the notation $\mathcal{A}=C[q,q^{-1}]$.

Definition 2.1: The quantum algebra $U_q(sl_2)$ is the associative algebra over $C(q)$ with generators e, f, K and K^{-1} and the following relations:

$$KK^{-1}=K^{-1}K=1,$$

$$KeK^{-1}=q^2e, \quad KfK^{-1}=q^{-2}f,$$

$$[e,f]=\frac{K-K^{-1}}{q-q^{-1}}.$$

Definition 2.2: The algebra $U_{\mathcal{A}}^{\mathrm{res}}(sl_2)$ is the $\mathcal{A}$-subalgebra of $U_q(sl_2)$ generated by the elements $e^{(r)}$, $f^{(r)}$, $K^{\pm 1}$ $(r\in N)$ for $r\geqslant 1$, where $e^{(r)}=e^r/[r]_q!$ and $f^{(r)}=f^r/[r]_q!$.

From now on we assume that ϵ is a primitive pth root of unity, where p is odd and greater than 1. When necessary, C is considered as $\mathcal{A}$-module via the the algebra homomorphism $\mathcal{A}\to C$ that takes q to ϵ. By definition, the restricted specialization of $U_q(sl_2)$ is

$$U_\epsilon^{\mathrm{res}}(sl_2)=U_{\mathcal{A}}^{\mathrm{res}}(sl_2)\otimes_{\mathcal{A}}C.$$

For simplicity, $e^{(r)}\otimes_{\mathcal{A}}1, f^{(r)}\otimes_{\mathcal{A}}1$ and $K^{\pm 1}\otimes_{\mathcal{A}}1$ will be identified with $e^{(r)}, f^{(r)}$ and $K^{\pm 1}$, respectively.

If V is a representation of $U_\epsilon^{\mathrm{res}}(sl_2)$ on which K is diagonalizable and $K^{\pm p}=1$, it is said to be of type 1.

Definition 2.3: Let m be an integer. The weight space V_m of a $U_\epsilon^{\mathrm{res}}(sl_2)$-module V of type 1 is defined by

$$V_m=\left\{v\in V \middle| Kv=\epsilon^m v, \quad \begin{bmatrix} K;0 \\ p \end{bmatrix}_q v=\begin{bmatrix} m \\ p \end{bmatrix}_\epsilon v\right\},$$

where

$$\begin{bmatrix} K;0 \\ p \end{bmatrix}_q=\prod_{s=1}^{p}\frac{Kq^{1-s}-K^{-1}q^{s-1}}{q^s-q^{-s}}$$

belongs to $U_{\mathcal{A}}^{\mathrm{res}}(sl_2)$ and is identified with $\left[\begin{smallmatrix} K;0 \\ p \end{smallmatrix}\right]_q\otimes_{\mathcal{A}}1$.

For any integer n, write $n=n_0+pn_1$, where n_0 and n_1 are integers and $0\leqslant n_0<p$. It is readily verified that

$$\begin{bmatrix} n \\ p \end{bmatrix}_\epsilon = n_1 .$$

Then by definition, $v\in V_m$ is a weight vector of weight m and we have

$$Kv=\epsilon^{m_0}v, \quad \begin{bmatrix} K;0 \\ p \end{bmatrix}_q v=m_1 v .$$

A $U_\epsilon^{\mathrm{res}}(sl_2)$-module V is called a highest module of type 1 if it is generated by a weight vector $v\in V_\lambda$ with $\lambda\in Z$ such that $ev=e^{(p)}v=0$. It follows by the usual argument that such a V has a unique irreducible quotient module.[1]

Denote by $V_\epsilon^{\mathrm{res}}(\lambda)$ the irreducible highest weight $U_\epsilon^{\mathrm{res}}(sl_2)$-module of type 1 and of highest weight λ. Then by the Verma module construction one can prove the following proposition.[1]

Proposition 2.1: $V_\epsilon^{\mathrm{res}}(\lambda)$ is isomorphic to $V_\epsilon^{\mathrm{res}}(\mu)$ if and only if $\lambda=\mu$.

III. RESTRICTED *q*-FOCK SPACES

The q-boson algebra $B_q(n)$ of rank n is the associative algebra over $C(q)$ generated by the elements a_i, a_i^+, $K_i^{\pm 1}$,1 $(i=1,2,\ldots,n)$ with the following relations:

$$a_i a_i^+ - q^2 a_i^+ a_i = 1, \quad [a_i, a_j^+]=0 \ (i\neq j),$$

$$[a_i, a_j]=[a_i^+, a_j^+]=0,$$

$$K_i a_j^+ K_i^{-1}=q^{\delta_{ij}}a_j^+, \quad K_i a_j K_i^{-1}=q^{-\delta_{ij}}a_j,$$

$$K_i K_i^{-1}=K_i^{-1}K_i=1,$$

where 1 is the unit.

We introduce the notations

$$a_i^{(n)}=\frac{a_i^n}{[n]_q!}, \quad a_i^{+(n)}=\frac{a_i^{+n}}{[n]_q!}$$

and the following definition.

Definition 3.1: The type 1 restricted q-boson algebra $B_q^{\mathrm{res1}}(2)$ of rank 2 is the $\mathcal{A}$-subalgebra of $B_q(2)$ generated by the elements a_i, $a_i^{+(r)}$, $K_i^{\pm 1}$,1 $(i=1,2; r\in N)$. The type 2 restricted q-boson algebra $B_q^{\mathrm{res2}}(2)$ of rank 2 is the $\mathcal{A}$-subalgebra of $B_q(2)$ generated by the elements a_1, $a_1^{+(r)}$, $a_2^{(r)}$, a_2^+, $K_1^{\pm 1}$, $K_2^{\pm 1}$,1 $(r\in N)$.

By induction one can prove the following three lemmas without difficulty.

Lemma 3.1:

$$\begin{bmatrix} r \\ k \end{bmatrix}_q = q^{-k}\begin{bmatrix} r-1 \\ k \end{bmatrix}_q + q^{r-k}\begin{bmatrix} r-1 \\ k-1 \end{bmatrix}_q \text{ for } r\geqslant k\geqslant 0.$$

Lemma 3.2:

$$\begin{bmatrix} r \\ k \end{bmatrix}_q \in C[q,q^{-1}] \text{ for } r\geqslant k\geqslant 0.$$

Lemma 3.3:

$$a_i^n a_i^{+(m)} = \sum_{s=0}^{m} q^{n(s+m)} q^{(s-m)(s+m+1)/2} \begin{bmatrix} n \\ m-s \end{bmatrix}_q a^{+(s)} a^{n-m+s},$$

$$a_i^{(n)} a_i^{+m} = \sum_{s=0}^{m} q^{n(s+m)} q^{(s-m)(s+m+1)/2} \begin{bmatrix} m \\ s \end{bmatrix}_q a^{+s} a^{(n-m+s)}.$$

Proposition 3.1: $\{a_1^{+(r_1)} a_2^{+(r_2)} a_1^{s_1} a_2^{s_2} K_1^{t_1} K_2^{t_2} | r_i, s_i \in Z^+, t_i \in Z; i=1,2\}$ is an $\mathcal{A}$-basis of $B_q^{\mathrm{res}1}(2)$; $\{a_1^{+(r_1)} a_2^{+r_2} a_1^{s_1} a_2^{(s_2)} K_1^{t_1} K_2^{t_2} | r_i, s_i \in Z^+, t_i \in Z; i=1,2\}$ is an $\mathcal{A}$-basis of $B_q^{\mathrm{res}2}(2)$.

Proof: It follows directly from Lemmas 3.2 and 3.3.

Corollary: $B_q^{\mathrm{res}1}(2)$ and $B_q^{\mathrm{res}2}(2)$ are two integral forms of $B_q(2)$.

Consider $B_q^{\mathrm{res}1}(2)$ as a $B_q^{\mathrm{res}1}(2)$-module as well as $C[q,q^{-1}]$-algebra. Let I be the left ideal of $B_q^{\mathrm{res}1}(2)$ generated by the elements

$$K_1 - 1, \quad K_2 - 1, \quad a_1, a_2.$$

Obviously, I is a $B_q^{\mathrm{res}1}(2)$-submodule. Let $\mathcal{F}_{\mathcal{A}}^1(2)$ denote the quotient module $B_q^{\mathrm{res}1}(2)/I$. It follows from Proposition 3.1 that $\mathcal{F}_{\mathcal{A}}^1(2)$ is a free $\mathcal{A}$-module and

$$\mathcal{F}_{\mathcal{A}}^1(2) = \mathrm{span}_{\mathcal{A}}\{a_1^{+(r_1)} a_2^{+(r_2)}|0\rangle | a_1|0\rangle = a_2|0\rangle = 0, \quad K_1|0\rangle = K_2|0\rangle = |0\rangle; r_1, r_2 \in Z^+\},$$

where $\{a_1^{+(r_1)} a_2^{+(r_2)}|0\rangle | r_1, r_2 \in Z^+\}$ is a basis of $\mathcal{F}_{\mathcal{A}}^1(2)$. $\mathcal{F}_{\mathcal{A}}^1(2)$ is called an $\mathcal{A}$-Fock module associated with $B_q^{\mathrm{res}1}(2)$. The $\mathcal{A}$-Fock module $\mathcal{F}_{\mathcal{A}}^2(2)$ associated with $B_q^{\mathrm{res}2}(2)$ can be defined in a similar way:

$$\mathcal{F}_{\mathcal{A}}^2(2) = \mathrm{span}_{\mathcal{A}}\{a_1^{+(r_1)} a_2^{+r_2}|0\rangle | a_1^r|0\rangle = a_2^{(r)}|0\rangle = 0, \quad r \in N; K_1|0\rangle = K_2|0\rangle = |0\rangle; r_1, r_2 \in Z^+\}.$$

It is easy to see that $\mathcal{F}_{\mathcal{A}}^1(2) \otimes_{\mathcal{A}} C(q) = \mathcal{F}_{\mathcal{A}}^2(2) \otimes_{\mathcal{A}} C(q) \triangleq \mathcal{F}_q(2)$ is the ordinary q-Fock space associated with $B_q(2)$. It is a vector space over the field $C(q)$. If we regard $\mathcal{F}_q(2)$ as an $\mathcal{A}$-module, then by identifying $\mathcal{F}_{\mathcal{A}}^1(2)$ with $\mathcal{F}_{\mathcal{A}}^1(2) \otimes_{\mathcal{A}} 1$, $\mathcal{F}_{\mathcal{A}}^1(2)$ becomes a submodule of $\mathcal{F}_q(2)$, and $\mathcal{F}_{\mathcal{A}}^2(2)$ likewise becomes a submodule of $\mathcal{F}_q(2)$. For convenience, in the subsequent discussion we will use the following notations:

$$f(r_1, r_2) = a_1^{+(r_1)} a_2^{+(r_2)}|0\rangle,$$

$$g(r_1, r_2) = a_1^{+(r_1)} a_2^{+r_2}|0\rangle.$$

We define

$$\mathcal{F}_{\epsilon}^1(2) = \mathcal{F}_{\mathcal{A}}^1(2) \otimes_{\mathcal{A}} C,$$

$$\mathcal{F}_{\epsilon}^2(2) = \mathcal{F}_{\mathcal{A}}^2(2) \otimes_{\mathcal{A}} C,$$

and identify $f(r_1, r_2) \otimes_{\mathcal{A}} 1$ and $g(r_1, r_2) \otimes_{\mathcal{A}} 1$ with $f(r_1, r_2)$ and $g(r_1, r_2)$, respectively. $\mathcal{F}_{\epsilon}^1(2)$ and $\mathcal{F}_{\epsilon}^2(2)$ will be referred to as restricted q-Fock spaces. In the following sections, we will construct irreducible representations of $U_{\epsilon}^{\mathrm{res}}(sl_2)$ on the restricted q-Fock spaces.

IV. FINITE DIMENSIONAL REPRESENTATIONS OF $U_{\epsilon}^{\mathrm{res}}(sl_2)$ VIA RESTRICTED q-FOCK SPACE

We recall that $U_q(sl_2)$ has the following realization on $\mathcal{F}_q(2)$:[8]

$$e = K_2^{-1} a_1^+ a_2, \quad f = K_1^{-1} a_1 a_2^+,$$

$$K=K_1K_2^{-1},\quad K^{-1}=K_1^{-1}K_2.$$

Remark: The above realization looks different from that presented in Ref. 8. This is because the generators of the q-boson algebra adopted in this article are slightly different from those in Ref. 8.

By the natural action $\mathcal{F}_q(2)$ becomes a $U_q(sl_2)$-module through this realization. Then naturally it becomes a $U_{\mathcal{A}}^{\mathrm{res}}(sl_2)$-module through the realization

$$e^{(r)}=q^{-r(r-1)/2}K_2^{-r}a_1^{+(r)}a_2^r,\quad f^{(r)}=q^{-r(r-1)/2}K_1^{-r}a_2^{+(r)}a_1^r.$$

It turns out that $\mathcal{F}_{\mathcal{A}}^1(2)$ is a $U_{\mathcal{A}}^{\mathrm{res}}(sl_2)$-submodule. In fact, the action of $U_{\mathcal{A}}^{\mathrm{res}}(sl_2)$ on $\mathcal{F}_{\mathcal{A}}^1(2)$ reads as follows:

$$Kf(r_1,r_2)=q^{r_1-r_2}f(r_1,r_2),\quad K^{-1}f(r_1,r_2)=q^{r_2-r_1}f(r_1,r_2),$$

$$e^{(r)}f(r_1,r_2)=\begin{bmatrix} r+r_1 \\ r \end{bmatrix}_q f(r_1+r,r_2-r),$$

$$f^{(r)}f(r_1,r_2)=\begin{bmatrix} r+r_2 \\ r \end{bmatrix}_q f(r_1-r,r_2+r).$$

Here we have used Lemma 3.3 and the formula

$$a_i^{+(m)}a_i^{+(n)}=\begin{bmatrix} m+n \\ m \end{bmatrix}_q a_i^{+(m+n)}\ \text{ for }\ i=1,2;\quad m,n\in N.$$

Thus it follows that $U_{\mathcal{A}}^{\mathrm{res}}(sl_2)\mathcal{F}_{\mathcal{A}}^1(2)\subset\mathcal{F}_{\mathcal{A}}^1(2)$. This proves the claim.

Clearly, $\mathcal{F}_\epsilon^1(2)$ is a $U_{\mathcal{A}}^{\mathrm{res}}(sl_2)$-module. It then follows that it is also a $U_\epsilon^{\mathrm{res}}(sl_2)$-module. Here the action of $U_\epsilon^{\mathrm{res}}(sl_2)$ on $\mathcal{F}_\epsilon^1(2)$ is induced from that of $U_{\mathcal{A}}^{\mathrm{res}}(sl_2)$ by identifying q with ϵ. Explicitly, we have

$$Kf(r_1,r_2)=\epsilon^{r_1-r_2}f(r_1,r_2),\quad K^{-1}f(r_1,r_2)=\epsilon^{r_2-r_1}f(r_1,r_2),$$

$$e^{(r)}f(r_1,r_2)=\begin{bmatrix} r+r_1 \\ r \end{bmatrix}_\epsilon f(r_1+r,r_2-r),$$

$$f^{(r)}f(r_1,r_2)=\begin{bmatrix} r+r_2 \\ r \end{bmatrix}_\epsilon f(r_1-r,r_2+r).$$

We observe that for $m\in N$ the subspace

$$V_m\triangleq\mathrm{span}_C\{f(r_1,r_2)\,|\,r_1+r_2=m\}$$

of $\mathcal{F}_\epsilon^1(2)$ is a $U_\epsilon^{\mathrm{res}}(sl_2)$-submodule. Define $v_i^{(m)}=f(m-i,i)$ for $i=0,1,\ldots,m$. Then $\{v_0^{(m)},\ldots,v_m^{(m)}\}$ is a basis of V_m.

The action of $U_\epsilon^{\mathrm{res}}(sl_2)$ on V_m is given by

$$Kv_r^{(m)}=\epsilon^{m-2r}v_r^{(m)},\quad K^{-1}v_r^{(m)}=\epsilon^{2r-m}v_r^{(m)},$$

$$ev_r^{(m)}=[m-r+1]_\epsilon v_{r-1}^{(m)},\quad fv_r^{(m)}=[r+1]_\epsilon v_{r+1}^{(m)},$$

$$e^{(p)}v_r^{(m)}=((m-r)_1+1)v_{r-p}^{(m)},\quad f^{(p)}v_r^{(m)}=(r_1+1)v_{r+p}^{(m)}.$$

Here $v_i^{(m)}$ is understood as the zero vector if $i<0$ or $i>m$. We notice that V_m is none other than the so called Weyl module $W_\epsilon^{\mathrm{res}}(m)$ with maximal weight m. Consequently, we have the following result.

Proposition 4.1: V_m is irreducible if and only if either $m<p$ or $m_0=p-1$. If V_m is reducible, it is not completely reducible.

A sketch of the proof of this proposition can be found in Ref. 1. The main point is the observation that

$$V' \triangleq \mathrm{span}_C\{v_r^{(m)} | m_0<r_0<p,\ \ r_1<m_1\}$$

is the unique proper $U_\epsilon^{\mathrm{res}}(sl_2)$-submodule of V_m.

Remark: It is an established fact that every finite dimensional irreducible $U_\epsilon^{\mathrm{res}}(sl_2)$-module of type 1 is a quotient module of Weyl module. As we have realized the Weyl module $W_\epsilon^{\mathrm{res}}(m)$ for an arbitrary $m \in N$ via the q-Fock space, we have actually presented q-Fock space construction for all finite dimensional irreducible representations of type 1 of $U_\epsilon^{\mathrm{res}}(sl_2)$.

V. INFINITE DIMENSIONAL REPRESENTATIONS OF $U_\epsilon^{\mathrm{res}}(sl_2)$ VIA RESTRICTED q-FOCK SPACE

In this section let us turn to consider q-Fock space construction for some infinite dimensional irreducible representations of $U_\epsilon^{\mathrm{res}}(sl_2)$. To this end, we need to use another q-boson realization of $U_q(sl_2)$. Our starting point is the following well-known q-boson realization of $U_q(sl_2)$ on $\mathcal{F}_q(2)$:[13]

$$K=q^{-1}K_1^{-1}K_2^{-1}, \quad K^{-1}=qK_1K_2,$$

$$e=K_1^{-1}K_2^{-1}a_1a_2, \quad f=-a_1^+a_2^+.$$

By definition $\mathcal{F}_q(2)$ is a $U_q(sl_2)$-module, and thus a $U_{\mathcal{A}}^{\mathrm{res}}(sl_2)$-module, the action on $\mathcal{F}_q(2)$ being the natural one. We have

$$e^{(r)}=q^{-r(r-1)}K_1^{-r}K_2^{-r}a_1^r a_2^{(r)}, \quad f^{(r)}=(-1)^r a_1^{+(r)}a_2^{+r}.$$

Then it follows from Lemma 3.3 that

$$e^{(r)}g(r_1,r_2)=\begin{bmatrix} r_2 \\ r_2-r \end{bmatrix}_q g(r_1-r,r_2-r),$$

$$f^{(r)}g(r_1,r_2)=(-1)^r\begin{bmatrix} r+r_1 \\ r \end{bmatrix}_q g(r_1+r,r_2+r),$$

namely, $U_{\mathcal{A}}^{\mathrm{res}}(sl_2)\mathcal{F}_{\mathcal{A}}^2(2)\subset\mathcal{F}_{\mathcal{A}}^2(2)$. Consequently, $\mathcal{F}_{\mathcal{A}}^2(2)$, and hence $\mathcal{F}_\epsilon^2(2)$, is a $U_{\mathcal{A}}^{\mathrm{res}}(sl_2)$-module. Finally, $\mathcal{F}_\epsilon^2(2)$ becomes a $U_\epsilon^{\mathrm{res}}(sl_2)$-module in the obvious way. Explicitly, the action of $U_\epsilon^{\mathrm{res}}(sl_2)$ on $\mathcal{F}_\epsilon^2(2)$ is as follows:

$$Kg(r_1,r_2)=\epsilon^{-(r_1+r_2+1)}g(r_1,r_2), \quad K^{-1}g(r_1,r_2)=\epsilon^{(r_1+r_2+1)}g(r_1,r_2),$$

$$e^{(r)}g(r_1,r_2)=\begin{bmatrix} r_2 \\ r_2-r \end{bmatrix}_\epsilon g(r_1-r,r_2-r),$$

$$f^{(r)}g(r_1,r_2)=(-1)^r\begin{bmatrix} r+r_1 \\ r \end{bmatrix}_\epsilon g(r_1+r,r_2+r).$$

On $\mathcal{F}_\epsilon^2(2)$, we have

$$\begin{bmatrix} K;0 \\ p \end{bmatrix}_q = \prod_{s=1}^{p} \frac{Kq^{1-s}-K^{-1}q^{s-1}}{q^s-q^{-s}} = \prod_{s=1}^{p} \frac{K_1^{-1}K_2^{-1}q^{-s}-K_1K_2q^s}{q^s-q^{-s}}.$$

Thus

$$\begin{bmatrix} K;0 \\ p \end{bmatrix}_q g(r_1,r_2) = \begin{bmatrix} -r_1-r_2-1 \\ p \end{bmatrix}_\epsilon g(r_1,r_2) = -(r_1+r_2+1)_1 g(r_1,r_2)$$

Hence, $g(r_1,r_2)$ is a weight vector of the weight $-(r_1+r_2+1)$ and $\mathcal{F}_\epsilon^2(2)$ is a $U_\epsilon^{\rm res}(sl_2)$-module of type 1.

For an arbitrary integer s, define

$$V^s = \mathrm{span}_C\{g(r_1,r_1+s)|r_1 \in Z^+\}.$$

We observe that V^s is a $U_\epsilon^{\rm res}(sl_2)$-submodule and there is the following decomposition:

$$\mathcal{F}_\epsilon^2(2) = \sum_{s\in Z} \oplus V^s.$$

For s that satisfies $s_0=0$, namely, $s=\pm rp (r\in Z^+)$, we have the following result.

Proposition 5.1: For $r\in Z^+$, $V^{\pm rp}$ is isomorphic to $V_\epsilon^{\rm res}(-(rp+1))$.

Proof: We only need to consider the case of V^{rp}. The other case is similar. We first show that V^{rp} is an infinite dimensional irreducible $U_\epsilon^{\rm res}(sl_2)$-module. For $m\in Z^+$ define $g(m)=g(m,m+rp)$. Then $\{g(m)|m\in Z^+\}$ is a basis of V^{rp}. We have

$$eg(m) = [m]_\epsilon g(m-1), \quad fg(m) = -[m+1]_q g(m+1)$$

and

$$e^{(p)}g(np) = ng((n-1)p), \quad f^{(p)}g(np-1) = (n-1)g((n+1)p-1)$$

for $n\in N$. Using these relations, one can easily show that as a $U_\epsilon^{\rm res}(sl_2)$-module V^{rp} can be generated by an arbitrary vector in it. The irreducibility is thus proved.

As shown above, $g(0)$ is a weight vector of the weight $-(1+rp)$. It is easy to see that it is actually a highest weight vector. On the other hand, it is clear that V^{rp} is a highest weight module: $V^{rp}= U_\epsilon^{\rm res}(sl_2)g(0)$. The claim then follows from the irreducibility of V^{rp}.

Now let us study V^s with $s_0\neq 0$. When $s>0$, define $v_m=g(m,m+s)$ and the subspace V' of V^s:

$$V' = \mathrm{span}_C\{v_m|p>m_0\geqslant p-s_0\}.$$

When $s<0$, we use W^s to denote V^s for convenience. Then

$$W^s = \mathrm{span}_C\{g(r_1+|s|,r_1)|r_1\in Z^+\}.$$

We define $w_m=g(m+|s|,m)$ and the subspace W' of W^s:

$$W' = \mathrm{span}_C\{w_m|0\leqslant m_0<p-s_0\}.$$

It is not difficult to see that V' and W' are proper submodules of V^s and W^s, respectively.

Proposition 5.2: V' is isomorphic to $V_\epsilon^{\rm res}(\lambda)$ with $\lambda=-(p-s_0+(s_1+1)p+1)$.

Proof: By the explicit action of $U_\epsilon^{\rm res}(sl_2)$ on $\mathcal{F}_\epsilon^2(2)$, it is not difficult to see that V' is irreducible and $V'=U_\epsilon^{\rm res}(sl_2)v_{p-s_0}$. Since v_{p-s_0} is the highest weight vector of V' of the weight $-(p-s_0+(s_1+1)p+1)$, the proposition then follows.

Proposition 5.3: V' is the unique maximal proper $U_\epsilon^{\rm res}(sl_2)$-submodule of V^s with $s>0$ and $s_0\neq 0$.

Proof: Let V'' be an arbitrary proper $U_\epsilon^{\rm res}(sl_2)$-submodule of V^s. To prove the proposition, we only need to show that it is included in V'. We observe that V'' has the vector space decomposition

$$V''=\sum_{\lambda\in\Lambda_s}\oplus(V_\lambda^s\cap V''),$$

where Λ_s stands for the weight set of V^s. Suppose v is a vector in V''. Define

$$\Lambda_s'=\{\lambda\in\Lambda_s|\lambda_0\geqslant p-s_0\},$$

$$\Lambda_s''=\{\lambda\in\Lambda_s|\lambda_0<p-s_0\}.$$

Then we can write $v=v_1+v_2$ where

$$v_1\in\sum_{\lambda\in\Lambda_s''}\oplus V_\lambda^s,\quad v_2\in\sum_{\lambda\in\Lambda_s'}\oplus V_\lambda^s\in V'.$$

Now due to the above vector space decomposition of V'', we have $v_1\in V''$. On the other hand, if v_1 is a nonzero vector, it is not difficult to show that $U_\epsilon^{\rm res}(sl_2)v_1=V^s$. Consequently, $v_1=0$ as V'' is a proper $U_\epsilon^{\rm res}(sl_2)$-submodule by assumption. This means $v=v_2\in V'$, namely, $V''\subset V'$. The proposition is thus proved.

Corollary: For V^s with $s>0$ and $s_0\neq 0$, V^s/V' is isomorphic to $V_\epsilon^{\rm res}(-(s+1))$.

Proof: Since V' is a maximal proper submodule, V^s/V' is irreducible. Moreover, V^s/V' is a highest module with the highest vector $\overline{v_0}\triangleq v_0+V'=g(0,s)+V'$ of the weight $-(s+1)$. The corollary thus follows.

Remark: Obviously, the above studied $U_\epsilon^{\rm res}(sl_2)$-modules V^{np}, V' and V^s/V' are all infinite dimensional. We notice that they are isomorphic to the modules $V_\epsilon^{\rm res}(\lambda)$ with λ negative. This should be the case. Actually, if λ is a positive integer $V_\epsilon^{\rm res}(\lambda)$ must be finite dimensional.

In the same way, we can prove the following result.

Proposition 5.4: W' is isomorphic to $V_\epsilon^{\rm res}(-(|s|+1))$; W^s/W' is isomorphic to $V_\epsilon^{\rm res}(\lambda)$ with $\lambda=-(p-|s|_0+(1+|s|_1)p+1)$.

From Proposition 5.1, the corollary to Proposition 5.3 and the remark at the end of Sec. IV we come to the conclusion that we have constructed all the representations $V_\epsilon^{\rm res}(\lambda)$ of $U_\epsilon^{\rm res}(sl_2)$ with $\lambda\in Z$ via the restricted q-Fock spaces. According to Proposition 2.1 they have exhausted all the irreducible highest representations of $U_\epsilon^{\rm res}(sl_2)$ of type 1. Obviously, the method presented in this article can readily be generalized to be applicable to the case of $U_\epsilon^{\rm res}(sl_n)$.

It might be interesting to probe the unitarity of the representations presented in this article. For this problem we wish to make the following comment. First, in the case of quantum algebras, the problem of unitarity of representations is not so important as in the case of Lie groups. One can clearly see this point from the literature of quantum algebras. Second, whether a representation is a unitary one depends not only on the inner product on the side of the representation space, but also on the so-called*-structure on the side of the quantum algebra. Besides, in our article, most of the irreducible representations that we present are defined on the quotient spaces of the restricted Fock spaces. Hence, it might be too simplistic to think that the question of unitarity can be addressed by simply asking whether $a^\dagger$ is the true adjoint of a.

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Chains of Frobenius subalgebras of so(M) and the corresponding twists

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Chains of extended Jordanian twists are studied for the universal enveloping algebras U(so(M)). The carrier subalgebra of a canonical chain $\mathcal{F}_{\mathcal{B}_{0<p\max}}$ cannot cover the maximal nilpotent subalgebra $N^+(\mathrm{so}(M))$. We demonstrate that there exist other types of Frobenius subalgebras in so(M) that can be large enough to include $N^+(\mathrm{so}(M))$. The problem is that the canonical chains $\mathcal{F}_{\mathcal{B}_{0<p}}$ do not preserve the primitivity on these new carrier spaces. We show that this difficulty can be overcome and the primitivity can be restored if one changes the basis and passes to the deformed carrier spaces. Finally, the twisting elements for the new Frobenius subalgebras are explicitly constructed. This gives rise to a new family of universal R-matrices for orthogonal algebras. For a special case of $g=\mathrm{so}(5)$ and its defining representation we present the corresponding matrix solution of the Yang–Baxter equation. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1402177]

I. INTRODUCTION

Quantizations of triangular Lie bialgebras with antisymmetric classical r-matrices $r=-r_{21}$ satisfying the classical Yang–Baxter equation (CYBE) form an important class of triangular Hopf algebras $\mathcal{A}(m,\Delta,S,\eta,\epsilon;\mathcal{R})$, with R-matrix satisfying the unitarity condition $\mathcal{R}_{21}\mathcal{R}=1$. These quantizations are defined by the twisting elements $\mathcal{F}=\Sigma f_{(1)}\otimes f_{(2)}\in\mathcal{A}\otimes\mathcal{A}$ that satisfy the twist equations:[1]

$$(\mathcal{F})_{12}(\Delta\otimes\mathrm{id})\mathcal{F}=(\mathcal{F})_{23}(\mathrm{id}\otimes\Delta)\mathcal{F},\quad(\epsilon\otimes\mathrm{id})\mathcal{F}=(\mathrm{id}\otimes\epsilon)\mathcal{F}=1. \tag{1}$$

The knowledge of the twisting element is quite important in applications giving (twisted) R-matrix $\mathcal{R}_F=\mathcal{F}_{21}\mathcal{R}\mathcal{F}^{-1}$ and twisted coproduct $\Delta_{\mathcal{F}}=\mathcal{F}\Delta\mathcal{F}^{-1}$.

Although for the general antisymmetric r-matrix the solution of the equation (1) was given in Ref. 1 in terms of Campbell–Hausdorf series quite few twisting elements were known in the explicit form: the Reshetikhin (Abelian) twists[2] and the Jordanian twist.[3,4] The explicit expressions of the more complicated twisting elements $\mathcal{F}$ were found in Ref. 5, for the carrier algebras **L** with special properties of their triangular decompositions. In the minimal case such algebras are four-dimensional. They can be considered as enlarged Heisenberg algebras with the defining relations

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$$[H,E]=E,\quad [H,A]=\alpha A,\quad [H,B]=\beta B,$$
$$[A,B]=E,\quad [E,A]=[E,B]=0,\qquad \alpha+\beta=1. \tag{2}$$

If the generators of $\mathbf{L}$ have primitive coproducts, the following group two-cocycle (twist) can be found as a solution of the Drinfeld equation (1):

$$\mathcal{F}_{\mathcal{E}(\alpha,\beta)}=\Phi_{\mathcal{E}(\alpha,\beta)}\Phi_j \tag{3}$$

with the Jordanian twist[3]

$$\Phi_j=\exp\{H\otimes\sigma\},\quad \sigma=\ln(1+E), \tag{4}$$

and the additional twisting factor[5,6]

$$\Phi_{\mathcal{E}(\alpha,\beta)}=\exp\{A\otimes Be^{-\beta\sigma}\}. \tag{5}$$

Such solutions (3) are called the extended Jordanian twists. They define the deformed Hopf algebra $\mathbf{L}_{\mathcal{E}(\alpha,\beta)}$ with the costructure

$$\Delta_{\mathcal{E}(\alpha,\beta)}(H)=H\otimes e^{-\sigma}+1\otimes H-A\otimes Be^{-(\beta+1)\sigma},$$
$$\Delta_{\mathcal{E}(\alpha,\beta)}(A)=A\otimes e^{-\beta\sigma}+1\otimes A,$$
$$\Delta_{\mathcal{E}(\alpha,\beta)}(B)=B\otimes e^{\beta\sigma}+e^{\sigma}\otimes B,$$
$$\Delta_{\mathcal{E}(\alpha,\beta)}(E)=E\otimes e^{\sigma}+1\otimes E=E\otimes 1+1\otimes E+E\otimes E. \tag{6}$$

In the simple Lie algebras of rank greater than 2 one can find not only the subalgebra $\mathbf{L}$ but also its multidimensional analog $\mathbf{L}_K$ $(K=0,1,\dots)$.[5,7] To construct the subalgebra $\mathbf{L}_0\subset g$ it is sufficient to choose an initial root λ_0 and consider the set π of its constituent roots

$$\pi=\{\lambda',\lambda''|\lambda'+\lambda''=\lambda_0,\quad \lambda'+\lambda_0,\lambda''+\lambda_0\notin\Lambda(g)\},$$
$$\pi=\pi'\cup\pi'',\quad \pi'\cap\pi''=0,\quad \pi'=\{\lambda'\},\pi''=\{\lambda''\}. \tag{7}$$

The subalgebra $\mathbf{L}_0$ is generated by the elements $\{E_{\lambda_0},E_\lambda|\lambda\in\pi\}$ and the Cartan generator H_{λ_0} dual to λ_0. The solution $\mathcal{F}_{\mathcal{E}_0\mathcal{J}_0}$ of the twist equations corresponding to the carrier subalgebra $\mathbf{L}_0$ is a multidimensional analog of (3). It also can be decomposed into the product of two factors, the Jordanian twist and the extension:

$$\mathcal{F}_{\mathcal{E}_0\mathcal{J}_0}=\Phi_{\mathcal{E}_0}\cdot\Phi_{\mathcal{J}_0}=\prod_{\lambda'\in\pi'}\exp\left\{E_{\lambda'}\otimes E_{\lambda_0-\lambda'}e^{-(1/2)\sigma_{\lambda_0}}\right\}\cdot\exp\{H_{\lambda_0}\otimes\sigma_{\lambda_0}\}. \tag{8}$$

Here $\sigma_{\lambda_0}=\ln(1+E_{\lambda_0})$ and $[H_{\lambda_0},E_{\lambda_0}]=E_{\lambda_0}$.

Each carrier subalgebra $\mathbf{L}_K$ is a semidirect sum $\mathbf{L}_K=\mathbf{L}\dot{\oplus}\mathbf{L}_{K-1}$. Thus the multidimensional subalgebras $\mathbf{L}_K$ can be constructed successively. To find a multidimensional carrier $\mathbf{L}_1$ in the simple algebra g consider the subset $\Lambda^{\perp}_{\lambda_0^0}$ of roots orthogonal to λ_0^0 and the corresponding subalgebra $g^{\perp}_{\lambda_0^0}\subset g$. In $g^{\perp}_{\lambda_0^0}$ a new initial root λ_0^1 can be chosen and its constituent roots $\pi^1\subset\Lambda(g^{\perp}_{\lambda_0^0})$ can be found according to the rules (7). The corresponding generators $\{H_{\lambda_0^1},E_{\lambda_0^1},E_{\lambda^1}|\lambda^1\in\pi^1\}$ form the subalgebra $\mathbf{L}(g^{\perp}_{\lambda_0^0})$ and $\mathbf{L}_1=\mathbf{L}(g^{\perp}_{\lambda_0^0})\dot{\oplus}\mathbf{L}_0$. The subalgebra $\mathbf{L}(g^{\perp}_{\lambda_0^0})$ commutes with $H_{\lambda_0^0},E_{\lambda_0^0}$ and acts on $\{E_\lambda|\lambda\in\pi^0=\pi\}\subset\mathbf{L}_0$ as on an ideal.

It was shown in Ref. 7 that for the classical Lie algebras g one can always find a subalgebra g_1 in $g^{\perp}_{\lambda_0}$ whose generators become primitive after the twist $\mathcal{F}_{\mathcal{E}_0\mathcal{J}_0}$. The root diagrams $\Lambda(g_1)$ and $\Lambda(g)$ are of the same type. So, it is always possible to the find the root λ^1_0 and the set π^1 in $\Lambda(g_1)$. Repeating this procedure we get the sequence of injections $g_p \subset \cdots \subset g_1 \subset g_0 = g$ and the corresponding sequence of subalgebras $\mathbf{L}_K$. The coproduct primitivization of $g_k \subset g_{k-1}$ (called the Matreshka effect) makes it possible to compose chains of extended twists of the type (8),

$$
\begin{aligned}
\mathcal{F}_{\mathcal{B}_{0<p}} &= \mathcal{F}_{\mathcal{E}_p\mathcal{J}_p} \cdot \cdots \cdot \mathcal{F}_{\mathcal{E}_0\mathcal{J}_0} \\
&= \prod_{\lambda' \in \pi'_p} \exp\{E_{\lambda'} \otimes E_{\lambda^p_0 - \lambda'} e^{-(1/2)\,\sigma_{\lambda^p_0}}\} \cdot \exp\{H_{\lambda^p_0} \otimes \sigma_{\lambda^p_0}\} \\
&\quad \cdot \prod_{\lambda' \in \pi'_{p-1}} \exp\{E_{\lambda'} \otimes E_{\lambda^{p-1}_0 - \lambda'} e^{-(1/2)\,\sigma_{\lambda^{p-1}_0}}\} \cdot \exp\{H_{\lambda^{p-1}_0} \otimes \sigma_{\lambda^{p-1}_0}\} \\
&\quad \cdot \ldots \\
&\quad \cdot \prod_{\lambda' \in \pi'_0} \exp\{E_{\lambda'} \otimes E_{\lambda^0_0 - \lambda'} e^{-(1/2)\,\sigma_{\lambda^0_0}}\} \cdot \exp\{H_{\lambda^0_0} \otimes \sigma_{\lambda^0_0}\}. \qquad (9)
\end{aligned}
$$

Consider the Bruhat decomposition $g = \mathbf{N}^+ + \mathbf{H} + \mathbf{N}^- = \mathbf{B}^+ + \mathbf{N}^-$. As it was demonstrated earlier, there exists the systematic structure governing the twists with the carriers in the Borel subalgebra $\mathbf{B}^+$ of g. On the other hand, it follows from our studies in Ref. 7 that this structure (a chain of extended twists) is insufficient to compose a solution of Drinfeld equations when the carrier algebra of the classical r-matrix is greater than $\mathbf{B}^+$. In the latter case the twisting element will contain the chain as a factor but as a whole the structure will be considerably different from that of a chain. Thus the twists that can be described by chains have their carriers in $\mathbf{B}^+$. Now let us look at the Cartan subalgebra H of g. In general the number of links of a chain is less than rank(g). For example, for sl(N) the number of links is $[N/2]$. Consider the largest possible twist for sl(N) with the structure of a chain. Its carrier contains $\mathbf{N}^+$. Still, in such chain the $N - [N/2] - 1$ Cartan generators remain uninvolved. This means that to characterize the size of the chain one must compare its carrier with the maximal nilpotent subalgebra $\mathbf{N}^+$ of g. This is why we call the chains *full* if their carriers contain $\mathbf{N}^+$. In the case $g = \mathrm{sl}(N)$ the subalgebras g_k (they remain primitive after the twisting by $\mathcal{F}_{\mathcal{E}_{k-1}\mathcal{J}_{k-1}}$) coincide with $g^{\perp}_{\lambda_{k-1}}$. The result is that the maximal canonical chain $\mathcal{F}_{\mathcal{B}_{0<p\max}}$ for $g = \mathrm{sl}(N)$ is full, and its carrier subalgebra contains all the generators of the nilpotent subalgebra $\mathbf{N}^+(g)$.

For the orthogonal simple algebras the situation is different. In this case $g^{\perp}_{\lambda_{k-1}} = g_k \oplus \mathrm{sl}^{(k)}(2)$ and the coproducts of generators in the space $g^{\perp}_{\lambda_{k-1}} > g_k$ are nontrivially deformed by the twist $\mathcal{F}_{\mathcal{E}_{k-1}\mathcal{J}_{k-1}}$. The next extended twist $\mathcal{F}_{\mathcal{E}_k\mathcal{J}_k}$ does not contain these generators in its carrier space. Such a chain cannot be full.

The canonical twists (9) correspond to solutions of the CYBE related with Frobenius subalgebras in g described by the coboundary bilinear forms $\omega^+_p = \Sigma^p_{k=0} E^*_{\lambda^k_0}([\ ,\ ])$.[8] In this article we show that for the orthogonal algebras these forms can be modified. The Frobenius subalgebras can be enlarged in order to include all nonzero root generators from $g^{\perp}_{\lambda_{k-1}} > g_k$. (Sec. II).

The problem is how to find the corresponding twists, i.e., to solve the equations (1) for the subalgebra $g^{\perp}_{\lambda_{k-1}}$ that contains the generators with deformed coproducts $\Delta_{\mathcal{F}_{\mathcal{E}_k\mathcal{J}_k}}$.

In Ref. 9 it was demonstrated that under certain conditions (while the coproducts in g are nontrivially twisted by $\mathcal{F}$) one can find in $U_{\mathcal{F}}(g)$ the deformed carrier subspace that is primitive and generates a subalgebra of g. Below we show that this effect is in some sense universal. The corresponding deformed spaces for orthogonal algebras can be found for any extended twist $\mathcal{F}_{\mathcal{E}_{k-1}\mathcal{J}_{k-1}}$. As a result the canonical chain of twists $\mathcal{F}_{\mathcal{B}_{0<p}}$ can be extended using some additional

factors (the deformed Jordanian twists). For the maximal value of p the corresponding chain $\mathcal{F}_{\mathcal{G}_{0<p}}$ becomes full and the corresponding carrier space contains all the generators of $\mathbf{N}^+(g)$ (Sec. III).

In Sec. IV we discuss the possible applications of the composed twists. The explicit form of the parametrized R-matrix in the defining representation of so(5) is given in the Appendix.

II. FROBENIUS SUBALGEBRAS

Here we deal with the universal enveloping algebras for simple classical Lie algebras over the field of characteristic zero. In particular we consider the complex orthogonal algebras $g=\mathrm{so}(M)$ of the series B_N (for $M=2N+1$) and D_N (for $M=2N$). The root system $\Lambda(g)$ will be fixed as follows:

$$\Lambda(g)=\begin{cases}\pm e_i,\ \pm e_j\pm e_k & \text{for } g=so(2N+1),\\ \pm e_i\pm e_j & \text{for } g=so(2N),\end{cases}\qquad i,j,k=1,\ldots,N. \tag{10}$$

Let $\mathcal{E}_{i,j}$ be the ordinary matrix units,

$$[\mathcal{E}_{i,j},\mathcal{E}_{k,l}]=\delta_{jk}\mathcal{E}_{i,l}-\delta_{il}\mathcal{E}_{k,j},$$

and $M_{i,j}$ be the antisymmetric ones,

$$[M_{a,b},M_{c,d}]=\delta_{bc}M_{a,d}+\delta_{ad}M_{b,c}-\delta_{ac}M_{b,d}-\delta_{bd}M_{a,c}.$$

The generators of $g=\mathrm{so}(M)$ can be realized as follows. The Cartan subalgebra $\mathcal{H}(g)$ is generated by

$$H_j=\left(-\frac{i}{2}\right)M_{2j-1,2j},\quad j=1,\ldots,N. \tag{11}$$

For Cartan generators we shall also use the notation

$$H_{j\pm(j+1)}=\left(-\frac{i}{2}\right)(M_{2j-1,2j}\pm M_{2j+1,2j+2}). \tag{12}$$

To the roots of $\Lambda(\mathrm{so}(M))$ we attribute the generators

$$\left.\begin{aligned}E_{i+j}&=\tfrac{1}{2}(-M_{2i,2j}+iM_{2i,2j-1}+iM_{2i-1,2j}+M_{2i-1,2j-1});\\ E_{i-j}&=\tfrac{1}{2}(-M_{2i,2j}-iM_{2i,2j-1}+iM_{2i-1,2j}-M_{2i-1,2j-1});\\ E_{-i+j}&=\tfrac{1}{2}(+M_{2i,2j}-iM_{2i,2j-1}+iM_{2i-1,2j}+M_{2i-1,2j-1});\\ E_{-i-j}&=\tfrac{1}{2}(+M_{2i,2j}+iM_{2i,2j-1}+iM_{2i-1,2j}-M_{2i-1,2j-1});\end{aligned}\right\}\quad i<j; \tag{13}$$

and

$$E_{\pm k}=\frac{1}{\sqrt{2}}(\pm M_{2k,2N+1}-iM_{2k-1,2N+1}),\quad k\leqslant N,\quad \text{for so}(2N+1). \tag{14}$$

The Borel subalgebras $B(g)$ are generated by the sets $\{H_i,E_i,E_{i\pm j}\}$ for $g=\mathrm{so}(2N+1)$ and $\{H_i,E_{i\pm j}\}$ for $g=\mathrm{so}(2N)$. To describe the chains of Frobenius subalgebras we shall also need the alternative realization of these generators through the ordinary matrix units. To get it let us renumerate the generators:

$$\left.\begin{aligned} A_{i,j} &\equiv -E_{i-j}, \\ A_{i,2N+2-j} &\equiv -E_{i+j}, \\ A_{i,N+1} &\equiv -E_i, \end{aligned}\right\} \quad \text{for so}(2N+1) \tag{15}$$

and

$$\left.\begin{aligned} A_{i,j} &\equiv -E_{i-j}, \\ A_{i,2N+1-j} &\equiv -E_{i+j}, \end{aligned}\right\} \quad \text{for so}(2N). \tag{16}$$

In these terms the Borel subalgebra $B(\mathrm{so}(M))$ is spanned by the set $\{A_{i,j}|i\leqslant j\}$ and we can also use the following matrix realization:

$$\begin{aligned} H_i &= \tfrac{1}{2}(\mathcal{E}_{i,i}-\mathcal{E}_{M+1-i,M+1-i}), \\ A_{i,j} &= \mathcal{E}_{i,j}-\mathcal{E}_{M+1-j,M+1-i}. \end{aligned} \tag{17}$$

The canonical chains of twists (9) for orthogonal simple Lie algebras are based on the sequence of injections

$$U(\mathrm{so}(M))\supset U(\mathrm{so}(M-4))\supset\cdots\supset U(\mathrm{so}(M-4k))\supset\cdots. \tag{18}$$

Each link of such chains [see (9)] contains the Jordanian twist $\Phi_{\mathcal{J}_k}=\exp\{H_{\lambda_0^k}\otimes\sigma_{\lambda_0^k}\}$ based on one of the long roots:

$$\lambda_0^k=e_1^k+e_2^k \quad (\text{for both } D_N \text{ and } B_N). \tag{19}$$

The hyperplane $V_{\lambda_0^k}^{\perp}$ orthogonal to λ_0^k coincides with the root space of the subalgebra $g_{\lambda_0^k}^{\perp}=\mathrm{so}(M-4(k+1))\oplus so^{(k+1)}(3)$. For each subalgebra $g_{k+1}=\mathrm{so}(M-4(k+1))$ we can again consider independently its root system Λ^{k+1} and choose the next initial root to be

$$\lambda_0^{k+1}=e_1^{k+1}+e_2^{k+1}.$$

On each step we can fix two vector subrepresentations $d^{v(a)}$ in the restriction (to g_{k+1}) of the adjoint representation ad_{g_k}:

$$d_{g_{k+1}}^{v(a)}\subset \mathrm{ad}_{g_k\downarrow g_{k+1}}, \quad a=1,2.$$

It is easy to check that the constituent roots form the weight diagrams for these representations. The representation space for $d_{g_{k+1}}^{v(a)}$ is spanned by the generators

$$\{E_a, E_{a\pm l}\} \text{ with the roots } \{e_a^k,\ e_a^k\pm e_l^k\in\pi_k\}$$

for $M-4k=2N+1$ and

$$\{E_{a\pm k}\} \text{ with the roots } \{e_a^k\pm e_l^k\in\pi_k\}$$

for $M-4k=2N$. In both cases $l=3,\ldots,N$.

For the representations $d_{g_{k+1}}^{v(a)}$ and $d_{g_{k+1}}^{v(a)}\otimes d_{g_{k+1}}^{v(b)}$ the following scalar and tensor invariants, I_{M-4k}^{a} and $I_{M-4k}^{a\otimes b}$ (with $a,b=1,2$), will be used in the construction of twists and twisted coproducts:

$$I^a_{2N+1}=\frac{1}{2}E_a^2+\sum_{l=3}^{N}(E_{a+l}E_{a-l}),$$

$$I^{a\otimes b}_{2N+1}=E_a\otimes E_b+\sum_{l=3}^{N}(E_{a+l}\otimes E_{b-l}+E_{a-l}\otimes E_{b+l}), \tag{20}$$

$$I^{a\wedge b}_{2N+1}=E_a\wedge E_b+\sum_{l=3}^{N}(E_{a+l}\wedge E_{b-l}+E_{a-l}\wedge E_{b+l}),$$

$$I^a_{2N}=\sum_{l=3}^{N}(E_{a+l}E_{a-l}),$$

$$I^{a\otimes b}_{2N}=\sum_{l=3}^{N}(E_{a+l}\otimes E_{b-l}+E_{a-l}\otimes E_{b+l}), \tag{21}$$

$$I^{a\wedge b}_{2N}=\sum_{l=3}^{N}(E_{a+l}\wedge E_{b-l}+E_{a-l}\wedge E_{b+l}).$$

The set of initial roots defines a natural gradation in the root space of the subalgebra $\mathbf{N}^+(\mathrm{so}(M))\subset\mathrm{so}(M)$:

$$\Lambda(\mathbf{N}^+(\mathrm{so}(M)))=\cup_{k=0}^{p_{\max}}(\lambda_0^k\cup\pi_k), \tag{22}$$

where $p_{\max}=[M/4]+[(M+1)/4]$.

The inverse of the map defined by the classical r-matrix is the Frobenius bilinear form. Let us study the Frobenius subalgebras in $B(\mathrm{so}(M))$.

Proposition 1: Let $\mathbf{L}$ *be a semi-direct sum of a subalgebra* $\mathbf{S}$ *and a commutative ideal* $\mathbf{N}$. *Then* $\mathbf{L}$ *is Frobenius if and only if the following conditions hold:*

(i) $\mathbf{L}$ *acts transitively on the space* $\mathbf{N}^*$ *with the generic point* A^*.
(ii) The stationary subalgebra $\mathbf{S}_{A^*}=\{s\in\mathbf{S}:A^*([s,x])=0,\ \text{for any } x\in\mathbf{N}\}$ *is Frobenius with a Frobenius homomorphism* $f_0:\mathbf{S}_{A^*}\to C$.

Moreover, in this case $f=f_0\oplus A^*$ *is a Frobenius homomorphism for* $\mathbf{L}$.

This statement can be obtained as a consequence of Proposition 1 and the Remark after it in Ref. 10. Here is how it can be used in the case of orthogonal simple Lie algebras.

Lemma 1: Let $\mathbf{L}_1\subset B(\mathrm{so}(M))$ *be a subalgebra generated by the set* $\{H_1,H_2,A_{i,j},i=1,2\}$. *Then* $\mathbf{L}_1$ *is Frobenius*.

Proof: In $\mathbf{L}_1$ the following subalgebras can be fixed: $\mathbf{N}_1=\{A_{1,j}\}$ and $\mathbf{S}_1=\{H_1,H_2,A_{2,j}\}$. The generators of the dual space $\mathbf{N}_1^*$ can be identified with the matrices $\{A_{i,1}\}$ defined according to the rule (17) and connected with $A_{1,j}$ through the bilinear form $\langle A,B\rangle=\mathrm{tr}\,(A,B)$ or by a Killing form in the general setting. Since $\dim\mathbf{N}_1=\dim\mathbf{S}_1$ it suffices to find a point $A^*\in\mathbf{N}_1^*$ such that $\mathbf{S}_{A^*}=0$. One can check directly that $A_0^*=\Sigma_{i=2}^{n-1}A_{i1}$ satisfies this condition. ■

This point A_0^* is not unique. If $G(\mathbf{S}_1)$ is the subgroup of $\mathrm{SO}(M)$ corresponding to the algebra $\mathbf{S}_1$, then for any $g\in G(\mathbf{S}_1)$ the point $\mathrm{Ad}^*(g)(A_0^*)=(A_0^*)^g$ satisfies the condition $\mathbf{S}_{(A_0^*)^g}=0$ since $\mathbf{S}_{(A_0^*)^g}=g^{-1}\mathbf{S}_{A_0^*}g=0$. For our purposes it is convenient to choose $A_0^*=A_{2,1}+A_{M-1,1}$ (One can check that this point satisfies the conditions of the Proposition 1.)

Lemma 2: Let $\mathbf{L}_{K,M}$ *be a subalgebra of* $B(\mathrm{so}(M))$ *generated by the set*

$$\{H_i,A_{i,j}|i=1,\ldots,2K;j=1,\ldots M;i<j;2K\leqslant[M/2]\}.$$

Then $\mathbf{L}_{K,M}$ *is Frobenius.*

Proof: The algebra $\mathbf{L}_{K,M}$ has the structure of a semidirect sum:

$$\mathbf{L}_{K,M}=\mathbf{S}_{K,M}\dot{\oplus}\mathbf{N}_{K,M},$$

where

$$\mathbf{N}_{K,M}=\{\{H_i|i=1,\ldots,2K;\}\{A_{i,j}|i=2,\ldots,2K;j=1,\ldots M;i<j\}\}.$$

Evidently $\mathbf{L}_{K,M}$ acts transitively on $\mathbf{N}^*_{K,M}$ with the generic point $A_1^*=A_{2,1}+A_{M-1,1}$. One can easily check that

$$(\mathbf{S}_{K,M})_{(A_0^*)}=\{H_i,A_{i,j}|i=3,\ldots,2K;i<j\}.$$

Thus

$$(\mathbf{S}_{K,M})_{(A_0^*)}\cong\mathbf{L}_{K-1,M-4}\subset B(\mathrm{so}(M-4)).$$

Obvious induction shows that $\mathbf{L}_{K,M}$ is Frobenius due to the Proposition 1. ■

The algebra $\mathbf{L}_{K,M}$ has a nontrivial second cohomology group $H^2(\mathbf{L}_{K,M})$. The latter contains $\Lambda^2(H^*_{K,M})$ where $H^*_{K,M}$ is the space dual to the Cartan subalgebra in $\mathbf{L}_{K,M}$, $H^*_{K,M}=\mathbf{L}_{K,M}\cap\mathcal{H}(\mathrm{so}(M))\subset B(\mathrm{so}(M))$. It is easy to see that all bilinear forms $H_i^*\wedge H_j^*$ are two-cocycles and not coboundaries. Here $H_i^*\in H^*_{K,M}$. Consequently $A^*_{K,M}+\zeta_{ij}H_i^*\wedge H_j^*$ are the nondegenerate two-cocycles on $\mathbf{L}_{K,M}$. The map $A^*_{K,M}$ is a Frobenius homomorphism, $A^*_{K,M}:\mathbf{L}_{K,M}\rightarrow\mathbf{C}$, because $A^*_{K,M}([x,y])$ is a nondegenerate bilinear form on $\mathbf{L}_{K,M}$. The induction procedure shows that $A^*_{K,M}$ can be chosen in the following form:

$$A^*_{K,M}=(A_{21}+A_{43}+A_{65}+\cdots)+(A_{M-1,1}+A_{M-3,3}+A_{M-5,5}+\cdots). \tag{23}$$

In the case of the orthogonal simple Lie algebras, chains of twists (9) introduced in Ref. 7 refer to the Frobenius subalgebras [contained in the corresponding $B(\mathrm{so}(M))$] with the coboundary nondegenerate bilinear forms,[8]

$$\omega_p^+=\sum_{k=0}^{p}\gamma_k(E^{(k)}_{1+2})^*([\,,\,]), \tag{24}$$

where p is the number of links in the chain $\mathcal{F}_{\mathcal{B}_{0<p}}$ and the parameters $\gamma_k=0,1$ indicate that we describe here the set of forms. It is obvious that the forms (24) ignore the subspaces of $\mathrm{so}^{(k)}(3)$ subalgebras that appear on each step of the sequence of injections in (22). According to the formula (23), to describe the maximal Frobenius subalgebras in $B(\mathrm{so}(M))$ the following form must be considered:

$$\omega_p^{\pm}=\sum_{k=0}^{p}(\gamma_k(E^k_{1+2})^*-\delta_k(E^k_{1-2})^*)([\,,\,]). \tag{25}$$

Here both parameters are discrete: $\gamma_k,\delta_k=0,1$. (Notice that this does not lead to the undesirable terms in the corresponding carrier space because in the Borel subalgebra $B(\mathrm{so}(M))$ (fixed by the choice of $\{\lambda_0^k\}$) there are no constituent roots for $e_1^k-e_2^k$. The form $\omega_p^{\pm}$ is considered on $B(\mathrm{so}(M))$. In terms of the integral root system $\Lambda(\mathrm{so}(M))$ (not split in the subsystems $\Lambda^{(k)}$) the generators $E^{(k)}_{1+2}$ and $E^{(k)}_{1-2}$ form the sequence

$$\{E_{1+2},E_{1-2},E_{3+4},E_{3-4},\ldots,E_{(2p+1)+(2p+2)},E_{(2p+1)-(2p+2)}\}$$
$$\approx\{A_{1,M-1},A_{1,2},A_{3,M-3},A_{3,4},\ldots A_{2p+1,M-(2p+1)},A_{2p+1,2p+2},\}.$$

Thus we come to the conclusion that there must be two sets of chains of twists for the orthogonal algebras corresponding to the two sets of the coboundary forms (24) and (25). The first set is the canonical chain of twists (9), whose twisting element can be rewritten in terms of invariants (20) and (21):

$$\begin{aligned}\mathcal{F}_{\mathcal{B}_{0<p}} &= \exp\{I^{1\otimes 2}_{M-4p}(1\otimes e^{-(1/2)\,\sigma^{p}_{1+2}})\}\\ &\quad\cdot\exp\{H^{(p)}_{1+2}\otimes\sigma^{p}_{1+2}\}\cdot\exp\{I^{1\otimes 2}_{M-4(p-1)}(1\otimes e^{-(1/2)\,\sigma^{p-1}_{1+2}})\}\cdot\exp\{H^{(p-1)}_{1+2}\otimes\sigma^{p-1}_{1+2}\}\\ &\quad\cdot\ldots\\ &\quad\cdot\exp\{I^{1\otimes 2}_{M}(1\otimes e^{-(1/2)\,\sigma^{0}_{1+2}})\}\cdot\exp\{H^{(0)}_{1+2}\otimes\sigma^{0}_{1+2}\}\\ &= \prod_{k=p}^{0}\exp\{I^{1\otimes 2}_{M-4k}(1\otimes e^{-(1/2)\,\sigma^{k}_{1+2}})\}\cdot\exp\{H^{(k)}_{1+2}\otimes\sigma^{k}_{1+2}\}\end{aligned}\tag{26}$$

[here $\sigma_{\lambda^k_0}$ are denoted by $\sigma^k_{1+2}=\ln(1+E^{(k)}_{1+2})$ according to (19) and for simplicity we put $\gamma_l=1$].

When dealing with the forms $\omega^{\pm}_p$ the problem is that in the process of twisting by a chain (26) the costructure of the subalgebras $\mathrm{so}^{(k)}$ (3) is considerably changed and the twist equations (1) become extremely difficult to solve.

III. CONSTRUCTION OF THE FULL CHAINS OF TWISTS

According to the general structure of a chain of twists[7] we can study its links separately. Let us assume that we have constructed the $k-1$ links of a chain and found the Matreshka effect. This means that after the chain twisting with $k-1$ links we get the subalgebra $g^{(k)}=\mathrm{so}(M-4k)$ with primitive generators. We shall show that it is possible to construct the next link of the chain so that the twist will correspond to the enlarged form $\omega^{\pm}_p$ [see (25)]. To start the construction of the kth link we have to choose the initial root λ^k_0 [as in (19)] and the subalgebra $\mathbf{L}_{K,M-4k}$ described in Lemma 2 (with $2K=[M/2]$). First we apply the following Jordanian twist to the subalgebra $\mathbf{L}_{K,M-4k}$:

$$\Phi_{\mathcal{J}_k}=\exp(H^k_{1+2}\otimes\sigma^k_{1+2}).\tag{27}$$

This results in the following deformed coproducts:

$$\Delta_{\mathcal{J}_k}(H^k_{1+2})=H^k_{1+2}\otimes e^{-\sigma^k_{1+2}}+1\otimes H^k_{1+2},$$

$$\Delta_{\mathcal{J}_k}(E^k_{1+2})=E^k_{1+2}\otimes e^{\sigma^k_{1+2}}+1\otimes E^k_{1+2},$$

$$\Delta_{\mathcal{J}_k}(E^k_{a\pm l})=E^k_{a\pm l}\otimes e^{1/2\,\sigma^k_{1+2}}+1\otimes E^k_{a\pm l},$$

$$l=3,\ldots,N;\quad a=1,2.$$

For $M=2N+1$ we also get

$$\Delta_{\mathcal{J}_k}(E^k_a)=E^k_a\otimes e^{(1/2)\,\sigma^k_{1+2}}+1\otimes E^k_a.$$

Notice that the generators $\{H^k_{1-2},E^k_{1-2},E^k_{2-1}\}$ remain primitive.

The second twisting factor must be the full canonical extension[5] for the Jordanian twist $\Phi_{\mathcal{J}_k}$ (27):

$$\Phi_{\mathcal{E}_k}=\exp(I^{1\otimes 2}_{M-4k}(1\otimes e^{-(1/2)\,\sigma^k_{1+2}})).\tag{28}$$

The successive application of these two factors performs the extended Jordanian twisting by the element $\Phi_{\mathcal{E}_k}\Phi_{\mathcal{J}_k}$ that leads to the following costructure in $\mathbf{L}_{K,M-4k}$:

$$\Delta_{\mathcal{E}_k\mathcal{J}_k}(H^k_{1+2})=H^k_{1+2}\otimes e^{-\sigma^k_{1+2}}+1\otimes H^k_{1+2}-(1\otimes e^{-(3/2)\,\sigma^k_{1+2}})I^{1\otimes 2}_{M-4k},$$

$$\Delta_{\mathcal{E}_k\mathcal{J}_k}(H^k_{1-2})=H^k_{1-2}\otimes 1+1\otimes H^k_{1-2},$$

$$\Delta_{\mathcal{E}_k\mathcal{J}_k}(E^k_{1+2})=E^k_{1+2}\otimes e^{\sigma^k_{1+2}}+1\otimes E^k_{1+2},$$

$$\Delta_{\mathcal{E}_k\mathcal{J}_k}(E^k_{1\pm k})=E^k_{1\pm k}\otimes e^{-(1/2)\,\sigma^k_{1+2}}+1\otimes E^k_{1\pm k},$$

$$\Delta_{\mathcal{E}_k\mathcal{J}_k}(E^k_{2\pm k})=E^k_{2\pm k}\otimes e^{(1/2)\,\sigma^k_{1+2}}+e^{\sigma^k_{1+2}}\otimes E^k_{2\pm k},$$

$$\Delta_{\mathcal{E}_k\mathcal{J}_k}(E^k_{1-2})=E^k_{1-2}\otimes 1+1\otimes E^k_{1-2}+(1\otimes e^{-(1/2)\,\sigma^k_{1+2}})I^{1\otimes 1}_{M-4k}+I^1_{M-4k}\otimes(e^{-\sigma^k_{1+2}}-1),$$

$$\Delta_{\mathcal{E}_k\mathcal{J}_k}(E^k_{2-1})=E^k_{2-1}\otimes 1+1\otimes E^k_{2-1}+(e^{\sigma^k_{1+2}}-1)\otimes I^2_{M-4k}e^{-\sigma^k_{1+2}}+(1\otimes e^{-(1/2)\,\sigma^k_{1+2}})I^{2\otimes 2}_{M-4k}.$$

And in the case of $M=2N+1$ for the short root generators we get

$$\Delta_{\mathcal{E}_k\mathcal{J}_k}(E^k_1)=E^k_1\otimes e^{-(1/2)\,\sigma^k_{1+2}}+1\otimes E^k_1,$$

$$\Delta_{\mathcal{E}_k\mathcal{J}_k}(E^k_2)=E^k_2\otimes e^{(1/2)\,\sigma^k_{1+2}}+e^{\sigma^k_{1+2}}\otimes E^k_2.$$

It would be necessary to have the coproducts for some of the invariants [see (20) and (21)]:

$$\Delta_{\mathcal{E}_k\mathcal{J}_k}(I^1_{M-4k})=I^1_{M-4k}\otimes e^{-\sigma^k_{1+2}}+1\otimes I^1_{M-4k}+I^{1\otimes 1}_{M-4k}(1\otimes e^{-(1/2)\,\sigma^k_{1+2}}), \tag{29}$$

$$\Delta_{\mathcal{E}_k\mathcal{J}_k}(I^2_{M-4k}e^{-\sigma^k_{1+2}})=I^2_{M-4k}e^{-\sigma^k_{1+2}}\otimes 1+e^{\sigma^k_{1+2}}\otimes I^2_{M-4k}e^{-\sigma^k_{1+2}}+I^{2\otimes 2}_{M-4k}(1\otimes e^{-(1/2)\,\sigma^k_{1+2}}). \tag{30}$$

We have two generators of $\mathbf{L}_{K,M-4k}$ that are not yet incorporated in the carrier subalgebra of the twist: H^k_{1-2} and E^k_{1-2}. The coproduct of the latter is deformed. So the canonical Jordanian factor cannot be used here. In Ref. 9 it was indicated that the reason for the nonprimitivity of the coproduct $\Delta_{\mathcal{E}_k\mathcal{J}_k}(E^k_{1-2})$ is that the generator E^k_{1-2} belongs to the long series of the initial root $\lambda^k_0=e^k_1+e^k_2$. It was shown there that in such a case the deformed carrier subspace must exist with primitive basic elements. In our situation such ''deformed'' generators must have the form

$$\begin{aligned} G^k_{1-2}&=E^k_{1-2}-I^1_{M-4k},\\ G^k_{2-1}&=E^k_{2-1}-I^2_{M-4k}e^{-\sigma^k_{1+2}}. \end{aligned} \tag{31}$$

Using the coproducts (29) and (30), it is easy to check that both G^k_{1-2} and G^k_{2-1} are primitive,

$$\begin{aligned} \Delta_{\mathcal{E}_k\mathcal{J}_k}(G^k_{1-2})&=\Delta_{\mathcal{E}_k\mathcal{J}_k}(E^k_{1-2})-\Delta_{\mathcal{E}_k\mathcal{J}_k}(I^1_{M-4k})\\ &=G^k_{1-2}\otimes 1+1\otimes G^k_{1-2}, \end{aligned}$$

$$\begin{aligned} \Delta_{\mathcal{E}_k\mathcal{J}_k}(G^k_{2-1})&=\Delta_{\mathcal{E}_k\mathcal{J}_k}(E^k_{2-1})-\Delta_{\mathcal{E}_k\mathcal{J}_k}(I^2_{M-4k})(e^{-\sigma^k_{1+2}}\otimes e^{-\sigma^k_{1+2}})\\ &=G^k_{2-1}\otimes 1+1\otimes G^k_{2-1}. \end{aligned}$$

Together with H^k_{1-2} the elements (31) generate a three-dimensional space V^k_G of primitive elements in the algebra $U_{\mathcal{E}_k\mathcal{J}_k}(\mathrm{so}(M-4k))$. Both G^k_{1-2} and G^k_{2-1} commute with $U(\mathrm{so}(M-4(k+1)))$ as well as H^k_{1-2} whose dual vector is orthogonal to the roots of $\mathrm{so}(M-4(k+1))$.

The subspace V^k_G spanned by $\{H^k_{1-2},G^k_{1-2},G^k_{2-1}\}$ is algebraically closed:

$$[H^k_{1-2},G^k_{1-2}]=G^k_{1-2},$$

$$[H^k_{1-2},G^k_{2-1}]=-G^k_{2-1},$$

$$[G^k_{1-2},G^k_{2-1}]=2H^k_{1-2}.$$

Let us denote this algebra by $\mathrm{so}^{(k)}_G(3)$. Clearly it is primitive, commutes with $U(\mathrm{so}(M-4(k+1)))$ and is realized on a deformed subspace. (This space is not orthogonal to H^k_{1+2}. Moreover, G^k_{2-1},G^k_{1-2} are not any longer eigenvectors of $\mathrm{ad}_{H^k_{1+2}}$.)

Another subalgebra which remains primitive after the composition $\Phi_{\mathcal{E}_k}\Phi_{\mathcal{J}_k}$ of twists (27) and (28) is $\mathrm{so}(M-4(k+1))$ (due to the Matreshka effect). We come to the conclusion that the twisted $U_{\mathcal{E}_k\mathcal{J}_k}(\mathrm{so}(M-4k))$ contains the primitive subalgebra $g^{\perp}_{\lambda^k_0}$,

$$U_{\mathcal{E}_k\mathcal{J}_k}(\mathrm{so}(M-4k))\supset g^{\perp}_{\lambda^k_0}=\mathrm{so}(M-4(k+1))\oplus\mathrm{so}^{(k)}_G(3).$$

Its Borel subalgebra is $\mathbf{L}_{K,M-4(k+1)}\oplus B(\mathrm{so}^{(k)}_G(3))$ and it is Frobenius (see Sec. II).

Remember that the subalgebra $g^{\perp}_{\lambda^k_0}$ has a structure of direct sum. Further, twisting by the next factors (such as $\Phi_{\mathcal{E}_{k+s}}\Phi_{\mathcal{J}_{k+s}}$) cannot affect the primitive subalgebra $\mathrm{so}^{(k)}_G(3)$. Each step produces (in the corresponding $g^{\perp}_{\lambda^k_0}$) the additional subalgebra $\mathrm{so}^{(k)}_G(3)$, $k=1,\ldots,p$. The primitive subalgebras that can be found in an orthogonal algebra after the chain twisting (26) with p links contain not only $\mathrm{so}(M-4(p+1))$ but also a direct sum of p copies of $\mathrm{so}_G(3)$:

$$U_{\mathcal{B}_{0<p}}(\mathrm{so}(M))\supset\mathcal{D}=\oplus^p_{k=1}\mathrm{so}^{(k)}_G(3).$$

The main consequence is that in the twisted $U_{\mathcal{B}_{0<p}}(\mathrm{so}(M))$ one can perform further twist deformations with the carrier subalgebra in $\mathcal{D}$. The most interesting among them are the Jordanian twists defined by

$$\Phi^G_{\mathcal{J}_k}=\exp(H^k_{1-2}\otimes\sigma^k_G) \tag{32}$$

that can be attributed to any number of copies $\mathrm{so}_G(3)$. Here $\sigma^k_G=\ln(1+G^k_{1-2})$. Thus in the general expression for the twisting element (26) one can insert in the appropriate k places the additional factors which are the Jordanian twisting elements on the deformed carrier spaces. This means that we can perform a substitution

$$\Phi_{\mathcal{E}_k}\Phi_{\mathcal{J}_k}\Rightarrow\Phi^G_{\mathcal{J}_k}\Phi_{\mathcal{E}_k}\Phi_{\mathcal{J}_k}=\Phi_{\mathcal{G}_k},$$

$$\exp\{I^{1\otimes 2}_{M-4k}(1\otimes e^{-1/2\,\sigma^k_{1+2}})\}\cdot\exp\{H^k_{1+2}\otimes\sigma^k_{1+2}\}$$
$$\Rightarrow\exp(H^k_{1-2}\otimes\sigma^k_G)\cdot\exp\{I^{1\otimes 2}_{M-4k}(1\otimes e^{-1/2\,\sigma^k_{1+2}})\}\cdot\exp(H^k_{1+2}\otimes\sigma^k_{1+2}).$$

Thus *the full chain* has the following form:

$$\mathcal{F}_{\mathcal{G}_{0<p}}=\prod^0_{k=p}\Phi_{\mathcal{G}_k}=\prod^0_{k=p}\exp(H^k_{1-2}\otimes\sigma^k_G)\cdot\exp\{I^{1\otimes 2}_{M-4k}(1\otimes e^{-1/2\,\sigma^k_{1+2}})\}\cdot\exp\{H^k_{1+2}\otimes\sigma^k_{1+2}\}. \tag{33}$$

This result means that we have constructed the explicit quantizations with a triangular universal R-matrix

$$\mathcal{R}_{\mathcal{G}_{0<p}}=(\mathcal{F}_{\mathcal{G}_{0<p}})_{21}(\mathcal{F}_{\mathcal{G}_{0<p}})^{-1}$$

for the following set of classical r-matrices:

$$r_{\mathcal{G}_{0<p}}=\sum_{k=0}^{p}\ \eta_k(H^k_{1+2}\wedge E^k_{1+2}+\xi_k H^k_{1-2}\wedge E^k_{1-2}+I^{1\wedge 2}_{M-4k}).$$

Here all the parameters are independent and continuous. Elementary computations show that these full chains (33) correspond to the coboundary forms (25). To illustrate these quantizations we present in the Appendix the matrix $\mathcal{R}_{\mathcal{G}_{0<p}}$ for the algebra so(5) in the defining representation.

In Sec. II we proved that adding $\zeta_{ij}H^*_i\wedge H^*_j$ to the forms of type (25) we obtain new nondegenerate two-cocycles, which are not coboundaries. We can also construct the corresponding twists for these modified cocycles:

$$\omega^{\pm}_p=\sum_{k=0}^{p}\ (\gamma_k(E^k_{1+2})^*-\delta_k(E^k_{1-2})^*)([,])+\sum_{i,j=0;\ i\neq j}^{p}\ \zeta_{ij}H^*_i\wedge H^*_j\,. \tag{34}$$

Notice that the subalgebras $\mathrm{so}^{(k)}_G(3)$ commute not only with $\mathrm{so}(M-4(k+1))$ but also with any $\{E^{(s)}_{1+2}\,|\,s\leqslant k\}$. This means that after having twisted $U(\mathrm{so}(M))$ by the chain (33) we obtain $p+1$ pairs of commuting primitive elements $\{\sigma^k_{1+2},\sigma^k_G|k=0,\ldots,p\}$. Therefore we can apply the Reshetikhin twist

$$\Phi_{\mathcal{R}}=\exp(\zeta_{ij}\sigma_i\otimes\sigma_j),\quad \sigma_i\in\{\sigma^k_{1+2},\sigma^k_G\,|\,k=0,\ldots,p\} \tag{35}$$

to the algebra $U_{\mathcal{G}_{0<p}}(\mathrm{so}(M))$.

Thus the element

$$\Phi_{\mathcal{R}}\mathcal{F}_{\mathcal{G}_{0<p}}$$

defines also a twist for $U(\mathrm{so}(M))$. It leads to the deformed Hopf algebra $U_{\mathcal{R}G_{0<p}}(\mathrm{so}(M))$ with the universal element

$$\mathcal{R}_{\mathcal{R}G_{0<p}}=(\Phi_{\mathcal{R}}\mathcal{F}_{\mathcal{G}_{0<p}})_{21}(\mathcal{F}_{\mathcal{G}_{0<p}})^{-1}(\Phi_{\mathcal{R}})^{-1}$$

and the classical r-matrix

$$r_{\mathcal{R}G_{0<p}}=\sum_{k=0}^{p}\ \eta_k(H^k_{1+2}\wedge E^k_{1+2}+\xi_k H^k_{1-2}\wedge E^k_{1-2}+I^{1\wedge 2}_{M-4k})+\sum_{i,j=0;\ i\neq j}^{p}\ \zeta_{ij}E^i_s\wedge E^j_t;$$

$$E^k_s,E^k_t\in\{E^k_{1+2},E^k_{1-2}|k=0,\ldots,p\}.$$

The dimensions of the nilpotent subalgebras $\mathbf{N}^+(\mathrm{so}(M))$ in the sequence $g^{\perp}_{\lambda^p_0}\subset g^{\perp}_{\lambda^{p-1}_0}\subset\cdots\subset g^{\perp}_{\lambda^0_0}\subset g$ are subject to the following simple relation:

$$\dim(\mathbf{N}^+(\mathrm{so}(M)))-\dim(\mathbf{N}^+(\mathrm{so}(M-4)))=2(\dim\, d^v_{\mathrm{so}(M-4)}+1). \tag{36}$$

Taking this into account we conclude [from the formula (22)] that the chains (33) are full. Furthermore, this means that for $p=p_{\max}=[M/4]+[(M+1)/4]$ the corresponding carrier spaces contain all the generators of the nilpotent subalgebra $\mathbf{N}^+(\mathrm{so}(M))$. When M is even-odd one can always find in $\mathrm{so}(M)$ one independent Cartan generator which cannot be included in the carrier

subalgebra of a chain. When M is even-even or odd the total number of Jordanian twists in a maximal full chain $\mathcal{F}_{\mathcal{G}_{0<p\ \max}}$ is equal to the rank of so(M). Thus in the latter case the carrier subalgebra is equal to the Borel subalgebra.

IV. CONCLUSIONS

The family of explicit twisting elements was constructed for the universal enveloping algebras $\mathcal{A}=U(\mathrm{so}(M))$ (series B and D) with full nilpotent subalgebras $\mathbf{N}^{+}(\mathrm{so}(M))$ included in the corresponding carrier spaces.

There are a variety of applications for explicitly known twisting elements $\mathcal{F}$. Using a particular (e.g., fundamental) representation for one of the factors of $\mathcal{A}\otimes\mathcal{A}$ we get from the universal R-matrix the L-operator of the FRT-formalism and this results in explicit relations among the generators of the original universal enveloping algebra and the FRT-generators of the twisted one.

Twisting of the coalgebra in $\mathcal{A}$ induces changes in Clebsch–Gordan coefficients of bases in the tensor products of irreducible representations $c_V\otimes d_W$. The evaluation of these coefficients is given by the direct action of the matrix F [F is the value of the twisting element in the corresponding representation: $F=c_V\otimes d_W(\mathcal{F})$] on the original CG coefficients.[11]

Due to the embedding of the simple Lie algebras g into the corresponding Yangians (as Hopf subalgebras) $U(g)\subset\mathcal{Y}(g)$ (Ref. 12), the Yangian R-matrix $R_{\mathcal{Y}}$ can be twisted by the same $\mathcal{F}$ defined for g.[13] As a result, for the case of orthogonal algebra $g=\mathrm{so}(M)$ the R-matrix [in the defining representation $d\subset\mathrm{Mat}(M,\mathbf{C})\otimes\mathrm{Mat}(M,\mathbf{C})$] will be changed:

$$ud(1\otimes 1)+\mathcal{P}-\frac{u}{u-1+M/2}\mathcal{K}\quad\rightarrow\quad ud(\mathcal{F}_{21}\mathcal{F}^{-1})+\mathcal{P}-\frac{u}{u-1+M/2}d(\mathcal{F}_{21})\mathcal{K}d(\mathcal{F}^{-1}).$$

(Here u is a spectral parameter and the operator $\mathcal{K}$ is obtained from the permutation $\mathcal{P}$ by transposing its first tensor factor.) For the canonical chains $\mathcal{F}=\mathcal{F}_{\mathcal{B}_{0<p}}$ the deformed solutions of the YBE were given in the explicit form in Ref. 14. Similarly to the case of canonical chains (9) the twists $\mathcal{F}_{\mathcal{G}_{0<p}}$ produce the sets of deformed Yangians and the new integrable Hamiltonians [cf. the sl(2)-case.[11]].

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APPENDIX

The simplest case where the full chain differs nontrivially from the canonical (the deformed carrier space is to be used) is $g=\mathrm{so}(5)$. Three deformation parameters can be intoduced in the corresponding chain of twists. Two of them (ξ and ζ) are continuous and describe the deformation scales in the Jordanian twisting factors. The discrete parameter $\kappa=0,1$ testifies that the extension factor in the chain can be switched off. The twisting element

$$\mathcal{F}_{\mathcal{G}_{0<p}}(\xi,\zeta,\kappa)=\exp(H_{1-2}\otimes\sigma_{G}(\xi,\zeta,\kappa))\cdot\exp\{(\xi\kappa)I_5^{1\otimes 2}(1\otimes e^{-(1/2)\sigma_{1+2}})\}\cdot\exp\{H_{1+2}\otimes\sigma_{1+2}(\xi)\}\tag{A1}$$

contains two Jordanian factors with

$$\sigma_{1+2}(\xi)=\ln(1+\xi E_{1+2})\quad\text{and}\quad\sigma_{G}(\xi,\zeta,\kappa)=\ln(1+\zeta(E_{1-2}-\tfrac{1}{2}\xi\kappa E_1^2)).$$

The corresponding universal $\mathcal{R}$-matrix is

$$\mathcal{R}_{\mathcal{G}_{0<p}}(\xi,\zeta,\kappa)=(\mathcal{F}_{\mathcal{G}_{0<p}}(\xi,\zeta,\kappa))_{21}(\mathcal{F}_{\mathcal{G}_{0<p}}(\xi,\zeta,\kappa))^{-1}.$$

We shall consider it in the defining five-dimensional representation d of so(5). This means that the following matrix realization will be used:

$$\begin{aligned} H_i&=\tfrac{1}{2}(\mathcal{E}_{i,i}-\mathcal{E}_{6-i,6-i}),\\ A_{i,j}&=\mathcal{E}_{i,j}-\mathcal{E}_{6-j,6-i};\\ i,j&=1,\ldots,5. \end{aligned} \tag{A2}$$

As a result we get the solution $d(\mathcal{R}_{\mathcal{G}_{0<p}}(\xi,\zeta,\kappa))$ of the matrix Yang–Baxter equation that can be written in terms of tensor products of 5×5 matrix units $\mathcal{E}_{i,j}$:

$$\begin{aligned} d(\mathcal{R}_{\mathcal{G}_{0<p}}(\xi,\zeta,\kappa))&=d(\mathcal{F}_{\mathcal{G}_{0<p}}(\xi,\zeta,\kappa))_{21}d(\mathcal{F}_{\mathcal{G}_{0<p}}(\xi,\zeta,\kappa))^{-1}\\ &=I\otimes I+(\mathcal{E}_{4,5}-\mathcal{E}_{1,2})\otimes\tfrac{1}{8}\zeta(4(\mathcal{E}_{1,1}-\mathcal{E}_{2,2}+\mathcal{E}_{4,4}-\mathcal{E}_{5,5})+2\zeta(\mathcal{E}_{4,5}-\mathcal{E}_{1,2})+\xi\zeta\kappa\mathcal{E}_{1,5})\\ &\quad+(\mathcal{E}_{4,5}+\mathcal{E}_{1,2})\otimes(-\tfrac{1}{8}\xi\zeta)(\zeta\mathcal{E}_{1,5}+2(\mathcal{E}_{2,5}+\mathcal{E}_{1,4}))+(\mathcal{E}_{3,5}-\mathcal{E}_{1,3})\otimes\xi\kappa(\mathcal{E}_{2,3}-\mathcal{E}_{3,4})\\ &\quad+(\mathcal{E}_{3,4}-\mathcal{E}_{2,3})\otimes\xi\kappa(\mathcal{E}_{3,5}-\mathcal{E}_{1,3})+(\mathcal{E}_{2,5}-\mathcal{E}_{1,4})\otimes\tfrac{1}{4}\xi(2(\mathcal{E}_{1,1}+\mathcal{E}_{2,2}-\mathcal{E}_{4,4}-\mathcal{E}_{5,5})\\ &\quad+\xi(\mathcal{E}_{2,5}-\mathcal{E}_{1,4}))+(\mathcal{E}_{2,5}+\mathcal{E}_{1,4})\otimes\tfrac{1}{8}\xi\zeta(\xi(\kappa-1)\mathcal{E}_{1,5}-2(\mathcal{E}_{4,5}+\mathcal{E}_{1,2}))\\ &\quad+(\mathcal{E}_{1,1}+\mathcal{E}_{2,2}-\mathcal{E}_{4,4}-\mathcal{E}_{5,5})\otimes\tfrac{1}{2}\xi(\mathcal{E}_{1,4}-\mathcal{E}_{2,5})+(\mathcal{E}_{1,1}-\mathcal{E}_{2,2}+\mathcal{E}_{4,4}-\mathcal{E}_{5,5})\\ &\quad\otimes\tfrac{1}{2}\zeta(\mathcal{E}_{1,2}-\mathcal{E}_{4,5})+\mathcal{E}_{1,3}\otimes(-\tfrac{1}{2}\xi\zeta\kappa)\mathcal{E}_{1,3}+\mathcal{E}_{3,5}\otimes(-\tfrac{1}{2}\xi\zeta\kappa)\mathcal{E}_{3,5}+\mathcal{E}_{2,5}\\ &\quad\otimes(-\xi^2\kappa(\mathcal{E}_{1,4})-\tfrac{1}{2}\xi^2\zeta\kappa(\mathcal{E}_{1,5}))(\tfrac{1}{2}\xi^2\kappa\mathcal{E}_{2,4}-\tfrac{1}{4}\xi^2\zeta\kappa\mathcal{E}_{1,4}\\ &\quad-\tfrac{1}{4}\xi\zeta(\kappa+1)(\mathcal{E}_{1,1}-\mathcal{E}_{2,2})+\tfrac{1}{4}\xi\zeta(1-\kappa)(\mathcal{E}_{4,4}-\mathcal{E}_{5,5}))\otimes\mathcal{E}_{1,5}+\mathcal{E}_{1,5}\\ &\quad\otimes(\tfrac{1}{4}\zeta\xi\kappa(\mathcal{E}_{1,1}-\mathcal{E}_{2,2}+\mathcal{E}_{4,4}-\mathcal{E}_{5,5})-\tfrac{1}{4}\xi\zeta(\mathcal{E}_{1,1}-\mathcal{E}_{2,2}-\mathcal{E}_{4,4}+\mathcal{E}_{5,5})+\tfrac{1}{2}\xi^2\kappa\mathcal{E}_{2,4}\\ &\quad+\tfrac{1}{8}\xi^2\zeta(3\kappa+1)\mathcal{E}_{1,4}+\tfrac{1}{8}\xi^2\zeta(\kappa+1)\mathcal{E}_{2,5}+\tfrac{1}{8}\xi\zeta^2(\kappa+1)\mathcal{E}_{4,5}\\ &\quad+\tfrac{1}{8}\xi\zeta^2(1-\kappa)\mathcal{E}_{1,2}+\tfrac{1}{16}\xi^2\zeta^2(3\kappa+1)\mathcal{E}_{1,5}). \end{aligned}$$

This expression presents the two-dimensional set of R-matrices. One can consider the submanifolds corresponding to the special values of the parameters. For $\zeta=0$, without the last (deformed) Jordanian factor, we get the R-matrix for the extended Jordanian twisted algebra $U_{\mathcal{E}J}(\mathrm{so}(5))$. For $\kappa=0$ we obtain the two-Jordanian R-matrix for $U_{\mathcal{J}_1\mathcal{J}_0}(\mathrm{so}(5))$. This is the result of two independent Jordanian twists [corresponding to two orthogonal long roots of so(5)]. For $\zeta=0$ with $\kappa=0$ and for $\xi=0$ we have two pure Jordanian R-matrices equivalent up to the renumeration of the generators.

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An algebraic approach to Macdonald–Koornwinder polynomials: Rodrigues-type formula and inner product identity

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We study Macdonald–Koornwinder polynomials in the context of double affine Hecke algebras. Nonsymmetric Macdonald–Koornwinder polynomials are constructed by use of raising operators provided by a representation theory of the double affine Hecke algebra associated with $A_{2l}^{(2)}$-type affine root system. This enables us to evaluate diagonal terms of scalar products of the nonsymmetric polynomials algebraically. The Macdonald–Koornwinder polynomials are expressed by linear combinations of the nonsymmetric counterparts. We show a new proof of the inner product identity of the Macdonald–Koornwinder polynomials without Opdam–Cherednik's shift operators. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Macdonald introduced a new class of orthogonal polynomials,[1–3] which are associated with root systems and are considered as q-deformations of Heckman–Opdam's Jacobi polynomials.[4–6] Since then, the Macdonald polynomials and their descendants have appeared in various areas of mathematics and physics and are studied from several viewpoints.[7–13] Macdonald gave some conjectures for his polynomials, i.e., constant terms, inner products, evaluations, and so on. Cherednik clarified an algebraic structure of the Macdonald polynomials by means of affine Hecke algebras.[14–17] He indeed proved several of the conjectures through a representation theory of the affine Hecke algebra. Among them, the shift operator approach, which was first developed by Opdam in the case of Jacobi polynomials, was generalized in the framework of double affine Hecke algebras to give a proof of Macdonald's inner product identity.

In our previous papers,[18–21] we presented Rodrigues-type formulas which give algebraic expressions for the nonsymmetric polynomials corresponding to the Jacobi and the Macdonald polynomials by use of raising operators. It is remarkable that our raising operators are provided by a representation theory of Cherednik's double affine Hecke algebras in a natural way and enable us to calculate diagonal terms of scalar products for the nonsymmetric polynomials except for those of their constant terms. Moreover we showed that Weyl-symmetrization of the nonsymmetric polynomials gives the Jacobi and the Macdonald polynomials algebraically and we evaluated their inner products without Opdam–Cherednik's shift operators.

Koornwinder introduced multivariable generalizations of the Askey–Wilson polynomials.[22] Koornwinder's polynomials reduce to two types of Macdonald polynomials associated with a *BC*-type nonreduced root system through a specialization of their parameters, which is a reason why they are called the Macdonald–Koornwinder polynomials nowadays. An explicit commutative family of difference operators which characterizes the Macdonald–Koornwinder polynomials and some properties of the polynomials in the self-dual point were investigated by van Diejen.[23,24]

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Noumi showed that Cherednik's affine Hecke algebraic approach can also be applied to the Macdonald–Koornwinder polynomials,[25] which was originally proposed by Macdonald[26] and was extensively studied by other people later.[27–30]

Although the Macdonald and Macdonald–Koornwinder polynomials share the similar affine Hecke algebraic approach we have mentioned previously, it seems that a unified approach to both polynomials has not been established. This is because, as for the latter polynomials, the relationship with root systems has not been clarified enough; namely, Noumi employed Lusztig's representation of the $C^{(1)}$-type Hecke algebra to study the Macdonald–Koornwinder polynomials while Koornwinder first introduced them as BC-type Askey–Wilson polynomials. Macdonald's $C^\vee C$-type nonreduced affine root system seems to give a solution on this problem.[26,29,30] However, in studying the Macdonald–Koornwinder polynomials with the $C^\vee C$-type root system, one has to consider the nonextended affine Weyl group and hence the Hecke algebra, since, if one extends the Hecke algebra to the affine one, two degrees of freedom in parameters of the polynomials are lost due to a nontrivial automorphism of the Dynkin diagram. In this paper, we introduce an affine Hecke algebra associated with an affine root system in an analogous way to Refs. 31 and 32. From our point of view, affine Hecke algebras employed by Cherednik in the study of the Macdonald polynomials are associated with affine root systems of nontwisted affine Lie algebras. An affine Hecke algebra associated with the $A_{2l}^{(2)}$-type affine root system enables us to treat the Macdonald–Koornwinder polynomials. We thus obtain a new and unified viewpoint for the Macdonald and Macdonald–Koornwinder polynomials. To give a new proof of an inner product identity for the Macdonald–Koornwinder polynomials is a goal of this paper.

This paper is organized as follows: In Sec. II, we briefly summarize known facts on affine root systems of affine Lie algebras[33] and introduce extended affine Weyl groups in such a way that they preserve the affine root systems.[31,32,34] We define the affine Hecke algebra as a deformation of group algebra of the extended affine Weyl group of type $X_N^{(r)}$ and refer to it as the affine Hecke algebra of type $X_N^{(r)}$. The Macdonald–Koornwinder polynomials are associated with the affine Hecke algebra of type $A_{2l}^{(2)}$ as we have described previously. In giving a representation of the affine Hecke algebra of type $A_{2l}^{(2)}$, we encounter a special situation discussed by Lusztig,[35] which is investigated in detail in the Appendix. After introducing the double affine Hecke algebra of $A_{2l}^{(2)}$-type in analogy with Cherednik's works,[14–17] we give its representation in the endomorphism of the Laurent polynomial ring (Theorem 2.16). In Sec. III, we consider nonsymmetric Macdonald–Koornwinder polynomials which are joint eigenvectors of commutative Cherednik operators. In a way similar to our previous papers, we provide a Rodrigues-type formula of the nonsymmetric polynomials (Theorem 3.14) and evaluate diagonal terms of their scalar products explicitly (Theorem 3.15 and Proposition 3.16). We construct the Macdonald–Koornwinder polynomials through the Weyl-symmetrization of the nonsymmetric polynomials (Proposition 3.21 and Corollary 3.22), and prove their inner product identities (Theorem 3.24). Section IV is devoted to concluding remarks.

II. DOUBLE AFFINE HECKE ALGEBRAS

A. Affine root systems and extended affine Weyl groups

We start to review affine root systems of affine Lie algebras.[33] Let $\mathfrak{g}$ be the affine Lie algebra of type $X_N^{(r)}$ associated with a generalized Cartan matrix $A=(a_{ij})_{i,j\in I}$ where $I:=\{0,1,2,\ldots,l\}$ is a set of indices, and let $S(A)$ be its Dynkin diagram. We denote by $\{a_i|i\in I\}$ the set of numerical labels of $S(A)$ and by $\{a_i^\vee|i\in I\}$ that of $S({}^tA)$. Let $\mathfrak{h}$ be the Cartan subalgebra of $\mathfrak{g}$. Let $R\subset\mathfrak{h}^*$ be the affine root system. We take the set of simple roots $\Pi:=\{\alpha_i|i\in I\}\subset\mathfrak{h}^*$ and the set of simple coroots $\Pi^\vee:=\{\alpha_i^\vee|i\in I\}\subset\mathfrak{h}$ such that $\langle\alpha_i,\alpha_j^\vee\rangle=a_{ij}$. Define the central element K of $\mathfrak{g}$ and a null-root $\delta\in R$ by $K:=\Sigma_{i\in I}\,a_i^\vee\alpha_i^\vee$ and $\delta:=\Sigma_{i\in I}\,a_i\alpha_i$, respectively. We fix elements $\Lambda_0^\vee\in\mathfrak{h}$ and $\Lambda_0\in\mathfrak{h}^*$ satisfying

$$\langle\alpha_i,\Lambda_0^\vee\rangle=\delta_{0i},\quad \langle\Lambda_0,\alpha_i^\vee\rangle=\delta_{0i},\quad \text{for } 0\leqslant i\leqslant l,\quad \langle\Lambda_0,\Lambda_0^\vee\rangle=0. \tag{2.1}$$

We introduce the root lattice Q, the coroot lattice $Q^\vee$, the weight lattice P, and the coweight lattice $P^\vee$, respectively, as

$$\begin{aligned} Q &:= \bigoplus_{i\in I} \mathbb{Z}\alpha_i \subset P := \bigoplus_{i\in I} \mathbb{Z}\Lambda_i \oplus \mathbb{C}\delta \subset \mathfrak{h}^*, \\ Q^\vee &:= \bigoplus_{i\in I} \mathbb{Z}\alpha_i^\vee \subset P^\vee := \bigoplus_{i\in I} \mathbb{Z}\Lambda_i^\vee \oplus \mathbb{C}K \subset \mathfrak{h}, \end{aligned} \tag{2.2}$$

where the fundamental weights Λ_i and coweights $\Lambda_i^\vee$ satisfy $\langle \alpha_i, \Lambda_j^\vee \rangle = \langle \Lambda_i, \alpha_j^\vee \rangle = \delta_{ij}$. We introduce a nondegenerate symmetric bilinear $\mathbb{C}$-value form $(.|.)$ on $\mathfrak{h}$, from which we have an isomorphism $\nu: \mathfrak{h} \to \mathfrak{h}^*$ defined by

$$\langle \nu(h), h' \rangle = (h|h') \quad \text{for } h, h' \in \mathfrak{h},$$

and the induced bilinear form $(.|.)$ on $\mathfrak{h}^*$. We have $a_i^\vee \nu(\alpha_i^\vee) = a_i \alpha_i$, $\nu(K) = \delta$ and $\nu(\Lambda_0^\vee) = a_0 \Lambda_0$.

Let $\mathring{I} := \{1,2,...,l\}$ be another set of indices, and let $\mathring{\Pi} := \{\alpha_i | i \in \mathring{I}\} (\subset \Pi)$ and $\mathring{\Pi}^\vee := \{\alpha_i^\vee | i \in \mathring{I}\}$ $(\subset \Pi^\vee)$. Let $\mathring{\mathfrak{h}}$ (respectively, $\mathring{\mathfrak{h}}_\mathbb{R}$) denote the linear span over $\mathbb{C}$ (respectively, $\mathbb{R}$) of $\mathring{\Pi}^\vee$. The dual notions $\mathring{\mathfrak{h}}^*$ and $\mathring{\mathfrak{h}}_\mathbb{R}^*$ are defined similarly. Set $\mathfrak{h}_\mathbb{R} = \mathring{\mathfrak{h}}_\mathbb{R} + \mathbb{R}K + \mathbb{R}\Lambda_0^\vee$ and $\mathfrak{h}_\mathbb{R}^* = \mathring{\mathfrak{h}}_\mathbb{R}^* + \mathbb{R}\Lambda_0 + \mathbb{R}\delta$. We define the "classical" root system by $\mathring{R} := R \cap \mathring{\mathfrak{h}}^*$, which corresponds to a root system for a finite-dimensional simple Lie algebra, and fix its decomposition by the disjoint union $\mathring{R} = \mathring{R}_+ \cup \mathring{R}_-$, where $\mathring{R}_+ (\subset \mathring{R})$ is the set of positive roots relative to $\mathring{\Pi}$ and $\mathring{R}_- := -\mathring{R}_+$. The sets of short and long roots in $\mathring{R}$ are, respectively, denoted by $\mathring{R}^s$ and $\mathring{R}^l$. We use the notation $\mathring{Q}$, $\mathring{Q}^\vee$, $\mathring{P}$, and $\mathring{P}^\vee$ for the classical root, the classical coroot, the classical weight, and the classical coweight lattices,

$$\begin{aligned} \mathring{Q} &:= \bigoplus_{i\in \mathring{I}} \mathbb{Z}\alpha_i \subset \mathring{P} := \bigoplus_{i\in \mathring{I}} \mathbb{Z}\overline{\Lambda_i} \subset \mathring{\mathfrak{h}}^*, \\ \mathring{Q}^\vee &:= \bigoplus_{i\in \mathring{I}} \mathbb{Z}\alpha_i^\vee \subset \mathring{P}^\vee := \bigoplus_{i\in \mathring{I}} \mathbb{Z}\overline{\Lambda_i^\vee} \subset \mathring{\mathfrak{h}}, \end{aligned} \tag{2.3}$$

where $\overline{\lambda}$ means the orthogonal projection of $\lambda \in \mathfrak{h}^*$ (respectively, $\lambda \in \mathfrak{h}$) on $\mathring{\mathfrak{h}}^*$ (respectively, $\mathring{\mathfrak{h}}$). Let $\mathring{Q}_+$, $\mathring{P}_+$, $\mathring{Q}_+^\vee$ and $\mathring{P}_+^\vee$ denote the corresponding lattices with $\mathbb{Z}_+$ instead of $\mathbb{Z}$.

The set of real roots $R^{\mathrm{re}} \subset R$ are given by

$$R^{\mathrm{re}} := \begin{cases} \{\alpha + n\gamma_\alpha \delta | \alpha \in \mathring{R}, n \in \mathbb{Z}\} & \text{if } A \text{ is not of type } A_{2l}^{(2)} \\ \{\alpha + n\gamma_\alpha \delta | \alpha \in \mathring{R}, n \in \mathbb{Z}\} & \\ \quad \cup \{\tfrac{1}{2}(\alpha + (2n+1)\delta) | \alpha \in \mathring{R}^l, n \in \mathbb{Z}\} & \text{if } A \text{ is of type } A_{2l}^{(2)} \end{cases}, \tag{2.4}$$

where $\gamma_\alpha = r$ if $\alpha \in R^l$ and $\gamma_\alpha = 1$ otherwise. Define the set of positive affine roots by $R_+ := \{\alpha + n\delta \in R^{\mathrm{re}} | \alpha \in \mathring{R}, n > 0\} \cup \mathring{R}_+$. Let $\theta := \delta - a_0 \alpha_0 (\in \mathring{Q})$. One sees that $(\theta|\theta) = 2a_0$, $\theta = a_0 \nu(\theta^\vee)$ and $(\theta^\vee|\theta^\vee) = 2a_0^{-1}$.

Next we consider Weyl groups which act on the root systems. Define a reflection on $\mathfrak{h}^*$ with respect to the hyperplane orthogonal to $\alpha \in R^{\mathrm{re}}$ by

$$s_\alpha(\lambda) := \lambda - \langle \lambda, \alpha^\vee \rangle \alpha \quad \text{for } \lambda \in \mathfrak{h}^*.$$

Simple reflections $\{s_i := s_{\alpha_i} | i \in I\}$ are related to each other by braid relations (Coxeter relations) $(s_i s_j)^{m_{ij}} = 1$,[36] where $m_{ij} = 2,3,4,6$ if α_i and α_j are connected by 0, 1, 2, 3 laces in the Dynkin

diagram $S(A)$, respectively. The reflections $\{s_\alpha|\alpha\in\Pi\}$ generate the affine Weyl group, which we denote by W. The affine Weyl group includes the Weyl group $\mathring{W}$, which is generated by $\{s_\alpha|\alpha\in\mathring{\Pi}\}$, as a subgroup. For $\alpha,\beta:=\delta-h\alpha\in R^{\mathrm{re}}$ with some h, one sees

$$s_\alpha s_\beta(\lambda)=\lambda+\langle\lambda,K\rangle\nu(\beta^\vee)-(\langle\lambda,\beta^\vee\rangle+\tfrac{1}{2}|\beta^\vee|^2\langle\lambda,K\rangle)\delta \quad \text{for } \lambda\in\mathfrak{h}^*.$$

Motivated by this formula, we introduce the following endomorphism $\tau_\mu,(\mu\in\mathring{\mathfrak{h}}^*)$ of $\mathfrak{h}^*$:

$$\tau_\mu(\lambda)=\lambda+\langle\lambda,K\rangle\mu-((\lambda|\mu)+\tfrac{1}{2}|\mu|^2\langle\lambda,K\rangle)\delta \quad \text{for } \lambda\in\mathfrak{h}^*.$$

They satisfy the additivity property $\tau_\lambda\tau_\mu=\tau_{\lambda+\mu}$, $(\lambda,\mu\in\mathring{\mathfrak{h}}^*)$. It is known that the affine Weyl group is isomorphic to the semidirect product $W\simeq\mathring{W}\ltimes\tau_M$ where $M:=\nu(\mathbb{Z}(\mathring{W}(\theta^\vee)))\subset\mathring{\mathfrak{h}}^*$.

Definition 2.1 (Extended affine Weyl groups): Let $\widetilde{M}:=\{\lambda\in\mathring{\mathfrak{h}}^*|\alpha\in R^{\mathrm{re}},(\alpha|\lambda)\in\gamma_\alpha\mathbb{Z}\}$. *The extended affine Weyl group of type* $X_N^{(r)}$ *is the semidirect product* $\widetilde{W}:=\mathring{W}\ltimes\tau_{\widetilde{M}}$.[31,32]

Indeed the lattice $\widetilde{M}$ is given by

$$\widetilde{M}=\begin{cases}\nu(\mathring{P}^\vee) & \text{if } r=1\\ \mathring{P} & \text{otherwise.}\end{cases} \tag{2.5}$$

Then we take a basis $\{\lambda_i|i\in\mathring{I}\}$ of $\widetilde{M}$ as $\lambda_i=\nu(\overline{\Lambda_i^\vee})$ if $r=1$ and $\lambda_i=\overline{\Lambda_i}$ otherwise. One finds that $\widetilde{W}$ is defined so as to preserve the affine root system R.

Proposition 2.2: Let $C^\vee:=\{\lambda\in\mathfrak{h}_{\mathbb{R}}^*|(\lambda|\alpha_i)\geqslant 0 \text{ for } 0\leqslant i\leqslant l\}$ *be the fundamental chamber and let* $\Omega:=\{w\in\widetilde{W}|w(C^\vee)=C^\vee\}$. *The extended affine Weyl group is isomorphic to the semidirect product* $\widetilde{W}\simeq\Omega\ltimes W$.

Let $\mathcal{O}$ be the set of indices of the image of α_0 by the automorphism of the Dynkin diagram $S(A)$. It is known that the elements in Ω are indexed by $r\in\mathcal{O}$[14–16] and each $\omega_r\in\Omega$ is distinguished by $\omega_r(\alpha_0)=\alpha_r$.

Define $\mathfrak{h}_s^*:=\{\lambda\in\mathfrak{h}_{\mathbb{R}}^*|\langle\lambda,K\rangle=s\}$ for $s\in\mathbb{R}$. The action of $\widetilde{W}$ on $\mathfrak{h}_{-1}^*\bmod\mathbb{R}\delta$ is faithful. We identify $\mathfrak{h}_{-1}^*\bmod\mathbb{R}\delta$ with $\mathring{\mathfrak{h}}_{\mathbb{R}}^*$ by projection and obtain an isomorphism af from $\widetilde{W}$ onto a group of affine transformation W_{af} of $\mathring{\mathfrak{h}}_{\mathbb{R}}^*$. Then we have the action of W_{af} on $\overline{\lambda}\in\mathring{\mathfrak{h}}_{\mathbb{R}}^*$,

$$\mathrm{af}(w)(\overline{\lambda})=\overline{w(\lambda)} \quad \text{for } \lambda\in\mathfrak{h}_{-1}^*,$$

from which we observe for $\lambda\in\mathring{\mathfrak{h}}_{\mathbb{R}}^*$ that

$$\mathrm{af}(w)(\lambda)=w(\lambda) \quad \text{for } w\in\mathring{W}, \quad \mathrm{af}(\tau_\mu)(\lambda)=\lambda-\mu \quad \text{for } \mu\in\widetilde{M}.$$

The action of W_{af} induces a function $(\lambda+n\delta)(\mu)=(\lambda|\mu)-n$ on $\mathring{\mathfrak{h}}_{\mathbb{R}}^*$ satisfying

$$(w(\lambda+n\delta))(\mu)=(\lambda+n\delta)(\mathrm{af}(w^{-1})(\mu)) \quad \text{for } \lambda+n\delta\in\mathfrak{h}_0^*, \quad \mu\in\mathring{\mathfrak{h}}_{\mathrm{R}}^*.$$

We define a length of an element $w\in\widetilde{W}$ by

$$\ell(w):=|R_w| \quad \text{where } R_w:=R_+\cap wR_-. \tag{2.6}$$

Here R_w is the set of positive roots which become negative roots by the action of w^{-1}. If we take a reduced expression of $w\in\widetilde{W}$ as $w=s_{i_1}s_{i_2}\ldots s_{i_k}\omega_r,(\ell(w)=k)$, the set R_w is explicitly given by $R_w=\{\alpha^{(1)}=\alpha_{i_1},\alpha^{(2)}=s_{i_1}(\alpha_{i_2}),\ldots,\alpha^{(k)}=s_{i_1}s_{i_2}\ldots s_{i_{k-1}}(\alpha_{i_k})\}$, which is independent of the decomposition of w. For $w=\tau_{-\lambda}$, $(\lambda\in\mathring{\mathfrak{h}}^*)$, we have

$$R_{\tau-\lambda}=\begin{cases}\left\{\alpha+n\gamma_\alpha\delta\,\middle|\,\alpha\in\mathring{R}_+,\frac{1}{\gamma_\alpha}(\lambda|\alpha)>n\geqslant 0,\ \text{or}\ \alpha\in\mathring{R}_-,\frac{1}{\gamma_\alpha}(\lambda|\alpha)\geqslant n>0\right\} & \text{if } A \text{ is not of type } A_{2l}^{(2)},\\ \left\{\alpha+n\gamma_\alpha\delta\,\middle|\,\alpha\in\mathring{R}_+,\frac{1}{\gamma_\alpha}(\lambda|\alpha)>n\geqslant 0,\ \text{or}\ \alpha\in\mathring{R}_-,\frac{1}{\gamma_\alpha}(\lambda|\alpha)\geqslant n>0\right\}\\ \quad\cup\left\{\frac{1}{2}(\alpha+(2n+1)\delta)\,\middle|\,\alpha\in\mathring{R}^l_+,\frac{1}{2}(\lambda|\alpha)>n\geqslant 0,\ \text{or}\ \alpha\in\mathring{R}^l_-,\frac{1}{2}(\lambda|\alpha)>n\geqslant 0\right\}\\ \quad\text{if } A \text{ is of type } A_{2l}^{(2)}\end{cases}. \tag{2.7}$$

We denote the set of distinct weights lying in the $\mathring{W}$-orbit of $\mu\in\tilde{M}$ by $\mathring{W}(\mu)$ and a unique dominant weight in $\mathring{W}(\mu)$ by $\mu^+(\in\tilde{M}_+)$. Define the isotropy group $\mathring{W}_\mu:=\{w\in\mathring{W}|w(\mu)=\mu\}$ for $\mu\in\tilde{M}_+$. In fact $\mathring{W}_\mu$ is genetrated by simple reflections s_i which it contains. Let $\{s_i|i\in\mathring{J}(\subset\mathring{I})\}$ be the set of simple reflections fixing $\mu\in\tilde{M}_+$ and let $\mathring{W}^\mu:=\{w\in\mathring{W}|\ell(ws_i)>\ell(w)\ \text{for all}\ i\in\mathring{J}\}$.

Proposition 2.3 (cf. Ref. 36): Given $w\in\mathring{W}$ and $\mu\in\tilde{M}_+$, there is a unique $u\in\mathring{W}^\mu$ and a unique $v\in\mathring{W}_\mu$ such that $w=uv$.

The above-given proposition shows that, for a general weight $\mu\in\tilde{M}$, there exists a unique element $w\in\mathring{W}^{\mu^+}$ such that $w(\mu^+)=\mu$.

B. Double affine Hecke algebras

We introduce affine Hecke algebras associated with affine root systems in an analogous way to Lusztig's works.[35] Let B be the braid group with generators $T_w,(w\in\tilde{W})$ satisfying braid relations:

$$T_{wv}=T_wT_v\quad\text{if}\ \ell(wv)=\ell(w)+\ell(v)\quad\text{for}\ w,v\in\tilde{W}. \tag{2.8}$$

We write $T_i,(i\in I)$ for T_{s_i}. One sees that, if a reduced expression of $w\in\tilde{W}$ is taken as $w=s_{i_1}s_{i_2}\cdots s_{i_k}\omega_r$, the corresponding element of the braid group B has an expression $T_w=T_{i_1}T_{i_2}\cdots T_{i_k}T_{\omega_r}$. Among the elements $\{T_w\in B|w\in\tilde{W}\}$, we define a set of elements $\{Y^\lambda\in B|\lambda\in\tilde{M}\}$ by

$$\begin{aligned}&(i)\quad Y^\lambda=T_{\tau_{-\lambda}}\ \text{for}\ \lambda\in\tilde{M}_+,\\ &(ii)\quad Y^\lambda=Y^\mu(Y^\nu)^{-1}\ \text{if}\ \lambda=\mu-\nu\in\tilde{M}\ \text{and}\ \mu,\nu\in\tilde{M}_+.\end{aligned} \tag{2.9}$$

The elements $\{Y^\lambda\}$ are well defined for all $\lambda\in\tilde{M}$. By definition (2.8), one has the additivity property $Y^{\lambda+\mu}=Y^\lambda Y^\mu$, $(\lambda,\mu\in\tilde{M})$, which provides the following significant proposition:

Proposition 2.4: The elements $\{Y^\lambda\in B|\lambda\in\tilde{M}\}$ are mutually commutative, and hence the braid group B includes a commutative subgroup generated by $\{Y^\lambda|\lambda\in\tilde{M}\}$.

Proposition 2.5: The elements $\{Y^\lambda,T_i|\lambda\in\tilde{M},i\in\mathring{I}\}$ generate B as a group.

In what follows, we restrict our discussions to the affine root system of type $A_{2l}^{(2)}$ since we are now interested in the Macdonald–Koornwinder polynomials; what it means here will soon be clear. Recall that there is no nontrivial automorphism of the Dynkin diagram $S(A)$ for the $A_{2l}^{(2)}$-type affine root system, that is, $\Omega=\{1\}$, while the corresponding Coxeter diagram has a nontrivial automorphism. The extended affine Weyl group of type $A_{2l}^{(2)}$ is isomorphic to the (nonextended) affine Weyl group of type $C_l^{(1)}$, that is, $\tilde{W}=W$, but structures of weight and coweight lattices they act on are different. We introduce the set of indeterminates $\{t_\alpha|\alpha\in R^{\mathrm{re}}\}$ such that $t_\alpha=t_{w(\alpha)}$ for $w\in\tilde{W}$. Indeed there exist three kinds of indeterminates corresponding to the following sets of real roots with different lengths:

$$(R^{\mathrm{re}})^s=\{\tfrac{1}{2}(\alpha+(2n+1)\delta)|\alpha\in\mathring{R}^l,n\in\mathbb{Z}\},$$

$$(R^{\mathrm{re}})^m=\{\alpha+n\delta|\alpha\in\mathring{R}^s,n\in\mathbb{Z}\},$$

$$(R^{\mathrm{re}})^l=\{\alpha+2n\delta|\alpha\in\mathring{R}^l,n\in\mathbb{Z}\}.$$

We denote the orthogonal projection of R^{re} on $\mathring{\mathfrak{h}}^*$ by $\overline{R^{\mathrm{re}}}$, which is nothing but the BC_l-type nonreduced root system. Note that $\overline{R^{\mathrm{re}}}$ has three kinds of root length, i.e., long, middle, and short roots. Let $\mathbb{C}_t=\mathbb{C}(\{t_\alpha^{1/2}\})$ denote the field of rational functions over $\mathbb{C}$ in square roots of these indeterminates $\{t_\alpha\}$.

Definition 2.6 (affine Hecke algebra): The affine Hecke algebra $H(\tilde{W})$ is the quotient of the group algebra $\mathbb{C}_t[B]$ by the two-sided ideal generated by

$$(T_i-t_i^{1/2})(T_i+t_i^{-1/2})\quad\text{for } 0\leqslant i\leqslant l,$$

where we write t_i for t_{α_i}.

The inverse element of T_i in $H(\tilde{W})$ is given by $T_i^{-1}=T_i-(t_i^{1/2}-t_i^{-1/2})$. One sees that the affine Hecke algebra $H(\tilde{W})$ is indeed generated over the field $\mathbb{C}_t$ by $\{T_i|i\in I\}$ satisfying

$$\begin{aligned}&\text{(i)}\quad (T_i-t_i^{1/2})(T_i+t_i^{-1/2})=0\quad\text{for } 0\leqslant i\leqslant l,\\ &\text{(ii)}\quad T_iT_jT_i\cdots=T_jT_iT_j\cdots,\quad m_{ij}\text{ factors on each side.}\end{aligned}\tag{2.10}$$

Proposition 2.7: Let $\lambda\in\tilde{M}$. In $H(\tilde{W})$, one sees

$$\begin{aligned}&(i)\quad T_iY^\lambda=Y^\lambda T_i\quad \textit{if } \langle\lambda,\alpha_i^\vee\rangle=0\ \textit{ for }\ \alpha_i\in\mathring{\Pi},\\ &(ii)\quad T_iY^{s_i(\lambda)}T_i=Y^\lambda\quad \textit{if } \langle\lambda,\alpha_i^\vee\rangle=1\ \textit{ for }\ \alpha_i\notin 2\tilde{M},\\ &(iii)\quad Y^{s_i(\lambda)}T_i-T_i^{-1}Y^\lambda+(t_{\tilde{\alpha}_i}^{1/2}-t_{\tilde{\alpha}_i}^{-1/2})Y^{\lambda-(1/2)\alpha_i}=0\quad \textit{if } \langle\lambda,\alpha_i^\vee\rangle=1\ \textit{ for }\ \alpha_i\in 2\tilde{M}.\end{aligned}\tag{2.11}$$

Here $\tilde{\alpha}\in R^{\mathrm{re}}$ is the root associated with the reflection $s_{\tilde{\alpha}}=\omega s_\alpha\omega^{-1}$ where ω is the automorphism of the Coxeter diagram corresponding to the Dynkin diagram $S(A)$.

We give a proof of Proposition 2.7 in Appendix.

Proposition 2.8: The affine Hecke algebra $H(\tilde{W})$ is also generated by the elements $\{T_i,Y^\lambda|i\in\mathring{I},\lambda\in\tilde{M}\}$ satisfying (2.10) and (2.11).[35]

By using Proposition 2.7 recursively, we have the following relations:

Proposition 2.9: For $\lambda\in\tilde{M}$, one has

$$T_iY^\lambda-Y^{s_i(\lambda)}T_i=\frac{(\check{t}_{\tilde{\alpha}_i}^{1/2}-\check{t}_{\tilde{\alpha}_i}^{-1/2})Y^{-(1/2)\alpha_i}+t_i^{1/2}-t_i^{-1/2}}{Y^{-\alpha_i}-1}(Y^{s_i(\lambda)}-Y^\lambda)\quad \textit{for }\ 1\leqslant i\leqslant l,\tag{2.12}$$

in $H(\tilde{W})$. Here we have put $\check{t}_\alpha=t_\alpha$ if $\alpha\in(R^{\mathrm{re}})^l$ and $\check{t}_\alpha=1$ otherwise.

Corollary 2.10: The element $Y^\lambda+Y^{s_\alpha(\lambda)},(\lambda\in\tilde{M},\alpha\in\mathring{\Pi})$ commutes with T_{s_α}.

Hence it is clear that elements from the $\mathring{W}$-invariant Laurent polynomial ring $\mathbb{C}_t[Y]^{\mathring{W}}$ are in the center of the affine Hecke algebra $\mathcal{Z}(H(\tilde{W}))$. In fact, the following stronger statement is known:

Theorem 2.11 (G. Lusztig): $\mathcal{Z}(H(\tilde{W}))=\mathbb{C}_t[Y]^{\mathring{W}}$.

We now define the double affine Hecke algebra $\mathcal{H}(\tilde{W})$ associated with the $A_{2l}^{(2)}$-type affine root system. We introduce another set of $\tilde{W}$-invariant indeterminates $\{u_\alpha|\alpha\in R^{\mathrm{re}}\}$ such that $u_\alpha=1$ if $\alpha\in(R^{\mathrm{re}})^m$, and put $u_i:=u_{\alpha_i}$. We take the field $\mathbb{K}:=\mathbb{C}(q^{1/2},\{t_\alpha^{1/2},u_\alpha^{1/2}\})$ of rational functions over $\mathbb{C}$ in square roots of indeterminates $\{q,t_\alpha,u_\alpha\}$.

Definition 2.12 (double affine Hecke algebra): The double affine Hecke algebra $\mathcal{H}(\tilde{W})$ *is generated over the field* $\mathbb{K}$ *by* $\{T_i, X^\mu | i \in I, \mu \in \mathring{P}\}$ *satisfying*

(i) *the relations* (2.10) *for* $\{T_i\}$,

(ii) $X^{\mu+\nu} = X^\mu X^\nu$ *for* $\mu, \nu \in \mathring{P}$,

(iii) $T_i X^\mu = X^\mu T_i$ *if* $\langle \mu, \alpha_i^\vee \rangle = 0$ *for* $\alpha_i \in \mathring{\Pi}$,

$$T_0 X^\mu = X^\mu T_0 \quad \text{if } \langle \mu, -\theta^\vee \rangle = 0,$$

(iv) $X^{s_i(\mu)} T_i^{-1} - T_i X^\mu - (u_{\tilde{\alpha}_i}^{1/2} - u_{\tilde{\alpha}_i}^{-1/2}) X^{\mu - (1/2)\alpha_i} = 0$ *if* $\langle \mu, \alpha_i^\vee \rangle = 1$ *for* $\alpha_i \in \mathring{\Pi}$,

$$X^{s_0(\mu)} T_0^{-1} - T_0 X^\mu - (u_l^{1/2} - u_l^{-1/2}) X^{\mu - \alpha_0} = 0 \quad \text{if } \langle \mu, -\theta^\vee \rangle = 1, \tag{2.13}$$

where

$$X^\mu = q^h \prod_{i \in \mathring{I}} (X^{\overline{\Lambda}_i})^{\mu_i} \quad \text{for } \mu = \sum_{i \in \mathring{I}} \mu_i \overline{\Lambda}_i + h\delta \in \mathring{P} \oplus \frac{1}{2}\mathbb{Z}\delta.$$

Proposition 2.13: For $\mu \in \mathring{P}$, *one has*

$$T_i X^\mu - X^{s_i(\mu)} T_i = \frac{(u_{\tilde{\alpha}_i}^{1/2} - u_{\tilde{\alpha}_i}^{-1/2}) X^{(1/2) n_i \alpha_i} + t_i^{1/2} - t_i^{-1/2}}{X^{n_i \alpha_i} - 1} (X^{s_i(\mu)} - X^\mu) \quad \text{for } 0 \leqslant i \leqslant l, \tag{2.14}$$

where $\{n_\alpha | \alpha \in R^{\mathrm{re}}\}$ *is defined by*

$$n_\alpha := \begin{cases} 2 & \text{if } \alpha \in (R^{\mathrm{re}})^s, \\ 1 & \text{otherwise,} \end{cases} \qquad n_i := n_{\alpha_i} \quad \text{for } 0 \leqslant i \leqslant l.$$

Proposition 2.14: The double affine Hecke algebra $\mathcal{H}(\tilde{W})$ *is also generated by the elements* $\{T_i, X^\mu, Y^\lambda | i \in \mathring{I}, \mu \in \mathring{P}, \lambda \in \tilde{M}\}$.

Proposition 2.15: There exists the following map which can be extended to the anti-involution $*: \mathcal{H}(\tilde{W}) \to \mathcal{H}(\tilde{W})$:

$$*: \ T_i \mapsto T_i^{-1}, \quad X^{\overline{\Lambda}_i} \mapsto X^{-\overline{\Lambda}_i}, \quad Y^{\lambda_i} \mapsto Y^{-\lambda_i} \quad \text{for } 1 \leqslant i \leqslant l,$$

$$q \mapsto q^{-1}, \quad t_\alpha \mapsto t_\alpha^{-1}, \quad u_\alpha \mapsto u_\alpha^{-1}. \tag{2.15}$$

We present a representation of the double affine Hecke algebra $\mathcal{H}(\tilde{W})$ in the endomorphism of the Laurent polynomial ring of variables $\{x^{\overline{\Lambda}_i} | i \in \mathring{I}\}$ over $\mathbb{K}$, which we denote by End $(\mathbb{K}[\mathring{P}])$. To begin with, we put $x^\delta = q$ and define the action of $w \in \tilde{W}$ on $\mathbb{K}[\mathring{P}]$ by

$$w(x^\mu) := x^{w(\mu)} \quad \text{for } x^\mu \in \mathbb{K}[\mathring{P}], \tag{2.16}$$

in particular, $\tau_\lambda(x^\mu) = q^{-(\lambda|\mu)} x^\mu$, $(\lambda \in \tilde{M})$.

Next, we introduce multiplication operators $\{\hat{X}^{\hat{\mu}} \in \mathrm{End}(\mathbb{K}[\mathring{P}]) | \hat{\mu} = \mu + h\delta \in \mathring{P} \oplus \frac{1}{2}\mathbb{Z}\delta\}$,

$$\hat{X}^{\hat{\mu}}(f) = q^h x^\mu f \quad \text{for } f \in \mathbb{K}[\mathring{P}], \tag{2.17}$$

and the Demazure–Lusztig operators $\{\hat{T}_i \in \mathrm{End}(\mathbb{K}[\mathring{P}]) | i \in I\}$:[25,35]

$$\hat{T}_i f := t_i^{1/2} s_i(f) + \frac{(u_{\tilde{\alpha}_i}^{1/2} - u_{\tilde{\alpha}_i}^{-1/2}) x^{(1/2)n_i\alpha_i} + t_i^{1/2} - t_i^{-1/2}}{x^{n_i\alpha_i} - 1}(s_i(f) - f) \quad \text{for } f \in \mathbb{K}[\mathring{P}]. \tag{2.18}$$

Indeed the Demazure–Lusztig operators are induced from Proposition 2.13.

Theorem 2.16: (*cf.* Refs. 25 and 35):

(*i*) *The map* $\pi: \mathcal{H}(\tilde{W}) \to \mathrm{End}(\mathbb{K}[\mathring{P}])$ *defined by*

$$\pi: X^\mu \mapsto \hat{X}^\mu, \quad T_i \mapsto \hat{T}_i \quad \textit{for } 0 \leqslant i \leqslant l,$$

induces a $\mathbb{K}$*-linear homomorphism from* $\mathcal{H}(\tilde{W})$ *to* $\mathrm{End}(\mathbb{K}[\mathring{P}])$.

(*ii*) *The map* π *provides a faithful representation of* $\mathcal{H}(\tilde{W})$.

Definition 2.17: The representation π *gives rise to a commutative family of difference operators* $\{\hat{Y}^\lambda := \pi(Y^\lambda) \in \mathrm{End}(\mathbb{K}[\mathring{P}]) | \lambda \in \tilde{M}\}$ *which we call the Cherednik operators.*

In Refs. 27, 29, and 30, a double affine Hecke algebra and the Cherednik operators are defined with a specific coordinate system for the corresponding root system. Note that we have defined them without using such a specific coordinate system. One sees shortly that the Demazure–Lusztig operators (2.18) include parameters we need for studying the Macdonald–Koornwinder polynomial.[25] We remark that, only in the representation of the double affine Hecke algebra of type $A_{2l}^{(2)}$, we can consider such additional parameters other than $\{t_\alpha\}$.

Definition 2.18: Define the order $\preccurlyeq$ *on* $\mathring{P}$ *by*

$$\nu \preccurlyeq \mu, (\mu, \nu \in \mathring{P}) \Leftrightarrow \begin{cases} \textit{if } \mu^+ \neq \nu^+ & \textit{then } \nu^+ < \mu^+ \\ \textit{if } \mu^+ = \nu^+ & \textit{then } \nu \leqslant \mu, \end{cases} \tag{2.19}$$

where

$$\nu < \mu \Leftrightarrow \mu - \nu \in \overline{Q}_+ = \nu(\mathring{Q}_+^\vee).$$

We show the triangularity of the Cherednik operators $\{\hat{Y}^\lambda | \lambda \in \tilde{M}\}$ in $\mathbb{K}[\mathring{P}]$.[14,17,29,37] Here the triangularity means that, in the expansion of $\hat{Y}^\lambda x^\mu$, only the terms x^ν appear whose weights ν are equal to or smaller than the original weight μ with respect to the order $\preccurlyeq$. Define $\{G_{\alpha_i}^\pm := \hat{T}_i^{\pm 1} s_i \in \mathrm{End}(\mathbb{K}[\mathring{P}]) | i \in I\}$. Since $\{G_\alpha^\pm | \alpha \in \Pi\}$ have a property $w G_\alpha^\pm w^{-1} = G_{w(\alpha)}^\pm$, they can be associated with all the real roots $\{\alpha \in R^{\mathrm{re}}\}$,

$$\begin{aligned} G_\alpha^+ &= t_\alpha^{1/2} + \frac{(u_{\tilde{\alpha}}^{1/2} - u_{\tilde{\alpha}}^{-1/2}) x^{(1/2)n_\alpha\alpha} + t_\alpha^{1/2} - t_\alpha^{-1/2}}{x^{n_\alpha\alpha} - 1}(1 - s_\alpha), \\ G_\alpha^- &= G_\alpha^+ - (t_\alpha^{1/2} - t_\alpha^{-1/2}) s_\alpha. \end{aligned} \tag{2.20}$$

Lemma 2.19: A reduced expression $\tau_{-\lambda} = s_{i_1} s_{i_2} \cdots s_{i_k} \in \tilde{W}$ *gives an expression* $Y^\lambda = T_{i_1}^{\varepsilon_1} T_{i_2}^{\varepsilon_2} \cdots T_{i_k}^{\varepsilon_k} \in H(\tilde{W})$ *where* $\varepsilon_i \in \{\pm 1\}$ *are determined by the set of affine roots* $R_{\tau_{-\lambda}}$, *that is,* $\varepsilon_i = 1$ *if the corresponding affine root is of the form* $\alpha^{(i)} = \alpha + h\delta$, $(\alpha \in \mathring{R}_+)$ *and* $\varepsilon_i = -1$ *otherwise.*

From this lemma, we have an expression of the Cherednik operators,

$$\hat{Y}^\lambda = \hat{T}_{i_1}^{\varepsilon_1} \hat{T}_{i_2}^{\varepsilon_2} \cdots \hat{T}_{i_k}^{\varepsilon_k} = G_{\alpha^{(1)}}^{\varepsilon_1} G_{\alpha^{(2)}}^{\varepsilon_2} \cdots G_{\alpha^{(k)}}^{\varepsilon_k} \tau_{-\lambda},$$

where $\tau_{-\lambda} = s_{i_1} s_{i_2} \cdots s_{i_k} \in \mathrm{End}(\mathbb{K}[\mathring{P}])$. Note that the affine roots $\{\alpha^{(i)} | i \in \{1,2,...,k\}\}$ appearing in the above-given expression run through the set $R_{\tau_{-\lambda}}$. We consider the Cherednik operators with $\lambda \in \tilde{M}_+$; in this case, all $\varepsilon_i = +1$, $(1 \leqslant i \leqslant k)$. Since each operator G_α^+ acts on $\mathbb{K}[\mathring{P}]$ as

$$G_\alpha^+ x^\mu = \begin{cases} t_\alpha^{1/2} x^\mu + \text{lower terms w.r.t. } \prec & \text{if } \langle \mu, \alpha^\vee \rangle \geqslant 0 \\ t_\alpha^{-1/2} x^\mu + \text{lower terms w.r.t. } \prec & \text{if } \langle \mu, \alpha^\vee \rangle < 0, \end{cases} \tag{2.21}$$

one finds that the Cherednik operators $\hat{Y}^\lambda, (\lambda \in \tilde{M}_+)$ have the triangularity in $\mathbb{K}[\mathring{P}]$,

$$\hat{Y}^\lambda x^\mu = c_{\mu\mu} x^\mu + \text{lower terms w.r.t.} \prec . \tag{2.22}$$

The coefficient of the top term x^μ is given by

$$c_{\mu\mu} = q^{(\lambda|\mu^*)},$$

$$\mu^* := \mu + \frac{1}{2} \sum_{\alpha \in R_+}^{\circ} (k_\alpha + \check{k}_{\tilde{\alpha}}) \gamma_\alpha^{-1} \alpha - \sum_{\substack{\alpha \in R_+ \\ \langle \mu, \alpha^\vee \rangle < 0}}^{\circ} (k_\alpha + \check{k}_{\tilde{\alpha}}) \gamma_\alpha^{-1} \alpha = \mu + w_\mu(\rho_k).$$

Here we have put $t_\alpha = q^{k_\alpha}$, $\check{t}_\alpha = q^{\check{k}_\alpha}$, and

$$\rho_k := \frac{1}{2} \sum_{\alpha \in R_+}^{\circ} (k_\alpha + \check{k}_{\tilde{\alpha}}) \gamma_\alpha^{-1} \alpha,$$

and we have denoted by w_μ a unique element in $\mathring{W}^{\mu^+}$ such that $w_\mu^{-1}(\mu) \in \mathring{P}_+$ to define $\rho_k(\mu) := w_\mu(\rho_k)$. We can also show the triangularity of $\hat{Y}^\lambda$ with general elements $\lambda \in \tilde{M}$ by the help of the decomposition $\hat{Y}^\lambda = \hat{Y}^\mu (\hat{Y}^\nu)^{-1}$ such that $\mu, \nu \in \tilde{M}_+$.

Proposition 2.20: The Cherednik operators $\{\hat{Y}^\lambda | \lambda \in \tilde{M}\}$ *have the triangularity in* $\mathbb{K}[\mathring{P}]$:

$$\hat{Y}^\lambda x^\mu = x^\mu q^{(\lambda|\mu + \rho_k(\mu))} + \sum_{\nu < \mu} c_{\mu\nu} x^\nu \quad \textit{for} \quad \mu \in \mathring{P}, \quad c_{\mu\nu} \in \mathbb{K}. \tag{2.23}$$

We remark that $\{G_\alpha^\pm\}$ satisfy the defining relation of Cherednik's root algebra,[38] which is considered as a generalization of the Yang–Baxter relation. A representation of the root algebra obtained by one of us produces the elliptic Ruijsenaars operators associated with affine root systems.[31,32,34,39]

III. MACDONALD–KOORNWINDER POLYNOMIALS

Macdonald gave a classification of his orthogonal polynomials in terms of irreducible admissible pairs.[2] The Macdonald–Koornwinder polynomials, which were not included in Macdonald's classification, were introduced as multivariable generalizations of the Askey–Wilson polynomials and they have five parameters *a, b, c, d, t* apart from *q*.[22] Macdonald proposed in his seminary notes that Cherednik's affine Hecke algebraic approach can be also applied to the Macdonald–Koornwinder polynomials.[26] By using the Demazure–Lusztig operators for the $C^{(1)}$-type Hecke algebra and Theorem 2.11 in Sec. II, Noumi actually constructed a set of commutative operators which characterizes the Macdonald–Koornwinder polynomials as their joint eigenvectors.[25] However his construction is slightly different from Cherednik's theory for the Macdonald polynomials in the sense that he used a (nonextended) affine Weyl group of type *C*, and hence it seems to be hard to give a unified viewpoint for both of them. In Sec. II, we defined the affine Hecke algebra such that the corresponding extended affine Weyl group preserves the affine root system. In our setting, the representation of the affine Hecke algebra associated with $A_{2l}^{(2)}$-type affine root system gave the Demazure–Lusztig operators (2.18) including parameters we need. Thus we obtain a classification of the Macdonald and Macdonald–Koornwinder polynomials in terms of affine root systems as

Affine root systems	Polynomials
$X_l^{(1)}$	X_l-type Macdonald
$A_{2l}^{(2)}$	Macdonald–Koornwinder (BC_l-type Macdonald)

We remark that Macdonald also implied this classification in Ref. 2. Cherednik studied the Macdonald polynomials associated with pairs $(\mathring{R},\mathring{R}^\vee)$ for nonsimply laced classical root systems,[16] which, in this classification, correspond to twisted affine root systems other than of type $A_{2l}^{(2)}$.

A. Nonsymmetric Macdonald–Koornwinder polynomials

First we consider the nonsymmetric Macdonald–Koornwinder polynomials.[18,27,29] Let ι be involution $\iota:\mathbb{K}[\mathring{P}]\to\mathbb{K}[\mathring{P}]$ defined by

$$\iota: q\mapsto q^{-1},\quad t_\alpha\mapsto t_\alpha^{-1},\quad u_\alpha\mapsto u_\alpha^{-1},\quad x^\mu\mapsto x^\mu,$$

and let $^-$ be bar-involution $^-:\mathbb{K}[\mathring{P}]\to\mathbb{K}[\mathring{P}]$ defined by

$$^-: q\mapsto q,\quad t_\alpha\mapsto t_\alpha,\quad u_\alpha\mapsto u_\alpha,\quad x^\mu\mapsto x^{-\mu}.$$

We define the following scalar products in $\mathbb{K}[\mathring{P}]$:

$$\langle f,g\rangle'_{q,t,u}:=[f\overline{g^\iota}\mu_{q,t,u}]_0,\quad (f,g)'_{q,t,u}:=[f\overline{g^\iota}\tilde{\mu}_{q,t,u}]_0, \tag{3.1}$$

where $[f]_0$ stands for the constant term (the coefficient of x^0) of f. The weight function $\mu_{q,t,u}$ is given by

$$\mu_{q,t,u}:=\prod_{\alpha\in R_+^{\mathrm{re}}}\frac{1-x^{n_\alpha\alpha}}{(1-t_\alpha^{1/2}u_{\tilde{\alpha}}^{1/2}x^{(1/2)n_\alpha\alpha})(1+t_\alpha^{1/2}u_{\tilde{\alpha}}^{-1/2}x^{(1/2)n_\alpha\alpha})}, \tag{3.2}$$

and $\tilde{\mu}_{q,t,u}=\mu_{q,t,u}/[\mu_{q,t,u}]_0$.

Proposition 3.1: Coefficients of $\mu_{q,t,u}$ are in the algebra $\mathbb{C}[\{t_\alpha^{1/2},u_\alpha^{1/2}\}][[q^{1/2}]]$ of formal power series in $q^{1/2}$ over polynomials in $\{t_\alpha^{1/2},u_\alpha^{1/2}\}$.

Proof: We give a proof of the proposition above following Ref. 2. Put

$$x_0:=x^{\alpha_0}=q^{1/2}x^{-(1/2)\theta},\quad x_i:=x^{\alpha_i}\quad\text{for } 1\leqslant i\leqslant l-1,\quad x_l:=x^{(1/2)\alpha_l},$$

and consider the polynomial ring $\mathbb{C}[x_0,\ldots,x_l]$. Due to $\theta=\Sigma_{i\in\mathring{I}}a_i\alpha_i=2\Sigma_{i=1}^{l-1}\alpha_i+\alpha_l$, we have $x^\theta=x_0^2x_1^2\cdots x_l^2$. Then $q^{1/2}=x_0x^{(1/2)\theta}=x_0x_1\cdots x_l$. We see that, for $\alpha\in\mathring{R}_+^l$ and $i\in\mathbb{N}$,

$$q^ix^{(1/2)\alpha}=x_0^{2i}x^{i\theta+(1/2)\alpha},\quad q^{i+1/2}x^{(1/2)\alpha}=x_0^{2i+1}x^{(i+1/2)\theta+(1/2)\alpha},$$

$$q^{i+1}x^{-(1/2)\alpha}=x_0^{2(i+1)}x^{(i+1)\theta-(1/2)\alpha},\quad q^{i+1/2}x^{-(1/2)\alpha}=x_0^{2i+1}x^{(i+1/2)\theta-(1/2)\alpha},$$

are monomials in $\mathbb{C}[x_0,\ldots,x_l]$ since $\alpha\leqslant\theta$. For $\alpha\in\mathring{R}^m$ and $i\in\mathbb{N}$,

$$q^ix^\alpha=x_0^{2i}x^{i\theta+\alpha},\quad q^{i+1}x^{-\alpha}=x_0^{2(i+1)}x^{(i+1)\theta-\alpha},$$

are also monomials in $\mathbb{C}[x_0,\ldots,x_l]$. Hence the weight function $\mu_{q,t,u}$ can be rewritten as

$$\mu_{q,t,u}=\sum_{\beta\in\mathbb{N}^{l+1}}b_\beta(t,u)x^\beta,$$

with $x^{\beta}:=x_0^{\beta_0}x_1^{\beta_1}\cdots x_l^{\beta_l}\in\mathbb{C}[x_0,\ldots,x_l]$ and $b_{\beta}(t,u)\in\mathbb{C}[\{t_\alpha^{1/2},u_\alpha^{1/2}\}]$. Moreover, from $x^{\beta}=q^{(1/2)\beta_0}x_1^{\beta_1-\beta_0}\cdots x_l^{\beta_l-\beta_0}(\in\mathbb{K}[\mathring{P}])$, we have

$$\mu_{q,t,u}=\sum_{\mu\in\mathring{P}}a_\mu(q,t,u)x^{\mu},$$

where $a_\mu(q,t,u)=\Sigma_{\beta_0\geqslant 0}q^{(1/2)\beta_0}b_\beta(t,u)\in\mathbb{C}[\{t_\alpha^{1/2},u_\alpha^{1/2}\}][[q^{1/2}]]$ and β is determined from $\mu\in\mathring{P}$ and $\beta_0\in\mathbb{N}$ by the condition $2\mu=2\Sigma_{i=1}^{l-1}(\beta_i-\beta_0)\alpha_i+(\beta_l-\beta_0)\alpha_l$. As a consequence, we see that the coefficients of $\mu_{q,t,u}$ are in $\mathbb{C}[\{t_\alpha^{1/2},u_\alpha^{1/2}\}][[q^{1/2}]]$. □

In terms of the classical root system $\mathring{R}$ corresponding to R, the weight function is rewritten as

$$\mu_{q,t,u}=\prod_{\alpha\in\mathring{R}_+^l}\frac{(x^\alpha,qx^{-\alpha};q)_\infty}{(ax^{(1/2)\alpha},bx^{(1/2)\alpha},cx^{(1/2)\alpha},dx^{(1/2)\alpha},aqx^{-(1/2)\alpha},bqx^{-(1/2)\alpha},cx^{-(1/2)\alpha},dx^{-(1/2)\alpha};q)_\infty}\times\prod_{\alpha\in\mathring{R}_+^s}\frac{(x^\alpha,qx^{-\alpha};q)_\infty}{(t_\alpha x^\alpha,t_\alpha qx^{-\alpha};q)_\infty},\tag{3.3}$$

where we have put $a=t_l^{1/2}u_0^{1/2}$, $b=-t_l^{1/2}u_0^{-1/2}$, $c=t_0^{1/2}u_l^{1/2}q^{1/2}$, $d=-t_0^{1/2}u_l^{-1/2}q^{1/2}$ in a way similar to Ref. 22 and have employed the q-shifted factorials

$$(z;q)_\infty:=\prod_{i=0}^{\infty}(1-zq^i),\quad (z_1,z_2,\ldots,z_k;q)_\infty:=\prod_{i=1}^{k}(z_i;q)_\infty.$$

Lemma 3.2 (cf. Refs. 40, 41). The constant term of $\mu_{q,t,u}$ is given by

$$\langle 1,1\rangle'_{q,t,u}=\prod_{\alpha\in\mathring{R}_+^l}\frac{(abcdq'^2_{0,\alpha};q)_\infty^2}{(qq'_{0,\alpha},abqq'_{0,\alpha},acq'_{0,\alpha},adq'_{0,\alpha},bcq'_{0,\alpha},bdq'_{0,\alpha},cdq'_{0,\alpha},abcdq'_{0,\alpha};q)_\infty}\times\prod_{\alpha\in\mathring{R}_+^s}\frac{(qq'^2_{0,\alpha};q)_\infty^2}{(t_\alpha qq_{0,\alpha}^2,t_\alpha^{-1}qq_{0,\alpha}^2;q)_\infty},\tag{3.4}$$

where $q_{0,\alpha}:=q^{(1/2)(\alpha|\rho_k)}$, $q'_{0,\alpha}:=q^{(1/2)(\alpha|\rho'_k)}$ and $\rho'_k:=(1/2)\Sigma_{\alpha\in\mathring{R}_+^s}k_\alpha\alpha$.

We admit this lemma which is verified from Gustafson's constant term identity,[40,42]

$$\langle 1,1\rangle_{q,t,u}=\prod_{i=1}^{l}\frac{(t,abcdt^{2l-i-1};q)_\infty}{(q,t^{l-i+1},abt^{l-i},act^{l-i},adt^{l-i},bct^{l-i},bdt^{l-i},cdt^{-i};q)_\infty},\tag{3.5}$$

together with Macdonald's identity for the Poincaré polynomials.[41] The definition of the inner product $\langle\cdot,\cdot\rangle_{q,t,u}$ in (3.5) will appear shortly (3.22). In order to see their explicit relation, we need the following identities:

$$\prod_{j<k}\frac{(t^{k-j},qt^{k-j};q)_\infty}{(t^{k-j+1},qt^{k-j-1};q)_\infty}=\prod_{i=1}^{l}\frac{(t,qt^{l-i};q)_\infty}{(q,t^{l-i+1};q)_\infty},$$

$$\prod_{j<k}\frac{(abcdt^{2l-j-k},abcdq^{-1}t^{2l-j-k};q)_\infty}{(abcdt^{2l-j-k+1},abcdq^{-1}t^{2l-j-k+1};q)_\infty}=\prod_{i=1}^{l}\frac{(abcdt^{2l-2i-1},abcdq^{-1}t^{l-i};q)_\infty}{(abcdt^{l-i-1},abcdq^{-1}t^{2(l-i)};q)_\infty},$$

where we put $t=t_i$, $(1\leqslant i\leqslant l-1)$. Another proof of the constant term identity is established by use of the shift operator.[29]

Definition 3.3 (nonsymmetric Macdonald–Koornwinder polynomials): The (monic) nonsymmetric Macdonald–Koornwinder polynomials $E_\mu := E_\mu(x;q,\{t_\alpha,u_\alpha\}) \in \mathbb{K}[\mathring{P}], (\mu \in \mathring{P})$ *are uniquely defined by the following conditions*:

$$\begin{aligned} &(i)\ \ E_\mu = x^\mu + \sum_{\nu \prec \mu} w_{\mu\nu} x^\nu \quad \text{for } w_{\mu\nu} \in \mathbb{K}, \\ &(ii)\ \ (E_\mu, x^\nu)'_{q,t,u} = 0 \quad \text{if } \nu \prec \mu. \end{aligned} \tag{3.6}$$

The weight function $\mu_{q,t,u}$ for the nonsymmetric Macdonald–Koornwinder polynomials were first introduced in Ref. 29. We remark that, by setting $u_\alpha = 1$ and $n_\alpha = 1$ in the weight function (3.2), we can also define nonsymmetric Macdonald polynomials associated with both nontwisted and twisted affine root systems other than of type $A_{2l}^{(2)}$.

Proposition 3.4: The adjoint operators of $\{\hat{T}_i, \hat{Y}^\lambda, \hat{X}^\mu \in \mathrm{End}(\mathbb{K}[\mathring{P}]) | i \in I, \lambda \in \widetilde{M}, \mu \in \mathring{P}\}$ *with respect to the scalar products (3.1) are given by*

$$(\hat{T}_i)^* = \hat{T}_i^{-1}, \quad (\hat{Y}^\lambda)^* = \hat{Y}^{-\lambda}, \quad (\hat{X}^\mu)^* = \hat{X}^{-\mu}.$$

Proof: $(\hat{X}^\mu)^* = \hat{X}^{-\mu}$ is straightforward from the definition of the scalar products (3.1). We show that $(\hat{T}_i)^* = \hat{T}_i^{-1}$. Since $(t_i)^* = t_i^{-1}$, it is sufficient to prove $(T_i - t_i^{1/2})^* = T_i - t_i^{1/2}$. Indeed, we see that

$$s_i^* = \mu_{q,t,u}^{-1} s_i \mu_{q,t,u} = \frac{(1-x^{-n_i\alpha_i})(1-t_i^{1/2}u_{\tilde{\alpha}_i}^{1/2}x^{(1/2)n_i\alpha_i})(1+t_i^{1/2}u_{\tilde{\alpha}_i}^{-1/2}x^{(1/2)n_i\alpha_i})}{(1-x^{n_i\alpha_i})(1-t_i^{1/2}u_{\tilde{\alpha}_i}^{1/2}x^{-(1/2)n_i\alpha_i})(1+t_i^{1/2}u_{\tilde{\alpha}_i}^{-1/2}x^{-(1/2)n_i\alpha_i})} s_i,$$

and hence we obtain

$$\begin{aligned} (\hat{T}_i - t_i^{1/2})^* &= (s_i^* - 1)t_i^{1/2} \frac{(1-t_i^{-1/2}u_{\tilde{\alpha}_i}^{-1/2}x^{-(1/2)n_i\alpha_i})(1+t_i^{-1/2}u_{\tilde{\alpha}_i}^{1/2}x^{-(1/2)n_i\alpha_i})}{1-x^{-n_i\alpha_i}} \\ &= (s_i^* - 1)t_i^{-1/2} \frac{(1-t_i^{1/2}u_{\tilde{\alpha}_i}^{1/2}x^{(1/2)n_i\alpha_i})(1+t_i^{1/2}u_{\tilde{\alpha}_i}^{-1/2}x^{(1/2)n_i\alpha_i})}{1-x^{n_i\alpha_i}} \\ &= \hat{T}_i - t_i^{1/2}. \end{aligned} \tag{3.7}$$

We see that $(\hat{Y}^\lambda)^* = \hat{Y}^{-\lambda}$ from its definition and $(\hat{T}_i)^* = \hat{T}_i^{-1}$. □

Theorem 3.5: *The nonsymmetric Macdonald–Koornwinder polynomials* $E_\mu \in \mathbb{K}[\mathring{P}]$ *are joint eigenvectors of the Cherednik operators* $\{\hat{Y}^\lambda \in \mathrm{End}(\mathbb{K}[\mathring{P}]) | \lambda \in \widetilde{M}\}$,

$$\hat{Y}^\lambda E_\mu = q^{(\lambda|\mu+\rho_k(\mu))} E_\mu. \tag{3.8}$$

Proof: Consider the nonsymmetric Macdonald–Koornwinder polynomial operated by the Cherednik operator $\hat{Y}^\lambda E_\mu, (\lambda \in \widetilde{M}, \mu \in \mathring{P})$. Due to the unitarity of the Cherednik operator $(\hat{Y}^\lambda)^* = \hat{Y}^{-\lambda}$ (Proposition 3.4) and their triangularity in $\mathbb{K}[\mathring{P}]$ (2.23), the polynomial $\hat{Y}^\lambda E_\mu$ satisfies condition (ii) in (3.6) and have the form (i) in (3.6) up to a constant factor $q^{(\lambda|\mu+\rho_k(\mu))}$. The uniqueness of the nonsymmetric Macdonald–Koornwinder polynomials shows that, for all λ $(\in \widetilde{M})$, $\widetilde{Y}^\lambda E_\mu$ coincides with E_μ up to the constant factor, which proves the theorem. □

Note that, since all the eigenvalues $\{q^{(\lambda|\mu+\rho_k(\mu))} | \lambda \in \widetilde{M}\}$ determine the weight $\mu \in \mathring{P}$ uniquely, all the simultaneous eigenspaces of the Cherednik operators $\{\hat{Y}^\lambda | \lambda \in \widetilde{M}\}$ are one dimensional.

Moreover, we see a proposition in the following.

Proposition 3.6 (cf. Refs. 27, 29): (i) We have the orthogonality of the nonsymmetric Macdonald–Koornwinder polynomials:

$$(E_\mu, E_\nu)'_{q,t,u} = 0 \quad \text{if } \mu \neq \nu. \tag{3.9}$$

In fact, the non-symmetric Macdonald–Koornwinder polynomials form an orthogonal basis in $\mathbb{K}[\mathring{P}]$ *with respect to the scalar product* $(\cdot,\cdot)'_{q,t,u}$ *in (3.1).*
(ii) Conditions (i) in (3.6) and (3.9) also determine the nonsymmetric Macdonald–Koornwinder polynomials E_μ *uniquely.*

Proposition 3.7: Applying the Demazure–Lusztig operators $\hat{T}_i, (1 \leqslant i \leqslant l)$ *to* $E_\mu, (\mu \in \mathring{P})$, *we obtain*

$$\hat{T}_i E_\mu = \begin{cases} \dfrac{t_i^{1/2} - t_i^{-1/2} + (\check{t}_{\tilde{\alpha}_i}^{-1/2} - \check{t}_{\tilde{\alpha}_i}^{-1/2}) q_{\mu,i}^{-1}}{1 - q_{\mu,i}^{-2}} E_\mu + t_i^{1/2} E_{s_i(\mu)} & \text{if } \langle \mu, \alpha_i^\vee \rangle < 0 \\ t_i^{1/2} E_\mu \quad \text{if } \langle \mu, \alpha_i^\vee \rangle = 0 \\ \dfrac{t_i^{1/2} - t_i^{-1/2} + (\check{t}_{\tilde{\alpha}_i}^{1/2} - \check{t}_{\tilde{\alpha}_i}^{-1/2}) q_{\mu,i}^{-1}}{1 - q_{\mu,i}^{-2}} E_\mu \\ \quad + \dfrac{t_i^{-1/2}(1 - t_i^{1/2}\check{t}_{\tilde{\alpha}_i}^{1/2} q_{\mu,i}^{-1})(1 + t_i^{1/2}\check{t}_{\tilde{\alpha}_i}^{-1/2} q_{\mu,i}^{-1})(1 - t_i^{-1/2}\check{t}_{\tilde{\alpha}_i}^{-1/2} q_{\mu,i}^{-1})(1 + t_i^{-1/2}\check{t}_{\tilde{\alpha}_i}^{1/2} q_{\mu,i}^{-1})}{(1 - q_{\mu,i}^{-2})^2} E_{s_i(\mu)} \quad \text{if } \langle \mu, \alpha_i^\vee \rangle > 0, \end{cases} \tag{3.10}$$

where $q_{\mu,i} := q^{(1/2)(\alpha_i | \mu + \rho_k(\mu))}$.

Proof: Let $f := (z\hat{T}_i + 1)E_\mu$ for $\langle \mu, \alpha_i^\vee \rangle \neq 0$. z is determined so that f has the same eigenvalues of $\{\hat{Y}^\lambda\}$ as those of $E_{s_i(\mu)}$. Each coefficient is determined by comparing their top terms. The case $\langle \mu, \alpha_i^\vee \rangle = 0$ follows from definition (3.6) and unitarity $(\hat{T}_i)^* = \hat{T}_i^{-1}$. □

Proposition 3.8 (cf. Ref. 27): The map ε *defined by*

$$\begin{gathered} \varepsilon : T_i \mapsto T_i^{-1}, \quad X^{\overline{\Lambda_i}} \mapsto Y^{\overline{\Lambda_i}}, \quad Y^{\overline{\Lambda_i}} \mapsto X^{\overline{\Lambda_i}}, \quad \text{for } 1 \leqslant i \leqslant l, \\ q \mapsto q^{-1}, \quad t_i \mapsto t_i^{-1}, \quad u_i \mapsto u_i^{-1} \quad \text{for } 1 \leqslant i \leqslant l, \\ t_0 \mapsto u_0^{-1}, \quad u_0 \mapsto t_0^{-1}, \end{gathered} \tag{3.11}$$

can be extended to the involution $\varepsilon : \mathcal{H}(\widetilde{W}) \to \mathcal{H}(\widetilde{W})$.

Proof: It is directly verified from the relations between generators of $\mathcal{H}(\widetilde{W})$ (2.13) and their image by the map ε. □

We have omitted details of the proof since the involution ε is essentially the same as that proved by Sahi for his double affine Hecke algebra.[27] The involution ε also provides

$$\varepsilon(T_0) = \varepsilon(T_{s_\theta}^{-1} Y^{(1/2)\theta}) = T_{s_\theta} X^{(1/2)\theta} = Y^{(1/2)\theta} T_0^{-1} X^{(1/2)\theta} =: U_0^{-1}, \tag{3.12}$$

which satisfy the following quadratic relation: $(U_0 - u_0^{1/2})(U_0 + u_0^{-1/2}) = 0$.

Proposition 3.9: Let $\lambda \in \widetilde{M}$. *In* $\mathcal{H}(\widetilde{W})$, *we have*

$$U_0 Y^\lambda - Y^{s_0(\lambda)} U_0 = \frac{(u_l^{1/2} - u_l^{-1/2}) Y^{-\alpha_0} + u_0^{1/2} - u_0^{-1/2}}{Y^{-2\alpha_0} - 1} (Y^{s_0(\lambda)} - Y^\lambda), \tag{3.13}$$

where $Y^\delta = q^{-1}$.

Definition 3.10: We call the following elements $\{S_i \in \mathcal{H}(\widetilde{W}) | i \in I\}$ *intertwiners:*[16,18,27]

$$S_0 := U_0^{-1} Y^{2\alpha_0} - (u_l^{1/2} - u_l^{-1/2}) Y^{\alpha_0} - U_0,$$
$$S_i := T_i^{-1} Y^{\alpha_i} - (\check{t}_{\tilde{\alpha}_i}^{1/2} - \check{t}_{\tilde{\alpha}_i}^{-1/2}) Y^{(1/2)\alpha_i} - T_i \quad \text{for } 1 \leqslant i \leqslant l. \tag{3.14}$$

Lemma 3.11: The elements $\{S_i \in \mathcal{H}(\tilde{W}) | i \in I\}$ *satisfy*

(*i*) $S_i S_j S_i \cdots = S_j S_i S_j \cdots$, m_{ij} *factors on each side,*

(*ii*) $S_i^2 = t_i^{-1}(1 - t_i^{1/2}\check{t}_{\tilde{\alpha}_i}^{1/2} Y^{(1/2)\alpha_i})(1 + t_i^{1/2}\check{t}_{\tilde{\alpha}_i}^{-1/2} Y^{(1/2)\alpha_i})(1 - t_i^{1/2}\check{t}_{\tilde{\alpha}_i}^{1/2} Y^{-(1/2)\alpha_i})$
$\times (1 + t_i^{1/2}\check{t}_{\tilde{\alpha}_i}^{-1/2} Y^{-(1/2)\alpha_i})$ *for* $1 \leqslant i \leqslant l$,

$$S_0^2 = u_0^{-1}(1 - u_0^{1/2}u_l^{1/2}Y^{\alpha_0})(1 + u_0^{1/2}u_l^{-1/2}Y^{\alpha_0})(1 - u_0^{1/2}u_l^{1/2}Y^{-\alpha_0})(1 + u_0^{1/2}u_l^{-1/2}Y^{-\alpha_0}). \tag{3.15}$$

Proof: We verify relations (i) and (ii) by applying the composite $\pi \circ \varepsilon$ to $\{S_i | i \in I\}$,

$$\pi \circ \varepsilon(S_i) = -t_i^{1/2}(1 + t_i^{-1/2}(u_{\tilde{\alpha}_i}^{1/2} - u_{\tilde{\alpha}_i}^{-1/2}) x^{-(1/2)n_i\alpha_i} - t_i^{-1} x^{-n_i\alpha_i}) s_i .$$

□

The concept of intertwiners in Hecke algebras has a long history, and intertwiners in double affine Hecke algebras were first introduced by Cherednik.[15,16] Motivated by Noumi's work,[25] Sahi introduced a set of intertwiners which gives a linear isomorphism between simultaneous eigenspaces of the Cherednik operators (Definition 2.17) to define the nonsymmetric Macdonald–Koornwinder polynomials.[27] In our previous paper,[18] we defined intertwiners by improving Sahi's operators so as to satisfy the braid relation (i) in Lemma 3.11, and we presented a Rodrigues-type formula of the nonsymmetric Macdonald–Koornwinder polynomials with a specific coordinate system for the associated affine root system. Here we have defined the intertwiners (3.14) to give the Rodrigues-type formula without using such a specific coordinate system.

Definition 3.12: For a reduced expression $w = s_{i_1} s_{i_2} \cdots s_{i_k} \in \tilde{W}$, $(k = \ell(w))$, *we define* $S_w := S_{i_1} S_{i_2} \cdots S_{i_k} (\in \mathcal{H}(\tilde{W}))$ *which is well defined for all* $w \in \tilde{W}$ *due to i) in Lemma 3.11. In particular, we write* $A_\mu := S_{\tau_{-\mu}}$ *for* $\mu \in \mathring{P}_+$. *We call* $\{\hat{A}_\mu := \pi(A_\mu) \in \mathrm{End}(\mathbb{K}[\mathring{P}])\}$ *the raising operators.*

Proposition 3.13: For $w \in \tilde{W}$ *and* $\lambda \in \tilde{M}$, *we have* $S_w Y^\lambda = Y^{w(\lambda)} S_w$.

Proof: The relations for $\{S_i | i \in I\}$ are verified from direct calculations, and hence they are extensible to the relations for $\{S_w | w \in \tilde{W}\}$. □

Theorem 3.14 (Rodrigues-type formula): *(i) For* $\mu \in \mathring{P}_+$, *we obtain the nonsymmetric Macdonald–Koornwinder polynomial* E_μ *by applying the raising operators* $\{\hat{A}_\mu | \mu \in \mathring{P}_+\}$ *to the reference state* $E_0 := 1$,

$$E_\mu = d_\mu^{-1} \hat{A}_\mu E_0, \tag{3.16}$$

where the coefficient of the top term is given by

$$d_\mu = q^{-(1/2)(\mu|\rho_k)} \prod_{\alpha \in R_{\tau_\mu}} t_\alpha^{1/2}(q^{n_\alpha \alpha(\rho_k)} - 1),$$

and $(\alpha + n\delta)(\rho_k) = (\alpha|\rho_k) - n$.

(ii) For $\mu \in \mathring{P}$, *we obtain the nonsymmetric Macdonald–Koornwinder polynomial* E_μ *by applying the operator* $\hat{S}_{w_\mu} := \pi(S_{w_\mu})$, $(w_\mu \in \mathring{W}^{\mu^+}, w_\mu^{-1}(\mu) = \mu^+ \in \mathring{P}_+)$ *to* E_{μ^+},

$$E_\mu = d_{w_\mu}^{-1} \hat{S}_{w_\mu} E_{\mu^+}, \tag{3.17}$$

where the coefficient of the top term is

$$d_{w_\mu} := \prod_{\alpha \in R_{w_\mu^{-1}}} \frac{-t_\alpha^{-1/2}(1-t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu^+,\alpha})(1+t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu^+,\alpha})(1-t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu^+,\alpha})(1+t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu^+,\alpha})}{1-q_{\mu^+,\alpha}^2},$$

and $q_{\mu^+,\alpha}=q^{(1/2)(\alpha|\mu^+ +\rho_k)}$.

Proof: (i) Let $E' := \hat{A}_\mu E_\nu, (\mu,\nu \in \mathring{P}_+)$. Due to Proposition 3.13, we have

$$\hat{Y}^\lambda E' = \hat{Y}^\lambda \hat{A}_\mu E_\nu = \hat{A}_\mu \hat{Y}^{\tau_\mu(\lambda)} E_\nu = q^{(\lambda|\mu)} \hat{A}_\mu \hat{Y}^\lambda E_\nu = q^{(\lambda|\mu+\nu+\rho_k)} E'.$$

Since all the simultaneous eigenspaces of $\hat{Y}^\lambda$ are one dimensional, E' coincides with the nonsymmetric Macdonald–Koornwinder polynomial $E_{\mu+\nu}$ up to a constant factor. Next we calculate coefficients of the top term d_μ. Using a reduced expression $\tau_{-\mu}=s_{i_1}s_{i_2}\cdots s_{i_k}$, $(\ell(\tau_{-\mu})=k)$, we take a set of weights $\{\mu^{(m)}\}=\{\mu^{(m)}=\mathrm{af}(s_{i_{m+1}}s_{i_{m+2}}\cdots s_{i_k})(0) | 1 \leqslant m \leqslant k\}$. For $\alpha_{i_m} \in \Pi$ associated with the simple reflection s_{i_m}, we have

$$\alpha_{i_m}(\mu^{(m)}) = (s_{i_1}\cdots s_{i_m}(\alpha_{i_m}))(\mu) = -(s_{i_1}\cdots s_{i_{m-1}}(\alpha_{i_m}))(\mu) = -\alpha^{(m)}(\mu) < 0,$$

since $\alpha^{(m)} = s_{i_1}\cdots s_{m-1}(\alpha_{i_m}) \in R_{\tau_{-\mu}} \subset R_+^{\mathrm{re}}$. Hence, in applying the operator $\hat{S}_{i_m}$ to the polynomial $E_{\mu^{(m)}}$, only the cases $\langle \mu^{(m)}, \alpha_{i_m}^\vee \rangle < 0$, $(i_m \neq 0)$ and $\langle \mu^{(m)}, -\theta^\vee \rangle < a_0^{-1}, (i_m = 0)$ appear. Then we have

$$\begin{aligned}
\hat{A}_\mu E_0 &= \prod_{\{m | i_m=0\}} q^{-(1/2)(\theta|\rho_k(\mu^{(m)}))} \prod_{m=1}^{k} t_{i_m}^{1/2}(q^{n_{i_m}\alpha_{i_m}(\mu^{(m)}+\rho_k(\mu^{(m)}))}-1)E_\mu \\
&= \prod_{\{m | i_m=0\}} q^{-(1/2)(\theta|\rho_k(\mu^{(m)}))} \prod_{m=1}^{k} t_{i_m}^{1/2}(q^{n_{i_m}(s_{i_k}\cdots s_{i_{m+1}}(\alpha_{i_m}))(\rho_k)}-1)E_\mu \\
&= q^{-(1/2)(\mu|\rho_k)} \prod_{\alpha \in R_{\tau_\mu}} t_\alpha^{1/2}(q^{n_\alpha \alpha(\rho_k)}-1)E_\mu .
\end{aligned}$$

(ii) We see that $E'' := \hat{S}_{w_\mu} E_{\mu^+}$ coincides with the nonsymmetric Macdonald–Koornwinder polynomial E_μ up to a constant factor, since Proposition 3.13 gives

$$\hat{Y}^\lambda E'' = \hat{Y}^\lambda \hat{S}_{w_\mu} E_{\mu^+} = \hat{S}_{w_\mu} \hat{Y}^{w_\mu^{-1}(\lambda)} E_{\mu^+} = q^{(w_\mu^{-1}(\lambda)|\mu^+ +\rho_k)} E'' = q^{(\lambda|w_\mu(\mu^+ +\rho_k))} E''.$$

Coefficients of the top term d_{w_μ} can be also calculated in a way similar to (i). □

It should be remarked that $\hat{S}_i E_\mu = 0$ for $s_i \in \widetilde{W}$ such that $s_i(\mu)=\mu$. We have constructed E_μ in two steps to avoid such situations. Indeed, for an expression $A_\mu = S_{i_1}S_{i_2}\cdots S_{i_k}$, one sees $i_k = 0$ since $\ell(\tau_{-\mu}s_i) = \ell(\tau_{-\mu})+1$, $(\mu \in \mathring{P}_+, i \in \mathring{I})$.

The Rodrigues-type formula we have obtained enables us to evaluate diagonal terms of scalar products for the nonsymmetric Macdonald–Koornwinder polynomials.

Theorem 3.15: *For a dominant weight* $\mu \in \mathring{P}_+$, *we have the scalar product:*

$$\begin{aligned}
\langle E_\mu, E_\mu \rangle'_{q,t,u} = &\prod_{\alpha \in \mathring{R}_+^l} \frac{(abcdq'^2_{\mu,\alpha};q)_\infty^2}{(qq'_{\mu,\alpha}, abqq'_{\mu,\alpha}, acq'_{\mu,\alpha}, adq'_{\mu,\alpha} bcq'_{\mu,\alpha}, bdq'_{\mu,\alpha}, cdq'_{\mu,\alpha}, abcdq'_{\mu,\alpha};q)_\infty} \\
&\times \prod_{\alpha \in \mathring{R}_+^s} \frac{(qq_{\mu,\alpha}^2;q)_\infty^2}{(t_\alpha qq_{\mu,\alpha}^2, t_\alpha^{-1}qq_{\mu,\alpha}^2;q)_\infty},
\end{aligned} \tag{3.18}$$

where $q_{\mu,\alpha}=q^{(1/2)(\alpha|\mu+\rho_k(\mu))}$ *and* $q'_{\mu,\alpha}=q^{(1/2)(\alpha|\mu+\rho'_k(\mu))}$.

Proof: First we calculate $(E_\mu,E_\mu)'_{q,t,u}$ in $\mathbb{K}$. Define $\{N(\alpha)\in\mathcal{H}(\tilde{W})\,|\,\alpha\in R^{\mathrm{re}}\}$ by

$$N(\alpha):=\tilde{t}_\alpha(1-\tilde{t}_\alpha^{-1/2}\tilde{u}_{\tilde{\alpha}}^{-1/2}Y^{(n_\alpha/2)\alpha})(1+\tilde{t}_\alpha^{-1/2}\tilde{u}_{\tilde{\alpha}}^{1/2}Y^{(n_\alpha/2)\alpha})(1-\tilde{t}_\alpha^{-1/2}\tilde{u}_{\tilde{\alpha}}^{-1/2}Y^{-(n_\alpha/2)\alpha})\times(1+\tilde{t}_\alpha^{-1/2}\tilde{u}_{\tilde{\alpha}}^{1/2}Y^{-(n_\alpha/2)\alpha}),\tag{3.19}$$

where we put $\tilde{t}_\alpha:=\varepsilon(t_\alpha)$ and $\tilde{u}_\alpha:=\varepsilon(u_\alpha)$. They satisfy the following properties:

$$N(\alpha_i)=S_i^2,\quad S_wN(\alpha)=N(w(\alpha))S_w\quad\text{for } w\in\tilde{W}.$$

If we take a reduced expression $\tau_{-\mu}=s_{i_1}s_{i_2}\cdots s_{i_k}$ the product $A_\mu^*A_\mu\in\mathcal{H}(\tilde{W})$ is written as

$$A_\mu^*A_\mu=S_{i_k}^*\cdots S_{i_2}^*S_{i_1}^*S_{i_1}S_{i_2}\cdots S_{i_k}=S_{i_k}\cdots S_{i_2}N(\alpha_{i_1})S_{i_2}\cdots S_{i_k}=\prod_{\alpha\in R_{\tau_\mu}}N(\alpha).$$

Thus we see that the operators $\hat{A}_\mu^*\hat{A}_\mu$ can be diagonalized by the nonsymmetric Macdonald–Koornwinder polynomials. The scalar product is calculated as

$$\begin{aligned}
&(E_\mu,E_\mu)'_{q,t,u}\\
&=(d_\mu^{-1}\hat{A}_\mu E_0,d_\mu^{-1}\hat{A}_\mu E_0)'_{q,t,u}=d_\mu^{-1}(d_\mu^{-1})^\iota(E_0,\hat{A}_\mu^*\hat{A}_\mu E_0)'_{q,t,u}\\
&=\prod_{\alpha\in R_{\tau_\mu}}\frac{(1-\tilde{t}_\alpha^{1/2}\tilde{u}_{\tilde{\alpha}}^{1/2}q^{-(n_\alpha/2)\alpha(\rho_k)})(1+\tilde{t}_\alpha^{1/2}\tilde{u}_{\tilde{\alpha}}^{-1/2}q^{-(n_\alpha/2)\alpha(\rho_k)})(1-\tilde{t}_\alpha^{-1/2}\tilde{u}_{\tilde{\alpha}}^{-1/2}q^{-(n_\alpha/2)\alpha(\rho_k)})(1+\tilde{t}_\alpha^{-1/2}\tilde{u}_{\tilde{\alpha}}^{1/2}q^{-(n_\alpha/2)\alpha(\rho_k)})}{(1-q^{-n_\alpha\alpha(\rho_k)})^2}\\
&=\prod_{\alpha\in\mathring{R}_+^l}\prod_{n=1}^{(1/2)(\alpha|\mu)}\frac{(1-t_l^{-1/2}t_0^{-1/2}q^{(1/2)(\alpha|\rho_k)+n})(1+t_l^{-1/2}t_0^{1/2}q^{(1/2)(\alpha|\rho_k)+n})(1-t_l^{1/2}t_0^{1/2}q^{(1/2)(\alpha|\rho_k)+n})(1+t_l^{1/2}t_0^{-1/2}q^{(1/2)(\alpha|\rho_k)+n})}{(1-q^{(\alpha|\rho_k)+2n})^2}\\
&\quad\times\frac{(1-u_0^{-1/2}u_l^{-1/2}q^{(1/2)(\alpha|\rho_k)+n-1/2})(1+u_0^{-1/2}u_l^{1/2}q^{(1/2)(\alpha|\rho_k)+n-1/2})(1-u_0^{1/2}u_l^{1/2}q^{(1/2)(\alpha|\rho_k)+n-1/2})(1+u_0^{1/2}u_l^{-1/2}q^{(1/2)(\alpha|\rho_k)+n-1/2})}{(1-q^{(\alpha|\rho_k)+2n-1})^2}\\
&\quad\times\prod_{\alpha\in\mathring{R}_+^s}\prod_{n=1}^{(\alpha|\mu)}\frac{(1-t_\alpha^{-1}q^{(\alpha|\rho_k)+n})(1-t_\alpha q^{(\alpha|\rho_k)+n})}{(1-q^{(\alpha|\rho_k)+n})^2}.
\end{aligned}$$

By use of the constant term identity (3.4), we have

$$\begin{aligned}
&\langle E_\mu,E_\mu\rangle'_{q,t,u}\\
&=\prod_{\alpha\in\mathring{R}_+^l}\frac{(1-qq_{\mu,\alpha}^2;q)_\infty^2}{(t_l^{-1/2}t_0^{-1/2}qq_{\mu,\alpha},-t_l^{-1/2}t_0^{1/2}qq_{\mu,\alpha},t_l^{1/2}t_0^{1/2}qq_{\mu,\alpha},-t_l^{1/2}t_0^{-1/2}qq_{\mu,\alpha};q)_\infty}\\
&\quad\times\frac{1}{(u_0^{-1/2}u_l^{-1/2}q^{1/2}q_{\mu,\alpha},-u_0^{-1/2}u_l^{1/2}q^{1/2}q_{\mu,\alpha},u_0^{1/2}u_l^{1/2}q^{1/2}q_{\mu,\alpha},-u_0^{1/2}u_l^{-1/2}q^{1/2}q_{\mu,\alpha};q)_\infty}\\
&\quad\times\prod_{\alpha\in\mathring{R}_+^s}\frac{(qq_{\mu,\alpha}^2;q)_\infty^2}{(t_\alpha^{-1}qq_{\mu,\alpha}^2,t_\alpha qq_{\mu,\alpha}^2q)_\infty}.
\end{aligned}\tag{3.20}$$

Hence we obtain (3.18) by rewriting this with a, b, c, and d. Note that we define the right-hand side of (3.20) by expanding them in $\mathbb{C}[\{t_\alpha^{1/2},u_\alpha^{1/2}\}][[q^{1/2}]]$. □

Proposition 3.16: For a weight $\mu\in\mathring{P}$ *lying in the* $\mathring{W}$*-orbit of* $\mu^+\in\mathring{P}_+$, *we have*

$$\frac{\langle E_\mu, E_\mu\rangle'_{q,t,u}}{\langle E_{\mu^+}, E_{\mu^+}\rangle'_{q,t,u}} = \prod_{\alpha\in R_{w_\mu^{-1}}} \frac{(1-q_{\mu^+,\alpha}^2)^2}{(1-t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu+,\alpha})(1+t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu^+,\alpha})(1-t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu^+,\alpha})(1+t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu^+,\alpha})}, \tag{3.21}$$

where $q_{\mu^+,\alpha}=q^{(1/2)(\alpha|\mu^+ +\rho_k)}$.

Proof: For a reduced expression $w_\mu=s_{i_1}s_{i_2}\cdots s_{i_k}\in \mathring{W}$, we have

$$S^*_{w_\mu}S_{w_\mu}=S^*_{i_k}\cdots S^*_{i_2}S^*_{i_1}S_{i_1}S_{i_2}\cdots S_{i_k}=S_{i_k}\cdots S_{i_2}N(\alpha_{i_1})S_{i_2}\cdots S_{i_k}=\prod_{\alpha\in R_{w_\mu^{-1}}}N(\alpha).$$

Using the Rodrigues-type formula (3.17), we calculate the scalar product,

$$\begin{aligned}\langle E_\mu, E_\mu\rangle'_{q,t,u}&=\langle d_{w_\mu}^{-1}\hat{S}_{w_\mu}E_{\mu^+}, d_{w_\mu}^{-1}\hat{S}_{w_\mu}E_{\mu^+}\rangle'_{q,t,u}\\ &=d_{w_\mu}^{-1}(d_{w_\mu}^{-1})^\iota\langle E_{\mu^+}, \hat{S}^*_{w_\mu}\hat{S}_{w_\mu}E_{\mu^+}\rangle'_{q,t,u}\\ &=d_{w_\mu}^{-1}(d_{w_\mu}^{-1})^\iota\langle E_{\mu^+}, E_{\mu^+}\rangle'_{q,t,u}\prod_{\alpha\in R_{w_\mu^{-1}}}t_\alpha^{-1}(1-t_\alpha^{1/2}t_{\tilde{\alpha}}^{1/2}q_{\mu^+,\alpha})(1+t_\alpha^{1/2}t_{\tilde{\alpha}}^{-1/2}q_{u^+,\alpha})\\ &\quad\times(1-t_\alpha^{1/2}t_{\tilde{\alpha}}^{1/2}q_{\mu^+,\alpha}^{-1})(1+t_\alpha^{1/2}t_{\tilde{\alpha}}^{-1/2}q_{\mu^+,\alpha}^{-1}),\end{aligned}$$

from which we obtain (3.21). □

B. Macdonald–Koornwinder polynomials

We turn to the main object of our interest, the Macdonald–Koornwinder polynomials. Define the following symmetric inner products in the $\mathring{W}$-invariant Laurent polynomial ring $\mathbb{K}[\mathring{P}]^{\mathring{W}}$:

$$\langle f,g\rangle_{q,t,u}:=\frac{1}{|\mathring{W}|}[f\overline{g}\Delta_{q,t,u}]_0,\quad (f,g)_{q,t,u}:=\frac{1}{|\mathring{W}|}[f\overline{g}\widetilde{\Delta}_{q,t,u}]_0, \tag{3.22}$$

where the weight function $\Delta_{q,t,u}$ is given by

$$\Delta_{q,t,u}:=\Delta^+_{q,t,u}\overline{\Delta^+_{q,t,u}},$$

$$\begin{aligned}\Delta^+_{q,t,u}&:=\prod_{\alpha\in\mathring{R}^l_+}\prod_{n=0}^{\infty}\frac{(1-x^{\alpha+2n\delta})(1-x^{\alpha+(2n+1)\delta})}{(1-t_l^{1/2}u_0^{1/2}x^{(1/2)\alpha+n\delta})(1+t_l^{1/2}u_0^{-1/2}x^{(1/2)\alpha+n\delta})(1-t_0^{1/2}u_l^{1/2}x^{(1/2)\alpha+(n+1/2)\delta})(1+t_0^{1/2}u_l^{-1/2}x^{(1/2)\alpha+(n+1/2)\delta})}\\ &\quad\times\prod_{\alpha\in\mathring{R}^s_+}\prod_{n=0}^{\infty}\frac{1-x^{\alpha+n\delta}}{1-t_\alpha x^{\alpha+n\delta}}\\ &=\prod_{\alpha\in\mathring{R}^l_+}\frac{(x^\alpha;q)_\infty}{(ax^{(1/2)\alpha},bx^{(1/2)\alpha},cx^{(1/2)\alpha},dx^{(1/2)\alpha};q)_\infty}\prod_{\alpha\in\mathring{R}^s_+}\frac{(x^\alpha;q)_\infty}{(t_\alpha x^\alpha;q)_\infty},\end{aligned} \tag{3.23}$$

and $\widetilde{\Delta}_{q,t,u}:=\Delta_{q,t,u}/[\mu_{q,t,u}]_0$.

Definition 3.17 (Macdonald–Koornwinder polynomials): The (monic) Macdonald–Koornwinder polynomials $P_\mu:=P_\mu(x;q,\{t_\alpha,u_\alpha\})\in\mathbb{K}[\mathring{P}]^{\mathring{W}}$, $(\mu\in\mathring{P}_+)$[22] *are uniquely defined by the following conditions*:

$$(i)\ \ P_\mu = m_\mu + \sum_{\nu<\mu} w_{\mu\nu} m_\nu \quad \text{for } w_{\mu\nu} \in \mathbb{K},$$
$$(ii)\ \ (P_\mu, m_\nu)_{q,t,u} = 0 \quad \text{if } \nu < \mu, \tag{3.24}$$

where $m_\mu(x) := \Sigma_{\nu \in \mathring{W}(\mu)} x^\nu \in \mathbb{C}[\mathring{P}]^{\mathring{W}}$ *is orbit sum.*

Proposition 3.18 (T. H. Koornwinder): (i) We have the orthogonality of the Macdonald–Koornwinder polynomials:

$$(P_\mu, P_\nu)_{q,t,u} = 0 \quad \text{if } \mu \neq \nu. \tag{3.25}$$

In fact, the Macdonald–Koornwinder polynomials form an orthogonal basis in $\mathbb{K}[\mathring{P}]^{\mathring{W}}$ *with respect to the inner product* $(\cdot,\cdot)_{q,t,u}$ *in (3.22).*
(ii) Conditions (i) in (3.24) and (3.25) also determine the Macdonald–Koornwinder polynomials P_μ *uniquely.*

To prove the above-mentioned proposition, one needs Koornwinder's difference operator which is Hermitian with respect to the inner products (3.22) and uniquely characterizes the Macdonald–Koornwinder polynomials as its eigenvectors.[22] An explicit commutative family of difference operators including the Koornwinder's operator were obtained in Ref. 23.

Lemma 3.19: For $f, g \in \mathbb{K}[\mathring{P}]^{\mathring{W}}$, *we have*

$$(f,g)'_{q,t,u} = \mathcal{W}(t)(f, g^\iota)_{q,t,u},$$

where

$$\mathcal{W}(t) = \sum_{w \in \mathring{W}} \prod_{\alpha \in R_{w^{-1}}} t_\alpha. \tag{3.26}$$

Proof: We decompose $\mu_{q,t,u}$ as

$$\mu_{q,t,u} = \Delta_{q,t,u} \prod_{\alpha \in \mathring{R}_+} \frac{(1 - t_\alpha^{1/2} u_{\tilde{\alpha}}^{1/2} x^{-(1/2)\alpha})(1 + t_\alpha^{1/2} u_{\tilde{\alpha}}^{-1/2} x^{-(1/2)\alpha})}{1 - x^{-\alpha}}.$$

Then we see that

$$\begin{aligned}
(f,g)'_{q,t,u} &= \frac{1}{|\mathring{W}|} \sum_{w \in \mathring{W}} [w(f\overline{g^\iota})\tilde{\mu}_{q,t,u}]_0 \\
&= \frac{1}{|\mathring{W}|} \sum_{w \in \mathring{W}} [f\overline{g^\iota} w(\tilde{\mu}_{q,t,u})]_0 \\
&= \frac{1}{|\mathring{W}|} \left[f\overline{g^\iota} \tilde{\Delta}_{q,t,u} \sum_{w \in \mathring{W}} w\left(\prod_{\alpha \in \mathring{R}_+} \frac{(1 - t_\alpha^{1/2} u_{\tilde{\alpha}}^{1/2} x^{-(1/2)\alpha})(1 + t_\alpha^{1/2} u_{\tilde{\alpha}}^{-1/2} x^{-(1/2)\alpha})}{1 - x^{-\alpha}} \right) \right]_0 \\
&= \frac{1}{|\mathring{W}|} \left[f\overline{g^\iota} \tilde{\Delta}_{q,t,u} \sum_{w \in \mathring{W}} \prod_{\alpha \in \mathring{R}_+} \frac{(1 - t_\alpha^{1/2} u_{\tilde{\alpha}}^{1/2} x^{-(1/2)w(\alpha)})(1 + t_\alpha^{1/2} u_{\tilde{\alpha}}^{-1/2} x^{-(1/2)w(\alpha)})}{1 - x^{-w(\alpha)}} \right]_0 \\
&= \frac{1}{|\mathring{W}|} [f\overline{g^\iota} \tilde{\Delta}_{q,t,u}]_0 \sum_{w \in \mathring{W}} \prod_{\alpha \in R_{w^{-1}}} t_\alpha.
\end{aligned} \tag{3.27}$$

In the last equality of (3.27), we have used the following identity:

$$\mathcal{W}(t)=\sum_{w\in\mathring{W}}\prod_{\alpha\in\mathring{R}_+}\frac{(1-t_\alpha^{1/2}u_{\tilde{\alpha}}^{1/2}x^{-(1/2)w(\alpha)})(1+t_\alpha^{1/2}u_{\tilde{\alpha}}^{-1/2}x^{-(1/2)w(\alpha)})}{1-x^{-w(\alpha)}}=\sum_{w\in\mathring{W}}\prod_{\alpha\in R_{w^{-1}}}t_\alpha. \tag{3.28}$$

This identity is obtained from expressions of the Poincaré polynomials associated with BC_1-type nonreduced root system $\overline{R^{\mathrm{re}}}$,[41]

$$\mathcal{W}(v)=\sum_{w\in\mathring{W}}\prod_{\alpha\in(R^{\mathrm{re}})_+}\frac{1-v_{2\alpha}^{1/2}v_\alpha x^{-w(\alpha)}}{1-v_{2\alpha}^{1/2}x^{-w(\alpha)}}=\sum_{w\in\mathring{W}}\prod_{\alpha\in R_{w^{-1}}}v_\alpha, \tag{3.29}$$

where $v_{2\alpha}=1$ if $2\alpha\notin\overline{R^{\mathrm{re}}}$. Indeed, by the following change of the indeterminates:

$$v_\alpha\to t_\alpha u_{\tilde{\alpha}}^{-1},\quad v_{(1/2)\alpha}\to u_{\tilde{\alpha}}\quad\text{for }\alpha\in\mathring{R},$$

we can verify (3.28). □

We remark that $\mathcal{W}(t)$ does not depend on u_α and agrees with the Poincaré polynomial associated with the Weyl group of type C_l.

Corollary 3.20: Proposition 3.1 with Lemma 3.19 shows that coefficients of $\Delta_{q,t,u}$ are in the algebra $\mathbb{C}(\{t_\alpha^{1/2},u_\alpha^{1/2}\})[[q^{1/2}]]$ of formal power series in $q^{1/2}$ over the field of rational functions in $\{t_\alpha^{1/2},u_\alpha^{1/2}\}$.

The Macdonald–Koornwinder polynomials $(P_\mu)^\iota$ mapped by involution ι satisfy the defining relations (3.24), since the weight function has the property $(\Delta_{q,t,u})^\iota=f\times\Delta_{q,t,u,}(f\in\mathbb{K})$. Hence $(P_\mu)^\iota=P_\mu$ from their top term. This fact and Lemma 3.19 show that, in defining the Macdonald–Koornwinder polynomials, we can employ the scalar product $(\cdot,\cdot)'_{q,t,u}$ instead of the inner product $(\cdot,\cdot)_{q,t,u}$.

Proposition 3.21: Let $P_\mu,(\mu\in\mathring{P}_+)$ be the following linear combination of the nonsymmetric Macdonald–Koornwinder polynomials $E_\nu,(\nu\in\mathring{P})$:

$$P_\mu=\sum_{\nu\in\mathring{W}(\mu)}a_{\mu\nu}E_\nu, \tag{3.30a}$$

where

$$a_{\mu\nu}:=\prod_{\alpha\in R_{w_\nu^{-1}}}\frac{1+t_\alpha^{-1/2}(\check{t}_{\tilde{\alpha}}^{1/2}-\check{t}_{\tilde{\alpha}}^{-1/2})q_{\mu,\alpha}-t_\alpha^{-1}q_{\mu,\alpha}^2}{1-q_{\mu,\alpha}^2}. \tag{3.30b}$$

The polynomials P_μ are elements in $\mathbb{K}[\mathring{P}]^{\mathring{W}}$. In fact, P_μ satisfy the definition of the Macdonald–Koornwinder polynomials (3.24).

Proof: We use the fact that conditions $\hat{T}_iP_\mu=t_i^{1/2}P_\mu,(1\leqslant i\leqslant l)$ are equivalent to $P_\mu\in\mathbb{K}[\mathring{P}]^{\mathring{W}}$ (see, for example, Ref. 17). If we take the expansion (3.30a), the coefficients $a_{\mu\nu}\in\mathbb{K}$ are uniquely determined under the conditions $\hat{T}_iP_\mu=t_i^{1/2}P_\mu$, $(1\leqslant i\leqslant l)$ and $a_{\mu\mu}=1$. Indeed, if we require

$$\hat{T}_iP_\mu=a_{\mu\nu}\hat{T}_iE_\nu+a_{\mu\nu'}\hat{T}_iE_{\nu'}+\cdots=t_i^{1/2}(a_{\mu\nu}E_\nu+a_{\mu\nu'}E_{\nu'}+\cdots),$$

for $\nu,\nu'=s_i(\nu)(\in\mathring{W}(\mu))$ satisfying $\nu'<\nu\leqslant\mu,(\mu\in\mathring{P}_+)$, we have

$$\frac{a_{\mu\nu'}}{a_{\mu\nu}}=\frac{1+t_i^{-1/2}(\check{t}_{\tilde{\alpha}_i}^{1/2}-\check{t}_{\tilde{\alpha}_i}^{-1/2})q_{\nu,i}-t_i^{-1}q_{\nu,i}^2}{1-q_{\nu,i}^2},$$

from (3.10). To consider $a_{\mu\nu}$ with a general weight $\nu=w_\nu(\mu)$ where $w_\nu\in\mathring{W}^\mu$ such that $w_\nu^{-1}(\nu)\in\mathring{P}_+$, we take a reduced expression $w_\nu=s_{i_1}s_{i_2}\cdots s_{i_k}$ and put $\mu^{(n)}:=s_{i_n}s_{i_{n+1}}\cdots s_{i_k}(\mu)$, $(1\leqslant n\leqslant k+1)$. We find

$$\begin{aligned}
a_{\mu\nu}&=\prod_{n=1}^{k}\frac{a_{\mu\mu^{(n)}}}{a_{\mu\mu^{(n+1)}}}\\
&=\prod_{n=1}^{k}\frac{1+t_{i_n}^{-1/2}(\check{t}_{\tilde{\alpha}_{i_n}}^{1/2}-\check{t}_{\tilde{\alpha}_{i_n}}^{-1/2})q_{\mu^{(n+1)},i_n}-t_{i_n}^{-1}q_{\mu^{(n+1)},i_n}^2}{1-q_{\mu^{(n+1)},i_n}^2}\\
&=\prod_{n=1}^{k}\frac{1+t_{i_n}^{-1/2}(\check{t}_{\tilde{\alpha}_{i_n}}^{1/2}-\check{t}_{\tilde{\alpha}_{i_n}}^{-1/2})q_{\mu,s_{i_k}s_{i_{k-1}}\cdots s_{i_{n+1}}(\alpha_{i_n})}-t_{i_n}^{-1}q_{\mu,s_{i_k}s_{i_{k-1}}\cdots s_{i_{n+1}}(\alpha_{i_n})}^2}{1-q_{\mu,s_{i_k}s_{i_{k-1}}\cdots s_{i_{n+1}}(\alpha_{i_n})}^2}.
\end{aligned}$$

One sees that the roots $\{s_{i_k}s_{i_{k-1}}\cdots s_{i_{n+1}}(\alpha_{i_n})\}$ run through the set $R_{w_\nu^{-1}}$ and hence does not depend on decomposition of w_ν. Then P_μ are of the form (i) in (3.24). They satisfy relation (ii) in (3.24) due to (3.6) and Lemma 3.19. □

Corollary 3.22: As a corollary of Proposition 3.14 and 3.21, we obtain algebraic expressions of the Macdonald–Koornwinder polynomials $P_\mu,(\mu\in\mathring{P}_+)$:

$$P_\mu=\sum_{\nu\in\mathring{W}(\mu)}a_{\mu\nu}d_{w_\nu}^{-1}d_\mu^{-1}\hat{S}_{w_\nu}\hat{A}_\mu E_0. \tag{3.31}$$

Now we consider the inner product identity of the Macdonald–Koornwinder polynomials. In the case of $l=1$, it reduces to that of the Askey–Wilson polynomials.[43] As for the higher rank setting, the identity is first proved at its self-dual point with expansion formulas[24] and a proof beyond the self-dual setting is given by combining van Diejen's work[24] and a duality of the polynomials.[27] Opdam–Cherednik's shift operator approach is also applied to the identity.[29] Although the shift operator approach is so powerful that it contains a proof of the constant term identity, its applications is restricted to the inner product identity with parameters satisfying $t_\alpha=q^{k_\alpha}$, $u_\alpha=q^{h_\alpha}$, $(k_\alpha,h_\alpha\in\mathbb{N})$ because of their properties. Our new proof shown here can be applied to the identity with indeterminates $\{q^{1/2},t_\alpha^{1/2},u_\alpha^{1/2}\}$, that is, we provide a proof of the identity in the algebra $\mathbb{C}(\{t_\alpha^{1/2},u_\alpha^{1/2}\})[[q^{1/2}]]$ of formal power-series in $q^{1/2}$ over the field of rational functions in $\{t_\alpha^{1/2},u_\alpha^{1/2}\}$.

We remark that, for certain renormalized nonsymmetric Macdonald–Koornwinder polynomials, there is an analytic approach to relate diagonal terms of their scalar products to residues of the weight function.[29,30] Using so-called symmetrizers, the results of the nonsymmetric polynomials lead to those of renormalized Macdonald–Koornwinder polynomials. However, in order to see the explicit inner product identity of monic Macdonald–Koornwinder polynomials (i.e., in the form of Theorem 3.24), it is necessary to use evaluation formulas of the polynomials and to put together residues of the weight function and several coefficients appearing in that process. Our approach gives direct and explicit calculation of the inner products for the monic Macdonald–Koornwinder polynomials (3.24) from Theorem 3.15, Proposition 3.16, 3.21 and Lemma 3.19, and hence it does not rely on the evaluation formula. Furthermore we can see that coefficients appearing in our process are nicely combined to produce the final result thanks to the following lemma.

Lemma 3.23: Let $\mu\in\mathring{P}_+$. We have

$$\sum_{\nu\in\mathring{W}(\mu)}\prod_{\alpha\in R_{w_\nu^{-1}}}\frac{t_\alpha(1-t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu,\alpha})(1+t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu,\alpha})}{(1-t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu,\alpha})(1+t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu,\alpha})}$$

$$=\mathcal{W}(t)\prod_{\alpha\in\mathring{R}_+}\frac{1-q_{\mu,\alpha}^2}{(1-t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu,\alpha})(1+t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu,\alpha})}. \tag{3.32}$$

Proof: There exists a $\mathbb{K}$-homomorphism $\varphi:\mathbb{C}(q^{1/2},\{t_\alpha^{1/2}\})[\{u_\alpha^{1/2}\},\frac{1}{2}\mathring{Q}]\to\mathbb{C}(q^{1/2},\{t_\alpha^{1/2}\})$ defined by

$$\varphi:x^{-(1/2)\alpha_i}\mapsto q^{(1/2)(\alpha_i|\mu+\rho_k)}=q_{\mu,\alpha_i}\quad\text{for } i\in\mathring{I},\quad u_\alpha\to\check{t}_\alpha.$$

Since $\mathcal{W}(t)\in\mathbb{C}(q^{1/2},\{t_\alpha^{1/2}\})[\{u_\alpha^{1/2}\},\frac{1}{2}\mathring{Q}]$ does not depend on $\{u_\alpha^{1/2},x^{1/2\alpha_i}\}$ as (3.28), we have

$$\begin{aligned}
&\varphi(\mathcal{W}(t))=\mathcal{W}(t)\\
&=\sum_{w\in\mathring{W}}\prod_{\alpha\in\mathring{R}_+}\varphi\left(\frac{(1-t_\alpha^{1/2}u_\alpha^{1/2}x^{-(1/2)w(\alpha)})(1+t_\alpha^{1/2}u_{\tilde{\alpha}}^{-1/2}x^{-(1/2)w(\alpha)})}{1-x^{-w(\alpha)}}\right)\\
&=\sum_{w\in\mathring{W}}\prod_{\alpha\in\mathring{R}_+}\frac{(1-t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu,w(\alpha)})(1+t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu,w(\alpha)})}{1-q_{\mu,w(\alpha)}^2}\\
&=\sum_{w\in\mathring{W}}\frac{\Pi_{\alpha\in R_w}(1-t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu,\alpha}^{-1})(1+t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu,\alpha}^{-1})\Pi_{\alpha\in\mathring{R}_+\setminus R_w}(1-t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu,\alpha})(1+t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu,\alpha})}{\Pi_{\alpha\in R_w}(1-q_{\mu,\alpha}^{-2})\Pi_{\alpha\in\mathring{R}_+\setminus R_w}(1-q_{\mu,\alpha}^2)}\\
&=\frac{\Sigma_{w\in\mathring{W}}\Pi_{\alpha\in R_w}t_\alpha(1-t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu,\alpha})(1+t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu,\alpha})\Pi_{\alpha\in\mathring{R}_+\setminus R_w}(1-t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu,\alpha})(1+t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu,\alpha})}{\Pi_{\alpha\in\mathring{R}_+}(1-q_{\mu,\alpha}^2)}.
\end{aligned}$$

Thus we obtain the following relation immediately:

$$\sum_{w\in\mathring{W}}\prod_{\alpha\in R_{w^{-1}}}\frac{t_\alpha(1-t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu,\alpha})(1+t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu,\alpha})}{(1-t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu,\alpha})(1+t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu,\alpha})}$$

$$=\mathcal{W}(t)\prod_{\alpha\in\mathring{R}_+}\frac{1-q_{\mu,\alpha}^2}{(1-t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{1/2}q_{\mu,\alpha})(1+t_\alpha^{1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q_{\mu,\alpha})}. \tag{3.33}$$

We show that the sum on the left-hand side of the equation above can be replaced by the sum on $\nu\in\mathring{W}(\mu)$. Consider the isotropy group $\mathring{W}_\mu=\{v\in\mathring{W}|v(\mu)=\mu\}$ for the dominant weight $\mu\in\mathring{P}_+$. Since an element $v\in\mathring{W}_\mu\setminus\{id\}$ can be written by the product of simple reflections fixing μ, $\{s_i|i\in\mathring{J}\subset\mathring{I}\}$ (see Ref. 36), there exists at least one simple root $\alpha_i\in\mathring{\Pi}$ associated with the reflection s_i in the set $R_{v^{-1}}$ if $\mathring{W}_\mu\neq\{id\}$. Hence, for $v\in\mathring{W}_\mu\setminus\{id\}$, we have

$$\begin{aligned}
&\prod_{\alpha\in R_{v^{-1}}}(1-t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q^{(1/2)(\alpha|\mu+\rho_k)})\\
&=(1-t_i^{-1/2}\check{t}_{\tilde{\alpha}_i}^{-1/2}q^{(1/2)(\alpha_i|\mu+\rho_k)})\prod_{\alpha\in R_{v^{-1}}\setminus\{\alpha_i\}}(1-t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q^{(1/2)(\alpha|\mu+\rho_k)})\\
&=(1-t_i^{-1/2}\check{t}_{\tilde{\alpha}_i}^{-1/2}t_i^{1/2}\check{t}_{\tilde{\alpha}_i}^{1/2})\prod_{\alpha\in R_{v^{-1}}\setminus\{\alpha_i\}}(1-t_\alpha^{-1/2}\check{t}_{\tilde{\alpha}}^{-1/2}q^{(1/2)(\alpha|\mu+\rho_k)})=0.
\end{aligned}$$

For $w \in \mathring{W}$, there is a unique $u \in \mathring{W}^{\mu}$ and a unique $v \in \mathring{W}_{\mu}$ such that $w=uv$. The formula $R_{w^{-1}} = R_{v^{-1}} \cup v^{-1} R_{u^{-1}}$ shows that, if $v \neq id$, the product on $\alpha \in R_{w^{-1}}$ in (3.33) vanishes. Thus we obtain the lemma above since the sum on $w \in \mathring{W}$ on the left-hand side of (3.33) can be replaced by that on $u \in \mathring{W}^{\mu}$ which is equivalent to that on $\nu \in \mathring{W}(\mu)$.

Theorem 3.24 (inner product identity): *Let $\mu, \nu \in \mathring{P}_+$. We have*

$$\begin{aligned}\langle P_{\mu}, P_{\nu} \rangle_{q,t,u} &= \delta_{\mu\nu} \prod_{\alpha \in \mathring{R}^l_+} \frac{(abcdq^{-1} q'^2_{\mu,\alpha}, abcdq'^2_{\mu,\alpha}; q)_{\infty}}{(qq'_{\mu,\alpha}, abq'_{\mu,\alpha}, acq'_{\mu,\alpha}, adq'_{\mu,\alpha}, bcq'_{\mu,\alpha}, bdq'_{\mu,\alpha}, cdq'_{\mu,\alpha}, abcdq^{-1} q'_{\mu,\alpha}; q)_{\infty}} \\ &\quad \times \prod_{\alpha \in \mathring{R}^s_+} \frac{(q^2_{\mu,\alpha}, qq^2_{\mu,\alpha}; q)_{\infty}}{(t_{\alpha} q^2_{\mu,\alpha}, t_{\alpha}^{-1} qq^2_{\mu,\alpha}; q)_{\infty}}, \end{aligned} \tag{3.34}$$

where $q_{\mu,\alpha} = q^{(1/2)(\alpha|\mu+\rho_k)}$ and $q'_{\mu,\alpha} = q^{(1/2)(\alpha|\mu+\rho'_k)}$.

Proof: The orthogonality in the case of $\mu \neq \nu$ follows from Lemma 3.19 and Proposition 3.6. Using the relation (3.26), the expansions (3.30a), and the definition of $E_{\nu}, (\nu \in \mathring{P})$ (3.6), we obtain

$$\begin{aligned}\langle P_{\mu}, P_{\mu} \rangle_{q,t,u} &= \mathcal{W}(t)^{-1} \langle P_{\mu}, P_{\mu} \rangle'_{q,t,u} \\ &= \mathcal{W}(t)^{-1} \sum_{\nu \in \mathring{W}(\mu)} a_{\mu\nu}(\alpha_{\mu\nu})^{\iota} \frac{\langle E_{\nu}, E_{\nu} \rangle'_{q,t,u}}{\langle E_{\mu}, E_{\mu} \rangle'_{q,t,u}} \langle E_{\mu}, E_{\mu} \rangle'_{q,t,u} \\ &= \mathcal{W}(t)^{-1} \sum_{\nu \in \mathring{W}(\mu)} \prod_{\alpha \in R_{w_{\nu}^{-1}}} \frac{t_{\alpha}(1 - t_{\alpha}^{-1/2} \check{t}_{\tilde{\alpha}}^{-1/2} q_{\mu,\alpha})(1 + t_{\alpha}^{-1/2} \check{t}_{\tilde{\alpha}}^{1/2} q_{\mu,\alpha})}{(1 - t_{\alpha}^{1/2} \check{t}_{\tilde{\alpha}}^{1/2} q_{\mu,\alpha})(1 + t_{\alpha}^{1/2} \check{t}_{\tilde{\alpha}}^{-1/2} q_{\mu.\alpha})} \langle E_{\mu}, E_{\mu} \rangle'_{q,t,u} \\ &= \prod_{\alpha \in \mathring{R}_+} \frac{1 - q^2_{\mu,\alpha}}{(1 - t_{\alpha}^{1/2} \check{t}_{\tilde{\alpha}}^{1/2} q_{\mu,\alpha})(1 + t_{\alpha}^{1/2} \check{t}_{\tilde{\alpha}}^{-1/2} q_{\mu,\alpha})} \langle E_{\mu}, E_{\mu} \rangle'_{q,t,u}, \end{aligned}$$

where the fourth equality follows from the Lemma 3.23. □

IV. CONCLUDING REMARKS

We have presented an algebraic approach to the Macdonald–Koornwinder polynomials. Let us summarize our results in this paper. First we have introduced the extended affine Weyl group which acts on the affine root system of type $X_N^{(r)}$ to define the affine Hecke algebra of type $X_N^{(r)}$. The affine Hecke algebra of type $X_N^{(r)}$ has provided a new and unified viewpoint for the Macdonald and Macdonald–Koornwinder polynomials. Introducing the double affine Hecke algebra of type $A_{2l}^{(2)}$, we have given its representation in End($\mathbb{K}[\mathring{P}]$), i.e., the Demazure–Lusztig operators. Second we have considered the nonsymmetric Macdonald–Koornwinder polynomials. We have provided the Rodrigues-type formula for the nonsymmetric Macdonald–Koornwinder polynomials by use of the raising operators. The formula enables us to evaluate diagonal terms of scalar products for the nonsymmetric polynomials in an algebraic manner. Third we have algebraically constructed the Macdonald–Koornwinder polynomials through the Weyl-symmetrization of the nonsymmetric polynomials. Their inner product identity has been proved by the Weyl-symmetrization of the scalar products of the nonsymmetric polynomials together with an expression of the Poincaré polynomials.

As we have already described, the Macdonald–Koornwinder polynomials include the Macdonald polynomials associated with admissible pairs (BC_l, B_l) and (BC_l, C_l) for the BC_l-type nonreduced root system.[2,22] Indeed we can see the relations by putting

$$q = x^{\delta}, \quad a = u_0, \quad b = t_l u_0^{-1}, \quad t_0 = u_l = 1 \quad \text{for } (BC_l, B_l)$$

$$q^2=x^{\delta},\quad a=u_0=u_l,\quad b=t_l u_0^{-1}=t_0 u_l^{-1}\quad \text{for } (BC_l,C_l),$$

in the first expression of the weight function (3.23). Then Rodrigues-type formulas, scalar products, Weyl-symmetrization of the nonsymmetric polynomials corresponding to the BC_l-type Macdonald polynomials immediately follow from the replacement above.

It is well-known fact that the Askey–Wilson polynomials play a role of a master family of orthogonal polynomials with one-variable in the Askey scheme.[44] The Macdonald–Koornwinder polynomials also give some known orthogonal polynomials through limit transitions and/or specialization of their parameters.[45–47] It is of interest to investigate multivariable extension of the Askey scheme for both symmetric and nonsymmetric cases from its algebraic structure like double affine Hecke algebras.

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APPENDIX: PROOF OF PROPOSITION 2.7

We present a proof of Proposition 2.7 following Lusztig.[35]

In what follows, we consider only the affine root system R of type $A_{2l}^{(2)}$, which contains real roots with three kinds of (square) lengths 1, 2, and 4. We use the following formulas for the length of an element of $\tilde{W}$:

Lemma A.1: For $w\in\tilde{W}$,

(i) $\ell(w^{-1})=\ell(w)$,

(ii) $\ell(ws_i)=\begin{cases}\ell(w)+1 & \text{if } w(\alpha_i)\in R_+\\ \ell(w)-1 & \text{if } w(\alpha_i)\in R_-,\end{cases}$ $\ell(s_iw)=\begin{cases}\ell(w)+1 & \text{if } w^{-1}(\alpha_i)\in R_+\\ \ell(w)-1 & \text{if } w^{-1}(\alpha_i)\in R_-,\end{cases}$

(iii) $\ell(\omega_r w)=\ell(w)$ *for* $r\in\mathcal{O}, w\in\tilde{W}$,

(iv) $\ell(\tau_\lambda)=\sum_{\alpha\in\mathring{R}_+}|(\lambda|\alpha)|$,

(v) $\ell(\tau_{\lambda+\mu})=\ell(\tau_\lambda)+\ell(\tau_\mu)$ *for* $\lambda,\mu\in\tilde{M}_+$.

Lemma A.2: Let $\lambda\in\tilde{M}_+,\alpha\in\mathring{\Pi}$ *be such that* $(\lambda|\alpha)=:p>0$. *Let* $s=s_\alpha$, $w=s\tau_\lambda s\tau_\lambda$. *One sees*

(i) $\ell(\tau_\lambda s)=\ell(\tau_\lambda)-1$,

(ii) $\lambda':=s(\lambda)+\lambda\in\tilde{M}_+$ *and* $\ell(w)=2\ell(\tau_\lambda)-2p$,

(iii) $\ell(\tau_\lambda s\tau_\lambda)=2\ell(\tau_\lambda)-2p+1$,

(iv) $T_sT_{s\tau_{-\lambda}}=T_{\tau_{-\lambda}}$, $T_{w^{-1}}T_s=T_{\tau_{-\lambda}s\tau_{-\lambda}}$,

(v) $T_{\tau_{-\lambda}}T_{s\tau_{-\lambda}}=T_{\tau_{-\lambda}s\tau_{-\lambda}}$ *for* $p=1$.

Proof: (i) We have $\tau_\lambda(\alpha)=\alpha-(\lambda|\alpha)\delta=\alpha-p\delta\in R_-$. Then (i) follows using Lemma A.1.

(ii) We have $w=\tau_{s(\lambda)+\lambda}=\tau_{2\lambda-(2p/|\alpha|^2)\alpha}=\tau_{\lambda'}$ and $\langle\lambda',\beta^\vee\rangle=2\langle\lambda,\beta^\vee\rangle-(2p/|\alpha|^2)\langle\alpha,\beta^\vee\rangle$ for $\beta\in\mathring{\Pi}$. One sees $\langle\lambda,\beta^\vee\rangle\geqslant 0$ since $\lambda\in\tilde{M}_+$. If $\alpha\neq\beta$, then $\langle\alpha,\beta^\vee\rangle<0$ so $\langle\lambda',\beta^\vee\rangle>0$. If $\alpha=\beta$, then $\langle\lambda,\beta^\vee\rangle=2p/|\alpha|^2$ and $\langle\alpha,\beta^\vee\rangle=2$ show $\langle\lambda',\beta^\vee\rangle=0$. Hence we find $\lambda'\in\tilde{M}_+$.

Using Lemma A.1, we have

$$\begin{aligned}\ell(w)&=\sum_{\beta\in\mathring{R}_+}|(s(\lambda)+\lambda|\beta)|\\&=\sum_{\beta\in\mathring{R}_+}(\lambda|s(\beta))+\sum_{\beta\in\mathring{R}_+}(\lambda|\beta)\\&=2\sum_{\beta\in\mathring{R}_+}(\lambda|\beta)-2(\lambda|\alpha)\\&=2\ell(\tau_\lambda)-2p.\end{aligned}$$

(iii) Using Lemma A.1 with $w^{-1}(\alpha)=\tau_{-\lambda'}(\alpha)=\alpha\in R_+$, we have $\ell(\tau_\lambda s\tau_\lambda)=\ell(sw)=\ell(w)+1$.
(iv) From $\ell(s)+\ell(s\tau_{-\lambda})=\ell(\tau_{-\lambda})$ and $\ell(w^{-1})+\ell(s)=\ell(w^{-1}s)=\ell(\tau_{-\lambda}s\tau_{-\lambda})$, we have

$$T_sT_{s\tau_{-\lambda}}=T_{\tau_{-\lambda}},\quad T_{w^{-1}}T_s=T_{\tau_{-\lambda}s\tau_{-\lambda}}.$$

(v) Set $p=1$. From $\ell(\tau_{-\lambda})+\ell(s\tau_{-\lambda})=\ell(\tau_{-\lambda}s\tau_{-\lambda})$, we have $T_{\tau_{-\lambda}}T_{s\tau_{-\lambda}}=T_{\tau_{-\lambda}s\tau_{-\lambda}}$.
□

Recall the definition of the lattice $\tilde{M}$ in (2.5). One sees easily that $\alpha\in 2\tilde{M}$ for $\alpha\in(R^{\mathrm{re}})^l$, which is very special situation discussed by Lusztig. We note that this situation does not occur in the $C_l^{(1)}$-type affine root system.

Lemma A.3: Assume that $\alpha\in 2\tilde{M}$. Tere is a unique element $\lambda\in\tilde{M}$ such that $(\lambda|\alpha)=2$ and $(\lambda|\beta)=0$ for all $\beta\in\mathring{\Pi}\backslash\{\alpha\}$. Moreover, in B, there exists elements $w',w''\in\tilde{W}$ and $\tilde{\alpha}\in R$ such that

$$T_{\tau_{-\lambda}s\tau_{-\lambda}}=T_{w'}T_{w''},\quad T_{\tau_{-2\lambda+(1/2)\alpha}}=T_{w'}T_{s_{\tilde{\alpha}}}T_{w''},\quad T_{\tau_{-\lambda}}T_{s\tau_{-\lambda}}=T_{w'}T_{s_{\tilde{\alpha}}}^2T_{w''}.$$

We give a proof of Lemma A.3 in several steps. For the $A_{2l}^{(2)}$-type affine root system, we have $\tilde{M}=\mathring{P}$. Let $\tilde{W}_1=\mathring{W}\ltimes\nu(\mathring{P}^\vee)$. The length of the elements of $\tilde{W}$ is extended to that of $\tilde{W}_1$ through the original definition (2.6). Let B_1 be the braid group corresponding to $\tilde{W}_1$. Then one sees that $\tilde{W}\subset\tilde{W}_1$ and $B\subset B_1$ in a natural way; moreover, if Ω_1 denotes the set of elements of length 0 in $\tilde{W}_1$, then $\Omega_1=\{1,\omega\}$ is a group of order 2 which is a complement of $\tilde{W}$ in $\tilde{W}_1$ and $\{1,T_\omega\}$ is a complement of B in B_1. In fact conjugation by ω stands for the nontrivial automorphism of the Coxeter diagram corresponding to the Dynkin diagram $S(A)$. Hence one sees $\omega s_\alpha\omega^{-1}=s_{\tilde{\alpha}}\in\tilde{W}$ and $\omega T_{s_\alpha}\omega^{-1}=T_{s_{\tilde{\alpha}}}\in B$ for $\tilde{\alpha}=\omega(\alpha)\in R$.

Lemma A.4: Let $\lambda_1\in\nu(\mathring{P}^\vee)$ such that $(\lambda_1|\alpha)=1$ and $(\lambda|\beta)=0$ for all $\beta\in\mathring{\Pi}\backslash\{\alpha\}$. Let $w'=\tau_{-3\lambda_1+(1/2)\alpha}\omega\in\tilde{W}_1$, $w''=\omega s\tau_{-\lambda_1}\in\tilde{W}_1$ and $\ell_1=\ell(\tau_{\lambda_1})$. Then $w',w''\in\tilde{W}$ and

$$\ell(\tau_{2\lambda-(1/2)\alpha})=4\ell_1-2,\quad \ell(\tau_\lambda s\tau_\lambda)=4\ell_1-3,\quad \ell(w')=3\ell_1-2,\quad \ell(w'')=\ell_1-1.$$

Proof: We have $\lambda_1\notin\mathring{P}$ since, if we have $\lambda_1\in\mathring{P}$, then it follows from $\alpha\in 2\mathring{P}$ that $(\lambda_1|\alpha)\in 2\mathbb{Z}$. Since $\mathring{P}$ has index 2 in $\nu(\mathring{P}^\vee)$, we have $2\lambda_1\in\mathring{P}$. In fact, if we set $\lambda=2\lambda_1$, then $(\lambda|\alpha)=2$ and $(\lambda|\beta)=0$ for all $\beta\in\mathring{\Pi}\backslash\{\alpha\}$. Uniqueness of this element λ is obvious since, if we have two such elements $\lambda,\mu\in\mathring{P}$, $(\lambda\neq\mu)$, then $(\lambda-\mu|\beta)=0$ for all $\beta\in\mathring{\Pi}$, contradicting $\lambda\neq\mu$. From $\lambda_1\in\nu(\mathring{P}^\vee)\backslash\mathring{P}$, we have $\tau_{\lambda_1}\in\omega\tilde{W}$ and $\tau_{3\lambda_1}\in\omega\tilde{W}$. Hence $w',w''\in\tilde{W}$.

Using Lemma A.1 and A.2 with $p=1$, we have $2\lambda_1$, $2\lambda_1-\frac{1}{2}\alpha=s(\lambda_1)+\lambda_1\in\mathring{P}_+$. Then

$$\ell(\tau_{2\lambda-(1/2)\alpha})=\ell(\tau_{2\lambda_1})+\ell(\tau_{2\lambda_1-(1/2)\alpha})=\ell(\tau_{2\lambda_1})+\ell(\tau_{s(\lambda_1)+\lambda_1})=2\ell_1+2\ell_1-2=4\ell_1-2.$$

If we set $p=2$ in (iii) of Lemma A.2, then we have

$$\ell(\tau_\lambda s \tau_\lambda) = 4\ell(\tau_\lambda) - 4 + 1 = 4\ell_1 - 3.$$

Using Lemma A.1 and A.2, we see

$$\ell(w') = \ell(\tau_{-3\lambda_1+(1/2)\alpha}\omega) = \ell(\tau_{-\lambda_1}) + \ell(\tau_{-2\lambda_1+(1/2)\alpha}) = \ell_1 + 2\ell_1 - 2 = 3\ell_1 - 2,$$

$$\ell(w'') = \ell(\omega s \tau_{-\lambda_1}) = \ell(\tau_{-\lambda_1}) - 1 = \ell_1 - 1.$$

□

Proof of Lemma A.3: We have already shown that $w', w'' \in \tilde{W}$ in Lemma A.4. We have

$$w'w'' = \tau_{-3\lambda_1+(1/2)\alpha} s \tau_{-\lambda_1} = \tau_{-2\lambda_1}(\tau_{-\lambda_1+(1/2)\alpha} s)\tau_{-\lambda_1} = \tau_{-2\lambda_1}(s\tau_{-\lambda_1})\tau_{-\lambda_1} = \tau_{-\lambda} s \tau_{-\lambda}.$$

Since Lemma A.2 and A.4 give rise to $\ell(w'w'') = \ell(w') + \ell(w'') = 4\ell_1 - 3$, we can verify $T_{\tau_{-\lambda} s \tau_{-\lambda}} = T_{w'} T_{w''}$.

In a way similar to Lemma. A.4, we find

$$w' s_{\tilde{\alpha}} w'' = \tau_{-3\lambda_1+(1/2)\alpha} \omega s_{\tilde{\alpha}} \omega s \tau_{-\lambda_1} = \tau_{-4\lambda_1+(1/2)\alpha} = \tau_{-2\lambda+(1/2)\alpha},$$

and $\ell(w' s_{\tilde{\alpha}} w'') = \ell(w') + \ell(s_{\tilde{\alpha}}) + \ell(w'') = 4\ell_1 - 2$. Then we have $T_{\tau_{-2\lambda+(1/2)\alpha}} = T_{w'} T_{s_{\tilde{\alpha}}} T_{w''}$.

We verify the last relation as

$$\begin{aligned} T_{\tau_{-\lambda}} T_{s\tau_{-\lambda}} &= T_{\tau_{-\lambda_1}} (T_{\tau_{-\lambda_1}} T_{s\tau_{-\lambda_1}}) T_{\tau_{-\lambda_1}} \\ &= T_{\tau_{-\lambda_1}} T_{\tau_{-\lambda_1} s \tau_{-\lambda_1}} T_{\tau_{-\lambda_1}} \\ &= T_{\tau_{-\lambda_1}} (T_{w^{-1}} T_s)(T_s T_{s\tau_{-\lambda_1}}) \\ &= T_{\tau_{-3\lambda_1+(1/2)\alpha}} T_s^2 T_{s\tau_{-\lambda_1}} \\ &= T_{w'} T_{s_{\tilde{\alpha}}}^2 T_{w''}. \end{aligned}$$

In the first equality, we have used $T_{\tau_{-\lambda}} = T_{\tau_{-\lambda_1}} T_{\tau_{-\lambda_1}}$ and $T_{s\tau_{-\lambda}} = T_{s\tau_{-\lambda_1}} T_{\tau_{-\lambda_1}}$ from (v) in Lemma A.1 and $\ell(\tau_{-\lambda}) = \ell(s\tau_{-\lambda_1}) + \ell(\tau_{-\lambda_1}) = 2\ell_1 - 1$, respectively. In the second and third equality, we have employed (v) and (iv) in Lemma A.2, respectively. The last equality follows immediately from $\omega T_{s_\alpha} \omega^{-1} = T_{s_{\tilde{\alpha}}}$. □

Proposition A.5: Let $\lambda, \mu \in \tilde{M}$ and $\alpha \in \mathring{\Pi}$,

(*i*) $Y^\lambda Y^\mu = Y^{\lambda+\mu}$

(*ii*) $T_s Y^\lambda = Y^\lambda T_s$ *if* $(\lambda|\alpha) = 0$,

(*iii*) $T_s Y^{s(\lambda)} T_s = Y^\lambda$ *if* $(\lambda|\alpha) = 1$ *for* $\alpha \notin 2\tilde{M}$.

(*iv*) *There exist elements* $b', b'' \in B$ *such that*

$$Y^{s(\lambda)} T_s = b' b'', \quad Y^{\lambda-(1/2)\alpha} = b' T_{s_{\tilde{\alpha}}} b'', \quad T_s^{-1} Y^\lambda = b' T_{s_{\tilde{\alpha}}}^2 b'',$$

if $(\lambda|\alpha) = 2$ *for* $\alpha \in 2\tilde{M}$.

Proof: (i) follows from the definition of Y^λ.

(ii) Using the definition of B and $\ell(\tau_{-\lambda} s_\alpha) = \ell(s_\alpha \tau_{-\lambda}) = \ell(\tau_{-\lambda}) + 1$, we have

$$Y^\lambda T_{s_\alpha} = T_{\tau_{-\lambda}} T_{s_\alpha} = T_{\tau_{-\lambda} s_\alpha} = T_{s_\alpha \tau_{-\lambda}} = T_{s_\alpha} T_{\tau_{-\lambda}} = T_{s_\alpha} Y^\lambda.$$

(iii) Using Lemma A.2, we have

$$T_s Y^{s(\lambda)} T_s = T_s (Y^{-\lambda} Y^{\lambda'}) T_s = T_s T_{\tau_{-\lambda}}^{-1} (T_{w^{-1}} T_s) = T_s T_{\tau_{-\lambda}}^{-1} T_{\tau_{-\lambda} s \tau_{-\lambda}} = T_s T_{\tau_{-\lambda}}^{-1} (T_{\tau_{-\lambda}} T_{s\tau_{-\lambda}}) = Y^\lambda.$$

(iv) Set $b'=T_{\tau_{-\lambda}}^{-1}T_{w'}$ and $b''=T_{w''}$. From $\lambda, s(\lambda)+\lambda\in\tilde{M}_+$, we have

$$Y^{s(\lambda)}=(Y^{\lambda})^{-1}Y^{s(\lambda)+\lambda}=T_{\tau_{-\lambda}}^{-1}T_{w^{-1}}=T_{\tau_{-\lambda}}^{-1}T_{\tau_{-\lambda}s\tau_{-\lambda}}T_s^{-1}=T_{\tau_{-\lambda}}^{-1}T_{w'}T_{w''}T_s^{-1}.$$

Then $Y^{s(\lambda)}T_s=T_{\tau_{-\lambda}}^{-1}T_{w'}T_{w''}=b'b''$.

From $\lambda-\frac{1}{2}\alpha\in\tilde{M}_+$ and $\ell(\tau_{-\lambda})+\ell(\tau_{-\lambda+(1/2)\alpha})=\ell(\tau_{-2\lambda+(1/2)\alpha})$, we have

$$Y^{\lambda-(1/2)\alpha}=T_{\tau_{-\lambda+(1/2)\alpha}}=T_{\tau_{-\lambda}}^{-1}T_{\tau_{-2\lambda+(1/2)\alpha}}=T_{\tau_{-\lambda}}^{-1}T_{w'}T_{s_{\tilde{\alpha}}}T_{w''}=b'T_{s_{\tilde{\alpha}}}b''.$$

In a similar way,

$$Y^{\lambda}=T_{\tau_{-\lambda}}=T_sT_{s\tau_{-\lambda}}=T_sT_{\tau_{-\lambda}}^{-1}T_{w'}T_{s_{\tilde{\alpha}}}^2T_{w''}=T_sb'T_{s_{\tilde{\alpha}}}^2b''.$$

Hence $T_s^{-1}Y^{\lambda}=b'T_{s_{\tilde{\alpha}}}^2b''$.

□

Proof of Proposition 2.7: The relations (i) and (ii) follow immediately from Proposition A.5. If we apply Proposition A.5 to case (iii), we have

$$Y^{s_i(\lambda)}T_i-(t_{\tilde{\alpha}_i}^{1/2}-t_{\tilde{\alpha}_i}^{-1/2})Y^{\lambda-(1/2)\alpha_i}-T_i^{-1}Y^{\lambda}=b'(1-(t_{\tilde{\alpha}_i}^{1/2}-t_{\tilde{\alpha}_i}^{-1/2})T_{s_{\tilde{\alpha}_i}}-T_{s_{\tilde{\alpha}_i}}^2)b''.$$

The last expression has image equal to zero in $H(\tilde{W})$. Hence we get (iii). □

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Quantal two-center Coulomb problem treated by means of the phase-integral method. I. General theory

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The present paper concerns the derivation of phase-integral quantization conditions for the two-center Coulomb problem under the assumption that the two Coulomb centers are fixed. With this restriction we treat the general two-center Coulomb problem according to the phase-integral method, in which one uses an *a priori* unspecified *base function*. We consider base functions containing three unspecified parameters $C, \tilde{C}$, and Λ. When the absolute value of the magnetic quantum number m is not too small, it is most appropriate to choose $\Lambda = |m| \neq 0$. When, on the other hand, $|m|$ is sufficiently small, it is most appropriate to choose $\Lambda = 0$. Arbitrary-order phase-integral quantization conditions are obtained for these choices of Λ. The parameters C and $\tilde{C}$ are determined from the requirement that the results of the first and the third order of the phase-integral approximation coincide, which makes the first-order approximation as good as possible. In order to make the paper to some extent self-contained, a short review of the phase-integral method is given in the Appendix. [DOI: 10.1063/1.1399294]

I. INTRODUCTION

The two-center Coulomb problem, that is, the problem of solving the Schrödinger equation for the motion of an electron with the charge $-e$ $(e>0)$ in the field of two fixed Coulomb centers with charges $Z_1 e$ and $Z_2 e$ at the distance r_{12} from each other, plays an important role in several fields of theoretical physics, e.g., in the theory of diatomic molecules, in scattering theory, and in the three-body problem. The two-center Coulomb problem has therefore been the subject of extensive studies both by numerical and by approximate analytical methods, and hence the literature on this problem is very comprehensive. In spite of this fact it is still of interest to continue the treatment of this problem for arbitrary values of Z_1, Z_2, and r_{12}. One reason for this is that the numerically exact solution of the problem meets with difficulties when $|Z_1 - Z_2|$ increases. Also, numerical difficulties appear for large values of r_{12}. For a general review of the problem we refer to Eyring *et al.*,[1] Herzberg,[2] Slater,[3] and Rosen.[4]

Ignoring the finiteness of the mass of the protons, Bates *et al.*[5] obtained important numerical results for the hydrogen molecule ion. Corresponding numerical results were obtained by Wallis and Hulburt[6] for the homonuclear one-electron two-center problem, by Bates and Carson[7] for the ion $HeH^{2+}(Z_1=1, Z_2=2)$, by Wind[8] for the ground state of the hydrogen molecule ion, by Peek[9] for the states $1s\sigma_g$ and $2p\sigma_u$ of the hydrogen molecule ion, and by Ponomarev and Puzynina[10,11]

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for several states of the Coulomb two-center system with $Z_1=1$ and $Z_2=2,3,\ldots,8$. Hunter and Pritchard[12] used a numerical procedure to compute nonadiabatic energies for the first few rotation–vibration levels of ${}^2\Sigma_g\, H_2^+$, ${}^2\Sigma\, HD^+$, and ${}^2\Sigma_g\, D_2^+$. For the hydrogen molecule ion Rosenthal and Bright Wilson, Jr.[13] calculated an accurate value of the ground state energy which is in agreement with the values obtained by Wind[8] and Peek.[9] For different internuclear distances Bates and Reid,[14] Murai,[15] and Murai and Takatsu[16] calculated electronic energies for various states of the hydrogen molecule ion under the assumption of infinite proton mass. For a large range of internuclear distances Winter *et al.*[17] made very accurate calculations for the lowest 20 states of the molecule ion HeH^{2+}. Klaus[18] studied the electronic energy of the ground state of the hydrogen molecule ion for small internuclear separation r_{12} and confirmed the remarkable discovery by Byers Brown and Steiner[19] that the electronic energy cannot be expanded in powers of r_{12} alone, but that powers of $\ln r_{12}$ must also be included. Klaus[18] also obtained for the hydrogen molecule ion further terms in the series given by Byers Brown and Steiner[19] for the general two-center Coulomb problem.

There exist also various approximate analytical methods for solving the quantal two-center Coulomb problem. Such approximate methods have great relevance for understanding the various physical aspects of the problem and also for the derivation of suitable accurate analytical expressions for physical quantities. In one of these methods one uses the quasiclassical approximation, that is, the first order of the phase-integral approximation. In using this method, one encountered in the early papers difficulties associated with the divergence of the phase-integral due to an inappropriate choice of the phase integrand (also called the quasimomentum), which is not determined quite uniquely. Different authors have mastered these difficulties in different ways, but no single unifying method has until now been proposed for the two-center Coulomb problem. An essential feature in our method is the use of the phase-integral approximation generated from an unspecified base function; see the Appendix.

The semiclassical quantization of the low-lying electronic states of the hydrogen molecule ion was treated by Strand and Reinhardt.[20] Pajunen[21] calculated the energy levels of the hydrogen molecule ion (under the assumption of infinitely heavy nuclei) in the first and the third order of the phase-integral approximation. Although he refers to one of the papers (his Ref. 10) in which the phase-integral approximation generated from an unspecified base function was introduced, he does not use the freedom to choose optimum expressions for the functions that he denotes by $Q_{\mathrm{mod}}(\mu)$ and $Q_{\mathrm{mod}}(\nu)$, and that in the present paper correspond to the more general base functions $\tilde{Q}(\xi)$ and $Q(\eta)$, respectively. In the present paper we shall make full use of the possibility to choose $\tilde{Q}(\xi)$ and $Q(\eta)$ most conveniently.

The phase-integral method, in which one uses the phase-integral approximation generated from an unspecified base function,[22] offers a method for mastering the previously mentioned difficulties in a unified way for an arbitrary order of the phase-integral approximation. In the present paper we shall apply this method to the quantal two-center Coulomb problem with fixed Coulomb centers. For the convenience of the reader a short review of the phase-integral method and formulas to be used are given in the Appendix.

Bearing in mind the relative ease of obtaining nowadays highly accurate values with the use of computers, one may ask for the purpose of treating the two-center Coulomb problem with the aid of the phase-integral method. When considering this question one should, however, remember that in the numerical methods there occur difficulties for large values of r_{12} as well as for large values $|Z_1-Z_2|$. The phase-integral formulas are, however, in general most accurate for large values of r_{12} and roughly as accurate for small as for large values of $|Z_1-Z_2|$. It may therefore be advantageous to use the phase-integral formulas for large values of r_{12} and $|Z_1-Z_2|$ instead of numerical results. These formulas can be expressed in terms of complete elliptic integrals, which can be evaluated easily with the use of standard computer programs. The latter formulas also have the advantage of making it possible to obtain for the energy and the separation constant accurate analytical expressions that for certain needs may be more useful than purely numerical results. They can, directly or after series expansion, be used to study the dependence of interesting physical quantities on the parameters of the problem. It seems possible that by means of such

analytical expressions one could refine the interesting investigations by Ponomarev[23] on configuration interaction of terms in the two-center Coulomb system and by Komarov and Solov'ev[24] on quasi-intersection of terms in the problem of two Coulomb centers with strongly different charges. The present work may thus be carried further to throw new light on interesting physical properties of the two-center Coulomb system.

A hydrogen atom in an electric field can be considered as the limiting case of an electron in the field of two Coulomb centers that lie far away from each other and have strongly different charges. It is therefore of interest to note the efficiency and accuracy of the phase-integral method in applications to the Stark effect of a hydrogen atom. For a state of a hydrogen atom with the principal quantum number 25 and the magnetic quantum number 1 in an electric field of 2514 V/cm Fröman and Fröman[25] obtained by means of the phase-integral method the energy with six digits already in the third-order approximation. For the same state Silverstone and Koch[26] had obtained the energy with six digits by the use of 24th-order Rayleigh–Schrödinger perturbation theory combined with a [12/12] Padé approximant, but the phase-integral results indicated that the last one of these digits was wrong by one unit. For a state of a hydrogen atom with the principal quantum number 30 and the magnetic quantum number 0 in an electric field of 800 V/cm, Fröman and Fröman[25] obtained by means of the phase-integral method the energy with nine digits already in the third-order approximation. For the same state, Damburg and Kolosov[25] obtained by means of an efficient purely numerical method the same energy with nine digits, but the phase-integral results indicated that the last one of these digits was wrong by one unit. For the same state, Silverstone and Koch[26] had earlier obtained the energy with six digits by the use of 24th-order Rayleigh–Schrödinger perturbation theory combined with a [12/12] Padé approximant, but the last digit was wrong by three units. One can therefore expect that states of the two-center Coulomb system that correspond to states of a hydrogen atom in an electric field with high principal quantum numbers, low magnetic quantum numbers, and large values of $|Z_1-Z_2|$ should be favorable for phase-integral treatment.

For particular single-well potentials one obtains the eigenvalues exactly from the phase-integral quantization condition of any order by determining the base function (which is defined in the Appendix) such that the eigenvalues coincide in the first- and third-order approximations; see Refs. 27–30. This is not possible for the two-center Coulomb problem, but by choosing the two base functions in this problem such that the values of the energy, as well as the values of the separation constant, coincide in the first- and third-order approximations, one obtains optimum results from the first-order quantization conditions. The study of the behavior of physical quantities can thus be performed with the use of the first-order formulas but with the accuracy of the more complicated third-order formulas. It is not possible to achieve this result if one uses the JWKB approximation, since there appears no *a priori* unspecified base function in that approximation. By making the above-mentioned exactness fulfilled in the limit of a parameter value, for which the phase-integral results without this adaptation would not be good, one can also extend the region of validity of the phase-integral treatment; see p. 12 in Ref. 30.

The present paper, referred to as paper I, constitutes the basis for further work by Athavan *et al.*,[31] (paper II), and Athavan *et al.*[32] (paper III), in which the contour integrals, occurring in the quantization conditions, will be expressed in terms of complete elliptic integrals, analogous to the papers by Lakshmanan and Kaliappan[33] and Lakshmanan *et al.*[34,35] In papers II and III calculations are made for the states $1s\sigma$ and $2p\sigma$ of the hydrogen molecule ion $(Z_1=Z_2=1)$, for two states with $Z_1=1$ and $Z_2=2$, for two states with $Z_1=1$ and $Z_2=5$, and for two states with $Z_1=1$ and $Z_2=8$. For the hydrogen molecule ion $(Z_1=Z_2=1)$ and the ion with $Z_1=1$ and $Z_2=2$ the phase-integral method cannot compete in terms of accuracy with the methods that have been used to obtain the extremely accurate numerical results for these ions, but the possibility of using the analytical phase-integral formulas expressed in terms of complete elliptic integrals is an alternative that for certain purposes may be preferable to the use of very accurate numerical results. For other ions the phase-integral method will probably yield results that for large values of r_{12} are more accurate than the results that have been obtained numerically, as can be seen from Tables III–VI in paper III. In fact, the phase-integral method constitutes an important complement to

perturbation theory and numerical methods. It can sometimes be used with significant advantage for problems where highly accurate numerical methods would be difficult to apply or where the analytical phase-integral formulas can give a deeper understanding of physical processes and provide guidance for numerical work. The investigations published in the present series of three papers give new information concerning the phase-integral method and also its potential power for applications to a wider class of physical problems.

II. SEPARATION OF THE SCHRÖDINGER EQUATION IN ELLIPTIC COORDINATES

We start by quoting some well-known results. The time-independent Schrödinger equation for the motion of an electron of mass μ and charge $-e$ $(e>0)$ in the field of two fixed Coulomb centers with charges Z_1e and Z_2e takes the following form:

$$\left(-\frac{\hbar^2}{2\mu}\Delta_{\vec{r}}-\frac{Z_1e^2}{r_1}-\frac{Z_2e^2}{r_2}\right)\Psi(\vec{r})=E\Psi(\vec{r}), \tag{2.1}$$

where r_1 and r_2 are the distances of the electron from the two centers, $\vec{r}$ is the position vector of the electron, and E is the electronic energy. To obtain the total energy one must add the potential energy of the two fixed charges, getting

$$E_{\text{total}}=\frac{Z_1Z_2e^2}{r_{12}}+E, \tag{2.2}$$

where r_{12} is the distance between the two centers. The differential equation (2.1) is separable in elliptic coordinates. If one introduces the variables

$$\xi=\frac{r_1+r_2}{r_{12}}, \quad 1\leqslant\xi<+\infty, \tag{2.3a}$$

$$\eta=\frac{r_1-r_2}{r_{12}}, \quad -1\leqslant\eta\leqslant+1, \tag{2.3b}$$

and puts

$$\Psi(\vec{r})=X(\xi)Y(\eta)e^{im\phi}, \tag{2.4}$$

where m is the magnetic quantum number (positive or negative integer or zero), and ϕ is the corresponding angle, the separation yields, in atomic units $(\hbar=e=\mu=1)$, the following two differential equations:

$$\frac{\mathrm{d}}{\mathrm{d}\xi}\left((\xi^2-1)\frac{\mathrm{d}X}{\mathrm{d}\xi}\right)+\left(-p^2\xi^2+b'\xi+A-\frac{m^2}{\xi^2-1}\right)X=0, \tag{2.5a}$$

$$\frac{\mathrm{d}}{\mathrm{d}\eta}\left((1-\eta^2)\frac{\mathrm{d}Y}{\mathrm{d}\eta}\right)+\left(p^2\eta^2+b\eta-A-\frac{m^2}{1-\eta^2}\right)Y=0, \tag{2.5b}$$

where A is the separation constant and

$$p^2=-\tfrac{1}{2}r_{12}^2E, \tag{2.6a}$$

$$b'=r_{12}(Z_2+Z_1), \tag{2.6b}$$

$$b=r_{12}(Z_2-Z_1). \tag{2.6c}$$

Putting

$$X(\xi)=\frac{f(\xi)}{(\xi^2-1)^{1/2}}, \tag{2.7a}$$

$$Y(\eta)=\frac{g(\eta)}{(1-\eta^2)^{1/2}}, \tag{2.7b}$$

we can transform the differential equations (2.5) into

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\xi^2}+\tilde{R}(\xi)\right)f(\xi)=0, \tag{2.8a}$$

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}\eta^2}+R(\eta)\right)g(\eta)=0, \tag{2.8b}$$

where

$$\tilde{R}(\xi)=-p^2+\frac{b'\xi+A'}{\xi^2-1}-\frac{m^2-1}{(\xi^2-1)^2}, \tag{2.9a}$$

$$R(\eta)=-p^2+\frac{b\eta-A'}{1-\eta^2}-\frac{m^2-1}{(1-\eta^2)^2}, \tag{2.9b}$$

with

$$A'=A-p^2. \tag{2.10}$$

The differential equations (2.8) are of the Schrödinger type. By solving them simultaneously under the boundary conditions that $f(+1)=f(+\infty)=0$ and $g(-1)=g(+1)=0$, one can obtain the energy and the separation constant as functions of the distance r_{12} and the quantum numbers.

When $Z_1=Z_2$ every bound-state wave function $Y(\eta)$ is either an even or an odd function of η, and when $\vec{r}$ is reflected at the center of symmetry for the two-center Coulomb problem, the wave function (2.4) remains unchanged when $Y(\eta)$ and m are both even or both odd, while the wave function (2.4) changes sign when one of $Y(\eta)$ and m is even and the other is odd.

III. APPLICATION OF THE PHASE-INTEGRAL METHOD

The essential features of the phase-integral method are briefly sketched in the Appendix. The phase-integral solutions of the differential equations (2.8a) and (2.8b), respectively, are linear combinations of the phase-integral functions

$$\tilde{q}^{-1/2}(\xi)\exp\left\{\pm i\int^{\xi}\tilde{q}(\xi)\mathrm{d}\xi\right\} \tag{3.1a}$$

and

$$q^{-1/2}(\eta)\exp\left\{\pm i\int^{\eta}q(\eta)\mathrm{d}\eta\right\}, \tag{3.1b}$$

respectively, where $\tilde{q}(\xi)$ and $q(\eta)$, respectively, are generated according to (A5a), (A5b), (A6a)–(A6c), (A3), and (A2) in the Appendix, with $R(z),Q(z)$ replaced by the appropriate functions $\tilde{R}(\xi),\tilde{Q}(\xi)$ and $R(\eta),Q(\eta)$, respectively, the quantities pertaining to the ξ-equation being characterized by a tilde.

A. Base functions generating phase-integral solutions

As is seen from (2.9a) and (2.9b), the functions $\tilde{R}(\xi)$ and $R(\eta)$ have poles at $\xi=\pm 1$ and $\eta=\pm 1$, respectively; these poles are of the second order if $m\neq\pm 1$, but of the first order if $m=\pm 1$. Furthermore, we note that when $m\neq 0$ the coefficients of the second-order poles differ from $\frac{1}{4}$, while for $m=0$ they are equal to $\frac{1}{4}$.

There are two main alternatives, discussed in the Appendix for the case of the radial Schrödinger equation, for choosing the base functions generating the phase-integral functions (3.1a) and (3.1b). Unifying these two alternatives, we choose the squares of the base functions to be

$$\tilde{Q}^2(\xi)=-p^2+\frac{A'-\tilde{C}+b'\xi}{\xi^2-1}-\frac{\Lambda^2}{(\xi^2-1)^2}, \tag{3.2a}$$

$$Q^2(\eta)=-p^2+\frac{-A'+C+b\eta}{1-\eta^2}-\frac{\Lambda^2}{(1-\eta^2)^2}, \tag{3.2b}$$

where C, $\tilde{C}$, and Λ are parameters, the choice of which we shall discuss in the following. The introduction of these parameters essentially increases the flexibility of the phase-integral formulas to be obtained.

By choosing $C=\tilde{C}=1/4$ one correctly obtains in the limit when $r_{12}\to 0$ the energy E and the reduced separation constant A' from the first-order phase-integral quantization conditions (to be derived in Sec. III B). For arbitrary values of r_{12} it is most appropriate to determine C and $\tilde{C}$ as functions of r_{12} such that one obtains the same value of p^2 (i.e., of the energy) and also of A' in the first and in the third order of the phase-integral approximation. One thereby achieves the optimum accuracy obtainable from the first-order quantization conditions. We emphasize that this can be achieved by the use of the phase-integral approximation generated from an unspecified base function (described in the Appendix), but cannot be achieved by means of the JWKB approximation, in which there is no unspecified base function. The decisive properties of the phase-integral approximation in question versus the JWKB approximation have been explained in some detail by Dammert and Fröman[36] and by Fröman and Fröman.[22]

When $|m|$ is not too small, we choose $\Lambda=|m|\neq 0$, but when $|m|$ is sufficiently small we choose $\Lambda=0$. For $m=0$ one should always choose $\Lambda=0$. The two alternatives $\Lambda=|m|\neq 0$ and $\Lambda=0$ yield solutions with different properties. When $\Lambda=|m|\neq 0$ the phase integral solutions of the differential equations (2.8a) and (2.8b) remain valid as $\xi\to\pm 1$ and $\eta\to\pm 1$, respectively. When $\Lambda=0$ the phase-integral solutions of the differential equations in question break down as $\xi\to\pm 1$ and $\eta\to\pm 1$, respectively, but the regular solutions of the ξ- and η-equations can be obtained at some distances from those points by the use of the connection formula described in Sec. 2 b of the Appendix, when one there replaces l by $(|m|-1)/2$; cf. (2.9a) and (2.9b). The wave functions obtained in that way are expected to be more accurate the stronger the Coulomb singularities of $\tilde{R}(\xi)$ and $R(\eta)$ at $\xi=\pm 1$ and $\eta=\pm 1$ are. However, even if the Coulomb singularities are strong, these wave functions are not expected to be good if $|m|$ is too large, in which case one should choose $\Lambda=|m|\neq 0$, as mentioned in the beginning of this paragraph.

Using the terminology ''classically allowed region'' and ''classically forbidden region'' in a generalized sense, viz. to characterize regions where $\tilde{Q}^2(\xi)$ or $Q^2(\eta)$ is larger than zero and less than zero, respectively, we shall now discuss the wave functions pertaining to the ξ-equation and the η-equation.

1. Wave functions pertaining to the ξ-equation

According to (3.2a) the function $-\tilde{Q}^2(\xi)$, where $1\leqslant\xi<+\infty$, always corresponds to a single-well potential.

For $\Lambda=|m|\neq 0$ there are four zeros of $\tilde{Q}^2(\xi)$, which we denote by ξ_1,ξ_2,ξ_3, and ξ_4; see Fig. 1(a). The zeros ξ_1 and ξ_2 may be real and both less than 1, or they may be complex conjugate. The zeros $\xi_3(>1)$ and $\xi_4(>\xi_3)$ are real. There is thus a classically allowed region between ξ_3 and ξ_4,

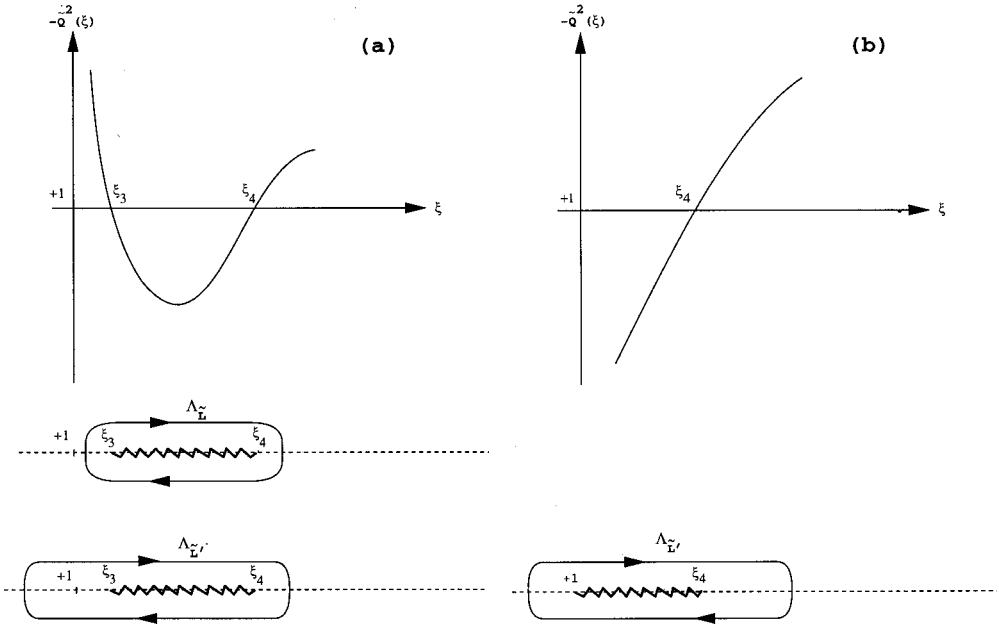

FIG. 1. Schematic pictures of $-\tilde{Q}^2(\xi)$ for $\xi>1$ and of the contours of integration in the complex ξ-plane. The cuts are indicated by wavy lines. On the upper lip of the cut $\tilde{Q}(\xi)$ is positive. Only those zeros of $\tilde{Q}^2(\xi)$ that are relevant for the contours of integration are shown. For $\Lambda=|m|\neq 0$ (a) always applies, and the relation between the integrals associated with the contours $\Lambda_{\tilde{L}}$ and $\Lambda_{\tilde{L}'}$ is $\tilde{L}'=\tilde{L}+|m|/2$; the zeros ξ_1 and ξ_2 of $\tilde{Q}^2(\xi)$, which are not shown, may be real or complex conjugate. For $\Lambda=0$ there are only two zeros, ξ_3 and ξ_4, of $\tilde{Q}^2(\xi)$, and either (a) or (b) may apply.

but classically forbidden regions for $1<\xi<\xi_3$ and $\xi>\xi_4$. The phase-integral wave functions generated from $\tilde{Q}(\xi)$ are good at $\xi=1$, and we can use the arbitrary-order connection formula, given by (A13) and (A14), for tracing the physically acceptable wave function from the classically forbidden region between 1 and ξ_3 to the classically allowed region, that is, the region between ξ_3 and $\xi_4(>\xi_3)$ where $\tilde{Q}^2(\xi)>0$; see Fig. 1(a).

For $\Lambda=0$ there are two zeros of $\tilde{Q}^2(\xi)$, which we denote by $\xi_3(<\xi_4)$ and $\xi_4(>1)$. The classically allowed region lies between ξ_3 and ξ_4 when $\xi_3>1$, but between 1 and ξ_4 when $\xi_3<1$; see Fig. 1. The phase-integral wave function is not good at $\xi=1$, but for the physically acceptable wave function one can obtain a phase-integral expression in the interior of the classically allowed region, when $\xi_3>1$ and the classically forbidden region between 1 and ξ_3 is sufficiently large, by means of the arbitrary-order connection formula given by (A13) and (A14), and when $\xi_3<1$ by means of the connection formula presented in Sec. 2 b of the Appendix.

Both when $\Lambda=|m|\neq 0$ and when $\Lambda=0$ the wave function, obtained in the classically allowed region to the left of ξ_4 as described previously, can be joined to the physically acceptable wave function traced from the classically forbidden region to the right of ξ_4 into the classically allowed region to the left of ξ_4 with the aid of the arbitrary-order connection formula given by (A13) and (A14). In this way, alternative quantization conditions, corresponding to $\Lambda=|m|\neq 0$ and $\Lambda=0$, can be obtained. They can be combined into one quantization condition. Figure 1 illustrates the two possible situations where the classically allowed region is delimited either by ξ_3 and ξ_4 [Fig. 1(a)] or by the pole at $\xi=+1$ and the turning point at $\xi=\xi_4$ [Fig. 1(b)].

2. Wave functions pertaining to the η-equation

The function $-Q^2(\eta)$ may correspond either to a single-well potential or to a double-well potential.

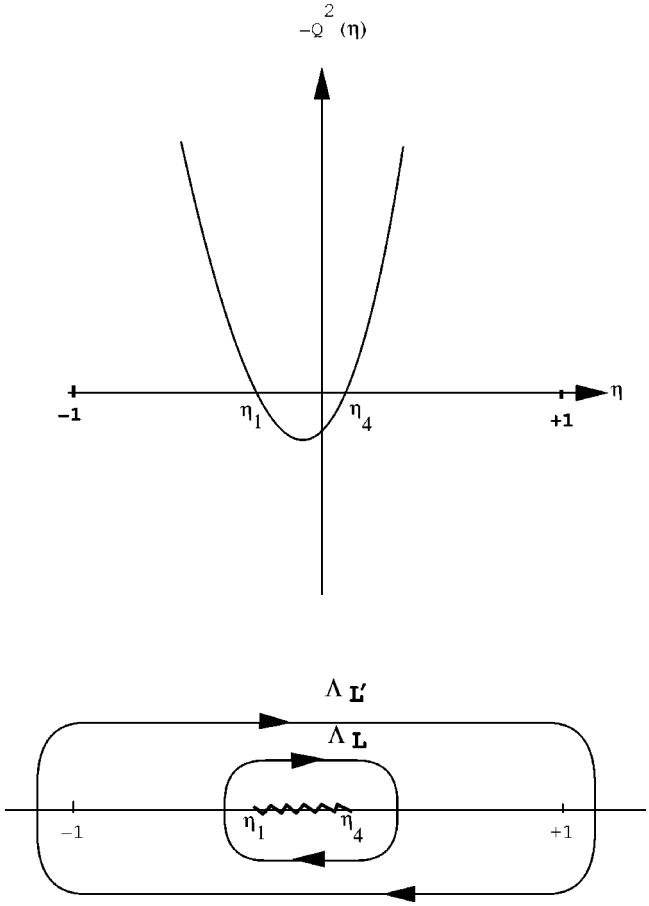

FIG. 2. Schematic pictures of $-Q^2(\eta)$ for $-1<\eta<1$ and of the contours of integration when $-Q^2(\eta)$ in the interval $-1<\eta<1$ is a single-well potential, which may occur for $\Lambda=|m|\neq 0$ as well as for $\Lambda=0$. The cut is indicated by a wavy line, on the upper lip of which $Q(\eta)$ is positive. The contour $\Lambda_{L'}$ can be used only when $\Lambda=|m|\neq 0$, and the relation between the integrals associated with the contours Λ_L and $\Lambda_{L'}$ is then $L'=L+|m|$. The quantization conditions, expressed in terms of complete elliptic integrals, for the situation with $\Lambda=|m|\neq 0$ are the same as the corresponding quantization conditions for the situation in Fig. 4(a). The quantization condition for the case given here with $\Lambda=0$ has so far not appeared in the applications.

For $\Lambda=|m|\neq 0$ the phase-integral solution is valid at the poles $\eta=\pm 1$ (which delimit classically forbidden regions) and can be traced into the classically allowed region closest to the pole in question with the aid of the connection formula given by (A13) and (A14). When there is only one classically allowed region, one obtains the quantization condition by identifying the two expressions for the wave function in that region. This case applies when $-Q^2(\eta)$ is a single-well potential (Fig. 2), or when the energy lies so far above the top of an underdense barrier [Fig. 4(b)] that it is appropriate to disregard the presence of the complex conjugate zeros η_2 and η_3 of $Q^2(\eta)$. When $-Q^2(\eta)$ corresponds to a double-well potential, the wave function can be traced from the region on one side of the barrier to the region on the other side with the aid of the arbitrary-order connection formula for a barrier described in Sec. 3 of the Appendix; see Figs. 3 and 4. Joining the two expressions for the wave function thus obtained to each other, one obtains the quantization condition.

When $\Lambda=0$ [Fig. 2 or Fig. 4(b)] the phase-integral wave function is not good at $\eta=\pm 1$, but at some distance from these points physically acceptable solutions can be obtained in the same classically allowed region by the use of the connection formulas presented in Secs. 2 and 3 of the

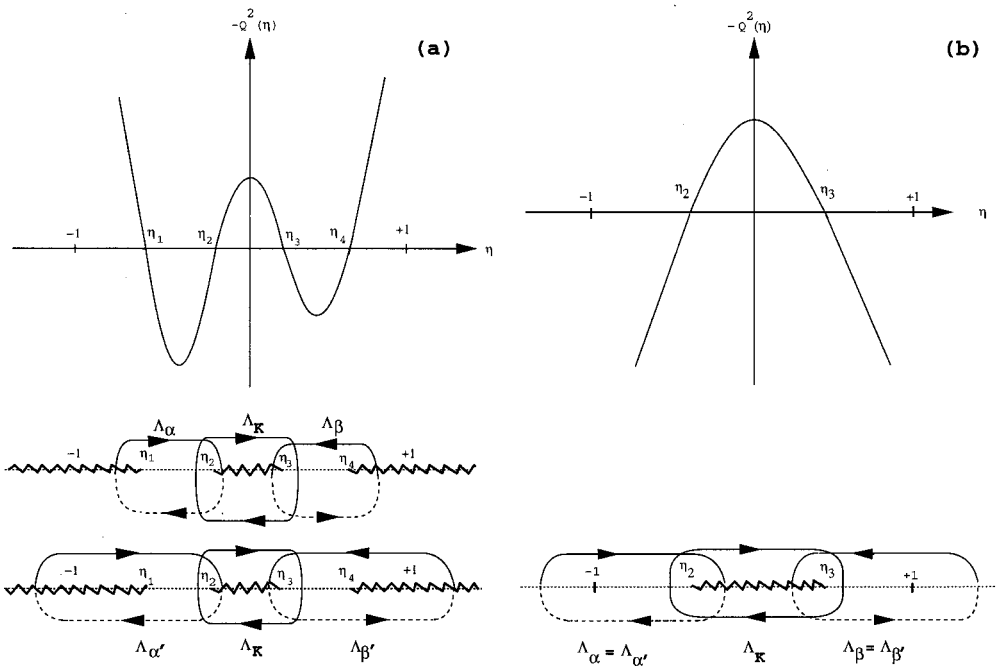

FIG. 3. Schematic pictures of $-Q^2(\eta)$ for $-1<\eta<1$ and of the contours of integration in the complex η-plane, when $-Q^2(\eta)$ corresponds to a double-well potential with a superdense barrier (subbarrier). In (a) $\Lambda=|m|\neq 0$ and in (b) $\Lambda=0$. The cuts are indicated by wavy lines, and the parts of the contours of integration that lie on Riemann sheets adjacent to the complex η-plane under consideration are dashed. In the left-hand classically allowed region $Q(\eta)$ is positive. Only those zeros of $Q^2(\eta)$ that are relevant for the contours of integration are shown. We recall the relations (3.18a) which mean that $\alpha'=\alpha+\Lambda\pi/2$ and $\beta'=\beta+\Lambda\pi/2$.

Appendix. Thus one obtains two expressions for the wave function, and by identifying these expressions one obtains a quantization condition.

B. Quantization conditions

1. Quantization conditions pertaining to the ξ-equation

For the differential equation (2.8a) the physically relevant interval is $1<\xi<\infty$. The phase-integral quantization condition for the situation in Fig. 1(a) involves a contour integral in the complex ξ-plane encircling ξ_3 and ξ_4, while the phase-integral quantization condition for the situation in Fig. 1(b) involves a contour integral encircling the simple pole at $\xi=1$ and the generalized classical turning point ξ_4. The quantization condition (A31) applies to the first situation, and the quantization condition (A32) applies to the second situation. Introducing the notations

$$\tilde{L}=\sum_{n=0}^{N}\tilde{L}^{(2n+1)}, \tag{3.3a}$$

$$\tilde{L}^{(2n+1)}=\frac{1}{2}\int_{\Lambda_{\tilde{L}}}\tilde{q}^{(2n+1)}(\xi)\mathrm{d}\xi, \tag{3.3b}$$

$$\tilde{L}'=\sum_{n=0}^{N}\tilde{L}'^{(2n+1)}, \tag{3.4a}$$

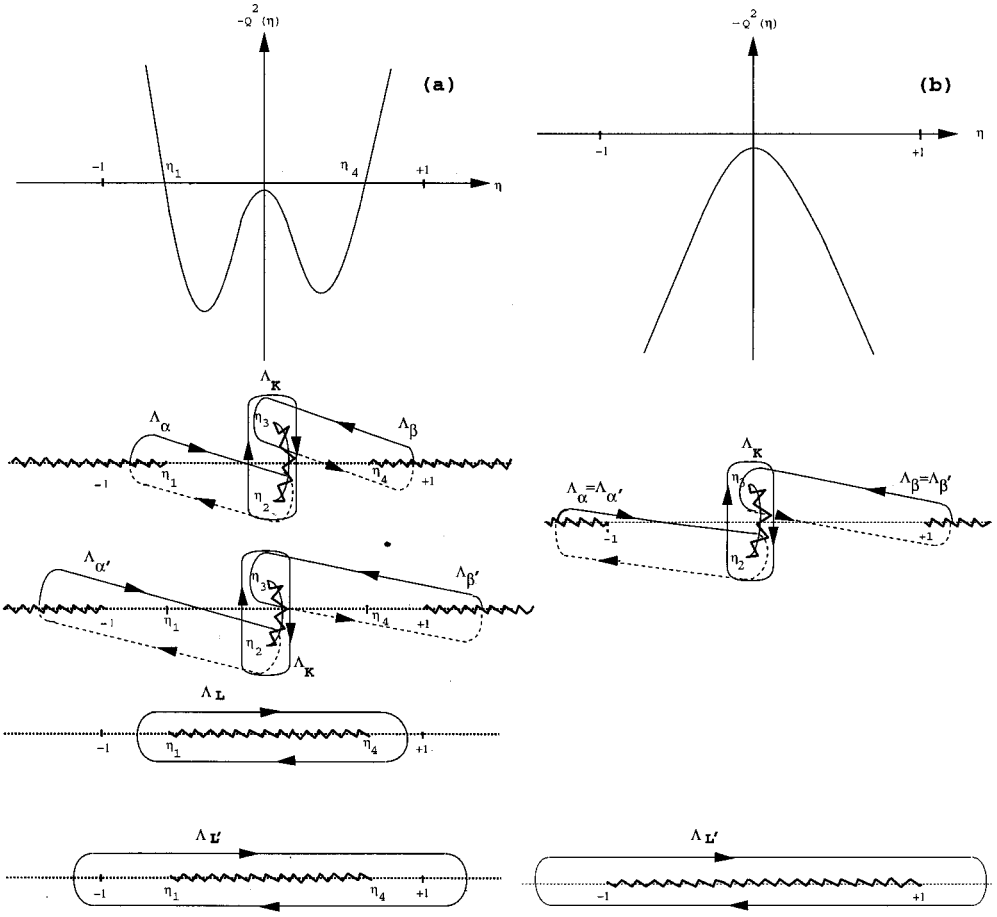

FIG. 4. Schematic pictures of $-Q^2(\eta)$ for $-1<\eta<1$ and of the contours of integration in the complex η plane, when $-Q^2(\eta)$ corresponds to a double-well potential with an under-dense barrier (superbarrier). In (a) $\Lambda=|m|\neq 0$ and in (b) $\Lambda=0$. The cuts are indicated by wavy lines, and the parts of the contours of integration that lie on Riemann sheets adjacent to the complex η-plane under consideration are dashed. In the left-hand classically allowed region $Q(\eta)$ is positive. Only those zeros of $Q^2(\eta)$ that are relevant for the contours of integration are shown. If the energy lies sufficiently far above the top of the barrier, one may treat the double-well potential problem as a single-well potential problem with the classically allowed region between η_1 and η_4 in (a) and between the poles at $\eta=-1$ and $\eta=+1$ in (b). One then introduces new cuts [between η_1 and η_4 in (a) and between -1 and $+1$ in (b)], on the upper lips of which $Q(\eta)$ is positive, and uses the contours Λ_L and $\Lambda_{L'}$. In (a) the relation between the corresponding integrals is $L'=L+|m|$. In both (a) and (b) L is related to α and β by the relation $L=\alpha+\beta$.

$$\tilde{L}'^{(2n+1)}=\frac{1}{2}\int_{\Lambda_{\tilde{L}'}}\tilde{q}^{(2n+1)}(\xi)\mathrm{d}\xi, \tag{3.4b}$$

where $\tilde{q}(\xi)$ is obtained according to (A5a), (A5b), (A6a)–(A6c), (A3), and (A2), and $\Lambda_{\tilde{L}}$ and $\Lambda_{\tilde{L}'}$ are the appropriate contours of integration pertaining to $\xi_3>1$ and $\xi_3<1$, respectively, and shown in Figs. 1(a) and 1(b), respectively, we can write the two quantization conditions corresponding to $\xi_3>1$ and $\xi_3<1$ as follows:

$$\tilde{L}=(\tilde{s}+\tfrac{1}{2})\pi, \quad \xi_3>1, \tag{3.5a}$$

$$\tilde{L}'=\left(\frac{|m|}{2}+\tilde{s}+\frac{1}{2}\right)\pi, \quad \xi_3<1, \tag{3.5b}$$

where $\tilde{s}$ is an integer. If, when $\Lambda=|m|\neq 0$ and hence $\xi_3>1$, we enlarge the contour of integration $\Lambda_{\tilde{L}}$ in Fig. 1(a), so that the new contour $\Lambda_{\tilde{L}'}$ encloses the turning points ξ_3 and ξ_4 as well as the pole at $\xi=1$, and if we compensate in (3.5a) along with (3.3a) and (3.3b) for this change by taking the residue of the integrand at $\xi=1$ into account, we obtain a general quantization condition, valid for both cases $\xi_3>1$ and $\xi_3<1$, i.e., for both situations depicted in Fig. 1, viz.

$$\tilde{L}'=\left(\frac{|m|}{2}+\tilde{s}+\frac{1}{2}\right)\pi, \quad \xi_3>1 \text{ or } \xi_3<1. \tag{3.6}$$

Besides condensing the two alternative quantization conditions (3.5a) and (3.5b) nicely into one formula, the quantization condition (3.6) has the further merit that, if the integration along the contour is made numerically (in cases where expressions in terms of complete elliptic integrals are not available), it may be advantageous to use the contour $\Lambda_{\tilde{L}'}$ instead of $\Lambda_{\tilde{L}}$ when $\xi_3>1$.

The quantization condition (3.6) yields the value of the reduced separation constant A' as a function of p^2 and $\tilde{C}$; see (3.2a).

2. Quantization conditions pertaining to the η-equation

In the physically relevant interval $-1<\eta<1$ the function $-Q^2(\eta)$ may correspond to a single-well potential (Fig. 2) or to a double-well potential with a superdense (Fig. 3) or underdense (Fig. 4) barrier. When, in the case of an underdense barrier, the energy lies sufficiently far above the top of the barrier, it may be preferable to disregard the barrier and to treat the double-well potential problem as a single-well potential problem.

When $\Lambda=|m|\neq 0$ or $\Lambda=0$, and $-Q^2(\eta)$ is or can be considered as a single-well potential, and the classically allowed region is delimited by two simple zeros of $Q^2(\eta)$, as shown in Figs. 2 and 4(a), we obtain from (A31) the single-well quantization condition

$$L=(s+\tfrac{1}{2})\pi, \quad s=\text{non-negative integer}, \tag{3.7}$$

where by definition

$$L=\frac{1}{2}\int_{\Lambda_L} q(\eta)\,\mathrm{d}\eta, \tag{3.8}$$

Λ_L being a closed contour encircling the generalized classical turning points. Note that in the derivation of (3.7) we have considered the classically forbidden regions to be thick also when $\Lambda=0$ (Fig. 2). When $\Lambda=|m|\neq 0$ we can with the aid of residue calculus write (3.7) along with (3.8) as

$$L'=(|m|+s+\tfrac{1}{2})\pi, \tag{3.9}$$

where L' is defined by

$$L'=\frac{1}{2}\int_{\Lambda_{L'}} q(\eta)\,\mathrm{d}\eta, \tag{3.10}$$

$\Lambda_{L'}$ being a closed contour encircling -1 and $+1$; see Figs. 2 and 4(a).

When $\Lambda=0$, and the classically allowed region is delimited by two first-order poles of $Q^2(\eta)$, as shown in Fig. 4(b), and the energy lies far above the top of the barrier, one can consider $-Q^2(\eta)$ as a single-well potential. From (A33) one then obtains the quantization condition (3.9) with L' defined by (3.10), where $\Lambda_{L'}$ is now the contour in Fig. 4(b).

We disregard the possibility that $\Lambda=0$ and the residues of $Q^2(\eta)$ at $\eta=-1$ and $\eta=+1$ have different signs, since this case has so far not appeared in the applications.

When $-Q^2(\eta)$ corresponds to a double-well potential (Figs. 3 and 4), which is usually the case, the quantization condition (A39) gives

$$\cos(\alpha+\beta+\tilde{\phi}-2a)=\frac{\cos(\alpha-\beta)}{[1+\exp(-2\pi\overline{K})]^{1/2}}, \tag{3.11}$$

where

$$a=\frac{\pi}{2} \quad \text{when} \quad \Lambda=|m|\neq 0, \tag{3.12a}$$

$$a=(|m|+1)\frac{\pi}{2} \quad \text{when} \quad \Lambda=0, \tag{3.12b}$$

$$\alpha=\sum_{n=0}^{N}\alpha^{(2n+1)}, \tag{3.13a}$$

$$\alpha^{(2n+1)}=\mathrm{Re}\,\frac{1}{2}\int_{\Lambda_\alpha} q^{(2n+1)}(\eta)\,\mathrm{d}\eta, \tag{3.13b}$$

$$\beta=\sum_{n=0}^{N}\beta^{(2n+1)}, \tag{3.14a}$$

$$\beta^{(2n+1)}=-\mathrm{Re}\,\frac{1}{2}\int_{\Lambda_\beta} q^{(2n+1)}(\eta)\,\mathrm{d}\eta, \tag{3.14b}$$

$$\overline{K}=\sum_{n=0}^{N}\overline{K}_{2n}, \tag{3.15a}$$

$$\overline{K}_{2n}=\frac{i}{2\pi}\int_{\Lambda_K} q^{(2n+1)}(\eta)\,\mathrm{d}\eta. \tag{3.15b}$$

For the superbarrier case (Fig. 4) we can instead of (3.15b) use the alternative formula

$$\overline{K}_{2n}=-2\,\mathrm{Im}\,\frac{1}{2\pi}\int_{\Lambda_\alpha} q^{(2n+1)}(\eta)\,\mathrm{d}\eta$$

$$=-2\,\mathrm{Im}\,\frac{1}{2\pi}\int_{\Lambda_\beta} q^{(2n+1)}(\eta)\,\mathrm{d}\eta, \tag{3.15b$'$}$$

which is useful in connection with the transformation to complete elliptic integrals. With the use of (3.13a), (3.13b), (3.14a), (3.14b), (3.15a), and (3.15b$'$) each one of the quantities α, β, and $\overline{K}$ is then obtained as the real or imaginary part of an integral over the contour Λ_α or Λ_β. The contours of integration $\Lambda_\alpha, \Lambda_\beta$, and Λ_K for subbarrier and superbarrier energies are shown in Figs. 3 and 4. The analytic expression for the quantity $\tilde{\phi}$ is given in terms of $\overline{K}$ and $\overline{K}_{2n}$ by (A28) and (A29a)–(A29c). The quantity $\tilde{\phi}$ is of decisive importance for energies in the neighborhood of the top of the barrier. The quantities α and β are positive. The quantity $\overline{K}_0$ is positive when η_2 and η_3 are real, it is equal to zero when η_2 and η_3 coincide, and it is negative when η_2 and η_3 are complex conjugate. The quantity $\overline{K}_2$ may be positive or negative irrespective of whether η_2 and η_3 are real or complex conjugate.

Analogously as we changed the original contour $\Lambda_{\tilde{L}}$ into $\Lambda_{\tilde{L}'}$, when dealing with the quantization condition (3.5a), we can, when $\Lambda=|m|\neq 0$, change the contours Λ_α and Λ_β depicted in Figs. 3(a) and 4(a), so that, instead of letting them enclose only η_1,η_2 and η_3,η_4, respectively, we make each one of them enclose also a pole, $\eta=-1$ or $\eta=+1$, respectively. Calling the new contours $\Lambda_{\alpha'}$ and $\Lambda_{\beta'}$ [see Figs. 3(a) and 4(a)] and defining

$$\alpha'=\sum_{n=0}^{N}\alpha'^{(2n+1)}, \tag{3.16a}$$

$$\alpha'^{(2n+1)}=\mathrm{Re}\frac{1}{2}\int_{\Lambda_{\alpha'}}q^{(2n+1)}(\eta)\,\mathrm{d}\eta, \tag{3.16b}$$

$$\beta'=\sum_{n=0}^{N}\beta'^{(2n+1)}, \tag{3.17a}$$

$$\beta'^{(2n+1)}=-\mathrm{Re}\frac{1}{2}\int_{\Lambda_{\beta'}}q^{(2n+1)}(\eta)\,\mathrm{d}\eta, \tag{3.17b}$$

and recalling that the functions Y_{2n} are regular analytic at $\eta=\pm 1$ when $\Lambda=|m|\neq 0$, we find with the use of residue calculus that for $\Lambda=|m|\neq 0$

$$\begin{aligned}\alpha'-\alpha&=\beta'-\beta\\&=\Lambda\pi/2,\end{aligned} \tag{3.18a}$$

$$\begin{aligned}\alpha'-\beta'&=\alpha-\beta\\&=-\frac{b\pi}{2p}.\end{aligned} \tag{3.18b}$$

With the aid of (3.18a) and (3.18b) we obtain from (3.11) along with (3.12a) for $\Lambda=|m|\neq 0$ the following quantization condition:

$$\cos[\alpha'+\beta'+\tilde{\phi}-(|m|+1)\pi]=\frac{\cos[b\pi/(2p)]}{[1+\exp(-2\pi\bar{K})]^{1/2}}, \tag{3.19}$$

which has the same merits, relative to the original form of the quantization condition, i.e., (3.11) with (3.12a), as were mentioned in connection with the quantization condition (3.6), pertaining to the ξ-equation. When $\Lambda=0$ we define

$$\alpha'=\sum_{n=0}^{N}\alpha'^{(2n+1)}, \tag{3.20a}$$

$$\alpha'^{(2n+1)}=\alpha^{(2n+1)}, \tag{3.20b}$$

$$\beta'=\sum_{n=0}^{N}\beta'^{(2n+1)}, \tag{3.21a}$$

$$\beta'^{(2n+1)}=\beta^{(2n+1)}, \tag{3.21b}$$

and note that (3.18a) is obviously valid also for $\Lambda=0$. With the use of the theory of complex integration one finds that also (3.18b) is valid for $\Lambda=0$. Then it follows from (3.11), (3.12b),

(3.18a), and (3.18b) that the quantization condition (3.19) is valid also when $\Lambda=0$. The quantization condition (3.19) thus covers in a unified and convenient form both cases $\Lambda=|m|\neq 0$ and $\Lambda=0$.

The quantization condition (3.19) can be rewritten as

$$\alpha'+\beta'+\tilde{\phi}-(|m|+1)\pi=\pm\arccos\frac{\cos[b\pi/(2p)]}{[1+\exp(-2\pi\bar{K})]^{1/2}}+2s'\pi, \tag{3.22}$$

where s' is an integer. As already mentioned, (3.18b) is valid for $\Lambda=|m|\neq 0$ as well as for $\Lambda=0$. When the plus sign in (3.22) applies, we use (3.18b) to express β' in terms of α', and when the minus sign in (3.22) applies, we use (3.18b) to express α' in terms of β'. Replacing s' by s_α or s_β, we thus obtain from (3.22) and (3.18b) the two quantization conditions

$$\alpha'=\left(\frac{|m|}{2}+s_\alpha+\frac{1}{2}\right)\pi-\frac{\tilde{\phi}}{2}-\frac{b\pi}{4p}+\frac{1}{2}\arccos\frac{\cos[b\pi/(2p)]}{[1+\exp(-2\pi\bar{K})]^{1/2}}, \tag{3.23a}$$

$$\beta'=\left(\frac{|m|}{2}+s_\beta+\frac{1}{2}\right)\pi-\frac{\tilde{\phi}}{2}+\frac{b\pi}{4p}-\frac{1}{2}\arccos\frac{\cos[b\pi/(2p)]}{[1+\exp(-2\pi\bar{K})]^{1/2}}, \tag{3.23b}$$

where we choose the branch of arccos such that the last two terms on the right-hand side of (3.23a) and (3.23b) cancel in the limit $\bar{K}\to+\infty$, that is, when the barrier becomes infinitely thick. In this limit, the formulas (3.23a) and (3.23b) simplify to

$$\alpha'=\left(\frac{|m|}{2}+s_\alpha+\frac{1}{2}\right)\pi, \tag{3.24a}$$

$$\beta'=\left(\frac{|m|}{2}+s_\beta+\frac{1}{2}\right)\pi. \tag{3.24b}$$

For the particular case that we have a symmetric two-center Coulomb problem, i.e., that $Z_1=Z_2$, as is the case for the ion H_2^+, the double-well potential pertaining to the η-equation becomes symmetric ($b=0$), and the quantization conditions (3.23a) and (3.23b) can be simplified:

$$\alpha'=\left(\frac{|m|}{2}+s_\alpha+\frac{1}{2}\right)\pi-\frac{\tilde{\phi}}{2}+\frac{1}{2}\arctan\exp(-\pi\bar{K}), \tag{3.25a}$$

$$\beta'=\left(\frac{|m|}{2}+s_\beta+\frac{1}{2}\right)\pi-\frac{\tilde{\phi}}{2}-\frac{1}{2}\arctan\exp(-\pi\bar{K}). \tag{3.25b}$$

The reduced separation constant A', obtained from (3.23a) and (3.23b) in the general case and from (3.25a) and (3.25b) in the symmetric case, is a function of p^2 and C.

3. Comments on the quantization conditions

In the existing semiclassical treatments, the quantization conditions derived on assumptions valid for $m\neq 0$ are in general extrapolated to $m=0$ (corresponding to a particularization of our case $\Lambda=0$) without any motivation. It is, however, not allowed one to obtain a quantization condition corresponding to $m=0$ from a quantization condition corresponding to $m\neq 0$ by letting m take continuous values and tend to zero by a limiting procedure. That the formulas obtained by

such an extrapolation are valid is an *a posteriori* conclusion. The correct justification of the quantization conditions for $\Lambda=0$ rests on the use of the connection formula in Sec. 2 b of the Appendix.

For given values of r_{12}, m and E one can, as already mentioned, obtain the possible values of the reduced separation constant A' in the differential equation (2.8a) with (2.9a) by applying phase-integral quantization conditions for a single-well potential, while to obtain the possible values of the reduced separation constant A' in the differential equation (2.8b) with (2.9b) one has to use quantization conditions either for a single-well potential or for a double-well potential. The appropriate quantization condition for the ξ-equation determines A' as a function of p^2 and $\tilde{C}$. The appropriate quantization condition for the η-equation determines A' as a function of p^2 and C. The eigenvalues of p^2, and hence the energy eigenvalues E, are obtained from the requirement that these two expressions for A' must be equal to each other. One then obtains A' from the quantization condition for the ξ-equation or the η-equation. The value thus obtained for A' depends obviously on the choice of C and $\tilde{C}$. One should choose these parameters as functions of r_{12} in such a way that very accurate values of p^2 and A' are obtained already in the first order of the phase-integral approximation. A practically useful criterion for this can be formulated as follows. For every value of r_{12} one determines C and $\tilde{C}$ such that the first-order approximation gives the same value as the third-order approximation for p^2 (and hence for the energy) as well as for A'. In this way one can make all calculations within the framework of the phase-integral method.

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APPENDIX: PHASE-INTEGRAL METHOD

Since the present paper is based on phase-integral formulas that are scattered in different publications, we collect in this Appendix the background material that is necessary for reading the paper.

The phase-integral method for solving differential equations of the type

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}z^2}+R(z)\psi=0 \tag{A1}$$

involves the following items.

(1) Arbitrary-order phase-integral approximation generated from an unspecified base function $Q(z)$, as described in Chap. 1 of Ref. 22; see also Dammert and Fröman.[36]
(2) The method for solving connection problems developed by Fröman and Fröman,[37] generalized to apply to the phase-integral approximation referred to in the above-given item.
(3) Supplementary quantities, expressed analytically in terms of phase-integrals. An example is the quantity $\tilde{\phi}$, which is a new notation for the quantity -2σ in Fröman *et al.*,[38] and which is of decisive importance, when two transition zeros lie close to each other.

We shall first briefly describe the phase-integral approximation referred to in item (1). Then we collect connection formulas pertaining to a single transition point [first-order zero or first-order pole of $Q^2(z)$] and to a real potential barrier, which can be derived by means of the method mentioned in item (2) combined with comparision equation technique for obtaining the supplementary quantity $\tilde{\phi}$ mentioned in item (3) and appearing in the connection formula for a real barrier. Finally we present quantization conditions for single-well and double-well potentials,

which can be derived by means of the connection formulas just mentioned. These quantization conditions are used in our treatment of the two-center Coulomb problem.

1. Phase-integral approximation generated from an unspecified base function

For a detailed description of the phase-integral approximation generated from an unspecified base function we refer to Chap. 1 in Ref. 22. A brief description is given in the following.

In the arbitrary-order phase-integral approximation in question there appears an unspecified function $Q(z)$ called the *base function*. This function is often chosen to be equal to $R^{1/2}(z)$, but in many physical problems it is important to use the possibility of choosing $Q(z)$ differently when there exist certain exceptional points, e.g., the origin in connection with the radial Schrödinger equation, and, correspondingly, the poles of $\tilde{Q}^2(\xi)$ and $Q^2(\eta)$ at $\xi=1$ and $\eta=\pm 1$ in the two-center Coulomb problem. In the present paper we introduce in the base functions a parameter Λ, chosen such that either $\Lambda=|m|\neq 0$ or $\Lambda=0$, and two parameters C and $\tilde{C}$ to be determined such that the first- and third-order results coincide, in order that the first-order approximation be as good as possible.

To be able to write the phase-integral approximation generated from an unspecified base function in condensed form one introduces the new independent variable

$$\zeta=\int^{z} Q(z)\mathrm{d}z \tag{A2}$$

and the function

$$\varepsilon_0=Q^{-3/2}(z)\frac{\mathrm{d}^2}{\mathrm{d}z^2}Q^{-1/2}(z)+\frac{R(z)-Q^2(z)}{Q^2(z)}. \tag{A3}$$

It can be shown that in a local region of the complex z-plane, where the absolute value of ε_0 is small, the differential equation (A1) has the approximate solutions

$$\psi=q^{-1/2}(z)\exp[\pm iw(z)], \tag{A4a}$$

$$w(z)=\int_{z_0}^{z} q(z)\mathrm{d}z, \tag{A4b}$$

where the lower limit of integration z_0 is an unspecified constant, and the function $q(z)$, pertaining to the phase-integral approximation of the order $2N+1$, is given by

$$q(z)=\sum_{n=0}^{N} q^{(2n+1)}(z), \tag{A5a}$$

$$q^{(2n+1)}(z)=Q(z)Y_{2n}, \tag{A5b}$$

with the first few functions Y_{2n} given by

$$Y_0=1, \tag{A6a}$$

$$Y_2=\tfrac{1}{2}\varepsilon_0, \tag{A6b}$$

$$Y_4=-\frac{1}{8}\varepsilon_0^2-\frac{1}{8}\frac{\mathrm{d}^2\varepsilon_0}{\mathrm{d}\zeta^2}. \tag{A6c}$$

The choice of the function $Q(z)$ does not affect the expressions for Y_{2n} in terms of ε_0 and ζ; only the expressions for ε_0 and ζ as functions of z are affected.

It is an essential advantage of the phase-integral approximation described previously versus the Carlini[39] (JWKB) approximation in higher order that the former approximation contains the unspecified base function $Q(z)$, which one can take advantage of in several ways. (As regards the motivation for the terminology Carlini approximation we refer to Ref. 39.) A criterion for the determination of the base function is that the function ε_0 be in some sense small in the region of the complex z-plane that is relevant for the problem under consideration. However, this criterion does not determine the base function $Q(z)$ uniquely; it turns out that, within certain limits, the results are not very sensitive to the choice of $Q(z)$, when the approximation is used in higher orders. With a convenient choice of $Q(z)$ already the first-order approximation can be very good. On the other hand an inconvenient, but possible, choice of $Q(z)$ introduces in the first-order approximation an unnecessarily large error that, however, in general becomes corrected already in the third-order approximation.

The freedom that one has in the choice of the base function $Q(z)$ will be illuminated in a concrete way in the following. For a radial Schrödinger equation the usual choice of $Q^2(z)$ is

$$Q^2(z)=R(z)-\frac{1}{4z^2}. \tag{A7a}$$

However, the replacement of (A7a) by

$$Q^2(z)=R(z)-\frac{1}{4z^2}-\frac{\text{const}}{z}, \tag{A7b}$$

where the coefficient of $1/z$ should be comparatively small, does not destroy the great accuracy of the results usually obtained with the phase-integral approximation in higher orders. There is thus a whole set of base functions that may be used, and there are various ways in which one can take advantage of this nonuniqueness to make the choice of the base function well adapted to the particular problem under consideration. For instance, by adapting the choice of $Q^2(z)$ to the analytical form of $R(z)$ one can sometimes achieve the result that the integrals occurring in the phase-integral approximation can be evaluated analytically. To give an example we assume that $R(z)$ contains only $\exp(z)$ but not z itself. In this case it is convenient to replace the choice (A7b) by the choice

$$Q^2(z)=R(z)-\frac{1}{4(e^z-1)^2}-\frac{\text{const}}{e^z-1}. \tag{A7c}$$

By a convenient choice, for instance of the unspecified coefficient in (A7b) or (A7c), one can sometimes attain the result that, for example, eigenvalues or phase shifts are obtained exactly for some particular parameter value in every order of the phase-integral approximation. As already mentioned in Sec. I, by making this exactness fulfilled in the limit of a parameter value, for which the phase-integral result without this adaptation would not be good, one can actually extend the region of validity of the phase-integral treatment; see p. 12 in Ref. 30. When the differential equation contains one or more parameters, the accurate calculation of the wave function may require different choices of the base function $Q(z)$ for different ranges of the parameter values. To illustrate this fact we consider the radial Schrödinger equation. For sufficiently large values of the angular momentum quantum number l we obtain an accurate phase-integral approximation (valid also close to $z=0$) if we choose $Q^2(z)$ according to (A7a) or (A7b). If the value of l is too small, this phase-integral approximation is not good. It can be considerably improved (except close to $z=0$), when the absolute value of the coefficient of $1/z$ in $R(z)$ is sufficiently large, if one chooses instead

$$Q^2(z)=R(z)+\frac{l(l+1)}{z^2}. \tag{A7d}$$

The corresponding phase-integral approximation is not valid close to $z=0$, but the wave function that is regular and tends to z^{l+1} as $z\to 0$ can be obtained sufficiently far away from $z=0$ by means of the connection formula that will be presented in Sec. 2 b of this Appendix.

The appearance of the unspecified base function $Q(z)$ in the phase-integral approximation is thus very important from several points of view. In our treatment of the two-center Coulomb problem we use two essentially different kinds of base function [corresponding to $\Lambda=|m|\neq 0$ and $\Lambda=0$ in (3.2a) and (3.2b)], which yield approximate solutions with different regions of validity.

When the first-order approximation is used, it is often convenient to choose the constant lower limit of integration z_0 in (A4b) to be a zero or a first-order pole of $Q^2(z)$. This is, however, in general not possible when a higher-order approximation is used, since the integral in (A4b) would then in general be divergent. If z_0 is an odd-order zero or an odd-order pole of $Q^2(z)$, it is therefore convenient to replace the definition (A4b) of $w(z)$ by the definition

$$w(z)=\frac{1}{2}\int_{\Gamma_{z_0}(z)} q(z)\mathrm{d}z, \tag{A8}$$

where $\Gamma_{z_0}(z)$ is a path of integration that starts at the point corresponding to z on a Riemann sheet adjacent to the complex z-plane under consideration, encircles z_0 in the positive or in the negative sense, and ends at z. It is immaterial for the value of the integral in (A8) if the path of integration encircles z_0 in the positive or in the negative sense, but the end point must be z. For the first-order approximation the definitions (A4b) and (A8) are identical.

It is useful to introduce a short-hand notation for the integral in the right-hand member of (A8) by the definition

$$\int_{(z_0)}^{z} q(z)\mathrm{d}z=\frac{1}{2}\int_{\Gamma_{z_0}(z)} q(z)\mathrm{d}z. \tag{A9}$$

For the first order of the phase-integral approximation one can replace (z_0) by z_0 in the left-hand member of (A9) and thus get an ordinary integral from z_0 to z instead of half of the integral along the contour $\Gamma_{z_0}(z)$. In analogy to (A9) one defines a short-hand notation for an integral in which the upper limit of integration is an odd-order zero or an odd-order pole of $Q^2(z)$. When one has two transition points of that kind as limits of integration, one requires that the contours of integration pertaining to the lower and upper limits of integration are encircled in the same direction, and the definition of the short-hand notation with both limits within parentheses implies then that the integral is equal to half of the integral along a closed loop enclosing both transition points. The simplified notation in the left-hand member of (A9) for the integral in the right-hand member of (A9) was introduced by Fröman *et al.*,[40] pp. 160–161. It makes it possible to use, for an arbitrary order of the phase-integral approximation, a similar simple notation and almost the same simple language (although in a generalized sense) as for the first order of the phase-integral approximation. One thus achieves a great formal and practical simplification in the treatment of concrete problems, when an arbitrary order of the phase-integral approximation is used.

We remark that the above-used notations differ from the notations in the original papers published up to the beginning of the 1980s in the respect that $Q^2(z)$ and $Q^2_{\mathrm{mod}}(z)$ in those papers correspond in the present paper to $R(z)$ and $Q^2(z)$, respectively.

2. Connection formulas associated with a single transition point

a. Connection formulas pertaining to a first-order, real transition zero

Before the phase-integral approximation generated from an unspecified base function had been introduced, Fröman[41] derived arbitrary-order connection formulas associated with a turning point for the particular phase-integral approximation of arbitrary order corresponding to $Q^2(z)=R(z)$. After the phase-integral approximation generated from an unspecified base function had

been introduced, it turned out that these connection formulas remain valid also when $Q^2(z) \neq R(z)$. In the following we shall present the general connection formulas.

The functions $R(z)$ and $Q^2(z)$ are assumed to be real on the real z-axis (the x-axis). On this axis there is a generalized classical turning point t, i.e., a simple zero of $Q^2(z)$, and there is, in a generalized sense, a classically allowed region on one side of t, i.e., a region where $Q^2(x)>0$, and a classically forbidden region on the other side of t, i.e., a region where $Q^2(x)<0$. Defining

$$w(x)=\int_{(t)}^{x} q(z)\mathrm{d}z, \tag{A10}$$

we can write the connection formula for tracing a phase-integral solution of (A1) from the classically allowed to the classically forbidden region as

$$A|q^{-1/2}(x)|\exp\left\{i\left[|w(x)|+\frac{\pi}{4}\right]\right\}+B|q^{-1/2}(x)|\exp\left\{-i\left[|w(x)|+\frac{\pi}{4}\right]\right\}$$
$$\rightarrow(A+B)|q^{-1/2}(x)|\exp[|w(x)|], \tag{A11}$$

where A and B are constants, which are arbitrary except for the requirement that $(A+B)/(|A|+|B|)$ must not be too close to zero. As a consequence of (A11) we have the connection formula

$$|q^{-1/2}(x)|\cos\left[|w(x)|+\delta-\frac{\pi}{4}\right]\rightarrow\sin\delta|q^{-1/2}(x)|\exp[|w(x)|], \tag{A12}$$

where δ is a real phase constant that must not be too close to a multiple of π. The connection formula for tracing a phase-integral solution of (A1) from the classically forbidden to the classically allowed region is

$$|q^{-1/2}(x)|\exp[-|w(x)|]+C|q^{-1/2}(x)|\exp[|w(x)|]$$
$$\rightarrow 2|q^{-1/2}(x)|\cos\left[|w(x)|-\frac{\pi}{4}\right], \tag{A13}$$

and it is valid provided that the condition

$$C\exp[|w(x)|]\lesssim\exp[-|w(x)|] \tag{A14}$$

is fulfilled. For a numerical study of the accuracy and the properties of the connection formula (A13) with $C=0$ we refer to Fröman and Mrazek.[42] We emphasize the one-directional character of the connection formulas (A11)–(A13), which means that the tracing of a solution must always be made in the direction of the arrow. This property of the connection formulas has been thoroughly investigated and even illustrated numerically by Fröman[43] for the first order of the Carlini[39] (JWKB) approximation. The whole discussion in Ref. 43 applies in principle to the connection formulas for the higher orders of the phase-integral approximation as well. The above-mentioned connection formulas for the phase-integral approximation of any order may in many cases be used for obtaining very accurate solutions of physical problems, when the classical turning points are well separated, and when there are no other transition points near the real axis in the region of the complex z-plane of interest. Within their range of applicability the connection formulas are very useful because of their simplicity and the great ease with which they can be used.

b. Connection formula pertaining to a first-order transition pole

Now we assume that in a certain region of the complex z-plane around a first-order transition pole t, i.e., a first-order pole of $Q^2(z)$, we have

$$R(z)=-\frac{l(l+1)}{(z-t)^2}+\frac{B}{z-t}+\text{a regular function of } z, \tag{A15}$$

$$Q^2(z)=\frac{\overline{B}}{z-t}+\text{a regular function of } z, \tag{A16}$$

where $2l+1$ is a non-negative integer. We assume that the absolute values of B and $\overline{B}$ are sufficiently large, while the absolute value of $B-\overline{B}$ and the absolute value of the difference between the two regular functions in (A15) and (A16) are sufficiently small. There is one particular curve on which $w(z)$, defined as

$$w(z)=\int_{(t)}^{z} q(z)\mathrm{d}z, \tag{A17}$$

is real. For the first order of the phase-integral approximation this is the anti-Stokes line that emerges from t. Therefore we use, also when a higher order of the phase-integral approximation is used, the terminology an *anti-Stokes line that emerges from t* in a generalized sense to denote the anti-Stokes line on which $w(z)$, defined in (A17), is real. For the first-order approximation (and under certain unnecessarily restrictive assumptions) Fröman and Fröman[37] obtained a phase-integral formula [their Eq. (7.28)], valid sufficiently far away from t on the anti-Stokes line that emerges from t, for the particular solution $\psi(z)$ of (A1) that fulfills the condition

$$\lim_{z\to t}\frac{\psi(z)}{(z-t)^{l+1}}=1. \tag{A18}$$

This formula can be generalized to be valid for an arbitrary order of the phase-integral approximation generated from an unspecified base function and can then be formulated as follows. On the lip of the anti-Stokes line emerging from t, where $\arg w(z)$ is smallest, the solution of (A1) that fulfills the condition (A18) is, sufficiently far away from t, given by the phase-integral formula

$$\psi(z)=\left(\pi c\frac{w(z)}{|w(z)|}\right)^{-1/2} q^{-1/2}(z)\cos\left[|w(z)|-\left(l+\frac{3}{4}\right)\pi\right], \tag{A19}$$

where c is the residue of $[\psi(z)]^{-2}$ at $z=t$ and is thus determined by the expansion of $\psi(z)$ in powers of $z-t$, and the sign of

$$\left[\pi c\frac{w(z)}{|w(z)|}\right]^{-1/2}$$

has to be chosen conveniently. For the special case that $l=0$ one finds that $c=B$. Formula (A19) can easily be particularized to the case that $R(z)$ and $Q^2(z)$ are real on the real z-axis (the x-axis) and t lies on that axis.

3. Connection formula for a real, smooth, single-hump potential barrier

Our starting point is a paper by Fröman and Fröman.[44] Although it was assumed in the treatment there that $Q^2(z)=R(z)$ with the notations in the present paper, the results obtained are valid also when $Q^2(z)\neq R(z)$. In the present paper it is convenient to introduce partly other notations than in Ref. 44. Thus we now denote by t' and t'' the two relevant zeros of $Q^2(z)$, i.e., the two generalized classical turning points in the subbarrier case ($t'<t''$) and the two complex conjugate transition zeros in the superbarrier case ($\mathrm{Im}\,t'\leqslant 0, \mathrm{Im}\,t''\geqslant 0$). Let x', called x_1 in Ref. 44,

be a point in the classically allowed region of the real z-axis to the left of the barrier, and let x'', called x_2 in Ref. 44, be a point in the classically allowed region of the real z-axis to the right of the barrier. We introduce the notations

$$\theta = |F_{22}| \exp(K), \tag{A20a}$$

$$\vartheta = \arg F_{22}, \tag{A20b}$$

$$\tilde{\phi} = -2\sigma = \frac{\pi}{2} - \arg F_{12}, \tag{A20c}$$

where F_{12} and F_{22} are defined in Ref. 44, and K is defined by Eq. (12) in Ref. 44. In the definitions (A20a)–(A20c) it is assumed that the phase of $q^{1/2}(z)$ is chosen as shown in Fig. 1 in Ref. 44. We shall, however, in the following write the formulas in such a way that they remain unchanged if one changes the phase of $Q^{1/2}(z)$ and hence the phase of $q^{1/2}(z)$; see (A5a) and (A5b). The quantity K in (A20a) is then given by

$$K = \frac{1}{2} i \int_{\Lambda} q(z)\,\mathrm{d}z$$

$$= i \int_{(t')}^{(t'')} q(z)\,\mathrm{d}z, \tag{A21}$$

where Λ [not to be confused with the parameter Λ in the base function $Q(\eta)$] is a closed contour of integration encircling both t' and t'', but no other transition point, and the integration is performed in the direction that in the *first-order approximation* yields $K>0$ for energies below the top of the barrier and $K<0$ for energies above the top of the barrier. If higher-order approximations are used, the quantity K may become negative also for energies below (but not too far from) the top of the barrier; see Table I in Ref. 45. We have replaced σ, defined by Eq. (28) in Ref. 44, by $-\tilde{\phi}/2$ [cf. (A20c)] in order to get better agreement with a notation used by other authors; see for instance Child.[46] Now we define

$$B' = A_1 \exp\left(-i\frac{\pi}{4}\right), \tag{A22a}$$

$$A' = B_1 \exp\left(+i\frac{\pi}{4}\right), \tag{A22b}$$

where the notations in the right-hand members are those used in Ref. 44. Using the short-hand notation defined in (A9), we obtain from Eqs. (25a) and (9a), with x_1 replaced by x', in Ref. 44 and (A22a) and (A22b) in the present paper

$$\psi(x') = A' |q^{-1/2}(x')| \exp\left(+i\left|\mathrm{Re}\int_{(t')}^{x'} q(z)\,\mathrm{d}z\right|\right)$$

$$+ B' |q^{-1/2}(x')| \exp\left(-i\left|\mathrm{Re}\int_{(t')}^{x'} q(z)\,\mathrm{d}z\right|\right), \tag{A23a}$$

and from Eqs. (25b) and (23), with x_2 replaced by x'', in Ref. 44 and (A20a)–(A20c), (A22a), and (A22b) in the present paper

$$\psi(x'')=A''|q^{-1/2}(x'')|\exp\left(+i\left|\mathrm{Re}\int_{(t'')}^{x''}q(z)\mathrm{d}z\right|\right)$$

$$+B''|q^{-1/2}(x'')|\exp\left(-i\left|\mathrm{Re}\int_{(t'')}^{x''}q(z)\mathrm{d}z\right|\right), \tag{A23b}$$

where

$$\begin{pmatrix}A''\\B''\end{pmatrix}=\tilde{M}\begin{pmatrix}A'\\B'\end{pmatrix}, \tag{A24}$$

$$\tilde{M}=\begin{pmatrix}\theta\exp\left[-i\left(\frac{\pi}{2}+\vartheta\right)\right] & (\theta^2+1)^{1/2}\exp(+i\tilde{\phi})\\ (\theta^2+1)^{1/2}\exp(-i\tilde{\phi}) & \theta\exp\left[+i\left(\frac{\pi}{2}+\vartheta\right)\right]\end{pmatrix}, \tag{A25a}$$

$$\det\tilde{M}=-1. \tag{A25b}$$

It is seen from (A23a) and (A23b) that the coefficients A' and A'' are associated with waves traveling away from the barrier, while the coefficients B' and B'' are associated with waves incoming toward the barrier. From (A25a) and (A25b) we obtain

$$\tilde{M}^{-1}=\begin{pmatrix}\theta\exp\left[-i\left(\frac{\pi}{2}-\vartheta\right)\right] & (\theta^2+1)^{1/2}\exp(+i\tilde{\phi})\\ (\theta^2+1)^{1/2}\exp(-i\tilde{\phi}) & \theta\exp\left[+i\left(\frac{\pi}{2}-\vartheta\right)\right]\end{pmatrix}. \tag{A26}$$

One thus obtains $\tilde{M}^{-1}$ from $\tilde{M}$ by replacing ϑ by $-\vartheta$. We emphasize that the above-mentioned formulas are in principle exact, provided that one knows the quantities θ, ϑ, and $\tilde{\phi}$, which depend slightly on x' and x''. Furthermore, the two transition zeros associated with the potential barrier need not lie far away from other possibly existing transition points; see Ref. 44. However, when one introduces for θ, ϑ, and $\tilde{\phi}$ the approximate values that will be given in the following, the barrier is assumed to be well separated (in the sense just described) from all transition points that are not associated with the barrier.

When A' and B' are given constants, associated with a wave function that is given at the point x', the coefficients A'' and B'', which are obtained from (A24) along with (A25a), depend slightly on x' and x'' via the quantities θ, ϑ, and $\tilde{\phi}$. One obtains the derivatives of $\psi(x')$ and $\psi(x'')$ from (A23a) and (A23b) by considering A',B',A'' and B'' *formally* as constants.

When the transition points that are *not* associated with the barrier lie sufficiently far away from t' and t'', it follows from Eq. (43a) in Ref. 44 and (A20a) and (A20b) that

$$\theta\approx\exp(K), \tag{A27a}$$

$$\vartheta\approx 0. \tag{A27b}$$

The quantity $\tilde{\phi}$ is particularly important when the energy is close to the top of the barrier, but it is important also for energies well below the top, if one with the use of higher orders of the phase-integral approximation wants to obtain very accurate results. In practice one cannot obtain useful expressions for $\tilde{\phi}$ from the exact formula (A20c). Under the assumption that $d^2R(z)/dz^2$ is not too close to zero at the top of the barrier, Fröman *et al.*[47] derived by means of comparision equation technique, adapted to yield formulas for supplementary quantities in the phase-integral

method, an approximate, but very accurate, formula in the $(2N+1)$th order of the phase-integral approximation [their eqs. (5.5.30), (5.5.25a)–(5.5.25g), (5.4.23), and (5.4.21)], from which we can obtain the formula

$$\tilde{\phi}=\arg\Gamma\left(\frac{1}{2}+i\overline{K}\right)-\overline{K}\ln|\overline{K}_0|+\sum_{n=0}^{N}\phi^{(2n+1)}, \tag{A28}$$

where

$$\phi^{(1)}=\overline{K}_0, \tag{A29a}$$

$$\phi^{(3)}=-\frac{1}{24\overline{K}_0}, \tag{A29b}$$

$$\phi^{(5)}=-\frac{7}{2880\overline{K}_0^3}+\frac{\overline{K}_2}{24\overline{K}_0^2}-\frac{\overline{K}_2^2}{2\overline{K}_0}, \tag{A29c}$$

with

$$\overline{K}_{2n}=\frac{1}{2\pi i}\int_{\Lambda}Y_{2n}Q(z)\mathrm{d}z, \quad n=0,1,2,\ldots,N, \tag{A30a}$$

$$\overline{K}=\sum_{n=0}^{N}\overline{K}_{2n}=\frac{K}{\pi}, \tag{A30b}$$

Λ being the previously described contour of integration encircling t' and t'' but no other transition point, with the integration performed in the direction that makes $\overline{K}_0$ positive when t' and t'' are real, i.e., when the barrier is superdense, but negative when t' and t'' are complex conjugate, i.e., when the barrier is underdense. [Note that we perform the integrations in (A21) and (A30a) in opposite directions in order to make these formulas agree with Eq. (12) in Ref. 44 and Eq. (5.4.21) in Ref. 47, respectively.] The result given by (A28), (A29a)–(A29c), and (A30a) and (A30b) can also be obtained from Ref. 38, where -2σ is the same as our $\tilde{\phi}$.

We emphasize again that for the validity of (A28) with the expressions (A29a)–(A29c) for $\phi^{(2n+1)}$ the essential restriction is that $|d^2R(z)/dz^2|$ must not be too small at the top of the barrier, which means that close to its top the barrier is approximately parabolic. However, when the energy is close to the top of the barrier, it is the slight deviation from parabolic shape close to the top of the barrier that determines the values of the quantities $\overline{K}_{2n}, n>0$, and one needs accurate values of these quantities for obtaining accurate values of $\tilde{\phi}$ in higher orders of the phase-integral approximation.

The barrier connection formula presented in this section is valid uniformly for all energies, below and above the top of the barrier. We would also like to emphasize that while the connection formulas pertaining to an isolated turning point (Fröman[41]) are one-directional, the barrier connection formula (A23a) and (A23b) with (A24) and (A25a), which is valid when the barrier is well isolated and has an approximately parabolic top, is bidirectional. However, the neighborhood of an energy that corresponds to a resonance requires a careful discussion.

4. Quantization conditions for single-well and double-well potentials

In this section we shall present quantization conditions for general single-well potentials[48–50] and double-well potentials,[38,50–52] valid for any conveniently chosen order of the phase-integral approximation, in forms especially adapted to the two-center Coulomb problem. In the quantiza-

tion conditions pertaining to the double-well potential there appears the supplementary quantity $\tilde{\phi}$, which was discussed in Sec. 3 of this Appendix, and which is of particular importance for energy eigenvalues in the neighborhood of the top of the barrier; cf. numerical results in Ref. 38, where Q^2, Q^2_{mod}, and σ correspond to R, Q^2, and $-\tilde{\phi}/2$, respectively, in the present paper. Comparision with numerical results[38] shows that all energy eigenvalues, also the low-lying ones and those in the neighborhood of the top of the barrier, are obtained very accurately from the phase-integral quantization conditions when the third- or fifth-order approximation is used.

Since arbitrary-order phase-integral quantization conditions for the single-well and for the double-well potential problems have been given in previous works, we restrict ourselves to quoting those results and taking into account the fact that we are dealing with the special potentials pertaining to the two-center Coulomb problem.

a. Quantization conditions for single-well potentials

We assume that $R(z)$ and $Q^2(z)$ are real on the real z-axis (the x-axis) and that there are two transition points t' and t'' $(>t')$ on this axis, each one of which may be either a first-order transition zero, i.e., a first-order zero of $Q^2(z)$, or a first-order transition pole, i.e., a first-order pole of $Q^2(z)$. These transition points are assumed to lie far away from all other transition points. On the real axis between t' and t'' it is assumed that $Q^2(x)$ is positive. With the aid of the connection formulas in Sec. 2 of this Appendix we can derive the quantization conditions that will be presented in the following.

When both t' and t'' are first-order transition zeros, we obtain the quantization condition[48,49]

$$\left| \int_{(t')}^{(t'')} q(z)\mathrm{d}z \right| = \left(s+\frac{1}{2} \right)\pi, \quad s=0,1,2,\ldots. \tag{A31}$$

When one of the transition points t' and t'' is a first-order transition zero, and the other is a first-order transition pole in the neighborhood of which $R(z)$ and $Q^2(z)$ can be expanded according to (A15) and (A16) with $l=(|m|-1)/2$, i.e., $l(l+1)=(m^2-1)/4$, we obtain under the assumptions introduced below those expansions the quantization condition[49]

$$\left| \int_{(t')}^{(t'')} q(z)\mathrm{d}z \right| = \left(\frac{|m|}{2}+s+\frac{1}{2} \right)\pi, \tag{A32}$$

where m is an integer (positive, negative or zero), and s is also an integer.

When both transition points t' and t'' are first-order transition poles, in the neighborhood of which $R(z)$ and $Q^2(z)$ can be expanded according to (A15) and (A16) with $l=(|m|-1)/2$, i.e., $l(l+1)=(m^2-1)/4$ for both transition poles but possibly with different coefficients B and $\overline{B}$ for the two transition poles, we obtain under the assumptions introduced below (A15) and (A16) the quantization condition[30]

$$\left| \int_{(t')}^{(t'')} q(z)\mathrm{d}z \right| = \left(|m|+s+\frac{1}{2} \right)\pi, \tag{A33}$$

where m is an integer (positive, negative, or zero), and s is also an integer.

b. Quantization conditions for double-well potentials

We assume that $R(z)$ and $Q^2(z)$ are real on the real z-axis (the x-axis) and that there are either two generalized classical turning points t' and t'' $(>t')$ [real, simple zeros of $Q^2(z)$] associated with a superdense potential barrier or two complex conjugate simple transition zeros t' and t'' [simple zeros of $Q^2(z)$; $\mathrm{Im}\,t'<0$, $\mathrm{Im}\,t''>0$] associated with an underdense potential barrier. The classically allowed region to the left of the barrier is to the left delimited by a transition point t_- (on the real axis), and the classically allowed region to the right of the barrier is to the right

delimited by a transition point t_+ (on the real axis), where t_- and t_+ are both either generalized classical turning points, i.e., simple zeros of $Q^2(z)$, or first-order transition poles, i.e., first-order poles of $Q^2(z)$. The points t_- and t_+, as well as other possibly existing transition points that are not associated with the barrier, are assumed to lie far away from t' and t''. When t_- and t_+ are simple transition poles we assume that in the neighborhood of $t_\pm$ we have

$$R(z)=\frac{(1-m^2)}{4(z-t_\pm)^2}+\frac{B_\pm}{z-t_\pm}+\text{a regular function of } z, \tag{A34}$$

$$Q^2(z)=\frac{\overline{B}_\pm}{z-t_\pm}+\text{a regular function of } z, \tag{A35}$$

where m is an integer (positive, negative, or zero), $B_\pm$ and $\overline{B}_\pm$ are sufficiently large to their absolute values, while the absolute values of $B_\pm-\overline{B}_\pm$, as well as the difference between the regular functions in (A34) and (A35), is not too large. Under the above-mentioned assumptions we obtain with the aid of connection formulas in Secs. 2 and 3 in this Appendix the quantization condition

$$\tan\left(\left|\operatorname{Re}\int_{(t_-)}^{(t')}q(z)\mathrm{d}z\right|+\frac{\tilde{\phi}}{2}-a\right)\tan\left(\left|\operatorname{Re}\int_{(t_+)}^{(t'')}q(z)\mathrm{d}z\right|+\frac{\tilde{\phi}}{2}-a\right)$$
$$=\frac{[1+\exp(-2K)]^{1/2}-1}{[1+\exp(-2K)]^{1/2}+1}, \tag{A36}$$

where

$$K=\frac{1}{2i}\int_\Lambda q(z)\mathrm{d}z, \tag{A37}$$

Λ being a closed contour, enclosing t' and t'', along which the integration is performed in the direction that makes the first-order contribution to K positive when the barrier is superdense but negative when the barrier is underdense, and

$$a=\begin{cases}\dfrac{\pi}{2} & \text{when } t_- \text{ and } t_+ \text{ are transition zeros}\\[2ex] (|m|+1)\dfrac{\pi}{2} & \text{when } t_- \text{ and } t_+ \text{ are transition poles.}\end{cases} \tag{A38}$$

The quantization condition (A36) can be rewritten into the form

$$\cos\left(\left|\operatorname{Re}\int_{(t_-)}^{(t')}q(z)\mathrm{d}z\right|+\left|\operatorname{Re}\int_{(t_+)}^{(t'')}q(z)\mathrm{d}z\right|+\tilde{\phi}-2a\right)$$
$$=\frac{\cos(|\operatorname{Re}\int_{(t_-)}^{(t')}q(z)\mathrm{d}z|-|\operatorname{Re}\int_{(t_+)}^{(t'')}q(z)\mathrm{d}z|)}{[1+\exp(-2K)]^{1/2}}. \tag{A39}$$

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Quantal two-center Coulomb problem treated by means of the phase-integral method. II. Quantization conditions in the symmetric case expressed in terms of complete elliptic integrals. Numerical illustration

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The contour integrals, occurring in the arbitrary-order phase-integral quantization conditions given in a previous paper, are in the first- and third-order approximations expressed in terms of complete elliptic integrals in the case that the charges of the Coulomb centers are equal. The evaluation of the integrals is facilitated by the knowledge of quasiclassical dynamics. The resulting quantization conditions involving complete elliptic integrals are solved numerically to obtain the energy eigenvalues and the separation constants of the $1s\sigma$ and $2p\sigma$ states of the hydrogen molecule ion for various values of the internuclear distance. The accuracy of the formulas obtained is illustrated by comparison with available numerically exact results. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1399295]

I. INTRODUCTION

In a previous paper[1] the general two-center Coulomb problem was treated according to the phase-integral method, briefly described in the appendix of that paper, and arbitrary-order quantization conditions were given, valid uniformly for all energies.

The symmetric case, where the charge numbers Z_1 and Z_2 of the two Coulomb centers are equal, represents for $Z_1=Z_2=1$ the hydrogen molecule ion H_2^+. This case has for natural reasons been studied more extensively than the general two-center problem. Thus, the H_2^+ ion was already the subject of treatments with the aid of the old quantum theory[2] and in the early days of quantum mechanics.[3,4] The simplicity of the hydrogen molecule ion grants it an analogous unique position in molecular physics as the hydrogen atom possesses in atomic physics. For instance, H_2^+ plays a role of fundamental significance in the theory of chemical bonding, and it is also of importance in the study of stellar atmospheres.

For the background of the present paper we refer to Ref. 1. In Sec. II of the present paper we present the quasiclassical dynamics of the associated particle system by setting up the equation of motion for a particle moving in the relevant potential and express the solution in terms of Jacobian elliptic functions. In Secs. III and IV we express the quantization conditions given in Ref. 1 in terms of complete elliptic integrals by using the solution in Sec. II. We introduce, analogously to Lakshmanan and Kaliappan,[5] Lakshmanan *et al.*,[6] and Lakshmanan *et al.*,[7] convenient transformations to elliptic functions, in order to be able to express both the real and the complex contour integrals, occurring in the quantization conditions, in terms of complete elliptic integrals. In choosing our transformations we exploit the symmetry of the functions $R(\eta)$ and $Q^2(\eta)$, introduced in Ref. 1, from the beginning of the calculations, since this is much simpler than to

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particularize formulas for the general case of arbitrary nuclear charge numbers Z_1 and Z_2 to the case $Z_1=Z_2$. Thus we obtain simple expressions for the quantities appearing in the quantization conditions in Ref. 1. It should be remarked that if one particularizes the η-quantization conditions involving complete elliptic integrals that are valid for arbitrary charge numbers Z_1 and Z_2 (to be derived in the subsequent paper[8]) to the case $Z_1=Z_2$, one must in general make further cumbersome transformations in order to bring the quantization conditions in question into the same form as those obtained by assuming from the begining that $Z_1=Z_2$. The functions $\tilde{R}(\xi)$ and $\tilde{Q}^2(\xi)$, introduced in Ref. 1, do not display an analogous symmetry as $R(\eta)$ and $Q^2(\eta)$ when $Z_1=Z_2$. The treatment of the ξ-equation is thus the same whether $Z_1=Z_2$ or $Z_1\neq Z_2$, and it is analogous to the treatment of the η-equation in the general case when Z_1 may be different from Z_2, which is treated in the third paper[8] in our series of papers concerning the phase-integral treatment of the quantal two-center Coulomb problem. All the contour integrals needed in the calculations are expressed in terms of complete elliptic integrals, corresponding to the use of the first- and third-order phase-integral approximations. Since complete elliptic integrals can easily be evaluated by means of standard computer programs, computational difficulties that may arise in direct numerical calculations (especially of higher-order terms) are thereby eliminated. One achieves also the possibility of being able to utilize well-known properties of complete elliptic integrals, for instance series expansions, for analytic studies on the basis of the quantization conditions. Some of the first-order contour integrals have previously been given in terms of complete elliptic integrals by Strand and Reinhardt,[9] but to the best knowledge of the present authors, even in the first-order approximation only partial results have been given.

The phase-integral formulas derived in this paper are quite flexible due to the presence of two arbitrary parameters C and $\tilde{C}$ introduced in the base functions $Q(\eta)$ and $\tilde{Q}(\xi)$ in Eqs. (3.2b) and (3.2a), respectively, in Ref. 1. In accordance with the discussion in Sec. III A of Ref. 1 we choose C and $\tilde{C}$ such that the first-order results are exactly equal to the third-order results, and we investigate in Sec. V of the present paper the accuracy of our phase-integral quantization conditions for the $1s\sigma$ and $2p\sigma$ states of the hydrogen molecule ion.

II. QUASICLASSICAL DYNAMICS

We have seen in Sec. III of Ref. 1 that the quantization conditions require the evaluation of various contour integrals. In the present section we shall restrict ourselves to the η-equation. The shape of the contours depends on the choice of Λ and on the real or complex nature of the zeros of $Q^2(\eta)$; see Figs. 2–4 in Ref. 1.

Letting, when $-Q^2(\eta)$ is a double-well potential, the zeros of $Q^2(\eta)$ be $\eta_1,\eta_2,\eta_3,\eta_4$ when $\Lambda=|m|\neq 0$ and η_2,η_3 when $\Lambda=0$, we shall evaluate the integrals $\alpha=\beta$ and $\overline{K}$ in the following cases separately.

(1) $\Lambda=|m|\neq 0$:
   (a) Subbarrier case (superdense) ($\eta_1=-\eta_4$ and $\eta_2=-\eta_3$ are real).
   (b) Superbarrier (under-dense) case (η_1,η_4 are real and η_2,η_3 are complex conjugate).

(2) $\Lambda=0$:
   (a) Subbarrier (superdense) case (only two zeros, $\eta_2=-\eta_3$; they are real).
   (b) Superbarrier (under-dense) case (only two zeros, η_2 and η_3; they are complex conjugate).

In each one of these cases the evaluation of the contour integrals in terms of complete elliptic integrals is facilitated by the knowledge of the associated quasiclassical dynamics. In particular the relevant substitution for the integration variable in the various contour integrals can be obtained with the help of, for example, Byrd and Friedman.[10] However, the meaning of these substitutions can be attributed to the associated solution of the equation of motion of the corresponding classical problem as in the case of three-dimensional anharmonic oscillators.[7]

To illustrate what has been said previously, we shall consider the subbarrier case of $\Lambda=|m|$

$\neq 0$. (For the other cases the analysis can be carried out in a similar way.) The base function $Q(\eta)$ for this case is

$$Q(\eta)=p\frac{[(a^2-\eta^2)(\eta^2-b^2)]^{1/2}}{1-\eta^2}, \tag{2.1}$$

where $a=\eta_4=-\eta_1$, $b=\eta_3=-\eta_2$, and $p^2=-(1/2)Er_{12}^2$. Let us define a new integration variable $\bar{u}$ by writing

$$\bar{u}=\int^{\eta}\frac{d\eta}{(1-\eta^2)Q(\eta)}; \tag{2.2}$$

then

$$\frac{d\eta}{d\bar{u}}=(1-\eta^2)Q(\eta)=\hat{Q}(\eta). \tag{2.3}$$

Before solving (2.3), we shall relate this differential equation to the equation of motion for the quasiclassical motion of a particle with a mass μ in a certain potential by differentiating (2.3) with respect to $\bar{u}$, getting

$$\frac{d^2\eta}{d\bar{u}^2}=\frac{1}{2}\frac{d\hat{Q}^2}{d\eta}. \tag{2.4}$$

Defining now the ''time'' variable u as

$$u=\bar{u}\sqrt{\mu}, \tag{2.5}$$

we obtain the equation of quasiclassical motion

$$\mu\frac{d^2\eta}{du^2}=-\frac{dU(\eta)}{d\eta}, \tag{2.6a}$$

$$U(\eta)=-\tfrac{1}{2}\hat{Q}^2(\eta). \tag{2.6b}$$

We can consider (2.6a) as representing the motion of a particle in the potential $U(\eta)$. We shall now solve the differential equation (2.3) in terms of Jacobian elliptic functions when $Q(\eta)$ is given by (2.1). The potential $U(\eta)$ is then given by

$$\begin{aligned}U(\eta)&=-\tfrac{1}{2}\hat{Q}^2(\eta)\\&=-\tfrac{1}{2}(1-\eta^2)^2Q^2(\eta)\\&=-\tfrac{1}{2}p^2(a^2-\eta^2)(\eta^2-b^2),\end{aligned} \tag{2.7}$$

and according to (2.3) and (2.1)

$$\frac{d\eta}{d\bar{u}}=p\sqrt{(a^2-\eta^2)(\eta^2-b^2)}. \tag{2.8}$$

By solving (2.8) with respect to η we obtain

$$\eta(\bar{u})=\frac{b}{\mathrm{dn}\left[\dfrac{p}{a}(\bar{u}-\bar{u}_0)\right]}, \tag{2.9}$$

where $\overline{u_0}$ is an integration constant, and the modulus k of the Jacobian elliptic function is given by

$$k^2=1-\frac{b^2}{a^2}. \tag{2.10}$$

Similarly we can for all other cases interpret the corresponding quasiclassical dynamics by the above-mentioned type of treatment.

III. CASE $\Lambda=|m|\neq 0$

In order to express the contour integrals, occurring in the quantization conditions pertaining to the ξ-equation and the η-equation, in terms of complete elliptic integrals, we transform the integrals in question from the ξ- or η-plane to another complex plane, the u-plane, on which the Jacobian elliptic functions $\mathrm{cn}\,u$, $\mathrm{sn}\,u$, and $\mathrm{dn}\,u$ are defined. We make frequent use of formulas in Ref. 10. As mentioned previously the transformation in question can be attributed to quasiclassical dynamics.

A. Four real zeros of $Q^2(\eta)$ and $\tilde{Q}^2(\xi)$

1. The quantities $\alpha=\beta$ and $\bar{K}$ pertaining to the η-equation: Subbarrier case [Fig. 3(a) in Ref. 1]

Putting $\eta_4=-\eta_1=a$ and $\eta_3=-\eta_2=b$, we have the base function (2.1), that is,

$$Q(\eta)=p\frac{[(a^2-\eta^2)(\eta^2-b^2)]^{1/2}}{1-\eta^2}. \tag{3.1}$$

Using the appropriate transformation on p. 54 in Ref. 10, or equivalently the quasiclassical solution given in Sec. II, we put

$$\eta=\frac{b}{\mathrm{dn}\,u}=\frac{b}{(1-k^2\mathrm{sn}^2\,u)^{1/2}},\quad k^2=1-\frac{b^2}{a^2}. \tag{3.2}$$

Noting that the loop $\eta_2\rightarrow\eta_1\rightarrow\eta_2$, that is $-b\rightarrow-a\rightarrow-b$, in the η-plane, denoted by $\Gamma_{-b,-a}$, represents the contour Λ_α in Fig. 3(a) of Ref. 1 which corresponds in the u plane to $0\rightarrow K\rightarrow 2K$, where K is the complete elliptic integral of the first kind, we obtain for the first-order contribution to α the following transformation of the original integral in the η-plane into an integral in the u-plane:

$$\begin{aligned}\alpha^{(1)}=\frac{1}{2}\int_{\Lambda_\alpha}Q(\eta)\mathrm{d}\eta&=\frac{1}{2}\int_{\Gamma_{-b,-a}}Q(\eta)\mathrm{d}\eta\\&=\frac{p}{g}\frac{1}{2}\int_0^{2K}\left(\frac{\mathrm{d}\eta}{\mathrm{d}u}\right)^2\frac{\mathrm{d}u}{1-\eta^2}\\&=p\frac{k^4b^2}{1-b^2}\frac{1}{2}\int_0^{2K}\frac{\mathrm{sn}^2\,u(1-\mathrm{sn}^2\,u)}{(1-k^2\,\mathrm{sn}^2\,u)(1-\nu^2\,\mathrm{sn}^2\,u)}\mathrm{d}u,\end{aligned} \tag{3.3}$$

which, after decomposition of the integrand into partial fractions and use of recurrence formulas in Ref. 10, yields

$$\alpha^{(1)}=\frac{p}{g}\left[E(k)-\left(1-\frac{k^2}{\nu^2}\right)K(k)+k^2\left(1-\frac{1}{\nu^2}\right)\Pi(\nu^2,k)\right], \tag{3.4a}$$

where

$$\nu^2=\frac{a^2-b^2}{a^2(1-b^2)}=\frac{k^2}{1-b^2},\quad g=\frac{1}{a},\quad k^2=\frac{a^2-b^2}{a^2}. \tag{3.5}$$

Here $K(k)$, $E(k)$, and $\Pi(\nu^2,k)$ are complete elliptic integrals of first, second, and third kind, respectively. Similarly we obtain for the third-order contribution to α [see Eqs. (3.13b), (A5b), (A6b), (A3), (2.9b), and (3.2b) of Ref. 1],

$$\begin{aligned}\alpha^{(3)}&=\frac{1}{2}\int_{\Lambda_\alpha} q^{(3)}(\eta)d\eta\\&=\frac{1}{2}\int_{\Lambda_\alpha}\left[\left(-C+\frac{1}{1-\eta^2}\right)\frac{1}{2Q(1-\eta^2)}-\frac{1}{8}Q^{-3}(\eta)\left(\frac{dQ(\eta)}{d\eta}\right)^2\right]d\eta,\end{aligned} \tag{3.6}$$

where C is the parameter introduced in the base function $Q(\eta)$ in Eq. (3.2b) of Ref. 1. After evaluation of the integrals we obtain

$$\begin{aligned}\alpha^{(3)}=&-\frac{gC}{2p}K(k)+\frac{g}{2p(1-b^2)\nu^2}[k^2K(k)+(\nu^2-k^2)\Pi(\nu^2,k)]\\&-\frac{g(1-b^2)}{8pb^2k^4}[P_1K(k)+P_2E(k)+P_3\Pi(\nu^2,k)],\end{aligned} \tag{3.4b}$$

where

$$P_1=\tfrac{1}{3}[-9k^4+k^2(8+5\nu^2)+4\nu^2-8], \tag{3.7a}$$

$$P_2=\tfrac{1}{3}[k^2(-4-\nu^2)+(8-4\nu^2)] \tag{3.7b}$$

and

$$P_3=4(\nu^2-k^2)^2. \tag{3.7c}$$

Analogous calculations can be performed to evaluate the quantity $\overline{K}$. For this purpose we make use of the appropriate transformation on p. 58 in Ref. 10, that is

$$\eta^2=b^2\,\mathrm{sn}^2\,u. \tag{3.8}$$

The first-order [see Eqs. (3.15b), (A5b), (A6a), and (3.2b) of Ref. 1] and the third-order [see Eqs. (3.15b), (A5b), (A6b), (A3), (2.9b), and (3.2b) of Ref. 1] contributions to $K(=\pi\overline{K})$ are

$$\begin{aligned}\pi\overline{K}_0&=\frac{i}{2}\int_{\Lambda_K}Q(\eta)d\eta\\&=\frac{p\nu^2}{g}\int_0^{2K}\frac{\mathrm{cn}^2\,u\,\mathrm{dn}^2\,u}{1-\nu^2\,\mathrm{sn}^2\,u}du\\&=\frac{p}{g}\left[E(k)+k^2\left(1-\frac{1}{\nu^2}\right)K(k)+(\nu^2-k^2)\left(1-\frac{1}{\nu^2}\right)\Pi(\nu^2,k)\right],\end{aligned} \tag{3.9a}$$

and

$$\pi\overline{K}_2=\frac{i}{2}\int_{\Lambda_K}q^{(3)}(\eta)\mathrm{d}\eta=\frac{i}{2}\int_{\Lambda_K}\left[\left(-C+\frac{1}{1-\eta^2}\right)\frac{1}{2Q(1-\eta^2)}-\frac{1}{8}Q^{-3}(\eta)\left(\frac{\mathrm{d}Q(\eta)}{\mathrm{d}\eta}\right)^2\right]\mathrm{d}\eta$$

$$=\frac{Cg}{p}K(k)-\frac{g}{p}\Pi(\nu^2,k)+\frac{g}{4b^2p}\left[\frac{1}{3k'^6}(-3\nu^2k^6-k^4+8\nu^2k^2-7\nu^2+1)E(k)\right.$$

$$\left.+\frac{3\nu^2-1}{3k'^2}K(k)+4\nu^2\Pi(\nu^2,k)\right], \tag{3.9b}$$

where

$$\nu^2=b^2,\quad g=\frac{1}{a},\quad k^2=\frac{b^2}{a^2},\quad k'^2=1-k^2=\frac{a^2-b^2}{a^2}. \tag{3.10}$$

The integrals α' and β' for the contours $\Lambda_{\alpha'}$ and $\Lambda_{\beta'}$ in Fig. 3(a) in Ref. 1 are obtained from the formulas $\alpha'=\alpha+\Lambda\pi/2$ and $\beta'=\beta+\Lambda\pi/2$, see Eq. (3.18a) in Ref. 1.

2. The quantities $\tilde{L}$ and $\tilde{L}'$ pertaining to the ξ-equation [Fig. 1(a) in Ref. 1]

Denoting the four real zeros $\xi_1<\xi_2<1<\xi_3<\xi_4$ of $\tilde{Q}^2(\xi)$ by the simpler notations $d<c<1<b<a$, respectively, used in Ref. 10, we have

$$\tilde{Q}(\xi)=p\frac{[(a-\xi)(\xi-b)(\xi-c)(\xi-d)]^{1/2}}{\xi^2-1}. \tag{3.11}$$

Using the appropriate transformation on p. 120 in Ref. 10, we obtain (cf. Sec. II)

$$\xi=\frac{b-c\nu_1^2\,\mathrm{sn}^2u}{1-\nu_1^2\,\mathrm{sn}^2u},\quad \nu_1^2=\frac{a-b}{a-c}<1. \tag{3.12}$$

Noting that the loop $\xi_3\to\xi_4\to\xi_3$, that is $b\to a\to b$, in the ξ-plane, denoted by $\Gamma_{b,a}$, represents the contour $\Lambda_{\tilde{L}}$ in Fig. 1(a) of Ref. 1 and corresponds to $0\to K\to 2K$ in the u-plane, and using the transformation (3.12), we obtain the first-order contribution to $\tilde{L}$ through the following transformation of the original integral in the ξ-plane to the u-plane:

$$\tilde{L}^{(1)}=\frac{1}{2}\int_{\Lambda_{\tilde{L}}}\tilde{Q}(\xi)\mathrm{d}\xi$$

$$=\frac{1}{2}\int_{\Gamma_{b,a}}\tilde{Q}(\xi)\mathrm{d}\xi$$

$$=\frac{p}{2g}\int_0^{2K}\left(\frac{\mathrm{d}\xi}{\mathrm{d}u}\right)^2\frac{\mathrm{d}u}{\xi^2-1}$$

$$=\frac{2p(\nu_2^2-\nu_1^2)(\nu_3^2-\nu_1^2)}{g}\int_0^{2K}\frac{\mathrm{sn}^2u(1-\mathrm{sn}^2u)(1-k^2\,\mathrm{sn}^2u)}{(1-\nu_1^2\,\mathrm{sn}^2u)^2(1-\nu_2^2\,\mathrm{sn}^2u)(1-\nu_3^2\,\mathrm{sn}^2u)}\mathrm{d}u, \tag{3.13}$$

where

$$\nu_1^2=\frac{a-b}{a-c},\quad \nu_2^2=\frac{1+c}{1+b}\nu_1^2,\quad \nu_3^2=\frac{1-c}{1-b}\nu_1^2, \tag{3.14}$$

$$g=\frac{2}{[(a-c)(b-d)]^{1/2}},\quad k^2=\frac{(a-b)(c-d)}{(a-c)(b-d)}. \tag{3.15}$$

Note that a, b, c, d, and hence also ν_1, ν_2, ν_3, g, k, depend on the choice of the parameter $\tilde{C}$ in the base function $\tilde{Q}(\xi)$; cf. Eq. (3.2a) in Ref. 1. Decomposing the integrand in (3.13) into partial fractions, and using recurrence formulas in Ref. 10, we obtain the final formula

$$\tilde{L}^{(1)} = -H^{(1)}(\nu_1,\nu_2,\nu_3,g,k,\tilde{C}) \tag{3.16a}$$

$$= \frac{2p}{g}\left[\left(1-2k^2+\frac{3k^2}{\nu_1^2}\right)K(k)-3E(k)\right.$$
$$\left.+\left(2(1+k^2)-\nu_1^2-\frac{3k^2}{\nu_1^2}\right)\Pi(\nu_1^2,k)-\sum_{i=1}^{3} C_i S_i\right], \tag{3.16b}$$

where we have introduced the "universal" function $H^{(1)}$, and

$$C_1 = \frac{2[2\nu_2^2\nu_3^2-\nu_1^2\nu_2^2-\nu_1^2\nu_3^2]}{(\nu_2^2-\nu_1^2)(\nu_1^2-\nu_3^2)}, \tag{3.17a}$$

$$C_2 = \frac{2\nu_2^2(\nu_3^2-\nu_1^2)}{(\nu_2^2-\nu_1^2)(\nu_3^2-\nu_2^2)}, \tag{3.17b}$$

$$C_3 = \frac{2\nu_3^2(\nu_2^2-\nu_1^2)}{(\nu_3^2-\nu_1^2)(\nu_2^2-\nu_3^2)}, \tag{3.17c}$$

$$S_i = \frac{1}{3k^2}\left[(\nu_i^2+2\nu_i^2k^2-3k^2)K(k)-(\nu_i^2+\nu_i^2k^2-3k^2)E(k)\right.$$
$$\left.+\frac{3k^2}{\nu_i^2}(1-\nu_i^2)(k^2-\nu_i^2)[\Pi(\nu_i^2,k)-K(k)]\right], \quad i=1,2,3, \tag{3.18}$$

which can also be written as

$$S_i = \frac{k'^2}{3}\left[\nu_i^2\frac{K(k)-E(k)}{k^2}+\frac{(3-2\nu_i^2)E(k)}{k'^2}-3\Pi\left(\frac{k^2-\nu_i^2}{1-\nu_i^2},k\right)\right], \quad i=1,2,3, \tag{3.18$'$}$$

the last formula being valid if ν_i^2 and k^2 fulfill the conditions stated in Sec. 117.03 in Ref. 10.

Similarly we get for the third-order contribution to $\tilde{L}$:

$$\tilde{L}^{(3)} = \frac{1}{2}\int_{\Lambda_{\tilde{L}}}\left[\left(\tilde{C}+\frac{1}{\xi^2-1}\right)\frac{1}{2\tilde{Q}(\xi)(\xi^2-1)}-\frac{1}{8}\tilde{Q}^{-3}(\xi)\left(\frac{d\tilde{Q}}{d\xi}\right)^2\right]d\xi,$$

that is

$$\tilde{L}^{(3)} = -H^{(3)}(\nu_1,\nu_2,\nu_3,g,k,\tilde{C}) \tag{3.16c}$$

$$= -\frac{g}{64p(\nu_2^2-\nu_1^2)(\nu_3^2-\nu_1^2)}\left[\sum_{i=1}^{4} C_i' K(k) + \sum_{i=1}^{4} D_i E(k)\right]$$
$$-\frac{g}{4p}\left[\tilde{C} + \frac{\nu_1^2(\nu_2^2-\nu_3^2)}{4\nu_2^2(\nu_1^2-\nu_3^2)} + \frac{\nu_1^2(\nu_2^2-\nu_3^2)}{4\nu_3^2(\nu_2^2-\nu_1^2)}\right]K(k), \tag{3.16d}$$

where $H^{(3)}$ is another "universal" function, $\tilde{C}$ is the parameter in the base function $\tilde{Q}(\xi)$ [cf. Eq. (3.2a) in Ref. 1], and

$$C_1' = \frac{4}{3k'^2}[k^4+2k^2-2+(2\nu_1^2+\nu_2^2+\nu_3^2)(1-2k^2)+\{2\nu_1^2(\nu_2^2+\nu_3^2)+\nu_2^2\nu_3^2+\nu_1^4\}(4-3k^2)]$$
$$+\frac{4}{3k'^2}\left[-\{2\nu_1^2\nu_2^2\nu_3^2+\nu_1^4(\nu_2^2+\nu_3^2)\}\frac{11-10k^2}{k^2}+\frac{\nu_1^4\nu_2^2\nu_3^2}{k^4}(14-6k^2-7k^4)\right], \tag{3.19a}$$

$$C_2' = \frac{4}{\nu_2^2\nu_3^2}\left[2\nu_2^4\nu_3^4+\nu_1^4\nu_2^4+\nu_1^4\nu_3^4-2\nu_1^4\nu_2^2\nu_3^2-\frac{2\nu_1^2\nu_2^4\nu_3^4}{k^2}\left(2-\frac{\nu_1^2}{3}\right)+\frac{4\nu_1^4\nu_2^4\nu_3^4}{3k^4}\right], \tag{3.19b}$$

$$C_3' = \frac{8\nu_2^2\nu_3^2}{3k^4}(3k^4-6\nu_1^2k^2+2\nu_1^4+k^2\nu_1^4), \tag{3.19c}$$

$$C_4' = 16\left[-(\nu_1^2\nu_2^2+\nu_2^2\nu_3^2+\nu_3^2\nu_1^2)-\frac{\nu_1^4\nu_2^2\nu_3^2}{k^4}(2+k^2)+\frac{\nu_1^2}{k^2}(\nu_1^2\nu_2^2+\nu_1^2\nu_3^2+4\nu_2^2\nu_3^2)\right], \tag{3.19d}$$

$$D_1 = \frac{4}{3k'^4}[2-3k^2-3k^4+2k^6-(2\nu_1^2+\nu_2^2+\nu_3^2)(1-4k^2+k^4)]$$
$$+\frac{4}{3k'^4}[-\{2\nu_1^2(\nu_2^2+\nu_3^2)+\nu_2^2\nu_3^2+\nu_1^4\}(1+k^2)]$$
$$+\frac{4}{3k'^4}\left[\frac{(11-20k^2+11k^4)\{2\nu_1^2\nu_2^2\nu_3^2+\nu_1^4(\nu_2^2+\nu_3^2)\}}{k^2}\right.$$
$$\left.-\frac{\nu_1^4\nu_2^2\nu_3^2}{k^4}(14-13k^2-13k^4+14k^6)\right], \tag{3.20a}$$

$$D_2 = \frac{16\nu_1^2\nu_2^2\nu_3^2}{3k^4}[3k^2-\nu_1^2(1+k^2)], \tag{3.20b}$$

$$D_3 = D_2, \tag{3.20c}$$

$$D_4 = \frac{16\nu_1^2}{k^2}\left[-(\nu_1^2\nu_2^2+\nu_1^2\nu_3^2+4\nu_2^2\nu_3^2)+\frac{2\nu_1^2\nu_2^2\nu_3^2}{k^2}(1+k^2)\right]. \tag{3.20d}$$

The integral $\tilde{L}'$ for the contour $\Lambda_{\tilde{L}'}$ in Fig. 1(a) in Ref. 1 is obtained from the formula $\tilde{L}' = \tilde{L} + (|m|/2)\pi$. Therefore $\tilde{L}'^{(1)}$ and $\tilde{L}'^{(3)}$ can be obtained from (3.16a)–(3.16d).

B. Two real and two complex conjugate zeros of $Q^2(\eta)$ and $\tilde{Q}^2(\xi)$

1. The quantities $\alpha=\beta$, $\tilde{K}$, L, and L' pertaining to the η-equation: Superbarrier case [Fig. 4(a) or Fig. 2 in Ref. 1]

Putting $\eta_4=-\eta_1=a$, $\eta_2=\eta_3^*=-ia_1$, we have

$$Q(\eta)=p\frac{[(a^2-\eta^2)(a_1^2+\eta^2)]^{1/2}}{1-\eta^2}. \tag{3.21}$$

Using the appropriate transformation on p. 133 of Ref. 10, that is,

$$\eta^2=a^2\,\mathrm{cn}^2\,u, \tag{3.22}$$

we now utilize the fact that the Jacobian elliptic functions are doubly periodic, one of the periods being complex. Thus, the loop $\eta_1\to\eta_2\to\eta_1$, that is $-a\to-ia_1\to-a$, in the η-plane, denoted by $\Gamma_{-a,-ia_1}$, represents the contour Λ_α in Fig. 4(a) of Ref. 1, and it corresponds in the u-plane to $0\to K+iK'\to 2K+2iK'$ where $K'=K(k')$. Denoting by $2\overline{G}^{(2n+1)}$ the integral occurring in the definitions (3.13b) and (3.15b′) in Ref. 1 when $Z_1=Z_2$, we have the following first-order expression:

$$\begin{aligned}\overline{G}^{(1)}&=\frac{1}{2}\int_{\Lambda_\alpha}Q(\eta)\,\mathrm{d}\eta\\&=\frac{1}{2}\int_{\Gamma_{-a,-ia_1}}Q(\eta)\,\mathrm{d}\eta,\end{aligned} \tag{3.23}$$

which when transformed to the variable u becomes

$$\overline{G}^{(1)}=\frac{pa^2}{2g}\int_0^{2K+2iK'}\frac{\mathrm{sn}^2\,u\,\mathrm{dn}^2\,u}{1-a^2\,\mathrm{cn}^2\,u}\,\mathrm{d}u. \tag{3.24}$$

After evaluation of the integral in (3.24) we obtain

$$\begin{aligned}\overline{G}^{(1)}=&\frac{p}{g}\left[E(k)+\frac{k^2}{a^2}(1-a^2)K(k)-\left(\frac{k^2}{a^2}+k'^2\right)\Pi(\nu^2,k)\right]\\&-\frac{p}{g}i\{E(k')+(k^2+a^2k'^2)[\Pi(1-\nu^2,k')-K(k')]\},\end{aligned} \tag{3.25a}$$

where

$$\nu^2=\frac{a^2}{a^2-1},\quad g=\frac{1}{(a^2+a_1^2)^{1/2}},\quad k^2=\frac{a^2}{a^2+a_1^2},\quad k'^2=1-k^2. \tag{3.26}$$

Similarly one obtains

$$\overline{G}^{(3)}=-\frac{Cg}{2p}K(k)+\left\{\frac{g}{2p(1-a^2)}+\frac{(\nu^2-1)g}{4p}\right\}\left[\Pi(\nu^2,k)-\frac{\pi}{2}\sqrt{\frac{a^2(1-a^2)}{k'^2a^2+k^2}}\right]$$
$$-\frac{g}{8\nu^2p}\left[\frac{1}{3}(-4k^2+4\nu^2-1)K(k)+\frac{1}{3k'^2}(-8k^4+8k^2(1-\nu^2)+1+7\nu^2)E(k)\right]$$
$$+i\left\{-\frac{Cg}{2p}K(k')+\left[\frac{g}{2p(1-a^2)}+\frac{(\nu^2-1)g}{4p}\right]\left[(1-a^2)K(k')-\nu^2\Pi(\nu^2-1,k')-\frac{\pi}{2}\right]\right.$$
$$-\frac{g}{8\nu^2p}\left[\frac{1}{3}(-4k^2+4\nu^2-1)K(k')\right.$$
$$\left.\left.+\frac{1}{3k'^2}(-8k^4+8k^2(1-\nu^2)+1+7\nu^2)[K(k')-E(k')]\right]\right\}. \tag{3.25b}$$

Recalling the definition of $\overline{G}^{(2n+1)}$ above (3.23) in the present paper, one sees that according to (3.13b) in Ref. 1 the first- and third-order contributions to α are

$$\alpha^{(1)}=\mathrm{Re}\,\overline{G}^{(1)}, \tag{3.27a}$$

$$\alpha^{(3)}=\mathrm{Re}\,\overline{G}^{(3)}, \tag{3.27b}$$

and that according to (3.15b′) in Ref. 1 the first- and third-order contributions to $K(=\pi\overline{K})$ are

$$\pi\overline{K}_0=-2\,\mathrm{Im}\,\overline{G}^{(1)}, \tag{3.28a}$$

$$\pi\overline{K}_2=-2\,\mathrm{Im}\,\overline{G}^{(3)}. \tag{3.28b}$$

The integrals $\alpha'=\beta'$ associated with the contours $\Lambda_{\alpha'}$ and $\Lambda_{\beta'}$ in Fig. 4 in Ref. 1 are obtained from the integrals $\alpha=\beta$ by means of the relations (3.18a) in Ref. 1, that is $\alpha'=\beta'=\alpha+\Lambda\pi/2=\beta+\Lambda\pi/2$. The integrals L and L' associated with the contours Λ_L and $\Lambda_{L'}$ in Fig. 4(a) in Ref. 1 can be obtained from the integrals $\alpha=\beta$ by means of the formulas $L=\alpha+\beta=2\alpha$ and $L'=L+|m|$.

The only essential difference between $-Q^2(\eta)$ in Fig. 4(a) in Ref. 1 and $-Q^2(\eta)$ in Fig. 2 in Ref. 1 is that in the former figure there is an underdense barrier of $-Q^2(\eta)$, while in the latter figure $-Q^2(\eta)$ has a single minimum. For the case in Fig. 2 one has therefore the formula $L^{(2n+1)}=\alpha^{(2n+1)}+\beta^{(2n+1)}=2\alpha^{(2n+1)}$, with expressions (3.27a) and (3.27b) for $\alpha^{(1)}$ and $\alpha^{(3)}$, and the formula $L'^{(2n+1)}=L^{(2n+1)}+|m|\,\delta_{n,0}$. The case in Fig. 2 has, however, not appeared in our applications.

2. The quantities $\tilde{L}$ and $\tilde{L}'$ pertaining to the ξ-equation [Fig. 1(a) in Ref. 1]

Denoting by $\xi_3=b$ and $\xi_4=a$ the real zeros of $\tilde{Q}^2(\xi)$, and by c and c^* the complex conjugate zeros ξ_1 and ξ_2 of $\tilde{Q}^2(\xi)$, we have

$$\tilde{Q}(\xi)=p\,\frac{[(a-\xi)(\xi-b)(\xi-c)(\xi-c^*)]^{1/2}}{\xi^2-1}. \tag{3.29}$$

Defining

$$c=b_1-ia_1,\quad c^*=b_1+ia_1, \tag{3.30}$$

$$A=[(a-b_1)^2+a_1^2]^{1/2},\quad B=[(b-b_1)^2+a_1^2]^{1/2}, \tag{3.31}$$

and using the appropriate transformation on p. 133 in Ref. 10, we get

$$\xi=\frac{aB+bA+(bA-aB)\operatorname{cn}u}{A+B+(A-B)\operatorname{cn}u}. \tag{3.32}$$

Noting that the loop $b\to a\to b$ in the ξ-plane (denoted by $\Gamma_{b,a}$ for the contour $\Lambda_{\tilde{L}}$) corresponds to the path $0\to 2K\to 4K$ in the u-plane, and using the transformation (3.32), we obtain for the first-order contribution to $\tilde{L}$ the formula [see Fig. 1(a) in Ref. 1],

$$\begin{aligned}\tilde{L}^{(1)}&=\frac{1}{2}\int_{\Lambda_{\tilde{L}}}\tilde{Q}(\xi)\mathrm{d}\xi\\&=\frac{1}{2}\int_{\Gamma_{b,a}}\tilde{Q}(\xi)\mathrm{d}\xi\\&=\frac{p(\nu_1-\nu_2)(\nu_1-\nu_3)}{g}\int_0^{4K}\frac{\operatorname{sn}^2u\,\operatorname{dn}^2u}{(1+\nu_1\operatorname{cn}u)^2+(1+\nu_2\operatorname{cn}u)(1+\nu_3\operatorname{cn}u)}\mathrm{d}u,\end{aligned} \tag{3.33}$$

where

$$\nu_1=\frac{A-B}{A+B},\quad \nu_2=\frac{(1+b)A-(1+a)B}{(1+b)A+(1+a)B},\quad \nu_3=\frac{(1-b)A-(1-a)B}{(1-b)A+(1-a)B}, \tag{3.34}$$

$$g=\frac{1}{\sqrt{AB}},\quad k^2=\frac{(a-b)^2-(A-B)^2}{4AB}. \tag{3.35}$$

By evaluating the last integral in (3.33), and introducing a new "universal" function $\overline{H}^{(1)}$, given by Eqs. (2.19), (2.20a)–(2.20c), and (2.21) in Ref. 8 with $j=0$, we obtain

$$\tilde{L}^{(1)}=-2\,\mathrm{Re}\,\overline{H}^{(1)}(\nu_1,\nu_2,\nu_3,g,k,\tilde{C})[\text{with } j=0] \tag{3.36a}$$

$$\begin{aligned}&=\frac{2p}{g}\left\{\frac{1}{\nu_1^2}\left[\left(2k^2+\frac{\nu_1^2}{1-\nu_1^2}\right)\Pi\left(\frac{\nu_1^2}{\nu_1^2-1},k\right)\right.\right.\\&\left.\left.+(\nu_1^2-2k^2)K(k)-2\nu_1^2E(k)+\nu_1k\pi\right]+\sum_{i=1}^{3}\overline{C}_i\overline{J}_i\right\},\end{aligned} \tag{3.36b}$$

where

$$\overline{C}_1=\frac{\nu_1^2(2\nu_3\nu_2-\nu_1\nu_3-\nu_1\nu_2)}{(\nu_1-\nu_2)(\nu_1-\nu_3)}, \tag{3.37a}$$

$$\overline{C}_2=\frac{(\nu_1-\nu_3)\nu_2^3}{(\nu_1-\nu_2)(\nu_2-\nu_3)}, \tag{3.37b}$$

$$\overline{C}_3=\frac{(\nu_1-\nu_2)\nu_3^3}{(\nu_1-\nu_3)(\nu_3-\nu_2)}, \tag{3.37c}$$

$$\overline{J_i}=\mathrm{Re}\,\overline{S_i}(\text{with } j=0)$$
$$=\frac{1}{\nu_i^4}\left[k^2(1-\nu_i^2)K(k)+\nu_i^2E(k)-(k^2+\nu_i^2k'^2)\Pi\left(\frac{\nu_i^2}{\nu_i^2-1},k\right)\right]$$
$$+\frac{1}{2k\nu_i^3}\left[k^2(\nu_i^2-1)-\frac{\nu_i^2}{2}\right]\pi, i=1,2,3; \tag{3.38}$$

cf. the definition of $\overline{S_i}$ in Eq. (2.21) in Ref. 8. The third-order contribution to $\tilde{L}$ is

$$\tilde{L}^{(3)}=-2\,\mathrm{Re}\,\overline{H}^{(3)}(\nu_1,\nu_2,\nu_3,g,k,\tilde{C})\ \ [\text{with } j=0] \tag{3.39a}$$
$$=-\frac{g}{8p}\left\{\left(4\tilde{C}+\frac{\nu_1^2(\nu_2-\nu_3)^2}{\nu_2\nu_3(\nu_1-\nu_3)(\nu_2-\nu_1)}\right)K(k)\right.$$
$$\left.+\frac{1}{(\nu_1-\nu_3)(\nu_1-\nu_2)}[XK(k)+YE(k)]\right\}, \tag{3.39b}$$

where $\overline{H}^{(3)}$ is another "universal" function, given by Eqs. (2.22) and (2.23a)–(2.23c) in Ref. 8 with $j=0$, and where thus

$$X=-\frac{(1+4k^2)}{3}+\frac{(3+4k'^2)}{3}(\nu_1^2+2\nu_1\nu_2+2\nu_1\nu_3+\nu_2\nu_3)-\frac{k'^2}{3k^2}(17-4k^2)\nu_1^2\nu_2\nu_3$$
$$-2\nu_1(\nu_1+\nu_2+\nu_3)+2\nu_2\nu_3+\nu_1^2\left(\frac{\nu_2}{\nu_3}+\frac{\nu_3}{\nu_2}\right), \tag{3.40a}$$

$$Y=\frac{1}{3k'^2}(1+8k^2-8k^4)+\frac{4}{3}(2k^2-1)(\nu_1^2+2\nu_1\nu_2+2\nu_1\nu_3+\nu_2\nu_3)$$
$$+\frac{\nu_1^2\nu_2\nu_3}{3k^2}(17-8k^2+8k^4). \tag{3.40b}$$

The integral $\tilde{L}'$ associated with the contour $\Lambda_{\tilde{L}'}$ in Fig. 1(a) in Ref. 1 is obtained from the formula $\tilde{L}'=\tilde{L}+(|m|/2)\pi$. One has therefore the formulas $\tilde{L}'^{(1)}=\tilde{L}^{(1)}+(|m|/2)\pi$ and $\tilde{L}'^{(3)}=\tilde{L}^{(3)}$ with $\tilde{L}^{(1)}$ and $\tilde{L}^{(3)}$ given by (3.39a) and (3.39b), respectively.

IV. CASE $\Lambda=0$

A. Two real zeros of $Q^2(\eta)$ and $\tilde{Q}^2(\xi)$

1. The quantities $\alpha=\beta$ and $\bar{K}$ pertaining to the η-equation: Subbarrier case [Fig. 3(b) in Ref. 1]

Putting $\eta_3=-\eta_2=b$ as before, we have

$$Q(\eta)=p\left[\frac{(\eta^2-b^2)}{1-\eta^2}\right]^{1/2}. \tag{4.1}$$

Using (3.2) with $a=1$, the first- and third-order contributions to α become

$$\alpha^{(1)}=p[E(k)-(1-k^2)K(k)], \tag{4.2a}$$

$$\alpha^{(3)}=\frac{1}{2pk^2}\left[(1-Ck^2)K(k)-E(k)-\frac{1}{12}\left((3k^2-8)K(k)-(7k^2-8)\frac{E(k)}{k'^2}\right)\right], \tag{4.2b}$$

where $k^2=1-b^2$.

The first- and third-order contributions to $K(=\pi\overline{K})$ are

$$\pi\overline{K}_0=2p[E(k)-(1-k^2)K(k)], \tag{4.3a}$$

$$\pi\overline{K}_2=\frac{1}{p}\left[CK(k)-\frac{E(k)}{k'^2}+\frac{1}{12k^2}\left(\frac{7k^2+1}{k'^2}E(k)-(3k^2+1)K(k)\right)\right], \tag{4.3b}$$

where $k^2=b^2$.

2. The quantities $\tilde{L}$ and $\tilde{L}'$ pertaining to the ξ-equation [Fig. 1 in Ref. 1]

If the real zeros of $\tilde{Q}^2(\xi)$ are $\xi_3=c(<a)$ and $\xi_4=a$, we have

$$\tilde{Q}(\xi)=p\left[\frac{(\xi-c)(a-\xi)}{(\xi+1)(\xi-1)}\right]^{1/2}. \tag{4.4}$$

We shall treat the three cases $1<c<a$, $-1<c<1<a$, and $c<-1<1<a$ separately.

a. Case $1<c<a$ [Fig. 1(a) in Ref. 1]. For this case we use the transformation on p. 120 of Ref. 10 and the formula in Sec. 256.19 with a suitable choice of parameters to obtain the first- and third-order contributions to $\tilde{L}$ as

$$\begin{aligned}\tilde{L}^{(1)}&=\int_c^a\tilde{Q}(\xi)\mathrm{d}\xi\\&=p\frac{(a-c)(c-1)g}{2\nu^2(\nu^2-k^2)}[(2\nu^2-\nu^4-k^2)\Pi(\nu^2,k)-\nu^2E(k)-(\nu^2-k^2)K(k)],\end{aligned} \tag{4.5a}$$

$$\begin{aligned}\tilde{L}^{(3)}=&\frac{\tilde{C}gK(k)}{2p}+\frac{g}{2(c^2-1)p}\left[\frac{2\nu^2}{k^4}(k^2-\nu^2)K(k)+\frac{1}{k^4k'^2}(k^2(k^2-\nu^4-2\nu^2)+2\nu^4)E(k)\right]\\&-\frac{g}{24\nu^4p(c-1)}[(-2+k^2+2\nu^2-\nu^4)K(k)+2(k^4-(1+\nu^2+\nu^4)k^2-\nu^2+2\nu^4+1)E(k)],\end{aligned} \tag{4.5b}$$

where

$$\nu^2=\frac{a-c}{a-1},\quad g=\frac{2}{[(a-1)(c+1)]^{1/2}},\quad k^2=\frac{2(a-c)}{(a-1)(c+1)}. \tag{4.6}$$

To obtain $\tilde{L}'$ one can use the formula $\tilde{L}'^{(2n+1)}=\tilde{L}^{(2n+1)}+(|m|/2)\delta_{n,0}$ with $\tilde{L}^{(1)}$ and $\tilde{L}^{(3)}$ given by (4.5a) and (4.5b).

b. Case $-1<c<1<a$ [Fig. 1(b) in Ref. 1]. We use in the appropriate transformation on p. 120 of Ref. 10 and the formula in Sec. 256.17 (with $b=1$ and $d=-1$) to obtain the first- and third-order contributions to $\tilde{L}'$ [see Fig. 1(b) in Ref. 1] as

$$\tilde{L}'^{(1)}=\frac{2p}{g}\left[\left(1-\frac{k^2}{\nu^2}\right)K(k)-E(k)+\left(\nu^2-2k^2+\frac{k^2}{\nu^2}\right)\Pi(\nu^2,k)\right], \tag{4.7a}$$

$$\tilde{L}'^{(3)}=\frac{g\tilde{C}K(k)}{2p}+\frac{g}{4p\nu^2(1-c)}\left[\left(1-\frac{\nu^4}{k^2}\right)K(k)+(k^2(2k^2-1-2\nu^2)+\nu^4)\frac{E(k)}{k^2k'^2}\right]$$
$$-\frac{g}{16(1-c)p\nu^2}\left[\frac{4}{3k^2}((2+\nu^4+2\nu^2)k^2-3k^4-2\nu^4)K(k)\right.$$
$$\left.+\frac{8}{3k'^2}\left(-(\nu^4+\nu^2-1)+k^2(\nu^4-\nu^2+2)+\frac{\nu^4}{k^2}\right)E(k)\right], \tag{4.7b}$$

where

$$\nu^2=\frac{a-1}{a-c},\quad g=\left(\frac{2}{a-c}\right)^{1/2},\quad k^2=\frac{(1+c)(a-1)}{2(a-c)}. \tag{4.8}$$

c. Case $c<-1<1<a$ [Fig. 1(b) in Ref. 1]. Using the transformation on p. 120 of Ref. 10 and the formula in Sec. 256.20 with a suitable choice of parameters, we obtain the first- and third-order contributions to $\tilde{L}'$ as

$$\tilde{L}'^{(1)}=\frac{(a-c)(1-c)gp}{2\nu^4}[-\nu^2E(k)+(\nu^2+k^2)K(k)+(\nu^4-k^2)\Pi(\nu^2,k)], \tag{4.9a}$$

$$\tilde{L}'^{(3)}=\frac{\tilde{C}gK(k)}{p}+\frac{g}{4p\nu^2}\left[\left(1-2\nu^2+\frac{\nu^4}{k^2}\right)K(k)-\left(1+\frac{\nu^4}{k^2}\right)E(k)\right]$$
$$-\frac{g}{32p\nu^2}\left\{\frac{4}{3k^2k'^2}[-k^4+k^2(2-\nu^4-2\nu^2)-\nu^4]K(k)\right.$$
$$\left.+\frac{8}{3k^2k'^4}[-k^6+k^4(\nu^2-\nu^4)+k^2(\nu^4+\nu^2-1)-\nu^4]E(k)\right\}, \tag{4.9b}$$

with

$$\nu^2=\frac{a-1}{a+1},\quad g=\frac{2}{[(a+1)(1-c)]^{1/2}},\quad k^2=\frac{(a-1)(-c-1)}{(a+1)(1-c)}. \tag{4.10}$$

B. Two complex conjugate zeros of $Q^2(\eta)$

The case of two complex conjugate zeros of the square of the base function occurs only for the η-equation.

The quantities $\alpha=\beta$ and $\overline{K}$ pertaining to the η-equation: Superbarrier case [Fig. 4(b) in Ref. 1]. With $\eta_2=-ia_1$ and $\eta_3=ia_1$ we have

$$Q(\eta)=p\frac{[(1-\eta^2)(a_1^2+\eta^2)]^{1/2}}{1-\eta^2}=p\left(\frac{a_1^2+\eta^2}{1-\eta^2}\right)^{1/2}. \tag{4.11}$$

Specializing to the case $a=1$ in (3.27a) and (3.27b) and (3.28a) and (3.28b) along with (3.25a) and (3.25b), we obtain the first- and third-order contributions to α as

$$\alpha^{(1)}=\mathrm{Re}\,\overline{G}^{(1)},\quad \alpha^{(3)}=\mathrm{Re}\,\overline{G}^{(3)} \tag{4.12}$$

and the first- and third-order contributions to $K(=\pi\overline{K})$ as

$$\pi\overline{K}_0=-2\,\mathrm{Im}\,\overline{G}^{(1)},\quad \pi\overline{K}_2=-2\,\mathrm{Im}\,\overline{G}^{(3)}, \tag{4.13}$$

where

$$\overline{G}^{(1)}=\frac{p}{g}\{E(k)+i[K(k')-E(k')]\}, \tag{4.14a}$$

$$\overline{G}^{(3)}=\frac{g}{2p}\left[(1-C)K(k)-E(k)-\frac{1}{12}\left(4K(k)+\frac{(8k^2-7)}{k'^2}E(k)\right)\right]$$
$$+i\frac{g}{2p}\left[-CK(k')+E(k')-\frac{1}{12}\left(4K(k')+\frac{(8k^2-7)}{k'^2}\{K(k')-E(k')\}\right)\right] \tag{4.14b}$$

with

$$g=\frac{1}{(1+a_1^2)^{1/2}}, \quad k^2=\frac{1}{1+a_1^2}. \tag{4.15}$$

The integral L' associated with the contour $\Lambda_{L'}$ in Fig. 4(b) in Ref. 1 is obtained from the formula $L'=\alpha+\beta=2\alpha$.

V. ACCURACY OF THE PHASE-INTEGRAL QUANTIZATION CONDITIONS FOR THE $1s\sigma$ AND $2p\sigma$ STATES OF THE HYDROGEN MOLECULE ION

For the $1s\sigma$ and $2p\sigma$ states of the hydrogen molecule ion one has to put $\Lambda=0$. The quantization conditions in Ref. 1 for the $1s\sigma$ state are (3.5a) with $\tilde{s}=0$ [Fig. 1(a) in Ref. 1] and (3.9) with $s=m=0$ [Fig. 4(b) in Ref. 1] when r_{12} is sufficiently small, but (3.5b) with $\tilde{s}=m=0$ [Fig. 1(b) in Ref. 1] and (3.25b) with $s_\alpha=s_\beta=m=0$ [Fig. 3(b) in Ref. 1] when r_{12} is sufficiently large. The quantization conditions in Ref. 1 for the $2p\sigma$ state are (3.5a) with $\tilde{s}=0$ [Fig. 1(a) in Ref. 1] and (3.9) with $s=1$ and $m=0$ [Fig. 4(b) in Ref. 1] when r_{12} is sufficiently small, but (3.5b) with $\tilde{s}=m=0$ [Fig. 1(b) in Ref. 1] and (3.25a) with $s_\alpha=s_\beta=m=0$ [Fig. 3(b) in Ref. 1] when r_{12} is sufficiently large. After having expressed these quantization conditions in the first order and third order of the phase-integral approximation in terms of complete elliptic integrals, as described in the previous sections, we have used these quantization conditions to calculate the energy E and the reduced separation constant A'. We have determined C and $\tilde{C}$ as function of r_{12} such that the first- and third-order quantization conditions give the same values of both E and A'. For the values of C and $\tilde{C}$ thus obtained, the choice of the base functions $Q(\eta)$ and $\tilde{Q}(\xi)$ is optimum in the sense that the most accurate first-order values of E and A' are obtained, since the first- and third-order approximations give the same values of E and A'. In this connection we remark that there are quantal systems for which one can obtain exact values of the energy by choosing the base function such that the first- and third-order results coincide; see p. 1826 in Ref. 11 and p. 16 in Ref. 12.

By determining C and $\tilde{C}$ for each value of r_{12} such that the first- and third-order quantization conditions give the same value of E as well as of A', we have obtained the results in Table I for the $1s\sigma$ state and in Table II for the $2p\sigma$ state of the hydrogen molecule ion; see also Figs. 1 and 2. Especially for large values of r_{12} the phase-integral values of E and A' in Tables I and II are in reasonable agreement with the numerically exact values obtained by Murai and Takatsu,[13,14] as is best seen from Fig. 1 for the state $1s\sigma$ and from Fig. 2 for the state $2p\sigma$. For these states the phase-integral method cannot compete with the numerical method used by Murai and Takatsu, but the possibility of using the analytical phase-integral formulas expressed in terms of complete elliptic integrals is an alternative that may sometimes be preferable to the use of the very accurate numerical results.

It is seen that in Figs. 1 and 2 there are sometimes some irregularities in the values of C, $\tilde{C}$, $|E-E_{\mathrm{MT}}|$ and $|A'-A'_{\mathrm{MT}}|$ for low r_{12} values. It should also be noted that C and $\tilde{C}$ approach the correct limiting value 1/4 as $r_{12}\to 0$.

To obtain the numerical results in Sec. V a general FORTRAN computer program using very rapid library routines was written at the Centre for Nonlinear Dynamics, Department of Physics,

TABLE I. For the state $1s\sigma$ of H_2^+ the values of C and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for E as well as for A'. With the use of these values of C and $\tilde{C}$, the values of E and A' have then been obtained from the quantization conditions that are appropriate depending on whether r_{12} is sufficiently small or sufficiently large. The numerically exact values obtained by Murai and Takatsu (Refs. 13 and 14) are given in the columns E_{MT} and A'_{MT}.

r_{12}	C	$\tilde{C}$	E	E_{MT}	$E-E_{\mathrm{MT}}$	A'	A'_{MT}	$A'-A'_{\mathrm{MT}}$
Sufficiently small r_{12}								
0.6	0.409 176 18 0	0.495 364 356 0	−1.618 424 439	−1.671 484 714 5	0.053 060 275	−0.199 240 748 9	−0.199 230 000 0	−0.000 010 748
0.8	0.443 152 899 0	0.488 457 984 4	−1.545 199 993	−1.554 480 091 5	0.009 280 098	−0.324 914 201 9	−0.327 900 000	0.002 985 799
1.0	0.468 177 174 4	0.490 208 142 0	−1.455 314 042	−1.451 786 313 0	−0.003 527 729	−0.470 687 972 1	−0.475 946 916 1	0.005 258 944
Sufficiently large r_{12}								
2.0	0.525 508 000 0	0.505 790 336 8	−1.109 450 173	−1.102 634 215 0	−0.006 815 958	−1.385 866 329	−1.393 538 844	0.007 672 515
3.0	0.534 795 590 0	0.514 686 014 0	−0.914 626 887 0	−0.910 896 197 4	−0.003 730 69	−2.451 736 492	−2.458 030 452	0.006 293 96
4.0	0.525 543 652 0	0.519 150 688 0	−0.798 198 554 4	−0.796 084 883 7	−0.002 113 671	−3.564 275 870	−3.569 090 310	0.004 814 44
5.0	0.509 534 415 3	0.521 027 659 1	−0.725 677 545 1	−0.724 420 295 2	−0.001 257 25	−4.673 981 394	−4.677 559 936	0.003 578 542
6.0	0.494 233 156 6	0.521 361 748 5	−0.679 416 283 8	−0.678 635 715 1	−0.000 780 568	−5.759 202 308	−5.761 839 130	0.002 636 822
7.0	0.482 991 774 0	0.520 850 534 0	−0.648 961 908 9	−0.648 451 147 1	−0.000 510 761	−6.817 236 218	−6.819 239 945	0.002 003 727
8.0	0.475 824 570 0	0.519 946 280 0	−0.627 926 537 2	−0.627 570 388 6	−0.000 356 149	−7.854 452 399	−7.856 077 820	0.001 625 421
9.0	0.471 507 673 0	0.518 905 760 0	−0.612 571 107 4	−0.612 306 564 0	−0.000 264 543	−8.878 337 258	−8.879 752 233	0.001 414 975
10.0	0.468 895 318 4	0.517 856 861 6	−0.600 785 980 7	−0.600 578 728 9	−0.000 207 251	−9.894 343 735	−9.895 643 269	0.001 299 534
15.0	0.464 171 046 0	0.513 368 645 0	−0.566 810 620 7	−0.566 715 605 2	−0.000 095 015	−14.932 033 45	−14.933 152 05	0.001 118 65
20.0	0.462 583 431 7	0.510 789 280 8	−0.550 074 045 2	−0.550 014 259 3	−0.000 059 786	−19.948 917 64	−19.949 960 67	0.001 043 03
25.0	0.461 735 080 0	0.508 920 020 0	−0.540 048 885 5	−0.540 005 800 8	−0.000 043 085	−24.958 994 30	−24.959 984 43	0.000 990 13

TABLE II. For the state $2p\sigma$ of H_2^+ the values of C and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for E as well as for A'. With the use of these values of C and $\tilde{C}$, the values of E and A' have then been obtained from the quantization conditions that are appropriate depending on whether r_{12} is sufficiently small or sufficiently large. The numerically exact values obtained by Murai and Takatsu (Refs. 13 and 14) are given in the columns E_{MT} and A'_{MT}.

r_{12}	C	$\tilde{C}$	E	E_{MT}	$E-E_{\mathrm{MT}}$	A'	A'_{MT}	$A'-A'_{\mathrm{MT}}$
Sufficiently small r_{12}								
0.2	0.263 395 978 0	0.246 516 819 0	−0.502 072 030 3	−0.502 680 000 0	−0.000 607 97	−2.005 074 078	−2.004 020 000	0.001 054 078
0.4	0.268 855 028 0	0.234 829 974	−0.509 130 292 8	−0.510 790 000 0	−0.001 659 708	−2.018 393 631	−2.016 330 000	0.002 063 631
0.6	0.275 068 547 0	0.209 525 191	−0.523 174 558 1	−0.524 305 000 0	−0.001 130 442	−2.041 072 959	−2.037 690 000	0.003 382 959
0.8	0.282 634 031 0	0.147 093 588 0	−0.552 425 793 5	−0.542 740 000 0	0.009 685 793	−2.075 482 537	−2.069 270 000	0.006 212 537
2.0	0.343 572 840 4	0.552 431 948 9	−0.657 183 769 2	−0.667 534 392 2	−0.010 350 623	−2.523 233 873	−2.521 958 177	0.001 275 696
3.0	0.391 523 598 0	0.526 004 845 9	−0.701 567 896 1	−0.701 418 333 4	0.000 149 563	−3.202 554 526	−3.196 382 289	0.006 172 237
Sufficiently large r_{12}								
4.0	0.427 994 195 0	0.524 934 545 0	−0.696 001 180 8	−0.695 550 639 4	0.000 450 542	−4.029 227 017	−4.025 940 635	0.003 286 382
5.0	0.448 161 632 0	0.523 892 464 0	−0.677 741 041 4	−0.677 291 613 2	0.000 449 428	−4.942 443 752	−4.941 274 459	0.001 169 293
6.0	0.459 123 373 0	0.522 676 096 0	−0.657 710 466 4	−0.657 310 559 0	0.000 399 907	−5.903 631 412	−5.903 659 889	−0.000 028 477
7.0	0.464 457 921 0	0.521 416 248 0	−0.639 467 418 3	−0.639 128 855 4	0.000 338 563	−6.890 343 283	−6.890 997 919	−0.000 654 636
8.0	0.466 614 486 0	0.520 178 914 0	−0.623 887 034 6	−0.623 606 015 6	0.000 280 969	−7.889 744 744	−7.890 707 161	−0.000 962 417
9.0	0.467 126 491 0	0.518 998 550 0	−0.610 887 601 2	−0.610 654 940 6	0.000 232 66	−8.894 778 515	−8.895 880 333	−0.001 101 818
10.0	0.466 877 089 0	0.517 893 123 0	−0.600 095 056 9	−0.599 901 068 6	0.000 193 989	−9.901 798 495	−9.902 954 530	−0.001 156 035
15.0	0.464 139 540 0	0.513 568 940 0	−0.566 803 604 6	−0.566 708 729 0	0.000 094 875	−14.932 144 72	−14.933 261 11	−0.001 116 39
20.0	0.462 583 050 0	0.510 789 280 0	−0.550 073 982 0	−0.550 014 197 7	0.000 059 785	−19.948 918 96	−19.949 961 91	−0.001 042 95
25.0	0.461 735 070 0	0.508 920 010 0	−0.540 048 885 0	−0.540 005 800 3	0.000 043 085	−24.958 994 32	−24.959 984 45	−0.000 990 13

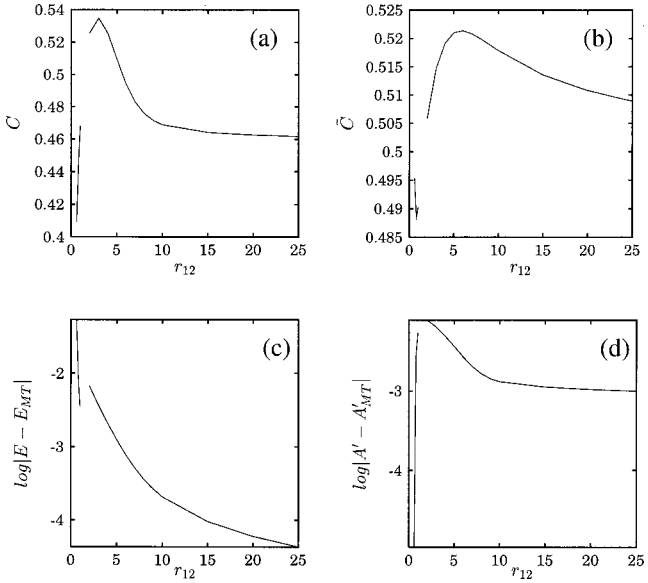

FIG. 1. Plots for the $1s\sigma$ state of the ion H_2^+ of (a) C vs r_{12}, (b) $\tilde{C}$ vs r_{12}, (c) $\log|E-E_{\mathrm{MT}}|$ vs r_{12}, and (d) $\log|A'-A'_{\mathrm{MT}}|$ vs r_{12}, when C and $\tilde{C}$ are determined as functions of r_{12} from the requirement that the first-order phase-integral results coincide with the third-order results. Here E and A' are the phase-integral values obtained in Table I, while E_{MT} and A'_{MT} are the corresponding numerically exact values obtained by Murai and Takatsu (Refs. 13 and 14) and quoted in Table I. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of r_{12} have been used.

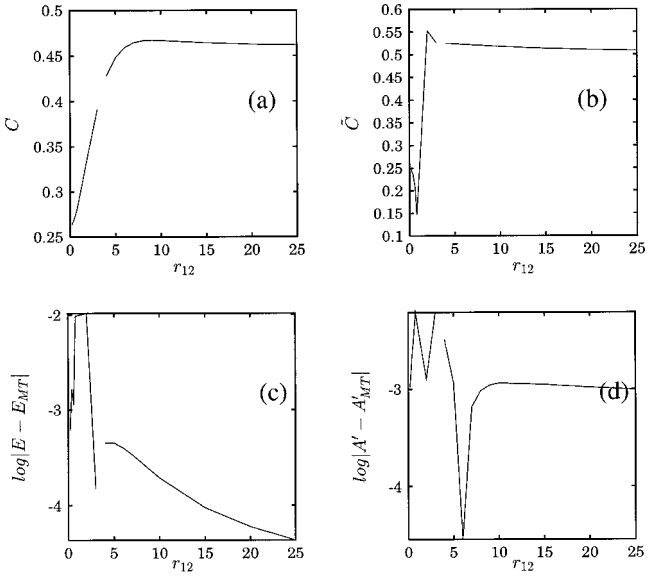

FIG. 2. Plots for the $2p\sigma$ state of the ion H_2^+ of (a) C vs r_{12}, (b) $\tilde{C}$ vs r_{12}, (c) $\log|E-E_{\mathrm{MT}}|$ vs r_{12}, and (d) $\log|A'-A'_{\mathrm{MT}}|$ vs r_{12}, when C and $\tilde{C}$ are determined as functions of r_{12} from the requirement that the first-order phase-integral results coincide with the third-order results. Here E and A' are the phase-integral values obtained in Table II, while E_{MT} and A'_{MT} are the corresponding numerically exact values obtained by Murai and Takatsu (Refs. 13 and 14) and quoted in Table II. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of r_{12} have been used.

Bharathidasan University, Tiruchirapalli, India. We have carried out the numerical calculations by Silicon Graphics Power Indigo 2 XZ Graphics Workstation (R8000, 64bit processor) using FORTRAN 77 compiler.

Some years ago, a direct numerical integration of the contour integrals in the phase-integral quantization conditions for the hydrogen molecule ion was carried out by Fil. lic. Anders Hökback at the Department of Theoretical Physics, University of Uppsala, Sweden. By means of this numerical material it was possible to make valuable checks of the correctness of the phase-integral quantization conditions expressed in terms of complete elliptic integrals.

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Quantal two-center Coulomb problem treated by means of the phase-integral method. III. Quantization conditions in the general case expressed in terms of complete elliptic integrals. Numerical illustration

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In this paper we take up the quantal two-center problem where the Coulomb centers have arbitrary positive charges. In analogy with the symmetric case, treated in the second paper of this series, we use the knowledge on the quasiclassical dynamics to express the contour integrals in the first- and third-order approximations of the phase-integral quantization conditions, given in the first paper of this series of papers, in terms of complete elliptic integrals. For various values of the distance between these charges the accuracy of the formulas obtained is illustrated by comparison with available numerically exact results. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1399296]

I. INTRODUCTION

In this third paper in a series of papers concerning the two-center Coulomb problem we take up the general case in which the charge numbers Z_1 and Z_2 of the two Coulomb centers are arbitrary. The study of such general systems is of considerable importance in the field of molecular physics and elementary particle physics. For example, the calculation of eigenvalues and electronic wave functions for one-electron diatomic molecules with fixed internuclear separation is the starting point for an accurate description of molecular vibrations and rotations and of ion–atom scattering.[1–4] Also the calculation of radiative transition probabilities for a π^- meson moving in the Coulomb field of two fixed nuclei[5] is a good example of the two-center Coulomb problem dealt with in elementary particle physics. Such calculations are of physical interest in connection with experimental[6–8] and theoretical[9] research on the absorption of π^- mesons stopped in substances containing hydrogen.

In the second paper in this series[10] the symmetric case, $Z_1=Z_2$, was considered. Using for the two-center Coulomb problem the general phase-integral quantization conditions derived in the first paper,[11] the relevant contour integrals for the first- and third-order approximations were expressed in terms of complete elliptic integrals so that numerical evaluation of energy eigenvalues and separation constants can easily be carried out. The evaluation of the various contour integrals was facilitated through suitable transformations of the ξ- and η-variables, which can be related to the quasiclassical motion of a particle. In the symmetric case, $Z_1=Z_2$, the squared base function $Q^2(\eta)$ has a symmetry, as discussed in Ref. 10. As a result of this, the evaluation of the quantities $\alpha=\beta$, L, L', and $\bar{K}$ pertaining to the η-quantization conditions was performed with the use of particular transformations in a rather simple way, while for the quantity $\tilde{L}$ in the ξ-quantization

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condition rather general transformations are necessary. However, in the general case, where Z_1 may be different from Z_2, no such symmetric structure exists for $Q^2(\eta)$, and $Q^2(\eta)$ and $\tilde{Q}^2(\xi)$, given by Eqs. (3.2a) and (3.2b) in Ref. 11, can have, besides the poles, the following structure of the zeros.

(1) Case $\Lambda=|m|\neq 0$:
   (a) Four real zeros.
   (b) Two real and two complex conjugate zeros.

(2) Case $\Lambda=0$:
   (a) Two real zeros.
   (b) Two complex conjugate zeros of $Q^2(\eta)$.

As a consequence, the evaluation of the contour integrals in the cases of the ξ-equation and the η-equation are analogous, except that certain coefficients change in the different subcases. This allows one to use the "universal" functions $H^{(2n+1)}$ and $\overline{H}^{(2n+1)}$, $n=0$ or 1, valid for the $(2n+1)$ th-order approximation, which were defined in Secs. III A 2 and III B 2 of Ref. 10. These functions depends on five parameters ν_1, ν_2, ν_3, g, and k, which are expressed in terms of the zeros of either $Q^2(\eta)$ or $\tilde{Q}^2(\xi)$, and on the parameter C or $\tilde{C}$ in the base function $Q(\eta)$ or $\tilde{Q}(\xi)$, respectively; see Eqs. (3.2a) and (3.2b) in Ref. 11. Different choices of these parameters allow one to express the relevant quantities α, β (which may now be different from α), L, L', $\overline{K}$, and $\tilde{L}$ in the first- and third-order phase integral approximation (apart possibly from a sign or a constant factor) as the appropriate "universal" function or its real or imaginary part with the appropriate parameters inserted. When the contour integrals are evaluated, one can solve the quantization conditions to obtain the energy levels accurately.

In principle one can specialize the results of the general case when Z_1 may be different from Z_2 to the particular case when $Z_1=Z_2$ in order to obtain the results of Ref. 10, but in practice this is cumbersome due to the different transformation formulas used for the η-part of the quantization conditions in Ref. 10. For the ξ-part such a specialization implies only that Z_1+Z_2 is replaced by $2Z_1$ but no essential simplification.

The plan of the present paper is as follows. In Sec. II A we express α, β, L, L', $\overline{K}$, and $\tilde{L}$ in terms of the "universal" functions appropriate for the subbarrier case with $\Lambda=|m|\neq 0$. In Sec. II B a similar treatment is given for the superbarrier case. In Sec. III an analogous procedure is applied to the case $\Lambda=0$. Finally, in Sec. IV a detailed numerical analysis of the phase-integral quantization conditions is carried out for $Z_1=1$ and different values of Z_2 (=2, 5, and 8), and comparision is made with existing numerically exact results for the energy and the reduced separation constant.

II. CASE $\Lambda=|m|\neq 0$

In this section we utilize for the case of four zeros of $Q^2(\eta)$ or $\tilde{Q}^2(\xi)$ the "universal" functions $H^{(2n+1)}$, $n=0$ or 1, introduced in Ref. 10 and related to the $(2n+1)$ th-order contribution, and the "universal" functions $\overline{H}^{(2n+1)}$, $n=0$ or 1, which will be introduced in Sec. II B 1. In the different cases one finds, as explained in Sec. I, that the forms of the evaluated contour integrals are similar, except for changes of the parameters. One obtains the expressions for the "universal" functions $H^{(1)}$, $H^{(3)}$, $\overline{H}^{(1)}$, and $\overline{H}^{(3)}$ by integrating one specific integral in each case explicitly and then modifying the definition of the parameters in these functions to obtain the other required quantities.

A. Four real zeros of $Q^2(\eta)$ or $\tilde{Q}^2(\xi)$

1. The quantities α, β, and $\overline{K}$ pertaining to the η-equation: Subbarrier case [Fig. 3(a) in Ref. 11]

Denoting the zeros η_1, η_2, η_3, and η_4 by a, b, c, and d, we write the base function for this case as

$$Q(\eta)=p\,\frac{[(\eta-a)(b-\eta)(c-\eta)(d-\eta)]^{1/2}}{1-\eta^2}. \tag{2.1}$$

Using the transformation on p. 103 in Ref. 12, we obtain

$$\eta=\frac{a-d\,\nu_1^2\,\mathrm{sn}^2\,u}{1-\nu_1^2\,\mathrm{sn}^2\,u}, \tag{2.2}$$

the parameter ν_1^2 being defined in (2.4). Noting that the loop $a\to b\to a$, that is $\eta_1\to\eta_2\to\eta_1$ in the η-plane, denoted by $\Gamma_{a,b}$, which represents the contour Λ_α in Fig. 3(a) of Ref. 11, corresponds to $0\to K\to 2K$ in the u-plane, one finds that the first-order contribution to α is

$$\begin{aligned}\alpha^{(1)}&=\frac{1}{2}\int_{\Lambda_\alpha}Q(\eta)\,\mathrm{d}\eta\\&=\frac{1}{2}\int_{\Gamma_{a,b}}Q(\eta)\,\mathrm{d}\eta\\&=\frac{p}{2g}\int_0^{2K}\left(\frac{\mathrm{d}\eta}{\mathrm{d}u}\right)^2\frac{\mathrm{d}u}{1-\eta^2}\\&=\frac{2p(a-d)^2\nu_1^4}{g(1-a^2)}\int_0^{2K}\frac{\mathrm{sn}^2\,u(1-\mathrm{sn}^2\,u)(1-k^2\,\mathrm{sn}^2\,u)\mathrm{d}u}{(1-\nu_1^2\,\mathrm{sn}^2\,u)^2(1-\nu_2^2\,\mathrm{sn}^2\,u)(1-\nu_3^2\,\mathrm{sn}^2\,u)},\end{aligned} \tag{2.3}$$

where

$$\nu_1^2=\frac{a-b}{d-b},\quad \nu_2^2=\frac{1+d}{1+a}\,\nu_1^2,\quad \nu_3^2=\frac{1-d}{1-a}\,\nu_1^2, \tag{2.4}$$

$$g=\frac{2}{[(d-b)(c-a)]^{1/2}},\quad k^2=\frac{(d-c)(b-a)}{(d-b)(c-a)}. \tag{2.5}$$

Decomposing the integrand in (2.3) into partial fractions and evaluating the integrals by means of recurrence formulas in Ref. 12, we obtain

$$\alpha^{(1)}=H^{(1)}(\nu_1,\nu_2,\nu_3,g,k,C), \tag{2.6}$$

where $H^{(1)}$ is the "universal" function defined in Eqs. (3.16a), (3.16b), (3.17a)–(3.17c), and (3.18) of Ref. 10 but with $\tilde{C}$ replaced by C and the parameters ν_i, $i=1,2,3$, given by (2.4), and g and k^2 given by (2.5). The evaluation of the quantity $\alpha^{(1)}$ in the present case is thus similar to the evaluation of the quantity $\tilde{L}^{(1)}$ in Sec. III A 2 of Ref. 10.

Proceeding in a similar way, the third-order contribution to α is found to be

$$\begin{aligned}\alpha^{(3)}&=\frac{1}{2}\int_{\Lambda_\alpha}\left(-C+\frac{1}{1-\eta^2}\right)\frac{\mathrm{d}\eta}{2Q(\eta)(1-\eta^2)}-\frac{1}{16}\int_{\Lambda_\alpha}Q^{-3}(\eta)\left(\frac{\mathrm{d}Q}{\mathrm{d}\eta}\right)^2\mathrm{d}\eta\\&=H^{(3)}(\nu_1,\nu_2,\nu_3,g,k,C),\end{aligned} \tag{2.7}$$

where $H^{(3)}$ is the "universal" function given in Eqs. (3.16c), (3.16d), (3.19a)–(3.19d), and (3.20a)–(3.20d) of Ref. 10 but with $\tilde{C}$ replaced by $-C$ and the parameters ν_i, $i=1,2,3$, given by (2.4), and g and k^2 given by (2.5).

In a similar manner as previously we proceed for the calculation of the first- and third-order contributions to β. The loop $d\to c\to d$, that is $\eta_4\to\eta_3\to\eta_4$ in the η-plane, denoted by $\Gamma_{d,c}$ and represented by the contour Λ_β in Fig. 3(a) of Ref. 11, corresponds to $0\to K\to 2K$ in the u-plane, and hence the first- and third-order contributions to β are

$$\begin{aligned}\beta^{(1)}&=\frac{1}{2}\int_{\Lambda_\beta}Q(\eta)\mathrm{d}\eta\\&=\frac{1}{2}\int_{\Gamma_{d,c}}Q(\eta)\mathrm{d}\eta\\&=H^{(1)}(\nu_1,\nu_2,\nu_3,k,C),\end{aligned}\tag{2.8a}$$

and

$$\beta^{(3)}=H^{(3)}(\nu_1,\nu_2,\nu_3,g,k,C),\tag{2.8b}$$

where now

$$\nu_1^2=\frac{d-c}{d-b},\quad \nu_2^2=\frac{1+b}{1+c}\,\nu_1^2,\quad \nu_3^2=\frac{1-b}{1-c}\,\nu_1^2,\tag{2.9}$$

and g and k^2 are given by (2.5).

Similarly one obtains

$$\pi\overline{K}_0=H^{(1)}(\nu_1,\nu_2,\nu_3,g,k,C),\tag{2.10a}$$

$$\pi\overline{K}_2=H^{(3)}(\nu_1,\nu_2,\nu_3,g,k,C),\tag{2.10b}$$

where now

$$\nu_1^2=\frac{c-b}{d-b},\quad \nu_2^2=\frac{1+d}{1+c}\,\nu_1^2,\quad \nu_3^2=\frac{1-d}{1-c}\,\nu_1^2,\tag{2.11}$$

and g is the same as given in (2.5) and k^2 is now given by

$$k^2=\frac{(c-b)(d-a)}{(d-b)(c-a)}.\tag{2.12}$$

According to Eq. (3.18a) in Ref. 11 the integrals α' and β' for the contours $\Lambda_{\alpha'}$ and $\Lambda_{\beta'}$ in Fig. 3(a) in Ref. 11 are obtained from the formulas $\alpha'=\alpha+\Lambda\pi/2$ and $\beta'=\beta+\Lambda\pi/2$.

2. The quantities $\tilde{L}$ and $\tilde{L}'$ pertaining to the ξ-equation [Fig. 1 in Ref. 11]

The formulas for the first- and third-order contributions to $\tilde{L}$ and $\tilde{L}'$ are derived and presented in Sec. III A 2 of Ref. 10, and they remain unchanged in the present case.

B. Two real and two complex conjugate zeros of $Q^2(\eta)$ or $\tilde{Q}^2(\xi)$

When there are two real and two complex conjugate zeros of $Q^2(\eta)$, the situation of either Fig. 4(a) or Fig. 2 in Ref. 11 may occur. However, the latter situation has so far not appeared in our applications, and therefore we disregard it in our treatment in the following of the η-equation.

1. The quantities α, β, $\bar{K}$, L, and L' pertaining to the η-equation: Superbarrier case [Fig. 4(a) in Ref. 11]

Denoting the real zeros of $Q^2(\eta)$ by $\eta_1=a$ and $\eta_4=d$ and the complex conjugate zeros η_2 and η_3 by c and c^*, we have the base function

$$Q(\eta)=p\frac{[(a-\eta)(\eta-d)(\eta-c)(\eta-c^*)]^{1/2}}{1-\eta^2}. \tag{2.13}$$

Defining

$$c=b_1-ia_1, \quad c^*=b_1+ia_1, \tag{2.14}$$

$$A=[(a-b_1)^2+a_1^2]^{1/2}, \tag{2.15a}$$

$$B=[(d-b_1)^2+a_1^2]^{1/2}, \tag{2.15b}$$

and using the transformation on p. 133 in Ref. 12, we get

$$\eta=\frac{aB+dA+(dA-aB)\operatorname{cn}u}{A+B+(A-B)\operatorname{cn}u}. \tag{2.16}$$

Here we exploit the fact that the Jacobian elliptic functions are doubly periodic, one of the periods being complex. Thus the loop $d\to a_1+ib_1\to d$, that is $\eta_4\to\eta_3\to\eta_4$ in the η-plane, denoted by Γ_{d,c^*}, for the contour Λ_β in Fig. 4(a) of Ref. 11, corresponds in the u-plane to the path $0\to K+iK'\to 2K+2iK'$, where K and K' are complete elliptic integrals of the modulus k, given in (2.18e), and of the complementary modulus $k'=\sqrt{1-k^2}$, respectively. Making use of the transformation (2.16), we obtain for the integral in the first-order expression for β,

$$\begin{aligned}\frac{1}{2}\int_{\Lambda_\beta}Q(\eta)\,\mathrm{d}\eta&=\frac{1}{2}\int_{\Gamma_{d,c^*}}Q(\eta)\,\mathrm{d}\eta\\&=-\frac{p(\nu_1-\nu_2)(\nu_1-\nu_3)}{2g}\int_0^{2K+2iK'}\frac{\operatorname{sn}^2u\,\operatorname{dn}^2u\,\mathrm{d}u}{(1+\nu_1\operatorname{cn}u)^2(1+\nu_2\operatorname{cn}u)(1+\nu_3\operatorname{cn}u)},\end{aligned} \tag{2.17}$$

where

$$\nu_1=\frac{A-B}{A+B}, \tag{2.18a}$$

$$\nu_2=\frac{(1+d)A-(1+a)B}{(1+d)A+(1+a)B}, \tag{2.18b}$$

$$\nu_3=\frac{(1-d)A-(1-a)B}{(1-d)A+(1-a)B}, \tag{2.18c}$$

$$g=\frac{1}{\sqrt{AB}}, \tag{2.18d}$$

$$k^2=\frac{(a-d)^2-(A-B)^2}{4AB}. \tag{2.18e}$$

Similarly one can treat the corresponding integrals in the first-order expressions for α, K, and $\tilde{L}$. When one then evaluates the integrals containing the elliptic functions [cf. (2.17)], one finds that all these integrals can be expressed in terms of a ''universal'' function $\bar{H}^{(1)}$ that is given by

$$\begin{aligned}\bar{H}^{(1)}(\nu_1,\nu_2,\nu_3,g,k,C)=-\frac{p}{g}\Bigg\{&\frac{1}{\nu_1^2}\Bigg[\left(2k^2+\frac{\nu_1^2}{1-\nu_1^2}\right)\Pi\left(\frac{\nu_1^2}{\nu_1^2-1},k\right)+(\nu_1^2-2k^2)K(k)-2\nu_1^2E(k)\\&+\nu_1k(2j+1)\pi-\frac{\nu_1^2(1-2k^2)+2k^2}{[(1-\nu_1^2)(k^2+\nu_1^2k'^2)]^{1/2}}\frac{\nu_1}{2}j\pi\Bigg]\\&+\sum_{i=1}^{3}\bar{C}_i\bar{S}_i+i\Bigg[\left(2k^2+\frac{\nu_1^2}{1-\nu_1^2}\right)\Pi\left(\frac{1}{1-\nu_1^2},k'\right)-2k^2K(k')+2E(k')\Bigg]\Bigg\},\end{aligned} \tag{2.19}$$

where $\bar{C}_1$, $\bar{C}_2$, and $\bar{C}_3$ are given by Eqs. (3.37a)–(3.37c) in Ref. 10, that is,

$$\bar{C}_1=\frac{\nu_1^2(2\nu_3\nu_2-\nu_1\nu_3-\nu_1\nu_2)}{(\nu_1-\nu_2)(\nu_1-\nu_3)}, \tag{2.20a}$$

$$\bar{C}_2=\frac{(\nu_1-\nu_3)\nu_2^3}{(\nu_1-\nu_2)(\nu_2-\nu_3)}, \tag{2.20b}$$

$$\bar{C}_3=\frac{(\nu_1-\nu_2)\nu_3^3}{(\nu_1-\nu_3)(\nu_3-\nu_2)}, \tag{2.20c}$$

and

$$\begin{aligned}\bar{S}_i=&\frac{1}{\nu_i^4}\left[k^2(1-\nu_i^2)K(k)+\nu_i^2E(k)-(k^2+\nu_i^2k'^2)\Pi\left(\frac{\nu_i^2}{\nu_i^2-1},k\right)\right]+\frac{1}{2k\nu_i^3}\\&\times\left[\left(k^2(\nu_i^2-1)-\frac{\nu_i^2}{2}\right)(2j+1)\pi+k[(1-\nu_i^2)(k^2+k'^2\nu_i^2)]^{1/2}j\pi\right]\\&+\frac{i}{\nu_i^2}\left\{-(k^2+\nu_i^2k'^2)\left[\Pi\left(\frac{1}{1-\nu_i^2},k'\right)-K(k')\right]-E(k')\right\},\quad i=1,2,3,\end{aligned} \tag{2.21}$$

j being an integer -1, 0, or $+1$, depending upon whether the quantity $\beta^{(1)}$, $L^{(1)}$, or $\alpha^{(1)}$, respectively, is evaluated, and originating from terms $\tan^{-1}(\mathrm{sd}\,u)$ and $\cos^{-1}(\mathrm{dn}\,u)$ while applying the limits of integration. Note that the quantity $\tilde{L}^{(1)}$, given by Eq. (3.36a) in Ref. 10, is just $-2\,\mathrm{Re}\,\bar{H}^{(1)}$ with $j=0$. For K, which is expressed in terms of the imaginary part of $\bar{H}^{(1)}$, the value of j, which appears only in the real part of $\bar{H}^{(1)}$, does not matter.

Similarly we also introduce the ''universal''function $\bar{H}^{(3)}$ given by

$$\overline{H}^{(3)}(\nu_1,\nu_2,\nu_3,g,k,C)=\frac{g}{16p}\left[\left(-4C+\frac{\nu_1^2(\nu_2-\nu_3)^2}{\nu_2\nu_3(\nu_1-\nu_3)(\nu_2-\nu_1)}\right)K(k)\right.$$
$$\left.+\frac{1}{(\nu_1-\nu_3)(\nu_1-\nu_2)}\left(XK(k)+YE(k)+\frac{2Zj}{k}\pi\right)\right]$$
$$+i\frac{g}{16p}\left[\left(-4C+\frac{\nu_1^2(\nu_2-\nu_3)^2}{\nu_2\nu_3(\nu_1-\nu_3)(\nu_2-\nu_1)}\right)K(k')\right.$$
$$\left.+\frac{1}{(\nu_1-\nu_3)(\nu_1-\nu_2)}\{XK(k')+Y[K(k')-E(k')]\}\right], \quad (2.22)$$

where C is the parameter in the square of the base function $Q(\eta)$ in Eq. (3.2b) of Ref. 11, and

$$X=-\frac{1+4k^2}{3}+\frac{3+4k'^2}{3}(\nu_1^2+2\nu_1\nu_2+2\nu_1\nu_3+\nu_2\nu_3)-\frac{k'^2}{3k^2}(17-4k^2)\nu_1^2\nu_2\nu_3$$
$$-2\nu_1(\nu_1+\nu_2+\nu_3)+2\nu_2\nu_3+\nu_1^2\left(\frac{\nu_2}{\nu_3}+\frac{\nu_3}{\nu_2}\right), \quad (2.23a)$$

$$Y=\frac{1}{3k'^2}(1+8k^2-8k^4)+\frac{4}{3}(2k^2-1)(\nu_1^2+2\nu_1\nu_2+2\nu_1\nu_3+\nu_2\nu_3)$$
$$+\frac{\nu_1^2\nu_2\nu_3}{3k^2}(17-8k^2+8k^4), \quad (2.23b)$$

$$Z=2\nu_1(\nu_1\nu_2+\nu_1\nu_3+4\nu_2\nu_3), \quad (2.23c)$$

where the parameters ν_1, ν_2, ν_3, g, and k^2 are defined in (2.18a)–(2.18e).

Then the first- and third-order contributions to the quantities α, β, and $K(=\pi\overline{K})$ are

$$\alpha^{(1)}=\mathrm{Re}\,\overline{H}^{(1)} \quad \text{with} \quad j=1, \quad (2.24)$$

$$\beta^{(1)}=\mathrm{Re}\,\overline{H}^{(1)} \quad \text{with} \quad j=-1, \quad (2.25)$$

$$\pi\overline{K}_0=-2\,\mathrm{Im}\,\overline{H}^{(1)}, \quad (2.26)$$

$$\alpha^{(3)}=\mathrm{Re}\,\overline{H}^{(3)} \quad \text{with} \quad j=1, \quad (2.27)$$

$$\beta^{(3)}=\mathrm{Re}\,\overline{H}^{(3)} \quad \text{with} \quad j=-1, \quad (2.28)$$

$$\pi\overline{K}_2=-2\,\mathrm{Im}\,\overline{H}^{(3)}, \quad (2.29)$$

where ν_1, ν_2, ν_3, g, and k^2 are still defined by (2.18a)–(2.18e). Since j appears only in the real part of $\overline{H}^{(2n+1)}$, we need not specify a value of j in (2.26) and (2.29).

The integrals α' and β' associated with the contours $\Lambda_{\alpha'}$ and $\Lambda_{\beta'}$ in Fig. 4(a) in Ref. 11 are obtained from α and β by means of the relations (3.18a) in Ref. 11, that is, $\alpha'=\alpha+\Lambda\pi/2$ and $\beta'=\beta+\Lambda\pi/2$. The integrals L and L' associated with the contours Λ_L and $\Lambda_{L'}$ in Fig. 4(a) in Ref. 11 can be obtained from α and β by means of the formulas $L=\alpha+\beta$ and $L'=L+|m|$.

2. The quantities $\tilde{L}$ and $\tilde{L}'$ pertaining to the ξ-equation [Fig. 1(a) in Ref. 11]

The formulas for the first- and third-order contributions to $\tilde{L}$ and $\tilde{L}'$ remain the same as the ones presented in Sec. III B 2 of Ref. 10.

III. CASE $\Lambda=0$

A. Two real zeros of $Q^2(\eta)$ or $\tilde{Q}^2(\xi)$

One should be able to obtain the formulas pertaining to the case $\Lambda=0$ by considering the limits of the "universal" functions $H^{(1)}$ and $H^{(3)}$ when $a\to-1$ and $d\to+1$ in the case of the η-equation. These specialization procedures are, however, much more cumbersome than the direct calculation of the quantities in question, and so we do not carry them out here. Instead we shall evaluate these quantities directly, and therefore no "universal" functions will appear in Sec. III A.

1. The quantities α, β, and $\bar{K}$ pertaining to the η-equation: Subbarrier case [Fig. 3(b) in Ref. 11]

We denote the two real zeros of $Q^2(\eta)$ by $\eta_2=b$ and $\eta_3=c$ and use transformations on pp. 103, 120, and 112 in Ref. 12 for calculating the first- and third-order contributions to α, β, and K, respectively. Here the base function reads

$$Q(\eta)=p\left[\frac{(\eta-b)(c-\eta)}{1-\eta^2}\right]^{1/2}. \tag{3.1}$$

The first- and third-order contributions to α are

$$\alpha^{(1)}=\frac{2p}{g\nu^2}[\nu^2E(k)-(k^2+\nu^2)K(k)+(k^2-\nu^4)\Pi(\nu^2,k)], \tag{3.2a}$$

and

$$\begin{aligned}\alpha^{(3)}=&-\frac{gCK(k)}{p}+\frac{g}{4p\nu^2}\left[\left(1-2\nu^2+\frac{\nu^4}{k^2}\right)K(k)-\left(1+\frac{\nu^4}{k^2}\right)E(k)\right]\\&-\frac{g}{32p\nu^2}\left\{\frac{1}{3k'^2}\left[\frac{1}{k^2}(4\nu^4-6\nu^2)+5\nu^4+4\nu^2+8-k^2(4+3\nu^4)-\frac{6\nu^4}{k^4}\right]K(k)\right.\\&\left.+\frac{1}{3k'^4}\left[-8k^4+(2+8\nu^2+4\nu^4)k^2-8+2\nu^4+\nu^2-\frac{1}{k^2}(2\nu^4+12\nu^2)+\frac{12\nu^4}{k^4}\right]E(k)\right\},\end{aligned} \tag{3.2b}$$

where

$$\nu^2=\frac{c+1}{c-1},\quad k^2=\frac{(1-b)(1+c)}{(1+b)(1-c)},\quad g=\frac{2}{[(1-c)(1+b)]^{1/2}}. \tag{3.3}$$

Similarly the first- and third-order contributions to β are

$$\beta^{(1)}=\frac{2p}{g\nu^2}[\nu^2E(k)+(k^2-\nu^2)K(k)+(\nu^4-k^2)\Pi(\nu^2,k)], \tag{3.4a}$$

and

$$\beta^{(3)}=-\frac{gCK(k)}{2p}+\frac{g}{4p\nu^2(1-c)}\left\{\left(1-\frac{\nu^4}{k^2}\right)K(k)+[k^2(2k^2-1-2\nu^2)+\nu^4]\frac{E(k)}{k^2k'^2}\right\}$$
$$-\frac{g}{16(1-c)p\nu^2}\left\{\frac{4}{3k^2}[(2+\nu^4+2\nu^2)k^2-3k^4-2\nu^4]K(k)\right.$$
$$\left.+\frac{8}{3k'^2}\left(-(\nu^4+\nu^2-1)+k^2(\nu^4-\nu^2+2)+\frac{\nu^4}{k^2}\right)E(k)\right\} \tag{3.4b}$$

with

$$\nu^2=\frac{1-b}{1-c} \tag{3.5}$$

and k^2 and g defined in (3.3).

The first- and third-order contributions to $K(=\pi\overline{K})$ are

$$\pi\overline{K}_0=\frac{2p}{gk^2}[(k^2-\nu^2)K(k)-\nu^2E(k)-(\nu^4-2\nu^2+k^2)\Pi(\nu^2,k)], \tag{3.6a}$$

and

$$\pi\overline{K}_2=-\frac{CgK(k)}{2p}+\frac{g}{2(c^2-1)p}\left[\frac{2\nu^2}{k^4}(k^2-\nu^2)K(k)+\frac{1}{k^4k'^2}\{k^2(k^2-\nu^4-2\nu^2)+2\nu^4\}E(k)\right]$$
$$-\frac{g}{24\nu^4p(c-1)}\{(-2+k^2+\nu^2-\nu^4)K(k)+2[k^4-(1+\nu^2+\nu^4)k^2-\nu^2+2\nu^4+1]E(k)\}, \tag{3.6b}$$

with

$$\nu^2=\frac{b-c}{b+1},\quad k^2=\frac{2(b-c)}{(1+b)(1-c)} \tag{3.7}$$

and g defined in (3.3).

2. The quantities $\tilde{L}$ and $\tilde{L}'$ pertaining to the ξ-equation [Fig. 1 in Ref. 11]

The formulas for the first- and third-order contributions to $\tilde{L}$ and $\tilde{L}'$ are the same as those derived and presented in Sec. IV A 2 of Ref. 10.

B. Two complex conjugate zeros of $Q^2(\eta)$

The situation of two complex conjugate transition zeros can occur only for $Q^2(\eta)$ but not for $\tilde{Q}^2(\xi)$.

The quantities α, β, and $\overline{K}$ pertaining to the η-equation: Superbarrier case [Fig. 4(b) in Ref. 11]. Specializing the general formulas (2.19) and (2.22) by putting $a=-1$, $d=+1$, we obtain

$$\overline{H}^{(1)}=\frac{p}{g}\left\{E(k)-K(k)+\frac{1}{1-\nu^2}\left[\Pi\left(\frac{\nu^2}{\nu^2-1},k\right)-\left(\frac{\nu^2(1-\nu^2)}{k^2+(1-k^2)\nu^2}\right)^{1/2}(2j+1)\pi\right]\right\}$$
$$+i\frac{p}{g}\left[K(k')-E(k')+\frac{\nu^2}{1-\nu^2}\Pi\left(\frac{1}{1-\nu^2},k'\right)\right] \tag{3.8a}$$

and

$$\overline{H}^{(3)}=\frac{g}{16p}\left\{\left(-4C+\frac{4\nu^2}{\nu^2-1}\right)K(k)+\frac{1}{\nu^2-1}\left(\overline{X}K(k)+\overline{Y}E(k)-\frac{16\nu j}{k}\pi\right)\right.$$
$$\left.+i\left[\left(-4C+\frac{4\nu^2}{\nu^2-1}\right)K(k')+\frac{1}{\nu^2-1}(\overline{X}K(k')+\overline{Y}[K(k')-E(k')])\right]\right\} \tag{3.8b}$$

where

$$\nu=\frac{A-B}{A+B},\quad g=\frac{1}{\sqrt{AB}},\quad k^2=\frac{4-(A-B)^2}{4AB} \tag{3.9}$$

with

$$A=[(1-b_1)^2+a_1^2]^{1/2},\quad B=[(1+b_1)^2+a_1^2)]^{1/2} \tag{3.10}$$

and

$$\overline{X}=-\frac{1}{3k^2}[k^2(14+9\nu^2)+17\nu^2], \tag{3.11a}$$

$$\overline{Y}=\frac{1}{3k^2k'^2}[-4k^4(1+\nu^2)+k^2(5+21\nu^2)-17\nu^2]. \tag{3.11b}$$

We now have

$$\alpha^{(1)}=\mathrm{Re}\,\overline{H}^{(1)}\ \text{ with }\ j=1, \tag{3.12a}$$

$$\alpha^{(3)}=\mathrm{Re}\,\overline{H}^{(3)}\ \text{ with }\ j=1, \tag{3.12b}$$

$$\beta^{(1)}=\mathrm{Re}\,\overline{H}^{(1)}\ \text{ with }\ j=-1, \tag{3.13a}$$

$$\beta^{(3)}=\mathrm{Re}\,\overline{H}^{(3)}\ \text{ with }\ j=-1, \tag{3.13b}$$

$$\pi\overline{K}_0=-2\,\mathrm{Im}\,\overline{H}^{(1)}, \tag{3.14a}$$

$$\pi\overline{K}_2=-2\,\mathrm{Im}\,\overline{H}^{(3)}. \tag{3.14b}$$

The integral L' associated with the contour $\Lambda_{L'}$ in Fig. 4(b) in Ref. 11 is obtained from the formula $L'=\alpha+\beta$.

IV. NUMERICAL ILLUSTRATION OF THE ACCURACY OF THE QUANTIZATION CONDITIONS

For the numerical illustration of the asymmetric case we have chosen $Z_1=1$ and considered three different values of Z_2, viz. $Z_2=2$, 5, and 8. The corresponding physical systems are the ions peHe^{2+}, peB^{5+}, and peO^{8+}, respectively, where p is a proton and e is an electron. For each one of these systems we have calculated the eigenvalue p and the reduced separation constant A' for two different σ-states and various values of r_{12}.

For the ion peHe^{2+} we have calculated the eigenvalue p and the reduced separation constant A' for the $1s\sigma$ and $2p\sigma$ states and various values of r_{12}, with appropriate quantization conditions and parameters. The quantization conditions in Ref. 11 for the $1s\sigma$ state are (3.5a) with $\tilde{s}=0$ [Fig. 1(a) in Ref. 11] and (3.9) with $s=m=0$ [Fig. 4(b) in Ref. 11] when r_{12} is sufficiently small, but (3.5b) with $\tilde{s}=m=0$ [Fig. 1(b) in Ref. 11] and (3.23b) with $s_\beta=m=0$ [Fig. 3(b) in Ref. 11] when r_{12} is sufficiently large. The quantization conditions in Ref. 11 for the $2p\sigma$ state are (3.5a) with

TABLE I. For the state $1s\sigma$ of the ion peHe^{2+} ($Z_1=1$, $Z_2=2$) the values of C and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for p as well as for A'. With the use of these values of C and $\tilde{C}$ the values of p and A' have then been obtained from the quantization conditions that are appropriate depending on whether r_{12} is sufficiently small or sufficiently large. The numerically exact values (accurate to all digits quoted) calculated by Winter, Duncan, and Lane (Ref. 4) and obtained as private communication from Professor Winter (see p. 288–289 in Ref. 4), are given in the columns p_{WDL} and A'_{WDL}.

r_{12}	C	$\tilde{C}$	p	p_{WDL}	$p-p_{\mathrm{WDL}}$	A'	A'_{WDL}	$A'-A'_{\mathrm{WDL}}$
Sufficiently small r_{12}								
0.2	0.429 636 290 0	0.498 615 930 0	0.291 383 595 7	0.290 953 422 8	0.000 430 173	−0.040 174 248 0	−0.049 553 118 6	0.009 378 87
0.4	0.493 861 021 0	0.499 134 204 7	0.554 673 563 1	0.554 404 047 7	0.000 269 516	−0.167 459 05	−0.175 244 393 5	0.007 785 348
0.6	0.501 452 965 0	0.502 193 641 8	0.794 973 025 6	0.794 506 105 6	0.000 466 92	−0.340 429 782 1	−0.347 538 152 2	0.007 108 37
0.8	0.502 367 219 5	0.504 529 183 1	1.018 520 819	1.018 366 017	−0.000 154 802	−0.541 765 53	−0.547 374 893 8	0.005 609 36
1.0	0.503 279 341 8	0.506 153 913 2	1.231 430 173	1.231 534 107	−0.000 103 934	−0.757 259 45	−0.762 414 748 1	0.005 155 3
2.0	0.505 914 555 0	0.508 360 674 0	2.241 478 757	2.241 514 227	−0.000 035 47	−1.870 558 067	−1.866 548 007	−0.004 010 06
Sufficiently large r_{12}								
3.0	0.495 165 115 0	0.509 990 487 0	3.241 389 959	3.241 868 168	−0.000 478 209	−2.918 225 629	−2.914 992 386	−0.003 233 243
4.0	0.490 440 911 0	0.509 430 828 0	4.243 060 447	4.243 211 413	−0.000 150 966	−3.938 607 817	−3.937 060 587	−0.001 547 23
5.0	0.487 819 713 0	0.508 527 279 0	5.244 268 024	5.244 326 655	−0.000 058 631	−4.950 729 976	−4.949 835 242	−0.000 894 734
6.0	0.486 158 619 0	0.507 663 201 0	6.245 131 490	6.245 159 553	−0.000 028 063	−5.958 842 182	−5.958 257 005	−0.000 585 177
7.0	0.485 014 520 0	0.506 911 980 0	7.245 774 185	7.245 789 653	−0.000 015 468	−6.964 658 345	−6.964 245 417	−0.000 412 928
8.0	0.484 180 140 0	0.506 273 720 0	8.246 269 561	8.246 278 979	−0.000 009 418	−7.969 033 663	−7.968 726 708	−0.000 306 955
9.0	0.483 545 672 0	0.505 732 525 0	9.246 662 366	9.246 668 544	−0.000 006 178	−8.972 444 904	−8.972 207 821	−0.000 237 083
10.0	0.483 047 591 0	0.505 271 252 0	10.246 981 13	10.246 985 42	−0.000 004 29	−9.975 179 205	−9.974 990 618	−0.000 188 587
11.0	0.482 646 613 0	0.504 875 107 0	11.247 244 80	11.247 247 92	−0.000 003 12	−10.977 419 91	−10.977 266 35	−0.000 153 56
12.0	0.482 317 160 0	0.504 532 116 0	12.247 466 43	12.247 468 78	−0.000 002 35	−11.979 289 63	−11.979 162 18	−0.000 127 45
13.0	0.482 041 888 0	0.504 232 758 0	13.247 655 26	13.247 657 09	−0.000 001 83	−12.980 873 44	−12.980 765 98	−0.000 107 46
14.0	0.481 808 600 0	0.503 969 520 0	14.247 818 04	14.247 819 49	−0.000 001 45	−13.982 232 27	−13.982 140 45	−0.000 091 82
15.0	0.481 808 600 0	0.503 736 437 0	15.247 959 78	15.247 960 97	−0.000 001 19	−14.983 410 87	−14.983 331 513	−0.000 079 36
20.0	0.503 205 646 0	0.502 884 623 0	20.248 460 92	20.248 461 08	−0.000 000 16	−19.987 542 06	−19.987 499 42	−0.000 042 64
40.0	0.501 581 890 0	0.501 502 700 0	40.249 224 10	40.249 224 14	−0.000 000 04	−39.993 759 65	−39.993 749 96	−0.000 009 69
60.0	0.501 050 490 0	0.501 015 330 0	60.249 481 50	60.249 481 48	−0.000 000 02	−59.995 837 79	−59.995 833 32	−0.000 004 47
80.0	0.500 786 200 0	0.500 766 500 0	80.249 610 66	80.249 610 66	−0.000 000 00	−79.996 877 47	−79.996 874 99	−0.000 002 48

TABLE II. For the state $2p\sigma$ of the ion peHe^{2+} ($Z_1=1$, $Z_2=2$) the values of C and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for p as well as for A'. With the use of these values of C and $\tilde{C}$ the values of p and A' have then been obtained from the quantization conditions that are appropriate depending on whether r_{12} is sufficiently small or sufficiently large. The numerically exact values (accurate to all digits quoted) calculated by Winter, Duncan, and Lane (Ref. 4), and obtained as private communication from Professor Winter (see p. 288 and 289 in Ref. 4), are given in the columns p_{WDL} and A'_{WDL}.

r_{12}	C	$\tilde{C}$	p	p_{WDL}	$p-p_{\mathrm{WDL}}$	A'	A'_{WDL}	$A'-A'_{\mathrm{WDL}}$
Sufficiently small r_{12}								
0.2	0.529 483 195 2	0.502 917 361 9	0.151 793 028 3	0.150 799 407 8	0.000 993 621	−2.009 318 372	−2.013 114 367	0.003 795 995
0.4	0.548 173 649 2	0.510 283 746 3	0.302 891 038 2	0.306 268 040 6	−0.003 377 002	−2.049 183 021	−2.053 824 124	0.004 641 103
0.6	0.592 837 408 1	0.527 910 282 7	0.468 491 904	0.469 837 259 7	−0.001 345 355	−2.120 325 324	−2.125 935 288	0.005 609 964 0
0.8	0.649 329 651 8	0.538 028 183 7	0.642 918 371	0.641 603 874 7	0.001 314 497	−2.226 301 818	−2.234 147 173	0.007 845 355
1.0	0.691 827 652 3	0.540 018 392 6	0.819 207 383	0.818 028 770 0	0.001 178 613	−2.382 017 327	−2.381 560 387	−0.000 456 94
2.0	0.729 184 714 2	0.541 064 392 9	1.641 039 285	1.640 235 157	0.000 804 128	−3.839 201 840	−3.846 791 567	0.007 589 727
Sufficiently large r_{12}								
3.0	0.793 129 854 7	0.542 632 985 6	2.304 295 844	2.303 194 434	0.001 101 41	−5.443 294 571	−5.444 185 235	0.000 890 664
4.0	0.836 843 296 1	0.542 917 392 1	2.869 430 632	2.872 046 343	−0.002 615 711	−7.447 320 938	−7.448 941 809	0.001 620 871
5.0	0.943 946 795 0	0.542 739 369 0	3.398 416 434	3.395 848 335	0.002 568 099	−9.524 254 856	−9.526 950 457	0.002 695 601
6.0	0.771 081 278 0	0.542 203 532 0	3.913 851 362	3.901 954 918	0.011 896 444	−11.586 707 82	−11.615 699 23	0.028 991 41
7.0	0.708 078 157 0	0.540 749 433 0	4.425 841 569	4.404 864 367	0.020 977 202	−13.633 853 83	−13.686 965 69	0.053 111 86
8.0	0.670 970 956 0	0.538 958 544 0	4.933 037 475	4.909 225 930	0.023 811 545	−15.676 830 67	−15.736 659 89	0.059 829 22
9.0	0.644 912 530 0	0.537 037 760 0	5.438 128 294	5.414 760 984	0.023 367 31	−17.713 140 08	−17.771 068 69	0.057 928 61
10.0	0.625 241 766 0	0.535 115 051 0	5.942 311 467	5.920 460 066	0.021 851 401	−19.742 854 83	−19.796 296 10	0.053 441 27
11.0	0.609 801 785 0	0.533 264 016 0	6.445 985 745	6.425 795 942	0.020 189 803	−21.767 156 93	−21.815 923 89	0.048 766 96
12.0	0.597 347 656 0	0.531 520 860 0	6.949 277 104	6.930 614 764	0.018 662 34	−23.787 269 83	−23.831 846 80	0.044 576 97
13.0	0.587 084 103 0	0.529 899 278 0	7.452 239 113	7.434 919 206	0.017 319 907	−25.804 162 11	−25.845 121 32	0.040 959 21
14.0	0.578 475 907 0	0.528 400 535 0	7.954 909 402	7.938 760 040	0.016 149 362	−27.818 547 86	−27.856 398 10	0.037 850 24
15.0	0.571 149 580 0	0.527 019 580 0	8.457 321 437	8.442 196 146	0.015 125 291	−29.830 949 19	−29.866 114 05	0.035 164 86
20.0	0.512 367 730 0	0.521 586 120 0	10.965 975 37	10.954 972 57	0.011 002 800	−39.875 040 33	−39.899 835 85	0.024 795 52
40.0	0.484 449 000 0	0.511 755 000 0	20.981 890 02	20.976 244 19	0.005 645 83	−79.937 707 97	−79.949 990 45	0.012 282 48
60.0	0.475 574 500 0	0.507 995 500 0	30.987 803 27	30.983 886 96	0.003 916 31	−119.958 467 1	−119.966 664 8	0.008 197 7
80.0	0.471 195 900 0	0.506 062 800 0	40.990 805 30	40.987 811 64	0.002 993 66	−159.968 799 1	−159.974 999 4	0.006 198 7

TABLE III. For the state $1s\sigma$ of the ion peB^{5+} ($Z_1=1$, $Z_2=5$) the values of C and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for p as well as for A'. With the use of these values of C and $\tilde{C}$ the values of p and A' have then been obtained from the quantization conditions that are appropriate depending on whether r_{12} is sufficiently small or sufficiently large. The numerically exact values obtained by Ponomarev and Puzynina (Ref. 13) are given in the columns p_{pp} and A'_{pp}. When r_{12} is so large that the phase integral values of p and A' are approximately as accurate or more accurate than the corresponding values in Ref. 13 we do not give values for $p-p_{\mathrm{pp}}$ and $A'-A'_{\mathrm{pp}}$, but denote them by three asterisks.

r_{12}	C	$\tilde{C}$	p	p_{pp}	$p-p_{\mathrm{pp}}$	A'	A'_{pp}	$A'-A'_{\mathrm{pp}}$
Sufficiently small r_{12}								
0.2	0.518 32	0.483 29	0.576 736	0.571 80	0.004 94	−0.102 639	−0.106 339	0.003 700
0.4	0.515 68	0.489 37	1.093 781	1.093 19	0.000 59	−0.318 422	−0.312 917	0.005 505
0.6	0.513 79	0.495 83	1.597 092	1.597 54	−0.000 49	−0.539 704	−0.533 666	−0.006 038
0.8	0.510 57	0.499 61	2.097 826	2.098 27	−0.000 44	−0.753 875	−0.749 331	−0.004 544
1.0	0.508 47	0.501 37	2.598 201	2.598 47	−0.000 27	−0.962 648	−0.959 583	−0.003 065
2.0	0.504 56	0.502 73	5.099 079	5.099 06	+0.000 02	−1.980 607	−1.979 97	−0.000 64
Sufficiently large r_{12}								
3.0	0.503 20	0.502 31	7.599 399	7.599 36	+0.000 04	−2.986 865	−2.986 66	−0.000 21
4.0	0.502 30	0.501 92	10.099 513	10.099 5	***	−3.990 163	−3.990 00	−0.000 16
5.0	0.500 81	0.501 64	12.599 680	12.599 6	***	−4.991 936	−4.992 00	+0.000 06
6.0	0.500 90	0.501 41	15.099 774	15.099 7	***	−5.993 175	−5.993 33	+0.000 16
7.0	0.500 82	0.501 24	17.599 832	17.599 7	***	−6.994 086	−6.994 28	+0.000 19
8.0	0.500 81	0.501 11	20.099 870	20.099 8	***	−7.994 774	−7.995 00	+0.000 23
9.0	0.500 80	0.501 00	22.599 897	22.599 8	***	−8.995 344	−8.995 56	+0.000 22
10.0	0.500 80	0.500 90	25.099 916	25.099 8	***	−9.995 783	−9.995 63	−0.000 15
11.0	0.500 70	0.500 83	27.599 930	27.599 8	***	−10.996 136	−10.996 0	***
12.0	0.500 70	0.500 80	30.099 941	30.099 8	***	−11.996 448	−11.996 4	***
13.0	0.500 60	0.500 67	32.599 950	32.599 8	***	−12.996 740	−12.996 6	***
14.0	0.500 70	0.500 60	35.099 957	35.099 8	***	−13.996 981	−13.996 9	***
15.0	0.500 60	0.500 60	37.599 962	37.599 9	***	−14.997 142	−14.997 1	***
16.0	0.500 62	0.500 59	40.099 873	40.099 9	***	−15.997 511	−15.997 3	***
17.0	0.500 59	0.500 55	42.599 883	42.599 9	***	−16.997 657	−16.997 4	***
18.0	0.500 56	0.500 53	45.099 889	45.099 9	***	−17.997 782	−17.997 6	***
19.0	0.500 50	0.500 40	47.599 912	47.599 9	***	−18.997 964	−18.997 7	***
20.0	0.500 60	0.500 50	50.099 978	50.099 9	***	−19.997 796	−19.997 8	***

TABLE IV. For the state $3s\sigma$ of the ion peB^{5+} ($Z_1=1$, $Z_2=5$) the values of C and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for p as well as for A'. With the use of these values of C and $\tilde{C}$ the values of p and A' have then been obtained from the quantization conditions that are appropriate depending on whether r_{12} is sufficiently small or sufficiently large. The numerically exact values obtained by Ponomarev and Puzynina (Ref. 13) are given in the columns p_{pp} and A'_{pp}. When r_{12} is so large that the phase integral values of p and A' are approximately as accurate or more accurate than the corresponding values in Ref. 13 we do not give values for $p-p_{\mathrm{pp}}$ and $A'-A'_{\mathrm{pp}}$, but denote them by three asterisks.

r_{12}	C	$\tilde{C}$	p	p_{pp}	$p-p_{\mathrm{pp}}$	A'	A'_{pp}	$A'-A'_{\mathrm{pp}}$
Sufficiently small r_{12}								
0.2	0.469 00	0.444 00	0.197 728	0.196 723	+0.001 005	0.118 904	0.077 870	+0.041 034
0.4	0.431 00	0.426 00	0.386 620	0.386 538	+0.000 082	0.277 525	0.286 919	−0.009 394
0.6	0.426 20	0.422 80	0.572 037	0.572 068	−0.000 031	0.570 774	0.579 790	−0.009 016
0.8	0.428 00	0.422 80	0.754 729	0.754 721	+0.000 008	0.916 385	0.921 649	−0.005 264
1.0	0.431 10	0.424 60	0.935 242	0.935 213	+0.000 029	1.290 323	1.293 12	−0.002 80
2.0	0.445 50	0.436 80	1.817 203	1.817 20	0.000 00	3.347 775	3.348 45	−0.000 68
Sufficiently large r_{12}								
3.0	0.456 80	0.447 62	2.680 126	2.680 08	+0.000 05	5.536 925	5.536 64	+0.000 29
4.0	0.464 00	0.456 00	3.533 310	3.533 28	+0.000 03	7.777 719	7.777 53	+0.000 19
5.0	0.468 70	0.462 35	4.380 874	4.380 88	−0.000 01	10.045 943	10.046 1	−0.000 2
6.0	0.473 20	0.467 30	5.224 967	5.224 94	+0.000 03	12.331 720	12.331 4	+0.000 3
7.0	0.476 08	0.471 19	6.066 647	6.066 62	+0.000 03	14.627 793	14.627 6	+0.000 2
8.0	0.478 20	0.474 30	6.906 648	6.906 65	−0.000 00	16.931 213	16.931 3	***
9.0	0.480 42	0.476 85	7.745 476	7.745 46	+0.000 02	19.240 602	19.240 5	***
10.0	0.482 02	0.478 98	8.583 369	8.583 35	+0.000 02	21.553 777	21.553 7	***
11.0	0.483 37	0.480 77	9.420 559	9.420 55	***	23.870 068	23.870 0	***
12.0	0.484 60	0.482 30	10.257 201	10.257 2	***	26.188 828	26.188 8	***
13.0	0.485 53	0.483 56	11.093 399	11.093 4	***	28.509 499	28.509 5	***
14.0	0.486 61	0.484 71	11.929 252	11.929 2	***	30.831 947	30.831 8	***
15.0	0.487 20	0.485 70	12.764 781	12.764 8	***	33.155 366	33.155 4	***
16.0	0.488 24	0.486 54	13.600 085	13.600 1	***	35.480 058	35.480 1	***
17.0	0.488 85	0.487 36	14.435 173	14.435 2	***	37.805 656	37.805 7	***
18.0	0.489 42	0.488 05	15.270 089	15.270 1	***	40.132 040	40.132 1	***
19.0	0.489 92	0.488 67	16.104 854	16.104 8	***	42.459 078	42.459 1	***
20.0	0.490 15	0.489 23	16.939 489	16.939 5	***	44.786 712	44.786 7	***

TABLE V. For the state $1s\sigma$ of the ion peO^{8+} ($Z_1=1$, $Z_2=8$) the values of C and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for p as well as for A'. With the use of these values of C and $\tilde{C}$ the values of p and A' have then been obtained from the quantization conditions that are appropriate depending on whether r_{12} is sufficiently small or sufficiently large. The numerically exact values obtained by Ponomarev and Puzynina (Ref. 13) are given in the columns p_{pp} and A'_{pp}. When r_{12} is so large that the phase integral values of p and A' are approximately as accurate or more accurate than the corresponding values in Ref. 13 we do not give values for $p-p_{\mathrm{pp}}$ and $A'-A'_{\mathrm{pp}}$, but denote them by three asterisks.

r_{12}	C	$\tilde{C}$	p	p_{pp}	$p-p_{\mathrm{pp}}$	A'	A'_{pp}	$A'-A'_{\mathrm{pp}}$
Sufficiently small r_{12}								
0.2	0.501 93	0.480 91	0.857 612	0.855 323	+0.002 289	−0.137 649	−0.142 128	+0.004 479
0.4	0.503 94	0.494 37	1.661 131	1.661 44	+0.000 09	−0.366 556	−0.361 348	−0.005 208
0.6	0.503 80	0.498 90	2.461 700	2.461 87	−0.000 17	−0.576 667	−0.573 808	0.002 859
0.8	0.503 35	0.500 43	3.261 920	3.261 97	−0.000 05	−0.782 022	−0.780 407	−0.001 615
1.0	0.502 80	0.501 00	4.062 060	4.062 06	0.000 00	−0.985 331	−0.984 350	−0.000 981
2.0	0.501 70	0.501 20	8.062 283	8.062 26	+0.000 02	−1.992 407	−1.992 19	−0.000 22
Sufficiently large r_{12}								
3.0	0.501 30	0.501 00	12.062 372	12.0623	***	−2.994 818	−2.994 79	−0.000 03
4.0	0.500 83	0.500 78	16.062 383	16.0624	***	−3.996 148	−3.996 09	−0.000 06
5.0	0.500 50	0.500 70	20.062 566	20.0624	***	−4.996 555	−4.996 87	+0.000 32
6.0	0.500 43	0.500 53	24.062 567	24.0624	***	−5.997 131	−5.997 24	+0.000 11
7.0	0.500 50	0.500 50	28.062 564	28.0624	***	−6.997 498	−6.997 64	+0.000 14
8.0	0.500 40	0.500 40	32.062 561	32.0624	***	−7.997 818	−7.997 93	+0.000 11
9.0	0.500 50	0.500 40	36.062 557	36.0624	***	−8.998 017	−8.998 16	+0.000 15
10.0	0.500 00	0.500 40	40.062 432	40.0624	***	−9.998 458	−9.998 34	−0.000 12
11.0	0.500 40	0.500 30	44.062 551	44.0624	***	−10.998 401	−10.998 5	***
12.0	0.500 00	0.500 30	48.062 446	48.0624	***	−11.998 716	−11.998 6	***
13.0	0.500 00	0.500 30	52.062 451	52.0625	***	−12.998 804	−12.998 7	***
14.0	0.500 10	0.500 30	56.062 455	56.0625	***	−13.998 861	−13.998 8	***
15.0	0.499 99	0.500 210	60.062 459	60.0625	***	−14.998 981	−14.998 9	***
16.0	0.500 24	0.500 23	64.062 466	64.0625	***	−15.999 028	−15.999 0	***
17.0	0.500 23	0.500 22	68.062 469	68.0625	***	−16.999 082	−16.999 0	***

TABLE VI. For the state $4d\sigma$ of the ion peO^{8+} ($Z_1=1$, $Z_2=8$) the values of C and $\tilde{C}$ have been obtained from the requirement that the first- and third-order phase-integral results coincide for p as well as for A'. With the use of these values of C and $\tilde{C}$ the values of p and A' have then been obtained from the quantization conditions that are appropriate depending on whether r_{12} is sufficiently small or sufficiently large. The numerically exact values obtained by Ponomarev and Puzynina (Ref. 13) are given in the columns p_{pp} and A'_{pp}. When r_{12} is so large that the phase integral values of p and A' are approximately as accurate or more accurate than the corresponding values in Ref. 13 we do not give values for $p-p_{\mathrm{pp}}$ and $A'-A'_{\mathrm{pp}}$, but denote them by three asterisks.

r_{12}	C	$\tilde{C}$	p	p_{pp}	$p-p_{\mathrm{pp}}$	A'	A'_{pp}	$A'-A'_{\mathrm{pp}}$
Sufficiently small r_{12}								
0.5	0.642 180	0.532 950	0.567 784	0.569 166	−0.001 382	−6.466 968	−6.457 64	−0.009 328
1.0	0.630 180	0.528 101	1.597 590	1.161 92	−0.002 16	−7.813 621	−7.822 20	+0.008 58
2.0	0.622 300	0.517 900	2.248 680	2.245 64	+0.003 04	−11.571 664	−11.589 9	+0.018 2
Sufficiently large r_{12}								
3.0	0.556 340	0.506 960	3.260 659	3.260 96	−0.000 30	−15.145 897	−15.1384	−0.0075
4.0	0.543 400	0.509 000	4.265 089	4.265 18	−0.000 09	−18.414 485	−18.4123	−0.0022
5.0	0.535 700	0.511 400	5.265 926	5.265 97	−0.000 04	−21.567 077	−21.5660	−0.0011
6.0	0.530 300	0.512 700	6.265 543	6.265 52	+0.000 02	−24.662 029	−24.6617	−0.0003
7.0	0.526 200	0.513 140	7.264 703	7.264 68	+0.000 02	−27.725 910	−27.7257	−0.0002
8.0	0.522 600	0.513 100	8.263 735	8.263 74	0.000 00	−30.771 316	−30.7710	−0.0003
9.0	0.520 450	0.512 760	9.262 851	9.262 83	+0.000 02	−33.804 409	−33.8043	***
10.0	0.518 610	0.512 300	10.261 986	10.262 0	***	−36.829 957	−36.8297	***
11.0	0.517 000	0.511 800	11.261 223	11.261 2	***	−39.849 843	−39.8497	***
12.0	0.515 200	0.511 300	12.260 537	12.260 5	***	−42.865 768	−42.8656	***
13.0	0.514 200	0.510 750	13.259 930	13.259 9	***	−45.878 744	−45.8787	***
14.0	0.513 180	0.510 270	14.259 369	14.259 4	***	−48.889 604	−48.8896	***
15.0	0.512 210	0.509 820	15.258 859	15.258 9	***	−51.898 778	−51.8987	***
16.0	0.511 740	0.509 390	16.258 398	16.258 4	***	−54.906 636	−54.9066	***
17.0	0.511 050	0.508 990	17.257 987	17.258 0	***	−57.913 363	−57.9133	***
18.0	0.510 440	0.508 620	18.257 608	18.257 6	***	−60.919 214	−60.9191	***
19.0	0.509 890	0.508 260	19.257 265	19.257 3	***	−63.924 359	−63.9243	***
20.0	0.509 400	0.507 900	20.256 969	20.256 9	***	−66.928 793	−66.9288	***

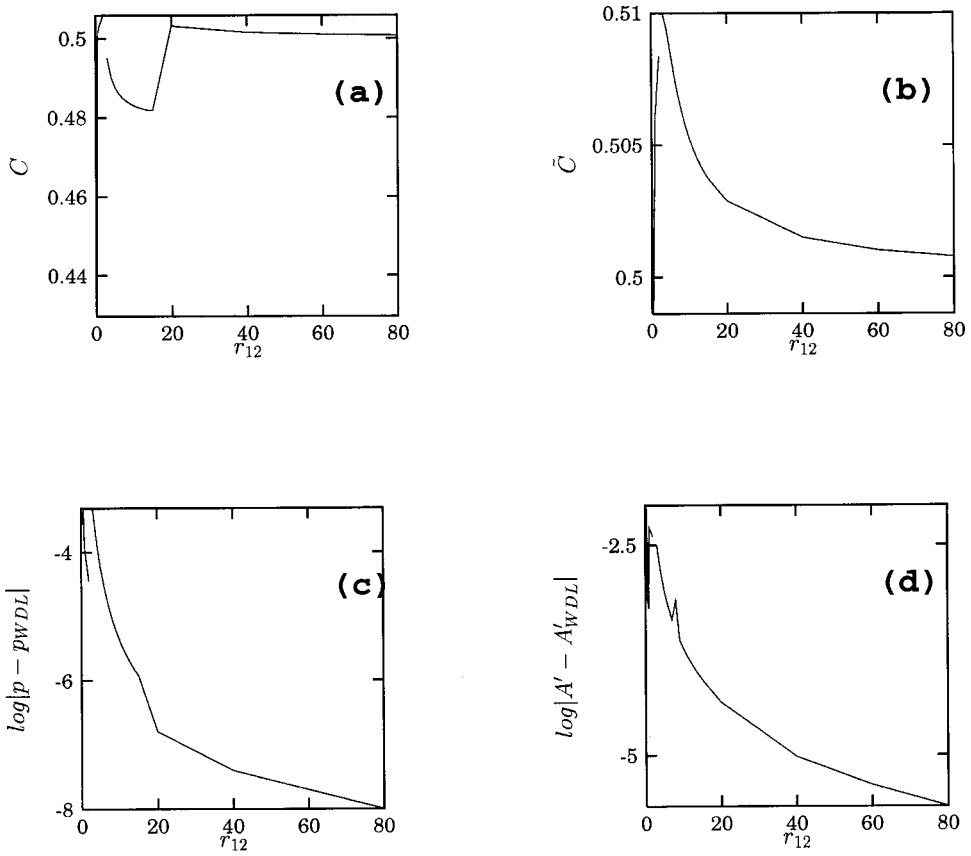

FIG. 1. Plots for the $1s\sigma$ state of the ion peHe^{2+} ($Z_1=1$, $Z_2=2$) of (a) C vs r_{12}, (b) $\tilde{C}$ vs r_{12}, (c) $\log|p-p_{\mathrm{WDL}}|$ vs r_{12}, and (d) $\log|A'-A'_{\mathrm{WDL}}|$ vs r_{12}, when C and $\tilde{C}$ are determined as functions of r_{12} from the requirement that the first-order and the third-order phase-integral results for p as well as for A' coincide. Here p and A' are the phase-integral values obtained in Table I, while p_{WDL} and A'_{WDL} are the corresponding numerically exact values (accurate to all digits quoted) calculated by Winter, Duncan, and Lane (Ref. 4, see pp. 288 and 289) and quoted in Table I. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of r_{12} have been used.

$\tilde{s}=0$ [Fig. 1(a) in Ref. 11] and (3.9) with $s=1$ and $m=0$ [Fig. 4(b) in Ref. 11] when r_{12} is sufficiently small, but (3.5b) with $\tilde{s}=m=0$ [Fig. 1(b) in Ref. 11] and (3.23a) with $s_\alpha=m=0$ [Fig. 3(b) in Ref. 11] when r_{12} is sufficiently large.

For the ion peB^{5+} we have computed the eigenvalue p and the reduced separation constant A' for the $1s\sigma$ and the $3s\sigma$ states and various values of r_{12}, with appropriate quantization conditions and parameters. The quantization conditions in Ref. 11 for the $1s\sigma$ state are (3.5a) with $\tilde{s}=0$ [Fig. 1(a) in Ref. 11] and (3.9) with $s=m=0$ [Fig. 4(b) in Ref. 11] when r_{12} is sufficiently small, but (3.5b) with $\tilde{s}=m=0$ [Fig. 1(b) in Ref. 11] and (3.23b) with $s_\beta=m=0$ [Fig. 3(b) in Ref. 11] when r_{12} is sufficiently large. The quantization conditions in Ref. 11 for the $3s\sigma$ state are (3.5a) with $\tilde{s}=2$ [Fig. 1(a) in Ref. 11] and (3.9) with $s=m=0$ [Fig. 4(b) in Ref. 11] when r_{12} is sufficiently small, but (3.5b) with $\tilde{s}=m=0$ [Fig. 1(b) in Ref. 11] and (3.23b) with $s_\beta=m=0$ [Fig. 3(b) in Ref. 11] when r_{12} is sufficiently large.

For the ion peO^{8+} we have calculated the eigenvalue p and the reduced separation constant A' for the $1s\sigma$ and the $4d\sigma$ states and various values of r_{12}, with appropriate quantization conditions and parameters. The quantization conditions in Ref. 11 for the $1s\sigma$ state are (3.5a) with $\tilde{s}=0$ [Fig. 1(a) in Ref. 11] and (3.9) with $s=m=0$ [Fig. 4(b) in Ref. 11] when r_{12} is sufficiently small, but (3.5b) with $\tilde{s}=m=0$ [Fig. 1(b) in Ref. 11] and (3.23b) with $s_\beta=m=0$ [Fig. 3(b) in Ref. 11] when r_{12} is sufficiently large. The quantization conditions in Ref. 11 for the $4d\sigma$ state are (3.5a) with

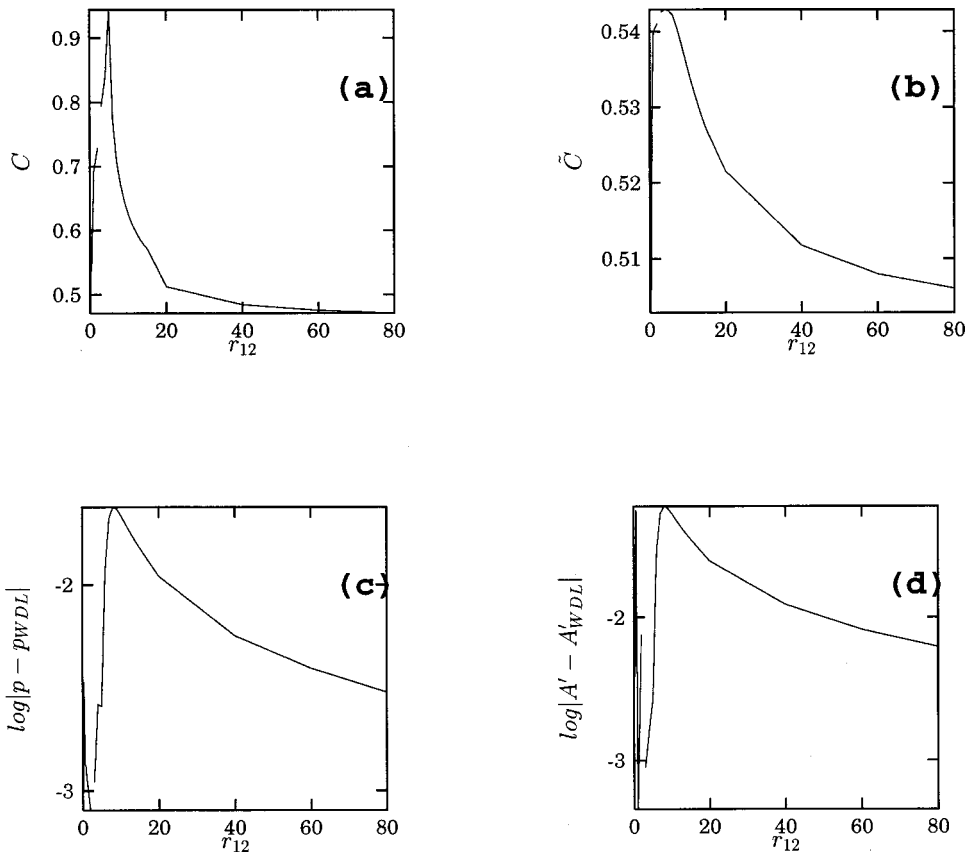

FIG. 2. Plots for the $2p\sigma$ state of the ion peHe^{2+} ($Z_1=1$, $Z_2=2$) of (a) C vs r_{12}, (b) $\tilde{C}$ vs r_{12}, (c) $\log|p-p_{\mathrm{WDL}}|$ vs r_{12}, and (d) $\log|A'-A'_{\mathrm{WDL}}|$ vs r_{12}, when C and $\tilde{C}$ are determined as functions of r_{12} from the requirement that the first-order and the third-order phase-integral results for p as well as for A' coincide. Here p and A' are the phase-integral values obtained in Table II, while p_{WDL} and A'_{WDL} are the corresponding numerically exact values (accurate to all digits quoted) calculated by Winter, Duncan, and Lane (Ref. 4, see pp. 288 and 289) and quoted in Table II. There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of r_{12} have been used.

$\tilde{s}=1$ [Fig. 1(a) in Ref. 11] and (3.9) with $s=2$ and $m=0$ [Fig. 4(b) in Ref. 11] when r_{12} is sufficiently small, but (3.5b) with $\tilde{s}=m=0$ [Fig. 1(b) in Ref. 11] and (3.23b) with $s_\beta=2$ and $m=0$ [Fig. 3(b) in Ref. 11] when r_{12} is sufficiently large.

In the calculations for the above-mentioned three ions we used the quantization conditions expressed in terms of complete elliptic integrals, obtained in the present paper, that correspond to the above-mentioned quantization conditions in Ref. 11.

We have determined the values of C and $\tilde{C}$ for several values of r_{12} such that the first- and third-order quantization conditions give the same value of p as well as of A'. These values are tabulated and compared with the numerically exact results obtained by Winter *et al.*[4] for the ion peHe^{2+} and by Ponomarev and Puzynina[13] for the ions peB^{5+} and peO^{8+}. In Tables I and II we give the results for the system peHe^{2+}. Although the phase-integral values of p and A' are very accurate for the $1s\sigma$ state of the ion peH^{2+} and large values of r_{12}, the phase-integral method cannot compete as regards accuracy with the method used by Winter *et al.*[4] to obtain the numerically exact values quoted in our Tables I and II. However, the possibility of using the analytical phase-integral formulas expressed in terms of complete elliptic integrals is an alternative that sometimes may be preferable to the use of very accurate numerical results. Tables III and IV present the results for the ion peB^{5+}. For the ion peO^{8+} the results are tabulated in Tables V and VI. From these four tables it is seen that for large values of r_{12} the phase-integral results are as

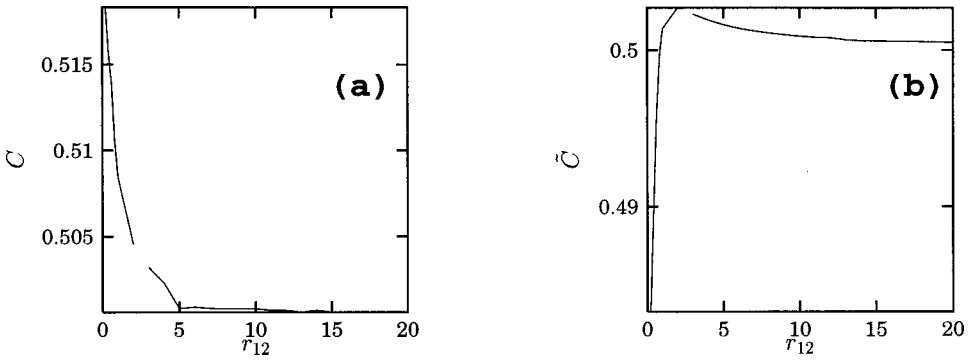

FIG. 3. Plots for the $1s\sigma$ state of the ion peB^{5+} ($Z_1=1$, $Z_2=5$) of (a) C vs r_{12}, (b) $\tilde{C}$ vs r_{12}, when C and $\tilde{C}$ are determined as functions of r_{12} from the requirement that the first-order and the third-order phase-integral results for p as well as for A' coincide (see Table III). There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of r_{12} have been used.

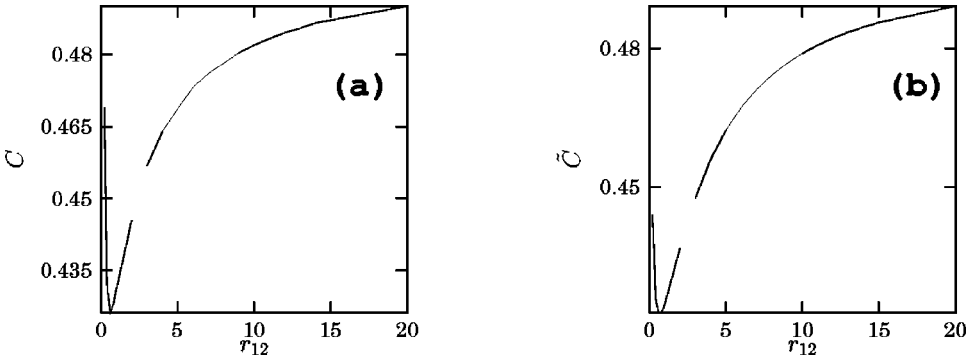

FIG. 4. Plots for the $3s\sigma$ state of the ion peB^{5+} ($Z_1=1$, $Z_2=5$) of (a) C vs r_{12}, (b) $\tilde{C}$ vs r_{12}, when C and $\tilde{C}$ are determined as functions of r_{12} from the requirement that the first-order and the third-order phase-integral results for p as well as for A' coincide (see Table IV). There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of r_{12} have been used.

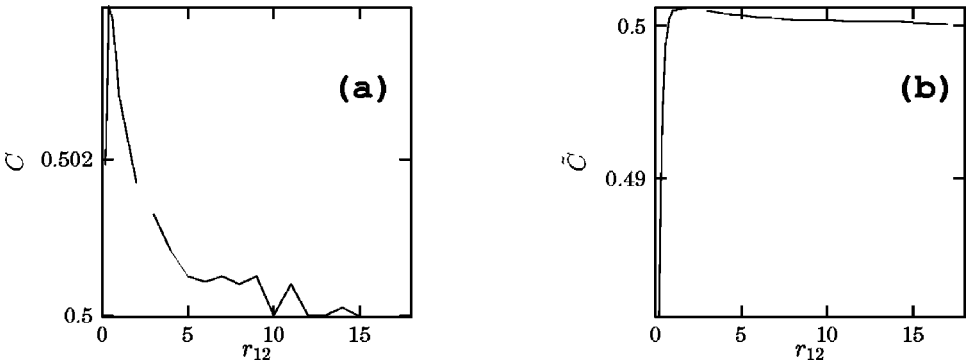

FIG. 5. Plots for the $1s\sigma$ state of the ion peO^{8+} ($Z_1=1$, $Z_2=8$) of (a) C vs r_{12}, (b) $\tilde{C}$ vs r_{12}, when C and $\tilde{C}$ are determined as functions of r_{12} from the requirement that the first-order and the third-order phase-integral results for p as well as for A' coincide (see Table V). There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of r_{12} have been used.

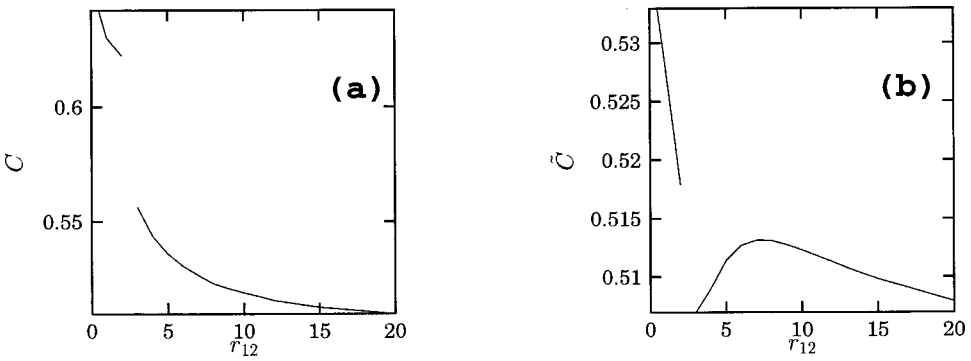

FIG. 6. Plots for the $4d\sigma$ state of the ion peO^{8+} ($Z_1=1$, $Z_2=8$) of (a) C vs r_{12}, (b) $\tilde{C}$ vs r_{12}, when C and $\tilde{C}$ are determined as functions of r_{12} from the requirement that the first-order and the third-order phase-integral results for p as well as for A' coincide (see Table VI). There is a break in each curve between the regions where the quantization conditions for sufficiently small and sufficiently large values of r_{12} have been used.

accurate or more accurate than the results that have been obtained numerically. In fact, the phase-integral values of p are at least as accurate as the numerically exact values of p[13] in Table III for $r_{12}>3$, in Table IV for $r_{12}>10$, in Table V for $r_{12}>2$, and in Table VI for $r_{12}>9$, and the phase-integral values of A' are at least as accurate as the numerically exact values of A'[13] in Table III for $r_{12}>10$, in Table IV for $r_{12}>7$, in Table V for $r_{12}>10$, and in Table VI for $r_{12}>8$. The results in Tables I–VI are presented graphically in Figs. 1–6.

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Multi-resolution analysis and fractional quantum Hall effect: An equivalence result

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In this article we prove that any multi-resolution analysis of $\mathcal{L}^2(\mathbf{R})$ produces, for some values of the filling factor, a single-electron wave function of the lowest Landau level (LLL) which, together with its (magnetic) translation, gives rise to an orthonormal set in the LLL. We also discuss the inverse construction. Moreover, we extend this procedure to the higher Landau levels and we discuss the analogies and the differences between this procedure and the one previously proposed by J.-P. Antoine and the author. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The role of wavelets in various applications of mathematics and to some physical problems like signal analysis is now completely established: the existence of a wide literature on this field is sufficient to give an idea of the amount of people involved in this and related topics. For a clear reading on this subject a standard quotation is Ref. 1. Reference 2 is an updated book where other interesting aspects of wavelets are discussed. What cannot be found in many textbooks, since is still to be understood, is the relevance of wavelets in quantum mechanics: at this moment, to our knowledge, very few of the applications proposed in this field (Ref. 3–8 among the others).

One of the most useful features of wavelets concerns their localization properties in both configuration and frequency space. This fact is at the basis of a series of papers[3–6] where different families of orthonormal (o.n.) bases in $\mathcal{L}^2(\mathbf{R})$ are used in the search for the ground state of a two-dimensional electron gas (2DEG) in a uniform positive background and subjected to a uniform electro-magnetic field. This is the physical system which produces the well-known fractional quantum Hall effect (FQHE). The key fact behind this approach is the existence of an unitary map between $\mathcal{L}^2(\mathbf{R})$ and the lowest Landau level (LLL), that is, the subspace of $\mathcal{L}^2(\mathbf{R}^2)$ corresponding to the lowest eigenvalue of the free Hamiltonian of the 2DEG. This implies that any o.n. basis in $\mathcal{L}^2(\mathbf{R})$ (not necessarily a wavelet one!) produces an o.n. basis in the LLL; for this reason the role of wavelets does not seem so crucial. We will comment again on this approach in Sec. V.

In this articles we establish a deeper connection between wavelets and FQHE. In particular we will show that any multi-resolution analysis (MRA) of $\mathcal{L}^2(\mathbf{R})$ produces *automatically* a wave function in $\mathcal{L}^2(\mathbf{R})$ and, as a second step, a wave function in the LLL which turns out to be o.n. to its own (magnetic) translation. This procedure, which works for an even value of the inverse filling factor, is only possible when we start from a MRA, contrary to what happens in Ref. 3, and can also be inverted: to any o.n. basis in the LLL which is generated by a single wave function via the action of magnetic translations can be associated a MRA.

The article is organized as follows:

In the next section we quickly review some of the main properties of a MRA and of the kq-representation,[9] which turns out to be a technical tool useful to implement the orthonormality condition.

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In Sec. III we state the problem of orthonormality of the single electron wave functions in connection with the FQHE.

In Sec. IV we show how, for fillings factors $\nu=1/2L$, $L\in\mathbf{N}$, a MRA produces in a completely natural way a wave function for the 2DEG with the desired orthonormality requirement. We also discuss the inverse procedure.

Section V is devoted to the comparison between this approach and the one proposed in Ref. 3. In particular, the example of the Haar o.n. basis is considered in detail. We also extend our procedure to higher Landau levels.

Section VI contains the conclusions and the plans for the future.

II. MATHEMATICAL TOOLS

In order to keep the article self-contained we now quickly review, for the reader's convenience, the main properties of the mathematical tools we will use in the rest of the article.

A. Multi-resolution analysis

The main result in the theory of MRA is the recipe which allows us to construct an orthonormal basis in $\mathcal{L}^2(\mathbf{R})$ starting from a single function ψ and acting on ψ with dilation and translation operators, generating the set

$$\{\psi_{j,k}(x)\equiv 2^{j/2}\psi(2^j x-k), j,k\in\mathbf{Z}\}. \tag{2.1}$$

Such a basis has the good properties of wavelets, including space *and* frequency localization. This is the key to their usefulness in many physical and mathematical applications. Let us now sketch the construction of these o.n. bases of wavelets. The full story may be found, for instance, in Ref. 1.

A *multi-resolution analysis* of $L^2(\mathbf{R})$ is an increasing sequence of closed subspaces

$$\cdots\subset V_{-2}\subset V_{-1}\subset V_0\subset V_1\subset V_2\subset\cdots, \tag{2.2}$$

with $\cup_{j\in Z}V_j$ dense in $L^2(\mathbf{R})$ and $\cap_{j\in Z}V_j=\{0\}$, and such that

(1) $f(x)\in V_j\Leftrightarrow f(2x)\in V_{j+1}$.
(2) There exists a function $\phi\in V_0$, called a *scaling* function, such that $\{\phi(x-k),k\in\mathbf{Z}\}$ is an o.n. basis of V_0.

Combining (1) and (2), one gets an o.n. basis of V_j, namely $\{\phi_{j,k}(x)\equiv 2^{j/2}\phi(2^j x-k),k\in\mathbf{Z}\}$. The role of V_j as an approximation space and in the direct decomposition of $\mathcal{L}(\mathbf{R})$ is discussed in Ref. 1.

Here we only need to know that the theory asserts the existence of a function ψ, called the *mother* of the wavelets, explicitly computable from ϕ, such that $\{\psi_{j,k}(x)\equiv 2^{j/2}\psi(2^j x-k),j,k\in\mathbf{Z}\}$ constitutes an orthonormal basis of $L^2(\mathbf{R})$: these are the *orthonormal wavelets*.

The construction of ψ proceeds as follows. First, the inclusion $V_0\subset V_1$ yields the relation

$$\phi(x)=\sqrt{2}\sum_{n=-\infty}^{\infty}h_n\phi(2x-n),\quad h_n=\langle\phi_{1,n}|\phi\rangle. \tag{2.3}$$

Taking Fourier transforms, this gives

$$\hat{\phi}(\omega)=m_o(\omega/2)\,\hat{\phi}(\omega/2), \tag{2.4}$$

where

$$m_o(\omega)=\frac{1}{\sqrt{2}}\sum_{-\infty}^{\infty}h_n e^{-in\omega} \tag{2.5}$$

is a 2π-periodic function. Iterating (2.4), one gets the scaling function as the (convergent!) infinite product

$$\hat{\phi}(\omega)=(2\pi)^{-1/2}\prod_{j=1}^{\infty} m_o(2^{-j}\omega). \tag{2.6}$$

Then one defines the function $\psi\in W_0\subset V_1$ by the relation

$$\hat{\psi}(\omega)=e^{i\omega/2}\overline{m_o(\omega/2+\pi)}\,\hat{\phi}(\omega/2), \tag{2.7}$$

or, equivalently,

$$\psi(x)=\sqrt{2}\sum_{n=-\infty}^{\infty}(-1)^{n-1}h_{-n-1}\phi(2x-n), \tag{2.8}$$

and proves that the function ψ indeed generates an o.n. basis with all the required properties.

Actually, this procedure does not produce a unique result. Another possibility, which is the one we will use in the example given later in this work, gives for the mother wavelet the following expansion:

$$\psi(x)=\sqrt{2}\sum_{n=-\infty}^{\infty}(-1)^{n}h_{-n+1}\phi(2x-n). \tag{2.9}$$

Various additional conditions may be imposed on the function ψ (hence on the basis wavelets): arbitrary regularity, several vanishing moments (in any case, ψ has always meant zero), fast decrease at infinity, even compact support. For instance, ψ has compact support if only finitely many h_n differ from zero.

Simple examples of this construction are the Haar basis, which comes from the scaling function $\phi(x)$ equal to 1 for $0\leqslant x<1$ and 0 otherwise, the spline functions,[1] and so on.

What is more interesting for our purposes is the role of the coefficients $\{h_n\}$ defining the two-scale relation (2.3). These are complex quantities which, if $\phi(x)$ is normalized, must satisfy the following relation:

$$\sum_{n\in\mathbf{Z}}|h_n|^2=1. \tag{2.10}$$

Furthermore, it can be proved using the 2π-periodicity of the function $m_o(\omega)$, together with the orthogonality of the set $\{\phi(x-k)\}$ for $k\in\mathbf{Z}$, that

$$|m_o(\omega)|^2+|m_o(\omega+\pi)|^2=1 \tag{2.11}$$

almost everywhere.[1] This equation can be written in two equivalent forms where the coefficients h_n explicitly appear:

$$\sum_{n\in\mathbf{Z}}h_n\overline{h_{n+2k}}=\delta_{k,0},\quad \forall k\in\mathbf{Z}, \tag{2.12}$$

or

$$\sum_{n,k\in\mathbf{Z}}h_n\overline{h_{n+2k}}e^{2,ik\omega}=1,\quad \text{a.e.}, \tag{2.13}$$

or yet, in a more convenient form,

$$\frac{1}{2}\sum_{n,l\in\mathbf{Z}} h_n\overline{h_l}e^{i(l-n)\omega}(1+(-1)^{l+n})=1, \quad \text{a.e.} \tag{2.14}$$

We end this rapid excursus on MRA with the following remark: the set of coefficients $\{h_n\}$ can be considered as the main ingredient of a MRA since it generates $m_o(\omega)$, $\hat{\phi}(\omega)$ and, finally, the mother wavelet $\psi(x)$.

B. kq-representation

The relevance of kq-representation in many-body physics has been established since its first appearance.[9] What was originally a physical tool has become, during the years, also a mathematical interesting object, widely analyzed in the literature, (see Refs. 10 and 11, for instance). We give here only a few definitions and refer to Refs. 9 and 11–13 for further reading and for applications.

The genesis of the kq-representation consists in the well-known possibility of a simultaneous diagonalization of any two commuting operators. In Ref. 12 it is shown that the following distributions,

$$\psi_{kq}(x)=\sqrt{\frac{2\pi}{a}}\sum_{n\in\mathbf{Z}} e^{ikna}\delta(x-q-na), \quad k\in[0,a[, \quad q\in\left[0,\frac{2\pi}{a}\right[, \tag{2.15}$$

are (generalized) eigenstates of both $T(a)=e^{ipa}$ and $\tau(2\pi/a)=e^{ix2\pi/a}$. Here a is a positive real number which plays the role of a lattice spacing.

How it is discussed in Ref. 12, these $\psi_{kq}(x)$ are Bloch-like functions corresponding to infinitely localized Wannier functions. They also satisfy orthogonality and closure properties. This implies that, roughly speaking, they can be used to define a new representation of the wave functions by means of the integral transform $Z:\mathcal{L}^2(\mathbf{R})\to\mathcal{L}^2(\square)$, where $\square=[0,a[\times[0,2\pi/a[$, defined as follows:

$$h(k,q):=(ZH)(k;q):=\int_{\mathbf{R}} d\omega\,\overline{\psi_{kq}(\omega)}H(\omega), \tag{2.16}$$

for all functions $H(\omega)\in\mathcal{L}^2(\mathbf{R})$. The result is a function $h(k,q)\in\mathcal{L}^2(\square)$.

To be more rigorous, Z should be defined first on the functions of $\mathcal{C}_0^\infty(\mathbf{R})$ and then extended to $\mathcal{L}^2(\mathbf{R})$ using its continuity.[10] In this way it is possible to give a rigorous meaning to formula (2.16).

From now on we will work in the following hypothesis:

$$a^2=2\pi, \tag{2.17}$$

which, also in view of the next section, will correspond to fixing the spacing of the lattice underlying the 2DEG.

Replacing $\psi_{kq}(x)$ with its explicit expression, formula (2.16) produces

$$h(k,q)=(ZH)(k,q):=\frac{1}{\sqrt{a}}\sum_{n\in\mathbf{Z}} e^{-ikna}H(q+na), \tag{2.18}$$

which can be inverted and gives the x-representation $H(\omega)\in\mathcal{L}^2(\mathbf{R})$ of a function $h(k,q)\in\mathcal{L}^2(\square)$ as follows:

$$H(\omega)=(Z^{-1}h)(\omega)=\int_{\square} dkdq\,\psi_{kq}(\omega)h(k,q). \tag{2.19}$$

Due to (2.15), this equation gives

$$H(x+na)=\frac{1}{\sqrt{a}}\int_0^a dk e^{ikna}h(k,x), \quad \forall x\in[0,a[, \quad \forall n\in\mathbf{Z}. \tag{2.20}$$

In all the literature concerning kq-representation, the role of the boundary conditions is widely discussed, also in connection with the continuity properties of the functions. For instance, in Ref. 14, a function $h(k,q)\in\mathcal{L}^2(\square)$ is said to be continuous if it is the restriction to the kq-cell of a function continuous in the *extended* kq-plane $(k,q\in\mathbf{R})$, and if it satisfies the following boundary conditions:

$$\begin{aligned} h(k+a,q)&=h(k,q),\\ h(k,q+a)&=e^{ika}h(k,q), \end{aligned} \tag{2.21}$$

which are typical of any function in kq-representation and which will always be assumed here.

III. STATING THE PROBLEM

In this section we will discuss a many-body model of the FQHE looking, in particular, for the single-electron wave function which generates the ground state of the physical system in the way described next. This system is simply a two-dimensional electron gas, 2DEG (that is a gas of electrons constrained in a two-dimensional layer), in a positive uniform background and subjected to a uniform magnetic field along z and an electric field along y.

The Hamiltonian of the system can be written as

$$H^{(N)}=H_0^{(N)}+\lambda(H_c^{(N)}+H_B^{(N)}) \tag{3.1}$$

where $H_0^{(N)}$ is the sum of N contributions:

$$H_0^{(N)}=\sum_{i=1}^{N} H_0(i). \tag{3.2}$$

Here $H_0(i)$ describes the minimal coupling of the electrons with the fields:

$$H_0=\frac{1}{2}(\underline{p}+\underline{A}(r))^2=\frac{1}{2}\left(p_x-\frac{y}{2}\right)^2+\frac{1}{2}\left(p_y+\frac{x}{2}\right)^2. \tag{3.3}$$

Notice that we are adopting here the symmetric gauge $\underline{A}=1/2(-y,x,0)$ and the same unit as in Ref. 15. $H_c^{(N)}$ is the canonical Coulomb interaction between charged particles:

$$H_c^{(N)}=\frac{1}{2}\sum_{i\neq j}^{N}\frac{1}{|\underline{r}_i-\underline{r}_j|} \tag{3.4}$$

and $H_B^{(N)}$ is the interaction of the charges with the background, whose explicit form can be found in Ref. 15.

In the following we will consider, as it is usually done in the literature, $\lambda(H_c^{(N)}+H_B^{(N)})$ as a perturbation of the free Hamiltonian $H_0^{(N)}$, and we will look for eigenstates of $H_0^{(N)}$ in the form of Slater determinant built up single electron wave functions. This approach is known to give good results for low electron (or hole) densities.[15] The easiest way to attack this problem consists in introducing the new variables

$$P'=p_x-y/2, \quad Q'=p_y+x/2. \tag{3.5}$$

In terms of P' and Q' the single electron Hamiltonian, H_0, can be written as

$$H_0 = \tfrac{1}{2}(Q'^2 + P'^2). \tag{3.6}$$

The transformation (3.5) can be seen as a part of a canonical map from (x,y,p_x,p_y) into (Q,P,Q',P') where

$$P = p_y - x/2, \quad Q = p_x + y/2. \tag{3.7}$$

These operators satisfy the following commutation relations:

$$[Q,P] = [Q',P'] = i, \quad [Q,P'] = [Q',P] = [Q,Q'] = [P,P'] = 0. \tag{3.8}$$

It is shown in Refs. 16 and 17 that a wave function in the (x,y)-space is related to its PP'-expression by the formula

$$\Psi(x,y) = \frac{e^{ixy/2}}{2\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{i(xP' + yP + PP')}\Psi(P,P')\, dP\, dP'. \tag{3.9}$$

The usefulness of the PP'-representation stems from the expression (3.6) of H_0. Indeed, in this representation, the single electron Schrödinger equation admits eigenvectors $\Psi(P,P')$ of H_0 of the form $\Psi(P,P') = f(P')h(P)$. Thus the ground state of (3.6) must have the form $f_0(P')h(P)$, where

$$f_0(P') = \pi^{-1/4} e^{-P'^2/2}, \tag{3.10}$$

and the function $h(P)$ is arbitrary, which manifests the degeneracy of the LLL. With f_0 as above, formula (3.9) becomes

$$\psi(x,y) = \frac{e^{ixy/2}}{\sqrt{2}\,\pi^{3/4}} \int_{-\infty}^{\infty} e^{iyP} e^{-(x+P)^2/2} h(P)\, dP. \tag{3.11}$$

It is worthwhile to stress that at this stage the Coulomb interaction has not yet been considered (and it will not in this article), but the common belief is that the explicit form of $h(P)$ should be fixed by this interaction.

Now the problem arises of how to construct the ground state of the free N-electron Hamiltonian $H_0^{(N)}$. We use a suggestion coming from the classical counterpart of this quantum problem. It is very well known that the ground state for a classical 2DEG is a (triangular) Wigner crystal: the classical electrons are sharply localized on the sites of a lattice whose lattice spacing is fixed by the electron density. What we expect, and what was proven in Ref. 15, is that, at least for certain regions of the filling factor, the quantum ground state should not be very different from this classical picture. Here we only sketch the procedure which is analyzed in more detail Refs. 15 and 3.

We start introducing the so-called magnetic translation operators $T(\vec{a}_i)$ defined by

$$T(\vec{a}_i) \equiv \exp(i\vec{\Pi}_c \cdot \vec{a}_i), \quad i = 1,2, \tag{3.12}$$

where $\vec{\Pi}_c \equiv (Q,P)$ and $\vec{a}_i$ are the lattice basis vectors [$\vec{a}_1 = a(1,0)$, $\vec{a}_2 = (a/2)(1,\sqrt{3})$ for a triangular lattice].

From now on, for simplicity we will work in a square lattice with unit cell of area 2π:

$$\vec{a}_1 = a(1,0), \quad \vec{a}_2 = a(0,1), \quad a^2 = 2\pi. \tag{3.13}$$

This choice is quite useful to keep the notation simple: moreover, its generalization to lattices of arbitrary shape is only a technical step.

The above *rationality* condition on the area has the following useful consequence:

$$[T(\vec{a}_1),T(\vec{a}_2)]=0. \tag{3.14}$$

This is not the only commutativity condition satisfied by the magnetic translations. Due to the commutation relations (3.8), we also find

$$[T(\vec{a}_1),H_0]=[T(\vec{a}_2),H_0]=0. \tag{3.15}$$

With the choice (3.13) of the lattice's basis the magnetic translations take a simple form

$$T_1:=T(\vec{a}_1)=e^{iaQ}, \quad T_2:=T(\vec{a}_2)=e^{iaP}, \tag{3.16}$$

and they act on a generic function $f(x,y)\in\mathcal{L}^2(\mathbf{R}^2)$ as follows

$$f_{m,n}(x,y):=T_1^mT_2^nf(x,y)=(-1)^{mn}e^{i(a/2)(my-nx)}f(x+ma,y+na). \tag{3.17}$$

We see from this formula that, if for instance $f(x,y)$ is localized around the origin, then $f_{m,n}(x,y)$ is localized around the lattice site $a(-m,-n)$.

Now we have all the ingredients to construct the ground state of $H_0^{(N)}$ mimiking the classical procedure. We simply start from the single electron ground state of H_0 given in (3.11), $\psi(x,y)$. Then we construct a set of copies $\psi_{m,n}(x,y)$ of ψ as in (3.17), with $m,n\in\mathbf{Z}$. All these functions still belong to the lowest Landau level for any choice of the function $h(P)$ due to (3.15). N of these wave functions $\psi_{m,n}(x,y)$ are finally used to construct a Slater determinant for the finite system:

$$\psi^{(N)}(\underline{r}_1,\underline{r}_2,\ldots,\underline{r}_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix} \psi_{m_1,n_1}(\underline{r}_1) & \psi_{m_1,n_1}(\underline{r}_2) & \ldots & \psi_{m_1,n_1}(\underline{r}_N) \\ \psi_{m_2,n_2}(\underline{r}_1) & \psi_{m_2,n_2}(\underline{r}_2) & \ldots & \psi_{m_2,n_2}(\underline{r}_N) \\ \cdot & \cdot & \ldots & \cdot \\ \cdot & \cdot & \ldots & \cdot \\ \cdot & \cdot & \ldots & \cdot \\ \psi_{m_N,n_N}(\underline{r}_1) & \psi_{m_N,n_N}(\underline{r}_2) & \ldots & \psi_{m_N,n_N}(\underline{r}_N) \end{vmatrix}. \tag{3.18}$$

It is known[15] that in order to get $\langle\psi^{(N)},\psi^{(N)}\rangle=1$ we need to have

$$\langle\psi_{m_i,n_i}\psi_{m_j,n_j}\rangle=\delta_{m_i,m_j}\delta_{n_in_j}. \tag{3.19}$$

In fact, if these translated functions were not o.n., then we would get $\|\psi^{(N)}\|=1+O(N)$, which is obviously divergent for N diverging. It is clear, therefore, that if we want to perform easily the thermodynamical limit, orthonormality between differently localized single electron wave functions must be required!

In the rest of this section we will discuss how the requirement (3.19) can be handled and, in particular, we will show that the use of kq-representation is quite a useful tool since it produces a very simple constraint. Some of the results we are now going to describe in this section are also due to G. Morchio and F. Strocchi,[18] while the original idea of using kq-representation in connection with an orthonormality constraint is already contained in Ref. 13 in the proof of completeness of lattice states proposed by the authors.

Let $\psi(x,y)$ be as in (3.11) and $\psi_{m,n}(x,y)=T_1^mT_2^n\psi(x,y)=(-1)^{mn}e^{i(a/2)(my-nx)}\psi(x+ma,y+na)$. After few computations and using the rationality condition $a^2=2\pi$ we obtain

$$\psi_{m,n}(x,y)=\frac{e^{i(xy/2)+iamy}}{\sqrt{2}\pi^{3/4}}\int_{-\infty}^{\infty}dP\,e^{i(y+na)P-(x+ma+P)^2/2}h(P). \tag{3.20}$$

We are interested now in finding some conditions on $h(P)$ such that condition (3.19), or its equivalent form

$$S_{m,n} := \langle \psi_{0,0}, \psi_{m,n} \rangle = \delta_{m,0}\delta_{n,0}, \tag{3.21}$$

is satisfied. With the previous definitions we find

$$S_{m,n} = \int_{-\infty}^{\infty} dp e^{inap} \overline{h(p+ma)} h(p), \tag{3.22}$$

which restates the problem of the orthonormality of the wave functions in terms of the PP'-representation. In particular we see that, for $m=n=0$, this equation implies that ψ in normalized in $\mathcal{L}^2(\mathbf{R}^2)$ if and only if $h(P)$ is normalized in $\mathcal{L}^2(\mathbf{R})$. This reflects the unitarity of the transformation (3.9), which, more in general, implies that any o.n. set in $\mathcal{L}^2(\mathbf{R})$ is mapped in an o.n. set in $\mathcal{L}^2(\mathbf{R}^2)$.

In order to use now kq-representation it is convenient to split the integral over $\mathbf{R}$ into an infinite sum of integrals restricted to $[ra,(r+1)a[, r \in \mathbf{Z}$, use the kq-representation, and, then, write everything in terms of a single integral over the unit cell $\square$. We have, using (2.20) and the well-known equality

$$\sum_{l \in \mathbf{Z}} e^{ixl(2\pi/c)} = c \sum_{l \in \mathbf{Z}} \delta(x - cl), \tag{3.23}$$

$$\begin{aligned} S_{m,n} &= \sum_{r \in \mathbf{Z}} \int_{ra}^{(r+1)a} dp e^{inap} \overline{h(p+ma)} h(p) \\ &= \sum_{r \in \mathbf{Z}} e^{inra^2} \int_0^a dp e^{inap} \overline{h(p+(r+m)a)} h(p+ra) \\ &= \sum_{r \in \mathbf{Z}} \frac{1}{a} \int_0^a dq \int_0^a dk \int_0^a dk' e^{ir(k-k')a} e^{inaq - ik'ma} h(k,q) \overline{h(k',q)}, \end{aligned}$$

so that

$$S_{m,n} = \int_{\square} dk dq e^{inaq - ikma} |h(k,q)|^2. \tag{3.24}$$

Due to the completeness of the set $\{e^{inaq-ikma}, n,m \in \mathbf{Z}\}$ in the unit cell $\square$, we conclude that $S_{m,n} = \delta_{m,0}\delta_{n,0}$ if and only if $h(k,q)$ is a phase, so that $|h(k,q)|$ is independent of k and q. This result can be considered as a slight generalization of the procedure discussed in Ref. 13 to the FQHE for filling factor $\nu = 1$.

It is easy to generalize this result to a filling $\nu = 1/2$. The idea is the following:

A filling factor $\nu = 1$ corresponds to all the sites of our square lattice (of spacing $a = \sqrt{2\pi}$) occupied. A $\nu = 1/2$ 2DEG can be seen, on the other hand, as if the same lattice was only partially occupied: one lattice site is free and the other is occupied. If we require the orthonormality of the related set of single electron wave functions, it is enough to ask for $S_{m,2n} = \delta_{m,0}\delta_{n,0}$. This is equivalent also to choose a different lattice, with a unit cell twice that before and basis vectors $a(1,0)$ and $2a(0,1)$. Of course, we would as well have chosen another lattice with basis vectors $a(0,1)$ and $2a(1,0)$, or also any other lattice with unit cell of area 4π. We use the first choice just to fix ideas. Equation (3.24) gives

$$S_{m,2n} = \int_{\square} dk dq e^{i2naq - ikma} |h(k,q)|^2 = \delta_{m,0}\delta_{n,0}, \tag{3.25}$$

which can be rewritten as

$$\frac{1}{2}\int_{\square} dkdq e^{inaq-ikma}\left(\left|h\left(k,\frac{q}{2}\right)\right|^2+\left|h\left(k,\frac{q+a}{2}\right)\right|^2\right). \tag{3.26}$$

This implies, again using the completeness of the functions $e^{inaq-ikma}, n,m\in\mathbf{Z}$, in $\square$, that

$$J_2(k,q):=\left|h\left(k,\frac{q}{2}\right)\right|^2+\left|h\left(k,\frac{q+a}{2}\right)\right|^2=\frac{1}{\pi}, \quad \text{almost everywhere for } k,q\in\square. \tag{3.27}$$

The generalization to $\nu=1/M$ is straightforward: we simply require the orthonormality of the wave functions located at a distance of M sites:

$$S_{m,Mn}=\int_{\square} dkdq e^{iMnaq-ikma}|h(k,q)|^2=\delta_{m,0}\delta_{n,0}$$

and, proceding as above, we deduce that $h(k,q)$ must satisfy the equality

$$J_M(k,q):=\left|h\left(k,\frac{q}{M}\right)\right|^2+\left|h\left(k,\frac{q+a}{M}\right)\right|^2+\cdots+\left|h\left(k,\frac{q+(M-1)a}{M}\right)\right|^2=\frac{M}{2\pi}, \tag{3.28}$$

almost everywhere for $k,q\in\square$.

The extension to a filling $\nu=L/M$, with L and M relatively prime, can be performed by imposing that condition $S_{m,n}=\delta_{m,0}\delta_{n,0}$ holds only for those (m,n) corresponding to a square lattice in which only L among M lattice sites are occupied. We will not consider this extension in this article.

IV. WHAT WE GET FROM MRA

In this section we will describe how two subjects which are so different, at a first sight, as the MRA and the orthonormality condition for a 2DEG discussed previously, are indeed very close.

Let us consider a given MRA of $\mathcal{L}^2(\mathbf{R})$. We have seen in Sec. II that to this MRA is associated a certain set of square-summable complex numbers $\{h_n\}_{n\in Z}$ satisfying, for instance, condition (2.12). This set produces a 2π-periodic function $m_o(\omega)$ and, through this, the scaling function $\hat{\phi}(\omega)$ and the mother wavelet.

Now we use the sequence $\{h_n\}_{n\in\mathbf{Z}}$ to define the following function, which strongly reminds us of $m_o(\omega)$:

$$T_2(\omega)=\begin{cases}\dfrac{1}{\sqrt{a}}\displaystyle\sum_{l\in\mathbf{Z}} h_l e^{-il\omega a}, & \omega\in[0,a[,\\ 0, \quad \text{otherwise.}\end{cases} \tag{4.1}$$

It is clear that $T_2(\omega)$ is square integrable and is not periodic. In particular, due to the normalization condition (2.10), we have $\|T_2\|_2^2=\int_{\mathbf{R}}|T_2(\omega)|^2\,d\omega=1$. Therefore the kq-transform of this function, $t_2(k,q)=(ZT_2)(k,q)$, is well defined in $\mathcal{L}^2(\square)$.

In particular, using (2.18) we find

$$t_2(k,q)=\frac{1}{\sqrt{a}}\sum_{n\in\mathbf{Z}} e^{-ikna}T_2(q+na). \tag{4.2}$$

The boundary conditions (2.21) are obviously satisfied: $t_2(k+a,q)=t_2(k,q)$ and $t_2(k,q+a)=e^{ika}t_2(k,q)$. It is easy to check that $t_2(k,q)$ satisfies also the orthonormality conditions (3.27). In fact, since we are interested to the value of $t_2(k,q)$ only in $\square$, and since $T_2(\omega)$ is different from zero only for $\omega\in[0,a[$, we conclude that, for $(k,q)\in\square$,

$$J_2(k,q)=\frac{1}{a}\left(\left|T\left(\frac{q}{2}\right)\right|^2+\left|T\left(\frac{q+a}{2}\right)\right|^2\right)=\frac{1}{a^2}\sum_{l,s} h_l\overline{h_s}e^{i(s-l)qa/2}(1+(-1)^{l+s}),$$

which is equal to $1/\pi$ a.e. in $k,q\in\square$, due to (2.14). This implies that $t_2(k,q)$ gives rise to a family of functions $\psi_{m,n}(x,y)$ in the LLL mutually orthonormal and corresponding to $\nu=\frac{1}{2}$. We will find the explicit form of these $\psi_{m,n}(x,y)$ in the next section, where we will also compare these results with the ones obtained in Ref. 3.

The above-mentioned procedure can be easily extended to fillings $\nu=1/2L$. The extension to odd denumerator is not so straightforward and will be given elsewhere.

The starting point is again the set $\{h_n\}_{n\in Z}$, producing a MRA of $\mathcal{L}^2(\mathbf{R})$, satisfying condition (2.12). Now we define

$$T_{2L}(\omega)=\begin{cases}\dfrac{1}{\sqrt{a}}\displaystyle\sum_{l\in\mathbf{Z}} h_l e^{-il\omega La}, & \omega\in[0,a[,\\ 0, \quad \text{otherwise.}\end{cases}\tag{4.3}$$

Again, this is a square-integrable function satisfying $\|T_{2L}\|^2=1$. Defining $t_{2L}(k,q)=(ZT_{2L})\times(k,q)$ we have, for $k,q\in\square$, $t_{2L}(k,q)=(1/\sqrt{a})T_{2L}(q)=(1/a)\Sigma_{l\in Z}h_l e^{-ilqLa}$. We also stress that $t_{2L}(k,q)$ satisfies the correct boundary conditions. With these definitions, using the rationality conditions $a^2=2\pi$ and collecting contributions of the form $|t_{2L}(k,q/2L)|^2$, $|t_{2L}(k,(q+2a)/2L)|^2,\ldots$, and the "odd ones," $|t_{2L}(k,(q+a)/2L)|^2,|t_{2L}(k,(q+3a)/2L)|^2,\ldots$, we obtain

$$\begin{aligned}J_{2L}(k,q)&:=\left|t_{2L}\left(k,\frac{q}{2L}\right)\right|^2+\left|t_{2L}\left(k,\frac{q+a}{2L}\right)\right|^2+\cdots+\left|t_{2L}\left(k,\frac{q+(2L-1)a}{2L}\right)\right|^2\\&=L\left(\left|t_{2L}\left(k,\frac{q}{2L}\right)\right|^2+\left|t_{2L}\left(k,\frac{q+a}{2L}\right)\right|^2\right)\\&=\frac{L}{a^2}\sum_{l,s} h_l\overline{h_s}e^{i(s-l)qa/2}(1+(-1)^{l+s}),\end{aligned}\tag{4.4}$$

which is again independent of k and q since it is equal to L/π a.e. in $\square$, due to condition (2.14). Finally, Eq. (3.28) is a consequence of the equality $\nu^{-1}=M=2L$. We conclude that $t_{2L}(k,q)$ produces, in the configuration space, a set of mutually orthonormal wave functions spanning the LLL for $\nu=1/2L$.

This result, which is in a certain sense rather unexpected because it relates two distant fields as MRA and FQHE, is only half of the surprise. In fact, in the rest of this section, we will also show that this relation works in the opposite direction. More in detail, we will show how to construct, starting from a function $h(k,q)$ which produces an o.n. set of translated functions in the LLL, a set of coefficients $\{h_n\}$ satisfying condition (2.14), and, therefore, generating a MRA.

The recipe is rather simple and requires only few lines: let us suppose to have a function $h(k,q)$ belonging to $\mathcal{L}^2(\square)$ satisfying the boundary conditions $h(k+a,q)=h(k,q)$ and $h(k,q+a)=e^{ika}h(k,q)$ and such that

$$|h(k,q/2)|^2+|h(k,(q+a)/2)|^2=\frac{1}{\pi}\quad\text{a.e. in }\square.\tag{4.5}$$

This means that in the configuration space the related set $\{\psi_{m,n}(x,y)\}$ is an o.n. set. Let us now define

$$h_n(k)=\int_0^a dq e^{inaq}h(k,q),\quad k\in[0,a[.\tag{4.6}$$

Even if $h_n(k)$ is, in general, a function of k, it is straightforward to check that if we take $h(k,q)$ coinciding with $t_2(k,q)$ in (4.2), then $h_n(k)=h_n$ for all $n\in\mathbf{Z}$. This means that the dependence on k may disappear in some relevant situation. It is not so surprising, therefore, to check that $\Sigma_{n\in\mathbf{Z}}h_n(k)\overline{h_{n+2l}(k)}$ does not depend on k for *any* choice of $h(k,q)$, if the equality (4.5) is satisfied. In fact, using equality (3.23) and condition (4.5), we find

$$\begin{aligned}\sum_{n\in\mathbf{Z}} h_n(k)\overline{h_{n+2l}(k)} &= a\int_0^a dq|h(k,q)|^2 e^{-2ilaq}\\ &= \frac{a}{2}\int_0^a dq e^{-ilaq}(|h(k,q/2)|^2+|h(k,(q+a)/2)|^2)\\ &= \frac{a}{2\pi}\int_0^a dq e^{-ilaq}=\delta_{l,0}. \end{aligned} \tag{4.7}$$

This result shows that any o.n. basis in the LLL for a filling factor $\nu=1/2$ produces a set of coefficients satisfying the summation rule (2.12) and, therefore, the basic condition giving rise to a MRA of $\mathcal{L}^2(\mathbf{R})$ (which, in general, will depend on an external parameter $k\in[0,a[$). The extension to a filling $\nu=1/2L$, $L\in\mathbf{N}$, is straightforward.

V. EXTENSION TO HIGHER LANDAU LEVELS AND FURTHER REMARKS

In the first part of this section we analyze the relation between the approach we have discussed here with the one originally proposed in Ref. 3 and further developed in Refs. 4 and 5. In those papers we used wavelet analysis in connection with the FQHE as we have done here. In Ref. 5, in particular, we discussed a toy model suggesting the relevance of single electron wave functions arising from wavelet theory in the construction of a Slater-like ground state for a 2DEG. This construction was carried out in detail for the FQHE in Refs. 3 and 4 using the canonical transformation (3.11) and the PP'-representation to generate an o.n. basis of functions in the LLL starting from an o.n. set of wavelets in $\mathcal{L}^2(\mathbf{R})$. This procedure is only apparently close to the one proposed in this article. The first difference is related to the possibility of extending the approach in Ref. 3 to *any* o.n. basis of $\mathcal{L}^2(\mathbf{R})$, a possibility which does not exist here since the procedure proposed in this article only works for an o.n. basis generated by a MRA. The second difference concerns the nature of the operators acting on the *mother* function which generates the o.n. set in the LLL: in Refs. 3 and 4 these operators are dilation and translation operators. Here, on the other hand, we use the magnetic translations defined in (3.12).

Since, however, these two procedures have something in common, we expect that the resulting wave functions should not be very different. And, in fact, this is the outcome of this section, where we will explore the details of the easiest example: the Haar wavelet. For this choice the set $\{h_n\}_{n\in\mathbf{Z}}$ reduces to $h_0=h_1=1/\sqrt{2}$, and all the other coefficients are zero. We have shown in Ref. 3 that this choice produces a function in the LLL localized around the origin which looks like

$$H_{00}(x,y)=\frac{e^{-ixy/2}e^{-y^2/2}}{2\pi^{1/4}}\left\{2\phi\left(\frac{x-iy+1/2}{\sqrt{2}}\right)-\phi\left(\frac{x-iy}{\sqrt{2}}\right)-\phi\left(\frac{x-iy+1}{\sqrt{2}}\right)\right\}, \tag{5.1}$$

where $\phi(z):=(2/\sqrt{\pi})\int_0^z e^{-t^2}dt$ is the error function.[19] The whole set $H_{mn}(x,y)$ is discussed in Ref. 3, where its asymptotic behavior is also discussed in connection with the localization of the electrons. Here we only state the result which will be compared with the one resulting by the approach proposed here. We have

$$H_{00}(x,y)\simeq\frac{e^{ixy/2}e^{-x^2/2}}{2\pi^{1/4}}\sqrt{\frac{2}{\pi}}\left(\frac{1}{x-iy}+\frac{e^{-1/2-x+iy}}{x-iy+1}-2\frac{e^{-1/8-(x-iy)/2}}{x-iy+1/2}\right), \tag{5.2}$$

which displays the Gaussian localization of the wave function in the variable x and shows the rather poor localization in y.

Let us now proceed in a different way. For a filling $\nu=1/2$ and a generic MRA, the function T_2 which produces an o.n. set of translates in the LLL is given in (4.1). Using the transformation rule (3.11) we obtain

$$T_2(x,y)=\frac{e^{ixy/2}}{\sqrt{2}\,\pi^{3/4}}\int_{-\infty}^{\infty}e^{iyQ-(x+Q)^2/2}T_2(Q)=\frac{\sqrt{a}e^{ixy/2}}{2\,\pi^{3/4}}\sum_{l\in\mathbf{Z}}h_l\int_0^a e^{iQ(y-la)-(x+Q)^2/2},$$

which, for the above choice of coefficients corresponding to the Haar wavelet, gives

$$T_2(x,y)=\frac{\sqrt{a}e^{ixy/2}}{2^{3/2}\pi^{5/4}}\int_0^a e^{iQy-(x+Q)^2/2}(1+e^{-iQa})\,dQ. \tag{5.3}$$

Here T_2 can be written in terms of error function $\phi(z)$ as follows:

$$T_2(x,y)=\frac{\sqrt{a}e^{-ixy/2-y^2/2}}{4\,\pi^{3/4}}\left(\phi\left(\frac{x+a-iy}{\sqrt{2}}\right)+\phi\left(\frac{x+a-i(y-a)}{\sqrt{2}}\right)-\phi\left(\frac{x-iy}{\sqrt{2}}\right)\right.$$
$$\left.-\phi\left(\frac{x-i(y-a)}{\sqrt{2}}\right)\right), \tag{5.4}$$

whose asymptotic behavior can be found with the help of Ref. 19:

$$T_2(x,y)\simeq\frac{\sqrt{a}e^{+ixy/2-x^2/2}}{2^{3/2}\pi^{5/4}}\left(\frac{1}{x-iy}+\frac{e^{\pi-ia(x-iy)}}{x-i(y-a)}-\frac{e^{-\pi-a(x-iy)}}{x+(a-iy)}-\frac{e^{-a(x-iy)(1+i)}}{x+a-i(y-a)}\right). \tag{5.5}$$

This formula shows that, even if the two procedures produce different results, the asymptotic behaviors, that is, the localization features of the electrons, coincide for H_{00} and T_2. This result can be considered as a consequence of the Balian–Low theorem applied to the present situation (see Refs. 1 and 6) and of the Battle theorem for our previous proposal (see Refs. 3, 20, and 6). Both these theorems give severe constraints on the localization properties of a wave function when orthonormality requirements of a different kind are imposed. We refer to Ref. 6 for a rather complete review of the localization problem in a generic Landau level.

The function T_2 can be used to construct a Slater determinant for the N-electron system as sketched above: we start considering its (magnetic) translated as in (3.17),

$$(T_2)_{m,n}(x,y)=\frac{\sqrt{a}e^{-ixy/2-ianx-(y+na)^2/2}}{4\,\pi^{3/4}}\left\{\phi\left(\frac{x+(m+1)a-i(y+na)}{\sqrt{2}}\right)-\phi\left(\frac{x+ma-i(y+na)}{\sqrt{2}}\right)\right.$$
$$\left.+\phi\left(\frac{x+(m+1)a-i(y+(n-1)a)}{\sqrt{2}}\right)-\phi\left(\frac{x+ma-i(y+(n-1)a)}{\sqrt{2}}\right)\right\}.$$

These are the functions used to build up the antisymmetric wave function

$$T^{(N)}(\underline{r}_1,\underline{r}_2,\ldots,\underline{r}_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}(T_2)_{m_1,n_1}(\underline{r}_1) & (T_2)_{m_1,n_1}(\underline{r}_2) & \ldots & (T_2)_{m_1,n_1}(\underline{r}_N)\\ (T_2)_{m_2,n_2}(\underline{r}_1) & (T_2)_{m_2,n_2}(\underline{r}_2) & \ldots & (T_2)_{m_2,n_2}(\underline{r}_N)\\ \cdot & \cdot & \ldots & \cdot\\ \cdot & \cdot & \ldots & \cdot\\ \cdot & \cdot & \ldots & \cdot\\ (T_2)_{m_N,n_N}(\underline{r}_1) & (T_2)_{m_N,n_N}(\underline{r}_2) & \ldots & (T_2)_{m_N,n_N}(\underline{r}_N)\end{vmatrix},$$

where (m_i,n_i) are those indexes compatible with an electron density $\nu=1/2$.

It is evident that our procedure produces many possible N-electron wave functions in the LLL, one for each different MRA of $\mathcal{L}^2(\mathbf{R})$. Among all these possibilities, the one physically relevant is that choice which minimizes the Coulomb energy. Of course, before comparing these results with those obtained using the Laughlin wave function, we first need to generalize our procedure to a triangular lattice. The details of this extension will be considered in a future work.

In the last part of this section we extend the orthonormality constraint (3.21) to levels higher than the lowest.

We begin this analysis with a general remark, which already suggests the final result: orthonormality is required on a set of functions obtained by a single wave function via the action of the magnetic translations T_i. On the other hand, the passage from a Landau level to the other is obtained with the action of the raising and lowering operators $A'^{\dagger}$ and A' defined by

$$A' = \frac{Q' + iP'}{\sqrt{2}}, \tag{5.6}$$

where Q' and P' are given in (3.5). We have already remarked that the translations T_i commute with Q' and P', and with A' and $A'^{\dagger}$ as a consequence, so that it is reasonable to expect that the orthonormality constraint does not change very much moving from the lowest to some higher Landau level. This is exactly what happens, as we will now show explicitly for the first excited level.

All the wave functions of the first Landau level, ILL, are given by formula (3.9) with $\Psi(P,P') = f_1(P')h(P)$. Here $f_1(P') = (\sqrt{2}/\pi^{1/4})P'e^{-P'^2/2}$ is the first excited function of the harmonic oscillator. Performing the integration in P' we obtain

$$\psi(x,y) = \frac{ie^{-ixy/2}}{\pi^{3/4}} \int_{-\infty}^{\infty} e^{iyP} e^{-P^2/2} P h(P-x)\, dP. \tag{5.7}$$

Acting on $\psi(x,y)$ with T_i as in (3.17) and defining $S_{m,n}$ as in (3.21) we obtain

$$\begin{aligned} S_{m,n} &= \frac{1}{\pi^{3/2}} \int d^2r \int_{-\infty}^{\infty} dp \int_{-\infty}^{\infty} dp' e^{-ianx - iyp + i(y+na)p' - (p^2+p'^2)/2} p p' \overline{h(p-x)} h(p'-x-ma) \\ &= \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dq e^{inaq} \overline{h(q)} h(q-ma)(q+x)^2 e^{-(q+x)^2} \\ &= \int_{-\infty}^{\infty} dp e^{inap} \overline{h(p+ma)} h(p), \end{aligned}$$

which coincides with the result obtained for the LLL. This means that, when passing to the kq-representation, the wave function originating the o.n. set in the ILL is exactly the same function originating the o.n. set in the LLL. Needless to say, this does not imply that in the configuration space the two different o.n. sets coincide, because they are generated by different $\psi(P,P')$, belonging to different Landau levels.

Even if the above-mentioned result has been obtained only for the ILL, it gives a strong indication that the orthonormality condition in terms of $h(P)$ takes exactly the same form for all the Landau levels. This also follows form our original remark on the commutativity among T_i and $A'^{\dagger}$.

VI. OUTCOME

In this article we have proven a deep connection between a MRA of $\mathcal{L}^2(\mathbf{R})$ and the FQHE. In particular we have shown how a single electron wave function, which, together with its magnetic translates, produces an o.n. set in the LLL, can be constructed starting from a MRA. This proce-

dure works for $\nu=1/2L, L\in\mathbf{N}$. We have also shown that this procedure can be essentially inverted since to any o.n. basis of translated functions of the LLL (corresponding to $\nu=1/2L$) corresponds a set of coefficients satisfying the main condition of a MRA of $\mathcal{L}^2(\mathbf{R})$. Moreover, we have compared this approach with a similar one, Ref. 3, which is close for the final result but is very different for the philosophy. We have finally extended this procedure to other Landau levels.

What is still to be done is a computation of the energy of the 2DEG for such a basis, in order to see if this procedure can give some hints about the ground state for the FQHE. We also plan to extend this procedure to filling ν of the form $\nu=1/(2L+1)$ and, more generally, $\nu=L/L'$, with L and L' relatively prime natural numbers.

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Berry phase in homogeneous Kähler manifolds with linear Hamiltonians

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We study the total [dynamical plus geometrical (Berry)] phase of cyclic quantum motion for coherent states over homogeneous Kähler manifolds $X=G/H$, which can be considered as the phase spaces of classical systems and which are, in particular cases, coadjoint orbits of some Lie groups G. When the Hamiltonian is linear in the generators of a Lie group, both phases can be calculated exactly in terms of *classical* objects. In particular, the geometric phase is given by the symplectic area enclosed by the (purely classical) motion in the space of coherent states. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1396837]

I. INTRODUCTION

Let us consider a quantum state $\psi(t)$ whose evolution follows a time-dependent Schrödinger equation. If the final state $\psi(T)$ coincides with the initial one $\psi(0)$, then the representative state vectors $|\psi(0)\rangle$ and $|\psi(T)\rangle$ differ one from another just by a phase factor $\exp(i\alpha)$. This phase factor can be split into two parts $\alpha=\beta+\gamma$, called, respectively, dynamical phase and geometrical phase. Both β and γ are important characteristics of the evolution of the system under consideration.

In particular the geometric phase turns out to depend on the Hamiltonian in a rather indirect way, as it is determined *only* by the closed loop traversed by the state in the state space. This geometrical phase associated to any quantum cyclic motion with time-dependent Hamiltonians appears, in addition to the well-known dynamical phase, due to the natural curvature of the line bundle over the projective Hilbert space of states. This was found by Berry[1] for adiabatic motion, interpreted by Simon[2] as above, and extended by Aharonov–Anandan in Ref. 3 (see also Refs. 4 and 5 for arbitrary cyclic motion). However, there are very few cases in which the calculation can be performed explicitly, and it would be nice to exhibit examples where the phases of a cyclic quantum motion can be calculated in closed terms.

We shall consider the important cases in which the Hamiltonian $H(t)$ is *linear* in the generators of a Lie algebra $\mathcal{G}$ acting through some unitary irreducible representation T^{λ} in a Hilbert space $\mathcal{H}^{\lambda}$, where λ labels the representation. The aim of this paper is to show that in these cases, explicit expressions for both β and γ can be given in terms of a related *classical* dynamical system. This is achieved by using the generalized coherent state technique,[6–8] and is done in a frame general enough to cover a wide variety of examples and particular cases, including the well-known situation for evolution of a spin 1/2 in a magnetic field, a standard example which is however an oversimplified one, because its quantum state space is the Riemann sphere $\mathbb{C}P^1$.

Therefore all information on *dynamical and geometrical phases* for these quantum systems

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can be obtained by studying the motion of a *purely classical* system in a suitable phase space. As we shall see these are the Kähler (and hence naturally symplectic) homogeneous spaces $X=G/H$, with G the Lie group of the Lie algebra $\mathcal{G}$. Important examples of such spaces are the orbits of the coadjoint representation of compact semisimple Lie groups. For $G=U(n)$ the generic (maximal dimension) coadjoint orbit is $\mathrm{U}(n)/\mathrm{U}(1)^n$; this space is called a flag manifold, and plays an important role in many areas.[9,10]

The setup of this paper is as follows: in Sec. II we present the main ideas leading to closed expressions for dynamical and geometrical phases, in terms of motion in the space X taken as a *classical* space. This is possible when the quantum Hamiltonian is linear in the generators of some representation of a Lie algebra $\mathcal{G}$ and besides X is an homogeneous Kähler manifold of the Lie group G. In Sec. III we describe some homogeneous Kähler manifolds; they include (i) coadjoint orbits of semisimple compact Lie groups, (ii) the so-called bounded symmetric domains which are not compact, and (iii) some other cases, like the Heisenberg ''plane.''

Finally in Appendix A we collect explicit expressions for the kernels which determine the Kähler potential, and we give some differential and topological information on Kähler manifolds, including the Poincaré polynomials. A resumé of relevant details on coherent states, extracted from Ref. 8 is also included as Appendix B.

II. THE GROUP THEORETICAL COMPUTATION OF PHASES

Let us consider the time-dependent Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle=\hat{H}(t)|\psi(t)\rangle, \tag{2.1}$$

with a Hamiltonian of the form

$$\hat{H}(t)=\sum_j a_j(t)X_j^\lambda, \quad X_j^\lambda=\mathcal{T}^\lambda(X_j), \tag{2.2}$$

where $\mathcal{T}^\lambda$ is a unitary irreducible representation of the Lie algebra $\mathcal{G}$, whose generators X_j are represented in $\mathcal{T}^\lambda$ by the (anti-Hermitian) operators iX_j^λ, and $a_j(t)$ is the arbitrary real functions of time. We consider here only those cases when the representation Hilbert space $\mathcal{H}^\lambda$ may be realized as a space $\mathcal{F}^\lambda$ of holomorphic functions on a complex homogeneous space $X=G/H$ which is also a Kähler one. We assume also that the initial state is a generalized coherent state $|x_0\rangle$ labeled by the point $x_0\in X$; for details, see Ref. 8.

In this case, under time evolution the initial coherent state remains a coherent state

$$|x(t)\rangle=U(t,0)|x(0)\rangle \tag{2.3}$$

and then $x(t)$ is a solution of the Hamilton equation for the corresponding *classical* system

$$\dot{x}=\{H(t),x\}^\lambda, \quad \dot{x}=\frac{dx}{dt}, \tag{2.4}$$

where $\{,\}^\lambda$ is the Poisson bracket induced on X by the representation $\mathcal{T}^\lambda$.

The mapping $X\to\mathcal{H}^\lambda$ which associates the point $x_0\in X$ to the coherent state $|x_0\rangle$ allows an isomorphic identification of actual quantum ''trajectories'' starting from $|x_0\rangle$ and obeying the usual Schrödinger equation

$$i\frac{d}{dt}|x(t)\rangle=\hat{H}(t)|x(t)\rangle \tag{2.5}$$

to some *classical* motions in X (taken as a *classical* phase space, not a configuration space), satisfying (2.4). Under this identification, if Γ is a closed loop in X with period T, it is still close

in the projective Hilbert space $\overline{\mathcal{H}}^{\lambda}$, which should be considered as the *true* state space, but not necessarily in the linear Hilbert space $\mathcal{H}^{\lambda}$. In this cyclic motion, the state *vector* picks up a phase

$$|\psi(T)\rangle = \exp(i\alpha)|\psi(0)\rangle, \quad \alpha = \beta + \gamma. \tag{2.6}$$

This can also be seen as follows.[4] Let Γ be a closed path (loop) in the projective Hilbert space $\overline{\mathcal{H}} = \mathbb{C}P^{\infty}$ of states; let $|\psi\rangle = |\psi(t)\rangle$ be a generic point in Γ. There is a tautological line bundle, whereby each point carries its vectors; this line bundle is Hermitian, by the Hermitian product in $\mathcal{H}$. Let $P(t)$ be in the fiber over $|\psi(t)\rangle$. The Hamiltonian $\hat{H}$ works in $\mathcal{H}$, and by projection in $\overline{\mathcal{H}}$ also, so the time evolution carries $P(0) \to P(t)$ and projects to $U(0,t): |\psi(0)\rangle \to |\psi(t)\rangle$. As $P(T)$ is the fibre over $\psi(T)$ which coincides with the fibre over $\psi(0)$, we must have

$$P(T) = \exp(i\alpha)P(0), \tag{2.7}$$

where α is the total phase for the cyclic motion. The lift of the path Γ through the connection of the line bundle L^{λ} would produce an U(1) holonomy γ; this is the *geometric phase*, and the difference, $\beta = \alpha - \gamma$ is the dynamical phase. As explained in detail in Ref. 2, we have the following explicit expressions for both parts of the total phase α:

$$\beta = \int \langle \psi(t)|\hat{H}(t)|\psi(t)\rangle dt, \quad \gamma = \int \langle \psi'(t)|\left(-i\frac{d}{dt}\right)|\psi'(t)\rangle dt, \tag{2.8}$$

where $|\psi'(t)\rangle$ is a trivializing section, i.e., there is no dynamical phase for the whole loop, see Refs. 4 and 11. The connection 1-form of this line bundle θ^{λ} is related locally to the symplectic 2-form as $\omega^{\lambda} = d\theta^{\lambda}$, and this symplectic 2-form is in turn induced by the imaginary part of the Hermitian scalar product in $\mathcal{H}^{\lambda}$.

Under the conditions stated, both phases can be computed directly in terms of the classical motion in X. For the dynamical part we have

$$\beta = \int \langle \psi(t)|\hat{H}(t)|\psi(t)\rangle dt = \int \langle x(t)|\hat{H}(t)|x(t)\rangle dt = \int a_j(t) X_j^{\lambda}(t) dt, \tag{2.9}$$

where $X_j^{\lambda}(t) = \langle x(t)|X_j^{\lambda}|x(t)\rangle$.

The geometric phase γ is given as the integral along Γ of the connection 1-form θ^{λ} which depends on the representation. Due to the Abelian nature of the U(1) group, the Stokes theorem applies and gives

$$\gamma = \gamma_{cl} = \int_{\Gamma} \theta^{\lambda} = \int_{\Sigma} \omega^{\lambda}, \tag{2.10}$$

where $\omega^{\lambda} = d\theta^{\lambda}$ and Σ is any surface having $\Gamma = \partial\Sigma$ as its boundary. Hence, we give the expression for the geometric phase in terms of symplectic area of any surface whose boundary is the given (classical) closed circuit in our Kähler manifold X.

Thus formula (2.10) is valid for arbitrary homogeneous Kähler manifolds. Now if F^{λ} denotes the Kähler potential,[12,13] the expressions for the connection and curvature forms are (see Appendix A)

$$\theta^{\lambda} = \frac{1}{i}\left(\frac{\partial F^{\lambda}}{\partial z_{\mu}} dz_{\mu} - \frac{\partial F^{\lambda}}{\partial \overline{z}_{\mu}} d\overline{z}_{\mu}\right), \quad \omega^{\lambda} = \frac{i}{2}\frac{\partial^2 F^{\lambda}}{\partial z_{\mu} \partial \overline{z}_{\nu}} dz_{\mu} \wedge \partial \overline{z}_{\nu} = d\theta^{\lambda}, \tag{2.11}$$

and the Kähler potential itself is related to the kernel, which generalizes Bergmann's kernel, as

$$F(z,\overline{z}) = \ln(K(z,\overline{w}))|_{w=z}. \tag{2.12}$$

The simplest closed loops are geodesic triangles. For them we can give explicit expressions.

Let us first consider the simplest case $\mathcal{G}=\mathrm{su}(2)$, where $X=\mathbb{C}P^1=\mathrm{SU}(2)/\mathrm{U}(1)$ is the Riemann sphere, and $\mathrm{U}(1)\to\mathrm{SU}(2)=S^3\to S^2$ is the second Hopf sphere bundle. In this case there is a single complex coordinate z, related with the point x on the sphere by the usual stereographic projection, and the Bergmann's kernel is given by

$$K(z,\overline{w})=1+z\overline{w}. \tag{2.13}$$

It is clear that any vertex can be carried to a prescribed point on the sphere, say the North pole, corresponding to $z=0$. Let $|x\rangle,|y\rangle$ denote the two coherent states determining the remaining triangle vertices, corresponding to points x,y on the sphere, and let us denote z,w the complex coordinates corresponding to x,y. The closed expression for the geometric phase associated to this closed loop is

$$\gamma=\frac{1}{2i}\ln\frac{K(\overline{z},w)}{K(z,\overline{w})}=\frac{1}{2i}\ln\frac{1+\overline{z}w}{1+z\overline{w}}=\frac{1}{2i}\ln\frac{\langle x|y\rangle}{\langle y|x\rangle}. \tag{2.14}$$

For $\mathcal{G}=\mathrm{su}(2)$ this result for the phase has been given already in Ref. 6 (see also Ref. 8). In this case the symplectic area is proportional to the Riemannian area for the standard Riemannian structure on S^2; this proportionality is however accidental and may be misleading because this does not hold in higher dimensions; for instance in $\mathbb{C}P^n$ $(n>1)$ the symplectic area of any finite triangle is not proportional to its Riemannian Fubini–Study area.

Let us now consider the general case where the generators X_j^λ close to a unitary irreducible representation of the Lie algebra $\mathcal{G}$. The symplectic area of any closed loop in $\overline{\mathcal{H}}$ is completely determined by the loop; this does not hold for the ''Riemannian'' area determined by a general Kähler metric, which depends essentially on the two-dimensional surface whose boundary is the prescribed loop. In this general case (with group $\mathcal{G}$), it suffices again to give a closed expression for the symplectic area of a triangular loop. If one vertex is carried to a prescribed point on the Kähler homogeneous manifold X (say determined by the complex coordinates $z_\mu=0$), the remaining vertices x,y will correspond to the complex coordinates z_μ,w_ν. The same argument as before leads in this case to the expression

$$\gamma\propto\frac{1}{2i}\ln\frac{K(\overline{z},w)}{K(z,\overline{w})}. \tag{2.15}$$

Appendix A contains explicit expressions for the kernels $K(z,\overline{w})$ for Hermitian symmetric spaces, taken from Ref. 8, where further details on the construction of the kernel $K(z_\mu,\overline{w_\nu})$ for homogeneous Kähler manifolds can be found.

In the case of complex Grassmannians, the usual choice for complex coordinates are called Pontrjagin coordinates and can be arranged as a complex rectangular matrix Z. After substituting for the relevant kernel, the basic expression (2.15) reduces to

$$\gamma\propto\frac{1}{2i}\ln\frac{\det(\mathrm{I}+ZW^\dagger)}{\det(\mathrm{I}+WZ^\dagger)} \tag{2.16}$$

and coincides with the formula for the geometric phase derived through explicit computation by Berceanu, who also points out the validity of a similar formula for any Hermitian symmetric space.[14] However, the arguments given in Ref. 8 appear to hold unrestrictedly for arbitrary homogeneous Kähler manifold X, and not only for Hermitian symmetric spaces.

In the well understood example (see, e.g., Refs. 15 and 16), of a spin 1/2 particle in a magnetic field,

$$i\frac{d}{dt}|\psi(t)\rangle=-\mu\mathbf{B}(t)\cdot\mathbf{S}|\psi(t)\rangle, \tag{2.17}$$

the Hamiltonian is a linear combination of three operators which span a Lie algebra su(2), and quantum evolution can be thus translated into a classical motion of a point on the homogeneous space SU(2)/U(1), the Riemann sphere again. The coadjoint orbits are 2-spheres and $x=\mathbf{x}$ is a unit vector in $\mathbb{R}^3$, so at any fixed time $\hat{H}(t)$ splits into two parts:

$$\hat{H}(t)=\hat{H}_{\parallel}+\hat{H}_{\perp}, \tag{2.18}$$

where

$$\hat{H}_{\perp}|\mathbf{x}(t)\rangle=0, \quad \hat{H}_{\parallel}|\mathbf{x}(t)\rangle=E(t)|\mathbf{x}(t)\rangle. \tag{2.19}$$

The longitudinal part produces only a dynamical phase, as the ray of $|\mathbf{x}\rangle$ and of $E(t)|\mathbf{x}\rangle$ are the same. The geometrical phase comes entirely from the transverse part. In particular, if the field is constant in direction:

$$H(t)=B(t)\sigma_z \tag{2.20}$$

and the initial state is $|\mathbf{x}\rangle=\cos(\theta/2)|+\rangle+\sin(\theta/2)|-\rangle$, the solution is readily obtained

$$|\psi(t)\rangle=a(t)|+\rangle+b(t)|-\rangle, \tag{2.21}$$

where $a(t)=a(0)\exp(-i\int B(t)dt)$, $b(t)=b(0)\exp(i\int B(t)dt)$. For $\theta=0$ or $\theta=\pi$ we have a purely dynamical phase, while for $\theta=\pi/2$ the phase is purely geometrical.

For arbitrary $\mathbf{B}(t)$ there is also a local splitting, and the "parallel" $H_{\parallel}$ and "perpendicular" $H_{\perp}$ parts of the Hamiltonian carry, respectively, the dynamical and geometric phases.

III. HOMOGENEOUS SYMPLECTIC MANIFOLDS AND KÄHLER MANIFOLDS

Relative to the definition of a symplectic manifold, see Ref. 17.

Definition: A symplectic manifold (M,ω) is called homogeneous if there exists on it a transitive action $\Phi_g: M\to M$ of some Lie group $G=\{g\}$ which acts as a group of symplectic transformations, i.e., it leaves invariant the form ω, $\Phi_g^*\omega=\omega$.

Theorem:[18] *Any homogeneous symplectic manifold on which a connected Lie group G acts transitively and by symplectic transformations is locally isomorphic to an orbit of a coadjoint representation of this group G or of a central extension of G by $\mathbb{R}$.*

Thus any coadjoint orbit of the group G is an homogeneous symplectic manifold.

Among the class of all homogeneous symplectic manifolds, the main important subclass is those of coadjoint orbits of *semisimple* Lie groups. These have an additional Kähler homogeneous structure. A Kähler manifold is defined as a complex manifold M endowed with a Kähler metric h, whose imaginary part is a closed 2-form. A Kähler metric is an Hermitian metric h which comes from a function $F(z,\bar{z})$ called the Kähler potential:

$$ds^2=h_{\mu\bar{\nu}}dz^{\mu}\,d\bar{z}^{\nu}, \quad h_{\mu\bar{\nu}}(z,\bar{z})=\partial_{\mu}\partial_{\bar{\nu}}F(z,\bar{z}), \quad \partial_{\mu}=\frac{\partial}{\partial z_{\mu}}, \quad \partial_{\bar{\nu}}=\frac{\partial}{\partial \bar{z}_{\nu}}. \tag{3.1}$$

The imaginary part of this metric is a symplectic 2-form

$$\omega=\frac{i}{2}h_{\mu\bar{\nu}}(z,\bar{z})dz^{\mu}\wedge d\bar{z}^{\nu}, \quad d\omega=0. \tag{3.2}$$

The connection between orbits of the coadjoint representation of compact simple Lie groups and Kähler homogeneous manifolds is stated in the following important result of Borel:

Theorem:[19] *Any orbit of the coadjoint representation of a compact simple Lie group is a compact Kähler homogeneous simply connected manifold, and any compact Kähler homogeneous simply connected manifold is some orbit of the coadjoint representation of the some compact simple Lie group.*

Orbits of the coadjoint representation of a compact Lie group are even rational manifolds.[20] Topologically they are compact and simply connected manifolds. Their topology is described, for example, in the review.[9] In the Appendix A we give some pertinent results.

Many examples of Kähler homogeneous manifolds with a compact group G are known; these spaces are compact, even-dimensional, simply connected and oriented. As the cohomology class $[\omega]\neq 0$, all the even Betti numbers are nonzero. Let us recall some simple examples.

For $G=\mathrm{SU}(2)=\mathrm{Spin}(3)\sim\mathrm{SO}(3)$, the generic coadjoint orbits in $\mathrm{su}(2)\approx\mathbb{R}^3$ are spheres S^2; there is an isolated orbit consisting of a single point, the origin. For each sphere the 2-form is just the area (volume) form, automatically closed by dimensionality. It is a complex (one-dimensional) manifold, the Riemann sphere.

For $G=\mathrm{SU}(3)$, there are three types of coadjoint orbits in $\mathrm{su}(3)\approx\mathbb{R}^8$: the origin, four-dimensional orbits isomorphic to $\mathbb{C}P^2=\mathrm{SU}(3)/\mathrm{SU}(2)\times\mathrm{U}(1)$, and six-dimensional maximal orbits, isomorphic to the flag manifold $\mathbb{F}^3=\mathrm{SU}(3)/\mathrm{U}(1)\times\mathrm{U}(1)$.

For $G=\mathrm{SU}(n)$, the description of the orbits is essentially given by the partitions of n (see Ref. 21).

The general calculation of Kähler metrics on the coadjoint orbits for any compact simple Lie group (the classical and exceptional structures of Cartan) was expelled in Ref. 21.

The main reason why these manifolds are Kähler is that the homogeneous structure is also obtained from the complex extension $G^{\mathbb{C}}$ of G. The role of the subgroup H here is played by some triangular (Borel) subgroup B; both $G^{\mathbb{C}}$ and B are analytic manifolds, and so is $G^{\mathbb{C}}/B$ which turns out to be isomorphic to G/H. The space X is also obviously simply connected, because G can be taken simply connected (for any X) and H is connected. This construction $X=G/H=G^{\mathbb{C}}/B$ is also basic in the Borel–Weil–Bott theory of analytic construction of irreducible representations of G as sections in some holomorphic bundles.

When G is a general simple or semisimple compact Lie group, the orbits of the coadjoint representation exhausts all the compact homogeneous Kähler manifolds.

Other examples of (noncompact) Kähler manifolds are the so-called bounded symmetric domains (see Ref. 22). Recall that a bounded domain $D\subset\mathbb{C}^n$ is called symmetric if each point in D is fixed by an involutive holomorphic diffeomorphism of D. These are characterized by the result.

Theorem: [Helgason,[22] p. 310] *(i) Each bounded symmetric domain D, when equipped with the Bergmann metric, is a Hermitian symmetric space of the noncompact type. In particular, a bounded symmetric domain is neccesarily simply connected.*

(ii) Let M be a Hermitian symmetric space of the noncompact type. Then there exists a bounded symmetric domain D and a holomorphic diffeomorphism of M onto D.

The paradigmatic example is the Lobachevsky plane. This is a Kähler manifold which is noncompact, and of constant negative curvature.

A complete classification of Kähler manifolds is still lacking. Hermitian symmetric spaces, which are completely classified, are examples of Kähler manifolds, while the remaining non-Hermitian symmetric spaces are not Kähler (e.g., the even dimensional spheres $S^{2n}, n>1$ are homogeneous and symmetric, but obviously not Kähler).

Some nonsemisimple groups also provide other Kähler manifolds. A very basic example is that obtained from the Heisenberg–Weyl algebra $\mathrm{hw}(1)$ generated by the usual operators $p,q,1$, by quotient by the subgroup generated by the subalgebra 1. This space is the basic ''quantum'' space q,p, whose noncompact Kähler character becomes obvious after introduction of the complex coordinate $z=p+iq$.

APPENDIX A: KÄHLER HOMOGENEOUS MANIFOLDS

We start by listing some examples of compact Kähler homogeneous manifolds. More details can be found in Refs. 19 and 21.

(1) $G=\mathrm{SO}(3)\sim\mathrm{SU}(2)$ is the rotation group of a three-dimensional vector space $\mathbb{R}^3$. Here the sign $\sim$ means a locally isomorphic group and $\mathcal{G}^*$ is the dual space to the Lie algebra $\mathcal{G}^*=\{\mathbf{x}|\mathbf{x}=(x_1,x_2,x_3)\}\approx\mathbb{R}^3$. There is a zero-dimensional orbit (the origin) while the remaining orbits are generic and are two-dimensional spheres $S_r^2=\{\mathbf{x}|\mathbf{x}^2=x_1^2+x_2^2+x_3^2=r^2\}$.

(2) $G=\mathrm{SU}(3)$. Here we have three types of coadjoint orbits in $\mathrm{su}(3)\approx\mathbb{R}^8$: First, the origin $\mathbf{x}=0$. Second, four-dimensional orbits (isomorphic to $\mathbb{C}P^2$)

$$\mathcal{O}=\frac{\mathrm{SU}(3)}{\mathrm{SU}(2)\times\mathrm{U}(1)}, \tag{A1}$$

and third, six-dimensional orbits isomorphic to the complex flag space $\mathbb{F}^3$

$$\mathcal{O}=\frac{\mathrm{SU}(3)}{\mathrm{U}(1)\times\mathrm{U}(1)}. \tag{A2}$$

(3) $G=\mathrm{SU}(n)$. Here, in addition to the trivial zero-dimensional orbit, we have orbits isomorphic to the complex projective space $\mathbb{C}P^{n-1}$,

$$\mathcal{O}=\frac{\mathrm{SU}(n)}{\mathrm{SU}(n-1)\times\mathrm{U}(1)}\sim\mathbb{C}P^{n-1}. \tag{A3}$$

There are also orbits isomorphic to the complex Grassmannians $\mathbb{C}G_{m,n}$,

$$\mathcal{O}=\frac{\mathrm{SU}(m+n)}{\mathrm{SU}(m)\times\mathrm{SU}(n)\times\mathrm{U}(1)}\sim\mathbb{C}G_{m,n}, \tag{A4}$$

and finally the generic maximal orbits are isomorphic to the complex flag manifold $\mathbb{F}^n$,

$$\mathcal{O}=\frac{\mathrm{SU}(n)}{\mathrm{U}(1)\times\mathrm{U}(1)\times\cdots\times\mathrm{U}(1)}\sim\mathbb{F}^n. \tag{A5}$$

(4) For compact simple Lie algebras, the coadjoint orbits of minimal nonzero dimension were investigated in Ref. 23, and are given in the following table:

G		$\dim\mathcal{O}_{\min}$	H
A_n	$\mathrm{SU}(n+1)$	$2n$	$A_{n-1}\times\mathrm{U}(1)$
B_n	$\mathrm{SO}(2n+1)$	$2(2n-1)$	$B_{n-1}\times\mathrm{SO}(2)$
C_n	$\mathrm{Sp}(n)$	$2(2n-2)$	$C_{n-1}\times\mathrm{U}(1)$
$D_n, n\neq 2$	$\mathrm{SO}(2n)$	$2(2n-2)$	$D_{n-1}\times\mathrm{SO}(2)$
G_2		10	$A_1\times\mathrm{SO}(2)$
F_4		30	$C_3\times\mathrm{SO}(2)$
E_6		32	$D_5\times\mathrm{SO}(2)$
E_7		54	$E_6\times\mathrm{SO}(2)$
E_8		114	$E_7\times\mathrm{SO}(2)$

1. Kernels for some Hermitian symmetric spaces

In this section we give the explicit expressions[24] for kernels of the Hermitian symmetric spaces of classical type, either compact or noncompact (bounded symmetric domains). They belong to four families, which in the Cartan notation are $A_{\mathrm{III}}, C_{\mathrm{I}}, D_{\mathrm{III}}$ and $BD_{\mathrm{I}}(q=2)$.[22] There are two further exceptional Hermitian symmetric spaces, $E_{\mathrm{III}}, E_{\mathrm{VII}}$ related to exceptional Lie algebras.

A_{III}**c**:

For the complex Grasmannians $\mathbb{C}G_{p,q}$ of p-planes in $\mathbb{C}^{p+q}$:

$$X=\mathrm{SU}(p+q)/(\mathrm{SU}(p)\otimes\mathrm{SU}(q)\otimes\mathrm{U}(1)),\quad p\geqslant q, \tag{A6}$$

in terms of the pq complex coordinates arranged in a rectangular $p\times q$ complex matrix Z:

$$K(z,\overline{w})=\det(I^{(p)}+ZW^{\dagger}). \tag{A7}$$

A_{III}**nc**:

The noncompact Cartan duals of the complex Grassmannians are the spaces:

$$X=\mathrm{SU}(p,q)/(\mathrm{SU}(p)\otimes\mathrm{SU}(q)\otimes\mathrm{U}(1)),\quad p\geqslant q, \tag{A8}$$

which can be realized as the bounded domain $I^{(p)}-ZZ^{\dagger}\geqslant 0$ with Z as above; its kernel is

$$K(z,\overline{w})=\det(I^{(p)}-ZW^{\dagger}). \tag{A9}$$

$C_{\mathrm{I}}\mathbf{c}$:

For the manifold of Lagrangian p-spaces in $\mathbb{C}^{2p}$, which is the compact symmetric Hermitian space,

$$X=\mathrm{Sp}(p)/\mathrm{U}(p), \tag{A10}$$

the kernel is given in terms of $p(p+1)/2$ complex coordinates arranged in a $p\times p$ complex symmetric matrix Z as

$$K(z,\overline{w})=\det(I^{(p)}+ZW^{\dagger}). \tag{A11}$$

$C_{\mathrm{I}}\mathbf{nc}$:

The Cartan dual to the previous space:

$$X=\mathrm{Sp}(2p,\mathbb{R})/\mathrm{U}(p) \tag{A12}$$

can be realized as the bounded domain $I^{(p)}-ZZ^{\dagger}\geqslant 0$ in terms of the coordinate matrix Z as above; its kernel is

$$K(z,\overline{w})=\det(I^{(p)}-ZW^{\dagger}). \tag{A13}$$

$D_{\mathrm{III}}\mathbf{c}$:

The kernel for the compact Hermitian symmetric space:

$$X=\mathrm{SO}(2p)/\mathrm{U}(p) \tag{A14}$$

is given in terms of $p(p-1)/2$ complex coordinates arranged in a rectangular $p\times p$ complex skew-symmetric matrix Z as

$$K(z,\overline{w})=\det(I^{(p)}+ZW^{\dagger}). \tag{A15}$$

$D_{\mathrm{III}}\mathbf{nc}$:

For the noncompact Cartan dual space:

$$X=\mathrm{SO}^{*}(2p)/\mathrm{U}(p) \tag{A16}$$

realized as the bounded domain $I^{(p)}-ZZ^{\dagger}\geqslant 0$ in terms of the coordinates Z as above, the kernel is

$$K(z,\overline{w})=\det(I^{(p)}-ZW^{\dagger}). \tag{A17}$$

$BD_{\mathrm{I}}\mathbf{c}$:

The real Grasmannian $\mathbb{R}G_{2,p}$ of 2-planes in $\mathbb{R}^{p+2}$:

$$X=\mathrm{SO}(p+2)/(\mathrm{SO}(p)\otimes\mathrm{SO}(2)). \tag{A18}$$

In terms of p complex coordinates arranged as a $p\times 1$ row complex vector $\mathbf{z}$, with $\mathbf{z}'$ denoting the transpose $1\times p$ column complex vector, then

$$K(z,\overline{w})=1+(\mathbf{z}\cdot\mathbf{z}')(\overline{\mathbf{w}}\cdot\overline{\mathbf{w}}')+2(\mathbf{z}\cdot\overline{\mathbf{w}}'). \tag{A19}$$

BD_{I}**nc**:
The noncompact dual space:

$$X=\mathrm{SO}(p,2)/(\mathrm{SO}(p)\otimes\mathrm{SO}(2)) \tag{A20}$$

can be realized as the bounded domain

$$|\mathbf{z}\cdot\mathbf{z}'|<1, \quad 1+|\mathbf{z}\cdot\mathbf{z}'|^2-2\overline{\mathbf{z}}\cdot\mathbf{z}'>0, \tag{A21}$$

where the p complex coordinates are arranged as a $p\times 1$ row complex vector $\mathbf{z}$, as above; the kernel is

$$K(z,\overline{w})=1+(\mathbf{z}\cdot\mathbf{z}')(\overline{\mathbf{w}}\cdot\overline{\mathbf{w}}')-2(\mathbf{z}\cdot\overline{\mathbf{w}}'). \tag{A22}$$

The two exceptional Hermitian symmetric spaces can be dealt with similarly, by using 3×3 octonionic matrices, as discussed by Hirzebruch.[25]

2. Topology of orbits

Orbits of a coadjoint representation of compact Lie groups are compact simply connected manifolds; this follows from the exact homotopy sequence. They have a nontrivial second homotopy group $\pi_2(X)$ because they are compact symplectic manifolds. Further information on their topology may be found, for example, in the review.[9]

Let $P_X(t)=\Sigma_{j=0}^{N} b_j t^j$ be the Poincaré polynomial of manifold X, b_j being the Betti numbers of the manifold X of dimension N. In our case $X=G/H$, where H is some compact semisimple subgroup of G, and rank $H=$rank $G=r$. In this case, the Hirsch formula (see Ref. 9) is valid

$$P_X(t)=\frac{\Pi_{j=1}^{r}(1-t^{2n_j})}{\Pi_{j=1}^{r}(1-t^{2m_j})}, \tag{A23}$$

where n_j and m_j are the degrees of basic invariants of the Weyl group W of the groups G and H (see Ref. 26). Let us give a few applications of this formula. We have

(i) For the complex projective space:

$$X=\mathbb{C}P^n, \quad P_X(t)=P_n(t)\equiv 1+t^2+t^4+\cdots+t^{2n}. \tag{A24}$$

(ii) For the complex flag manifold $\mathbb{F}^n$:

$$X=\mathbb{F}^n=\frac{\mathrm{SU}(n)}{U(1)\times\cdots\times U(1)}, \quad P_X(t)=P_1(t)P_2(t)\cdots P_{n-1}(t), \tag{A25}$$

where the polynomial $P_n(t)$ was defined above.

(iii) An example of a real Grassmannian $\mathbb{R}G_{3,2}$:

$$X=\frac{\mathrm{SO}(5)}{\mathrm{SO}(3)\times\mathrm{SO}(2)}, \quad P_X(t)=P_3(t). \tag{A26}$$

(iv) An example of a real "flag-like" manifold:

$$X=\frac{\mathrm{SO}(5)}{\mathrm{SO}(2)\times\mathrm{SO}(2)}, \quad P_X=P_1(t)P_3(t). \tag{A27}$$

(v) For the minimal orbits of the coadjoint representation of G_2,

$$X=\frac{G_2}{\mathrm{SU}(2)\times\mathrm{U}(1)}, \quad P_X=P_5(t). \tag{A28}$$

(vi) For the octonionic "flag-like" coadjoint orbit of G_2:

$$X=\frac{G_2}{U(1)\times U(1)},\quad P_X=\frac{(1-t^4)(1-t^{12})}{(1-t^2)(1-t^2)}=P_1(t)P_5(t). \tag{A29}$$

(vii) For the complex Grassmann manifolds $\mathbb{C}G_{m,n}$

$$X=\mathbb{C}G_{m,n}=\frac{\mathrm{SU}(m+n)}{\mathrm{SU}(m)\times\mathrm{SU}(n)\times\mathrm{U}(1)}, \tag{A30}$$

$$P_X=\frac{(1-t^4)\cdots(1-t^{2(m+n)})}{(1-t^2)[(1-t^4)\cdots(1-t^{2m})][(1-t^4)\cdots(1-t^{2n})]}. \tag{A31}$$

For example, for the lowest dimensional complex Grassmann manifold, $\mathbb{C}G_{2,2}$, we have

$$X=\mathbb{C}G_{2,2}=\frac{\mathrm{SU}(4)}{\mathrm{SU}(2)\times\mathrm{SU}(2)\times\mathrm{U}(1)}, \tag{A32}$$

$$P_X=\frac{(1-t^6)(1-t^8)}{(1-t^2)(1-t^4)}=(1+t^4)(1+t^2+t^4)=1+t^2+2t^4+t^6+t^8. \tag{A33}$$

(viii) For the octonionic Cayley plane,

$$X=\frac{F_4}{C_3\times\mathrm{SO}(2)},\quad P_X=\frac{(1-t^{16})(1-t^{24})}{(1-t^2)(1-t^8)}, \tag{A34}$$

$$P_X=(1+t^8)(1+t^2+t^4+\cdots+t^{22})=1+t^2+t^4+\cdots+2t^8+2t^{10}+\cdots+2t^{22}+t^{24}+\cdots+t^{30}.$$

APPENDIX B: COHERENT STATES

As discussed in Sec. II, we consider here classical Hamiltonian systems which correspond to quantum systems of a special type for which the quantum properties are expressed simply in terms of classical ones.

Let (X,ω) be a compact simply connected symplectic manifold on which the semisimple compact Lie group G act transitively.

As it was shown by Borel,[19] this class of manifolds coincides with the class of orbits of a coadjoint or (what is equivalent) adjoint representation of the compact semisimple Lie group G. These manifolds are Kähler homogeneous manifolds, and have even dimension. This means that they admit a Hermitian G-invariant metric, as given in (3.1), whose imaginary part is a closed 2-form given in (3.2). Both are determined by a single function $F(z,\overline{z})$, called the potential of the Kähler metric, which may be found from the Gauss decomposition of the group G.

The G-invariant Hermitian metric (and the G-invariant symplectic structure) on the orbits of coadjoint actions is not uniquely determined. The most general ones are a linear combination of a number r of basic metrics or symplectic forms, the number r being equal to the rank of the manifold.

Let us recall now the construction of unitary irreducible representations of simple compact Lie groups G of rank r. Such representation is characterized by an r-dimensional vector $\lambda=(\lambda_1,\ldots,\lambda_r)$—the so-called highest weight: $T(g)=T^{\lambda}(g)$, where $\lambda=\Sigma\lambda_j w_j$, w_j are the fundamental weights and λ_j are non-negative integers.

Correspondingly, in the representation space $\mathcal{H}^{\lambda}$, there exists a vector (the highest vector) $|\lambda\rangle$ satisfying the conditions

$$\hat{E}_{\alpha}|\lambda\rangle=0,\quad \alpha\in R_+,\quad \hat{H}_j|\lambda\rangle=\lambda_j|\lambda\rangle, \tag{B1}$$

where $\hat{E}_{\alpha}$ and $\hat{H}_j$ are operators in $\mathcal{H}^{\lambda}$ which represent the Chevalley basis for $\mathcal{G}^C$.

In the space $\mathcal{H}^{\lambda}$, there exists a basis $\{|\mu\rangle\}$, where μ is a weight vector, i.e., an eigenvector of all operators H_j:

$$H_j|\mu\rangle=\mu_j|\mu\rangle. \tag{B2}$$

A general representation $T^{\lambda}(g)$ characterized by the highest weight $\lambda=(\lambda_1,\ldots,\lambda_r)$ corresponds to a fiber bundle over $X=G/H=G^{C}/B_{+}=X_{-}$, with the circle as a fiber, with connection and curvature forms:

$$\theta^{\lambda}=\frac{1}{2i}\left(\frac{\partial F^{\lambda}}{\partial z_{\mu}}dz_{\mu}-\frac{\partial F^{\lambda}}{\partial \overline{z}_{\mu}}d\overline{z}_{\mu}\right),\quad \omega^{\lambda}=\frac{1}{2i}\frac{\partial^2 F^{\lambda}}{\partial z_{\mu}\partial \overline{z}_{\nu}}dz_{\mu}\wedge\partial\overline{z}_{\nu}=d\theta^{\lambda}, \tag{B3}$$

where $F=\Sigma_l \lambda_l F^l$, $l=1,2,\ldots,r$. The representation $T^{\lambda}(g)$ with the highest weight λ may be realized in the space of polynomials $\mathcal{F}^{\lambda}$ over X_{-}. Namely,

$$T^{\lambda}(g)f(z)=\alpha_{\lambda}(z,g)f(z_g), \tag{B4}$$

where the quantities $\alpha_{\lambda}(z,g)$ and z_g may be found from the Gaussian decomposition

$$zg=\zeta_1 h_1 z_1, \tag{B5}$$

$$z_g=z_1,\quad \alpha_{\lambda}(z,g)=\delta_1^{\lambda_1}\cdots\delta_r^{\lambda_r}. \tag{B6}$$

The invariant scalar product $\mathcal{F}^{\lambda}$ is introduced by the formulas

$$(f_1,f_2)=d_{\lambda}\int \overline{f_1}(z)f_2(z)d\mu_{\lambda}(z), \tag{B7}$$

where d_{λ} is the dimension of the representation T^{λ}. In this case we have

$$T^{\lambda}(g)f(z)=\exp[iS^{\lambda}(z,g)]f(z_g), \tag{B8}$$

where

$$S^{\lambda}(z,g)=\int_0^z(\theta^{\lambda}-g_{*}\cdot\theta^{\lambda})+S^{\lambda}(0,g), \tag{B9}$$

and the Kähler potential is

$$F^{\lambda}=\sum \lambda_l F_l^{\lambda}(z,\overline{z})=-\ln\langle\lambda|T^{\lambda}(zz^{+})|\lambda\rangle, \tag{B10}$$

which determines after (B3) the connection θ^{λ} and curvature ω^{λ} forms in the fiber bundle with base X, a circle as a fiber, and related to the representation $T^{\lambda}(g)$.

A similar construction works also for degenerate representations for which the highest weight λ is singular, i.e., $(\lambda,\alpha)=0$ for one or several roots α. Then the *isotropy* subgroup $\tilde{B}$ of a vector $|\psi_0\rangle$ is one of the so-called parabolic subgroups. This means that $\tilde{B}$ contains the Borel subgroup B, i.e., the maximal solvable subgroup. The coset space $X=G^{C}/\tilde{B}$ is the degenerate orbit of the coadjoint representation, but this space is still the homogeneous Kähler manifold.[19] Hence the construction considered above is valid completely also in this case.

Following Refs. 6–8, let us now construct the coherent state (hereafter CS) systems for an arbitrary compact Lie group.

To this aim one has to take an initial vector $|0\rangle$ in the space $\mathcal{H}^{\lambda}$. Note first of all that the isotropy subgroup H_{μ} for any state $|\mu\rangle$ corresponding to weight vector μ contains the Cartan subgroup $H=\mathrm{U}(1)\times\cdots\times\mathrm{U}(1)=T^r$, where r is the number of $\mathrm{U}(1)$ factors entering in H, and is called the rank of group G. For generic weight vectors subgroup H_{μ} coincides with H.

In general, the isotropy subgroup for a linear combination of weight vector is a subgroup of the Cartan subgroup. Therefore it is convenient to choose a weight vector $|\mu\rangle$ as an initial element of the CS system. In the general case, the isotropy subgroup H_μ is isomorphic to the Cartan subgroup H, and a CS is characterized by a point of $X=G/H$.

For the degenerate representation, where the highest weight λ is orthogonal to some root $\alpha:(\lambda,\alpha)=0$, the isotropy subgroup H_μ may be larger than T^r for some state vector $|\mu\rangle$. Then any CS $|x\rangle$ is characterized by a point of a degenerate orbit of the adjoint representation. Indeed, in all cases,

$$H_j'|x\rangle=[T(g)H_jT^{-1}(g)]|x\rangle=\mu_j|x\rangle, \quad |x\rangle=T(g)|\mu\rangle. \tag{B11}$$

Therefore if we take a state vector $|\mu\rangle$ as the initial vector $|0\rangle$, then the coherent state $|x\rangle$ is characterized by a point of an orbit of adjoint representation, and the orbit may be degenerate.

Now suppose that $T^\lambda(g)$ is a nondegenerate representation of the compact Lie group G with the highest weight λ, i.e., $(\lambda,\alpha)\neq 0$ for any $\alpha\in R$. We take the vector with the lowest weight $|-\lambda\rangle$ as the initial vector $|0\rangle$ for the CS system. Let us consider the action on this state of operators H_j, E_α, and $E_{-\alpha}(\alpha\in R_+)$ representing the Lie algebra $\mathcal{G}^C$. One can see that subalgebra $\mathcal{B}_-=\{H_j,E_{-\alpha}\},\alpha\in R_+$ is the isotropy subalgebra for the vector $|\lambda\rangle$. The corresponding group B_- is a subgroup of G^C.

Taking the lowest weight vector $|\lambda\rangle$ as $|0\rangle$, applying operators $T^\lambda(g)$ and using the Gaussian decomposition $g=\zeta hz$, with $\zeta\in Z_+$, we obtain the CS system

$$|\zeta\rangle=NT^\lambda(\zeta)|0\rangle=N\exp\left(\sum_{\alpha\in R_+}\zeta_\alpha E_\alpha\right)|0\rangle, \quad N=\langle 0|T^\lambda(g)|0\rangle, \tag{B12}$$

or in another form

$$|\zeta\rangle=D(\xi)|0\rangle, \quad D(\xi)=\exp\left[\sum\ (\xi_\alpha E_\alpha-\overline{\xi}_\alpha E_{-\alpha})\right]. \tag{B13}$$

Note that the unitary operators $D(\xi)$ do not form a group but their multiplication law is

$$D(\xi_1)D(\xi_2)=D(\xi_3)\exp\left(i\sum_j\ \varphi_jH_j\right). \tag{B14}$$

Note also that these CS are eigenstates of operators

$$T(g)H_jT^{-1}(g)=\tilde{H}_j, \quad \tilde{H}_j|x\rangle=-\lambda_j|x\rangle. \tag{B15}$$

The last equations determine the CS up to a phase factor $\exp(i\alpha)$. The constructed CS system has all properties of a general CS system. Some of the most important ones are noted below.

(1) Operators $T^\lambda(g)$ transform one CS into another,

$$T^\lambda(g)|x\rangle=\exp(i\phi_\lambda(x,g))|x_g\rangle, \tag{B16}$$

where $\phi_\lambda(x,g)$ is a phase shift.

(2) CS are not mutually orthogonal. The scalar product is

$$\langle\zeta_1|\zeta_2\rangle=N_1N_2\langle 0|T^+(\zeta_1)T(\zeta_2)|0\rangle=N_1N_2\langle 0|T(\zeta_1^+\zeta_2)|0\rangle=K_\lambda(\zeta_1^+\zeta_2)[K_\lambda(\zeta_1^+\zeta_1)K_\lambda(\zeta_2^+\zeta_2)]^{-1/2}, \tag{B17}$$

where

$$K_\lambda(\zeta_1^+\zeta_2)=\Delta_1^{\lambda_1}(\zeta_1^+\zeta_2)\cdots\Delta_r^{\lambda r}(\zeta_1^+\zeta_2)$$

and quantities Δ_j may be found from the Gaussian decomposition. For the group $G=\mathrm{SU}(n)$, $G^C=\mathrm{SL}(n,\mathbb{C})$, the quantity Δ_j is the lower angular minor of order j of the matrix $\zeta_1^+\zeta_2$.

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Quantum physical systems as classical systems

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A physical system showing a classical (deterministic) behavior to an observer can appear to be a quantum system to another observer unable to distinguish between some distinct states. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Summary 1: Quantum mechanics is a very precise and powerful physical theory but is accompanied with the negative hypothesis that the measuring process can have only an essentially statistical, nondeterministic character.

It is hard to believe that in the future this assumption will not be overcome or reduced in some way by new experiments or new theories: it does not seem there is any conclusive reason to exclude it.

But is a theory conceivable where the outcomes of the measurements are uniquely defined and the statistical previsions of quantum mechanics exactly respected?

From a mathematical viewpoint it is not difficult to produce an object with these properties. More difficult would be to justify in physical terms the artificial construction we propose; however, we give a general argument showing how the interplay between the classical and quantum mechanics we offer is interpretable as the difference between an imaginary very expert observer and another nonexpert observer compelled to confuse different states or different observables.

The main goal of this article is precisely to give a rigorous meaning to this interplay and a proof that the general quantum system, with all its states and observables, can be obtained from some classical system.

We cannot offer any physical representation for this classical system; we confine here proving that besides the well known theorems concerning the impossibility of hidden variables (Refs. 1 and 2) there is also room for a result in favor of the possibility.

All this is made inside the usual descriptions of the standard quantum physical systems via quantum logic (Refs. 3–5, etc.) and, except for the requirement of hidden variables, does not refer to any nonorthodoxical physical theory.

II. REDUCTION

Definition 2: A (model for a) **classical physical system** is a couple $(S,\mathcal{L})$ of a set S (the **set of pure states**) and a family $\mathcal{L}$ of subets of S (the family of **propositions** of S) distinguishing the elements of S (that is for every couple of different states there is a proposition in $\mathcal{L}$ not containing both of them).

Every L in $\mathcal{L}$ represents the subset where a proposition (an observable taking only the value 0 and 1) is true.

The hypothesis that $\mathcal{L}$ distinguishes the elements of S is made to simplify the situation; we can always suppose this hypothesis verified because otherwise we pass to consider as states the classes of the following equivalence relation: two elements of S are equivalent if every time a proposition contains one of them it contains them both.

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Example 3: Usually $\mathcal{L}$, in the classical case, is the set of all parts of S or the set of all measurable Borel subset of a Borel family.

We are not going to make any restriction on the family $\mathcal{L}$.

Definition 4: An **observable** for a classical system $(S,\mathcal{L})$ is a function $f:S\to\mathbf{R}$ such that for every Borel subset B in the Borel family $\mathcal{B}(\mathbf{R})$ of $\mathbf{R}$ the inverse image $f^{-1}(B)$ is in $\mathcal{L}$.

Example 5: In particular the characteristic functions of the subsets L in $\mathcal{L}$ are observable functions.

Let us denote by $\mathcal{F}$ the set of all the observable functions of the system $(S,\mathcal{L})$.

Remark 6: If f is an observable function of $(S,\mathcal{L})$ and $g:\mathbf{R}\to\mathbf{R}$ is a Borel function, the function $g\circ f:S\to\mathbf{R}$ is an observable. In fact, for every Borel subset B the set $(g\circ f)^{-1}(B)=f^{-1}(g^{-1}(B))$ is in $\mathcal{L}$.

These definitions are given to idealize the situation of an observer (that we will call the precise observer) able to prepare with extreme precision a physical system in a variety of different (pure) states and to perform on the system several measures in such a way that when he prepares the state s and performs the observable f he can get the exact value $f(s)$. Our observer knows all the time and exactly what state is preparating and what observable is performing.

To have a more precise idea of this kind of situation let us suppose that the precise observer has a very huge and efficient laboratory where he can prepare every sort of state of the physical system under consideration and use every sort of measuring apparatus: all he has to do is to give to the laboratory's computer a ''string'' specifying completely and exactly the state to prepare and another ''string'' specifying the observable to measure and the fantastic laboratory does all the work.

The observer checks that given a ''state string'' and an ''observable string'' he always gets the same value and so he can state with certainty that the physical system considered is classical (deterministic).

Let us consider now another observer (that we will call the imprecise observer) studying the same physical system but with a poorer ability; this second observer can produce all the states and observables of the previous one but he does not know exactly what he makes: he gives a ''procedure'' to produce a certain state and another ''procedure'' to produce the measuring apparatus but if he repeats the given procedures he can get different values in a random and, for him, unavoidable way.

Let us suppose, moreover, that the precise observer can describe precisely what the problem is with the imprecise observer: when this second one chooses a ''procedure'' he produces a state among several different ones in a given class of equivalence of S with a certain probability: there is an equivalence relation (the **confusion** relation) $\mathcal{R}$ on the classical system $(S,\mathcal{L})$ and a probability measure μ_p on every equivalence class p in the quotient set $P=S/\mathcal{R}$. When the imprecise observer tries to prepare the system with a given procedure p he does not know which one of the states in the class $p=[s]$ he is really preparing, therefore when he evaluates the observable f he can get any one of the values in the subset $f([s])$. Making several trials he experiments all these values with different frequencies arriving in the end at the conclusion that the measure of the observable f on the ''preparation'' p has a statistical character and that he cannot get anything more that the probability $\pi(f,p,B)$ that the measure of f on p lies in the Borel subset B of $\mathbf{R}$.

For the precise observer it is obvious that

$$\pi(f,p,B)=\mu_p(f^{-1}(B)\cap p).$$

If the imprecise observer is left unaware of his ''confusion'' and convinced that he cannot get any more information on the system, he will decide, coherently, not to distinguish between preparations or measuring apparatuses giving the same probabilities. Therefore, he will define the following concept:

Definition 7: A (model for a) **statistical physical system** is a triple $(P,\mathcal{O},\pi)$ of a set P (the set of statisical **states**), another set $\mathcal{O}$ (the set of statistical **observables**) and a function:

$\pi:\mathcal{O}\times\mathcal{P}\times\mathcal{B}(\mathbf{R})\to[0,1]$ (the **probability** that the measure of an observable on a state lies in a Borel subset of $\mathbf{R}$) such that

(1) $\pi(T',p,B)=\pi(T'',p,B)$ for every p in P and B in $\mathcal{B}(\mathbf{R})$ implies $T'=T''$ and
(2) $\pi(T,p',B)=\pi(T,p'',B)$ for every T in $\mathcal{O}$ and B in $\mathcal{B}(\mathbf{r})$ implies $p'=p''$.

From the viewpoint of the precise observer this means that two states s' and s'' are equivalent in the equivalence relation of confusion if and only if

$$\mu_{[s']}(f^{-1}(B)\cap[s'])=\mu_{[s'']}(f^{-1}(B)\cap[s''])$$

for every f in $\mathcal{F}$ and every B in $\mathcal{B}(\mathbf{R})$.

Moreover, the precise observer makes a discovery: the imprecise observer confuses not only the states but also the observables.

The set of statistical observables $\mathcal{O}$ is the quotient set of $\mathcal{F}$ modulo the equivalence relation stating that two functions f' and f'' of $\mathcal{F}$ are equivalent if

$$\mu_{[s]}(f'^{-1}(B)\cap[s])=\mu_{[s]}(f''^{-1}(B)\cap[s])$$

for every s in S and every B in $\mathcal{B}(\mathbf{R})$.

Therefore, the precise observer can give the following:

Definition 8: A **confusion** relation for a classical system $(S,\mathcal{L})$ is given assigning an equivalence relation $\mathcal{R}$ on S and a probability measure μ_p on every equivalence class in such a way that for every couple of inequivalent elements s' and s'' in S there exists a proposition L in $\mathcal{L}$ with $\mu_{[s']}(L\cap[s'])\neq\mu_{[s'']}(L\cap[s''])$.

It is clear that for every confusion relation $\mathcal{R}$ there is also defined an equivalence relation $\mathcal{M}$ on the set $\mathcal{F}$ of observable functions by taking $f'\mathcal{M}f''$ if

$$\mu_{[s]}(f'^{-1}(B)\cap[s])=\mu_{[s]}(f''^{-1}(B)\cap[s])$$

for every s in S and every B in $\mathcal{B}(\mathbf{R})$.

Therefore a statistical system is well defined by taking

(1) $\hat{S}=S/\mathcal{R}$,
(2) $\hat{\mathcal{F}}=\mathcal{F}/\mathcal{M}$,
(3) $\hat{\mu}:\hat{\mathcal{F}}\times\hat{S}\times\mathcal{B}(\mathbf{R})\to[0,1]$ given by $\hat{\mu}([f],[s],B)=\mu_{[s]}(f^{-1}(B)\cap[s])$.

Definition 9: Given a classical system $(S,\mathcal{L})$ and a confusion relation $(\mathcal{R},\{\mu_p\}_{p\in S/\mathcal{R}})$, the statistical system $(\mathcal{F}/\mathcal{M},\mathcal{S}/\mathcal{R},\hat{\mu})$ is called the **system reduced** by the confusion relation.

Remark 10: We call the procedure given above the reduction just because we pass from a state space to another making a quotient along (essentially) one-dimensional fibers as when we reduce a contact manifold producing a symplectic manifold.

When a statistical system can be obtained as a reduced system of a classical system there is at least a mathematical reason to talk of **hidden variables** (the ''variables'' describing the elements in each equivalence class of the state set of the classical system): under every statistical state $p=[s]$ are ''hidden'' the elements of $[s]$, the ''true states.''

It is possible to make precise this assertion considering the following (Ref. 6, p. 262):

Definition 11: Let $(\mathcal{O},P,\pi)$ be a statistical system. A **model for a system with hidden variables with respect to** $(\mathcal{O},P,\pi)$ is given assigning

(1) a set S (the **space of hidden states**) a surjective map $\rho:S\to P$ (associating to a ''hidden state'' its ''apparent state'');

(2) for each ''apparent'' state $p\in P$ a probability measure μ_p on S (representing the probability to find in a measurable subset of S a ''hidden state'' representing p); and

(3) for each observable $T \in \mathcal{O}$ a function $f_T : S \to \mathbf{R}$ (representing a classical observable giving the values that appear randomly for the statistical observable T) such that for every Borel subset B of $\mathbf{R}$:

$$\pi(T,p,B) = \mu_p(f_T^{-1}(B))$$

(that is the probability that the value of T on p lies in B is given by the probability to find a hidden state of p between the states where the observable f_T takes a value in B).

In fact, in the case of a reduced system, we can take as $\rho : S \to P$ the quotient map and for every p in P as probability measure μ_p, the measure μ_p seen as a measure on all S and not only on $\rho^{-1}(p)$.

We are going to prove that the general quantum system (given by a Hilbert space) is a reduced system of a classical system.

This kind of property is sometimes considered impossible to be proved or in contradiction with the principles of the standard quantum mechanics.

On the contrary, the same property can be considered ''well known'' and quite obvious: if you want a ''hidden variable'' function giving the right statistical outcomes for a self-adjoint operator T of the Hilbert space $\mathbf{H}$ simply take the ''quasi-inverse'' function $f : \mathbf{P}(\mathbf{H}) \times]0,1[\to \mathbf{R}$ (cf. the proof of the following theorem) defined by

$$f([h],t) = sup\{u : \langle E^T_{]-\infty,u]} \rangle_h \geqslant t\}.$$

It seems that all depends on what you mean. In this section we have just tried to suggest a plausible interpretation that can save determinism in observations.

III. THE QUANTUM SYSTEM AS A REDUCED SYSTEM

Definition 12: The (model) for the (irreducible) **quantum system** is given assigning:

(1) the (complex) projective space $\mathbf{P}(\mathbf{H})$ of a Hilbert space $\mathbf{H}$ (of dimension at least two) as state space;

(2) the set $SA(\mathbf{H})$ of self-adjoint operators on $\mathbf{H}$ as observable space; and

(3) the function $\pi : SA(\mathbf{H}) \times \mathbf{P}(\mathbf{H}) \times \mathcal{B}(\mathbf{R}) \to [0,1]$ defined by

$$\boldsymbol{\pi}(T,[h],B) = \langle E^T_B \rangle_h = \frac{\langle h, E^T_B(h) \rangle}{\langle h,h \rangle}$$

(where $E^T_B = \chi_B \circ T$ is the projector operator associated to the Borel subset B of $\mathbf{R}$ in the spectral measure of T) as probability function.

Theorem 13: The quantum system is the reduced system of a classical system.

Proof: For every $[h]$ in $\mathbf{P}(\mathbf{H})$ let us consider a complete separable metric space $S_{[h]}$ with a Borel measure $\mu_{[h]}$ such that $\mu_{[h]}(S_{[h]}) = 1$ and $\mu_{[h]}(\{s\}) = 0$ for every s in $S_{[h]}$. For every such space there is a measurable map $\phi_{[h]} : S_{[h]} \to]0,1[$ such that $\phi_{[h]*}(\mu_{[h]}) = \lambda$, where λ denotes the Lebesgue measure on the interval (cf. Ref. 7, Theorem 9, p. 327).

Let S be the disjoint union of the $\{S_{[h]}\}_{[h] \in \mathbf{P}(\mathbf{H})}$. We will call a subset L of S a proposition if $L \cap S_{[h]}$ is a measurable set for every $[h]$ in $\mathbf{P}(\mathbf{H})$ and if there exists a projector E of $\mathbf{H}$ such that $\mu_{[h]}(L \cap S_{[h]}) = \langle E \rangle_h$ for every $[h]$ in $\mathbf{P}(\mathbf{H})$.

Let $\mathcal{L}$ be the set of all propositions in S.

Every proposition L determines the set of all $[h]$ where $\mu_{[h]}(L \cap S_{[h]}) = 1$ and therefore the projector E. If we denote by $\mathcal{E}$ the set of all projectors of $\mathbf{H}$, it is a map $\varepsilon : \mathcal{L} \to \mathcal{E}$ associating to a proposition its projector is well defined.

The map ε is surjective; fixed E is enough to take in $S_{[h]}$ a measurable subset $L_{[h]}$ such that $\mu_{[h]}(L_{[h]} \cap S_{[h]}) = \langle E \rangle_h$ and then take L as the disjoint union of all the $L_{[h]}$. It is not difficult to prove, in a similar way, that the propositions distinguish the elements in S.

Let us denote by $\mathcal{F}$, as usual, the set of all observable functions for $(S,\mathcal{L})$; we want to prove that to each of these functions f is associated a self-adjoint operator T such that

$$\mu_{[h]}(f^{-1}(B)\cap S_{[h]})=\langle E_B^T\rangle_h$$

for every $[h]$ in $\mathbf{P}(\mathbf{H})$ and B in $\mathcal{B}(\mathbf{R})$.

For every real number t the proposition $L_t=f^{-1}(]-\infty,t])$ determines a projector E_t. The family $\{E_t\}_{t\in\mathbf{R}}$ is a spectral family of projectors of $\mathbf{H}$ [cf. Ref. 8, Definition (7.11), p. 180]; in fact, $\langle E_t\rangle_h= =(f|_{S_{[h]}*}\mu_{[h]})(]-\infty,t])$ for every h and therefore the monotonicity, the left-continuity and the convergence to 0 and 1 properties for the projection operators follow from the analogous properties of cumulative distribution functions for Borel probabilitity measures (cf. Ref. 7, Lemma 10, p. 262).

Hence the spectral family $\{E_t\}_{t\in\mathbf{R}}$ defines a self-adjoint operator T such that for every t in $\mathbf{R}$,

$$\mu_{[h]}(f^{-1}(]-\infty,t])\cap S_{[h]})=\langle E^T_{]-\infty,t]}\rangle_h,$$

and therefore for every Borel subset B of $\mathbf{R}$,

$$\mu_{[h]}(f^{-1}(B)\cap S_{[h]})=\langle E_B^T\rangle_h.$$

The operator T is unambiguously defined by the function f. Let us denote by $\tau:\mathcal{F}\to SA(\mathbf{H})$ the map so defined. Let us prove this map is surjective.

For every $[h]$ let us denote by $F_{[h]}:\mathbf{R}\to]0,1[$ the distribution function $F_{[h]}(u)=\langle E^T_{]-\infty,u]}\rangle_h$; its induced Borel measure $\nu_{F_{[h]}}$ has the property that $\nu_{F_{[h]}}(B)=\langle E_B^T\rangle_h$ for every Borel subset B.

Its quasi-inverse $\widetilde{F_{[h]}}:]0,1[\to\mathbf{R}$ verifies $\widetilde{F_{[h]}}_*(\lambda)=\nu_{F_{[h]}}$ (cf. Ref. 9, Theorem 4, p. 94) and therefore $(\widetilde{F_{[h]}}\circ\phi_{[h]*}(\mu_{[h]})=\nu_{F_{[h]}}$, that is,

$$(\widetilde{F_{[h]}}\circ\phi_{[h]*}(\mu_{[h]})(]a,b=F_{[h]}(b)-F_{[h]}(a)=\langle E^T_{]a,b]}\rangle_h$$

for every $a<b$ in $\mathbf{R}$.

The function $f:S\to\mathbf{R}$ defined by $f(s)=\widetilde{F_{[h]}}(\phi_{[h]}(s))$ (where $[h]$ contains s) has the desired property: $\tau(f)=T$.

Let us prove that the reduced system of $(S,\mathcal{L})$ is the quantum system. Two elements r in $[h]$ and s in $[k]$ are equivalent if and only if $\mu_{[h]}(L\cap S_{[h]})=\mu_{[k]}(L\cap S_{[k]})$ for every proposition L, therefore, if and only if $\langle E\rangle_h=\langle E\rangle_k$ for every projector E of $\mathbf{H}$, that is, if and only if $[h]=[k]$.

Two functions f and g in $\mathcal{L}$ are equivalent if and only if $\langle E_B^{\tau(f)}\rangle_h=\langle E_B^{\tau(g)}\rangle_h$ for every h and B. This means $E_B^{\tau(f)}=E_B^{\tau(g)}$ for every B, that is, $\tau(f)=\tau(g)$. In the end, $\hat{\mu}([f],[h],B)=\mu_{[h]}(f^{-1}(B)\cap S_{[h]})=\langle E_B^{\tau(f)}\rangle_h=\pi(\tau(f),[h],B)$. ■

From now on we will denote by $(S,\mathcal{L})$ a classical system giving the (irreducible) quantum system as reduction, by $\mathcal{F}$ its set of observable functions and by $\rho:S\to\mathbf{P}(\mathbf{H})$, $\tau:\mathcal{F}\to SA(\mathbf{H})$ and $\varepsilon:\mathcal{L}\to\mathcal{E}$ the quotient maps.

Remark 14: If L is in $\mathcal{L}$, then also $(S\backslash L)$ is in $\mathcal{L}$ and $\varepsilon(S\backslash L)=I-\varepsilon(L)$.

Remark 15: If T is a self-adjoint operator with spectral measure $\{B\mapsto E_B\}$ and $g:\mathbf{R}\to\mathbf{R}$ is a Borel function, then a self-adjoint operator $g(T)$ with spectral measure $\{B\mapsto E_{g^{-1}(B)}\}$ is well defined.

Theorem 16: *If f is an observable function of a classical system $(S,\mathcal{L})$ reducing to the quantum system and $g:\mathbf{R}\to\mathbf{R}$ is any Borel function, it holds $\tau(g\circ f)=g(\tau(f))$.*

Proof: The function f gives the operator $\tau(f)=T$ with spectral measure $\{B\mapsto E_B=\varepsilon(f^{-1}(B))\}$. The observable function $g\circ f$ defines the spectral measure $\{B\mapsto\varepsilon(f^{-1}(g^{-1}(B)))\}$ and this is exactly the spectral measure of $g(T)$. ■

Theorem 17: *If f is an observable function of a classical system $(S,\mathcal{L})$ reducing to the quantum system and $g:\mathbf{R}\to\mathbf{R}$ is any Borel function, it holds*

(1) $\langle g(\tau(f))\rangle_h=\int_0^1 g(f([h],t))\cdot d\lambda(t)$,
(2) $\langle \tau(f)\rangle_h=\int_0^1 f([h],t)\cdot d\lambda(t)$.

Proof: The point (2) follows from (1) taking $g=id_{\mathbf{R}}$. Let us prove (1):

$$\langle g(\tau(f))\rangle_h=\int_{\mathbf{R}} g(u)\cdot d\nu_{\langle E^{\tau(f)}_{]-\infty,.]}\rangle_h}=\int_{\mathbf{R}} g(u)\cdot(df_{[h]*}\lambda_{]0,1[})=\int_{]0,1[} g(u)\circ f_{[h]}\cdot d\lambda,$$

cf. Ref. 8, Theorem 7.14(e) and Ref. 9, Corollary 3, p. 93 for the passages. ■

Theorem 18: *Given two projectors E and F, if there exist two propositions L and M in $\mathcal{L}$ such that*

(1) the (finite) Boolean algebra of subsets $\mathcal{A}$ generated by L and M is contained in $\mathcal{L}$ and
(2) the map $\varepsilon:\mathcal{A}\to\mathcal{E}$ sends L in E, M in F transforming the operation $\wedge$ in $\cap$, $\vee$ in $\cup$ and the complementation in the orthogonality,

then the projectors E and F are compatible (that is commute).

Proof: The union $L\cup M=L\cup(\mathsf{C}L\cap M)=M\cup(\mathsf{C}M\cap L)$ belongs to L and

$$\varepsilon(L\cup M)=E\vee F=\varepsilon(L\cup(\mathsf{C}L\cap M))=E\vee(E'\wedge F)=\varepsilon(M\cup(\mathsf{C}M\cap L))=F\vee(F'\wedge E).$$

This proves that E and F are compatible (cf. Ref. 4, Problem 2 of 5–8, p. 87). ■

Remark 19: Therefore, whenever you consider two noncommuting projectors E and F it is impossible to find two propositions L and M with the properties (1) and (2) of the previous theorem.

Definition 20: Let E_1,E_2 and F_1,F_2 be two couples of projectors in $\mathcal{E}$. We will say that the couples **admit proposition intersections** if there are two couples of propositions A_1,A_2 and B_1,B_2 with $\varepsilon(A_i)=E_i$ and $\varepsilon(B_j)=F_j$ for $i,j=1,2$ and such that the 16 intersections $A_i\cap B_j$, $\mathsf{C}A_i\cap B_j$, $A_i\cap\mathsf{C}B_j$, $\mathsf{C}A_i\cap\mathsf{C}B_j$ are all in $\mathcal{L}$ and $\varepsilon(A_i\cap B_j)=E_i\wedge F_j$, $\varepsilon(\mathsf{C}A_i\cap B_j)=(I-E_i)\wedge F_j$, $\varepsilon(A_i\cap\mathsf{C}B_j)=E_i\wedge(I-F_j)$, and $\varepsilon(\mathsf{C}A_i\cap\mathsf{C}B_j)=(I-E_i)\wedge(I-F_j)$.

Notation 21: In this situation we will consider the self-adjoint operators

$$\begin{aligned}T_{ij}(E,F)&=E_i\wedge F_j+(I-E_i)\wedge(I-F_j)-(I-E_i)\wedge F_j-E_i\wedge(I-F_j)\\&=\varepsilon(A_i\cap B_j)+\varepsilon(\mathsf{C}A_i\cap\mathsf{C}B_j)-\varepsilon(\mathsf{C}A_i\cap B_j)-\varepsilon(A_i\cap\mathsf{C}B_j).\end{aligned}$$

Theorem 22: *If E_1,E_2 and F_1,F_2 are two couples of projectors in $\mathcal{E}$ admitting proposition intersections, then for every h in $\mathbf{H}\backslash\{0\}$ it holds the inequality*

$$|\langle T_{11}(E,F)\rangle_h-\langle T_{12}(E,F)\rangle_h|+|\langle T_{21}(E,F)\rangle_h+\langle T_{22}(E,F)\rangle_h|\leqslant 2.$$

Proof: The functions: $f_{ij}=\chi_{A_i\cap B_j}+\chi_{(S\backslash A_i)\cap(S\backslash B_j)}-\chi_{(S\backslash A_i)\cap B_j}-\chi_{A_i\cap(S\backslash B_j)}$ are functions on S with $\int_0^1 f_{ij}([h],t)\cdot d\lambda(t)=\langle T_{ij}(E,F)\rangle_h$. It is not difficult to check in S the following equality: $|f_{11}-f_{12}|+|f_{21}+f_{22}|=2$.

Therefore,

$$\begin{aligned}&|\langle T_{11}(E,F)\rangle_h-\langle T_{12}(E,F)\rangle_h|+|\langle T_{21}(E,F)\rangle_h+\langle T_{22}(E,F)\rangle_h|\\&\quad=\left|\int_0^1 f_{11}([h],t)\cdot d\lambda(t)-\int_0^1 f_{12}([h],t)\cdot d\lambda(t)\right|+\left|\int_0^1 f_{21}([h],t)\cdot d\lambda(t)+\int_0^1 f_{22}([h],t)\cdot d\lambda(t)\right|\\&\quad\leqslant\int_0^1(|f_{11}-f_{12}|+|f_{21}+f_{22}|)([h],t)\cdot d\lambda(t)=2.\end{aligned}$$

■

Remark 23: The proof of the previous theorem mimics the usual one given to prove one of the Bell inequalities and, in fact, if you take in a quantum system two couples of projections not verifying the Bell inequality for some state, you have two couples of projections not admitting proposition intersections.

Problem 24: When we have two couples of projections not admitting proposition intersections we can consider the system as the reduction of a classical system and replace the projectors E_1, E_2, F_1, F_2 with some propositions A_1, A_2, B_1, B_2, but we do not dispose of for example, the proposition $A_1 \cap B_1$ (or this intersection does not correspond to the projector $E_1 \wedge F_1$).

The absence of $A_1 \cap B_1$ is in contrast with the possibility, considered natural in a classical physical theory, to check ''in the same time'' two properties of a system.

This is undoubtly strange and uncomfortable; however, if we take seriously the hypothesis of the precise observer, any objection to this eventuality cannot be considered definitive unless expressed in terms of his physics: in other words, we should be able first to know his description of the physical reality and how he can explain, for example, a possible absence of intersections.

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Existence of multivortex solutions in the self-dual Chern–Simons–Higgs theory in a background metric

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In this paper we show the existence of the multiple multivortex solutions of the self-duality equations of $(2+1)$ dimensional Chern–Simons–Higgs model in a background metric of the form $g_{\mu\nu}=\mathrm{diag}(1,-b(x),-b(x))$ with $b(x)=O(|x|^{-l})$ as $|x|\to\infty$ for some $l>2$. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The first Abelian Chern–Simons–Higgs model in the $(2+1)$ dimensional gauge theory was obtained by Hong, Kim, and Pac,[1] and Jackiw and Weinberg[2] independently. In Ref. 3, Schiff reformulated the Chern–Simons–Higgs model in the background metric of the form $g_{\mu\nu}=\mathrm{diag}(1,-b,-b)$, $b=b(x^1,x^2)$, and obtained self-dual equations by choosing the same Higgs potential as that of Refs. 1 and 2.

The Lagrangian in Schiff's theory is given by (after a rescaling of constants)

$$\mathcal{L}=\frac{\kappa}{4\sqrt{g}}\epsilon^{\mu\nu\rho}F_{\mu\nu}A_\rho+g^{\mu\nu}(D_\mu\phi)(D_\nu\phi)^*-\frac{1}{\kappa^2}|\phi|^2(1-|\phi|^2)^2,$$

where $A=A_\mu\,\mathrm{d}x^\mu$ is a gauge field, $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$ is its curvature tensor, $D_\mu=\partial_\mu-iA_\mu$ is the gauge covariant derivative, ϕ is a complex scalar field called the Higgs field, $\epsilon^{\mu\nu\rho}$ is a totally skew-symmetric tensor with $\epsilon^{012}=1$, $\kappa>0$ is a Chern–Simons coupling constant, and $g_{\mu\nu}=\mathrm{diag}(1,-b,-b)$ is a background metric.

The corresponding Euler–Lagrange equations are

$$\begin{aligned}&\frac{\kappa}{2\sqrt{g}}\epsilon^{\mu\nu\rho}F_{\mu\nu}=J^\rho,\quad J^\rho=ig^{\mu\rho}(\phi(D_\mu\phi)^*-\phi^*(D_\mu\phi)),\\&D_\mu(\sqrt{g}g^{\mu\nu}D_\nu\phi)=-\frac{1}{\kappa^2}\sqrt{g}(|\phi|^2-1)(3|\phi|^2-1)\phi.\end{aligned}\tag{1.1}$$

.

We seek the static solution of (1.1), i.e., A_μ and ϕ are functions of (x^1,x^2) only. If $\rho=0$, we obtain a Chern–Simons Gauss law

$$\kappa F_{12}=-2bA_0|\phi|^2.\tag{1.2}$$

Let Φ be the total magnetic flux and Q be the electric charge,

$$\Phi=\int \mathrm{d}^2x F_{12},\quad Q=\int \mathrm{d}^2x\sqrt{g}J^0.$$

Taking (1.2) into account, $Q=\kappa\Phi$. The energy-momentum tensor $T_{\mu\nu}$ is given by

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$$T_{\mu\nu}=(D_\mu\phi)(D_\nu\phi)^*+(D_\mu\phi)^*(D_\nu\phi)-g_{\mu\nu}g^{\alpha\beta}(D_\alpha\phi)(D_\beta\phi)^*+g_{\mu\nu}\frac{1}{\kappa^2}|\phi|^2(1-|\phi|^2)^2.$$

If we assume that $|\phi D_1\phi|+|\phi D_2\phi|=o(|x|^{-1})$ as $|x|\to\infty$, the energy is given by

$$\begin{aligned}E&=\int d^2x\sqrt{g}\,T_{00}=\int d^2x\left(b|D_0\phi|^2+|D_1\phi|^2+|D_2\phi|^2+\frac{1}{\kappa^2}b|\phi|^2(1-|\phi|^2)^2\right)\\&=\int d^2x\left\{\left|\frac{\kappa F_{12}}{2\sqrt{b}|\phi|}\right|\pm\frac{\sqrt{b}}{\kappa}|\phi|(|\phi|^2-1)\right|^2+|D_1\phi\pm iD_2\phi|^2\Bigg\}\pm\int d^2xF_{12}\\&\geqslant\pm\int d^2xF_{12}.\end{aligned}$$

Without loss of generality we may assume that the conserved quantity $\int d^2xF_{12}$ is non-negative, so we choose the upper sign. Then the minimun is saturated if and only if (A,ϕ) satisfy the following self-duality equations:

$$\begin{aligned}D_1\phi+iD_2\phi&=0,\\F_{12}+\frac{2}{\kappa^2}b|\phi|^2(|\phi|^2-1)&=0.\end{aligned}\tag{1.3}$$

When $b\equiv1$, the energy density T_{00} implies that the finite energy solution of (1.2) and (1.3) satisfies either $\phi\to0$ (nontopological solution) or $|\phi|\to1$ (topological solution) as $|x|\to\infty$. For the nontopological solution, Spruck and Yang[4] obtained a radially symmetric N-vortex solution (A,ϕ) with

$$|\phi(x)|^2=O(|x|^{-(2N+4+\beta)})\quad\text{as}\quad|x|\to\infty\tag{1.4}$$

for some constant $\beta>0$. In Ref. 5, Chen *et al.* showed that for every $\beta\in(0,\infty)$, (1.3) admits a radially symmetric N-vortex solution satisfying (1.4). Recently, Chae and Imanuvilov[6] showed that for arbitrary N-vortices, there is a constant $\beta_0>0$ such that for each $\beta\in(0,\beta_0)$, the system (1.2)–(1.3) admits a solution with the decay (1.4).

For the system with $b\equiv1$ and the periodic boundary condition, Caffarelli and Yang[7] showed there is a critical value κ_c such that the system (1.3) admits a maximal solution if $0<\kappa<\kappa_c$. Later, Tarantello[8] showed that if $\kappa=\kappa_c$ (1.3) admits a solution and if $\kappa<\kappa_c$ (1.3) admits a ''mountain pass'' type solution different from the maximal one. Furthermore, she gave the asymptotic behavior of the second solution as $\kappa\to0$ when $N=1$.

When b is non-negative, Hölder continuous, and $b(x)=O(|x|^{-l})$ as $|x|\to\infty$ for some $l>2$, Kurata[9] showed that if $0\leqslant N\leqslant1$ then for each $2(N-2)<\alpha<\min\{0,l-4\}$ there exists a solution of (1.3) such that $|\phi(x)|^2=O(|x|^\alpha)$ as $|x|\to\infty$. He considered a variational formulation in the weighted space introduced in Ref. 10 and used the Moser–Trudinger inequality, which restricted the values of N and α.

In this paper, we show that the values of N and α in Ref. 9 can be extended. We use the supersubsolution method to show that for each $N\geqslant0$ and $\alpha\leqslant0$, (1.3) admits a maximal solution (A,ϕ) such that $|\phi|=O(|x|^\alpha)$ as $|x|\to\infty$. More precisely, we have

Theorem 1.1: *Suppose that b is non-negative, Hölder continuous, $b(0)>0$ and $b(x)=O(|x|^{-l})$ for some $l>2$ as $|x|\to\infty$. For $\alpha\leqslant0$ and $p_1,\ldots,p_N\in\mathbb{R}^2$, there exists a critical value*

$$\kappa_\alpha\in\left(0,\sqrt{\frac{\int b\,dx}{2\pi(2N-\alpha)}}\right)$$

such that for $0<\kappa\leqslant\kappa_\alpha$ *the system (1.2)–(1.3) admits a solution* (A_κ,ϕ_κ) *with the following properties:*

(i) The zeros of ϕ_κ *are* $p_1,\cdots,p_N$.

(ii) (A_κ,ϕ_κ) *satisfies the decay estimates*

$$|\phi_\kappa|^2=O(|x|^\alpha),\quad F_{12}=O(|x|^{-l+\alpha})\quad as\ \ |x|\to\infty.$$

Moreover, if $\alpha<0$ *then* $|D_1\phi_\kappa|^2+|D_2\phi_\kappa|^2=O(|x|^{-2+\alpha})$ *as* $|x|\to\infty$ *and if* $\alpha=0$ *then* $|D_1\phi_\kappa|^2+|D_2\phi_\kappa|^2=O(|x|^{-2-2t})$ *for every* $t<\min\{l-2,1\}$ *as* $|x|\to\infty$.

(iii) The energy, the magnetic flux, and the electric charge are given by

$$E=\Phi=\pi(2N-\alpha),\quad Q=\pi\kappa(2N-\alpha).$$

(iv) (A_κ,ϕ_κ) *is maximal in the sense that* $|\phi_\kappa|$ *takes the largest possible value among the solutions of (1.2)–(1.3) with the same zero set.*

(v) If $b>0$ *then* $|\phi_\kappa|\to1$ *pointwise a.e. and* $\partial_1A_2^{(\kappa)}-\partial_2A_1^{(\kappa)}\to2\pi\Sigma_{j=1}^N\delta_{p_j}$ *in the measure sense as* $\kappa\to0$.

Furthermore, if $N-\alpha>0$ *and* $0<\kappa<\kappa_\alpha$, *there exists a second solution* $(\tilde A_\kappa,\tilde\phi_\kappa)$ *of (1.2)–(1.3) such that* $|\tilde\phi_\kappa|<|\phi_\kappa|$ *in* $\mathbb{R}^2\backslash\{p_1,\cdots,p_N\}$.

Theorem 1.1 is our main result. This theorem will be proved with the help of a reduction of (1.3) to a single elliptic equation. Following Jaffe and Taubes,[11] we find that the set of zeros of ϕ is discrete. Furthermore, for any set $Z(\phi)=\{p_1,\ldots,p_N\}$ of zeros of ϕ, the system (1.3) reduces to a single elliptic equation

$$\Delta u=\frac{4}{\kappa^2}be^u(e^u-1)+4\pi\sum_{i=1}^N\delta_{p_i}\tag{1.5}$$

with unknown $u=\ln|\phi|^2$. Conversely if u is a solution of (1.5), then the solution (A,ϕ) is recovered by

$$\phi(x)=\exp\left(\frac{1}{2}u(x)+i\sum_{j=1}^N\arg(x-p_j)\right),$$

$$A_1=-\operatorname{Re}(2i\partial^*\ln\phi),\quad A_2=-\operatorname{Im}(2i\partial^*\ln\phi),\tag{1.6}$$

$$A_0=\frac{1}{\kappa}(|\phi|^2-1),$$

where $\partial^*=(\partial_1+i\partial_2)/2$.

Let us define some background functions

$$u_0(x)=\sum_{j=1}^N\ln\left(\frac{|x-p_j|^2}{1+|x-p_j|^2}\right),\quad w_0(x)=\sum_{j=1}^N\ln(1+|x-p_j|^2),$$

$$u_\alpha(x)=\ln(1+|x|^2)^{\alpha/2},\quad \alpha\in\mathbb{R}.$$

Set $\lambda=4/\kappa^2$ and $v=u-u_0-u_\alpha$. Then v satisfies

$$\Delta v=\lambda bU_\alpha e^v(U_\alpha e^v-1)+f_\alpha,\tag{1.7}$$

where $U_\alpha=e^{u_0+u_\alpha}$ and $f_\alpha=\Delta(w_0-u_\alpha)$.

Equation (1.7) is the main equation to study in this paper. We shall establish the following:

Proposition 1.1: Suppose that $b\geqslant0$, $b(0)>0$, $b\in C^\nu_{\rm loc}$, *and* $b(x)=O(|x|^{-l})$ *as* $|x|\to\infty$ *for some* $l>2$. *For* $\alpha\leqslant0$ *and* $p_1,\ldots,p_N\in\mathbb{R}^2$, *there is a constant* $\lambda_\alpha\geqslant8\pi(2N-\alpha)/\int b\,dx$ *such that:*

(i) If $\lambda>\lambda_\alpha$ *then (1.7) has a maximal bounded solution and if* $\lambda<\lambda_\alpha$ *then (1.7) has no nontrivial bounded solution. If* $\lambda=\lambda_\alpha$ *then (1.7) has a bounded solution* v_*.

(ii) If $N-\alpha>0$ *and* $\lambda>\lambda_\alpha$ *then (1.7) has at least two bounded solutions* v_2 *and* $\overline{v}_{\lambda,\alpha}$ *such that* $\overline{v}_{\lambda,\alpha}$ *is maximal and* $v_2<\overline{v}_{\lambda,\alpha}$.

Furthermore, for each $t<\min\{1,l-2-\alpha\}$ *and a bounded solution* v *of (1.7), there exists a constant* C *such that*

$$\|(1+|x|^2)^{(t+1)/2}\nabla v\|_{L^\infty(\mathbb{R}^2)}\leqslant C. \tag{1.8}$$

Proposition 1.2: Suppose that b *is positive. The maximal bounded solution* $\overline{v}_{\lambda,\alpha}$ *of (1.7) satisfies*

(i) $\overline{v}_{\lambda,\alpha}\to -u_0-u_\alpha$ *a.e. in* $\mathbb{R}^2$ *as* $\lambda\to\infty$.

(ii) $\lambda b U_\alpha e^{\overline{v}_{\lambda,\alpha}}(1-U_\alpha e^{\overline{v}_{\lambda,\alpha}})\to 4\pi\Sigma_{j=1}^N\delta_{p_j}$ *in the measure sense as* $\lambda\to\infty$.

(iii) $\|u_0+u_\alpha+\overline{v}_{\lambda,\alpha}\|_{C^{2,\nu}(\Omega)}\to 0$ *as* $\lambda\to\infty$ *for any compact domain* $\Omega\subset\mathbb{R}^2\setminus\{p_1,\ldots,p_N\}$. *In fact, there exist positive constants* $c_j=c_j(\Omega)$, $j=1,2$ *such that*

$$\|u_0+u_\alpha+\overline{v}_{\lambda,\alpha}\|_{C^{2,\nu}(\Omega)}\leqslant c_1 e^{-c_2\sqrt{\lambda}}. \tag{1.9}$$

The proof of Proposition 1.1 is mainly based on the supersubsolution method and the variational method used in Ref. 8.

For a bounded solution $v_{\lambda,\alpha}$ of (1.7), the pair (A_μ,ϕ) defined as (1.6) with $u=u_0+u_\alpha+v_{\lambda,\alpha}$ gives rise to a solution of (1.2)–(1.3) such that

$$\begin{aligned}|\phi|^2&=e^u=O(|x|^\alpha),\\ F_{12}&=\frac{\lambda}{2}be^u(1-e^u)=O(|x|^{-l+\alpha})\quad\text{as } |x|\to\infty.\end{aligned} \tag{1.10}$$

Furthermore if $\alpha<0$ then

$$|D_1\phi|^2+|D_2\phi|^2=\tfrac{1}{2}e^u|\nabla u|^2=O(|x|^{-2+\alpha})\quad\text{as } |x|\to\infty \tag{1.11}$$

and if $\alpha=0$ then

$$|D_1\phi|^2+|D_2\phi|^2=O(|x|^{-2-2t})\quad\text{as } |x|\to\infty \tag{1.12}$$

for every $t<\min\{1,l-2\}$. Moreover, in view of (1.3), (1.8) and (1.10)–(1.12), the energy is finite and given by

$$E=\int_{\mathbb{R}^2}\frac{\lambda}{2}be^u(1-e^u)\,dx=\lim_{R\to\infty}\int_{|x|=R}\frac{1}{2}\frac{\partial}{\partial\nu}(w_0-u_\alpha-v_{\lambda,\alpha})d\sigma=\pi(2N-\alpha),$$

where $\partial/\partial\nu$ denotes the outward normal derivative.

Thus we conclude that Theorem 1.1 is an immediate consequence of Propositions 1.1 and 1.2. In Sec. II we will prove Propositions 1.1 and 1.2 in several steps.

II. PROOF OF THEOREM 1.1

We recall some results about weighted space $M^2_{s,\delta}$ which is the closure of $C_0^\infty(\mathbb{R}^2)$ with respect to the norm

$$\|\phi\|_{M^2_{s,\delta}}=\sum_{|\alpha|\leqslant s}\|\sigma^{(\delta+|\alpha|)}\partial_x^\alpha\phi\|_{L^2},$$

where $\sigma(x)=(1+|x|^2)^{1/2}$, s is a non-negative integer, $\delta\in\mathbb{R}$, and $\phi\in C_0^\infty(\mathbb{R}^2)$. $M^2_{s,\delta}$ has the following properties.

Lemma 2.1:

McOwen—Refs. 12 and 10.

(a) $M^2_{s',\delta'}\subset M^2_{s,\delta}$ *if* $s'\geqslant s$ *and* $\delta'\geqslant\delta$. *If* $s'>s$ *and* $\delta'>\delta$, *the inclusion is compact.*

(b) If $-1<\delta<0$ *then the Laplacian* Δ, $\Delta: M^2_{2,\delta}\to M^2_{0,\delta+2}$ *is an injection with closed range* $\{f\in M^2_{0,\delta+2}\,|\int_{\mathbb{R}^2} f=0\}$, *and* $\|u\|_{M^2_{2,\delta}}\leqslant C\|\Delta u\|_{M^2_{0,\delta+2}}$ *with* C *independent of* u.

Cantor—Ref. 13:

(c) For any $\delta,l\in\mathbb{R}$, *the map* $f\mapsto f\sigma^l$ *is a continuous map from* $M^2_{2,\delta}$ *into* $M^2_{2,\delta-l}$.

(d) Let $s>1$ *and* $\delta<1$. *There is a constant* $C>0$ *such that* $\|f\sigma^\delta\|_{L^\infty}\leqslant C\|f\|_{M^2_{s,0}}$ *for all* $f\in C_0^\infty$. *Therefore, if* $\delta>-1$ *and* $f\in M^2_{2,\delta}$ *then* $\|f\sigma^\beta\|_{L^\infty}\leqslant C\|f\|_{M^2_{2,\delta}}$ *for* $\beta<1+\delta$.

With the help of the function space $M^2_{s,\delta}$, we present the asymptotic behavior at infinity of the bounded solution of (1.7).

Lemma 2.2: Suppose $l>2$, $\alpha\leqslant 0$ *and* $v\in C^2_{loc}$ *is a solution of (1.7).*

(i) If $bU_\alpha e^v(U_\alpha e^v-1)$ *belongs to* $M^2_{0,\delta+2}$ *for some* $\delta\in(-1,0)$, *there exist constants* β *and* v_∞ *such that* v *satisfies the asymptotic behavior*

$$v(x)=\beta\ln|x|+v_\infty+o(|x|^\gamma)\quad\text{as}\quad|x|\to\infty \tag{2.1}$$

for every $\gamma>-1-\delta$ *and*

$$\int_{\mathbb{R}^2} bU_\alpha e^v(1-U_\alpha e^v)\,dx=\frac{2\pi}{\lambda}(2N-\alpha-\beta).$$

(ii) Suppose that $u:=u_0+u_\alpha+v$ *is bounded above. If* $\alpha<0$ *then* $u<0$. *If* $\alpha=0$ *and* $N>0$ *then* $u<0$ *and* $\lim_{|x|\to\infty}u(x)<0$.

Remark: It follows from Lemma 2.2 that if (1.7) admits a nontrivial bounded solution then necessarily $\lambda>8\pi(2N-\alpha)/\int b\,dx$.

Proof of Lemma 2.2: Define

$$\beta=\frac{1}{2\pi}\int_{\mathbb{R}^2}\lambda bU_\alpha e^v(U_\alpha e^v-1)\,dx+2N-\alpha.$$

Then Lemma 2.1 implies that there exists $w\in M^2_{2,\delta}\subset C_0(\mathbb{R}^2)$ such that

$$\Delta w=\lambda bU_\alpha e^v(U_\alpha e^v-1)+f_{\alpha+\beta},$$

where $f_{\alpha+\beta}=f_\alpha-\Delta u_\beta$, $u_\beta(x)=\ln(1+|x|^2)^{\beta/2}$.

Then $v=u_\beta+w+h$ for some harmonic function h. Since $bU_\alpha e^v(U_\alpha e^v-1)$ belongs to $M^2_{0,\delta+2}$, h must be constant. The decay estimate of w is an immediate consequence of lemma 2.1. This proves (i).

(ii) can be proved from maximum principle and we will prove only the second part of (ii). For sufficiently large $R>0$, choose a smooth function $\psi>0$ such that $\psi\equiv 1$ for $|x|<R$, $\psi\equiv 0$ for $|x|>2R$, and $\|\nabla\psi\|_{L^\infty}\leqslant 2/R$. Then we obtain

$$0\leqslant\int_{\mathbb{R}^2}u^+\psi\Delta u\,dx=-\int_{\mathbb{R}^2}\psi|\nabla u^+|^2\,dx-\int_{R\leqslant|x|\leqslant 2R}u^+\nabla\psi\cdot\nabla u\,dx,$$

where $u^+=\max\{u,0\}$. Lemma 2.1 (i) implies that there are constants $\beta\leqslant 0$ and v_∞ such that

$$u=u_0+u_\beta+\xi+v_\infty,$$

where $\xi\in M^2_{2,\delta}$ for some $-1<\delta<0$. Without loss of generality, we may assume that $\beta=0$. Then

$$\left|\int_{R\leqslant|x|\leqslant 2R} u^+\nabla\psi\cdot\nabla u\,dx\right| \leqslant C\int_{R\leqslant|x|\leqslant 2R}|x|^{-2-\delta}u^+|\nabla\xi||x|^{1+\delta}\,dx + CR^{-2}$$

$$\leqslant C_\delta R^{-1-\delta}(1+\|u^+\|_{L^\infty}\|\xi\|_{M^2_{2,\delta}}).$$

Letting $R\to\infty$, we obtain $u^+\equiv 0$, which implies that $u<0$.

Suppose that $\lim_{|x|\to\infty}u(x)=0$. Fix a constant $\gamma\in(\max\{-1,-l+2\},0)$ and introduce a comparison function $w=C_0|x|^{\gamma/2}$.

There exists an $R>0$ such that

$$\Delta(u+w)=\lambda b e^u(e^u-1)+\frac{\gamma^2}{4}|x|^{-2}w\geqslant\lambda b(u+w)\quad\text{for } |x|>R.$$

It follows from maximum principle that $u+w\leqslant(u+w)|_{|x|=R}<0$ for $|x|>R$ if C_0 is sufficiently small. But this leads to a contradiction since $u(x)=o(|x|^\gamma)$ as $|x|\to\infty$ from (i). □

We now construct a supersolution of (1.7). Consider the following:

$$\Delta v=\lambda b(U_\alpha e^v-1)+f_\alpha. \tag{2.2}$$

It is easily seen that the bounded solution of (2.2) is a supersolution of (1.7). Moreover it follows from maximum principle that every bounded solution v of (2.2) satisfies that $U_\alpha e^v<1$ in $\mathbb{R}^2$.

Lemma 2.3: For each $\alpha<l-2$, there is a constant $\beta_0\geqslant 0$ such that if $\lambda>\beta_0$ then Eq. (2.2) has a unique bounded solution $v^+_{\lambda,\alpha}\in C^{2,\nu}_{\text{loc}}$ with the following properties:

(i) $v^+_{\lambda,\alpha_1}+u_{\alpha_1}>v^+_{\lambda,\alpha_2}+u_{\alpha_2}$ if $\alpha_2<\alpha_1<l-2$.

(ii) For each λ, $v^+_{\lambda,\beta}\to v^+_{\lambda,\alpha}$ uniformly on any bounded domain as $\beta\to\alpha$. Moreover, if $\alpha\leqslant 0$ then

(iii) $v^+_{\lambda,\alpha}>v^+_{\mu,\alpha}$ if $\lambda>\mu$.

(iv) If $v_{\lambda,\alpha}$ is a bounded solution of (1.7), then $v_{\lambda,\alpha}<v^+_{\lambda,\alpha}$.

The proof of Lemma 2.3 is based on the following theorem and maximum principle.

Theorem 2.2:

McOwen—Ref. 12. If $K\leqslant 0$ in $\mathbb{R}^2$, $K(0)<0$ and $K(x)\geqslant -C|x|^{-l}$ near ∞ for some constant $l>2$, then for every $0<\beta<l-2$, there exists a solution u of

$$\Delta u+Ke^u=0\quad\text{in } \mathbb{R}^2 \tag{2.3}$$

and a constant u_∞ such that

$$u(x)=\beta\ln|x|+u_\infty+O(|x|^\gamma)\quad\text{as } |x|\to\infty \tag{2.4}$$

for every $\gamma>\max\{-1,2-l+\beta\}$.

Cheng and Ni—Ref. 14. For each $0<\beta<l-2$, (2.3) possesses a unique solution u satisfying (2.4).

In view of Theorem 2.2 we can prove Lemma 2.3.

Proof of Lemma 2.3: Define

$$\beta_0=\max\left\{0,\frac{2\pi(2N-\alpha)}{\int_{\mathbb{R}^2}b(y)dy}\right\}$$

and assume that $\lambda>\beta_0$. Define a function h by

$$h(x)=\frac{1}{2\pi}\int_{\mathbb{R}^2}\ln|x-y|\,b(y)\,dy.$$

Let $\gamma=-2N+(\lambda/2\pi)\int_{\mathbb{R}^2}b$. Since h satisfies the asymptotic behavior

$$h(x)=\left(\frac{1}{2\pi}\int_{\mathbb{R}^2} b(y)dy\right)\ln|x|+O(1) \quad \text{as } |x|\to\infty,$$

the function defined by $K_\lambda=\lambda b U_\alpha e^{w_0-u_\alpha-\lambda h}$ satisfies the decay estimate

$$K_\lambda(x)=O(|x|^{-(l+\gamma)}) \quad \text{as } |x|\to\infty.$$

Since $l+\gamma>2$, theorem 2.2 implies that

$$\Delta u-K_\lambda e^u=0 \quad \text{in } \mathbb{R}^2$$

has a unique solution $\tilde{u}$ such that

$$\tilde{u}(x)=(\gamma+\alpha)\ln|x|+u_\infty+o(1) \quad \text{as } |x|\to\infty$$

for some constant u_∞. Then $v^+_{\lambda,\alpha}=\tilde{u}+w_0-u_\alpha-\lambda h$ is the unique bounded solution of (2.2) and elliptic regularity estimate implies that $v^+_{\lambda,\alpha}\in C^{2,\nu}_{\text{loc}}$.

Let $w^+_{\lambda,\alpha}=v^+_{\lambda,\alpha}+u_\alpha$. Then $w^+_{\lambda,\alpha}$ satisfies

$$\Delta w^+_{\lambda,\alpha}=\lambda b(e^{u_0+w^+_{\lambda,\alpha}}-1)+\Delta w_0 \quad \text{in } \mathbb{R}^2. \tag{2.5}$$

It follows from maximum principle that $w^+_{\lambda,\alpha}>w^+_{\lambda,\beta}$ for $\alpha>\beta$, which proves (i).

We can prove (ii) from standard diagonal process and Rellich theorem. Indeed, for any sequence $\{\beta_n\}$ converging to α, Sobolev embedding theorem and Schauder estimates imply that $\|w^+_{\lambda,\beta_n}\|_{C^{2,\nu}(\bar{\Omega})}\leqslant C(\alpha,\Omega)$ for any bounded domain Ω. Then there exists a subsequence $\{w^1_n\}$ of $\{w^+_{\lambda,\beta_n}\}$ and $w^1\in C^2(\overline{B_1(0)})$ such that w^1_n converges to w^1 in $C^2(\overline{B_1(0)})$.

Any sequence $\{w^i_n\}\subset C^2(\overline{B_i(0)})$ converging to $w^i\in C^2(\overline{B_i(0)})$ contains a subsequence $\{w^{i+1}_n\}$ converging to $w^{i+1}\in C^2(\overline{B_{i+1}(0)})$. Rellich theorem implies that $w^i=w^{i+1}$ in $B_i(0)$ for all $i\geqslant 1$.

For $x\in B_N(0)$, define $w_*(x)=w^N(x)$. Then w_* is a well-defined C^2-solution of Eq. (1.7). As shown implicitly in Lemma 2.2, every bounded solution of (2.2) satisfies (2.1) with $\beta=0$ and $\gamma>\max\{-1,-l+2\}$. Then it is easily seen from (i) that w_* satisfies

$$w_*(x)=\alpha\ln|x|+O(1) \quad \text{near } \infty,$$

and w^+_{λ,β_n} converges to w_* uniformly on any bounded domain. Since $\{\beta_n\}$ is arbitrary and the bounded solution of (2.2) is unique, we obtain (ii).

Note that $U_\alpha e^{v^+_{\lambda,\alpha}}<1$ for $\alpha\leqslant 0$. Then it follows from maximum principle that $w^+_{\lambda,\alpha_1}>w^+_{\mu,\alpha_2}$ if $\lambda>\mu$ and $\alpha_2<\alpha_1\leqslant 0$. Then (iii) is an immediate consequence of (ii) and maximum principle.

Suppose that $\alpha\leqslant 0$ and $v_{\lambda,\alpha}$ is any bounded solution of Eq. (1.7). Let $w_{\lambda,\alpha}=v_{\lambda,\alpha}+u_\alpha$ and choose a $\beta\in(\alpha,l-2)$. Since

$$\Delta(w_{\lambda,\alpha}-w^+_{\lambda,\beta})\geqslant\lambda b e^{u_0}(e^{w_{\lambda,\alpha}}-e^{w^+_{\lambda,\beta}}) \quad \text{in } \mathbb{R}^2,$$

$$(w_{\lambda,\alpha}-w^+_{\lambda,\beta})(x)<0 \quad \text{if } |x| \text{ is sufficiently large,}$$

maximum principle implies that $w_{\lambda,\alpha}<w^+_{\lambda,\beta}$ in $\mathbb{R}^2$. Then (ii) and maximum principle imply (iv).□

We now construct a subsolution of (1.7) for each $\alpha\leqslant 0$. Choose a smooth function ρ_α and an open set Ω such that $(\text{supp}\,\rho_\alpha)\subset\Omega\subset(\text{supp}\,b)\setminus\{p_1,\ldots,p_N\}$ and $\int_{\mathbb{R}^2}(f_\alpha-\rho_\alpha)=0$. Let v^- be a bounded solution of

$$\Delta v=f_\alpha-\rho_\alpha \quad \text{in } \mathbb{R}^2. \tag{2.6}$$

Since the bounded solution of (2.6) is unique up to an additive constant, we can choose v^- so that

$$U_\alpha e^{v^-} \leqslant 1/2, \quad v^- < v^+_{\mu,\alpha} \quad \text{for some} \quad \mu > \beta_0 = \frac{2\pi(2N-\alpha)}{\int_{\mathbb{R}^2} b\, dx}.$$

Then

$$bU_\alpha e^{v^-}(U_\alpha e^{v^-} - 1) \leqslant C_0 < 0 \quad \text{in } \Omega$$

for some constant C_0. Thus if $\lambda \geqslant \mu$ is sufficiently large, then $v^- < v^+_{\lambda,\alpha}$ and

$$\Delta v^- = f_\alpha - \rho_\alpha \geqslant \lambda b U_\alpha e^{v^-}(U_\alpha e^{v^-} - 1) + f_\alpha \quad \text{in } \Omega.$$

Moreover,

$$\Delta v^- = f_\alpha \geqslant \lambda b U_\alpha e^{v^-}(U_\alpha e^{v^-} - 1) + f_\alpha \quad \text{in } \mathbb{R}^2 \setminus \Omega$$

for all $\lambda > 0$. Therefore v^- is a subsolution of Eq. (1.7) and $v^- < v^+_{\lambda,\alpha}$ if λ is sufficiently large.

We are now ready to construct a maximal bounded solution of (1.7). Let us consider the following boundary value problem:

$$\begin{cases} \Delta v = \lambda b U_\alpha e^v (U_\alpha e^v - 1) + f_\alpha, & \Omega, \\ v = v^+_{\lambda,\alpha}, & \partial\Omega, \end{cases} \tag{2.7}$$

where Ω is a smooth bounded domain.

Lemma 2.4: There exists a solution v_Ω of (2.7) satisfying $v^- \leqslant v_\Omega \leqslant v^+_{\lambda,\alpha}$ if λ is sufficiently large.

Proof: Let $d = 3\lambda \|b\|_{L^\infty} + 1$ and apply the following iterative scheme

$$(\Delta - d)v_{n+1} = \lambda b U_\alpha e^{v_n}(U_\alpha e^{v_n} - 1) - d v_n + f_\alpha, \quad \Omega \quad (n = 0,1,2,\ldots) \tag{2.8}$$

$$v_{n+1} = v^+_{\lambda,\alpha}, \quad \partial\Omega$$

$$v_0 = v^+_{\lambda,\alpha}.$$

For each $n = 1,2,\ldots$, (2.8) has a solution $v_n \in C^2(\bar{\Omega})$ satisfying $v^- \leqslant v_{n+1} \leqslant v_n$ in Ω. Standard bootstrap argument shows that $v_\Omega = \lim_{n\to\infty} v_n$ is a solution of (2.7). □

We can construct a solution $\bar{v}_{\lambda,\alpha}$ of (1.7) from $\{v_\Omega\}$ by means of standard diagonal process and Rellich theorem. Moreover, $\bar{v}_{\lambda,\alpha}$ is maximal. Indeed, if $v_{\lambda,\alpha}$ is another bounded solution of Eq. (1.7), then $v_{\lambda,\alpha} < v^+_{\lambda,\alpha}$ in $\mathbb{R}^2$ by Lemma 2.3(iv). From the iteration process (2.8), we can show that $v_{\lambda,\alpha} \leqslant v_n$ in each step and conclude that $v_{\lambda,\alpha} \leqslant v_\Omega$ for any bounded domain Ω. Since Ω is arbitrary, $v_{\lambda,\alpha} \leqslant \bar{v}_{\lambda,\alpha}$ in $\mathbb{R}^2$.

Therefore we conclude that if λ is sufficiently large, then (1.7) has a maximal solution $\bar{v}_{\lambda,\alpha}$. Following Caffarelli and Yang,[7] we can also verify that for each $\alpha \leqslant 0$ there exists a critical value $\lambda_\alpha \geqslant 8\pi(2N-\alpha)/\int_{\mathbb{R}^2} b\, dx$ such that if $\lambda > \lambda_\alpha$, Eq. (1.7) has a maximal bounded solution and if $\lambda < \lambda_\alpha$, (1.7) has no nontrivial bounded solution.

Moreover, $\bar{v}_{\lambda,\alpha}$ satisfies the following monotonicity property.

Lemma 2.5: Suppose that $\lambda > \mu > \lambda_\alpha$. If $\alpha < 0$, then there holds

$$\bar{v}_{\lambda,\alpha} > \bar{v}_{\mu,\alpha} \quad \text{and} \quad \lim_{|x|\to\infty} \bar{v}_{\lambda,\alpha}(x) > \lim_{|x|\to\infty} \bar{v}_{\mu,\alpha}(x). \tag{2.9}$$

Equation (2.9) remains true if $\alpha = 0$ and $N > 0$.

Proof: We can use $\bar{v}_{\mu,\alpha}$ (*respectively* $v^+_{\lambda,\alpha}$) as a subsolution (*respectively*, supersolution) of (1.7) to construct $\bar{v}_{\lambda,\alpha}$ such that $\bar{v}_{\mu,\alpha} < \bar{v}_{\lambda,\alpha} < v^+_{\lambda,\alpha}$, which proves the first inequality.

If $\alpha<0$ there exists an R such that $U_\alpha e^{\bar{v}_{\lambda,\alpha}}<1/2$ for $|x|>R$. Choose $\epsilon>0$ such that $w:=\bar{v}_{\mu,\alpha}-\bar{v}_{\lambda,\alpha}+\epsilon<0$ for $|x|=R$. Let ψ be the smooth function such that $\psi\equiv 1$ for $|x|\leqslant R$, $\psi\equiv 0$ for $|x|>2R$, and $\|\nabla\psi\|_{L^\infty}\leqslant 2/R$.

It follows from Lemma 2.2 that there exists a constant c_∞ such that $w=\xi+c_\infty$ for some $\xi\in M^2_{2,\delta}$ with $-1<\delta<\min\{0,l-3-\alpha\}$. Then we obtain

$$0\leqslant\int_{|x|\geqslant R} w^+\psi\Delta w\,dx=-\int_{|x|\geqslant R}\psi|\nabla w^+|^2\,dx-\int_{R\leqslant|x|\leqslant 2R} w^+\nabla\psi\cdot\nabla w\,dx,$$

where $w^+=\max\{w,0\}$. Letting $R\to\infty$, we obtain the result.

If $\alpha=0$ and $N>0$ choose R such that $R>\sup_i|p_i|$. Let

$$K=\frac{(U_0e^{\bar{v}_{\mu,0}}(U_0e^{\bar{v}_{\mu,0}}-1)-U_0e^{\bar{v}_{\lambda,0}}(U_0e^{\bar{v}_{\lambda,0}}-1))}{\bar{v}_{\mu,0}-\bar{v}_{\lambda,0}}.$$

Note that $|K|\leqslant 1$ and $U_0e^{\bar{v}_{\lambda,0}}(U_0e^{\bar{v}_{\lambda,0}}-1)\leqslant -C_0<0$ for $|x|>R$. Choose $\epsilon>0$ such that $w:=\bar{v}_{\mu,0}-\bar{v}_{\lambda,0}+\epsilon<0$ for $|x|=R$ and $-2\mu\epsilon+(\lambda-\mu)C_0>0$. Then we obtain

$$\Delta w-\mu b(K+1)w=b[-\epsilon\mu(K+1)-\mu(\bar{v}_{\mu,0}-\bar{v}_{\lambda,0})+(\mu-\lambda)U_0e^{\bar{v}_{\lambda,0}}(U_0e^{\bar{v}_{\lambda,0}}-1)]$$

$$\geqslant 0\quad\text{for } |x|>R. \tag{2.10}$$

Multiplying both sides of (2.10) by ψw^+ and integrating by parts, we obtain the desired result.□

Lemma 2.5 enables us to obtain a function given by

$$v_*(x)=\inf_{\lambda>\lambda_\alpha}\bar{v}_{\lambda,\alpha}(x).$$

Lemma 2.6: v_* belongs to $C^{2,\nu}_{\mathrm{loc}}$ and it is a bounded solution of (1.7) for $\lambda=\lambda_\alpha$.

Proof: By a result of Brezis and Merle[15] it is possible to show that $\{\bar{v}_{\lambda,\alpha}\}_{\lambda_\alpha<\lambda<2\lambda_\alpha}$ is uniformly bounded on a compact domain of $\mathbb{R}^2$. Indeed, if we define $z_{\lambda,\alpha}=\bar{v}_{\lambda,\alpha}+u_\alpha-w_0$, then $z_{\lambda,\alpha}$ satisfies

$$-\Delta z_{\lambda,\alpha}=\lambda be^{u_0+w_0+z_{\lambda,\alpha}}(1-e^{u_0+w_0+z_{\lambda,\alpha}}).$$

Moreover, $\lambda be^{u_0+w_0}(1-e^{u_0+w_0+z_{\lambda,\alpha}})$ is uniformly bounded in B_r and $\int_{B_r}e^{z_{\lambda,\alpha}}\leqslant C_r$ for each $r>0$. Then $\{z_{\lambda,\alpha}\}$ has a subsequence $z_n=z_{\lambda_n,\alpha}$ ($\lambda_n\to\lambda_\alpha$ as $n\to\infty$) satisfying the following alternative:

(a) z_n is bounded on B_r.

(b) $z_n\to-\infty$ uniformly on B_r.

(c) There exists a set $S=\{a_1,\ldots,a_m\}\subset B_r$ and sequences $x_n^i\to a_i$ ($i=1,\ldots,m$) such that $z_n(x_n^i)\to\infty$ and $z_n\to-\infty$ uniformly on compact subsets of $\mathbb{R}^2\setminus S$.

Note that

$$bU_\alpha e^{\bar{v}_{\lambda,\alpha}}(1-U_\alpha e^{\bar{v}_{\lambda,\alpha}})\leqslant b\quad\text{in } \mathbb{R}^2. \tag{2.11}$$

In view of (2.11), Lemma 2.2(i), and the monotonicity property (2.9), (b) and (c) are excluded and we conclude that $\{z_{\lambda,\alpha}\}$ is uniformly bounded on B_r for each $r>0$. Then the diagonal process and standard elliptic theory imply that v_* belongs to $C^{2,\nu}_{\mathrm{loc}}$ and it is a solution of (1.7) when $\lambda=\lambda_\alpha$.

Moreover, Lemma 2.2 implies that v_* satisfies

$$v_*(x)=\delta\ln|x|+v_\infty+o(1)\quad\text{as}|x|\to\infty$$

and

$$\int_{\mathbb{R}^2} bU_\alpha e^{v_*}(1-U_\alpha e^{v_*}) = \frac{2\pi}{\lambda_\alpha}(2N-\alpha-\delta)$$

for some constants δ and v_∞. It follows from dominated convergence theorem that $\delta=0$, which in turn implies that v_* is bounded. □

We now show that if $\alpha\leqslant 0$, $N-\alpha>0$, and $\lambda>\lambda_\alpha$ then there exists a second solution v_2 of (1.7) such that $v_2<\overline{v}_{\lambda,\alpha}$.

Given $l>2$, fix $\epsilon\in(2,\min\{l,4\})$ and define $h(x)=(1+|x|^2)^{-\epsilon/2}$. We recall some results about the weighted space $\mathcal{H}$[10] which is the Hilbert space of L^2_{loc}-functions for which

$$\|v\|_{\mathcal{H}}=(\|\nabla v\|^2_{L^2(\mathrm{d}x)}+\|v\|^2_{L^2(\mathrm{d}\mu)})^{1/2}<\infty, \tag{2.12}$$

where $\mathrm{d}\mu=h\,\mathrm{d}x$. Note that $\mathcal{H}\subset M^2_{1,-\epsilon/2}$.

Let $\mathcal{H}'=\{v\in\mathcal{H}|\int_{\mathbb{R}^2}v\,\mathrm{d}\mu=0\}$.

Lemma 2.7:

McOwen—Ref. 10.

(i) Let $\eta>0$. Then there exists a constant C_η such that

$$\|v\|_{M^2_{0,-1-\eta}}\leqslant C_\eta\|\nabla v\|_{L^2}$$

for every $v\in\mathcal{H}'$.

(ii) For $\beta\in(0,\min\{4\pi,2\pi(\epsilon-2)\})$, there exists a constant C_β such that

$$\int_{\mathbb{R}^2} e^{|v|}\,\mathrm{d}\mu\leqslant C_\beta\exp\left(\frac{1}{4\beta}\|\nabla v\|^2_{L^2}\right)$$

for every $v\in\mathcal{H}'$.

Note that Eq. (1.7) has a variational structure. In a similar way as in Tarantello,[8] we consider the functional

$$I_\lambda(v)=\frac{1}{2}\|\nabla v\|^2_{L^2}+\frac{\lambda}{2}\int_{\mathbb{R}^2}K(U_\alpha e^v-1)^2\,\mathrm{d}\mu+\int_{\mathbb{R}^2}Fv\,\mathrm{d}\mu$$

defined on the set

$$\Lambda=\{\,v\in\mathcal{H}|v\geqslant v_*\quad a.e.\,\},$$

where $K=bh^{-1}$, $F=f_\alpha h^{-1}$, and $v_*=\inf_{\lambda>\lambda_\alpha}\overline{v}_{\lambda,\alpha}$. It is easily verified that I_λ is bounded below, coercive and lower semicontinuous on Λ. Then there exists $v_0\in\Lambda$ such that $I_\lambda(v_0)=\inf_{v\in\Lambda}I_\lambda(v)$. It can be shown[8] that v_0 is a C^2-solution of (1.7) and $v_0>v_*$.

Fix $t\in(0,-1+\epsilon/2)$. Let us denote $\mathcal{V}$ the Banach space of C^1-functions for which

$$\|v\|_{\mathcal{V}}=(\|\sigma^{1+t}\nabla v\|_{L^\infty}+\|v\|_{L^\infty})<\infty,\quad \sigma(x)=(1+|x|^2)^{1/2}.$$

Note that I_λ is well defined on $\mathcal{V}$ as well as $\mathcal{H}$.

Lemma 2.8: The function v_0 is a local minimum of I_λ in $\mathcal{H}$.

Proof: We follow Ref. 8 and argue by contradiction. Suppose that for each $n=1,2,\ldots$, there exists $v_n\in\mathcal{H}$ such that

$$I_\lambda(v_0)>I_\lambda(v_n)=\inf_{\|v_n-v_0\|_{\mathcal{H}}\leqslant 1/n}I_\lambda(v).$$

Then v_n satisfies

$$-\Delta v_n+\lambda bU_\alpha e^{v_n}(U_\alpha e^{v_n}-1)+f_\alpha=\eta_n(-\Delta(v_n-v_0)+h(v_n-v_0)). \tag{2.13}$$

Clearly $\eta_n \leqslant 0$. We rewrite (2.13) as

$$\Delta(v_n - v_0) = \frac{\lambda}{1+|\eta_n|} b U_\alpha^2 (e^{2v_n} - e^{2v_0}) - \frac{\lambda}{1+|\eta_n|} b U_\alpha (e^{v_n} - e^{v_0}) + \frac{|\eta_n|}{1+|\eta_n|} h(v_n - v_0)$$
$$:= \xi_n \quad \text{in } \mathbb{R}^2.$$

Since ξ_n belongs to $M^2_{0,\epsilon/2}$, there exist $\phi_n \in C^1 \cap M^2_{2,-2+\epsilon/2} \subset C_0(\mathbb{R}^2)$ and a constant c_n such that

$$v_n - v_0 = \frac{\beta_n}{2} \ln(|x|^2+1) + \phi_n + c_n$$

with

$$\beta_n = \frac{1}{2\pi} \int_{\mathbb{R}^2} \xi_n \, dx.$$

Since $v_n - v_0 \in \mathcal{H}$, $\beta_n = 0$. Note that by the inequality $|e^s - 1| \leqslant |s| e^{|s|}$, $s \in \mathbb{R}$, ξ_n satisfies

$$|\xi_n| \leqslant Ch |v_n - v_0| (e^{2|v_n - v_0|} + 1).$$

Decompose $v_n - v_0 = w_n + a_n$, $w_n \in \mathcal{H}'$, and $a_n \in \mathbb{R}$. Then we have $\|\nabla w_n\|_{L^2} + |a_n| \leqslant C/n$ from our assumption.

It follows from Lemma 2.1 that

$$\|\sigma^t \phi_n\|^2_{L^\infty} \leqslant C \|\phi_n\|^2_{M^2_{2,-2+\epsilon/2}} \leqslant C \|\xi_n\|^2_{M^2_{0,\epsilon/2}} \leqslant C \int_{\mathbb{R}^2} (|w_n|^2 + |a_n|^2) e^{4(|w_n| + |a_n|)} d\mu$$
$$\leqslant C(\|w_n\|_{L^2(d\mu)} + |a_n|^2) \left(\int_{\mathbb{R}^2} e^{10(|w_n| + |a_n|)} d\mu \right)^{1/2}$$
$$\leqslant C(\|\nabla w_n\|_{L^2} + |a_n|^2) \exp(C \|\nabla w_n\|^2_{L^2}) \leqslant C/n.$$

Moreover we obtain

$$\int_{\mathbb{R}^2} |v_n - v_0|^2 \, d\mu = \int_{\mathbb{R}^2} |c_n + \phi_n|^2 \, d\mu \geqslant \int_{\mathbb{R}^2} \left(\frac{c_n^2}{2} - \|\phi_n\|^2_{L^\infty} \right) d\mu,$$

which implies that $|c_n| \leqslant C/\sqrt{n}$.

Given $x_0 \in \mathbb{R}^2$, let $\Omega = \{y \in \mathbb{R}^2 | \frac{1}{2}|x_0| < |y| < \frac{3}{2}|x_0|\}$ if $|x_0| > 1$ and let $\Omega = \{y \in \mathbb{R}^2 | |y| < 2\}$ if $|x_0| \leqslant 1$. Then we obtain

$$\sigma(x_0) |\nabla \phi_n(x_0)| \leqslant C(\sup_\Omega |\phi_n| + \sigma^2(x_0) \sup_\Omega |\Delta \phi_n|)$$
$$\leqslant C(|\phi_n(y)| + \sigma^2(x_0) h(z) |c_n + \phi_n(z)|) \quad \text{for some } y, z \in \overline{\Omega}$$
$$\leqslant \frac{C}{\sqrt{n}} (\sigma^{-t}(y) + \sigma^2(x_0) \sigma^{-\epsilon}(z))$$
$$\leqslant \frac{C}{\sqrt{n}} \sigma^{-t}(x_0)$$

with C independent of x_0 and n. Since $x_0 \in \mathbb{R}^2$ is arbitrary, we obtain $\|\sigma^{1+t} \nabla \phi_n\|_{L^\infty} \leqslant C/\sqrt{n}$.

Therefore $v_n - v_0$ belongs to $\mathcal{V}$ and $\|v_n - v_0\|_{\mathcal{V}} \to 0$ as $n \to \infty$, which leads to a contradiction since v_0 is a local minimum of I_λ in $\mathcal{V}$. Indeed, note that $bU_\alpha e^{v_0}(U_\alpha e^{v_0} - 1) + f_\alpha$ belongs to $M^2_{0,\epsilon/2}$. Then we can prove that $v_0 \in \mathcal{V}$ by using the argument similar to the one above. Moreover a slight modification of the proof of Lemma 2.5 shows that $\lim_{|x|\to\infty} v_0(x) > \lim_{|x|\to\infty} v_*(x)$. □

We may assume that the maximal solution $\overline{v}_{\lambda,\alpha}$ is a local minimum of I_λ in $\mathcal{H}$ and $I_\lambda(\overline{v}_{\lambda,\alpha}) < \inf_{\|v - v_0\|_{\mathcal{H}} = r} I_\lambda(v)$ for some $r > 0$.

Note that the functional I_λ has a mountain pass structure, i.e., $I_\lambda(\overline{v}_{\lambda,\alpha} + c) \to -\infty$ as $c \to -\infty$. Moreover, it can be shown similar to Ref. 8 that I_λ satisfies the Palais–Smale condition in $\mathcal{H}$. Therefore we obtain a second solution $v_2 \in \mathcal{H}$ of (1.7) such that

$$I_\lambda(v_2) = \inf_{s \in \mathcal{P}} \max_{t \in [0,1]} I_\lambda(s(t))$$

where $\mathcal{P} = \{s : [0,1] \to \mathcal{H} \mid s \text{ is continuous, } s(0) = \overline{v}_{\lambda,\alpha}, \text{ and } s(1) = \overline{v}_{\lambda,\alpha} + c_\lambda\}$ and c_λ is a fixed constant so that $I_\lambda(\overline{v}_{\lambda,\alpha} + c_\lambda) < I_\lambda(\overline{v}_{\lambda,\alpha})$. Maximum principle implies that $v_2 < \overline{v}_{\lambda,\alpha}$.

We are ready to prove Proposition 1.1.

Proof of Proposition 1.1: We have only to prove the inequality (1.8). If v is a bounded solution of (1.7), then $\lambda b U_\alpha e^v (U_\alpha e^v - 1) + f_\alpha$ belongs to $M^2_{0,\delta+2}$ for every $-1 < \delta < \min\{0, l - \alpha - 3\}$. Then a slight modification of the proof of Lemma 2.8 proves the inequality (1.8). □

Proof of Proposition 1.2: Since (i) and (ii) are similarly proved as in Ref. 8, we prove (iii) only. Let $\overline{u}_{\lambda,\alpha} = u_0 + u_\alpha + \overline{v}_{\lambda,\alpha}$. Let $d = \frac{1}{3}\mathrm{dist}(\{p_j\}, \Omega) > 0$ and $\Omega_r = \{x \in \mathbb{R}^2 \mid \mathrm{dist}(x, \Omega) < r\}$ for $r > 0$. Define two constants

$$m_1 = \inf_{x \in \Omega_{2d}} \overline{u}_{\lambda_\alpha,\alpha}, \quad m_2 = \inf_{x \in \Omega_{2d}} b(x).$$

Hence if $\lambda > \lambda_\alpha$ then

$$b e^{\overline{u}_{\lambda,\alpha}}(e^{\overline{u}_{\lambda,\alpha}} - 1) < m_2 e^{2m_1} \overline{u}_{\lambda,\alpha} \quad \text{in } \Omega_{2d}.$$

Letting $m = m_2 e^{2m_1}$, we obtain $\Delta \overline{u}_{\lambda,\alpha} - \lambda m \overline{u}_{\lambda,\alpha} < 0$ in Ω_{2d}.

Given $x_0 \in \Omega_d$, define

$$w(x) = (1 - m_1)\exp\left(\frac{\sqrt{\lambda m}}{4\mathrm{d}}(|x - x_0|^2 - d^2)\right), \quad |x - x_0| \leqslant d.$$

If $\lambda > 2/m\mathrm{d}^2$, w satisfies

$$\Delta w - \lambda m w = \left(\frac{\lambda m}{4\mathrm{d}^2}\left|x - x_0\right|^2 + \frac{\sqrt{\lambda m}}{d} - \lambda m\right) w < 0 \quad \text{in } B_d(x_0).$$

Then we obtain

$$\Delta(\overline{u}_{\lambda,\alpha} + w) - \lambda m(\overline{u}_{\lambda,\alpha} + w) < 0, \quad B_d(x_0)$$

$$\overline{u}_{\lambda,\alpha} + w > 0, \quad \partial B_d(x_0).$$

Maximum principle implies that $\overline{u}_{\lambda,\alpha} > -w$ in $B_d(x_0)$. In particular, this inequality holds for $x = x_0$ and hence we obtain

$$\overline{u}_{\lambda,\alpha} > -(1 - m_1)\exp\left(-\frac{\sqrt{\lambda m}}{4} d\right) \text{in } \Omega_d,$$

since $x_0 \in \Omega_d$ is arbitrary. Since $\|\Delta \overline{u}_{\lambda,\alpha}\|_{L^2(\Omega_d)} \leqslant c_1 e^{-c_2\sqrt{\lambda}}$ for some constants $c_j = c_j(\Omega) > 0$ $(j = 1,2)$, then Sobolev embedding theorem and interior Schauder estimate imply (1.9). □

The proof of Theorem 1.1 is complete.

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To what extent do the classical equations of motion determine the quantization scheme?

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A simple example of one particle moving in a $(1+1)$ space–time is considered. As an example we take the harmonic oscillator. We confirm the statement that the classical equations of motion do not determine at all the quantization scheme. To this aim we use two inequivalent Lagrange functions, yielding Euler–Lagrange equations, having the same set of solutions. We present in detail the calculations of both cases to emphasize the differences occuring between them. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1405125]

I. INTRODUCTION

In classical physics the content of dynamical process is mainly characterized by the equations of motion of the physical system. It may happen that these equations can be derived from a certain Lagrange function as the Euler–Lagrange equations. If this is the case we may expect that there can be many (even infinitely many!) nonequivalent Lagrange functions linked to these equations of motion, yielding the same set of solutions—so called s-equivalent equations. This fact is well known.[1,2]

Two nonequivalent but s-equivalent Lagrange functions lead to two distinct Hamilton functions and distinct canonical momentum variables. If we take as the starting point for our consideration these two Hamilton functions as well as these two sets of canonical momenta and try to quantize them in a standard way we get, in general, two distinct quantization schemes, differing essentially from each other, althought both having common roots coming from the same equations of motion. This fact is not new and well known to some physicists,[1,2] but—strange enough—not much attention was paid by them to this problem.

From what was said so far we may infer that the answer to the question posed in the title is that the equations of motion do not determine the quantization scheme.

Below we shall present an elucidating example in favor of the statement made above.

One remark is in order here. If we choose two inequivalent but s-equivalent Lagrange functions, say, L, and L', we get two sets of canonical variables

$$\left(x,p\equiv\frac{\partial L}{\partial\dot{x}}\right) \quad \text{and} \quad \left(x,p'\equiv\frac{\partial L'}{\partial\dot{x}}\right). \tag{1.1}$$

Notice that those canonical variables are not connected to each other by a canonical transformation, viz.

$$(x,p)\rightarrow(X(x,p),P(x,p)). \tag{1.2}$$

Should they be linked to each other by a point transformation

$$(x,p)\rightarrow(x,p'(x,p)) \tag{1.3}$$

it would follow from the canonical Poisson brackets that

$$p' = p + f(x), \quad f(x) - \text{arbitrary function}, \tag{1.4}$$

which is not the case considered by us in this note.

II. THE CASE OF ONE CLASSICAL PARTICLE IN A (1+1) SPACE–TIME. THE MASTER EQUATION FOR $H'(x,p')$

To buttress the above observations and make plain the goal of this note, we shall investigate a very simple problem of classical mechanics. So let us restrict ourselves to the case of one classical particle, moving in a $(1+1)$ space–time. Let us take sufficiently smooth equation of motion

$$\ddot{x} = f(x,\dot{x},t), \tag{2.1}$$

where $x(t)$ denotes the location of the particle and $\dot{x} \equiv dx/dt$ and $\ddot{x} \equiv d^2x/dt^2$ denote its velocity and acceleration, respectively, t being the independent time variable. To every such equation belongs a Lagrange function,[2,3] $L(x,\dot{x},t)$. Let us further restrict ourselves for simplicity reasons to automonous Lagrange functions. It is known[2,4] that the most general expression for Lagrange function $L'(x,\dot{x})$, s-equivalent to $L(x,\dot{x})$, is

$$L' = \dot{x} \int_c^{\dot{x}} \frac{d\Sigma(H)}{dH} \frac{\partial^2 L}{\partial \dot{x}^2}\bigg|_{\dot{x}=u} du - \Sigma(H), \tag{2.2}$$

where $\Sigma(H)$ is an arbitrary differentiable function of H, different from zero a.e., and

$$H \equiv \dot{x}\frac{\partial L}{\partial \dot{x}} - L, \tag{2.3}$$

the Hamilton function. The constant c is so chosen that the integral on the rhs of (2.2) does not diverge. It is easy to see that we have

$$\frac{\partial L'}{\partial x} - \dot{x}\frac{\partial^2 L'}{\partial \dot{x}\partial x} - \ddot{x}\frac{\partial^2 L'}{\partial \dot{x}^2} = \frac{d\Sigma(H)}{dH}\left(\frac{\partial L}{\partial x} - \dot{x}\frac{\partial^2 L}{\partial \dot{x}\partial x} - \ddot{x}\frac{\partial^2 L}{\partial \dot{x}^2}\right). \tag{2.4}$$

[The presence of $d\Sigma(H)/dH$ in (2.4) causes the set of solutions of equation on the lhs of (2.4) and the one on the rhs to differ by a set of measure zero.] Thus L' is, indeed, s-equivalent to L. We have

$$H' \equiv \dot{x}\frac{\partial L'}{\partial \dot{x}} - L' = \Sigma(H). \tag{2.5}$$

We get also

$$p' \equiv \frac{\partial L'}{\partial \dot{x}}. \tag{2.6}$$

It is trivial to find H' and p' for given Σ and L as functions of x and $\dot{x}$. It is, however, not so simple to get H' as a function of x and p'. To get that let us observe that from (2.6) and (2.2) follows

$$1 = \frac{d\Sigma}{dH}\frac{\partial^2 L}{\partial \dot{x}^2}\frac{\partial \dot{x}(x,p')}{\partial p'}. \tag{2.7}$$

Taking into account the relation

$$\frac{\partial H'(x,p')}{\partial p'} = \dot{x}(x,p') \tag{2.8}$$

we get from (2.7) and (2.8)

$$\frac{\partial^2 H'(x,p')}{\partial p'^2} = \frac{\partial \dot{x}(x,p')}{\partial p'} = \left(\frac{dH'}{dH} \frac{\partial^2 L}{\partial \dot{x}^2}\bigg|_{\dot{x}=\partial H'/\partial p'} \right)^{-1}. \tag{2.9}$$

This is the master equation for H' as a function of p' and x; it is, in general, nonlinear.

The solutions of this master equation have to satisfy a physically justified requirement that p' has to tend to zero as $\dot{x}$ tends to zero and vice versa, or, in other words,

$$\frac{\partial H'}{\partial p'}\bigg|_{p'=0} = 0. \tag{2.10}$$

III. APPLICATION OF THE MASTER EQUATION

To make use of this master equation one has, of course, to specify what L and Σ are. This will be done now. We choose

$$L = \tfrac{1}{2}\dot{x}^2 - V(x), \tag{3.1}$$

where $V(x)$ is a non-negative function of x and

$$\Sigma(H) = H' = \sqrt{2H}. \tag{3.2}$$

[In case $V(x)$ is just bounded from below we may make it non-negative for each x by adding to it a suitably choosen positive constant.]

Square root means non-negative root. [The equality (3.2) should be understood as follows:

$$H' = \alpha\sqrt{2H}, \quad \alpha - \text{const.}$$

As H' as well H should have the same dimensions it follows that the constant α has to have the dimension

$$[\alpha] = g^{1/2} \text{ cm/s}.$$

The equation (3.3) reads

$$\frac{\partial^2 H'}{\partial p^2} = \frac{1}{\alpha^2 m} H'$$

as L in (3.1) becomes

$$L = \tfrac{1}{2} m\dot{x}^2 - V(x),$$

where m denotes the mass of the particle. In this note we put

$$a = m = 1.]$$

For this choice of L and Σ Eq. (2.9) reduces to

$$\frac{\partial^2 H'}{\partial p'^2} = H'. \tag{3.3}$$

The solution of (3.3) reads

$$H' = \alpha(x)\sinh p' + \beta(x)\cosh p'. \tag{3.4}$$

This solution has to satisfy the requirement (2.10) and therefore

$$\alpha(x) = 0. \tag{3.5}$$

From (3.1) and the Hamilton equation, we obtain

$$\frac{d}{dt}\frac{\partial H'}{\partial p'} = \ddot{x} = -\frac{\partial V}{\partial x}. \tag{3.6}$$

If we insert in (3.6)

$$\dot{x} = \beta(x)\sinh p', \tag{3.7}$$

$$\dot{p}' = -\frac{\partial H'}{\partial x} = -\frac{\partial \beta}{\partial x}\cosh p', \tag{3.8}$$

following from the Hamilton equations, we obtain

$$\frac{1}{2}\frac{\partial}{\partial x}\beta^2 = \frac{\partial V}{\partial x}$$

or

$$\beta = \pm\sqrt{2(V+C)}, \tag{3.9}$$

C being a constant. Hence

$$H' = \pm\sqrt{2(V(x)+C)}\cosh p'. \tag{3.10}$$

According to our choice (3.2) taking into account (3.9), we should have

$$\pm\sqrt{2(V+C)}\cosh p' = \sqrt{2(\dot{x}^2/2+V)}. \tag{3.11}$$

To keep both sides of the relation (3.11) compatible with each other we have to choose the $(+)$ sign on the lhs of (3.11). Since for p' tending to zero $\dot{x}$ should also tend to zero we conclude that $C=0$. Thus eventually we have

$$H' = \sqrt{2V(x)}\cosh p'. \tag{3.12}$$

Notice that we could as well choose in the definition on the rhs of (3.2) the $(-)$ sign in front of the root or use both signs suitable for certain nonoverlapping intervals of the variable x. This would cause a change of our model. In each case, mentioned earlier, the Hamilton equations are s-equivalent to original equations of motions and the Hamilton functions are constants of motion.

The original Hamilton function reads

$$H = \tfrac{1}{2}p^2 + V(x). \tag{3.13}$$

IV. EXAMPLE OF THE HARMONIC OSCILLATOR

For the case of the harmonic oscillator

$$V(x) = \tfrac{1}{2}x^2, \tag{4.1}$$

and we choose the model

$$H' = \sqrt{x^2}\cosh p'. \tag{4.2}$$

[Relation (4.2) has to be understood as follows

$$H' = \sqrt{m}\omega\alpha x \cosh\left(\frac{p'}{\sqrt{m}\alpha}\right)$$

as we have $L = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2x^2$, $[\omega] = 1/\mathrm{s}$. We put $m = \alpha = \omega = 1$.] H' is bounded from below. As H' is a conserved quantity the singularity of the trajectory appears at $x = 0$. It can be easily removed by taking as the potential

$$V(x) = \tfrac{1}{2}x^2 + a, \tag{4.3}$$

a an arbitrary positive constant. We are not going to use this procedure as it would essentially complicate our further calculations. For the case (4.2) the classical trajectories would be given by

$$\sqrt{x^2}\cosh p' = b, \quad b - a \text{ const.} \tag{4.4}$$

For $b > 0$ the phase trajectory lies in the strip $0 < x \leqslant b$ and $-b \leqslant x < 0$, while $-\infty < p' < +\infty$. If $|x| \to b$, then $dp'/dx \to \infty$. In the following we shall use one branch,

$$x\cosh p' = b, \tag{4.5}$$

for simplicity reasons.

It is easy to see that (4.2) gives rise to the equation

$$\ddot{x} + x = 0. \tag{4.6}$$

Indeed, we have

$$\frac{\partial H'}{\partial x} = \cosh p' = -\dot{p}', \quad \frac{\partial H'}{\partial p'} = x\sinh p' = \dot{x}. \tag{4.7}$$

Then

$$\ddot{x} = \dot{x}\sinh p' + \dot{p}'x\cosh p' = x(\sinh p')^2 - x(\cosh p')^2 = -x. \tag{4.8}$$

V. QUANTIZATION

Let us now try to quantize H and H'. We assume that the operators $(x, \hat{p})$ and $(x, \hat{p}')$ satisfy the standard canonical commutation relations. Then $\hat{p}$ as well as $\hat{p}'$ can be replaced by

$$-i\partial_x \tag{5.1}$$

in formulas (3.13) and (3.12), respectively. We get the following differential expressions, viz.

$$H_Q = -\tfrac{1}{2}(\partial_x)^2 + V(x) \tag{5.2}$$

$$H'_Q = \sqrt{\tfrac{1}{2}V(x)}\cos(\partial_x) + \cos(\partial_x)\sqrt{\tfrac{1}{2}V(x)}. \tag{5.3}$$

These expressions applied to $C_0^\infty(\mathbf{R})$ define symmetric operators in $L^2(\mathbf{R})$. (As it is well known, H_Q can be extended to a self-adjoint operator.) Notice that the operator (5.3) is not local, viz.

$$\cos(\partial_x)\Psi(x)=\tfrac{1}{2}(\Psi(x+i)+\Psi(x-i)) \tag{5.4}$$

and therefore (we denote the operator also by H'_Q)

$$H'_Q\Psi(x)=\frac{1}{\sqrt{2}}(\sqrt{V(x)}+\sqrt{V(x+i)})\Psi(x+i)+\frac{1}{\sqrt{2}}(\sqrt{V(x)}+\sqrt{V(x-i)})\Psi(x-i). \tag{5.5}$$

VI. HARMONIC OSCILLATOR

The potential is given by (4.1). As it is well known the eigenvalues for H_Q are

$$n+\tfrac{1}{2}, \quad n-\text{natural number or } 0, \tag{6.1}$$

and the eigenfunctions are the Hermitian functions

$$\Psi_n=\exp(-x^2/2)H_n(x), \tag{6.2}$$

where H_n are the Hermitian polynomials.[5]

For the case H'_Q we have [see (5.3)]

$$H'_Q=\tfrac{1}{2}(x\cos(\partial_x)+\cos(\partial_x)x). \tag{6.3}$$

The case of nonlocal H'_Q will be investigated in Sec. VII.

It seems more convenient to start the discussion by using different canonically conjugate variables, namely (hereafter we shall use the letter p instead of p')

$$-i\partial_x\to p \quad \text{and} \quad x\to i\partial_p. \tag{6.4}$$

Notice that the two systems of variables are linked by a Fourier transformation.

Let us denote the new Hamilton operator by K. Then we get from (6.3)

$$K=\frac{i}{2}(\partial_p\cosh(p)+\cosh(p)\partial_p). \tag{6.5}$$

The differential expression (6.5) when applied to $C_0^\infty(\mathbf{R})$ defines a symmetric operator in $L^2(\mathbf{R})$, which we shall also denote by K. This statement as well as the following results are dicussed *in extenso* in the Appendix. It is shown that for real γ,

$$0\leqslant\gamma<2, \tag{6.6}$$

the system of functions

$$\{\Psi_{2n+\gamma}(p)\}_{n\in\mathbf{Z}}, \tag{6.7}$$

where

$$\Psi_{2n+\gamma}(p)=\frac{1}{\sqrt{\pi\cosh p}}\exp(-i(2n+\gamma)\operatorname{arctan}\sinh p) \tag{6.8}$$

are the solution of the equations

$$K\Psi_{2n+\gamma}(p)=(2n+\gamma)\Psi_{2n+\gamma}(p), \tag{6.9}$$

is an orthonormal basis for $L^2(\mathbf{R})$. Thus for each fixed γ of the interval (6.6) K has a self-adjoint extension K_α, $\alpha\equiv\exp(-i\gamma\pi)$.

VII. FOURIER TRANSFORM OF THE EIGENFUNCTIONS

In this section we investigate Fourier transforms of eigenfunctions of the Hamilton operator (6.5). We find an expression for the Fourier transform in the case when eigenvalues are equal to $n+1/2$, where n is an integer. However, we do not see how to solve the problem for other eigenvalues. We show that in the considered case the Fourier transforms are eigenfunctions of nonlocal Hamilton operator (6.3). These eigenfunctions form two bases in the Hilbert space. They are expressed by the polynomial of Meixner and Pollaczek.

Let us rewrite the result (6.8). The normalized eigenfunction belonging to the eigenvalue λ reads

$$\Psi_\lambda(p)=\frac{1}{\sqrt{\pi\cosh p}}\ \exp(-i\lambda\ \text{arctan}\ \sinh p). \tag{7.1}$$

We start with two identities:

$$\frac{1}{\sqrt{\cosh p}}\ \exp\left(-\frac{i}{2}\text{arctan}\ \sinh p\right)=\frac{1+i}{1+ie^p}e^{p/2}, \tag{7.2}$$

$$\exp(-i\ \text{arctan}\ \sinh p)=i\frac{1-ie^p}{1+ie^p}. \tag{7.3}$$

To check these identities it is most simple to compare the moduli and arguments of the complex number on both sides of the equalities.

Mulitiplying the first identity by the nth power of the second identity we obtain

$$\Psi_{n+1/2}(p)=\frac{1}{\sqrt{\pi}}\left(i\frac{1-ie^p}{1+ie^p}\right)^n\frac{1+i}{1+ie^p}e^{p/2}. \tag{7.4}$$

To get the Fourier transform of (7.4),

$$\Phi_\lambda(x)\equiv\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi_\lambda(p)e^{ipx}dp, \tag{7.5}$$

we employ the method of generating function. We define

$$\Psi(p,t)\equiv\sum_{n=0}^{\infty}\Psi_{n+1/2}(p)t^n=\frac{1}{\sqrt{\pi}}\frac{1+i}{(1-it)+i(1+it)e^p}e^{p/2}. \tag{7.6}$$

The computation of (7.6) amounts to summing up the geometrical series covergent for $|t|<1$. The Fourier transform of the generating function (7.6) yields the generating function for the Fourier transforms of the eigenfunctions:

$$\Phi(x,t)\equiv\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi(p,t)e^{ipx}dp=\sum_{n=0}^{\infty}\Phi_{n+1/2}(x)t^n. \tag{7.7}$$

To evaluate the integral (7.7) we shall use the method of complex analysis. Let us consider the function

$$\frac{1}{\sqrt{2\pi}}\Psi(p,t)e^{ipx} \tag{7.8}$$

as the function of a complex variable p and let us compute the integral of function (7.8) along the contour of the rectangle with the vertices located at the points $(-a,0)$, $(a,0)$, $(a,2\pi i)$, $(-a,2\pi i)$, $a>0$, running in the counter-clockwise direction. In the limit when a tends to infinity, the integral along the lower side yields $\Phi(x,t)$. To get the integral along the upper side of the rectangle we exploit the relation

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi(p+2\pi i,t)e^{i(p+2\pi i)x}dp=-\Phi(x,t)e^{-2\pi x}, \tag{7.9}$$

which follows from the property

$$\Psi(p+2\pi i,t)=-\Psi(p,t). \tag{7.10}$$

In the limit the contributions from both remaining sides of the rectangle vanish. Then the integral along the rectangle in the limit is equal to

$$\Phi(x,t)+\Phi(x,t)e^{-2\pi x}. \tag{7.11}$$

Function (7.6) is a meromorphic function and has inside of the rectangle a simple pole at the point

$$\tilde{p}=\frac{i\pi}{2}-2i\arctan t. \tag{7.12}$$

We can express the integral of the function (7.6) along the rectangle by residuum of the function at the point $\tilde{p}$ which is equal to

$$-\frac{i}{\pi}e^{-\pi x/2}\frac{1}{\sqrt{1+t^2}}\exp(2x\arctan t). \tag{7.13}$$

The integral (7.11) is the product of $2\pi i$ and the residuum (7.13). Finally, we get

$$\Phi(x,t)=\frac{2e^{-\pi x/2}}{1+e^{-2\pi x}}\frac{1}{\sqrt{1+t^2}}\exp(2x\arctan t). \tag{7.14}$$

Let us set

$$W(x,t)\equiv\frac{1}{\sqrt{1+t^2}}\exp(2x\arctan t)=\sum_{n=0}^{\infty}W_n(x)\frac{t^n}{n!}. \tag{7.15}$$

The formula (7.15) defines the sequence of polynomials $W_n(x)$. Degree of the polynomial $W_n(x)$ equals n. The polynomials $W_n(x)$ are even functions for even n and odd functions for odd n.

Comparing definitions (7.7) and (7.15) and the formula (7.14) we can write

$$\Phi_{n+1/2}(x)=\frac{2e^{-\pi x/2}}{1+e^{-2\pi x}}\frac{W_n(x)}{n!}=\Phi_{1/2}(x)\frac{W_n(x)}{n!}. \tag{7.16}$$

This formula holds for non-negative integer n. From the definition of the Fourier transformation (7.5) and from the relation

$$\Psi_{-\lambda}(p)=\overline{\Psi_{\lambda}(p)} \tag{7.17}$$

follows

$$\Phi_{-\lambda}(x)=\Phi_{\lambda}(-x). \tag{7.18}$$

Thus for non-negative integer n we have

$$\Phi_{-n-1/2}(x)=(-1)^n\frac{2e^{\pi x/2}}{1+e^{2\pi x}}\frac{W_n(x)}{n!}=(-1)^n\Phi_{-1/2}(x)\frac{W_n(x)}{n!}, \tag{7.19}$$

which supplements relation (7.16).

Let us investigate the polynomials $W_n(x)$. For this aim we differentiate $W(x,t)$, given by (7.15), with respect to t. We get

$$\frac{\partial W(x,t)}{\partial t}=\frac{2x-t}{1+t^2}W(x,t). \tag{7.20}$$

If we multiple both sides of (7.20) by $(1+t^2)$ and compare the coefficients of the same power of t on both sides of (7.20), we obtain

$$\begin{aligned} W_0(x)&=1,\\ W_1(x)&=2x,\\ W_2(x)&=4x^2-1,\\ W_3(x)&=8x^3-10x,\\ W_4(x)&=16x^4-56x^2+9, \quad \text{etc.}, \end{aligned} \tag{7.21}$$

as well as recurrence formula

$$W_{n+1}(x)+n^2W_{n-1}(x)=2xW_n(x), \quad n>0. \tag{7.22}$$

Now we are going to show that the Fourier transformed functions $\Phi_{n+1/2}$ are eigenfunctions of the nonlocal Hamilton operator (6.3):

$$H'_Q\Phi_{n+1/2}(x)\equiv\frac{i}{2}\left(\frac{1}{2}-ix\right)\Phi_{n+1/2}(x+i)-\frac{i}{2}\left(\frac{1}{2}+ix\right)\Phi_{n+1/2}(x-i)=(n+1/2)\Phi_{n+1/2}(x). \tag{7.23}$$

We shall prove (7.23) for non-negative integer n; for negative ones the proof is very similar to that for non-negative.

Taking into account the relation

$$\Phi_{1/2}(x\pm i)=\mp i\Phi_{1/2}(x) \tag{7.24}$$

and the formula (7.16) we conclude that (7.23) holds iff

$$hW_n(x)\equiv\tfrac{1}{2}(\tfrac{1}{2}-ix)W_n(x+i)+\tfrac{1}{2}(\tfrac{1}{2}+ix)W_n(x-i)=(n+1/2)W_n(x). \tag{7.25}$$

To prove relation (7.25) let us apply the expression h upon $W(x,t)$, namely,

$$\begin{aligned} hW(x,t)&=\frac{1}{2}\left(\frac{1}{2}-ix\right)W(x+i,t)+\frac{1}{2}\left(\frac{1}{2}+ix\right)W(x-i,t)\\ &=\left(\frac{1}{2}+t\frac{2x-t}{1+t^2}\right)W(x,t)=\frac{1}{2}W(x,t)+t\frac{\partial W(x,t)}{\partial t}. \end{aligned} \tag{7.26}$$

The last equality follows from the formula (7.20). If we compare the coefficients of the same power of t on both sides of (7.26), we get (7.25). This completes the proof.

Let us return to the consideration of the previous section. There we learned that for any fixed λ the functions $\Psi_{2n+\gamma}$, $n=0,\pm1,\pm2,\pm3,\ldots$, form an orthonormal basis in $L^2(\mathbf{R})$. It is known that the Fourier transformation maps an orthonormal basis into a new orthonormal basis.

We have found the Fourier transforms of the eigenfunctions only for $\gamma=1/2$ and $\gamma=3/2$. Further, we choose $\gamma=1/2$ and consider an orthonormal basis:

$$\Phi_{2n+1/2}, \quad n=0,\pm1,\pm2,\pm3,\ldots. \tag{7.27}$$

Taking into account the definition (7.16) and (7.18) and property of polynomials $W_m(-x)=(-1)^m W_m(x)$ we get for non-negative integer n and k

$$\int_{-\infty}^{+\infty}\Phi_{2n+1/2}(x)\Phi_{2k+1/2}(x)dx=\int_{-\infty}^{+\infty}\frac{1}{2}(\Phi_{2n+1/2}(x)\Phi_{2k+1/2}(x)+\Phi_{2n+1/2}(-x)\Phi_{2k+1/2}(-x))dx$$

$$=\int_{-\infty}^{+\infty}\frac{W_{2n}(x)}{(2n)!}\frac{W_{2k}(x)}{(2k)!}\frac{dx}{\cosh\pi x}. \tag{7.28}$$

Similar computation for positive integers n and k gives

$$\int_{-\infty}^{+\infty}\Phi_{-2n+1/2}(x)\Phi_{-2k+1/2}(x)dx=\int_{-\infty}^{+\infty}\frac{W_{2n-1}(x)}{(2n-1)!}\frac{W_{2k-1}(x)}{(2k-1)!}\frac{dx}{\cosh\pi x}. \tag{7.29}$$

Functions on the left sides of (7.28) and (7.29) are orthonormal. Therefore for non-negative integer n and k, both odd or even, we have

$$\int_{-\infty}^{+\infty}\frac{W_n(x)W_k(x)}{\cosh\pi x}dx=(n!)^2\delta_{n,k}. \tag{7.30}$$

If n is odd and k is even, then the integrated function is odd and the integral vanish.

We may regard the set of polynomials $W_n(x)$ as the system of orthogonal polynomials with respect to the scalar product

$$\langle f,g\rangle\equiv\int_{-\infty}^{+\infty}\frac{\overline{f(x)}g(x)}{\cosh\pi x}dx. \tag{7.31}$$

We may prove orthogonality relation (7.30) directly, not refering to Fourier transformation. We are going to use the generating function $W(x,t)$.

Let us calculate in two different ways an integral

$$\int_{-\infty}^{+\infty}\frac{W(x,s)W(x,t)}{\cosh\pi x}dx. \tag{7.32}$$

On the one hand, we have

$$\sum_{n=0}^{\infty}\sum_{k=0}^{\infty}s^n t^k\int_{-\infty}^{+\infty}\frac{W_n(x)W_k(x)}{\cosh\pi x}dx. \tag{7.33}$$

On the other hand, we have

$$\int_{-\infty}^{+\infty}\frac{\exp(2x(\arctan s+\arctan t))}{\sqrt{1+s^2}\sqrt{1+t^2}\cosh\pi x}dx=\frac{1}{1-st}=\sum_{n=0}^{\infty}s^n t^n. \tag{7.34}$$

Comparing the coefficent of the same power s and t in the formulas (7.33) and (7.34) we get (7.30). To compute the integral (7.34) we exploit the relations

$$\int_{-\infty}^{+\infty} \frac{e^{2x\theta}}{\cosh \pi x} dx = \frac{1}{\cos \theta}, \quad -\frac{\pi}{2} < \theta < \frac{\pi}{2}, \tag{7.35}$$

and

$$\cos(\arctan s + \arctan t) = \frac{1 - st}{\sqrt{1+s^2}\sqrt{1+t^2}}. \tag{7.36}$$

The integral (7.35) we can calculate using the complex analysis method in a very similar way to the way we calculated the Fourier transform of the generating function (7.7). We exploit the following property of integrated function $f(x) \equiv \exp(2x\theta)/\cosh \pi x$:

$$f(x+i) = -f(x)e^{2i\theta}. \tag{7.37}$$

VIII. FINAL REMARKS

(1) Let us define the expression:

$$Rf(x) \equiv \frac{i}{2}\left(\frac{1}{2} - ix\right) f(x+i) - \frac{i}{2}\left(\frac{1}{2} + ix\right) f(x-i) + xf(x). \tag{8.1}$$

Then R behaves as a ''creation operator''

$$[h, R] = R, \tag{8.2}$$

where h is defined by formula (7.25). Therefore,

$$hf = \lambda f \quad \text{implies} \quad hRf = (\lambda + 1)Rf. \tag{8.3}$$

That confirms the designation ''creation operator'' for R. More exactly, we have

$$RW_n = W_{n+1}. \tag{8.4}$$

(2) The equation

$$\frac{i}{2}\left(\frac{1}{2} - ix\right)\Phi(x+i) - \frac{i}{2}\left(\frac{1}{2} + ix\right)\Phi(x-i) = \frac{1}{2}\Phi(x) \tag{8.5}$$

is not only solved by the function

$$\Phi_{1/2}(x) = \frac{2e^{-\pi x/2}}{1 + e^{-2\pi x}}, \tag{8.6}$$

but also by the function

$$\Phi(x) \equiv \Phi_{1/2}(x + a). \tag{8.7}$$

The Fourier transform of Φ reads

$$\Psi(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Phi(x) e^{-ipx} dx = \Psi_{1/2}(p) e^{-ipa}, \tag{8.8}$$

where

$$\Psi_{1/2}(p)=\frac{1+i}{1+ie^{p}}e^{p/2}. \tag{8.9}$$

We have

$$K\Psi(p)=(\tfrac{1}{2}+a\cosh p)\Psi(p), \tag{8.10}$$

and for $a\neq 0$ the function $\Psi(p)$ is not an eigenfunction of K.

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APPENDIX

Let us start with (6.5), viz.

$$K=\frac{i}{2}(\partial_p\cosh(p)+\cosh(p)\partial_p). \tag{A1}$$

This differential expression when applied to $C_0^{\infty}(\mathbf{R})$ defines a symmetric operator in $L^2(\mathbf{R})$ as stated in Sec. VI. We shall denote this operator also by K. Indeed, if Ψ and Φ belong to $C_0^{\infty}(\mathbf{R})$, then

$$\int_{-\infty}^{+\infty}\overline{\Psi(p)}K\Phi(p)dp-\int_{-\infty}^{+\infty}\overline{K\Psi(p)}\Phi(p)dp=i\int_{-\infty}^{+\infty}\frac{d}{dp}(\cosh(p)\overline{\Psi(p)}\Phi(p))dp$$
$$=i\cosh(p)\overline{\Psi(p)}\Phi(p)\Big|_{-\infty}^{+\infty}=0. \tag{A2}$$

Let λ belong to $\mathbf{C}$. Then the equation

$$K\Psi_{\lambda}(p)=\lambda\Psi_{\lambda}(p) \tag{A3}$$

has the solution

$$\Psi_{\lambda}(p)=C_{\lambda}\frac{1}{\sqrt{\cosh p}}\exp(-i\lambda\ \text{arctan sinh}\,p), \tag{A4}$$

which is unique up to the multiplicative constant C_{λ}. We may use this constant to normalize Ψ_{λ}. Clearly Ψ_{λ} belongs to $L^2(\mathbf{R})$ as (for λ, $\mu\in\mathbf{R}$ and $\lambda\neq\mu$ we have $\int_{-\infty}^{+\infty}\overline{\Psi_{\lambda}(p)}\Psi_{\mu}(p)dp=\overline{C_{\lambda}}C_{\mu}[\sin(\lambda-\mu)\pi/2]/[(\lambda-\mu)\pi/2]$)

$$\int_{-\infty}^{+\infty}\overline{\Psi(p)}\Psi(p)dp=|C_{\lambda}|^2\int_{-\infty}^{+\infty}\frac{dp}{\cosh p}=|C_{\lambda}|^2\pi. \tag{A5}$$

Thus the defect subspaces for the adjoint operator, K^{+}, are one dimensional and the defect indices are $\{-1,1\}$. Hence K has the one-parameter family of self-adjoint extensions, which can be defined as follows. Let

$$\alpha\in\mathbf{C},\quad |\alpha|=1, \tag{A6}$$

and define

$$M_\alpha=\left\{\Phi\in C^\infty(\mathbf{R}):\ \lim_{p\to-\infty}(\sqrt{\cosh p}\Phi(p))=\alpha\lim_{p\to+\infty}(\sqrt{\cosh p}\Phi(p))\right\}. \tag{A7}$$

Let us further define the operator K_α as

$$K_\alpha\Phi(p)=\frac{i}{2}\left(\sinh(p)+2\cosh(p)\frac{d}{dp}\right)\Phi(p),\quad \Phi\in M_\alpha. \tag{A8}$$

The operator K_α is essentially self-adjoint. To see this we observe that

$$\mathrm{Ran}(K_\alpha\pm i\mathbb{1})$$

is dense in $L^2(\mathbf{R})$. Indeed, taking

$$\Psi=\Psi_{\pm i},$$

we see that (A2) does not hold for all $\Phi\in M_\alpha$. Thus Ψ do not belong to the domain $D(K_\alpha^+)$ of K_α^+. Consequently, if $\Psi\in D(K_\alpha^+)$, then

$$K\Psi=K_\alpha^+\Psi=\pm i\Psi\quad\text{implies}\quad\Psi=0. \tag{A9}$$

This implies that if

$$(\Psi,(K_\alpha\mp i\mathbb{1})\Phi)=((K_\alpha^+\pm i\mathbb{1})\Psi,\Phi)=0 \tag{A10}$$

for all $\Phi\in M_\alpha$, then $\Psi=0$ and hence

$$\mathrm{Ran}(K_\alpha\pm i\mathbb{1}) \tag{A11}$$

is dense and K_α is essentially self-adjoint. We shall denote the closure of K_α by $\overline{K_\alpha}$.

Let us now consider the function (A4). For real λ we have

$$\lim_{p\to-\infty}(\sqrt{\cosh p}\ \Psi_{2n+\gamma}(p))=\alpha\lim_{q\to+\infty}(\sqrt{\cosh p}\ \Psi_{2n+\gamma}(p)), \tag{A12}$$

where

$$\alpha=e^{i\pi\gamma}.$$

We conclude that for any $0\leqslant\gamma<2$ the functions

$$\{\Psi_{2n+\gamma}\}_{n\in\mathbf{Z}} \tag{A13}$$

form a system of eigenvectors for the self-adjoint operator

$$\overline{K_\alpha},\quad \alpha=e^{-i\gamma\pi}. \tag{A14}$$

The corresponding eigenvalues are

$$\{2n+\gamma\}_{n\in\mathbf{Z}}. \tag{A15}$$

It follows from (A5) that if $C_{2n+\gamma}=1/\sqrt{\pi}$, then $\Psi_{2n+\gamma}$ are normalized. We show that for any

$$0\leqslant\gamma<2$$

the system

$$\{\Psi_{2n+\gamma}\}_{n\in\mathbf{Z}}$$

is an orthonormal basis for $L^2(\mathbf{R})$. It is sufficient to show that for any

$$f \in L^2(\mathbf{R})$$

there is

$$\sum_{n \in \mathbf{Z}} |(f, \Psi_{2n+\gamma})|^2 = \|f\|^2, \tag{A16}$$

where $(.,.)$ and $\|.\|$ denote the inner product and the norm in L^2, respectively. To prove (A16) let us observe that

$$(f, \Psi_{2n+\gamma}) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \overline{f(p)} (\cosh\, p)^{-1/2} \exp(-i(2n+\gamma) \operatorname{arctan} \sinh p) dp. \tag{A17}$$

Let us change the variables as follows

$$\begin{aligned} &\sinh p = \tan \frac{\theta}{2}, \quad -\pi \leqslant \theta \leqslant \pi, \\ &\cosh p = \frac{1}{\cos\, \theta/2}, \quad dp = \frac{d\theta}{\cos\, \theta/2}. \end{aligned} \tag{A18}$$

Then (A17) takes the form

$$(f, \Psi_{2n+\gamma}) = \frac{1}{2\sqrt{\pi}} \int_{-\pi}^{+\pi} \overline{f\left(\operatorname{arcsinh} \tan \frac{\theta}{2} \right)} \left(\cos \frac{\theta}{2} \right)^{-1/2} \exp\left(\frac{-i\gamma\theta}{2} \right) \exp(-in\theta) d\theta. \tag{A19}$$

We get further

$$\sum_{n \in \mathbf{Z}} |(f, \Psi_{2n+\gamma})|^2 = \frac{1}{4\pi} \sum_{n \in \mathbf{Z}} \left| \int_{-\pi}^{\pi} \overline{\tilde{f}(\theta)} e^{-in\theta} d\theta \right|^2 = \frac{1}{2} \int_{-\pi}^{\pi} |\tilde{f}(\theta)|^2 d\theta = \int_{-\infty}^{+\infty} |f(q)|^2 dq = \|f\|^2, \tag{A20}$$

where

$$\tilde{f}(\theta) \equiv f\left(\operatorname{arcsinh} \tan \frac{\theta}{2} \right) \left(\cos \frac{\theta}{2} \right)^{-1/2} e^{i\gamma\theta/2}. \tag{A21}$$

Formula (A20) is the Parseval equality.

Note: Notice that the model linked to formula (4.5) is not s-equivalent to the initial model.

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Trions in a periodic potential

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The group-theoretical classification of trion states (charged excitons $X^{\pm}$) is presented. It is based on considerations of products of irreducible projective representations of the two-dimensional translation group. For a given BvK period N degeneracy of obtained states is N^2. Trions $X^{\pm}$ consist of two identical particles (holes or electrons), so the symmetrization of states with respect to particles transposition is considered. There are $N(N+1)/2$ symmetric and $N(N-1)/2$ antisymmetric states. Completely antisymmetric states can be constructed by introducing antisymmetric and symmetric spin functions, respectively. Two symmetry-adapted bases are considered: The first is obtained from a direct conjugation of three representations, whereas in the second approach the states of an electrically neutral pair hole–electron are determined in the first step. The third possibility, a conjugation of representations corresponding to identical particles in the first step, is presented elsewhere. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1409350]

I. INTRODUCTION

The quantum Hall effect and high temperature superconductivity have given rise to interest in properties of the two-dimensional electron gas subjected to electric and magnetic fields. The observation of (negatively) charged excitons[1] has recalled a 40-year-old concept of excitons ''trions'' or ''charged excitons'' introduced by Lampert in 1958.[2] Recently, such excitons, consisting of two holes and an electron or two electrons and hole (denoted $X^{\pm}$, respectively), have been investigated both experimentally and theoretically.[3–5]

In this paper classification based on translational symmetry in the presence of a periodic potential and an external magnetic field is presented. To perform this task the so-called magnetic translation operators, introduced by Brown[6] and Zak,[7] are used. These operators commute with the standard Hamiltonian of an electron in the magnetic field $\mathbf{H}=\nabla\times\mathbf{A}$ and a periodic potential $V(\mathbf{r})$,

$$\mathcal{H}=\frac{1}{2m}\left(\mathbf{p}+\frac{e}{c}\mathbf{A}\right)^2+V(\mathbf{r}). \tag{1}$$

Brown and Zak's concepts can be generalized to a local gauge of the vector potential $\mathbf{A}$,[8,9] N-dimensional lattices,[10,11] and the spatially inhomogeneous magnetic field.[12] This paper exploits the fact that after imposing the Born–von Kármán (BvK) periodic conditions the magnetic translations form a finite-dimensional projective representation of the two-dimensional (2D) translation group. Kronecker products of irreducible projective representations can be applied to description of multiparticle states.[13,14]

Considering problems which involve the magnetic field $\mathbf{H}$ determined by the vector potential $\mathbf{A}$, one has to keep in mind that some results may depend on a chosen gauge, though physical properties should be gauge independent. Two gauges are most frequently used in the description of 2D electron systems: the Landau gauge with $\mathbf{A}=[0,xH,0]$ and the antisymmetric one with $\mathbf{A}=(\mathbf{H}\times\mathbf{r})/2$. The relations between these gauges were discussed in the earlier article,[9] so this problem is left out in the present considerations. However, it should be underlined that form

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representation matrices depend on the chosen gauge and, moreover, obtained representations are inequivalent, which means, among other things, that their bases are not related by a unitary transformation. This question is briefly discussed in Sec. IV.

II. IRREDUCIBLE PROJECTIVE REPRESENTATIONS OF THE 2D TRANSLATION GROUP

All finite-dimensional irreducible projective representations of the 2D translation for a given BvK period N are labeled n,l,k_1,k_2, where n is a divisor of N, $0<l<n$ is mutually prime with n, and $\mathbf{k}=(k_1,k_2)$ labels irreducible representations of 2D translation group with the BvK period N/n, so $k_1,k_2=0,1,\ldots,(N/n)-1$. In the special case $n=N$ matrix elements are given by the following formula:[14]

$$D^l_{jk}[n_1,n_2]=\delta_{j,k-n_2}\omega_N^{ln_1j}, \tag{2}$$

where l is mutually prime with N, $\omega_N=\exp(2\pi i/N)$, $j,k,n_1,n_2=0,1,\ldots,N-1$ (so all expressions are calculated modulo N), and $[n_1,n_2]$ denotes a vector of the 2D translation group (strictly speaking, their coordinates in the lattice basis $\{\mathbf{a}_1,\mathbf{a}_2\}$). For the sake of simplicity the considerations are limited to this case and the results presented correspond to the limit of high magnetic fields, i.e., there is no mixing of the Landau levels. The other special case $n=1$ leads to the standard (vector) representations of the translation group, i.e.,

$$D^{\mathbf{k}}[n_1,n_2]=\omega_N^{k_1n_1+k_2n_2}. \tag{3}$$

It has been shown in the earlier paper[14] that for a given magnetic field $\mathbf{H}$ the indices l and n are related to the charge of a moving particle. In the considered case it is assumed that the representation D^l corresponds to a hole, whereas D^{-l} corresponds to an electron. The vector representation $D^{\mathbf{k}}$ corresponds to a neutral particle or to an electron–hole pair, which is a case considered here. Hence, trions $X^{\pm}$ correspond to the Kronecker product of three representations: $D^{\pm l}\otimes D^{\pm l}\otimes D^{\mp l}$.

III. TRION STATES AND THEIR SYMMETRIZATION

A. Direct conjugation

The trions $X^{\pm}$ are charged excitons with the charge $\pm e$ equal to that of a single hole or electron, so, from the group-theoretical point of view, their states have to transform as vectors of the irreducible projective representation $D^{\pm l}$. Since representations $D^{\pm l}$ are N-dimensional then the following decomposition is true (see also Ref. 14):

$$D^{\pm l}\otimes D^{\pm l}\otimes D^{\mp l}=N^2D^{\pm l}. \tag{4}$$

This relation expressed in terms of the basis vectors has a form

$$|w\rangle_{\pm}^{pq}=\sum_{stu} a^{pq}_{stu,w}|stu\rangle_{\pm\pm\mp}, \tag{5}$$

where $s,t,u,w,p,q=0,1,\ldots,N-1$, $|w\rangle_{\pm}$ is a state of the trion $X^{\pm}$, $|stu\rangle_{\pm\pm\mp}$ is a three-particle state with s,t labeling states of two holes (electrons), u being a label of a single electron (hole), and the pair p,q plays a role of a repetition index. The state $|w\rangle_{\pm}$ should behave as a basis vector of the representation $D^{\pm l}$, so

$$D^{\pm l}[n_1,n_2]|w\rangle_{\pm}=\omega_N^{\pm ln_1(w-n_2)}|w-n_2\rangle_{\pm}; \tag{6}$$

it is satisfied if $a^{pq}_{stu,w}=\delta_{s,w+p}\delta_{t,w+q}\delta_{u,w+p+q}$, or

$$|w\rangle_{\pm}^{pq}=|(w+p)\,(w+q)\,(w+p+q)\rangle_{\pm\pm\mp}. \tag{7}$$

Namely, for each pair p,q the product (4) acts on a ket $|w\rangle_{\pm}^{pq}$ as follows:

$$\begin{aligned} D^{\pm l}\otimes D^{\pm l}\otimes D^{\mp l}[n_1,n_2]|w\rangle_{\pm}^{pq} &= D^{\pm l}[n_1,n_2]|w+p\rangle D^{\pm l}[n_1,n_2]|w+q\rangle D^{\mp l}[n_1,n_2]|w+p+q\rangle \\ &= \omega_N^{\pm ln_1(w-n_2)}|(w+p-n_2)(w+q-n_2)(w+p+q-n_2)\rangle_{\pm\pm\mp} \\ &= \omega_N^{\pm ln_1(w-n_2)}|w-n_2\rangle_{\pm}^{pq}. \end{aligned}$$

For $p=q$ the states obtained are symmetric with respect to the transposition of identical particles (holes or electrons). In the other cases ($p\neq q$) it is easy to form symmetric and antisymmetric combinations:

$$|w\rangle_{\pm}^{pq\pm}=2^{-1/2}(|w\rangle_{\pm}^{pq}\pm|w\rangle_{\pm}^{qp}), \tag{8}$$

where now $q>p=0,1,\ldots,N-1$. In this way one obtains $N(N-1)/2$ antisymmetric states and (together with those for $p=q$) $N(N+1)/2$ symmetric ones. Completely antisymmetric states can be constructed by introducing symmetric and antisymmetric spin functions, respectively. Noninteracting trions, therefore, will be described by a similar Hamiltonian as for free holes (electrons) [cf. Eq. (1)] with a modified effective mass and, if necessary, an appropriate potential $V(\mathbf{r})$. However, the degeneracy of energy levels is N^2 times larger.

Another form of the irreducible basis can be obtained when one considers at first conjugation of two representations and next conjugation of the resultant representation with the third one. The first step can be done in two ways: (i) two identical representations are conjugated, i.e., one considers a product $D^l\otimes D^l$ or $D^{-l}\otimes D^{-l}$ and (ii) states of a pair hole–electron are determined. The first method is more interesting since it can be used in problems where pairs of identical particles come into play (e.g., superconducting states). However, the considerations are a bit more complicated since the parity of N has to be taken into account.[15] Hence, in this paper the second possibility will be investigated, whereas the first is presented elsewhere.[16]

B. States of a hole–electron pair

We start the considerations from constructing states of a hole–electron pair (in a general case: a particle–antiparticle pair). Since such a pair has the charge zero, then its behavior in the external magnetic field should be similar (up to effective mass, etc.) to this of a noncharged particle. It means that in the algebraic picture ordinary (vector) representations of the translation group have to appear. This is confirmed by the brief outlook presented previously: Projective representations used to labeling of electron and hole states differ in the sign of l only. When both particles move in the same magnetic field then corresponding representations are D^{+l} and D^{-l} (of course, the BvK period N is identical in both cases). In this case matrix elements of these representations are given by (2) and those of their product are

$$(D^{+l}\otimes D^{-l})_{jj',kk'}[n_1,n_2]=D_{jk}^{+l}[n_1,n_2]D_{j'k'}^{-l}[n_1,n_2]=\delta_{j,k-n_2}\delta_{j+k',k+j'}\omega_N^{ln_1(j-j')}. \tag{9}$$

The product of representations $D^{+l}\otimes D^{-l}$ is a reducible representation, which can be decomposed into the irreducible one-dimensional vector representations (3),

$$D^{+l}\otimes D^{-l}=\bigoplus_{\mathbf{k}} D^{\mathbf{k}}. \tag{10}$$

There is no need to use the repetition index, because each representation appears only once. We are looking for such N^2 linear combinations

$$|0\rangle_{\mathbf{k}}=\sum_{s,t} a_{st}^{\mathbf{k}}|s\rangle_{+}|t\rangle_{-},$$

each of which behaves as a basis vector of a given irreducible representation $D^{\mathbf{k}}$. It can be shown that $a_{st}^{\mathbf{k}}=\delta_{t,s-xk_1}\omega_N^{sk_2}$, where x is the inverse of l modulo N (since l is mutually prime with N, then x is well determined), i.e., $xl=1 \bmod N$. Namely one obtains

$$\begin{aligned}(D^{+l}\otimes D^{-l})[n_1,n_2]|0\rangle_{\mathbf{k}} &= \sum_s \omega_N^{sk_2} D^{+l}[n_1,n_2]|s\rangle_{+} D^{-l}[n_1,n_2]|s-xk_1\rangle_{-} \\ &= \sum_s \omega_N^{sk_2}\omega_N^{ln_1(s-n_2)}|s-n_2\rangle_{+}\omega_N^{ln_1(n_2+xk_1-s)}|s-xk_1-n_2\rangle_{-} \\ &= \omega_N^{k_1n_1+k_2n_2}\sum_{s'} \omega_N^{s'k_2}|s'\rangle_{+}|s'-xk_1\rangle_{-} \\ &= D^{\mathbf{k}}[n_1,n_2]|0\rangle_{\mathbf{k}}.\end{aligned}$$

C. Trion states

The results presented in the previous section yield

$$|0\rangle_{\mathbf{k}}=\sum_s \omega_N^{sk_2}|s\,(s-xk_1)\rangle_{+-}, \quad xl=1 \bmod N. \tag{11}$$

Therefore,

$$D^{+l}\otimes D^{-l}\otimes D^{\pm l}=\bigoplus_{\mathbf{k}} D^{\mathbf{k}}\otimes D^{\pm l}$$

and trion states $|w\rangle_{\pm}^{\mathbf{k}}$, $w=0,1,\ldots,N-1$, can be written as

$$|w\rangle_{\pm}^{\mathbf{k}}=\sum_{s,t,u} b_{stu}^{w;\mathbf{k}}|stu\rangle_{+-\pm},$$

where s,t label states of a pair and u those of the second hole (electron) for a trion $X^{\pm}$. The repetition index $\mathbf{k}$ follows from the way in which the final states are constructed: at first states $|s\rangle_{+}$ and $|t\rangle_{-}$ are conjugated to the states $|0\rangle_{\mathbf{k}}$ according to Eq. (11) and next linear combinations of pairs $|0\rangle_{\mathbf{k}}|u\rangle_{\pm}$ are considered. Therefore, one can write

$$|w\rangle_{\pm}^{\mathbf{k}}=\sum_u c_u^{w;\mathbf{k}}|0\rangle_{\mathbf{k}}|u\rangle_{\pm}.$$

Since for each $\mathbf{k}=(k_1,k_2)$, $k_1,k_2=0,1,\ldots,N-1$ one has[13,14]

$$D^{\mathbf{k}}\otimes D^{\pm l}=D^{\pm l},$$

then each such product yields states $|w\rangle_{\pm}$, but the coefficients c_u^w depend on $\mathbf{k}$ and are given as

$$c_u^{w;\mathbf{k}}=\omega_N^{-wk_2}\delta_{u,w\mp xk_1},$$

where, again, $xl=1 \bmod N$, so

$$|w\rangle_{\pm}^{\mathbf{k}}=\omega_N^{-wk_2}|0\rangle_{\mathbf{k}}|w\mp xk_1\rangle_{\pm}\,. \tag{12}$$

Taking into account Eqs. (3) and (6) one obtains

$$\begin{aligned}(D^{\mathbf{k}}\otimes D^{\pm l})[n_1,n_2]|w\rangle_{\pm}^{\mathbf{k}}&=\omega_N^{-wk_2}D^{\mathbf{k}}[n_1,n_2]|0\rangle_{\mathbf{k}}D^{\pm l}[n_1,n_2]|w\mp xk_1\rangle_{\pm}\\&=\omega_N^{-(w-n_2)k_2}\omega_N^{\pm ln_1(w-n_2)}|0\rangle_{\mathbf{k}}|w\mp xk_1-n_2\rangle_{\pm}\\&=\omega_N^{\pm ln_1(w-n_2)}|w-n_2\rangle_{\pm}=D^{\pm l}[n_1,n_2]|w\rangle_{\pm}\,.\end{aligned}$$

Equations (11) and (12) lead to the final expression ($xl=1 \bmod N$, $N^{-1/2}$ is a normalization factor)

$$|w\rangle_{\pm}^{\mathbf{k}}=N^{-1/2}\omega_N^{-wk_2}\sum_s\ \omega_N^{sk_2}|s\ (s-xk_1)\ (w\mp xk_1))\rangle_{+-\pm}\,. \tag{13}$$

In such a state there is a kind of symmetry between an electron and a hole forming the neutral pair electron–hole, but there is no symmetry between two holes (electrons) in the trion $X^{\pm}$. Since there are N^2 trion states labeled by w then it is possible to construct states symmetric and antisymmetric with respect to transposition of particles. One of the possible ways is presented in Sec. III A and it is easy to determine a transformation between the basis obtained earlier and that presented previously.

Let us consider states of a trion X^+. The results of Sec. III A read

$$|w\rangle_+^{pq}=|(w+p)\ (w+q)\ (w+p+q))\rangle_{++-}\,, \tag{14}$$

where the first two indices correspond to the states of a hole and a third one to the state of an electron. In the above-presented formula (13) holes are labeled by the first and the third indices, whereas the middle one corresponds to an electron. Therefore, to calculate scalar products the order of indices has to be changed in one of these formulas. Having this done one obtains

$$\begin{aligned}{}_+^{\mathbf{k}}\langle w|w\rangle_+^{pq}&=N^{-1/2}\omega_N^{wk_2}\sum_s\ \omega_N^{-sk_2}{}_{+-+}\langle s\ (s-xk_1)\ (w-xk_1)|(w+p)\ (w+p+q)\ (w+q)\rangle_{+-+}\\&=N^{-1/2}\omega_N^{-pk_2}\delta_{q+xk_1,0}\,.\end{aligned} \tag{15}$$

In the simplest case $N=2$ this formula yields [the unique representation is obtained for $l=x=1$; $\mathbf{k}=(k_1,k_2)$]

$$|w\rangle_+^{00}=2^{-1/2}(|w\rangle_+^{(0,0)}+|w\rangle_+^{(1,0)}),$$

$$|w\rangle_+^{01}=2^{-1/2}(|w\rangle_+^{(0,0)}-|w\rangle_+^{(1,0)}),$$

$$|w\rangle_+^{10}=2^{-1/2}(|w\rangle_+^{(0,1)}+|w\rangle_+^{(1,1)}),$$

$$|w\rangle_+^{11}=2^{-1/2}(|w\rangle_+^{(0,1)}-|w\rangle_+^{(1,1)}).$$

The second and the third formulas can be symmetrized, which yields

$$|w\rangle_+^{01+}=2^{-1}(|w\rangle_+^{(0,0)}-|w\rangle_+^{(1,0)}+|w\rangle_+^{(0,1)}+|w\rangle_+^{(1,1)}),$$

$$|w\rangle_+^{01-}=2^{-1}(|w\rangle_+^{(0,0)}-|w\rangle_+^{(1,0)}-|w\rangle_+^{(0,1)}-|w\rangle_+^{(1,1)}).$$

IV. OTHER GAUGES

A trivial factor system θ (of an extension of groups or a projective representation) is determined by any mapping $\phi: G \to \mathrm{U}(1)$ by[9,17]

$$\theta(\mathbf{R},\mathbf{R}') = \phi(\mathbf{R})\,\phi(\mathbf{R})/\phi(\mathbf{R}+\mathbf{R}');$$

the factor system θ is standard if $\phi(\mathbf{0})=1$. If $\mu'(\mathbf{R},\mathbf{R}') = \mu(\mathbf{R},\mathbf{R}')\,\theta(\mathbf{R},\mathbf{R}')$ then factor systems μ and μ' are called equivalent. It can be easily shown[9] that these factor systems lead to the same value of the magnetic flux encircled by a loop formed by the vectors $\mathbf{R}$, $\mathbf{R}'$, $-\mathbf{R}$, and $-\mathbf{R}'$ and, therefore, is related to the magnitude of the magnetic field and is gauge independent (i.e., does not depend on the vector potential $\mathbf{A}$). Let θ be a standard trivial factor system determined by a mapping ϕ and let D be a projective representation with a factor system μ, i.e.,

$$D(\mathbf{R})D(\mathbf{R}') = \mu(\mathbf{R},\mathbf{R}')D(\mathbf{R}+\mathbf{R}').$$

A new representation D' determined as $D'(\mathbf{R}) = \phi(\mathbf{R})D(\mathbf{R})$ has an equivalent factor system $\mu' = \theta\mu$. On the other hand, for any unitary operator S and $D''(\mathbf{R}) = SD(\mathbf{R})S^{-1}$ one obtains

$$D''(\mathbf{R})D''(\mathbf{R}') = \mu(\mathbf{R},\mathbf{R}')D''(\mathbf{R}+\mathbf{R}'),$$

so *equivalent* representations have *identical* factor systems. It means that bases introduced for representations with equivalent (but different) factor systems are *not* related to each other by means of a *global* unitary transformation.[17] The relation between representations D and D' is *local*, since it depends on a vector $\mathbf{R}$ of the translation group.

These considerations give rise to the problem in which way bases obtained for different choices of the vector potential (different gauges) are related to each other. The most popular gauges, i.e., the Landau and the symmetric ones, are the special cases of the so-called linear gauge,[11] which in the 2D case has the form

$$\mathbf{A}(\mathbf{r}) = H[-\beta y, (1-\beta)x],$$

where H is a magnitude of the magnetic field $\mathbf{H}=[0,0,H]$. The relation between the vector potential $\mathbf{A}$ and the factor system of a projective representation shown in Ref. 8 yields that $\beta = 0$ corresponds to the representation (2), whereas $\beta=1$ and $\beta=1/2$, determining the other form of the Landau gauge and the (anti)symmetric one $\mathbf{A}=(\mathbf{H}\times\mathbf{r})/2$, lead to matrices

$${}^{1}D^{l}_{jk}[n_1,n_2] = \delta_{j,k-n_2}\omega_N^{ln_1k}, \quad {}^{1/2}D^{l}_{jk}[n_1,n_2] = \delta_{j,k-n_2}\omega_N^{ln_1(j+k)/2}.$$

In a general case one obtains

$${}^{\beta}D^{l}_{jk}[n_1,n_2] = \delta_{k-j,n_2}\omega_N^{ln_1[(1-\beta)j+\beta k]} = \delta_{k-j,n_2}\omega_N^{ln_1(j+\beta n_2)} = \omega_N^{ln_1n_2\beta}\,{}^{0}D^{l}_{jk}[n_1,n_2]. \tag{16}$$

The action of operators ${}^{\beta}D^{l}$ for vectors $[n_1,0]$ and $[0,n_2]$ on the basis vectors yields

$${}^{\beta}D^{l}[n_1,0]|j\rangle = \omega_N^{ln_1j}|j\rangle, \quad {}^{\beta}D^{l}[0,n_2]|j\rangle = |j-n_2\rangle.$$

Therefore, they behave in the same way for all real numbers β. The differences can only be noticed for general translations $[n_1,n_2]$ and, moreover, the nonzero matrix elements obtained for different β appear in the same places (it is controlled by the δ_{k-j,n_2}), but are multiplied by different powers of ω_N^l. Let us recall the former name of projective representations, used especially by physicists (see, e.g., Ref. 6). They were called *ray* representations, which was strongly related to the notion of *rays* in quantum mechanics.[18] Since only a module of a bracket $\langle j|k\rangle$ has

a physical meaning, then vectors (complex functions) $|j\rangle$, $|k\rangle$ are determined up to factors $\lambda \in U(1)$. Therefore, a chosen state $|j\rangle$ represents in fact a ray, i.e., the set $||j\rangle\rangle=\{\lambda|j\rangle|\lambda \in U(1)\}$. In a general case

$$ {}^{\beta}D^{l}_{jk}[n_1,n_2]=\langle j|{}^{\beta}D^{l}[n_1,n_2]|k\rangle=\delta_{k-j,n_2}\omega_N^{-ln_1j\beta}\omega_N^{ln_1j}\omega_N^{ln_1k\beta}. $$

Therefore, replacing each vector $|j\rangle$ by an element of the same ray $|j'\rangle=\omega_N^{-ln_1j\beta}$ one obtains

$$ \langle j'|{}^{\beta}D^{l}[n_1,n_2]|k'\rangle=\omega_N^{ln_1(j-k)\beta}\langle j|{}^{\beta}D^{l}[n_1,n_2]|k\rangle=\delta_{k-j,n_2}\omega_N^{ln_1j}={}^{0}D^{l}_{jk}[n_1,n_2]. $$

However, this transformation is *local*, because it depends on n_1 and, in fact, n_2, since $k-j=n_2$ for nonzero matrix elements. If can be verified that Eq. (7) is invariant under this transformation, so all relations derived here for the Landau gauge are valid for other linear gauges.

V. FINAL REMARKS

The presented considerations have shown that free trions should behave in a similar way to free electrons or holes. However, due to their internal structure the degeneracy is higher and there are many possibilities to construct states $|w\rangle_{\pm}$, two of which have been discussed previously. In these simplified considerations there are no interactions between trions or mixing of Landau levels and the spin or angular momentum numbers have not been considered. Taking into account spins will allow one to construct states completely antisymmetric with respect to the permutational symmetry. Such problem has been discussed lately by Dzyubenko *et al.*[5] for the case of free trions (i.e., without a periodic potential, so there is no discrete translational symmetry). A sum of indices on the right-hand side of (14), taking into account signs of charges, is $(2w+p+q)-(w+p+q)=w$, which is equal to the index on the left-hand side of this equation. This is the same result as presented in Ref. 5, where the total angular momentum projection of a trion equals $(n_1-m_1)+(n_2-m_2)-(n_3-m_3)$, where (n_j-m_j) is the total angular momentum projection for holes ($j=1,2$) and an electron ($j=3$), with n and m being the Landau level and the oscillator quantum numbers, respectively. It is interesting that Dzyubenko *et al.* obtained their results in the antisymmetric gauge $\mathbf{A}=(\mathbf{H}\times\mathbf{r})/2$, whereas in the presented considerations the Landau gauge has been used. It confirms that the physical properties are gauge independent. On the other hand, the actual form of wave functions is not discussed here, but the relations between representations and their product are taken into account only. These relations are independent of the matrix representations and, similarly, the form of resultant basis is independent of the function form: for a given BvK period N and any linear gauge irreducible projective representations are N-dimensional and their action on basis vectors are similar (up to a factor system).[6,7,9,19]

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Finite size effects in the anisotropic $(\lambda/4!)(\varphi_1^4+\varphi_2^4)_d$ model

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We consider the $(\lambda/4!)(\varphi_1^4+\varphi_2^4)$ model on a d-dimensional Euclidean space, where all but one of the coordinates are unbounded. Translation invariance along the bounded coordinate, z, which lies in the interval $[0,L]$, is broken because of the boundary conditions (BCs) chosen for the hyperplanes $z=0$ and $z=L$: DD and NN, where D denotes Dirichlet and N Neumann, respectively. The renormalization procedure up to one-loop order in the two-point function is applied, obtaining two main results. The first is the fact that the renormalization program requires the introduction of counterterms which are surface interactions. The second one is that the tadpole graphs for DD and NN have the same z dependent part in modulus but with opposite signs. We investigate the relevance of this fact to the elimination of surface divergences. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In this article we consider an interacting quantum field theory model in the presence of boundaries. We shall assume that the system is finite along one dimension $z\in[0,L]$, and infinitely extended along the remaining $(d-1)$ directions.

The presence of geometric restrictions on the domain of one of the coordinates of the system demands the introduction of classical boundary conditions, to be satisfied by the fields on the two hypersurfaces at $z=0$ and $z=L$. If we restrict ourselves to a real scalar field, Hermiticity of the Hamiltonian leads us to five different (inequivalent) choices for the BCs, namely, DD, NN, DN, periodic and antiperiodic. The last two choices are usual in the finite-temperature literature and shall not be dealt with here since they do not break translation invariance, which is the phenomenon we are concerned with.

Physical systems will be, in general, finite along several directions. For the sake of simplicity we will consider a d-dimensional layered geometry. Although the highly idealized case of planar boundaries misses a whole series of features that are present in the general, curved boundary case, for more general shapes the multiple reflection method can be used to find the correlation functions of the model.[1]

Most of the papers in the literature deal with periodic or antiperiodic boundary conditions, where translation symmetry is maintained and surface effects avoided. Moreover, in quantum systems where translation symmetry is broken, the renormalization procedure is more involved than for translation invariant systems, either bounded or unbounded. The diagrammatic expansion and the renormalization program for an unbounded system are conveniently performed in momentum space. On the other hand, when DD or NN BCs are implemented, one may still work with Green's functions at fixed $(d-1)$-dimensional momenta, since there is translation symmetry along those dimensions. In this case a convenient representation for the Green functions is a mixed $(\vec{p},z)$ space.

It is well known that the electromagnetic field confined between two parallel plates has a finite

renormalized stress-tensor near the boundaries without surface divergences. In the Casimir subtraction, one finds that when $\langle 0|\vec{E}^2|0\rangle$ and $\langle 0|\vec{B}^2|0\rangle$ are added their boundary singularities cancel. In this article we reexaminate this result and we will use two different facts to rederive it:

(i) First it was shown that for an electromagnetic field confined in a perfectly conducting cavity it is possible to treat the electric and magnetic modes separately where each one satisfies Dirichlet and Neumann boundary conditions, respectively.[2]
(ii) Second is the fact that the size-dependent parts of the tadpole for *DD* and *NN* BC have the same functional form and opposite signs.

Consequently, the study of two mutually noninteracting scalar fields subject to different boundary conditions reproduces exactly the electromagnetic case. It is a different way to rederive the case of finiteness of the renormalized electromagnetic stress-tensor near a perfectly conducting plate.

In this article we will consider a massive scalar theory subject to two different classical BCs: *DD* and *NN* (the mass acts just as an infrared regulator). Besides the lack of translational invariance, we shall face the problem of surface divergences. One way to avoid them is to smooth out the plates surface. But in this case an ambiguity appears, since loop-graphs will depend on an *ad hoc* model assumption, namely, the particular features of the smooth walls. Consequently, we prefer to maintain the hard walls assumption. In the context of the Casimir energy of minimally coupled scalar fields, many authors used soft, hard and semi-hard BCs.[3] Different questions sometimes require more complicated BCs, like the quantum mechanical treatment of the boundary conditions presented by Ford and Svaiter,[4] a device implemented to solve a long standing paradox concerning the renormalized energy of minimally and conformally coupled scalar fields.

For translation invariant systems, because of Poincaré invariance, one should expect that overlapping divergences will not obstruct the implementation of the renormalization program.[5] In systems where Poincaré invariance does not hold, these proofs do not apply, and one must show that it is still possible to implement such program. A technical difficulty is also met here, since the presence of geometric restrictions makes Feynman diagrams harder to compute than is ordinary quantum field theory in unbounded systems. A crucial work on this subject has been presented by Symanzik.[6] Of particular importance are also the papers by Nemirovsky and Freed, and Krech and Dietrich.[7]

The organization of the article is as follows: In Sec. II we discuss the slab configurations, dealing with the two-point and four-point functions, both for *DD* and *NN* BCs. In Sec. III we analyze the divergences of the translational invariant part of the tadpoles. Section IV deals with the analysis of the ultraviolet and infrared divergences of the z-dependent part of the tadpoles. Finally, Sec. V contains our conclusions. Throughout this article we use $\hbar = c = 1$.

II. FINITE SIZE EFFECTS AND CLASSICAL BOUNDARY CONDITIONS

Let us consider a d-dimensional Euclidean space with the anisotropic Landau–Ginzburg model for an $N=2$ component order parameter with a Lagrange density $\mathcal{L}=\mathcal{L}_0+\mathcal{L}_{\rm int}$, where

$$\mathcal{L}_0(\varphi_1,\varphi_2)=\tfrac{1}{2}(\partial\varphi_1)^2+\tfrac{1}{2}(\partial\varphi_2)^2+\tfrac{1}{2}m^2\varphi_1^2+\tfrac{1}{2}m^2\varphi_2^2 \tag{1}$$

and

$$\mathcal{L}_{\rm int}=\frac{\lambda}{4!}(\varphi_1^4+\varphi_2^4). \tag{2}$$

As discussed before, we will assume that the system is confined between two parallel plates localized at $z=0$ and $z=L$, and use the Cartesian coordinates $x^\mu=(\vec{r},z)$ where $\vec{r}$ is a

$(d-1)$-dimensional vector perpendicular to the z direction. For the cubic anisotropic model, we define the boundary conditions over the plates for the fields $\varphi_1(x)$ and $\varphi_2(x)$. For the $\varphi_1(x)$ field we assume Dirichlet–Dirichlet boundary conditions, i.e.,

$$\varphi_1(\vec{r},z)|_{z=0}=\varphi_1(\vec{r},z)|_{z=L}=0, \tag{3}$$

and for the $\varphi_2(x)$ we will assume Neumann–Neumann boundary conditions, i.e.,

$$\frac{\partial}{\partial z}\varphi_2(\vec{r},z)\bigg|_{z=0}=\frac{\partial}{\partial z}\varphi_2(\vec{r},z)\bigg|_{z=L}=0. \tag{4}$$

It is well known that ^{4}He films close to the λ transition satisfy DD BCs. Another well known example of such kind of boundary conditions is the electromagnetic field. It was shown that for an electromagnetic field confined in a perfectly conducting cavity, it is possible to treat the electric and magnetic modes separately, where each one satisfies Dirichlet and Newmann BCs, respectively.[2] Going back to our discussion, since the translational invariance is not preserved, let us use a Fourier expansion of the fields in the following form:

$$\varphi(\vec{r},z)=\frac{1}{(2\pi)^{(d-1)/2}}\int d^{d-1}p\sum_n \phi_n(\vec{p})e^{i\vec{p}\cdot\vec{r}}u_n(z), \tag{5}$$

where the $u_n(z)$ are the normalized eigenfunctions of the operator $-d^2/dz^2$ satisfying the completeness and orthonormality relations, i.e.,

$$\sum_n u_n(z)u_n^*(z')=\delta(z-z'), \tag{6}$$

$$\int_0^L dz u_n(z)u_{n'}^*(z)=\delta_{n,n'}, \tag{7}$$

and finally

$$-\frac{d}{dz^2}u_n(z)=k_n^2u_n(z), \tag{8}$$

where $k_n=n\pi/L$, $n=1,2,...$, for DD BCs and $n=0,1,2,...$,for NN BCs.

Coming back to the case of DD and NN boundary conditions, the eigenfunctions are, respectively,

$$u_n(z)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi z}{L}\right), \quad n=1,2,..., \tag{9}$$

and

$$u_n(z)=\sqrt{\frac{2}{L}}\cos\left(\frac{n\pi z}{L}\right), \quad n=1,2,\dots . \tag{10}$$

For NN BCs, we also have the zeroth mode $u_0(z)=1/\sqrt{L}$. The free propagator can be expressed in the following form:

$$G_0^{(2)}(\vec{r},z,z')=\frac{1}{(2\pi)^{d-1}}\int d^{d-1}p\sum_n e^{i\vec{p}\cdot\vec{r}}u_n(z)u_n^*(z')G_{0,n}(\vec{p}), \tag{11}$$

where it is not difficult to show that $G_{0,n}(\vec{p})$ is given by

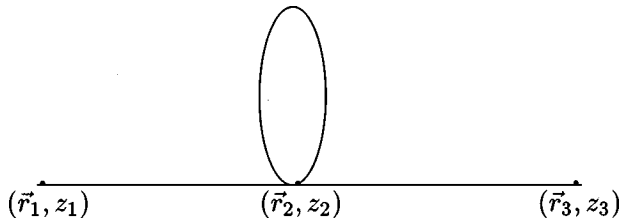

FIG. 1. The two-point function for $\varphi_1(x)$.

$$G_{0,n}(\vec{p}) = (\vec{p}^2 + k_n^2 + m^2)^{-1}. \tag{12}$$

As we discussed before, for translational invariant systems we have $G_0^{(2)}(x,x') = G_0^{(2)}(x - x')$ and from coordinate space Feynman rules we can go to momentum space representation, which is the more convenient framework to analyze the divergences of the theory. Translation invariance is reflected in momentum conservation conditions. Since our system possesses translation invariance along the direction parallel to the plates, the parallel momentum, $\vec{p}$, is conserved. In this case a convenient representation is a mixed $(\vec{p},z)$ space. The Feynman rules for different boundary conditions were derived in many references and we will not repeat the rules here. For a careful study of Feynman rules in such systems, see, for example, Ref. 8. Let us study the one-loop correction to the bare two-point function $G_0^{(2)}(x,x')$, both for the *DD* and *NN* cases. Using the Feynman rules (see Fig. 1) we have

$$G_0^{(2)}(\lambda,\vec{r}_1,z_1,\vec{r}_3,z_3) = \frac{\lambda}{2}\int d^{d-1}r_2 \int_0^L dz_2 G_0^{(2)}(\vec{r}_1,z_1;\vec{r}_2,z_2) \times G_0^{(2)}(\vec{r}_2,z_2;\vec{r}_2,z_2) G_0^{(2)}(\vec{r}_2,z_2;\vec{r}_3,z_3). \tag{13}$$

Each of these expressions can, for the case of *DD* BCs, be expanded as

$$G_0^{(2)}(\vec{r}_1 - \vec{r}_2, z_1, z_2) = \frac{2}{L}\frac{1}{(2\pi)^{d-1}} \sum_{n=1}^{\infty} \sin\left(\frac{n\pi z_1}{L}\right) \sin\left(\frac{n\pi z_2}{L}\right) \int d^{d-1}p \, \frac{e^{i\vec{p}.(\vec{r}_1 - \vec{r}_2)}}{(\vec{p}^2 + (n\pi/L)^2 + m^2)}. \tag{14}$$

$$G_0^{(2)}(\vec{r}_2 - \vec{r}_3, z_2, z_3) = \frac{2}{L}\frac{1}{(2\pi)^{d-1}} \sum_{n'=1}^{\infty} \sin\left(\frac{n\pi z_2}{L}\right) \sin\left(\frac{n\pi z_3}{L}\right) \int d^{d-1}p \, \frac{e^{i\vec{p}.(\vec{r}_2 - \vec{r}_3)}}{(\vec{p}^2 + (n'\pi/L)^2 + m^2)}, \tag{15}$$

and finally using the notation $G_0^{(2)}(\vec{r}_2,z_2;\vec{r}_2,z_2) = G_0^{(2)}(\vec{0},z_2)$ we have

$$G_0^{(2)}(\vec{0},z_2) = \frac{2}{L}\frac{1}{(2\pi)^{d-1}} \sum_{n''=1}^{\infty} \sin^2\frac{n''\pi z_2}{L} \int d^{d-1}p \, \frac{1}{(\vec{p}^2 + (n''\pi/L)^2 + m^2)}. \tag{16}$$

Although the functions $G_0^{(2)}(\vec{r}_1 - \vec{r}_2, z_1, z_2)$ and $G_0^{(2)}(\vec{r}_2 - \vec{r}_3, z_2, z_3)$ are singular at $\vec{r}_1 = \vec{r}_2$, $z_1 = z_2$ and $\vec{r}_2 = \vec{r}_3$, $z_2 = z_3$, the singularities are integrable (for points outside the plates), consequently only the tadpole is divergent and needs a regularization and renormalization procedure. A straightforward calculation yields the order λ correction to the bare two-point function in the one-loop approximation:

$$G_0^{(2)}(\lambda,\vec{r}_1-\vec{r}_3,z_1,z_3)=\frac{2}{L^2}\frac{1}{(2\pi)^{d-1}}\int_0^L dz_2\sum_{n,n'=1}^{\infty}\sin\left(\frac{n\pi z_1}{L}\right)\times\sin\left(\frac{n\pi z_2}{L}\right)\sin\left(\frac{n'\pi z_2}{L}\right)\sin\left(\frac{n'\pi z_3}{L}\right)\times\int d^{d-1}p\,\frac{e^{i\vec{p}(\vec{r}_1-\vec{r}_3)}}{(\vec{p}^2+(n\pi/L)^2+m^2)(\vec{p}^2+(n'\pi/L)^2+m^2)}T_{DD}(L,m,d,z_2),\tag{17}$$

where, since we will use dimensional regularization, we introduce a dimensional parameter μ, and define $g=\lambda\mu^{4-d}$. The expression for the tadpole $T_{DD}(L,m,d,z)$ is then

$$T_{DD}(L,m,d,z)=\frac{2g}{L}\frac{1}{(2\pi)^{d-1}}\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi z}{L}\right)\int d^{d-1}p\,\frac{1}{(\vec{p}^2+(n\pi/L)^2+m^2)}.\tag{18}$$

The tadpole graph in the case of NN BCs can also be easily found, and it is given by

$$T_{NN}(L,m,d,z)=\frac{g}{L}\frac{1}{(2\pi)^{d-1}}\int d^{d-1}k\,\frac{1}{(\vec{k}^2+m^2)}+\frac{2g}{L}\frac{1}{(2\pi)^{d-1}}\sum_{n=1}^{\infty}\cos^2\left(\frac{n\pi z}{L}\right)\int d^{d-1}p\,\frac{1}{(\vec{p}^2+(n\pi/L)^2+m^2)}.\tag{19}$$

Note that both $T_{DD}(L,m,d,z)$ and $T_{NN}(L,m,d,z)$ diverge in their continuum momenta integrals and also in the n summation. In the next section we will analyze the ultraviolet behavior of the bare two-point functions, i.e., $T_{DD}(L,m,d,z)$ and $T_{NN}(L,m,d,z)$.

III. ANALYSIS OF THE ULTRAVIOLET DIVERGENCES OF $T_{DD}(L,m,d,z)$ AND $T_{NN}(L,m,d,z)$

The aim of this section is to analyze the structure of the divergences of the bare two-point functions for cases of both DD and NN boundary conditions. Let us start from the expression of the vacuum activity for the case of DD boundary conditions, i.e.,

$$T_{DD}(L,m,d,z)=\frac{2g}{L}\frac{1}{(2\pi)^{d-1}}\sum_{n=1}^{\infty}\sin^2\left(\frac{n\pi z}{L}\right)\int d^{d-1}p\,\frac{1}{(\vec{p}^2+(n\pi/L)^2+m^2)}.\tag{20}$$

Using trigonometric identities and also the relation[9]

$$\sum_{n=1}^{\infty}\frac{\cos nx}{n^2+a^2}=-\frac{1}{2a^2}+\frac{\pi}{2a}\frac{\cosh a(\pi-x)}{\sinh\pi a},\tag{21}$$

which is valid for $0\leqslant x\leqslant 2\pi$, it is easy to show that the vacuum activity in the case of DD BCs is given by

$$T_{DD}(L,m,d,z)=\frac{g}{2L}\frac{1}{(2\pi)^{d-1}}\sum_{n=-\infty}^{\infty}\int d^{d-1}p\,\frac{1}{(\vec{p}^2+(n\pi/L)^2+m^2)}-gf_2(d,L,m,z),\tag{22}$$

where

$$f_2(L,m,d,z)=\frac{1}{2}\frac{1}{(2\pi)^{d-1}}\int d^{d-1}p\,\frac{1}{(\vec{p}^2+m^2)^{1/2}}\frac{\cosh\left((L-2z)(\vec{p}^2+m^2)^{1/2}\right)}{\sinh\left(L(\vec{p}^2+m^2)^{1/2}\right)}. \tag{23}$$

In an analogous way, it is also possible to calculate the vacuum activity for the NN BCs, i.e., $T_{NN}(L,m,d,z)$ and we obtain

$$T_{NN}(L,m,d,z)=\frac{g}{2L}\frac{1}{(2\pi)^{d-1}}\sum_{n=-\infty}^{\infty}\int d^{d-1}p\,\frac{1}{(\vec{p}^2+(n\pi/L)^2+m^2)}+g f_2(L,m,d,z). \tag{24}$$

Since $T_{DD}(L,m,d,z)$ and $T_{NN}(L,m,d,z)$ have the same functional form, both have the same kind of ultraviolet divergences. Let us define $f_1(L,m,d)$ by

$$f_1(L,m,d)=\frac{1}{2L}\frac{1}{(2\pi)^{d-1}}\sum_{n=-\infty}^{\infty}\int d^{d-1}p\,\frac{1}{(\vec{p}^2+(n\pi/L)^2+m^2)}. \tag{25}$$

The equation above has ultraviolet divergences, but it is (formally) proportional to the tadpole in finite temperature field theory, after the identification: $\beta\equiv 2L$. To deal with the divergences of the one-loop two-point function at finite temperature we have to do frequency sums and $(d-1)$-dimensional integrals for the continuum momenta. The most popular method to deal with Matsubara sums is analytic extension away from the discrete complex energies down to real axis with the replacement of the energy sums by contour integrals.[10] We prefer to use dimensional regularization in the continuum,[11] and afterwards to analytically extend the modified Epstein zeta function which appears after the dimensional regularization.[12] Since the formalism has already been developed by Malbouisson and Svaiter in Ref. 13, we will only sketch the procedure here. First we have to use a well known result of dimensional regularization, i.e.,

$$\int\frac{d^dk}{(k^2+a^2)^s}=\frac{\pi^{d/2}}{\Gamma(s)}\Gamma\left(s-\frac{d}{2}\right)\frac{1}{a^{2s-d}}, \tag{26}$$

and let us define the modified Epstein zeta function $\zeta(z,a)$ by

$$\zeta(z,a)=\sum_{n=-\infty}^{\infty}\frac{1}{(n^2+a^2)^z},\quad a^2>0, \tag{27}$$

which is analytic for $\mathrm{Re}(z)>\frac{1}{2}$. It is possible to analytically extend the modified Epstein zeta function where the integral representation is valid for $\mathrm{Re}(z)<1$[14]

$$\sum_{n=-\infty}^{\infty}(n^2+a^2)^{-z}=a^{1-2z}\left[\sqrt{\pi}\frac{\Gamma\left(z-\frac{1}{2}\right)}{\Gamma(z)}+4\sin\pi z\int_1^{\infty}\frac{(t^2-1)^{-z}dt}{e^{2\pi at}-1}\right]. \tag{28}$$

Using Eqs. (26) and (28) in Eq. (25), we get a polar part (size independent) plus a size dependent analytic correction. It is clear that the mass counterterm generated by $f_1(L,m,d)$ is size independent, as the finite temperature field theory has no temperature dependent counterterm. The first interesting result of the article is given by Eqs. (22) and (24). The tadpole graphs expressed by $T_{DD}(L,m,d,z)$ and $T_{NN}(L,m,d,z)$ have the same z dependent part in modulus but with opposite signs. From the previous discussion it is possible to understand the finiteness of the renormalized stress-tensor of an electromagnetic field near a flat prefectly conducting plate. Although the expectation values of the squared electric and magnetic field are divergent, a delicate cancellation makes the renormalized stress-tensor finite. As the size dependent parts of $T_{DD}(L,m,d,z)$ and $T_{NN}(L,m,d,z)$ have the same functional form and opposite signs, and recalling that it is possible to treat the electric and magnetic modes separately (where one obeys DD and the other NN BCs),

we automatically obtain a finite result for the vacuum expectation value of the stress-tensor of the electromagnetic field. It is important to stress that when the conducting boundary is curved, the energy density diverges on the boundary.[15]

We shall deal with the renormalization program in the one-loop approximation in the next section, also discussing, for the sake of completeness, the issue of infrared (IR) divergencies in different numbers of dimensions.

IV. ANALYSIS OF THE ULTRAVIOLET AND INFRARED DIVERGENCES OF THE *z*-DEPENDENT PART OF THE TADPOLES

Let us use the fact that $d^{d-1}p=p^{d-2}dpd\Omega_{d-1}$ and $\int d\Omega_{d-1}=2\pi^{(d-1)/2}/\Gamma((d-1)/2)$. It should be noted that, had we chosen $m^2=0$, the ultraviolet divergences would have kept the same polar structure. Consequently, for simplicity let us choose again $m=0$, and, for reasons that will become evident later, we first assume $d>3$. The special case $d=3$ is discussed at the end of this section. Defining $h_2(d)$ by

$$h_2(d)=\frac{1}{2^{d-2}}\,\frac{1}{\pi^{(d-1)/2}}\,\frac{1}{\Gamma((d-1)/2)}, \tag{29}$$

it is possible to write $f_2(L,m,d,z)|_{m=0}$ as

$$f_2(L,m,d,z)|_{m=0}=\frac{1}{2}h_2(d)\int_0^\infty dk k^{d-3}\coth kL\cosh 2kz-h_2(d)\int_0^\infty dk k^{d-3}\cosh kz\sinh kz. \tag{30}$$

In a general way, the regularization process is achieved by introducing exponential cut-off regulators and after that the identification of the poles of the regularized quantity by means of the Laurent series expansion around some point, i.e., the negative power portion of such series. Note that instead of imposing renormalization conditions over the 1PI correlation functions, we can simply subtract the singular part of the Laurent series around some point, by the introduction of the counterterms. Let us assume $z\neq 0$ and $z\neq L$. A straightforward calculation gives

$$f_2(L,m,d,z)|_{m=0}=\frac{1}{2}h_2(d)\left[\int_0^\infty dk k^{d-3}(\coth kL-1)\cosh 2kz + \int_0^\infty dk k^{d-3}(\cosh 2kz-\sinh 2kz)\right]. \tag{31}$$

In the first integral for large k, $(\coth kL-1)$ has the behavior $(\coth kL-1)\sim e^{-2kL}$. Moreover, the second integral in Eq. (31) is ultraviolet finite for $z\neq 0$. Let us define $x=kL$ and $q=kz$ in the first and second integrals above, respectively. Then Eq. (31) becomes

$$f_2(L,m,d,z)|_{m=0}=\frac{1}{2}h_2(d)\frac{1}{L^{d-2}}\int_0^\infty dx x^{d-3}(\coth x-1)\cosh\left(\frac{2z}{L}x\right) + \frac{1}{2}h_2(d)\frac{1}{z^{d-2}}\int_0^\infty dq q^{d-3}(\cosh 2q-\sinh 2q). \tag{32}$$

The second term in the above equation gives us the well known result that for a massless minimal coupled scalar field $\langle\varphi^2(x)\rangle$ diverges as $1/z^2$ if we approach the plate.[16] In order to analyze the polar part of $f_2(L,0,d,z)$, we use the definition of the gamma function. Let us define $I_1(\nu,\mu)$ and $I_2(\mu,\beta)$ by

$$I_1(\mu,\nu)=\int_0^\infty dx x^{\mu-1}e^{-\nu x}=\frac{1}{\nu^\mu}\Gamma(\mu),\quad \mathrm{Re}(\mu)>0,\quad \mathrm{Re}(\nu)>0, \tag{33}$$

and

$$I_2(\mu,\beta)=\int_0^\infty dx x^{\mu-1}e^{-\beta x}(\coth x-1)=2^{1-\mu}\Gamma(\mu)\zeta\left(\mu,\frac{\beta}{2}+1\right),\quad \mathrm{Re}(\beta)>0,\quad \mathrm{Re}(\mu)>1, \tag{34}$$

where $\zeta(z,a)$ is the Riemann zeta function defined by[9]

$$\zeta(z,a)=\sum_{n=0}^{\infty}\frac{1}{(n+a)^z},\quad \mathrm{Re}(z)>1,\quad a\neq 0,-1,-2,\ldots . \tag{35}$$

Then, using Eqs. (33)–(35) in Eq. (32) we have that

$$f_2(L,m,d,z)|_{m=0}=\frac{1}{2}h_2(d)\frac{1}{L^{d-2}}\left[2^{2-d}\Gamma(d-2)\left(\zeta\left(d-2,\frac{z}{L}+1\right)+\zeta\left(d-2,-\frac{z}{L}+1\right)\right)\right]+\frac{1}{(2z)^{d-2}}h_2(d)\Gamma(d-2). \tag{36}$$

Using the definition of the zeta function, it is evident that

$$\frac{1}{L^{d-2}}\left(\zeta\left(d-2,\frac{z}{L}+1\right)+\zeta\left(d-2,-\frac{z}{L}+1\right)\right)=\frac{1}{L^{d-2}}\sum_{n=0}^{\infty}\frac{1}{(n+(1+z/L))^{d-2}}+\frac{1}{(L-z)^{d-2}}+\frac{1}{L^{d-2}}\sum_{n=1}^{\infty}\frac{1}{(n+(1-z/L))^{d-2}}. \tag{37}$$

We see that the regularized $f_2(L,0,d,z)$ has two poles of order $(d-2)$ in $z=0$ and in $z=L$. Note that the residues of the poles in $z=0$ and in $z=L$ are L independent. Since the domain of analyticity of the zeta function is $d>3$, the case $d=3$ must be studied separately. Different treatments for $d=3$ and $d=4$ simply express the fact that infrared divergences are more severe in lower dimensions.

We will go back to Eq. (23), studying the case $m^2\neq 0$, to see how the IR divergences pop up in the $m^2\to 0$ limit. It is important to stress that, only in the *NN* BC case, we have IR divergences for massless fields, coming from the term $n=0$, i.e., Eq. (22) is IR finite for $m=0$. A straightforward calculation yields

$$f_2(L,m,d,z)=\frac{1}{2}h_2(d)\int_0^\infty d\rho\,\frac{\rho^{d-2}}{(\rho^2+m^2)^{1/2}}\,\frac{\cosh\left((L-2z)(\rho^2+m^2)^{1/2}\right)}{\sinh(L(\rho^2+m^2)^{1/2})}. \tag{38}$$

Defining $\sigma=(\rho^2+m^2)^{1/2}$ and using the fact that $d=3$, we have

$$f_2(L,m,d,z)|_{d=3}=\frac{1}{2}h_2(3)\left[\int_m^\infty d\sigma(\coth\sigma L-1)\cosh 2\sigma z+\int_m^\infty d\sigma(\cosh 2\sigma z-\sinh 2\sigma z)\right]. \tag{39}$$

The second integral in the above expression is convergent for $z\neq 0$, and, defining $v=2\sigma z$, it becomes

$$\frac{1}{4z}h_2(3)\int_{2mz}^{\infty}dv\,e^{-v}=\frac{1}{4z}h_2(3)\Gamma(1,2mz), \tag{40}$$

where $\Gamma(a,x)$ is the incomplete gamma function. Consequently, we have a simple pole for $z=0$. Again, the residue of this pole is L independent. To complete the regularization procedure we now have to analyze the first integral of Eq. (39):

$$\frac{1}{2}h_2(3)\int_m^{\infty}d\sigma(\coth\sigma L-1)\cosh 2\sigma z=\frac{1}{8L}h_2(3)\int_{2mL}^{\infty}du\,\frac{e^{(z/L)\,u}}{e^u-1}+\frac{1}{8L}h_2(3)\int_{2mL}^{\infty}du\,\frac{e^{-(z/L)\,u}}{e^u-1}. \tag{41}$$

The second integral on the right side of Eq. (41) is convergent and the first one has a simple pole at $z=L$, again with an L independent residue.

As we have already taken care of the ultraviolet divergences, let us study the infrared divergent piece (for $m=0$) of $f_2(L,m,d,z)|_{d=3}$. Let us call this piece $f_2^*(L,m,d,z)|_{d=3}$. Note that we introduce an ultraviolet cut-off in order to use the Bernoulli representation of the integrand:

$$f_2^*(L,m,d,z)|_{d=3}=\frac{1}{4L}h_2(3)\left(\int_{mL}^{2\pi}du\,\frac{e^{(z/L)\,u}}{e^u-1}+\int_{mL}^{2\pi}du\,\frac{e^{-(z/L)\,u}}{e^u-1}\right). \tag{42}$$

Writing the integrand using the Bernoulli polynomials it is not difficult to show that

$$f_2^*(L,m,3,z)=\frac{1}{2L}h_2(3)B_0\left(\frac{z}{L}\right)\ln\left(\frac{2\pi}{mL}\right)+\text{regular part}\ \ (f_2^*(L,m,z)). \tag{43}$$

From the previous discussion, we can conclude that, in order to eliminate the ultraviolet divergences of the theory we have to introduce counterterms as surface interactions, and consequently the full action will have the following form for both fields φ_1 and φ_2:

$$S(\varphi)=\int_0^L dz\int d^{d-1}r\left(\frac{1}{2}(\partial\varphi)^2+\frac{1}{2}m^2\varphi^2+\frac{1}{4!}\lambda\varphi^4\right)+\int d^{d-1}r(c_1\varphi^2(\vec{r},0)+c_2\varphi^2(\vec{r},L)). \tag{44}$$

We have seen that, to renormalize the theory, counterterms corresponding to surface interactions are required. We conjecture that one can avoid this difficulty by equipping the model with a $\varphi_1^2\varphi_2^2$ interaction. Then, the z dependent pieces of each tadpole may cancel each other out, and the two fields develop a size dependent mass Δm^2 proportional to gL^{-2}, as for the single φ^4 model at finite temperature. The study of the $O(2)$ symmetric model is under investigation by the authors.

V. CONCLUSIONS

In this article we studied finite size effects in an interacting field theory, with broken translation invariance. We calculated the vacuum activity for an anisotropic model, between two parallel plates in a d dimensional Euclidean space. It has been possible to obtain closed expressions for $\langle\varphi_1^2(x)\rangle$ and $\langle\varphi_2^2(x)\rangle$, for fields satisfying DD and NN BCs, respectively. We presented a model having the interesting property that the z-dependent part of the tadpole graphs for DD and NN BCs have the same modulus and opposite signs. This fact could explain the boundedness of the renormalized vacuum expectation value of the energy-stress tensor of the electromagnetic field in the Casimir-like configuration.

There are several directions in which the finite size effects for systems with breaking of translational invariance which may deserve further research. They are, to mention a few of them: the study ofinteracting fermions, the nonlinear σ model in domains with one finite direction and $(d-1)$ infinite directions,[17] and, finally, as a straightforward extension of this work, the study of

the $O(2)$ symmetric model at the two-loop approximation. As discussed in the Introduction, one should prove that the the renormalization program can be implemented beyond the one-loop approximation, where overlapping divergences emerge.

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Cosmological implications of a nonseparable 5D solution of the vacuum Einstein field equations

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An exact class of solutions of the 5D vacuum Einstein field equations (EFEs) is obtained. The metric coefficients are found to be nonseparable functions of time and the extra coordinate l and the induced metric on $l=$const hypersurfaces has the form of a Friedmann–Robertson–Walker cosmology. The 5D manifold and 3D and 4D submanifolds are in general curved, which distinguishes this solution from previous ones in the literature. The singularity structure of the manifold is explored: some models in the class do not exhibit a big bang, while others exhibit a big bang and a big crunch. For the models with an initial singularity, the equation of state of the induced matter evolves from radiation-like at early epochs to Milne-like at late times and the big bang manifests itself as a singular hypersurface in 5D. The projection of comoving 5D null geodesics onto the 4D submanifold is shown to be compatible with standard 4D comoving trajectories, while the expansion of 5D null congruences is shown to be in line with conventional notions of the Hubble expansion. [DOI: 10.1063/1.1407836]

I. INTRODUCTION

The vacuum EFEs for space–time plus an extra dimension are given in terms of the Ricci tensor by $R_{AB}=0$ $(A,B=0-3,4)$. These contain the field equations of general relativity, which in terms of the Einstein tensor and an induced energy-momentum tensor are $G_{\alpha\beta}=8\pi T_{\alpha\beta}$ $(\alpha,\beta=0-3)$. The latter is obtained by a well-known technique.[1] Mathematically it can depend on $g_{4\alpha}$, g_{44} and derivatives of $g_{\alpha\beta}$ with respect to $x^4=l$, while physically it can describe a perfect fluid with density ρ and pressure p. If there is no dependency on l, the equation of state is that of radiation or ultrarelativistic particles, $p=\rho/3$.[2] If there is dependency on l, a wide range is available for the equation of state.[3] What are often referred to as the standard 5D cosmological models were found as a class of solutions of $R_{AB}=0$ by Ponce de Leon.[4] These solutions are separable in the time (t), space (r,θ,ϕ) and the extra coordinate (l). On the hypersurfaces $l=$const, which we label Σ_l; they reduce to the standard Friedmann–Robertson–Walker (FRW) models of 4D cosmology with flat space sections $(k=0)$. The class depends on one dimensionless parameter which fixes the scale-factor a for the dynamics and the equation of state for the matter. It includes the $a=t^{2/3}$, $p=0$ Einstein–de Sitter solution for the late universe, and the $a=t^{1/2}$, $p=\rho/3$ radiation solution for the early universe. However, the Ponce de Leon solutions are not unique as the 5D analysis of the standard 4D FRW solutions.

In Sec. II, we obtain a nonseparable solution of the scale factor. Sections III and IV are devoted to cosmological implications, i.e., singularities and geodesics, respectively. Section V is for comments.

II. NONSEPARABLE SOLUTION

A class of solutions which is mathematically different and physically reasonable has a 5D line element given by

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$$dS^2=\sigma\left\{dt^2-a^2\left[\frac{dr^2}{(1-kr^2)}+r^2d\Omega^2\right]\right\}+\epsilon b^2dl^2. \tag{1}$$

Here $k=\pm1,0$ describes the 3D curvature, $d\Omega^2\equiv d\theta^2+\sin^2\theta d\phi^2$ describes the 2D spherical geometry, and $\epsilon=\pm1$ describes the nature of the extra dimension. The functions $\sigma=\sigma(l)$, $a=a(t,l)$, $b=b(t,l)$ are to be fixed by the 5D field equations. We have studied the latter, particularly with regard to the 4D properties of matter. Hereafter we employ $c=G=1$ unit system, that is, $L=M=T$.

A simple class of solutions of $G_{AB}=0$ is obtained if we write $\sigma=\text{const}\equiv\sigma_0$, $\hat{a}\equiv\partial a/\partial l=f(l)b$ (here and henceforth, we use hats to denote $\partial/\partial l$). Then the scale factors for ordinary space–time and the extra dimension are

$$a=\sqrt{-Ft^2+gt+h}, \tag{2}$$

$$b=\frac{-2\epsilon\sigma_0f\hat{f}t^2+\hat{g}t+\hat{h}}{2fa}. \tag{3}$$

Here $F\equiv\epsilon\sigma_0f^2+k$, $g=g(l)$ and $h=h(l)$ are functions, so including $f=f(l)$ we have three such. There exists a relation between these, set by the field equations. It is

$$h=-\frac{g^2+\kappa}{4F}, \tag{4}$$

where κ is a constant with the physical dimensions of (length)^2. In terms of this, the 3D scale factor (2) is given by

$$a^2=-\frac{[(2Ft-g)^2+\kappa]}{4F}. \tag{5}$$

The extra-dimensional scale-factor (3) is given by

$$b=-\frac{[4\epsilon\sigma_0f\hat{f}Ft^2-2\hat{g}F^2t+g\hat{g}F-\epsilon\sigma_0f\hat{f}(g^2+\kappa)]}{4afF^2}. \tag{6}$$

The new solutions have some properties in common with the Ponce de Leon cosmologies[4] and some which are different. The Ponce de Leon solutions only exist for $\epsilon=-1$, but the new ones have $\epsilon=\pm1$ so the extra dimension can be spacelike or timelike. Other (wavelike) solutions are known for $\epsilon=+1$,[5] but the new solutions open the way to testing the signature of the 5D manifold by observations of the 4D properties of matter as given by (8) and (9). The solution (6) is in general somewhat complicated, but we will not be much concerned with it because it is (5) which, via the Friedmann equations, determines the properties of matter. These for perfect fluid mean that Einstein's equations read as usual

$$G_{\alpha\beta}=8\pi T_{\alpha\beta}=8\pi[(\rho+p)u_\alpha u_\beta-pg_{\alpha\beta}]. \tag{7}$$

Here the four-velocities $u^\alpha\equiv dx^\alpha/ds$ are defined in terms of the 4D interval s, which is included in S of (1), and we have $u^\alpha=(1,0,0,0)$. Then the density and pressure are given by

$$\frac{8\pi\rho}{3}=-\frac{\epsilon f^2}{a^2}-\frac{\kappa}{4\sigma_0a^4}, \tag{8}$$

$$8\pi p=\frac{\epsilon f^2}{a^2}-\frac{\kappa}{4\sigma_0a^4}. \tag{9}$$

We recover FRW-like models on Σ_l that contain an exotic type of induced matter, with an equation of state which follows from (8) and (9),

$$p=\frac{\rho}{3}\left[1-\frac{8\epsilon\sigma_0 a^2 f^2}{(4\epsilon\sigma_0 a^2 f^2+\kappa)}\right]. \tag{10}$$

This equation of state is manifestly dependent on time and completes the formal part of our analysis, which a fast computer package[6] has confirmed. The form of these relations suggests a two-fluid model as used in solutions of straight general relativity. The first terms in (8) and (9) by themselves imply $(\rho+3p)=0$, which is the 4D signature of matter with zero gravitational density.[1,7] This kind of matter has been suggested as relevant to cosmic strings, i.e., open strings with subrelativity transverse motions,[8] and K-matter which existence mentions the possibility of a universe dominated by cosmic strings,[9] to zero-point fields required by quantum theory[10,11] and to extreme sources for the Reissner–Nordström metric which require that the material contents of the sphere has no effect on gravitational interactions at its center.[12] The second terms in (8) and (9) by themselves imply $p=\rho/3$, which of course means photon-like matter. These identifications are supported by the behavior of the scale-factor (2) or (5), where the latter may vary as $t^{1/2}$ in the radiation model or as t in the empty (Milne) model. They become exact when in (8) and (9) $f\to 0$, and $\kappa\to 0$, respectively. Or on a given Σ_l hypersurface, we find in (2) that as $t\to\infty$, $a(t,l)\to\infty$—provided that $F<0$—which implies in (10) that $p\to-\rho/3$. This is the equation of state of the Milne, or empty universe where the gravitational density of matter is zero. Hence, it might be understood that the 4D cosmologies on the Σ_l hypersurface are asymptotically empty as $t\to\infty$. However, it should be noted that ρ, p of (8) and (9) refer to the total density and pressure, and that any split is in general arbitrary in the absence of information about the particles which make up the matter. Some of the latter may, in principle, be of nonstandard type, since $g_{44}=\epsilon b^2(t,l)$ describes a 3D homogeneous scalar-field.[1] This can manifest itself in 4D as a time-dependent cosmological "constant," as required to harmonize astrophysical data on the age of the universe.[13,14] A time-dependent scalar field generalizes the constant vacuum of Einstein's theory, whose density and pressure are given in terms of the cosmological constant by $\rho=-p=\Lambda/8\pi$. The positive Λ is concluded by revisiting the Tinsley diagram with the recent determinations of the Hubble constants.[15]

III. SINGULARITIES

The age of the universe is defined in 4D models as the time elapsed since the big bang, but the latter concept has to be treated carefully in 5D models. In solutions of the 5D field equations which are flat in 5D but contain a curved space which is singular in 4D, the big bang has to be identified as a defect of the geometry.[1,4]

To analyze the early behavior of the 4D cosmologies embedded in (1), we need to establish whether or not these models contain big bang singularities. Related to this issue is the nature of the singularity structure of 5D manifold as related to the singularity structure of the 4D submanifolds. It is well known that the 5D Ponce de Leon cosmological metrics contain 4D Σ_l hypersurfaces that precisely mimic standard FRW cosmologies complete with a big bang singularity. However, the 5D manifold is flat $R^A_{BCD}=0$, which suggests that the 4D big bang is merely a consequence of the way in which the Σ_l hypersurfaces are embedded in 5D Minkowski space, or, equivalently, the choice of 5D coordinates. The Ponce de Leon solutions are flat in 3D, curved in 4D and (perhaps surprisingly) flat in 5D.[1,16] That is, the Riemann–Christoffel tensors for 5D and 4D are $R^A_{BCD}=0$ and $R^\alpha_{\beta\gamma\delta}\neq 0$, so a flat manifold smoothly embeds a curved one (locally), like 3D Euclidean space embeds the 2D surface of the Earth. We wish to address the issue of whether or not the present manifold (1) is curved or flat, and whether or not it contains a genuine singularity.

A direct attack on the problem could entail the calculation of the 5D Kretschmann curvature invariant $K\equiv R^{ABCD}R_{ABCD}$ for (1). The divergence of this quantity is usually interpreted as being indicative of a curvature singularity in the manifold.[1,17] However, the calculation of K for (1) is difficult, even by computer. We can make some headway by considering a special case defined by

$$\epsilon=-1,\ \ k=0,\ \ f(l)=1/\sqrt{2\sigma_0},\ \ g(l)=l. \tag{11}$$

In this model we have

$$a(t,l)=\sqrt{\frac{(t+l)^2+\kappa}{2}}. \tag{12}$$

The associated curvature invariant is

$$K=\frac{72\kappa^2}{\sigma_0^2[(t+l)^2+\kappa]^4}. \tag{13}$$

The scale factor $a(t,l)$ goes to zero and the Kretschmann scalar K becomes infinity along the hypersurfaces

$$0=t+l\pm\sqrt{-\kappa}. \tag{14}$$

Clearly, there will be no curvature singularity for $\kappa>0$. Therefore, for at least one specific case, we find that the manifold (1) is curved in 5D and singular where the scale factor $a(t,l)$ vanishes, in sharp contrast with the Ponce de Leon solutions. For the present model, the density and pressure of (8) and (9) will diverge in general as $a\to 0$ along the hypersurfaces of (14).

It is interesting to note that $K=0$ for $\kappa=0$ in the model presented above. Indeed, an analysis of the general metric (1) via computer shows that $R^A_{BCD}=0$ for $\kappa=0$. In this eventuality, the scale factor (2) with (4) becomes

$$a(t,l)=\frac{g(l)t+2h(l)}{2h^{1/2}(l)}, \tag{15}$$

which is linear in time, just like the scale factor for the Milne universe (indeed, the equation of state of the induced matter is $p=-\rho/3$). So the $\kappa=0$ case entails induced matter with zero gravitational density, is curved in 4D and is flat in 5D. However, it bears repeating that when $\kappa\neq 0$, it is possible to have curved 5D solutions.

Now, by analogy with the standard FRW model, it is obvious that the 4D submanifolds on Σ_l will be singular for times $t_*(l)$ such that $a(t_*,l)=0$, an epoch commonly referred as the big bang. Solving $a(t_*,l)=0$ in (5) for t_* gives two solutions:

$$t_*^{\pm}(l)=\frac{g(l)\pm\sqrt{-\kappa}}{2F}. \tag{16}$$

Two things are apparent from this result. First, there can be no 4D big bang if $\kappa>0$. This is in agreement with the special case presented above, where the scale factor can only vanish if $\kappa\leqslant 0$. Second, we see that if $\kappa<0$, there are two separate singularities, or, in other words, two big bangs in $F<0$. These 4D events are located on the two 4D hypersurfaces defined by (16). In the neighborhood of the big bang, $a^2(t_*^{\pm}+\delta t,l)\sim a_*(l)\,\delta t$ where $a_*(l)$ is some function of l at $t=t_*^{\pm}$. The equation of state of the cosmological matter is then

$$p=\frac{\rho}{3}\left[\frac{\kappa-\tilde{a}_*(l)\,\delta t}{\kappa+\tilde{a}_*(l)\,\delta t}\right]=\frac{\rho}{3}-O(\delta t), \tag{17}$$

where $\tilde{a}_*(l)$ is some other function of l. As $\delta t\to 0$, we recover $p=\rho/3$. So, near the big bang(s), the induced matter behaves like radiation while at late times it behaves like the matter in the Milne model.

Finally, we consider the case $F>0$, which is guaranteed for $\epsilon=1$ and $k=0,1$ since we must have $\sigma_0>0$. If we also have $\kappa<0$, it is clear that on Σ_l, $a(t,l)$ is real only between t_*^- and t_*^+. This is a cosmological model with both a big bang and a big crunch, similar to the standard $k=+1$ FRW metrics. There therefore exists a hiearchy of 4D cosmologies on the Σ_l hypersurfaces.

TABLE I. Characteristics of the 5D manifold and the 4D cosmologies embedded on the Σ_l hypersurfaces.

	$F<0$	$F>0$
$\kappa>0$ and $R^A_{BCD}\neq 0$ in general	no big bang	$a(t,l)$ is complex
$\kappa=0$, $R^A_{BCD}=0$	one big bang	$a(t,l)$ is complex
$\kappa<0$ and $R^A_{BCD}\neq 0$ in general	two big bangs	big bang and big crunch

If $\kappa<0$, then the issue of whether each of the cosmologies is forever expanding or destined to end in a big crunch is entirely determined by the value of $f(l)$ on that hypersurface. If $\kappa\geqslant 0$, the quantity inside the radical in the definition of $a(t,l)$ in (5) will be less than or equal to zero for all times, which makes $a(t,l)$ complex and has the effect of switching the signature of the (x^1,x^2,x^3) coordinates from spacelike to timelike (this also happens for $t\notin[t_*^-,t_*^+]$ if $\kappa<0$). Table I summarizes all the cases discussed in this section for both the global 5D geometry and the type of cosmology embedded on the Σ_l hypersurfaces.

IV. GEODESICS

The possibility the test particles move on higher dimensional geodesics has been studied by many authors.[1,18–20] In particular, it has recently been demonstrated that particles that are massless in 5D appear to be massive in 4D.[21] In this section, we examine the 5D null and comoving geodesics of the metric (1) for the $\epsilon=-1$ case and identify the 4D GR limit.

We take $\epsilon=-1$ and define $\Sigma^2\equiv\sigma_0$. Then, the metric (1) may be written as

$$dS^2=[\Sigma dt+b(t,l)dl][\Sigma dt-b(t,l)dl]-\Sigma^2a^2(t,l)ds_3^2, \tag{18}$$

where $\Sigma^2a^2(t,l)ds_3^2$ represents the spatial three-metric, with

$$ds_3^2=\frac{dr^2}{1-kr^2}+r^2d\Omega^2. \tag{19}$$

Now, since the terms in square brackets represent a two-dimensional manifold, which must be conformally flat, it is in principle possible to find a coordinate transformation

$$\eta=\eta(t,l),\quad \xi=\xi(t,l) \tag{20}$$

that will cast the metric in the form

$$dS^2=C(\eta,\xi)d\eta d\xi-\Sigma^2a^2(\eta,\xi)ds_3^2. \tag{21}$$

Then, the null geodesics of the manifold that are spatially comoving ($ds_3^2=0$) are just the $d\eta=0$ or $d\xi=0$ trajectories. However, the transformation (20) is not immediately obvious. Therefore, we must be content with an indirect analysis of the properties of the 5D null-comoving paths.

Consider the vectors

$$k^A\partial_A=\frac{1}{\sqrt{2}\Sigma}\partial_t+\frac{1}{\sqrt{2}b(t,l)}\partial_l, \tag{22}$$

$$N^A\partial_A=\frac{1}{\sqrt{2}\Sigma}\partial_t-\frac{1}{\sqrt{2}b(t,l)}\partial_l. \tag{23}$$

They satisfy

$$k^Ak_A=0,\quad N^AN_A=0,\quad k^AN_A=1. \tag{24}$$

Both k^A and N^A are tangent to null geodesics and can be thought of as the principal and auxiliary vectors of a null congruence. They both share the same parametrization, defined by

$$\frac{dt}{d\lambda} = \frac{1}{\sqrt{2}\Sigma},$$

$$\frac{dl}{d\lambda} = +\frac{1}{\sqrt{2}b(t,l)} \quad (\text{for } k^A),$$

$$= -\frac{1}{\sqrt{2}b(t,l)} \quad (\text{for } N^A). \tag{25}$$

In order to determine if λ is a 5D affine parameter, we calculate

$$k^A \nabla_A k^B = \left[\frac{1}{\sqrt{2}\Sigma}\frac{\partial}{\partial t}\ln b(t,l)\right] k^B, \tag{26}$$

with a similar expression for N^A. ∇_A is the 5D covariant derivative operator. This shows that λ is not a 5D affine parameter. However, it is easy to see that the 4D projections of k^A and N^A onto Σ_l satisfy the 4D geodesic equation for timelike geodesics. Therefore, λ is the 4D proper time $\tau = \Sigma t$ comoving geodesics (up to a constant prefactor). This is an excellent example of how a null path in 5D can appear to be the trajectory of a massive particle in 4D.

We now explore the possibility that galaxies travel along 5D trajectories described by (22) or (23). The tangent space to the null vectors k^A and N^A is necessarily three dimensional and has the metric

$$q_{AB} = g_{AB} - k_A N_B - k_B N_A, \tag{27}$$

which gives

$$q_{AB} dx^A dx^B = -\Sigma^2 a^2(t,l) ds_3^2. \tag{28}$$

It is clear that the tangent space of k^A and N^A is equivalent to the $t = \text{const}$, $l = \text{const}$ three-surface of the 5D manifold. Hence, observers traveling along 5D null-comoving geodesics 4D comoving geodesics (confined to Σ_l) share the same tangent space, which suggests that they will observe the world around them in the same manner. In particular, we can calculate the expansion Θ of a congruence of 5D geodesics with tangent vector k^A. For nonaffinity parametrized geodesics, Θ is given by

$$\Theta = \nabla^A k_A - N_B k^A \nabla_A k^B. \tag{29}$$

Plugging in expression for k^A and N^A, we get

$$\Theta = \frac{3}{a}\left(\frac{1}{\sqrt{2}\Sigma}\frac{\partial a}{\partial t} + \frac{1}{\sqrt{2}b(t,l)}\frac{\partial a}{\partial l}\right) = \frac{3}{a}\frac{da}{d\lambda}. \tag{30}$$

Since the expansion scalar represents the fractional rate of change in the three-volume δV of the congruence, i.e., $\Theta = (\delta V)^{-1} d(\delta V)/d\lambda$, we see that $\delta V \sim a^3(\lambda)$ as expected. That is, an observer in a galaxy traveling along a 5D null-comoving geodesic will see the other galaxies receding away in a Hubble-like expansion with scale factor $a(\lambda)$ (recall that $\lambda = \sqrt{2}\tau$).

We are now in a position to identify the 4D limit of the theory. The geodesic paths described by k^A and N^A would be identical to 4D geodesics if $dl = 0$, that is, they are confined to Σ_l hypersurfaces. This will be true if $|dl/d\tau| = b^{-1}(t,l) \ll 1$, which can be physically interpreted as

demanding that large changes in the 4D proper time τ be accompanied by small changes in the extra coordinate l. This can be accomplished in the $\epsilon=-1$ case by choosing $f(l)$ and σ_0 such that $|f(l)|\ll 1$ and $[f^2(l)\sigma_0-k]>0$, which ensures that $a(t,l)$ is real as $t\to\infty$. In terms of the toy model (11), we recover the 4D limit for $\Sigma\to\infty$.

V. COMMENTS

The new nonseparable solution (2) gives a physical meaning of the coefficients K_1 and K_2 which appear in the solution of the scale factor.[22] That is, these constants and the coefficient of t^2 as well are originated in $f(l),g(l)$ and $h(l)$ on the hypersurface Σ_l. This helps us to consider the special case (11).

The physical big bang in 4D is a hypersurface in 5D. This kind of behavior has been observed in other 5D solutions, e.g., in a ''wavelike'' class of exact cosmological solutions which look like waves propagating in the fifth dimension.[23] For the example just considered, the 4D big bang is akin to a 5D shock wave.[24] It is different to what happens in the Ponce de Leon cosmologies,[4] because of the nonseparable nature of the solutions. In general, 5D cosmologies where the 4D big bang is a geometrical effect have major implications for the early universe, notably in regard to particle masses during the inflationary epoch[25] and the thermalization of photons by the particle mass varying quadratically with the time during the subsequent radiation epoch.[26] The 5D cosmologies imply the variability of the masses of all particles.[1] The precise nature of the transformation (20) for general choices of $f(l),g(l)$ and $h(l)$ will naturally give us closed form solutions for the comoving null geodesic equation and enable us to study those cosmological phenomena in the early universe. These studies and a study of timelike 5D geodesics ($\epsilon=1$) are left for future work.

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Batalin–Tyutin quantization of the spinning particle model

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The spinning particle model for anyon is analyzed in the Batalin–Tyutin scheme of quantization in extended phase space. Here additional degrees of freedom are introduced in the phase space such that all the constraints in the theory are rendered first class, that is, commuting in the sense of Poisson brackets. Thus the theory can be studied without introducing the Dirac brackets which appear in the presence of noncommuting or second class constraints. In the present case the Dirac brackets make the configuration space of the anyon noncanonical and also, being dynamical variable dependent, poses problems for the quantization program. We show that previously obtained results (e.g., gyromagnetic ratio of anyon being 2) are recovered in the Batalin–Tyutin variable independent sector in the extended space. The Batalin–Tyutin variable contributions are significant and are computable in a straightforward manner. The latter can be understood as manifestations of the noncommutative space–time in the enlarged phase space. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1405847]

I. INTRODUCTION

Theoretical models for anyons,[1] excitations of arbitrary spin and statistics in $2+1$-dimensions, have been proposed from different perspectives, the most popular ones being the point-charge Chern–Simons gauge field interacting theory[2] and the later symplectic models (SMs)[3,4] and the spinning particle models (SPMs).[5,6] The SM and SPM can be related to the anyon field equation proposed in Ref. 7. It has been questioned[8] whether the former interacting theory is a minimal description of the anyon. The latter models are free from complications of this type and both of them agree regarding results [such as rigidity of the angular momentum and the gyromagnetic ratio (g) being equal to 2] for free anyons as well as anyons interacting with Abelian external gauge field, respectively.

However, the SMs or SPMs are also interesting from another point of view. They have a close connection with the noncommutative space–time theories, which have created a lot of interest lately.[9]

In SMs,[4] the symplectic structure has been posited, which gives rise to the noncommutativity in the particle configuration space. On the other hand, in SPMs,[5,6] the above mentioned feature is a result of the constraint structure of the model. The set of second class constraints (SCCs), with noncommuting Poisson brackets (PBs) (in the sense of Dirac classification scheme[10]), induces nontrivial Dirac brackets (DBs) among the coordinate variables. Since we will concentrate on SPMs[6] in the present work, these comments will be elaborated.

Let us now impose a bit of caution on the methodology of evaluation of the g value of anyon in SMs and SPMs. One compares the Hamiltonian (in the former[4]) and equations of motion (in the latter[6]) with the corresponding expressions obtained for a charged particle with spin in background electromagnetic field *in conventional (commuting) configuration space*. The validity of this matching procedure can be questioned on the grounds that the nature of the configuration spaces in the two systems that are being compared are qualitatively different. But more importantly, the quantization procedure runs into trouble due to operator ordering ambiguities in the DBs in SPs and

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SPMs. This complication arises since in theories with nonlinear constraints, the DBs can involve dynamical variables, which is true for the present case. When these DBs are elevated to commutation relations in the process of quantization, the above mentioned feature creates problems.

Finally (as has been pointed out before[5,6]), the induced nonvanishing DB algebra $[A_a(\mathbf{x},t), A_b(\mathbf{y},t)]$ between supposedly ''external'' electromagnetic field variables makes us wonder as to how far the treatment of the gauge fields being nondynamical is justified. The problems related to the noncanonical nature of the coordinate system have also been discussed in Ref. 11.

Now we come to the motivation of the present work. All of the above problems can be naturally addressed in the Batalin–Tyutin (BT) quantization scheme[12] (which is a particular type of the more general quantization method[13]), where additional phase space degrees of freedom (BT variables) are introduced in such a way that existing SCCs are converted into (Abelian) first class constraints (FCCs, see Ref. 10), thereby enhancing the gauge symmetry of the extended system. Thus the problematic DBs can be avoided. One can resort to Dirac quantization of FCC systems by requiring that the physical states obey the FCCs (i.e., $FCC|physical\ state\rangle=0$). Or else one can work in a convenient gauge where the problematic DBs do not appear. Later on we will use the first alternative.

Apart from the above reasons, we will find that by its own right, the problem of BT extension of SPMs has several interesting features, some of them not addressed in the literature. First, the SCC system in SPMs can be expressed[5,6] in a covariant (and neat) form which, however, is reducible, that is, the SCCs, are not independent. The BT formulation has been developed for irreducible or independent set of SCCs only. This forces us to choose an independent set of SCCs, thereby losing manifest covariance. As an unsolved problem, it will be interesting to study the BT extension of a generic reducible SCC system.

Let us put the present work in its proper perspective. We have developed a framework for treating the spinning particle model as an FCC system in a BT-extended phase space where the background space–time is normal (that is, commuting), so that comparison between results obtained for anyons and analogous models in conventional space–time do not pose any ambiguity. (In particular, we will recover the result that for anyons $g=2$, but will indicate the presence of correction terms as well.) Also the canonical quantization program is rigorous since DBs do not appear and so operator ordering problems are absent in the canonical commutation relations.

Lastly we note that the present BT extension is classical in the sense that operator ordering problems in the extended system have not been addressed.[14]

The article is organized as follows: in Sec. II we briefly reproduce the skeleton of BT formalism. This will also help us to fix the notations. We quickly introduce the SPM in Sec. III for completeness. Section IV is devoted to developing the BT extension of SPMs. This constitutes the main body of our work. Section V deals with the quantization procedure and recovering of previous results. In Sec. VI we conclude with a discussion and some future lines of work.

II. BATALIN–TYUTIN FORMULATION

In this section we state the main results of BT prescription[12] to be used. The basic idea behind the scheme is to introduce additional phase space variables (BT variables) ϕ_a^α, besides the existing physical degrees of freedom (q,p), such that *all* the constraints in the extended system are reduced to FCCs. This means that one has to modify the original constraints and Hamiltonian accordingly by putting BT-extension terms in them. The way to achieve this at the classical level has been proved in Ref. 12. Let us consider a set of constraints $(\Theta_\alpha^a, \Psi_l)$ and a Hamiltonian operator H with the following Poisson Bracket (PB) relations,

$$\{\Theta_\alpha^a(q,p),\Theta_\beta^b(q,p)\}\approx\Delta_{\alpha\beta}^{ab}(q,p)\neq 0,\ \{\Theta_\alpha^a(q,p),\Psi_\beta^l(q,p)\}\approx 0,$$
$$\{\Psi_l(q,p),\Psi_n(q,p)\}\approx 0,\ \{\Psi_l(q,p),H(q,p)\}\approx 0. \tag{1}$$

In the above (q,p) are referred to as physical variables and "$\approx$" means that the equality holds on the constraint surface and $\{p_a,x_b\}=g_{ab}$; $g_{ab}=\mathrm{diag}(1,-1,-1)$. Clearly Θ^a_α and Ψ_l are SCC and FCC,[10] respectively. The latter are responsible for gauge invariance and the former can be used as operator identities provided one uses the DBs[10] as defined:

$$\{A(q,p),B(q,p)\}_{\mathrm{DB}}=\{A,B\}-\{A,\Theta^a_\alpha\}\Delta^{\alpha\beta}_{ab}\{\Theta^b_\beta,B\},\quad \Delta^{ab}_{\alpha\beta}\Delta^{\beta\gamma}_{bc}=\delta^a_c\delta^\alpha_\gamma. \tag{2}$$

However, in systems with nonlinear SCCs, in general the DBs can become dynamical variable dependent[5,6,15] due to the $\{A,\Theta^a_\alpha\}$ and $\Delta^{\alpha\beta}_{ab}$ terms, leading to problems for the quantization program. To cure this type of pathology, BT formalism is a systematic framework where one introduces the BT variables ϕ^α_a, obeying

$$\{\phi^\alpha_a,\phi^\beta_b\}=\omega^{\alpha\beta}_{ab}=-\omega^{\beta\alpha}_{ba}, \tag{3}$$

where $\omega^{\alpha\beta}_{ab}$ is a constant (or at most a c-number funtion) matrix, with the aim of modifying the SCC $\Theta^a_\alpha(q,p)$ to $\tilde{\Theta}^a_\alpha(q,p,\phi^\alpha_a)$ such that

$$\{\tilde{\Theta}^a_\alpha(q,p,\phi),\tilde{\Theta}^b_\beta(q,p,\phi)\}=0,\ \ \tilde{\Theta}^a_\alpha(q,p,\phi)=\Theta^a_\alpha(q,p)+\Sigma^\infty_{n=1}\tilde{\Theta}^{a(n)}_\alpha(q,p,\phi),\ \ \tilde{\Theta}^{a(n)}\approx O(\phi^n). \tag{4}$$

The explicit terms in the above expansion are[12]

$$\tilde{\Theta}^{a(1)}_\alpha=X^{ab}_{\alpha\beta}\phi^\beta_b,\quad \Delta^{ab}_{\alpha\beta}+X^{ac}_{\alpha\gamma}\omega^{\gamma\delta}_{cd}X^{bd}_{\beta\delta}=0, \tag{5}$$

$$\tilde{\Theta}^{a(n+1)}_\alpha=-\frac{1}{n+2}\phi^\delta_d\omega^{dc}_{\delta\gamma}X^{\gamma\beta}_{cb}B^{ba(n)}_{\beta\alpha},\quad n\geqslant 1, \tag{6}$$

$$B^{ba(1)}_{\beta\alpha}=\{\tilde{\theta}^{b(0)}_\beta,\tilde{\theta}^{a(1)}_\alpha\}_{(q,p)}-\{\tilde{\theta}^{a(0)}_\alpha,\tilde{\theta}^{b(1)}_\beta\}_{(q,p)}, \tag{7}$$

$$B^{ba(n)}_{\beta\alpha}=\Sigma^n_{m=0}\{\tilde{\theta}^{b(n-m)}_\beta,\tilde{\theta}^{a(m)}_\alpha\}_{(q,p)}+\Sigma^n_{m=0}\{\tilde{\theta}^{b(n-m)}_\beta,\tilde{\theta}^{a(m+2)}_\alpha\}_{(\phi)},\quad n\geqslant 2. \tag{8}$$

In the above, we have defined

$$X^{ab}_{\alpha\beta}X^{\beta\gamma}_{bc}=\omega^{ab}_{\alpha\beta}\omega^{\beta\gamma}_{bc}=\delta^\gamma_\alpha\delta^a_c. \tag{9}$$

A very useful idea is to introduce the improved variable $\tilde{f}(q,p)$ (Ref. 12) corresponding to each $f(q,p)$,

$$\tilde{f}(q,p,\phi)\equiv f(\tilde{q},\tilde{p})=f(q,p)+\Sigma^\infty_{n=1}\tilde{f}(q,p,\phi)^{(n)},\ \ \tilde{f}^{(1)}=-\phi^\beta_c\omega^{cb}_{\beta\gamma}X^{\gamma\delta}_{bd}\{\theta^a_\delta,f\}_{(q,p)}, \tag{10}$$

$$\tilde{f}^{(n+1)}=-\frac{1}{n+1}\phi^\beta_c\omega^{cb}_{\beta\gamma}X^{\gamma\delta}_{bd}G(f)^{d(n)}_\delta,\quad n\geqslant 1, \tag{11}$$

$$G(f)^{b(n)}_\beta=\Sigma^n_{m=0}\{\tilde{\theta}^{b(n-m)}_\beta,\tilde{f}^{(m)}\}_{(q,p)}+\Sigma^{(n-2)}_{m=0}\{\tilde{\theta}^{b(n-m)}_\beta,\tilde{f}^{(m+2)}\}_{(\phi)}+\{\tilde{\theta}^{b(n+1)}_\beta,\tilde{f}^{(1)}\}_{(\phi)}, \tag{12}$$

which have the property $\{\tilde{\Theta}^a_\alpha(q,p,\phi),\tilde{f}(q,p,\phi)\}=0$. It can be proved that extensions of the original FCC Ψ_l and Hamiltonian H are simply

$$\tilde{\Psi}_l=\Psi(\tilde{q},\tilde{p}),\ \ \tilde{H}=H(\tilde{q},\tilde{p}). \tag{13}$$

One can also reexpress the converted SCCs as $\tilde{\Theta}^a_\alpha\equiv\Theta^a_\alpha(\tilde{q},\tilde{p})$. The following identification theorem,

$$\{\tilde{A},\tilde{B}\}=\{\widetilde{A,B}\}_{\mathrm{DB}},\ \ \{\tilde{A},\tilde{B}\}|_{\phi=0}=\{A,B\}_{\mathrm{DB}},\ \ \tilde{0}=0, \tag{14}$$

will play a crucial role in our later application. Hence the outcome of the BT extension is the closed system of FCCs with the FC Hamiltonian given by

$$\{\tilde{\Theta}^a_\alpha,\tilde{\Theta}^b_\beta\}=\{\tilde{\Theta}^a_\alpha,\tilde{\Psi}_l\}=\{\tilde{\Theta}^a_\alpha,H\}=0,\ \ \{\tilde{\Psi}_l,\tilde{\Psi}_n\}\approx 0,\ \ \{\tilde{\Psi}_l,H\}\approx 0. \tag{15}$$

We will see that due to the nonlinearity in the SCCs, the extensions in the improved variables (and subsequently in the FCCs and FC Hamiltonian) turn out to be infinite series. This type of situation has been encountered before.[15]

III. SPINNING PARTICLE MODEL REVISITED

The SPM proposed by us[6] where an anyon interacts with a $U(1)$ gauge field in $2+1$-dimensions is given by the Lagrangian

$$L=\left(m^2U^aU_a+\frac{j^2}{2}\sigma^{ab}\sigma_{ab}+mj\epsilon^{abc}U_a\sigma_{bc}\right)^{1/2}+eU_aA^a, \tag{16}$$

where

$$U^a=\frac{dx^a}{d\tau},\ \ \sigma^{ab}=\frac{1}{2}\epsilon^{abc}\sigma_c=\Lambda^a_c\frac{d\Lambda^{cb}}{d\tau},\ \ \Lambda^a_c\Lambda^{cb}=\Lambda^a_c\Lambda^{bc}=g^{ab}.$$

Here (x^a,Λ^{ab}) is a Poincaré group element and also a set of dynamical variables of the theory. The canonical momenta are defined in the following way:[5,6]

$$p^a=-\frac{\partial L}{\partial U_a}\equiv\pi^a-eA^a,\ \ S^{ab}=-\frac{\partial L}{\partial\sigma_{ab}}\equiv\frac{1}{2}\epsilon^{abc}S_c. \tag{17}$$

The phase space algebra is

$$\{x_a,x_b\}=0,\ \ \{p_a,x_b\}=g_{ab},\ \ \{\pi_a,\pi_b\}=eF_{ab}=e(\partial_aA_b-\partial_bA_a), \tag{18}$$

$$\{S^a,S^b\}=\epsilon^{abc}S_c,\ \ \{S^a,\Lambda^{0b}\}=\epsilon^{abc}\Lambda^0{}_c,\ \ \{\Lambda^{0a},\Lambda^{0b}\}=0. \tag{19}$$

In the free theory, one encounters the following set of FCC and SCC, respectively:

$$\Psi_1\equiv\pi_a\pi^a-m^2\approx 0,\ \ \Psi_2\equiv\pi.S-\frac{mj}{2}\approx 0,$$

$$\Theta^a_1\equiv\Lambda^{0a}-\frac{p^a}{m}\approx 0,\ \ \theta^a_2\equiv S^{ab}p_b=\epsilon^{abc}p_bS_c\approx 0.$$

In the free theory, Ψ_1 and Ψ_2 are respectively the mass-shell condition and the Pauli–Lubanski relation.

In the interacting theory, one obtains to $O(e)$ the following set of FCCs and SCCs:

$$\Psi_1\equiv\pi_a\pi^a-m^2+\frac{2eF_{ab}\pi^a}{\pi^2}\Theta^b_2\approx 0,\ \ \Psi_2\equiv\pi.S-\frac{mj}{2}+\frac{ejF_{ab}\pi^a}{2m\pi^2}\Theta^b_2\approx 0, \tag{20}$$

$$\Theta^a_1\equiv\Lambda^{0a}-\frac{\pi^a}{m}\approx 0,\ \ \theta^a_2\equiv S^{ab}\pi_b=\epsilon^{abc}\pi_bS_c\approx 0. \tag{21}$$

Actually one can check that $S^aS_a=j^2/4$, but this is not independent of Ψ_l given above (20). To verify the constraint algebra after computing the PBs, one has to invoke the relation $S^a=(j/2m)\,\pi^a$, which is consistent with the SCC Θ_2^a and the normalization agrees with the free theory. The above relation is valid also at the level of DBs.[6]

Note that in the above set of SCCs, Θ_1^a has been imposed from outside such that the angular coordinates are properly restricted. It is easy to ascertain that the SCCs Θ_α^a form a reducible set, since

$$\pi^a\Theta_{1a}=-\tfrac{1}{2}m\Theta^{1a}\Theta_{1a},\quad \pi^a\Theta_{2a}=0.$$

(With $e=0$, these features are true for the free theory stated earlier.) However, one works with this reducible set because the manifestly covariant structure simplifies calculations and one can invert[5,6] the SCC algebra matrix perturbativly to get the DBs. To $O(e)$ we obtain the DB between two generic field as[6]

$$\{A,B\}_{\mathrm{DB}}=\{A,B\}+\frac{eF_{ab}}{m^2}\{A,\Theta_2^a\}\{\Theta_2^b,B\}-\frac{1}{2}\epsilon^{abc}S_c\{A,\Theta_{1a}\}\{\Theta_{1b},B\}$$

$$+\frac{1}{2m}\{A,\Theta_2^a\}\{\Theta_{1a},B\}-\frac{1}{2m}\{A,\Theta_1^a\}\{\Theta_{2a},B\}. \tag{22}$$

In particular, the following DB,

$$\{x^a,x^b\}_{\mathrm{DB}}=-\frac{1}{2m^2}\epsilon^{abc}S_c+O(e), \tag{23}$$

gives rise to the noncommutative space–time, which in turn generates the arbitrary spin contribution in the angular momentum. Note that the algebra (23) is nontrivial in the free theory as well. Fixing the gauge condition $x_0=\tau$ as the proper time and using Ψ_1 one ends up with the Hamiltonian,

$$H=(m^2-\pi^i\pi_i)^{1/2}-eA_0, \tag{24}$$

where the Θ_2^a dependent term has been dropped since we used DBs.[6,5] To $O(e)$ the $2+1$-dimensional analog of the $3+1$-dimensional Bargmann–Michel–Telegdi equation[16] is

$$\dot{S}^a=\{H,S^a\}_{\mathrm{DB}}=\frac{e}{m}F^{ab}S_b. \tag{25}$$

Comparison with the original equation[16] reveals that $g=2$ for the particle.

As we have mentioned before, the comparison has been carried out between the present system in noncommutative configuration space and the original Bargmann–Michel–Telegdi equation in normal coordinate system.

The connection between our result and that of the SM[4] is very direct but subtle. Remember that in SMs,[4] a modified expression [with an $O(eF)$ term] for the ''mass-shell'' condition is used. [In our analysis, an analogous Θ_2^a-dependent term in (24) was ''strongly'' put to zero since it was proportional to the SCCs and we use DBs.] The analysis in the SM is for the FCC system, according to Dirac, where one demands that the FCCs annihilate the physical states. (In our BT extended theory, we will also follow this route.) Now in Ref. 4, one solves perturbatively, for small e, the noncanonical symplectic algebra (which is equivalent to our DBs), in terms of a set of canonical phase space variables, and rewrites the Hamiltonian in terms of these *new* variables and finally compares this expression with the Hamiltonian of a charged particle in ordinary

space–time. Again the $g=2$ result[4] is reproduced. Obviously this derivation[4] also suffers from the same conceptual drawback as the previous one.[6] With this background, we now move on to the BT extension of the SPM.

IV. BATALIN–TYUTIN EXTENSION OF THE SPINNING PARTICLE MODEL

This section comprises of the main body of our work where we introduce the BT machinery[12] in order to take into account the SCCs of the theory but at the same time avoid using a noncanonical coordinate. As mentioned before, we now use a smaller set of SCCs which are irreducible. Also note that in the extended space the constraints will be modified and we can no longer use the original constraints to simplfy the SCC algebra. Choosing Θ^i_α as the irreducible set of SCCs, the PB algebra is

$$\{\Theta^i_\alpha,\Theta^j_\beta\}=\Delta^{ij}_{\alpha\beta}, \tag{26}$$

$$\Delta^{ij}_{11}=\frac{eF^{ij}}{m^2}, \tag{27}$$

$$\Delta^{ij}_{12}=-\left[(\pi.\Lambda)g^{ij}-\pi^i\Lambda^{0j}+\frac{e}{m}\epsilon^{jbc}F^i{}_bS_c\right]=-\Delta^{ji}_{21},\quad \pi.\Lambda=\pi_a\Lambda^{0a}, \tag{28}$$

$$\Delta^{ij}_{22}=[\pi_0(\pi.S)\epsilon^{ij}+e(F^{ij}S^2+S_bF^{bi}S^j+S^iF^{jb}S_b],\quad S^2=S_aS^a. \tag{29}$$

Next, following (5), we need to compute $X^{ij}_{\alpha\beta}$ as the whole calculational scheme rests on this quantity and its inverse. This we do perturbatively by first considering the free theory (i.e., $e=0$), where

$$\Theta^i_1\equiv\Lambda^{0i}-\frac{p^i}{m},\quad \Theta^i_2\equiv\epsilon^{ibc}p_bS_c, \tag{30}$$

$$\{\Theta^i_\alpha,\Theta^j_\beta\}=\Delta^{ij}_{\alpha\beta}=\begin{pmatrix}0 & -((p.\Lambda)g^{ij}-p^i\Lambda^{0j})\\ ((p.\Lambda)g^{ij}-p^j\Lambda^{0i}) & p_0(p.S)\epsilon^{ij}\end{pmatrix}. \tag{31}$$

For the free theory we propose

$$X^{ij}_{\alpha\beta}|_{e=0}\equiv x^{ij}_{\alpha\beta}=\begin{pmatrix}0 & -((p.\Lambda)g^{ij}-p^i\Lambda^{0j})\\ g^{ij} & \frac{1}{2}p_0(p.S)\epsilon^{ij}\end{pmatrix}. \tag{32}$$

One can check that $x^{ij}_{\alpha\beta}$ satisfies (5) for the free theory, provided we choose $\omega^{\alpha\beta}_{ab}=\epsilon^{\alpha\beta}g_{ab}$, $\epsilon^{12}=1$. Since there is some arbitrariness involved in $x^{ij}_{\alpha\beta}$ and $\omega^{\alpha\beta}_{ab}$, their choices are dictated by convenience. The inverse is defined

$$\begin{gathered}x^{\alpha\beta}_{ij}x^{jk}_{\beta\gamma}=\delta^\alpha_\gamma g^i_k,\\ x^{\gamma\delta}_{jk}=\begin{pmatrix}\frac{p_0(p.S)}{2(p.\Lambda)}\left(\epsilon_{jk}-\frac{\epsilon_{jl}p_l\Lambda_{0k}}{p_0\Lambda_{00}}\right) & g_{jk}\\ -\frac{1}{(p.\Lambda)}\left(g_{jk}+\frac{p_j\Lambda_{0k}}{p_0\Lambda_{00}}\right) & 0\end{pmatrix}.\end{gathered} \tag{33}$$

This is an exact result. Now, for the interacting theory, we find to $O(e)$,

$$X^{ij}_{\alpha\beta}=x^{ij}_{\alpha\beta}(p_a\to\pi_a)+ey^{ij}_{\alpha\beta}, \tag{34}$$

$$y_{11}^{ij}=\frac{F^{il}\Lambda_{0l}p^j}{m^2p_0\Lambda_{00}(p^k\Lambda_{0k})};\quad y_{22}^{ij}=\frac{1}{2}\,(S_0)^2F^{ij}, \tag{35}$$

$$y_{21}^{ij}=\frac{S_0\epsilon^{rl}F^{0r}S^l}{p_0(p.S)}g^{ij}, \tag{36}$$

$$y_{12}^{ij}=-\frac{1}{m}\,F^i{}_b\epsilon^{jbc}S_c+\frac{F^{il}\Lambda_{0l}p_k\epsilon^{jk}p_0(p.S)}{2m^2p_0\Lambda_{00}(p^k\Lambda_{0k}}+\frac{S_0\epsilon^{rl}F^{0r}S^l}{p_0(p.S)}\,((p.\Lambda)g^{ij}-p^i\Lambda^{0j}). \tag{37}$$

The inverse, to $O(e)$, is of the form

$$X_{ij}^{\alpha\beta}=x_{ij}^{\alpha\beta}(p_a\to\pi_a)-ex_{ik}^{\alpha\mu}(p)y_{\mu\nu}^{kl}(p)x_{lj}^{\nu\beta}(p). \tag{38}$$

In the present work the explicit form of $X_{ij}^{\alpha\beta}$ will not be utilized. From the relation

$$\tilde{\Theta}_\alpha^{i(1)}=X_{\alpha\beta}^{ij}\phi_j^\beta, \tag{39}$$

the explicit expressions for $\tilde{\Theta}_\alpha^{i(1)}$ (i.e., one BT variable extension term) are

$$\tilde{\Theta}_1^{i(1)}=-(g^{ik}(\pi.\Lambda)-\pi^i\Lambda^{0k})\phi_k^2+e(y_{12}^{ik}\phi_k^2+y_{11}^{ik}\phi_k^1), \tag{40}$$

$$\tilde{\Theta}_2^{i(1)}=\tfrac{1}{2}\,\pi_0(\pi.S)\epsilon^{ik}\phi_k^2+\phi^{1i}+e(y_{21}^{ik}\phi_k^1+y_{22}^{ik}\phi_k^2). \tag{41}$$

We emphasize that the series for $\tilde{\Theta}_1^i$ and $\tilde{\theta}_2^i$ do not terminate and the higher order terms in ϕ_i^α can be derived by a straightforward but extremely tedious calculation. However, to check whether our target of converting SCCs to FCCs has really been achieved (to $O(e)$), one can convince oneself that

$$\{(\Theta_\alpha^i+\tilde{\Theta}_\alpha^{i(1)}),(\Theta_\beta^j+\tilde{\Theta}_\beta^{j(1)})\}=0+O(\phi).$$

To check the cancellation of $O(\phi)$ terms, $\Theta_\alpha^{i(2)}$ terms are required.

Now we move on to the *one BT extension* of the physical degrees of freedom, i.e., the improved variables. The BT extensions of the BT variables themselves will vanish. Let us start by constructing the extensions for π^a. From the generic expression given in (10), we have

$$\begin{aligned}\tilde{\pi}^{a(1)}&=-\phi_c^\beta\omega_{\beta\gamma}^{cb}X_{bd}^{\gamma\delta}\{\Theta_\delta^d,\pi^a\}_{(q,p)}\\&=\frac{e}{m}\,(\phi^{2j}x_{ji}^{11}-\phi^{1j}x_{ji}^{21})F^{ia}-e\phi_i^2\epsilon^{ide}S_eF_d{}^a\\&=\frac{e}{m}\,F^{ia}\left[\left(\phi^{2j}\,\frac{p_0(p.S)}{2(p.\Lambda)}\left(\epsilon_{ji}-\frac{\epsilon_{jl}p_l\Lambda^0{}_i}{p_0\Lambda_{00}}\right)+\phi^{ij}\,\frac{1}{(p.\Lambda)}\left(g_{ij}+\frac{p_j\Lambda_{0i}}{p_0\Lambda_{00}}\right)\right)\right]-e\phi_i^2\epsilon^{ide}S_eF_d{}^a\,.\end{aligned} \tag{42}$$

In a straightforward manner, one can compute the rest of the improved variables, from the structures given here:

$$\tilde{x}^{a(1)}=-\phi_c^\beta\omega_{\beta\gamma}^{cb}X_{bd}^{\gamma\delta}\{\Theta_\delta^d,x^a\}_{(q,p)}=\frac{g^{ai}}{m}\,(\phi^{2j}x_{ji}^{11}-\phi^{1j}x_{ji}^{21})+\epsilon^{aic}S_c(\phi^{2j}X_{ji}^{12}-\phi^{1j}X_{ji}^{22}), \tag{43}$$

$$\begin{aligned}\tilde{S}^{a(1)}&=-\phi_c^\beta\omega_{\beta\gamma}^{cb}X_{bd}^{\gamma\delta}\{\Theta_\delta^d,S^a\}_{(q,p)}\\&=\epsilon^{aic}\Lambda_{0c}(-\phi^{1j}X_{ji}^{21}+\phi^{2j}X_{ji}^{11})-(g^{ai}(\pi.S)-S^i\pi^a)(\phi^{2j}X_{ji}^{12}-\phi^{1j}X_{ji}^{22}),\end{aligned} \tag{44}$$

$$\tilde{\Lambda}^{0a(1)} = -\phi_c^\beta \omega_{\beta\gamma}^{cb} X_{bd}^{\gamma\delta} \{\Theta_\delta^d, \Lambda^{0a}\}_{(q,p)} = (g^{ai}(\pi.\Lambda) - \Lambda^{0i}\pi^a)(\phi^{1j} X_{ji}^{22} - \phi^{2j} X_{ji}^{12}). \tag{45}$$

These improved variables also comprise of infinite sequences of higher order ϕ_i^α terms. As a nontrivial consistency check, we have tested the validity of the assertion that, to $O(\phi)$, $\tilde{\Theta}_\alpha^a \equiv \Theta_\alpha^a(\tilde{q},\tilde{p})$ holds. To examine the *two*-ϕ-term, $O(\phi^2)$-terms in $\tilde{\Theta}_\alpha^i$ and $\tilde{f}(q,p)$ are required. In the next section we will make use of these results to redetermine the g-value for the anyon in the extended phase space. However, as we have stressed before, the main achievement is that a consistent framework has been provided wherein quantization of the SPM is unambiguous and derivation of the previous results are more transparent.

V. APPLICATION—*g* IN EXTENDED SPACE

Let us start by recovering the ''mass shell'' condition $\tilde{\Psi}_1$ in BT extended space, which is simply given by

$$\tilde{\Psi}_1 \equiv \tilde{\pi}_a \tilde{\pi}^a - m^2 + \frac{2e\tilde{F}_{ab}\tilde{\pi}^a}{\tilde{\pi}^2}\tilde{\Theta}_2^b \approx 0. \tag{46}$$

Remembering that *all* the improved variables are of the form

$$\tilde{\mathcal{A}}(q,p,\phi) = \mathcal{A}(q,p) + O(\phi) + \ldots, \quad \tilde{F} = F(\tilde{x}) = F(x) + (\partial F)\phi + \ldots,$$

and neglecting ∂F terms, it is clear that ϕ-independent *polynomial* expressions of relevant operators will remain intact and, so, up to non-ϕ terms, the previous relations survive. Hence proceeding in the same way as before, in the extended space, one can compare the Schrödinger equation to derive $g = 2 + O(\phi)$ for anyons. However, more work is to be done to ascertain whether the ϕ-terms can contribute to g even in the nonrelativistic limit $p_0 \approx m \gg |\mathbf{p}|$ used in Ref. 4. Notice that the Pauli–Lubanski relation is modified to

$$\tilde{\Psi}_2 \equiv \tilde{\pi}.\tilde{S} - \frac{mj}{2} + \frac{ej\tilde{F}_{ab}\tilde{\pi}^a}{2m\tilde{\pi}^2}\tilde{\Theta}_2^b \approx 0.$$

This discussion corresponds to the SM model.[4]

Returning to our SPM model,[6] we follow the discussion in Sec. III and introduce the gauge fixing condition for $\tilde{\Psi}_1$ to be $\tilde{x}_0 - \tau = 0$ and obtain the Hamiltonian as

$$\tilde{H} = (m^2 - \tilde{\pi}^i\tilde{\pi}_i + \tilde{\Theta}_2^a - \text{term})^{1/2} - e\tilde{A}_0. \tag{47}$$

We immediately notice that the Hamiltonian in extended space is not a rational function of the phase space variables and also that the Θ_2^a term cannot be dropped. But the theorem in (14) comes to the rescue. The Θ_2^a can contribute to the equations of motion of the generic form $\dot{\tilde{\mathcal{A}}} = \{\tilde{H}, \tilde{\mathcal{A}}\}$ by terms proportional to $\tilde{\Theta}_2^a$ only since PBs in extended space with $\tilde{\Theta}_\alpha^i$ vanish. So long as we are concerned with computing PBs, the theorem (14) can be applied without going to the details of the explicit structure of the respective operators in the PB. Hence utilizing (14), we can simply transform the BMT equation of motion for the spin variable,[6] in terms of the improved variables, and get

$$\dot{\tilde{S}}^a = \frac{e}{m}\tilde{F}^{ab}\tilde{S}_b \approx \frac{e}{m}F^{ab}\tilde{S}_b. \tag{48}$$

This is our cherished Bargmann–Michel–Telegdi equation for anyon in BT-extended space. Obviously in the the BT-extended space, the expression for g is modified to $g = 2 + O(\phi)$ for anyons, with the additional terms coming from the BT-variable dependent terms.

To facilitate a comparison with the results obtained in the physical variable sector (without introducing BT variables), we can rewrite the improved variables by their physical counterpart and the BT extension terms. Since the phase space PB algebra (18), (19), and (3) is trivially known, we can compute $\dot{S}^a$ from (51) in a straightforward way. Obviously it will be of the form

$$\dot{\tilde{S}}^a \approx \frac{e}{m} F^{ab} \tilde{S}_b + O(\phi). \tag{49}$$

In a restricted way, we can eliminate the BT variables in terms of the physical variables if we adopt the Dirac quantization prescription for systems with FCCs only, where the physical sector of Hilbert space is required to satisfy $FCC\ |physical\ state\rangle = 0$.[17] In the present case, this reduces to

$$\tilde{\Theta}^i_\alpha |ph.\ \ st.\rangle = \tilde{\Psi}_l |ph.\ \ st.\rangle = 0. \tag{50}$$

Since we are interested in substituting the BT variables in the expression of the Hamiltonian in (47), we can solve the constraints for $e=0$ as the terms involving BT variables are already of $O(e)$. This leads to the set of equations

$$\begin{aligned} \tilde{\Theta}^i_1|_{e=0} &= \Theta^i_1|_{e=0} - (g^{ij}(p.\Lambda) - p^i \Lambda^{oj})\phi^2_j = 0, \\ \tilde{\Theta}^i_2|_{e=0} &= \Theta^i_2|_{e=0} + \phi^{1i} + \tfrac{1}{2} m^2 S_0 \epsilon^{ik} \phi^2_k = 0. \end{aligned} \tag{51}$$

From the solutions of the above equations, we find

$$\begin{aligned} \phi^{1i} &= -\Theta^i_2 - \tfrac{1}{2} m^2 S_0 \epsilon^{ij} \phi^2_j, \\ \phi^{2i} &= \frac{\Theta_{1j}}{(p.\Lambda)} \left(g^{ij} + \frac{p^i \Lambda^{0j}}{p_0 \Lambda_{00}} \right). \end{aligned} \tag{52}$$

Notice that the BT variables in this restricted derivation, being proportional to Θ^i_α, are nonvanishing even in the free theory since in the extended sector Θ^i_α are no longer the constraints. It should be emphasized that this is not the whole story since $\tilde{\Theta}^i_\alpha$ consists of an infinite number of terms. Also there are indications that higher order terms will survive even if, on top of our small e restriction, we incorporate the nonrelativistic limit (that is, $p_0 \approx m \gg |\mathbf{p}|$, as has been done in Ref. 4). On the other hand, putting these expressions in the BMT equation shows the leading term in $g=2$ survives but there can be nontrivial velocity dependent corrections. Putting the BT variables back in (49) we get the BMT equation completely in the physical sector.

VI. CONCLUSION

To conclude, in the present work we have formulated an extension of the spinning particle model for anyon[6] along the lines of Batalin–Tyutin quantization scheme.[12] The reason behind working in the extended phase space lies in the presence of nonlinear second class constraints in the model, which induce a noncanonical structure in the particle coordinate. Specifically, the position coordinates become noncommuting, which creates a problem for the quantization programs. Also this makes the comparison between results obtained here and in conventional space–time models difficult. The gyromagnetic ratio of anyon was obtained to be 2[4,6] by invoking precisely this type of matching.

To avoid this type of nontrivial structure in the space–time, the Batalin–Tyutin formalism[12] is adopted where extra BT variables are introduced in the phase space in such a way that all the constraints become first class in the extended space and the problematic Dirac brackets can be avoided. Hence the commuting space–time structure is kept intact. However, the price to pay is that the extensions of the constraints and relevant variables turn out to be infinite series (even to

lowest order in e, the electromagnetic coupling), with higher powers of BT variables. One has to be very careful in taking the nonrelativistic limit[4] and *a prior* it is difficult to determine whether the series will terminate or not.

In the present work we have computed explicitly the one-ϕ extensions of *all* the constraints and degrees of freedom. From the nature of the extensions, it is clear the BT-variable independent relations remain the same as the original ones. Hence one might say that the BT terms are effects of the noncommuting space–time algebra. However, we note that these results are partial in the sense that higher BT-variable terms may also contribute to this order of accuracy. One of our immediate goals in this area is to compute explicitly effect of the BT-variable terms in observable quantities, e.g., g.

From another point of view, this work is significant since it may provide a mapping between theories in *noncommuting* space–time on one hand, and theories in conventional configuration space with extra *spin* degrees of freedom. Subsequently, Batalin–Tyutin extension can be introduced and one can check if results of simple noncommutative models[9] are reproduced.

Another interesting problem of the formal kind is to develop the Batalin–Tyutin scheme for reducible second class constraint systems, such as the spinning particle model in manifestly covariant form. One has to be careful in introducing the BT variables since reducibility in the system will be reflected in the number of these degrees of freedom.

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Sequential quantum measurements

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A quantum effect is an operator A on a complex Hilbert space H that satisfies $0 \leqslant A \leqslant I$. We denote the set of quantum effects by $\mathcal{E}(H)$. The set of self-adjoint projection operators on H corresponds to sharp effects and is denoted by $\mathcal{P}(H)$. We define the sequential product of $A,B \in \mathcal{E}(H)$ by $A \circ B = A^{1/2}BA^{1/2}$. The main purpose of this article is to study some of the algebraic properties of the sequential product. Many of our results show that algebraic conditions on $A \circ B$ imply that A and B commute for the usual operator product. For example, if $A \circ B$ satisfies certain distributive or associative laws, then $AB = BA$. Moreover, if $A \circ B \in \mathcal{P}(H)$, then $AB = BA$ and $A \circ B = B$ or $B \circ A = B$ if and only if $AB = BA = B$. A natural definition of stochastic independence is introduced and briefly studied. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1407837]

I. INTRODUCTION

Two measurements A and B cannot be performed simultaneously in general, so they are frequently executed sequentially. We denote by $A \circ B$ a sequential measurement in which A is performed first and B second. We restrict our attention to yes–no measurements that have only two possible results usually taken to be 0 and 1. A paradigm situation is an optical bench in which a beam of particles prepared in a certain state is injected at the left and then subjected to a sequence of filters $F_1,\ldots,F_n$. An individual particle either passes through a filter F_i or does not so the filters can be thought of as yes–no measurements. Particles that pass through all the filters enter a detection device at the right of F_n and are counted. Because of quantum interference, the order of placement of the filters usually makes a difference. The resulting sequential measurement is $F_1 \circ F_2 \circ \cdots \circ F_n$ and the probability that a particle is detected is denoted by $P(F_1 \circ F_2 \circ \cdots \circ F_n)$. In practice, this probability is usually approximated by a relative long-run frequency. Thus, if a large number N_{in} of particles is injected and N_{out} particles are detected, then

$$P(F_1 \circ F_2 \circ \cdots \circ F_n) \approx \frac{N_{\text{in}}}{N_{\text{out}}}.$$

Following the standard terminology, we call yes–no measurements **effects**.[1–3] For effects A and B, it is reasonable to assume that

$$P(A \circ B) = P(A)P(B|A). \tag{1.1}$$

For a classical system, A and B are represented by sets and P is represented by a probability measure. In this case we have

$$P(A \circ B) = \frac{P(A)P(A \cap B)}{P(A)} = P(A \cap B)$$

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when $P(A)\neq 0$. Hence, $A\circ B$ is represented by $A\cap B$ and we write $A\circ B=A\cap B$. But then

$$A\circ B=A\cap B=B\cap B=B\circ A$$

and this does not describe quantum interference. For this reason, we must abandon classical probability theory and we are forced to employ quantum probability theory. For example, let A and B be polarizing filters in planes perpendicular to the particle beam, where A polarizes vertically and B at a 45° angle. If the incoming beam is prepared in a state of horizontal polarization, then $A\circ B$ will transmit no particles, while $B\circ A$ will transmit particles. In this case, $A\circ B\neq B\circ A$.

In quantum mechanics, sharp effects are represented by self-adjoint projection operators on a complex Hilbert space H and general effects that may be unsharp (imprecise) are represented by operators on H satisfying $0\leqslant A\leqslant I$.[1–3] This latter condition means that

$$0\leqslant\langle Ax,x\rangle\leqslant\langle x,x\rangle$$

for all $x\in H$ and it easily follows that A is self-adjoint. We denote the set of sharp effects by $\mathcal{P}(H)$ and the set of general effects by $\mathcal{E}(H)$. If $W\in\mathcal{E}(H)$ is of trace class and satisfies $\mathrm{tr}(W)=1$, then W is called a **density operator**. We denote the set of density operators by $\mathcal{D}(H)$. Each $W\in\mathcal{D}(H)$ represents a quantum state and $P_W(A)=\mathrm{tr}(AW)$ is the probability that the effect A occurs (has value 1) when the system is prepared in the state W.

For $A,B\in\mathcal{E}(H),W\in\mathcal{D}(H)$, we define the **conditional probability of** B **given** A by

$$P_W(B|A)=\frac{\mathrm{tr}(BA^{1/2}WA^{1/2})}{\mathrm{tr}(AW)}=\frac{\mathrm{tr}(A^{1/2}BA^{1/2}W)}{\mathrm{tr}(AW)} \tag{1.2}$$

when $\mathrm{tr}(AW)\neq 0$.[1,4,5] As usual, $A^{1/2}$ is the unique positive square root of A. Equation (1.2) generalizes the well-known von Neumann–Lüders formula[6]

$$P_W(B|A)=\frac{\mathrm{tr}(BAWA)}{\mathrm{tr}(AW)}$$

for $A,B\in\mathcal{P}(H)$. Applying Eqs. (1.1) and (1.2) we have

$$P_W(A\circ B)=P_W(A)P_W(B|A)=\mathrm{tr}(A^{1/2}BA^{1/2}W)=P_W(A^{1/2}BA^{1/2}). \tag{1.3}$$

Notice that $A^{1/2}BA^{1/2}\in\mathcal{E}(H)$ because

$$0\leqslant\langle A^{1/2}BA^{1/2}x,x\rangle=\langle BA^{1/2}x,A^{1/2}x\rangle\leqslant\langle A^{1/2}x,A^{1/2}x\rangle=\langle Ax,x\rangle\leqslant\langle x,x\rangle.$$

Since (1.3) holds for every $W\in\mathcal{D}(H)$, we define $A\circ B=A^{1/2}BA^{1/2}$ and we have just shown that $A\circ B\leqslant A$. We call $A\circ B$ the **sequential product** of A and B.

We say that $A,B\in\mathcal{E}(H)$ are **compatible** if $AB=BA$. The sequential product illustrates why it is important to consider unsharp effects. Even if $A,B\in\mathcal{P}(H)$ are sharp, $A\circ B=ABA\notin\mathcal{P}(H)$ unless A and B are compatible. In this article, we shall study various properties of the sequential product. Many of our results show that if one tries to impose classical conditions on $A\circ B$, then it forces A and B to be compatible.

II. SEQUENTIAL INDEPENDENCE

It is clear that the sequential product satisfies $0\circ A=0$, $I\circ A=A$, $A\circ(B+C)=A\circ B+A\circ C$ whenever $B+C\leqslant I$, and $(\lambda A)\circ B=A\circ(\lambda B)=\lambda(A\circ B)$ for every $0\leqslant\lambda\leqslant 1$. We shall show that $A\circ B$ has practically no other algebraic properties unless compatibility conditions are imposed. To illustrate the fact that $A\circ B$ does not have properties that one might expect, we now show that $A\circ B=A\circ C$ does not imply $B\circ A=C\circ A$ even for $A,B,C\in\mathcal{P}(H)$. In $H=\mathbb{C}^2$, consider $A,B,C\in\mathcal{P}(H)$ given by the following matrices:

$$A=\frac{1}{2}\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix},\quad B=\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix},\quad C=\begin{bmatrix}0 & 0\\ 0 & 1\end{bmatrix}.$$

We then have

$$A\circ B=ABA=\tfrac{1}{2}A=ACA=A\circ C.$$

However,

$$B\circ A=BAB=\tfrac{1}{2}B\neq\tfrac{1}{2}C=CAC=C\circ A.$$

This example also shows that $A\circ B\not\leqslant B$ in general, even though we always have $A\circ B\leqslant A$.

We say that $A,B\in\mathcal{E}(H)$ are **sequentially independent** if $A\circ B=B\circ A$. It is clear that if A and B are compatible, then they are sequentially independent. To prove the converse, we shall need the following result due to Fuglede–Putnam–Rosenblum.[7]

Theorem 2.1: *If M, N, T are bounded linear operators on H with M and N normal, then $MT=TN$ implies $M^*T=TN^*$.*

Although the next result was given in Ref. 5 we include the proof because it is very short.

Corollary 2.2: For $A,B\in\mathcal{E}(H)$, $A\circ B=B\circ A$ implies $AB=BA$.

Proof: Since $A\circ B=B\circ A$, we have

$$A^{1/2}B^{1/2}B^{1/2}A^{1/2}=B^{1/2}A^{1/2}A^{1/2}B^{1/2}.$$

Hence, $M=A^{1/2}B^{1/2}$ and $N=B^{1/2}A^{1/2}$ are normal. Letting $T=A^{1/2}$, we have $MT=TN$. Applying Theorem 2.1 we conclude that $B^{1/2}A=AB^{1/2}$. It immediately follows that $BA=AB$. □

Sequential independence for three or more effects was considered in Ref. 5 and a more general result was proved. Our next result shows that if $A\circ B$ is sharp, then A and B are compatible (and hence, sequentially independent).

Theorem 2.3: *For $A,B\in\mathcal{E}(H)$, if $A\circ B\in\mathcal{P}(H)$, then $AB=BA$.*

Proof: Assume that $A^{1/2}BA^{1/2}=A\circ B\in\mathcal{P}(H)$. Suppose that $A\circ Bx=x$ where $\|x\|=1$. We then have $\langle BA^{1/2}x,A^{1/2}x\rangle=1$. By Schwarz's inequality we have $BA^{1/2}x=A^{1/2}x$ and, hence, $Ax=A\circ Bx=x$. Since x is an eigenvector of A with eigenvalue 1, the same holds for $A^{1/2}$. Thus, $A^{1/2}x=x$ so that $BA^{1/2}x=A\circ Bx$. We conclude that $BA^{1/2}x=A\circ Bx$ for every x in the range $R(A\circ B)$. Now suppose that $A\circ Bx=0$. We then have

$$\|B^{1/2}A^{1/2}x\|^2=\langle B^{1/2}A^{1/2}x,B^{1/2}A^{1/2}x\rangle=\langle A\circ Bx,x\rangle=0$$

so that $B^{1/2}A^{1/2}x=0$. Hence, $BA^{1/2}x=0$ and it follows that $BA^{1/2}x=A\circ Bx$ for every x in the null space $N(A\circ B)$. We conclude that $BA^{1/2}=A\circ B$. Hence,

$$BA^{1/2}=A\circ B=(A\circ B)^*=A^{1/2}B$$

so that $AB=BA$. □

Simple examples show that the converse of Theorem 2.3 does not hold. However, the converse does hold for sharp effects.

Corollary 2.4: For $A,B\in\mathcal{P}(H)$, $A\circ B\in\mathcal{P}(H)$ if and only if $AB=BA$.

This last result shows that $\mathcal{P}(H)$ is not closed under sequential products. Theorem 2.3 can be stated in the following equivalent form. For $A,B\in\mathcal{E}(H)$, if $ABA\in\mathcal{P}(H)$, then $AB=BA$. It is interesting to note that this form does not hold for arbitrary bounded self-adjoint operators.

Example: In $\mathbb{C}^3$ consider the self-adjoint operators $B=\mathrm{diag}(0,1,1)$ and

$$A=\begin{bmatrix}0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 0\end{bmatrix}.$$

Then $AB \neq BA$ but $ABA = \mathrm{diag}(1,0,0) \in \mathcal{P}(H)$. □

It follows from Corollary 2.4 that for $A,B \in \mathcal{P}(H)$ we have $A \circ B = B$ if and only if $AB = BA = B$. We now generalize this result to arbitrary effects.

Theorem 2.5: *For $A,B \in \mathcal{E}(H)$ the following statements are equivalent.* (a) $A \circ B = B$. (b) $B \circ A = B$. (c) $AB = BA = B$.

Proof: It is clear that (c) implies both (a) and (b). It then suffices to show that (a) and (b) each imply (c). If $A \circ B = B$ we have

$$A^{1/2}B^2A^{1/2} = A^{1/2}BA^{1/2}BA = B^2A.$$

Taking adjoints gives $B^2A = AB^2$. It follows that $AB = BA = B$. If $B \circ A = B$, then for any $x \in H$ we have

$$\langle AB^{1/2}x, B^{1/2}x\rangle = \langle B \circ Ax, x\rangle = \langle Bx, x\rangle = \|B^{1/2}x\|^2.$$

If $B^{1/2}x \neq 0$, then

$$\left\langle A\frac{B^{1/2}x}{\|B^{1/2}x\|}, \frac{B^{1/2}x}{\|B^{1/2}x\|}\right\rangle = 1.$$

It follows from Schwarz's inequality that $AB^{1/2}x = B^{1/2}x$. Hence, $AB^{1/2} = B^{1/2}$ so that $AB^{1/2} = B^{1/2}A = B^{1/2}$. We conclude that $AB = BA = B$. □

Theorem 2.5(a) cannot be strengthened to the case $A \circ B \leqslant B$. That is, $A \circ B \leqslant B$ does not imply $AB = BA$.

Example: In $\mathbb{C}^2$ let

$$A = \frac{1}{4}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{bmatrix}.$$

Then $A \circ B \leqslant B$ but $AB \neq BA$. □

The next result strengthens Theorem 2.5 for certain special cases.

Theorem 2.6: (a) *For $A,B \in \mathcal{P}(H)$ we have $A \circ B \leqslant B$ if and only if $AB = BA$.* (b) *For $A,B \in \mathcal{P}(H)$ we have $A \circ B \geqslant B$ if and only if $AB = BA = B$.* (c) *If $A,B \in \mathcal{E}(H)$ with $\dim H < \infty$ and $A \circ B \geqslant B$, then $AB = BA = B$.*

Proof: (a) Clearly, $AB = BA$ implies $A \circ B \leqslant B$. Conversely, if

$$ABA = A \circ B \leqslant B,$$

then it follows that

$$BABA = ABAB = ABA.$$

Now $ABA \in \mathcal{P}(H)$ because

$$ABAABA = ABABA = BABA = ABA.$$

Applying Theorem 2.3 we have $AB = BA$.

(b) Again it is clear that $AB = BA = B$ implies $A \circ B \geqslant B$. Conversely, if

$$ABA = A \circ B \geqslant B,$$

then we have

$$BABA = ABAB = B.$$

As before, $(A\circ B)^2=BABA=B$ so that $A\circ B=B$. Hence, $AB=BA=B$. (c) Let $x_1,\ldots,x_n$ be an orthonormal basis of eigenvectors of $A^{1/2}$ with corresponding eigenvalues $\lambda_1,\ldots,\lambda_n$. Since

$$\langle Bx_i,x_i\rangle\leqslant\langle BA^{1/2}x_i,A^{1/2}x_i\rangle=\lambda_i^2\langle Bx_i,x_i\rangle$$

we have $Bx_i=0$ if $\lambda_i<1$. Moreover, if $\lambda_i=1$, we have

$$\langle(A^{1/2}BA^{1/2}-B)x_i,x_i\rangle=0. \tag{2.1}$$

Hence, (2.1) holds for $i=1,2,\ldots,n$. Since $A^{1/2}BA^{1/2}-B\geqslant 0$, we conclude that $(A\circ B-B)x_i=0$ for $i=1,2,\ldots,n$. Hence, $A\circ B=B$ and the result follows from Theorem 2.5(a). □

Theorem 2.6(c) says that when $\dim H<\infty$ we cannot amplify an effect by preceding it by another effect. It is an open problem whether this result holds when $\dim H=\infty$.

III. ASSOCIATIVITY

For a unit vector $x\in H$, we denote the self-adjoint projection onto the one-dimensional subspace spanned by x by P_x. We first prove a lemma that is needed for the following theorem on associativity.

Lemma 3.1: (a) *If* $|\langle y,x\rangle|=|\langle z,x\rangle|$ *for every* $x\in H$, *then* $y=cz$ *where* $|c|=1$. (b) *If* $f:H\to\mathbb{C}$, T *is a nonzero bounded linear operator on* H, *and* $Mx=f(x)Tx$ *is linear, then* $f(x)=f(y)$ *for every* $x,y\neq 0$.

Proof: (a) The result clearly holds if $y=0$ so suppose that $y\neq 0$. We then have

$$\|y\|^2=\langle y,y\rangle=|\langle z,y\rangle|=|\langle y,z\rangle|=\langle z,z\rangle=\|z\|^2.$$

Hence, $\|y\|=\|z\|$ and we have $|\langle y,z\rangle|=\|z\|\|y\|$. We conclude that $y=cz$ with $|c|=1$.

(b) For $\alpha\in\mathbb{C}$ we have

$$\alpha f(\alpha x)Tx=f(\alpha x)T(\alpha x)=M(\alpha x)=\alpha Mx=\alpha f(x)Tx.$$

Hence, $f(\alpha x)=f(x)$ for every $\alpha\in\mathbb{C}$ with $\alpha\neq 0$. Moreover,

$$f(x+y)Tx+f(x+y)Ty=M(x+y)=Mx+My=f(x)Tx+f(y)Ty.$$

If Tx and Ty are linearly independent, we conclude that $f(x)=f(y)$. Suppose that $Tx\neq 0$ and $Ty\neq 0$ are linearly dependent. If T has one-dimensional range, then T is essentially a linear functional and the result follows. Otherwise, there exists a $z\in H$ such that Tz and Tx are linearly independent and hence Tz and Ty are linearly independent. But then $f(y)=f(z)=f(x)$. □

Theorem 3.2: *For* $A,B\in\mathcal{E}(H)$ *we have* $A\circ(B\circ C)=(A\circ B)\circ C$ *for every* $C\in\mathcal{E}(H)$ *if and only if* $AB=BA$.

Proof: If $AB=BA$, then clearly $A\circ(B\circ C)=(A\circ B)\circ C$ for every $C\in\mathcal{E}(H)$. Conversely, suppose that $A\circ(B\circ C)=(A\circ B)\circ C$ for every $C\in\mathcal{E}(H)$. Then $A\circ(B\circ P_x)=(A\circ B)\circ P_x$ for every unit vector $x\in H$. For any $x,y\in H$ with $\|x\|=1$ we have

$$\begin{aligned}|\langle B^{1/2}A^{1/2}y,x\rangle|^2&=\langle B^{1/2}A^{1/2}y,x\rangle\langle x,B^{1/2}A^{1/2}y\rangle=\langle P_xB^{1/2}A^{1/2}y,B^{1/2}A^{1/2}y\rangle=\langle A\circ(B\circ P_x)y,y\rangle\\&=\langle(A\circ B)\circ P_xy,y\rangle=\langle(A^{1/2}BA^{1/2})^{1/2}P_x(A^{1/2}BA^{1/2})^{1/2}y,y\rangle\\&=\langle P_x(A^{1/2}BA^{1/2})^{1/2}y,(A^{1/2}BA^{1/2})^{1/2}y\rangle=|\langle(A^{1/2}BA^{1/2})^{1/2}y,x\rangle|^2.\end{aligned}$$

Applying Lemma 3.1(a), we conclude that

$$(A^{1/2}BA^{1/2})^{1/2}x=f(x)B^{1/2}A^{1/2}x$$

for every $x\in H$ where $f:H\to\mathbb{C}$ satisfies $|f(x)|=1$. It follows from Lemma 3.1(b) that

$$(A^{1/2}BA^{1/2})^{1/2}=cB^{1/2}A^{1/2}$$

for some $c\in\mathbb{C}$ with $|c|=1$. Taking adjoints gives $cB^{1/2}A^{1/2}=c^*A^{1/2}B^{1/2}$. Hence, $A^{1/2}B^{1/2}=B^{1/2}(dA^{1/2})$ where $|d|=1$. Applying Theorem 2.1, we have $A^{1/2}B^{1/2}=B^{1/2}(d^*A^{1/2})$ so that $dB^{1/2}A^{1/2}=d^*B^{1/2}A^{1/2}$. Hence, either $B^{1/2}A^{1/2}=0$ or $d=d^*$. In the first case,

$$B^{1/2}A^{1/2}=A^{1/2}B^{1/2}=0$$

so that $AB=BA$. In the second case, d is real so that $d=\pm 1$. If $d=1$, we again have $AB=BA$. If $d=-1$, we have $A^{1/2}B^{1/2}=-B^{1/2}A^{1/2}$. But then $A^{1/2}B^{1/2}A^{1/2}=-B^{1/2}A$ which implies $AB^{1/2}=B^{1/2}A$. Hence, $AB=BA$. □

The fact that $A\circ(B\circ C)\neq(A\circ B)\circ C$, in general, presents a puzzling quantum paradox. In applications, one always uses

$$A\circ(B\circ C)=A^{1/2}B^{1/2}CB^{1/2}A^{1/2}$$

to describe a sequential measurement (A,B,C). This prescription for (A,B,C) states that A is measured first and then the sequential measurement $B\circ C$ is performed. The expression

$$(A\circ B)\circ C=(A^{1/2}BA^{1/2})^{1/2}C(A^{1/2}BA^{1/2})^{1/2}$$

is never used to describe (A,B,C). This latter prescription states that the sequential measurement $A\circ B$ is performed first and then C is measured. Physically, one would expect that these two procedures should give the same result. The fact that the results may be different mathematically indicates that both of these procedures should be described by $A\circ(B\circ C)$ and that $(A\circ B)\circ C$ is simply a nonphysical mathematical construct. However, if it turns out that $(A\circ B)\circ C$ does have a physical meaning, then the fact that these two procedures are different would be quite interesting.

We have seen that the associative law $A\circ(B\circ C)=(A\circ B)\circ C$ holds for every $C\in\mathcal{E}(H)$ if and only if A and B are compatible. It is interesting that we obtain a stronger result if $A\circ(C\circ B)=(A\circ C)\circ B$ for every $C\in\mathcal{E}(H)$. In order to prove this result we shall need a preliminary theorem.

Lemma 3.3: If $\alpha_i,\beta_i,\gamma_i\in\mathbb{R}$, $i=1,2,...,n$, *satisfy*

$$\left(\sum_{j=1}^{n} d_jt_j\right)\left(\sum_{k=1}^{n}\beta_kt_k\right)=\left(\sum_{j=1}^{n}\gamma_jt_j\right)\left(\sum_{k=1}^{n}t_k\right) \tag{3.1}$$

for all $t_i\in\mathbb{R}$, $i=1,2,...,n$, *then either* $\alpha_1=\alpha_2=\cdots=\alpha_n$ *or* $\beta_1=\beta_2=\cdots=\beta_n$.

Proof: Identifying coefficients (or taking second partial order derivatives), (3.1) gives

$$\alpha_j\beta_k+\alpha_k\beta_j=\gamma_j+\gamma_k$$

for all $j,k\in\{1,...,n\}$. In particular, we have $\gamma_j=\alpha_j\beta_j$ for all $j\in\{1,...,n\}$. Hence, if $j\neq k$ we obtain

$$(\alpha_j-\alpha_k)(\beta_j-\beta_k)=(\alpha_j\beta_j+\alpha_k\beta_k)-(\alpha_j\beta_k+\alpha_k\beta_j)=0.$$

Thus, either $\alpha_j=\alpha_k$ or $\beta_j=\beta_k$ for all $j,k\in\{1,...,n\}$. Now let $M\subseteq\{1,...,n\}$ be a maximal set of indices such that either $\alpha_j=\alpha_k$ for all $j,k\in M$ or $\beta_j=\beta_k$ for all $j,k\in M$. Suppose that $M\neq\{1,...,n\}$ and let $m\in\{1,...,n\}\backslash M$. Assume without loss of generality that $\alpha_j=\alpha_k$ for all $j,k\in M$. By the maximality of M, we have that $\alpha_m\neq\alpha_j$ for all $j\in M$ but this forces $\beta_j=\beta_m$ for all $j\in M$. Since $\beta_j=\beta_k$ for all $j,k\in M\cup\{m\}$, this contradicts the maximality of M. Hence, $M=\{1,...,n\}$. □

Theorem 3.4: *Let A,B,C be bounded self-adjoint operators on a complex Hilbert space H with the property*

$$\langle Ax,x\rangle\langle Bx,x\rangle=\langle Cx,x\rangle \tag{3.2}$$

for all $x \in H$ with $\|x\| = 1$. Then $A = cI$ or $B = cI$ for some $c \in \mathbb{R}$.

Proof: Notice that (3.2) has the following equivalent version,

$$\langle Ax,x\rangle\langle Bx,x\rangle = \langle Cx,x\rangle\langle x,x\rangle, \tag{3.3}$$

for all $x \in H$. We first assume that H is finite dimensional. In this case, we can diagonalize C and represent A,B,C by self-adjoint matrices $A = [\alpha_{jk}]$, $B = [\beta_{jk}]$, $C = \operatorname{diag}(\gamma_1,...,\gamma_n)$ on $\mathbb{C}^n$ where $\gamma_1,\ldots,\gamma_n \in \mathbb{R}$. Then (3.3) becomes

$$\left(\sum_{j,k=1}^{n} \alpha_{jk}\overline{\lambda}_j\lambda_k\right)\left(\sum_{j,k=1}^{n} \beta_{jk}\overline{\lambda}_j\lambda_k\right) = \left(\sum_{j=1}^{n} \gamma_j|\lambda_j|^2\right)\left(\sum_{j=1}^{n} |\lambda_j|^2\right) \tag{3.4}$$

for every $(\lambda_1,\ldots,\lambda_n) \in \mathbb{C}^n$. Suppose that $j \neq k$ and let $\lambda_m = 0$ for all $m \in \{1,...,n\}\backslash\{j,k\}$. Then (3.4) gives

$$\begin{aligned}&(\alpha_{jj}|v|^2 + \alpha_{kk}|w|^2 + \alpha_{jk}\overline{v}w + \overline{\alpha}_{jk}v\overline{w})(\beta_{jj}|v|^2 + \beta_{kk}|w|^2 + \beta_{jk}\overline{v}w + \overline{\beta}_{jk}v\overline{w})\\ &\quad = (\gamma_j|v|^2 + \gamma_k|w|^2)(|v|^2 + |w|^2)\end{aligned}$$

for all $v,w \in \mathbb{C}$. If we take $w = 1$ and $|v| = 1$, the previous equation becomes

$$(u_0 + u_1\overline{v} + \overline{u_1}v)(z_0 + z_1\overline{v} + \overline{z_1}v) = 2(\gamma_j + \gamma_k) \tag{3.5}$$

for all $v \in \mathbb{C}$ with $|v| = 1$, where $u_0 = \alpha_{jj} + \alpha_{kk}$, $z_0 = \beta_{jj} + \beta_{kk}$, $u_1 = \alpha_{jk}$, $z_1 = \beta_{jk}$. But (3.5) implies that $u_1 = z_1 = 0$ and we conclude that

$$\alpha_{jk} = \beta_{jk} = 0, \quad j \neq k. \tag{3.6}$$

Applying (3.6), (3.4) becomes

$$\left(\sum_{j=1}^{n} \alpha_{jj}|\lambda_j|^2\right)\left(\sum_{j=1}^{n} \beta_{jj}|\lambda_j|^2\right) = \left(\sum_{j=1}^{n} \gamma_j|\lambda_j|^2\right)\left(\sum_{j=1}^{n} |\lambda_j|^2\right).$$

Applying Lemma 3.3, it follows that either $\alpha_{11} = \cdots = \alpha_{nn}$ or $\beta_{11} = \cdots = \beta_{nn}$. Hence, the result holds if H is finite dimensional.

We now assume that H is infinite dimensional. Denote by $\mathcal{F}(H)$ the set of all finite dimensional subspaces in H. For every $F \in \mathcal{F}(H)$ we define P_F to be the orthogonal projection onto F and we define the self-adjoint operators $A_F = P_FAP_F$, $B_F = P_FBP_F$ and $C_F = P_FCP_F$. For every $F \in \mathcal{F}(H)$ and every $x \in F$ with $\|x\| = 1$, (3.2) gives

$$\langle A_Fx,x\rangle\langle B_Fx,x\rangle = \langle Ax,x\rangle\langle Bx,x\rangle = \langle Cx,x\rangle = \langle C_Fx,x\rangle.$$

It follows from our work in the previous paragraph that either there exists an $\alpha_F \in \mathbb{R}$ such that $A_Fx = \alpha_Fx$ for every $x \in F$ or there exists a $\beta_F \in \mathbb{R}$ such that $B_Fx = \beta_Fx$ for every $x \in F$. Thus, either $A_F = \alpha_FP_F$ or $B_F = \beta_FP_F$. For every $F \in \mathcal{F}(H)$, define

$$\lambda_F = \begin{cases} \alpha_F & \text{if } A_F = \alpha_FP_F, \\ \|A\| + 1 & \text{otherwise,} \end{cases} \quad \mu_F = \begin{cases} \beta_F & \text{if } B_F = \beta_FP_F, \\ \|B\| & \text{otherwise.} \end{cases}$$

It is clear that $\lambda_F \leqslant \|A\| + 1$ and $\mu_F \leqslant \|B\| + 1$. If we order $\mathcal{F}(H)$ by inclusion, we have a bounded net (λ_F,μ_F) in $\mathbb{R}^2$. By compactness, this net has a convergent subnet. Hence, there exists a directed set $(\Sigma, \leqslant)$ and a map $\phi:\Sigma \to \mathcal{F}(H)$ such that for every $F \in \mathcal{F}(H)$ there exists a $\sigma_F \in \Sigma$ such that $F \leqslant \phi(\sigma)$ for every $\sigma_F \leqslant \sigma$ and

$$\lim_{\sigma\in\Sigma} (\lambda_{\phi(\sigma)},\mu_{\phi(\sigma)}) = (\alpha,\beta)$$

for some $(\alpha,\beta)\in\mathbb{R}^2$. If $\alpha\neq\|A\|+1$, then for σ sufficiently large we have $\lambda_{\phi(\sigma)}=\alpha_{\phi(\sigma)}\leqslant\|A\|$. In this case $A_{\phi(\sigma)}=\alpha_{\phi(\sigma)}P_{\phi(\sigma)}$. Since the net $P_{\phi(\sigma)}$ converges in the strong operator topology to I, it follows that the net $A_{\phi(\sigma)}$ converges in the strong operator topology to A. It follows that $A=\alpha I$. If $\alpha=\|A\|+1$, then for σ sufficiently large we must have $\lambda_{\phi(\sigma)}=\|A\|+1$. Hence, $\mu_{\phi(\sigma)}\neq\|B\|+1$ so $\mu_{\phi(\sigma)}=\beta_{\phi(\sigma)}$. Arguing as before, we conclude that $B=\beta I$. □

We now apply this theorem to prove the following result about associativity.

Theorem 3.5: *For $A,B\in\mathcal{E}(H)$, the following statements are equivalent.* (a) $A\circ(C\circ B)=(A\circ C)\circ B$ *for every* $C\in\mathcal{E}(H)$. (b) $C\circ(A\circ B)=(C\circ A)\circ B$ *for every* $C\in\mathcal{E}(H)$. (c) $\langle A\circ Bx,x\rangle=\langle Ax,x\rangle\times\langle Bx,x\rangle$ *for every* $x\in H$ *with* $\|x\|=1$. (d) $A=cI$ *or* $B=cI$ *for some* $0\leqslant c\leqslant 1$.

Proof: If (a) holds, then $A\circ(P_x\circ B)=(A\circ P_x)\circ B$ holds for every unit vector $x\in H$. If $A^{1/2}x\neq 0$, let $y=A^{1/2}x/\|A^{1/2}x\|$. We then have for every $z\in H$ that

$$A\circ(P_x\circ B)z=A^{1/2}P_xBP_xA^{1/2}z=\langle A^{1/2}z,x\rangle A^{1/2}P_xBx=\langle A^{1/2}z,x\rangle\langle Bx,x\rangle A^{1/2}x=\langle Bx,x\rangle\|A^{1/2}x\|^2P_yz.$$

Hence, $A\circ(P_x\circ B)=\langle Bx,x\rangle\|A^{1/2}x\|^2P_y$. Moreover,

$$A\circ P_xz=A^{1/2}P_xA^{1/2}z=\langle A^{1/2}z,x\rangle A^{1/.2}x=\|A^{1/2}x\|^2P_yz$$

so that $A\circ P_x=\|A^{1/2}x\|^2P_y$. Hence,

$$(A\circ P_x)\circ B=(A\circ P_x)^{1/2}B(A\circ P_x)^{1/2}=\|A^{1/2}x\|^2P_yBP_y.$$

We conclude that $P_yBP_y=\langle Bx,x\rangle P_y$. It follows that

$$\langle Bx,x\rangle y=P_yBy=\langle By,y\rangle y$$

so that $\langle Bx,x\rangle=\langle By,y\rangle$. Since $y=A^{1/2}x/\|A^{1/2}x\|$, this last expression becomes

$$\langle A\circ Bx,x\rangle=\langle Ax,x\rangle\langle Bx,x\rangle,$$

so (a) implies (c).

If (b) holds, then for any unit vector $x\in H$ we have

$$\begin{aligned}(A\circ Bx,x)P_x&=P_x(A\circ B)P_x=P_x\circ(A\circ B)=(P_x\circ A)\circ B=(P_xAP_x)^{1/2}B(P_xAP_x)^{1/2}\\&=\langle Ax,x\rangle P_xBP_x=\langle Ax,x\rangle\langle Bx,x\rangle P_x.\end{aligned}$$

Hence, (b) implies (c). It follows from Theorem 3.4 that (c) implies (d). Finally, it is clear that (d) implies both (a) and (b). □

IV. STOCHASTIC INDEPENDENCE AND TOTAL PROBABILITY

We say that $A,B\in\mathcal{E}(H)$ are **stochastically independent relative to the state** $W\in\mathcal{D}(H)$ if $P_W(A\circ B)=P_W(A)P_W(B)$. We can also write this condition in the form

$$\mathrm{tr}[(A\circ B)W]=\mathrm{tr}(AW)\mathrm{tr}(BW). \tag{4.1}$$

In the case of a pure state $W=P_x$, (4.1) becomes

$$\langle A\circ Bx,x\rangle=\langle Ax,x\rangle\langle Bx,x\rangle. \tag{4.2}$$

Notice that (4.2) appears in condition (c) of Theorem 3.5

Corollary 4.1: For $A,B\in\mathcal{E}(H)$ the following statements are equivalent. (a) *A and B are stochastically independent relative to every state $W\in\mathcal{D}(H)$.* (b) *A and B are stochastically independent relative to every pure state P_x.* (c) $A=cI$ *or* $B=cI$ *for some* $0\leqslant c\leqslant 1$.

Proof: This follows directly from Theorem 3.5. □

It is interesting to note that the classical counterpart to Corollary 4.1 holds. Recall that two bounded random variables f,g are **uncorrelated relative to a probability measure** μ if $\int fg\,d\mu = \int f\,d\mu \int g\,d\mu$.

Theorem 4.2: *Two bounded random variables f,g are uncorrelated relative to every probability measure on their sample space if and only if f or g is constant.*

Proof: It is clear that if f or g is constant, then they are uncorrelated. Conversely, assume that f,g are uncorrelated relative to every probability measure and that g is not constant. Then there exist an x and y in their sample space Ω such that $g(x)\neq g(y)$. Let μ be the probability measure $\mu = 1/2\,\delta_x + 1/2\,\delta_y$ where δ_x denotes the Dirac measure concentrated at x. We then have

$$\frac{1}{2}f(x)g(x)+\frac{1}{2}f(y)g(y)=\int fg\,d\mu=\int f\,d\mu\int g\,d\mu=\frac{1}{4}[f(x)+f(y)][g(x)+g(y)].$$

It follows that

$$f(x)g(x)+f(y)g(y)=f(y)g(x)+f(x)g(y).$$

Hence,

$$f(x)[g(x)-g(y)]=f(y)[g(x)-g(y)]$$

so that $f(x)=f(y)$. Let $z\in\Omega$ with $z\neq x, z\neq y$. Then either $g(z)\neq g(x)$ or $g(z)\neq g(y)$. In either case, by the previous reasoning we have $f(z)=f(x)$. Hence, f is constant. □

Stochastic independence appears to be quite rare. One case in which it does occur is in a tensor product space $\mathcal{E}(H\otimes H)$. In this case any two effects of the form $A\otimes I, I\otimes B$ are stochastically independent relative to a pure tensor state $x\otimes y$. Indeed,

$$\begin{aligned}\langle (A\otimes I)\circ(I\otimes B)x\otimes y, x\otimes y\rangle &= \langle Ax\otimes By, x\otimes y\rangle\\ &= \langle Ax,x\rangle\langle By,y\rangle\\ &= \langle A\otimes Ix\otimes y, x\otimes y\rangle\langle I\otimes Bx\otimes y, x\otimes y\rangle.\end{aligned}$$

Another case is when x is a unit eigenvector of A. In this case A,B are stochastically independent relative to P_x for every $B\in\mathcal{E}(H)$. The next result generalizes this situation.

Theorem 4.3: (*i*) *The following statements are equivalent.* (a) $P_W(A)=1$. (b) $WA=AW=W$. (c) $P_W(A\circ B)=P_W(B)$ *for every* $B\in\mathcal{E}(H)$. (*ii*) $P_W(A)=P_W(B)=1$ *if and only if* $P_W(A\circ B)=1$.

Proof: (*i*) Suppose that (a) holds. If λ_i, $i=1,2,...$, are the nonzero eigenvalues of W (including multiplicity) and x_i are the corresponding unit eigenvectors, then $\Sigma\lambda_i=1$ and

$$\sum \lambda_i\langle Ax_i, x_i\rangle = \mathrm{tr}(AW)=1.$$

It follows that $\langle Ax_i, x_i\rangle = 1$ and hence $Ax_i = x_i$, $i=1,2,...$. Thus, $AWx_i = Wx_i$. It follows that $AW=WA=W$ so (a) implies (b). If (b) holds, we have for every $B\in\mathcal{E}(H)$ that

$$P_W(A\circ B)=\mathrm{tr}(BA^{1/2}WA^{1/2})=\mathrm{tr}(BWA)=\mathrm{tr}(BW)=P_W(B).$$

Hence, (b) implies (c). Finally (c) implies (a) because we can let $B=I$.

(*ii*) If $P_W(A)=P_W(B)=1$, then by (c) we have $P_W(A\circ B)=P_W(B)=1$. Conversely if $P_W(A\circ B)=1$, then since $A\circ B\leqslant A$ we have $P_W(A)=1$. By (c) we have $P_W(B)=P_W(A\circ B)=1$. □

Notice that Theorem 4.3(c) says that if $P_W(A)=1$, then A and B are stochastically independent relative to W for every $B\in\mathcal{E}(H)$. The next example shows that if $P_W(A)=1$, then we need not have that $P_W(B\circ A)=P_W(B)$. Moreover, $P_W(B\circ A)\neq P_W(B)P_W(A)$ so B and A are not stochastically independent relative to W. This shows that stochastic independence is not a symmetric relation.

Example: Let $\dim H \geqslant 2$ and let x and y be linearly independent, nonorthogonal, unit vectors. Letting $W = P_x$ we have

$$P_W(P_x) = \mathrm{tr}(P_x) = 1.$$

We then obtain

$$P_W(P_x \circ P_y) = P_W(P_y) = |\langle x,y\rangle|^2 \neq 0,1.$$

However,

$$P_W(P_y \circ P_x) = \langle P_y P_x P_y x, x\rangle = |\langle x,y\rangle|^4 \neq |\langle x,y\rangle|^2 = P_W(P_y).$$

□

The simplest version of the law of total probability would say that

$$P_W(B) = P_W(A)P_W(B|A) + P_W(I-A)P_W(B|I-A).$$

In terms of the sequential product this can be stated as

$$P_W(B) = P_W(A \circ B) + P_W((I-A)\circ B) = P_W(A \circ B + (I-A)\circ B).$$

Does this equation hold for every $W \in \mathcal{D}(H)$? Equivalently, does the following equation hold?

$$B = A \circ B + (I-A)\circ B. \tag{4.3}$$

The next result is proved in Ref. 8. However, our proof is slightly different and perhaps simpler.

Theorem 4.4: *For $A,B \in \mathcal{E}(H)$, (4.3) holds if and only if $AB = BA$.*

Proof: It is clear that (4.3) holds if $AB = BA$. Conversely, assume that (4.3) holds and write it as

$$B = A^{1/2}BA^{1/2} + (I-A)^{1/2}B(I-A)^{1/2}.$$

Multiplying by $A^{1/2}$ on the left and right, we obtain

$$\begin{aligned} A^{1/2}BA^{1/2} &= ABA + A^{1/2}(I-A)^{1/2}B(I-A)^{1/2}A^{1/2} \\ &= ABA + (I-A)^{1/2}A^{1/2}BA^{1/2}(I-A)^{1/2} \\ &= ABA + (I-A)^{1/2}[B - (I-A)^{1/2}B(I-A)^{1/2}](I-A)^{1/2} \\ &= ABA - (I-A)B(I-A) + (I-A)^{1/2}B(I-A)^{1/2} \\ &= ABA - (I-A)B(I-A) + B - A^{1/2}BA^{1/2}. \end{aligned}$$

Hence,

$$2A^{1/2}BA^{1/2} = ABA - (I-A)B(I-A) + B = AB + BA. \tag{4.4}$$

Using the commutator notation $[X,Y] = XY - YX$ (4.4) gives

$$[A^{1/2},[A^{1/2},B]] = A^{1/2}(A^{1/2}B - BA^{1/2}) - (A^{1/2}B - BA^{1/2})A^{1/2} = AB - 2A^{1/2}BA^{1/2} + BA = 0.$$

If follows that for every spectral projection E of A we have

$$[E,[A^{1/2},B]] = 0.$$

By the Jacobi identity

$$[E,[A^{1/2},B]]+[B,[E,A^{1/2}]]+[A^{1/2},[B,E]]=0$$

we have that $[A^{1/2},[E,B]]=0$. As before we obtain $[E,[E,B]]=0$. Hence,

$$0=E(EB-BE)-(EB-BE)E=EB+BE-2EBE,$$

which we can write as

$$EB=2EBE-BE.$$

Multiplying on the left by E gives $EB=EBE$. Hence,

$$EB=(EBE)^*=BE.$$

It follows that $AB=BA$. □

Although the sequential product is always distributive on the right, Theorem 4.4 shows that it is not always distributive on the left. That is, $(A+B)\circ C\neq A\circ C+B\circ C$ in general, when $A+B\leqslant I$. Indeed, if $AC\neq CA$, then by Theorem 4.4 we have

$$A\circ C+(I-A)\circ C\neq C=(A+(I-A))\circ C.$$

Example: One might conjecture that the following generalization of Theorem 4.4 holds. If $A+B\leqslant I$ and $(A+B)\circ C=A\circ C+B\circ C$, then $CA=AC$ or $CB=BC$. However, this conjecture is false. Suppose that $CB\neq BC$. Nevertheless, we have

$$(\tfrac{1}{2}B+\tfrac{1}{2}B)\circ C=B\circ C=\tfrac{1}{2}B\circ C+\tfrac{1}{2}B\circ C=(\tfrac{1}{2}B)\circ C+(\tfrac{1}{2}B)\circ C.$$

□

We close with an open problem that generalizes Theorem 4.4. Suppose that $A_i\in\mathcal{E}(H)$, $i=1,...,n$, with $\Sigma A_i=I$ and that $B=\Sigma A_i\circ B$. Does this imply that $BA_i=A_iB$, $i=1,...,n$? Notice that the answer is affirmative if $A_i\in\mathcal{P}(H)$, $i=1,...,n$. In fact, we only need $A_i\in\mathcal{P}(H)$, $i=1,...,n$, and $\Sigma A_i\leqslant I$. In this case, we have $A_iA_j=A_jA_i=0$ for $i\neq j$. Hence, if $B=\Sigma A_i\circ B$, then $A_iB=BA_i=A_i\circ B$, $i=1,...,n$. It is shown in Ref. 8 that the answer is affirmative when B has discrete spectrum with a strictly decreasing sequence of eigenvalues.

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Some exact nontrivial global solutions with values in unit sphere for two-dimensional Landau–Lifshitz equations

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We present some exact global solutions with values in unit sphere for two-dimensional Landau–Lifshitz equations with initial-boundary conditions, and obtained a continuum which can be made from those solutions of a tuft of Landau–Lifshitz equations. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In 1986, Zhou and Guo[1] proved the global existence of weak solution for generalized Landau–Lifhsitz equations without Gilbert term in multidimensions. They considered the homogeneous boundary problem

$$\vec{u}(x,t)=0, \quad \text{for } x\in\partial\Omega, \quad 0\leqslant 1\leqslant T \tag{1}$$

with the initial value condition

$$\vec{u}(x,0)=\phi(x), \quad \text{for } x\in\Omega \tag{2}$$

for the system of ferromagnetic chain with several variables

$$\vec{u}_t=\vec{u}\times\Delta\vec{u}+\vec{f}(x,t,\vec{u}), \tag{3}$$

where $\vec{f}(x,t,\vec{u})$ is a given three-dimensional vector function in $x\in R^n$, $t\in R^+$, $\vec{u}\in R^3$. $\phi(x)$ is a given three-dimensional initial value function on $\overline{\Omega}$, Ω is a bounded domain in n-dimensional Euclidean space R^n. Under some conditions on $\vec{f}(x,t,\vec{u})$ and $\phi(x)$, they proved that the initial homogeneous boundary problem (1), (2) with the system of ferromagnetic chain (3) has at least one global weak solution

$$\vec{u}(x,t)\in L^{\infty}(0,T;H_0^1(\Omega))\cap C^{(0,1/(3+[n/2]))}(0,T;L^2(\Omega)).$$

Whether the global existence of the smooth solution for a Landau–Lifshitz equation in multidimensions ($n\geqslant 2$) is still an important open problem.

In 1999, Chang, Shatah, and Uhlenbeck[2] considered the following initial value problem for the two-dimensional cylindrical symmetric Landau–Lifshitz equations:

$$\vec{Z}_t=\vec{Z}\times\vec{Z}_{rr}+\frac{1}{r}\vec{Z}\times\vec{Z}_r. \tag{4}$$

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Under the small energy initial condition, they proved that there exists one global smooth solution for Eq. (4). We constructed one exact blow-up solution for two-dimensional Landau–Lifshitz equations (4) in Ref. 4. In Ref. 3, we constructed some exact blow-up solutions for n-dimensional Landau-Lifshitz equations:

$$\vec{Z}_t=\vec{Z}\times\vec{Z}_{rr}+\frac{n-1}{r}\vec{Z}\times\vec{Z}_r, \quad n\geqslant 2 \tag{5}$$

and

$$\vec{Z}_t=\vec{Z}\times\Delta Z \tag{6}$$

where

$$\Delta=\sum_{i=1}^{n}\frac{\partial^2}{\partial x_i^2}, \quad n\geqslant 2.$$

In this paper, we will construct some exact nontrivial global solutions with values in unit sphere for Eq. (4), and get a continuum from those global smooth solutions of a tuft of Landau–Lifshitz Equations on unit sphere.

II. SOME EXACT GLOBAL SOLUTIONS OF (4)

Theorem 1: *Let* $\Omega_a=(0,a)(0<a<\infty)$, $S=\{(u_1,u_2,u_3)|u_1^2+u_2^2+u_3^2=1,u_1,u_2,u_3\in R\}$, *if* $n=2$, *for every nonzero constant* C,

$$\vec{Z}(r,t)=\left(\frac{\cos\dfrac{Cr^2}{4\sqrt{1+C^2t^2}}}{\sqrt{1+C^2t^2}},\frac{\sin\dfrac{Cr^2}{4\sqrt{1+C^2t^2}}}{\sqrt{1+C^2t^2}},\frac{Ct}{\sqrt{1+C^2t^2}}\right), \tag{7}$$

is an exact global solution of (4) with the initial-boundary conditions:

(i) Initial condition,

$$\vec{Z}(r,0)=\left(\cos\frac{Cr^2}{4},\sin\frac{Cr^2}{4},0\right)\in S, \quad (r,0)\in\Omega_a\times\{0\},$$

(ii) boundary conditions,

$$\vec{Z}(0,t)=\left(\frac{1}{\sqrt{1+C^2t^2}},0,\frac{Ct}{\sqrt{1+C^2t^2}}\right), \quad (0,t)\in\{0\}\times[0,\infty),$$

$$\vec{Z}(a,t)=\left(\frac{\cos\dfrac{Ca^2}{4\sqrt{1+C^2t^2}}}{\sqrt{1+C^2t^2}},\frac{\sin\dfrac{Ca^2}{4\sqrt{1+C^2t^2}}}{\sqrt{1+C^2t^2}},\frac{Ct}{\sqrt{1+C^2t^2}}\right), \quad (a,t)\in\{a\}\times[0,\infty),$$

and $\vec{Z}(r,t)$ *satisfy*

(iii)

$$\vec{Z}(r,t)\in C^\infty(\Omega_a\times(0,\infty)), \quad (\forall 0<a<\infty).$$

(iv) Let

$$E(t)=\int_0^\infty |Z_r|^2 r\,\mathrm{d}r.$$

Then

$$E(t)=\frac{C^2a^4}{4(1+C^2t^2)^2}$$

and

$$\sup_{t\in[0,\infty)} E(t)=E(0)=\tfrac{1}{4}C^2a^4,$$

(v)

$$\lim_{t\to\infty}\vec{Z}(r,t)=(0,0,1)\in S,\quad (\forall C\neq 0)$$

and (0, 0, 1) *is a trivial solution of (4).*

(vi)

$$\vec{Z}(r,t)\in S,\quad (r,t)\in[0,a]\times[0,\infty].$$

Proof: We only verify that $\vec{Z}(r.t)$ are all solutions of (4), for all nonzero constants C,

$$\vec{Z}_t=\left(-\frac{C^2t\cos\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{\sqrt{(1+C^2t^2)^3}}+\frac{C^3r^2t\sin\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{4(1+C^2t^2)^2},-\frac{C^2t\sin\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{\sqrt{(1+C^2t^2)^3}}-\frac{C^3r^2t\cos\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{4(1+C^2t^2)^2},\frac{C}{\sqrt{(1+C^2t^2)^3}}\right),$$

$$\vec{Z}_r=\left(-\frac{Cr\sin\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{2(1+C^2t^2)},\frac{Cr\cos\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{2(1+C^2t^2)},0\right),$$

$$\vec{Z}_{rr}=\left(-\frac{C\sin\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{2(1+C^2t^2)}-\frac{C^2r^2\cos\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{4\sqrt{(1+C^2t^2)^3}},\frac{C\cos\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{2(1+C^2t^2)}-\frac{C^2r^2\sin\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{4\sqrt{(1+C^2t^2)^3}},0\right).$$

Therefore,

$$\vec{Z}\times\vec{Z}_{rr}+\frac{1}{r}\vec{Z}\times\vec{Z}_r$$

$$=\left(-\frac{C^2t\cos\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{\sqrt{(1+C^2t^2)^3}}+\frac{C^3r^2t\sin\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{4(1+C^2t^2)^2},-\frac{C^2t\sin\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{\sqrt{(1+C^2t^2)^3}}\right.$$

$$\left.-\frac{C^3r^2t\cos\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{4(1+C^2t^2)^2},\frac{C}{\sqrt{(1+C^2t^2)^3}}\right)=\vec{Z}_t.$$

Consequently (8) satisfy (4). □

One can verify following general theorem

Theorem 2: *Let*

$$A=\begin{pmatrix}a_{11}&a_{12}&a_{13}\\a_{21}&a_{22}&a_{23}\\a_{31}&a_{32}&a_{33}\end{pmatrix}$$

be any fixed third-order constant orthogonal matrix, then for every nonzero constant C,

$$\vec{Z}(r,t)=\left(\frac{\cos\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{\sqrt{1+C^2t^2}},\frac{\sin\frac{Cr^2}{4\sqrt{1+C^2t^2}}}{\sqrt{1+C^2t^2}},\frac{Ct}{\sqrt{1+C^2t^2}}\right)A \tag{8}$$

is an exact global solution of (4) with the initial-boundary conditions:

(i) Initial condition,

$$\vec{Z}(r,0)=\left(\cos\frac{Cr^2}{4},\sin\frac{Cr^2}{4},0\right)A\in S,\quad r\in\Omega_a,$$

(ii) boundary conditions,

$$\vec{Z}(0,t)=\left(\frac{1}{\sqrt{1+C^2t^2}},0,\frac{Ct}{\sqrt{1+C^2t^2}}\right)A,\quad t\in[0,\infty),$$

$$\vec{Z}(a,t)=\left(\frac{\cos\frac{Ca^2}{4\sqrt{1+C^2t^2}}}{\sqrt{1+C^2t^2}},\frac{\sin\frac{Ca^2}{4\sqrt{1+C^2t^2}}}{\sqrt{1+C^2t^2}},\frac{Ct}{\sqrt{1+C^2t^2}}\right)A,\quad t\in[0,\infty),$$

and $\vec{Z}(r,t)$ *satisfy*

(iii)

$$\vec{Z}(r,t)\in C^\infty(\Omega_a\times(0,\infty)),\quad(\forall 0<a<\infty).$$

(iv) Let

$$E(t)=\int_0^\infty|Z_r|^2r\,dr.$$

Then

$$E(t)=\frac{C^2a^4}{4(1+C^2t^2)^2}$$

and

$$\sup_{t\in[0,\infty)} E(t)=E(0)=\tfrac{1}{4}C^2a^4.$$

(v)

$$\lim_{t\to\infty}\vec{Z}(r,t)=(a_{31},a_{32},a_{33})\in S,\quad(\forall C\neq 0)$$

and (a_{31},a_{32},a_{33}) *is a trivial solution of (4).*

(vi)

$$\vec{Z}(r,t)\in S,\quad (r,t)\in[0,a]\times[0,\infty).$$

Remark 1: Theorems 1 and 2 reply partly to the open problem about the existence of global smooth solution for multidimensional Landau–Lifshitz equations under the initial-boundary conditions.

Remark 2: In Landau–Lifshitz equations $\vec{Z}$ *is the spin field, it describes the evolution of spin field in continuum ferromagnets,* $\vec{Z}_{rr}+(1/r)\vec{Z}_r$ *is an effective field. Theorem 1 shows that there exists at least a global smooth solution, though the initial energy is not small. Theorem 2 implies that there exists a continuum which can be made from those global smooth solutions of a tuft of Landau–Lifshitz equations on unit sphere.*

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Energy bounds for the spinless Salpeter equation

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We study the spectrum of the Salpeter Hamiltonian $H=\beta\sqrt{m^2+\mathbf{p}^2}+V(r)$, where $V(r)$ is an attractive central potential in three dimensions. If $V(r)$ is a convex transformation of the Coulomb potential $-1/r$ and a concave transformation of the harmonic-oscillator potential r^2, then both upper and lower bounds on the discrete eigenvalues of H can be constructed, which may all be expressed in the form $E=\min_{r>0}[\beta\sqrt{m^2+P^2/r^2}+V(r)]$ for suitable values of P here provided. At the critical point $r=\hat{r}$ the relative growth to the Coulomb potential $h(r)=-1/r$ must be bounded by $\mathrm{d}V/\mathrm{d}h<2\beta/\pi$. © *2001 American Institute of Physics.*
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I. INTRODUCTION

We study the (semirelativistic) ''spinless-Salpeter'' Hamiltonian

$$H=\beta\sqrt{m^2+\mathbf{p}^2}+V(r), \quad \beta>0, \tag{1}$$

in which $V(r)$ is a central potential in three spatial dimensions. The eigenvalue equation of this operator is called the ''spinless Salpeter equation.'' This equation of motion arises as a well-defined standard approximation to the Bethe–Salpeter formalism[1] for the description of bound states within a (relativistic) quantum field theory and is arrived at by the following simplifying steps:

(1) Eliminate all timelike variables by assuming the Bethe–Salpeter kernel that describes the interactions between the bound-state constituents to be static, i.e., instantaneous; the result of this reduction step is called the ''instantaneous Bethe–Salpeter equation'' or the ''Salpeter equation.'' [2]
(2) Neglect the spin of the bound-state constituents, assume the Bethe–Salpeter kernel to be of convolution type (as is frequently the case), and consider merely positive-energy solutions ψ, in order to arrive at the so-called ''spinless Salpeter equation'' $H\psi=E\psi$, with a Hamiltonian H of the form (1). (For two particles, this form of the Hamiltonian H holds only for equal masses m of the bound-state constituents.)

(For a more detailed account of the reduction of the Bethe–Salpeter equation to the spinless

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Salpeter equation, consult, e.g., the introductory sections of Refs. 3 and 4.) This wave equation describes the bound states of spin-zero particles (scalar bosons) as well as the spin-averaged spectra of the bound states of fermions.

In this article we consider potentials which are at the same time convex transformations $V(r)=g(h(r))$ of the Coulomb potential $h(r)=-1/r$ and concave transformations of the harmonic-oscillator potential $h(r)=r^2$. The reason for this is that spectral information is known for these two ''basis'' potentials $h(r)$. Thus the class of potentials is those $V(r)$ that have a dual representation

$$V(r)=g^{(1)}\left(-\frac{1}{r}\right)=g^{(2)}(r^2),$$

in which $g^{(1)}$ is convex ($g^{(1)\prime\prime}>0$) and $g^{(2)}$ is concave ($g^{(2)\prime\prime}<0$). An example of a potential in this class is

$$V(r)=-\frac{c_1}{r}+c_2\ln r+c_3 r+c_4 r^2, \tag{2}$$

where the coefficients $\{c_i\}$ are not negative and are not all zero. Thus tangent lines to the transformation function $g(h)$ are of the form $ah+b$ and are either Coulomb potentials lying below V, or harmonic-oscillator potentials lying above V. This geometrical idea is the basis for our approach to the spectral problem posed by H. We recall the application of this idea to the (nonrelativistic) Schrödinger problem in Sec. III. The general envelope formalism for the derivation of upper and lower bounds on the eigenvalues of the semirelativistic Salpeter Hamiltonian H of Eq. (1) is established in Sec. IV.

It is fundamental to our method that we first know something about the spectrum of H in those cases where $V(r)$ is one of the basis potentials, i.e., the Coulomb and the harmonic oscillator. These two spectra are discussed in Sec. II. In Sec. V we look at the example of the Coulomb-plus-linear potential.

II. THE COULOMB AND HARMONIC-OSCILLATOR POTENTIALS

A. Scaling behavior

Since the two basis potentials are both pure powers, it is helpful first to determine what can be learned about the corresponding eigenvalues by the use of standard scaling arguments. By employing a wave function $\phi(cr)$ depending on a scale variable $c>0$, we find the following scaling rule for the eigenvalues corresponding to attractive pure power potentials $v\ \mathrm{sgn}(q)r^q$. The Hamiltonian

$$H=\beta\sqrt{m^2+\mathbf{p}^2}+v\ \mathrm{sgn}(q)r^q$$

has the (energy) eigenvalues $E(v,\beta,m)$, where

$$E(v,\beta,m)=\beta m E\left(\frac{v}{\beta m^{1+q}},1,1\right),\quad q\geqslant -1.$$

The scaling behavior described by the above formula allows us to consider the one-particle, unit-mass special case $m=\beta=1$ initially, that is to say, to work w.l.o.g. with the operator

$$H=\sqrt{1+\mathbf{p}^2}+v\ \mathrm{sgn}(q)r^q.$$

B. Coulomb potential

In the case of the Coulomb potential $V(r)=-v/r$ it is well known[5] that the Hamiltonian H has a Friedrichs extension provided the coupling constant v is not too large. Specifically, it is necessary in this case that v is smaller than a critical value v_c of the coupling constant:

$$v<v_c=\frac{2}{\pi}.$$

With this restriction, a lower bound to the bottom of the spectrum is provided by Herbst's formula

$$E_0\geqslant\sqrt{1-(\sigma v)^2},\quad \sigma\equiv\frac{\pi}{2}. \tag{3}$$

By comparing the spinless Salpeter problem to the corresponding Klein–Gordon equation, Martin and Roy[6] have shown that if the coupling constant is further restricted by $v<\frac{1}{2}$, then an improved lower bound is provided by the expression

$$E_0\geqslant\sqrt{\frac{1+\sqrt{1-4v^2}}{2}},\quad v<\frac{1}{2}. \tag{4}$$

It turns out that our lower-bound theory has a simpler form when the Coulomb eigenvalue formula has the form of Eq. (3) rather than that of Eq. (4). For this reason, we have derived from Eq. (4) a family of Coulomb bounds which, by rather elementary methods, is found to read

$$E_0\geqslant\sqrt{1-(\sigma v)^2},\quad v\leqslant\frac{\sqrt{\sigma^2-1}}{\sigma^2}<\frac{1}{2}. \tag{5}$$

All these (lower) bounds are slightly weaker than the Martin–Roy bound (4) but above the Herbst bound (3). We note that these functions of the coupling constant v are all monotone and *concave*.

C. Harmonic-oscillator potential

In the case of the harmonic-oscillator potential, i.e., $V(r)=vr^2$, much more is known.[7,8] In momentum-space representation the operator $\mathbf{p}$ becomes a c-variable and, thus, from the spectral point of view, the Hamiltonian $H=\sqrt{1+\mathbf{p}^2}+vr^2$ is equivalent to the Schrödinger operator

$$H=-v\Delta+\sqrt{1+r^2}. \tag{6}$$

Since the potential $V(r)$ increases without bound, the spectrum of H is entirely discrete.[9] We denote its eigenvalues by $\mathcal{E}_{n\mathrm{l}}(v)$, where $n=1,2,3,\ldots$ "counts" the radial states in each angular-momentum subspace labeled by $\mathrm{l}=0,1,2,\ldots$. Later we shall either approximate the eigenvalues $\mathcal{E}(v)$ analytically or assume them to be known numerically. The eigenvalues $\mathcal{E}(v)$ of such Schrödinger operators are *concave* functions of the coupling constant v.[10,11]

D. The spectral comparison theorem

For the class of interaction potentials given by (2) with the coefficient of the Coulombic term not too large, that is, for all potentials which satisfy the constraint $\lim_{r\to 0}r^2V'(r)<2\beta/\pi$, the semirelativistic Salpeter Hamiltonian H is bounded below and is essentially self-adjoint.[5] Consequently, the discrete spectrum of H is characterized variationally[9] and it follows immediately from this that, if we compare two such Hamiltonians H having the potentials $V^{(1)}(r)$ and $V^{(2)}(r)$, respectively, and we know that $V^{(1)}(r)<V^{(2)}(r)$, then we may conclude that the corresponding discrete eigenvalues $E_{n\mathrm{l}}$ satisfy the inequalities $E_{n\mathrm{l}}^{(1)}<E_{n\mathrm{l}}^{(2)}$. We shall refer to this fundamental result as the "spectral comparison theorem." In the more common case of nonrelativistic dynam-

ics, i.e., for a (nonrelativistic) kinetic term of the form $\beta \mathbf{p}^2/2m$ in the Hamiltonian H, a constraint similar to the above would hold for the coefficient of a possible additional (attractive) $-1/r^2$ term in the potential $V(r)$.

III. GENERAL ENVELOPE THEORY OF SCHRÖDINGER OPERATORS

In nonrelativistic envelope theory,[11–13] if the potential V is a smooth transformation $V(r) = g(\mathrm{sgn}(q) r^q)$ of the power-law potential $\mathrm{sgn}(q) r^q$, the eigenvalues of $H = -\Delta + V(r)$ are approximated by

$$E_{nl} \approx \min_{r>0} \left[\frac{P_{nl}^2(q)}{r^2} + V(r) \right]. \tag{7}$$

The numbers $P_{nl}(q)$ can be derived from the eigenvalues of $-\Delta + \mathrm{sgn}(q) r^q$.[13] If g is convex ($g'' > 0$), Eq. (7) yields lower bounds; if g is concave ($g'' < 0$), the results are upper bounds.

As an immediate application we consider the (nonrelativistic) Schrödinger Hamiltonian (6) for the (relativistic) Salpeter harmonic-oscillator problem (1). Here we have $H = -v\Delta + V(r)$, with $V(r) = \beta\sqrt{m^2 + r^2}$; hence, the potential is a convex transformation of a linear potential and a concave transformation of a harmonic-oscillator potential. We conclude therefore from (7)

$$\min_{r>0} \left[v \frac{P_{nl}^2(1)}{r^2} + \beta\sqrt{m^2 + r^2} \right] \leqslant \mathcal{E}_{nl}(v) \leqslant \min_{r>0} \left[v \frac{P_{nl}^2(2)}{r^2} + \beta\sqrt{m^2 + r^2} \right]; \tag{8}$$

the numbers $P_{nl}(1)$ are given in Table 1 of Ref. 14, and $P_{nl}(2) = 2n + l - \frac{1}{2}$. Interestingly the upper and lower bounds (8) are equivalent to the corresponding bounds obtained in Ref. 8; however, these earlier specific bounds were not derived as part of a general theory.

IV. GENERAL ENVELOPE THEORY OF SALPETER HAMILTONIANS

Let us now turn to our main topic and consider the spinless-Salpeter Hamiltonian of Eq. (1),

$$H = \beta\sqrt{m^2 + \mathbf{p}^2} + V(r),$$

and its eigenvalues E. We shall assume that the potential $V(r)$ is a smooth transformation $V(r) = g(h(r))$ of another potential $h(r)$ and that g has definite convexity so that we obtain bounds to the energy eigenvalues E. We suppose that the "basis" potential $h(r)$ generates a "tangential" Salpeter problem

$$\mathcal{H} = \beta\sqrt{m^2 + \mathbf{p}^2} + v\,h(r),$$

for which the eigenvalues $e(v)$, or bounds to them, are known. We shall follow here as closely as possible the development in Refs. 11–13 for the corresponding Schrödinger problem. We express our results in the form of two theorems.

(1) The approximations we shall use from Sec. II, regarded as functions of the coupling v, and also the (unknown) energy functions $e(v)$ of the "tangential" Salpeter problem are all *concave*: $e''(v) < 0$. The latter result represents the principal claim of Theorem 1.
(2) In Theorem 2 we begin by using an envelope representation for the potential $V(r)$ and then demonstrate that all the spectral formulas that follow possess a certain structure.

Finally, as an application, we specialize to the case of pure power-law "basis" potentials $h(r)$ and, more particularly, to the Coulomb potential and the harmonic-oscillator potential for which, at this time, we have spectral information (cf. the discussions in Secs. II B and II C).

A. Convexity of the energy function

We begin by proving the following.

Theorem 1: *The function $e(v)$ is concave, that is, $e''(v)<0$.*

Proof: Suppose the exact eigenvalue and (normalized) eigenvector for the problem posed by $\mathcal{H}=\beta\sqrt{m^2+\mathbf{p}^2}+vh(r)$ are $e(v)$ and $\psi(v,r)$. By differentiating $(\psi,\mathcal{H}\psi)$ with respect to v we find $e'(v)=(\psi,h\psi)$. If we now apply $\psi(v,r)$ as a trial vector to estimate the energy of the operator $\beta\sqrt{m^2+\mathbf{p}^2}+uh(r)$, in which v has been replaced by u, we obtain an upper bound to $e(u)$ which may be written in the form $e(u)\leqslant e(v)+(u-v)e'(v)$. This inequality tells us that the function $e(u)$ lies beneath its tangents; that is to say, $e(u)$ is *concave*. □

B. The principal envelope formula

With the help of Theorem 1 we are able to prove the following theorem.

Theorem 2 (principal envelope formula): *Suppose that the operator $\beta\sqrt{m^2+\mathbf{p}^2}+vh(r)$ has the exact lowest eigenvalue $e(v)$, and suppose that the operator $\beta\sqrt{m^2+\mathbf{p}^2}+g(h(r))$ has the exact lowest eigenvalue E. Then*

$$E\approx\mathcal{E}\equiv\min_{v>0}[e(v)-ve'(v)+g(e'(v))]. \tag{9}$$

If g is concave (that is, $g''<0$), then $E\leqslant\mathcal{E}$; if g is convex (that is, $g''>0$), then $E\geqslant\mathcal{E}$.

Proof: All tangential potentials we shall employ have the form $V^{(t)}(r)=a(t)h(r)+b(t)$, where the coefficients $a(t)$ and $b(t)$ are given by

$$a(t)=\frac{V'(t)}{h'(t)}=g'(h(t)),\quad b(t)=V(t)-a(t)h(t)=g(h(t))-g'(h(t))h(t),$$

and $r=t$ is the point of contact of the potential $V(r)$ and its tangent $V^{(t)}(r)$. If, for definiteness, we assume that $V=g(h)$ with g concave (i.e., $g''<0$), we obtain a family of upper bounds given by

$$E\leqslant\varepsilon(t)=e(a(t))+b(t).$$

The best of these is given by optimizing over t:

$$E\leqslant\varepsilon(\hat{t})=e(a(\hat{t}))+b(\hat{t}),$$

where $\hat{t}$, the value of t which optimizes these bounds, is to be determined as the solution of

$$e'(g'(h(\hat{t})))=h(\hat{t}).$$

In the spirit of the Legendre transformation[15] we now consider another problem which has the same solution; this second problem is the one that provides us with our basic eigenvalue formula. We consider

$$\mathcal{E}=\min_{v>0}[e(v)-ve'(v)+g(e'(v))],$$

which is well defined since $e(v)$ is concave. The solution has the critical point $\hat{v}=g'(e'(\hat{v}))$. If we now apply the correspondence $h(\hat{t})=e'(\hat{v})$, the critical point $\hat{v}$ becomes $\hat{v}=g'(h(\hat{t}))$ and the tangential-potential coefficients a and b become

$$a(\hat{t})=g'(e'(v))=v,\quad b(\hat{t})=g(e'(v))-ve'(v),\quad v=\hat{v}. \tag{10}$$

Meanwhile, the original critical (energy) value is given by

$$\varepsilon(\hat{t}) = e(a(\hat{t})) + b(\hat{t}) = e(v) - ve'(v) + g(e'(v)), \quad v = \hat{v}.$$

□

From the proof of Theorem 2 it follows immediately that, if the *exact* energy function $e(v)$ corresponding to the basis potential h is not available, then, for $g(h)$ concave, concave *upper* approximations $e_u(v) > e(v)$ or, for $g(h)$ convex, concave *lower* approximations $e_l(v) < e(v)$ may be used instead of the exact energy function $e(v)$ in the principal envelope formula (9). Then all the lower tangents will lie even lower and all the upper tangents will lie even higher. If g is convex, we obtain a lower bound; if g is concave, we obtain an upper bound; because of the concavity of $e(v)$, *this* extremum is a minimum in *both* cases. If we wish to use numerical solutions to the "basis" problem [generated by $h(r)$], or if a completely new energy-bound expression becomes available, the principal envelope formula (9) is what would be used first.

Interestingly, in the formula (9) the tangential-potential apparatus is no longer evident; only the correct convexity is required. As in the Schrödinger case,[11] once we have the basic result, the reformulation in terms of "kinetic potentials" is often useful: the kinetic potential $\overline{h}(s)$ corresponding to some basis potential $h(r)$ is given by the Legendre transformation[15]

$$\overline{h}(s) = e'(v), \quad s = e(v) - ve'(v).$$

Meanwhile the envelope approximation has the kinetic-potential expression $\overline{V}(s) \approx g(\overline{h}(s))$.

For both the Coulomb lower bounds (3) or (5) and the harmonic-oscillator upper bounds (8) which we have at present, we may express our general results in a special common form which will now be derived.

C. The Coulomb lower bound

We consider first the Coulomb lower bound in which we assume that the potential $V(r)$ is a convex transformation $V(r) = g(h(r))$ of the Coulomb potential $h(r) = -1/r$. According to Sec. II B, in this case all the "lower" $e_l(v)$ have been arranged—with the parameters β and m returned—in the form

$$e_l(v) = \beta m \sqrt{1 - \left(\frac{\sigma v}{\beta}\right)^2}.$$

From this it follows by elementary algebra that if we define a new optimization variable r by $e_l'(v) = h(r) = -1/r$, we have

$$e_l(v) - ve_l'(v) = \beta \sqrt{m^2 + \frac{P^2}{r^2}}, \quad P \equiv \frac{1}{\sigma}.$$

Consequently, the lower bound on the energy eigenvalues E of the spinless Salpeter equation becomes

$$E \geqslant \min_{r>0} \left[\beta \sqrt{m^2 + \frac{P^2}{r^2}} + V(r) \right], \quad v < \beta v_P. \tag{11}$$

Here the boundary value v_P of the Coulomb coupling v is given, when simply determined by the requirement of boundedness from below of the operator (1), by the critical coupling v_c,

$$v_P = v_c = \frac{2}{\pi},$$

and, when arising from the region of validity of our Coulomb-like family of lower bounds (5), via $P = 1/\sigma$, by

$$v_P = P\sqrt{1-P^2} < \tfrac{1}{2}. \tag{12}$$

$\{P, v_P\}$ pairs may be easily generated from the upper bound on the coupling v in Eq. (12). The meaning of the Coulomb-coupling constraint is $a(\hat{t}) < \beta v_P$, where a is the coefficient in the tangential Coulomb potential given by (10).

D. The harmonic-oscillator upper bounds

Next, let us turn to the harmonic-oscillator upper bounds. Our main assumption here is that $V(r) = g(r^2)$, with $g'' < 0$. In this case the only difficulty is that the basis problem $h(r) = r^2$ is equivalent to a Schrödinger problem whose solution $\mathcal{E}_{nl}(v)$ is not known exactly. Following the discussion after the proof of Theorem 2, let us call the upper bound provided by Eq. (8) $e_u(v)$ and let us introduce the shorthand notation $P_{nl}(2) = 2n + l - \frac{1}{2} = P$. Then we have the following parametric equations for $e_u(v)$:

$$e_u(v) = v\,\frac{P^2}{r^2} + \beta\sqrt{m^2 + r^2}, \quad v = \frac{\beta r^4}{2P^2\sqrt{m^2+r^2}}, \quad e_u'(v) = \frac{P^2}{r^2}.$$

By substituting these expressions into the fundamental envelope formula (9) we obtain the following upper bound on all the eigenvalues E_{nl} of the spinless-Salpeter problem with potential $V(r) = g(r^2)$ and $g'' < 0$:

$$E_{nl} \leqslant \min_{r>0}\left[\beta\sqrt{m^2 + \frac{P^2}{r^2}} + V(r)\right], \quad P = P_{nl}(2) = 2n + l - \frac{1}{2}. \tag{13}$$

V. THE COULOMB-PLUS-LINEAR (OR "FUNNEL") POTENTIAL

In order to illustrate the above results by a physically motivated example, let us apply these considerations to the Coulomb-plus-linear or (in view of its shape) "funnel" potential

$$V(r) = -\frac{c_1}{r} + c_2 r, \quad c_1 \geqslant 0, \quad c_2 \geqslant 0.$$

(This potential provides a reasonable overall description of the strong interactions of quarks in hadrons. For the phenomenological description of hadrons in terms of both nonrelativistic and semirelativistic potential models, see, e.g., Refs. 16 and 17.) By choosing as basis potential $h(r) = -1/r$, we may write $V(r) = g(h(r))$ with

$$g(h) = c_1 h - \frac{c_2}{h},$$

which is clearly a convex function of $h < 0$: $g'' > 0$. Thus the convexity condition is satisfied. However, we are not free to choose the coupling constants c_1 and c_2 as large as we please. It is immediately obvious that, for a particular $\{P, v_P\}$ pair, we must in any case have $c_1 < \beta v_P$. For the full problem the coefficient c_2 of the linear term will also be involved. The coupling v we are concerned about is given by (10). We have

$$v = g'(e'(v)) = \frac{\beta P^2}{r\sqrt{m^2 + (P/r)^2}} = c_1 + \frac{c_2}{h^2} = c_1 + c_2 r^2.$$

From this we obtain, for given values of the parameters m and β and for a given $\{P, v_P\}$ pair, as a sufficient condition for $v < \beta v_P$ the "Coulomb coupling constant constraint" on the two coupling strengths c_1 and c_2 in the funnel potential:

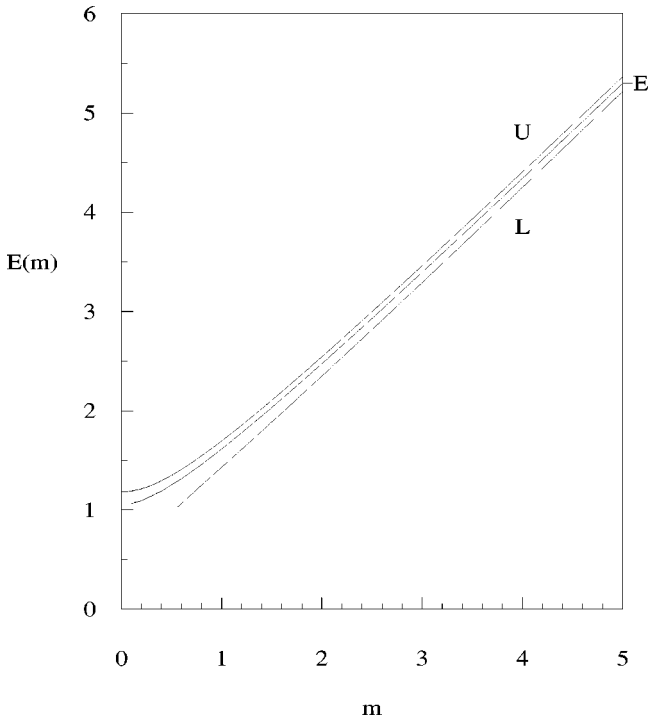

FIG. 1. Lower bounds (L), according to (11), and upper bounds (U), according to (13), on the energy eigenvalue E of the ground state $[(n,l)=(1,0)]$ of the spinless Salpeter equation with a Coulomb-plus-linear potential $V(r)=-c_1/r+c_2 r$, for $\beta=1$, $c_1=0.1$, and $c_2=0.25$. The lower bound is given by the general result (11) with the "best" $P(m)$ provided by (15). In order to satisfy the Coulomb coupling constraint (15), the mass m must fulfil $m>\sqrt{5}/4$. For comparison, a (very accurate) Rayleigh–Ritz variational upper bound E is depicted, too.

$$c_1+\frac{P^2}{m^2}\left(\frac{P^2}{v_P^2}-1\right)c_2<\beta v_P\,. \tag{14}$$

In the case $\{P=1/\sqrt{2}, v_P=\frac{1}{2}\}$ and $\beta=m=1$ this condition reduces to $c_1+\frac{1}{2}c_2<\frac{1}{2}$. For Herbst's lower bound (3), i.e., $P=v_P=v_c=2/\pi$, this constraint clearly yields $c_1<\beta v_P$. There is no escaping this feature of all energy bounds involving the Coulomb potential: the constraint derives from the fundamental observation that the Coulomb coupling v must not be too large, so that the (relativistic) kinetic energy is able to counterbalance the Coulomb potential in order to maintain the Hamiltonian (1) with $V(r)=-v/r$ bounded from below.

For example, if we seek the largest allowed value of the parameter P by solving Eqs. (12) and (14) together, we find that this largest P is given by

$$\frac{c_2\sin^4 t}{\cos^2 t(\beta\sin t\cos t-c_1)}=m^2,\quad P\equiv\sin t. \tag{15}$$

For the Coulomb-plus-linear potential $V(r)=-c_1/r+c_2 r$ under consideration, Fig. 1 shows the lower and upper bounds on the lowest energy eigenvalue E of the spinless Salpeter equation, given by the envelopes of the lower and upper families of tangential energy curves (11) and (13). In the case of the lower bound (11), we have used for each m the best possible $P(m)$ provided by (15). As $m\to 0$, the "basis" Coulomb problem $H=\beta\sqrt{m^2+\mathbf{p}^2}-v/r$ has energy $e(m)\to 0$; thus the Coulomb lower bound for a non-Coulomb problem becomes very weak for small values of m. Of course, Eq. (13) provides us with rigorous upper bounds for *every* energy level.

In order to get an idea of the location of the exact energy eigenvalues E, Fig. 1 also shows the ground-state energy curve $E(m)$ obtained by the Rayleigh–Ritz variational technique[9] with the

Laguerre basis states for the trial space defined in Ref. 18. Strictly speaking, this energy curve represents only an upper bound to the precise eigenvalue E. However, from the findings of Ref. 18 the deviations of these Laguerre bounds from the exact eigenvalues may be estimated, for the superposition of 25 basis functions used here, to be of the order of 1%.

VI. SUMMARY AND CONCLUSION

In this analysis we have studied the discrete spectrum of semirelativistic ''spinless-Salpeter'' Hamiltonians H, defined in Eq. (1), by an approach which is based principally on convexity. We have at our disposal very definite information concerning, on the one hand, the bottom of the spectrum of H for the Coulomb potential, $h(r)=-1/r$, and, on the other hand, the entire spectrum of H for the harmonic-oscillator potential, $h(r)=r^2$. The class of potentials that are at the same time a convex transformation of $-1/r$ and a concave transformation of r^2 includes, for example, arbitrary linear combinations of Coulomb, logarithmic, linear, and harmonic-oscillator terms. The envelope technique applied here takes advantage of the fact that all ''tangent lines'' to the interaction potential $V(r)=g(h(r))$ in H are potentials of the form $ah(r)+b$, and that, by convexity and the comparison theorem recalled in Sec. II D, the energy eigenvalues corresponding to these ''tangent'' potentials provide rigorous bounds to the unknown exact eigenvalues E of H. If $e(v)$ denotes the energy function—or a suitable bound to it—corresponding to the problem posed by a ''basis'' potential $vh(r)$, where v is a positive coupling parameter, the envelopes of upper and lower families of energy curves may be found with the help of the ''principal envelope formula''

$$E \approx \min_{v>0}[e(v)-ve'(v)+g(e'(v))].$$

Here, a sign of approximate equality is used to indicate that, for a definite convexity of $g(h)$, the envelope theory yields lower bounds for convex $g(h)$ and upper bounds for concave $g(h)$. With the above principal envelope formula at hand, all new spectral pairs $\{h(r),e(v)\}$ which may become available at some future time can immediately be used to enrich our collection of energy bounds. If the basis potential $h(r)$ is a pure power, these bounds can be written as

$$E_{nl} \approx \min_{r>0}\left[\beta\sqrt{m^2+\frac{P_{nl}^2}{r^2}}+V(r)\right],$$

where the numbers P_{nl} are obtained from the corresponding underlying basis problems. The power of this technique is illustrated, in Sec. V, by our application to the so-called funnel potential, $V(r)=-c_1/r+c_2 r$. For this problem, we have employed both the semirelativistic Coulomb and harmonic-oscillator problems to calculate, respectively, lower and upper bounds on the energy eigenvalues of the spinless Salpeter equation.

We expect that such results would provide bounds on the energy eigenvalues for general theoretical discussions, or be used as guides for more tightly focused analytic or numerical studies of the spectra of semirelativistic ''spinless-Salpeter'' Hamiltonians.

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Generalized Yang–Mills actions from Dirac operator determinants

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We consider the quantum effective action of Dirac fermions on four-dimensional flat Euclidean space coupled to external vector- and axial Yang–Mills fields, i.e., the logarithm of the (regularized) determinant of a Dirac operator on flat $\mathbb{R}^4$ twisted by generalized Yang–Mills fields. According to physics folklore, the logarithmic divergent part of this effective action in the pure vector case is proportional to the Yang–Mills action. We present a simple explicit computation proving this fact and extending it to the chiral case. We use an efficient computation method for quantum effective actions which is based on calculation rules for pseudo-differential operators and which yields an expansion of the logarithm of Dirac operators in local and quasi-gauge invariant polynomials of decreasing scaling dimension. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1399297]

I. INTRODUCTION

Determinants of differential operators arise as (exponentials of) effective actions in quantum field theory. The precise definition and investigation of such objects is an interesting and challenging mathematical problem which has led to an active and fruitful interplay between mathematics and physics.

In this paper we compute the logarithmic divergent part, $S_{\log}(A)$, of the logarithm of the regularized determinant for Dirac operators D_A describing Dirac fermions coupled to a generalized Yang–Mills field A on four-dimensional spacetime. For simplicity we assume spacetime to be flat $\mathbb{R}^4$ with Euclidean signature and the natural spin structure. The Yang–Mills fields we consider contain, besides the vector part V, also a chiral (axial) part C [for precise definitions see Eq. (7) *ff.* below]; we write $A=(V,C)$. Our definition of $S_{\log}$ is motivated by physical considerations and will be explained further below. To indicate the mathematical significance of our calculation, we note that $S_{\log}(A)$ is (essentially) the noncommutative residue [Wodzicki (1985)] of the logarithm of D_A [see Eq. (3) for the precise statement]. A main motivation for this work is to present a computation method for effective fermion actions which at the same time is mathematically rigorous, close to standard Feynman diagram computations in quantum field theory [see, e.g., Itzykson and Zuber (1985) and Weinberg (1996)], and simple to use. We believe that this method is a useful alternative to other methods like the ζ-function regularizations or the heat kernel expansions [see, e.g., Gilkey (1995) and Berline *et al.* (1992)]. We, therefore, made some effort to present this method in a self-contained way, in the hope that this is useful also for readers who are mainly interested in learning how to compute effective actions.

We now discuss our computation method [parts of this method were used previously by us in Langmann (1995) and Langmann and Mickelsson (1996)]. We regard the Dirac operator D_A as a PSDO (pseudo-differential operator) on a Hilbert space of square-integrable functions on $\mathbb{R}^4$. Our starting point is the following definition for the regularized effective fermion action:

$$S_\Lambda(A) := \mathrm{Tr}_\Lambda\left(\log\left(\frac{\mathsf{D}_A+\mathrm{i}m}{\Lambda_0}\right)-\log\left(\frac{\mathsf{D}_0+\mathrm{i}m}{\Lambda_0}\right)\right), \tag{1}$$

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where m is a real parameter which has the physical interpretation of a fermion mass, and Λ is a positive regularization parameter which we call UV (ultraviolet) *cutoff*. The role of the nonzero and complex parameter Λ_0 is twofold. Firstly, it makes the argument of the logarithm dimensionless, and secondly, setting $\Lambda_0 = |\Lambda_0|/(1+i0^+)$ avoids possible ambiguities due to the branch cuts of the logarithm which otherwise can arise. (Of course, all results must be independent of $|\Lambda_0|$, and this is a useful check.) This definition above has three ingredients. Firstly, a definition of the log of an operator a as an integral of the resolvent of a. Secondly, some basic facts about PSDO which imply a simple and powerful formula for the symbol of the resolvent of the Dirac operator D_A. And thirdly, a definition of a regularized Hilbert space trace Tr_Λ (where removing the regularization corresponds to the limit $\Lambda \to \infty$). Combining these ingredients we obtain an expansion of $S_\Lambda(A)$ in local and quasi-gauge invariant polynomials of decreasing scaling dimension. We find

$$S_\Lambda(A) = \Lambda^2 S^{(2)}(A) + \log\left(\frac{\Lambda}{|m|}\right) S_{\log}(A) + S^{(0)}(A) + \mathcal{O}(\Lambda^{-1}), \tag{2}$$

and this provides our definition of $S_{\log}(A)$. Our results for $S_{\log}(A)$ and $S^{(2)}(A)$ will be presented in the next Section. We shall also demonstrate on our way that $S_{\log}(A)$ is proportional to the noncommutative residue Wodzicki (1985) of the logarithm of the Dirac operator D_A:

$$S_{\log}(A) = 4\,\mathrm{Res}\left(\log\left(\frac{\mathsf{D}_A + \mathrm{i}m}{\Lambda_0}\right) - \log\left(\frac{\mathsf{D}_0 + \mathrm{i}m}{\Lambda_0}\right)\right). \tag{3}$$

The logarithm of the regularized trace of the determinant of the Dirac operator can then be defined as

$$S^{(0)}(A) = \mathrm{TR}\left(\log\left(\frac{\mathsf{D}_A + \mathrm{i}m}{\Lambda_0}\right) - \log\left(\frac{\mathsf{D}_0 + \mathrm{i}m}{\Lambda_0}\right)\right), \tag{4}$$

where TR is the renormalized trace which we will define, and we will provide all mathematical tools necessary for computing $S^{(0)}(A)$ explicitly.

We note that our computation method is closely related to methods which have been used in the physics literature for a long time [see, e.g., DeWitt (1965), Itzykson and Zuber (1985), and Weinberg (1996)]. The regularization we use is simple and close to how regularizations are often done in Feynman diagram computations, i.e., by introducing a sharp UV cutoff [see Eq. (32)]. We believe, however, that we can offer some improvements in detail which make computations easier, more transparent in structure, but nevertheless such that each step can be easily justified with mathematical rigor.

We now discuss some motivation for our computation from a quantum field theory point of view. As was known already to Schwinger for the Abelian case, the effective action of fermions coupled to a Yang–Mills field $A = V$ (i.e., $C = 0$) contains a logarithmic divergence, $\log(\Lambda/m)\, S_{\log}(A)$, and $S_{\log}(A)$ (for $C = 0$) is proportional to the usual Yang–Mills (YM) action

$$S_{\mathrm{YM}}(A) = \frac{1}{2g^2} \int_{\mathbb{R}^4} \mathrm{d}^4x\, \mathrm{tr}\, \mathcal{F}_{\mu\nu}\mathcal{F}^{\mu\nu},$$

[see, e.g., Itzykson and Zuber (1985) Eq. (12.123) where $1/\epsilon$ corresponds to $\log(\Lambda/m)$]. This is important since it implies that a change in the cutoff in the gauge theory, $\Lambda \to \Lambda'$, leads to a finite change of the effective fermion action which can be absorbed by changing the Yang–Mills coupled constant, $g^{-2} \to (g')^{-2} = g^{-2} + const.\log(\Lambda'/\Lambda)$. The logarithmic dependence of the Yang–Mills coupling constant on the UV cutoff is remarkable and distinguishes four space–time dimensions from all others.

Our computation is closely related to more recent ideas which have led to a deeper geometric understanding of the standard model of elementary particle physics (including Higgs sector). This approach is based on Connes' NCG [noncommutative geometry; textbooks on this subject are

Connes (1994) and Gracia-Bondia *et al.* (2001)]. One important ingredient of this approach is to define a generalized Dirac operator D_A, and this Dirac operator not only specifies the fermion part of the action of the model but also the Yang–Mills part $S_{\rm YM}(A)$: There is a definition of $S_{\rm YM}(A)$ in terms of D_A [see Chamseddine and Connes (1997) and references therein]. Our discussion above suggests a simple physical interpretation of this *spectral action principle* [Chamseddine and Connes (1997)]: The logarithmic divergence of the fermion effective action is potentially ''dangerous'' since it can make the model ambiguous: There is no preferred choice for the cut-off, and changing it generates a term proportional to $S_{\log}(A)$. However, the fact that $S_{\log}(A)$ is proportional to the Yang–Mills action resolves this problem for the standard (purely vector) Yang–Mills theory on $\mathbb{R}^4$, as discussed above. It, therefore, is natural to *require that the Yang–Mills action is proportional to the logarithmic divergent part of the fermion effective action in any gauge theory models*. In particular this suggests the following definition of the generalized (vector and chiral) Yang–Mills action in terms of the generalized Dirac operators D_A

$$S_{\rm YM}(A) := const.\,\frac{1}{2g^2}\,S_{\log}(A), \tag{5}$$

(for one fermion flavor $const. = 24\pi^2$). Equation (3) shows that for flat Euclidean space $\mathbb{R}^4$, this definition is equivalent to the one given in Chamseddine and Connes (1997). We conjecture that this is true for other four dimensional spin manifolds as well.

The plan of this paper is as follows. We summarize our notation and results in Sec. II. Section III contains a summary of the mathematical prerequisites, i.e., the three ingredients of our method mentioned above. The computations of $S_{\log}(A)$ is presented in Section IV with some computation details deferred to Appendix B. We conclude with some remarks in Sec. V. Appendix A contains some discussion on regularized traces and the noncommutative residue.

Notation: We write gl_N for the complex $N\times N$ matrices and GL_N for the invertible matrices in gl_N. We sometimes write I_V or I for the identity operator on a vector space V but often abuse notation and do not distinguish between cI and c for complex numbers. For V, W vector spaces and a an operator on V, we often use the same symbols a to also denote the corresponding operator $a\otimes I_W$ and $I_W\otimes a$ on $V\otimes W$ and $W\otimes V$, respectively. The real part of a complex number c is denoted as $\Re c$.

II. DEFINITIONS AND RESULTS

For simplicity we assume spacetime $M^4=\mathbb{R}^4$ with Euclidean signature (the extension of our calculation to other four–dimensional spin manifolds should be possible using symbol calculus of pseudo–differential operators [Hörmander (1995)]).

We consider the Hilbert

$$\mathcal{H} = L^2(\mathbb{R}^4)\otimes\mathbb{C}^4_{\rm spin}\otimes\mathbb{C}^N_{\rm color}, \tag{6}$$

which has the physical interpretation as space of the one–particle states of the fermions. We also introduce the space $\mathcal{D}$ of functions in $\mathcal{H}$ which are smooth (i.e., C^∞) and L^1; $\mathcal{D}$ is a convenient dense domain in $\mathcal{H}$.

The Dirac operators of interest to us are of the form

$$\hat{D}_A = \gamma^\nu(-\mathrm{i}\partial_\nu + V_\nu(x) + \mathrm{i}\gamma_5 C_\nu(x)), \tag{7}$$

where $A=(V,C)$ (repeated indices $\nu,\mu\ldots=1,2,3,4$ are summed over; $x=(x^1,x^2,x^3,x^4)\in\mathbb{R}^4$), with $\partial_\nu=\partial/\partial x^\nu$ and γ^ν the Dirac spin matrices acting on $\mathbb{C}^4_{\rm spin}$ and obeying

$$\gamma^\mu\gamma^\nu+\gamma^\nu\gamma^\mu = 2\,\eta^{\mu\nu}, \tag{8}$$

for $\mu,\nu=1,2,3,4$, where $\eta^{\mu\nu}=\eta_{\mu\nu}=diag(1,1,1,1)$ is the metric tensor, and

$$\gamma_5 := \gamma^1\gamma^2\gamma^3\gamma^4, \tag{9}$$

as usual (for the convenience of the reader, explicit formulas for these matrices are given in Appendix A 1).

For simplicity we assume that the functions V_ν and C_ν, $\mathbb{R}^4 \to \mathrm{gl}_N$, are *regular*, i.e., they are C^∞ and vanish like $\mathcal{O}(|x|^{-4-\varepsilon})$, for some $\varepsilon > 0$, as $|x| \to \infty$ (the latter condition is to ensure that integrals of regular functions over $\mathbb{R}^4$ absolutely converge).

In particular, the free Dirac operator is defined by the differential operator

$$\hat{D}_0 = -\mathrm{i}\gamma^\nu \partial_\nu . \tag{10}$$

We define the *gauge group* $\mathcal{G}$ as follows. Let GL_N be the group of all invertible matrices in gl_N. Then $\mathcal{G}$ is the group of all GL_N-valued functions U on $\mathbb{R}^4$ such that $U(x) - 1$ is a regular function. Note that one can write

$$\hat{D}_A = \tfrac{1}{2}(1-\gamma_5)\gamma^\nu(-\mathrm{i}\partial_\mu + V_\mu + \mathrm{i}C_\mu) + \tfrac{1}{2}(1+\gamma_5)\gamma^\nu(-\mathrm{i}\partial_\mu + V_\mu - \mathrm{i}C_\mu),$$

where $V_\mu \pm \mathrm{i}C_\mu$ are the *chiral* components of the gauge field. This representation shows that it is natural to consider two kinds of gauge transformations,

$$V_\mu \pm \mathrm{i}C_\mu \to (U_\pm)^{-1}(V_\mu \pm \mathrm{i}C_\mu)U_\pm - \mathrm{i}(U_\pm)^{-1}\partial_\mu U_\pm , \quad U_\pm \in \mathcal{G}. \tag{11}$$

For $U_+ = U_- = U$ we denote these as *vector gauge transformation*, otherwise as *chiral gauge transformation*.

Note that $\hat{D}_A$ in Eq. (7) is well-defined on the domain $\mathcal{D} \subset \mathcal{H}$, and we find it useful to distinguish this formally self-adjoint differential operator in notation from the corresponding self-adjoint extension on $\mathcal{H}$ which we denote as D_A, i.e., $(\mathsf{D}_A f)(x) = \hat{D}_A f(x)$ for all $f(x) \in \mathcal{D}$. We also write

$$\mathsf{D}_A = \mathsf{D}_0 + \mathsf{A}, \tag{12}$$

where D_0 is the free Dirac operator (i.e., self-adjoint extension of $\hat{D}_0$) and A the operator defined by multiplication with the generalized Yang–Mills field

$$\hat{A}(x) = \gamma^\nu(V_\nu(x) + \mathrm{i}\gamma_5 C_\nu(x)). \tag{13}$$

We will compute the fermion effective action $S_\Lambda(A)$ defined in Eq. (1), and we will show that it can be expanded as in Eq. (2). As discussed, Tr_Λ is a Hilbert space trace with an UV cutoff $\Lambda > 0$, and Λ_0 is an arbitrary, in general complex, parameter making the argument of the logarithm dimensionless. Moreover, the real (positive or negative) parameter m corresponds to a fermion mass and serves as an infrared (IR) regulator in our computation. Our main result is an explicit formula for $S_{\log}(A)$.

Proposition: *The logarithmic divergent piece* $S_{\log}(\mathrm{A})$ *of the logarithm of the (regularized) determinant of the Dirac operator* D_A *equals*

$$S_{\log}(A) = \frac{1}{24\pi^2}\int_{M^4} d^4x\, \mathrm{tr}_N\left(\tfrac{1}{2}\mathcal{F}^+_{\mu\nu}(\mathcal{F}^+)^{\mu\nu} + \tfrac{1}{2}\mathcal{F}^-_{\mu\nu}(\mathcal{F}^-)^{\mu\nu} - 6m^2 C^\mu C_\mu\right), \tag{14}$$

where tr_N *is the usual matrix trace in* gl_N *and* ($[a,b] := ab - ba$)

$$\mathcal{F}^\pm_{\mu\nu} := \partial_\mu A^\pm_\nu - \partial_\nu A^\pm_\mu + \mathrm{i}[A^\pm_\mu, A^\pm_\nu], \quad A^\pm_\mu := V_\mu \pm C_\mu , \tag{15}$$

is the curvature associated with the chiral component $A^\pm$ *of the Yang–Mills field.*

(*Proof in Sec.* IV *with some details deferred to Appendix B.*)

For $C=0$ (no chiral field) we obtain

$$S_{\log}(A)=\frac{1}{24\pi^2}\int_{M^4}d^4x\,\mathrm{tr}_N\mathcal{F}_{\mu\nu}\mathcal{F}^{\mu\nu},$$

with

$$\mathcal{F}_{\mu\nu}=\partial_\mu V_\nu-\partial_\nu V_\mu+\mathrm{i}[V_\mu,V_\nu], \tag{16}$$

which is the standard Yang–Mills action. Note that $\mathcal{F}_{\mu\nu}=\mathrm{i}[D_\mu,D_\nu]$ with

$$D_\nu:=-\mathrm{i}\partial_\nu+V_\nu(x), \tag{17}$$

the covariant derivative, and similarly

$$\mathcal{F}^{\pm}_{\mu\nu}=\mathrm{i}[D_\mu\pm\mathrm{i}C_\mu,D_\nu\pm\mathrm{i}C_\nu]. \tag{18}$$

It is important to note that for $m=0$, $S_{\log}(A)$ in Eq. (14) this is manifestly invariant under all gauge transformations Eq. (11). For $m\neq 0$, there is also a mass term $\propto C^\mu C_\mu$ for the chiral gauge field which is only invariant under vector gauge transformations, i.e., only the transformations Eq. (11) with $U_+=U_-=U$. The parameter in front of this term is fixed by the fermion mass. There is no similar term for the vector gauge field (note that such a term would spoil vector gauge invariance).

It is interesting to note that the result of our computation in Sec. IV suggests that for manifolds M^4 with boundary ∂M^4, $S_{\log}(A)$ has an additional contribution

$$\Delta S_{\log}(A)=\frac{1}{24\pi^2}\int_{M^4}d^4x\,\partial^\mu\mathrm{tr}_N J_\mu, \tag{19}$$

with

$$J_\mu:=2C_\mu\mathrm{i}[D_\nu,C^\nu]-2C^\nu\mathrm{i}[D_\nu,C_\mu]+2\mathrm{i}[D_\mu,C^\nu C_\nu]. \tag{20}$$

This is a boundary term (by Stokes's theorem). Note that this term is also invariant under vector gauge transformations, and it vanishes if the axial Yang–Mills field C_μ is zero.

It is also worth noting that, as a by-product, we also obtain the explicit expression for the quadratic divergent part of the effective action:

$$S^{(2)}(A)=\frac{1}{16\pi^2}\int_{M^4}d^4x\,\mathrm{tr}_N(-V^\mu V_\mu+C^\mu C_\mu). \tag{21}$$

In contrast to $S_{\log}(A)$ this term is not gauge invariant (as already mentioned, the term $\propto V^\mu V_\mu$ spoils vector gauge invariance)! This highlights the fact that the regularization procedure we use is not manifestly gauge invariant but only quasi-gauge invariant. It shows that the vector gauge invariance of our result for $S_{\log}$ is somewhat remarkable. It is also interesting to note that for $V_\mu=\pm C_\mu$, $S^{(2)}(A)=0$.

III. CALCULATION TOOLS

In this Section we collect the mathematical prerequisites for our computation. We will explain the three ingredients for our method: Firstly, a definition of the logarithm of operators a in terms of an integral of the resolvent of a. Secondly, a few basic definitions for PSDO which imply a simple and elegant formula for the symbol of the resolvent of Dirac operators D_A. And finally, a

definition of a regularized Hilbert space trace Tr_Λ (corresponding to introducing an UV cutoff Λ). In the next Section we will put these ingredients together and obtain an expansion of the effective action as described in the Introduction.

A. The logarithm of operators

Let a be a bounded operator on a Hilbert space $\mathcal{H}$ with norm less than one. Then ($I=I_{\mathcal{H}}$ is the identity operator)

$$\log(I+a)=\int_0^1 \frac{\mathrm{d}s}{s}(I-(I+sa)^{-1}), \tag{22}$$

as can be seen by a Taylor expansion,

$$\log(I+a)=\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{n}a^n=-\sum_{n=1}^{\infty}\int_0^1\frac{\mathrm{d}s}{s}(-sa)^n,$$

interchanging summation and integration, and using the geometric series.

We take this as a motivation to *define*

$$\log\left(\frac{\mathsf{D}_A+\mathrm{i}m}{\Lambda_0}\right):=\int_0^1\frac{\mathrm{d}s}{s}\left(I-\left(I+s\left[\frac{\mathsf{D}_A+\mathrm{i}m}{\Lambda_0}-I\right]\right)^{-1}\right), \tag{23}$$

where Λ_0 is a some complex number. This representation of the logarithm as integral of a resolvent will be convenient for us since there is a simple formula for the resolvent of (generalized) Dirac operators, as discussed below.

B. Pseudo–differential operators

1. Generalities

We summarize some basic facts about pseudo-differential operators (PSDO) on $\mathbb{R}^4$ [a discussion for general manifolds can be found, e.g., in Hörmander (1985)]. We consider PSDO a on $\mathcal{H}$ which can be represented by their *symbol* $\sigma[a](p,x)$, i.e., a $\mathrm{gl}_4\otimes\mathrm{gl}_N$–valued functions on phase space $\mathbb{R}^4\times\mathbb{R}^4$ defined such that [Hörmander (1985)]

$$(af)(x)=\int_{\mathbb{R}^4}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}d^4y\,e^{ip\cdot(x-y)}\sigma[a](p,x)f(y), \tag{24}$$

for all $f(y)\in\mathcal{D}$ (matrix multiplication is understood; $p\cdot x=x^\nu p_\nu$). In particular, D_0 and A are PSDO with symbols

$$\sigma[\mathsf{D}_0](p,x)=\not{p}:=\gamma^\nu p_\nu,\quad \sigma[\mathsf{A}](p,x)=\hat{A}(x). \tag{25}$$

Eq. (24) implies the following equation which encodes the product of operators in terms of their symbols:

$$\sigma[ab](p,x)=\int_{\mathbb{R}^4}\frac{\mathrm{d}^4q}{(2\pi)^4}\int_{\mathbb{R}^4}d^4y\,\mathrm{e}^{\mathrm{i}(x-y)\cdot(p-q)}\sigma[a](q,x)\sigma[b](p,y). \tag{26}$$

We will encounter PSDO a which allow an asymptotic expansion

$$\sigma[a]\sim\sum_{j=0}^{\infty}\sigma_{K-j}[a], \tag{27}$$

where $\sigma_{K-j}[a](p,x)$ is homogeneous of degree $K-j$ in p, [i.e., $\sigma_{K-j}[a](sp,x) = s^{K-j}\sigma_{K-j}[a](p,x)$ for all $s>0$ and $|p|>0$] and behaves as $|p|^{K-j}$ for $|p|\to\infty$ ($|p| := \sqrt{p\cdot p}$). We write

$$\sigma[a](p,x) = \sum_{j=0}^{n} \sigma_{K-j}[a](p,x) + \mathcal{O}(|p|^{K-n-1}), \tag{28}$$

for all integers n. Eq. (26) implies

$$\sigma[ab](p,x) \sim \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \frac{\partial^n \sigma[a](p,x)}{\partial p_{i_1}\cdots\partial p_{i_n}} \frac{\partial^n \sigma[b](p,x)}{\partial x_{i_1}\cdots\partial x_{i_n}}. \tag{29}$$

This equation allows to determine the asymptotic expansions of $\sigma[ab]$ and $\sigma[a^{-1}]$ from the ones of $\sigma[a]$ and $\sigma[b]$.

2. The symbol of the resolvent

Equation (23) expresses $\log(\mathsf{D}_A + \mathrm{i}m)$ as an integral of resolvents of the Dirac operator D_A, i.e., of operators $(c_1 I + c_2 \mathsf{D}_A)^{-1}$ with $c_{1,2}$ complex numbers. We will therefore need the symbol of such a resolvent. To determine this we note that

$$\sigma[c_1 I + c_2 \mathsf{D}_A](p,x) = c_1 + c_2[\not{p} + \hat{A}(x)]. \tag{30}$$

We then could use Eq. (29) to find the expansion for $\sigma[(c_1 I + c_2 \mathsf{D}_A)^{-1}](p,x)$. We now present a useful result summarizing this expansion in a simple formula.

Lemma: The following holds for all $c_1, c_2 \in \mathbb{C}$

$$\sigma[(c_1 I + c_2 \mathsf{D}_A)^{-1} a](p,x) = (c_1 + c_2[\not{p} + \hat{D}_A])^{-1} \sigma[a](x,p). \tag{31}$$

Remark: The proper interpretation of this equation is as follows:

$$\sigma[(c_1 I + c_2 \mathsf{D}_A)^{-1} a](p,x) \sim \sum_{n=0}^{\infty} (-1)^n (c_1 + c_2 \not{p})^{-1} [\hat{D}_A (c_1 + c_2 \not{p})^{-1}]^n \sigma[a](x,p),$$

where the differential operators ∂_ν in $\hat{D}_A = -\mathrm{i}\gamma^\mu \partial_\nu + \hat{A}(x)$ act to the right on the functions $\hat{A}(x)$ according to the Leibniz rule. We note that we will need this equation only for $a = I$.

Proof of the Lemma: One can check Eq. (31) by using Eqs. (27) and (29), taking $c_1 I + c_2 \mathsf{D}_A$ for a and $[c_1 I + c_2 \mathsf{D}_A]^{-1} a$ for b, and inserting Eq. (30). A simpler argument avoiding tedious expansions is as follows: Note that by definition, $(\mathsf{D}_A f)(x) = [\hat{D}_0 + \hat{A}(x)] f(x)$ for all $f \in \mathcal{D}$, thus

$$((c_1 I + c_2 \mathsf{D}_A) a f)(x) = (c_1 + c_2[\hat{D}_0 + \hat{A}(x)])(af)(x) = \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4} \int_{\mathbb{R}^4} d^4 y\, e^{ip\cdot(x-y)} (c_1 + c_2[\not{p} + \hat{D}_0 + \hat{A}(x)]) \sigma[a](p,x) f(y),$$

where we used Eq. (24) and the Leibniz rule. Replacing a in this equation by $(c_1 I + c_2 \mathsf{D}_A)^{-1} a$, we see that this is equivalent to Eq. (31). [Note that this argument implies the interpretation of Eq. (31) as given above!] □

Remark: We believe that our expansion in powers of the differential operator $\hat{D}_A$ is very natural for at least two reasons. Firstly, since under a vector gauge transformation, $\hat{D}_A \to U^{-1} \hat{D}_A U$, such an expansion is close to being manifestly gauge invariant (we will discuss this point in more detail below). Secondly, it is natural from the point of view of power counting: In

contrast to an expansion in $\hat{A}$, the nth order term in our expansion includes precisely those local polynomials in V_μ and C_ν (and derivatives thereof) which all have the same scaling dimension $4-n$.

Remark: Loosely speaking, PSDO are useful since they allow to interpolate between Fourier- and position space: Generically in quantum theory one deals with operators H on some Hilbert space of L^2-functions on $\mathbb{R}^n$ which are a sum of a free part H_0 diagonal in Fourier space, [$\hat{f}(p) = \int_{\mathbb{R}^n} \mathrm{d}^n x\, e^{ip\cdot x} f(x)$ denotes the Fourier transform], $\widehat{(H_0 f)}(p) = E_0(p)\hat{f}(p)$, and a potential term V diagonal in position space, $(Vf)(x) = V(x)f(x)$. The symbol of H is then simply the sum of $E_0(p)$ and $V(x)$, which is an attractive feature. The price one has to pay is that the symbol of ("nice") functions F of H are somewhat complicated: In a first approximation, $\sigma[F(H)](p,x) \sim F(E_0(p)+V(x))+\cdots$, but there are correction terms $\cdots$ depending on derivatives. The Lemma above is a special case of the following formula,

$$\sigma[F(H)](p,x) \sim F(E_0(p-\mathrm{i}\partial)+V(x))1,$$

nicely summarizing the systematic derivative expansion of functions of H.

C. Regularized traces and the noncommutative residue

We now define the regularized trace which we will use. We first note that due to our technical assumptions on the gauge fields all operators a which we will encounter are PSDO which have symbols $\sigma[a](p,x)$ which go at least like $\mathcal{O}(|x|^{-4-\varepsilon})$, some $\varepsilon>0$, for fixed p and $|x|\to\infty$, and are finite for finite p. Thus

$$\mathrm{Tr}_\Lambda(a) := \int_{|p|\leqslant\Lambda} \frac{\mathrm{d}^4 p}{(2\pi)^4} \int_{\mathbb{R}^4} d^4x\, \mathrm{tr}\, \sigma[a](x,p), \tag{32}$$

where tr is the full matrix trace (including the trace tr_ν in gl_4 and the trace tr_N in gl_N), is well-defined for $\Lambda<\infty$, and this defines a regularized Hilbert space trace: If a is a trace–class operator then $\mathrm{Tr}_\Lambda(a)$ has a well-defined limit $\Lambda\to\infty$ which is equal to the Hilbert space trace of a [Hörmander (1985)]. More generally one can consider PSDO a for which $\mathrm{Tr}_\Lambda(a)$ can be expanded as

$$\mathrm{Tr}_\Lambda(a) = c^{(K)}(a)\Lambda^K + c^{(K-1)}(a)\Lambda^{K-1} + \cdots + c^{(1)}(a)\Lambda + c_{\log}(a)\log\left(\frac{\Lambda}{|m|}\right) + c^{(0)}(a) + \mathcal{O}(\Lambda^{-1}), \tag{33}$$

with K some non-negative integer.

We recall that the noncommutative residue [Wodzicki (1985)] of a PSDO a with an asymptotic expansion as in Eq. (27) can be defined as [see, e.g., Eq. (2.7) in Varilly and Gracia-Bondia (1993)]

$$\mathrm{Res}(a) := \frac{1}{4}\int_{\mathbb{R}^4} \frac{\mathrm{d}^4 p}{(2\pi)^4}\, \delta(|p|-1) \int_{\mathbb{R}^4} d^4x\, \mathrm{tr}\sigma_{-4}[a](x,p), \tag{34}$$

and for PSDO a as above:

$$\mathrm{Res}(a) = \tfrac{1}{4} c_{\log}(a), \tag{35}$$

i.e., the residue is equal, up to a constant, to the logarithmic divergent part of the regularized trace of a. (An elementary proof of this latter fact is outlined in Appendix A.)

Remark: In our definition of Tr_Λ we use a sharp cutoff, i.e.,

$$\mathrm{Tr}_\Lambda(a)=\int_{\mathbb{R}^4}\frac{\mathrm{d}^4p}{(2\pi)^4}f\left(\frac{|p|}{\Lambda}\right)\int_{|p|\leqslant\Lambda}d^4x\,\mathrm{tr}\sigma[a](x,p), \tag{36}$$

where $f(t)$ equals the Heaviside step function $\theta(1-t)$. In principle one could define a regularized trace using Eq. (36) and choosing any non-negative, piece-wise smooth, function $f(t)$ which vanishes exponentially fast for $|t|\to\infty$ and is such that $f(0)=1$. For example, the choice $f(t)=\exp(-t^2)$ would correspond to the standard heat kernel regularization.

We will show in Appendix A that $c_{\log}(a)$ is in fact independent of f.

Using any such regularization one can define the *renormalized trace* as the finite part of the regularized trace:

$$\mathrm{TR}(a):=c_0(a), \tag{37}$$

but this is not quite independent of the regularization: As also discussed in Appendix A, changing the regularization function $f\to\tilde{f}$ amounts to changing

$$\mathrm{TR}(a)\to\mathrm{TR}(a)+\log(s)\,c_{\log}(a), \tag{38}$$

with some constant $s>0$ depending on f and $\tilde{f}$: The logarithmic divergent piece accounts for the regularization dependence of the renormalized trace, and this is the reason for our interest in it, as discussed in the Introduction.

Remark: We note Eq. (36) is equivalent to

$$\mathrm{Tr}_\Lambda(a)=\mathrm{Tr}(P_\Lambda a),\quad P_\Lambda:=f(|\mathsf{D}_0|/\Lambda), \tag{39}$$

(using the spectral theorem for self-adjoint operators). This naturally extends the definition of Tr_Λ from PSDO to a large class of operators on $\mathcal{H}$. More generally, one could change the regularization by changing $\mathsf{D}_0\to\mathsf{D}_B$ in the definition of P_Λ, for some fixed Yang–Mills field B. One can show that this would change $\mathrm{TR}(a)$ by a term proportional to $\mathrm{Res}([\log(\mathsf{D}_B)-\log(\mathsf{D}_0)]a)$ [see, e.g., Eq. (1.6) in Cardona *et al.* (2000)]. It would be interesting to explore this possibility in more detail.

IV. COMPUTATION OF EFFECTIVE FERMION ACTION

In this Section we present the explicit computation of the effective fermion action and thus prove the proposition in Sec. II. Our computation amounts to a quasi-gauge invariant gradient expansion, which is essentially an expansion in powers of the UV cutoff Λ. This allows us to extract, in a simple manner, the quadratic and logarithmic divergent pieces which is what we are interested in.

A. Quasi-gauge covariant expansion

We write

$$S_\Lambda(A)=\int_{|p|\leqslant\Lambda}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_{\mathbb{R}^4}d^4x\,\mathrm{tr}\,\mathcal{S}(x,p)\,1, \tag{40}$$

where $\mathcal{S}(x,p)$ is obtained by computing the symbol of the operator $\log(\mathsf{D}_A+\mathrm{i}m)/\Lambda_0-\log(\mathsf{D}_0+\mathrm{i}m)/\Lambda_0$ as explained in the last Section, i.e.,

$$\begin{aligned}\mathcal{S}(x,p)&=\int_0^1\frac{\mathrm{d}s}{s}([1-s+s\not{p}+s\not{a}]^{-1}-[1-s+s\not{p}]^{-1})\\&=\int_0^\infty\frac{\mathrm{d}u}{u}([1+u\not{p}+u\not{a}]^{-1}-[1+u\not{p}]^{-1}),\end{aligned} \tag{41}$$

where we used Eqs. (22) and (31), introduced the convenient short-hand notion

$$\tilde{\not{p}} := \frac{\not{p} + \mathrm{i}m}{\Lambda_0}, \quad \tilde{\not{a}} := \frac{-\mathrm{i}\not{\partial} + \hat{\not{A}}}{\Lambda_0}, \tag{42}$$

and changed integration variables, $s = u/(1+u)$. The 1 on the right-hand side (r.h.s.) of Eq. (40) is the symbol of the identity operator. As explained in more detail below, $\mathcal{S}$ here is to be regarded as a differential operator acting on 1. It is straightforward to expand the integrand in this equation in powers of $\tilde{\not{a}}$:

$$\mathcal{S} = \sum_{n=1}^{L} (-1)^{n-1} \mathcal{S}_n + \mathcal{R}_{L+1}, \tag{43}$$

where

$$\mathcal{S}_n = (-1)^{n-1} \int_0^\infty \frac{\mathrm{d}u}{u} \frac{1}{1+u\tilde{\not{p}}} \left(u\tilde{\not{a}} \frac{1}{1+u\tilde{\not{p}}} \right)^n \tag{44}$$

and

$$\mathcal{R}_{L+1} = \int_0^\infty \frac{\mathrm{d}u}{u} \frac{1}{1+u\tilde{\not{p}}} \left(u\tilde{\not{a}} \frac{1}{1+u\tilde{\not{p}}} \right)^L u\tilde{\not{a}} [1 + u(\tilde{\not{p}} + \tilde{\not{a}})]^{-1}, \tag{45}$$

is a remainder term.

In the following we find it convenient to use the short-hand notation and write:

$$\hat{D}_A = \sum_{s=0,5} \gamma_s^\nu D_\nu^s \tag{46}$$

where

$$D_\nu^0 := D_\nu \quad D_\nu^5 := C_\nu \tag{47}$$

and

$$\gamma_0^\nu := \gamma^\nu, \quad \gamma_5^\nu := \mathrm{i}\gamma^\nu \gamma_5. \tag{48}$$

We then define

$$\mathcal{M}_{n;s_1\cdots s_n}^{\nu_1\cdots\nu_n} := (\Lambda_0)^{-n} \int_{|p|\leqslant\Lambda} \frac{\mathrm{d}^4 p}{(2\pi)^4} \mathrm{tr}_\nu \int_0^\infty \mathrm{d}u u^{n-1} \frac{1}{1+u\tilde{\not{p}}} \gamma_{s_1}^{\nu_1} \frac{1}{1+u\tilde{\not{p}}} \cdots \gamma_{s_n}^{\nu_n} \frac{1}{1+u\tilde{\not{p}}}, \tag{49}$$

where $s_j = 0,5$ and $\nu_j = 1,2,3,4$. This allows us to write

$$\mathcal{S}_n := \int_{|p|\leqslant\Lambda} \frac{\mathrm{d}^4 p}{(2\pi)^4} \int_{\mathbb{R}^4} d^4x \mathrm{tr}\, \mathcal{S}_n(x,p) = \sum_{\underline{s}} \mathcal{M}_{n;\underline{s}}^{\nu_1\cdots\nu_n} \int_{\mathbb{R}^4} d^4x \mathrm{tr}_N D_{\nu_1}^{s_1} \cdots D_{\nu_n}^{s_n}: \tag{50}$$

here and in the following, $\underline{s}$ is short for $(s_1,..,s_n)$.

The following Lemma simplifies the computation significantly: It implies that the $\mathcal{S}_n$ for *odd* integers n all vanish, and that a series expansion in the mass m only has nonzero *even* powers.

Lemma: The coefficients $\mathcal{M}_{n;\underline{s}}^{\nu}$ in Eq. (49) are nonzero only for even integers n, and they are invariant under $m \to -m$, i.e., they are independent of the sign of the mass.
(Proof in Appendix B.)

Remark: We now can explain why we denote our expansion quasi–gauge invariant. This is because the operators D_ν^s transform gauge covariantly under a vector gauge transformation U,

$D^s_\nu \to U^{-1} D^s_\nu U$. This implies that the differential operators defined in Eq. (50) all are gauge invariant. However, the action is a polynomial which is obtained by applying these differentiation operators to 1 [cf. Eqs. (40)] using Leibniz rule and $\partial_\nu 1 = 0$, e.g.,

$$\begin{aligned} D_\nu 1 &= V_\nu(x), \\ D_{\nu_1} C_{\nu_2} 1 &= -\mathrm{i}[\partial_{\nu_1} C_{\nu_2}(x)] + V_{\nu_1}(x) C_{\nu_2}(x), \\ D_{\nu_1} D_{\nu_2} 1 &= -\mathrm{i}[\partial_{\nu_1} V_{\nu_2}(x)] + V_{\nu_1}(x) V_{\nu_2}(x), \end{aligned} \tag{51}$$

etc. The result will be gauge invariant only if the differential operator in Eq. (50) is already a polynomial. This happens, e.g., if the differential operators D_ν only appear in combinations $[D_\nu, D_\mu]$ and $[D_\nu, C_\mu]$. This is not obvious. However, we will see below that this happens for the terms leading to logarithmic divergent part.

B. Expansion in powers of the UV cutoff

We now show that our expansion above is essentially an expansion in powers of the UV cutoff Λ. Our computation can be simplified by the following argument (this argument is refined and justified in detail in Appendix B). As mentioned, m serves as a particular IR cutoff for momentum integrals. We expect that our result is independent of the precise form of the IR regularization. Thus we use instead the following, simpler one: we set $m = 0$ in $\not{p}$ but restrict integrations over p to $m \leqslant |p| \leqslant \Lambda$. *We stress that we use this simplification in the main text only to ease our presentation, and that it is appropriate only for computing the diverging contributions to the regularized determinant: The computation of the finite part should be done with the method explained in Appendix B.* Below we shall see that this simplified procedure gives an IR regularization provided we also set $\Lambda_0 = |\Lambda_0|/(1 + \mathrm{i}0^+)$ (a justification of this can be also found in the Appendix B). Using then

$$\frac{1}{1 + u\not{p}} = \frac{1}{1 - u^2 |p|^2 (\Lambda_0)^{-2}} [1 - u\not{p}(\Lambda_0)^{-1}],$$

and rescaling $u|p|(\Lambda_0)^{-1} \to u(1 + \mathrm{i}0^+)$ we see that $\mathcal{M}_n$ in Eq. (49) becomes (we use the different symbol $\tilde{\mathcal{M}}_n$ to indicate that these numbers are obtained with a simplified IR regularization.)

$$\tilde{\mathcal{M}}^\nu_{n;\underline{s}} = \frac{1}{8\pi^2} \int_{|m|}^{\Lambda} \mathrm{d}|p| |p|^{3-n} \mathcal{J}^\nu_{n;\underline{s}}(p), \tag{52}$$

where

$$\mathcal{J}^{\nu_1 \cdots \nu_n}_{n;\underline{s}} := \int_0^\infty \mathrm{d}u\, u^{n-1} \left(\frac{1}{1 - [u(1 + \mathrm{i}0^+)]^2} \right)^{n+1} \langle \mathrm{tr}_\nu (1 - u\not{\xi}) \gamma^{\nu_1}_{s_1} (1 - u\not{\xi}) \cdots \gamma^{\nu_n}_{s_n} (1 - u\not{\xi}\not{\xi}) \rangle, \tag{53}$$

and we used $(2\pi)^{-4} \int_{m \leqslant |p| \leqslant \Lambda} \mathrm{d}^4 p\, g(p) = (8\pi^2)^{-1} \int_{|m|}^{\Lambda} \mathrm{d}|p| |p|^3 \langle g(|p|\xi) \rangle$ with

$$\langle g(\xi) \rangle := \frac{1}{2\pi^2} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4 \xi}{(2\pi)^4}\, \delta(|\xi| - 1)\, g(\xi), \tag{54}$$

the angular average (i.e., integration over the unit sphere in $\mathbb{R}^4$). We now see that $\Lambda_0 = |\Lambda_0|/(1 + \mathrm{i}0^+)$ is needed to specify how to treat the singularity in the u-integral. These u-integrals are then finite [see Eqs. (56) and (57) below]. The result we get is independent of $|\Lambda_0|$, as expected. It shows explicitly that our expansion leads to an expansion of the action in powers of Λ. We are

interested in $\Lambda\to\infty$. In this limit, $\tilde{\mathcal{M}}_n \propto |\Lambda|^{n-4}$ for $n<4$ and $\propto |m|^{4-n}$ for $n>4$: The former terms are divergent in the UV (i.e., for $\Lambda\to\infty$), the latter in the IR (i.e., for $m\to 0$). It is precisely the "boundary case" $n=4$ which gives rise to the logarithmic divergence.

This result obtained with the simplified IR treatment is correct only in leading order in Λ. In Appendix B we show how to do the computation without this simplification, and that

$$\mathcal{M}_n = \tilde{\mathcal{M}}_n + \mathcal{O}(m^2 \Lambda^{2-n}), \quad n>2, \tag{55}$$

showing that the simplified IR treatment gives the correct result for the diverging terms for all n but $n=2$. For $n=2$ there are corrections $\propto m^2 \log(\Lambda/m)$ which contribute to $S_{\log}$ and which we, therefore, have to compute exactly.

C. Computation of diverging parts of the effective action

We now proceed to compute the coefficients $\mathcal{J}_n$ Eq. (53) for those terms we are interested in, i.e., for $n=1,2,3,4$. Using Eq. (52) this is straightforward: One only needs to evaluate the integrals

$$\mathcal{N}_{n,k} = \int_0^\infty du\, u^{n+k-1} (1-[u(1+i0^+)]^2)^{-n-1}, \tag{56}$$

the angular averages $\langle \xi_{\nu_1} \cdots \xi_{\nu_k} \rangle$, and traces of products of Dirac matrices. The integrals in Eq. (56) are [cf., e.g., Eq. 3.251(11.) in Gradshteyn and Ryzhik (1980)]

$$\mathcal{N}_{n,k} = -(-1)^{(n-k)/2} B\left(\frac{n+k}{2}, \frac{n-k}{2}+1\right), \tag{57}$$

where $B(x,y)=\Gamma(x)\Gamma(y)/\Gamma(x+y)$. We only need

$$\mathcal{N}_{2,0} = \tfrac{1}{4}, \quad \mathcal{N}_{2,2} = -\tfrac{1}{4},$$

$$\mathcal{N}_{4,0} = \tfrac{1}{24}, , \quad \mathcal{N}_{4,2} = -\tfrac{1}{24}, \quad \mathcal{N}_{4,4} = \tfrac{1}{8}.$$

The computation of the traces of Dirac matrices is simplified using the following relations:

$$(1-u\xi)\gamma^\nu = \gamma^\nu (1+u\xi) - 2u\xi^\nu, \quad \nu = 1,2,3,4,$$

$$\gamma_5 \xi \gamma_5 = -\xi, \quad \xi^2 = |\xi|^2, \tag{58}$$

which follow from Eq. (8). We also need

$$\langle 1 \rangle = 1, \quad \langle \xi_{\mu_1} \xi_{\mu_2} \rangle = \tfrac{1}{4} \eta_{\mu_1\mu_2}$$

$$\langle \xi_{\mu_1} \xi_{\mu_2} \xi_{\mu_3} \xi_{\mu_4} \rangle = \tfrac{1}{24} (\eta_{\mu_1\mu_2}\eta_{\mu_3\mu_4} + \eta_{\mu_1\mu_3}\eta_{\mu_2\mu_4} + \eta_{\mu_1\mu_4}\eta_{\mu_2\mu_3}), \tag{59}$$

and that the angular average for a product of an odd number of components ξ_{μ_j} is zero. Moreover,

$$\mathrm{tr}_\nu(\gamma^{\mu_1}\gamma^{\mu_2}) = 4\eta^{\mu_1\mu_2},$$

$$\mathrm{tr}_\nu(\gamma^{\mu_1}\gamma^{\mu_2}\gamma^{\mu_3}\gamma^{\mu_4}) = 4(\eta^{\mu_1\mu_2}\eta^{\mu_3\mu_4} - \eta^{\mu_1\mu_3}\eta^{\mu_2\mu_4} + \eta^{\mu_1\mu_4}\eta^{\mu_2\mu_3}), \tag{60}$$

$$\mathrm{tr}_\nu(\gamma_5\gamma^{\mu_1}\gamma^{\mu_2}\gamma^{\mu_3}\gamma^{\mu_4}) = 4\epsilon^{\mu_1\mu_2\mu_3\mu_4},$$

where $\epsilon^{\mu_1\mu_2\mu_3\mu_4}$ is the completely antisymmetric symbol with $\epsilon^{1234}=1$. Note that $\mathrm{tr}_\nu(\gamma_\mu^s) = \mathrm{tr}_\nu(\gamma_{\mu_1}^{s_1}\gamma_{\mu_2}^{s_2}\gamma_{\mu_3}^{s_3}) = 0$ always.

TABLE I. Parameters in Eq. (65) where $\underline{s}=(s_1,s_2,s_3,s_4)$.

s_1	1	1	1	1	5	5	5	5	1	1	1	1	5	5	5	5
s_2	1	1	5	5	1	1	5	5	1	1	5	5	1	1	5	5
s_3	1	5	1	5	1	5	1	5	1	5	1	5	1	5	1	5
s_4	1	5	5	1	5	1	1	5	5	1	1	5	1	5	5	1
$A_{\underline{s}}$	0	−2	−2	2	−2	−2	−2	0	0	0	0	0	0	0	0	0
$B_{\underline{s}}$	−2	2	2	0	4	2	2	−2	0	0	0	0	0	0	0	0
$C_{\underline{s}}$	2	−2	0	2	−2	0	−2	2	0	0	0	0	0	0	0	0
$D_{\underline{s}}$	0	0	0	0	0	0	0	0	−i	−i	i	i	i	i	−i	−i

It is now easy to see that $\mathcal{J}^{\mu}_{1,s}=\mathcal{J}^{\mu_1\mu_2\mu_3}_{3;s_1s_2s_3}=0$, thus

$$\mathcal{S}_1=\mathcal{S}_3=0. \tag{61}$$

The simplest nonzero terms are for $n=2$. Combining the formulas given above it is easy to see that

$$\mathcal{J}^{\mu_1\mu_2}_{2;s_1s_2}=\frac{1}{8\pi^2}A_{s_1s_2}\eta^{\mu_1\mu_2},$$

$$A_{55}=-A_{00}=1,\quad A_{50}=A_{05}=0. \tag{62}$$

Thus

$$\tilde{\mathcal{S}}_2=\Lambda^2\frac{1}{16\pi^2}\int d^4x\,\mathrm{tr}_N(-D^{\mu}D_{\mu}+C^{\mu}C_{\mu}). \tag{63}$$

This is a gauge invariant differential operator. When acting on 1 [cf. Eq. (51)] we obtain the quadratic divergent part of the effective action Eq. (21) which is not gauge invariant.

As mentioned, $\tilde{\mathcal{S}}^{(2)}$ is only the leading order contribution to $\mathcal{S}^{(2)}$. A more careful computation without the simplified IR regularization gives (see Appendix B)

$$\mathcal{S}_2=\tilde{\mathcal{S}}_2-m^2\log\left(\frac{\Lambda}{|m|}\right)\frac{1}{8\pi^2}\int d^4x\,\mathrm{tr}_N(C^{\mu}C_{\mu})+\cdots, \tag{64}$$

where "$\cdots$" are terms which remain finite for $\Lambda\to\infty$. We see that the subleading term which was missed by the naive IR regularization contributes to $S_{\log}$. As discussed in Sec. II, this term is gauge invariant.

We now turn to the case $n=4$ which leads to the logarithmic divergence. All relations needed to compute the $\mathcal{J}^{\nu_1\nu_2\nu_3\nu_4}_{\underline{s}}$ were listed above. The result can be written as follows:

$$\mathcal{J}^{\nu_1\nu_2\nu_3\nu_4}_{\underline{s}}=\tfrac{1}{3}(A_{\underline{s}}\eta^{\nu_1\nu_2}\eta^{\nu_3\nu_4}+B_{\underline{s}}\eta^{\nu_1\nu_3}\eta^{\nu_2\nu_4}+C_{\underline{s}}\eta^{\nu_1\nu_4}\eta^{\nu_2\nu_3}+D_{\underline{s}}\epsilon^{\nu_1\nu_2\nu_3\nu_4}), \tag{65}$$

where $\underline{s}=(s_1,s_2,s_3,s_4)$. The numbers $A_{\underline{s}},B_{\underline{s}},C_{\underline{s}},D_{\underline{s}}$ are all given in Table I. (We have checked this result extensively using the symbolic programming language MAPLE.) We note that the numbers $A_{\underline{s}},B_{\underline{s}},C_{\underline{s}}$ ($D_{\underline{s}}$) all are real (purely imaginary) and nonzero only if an even (odd) number of the s_j equal 5.

Combining these results we find

$$\tilde{S}_4=\log\left(\frac{\Lambda}{|m|}\right)\frac{1}{24\pi^2}\int_{\mathbb{R}^4}d^4x\,\mathrm{tr}_N[\mathcal{P}_R+\mathcal{P}_I], \tag{66}$$

where

$$\mathcal{P}_R=\sum_{\underline{s}}\ (A_{\underline{s}}\eta^{\nu_1\nu_2}\eta^{\nu_3\nu_4}+B_{\underline{s}}\eta^{\nu_1\nu_3}\eta^{\nu_2\nu_4}+C_{\underline{s}}\eta^{\nu_1\nu_4}\eta^{\nu_2\nu_3})D^{s_1}_{\nu_1}D^{s_2}_{\nu_2}D^{s_3}_{\nu_3}D^{s_4}_{\nu_4}$$

$$\mathcal{P}_I=\sum_{\underline{s}}\ D_{\underline{s}}\epsilon^{\nu_1\nu_2\nu_3\nu_4}D^{s_1}_{\nu_1}D^{s_2}_{\nu_2}D^{s_3}_{\nu_3}D^{s_4}_{\nu_4}, \tag{67}$$

with the coefficients given in Table I. $\mathcal{P}_R$ is a sum of 19 nonzero terms. We now claim that it is possible to write $\mathcal{P}_R=\mathcal{P}_{R,1}+\mathcal{P}_{R,2}$ where

$$\begin{aligned}\mathcal{P}_{R,1}=&-[D^\mu,D^\nu][D_\mu,D_\nu]-[C^\mu,C^\nu][C_\mu,C_\nu]+[D^\mu,D^\nu][C_\mu,C_\nu]+[C^\mu,C^\nu][D_\mu,D_\nu]\\&+2[D^\mu,C^\nu][D_\mu,C_\nu]+2[D^\mu,C^\nu][C_\mu,D_\nu]\end{aligned} \tag{68}$$

and

$$\mathcal{P}_{R,2}=\mathrm{i}[D^\mu,J_\mu]+[[D^\mu,D^\nu],[C_\mu,C_\nu]]-2[C^\mu,[D_\mu,D_\nu]C^\nu] \tag{69}$$

with J_μ given in Eq. (20). Similarly

$$\mathcal{P}_I=\frac{\mathrm{i}}{2}\epsilon^{\nu_1\nu_2\nu_3\nu_4}[[D_{\nu_1},D_{\nu_2}]+[C_{\nu_1},C_{\nu_2}],[D_{\nu_3},C_{\nu_4}]]. \tag{70}$$

[The proof of Eqs. (68)–(70) are straightforward calculation which we skip.]

We see that, $\mathcal{P}_{R,1}$ equals $\frac{1}{2}(\mathcal{F}^+_{\mu\nu}(\mathcal{F}^+)^{\mu\nu}+\mathcal{F}^-_{\mu\nu}(\mathcal{F}^-)^{\mu\nu})$ with $\mathcal{F}^\pm_{\mu\nu}$ defined in Eq. (15). The remaining terms are linear combinations of commutators! Using the cyclicity of the matrix trace we thus obtain

$$\mathrm{tr}_N\mathcal{P}_{R,2}=\partial^\mu\mathrm{tr}_N J_\mu,\quad \mathrm{tr}_N\mathcal{P}_I=0. \tag{71}$$

This implies Eqs. (14)–(20) and completes our computation. □

Remark: Note that $\mathcal{P}_R$ and $\mathcal{P}_I$ are not differential operators but polynomials [i.e., there are no terms $(\cdots)D_\mu$]. This implies that both these terms are gauge covariant which, as we believe, is remarkable.

V. CONCLUSIONS

The regularization which we used was simple but not manifestly gauge invariant. For the result computed in this paper the latter property is irrelevant: since the logarithmic divergence is regularization dependent one can compute it using any regularization. However, we believe that our method is useful even for computing the finite part of the effective action, i.e., $S^{(0)}(A)$ in Eq. (4). We stress again that the simplified IR regularization used in the main text is not appropriate in this computation but the formulas given in Appendix B should be used. We conjecture that $S^{(0)}(A)$ computed in this way is gauge invariant.

As mentioned in the Remark at the end of Sec. 3, we defined a renormalized trace $\mathrm{TR}_{|\mathsf{D}_0|}$ using the free Dirac operator D_0. More general we could use the Dirac operator D_B with some fixed nontrivial Yang–Mills field B. In particular, we expect that the standard ζ-function regularization of the logarithm of the determinant of D_A should be identical with

$$\mathrm{TR}_{|\mathsf{D}_A|}\log\left(\frac{\mathsf{D}_A+\mathrm{i}m}{\Lambda_0}\right),$$

where the regularization function is $f(t)=\exp(-t^2)$. The latter definition has the advantage that it is manifestly gauge invariant, but it seems less easy to use for explicit computations as ours. It is natural to expect that the difference between the latter definition and $S^{(0)}(A)$ in Eq. (4) is also proportional to $S_{\log}(A)$.

Effective action computations are used in many applications of quantum field theory. We believe that the methods which we presented should be useful in other such contexts as well.

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APPENDIX A: MORE ON REGULARIZED TRACES

In this Appendix we outline elementary proofs of some facts about regularized traces stated in the main text.

1. The logarithmic divergence

We compute the regularized trace in Eq. (36) for an operator a with a symbol allowing for an asymptotic expansion as in Eq. (27). It is easy to see that the contribution of $\sigma_k[a](p,x)$ to $\mathrm{Tr}_\Lambda(a)$ is

$$\int_0^\infty d|p||p|^{k+3} f\left(\frac{|p|}{\Lambda}\right) \int_{\mathbb{R}^4} \frac{\mathrm{d}^4\xi}{(2\pi)^4}\, \delta(|\xi|-1) \int_{\mathbb{R}^4} d^4x\, \mathrm{tr}\sigma_k[a](\xi,x),$$

where we used the homogeneity of $\sigma_k[a]$. Changing variables, $|p|\to u=|p|/\Lambda$, and comparing with Eq. (33) we see that for all $k\geqslant -3$

$$c_{k+4}(a)=N_k \int_{\mathbb{R}^4} \frac{\mathrm{d}^4\xi}{(2\pi)^4}\, \delta(|\xi|-1)\, \mathrm{tr}\sigma_k[a](\xi,x), \tag{A1}$$

with $N_k=\int_0^\infty \mathrm{d}u u^{k+3} f(u)$ constants depending on f. For $k=-4$ the computation above does not make sense (the constant N_{-4} diverges), but we can compute $c_{\log}(a)$ as follows. We first subtract from the symbol of a the diverging part which we already accounted for and define

$$\sigma^\perp_{-3}[a](p,x) := \sigma[a](p,x) - \sum_{j=0}^{K+3} \sigma_{K-j}[a](p,x) = \sigma_{-4}[a](p,x) + \mathcal{O}(|p|^{-5}). \tag{A2}$$

Equation (33) then suggests that

$$c_{\log}(a) = \lim_{\Lambda\to\infty} \frac{1}{\log(\Lambda)} \int_{\mathbb{R}^4} \frac{\mathrm{d}^4p}{(2\pi)^4} f\left(\frac{|p|}{\Lambda}\right) \int_{\mathbb{R}^4} d^4x\, \mathrm{tr}\, \sigma[a]^\perp_{-3}(p,x).$$

Computing this using L'Hospital's rule we obtain

$$\begin{aligned} c_{\log}(a) &= \lim_{\Lambda\to\infty} \Lambda \int_{\mathbb{R}^4} \frac{\mathrm{d}^4p}{(2\pi)^4} f'\left(\frac{|p|}{\Lambda}\right)\left(-\frac{|p|}{\Lambda^2}\right) \int_{\mathbb{R}^4} d^4x\, \mathrm{tr}\, \sigma[a]^\perp_{-3}(p,x) \\ &= \lim_{\Lambda\to\infty} \left(\int_{\mathbb{R}^4} \frac{\mathrm{d}^4p}{(2\pi)^4} \left(-f'\left(\frac{|p|}{\Lambda}\right)\frac{|p|}{\Lambda}\right) \int_{\mathbb{R}^4} d^4x\, \mathrm{tr}\, \sigma[a]_{-4}(p,x) + \mathcal{O}(\Lambda^{-1}) \right). \end{aligned}$$

Changing variables etc. as above and using $\int_0^\infty du(-f'(u))=f(0)=1$ (independent of f!) we obtain

$$c_{\log}(a) = \int_{\mathbb{R}^4} \frac{\mathrm{d}^4\xi}{(2\pi)^4}\, \delta(|\xi|-1) \int_{\mathbb{R}^4} d^4x\, \mathrm{tr}\sigma_{-4}(a)(\xi,x). \tag{A3}$$

Recalling Eq. (34) we obtain Eq. (35). □

2. Renormalized traces

It is obvious that changing the regularization functions $f(t)\to\tilde{f}(t)=f(t/s)$ for some fixed $s>0$, amounts to changing $\Lambda\to s\Lambda$, and thus changes $c^{(0)}\to c^{(0)}+\log(s)\,c_{\log}$. Thus (33) is obvious for this special case. For more general changes $f(t)\to\tilde{f}(t)$ of the regularization function, Eq. (33) can be shown using

$$\int_{\mathbb{R}^4}\frac{\mathrm{d}^4p}{(2\pi)^4}f\left(\frac{|p|}{\Lambda}\right)\int_{\mathbb{R}^4}d^4x\,\mathrm{tr}\,\sigma[a]^{\perp}_{-3}(p,x)=c_{\log}(a)\log\left(\frac{\Lambda}{|m|}\right)+c^{(0)}(a)+\mathcal{O}(\Lambda^{-1}),$$

which follows from our discussion above.

APPENDIX B: COMPUTATION DETAILS

In this Appendix we present some details concerning our computations discussed in the main text. In particular, we give explicit formulas for the Dirac matrices, and we also show show how to compute the structure constants $\mathcal{M}_n$ in Eq. (49) exactly, i.e., without the simplified IR regularization. We also prove the Lemma in Sec. IV A and Eq. (55), and we give some details about the computation yielding Eq. (64).

1. Dirac matrices

A convenient representation for the Dirac matrices is as follows:

$$\gamma^j=\begin{pmatrix}\mathbf{0}&\sigma_j\\ \sigma_j&\mathbf{0}\end{pmatrix},\quad j=1,2,3,\quad \gamma^4=\begin{pmatrix}\mathbf{0}&\mathrm{i}\mathbf{1}\\ -\mathrm{i}\mathbf{1}&\mathbf{0}\end{pmatrix},\quad \gamma_5=\begin{pmatrix}\mathbf{1}&\mathbf{0}\\ \mathbf{0}&-\mathbf{1}\end{pmatrix},\tag{B1}$$

where $\mathbf{1}$ and $\mathbf{0}$ are the 2×2 unit- and zero matrices and

$$\sigma_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_2=\begin{pmatrix}0&-\mathrm{i}\\ \mathrm{i}&0\end{pmatrix},\quad \sigma_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix},$$

the Pauli sigma matrices as usual.

2. Details about the gradient expansion

We start by rewriting the $\mathcal{M}_n$ in a convenient form. We define

$$P_\varepsilon:=\frac{1}{2}\left(1+\varepsilon\frac{\not{p}}{|p|}\right),\quad \varepsilon=\pm,\tag{B2}$$

which are orthogonal projections, $P_\varepsilon P_{-\varepsilon}=0$ and $P_\varepsilon^2=P_\varepsilon$, satisfying $P_++P_-=1$. We then can write

$$(1-u\not{p})^{-1}=\sum_{\varepsilon=\pm}P_\varepsilon\frac{1}{1+u\dfrac{\varepsilon|p|+\mathrm{i}m}{\Lambda_0}},$$

which we insert $n+1$ times in Eq. (49)

$$\mathcal{M}^{\nu_1\cdots\nu_n}_{n;s_1\cdots s_n}=(\Lambda_0)^{-n}\int_{|p|\leqslant\Lambda}\frac{\mathrm{d}^4p}{(2\pi)^4}\int_0^\infty \mathrm{d}u\,u^{n-1}$$
$$\times\sum_{\varepsilon_1,\ldots,\varepsilon_{n+1}=\pm}\left(\prod_{j=1}^{n+1}\frac{1}{1+u\dfrac{\varepsilon_j|p|+\mathrm{i}m}{\Lambda_0}}\right)\mathrm{tr}_\nu(P_{\varepsilon_1}\gamma_{s_1}^{\nu_1}P_{\varepsilon_2}\cdots\gamma_{s_n}^{\nu_n}P_{\varepsilon_{n+1}}).$$

We thus obtain

$$\mathcal{M}^{\nu_1\cdots\nu_n}_{n;s_1\cdots s_n}=\sum_{\varepsilon_1,\ldots,\varepsilon_{n+1}=\pm}\mathcal{I}_{n;\varepsilon_1,\ldots,\varepsilon_{n+1}}\mathrm{tr}_\nu\langle P_{\varepsilon_1}\gamma_{s_1}^{\nu_1}P_{\varepsilon_2}\cdots\gamma_{s_n}^{\nu_n}P_{\varepsilon_{n+1}}\rangle, \tag{B3}$$

with

$$\mathcal{I}_{n;\varepsilon_1,\ldots,\varepsilon_{n+1}}=\mathcal{I}_{n;k},\quad k\ \text{ such that }\ \sum_{j=1}^{n+1}\varepsilon_j=n+1-2k \tag{B4}$$

and

$$\mathcal{I}_{n;k}=(\Lambda_0)^{-n}\frac{1}{8\pi^2}\int_0^\Lambda \mathrm{d}|p||p|^3\int_0^\infty \mathrm{d}u\,u^{n-1}\left(\frac{1}{1+u\dfrac{|p|+\mathrm{i}m}{\Lambda_0}}\right)^{n+1-k}\left(\frac{1}{1+u\dfrac{-|p|+\mathrm{i}m}{\Lambda_0}}\right)^{k}.$$

Rescaling $u\Lambda/\Lambda_0\to u$ and introducing $\xi=|p|/\Lambda$ yields

$$\mathcal{I}_{n;k}=(\Lambda)^{4-n}\frac{1}{8\pi^2}\int_0^1 \mathrm{d}\xi\xi^3\int_0^\infty \mathrm{d}u\,u^{n-1}\left(\frac{1}{1+u\left[\xi+\mathrm{i}\dfrac{m}{\Lambda}\right]}\right)^{n+1-k}\left(\frac{1}{1+u\left[-\xi+\mathrm{i}\dfrac{m}{\Lambda}\right]}\right)^{k}. \tag{B5}$$

Proof of the Lemma in Sec. IV A: We note that

$$\mathrm{tr}_\nu\langle P_{\varepsilon_1}\gamma_{s_1}^{\nu_1}P_{\varepsilon_2}\cdots\gamma_{s_n}^{\nu_n}P_{\varepsilon_{n+1}}\rangle=:T^\nu_{\underline{\varepsilon},\underline{s}},$$

is invariant under $\varepsilon_j\to-\varepsilon_j$ [since the latter transformation amounts to the variable change $\xi\to-\xi$ in the integral Eq. (54) defining the angular average]. Moreover, the cyclicity of trace and $\gamma_5^2=1$ implies that $T^\nu_{\underline{\varepsilon},\underline{s}}$ does not change if we replace all P_{ε_j} and $\gamma_{s_j}^{\nu_j}$ by $\gamma_5P_{\varepsilon_j}\gamma_5$ and $\gamma_5\gamma_{s_j}^{\nu_j}\gamma_5$, respectively. Using $\gamma_5P_\varepsilon\gamma_5=P_{-\varepsilon}$ and $\gamma_5\gamma_s^\nu\gamma_5=-\gamma_s^\nu$ we obtain $T^\nu_{\underline{\varepsilon},\underline{s}}=(-1)^nT^\nu_{-\underline{\varepsilon},\underline{s}}$, and using $T^\nu_{-\underline{\varepsilon},\underline{s}}=T^\nu_{\underline{\varepsilon},\underline{s}}$ this proves that $T^\nu_{\underline{\varepsilon},\underline{s}}$— and thus $\mathcal{M}_n$ in Eq. (49)—is nonzero only for even n.

From Eq. (B4) it is obvious that $\varepsilon_j\to-\varepsilon_j$ corresponds to $k\to n+1-k$, and thus $T^\nu_{\underline{\varepsilon},\underline{s}}=T^\nu_{-\underline{\varepsilon},\underline{s}}$ implies that we can replace $\mathcal{I}_{n;k}$ by $[\mathcal{I}_{n;k}+\mathcal{I}_{n;n+1-k}]/2$ in Eq. (B3). We can write the latter as a sum of the terms which are even and odd under the change of the sign of the mass $m\to-m$. A simple change of variables shows that u-integrals in the odd term

$$\tfrac{1}{4}[\mathcal{I}_{n;k}(m)+\mathcal{I}_{n;n+1-k}(m)-\mathcal{I}_{n;k}(-m)-\mathcal{I}_{n;n+1-k}(-m)],$$

can be written as follows (n even):

$$\frac{1}{4}\int_{-\infty}^\infty \mathrm{d}u\,u^{n-1}\left(\frac{1}{1+u\left[\xi+\mathrm{i}\dfrac{m}{\Lambda}\right]}\right)^{n+1-k}\left(\frac{1}{1+u\left[-\xi+\mathrm{i}\dfrac{m}{\Lambda}\right]}\right)^{k},$$

plus the same integral but with k and $n+1-k$ interchanged. The latter integrals can be computed using Cauchy's theorem: The poles of the integrand are in $u=-1/(\xi+\mathrm{i}m/\Lambda)$ and $u=1/(\xi-\mathrm{i}m/\Lambda)$ and thus both always in the same half of the complex u-plane (upper or lower, depending on the sign of m). Computing the integral by closing the integration path in the half plane where the integrand is analytic (which is possible since the integrand vanishes like $\mathcal{O}(|u|^{-2})$ for $|u|\to\infty$) one sees that the integral is zero. This implies $\mathcal{M}_n(-m)=\mathcal{M}_n(m)$. □

Proof of Eq. (55): Our discussion above implies that we can replace $\mathcal{I}_{n;k}$ in Eq. (B3) by $\Re\mathcal{I}_{n;k}=[\mathcal{I}_{n;k}(m)+\mathcal{I}_{n;k}(-m)]/2$.

We are interested in the terms which diverge for $\Lambda\to\infty$. To isolate them it is convenient to determine $\partial\mathcal{M}_n/\partial\Lambda$. We thus compute

$$\frac{\partial}{\partial\Lambda}\Re\mathcal{I}_{n;k}=\Lambda^{3-n}\frac{1}{8\pi^2}I_{n,k}\left(\frac{m}{\Lambda}\right), \tag{B6}$$

where we introduced the functions

$$I_{n,k}(\eta)=\Re\int_0^\infty \mathrm{d}u\,u^{n-1}\left(\frac{1}{1+u[1+\mathrm{i}\eta]}\right)^{n+1-k}\left(\frac{1}{1+u[-1+\mathrm{i}\eta]}\right)^{k}. \tag{B7}$$

Note that the functions $I_{n,k}(\eta)$ are well-defined for all real $\eta\neq 0$, have a finite limit $I_{n,k}(0^+)$ as $\eta\to 0$, and they have series expansions in η^2. [To see this note that $I_{n,k}(\eta)=\Re\int_0^\infty \mathrm{d}s(1/(s+1+\mathrm{i}\eta))^{n+1-k}(1/(s-1+\mathrm{i}\eta))^k$.]

It is easy to see that with the simplified regularization used in the main text we can obtain a formula for $\tilde{\mathcal{M}}^{\nu_1\cdots\nu_n}_{n;s_1\cdots s_n}$ as in Eqs. (B3) and (B4) but with $\mathcal{I}_{n;k}$ replaced by

$$\tilde{\mathcal{I}}_{n;k}=\frac{1}{8\pi^2}\int_0^\Lambda \mathrm{d}|p||p|^{3-n}I_{n;k}(0^+). \tag{B8}$$

We thus get

$$\frac{\partial}{\partial\Lambda}(\mathcal{I}_{n;k}-\tilde{\mathcal{I}}_{n;k})=\frac{1}{8\pi^2}\Lambda^{3-n}\left(I_{n;k}\left(\frac{m}{\Lambda}\right)-I_{n;k}(0^+)\right)=\mathcal{O}(m^2\Lambda^{1-n}), \tag{B9}$$

which proves Eq. (55). □

Remark: We now can explain the reason for our choice $\Lambda_0=|\Lambda_0|/(1+\mathrm{i}0^+)$ in the main text: This yields a regularization specifying the otherwise undefined integrals $I_{n;k}(0)$, and from Eq. (B9) it is clear that this is the regularization yielding a result identical with the one obtained with the proper regularization, up to lower order terms.

Computation of $\boldsymbol{\mathcal{S}}_2$: For $n=2$ we need to compute $\mathcal{M}_2$ in Eq. (49) exactly, using the formulas given above.

Similarly as explained in the main text we compute [cf. Eq. (B3)]

$$\mathrm{tr}_\nu\langle P_{\varepsilon_1}\gamma_{s_1}^{\nu_1}P_{\varepsilon_2}\cdots\gamma_{s_2}^{\nu_2}P_{\varepsilon_3}\rangle=\delta_{\varepsilon_1,\varepsilon_3}\eta^{\nu_1\nu_2}(1-\varepsilon_1\varepsilon_2(-1)^{s_1}).$$

Moreover, the integrals defined in Eq. (B7) for $n=2$ and $k=0,1$ are

$$I_{2,0}(\eta)=\Re\frac{1}{2(1+\mathrm{i}\eta)^2}=\frac{1}{2}-\frac{3}{2}\eta^2+\mathcal{O}(\eta^4),$$

$$I_{2,1}(\eta)=\Re\frac{1}{4(1+\mathrm{i}\eta)}\left((1+\mathrm{i}\eta)\log\left(\frac{1+\mathrm{i}\eta}{1-\mathrm{i}\eta}\right)-2\right)=\frac{1}{2}+\frac{1}{2}\eta^2+\mathcal{O}(\eta^4),$$

and with Eqs. (B6), (B3), and (B4) we can compute $\partial\mathcal{M}_2/\partial\Lambda$. Straightforward computations yield

$$\mathcal{M}^{\nu_1\nu_2}_{2;s_1s_2} = \delta_{s_1s_2}\eta^{\nu_1\nu_2}\frac{1}{16\pi^2}\left(\Lambda^2 A_{s_1s_2} + m^2\log\left(\frac{\Lambda}{|m|}\right)A^{(0)}_{s_1s_2} + \mathcal{O}(\Lambda^0)\right),$$

$$A_{55} = -A_{00} = 1, \quad A^{(0)}_{55} = -2, \quad A^{(0)}_{00} = 0, \tag{B10}$$

and with Eq. (50) we obtain Eqs. (63)–(64).

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On the classification of *N*-extended supersymmetric quantum mechanical systems

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In this paper some properties of the irreducible multiplets of representation for the $N=(p,q)$-extended supersymmetry in one dimension are discussed. Essentially two results are presented. At first a peculiar property of the one dimension is exhibited, namely that any multiplet containing $2d$ (d bosonic and d fermionic) particles in M different spin states is equivalent to a $\{\mathbf{d},\mathbf{d}\}$ multiplet of just two spin states (all bosons and all fermions being grouped in the same spin). Later, it is shown that the classification of all multiplets of this kind carrying an irreducible representation of the N-extended supersymmetry is in one-to-one correspondence with the classification of real-valued Clifford Γ-matrices of Weyl type. In particular, $p+q$ is mapped into D, the space–time dimensionality, while $2d$ is determined to be the dimensionality of the corresponding Γ-matrices. The implications of these results to the theory of spinning particles are analyzed. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1409349]

I. INTRODUCTION

Recently we have assisted in renewing interest in the theory of supersymmetric and superconformal quantum mechanics due to different physical motivations and viewpoints. Supersymmetric and superconformal[1] (see also Ref. 2) quantum mechanical models succeed in describing the low-energy effective dynamics, as well as the moduli space, of a certain class of black holes. Particle models with extended world-line supersymmetries naturally describe the related geometries, see Ref. 3. Another scenario involving supersymmetric quantum mechanics (SQM) concerns the light–cone quantization of supersymmetric theories.[4] Besides that, SQM models offer a natural setup for testing, under a rigorous mathematical framework, some conjectures (like the AdS/CFT correspondence for AdS_2) or properties and consequences of dimensionally reduced supersymmetric field theories[5] and such phenomena as their spontaneous supersymmetry breaking,[6,7] including the partial breaking.[8,9] Having this in mind, the importance of the investigation of large N-extended (SQM) models cannot be overestimated. Indeed, since the reduced version to a one (temporal) dimension of a supersymmetric $4d$ theory gets four times the number of supersymmetries of the original model, $N=2,4$ super-Yang–Mills are reduced to, respectively, $N=8$ and $N=16$ SQM models, while the $N=8$ supergravity is associated with the $N=32$ SQM theory.

However, not much attention has been paid to such large-N SUSY quantum models and only partial results are known.[10,5] The reason however is clear—$N=4$ is the largest number of extended supersymmetry for which a superfield formalism is known. Investigating the $N>4$ case requires the use of component fields and computations soon become cumbersome.

In this paper we attack the problem of investigating large N SQM models from a different

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viewpoint. We are able to classify the irreducible multiplets of representations of the N extended supersymmetry. We prove at first that all such multiplets are associated with fundamental short multiplets in which all bosons and all fermions are accommodated into just two spin states. As a consequence of that, differently presented dynamical systems turn out to be expressions of the same algebraic structure. Later, we give the full classification of the short multiplets. We further mention how the above-mentioned results find application to the theory of the particles with spin.

The closest references to the results presented here are given in Refs. 11 and 12 in which the classification of (in our language) the short multiplets for the Euclidean supersymmetry was derived, i.e., representations of the (1.2) algebra with positive eigenvalues only. See also Ref. 13 for explicit constructions of multiplets of extended supersymmetries.

In our work we further prove that all multiplets fit into equivalence classes characterized by the short multiplets. Besides that, we extend the classification of Refs. 11 and 12 to the pseudo-Euclidean supersymmetry [arbitrary signatures of the eigenvalues of the ω_{ij} matrix in formula (1.2)]. Indeed, as we will prove in the following, it is in this larger class that symmetries of the particles with spin moving in a Minkowskian or AdS-like background should be looked for. The analysis which follows is based on the results for the classification of real-valued Clifford algebras as presented in Ref. 14.

It is well known that the SQM, being the simplest example of a theory which includes simultaneously commuting and anticommuting variables, realizes as its symmetry group the one-dimensional supersymmetry. In general this supersymmetry is generated by N supercharges $Q_i, i=1,2,\ldots,N$ and the Hamiltonian

$$H=-i\frac{\partial}{\partial t} \tag{1.1}$$

with the following algebra:

$$\{Q_i,Q_j\}=\omega_{ij}H, \tag{1.2}$$

where the constant tensor ω_{ij} has p positive and q negative eigenvalues. Usually all eigenvalues are positive and the above-mentioned algebra is named the N-extended one-dimensional supersymmetry. Nevertheless, in general, reasons can exist leading to an indefinite tensor ω_{ij}.[15] In the following, without loss of generality, the algebra of supercharge Q_i's will be conveniently diagonalized and normalized in such a way that the tensor ω_{ij} can be expressed as

$$\omega_{ij}=\eta_{ij}, \tag{1.3}$$

where η_{ij} is a pseudo-Euclidean metric with the signature (p,q).

The representation of the algebra (1.2) is formed by commuting (Bosonic) and anticommuting (Fermionic before the quantization and Clifford after it) variables. Some of them are true physical variables, others play an auxiliary role. Usually all these variables are taken to be the components of irreducible superfields.

The simplest way to construct a classical Lagrangian for the SQM in D dimensions is to consider the superfields $(A=1,2,\ldots,D)$,

$$\Phi_A(\tau,\eta^\alpha)=\Phi^0_A(\tau)+\eta^\alpha\Phi^1_{A\alpha}(\tau)+\eta^{\alpha_1}\eta^{\alpha_2}\Phi^2_{A\alpha_1\alpha_2}(\tau)+\cdots+\eta^{\alpha_1}\eta^{\alpha_2}\cdots\eta^{\alpha_N}\Phi^N_{A\alpha_1\alpha_2\cdots\alpha_N}(\tau), \tag{1.4}$$

in the superspace (τ,η^α) with one bosonic coordinate τ and N Grassmann coordinates η^α. Such superfields for general N are highly reducible and only lower values of N were investigated in detail. The first components of the superfields are the usual bosonic coordinates $\Phi^0_A(\tau)$, the next ones $\Phi^1_{A\alpha}(\tau)$ are the Grassmann coordinates. All the other components of the superfields are auxiliary. So, the classical Lagrangian of the SQM describes the evolution of bosonic and addi-

tional Grassmann degrees of freedom, which after quantization become generators of the Clifford algebra. This fact naturally leads to the matrix realization of the Hamiltonian and supercharges of SQM.[6,16,17]

The dimensionality of such realization depends on the total number of Grassmann variables. In the case of scalar superfields (1.4) the dimensionality is $2^{[DN/2]}$. So, it rapidly grows for extended supersymmetry. The way out of this difficulty is to use more complicated representations of the extended supersymmetry.[18–23] The simplest of them is given by the chiral superfield, which contains one complex bosonic and $N/2$ complex Grassmann fields. The Lagrangian for such superfield naturally describes the two-dimensional SQM. The ratio of numbers (Fermi/boson) in this case is $N/2$ instead of N as for scalar superfields. For more complicated representations this ratio grows even more slowly.[19–23] This fact has an essential influence on the dimensionality of the matrix realizations of the Hamiltonian and supercharges—they are smaller for the same number of bosonic coordinates Φ^0_A. The distinguishing feature of such representations is the fact that the lowest components $\Phi^0_A(\tau)$ $(A=1,2,\ldots,D)$ of the superfields (1.4) *all together* form an irreducible representation of some subgroup of the automorphism group of the algebra (1.2). The corresponding actions are also invariant under the transformations of this subgroup, which thus plays the role of space (or space–time) rotations. In particular the inclusion of the time coordinate $t(\tau)$ along with the space ones $x^a(\tau)$ in an irreducible representation $\Phi^0_A(\tau)$ of such subgroup means that such a subgroup, as well as the whole automorphism group of the algebra (1.2), is pseudo-Euclidean.[15] In consequence of that the metric tensor η_{ij} in (1.3) is pseudo-Euclidean too.

So, the number of bosonic and fermionic physical components and, correspondingly, the dimensionality of quantum Hamiltonian and supercharges realized as matrices, crucially depend on the choice of the irreducible superfield or, equivalently, irreducible representation of the algebra (1.2). In this sense the classification of all such representations is very useful.

II. THE EQUIVALENCE RELATIONS

In this section we analyze the structure of the supermultiplets of the N-extended supersymmetry in one-dimensional space. We will show in which sense all irreducible representations are equivalent to the representations with a definite structure of the multiplets. To fix the notation, let N denote the number of extended supersymmetries and $2d$ (d bosons and d fermions) the dimensionality of the corresponding multiplet, (may be reducible), carrying the N-extended SUSY representation. In general such multiplet can be represented in the form of a chain

$$\Phi^0_{a_0}, \quad \Phi^1_{a_1},\ldots,\Phi^{M-1}_{a_{M-1}}, \quad \Phi^M_{a_M} \tag{2.1}$$

whose components $\Phi^I_{a_I}$, $(a_I=1,2,\ldots,d_I)$ are real. All the components with even I have the same Grassmann parity as that of $\Phi^0_{a_0}$, while the components with odd values of I have the opposite one. Such structure of the multiplet is closely related to the superfield representations; the upper index I, numbering the elements of the chain, corresponds to their place in the superfield expansion (1.4) or to their dimensionality which decreases by 1/2 at each step along the chain if one chooses

$$\dim(\tau)=1, \quad \dim(\eta)=\tfrac{1}{2}. \tag{2.2}$$

The number $M+1$ is the length of the supermultiplet, M being subjected to the constraint $M \leqslant N$ since, for example in the case of irreducible representations, not all the components of the superfield (1.4) are independent—some of the higher components are expressed in terms of time derivatives of the lower ones.

For the supermultiplet (2.1) we will also use the short notation $\{\mathbf{d_0},\mathbf{d_1},\ldots,\mathbf{d_M}\}$. As an example, in the case of $N=2$ one can consider the irreducible representations $\{\mathbf{1},\mathbf{2},\mathbf{1}\}$ (real superfield)

$$\Phi=\Phi(\tau,\eta_1,\eta_2)=\Phi^0(\tau)+i\,\eta^\alpha\Phi^1_\alpha(\tau)+i\,\eta^1\eta^2\Phi^2(\tau), \tag{2.3}$$

and $\{\mathbf{2},\mathbf{2}\}$ (chiral superfield)

$$\tilde{\Phi}(\tau,\eta,\overline{\eta})=\tilde{\Phi}^0(\tau)+\eta\tilde{\Phi}^1(\tau)+\frac{i}{2}\overline{\eta}\eta\dot{\tilde{\Phi}}^0(\tau), \tag{2.4}$$

where $\eta=\eta_1+i\,\eta_2$, $\overline{\eta}=\eta_1-i\,\eta_2$ are complex Grassmann coordinates. The last component in expression (2.4) is proportional to the time derivative of the first one. Both $\tilde{\Phi}^0(\tau)$ and $\tilde{\Phi}^1(\tau)$ in (2.4) are complex. Obviously, in both cases (2.3) and (2.4), $\Sigma_I\,d_I=2$ separately for real bosonic and fermionic components.

Due to dimensionality arguments the supersymmetry transformation law for the components $\Phi^I_{a_I}$ is of the following form (ε^i are infinitesimal Grassmann parameters):

$$\delta_\varepsilon\Phi^I_{a_I}=\varepsilon^i(C^I_i)_{a_I}{}^{a_{I+1}}\Phi^{I+1}_{a_{I+1}}+\varepsilon^i(\tilde{C}^I_i)_{a_I}{}^{a_{I-1}}\frac{d}{d\tau}\Phi^{I-1}_{a_{I-1}}. \tag{2.5}$$

Evidently, due to the absence in (2.1) of the components with $I=-1$, $I=M+1$, the transformation laws for the end components of the chain are simpler:

$$\delta_\varepsilon\Phi^0_{a_0}=\varepsilon^i(C^0_i)_{a_0}{}^{a_1}\Phi^1_{a_1},\quad \delta_\varepsilon\Phi^M_{a_M}=\varepsilon^i(\tilde{C}^M_i)_{a_M}{}^{a_{M-1}}\frac{d}{d\tau}\Phi^{M-1}_{a_{M-1}}. \tag{2.6}$$

The transformation law for the last component of the multiplet reads that it transforms as a total derivative. It is a very essential property, because the integral of this component is invariant under the supersymmetry transformations and can be used to construct invariant actions.

Another very important consequence of the transformation law of the last components is present only in one dimension. Just in this case one can redefine this component

$$\Phi^M_{a_M}=\frac{\mathrm{d}}{\mathrm{d}\tau}\Psi^{M-2}_{a_M} \tag{2.7}$$

in terms of some functions $\Psi^{M-2}_{a_M}$. This correspondence is exact up to some constants $C^M_{a_M}$ which describe the trivial representations of the supersymmetry algebra. The dimensionality of the new components $\Psi^{M-2}_{a_M}$ coincides with the dimensionality of the components $\Phi^{M-2}_{a_{M-2}}$. Moreover, their transformation law is of the same type—they transform through the components $\Phi^{M-1}_{a_{M-1}}$ and $\Phi^{M-3}_{a_{M-3}}$ (with vanishing coefficients before the time derivative of the latter),

$$\delta_\varepsilon\Psi^{M-2}_{a_M}=\varepsilon^i(\tilde{C}^M_i)_{a_M}{}^{a_{M-1}}\Phi^{M-1}_{a_{M-1}}. \tag{2.8}$$

So, we have shown that up to trivial representations of the supersymmetry algebra the supermultiplet $\{\mathbf{d_0},\mathbf{d_1},\ldots,\mathbf{d_{M-2}},\mathbf{d_{M-1}},\mathbf{d_M}\}$ is equivalent to the supermultiplet $\{\mathbf{d_0},\mathbf{d_1},\ldots,\mathbf{d_{M-2}}+\mathbf{d_M},\mathbf{d_{M-1}},\mathbf{0}\}$. It means that the initial supermultiplet of length $M+1$ is equivalent to a shorter multiplet of length M. Evidently, the total number of bosonic and fermionic components in both supermultiplets is the same. This procedure can obviously be repeated $M-1$ times, so that at the end one reaches the shortest multiplet of length 2—the multiplet $\{\mathbf{d},\mathbf{d}\}$.

The simplest example of such shortening of the length is given in the case of $N=2$. The component $\Phi^2(\tau)$ in the real superfield (2.3) transforms as a total derivative of some new field $\Psi^0(\tau)$ which, together with $\Phi^0(\tau)$, forms the complex $\tilde{\Phi}^0(\tau)$ of (2.4). A more complicated example is furnished by the $N=4$ representation multiplets $\{\mathbf{1},\mathbf{4},\mathbf{3}\}$, $\{\mathbf{2},\mathbf{4},\mathbf{2}\}$, and $\{\mathbf{3},\mathbf{4},\mathbf{1}\}$ which were used in Refs. 19, 20, and 8 for one-dimensional,[23] two-dimensional,[21,22] and three-dimensional

SQM, respectively. The corresponding components of these representations are interconnected by the transformation (2.7). To our knowledge, the multiplet (4,4) which should be useful in the four-dimensional case was not considered in the literature.

In principle, one can consider the inverse procedure—the lengthening of the multiplet starting from the one for $\{\mathbf{d},\mathbf{d}\}$. Only the first step is trivial—the transition from the $\{\mathbf{d},\mathbf{d}\}$ multiplet to the $\{\mathbf{d}-\mathbf{d_1},\mathbf{d},\mathbf{d_1}\}$ multiplet can always be done with the help of the transformation inverse to (2.7) applied to an arbitrary number $d_1 \leqslant d$ of the first components of the initial multiplet. The possibility of further lengthening must be analyzed separately in each particular case and will be shortly discussed at the end of the paper.

It should be noticed that $d_1 = d$ is allowed. The corresponding transformation links two length-2 multiplets, the one in which bosons have higher spin, to the one in which fermions have higher spins. Explicitly we have

$$\delta_\varepsilon \Phi_a = \varepsilon^i (C_i)_a^{\ b} \Psi_b, \quad \delta_\varepsilon \Psi_a = \varepsilon^i (\tilde{C}_i)_a^{\ b} \frac{\mathrm{d}}{\mathrm{d}\tau} \Phi_b, \tag{2.9}$$

while for $\Xi_a = (\mathrm{d}/\mathrm{d}\tau)\,\Psi_a$ we get

$$\delta_\varepsilon \Xi_a = \varepsilon^i (C_i)_a^{\ b} \Phi_b, \quad \delta_\varepsilon \Phi_a = \varepsilon^i (\tilde{C}_i)_a^{\ b} \frac{\mathrm{d}}{\mathrm{d}\tau} \Xi_b. \tag{2.10}$$

We finally comment that, due to the previous considerations, the classification of all supermultiplets of length 2 automatically provides the classification of all supermultiplets of length 3. In many physical applications of interest, this is quite sufficient.

III. EXTENDED SUPERSYMMETRIES AND REAL-VALUED CLIFFORD ALGEBRAS

The main result of Sec. II is that the problem of classifying all N-extended supersymmetric quantum mechanical systems is reduced to the problem of classifying the irreducible representations (2.1) of length 2. Having this in mind we simplify the notations. Let the indices $a, \alpha = 1,\ldots,d$ number the bosonic (and, respectively, fermionic) elements in the SUSY multiplet. All of them are assumed to depend on the time coordinate τ ($X_a \equiv X_a(\tau)$, $\theta_\alpha \equiv \theta_\alpha(\tau)$).

In order to be definite and without loss of generality let us take the bosonic elements to be the first ones in the chain $\{\mathbf{d},\mathbf{d}\}$, which can be conveniently represented also as a column

$$\Psi = \begin{pmatrix} X_a \\ \theta_\alpha \end{pmatrix}. \tag{3.1}$$

Equation (2.5) is reduced to the following set of equations:

$$\begin{aligned} \delta_\varepsilon X_a &= \varepsilon^i (C_i)_a^{\ \alpha} \theta_\alpha \equiv i(\varepsilon^i Q_i \Psi)_a, \\ \delta_\varepsilon \theta_\alpha &= \varepsilon^i (\tilde{C}_i)_\alpha^{\ b} \frac{\mathrm{d}}{\mathrm{d}\tau} X_b \equiv i(\varepsilon^i Q_i \Psi)_\alpha, \end{aligned} \tag{3.2}$$

where, as a consequence of (1.2),

$$C_i \tilde{C}_j + C_j \tilde{C}_i = i\,\eta_{ij} \tag{3.3}$$

and

$$\tilde{C}_i C_j + \tilde{C}_j C_i = i\,\eta_{ij}. \tag{3.4}$$

Since $\varepsilon_i, X_a, \theta_\alpha$ are real, the matrices C_i, $\tilde{C}_i$ have to be imaginary and real, respectively. If we set (just for normalization)

$$C_i=\frac{i}{\sqrt{2}}\sigma_i,$$
$$\tilde{C}_i=\frac{1}{\sqrt{2}}\tilde{\sigma}_i \tag{3.5}$$

and accommodate $\sigma_i,\tilde{\sigma}_i$ into a single matrix

$$\Gamma_i=\begin{pmatrix}0 & \sigma_i\\ \tilde{\sigma}_i & 0\end{pmatrix}, \tag{3.6}$$

they form a set of real-valued Clifford Γ-matrices of Weyl type (i.e., block antidiagonal), obeying the (pseudo-) Euclidean anticommutation relations

$$\{\Gamma_i,\Gamma_j\}=2\eta_{ij}. \tag{3.7}$$

Conversely, given a set of (pseudo-) Euclidean real-valued Clifford Γ-matrices of Weyl type, one can invert the above-mentioned procedure and reconstruct the supercharges Q_i,

$$Q_i=\frac{1}{\sqrt{2}}\begin{pmatrix}0 & \sigma_i\\ \tilde{\sigma}_i\cdot H & 0\end{pmatrix}, \tag{3.8}$$

in the basis (3.1).

In addition to the matrices Γ^i (3.6) in the space of vectors (3.1) the further matrix Γ^{N+1}, which anticommutes with the supercharges and corresponds to the fermionic number, exists

$$\Gamma_{N+1}=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{3.9}$$

Altogether the matrices (3.6) and (3.9) form the real-valued representation Γ_I of the (pseudo-) Euclidean Clifford algebra with the signature $(p+1,q)$.

Instead of (3.5) one can take

$$C_i=\frac{i}{\sqrt{2}}\sigma_i,$$
$$\tilde{C}_i=-\frac{1}{\sqrt{2}}\tilde{\sigma}_i, \tag{3.10}$$

and accommodate $\sigma_i,\tilde{\sigma}_i$ into the matrices (3.6), which now obey the (pseudo-) Euclidean anticommutation relations

$$\{\tilde{\Gamma}_i,\tilde{\Gamma}_j\}=-2\eta_{ij} \tag{3.11}$$

with opposite to (3.7) sign of the right-hand side. Together with fermion number matrix (3.9) the new matrix $\tilde{\Gamma}_i$ forms the real-valued representation of the (pseudo-) Euclidean Clifford algebra with the signature $(q+1,p)$. This fact means that the representations of $C_{p+1,q}$ and $C_{q+1.p}$ should be connected one with the other. Indeed, this connection is established by the correspondence

$$\tilde{\Gamma}_i = \Gamma_{N+1}\Gamma_i . \tag{3.12}$$

Thus, the representations of the (p,q)- extended supersymmetry algebra (1.2) are in one-to-one correspondence with the real-valued representations of the Clifford algebra $C_{p+1,q} \sim C_{q+1,p}$.

In general the real Clifford algebras were classified in Ref. 24 (for the compact case $q=0$) and in Ref. 25 (for the noncompact case). The construction along the lines (3.2)–(3.9) for representations of the type $\{\mathbf{d},\mathbf{d}\}$ in the case of positively definite signature $(p,q)=(N,0)$ was performed in Ref. 11 (see also Ref. 12) where the dimensionalities as well as realizations of the Γ-matrices (3.6) were described. In the case of pseudo-Euclidean metric with signature (p,q) such construction extensively uses the considerations of Ref. 14. The results will be presented in Sec. IV.

IV. CLASSIFICATION OF THE IRREDUCIBLE REPRESENTATIONS

According to the results of Sec. III the classification of irreducible multiplets of representation of a (p,q) extended supersymmetry is in one-to-one correspondence with the classification of the real Clifford algebras $C_{p,q}$ with the further property that the Γ matrices can be realized in Weyl (i.e., block antidiagonal) form.

For what concerns real matrix representations of the Clifford algebras we borrow the results of Ref. 14. Three cases have to be distinguished for real representations, specified by the type of most general solution allowed for a real matrix S commuting with all the Clifford Γ_i matrices, i.e.,

(i) the normal case, realized when S is a multiple of the identity,
(ii) the almost complex case, for S being given by a linear combination of the identity and of a real $J^2=-\mathbf{1}$ matrix,
(iii) finally the quaternionic case, for S being a linear combination of real matrices satisfying the quaternionic algebra.

Real irreducible representations of normal type exist whenever the condition $p-q=0,1,2 \bmod 8$ is satisfied (their dimensionality being given by $2^{[N/2]}$, where $N=p+q$), while the almost complex and the quaternionic type representations are realized in the $p-q=3,7 \bmod 8$ and in the $p-q=4,5,6 \bmod 8$ cases, respectively. The dimensionality of these representations is given in both cases by $2^{[N/2]+1}$.

We further require the extra condition that the real representations should admit a block antidiagonal realization for the Clifford Γ matrices. This condition is met for $p-q=0 \bmod 8$ in the normal case (it corresponds to the standard Majorana–Weyl requirement), $p-q=7 \bmod 8$ in the almost complex case and $p-q=4,6 \bmod 8$ in the quaternionic case. In all these cases the real irreducible representation is unique.

The above-mentioned results can be summarized as follows, expressing the dimensionality of the irreducible representations of the algebra (1.2) [independently of the length $M+1$ of the chain (2.1)] as function of the signature (p,q). Let $q=8k+m$, $0\leqslant m\leqslant 7$, and $p=8l+m+n$, $1\leqslant n\leqslant 8$ ($l=-1$ when $k=0$ and $p\leqslant q$). Then, the dimensionalities of the bosonic (fermionic) spaces are given by

$$d=2^{4k+4l+m}\cdot G(n), \tag{4.1}$$

where the so-called Radon–Hurwitz function $G(n)$ is defined with the help of the table which can be encountered in Ref. 12

$$\begin{array}{cccccccccc} n & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\ G(n) & 1 & 2 & 4 & 4 & 8 & 8 & 8 & 8 \end{array}. \tag{4.2}$$

In words, $G(n)=2^r$, where r is the nearest integer which is greater or equal to $\log_2 n$.

Conversely, a second useful table expresses which kind of signatures (p,q) are possible for a given dimensionality of the bosonic and fermionic spaces. In order to do so it is convenient to introduce the notion of maximally extended supersymmetry. The $C_{p,q}$ $(p-q=6 \bmod 8)$ real representation for the quaternionic case can be recovered from the 7 mod 8 almost complex $C_{p+1,q}$ representation by deleting one of the Γ matrices; in turn the latter representation is recovered from the $C_{p+2,q}$ normal Majorana–Weyl representation by deleting another Γ matrix. The dimensionality of the three representations mentioned previously being the same, the normal Majorana–Weyl representation realizes the maximal possible extension of supersymmetry compatible with the dimensionality of the representation. In search for the maximal extension of supersymmetry we can therefore limit ourselves to consider the normal Majorana–Weyl representations, as well as the quaternionic ones satisfying the $p-q=4 \bmod 8$ condition.

Therefore let $p=8l+m+8+4\epsilon$ and $q=8k+m$, where the range of values for k,l,m is the same as before, while ϵ assumes two values, distinguishing the Majorana–Weyl $(\epsilon=0)$ and the quaternionic case $(\epsilon=1)$. A space of $d=2^t$ bosonic and $d=2^t$ fermionic states can carry the following set of maximally extended supersymmetries:

$$(p=t-4z+5-3\epsilon, q=t+4z+\epsilon-3), \tag{4.3}$$

where the integer $z=k-l$ must take values in the interval

$$\tfrac{1}{4}(3-t-\epsilon)\leqslant z\leqslant \tfrac{1}{4}(t+5-3\epsilon) \tag{4.4}$$

in order to guarantee the $p\geqslant 0$ and $q\geqslant 0$ requirements. It is also convenient to represent the answer by the following table:

d	(p,q)
2^{4l}	$(8l-4k+1,4k+1),(8l-4k-2,4k+2)$
2^{4l+1}	$(8l-4k+2,4k+2),(8l-4k-1,4k+3)$
2^{4l+2}	$(8l-4k+4,4k),(8l-4k+3,4k+3)$
2^{4l+3}	$(8l-4k+8,4k),(8l-4k+5,4k+1),$

(4.5)

where k is an integer satisfying the conditions $p\geqslant 0$, $q\geqslant 0$.

For the lowest values of dimensionality d the solutions are given by the table:

d	(p,q)
1	(1,1)
2	(2,2)
4	(4,0),(3,3),(0,4) (4,6)
8	(8,0),(5,1),(4,4),(1,5),(0,8)
16	(9,1),(6,2),(5,5),(2,6),(1,9)
32	(10,2),(7,3),(6,6),(3,7),(2,10).

(4.6)

As already recalled, obviously the representations (p',q') with $p'\leqslant p, q'\leqslant q$ also exist for the same dimensionality d. These representations are also irreducible unless either p' or q' becomes too small. For example, the $d=16$-dimensional representations are irreducible not only for the signature $(p,q)=(5,5)$, but also for the pairs (5,4),(5,3),(5,2),(4,5),(3,5),(2,5), while the irreducible representations for the signatures (5,1),(4,4),(1,5) are encountered in $d=8$ dimensions.

V. EXAMPLES OF REPRESENTATIONS FOR SUPERCHARGES

For the case $(p,q)=(4,0)$ the following matrices realize four supercharges:

$$Q_1=\frac{1}{\sqrt{2}}\begin{vmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & H & 0 & 0 & 0 & 0 \\ 0 & 0 & H & 0 & 0 & 0 & 0 & 0 \\ 0 & H & 0 & 0 & 0 & 0 & 0 & 0 \\ H & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix},$$

$$Q_2=\frac{1}{\sqrt{2}}\begin{vmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & H & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -H & 0 & 0 & 0 & 0 \\ H & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -H & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix}, \tag{5.1}$$

$$Q_3=\frac{1}{\sqrt{2}}\begin{vmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ H & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & H & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -H & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -H & 0 & 0 & 0 & 0 \end{vmatrix},$$

$$Q_4=\frac{1}{\sqrt{2}}\begin{vmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & -H & 0 & 0 & 0 & 0 & 0 & 0 \\ H & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & H & 0 & 0 & 0 & 0 \\ 0 & 0 & -H & 0 & 0 & 0 & 0 & 0 \end{vmatrix}.$$

These supercharges act in the space with four bosonic and four fermionic coordinates forming the representation {**4**,**4**}. The automorphism group SO(p,q) of the algebra (1.2) is now SO(4).

Besides the transformations of the automorphism group $Q_i' = \Lambda_i^j Q_j$ the algebra of supercharges is invariant under the more general transformations of the type

$$Q_i' = U Q_i U^{-1} \tag{5.2}$$

with block-diagonal 8×8 matrices U. When the matrix U is nonsingular and real the transformation (5.2) simply means a change of basis in bosonic and fermionic sectors. On the other hand this transformation drastically changes the representation when U depends on the operator $H = -i\mathrm{d}/\mathrm{d}\tau$. In this case the transformation (5.2) is in general nonlocal. Nevertheless, transformations exist which do not lead to any nonlocality. In particular, in the framework of the example (5.1) one can take

$$U_1 = \mathrm{diag}\{1,1,1,H,1,1,1,1\} \tag{5.3}$$

and obtain the new realization for the operators Q_i,

$$Q_1 = \frac{1}{\sqrt{2}} \begin{vmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & H & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & H & 0 & 0 & 0 & 0 & 0 \\ 0 & H & 0 & 0 & 0 & 0 & 0 & 0 \\ H & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix},$$

$$Q_2 = \frac{1}{\sqrt{2}} \begin{vmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -H & 0 & 0 \\ 0 & 0 & H & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ H & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -H & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix}, \tag{5.4}$$

$$Q_3 = \frac{1}{\sqrt{2}} \begin{vmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -H \\ H & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & H & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -H & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \end{vmatrix},$$

$$Q_4=\frac{1}{\sqrt{2}}\begin{vmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & H & 0 \\ 0 & -H & 0 & 0 & 0 & 0 & 0 & 0 \\ H & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -H & 0 & 0 & 0 & 0 & 0 \end{vmatrix}$$

in which all the elements of the last column in the left off-diagonal block have lost the multiplier H. Instead, all the elements of the last arrow in the right off-diagonal block acquired H as a multiplier. This representation of the supercharges corresponds to the irreducible supermultiplet $\{\mathbf{3},\mathbf{4},\mathbf{1}\}$ which was used in Refs. 21 and 22 for constructing the three-dimensional $N=4$ extended SQM. The supermultiplets $\{\mathbf{2},\mathbf{4},\mathbf{2}\}$ and $\{\mathbf{1},\mathbf{4},\mathbf{3}\}$ are derived with the help of the following matrices U:

$$U_2=\mathrm{diag}\{1,1,H,H,1,1,1,1\}, \quad U_3=\mathrm{diag}\{1,H,H,H,1,1,1,1\}. \tag{5.5}$$

The next one in this sequence

$$U_4=\mathrm{diag}\{H,H,H,H,1,1,1,1\} \tag{5.6}$$

again gives the supermultiplet $\{\mathbf{4},\mathbf{4}\}$ but with the opposite grading—the first in the chain is the fermionic subspace. This completes the classification of the irreducible supermultiplets of the $N=4$ extended SQM. One can show that all the irreducible supermultiplets of the (p,q) extended SQM are of length which does not exceed 3 when the constraint

$$d\leqslant p+q \tag{5.7}$$

is fulfilled. The determination of the possible values of the lengths of irreducible supermultiplets, as well as their detailed structure, in the case when (5.7) is not fulfilled needs a separate investigation.

A simple example of an irreducible supermultiplet of length 4 is given by the $(p,q)=(3,0)$ case, in which the irreducible representation has also $d=4$ and supercharges in the $\{\mathbf{4},\mathbf{4}\}$ representation are given by Q_1,Q_2,Q_3 in (5.1). Taking

$$U_5=\mathrm{diag}\{1,H,H,H,1,H,1,1\} \tag{5.8}$$

one derives the expressions for all four supercharges

$$Q_1=\frac{1}{\sqrt{2}}\begin{vmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & H & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & H & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & H & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ H & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{vmatrix},$$

$$
Q_2=\frac{1}{\sqrt{2}}\begin{vmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -H\\
0 & 0 & 0 & 0 & H & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & -1 & 0 & 0\\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & -H & 0 & 0 & 0 & 0\\
H & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0
\end{vmatrix},
$$

$$
Q_3=\frac{1}{\sqrt{2}}\begin{vmatrix}
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & -H & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -H\\
H & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & H & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0
\end{vmatrix},
\tag{5.9}
$$

$$
Q_4=\frac{1}{\sqrt{2}}\begin{vmatrix}
0 & 0 & 0 & 0 & 0 & H^{-1} & 0 & 0\\
0 & 0 & 0 & 0 & -H & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -H\\
0 & 0 & 0 & 0 & 0 & 0 & H & 0\\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0\\
H^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0\\
0 & 0 & -1 & 0 & 0 & 0 & 0 & 0
\end{vmatrix}
$$

from which one can easily see that the fourth supercharge Q_4 becomes singular after the transformation. Indeed, just the first three supercharges in (5.9) are realized in the irreducible representation $\{\mathbf{1},\mathbf{3},\mathbf{3},\mathbf{1}\}$ of length 4.

The Weyl-type $C_{0,4}$ representation has been explicitly presented in Ref. 14. Due to the mod 8 property of Γ matrices, it allows, together with $C_{4,0}$, one to construct all quaternionic representations of Weyl type for the allowed values of (p,q). For what concerns the Majorana–Weyl representations, an algorithm to explicitly construct them can be found, e.g., in Ref. 26. Moreover, the following symmetry property

$$
\Gamma_i^T=\begin{cases}\Gamma_i, & i\leqslant p\\ -\Gamma_i, & (p+1)\leqslant i\leqslant(p+q)\end{cases}
\tag{5.10}
$$

can always be assumed to be valid.

VI. AN APPLICATION: SUPERSYMMETRIES OF THE FREE KINETIC LAGRANGIANS OF THE "SPINNING" PARTICLE

We present for completeness the analysis of the extended supersymmetric invariances for the simplest action of the ''spinning'' particle model, given by the free kinetic term. We use the quotation marks in the word ''spinning'' because actually the considered actions describe particles

with spin and are different from the spinning particle models in which both fermions and bosons are space–time vectors and bosons, in addition, are scalars with respect to the supersymmetry transformations.

In general the most significant dynamical systems are σ-models presenting a nonlinear kinetic term; for such systems the extended supersymmetries put constraints on the metric of the target. We avoid entering this problem here and just limit ourselves to illustrate how invariances under pseudo-Euclidean supersymmetries can arise. We show in fact that a ''spinning'' particle evolving in a non-Euclidean background in general admits invariances under pseudo-Euclidean supersymmetries.

We consider the models involving d bosonic fields X_a and d spinors Θ_α collected in the vector Ψ (3.1) (no auxiliary fields are present).

The free kinetic action is given by

$$S_K=\int \mathrm{d}t\, \mathcal{L}=\frac{1}{2}\int \mathrm{d}t \Psi^T \Lambda \Psi=\frac{1}{2}\int \mathrm{d}t (X,\Theta)\begin{pmatrix} \lambda_1 H^2 & 0 \\ 0 & \lambda_2 H \end{pmatrix}\begin{pmatrix} X \\ \Theta \end{pmatrix} \tag{6.1}$$

$$=\frac{1}{2}\int \mathrm{d}t(\dot{X}_a \lambda_1^{ab}\dot{X}_b - i\Theta_\alpha \lambda_2^{\alpha\beta}\dot{\Theta}_\beta), \tag{6.2}$$

where the structure of the matrix Λ is dictated by the conservation of the fermion number and by dimensional arguments. Both λ_1,λ_2 should be symmetrical in addition: $\lambda_M^T=\lambda_M$.

The invariance of the action under the supersymmetry transformations (3.2),

$$\delta S_K=\frac{i}{\sqrt{2}}\varepsilon^i X_a(\lambda_1\sigma_i-\tilde{\sigma}_i^T\lambda_2)^{a\alpha}H^2\Theta_\alpha=0, \tag{6.3}$$

means that the following property of λ's,

$$\lambda_1\sigma_i-\tilde{\sigma}_i^T\lambda_2=0, \tag{6.4}$$

should be valid, in accordance with (5.10)

$$\tilde{\sigma}_i^T=\eta^{ii}\sigma_i. \tag{6.5}$$

It means that in the case of Euclidean supersymmetry ($q=0$) we get

$$\lambda_1=\lambda_2=I, \tag{6.6}$$

where I is a d dimensional identity matrix (see also Ref. 12). In the general case ($q\geqslant 1$) the following representation for the Γ_i matrices[14] is useful

$$\Gamma_\mu=\begin{pmatrix} 0 & \gamma_\mu \\ \gamma_\mu & 0 \end{pmatrix},\quad \mu=1,2,\ldots,p+q-1,\quad \Gamma_{p+q}=\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \tag{6.7}$$

where γ_μ form a real valued representation of the Clifford algebra $C_{p,q-1}$ with the symmetry property (5.10). So, the conditions (6.4) give, in particular, $\lambda_1=-\lambda_2\equiv C$ and

$$C\gamma_\mu+\gamma_\mu^T C=0, \tag{6.8}$$

which means that the matrix C is the charge conjugation matrix for the Clifford algebra $C_{p,q-1}$. The additional property of symmetry for this matrix $C^T=C$ limits the possible signatures (p,q) for which the free action (6.1) is invariant under all $p+q$ supersymmetries. These possible signatures (p,q) can be represented by the following table:

$p\backslash q$	0	1	2	3	4	5	6	7	8
0	+	+	+	+	+	+	+	+	+
1	+		+		+		+	+	+
2	+			+	+	+	+	+	+
3	+				+	+	+		+
4	+	+	+	+	+	+	+	+	+
5	+		+	+	+		+		+
6	+	+	+	+	+			+	+
7	+	+	+		+				+
8	+	+	+	+	+	+	+	+	+

(6.9)

which together with the modulo-8 periodicity gives the total answer. Therefore, for the cases of empty entries of the table it should be checked separately for each specific choice of the matrices λ_1, λ_2 which supersymmetries survive as invariances of the action.

The first nontrivial example concerns a two-dimensional "spinning" particle ($d=2$). Its two bosonic and two fermionic degrees of freedom carry the $\{\mathbf{2},\mathbf{2}\}$ representation of (2,2) extended supersymmetry. However, due to the condition (6.4) only half of these supersymmetries can be invariances of the action. We obtain in fact invariance under either the (2,0) or the (1,1) extended supersymmetries, whether the target space is, respectively, Euclidean or Minkowskian. Therefore already for the two-dimensional Minkowskian "spinning" particle we observe the arising of the pseudo-Euclidean supersymmetry invariance.

More generally, in all the cases except the Euclidean one ($q=0$ *or* $p=0$), exactly half of the eigenvalues of the charge conjugation matrix C are negative. It means that the action (6.1) describes the free motion in the space–time with signature $(d/2,d/2)$ with equal numbers of spacelike and timelike coordinates. Both of them transform as irreducible spinors of the isomorphisms group $\mathrm{SO}(p,q)$ generated by

$$J_{ik}=\tfrac{1}{4}[\Gamma_i,\Gamma_k]. \tag{6.10}$$

If one wants to have another space–time signature, some of the bosonic coordinates can be converted into the auxiliary ones with the help of the procedure described at the end of Sec. V. Formally it means that in the action (6.1) the time derivatives of some bosonic coordinates $\dot{X}_a$ are replaced by new auxiliary variables F_a.

The resulting representation $\{\mathbf{D},\mathbf{d},\mathbf{d}-\mathbf{D}\}$ can, for example, contain only 1 timelike and $D-1$ spacelike bosonic dynamical coordinates. Its corresponding action describes the "spinning" particle with all its space–time coordinates belonging to *one* irreducible representation of the extended supersymmetry. All the additional $d-D$ bosonic coordinates are auxiliary. The example of such description of the four-dimensional spinning particle with (4,4) extended supersymmetry was given in Ref. 15.

VII. CONCLUSIONS

In this paper we presented some results concerning the representation theory for irreducible multiplets of the one-dimensional $N=(p,q)$-extended supersymmetry. As pointed out in the text, a peculiar feature of the one-dimensional supersymmetric algebras consists in the fact that the supermultiplets formed by d bosonic and d fermionic degrees of freedom accommodated in a chain with $M+1$ $(M\geqslant 2)$ different spin states such as (2.1) uniquely determines a two-chain multiplet of the form $\{\mathbf{d},\mathbf{d}\}$ which carries a representation of the N extended supersymmetry. Furthermore, it is shown that all such two-chain irreducible multiplets of the (p,q) extended supersymmetry are fully classified; when, e.g., the condition $p-q=0 \bmod 8$ is satisfied, their classification is equivalent to those of Majorana–Weyl spinors in any given space–time, the number $p+q$ of extended supersymmetries being associated with the dimensionality D of the space–time, while the $2d$ supermultiplet dimensionality is the dimensionality of the corresponding Γ matrices. The more general case for arbitrary values of p and q has also been fully discussed.

These mathematical properties can find a lot of interesting applications in connection with the construction of supersymmetric and superconformal quantum mechanical models. These theories are vastly studied due to their relevance in many different physical domains. To name just a few we mention the low-energy effective dynamics of black-hole models, the dimensional reduction of higher-dimensional superfield theories, which are a laboratory for the investigation of the spontaneous breaking of the supersymmetry (for such investigations the extended supersymmetry is an essential ingredient), as well as many others. As recalled in Sec. I, it is very crucial to build extended supersymmetric models realized with the lowest-dimensional representations.

Another area in which we have started applying the tools here elaborated is that one of supersymmetric integrable hierarchies in $1+1$ dimensions. They are globally supersymmetric nonlinear nonrelativistic theories, the one-dimensional susy's being realized through charges obtained by integrating the supercurrents along the spatial line.

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Four-dimensional lattice gauge theory with ribbon categories and the Crane–Yetter state sum

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Lattice Gauge Theory in four-dimensional Euclidean space–time is generalized to ribbon categories which replace the category of representations of the gauge group. This provides a framework in which the gauge group becomes a quantum group while space–time is still given by the ''classical'' lattice. At the technical level, this construction generalizes the spin foam model dual to lattice gauge theory and defines the partition function for a given triangulation of a closed and oriented piecewise-linear four-manifold. This definition encompasses both the standard formulation of $d=4$ pure Yang–Mills theory on a lattice and the Crane–Yetter invariant of four-manifolds. The construction also implies that certain classes of spin foam models formulated using ribbon categories are well-defined even if they do not correspond to a topological quantum field theory. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1398063]

I. INTRODUCTION

The formulation of gauge theory on a lattice[1] combines manifest gauge symmetry with the path integral approach although space–time cannot be retained as a smooth manifold and is replaced instead by a discrete structure. In the present article lattice gauge theory (LGT) always refers to pure gauge theory in Euclidean space–time.

LGT offers a number of generalizations that do not have a naïve continuum analogy such as gauge theory with finite gauge groups. Furthermore, in three dimensions it is possible to define LGT for quantum groups.[2,3] Combining the various actions and Boltzmann weights with suitable ''gauge groups'' (finite groups, Lie groups or quantum groups), this model has several special cases that belong to different branches of physics and mathematics. It is at the center of the relation between LGT with Yang–Mills[1] or with Chern–Simons action,[4,5] the Turaev–Viro invariant of three-manifolds,[6,7] a purely algebraic construction of Topological Quantum Field Theory[4,6] and three-dimensional Euclidean quantum gravity without or with cosmological constant.[8]

At least some of the above constructions are known to have analogies in four dimensions. Even though the question of which is a suitable unified model remains unsolved in full generality, some of the relations known from three dimensions persist also in four dimensions. In the present article we concentrate on the standard formulation of LGT and on the Crane–Yetter state sum.[9,10] We present a definition which encompasses both and generalizes four-dimensional LGT to quantum groups. Technically this is realized for ribbon categories which arise as the categories of representations of certain quantum groups and which replace the category of representations of the gauge group of LGT.

The main result of the present article is the existence of such a generalized LGT in four-dimensional Euclidean space–time using ribbon categories. This model contains the Crane–Yetter state sum as a special case for a particular Boltzmann weight and agrees on the other hand with the spin foam model which is strong-weak dual to LGT if the ribbon category is the category of

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finite-dimensional representations of a compact Lie group. Beyond this, it provides a definition of spin foam models in $d=4$ using ribbon categories which includes in particular the proof that this construction is well-defined even in cases in which the model does not correspond to a Topological Quantum Field Theory.

At the technical level, the construction of these spin foam models using ribbon categories can be motivated from the following observations. From the study of nonperturbative quantum gravity it has emerged that LGT admits a reformulation as a spin foam model—see, for example, Refs. 8, 11, and 12. Many models of interest in quantum gravity are either Topological Quantum Field Theories and use ''delta-functions'' as Boltzmann weights (for example, Ref. 13), or they are topological up to constraints which do not change the weights, but restrict the set of admissible representations. This is the case for some versions of the Barrett–Crane model.[14]

LGT, however, admits more general Boltzmann weights,

$$w: G \to \mathbb{R}, \quad g \mapsto \exp(-s(g)). \tag{1.1}$$

Here the compact Lie group G is the gauge group, the (local) action $s: G \to \mathbb{R}$ is a real, bounded and L^2-integrable class function, and the Boltzmann weight $w(g)$ is evaluated for each plaquette of the lattice. This model encompasses lattice Yang–Mills theory, for example using Wilson's action, but it is not restricted to this case. For general background on LGT the reader is referred to standard textbooks, for example, Refs. 15 and 16.

The spin foam model corresponding to the standard formulation of LGT on a hypercubic lattice was constructed in detail in Ref. 17, where it was found that it generalizes the strong-weak dual of LGT which had been known only in the Abelian case[18,19] and for SU(2) in $d=3$ (Ref. 20) before. The Boltzmann weight (1.1) enters the spin foam model via the coefficients $\hat{w}_\rho$ of its character expansion,

$$w(g) = \sum_{\rho \in \mathcal{R}} \hat{w}_\rho \chi^{(\rho)}(g), \quad \hat{w}_\rho = \dim V_\rho \int_G \overline{\chi^{(\rho)}(g)} w(g)\, dg. \tag{1.2}$$

Here $\chi^{(\rho)}: G \to \mathbb{C}$ denotes the character of the finite-dimensional irreducible representation V_ρ, the sum is over equivalence classes of finite-dimensional irreducible representations of G, and $\int_G$ is the normalized Haar measure on G.

The way the coefficients $\hat{w}_\rho$ appear in the spin foam model dual to LGT[17] compared with the Ooguri state sum[13] indicates that there exists a unified construction encompassing both. In addition, the fact that the Crane–Yetter state sum[9,10] can be understood as a generalization of the Ooguri model to quantum groups suggests the construction given in the present article.

The strategy for the definition of $d=4$ LGT using ribbon categories is as follows. The construction is based on a triangulation of a closed and oriented piecewise-linear four-manifold M which is specified by an abstract combinatorial complex. In the special case of a Lie group symmetry, the definition shall coincide with the spin foam model dual to LGT if that LGT is formulated on the two-complex dual to the triangulation (note that we formulate the spin foam model on the triangulation itself, following Ref. 10). In the Lie group case, both pictures are available: the spin foam model on the triangulation and LGT on the dual two-complex. They are dual to each other in the sense of Ref. 17. Physically this means strong-weak duality between LGT and the spin foam model while on the mathematical side the two models are related by a Tannaka–Krein-like reconstruction theorem relating LGT (formulated in terms of the gauge group G) with the spin foam model (formulated in terms of the category of representations Rep G). For details on quantum groups, ribbon categories and the reconstruction theorems, the reader is referred to standard textbooks such as Refs. 21 and 22.

The generalization takes place in the spin foam picture where the category Rep G is replaced by a suitable ribbon category $\mathcal{C}$. Loosely speaking, using the reconstruction theorems, this provides a definition of LGT in which the gauge group is replaced by a quantum group. Technically, the

notion of gauge group is lost, but one can think of replacing the algebra of representation functions $C_{\mathrm{alg}}(G)$ by a noncommutative algebra (a suitable ribbon Hopf algebra) while space–time is still given by the 'classical' lattice.

The generalization from Rep G to a generic ribbon category $\mathcal{C}$ involves choices of the ordering of tensor factors and choices of the braiding whenever tensor factors are exchanged. These choices are not at all obvious from the Lie group case which involves only the symmetric category Rep G.

The method to achieve a consistent definition in the spin foam picture is to choose a linear order of vertices for the combinatorial complex and to define the partition function in a way that employs special choices and that refers explicitly to that order. It is then possible to show in a second step that the partition function is actually independent of the order (combinatorially invariant) and is thus well-defined for a given triangulation. This approach can be seen as a generalization to four dimensions of the strategy which Barrett and Westbury[7] employ in their approach to the Turaev–Viro invariant.[6]

Another point of view on the definition given in the present article is related to the construction of the Crane–Yetter state sum in Ref. 10. The authors of Ref. 10 first show that the state sum is independent of the triangulation, which in our terminology relies on the choice of a particular Boltzmann weight. Triangulation independence then implies combinatorial invariance and thus establishes that the state sum is well-defined. As an alternative proof, it is conceivable to show combinatorial invariance in the first step. This holds for any choice of Boltzmann weights. One could then prove in a second step that the choice of special Boltzmann weights implies triangulation independence by standard arguments as in Refs. 9, 10, and 13. The construction presented in the present article can be viewed as the first of these two steps.

Finally, we would like to mention D. V. Boulatov's approach to LGT for quantum groups in three dimensions.[2] His construction makes use of the general result of Reshetikhin and Turaev[23] establishing a functor from the category of ribbon graphs in $\mathbb{R}^3$ to the ribbon category $\mathcal{C}$. The strategy in Ref. 2 is to construct a suitable ribbon graph in the triangulated manifold which then yields a well-defined partition function as the quantum trace of a ribbon morphism.

A related definition of $d=3$ LGT for quantum groups was developed by R. Oeckl[3] in which the duality between LGT and its dual spin foam model is understood entirely in terms of manipulations of ribbon graphs. The approach of Ref. 3 also develops the correspondence of ribbon categories with suitable quantum groups, namely coribbon Hopf algebras, in a way that transparently generalizes the duality transformation of the Lie group case.

However, since the Reshetikhin–Turaev functor is available only for ribbon graphs in $\mathbb{R}^3$, these approaches do not have a direct generalization to higher dimension. In the present article, we use the functor mainly to justify diagrammatic calculations.

The present article is organized as follows. In Sec. II, we review some mathematical background on the Peter–Weyl theory for compact Lie groups and on ribbon categories, and we introduce our notation for combinatorial and simplicial complexes. The duality transformation for LGT with Lie gauge groups which was derived in Ref. 17 on a cubic lattice is reviewed in Sec. III and formulated there on a two-complex. In Sec. IV, we define the spin foam model generalizing the dual of LGT to suitable ribbon categories. This section contains the definition of the partition function, the proof that it is well-defined and comments on the construction of observables and on the role played by the gauge transformations in the spin foam model. In Sec. V, we indicate how these definitions specialize to the standard formulation of LGT with a compact Lie group (or a finite group) as the gauge group and to the Crane–Yetter invariant. We also comment on possible generalizations and relations with other spin foam models. Section VI contains a conclusion and comments on open questions.

II. PRELIMINARIES

A. Peter–Weyl theory

In this section, we briefly summarize definitions and basic statements related to the algebra of representation functions $C_{\mathrm{alg}}(G)$ of G where G is a compact Lie group (or a finite group). These

results are needed in Sec. III in order to present the duality transformation relating LGT and the spin foam model. For more details, the reader is referred to the Introduction of Ref. 17 or to textbooks such as Refs. 24 and 25.

1. Representation functions

Finite-dimensional complex vector spaces on which G is represented are denoted by V_ρ and by $\rho: G \to \mathrm{Aut}V_\rho$ the corresponding group homomorphism. Let $\tilde{\mathcal{R}}$ denote a set containing one unitary representative of each class of finite-dimensional representations and $\mathcal{R}$ the subset of irreducible representations. For a representation $\rho \in \tilde{\mathcal{R}}$, the dual representation is denoted by ρ^*, and the dual vector space of V_ρ by V_ρ^*. The dual representation is given by $\rho^*: G \mapsto \mathrm{Aut}V_\rho^*$, where $\rho^*(g): V_\rho^* \to V_\rho^*$, $\eta \mapsto \eta \circ \rho(g^{-1})$, i.e., $(\rho^*(g)\eta)(v) = \eta(\rho(g^{-1})v)$ for all $v \in V_\rho$. There exists a one-dimensional "trivial" representation of G which is denoted by $V_{[1]} \cong \mathbb{C}$.

For the unitary representations V_ρ, $\rho \in \tilde{\mathcal{R}}$, there exist standard sesquilinear scalar products $\langle \cdot ; \cdot \rangle$ and orthonormal bases (v_j) in such a way that the basis (v_j) of V_ρ is dual to the basis (η^j) of V_ρ^*, i.e., $\eta^j(v_k) = \delta_k^j$. Duality is here given by the scalar product, i.e., $\langle v_j ; v_k \rangle = \eta^j(v_k)$ and $\langle \eta^j ; \eta^k \rangle = \eta^k(v_j)$, $1 \leqslant j,k \leqslant \dim V_\rho$.

The complex-valued functions

$$t^{(\rho)}_{\eta,v} : G \to \mathbb{C}, \quad g \mapsto \eta(\rho(g)v), \tag{2.1}$$

where $\rho \in \tilde{\mathcal{R}}$, $v \in V_\rho$ and $\eta \in V_\rho^*$, are called *representation functions* of G. They form a commutative and associative unital algebra over $\mathbb{C}$,

$$C_{\mathrm{alg}}(G) := \{\, t^{(\rho)}_{\eta,v} : \quad \rho \in \tilde{\mathcal{R}}, v \in V_\rho, \eta \in V_\rho^* \,\}, \tag{2.2}$$

whose operations are given by

$$(t^{(\rho)}_{\eta,v} + t^{(\sigma)}_{\vartheta,w})(g) := t^{(\rho \oplus \sigma)}_{\eta + \vartheta, v+w}(g), \tag{2.3a}$$

$$(t^{(\rho)}_{\eta,v} \cdot t^{(\sigma)}_{\vartheta,w})(g) := t^{(\rho \otimes \sigma)}_{\eta \otimes \vartheta, v \otimes w}(g), \tag{2.3b}$$

for $\rho, \sigma \in \tilde{\mathcal{R}}$ and $v \in V_\rho$, $w \in V_\sigma$, $\eta \in V_\rho^*$, $\vartheta \in V_\sigma^*$ and $g \in G$. The zero element of $C_{\mathrm{alg}}(G)$ is $t^{[1]}_{0,0}(g) = 0$ and its unit element $t^{[1]}_{\eta,v}(g) = 1$ where the normalization is such that $\eta(v) = 1$.

The algebra $C_{\mathrm{alg}}(G)$ is furthermore equipped with a Hopf algebra structure employing the coproduct $\Delta: C_{\mathrm{alg}}(G) \to C_{\mathrm{alg}}(G) \otimes C_{\mathrm{alg}}(G) \cong C_{\mathrm{alg}}(G \times G)$, the co-unit $\varepsilon: C_{\mathrm{alg}}(G) \to \mathbb{C}$ and the antipode $S: C_{\mathrm{alg}}(G) \to C_{\mathrm{alg}}(G)$, which are defined by

$$\Delta t^{(\rho)}_{\eta,v}(g,h) := t^{(\rho)}_{\eta,v} g(\cdot h), \tag{2.4a}$$

$$\varepsilon t^{(\rho)}_{\eta,v} := t^{(\rho)}_{\eta,v}(1), \tag{2.4b}$$

$$S t^{(\rho)}_{\eta,v}(g) := t^{(\rho)}_{\eta,v}(g^{-1}), \tag{2.4c}$$

for $\rho \in \tilde{\mathcal{R}}$ and $v \in V_\rho$, $\eta \in V_\rho^*$ and $g,h \in G$. For unitary representations, the antipode relates a representation with its dual which is just the conjugate representation,

$$S t^{(\rho)}_{mn}(g) = t^{(\rho^*)}_{nm}(g) = \overline{t^{(\rho)}_{nm}(g)}. \tag{2.5}$$

The bar denotes complex conjugation.

2. Peter–Weyl decomposition and theorem

The structure of the algebra $C_{\mathrm{alg}}(G)$ can be understood if $C_{\mathrm{alg}}(G)$ is considered as a representation of $G \times G$ by combined left and right translation of the function argument.

Theorem 2.1 (Peter–Weyl decomposition): Let G be a compact Lie group (or a finite group).

(1) There is an isomorphism

$$C_{\mathrm{alg}}(G) \cong_{G\times G} \bigoplus_{\rho\in\mathcal{R}} (V_\rho^* \otimes V_\rho) \tag{2.6}$$

of representations of $G\times G$. Here the direct sum is over one unitary representative of each equivalence class of finite-dimensional irreducible representations of G. The direct summands $V_\rho^*\otimes V_\rho$ are irreducible as representations of $G\times G$.

(2) The direct sum in (2.6) is orthogonal with respect to the L^2-scalar product on $C_{\mathrm{alg}}(G)$, which is formed using the Haar measure on G on the left hand side, and using the standard scalar products on the right hand side, namely

$$\langle t^{(\rho)}_{\eta,v}; t^{(\sigma)}_{\vartheta,w}\rangle_{L^2} = \int_G \overline{t^{(\rho)}_{\eta,v}(g)}\cdot t^{(\sigma)}_{\vartheta,w}(g)\, dg = \frac{1}{\dim V_\rho}\,\delta_{\rho\sigma}\overline{\langle \eta;\vartheta\rangle}\langle v;w\rangle, \tag{2.7}$$

where $\rho,\sigma\in\mathcal{R}$ are irreducible. The Haar measure is denoted by $\int_G$ and normalized such that $\int_G dg = 1$.

Each representation function $f\in C_{\mathrm{alg}}(G)$ can thus be decomposed according to (2.6) such that its L^2-norm is given by

$$\|f\|_{L^2}^2 = \sum_{\rho\in\mathcal{R}} \frac{1}{\dim V_\rho}\|f_\rho\|^2, \tag{2.8}$$

where $f_\rho\in V_\rho^*\otimes V_\rho \cong \mathrm{Hom}(V_\rho,V_\rho)$, $\rho\in\mathcal{R}$, and all except finitely many f_ρ are zero.

Theorem 2.2 (Peter–Weyl theorem): Let G be a compact Lie group. Then $C_{\mathrm{alg}}(G)$ forms a dense subset of $L^2(G)$.

The characters $\chi^{(\rho)}: G\to\mathbb{C}$ associated with the finite-dimensional unitary representations $\rho\in\widetilde{\mathcal{R}}$ of G are given by the traces,

$$\chi^{(\rho)} := \sum_{j=1}^{\dim V_\rho} t^{(\rho)}_{jj}. \tag{2.9}$$

Each class function $f\in C_{\mathrm{alg}}(g)$ can be character-decomposed

$$f(g) = \sum_{\rho\in\mathcal{R}} \chi^{(\rho)}(g)\,\hat{f}_\rho, \quad \text{where} \quad \hat{f}_\rho = \dim V_\rho \int_G \overline{\chi^{(\rho)}(g)} f(g)\, dg, \tag{2.10}$$

such that the completion of $C_{\mathrm{alg}}(G)$ to $L^2(G)$ is compatible with this decomposition.

3. The Haar measure

The Haar measure on G can be understood in terms of the Peter–Weyl decomposition (2.6) as follows.

Proposition 2.3: Let G be a compact Lie group (or a finite group) and $\rho\in\widetilde{\mathcal{R}}$ be a finite-dimensional unitary representation of G with the orthogonal decomposition

$$V_\rho \cong \bigoplus_{j=1}^{k} V_{\tau_j}, \quad \tau_j\in\mathcal{R}, k\in\mathbb{N}, \tag{2.11}$$

into irreducible components τ_j. Let $P^{(j)}: V_\rho \to V_{\tau_j} \subseteq V_\rho$ be the G-invariant orthogonal projectors associated with the above decomposition. Assume that precisely the first l components $\tau_1, \ldots, \tau_l$, $0 \leqslant l \leqslant k$, are equivalent to the trivial representation. Then the Haar measure of a representation function $t^{(\rho)}_{mn}$, $1 \leqslant m,n \leqslant \dim V_\rho$, is given by

$$\int_G t^{(\rho)}_{mn}(g)\, dg = \sum_{j=1}^{l} P^{(j)m} P^{(j)}_n, \quad P^{(j)m} = \eta^m(w^{(j)}), \quad P^{(j)}_n = \vartheta^{(j)}(v_n). \tag{2.12}$$

Here (v_n) and (η^m) are dual bases of V_ρ and V^*_ρ, the $w^{(j)}$ are normalized vectors in $V_{\tau_j} \subseteq V_\rho$, and $\vartheta^{(j)}$ denotes the linear form dual to $w^{(j)}$.

B. Ribbon categories

Ribbon categories are used in the present article as a generalization of the category of representations of the gauge group. A ribbon category is a braided monoidal category with some additional structure. In this section, we summarize the basic definitions with emphasis on a convenient diagrammatic notation. We refer the reader to the literature for more details, for example, to Refs. 21 and 22. Our presentation is similar to that of Ref. 3; we essentially follow Ref. 22, but use the diagrams of Ref. 21. Also relevant in the context of the present article are the results of Reshetikhin and Turaev.[23,26]

1. Basic definitions

Definition 2.4: A *strict monoidal category* is a category $\mathcal{C}$ together with a covariant functor $\otimes: \mathcal{C} \times \mathcal{C} \to \mathcal{C}$ and a *unit object* $\mathbf{1}$ such that

$$U \otimes (V \otimes W) = (U \otimes V) \otimes W, \tag{2.13a}$$

$$V \otimes \mathbf{1} = V = \mathbf{1} \otimes V, \tag{2.13b}$$

for all objects U, V, W.

Definition 2.5: A *strict braided monoidal category* is a strict monoidal category with natural isomorphisms (the *braiding*),

$$\psi_{V,W}: V \otimes W \to W \otimes V, \tag{2.14}$$

such that

$$\psi_{U \otimes V, W} = (\psi_{U,W} \otimes \mathrm{id}_V) \circ (\mathrm{id}_U \otimes \psi_{V,W}), \tag{2.15a}$$

$$\psi_{U, V \otimes W} = (\mathrm{id}_V \otimes \psi_{U,W}) \circ (\psi_{U,V} \otimes \mathrm{id}_W), \tag{2.15b}$$

$$\psi_{V,\mathbf{1}} = \mathrm{id}_V = \psi_{\mathbf{1},V}, \tag{2.15c}$$

for all objects U, V, W. The category is called *symmetric* if in addition

$$\psi_{W,V} \circ \psi_{V,W} = \mathrm{id}_{V \otimes W}. \tag{2.16}$$

Definition 2.6: A strict monoidal category $\mathcal{C}$ is called *rigid* if for each object V there exists an object V^* (the *left dual*) and if there are natural isomorphisms

$$\mathrm{ev}_V: V^* \otimes V \to \mathbf{1}, \quad \text{(evaluation)}, \tag{2.17a}$$

$$\mathrm{coev}_V: \mathbf{1} \to V \otimes V^* \quad \text{(co-evaluation)}, \tag{2.17b}$$

which satisfy for all objects V,

$$\mathrm{id}_V = (\mathrm{id}_V \otimes \mathrm{ev}_V) \circ (\mathrm{coev}_V \otimes \mathrm{id}_V), \tag{2.18a}$$

$$\mathrm{id}_{V^*} = (\mathrm{ev}_V \otimes \mathrm{id}_{V^*}) \circ (\mathrm{id}_{V^*} \otimes \mathrm{coev}_V). \tag{2.18b}$$

For a given morphism $f: V \to W$, the dual morphism $f^*: W^* \to V^*$ is defined by

$$f^* := (\mathrm{ev}_W \otimes \mathrm{id}_{V^*}) \circ (\mathrm{id}_{W^*} \otimes f \otimes \mathrm{id}_{V^*}) \circ (\mathrm{id}_{W^*} \otimes \mathrm{coev}_V). \tag{2.19}$$

Left duality thus defines a contravariant functor $*: \mathcal{C} \to \mathcal{C}$.

Definition 2.7: A *strict ribbon category* $\mathcal{C}$ is a strict rigid braided monoidal category with natural isomorphisms (the *twist*),

$$\nu_V : V \to V, \tag{2.20}$$

such that for all objects V, W,

$$\nu_{V \otimes W} = (\nu_V \otimes \nu_W) \circ \psi_{W,V} \circ \psi_{V,W}, \tag{2.21a}$$

$$(\nu_V)^* = \nu_{V^*}, \tag{2.21b}$$

$$\nu_{\mathbf{1}} = \mathrm{id}_{\mathbf{1}}. \tag{2.21c}$$

It is now possible to construct right duals ${}^*V$ from the braiding, the twist and the left duals. The right dual objects agree in this case with the left duals, ${}^*V = V^*$, and right evaluation and right co-evaluation are given by

$$\widetilde{\mathrm{ev}}_V : V \otimes V^* \to \mathbf{1}, \quad \widetilde{\mathrm{ev}}_V := \mathrm{ev}_V \circ \psi_{V,V^*} \circ (\nu_V \otimes \mathrm{id}_{V^*}), \tag{2.22a}$$

$$\widetilde{\mathrm{coev}}_V : \mathbf{1} \to V^* \otimes V, \quad \widetilde{\mathrm{coev}}_V := (\nu_{V^*} \otimes \mathrm{id}_V) \circ \psi_{V,V^*} \circ \mathrm{coev}_V. \tag{2.22b}$$

Finally, right and left duals can be employed in order to define the analog of trace and dimension.

Definition 2.8: Let $\mathcal{C}$ be a strict ribbon category, V an object of $\mathcal{C}$ and $f: V \to V$.

(1) The *quantum trace* of f is defined by

$$\mathrm{qtr}(f) := \widetilde{\mathrm{ev}}_V \circ (f \otimes \mathrm{id}_{V^*}) \circ \mathrm{coev}_V. \tag{2.23}$$

(2) The *quantum dimension* of V is defined by

$$\mathrm{qdim} V := \mathrm{qtr}(\mathrm{id}_V) = \widetilde{\mathrm{ev}}_V \circ \mathrm{coev}_V. \tag{2.24}$$

Note that the quantum trace satisfies $\mathrm{qtr}(g \circ f) = \mathrm{qtr}(f \circ g)$ for $f: V \to W$ and $g: W \to V$. Furthermore, for $h: V \to V$ and $k: W \to W$, $\mathrm{qtr}(h \otimes k) = \mathrm{qtr}(h) \circ \mathrm{qtr}(k)$ and $\mathrm{qdim}(V \otimes W) = \mathrm{qdim} V \circ \mathrm{qdim} W$, where the compositions are in $\mathrm{Hom}(\mathbf{1}, \mathbf{1})$.

All monoidal categories defined above, starting from Definition 2.4, are strict. If a non-strict category is given, there exists an equivalent strict version[23] which can be used instead. As a consequence of the coherence conditions on associativity and unit constraints in the definition of a (nonstrict) monoidal category, it would also be possible to make a choice of parentheses in all definitions and to insert the constraints in a consistent way in all equations. The same would apply to the calculations and results presented in the following sections of this paper.

Furthermore, all categories of interest in this article, are $\mathbb{C}$-linear (for details see, for example, Refs. 21 and 27). This means that there is the notion of a (finite) direct sum of objects, that, furthermore, for given objects V, W the sets $\mathrm{Hom}(V, W)$ form $\mathbb{C}$-vector spaces and that composition of morphisms is $\mathbb{C}$-bilinear. Additionally, there are notions of monomorphism and epimorphism which have the usual properties known from linear algebra. The reader might think of the

case where all objects are $\mathbb{C}$-vector spaces. Finally, the additional structures such as tensor product, braiding, duality and twist are required to be compatible with the $\mathbb{C}$-linear structure, in particular $\mathrm{Hom}(\mathbf{1},\mathbf{1})\cong\mathbb{C}$ such that composition corresponds to multiplication.

As a consequence, $\mathrm{Hom}(U\otimes V,W)\cong\mathrm{Hom}(V,W\otimes U^*)$ are isomorphic as $\mathbb{C}$-vector spaces. We also need the dual space of $\mathrm{Hom}(V,W)$. One can make use of a nondegenerate $\mathbb{C}$-bilinear pairing

$$\mathrm{Hom}(V^*,W^*)\otimes_{\mathbb{C}}\mathrm{Hom}(V,W)\to\mathbb{C},\ f\otimes g\mapsto \mathrm{ev}_W\circ(g\otimes f)\circ\widetilde{\mathrm{coev}}_V, \tag{2.25}$$

in order to define the dual space $\mathrm{Hom}(V,W)^*$ up to isomorphism. Here we use $\mathrm{Hom}(V^*,W^*)$ rather than $\mathrm{Hom}(W,V)$ because some diagrams in the following sections are then related by a mirror symmetry.

All conditions that are required for the construction of the spin foam model are summarized in the following definition.

Definition 2.9: An *admissible* ribbon category is a $\mathbb{C}$-linear strict ribbon category which satisfies the following conditions.

(1) For all objects V, W of $\mathcal{C}$ the space $\mathrm{Hom}(V,W)$ is finite-dimensional as a $\mathbb{C}$-vector space.
(2) The pairing (2.25) is nondegenerate for all objects V, W of $\mathcal{C}$.

A *set of colors* $\mathcal{C}_0$ is a countable set of objects of $\mathcal{C}$ such that

(1) no two elements of $\mathcal{C}_0$ are isomorphic, and
(2) for each object $V\in\mathcal{C}_0$, the set $\mathcal{C}_0$ also contains an object which is isomorphic to V^*.

There are two cases in which one wants to require stronger conditions. First, in order to have a correspondence of the spin foam model with LGT, one seeks a categorical version of the Peter–Weyl theorem and of the Haar measure.

The role of the irreducible representations in the Peter–Weyl theory is now played by the simple objects:

Definition 2.10: Let $\mathcal{C}$ be a $\mathbb{C}$-linear strict ribbon category.

(1) An object V of $\mathcal{C}$ is called *simple* if each nonzero monomorphism $f:U\to V$ is an isomorphism and each nonzero epimorphism $f:V\to W$ is an isomorphism.
(2) $\mathcal{C}$ is called *semi-simple* if each object V of $\mathcal{C}$ is isomorphic to a (finite) direct sum of simple objects.
(3) $\mathcal{C}$ is called *finitely* (*countably*) *semi-simple* if $\mathcal{C}$ is semi-simple and if there are only finitely (countably) many simple objects up to isomorphism.

Corollary 2.11: Let $\mathcal{C}$ be a countably semi-simple and admissible ribbon category such that the unit object $\mathbf{1}$ is simple and such that for each simple object J we have $\mathrm{Hom}(J,J)\cong\mathbb{C}$. Let $\mathcal{C}_0$ denote a set containing one representative per equivalence class of simple objects of $\mathcal{C}$ and let V, W be objects of $\mathcal{C}$. Then the natural map given by composition of morphisms,

$$\bigoplus_{J\in\mathcal{C}_0}\mathrm{Hom}(V,J)\otimes_{\mathbb{C}}\mathrm{Hom}(J,W)\to\mathrm{Hom}(V,W), \tag{2.26}$$

is an isomorphism of $\mathbb{C}$-vector spaces.

The direct sum in (2.26) plays the role of the Peter–Weyl decomposition (2.6) in the categorical framework.

Remark 2.12: Under the conditions of Corollary 2.11, there exists furthermore for each natural transformation $f_V:V\to V$ another natural transformation $(Tf)_V:V\to V$ which is defined by the projection onto the direct summand labeled by $J=\mathbf{1}$ in (2.26),

$$T:\mathrm{Hom}(V,V)\to\mathrm{Hom}(V,\mathbf{1})\otimes\mathrm{Hom}(\mathbf{1},V)\subseteq\mathrm{Hom}(V,V). \tag{2.27}$$

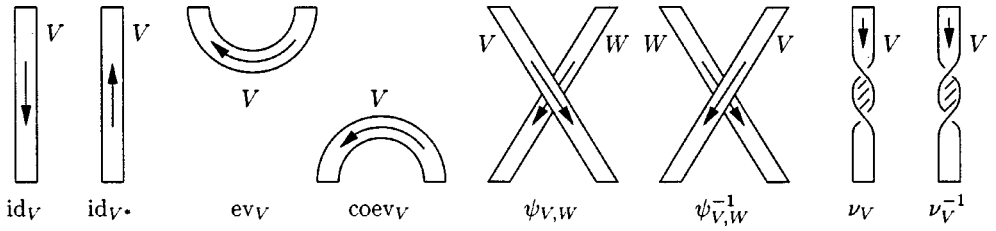


FIG. 1. Some basic ribbon diagrams: The identity morphisms id_V and id_{V^*}, evaluation ev_V and coevaluation coev_V, the braiding $\psi_{V,W}$, the twist ν_V and their inverses, cf. Definitions 2.4–2.7.

These $(Tf)_V$ satisfy, for example, $(Tf)_J=0$ for all simple objects J which are not isomorphic to the unit object **1**.

The projection T can be viewed as the translation of the Haar measure $\int: C_{\mathrm{alg}}(G)\to\mathbb{C}$ into the categorical language, cf. (2.12).

A detailed explanation of how Corollary 2.11 and Remark 2.12 are related with Peter–Weyl decomposition and Haar measure in the Lie group case can be found in Ref. 3. In the picture of Ref. 3, the algebra of representation functions $C_{\mathrm{alg}}(G)$ of the Lie group G co-acts on the vector spaces dual to the representations V_ρ of G.

A second situation in which one sometimes requires semi-simplicity is the case when the spin foam model defines a topological invariant; see, for example, Ref. 10. Recall, however, that the categories of finite-dimensional representations of the quantum groups $U_q(\mathfrak{g})$, q a root of unity, which form important examples, are not semi-simple.[21] I thank R. Oeckl for pointing out that the weaker notions of quasi-dominance and dominance (Chapt. XI of Ref. 26) can be used to establish a uniform treatment of all interesting cases.

The problem of the definition of the spin foam model with ribbon categories which is the subject of the present article is, however, not affected by these subtleties since it relies only on Definition 2.9.

2. Ribbon diagrams

There exists a very convenient notation for morphisms of a ribbon category $\mathcal{C}$ in terms of *ribbon diagrams* (Fig. 1). The diagrams consist of ribbons which have a white side (normally facing up) and a black side (facing down). They are directed which is denoted by arrows, and they are labeled with objects of $\mathcal{C}$.

The identity morphism id_V is represented by a ribbon labeled V with the arrow pointing down. The identity morphism id_{V^*} of the dual object has the same label V, but an arrow pointing up. The diagrams are generally read from top to bottom. Putting diagrams below each other denotes composition of morphisms while putting them next to each other denotes the tensor product of

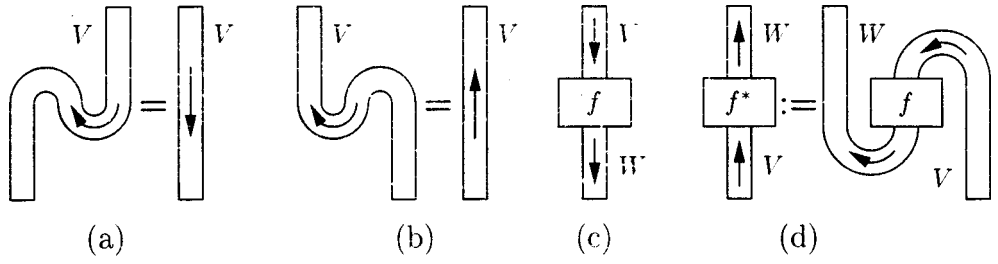


FIG. 2. The conditions (2.18a) and (2.18b) on evaluation and coevaluation are depicted in diagrams (a) and (b). A morphism $f: V\to W$ is represented by a coupon as in (c). Diagram (d) shows the definition of the dual morphism f^* as given by (2.19).

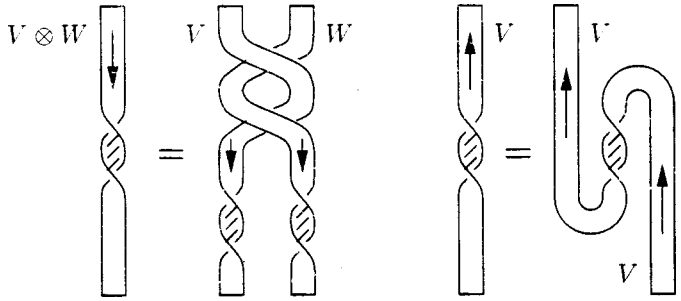


FIG. 3. The conditions (2.21a) and (2.21b) on the twist ν_V in diagrammatic notation.

morphisms. Figure 1 also shows the natural isomorphisms ev_V, coev_V of (2.17), the braiding $\psi_{V,W}$ of (2.14), the twist ν_V of (2.20) and their inverses, respectively. The unit object **1** is invisible in the diagrams which is justified by (2.13b), (2.15c) and (2.21c).

Figure 2 shows the conditions (2.18a) and (2.18b) on evaluation and coevaluation in (a) and (b). Morphisms $f: V \to W$ are represented by a *coupon* labeled f with an incoming and an outgoing ribbon as in (c). Figure 2 also shows the definition of the dual morphism (2.19) in diagram (d).

The conditions (2.21a) and (2.21b) on the twist ν_V in a ribbon category are depicted in Fig. 3. Figure 4 shows the definition of right duals via $\widetilde{\mathrm{ev}}_V$ and $\widetilde{\mathrm{coev}}_V$ of (2.22), the quantum trace (2.23) and the quantum dimension (2.24).

The main purpose of the ribbon diagrams presented in this section is that they have an immediate translation into algebraic language in terms of morphisms of the ribbon category $\mathcal{C}$ and at the same time provide an intuitive way of dealing with the algebraic manipulations. One can imagine that the ribbons shown in the diagrams are embedded in $\mathbb{R}^3$. The obvious isotopies then correspond to relations in $\mathcal{C}$. This is a direct consequence of the functor constructed by Reshetikhin and Turaev in Ref. 23 where more details can be found. In the following, we present many calculations in the diagrammatic language. If required, they can be translated at any stage into the corresponding algebraic expressions.

In the remaining parts of the article, we employ a simplified notation in which the ribbons are represented by single directed lines, and it is understood that their white side always faces up. This is known as *blackboard framing*. It is particularly convenient here because it turns out that the relevant diagrams in the following sections can be drawn without twists.

3. Quantum groups and ribbon categories

The ribbon categories arising in Ref. 23 are constructed as the categories of finite-dimensional representations of suitable ribbon Hopf algebras (see also Refs. 21, 22, and 26).

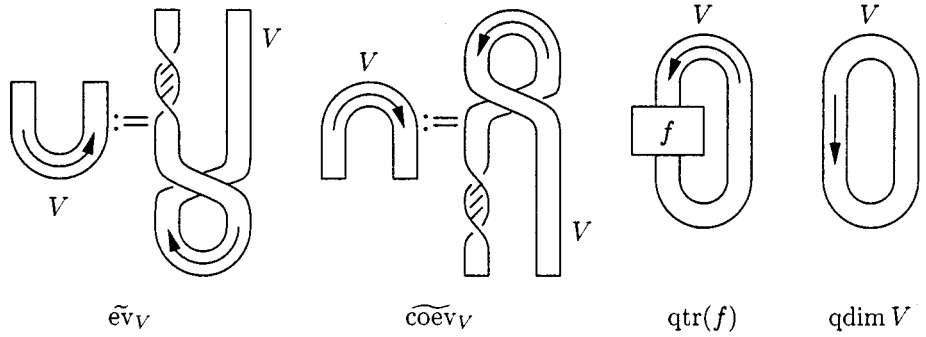


FIG. 4. Definition of right duality, $\widetilde{\mathrm{ev}}_V$ and $\widetilde{\mathrm{coev}}_V$ of (2.22), the quantum trace (2.23) and the quantum dimension (2.24).

An alternative picture is developed in Ref. 3. It is dual to the former in the sense that it uses the dual Hopf algebra co-acting on the dual spaces of the representations. It is thus based on coribbon Hopf algebras and their ribbon category of corepresentations. This point of view is much closer to the duality transformation for LGT with Lie groups (see Sec. III or Ref. 17) since the algebra of representation functions $C_{\mathrm{alg}}(G)$ of the gauge group naturally coacts on the dual spaces of the representations of G and can be replaced by a suitable coribbon Hopf algebra.[3]

C. Combinatorial and simplicial complexes

1. Triangulations

For the construction of the spin foam model using ribbon categories, we need combinatorial complexes and simplicial complexes. Combinatorial complexes contain the information of which simplices are contained in the boundary of a given simplex while simplicial complexes also provide a linear order of the vertices and keep track of all relative orientations. This terminology follows Ref. 7. In order to construct a spin foam model for ribbon categories, we aim for a definition of the partition function which takes the relative orientations into account, but which does not depend on the linear order of vertices.

For the purpose of the present article, it is furthermore sufficient to deal with abstract complexes. The details of how their simplices are mapped to the given manifold are not discussed here except for a few restrictions that apply if the complex corresponds to a closed and oriented manifold.

Definition 2.13: For a given set Λ of *vertices*, a *combinatorial complex* $\Lambda^{(*)}$ is a nonempty set of subsets of Λ,

$$\varnothing \neq \Lambda^{(*)} \subseteq \mathcal{P}\Lambda, \tag{2.28}$$

such that for each $v \in \Lambda$, $\{v\} \in \Lambda^{(*)}$ and for each set $X \in \Lambda^{(*)}$, all its nonempty subsets are also contained in $\Lambda^{(*)}$, i.e.,

$$X \in \Lambda^{(*)} \quad \text{and} \quad \varnothing \neq Y \subseteq X \Rightarrow Y \in \Lambda^{(*)}. \tag{2.29}$$

The sets $X \in \Lambda^{(*)}$ are called *simplices*. The subsets $\varnothing \neq Y \subseteq X$ are the *faces of* X. The elements of the set

$$\Lambda^{(k)} := \{X \in \Lambda^{(*)}: \quad |X| = k+1\}, \quad k \in \mathbb{N}, \tag{2.30}$$

are called k-simplices. Here $|\cdot|$ denotes the cardinality of a set. A *combinatorial k-complex* is a combinatorial complex for which $\Lambda^{(j)} = \varnothing$ for all $j > k$. For each k-simplex $X \in \Lambda^{(k)}$, its *boundary* is defined as the collection of $(k-1)$-simplices,

$$\partial X := \{Y \subseteq X: \ |Y| = k\}. \tag{2.31}$$

A combinatorial complex is called *finite* if $\Lambda^{(*)}$ is a finite set.

Definition 2.14: A *simplicial complex* $(\Lambda^{(*)}, <)$ is a combinatorial complex $\Lambda^{(*)}$ with a linear order $(<)$ of the vertices Λ. The k-simplices $X \in \Lambda^{(k)}$ can then be represented by $(k+1)$-tuples $(v_0, v_1, \ldots, v_k)$ of vertices $v_j \in \Lambda$ in standard order $v_0 < v_1 < \ldots < v_k$. In the free $\mathbb{Z}$-module generated by $\Lambda^{(*)}$, the boundary of a k-simplex is given as a sum over the $(k-1)$-simplices in ∂X,

$$\partial(v_0, v_1, \ldots, v_k) := \sum_{j=0}^{k} (-1)^j (v_0, v_1, \ldots, \hat{v}_j, \ldots, v_k), \tag{2.32}$$

where the hat $(\hat{\ })$ indicates that a symbol is omitted. An abbreviated notation is

$$(01\cdots k) := (v_0, v_1, \ldots, v_k). \tag{2.33}$$

In the following we also use the notation $(v_0,v_1,\ldots,v_k)$ with arbitrary vertex order. In the simplicial complex this denotes an oriented k-simplex $\mathrm{sgn}\tau\cdot(v_{\tau(0)},\ldots,v_{\tau(k)})$ where the sign depends on the sign of the permutation $\tau\in\mathcal{S}_{k+1}$ which is required to sort the vertices such that $v_{\tau(0)}<\ldots<v_{\tau(k)}$.

The triangulations of a compact piecewise-linear k-manifold M can be chosen to have only finitely many simplices. In this case their combinatorics are described by a finite combinatorial k-complex for which there always exists a linear order of vertices.

For a simplicial k-complex which corresponds to the triangulation of a closed and oriented k-manifold M, the relative orientation of each simplex σ with respect to M is given, i.e., whether $+\sigma$ or $-\sigma$ is isomorphic to a simplex in M. Observe further that in this case each $(k-1)$-simplex is contained in the boundary of exactly two k-simplices: once with positive and once with negative relative orientation.

2. The dual two-complex

In the present article the spin foam model is defined on a combinatorial complex $\Lambda^{(*)}$. This point of view agrees with, Refs. 7 and 10, but is dual to the definition given in Ref. 12.

In order to compare the spin foam model on $\Lambda^{(*)}$ with LGT, this LGT has to be formulated on the two-complex dual to $\Lambda^{(*)}$. In this section, we define a generalized notion of two-complexes which includes polygons rather than just triangles and which makes the cyclic ordering of edges around the polygons explicit. This ordering is necessary to arrange the factors of the group products which are used in the definition of LGT.

Definition 2.15: A *finite generalized two-complex with cyclic structure* (V,E,F) consists of finite sets V (*vertices*), E (*edges*) and F (*polygons*) together with maps

$$\partial_+ : E\to V \quad \text{(end point of an edge)}, \tag{2.34a}$$

$$\partial_- : E\to V \quad \text{(starting point of an edge)}, \tag{2.34b}$$

$$N: F\to\mathbb{N} \quad \text{(number of edges in the boundary of a polygon)}, \tag{2.34c}$$

$$\partial_j : F\to E \quad \text{(the } j\text{th edge in the boundary)}, \tag{2.34d}$$

$$\varepsilon_j : F\to\{-1,+1\} \quad \text{(its orientation)} \tag{2.34e}$$

such that

$$\partial_{-\varepsilon_j f}\partial_j f=\partial_{\varepsilon_{j+1}f}\partial_{j+1}f, \quad 1\leqslant j\leqslant N(f)-1, \tag{2.35a}$$

$$\partial_{-\varepsilon_{N(f)}f}\partial_{N(f)}f=\partial_{\varepsilon_1 f}\partial_1 f, \tag{2.35b}$$

for all $f\in F$.

The conditions (2.35) state that the edges in the boundary of a polygon $f\in F$ are in cyclic ordering from $\partial_1 f$ to $\partial_{N(f)}f$ where one encounters the edges with a relative orientation given by $-\varepsilon_j f$, (see Fig. 5). Observe that (2.35) can be used to generalize the condition $\partial\circ\partial=0$ to the situation where the edges are labeled with noncommutative variables.

Given a finite simplicial k-complex $\Lambda^{(*)}$, one can construct the dual two-complex (V,E,F) in the standard way: The dual vertices are just the k-simplices, $V:=\Lambda^{(k)}$. The dual edges are the $(k-1)$-simplices, $E:=\Lambda^{(k-1)}$, and the dual polygons are given by the $(k-2)$-simplices, $F:=\Lambda^{(k-2)}$. Observe that the $(k-2)$-simplices $\Lambda^{(k-2)}$ are in general contained in the boundaries of more than three $(k-1)$-simplices which implies that the polygons F have in general more than three edges. The maps ∂_j, ε_j, etc. of (2.34) can be constructed inductively from the boundary relation of the simplicial complex.

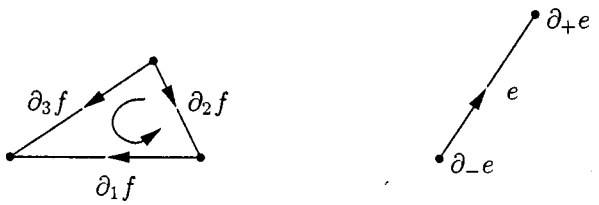


FIG. 5. The maps ∂_j and ε_j and the conditions (2.35). Here $N(f)=3$, $\varepsilon_1 f=+1$, $\varepsilon_2 f=+1$ and $\varepsilon_3 f=(-1)$.

In the calculations of the next section, the following abbreviations are convenient: For a given edge $e \in E$, the sets

$$e_+ := \{f \in F:\ e=\partial_j f,\quad \varepsilon_j f=(+1)\quad \text{for some } j,\quad 1 \leqslant j \leqslant N(f)\}, \tag{2.36a}$$

$$e_- := \{f \in F:\ e=\partial_j f,\quad \varepsilon_j f=(-1)\quad \text{for some } j,\quad 1 \leqslant j \leqslant N(f)\}, \tag{2.36b}$$

contain all polygons that have the edge e in their boundary with positive $(+)$ or negative $(-)$ orientation. For a given polygon $f \in F$, the set

$$f_0 := \{v \in V:\ v=\delta_- \delta_j f \quad \text{for some } j,\quad 1 \leqslant j \leqslant N(f)\} \tag{2.37}$$

denotes all vertices that are contained in the boundary of the polygon f. Finally, the sets

$$f_+ := \{e \in E:\ e=\partial_j f,\quad \varepsilon_j f=(+1)\quad \text{for some } j,\quad 1 \leqslant j \leqslant N(f)\}, \tag{2.38a}$$

$$f_- := \{e \in E:\ e=\partial_j f,\quad \varepsilon_j f=(-1)\quad \text{for some} j,\quad 1 \leqslant j \leqslant N(f)\}, \tag{2.38b}$$

denote all edges in the boundary of the polygon f with positive $(+)$ or negative $(-)$ orientation.

III. THE DUALITY TRANSFORMATION

In this section, we recall the duality transformation relating LGT for Lie groups on the dual generalized two-complex (V,E,F) with a spin foam model. This transformation was carried out in Ref. 17 on a hypercubic lattice and is formulated here for generic two-complexes.

The calculation is presented entirely in terms of the two-complex (V,E,F) and does not refer to the simplicial complex $\Lambda^{(*)}$. Its relation with $\Lambda^{(*)}$ will be discussed in the following section. The calculation is furthermore valid in arbitrary dimension $d \geqslant 2$.

Definition 3.1: Let G be a compact Lie group (or a finite group). The partition function of LGT on the finite generalized two-complex (V,E,F) with cyclic structure is defined by

$$Z = \left(\prod_{e \in E} \int_G dg_e \right) \prod_{f \in F} w(g_f), \quad g_f := g_{\partial_1 f}^{\varepsilon_1 f} \cdots g_{\partial_{N(f)} f}^{\varepsilon_{N(f)} f}. \tag{3.1}$$

Here $\int_G$ denotes the normalized Haar measure on G, $w: G \to \mathbb{R}$ is the Boltzmann weight (1.1), and g_f is the cyclicly ordered product of the group elements attached to the edges in the boundary of the polygon $f \in F$.

Remark 3.2: (1) Observe that even though this definition explicitly refers to the cyclic structure, the value of Z is actually independent of it. The starting point for the cyclic numbering of edges in the boundary of a polygon does not matter because the Boltzmann weight is given by a class function and thus invariant under cyclic permutation of the factors of g_f. Reversal of the orientation is also a symmetry because it replaces g_f by g_f^{-1} which yields the complex conjugate of the class function, but this function is real.

(2) Let $h: V \to G, v \mapsto h_v$ associate a group element to each vertex. The weight $w(g_f)$ in (3.1) is invariant under the *local gauge transformations*,

$$g_e \mapsto h_{\partial_+ e} \cdot g_e \cdot h_{\partial_- e}^{-1}. \tag{3.2}$$

In order to prove this invariance, one has to make use of the conditions (2.35).

The first step of the duality transformation is to insert the character expansion (1.2) of the Boltzmann weight into (3.1),

$$Z = \left(\prod_{e \in E} \int_G dg_e \right) \prod_{f \in F} \sum_{\rho_f \in \mathcal{R}} \hat{w}_{\rho_f} \sum_{n_f=1}^{\dim V_{\rho_f}} t^{(\rho_f)}_{n_f n_f}(g_f). \tag{3.3}$$

The trace of the character is responsible for summations over one index n_f per polygon $f \in F$. The application of coproduct and antipode [Eqs. (2.4a) and (2.4c)] to the product g_f [Eq. (3.1)] yields further vector index summations. In total there is one summation per polygon and per vertex of that polygon. These summation variables are denoted by $n(f,v)$ where $f \in F$ and $v \in f_0$,

$$\begin{aligned} Z = \left(\prod_{e \in E} \int_G dg_e \right) \prod_{f \in F} \sum_{\rho_f \in \mathcal{R}} \hat{w}_{\rho_f} \sum_{n(f,\partial_- \partial_1 f)=1}^{\dim V_{\rho_f}} \cdots \sum_{n(f,\partial_- \partial_{N(f)} f)=1}^{\dim V_{\rho_f}} \\ t^{(\rho_f)}_{n(f,\partial_+ \partial_1 f), n(f,\partial_- \partial_1 f)}(g_{\partial_1 f}^{\varepsilon_1 f}) \cdots t^{(\rho_f)}_{n(f,\partial_+ \partial_{N(f)} f), n(f,\partial_- \partial_{N(f)} f)}(g_{\partial_{N(f)} f}^{\varepsilon_{N(f)} f}). \end{aligned} \tag{3.4}$$

Recall that the conditions (2.35) of the two-complex apply here. The above expression can now be reorganized, moving all summations to the left,

$$\begin{aligned} Z = \left(\prod_{e \in E} \int_G dg_e \right) \left(\prod_{f \in F} \sum_{\rho_f \in \mathcal{R}} \right) \left(\prod_{f \in F} \hat{w}_{\rho_f} \right) \left(\prod_{f \in F} \prod_{v \in f_0} \sum_{n(f,v)=1}^{\dim V_{\rho_f}} \right) \\ \prod_{f \in F} \left(\prod_{e \in f_+} t^{(\rho_f)}_{n(f,\partial_+ e), n(f,\partial_- e)}(g_e) \right) \left(\prod_{e \in f_-} t^{(\rho_f^*)}_{n(f,\partial_- e), n(f,\partial_+ e)}(g_e) \right). \end{aligned} \tag{3.5}$$

Here the notation

$$\left(\prod_{f \in F} \sum_{\rho_f \in \mathcal{R}} \right) := \sum_{\rho_f \in \mathcal{R}} \cdots \sum_{\rho_f \in \mathcal{R}} \tag{3.6}$$

denotes one summation per polygon $f \in F$. Sorting the product of representation functions by edge rather than by polygon amounts to just a slight change in the enumeration of polygons and edges,

$$\begin{aligned} Z = \left(\prod_{f \in F} \sum_{\rho_f \in \mathcal{R}} \right) \left(\prod_{f \in F} \hat{w}_{\rho_f} \right) \left(\prod_{f \in F} \prod_{v \in f_0} \sum_{n(f,v)=1}^{\dim V_{\rho_f}} \right) \\ \prod_{e \in E} \int_G dg_e \left[\prod_{e \in E} \left(\prod_{f \in e_+} t^{(\rho_f)}_{n(f,\partial_+ e), n(f,\partial_- e)}(g_e) \right) \left(\prod_{f \in e_-} t^{(\rho_f^*)}_{n(f,\partial_- e), n(f,\partial_+ e)}(g_e) \right) \right]. \end{aligned} \tag{3.7}$$

The integrals can now be evaluated using the formula (2.12),

$$\int_G dg_e [\cdots] = \sum_{P^{(e)} \in \mathcal{P}_e} P^{(e) \overbrace{n(f,\partial_+ e),\ldots}^{f \in e_+} \overbrace{n(f,\partial_- e),\ldots}^{f \in e_-}} P^{(e)}_{\underbrace{n(f,\partial_- e),\ldots}_{f \in e_+} \underbrace{n(f,\partial_+ e),\ldots}_{f \in e_-}}, \tag{3.8}$$

where $\mathcal{P}_e$ denotes a basis of orthogonal G-invariant projectors onto the trivial components in the complete decomposition of

$$\left(\bigotimes_{f\in e_+}\rho_f\right)\otimes\left(\bigotimes_{f\in e_-}\rho_f^*\right). \tag{3.9}$$

The curly brackets in (3.8) indicate that there is one index $n(f,\partial_+ e)$ for each $f\in e_+$ etc. Finally, the sums over projectors are moved to the left of the expression,

$$Z=\left(\prod_{f\in F}\sum_{\rho_f\in\mathcal{R}}\right)\left(\prod_{e\in E}\sum_{P^{(e)}\in\mathcal{P}_e}\right)\left(\prod_{f\in F}\hat{w}_{\rho_f}\right)\left(\prod_{f\in F}\prod_{v\in f_0}\sum_{n(f,v)=1}^{\dim V_{\rho_f}}\right)$$
$$\prod_{e\in E}P^{(e)\overbrace{n(f,\partial_+e),\ldots}^{f\in e_+}\overbrace{n(f,\partial_-e),\ldots}^{f\in e_-}}P^{(e)}_{\underbrace{n(f,\partial_-e),\ldots}_{f\in e_+}\underbrace{n(f,\partial_+e),\ldots}_{f\in e_-}}. \tag{3.10}$$

This formula can now be reorganized and yields the final result:

Theorem 3.3: The partition function (3.1) of LGT on the finite generalized two-complex (V,E,F) with cyclic structure is equal to the expression

$$Z=\left(\prod_{f\in F}\sum_{\rho_f\in\mathcal{R}}\right)\left(\prod_{e\in E}\sum_{P^{(e)}\in\mathcal{P}_e}\right)\left(\prod_{f\in F}\hat{w}_{\rho_f}\right)\left(\prod_{v\in V}C(v)\right). \tag{3.11}$$

Here $\mathcal{P}_e$ denotes a basis of orthogonal G-invariant projectors onto the trivial components in the complete decomposition of (3.9). The weights per polygon $\hat{w}_{\rho_f}$ are the coefficients of the character expansion (1.2) of the original Boltzmann weight. The weights per vertex $C(v)$ are given by a trace involving representations and projectors in the neighborhood of the vertex $v\in V$,

$$C(v)=\left(\prod_{\substack{f\in F:\\ v\in f_0}}\sum_{n_f=1}^{\dim V_{\rho_f}}\right)\left(\prod_{\substack{e\in E:\\ v=\partial_+e}}P^{(e)\overbrace{n_fn_f\ldots}^{f\in e_+}\overbrace{n_fn_f\ldots}^{f\in e_-}}\right)\left(\prod_{\substack{e\in E:\\ v=\partial_-e}}P^{(e)}_{\underbrace{n_fn_f\ldots}_{f\in e_+}\underbrace{n_fn_f\ldots}_{f\in e_-}}\right). \tag{3.12}$$

Remark 3.4: (1) The projectors onto the trivial representations,

$$P^{(e)}:\left(\bigotimes_{f\in e_+}\rho_f\right)\otimes\left(\bigotimes_{f\in e_-}\rho_f^*\right)\to\mathbb{C}, \tag{3.13}$$

can be replaced via the isomorphisms $\mathrm{Hom}(V\otimes W^*,\mathbb{C})\cong\mathrm{Hom}(V,W)$ by representation morphisms

$$\varphi^{(e)}:\bigotimes_{f\in e_+}\rho_f\to\bigotimes_{f\in e_-}\rho_f. \tag{3.14}$$

The partition function then contains a sum over a basis of the space of representation morphisms for each edge $e\in E$,

$$\mathrm{Hom}\left(\bigotimes_{f\in e_+}\rho_f\,,\ \bigotimes_{f\in e_-}\rho_f\right). \tag{3.15}$$

(2) The expression $C(v)$ is a trace in the category of finite dimensional representations Rep G, cf. Fig. 6(a). Observe that all vector indices n_f are contracted. The complexity of the $C(v)$ depends on the number of edges which contain $v\in V$ in their boundary. In order to generalize this spin foam model to ribbon categories, $C(v)$ has to be replaced by a quantum trace. The main motivation for formulating LGT on the two-complex dual to a triangulation is that it is now guaranteed that in dimension 4 there are always precisely five edges which contain v. Without this restriction, the generalization of $C(v)$ to the ribbon case would be much harder.

(3) Observe that for $G=\mathrm{SU}(2)$ in three dimensions, the $C(v)$ are essentially the $6j$-symbols of SU(2).

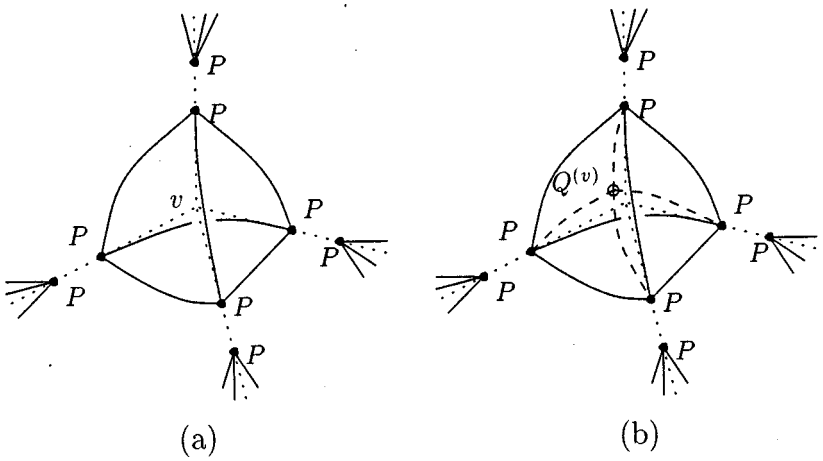


FIG. 6. The neighborhood of a vertex $v \in V$ on the dual two-complex in the three-dimensional case. The dotted lines denote the four edges attached to the vertex. Diagram (a) shows the weight $C(v)$ per vertex $v \in V$ occurring in the spin foam model where the full dots denote projectors $P^{(e)}$, and the solid lines the representations V_ρ. Diagram (b) visualizes the weight $\tilde{C}(v)$ in the spin network expectation value. Here $Q^{(v)}$ is the morphism attached to v, and the dashed lines denote the representations τ_e.

The generic observables of LGT that have nonvanishing expectation values under the path integral are *spin networks*, the generalization of Wilson loops to the non-Abelian case.

Definition 3.5: Let G be a compact Lie group (or a finite group), (V,E,F) be a finite generalized two-complex with cyclic structure and Z denote the partition function of LGT of Definition 3.1. Let $\tau: E \to \mathcal{R}$ assign a unitary finite-dimensional irreducible representation τ_e to each edge $e \in E$ and for each vertex $v \in V$, let

$$Q^{(v)}: \bigotimes_{\substack{e \in E: \\ v = \partial_+ e}} \tau_e \to \bigotimes_{\substack{e \in E: \\ v = \partial_- e}} \tau_e \tag{3.16}$$

denote a representation morphism. The *spin network* labeled by τ_e and $Q^{(v)}$ associates to each configuration $E \to G, e \mapsto g_e$ the value

$$W(\tau,Q) := \frac{1}{Z}\left(\prod_{e \in E} \sum_{k_e,l_e=1}^{\dim V_{\tau_e}}\right)\left(\prod_{e \in E} t^{(\tau_e)}_{k_e l_e}(g_e)\right)\left(\prod_{v \in V} Q^{(v)}_{\underbrace{k_e \cdots}_{\substack{e \in E: \\ v = \partial_+ e}} \ \underbrace{l_e \cdots}_{\substack{e \in E: \\ v = \partial_- e}}}\right). \tag{3.17}$$

For more details on this definition and for the proof of the following result, we refer the reader to Ref. 17.

Theorem 3.6: Let G be a compact Lie group (or a finite group) and (V,E,F) be a finite generalized two-complex with cyclic structure. Let τ_e and $Q^{(v)}$ define a spin network as in Definition 3.5. The expectation value of the spin network,

$$\langle W(\tau,Q)\rangle = \left(\prod_{e \in E} \int_G dg_e\right)\left[W(\tau,Q)\prod_{f \in F} w(g_f)\right], \tag{3.18}$$

TABLE I. The partition function of the spin foam model dual to LGT (3.11) is a sum over all colorings where the summands contain certain weights. Here colorings and weights are given for LGT living on the two-complex dual to the triangulation.

Triangulation	Dual two-complex	Coloring	Weights
four-simplex	vertex	-	$C(v)$
tetrahedron	edge	morphism	-
triangle	polygon	simple object	$\hat{w}_\rho$
edge	-	-	-
vertex	-	-	-

is equal to

$$\langle W(\tau,Q)\rangle = \frac{1}{Z}\left(\prod_{f\in F}\sum_{\rho_f\in\mathcal{R}}\right)\left(\prod_{e\in E}\sum_{P^{(e)}\in\tilde{\mathcal{P}}_e}\right)\left(\prod_{f\in F}\hat{w}_{\rho_f}\right)$$
$$\prod_{v\in V}\left[\left(\prod_{\substack{e\in E\\ v=\partial_+ e}}\sum_{k_e=1}^{\dim V_{\tau_e}}\right)\left(\prod_{\substack{e\in E\\ v=\partial_- e}}\sum_{l_e=1}^{\dim V_{\tau_e}}\right)\tilde{C}(v)\cdot Q^{(v)}_{\underbrace{k_e\ldots}_{\substack{e\in E:\\ v=\partial_+ e}}\ \underbrace{l_e\ldots}_{\substack{e\in E:\\ v=\partial_- e}}}\right]. \tag{3.19}$$

Here $\tilde{\mathcal{P}}_e$ is a basis of orthogonal G-invariant projectors onto the trivial components in the complete decomposition of

$$\left(\bigotimes_{f\in e_+}\rho_f\right)\otimes\left(\bigotimes_{f\in e_-}\rho_f^*\right)\otimes\tau_e\,. \tag{3.20}$$

The weights per polygon $\hat{w}_{\rho_f}$ are the coefficients of the character expansion (1.2) of the original Boltzmann weight. The weights per vertex $\tilde{C}(v)$ are given by the trace

$$\tilde{C}(v)=\left(\prod_{\substack{f\in F:\\ v\in f_0}}\sum_{n_f=1}^{\dim V_{\rho_f}}\right)\left(\prod_{\substack{e\in E:\\ v=\partial_+ e}}P^{(e)\overbrace{n_f n_f\ldots}^{f\in e_+}\overbrace{n_f n_f\ldots}^{f\in e_-}k_e}\right)\left(\prod_{\substack{e\in E:\\ v=\partial_- e}}P^{(e)}_{\underbrace{n_f n_f\ldots}_{f\in e_+}\underbrace{n_f n_f\ldots}_{f\in e_-}l_e}\right). \tag{3.21}$$

Remark 3.7: (1) The Theorem 3.6 is an example for an explicit calculation how the spin foams that are the configurations in the partition function couple to the spin network $W(\tau,Q)$. Figure 6(b) visualizes the trace which gives the weights per vertex $\tilde{C}(v)$.

(2) If the set of edges for which the representations τ_e are nontrivial forms a closed loop, then $W(\tau,Q)$ is nonzero only if the non-trivial τ_e are all isomorphic. The morphisms $Q^{(v)}$ are then unique up to normalization. In this case $W(\tau,Q)$ describes a Wilson loop.

IV. THE SPIN FOAM MODEL FOR RIBBON CATEGORIES

In Sec. III, the spin foam model dual to LGT was derived for the case in which the gauge group G is a Lie group. If LGT is defined on the two-complex dual to the triangulation, the partition function of the spin foam model consists of a sum over all labelings of triangles with irreducible representations (simple objects) and of all tetrahedra with invariant projectors (representation morphisms) (see Table I).

This spin foam model shall be generalized to a ribbon category $\mathcal{C}$ which replaces the category of representations Rep G of the gauge group G. The partition function will contain the sum over all colorings of triangles with simple objects explicitly while the sum over all colorings of tetrahedra with morphisms will be implemented as a trace over suitable state spaces.

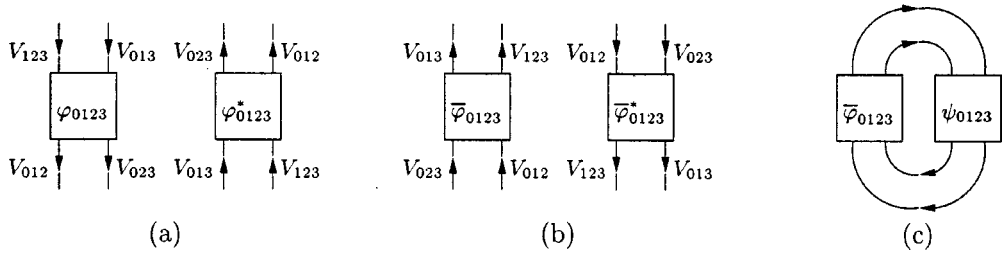


FIG. 7. (a) The coupons denoting morphisms $\varphi_{0123}\in H_{0123}$ and their duals φ^*_{0123} (4.4a) as well as (b) morphisms of the dual state spaces, $\overline{\varphi}_{0123}\in H^*_{0123}$ and their duals $\overline{\varphi}^*_{0123}$ (4.3b). Diagram (c) shows the pairing (4.5). All ribbons are drawn in blackboard framing.

The definition of the spin foam model is formulated in a first step for a given simplicial four-complex. The definition thus refers explicitly to the linear order of vertices. In a second step we will prove that it does not depend on that order and that it is thus well-defined for any combinatorial complex that corresponds to the triangulation of a closed and oriented piecewise-linear four-manifold.

A. Definition of the partition function

First we define the colorings which will be explicitly summed over in the partition function.

Definition 4.1: Let $\Lambda^{(*)}$ denote a simplicial complex, $\mathcal{C}$ be an admissible ribbon category (Definition 2.9) and $\mathcal{C}_0$ be a set of colors.

(1) A *coloring* $V:\Lambda^{(2)}\to\mathcal{C}_0$ associates an object $V(v_0,v_1,v_2)\in\mathcal{C}_0$ to each triangle $(v_0,v_1,v_2)\in\Lambda^{(2)}$ with standard vertex order $v_0<v_1<v_2$.

(2) For any permutation $\sigma\in\mathcal{S}_3$ (acting on $\{0,1,2\}$) define

$$V(v_{\sigma(0)},v_{\sigma(1)},v_{\sigma(2)}):=\begin{cases} V(v_0,v_1,v_2), & \text{if} \quad \operatorname{sgn}\sigma=1,\\ V(v_0,v_1,v_2)^*, & \text{if} \quad \operatorname{sgn}\sigma=-1. \end{cases} \tag{4.1}$$

For given vertices $v_0,v_1,v_2\in\Lambda$, we use the abbreviated notation

$$V_{012}:=V(v_0,v_1,v_2), \quad V_{021}:=V(v_0,v_2,v_1), \tag{4.2}$$

and so on, for example, $V_{021}=V^*_{012}$.

Recall that $(V^*)^*\cong V$ is isomorphic in $\mathcal{C}$, but in general not equal. The Definition 4.1 therefore describes an action of the symmetric group $\mathcal{S}_3$ only up to isomorphism.

The state spaces are defined in the next step. A trace over these spaces will yield the summation over colorings of the tetrahedra with morphisms.

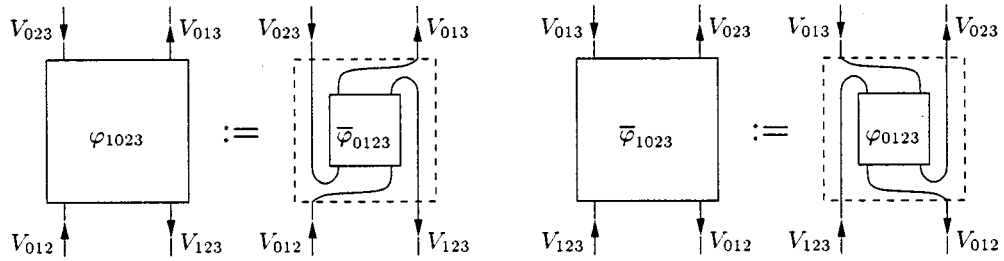


FIG. 8. The definition of the morphisms $\varphi_{1023}:=\tau_0^{*-1}(\overline{\varphi}_{0123})\in H_{1023}$ and $\overline{\varphi}_{1023}:=\tau_0(\varphi_{0123})\in H^*_{1023}$ for given $\overline{\varphi}_{0123}\in H^*_{0123}$ and $\varphi_{0123}\in H_{0123}$ [see (4.6a)].

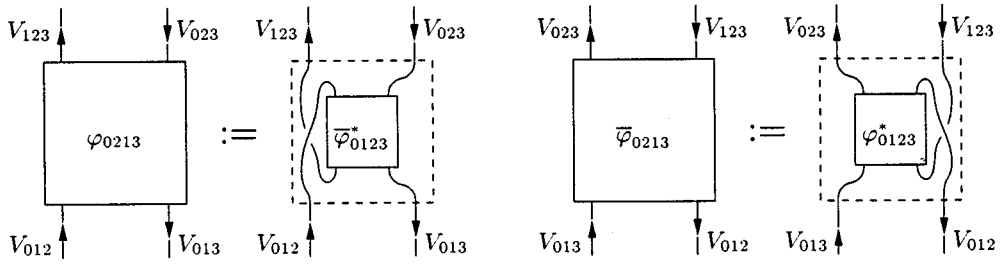


FIG. 9. The definition of the morphisms $\varphi_{0213} := \tau_1^{*-1}(\overline{\varphi}_{0123}) \in H_{0213}$ and $\overline{\varphi}_{0213} := \tau_1(\varphi_{0123}) \in H^*_{0213}$ for given $\overline{\varphi}_{0123} \in H^*_{0123}$ and $\varphi_{0123} \in H_{0123}$ [see (4.6b)].

Definition 4.2: Let $V: \Lambda^{(2)} \to \mathcal{C}_0$ denote a coloring. The *state space* associated with a tetrahedron (v_0, v_1, v_2, v_3) with arbitrary vertex order is defined by

$$H^{(V)}(v_0, v_1, v_2, v_3) := \mathrm{Hom}(V(v_1, v_2, v_3) \otimes V(v_0, v_1, v_3), V(v_0, v_1, v_2) \otimes V(v_0, v_2, v_3)). \tag{4.3a}$$

The dual state space is then given up to isomorphism by the pairing (2.25),

$$H^{(V)}(v_0, v_1, v_2, v_3)^* := \mathrm{Hom}(V(v_0, v_1, v_3)^* \otimes V(v_1, v_2, v_3)^*, V(v_0, v_2, v_3)^* \otimes V(v_0, v_1, v_2)^*). \tag{4.3b}$$

The following abbreviated notation is used,

$$H_{0123} = \mathrm{Hom}(V_{123} \otimes V_{013}, V_{012} \otimes V_{023}), \tag{4.4a}$$

$$H^*_{0123} = \mathrm{Hom}(V^*_{013} \otimes V^*_{123}, V^*_{023} \otimes V^*_{012}), \tag{4.4b}$$

so that the pairing (2.25) reads in this case

$$\langle \cdot, \cdot \rangle_{0123} : H^*_{0123} \otimes H_{0123} \to \mathbb{C}, (\overline{\varphi}_{0123}, \psi_{0123}) \mapsto \langle \overline{\varphi}_{0123}, \psi_{0123} \rangle_{0123}. \tag{4.5}$$

The ribbon diagrams corresponding to a morphism $\varphi_{0123} \in H_{0123}$ and its dual φ^*_{0123} are depicted in Fig. 7(a). The morphism of the dual state space $\overline{\varphi}_{0123} \in H^*_{0123}$ and its dual $\overline{\varphi}^*_{0123}$ are represented diagrammatically as in Fig. 7(b). Dual morphisms are denoted by a star (*) whereas we indicate by a bar ($\overline{\ }$) that a morphism belongs to a dual state space. Figure 7(c) shows the pairing (4.5) for morphisms $\overline{\varphi}_{0123} \in H^*_{0123}$ and $\psi_{0123} \in H_{0123}$. In Fig. 7 and in the following we use blackboard framing (see Sec. II B 2).

Remark 4.3: (1) Definition 4.2 applies to any order of vertices. In particular, the definition of H_{0123} involves $V(v_0, v_1, v_2)$ etc., as given by (4.1).

(2) The definition (4.3b) implements a special choice of isomorphism between H_{0123} and H^*_{0123} via the pairing (4.5). This choice is used consistently in the following.

The state spaces of Definition 4.2 for different vertex order are related by linear isomorphisms which are defined in the next step.

Definition 4.4: Let H_{0123} and H^*_{0123} denote the state space and its dual for a tetrahedron (v_0, v_1, v_2, v_3). The linear maps

$$\tau_0 : H_{0123} \to H^*_{1023}, \quad \tau_0^{*-1} : H^*_{0123} \to H_{1023}, \tag{4.6a}$$

$$\tau_1 : H_{0123} \to H^*_{0213}, \quad \tau_1^{*-1} : H^*_{0123} \to H_{0213}, \tag{4.6b}$$

$$\tau_2 : H_{0123} \to H^*_{0132}, \quad \tau_2^{*-1} : H^*_{0123} \to H_{0132}, \tag{4.6c}$$

are defined by the diagrams in Figs. 8–10.

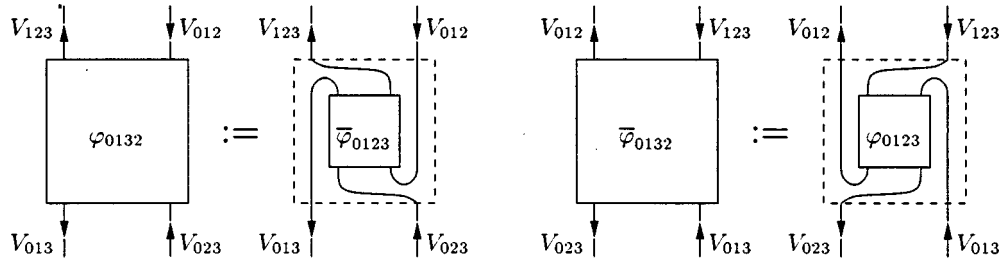


FIG. 10. The definition of the morphisms $\varphi_{0132} := \tau_2^{*-1}(\overline{\varphi}_{0123}) \in H_{0132}$ and $\overline{\varphi}_{0132} := \tau_2(\varphi_{0123}) \in H_{0132}^*$ for given $\overline{\varphi}_{0123} \in H_{0123}^*$ and $\varphi_{0123} \in H_{0123}$ [see (4.6c)].

Note that τ_j exchanges the jth and the $(j+1)$-th vertices of the four arguments of $H(v_0, v_1, v_2, v_3)$, counting from zero. These need not be the vertices with number j and $j+1$, for example,

$$\tau_0 : H_{1234} \to H_{2134}^*, \quad \tau_1 : H_{0214} \to H_{0124}^*. \tag{4.7}$$

Lemma 4.5: Let τ_j, $0 \leqslant j \leqslant 2$, denote the linear maps of Definition 4.4.

(1) The τ_j satisfy $\tau_j^{*-1} \circ \tau_j = \mathrm{id}$ and $\tau_j \circ \tau_j^{*-1} = \mathrm{id}$. In particular, the τ_j and τ_j^{*-1} form linear isomorphisms.

(2) The τ_j satisfy $\langle \tau_j^{*-1}(\psi_{0123}), \tau_j(\overline{\varphi}_{0123}) \rangle_{1023} = \langle \overline{\varphi}_{0123}, \psi_{0123} \rangle_{0123}$ for all $\overline{\varphi}_{0123} \in H_{0123}^*$ and $\psi_{0123} \in H_{0123}$ which motivates the notation τ_j^{*-1}.

Proof: (1) The relations $\tau_j^{*-1} \circ \tau_j = \mathrm{id}$ can be verified diagrammatically using the identities that hold in ribbon categories. Figure 11 shows the calculation for $\tau_1^{*-1} \circ \tau_1 = \mathrm{id}_{H_{0123}}$. The other cases are analogous.

(2) This claim can also be verified diagrammatically. It is essentially a consequence of the fact that the maps τ_j on the dual state spaces in Figs. 8–10 are given by the mirror images of the maps on the original state spaces. □

Remark 4.6: In analogy with the three-dimensional case, one could conjecture that the τ_j generate an action of the symmetric group $\mathcal{S}_4$ on some collection of state spaces. This is not the case. Only in the final step we will have an action of the symmetric group when it is proved that the partition function is well-defined.

At this point, the colorings V_{jkl} and the spaces H_{jklm} are defined for a generic vertex order. The summation over all coulorings of tetrahedra with morphisms, which is part of the partition function, will be implemented as a trace. This trace is over the tensor product of maps $Z_{01234}^{(V)}$ for all four-simplices $(v_0, \ldots, v_4) \in \Lambda^{(4)}$. These building blocks $Z_{01234}^{(V)}$ are defined first.

Definition 4.7: Let $V : \Lambda^{(2)} \to \mathcal{C}_0$ be a coloring and the state spaces for the tetrahedra be given by Definition 4.2.

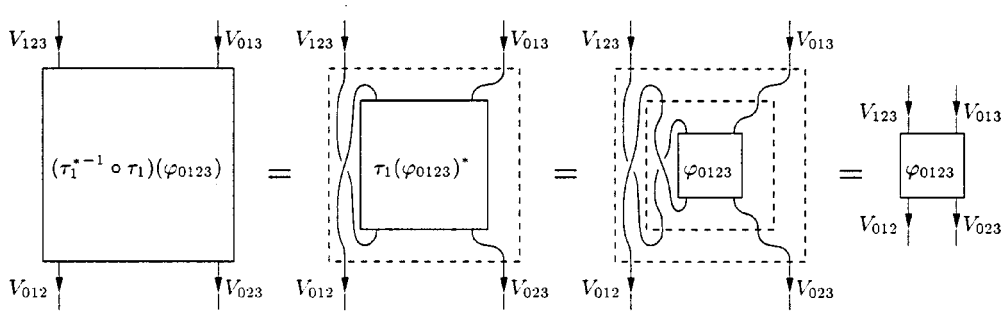


FIG. 11. Diagrammatic proof of the identity $\tau_1^{*-1} \circ \tau_1 = \mathrm{id}_{H_{0123}}$ in Lemma 4.5. Here $\varphi_{0123} \in H_{0123}$.

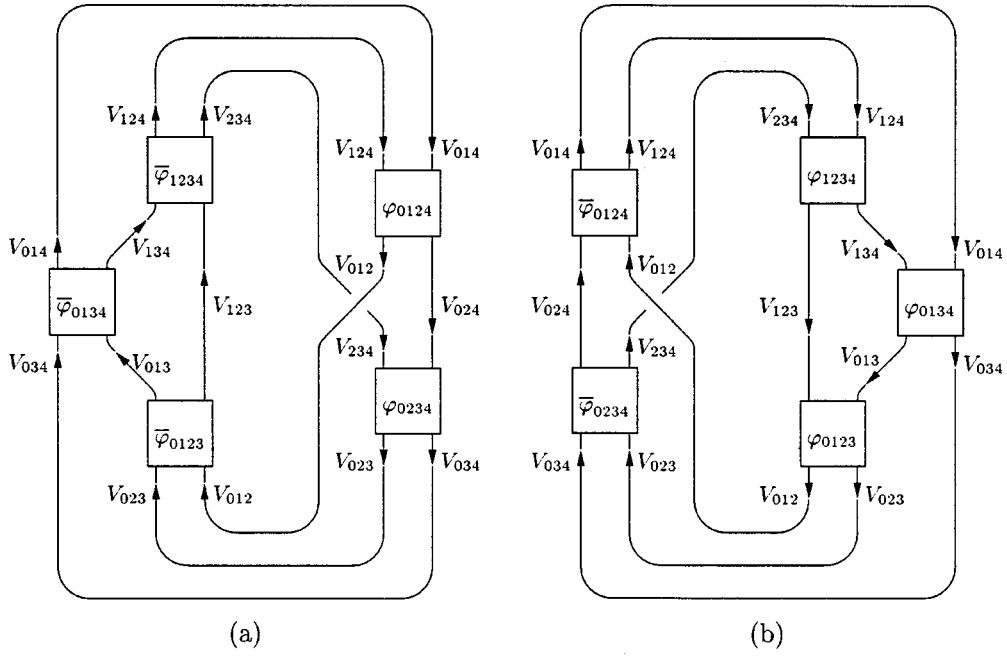


FIG. 12. (a) The quantum trace (4.8b) defining the four-simplex map for a four-simplex with positive relative orientation in M. (b) The quantum trace (4.9b) for negative relative orientation. The morphisms are denoted by $\varphi_{jklm} \in H_{jklm}$ and $\overline{\varphi}_{jklm} \in H^*_{jklm}$ and represented by the coupons of Fig. 7.

(1) For any four-simplex $(v_0,\ldots,v_4)$ whose relative orientation in the manifold M is positive, define the four-*simplex map*

$$Z^{(V),(+)}_{01234} : H_{0234} \otimes H_{0124} \to H_{1234} \otimes H_{0134} \otimes H_{0123} \tag{4.8a}$$

to be the linear map that is related by the pairing (2.25) to the quantum trace

$$Z'^{(V),(+)}_{01234} : H^*_{1234} \otimes H_{0234} \otimes H^*_{0134} \otimes H_{0124} \otimes H^*_{0123} \to \mathbb{C}, \tag{4.8b}$$

which is depicted in Fig. 12(a).

(2) For any four-simplex with negative relative orientation in M, the four-*simplex map*

$$Z^{(V),(-)}_{01234} : H_{1234} \otimes H_{0134} \otimes H_{0123} \to H_{0234} \otimes H_{0124} \tag{4.9a}$$

is defined by the quantum trace

$$Z'^{(V),(-)}_{01234} : H_{1234} \otimes H^*_{0234} \otimes H_{0134} \otimes H^*_{0124} \otimes H_{0123} \to \mathbb{C}, \tag{4.9b}$$

which is depicted in Fig. 12(b).

Remark 4.8: (1) The assignment of the H_{jklm} to domain or codomain and the assignment of duality stars (*) in the above definitions is according to the orientation of the tetrahedra in the boundary of the four-simplex,

$$\partial(01234) = (1234) - (0234) + (0134) - (0124) + (0123). \tag{4.10}$$

(2) Observe that Fig. 12(b) is the mirror image of (a) with all arrows reversed. This is different from the quantum trace of the dual morphism which would also replace the over-crossing by an under-crossing.

In order to obtain a summation over a basis of each state space H_{jklm}, the partition function is defined as a trace over the tensor product of all four-simplex maps.

Definition 4.9: Let $\Lambda^{(*)}$ be a finite combinatorial four-complex corresponding to a triangulation of a closed oriented piecewise-linear four-manifold M. Choose a fixed linear order of the vertices of Λ. Let $V:\Lambda^{(2)}\to\mathcal{C}_0$ be a coloring and let the four-simplex maps $Z^{(V),(\pm)}_{jklmn}$ be given by Definition 4.7.

The *partition function per coloring* is defined as

$$Z^{(V)}:=\mathrm{tr}_{\mathcal{H}}\left[P\circ\left(\bigotimes_{(v_0,\ldots,v_4)\in\Lambda^{(4)}} Z^{(V),(\varepsilon_{01234})}_{01234}\right)\right]. \tag{4.11}$$

Here $\varepsilon_{01234}\in\{+1,-1\}$ denotes the relative orientation of the four-simplex $(v_0,\ldots,v_4)\in\Lambda^{(4)}$ in M. Since every tetrahedron occurs precisely twice in the boundary of a four-simplex, once with positive and once with negative relative orientation, both domain and codomain of the tensor product over the $Z^{(V),(\pm)}_{01234}$ are permutations of the tensor factors of

$$\mathcal{H}:=\bigotimes_{(v_0,v_1,v_2,v_3)\in\Lambda^{(3)}} H^{(V)}(v_0,v_1,v_2,v_3). \tag{4.12}$$

The permutation operator P in (4.11) is the unique permutation which sorts the tensor factors of the codomain such that their ordering agrees with the ordering of factors in the domain.

Remark 4.10: The trace over the tensor product $\mathcal{H}$ in the above definition essentially contains the quantum traces (4.8b) or (4.9b) for all four-simplices plus an additional summation over bases of all state spaces. In the partition function the traces generalize the weights $C(v)$, cf. Table I and (3.12). Figure 12 is the four-dimensional analogue of Fig. 6(a) with a particular choice of over- and under-crossings.

Definition 4.11: Let $\Lambda^{(*)}$ be a finite combinatorial four-complex corresponding to a triangulation of a closed oriented piecewise-linear four-manifold M. Choose a fixed linear order of the vertices of Λ. For each coloring $V:\Lambda^{(2)}\to\mathcal{C}_0$, let the partition function per coloring, $Z^{(V)}$, be given by Definition 4.9. The *partition function* is defined as

$$Z:=\sum_{V:\Lambda^{(2)}\to\mathcal{C}_0}\left(\prod_{(v_0,v_1,v_2)\in\Lambda^{(2)}}\hat{w}(v_0,v_1,v_2)(V_{012})\right)Z^{(V)}. \tag{4.13}$$

The weights $\hat{w}(v_0,v_1,v_2):\mathcal{C}_0\to\mathbb{R}$ assign a real number to the object associated with the triangle $(v_0,v_1,v_2)\in\Lambda^{(2)}$ and are required to satisfy the *reality condition*,

$$\hat{w}(v_0,v_1,v_2)(V^*)=\hat{w}(v_0,v_1,v_2)(V), \tag{4.14}$$

and to be functions on equivalence classes of isomorphic objects, i.e.,

$$\hat{w}(v_0,v_1,v_2)(V)=\hat{w}(v_0,v_1,v_2)(\tilde{V}) \quad \text{if} \quad V\cong\tilde{V}. \tag{4.15}$$

Section IV B is devoted to proving that this definition is actually independent of the linear order of vertices and of the choice of colors $\mathcal{C}_0$ up to isomorphism. The partition function is therefore well-defined for a combinatorial complex that corresponds to the triangulation of a closed and oriented manifold. In Sec. V, we discuss some relevant special cases in more detail that are covered by (4.13), in particular the relation with the standard formulation of LGT for Lie groups and the Crane–Yetter state sum. There, we also comment on the convergence of (4.13) if $\mathcal{C}_0$ is not a finite set.

B. Properties of the partition function

First we show that the partition function (4.13) does not depend on the choice of colors $\mathcal{C}_0$ up to isomorphism.

Theorem 4.12: Let $V:\Lambda^{(2)}\to\mathcal{C}_0$ denote a coloring, and for each triangle $(v_0,v_1,v_2)\in\Lambda^{(2)}$, $v_0<v_1<v_2$, let

$$\Phi(v_0,v_1,v_2):V(v_0,v_1,v_2)\to\tilde{V}(v_0,v_1,v_2) \tag{4.16}$$

be an isomorphism in $\mathcal{C}$ for some object $\tilde{V}(v_0,v_1,v_2)$. Then the partition functions per coloring (4.11) for V and $\tilde{V}$ agree,

$$Z^{(V)}=Z^{(\tilde{V})}. \tag{4.17}$$

Proof: Using the standard abbreviations, the given isomorphisms are of the form $\Phi_{012}:V_{012}\to\tilde{V}_{012}$ for all triangles (v_0,v_1,v_2) with standard vertex order $v_0<v_1<v_2$. For any permutation $\sigma\in\mathcal{S}_3$ we define isomorphisms $\Phi_{\sigma(0)\sigma(1)\sigma(2)}:V_{\sigma(0)\sigma(1)\sigma(2)}\to\tilde{V}_{\sigma(0)\sigma(1)\sigma(2)}$ by

$$\Phi_{\sigma(0)\sigma(1)\sigma(2)}:=\begin{cases}\Phi_{012}:V_{012}\to\tilde{V}_{012}, & \text{if } \operatorname{sgn}\sigma=1,\\ \Phi^{*-1}_{012}:V^*_{012}\to\tilde{V}^*_{012}, & \text{if } \operatorname{sgn}\sigma=-1.\end{cases} \tag{4.18}$$

Observe that this assignment is compatible with Definition 4.1. These definitions provide us with isomorphisms $\Phi_{012}:V_{012}\to\tilde{V}_{012}$ and with their dual maps $\Phi^*_{012}:\tilde{V}^*_{012}\to V^*_{012}$ for all triangles (v_0,v_1,v_2) with arbitrary vertex order.

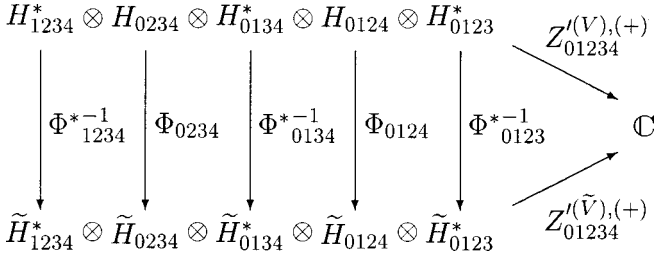
Furthermore, there are induced linear isomorphisms of the state spaces,

$$\begin{gathered}\Phi_{0123}:\operatorname{Hom}(V_{123}\otimes V_{013},V_{012}\otimes V_{023})\to\operatorname{Hom}(\tilde{V}_{123}\otimes\tilde{V}_{013},\tilde{V}_{012}\otimes\tilde{V}_{023}),\\ \varphi_{0123}\mapsto(\Phi_{012}\otimes\Phi_{023})\circ\varphi_{0123}\circ(\Phi^{-1}_{123}\otimes\Phi^{-1}_{013}),\end{gathered} \tag{4.19a}$$

and

$$\begin{gathered}\Phi^*_{0123}:\operatorname{Hom}(\tilde{V}^*_{013}\otimes\tilde{V}^*_{123},\tilde{V}^*_{023}\otimes\tilde{V}^*_{012})\to\operatorname{Hom}(V^*_{013}\otimes V^*_{123},V^*_{023}\otimes V^*_{012}),\\ \overline{\varphi}_{0123}\mapsto(\Phi^*_{023}\otimes\Phi^*_{012})\circ\overline{\varphi}_{0123}\circ(\Phi^{*-1}_{013}\otimes\Phi^{*-1}_{123}).\end{gathered} \tag{4.19b}$$

A convenient abbreviated notation for these maps is $\Phi_{0123}:H_{0123}\to\tilde{H}_{0123}$, $\Phi^*_{0123}:\tilde{H}^*_{0123}\to H^*_{0123}$ writing $\tilde{H}_{0123}:=\operatorname{Hom}(\tilde{V}_{123}\otimes\tilde{V}_{013},\tilde{V}_{012}\otimes\tilde{V}_{023})$ etc. Now the following diagram for the traces $Z'^{(V),(+)}_{01234}$ commutes:



To see this, imagine Fig. 12(a) drawn for maps $\tilde{\varphi}_{jklm}\in\tilde{H}_{jklm}$ etc. and insert the definitions of the linear isomorphisms Φ_{jklm} of (4.19). Then the isomorphisms in $\mathcal{C}$, $\Phi_{jkl}:V_{jkl}\to\tilde{V}_{jkl}$, appear twice in each ribbon in a way such that they cancel.

Let $\langle\cdot,\cdot\rangle^{\sim}:\tilde{H}^*_{0123}\otimes\tilde{H}_{0123}\to\mathbb{C}$ denote the pairing (4.5) applied to the state spaces which use the coloring $\tilde{V}$. We find

$$\langle \Phi^{*-1}_{0123}(\overline{\varphi}_{0123}), \Phi_{0123}(\psi_{0123})\rangle^{\sim} = \langle \overline{\varphi}_{0123}, \psi_{0123}\rangle, \tag{4.20}$$

for all $\overline{\varphi}_{0123} \in H^*_{0123}$ and $\psi_{0123} \in H_{0123}$. As a consequence the following diagram involving the four-simplex maps themselves also commutes:

$$\begin{array}{ccc}
H_{0234} \otimes H_{0124} & \xrightarrow{Z^{(V),(+)}_{01234}} & H_{1234} \otimes H_{0134} \otimes H_{0123} \\
\downarrow \Phi_{0234} \quad \downarrow \Phi_{0124} & & \downarrow \Phi_{1234} \quad \downarrow \Phi_{0134} \quad \downarrow \Phi_{0123} \\
\widetilde{H}_{0234} \otimes \widetilde{H}_{0124} & \xrightarrow{Z^{(\tilde{V}),(+)}_{01234}} & \widetilde{H}_{1234} \otimes \widetilde{H}_{0134} \otimes \widetilde{H}_{0123}
\end{array}$$

Analogous diagrams are available for $Z^{(V),(-)}_{01234}$ and Fig. 12(b) in the case of opposite orientation.

Finally, each tetrahedron occurs precisely twice in the boundaries of four-simplices, once with positive and once with negative relative orientation. Therefore the tensor product of all four-simplex maps in (4.11) is conjugated by a linear isomorphism Φ which can be obtained from a tensor product of the Φ_{jklm},

$$P \circ \left(\bigotimes_{\sigma \in \Lambda^{(4)}} Z^{(V),(\varepsilon_\sigma)}_{\sigma} \right) = \Phi \left[P \circ \left(\bigotimes_{\sigma \in \Lambda^{(4)}} Z^{(\tilde{V}),(\varepsilon_\sigma)}_{\sigma} \right) \right] \Phi^{-1}. \tag{4.21}$$

Since $Z^{(V)}$ is the trace of (4.21), it agrees with $Z^{(\tilde{V})}$. □

Corollary 4.13: The partition function (4.13) does not depend on the choice of colors $\mathcal{C}_0$ up to isomorphism.

Proof: Consider another set of colors $\widetilde{\mathcal{C}}_0$ such that each coloring $V:\Lambda^{(2)} \to \mathcal{C}_0$ induces a coloring $\tilde{V}:\Lambda^{(2)} \to \widetilde{\mathcal{C}}_0$ for which $V_{012} \cong \tilde{V}_{012}$ are isomorphic in $\mathcal{C}$ for all triangles $(v_0, v_1, v_2) \in \Lambda^{(2)}$. The partition function (4.13) defined using $\mathcal{C}_0$ agrees with that one defined using $\widetilde{\mathcal{C}}_0$ because the weights satisfy $\hat{w}(v_0, v_1, v_2)(V_{012}) = \hat{w}(v_0, v_1, v_2)(\tilde{V}_{012})$ and because $Z^{(V)} = Z^{(\tilde{V})}$ according to Theorem 4.12. □

In order to prove the independence of the partition function (4.13) of the linear order of vertices, a generic four-simplex (01234) is considered. It is proved that any permutation of its vertices that results in different four-simplex maps H_{jklm} according to Definitions 4.2 and 4.7 does not change the partition function (4.13).

This statement is verified for the four elementary transpositions of $\mathcal{S}_5$ (acting on the vertices {0,1,2,3,4}). The following lemmas prepare the proof. They establish diagrammatical isotopies which permute the coupons in Fig. 12(a) in order to reach a configuration similar to Fig. 12(b). Recall that the orientation of the four-simplex changes if an odd permutation is applied to its vertices.

Lemma 4.14: For any coloring $V:\Lambda^{(2)} \to \mathcal{C}_0$ and morphisms $\varphi_{jklm} \in H_{jklm}$ and $\overline{\varphi}_{jklm} \in H^*_{jklm}$, the quantum trace in Fig. 12(a) is equal to the quantum trace in Fig. 13.

Proof: The calculation is described in diagrammatic language and can be translated into equalities for morphisms of the ribbon category $\mathcal{C}$ as described in Sec. II B. First, a number of coupons are moved around in the plane without twisting or braiding any ribbons: Move the coupon φ_{0124} to the left and place it above $\overline{\varphi}_{1234}$, then move $\overline{\varphi}_{0134}$ down and to the right and place it below and right of φ_{0234}. Move $\overline{\varphi}_{0123}$ to the right and place it below $\overline{\varphi}_{0123}$ and below and left of $\overline{\varphi}_{0134}$. Rotate the coupon $\overline{\varphi}_{0123}$ by 360 degrees in order to place its ribbons as depicted in Fig. 13. Finally, lift the ribbon labeled V_{014} out of the plane, move it across the entire diagram, and place it as shown in Fig. 13. □

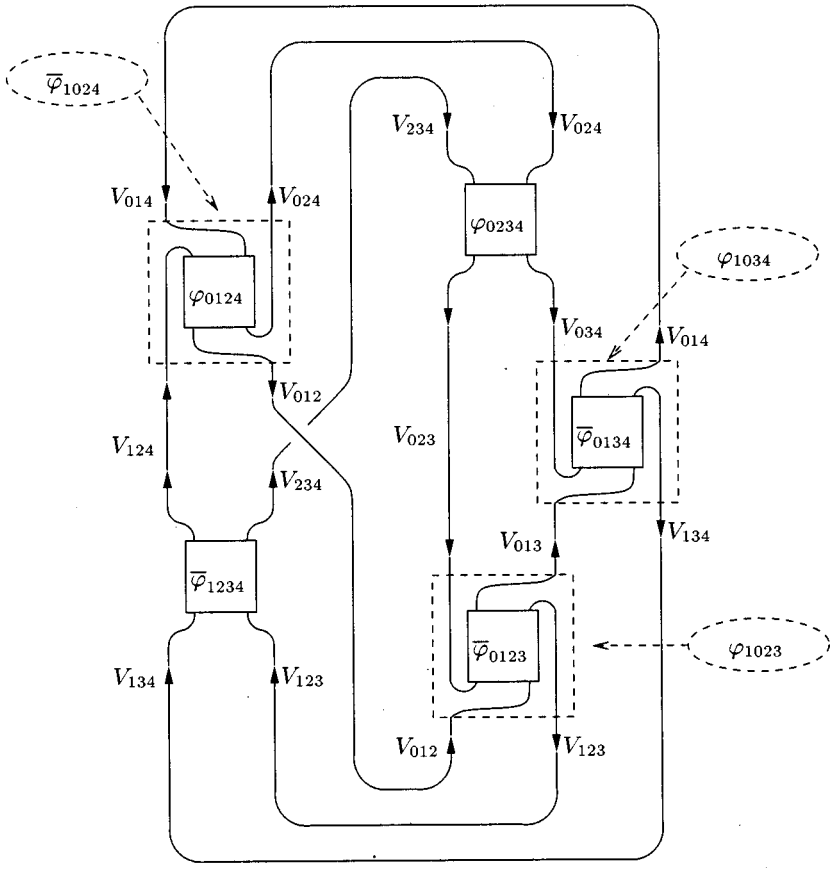


FIG. 13. This diagram is isotopic to the quantum trace $Z'^{(V),(+)}_{01234}$ in Figure 12(a), cf. Lemma 4.14 and Lemma 4.16. The morphisms in the dashed boxes are by definition of τ_0 (Definition 4.4) just morphisms $\overline{\varphi}_{1024} \in H^*_{1024}$, $\varphi_{1034} \in H_{1034}$ and $\varphi_{1023} \in H_{1023}$. With these replacements this quantum trace is similar to Figure 12(b) defining $Z^{(V),(-)}_{10234}$ for opposite relative orientation with a non-standard order (10234) of vertices. Note that the permutation $(01) \in \mathcal{S}_5$ also replaces V_{012}, V_{013} and V_{014} by their duals according to Definition 4.1.

Lemma 4.15: For any coloring $V:\Lambda^{(2)} \to \mathcal{C}_0$ and morphisms $\varphi_{jklm} \in H_{jklm}$ and $\overline{\varphi}_{jklm} \in H^*_{jklm}$, the quantum trace in Fig. 12(a) is equal to the quantum trace in Fig. 14.

Proof: The proof is again explained diagrammatically: Start with Fig. 12(a). Lift the ribbon V_{012} out of the plane and move it across the coupon φ_{1234} so that V_{012} now over-crosses V_{123}, V_{134} and V_{124} rather than V_{234}. Then the coupons can be moved around in the plane without introducing twists or braidings such that the configuration in Fig. 14 is obtained. □

There exist two more lemmas that deal with the elementary transpositions (23) and (34) as well as four lemmas dealing with the case of opposite relative orientation. They are not stated explicitly here since they are very similar and completely analogous to prove.

The results of the preceding lemmas, Figs. 13 and 14, are furthermore related to the quantum trace of Fig. 12(b) for a four-simplex with a different order of vertices. This is stated in the following lemmas.

Lemma 4.16: Let $\tau = (01)$ and consider the four-simplex (01234). Let $V:\Lambda^{(2)} \to \mathcal{C}_0$ denote a coloring. Then there exists another coloring $\tilde{V}$ with isomorphic objects for each triangle, $\tilde{V}_{012} \cong V_{012}$, such that the following diagram commutes:

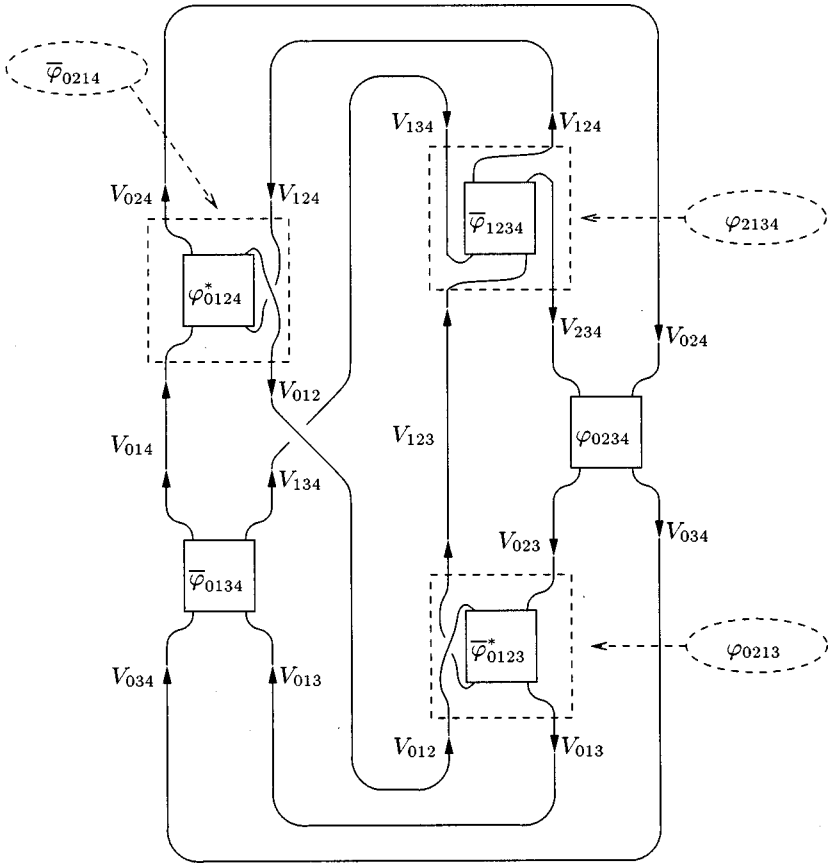


FIG. 14. This diagram is isotopic to the quantum trace defining $Z^{(V),(+)}_{01234}$ in Figure 12(a), cf. Lemma 4.15 and Lemma 4.17.

$$\begin{array}{ccc} H_{0234}\otimes H_{0124} & \xrightarrow{Z^{(V),(+)}_{01234}} & H_{1234}\otimes H_{0134}\otimes H_{0123} \\ \downarrow \mathrm{id} \quad \downarrow \tau_0 & & \downarrow \mathrm{id} \quad \downarrow \tau_0 \quad \downarrow \tau_0 \\ H_{0234}\otimes H^*_{1024} & \longrightarrow & H_{1234}\otimes H^*_{1034}\otimes H^*_{1023} \end{array}$$

Here $Z^{(V),(+)}_{01234}$ is the four-simplex map of Definition 4.7, the maps τ_0 are given in Definition 4.4, and the bottom horizontal map is determined, using the pairing (4.5), by the four-simplex map

$$Z^{(\tilde{V})(-)}_{10234}: H_{0234}\otimes H_{1034}\otimes H_{1023}\to H_{1234}\otimes H_{1024}. \tag{4.22}$$

Proof: Consider Fig. 13 whose quantum trace agrees with $Z'^{(V),(+)}_{01234}$ of Fig. 12(a) according to Lemma 4.14. The linear isomorphisms τ_0 of Definition 4.4 can now be used to replace the dashed boxes of Fig. 13 by morphisms of the state spaces H_{jklm} with a different vertex order. The result is very similar to the trace $Z'^{(V)(-)}_{10234}$ of Fig. 12(b) for the four-simplex (10234).

Observe, however, that in Fig. 12(b) the arrows of the ribbons corresponding to the triangles (012), (013) and (014) are reversed compared with Fig. 13. We can reverse these arrows in Fig. 13 if we label them instead by V^*_{012}, V^*_{013} and V^*_{014}, respectively.

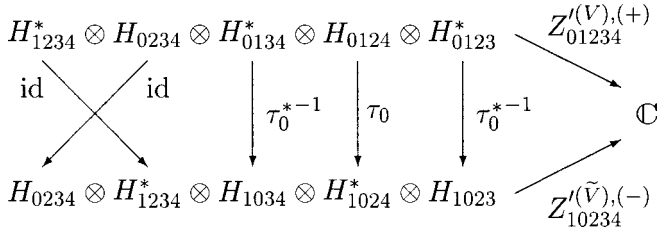
Consider the triangle (012). If (v_0,v_1,v_2) is an even permutation of the standard vertex order, then Fig. 13 contains $V_{012}=V$ for some object $V\in\mathcal{C}_0$, i.e., upon reversal of the arrows this label changes to $V^*_{012}=V_{102}$. This is the same label as the label arising in $Z'^{(V)(-)}_{10234}$.

If, however, (v_0,v_1,v_2) is an odd permutation of the standard vertex order, then Fig. 13 contains $V_{012}=V^*$ for some object $V\in\mathcal{C}_0$, i.e., upon arrow reversal this becomes $V^*_{012}=(V^*)^*$. This is in general not identical, but still isomorphic to V which arises in $Z'^{(V)(-)}_{10234}$ in this case. This is the reason why the present lemma holds only for a coloring $\tilde{V}$ with isomorphic objects at all triangles.

Let (w_0,w_1,w_2) denote any triangle in standard vertex order, $w_0<w_1<w_2$. Define the coloring $\tilde{V}$ by

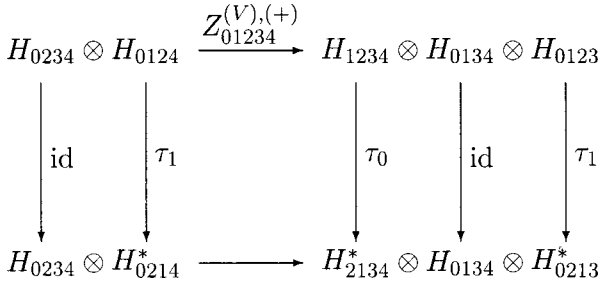
$$\tilde{V}_{\sigma(0)\sigma(1)\sigma(2)}:=\begin{cases}(V^*_{012})^*, & \text{if} \quad \mathrm{sgn}\sigma=1,\\ V^*_{012}, & \text{if} \quad \mathrm{sgn}\sigma=-1,\end{cases} \tag{4.23}$$

if $\{w_0,w_1,w_2\}\in\{\{v_0,v_1,v_2\},\{v_0,v_1,v_3\},\{v_0,v_1,v_4\}\}$ and by $\tilde{V}_{\sigma(0)\sigma(1)\sigma(2)}:=V_{\sigma(0)\sigma(1)\sigma(2)}$ for the other triangles. Then the quantum trace of Fig. 13 with arrows (012), (013) and (014) reversed agrees with the trace of Fig. 12(b) for the coloring $\tilde{V}$. The following diagram therefore commutes:



Using Lemma 4.5, this implies the commutativity of the diagram claimed in the present lemma.□

Lemma 4.17: Let $\tau=(12)$ and $V:\Lambda^{(2)}\to\mathcal{C}_0$ be a coloring. Then there exists another coloring $\tilde{V}$ with isomorphic objects for each triangle such that the following diagram commutes:

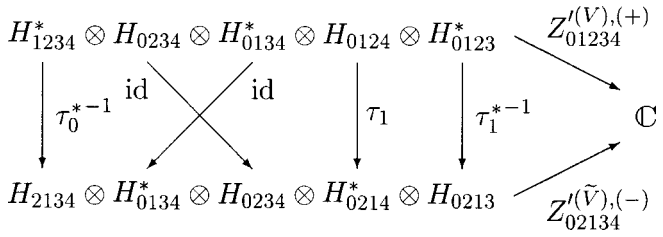


Here the τ_j are the isomorphisms given in Definition 4.4, and the bottom horizontal map is determined, using the pairing (4.5), by the four-simplex map

$$Z^{(\tilde{V}),(-)}_{02134}:H_{2134}\otimes H_{0234}\otimes H_{0213}\to H_{0134}\otimes H_{0214}. \tag{4.24}$$

Proof: Consider Fig. 14 whose quantum trace agrees with $Z'^{(V),(+)}_{01234}$ of Fig. 12(a) according to Lemma 4.15. The linear isomorphisms τ_0 and τ_1 of Definition 4.4 can now be used to replace the dashed boxes of Fig. 14 by morphisms of the state spaces H_{jklm} with a different vertex order. The result is the trace $Z'^{(\tilde{V}),(-)}_{02134}$ of Fig. 12(b) for the four-simplex (02134) up to the choice of isomorphic objects for the triangles (012), (123) and (124). These isomorphisms arise from double dualization as in Lemma 4.16.

The following diagram therefore commutes:



Employing Lemma 4.5, this proves the claim. □

There exist similar lemmas for the other elementary transpositions (23) and (34) as well as for the corresponding statements with opposite relative orientations, i.e., where $Z^{(V),(+)}$ and $Z^{(V),(-)}$ are exchanged. Their proofs are entirely analogous.

Theorem 4.18: The partition function (4.13) does not depend on the choice of the linear order of vertices.

Proof: Equip the set of vertices with a different linear order which is induced from the given one by a permutation τ of the vertices. The partition function using this new order can be expressed in terms of the original order if τ is applied both to the vertices and to the coloring,

$$Z_\tau = \sum_{V:\Lambda^{(2)}\to\mathcal{C}_0} \left(\prod_{(v_0,v_1,v_2)\in\Lambda^{(2)}} \hat{w}(v_{\tau^{-1}(0)}, v_{\tau^{-1}(1)}, v_{\tau^{-1}(2)})((\tau V)_{012}) \right) Z_\tau^{(\tau V)}. \tag{4.25}$$

Here

$$Z_\tau^{(\tau V)} = \mathrm{tr}_{\mathcal{H}}\left[P \circ \left(\bigotimes_{s\in\Lambda^{(4)}} Z_{\tau(s)}^{(\tau V),(\varepsilon_{\tau(s)})} \right) \right] \tag{4.26}$$

replaces the partition function per coloring in the case of the new vertex order, $\tau(s)$ denotes $(\tau^{-1}(0)\cdots\tau^{-1}(4))$ for a given four-simplex $s=(01234)$, and τV is the coloring induced by τ, i.e., $(\tau V)_{012} = V_{\tau^{-1}(0)\tau^{-1}(1)\tau^{-1}(2)}$ for all triangles $(v_0,v_1,v_2)\in\Lambda^{(2)}$.

The permutation τ replaces triangles (012) by $(\tau^{-1}(0)\tau^{-1}(1)\tau^{-1}(2))$ and therefore just permutes the factors of the product in (4.25). This product can be reorganized so that we obtain

$$Z_\tau = \sum_{V:\Lambda^{(2)}\to\mathcal{C}_0} \left(\prod_{(v_0,v_1,v_2)\in\Lambda^{(2)}} \hat{w}(v_0,v_1,v_2)(V_{012}) \right) Z_\tau^{(\tau V)}, \tag{4.27}$$

where the vertex order of the triangles does not matter because of the reality condition (4.14).

Any permutation τ which just permutes the four-simplices but does not change the vertex order of these four-simplices, permutes the tensor factors in (4.26) and therefore leaves the trace invariant. It is thus sufficient to prove invariance under permutations τ that change the vertex order for fixed four-simplices.

Consider a four-simplex $s=(01234)$ and and let τ be an elementary transposition, $\tau \in \{(01),(12),(23),(34)\}$. The colouring τV associates with each triangle $(w_0,w_1,w_2)\in\Lambda^{(2)}$ either the object $V(w_3,w_4,w_5)$ assigned to some triangle $(w_3,w_4,w_5)\in\Lambda^{(2)}$ or the dual of that object.

Since the set of colors $\mathcal{C}_0$ contains for each given object V exactly one object that is isomorphic to V^*, there exists a unique coloring $\overline{V}:\Lambda^{(2)}\to\mathcal{C}_0$ such that $\overline{V}_{012}\cong(\tau V)_{012}$ for all triangles. Moreover, since τ is a transposition, $(\tau\overline{V})_{012}\cong V_{012}$ so that τ induces an involution on the set of colorings $\Lambda^{(2)}\to\mathcal{C}_0$. We can now sum over $\overline{V}$ rather than V in (4.27) and obtain

$$Z_\tau = \sum_{V:\Lambda^{(2)}\to\mathcal{C}_0} \left(\prod_{(v_0,v_1,v_2)\in\Lambda^{(2)}} \hat{w}(v_0,v_1,v_2)(V_{012}) \right) Z_\tau^{(V)}, \tag{4.28}$$

$$Z_\tau^{(V)} = \mathrm{tr}_{\mathcal{H}}\left[P\circ\left(\bigotimes_{s\in\Lambda^{(4)}} Z_{\tau(s)}^{(V),(\varepsilon_{\tau(s)})} \right) \right], \tag{4.29}$$

where we have used (4.14) and where we have written V instead of $\overline{V}$ for simplicity.

In the preceding lemmas we have constructed linear isomorphisms which form the vertical maps in commutative diagrams of the following form:

$$\begin{array}{ccc} H_{0234}\otimes H_{0124} & \xrightarrow{Z_{01234}^{(V),(+)}} & H_{1234}\otimes H_{0134}\otimes H_{0123} \\ \downarrow \Phi_1 \quad \downarrow \Phi_2 & & \downarrow \Phi_3 \quad \downarrow \Phi_4 \quad \downarrow \Phi_5 \\ H^{(1)}\otimes H^{(2)} & \longrightarrow & H^{(3)}\otimes H^{(4)}\otimes H^{(5)} \end{array}$$

Here the $H^{(j)}$ are suitable state spaces such that the bottom horizontal map is related to the four-simplex map $Z_{\tau(s)}^{(\tilde{V})(-)}$ by the pairing (4.5). The coloring $\tilde{V}$ is such that $\tilde{V}_{012}\cong V_{012}$ for all triangles (012).

Since each tetrahedron occurs twice in the boundary of some four-simplices, once with positive and once with negative relative orientation, each state space $H_{\tau(jklm)}$ occurs twice among the $H^{(j)}$, once as $H_{\tau(jklm)}$ and once as the dual state space $H^*_{\tau(jklm)}$. In both cases, the corresponding map Φ_j is the same, either one of the τ_i or the identity. Therefore the tensor product of all four-simplex maps is conjugated by a linear isomorphism Φ which can be obtained from a tensor product of these Φ_j,

$$P\circ\left(\bigotimes_{s\in\Lambda^{(4)}} Z_s^{(V),(\varepsilon_s)} \right) = \Phi\left[P\circ\left(\bigotimes_{s\in\Lambda^{(4)}} Z_{\tau(s)}^{(V),(\varepsilon_{\tau(s)})} \right) \right] \Phi^{-1}. \tag{4.30}$$

Observe that here $\varepsilon_{\tau(s)} = -\varepsilon_s$ and that the coloring $\tilde{V}$ can be replaced by V as a consequence of Theorem 4.12.

Since $Z_\tau^{(V)}$ is the trace over (4.30), we find $Z_\tau^{(V)} = Z^{(V)}$ and therefore $Z_\tau = Z$. □

C. Gauge symmetry

In order to understand the gauge symmetry of LGT in the picture of the spin foam model, consider first the case in which $\mathcal{C}$ is the category of finite-dimensional representations of the gauge group G. The group then acts on its representations via natural equivalences $(t_g^{(V)})_V$, $g\in G$, i.e., natural isomorphisms $t_g^{(V)}: V\to V$ for all objects V.

In LGT on the two-complex (V,E,F) dual to the simplicial complex $\Lambda^{(*)}$, consider a gauge transformation involving only one vertex $v\in V$. This means that the group elements g_e attached to the edges $e\in E$ are transformed as

$$g_e \mapsto g_e\cdot h_v^{-1}, \quad \text{if} \quad v=\partial_- e, \tag{4.31a}$$

$$g_e \mapsto h_v\cdot g_e, \quad \text{if} \quad v=\partial_+ e, \tag{4.31b}$$

for $h_v\in G$ while all other variables g_e remain unchanged. For each polygon containing the vertex v in its boundary, precisely two edges are affected in such a way that the effect of the transformation cancels for the polygon.

In the spin foam picture, only the four-simplex dual to the vertex $v \in V$ is affected. Let (v_0, v_1, v_2) denote the triangle to which a polygon is dual. The gauge transformation then inserts natural isomorphisms $t_g^{(V_{012})}$ and $(t_g^{(V_{012})})^{-1}$ into the ribbon corresponding to that triangle, i.e., to the ribbon labeled by the object V_{012}. These isomorphisms cancel.

In the categorical picture, however, this symmetry can be understood in other terms. Let now $\mathcal{C}$ denote any admissible ribbon category and choose a coloring $V: \Lambda^{(2)} \to \mathcal{C}_0$. Consider a morphism $\varphi_{0123} \in H_{0123}$, i.e., $\varphi_{0123}: V_{123} \otimes V_{013} \to V_{012} \otimes V_{023}$. Then for any natural equivalence $(t^{(V)})_V$, naturality means

$$\varphi_{0123} = (t^{(V_{013})} \otimes t^{(V_{012})}) \circ \varphi_{0123} \circ (t^{(V_{123})^{-1}} \otimes t^{(V_{013})^{-1}}). \tag{4.32}$$

If this transformation for the natural equivalence $(t^{(V)})_V$ is applied simultaneously to all morphisms φ_{jklm} in Fig. 12(a) or 12(b), the isomorphisms $t^{(V_{jkl})}$ cancel pairwise in each ribbon, and the quantum trace remains unchanged.

In the categorical description of the spin foam model, the gauge symmetry is therefore automatically implemented. It is just the naturality property of natural equivalences together with the fact that all ribbon diagrams used in the definition of the partition function are quantum traces.

D. Wilson loop and spin networks

Having generalized the partition function of LGT to ribbon categories, it is desirable to understand the corresponding generalization for the observables of LGT, namely for Wilson loops and spin networks (Definition 3.5).

In order to define the expectation value of a spin network, recall that the quantum traces in Fig. 12 generalize the four-dimensional version of Fig. 6(a). One should therefore extend Fig. 12 and include five additional ribbons and one coupon for the spin network as Fig. 6(b) suggests. However, it seems to be impossible to find a ribbon diagram which has the symmetries required in Sec. IV B.

A possible explanation is the following argument. In the Lie group case, the spin network (3.17) attaches representations to the edges and morphisms to the vertices of the two-complex (V, E, F). Its generalization to the ribbon case should therefore be given by a ribbon graph in four dimensions. In four dimensions, however, there is no canonical way of associating to each ribbon graph a morphism in the ribbon category $\mathcal{C}$ because there is no four-dimensional analogs of the Reshetikhin–Turaev functor. It is conceivable that the notion of a spin network in four dimensions using ribbon categories is not a good definition.

For the constructions of observables that generalize Definition 3.5 to the case of ribbon categories, one therefore has to choose a linear order of vertices on which the result will then depend in a crucial way. Spin network observables are thus defined for simplicial complexes, but not in general for combinatorial complexes.

These restrictions are important if one wants to construct particular physical models which are based on a spin foam model using ribbon categories. It remains to be studied under which conditions one can define at least a certain class of observables and how the dependence on the vertex order can be interpreted. The reader is also referred to the diagrammatic approach to observables in three dimensions in Ref. 3.

V. SPECIAL CASES AND GENERALIZATIONS

The partition function (4.13) of the spin foam model using ribbon categories covers a number of special cases which were already known in other contexts. In this section, we comment on the relations between these models.

A. Lattice gauge theory

The category $\mathcal{C}=\mathrm{Rep}\ G$ of finite-dimensional representations of a compact Lie group G forms a semi-simple admissible ribbon category. The relation of the spin foam model with LGT holds if the set of colors $\mathcal{C}_0$ is a set containing one representative of each equivalence class of simple objects.

In this case one can use the generic Boltzmann weight (1.1) for any action which is local, i.e., evaluated once for each polygon, and which is a real and bounded L^2-integrable class function of G. In particular, the standard *Wilson action* and the *heat kernel* or *generalized Villain action* are of this form. For details about these actions and about their character expansion, we refer the reader to standard textbooks such as Refs. 15 and 16.

In general the set of representatives $\mathcal{C}_0$ of the simple objects is countably infinite. However, the partition function (4.13) is a convergent series because the Boltzmann weight is an L^2-function, and its character expansion therefore forms a square summable series due to the Peter–Weyl theorem. For more details, see Refs. 17 and 25.

In this case both pictures, LGT and the spin foam model, are well-defined and are dual to each other in the sense of Ref. 17. A comparison of the spin foam model dual to LGT (3.11) and the generalization (4.13) shows the following correspondences, cf. Table I. The sum over colorings of triangles/polygons and the weights $\hat{w}$ are explicitly contained in the partition function. The sum over colorings of tetrahedra/edges with morphisms is explicit in (3.11) and it is the result of the trace over the tensor product $\mathcal{H}$ in (4.11). The weights $C(v)$ per four-simplex/vertex are given by the formula (3.12) and agree with the quantum traces of Fig. 12 which appear as a result of the trace over the four-simplex maps in (4.11).

For standard actions of LGT such as Wilson's action or the heat kernel action, the character expansion coefficients behave qualitatively like $\exp((1/\beta)\, s^*(V_\rho))$ if the Boltzmann weight is of the form $\exp(\beta s(g))$. Here β is the *inverse temperature*, $s(g)$ denotes the action and $s^*(V_\rho)$ the *dual action*, a function assigning a real number to each finite-dimensional irreducible representation of G. The transformation between LGT and the spin foam model thus realizes a low temperature–high temperature duality or a strong-weak duality in the bare coupling g_0 if $\beta = 1/g_0^2$.

For the heat kernel action, the dual action $s^*(V_\rho) \sim C_\rho^{(2)}$ is essentially given by the second order Casimir operator $C_\rho^{(2)}$ of the representation. One can thus sort the configurations of the spin foam model by the sum of the Casimir eigenvalues over all triangles, and recovers the full strong coupling expansion of non-Abelian LGT.

Observe finally that LGT was formulated here on the two-complex dual to a generic triangulation. In order to obtain the usual continuum limit, the Boltzmann weight $\hat{w}(v_0,v_1,v_2)$ should now depend on the geometry of the triangle (v_0,v_1,v_2) in a suitable way.

B. Gauge theory with finite groups

If $\mathcal{C}=\mathrm{Rep}\, G$ is the category of representations of a finite group G, all comments of Sec. V A still apply. In this case, there are only finitely many simple objects up to isomorphism and the partition functions in both pictures, in LGT and in the spin foam model, are well-defined.

It is now also possible to study the "topological" Boltzmann weight

$$w(g)=\delta(g):=\begin{cases} |G|, & \text{if} \quad g=1, \\ & \\ 0 & \text{else,} \end{cases} \qquad \text{i.e.,} \quad \hat{w}_\rho=\dim V_\rho\,. \tag{5.1}$$

With suitable prefactors, the partition function is then independent of the triangulation and thus forms a topological invariant which is well known and depends only on the gauge group and on the first fundamental group of the manifold. See, for example, the comments in Sec. 2.2 of Ref. 28.

C. The Crane–Yetter state sum

Let $\mathcal{C}$ be a finitely semi-simple and admissible ribbon category satisfying the conditions of Corollary 2.11 and $\mathcal{C}_0$ be a set containing one representative for each equivalence class of simple objects. This case is beyond the standard formulation of LGT, and only the spin foam model (4.13) makes sense. The partition function is a finite sum. It is again possible to choose ''topological'' Boltzmann weights which here means the quantum dimension of the simple objects,

$$\hat{w}(V) = \mathrm{qdim} V. \tag{5.2}$$

With suitable prefactors the partition function (4.13) agrees with the Crane–Yetter invariant.[10] For a comparison of Fig. 12(a) with the main diagram in Ref. 10, observe that the state spaces H_{0123} used in the present article can be further decomposed employing semi-simplicity (2.26), for example,

$$H_{0123} = \mathrm{Hom}(V_{123} \otimes V_{013}, V_{012} \otimes V_{023}) \cong \oplus_{J \in \mathcal{C}_0} \mathrm{Hom}(V_{123} \otimes V_{013}, J) \otimes \mathrm{Hom}(J, V_{012} \otimes V_{023}). \tag{5.3}$$

If this decomposition is applied to the state spaces associated with all tetrahedra, one has to color in addition the tetrahedra with simple objects [the J in (5.3)] and the tetrahedra (0123) with two types of morphisms, $\mathrm{Hom}(V_{123} \otimes V_{013}, J)$ and $\mathrm{Hom}(J, V_{012} \otimes V_{023})$. These colorings are used in the standard formulation of the Crane–Yetter state sum in Ref. 10. Note that the additional weight $1/J$ per tetrahedron in Ref. 10 is a consequence of the choice of bases of $\mathrm{Hom}(V_{123} \otimes V_{013}, J)$ and $\mathrm{Hom}(J, V_{012} \otimes V_{023})$.

D. The generic case

The construction presented generalizes LGT and the Crane–Yetter state sum, but also contains the generic case. Here $\mathcal{C}$ is any admissible ribbon category, in particular not required to be semi-simple, and the weights $\hat{w}(V)$ for given simple objects V can be quite freely chosen. If the set of colors $\mathcal{C}_0$ is finite, the partition function is a finite sum and thus well-defined for any choice of weights. If $\mathcal{C}_0$ is a countable set, similar convergence issues arise as for Lie groups.[17] Note that here it is also necessary to examine the quantum traces of Fig. 12 in order to prove convergence of the partition function.

E. Generalizations and the Barrett–Crane model

If $\mathcal{C} = \mathrm{Rep}\, G$ for a compact Lie group, for example, $G = \mathrm{SU}(2)$, and if the Boltzmann weight is chosen to be ''topological,''

$$w(g) = \delta(g), \quad \hat{w}(V_\rho) = \dim V_\rho, \tag{5.4}$$

the partition function is just a (divergent) formal expression. This is the case for the Ooguri model[13] which can be formulated in the LGT or in the spin foam picture.

The simplest version of a spin foam model of Barrett–Crane type[14] is obtained from the Ooguri model for SO(4) in the spin foam picture by restricting the representations in all sums to the *simple* representations of SO(4). Simple here means that the representation is of the form $V \otimes V$ as a representation of $\mathrm{SU}(2) \times \mathrm{SU}(2)$ for some irreducible representation V of SU(2).

In order to implement this restriction one can choose the set of colors $\mathcal{C}_0$ to contain one representative per isomorphism class of simple representations of SO(4). However, in addition one has to restrict the sum over J in (5.3) to simple representations. As a consequence the state spaces H_{0123} are certain subspaces of $\mathrm{Hom}(V_{123} \otimes V_{013}, V_{012} \otimes V_{023})$.

The results of the present article can be generalized to state spaces that are subspaces of $\mathrm{Hom}(V_{123} \otimes V_{013}, V_{012} \otimes V_{023})$ as long as the pairing (4.5) and the maps τ_j of Definition 4.4 can be consistently restricted to these subspaces. The correspondence with LGT with a partition function (3.1) is, however, lost as a consequence of this generalization.

VI. CONCLUSION AND OUTLOOK

The spin foam model for ribbon categories defined in the present article generalizes the spin foam model dual to lattice gauge theory (LGT) and can be used as a definition of LGT for gauge groups which are quantum groups rather than Lie groups. Furthermore, the definition presented here encompasses state sum models that are of interest both in topology and in quantum gravity. The definition presented provides a bridge between the standard (Lie group) formulation of LGT and the Crane–Yetter invariant which uses ribbon categories. It can also be used to construct other spin foam models that do not correspond to topological quantum field theories and provides proofs that they are well-defined. This work might finally help to make the relation of LGT and the spin foam models used in other areas more transparent and the common concepts and open questions more accessible.

If one seeks to construct even more general spin foam models than defined here, it is worth pointing out that consistency of the definition restricts the quantum traces of Fig. 12 very tightly. The introduction of further weights, however, seems to be much easier to achieve.

The definition of LGT with ribbon categories presented here is restricted to four dimensions. Technically, this is due to the fact that the key diagrams in Fig. 12 are handmade for this construction. Due to the generality of ribbon categories it involves choices of over- or undercrossings, and only with a good choice is the partition function well-defined. While the corresponding approaches in $d=3$[2,3] are canonical in the sense that their construction is well-defined due to general principles, the $d=4$ construction presented here involves choices and one has to verify *a posteriori* that it is consistent. It is not obvious whether the result of Ref. 29 in arbitrary dimension in the Lie group case can be generalized to ribbon categories. It is, in any case, a striking observation that there exist constructions in $d=3$ (Ref. 3) and in $d=4$ (presented here) which both generalize the spin foam model dual to LGT. Notice, however, that the $d=3$ case can be handled with spherical categories[7] which are more general than ribbon categories. For the construction in $d=4$, we make explicit use of ribbon categories because the basic diagrams in Fig. 12 always contain a crossing. If ribbon categories are used in the construction in $d=3$, all spin network observables can be defined[3] whereas in $d=4$ there are no canonical expressions for the spin network observables anymore. It therefore seems that one has to use more and more restrictive structures if one wishes to increase the dimension.

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A new class of entanglement measures

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We introduce new entanglement measures on the set of density operators on tensor product Hilbert spaces. These measures are based on the greatest cross norm on the tensor product of the sets of trace class operators on Hilbert space. We show that they satisfy the basic requirements on entanglement measures discussed in the literature, including convexity, invariance under local unitary operations and nonincrease under local quantum operations and classical communication. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1398062]

I. INTRODUCTION

This paper is devoted to the study of entanglement of quantum states, which is one of the most decisively nonclassical features in quantum theory. The question of quantifying entanglement in the case of mixed quantum states represented by density operators on finite dimensional Hilbert spaces has recently been studied extensively in the context of quantum information theory, see, e.g., Refs. 1–10, and references therein.

An *entanglement measure* is a real-valued function defined on the set of density operators on some tensor product Hilbert space subject to further physically motivated conditions, see, e.g., Refs. 3–7 and below. A number of entanglement measures have been discussed in the literature, such as the von Neumann reduced entropy, the relative entropy of entanglement,[4] the entanglement of distillation and the entanglement of formation.[2] Several authors proposed physically motivated postulates to characterize entanglement measures, see below. These postulates (although they vary from author to author in the details) have in common that they are based on the concepts of the operational formulation of quantum mechanics.[11] We shall discuss one version of these *operational characterizations* of entanglement measures in Sec. IV.

In this paper we introduce new entanglement measures based on the greatest cross norm on the tensor product of the sets of trace class operators on Hilbert space (see Secs. V and VI). We shall show that the measures introduced in this work satisfy all the basic requirements for entanglement measures. These include convexity, invariance under local unitary transformations, and nonincrease under procedures composed of local quantum operations and classical communication.

Throughout this paper the set of trace class operators on some Hilbert space $\mathcal{H}$ is denoted by $\mathcal{T}(\mathcal{H})$ and the set of bounded operators on $\mathcal{H}$ by $\mathcal{B}(\mathcal{H})$. A density operator is a positive trace class operator with trace one.

II. PRELIMINARIES

In this section we collect some basic definitions and results which are used in the course of this paper.

In the present paper we restrict ourselves mainly to the situation of a composite quantum system consisting of two subsystems with Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ where $\mathcal{H}_1$ and $\mathcal{H}_2$ denote the Hilbert spaces of the subsystems (except in Sec. VI). The states of the system are identified with the density operators on $\mathcal{H}_1 \otimes \mathcal{H}_2$.

Definition 1: Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two Hilbert spaces of arbitrary dimension. A density operator ρ on the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_2$ is called separable *or* disentangled *if there exist a family $\{\omega_i\}$ of*

positive real numbers, a family $\{\rho_i^{(1)}\}$ *of density operators on* $\mathcal{H}_1$ *and a family* $\{\rho_i^{(2)}\}$ *of density operators on* $\mathcal{H}_2$ *such that*

$$\rho = \sum_i \omega_i \rho_i^{(1)} \otimes \rho_i^{(2)}, \tag{1}$$

where the sum converges in trace class norm.

The set of states is a convex set and its extreme points, which are also called *pure states*, are the projection operators. Every pure state obviously corresponds to a unit vector ψ in $\mathcal{H}_1 \otimes \mathcal{H}_2$. We denote the projection operator onto the subspace spanned by the unit vector ψ by P_ψ.

The Schmidt decomposition is of central importance in the characterization and quantification of entanglement associated with pure states.

Lemma 2: Let $\mathcal{H}_1$ *and* $\mathcal{H}_2$ *be Hilbert spaces of arbitrary dimension and let* $\psi \in \mathcal{H}_1 \otimes \mathcal{H}_2$. *Then there exist a family of non-negative real numbers* $\{p_i\}_i$ *and orthonormal bases* $\{a_i\}_i$ *and* $\{b_i\}_i$ *of* $\mathcal{H}_1$ *and* $\mathcal{H}_2$, *respectively, such that*

$$\psi = \sum_i \sqrt{p_i} a_i \otimes b_i .$$

The family of positive numbers $\{p_i\}_i$ is called the family of *Schmidt coefficients* of ψ. For pure states the family of Schmidt coefficients of a state completely characterizes the amount of entanglement of that state. A pure state ψ is separable if and only if $\psi = a \otimes b$ for some $a \in \mathcal{H}_1$ and $b \in \mathcal{H}_2$.

The *von Neumann* (vN) *reduced entropy* for density operators σ on a tensor product Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ is defined as

$$S_{\mathrm{vN}}(\sigma) := -\mathrm{Tr}_{\mathcal{H}_1}(\mathrm{Tr}_{\mathcal{H}_2}\sigma \ln(\mathrm{Tr}_{\mathcal{H}_2}\sigma)), \tag{2}$$

where $\mathrm{Tr}_{\mathcal{H}_1}$ and $\mathrm{Tr}_{\mathcal{H}_2}$ denote the partial traces over $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. In the case of pure states $\sigma = P_\psi$, it can be shown that $-\mathrm{Tr}_{\mathcal{H}_1}(\mathrm{Tr}_{\mathcal{H}_2} P_\psi \ln(\mathrm{Tr}_{\mathcal{H}_2} P_\psi)) = -\mathrm{Tr}_{\mathcal{H}_2}(\mathrm{Tr}_{\mathcal{H}_1} P_\psi \ln(\mathrm{Tr}_{\mathcal{H}_1} P_\psi)) = -\Sigma_i p_i \ln p_i$ where $\{p_i\}_i$ denotes the family of Schmidt coefficients of ψ. However, for a general mixed state σ we have $\mathrm{Tr}_{\mathcal{H}_1}(\mathrm{Tr}_{\mathcal{H}_2}\sigma \ln(\mathrm{Tr}_{\mathcal{H}_2}\sigma)) \neq \mathrm{Tr}_{\mathcal{H}_2}(\mathrm{Tr}_{\mathcal{H}_1}\sigma \ln(\mathrm{Tr}_{\mathcal{H}_1}\sigma))$.

III. EFFECTS AND OPERATIONS

In this section we recall some of the fundamental concepts and definitions in the operational approach to quantum theory and in quantum measurement theory.[11–15] The quantum mechanical *state* of a quantum system is described by a density operator ρ on the system's Hilbert space $\mathcal{H}$, i.e., by a positive trace class operator with trace one. Let $\mathcal{K}$ be another Hilbert space. An *operation* is a positive linear map $T: \mathcal{T}(\mathcal{H}) \to \mathcal{T}(\mathcal{K})$ such that T is trace nonincreasing for positive trace class operators, i.e., $0 \leq \mathrm{Tr}(T(\sigma)) \leq \mathrm{Tr}(\sigma)$ for all positive $\sigma \in \mathcal{T}(\mathcal{H})$. Following Refs. 2 and 7 we adopt the point of view that allowed operations in a laboratory are (O1) adding an ancilla, (O2) tracing out part of the system, (O3) performing unitary operations, and (O4) performing possibly selective yes–no experiments. It can be shown (for a detailed proof see, e.g., Ref. 16) that the class of operations $T: \mathcal{T}(\mathcal{H}) \to \mathcal{T}(\mathcal{K})$ composed out of operations of the form (O1)–(O4) coincides with the class of trace nonincreasing *completely positive* operations, i.e., has the property that for all $n \geq 0$ the map T_n on $\mathcal{T}(\mathcal{H} \otimes \mathbb{C}^n)$ defined by $T_n := T \otimes 1_n$, where $1_n \in \mathcal{B}(\mathbb{C}^n)$ denotes the unit matrix, is positive. For a further physical motivation of the requirement of complete positivity see, e.g., Ref. 11. In the sequel it is always understood that all operations are completely positive. If $\mathcal{H}$ and $\mathcal{K}$ are both finite dimensional Hilbert spaces, then it follows from the Choi–Kraus representation theorem for operations[11,13,17] that for every operation $T: \mathcal{T}(\mathcal{H}) \to \mathcal{T}(\mathcal{K})$ there exists a family of bounded operators $\{A_k : \mathcal{H} \to \mathcal{K}\}_k$ with $\Sigma_k A_k A_k^\dagger \leq 1_\mathcal{K}$ such that T can be expressed as

$$T(\sigma)=\sum_k A_k^\dagger \sigma A_k, \tag{3}$$

for all $\sigma\in\mathcal{T}(\mathcal{H})$. If $\mathcal{H}=\mathcal{K}$, the Choi–Kraus representation is also valid for infinite dimensional Hilbert spaces (all sums converge in trace class norm). The family $\{A_k\}_k$ is not unique. However, the operator $E:=\Sigma_k A_k A_k^\dagger = T^*(1)$ is independent of the family $\{A_k\}_k$ chosen and is called the *effect* corresponding to the operation T and its associated yes-no measurement (T^* denotes the adjoint of T[11]). Generally, an operator E is called an *effect operator* if E is bounded and Hermitean and if $0\leqslant E\leqslant 1$. *Effect operator valued measures* are then the most general *observables* in the theory.[14] They are also called *positive operator valued (POV) measures*. A *Lüders–von Neumann operation* is an operation of the form $T_L(\sigma)=\Sigma_k P_k\sigma P_k$ where $\{P_k\}_k$ is a set of mutually orthogonal projection operators on $\mathcal{H}$. Lüders–von Neumann operations are repeatable. In the case of a general operation, it is possible to view the terms in its Choi–Kraus representation as representing different possible measurement outcomes. In the terminology of operational quantum theory the individual terms in the Choi–Kraus representation (3) form a set of operations corresponding to coexistent effects, see Refs. 11 and 14: Two effect operators E_1 and E_2 are called *coexistent* if there exist effect operators F,G,H with $F+G+H\leqslant 1$ such that $E_1=F+G$ and $E_2=F+H$ (in general $F,G,$ and H will not be unique, however). Therefore, in general two coexistent effect operators E_1 and E_2 do not correspond to mutually complementary measurement outcomes but instead may have some ''overlap'' represented by the operator F even if $E_1+E_2\leqslant 1$. Coexistent effect operators need not commute.

IV. ENTANGLEMENT MEASURES

An entanglement measure is a functional E defined on the set of density operators on the Hilbert space of a composite quantum system measuring the degree of entanglement of every given density operator. Every measure of entanglement E should satisfy the following requirements:[2–4,6,7]

(E0) An entanglement measure is a positive real-valued functional E which for any given two systems is well-defined on the set $\mathcal{D}(\mathcal{H}_1\otimes\mathcal{H}_2)$ of density operators on the tensor product $\mathcal{H}_1\otimes\mathcal{H}_2$ of the Hilbert spaces of the two systems. Moreover, E is *expansible*, i.e., whenever $\rho\in\mathcal{D}(\mathcal{H}_1\otimes\mathcal{H}_2)\subset\mathcal{D}(\mathsf{H}_1\otimes\mathsf{H}_2)$ with embeddings $\mathcal{H}_1\hookrightarrow\mathsf{H}_1$ and $\mathcal{H}_2\hookrightarrow\mathsf{H}_2$ of Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ into larger Hilbert spaces H_1 and H_2 respectively, then $E|_{\mathcal{H}_1\otimes\mathcal{H}_2}(\rho)=E|_{\mathsf{H}_1\otimes\mathsf{H}_2}(\rho)$;

(E1) if σ is separable, then $E(\sigma)=0$;

(E2) local unitary transformations leave E invariant, i.e.,
$$E(\sigma)=E((U_1\otimes U_2)\sigma(U_1^\dagger\otimes U_2^\dagger))$$
for all unitary operators U_1 and U_2 acting on $\mathcal{H}_1$ or $\mathcal{H}_2$ respectively,

(E3) entanglement cannot increase under procedures consisting of local operations on the two quantum systems and classical communication. If T is an operation which is trace-preserving on positive operators and can be realized by means of local operations and classical communication, i.e., is composed out of local operations of the form (O1)–(O4) and classical communication, then
$$E(T(\sigma))\leqslant E(\sigma), \tag{4a}$$
for all $\sigma\in\mathcal{D}(\mathcal{H}_1\otimes\mathcal{H}_2)$. It is clear that every procedure acting on an individual single quantum system $\mathcal{H}_1\otimes\mathcal{H}_2$ composed only of local operations and classical communication can formally be represented as a finite sequence of operations of the form $T_1\otimes T_2$, where T_1 and T_2 are local operations on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. The requirement that entanglement cannot increase under local operations and classical communication is thus equivalent to
$$E((T_1\otimes T_2)(\sigma))\leqslant E(\sigma), \tag{4b}$$
for all $\sigma\in\mathcal{D}(\mathcal{H}_1\otimes\mathcal{H}_2)$.

Remark 3: Equation 4(b) stipulates that local operations cannot increase entanglement. In the quantum information literature most authors replace Eqs. (4a) and (4b) by the stronger requirement

$$\sum_i p_i E(\sigma_i) \leqslant E(\sigma). \tag{5}$$

Equation (5) stipulates that after the measurement the entanglement (as measured by E) averaged over the possible output states σ_i is less than or equal to the original entanglement. Here p_i denotes the probability that the final state σ_i occurs. In the literature Eq. (5) is normally taken as the formal expression for the paradigm that it is impossible to create or increase entanglement by performing procedures composed of local quantum operations and classical communication alone. A disadvantage of Eq. (5) is that it makes sense only in measurement situations and that the "possible output states" corresponding to a given operation T are not uniquely defined. Mathematically this corresponds to the fact that the Choi–Kraus representation of an operation T is in general not unique. The difference between Eqs. (4a) and (5) is that Eq. (5) stipulates that entanglement cannot increase on average under local operations and classical communications (for a detailed discussion of this point see Ref. 7). In contrast Eq. (4a) says that entanglement cannot increase for any operation which acts on individual systems and is composed of local operations and classical communication. If one takes up the former (ensemble) point of view of Eq. (5), then Eq. (4b) does no longer represent the most general condition because from the ensemble point of view the most general operations composed out of local operations and classical communications can contain correlations between terms of the Choi–Kraus representations of subsequent local operations. A precise definition can be found, e.g., in Ref. 16. Some authors consider also other classes of local operations, most prominently the class of separable *operations considered in Ref. 3;*

(E4) mixing of states does not increase entanglement, i.e., E is convex

$$E(\lambda\sigma+(1-\lambda)\tau) \leqslant \lambda E(\sigma)+(1-\lambda)E(\tau)$$

for all $0 \leqslant \lambda \leqslant 1$ and all $\sigma, \tau \in \mathcal{D}(\mathcal{H}_1 \otimes \mathcal{H}_2)$.

Apart from the requirements (E0)–(E4) on entanglement measures many authors add further requirements to the definition of entanglement measures but we are not going to discuss them in this paper. For details, see Ref. 16. In the sequel we exclude the trivial functional $E \equiv 0$ which also satisfies (E0)–(E4).

Remark 4: Postulate (E2) is an immediate consequence of (E3).

Remark 5: It has been argued in Ref. 8 that the entanglement of distillation E_D introduced in Ref. 2 does vanish for certain nonseparable states (so-called bound entangled states). Therefore, it has been pointed out in Ref. 6 that replacing (E1) by the stronger requirement that for every entanglement measure $E(\sigma)=0$ if and only if σ is separable might exclude interesting entanglement measures. For more information the reader is referred to the references.

Example 6: Post selection of a subensemble means selecting a (non-normalized) output state of a quantum operation and normalizing its trace to 1. This procedure can lead to an increase in entanglement. This can be seen by considering a very simple example. Consider a composite quantum system composed of two three-level quantum systems and the state

$$\rho_\varepsilon = (1-\varepsilon)|00\rangle\langle 00| + \frac{\varepsilon}{2}(|12\rangle - |21\rangle)(\langle 12| - \langle 21|).$$

For ε small it is intuitively obvious that this state does not contain "much" entanglement and every entanglement measure should reflect this. Indeed consider, for example, the relative entropy of entanglement introduced in Ref. 3 defined by:

$$E_S(\sigma) := \inf_{\rho}(\mathrm{Tr}(\sigma \ln \sigma - \sigma \ln \rho)), \tag{6}$$

where the infimum runs over all separable states ρ for which $\mathrm{Tr}(\sigma \ln \rho)$ is well-defined and finite. Elementary estimates using the results of Ref. 3 show that

$$E_S(\rho_\varepsilon) \leqslant \varepsilon \ln 2.$$

If we subject the system to an operation testing whether or not the system is in the state $|00\rangle$ and select after the measurement the subensemble corresponding to the negative outcome (system is not in the state $|00\rangle$), then clearly the final state after the operation and post selection is given by $\frac{1}{2}(|12\rangle - |21\rangle)(\langle 12| - \langle 21|)$. Notice that this operation can be achieved by local operations and classical communication. We find

$$E_S(\tfrac{1}{2}(|12\rangle - |21\rangle)(\langle 12| - \langle 21|)) = \ln 2 > E_S(\rho_\varepsilon).$$

Similarly it can be shown that the entanglement measure $\|\cdot\|_\gamma$ to be introduced below may increase under post selection of subensembles. Therefore, we see that we must not replace the operation in Eq. (4a) by some normalized nonlinear operation $\rho \mapsto T(\rho)/\mathrm{Tr}(T(\rho))$ corresponding to post selection of a subensemble.

V. A NEW CLASS OF ENTANGLEMENT MEASURES

Consider the situation that the two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ are both finite dimensional and consider the spaces $\mathcal{T}(\mathcal{H}_1)$ and $\mathcal{T}(\mathcal{H}_2)$ of trace class operators on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. Both spaces are Banach spaces when equipped with the trace class norm $\|\cdot\|_1^{(1)}$ or $\|\cdot\|_1^{(2)}$, respectively, see, e.g., Schatten.[18] In the sequel we shall drop the superscript and write $\|\cdot\|_1$ for both norms, slightly abusing the notation; it will always be clear from the context which norm is meant. The algebraic tensor product $\mathcal{T}(\mathcal{H}_1) \otimes_{\mathrm{alg}} \mathcal{T}(\mathcal{H}_2)$ of $\mathcal{T}(\mathcal{H}_1)$ and $\mathcal{T}(\mathcal{H}_2)$ is defined as the set of all finite linear combinations of elementary tensors $u \otimes v$, i.e., the set of all finite sums $\Sigma_{i=1}^n u_i \otimes v_i$ where $u_i \in \mathcal{T}(\mathcal{H}_1)$ and $v_i \in \mathcal{T}(\mathcal{H}_2)$ for all i.

It is well known that we can define a cross norm on $\mathcal{T}(\mathcal{H}_1) \otimes_{\mathrm{alg}} \mathcal{T}(\mathcal{H}_2)$ by[19]

$$\|t\|_\gamma := \inf\left\{ \sum_{i=1}^n \|u_i\|_1 \|v_i\|_1 \,\middle|\, t = \sum_{i=1}^n u_i \otimes v_i \right\}, \tag{7}$$

where $t \in \mathcal{T}(\mathcal{H}_1) \otimes_{\mathrm{alg}} \mathcal{T}(\mathcal{H}_2)$ and where the infimum runs over all finite decompositions of t into elementary tensors. It is also well known that $\|\cdot\|_\gamma$ majorizes any subcross seminorm on $\mathcal{T}(\mathcal{H}_1) \otimes_{\mathrm{alg}} \mathcal{T}(\mathcal{H}_2)$. We denote the completion of $\mathcal{T}(\mathcal{H}_1) \otimes_{\mathrm{alg}} \mathcal{T}(\mathcal{H}_2)$ with respect to $\|\cdot\|_\gamma$ by $\mathcal{T}(\mathcal{H}_1) \otimes_\gamma \mathcal{T}(\mathcal{H}_2)$. $\mathcal{T}(\mathcal{H}_1) \otimes_\gamma \mathcal{T}(\mathcal{H}_2)$ is a Banach algebra.[19]

As both $\mathcal{H}_1$ and $\mathcal{H}_2$ are finite dimensional, $\mathcal{T}(\mathcal{H}_1) = \mathcal{B}(\mathcal{H}_1)$ and $\mathcal{T}(\mathcal{H}_2) = \mathcal{B}(\mathcal{H}_2)$ and $\mathcal{B}(\mathcal{H}_1) \otimes_{\mathrm{alg}} \mathcal{B}(\mathcal{H}_2) = \mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$, see, e.g., Ref. 20, Example 11.1.6. In finite dimensions all Banach space norms on $\mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$, in particular the operator norm $\|\cdot\|$, the trace class norm $\|\cdot\|_1$, and the norm $\|\cdot\|_\gamma$, are equivalent, i.e., generate the same topology on $\mathcal{B}(\mathcal{H}_1 \otimes \mathcal{H}_2)$.

For later reference we compute the value of $\|P_\psi\|_\gamma$ for one-dimensional projection operators $P_\psi = |\psi\rangle\langle\psi|$ on $\mathcal{H}_1 \otimes \mathcal{H}_2$ in terms of the coefficients in the Schmidt representation of $|\psi\rangle$. In this section we make extensive use of the Dirac bra-ket notation.

Proposition 7: Let $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ be a unit vector and $|\psi\rangle = \Sigma_i \sqrt{p_i} |\phi_i\rangle \otimes |\chi_i\rangle$ its Schmidt representation, where $\{|\phi_i\rangle\}_i$ and $\{|\chi_i\rangle\}_i$ are orthonormal bases of $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively and where $p_i \geqslant 0$ and $\Sigma_i p_i = 1$. Let P_ψ denote the one-dimensional projection operator onto the subspace spanned by $|\psi\rangle$. Then

$$\|P_\psi\|_\gamma = \sum_{ij} \sqrt{p_i p_j} = \left(\sum_i \sqrt{p_i} \right)^2.$$

Proof: Without loss of generality we assume that $\mathcal{H}_1=\mathcal{H}_2$ which can always be achieved by possibly suitably enlarging one of the two Hilbert spaces. Further, we identify $\mathcal{H}_1=\mathcal{H}_2$ with $\mathbb{C}^n$, where $n=\dim\mathcal{H}_1$, i.e., we fix an orthonormal basis in $\mathcal{H}_1$ which we identify with the canonical real basis in $\mathbb{C}^n$. With respect to this canonical real basis in $\mathbb{C}^n$ we can define complex conjugates of elements of $\mathcal{H}_1$ and the complex conjugate as well as the transpose of a linear operator acting on $\mathcal{H}_1$. From the Schmidt decomposition it follows that:

$$P_\psi=|\psi\rangle\langle\psi|=\sum_{ij}\sqrt{p_ip_j}|\phi_i\rangle\langle\phi_j|\otimes|\chi_i\rangle\langle\chi_j|. \tag{8}$$

From the definition of $\|\cdot\|_\gamma$ it is thus obvious that $\|P_\psi\|_\gamma\leqslant\Sigma_{ij}\sqrt{p_ip_j}$. Now consider the Hilbert space $\mathfrak{H}$ of Hilbert–Schmidt operators on $\mathcal{H}_1\otimes\mathcal{H}_2$ equipped with the Hilbert–Schmidt inner product $\langle f|g\rangle=\mathrm{Tr}(f^\dagger g)$. Equation (8) induces an operator $\mathfrak{A}_\psi$ on $\mathfrak{H}$ as follows. Every element ζ in $\mathfrak{H}$ can be written $\zeta=\Sigma_k x_k\otimes y_k$ where x_k and y_k are trace class operators on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. Then $\mathfrak{A}_\psi$ is defined on ζ as $\mathfrak{A}_\psi(\zeta):=\Sigma_{ijk}\sqrt{p_ip_j}\langle\chi_i^*|x_k|\chi_j^*\rangle|\phi_i\rangle\langle\phi_j|\otimes y_k$ where $|\chi_i^*\rangle$ denotes the complex conjugate of the vector $|\chi_i\rangle$ with respect to the canonical real basis in $\mathbb{C}^n$. Proposition 11.1.8 in Ref. 20 implies that $\mathfrak{A}_\psi(\zeta)$ is independent of the representation of ζ. Consider a representation $P_\psi=\Sigma_{i=1}^r u_i\otimes v_i$ of P_ψ as sum over simple tensors. Denote the transpose of v_i by v_i^T. Then the operator defined by

$$\mathcal{A}_\psi(\zeta):=\sum_{i,k=1}^{r}\mathrm{Tr}(v_i^Tx_k)u_i\otimes y_k, \tag{9}$$

is equal to $\mathfrak{A}_\psi$ (by virtue of Proposition 11.1.8 in Ref. 20). We denote the trace norm on $\mathcal{T}(\mathfrak{H})$ by $\tau(\cdot)$. The operator $\mathfrak{A}_\psi$ is of trace class and the right-hand side of Eq. (8) is the so-called polar representation of $\mathfrak{A}_\psi$ which implies $\tau(\mathfrak{A}_\psi)=\Sigma_{ij}\sqrt{p_ip_j}$, see Ref. 18. $\mathfrak{A}_\psi$ admits also many other representations $\mathfrak{A}_\psi=\Sigma_i f_i\otimes g_i$ with families of operators $\{f_i\}$ and $\{g_i\}$ acting on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. It is well known that

$$\tau(\mathfrak{A}_\psi)=\inf\left\{\sum_i\|f_i\|_2\|g_i\|_2\,\middle|\,\mathfrak{A}_\psi=\sum_i f_i\otimes g_i\right\}\leqslant\|P_\psi\|_\gamma,$$

where $\|\cdot\|_2$ denotes the Hilbert–Schmidt norm and where the latter inequality follows from $\|z\|_2\leqslant\|z\|_1$ and from the fact that each decomposition of $\mathfrak{A}_\psi$ corresponds in an obvious one-to-one fashion to a decomposition of P_ψ. This proves the proposition. □

Corollary 8: Let ρ be a density operator on $\mathcal{H}_1\otimes\mathcal{H}_2$, where $\mathcal{H}_1$ and $\mathcal{H}_2$ are finite dimensional Hilbert spaces. If $\rho=\Sigma_{ij}a_{ij}|\phi_i\rangle\langle\phi_j|\otimes|\chi_i\rangle\langle\chi_j|$, then $\|\rho\|_\gamma=\Sigma_{ij}|a_{ij}|$.

An immediate corollary of Proposition 7 is that a pure state $|\psi\rangle\in\mathcal{H}_1\otimes\mathcal{H}_2$ is separable if and only if $\|P_\psi\|_\gamma=1$. In Ref. 1 it has been proven that more generally all separable density matrices can be characterized by $\|\cdot\|_\gamma$.

Theorem 9: *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be finite dimensional Hilbert spaces and ρ be a density operator on $\mathcal{H}_1\otimes\mathcal{H}_2$. Then ρ is separable if and only if $\|\rho\|_\gamma=1$.*

In Ref. 1 it has been tentatively suggested that $\|\cdot\|_\gamma$ can be considered as a quantitative measure of entanglement. In the present work we substantiate this claim by proving

Proposition 10: The function

$$E_\gamma(\sigma):=\|\sigma\|_\gamma\log\|\sigma\|_\gamma,$$

satisfies the criteria $(E0)$–$(E4)$ for entanglement measures.

Proof: (E1) is an immediate consequence of Theorem 9 and (E0) and (E2) are clear. (E3): Let T be an operation composed of local operations, and classical communication. As we have argued above every such T can be realized as a sequence of operations of the form $T_1\otimes T_2$ where T_1 and T_2 are local operations on system 1 and 2, respectively. We show that $\|(T_1\otimes T_2)(\sigma)\|_\gamma\leqslant\|\sigma\|_\gamma$. By

linearity of $T_1\otimes T_2$ every decomposition of σ into finite sums of simple tensors $\sigma=\Sigma_{i=1}^r x_i\otimes y_i$, where x_i and y_i are trace class operators on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, induces a decomposition of $(T_1\otimes T_2)(\sigma)$ into a sum of simple tensors $(T_1\otimes T_2)(\sigma)=\Sigma_{i=1}^r T_1(x_i)\otimes T_2(y_i)$. Thus

$$\begin{aligned}\|(T_1\otimes T_2)(\sigma)\|_\gamma &= \inf\left\{\sum_{i=1}^r \|X_i\|_1\|Y_i\|_1 \,\middle|\, (T_1\otimes T_2)(\sigma)=\sum_{i=1}^r X_i\otimes Y_i\right\}\\ &\leqslant \inf\left\{\sum_{i=1}^r \|T_1(x_i)\|_1\|T_2(y_i)\|_1 \,\middle|\, \sigma=\sum_{i=1}^r x_i\otimes y_i\right\}\\ &\leqslant \|T_1\|\|T_2\|\inf\left\{\sum_{i=1}^r \|x_i\|_1\|y_i\|_1 \,\middle|\, \sigma=\sum_{i=1}^r x_i\otimes y_i\right\}\\ &\leqslant \inf\left\{\sum_{i=1}^r \|x_i\|_1\|y_i\|_1 \,\middle|\, \sigma=\sum_{i=1}^r x_i\otimes y_i\right\}\\ &= \|\sigma\|_\gamma,\end{aligned}$$

where we have used that both T_1 and T_2 are bounded maps on the space of trace class operators on $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively and that

$$\|T_i\|=\sup\{\mathrm{Tr}(T_i(\rho))\,|\,\rho\in\mathcal{T}(\mathcal{H}_i),\rho\geqslant 0 \ \text{ and } \ \mathrm{Tr}(\rho)=1\}\leqslant 1,$$

see, e.g., Lemma 2.2.1 in Ref. 12. (E3) follows from the fact that $[1,\infty[\ni s\mapsto s\log s$ is monotone. Finally, (E4) follows from the facts that $\|\cdot\|_\gamma$ is subadditive and that $[1,\infty[\ni s\mapsto s\log s$ is monotone and convex. □

Remark 11: It follows from the proof of Proposition 10 that if f is a convex, monotonously increasing function on $[1,\infty[$ with $f(1)=0$, then

$$E_f(\sigma):=f(\|\sigma\|_\gamma),$$

is an entanglement measure satisfying the requirements $(E0)$–$(E4)$. A possible choice is $f_1(x)=x-1$ leading to the entanglement measure $E_{f_1}(\sigma)=\|\sigma\|_\gamma-1$. This shows that indeed (as claimed in Ref. 1) the function $\|\sigma\|_\gamma-1$ is an entanglement measure on the space of density operators. Other possible choices for f are $f_2(x)=x\ln x-x+1$, $f_3(x)=e^{a(x-1)}, a>0$ and so forth.

Corollary 12: The entanglement measures constructed in Remark 11 (including the measure E_γ from Proposition 10) satisfy that $E_f(\sigma)=0$ if and only if σ is separable.

Proof: This is an immediate consequence of Theorem 9. □

Proposition 13: Let T_1 and T_2 be two trace-preserving Lüders–von Neumann operations on finite dimensional Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively, and let *$T_L=T_1\otimes T_2$ denote the corresponding Lüders–von Neumann operation acting locally on $\mathcal{H}_1\otimes\mathcal{H}_2$. Let $T_1(\sigma_1)=\Sigma_i P_i\sigma_1 P_i$ and $T_2(\sigma_2)=\Sigma_j Q_j\sigma_2 Q_j$ be Choi–Kraus representations of T_1 and T_2, respectively, in terms of families $\{P_i\}$ and $\{Q_j\}$ of, respectively, mutually orthogonal projection operators. Then the entanglement measure $E_{f_1}=\|\cdot\|_\gamma-1$ as in Remark 11 satisfies*

$$\sum_{ij} p_{ij}(\|\sigma_{ij}\|_\gamma-1)\leqslant\|\sigma\|_\gamma-1,$$

where $p_{ij}:=\mathrm{Tr}((P_i\otimes Q_j)\sigma(P_i\otimes Q_j))$ and $\sigma_{ij}=(P_i\otimes Q_j)\sigma(P_i\otimes Q_j)/p_{ij}$ and where σ is a density operator on $\mathcal{H}_1\otimes\mathcal{H}_2$.

Proof: Let P and P' be orthogonal projection operators. Then $\|PxP+P'yP'\|_1=\|PxP\|_1+\|P'yP'\|_1$ for all operators x,y. This follows from considering the spectral resolutions of PxP and $P'yP'$. Hence $\Sigma_i\|P_ix_kP_i\|_1=\|\Sigma_iP_ix_kP_i\|_1\leq\|x_k\|_1$. A similar argument shows that $\Sigma_j\|Q_j\tilde{z}Q_j\|_1\leq\|\tilde{z}\|_1$ for all $\tilde{z}\in\mathcal{B}(\mathcal{H}_2)$. Hence

$$\begin{aligned}\sum_{ij}p_{ij}(\|\sigma_{ij}\|_\gamma-1)&\leq\inf\left\{\sum_{ijk}\|P_ix_kP_i\|_1\|Q_jy_kQ_j\|_1\,\middle|\,\sigma=\sum_k x_k\otimes y_k\right\}-1\\&\leq\inf\left\{\sum_k\|x_k\|_1\|y_k\|_1\,\middle|\,\sigma=\sum_k x_k\otimes y_k\right\}-1\\&=\|\sigma\|_\gamma-1.\end{aligned}$$

□

It is known that some physically interesting entanglement measures coincide with the von Neumann reduced entropy on pure states, for instance the relative entropy of entanglement.[4] However, it follows immediately from Proposition 7 that E_γ does not coincide with the von Neumann reduced entropy on pure states: It follows from Ref. 4 that the entropy of entanglement for a pure state of the form $|\phi\rangle=\alpha|00\rangle+\beta|11\rangle$ is equal to $-|\alpha|^2\ln|\alpha|^2-|\beta|^2\ln|\beta|^2$, whereas it follows from Proposition 7 that $E_\gamma(|\phi\rangle\langle\phi|)=2(|\alpha|+|\beta|)^2\ln(|\alpha|+|\beta|)$. Therefore, we have explicitly constructed an entanglement measure satisfying a physically reasonable set of requirements which is not equal to the von Neumann reduced entropy on pure states. We have proven

Proposition 14: E_γ and S_{vN} do not coincide on pure states.

In Ref. 16 necessary and sufficient conditions for an entanglement measure to coincide with S_{vN} on pure states were derived. It is easy to see that, e.g., E_γ does not satisfy the additivity condition (P4) considered in Ref. 16.

VI. HIGHER TENSOR PRODUCT HILBERT SPACES

So far we restricted ourselves to tensor product Hilbert spaces of two finite dimensional Hilbert spaces. It is straightforward, however, to generalize our results to the situation of tensor products of more than two, but at most finitely many, finite dimensional Hilbert spaces. To this end consider the tensor product $\mathcal{H}=\mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_n$ of n finite dimensional Hilbert spaces $\mathcal{H}_1,\ldots,\mathcal{H}_n$. The obvious generalization of the definition of $\|\cdot\|_\gamma$ is

$$\|t\|_\gamma^{(n)}:=\inf\left\{\sum_{i=1}^r\|u_i^{(1)}\|_1\cdots\|u_i^{(n)}\|_1\,\middle|\,t=\sum_{i=1}^r u_i^{(1)}\otimes\cdots\otimes u_i^{(n)}\right\},\tag{10}$$

where t is a trace class operator on $\mathcal{H}$.

It is straightforward to generalize the main result of Ref. 1 to n-fold tensor product Hilbert spaces $\mathcal{H}=\mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_n$.

Definition 15: Let $\mathcal{H}_1,\ldots,\mathcal{H}_n$ be Hilbert spaces of arbitrary dimension. A density operator ρ on the tensor product $\mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_n$ is called disentangled *or* separable *(with respect to $\mathcal{H}_1,\ldots,\mathcal{H}_n$) if there exist a family $\{\omega_i\}$ of positive real numbers, and families $\{\rho_i^{(k)}\}$ of density operators on $\mathcal{H}_k$ respectively, where $1\leq k\leq n$, such that*

$$\rho=\sum_i\omega_i\rho_i^{(1)}\otimes\cdots\otimes\rho_i^{(n)},\tag{11}$$

where the sum converges in trace class norm.

Theorem 16: *Let $\mathcal{H}_1,\ldots,\mathcal{H}_n$ be finite dimensional Hilbert spaces and ρ be a density operator on $\mathcal{H}=\mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_n$. Then ρ is separable if and only if $\|\rho\|_\gamma^{(n)}=1$.*

We now consider the situation that $\mathcal{H}$ is the m-fold tensor product of $\mathfrak{H}_1 \otimes \mathfrak{H}_2$ with two finite dimensional Hilbert spaces $\mathfrak{H}_1$ and $\mathfrak{H}_2$. The functional E_γ from Proposition 10 admits an obvious extension

$$E_\gamma(\sigma) := \|\sigma\|_\gamma^{(n)} \ln \|\sigma\|_\gamma^{(n)}, \tag{12}$$

for all trace class operators σ on $\mathcal{H}$.

Proposition 17: The functional defined by Eq. (12) satisfies the criteria $(E0)$–$(E4)$ *for entanglement measures.*

VII. CONCLUSION

To conclude, in this paper we have introduced a new class of entanglement measures on the space of density operators on tensor product Hilbert spaces. Our entanglement measures are based on the greatest cross norm $\|\cdot\|_\gamma$ on the set of trace class operators on the tensor product Hilbert space. We showed that our entanglement measures satisfy a number of physically desirable requirements, in particular that they do not increase under local quantum operations.

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Superalgebras for the Penning trap

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The Hamiltonian describing a single fermion in a Penning trap is shown to be supersymmetric in certain cases. The supersymmetries of interest occur when the ratio of the cyclotron frequency to the axial frequency is $\frac{3}{2}$ and the particle has anomalous magnetic moment $\frac{4}{3}$ or $\frac{2}{3}$. At these supersymmetric points, the spectrum shows uniformly spaced crossed levels. The associated superalgebras are su$(2|1)$ and su$(1|1)$. The phase space for this problem has an osp$(2|6)$ structure and contains all the degeneracy superalgebras. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1404386]

I. INTRODUCTION

The Penning trap[1,2] is an impressive tool for precision spectroscopy of charged particles. High-precision measurements conducted on particles in a Penning trap include a comparison of the anomalous magnetic moments for the electron and positron to a precision of 10^{-12},[3] a measurement of the charge-to-mass ratio for protons and antiprotons to 10^{-10},[4] and a search for time dependence in the anomaly frequency of a trapped electron.[5] Comparable precisions have been attained in measurements of the mass ratio of the proton to the electron,[6] the masses of molecular ions,[7] and bounds on the anisotropy of space.[8] Recent theoretical investigations indicate that Penning-trap experiments can constrain Lorentz and CPT violation at the level of 10^{-20} in the context of a general standard-model extension.[9] Numerous other applications of Penning traps exist.[10]

In the present article, we investigate the symmetries of the Hamiltonian describing a single charged fermionic particle confined in a Penning trap with hyperbolic electrodes. The symmetry depends on the relative values of the magnetic and electric fields and on the gyromagnetic ratio of the trapped particle. For certain values of these parameters, superalgebras[11] arise.

There are relatively few physical manifestations of superalgebras. One arises in nuclear physics.[12] Another exists in atomic systems,[13,14] where a broken quantum-mechanical supersymmetry has been shown to underlie the properties of the chemical elements. It has recently been suggested that a supersymmetry also exists in the context of traps.[15] In this case, a radial supersymmetry for the trap wave functions provides a description of a small cloud of particles in a trap via an effective single-particle formalism. The associated parallels between traps and atoms in the context of quantum-mechanical supersymmetry have been studied in some detail.[16] Some other results in quantum-mechanical supersymmetry are reviewed in Ref. 17.

The supersymmetries discussed in this article for the Penning trap are of a different type. The idea is to consider the full Hamiltonian written in terms of creation and annihilation operators. The (anti)commutation relations satisfied by quadratic combinations of these operators define the superalgebras relevant to the problem.

In Sec. II, the relevant features of the Penning trap are reviewed and some definitions are given. The relative strengths of the trapping fields required for degeneracies to occur are discussed in Sec. III. The central algebra common to all cases is given in Sec. IV, and each of the five relevant superalgebras are presented in turn in Secs. V–IX. In Sec. X we summarize and discuss the results.

II. THE PENNING TRAP

In most situations, the dynamics of a particle in a Penning trap is dominated by its interaction with a uniform magnetic field **B**. For convenience, we work in cylindrical coordinates (ρ,ϕ,z) with $\mathbf{B}=B\hat{\mathbf{z}}$. A suitable choice of vector potential is $\mathbf{A}=(B\rho/2)\hat{\phi}$.

The quadrupole electric field of the trap is produced by electrodes in one of several possible forms.[18,19] We restrict attention to the case with electrode surfaces given in cylindrical coordinates by the expressions

$$z^2=\rho^2/2\pm d^2, \tag{1}$$

where d is a constant. The upper equation is a hyperboloid of two sheets and describes the endcap surfaces, which intersect the z axis at $z=\pm d$ and have potential $V/2$. The remaining electrode surface has potential $-V/2$ and has shape determined by the lower sign in Eq. (1). It is a hyperboloid of one sheet encircling the z axis with waist radius $\sqrt{2}d$ in the $z=0$ plane. The electrostatic potential is

$$\phi(\rho,\phi,z)=\frac{V}{2d^2}(z^2-\rho^2/2) \tag{2}$$

in the trapping region.

Let the trapped particle have charge q and mass m. We assume that q and V have the same sign, thereby ensuring axial trapping. Defining the axial frequency $\omega_z=(qV/md^2)^{1/2}$ and the cyclotron frequency $\omega_c=|qB|/m$, the Hamiltonian for $q>0$ is

$$\tilde{H}=-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2+\frac{1}{8}m\Omega^2\rho^2+\frac{1}{2}m\omega_z^2z^2+\frac{1}{2}\hbar\omega_c i\frac{\partial}{\partial\phi}, \tag{3}$$

where $\Omega=(\omega_c^2-2\omega_z^2)^{1/2}$. For $q<0$, the last term would be negative. The algebraic structure of the problem turns out to be independent of the sign of q, and to avoid carrying two signs in the expressions that follow, we restrict attention to the case $q>0$.

Equation (3) separates by defining $\Psi(\rho,\phi,z)\equiv(r_0/\rho)^{1/2}W(\rho)\Theta(\theta,z)$, where $r_0=(\hbar/m\omega_c)^{1/2}$. The equation in ρ is

$$\left\{-\frac{\hbar^2}{2m}\frac{d^2}{d\rho^2}+\frac{\hbar^2}{2m}\frac{(\hat{M}^2-\frac{1}{4})}{\rho^2}+\frac{1}{8}m\Omega^2\rho^2-\left[E-\left(\hat{K}+\frac{1}{2}\right)\hbar\omega_z+\frac{1}{2}\hat{M}\hbar\omega_c\right]\right\}W(\rho)=0, \tag{4}$$

where $\hat{M}$ and $\hat{K}$ are separation constants taking values $\hat{M}=0,\pm1,\pm2,\ldots$ and $\hat{K}=0,1,2,\ldots$. The energy eigenvalues E for this problem are

$$E_{N,\hat{K},\hat{M}}=\frac{\hbar}{2}[\Omega N+2\omega_z\hat{K}-\omega_c\hat{M}+(\Omega+\omega_z)], \tag{5}$$

where N takes values $N=|\hat{M}|,|\hat{M}|+2,|\hat{M}|+4,\ldots$. The full solution to the stationary problem $\tilde{H}\Psi=E\Psi$ involves generalized Laguerre and Hermite polynomials,

$$\Psi_{N,\hat{K},\hat{M}}(\rho,\phi,z)=C_{N,\hat{K},|\hat{M}|}\left(\frac{\rho}{r_0}\right)^{|\hat{M}|}\exp\left[-\frac{k}{4}\left(\frac{\rho}{r_0}\right)^2-\frac{1}{2}\left(\frac{z}{s_0}\right)^2+i\hat{M}\phi\right]$$
$$\times L_{N/2-|\hat{M}|/2}^{(|\hat{M}|)}\left(\frac{k}{2}\left(\frac{\rho}{r_0}\right)^2\right)H_{\hat{K}}\left(\frac{z}{s_0}\right), \tag{6}$$

where $k=\Omega/\omega_c$, $s_0=(\hbar/m\omega_z)^{1/2}$, and the normalization coefficient is

$$C_{N,\hat{K},|\hat{M}|}=\left[\frac{\sqrt{k}}{r_0^2 s_0 2^{\hat{K}}\pi^{3/2}}\left(\frac{k}{2}\right)^{|\hat{M}|+1/2}\frac{\Gamma(N/2-|\hat{M}|/2+1)}{\Gamma(N/2+|\hat{M}|/2+1)\Gamma(\hat{K}+1)}\right]^{1/2}. \tag{7}$$

For the special case $k=0$, the coefficient of the ρ^2 term in Eq. (4) would vanish and the above solutions would change. We exclude this case because it does not allow long-term confinement. In the initial stages of trapping before significant cooling has occurred, the motion of the particle can be understood classically. The possible trajectories are either circles about the central axis or curves that exit the trap. The former are unstable to radial perturbations. We therefore restrict attention to the range of values $0<k\leqslant 1$, or, equivalently, $0<\Omega\leqslant\omega_c$.

The Hamiltonian $\tilde{H}$ can be expressed in terms of creation and annihilation operators. A transformation of the phase space yields six dimensionless operators

$$\begin{aligned}
a,a^\dagger &= \frac{r_0}{\sqrt{2k}}(\pm\partial_x+i\partial_y)+\sqrt{\frac{k}{8}}\frac{1}{r_0}(x\pm iy),\\
b,b^\dagger &= \frac{r_0}{\sqrt{2k}}(\mp\partial_x+i\partial_y)-\sqrt{\frac{k}{8}}\frac{1}{r_0}(x\mp iy),\\
c,c^\dagger &= \pm\frac{s_0}{\sqrt{2}}\partial_z+\frac{1}{\sqrt{2}\,s_0}z.
\end{aligned} \tag{8}$$

They commute with each other except for the cases

$$[a,a^\dagger]=1,\quad [b,b^\dagger]=1,\quad [c,c^\dagger]=1. \tag{9}$$

The transformation (8) preserves the canonical properties of the phase space, including the commutation relations for the momentum and position operators. Therefore, it is symplectic.[20]

The symplectic transformation casts the Hamiltonian into the form

$$\tilde{H}=\hbar\omega_+(a^\dagger a+\tfrac{1}{2})-\hbar\omega_-(b^\dagger b+\tfrac{1}{2})+\hbar\omega_z(c^\dagger c+\tfrac{1}{2}), \tag{10}$$

where $\omega_+=(\omega_c+\Omega)/2$ and $\omega_-=(\omega_c-\Omega)/2$ are called the modified cyclotron frequency and the magnetron frequency, respectively. The negative sign in Eq. (10) reveals an inverted oscillator in the system, which in principle could lead to an instability in the presence of radiation. However, in practical situations this energy loss is controlled by ensuring $\omega_+\gg\omega_-$, so particles may be trapped "indefinitely."[18]

For particles with spin $\frac{1}{2}$, a term H' must be added to the Hamiltonian (3),

$$H'\equiv-\vec{\mu}\cdot\mathbf{B}=-\frac{g}{4}\hbar\omega_c\sigma_3, \tag{11}$$

where g is the Landé factor relating the spin to the magnetic dipole moment and σ_3 is the third Pauli matrix. The operators $f\equiv(\sigma_1+i\sigma_2)/2$ and $f^\dagger\equiv(\sigma_1-i\sigma_2)/2$ have one nonzero anticommutation relation,

$$\{f,f^\dagger\}\equiv ff^\dagger+f^\dagger f=1, \tag{12}$$

and they provide a formalism for describing the spin degree of freedom. The additional term in the Hamiltonian is $H'=\hbar\omega_g(f^\dagger f-\frac{1}{2})$, where $\omega_g=|g|\omega_c/2$. The sign of this term assumes $gq>0$.

Combining the bosonic and fermionic degrees of freedom we obtain the full Hamiltonian $H\equiv\tilde{H}+H'$ in operator form:

$$H=\hbar\omega_+(a^\dagger a+\tfrac{1}{2})-\hbar\omega_-(b^\dagger b+\tfrac{1}{2})+\hbar\omega_z(c^\dagger c+\tfrac{1}{2})+\hbar\omega_g(f^\dagger f-\tfrac{1}{2}). \tag{13}$$

The basis states for this problem can be denoted by $|N_a,N_b,N_c,N_f\rangle$, where $N_a,N_b,N_c \in\{0,1,2,\ldots\}$ are the eigenvalues of the number operators $a^\dagger a$, $b^\dagger b$, and $c^\dagger c$, and where $N_f \in\{0,1\}$ is the eigenvalue of $f^\dagger f$.

The energy eigenvalues of the system follow from Eq. (13):

$$E(N_a,N_b,N_c,N_f;\omega_c,\omega_z,g)/\hbar\equiv\omega_+(N_a+\tfrac{1}{2})-\omega_-(N_b+\tfrac{1}{2})+\omega_z(N_c+\tfrac{1}{2})+\omega_g(N_f-\tfrac{1}{2}). \tag{14}$$

The quantum numbers used here are related to the ones in Eq. (5) by $N_a=(N-\hat{M})/2$, $N_b=(N+\hat{M})/2$, and $N_c=\hat{K}$.

The relative values of the frequencies in Eq. (14) play an important part in the superalgebra structures considered later in this work. To this end, it is useful to define the ratio σ of the cyclotron and axial frequencies,

$$\sigma\equiv\omega_c/\omega_z=\left(\frac{qB^2d^2}{mV}\right)^{1/2}. \tag{15}$$

This parameter contains information about the relative values of B and V. For experiments with single trapped electrons, typical values[18] are $d\simeq 0.3$ cm, $B\simeq 6$ T, and $V\simeq 10$ V, giving $\sigma\simeq 3\times 10^3$. In this limit of $\sigma\gg 1$, the motion of the trapped particle is dominated by its interaction with the magnetic field, and Eq. (14) becomes

$$\lim_{\sigma\to\infty}E(N_a,N_b,N_c,N_f;\omega_c,\omega_z,g)=\hbar\omega_c\left[\left(N_a+\frac{1}{2}gN_f\right)-\frac{1}{2}\left(\frac{g-2}{2}\right)\right]. \tag{16}$$

For experiments with single trapped protons, typical values[18] are $d\simeq 0.1$ cm, $B\simeq 5$ T, and $V\simeq 50$ V, giving the lower value $\sigma\simeq 8$. As σ is decreased, the confining effect of the magnetic field is weakened, and trapping becomes impractical when $\sigma=\sqrt{2}$. This corresponds to the excluded case $k=0$. Exceptional measurement precisions are possible: for trapped protons, cyclotron-frequency precisions are at the 90 parts per trillion level,[4] making it feasible to probe minuscule effects such as Lorentz violation.[21]

III. DEGENERACY SUPERALGEBRAS AND FREQUENCY EQUALITIES

The algebraic structures that arise for the single-particle Penning trap are superalgebras because both fermionic and bosonic operators are involved. We focus on *degeneracy* superalgebras formed from operators that commute with the Hamiltonian, thereby linking degenerate eigenstates.

All the symmetries we consider are based on the Hamiltonian (13). Superalgebras arise for special values of the two parameters g and σ, which in turn determine the four characteristic frequencies $\omega_\pm$, ω_z, and ω_g up to an overall factor. As an illustrative example, consider the case of $g=\frac{2}{3}$ and $\sigma=\frac{3}{2}$. The Penning-trap Hamiltonian is

$$H/\hbar\omega_z=(a^\dagger a+c^\dagger c+1)-\tfrac{1}{2}(b^\dagger b-f^\dagger f+1), \tag{17}$$

and there are two distinct frequencies, $\omega_+=\omega_z=2\omega_-=2\omega_g$. The generator $b^\dagger f$ increases N_b by one unit while decreasing N_f by the same amount. It commutes with the Hamiltonian because of the equality of ω_g and ω_-.

In the most general case, $\omega_\pm$, ω_z, and ω_g are distinct. There are four generators constructed from quadratic combinations of creation and annihilation operators that commute with the Hamiltonian: $a^\dagger a$, $b^\dagger b$, $c^\dagger c$, and $f^\dagger f$. They generate an Abelian algebra $\mathrm{u}(1)\times\mathrm{u}(1)\times\mathrm{u}(1)\times\mathrm{u}(1)$ and form a complete set of commuting operators. Their interpretation as constants of the motion is considered in the next section. The generators of this Abelian algebra commute with the Hamil-

tonian and with any other degeneracy operators regardless of the values of g and σ. Therefore, all the degeneracy superalgebras considered below contain this four-dimensional central algebra.

Even with four distinct frequencies, degeneracies in the energies can occur. Consider the case of $\sigma=\frac{9}{4}$ and $g=\frac{2}{3}$. The corresponding Hamiltonian is

$$H/\hbar\omega_z=2(a^\dagger a+\tfrac{1}{2})-\tfrac{1}{4}(b^\dagger b+\tfrac{1}{2})+(c^\dagger c+\tfrac{1}{2})+\tfrac{3}{4}(f^\dagger f-\tfrac{1}{2}). \tag{18}$$

The point is that the associated frequencies are all rational multiples of each other. By taking combinations higher than quadratic in the creation or annihilation operators, generators can be constructed that commute with the Hamiltonian. Take, for example, the operator $a^\dagger c^2$. It increases N_a by one unit and decreases N_c by two units. This ensures commutation with the Hamiltonian because the associated frequencies ω_+ and ω_z are in the ratio 2:1. Other generators that commute with this Hamiltonian are $a(c^\dagger)^2$, $(b^\dagger)^4c^\dagger$, b^4c, ab^8, $a^\dagger(b^\dagger)^8$, and $bcf^\dagger$. A detailed study of the algebraic structures associated with cubic and higher combinations of creation or annihilation operators lies beyond the scope of the present work.

Next, consider the case of three distinct frequencies. For a superalgebra to arise, ω_g must be equated with another frequency. We give a few examples. For $\sigma=\frac{9}{4}$ and $g=\frac{2}{9}$, we find that the ratio $\omega_+:\omega_-:\omega_z:\omega_g$ is 8 : 1 : 4 : 1, so that $\omega_g=\omega_-$. For $\sigma=\frac{11}{6}$ and $g=\frac{18}{11}$, the frequency ratio is 9 : 2 : 6 : 9, so that $\omega_g=\omega_+$. For $\sigma=\frac{9}{4}$ and $g=\frac{8}{9}$, the frequency ratio is 8 : 1 : 4 : 4, so that $\omega_g=\omega_z$. The superalgebras that arise are all isomorphic and are discussed in Sec. V.

Next, consider ways in which the single-particle Penning-trap system can have two distinct characteristic frequencies in a rational ratio. Of these, we focus on the simplest possible ratio, 2:1. It turns out that there are only two cases. One arises for $g=\frac{2}{3}$ and $\sigma=\frac{3}{2}$ and the corresponding Hamiltonian is given in Eq. (17). This case is considered in Sec. VI. The other arises for $\sigma=\frac{3}{2}$ and $g=\frac{4}{3}$. It is the intersection point of the curves ω_+, ω_z, and ω_g as functions of σ, and is illustrated in Fig. 1. For this case, the frequencies are $\omega_+=\omega_z=\omega_g=2\omega_-$ and the associated supersymmetries are considered in detail in Sec. VII.

It is not possible to equate all four frequencies to yield a single characteristic frequency for the system. This can be seen in Fig. 1, which shows that ω_z cannot equal ω_-.

The two cases with two distinct characteristic frequencies are special. They represent the largest possible superalgebras that can be constructed from quadratic generators for the single-particle Penning trap. Both cases have $\sigma=\frac{3}{2}$, but differ in the values of g.

IV. CONSTANTS OF THE MOTION FOR THE SUPERSYMMETRIC CONFIGURATION

For the supersymmetric point $\sigma=\frac{3}{2}$, the Hamiltonian can be written in terms of four constants of the motion H_ρ, H_ϕ, H_z, and H_f to be defined next:

$$H=H_\rho+H_\phi+H_z+H_f. \tag{19}$$

These operators have simple physical interpretations.

The first one is the energy operator of a harmonic oscillator in the xy plane with frequency $\omega_z/4$:

$$\begin{aligned} H_\rho &\equiv -\frac{\hbar^2}{2m}\left(\partial_\rho^2+\frac{1}{\rho}\partial_\rho+\frac{1}{\rho^2}\partial_\phi^2\right)+\frac{1}{2}m\left(\frac{\omega_z}{4}\right)^2\rho^2 \\ &=\frac{\hbar\omega_z}{4}(a^\dagger a+b^\dagger b+1). \end{aligned} \tag{20}$$

The operator H_ϕ is a rotational energy about the z axis:

$$H_\phi\equiv\tfrac{1}{2}\hbar\omega_c i\partial_\phi=-\tfrac{1}{2}\omega_c L_z, \tag{21}$$

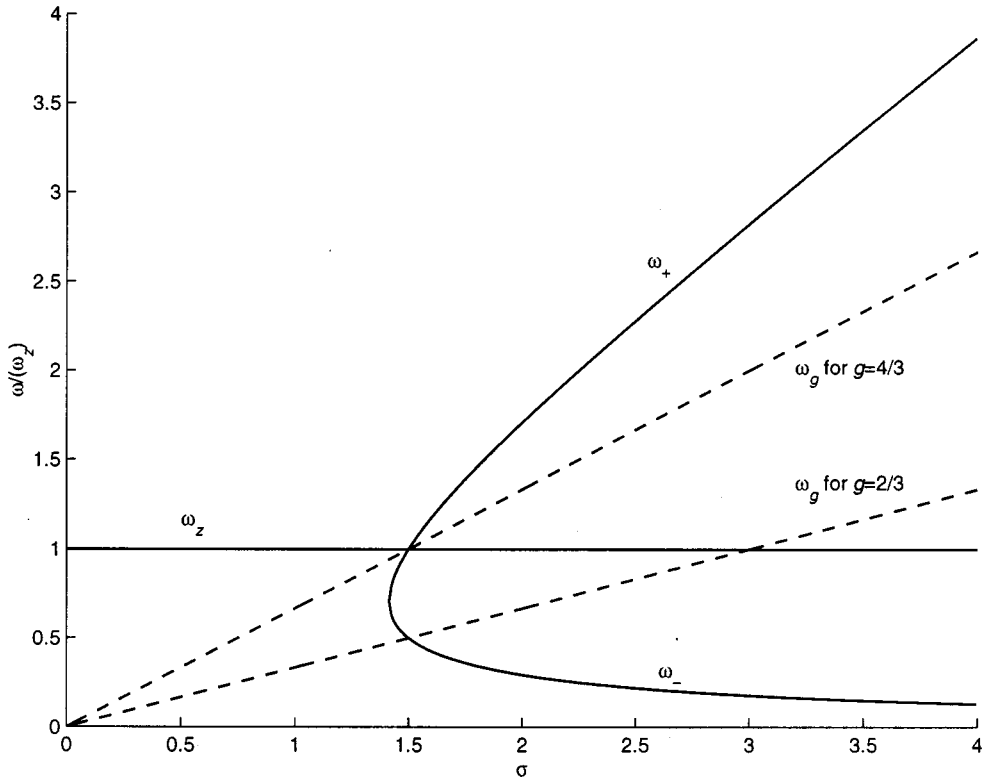

FIG. 1. The four Penning-trap frequencies ω_+, ω_-, ω_g, and ω_z as functions of the parameter $\sigma=\omega_c/\omega_z$. The dashed lines show ω_g for $g=\frac{4}{3}$ and $g=\frac{2}{3}$. For $g=\frac{4}{3}$, there are three equal frequencies $\omega_+=\omega_z=\omega_g=2\omega_-$ at the supersymmetric point $\sigma=\frac{3}{2}$. For $g=\frac{3}{2}$, there are two pairs of distinct equal frequencies at the supersymmetric point. The frequencies ω_+ and ω_- have infinite slopes where they meet at $\sigma=2^{1/2}$.

where $\omega_c=3\omega_z/2$. This term has negative eigenvalues for L_z in the $+z$ direction. This is consistent with the presence of an inverted harmonic oscillator in the Penning trap. The angular momentum about the z axis can be expressed in terms of the creation and annihilation operators[22] as

$$L_z=\hbar(b^\dagger b-a^\dagger a). \tag{22}$$

The operator H_z is the energy operator of a harmonic oscillator with frequency ω_z on the z axis:

$$H_z\equiv-\frac{\hbar^2}{2m}\partial_z^2+\frac{1}{2}m\omega_z^2z^2=\hbar\omega_z\left(c^\dagger c+\frac{1}{2}\right). \tag{23}$$

The operator H_f is the energy operator for the splitting between the two spin projections onto the z axis:

$$H_f\equiv\hbar\omega_g(f^\dagger f-\tfrac{1}{2}). \tag{24}$$

The four operators H_ρ, H_ϕ, H_z, and H_f form an alternative complete set of commuting operators for the single-particle Penning trap. They form a basis of the Abelian center of all the degeneracy superalgebras for this system, and their associated energies are independent of each other.

V. THREE DISTINCT FREQUENCIES

For this case, ω_g must equal one of the other frequencies and the remaining two frequencies must each be distinct from this value and from each other. This can occur in numerous ways. As an example, consider the case with $\sigma=\frac{11}{6}$ and $g=\frac{18}{11}$ mentioned in Sec III. The Hamiltonian is

$$H/\hbar\omega_z=\tfrac{3}{2}(a^\dagger a+f^\dagger f)-\tfrac{1}{3}(b^\dagger b+\tfrac{1}{2})+(c^\dagger c+\tfrac{1}{2}). \tag{25}$$

Define the operators

$$\begin{aligned} J&\equiv a^\dagger a+f^\dagger f,\\ \overline{J}&\equiv a^\dagger a-f^\dagger f+1,\\ F_{+1}&\equiv a^\dagger f,\\ F_{-1}&\equiv a f^\dagger. \end{aligned} \tag{26}$$

Note from Eq. (8) that they depend on the value of k, and that for this case $k=\sqrt{\sigma^2-2}/\sigma=\frac{7}{11}$. They commute with the Hamiltonian and generate a superalgebra. The only nonzero relations are

$$[\overline{J},F_{\pm1}]=\pm 2F_{\pm1},\quad \{F_{+1},F_{-1}\}=J. \tag{27}$$

This algebra has a nontrivial ideal spanned by $J,F_{\pm1}$ and so is not simple. The ideal is the nilpotent superalgebra su$(1|1)$ with Lie part u(1) generated by J. The operator $\overline{J}$ does not commute with the odd operators $F_{\pm1}$, so we denote the superalgebra by u$(1)\oslash$su$(1|1)$ to indicate the absence of a direct product.

The full degeneracy algebra for the Hamiltonian Eq. (25) includes elements which complete the basis of the center. The structure is u$(1)\times$u$(1)\times$u$(1)\oslash$su$(1|1)$, generated by $b^\dagger b$, $c^\dagger c$, $\overline{J}$, and $\{J,F_{\pm1}\}$.

Given a pair $F_{\pm1}$ of mutually Hermitian-conjugate generators, (self-)Hermitian generators are obtained by the combinations $T_1=(F_{+1}+F_{-1})/2$ and $T_2=i(F_{+1}-F_{-1})/2$. We define non-Hermitian ladder generators because they are useful for calculations. The actual Hermitian generators within the superalgebras can always be constructed by this method.

Another way to obtain a supersymmetry with three distinct frequencies in the system is to set $\omega_g=\omega_-$. Consider the example mentioned in Sec. III with $g=\frac{2}{9}$ and $\sigma=\frac{9}{4}$, which corresponds to $k=\frac{7}{9}$. The Hamiltonian is

$$H/\hbar\omega_z=2(a^\dagger a+\tfrac{1}{2})-\tfrac{1}{4}(b^\dagger b-f^\dagger f+1)+(c^\dagger c+\tfrac{1}{2}). \tag{28}$$

We define four operators that commute with the Hamiltonian:

$$\begin{aligned} K&\equiv b^\dagger b+f^\dagger f,\\ \overline{K}&\equiv b^\dagger b-f^\dagger f+1,\\ F_{+2}&\equiv b^\dagger f^\dagger,\\ F_{-2}&\equiv bf. \end{aligned} \tag{29}$$

They generate a superalgebra with nonzero relations

$$[K,F_{\pm2}]=\pm 2F_{\pm2},\quad \{F_{+2},F_{-2}\}=\overline{K}. \tag{30}$$

Comparison of these relations with those in Eq. (27) shows that the two algebras are isomorphic. The full superalgebra for this example is $u(1)\times u(1)\times u(1)\oslash su(1|1)$, generated by $a^\dagger a$, $c^\dagger c$, K, and $\{\overline{K},F_{\pm 2}\}$.

One might expect different superalgebras to arise for the Hamiltonians (25) and (28) because of the opposite signs of $a^\dagger a$ and $b^\dagger b$ relative to $f^\dagger f$. However, this is not the case, and the isomorphism relating the operators in Eqs. (26) and (29) is given explicitly by

$$a\leftrightarrow b, \quad a^\dagger\leftrightarrow b^\dagger, \quad f\leftrightarrow f^\dagger. \tag{31}$$

It follows from this observation that the *only* superalgebra that can arise for three distinct frequencies is $u(1)\oslash su(1|1)$. In all cases of this type, the full symmetry is $u(1)\times u(1)\times u(1)\oslash su(1|1)$.

This supersymmetry is relevant to experiments with electrons or positrons, where $\sigma\gg 1$ and $g\simeq 2$. Taking $g=2$, the Hamiltonian for $\sigma\gg 1$ is

$$H/\hbar\approx\omega_c(a^\dagger a+f^\dagger f)+\omega_z(c^\dagger c+\tfrac{1}{2})-\omega_-(b^\dagger b+\tfrac{1}{2}), \tag{32}$$

with $\omega_c\gg\omega_z\gg\omega_-$. However, the supersymmetry is broken because in the physical situation g is slightly larger than 2, so ω_+ is always slightly less than ω_g no matter how strong the magnetic field. The value of the g factor determines the degree to which this supersymmetry is broken in the strong-B limit. In this regime, the particle experiences a uniform magnetic field and has associated supercoherent states.[23] If g were exactly equal to 2, the anomaly $a_e=(g-2)/2\simeq 10^{-3}$ would be zero, and the spin-up and spin-down ladders would have no relative energy shift.[24]

VI. TWO PAIRS OF EQUAL FREQUENCIES: $\omega_+=\omega_z=2\omega_-=2\omega_g$

For $g=\frac{2}{3}$ and $\sigma=\frac{3}{2}$, the Penning-trap Hamiltonian is given in Eq. (17). Four linearly independent generators constructed from a, $a^\dagger$, c, and $c^\dagger$ that commute with this Hamiltonian are

$$\begin{gathered}\overline{L}\equiv a^\dagger a+c^\dagger c+1,\\ L\equiv\tfrac{1}{2}(a^\dagger a-c^\dagger c), \quad E_{+2}\equiv a^\dagger c, \quad E_{-2}\equiv ac^\dagger.\end{gathered} \tag{33}$$

The generator $\overline{L}$ commutes with the other three, forming a $u(1)$ subalgebra. The generators E_{+2} and E_{-2} are Hermitian conjugates and are themselves non-Hermitian. They are ladder operators, which together with L give the Lie algebra $so(3)$:

$$[L,E_{\pm 2}]=\pm E_{\pm 2}, \quad [E_{+2},E_{-2}]=2L. \tag{34}$$

The remaining generators of the superalgebra are K, $\overline{K}$, and $F_{\pm 2}$ defined in Eq. (29), but with $k=\frac{1}{3}$. They span the superalgebra $u(1)\oslash su(1|1)$ with nonzero relations given in Eq. (30).

Combining the relations of Eqs. (34) and (30), the full degeneracy superalgebra for the Hamiltonian in (17) is $u(1)\times so(3)\times u(1)\oslash su(1|1)$, generated by $\overline{L}$, $\{L,E_{\pm 2}\}$, $\overline{K}$, and $\{K,F_{\pm 2}\}$. It is implicit that for this case $k=\frac{7}{9}$ in the definitions (29).

For $gq<0$, the second term of the Hamiltonian (17) becomes $-(b^\dagger b+f^\dagger f)/2$. A full set of generators that commute with the Hamiltonian is obtained from Eq. (33) and by making the replacements $f\rightarrow f^\dagger$ and $f^\dagger\rightarrow f$ in Eq. (29). This operation is an automorphism, leaving the relations (30) and (34) unchanged.

From a given state $|N_a,N_b,N_c,N_f\rangle$, the elements defined in Eqs. (29) and (33) generate all the states in the degenerate subspace. The Lie algebra $so(3)$ generates states differing in the N_a and N_c eigenvalues. For example,

$$E_{+2}|N_a,N_b,N_c,N_f\rangle\sim|N_a+1,N_b,N_c-1,N_f\rangle. \tag{35}$$

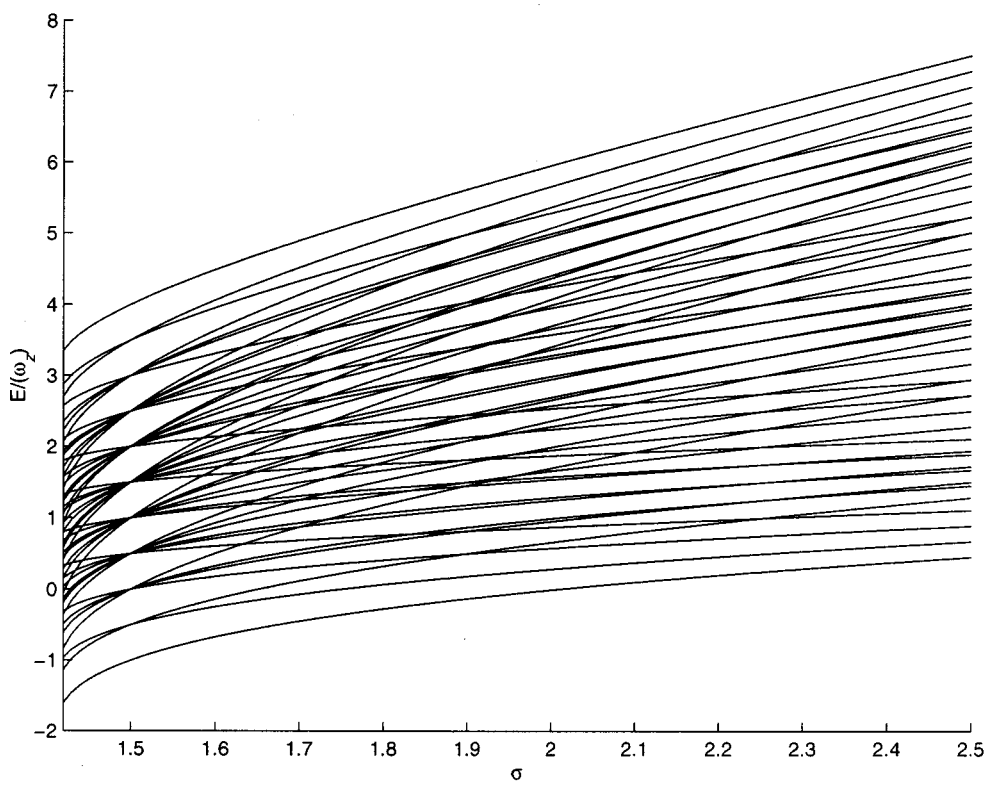

FIG. 2. Penning-trap energies as a function of σ for various states, with $g=\frac{2}{3}$. There are conspicuous degeneracies of the levels at the supersymmetric point $\sigma=\frac{3}{2}$, arising from the superalgebra structure discussed in Sec. VI. Another degeneracy occurs at $\sigma=2.25$. In this plot, $\hbar=1$.

In contrast, the subsuperalgebra su$(1|1)$ acts to give states differing only in N_b and N_f. For example,

$$F_{+2}|N_a,N_b,N_c,N_f\rangle\sim((N_f+1)\text{mod }2)|N_a,N_b+1,N_c,(N_f+1)\text{mod }2\rangle. \tag{36}$$

Insight into the physical implications of the superalgebra can be gained from Fig. 2. It plots the energy levels of the Penning trap versus σ for the states with quantum numbers $N_a=0,1,2$, $N_b=0,...,3$, $N_c=0,1$, and $N_f=0,1$. At $\sigma=\frac{3}{2}$, the Hamiltonian has the form of Eq. (17). The coefficients of the two terms show that the frequencies are in the ratio 2:1. This gives the uniform spacing of the energy levels and creates the sharply defined crossing features at this supersymmetry point on the plot.

Figure 2 also reveals the set of evenly spaced degenerate levels at $\sigma=2.25$, for which the Hamiltonian has the form in Eq. (18).

The operators L, $\overline{L}$, K, and $\overline{K}$ form a complete set of commuting operators for the system. They can be expressed in terms of the more physical operators defined in Sec. IV:

$$\hbar\omega_z\overline{L}=2H_\rho+\tfrac{2}{3}H_\phi+H_z, \tag{37}$$

$$\hbar\omega_z L=H_\rho+\tfrac{1}{3}H_\phi-\tfrac{1}{2}H_z, \tag{38}$$

$$\hbar\omega_z\overline{K}=2H_\rho-\tfrac{2}{3}H_\phi-2H_f, \tag{39}$$

$$\hbar\omega_z K=2H_\rho+\tfrac{2}{3}H_\phi+2H_f. \tag{40}$$

VII. THREE EQUAL FREQUENCIES: $\omega_+=\omega_z=\omega_g=2\omega_-$

Three frequencies can be equated by setting $g=\frac{4}{3}$ and $\sigma=\frac{3}{2}$, giving the Hamiltonian

$$H/\hbar\omega_z=(a^\dagger a+c^\dagger c+f^\dagger f+\tfrac{1}{2})-\tfrac{1}{2}(b^\dagger b+\tfrac{1}{2})\equiv M-\tfrac{1}{2}\overline{M}. \tag{41}$$

The generators M and $\overline{M}$, defined by the expressions in parentheses, commute with each other and with H. They therefore form an independent $\mathrm{u}(1)\times\mathrm{u}(1)$ subalgebra of the full degeneracy superalgebra.

In addition to M and $\overline{M}$, there are four independent even elements given by

$$\tilde{L}\equiv\tfrac{1}{2}(a^\dagger a+c^\dagger c)+f^\dagger f \tag{42}$$

and by $L,E_{\pm2}$ defined in Eq. (33). The generator $\tilde{L}$ commutes with the even elements $L,E_{\pm2}$, which in turn satisfy the commutation relations (34) for the compact Lie algebra su(2).

There are four odd elements that commute with the Hamiltonian: $F_{\pm1}$ as defined in Eq. (26) but with $k=\frac{1}{3}$, and

$$F_{+3}\equiv c^\dagger f,\quad F_{-3}\equiv c f^\dagger. \tag{43}$$

Their nonzero anticommutation relations are

$$\{F_{+1},F_{-1}\}=\tilde{L}+L,\quad \{F_{+3},F_{-3}\}=\tilde{L}-L,\quad \{F_{\pm1},F_{\mp3}\}=E_{\pm2}, \tag{44}$$

and their nonzero commutation relations with the even elements are

$$\begin{aligned}
&[\tilde{L},F_{\pm1}]=\mp\tfrac{1}{2}F_{\pm1},\quad [\tilde{L},F_{\pm3}]=\mp\tfrac{1}{2}F_{\pm3},\\
&[L,F_{\pm1}]=\pm\tfrac{1}{2}F_{\pm1},\quad [L,F_{\pm3}]=\mp\tfrac{1}{2}F_{\pm3},\\
&[E_{\pm2},F_{\pm3}]=\pm F_{\pm1},\quad [E_{\pm2},F_{\mp1}]=\mp F_{\mp3}.
\end{aligned} \tag{45}$$

The superalgebra with generators given in Eqs. (33), (42), and (43) is $\mathrm{su}(2|1)$, with Lie part $\mathrm{u}(1)\times\mathrm{su}(2)$. The first component is generated by $\tilde{L}$ and the second by $\{L,E_{\pm2}\}$. The action of these generators on the eigenstates of the Hamiltonian is similar to that displayed in Eqs. (35) and (36), except that here the values of N_a, N_c, and N_f are affected.

The full degeneracy structure of the Hamiltonian (41) is $\mathrm{u}(1)\times\mathrm{u}(1)\times\mathrm{su}(2|1)$. It has three subalgebras, generated by the sets $\{\overline{M}\}$, $\{M\}$, and $\{L,\tilde{L},E_{\pm2},F_{\pm1},F_{\pm3}\}$.

The Hamiltonian for $gq<0$ is found by replacing $(f^\dagger f-\frac{1}{2})\to-(f^\dagger f-\frac{1}{2})$ in (41). To obtain the generators commuting with this Hamiltonian, the replacements $f\to f^\dagger$ and $f^\dagger\to f$ are made in the definitions for all the operators. This automorphism leaves unchanged the superalgebra relations. Thus, the algebraic structure is again independent of the sign of gq for the trapped particle.

Figure 3 plots the energy levels versus σ for the states with quantum numbers $N_a=0,1,2$, $N_b=0,1,2$, $N_c=0,1$, and $N_f=0,1$. Because the frequencies are in a rational ratio, the supersymmetry point has uniformly spaced crossings at $\sigma=\frac{3}{2}$.

The operators $\overline{M}$, M, $\tilde{L}$, and L form a complete set of commuting operators for the system. They can be expressed in terms of the alternative basis of Sec. IV:

$$\hbar\omega_z\overline{M}=2H_\rho-\tfrac{2}{3}H_\phi, \tag{46}$$

$$\hbar\omega_z M=2H_\rho+\tfrac{2}{3}H_\phi+H_z+H_f, \tag{47}$$

$$\hbar\omega_z\tilde{L}=H_\rho+\tfrac{1}{3}H_\phi+\tfrac{1}{2}H_z+H_f, \tag{48}$$

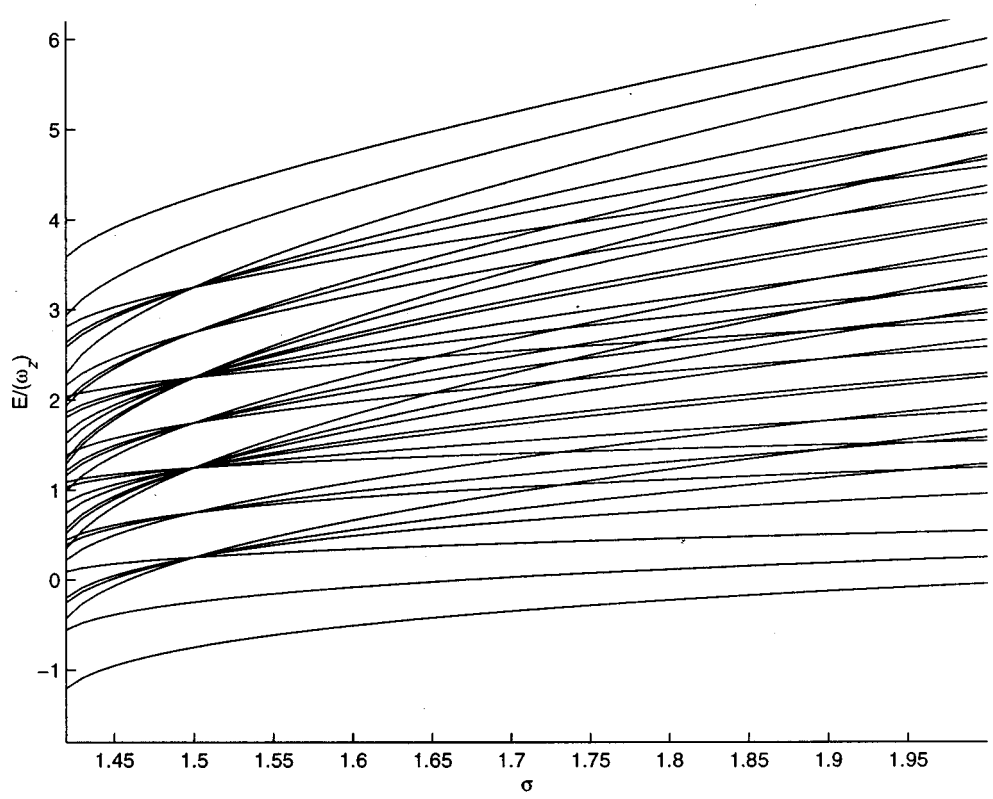

FIG. 3. Penning-trap energies as a function of σ for various states, with $g=\frac{4}{3}$. The evenly spaced crossings at the supersymmetric point $\sigma=\frac{3}{2}$ are discussed in Sec. VII. For this plot, $\hbar=1$.

$$\hbar\omega_z L = H_\rho + \tfrac{1}{3}H_\phi - \tfrac{1}{2}H_z\,. \tag{49}$$

These expressions can be inverted. For example, the spin-splitting operator H_f can be shown to be $H_f=\hbar\omega_z(2\tilde{L}-M)$.

VIII. HYPOTHETICAL CASE OF FOUR EQUAL FREQUENCIES

The largest possible degeneracy superalgebra in a system of the form of (13) would arise if all the frequencies could be set equal. No choices of g and σ allow this in the Penning trap, as can be seen from Fig. 1. Nonetheless, it is of interest to consider the degeneracy superalgebra that would arise from a Hamiltonian of the form

$$H_0 \equiv a^\dagger a - b^\dagger b + c^\dagger c + f^\dagger f, \tag{50}$$

where f and $f^\dagger$ are fermionic and the other operators are bosonic, because this superalgebra contains all the superalgebras discussed in Secs. V–VII as subsuperalgebras. This superalgebra is $\mathrm{u}(1)\times\mathrm{su}(2,1|1)$, as shown later in this work.

The Hamiltonian H_0 forms an independent u(1) subalgebra by definition. There are eight other independent generators commuting with this Hamiltonian that are constructed only from bosonic operators. Expressed in the Cartan–Weyl basis, they are $E_{\pm 2}$ already defined in Eq. (33), and

$$H_1 \equiv b^\dagger b + c^\dagger c + 1, \quad H_2 \equiv a^\dagger a + b^\dagger b + 1,$$

$$E_{+1} \equiv b^\dagger c^\dagger, \quad E_{-1} \equiv bc, \tag{51}$$

$$E_{+3} \equiv a^\dagger b^\dagger, \quad E_{-3} \equiv ab,$$

and they satisfy the nonzero commutation relations

$$\begin{gathered}
[H_1, E_{\pm 1}] = \pm 2E_{\pm 1}, \quad [H_1, E_{\pm 2}] = \mp E_{\pm 2}, \quad [H_1, E_{\pm 3}] = \pm E_{\pm 3}, \\
[H_2, E_{\pm 1}] = \pm E_{\pm 1}, \quad [H_2, E_{\pm 2}] = \pm E_{\pm 2}, \quad [H_2, E_{\pm 3}] = \pm 2E_{\pm 3}, \\
[E_{\pm 2}, E_{\mp 3}] = \mp E_{\mp 1}, \quad [E_{\pm 3}, E_{\mp 1}] = \mp E_{\pm 2}, \quad [E_{\pm 1}, E_{\pm 2}] = \mp E_{\pm 3}, \\
[E_{+1}, E_{-1}] = -H_1, \quad [E_{+2}, E_{-2}] = -H_1 + H_2, \quad [E_{+3}, E_{-3}] = -H_2.
\end{gathered} \tag{52}$$

These generators provide a description of the Lie algebra su(2,1).

Including the two fermionic operators f and $f^\dagger$ allows the introduction of seven more generators that commute with the Hamiltonian (50), of which one,

$$H_3 \equiv a^\dagger a - b^\dagger b + c^\dagger c + 3f^\dagger f - 1, \tag{53}$$

is even and commutes with the eight other even generators. The six others are odd generators defined earlier: $F_{\pm 1}$, $F_{\pm 2}$, and $F_{\pm 3}$. They satisfy anticommutation relations, of which the only nonzero ones are

$$\begin{gathered}
\{F_{\pm 2}, F_{\pm 3}\} = E_{\pm 1}, \qquad \{F_{\pm 1}, F_{\mp 3}\} = E_{\pm 2}, \qquad \{F_{\pm 1}, F_{\pm 2}\} = E_{\pm 3}, \\
\{F_{+1}, F_{-1}\} = -\tfrac{1}{3}H_1 + \tfrac{2}{3}H_2 + \tfrac{1}{3}H_3, \\
\{F_{+2}, F_{-2}\} = \tfrac{1}{3}H_1 + \tfrac{1}{3}H_2 - \tfrac{1}{3}H_3, \\
\{F_{+3}, F_{-3}\} = \tfrac{2}{3}H_1 - \tfrac{1}{3}H_2 + \tfrac{1}{3}H_3.
\end{gathered} \tag{54}$$

Note that these anticommutators yield elements within the even part of the superalgebra, as expected. Commutation relations between even and odd generators produce generators in the odd part of the superalgebra. The nonzero cases are

$$\begin{gathered}
[H_3, F_{\pm 1}] = \mp 2F_{\pm 1}, \quad [H_3, F_{\pm 2}] = \pm 2F_{\pm 2}, \quad [H_3, F_{\pm 3}] = \mp 2F_{\pm 3}, \\
[H_1, F_{\pm 2}] = \pm F_{\pm 2}, \quad [H_1, F_{\pm 3}] = \pm F_{\pm 3}, \\
[H_2, F_{\pm 1}] = \pm F_{\pm 1}, \quad [H_2, F_{\pm 2}] = \pm F_{\pm 2}, \\
[E_{\pm 1}, F_{\mp 2}] = \mp F_{\pm 3}, \quad [E_{\pm 1}, F_{\mp 3}] = \mp F_{\pm 2}, \\
[E_{\pm 3}, F_{\mp 1}] = \mp F_{\pm 2}, \quad [E_{\pm 3}, F_{\mp 2}] = \mp F_{\pm 1},
\end{gathered} \tag{55}$$

and the last two relations of (45). The fifteen-dimensional superalgebra su(2,1|1) considered here has Lie subalgebra u(1)$\times$su(2,1), with the first component generated by H_3. The su(2,1) subalgebra has eight dimensions, with basis given in Eq. (51).

Including the u(1) algebra generated by H_0, the full degeneracy superalgebra for the Hamiltonian (50) is u(1)$\times$su(2,1|1).

IX. PHASE-SPACE SUPERALGEBRA

The degeneracy superalgebras considered above are subsuperalgebras of a still larger superalgebra $\mathcal{A}$, where the generators are formed from *all* possible independent quadratic combinations of creation or annihilation operators. This algebra is not a degeneracy superalgebra, although it contains the degeneracy superalgebras mentioned in the previous sections. In the superalgebra $\mathcal{A}$,

TABLE I. Penning-trap superalgebras for the supersymmetric configuration $\sigma=\frac{3}{2}$. The particle g factor is given in the first column, and the four frequencies in units of ω_z are given in the next four columns. The algebraic structures found and the sections where they are discussed are given in the final two columns. The symbol $\oslash$ is defined in Sec. V. The bottom row represents the hypothetical case with four equal frequencies.

g	ω_+	ω_-	ω_z	ω_g	Structure	Section
$\frac{2}{9}$	2	$\frac{1}{4}$	1	$\frac{1}{4}$	$u(1)\times u(1)\times u(1)\oslash su(1\|1)$	V
$\frac{2}{3}$	1	$\frac{1}{2}$	1	$\frac{1}{2}$	$u(1)\times so(3)\times u(1)\oslash su(1\|1)$	VI
$\frac{4}{3}$	1	$\frac{1}{2}$	1	1	$u(1)\times u(1)\times su(2\|1)$	VII
	1	1	1	1	$u(1)\times su(2,1\|1)$	VIII

there are 12 odd generators formed by pairing each of the six bosonic operators $a,a^\dagger,b,b^\dagger,c,c^\dagger$, with each of the fermionic operators $f,f^\dagger$. There are 21 even generators formed from pairs of bosonic operators including, for example, $a^\dagger a^\dagger,a^\dagger b,bb,bc^\dagger$. These generate an $sp(6)$ subalgebra. A further even generator, $f^\dagger f$, is formed from the fermionic operators. Taken together, the 34 generators define the superalgebra $osp(2|6)$, which has even part $sp(6)\times so(2)$.

The $osp(2|6)$ superalgebra $\mathcal{A}$ is not unique to the Penning-trap system, since it would arise for any combination of signs for the number operators in the Hamiltonian (13). The point is that $\mathcal{A}$ exists even before a potential for the physical problem is defined. The only requirement for $\mathcal{A}$ to be a relevant algebra is that the system describe a single fermion in a phase space with three space and three momentum dimensions. Thus, the superalgebra $osp(2|6)$ describes the properties of the phase space for the problem.

The Hamiltonian for the Penning trap is fixed by specifying the parameters ω_c, ω_z, and g. For each of the cases in Secs. V–VII, the degeneracy superalgebra is a subsuperalgebra of the phase-space superalgebra. We therefore find a hierarchy of nested superalgebras: $\mathcal{A}=osp(2|6)\supset so(2,1|1)\supset\mathcal{D}$, where $\mathcal{D}$ is any of the degeneracy superalgebras of Secs. V–VII.

We have considered only structures arising from *quadratic* combinations of creation or annihilation operators. The issue of the role played by higher-order combinations, such as those commuting with Eq. (18), is related to Clifford-algebra theory[25] but lies outside the scope of this article.

X. SUMMARY AND DISCUSSION

Several superalgebras are associated with the single-particle Penning trap. The various cases depend on the gyromagnetic ratio of the trapped particle and the relative strengths of the magnetic and electric fields. This article considers the degeneracy superalgebras of operators that commute with the Hamiltonian. The relevant superalgebras are summarized in Table I.

In general, superalgebra descriptions might be expected for trap systems having energy separations between spin states equal to the separations between the bosonic oscillator levels. This guarantees the existence of odd generators that commute with the Hamiltonian. Traps in which the spin cannot be reversed, such as the TOP or Ioffe-Pritchard traps,[15] are therefore unlikely to have superalgebra structures of the type described here. Superalgebras of this kind are also unlikely for traps where the spin states are independent of a magnetic field, as is the case for the Paul trap.[15] However, supersymmetries of another type do appear in these systems.[15]

Some other issues beyond the scope of this article are of potential interest. In particular, the spectrum-generating superalgebras would be relevant to a complete study of the properties of the Penning trap. Furthermore, higher-rank combinations of operators, such as those mentioned for the $\sigma=\frac{9}{4}$ point in Fig. 1, can be expected to arise in a study of the relevant Clifford algebras.

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Quadratic algebra associated with rational Calogero-Moser models

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Classical Calogero–Moser models with rational potential are known to be superintegrable. That is, on top of the r involutive conserved quantities necessary for the integrability of a system with r degrees of freedom, they possess an additional set of $r-1$ algebraically and functionally independent globally defined conserved quantities. At the quantum level, Kuznetsov uncovered the existence of a quadratic algebra structure as an underlying key for superintegrability for the models based on A type root systems. Here we demonstrate in a universal way the quadratic algebra structure for quantum rational Calogero–Moser models based on any root systems. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1404387]

I. INTRODUCTION

Calogero–Moser models[1–3] with the rational potentials, without the harmonic confining force, have the simplest and best understood dynamical structures among models with the other types of potentials. Their superintegrability, that is the existence of $2r-1$ global, functionally independent conserved quantities (constants of motion) for a system of r degrees of freedom, is one of the most striking features. It was found at the classical level by Wojciechowski[4] and at the quantum level by Kuznetsov[5] and Ujino–Wadati–Hikami[6] for models based on the A type root systems. Kuznetsov[5] uncovered an interesting algebraic structure, the so-called *quadratic algebra* as a hidden symmetry of the superintegrability. Ujino–Wadati–Hikami[6] introduced a similar algebraic structure. The concept of superintegrability is closely related with that of *algebraic linearizability* formulated by Caseiro–Françoise[7] and developed further by Caseiro–Françoise–Sasaki[8] for the models based on any root systems. We follow the notation of our previous paper unless otherwise stated.

In this article we show, at the quantum level, that the quadratic algebra is ''universal,'' namely, it is enjoyed by all the rational Calogero–Moser models based on *any* root systems including the noncrystallographic ones. The same assertion at the classical level simply follows as the classical limit of replacing the quantum commutator by the Poisson bracket. The generators of the quadratic algebra are the above mentioned conserved quantities of the superintegrable theory. Among them, the involutive subset of r conserved quantities, which characterize the Liouville integrability of the system with r degrees of freedom, constitute the Cartan subalgebra and an ideal among the conserved quantities. Commutators among the additional conserved quantities turn out to be bi-linear (quadratic) combinations of the two types of conserved quantities. This nonlinear algebra seems to be closely related to the W-algebras,[9] extensions of the Virasoro algebra, or to the algebras related with the R-matrices of integrable theories,[10] but the precise relationship remains to be clarified.

Calogero–Moser models for any root systems were formulated by Olshanetsky and Perelomov,[11] who provided Lax pairs for the models based on the classical root systems, i.e., the A, B, C, D and BC type root systems. A universal *classical* Lax pair applicable to all the Calogero–Moser models based on any root systems including the E_8 and the noncrystallographic

root systems was derived by Bordner–Corrigan–Sasaki[12] which unified various types of Lax pairs known at that time.[13,14] A universal *quantum* Lax pair applicable to all the Calogero–Moser models based on any root systems and for degenerate potentials was derived by Bordner–Manton–Sasaki[15] which provided the basic tools for the present article.

The purpose of the present article is twofold. First, it is to derive and present the *quadratic algebra* for rational Calogero–Moser models based on any root systems in its fullest universality based on the universal Lax pair.[15] Extracting detailed information from the quadratic algebra to elucidate dynamical properties of each specific system would require formulations suitable for the particular systems. This would not be discussed here. Second, we formulate and present the quantum versions of various concepts and formulas related to the algebraic linearizability introduced and developed in Ref. 8. As has been noticed from the earliest days of Calogero–Moser models, the quantum and classical integrability are very closely related. Many formulas related to the algebraic linearizability take the same form at the classical and quantum levels, with some notable exceptions as will be mentioned in the article.

This article is organized as follows. In Sec. II we introduce the model and notations with an emphasis on the difference between the quantum and classical versions. The quantum theorem of the algebraic linearizability for the rational model is derived based on the Lax pair formalism. In Sec. III we evaluate fundamental commutation relations which are necessary for the quadratic algebra. This will be carried out with the help of the Dunkl operators, or the so-called l operators which are equivalent to the quantum L operator. The quantum theorem of the algebraic linearizability for the higher Hamiltonians of the rational model is derived. In Sec. IV the quadratic algebra for rational Calogero–Moser models is derived and presented in its fullest universality. Section V gives the quantum version of the algebraic linearizability of the rational potential model with harmonic confining force. The problem of quantum integrability of rational Calogero–Moser model with quartic interactions is not yet settled. In Sec. VI we present a partial result that the quantum equations of motion can be cast into Lax type matrix equations. The existence of quantum conserved quantities, however, does not follow from these matrix equations. The final section is for comments on the Hermiticity of the algebra generators.

II. QUANTUM CALOGERO–MOSER MODELS WITH RATIONAL POTENTIAL

Let us start with the Hamiltonian of *quantum* Calogero–Moser model with rational potential based on any root system, which could be any one of the crystallographic root systems, A_r, B_r, C_r, D_r, (BC_r), E_6, E_7, E_8, F_4 and G_2 or the noncrystallographic H_3, H_4 and $I_2(m)$, which is the dihedral root system associated with a regular m-gon. The existing works on the quadratic algebras are all for the A_r root system.[5,6,16] Let us denote by Δ a root system of rank r. The dynamical variables are the coordinates $q_i, i=1,\ldots,r$, and their canonically conjugate momenta $p_i, i=1,\ldots,r$, with the canonical commutation relations:

$$[q_j,p_k]=i\delta_{jk}, \quad [q_j,q_k]=[p_j,p_k]=0, \quad j,k=1,\ldots,r. \tag{2.1}$$

As usual the momentum operator, p_j acts as a derivative operator on a (wave) function f of q:

$$f\to p_j f: \quad (p_j f)(q)=-i\frac{\partial f(q)}{\partial q_j}, \quad j=1,\ldots,r.$$

The Hamiltonian for the *quantum* Calogero–Moser model with rational potential is very simple:

$$\mathcal{H}=\frac{1}{2}p^2+\frac{1}{2}\sum_{\rho\in\Delta_+}\frac{g_{|\rho|}(g_{|\rho|}-1)|\rho|^2}{(\rho\cdot q)^2}, \quad \Delta_+ : \text{set of positive roots}, \tag{2.2}$$

in which the real coupling constants $g_{|\rho|}>0$ are defined on orbits of the corresponding finite reflection group, i.e., they are identical for roots in the same orbit. The only difference with the

classical Hamiltonian is the coupling constant dependence, $g_{|\rho|}(g_{|\rho|}-1)$ instead of $g_{|\rho|}^2$ in the classical case. The Hamiltonian is invariant under reflections of the phase space variables about a hyperplane perpendicular to any root

$$\mathcal{H}(s_\alpha(p),s_\alpha(q))=\mathcal{H}(p,q), \quad \forall \alpha\in\Delta, \tag{2.3}$$

with the action of s_α on any vector $\gamma\in\mathbf{R}^r$ defined by

$$s_\alpha(\gamma)=\gamma-(\alpha^\vee\cdot\gamma)\alpha, \quad \alpha^\vee\equiv 2\alpha/|\alpha|^2. \tag{2.4}$$

The integrability is best understood in terms of the quantum Lax pair[15] or the Dunkl operators,[17,18] which are known to be equivalent with the Lax operator.[19] Let us choose a set of $\mathbf{R}^r$ vectors $\mathcal{R}=\{\mu^{(k)}\in\mathbf{R}^r,\ k=1,\ldots,D\}$, which form a single orbit of the Coxeter group with D elements, that is, they are permuted under the action of the Coxeter group. For example, we can choose the set of vector (minimal) weights for A_r or D_r, or the set of short (long) roots for B_r, C_r or F_4, G_2, or the set of all roots for E_6 to E_8. Then the Lax operators are $D\times D$ dimensional matrices

$$\begin{aligned} L(p,q)&=p\cdot\hat{H}+X(q), \quad X(q)=i\sum_{\rho\in\Delta_+} g_{|\rho|}\frac{\rho.\hat{H}}{\rho\cdot q}\hat{s}_\rho,\\ M(q)&=-\frac{i}{2}\sum_{\rho\in\Delta_+} g_{|\rho|}\frac{|\rho|^2}{(\rho.q)^2}(\hat{s}_\rho-I), \end{aligned} \tag{2.5}$$

consisting of operators $\{\hat{H}_j\}$, $(j=1,\ldots,r)$, $\{\hat{s}_\rho\}$ and the identity operator I. Their matrix elements are defined by

$$(\hat{H}_j)_{\mu\nu}=\mu_j\delta_{\mu\nu}, \quad (\hat{s}_\rho)_{\mu\nu}=\delta_{\mu,s_\rho(\nu)}=\delta_{\nu,s_\rho(\mu)}, \quad \mu,\nu\in\mathcal{R}. \tag{2.6}$$

The Lax operators are Coxeter covariant:

$$L(s_\alpha(p),s_\alpha(q))=\hat{s}_\alpha L(p,q)\hat{s}_\alpha, \quad M(s_\alpha(q))=\hat{s}_\alpha M(q)\hat{s}_\alpha, \tag{2.7}$$

and L is Hermitian $L^\dagger=L$ and M is anti-Hermitian $M^\dagger=-M$.

We see that the Heisenberg equations of motion are equivalent to a matrix equation[15,19]

$$\frac{dL}{dt}\equiv\dot{L}=i[\mathcal{H},L]=[L,M], \tag{2.8}$$

in which the matrix elements are quantum operators. This means that in general the *trace* of the product of two matrix operators $A(p,q)$ and $B(p,q)$ is not commutative, $\mathrm{Tr}AB\neq\mathrm{Tr}BA$, or $\mathrm{Tr}[A,B]\neq 0$, implying that $\mathrm{Tr}L^n$ is not *conserved* in quantum theory. However, thanks to the special property of the above M matrix

$$\sum_{\mu\in\mathcal{R}} M_{\mu\nu}=\sum_{\nu\in\mathcal{R}} M_{\mu\nu}=0, \tag{2.9}$$

the *total sum* of the powers of the Lax operator L defined by

$$F_j=\mathrm{Ts}(L^j)\equiv\sum_{\nu,\mu\in\mathcal{R}}(L^j)_{\mu\nu}, \quad j=0,1,\ldots,D-1, \tag{2.10}$$

is conserved:

$$\frac{d}{dt}\mathrm{Ts}(L^j)=\sum_{\mu,\nu\in\mathcal{R}}[(L^jM)_{\mu\nu}-(ML^j)_{\mu\nu}]$$

$$=\sum_{\mu,\nu,\kappa\in\mathcal{R}}[L^j_{\mu\kappa}M_{\kappa\nu}-M_{\mu\kappa}L^j_{\kappa\nu}]$$

$$=\sum_{\mu,\kappa\in\mathcal{R}}L^j_{\mu\kappa}\left(\sum_{\nu\in\mathcal{R}}M_{\kappa\nu}\right)-\sum_{\nu,\kappa\in\mathcal{R}}\left(\sum_{\mu\in\mathcal{R}}M_{\mu\kappa}\right)L^j_{\kappa\nu}=0.$$

It is easy to see from (2.7) that $\{F_j\}$'s are Coxeter invariant. These form the involutive set of conserved quantities of the theory. Not all of them are independent. As is well-known, the independent conserved quantities appear for such j as 1 plus *exponent* of the root system, (see, for example, Refs. 19 and 20). For some choice of the set of vectors $\mathcal{R}$ for some root system Δ, F_j can be vanishing for certain j's. For example, if $\mathcal{R}$ contains a vector μ and $-\mu$ at the same time, then $F_{\mathrm{odd}}\equiv 0$.

The Hamiltonian (2.2) is proportional to F_2,

$$\mathcal{H}=\frac{1}{2C_{\mathcal{R}}}F_2=\frac{1}{2C_{\mathcal{R}}}\mathrm{Ts}(L^2), \tag{2.11}$$

in which the coefficient $C_{\mathcal{R}}$ is defined by

$$\mathrm{Ts}(\hat{H}_j\hat{H}_k)=\sum_{\mu\in\mathcal{R}}\mu_j\mu_k=\delta_{jk}C_{\mathcal{R}}. \tag{2.12}$$

Following the line of argument of Ref. 8 we define

$$Q=q\cdot\hat{H},\quad G_j=\mathrm{Ts}(QL^j),\quad G_j^{(2)}=\mathrm{Ts}(Q^2L^j),\quad j=0,1,\ldots,D-1, \tag{2.13}$$

in which the last quantity Q^2L^j was introduced by Rañada.[21] Under the reflection, Q transforms in the same way as L and M, (2.7):

$$q\to s_\alpha(q),\quad Q(s_\alpha(q))=\hat{s}_\alpha Q(q)\hat{s}_\alpha. \tag{2.14}$$

Thus G_j and $G_j^{(2)}$ are Coxeter invariant, too. The time evolution of Q is exactly the same as in the classical case[8]

$$\dot{Q}=[Q,M]+L, \tag{2.15}$$

leading to the corresponding result:

$$\begin{aligned}\dot{G}_j&=\mathrm{Ts}(\dot{Q}L^j+Q\dot{L}^j)\\&=\mathrm{Ts}(QML^j-MQL^j+L^{j+1}+QL^jM-QML^j)\\&=\mathrm{Ts}(L^{j+1})-\sum_{\nu,\kappa\in\mathcal{R}}\left(\sum_{\mu\in\mathcal{R}}M_{\mu\kappa}\right)(QL^j)_{\kappa\nu}+\sum_{\mu,\kappa\in\mathcal{R}}(QL^j)_{\mu\kappa}\left(\sum_{\nu\in\mathcal{R}}M_{\kappa\nu}\right)\\&=\mathrm{Ts}(L^{j+1})=F_{j+1}.\end{aligned} \tag{2.16}$$

Like $\{F_j\}$'s not all of $\{G_j\}$'s are independent. Independent $\{G_j\}$ appear when $\{j\}$ are the exponents of Δ. This provides the algebraic linearization of the quantum models. Like in the classical theory, we have the following.

Proposition II.1: The quantum Calogero–Moser system (2.2) is superintegrable for any root system.

Proof: On top of the D first integrals F_k which are in involution, we have the $D(D-1)/2$ extra first integrals defined by

$$H_{k,k'}=F_{k+1}G_{k'}-F_{k'+1}G_k, \tag{2.17}$$

$$\dot{H}_{k,k'}=i[\mathcal{H},H_{k,k'}]=0. \tag{2.18}$$

Like in our previous paper for the classical systems,[8] we do not demonstrate that these $D(D-1)/2$ $\{H_{k,k'}\}$'s contain $r-1$ algebraically independent ones. That would require detailed exhaustive arguments for each root system. We refer to Ref. 20 for general arguments of independence of $\{F_j\}$ type conserved quantities.

For the quantum models based on the A type root system, a similar result was derived by Gonera[16] based on a sl(2,**R**) representation. The time evolution of $G_j^{(2)}$ is slightly complicated:

$$\begin{aligned}\dot{G}_j^{(2)}&=\mathrm{Ts}(\dot{Q}QL^j)+\mathrm{Ts}(Q\dot{Q}L^j)+\mathrm{Ts}(Q^2\dot{L}^j)\\&=\mathrm{Ts}(LQL^j)+\mathrm{Ts}(QL^{j+1}).\end{aligned} \tag{2.19}$$

Since L and Q do not commute in quantum theory, the classical relation $\dot{G}_j^{(2)}=2\mathrm{Tr}(QL^{j+1})=2G_{j+1}$ does not hold any longer. In quantum theory we have

$$QL-LQ=i\delta_{kl}\hat{H}_k\hat{H}_l+iK, \quad K\equiv\sum_{\rho\in\Delta_+} g_{|\rho|}(\rho\cdot\hat{H})(\rho^\vee\cdot\hat{H})\hat{s}_\rho. \tag{2.20}$$

The right hand side gives the ''quantum corrections.'' Thus we arrive at

$$\dot{G}_j^{(2)}=2\,\mathrm{Ts}(QL^{j+1})-i\delta_{kl}\mathrm{Ts}(\hat{H}_k\hat{H}_lL^j)-i\,\mathrm{Ts}(KL^j). \tag{2.21}$$

The second term is easy to evaluate, since

$$\delta_{kl}\mathrm{Ts}(\hat{H}_k\hat{H}_lL^j)=\delta_{kl}\sum_{\mu,\nu\in\mathcal{R}}(\mu_k\mu_l(L^j)_{\mu\nu})=\mu^2\mathrm{Ts}(L^j), \tag{2.22}$$

in which μ^2 is the same for all $\mu\in\mathcal{R}$. The third term reads

$$\mathrm{Ts}(KL^j)=\sum_{\rho\in\Delta_+}\sum_{\mu,\nu\in\mathcal{R}} g_{|\rho|}(\rho\cdot\mu)(\rho^\vee\cdot\mu)(L^j)_{\mu\nu},$$

and for any vector $\mu\in\mathbf{R}^r$ we have

$$\sum_{\rho\in\Delta_+} g_{|\rho|}(\rho\cdot\mu)(\rho^\vee\cdot\mu)=\frac{2}{r}\mu^2\sum_{\rho\in\Delta_+} g_{|\rho|}, \tag{2.23}$$

in which

$$\frac{2}{r}\sum_{\rho\in\Delta_+} g_{|\rho|} \tag{2.24}$$

can be considered as a *deformed Coxeter number*. For $g_{|\rho|}\equiv 1$ it reduces to the Coxeter number. Thus we arrive at a quantum formula

$$\dot{G}_j^{(2)} = 2G_{j+1} - i\mu^2\left(1 + \frac{2}{r}\sum_{\rho\in\Delta_+} g_{|\rho|}\right)F_j$$

$$= 2G_{j+1} - i\mu^2\frac{2}{r}\tilde{\mathcal{E}}_0 F_j\,. \tag{2.25}$$

Here, the coefficient of the quantum corrections term $\tilde{\mathcal{E}}_0$ is defined by

$$\tilde{\mathcal{E}}_0 = \frac{r}{2} + \sum_{\rho\in\Delta_+} g_{|\rho|}\,, \tag{2.26}$$

which characterizes the ground state energy of the rational Calogero–Moser model with harmonic confining force [see, for example, (2.21) of Ref. 19]. This fact is closely related with the sl(2,**R**) algebra for rational Calogero–Moser models discussed by many authors (see, for example, Refs. 22–24, 18, and 16). We will not discuss $G_j^{(2)}$ any longer in this article, except for some comments in the final section.

III. BASIC COMMUTATION RELATIONS

Typical generators of the quadratic algebra are $\{F_j\}$'s (2.10) and $\{H_{k,l}\}$'s (2.17). Namely they are either linear in $\{F_j\}$'s or bi-linear combinations of $\{F_j\}$'s and $\{G_k\}$'s. As will be clear in later discussions, see, for example, (4.10), the set of $\{F_j\}$'s must be understood in the broadest sense to include the dependent ones. That is, any polynomials in the independent r involutive conserved quantities are allowed. For example, F_j for $j \neq 1 + exponent$ or $j > h$ (the Coxeter number) enter into the theory naturally. Likewise, the set of $\{G_j\}$'s include the dependent ones, which are independent ones times any polynomial in $\{F_k\}$'s. In order to explore and present the full content of the quadratic algebra, we need to evaluate the commutators such as

$$[F_j, F_k], \quad [F_j, G_k], \quad [G_j, G_k]. \tag{3.1}$$

For this purpose the Dunkl operators[17] or l operators which are the *vector* version of the Lax matrix operator L (Ref. 19) are useful:

$$\mathrm{l}_\mu = \mathrm{l}\cdot\mu = p\cdot\mu + i\sum_{\rho\in\Delta_+} g_{|\rho|}\frac{\rho.\mu}{\rho.q}\check{s}_\rho\,, \quad \mu\in\mathcal{R}, \tag{3.2}$$

in which another reflection operator $\check{s}_\rho$ acts on a (wave) function f of q as

$$f \to \check{s}_\rho f\colon \quad (\check{s}_\rho f)(q) = f(s_\rho(q)). \tag{3.3}$$

The l operator is linear in μ, Coxeter covariant and Hermitian:

$$\check{s}_\rho \mathrm{l}_\mu \check{s}_\rho = \mathrm{l}_{s_\rho(\mu)}\,, \quad \mathrm{l}_\mu = \mathrm{l}_\mu^\dagger\,, \quad \forall\rho\in\Delta. \tag{3.4}$$

It is shown[19] that the Hilbert space of any quantum Calogero–Moser system consists of Coxeter invariant wavefunctions. That is, they satisfy

$$\check{s}_\rho\psi = \psi, \quad \forall\rho\in\Delta. \tag{3.5}$$

It is well-known that the l operators for the rational Calogero–Moser models commute:

$$[\mathrm{l}_\mu, \mathrm{l}_\nu] = 0, \quad \forall\mu,\nu\in\mathcal{R}. \tag{3.6}$$

The relationship between L and l is simple. For any Coxeter invariant function ψ, $F_k\psi$ and $G_k\psi$ are Coxeter invariant, too, and we have[19]

$$F_k\psi \equiv \mathrm{Ts}(L^k)\psi = \sum_{\mu\in\mathcal{R}} \mathrm{l}_\mu^k \psi, \quad \forall k \in \mathbf{Z}_+, \tag{3.7}$$

$$G_k\psi \equiv \mathrm{Ts}(QL^k)\psi = \sum_{\mu\in\mathcal{R}} q\cdot\mu \mathrm{l}_\mu^k \psi, \quad \forall k \in \mathbf{Z}_+. \tag{3.8}$$

The involution of $\{F_j\}$'s is a simple consequence of (3.6) and (3.7):

$$[F_j, F_k] = 0, \quad \forall j,k \in \mathbf{Z}_+, \tag{3.9}$$

which is a well-known result.

For the evaluation of the second and third types of commutators in (3.1) we need to know in general

$$[\mathrm{l}_\mu^n, q\cdot\nu \mathrm{l}_\nu^m]. \tag{3.10}$$

It is straightforward to show by induction

$$[\mathrm{l}_\mu^j, q\cdot\nu] = -i\left[j\mu\cdot\nu \mathrm{l}_\mu^{j-1} + \sum_{\rho\in\Delta_+} g_{|\rho|}(\rho\cdot\mu)(\rho^\vee\cdot\nu)\frac{\mathrm{l}_\mu^j - \mathrm{l}_{s_\rho(\mu)}^j}{\mathrm{l}_\mu - \mathrm{l}_{s_\rho(\mu)}}\check{\mathrm{s}}_\rho\right], \tag{3.11}$$

starting from

$$[\mathrm{l}_\mu, q\cdot\nu] = -i\left[\mu\cdot\nu I + \sum_{\rho\in\Delta_+} g_{|\rho|}(\rho\cdot\mu)(\rho^\vee\cdot\nu)\check{s}_\rho\right], \tag{3.12}$$

and

$$[\mathrm{l}_\mu^2, q\cdot\nu] = -i\left[2(\mu\cdot\nu)\mathrm{l}_\mu + \sum_{\rho\in\Delta_+} g_{|\rho|}(\rho\cdot\mu)(\rho^\vee\cdot\nu)\frac{\mathrm{l}_\mu^2 - \mathrm{l}_{s_\rho(\mu)}^2}{\mathrm{l}_\mu - \mathrm{l}_{s_\rho(\mu)}}\check{\mathrm{s}}_\rho\right]. \tag{3.13}$$

Here the fraction of operators, $\mathrm{l}_\mu^j - \mathrm{l}_{s_\rho(\mu)}^j / \mathrm{l}_\mu - \mathrm{l}_{s_\rho(\mu)}$, is well defined since the l operators commute with each other, (3.6). For example, we have $\mathrm{l}_\mu^2 - \mathrm{l}_{s_\rho(\mu)}^2 / \mathrm{l}_\mu - \mathrm{l}_{s_\rho(\mu)} = \mathrm{l}_\mu + \mathrm{l}_{s_\rho(\mu)}$. Thus we arrive at

$$\begin{aligned}[\mathrm{l}_\mu^j, q\cdot\nu \mathrm{l}_\nu^k] &= [\mathrm{l}_\mu^j, q\cdot\nu]\mathrm{l}_\nu^k \\ &= -i\left[j\mu\cdot\nu \mathrm{l}_\mu^{j-1}\mathrm{l}_\nu^k + \sum_{\rho\in\Delta_+} g_{|\rho|}(\rho\cdot\mu)(\rho^\vee\cdot\nu)\frac{\mathrm{l}_\mu^j - \mathrm{l}_{s_\rho(\mu)}^j}{\mathrm{l}_\mu - \mathrm{l}_{s_\rho(\mu)}}\mathrm{l}_{s_\rho(\nu)}^k\check{\mathrm{s}}_\rho\right].\end{aligned} \tag{3.14}$$

The second term on the right hand side of (3.14) vanishes when summed over μ:

$$V \equiv \sum_{\mu\in\mathcal{R}} g_{|\rho|}(\rho\cdot\mu)(\rho^\vee\cdot\nu)\frac{\mathrm{l}_\mu^j - \mathrm{l}_{s_\rho(\mu)}^j}{\mathrm{l}_\mu - \mathrm{l}_{s_\rho(\mu)}}\mathrm{l}_{s_\rho(\nu)}^k\check{\mathrm{s}}_\rho = 0. \tag{3.15}$$

This can be seen as follows. The set $\mathcal{R}$ is Coxeter invariant, i.e., $s_\rho(\mathcal{R}) = \mathcal{R}$. Consider the change of variables $\mu' = s_\rho(\mu)$. Then $\mu = s_\rho(\mu')$ and

$$V=\sum_{\mu'\in\mathcal{R}} g_{|\rho|}(\rho\cdot s_\rho(\mu'))(\rho^\vee\cdot\nu)\frac{l^j_{s_\rho(\mu')}-l^j_{\mu'}}{l_{s_\rho(\mu')}-l_{\mu'}}l^k_{s_\rho(\nu)}\check{s}_\rho$$

$$=\sum_{\mu'\in\mathcal{R}} g_{|\rho|}(-\rho\cdot\mu')(\rho^\vee\cdot\nu)\frac{l^j_{\mu'}-l^j_{s_\rho(\mu')}}{l_{\mu'}-l_{s_\rho(\mu')}}l^k_{s_\rho(\nu)}\check{s}_\rho=-V.$$

By summing over μ and ν, we obtain from (3.14)

$$\left[\sum_{\mu\in\mathcal{R}} l^j_\mu,\sum_{\nu\in\mathcal{R}} q\cdot\nu l^k_\nu\right]=-ij\sum_{\mu,\nu\in\mathcal{R}}(\mu\cdot\nu)l^{j-1}_\mu l^k_\nu. \tag{3.16}$$

The right hand side is a Coxeter invariant polynomial in l_μ, which corresponds to a polynomial in $\{F_j\}$ to be denoted by $F_{k,j}$:

$$\sum_{\mu,\nu\in\mathcal{R}}(\mu\cdot\nu)l^{j-1}_\mu l^k_\nu\psi\equiv F_{k,j}\psi,\quad \psi:\ \text{Coxeter invariant.} \tag{3.17}$$

Thus we arrive at

$$i[F_j,G_k]=jF_{k,j} \tag{3.18}$$

$$[F_n,F_{k,j}]=0,\quad \forall n\in\mathbf{Z}. \tag{3.19}$$

When the set of vectors $\mathcal{R}$ consists of orthonormal vectors, for example, the vector representation of A_r embedded in an $r+1$ dimensional space, or vector representations of C_r and D_r, or the set of short roots of B_r, the above $F_{k,j}$ has a simpler expression. In such cases, only $\mu=\pm\nu$ terms in (3.17) survive and we have

$$\sum_{\mu,\nu\in\mathcal{R}}(\mu\cdot\nu)l^{j-1}_\mu l^k_\nu=\begin{cases} C_{\mathcal{R}}\sum_{\nu\in\mathcal{R}} l^{j+k-1}_\nu, \\ 0, \end{cases} \tag{3.20}$$

in which $C_{\mathcal{R}}$ is defined by (2.12). That is, (3.18) is replaced by a more explicit formula

$$i[F_j,G_k]=jC_{\mathcal{R}}F_{j+k-1}, \tag{3.21}$$

which was reported in Kuznetsov's paper for A_r case[5] ($C_{\mathcal{R}}=1$). (In the above formula we assume that neither F_j nor G_k vanish.) As for the extra exponent at $r-1$ in D_r theory, the corresponding F and G operators are best expressed by l operators in the orthonormal basis:

$$F_{r'}\leftrightarrow l_1\cdots l_r,\quad G_{r'-1}\leftrightarrow\sum_{j=1}^{r} q_j l_1\cdots\tilde{l}_j\cdots l_r, \tag{3.22}$$

in which $\tilde{l}_j$ means that the factor is missing.

The general commutation relations (3.18) and (3.19) provide the algebraic linearization of the Hamiltonian systems generated by the higher conserved quantities $\{F_j\}$.

Proposition III.1: The Hamiltonian system generated by the higher conserved quantity F_j (2.10) of quantum Calogero–Moser system (2.2) is superintegrable for any root system.

Proof: On top of the D first integrals F_k, we have the $D(D-1)/2$ extra first integrals for the Hamiltonian F_j:

$$H^{(j)}_{k,k'}=F_{k,j}G_{k'}-F_{k',j}G_k, \tag{3.23}$$

$$\frac{dH^{(j)}_{k,k'}}{dt_j}=i[F_j,H^{(j)}_{k,k'}]=0. \tag{3.24}$$

IV. QUADRATIC ALGEBRA

In order to evaluate the commutators among various $\{H^{(j)}_{k,k'}\}$'s we need the knowledge of the third type of commutators in (3.1), that is, $[G_j,G_k]$. From (3.14) we have

$$\begin{aligned}
&[q\cdot\mu \mathrm{l}^j_\mu, q\cdot\nu \mathrm{l}^k_\nu]\\
&\quad=q\cdot\mu[\mathrm{l}^j_\mu, q\cdot\nu \mathrm{l}^k_\nu]+[q\cdot\mu, q\cdot\nu \mathrm{l}^k_\nu]\mathrm{l}^j_\mu\\
&\quad=-i\left\{(\mu\cdot\nu)j(q\cdot\mu)\mathrm{l}^{j-1}_\mu \mathrm{l}^k_\nu+\sum_{\rho\in\Delta_+} g_{|\rho|}(q\cdot\mu)(\rho\cdot\mu)(\rho^\vee\cdot\nu)\frac{\mathrm{l}^j_\mu-\mathrm{l}^j_{s_\rho(\mu)}}{\mathrm{l}_\mu-\mathrm{l}_{s_\rho(\mu)}}\mathrm{l}^k_{s_\rho(\nu)}\check{s}_\rho\right\}\\
&\qquad+i\left\{(\mu\cdot\nu)k(q\cdot\nu)\mathrm{l}^{k-1}_\nu \mathrm{l}^j_\mu+\sum_{\rho\in\Delta_+} g_{|\rho|}(q\cdot\nu)(\rho\cdot\nu)(\rho^\vee\cdot\mu)\frac{\mathrm{l}^k_\nu-\mathrm{l}^k_{s_\rho(\nu)}}{\mathrm{l}_\nu-\mathrm{l}_{s_\rho(\nu)}}\mathrm{l}^j_{s_\rho(\mu)}\check{s}_\rho\right\}.
\end{aligned} \tag{4.1}$$

As in the previous case (3.15), the coupling constant dependent terms, that is the second and fourth terms in (4.1), cancel with each other when summed over μ and ν:

$$\left[\sum_{\mu\in\mathcal{R}}(q\cdot\mu)\mathrm{l}^j_\mu,\sum_{\nu\in\mathcal{R}}(q\cdot\nu)\mathrm{l}^k_\nu\right]=-i\sum_{\mu,\nu\in\mathcal{R}}\{j(\nu\cdot\mu)(q\cdot\mu)\mathrm{l}^{j-1}_\mu \mathrm{l}^k_\nu-k(\mu\cdot\nu)(q\cdot\nu)\mathrm{l}^{k-1}_\nu \mathrm{l}^j_\mu\}. \tag{4.2}$$

Both terms on the right hand side are Coxeter invariant polynomials in q and l which are linear in q and of degree $j+k-1$ in l. Therefore, they are expressible as linear combination of $\{G_l\}$'s or polynomials in $\{F_m\}$'s multiplied on them. This can be checked by direct calculation or by using the Jacobi identity on the left hand side. Thus we express

$$\begin{aligned}
&\sum_{\mu,\nu\in\mathcal{R}}(\mu\cdot\nu)(q\cdot\mu)\mathrm{l}^{j-1}_\mu \mathrm{l}^k_\nu\psi\equiv G_{j,k}\psi,\\
&\qquad\qquad\qquad\qquad\qquad\qquad\psi\text{: Coxeter invariant.}\\
&\sum_{\mu,\nu\in\mathcal{R}}(\mu\cdot\nu)(q\cdot\nu)\mathrm{l}^j_\mu \mathrm{l}^{k-1}_\nu\psi\equiv G_{k,j}\psi,
\end{aligned} \tag{4.3}$$

We arrive at the following general commutation relation

$$i[G_j,G_k]=jG_{j,k}-kG_{k,j}. \tag{4.4}$$

These $\{G_{j,k}\}$'s satisfy the same type of commutation relations as above.

When the set of vectors $\mathcal{R}$ consists of orthonormal vectors, we have

$$\sum_{\mu,\nu\in\mathcal{R}}(\mu\cdot\nu)(q\cdot\mu)\mathrm{l}^{j-1}_\mu \mathrm{l}^k_\nu=\sum_{\mu,\nu\in\mathcal{R}}(\mu\cdot\nu)(q\cdot\nu)\mathrm{l}^j_\mu \mathrm{l}^{k-1}_\nu=\begin{cases}C_{\mathcal{R}}\displaystyle\sum_{\nu\in\mathcal{R}}(q\cdot\nu)\mathrm{l}^{j+k-1}_\nu,\\ 0.\end{cases} \tag{4.5}$$

This leads to a simplified commutation relation

$$i[G_j,G_k]=(j-k)C_{\mathcal{R}}G_{j+k-1}, \tag{4.6}$$

which was reported in Kuznetsov's paper for A_r case[5] ($C_{\mathcal{R}}=1$).

To sum up, we have obtained the following general commutation relations:

$$[F_j,F_k]=0, \tag{4.7}$$

$$i[F_j,G_k]=jF_{k,j}, \tag{4.8}$$

$$i[G_j,G_k]=jG_{j,k}-kG_{k,j}. \tag{4.9}$$

By using these the operators $\{F_j\}$'s and $\{H^{(m)}_{k,l}\}$'s defined by

$$H^{(m)}_{k,l}=F_{k,m}G_l-F_{l,m}G_k, \quad H^{(m)}_{k,l}=-H^{(m)}_{l,k}, \tag{4.10}$$

generate a quadratic algebra

$$[F_j,F_k]=0, \tag{4.11}$$

$$i[F_j,H^{(m)}_{k,l}]=j(F_{k,m}F_{l,j}-F_{l,m}F_{k,j}), \tag{4.12}$$

$$i[H^{(m)}_{k,l},H^{(m')}_{k',l'}]=\text{quadratic in } H^{(n)}_{r,s} \text{ and } F_t. \tag{4.13}$$

This is the quadratic algebra of the quantum rational Calogero–Moser models based on any root systems. For the classical root systems it can be simplified by using the relations (3.21) and (4.6) to the forms given in Kuznetsov's paper.[5] It characterizes the superintegrability structure of quantum models. In applications for specific models, the indices of $\{F\}$'s and $\{G\}$'s and $\{H\}$'s must be chosen properly. This would give more specific forms of the quadratic algebra relations.

V. RATIONAL POTENTIAL MODEL WITH HARMONIC CONFINING FORCE

The arguments for the algebraic linearization for the *quantum* rational potential model with harmonic confining force go almost parallel with the classical ones. So we present only the key formulas. We have to note the coupling dependence is changed from $g^2_{|\rho|}$ (classical) to $g_{|\rho|}(g_{|\rho|}-1)$ (quantum) and instead of *trace* (Tr, classical) we need the *total sum* (Ts, quantum). The Hamiltonian is now

$$\mathcal{H}_\omega=\frac{1}{2}p^2+\frac{1}{2}\omega^2q^2+\frac{1}{2}\sum_{\rho\in\Delta_+}\frac{g_{|\rho|}(g_{|\rho|}-1)|\rho|^2}{(\rho\cdot q)^2}. \tag{5.1}$$

With the same matrix operators L, M and Q as in the rational case the equations of motion can be expressed in matrix forms:

$$\dot{L}=[L,M]-\omega^2Q, \quad \dot{Q}=[Q,M]+L. \tag{5.2}$$

Introduce the matrices

$$L^{\pm}=L\pm i\omega Q \tag{5.3}$$

whose time evolution reads

$$\dot{L}^{\pm}=[L^{\pm},M]\pm i\omega L^{\pm}. \tag{5.4}$$

They can be cast into a Lax form for $\mathcal{L}=L^+L^-$ as

$$\dot{\mathcal{L}}=[\mathcal{L},M]. \tag{5.5}$$

Consider then the functions

$$F_k = \mathrm{Ts}(L^+ \mathcal{L}^k), \quad G_k = \mathrm{Ts}(L^- \mathcal{L}^k). \tag{5.6}$$

The time evolution yields

$$\dot{F}_k = i\omega F_k, \quad \dot{G}_k = -i\omega G_k. \tag{5.7}$$

Thus these functions provide the algebraic linearization of the quantum system.

VI. RATIONAL MODEL WITH A QUARTIC POTENTIAL

As proved by Françoise and Ragnisco[25] for the models based on the A type root systems and by us[8] for the models based on any root systems, the rational Calogero–Moser model can be deformed into an integrable system by adding a quartic potential at the *classical* level. Here we provide a partial result at the quantum level. The equation of motion can be cast into Lax type equations but they fail to produce conserved quantities.

Define again the same matrices L, Q, X and M. Let

$$h(Q) = aQ + bQ^2 \tag{6.1}$$

be a matrix quadratic in Q; (a,b) are just two new independent parameters. The perturbed Hamiltonian is now

$$\mathcal{H}_h \propto \mathrm{Ts}(L^2 + h(Q)^2). \tag{6.2}$$

Like in the classical theory, the equations of motion can be cast into matrix forms by defining

$$L^\pm = L \pm \mathrm{i}h(Q), \quad \mathcal{L}_1 = L^+ L^-, \quad \mathcal{L}_2 = L^- L^+. \tag{6.3}$$

Though care is needed for the quantum noncommutativity, the calculation is essentially the same as in the classical theory and we arrive at the time evolution of $L^\pm$ and $\mathcal{L}_1$, $\mathcal{L}_2$:

$$\dot{L}^\pm = [L^\pm, M] \pm i\,\tfrac{1}{2}(h'(Q)L^\pm + L^\pm h'(Q)), \tag{6.4}$$

$$\dot{\mathcal{L}}_1 = \left[\mathcal{L}_1, M - \frac{i}{2}h'(Q)\right], \quad \dot{\mathcal{L}}_2 = \left[\mathcal{L}_2, M + \frac{i}{2}h'(Q)\right]. \tag{6.5}$$

Because of the term $\pm(i/2)\,h'(Q)$ added to the M matrix, it loses the sum up to zero property (2.9) and thus *neither trace nor total sum* of the powers of $\mathcal{L}_{1,2}$ are conserved at the quantum level.

For the superintegrability of the trigonometric (hyperbolic) potential models, we refer to Refs. 26 and 27.

VII. COMMENTS ON THE HERMITICITY OF ALGEBRA GENERATORS

In quantum mechanics physical quantities or the observables are described by Hermitian operators in Hilbert space.[16] The hermiticity of F_j, (2.10), is obvious from that of L. The original definition of G_j, (2.13), is not Hermitian. With the following redefinition of Hermitian G_j,

$$G_j = \mathrm{Ts}\sum_{k=0}^{j} (L^k Q L^{j-k})/(j+1), \tag{7.1}$$

it satisfies the same formula (2.16). Whereas the definition of $F_{k,j}$ (3.17) remains the same, that of $H^{(j)}_{k,k'}$ (3.23) should be changed to a Hermitian form

$$2H^{(j)}_{k,k'} = F_{k,j}G_{k'} + G_{k'}F_{k,j} - F_{k',j}G_k - G_k F_{k',j}. \tag{7.2}$$

A formulation with explicitly Hermitian G_j could have been achieved by

$$G_{j-1} \propto i[q^2, F_j], \tag{7.3}$$

which is closely related with the extension of the sl(2,**R**) algebra.[22–24,6,18,16] This also explains the assertion that independent $\{G_j\}$'s appear at $j=$exponent.

We chose the current presentation in order to avoid excessively complicated looking formulas and to allow an easy comparison with the original work, Ref. 5, on the quadratic algebra.

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Symmetry classification of diatomic molecular chains

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A symmetry classification of possible interactions in a diatomic molecular chain is provided. For nonlinear interactions the group of Lie point transformations, leaving the lattice invariant and taking solutions into solutions, is at most five-dimensional. An example is considered in which subgroups of the symmetry group are used to reduce the dynamical differential-difference equations to purely difference ones. [DOI: 10.1063/1.1398583]

I. INTRODUCTION

The purpose of this article is to analyze possible interactions in a long one-dimensional molecule consisting of two types of atoms. The model we consider is a very general one, described by the equations

$$E_1 \equiv \ddot{x}_n - F_n(\xi_n, t) - G_n(\eta_{n-1}, t) = 0,$$
$$E_2 \equiv \ddot{y}_n - K_n(\xi_n, t) - P_n(\eta_n, t) = 0, \tag{1.1}$$

where the overdots denote time derivatives and x_n, y_n can be interpreted as the displacement of the nth atom of type X or Y, respectively, from their equilibrium positions. We define

$$\xi_n \equiv y_n - x_n, \quad \eta_n \equiv x_{n+1} - y_n \tag{1.2}$$

and t is time. The functions F_n, G_n, K_n and P_n are as yet unspecified smooth functions. Indeed, our aim is to classify such systems according to the Lie point symmetries that they allow, that is, to classify these functions F_n, G_n, K_n and P_n.

The assumptions built into the model are the following.

(1) The atoms of type X and Y alternate along a fixed uniform one-dimensional chain with positions labeled by the integers n (see Fig. 1).
(2) Only nearest neighbor interactions are considered, i.e., the atom X_n interacts only with Y_{n-1} and Y_n, and Y_n interacts only with X_n and X_{n+1} (see Fig. 1).
(3) The system is invariant under a uniform translation of all atoms in the molecule and also under a Galilei transformations of the chain.

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FIG. 1. Interactions between atoms of type X and Y along a molecular chain.

(4) The systems are strongly coupled, i.e., we assume

$$\frac{\partial F_n}{\partial \xi_n} \neq 0, \quad \frac{\partial G_n}{\partial \eta_{n-1}} \neq 0, \quad \frac{\partial K_n}{\partial \xi_n} \neq 0, \quad \frac{\partial P_n}{\partial \eta_n} \neq 0. \tag{1.3}$$

(5) In the bulk of the article we assume that the interactions are nonlinear, i.e., at least one of the four functions F_n, G_n, K_n or P_n depends nonlinearly on the argument ξ or η, respectively. The linear case will be treated separately.

(6) A discrete symmetry is built into the model. Indeed, the two equations (1.1) are permuted by the transformation

$$\begin{gathered} x_n \to y_n, \quad y_n \to x_{n+1}, \\ F_n \to P_n, \quad G_n \to K_n, \quad K_{n-1} \to G_n, \quad P_{n-1} \to F_n. \end{gathered} \tag{1.4}$$

Models of this type have many applications in classical mechanics, in molecular physics, or mathematical biology.[1–3] In applications, the form of the functions in Eq. (1.1) are usually *a priori* fixed.

The formalism used in this article is the one called ''intrinsic method'' in earlier articles.[4,5] It has already been applied to monoatomic molecular chains[6] and to a model with two species, or two types of atoms, distributed along a double chain.[7]

In this approach the dependent variables x and y depend on one discrete variable n and one continuous variable t. Symmetry transformations, taking solutions into solutions, act on the variables x, y and t, not, however, on the lattice variable n. The Lie algebra of the symmetry group is realized by vector fields of the form

$$\hat{X} = \tau(x_n, y_n, t)\partial_t + \phi_n(x_n, y_n, t)\partial_{x_n} + \psi_n(x_n, y_n, t)\partial_{y_n}. \tag{1.5}$$

The functions τ, ϕ_n and ψ_n are determined from the requirement that the second prolongation of the vector field $\hat{X}$ should annihilate Eqs. (1.1) on their solution surface. Explicitly we have[4–7]

$$\mathrm{pr}^{(2)}\hat{X} = \tau(t, x_n, y_n)\partial_t + \sum_{k=n-1}^{n+1} \phi_k(t, x_n, y_n)\partial_{x_k} + \sum_{k=n-1}^{n+1} \psi_k(t, x_n, y_n)\partial_{y_k} + \phi_n^{tt}\partial_{\ddot{x}_n} + \psi_n^{tt}\partial_{\ddot{y}_n} \tag{1.6}$$

with

$$\begin{aligned} \phi_n^{tt} &= D_t^2\phi_n - (D_t^2\tau)\,\dot{x}_n - 2(D_t\tau)\,\ddot{x}_n, \\ \psi_n^{tt} &= D_t^2\psi_n - (D_t^2\tau)\,\dot{y}_n - 2(D_t\tau)\,\ddot{y}_n \end{aligned} \tag{1.7}$$

(D_t is the total time derivative). In Eq. (1.6) we have spelled out only those terms which act on Eq. (1.1).

The use of this formalism is not obligatory. Indeed, the group transformations can also act on the lattice[8–11] and generalized symmetries can be very useful.[12] In this article we restrict ourselves to the intrinsic formalism, described earlier in this work.

The present article is organized as follows. In Sec. II we establish the general form of the vector fields (1.5) that realize the symmetry algebra of Eq. (1.1). We also derive the determining

equations for the symmetries and introduce a ''group of allowed transformations.'' Allowed transformations take equations of the type (1.1) into other equations of the same type. They can change the functions F_n, G_n, K_n and P_n into other functions of the same arguments. As in previous articles, we classify equations into symmetry classes under the action of allowed transformations.[6,7,13,14] We also establish that Eqs. (1.1) are invariant under a two-dimensional Abelian group for any functions $F_n,\ldots,P_n$. Section III is devoted to Abelian symmetry algebras. We denote them $A_{j,k,}$, where A means Abelian, j denotes the dimension and $k=1,2,3,\ldots$ enumerates algebras of the same dimension. For each interaction we list only the maximal symmetry algebra. Section IV is devoted to nilpotent symmetry algebras, denoted by $N_{j,k}$ with the same conventions as in Sec. III. In Sec. V we find all solvable symmetry algebras with non-Abelian nilradicals ($SN_{j,k}$). In Sec. VI we find those with Abelian nilradicals ($SA_{j,k}$). All nonsolvable symmetry algebras are listed in Sec. VII ($NS_{j,k}$). In Secs. III–VII we consider only nonlinear interactions. Symmetries of the linear case are discussed in Sec. VIII. Conclusions and some applications of the symmetries are summed up in Sec. IX.

II. DETERMINING EQUATIONS AND ALLOWED TRANSFORMATIONS

The algorithm for finding the symmetry algebra of Eq. (1.1) is

$$\mathrm{pr}\hat{X}\,E_a|_{E_b=0}=0,\quad a=1,2,\quad b=1,2. \tag{2.1}$$

The coefficients of all terms of the type $\dot{x}_n^p\dot{y}_n^q$ must vanish independently and we find that the vector field (1.5) must actually have the form

$$\hat{X}=\tau(t)\partial_t+\left[\left(a+\frac{\dot{\tau}(t)}{2}\right)x_n+\lambda_n(t)\right]\partial_{x_n}+\left[\left(a+\frac{\dot{\tau}(t)}{2}\right)y_n+\mu_n(t)\right]\partial_{y_n}, \tag{2.2}$$

where a is a constant and $\lambda_n(t),\mu_n(t)$ and $\tau(t)$ are functions of the indicated variables. This form (2.2) is valid for any interactions F_n, G_n, K_n and P_n in Eq. (1.1). Moreover, we have

$$\tau=\tau_0+\tau_1 t+\tau_2 t^2, \tag{2.3}$$

where τ_0,τ_1 and τ_2 are constants.

The constants a, τ_i and the functions $\lambda_n(t)$ and $\mu_n(t)$ are subject to two further determining equations that involve the interaction functions explicitly. They are

$$\ddot{\lambda}_n+\left(a-\frac{3}{2}\dot{\tau}\right)(F_n+G_n)+\left[\lambda_n-\mu_n-\left(a+\frac{\dot{\tau}}{2}\right)\xi_n\right]F_{n,\xi_n}+\left[\mu_{n-1}-\lambda_n-\left(a+\frac{\dot{\tau}}{2}\right)\eta_{n-1}\right]G_{n,\eta_{n-1}}$$
$$-\tau(F_{n,t}+G_{n,t})=0, \tag{2.4}$$

$$\ddot{\mu}_n+\left(a-\frac{3}{2}\dot{\tau}\right)(K_n+P_n)+\left[\lambda_n-\mu_n-\left(a+\frac{\dot{\tau}}{2}\right)\xi_n\right]K_{n,\xi_n}+\left[\mu_n-\lambda_{n+1}-\left(a+\frac{\dot{\tau}}{2}\right)\eta_n\right]P_{n,\eta_n}$$
$$-\tau(K_{n,t}+P_{n,t})=0. \tag{2.5}$$

Our task is to perform a complete analysis of Eqs. (2.4) and (2.5). Conceptually, this is very similar to the problem considered in Ref. 7. However, the functions figuring in Eq. (1.1) are less general than those of Ref. 7, hence the computations are simpler.

We shall classify the equations of type (1.1) into equivalence classes under the action of a group of ''allowed transformations.'' These are transformations of the form

$$x_n=\Phi_n(\tilde{x}_n,\tilde{y}_n,\tilde{t}),\quad y_n=\Psi_n(\tilde{x}_n,\tilde{y}_n,\tilde{t}),\quad t=T(\tilde{t}) \tag{2.6}$$

that transform Eqs. (1.1) into equations of the same form, but do not preserve the functions on the right hand side of Eq. (1.1). The requirement that no first derivatives should appear and that the transformed functions $\tilde{F}_n$ and $\tilde{K}_n$ should depend only on $\tilde{\xi}_n$ and $\tilde{t}$, and $\tilde{G}_n$ and $\tilde{P}_n$ only on $\tilde{t}$ and $\tilde{\eta}_{n-1}$ or $\tilde{\eta}_n$, respectively, implies that the transformations actually have the form

$$\begin{pmatrix} x_n(t) \\ y_n(t) \end{pmatrix} = q\,\dot{\tilde{t}}^{-1/2} \begin{pmatrix} \tilde{x}_n(\tilde{t}) \\ \tilde{y}_n(\tilde{t}) \end{pmatrix} + \begin{pmatrix} \alpha_n(t) \\ \beta_n(t) \end{pmatrix}, \tag{2.7}$$

$$\tilde{t} = \frac{c_1 t + c_2}{c_3 t + c_4}, \quad c_1 c_4 - c_2 c_3 = 1, \quad q \neq 0, \tag{2.8}$$

where $q, c_1, \ldots, c_4$ are constants and α_n and β_n are arbitrary functions of n and t.

The transformed system is

$$\begin{aligned} \ddot{\tilde{x}}_n(\tilde{t}) &= \tilde{F}_n(\tilde{\xi}_n, \tilde{t}) + \tilde{G}_n(\tilde{\eta}_{n-1}, \tilde{t}), \\ \ddot{\tilde{y}}_n(\tilde{t}) &= \tilde{K}_n(\tilde{\xi}_n, \tilde{t}) + \tilde{P}_n(\tilde{\eta}_n, \tilde{t}), \end{aligned} \tag{2.9}$$

with

$$\begin{pmatrix} \tilde{F}_n + \tilde{G}_n \\ \tilde{K}_n + \tilde{P}_n \end{pmatrix} = \frac{\dot{\tilde{t}}^{-3/2}}{q} \left[\begin{pmatrix} F_n(\xi_n, t) + G_n(\eta_{n-1}, t) \\ K_n(\xi_n, t) + P_n(\eta_n, t) \end{pmatrix} - \begin{pmatrix} \ddot{\alpha}_n(t) \\ \ddot{\beta}_n(t) \end{pmatrix} \right], \tag{2.10}$$

where

$$\xi_n = y_n - x_n = q\,\dot{\tilde{t}}^{-1/2}(\tilde{x}_n - \tilde{y}_n) + \alpha_n(t) - \beta_n(t), \tag{2.11}$$

$$\eta_n = x_{n+1} - y_n = q\,\dot{\tilde{t}}^{-1/2}(\tilde{x}_{n+1} - \tilde{y}_n) + \alpha_{n+1}(t) - \beta_n(t), \tag{2.12}$$

$$t = \frac{c_4 \tilde{t} - c_2}{-c_3 \tilde{t} + c_1}. \tag{2.13}$$

The vector field $\hat{X}$ of Eq. (2.2) is transformed into a similar field with

$$\tilde{\tau}(\tilde{t}) = \tau(t(\tilde{t}))\,\dot{\tilde{t}}, \quad \tilde{a} = a, \tag{2.14}$$

$$\begin{pmatrix} \tilde{\lambda}_n(\tilde{t}) \\ \tilde{\mu}_n(\tilde{t}) \end{pmatrix} = \frac{\dot{\tilde{t}}^{1/2}}{q} \left[\left(a + \frac{\dot{\tau}}{2} \right) \begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix} - \tau \begin{pmatrix} \dot{\alpha}_n \\ \dot{\beta}_n \end{pmatrix} + \begin{pmatrix} \lambda_n \\ \mu_n \end{pmatrix} \right]. \tag{2.15}$$

The transformed functions and constants must satisfy the same determining equations (2.4) and (2.5).

As mentioned in the Introduction, translational and Galilei invariance are built into the model. That is easy to check. Indeed $\lambda_n = \mu_n = 1$, $a = 0$, $\tau(t) = 0$ and $\lambda_n = \mu_n = t$, $a = 0$, $\tau(t) = 0$ are solutions of Eqs. (2.4) and (2.5) for F_n, G_n, K_n and P_n arbitrary. No other symmetries exist, unless some constraints on the interactions are imposed.

We shall use the allowed transformations to simplify the vector fields that occur. In particular the coefficient $\tau(t)$ of a given vector field can be transformed into one of the following expressions: 0, 1, t or $t^2 + 1$.

Our strategy will be to first find all Abelian symmetry algebras, then all nilpotent (non-Abelian) ones. Once these are known, we can determine all solvable ones, having the corresponding Abelian or nilpotent ones as nilradicals.[15] Finally, all nonsolvable symmetry algebras will be determined, making use of their Levi decomposition.[15]

Any symmetry algebra will contain the algebra

$$\mathbf{A_{2,1}}: \quad \hat{X}_1=\partial_{x_n}+\partial_{y_n}, \quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}), \tag{2.16}$$

as a subalgebra. Allowed transformations leave the algebra (2.16) invariant. Any further element of the symmetry algebra can be transformed into one of the following ones:

$$\hat{Y}_1=\partial_t+a(x_n\,\partial_{x_n}+y_n\,\partial_{y_n}), \quad a=0,1, \tag{2.17}$$

$$\hat{Y}_2=t\,\partial_t+(a+\tfrac{1}{2})(x_n\,\partial_{x_n}+y_n\,\partial_{y_n}), \tag{2.18}$$

$$\hat{Y}_3=(t^2+1)\,\partial_t+(a+t)(x_n\,\partial_{x_n}+y_n\,\partial_{y_n}), \tag{2.19}$$

$$\hat{Y}_4=\lambda_n(t)(\partial_{x_n}+\partial_{y_n}), \quad \ddot{\lambda}_n\neq 0, \quad \lambda_{n+1}\neq\lambda_n, \tag{2.20}$$

$$\hat{Y}_5=\lambda_n(t)\,\partial_{x_n}+\lambda_{n+1}(t)\,\partial_{y_n}, \quad \ddot{\lambda}_n\neq 0, \quad \lambda_{n+1}\neq\lambda_n. \tag{2.21}$$

The interactions that allow these additional terms can easily be determined from Eqs. (2.4) and (2.5). Once this is done, we determine whether the considered interactions allow further symmetries. For each interaction, we shall only list the maximal symmetry algebra allowed, not lower-dimensional subalgebras.

III. ABELIAN SYMMETRY ALGEBRAS

The lowest dimensional maximal symmetry algebra is $A_{2,1}$ of Eq. (2.16), present for any interactions in Eq. (1.1). This algebra can be enlarged into a higher dimensional Abelian algebra by adding elements of the type (2.20) or (2.21). The determining equations for a nonlinear system allow at most four commuting symmetry generators. Moreover, the three-dimensional symmetry algebras are never maximal.

Finally, we obtain two different four-dimensional Abelian symmetry algebras together with the interactions that allow them. They are

$$\mathbf{A_{4,1}}: \quad \hat{X}_1=\lambda_{1,n}(t)(\partial_{x_n}+\partial_{y_n}), \quad \hat{X}_2=\lambda_{2,n}(t)(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{X}_3=\partial_{x_n}+\partial_{y_n}, \quad \hat{X}_4=t(\partial_{x_n}+\partial_{y_n}),$$

$$F_n=F_n(\xi_n,t), \quad G_n=\frac{\ddot{\lambda}_{1,n}}{\lambda_{1,n}-\lambda_{1,n-1}}\,\eta_{n-1},$$

$$K_n=K_n(\xi_n,t), \quad P_n=\frac{\ddot{\lambda}_{1,n}}{\lambda_{1,n+1}-\lambda_{1,n}}\,\eta_n,$$

$$\ddot{\lambda}_{1,n}\neq 0, \quad \ddot{\lambda}_{2,n}\neq 0, \quad \lambda_{1,n+1}\neq\lambda_{1,n},$$

$$\frac{\ddot{\lambda}_{2,n}}{\ddot{\lambda}_{1,n}}=\frac{\lambda_{2,n}-\lambda_{2,n-1}}{\lambda_{1,n}-\lambda_{1,n-1}}=\frac{\lambda_{2,n+1}-\lambda_{2,n}}{\lambda_{1,n+1}-\lambda_{1,n}};$$

$$\mathbf{A_{4,2}}: \quad \hat{X}_1=\lambda_{1,n}(t)\partial_{x_n}+\lambda_{1,n+1}(t)\partial_{y_n}, \quad \hat{X}_2=\lambda_{2,n}(t)\partial_{x_n}+\lambda_{2,n+1}(t)\partial_{y_n},$$

$$\hat{X}_3=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_4=t(\partial_{x_n}+\partial_{y_n}),$$

$$F_n=\frac{\ddot{\lambda}_{1,n}}{\lambda_{1,n+1}-\lambda_{1,n}}\xi_n,\quad G_n=G_n(\eta_{n-1},t),$$

$$K_n=\frac{\ddot{\lambda}_{1,n+1}}{\lambda_{1,n+1}-\lambda_{1,n}}\xi_n,\quad P_n=P_n(\eta_n,t),$$

$$\ddot{\lambda}_{1,n}\neq 0,\quad \ddot{\lambda}_{2,n}\neq 0,\quad \lambda_{1,n+1}\neq\lambda_{1,n},$$

$$\frac{\ddot{\lambda}_{2,n}}{\ddot{\lambda}_{1,n}}=\frac{\lambda_{2,n}-\lambda_{2,n-1}}{\lambda_{1,n}-\lambda_{1,n-1}}=\frac{\lambda_{2,n+1}-\lambda_{2,n}}{\lambda_{1,n+1}-\lambda_{1,n}}.$$

The algebras $A_{4,1}$ and $A_{4,2}$ are actually related by the discrete symmetry (1.4). Algebra $A_{4,1}$ is transformed into $A_{4,2}$ by the substitutions

$$\begin{gathered}F_n(\xi_n)\to P_n(\eta_n),\quad G_n(\eta_{n-1})\to K_n(\xi_n),\\ K_{n-1}(\xi_{n-1})\to G_n(\eta_{n-1}),\quad P_{n-1}(\eta_{n-1})\to F_n(\xi_n),\\ \sigma_n(t)\,\partial_{x_n}\to\sigma_{n+1}(t)\,\partial_{y_n},\quad \sigma_n(t)\,\partial_{y_n}\to\sigma_n(t)\,\partial_{x_n}.\end{gathered}\tag{3.1}$$

The functions $\lambda_{1,n}(t)$ and $\lambda_{2,n}(t)$ in algebras $A_{4,1}$, $A_{4,2}$ satisfy the equations

$$\frac{\ddot{\lambda}_{2,n}}{\ddot{\lambda}_{1,n}}=\frac{\lambda_{2,n}-\lambda_{2,n-1}}{\lambda_{1,n}-\lambda_{1,n-1}}=\frac{\lambda_{2,n+1}-\lambda_{2,n}}{\lambda_{1,n+1}-\lambda_{1,n}}.\tag{3.2}$$

These equations can be solved and we obtain

$$\begin{gathered}\lambda_{1,n}=f(t)\lambda_{2,n}+g(t),\quad \lambda_{2,n}=\frac{\gamma_n}{\dot{f}(t)^{1/2}}-\frac{1}{2\,\dot{f}(t)^{1/2}}\int_{t_0}^{t}\frac{\ddot{g}(s)}{\dot{f}(s)^{1/2}}\,ds,\\ \dot{f}(t)\neq 0,\quad \gamma_{n+1}\neq\gamma_n,\end{gathered}\tag{3.3}$$

where $f(t)$, $g(t)$ are arbitrary smooth functions of t and γ_n is an arbitrary function of n.

Notice that the quantities $\lambda_{1,n}(t)$ and $\lambda_{2,n}(t)$ [or $f(t)$, $g(t)$ and γ_n] figure explicitly in the interaction functions G_n and P_n of $A_{4,1}$, or respectively in F_n and K_n of $A_{4,2}$. The two algebras are thus indeed four-dimensional and completely specified.

IV. NILPOTENT NON-ABELIAN SYMMETRY ALGEBRAS

Nilpotent Lie algebras exist for all dimensions $\dim L\geqslant 3$. For $\dim L=3$ only one type exists, namely the Heisenberg algebra. It has a two-dimensional Abelian ideal. Maximality requires that this ideal be the algebra $A_{2,1}$ of Eq. (2.16). The Heisenberg algebra is obtained by adding the operator $\hat{T}=\partial_t$. We then calculate the interaction allowing this symmetry algebra, and obtain

$$\mathbf{N_{3,1}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),\quad \hat{T}=\partial_t,$$

$$F_n=f_n(\xi_n),\quad G_n=g_n(\eta_{n-1}),$$

$$K_n = k_n(\xi_n), \quad P_n = p_n(\eta_n).$$

We mention that this algebra is invariant under the substitution (3.1).

Every nilpotent non-Abelian Lie algebra contains the Heisenberg algebra as a subalgebra. We can hence proceed by adding further operators to $N_{3,1}$. Moreover, they can only be added to the Abelian ideal. The determining equations (2.4) and (2.5) allow us to add at most two operators. Maximality requires that we add precisely two. We thus obtain two mutually isomorphic five-dimensional nilpotent Lie algebras with four-dimensional Abelian ideals, namely,

$$\mathbf{N_{5,1}}: \ \hat{X}_1 = \partial_{x_n} + \partial_{y_n}, \quad \hat{X}_2 = t(\partial_{x_n} + \partial_{y_n}), \quad \hat{T} = \partial_t,$$

$$\hat{X}_3 = (\sigma_n + t^2)(\partial_{x_n} + \partial_{y_n}), \quad \hat{X}_4 = \left(\sigma_n t + \frac{t^3}{3}\right)(\partial_{x_n} + \partial_{y_n}),$$

$$F_n = f_n(\xi_n), \quad G_n = \frac{2}{\sigma_n - \sigma_{n-1}}\eta_{n-1},$$

$$K_n = k_n(\xi_n), \quad P_n = \frac{2}{\sigma_{n+1} - \sigma_n}\eta_n, \quad \sigma_{n+1} \neq \sigma_n,$$

where σ_n is an arbitrary function of n.

The second algebra $N_{5,2}$ is obtained from $N_{5,1}$ by the substitution (3.1). We mention that the interactions allowing the symmetry algebra $N_{5,1}$ are special cases of those allowing the Abelian algebra $A_{4,1}$. Similarly for $N_{5,2}$ and $A_{4,2}$.

V. SOLVABLE NON-NILPOTENT SYMMETRY ALGEBRAS WITH NON-ABELIAN NILRADICALS

A solvable Lie algebra L always has a uniquely defined maximal nilpotent ideal, the nilradical $NR(L)$.[15] If a solvable symmetry algebra of the system (1.1) has a non-Abelian nilradical, it must be $N_{3,1}$, $N_{5,1}$ or $N_{5,2}$ of Sec. IV, or a four-dimensional subalgebra of $N_{5,1}$ or $N_{5,2}$.

The determining equations (2.4) and (2.5) do not allow any extension of the four and five-dimensional nilpotent symmetry algebras to solvable ones.

The Heisenberg algebra $N_{3,1}$, on the other hand, leads to three different four-dimensional solvable symmetry algebras. The Lie algebras are given by four basis elements, $\hat{X}_1$, $\hat{X}_2$ and $\hat{T}$ of $N_{3,1}$ and an additional operator $\hat{Y}$. Below we list these elements $\hat{Y}$ together with the invariant interactions that allow the corresponding symmetry groups. In each case we present a matrix A defining the action of $\hat{Y}$ on the nilradical $N_{3,1}$ (i.e., $[\hat{X}, \hat{Y}] = A_{i1}\hat{X} + A_{i2}\hat{T} + A_{i3}\hat{X}_2$).

$$\mathbf{SN_{4,1}}: \ \hat{Y} = t\partial_t + (a + \tfrac{1}{2})(x_n\partial_{x_n} + y_n\partial_{y_n}),$$

$$F_n = (\xi_n)^{(2a-3)/(2a+1)} f_n, \quad G_n = (\eta_{n-1})^{(2a-3)/(2a+1)} g_n,$$

$$K_n = (\xi_n)^{(2a-3)/(2a+1)} k_n, \quad P_n = (\eta_n)^{(2a-3)/(2a+1)} p_n,$$

$$A = \mathrm{diag}\,(a + \tfrac{1}{2}, 1, a - \tfrac{1}{2}), \quad a \neq -\tfrac{1}{2}, \tfrac{3}{2};$$

$$\mathbf{SN_{4,2}}: \ \hat{Y} = t\partial_t + (2x_n + t^2)\partial_{x_n} + (2y_n + t^2)\partial_{y_n},$$

$$F_n = f_n + \tfrac{1}{2}\ln(\xi_n), \quad G_n = \tfrac{1}{2}\ln(\eta_{n-1}),$$

$$K_n = k_n + \tfrac{1}{2}\ln(\xi_n), \quad P_n = \tfrac{1}{2}\ln(\eta_n),$$

$$A = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 1 & 2 \\ 0 & 0 & 1 \end{pmatrix};$$

$$\mathbf{SN_{4,3}}: \quad \hat{Y} = t\partial_t + \sigma_{1,n}\partial_{x_n} + \sigma_{2,n}\partial_{y_n},$$

$$F_n = f_n \exp\left(\frac{2\xi_n}{\sigma_{1,n}-\sigma_{2,n}}\right), \quad G_n = g_n \exp\left(\frac{-2\eta_{n-1}}{\sigma_{1,n}-\sigma_{2,n-1}}\right),$$

$$K_n = k_n \exp\left(\frac{2\xi_n}{\sigma_{1,n}-\sigma_{2,n}}\right), \quad P_n = p_n \exp\left(\frac{-2\eta_n}{\sigma_{1,n+1}-\sigma_{2,n}}\right),$$

$$A = \mathrm{diag}\,(0,1,-1), \quad \sigma_{1,n} \neq \sigma_{2,n}, \quad \sigma_{1,n+1} \neq \sigma_{2,n}.$$

The quantities $f_n, g_n, p_n, k_n, \sigma_{1,n}$ and $\sigma_{2,n}$ depend on n alone.

The transformation (3.1) does not lead to any new algebras or interactions. In the case of the algebra $SN_{4,3}$ we may have $\sigma_{2,n+1} = \sigma_{2,n}$. Then σ_2 can be transformed into $\sigma_{2,n} = \sigma = 0$, and similarly, for $\sigma_{2,n+1} \neq \sigma_{2,n}$, but $\sigma_{1,n+1} = \sigma_{1,n} \equiv \sigma$, we can transform σ_1 into $\sigma_1 = \sigma = 0$.

VI. SOLVABLE NON-NILPOTENT SYMMETRY ALGEBRAS WITH ABELIAN NILRADICALS

A large number of symmetry algebras of the system (1.1) are of this type. To identify and classify them, we use several known results on the structure of solvable Lie algebras.[15]

(1) The nilradical $NR(L)$ is unique and its dimension satisfies

$$\dim NR(L) \geqslant \tfrac{1}{2}\dim L. \tag{6.1}$$

(2) Any solvable Lie algebra L can be written as the algebraic sum of the nilradical $NR(L)$ and a complementary linear space F, i.e., $L = F \dot{+} NR(L)$.

(3) The derived algebra is contained in its nilradical: $[L,L] \subseteq NR(L)$.

(4) For an Abelian nilradical $\{\hat{X}_1, \ldots, \hat{X}_n\}$, the commutation relations can be written as

$$[\hat{X}_i, \hat{Y}_k] = (A_k)_{ij}\hat{X}_j, \quad [A_k, A_l] = 0, \quad [\hat{Y}_i, \hat{Y}_k] = c_{ik}^l \hat{X}_l, \quad [\hat{X}_i, \hat{X}_k] = 0, \tag{6.2}$$

where the elements $\hat{Y}_k$ are the non-nilpotent elements (outside the nilradical). The matrices A_k commute and are linearly nilindependent (i.e., no nontrivial linear combination of them is a nilpotent matrix). If only one element $\hat{Y}$ outside the nilradical exists, the non-nilpotent matrix A can be taken in Jordan canonical form.

In our case we can add that the Abelian nilradical must be one of the algebras found in Sec. III. In principle, the nilradical could be a three-dimensional subalgebra of $A_{4,1}$, or $A_{4,2}$, containing $A_{2,1}$ as a subalgebra. However, it turns out that all choices of this type lead to symmetry algebras that are not maximal for the interactions that they allow.

The following solvable symmetry algebras occur.

A. dim NR(L)=2

The only two-dimensional nilradical that leads to solvable Lie algebras that are maximal for the obtained interaction is $A_{2,1}$. The solvable Lie algebras are always three-dimensional. A basis for them consists of $\hat{X}_1$ and $\hat{X}_2$ of Eq. (2.16) and an additional element $\hat{Y}$. In each case we give the element $\hat{Y}$ and the matrix A representing the action of $\hat{Y}$ on the nilradical:

$$\mathbf{SA_{3,1}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),\quad \hat{Y}=\partial_t+x_n\partial_{x_n}+y_n\partial_{y_n},$$

$$F_n=\xi_n f_n(\omega_n),\quad G_n=\eta_{n-1}g_n(\zeta_{n-1}),$$

$$K_n=\xi_n k_n(\omega_n),\quad P_n=\eta_n p_n(\zeta_n),$$

$$\omega_n=\xi_n \mathrm{e}^{-t},\quad \zeta_n=\eta_n \mathrm{e}^{-t},\quad A=\begin{pmatrix}1 & -1\\ 0 & 1\end{pmatrix};$$

$$\mathbf{SA_{3,2}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),\quad \hat{Y}=t\partial_t+(a+\tfrac{1}{2})(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$F_n=t^{-2}\xi_n f_n(\omega_n),\quad G_n=t^{-2}\eta_{n-1}g_n(\zeta_{n-1}),$$

$$K_n=t^{-2}\xi_n k_n(\omega_n),\quad P_n=t^{-2}\eta_n p_n(\zeta_n),$$

$$\omega_n=\xi_n t^{-(a+1/2)},\quad \zeta_n=\eta_n t^{-(a+1/2)},\quad A=\mathrm{diag}\,(a-\tfrac{1}{2},a+\tfrac{1}{2});$$

$$\mathbf{SA_{3,3}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),\quad \hat{Y}=(t^2+1)\partial_t+(a+t)(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$F_n=(t^2+1)^{-2}\xi_n f_n(\omega_n),\quad G_n=(t^2+1)^{-2}\eta_{n-1}g_n(\zeta_{n-1}),$$

$$K_n=(t^2+1)^{-2}\xi_n k_n(\omega_n),\quad P_n=(t^2+1)^{-2}\eta_n p_n(\zeta_n),$$

$$\omega_n=\xi_n(t^2+1)^{-1/2}\exp[-a\arctan(t)],\quad \zeta_n=\eta_n(t^2+1)^{-1/2}\exp[-a\arctan(t)],$$

$$A=\begin{pmatrix}a & -1\\ 1 & a\end{pmatrix}.$$

These three algebras are nonisomorphic (since the corresponding matrices A are not mutually conjugate). Each of these three cases is self-conjugate under the substitution (3.1).

B. dim NR(L)=4

The nilradical could be three-dimensional, however the obtained solvable Lie algebra is never maximal. We only need to deal with four-dimensional Abelian ideals of the form $A_{4,1}$ and $A_{4,2}$. An extension to a solvable Lie algebra is only possible for special cases of the functions $\lambda_{1,n}(t)$ and $\lambda_{2,n}(t)$ figuring in the vector fields and interactions. Next we list all inequivalent extensions of $A_{4,1}$. There are precisely nine of them. The corresponding extensions of $A_{4,2}$ are obtained by the substitution (3.1). The action of $\hat{Y}$ on $\{\hat{X}_1,\ldots,\hat{X}_4\}$ is represented by the matrix A:

$$\mathbf{SA_{5,1}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{X}_3=\sigma_n \mathrm{e}^{t}(\partial_{x_n}+\partial_{y_n}),\quad \hat{X}_4=\sigma_n \mathrm{e}^{-t}(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{Y}=\partial_t+a(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$F_n=\xi_n f_n(\omega_n),\quad G_n=\frac{\sigma_n}{\sigma_n-\sigma_{n-1}}\,\eta_{n-1},$$

$$K_n=\xi_n k_n(\omega_n),\quad P_n=\frac{\sigma_n}{\sigma_{n+1}-\sigma_n}\,\eta_n,$$

$$\omega_n=\xi_n e^{-at},\quad \sigma_{n+1}\neq\sigma_n,\quad A=\begin{pmatrix} a-1 & 0 & 0 & 0\\ 0 & a+1 & 0 & 0\\ 0 & 0 & a & 0\\ 0 & 0 & -1 & a\end{pmatrix};$$

$$\mathbf{SA_{5,2}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{X}_3=\sigma_n\cos(t)(\partial_{x_n}+\partial_{y_n}),\quad \hat{X}_4=\sigma_n\sin(t)(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{Y}=\partial_t+a(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$F_n=\xi_n f_n(\omega_n),\quad G_n=\frac{-\sigma_n}{\sigma_n-\sigma_{n-1}}\eta_{n-1},$$

$$K_n=\xi_n k_n(\omega_n),\quad P_n=\frac{-\sigma_n}{\sigma_{n+1}-\sigma_n}\eta_n,$$

$$\omega_n=\xi_n e^{-at},\quad \sigma_{n+1}\neq\sigma_n,\quad A=\begin{pmatrix} a & 1 & 0 & 0\\ -1 & a & 0 & 0\\ 0 & 0 & a & 0\\ 0 & 0 & -1 & a\end{pmatrix};$$

$$\mathbf{SA_{5,3}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{X}_3=(\sigma_n+t^2)(\partial_{x_n}+\partial_{y_n}),\quad \hat{X}_4=\left(\sigma_n t+\frac{t^3}{3}\right)(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{Y}=\partial_t+a(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$F_n=\xi_n f_n(\omega_n),\quad G_n=\frac{2\eta_{n-1}}{\sigma_n-\sigma_{n-1}},$$

$$K_n=\xi_n k_n(\omega_n),\quad P_n=\frac{2\eta_n}{\sigma_{n+1}-\sigma_n},$$

$$\omega_n=\xi_n e^{-at},\quad \sigma_{n+1}\neq\sigma_n,\quad A=\begin{pmatrix} a & 0 & 0 & -2\\ -1 & a & 0 & 0\\ 0 & 0 & a & 0\\ 0 & 0 & -1 & a\end{pmatrix};$$

$$\mathbf{SA_{5,4}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{X}_3=\sigma_n t^{\alpha}(\partial_{x_n}+\partial_{y_n}),\quad \hat{X}_4=\sigma_n t^{1-\alpha}(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{Y}=t\partial_t+(a+\tfrac{1}{2})(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$F_n=t^{-2}\xi_n f_n(\omega_n),\quad G_n=\alpha(\alpha-1)t^{-2}\frac{\sigma_n}{\sigma_n-\sigma_{n-1}}\eta_{n-1},$$

$$K_n=t^{-2}\xi_n k_n(\omega_n),\quad P_n=\alpha(\alpha-1)t^{-2}\frac{\sigma_n}{\sigma_{n+1}-\sigma_n}\eta_n,$$

$$\omega_n=\xi_n t^{-(a+1/2)},\quad \sigma_{n+1}\neq\sigma_n,\quad \alpha\neq 0,1,$$

$$A=\mathrm{diag}\,(a-\alpha+\tfrac{1}{2},a+\alpha-\tfrac{1}{2},a+\tfrac{1}{2},a-\tfrac{1}{2});$$

$$\mathbf{SA_{5,5}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{X}_3=\sigma_n t^{1/2}\ln(t)(\partial_{x_n}+\partial_{y_n}),\quad \hat{X}_4=\sigma_n t^{1/2}(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{Y}=t\partial_t+(a+\tfrac{1}{2})(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$F_n=t^{-2}\xi_n f_n(\omega_n),\quad G_n=-\tfrac{1}{4}t^{-2}\frac{\sigma_n}{\sigma_n-\sigma_{n-1}}\eta_{n-1},$$

$$K_n=t^{-2}\xi_n k_n(\omega_n),\quad P_n=-\tfrac{1}{4}t^{-2}\frac{\sigma_n}{\sigma_{n+1}-\sigma_n}\eta_n,$$

$$\omega_n=\xi_n t^{-(a+1/2)},\quad \sigma_{n+1}\neq\sigma_n,\quad A=\begin{pmatrix} a & -1 & 0 & 0\\ 0 & a & 0 & 0\\ 0 & 0 & a+\frac{1}{2} & 0\\ 0 & 0 & 0 & a-\frac{1}{2}\end{pmatrix};$$

$$\mathbf{SA_{5,6}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{X}_3=\sigma_n t^{1/2}\cos[\ln(t)](\partial_{x_n}+\partial_{y_n}),\quad \hat{X}_4=\sigma_n t^{1/2}\sin[\ln(t)](\partial_{x_n}+\partial_{y_n}),$$

$$\hat{Y}=t\partial_t+(a+\tfrac{1}{2})(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$F_n=t^{-2}\xi_n f_n(\omega_n),\quad G_n=-\frac{5}{4}t^{-2}\frac{\sigma_n}{\sigma_n-\sigma_{n-1}}\eta_{n-1},$$

$$K_n=t^{-2}\xi_n k_n(\omega_n),\quad P_n=-\frac{5}{4}t^{-2}\frac{\sigma_n}{\sigma_{n+1}-\sigma_n}\eta_n,$$

$$\omega_n=\xi_n t^{-(a+1/2)},\quad \sigma_{n+1}\neq\sigma_n,\quad A=\begin{pmatrix} a & 1 & 0 & 0\\ -1 & a & 0 & 0\\ 0 & 0 & a+\frac{1}{2} & 0\\ 0 & 0 & 0 & a-\frac{1}{2}\end{pmatrix};$$

$$\mathbf{SA_{5,7}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{X}_3=[\sigma_n-\ln(t)](\partial_{x_n}+\partial_{y_n}),\quad \hat{X}_4=t[\sigma_n+\ln(t)](\partial_{x_n}+\partial_{y_n}),$$

$$\hat{Y}=t\partial_t+(a+\tfrac{1}{2})(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$F_n=t^{-2}\xi_n f_n(\omega_n),\quad G_n=-t^{-2}\frac{\eta_{n-1}}{\sigma_n-\sigma_{n-1}},$$

$$K_n=t^{-2}\xi_n k_n(\omega_n),\quad P_n=-t^{-2}\frac{\eta_n}{\sigma_{n+1}-\sigma_n},$$

$$\omega_n=\xi_n t^{-(a+1/2)},\quad \sigma_{n+1}\neq\sigma_n,\quad A=\begin{pmatrix} a+\frac{1}{2} & 0 & 1 & 0\\ 0 & a-\frac{1}{2} & 0 & -1\\ 0 & 0 & a+\frac{1}{2} & 0\\ 0 & 0 & 0 & a-\frac{1}{2}\end{pmatrix};$$

$$\mathbf{SA_{5,8}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{X}_3=\lambda_{1,n}(t)(\partial_{x_n}+\partial_{y_n}),\quad \lambda_{1n}=\sigma_n(t^2+1)^{1/2}\exp[\alpha\arctan(t)],$$

$$\hat{X}_4=\lambda_{2,n}(t)(\partial_{x_n}+\partial_{y_n}),\quad \lambda_{2n}=\sigma_n(t^2+1)^{1/2}\exp[-\alpha\arctan(t)],$$

$$\hat{Y}=(t^2+1)\partial_t+(a+t)(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$F_n=(t^2+1)^{-2}\xi_n f_n(\omega_n),\quad G_n=(\alpha^2+1)(t^2+1)^{-2}\frac{\sigma_n}{\sigma_n-\sigma_{n-1}}\eta_{n-1},$$

$$K_n=(t^2+1)^{-2}\xi_n k_n(\omega_n),\quad P_n=(\alpha^2+1)(t^2+1)^{-2}\frac{\sigma_n}{\sigma_{n+1}-\sigma_n}\eta_n,$$

$$\omega_n=\xi_n(t^2+1)^{-1/2}\exp[-a\arctan(t)],\quad \sigma_{n+1}\neq\sigma_n,\quad \alpha\neq 0,$$

$$A=\begin{pmatrix} a-\alpha & 0 & 0 & 0\\ 0 & a+\alpha & 0 & 0\\ 0 & 0 & a & 1\\ 0 & 0 & -1 & a\end{pmatrix};$$

$$\mathbf{SA_{5,9}}:\ \hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{X}_3=\sigma_n(t^2+1)^{1/2}(\partial_{x_n}+\partial_{y_n}),\quad \hat{X}_4=\sigma_n(t^2+1)^{1/2}\arctan(t)(\partial_{x_n}+\partial_{y_n}),$$

$$\hat{Y}=(t^2+1)\partial_t+(a+t)(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$F_n=(t^2+1)^{-2}\xi_n f_n(\omega_n),\quad G_n=(t^2+1)^{-2}\frac{\sigma_n}{\sigma_n-\sigma_{n-1}}\eta_{n-1},$$

$$K_n=(t^2+1)^{-2}\xi_n k_n(\omega_n),\quad P_n=(t^2+1)^{-2}\frac{\sigma_n}{\sigma_{n+1}-\sigma_n}\eta_n,$$

$$\omega_n=\xi_n(t^2+1)^{-1/2}\exp[-a\arctan(t)],\quad \sigma_{n+1}\neq\sigma_n,\quad \alpha\neq 0,$$

$$A=\begin{pmatrix} a & 0 & 0 & 0\\ -1 & a & 0 & 0\\ 0 & 0 & a & 1\\ 0 & 0 & -1 & a\end{pmatrix}.$$

In all cases the interaction terms G_n and P_n are specified, whereas F_n and K_n each involve an arbitrary function of one variable ω_n. The time dependence of the variable ω_n and the functions F_n and K_n depends on the form of the generator $\hat{Y}$.

After the substitution (3.1) we have altogether 18 five-dimensional Lie algebras. No further symmetry generators can be added, at least in the nonlinear case studied so far.

VII. NONSOLVABLE SYMMETRY ALGEBRAS

Any finite dimensional Lie algebra L that is not solvable is either semisimple, or has a nontrivial and unique Levi decomposition

$$L=S\triangleright R, \tag{7.1}$$

where S is semisimple and R is the radical, i.e., the maximal solvable ideal. The only semisimple Lie algebra that can be realized in terms of the vector fields (2.2) is actually simple, namely $\mathrm{sl}(2,\mathbb{R})$. Up to allowed transformations the realization is unique (and given below by the operators $\hat{Y}_1$, $\hat{Y}_2$ and $\hat{Y}_3$). The determining equations (2.4) and (2.5) can be used to obtain the interaction invariant under the corresponding group $\mathrm{SL}(2,\mathbb{R})$. Equations (1.1) will then be invariant under a five-dimensional group that contains the subalgebra $A_{2,1}$. We have

$$\mathbf{NS_{5,1}}:\ \hat{Y}_1=\partial_t,\quad \hat{Y}_2=t\partial_t+\tfrac{1}{2}(x_n\partial_{x_n}+y_n\partial_{y_n}),\quad \hat{Y}_3=t^2\partial_t+t(x_n\partial_{x_n}+y_n\partial_{y_n}),$$

$$\hat{X}_1=\partial_{x_n}+\partial_{y_n},\quad \hat{X}_2=t(\partial_{x_n}+\partial_{y_n}),$$

$$F_n=\xi_n^{-3}f_n,\quad G_n=\eta_{n-1}^{-3}g_n,$$

$$K_n=\xi_n^{-3}k_n,\quad P_n=\eta_n^{-3}p_n.$$

The Lie algebra $NS_{5,1}$ is isomorphic to the special affine algebra $\mathrm{saff}(2,\mathbb{R})$. This is the only maximal nonsolvable symmetry algebra that occurs.

This completes our analysis of possible symmetries of the system (1.1) with nonlinear interactions.

VIII. SYMMETRIES OF LINEAR INTERACTIONS

In Secs. III–VII we have excluded the case of linear interactions. Let us turn to this case now. We specify Eqs. (1.1) to be

$$\begin{aligned}\ddot{x}_n&=A_n(t)\,\xi_n+B_n(t)\,\eta_{n-1}+U_n(t),\\ \ddot{y}_n&=C_n(t)\,\xi_n+D_n(t)\,\eta_n+V_n(t).\end{aligned} \tag{8.1}$$

The system is still strongly coupled, i.e., the functions A_n, B_n, C_n, D_n are all nonzero. The determining equations reduce to

$$\ddot{\lambda}_n-(\mu_n-\lambda_n)A_n-(\lambda_n-\mu_{n-1})B_n+(a-\tfrac{3}{2}\dot{\tau})U_n-\tau\dot{U}_n=0, \tag{8.2}$$

$$\ddot{\mu}_n-(\mu_n-\lambda_n)C_n-(\lambda_{n+1}-\mu_n)D_n+(a-\tfrac{3}{2}\dot{\tau})V_n-\tau\dot{V}_n=0, \tag{8.3}$$

$$2\dot{\tau}A_n+\tau\dot{A}_n=0, \tag{8.4}$$

$$2\dot{\tau}B_n+\tau\dot{B}_n=0, \tag{8.5}$$

$$2\dot{\tau}C_n+\tau\dot{C}_n=0, \tag{8.6}$$

$$2\dot{\tau}D_n+\tau\dot{D}_n=0, \tag{8.7}$$

$$\tau=\tau_0+\tau_1+\tau_2 t^2, \tag{8.8}$$

since the coefficients of ξ_n, η_n, η_{n-1} and 1 vanish separately.

For $A_n(t),\ldots,D_n(t)$ generic, we obtain $\tau=0$ and then only Eqs. (8.2) and (8.3) (with $\tau=0$) survive. These equations can be solved in the generic case and we obtain two types of symmetries, both just a consequence of linearity.

(1) We take $a=0$ and denote $(\lambda_{h,n},\mu_{h,n})$ the general solution of the homogeneous equations, i.e., Eq. (8.1) with $U_n=V_n=0$. The vector field is

$$\hat{X}_h=\lambda_{h,n}(t)\,\partial_{x_n}+\mu_{h,n}(t)\,\partial_{y_n}. \tag{8.9}$$

(2) For $a\neq 0$ we choose $a=-1$ and denote some chosen particular solution of the inhomogeneous system (8.1) $(\lambda_{p,n},\mu_{p,n})$. The vector field is

$$\hat{X}_p=[x_n-\lambda_{p,n}(t)]\partial_{x_n}+[y_n-\mu_{p,n}(t)]\partial_{y_n}. \tag{8.10}$$

In particular, if we have $U_n=V_n=0$, then we take $\lambda_{p,n}=\mu_{p,n}=0$ in Eq. (8.10).

The symmetry (8.9) only means that we can add any solution of the homogeneous equations to a solution of Eq. (8.1). The symmetry (8.10) corresponds to the fact that a solution of the homogeneous system can be multiplied by a constant.

Let us now assume that a further symmetry generator exists. It is of the form (2.2) with $\tau(t)$ as in Eq. (8.8). Allowed transformations can be used to transform τ into one of four cases. Let us consider them separately.

A. $\tau=0$

No symmetries beyond the generic ones are obtained.

B. $\tau=1$

Using allowed transformations we simplify the additional vector field into

$$\hat{T}=\partial_t+a(x_n\,\partial_{x_n}+y_n\,\partial_{y_n}). \tag{8.11}$$

The determining equations restrict the time dependence of the coefficients in Eq. (8.1) and the system reduces to

$$\ddot{x}_n = f_n\,\xi_n + g_n\,\eta_{n-1} + u_n e^{at},$$
$$\ddot{y}_n = k_n\,\xi_n + p_n\,\eta_n + v_n e^{at}. \tag{8.12}$$

C. $\tau = t$

The additional vector field and invariant equations are reduced to

$$\hat{D} = t\,\partial_t + (a + \tfrac{1}{2})(x_n\,\partial_{x_n} + y_n\,\partial_{y_n}), \tag{8.13}$$

$$\ddot{x}_n = \frac{f_n}{t^2}\,\xi_n + \frac{g_n}{t^2}\,\eta_{n-1} + u_n t^{a-3/2},$$
$$\ddot{y}_n = \frac{k_n}{t^2}\,\xi_n + \frac{p_n}{t^2}\,\eta_n + v_n t^{a-3/2}. \tag{8.14}$$

D. $\tau = t^2 + 1$

The additional vector field and invariant equations are

$$\hat{C} = (t^2+1)\partial_t + (a+t)(x_n\partial_{x_n} + y_n\partial_{y_n}), \tag{8.15}$$

$$\ddot{x}_n = \frac{f_n}{(t^2+1)^2}\,\xi_n + \frac{g_n}{(t^2+1)^2}\,\eta_{n-1} + \frac{u_n}{(t^2+1)^{3/2}}\exp[a\arctan(t)],$$
$$\ddot{y}_n = \frac{k_n}{(t^2+1)^2}\,\xi_n + \frac{p_n}{(t^2+1)^2}\,\eta_n + \frac{v_n}{(t^2+1)^{3/2}}\exp[a\arctan(t)]. \tag{8.16}$$

In all cases f_n, g_n, k_n, p_n, u_n and v_n are independent of t. No further symmetries exist for any of the interactions (8.12), (8.14) or (8.16).

IX. CONCLUSIONS

Let us sum up the results obtained earlier.

For nonlinear interactions the symmetry algebra is at most five-dimensional. The following cases occur.

(1) The nonsolvable algebra $NS_{5,1}$ of Sec. VII. The dependence of the right hand side of Eq. (1.1) on ξ_n and η_n is completely specified by an inverse cube relation. The dependence on the discrete variable n remains arbitrary. The interactions are time independent.

(2) The solvable Lie algebras with Abelian nilradicals $SA_{5,1},\ldots,SA_{5,9}$ [and $SA_{5,10},\ldots,SA_{5,18}$ by the substitution (3.1)] of Sec. VI B. The interactions are all "semilinear." By this we mean that the dependence on one variable η_n is specified to be linear, whereas the dependence on ξ_n remains arbitrary (and vice versa for $SA_{5,10},\ldots,SA_{5,18}$). The time dependence of the nonlinear terms in the interaction depends crucially on the form of the non-nilpotent element $\hat{Y}$. Any attempt to enlarge the symmetry algebra by further elements leads to linear interactions.

(3) The nilpotent five-dimensional Lie algebras $N_{5,1}$ and the related algebra $N_{5,2}$ of Sec. IV. For $N_{5,1}$ the interaction is again semilinear with G_n and P_n linear in η_{n-1} and η_n, respectively, and F_n and K_n arbitrary functions of ξ_n (and vice versa for $N_{5,2}$). The interaction is time independent.

(4) Four-dimensional maximal symmetry algebras are either Abelian, or solvable with the Heisenberg algebra as a nilradical. For $A_{4,1}$ and $A_{4,2}$ the interaction is semilinear with an arbitrary

time dependence in the nonlinear terms. For $SN_{4,1}$, $SN_{4,2}$ and $SN_{4,3}$ the dependence on ξ_n and η_n is completely specified as being monomial, logarithmic or exponential, respectively. There is no time dependence.

(5) A three-dimensional maximal symmetry algebra is either nilpotent, or solvable with an Abelian nilradical. For $N_{3,1}$, the Heisenberg algebra, the interaction is time independent, otherwise arbitrary. The model, studied by Campa *et al.*,[1] namely,

$$F_n(\xi_n)=\frac{1}{M_1}(k_1\xi_n+\varepsilon\beta_1\xi_n^2), \quad K_n(\xi_n)=-\frac{M_1}{M_2}F_n(\xi_n),$$

$$G_n(\eta_{n-1})=-\frac{1}{M_1}(k_2\eta_{n-1}+\varepsilon\beta_2\eta_{n-1}^2), \quad P_n(\eta_n)=-\frac{M_1}{M_2}G_{n+1}(\eta_{n+1}),$$

is of this type. For $SA_{3,1}$, $SA_{3,2}$ and $SA_{3,3}$ the interactions involve four arbitrary functions of one variable. The interaction is entirely specified by the element $\hat{Y}$.

(6) As mentioned earlier, the general interaction in Eq. (1.1) is invariant under the group of global translations and Galilei transformations, corresponding to the algebra $A_{2,1}$ of Eq. (2.16).

The symmetries found in this article can be used to perform symmetry reduction on one hand, and to obtain new solutions from known ones on the other.

Let us look at the example of algebra $NS_{5,1}$. The system (1.1) in this case reduces to

$$\ddot{x}_n=\frac{f_n}{\xi_n^3}+\frac{g_n}{\eta_{n-1}^3}, \quad \ddot{y}_n=\frac{k_n}{\xi_n^3}+\frac{p_n}{\eta_n^3}. \tag{9.1}$$

The algebra sl(2,$\mathbb{R}$) has three inequivalent one-dimensional subalgebras, namely $\hat{Y}_1$, $\hat{Y}_2$ and $\hat{Y}_3+\hat{Y}_1$. Each of them can be used to reduce the system (9.1) to a system of two difference equations. Let us look at the three individual cases separately.

A. Subalgebra $\hat{Y}_1$

This algebra leads to stationary solutions. We have

$$x_n=x_{n,0}, \quad y_n=y_{n,0} \tag{9.2}$$

and hence

$$\xi_{n,0}=\left(-\frac{f_n}{g_n}\right)^{1/3}\eta_{n-1,0}=\left(-\frac{k_n}{p_n}\right)^{1/3}\eta_{n,0}. \tag{9.3}$$

B. Subalgebra $\hat{Y}_2$

The reduction formulas in this case are

$$x_n=x_{n,0}\sqrt{t}, \quad y_n=y_{n,0}\sqrt{t} \tag{9.4}$$

and the recursion relations are

$$-\frac{x_{n,0}}{4}=\frac{f_n}{\xi_{n,0}^3}+\frac{g_n}{\eta_{n-1,0}^3}, \quad -\frac{y_{n,0}}{4}=\frac{k_n}{\xi_{n,0}^3}+\frac{p_n}{\eta_{n,0}^3}. \tag{9.5}$$

C. Subalgebra $\hat{Y}_3+\hat{Y}_1$

We put

$$x_n=x_{n,0}\sqrt{t^2+1}, \quad y_n=y_{n,0}\sqrt{t^2+1} \tag{9.6}$$

and obtain the recursion relations

$$x_{n,0}=\frac{f_n}{\xi_{n,0}^3}+\frac{g_n}{\eta_{n-1,0}^3}, \quad y_{n,0}=\frac{k_n}{\xi_{n,0}^3}+\frac{p_n}{\eta_{n,0}^3}. \tag{9.7}$$

In all three cases we can express ξ_n in terms of η_n and obtain a two term recursion relation for η_n. These can be solved, but we will not go into the details here.

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On the structure of Picard–Fuchs type equations for Liouville–Arnold integrable Hamiltonian system on cotangent phase spaces

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There are studied in detail the structure properties of integral submanifold imbedding mapping for a class of algebraically Liouville integrable Hamiltonian systems on cotangent phase spaces and related with it so called Picard–Fuchs type equations. It is shown that these equations can be in general regularly constructed making use of a given *a priori* system of involutive invariants and proved that their solutions in the Hamolton–Jacobi separable variable case give rise exactly to the integral submanifold imbedding mapping being as known a main ingredient for Liouville–Arnold integrability by quadratures of the Hamiltonian system under regard. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1409961]

I. INTRODUCTION

We consider a completely integrable via Liouville–Arnold[1,2] Hamiltonian system on a cotangent canonically symplectic manifold $(T^*(\mathbb{R}^n), \omega^{(2)})$, $n \in \mathbb{Z}_+$, possessing exactly $n \in \mathbb{Z}_+$ functionally independent and Poisson commuting algebraic polynomial invariants $H_j : T^*(\mathbb{R}^n) \to \mathbb{R}$, $j = \overline{1,n}$. Due to the Liouville–Arnold theorem[1,2] this Hamiltonian system can be completely integrated by quadratures in quasiperiodic functions on its integral submanifold when taken compact. It is equivalent to the statement that this compact integral submanifold is diffeomorphic to a torus $\mathbb{T}^n$, which makes it possible to formulate the problem of integrating the system by means of searching the corresponding integral submanifold imbedding mapping $\pi_h : M_h^n \to T^*(\mathbb{R}^n)$, where by definition

$$M_h^n := \{(q,p) \in T^*(\mathbb{R}^n): \quad H_j(q,p) = h_j \in \mathbb{R}, \quad j = \overline{1,n}\}. \tag{1.1}$$

Since $M_h^n \simeq \mathbb{T}^n$, and the integral submanifold (1.1) is invariant subject to all Hamiltonian flows $K_j : T^*(\mathbb{R}^n) \to T(T^*(\mathbb{R}^n))$, $j = \overline{1,n}$, where

$$i_{K_j} \omega^{(2)} = -dH_j, \tag{1.2}$$

there exist[1,2] corresponding "action-angle"-coordinates $(\varphi, \gamma) \in (\mathbb{T}_\gamma^n, \mathbb{R}^n)$ on the torus $\mathbb{T}_\gamma^n \simeq M_h^n$, specifying its imbedding $\pi_\gamma : \mathbb{T}_\gamma^n \to T^*(\mathbb{R}^n)$ by means of a set of smooth functions $\gamma \in \mathcal{D}(\mathbb{R}^n)$, where

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$$\mathbb{T}^n_\gamma := \{(q,p) \in T^*(\mathbb{R}^n): \quad \gamma_j(h) = \gamma_j \in \mathbb{R}, \quad j = \overline{1,n}\}. \tag{1.3}$$

The induced by (1.3) mapping $\gamma: \mathbb{R}^n \ni h \to \mathbb{R}^n$ is of great interest for many applications and was studied still earlier by Picard and Fuchs subject to the corresponding differential equations it satisfies:

$$\partial \gamma_j(h)/\partial h_i = F_{ij}(\gamma; h), \tag{1.4}$$

where $h \in \mathbb{R}^n$ and $F_{ij}: \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$, $i,j = \overline{1,n}$, are some smooth almost everywhere functions. In the case when the right-hand side of (1.4) is a set of algebraic functions on $\mathbb{C}^n \times \mathbb{C}^n \ni (\gamma; h)$, all Hamiltonian flows $K_j: T^*(\mathbb{R}^n) \to T(T^*(\mathbb{R}^n))$, $j = \overline{1,n}$, are said to be algebraically completely integrable[3–6] in quadratures. In general equations like (1.4) were studied in Refs. 7, 3, and 8, a recent interesting example can be found in Refs. 9 and 10. It is necessary to mention here that the problem of describing integral submanifold imbedding mappings within the canonical transformation approach subject to algebraically integrable Hamiltonian systems on $T^*(\mathbb{R}^n)$ had arisen some time before in artful articles,[3,11,4,12,5] where in particular these mappings were called ''quasi-point transformations.'' The main impact into understanding the role of Picard–Fuchs equations as equations on moduli space of the corresponding algebraic curves was done by Francoise.[9,3,13] There was devised an effective differential-geometric approach to treating the corresponding integral submanifold imbedding mappings by means of specially constructed vector fields on the moduli space of algebraic curves naturally related with a given algebraically integrable Hamiltonian system. His construction was further developed and substantially improved by Tsiganov[14–16] in the framework of his general approach to separation of variables.

II. CANONICAL TRANSFORMATIONS PROPERTIES

It is clear enough that Picard–Fuchs equations (1.4) are related to the associated canonical transformation of the symplectic two-form $\omega^{(2)} \in \Lambda^2(T^*(\mathbb{R}^n))$ in a neighborhood $U(M^n_h)$ of the integral submanifold $M^n_h \subset T^*(\mathbb{R}^n)$. To make it more precise, denote $\omega^{(2)}(q,p) = dpr^*\alpha^{(1)}(q;p)$, where for $(q,p) \in T^*(\mathbb{R}^n)$

$$\alpha^{(1)}(q;p) := \sum_{j=1}^{n} p_j \, dq_j = \langle p, dq \rangle \in \Lambda^1(\mathbb{R}^n) \tag{2.1}$$

is the canonical Liouville one-form on $\mathbb{R}^n$, $\langle \cdot, \cdot \rangle$ is the usual scalar product in $\mathbb{R}^n$, $\mathrm{pr}: T^*(\mathbb{R}^n) \to \mathbb{R}^n$ is the bundle projection. One can now define a mapping

$$dS_q: \mathbb{R}^n \to T^*_q(\mathbb{R}^n), \tag{2.2}$$

such that $dS_q(h) \in T^*_q(\mathbb{R}^n)$ is an exact one-form for all $q \in M^n_h$ and $h \in \mathbb{R}^n$, yielding

$$(dS_q)^*(dpr^*\alpha^{(1)}) = (dS_q)^*\omega^{(2)} := d^2 S_q \equiv 0. \tag{2.3}$$

Thereby the mapping (2.2) defines a so-called generating function[1,2] $S_q: \mathbb{R}^n \to \mathbb{R}$, satisfying on M^n_h the relationship

$$\mathrm{pr}^*\alpha^{(1)}(q;p) + \langle t, dh \rangle = dS_q(h), \tag{2.4}$$

where $t \in \mathbb{R}^n$ is the set of evolution parameters. From (2.4) one gets right away that the equality

$$S_q(h) = \int_{q^{(0)}}^{q} \langle p, dq \rangle \Big|_{M^n_h} \tag{2.5}$$

holds for any $q,q^{(0)}\in M_h^n$. On the other hand, one can define a one more generating function $S_\mu:\mathbb{R}^n\to\mathbb{R}$, such that

$$\mathrm{d}S_\mu:\mathbb{R}^n\to T^*_\mu(M_h^n),$$

where $\mu\in M_h^n\simeq\otimes_{j=1}^n\mathbb{S}_j^1$ are global separable coordinates existing on M_h^n owing to the Liouville–Arnold theorem. Thus one can write down the following canonical relationship:

$$\langle w,\mathrm{d}\mu\rangle+\langle t,\mathrm{d}h\rangle=\mathrm{d}S_\mu(h), \tag{2.6}$$

where $w_j:=w_j(\mu_j;h)\in T^*_{\mu_j}(\mathbb{S}_j^1)$ for every $j=\overline{1,n}$. Whence one follows readily that

$$S_\mu(h)=\sum_{j=1}^n\int_{\mu_j^{(0)}}^{\mu_j}w(\lambda;h)\mathrm{d}\lambda, \tag{2.7}$$

satisfying on $M_h^n\subset T^*(\mathbb{R}^n)$ the following relationship:

$$\mathrm{d}S_\mu+\mathrm{d}\mathcal{L}_\mu=\mathrm{d}S_q|_{q=q(\mu;h)} \tag{2.8}$$

for some mapping $\mathcal{L}_\mu:\mathbb{R}^n\to\mathbb{R}$. As a result of (??) and (2.8) one gets that the following important expressions

$$t_i=\partial S_\mu(h)/\partial h_i,\quad \langle p,\partial q/\partial\mu_i\rangle=w_i+\partial\mathcal{L}_\mu/\partial\mu_i \tag{2.9}$$

hold for all $i=\overline{1,n}$. A construction similar to the above-mentioned one can be done subject to the imbedded torus $\mathbb{T}_\gamma^n\subset T^*(\mathbb{R}^n)$:

$$\mathrm{d}\tilde{S}_q(\gamma):=\sum_{j=1}^n p_j\,\mathrm{d}q_j+\sum_{i=1}^n\varphi_i\,\mathrm{d}\gamma_i, \tag{2.10}$$

where owing to (2.2) $\tilde{S}_q(\gamma):=S_q(\xi\cdot\gamma)$, $\xi\cdot\gamma(h)=h$, for all $(q;\gamma)\in U(M_h^n)$. For angle coordinates $\varphi\in\mathbb{T}_\gamma^n$ one obtains from (2.10) that

$$\varphi_i=\partial\tilde{S}_q(\gamma)/\partial\gamma_i \tag{2.11}$$

for all $i=\overline{1,n}$. As $\varphi_i\in\mathbb{R}/2\pi\mathbb{Z}$, $i=\overline{1,n}$, from (2.12) one derives that

$$\frac{1}{2\pi}\oint_{\sigma_j^{(h)}}\mathrm{d}\varphi_i=\delta_{ij}=\frac{1}{2\pi}\frac{\partial}{\partial\gamma_i}\oint_{\sigma_j^{(h)}}\mathrm{d}\tilde{S}_q(\gamma)=\frac{1}{2\pi}\frac{\partial}{\partial\gamma_i}\oint_{\sigma_j^{(h)}}\langle p,\mathrm{d}q\rangle \tag{2.12}$$

for all canonical cycles $\sigma_j^{(h)}\subset M_h^n$, $j=\overline{1,n}$, constituting a basis of the one-dimensional homology group $H^1(M_h^n;\mathbb{Z})$. Thereby, owing to (2.12), it follows that for all $i=\overline{1,n}$ "action" variables can be found as

$$\gamma_i=\frac{1}{2\pi}\oint_{\sigma_i^{(h)}}\langle p,\mathrm{d}q\rangle. \tag{2.13}$$

Recall now that $M_h^n\simeq\mathbb{T}_\gamma^n$ are diffeomorphic also to $\otimes_{j=1}^n\mathbb{S}_j^1$, where $\mathbb{S}_j^1$, $j=\overline{1,n}$, are some one-dimensional real circles. The evolution along any of vector fields $K_j:T^*(\mathbb{R}^n)\to T(T^*(\mathbb{R}^n))$, $j=\overline{1,n}$, on $M_h^n\subset T^*(\mathbb{R}^n)$ is known[17,18] to be a linear winding around the torus $\mathbb{T}_\gamma^n$, that can be interpreted also in the following way: The above-introduced independent of each other global coordinates on circles $\mathbb{S}_j^1$, $j=\overline{1,n}$, are such that the resulting evolution undergoes a quasiperiodic

motion. These coordinates—still being called Hamilton–Jacobi—prove to be very important for accomplishing the complete integrability by quadratures via solving the corresponding Picard—Fuchs type equations.

Let us denote these separable coordinates on the integral submanifold $M_h^n \simeq \otimes_{j=1}^n \mathbb{S}_j^1$ by $\mu_j \in \mathbb{S}_j^1$, $j=\overline{1,n}$, and define the corresponding imbedding mapping $\pi_h: M_h^n \to T^*(\mathbb{R}^n)$ as

$$q=q(\mu;h), \quad p=p(\mu;h). \tag{2.14}$$

Such a general kind of imbedding mappings was also considered before in Refs. 12, 17–20. There exist two important cases subject to the imbedding (2.14).

The first case is related to the integral submanifold $M_h^n \subset T^*(\mathbb{R}^n)$, which can be parametrized as a manifold by means of the base coordinates $q \in \mathbb{R}^n$ of the cotangent bundle $T^*(\mathbb{R}^n)$. This can be explained as follows: The canonical Liouville one-form $\alpha^{(1)} \in \Lambda^1(\mathbb{R}^n)$, in accordance with the diagram

$$\begin{array}{ccccc} T^*(M_h^n) & \simeq & T^*(\otimes_{j=1}^n \mathbb{S}_j^1) & \overset{\overline{\pi}_h^*}{\leftarrow} & T^*(\mathbb{R}^n) \\ \mathrm{pr}\downarrow & & \mathrm{pr}\downarrow & & \mathrm{pr}\downarrow \\ M_h^n & \simeq & \otimes_{j=1}^n \mathbb{S}_j^1 & \overset{\overline{\pi}_h}{\rightarrow} & \mathbb{R}^n \end{array} \tag{2.15}$$

is mapped by the imbedding mapping $\overline{\pi}_h = \mathrm{pr} \cdot \pi_h : M_h^n \to \mathbb{R}^n$ not depending on a set of parameters $h \in \mathbb{R}^n$, into the one-form

$$\alpha_h^{(1)} = \overline{\pi}_h^* \alpha^{(1)} = \sum_{j=1}^n w_j(\mu_j;h)\mathrm{d}\mu_j, \tag{2.16}$$

where $(\mu,w) \in T^*(\otimes_{j=1}^n \mathbb{S}_j^1) \simeq \otimes_{j=1}^n T^*(\mathbb{S}_j^1)$. The imbedding mapping $\overline{\pi}_h: M_h^n \to \mathbb{R}^n$ due to the equality (2.16) makes the function $\mathcal{L}_\mu: \mathbb{R}^n \to \mathbb{R}$ to be zero giving rise to the generating function $S_\mu: \mathbb{R}^n \to \mathbb{R}$, enjoying the condition

$$\mathrm{d}S_\mu = \mathrm{d}S_q\big|_{q=q(\mu)}, \tag{2.17}$$

where as before

$$S_\mu(h) = \sum_{j=1}^n p_j \, \mathrm{d}q_j + \sum_{j=1}^n t_j \, \mathrm{d}h_j \tag{2.18}$$

and $\det\|\partial q(\mu)/\partial\mu\| \neq 0$ almost everywhere on M_h^n for all $h \in \mathbb{R}^n$. Similarly to (2.9), one gets from (2.18) that

$$t_j = \partial S_\mu(h)/\partial h_j \tag{2.19}$$

for $j=\overline{1,n}$. Concerning the second part of the imbedding mapping (2.14) we arrive at the following simple result due to the equality (2.16):

$$p_i = \sum_{j=1}^n w_j(\mu_j;h)\partial\mu_j/\partial q_i, \tag{2.20}$$

where $i=\overline{1,n}$ and $\det\|\partial\mu/\partial q\| \neq 0$ almost everywhere on $\pi(M_h^n)$ due to the local invertibility of the imbedding mapping $\pi: M_h^n \to \mathbb{R}^n$. Thus, we can claim that the problem of complete integrability in the first case is solved if the only imbedding mapping $\pi: M_h^n \to \mathbb{R}^n \subset T^*(\mathbb{R}^n)$ is constructed. This

case was in detail considered in Ref. 21 where the corresponding Picard–Fuchs type equations were built based on a one extension of Galissot–Reeb (see the Theorem of Galissot–Reeb in Ref. 6) and modern Francoise results.[9,3,13] Namely, similar to (1.4), these equations are defined as follows:

$$\partial w_j(\mu_j;h)/\partial h_k = P_{kj}(\mu_j, w_j;h), \tag{2.21}$$

where $P_{kj}: T^*(\otimes_{j=1}^n \mathbb{S}_j^1)\times\mathbb{C}^n \to \mathbb{C}$, $k,j=\overline{1,n}$, are some algebraic functions of their arguments.

Concerning *the second case* when the integral submanifold $M_h^n \subset T^*(\mathbb{R}^n)$ *cannot be* imbedded almost everywhere into the base space $\mathbb{R}^n \subset T^*(\mathbb{R}^n)$, a relationship like (2.18) does not take place, and we are forced to consider the usual canonical transformation from $T^*(\mathbb{R}^n)$ to $T^*(\mathbb{R}^n)$ based on a mapping $d\mathcal{L}_q: \otimes_{j=1}^n \mathbb{S}_j^1 \to T^*(\mathbb{R}^n)$, where $\mathcal{L}_q: \otimes_{j=1}^n \mathbb{S}_j^1 \to \mathbb{R}$ enjoys for all $\mu \in \otimes_{j=1}^n \mathbb{S}_j^1 \simeq M_h^n \ni q$ the following relationship:

$$\mathrm{pr}^*\, \alpha^{(1)}(q;p) = \sum_{j=1}^n w_j\, d\mu_j + d\mathcal{L}_q(\mu). \tag{2.22}$$

In this case we can derive for any $\mu \in \otimes_{j=1}^n \mathbb{S}_j^1$ the introduced before hereditary generating function $\mathcal{L}_\mu: \mathbb{R}^n \to T^*(\otimes_{j=1}^n \mathbb{S}_j^1)$ as

$$d\mathcal{L}_\mu = d\mathcal{L}_q|_{q=q(\mu;h)}, \tag{2.23}$$

satisfying evidently the following canonical transformation condition:

$$dS_q(h) = \sum_{j=1}^n w_j(\mu_j;h)d\mu_j + \sum_{j=1}^n t_j\, dh_j + d\mathcal{L}_\mu(h) \tag{2.24}$$

for almost all $\mu \in \otimes_{j=1}^n \mathbb{S}_j^1$ and $h \in \mathbb{R}^n$. Based on (2.24) one can derive the following relationships:

$$\partial \mathcal{L}_\mu(h)/\partial h_j = \langle p, \partial q/\partial h_j\rangle|_{M_h^n} \tag{2.25}$$

for all $j=\overline{1,2}$, $\mu \in \otimes_{j=1}^n \mathbb{S}_j^1$ and $h \in \mathbb{R}^n$. Whence the following important analytical result

$$\begin{aligned} t_s &= \sum_{j=1}^n \int_{\mu_j^{(0)}}^{\mu_j} (\partial w_j(\lambda;h)/\partial h_s)d\lambda, \\ \sum_{j=1}^n p_j(\mu;h)(\partial q_j/\partial \mu_s) &= w_s + \partial \mathcal{L}_\mu(h)/\partial \mu_s \end{aligned} \tag{2.26}$$

holds for all $s=\overline{1,2}$ and $\mu, \mu^{(0)} \in \otimes_{j=1}^n \mathbb{S}_j^1$ with parameters $h \in \mathbb{R}^n$ being fixed. Thereby we have found a natural generalization of the relationships (2.20) subject to the extended integral submanifold imbedding mapping $\pi_h: M_h^n \to T^*(\mathbb{R}^n)$ in the form (2.14).

Assume now that functions $w_j: \mathbb{C}\times\mathbb{C}^n \to \mathbb{C}$, $j=\overline{1,n}$, satisfy in general Picard–Fuchs equations like (2.21), having due to Refs. 7, 3, 22 the following algebraic solutions:

$$w_j^{n_j} + \sum_{k=0}^{n_j-1} c_{j,k}(\lambda;h) w_j^k = 0, \tag{2.27}$$

where $c_{j,k}: \mathbb{C}\times\mathbb{C}^n \to \mathbb{C}$, $k=\overline{0,n_j-1}$, $j=\overline{1,n}$, are some polynomials in $\lambda \in \mathbb{C}$. Each algebraic curve of (2.27) is known to be in general topologically equivalent due to the Riemann theorem[7,22] to some Riemannian surface $\Gamma_h^{(j)}$ of genus $g_j \in \mathbb{Z}_+$, $j=\overline{1,n}$. Thereby, one can realize the local

diffeomorphism $\rho: M_h^n \to \otimes_{j=1}^n \Gamma_h^{(j)}$, mapping homology group basis cycles $\sigma_j^{(h)} \subset M_h^n$, $j=\overline{1,n}$, into homology subgroup $H_1(\otimes_{j=1}^n \Gamma_h^{(j)};\mathbb{Z})$ basis cycles $\sigma_j(\Gamma_h) \subset \Gamma_h^{(j)}$, $j=\overline{1,n}$, satisfying the following relationships:[23]

$$\rho(\sigma_j^{(h)}) = \sum_{k=1}^{n} n_{jk} \sigma_k(\Gamma_h), \tag{2.28}$$

where $n_{jk} \in \mathbb{Z}$, $k=\overline{1,j}$ and $j=\overline{1,n}$, are some fixed integers. Based on (2.28) and (2.23) one can write down, for instance, expressions (2.13) as follows:

$$\gamma_i = \frac{1}{2\pi} \sum_{j=1}^{n} n_{ij} \oint_{\sigma_j(\Gamma_h)} w_j(\lambda;h)\mathrm{d}\lambda, \tag{2.29}$$

where $i=\overline{1,n}$. Subject to the evolution on $M_h^n \subset T^*(\mathbb{R}^n)$ one can easily obtain from (2.25) that

$$\mathrm{d}t_i = \sum_{j=1}^{n} (\partial w_j(\mu_j;h)/\partial h_i)\mathrm{d}\mu_j \tag{2.30}$$

at $\mathrm{d}h_i = 0$ for all $i=\overline{1,n}$, giving rise evidently to a global τ parametrization of the set of circles $\otimes_{j=1}^n \mathbb{S}_j^1 \subset \otimes_{j=1}^n \Gamma_h^{(j)}$, that is one can define some inverse algebraic functions to Abelian type integrals (2.23) as

$$\mu = \mu(\tau;h), \tag{2.31}$$

where as before, $\tau=(t_1,t_2,\ldots,t_n) \in \mathbb{R}^n$ is a vector of evolution parameters. Recalling now expression (2.14) for integral submanifold mapping $\pi_h: M_h^n \to T^*(\mathbb{R}^n)$, one can at last write down final expressed by ''quadratures'' mappings for evolutions on $M_h^n \subset T^*(\mathbb{R}^n)$ as follows:

$$q = q(\mu(\tau;h)) = \tilde{q}(\tau;h), \quad p = p(\mu(\tau;h)) = \tilde{p}(\tau;h), \tag{2.32}$$

where obviously a vector $(\tilde{q},\tilde{p}) \in T^*(\mathbb{R}^n)$ is quasiperiodic in each variable $t_i \in \tau$, $i=\overline{1,n}$. Thus the following theorem holds.

Theorem 2.1: *Every completely integrable Hamiltonian system admitting an algebraic submanifold $M_h^n \subset T^*(\mathbb{R}^n)$ possesses a separable canonical transformation (2.24) which is described by differential algebraic Picard–Fuchs type equations whose solution is a set of algebraic curves (2.27).*

Therefore, the main ingredient of this scheme of integrability by quadratures is finding the Picard–Fuchs type equations (2.21) corresponding to the integral submanifold imbedding mapping (2.14) depending in general on $\mathbb{R}^n \ni h$-parameters for the case when the integral submanifold $M_h^n \subset T^*(\mathbb{R}^n)$ cannot be imbedded into the base space $\mathbb{R}^n \subset T^*(\mathbb{R}^n)$ of the phase space $T^*(\mathbb{R}^n)$.

Similar to the differential-geometric approach developed in Refs. 9, 21, and 13, one can find one-forms $h_j^{(1)} \in \Lambda^1(T^*(\mathbb{R}^n))$, $j=\overline{1,n}$, enjoying the following identity on $T^*(\mathbb{R}^n)$:

$$\omega^{(2)}(q,p) := \sum_{j=1}^{n} \mathrm{d}p_j \wedge \mathrm{d}q_j = \sum_{j=1}^{n} \mathrm{d}H_j \wedge h_j^{(1)}. \tag{2.33}$$

The one-forms $h_j^{(1)} \in \Lambda^1(T^*(\mathbb{R}^n))$, $j=\overline{1,n}$, possess the following important properties when pulled back to the integral submanifold (1.1):

$$\pi_h^* h_j^{(1)} := \overline{h_j^{(1)}} = \mathrm{d}t_j, \tag{2.34}$$

where $\overline{h_j^{(1)}} \in \Lambda^1(M_h^n)$, and $\pi_{h*}\mathrm{d}/\mathrm{d}t_j = K_j \cdot \pi_h$ for all $j=\overline{1,n}$. Expression (2.34) combined with (2.30) gives rise easily to the following set of relationships:

$$\overline{h}_j^{(1)} = \sum_{j=1}^{n} (\partial w_j(\mu_j;h)/\partial h_i)\mathrm{d}\mu_j \tag{2.35}$$

at $\mathrm{d}h_j = 0$ for all $j = \overline{1,n}$ on $M_h^n \otimes_{j=1}^n \mathbb{S}_j^1 \subset \otimes_{j=1}^n \Gamma_h^{(j)}$ for all $j = \overline{1,n}$. Since we are interested in the integral submanifold imbedding mapping (2.11) being locally diffeomorphic in a neighborhood $U(M_h^n) \subset T^*(\mathbb{R}^n)$, the Jacobian $\det\|\partial q(\mu;h)/\partial\mu\| \neq 0$ almost everywhere in $U(M_h^n)$. On the other hand, as was shown in Refs. 9, 21, and 13, the set of one-forms $\overline{h}_j^{(1)} \in \Lambda^1(M_h^n)$, $j = \overline{1,n}$, can be, in general, represented in $U(M_h^n)$ as

$$\overline{h}_j^{(1)} = \sum_{k=1}^{n} \overline{h}_{jk}^{(1)}(q,p)\mathrm{d}q_k|_{M_h^n}, \tag{2.36}$$

where $\overline{h}_{jk}^{(1)} : T^*(\mathbb{R}^n) \to \mathbb{R}$, $k,j = \overline{1,n}$, are some algebraic expressions of their arguments. Thereby, one easily finds from (2.36) and (2.35) that

$$\partial w_i(\mu_i;h)/\partial h_j = \sum_{k=1}^{n} \overline{h}_{jk}^{(1)}(q(\mu;h),p(\mu;h))(\partial q_k(\mu;h)/\partial\mu_i) \tag{2.37}$$

for all $i,j = \overline{1,n}$. Subject to p-variables in (2.37) we must owing to (2.26) use the expressions

$$\begin{gathered} \sum_{j=1}^{n} p_j(\mu;h)(\partial q_j/\partial\mu_s) = w_s + \partial\mathcal{L}_\mu(h)/\partial\mu_s, \\ \partial\mathcal{L}_\mu(h)/\partial h_j = \langle p, \partial q/\partial h_j\rangle|_{M_h^n}, \end{gathered} \tag{2.38}$$

being true for $s = \overline{1,n}$ and all $\mu \in \otimes_{j=1}^n \mathbb{S}_j$, $h \in \mathbb{R}^n$ in the neighborhood $U(M_h^n) \subset T^*(\mathbb{R}^n)$ chosen before. Thereby, we arrived at the following form of (2.37):

$$\partial w_i(\mu_i;h)/\partial h_j = \overline{P}_{ji}(\mu,w;h), \tag{2.39}$$

where for all $i,j = \overline{1,n}$,

$$\overline{P}_{ji}(\mu,w;h) := \sum_{k=1}^{n} \overline{h}_{jk}^{(1)}(q(\mu;h),p(\mu;h))\partial q_k/\partial\mu_i) \tag{2.40}$$

depend correspondingly only on $\overset{<(i)}{\neq h} \ni (\mu_i,w_i)$-variables for each $i \in \{\overline{1,n}\}$ and all $j = \overline{1,n}$. This condition can be evidently written down as follows:

$$\partial\overline{P}_{ji}(\mu,w;h)/\partial\mu_k = 0 \tag{2.41}$$

for $j,i \neq k \in \{\overline{1,n}\}$ at almost all $\mu \in \otimes_{j=1}^n \mathbb{S}_j^1$ and $h \in \mathbb{R}^n$. The set of conditions (2.37) gives rise in general to a system of algebraic-differential equations subject to the imbedding mapping $\mathrm{pr}\,\pi_h : M_h^n \to \mathbb{R}^n$ defined analytically by (2.14) and the generating function (2.23). As a result of solving these equations we obtain, evidently owing to (2.39) and (2.41), the following system of Picard–Fuchs type equations:

$$\partial w_i(\mu_i;h)/\partial h_j = P_{ji}(\mu_i,w_i;h) \tag{2.42}$$

where, in general, the mappings

$$P_{ji} : \Gamma_h^{(i)} \times \mathbb{R}^n \to \mathbb{C} \tag{2.43}$$

are some algebraic expressions. Since the set of algebraic curves (2.27) must enjoy the Picard–Fuchs type system (2.42), we can retrieve this set just solving them. The latter gives rise due to (2.25) and (2.14) to the integrability of all flows on $M_h^n \subset T^*(\mathbb{R}^n)$ by quadratures as was mentioned in Sec. 1.

Theorem 2.2: *Let there be given a completely integrable Hamiltonian system on the coadjoint manifold $T^*(\mathbb{R}^n)$ whose integral submanifold $M_h^n \subset T^*(R^n)$ is described by Picard–Fuchs type algebraic equations (2.42). The corresponding imbedding mapping $\pi_h : M_h^n \to T^*(R^n)$ (2.14) is a solution of a compatibility condition subject to the differential-algebraic relationships (2.41) on the canonical transformations generating function (2.23).*

In the following we shall show that the scheme described previously really leads to an algorithmic procedure of constructing the Picard–Fuchs type equations (2.42) and the corresponding integral submanifold imbedding mappings $\pi_h : M_h^n \to T^*(\mathbb{R}^n)$ in the form (2.14) applying it to the so called Henon–Heiles and truncated Focker–Plank Hamiltonian systems on the canonically symplectic cotangent space $T^*(\mathbb{R}^2)$.

III. EXAMPLES

A. The Henon–Heiles system

This flow is governed by the Hamiltonian

$$H_1 = \tfrac{1}{2}p_1^2 + \tfrac{1}{2}p_2^2 + q_1 q_2^2 + \tfrac{1}{3}q_1^3 \tag{3.1}$$

on the canonically symplectic phase space $M^4 = T^*(\mathbb{R}^2)$ with the symplectic structure

$$\omega^{(2)} = \sum_{j=1}^{2} \mathrm{d}p_j \wedge \mathrm{d}q_j . \tag{3.2}$$

As is well known, there exists the following additional invariant that commutes with (3.1):

$$H_2 = p_1 p_2 + 1/3 q_2^3 + q_1^2 q_2 , \tag{3.3}$$

that is $\{H_1, H_2\} = 0$ on the entire space M^4. Put $H_j = h_j \in \mathbb{R}$, $j = \overline{1,2}$, thereby defining the integral submanifold

$$M_h^2 := \{(q,p) \in M^4 : h(H_j) = h_j \in \mathbb{R}, j = \overline{1,2}\},$$

if compact and connected, being diffeomorphic to the standard torus $\mathbb{T}^2 \simeq \mathbb{S}^1 \times \mathbb{S}^1$ owing to the Liouville–Arnold theorem. One can therefore find cyclic (separable) coordinates $\mu_j \in \mathbb{S}^1$, $j = \overline{1,2}$, on the torus $\mathbb{T}^2$ such that the symplectic structure (6.2) will take the form:

$$\omega^{(2)} = \sum_{j=1}^{2} \mathrm{d}w_j \wedge \mathrm{d}\mu_j , \tag{3.4}$$

where the conjugate variables $w_j \in T^*(\mathbb{S}^1)$, $j = \overline{1,2}$, on M_h^2 depend only on the corresponding variables $\mu_j \in \mathbb{S}_j^1$, $j = \overline{1,2}$. In this case it is evident that the evolution along M_h^2 will be separable and representable by means of quasiperiodic functions of the evolution parameters. To show this, recall that the fundamental determining equations (2.41) are based on the one-forms $\overline{h}_j^{(1)} \in \Lambda(M_h^2)$, $j = \overline{1,2}$, satisfying the identity

$$\sum_{j=1}^{2} \mathrm{d}H_j \wedge_j \overline{h}_j^{(1)} = \sum_{j=1}^{2} \mathrm{d}p_j \wedge \mathrm{d}q_j . \tag{3.5}$$

Here

$$\overline{h}_j^{(1)}=\sum_{k=1}^{2}\overline{h}_{jk}(q,p)\mathrm{d}q_k, \tag{3.6}$$

where $j=\overline{1,2}$. Substituting (3.7) into (3.6), one obtains

$$\overline{h}_1^{(1)}=\frac{p_1\mathrm{d}q_1}{p_1^2-p_2^2}+\frac{p_2\mathrm{d}q_2}{p_1^2-p_2^2},\quad \overline{h}_2^{(1)}=\frac{p_2\mathrm{d}q_1}{p_{21}^2-p_1^2}+\frac{p_1\mathrm{d}q_2}{p_1^2-p_2^2}. \tag{3.7}$$

On the other hand, the following implication holds on $M_h^2\subset M^4$:

$$\alpha_h^{(1)}=\sum_{j=1}^{2}w_j(\mu_j;h)\mathrm{d}\mu_j\Rightarrow\sum_{j=1}^{2}p_j\,\mathrm{d}q_j:=\alpha^{(1)}, \tag{3.8}$$

where we have assumed that the integral submanifold M_h^2 admits the local coordinates in the base manifold $\mathbb{R}^2$ endowed with the canonical one-form $\alpha_h^{(1)}\in\Lambda(M_h^2)$ as given in (3.9). Thus, making use of the imbedding mapping $\pi_h:M_h^2\to T^*(\mathbb{R}^2)$ in the form

$$q_j=q_j(\mu),\quad p_j=p_j(\mu), \tag{3.9}$$

$j=\overline{1,2}$, one readily finds that the equalities

$$p_j=\sum_{k=1}^{2}w_k(\mu_k;h)\partial\mu_k/\partial q_j \tag{3.10}$$

hold for $j=\overline{1,2}$ on the entire integral submanifold M_h^2.

Substituting (3.11) into (3.8) and using the characteristic relationships (2.41), one obtains after simple but cumbersome calculations the following differential-algebraic expressions:

$$\partial q_1/\partial\mu_1-\partial q_2/\partial\mu_1=0,\quad \partial q_1/\partial\mu_2+\partial q_2/\partial\mu_2=0, \tag{3.11}$$

whose simplest solutions are

$$q_1=(\mu_1+\mu_2)/2,\quad q_2=(\mu_1-\mu_2)/2. \tag{3.12}$$

Using (3.11) one finds that

$$p_1=w_1+w_2,\quad p_2=w_1-w_2, \tag{3.13}$$

where

$$w_1=\sqrt{h_1+h_2-4/3\mu_1^3},\quad w_2=\sqrt{h_1-h_2-4/3\mu_2^3}. \tag{3.14}$$

Consequently, one obtains the separable[11,17,14] Hamiltonian functions (3.1) and (3.3) in some open vicinity of the cotangent space $T^*(M_h^2)$:

$$h_1=\tfrac{1}{2}w_1^2+\tfrac{1}{2}w_2^2+\tfrac{2}{3}(\mu_1^3+\mu_2^3),\quad h_2=\tfrac{1}{2}w_1^2-\tfrac{1}{2}w_2^2+\tfrac{2}{3}(\mu_1^3-\mu_2^3), \tag{3.15}$$

which generate the following separable motions on $M_h^2\subset T^*(\mathbb{R}^2)$:

$$\begin{aligned}\mathrm{d}\mu_1/\mathrm{d}t&:=\partial h_1/\partial w_1=\sqrt{h_1+h_2-4/3\mu_1^3},\\ \mathrm{d}\mu_2/\mathrm{d}t&:=\partial h_1/\partial w_2=\sqrt{h_1-h_2-4/3\mu_2^3}\end{aligned} \tag{3.16}$$

for the Hamiltonian (3.1), and

$$\begin{aligned} \mathrm{d}\mu_1/\mathrm{d}x &:= \partial h_2/\partial w_1 = \sqrt{h_1+h_2-4/3\mu_1^3}, \\ \mathrm{d}\mu_2/\mathrm{d}t &:= \partial h_1/\partial w_2 = -\sqrt{h_1-h_2-4/3\mu_2^3} \end{aligned} \tag{3.17}$$

for the Hamiltonian (3.3), where $x,t\in\mathbb{R}$ are the corresponding evolution parameters.

Analogously, one can show that there exists[12,17,18,20] an integral submanifold imbedding mapping in the form (2.14) for the following integrable modified Henon–Heiles involutive system:

$$\begin{aligned} H_1 &= \tfrac{1}{2}p_1^2+\tfrac{1}{2}p_2^2+q_1q_2^2+\tfrac{16}{3}q_1^3, \\ H_2 &= 9p_2^4+36q_1p_2^2q_2^2-12p_1p_2q_2^3-2q_2^4(q_2^2+6q_1^2), \end{aligned} \tag{3.18}$$

where $\{H_1,H_1\}=0$ on the entire phase space $M^4=T^*(\mathbb{R}^2)$. Based on considerations similar to the above-mentioned ones, one can deduce the following[17,18,20] expressions:

$$\begin{aligned} q_1 &= -\frac{1}{4}(\mu_1+\mu_2)-\frac{3}{8}\left(\frac{w_1+w_2}{\mu_1-\mu_2}\right)^2, \\ q_2^2 &= -2\sqrt{h_2}/(\mu_1-\mu_2), \quad w_1=\sqrt{2/3\mu_1^3-4/3\sqrt{h_2}-8h_1}, \\ p_1 &= \frac{1}{2\sqrt{-6(\mu_1+\mu_2+4q_1)}}\left[\frac{-2\sqrt{h_2}}{\mu_1-\mu_2}-\mu_1\mu_2+4(\mu_1+\mu_2)q_1+32q_1^2\right], \\ p_2 &= \sqrt{h_2}(\mu_{1+}\mu_2+4q_1)/(3(\mu_{1-}\mu_2)), \quad w_2=\sqrt{2/3\mu_2^3+4/3\sqrt{h_2}-8h_1}, \end{aligned} \tag{3.19}$$

thereby solving explicitly the problem of finding the corresponding integral submanifold imbedding $\pi_h: M_h^2\to T^*(\mathbb{R}^2)$ that generates separable flows in the variables $(\mu,w)\in T^*(M_h^2)$.

B. A four-dimensional truncated Focker–Plank Hamiltonian system

Let us consider the flow

$$\left.\begin{aligned} \mathrm{d}q_1/\mathrm{d}t = p_1+\alpha(q_1+p_2)(q_2+p_1), \quad \mathrm{d}q_2/\mathrm{d}t = p_2, \\ \mathrm{d}p_1/\mathrm{d}t = -(q_1+p_2)-\alpha[q_2p_1+1/2(p_1^2+p_2^2+q_2^2)], \\ \mathrm{d}p_2/\mathrm{d}t = -(q_2+p_1), \end{aligned}\right\} = K_1(q,p), \tag{3.20}$$

where $K_1: T^*(\mathbb{R}^2)\to T(T^*(\mathbb{R}^2))$ is the corresponding vector field on $T^*(\mathbb{R}^2)\ni(q,p)$, $t\in\mathbb{R}$ is an evolution parameter, called a truncated four-dimensional Focker–Plank flow. It is easy to verify that functions $H_j: T^*(\mathbb{R}^2)\to\mathbb{R}$, $j=\overline{1,2}$, where

$$H_1 = 1/2(p_1^2+p_2^2+q_1^2)+q_1p_2+\alpha(q_1+p_2)[q_2p_1+1/2(p_1^2+p_2^2+q_2^2)] \tag{3.21}$$

and

$$H_2 = 1/2(p_1^2+p_2^2+q_2^2)+q_2p_1 \tag{3.22}$$

are functionally independent invariants with respect to the flow (3.21). Moreover, the invariant (3.21) is the Hamiltonian function for (3.21), that is the relationship

$$i_{k_1}\omega^{(2)} = -\mathrm{d}H_1 \tag{3.23}$$

holds on $T^*(\mathbb{R}^2)$, where the symplectic structure $\omega^{(2)}\in\Lambda^2(T^*(\mathbb{R}^2))$ is given as follows:

$$\omega^{(2)} := \mathrm{d}pr^*\alpha^{(1)} = \sum_{j=1}^{2} \mathrm{d}p_j \wedge \mathrm{d}q_j, \tag{3.24}$$

with $\alpha^{(1)} \in \Lambda^1(\mathbb{R}^2)$ being the canonical Liouville form on $\mathbb{R}^2$:

$$\alpha^{(1)}(q;p) = \sum_{j=1}^{2} p_j \, \mathrm{d}q_j \tag{3.25}$$

for any $(q,p) \in T^*(\mathbb{R}^2) \simeq \Lambda^1_q(\mathbb{R}^2)$.

The invariants (3.22) and (3.23) evidently commute with each other subject to the associated Poisson bracket on $T^*(\mathbb{R}^2)$:

$$\{H_1, H_2\} = 0. \tag{3.26}$$

Thereby, owing to the Abelian Liouville–Arnold theorem[1,2] the dynamical system (3.21) is completely integrable by quadratures on $T^*(\mathbb{R}^2)$, and we can apply the scheme devised in Sec. II to the commuting invariants (3.22) and (3.23) subject to the symplectic structure (3.25). One easily calculates that

$$\omega^{(2)} = \sum_{i=1}^{2} \mathrm{d}H_i \wedge h_i^{(1)}, \tag{3.27}$$

where the corresponding one-forms $\pi_h^* h_i^{(1)} := \overline{h}_i^{(1)} \in \Lambda^1(M_h^2)$, $i = \overline{1,2}$, are given as

$$\begin{aligned} \overline{h}_1^{(1)} &= \frac{p_2 \mathrm{d}q_1 - (p_1+q_2)\mathrm{d}q_2}{p_1p_2 - (p_1+q_2)(q_1+p_2) - \alpha h_2(p_1+q_2)}, \\ \overline{h}_2^{(1)} &= \frac{-[(q_1+p_2)(1+\alpha p_2)+\alpha h_2]\mathrm{d}q_1 + (p_1+\alpha[h_2+(q_2+p_1)(q_1+p_2)])\mathrm{d}q_2}{p_1p_2 - (q_2+p_1)(\alpha h_2 + q_1 + p_2)}, \end{aligned} \tag{3.28}$$

and an invariant submanifold $M_h^2 \subset T^*(\mathbb{R}^2)$ is defined as

$$M_h^2 := \{(q,p) \in T^*(\mathbb{R}^2) : H_i(q,p) = h_i \in \mathbb{R}, i = \overline{1,2}\} \tag{3.29}$$

for some parameters $h \in \mathbb{R}^2$. Based now on expressions (3.29) and (2.37) one can easily construct functions $\overline{P}_{ij}(w;h)$, $i,j = \overline{1,2}$, in (2.39), defined on $T^*(M_h^2) \simeq T^*(\otimes_{j=1}^2 \mathbb{S}_j^1)$ subject to the integral submanifold imbedding mapping $\pi_h : M_h^2 \to T^*(\mathbb{R}^2)$ in coordinates $\mu \in \otimes_{j=1}^2 \mathbb{S}_j^1 \subset \otimes_{j=1}^2 \Gamma_h^{(j)}$, which we do not write down in detail due to their a bit long and cumbersome form. Having applied then the criterion (2.41), we arrive at the following compatibility relationships subject to the mappings $q : (\otimes_{j=1}^2 \mathbb{S}_j^1) \times \mathbb{R}^2 \to \mathbb{R}^2$ and $p : (\otimes_{j=1}^2 \mathbb{S}_j^1) \times \mathbb{R}^2 \to T_q^*(\mathbb{R}^2)$:

$$\begin{aligned} &\partial q_1 / \partial \mu_1 - \partial q_2 / \partial \mu_2 = 0, \\ &\partial w_1 / \partial h_1 (\partial q_1 / \partial h_1) = \partial w_2 / \partial h_1 (\partial q_2 / \partial h_1), \\ &\partial w_1 / \partial h_2 (\partial q_1 / \partial h_2) = \partial w_2 / \partial h_2 (\partial q_2 / \partial h_2), \\ &w_1 \partial w_1 / \partial h_1 - w_2 \partial w_2 / \partial h_2 = 0, \\ &\partial (w_1 \partial w_1 / \partial h_2) / \partial \mu_1 + \alpha \partial q_1 / \partial \mu_1 = 0 \end{aligned} \tag{3.30}$$

and so on, for all $\mu \in \otimes_{j=1}^2 \mathbb{S}_j^1$. Solving equations like (3.11), one can find right away that

$$p_1 = w_1, \quad p_2 = w_2,$$

$$q_1 = c_1 + \mu_1 - w_2(\mu_1;h), \qquad (3.31)$$
$$q_2 = c_2 + \mu_2 - w_1(\mu_2;h),$$

where $c_j(h_1,h_2) \in \mathbb{R}^1$, $j=\overline{1,2}$, are constant, hold on $T^*(M_h^2)$, giving rise to the following Picard–Fuchs type equations in the form (2.42):

$$\begin{gathered}\partial w_1(\mu_1;h)/\partial h_1 = 1/w_1,\\ \partial w_1(\mu_1;h)/\partial h_2 = -\alpha/\mu_1,\\ \partial w_2(\mu_2;h)/\partial h_1 = 0,\\ \partial w_2(\mu_2;h)/\partial h_2 = 1/w_2.\end{gathered} \qquad (3.32)$$

The Picard–Fuchs equations (3.33) can be easily integrated by quadratures as follows:

$$\begin{gathered}w_1^2 + k_1(\mu_1) - 2h_1 = 0,\\ w_2^2 + k_2(\mu_2) - 2h_2 = 0,\end{gathered} \qquad (3.33)$$

where $k_j : \mathbb{S}_j^1 \to \mathbb{C}$, $j=\overline{1,2}$ are still unknown functions. For the to be determined explicitly, it is necessary to substitute (3.12) into expressions (3.22) and (3.23), making use of (3.34) that amounts to the following results:

$$k_1 = \mu_1^2 + \alpha h_2, \quad k_2 = \mu_2^2 \qquad (3.34)$$

under the condition that $c_1=0$, $c_2=0$. Thereby, we have constructed, owing to (3.34), the corresponding (2.27) algebraic curves $\Gamma_h^{(j)}$, $j=\overline{1.2}$, in the explicit form:

$$\begin{gathered}\Gamma_h^{(1)} := \{(\lambda, w_1) : w_1^2 + \lambda^2 + \lambda h_2 - 2h_1) = 0\},\\ \Gamma_h^{(2)} := \{(\lambda, w_2) : w_2^2 + \lambda^2 - 2h^2 = 0\},\end{gathered} \qquad (3.35)$$

where $(\lambda, w_j) \in \mathbb{C}\times\mathbb{C}$, $j=\overline{1,2}$, and $h \in \mathbb{R}^2$ are arbitrary parameters. Making use now of expressions (3.36) and (3.32), one can construct in explicit form the integral submanifold imbedding mapping $\pi_h : M_h^2 \to T^*(\mathbb{R}^2)$ for the flow (3.21):

$$\begin{gathered}q_1 = \mu_1 - \sqrt{2h_2 - \mu_2^2}, \quad p_1 = w_1(\mu_1;h),\\ q_2 = \mu_2 - \sqrt{2h_1 - 2h_2\mu_1 - \mu_1^2}, \quad p_2 = w_2(\mu_2;h),\end{gathered} \qquad (3.36)$$

where $(\mu, w) \in \otimes_{j=1}^2 \Gamma_h^{(j)}$. As was mentioned before in Sec. II, (3.37) together with explicit expressions like (2.26) make it possible right away to find solutions to the truncated Focker–Plank flow (3.21) by quadratures, thereby completing its integrability.

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Asymptotic expansion of ${}_2F_1(a,b;c;x)$ in terms of confluent hypergeometric functions

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We have developed a new asymptotic formula for ${}_2F_1(a,b;c;x)$ in which a and c are finite, $|b|$ tends to infinity and the argument x tends to zero. We make use of this result to obtain asymptotic expansions of the electric dipole ($E1$) *quantal differential* excitation function for the adiabaticity parameter $\xi=\eta_f-\eta_i$ and the Sommerfeld parameter η_f tending to infinity simultaneously, while the parameter η_i remains finite. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The motivation and some of the groundwork for the present article derive from an earlier article,[1] henceforth referred to as I.

We begin our discussion with the quantal expression[2,3] of the differential excitation function,

$$\mathrm{d}f_{E1}(\theta,\eta_i,\xi)=\frac{8\pi^3\eta_i\eta_f}{9\xi^2}\frac{e^{\mp\pi|\xi|}}{\sinh(\pi\eta_i)\sinh(\pi\eta_f)}\frac{d}{dx}\left(-x\frac{d}{dx}|{}_2F_1(-i\eta_i,-i\eta_f;1;x)|^2\right)\mathrm{d}\Omega, \tag{1.1}$$

which determines the angular distribution of inelastically scattered particles in Coulomb excitation.[4,5] We make explicit the distinction between the repulsive and attractive cases by writing ξ as $\mp|\xi|$. We can convert the repulsive case ($\eta_i>0$) to the attractive case ($\eta_i<0$) by simply switching the signs of η_i, η_f and ξ. The total effect of this transformation is to replace the factor of $\exp(-\pi|\xi|)$, for repulsive potentials, by a factor of $\exp(+\pi|\xi|)$ for attractive potentials. The argument x is defined by

$$x=-\frac{4\eta_i\eta_f}{\xi^2}\sin^2\left(\frac{\theta}{2}\right), \tag{1.2}$$

where θ is the deflection angle of the scattered particle. Gauss' hypergeometric function ${}_2F_1(a,b;c;z)$ is defined by

$${}_2F_1(a,b;c;z)=\sum_{n=0}^{\infty}\frac{(a)_n(b)_n}{n!(c)_n}z^n \tag{1.3}$$

within the circle of convergence of this series ($|z|<1$) and by analytic continuation elsewhere. We will henceforth omit the subscripts and write ${}_2F_1(\cdots)$ simply as $F(\cdots)$. The dimensionless Sommerfeld parameter η_i is defined by

$$\eta_i=\frac{Z_1Z_2\mathrm{e}^2}{\hbar v_i}=Z_1Z_2\sqrt{\frac{M}{E_i}}, \tag{1.4}$$

where $Z_1(Z_2)$ is the charge number of the projectile (atomic system), v_i is the relative velocity, M is the reduced mass in electron-mass units, and E_i is the initial kinetic energy of relative motion measured in Rydbergs (13.6 eV). The dimensionless adiabaticity parameter ξ is defined by

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$$\xi=\eta_f-\eta_i=\eta_i\left[\left(1-\frac{E_{if}}{E_i}\right)^{-1/2}-1\right]=Z_1Z_2\sqrt{\frac{M}{E_i}}\left[\left(1-\frac{E_{if}}{E_i}\right)^{-1/2}-1\right], \tag{1.5}$$

where the indices i and f refer to the initial and final states, respectively, and $E_{if}=E_i-E_f$. In order to evaluate Eq. (1.1), we first expand the derivatives

$$\begin{aligned}\frac{d}{dx}\left(-x\frac{d}{dx}|F|^2\right)&=\frac{d}{dx}\left[-x\frac{d}{dx}(FF^*)\right]=\frac{d}{dx}\left[-x\left(\frac{dF}{dx}F^*+F\frac{dF^*}{dx}\right)\right]=-\left[\frac{dF}{dx}F^*+F\frac{dF^*}{dx}\right]\\&\quad-x\left[\frac{d^2F}{dx^2}F^*+2\frac{dF}{dx}\frac{dF^*}{dx}+F\frac{d^2F}{dx^2}\right]=-2\mathbf{Re}\left(\frac{dF}{dx}F^*\right)-2x\mathbf{Re}\left(\frac{d^2F}{dx^2}F^*\right)\\&\quad-2x\left|\frac{dF}{dx}\right|^2.\end{aligned} \tag{1.6}$$

We notice that $F^*(a,b;c;z)=F(a^*,b^*;c^*;z^*)$, so that

$$F^*(-i\eta_i,-i\eta_f;1;x)=F(i\eta_i,i\eta_f;1;x). \tag{1.7}$$

With this in place, we can perform the differentiation using equation 15.2.2 of Ref. 6,

$$\frac{d^n}{dz^n}{}_2F_1(a,b;c;z)=\frac{(a)_n(b)_n}{c_n}{}_2F_1(a+n,b+n;c+n;z), \tag{1.8}$$

to obtain

$$\begin{aligned}df_{E1}(\theta,\eta_i,\xi)&=\frac{8\pi^3(\eta_i\eta_f)^2}{9\xi^2}\frac{e^{\mp\pi|\xi|}}{\sinh(\pi\eta_i)\sinh(\pi\eta_f)}\times\{2\mathbf{Re}[F(1-i\eta_i,1\\&\quad-i\eta_f;2;x)F(i\eta_i,i\eta_f;1;x)]+x[\mathbf{Re}\{(1-i\eta_i)(1-i\eta_f)\\&\quad\times F(2-i\eta_i,2-i\eta_f;3;x)F(i\eta_i,i\eta_f;1;x)\}\\&\quad-2\eta_i\eta_f|F(1-i\eta_i,1-i\eta_f;2;x)|^2]\}d\Omega.\end{aligned} \tag{1.9}$$

Using Gauss' relations for contiguous functions and eq. 15.3.3 of Ref. 6 in the previous equation yields

$$\begin{aligned}df_{E1}(\theta,\eta_i,\xi)&=\frac{16\pi^3(\eta_i\eta_f)^2}{9\xi^2}\frac{e^{\mp\pi|\xi|}}{\sinh(\pi\eta_i)\sinh(\pi\eta_f)}\times\left\{\mathbf{Re}\left[\left(1+\frac{4\eta_i\eta_f\sin^2(\theta/2)}{\xi^2}\right)^{1-i(\eta_i+\eta_f)}\right.\right.\\&\quad\times[(1-i\eta_f)\times F(1-i\eta_i,2-i\eta_f;2;x)F(1-i\eta_i,1-i\eta_f;2;x)\\&\quad+i\eta_fF^2(1-i\eta_i,1-i\eta_f;2;x)]-\left(1+\eta_f{}^2+(1-i\eta_i)(1-i\eta_f)\frac{4\eta_i\eta_f\sin^2(\theta/2)}{\xi^2}\right)\\&\quad\times F(1-i\eta_i,2-i\eta_f;2;x)F(1+i\eta_i,1+i\eta_f;2;x)+i\eta_f(1+i\eta_f)\\&\quad\left.\times\left(1+\frac{4\eta_i\eta_f\sin^2(\theta/2)}{\xi^2}\right)\times F(1+i\eta_i,2+i\eta_f;2;x)F(1-i\eta_i,1-i\eta_f;2;x)\right]\\&\quad+(1+\eta_f^2)\left(1+\frac{4\eta_i\eta_f\sin^2(\theta/2)}{\xi^2}\right)|F(1-i\eta_i,2-i\eta_f;2;x)|^2\\&\quad\left.+\eta_f^2|F(1-i\eta_i,1-i\eta_f;2;x)|^2\right\}d\Omega.\end{aligned} \tag{1.10}$$

It is now possible to take the limit as $\theta\to0$ in Eqs. (1.9) and (1.10), respectively, provided we also assume that $\xi\neq0$, i.e., the collision is inelastic. Under these conditions $x=0$, and since all of the hypergeometric functions then have the value of unity, we obtain the following result

$$df_{E1}(\theta=0,\eta_i,\xi)=\frac{16}{9}\frac{\pi^3(\eta_i\eta_f)^2}{\xi^2}\frac{e^{\mp\pi|\xi|}}{\sinh(\pi\eta_i)\sinh(\pi\eta_f)}\,d\Omega. \tag{1.11}$$

In the limiting case $E_f\to 0$ and $\theta\neq 0$, the parameters η_f, ξ both tend to ∞ simultaneously, whereas the parameter η_i remains finite and the argument $x\to 0$. We first obtain an expansion for the ordinary hypergeometric function in terms of confluent hypergeometric functions. One should be aware that some leading and first-order terms cancel out in the subexpressions of Eq. (1.10), and quadratic factors in ξ mean that the second-order terms in ξ^{-1} become important as $\xi\to\infty$.

We used the symbolic computation program MAPLE VI[7] in order to carry out the algebra in this work. Numerical results of Eq. (1.10), for moderate values of ξ, obtained with MAPLE and the FORTRAN code written by Burgess[8] agree to six-decimal figures.

II. EXPANSION FOR HYPERGEOMETRIC FUNCTION

It is well-known (Ref. 9 §2.3.2 and §6.1, Ref. 10 §1.1, and Ref. 11 §3.1) that

$$\lim_{b\to\infty}F\left(a,b;c;\frac{z}{b}\right)={}_1F_1(a,c;z), \tag{2.1}$$

where ${}_1F_1(a,c;z)$ is the confluent hypergeometric function.

We now derive a second-order correction to this result.

By definition

$$F\left(a,b;c;\frac{z}{b}\right)=\sum_{n=0}^{\infty}\frac{(a)_n}{(c)_n n!}z^n\frac{(b)_n}{b^n}, \tag{2.2}$$

but, as was discussed in paper I (§II of Ref. 1)

$$\frac{(b)_n}{b^n}=\prod_{r=1}^{n-1}\left(1+\frac{r}{b}\right)=1+\frac{1}{2}n(n-1)\frac{1}{b}+n(n-1)\left[\frac{1}{3}(n-2)+\frac{1}{8}(n-2)(n-3)\right]\frac{1}{b^2}+\cdots, \tag{2.3}$$

so

$$F\left(a,b;c;\frac{z}{b}\right)=\sum_{n=0}^{\infty}\frac{(a)_n}{(c)_n n!}z^n\left\{1+\frac{1}{2}n(n-1)\frac{1}{b}+n(n-1)\left[\frac{1}{3}(n-2)+\frac{1}{8}(n-2)(n-3)\right]\frac{1}{b^2}\right\}$$
$$+\cdots. \tag{2.4}$$

Interchanging the two summations, we see that the first term sums to $f(z)={}_1F_1(a,c;z)$. To sum the second, third and fourth terms, we note that

$$z^2f''(z)=\sum_{n=0}^{\infty}n(n-1)\frac{(a)_n}{(c)_n n!}z^n,$$

$$z^3f'''(z)=\sum_{n=0}^{\infty}n(n-1)(n-2)\frac{(a)_n}{(c)_n n!}z^n, \tag{2.5}$$

$$z^4f^{(4)}(z)=\sum_{n=0}^{\infty}n(n-1)(n-2)(n-3)\frac{(a)_n}{(c)_n n!}z^n.$$

We can use the differentiation formula (equation 13.4.9 of Ref. 6) to obtain the following expressions for $f''(z)$, $f'''(z)$ and $f^{(4)}(z)$:

$$f''(z)=\frac{d^2}{dz^2}{}_1F_1(a,c;z)=\frac{a(a+1)}{c(c+1)}{}_1F_1(a+2,c+2;z),$$

$$f'''(z)=\frac{d^3}{dz^3}{}_1F_1(a,c;z)=\frac{a(a+1)(a+2)}{c(c+1)(c+2)}{}_1F_1(a+3,c+3;z), \tag{2.6}$$

$$f^{(4)}(z)=\frac{d^4}{dz^4}{}_1F_1(a,c;z)=\frac{a(a+1)(a+2)(a+3)}{c(c+1)(c+2)(c+3)}{}_1F_1(a+4,c+4;z).$$

So, we have the asymptotic expression

$$F\left(a,b;c;\frac{z}{b}\right)\sim{}_1F_1(a,c;z)+\frac{a(a+1)}{c(c+1)}\frac{z^2}{2}{}_1F_1(a+2,c+2;z)\frac{1}{b}+\left[\frac{a(a+1)(a+2)}{c(c+1)(c+2)}\frac{z^3}{3}{}_1F_1(a+3,\right.$$

$$\left.c+3;z)+\frac{a(a+1)(a+2)(a+3)}{c(c+1)(c+2)(c+3)}\frac{z^4}{8}{}_1F_1(a+4,c+4;z)\right]\frac{1}{b^2}, \tag{2.7}$$

for $|b|$ large.

III. SPECIALIZATION TO THE PRESENT CASE

Equations (1.9) and (1.10) have hypergeometric functions with the following form

$$F(\alpha-i\eta_i,\beta-i\eta_f;\gamma;x)=F(\alpha-i\eta,\beta-i(\eta+\xi);\gamma;x), \tag{3.1}$$

or those of the form

$$F(\alpha+i\eta_i,\beta+i\eta_f;\gamma;x)=F(\alpha+i\eta,\beta+i(\eta+\xi);\gamma;x). \tag{3.2}$$

The form (3.1) may be converted to that of (3.2) by making the substitution $\eta\rightarrow-\eta$ and $\xi\rightarrow-\xi$. For this reason, we concern ourselves with expanding only the form (3.1) and make use of this transformation in order to deal with the form (3.2).

Applying (2.7) to (3.1) gives

$$\begin{aligned}F(\alpha-i\eta,\beta-i(\eta+\xi);\gamma;x)\sim{}&{}_1F_1(\alpha-i\eta,\gamma;z)+\frac{(\alpha-i\eta)(\alpha+1-i\eta)}{2\gamma(\gamma+1)}z^2\\&\times{}_1F_1(\alpha+2-i\eta,\gamma+2;z)\frac{1}{\beta-i(\eta+\xi)}\\&+\left\{\frac{(\alpha-i\eta)(\alpha+1-i\eta)(\alpha+2-i\eta)}{3\gamma(\gamma+1)(\gamma+2)}z^3\right.\\&\times{}_1F_1(\alpha+3-i\eta,\gamma+3;z)\\&+\frac{(\alpha-i\eta)(\alpha+1-i\eta)(\alpha+2-i\eta)(\alpha+3-i\eta)}{8\gamma(\gamma+1)(\gamma+2)(\gamma+3)}z^4\\&\left.\times{}_1F_1(\alpha+4-i\eta,\gamma+4;z)\right\}\frac{1}{[\beta-i(\eta+\xi)]^2},\end{aligned} \tag{3.3}$$

where

$$z=[\beta-i(\eta+\xi)]x,$$

and the argument x is defined by Eq. (1.2). The term z is a nonconstant function of ξ. Thus, in addition to the limiting process associated with the expansion of the hypergeometric function, there are additional terms associated with the variation of z as $\xi\to\infty$. We note that

$$z=4i\eta\sin^2\left(\frac{\theta}{2}\right)-4(\beta-2i\eta)\sin^2\left(\frac{\theta}{2}\right)\frac{\eta}{\xi}-4(\beta-i\eta)\sin^2\left(\frac{\theta}{2}\right)\frac{\eta^2}{\xi^2}. \tag{3.4}$$

We also expand, to second-order in powers of ξ^{-1}, quantities related to z and x and obtain

$$\begin{aligned} zx &\sim -16i\frac{\eta^2}{\xi}\sin^4\left(\frac{\theta}{2}\right)+16\frac{\eta^2}{\xi^2}(\beta-3i\eta)\sin^4\left(\frac{\theta}{2}\right),\\ zx^2 &\sim 64i\frac{\eta^3}{\xi^2}\sin^6\left(\frac{\theta}{2}\right),\\ zx^3 &\sim -256\frac{\eta^4}{\xi^2}\sin^8\left(\frac{\theta}{2}\right). \end{aligned} \tag{3.5}$$

Using the differentiation formula (13.4.9) of Ref. 6 and expanding the hypergeometric functions in Eq. (3.3) as a Taylor series about $z_0=4i\eta\sin^2(\theta/2)$, leads to the asymptotic behavior

$$\begin{aligned} F(\alpha-i\eta,\beta-i(\eta+\xi);\gamma;x)\sim{}& {}_1F_1(\alpha-i\eta,\gamma;z_0)-4\frac{\eta}{\xi}\sin^2\left(\frac{\theta}{2}\right)\frac{(\alpha-i\eta)}{\gamma}\Bigg\{(\beta-2i\eta){}_1F_1(\alpha+1\\ &-i\eta,\gamma+1;z_0)+2i\eta\sin^2\left(\frac{\theta}{2}\right)\frac{(\alpha+1-i\eta)}{(\gamma+1)}{}_1F_1(\alpha+2-i\eta,\gamma\\ &+2;z_0)\Bigg\}+4\frac{\eta^2}{\xi^2}\sin^2\left(\frac{\theta}{2}\right)\frac{(\alpha-i\eta)}{\gamma}\Bigg\{-(\beta-i\eta){}_1F_1(\alpha+1-i\eta,\gamma\\ &+1;z_0)+2\sin^2\left(\frac{\theta}{2}\right)(\beta-2i\eta)^2\frac{(\alpha+1-i\eta)}{(\gamma+1)}{}_1F_1(\alpha+2-i\eta,\gamma\\ &+2;z_0)+2\sin^2\left(\frac{\theta}{2}\right)\frac{(\alpha+1-i\eta)}{\gamma+1}\Bigg[(\beta-3i\eta){}_1F_1(\alpha+2-i\eta,\gamma\\ &+2;z_0)+4i\eta\sin^2\left(\frac{\theta}{2}\right)(\beta-2i\eta)\frac{(\alpha+2-i\eta)}{(\gamma+2)}{}_1F_1(\alpha+3-i\eta,\gamma\\ &+3;z_0)\Bigg]+8\eta\sin^4\left(\frac{\theta}{2}\right)\frac{(\alpha+1-i\eta)(\alpha+2-i\eta)}{(\gamma+1)(\gamma+2)}\Bigg[i\frac{2}{3}{}_1F_1(\alpha+3\\ &-i\eta,\gamma+3;z_0)-\eta\sin^2\left(\frac{\theta}{2}\right)\frac{(\alpha+3-i\eta)}{(\gamma+3)}{}_1F_1(\alpha+4-i\eta,\gamma\\ &+4;z_0)\Bigg]\Bigg\}, \end{aligned} \tag{3.6}$$

for $\eta/\xi\ll 1$.

IV. APPLICATION TO DIPOLE EXCITATION FUNCTION

Upon applying the asymptotic expansion of the hypergeometric function [Eq. (3.6)] to Eq. (1.10) we find, for an attractive Coulomb field, the zeroth-order approximation

$$
\begin{aligned}
df_{E1}(\theta,\eta,\xi\to\infty)=\frac{64}{9}\pi^3\eta^2\exp(-2\pi\eta)[1-\exp(-2\pi\eta)]^{-1}\times\Bigg[\mathbf{Re}\Bigg\{\exp\Bigg[-4i\eta\sin^2\left(\frac{\theta}{2}\right)\Bigg]\\
\times\Bigg[({}_1F_1(1-i\eta,2;z_0))^2+2i\eta(1-i\eta)\sin^2\left(\frac{\theta}{2}\right){}_1F_1(2-i\eta,3;z_0){}_1F_1(1\\
-i\eta,2;z_0)\Bigg\}\Bigg]-2\eta\sin^2\left(\frac{\theta}{2}\right)\mathbf{Re}\{i(1+i\eta){}_1F_1(2+i\eta,3;-z_0){}_1F_1(1-i\eta,2;z_0)\}\\
-8\eta^2\sin^4\left(\frac{\theta}{2}\right)\mathbf{Re}\{(1+i\eta){}_1F_1(2+i\eta,3;-z_0){}_1F_1(1-i\eta,2;z_0)\}\\
+4\eta^2\sin^2\left(\frac{\theta}{2}\right)[|{}_1F_1(1-i\eta,2;z_0)|^2+(1+\eta^2)|{}_1F_1(2-i\eta,3;z_0)|^2]\Bigg]d\Omega, \quad (4.1)
\end{aligned}
$$

where $z_0=4i\eta\sin^2(\theta/2)$.

Using the leading order of Eq. (3.6) in Eq. (1.9) gives the equivalent limit of the exact quantal excitation function as $\xi\to\infty$,

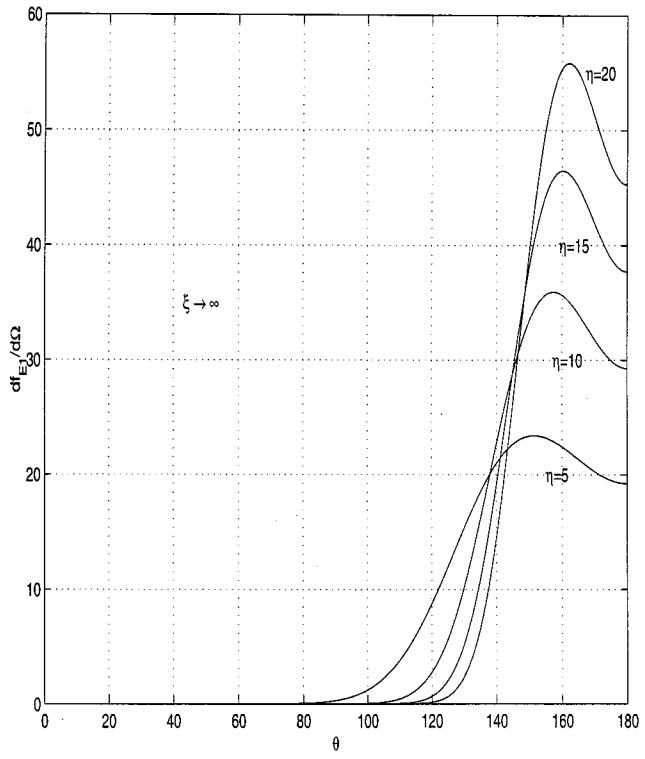

FIG. 1. Asymptotic differential excitation function for an attractive Coulomb field. The functions $df_{E1}(\theta,\eta,\xi\to\infty)/d\Omega$ are plotted as a function of θ for fixed values of η. As $\eta\to\infty$ the function becomes more and more sharply peaked, eventually attaining the singular behavior of the semiclassical approximation.

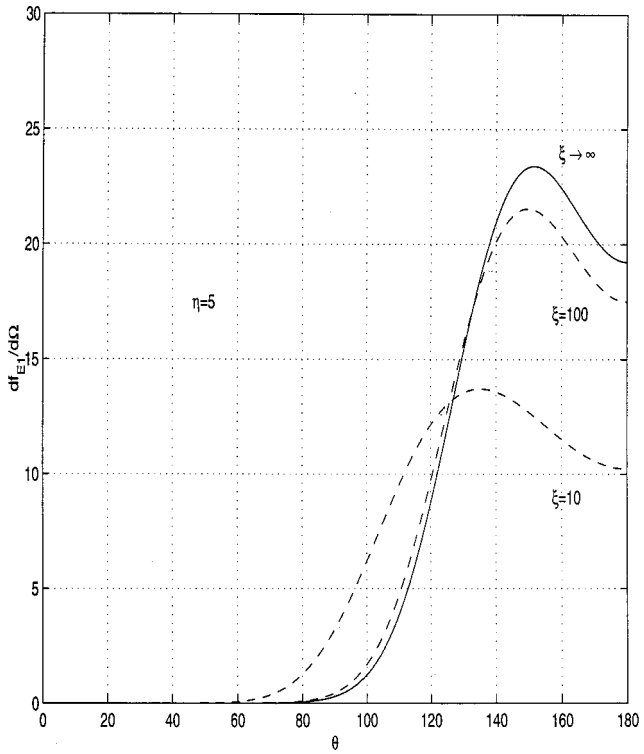

FIG. 2. Differential excitation functions, for an attractive Coulomb field, plotted as a function of θ. $--$, functions $\mathrm{d}f_{E1}(\theta,\eta=5,\xi)/\mathrm{d}\Omega$ for fixed values of ξ; $-$, asymptotic function $\mathrm{d}f_{E1}(\theta,\eta=5,\xi\to\infty)/\mathrm{d}\Omega$.

$$df_{E1}(\theta,\eta,\xi\to\infty)=\frac{64}{9}\,\pi^3\eta^2\exp(-2\pi\eta)[1-\exp(-2\pi\eta)]^{-1}\times\mathbf{Re}\Big\{{}_1F_1(1-i\eta,2;z_0)\,{}_1F_1(i\eta,1;$$
$$-z_0)+2i\eta(1-i\eta)\sin^2\left(\frac{\theta}{2}\right)\,{}_1F_1(2-i\eta,3;z_0)\times{}_1F_1(i\eta,1;-z_0)$$
$$+4\eta^2\sin^2\left(\frac{\theta}{2}\right)|{}_1F_1(1-i\eta,2;z_0)|^2\Big\}\,\mathrm{d}\Omega. \tag{4.2}$$

At this point, we can easily take the limit as $\theta\to 0$ in Eqs. (4.1) and (4.2), and the result is

$$df_{E1}(\theta=0,\eta,\xi\to\infty)=\tfrac{64}{9}\,\pi^3\eta^2\exp(-2\pi\eta)[1-\exp(-2\pi\eta)]^{-1}, \tag{4.3}$$

which is identical to Eq. (1.11), taken in the limit as $\xi\to\infty$. In the repulsive case, the excitation function is everywhere 0, as $\xi\to\infty$. This is expected, since, in that case, the projectile wave function is excluded from being very near the target by the Coulomb barrier. Equations (4.1) and (4.2) are also finite at $\theta=\pi$.

In Fig. 1 we present results for the quantal differential excitation function, using the asymptotic expression [Eq. (4.1)], for different values of the parameter η. As $\eta\to\infty$, the function becomes more and more sharply peaked, eventually attaining the singular behavior of the semiclassical approximation, viz.,

$$\frac{\mathrm{d}f_{E1}}{\mathrm{d}\Omega}(\theta,\eta\to\infty,\xi\to\infty)=\begin{cases}0, & 0\leqslant\theta<\pi,\\ \infty, & \theta=\pi.\end{cases} \tag{4.4}$$

In Fig. 2, we show values of the exact expression [Eq. (1.10)], for $\eta=5$ and different values

of the parameter ξ, and the asymptotic expression [Eq. (4.1)]. In the limit of large values for ξ, the differential excitation function approaches values obtained using the *asymptotic* differential function.

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Checkerboard composites with separated phases

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Recently the authors have developed a method [SIAM J. Appl. Math. **61**, 1839–1556 (2001)] capable of solving, in closed form, boundary value problems for four-phase doubly periodic checkerboard composites with continuity between the different phases. The method is based upon a novel conformal mapping that preserves the doubly periodic nature of the physical problem. The aim of the current article is to explore generalizations of that approach where we now replace continuity between some phases by nonconducting or perfectly conducting strips, thereby modeling debonding or electrodes in electrochemical devices. The specific objective is to determine effective resistivities and related parameters for these four-phase objects in a concise and explicit form. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1398336]

I. INTRODUCTION

We shall consider doubly periodic boundary value problems in electrostatics, or other analogous subjects whose underlying governing equation is Laplace's equation. There are many applications in physics: heat transfer, electrostatics, flow in porous media and composite materials; explicit closed-form solutions for model structures are useful benchmarks and can demonstrate theoretical ideas and relations useful either for refining numerical work, or of interest in their own right. We concentrate upon checkerboard structures, and in each repeating checkerboard cell we shall have distinct differing phases and we aim to calculate effective properties, such as effective resistivities and dissipation, when the medium is subjected to some external applied field. Since the problems are harmonic, the most natural approach is to use complex variable techniques; however, there is a fundamental difficulty in that it is very difficult to satisfy all the continuity or boundary conditions between the distinct phases while simultaneously maintaining the periodicity conditions. It is this difficulty that our efforts have been focused upon.

If we have, say, a two-phase material and one phase is perfectly conducting, or of infinite resistivity, then much progress can be made using standard conformal mapping techniques[1] or the method of images.[2] But outside these limits, distinct phases pose a considerable challenge and the only exact solutions to boundary value problems, and corresponding formulas for effective properties, of this doubly periodic class are the classical Rayleigh[3] and Maxwell[4] solutions, and for checkerboard two-phase geometries previous analyses exist for square,[5] or rectangular,[6,7] cells. These checkerboard analyses rest upon solving complicated Markushevich conjugate Riemann–Hilbert problems. Recently the authors[8,9] have bypassed this approach and have been able to consider three- and four-phase rectangular checkerboard geometries. This enabled the present authors to prove the Mortola and Steffé[10] conjecture for the effective resistivities of a four-phase square checkerboard structure as an interesting subcase of rectangular checkerboards. Square checkerboards have the advantage of some additional geometrical symmetry, and for two phases this has led to the well-known geometric mean law and generalizations that emerge from using

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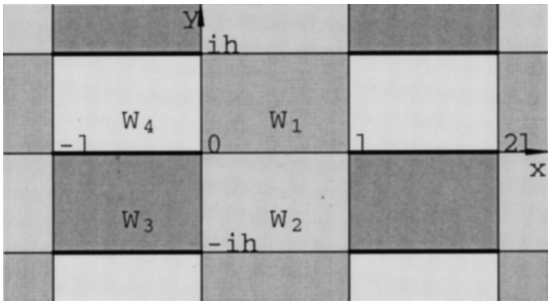

FIG. 1. The geometry for a doubly periodic four-phase checkerboard with a nonconducting strip, the thicker lines lying along $-l<x<0$, $y=\pm nh$, $n=0,1,...$, inserted between phases 3 and 4.

reciprocal relations.[11–13] Very recently Milton[14] extended this approach to also prove the Mortola and Steffé conjecture using a method completely independent of ours.

Our recent approach rests upon a piece of mathematical origami using conformal mapping into a simple object, on a two-sheeted Riemann surface, from the doubly periodic boundary value problem. The purpose of the present article is to explore this further, by considering some phases to be separated by nonconducting or perfectly conducting slits, thereby modeling delamination or electrochemical devices,[15] albeit in a simple model.

It should also be mentioned that an analytical approach using complex analysis is by no means the only avenue open for tackling this type of problem. Estimates of effective parameters are important in several areas of physics and engineering, thus numerical,[16–18] asymptotic,[19] network analogies,[20] variational bounds,[21] and other approaches complementary to ours have been developed, although in most cases two-phase structures have been considered, and the insertion of nonconducting or superconducting strips is a further complication that appears not to have been attempted. In some cases these approaches allow extensions to nonlinear composites.[22] Nonetheless, it is important and, we think, interesting to have some benchmark closed-form solutions available.

II. FORMULATION

We begin from the governing equations for a static electric field $\mathbf{E}$: $\nabla\cdot(\sigma\mathbf{E})=0$, $\nabla\times\mathbf{E}=0$, with the conductivity, σ, constant in each homogeneous region; hereon we exclusively use the language of electrostatics. Then at an interface between dissimilar media we have no jump in the tangential component of the field or the normal component of the current density leading to: $[\![\sigma E_n]\!]=0$, $[\![E_t]\!]=0$, where the $[\![\ ]\!]$ denote jumps in a quantity and the subscripts t, n denote tangential and normal components of the field, $\mathbf{E}=(E_n,E_t)$. As the conductivity, σ, is constant in each cell we can define a potential ϕ such that $\mathbf{E}=-\nabla\phi$ and thus $\nabla^2\phi=0$; ϕ is harmonic and this motivates the complex variable approach.

We choose to use a vector $\mathbf{w}=\sigma\mathbf{E}$, and thus $\nabla\cdot\mathbf{w}=0$, $\nabla\times(\rho\mathbf{w})=0$, with ρ as the resistivity, constant in each cell. The vector $\mathbf{w}$ has interface conditions $[\![\rho w_t]\!]=0$, $[\![w_n]\!]=0$. In each phase, distinguished by the subscript k where we number the phases clockwise and $k=1,...,4$, we find it is most convenient to utilize complex variables, that is, $z=x+iy$ and $w_k(z)=w_{kx}-iw_{ky}$ where $\mathbf{w}_k=(w_{kx},w_{ky})$.

In each problem that we shall consider we apply mean fluxes, a, b in (2.1), across each cell (see for instance the geometry of Fig. 1), $W=[-l,l]\times[-h,h]$, and then calculate the effective resistivities, $\rho_{x,y}$ as defined in (2.2), that in turn can be utilized to find the dissipation and a resistivity tensor. In our evaluations we take integrals for the effective resistivities along the axes themselves, although there is no loss of generality in doing so. That is, ρ_y is the same if calculated as the integral from $y=-h$ to $y=h$ for any $-l<x<l$, and similarly for ρ_x integrated over $x=-l,l$ for $-h<y<h$. This has some bearing upon our later analysis as we shall, for nonconducting boundary conditions along $-l<x<0$, $y=\pm nh$, have three unknowns and apparently only

two imposed mean fluxes; the extra constraint is that the potential, ϕ, is continuous at the ends of the nonconducting strips and thus ρ_x is independent of y. A similar constraint holds for superconducting strips.

For the applied mean fluxes we use $\nabla \cdot \mathbf{w}_k = 0$ in each subcell, with the divergence theorem to show that

$$\int_{W'} \nabla \cdot \mathbf{w}_k \, dV = \int_{S'} \mathbf{w}_k \cdot \mathbf{n} \, dS = 0$$

for any closed surface S' enclosing area W', with outward pointing normal $\mathbf{n}$, within a subcell W_k. Utilizing the continuity conditions across each cell (or $w_y = 0$ on $-l < x < 0$, $y = \pm nh$ for the nonconducting strips) it is clear that

$$\int_{S''} \mathbf{w}_k \cdot \mathbf{n} \, dS = 0$$

with S'' as a closed surface within the cell. After utilizing the double periodicity, it is evident that the mean fluxes a and b defined as

$$a = \frac{1}{2h} \int_{-h}^{h} \mathrm{Re}[w_k(x+iy)] dy, \quad b = \frac{1}{2l} \int_{-l}^{l} \mathrm{Im}[w_k(x+iy)] dx, \tag{2.1}$$

are independent of $x = x_0$ and $y = y_0$, for x_0, y_0 constant, respectively, which is a statement of conservation of charge in each cell.

For the effective resistivities we first define vectors $\mathbf{q}_k = (\rho_k w_{ky}, -\rho_k w_{kx})$ in each phase and, from $\nabla \times (\rho_k \mathbf{w}_k) = 0$, noting that $\nabla \cdot \mathbf{q}_k = 0$, we have

$$\int_{S''} \mathbf{q}_k \cdot \mathbf{n} \, dS = 0$$

around the whole cell. Strictly speaking we should subdivide the region into the subcells, but again continuity means that all those contributions disappear. Utilizing the periodicity and continuity at the edges of the cell, the effective resistivities ρ_x and ρ_y defined as

$$\rho_x = \frac{1}{2la} \int_{-l}^{l} \mathrm{Re}[\rho_k w_k(x+iy)] \, dx, \quad \rho_y = \frac{1}{2hb} \int_{-h}^{h} \mathrm{Im}[\rho_k w_k(x+iy)] \, dy, \tag{2.2}$$

are independent of $y = y_0$ and $x = x_0$ (for x_0, y_0 constant), respectively. If we insert nonconducting strips along $-l < x < 0$, $y = \pm nh$, then

$$\rho_x|_{y_0>0} - \rho_x|_{y_0<0} = [\phi(0,y)]_{y=0-}^{y=0+} - [\phi(-l,y)]_{y=0-}^{y=0+}, \tag{2.3}$$

and from continuity of ϕ this is zero and ρ_x is still independent of y. We use this constraint as an additional condition that our later solution must obey.

Thus, trivially, we have the effective resistivity tensor ρ as

$$\rho = \int_W \rho_k w_k(z) \, dV \Big/ \int_W w_k(z) \, dV \equiv \frac{a\rho_x - ib\rho_y}{a - ib}. \tag{2.4}$$

To calculate the dissipation we define vectors $\mathbf{p}_k$ in each phase as $\mathbf{p}_k = -(\phi w_{kx}, \phi w_{ky})$; notably $\nabla \cdot \mathbf{p}_k = \rho_k (w_{kx}^2 + w_{ky}^2)$ and thus using the divergence theorem, double periodicity, and the conditions across the phases, the dissipation is

$$D=\frac{1}{4lh}\int_W \rho_k |w_k(z)|^2 \,\mathrm{d}V=\frac{1}{4lh}\int_S \mathbf{p}_k\cdot\mathbf{n}\,\mathrm{d}S, \tag{2.5}$$

where S is the boundary of the whole cell enclosing area W. Using periodicity across the cell,

$$4lhD=-\int_{-h}^{h}[\,\phi(x,y)\,]_{x=-l}^{x=l} w_x\,\mathrm{d}y-\int_{-l}^{l}[\,\phi(x,y)\,]_{y=-h}^{y=h} w_y\,\mathrm{d}x, \tag{2.6}$$

and the jumps in the potential across the cell follow from the definition of ρ_x, ρ_y and the dissipation is found to be

$$D=a^2\rho_x+b^2\rho_y. \tag{2.7}$$

These reductions of the resistivity tensor and dissipation to line integrals mean that these are quite general results for doubly periodic systems and the explicit evaluation of various area integrals is unnecessary.

Thus for four-phase rectangular checkerboards, with each phase a different constant resistivity and connected via continuity conditions, for which we have previously calculated[8] ρ_x and ρ_y as

$$\rho_x=\frac{\sigma(\lambda,1-m)}{\sigma(\lambda,m)}\left[\frac{(\rho_2+\rho_3)(\rho_4+\rho_1)}{(\rho_1+\rho_2)(\rho_3+\rho_4)}\right]^{1/2}\left(\frac{\sigma_3}{\sigma_1}\right)^{1/2}, \tag{2.8}$$

$$\rho_y=\frac{\sigma(\lambda,m)}{\sigma(\lambda,1-m)}\left[\frac{(\rho_1+\rho_2)(\rho_3+\rho_4)}{(\rho_2+\rho_3)(\rho_4+\rho_1)}\right]^{1/2}\left(\frac{\sigma_3}{\sigma_1}\right)^{1/2}, \tag{2.9}$$

the dissipation and resistivity now follow instantly; the Mortola and Steffé conjecture is proved by setting $l=h\mapsto m=\frac{1}{2}$ in Eqs. (2.8) and (2.9). These general formulas depend upon the resistivities and the geometry in a nontrivial manner and contain several functions and parameters that require definition: The parameters $\sigma_{1,\ldots,4}$ (σ_2, σ_4 are required later) are given entirely in terms of the resistivities as

$$\begin{gathered}\sigma_1=\rho_1+\rho_2+\rho_3+\rho_4,\quad \sigma_2=\rho_1\rho_3-\rho_2\rho_4,\\ \sigma_3=\rho_1\rho_2\rho_3+\rho_1\rho_2\rho_4+\rho_1\rho_3\rho_4+\rho_2\rho_3\rho_4,\quad \sigma_4=\rho_1^2(\rho_2+\rho_3)+\rho_2^2(\rho_1+\rho_4).\end{gathered} \tag{2.10}$$

An important parameter in the general formulas is $\sigma(\lambda,m)$ defined as

$$\sigma(\lambda,m)=\frac{(2/\pi)K(m)}{P_{\lambda/2-1/2}(1-2m)}, \tag{2.11}$$

wherein we use the Legendre function of the first kind, $P_\nu(1-2m)$, and $K(m)$ is the complete elliptic integral of the first kind with m implicitly defined from $K(m)/K(1-m)=l/h$. The ratio $\sigma(\lambda,m)/\sigma(\lambda,1-m)$ is ubiquitous in the expressions associated with effective parameters and is

$$\frac{\sigma(\lambda,m)}{\sigma(\lambda,1-m)}=\frac{l}{h}\frac{P_{\lambda/2-1/2}(2m-1)}{P_{\lambda/2-1/2}(1-2m)}; \tag{2.12}$$

the geometric dependence in this ratio is encapsulated in the l/h terms and, of course, in m, and the material dependence in each phase is encapsulated in λ defined from

$$\cos\pi\lambda=1-2\Delta^2,\quad \Delta^2=\frac{\sigma_2^2}{\sigma_1\sigma_3+\sigma_2^2}. \tag{2.13}$$

Similar functions and parameters also appear in later calculations.

III. INTERFACIAL GENERALIZATION

Our previous article[8] was a progression from earlier works on checkerboards,[5–7] but we developed the novel concept[9] that much of the previous analysis could be sidestepped by a conformal mapping at the outset of the analytical work. In all of these papers the basic geometry consists of two-, three-, or four-phase rectangles all linked by continuity across their adjoining interfaces. However, real materials in contact may debond due to applied stresses, or thermal stresses during/after fabrication, and the net effect may be to alter these continuity conditions. An extreme example would be to have a nonconducting (or super-conducting) barrier appear between some of the phases. We model this in order to assess the importance of the interface conditions upon the formulas for the effective parameters, and also to assess how easily we can generalize our earlier study.

A. The mapping

We consider the geometry shown in Fig. 1 where four phases exist, but between the phases labeled as 3 and 4 there lies a nonconducting barrier, or for Sec. III C a superconducting strip.

We can map this checkerboard geometry, together with the periodicity conditions, into four joined quarter planes on a two-sheeted Riemann surface. As in our earlier papers[8,9] we search for a doubly periodic function that maps horizontal boundaries to adjoining segments of the real axis in the ζ plane and, in addition, maps the vertical boundaries to the imaginary axis in the ζ plane. If we can achieve this, then we can simply solve a basic four-quarter plane solution and deduce the checkerboard solution. The mapping required is[8,9]

$$\zeta(z)=\left[\frac{1-\mathrm{cn}([2K(m)z/l]|m)}{1+\mathrm{cn}([2k(m)z/l]|m)}\right]^{1/2}, \tag{3.14}$$

where the cn are the Jacobi elliptic cosinus functions. For more details on these functions, see, for instance, Ref. 23. This mapping is built using the initial mapping of the rectangular region consisting of four cells into a four-quarter plane structure using the elliptic sinus

$$\mathrm{sn}\left(\frac{K(m)z}{l}\middle|m\right).$$

But importantly this does not map the continuity conditions on the vertical boundaries correctly, and a further manipulation of this is required that leads to (3.14). The noteworthy feature of this mapping is that we get a two-sheeted Riemann surface, where the boundary conditions on each overlying interface are the same on each sheet. This is important as it allows us to utilize a simpler solution for four joined quarter planes. If this were not the case, we would be severely hampered, and it is not clear if such problems would be solvable. An example would be to consider the same geometry, but to omit alternating nonconducting barriers, that is, remove those at $y=\pm 2nh$ for n integer. Further details of the required mapping can be found in Ref. 8.

B. Basic solution

For four joined quarter planes, with a nonconducting barrier inserted along the negative real axis, and in terms of our complex variable approach, the boundary conditions are that

$$\mathrm{Im}[i(\rho_1 w_1(x)-\rho_2 w_2(x))]=0, \quad \mathrm{Im}[w_1(x)-w_2(x)]=0, \quad \text{on } 0<x<\infty, \tag{3.15}$$

$$\mathrm{Im}[w_3(x)]=\mathrm{Im}[w_4(x)]=0, \quad \text{on} -\infty<x<0, \tag{3.16}$$

$$\mathrm{Im}[i(w_4(\mathrm{i}y)-w_1(\mathrm{i}y))]=0, \quad \mathrm{Im}[\rho_4 w_4(\mathrm{i}y)-\rho_1 w_1(\mathrm{i}y)]=0, \quad \text{on } 0<y<\infty, \tag{3.17}$$

$$\mathrm{Im}[i(w_2(\mathrm{i}y)-w_3(\mathrm{i}y))]=0, \quad \mathrm{Im}[\rho_2 w_2(\mathrm{i}y)-\rho_3 w_3(\mathrm{i}y)]=0, \quad \text{on } -\infty<y<0. \tag{3.18}$$

Following Appendix A of Ref. 8 with minor changes, the solution is found by solving a Riemann–Hilbert problem for four joined quarter planes, and the solution emerges as

$$w_k(\zeta)=C_0 w_{k0}+C_1 A_k(\lambda^{(nc)})\zeta^{\lambda^{(nc)}}+C_2\overline{A_k(\lambda^{(nc)})}\zeta^{-\lambda^{(nc)}},\quad k=1,...,4. \tag{3.19}$$

There is considerable notation embedded within this closed form solution. Since we have three sets of solutions and formulas associated with either continuous interface conditions, or with inserted superconducting, nonconducting strips, we introduce a superscript notation to distinguish them; we use (nc) and (c) for nonconducting and superconducting cases, respectively, and we do not label the formulas for the continuous case.

The general solution (3.19) contains arbitrary real constants C_0, C_1, C_2, to be determined in terms of the applied mean fluxes and continuity of ϕ, and the w_{k0} are explicitly

$$w_{10}=w_{40}=\rho_2,\quad w_{20}=w_{30}=\rho_1.$$

The powers $\lambda^{(nc)}$ follow from

$$e^{\mp i\pi\lambda^{(nc)}}=\frac{\sigma_3-\sigma_4\mp 2i\sqrt{\sigma_3\sigma_4}}{\sigma_3+\sigma_4}, \tag{3.20}$$

where $0<\lambda^{(nc)}\leqslant 1$. The $A_k(\lambda^{(nc)})$ are

$$\begin{aligned} A_1(\lambda^{(nc)})&=\frac{\rho_2\sigma_2-\mathrm{i}\sqrt{\sigma_3\sigma_4}}{\sigma_3+\sigma_4},\quad A_2(\lambda^{(nc)})=\frac{\rho_1\sigma_2-\mathrm{i}\sqrt{\sigma_3\sigma_4}}{\sigma_3+\sigma_4},\\ A_3(\lambda^{(nc)})&=-\mathrm{e}^{\mathrm{i}\pi\lambda^{(nc)}}\frac{\rho_2}{\rho_2+\rho_3},\quad A_4(\lambda^{(nc)})=\mathrm{e}^{-\mathrm{i}\pi\lambda^{(nc)}}\frac{\rho_1}{\rho_1+\rho_4}. \end{aligned} \tag{3.21}$$

Given this general solution we use the doubly periodic mapping (3.14) to perform the mathematical origami folding this four joined quarter plane solution into the doubly periodic cells. Thus (3.19) is the solution to the doubly periodic problem, but with $\zeta(z)$ given by (3.14) and the three unknown constants $C_{0,1,2}$ that we need to determine. We do this by prescribing mean fluxes a and b and using continuity of ϕ which leads to ρ_x being independent of y. We also require various integrals from Obnosov,[6] which we use freely.

The upshot, after some algebra, is that

$$\begin{aligned} C_0&=\frac{2a}{(\rho_1+\rho_2)+\alpha(m)\sigma_2},\quad C_{1,2}=a\,\frac{\alpha(m)(\sigma_3+\sigma_4)}{[(\rho_1+\rho_2)+\alpha(m)\sigma_2]}\,\frac{\sigma(\lambda^{(nc)},1-m)}{(\rho_1+\rho_2)}\\ &\quad\mp b\sqrt{\frac{\sigma_3+\sigma_4}{\sigma_4}}\,\sigma(\lambda^{(nc)},m), \end{aligned} \tag{3.22}$$

where

$$\alpha(m)=\frac{\sigma(\lambda^{(nc)},m)}{\sigma(\lambda^{(nc)},1-m)}\,\frac{\sigma_2}{\sqrt{\sigma_3(\sigma_3+\sigma_4)}}.$$

C. Perfectly conducting strips

A doubly periodic array of perfectly conducting strips inserted between the phases could be used to model arrays of microelectrodes,[15] and is a simple extension of the last section. If we now replace the nonconducting strips by perfect conductors (electrodes), we need only change the boundary conditions on $-\infty<x<0$ to $\mathrm{Im}(iw_3)=0$, $\mathrm{Im}(iw_4)=0$, in the simplified quarter plane problem (3.15)–(3.18). The general solution of the problem has the same form as (3.19), but now

$$w_{10}=w_{20}=\mathrm{i}\rho_3\rho_4, \quad w_{30}=\mathrm{i}\rho_2\rho_4, \quad w_{40}=\mathrm{i}\rho_1\rho_3$$

and

$$A_1(\lambda^{(c)})=\frac{\beta\sqrt{\rho_1\rho_2\sigma_1}-\mathrm{i}\rho_1\sigma_2}{\rho_1(\rho_1+\rho_2)(\rho_2+\rho_3)}, \quad A_2(\lambda^{(c)})=\frac{\beta\sqrt{\rho_1\rho_2\sigma_1}-\mathrm{i}\rho_2\sigma_2}{\rho_2(\rho_1+\rho_2)(\rho_2+\rho_3)},$$

$$A_3(\lambda^{(c)})=-\mathrm{i}\frac{(\rho_1+\rho_4)}{(\rho_2+\rho_3)}\mathrm{e}^{\mathrm{i}\pi\lambda^{(c)}}, \quad A_4(\lambda^{(c)})=\mathrm{i}\mathrm{e}^{-\mathrm{i}\pi\lambda^{(c)}},$$

with

$$\beta=\sqrt{\sigma_3+\sigma_4-\rho_1\rho_2\sigma_1}.$$

The powers in the general solution change to

$$\mathrm{e}^{\mp\mathrm{i}\pi\lambda^{(c)}}=\frac{\rho_1\rho_2\sigma_1-\beta^2\mp 2\mathrm{i}\beta\sqrt{\rho_1\rho_2\sigma_1}}{\sigma_3+\sigma_4}, \tag{3.23}$$

and the superscript (c) used here denotes those solutions, and formulas, associated with perfectly conducting strips. If the full solution is required to, for instance, draw lines of equipotential, one also requires the constants

$$C_0=2b\frac{\rho_1+\rho_2}{\beta^2}, \quad C_{1,2}=\frac{\rho_2+\rho_3}{\beta}\sqrt{\frac{\rho_1\rho_2}{\sigma_1}}\left(a\sigma(1-m)\mp b\sigma(m)\frac{\sigma_2(\rho_1+\rho_2)}{\beta\sqrt{\sigma_3+\sigma_4}}\right). \tag{3.24}$$

D. Effective properties

Given the general solution together with the constants (3.22) and (3.24), we can evaluate the effective resistivities using the definitions (2.2), the first of which gives

$$\rho_x^{(nc)}=\frac{\sigma_4}{[\rho_1+\rho_2+\alpha(m)\sigma_2](\rho_1+\rho_2)}, \quad \rho_x^{(c)}=\frac{\rho_1\rho_2}{(\rho_1+\rho_2)}\frac{\sigma(\lambda^{(c)},1-m)}{\sigma(\lambda^{(c)},m)}\left[\frac{\sigma_3+\sigma_4}{\rho_1\rho_2\sigma_1}\right]^{1/2}. \tag{3.25}$$

The first of these, $\rho_x^{(nc)}$, is quite different from the situation with continuous interface conditions, ρ_x, as the factor $\sigma(\lambda^{(nc)},1-m)/\sigma(\lambda^{(nc)},m)$ is now embedded within the formula $\rho_x^{(nc)}$, rather than as a rescaling prefactor, which implies a more involved dependence upon the cell dimensions h and l. Another notable point is that, for the continuous cases, $\rho_{x,y}$, there exists a solution independent of the aspect ratio, h/l; this emerges if $\rho_1\rho_3=\rho_2\rho_4$ as then $\lambda=0$. For this relation between the resistivities the solution for $\rho_x^{(nc)}$ is also independent of l/h. For $\rho_y^{(nc)}$ the prefactor $\sigma(\lambda^{(nc)},1-m)/\sigma(\lambda^{(nc)},m)$ emerges again and we find that

$$\rho_y^{(nc)}=\frac{\sigma(\lambda^{(nc)},m)}{\sigma(\lambda^{(nc)},1-m)}\left[\frac{(\rho_1+\rho_2)\sigma_3}{(\rho_1+\rho_4)(\rho_3+\rho_4)}\right]^{1/2},$$

$$\rho_y^{(c)}=\frac{(\rho_1+\rho_2)^2}{\beta^2}\left(\rho_3\rho_4+\frac{\sigma_2^2}{(\rho_1+\rho_2)}\frac{\sigma(m)}{\sigma(1-m)}\sqrt{\frac{\rho_1\rho_2}{\sigma_1(\sigma_3+\sigma_4)}}\right) \tag{3.26}$$

with no aspect ratio independence for $\rho_1\rho_3=\rho_2\rho_4$. If ρ_3 (or ρ_4) $\to\infty$, that is, one of the phases sandwiched between the nonconducting strips is itself completely nonconducting, then the expressions $\rho_{x,y}$ and $\rho_{x,y}^{(nc)}$ are equal, as we would also expect. Similarly if we replace either ρ_3 or ρ_4 by

zero, so that phase is perfectly conducting, $\rho_{x,y}\equiv\rho_{x,y}^{(c)}$. The practical computation of these formulas is straightforward; it requires m, found using a standard rootfinding algorithm, and the evaluation of the Legendre functions, using quadrature.

For comparison with numerical simulations, and also from the point of view of physical interpretation, it is useful to consider the extreme limits of very elongated short or long strips, that is, $h\gg l$, $h\ll l$.

For short strips, where $h\gg l$ we can extract asymptotic formulas, from (3.25) and (3.26), for the effective resistivities

$$\rho_x^{(nc),(c)}=\frac{(\rho_1+\rho_4)(\rho_2+\rho_3)}{(\rho_1+\rho_2+\rho_3+\rho_4)},\quad \rho_y^{(nc),(c)}=\left(\frac{\rho_2\rho_3}{\rho_2+\rho_3}+\frac{\rho_1\rho_4}{\rho_1+\rho_4}\right), \tag{3.27}$$

to order $O(l/h)$, if required, and those leading order corrections can be found as in Ref. 9. To leading order these results are exactly those which would be obtained if the strips were absent and replaced by continuity. These $h\gg l$ results can be interpreted in terms of resistors in parallel, series, and combinations thereof.

For long strips, $h\ll l$, and the nonconducting strips now play a major role, and one finds that

$$\rho_x^{(nc)}=\frac{\rho_1\rho_2}{(\rho_1+\rho_2)}+\frac{\rho_3\rho_4}{(\rho_3+\rho_4)},\quad \rho_y^{(nc)}=(\rho_1+\rho_2). \tag{3.28}$$

Notably, to leading order the result for $\rho_y^{(nc)}$ is that which would be obtained if regions 3 and 4 were completely replaced by regions of infinite resistivity. The resistivity in the direction of the x axis is that we would obtain if the nonconducting strips were replaced by continuity conditions, suggesting that ρ_x is not strongly affected by the change in interface conditions, at least for $h\ll l$. For perfectly conducting strips, and $h\ll l$, we obtain

$$\rho_x^{(c)}=\frac{\rho_1\rho_2}{(\rho_1+\rho_2)},\quad \rho_y^{(c)}=\frac{(\rho_4+\rho_3)(\rho_1+\rho_2)}{(\rho_1+\rho_2+\rho_3+\rho_4)}; \tag{3.29}$$

now, conversely to $\rho_{x,y}^{(nc)}$, the former is identical to situation where regions 3 and 4 are completely replaced, now, by regions of zero resistivity, and the latter identical with ρ_y in this limit.

If the checkerboards are square ($h=l$), we no longer have the h,l dependence and $m=\frac{1}{2}$. The results are then that

$$\rho_x^{(nc)}=\frac{\sigma_4\sqrt{\sigma_3(\sigma_3+\sigma_4)}}{(\rho_1+\rho_2)[\sigma_2^2+(\rho_1+\rho_2)\sqrt{\sigma_3(\sigma_3+\sigma_4)}]},\quad \rho_y^{(nc)}=\left[\frac{(\rho_1+\rho_2)\sigma_3}{(\rho_1+\rho_4)(\rho_3+\rho_4)}\right]^{1/2}, \tag{3.30}$$

$$\rho_x^{(c)}=\left[\frac{\rho_1\rho_2(\rho_1+\rho_4)(\rho_2+\rho_3)}{(\rho_1+\rho_2)\sigma_1}\right]^{1/2},$$

$$\rho_y^{(c)}=[\rho_3\rho_4(\rho_1+\rho_2)\sqrt{\sigma_1(\sigma_3+\sigma_4)}+\sigma_2^2\sqrt{\rho_1\rho_2}]\frac{(\rho_1+\rho_2)}{\beta^2\sqrt{\sigma_1(\sigma_3+\sigma_4)}}. \tag{3.31}$$

For continuous interface conditions using (2.8) and (2.9), and limiting to square checkerboards, one can interchange the phases ρ_2 and ρ_4 to translate between ρ_x and ρ_y. Clearly the insertion of perfectly conducting or nonconducting strips removes this simple symmetry. The formulas in (3.30) and (3.31) are the generalizations of the classical Dykhne [12] formulas, or the Mortola and Steffé[10] conjecture, to four-phase media, but additionally with perfectly conducting or nonconducting strips inserted.

Comparing the situation with and without nonconducting strips, the effective resistivity in the x direction is, in general, not too severely affected. However, in the y direction the strips completely block the field between phases 3 and 4, and the effective resistivity rises. A sample

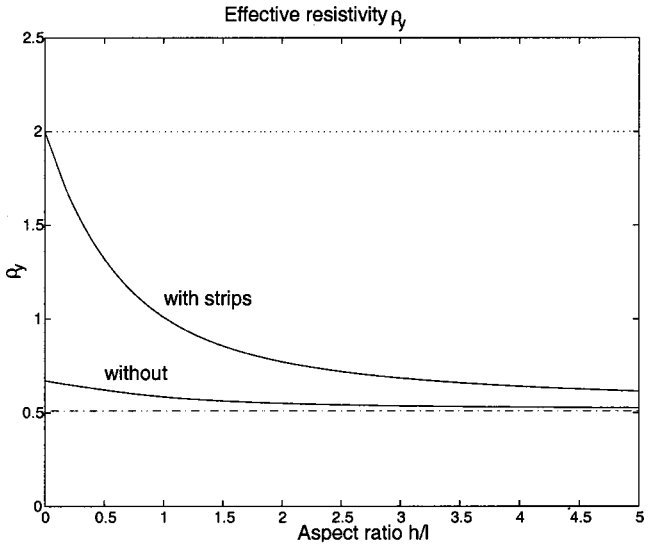

FIG. 2. The effective resistivity ρ_y versus aspect ratio h/l where $\rho_1=\rho_2=\rho_4=1$, $\rho_3=0.01$. The solid lines show ρ_y for continuous phases or inserted nonconducting strips, the dotted and dot–dash lines show the $h \ll l$ and $h \gg l$ limits (3.28) and (3.27).

calculation demonstrating the large changes that can potentially occur is shown in Fig. 2 for the situation when one phase (3) is of low resistivity while the others are all equal to unity. For perfectly conducting strips the converse occurs; the effective resistivity in the y direction is relatively unaffected whereas that in the x direction can vary considerably.

IV. CONCLUDING REMARKS

Conductive and nonconductive strips inserted in doubly periodic structures are simple models for debonding or perfect transmission across interfaces for composite structures. Estimates of the changes in effective properties away from those found with continuous conditions are thus far missing from the literature, as are formulas for four distinct phases; the current article provides those formulas explicitly for four-phase model checkerboard media. Apart from providing general formulas valid for all aspect ratios we also provide simple formulas valid for the useful limiting cases of very elongated geometries and square checkerboards. Many other limiting and special cases emerge from these results, for instance, reductions to three, two, or single phase media are easily possible; in the last case we recover the well-known results for an array of cracks in antiplane elasticity, namely that $\rho_x^{(nc)}=\rho$, that is, it is unaffected by the cracks. The results giving the general solution can also be exploited to show lines of equipotential or any other detail required.

A useful reduction of the power dissipation integral to a line integral is also briefly described; this should be of wide utility in related situations.

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Representations of the q-deformed algebra $\mathrm{U}_q'(\mathrm{so}_4)$

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We study the nonstandard q-deformation $\mathrm{U}_q'(\mathrm{so}_4)$ of the universal enveloping algebra $\mathrm{U}(\mathrm{so}_4)$ obtained by deforming the defining relations for skew-symmetric generators of $\mathrm{U}(\mathrm{so}_4)$. This algebra is used in quantum gravity and algebraic topology. We construct a homomorphism ϕ of $\mathrm{U}_q'(\mathrm{so}_4)$ to the certain nontrivial extension of the Drinfeld–Jimbo quantum algebra $\mathrm{U}_q(\mathrm{sl}_2)^{\otimes 2}$ and show that this homomorphism is an isomorphism. By using this homomorphism we construct irreducible finite-dimensional representations of the classical type and of the nonclassical type for the algebra $\mathrm{U}_q'(\mathrm{so}_4)$. It is proved that for q not a root of unity each irreducible finite-dimensional representation of $\mathrm{U}_q'(\mathrm{so}_4)$ is equivalent to one of these representations. We prove that every finite-dimensional representation of $\mathrm{U}_q'(\mathrm{so}_4)$ for q not a root of unity is completely reducible. It is shown how to construct (by using the homomorphism ϕ) tensor products of irreducible representations of $\mathrm{U}_q'(\mathrm{so}_4)$. [Note that no Hopf algebra structure is known for $\mathrm{U}_q'(\mathrm{so}_4)$.] These tensor products are decomposed into irreducible constituents.
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I. INTRODUCTION

In Ref. 1 a q-deformation of the universal enveloping algebra $\mathrm{U}(\mathrm{so}_n)$ was introduced which uses a realization of the Lie algebra so_n by skew-symmetric matrices (rather than by root elements and the diagonal Cartan subalgebra). If $I_{ij}=E_{ij}-E_{ij}$ are the skew-symmetric matrices of so_n, where $(E_{ij})_{sr}:=\delta_{is}\delta_{jr}$, then so_n is generated by the matrices $I_{21},I_{32},\ldots,I_{n,n-1}$ (other basis matrices are obtained by taking commutators of these matrices). The following Serre-type theorem is true (see Ref. 2): *The universal enveloping algebra* $\mathrm{U}(\mathrm{so}_n)$ *is isomorphic to the associative algebra generated by (abstract) elements* $I_{21},I_{32},\ldots,I_{n,n-1}$ *satisfying the relations*

$$I_{i,i-1}^2 I_{i+1,i}-2I_{i,i-1}I_{i+1,i}I_{i,i-1}+I_{i+1,i}I_{i,i-1}^2=-I_{i+1,i},$$

$$I_{i,i-1}I_{i+1,i}^2-2I_{i+1,i}I_{i,i-1}I_{i+1,i}+I_{i+1,i}^2I_{i,i-1}=-I_{i,i-1},$$

$$I_{i,i-1}I_{j,j-1}=I_{j,j-1}I_{i,i-1}\quad \text{for } |i-j|>1.$$

Now we q-deform these relations by $2\to[2]_q\equiv q+q^{-1}$. As a result, we obtain the associative algebra generated by elements $I_{21},I_{32},\ldots,I_{n,n-1}$ satisfying the relations

$$I_{i,i-1}^2 I_{i+1,i}-(q-q^{-1})I_{i,i-1}I_{i+1,i}I_{i,i-1}+I_{i+1,i}I_{i,i-1}^2=-I_{i+1,i},$$

$$I_{i,i-1}I_{i+1,i}^2-(q+q^{-1})I_{i+1,i}I_{i,i-1}I_{i+1,i}+I_{i+1,i}^2I_{i,i-1}=-I_{i,i-1},$$

$$I_{i,i-1}I_{j,j-1}=I_{j,j-1}I_{i,i-1} \quad \text{for} \quad |i-j|>1.$$

We denote this algebra by $U_q'(so_n)$. Associative algebras isomorphic to $U_q'(so_n)$ appear in quantum gravity,[3–5] in discrete Schrödinger equation,[6] in algebraic topology,[7,8] in the theory of q-orthogonal polynomials,[9] and in the theory of q-Laplace operators and q-harmonic polynomials.[10] For this reason, studying the algebra $U_q'(so_n)$ (especially for small numbers n) is of great importance. There are several problems which have to be solved. The most important are the following ones:

(a) relation of $U_q'(so_n)$ to Drinfeld–Jimbo quantum algebras;
(b) structure of the algebra $U_q'(so_n)$ (including explicit form of the center, Casimir elements, automorphism group, etc.); and
(c) construction and classification of irreducible finite-dimensional representations.

Parts of the main problems are solved. For example, it is shown (see Refs. 11 and 12) that $U_q'(so_n)$ can be embedded as a subalgebra into the Drinfeld–Jimbo quantum algebra $U_q(sl_n)$. [Recall that the Drinfeld–Jimbo quantum algebra $U_q(so_n)$ is not contained in $U_q(sl_n)$.] The main classes of irreducible finite-dimensional representations of $U_q'(so_n)$ are constructed for q not a root of unity (see Refs. 13 and 14) and for q a root of unity (see Refs. 12 and 15). But the corresponding classification theorem for the representation theory of $U_q'(so_n)$ is not proved. Casimir elements were constructed for q not a root of unity (see Refs. 16 and 17) and for q a root of unity (see Ref. 18). But it is not known whether they generate the center.

Most problems are solved[19–22] for the algebra $U_q'(so_3)$. In particular, it was shown that $U_q'(so_3)$ can be embedded into a certain extension of the Drinfeld–Jimbo algebra $U_q(sl_2)$ [but $U_q'(so_3)$ is not isomorphic to $U_q(sl_2)$]. The classification theorem for representation theory of $U_q'(so_3)$ were proved.[22] It was shown that the automorphism group of $U_q'(so_3)$ contains a group isomorphic to the modular group $SL(2,Z)$.

The aim of this article is to solve the main problems for the algebra $U_q'(so_4)$ naturally appearing in algebraic topology.[8] [Note that, unlike the classical case, the algebra $U_q'(so_4)$ is not isomorphic to the product of two copies of $U_q'(so_3)$.] The algebra $U_q'(so_4)$ and its irreducible finite-dimensional representations were studied in several paper.[23–25] Nevertheless, the main problems were not solved. The main results of this article are the following:

(I) We construct a homomorphism from $U_q'(so_4)$ to some extension of the Drinfeld–Jimbo quantum algebra $U_q(sl_2)^{\otimes 2}\equiv U_q(sl_2)\otimes U_q(sl_2)$. It is shown that this homomorphism is injective. Thus, $U_q'(so_4)$ is embedded into this extension of $U_q(sl_2)^{\otimes 2}$. This solves for $U_q'(so_4)$ the problem (a).

(II) The theorem classifying irreducible finite-dimensional representations of $U_q'(so_4)$ is proved, when q is not a root of unity. According to this theorem, irreducible representations of the classical type (q-analog of the irreducible representations of the Lie algebra so_4) and irreducible representations of the nonclassical type (these representations do not have any classical analogue) exhaust all irreducible finite-dimensional representations of $U_q'(so_4)$. This solves for $U_q'(so_4)$, when q is not a root of unity, the problem (c).

(III) It is proved that if q is not a root of unity, then any finite-dimensional representation of $U_q'(so_4)$ is completely reducible.

(IV) It is shown how to construct tensor products of irreducible finite-dimensional representations of $U_q'(so_4)$. [Note that no Hopf algebra structure is known on $U_q'(so_4)$.]

In Secs. II–IV q is any complex number different from ± 1. In other sections it is assumed that q is not a root of unity.

II. THE ALGEBRA $U_q'(so_4)$

We first define the q-deformed algebra $U_q'(so_3)$ which is a subalgebra of $U_q'(so_4)$. The algebra $U_q'(so_3)$ is obtained[26] by a q-deformation of the standard commutation relations

$$[I_{21},I_{32}]=I_{31},\quad [I_{32},I_{31}]=I_{21},\quad [I_{31},I_{21}]=I_{32}$$

of the Lie algebra so_3. So, the algebra $U'_q(so_3)$ is the complex associative algebra (with unit element) generated by the elements I_{21}, I_{32}, I_{31} satisfying the defining relations

$$[I_{21},I_{32}]_q:=q^{1/2}I_{21}I_{32}-q^{-1/2}I_{32}I_{21}=I_{31}. \tag{1}$$

$$[I_{32},I_{31}]_q:=q^{1/2}I_{32}I_{31}-q^{-1/2}I_{31}I_{32}=I_{21}, \tag{2}$$

$$[I_{31},I_{21}]_q:=q^{1/2}I_{31}I_{21}-q^{-1/2}I_{21}I_{31}=I_{32}. \tag{3}$$

Note that by (1) the element I_{31} is not independent: it depends on the elements I_{21} and I_{32}. Substituting the expression (1) for I_{31} into (2) and (3) we obtain the relations

$$I_{21}I_{32}^2-(q+q^{-1})I_{32}I_{21}I_{32}+I_{32}^2I_{21}=-I_{21}, \tag{4}$$

$$I_{32}I_{21}^2-(q+q^{-1})I_{21}I_{32}I_{21}+I_{21}^2I_{32}=-I_{32}. \tag{5}$$

The relations (4) and (5) restore the relations (2) and (3) if we introduce the element I_{31} defined by (1). The algebra $U'_q(so_3)$ can be defined as the associative algebra generated by the elements I_{21} and I_{32} satisfying the defining relations (4) and (5).

Starting from the definition of $U'_q(so_3)$ by relations (4) and (5), we give the following definition of the q-deformed algebra $U'_q(so_4)$. It is an associative algebra (with unit element) generated by the elements I_{21}, I_{32}, I_{43} satisfying the defining relations

$$I_{21}I_{32}^2-(q+q^{-1})I_{32}I_{21}I_{32}+I_{32}^2I_{21}=-I_{21}, \tag{6}$$

$$I_{32}I_{21}^2-(q+q^{-1})I_{21}I_{32}I_{21}+I_{21}^2I_{32}=-I_{32}, \tag{7}$$

$$I_{32}I_{43}^2-(q+q^{-1})I_{43}I_{32}I_{43}+I_{43}^2I_{32}=-I_{32}. \tag{8}$$

$$I_{43}I_{32}^2-(q+q^{-1})I_{32}I_{43}I_{32}+I_{32}^2I_{43}=-I_{43}, \tag{9}$$

$$I_{21}I_{43}-I_{43}I_{21}=0. \tag{10}$$

It is clear that $U'_q(so_4)$ contains at least two subalgebras isomorphic to $U'_q(so_3)$. The first one is generated by I_{21} and I_{32}, and the second one by I_{32} and I_{43}.

We can introduce in $U'_q(so_4)$ the elements I_{31}, I_{42}, and I_{41}. They are defined as in (1):

$$I_{31}:=[I_{21},I_{32}]_q,\quad I_{42}:=[I_{32},I_{43}]_q,\quad I_{41}:=[I_{21},I_{42}]_q=[I_{31},I_{43}]_q,$$

where $[A,B]_q:=q^{1/2}AB-q^{-1/2}BA$ is the q-commutator of A and B. Then the elements I_{ij}, $4\geqslant i>j\geqslant 1$, satisfy the relations[13]

$$[I_{21},I_{32}]_q=I_{31},\quad [I_{32},I_{31}]_q=I_{21},\quad [I_{31},I_{21}]_q=I_{32}, \tag{11}$$

$$[I_{32},I_{43}]_q=I_{42},\quad [I_{43},I_{42}]_q=I_{32},\quad [I_{42},I_{32}]_q=I_{43}, \tag{12}$$

$$[I_{31},I_{43}]_q=I_{41},\quad [I_{43},I_{41}]_q=I_{31},\quad [I_{41},I_{31}]_q=I_{43}. \tag{13}$$

$$[I_{21},I_{42}]_q=I_{41},\quad [I_{42},I_{41}]_q=I_{21},\quad [I_{41},I_{21}]_q=I_{42}. \tag{14}$$

$$[I_{21},I_{43}]=0,\quad [I_{32},I_{41}]=0,\quad [I_{42},I_{31}]=(q-q^{-1})(I_{21}I_{43}-I_{32}I_{41}). \tag{15}$$

As in the case of the algebra $U_q'(so_3)$, the relations (11)–(15) are equivalent to the relations (6)–(10). Note that the relations (11)–(15) define the algebra appearing in algebraic topology.[8]

Four sets of relations (11)–(14) gives four subalgebras of $U_q'(so_4)$ isomorphic to $U_q'(so_3)$. They are generated by triples (I_{21},I_{32},I_{31}), (I_{32},I_{43},I_{42}), (I_{31},I_{43},I_{41}), and (I_{21},I_{42},I_{41}), respectively.

The Poincaré–Birkhoff–Witt theorem is true for $U_q'(so_4)$. It can be formulated as: *The elements* $I_{31}^{m_{31}}I_{32}^{m_{32}}I_{41}^{m_{41}}I_{42}^{m_{42}}I_{43}^{m_{43}}I_{21}^{m_{21}}$, $m_{ij}=0,1,2,...$, *form a basis of* $U_q'(so_4)$. This theorem is proved by means of the diamond lemma (see Ref. 27, subsection 4.1.5). As in the case of an ordinary simple Lie algebra, the same theorem holds for any other ordering of the six generators.

We shall need Casimir elements of $U_q'(so_4)$. In order to give them we introduce also the elements $I_{31}^-:=[I_{21},I_{32}]_{q^{-1}}$, $I_{42}^-:=[I_{32},I_{43}]_{q^{-1}}$, and $I_{41}^-:=[I_{31},I_{43}]_{q^{-1}}$, where $[A,B]_{q^{-1}}:=q^{-1/2}AB-q^{1/2}BA$. Then[16]

$$C_4=q^{-1}I_{21}I_{43}-I_{31}I_{42}+qI_{32}I_{41},$$

$$C_4'=q^{-2}I_{21}^2+I_{32}^2+q^2I_{43}^2+q^{-1}I_{31}I_{31}^-+qI_{42}I_{42}^-+I_{41}I_{41}^-$$

are two independent elements of the center of the algebra $U_q'(so_4)$. Using the Poincaré–Birkhoff–Witt theorem the element C_4' can be represented in the form

$$\begin{aligned}C_4'=&q^2I_{21}^2+I_{41}^2+I_{32}^2+q^{-2}(I_{43}^2+I_{21}^2+I_{31}^2)-(q-q^{-1})q^{-3/2}(I_{31}I_{32}I_{21}+I_{31}I_{41}I_{43})\\&-(q-q^{-1})q^{1/2}(I_{32}I_{42}I_{43}+I_{41}I_{42}I_{21})+(q-q^{-1})^2I_{32}I_{41}I_{43}I_{21}.\end{aligned}$$

III. THE ALGEBRA $U_q(sl_2)^{\otimes 2,ext}$

Let e_1, f_1, q^{H_1} and e_2, f_2, q^{H_2} be generating elements of two copies of the quantum algebra $U_q(sl_2)$ satisfying the relations

$$q^{H_i}e_i=qe_iq^{H_i},\quad q^{H_i}f_i=q^{-1}f_iq^{H_i},\quad [e_i,f_i]=\frac{q^{2H_i}-q^{-2H_i}}{q-q^{-1}}.$$

The expressions

$$c_i=e_if_i+\frac{q^{2H_i-1}+q^{-2H_i+1}}{(q-q^{-1})^2},\quad i=1,2,$$

give Casimir elements of these algebras $U_q(sl_2)$. The comultiplication Δ is given in $U_q(sl_2)$ by the formulas

$$\Delta(q^{\pm H_i})=q^{\pm H_i}\otimes q^{\pm H_i},\quad \Delta(e_i)=e_i\otimes q^{H_i}+q^{-H_i}\otimes e_i,\quad \Delta(f_i)=f_i\otimes q^{H_i}+q^{-H_i}\otimes f_i.$$

Let us consider the polynomials

$$p_i(x_i)=q^{-1}x_i^4-c_i(q-q^{-1})^2x_i^2+q,$$

where c_i are the Casimir elements. They are irreducible in $U_q(sl_2)$, that is, there exists no element $a\in U_q(sl_2)$ such that $p_i(a)=0$. Therefore, we can define the quartic algebraic extension $\hat{U}_q(sl_2)$ of the algebra $U_q(sl_2)$ by means of the element x_i commuting with all elements of $U_q(sl_2)$:

$$\hat{U}_q(sl_2)=\{a_3x_i^3+a_2x_i^2+a_1x_i+a_0|a_j\in U_q(sl_2)\},$$

assuming that $p_i(x_i)=0$, that is, $x_i^4=qc_i(q-q^{-1})^2x_i^2-q^2$. This equation is equivalent to the following one

$$c_i=\frac{x_i^2q^{-1}+x_i^{-2}q}{(q-q^{-1})^2}. \tag{16}$$

Note that the element x_i has an inverse in $\hat{U}_q(sl_2)$ since $x_i(-x_i^3q^{-1}+c_i(q-q^{-1})^2x_i)q^{-1}=1$, that is,

$$x_i^{-1}=(-x_i^3q^{-1}+c_i(q-q^{-1})^2x_i)q^{-1}. \tag{17}$$

We consider two algebras $\hat{U}_q(sl_2)$ generated by the elements e_1, f_1, $q^{\pm H_1}$, x_1 and by the elements e_2, f_2, $q^{\pm H_2}$, x_2, respectively. Let $\hat{U}_q(sl_2)^{\otimes 2}$ be the tensor product of these algebras. Then we extend (in the sense of Ref. 28) this algebra $\hat{U}_q(sl_2)^{\otimes 2}$ by adding to it the commuting elements

$$(q^{H_1}q^{H_2}q^j+q^{-H_1}q^{-H_2}q^{-j})^{-1},\quad (q^{H_1}q^{-H_2}q^j+q^{-H_1}q^{H_2}q^{-j})^{-1},\quad j=0,\pm 1,\pm 2,\ldots. \tag{18}$$

This extended algebra will be denoted by $\hat{U}_q(sl_2)^{\otimes 2,\mathrm{ext}}$. It is the associative algebra generated by the elements e_i, f_i, $q^{\pm H_1}$, x_i, $i=1,2$, and by elements (18) such that e_1, f_1, $q^{\pm H_1}$, x_1 and e_2, f_2, $q^{\pm H_2}$, x_2 satisfy the relations determined in the algebra $\hat{U}_q(sl_2)$, each of the elements e_1, f_1, $q^{\pm H_1}$, x_1 commute with each of the elements e_2, f_2, $q^{\pm H_2}$, x_2, each of the elements $q^{\pm H_1}$ and $q^{\pm H_2}$ commutes with each of elements (18), and

$$(q^{H_1+H_2+j}+q^{-H_1-H_2-j})^{-1}e_i=e_i(q^{H_1+H_2+j+1}+q^{-H_1-H_2-j-1})^{-1},$$

$$(q^{H_1+H_2+j}+q^{-H_1-H_2-j})^{-1}f_i=f_i(q^{H_1+H_2+j-1}+q^{-H_1-H_2-j+1})^{-1},$$

$$(q^{H_1-H_2+j}+q^{-H_1+H_2-j})^{-1}e_i=e_i(q^{H_1-H_2+j+\varepsilon}+q^{-H_1+H_2-j-\varepsilon})^{-1},$$

$$(q^{H_1-H_2+j}+q^{-H_1+H_2-j})^{-1}f_i=f_i(q^{H_1-H_2+j-\varepsilon}+q^{-H_1+H_2-j+\varepsilon})^{-1},$$

$$(q^{H_1+H_2+j}+q^{-H_1-H_2-j})^{-1}(q^{H_1+H_2+j}+q^{-H_1-H_2-j})=1,$$

$$(q^{H_1-H_2+j}+q^{-H_1+H_2-j})^{-1}(q^{H_1-H_2+j}+q^{-H_1+H_2-j})=1,$$

where $\varepsilon=1$ if $i=1$ and $\varepsilon=-1$ if $i=2$.

Let us find irreducible finite-dimensional representations of the algebra $U_q(sl_2)^{\otimes 2,\mathrm{ext}}$ for q not a root of unity. For these values of q the algebra $U_q(sl_2)$ has finite-dimensional irreducible representations $T_l\equiv T_l^{(1)}$, $T_l^{(-1)}$, $T_l^{(\mathrm{i})}$, $T_l^{(-\mathrm{i})}$, $l=0,\frac{1}{2},1,\frac{3}{2},\ldots$, acting on the vector space $\mathcal{H}_l$ with basis $|l,m\rangle$, $m=-l,-l+1,\ldots,l$. These representations are given by the formulas

$$T_l^{(1)}(q^H)|l,m\rangle=q^m|l,m\rangle,\quad T_l^{(1)}(e)|l,m\rangle=[l-m]|l,m+1\rangle, \tag{19}$$

$$T_l^{(1)}(f)|l,m\rangle=[l+m]|l,m-1\rangle, \tag{20}$$

where numbers in square brackets mean q-numbers determined by

$$[a]=\frac{q^a-q^{-a}}{q-q^{-1}},$$

and by the formulas

$$T_l^{(-1)}(q^H)|l,m\rangle=-q^m|l,m\rangle,\quad T_l^{(-1)}(X)=T_l^{(1)}(X),\quad X=e,f, \tag{21}$$

$$T_l^{(\mathrm{i})}(q^H)|l,m\rangle=\mathrm{i}q^m|l,m\rangle,\quad T_l^{(\mathrm{i})}(e)=T_l^{(1)}(e),\quad T_l^{(\mathrm{i})}(f)=-T_l^{(1)}(f), \tag{22}$$

$$T_l^{(-\mathrm{i})}(q^H)|l,m\rangle=-\mathrm{i}q^m|l,m\rangle,\quad T_l^{(-\mathrm{i})}(e)=T_l^{(1)}(e),\quad T_f^{(-\mathrm{i})}(f)=-T_l^{(1)}(f) \tag{23}$$

(see, for example, Ref. 27, Chap. 3). The representations $T_l^{(1)},T_l^{(-1)},T_l^{(\mathrm{i})},T_l^{(-\mathrm{i})}$, $l=0,\frac{1}{2},1,\frac{3}{2},\ldots$, are pairwise nonequivalent and any irreducible finite-dimensional representation of $\mathrm{U}_q(\mathrm{sl}_2)$ is equivalent to one of these representations. Values of the Casimir element c on these representations are given by

$$T_l^{(1)}(c)=T_l^{(-1)}(c)=\frac{q^{2l+1}+q^{-2l-1}}{(q-q^{-1})^2},\quad T_l^{(i)}(c)=T_l^{(-i)}(c)=-\frac{q^{2l+1}+q^{-2l-1}}{(q-q^{-1})^2}.$$

Since the Casimir element of $\mathrm{U}_q(\mathrm{sl}_2)$ is multiple to the unit operator on the space $\mathcal{H}_l$, then each of the representations $T_l^{(1)},T_l^{(-1)},T_l^{(\mathrm{i})},T_l^{(-\mathrm{i})}$, $l=0,\frac{1}{2},1,\frac{3}{2},\ldots$, can be extended to a representation of $\hat{\mathrm{U}}_q(\mathrm{sl}_2)$. In order to determine these extensions we have to determine the operators $T_l^{(\varepsilon)}(x)$, $\varepsilon=\pm1,\pm\mathrm{i}$, corresponding to the element x from (16). It follows from (16) that

$$T_l^{(\varepsilon)}(c)=\frac{T_l^{(\varepsilon)}(x)^2q^{-1}+T_l^{(\varepsilon)}(x)^{-2}q}{(q-q^{-1})^2}.$$

If some operator $T_l^{(\varepsilon)}(x)$ is a solution of this equation, then the operators

$$\tilde{T}_l^{(\varepsilon)}(x)=-T_l^{(\varepsilon)}(x),\quad T_l^{(\varepsilon)}(x)^{-1}q,\quad -T_l^{(\varepsilon)}(x)^{-1}q$$

are also its solutions. Each of them can be taken for extension of the representation $T_l^{(\varepsilon)}$ of $\mathrm{U}_q(\mathrm{sl}_2)$. Since the element x commutes with all elements of $\mathrm{U}_q(\mathrm{sl}_2)$, then different extensions of $T_l^{(\varepsilon)}$ (obtained by using different solutions of the previous equation) do not essentially differ from each other. For this reason, we shall use only the solution $T_l^{(\varepsilon)}(x)=q^{-l}I$, where I is the unit operator. We denote the extended representations of $\hat{\mathrm{U}}_q(\mathrm{sl}_2)$, extended by using the solution $T_l^{(\varepsilon)}(x)=q^{-l}I$, by the same symbols $T_l^{(1)},T_l^{(-1)},T_l^{(\mathrm{i})},T_l^{(-\mathrm{i})}$.

It is clear that irreducible finite-dimensional representations of $\hat{\mathrm{U}}_q(\mathrm{sl}_2)^{\otimes2}$ are equivalent to the following ones:

$$T_l^{(\varepsilon)}\otimes T_{l'}^{(\varepsilon')},\quad l,l'=0,\tfrac{1}{2},1,\tfrac{3}{2},\ldots,\quad \varepsilon,\varepsilon'=1,-1,\mathrm{i},-\mathrm{i},$$

where $T_l^{(\varepsilon)}$ and $T_{l'}^{(\varepsilon')}$ are irreducible representations of two copies of the algebra $\hat{\mathrm{U}}_q(\mathrm{sl}_2)$, respectively. Now we wish to extend these representations of $\hat{\mathrm{U}}_q(\mathrm{sl}_2)^{\otimes2}$ to representations of the algebra $\hat{\mathrm{U}}_q(\mathrm{sl}_2)^{\otimes2,\mathrm{ext}}$ by using the relation

$$\begin{aligned}&(T_l^{(\varepsilon)}\otimes T_{l'}^{(\varepsilon')})((q^{H_1+H_2+j}+q^{-H_1-H_2-j})^{-1})\\&\quad=(q^jT_l^{(\varepsilon)}(q^{H_1})\otimes T_{l'}^{(\varepsilon')}(q^{H_2})+q^{-j}T_l^{(\varepsilon)}(q^{H_1})\otimes T_{l'}^{(\varepsilon')}(q^{-H_2}))^{-1},\\&(T_l^{(\varepsilon)}\otimes T_{l'}^{(\varepsilon')})((q^{H_1-H_2+j}+q^{-H_1+H_2-j})^{-1})\\&\quad=(q^jT_l^{(\varepsilon)}(q^{H_1})\otimes T_{l'}^{(\varepsilon')}(q^{-H_2})+q^{-j}T_l^{(\varepsilon)}(q^{-H_1})\otimes T_{l'}^{(\varepsilon')}(q^{H_2}))^{-1}.\end{aligned}$$

Clearly, only those irreducible representations $T_l^{(\varepsilon)}\otimes T_{l'}^{(\varepsilon')}$ of $\hat{\mathrm{U}}_q(\mathrm{sl}_2)^{\otimes2}$ can be extended to representations of $\hat{\mathrm{U}}_q(\mathrm{sl}_2)^{\otimes2,\mathrm{ext}}$ for which all the operators

$$q^jT_l^{(\varepsilon)}(q^{H_1})\otimes T_{l'}^{(\varepsilon')}(q^{H_2})+q^{-j}T_l^{(\varepsilon)}(q^{-H_1})\otimes T_{l'}^{(\varepsilon')}(q^{-H_2}),\quad j=0,\pm1,\ldots,$$

$$q^j T_l^{(\varepsilon)}(q^{H_1}) \otimes T_{l'}^{(\varepsilon')}(q^{-H_2}) + q^{-j} T_l^{(\varepsilon)}(q^{-H_1}) \otimes T_{l'}^{(\varepsilon')}(q^{H_2}), \quad j = 0, \pm 1, \ldots,$$

are invertible. From formulas (19)–(23) it follows that these operators are always invertible for the representations $T_l^{(\varepsilon)} \otimes T_{l'}^{(\varepsilon')}$ such that $\varepsilon, \varepsilon' = 1, -1$ or ε, $\varepsilon' = \mathrm{i}, -\mathrm{i}$, and also for all the representations $T_l^{(\varepsilon)} \otimes T_{l'}^{(\varepsilon')}$ such that $l + l'$ is a half-integral (but not integral) number and $\varepsilon = \pm 1$, $\varepsilon' = \pm \mathrm{i}$ or $\varepsilon = \pm \mathrm{i}$, $\varepsilon' = \pm 1$. For the representations $T_l^{(\varepsilon)} \otimes T_{l'}^{(\varepsilon')}$ with $\varepsilon = \pm 1$, $\varepsilon' = \pm \mathrm{i}$ or $\varepsilon = \pm \mathrm{i}$, $\varepsilon' = \pm 1$ and $l + l' \in Z$ some of these operators are not invertible since they have zero eigenvalue. Denoting the extended representations by the same symbols, we can formulate the following assertion:

Theorem 1: *If q is not a root of unity, then the algebra $\hat{U}_q(sl_2)^{\otimes 2,\mathrm{ext}}$ has irreducible finite-dimensional representations*

$$T_l^{(\varepsilon)} \otimes T_{l'}^{(\varepsilon')}, \quad l, l' = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots, \quad \varepsilon, \varepsilon' = \pm 1 \quad \text{or} \quad \varepsilon, \varepsilon' = \pm \mathrm{i},$$

$$T_l^{(\varepsilon)} \otimes T_{l'}^{(\varepsilon')}, \quad l + l' \in \tfrac{1}{2} Z, \quad l + l' \notin Z, \quad \varepsilon = \pm 1, \varepsilon' = \pm \mathrm{i} \quad \text{or} \quad \varepsilon = \pm \mathrm{i}, \ \varepsilon' = \pm 1$$

(all four combinations of signs are possible). Up to values of the operators corresponding to the elements $x_1^k \otimes x_2^s$, $k, s = 1,2,3$, any irreducible finite-dimensional representation of $\hat{U}_q(sl_2)^{\otimes 2,\mathrm{ext}}$ is equivalent to one of these representations.

IV. THE ALGEBRA HOMOMORPHISM $U'_q(so_4) \to \hat{U}_q(sl_2)^{\otimes 2,\mathrm{ext}}$

The aim of this section is to give in an explicit form the algebra homomorphism of $U'_q(so_4)$ to $\hat{U}_q(sl_2)^{\otimes 2,\mathrm{ext}}$. This homomorphism is given by the following theorem:

Theorem 2: *There exists a unique algebra homomorphism ϕ: $U'_q(so_4) \to \hat{U}_q(sl_2)^{\otimes 2,\mathrm{ext}}$ such that*

$$\phi(I_{21}) = \mathrm{i}[H_1 + H_2]_q, \quad \phi(I_{43}) = \mathrm{i}[H_1 - H_2]_q, \tag{24}$$

$$\begin{aligned}
\phi(I_{32}) = &- \frac{x_1^{-1} q^{-H_2+1} + x_1 q^{H_2-1}}{(q^{H_1+H_2-1} + q^{-H_1-H_2+1})(q^{H_1-H_2+1} + q^{-H_1+H_2-1})} E_2 \\
&+ \frac{x_1^{-1} q^{H_2+1} + x_1 q^{-H_2-1}}{(q^{H_1+H_2+1} + q^{-H_1-H_2-1})(q^{H_1-H_2-1} + q^{-H_1+H_2+1})} F_2 \\
&+ \frac{x_2^{-1} q^{-H_1+1} + x_2 q^{H_1-1}}{(q^{H_1+H_2-1} + q^{-H_1-H_2+1})(q^{H_1-H_2-1} + q^{-H_1+H_2+1})} E_1 \\
&- \frac{x_2^{-1} q^{H_1+1} + x_2 q^{-H_1-1}}{(q^{H_1+H_2+1} + q^{-H_1-H_2-1})(q^{H_1-H_2+1} + q^{-H_1+H_2-1})} F_1 .
\end{aligned} \tag{25}$$

Proof: We have to show that three elements $\phi(I_{21})$, $\phi(I_{32})$, and $\phi(I_{43})$ from (24) and (25) satisfy the defining relations (6)–(10). It is made by direct verification. Namely, we substitute the expressions (24) and (25) for $\phi(I_{21}), \phi(I_{43}), \phi(I_{32})$ into (6)–(10) and then permute the generating elements $(q^{H_i})^{\pm 1}, e_i, f_i$ in numerators [using the defining relations of the algebra $U_q(sl_2)$], reducing them to the form $(q^{H_1})^r (q^{H_2})^s e_1^{a_1} e_2^{b_1} f_1^{a_2} f_2^{b_2}, r, s \in Z$. $a_1, b_1, a_2, b_2 \in Z_+$. Then it is directly seen that the relations (7), (8), and (10) are fulfilled. So, we have to prove the relations (6) and (9). We cancel in these relations separately terms ending with e_1^2, e_2^2, f_1^2, and f_2^2. Now in the relation (6) we cancel terms ending with $e_1 e_2, f_1 f_2, f_1 e_2$ and in the relation (9) terms ending with $e_1 f_2, f_1 e_2$. Then we multiply both sides of (6) by

$$(q^{H_1+H_2-1} + q^{-H_1-H_2+1})^{-1} (q^{H_1+H_2+1} + q^{-H_1-H_2-1})^{-1}$$

and both sides of (9) by

$$(q^{H_1-H_2-1}+q^{-H_1+H_2+1})^{-1}(q^{H_1-H_2+1}+q^{-H_1+H_2-1})^{-1}.$$

After that we cancel in (6) terms ending with e_1f_2 and in (9) terms ending with e_1e_2 and f_1f_2. Now we have in (6) and (9) only the terms ending with e_1f_1 and e_2f_2 and terms without any e_jf_k, $j\neq k$. We replace e_1f_1 and e_2f_2 by the expressions following from the expression for the Casimir elements, that is, by $c_i-(q^{2H_i-1}+q^{-2H_i+1})/(q-q^{-1})^2$, respectively, and multiply both sides of both relations by

$$(q^{H_1+H_2-1}+q^{-H_1-H_2+1})(q^{H_1+H_2+1}+q^{-H_1-H_2-1})(q^{H_1+H_2}+q^{-H_1-H_2})(q^{H_1-H_2-1}$$
$$+q^{-H_1+H_2+1})(q^{H_1-H_2+1}+q^{-H_1+H_2-1})(q^{H_1-H_2}+q^{-H_1+H_2}).$$

We obtain the relations, both sides of which are cancelled. The theorem is proved.

V. PROPERTIES OF REPRESENTATIONS OF $U_q'(so_4)$

We assume everywhere below that q is not a root of unity.

Our aim is to obtain irreducible finite-dimensional representations of $U_q'(so_4)$ by using the homomorphism of Theorem 2. But before we need some statements on such representations of $U_q'(so_4)$.

Let $U_q'(so_3)_1$ and $U_q'(so_3)_2$ denote the subalgebras of $U_q'(so_4)$ generated by I_{21}, I_{32} and by I_{32}, I_{43}, respectively. It is known that the restriction of a finite-dimensional representation T of $U_q'(so_4)$ to any of these subalgebras is a completely reducible representation since any finite-dimensional representation of $U_q'(so_3)$ for q not a root of unity is completely reducible (see Ref. 29). Let

$$T\downarrow U_q'(so_3)_1=R_1\oplus R_2\oplus\cdots\oplus R_k, \tag{26}$$

$$T\downarrow U_q'(so_3)_2=R_1'\oplus R_2'\oplus\cdots\oplus R_{k'}'. \tag{27}$$

Next we shall prove some assertions characterizing these decompositions. Using the classification of irreducible finite-dimensional representations of $U_q'(so_3)$ for q not a root of unity (see Ref. 22), we can state that each of the irreducible representations R_i and R_j' in (26) and (27) is a representation of the classical type or a representation of the nonclassical type.

Proposition 1: The decomposition (26), as well as the decomposition (27), contains only irreducible representations of the classical type or only irreducible representations of the nonclassical type.

Proof: Let us prove our proposition for the decomposition (26). It follows from the results of Ref. 30 that the operators $T(I_{41}), T(I_{42}), T(I_{43})$ form a tensor operator transforming under the vector (three-dimensional) representation of $U_q'(so_3)_1$. It is known from Ref. 21 that a tensor product of a classical- (nonclassical) type irreducible representation by the vector representation contains in the decomposition classical- (respectively, nonclassical) type representations. For this reason, if, for example, the representation R_1 in (26) is of the classical type and $|l_1,m_1\rangle$, $m_1=-l_1,-l_1+1,...,l_1$, are basis elements of its representation subspace, then according to the Wigner–Eckart theorem[30] for vector tensor operator $\{T(I_{41}), T(I_{42}), T(I_{43})\}$, the vectors $T(I_{4i})|l_1,m_1\rangle$, $i=1, 2, 3$, are linear combinations of vectors belonging to subspaces of irreducible representations of $U_q'(so_3)_1$ of the classical type. The same assertion is true for vectors belonging to subspaces of representations of the nonclassical type: that is, if R_1 is of the nonclassical type, then the vectors $T(I_{4i})|l_1,m_1\rangle$ are linear combinations of vectors belonging to subspaces of irreducible representations of the nonclassical type. Thus, if in the decomposition (26) there exists an irreducible representation of the classical type, then acting upon vectors of the corresponding subspace by the operators $T(I_{4i})$, $i=1, 2, 3$, we obtain vectors belonging to subspaces on which irreducible representations of the classical type are realized. Since the representation T of $U_q'(so_4)$ is irreducible, then in this case the decomposition (26) contains only irreducible representations of

the classical type. If the decomposition (26) does not contain an irreducible representation of the classical type, then all representations in this decomposition are of the nonclassical type. The proposition is proved.

Proposition 2: Both decompositions (26) and (27) contain irreducible representations of the same type (classical or nonclassical).

Proof: In order to prove this proposition we note (see Ref. 22) that eigenvalues of the operator $R(I_{21})$ of an irreducible representation R of $U'_q(so_3)$ are of the form $i[m], i[m-1], \ldots$ with integral or half-integral $m, m-1, \ldots$ if R is of the classical type, and of the form $\pm[m]_+, \pm[m-1]_+, \ldots$ with only half-integral $\pm m, \pm m-1, \ldots$ if R is of the nonclassical type, where

$$[m]_+ = \frac{q^m + q^{-m}}{q - q^{-1}}. \tag{28}$$

Let the decomposition (26) consist of irreducible representations of the classical type. Then eigenvalues of the operators $R_i(I_{21})$ are of the form $i[m], i[m-1], \ldots$. We state that then the operators $R_i(I_{32})$ can be diagonalized and their eigenvalues are also of this form. Really, the algebra $U'_q(so_3)_1$ has the automorphism τ such that $\tau(I_{21}) = I_{32}$ and $\tau(I_{32}) = I_{21}$. Since $\mathrm{Tr} R_i(I_{21}) = \mathrm{Tr} R_i(I_{32}) = 0$ (this equality characterizes[21] irreducible representations of the classical type), then the representations $R'_i = R_i \circ \tau$ are of the classical type. Moreover, $R'_i \sim R_i$ (since up to equivalence there exists a single irreducible representation of the classical type with a fixed dimension). Then the operators $R'_i(I_{21}) = R_i(I_{32})$ are diagonalizable and the spectrum of $R_i(I_{32})$ coincides with that of $R_i(I_{21})$. Our statement concerning the operator $R_i(I_{32})$ is proved.

Now we consider the decomposition (27). The operator $T(I_{32}) = \Sigma_i \oplus R_i(I_{32})$ coincides with the operator $T(I_{32}) = \Sigma_i \oplus R'_i(I_{32})$. We have found a form of the spectrum of the operator $T(I_{32})$. Now we can conclude that the operators $R'_i(I_{32})$ have eigenvalues of the form $i[m], i[m-1], \ldots$. This means that the irreducible representations R'_i in (27) are of the classical type.

If the decomposition (26) consists of irreducible representations of the nonclassical type, the decomposition (27) consists of representations of the same type. Really, if the decomposition (27) would consist of representations of the classical type, then conducting the above reasoning in the converse order, we would conclude that the decomposition (26) consists of representations of the classical type. The proposition is proved.

Corollary: If T is an irreducible finite-dimensional representation of $U'_q(so_4)$, then both operators $T(I_{21})$ and $T(I_{43})$ can be simultaneously diagonalized and eigenvalues of both these operators are either of the form $i[m], i[m-1], \ldots$ with integral or half-integral $m, m-1, \ldots$ or of the form $[m]_+, [m-1]_+, \ldots$ with half-integral $m, m-1, \ldots$.

Proof: The operators $T(I_{21})$ and $T(I_{43})$ can be simultaneously diagonalized since the operators $R_i(I_{21})$ and $R'_j(I_{43})$ in the decompositions (26) and (27) can be simultaneously diagonalized. [Note that elements I_{21} and I_{43} are commuting in $U'_q(so_4)$.] Since decompositions (26) and (27) consist only of irreducible representations of the classical type or only irreducible representations of the nonclassical type, then the second assertion of the corollary follows. Corollary is proved.

VI. IRREDUCIBLE REPRESENTATIONS OF $U'_q(so_4)$ OF THE CLASSICAL TYPE

If T is a representation of the algebra $\hat{U}_q(sl_2)^{\otimes 2,\mathrm{ext}}$ on a finite-dimensional linear space $\mathcal{H}$, then the mapping

$$R: U'_q(so_4) \to \mathcal{L}(\mathcal{H}) \tag{29}$$

[where $\mathcal{L}(\mathcal{H})$ is the space of linear operators on $\mathcal{H}$] defined by the composition $R = T \circ \phi$ (where ϕ is the homomorphism of Theorem 2) is a representation of $U'_q(so_4)$. Let us consider the representations

$$R_{jj'} \equiv R^{(1,1)}_{jj'} = (T^{(1)}_j \otimes T^{(1)}_{j'}) \circ \phi, \quad j, j' = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots, \tag{30}$$

of $\mathrm{U}_q'(\mathrm{so}_4)$, where $T_j^{(1)}\otimes T_{j'}^{(1)}$ are irreducible representations of $\hat{\mathrm{U}}_q(\mathrm{sl}_2)^{\otimes 2,\mathrm{ext}}$ from Theorem 1.

Using formulas for the representations $T_j^{(1)}\otimes T_{j'}^{(1)}$ of $\hat{\mathrm{U}}_q(\mathrm{sl}_2)^{\otimes 2,\mathrm{ext}}$ from Theorem 1 and the expressions (24) and (25) for $\phi(I_{i,i-1})$, $i=2,3,4$, we find that

$$R_{jj'}(I_{21})|k,l\rangle = \mathrm{i}[k+l]|k,l\rangle, \tag{31}$$

$$R_{jj'}(I_{43})|k,l\rangle = \mathrm{i}[k-l]|k,l\rangle, \tag{32}$$

$$\begin{aligned} R_{jj'}(I_{32})|k,l\rangle = {} & \frac{1}{(q^{k+l}+q^{-k-l})(q^{k-l}+q^{-k+l})}\{-(q^{j-l}+q^{-j+l})[j'-l]|k,l+1\rangle \\ & +(q^{j+l}+q^{-j-l})[j'+l]|k,l-1\rangle+(q^{j'-k}+q^{-j'+k})[j-k]|k+1,l\rangle \\ & -(q^{j'+k}+q^{-j'-k})[j+k]|k-1,l\rangle\}, \end{aligned} \tag{33}$$

where numbers in square brackets are corresponding q-numbers and $|k,l\rangle$ denote the basis vector

$$|k,l\rangle \equiv |j,k\rangle\otimes|j',l\rangle$$

of the space $\mathcal{H}_j\otimes\mathcal{H}_{j'}$ of the representation $T_j^{(1)}\otimes T_{j'}^{(1)}$ of $\hat{\mathrm{U}}_q(\mathrm{sl}_2)^{\otimes 2,\mathrm{ext}}$.

Remark: Taking instead of $T_j^{(1)}\otimes T_{j'}^{(1)}$ the irreducible representations with other values of the operators corresponding to the elements $x_1^k\otimes x_2^s$, $k,s=1,2,3$ (see Theorem 1), we would obtain representations of $\mathrm{U}_q'(\mathrm{so}_4)$ equivalent to $R_{jj'}$.

The representation $R_{jj'}$ of $\mathrm{U}_q'(\mathrm{so}_4)$ is equivalent to the representation T_{rs}, $r=j+j'$, $s=j-j'$ from Ref. 24 which in the $\mathrm{U}_q'(\mathrm{so}_3)$ basis $|j'',m\rangle$, $|s|\leqslant j''\leqslant r$, $m=-j'',\ -j''+1,\ldots,j''$, is given by the formulas

$$T_{rs}(I_{21})|j'',m\rangle = i[m]|j'',m\rangle, \tag{34}$$

$$T_{rs}(I_{32})|j'',m\rangle = \frac{1}{q^m+q^{-m}}([j''-m]|j'',m+1\rangle-[j''+m]|j'',m-1\rangle), \tag{35}$$

$$\begin{aligned} T_{rs}(I_{43})|j'',m\rangle = {} & \mathrm{i}\frac{[r+1][s][m]}{[r''][j''+1]}|j'',m\rangle+\frac{[r-j''][j''+s+1]}{[j''+1][2j''+1]}|j''+1,m\rangle \\ & -\frac{[r+j''+1][j''-s][j''-m][j''+m]}{[j''][2j''+1]}|j''-1,m\rangle \end{aligned} \tag{36}$$

[note that our basis elements $|j'',m\rangle$ differ from the basis elements in formula (19) of Ref. 24 by the appropriate multipliers; for this reason, formula (36) differs from formula (19) in Ref. 24]. It was shown[24] that under diagonalization of the operator $T_{rs}(I_{43})$ we obtain a new basis $\{|x,m\rangle\}$ on which the operators $T_{rs}(I_{21}), T_{rs}(I_{43}), T_{rs}(I_{32})$ are given by formulas

$$T_{rs}(I_{21})|x,m\rangle = \mathrm{i}[m]|x,m\rangle, \quad T_{rs}(I_{43})|x,m\rangle = \mathrm{i}[x]|x,m\rangle \tag{37}$$

and by formula (33) in Ref. 24. Under the renotation of the basis elements and multiplying them by the appropriate multipliers we obtain formulas for the representation $R_{jj'}$ obtained earlier in this work. This proves the equivalence stated earlier.

The irreducible representations $R_{jj'}$ are called representations of *the classical type*.[14] If $q\to 1$, then the operators $R_{jj'}(I_{i,i-1})$, $i=2,3,4$, tend to the corresponding operators of the irreducible representations of the Lie algebra so_4.

VII. IRREDUCIBLE REPRESENTATIONS OF $U'_q(so_4)$ OF THE NONCLASSICAL TYPE

Now we apply the method of the previous section to the irreducible representations $T_j^{(-i)} \otimes T_{j'}^{(1)}$ of the algebra $\hat{U}_q(sl_2)^{\otimes 2,ext}$ with j half-integral and j' integral or with j integral and j' half-integral. Then we obtain the representations

$$R_{jj'}^{(-i,1)} = (T_j^{(-i)} \otimes T_{j'}^{(1)}) \circ \phi, \tag{38}$$

of $U'_q(so_4)$ with

$$j = \tfrac{1}{2}, \tfrac{3}{2}, \tfrac{5}{2}, \ldots, \quad j' = 0,1,2,..., \quad \text{or} \quad j = 0,1,2,..., \quad j' = \tfrac{1}{2}, \tfrac{3}{2}, \tfrac{5}{2}, \ldots . \tag{39}$$

Using formulas for the representations $T_j^{(-i)}$ and $T_{j'}^{(1)}$ of $U_q(sl_2)$ and the expression (24) and (25) for $\phi(I_{i,i-1})$, $i=2,3,4$, we find that

$$R_{jj'}^{(-i,1)}(I_{21})|k,l\rangle = [k+l]_+ |k,l\rangle, \tag{40}$$

$$R_{jj'}^{(-i,1)}(I_{43})|k,l\rangle = [k-l]_+ |k,l\rangle, \tag{41}$$

$$R_{jj'}^{(-i,1)}(I_{32})|k,l\rangle = \frac{1}{[k+l][k-l](q-q^{-1})} \{-i[j-l][j'-l]|k,l+1\rangle + i[j+l][j'+l]|k,l-1\rangle$$
$$- i[j'-k][j-k]|k+1,l\rangle + i[j'+k][j+k]|k-1,l\rangle\}, \tag{42}$$

where the numbers in square brackets are the corresponding q-numbers, $[a]_+$ are defined in (28), and $|k, l\rangle$ denotes the basis vectors

$$|k,l\rangle = |j,k\rangle \otimes |j',l\rangle \tag{43}$$

of the space $\mathcal{H}_j \otimes \mathcal{H}_{j'}$ of the representation $T_j^{(-i)} \otimes T_{j'}^{(1)}$ of $\hat{U}_q(sl_2)^{\otimes 2,ext}$. Note that both $j+j'$ and $k+l$ are half-integral.

In this case we have the equalities $[k+l]_+ = [-k-l]_+$, $[k-l]_+ = [-k+l]_+$ and for this reason the operators $R_{jj'}^{(-i,1)}(I_{21})$ and $R_{jj'}^{(-i,1)}(I_{43})$ have multiple eigenvalues. Namely, all pairs of the vectors $|k, l\rangle$ and $|-k,-l\rangle$ have the same eigenvalues:

$$R_{jj'}^{(-i,1)}(I_{21})|k,l\rangle = [k+l]_+ |k,l\rangle, \quad R_{jj'}^{(-i,1)}(I_{43})|k,l\rangle = [k-l]_- |k,l\rangle,$$

$$R_{jj'}^{(-i,1)}(I_{21})|-k,-l\rangle = [k+l]_+ |-k,-l\rangle, \quad R_{jj'}^{(-i,1)}(I_{43})|-k,-l\rangle = [k-l]_+ |-k,-l\rangle.$$

The representation $R_{jj'}^{(-i,1)}$ is reducible. In order to show this we distinguish two case:

(a) j is half-integral and j' integral and
(b) j is integral and j' half-integral.

We consider first the case (a). In order to decompose $R_{jj'}^{(-i,1)}$ into irreducible constituents we choose a new basis in the representation space consisting of the vectors

$$|k,l\rangle^+ = |k,l\rangle + (-1)^l |-k,-l\rangle, \quad k>0,$$

$$|k,l\rangle^- = |k,l\rangle + (-1)^{l+1} |-k,-l\rangle, \quad k>0.$$

Using formulas (40)–(42) we easily find that

$$R_{jj'}^{(-i,1)}(I_{21})|k,l\rangle^\pm = [k+l]_- |k,l\rangle^\pm, \quad R_{jj'}^{(-i,1)}(I_{43})|k,l\rangle^\pm = [k-l]_+ |k,l\rangle^\pm, \tag{44}$$

$$R^{(-\mathrm{i},1)}_{jj'}(I_{32})|k,l\rangle^+=\frac{1}{[k+l][k-l](q-q^{-1})}\{-\mathrm{i}[j-l][j'-l]|k,l+1\rangle^+ +\mathrm{i}[j+l][j'+l]|k,l-1\rangle^+$$
$$-\mathrm{i}[j'-k][j-k]|k+1,l\rangle^+ +\mathrm{i}[j'+k][j+k]|k-1,l\rangle^+\},\quad k\neq\tfrac{1}{2}, \tag{45}$$

$$R^{(-\mathrm{i},1)}_{jj'}(I_{32})\left|\frac{1}{2},l\right\rangle^+=\frac{-1}{[l+\frac{1}{2}][l-\frac{1}{2}](q-q^{-1})}\left\{-\mathrm{i}[j-l][j'-l]\left|\frac{1}{2},l+1\right\rangle^+\right.$$
$$+\mathrm{i}[j+l][j'+l]\left|\frac{1}{2},l-1\right\rangle^+ -\mathrm{i}[j'-\tfrac{1}{2}][j-\tfrac{1}{2}]\left|\frac{3}{2},l\right\rangle^+$$
$$\left.+\mathrm{i}[j'+\tfrac{1}{2}][j+\tfrac{1}{2}](-1)^l\left|\frac{1}{2},-l\right\rangle^+\right\}. \tag{46}$$

The operator $R^{(-\mathrm{i},1)}_{jj'}(I_{32})$ acts on the vectors $|k,l\rangle^-$ by formulas (45) and (46) if to replace all $|k,l\rangle^+$ by the corresponding $|k,l\rangle^-$, and in (46) to replace $(-1)^l$ by $(-1)^{l+1}$.

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be the subspaces of the representation space of $R^{(-\mathrm{i},1)}_{jj'}$ spanned by the vectors $|k,l\rangle^+$ and by the vectors $|k,l\rangle^-$, respectively. We see from the previous formulas that these subspaces are invariant with respect to the representation $R^{(-\mathrm{i},1)}_{jj'}$. We denote the restrictions of $R^{(-\mathrm{i},1)}_{jj'}$ to $\mathcal{H}_1$ and $\mathcal{H}_2$ by $R^{(+,+,+)}_{jj'}$ and $R^{(+,+,-)}_{jj'}$, respectively. Note that

$$R^{(+,+,+)}_{jj'}(I_{32})\left|\frac{1}{2},0\right\rangle^+=\frac{1}{[\frac{1}{2}]^2(q-q^{-1})}\left\{-\mathrm{i}[j][j']\left|\frac{1}{2},1\right\rangle^+ +i[j][j']\left|\frac{1}{2},-1\right\rangle^+ -\mathrm{i}[j'-\tfrac{1}{2}][j-\tfrac{1}{2}]\right.$$
$$\left.\times\left|\frac{3}{2},0\right\rangle^+ +i[j'+\tfrac{1}{2}][j+\tfrac{1}{2}]\left|\frac{1}{2},0\right\rangle^+\right\}, \tag{47}$$

that is, the operator $R^{(+,+,+)}_{jj'}(I_{32})$ has nonzero diagonal element

$$^+\left\langle\frac{1}{2},0\right|R^{(+,+,+)}_{jj'}(I_{32})\left|\frac{1}{2},0\right\rangle^+=i\frac{[j'+\frac{1}{2}][j+\frac{1}{2}]}{[\frac{1}{2}]^2(q-q^{-1})}.$$

In the same way it is shown that

$$^-\left\langle\frac{1}{2},0\right|R^{(+,+,-)}_{jj'}(I_{32})\left|\frac{1}{2},0\right\rangle^-=-\mathrm{i}\frac{[j'+\frac{1}{2}][j+\frac{1}{2}]}{[\frac{1}{2}]^2(q-q^{-1})}.$$

Now we consider the case (b). The new basis of the representation space is

$$|k,l\rangle^+=|k,l\rangle+(-k)^l|-k,-l\rangle,\quad l>0,$$

$$|k,l\rangle^-=|k,l\rangle+(-1)^{k+1}|-k,-l\rangle,\quad l>0.$$

Then formulas for $R^{(-\mathrm{i},1)}_{jj'}(I_{21})$ and $R^{(-\mathrm{i},1)}_{jj'}(I_{43})$ are the same as in case (a). Formula (45) is the same, but we have consider it for $l\neq 1/2$. Instead of (46) we have the formula

$$R^{(-\mathrm{i},1)}_{jj'}(I_{32})\left|k,\frac{1}{2}\right\rangle^{+}=\frac{1}{[k+\frac{1}{2}][k-\frac{1}{2}](q-q^{-1})}\left\{-\mathrm{i}[j-\tfrac{1}{2}][j'-\tfrac{1}{2}]\left|k,\frac{3}{2}\right\rangle^{+}+\mathrm{i}[j+\tfrac{1}{2}][j'+\tfrac{1}{2}](-1)^{k}\right.$$
$$\left.\left|-k,\frac{1}{2}\right\rangle^{+}-\mathrm{i}[j'-k][j-k]\left|k+1,\frac{1}{2}\right\rangle^{+}+\mathrm{i}[j'+k][j+k]\left|k-1,\frac{1}{2}\right\rangle^{+}\right\}. \tag{48}$$

The operator $R^{(-\mathrm{i},1)}_{jj'}(I_{32})$ acts on the vectors $|k,l\rangle^{-}$ by formulas (45) and (48) if to replace all $|k,l\rangle^{+}$ by $|k,l\rangle^{-}$, respectively, and in (48) to replace $(-1)^k$ by $(-1)^{k+1}$.

We denote the subspaces spanned by the vectors $|k,l\rangle^{+}$ and by the vectors $|k,l\rangle^{-}$ as $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. As we see from the previous formulas, these subspaces are invariant with respect to the representation $R^{(-\mathrm{i},1)}_{jj'}$. We denote the corresponding subrepresentations by $R^{(+,+,-)}_{jj'}$ and $R^{(+,+,+)}_{jj'}$, respectively. In particular, we have

$$R^{(+,+,-)}_{jj'}(I_{32})\left|0,\frac{1}{2}\right\rangle^{+}=\frac{-1}{[\frac{1}{2}]^2(q-q^{-1})}\left\{-\mathrm{i}[j-\tfrac{1}{2}][j'-\tfrac{1}{2}]\left|0,\frac{3}{2}\right\rangle^{+}+\mathrm{i}[j+\tfrac{1}{2}][j'+\tfrac{1}{2}]\left|0,\frac{1}{2}\right\rangle^{+}\right.$$
$$\left.-\mathrm{i}[j'][j]\left|1,\frac{1}{2}\right\rangle^{+}+\mathrm{i}[j'][j]\left|-1,\frac{1}{2}\right\rangle^{+}\right\}, \tag{49}$$

that is, the operator $R^{(+,+,-)}_{jj'}(I_{32})$ has nonzero diagonal element

$${}^{+}\left\langle 0,\frac{1}{2}\right|R^{(+,+,-)}_{jj'}(I_{32})\left|0,\frac{1}{2}\right\rangle^{+}=-\mathrm{i}\frac{[j'+\frac{1}{2}][j+\frac{1}{2}]}{[\frac{1}{2}]^2(1-q^{-1})}.$$

For the operator $R^{(+,+,+)}_{jj'}(I_{32})$ we have

$${}^{-}\left\langle 0,\frac{1}{2}\right|R^{(+,+,+)}_{jj'}(I_{32})\left|0,\frac{1}{2}\right\rangle^{-}=\mathrm{i}\frac{[j'+\frac{1}{2}][j+\frac{1}{2}]}{[\frac{1}{2}]^2(1-q^{-1})}.$$

Now we consider in the same way the representations

$$R^{(-\mathrm{i},-1)}_{jj'}=(T^{(-\mathrm{i})}_{j}\otimes T^{(-1)}_{j'})\circ\phi$$

of $U'_q(so_4)$. As a result, we obtain for these representations formulas (40)–(42) in which the right-hand sides of (40) and (41) are multiplied by -1 and the right-hand side of (42) is left without any change. These representations are reducible and we have

$$R^{(-\mathrm{i},-1)}_{jj'}=R^{(-,-,+)}_{jj'}\oplus R^{(-,-,-)}_{jj'},$$

where the representations $R^{(-,-,+)}_{jj'}$ and $R^{(-,-,-)}_{jj'}$ act on such subspaces as in the previous case, with these difference that

$$R^{(-,-,\pm)}_{jj'}(I_{21})=-R^{(+,+,\pm)}_{jj'}(I_{21}),\quad R^{(-,-,\pm)}_{jj'}(I_{43})=-R^{(+,+,\pm)}_{jj'}(I_{43}),$$

that is,

$$R^{(-,-,\pm)}_{jj'}(I_{21})|k,l\rangle^{\pm}=-[k+l]_{+}|k,l\rangle^{\pm},\quad R^{(-,-,\pm)}_{jj'}(I_{43})|k,l\rangle^{\pm}=-[k-l]_{+}|k,l\rangle^{\pm}.$$

The operators $R^{(-,-,Z\pm)}_{jj'}(I_{32})$ coincide with the corresponding operators $R^{(+,+,\pm)}_{jj'}(I_{32})$.

Similarly, the representation $R^{(\mathrm{i},1)}_{jj'}=(T^{(\mathrm{i})}_{j}\otimes T^{(1)}_{j'})\circ\phi$ of $U'_q(so_4)$ is reducible and decomposes as

$$R^{(\mathrm{i},1)}_{jj'}=R^{(-,-,+)}_{jj'}\oplus R^{(-,-,-)}_{jj'},$$

where $R^{(-,-,\pm)}_{jj'}$ are such as earlier in this work, and the representation $R^{(\mathrm{i},-1)}_{jj'}=(T^{(\mathrm{i})}_{j}\otimes T^{(-1)}_{j'})\circ\phi$ of $\mathrm{U}'_q(\mathrm{so}_4)$ is reducible and decomposes as

$$R^{(\mathrm{i},-1)}_{jj'}=R^{(+,+,+)}_{jj'}\oplus R^{(+,+,-)}_{jj'},$$

where $R^{(+,+,\pm)}_{jj'}$ are such as earlier in this work.

Let us consider the representation

$$R^{(1,\mathrm{i})}_{j'j}=(T^{(1)}_{j'}\otimes T^{(\mathrm{i})}_{j})\circ\phi$$

of $\mathrm{U}'_q(\mathrm{so}_4)$ (for convenience we take first the index j' and then j). We have

$$R^{(1,\mathrm{i})}_{j'j}(I_{21})|l,k\rangle=-[k+l]_+|l,k\rangle,\quad R^{(1,\mathrm{i})}_{j'j}(I_{43})|l,k\rangle=[k-l]_+|l,k\rangle,$$

$$R^{(1,\mathrm{i})}_{j'j}(I_{32})|l,k\rangle=\frac{1}{[k+l][l-k](q-q^{-1})}\{-\mathrm{i}[j-l][j'-l]|l+1,k\rangle+\mathrm{i}[j+l][j'+l]|l-1,k\rangle-\mathrm{i}[j'-k][j-k]|l,k+1\rangle+\mathrm{i}[j'+k][j+k]|l,k-1\rangle\}.$$

In order to have a similarity with formulas (40)–(42) we denote the vectors $|l,\,k\rangle$ by $|k,\,l\rangle$ and the representation $R^{(1,\mathrm{i})}_{j'j}$ by $\hat{R}^{(\mathrm{i},1)}_{jj'}$.

The operators $\hat{R}^{(\mathrm{i},1)}_{jj'}(I_{21})$ and $\hat{R}^{(\mathrm{i},1)}_{jj'}(I_{43})$ have multiple common eigenvectors $|k,\,l\rangle$ and $|-k,-l\rangle$. The representation $\hat{R}^{(\mathrm{i},1)}_{jj'}$ is analyzed as the representation $R^{(-\mathrm{i},1)}_{jj'}$ given earlier and we have the following result. The representation $\hat{R}^{(\mathrm{i},1)}_{jj'}$ is reducible and decomposes into irreducible subrepresentations as

$$\hat{R}^{(\mathrm{i},1)}_{jj'}=R^{(-,+,+)}_{jj'}\oplus R^{(-,+,-)}_{jj'},$$

where the representations $R^{(-,+,\pm)}_{jj'}$ differ from the representations $R^{(+,+,\pm)}_{jj'}$, respectively, only by the operator $R^{(-,+,\pm)}_{jj'}(I_{21})$ and

$$R^{(-,+,\pm)}_{jj'}(I_{21})=-R^{(+,+,\pm)}_{jj'}(I_{21}).$$

Similarly, the representation

$$R^{(1,-\mathrm{i})}_{j'j}\equiv\hat{R}^{(-\mathrm{i},1)}_{jj'}=(T^{(1)}_{j'}\otimes T^{(-\mathrm{i})}_{j})\circ\phi$$

of $\mathrm{U}'_q(\mathrm{so}_4)$ is reducible and decomposes into irreducible components as

$$\hat{R}^{(-\mathrm{i},1)}_{jj'}=R^{(+,-,+)}_{jj'}\oplus R^{(+,-,-)}_{jj'},$$

where the representations $R^{(+,-,\pm)}_{jj'}$ differ from the representations $R^{(+,+,\pm)}_{jj'}$, respectively, only by the operator $R^{(+,-,\pm)}_{jj'}(I_{43})$ and

$$R^{(+,-,\pm)}_{jj'}(I_{43})=-R^{(+,+,\pm)}_{jj'}(I_{43}).$$

We do not consider other representations $R^{(\pm1,\pm\mathrm{i})}_{j'j}=(T^{(\pm1)}_{j'}\otimes T^{(\pm\mathrm{i})}_{j})$ since they do not give new irreducible representations of $\mathrm{U}'_q(\mathrm{so}_4)$.

Thus, for every value of j and j' such that

$$j=0,1,2,\ldots,\ \ j'=\tfrac{1}{2},\tfrac{3}{2},\tfrac{5}{2},\ldots,\quad\text{or}\quad j=\tfrac{1}{2},\tfrac{3}{2},\tfrac{5}{2},\ldots,\ \ j'=0,1,2,\ldots.$$

we constructed eight representations $R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}$, $\varepsilon_i=\pm$. These representations act on the linear space $\mathcal{H}$ with the basis

$$|k,l\rangle, \quad k=j,j-1,...,\tfrac{1}{2}, \quad l=j', \ j'-1,...,-j'$$

if j' is integral, and with the basis

$$|k,l\rangle, \quad k=j,j-1,...,-j, \quad l=j', \ j'-1,...,\tfrac{1}{2}$$

if j is integral. The representations are given by the formulas

$$R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}(I_{21})|k,l\rangle=\varepsilon_1[k+l]_+|k,l\rangle, \tag{50}$$

$$R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}(I_{43})|k,l\rangle=\varepsilon_2[k-l]_+|k,l\rangle, \tag{51}$$

$$\begin{aligned}R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}(I_{32})|k,l\rangle=&\frac{1}{[k+l][k-l](q-q^{-1})}\{-\mathrm{i}[j'-l][j-l]|k,l+1\rangle+\mathrm{i}[j'+l][j+l]|k,l-1\rangle\\&-\mathrm{i}[j'-k][j-k]|k+1,l\rangle+\mathrm{i}[j'+k][j+k]|k-1,l\rangle\},\end{aligned} \tag{52}$$

where $k\neq\frac{1}{2}$ if j is half-integral and $l\neq\frac{1}{2}$ if j' is half-integral, and by

$$\begin{aligned}R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}(I_{32})\left|\frac{1}{2},l\right\rangle=&\frac{1}{[l+\frac{1}{2}][l-\frac{1}{2}](q-q^{-1})}\left\{-\mathrm{i}[j-l][j'-l]\left|\frac{1}{2},l+1\right\rangle+\mathrm{i}[j+l][j'+l]\right.\\&\left.\times\left|\frac{1}{2},l-1\right\rangle-\mathrm{i}[j'-\tfrac{1}{2}][j-\tfrac{1}{2}]\left|\frac{3}{2},l\right\rangle+\mathrm{i}[j'+\tfrac{1}{2}][j+\tfrac{1}{2}]\varepsilon_3(-1)^l\left|\frac{1}{2},-l\right\rangle\right\}\end{aligned} \tag{53}$$

if j is half-integral and by

$$\begin{aligned}R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}(I_{32})\left|k,\frac{1}{2}\right\rangle=&\frac{1}{[k+\frac{1}{2}][k-\frac{1}{2}](q-q^{-1})}\left\{-\mathrm{i}[j-\tfrac{1}{2}][j'-\tfrac{1}{2}]\left|k,\frac{3}{2}\right\rangle+\mathrm{i}[j+\tfrac{1}{2}][j'+\tfrac{1}{2}]\varepsilon_3\right.\\&\left.(-1)^k\left|-k,\frac{1}{2}\right\rangle-\mathrm{i}[j'-k][j-k]\left|k+1,\frac{1}{2}\right\rangle+\mathrm{i}[j'+k][j+k]\left|k-1,\frac{1}{2}\right\rangle\right\}\end{aligned} \tag{54}$$

if j' is half-integral.

It is seen from formulas for representations that the representations $R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}$ and $R^{(\varepsilon_1,-\varepsilon_2,\varepsilon_3)}_{j'j}$ are equivalent. The equivalence operator A is given by the formula $A|k,l\rangle=|l,k\rangle$. For this reason, we consider the representations $R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}$ only for $j\geqslant j'$.

Theorem 3: *The representations* $R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}$, $j\geqslant j'$, *are irreducible and pairwise nonequivalent.*

Proof: Irreducibility of these representations will be proved in Sec. VIII. In order to prove their pairwise nonequivalence we note that finite-dimensional representations T and T' of $U'_q(so_4)$ cannot be equivalent if for at least one pair $T(I_{i,i-1})$, $T'(I_{i,i-1})$, $i=2,3,4$, we have $\mathrm{Tr}T(I_{i,i-1})\neq\mathrm{Tr}T'(I_{i,i-1})$. For this reason, the representations $R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}$ and $R^{(\varepsilon'_1,\varepsilon'_2,\varepsilon'_3)}_{ss'}$ with $(\varepsilon_1,\varepsilon_2,\varepsilon_3)\neq(\varepsilon'_1,\varepsilon'_2,\varepsilon'_3)$ or/and with $(j,j')\neq(s,s')$ are not equivalent.

Irreducible representations $R_{jj'}^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}$ are called *representations of the nonclassical type*. They have no classical analogue. They are characterized by the property that the operators $R_{jj'}^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)} \times (I_{i,i-1})$, $i=2,3,4$, have a nonzero trace. Note that there exist eight nontrivial one-dimensional representations of the nonclassical type. They coincide with the representations $R_{(1/2)0}^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}$.

VIII. THE CLASSIFICATION THEOREM

The main aim of this section is to prove that previously constructed irreducible representations of the classical type and of the nonclassical type exhaust all irreducible finite-dimensional representations of the algebra $\mathrm{U}_q'(\mathrm{so}_4)$. We also prove that pairs of the irreducible representations of Theorem 3 are not equivalent. But first we study some auxiliary operators.

Let R be a finite-dimensional representation of $\mathrm{U}_q'(\mathrm{so}_4)$ on a linear vector space $\mathcal{H}$. We suppose that the operators $R(I_{21})$ and $R(I_{43})$ have eigenvalues only of the classical type, that is, of the form $\mathrm{i}[m]$, where $[m]$ means a q-number. Let $|k,\, l\rangle$ be an eigenvector such that

$$R(I_{21})|k,l\rangle = \mathrm{i}[k+l]|k,l\rangle, \quad R(I_{43})|k,l\rangle = \mathrm{i}[k-l]|k,l\rangle.$$

We associate with this eigenvector the operators

$$X_1^{(k,l)} = -R(I_{41}) + q^{-2k}R(I_{32}) - \mathrm{i}q^{-k-l+1/2}R(I_{42}) - \mathrm{i}q^{-k+l-1/2}R(I_{31}), \tag{55}$$

$$X_2^{(k,l)} = -R(I_{41}) + q^{2k}R(I_{32}) + \mathrm{i}q^{k+l+1/2}R(I_{42}) + \mathrm{i}q^{k-l-1/2}R(I_{31}), \tag{56}$$

$$X_3^{(k,l)} = R(I_{41}) + q^{-2l}R(I_{32}) + \mathrm{i}q^{-k-l+1/2}R(I_{42}) - \mathrm{i}q^{k-l-1/2}R(I_{31}), \tag{57}$$

$$X_4^{(k,l)} = R(I_{41}) + q^{2l}R(I_{32}) - \mathrm{i}q^{k+l+1/2}R(I_{42}) + \mathrm{i}q^{-k+l-1/2}R(I_{31}). \tag{58}$$

Note that later we shall use the explicit form of the operators $X_1^{(k,l)}$, $X_2^{(k,l)}$, $X_3^{(k,l)}$, $X_4^{(k,l)}$ under action on the vector $|k,\, l\rangle$. In this case we may consider formulas (55)–(58) as a system of linear equations with unknown vectors $R(I_{32})|k,l\rangle$, $R(I_{31})|k,l\rangle$, $R(I_{42})|k,l\rangle$, and $R(I_{41})|k,l\rangle$. The determinant of this system can be easily calculated:

$$\det\begin{pmatrix} -1 & q^{-2k} & -\mathrm{i}q^{-k-l+1/2} & -\mathrm{i}q^{-k+l-1/2} \\ -1 & q^{2k} & \mathrm{i}q^{k+l+1/2} & \mathrm{i}q^{k-l-1/2} \\ 1 & q^{-2l} & \mathrm{i}q^{-k-l+1/2} & -\mathrm{i}q^{k-l-1/2} \\ 1 & q^{2l} & -\mathrm{i}q^{k+l+1/2} & \mathrm{i}q^{-k+l-1/2} \end{pmatrix} = (q^{k+l}+q^{-k-l})(q^{k-l}+q^{-k+l}).$$

If q is not a root of unity, then this determinant does not vanish for any integral or half-integral k and l. This means that the system of above equations can be solved and we can find how the operators $R(I_{32})$, $R(I_{31})$, $R(I_{42})$, and $R(I_{41})$ act on the vector $|k,\, l\rangle$. This reasoning will be used below.

Lemma 1: The vectors $X_i^{(k,l)}|k,l\rangle$ are eigenvectors of the operators $R(I_{21})$ and $R(I_{43})$:

$$R(I_{21})(X_1^{(k,l)}|k,l\rangle) = \mathrm{i}[k+l+1](X_1^{(k,l)}|k,l\rangle), \quad R(I_{43})(X_1^{(k,l)}|k,l\rangle) = \mathrm{i}[k-l-1](X_1^{(k,l)}|k,l\rangle),$$

$$R(I_{21})(X_2^{(k,l)}|k,l\rangle) = \mathrm{i}[k+l-1](X_2^{(k,l)}|k,l\rangle), \quad R(I_{43})(X_2^{(k,l)}|k,l\rangle) = \mathrm{i}[k-l+1](X_2^{(k,l)}|k,l\rangle),$$

$$R(I_{21})(X_3^{(k,l)}|k,l\rangle) = \mathrm{i}[k+l+1](X_3^{(k,l)}|k,l\rangle), \quad R(I_{43})(X_3^{(k,l)}|k,l\rangle) = \mathrm{i}[k-l+1](X_3^{(k,l)}|k,l\rangle),$$

$$R(I_{21})(X_4^{(k,l)}|k,l\rangle) = \mathrm{i}[k+l-1](X_4^{(k,l)}|k,l\rangle), \quad R(I_{43})(X_4^{(k,l)}|k,l\rangle) = \mathrm{i}[k-l-1](X_4^{(k,l)}|k,l\rangle).$$

Proof: The lemma is proved by direct calculation using the defining relations for the elements $I_{ij} \in U_q'(\mathrm{so}_4)$, $i>j$. For example, by using relations (11)–(14) we have

$$R(I_{21})(X_1^{(k,l)}|k,l\rangle)=R(-qI_{41}+q^{-2k-1}I_{32}-iq^{-k-l-1/2}I_{42}-iq^{k+l+1/2}I_{31})R(I_{21})|k,l\rangle$$
$$+R(iq^{-k-l}I_{41}-iq^{l-k}I_{32}+q^{1/2}I_{42}+q^{-2k-1/2}I_{31})|k,l\rangle$$
$$=i[k+l+1](X_1^{(k,l)}|k,l\rangle).$$

The lemma is proved.

Lemma 1 means that the operators $X_1^{(k,l)}$ and $X_3^{(k,l)}$ increase k and l in the eigenvalues of $R(I_{21})$ and $R(I_{43})$, respectively, and the operators $X_2^{(k,l)}$ and $X_4^{(k,l)}$ decrease these numbers in these eigenvalues. Symbolically we write this in the form

$$X_1:\ l\to l+1,\quad X_2: l\to l-1,$$

$$X_3:\ k\to k+1,\quad X_4: k\to k-1.$$

Lemma 2: The operators (55)–(58) have the properties

$$X_3^{(k,l+1)}X_1^{(k,l)}|k,l\rangle=X_1^{(k+1,l)}X_3^{(k,l)}|k,l\rangle,\quad X_4^{(k,l-1)}X_2^{(k,l)}|k,l\rangle=X_2^{(k-1,l)}X_4^{(k,l)}|k,l\rangle,$$

$$X_4^{(k,l+1)}X_1^{(k,l)}|k,l\rangle=X_1^{(k-1,l)}X_4^{(k,l)}|k,l\rangle,\quad X_3^{(k,l-1)}X_2^{(k,l)}|k,l\rangle=X_2^{(k+1,l)}X_3^{(k,l)}|k,l\rangle.$$

Proof: The first of these relations is proved as follows. Using the expressions (55) and (57) for X_1 and X_3 we express [by using relations (11)–(15)] the elements $X_3^{(k,l+1)}X_1^{(k,l)}$ and $X_1^{(k+1,l)}X_3^{(k,l)}$ as a linear combination of the basis elements from Poincaré–Birkhoff–Witt theorem. As a result, we receive the first relation. Other relations are proved in the same way. The lemma is proved.

Lemma 2 means that the pairs of operators X_1 and X_3, X_2 and X_4, X_1 and X_4, and X_2 and X_3 (with appropriate upper indices) commute under action on the vector $|k,\ l\rangle$.

Lemma 3: The operators (55)–(58) have the properties

$$X_2^{(k,l+1)}X_1^{(k,l)}|k,l\rangle=(C_4'-(q^{2l+1}+q^{-2l-1})C_4+[2l][2(l+1)])|k,l\rangle,$$

$$X_1^{(k,l-1)}X_2^{(k,l)}|k,l\rangle=(C_4'-(q^{2l-1}+q^{-2l+1})C_4+[2l][2(l-1)])|k,l\rangle,$$

$$X_4^{(k+1,l)}X_3^{(k,l)}|k,l\rangle=(C_4'+(q^{2k+1}+q^{-2k-1})C_4+[2k][2(k+1)])|k,l\rangle,$$

$$X_3^{(k-1,l)}X_4^{(k,l)}|k,l\rangle=(C_4'+(q^{2k-1}+q^{-2k+1})C_4+[2k][2(k-1)])|k,l\rangle,$$

where C_4 and C_4' *are the Casimir elements of* $U'_q(so_4)$ *from Sec. II.*

The proof is given in the same way as that of Lemma 2, taking into account expressions for the Casimir elements.

Lemma 3 can be used for evaluation of eigenvalues of Casimir elements C_4 and C_4' on irreducible representations R when the operators $R(I_{21})$ and $R(I_{43})$ have eigenvalues of the classical type. Eigenvectors $|k,\ l\rangle$ of the operators $R(I_{21})$ and $R(I_{43})$ are called *weight vectors* of the representation R. A weight vector $|j,j'\rangle$ is called *a highest weight vector* if

$$X_1^{(j,j')}|j,j'\rangle=0,\quad X_3^{(j,j')}|j,j'\rangle=0.$$

If R is an irreducible representation with classical-type eigenvalues of the operators $R(I_{21})$ and $R(I_{43})$, then we apply both sides of the first and the third relations of Lemma 3 to the vector of highest weight $|j,j'\rangle$. The left-hand sides send this vector to zero, and then the right-hand sides (equating to zero) give the following eigenvalues for C_4 and C_4':

$$C_4=[j+j'+1][j'-j]I,$$

$$C_4'=\{(q^{2j+1}+q^{-2j-1})[j-j'][j+j'+1]-[2j][2j+2]\}I,$$

where I is the unit operator on the representation space. In particular, such eigenvalues have Casimir operators of the classical-type representation $R_{jj'}$.

Later in this work where we prove assertions concerning finite-dimensional representations of $U_q(so_4)$, we shall have in mind the following properties of the operators $X_i^{(k,l)}$ from (55)–(58), which are derived from Lemmas 1–3:

(A) Let $|k,l\rangle$ be such as in Lemma 1. Acting on $|k,l\rangle$ by the operators X_i, $i=1,2,3,4$, with appropriate upper indices, we can obtain a vector $|k,l\rangle'$ with eigenvalues of the operators $R(I_{21})$ and $R(I_{43})$ coinciding with those of the vector $|k,l\rangle$. Then $|k,l\rangle'=a|k,l\rangle$ for some complex number a.

(B) Let $|k,l\rangle$ be such as in Lemma 1. If $X_1^{(k,l)}|k,l\rangle=|k,l+1\rangle=0$ and $|k',l\rangle$ is another weight vector of the operators $R(I_{21})$ and $R(I_{43})$ obtained by action of the operators X_i, $i=1,2,3,4$, with appropriate upper indices, then $X_1^{(k',l)}|k',l\rangle=|k',l+1\rangle=0$. The same assertion is valid for the vectors $X_2^{(k,l)}|k,l\rangle$, $X_3^{(k,l)}|k,l\rangle$, and $X_4^{(k,l)}|k,l\rangle$. This means that by acting on $|k,l\rangle$ by the operators X_i, $i=1,2,3,4$, with appropriate upper indices, we obtain the set of nonzero vectors $|k',l'\rangle$ such that their values (k',l') constitute a parallelogram with vertices (j,j'), $(j,-j')$, $(-j,j')$, and $(-j,-j')$ under some values of j and j'.

Now let R' be a finite-dimensional representation of $U_q'(so_4)$ on a linear space $\mathcal{H}'$. Suppose that the operators $R'(I_{21})$ and $R'(I_{43})$ have eigenvalues only of the nonclassical type, that is, of the form $\pm[m]_+$, where $[m]_+=(q^m+q^{-m})/(q-q^{-1})$ and m are half-integral. If $|k,l\rangle$ is an eigenvector such that

$$R'(I_{21})|k,l\rangle=\varepsilon_1[k+l]_+|k,l\rangle,\quad R'(I_{43})|k,l\rangle=\varepsilon_2[k-l]_-|k,l\rangle,$$

then we associate with it the operators

$$X_1^{(k,l)}=R'(I_{41})+q^{-2k}R'(I_{32})-q^{-k-l+1/2}R'(I_{42})-q^{-k+l-1/2}R'(I_{31}), \tag{59}$$

$$X_2^{(k,l)}=R'(I_{41})+q^{2k}R'(I_{32})-q^{k+l+1/2}R'(I_{42})-q^{k-l-1/2}R'(I_{31}), \tag{60}$$

$$X_3^{(k,l)}=-R'(I_{41})-q^{-2l}R'(I_{32})+q^{-k-l+1/2}R'(I_{42})+q^{-k-l-1/2}R'(I_{31}), \tag{61}$$

$$X_4^{(k,l)}=-R'(I_{41})-q^{2l}R'(I_{32})+q^{k+l+1/2}R'(I_{42})+q^{-k+l-1/2}R'(I_{31}). \tag{62}$$

Next we shall consider relations (59)–(62) as a system of linear equations. The determinant of the matrix of this system is equal to

$$\det\begin{pmatrix} 1 & q^{-2k} & -q^{-k-l+1/2} & -q^{-k+l-1/2} \\ 1 & q^{2k} & -q^{k+l+1/2} & -q^{k-l-1/2} \\ -1 & -q^{-2l} & q^{-k-l+1/2} & q^{k-l-1/2} \\ -1 & -q^{2l} & q^{k+l+1/2} & q^{-k+l-1/2} \end{pmatrix}=(q^{k+l}-q^{-k-l})(q^{k-l}-q^{-k+l}).$$

If q is not a root of unity, then this determinant does not vanish for any half-integral $k\pm l$. Hence, the previous system of equations can be solved and we can find how the operators $R'(I_{32})$, $R'(I_{31})$, $R'(I_{42})$, and $R'(I_{41})$ act on the vector $|k,l\rangle$.

Next we formulate three lemmas for these operators analogous to Lemma 1–3. Proofs of these lemmas are the same as in the case of Lemmas 1–3 and we omit them.

Lemma 4: The vectors $X_i^{(k,l)}|k,l\rangle$ are eigenvectors of the operators $R'(I_{21})$ and $R'(I_{43})$:

$$R'(I_{21})(X_1^{(k,l)}|k,l\rangle)=\varepsilon_1[k+l+1]_+(X_1^{(k,l)}|k,l\rangle),$$

$$R'(I_{43})(X_1^{(k,l)}|k,l\rangle)=\varepsilon_2[k-l-1]_+(X_1^{(k,l)}|k,l\rangle),$$

$$R'(I_{21})(X_2^{(k,l)}|k,l\rangle)=\varepsilon_1[k+l-1]_+(X_2^{(k,l)}|k,l\rangle),$$

$$R'(I_{43})(X_2^{(k,l)}|k,l\rangle)=\varepsilon_2[k-l+1]_+(X_2^{(k,l)}|k,l\rangle),$$

$$R'(I_{21})(X_3^{(k,l)}|k,l\rangle)=\varepsilon_1[k+l+1]_+(X_3^{(k,l)}|k,l\rangle),$$

$$R'(I_{43})(X_3^{(k,l)}|k,l\rangle)=\varepsilon_2[k-l+1]_+(X_3^{(k,l)}|k,l\rangle),$$

$$R'(I_{21})(X_4^{(k,l)}|k,l\rangle)=\varepsilon_1[k+l-1]_+(X_4^{(k,l)}|k,l\rangle),$$

$$R'(I_{43})(X_4^{(k,l)}|k,l\rangle)=\varepsilon_2[k-l-1]_+(X_4^{(k,l)}|k,l\rangle).$$

Lemma 5: The operators (59)–(62) have the properties

$$X_3^{(k,l+1)}X_1^{(k,l)}|k,l\rangle=X_1^{(k+1,l)}X_3^{(k,l)}|k,l\rangle,\quad X_4^{(k,l-1)}X_2^{(k,l)}|k,l\rangle=X_2^{(k-1,l)}X_4^{(k,l)}|k,l\rangle,$$

$$X_4^{(k,l+1)}X_1^{(k,l)}|k,l\rangle=X_1^{(k-1,l)}X_4^{(k,l)}|k,l\rangle,\quad X_3^{(k,l-1)}X_2^{(k,l)}|k,l\rangle=X_2^{(k+1,l)}X_3^{(k,l)}|k,l\rangle.$$

Lemma 6: For the operators (59)–(62) we have

$$X_2^{(k,l+1)}X_1^{(k,l)}|k,l\rangle=(C_4'-(q^{2l+1}+q^{-2l-1})C_4+[2l][2(l+1)])|k,l\rangle,$$

$$X_1^{(k,l-1)}X_2^{(k,l)}|k,l\rangle=(C_4'-(q^{2l-1}+q^{-2l+1})C_4+[2l][2(l-1)])|k,l\rangle,$$

$$X_4^{(k+1,l)}X_3^{(k,l)}|k,l\rangle=(C_4'-(q^{2k+1}+q^{-2k-1})C_4+[2k][2(k+1)])|k,l\rangle,$$

$$X_3^{(k-1,l)}X_4^{(k,l)}|k,l\rangle=(C_4'-(q^{2k-1}+q^{-2k+1})C_4+[2k][2(k-1)])|k,l\rangle,$$

where C_4 and C_4' are the Casimir elements of $U'_q(so_4)$ *from Sec. II.*

Lemma 6 can be used for evaluation of eigenvalues of Casimir elements C_4 and C_4' on irreducible representations R' when the operators $R'(I_{21})$ and $R'(I_{43})$ have eigenvalues of the nonclassical type. Eigenvectors $|k,l\rangle$ of the operators $R'(I_{21})$ and $R'(I_{43})$ are called *weight vectors* of the representation R'. A weight vector $|j,j'\rangle$ is called *a highest weight vector* if

$$X_1^{(j,j')}|j,j'\rangle=0,\quad X_3^{(j,j')}|j,j'\rangle=0.$$

If R' is an irreducible representation with nonclassical type eigenvalues of the operators $R'(I_{21})$ and $R'(I_{43})$, then applying both sides of the first and third relations of Lemma 6 to the vector of highest weight $|j,j'\rangle$ we derive that

$$C_4=[j+j'+1]_+[j-j']_+I,$$

$$C_4'=\{(q^{2j+1}+q^{-2j-1})[j-j']_+[j+j'+1]_+-[2j][2j+2]\}I,$$

where I is the identity operator on the representation space. In particular, such eigenvalues have Casimir operators of the nonclassical type representation $R_{jj'}^{\varepsilon_1,\varepsilon_2,\varepsilon_3}$.

The operators $X_i^{(k,l)}$ from (59)–(62) have the properties similar to the properties (A) and (B).

Proof of the first part of Theorem 3: Let $R_{jj'}^{\varepsilon_1,\varepsilon_2,\varepsilon_3}$ be a representation of the nonclassical type on the vector space $\mathcal{H}$. Then the commuting operators $R_{jj'}^{\varepsilon_1,\varepsilon_2,\varepsilon_3}(I_{21})$ and $R_{jj'}^{\varepsilon_1,\varepsilon_2,\varepsilon_3}(I_{43})$ are simultaneously diagonalized. Since q is not a root of unity, the eigenvalues $(\varepsilon_1[k+l]_+,\varepsilon_2[k-l]_+)$ for the corresponding vector $|k,l\rangle$ are of multiplicity 1. Let $\mathcal{H}'$ be a nontrivial invariant subspace of the representation space $\mathcal{H}$, and let $\Sigma_{k,l}\alpha_{k,l}|k,l\rangle$ be a nonzero vector from $\mathcal{H}'$. Since eigenvalues $(\varepsilon_1[k+l]_+,\varepsilon_2[k-l]_+)$ are of multiplicity 1, then each $|k,l\rangle$ from this linear combination belongs

to $\mathcal{H}'$. Let $|k',l'\rangle$ be one of these vectors. Applying the operators X_1 and X_3 (with appropriate upper indices) to $|k',l'\rangle$ we obtain the vector of highest weight $|j,j'\rangle$ of the representation $R^{\varepsilon_1,\varepsilon_2,\varepsilon_3}_{jj'}$. Applying to $|j,j'\rangle$ the operators X_2 and X_4 (with appropriate indices) we obtain all basis vectors of the space $\mathcal{H}$. Hence, the representation $R^{\varepsilon_1,\varepsilon_2,\varepsilon_3}_{jj'}$ is irreducible. The theorem is proved.

Now we can prove the theorem on classification of irreducible finite-dimensional representations of $\mathrm{U}'_q(\mathrm{so}_4)$.

Theorem 4: *If q is not a root of unity, then each irreducible finite-dimensional representation R of $\mathrm{U}'_q(\mathrm{so}_4)$ is equivalent to one of the irreducible representations of the classical type or to one of the irreducible representations of the nonclassical type.*

Proof: Let us first prove the following assertion: *if eigenvalues of the operators $R(I_{21})$ and $R(I_{43})$ of an irreducible finite-dimensional representation R of $\mathrm{U}'_q(\mathrm{so}_4)$ are of the classical type (that is, of the form $i[m]$, $m\in\frac{1}{2}Z$), then R is equivalent to one of the irreducible representations of the classical type.* We diagonalize both operators $R(I_{21})$ and $R(I_{43})$ and represent their eigenvectors in the form $|k,l\rangle$, where

$$R(I_{21})|k,l\rangle=i[k+l]|k,l\rangle,\quad R(I_{43})|k,l\rangle=i[k-l]|k,l\rangle.$$

(These eigenvectors are called weight vectors.) Due to Lemmas 1 and 2, there exists an eigenvector of highest weight (we denote it by $|j,j'\rangle$), that is such that

$$R(I_{21})|j,j'\rangle=i[j+j']|j,j'\rangle,\quad R(I_{43})|j,j'\rangle=i[j-j']|j,j'\rangle,$$

$$X_1^{(j,j')}|j,j'\rangle=0,\quad X_3^{(j,j')}|j,j'\rangle=0.$$

Applying the first and third relations of Lemma 3 to the vector $|j,j'\rangle$ we find eigenvalues of the Casimir operators $R(C_4)$ and $R(C'_4)$ on the representation R:

$$R(C_4)=[j+j'+1][j'-j], \tag{63}$$

$$R(C'_4)=(q^{2j+1}+q^{-2j-1})[j-j'][j+j'+1]-[2j][2j+2]. \tag{64}$$

Acting on the vector $|j,j'\rangle$ by the operators X_2 (with appropriate upper indices) we construct recursively the vectors

$$|j,j'-s\rangle:=X_2^{(j,j'-s+1)}\cdots X_2^{(j,j'-1)}X_2^{(j,j')}|j,j'\rangle,\quad s=0,1,2,\ldots.$$

Since the representation R is finite dimensional and (by Lemma 1) these vectors have different eigenvalues, there exists smallest positive integer n such that

$$|j,j'-n\rangle:=X_2^{(j,j'-n+1)}|j,j'-n+1\rangle=0. \tag{65}$$

Similarly, between vectors

$$|j-r,j'\rangle:=X_4^{(j-r+1,j')}\cdots X_4^{(j-1,j')}X_4^{(j,j')}|j,j'\rangle,\quad r=0,1,2,\ldots,$$

there exists a nonzero vector with smallest positive integer m such that

$$|j-m,j'\rangle:=X_4^{(j-m+1,j')}|j-m+1,j'\rangle=0. \tag{66}$$

Then using the second and fourth relations of Lemma 3, we find from (63)–(66) that

$$X_1^{(j,j'-n)}X_2^{(j,j'-n+1)}|j,j'-n+1\rangle=[n][n-2j'-1](q^{j'-j-n}+q^{-j'+j+n})(q^{j+j'-n+1}+q^{-j-j'+n-1})|j,j'-n+1\rangle=0,$$

$$X_3^{(j-m,j')}X_4^{(j-m+1,j')}|j-m+1,j'\rangle=[m][m-2j-1](q^{m-j-j'-1}+q^{-m+j+j'+1})(q^{m-j+j'}+q^{-m+j-j'})|j-m+1,j'\rangle=0.$$

Therefore, $[n-2j'-1]=0$ and $[m-2j-1]=0$, that is,

$$m=2j+1, \quad n=2j'+1.$$

Now we act successively on the vectors $|j,j'\rangle,|j,j'-1\rangle,|j,j'-2\rangle,\ldots,|j,-j'\rangle$ by the operators X_4 with the appropriate upper indices. As a result, we construct the vectors

$$|j,j'\rangle, \quad |j-1,j'\rangle, \quad \ldots, \quad -j,j'\rangle,$$

$$|j,j'-1\rangle, \quad |j-1,j'-1\rangle, \quad \ldots, \quad |-j,j'-1\rangle,$$

$$\ldots \quad \ldots \quad \ldots \quad \ldots$$

$$|j,-j'\rangle, \quad |j-1,-j'\rangle, \quad \ldots, \quad |-j,j'\rangle,$$

for which

$$R(I_{21})|k,l\rangle=i[k+l]|k,l\rangle, \quad R(I_{43})|k,l\rangle=i[k-l]|k,l\rangle.$$

We can find how the operators X_i, $i=1,2,3,4$, with appropriate indices act on these vectors:

$$X_2^{(k,l)}|k,l\rangle=|k,l-1\rangle, \quad X_4^{(k,l)}|k,l\rangle=|k-1,l\rangle,$$

$$X_1^{(k,l)}|k,l\rangle=X_1^{(k,l)}X_2^{(k,l+1)}|k,l+1\rangle=(R(C_4')-(q^{2l+1}+q^{-2l-1})R(C_4)+[2l+2][2l])|k,l+1\rangle,$$

$$X_3^{(k,l)}|k,l\rangle=X_3^{(k,l)}X_4^{(k+1,l)}|k+1,l\rangle=(R(C_4')+(q^{(2k+1)}+q^{-2k-1})R(C_4)+[2k+2][2k])|k+1,l\rangle.$$

Putting here the explicit expression for the Casimir operators, substituting these expressions for $X_i^{(k,l)}|k,l\rangle$ to (55)–(58), and considering (55)–(58) as a system of linear equations with unknown $R(I_{32})|k,l\rangle$, $R(I_{31})|k,l\rangle$, $R(I_{42})|k,l\rangle$, and $R(I_{41})|k,l\rangle$, we solve this system and find that

$$R(I_{32})|k,l\rangle=\frac{1}{(q^{k+l}+q^{-k-l})(q^{k-l}+q^{-k+l})}\{|k-1,l\rangle+|k,l-1\rangle-(q^{j-l}+q^{j+l})(q^{j+l+1}+q^{-j-l-1})\times[j'-l][j'+l+1]|k,l+1\rangle-(q^{j'-k}+q^{j+k})(q^{j'+k+1}+q^{-j'-k-1})\times[j-k][j+k+1]|k+1,l\rangle\}.$$

Thus, the vectors $|k,l\rangle$, $-j\leqslant k\leqslant j$, $-j'\leqslant l\leqslant j'$, constitute a basis of the representation space $\mathcal{H}$. Introducing a new basis $\{|k,l\rangle'\}$ such that

$$|k,l\rangle=(-1)^{k+l}\prod_{r=-j}^{k}(q^{j'+r}+q^{-j'-r})^{-1}[j+r]^{-1}\prod_{s=-j'}^{k}(q^{j+s}+q^{-j-s})^{-1}[j'+s]^{-1}|k,l\rangle',$$

we shall obtain for $R(I_{21})$, $R(I_{32})$, and $R(I_{43})$ the operators of the irreducible representation $R_{jj'}$ of the classical type from Sec. IV. Thus, in this case the theorem is proved.

Now we prove the second part of the theorem which can be formulated as follows: *if eigenvalues of the operators $R(I_{21})$ and $R(I_{43})$ of an irreducible finite-dimensional representation R are of the nonclassical type, that is, of the form $\pm[m]_+$, $m\in\frac{1}{2}Z, m\notin Z$, then R is equivalent to one of the irreducible representations of the nonclassical type.*

We first prove that if eigenvalues of the operators $R(I_{21})$ and $R(I_{43})$ are of the form $[m]_+$ (only sign + is taken), then R is equivalent to one of the irreducible representations of the nonclassical type. A proof is similar to that of the previous case and for this reason we do not give details.

Due to Lemmas 4 and 5, there exists an eigenvector of highest weight $|j,j'\rangle$ such that

$$R(I_{21})|j,j'\rangle=[j+j']_+|j,j'\rangle, \quad R(I_{43})|j,j'\rangle=[j-j']_+|j,j'\rangle,$$

$$X_1^{(j,j')}|j,j'\rangle=X_3^{(j,j')}|j,j'\rangle=0.$$

Applying relations of Lemma 6 to $|j,j'\rangle$ we find eigenvalues of the Casimir operators $R(C_4)$ and $R(C_4')$:

$$R(C_4)=[j+j'+1]_+[j-j']_+, \tag{67}$$

$$R(C_4')=(q^{2j+1}+q^{-2j-1})[j-j']_+[j+j'+1]_+-[2j][2j+2]. \tag{68}$$

Now we construct recursively the vectors

$$|j-r,j'-s\rangle:=X_4^{(j-r+1,j'-s)}\cdots X_4^{(j,j'-s)}X_2^{(j,j'-s+1)}\cdots X_2^{(j,j'-1)}X_2^{(j,j')}|j,j'\rangle, \tag{69}$$

$$r,s=0,1,2,\ldots.$$

By Lemma 4, for these vectors we have

$$R(I_{21})|k,l\rangle=[k+l]_+|k,l\rangle, \quad R(I_{43})|k,l\rangle=[k-l]_+|k,l\rangle. \tag{70}$$

These vectors satisfy the relations

$$X_2^{(k,l)}|k,l\rangle=|k,l-1\rangle, \quad X_4^{(k,l)}|k,l\rangle=|k-1,l\rangle, \tag{71}$$

$$\begin{aligned}X_1^{(k,l)}|k,l\rangle&=X_1^{(k,l)}X_2^{(k,l+1)}|k,l+1\rangle\\&=(R(C_4')-(q^{2l+1}+q^{-2l-1})R(C_4)+[2l+2][2l])|k,l+1\rangle,\end{aligned} \tag{72}$$

$$\begin{aligned}X_3^{(k,l)}|k,l\rangle&=X_3^{(k,l)}X_4^{(k+1,l)}|k+1,l\rangle\\&=(R(C_4')-(q^{(2k+1}+q^{-2k-1})R(C_4)+[2k+2][2k])|k+1,l\rangle.\end{aligned} \tag{73}$$

Since the operators $X_1^{(k,l)}$, $X_2^{(k,l)}$, $X_3^{(k,l)}$, and $X_4^{(k,l)}$ acting on the vector $|k,\,l\rangle$ determine the action of the operators $R(I_{32})$, $R(I_{31})$, $R(I_{42})$, and $R(I_{41})$ on this vector, then the vectors

$$|j,j'\rangle, \quad |j-1,j'\rangle, \quad |j-2,j'\rangle, \quad \ldots,$$

$$|j,j'-1\rangle, \quad |j-1,j'-1\rangle \quad |j-2,j'-1\rangle, \quad \ldots,$$

$$|j,j'-2\rangle, \quad |j-1,j'-2\rangle, \quad |j-2,j'-2\rangle, \quad \ldots,$$

$$\ldots \quad \ldots \quad \ldots \quad \ldots$$

span an invariant subspace in the representation space $\mathcal{H}$. Since the representation R is irreducible, they span the whole space $\mathcal{H}$. It follows from (70) that only pairs of vectors $|k,\,l\rangle$ and $|-k,-l\rangle$ have the same eigenvalues for the operators $R(I_{21})$ and $R(I_{43})$.

In order to determine which possibilities exist for the representation R, we proceed as follows. For definiteness we suppose that j is half-integral. Using formula (69) we first create the set of all

possible vectors $|k, l\rangle$, which does not contain pairs $|k, l\rangle$ and $|-k,-l\rangle$. For example, we create all the vectors $|k, l\rangle$ with $k>0$. This set contains the vector $|\frac{1}{2},0\rangle$. There are two possibilities:

(a) The vectors $|\frac{1}{2},0\rangle$ and $|-\frac{1}{2},0\rangle$ are linearly dependent, that is, $X_4^{(1/2,0)}|\frac{1}{2},0\rangle=a|\frac{1}{2},0\rangle$.
(b) The vectors $|\frac{1}{2},0\rangle$ and $|-\frac{1}{2},0\rangle$ are linearly independent.

In the case (a) all pairs $|k, l\rangle$ and $|-k,-l\rangle$ consist of linearly dependent vectors. The reason for this is that

$$X_1^{(k,l)}=X_2^{(-k,-l)}, \quad X_3^{(k,l)}=X_4^{(-k,-l)} \tag{74}$$

[as it follows from expressions (59)–(62) for the operators X_i, $i=1,2,3,4$]. Therefore, for every positive integral r and s the vectors

$$X_3^{(r+1/2,s)}\cdots X_3^{(r+1/2,0)}X_1^{(r-1/2,0)}\cdots X_1^{(1/2,0)}|\tfrac{1}{2},0\rangle,$$

$$X_4^{(-r-1/2,-s)}\cdots X_4^{(-r-1/2,0)}X_2^{(-r+1/2,0)}\cdots X_2^{(-1/2,0)}|\tfrac{1}{2},0\rangle$$

are linearly dependent with the same constant a. The constant a can be explicitly calculated. Namely, since $X_4^{(1/2,0)}|1/2,0\rangle=|-1/2,0\rangle=a|1/2,0\rangle$ and $X_3^{(-1/2,0)}=X_4^{(1/2,0)}$, we have

$$\begin{aligned}X_3^{(-1/2,0)}|-\tfrac{1}{2},0\rangle&=X_3^{(-1/2,0)}X_4^{(-1/2,0)}|\tfrac{1}{2},0\rangle=R(C_4'-2C_4-1)|\tfrac{1}{2},0\rangle\\&=X_3^{(-1/2,0)}\,a|\tfrac{1}{2},0\rangle=aX_4^{(1/2,0)}|\tfrac{1}{2},0\rangle=a^2|\tfrac{1}{2},0\rangle,\end{aligned}$$

that is, $a^2=R(C_4'-2C_4-1)$. This means that a is determined up to a sign. Using expressions for values of the Casimir elements of $U'_q(so_4)$ on irreducible representations with highest weight vector $|j,j'\rangle$, we find that $a=\varepsilon_3(q-q^{-1})[j+\frac{1}{2}][j'+\frac{1}{2}]$, where ε_3 takes one of the values ± 1.

Thus, we received the following set of linear independent vectors of the representation space $\mathcal{H}$:

$$|j,j'\rangle, \quad |j-1,j'\rangle, \quad \cdots, \quad |\tfrac{1}{2},j'\rangle,$$

$$|j,j'-1\rangle, \quad |j-1,j'-1\rangle, \quad \cdots, \quad |\tfrac{1}{2},j'-1\rangle,$$

$$\cdots \quad \cdots \quad \cdots \quad \cdots$$

$$|j,-j'\rangle, \quad |j-1,-j'\rangle, \quad \cdots, \quad |\tfrac{1}{2},-j'\rangle.$$

These vectors constitute a basis of the space $\mathcal{H}$. We introduce a new basis $\{|k,l\rangle'\}$ such that

$$|k,l\rangle=\prod_{r=1/2}^{k}(q^{j'+r}-q^{-j'-r})^{-1}[j+r]^{-1}\prod_{s=-j'}^{k}(q^{j+s}-q^{-j-s})^{-1}[j'+s]^{-1}|k,l\rangle'.$$

Rewriting the relations (71)–(73) for this new basis we obtain a system of linear equations with unknown $R(I_{32})|k,l\rangle'$, $R(I_{42})|k,l\rangle'$, $R(I_{41})|k,l\rangle'$, and $R(I_{31})|k,l\rangle'$. Solving this system we find that the operator $R(I_{32})$ acts on the basis vectors by the formulas for the irreducible nonclassical type representation $R_{jj'}^{(+,+,+)}$ or the irreducible nonclassical type representation $R_{jj'}^{(+,+,-)}$.

Now we consider case (b). Due to the relation (74) we conclude that the vectors

$$|k,l\rangle, \quad k=j,j-1,j-2,\cdots,-j, \quad l=j',j'-1,j'-2,\cdots,-j',$$

are linearly independent and constitute a basis of the representation space $\mathcal{H}$. Solving the system of linear equations (71)–(73) we obtain a representation of $\mathrm{U}_q'(\mathrm{so}_4)$ equivalent to one of the representations $R_{jj'}^{(\pm\mathrm{i},\pm 1)}$ or $R_{jj'}^{(\pm 1,\pm\mathrm{i})}$ from Sec. VI. These representations are reducible. So, case (b) is not possible for our irreducible representation R.

We have considered the case when all eigenvalues of the operators $R(I_{21})$ and $R(I_{43})$ are of the form $[m]_+$ (with sign +). However, due to automorphisms ψ_1 and ψ_2, mapping $I_{21}\to -I_{21}$ and $I_{43}\to -I_{43}$, respectively, and conserving all other generating elements in $\{I_{21},I_{32},I_{43}\}$, to every such irreducible representation R there correspond the representations $R^{(+,-)}=R\circ\psi_2$, $R^{(-,+)}=R\circ\psi_1$, $R^{(-,-)}=R\circ\psi_1\psi_2$ such that

$$R^{(+,-)}(I_{21})|k,l\rangle=[k+l]_+|k,l\rangle,\quad R^{(+,-)}(I_{43})|k,l\rangle=-[k-l]_+|k,l\rangle, \tag{75}$$

$$R^{(-,+)}(I_{21})|k,l\rangle=-[k+l]_+|k,l\rangle,\quad R^{(-,+)}(I_{43})|k,l\rangle=[k-l]_+|k,l\rangle, \tag{76}$$

$$R^{(-,-)}(I_{21})|k,l\rangle=-[k+l]_+|k,l\rangle,\quad R^{(-,-)}(I_{43})|k,l\rangle=-[k-l]_+|k,l\rangle. \tag{77}$$

Conversely, to any of the representations $R^{(+,-)},R^{(-,+)},R^{(-,-)}$ with these properties there corresponds a unique representation R such that

$$R(I_{21})|k,l\rangle=[k+l]_+|k,l\rangle,\quad R(I_{43})|k,l\rangle=[k-l]_+|k,l\rangle \tag{78}$$

for all eigenvactors $|k,l\rangle$. This means that the classification of irreducible representations R with property (78) automatically leads to the classification of irreducible representations with any of the properties (75)–(77) and vice versa. Therefore, any of irreducible representations of $\mathrm{U}_q'(\mathrm{so}_4)$ with one of the properties (75)–(77) is equivalent to one of the irreducible representations of the nonclassical type. The theorem is proved.

In Sec. IV we constructed the homomorphism $\phi:\mathrm{U}_q'(\mathrm{so}_4)\to\hat{\mathrm{U}}_q(\mathrm{sl}_2)^{\otimes 2,\mathrm{ext}}$ (see Theorem 2). Now we are able to prove a stronger assertion:

Corollary: If q is not a root of unity, then the homomorphism $\mathrm{U}_q'(\mathrm{so}_4)\to\hat{\mathrm{U}}_q(\mathrm{sl}_2)^{\otimes 2,\mathrm{ext}}$ of Theorem 2 is injective.

Proof: If the assertion of our corollary is not true, then there exists nonzero element $a\in\mathrm{U}_q'(\mathrm{so}_4)$ such that $\phi(a)=0$. Then for any finite-dimensional representation T of the algebra $\hat{\mathrm{U}}_q(\mathrm{sl}_2)^{\otimes 2,\mathrm{ext}}$ we have $T(\phi(a))=0$. Taking the representations $T_{jj'}^{(\pm 1,\pm 1)}$, $T_{jj'}^{(\pm\mathrm{i},\pm 1)}$ and $T_{jj'}^{(\pm 1,\pm\mathrm{i})}$, where $T_{jj'}^{(\pm\varepsilon_1,\pm\varepsilon_2)}\equiv T_j^{(\pm\varepsilon_1)}\otimes T_{j'}^{(\pm\varepsilon_2)}$ (see Secs. VI and VII), as a representation T, we obtain $T_{jj'}^{(\pm 1,\pm 1)}(\phi(a))=0$, $T_{jj'}^{(\pm\mathrm{i},\pm 1)}(\phi(a))=0$, and $T_{jj'}^{(\pm 1,\pm\mathrm{i})}(\phi(a))=0$ for all admissible values of j and j'. As we have previously seen, any irreducible finite-dimensional representation of $\mathrm{U}_q'(\mathrm{so}_4)$ is equivalent to the representation $T_{jj'}^{(1,1)}\circ\phi$ with appropriate values of j and j' or to one of the irreducible constituents of the representations $T_{jj'}^{(\pm\mathrm{i},\pm 1)}\circ\phi$ and $T_{jj'}^{(\pm 1,\pm\mathrm{i})}\circ\phi$. This means that $R(a)=0$ for any irreducible finite-dimensional representation of $\mathrm{U}_q'(\mathrm{so}_4)$. But it was shown in Ref. 13 (see also Ref. 2) that irreducible finite-dimensional representations of $\mathrm{U}_q'(\mathrm{so}_4)$ separate elements of this algebra. Thus, for our element a there exists an irreducible finite-dimensional representation R such that $R(a)\neq 0$. This contradiction proves the corollary.

IX. COMPLETE REDUCIBILITY OF FINITE-DIMENSIONAL REPRESENTATIONS

It was proved in Ref. 29 that if q is not a root of unity, then every finite-dimensional representation of the algebra $\mathrm{U}_q'(\mathrm{so}_3)$ is completely reducible. The aim of this section is to prove the corresponding theorem for the algebra $\mathrm{U}_q'(\mathrm{so}_4)$.

We denote values of the Casimir operators C_4 and C_4' on irreducible representations of the classical and nonclassical types as follows:

$$C_4(R_{jj'})=C_{jj'},\quad C_4'(R_{jj'})=C_{jj'}',\quad C_4(R_{jj'}^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)})=\tilde{C}_{jj'},\quad C_4'(R_{jj'}^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)})=\tilde{C}_{jj'}'.$$

Then the values $C_{jj'}$ and $C'_{jj'}$ are given by formulas (63) and (64) whereas $\tilde{C}_{jj'}$ and $\tilde{C}'_{jj'}$ are given by (67) and (68). The following assertion will be used for proving the theorem on complete irreducibility.

Proposition 3: If for irreducible representations $R_{jj'}$ and $R_{kk'}$ we have $C_{jj'}=C_{kk'}$ and $C'_{jj'}=C'_{kk'}$, then these representations are equivalent, that is, $(j,j')=(k,k')$. If for irreducible representations $R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}$ and $R^{(\varepsilon'_1,\varepsilon'_2,\varepsilon'_3)}_{kk'}$ we have $\tilde{C}_{jj'}=\tilde{C}_{kk'}$ and $\tilde{C}'_{jj'}=\tilde{C}'_{kk'}$, then $(j,j')=(k,k')$. For any irreducible representations $R_{jj'}$ and $R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{kk'}$ the simultaneous equalities $C_{jj'}=\tilde{C}_{kk'}$ and $C'_{jj'}=\tilde{C}'_{kk'}$ are not possible.

Proof: We prove only the first part of the proposition (other ones are proved similarly). Let $C_{jj'}=C_{kk'}$ and $C'_{jj'}=C'_{kk'}$. We have from (63) and (64) that

$$C'_{kk'}=-(q^{2k+1}+q^{-2k-1})C_{kk'}-[2k][2k+2].$$

Substituting here $C_{kk'}=C_{jj'}$ we obtain from $C'_{jj'}=C'_{kk'}$ that

$$-(q^{2j+1}+q^{-2j-1})C_{jj'}-[2j][2j+2]=-(q^{2k+1}+q^{-2k-1})C_{jj'}-[2k][2k+2].$$

It can be simplified and factorized to the following form:

$$(q^{k+j+1}-q^{-k-j-1})(q^{k-j}-q^{-k+j})(q^{j'+k+1}+q^{-j'-k-1})(q^{j'-k}+q^{-j'+k})=0.$$

Since q is not a root of unity and j,j',k must be non-negative and integral or half-integral, this equality is true only for $k=j$. The relation $C_{jk'}=C_{jj'}$ can also be factorized and we obtain $(q^{k'+j'+1}-q^{-k'-j'-1})(q^{j'-k'}-q^{-j'+k'})=0$. Using similar argumentation, we derive from here that $j'=k'$. The proposition is proved.

Theorem 5: *If q is not a root of unity, then each finite-dimensional representation of $U'_q(so_4)$ is completely reducible.*

Proof: In order to prove this theorem it is enough to show that every finite-dimensional representation R of $U'_q(so_4)$, containing only two irreducible constituents, is completely reducible.

Let R be a finite-dimensional representation of $U'_q(so_4)$ containing only two irreducible constituents R' and R''. It is known that if $C_4(R')\neq C_4(R'')$ or $C'_4(R')\neq C''_4(R'')$, then R is a direct sum of its subrepresentations R' and R''. Thus, we have to consider only the case when $C_4(R')=C_4(R'')$ and $C'_4(R')=C'_4(R'')$. According to Proposition 3, we have to prove the theorem for two cases:

(a) Both constituents R' and R'' are equivalent and belong to the classical type.

(b) Both constituents R' and R'' are of the nonclassical type and are of the form $R^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}_{jj'}$ and $R^{(\varepsilon'_1,\varepsilon'_2,\varepsilon'_3)}_{jj'}$.

Each case will be proved separately.

Case (a). We denote our constituents by $R_{jj'}$ and $R'_{jj'}$, respectively. Since restriction of the representation R to the subalgebra $U'_q(so_3)$ is completely reducible, there exists a basis in the space of the representation R consisting of eigenvectors for both operators $R(I_{21})$ and $R(I_{43})$. In this basis there exist exactly two vectors of highest weight. Let $|j,j'\rangle$ and $|j,j'\rangle'$ be these vectors. We create two sets of vectors

$$X_2^r X_4^t|j,j'\rangle, \quad r,t=0,1,2,\ldots, \quad \text{and} \quad X_2^r X_4^t|j,j'\rangle', \quad r,t=0,1,2,\ldots,$$

where each of the operators X_2 and X_4 is taken with the appropriate upper indices. Due to the properties of the operators X_2 and X_4, these two sets span two subspaces V_1 and V_2 which are invariant with respect to the operators $R(I_{21})$, $R(I_{32})$, and $R(I_{43})$. Moreover, we have $V=V_1\oplus V_2$ and the theorem is proved in this case.

Case (b). We distinguish here the following subcases:

(I) two constituents are equivalent;

(II) two constituents are $R_{jj'}^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}$ and $R_{jj'}^{(\varepsilon_1',\varepsilon_2',\varepsilon_3')}$, where $\varepsilon_1\neq\varepsilon_1'$ or/and $\varepsilon_2\neq\varepsilon_2'$; and

(III) two constituents are $R_{jj'}^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}$ and $R_{jj'}^{(\varepsilon_1,\varepsilon_2,-\varepsilon_3)}$.

For subcase (I) a proof is such as in case (a). Let us consider subcase (II). Let $\varepsilon_1\neq\varepsilon_1'$. In the representation space V, there exist two linearly independent vectors $|j,j'\rangle$ and $|j,j'\rangle'$ which are of highest weights, that is,

$$X_1^{(i,j')}|j,j'\rangle=X_1^{(j,j')}|j,j'\rangle'=0,\quad X_3^{(jj')}|j,j'\rangle=X_3^{(jj')}|j,j'\rangle'=0,$$

and such that

$$R(I_{21})|j,j'\rangle=\varepsilon_1[j+j']_+|j,j'\rangle,\quad R(I_{21})|j,j'\rangle'=\varepsilon_1'[j+j']_+|j,j'\rangle.$$

We create two sets of vectors

$$X_2^rX_4^t|j,j'\rangle,\quad r,t=0,1,2,\cdots,\quad \text{and}\quad X_2^rX_4^t|j,j'\rangle',\quad r,t=0,1,2,...,$$

where the operators X_2 and X_4 are taken with the appropriate upper indices. No nonzero vector of the first set is a multiple of some vector of the second set (since otherwise these two sets span the same vector subspace of the representation space V). These two sets of vectors span two invariant linear subspaces V_1 and V_2 of V. Since $V=V_1\oplus V_2$, then the representation R is a direct sum of the subrepresentations $R_{jj'}^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}$ and $R_{jj'}^{(\varepsilon_1',\varepsilon_2',\varepsilon_3')}$.

Let us prove the theorem in subcase (III). We suppose that the representation $R_{jj'}^{(\varepsilon_1,\varepsilon_2,\varepsilon_3)}$ is realized on an invariant subspace V_1 and denote weight vectors for this representation by $|k,l\rangle$. We have $R(I_{32})|\frac{1}{2},0\rangle=\varepsilon_3a|\frac{1}{2},0\rangle+\cdots$, where a is the appropriate constant, and a linear combination of weight vectors with weights, different from that of the vector $|\frac{1}{2},0\rangle$, is denoted by dots. In the space V of the representation R there exists another vector $|\frac{1}{2},0\rangle'$ such that

$$R(I_{32})|\tfrac{1}{2},0\rangle'=-\varepsilon_3a|\tfrac{1}{2},0\rangle'+r|\tfrac{1}{2},0\rangle+\cdots,$$

where dots mean the same as earlier. Then we easily verify that

$$R(I_{32})\left(\left|\frac{1}{2},0\right\rangle'-\frac{r}{2a\varepsilon_3}\left|\frac{1}{2},0\right\rangle\right)=-a\varepsilon_3\left(\left|\frac{1}{2},0\right\rangle'-\frac{r}{2a\varepsilon_3}\left|\frac{1}{2},0\right\rangle\right)+\cdots$$

with the same meaning for dots. Denoting the vector $|\frac{1}{2},0\rangle'-(r/2a\varepsilon_3)|\frac{1}{2},0\rangle$ by $|\frac{1}{2},0\rangle''$ we create the vectors

$$X_1^rX_3^t|\tfrac{1}{2},0\rangle'',\quad r,t=0,1,2,...,$$

then take the vector of highest weight in this set (we denote it by $|j,j'\rangle''$) and create the vectors

$$X_1^rX_3^t|j,j'\rangle'',\quad r,t=0,1,2,...$$

(the operators X_1 and X_3 are taken with the appropriate upper indices). The linear subspace V_2 spanned by the last vectors is invariant and irreducible. Since $V=V_1\oplus V_2$, the theorem is proved also in this subcase.

X. TENSOR PRODUCTS OF REPRESENTATIONS

As in the case of the algebra $U_q'(so_3)$ (see Ref. 21), the homomorphism of Theorem 2 allows us to determine tensor products of irreducible finite-dimensional representations of the algebra $U_q'(so_4)$ and decompose them into irreducible constituents.

Let us explain this on the example of the classical type irreducible representations of $U_q'(so_4)$. Let $T^{(1,1)}_{jj'}=T^{(1)}_j\otimes T^{(1)}_{j'}$ be the irreducible representation of $U_q(sl_2)^{\otimes 2,\mathrm{ext}}$. Then the tensor product $T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'}$ is a well-defined representation of the algebra $U_q(sl_2)^{\otimes 2}$. Thus, we have to determine the operators $(T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'})(x_i)$, $i=1, 2$. For this we use the determined operators $(T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'})(c_i)$, $i=1, 2$, where c_i are Casimir elements from Sec. III. We define the operators $(T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'})(x_i)$ as solutions of quartic equations

$$q^{-1}\{(T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'})(x_i)\}^4-(T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'})(c_i)(q-q^{-1})^2\{(T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'})(x_i)\}^2+q=0 \quad (79)$$

(see the equation for the elements x_i in Sec. III). In order to find these solutions we may diagonalize the operators $(T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'})(c_i)$, which is always possible because the representation $T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'}$ is completely reducible. These operators turn to the block diagonal form with multiples of identity on the diagonal and the solutions of Eqs. (79) can be easily calculated. The solutions $(T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'})(x_i)$ have the same form and therefore clearly commute with all other operators which now have block diagonal form. Composing the representation $T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'}$ of $U_q(sl_2)^{\otimes 2,\mathrm{ext}}$ with the homomorphism ϕ from Theorem 2 we obtain the representation

$$R_{jj'}\otimes R_{ss'}=\{T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'}\}\circ\phi,$$

which is treated as the tensor product of irreducible representations $R_{jj'}$ and $R_{ss'}$ of the algebra $U_q'(so_4)$.

For the representation $T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'}$ of $U_q(sl_2)^{\otimes 2,\mathrm{ext}}$ we have the decomposition

$$T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'}=\bigoplus_{k=|j-s|}^{j+s}\ \bigoplus_{k'=|j'-s'|}^{j'+s'} T^{(1,1)}_{kk'}.$$

Composing the left- and the right-hand sides of this relation with the homomorphism ϕ from Theorem 2,

$$T^{(1,1)}_{jj'}\otimes T^{(1,1)}_{ss'})\circ\phi=\left(\bigoplus_k\ \bigoplus_k T^{(1,1)}_{kk'}\right)\circ\phi,$$

we obtain the decomposition of the tensor product $R_{jj'}\otimes R_{ss'}$:

$$R_{jj'}\otimes R_{ss'}=\bigoplus_{k=|j-s|}^{j+s}\ \bigoplus_{k'=|j'-s'|}^{j'+s'} R_{kk'}.$$

As in the case of the algebra $U_q'(so_3)$ in Ref. 21, we can also determine in a similar way tensor products of irreducible representations of the classical and the nonclassical types and tensor products of irreducible representations of the nonclassical type.

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Transformation formulas for double hypergeometric series related to 9-*j* coefficients and their basic analogs

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In a recent paper, Ališauskas deduced different triple sum expressions for the 9-*j* coefficient of su(2) and $su_q(2)$. For a singly stretched 9-*j* coefficient, these reduce to different double sum series. Using these distinct series, we deduce a set of new transformation formulas for double hypergeometric series of Kampé de Fériet type and their basic analogs. These transformation formulas are valid for rather general parameters of the series, although a common feature is that all the series appearing here are terminating. It is also shown that the transformation formulas deduced here generate a group of transformation formulas, thus yielding an invariance group or symmetry group of particular double series. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1405126]

I. INTRODUCTION

The Wigner 9-*j* coefficients (or 9-*j* symbols) arise as recoupling coefficients in the coupling (tensor product) of four irreducible representations of su(2), and play an important role in the quantum theory of angular momentum.[1–3] Although the relation between recoupling coefficients, such as the 3-*j* coefficient and the 6-*j* coefficient, and hypergeometric series or (discrete) orthogonal polynomials of hypergeometric type is well understood,[3–6] the 9-*j* coefficient remains somewhat a mystery in this respect. There are many known expressions for the 9-*j* coefficient as a multiple hypergeometric series. The most compact formula is the so-called triple sum series, originally derived by Ališauskas and Jucys,[7] and rederived in Ref. 8. Whether a triple sum expression is really the best one can do for the 9-*j* coefficient is not known; specialists in the field still guess that a double sum series might exist.[9]

The triple sum series of Ališauskas and Jucys was recognized as a special case[5,10] of a triple hypergeometric series defined by Srivastava.[11] It was used to speed up the numerical computation of 9-*j* coefficients,[10] and to derive certain summation and reduction formulas for hypergeometric series by using particular classes of 9-*j* coefficients.[12–14]

Ališauskas and Jucys's triple sum series was recently rederived in two ways. In Ref. 15, Rosengren deduced the triple sum series for 9-*j* coefficients [of su(1,1) rather than of su(2)] based upon the use of coupling kernels; in Ref. 16, he showed that the same formula can be deduced starting from the classical expansion of the 9-*j* coefficient in terms of 6-*j* coefficients and performing Dougall's summation formula[17] for a very well-poised ${}_4F_3(-1)$ series. In a recent paper,[18] Ališauskas realized that this technique can be applied for several distinct expansions of the 9-*j* coefficient in terms of 6-*j* coefficients. Thus he obtained seven different triple sum formulas for the 9-*j* coefficient of su(2). At the same time, he showed that this technique has a basic analogue (or *q*-analog), depending upon a *q*-analog of Dougall's summation formula.[19] So, he also obtained seven triple sum formulas for the 9-*j* coefficient of $su_q(2)$, i.e., for the *q*-9-*j* coefficients.

The study of these different triple sum formulas from the point of view of multiple hypergeo-

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metric series would be interesting, though rather tedious because of the complicated structure of the formulas. However, when considering the class of singly stretched 9-j coefficients (i.e., one of the arguments in the 9-j coefficient is the sum of two others), most of these triple sum formulas reduce to double sum formulas which are less complicated and easier to handle. Ališauskas actually wrote down these double sum formulas (Ref. 18, Sec. IV B), and used them to derive certain rearrangement formulas of double sum series and their basic analogs.

In the present article we shall show that the double sum formulas for the singly stretched 9-j coefficient actually give rise to a fairly complete theory of transformation formulas for terminating double hypergeometric series of Kampé de Fériet type. This is particularly interesting because until now not many transformation formulas for multiple hypergeometric series are known, even though transformation formulas for hypergeometric series of a single variable play an important role.[17,20] The double hypergeometric series appearing in this context are proper Kampé de Fériet functions $F_{q:s;s}^{p:r;r}$ with $q+s=2$ and $p+r=3$. Such functions have been defined in Refs. 21 and 22, and studied by Srivastava and Karlsson,[23] whose notation we follow. This notation is a rather straightforward extension of that for single hypergeometric series, e.g.,

$$F_{0:2;2}^{1:2;2}\left[\begin{matrix} e:a,b;a',b'; \\ :c,d;c',d'; \end{matrix} x,y\right]=\sum_{j,k=0}^{\infty}(e)_{j+k}\frac{(a)_j(b)_j}{(c)_j(d)_j}\frac{(a')_k(b')_k}{(c')_k(d')_k}\frac{x^j}{j!}\frac{y^k}{k!}, \tag{1}$$

and

$$F_{1:1;1}^{1:2;2}\left[\begin{matrix} e:a,b;a',b'; \\ d:\ c\ ;\ c'\ ; \end{matrix} x,y\right]=\sum_{j,k=0}^{\infty}\frac{(e)_{j+k}}{(d)_{j+k}}\frac{(a)_j(b)_j}{(c)_j}\frac{(a')_k(b')_k}{(c')_k}\frac{x^j}{j!}\frac{y^k}{k!}. \tag{2}$$

Herein, $(a)_k$ is the classical Pochhammer symbol,[17,20]

$$(a)_k=a(a+1)\cdots(a+k-1); \tag{3}$$

$a,b,\ldots$ are referred to as the parameters of the series, and x, y as the variables. Observe that factors of the form $(d)_{j+k}$ or $(e)_{j+k}$ are responsible for the fact that such double series cannot simply be written as the product of two single hypergeometric series. The Kampé de Fériet series appearing in the context of double sums related to the 9-j coefficients are those of type $F_{0:2;2}^{1:2;2}$, $F_{1:1;1}^{1:2;2}$ and $F_{1:1;1}^{0:3;3}$.

Convergence properties of such Kampé de Fériet series have been considered in Ref. 24. In this article, however, all the series dealt with are *terminating* series and hence there are no convergence conditions. Note that the termination of Kampé de Fériet series such as (1) or (2) can be assured in two ways:

(i) A common numerator parameter equals a negative integer: e.g., $e=-n$, with n a positive integer, in (1) or (2) yields a terminating series irrespective of the value of the other parameters.

(ii) Two separate numerator parameters are equal to negative integers: e.g., $a=-n$ and $a'=-m$ in (1) or (2), with m and n positive integers.

In both cases the denominator parameters of the Kampé de Fériet series should not be negative integers. If some of the denominator parameters are nevertheless negative integers, then they should be smaller (or equal) than the parameters responsible for the termination of the series.

The transformation formulas deduced here from the double sum expressions for 9-j coefficients turn out to be of a quite general nature. Apart from the parameter(s) responsible for the termination, the remaining parameters of the series are completely general. Furthermore, the transformation formulas, together with trivial permutation symmetries, are shown to generate a *symmetry group* for the double hypergeometric series. In other words, we shall show that for each of the double hypergeometric series considered here, there exists a whole set of transformation formulas related to a group action on the parameters of the double series.

In the paper by Ališauskas,[18] the emphasis is on the q-9-j coefficients, i.e., the 9-j coefficients of $\mathrm{su}_q(2)$. So it would be interesting to see if the transformation theory developed here could be generalized to the basic analog (i.e., the q-analogue). This is indeed the case. We shall give and prove a set of new transformation formulas for basic double series. For the notation related to q-series and single basic hypergeometric series, we refer to the standard book of Gasper and Rahman.[25] The double series appearing in this context, however, are special cases of general basic double series defined by Srivastava and Karlsson (Ref. 23, p. 349).

II. THE STRETCHED 9-j COEFFICIENT AND DOUBLE SERIES

Ališauskas[18] considers the stretched 9-j coefficient denoted by

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j_{12}+j_{34} \end{Bmatrix}, \tag{4}$$

which is a transformation coefficient connecting two different ways in which four angular momenta j_1, j_2, j_3 and j_4 can be coupled. Since they stand for angular momenta, all the arguments in (4) are non-negative integers or half-integers. In fact, in Ref. 18, the q-analogs of such 9-j coefficients are considered, but here we first treat the classical case ($q=1$).

In Ref. 18, Sec. IV B, a list of double sum expressions is determined for (4). It is not difficult to rewrite these in terms of double hypergeometric series of Kampé de Fériet type. For example, from Ref. 18, (4.3d), one deduces

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j_{12}+j_{34} \end{Bmatrix}$$

$$= C F^{1:2;2}_{0:2;2}\left[\begin{matrix} -j_1-j_2+j_{12} : -j_2-j_4+j_{24}, -j_2-j_4-j_{24}-1 ; j_{13}-j_1+j_3+1, -j_1-j_3+j_{13}; \\ : -2j_2, -j_2-j_4+j_{12}+j_{34}-j_{13} ; -2j_1, j_4-j_1-j_{34}+j_{13}+1 ; \end{matrix} 1,1\right], \tag{5}$$

where C is some constant. Similarly, Ref. 18, (4.4b), yields

$$\begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j_{12}+j_{34} \end{Bmatrix}$$

$$= C' F^{1:2;2}_{1:1;1}$$

$$\times\left[\begin{matrix} -j_1-j_2+j_{12} & : -j_2-j_4+j_{24}, 1+j_4-j_2+j_{24}; j_{13}-j_1+j_3+1, -j_1-j_3+j_{13}; \\ 1-j_1-j_{34}+j_{13}-j_2+j_{24}: & -2j_2 \quad ; \quad -2j_2 \quad ; \end{matrix} 1,1\right], \tag{6}$$

where C' is another constant. Upon equating the rhs's of (5) and (6), using the actual values of C and C', and relabelling the parameters of the series, one finds

$$F^{1:2;2}_{0:2;2}\left[\begin{matrix} -n : a,b ; a',b' ; \\ : c,d ; c',d' ; \end{matrix} 1,1\right] = \frac{(d-a+n-1)!(d-1)!}{(d-a-1)!(d+n-1)!} F^{1:2;2}_{1:1;1}\left[\begin{matrix} -n \ : a, c-b ; a', b' ; \\ d'+a : \quad c \quad ; \quad c' \quad ; \end{matrix} 1,1\right]. \tag{7}$$

Herein, the parameters satisfy $d+d'=1-n$, so there are in total eight free parameters [as there are in (4)]. Since all the parameters in (4) are non-negative integers or half-integers, the param-

eters in (7) in first instance all correspond to integers. In particular, $-n$ corresponds to a negative integer (due to triangular conditions satisfied by the angular momentum coefficients). However, once the equation is rewritten in the form (7), with

$$\frac{(d-a+n-1)!(d-1)!}{(d-a-1)!(d+n-1)!}=\frac{(d-a)_n}{(d)_n},$$

it is obvious that this is a *rational identity* in the remaining parameters a, b, c, d, a', b', c' and d', once $-n$ is a fixed negative integer. Therefore, (8a) holds for arbitrary parameters a, b, c, d, a', b', c' and d' (but still subject to the constraint $d+d'=1-n$). As such, we have found a rather general transformation formula between two terminating Kampé de Fériet series. This proves the first formula of the following theorem:

Theorem 1: *Let n be a non-negative integer and a, b, c, d, a′, b′, c′ and d′ arbitrary parameters with $d+d'=1-n$. Then the following transformation formulas hold*:

$$F^{1:2;2}_{0:2;2}\left[\begin{matrix}-n:a,b\,;a',b'\,;\\ :c,d\,;c',d'\,;\end{matrix}1,1\right]=\frac{(d-a)_n}{(d)_n}F^{1:2;2}_{1:1;1}\left[\begin{matrix}-n\ :a,c-b\,;a',b'\,;\\ d'+a:\ c\ ;\ c'\ ;\end{matrix}1,1\right] \tag{8a}$$

$$=\frac{(d-b+b')_n}{(d)_n}F^{1:2;2}_{0:2;2}\left[\begin{matrix}-n:c-a,b\ ;c'-a',b'\ ;\\ :c,d'-b'+b\,;c',d-b+b'\,;\end{matrix}1,1\right], \tag{8b}$$

and

$$F^{1:2;2}_{1:1;1}\left[\begin{matrix}-n:a,b\,;a',b'\,;\\ d\ :\ c\ ;\ c'\ ;\end{matrix}1,1\right]=\frac{(d-b-b')_n}{(d)_n}F^{1:2;2}_{1:1;1}\left[\begin{matrix}-n\ :c-a,b\,;c'-a',b'\,;\\ 1-n-d+b+b':\ c\ ;\ c'\ ;\end{matrix}1,1\right]. \tag{9}$$

Proof: The transformation formula (8b) was deduced recently in a different context.[26] This equation can now also be seen in the context of the stretched 9-j coefficient. In fact, it corresponds to a symmetry of this 9-j coefficient [namely a transposition of the first and second column in (4)], reexpressed by means of (5). Finally, applying (8a) to the rhs of (8b) and equating the resulting expression with the rhs of (8a) yields (9) (after appropriate relabelling of the parameters). □

Observe that in this section all Kampé de Fériet series are terminating because a common numerator parameter equals a negative integer. In the following section we shall consider some transformation formulas, also deduced from the stretched 9-j coefficient, for Kampé de Fériet series that are terminating because of the appearance of two negative integers as separate numerator parameters.

III. KAMPÉ DE FÉRIET SERIES WITH TWO NEGATIVE INTEGERS AS PARAMETER

Though the transformation formulas with a single common numerator parameter as a negative integer (i.e., Theorem 1) are new, there do exist some transformation formulas for Kampé de Fériet series with two separate numerator parameters as negative integers. One of these formulas is given by Singh,[27] and reads

$$F^{0:3;3}_{1:1;1}\left[\begin{matrix}:-n,a,b\,;-m,a',b'\,;\\ d:\ c\ ;\ c'\ ;\end{matrix}1,1\right]$$

$$=\frac{(c-a)_n(c'-a')_m}{(c)_n(c')_m}F^{0:3;3}_{1:1;1}\left[\begin{matrix}:\ -n,a,b'\ ;\ -m,a',b\ ;\\ d:1+a-c-n\,;1+a'-c'-m\,;\end{matrix}1,1\right], \tag{10}$$

where n and m are non-negative integers and $b+b'=d$. This, and some other transformation formulas of similar type, can be found in or deduced from Ref. 18, Appendix C.

Let us first consider some transformation formulas that express a Kampé de Fériet series of type $F^{1:2;2}_{0:2;2}$ into a series of a different type:

Theorem 2: *Let m and n be non-negative integers, and a, b, c, d, a′, b′ and c′ be arbitrary parameters with c+c′=1+d. Then*

$$F^{1:2;2}_{0:2;2}\left[\begin{matrix} d:-n,a\,;-m,a'\,; \\ :\ b,c\ ;\ b',c'\ ; \end{matrix}1,1\right]$$
$$=\frac{(b-a)_n(1-c)_m}{(b)_n(c')_m}F^{0:3;3}_{1:1;1}\left[\begin{matrix} :-n,a,-d+c\,;-m,b'-a',d\,; \\ c-m:-n+a-b+1\,; \quad b' \quad ; \end{matrix}1,1\right] \tag{11a}$$

$$=\frac{(1-c)_m}{(c')_m}F^{1:2;2}_{1:1;1}\left[\begin{matrix} d\ :-n,a\,;-m,b'-a'\,; \\ c-m:\ b\ ;\quad b' \quad ; \end{matrix}1,1\right]. \tag{11b}$$

The proof of (11a) follows by comparing Eqs. (4.3c) and (4.3e) of Ref. 18, making appropriate relabellings, and using the same rational expression argument as in the proof of Theorem 1. In a similar way, (11b) follows from (4.3b) and (4.4c) of Ref. 18.

It is worth mentioning that transformation formulas (8a) and (11b) are formally equivalent [after rewriting the Pochhammer symbols in terms of gamma functions and using the constraint $1-c=c'-d$ to eliminate c from the gamma functions in (11b)].

We can now present three results, giving transformation formulas for Kampé de Fériet series of a particular type into series of the same type, for each of the types $F^{1:2;2}_{0:2;2}$, $F^{1:2;2}_{1:1;1}$ and $F^{0:3;3}_{1:1;1}$.

Theorem 3: *Let n and m be non-negative integers and a, b, c, a, b′, c′ and d be arbitrary parameters with c+c=d+1. Then*

$$F^{1:2;2}_{0:2;2}\left[\begin{matrix} d:-n,a\,;-m,a'\,; \\ :\ b,c\ ;\ b',c'\ ; \end{matrix},1,1\right]$$
$$=\frac{(-1)^m(d)_n(b-a)_n(a')_m}{(b)_n(c')_m(b')_m(c)_{n-m}}$$
$$\times F^{1:2;2}_{0:2;2}\left[\begin{matrix} -m-c'+1: & -n,-n-b+1 & ; & -m,-a'+b' & ; \\ & :-n+a-b+1,-n-d+1\,; & & -m-a'+1,-m+n+c\,; \end{matrix}1,1\right] \tag{12a}$$

$$=\frac{(-1)^m(d)_m(b-a)_n(a')_m}{(b)_n(b')_m(c')_m}$$
$$\times F^{1:2;2}_{0:2;2}\left[\begin{matrix} -m-c'+1: & -n,a & ; & -m,1-m-b' & ; \\ & :-n+a-b+1,c\,; & & 1-m-a',1-m-d\,; \end{matrix}1,1\right]. \tag{12b}$$

Proof: The first formula, (12a), follows by comparing expressions (4.3a) and (4.3d) of Ref. 18, and using the rational expression argument. The second formula is derived using (11a) and Singh's formula (10). □

In (12a) the difference $n-m$ might be negative, and then $c_{n-m}=(-1)^{m-n}/(1-c)_{m-n}$, which is the natural extension of the Pochhammer symbol.

Using the above two formulas and (11b) yields the following.

Theorem 4: *Let n and m be non-negative integers and let a, b, a′, b′, c and d be arbitrary parameters. Then*

$$F^{1:2;2}_{1:1;1}\left[\begin{matrix} c: -n,a\,; -m,a'\,; \\ d: b\quad\;\; ; b'\quad\;\; ; \end{matrix} 1,1\right]$$

$$= \frac{(c)_{n+m}(b-a)_n(b'-a')_m}{(d)_{n+m}(b)_n(b')_m}$$

$$\times F^{1:2;2}_{1:1;1}\left[\begin{matrix} d-c & : -n,-n-b+1\,; -m,-m-b'+1\,; \\ -n-m-c+1: & -n+a-b+1\,; -m+a'-b'+1\,; \end{matrix} 1,1\right] \tag{13a}$$

$$= \frac{(b-a)_n(b'-a')_m}{(b)_n(b')_m} F^{1:2;2}_{1:1;1}\left[\begin{matrix} d-c: & -n,a & ; & -m,a' & ; \\ d & : -n+a-b+1\,; & & -m+a'-b'+1\,; & \end{matrix} 1,1\right]. \tag{13b}$$

As a third and final result, we give the transformation formulas for Kampé de Fériet series of type $F^{0:3;3}_{1:1;1}$. The first formula follows from (12a) and (11a); the second is just Singh's formula (10).

Theorem 5: *Let n and m be non-negative integers and let a, b, c, a′, b′, c′ and d be arbitrary parameters such that b+b′=d. Then*

$$F^{0:3;3}_{1:1;1}\left[\begin{matrix} : -n,a,b\,; -m,a',b'\,; \\ d: \quad c \quad ; \quad c' \quad ; \end{matrix} 1,1\right]$$

$$= \frac{(b')_{n+m}(a)_n(c'-a')_m}{(d)_{n+m}(c)_n(c')_m}$$

$$\times F^{0:3;3}_{1:1;1}\left[\begin{matrix} & : -n,c-a,1-n-m-d\,; -m,-c'-m+1,b\,; \\ -n-m+1-b': & -n-a+1 \quad ; & -m+a'-c'+1 \quad ; \end{matrix} 1,1\right] \tag{14a}$$

$$= \frac{(c-a)_n(c'-a')_m}{(c)_n(c')_m} F^{0:3;3}_{1:1;1}\left[\begin{matrix} : & -n,a,b' & ; & -m,a',b & ; \\ d: 1+a-c-n\,; & & & 1+a'-c'-m\,; & \end{matrix} 1,1\right]. \tag{14b}$$

IV. SYMMETRY GROUPS OF TERMINATING KAMPÉ DE FÉRIET SERIES

In the previous sections we have determined transformation formulas between (terminating) Kampé de Fériet series of the same type. It is known that transformation formulas of hypergeometric series of a single variable can give rise to a transformation group.[28] This transformation group, known as the symmetry group or invariance group of the series, arises as a finite group acting on the parameters of the series. The existing transformation formulas are then expressed as the invariance of a certain hypergeometric series under the action of group elements on its parameters. For single hypergeometric series (and basic series), this idea has been expanded in Ref. 28.

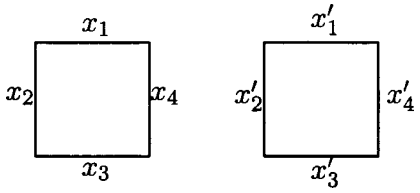
So, it would be interesting to see whether there are any invariance groups behind the transformation formulas for double hypergeometric series, as the ones we are dealing with in this article. One such invariance group for a double series has recently been discussed.[26] This concerns the invariance group related to the transformation formula (8b). Observe that (8b) gives a transformation between two series of the type $F^{1:2;2}_{0:2;2}$. Apart from this transformation, there are also trivial transformations for

$$F^{1:2;2}_{0:2;2}\left[\begin{matrix} -n: a,b\,; a',b'\,; \\ \quad : c,d\,; c',d'\,; \end{matrix} 1,1\right] \quad \text{with} \quad d+d'=1-n, \tag{15}$$

namely the transposition of a and b, or the transposition of a' and b', or the exchange of all primed with the corresponding unprimed parameters. It was shown in Ref. 26 that superposing

such trivial transformations with (8b) gives rise to a set of 64 transformations for the series $F^{1:2;2}_{0:2;2}$ (with one common numerator parameter equal to $-n$). These 64 transformations correspond to a group G of order 64, which we shall briefly describe because it also plays a role in other transformations considered in this article.

First, consider the permutation group S_8 acting on $(x_1,x_2,x_3,x_4,x_1',x_2',x_3',x_4')$, and its subgroup $D_8\times D_8'$. Herein, D_8 stands for the dihedral group[29] (sometimes denoted by D_4) consisting of the eight symmetries of the square (i.e., those permutations of $x_1,\ldots,x_4$ that preserve the square whose sides are labeled by $x_1,\ldots,x_4$). Similarly, D_8' is the same dihedral group but acting on the primed labels $x_1',\ldots,x_4'$. The group $D_8\times D_8'$ consists of 64 elements; superposing on this group the interchange of primed and unprimed elements yields a group of order 128, denoted by $S_2\times(D_8\times D_8')$. This is the invariance group of two squares whose sides are labeled as follows:



The group G now consists of those 64 elements of $S_2\times(D_8\times D_8')$ that preserve the constraint

$$x_1+x_3+x_1'+x_3'-x_2-x_4-x_2'-x_4'=0, \tag{16}$$

i.e., those elements that map $X=x_1+x_3+x_1'+x_3'-x_2-x_4-x_2'-x_4'$ into $\pm X$ by permuting the indices. The following proposition[26] then describes the invariance group generated by the transformation (8b):

Proposition 6: Let x_i, x_i' $(i=1,\ldots,4)$ be arbitrary parameters such that $x_1+x_3+x_1'+x_3'=x_2+x_4+x_2'+x_4'$ and let n be a non-negative integer. Then the expression

$$f_1(x)=\left(\frac{1-n}{2}+x_2-x_2'\right)_n \times F^{1:2;2}_{0:2;2}\left[\begin{matrix} -n: x_2+x_3, x_1+x_2 & ; x_2'+x_3', x_1'+x_2' & ; \\ : \sum_i x_i,\ \frac{1-n}{2}+x_2-x_2' & ; \sum_i x_i',\ \frac{1-n}{2}+x_2'-x_2 & ; \end{matrix}1,1\right]$$

is (up to a sign) invariant under the action of G. The action of an element g of G is by permuting the indices of $x_1,\ldots,x_4'$, and we can write

$$f_1(g\cdot x)=\epsilon^n f_1(x),$$

where $\epsilon=\pm 1$ is determined by $g(X)=\epsilon X$.

When determining the invariance group of the series

$$F^{1:2;2}_{1:1;1}\left[\begin{matrix} -n: a,b; a',b'; \\ d \ : \ c \ ; \ c' \ ; \end{matrix}1,1\right] \tag{17}$$

the following relabeling is appropriate:

$$a=x_2+x_3,\quad b=x_1+x_2,\quad c=\sum_i x_i,$$
$$a'=x_2'+x_3',\quad b'=x_1'+x_2',\quad c'=\sum_i x_i',\quad d=\frac{1-n}{2}+x_2+x_2'. \tag{18}$$

Here again, $-n$ is a negative integer and $x_1,\ldots x_4'$ are arbitrary parameters satisfying (16). Using this relabeling in (17), the transformation (9) corresponds (apart from a factor) to the permutation $g_1=(x_1\,x_2)(x_3\,x_4)(x_1'\,x_2')(x_3'\,x_4')$. The trivial transposition of a and b in (17) corresponds to the permutation $g_2=(x_1\,x_3)$. And the interchange of primed and unprimed parameters in (17) corresponds to the permutation $g_3=(x_1\,x_1')(x_2\,x_2')(x_3\,x_3')(x_4\,x_4')$. It is now easy to see that the elements g_1, g_2 and g_3 generate the group G described earlier. Thus we have the following result:

Proposition 7: Let x_i, x_i' $(i=1,\ldots,4)$ be arbitrary parameters such that $x_1+x_3+x_1'+x_3'=x_2+x_4+x_2'+x_4'$ and let n be a non-negative integer. Then the expression

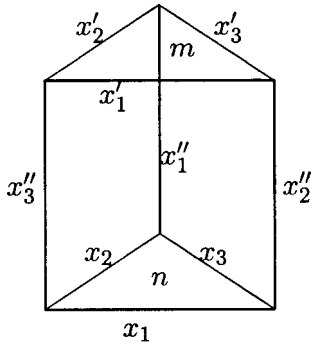
$$f_2(x)=\left(\frac{1-n}{2}+x_2+x_2'\right)_n F^{1:2;2}_{1:1;1}\left[\begin{matrix}-n & : x_2+x_3,x_1+x_2;\ x_2'+x_3',x_1'+x_2';\\ \frac{1-n}{2}+x_2+x_2' : \sum_i x_i & ;\ \sum_i x_i' \end{matrix};1,1\right]$$

is (up to a sign) invariant under the action of G, i.e., $f_2(g\cdot x)=\epsilon^n f_2(x)$, where $\epsilon=\pm 1$ is determined by $g(X)=\epsilon X$.

So the invariance groups of (15) and (17) are the same: both series have 64 symmetries. Moreover, the two nontrivial transformations (8b) and (9) both correspond to the same element, namely g_1, of G.

Now we shall show that also the transformations with two numerator parameters $-n$ and $-m$ being negative integers give rise to an interesting symmetry group. It will be convenient to first describe the group, and then show that under a certain relabeling of the parameters it is indeed the symmetry group of the transformations given in Theorems 3–5.

Consider a prism with an equiangular triangle as basis and edges orthogonal to this basis. The sides of the triangles are labeled by x_1, x_2, x_3 and x_1', x_2', x_3'; the three edges are labeled by x_1'', x_2'', x_3''. For convenience we shall also label the basis triangle by n and the opposite triangle by m:



The symmetry group H of this prism is generated by four planes of symmetry: the three planes of symmetry through an edge $x_i''(i=1,2,3)$ and the plane of symmetry parallel with the basis. Let $r_i(i=1,2,3)$ denote the reflection about a plane of symmetry through an edge x_i'', and let r_0 denote the reflection about the plane of symmetry that is parallel with the basis. These four reflections map the prism into itself, and they generate the symmetry group of the prism. This symmetry group H is a group of order 12, and it is easy to verify that it is isomorphic to the dihedral group D_{12} (i.e., the symmetries of the hexagon). The generating reflections correspond to permutations of $x_1,x_2,\ldots,x_3''$ (and possibly an interchange of n and m):

$$r_1:(x_2\,x_3)(x_2'\,x_3')(x_2''\,x_3''),$$

$$r_2:(x_1\,x_3)(x_1'\,x_3')(x_1''\,x_3''),$$

$$r_3:(x_1\,x_2)(x_1'\,x_2')(x_1''\,x_2''),$$

$$r_0:(x_1\,x_1')(x_2\,x_2')(x_3\,x_3')(n\,m).$$

It turns out that the transformations given in Theorems 3–5 all have the same symmetry group, described by H. Thus we can state the following:

Proposition 8: Let m and n be nonnegative integers, and let x_i, x_i', x_i'' $(i=1,2,3)$ *be arbitrary parameters such that* $\Sigma_{i=1}^3 x_i=0$, $\Sigma_{i=1}^3 x_i'=0$, $\Sigma_{i=1}^3 x_i''=0$. *Then the following expressions,*

$$g_1(x)$$

$$=\left(\frac{2(1-n)}{3}-x_1\right)_n\left(\frac{2-2n+m}{3}-x_2''\right)_n\left(\frac{2(1-m)}{3}-x_1'\right)_m\left(\frac{2-2m+n}{3}-x_3''\right)_m$$

$$\times F^{1:2;2}_{0:2;2}\left[\begin{matrix}\dfrac{1-n-m}{3}+x_1'': -n, \dfrac{1-n}{3}+x_2 & ; -m, \dfrac{1-m}{3}+x_3' & ; \\ : \dfrac{2(1-n)}{3}-x_1, \dfrac{2-2n+m}{3}-x_2''; & \dfrac{2(1-m)}{3}-x_1', \dfrac{2-2m+n}{3}-x_3'' & ;\end{matrix}\ 1,1\right], \tag{19}$$

$$g_2(x)=\left(\frac{2(1-n-m)}{3}+x_2''\right)_{n+m}\left(\frac{2(1-n)}{3}-x_3\right)_n\left(\frac{2(1-m)}{3}-x_3'\right)_m$$

$$\times F^{1:2;2}_{1:1;1}\left[\begin{matrix}\dfrac{1-n-m}{3}-x_3'' & : -n, \dfrac{1-n}{3}+x_2; -m, \dfrac{1-m}{3}+x_2'; \\ \dfrac{2(1-n-m)}{3}+x_2'': \dfrac{2(1-n)}{3}-x_3 & ; \dfrac{2(1-m)}{3}-x_3' \quad ;\end{matrix}\ 1,1\right], \tag{20}$$

$$g_3(x)$$

$$=\left(\frac{2(1-n-m)}{3}-x_1''\right)_{n+m}\left(\frac{2(1-n)}{3}+x_2\right)_n\left(\frac{2(1-m)}{3}+x_3'\right)_m F^{0:3;3}_{1:1;1}$$

$$\times\left[\begin{matrix} & : -n, \dfrac{1-n}{3}-x_1, \dfrac{1-n-m}{3}+x_2''; -m, \dfrac{1-m}{3}-x_1', \dfrac{1-n-m}{3}+x_3''; \\ \dfrac{2(1-n-m)}{3}-x_1'': \dfrac{2(1-n)}{3}+x_2 & ; \dfrac{2(1-m)}{3}+x_3' & ;\end{matrix}\ 1,1\right], \tag{21}$$

are (up to a sign) invariant under the action of H, the symmetries of the prism, i.e., $g_1(h\cdot x)=(-1)^{l_0(n+m)}g_1(x)$, $g_2(h\cdot x)=(-1)^{l(n+m)}g_2(x)$ *and* $g_3(h\cdot x)=(-1)^{l_0(n+m)}g_3(x)$, *where l is the number of reflections* r_1, r_2, r_3 *in the expression of h and* l_0 *is the number of reflections* r_0, r_1, r_2, r_3 *in the expression of h.*

Proof: Consider (19). Equation (12a) of Theorem 3 expresses that $g_1(h_1\cdot x)=g_1(x)$, with $h_1=(x_1\,x_3\,x_2)(x_1'\,x_3'\,x_2')(x_1''\,x_3''\,x_2'')$. Similarly, Eq. (12b) of Theorem 3 expresses that $g_1(h_2\cdot x)$

$=(-1)^{m+n}g_1(x)$, with $h_2=(x_1\,x_3)(x_1'\,x_3')(x_1''\,x_3'')$. Apart from the two transformations given in Theorem 3, there is of course also the trivial transformation interchanging $-n,a,b,c$ with $-m,a',b',c'$; this expresses that $g_1(h_3\cdot x)=g_1(x)$ with $h_3=(x_1\,x_1')(x_2\,x_3')(x_3\,x_2')(x_2''\,x_3'')\times(n\,m)$. It is now easy to verify that h_1, h_2 and h_3 generate H, i.e., the same group as generated by r_i $(i=0,1,2,3)$. Thus the symmetry statement for (19) follows. The remaining cases (20) and (21) follow in a similar way from Theorems 4 and 5. □

V. BASIC ANALOGS OF SOME TRANSFORMATION FORMULAS

In this section we shall be dealing with the basic analogs (or q-analogs) of some of the transformation formulas for double hypergeometric series considered in Secs. II and III. For a general introduction and background to basic hypergeometric series, see Ref. 25, whose notation we follow: thus q is a parameter with $|q|<1$; $(a;q)_n$ is the q-shifted factorial; $(a,b,c;q)_n$ stands for $(a;q)_n(b;q)_n(c;q)_n$; ${}_{p+1}\Phi_p$ is the common notation for a basic hypergeometric series in one variable; etc.

The double basic hypergeometric series appearing in the present context is a special case of general double basic series defined by Srivastava and Karlsson (Ref. 23, p. 349). So, we use their notation to define the series

$$\Phi^{1:2;2}_{0:2;2}\left[\begin{matrix} e:a,b\,;\,a',b'\,;\,q;x,y \\ :c,d\,;\,c',d'\,;\,\lambda,\mu,\nu \end{matrix}\right]$$

$$=\sum_{j,k=0}^{\infty} q^{\lambda\, j(j-1)/2+\mu k(k-1)/2+\nu jk}(e;q)_{j+k}\frac{(a;q)_j(b;q)_j}{(c;q)_j(d;q)_j}\frac{(a';q)_k(b';q)_k}{(c';q)_k(d';q)_k}\frac{x^j}{(q;q)_j}\frac{y^k}{(q;q)_k}; \quad (22)$$

the definition of $\Phi^{1:2;2}_{1:1;1}$ and $\Phi^{0:3;3}_{1:1;1}$ is completely analogous. For double basic series such as (22), ν is usually taken to be 0, in which case this is a straightforward double series analog of the basic series ${}_3\Phi_2$. However, also the cases with $\nu=+1$ or $\nu=-1$ appear in the literature,[27,30] and will play a role in the transformation formulas given here.

The main purpose of this section is to show that the different expressions of q-9-j coefficients of Ref. 18, in the singly stretched case, give rise to new transformation formulas for double basic hypergeometric series of the type $\Phi^{1:2;2}_{0:2;2}$, $\Phi^{1:2;2}_{1:1;1}$ and $\Phi^{0:3;3}_{1:1;1}$. Ališauskas actually realized that his expressions gave rise to ''rearrangement formulas of double sums'' (see Ref. 18, Appendix C), but he did not write them as transformation formulas of series of the type (22). Furthermore, he did not recognize that some of these formulas allow for a set of very general parameters.

In this section we shall discuss some of the q-analogs of theorems given in Secs. II and III. Rather than derive these q-analogs from the different double series expressions of Ališauskas,[18] a direct proof is given. It turns out that the direct proofs of such transformation formulas are fairly easy, and all rely on the same technique.

We know of two genuine transformation formulas for double basic hypergeometric series that have appeared in the literature (by a genuine transformation formula, we mean a formula expressing a basic double series of a particular type into another series of the same type). One of these was given by Singh:[27] if m and n are non-negative integers, and a,b,c,a',b',c' and d arbitrary parameters with $bb'=d$, then

$$\Phi^{0:3;3}_{1:1;1}\left[\begin{matrix} :q^{-n},a,b\,;\,q^{-m},a',b'q\,;\,cdq^n/ab,c'dq^m/a'b' \\ d: \quad c \quad ; \quad c' \quad ; \quad 0,0,1 \end{matrix}\right]$$

$$=\frac{(c/a;q)_n(c'/a';q)_m}{(c;q)_n(c';q)_m}\Phi^{0:3;3}_{1:1;1}\left[\begin{matrix} :q^{-n},a,b'\,;\,q^{1-m},a',b;q\,;\;q,q \\ d:\,q^{1-n}a/c\;;\;q^{1-m}a'/c'\;;0,0,0 \end{matrix}\right]. \quad (23)$$

The other was the topic of a recent paper:[26] if n is a non-negative integer, and a,b,c,d,a',b',c' and d' are arbitrary parameters with $dd'=q^{1-n}$, then

$$\Phi_{0:2;2}^{1:2;2}\left[\begin{matrix} q^{-n}:a,b;a',b';q;cdq^n/ab,c'd'q^n/a'b' \\ :c,d;c',d'; \qquad 0,0,-1 \end{matrix}\right]$$
$$=\frac{(d'b/b';q)_n}{(d';q)_n}b^{-n}\,\Phi_{0:2;2}^{1:2;2}\left[\begin{matrix} q^{-n}: \quad c/a,b \quad ;c'/a',b';q;q,q \\ :c,d'b/b';c',db'/b;\ 0,0,0 \end{matrix}\right]. \tag{24}$$

Observe that (23) is the basic analog of (14b), and (24) is the basic analog of (8b).

We shall now indicate how such formulas, and others, can be derived directly. First, we shall deduce two basic analogs of (8a); namely, if $dd'=q^{1-n}$, then

$$\Phi_{0:2;2}^{1:2;2}\left[\begin{matrix} q^{-n}:a,b;a',b';q;cdq^n/ab,y \\ :c,d;\ c',d' \ ;\ 0,0,-1 \end{matrix}\right]=\frac{(d/a;q)_n}{(d;q)_n}\Phi_{1:1;1}^{1:2;2}\left[\begin{matrix} q^{-n}:a,c/b;a',b';q;q,ay \\ ad':\quad c \quad ;\quad c' \quad ;\ 0,0,0 \end{matrix}\right], \tag{25}$$

and

$$\Phi_{0:2;2}^{1:2;2}\left[\begin{matrix} q^{-n}:a,b;a',b';q;q,y \\ :c,d;c',d';\ 0,0,0 \end{matrix}\right]=\frac{a^n(d/a;q)_n}{(d;q)_n}\Phi_{1:1;1}^{1:2;2}\left[\begin{matrix} q^{-n}:a,c/b;a',b';q;bq/d,y \\ ad':\quad c \quad ;\quad c' \quad ;\ 0,0,0 \end{matrix}\right], \tag{26}$$

Herein, as usual, n is a non-negative integer, a,b,c,d,a',b',c' and d are arbitrary parameters (subject to $dd'=q^{1-n}$), and y is an arbitrary variable.

For a proof, expand the lhs L of (25) into a double series:

$$L=\sum_{j,k}\frac{(q^{-n};q)_{j+k}(a,b;q)_j(a',b';q)_k}{(q,c,d;q)_j(q,c',d';q)_k}\left(\frac{cdq^n}{ab}\right)^j y^k q^{-jk}$$
$$=\sum_k\frac{(q^{-n},a',b';q)_k}{(q,c',d';q)_k}y^k\,{}_3\Phi_2\left[\begin{matrix} q^{-n+k},a,b; \\ c,d \quad ;q,cdq^{n-k}/ab \end{matrix}\right].$$

Now apply Sears' transformation formula [Ref. 25, (III.13)], and expand again:

$$L=\sum_k\frac{(q^{-n},a',b';q)_k}{(q,c',d';q)_k}y^k\frac{(d/a;q)_{n-k}}{(d;q)_{n-k}}\,{}_3\Phi_2\left[\begin{matrix} q^{-n+k},a,c/b; \\ c,aq^{1-n+k}/d; \end{matrix}q,q\right]$$
$$=\sum_{j,k}\frac{(q^{-n};q)_{j+k}(a,c/b;q)_j(a',b';q)_k}{(q,c,aq^{1-n+k}/d;q)_j(q,c',d';q)_k}y^k q^j\frac{(d/a;q)_{n-k}}{(d;q)_{n-k}}. \tag{27}$$

Using $d'=q^{1-n}/d$, and elementary properties of q-shifted factorials, there comes

$$\frac{1}{(aq^{1-n+k}/d;q)_j(d';q)_k}\frac{(d/a;q)_{n-k}}{(d;q)_{n-k}}=\frac{a^k}{(aq^{1-n}/d;q)_{j+k}}\frac{(d/a;q)_n}{(d;q)_n}.$$

Plugging this in (27) yields the rhs of (25). The proof of (26) is completely analogous.

Now we can give the basic analog of (9):

Proposition 9: Let n be a non-negative integer and a,b,c,a′,b′,c′ and d be arbitrary parameters. Then

$$\Phi_{1:1;1}^{1:2;2}\left[\begin{matrix} q^{-n}:a,b;a',b';q;q,dc'q^n/a'b' \\ d\ :\ c\ ;\ c'\ ; \qquad 0,0,0 \end{matrix}\right]$$
$$=\frac{b^n(d/bb';q)_n}{(d;q)_n}\Phi_{1:1;1}^{1:2;2}\left[\begin{matrix} q^{-n} \quad :c/a,b;c'/a',b';q;b'aq/d,q \\ q^{1-n}bb'/d:\quad c \quad ;\quad c' \quad ;\quad 0,0,0 \end{matrix}\right]. \tag{28}$$

Proof: This is now straightforward: apply (25) to the lhs of (24) and (26) to the rhs of (24). Comparing these expressions yields (28). □

With this, we have given basic analogs of all transformation formulas of Sec. II. Also for the transformation formulas with two separate numerator parameters as negative integers, given in Sec. III, the basic analogs can be deduced. The proof of such formulas uses similar steps as illustrated in the proof of (25):

(a) Rewrite the double sum as a single sum over a term containing a ${}_3\Phi_2$ series.
(b) Perform one of Sears' transformation formulas on the ${}_3\Phi_2$ and rewrite the result as a double sum.
(c) Make certain simplifications, using the constraint (if present) between the parameters.
(d) If necessary, repeat (a), (b) and (c) on the double sum obtained so far, and finally rewrite it in the standard notation of a double basic hypergeometric series.

Detailed proofs of the remaining formulas in this section will not be given, since they all follow the above technique. In fact, we will not even give the basic analogs of all of the formulas of Sec. III, but just list those corresponding to the transformation formulas of Theorems 3, 4 and 5.

Here are the basic analogs of (12a) and (12b), given in Theorem 3. The first, (12a), has two basic analogs, namely,

$$\Phi_{0:2;2}^{1:2;2}\left[\begin{matrix} d:q^{-n},a\,;q^{-m},a'\,;q;bcq^n/ad,b'c'q^m/a'd \\ :\ b,c\ ;\ b',c'\ ; \qquad 0,0,-1 \end{matrix}\right]$$
$$=\frac{(-1)^m(d;q)_n(b/a;q)_n(a';q)_m(b'/a'c)^m(c/d)^n q^{\binom{m+1}{2}-mn}}{(b;q)_n(c';q)_m(b';q)_m(c;q)_{n-m}}$$
$$\times\Phi_{0:2;2}^{1:2;2}\left[\begin{matrix} q^{1-m}/c':\ q^{-n},q^{1-n}/b\ ;\ q^{-m},b'/a'\ ;q;aq^{m+1}/c,dq^{n+1}/b' \\ :aq^{1-n}/b,q^{1-n}/d\,;q^{1-m}/a',cq^{n-m}\,; \qquad 0,0,-1 \end{matrix}\right] \tag{29}$$

and

$$\Phi_{0:2;2}^{1:2;2}\left[\begin{matrix} d:q^{-n},a\,;q^{-m},a'\,;q;q,q \\ :\ b,c\ ;\ b',c'\ ;\ 0,0,0 \end{matrix}\right]$$
$$=\frac{(-1)^m(d;q)_n(b/a;q)_n(a';q)_m(d/c)^m a^n q^{\binom{m+1}{2}}}{(b;q)_n(c';q)_m(b';q)_m(c;q)_{n-m}}$$
$$\times\Phi_{0:2;2}^{1:2;2}\left[\begin{matrix} q^{1-m}/c':\ q^{-n},q^{1-n}/b\ ;\ q^{-m},b'/a'\ ;q;q,q \\ :aq^{1-n}/b,q^{1-n}/d\,;q^{1-m}/a',cq^{n-m}\,;\ 0,0,0 \end{matrix}\right], \tag{30}$$

where in both formulas $cc'=qd$. The basic analog of (12b) is

$$\Phi_{0:2;2}^{1:2;2}\left[\begin{matrix} d:q^{-n},a\,;q^{-m},a'\,;q;cbq^n/ad,y \\ :\ b,c\ ;\ b',c'\ ; \quad 0,0,-1 \end{matrix}\right]$$
$$=\frac{(-1)^m(b/a;q)_n(a',d;q)_m q^{-\binom{m+1}{2}}y^m}{(b;q)_n(b',c';q)_m}$$
$$\times\Phi_{0:2;2}^{1:2;2}\left[\begin{matrix} q^{1-m}/c':\ q^{-n},a\ ;\ q^{-m},q^{1-m}/b'\ ;q;q,b'q^{m+2}/a'cy \\ :c,aq^{1-n}/b\,;q^{1-m}/a',q^{1-m}/d\,; \qquad 0,0,0 \end{matrix}\right], \tag{31}$$

where again $cc'=qd$.

The basic analogs of the formulas in Theorem 4 are given by

$$\Phi^{1:2;2}_{1:1;1}\left[\begin{matrix} c : q^{-n},a\,;\, q^{-m},a'\,;\, q;bdq^n/ac,q \\ d: \quad b \quad ;\quad b' \quad ;\quad 0,0,0 \end{matrix}\right]$$
$$= \frac{(b/a;q)_n (b'/a';q)_m (c;q)_{n+m} (a')^m (d/c)^n}{(b;q)_n (b';q)_m (d;q)_{n+m}}$$
$$\times \Phi^{1:2;2}_{1:1;1}\left[\begin{matrix} d/c \quad : q^{-n},q^{1-n}/b\,;\, q^{-m},q^{1-m}/b'\,;\, q;aq^{1-m}/d,q \\ q^{1-n-m}/c: \quad aq^{1-n}/b \quad ;\quad a'q^{1-m}/b' \quad ;\quad 0,0,0 \end{matrix}\right] \tag{32}$$

and

$$\Phi^{1:2;2}_{1:1;1}\left[\begin{matrix} c : q^{-n},a\,;\, q^{-m},a'\,;\, q;dbq^n/ac,q \\ d: \quad b \quad ;\quad b' \quad ;\quad 0,0,0 \end{matrix}\right]$$
$$= \frac{(a')^m (b/a;q)_n (b'/a';q)_m}{(b;q)_n (b';q)_m} \Phi^{1:2;2}_{1:1;1}\left[\begin{matrix} d/c: \quad q^{-n},a \quad ;\quad q^{-m},a' \quad ;q;q,cq/b' \\ d \quad : aq^{1-n}/b'\,;\, a'q^{1-m}/b'\,; \quad 0,0,0 \end{matrix}\right]. \tag{33}$$

Finally, the basic analogs of the transformation formulas (14a) and (14b) of Theorem 5 are given by

$$\Phi^{0:3;3}_{1:1;1}\left[\begin{matrix} \quad : q^{-n},a,b\,;\, q^{-m},a',b'\,;\, q;q,q \\ d: \quad c \quad ;\quad c' \quad ;\, 0,0,0 \end{matrix}\right]$$
$$= \frac{(a')^m b^n (b';q)_{n+m} (a';q)_n (c'/a';q)_m}{(d;q)_{n+m} (c;q)_n (c';q)_m}$$
$$\times \Phi^{0:3;3}_{1:1;1}\left[\begin{matrix} \quad : q^{-n},c/a,q^{1-n-m}/d\,;\, q^{-m},q^{1-m}/c',b\,;\, q;q,q \\ q^{1-n-m}/b': \quad q^{1-n}/a \quad ;\quad q^{1-m}a'/c' \quad ;\, 0,0,0 \end{matrix}\right] \tag{34}$$

and (23), where $bb'=d$ in both formulas.

This completes the list of q-analogs of the transformation formulas of Kampé de Fériet series with two non-negative integers as parameters, as given in Theorems 3–5.

VI. SUMMARY

Using the different double sum expressions of Ališauskas[18] for a singly stretched 9-j coefficient of su(2) or su$_q$(2), we have deduced a set of new transformation formulas for double hypergeometric series of Kampé de Fériet type and their basic analogs. An important observation is that these transformation formulas are valid for quite general parameters, even though the original 9-j coefficients assume only non-negative integer or half-integer values as arguments. The transformation formulas given here for double hypergeometric series of Kampé de Fériet type are all terminating, which means that either a common numerator parameter or else two separate numerator parameters are negative integers.

The transformation formulas seem to inherit some of the symmetries of the 9-j coefficient. In particular, we have shown that the given transformation formulas for a double series of a particular type generate a symmetry group, acting on the parameters of the series. These symmetry groups are explicitly determined and described as subgroups of permutation groups, or as symmetry groups of some geometric object.

In the case of basic double hypergeometric series, corresponding to different expressions of $9\text{-}j$ coefficients of $\mathrm{su}_q(2)$, the relevant series is a double q-series as defined in Ref. 23. Also for these series, the transformation formulas are listed, and we have shown that an independent proof of such transformations is easy.

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On the biparametric quantum deformation of GL(2)⊗GL(1)

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We study the biparametric quantum deformation of GL(2)⊗GL(1) and exhibit its cross-product structure. We derive explicitly the associated dual algebra, i.e., the quantized universal enveloping algebra employing the *R*-matrix procedure. This facilitates construction of a bicovariant differential calculus which is also shown to have a cross-product structure. Finally, a Jordanian analog of the deformation is presented as a cross-product algebra. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1407280]

I. INTRODUCTION

The biparametric quantum deformation of GL(2)⊗GL(1) was introduced in Ref. 1 as a novel Hopf algebra involving five generators $\{a,b,c,d,f\}$ and two deformation parameters $\{r,s\}$. From among the five generators, four $\{a,b,c,d\}$ correspond to GL(2) and the fifth one f is related to GL(1). These can be arranged in the matrix of generators

$$\mathcal{T}=\begin{pmatrix} f & 0 & 0 \\ 0 & a & b \\ 0 & c & d \end{pmatrix} \tag{1}$$

with the labelling 0, 1, 2. The associated solution of the quantum Yang–Baxter equation is

$$R=\begin{pmatrix} r & 0 & 0 & 0 \\ 0 & \mathsf{S}^{-1} & 0 & 0 \\ 0 & \Lambda & \mathsf{S} & 0 \\ 0 & 0 & 0 & R_r \end{pmatrix} \tag{2}$$

in block form, i.e., in the order (00), (01), (02), (10), (20), (11), (12), (21), (22) (which is chosen in conjunction with the block form of the $\mathcal{T}$-matrix) where

$$R_r=\begin{pmatrix} r & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & \Lambda & 1 & 0 \\ 0 & 0 & 0 & r \end{pmatrix}; \quad \mathsf{S}=\begin{pmatrix} s & 0 \\ 0 & 1 \end{pmatrix}; \quad \Lambda=\begin{pmatrix} \lambda & 0 \\ 0 & \lambda \end{pmatrix}; \quad \lambda=r-r^{-1}.$$

The $R\mathcal{T}\mathcal{T}$ relations

$$R\mathcal{T}_1\mathcal{T}_2=\mathcal{T}_2\mathcal{T}_1R \tag{3}$$

(where $\mathcal{T}_1=\mathcal{T}\otimes\mathbf{1}$ and $\mathcal{T}_2=\mathbf{1}\otimes\mathcal{T}$) give the commutation relations between the generators *a, b, c, d,* and *f*

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$$ab=r^{-1}ba, \quad bd=r^{-1}db,$$
$$ac=r^{-1}ca, \quad cd=r^{-1}dc, \tag{4}$$
$$bc=cb, \quad [a,d]=(r^{-1}-r)bc,$$

and

$$af=fa, \quad cf=sfc,$$
$$bf=s^{-1}fb, \quad df=fd. \tag{5}$$

Note that the first set of these relations is exactly the q-deformation of GL(2) with deformation parameter r while the second set involves the fifth generator f and the second deformation parameter s. This results in a biparametric q-deformation of GL(2)$\otimes$GL(1), say, $\mathcal{A}_{r,s}$. The coproduct and counit is given as

$$\Delta(\mathcal{T})=\mathcal{T}\otimes\mathcal{T},$$
$$\varepsilon(\mathcal{T})=\mathbf{1}. \tag{6}$$

The Casimir operator $\delta=ad-r^{-1}bc$ is invertible and determines the antipode

$$S(f)=f^{-1}, \quad S(a)=\delta^{-1}d, \quad S(b)=-\delta^{-1}rb, \quad S(c)=-\delta^{-1}r^{-1}c, \quad S(d)=\delta^{-1}a. \tag{7}$$

The quantum determinant $\mathcal{D}=\delta f$ is grouplike but not central. Some of the interesting features of the above quantum deformation are the following:

(i) If we write the set of generators $\{a,b,c,d,f\}$ as $\{f^Na, f^Nb, f^Nc, f^Nd\}$ (N being a fixed nonzero integer), i.e., reducing the five-dimensional set to the four-dimensional set, then we obtain an exact realization of the biparametric (p,q)-deformation of GL(2), i.e., $\mathrm{GL}_{p,q}(2)$ subject to the relations

$$p=r^{-1}s^N \quad \text{and} \quad q=r^{-1}s^{-N}. \tag{8}$$

This realization also reproduces the full Hopf algebraic structure underlying $\mathrm{GL}_{p,q}(2)$.

(ii) Another interesting feature of the $\mathcal{A}_{r,s}$ deformation is that it can be contracted (by means of the contraction procedure[2] based on the concept of singular limit of a similarity transformation) to yield the corresponding biparametric Jordanian deformation of GL(2)$\otimes$GL(1), which in turn provides a complete realization of the biparametric (h,h')-deformation of GL(2), i.e., $\mathrm{GL}_{h,h'}(2)$ in a manner similar to that for the q-deformed case.[3]

(iii) Both the biparametric quantum and Jordanian deformations of GL(2)$\otimes$GL(1) admit colored extensions[3] which also commute with the contraction procedure.

(iv) The physical interest in studying $\mathcal{A}_{r,s}$ lies in the observation that when endowed with a $*$-structure, this specializes to its compact form, i.e., provides a biparametric q-deformation of SU(2)$\otimes$U(1), which is precisely the gauge group for the theory of electroweak interactions.

Another deformation similar to $\mathcal{A}_{r,s}$ has also been recently given in Ref. 4, though in a different context. In the present article, we give an explicit description of the algebra dual to $\mathcal{A}_{r,s}$ as a starting point in further investigation of this quantum group structure. Motivated by the relation of this deformation with gauge theory, we also construct a bicovariant differential calculus since gauge theories have an obvious differential geometric description. This would then provide insights into possible scenarios for constructing q-gauge theories based on this deformation. In pursuing our aim, we follow the convenient R-matrix approach.[5,6] In Sec. II, we give the cross-product structure and go over to the R-matrix duality in Sec. III. The constructive calculus is presented in Sec. IV, while Sec. V is a brief description of the Jordanian analog. The results are discussed in Sec. VI.

II. CROSS-PRODUCT STRUCTURE

The biparametric q-deformation $\mathcal{A}_{r,s}$ can also be considered as the semidirect or cross-product $\mathrm{GL}_r(2)\underset{s}{\rtimes}\mathbb{C}[f,f^{-1}]$ built on the vector space $\mathrm{GL}_r(2)\otimes\mathbb{C}[f,f^{-1}]$ where $\mathrm{GL}_r(2)=\mathbb{C}[a,b,c,d]$ modulo the relations (4) and $\mathbb{C}[f,f^{-1}]$ has the cross relations (5). Then, $\mathcal{A}_{r,s}$ can also be interpreted as a skew Laurent polynomial ring $\mathrm{GL}_r[f,f^{-1};\sigma]$ where σ is the automorphism given by the action of element f on $\mathrm{GL}_r(2)$. Knowing properties of cross-product algebras (general theory given in Refs. 7 and 8), we already know that the algebra dual to $\mathcal{A}_{r,s}$ would be the cross-coproduct coalgebra $\mathcal{U}_{r,s}=\mathrm{U}_r(\mathrm{gl}(2))\underset{s}{\rtimes}\mathbb{C}[[\phi]]$ with ϕ as an element dual to f. If we let $A=\mathrm{GL}_r(2)$ and $H=\mathbb{C}[f,f^{-1}]$, then A is a left H-module algebra and the action of f on $\mathrm{GL}_r(2)$ is given by

$$f\triangleright a=a,\quad f\triangleright b=sb,\quad f\triangleright c=s^{-1}c,\quad f\triangleright d=d. \tag{9}$$

As a vector space, the dual is $\mathcal{U}_{r,s}=\mathrm{U}_r(\mathrm{gl}(2))\otimes\mathrm{U}(\mathrm{u}(1))$. Now, the duality relation between $\langle \mathrm{GL}_r(2),\mathrm{U}_r(\mathrm{gl}(2))\rangle$ is already well known,[9] while that between $\langle\mathbb{C}[f,f^{-1}],\mathrm{U}(\mathrm{u}(1))\rangle$ is given by $\langle f,\phi\rangle=1$, i.e., $\mathrm{U}(\mathrm{u}(1))=\mathbb{C}[[\phi]]$. More precisely, we work algebraically with $\mathbb{C}[s^{\phi},s^{-\phi}]$ where $\langle f,s^{\phi}\rangle=s$ (this is a standard notational convention which we adopt). This induces duality on the vector space tensor products and the left action dualizes to the left coaction. This results in the dual algebra being a cross-coproduct $\mathcal{U}_{r,s}=\mathrm{U}_r(\mathrm{gl}(2))\underset{s}{\rtimes}\mathbb{C}[[\phi]]$. Let us recall[9] that $\mathrm{U}_r(\mathrm{gl}(2))$, the algebra dual to $\mathrm{GL}_r(2)$, is isomorphic to the tensor product $\mathrm{U}_r(\mathrm{sl}(2))\otimes\tilde{U}(\mathrm{u}(1))$ where $\mathrm{U}_r(\mathrm{sl}(2))$ has the usual generators $\{H,X_{\pm}\}$ and $\tilde{U}(u(1))=\mathbb{C}[[\xi]]=\mathbb{C}[r^{\xi},r^{-\xi}]$ with ξ central. Therefore, $\mathcal{U}_{r,s}$ is nothing but $\mathrm{U}_r(\mathrm{sl}(2))$ and two central generators ξ and ϕ, where ξ is the generating element of $\tilde{U}(\mathrm{u}(1))$ and ϕ is the generating element of $\mathrm{U}(\mathrm{u}(1))$. Also note that s^{ϕ} (s being the second deformation parameter) is dually paired with the element f of $\mathcal{A}_{r,s}$. Defining the left coaction $\mathrm{U}_r(\mathrm{gl}(2))\to\mathrm{U}(\mathrm{u}(1))\otimes\mathrm{U}_r(\mathrm{gl}(2))$ we have

$$X_+\to s^{\phi}\otimes X_+,\quad X_-\to s^{-\phi}\otimes X_-,\quad H\to 1\otimes H,\quad \xi\to 1\otimes\xi. \tag{10}$$

It can be checked that this gives the correct duality pairings. For example, we have for X_+

$$\begin{aligned}
&\left\langle \Delta_L(X_+),1\otimes\begin{pmatrix}a&b\\c&d\end{pmatrix}\right\rangle=\left\langle s^{\phi}\otimes X_+,1\otimes\begin{pmatrix}a&b\\c&d\end{pmatrix}\right\rangle=\langle s^{\phi},1\rangle\left\langle X_+,\begin{pmatrix}a&b\\c&d\end{pmatrix}\right\rangle=\begin{pmatrix}0&1\\0&0\end{pmatrix},\\
&\left\langle \Delta_L(X_+),f\otimes\begin{pmatrix}a&b\\c&d\end{pmatrix}\right\rangle=\left\langle s^{\phi}\otimes X_+,f\otimes\begin{pmatrix}a&b\\c&d\end{pmatrix}\right\rangle=\langle s^{\phi},f\rangle\left\langle X_+,\begin{pmatrix}a&b\\c&d\end{pmatrix}\right\rangle=s\begin{pmatrix}0&1\\0&0\end{pmatrix},\\
&\left\langle X_+,f\triangleright\begin{pmatrix}a&b\\c&d\end{pmatrix}\right\rangle=\left\langle X_+,\begin{pmatrix}a&sb\\s^{-1}c&d\end{pmatrix}\right\rangle=s\begin{pmatrix}0&1\\0&0\end{pmatrix}.
\end{aligned} \tag{11}$$

Therefore, the coalgebra structure of $\mathcal{U}_{r,s}$ is given as

$$\Delta(X_+)=X_+\otimes r^{H/2}+r^{-H/2}s^{\phi}\otimes X_+, \tag{12}$$

$$\Delta(X_-)=X_-\otimes r^{-H/2}+r^{H/2}s^{-\phi}\otimes X_+, \tag{13}$$

$$\Delta(H)=H\otimes 1+1\otimes H, \tag{14}$$

$$\Delta(\xi)=\xi\otimes 1+1\otimes\xi, \tag{15}$$

$$\Delta(\phi)=\phi\otimes 1+1\otimes\phi. \tag{16}$$

In this way, we have obtained the Drinfeld–Jimbo form of the dual algebra $\mathcal{U}_{r,s}$ using the cross-product construction. Given other approaches to the problem of duality for quantum groups, we also construct explicitly the dual algebra using the *R*-matrix procedure.

III. *R*-MATRIX DUALITY

The biparametric (r,s)-deformation, $\mathcal{A}_{r,s}$, of GL(2)⊗GL(1) has been defined in the previous section at the group level, i.e., as the q-deformation of algebra of functions on GL(2)⊗GL(1). In this section, we derive explicitly the corresponding quantised universal enveloping algebra, i.e., its dual within the framework of the *R*-matrix formulation. We first construct functionals (matrices) $\mathcal{L}^+$ and $\mathcal{L}^-$ which are dual to the matrix of generators in the fundamental representation. The linear functionals $(\mathcal{L}^\pm)^a_b$ (following the method of Refs. 5 and 7) are defined by their value on the elements of the matrix of generators $\mathcal{T}$

$$\langle (\mathcal{L}^\pm)^a_b, \mathcal{T}^c_d \rangle = (R^\pm)^{ac}_{bd}, \tag{17}$$

where

$$(R^+)^{ac}_{bd} = c^+ (R)^{ca}_{db}, \tag{18}$$

$$(R^-)^{ac}_{bd} = c^- (R^{-1}))^{ac}_{bd}, \tag{19}$$

and c^+, c^- are free parameters. Matrices $(\mathcal{L}^\pm)^a_b$ satisfy

$$\langle (\mathcal{L})^a_b, uv \rangle = \langle (\mathcal{L}^\pm)^a_c \otimes (\mathcal{L}^\pm)^c_d, u \otimes v \rangle = (\mathcal{L}^\pm)^a_c(u)(\mathcal{L}^\pm)^c_d(v), \tag{20}$$

$$\text{i.e.,} \quad \Delta(\mathcal{L}^\pm)^a_b = (\mathcal{L}^\pm)^a_c \otimes (\mathcal{L}^\pm)^c_b .$$

For $\mathcal{A}_{r,s}$, the (R^+) and (R^-) matrices read

$$(R^+) = c^+ \begin{pmatrix} r & 0 & 0 & 0 \\ 0 & \mathsf{S} & \Lambda & 0 \\ 0 & 0 & \mathsf{S}^{-1} & 0 \\ 0 & 0 & 0 & R_r^T \end{pmatrix}; \quad (R^-) = c^- \begin{pmatrix} r^{-1} & 0 & 0 & 0 \\ 0 & \mathsf{S} & 0 & 0 \\ 0 & -\Lambda & \mathsf{S}^{-1} & 0 \\ 0 & 0 & 0 & R_r^{-1} \end{pmatrix}, \tag{21}$$

where R_r, Λ, and S are the same as before and $R_r^{-1} = R_{r^{-1}}$. Before proceeding further, it is pertinent to make the following remark about the $\mathcal{L}^\pm$ functionals. Let $\mathrm{A}(R)$ be a bialgebra or a Hopf algebra underlying a 3×3 quantum matrix and let $\tilde{U}(R)$ be a similar matrix bialgebra with two full matrices $\mathcal{L}^\pm$ of generators. These may be viewed as functionals $\mathrm{A}(R) \to \mathbb{C}$ via (17), but duality pairing at this level may be degenerate. So, we look at appropriate quotients of these such that the pairing is non degenerate. In our case, upon quotienting $\mathrm{A}(R)$ would descend to $\mathcal{A}_{r,s}$, and likewise $\tilde{U}(R)$ to the dual of $\mathcal{A}_{r,s}$. The quotient on $\mathrm{A}(R)$ is obtained by setting certain entries of the T-matrix to zero. The most general 3×3 quantum matrix has nine elements

$$\mathcal{T} = \begin{pmatrix} \mathcal{T}^0_0 & \mathcal{T}^0_1 & \mathcal{T}^0_2 \\ \mathcal{T}^1_0 & \mathcal{T}^1_1 & \mathcal{T}^1_2 \\ \mathcal{T}^2_0 & \mathcal{T}^2_1 & \mathcal{T}^2_2 \end{pmatrix}. \tag{22}$$

Now, let $\mathcal{T}^0_1 = 0 = \mathcal{T}^0_2$ and $\mathcal{T}^1_0 = 0 = \mathcal{T}^2_0$. Checking the coideal property (via coproduct of $\mathcal{T}$), we have

$$\Delta(\mathcal{T}^0_1) = \mathcal{T}^0_0 \otimes \mathcal{T}^0_1 + \mathcal{T}^0_1 \otimes \mathcal{T}^1_1 + \mathcal{T}^0_2 \otimes \mathcal{T}^2_1,$$

$$\begin{aligned}\Delta(\mathcal{T}_2^0)&=\mathcal{T}_0^0\otimes\mathcal{T}_2^0+\mathcal{T}_1^0\otimes\mathcal{T}_2^1+\mathcal{T}_2^0\otimes\mathcal{T}_2^2,\\ \Delta(\mathcal{T}_0^1)&=\mathcal{T}_0^1\otimes\mathcal{T}_0^0+\mathcal{T}_1^1\otimes\mathcal{T}_0^1+\mathcal{T}_2^1\otimes\mathcal{T}_0^2,\\ \Delta(\mathcal{T}_0^2)&=\mathcal{T}_0^2\otimes\mathcal{T}_0^0+\mathcal{T}_1^2\otimes\mathcal{T}_0^1+\mathcal{T}_2^2\otimes\mathcal{T}_0^2.\end{aligned}\tag{23}$$

These generate biideals. Therefore, setting them to zero gives the quotient of $\mathrm{A}(R)$

$$\mathcal{T}=\begin{pmatrix}\mathcal{T}_0^0 & 0 & 0\\ 0 & \mathcal{T}_1^1 & \mathcal{T}_2^1\\ 0 & \mathcal{T}_1^2 & \mathcal{T}_2^2\end{pmatrix}=\begin{pmatrix}f & 0 & 0\\ 0 & a & b\\ 0 & c & d\end{pmatrix}=\mathcal{T}(\mathcal{A}_{r,s}).\tag{24}$$

Similarly, the quotient on $\tilde{U}(R)$ is obtained by setting certain entries of $\mathcal{L}^{\pm}$ matrices to zero. Starting with

$$\mathcal{L}^{+}=\begin{pmatrix}\mathcal{L}_0^{+0} & \mathcal{L}_1^{+0} & \mathcal{L}_2^{+0}\\ \mathcal{L}_0^{+1} & \mathcal{L}_1^{+1} & \mathcal{L}_2^{+1}\\ \mathcal{L}_0^{+2} & \mathcal{L}_1^{+2} & \mathcal{L}_2^{+2}\end{pmatrix},\quad \mathcal{L}^{-}=\begin{pmatrix}\mathcal{L}_0^{-0} & \mathcal{L}_1^{-0} & \mathcal{L}_2^{-0}\\ \mathcal{L}_0^{-1} & \mathcal{L}_1^{-1} & \mathcal{L}_2^{-1}\\ \mathcal{L}_0^{-2} & \mathcal{L}_1^{-2} & \mathcal{L}_2^{-2}\end{pmatrix},\tag{25}$$

we make the ansatz

$$\begin{aligned}\mathcal{L}_1^{+2}&=0=\mathcal{L}_2^{-1},\\ \mathcal{L}_1^{+0}=\mathcal{L}_2^{+0}&=\mathcal{L}_0^{+1}=\mathcal{L}_0^{+2}=0,\\ \mathcal{L}_1^{-0}=\mathcal{L}_2^{-0}&=\mathcal{L}_0^{-1}=\mathcal{L}_0^{-2}=0,\end{aligned}\tag{26}$$

and, similar to the above for $\mathrm{A}(R)$, check the coideal property. We also verify explicitly[7] that this ansatz is compatible with the duality pairing

$$\begin{aligned}\langle\mathcal{L}_1^{+2},\mathcal{T}_j^i\rangle&=R_{1j}^{+2i}=R_{j1}^{i2}=0,\\ \langle\mathcal{L}_2^{-1},\mathcal{T}_j^i\rangle&=R_{2j}^{-1i}=(R^{-1})_{2j}^{1i}=0,\end{aligned}\tag{27}$$

and so on for their pairing with products of the $\mathcal{T}_j^i$. Therefore, setting these elements to zero yields a quotient bialgebra $\mathrm{U}(R)$ of $\tilde{\mathrm{U}}(R)$

$$\mathcal{L}^{+}=\begin{pmatrix}\mathcal{L}_0^{+0} & 0 & 0\\ 0 & \mathcal{L}_1^{+1} & \mathcal{L}_2^{+1}\\ 0 & 0 & \mathcal{L}_2^{+2}\end{pmatrix},\quad \mathcal{L}^{-}=\begin{pmatrix}\mathcal{L}_0^{-0} & 0 & 0\\ 0 & \mathcal{L}_1^{-1} & 0\\ 0 & \mathcal{L}_1^{-2} & \mathcal{L}_2^{-2}\end{pmatrix}.\tag{28}$$

Therefore, the initial pairing $\langle\mathrm{A}(R),\tilde{\mathrm{U}}(R)\rangle$ descends to $\langle\mathcal{A}_{r,s},\mathrm{U}(R)\rangle$. So, for $\mathcal{U}_{r,s}$ [or $\mathrm{U}(R)$] we make the following ansatz for the $\mathcal{L}^{\pm}$ matrices:

$$\mathcal{L}^{+}=c^{+}r\begin{pmatrix}s^{-1/2(\tilde{F}-H_2-1)}r^{1/2(\tilde{F}-H_1-1)} & 0 & 0\\ 0 & s^{-1/2(\tilde{F}-H_1+1)}r^{1/2(-\tilde{F}+H_2-1)} & r^{-1}\lambda\tilde{C}\\ 0 & 0 & s^{-1/2(\tilde{F}+H_1-1)}r^{1/2(-\tilde{F}-H_2-1)}\end{pmatrix},$$

$$\mathcal{L}^{-}=c^{-}r^{-1}\begin{pmatrix}s^{-1/2(\tilde{F}-H_2-1)}r^{-1/2(\tilde{F}-H_1-1)} & 0 & 0\\ 0 & s^{-1/2(\tilde{F}-H_1+1)}r^{-1/2(-\tilde{F}+H_2-1)} & 0\\ 0 & -r\lambda\tilde{B} & s^{-1/2(\tilde{F}+H_1-1)}r^{-1/2(-\tilde{F}-H_2-1)}\end{pmatrix},$$

where $H_1=\tilde{A}+\tilde{D}$, $H_2=\tilde{A}-\tilde{D}$, and $\{\tilde{A},\tilde{B},\tilde{C},\tilde{D},\tilde{F}\}$ is the set of generating elements of the dual algebra. This is consistent with the action on the generators of $\mathcal{A}_{r,s}$ and gives the correct duality pairings. More conveniently,

$$\mathcal{L}^+=\begin{pmatrix} J & 0 & 0 \\ 0 & M & P \\ 0 & 0 & N \end{pmatrix} \quad \text{and} \quad \mathcal{L}^-=\begin{pmatrix} J' & 0 & 0 \\ 0 & M' & 0 \\ 0 & Q & N' \end{pmatrix}, \tag{29}$$

where

$$\begin{aligned} J&=s^{-(1/2)(\tilde{F}-H_2-1)}r^{(1/2)(\tilde{F}-H_1+1)}, \\ M&=s^{-(1/2)(\tilde{F}-H_1+1)}r^{(1/2)(-\tilde{F}+H_2+1)}, \\ N&=s^{-(1/2)(\tilde{F}+H_1-1)}r^{(1/2)(-\tilde{F}-H_2+1)}, \\ J'&=s^{-(1/2)(\tilde{F}-H_2-1)}r^{-(1/2)(\tilde{F}-H_1+1)}, \\ M'&=s^{-(1/2)(\tilde{F}-H_1+1)}r^{-(1/2)(-\tilde{F}+H_2+1)}, \\ N'&=s^{-(1/2)(\tilde{F}+H_1-1)}r^{-(1/2)(-\tilde{F}-H_2+1)}, \end{aligned} \tag{30}$$

and

$$\begin{aligned} P&=\lambda\tilde{C}, \\ Q&=-\lambda\tilde{B}. \end{aligned} \tag{31}$$

These can also be arranged in terms of smaller L^+ and L^- matrices:

$$\begin{aligned} \mathcal{L}^+&=c^+\begin{pmatrix} J & 0 \\ 0 & L^+ \end{pmatrix}, \quad \text{where } L^+=\begin{pmatrix} M & P \\ 0 & N \end{pmatrix}, \\ \mathcal{L}^-&=c^-\begin{pmatrix} J' & 0 \\ 0 & L^- \end{pmatrix}, \quad \text{where } L^-=\begin{pmatrix} M' & 0 \\ Q & N' \end{pmatrix}. \end{aligned} \tag{32}$$

A. Commutation relations of the dual

The dual algebra is generated by $\mathcal{L}^\pm$ functionals which satisfy the q-commutation relations (the so-called $R\mathcal{L}\mathcal{L}$ relations)

$$R_{12}\mathcal{L}_2^\pm\mathcal{L}_1^\pm=\mathcal{L}_1^\pm\mathcal{L}_2^\pm R_{12}, \tag{33}$$

$$R_{12}\mathcal{L}_2^+\mathcal{L}_1^-=\mathcal{L}_1^-\mathcal{L}_2^+R_{12}, \tag{34}$$

where $\mathcal{L}_1^\pm=\mathcal{L}^\pm\otimes\mathbf{1}$ and $\mathcal{L}_2^\pm=\mathbf{1}\otimes\mathcal{L}^\pm$. Since $\mathcal{A}_{r,s}$ is a quotient Hopf algebra, it is necessary to amend the R-matrix to eliminate relations that are inconsistent with the quotient structure. Consequently, the R-matrix for the $R\mathcal{L}\mathcal{L}$ relations is different from the one used in the $R\mathcal{T}\mathcal{T}$ relations. The $R\mathcal{L}\mathcal{L}$ relations are constructed with the R-matrix:

$$R_{12}=c^{-}\langle \mathcal{L}^{-},\mathcal{T}\rangle^{-1}=\begin{pmatrix} r & 0 & 0 & 0 \\ 0 & \mathsf{S}^{-1} & 0 & 0 \\ 0 & 0 & \mathsf{S} & 0 \\ 0 & 0 & 0 & R_r \end{pmatrix}. \tag{35}$$

Evaluating $\mathcal{L}_1^{\pm},\mathcal{L}_2^{\pm}$ matrices and substituting in the above $R\mathcal{L}\mathcal{L}$-relations yields the dual algebra commutation relations. From $R_{12}\mathcal{L}_2^{-}\mathcal{L}_1^{-}=\mathcal{L}_1^{-}\mathcal{L}_2^{-}R_{12}$ and $R_{12}\mathcal{L}_2^{+}\mathcal{L}_1^{+}=\mathcal{L}_1^{+}\mathcal{L}_2^{+}R_{12}$ we obtain

$$R_rL_2^{-}L_1^{-}=L_1^{-}L_2^{-}R_r, \tag{36}$$

$$R_rL_2^{+}L_1^{+}=L_1^{+}L_2^{+}R_r, \tag{37}$$

$$MJ=JM,\quad M'J'=J'M',$$

$$NJ=JN,\quad N'J'=J'N', \tag{38}$$

$$PJ=sJP,\quad J'Q=sQJ',$$

where

$$\begin{gathered} R_rL_2^{-}L_1^{-}=L_1^{-}L_2^{-}R_r\Rightarrow QM'=rM'Q,\quad N'Q=rQN',\quad \text{and}\quad N'M'=M'N' \\ R_rL_2^{+}L_1^{+}=L_1^{+}L_2^{+}R_r\Rightarrow PM=rMP,\quad NP=rPN,\quad \text{and}\quad NM=MN. \end{gathered} \tag{39}$$

In addition, the cross relation $R_{12}\mathcal{L}_2^{+}\mathcal{L}_1^{-}=\mathcal{L}_1^{-}\mathcal{L}_2^{+}R_{12}$ yields

$$\begin{gathered} NJ'=J'N,\quad MJ'=J'M,\quad PJ'=sJ'P, \\ N'J=JN',\quad M'J=JM',\quad JQ=sQJ, \end{gathered} \tag{40}$$

and $R_rL_2^{+}L_1^{-}=L_1^{-}L_2^{+}R_r$ which further implies

$$QP-PQ=-\lambda(N'M-NM'). \tag{41}$$

Simplifying the above, we get the following commutation relations

$$[\tilde{A},\tilde{B}]=\tilde{B},\quad [\tilde{A},\tilde{C}]=-\tilde{C},$$

$$[\tilde{D},\tilde{B}]=-\tilde{B},\quad [\tilde{D},\tilde{C}]=\tilde{C}, \tag{42}$$

$$[\tilde{A},\tilde{D}]=0,\quad [\tilde{F},\bullet]=0,$$

and

$$[\tilde{B},\tilde{C}]=\frac{r^{\tilde{A}-\tilde{D}}s^{-\tilde{F}}-r^{-(\tilde{A}-\tilde{D})}s^{-\tilde{F}}}{r-r^{-1}}=\frac{r^{\gamma^{\tilde{F}}}}{r-r^{-1}}[r^{\tilde{A}-\tilde{D}}-r^{-(\tilde{A}-\tilde{D})}], \tag{43}$$

where $\gamma=(\ln s/\ln r)$. So, we obtain a single-parameter deformation of $\mathrm{U}(\mathrm{gl}(2)\otimes\mathrm{U}(\mathrm{u})(1))$ as an algebra. Including the coproduct, we again obtain a semidirect product $\mathrm{U}_r(\mathrm{gl}(2))\underset{s}{\rtimes}\mathrm{U}(\mathrm{u}(1))$, as expected.

IV. CONSTRUCTIVE CALCULUS

In order to investigate the differential geometric structure of the (r,s)-deformation, $\mathcal{A}_{r,s}$, of $\mathrm{GL}(2)\otimes\mathrm{GL}(1)$, we use Jurčo's constructive procedure[6] based on the R-matrix formulation. This method has so far been applied only to full matrix quantum groups, but we demonstrate here that it works equally well for appropriate quotients of these. For $\mathcal{A}_{r,s}$, we obtain a first-order bicovariant differential calculus employing the ansatz for $\mathcal{L}^{\pm}$ introduced in Sec. III.

A. One-forms

Let $\{\omega\}$ be the basis of all left-invariant quantum one-forms. So, we have

$$\Delta_L(\omega)=\mathbf{1}\otimes\omega. \tag{44}$$

This defines the left action on the bimodule Γ (space of quantum one-forms). The bimodule Γ is further characterized by the commutation relations between ω and $a\in\mathcal{A}(\equiv\mathcal{A}_{r,s})$,

$$\omega a=(f*a)\omega. \tag{45}$$

The left convolution product is

$$f*a=(\mathbf{1}\otimes f)\Delta(a), \tag{46}$$

where $f\in\mathcal{A}'[=\mathrm{Hom}(\mathcal{A},\mathbf{C})]$ belongs to the dual. This means

$$\omega a=(\mathbf{1}\otimes f)\Delta(a)\omega. \tag{47}$$

Now the linear functional f is defined in terms of the $\mathcal{L}^{\pm}$ matrices as

$$f=S(\mathcal{L}^{+})\mathcal{L}^{-}. \tag{48}$$

Thus we have

$$\omega a=[(\mathbf{1}\otimes S(\mathcal{L}^{+})\mathcal{L}^{-})\Delta(a)]\omega. \tag{49}$$

In terms of components,

$$\omega_{ij}a=[(\mathbf{1}\otimes S(l^{+}_{ki})l^{-}_{jl})\Delta(a)]\omega_{kl} \tag{50}$$

using the expressions $\mathcal{L}^{\pm}=l^{\pm}_{ij}$ and $\omega=\omega_{ij}$ where $i,j=1,...,3$. For Γ to be a bicovariant bimodule, the right coaction is given by

$$\Delta_R(\omega)=\omega\otimes M \tag{51}$$

where functionals M are defined in terms of the matrix of generators $\mathcal{T}$.

$$M=\mathcal{T}S(\mathcal{T}). \tag{52}$$

Again, in component form, we can write

$$\Delta_R(\omega_{ij})=\omega_{kl}\otimes t_{ki}S(t_{jl}). \tag{53}$$

Using the above formulas, we obtain the commutation relations of all the left-invariant one-forms with the generating elements $\{a,b,c,d,f\}$ of $\mathcal{A}_{r,s}$:

$$\omega^0 a=a\omega^0,\quad \omega^0 b=b\omega^0,$$

$$\omega^1 a=r^{-2}a\omega^1,\quad \omega^1 b=b\omega^1,$$

$$\omega^+ a = r^{-1} a \omega^+, \quad \omega^+ b = r^{-1} b \omega^+ - \lambda r^{-1} a \omega^1, \tag{54}$$

$$\omega^- a = r^{-1} a \omega^- - \lambda r^{-1} b \omega^1, \quad \omega^- b = r^{-1} b \omega^-,$$

$$\omega^2 a = a \omega^2 - \lambda b \omega^+, \quad \omega^2 b = r^{-2} b \omega^2 - \lambda r^{-1} a \omega^- + \lambda^2 b \omega^1,$$

$$\omega^0 c = c \omega^0, \quad \omega^0 d = d \omega^0,$$

$$\omega^1 c = r^{-2} c \omega^1, \quad \omega^1 d = d \omega^1,$$

$$\omega^+ c = r^{-1} c \omega^+, \quad \omega^+ d = r^{-1} d \omega^+ - \lambda r^{-1} c \omega^1, \tag{55}$$

$$\omega^- c = r^{-1} c \omega^- - \lambda r^{-1} d \omega^1, \quad \omega^- d = r^{-1} d \omega^-,$$

$$\omega^2 c = c \omega^2 - \lambda d \omega^+, \quad \omega^2 d = r^{-2} d \omega^2 - \lambda r^{-1} c \omega^- + \lambda^2 d \omega^1,$$

$$\omega^0 f = r^{-2} f \omega^0,$$

$$\omega^1 f = f \omega^1,$$

$$\omega^+ f = s f \omega^+, \tag{56}$$

$$\omega^- f = s^{-1} f \omega^-,$$

$$\omega^2 f = f \omega^2,$$

where $\omega^0 = \omega_{11}$, $\omega^1 = \omega_{22}$, $\omega^+ = \omega_{23}$, $\omega^- = \omega_{32}$, $\omega^2 = \omega_{33}$ and the components $\omega_{12}, \omega_{13}, \omega_{21}, \omega_{31}$ have null contribution, given the structure of the $\mathcal{T}$ matrix (i.e., $t_{12} = t_{13} = t_{21} = t_{31} = 0$).

B. Vector fields

The linear space Γ (space of all left invariant one-forms) contains a bi-invariant element $\tau = \Sigma_i \omega_{ii}$ which can be used to define a derivative on $\mathcal{A}$. For $a \in \mathcal{A}$, one sets

$$\mathbf{d}a = \tau a - a \tau. \tag{57}$$

Now

$$\omega_{ii} a = [(\mathbf{1} \otimes S(l^+_{ki}) l^-_{il}) \Delta(a)] \omega_{kl}. \tag{58}$$

So,

$$\mathbf{d}a = [(\mathbf{1} \otimes \chi_{kl}) \Delta(a)] \omega_{kl}, \tag{59}$$

where $\chi_{kl} = S(l^+_{ki}) l^-_{il} - \delta_{kl} \varepsilon, \varepsilon$ being the counit. Denote

$$\chi_{ij} = S(l^+_{ik}) l^-_{kj} - \delta_{ij} \varepsilon \tag{60}$$

or more compactly

$$\chi = S(\mathcal{L}^+) \mathcal{L}^- - \mathbf{1} \varepsilon \tag{61}$$

the matrix of left-invariant vector fields χ_{ij} on $\mathcal{A}$. The action of the vector fields on the generating elements is

$$\chi_{ij} a = (S(l^+_{ik}) l^-_{kj} - \delta_{ij} \varepsilon) a, \tag{62}$$

$$\chi_{ij}a=\langle S(l^{+}_{ik})l^{-}_{kj},a\rangle-\delta_{ij}\varepsilon(a). \tag{63}$$

Explicitly, we obtain

$$\chi_0(a)=0,\quad \chi_0(b)=0,$$

$$\chi_1(a)=r^{-2}-1,\quad \chi_1(b)=0,$$

$$\chi_+(a)=0,\quad \chi_+(b)=0, \tag{64}$$

$$\chi_-(a)=0,\quad \chi_-(b)=-(r-r^{-1}),$$

$$\chi_2(a)=0,\quad \chi_2(b)=0,$$

$$\chi_0(c)=,\quad \chi_0(d)=0,$$

$$\chi_1(c)=0,\quad \chi_1(d)=(r-r^{-1})^2,$$

$$\chi_+(c)=-(r-r^{-1}),\quad \chi_+(d)=0, \tag{65}$$

$$\chi_-(c)=0,\quad \chi_-(d)=0,$$

$$\chi_2(c)=0,\quad \chi_2(d)=r^{-2}-1,$$

$$\chi_0(f)=r^{-2}-1,$$

$$\chi_1(f)=0,$$

$$\chi_+(f)=0, \tag{66}$$

$$\chi_-(f)=0,$$

$$\chi_2(f)=0,$$

where $\chi_0=\chi_{11}$, $\chi_1=\chi_{22}$, $\chi_+=\chi_{23}$, $\chi_-=\chi_{32}$, $\chi_2=\chi_{33}$ and again (by previous argument) the components $\chi_{12},\chi_{13},\chi_{21},\chi_{31}$ have null contribution. The left convolution products are given as

$$\chi_0*a=0,\quad \chi_0*b=0,$$

$$\chi_1*a=(r^{-2}-1)a,\quad \chi_1*b=((r-r^{-1})^2)b,$$

$$\chi_+*a=-(r-r^{-1})b,\quad \chi_+*b=0, \tag{67}$$

$$\chi_-*a=0,\quad \chi_-*b=-(r-r^{-1})a,$$

$$\chi_2*a=0,\quad \chi_2*b=(r^{-2}-1)b,$$

$$\chi_0*c=0,\quad \chi_0*d=0,$$

$$\chi_1*c=(r^{-2}-1)c,\quad \chi_1*d=((r-r^{-1})^2)d,$$

$$\chi_+*c=-(r-r^{-1})d,\quad \chi_+*d=0, \tag{68}$$

$$\chi_-*c=0,\quad \chi_-*d=-(r-r^{-1})c,$$

$$\chi_2 * c = 0, \quad \chi_2 * d = (r^{-2}-1)d,$$

$$\chi_0 * f = (r^{-2}-1)f,$$

$$\chi_1 * f = 0,$$

$$\chi_+ * f = 0, \tag{69}$$

$$\chi_- * f = 0,$$

$$\chi_2 * f = 0.$$

C. Exterior derivatives

Using $\mathbf{d}a = \Sigma_i (\chi_i * a)\omega^i$ for $a \in \mathcal{A}$, we obtain the action of the exterior derivatives:

$$\mathbf{d}a = (r^{-2}-1)a\omega^1 - \lambda b\omega^+, \tag{70}$$

$$\mathbf{d}b = \lambda^2 b\omega^1 - \lambda a\omega^- + (r^{-2}-1)b\omega^2, \tag{71}$$

$$\mathbf{d}c = (r^{-2}-1)c\omega^1 - \lambda d\omega^+, \tag{72}$$

$$\mathbf{d}d = \lambda^2 d\omega^1 - \lambda c\omega^- + (r^{-2}-1)d\omega^2, \tag{73}$$

$$\mathbf{d}f = (r^{-2}-1)f\omega^0, \tag{74}$$

where $\lambda = r - r^{-1}$. The exterior derivative $\mathbf{d}: \mathcal{A} \to \Gamma$ satisfies the Leibniz rule and $\mathbf{d}\mathcal{A}$ generates Γ as a left $\mathcal{A}$-module. This then defines a first-order differential calculus $(\Gamma, \mathbf{d})$ on $\mathcal{A}_{r,s}$. Furthermore, the calculus is bicovariant due to the coexistence of the left and the right actions,

$$\Delta_L : \Gamma \to \mathcal{A} \otimes \Gamma, \tag{75}$$

$$\Delta_R : \Gamma \to \Gamma \otimes \mathcal{A}, \tag{76}$$

since $\mathbf{d}$ has the invariance property

$$\Delta_L \mathbf{d} = (\mathbf{1} \otimes \mathbf{d})\Delta, \tag{77}$$

$$\Delta_R \mathbf{d} = (\mathbf{d} \otimes \mathbf{1})\Delta. \tag{78}$$

The bicovariance holds also due to the existence of the bi-invariant element $\tau = \Sigma_i \omega_{ii}$ [Eq. (57)] of the linear space of left-invariant one-forms. If we rewrite the derivatives $\{\mathbf{d}a, \mathbf{d}b, \mathbf{d}c, \mathbf{d}d, \mathbf{d}f\}$ as $\{\mathbf{d}(f^N a), \mathbf{d}(f^N b), \mathbf{d}(f^N c), \mathbf{d}(f^N d)\}$, i.e., reducing from the five-dimensional to the four-dimensional algebra, then the latter set of exterior derivatives provides a realization of the differential calculus on the biparametric (p,q)-deformation of GL(2), i.e., $\mathrm{GL}_{p,q}(2)$, with the defining relations between the two sets of deformation parameters (p,q) and (r,s) as before. Furthermore, the differential calculus also respects the cross-product structure of $\mathcal{A}_{rs}$. It can be checked (using the Leibniz rule) that

$$\mathbf{d}(af - fa) = 0, \quad \mathbf{d}(cf - sfc) = 0, \quad \mathbf{d}(bf - s^{-1}fb) = 0, \quad \mathbf{d}(df - fd) = 0, \tag{79}$$

which is consistent with the cross relations (5).

V. JORDANIAN ANALOG

It was shown in Ref. 3 that the $\mathcal{A}_{r,s}$ deformation could be contracted (by means of singular limit of similarity transformations) to obtain a nonstandard or Jordanian analog, say $\mathcal{A}_{m,k}$, with deformation parameters $\{m,k\}$ and the associated R-matrix is triangular. In analogy with $\mathcal{A}_{r,s}$, $\mathcal{A}_{m,k}$ can also be considered as the semidirect or cross-product $\mathrm{G}\mathcal{L}_m(2)\underset{k}{\rtimes}\mathbb{C}[f,f^{-1}]$ where $\mathrm{GL}_m(2)=\mathbb{C}[a,b,c,d]$ modulo the relations

$$\begin{gathered}[c,d]=-mc^2, \quad [c,b]=-m(ac+cd)=-m(ca+dc),\\ [c,a]=-mc^2, \quad [d,a]=-m(d-a)c=-mc(d-a),\end{gathered} \tag{80}$$

$$\begin{gathered}[d,b]=-m(d^2-\delta),\\ [b,a]=-m(\delta-a^2),\end{gathered} \tag{81}$$

where $\delta=ad-bc+mac=ad-cb-mcd$, and $\mathbb{C}[f,f^{-1}]$ has the cross relations

$$\begin{gathered}[f,a]=kcf, \quad [f,b]=k(df-fa),\\ [f,c]=0, \quad [f,d]=-kcf.\end{gathered} \tag{82}$$

Thus, $\mathcal{A}_{m,k}\simeq\mathrm{GL}_m(2)\underset{k}{\rtimes}\mathbb{C}[f,f^{-1}]$ can also be interpreted as a skew Laurent polynomial ring $\mathrm{GL}_m[f,f^{-1};\sigma]$ where σ is the automorphism given by the action of element f on $\mathrm{GL}_m(2)$. The (left) action is given by

$$f\triangleright a=a+kc, \quad f\triangleright b=b+k(d-a)-k^2c, \quad f\triangleright c=c, \quad f\triangleright d=d-kc. \tag{83}$$

VI. DISCUSSION

In this article, we have investigated the algebro-geometric structure of the biparametric quantum deformation of GL(2)⊗GL(1), namely, $\mathcal{A}_{r,s}$. A particular feature of this deformation is that it has an interpretation as a semidirect or cross-product algebra. We exhibit this cross-product structure and establish a picture of duality in this setting. Using the R-matrix formalism, we have given an explicit derivation of the corresponding dual algebra, i.e., the quantized universal enveloping algebra, and also constructed a bicovariant differential calculus. The dual algebra obtained via R-matrices is isomorphic to the dual algebra obtained by the cross-product construction. We note that the differential calculus satisfies the required axioms, contains the calculus on $\mathrm{GL}_q(2)$, and our results match with those given in Ref. 10. Besides, the calculus is also consistent with the cross-product structure of $\mathcal{A}_{r,s}$. We expect that the calculus could as well be obtained by projection from the calculus on multiparameter q-deformed GL(3). The differential calculus obtained on $\mathcal{A}_{r,s}$ enables us to investigate the associated gauge theory from a noncommutative perspective. It would be useful to repeat the analysis presented in this article for the biparametric Jordanian deformation of GL(2) ⊗GL(1) obtained in Ref. 3 and also to investigate corresponding hybrid (q, h)-deformations.[11,12] Furthermore, it would indeed be interesting to generalize the setting to the case of colored quantum and Jordanian deformations.

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Weakly primitive vectors of Kac-modules of the Lie superalgebras $sl(m/n)$

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It was conjectured by Hughes *et al.* [J. Math. Phys. **33**, 470–491 (1992)] that there exists a bijection between the composition factors of a Kac-module and the so-called permissible codes. In a previous paper it was proved that to any unlinked code, there corresponds a composition factor of the Kac-module. Here it is proved that to any linked code, there corresponds a composition factor of the Kac-module.
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I. INTRODUCTION

Lie superalgebras are important generalizations of Lie algebras, of interest to both mathematicians and physicists. In the classification of finite-dimensional modules of the basic classical Lie superalgebras,[1–3] Kac distinguished between typical and atypical modules. He also introduced the Kac-module $\overline{V}(\Lambda)$, which was shown to be simple if and only if Λ is typical. For Λ being atypical, the problem of the structure of $\overline{V}(\Lambda)$, or equivalently, the character of the simple module $V(\Lambda)$, has been the subject of intensive study.[3–7] More generally, the problem of classifying indecomposable modules has received much attention in the literature.[8–10] Kac obtained a character formula for typical modules.[3] The problem for atypical $sl(m/n)$-modules has seemed to be difficult, though several partial solutions have been achieved.[6,11]

Serganova[4] found a solution for the characters of simple $gl(m/n)$-modules, which described the multiplicities $a_{\Lambda\Sigma}$ of composition factors $V(\Sigma)$ of $\overline{V}(\Lambda)$ in terms of Kazhdan–Lusztig polynomials. However, her algorithm of describing $a_{\Lambda\Sigma}$ turns out to be rather complicated. The structure of $\overline{V}(\Lambda)$ is still not so apparent. Hughes *et al.*[11] derived an algorithm to determine all the composition factors of $sl(m/n)$-Kac-modules $\overline{V}(\Lambda)$. They conjectured that there exists a bijection between the composition factors of $\overline{V}(\Lambda)$ and the permissible codes. This conjecture clearly describes the structure of $\overline{V}(\Lambda)$. In Ref. 12, the authors proved that to any unlinked code, there corresponds a composition factor of $\overline{V}(\Lambda)$, by constructing explicitly a primitive vector corresponding to the unlinked code. Here we first determine the bottom composition factor of the Kac-module $\overline{V}(\Lambda)$, then prove that to any linked code, there corresponds a composition factor. Thus, this will give a half proof of the conjecture. Our main results are summarized in Theorems 3.2, 3.5, 3.7, and 4.1.

II. THE LIE SUPERALGEBRA $sl(m+1/n+1)$

We shall only give necessary definitions and notations. For detail, please refer to Ref. 12. Denote $G=sl(m+1/n+1)=\{x=\binom{AB}{CD} | \mathrm{str}(x)=\mathrm{tr}(A)-\mathrm{tr}(D)=0\}$, where A,B,C,D are $(m+1)\times(m+1),(m+1)\times(n+1),(n+1)\times(m+1),(n+1)\times(n+1)$ matrices, respectively. Let $G_{\bar{0}}=\{\binom{A0}{0D}\}$, $G_{\bar{1}}=\{\binom{0B}{C0}\}$. Let H be the Cartan subalgebra of G, H^* the dual of H spanned by

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$\epsilon_a\,(a=1,\ldots,m+1),\epsilon'_b\,(b=1,\ldots,n+1)$, where $\epsilon_a:x\to A_{aa}$, $\epsilon'_b:x\to D_{bb}$ for $x=\binom{AB}{CD}$, with $\Sigma_{a=1}^{m+1}\epsilon_a-\Sigma_{b=1}^{n+1}\epsilon'_b=0$; it has an inner product: $\langle\epsilon_a|\epsilon_b\rangle=\delta_{ab},\langle\epsilon_a|\epsilon'_b\rangle=0,\langle\epsilon'_a|\epsilon'_b\rangle=-\delta_{ab}$. Let Δ,Δ_0,Δ_1 be sets of roots, even, odd roots, respectively. Set

$$I_1=\{\bar{m},\ldots,\bar{1}\},\quad I_2=\{1,\ldots,n\},\quad I=I_1\cup\{0\}\cup I_2,\quad \text{where } \bar{i}=-i \text{ for } i\in\mathbb{Z}_+. \tag{2.1}$$

Choose a basis for H: $h_i=E_{m+i+1,m+i+1}-E_{m+i+2,m+i+2}, i\in I_1\cup I_2, h_0=E_{m+1,m+1}+E_{m+2,m+2}$. The simple roots in H^* are: $\alpha_i=\epsilon_{m+i+1}-\epsilon_{m+i+2}, i\in I_1, \alpha_0=\epsilon_{m+1}-\epsilon'_1, \alpha_i=\epsilon'_i-\epsilon'_{i+1}, i\in I_2$. Thus α_0 is the only odd simple root. The symmetric inner product satisfies

$$\begin{gathered}\langle\alpha_i|\alpha_i\rangle=2,\quad i\in I_1,\quad \langle\alpha_0|\alpha_0\rangle=0,\quad \langle\alpha_i|\alpha_i\rangle=-2,\quad i\in I_2,\\ \langle\alpha_{i-1}|\alpha_i\rangle=-1,\quad i\in I_1,\quad \langle\alpha_0|\alpha_{\pm1}\rangle=\pm1,\quad \langle\alpha_i|\alpha_{i+1}\rangle=1,\quad i\in I_2,\end{gathered} \tag{2.2}$$

and $\langle\alpha_i|\alpha_j\rangle=0$, $j\neq i,i\pm1$, and $h_i(\alpha_j)=\alpha_j(h_i)=\langle\alpha_i|\alpha_j\rangle, i\leqslant0$ or $-\langle\alpha_i|\alpha_j\rangle, i>0$. Let $\Delta^{\pm}(\Delta_0^{\pm},\Delta_1^{\pm})$ be sets of positive/negative roots (even, odd roots). Let $\alpha_{ij}=\Sigma_{k=i}^{j}\alpha_k$, then $\Delta_0^{\pm}=\{\pm\alpha_{ij}|i\leqslant j,i,j\in I_1 \text{ or } i,j\in I_2\}$, $\Delta_1^{\pm}=\{\pm\alpha_{ij}|i\in I_1\cup\{0\},j\in\{0\}\cup I_2\}$. The root vectors $e_{ij}=e(\alpha_{ij}),f_{ij}=f(\alpha_{ij})=e(-\alpha_{ij})$ and the elements h_{ij} of H are

$$e_{ij}=E_{m+i+1,m+j+2},\quad f_{ij}=E_{m+j+2,m+i+1},\quad h_{ij}=E_{m+i+1,m+i+1}-(-1)^{\sigma_{ij}}E_{m+j+2,m+j+2}, \tag{2.3}$$

where $\sigma_{ij}=0$ or $1\Leftrightarrow\alpha_{ij}$ is even or odd. Set $e_i=e_{ii},f_i=f_{ii}$. The set $\{e_{ij},f_{ij},h_i|i,j\in I,i\leqslant j\}$ yields a basis for G, with the following nontrivial relations:

$$[e_{ij},e_{j+1,\not}]=e_{i\not},\quad [f_{ij},f_{j+1,\not}]=-f_{i\not},\quad [e_{ij},f_{ij}]=h_{ij},$$

$$[e_{ij},f_{ik}]=\begin{cases}-(-1)^{\sigma_{ij}\sigma_{ik}}f_{j+1,k} & \text{if } j<k\\ -(-1)^{\sigma_{ij}\sigma_{ik}}e_{k+1,j} & \text{if } j>k\end{cases},$$

$$[e_{ik},f_{jk}]=\begin{cases}e_{i,j-1} & \text{if } i<j\\ f_{j,i-1} & \text{if } i>j\end{cases},$$

$$[h_{ij},e_{k\not}]=\mu e_{k\not},\quad [h_{ij},f_{k\not}]=-\mu f_{k\not},\quad \mu=\delta_{i,k}-\delta_{i,\not+1}-(-1)^{\sigma_{ij}}\delta_{j,k-1}+(-1)^{\sigma_{ij}}\delta_{j,\not}. \tag{2.4}$$

Set $G_0^{\pm}=\text{span}\{e(\alpha)|\alpha\in\Delta_0^{\pm}\},G_{\pm1}=\text{span}\{e(\beta)|\beta\in\Delta_1^{\pm}\},G^{\pm}=G_0^{\pm}\oplus G_1^{\pm}$. Note that $G_1^{\pm}=G_{\pm1},G_0^{-}=G_0^{-}\oplus H\oplus G_0^{+},G=G^{-}\oplus H\oplus G^{+}$. For $\lambda\in H^*$, define its *Dynkin labels* to be $a_i=\lambda(h_i),i\in I$. These uniquely determine λ, which can then be represented as $\lambda=[a_{\bar{m}},\ldots,a_{\bar{1}};a_0;a_1,\ldots,a_n]$. λ is called *dominant* if $a_i\geqslant0$ for all $i\neq0$, *integral* if $a_i\in\mathbb{Z}$ for all $i\neq0$.

Let $V^0(\Lambda)$ be the simple G_0^{-}-module with integral dominant highest weight Λ and vector v_Λ. Extend $V^0(\Lambda)$ to be a $G_0^{-}\oplus G_{+1}$ module by setting $G_{+1}V^0(\Lambda)=0$. The *Kac-module*[3] is

$$\overline{V}(\Lambda)=\text{Ind}_{G_0\oplus G_{+1}}^{G}V^0(\Lambda)=\mathbf{U}(G)\otimes_{G_0\oplus G_{+1}}V^0(\Lambda), \tag{2.5}$$

where $\mathbf{U}(G)$ is the universal enveloping algebra of G. Since $\mathbf{U}(G)=\mathbf{U}(G_{-1})\otimes\mathbf{U}(G_0)\otimes\mathbf{U}(G_{+1})$, it implies $\overline{V}(\Lambda)\cong\mathbf{U}(G_{-1})\otimes V^0(\Lambda)$. Set $M=\{v\in\overline{V}(\Lambda)|v_\Lambda\notin\mathbf{U}(G)v\}$, then $V(\Lambda)=\overline{V}(\Lambda)/M$ is a finite-dimensional simple module with highest weight Λ. Define $\rho=\rho_0-\rho_1$, where $\rho_0=\frac{1}{2}\Sigma_{\alpha\in\Delta_0^+}\alpha,\rho_1=\frac{1}{2}\Sigma_{\beta\in\Delta_1^+}\beta$.

Definition 2.1: $\Lambda,\overline{V}(\Lambda),V(\Lambda)$ are called *typical* if $\langle\Lambda+\rho|\beta\rangle\neq0$ for all $\beta\in\Delta_1^+$. If $\beta\in\Delta_1^+$ such that $\langle\Lambda+\rho|\beta\rangle=0$, then $\Lambda,\overline{V}(\Lambda),V(\Lambda)$ are called *atypical* and β is an *atypical root* for Λ. If there exist precisely r distinct atypical roots for Λ, we call $\Lambda,\overline{V}(\Lambda),V(\Lambda)$ *r-fold atypical*.

It is proved[3] that every finite-dimensional simple G-module is isomorphic to a $V(\Lambda)$, characterized by its integral dominant highest weight Λ and that $\overline{V}(\Lambda)$ is simple$\Leftrightarrow\Lambda$ is typical.

A *composition series* of $\overline{V}(\Lambda)$ is a sequence $\overline{V}(\Lambda)=V_0\supset V_1\supset\cdots$ with each V_i/V_{i+1} isomorphic to some simple module $V(\Sigma)$, called a *composition factor* of $\overline{V}(\Lambda)$. A conjecture was made in Ref. 11, giving all the composition factors of $\overline{V}(\Lambda)$. We aim to prove the existence of all these composition factors; for this, important concepts are those defined as follows.

Definition 2.2: A vector $v\neq 0$ in a G-module V is called *weakly G-primitive* if there exists a G-submodule U of V such that $v\notin U$ and $G^+v\subset U$. If $U=0$, v is called *G-primitive*.

We are only concerned with finite-dimensional modules and so we always suppose Λ is an integral dominant weight. Thus, weakly $G_{\bar{0}}$-primitive vectors are in fact $G_{\bar{0}}$-primitive and integral dominant. A *cyclic module* is an indecomposable module generated by a weakly primitive vector. A weakly primitive vector v will determine a cyclic submodule $\mathbf{U}(G)v$ and a composition factor. An important construct in classifying composition factors is the following concept.

Definition 2.3: The *atypicality matrix* $A(\Lambda)$ is the $(m+1)\times(n+1)$ matrix with (b,c)-entry $A(\Lambda)_{bc}=\langle\Lambda+\rho|\beta_{bc}\rangle=\Sigma_{k=\overline{m-b+1}}^{0}a_k-\Sigma_{k=1}^{c-1}\ a_k+m-b-c+2$, where $\beta_{bc}=\alpha_{\overline{m-b+1},c-1}$.

For example, for $G=sl(3/5)$, $\Lambda=[31;0;0020]$ is three-fold atypical and

$$A(\Lambda)=\begin{pmatrix} 6 & 5 & 4 & 1 & 0 \\ 2 & 1 & 0 & \overline{3} & \overline{4} \\ 0 & \overline{1} & \overline{2} & \overline{5} & \overline{6} \end{pmatrix}. \tag{2.6}$$

If Λ is r-fold atypical, we label the atypical roots $\gamma_1<\cdots<\gamma_r$ according to the partial ordering: $\lambda,\mu\in H^*$: $\lambda\geqslant\mu\Leftrightarrow\lambda-\mu=\Sigma_{i\in I}k_i\alpha_i$ with all $k_i\geqslant 0$. For $1\leqslant s<t\leqslant r$, denote by x_{st} the entry in $A(\Lambda)$ at the intersection of the column containing the γ_s zero with the row containing the γ_t zero, and h_{st} the number of steps to go from the γ_s zero via x_{st} to the γ_t zero with the zeros themselves included in the count. Important concepts in the classification of composition factors are the following (we give these concepts in term of mathematical expressions and refer the reader to Refs. 11 and 12 for descriptions and examples if these are not familiar to the reader).

Definition 2.4: Let Λ be r-fold atypical with atypical roots $\{\gamma_1,\ldots,\gamma_r\}$, $1\leqslant s<t\leqslant r$. Define:

(1) γ_s,γ_t are called *n-*, *q-*, or *c-related*$\Leftrightarrow x_{st}>h_{st}-1$, $x_{st}=h_{st}-1$, or $x_{st}<h_{st}-1$.

(2) The *nqc-type* $nqc(\Lambda)$ of Λ is a triangular array of r columns such that for $1\leqslant s\leqslant t\leqslant r$, the $(r-t+1,s)$-entry $nqc(\Lambda)_{st}$ is zero if $s=t$ and $nqc(\Lambda)_{st}=n,q,c\Leftrightarrow\gamma_s,\gamma_t$ are *n-*, *q-*, *c*-related if $s<t$.

(3) A *code* Σ^c for Λ is an array of length r, each element of the array consisting of a nonempty column of increasing labels taken from $\{0,1,\ldots,r\}$ subject to the order relation $1<\cdots<r<0$, such that the (s,t)-entry is either empty (in this case, we set $c_{st}=\varnothing$) or c_{st} with $0\leqslant c_{st}\leqslant r$ satisfying the following rules:

(i) $c_{1s}=0$, s, or a with $s<a\leqslant r$; and $c_{1s}=a\Rightarrow nqc(\Lambda)_{sa}=q$.
(ii) $s<t, nqc(\Lambda)_{st}=\cdots=nqc(\Lambda)_{t-1,t}=c$ and $c_{1t}=a\geqslant t\Rightarrow\exists\ u>1$, $c_{us}=a$ and $c_{1s}\neq 0,a$.
(iii) $u<v$, $c_{uw}=s\neq 0$, and $c_{vw}=t\Rightarrow s<t$, $c_{1t}=t$ and $nqc(\Lambda)_{st}=c$.
(iv) $c_{uv}=c_{wx}\neq\varnothing,0$ and $c_{u+1,v}\neq\varnothing\Rightarrow c_{w+1,x}=c_{u+1,v}$.
(v) $s<t<u, nqc(\Lambda)_{st}=nqc(\Lambda)_{tu}=q$, and $c_{1s}=c_{1u}\neq 0\Rightarrow c_{1t}\neq 0$.
(vi) $s<t<u<v$, $c_{1s}=c_{1u}=a\neq 0$ and $c_{1t}=c_{1v}=b\neq 0\Rightarrow\exists\ w,x$, $c_{ws}=c_{xu}=b$ if $a<b$, or $c_{wt}=c_{xv}=a$ if $a>b$.

(4) A code Σ^c is called a *linked* code if there exist γ_s,γ_t which are linked, i.e., columns s and t have the same nonzero top entry (and in this case we say column s *is linked to* column t in code Σ^c). Otherwise, it is called an *unlinked* code.

(5) A code is called *indecomposable* if all nonzero columns contain a common nonzero entry.

(6) Denote $D=\{(b,c)|1\leqslant b\leqslant m+1, 1\leqslant c\leqslant n+1\}$, $\Gamma_\Lambda=\{(b_s,c_s)|s=1,\ldots,r\}$ the set of, respectively, positions, positions of zeros, of $A(\Lambda)$ (so $\gamma_s=\beta_{b_s,c_s}, s=1,\ldots,r$) and define $\hat{K}$

$=\{\beta_{bc}|(b,c)\in K\}$ for any subset K of D (so $\hat{D}=\Delta_1^+$ and $\hat{\Gamma}_\Lambda=\{\gamma_1,\ldots,\gamma_r\}$). For $1\leqslant s\leqslant r$, set

$$W_\Lambda^e(s)=\left\{(b,c)\in D\,\middle|\,1\leqslant c\leqslant c_s, b=b_s+\sum_{t=c}^{c_s-1}a_t\right\},$$

$$S_\Lambda^e(s)=\left\{(b,c)\in D\,\middle|\,b_s\leqslant b\leqslant m+1, c=c_s-\sum_{t=b_s}^{b-1}a_{\overline{m-t+1}}\right\},$$

$$W_\Lambda(s)=\{(b,c)\in W_\Lambda^e(s)|b<d \text{ or } c<e, \forall\,(d,e)\in S_\Lambda^e(s)\}\cup\{(b_s,c_s)\}, \tag{2.7}$$

$$S_\Lambda(s)=\{(d,e)\in S_\Lambda^e(s)|b<d \text{ or } c<e, \forall\,(b,c)\in W_\Lambda^e(s)\}\cup\{(b_s,c_s)\},$$

$$SW_\Lambda(s)=W_\Lambda(s)\cup S_\Lambda(s).$$

$SW_\Lambda(s)$ is called the *southwest chain* emanating from (b_s,c_s) and $SW_\Lambda=\cup_{s=1}^r SW_\Lambda(s)$ is called the set of all south west chains.

(7) For an unlinked code Σ^c with nonzero columns $C_{s_1},\ldots,C_{s_p}$, define $D_\Sigma=\varnothing$ if $p=0$ or $\cup_{i=1}^p SW_\Lambda(s_i)$ otherwise. The *weight corresponding to* Σ^c is defined by $\Sigma=\Lambda-\Sigma_{\beta\in\hat{D}_\Sigma}\beta$.

(8) For $1\leqslant t\leqslant r$, suppose $W_\Lambda(t),S_\Lambda(t)$ end at $(d_t,e_t),(d_t',e_t')$, respectively, $d_t'\geqslant d_t, e_t'\geqslant e_t$. Define $D(t)$ to be the region of D within or on the boundary consisting of $SW_\Lambda(t)$, the vertical line joining (d_t',e_t) to (d_t,e_t) and the horizontal line joining (d_t',e_t) to (d_t',e_t'). Then it is proved in Ref. 12 that the indecomposable unlinked codes are in 1–1 correspondence with $D(t)$ for $1\leqslant t\leqslant r$.

For the example given in (2.6), $r=3$ with $\gamma_1=\beta_{31},\gamma_2=\beta_{23},\gamma_3=\beta_{15}$, and

$$nqc(\Lambda)=\begin{matrix}q & n & 0\\ c & 0 & \\ 0 & & \end{matrix}.$$

Below we list all seven codes and indicate positions of the chain $SW_\Lambda(s)$ by s:

$$\begin{matrix}000 & 100 & 003 & 103 & 120 & 123 & 303\\ & & & & 2 & 2 & \end{matrix},\quad A(\Lambda)\to\begin{pmatrix}. & . & . & 3 & 3\\ 2 & 2 & 2 & . & .\\ 1 & 2 & . & . & .\end{pmatrix}, \tag{2.8}$$

where the first six codes are unlinked codes corresponding to weights Λ, $\Lambda-\beta_{31}$, $\Lambda-(\beta_{14}+\beta_{15})$, $\Lambda-\beta_{31}-(\beta_{14}+\beta_{15})$, $\Lambda-\beta_{31}-(\beta_{21}+\beta_{22}+\beta_{23}+\beta_{32})$, $\Lambda-\beta_{31}-(\beta_{21}+\beta_{22}+\beta_{23}+\beta_{32})-(\beta_{14}+\beta_{15})$, respectively. It is proved[12] that an unlinked code corresponds to a primitive vector, thus a composition factor of $\overline{V}(\Lambda)$. In this paper, we shall prove that a linked code corresponds to a weakly primitive vector, and is thus a composition factor.

III. THE BOTTOM COMPOSITION FACTOR

Now we are in a position to prove a result about the bottom composition factor of a Kac-module; this will play an important role in the proof of the existence of weakly primitive vectors corresponding to linked codes. Suppose Λ is a r-fold atypical with atypical roots $\gamma_1,\ldots,\gamma_r$. As in Ref. 12, without loss of generality, we can suppose $\gamma_r=\beta_{1,n+1}$ (recall that $\beta_{bc}=\alpha_{\overline{m-b+1,c-1}}$). Let Σ_-^c be the code such that $D_{\Sigma_-}=SW_\Lambda$ [*cf.* Definition 2.4(7)], i.e., Σ_-^c is the unique code containing all numbers $1,\ldots,r$, therefore $\Sigma_-=\Lambda-\Sigma_{\beta\in\widehat{SW}_\Lambda}\beta$. By Definition 2.4, this is clearly an unlinked code, and so, as proved in Ref. 12, it corresponds to a primitive vector v_{Σ_-}.

Define a total ordering on Δ: $\alpha_{ij}<\alpha_{kl}\Leftrightarrow j-i<l-k$ or $j-i=l-k$ but $i>k$. It implies that $\beta_{bc}<\beta_{de}\Leftrightarrow c-b<d-e$ or $c-b=d-e$ but $b>d$. Recalling the notation (2.3), choose a basis B of $\mathbf{U}(G_{-1})$: $B=\{b=\Pi_{\beta\in S} f(\beta)|S\subset\Delta_1^+\}$, where the product $b=f(\beta_1)\cdots f(\beta_s)$ is written in the *proper order:* $\beta_1<\cdots<\beta_s$. Define a total ordering on B by $b>b'=f(\beta_1')\cdots f(\beta_{s'}')\Leftrightarrow s>s'$ or $s=s'$ but $\beta_k>\beta_k'$ and $\beta_i=\beta_i', 1\leqslant i\leqslant k-1$ for some k, where b,b' are in proper order. Recall that an element $v\in\overline{V}(\Lambda)$ can be uniquely written as

$$v=b_1y_1v_\Lambda+b_2y_2v_\Lambda+\cdots b_i\in B, b_1>b_2>\cdots, 0\neq y_i\in\mathbf{U}(G_0^-). \tag{3.1}$$

Clearly, $v\neq 0\Leftrightarrow t=0$. If $v\neq 0$, we call $b_1y_1v_\Lambda$ the *leading term* and we call a term $b_iy_iv_\Lambda$ a *prime term* if y_i is a nonzero scalar. Define a partial ordering on D by: $(b,c)<(d,e)\Leftrightarrow(b,c)$ is located below and to the left of (d,e), i.e., $b>d, c\leqslant e$ or $b=d, c<e$.

Lemma 3.1: Given any $(b,c)\in D$, let K be any subset of $D\backslash SW_\Lambda$ satisfying: (i) $(d,e)\in K\Rightarrow(d,e)<(b,c)$; (ii) $(d,e)\in K\Rightarrow(d',e')\in K\cup SW_\Lambda$ for all $(d',e')<(d,e)$. Then we have

$$e(\beta_{bc})\prod_{\beta\in\hat{K}} f(\beta)v_{\Sigma_-}=0. \tag{3.2}$$

Proof: We shall use induction on $\#K$. If $\#K=0$, i.e., $K=\varnothing$, then it is obvious since v_{Σ_-} is a primitive vector. Suppose now $\#K\geqslant 1$, and suppose that (3.2) holds for all K' such that $\#K'<\#K$. Choose $(d,e)\in K$ first to be topmost and then to be rightmost in K. Let $K'=K\backslash\{(d,e)\}$, then clearly K' still satisfies (i) and (ii); by the inductive hypothesis we have

$$e(\beta_{bc})\prod_{\beta\in\hat{K}} f(\beta)v_{\Sigma_-}=[e(\beta_{bc}),f(\beta_{de})]\prod_{\beta\in\hat{K}'} f(\beta)v_{\Sigma_-}, \tag{3.3}$$

which is equal to zero if both $d\neq b$ and $e\neq c$. Suppose now $d=b$ and hence $e<c$ (the case for $d>b$ and $e=c$ is similar). Then by (2.4),

$$[e(\beta_{bc}),f(\beta_{de})]=e(\alpha_{e+1,c}) \quad \text{is a positive root vector.} \tag{3.4}$$

Write $\Pi_{\beta\in\hat{K}'} f(\beta)v_{\Sigma_-}$ in the form of (3.1),

$$\prod_{\beta\in\hat{K}'} f(\beta)v_{\Sigma_-}=b_1y_1v_\Lambda+b_2y_2v_\Lambda+\cdots, \tag{3.5}$$

where $y_i\in\mathbf{U}(G_0^-), b_1<b_2<\cdots$; then by property (ii) of K' one can see that every b_i can be written as (up to a sign)

$$b_i=\prod_{\beta\in\hat{K}'} f(\beta)\prod_{\beta\in\hat{E}_i} f(\beta)=\prod_{\beta\in\hat{D}_i} f(\beta), \quad \hat{D}_i=\hat{K}'\cup\hat{E}_i \tag{3.6}$$

for some $\hat{E}_i\subset\hat{D}$, where D_i satisfies the following property:

$$(d',e')\in D_i \text{ and } (d',e')<(b,c)\Rightarrow(d'',e'')\in D_i \text{ for all } (d'',e'')<(d',e'). \tag{3.7}$$

Now applying (3.4) to (3.5), noting that applying (3.4) to v_{Σ_-} is zero, we see that the right-hand side of (3.3) is a linear combination of the form

$$[e(\alpha_{e+1,c}),f(\beta)]\prod_{\beta'\in\hat{K}'\backslash\{\beta\}} f(\beta')v_{\Sigma_-}, \quad \beta\in\hat{K}'. \tag{3.8}$$

Using (3.5), (3.6), and (3.7), we see that (3.8) can be written as a linear combination of the form

$$[e(\alpha_{e+1,c}),f(\beta)]\prod_{\beta'\in\hat{D}_i\setminus\{\beta\}} f(\beta')y_i v_\Lambda, \quad \beta\in\hat{K}'. \tag{3.9}$$

Note that by (2.4), for $(d',e')\in K',\beta=\beta_{d',e'}\in\hat{K}'$, $[e(\alpha_{e+1,c}),f(\beta)]$ is either zero or up to a sign equal to $f(\beta_{d'',e''})$ for some $(d'',e'')\prec(d',e')$; by (i) $(d',e')\prec(b,c)$, thus by (3.7) $(d'',e'')\in\hat{D}_i\setminus\{\beta\}$, and so $f(\beta_{d'',e''})$ appears twice, therefore we obtain that (3.9) is zero. This proves (3.2). ■

Theorem 3.2: v_{Σ_-} is contained in every submodule of $\overline{V}(\Lambda)$. Thus it is the primitive vector corresponding to the bottom composition factor.

Proof: Set

$$v'_{\Sigma_-}=\prod_{(b,c)\notin SW_\Lambda} e(\beta_{bc})T_- v_\Lambda, \quad \text{where} \quad T_-=\prod_{(b,c)\in D} f(\beta_{bc}). \tag{3.10}$$

By rewriting v'_{Σ_-}, we have (up to a sign)

$$\begin{aligned} v'_{\Sigma_-}&=\prod_{(b,c)\notin SW_\Lambda} e(\beta_{bc})\prod_{(b,c)\notin SW_\Lambda} f(\beta_{bc})\prod_{(b,c)\in SW_\Lambda} f(\beta_{bc})v_\Lambda \\ &=\prod_{(b,c)\notin SW_\Lambda} e(\beta_{bc})\prod_{(b,c)\notin SW_\Lambda} f(\beta_{bc})v_{\Sigma_-}, \end{aligned} \tag{3.11}$$

where the second equality follows from the fact that when writing v_{Σ_-} in the form of (3.1), other than its leading term, each term contains some factor $f(\beta_{bc})$ with $(b,c)\notin SW_\Lambda$, which therefore appears twice and so vanishes. From (3.11), we have

$$\begin{aligned} v'_{\Sigma_-}&=\prod_{(b,c)\notin SW_\Lambda,b\neq 1} e(\beta_{bc})e(\beta_{11})\cdots e(\beta_{1k})f(\beta_{1k})\cdots f(\beta_{11})\prod_{(b,c)\notin SW_\Lambda,b\neq 1} f(\beta_{bc})v_{\Sigma_-} \\ &=\prod_{(b,c)\notin SW_\Lambda,b\neq 1} e(\beta_{bc})e(\beta_{11})\cdots e(\beta_{1,k-1}) \\ &\quad\times[e(\beta_{1k}),f(\beta_{1k})]f(\beta_{1,k-1})\cdots f(\beta_{11})\prod_{(b,c)\notin SW_\Lambda,b\neq 1} f(\beta_{bc})v_{\Sigma_-}, \end{aligned} \tag{3.12}$$

where we have supposed $\{(1,c)\notin SW_\Lambda\}=\{(1,1),\ldots,(1,k)\}$, and where the last equality follows from Lemma 3.1. Recall that $\beta_{bc}=\alpha_{\overline{m-b+1},c-1}$, by (2.4),

$$h'=[e(\beta_{1k}),f(\beta_{1k})]=h_{\bar{m},k-1}=h_{\bar{m}}+\cdots+h_{\bar{0}}-h_1-\cdots-h_{k-1}. \tag{3.13}$$

Note that in (3.12), $h'=[e(\beta_{1k}),f(\beta_{1k})]$ precedes an element of $\overline{V}(\Lambda)$ which has the weight $\lambda=\Lambda-2\rho_1+\beta_{1k}$. A straightforward computation gives (recall Definition 2.3)

$$\lambda(h')=A(\Lambda)_{1k}-(n-k+1). \tag{3.14}$$

Recall that we assume that $\gamma_r=\beta_{1,n+1}$, we have $A(\Lambda)_{1,n+1}=0$ and by (2.7), $(1,c)\in SW_\Lambda\Leftrightarrow A(\Lambda)_{1,c}=n-c+1$ and $(1,c)\notin SW_\Lambda\Leftrightarrow A(\Lambda)_{1,c}>n-c+1$, thus (3.14) is nonzero. Therefore we can replace $[e(\beta_{1k}),f(\beta_{1k})]$ in (3.12) by a nonzero scalar. Using induction on k, we have

$$v'_{\Sigma_-}=c\prod_{(b,c)\notin SW_\Lambda,b\neq 1} e(\beta_{bc})\prod_{(b,c)\notin SW_\Lambda,b\neq 1} f(\beta_{bc})v_{\Sigma_-}, \tag{3.15}$$

for some nonzero $c\in\mathbb{C}$. By repeating the process, we obtain that $v'_{\Sigma_-}=c'v_{\Sigma_-}$ for some nonzero $c'\in\mathbb{C}$. Since every submodule U of $\overline{V}(\Lambda)$ contains T_-v_Λ, and therefore by (3.10), it contains v'_{Σ_-}, and so contains v_{Σ_-}. This proves the theorem. ■

Using Theorem 3.2, we can prove a theorem, which appears as a conjecture in Ref. 11. First we give the notion of the northeast chains,[11] which will also be important in establishing the relation between linked codes and weakly primitive vectors in Sec. IV.

Definition 3.3: (*cf.* Definition 2.4(6).) For $1\leqslant s\leqslant r$, set

$$E^e_\Lambda(s)=\left\{(b,c)\in D\middle|c_s\leqslant c\leqslant n+1,b=b_s-\sum_{t=c_s}^{c-1}a_t\right\},$$

$$N^e_\Lambda(s)=\left\{(b,c)\in D\middle|1\leqslant b\leqslant b_s,c=c_s+\sum_{t=b}^{b_s-1}a_{\overline{m-t+1}}\right\},$$

$$E_\Lambda(s)=\{(b,c)\in E^e_\Lambda(s)\,|\,b>d \text{ or } c>e,\forall(d,e)\in N^e_\Lambda(s)\}\cup\{(b_s,c_s)\},\tag{3.16}$$

$$N_\Lambda(s)=\{(d,e)\in N^e_\Lambda(s)\,|\,b>d \text{ or } c>e,\forall(b,c)\in E^e_\Lambda(s)\}\cup\{(b_s,c_s)\},$$

$$NE_\Lambda(s)=E_\Lambda(s)\cup N_\Lambda(s).$$

$NE_\Lambda(s)$ is called the set of *northeast chains* emanating from (b_s,c_s). Denote $NE_\Lambda=\cup_{s=1}^r NE_\Lambda(s)$.

For the example given in (2.6), the northeast chains can be expressed by

$$A(\Lambda)\to\begin{pmatrix}.&.&.&.&3\\.&1&2&.&.\\1&1&1&.&.\end{pmatrix}.\tag{3.17}$$

Remark 3.4: Similar to codes, we can define *opposite codes* corresponding to northeast chains and define $D'(t)$ to be the region of D within or on the boundary consisting of $NE_\Lambda(t)$, the vertical line joining (u_t,v_t) to (u'_t,v_t) and the horizontal line joining (u'_t,v'_t) to (u'_t,v_t), where $(u_t,v_t),(u'_t,v'_t)$ are, respectively, the end points of $E_\Lambda(t),N_\Lambda(t),u_t\geqslant u'_t,v_t\geqslant v'_t$. Then indecomposable unlinked opposite codes are in 1–1 correspondence with $D'(t)$ for $1\leqslant t\leqslant r$ [*cf.* Definition 2.4(8)].

Theorem 3.5: The lowest G_0^--highest weight Π of $V(\Lambda)$ is $\Lambda_-+\Sigma_{\beta\in\widehat{NE}_\Lambda}\beta$, where $\Lambda_-=\Lambda-2\rho_1$.

Proof: Set $\Pi_+=\Lambda+\Sigma_{\beta\in\widehat{NE}_\Lambda}\beta$. We have[11] $NE_\Lambda=SW_{\Pi_+}$ and hence by Theorem 3.2, $\Lambda=\Pi_+-\Sigma_{\beta\in\widehat{SW}_{\Pi_+}}\beta$ is the highest weight of the bottom composition factor of $\overline{V}(\Pi_+)$. So $\Pi=\Pi_+-2\rho_1$ (the lowest G_0^--highest weight of $\overline{V}(\Pi_+)$) is the lowest G_0^--highest weight of $V(\Lambda)$. ■

Definition 3.6: Let Σ^c_1,Σ^c be two codes for Λ. We call Σ^c_1 a *subcode* of Σ^c (denoted by $\Sigma^c_1\leqslant\Sigma^c$ and denoted by $\Sigma^c_1<\Sigma^c$ if $\Sigma^c_1\leqslant\Sigma^c$ and $\Sigma^c_1\neq\Sigma^c$), if each nonzero entry in a column of Σ^c_1 is contained as an entry in the same column of Σ^c and if this column of Σ^c corresponding to a nonzero element of Σ^c_1 is linked to another column of Σ^c, then these columns are linked in Σ^c_1.

For example, the first five codes in (2.8) are subcodes of the sixth but no code except the first is a subcode of the seventh. Another example is that $0230<\begin{smallmatrix}4234\\44\end{smallmatrix}$. For any unlinked code Σ^c, we can write it as $\Sigma^c=\Sigma^c_1\cdots\Sigma^c_k$ such that each Σ^c_i is indecomposable. Such Σ^c_i are called *indecomposable components* of Σ^c. For a code Σ^c for Λ, to avoid confusion, sometimes, we need to denote it as $\Sigma^c(\Lambda)$ and denote the corresponding weight as $\Sigma(\Lambda)$. For example, if $\Sigma^c=\Sigma^c_1\Sigma^c_2$ and $\Sigma^c,\Sigma^c_1,\Sigma^c_2$ are unlinked, then we have primitive weights Σ,Σ_1,Σ_2 of Λ, and we have code $\Sigma^c_1(\Sigma_2)$ and primitive weight $\Sigma_1(\Sigma_2)$ of Σ_2.

Theorem 3.7: Let Σ_1^c,Σ^c be unlinked codes for Λ such that $\Sigma_1^c \leqslant \Sigma^c$. Suppose v_{Σ_1},v_Σ are primitive vectors of $\overline{V}(\Lambda)$ corresponding to Σ_1^c,Σ^c, respectively, then $v_\Sigma \in \mathbf{U}(G^-)v_{\Sigma_1}$.

Proof: By Serganova's Theorem,[13] an r-fold atypical indecomposable module over $sl(m+1/n+1)$ is equivalent to an r-fold atypical indecomposable module over $sl(r/r)$; in particular, the structure of an r-fold atypical Kac-module over $sl(m+1/n+1)$ is equivalent to the structure of an r-fold atypical Kac-module over $sl(r/r)$. Thus we can suppose that $G=sl(r/r)$ and that Λ is an r-fold atypical weight with atypical root $\gamma_1<\cdots<\gamma_r$ such that $\gamma_s=\beta_{r+1-s,s}=\alpha_{\overline{s-1,s-1}},s=1,\ldots,r$.

First we would like to make the following remark. In the proof of Theorem 6.6 of Ref. 12, we constructed two weight vectors v_Σ and $\tilde{v}_\Sigma$ and proved that at least one of them is primitive. Now in our case here, since $G=sl(r/r)$, by symmetry, we see that both vectors are primitive. Since both vectors have the same prime term (i.e., the leading term) up to a nonzero scalar, by Lemma 5.1(ii) of Ref. 12, we see that $v_\Sigma=\tilde{v}_\Sigma$ up to a nonzero scalar.

Now we shall use induction on r. If $\Sigma_1^c=\Sigma^c$ or $\Sigma^c=\Sigma_-^c$, then the proof is trivial. Thus suppose $\Sigma_1^c<\Sigma^c<\Sigma_-^c$.

Case 1: Σ^c is indecomposable.

Subcase (i): Column r of Σ^c is zero. Then as in the proof of Theorem 6.6 in Ref. 12, we can regard Σ^c as a code of the weight $\Lambda^{(r-1/r-1)}$ [which is the restriction of Λ to $G^{(r-1/r-1)}=sl(r-1/r-1)$]. The atypicality matrix $A(\Lambda^{(r-1/r-1)})$ is obtained from $A(\Lambda)$ by removing the first row and the last column. So $\Lambda^{(r-1/r-1)}$ is $(r-1)$-fold atypical, and the theorem is obtained by induction on r.

Subcase (ii): Column r of Σ^c is nonzero. Since Σ^c is an indecomposable unlinked code and $\Sigma^c\neq\Sigma_-^c$, every nonzero column of Σ^c must contain r, so column 1 of Σ^c must be zero. Let $I'=I\backslash\{\overline{1},0,1\}$. Let G' be the Lie supersubalgebra of G generated by $\{e_i,f_i,e_0'=e_{\overline{1,1}},f_0'=f_{\overline{1,1}}|i\in I'\}$ (i.e., we regard $\alpha_0'=\alpha_{\overline{1}}+\alpha_0+\alpha_1$ as the odd simple root in G' and simple roots $\alpha_{\overline{1}},\alpha_1$ of G are eliminated in G'). Thus obviously, $G'\cong sl(r-1/r-1)$ and $H'=\mathrm{span}\{h_i,h_0'=h_{\overline{1}}+h_0-h_1|i\in I'\}$ is the Cartan subalgebra of G'. We see that $\Lambda'=\Lambda|_{H'}$ is an $(r-1)$-fold atypical weight of G' whose atypicality matrix $A(\Lambda')$ is obtained from $A(\Lambda)$ by removing the first column and the last row. Thus Σ^c corresponds to a code Σ'^c of G' such that column i of Σ'^c is obtained from column $(i+1)$ of Σ^c with each nonzero label c substituted by $c-1$ for $i=1,\ldots,r-1$. For example, $G=sl(3/3),\Lambda=[02;0;20]$ and $\Sigma^c=\begin{smallmatrix}023\\3\end{smallmatrix}$, then $G'=sl(2/2),\Lambda'=[0;0;0]$ and $\Sigma'^c=\begin{smallmatrix}12\\2\end{smallmatrix}$, and we have the atypicality matrices as follows:

$$A(\Lambda)=\begin{pmatrix}4&1&0\\3&0&\overline{1}\\0&\overline{3}&\overline{4}\end{pmatrix}\rightarrow\begin{pmatrix}.&3&3\\.&2&3\\1&.&.\end{pmatrix},$$

$A(\Lambda')=\left(\begin{smallmatrix}10\\01\end{smallmatrix}\right)\rightarrow\left(\begin{smallmatrix}22\\12\end{smallmatrix}\right)$, where in the final array, we have specified all positions of the southwest chains of Λ and Λ' (keeping this example in mind will help understand the arguments that follow). Similarly, Σ_1^c corresponds to a code Σ'^c_1 of G' and $\Sigma'^c_1<\Sigma'^c$ (for the example we just mentioned, we have $\Sigma_1^c=020$, then $\Sigma'^c_1=10<\Sigma'^c=\begin{smallmatrix}12\\2\end{smallmatrix}$). Observe that the G'-submodule generated by v_Λ in $\overline{V}(\Lambda)$ is the G'-Kac-module $\overline{V}(\Lambda')$. Thus there exists $g_{\Sigma_1'},g_{\Sigma'}\in\mathbf{U}(G'^-)$ such that $v_{\Sigma_1'}=g_{\Sigma_1'}v_\Lambda,v_{\Sigma'}=g_{\Sigma'}v_\Lambda$ are G'-primitive vectors, and by inductive assumption, $v_{\Sigma'}\in\mathbf{U}(G'^-)v_{\Sigma_1'}$, i.e., there exists $g'\in\mathbf{U}(G'^-)$ such that $v_{\Sigma'}=g'v_{\Sigma_1'}=g'g_{\Sigma_1'}v_\Lambda$. Note that by the proof of Theorem 6.6 of Ref. 12, we see that we can label the roots associated with the positions in $D_{\Sigma_1'}$ by $\beta_p=\alpha_{\overline{m_p,n_p}},p=1,\ldots,s$, where $s=\#D_{\Sigma_1'}$, such that $\Lambda_0=\Lambda,\Lambda_p=\Lambda-\Sigma_{q=1}^p\beta_q$, and $v_{\Lambda_p}=\chi_{J_p}^{(m_p+1/n_p+1)}f(\beta_p)v_{\Lambda_{p-1}}$ for $p=1,\ldots,s$, and $\Sigma_1'=\Lambda_s,v_{\Sigma_1'}=v_{\Lambda_s}$. Here $J_p=\{\overline{m_p-y_p+1,\ldots,\overline{2}};2,\ldots,n_p-x_p+1\}\subset I'$, where x_p,y_p are defined as those x,y in (6.2) of Ref. 12 [cf. (6.4) of Ref. 12, note that since in G', $\alpha_0'=\alpha_{\overline{1}}+\alpha_0+\alpha_1$ and we do not have simple roots $\alpha_{\overline{1}},\alpha_1$ in G', thus we do not have elements $\overline{1},1$ in J_p]. Similarly, g' can be written as a

product of the form $\Pi_{p=1}^{s'}\chi_{J'_p,C_p}^{(m'_p+1,n'_p+1)}f(\beta'_p)$ for some $J'_p\subset I'$ and some $C_p\in\mathbb{C}^{\otimes\#J'_p}$ [cf. (6.5a) of Ref. 12], where $s'=\#(D_{\Sigma'}\backslash D_{\Sigma'_1})$ and $\beta'_p=\alpha_{\overline{m}'_p,n'_p}$ are roots associated with the positions in $D_{\Sigma'}\backslash D_{\Sigma'_1}$, for $p=1,\ldots,s'$, such that g' commutes with G'^{+}_0. Now if we set $\tilde{J}_p=J_p\cup\{\overline{1},1\}$ and let $\tilde{v}_{\Lambda_p}=\chi_{\tilde{J}_p}^{(m_p+1/n_p+1)}f(\beta_p)v_{\Lambda_{p-1}}$, then by the proof of Theorem 6.6 of Ref. 12 and the remark in the second paragraph of the proof, we see that $\tilde{v}_{\Sigma'_1}=\tilde{v}_{\Lambda_s}$ is precisely the G-primitive vector corresponding to the code Σ_1 of G. Similarly, if we set $\tilde{J}'_p=J'_p\cup\{\overline{1},1\}$ and let $\tilde{g}'=\Pi_{p=1}^{s'}\chi_{\tilde{J}'_p,\tilde{C}_p}^{(m'_p+1,n'_p+1)}f(\beta'_p)$ for some $\tilde{C}_p\in\mathbb{C}^{\otimes\#\tilde{J}'_p}$ (such that the ith coordinate of $\tilde{C}_p$ is the same as the ith coordinate of C_p for all $i\in J'_p$), then $\tilde{g}'$ commutes with G_0^{+}. Now set $\tilde{v}_{\Sigma'}=\tilde{g}'\tilde{v}_{\Sigma'_1}$, we see that $\tilde{v}_{\Sigma'}$ has the same (up to a nonzero scalar) prime terms as those of $v_{\Sigma'}$, so it is nonzero. By our construction, $\tilde{v}_{\Sigma'}$ must be the G-primitive vector v_Σ corresponding to the code Σ^c of G [since $\tilde{v}_{\Sigma'}$ has the same (up to a nonzero scalar) prime terms as those of v_Σ (in fact, the only prime term is the leading term), and they both are G_0-primitive, thus by Lemma 5.1(ii) of Ref. 12, they must be equal up to a nonzero scalar], and we have the theorem in this case.

Case 2: Suppose that $\Sigma^c=\Sigma'^c\Sigma''^c$ is decomposable and both Σ'^c,Σ''^c are subcodes of Σ^c.

Then we can also write $\Sigma_1^c=\Sigma'^c_1\Sigma''^c_1$ (one of Σ'^c_1,Σ''^c_1 may be zero) such that $\Sigma'^c_1\leqslant\Sigma'^c$ and $\Sigma''^c_1\leqslant\Sigma''^c$. The code $\Sigma'^c_1(\Sigma'')$ for Σ'' is a subcode of $\Sigma'^c(\Sigma'')$. Thus in $\overline{V}(\Sigma'')$, by induction on number of indecomposable components, we have

$$v_{\Sigma'^c(\Sigma')}\in\mathbf{U}(G^-)v_{\Sigma'^c_1(\Sigma'')}. \tag{3.18}$$

As in Ref. 12, define the module homomorphism $\overline{V}(\Sigma'')\to\overline{V}(\Lambda)$ by mapping $v_{\Sigma''}$ in $\overline{V}(\Sigma'')$ to $v_{\Sigma''(\Lambda)}$ in $\overline{V}(\Lambda)$ [Note that[3] every highest weight module with highest weight Σ'' is a quotient module of the Kac-module $\overline{V}(\Sigma'')$ and $\mathbf{U}(G^-)v_{\Sigma''(\Lambda)}$ is a highest weight module with highest weight Σ'', thus there exists a module homomorphism $\overline{V}(\Sigma'')\to\mathbf{U}(G^-)v_{\Sigma''(\Lambda)}\subset\overline{V}(\Lambda)$]. From the proof of Theorem 6.12 of Ref. 12, we see that if we set Σ_0 to be the primitive weight of Λ corresponding to code $\Sigma'^c_1\Sigma''^c$, then the primitive vectors v_Σ,v_{Σ_0} of $\overline{V}(\Lambda)$ are precisely the images of $v_{\Sigma'^c(\Sigma'')},v_{\Sigma'^c_1(\Sigma'')}$. Thus by (3.18),

$$v_\Sigma\in\mathbf{U}(G^-)v_{\Sigma_0}. \tag{3.19}$$

On the other hand, in $\overline{V}(\Lambda)$, the proof of Theorem 6.12 of Ref. 12 shows that there exists $g_{\Sigma''},g_{\Sigma''_1},g_{\Sigma'}\in\mathbf{U}(G^-)$ such that

$$v_{\Sigma''}=g_{\Sigma''}v_\Lambda,\quad v_{\Sigma''_1}=g_{\Sigma''_1}v_\Lambda,\quad v_{\Sigma_0}=g_{\Sigma'_1}v_{\Sigma''},\quad v_{\Sigma_1}=g_{\Sigma'_1}v_{\Sigma''_1}. \tag{3.20}$$

By case 1 and induction on number of indecomposable components, $v_{\Sigma''}\in\mathbf{U}(G^-)v_{\Sigma''_1}$, i.e., we can write $g_{\Sigma''}=g''g_{\Sigma''_1}$ for some $g''\in\mathbf{U}(G^-)$. Then we have

$$\begin{aligned}v_{\Sigma_0}&=g_{\Sigma'_1}v_{\Sigma''}=g_{\Sigma'_1}g_{\Sigma''}v_\Lambda=c_1g_{\Sigma''}g_{\Sigma'_1}v_\Lambda=c_1g''g_{\Sigma''_1}g_{\Sigma'_1}v_\Lambda\\&=c_2g''g_{\Sigma'_1}g_{\Sigma''_1}v_\Lambda=c_2g''v_{\Sigma_1}\in\mathbf{U}(G^-)v_{\Sigma_1},\end{aligned} \tag{3.21}$$

for some $c_1, c_2 \in \mathbb{C}$, where the third, fifth equalities follow from Lemma 5.1 of Ref. 12 since they are primitive vectors of the same weights with the same prime terms (i.e., the leading term) up to scalars. Now the proof is completed by (3.19), (3.21). ■

IV. WEAKLY PRIMITIVE VECTORS

Our main result in this section is the following theorem.

Theorem 4.1: To any linked code Σ^c for Λ, there corresponds a weakly primitive vector v_Σ in $\overline{V}(\Lambda)$. Furthermore, if $\Sigma_1^c \leqslant \Sigma^c$, then $v_\Sigma \in \mathbf{U}(G^-)v_{\Sigma_1}$.

Proof: As in the proof of Theorem 3.7, we suppose $G=sl(r/r)$ and Λ is an r-fold atypical weight with atypical root $\gamma_1<\cdots<\gamma_r$ such that $\gamma_s=\beta_{r+1-s,s}=\alpha_{\overline{s-1,s-1}}, s=1,\ldots,r$.

By introducing the Young diagram for Λ, it was proved in Ref. 11 that all codes (linked or unlinked) for Λ are in 1–1 correspondence with the standard boundary strip removals in the Young diagram for Λ. In Diagram 1, we list the Young diagrams for some Λ and some codes Σ^c, and specify all positions on the boundary removals corresponding to column i of code Σ^c by an entry i for $i=1,2,\ldots,r$. Observe that in Diagram 1(i), column s is wrapped by column t for all s and t with $s<t$ (we say column s *is wrapped by* column t for $s<t$ if the top entry of column t appears somewhere below the top entry in column s); in Diagram 1(ii), column 1 is linked to column 2 and these two columns are wrapped by columns 3 and 4, in this case we say that this link *is wrapped by* column 4; in Diagram 1(iii), columns 1, 2, and 3 appear to be linked to columns 4, 5, and 6,

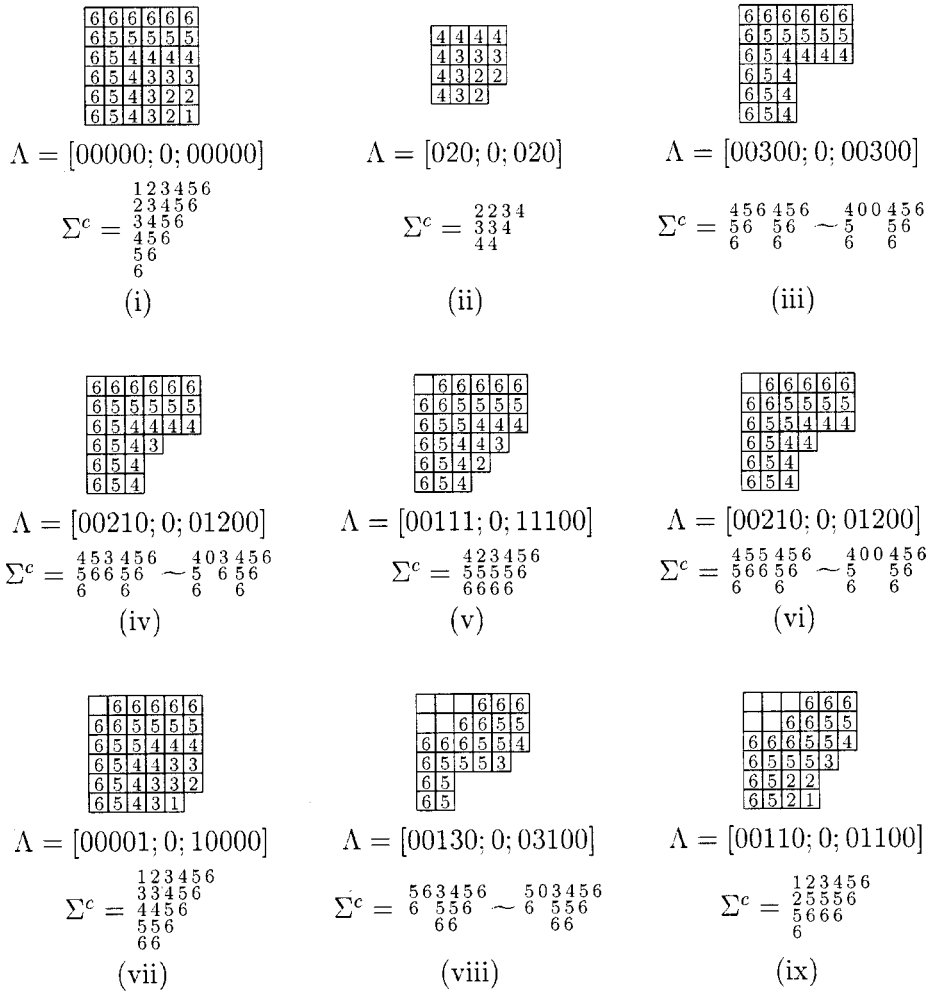


Diagram 1.

respectively, however, the shape of the corresponding boundary removals of the Young diagram just looks like that of Diagram 1(ii): In general if column s is linked to column t for $s<t$ and column u is linked to column v for $s<u<t<v$, then by rule (vi) of code definition, the link of column s to column t is wrapped by column v. This leads us to the following definition:

For any code Σ^c, we denote by $\tilde{\Sigma}^c$ the array obtained from Σ^c obeying the rule: if $s<t<u<v$ and $c_{1s}=c_{1u}=a<b=c_{1t}=c_{1v}$ [cf. Definition 2.4(3.vi)], then column t of $\tilde{\Sigma}^c$ is set to be zero. We call $\tilde{\Sigma}^c$ the *reduced code* of Σ^c and denote $\Sigma^c \sim \tilde{\Sigma}^c$. In particular, $\Sigma^c=\tilde{\Sigma}^c$ if Σ^c is an unlinked code. In general, $\tilde{\Sigma}^c$ is not a code by Definition 2.4(3).

Using this definition, the code in Diagram 1(iii) can be better reinterpreted as: Column 1 is linked to column 4 and this link is wrapped by columns 5 and 6. Thus we have the reduced code in the right-hand side of the symbol $\sim$, which is simply the same code as in Diagram 1(ii) if we delete the columns which are zero (i.e., columns 2 and 3). Similarly, we have other reduced codes in Diagram 1. By the definition of reduced codes, we obtain the following observation.

Observation 1: Suppose $1\leqslant s\leqslant u\leqslant t$ such that column s is linked to column t in a reduced code $\tilde{\Sigma}^c$, then column u cannot be linked to column v for any v such that $v<s$ or $v>t$.

We set

$$B_{\tilde{\Sigma}^c}=\{(s,t)\,|\,1\leqslant s<t\leqslant r,\ \text{columns } s \text{ and } t \text{ of } \tilde{\Sigma}^c \text{ contain a common nonzero top entry}\}. \tag{4.1}$$

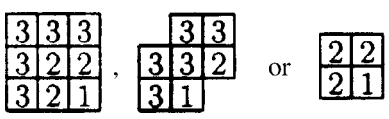
Define the *link number* to be $i_{\tilde{\Sigma}^c}=\#B_{\tilde{\Sigma}^c}$. We shall prove the theorem by induction on $i_{\tilde{\Sigma}^c}$. If $i_{\tilde{\Sigma}^c}=0$, then $\tilde{\Sigma}^c$ is an unlinked reduced code, thus $\Sigma^c=\tilde{\Sigma}^c$, and so Σ^c corresponds to a primitive vector.[12] If $\Sigma_1^c\leqslant\Sigma^c$, then Σ_1^c is also an unlinked code and the second statement of Theorem 4.1 follows from Theorem 3.7.

Now suppose $i_{\tilde{\Sigma}^c}>0$. Define a total ordering on $B_{\tilde{\Sigma}^c}$ by

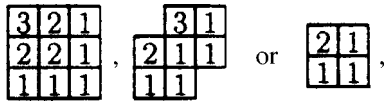
$$(s,t)\leqslant(u,v)\Leftrightarrow t<v \text{ or } t=v \text{ but } s>u. \tag{4.2}$$

Choose $(s,t)\in B_{\tilde{\Sigma}^c}$ to be the smallest pair with respect to the ordering (4.2). Let u be the smallest number such that $s<u<t$ and such that column u of $\tilde{\Sigma}^c$ is nonzero. If such u does not exist, we set $u=t$.

Case 1: $u=t$ or $u<t$ but column u contains the top entry of column t as an entry [thus column v is wrapped by column t for $u\leqslant v<t$ by rule (ii) of code definition]. For any w with $s<w<u$ (if such w exists), by rule (v) of code definition, $nqc(\Lambda)_{wt}\neq q$, and by rule (ii), $nqc(\Lambda)_{wt}\neq c$; thus $nqc(\Lambda)_{wt}=n$ and so $nqc(\Lambda)_{sw}=c$ (since $nqc(\Lambda)_{st}=q$). This shows that $D'(s)=\Sigma_{i=s}^{u-1}NE_\Lambda(i)$ corresponds to an opposite (unlinked) code for Λ, and $\Lambda'=\Lambda+\Sigma_{(b,c)\in D'(s)}\beta_{bc}$ is an integral dominant r-fold atypical root. For example, if the pair (Λ,Σ^c) is shown in Diagram 1(iii), 1(vi), or 1(viii), then Λ' is shown in Diagram 1(i), 1(vii) or 1(ix), respectively (to indicate the boxes in the Young diagram for Λ' corresponding to the northeast chain $D'(s)$, the boxes on the right-bottom corner of the Young diagram labeled as



should be re-labeled as



respectively). Now for the weight Λ', by construction, we have $nqc(\Lambda')_{w,u-1}=c$ for all $s\leqslant w<u-1$. Note that we have

Claim 1. Suppose $1\leqslant s<u'\leqslant r$ such that $D'(s)=\Sigma_{i=s}^{u'}NE_{\Lambda}(i)$ corresponds to an opposite (unlinked) code for Λ, and $\Lambda'=\Lambda+\Sigma_{(b,c)\in D'(s)}\beta_{bc}$ is an integral dominant r-fold atypical root. Then there exists an unlinked code $\Sigma_0^c(\Lambda')$ for Λ', such that $D_{\Sigma_0(\Lambda')}=\Sigma_{i=s}^{u'}SW_{\Lambda'}(i)$ is equal to $D'(s)$.

To obtain this claim, we can restrict our attention to $G^{(u'/u')}=sl(u'/u')$ so that we can suppose $u'=r$. Furthermore, by letting G' be the Lie supersubalgebra of $G^{(u'/u')}$ generated by $\{e_i,f_i,e_0'=e_{\overline{s-1},s-1},f_0'=f_{\overline{s-1},s-1}|i=s,\ldots,u'-1\}$ as in the proof of Theorem 3.7, we can suppose $s=1$. But then, $D'(s)$ is simply the set of northeast chains and the claim is obtained from the proof of Theorem 3.5.

By Claim 1, there exists an unlinked code $\Sigma_0^c(\Lambda')$ for Λ', such that $D_{\Sigma_0(\Lambda')}=\Sigma_{i=s}^{u-1}SW_{\Lambda'}(i)$ is equal to $D'(s)$. For the example we have just given,

$$\Sigma_0^c(\Lambda')=\begin{array}{ccc}1&2&3\\2&3&\\3&&\end{array},\quad\begin{array}{ccc}1&2&3\\3&3&\end{array}\quad\text{or}\quad\begin{array}{cc}1&2\\2&\end{array},$$

respectively. From this and Ref. 12, we obtain the following important fact.

Fact 1: Λ is the primitive weight of Λ' corresponding to the code $\Sigma_0^c(\Lambda')$.

Similarly, we have $nqc(\Lambda')_{vt}=c$ for all $s\leqslant v<t$ and there exists a code $\Sigma^c(\Lambda')$ for Λ' which is obtained from the code $\Sigma_0^c(\Lambda')$ and the code Σ^c by the following rules:

(i) if $w\geqslant t$ or $w<s$, then column w of $\Sigma^c(\Lambda')$ is the same as column w of Σ^c.
(ii) if $s\leqslant v\leqslant t-1$, then column v of $\Sigma^c(\Lambda')$ contains all nonzero entries of column v of $\Sigma_0^c(\Lambda')$ and also contains a as an entry, where a is the top entry of column t of Σ^c (thus contains all entries of column t of Σ^c).

Note that these rules uniquely determine the code $\Sigma^c(\Lambda')$. For the example we have just given, the code $\Sigma^c(\Lambda')$ is given in Diagram 1(i), 1(vii), or 1(ix), respectively. Now the link number for $\Sigma^c(\Lambda')$ is $i_{\tilde{\Sigma}^c(\Lambda')}=i_{\tilde{\Sigma}^c}-1$. By induction, there exists a weakly primitive vector $v_{\Sigma^c(\Lambda')}\in\overline{V}(\Lambda')$. As in the proof of Theorem 3.7, we define a module homomorphism $\overline{V}(\Lambda)\to\overline{V}(\Lambda')$ which maps v_Λ in $\overline{V}(\Lambda)$ to $v_{\Sigma_0(\Lambda')}$ in $\overline{V}(\Lambda')$. Under this homomorphism the preimage of $v_{\Sigma(\Lambda')}$ is a weakly primitive vector of $\overline{V}(\Lambda)$ corresponding to the code Σ [since $\Sigma_0^c(\Lambda')\leqslant\Sigma^c(\Lambda')$ and so $v_{\Sigma(\Lambda')}\in\mathbf{U}(G^-)v_{\Sigma_0(\Lambda')}$). Suppose $\Sigma_1^c\leqslant\Sigma^c$. Then as above we can write a code $\Sigma_1^c(\Lambda')$ for Λ' such that $\Sigma_0^c(\Lambda')\leqslant\Sigma_1^c(\Lambda')\leqslant\Sigma^c(\Lambda')$ and so $v_{\Sigma(\Lambda')}\in\mathbf{U}(G^-)v_{\Sigma_1(\Lambda')}\subset\mathbf{U}(G^-)v_{\Sigma_0(\Lambda')}$. Thus we obtain the second statement of Theorem 4.1.

Case 2: $u<t$ and column u does not contain the top entry of column t as an entry. Let $v<t$ be the largest number such that the top entry of column t does not appear as an entry in column v. Let $\Sigma'^c\leqslant\Sigma^c$ be the subcode of Σ^c such that for $w<u$ or $w>v$, column w is zero and for $u\leqslant w\leqslant v$, column w consists of those entries a of column w of Σ^c such that $u\leqslant a\leqslant v$ (if there is no such a, then column w is set to be zero). Let Λ' be the primitive weight of $\overline{V}(\Lambda)$ corresponding to code Σ'^c. Let $\Sigma^c(\Lambda')$ be a code for Λ' obtained from Σ^c by removing all entries appearing in Σ'^c (if in a column there is no entry after removing, then this column is set to be zero). By code definition, one can verify that $\Sigma^c(\Lambda')$ is indeed a code for Λ' (note that in the code Σ^c since the top entry of column t does not appear in column w for all w with $u\leqslant w\leqslant v$, column w of Σ^c can only contain those entries a with $u\leqslant a\leqslant v$ by code definition; thus column w of $\Sigma^c(\Lambda')$ is in fact zero for all w with $u\leqslant w\leqslant v$). For example, if the pair (Λ,Σ^c) is given in Diagram 1(iv) or 1(v), then $\Sigma'^c=00300$ or 02300 and the pair $(\Lambda',\Sigma^c(\Lambda'))$ is shown in Diagram 1(iii) or 1(vi), respectively. Now $\Sigma^c(\Lambda')$ is a code in Case 1, therefore, there exists a weakly primitive vector $v_{\Sigma(\Lambda')}$

in $\overline{V}(\Lambda')$. Define a module homomorphism: $\overline{V}(\Lambda')\to\overline{V}(\Lambda)$ mapping $v_{\Lambda'}$ in $\overline{V}(\Lambda')$ to $v_{\Sigma'^c}$ (having the same weight Λ') in $\overline{V}(\Lambda)$. We claim that the image of $v_{\Sigma(\Lambda')}$ is nonzero by calculating the coefficient of the leading term as we did in Ref. 12. This image is then the weakly primitive vector corresponding to the code Σ^c for Λ. Similarly, we obtain the second statement of Theorem 4.1. ■

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Soliton solutions of XXZ lattice Landau–Lifshitz equation

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Multisoliton solutions of the partially isotropic (classical) lattice Landau–Lifshitz equation are constructed. A trigonometric version of the dressing method is proposed to this aim. The dressing matrix is a matrix valued periodic function of the spectral parameter, and takes almost the same form as the L-matrix except for the number of poles. Both the easy-axis ($J_1=J_2<J_3$) and easy-plane ($J_1<J_2=J_3$) cases can be treated in a parallel way. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1407839]

I. INTRODUCTION

The Landau–Lifshitz (LL) equation is an equation that describes the motion of the classical ferromagnetic spins on a continuous space. It is known that the LL equation is a universal equation in the sense that it reduces to integrable systems in special cases, such as the sine-Gordon (SG) model and the nonlinear Schrödinger (NLS) equation. Sklyanin established that the LL equation itself is a completely integrable Hamiltonian system by constructing the Lax pair.[1]

For an application to the theory of condensed-matter physics, it will be more natural that the spins are configured on a lattice rather than on a continuous space. Although the solitary excitations in one-dimensional magnets have been extensively studied from that point of view,[2] it is known that a ''naive'' discretization does not inherit the complete integrability of the LL equation.[3] A completely integrable lattice version of the LL equation (the LLL equation) has been proposed by an approach from the r-matrix.[4,5] The lattice version, like the continuous case, contains a lattice SG model[6] and a lattice versions of NLS equation[7,8] as its special cases.

In this article, we construct the soliton solutions of the LLL equation by a dressing method. Because the Lax formalism of the LLL equation (as well as the continuous LL equation) contains elliptic functions of the spectral parameters, the usual dressing method[9] has to be modified. Bobenko developed such a variant of the dressing method to construct multisoliton solutions of the continuous LL equation.[10] Volkov applied Bobenko's method to the LLL equation and obtained the one-soliton solution,[11] but did not present an explicit form of multisoliton solutions. This will probably be due to technical difficulties—in Bobenko's approach, multisoliton solutions are obtained by a sequence of dressing transformations, which becomes more complicated as one proceeds. We propose a new dressing method to overcome this difficulty.

Our approach is based on a single dressing matrix rather than a sequence of dressing transformations. This dressing matrix is characterized by several analytic properties, which we shall derive from those of the L-matrix. In order to make the calculations not too complicated, we consider the partially isotropic (XXZ) LLL equation. The dressing matrix for this case is a linear combination of the trigonometric functions, and the coefficients are determined by a procedure similar to the usual dressing method.

This paper is organized as follows. In Sec. II we provide a brief review of the LLL equation and its Lax pair. In Sec. III we illustrate the construction of the multisoliton solution of the easy-axis LLL equation by the dressing method. The easy-plane case is also mentioned in Sec. IV. Section V is for conclusion and discussion.

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II. LATTICE LANDAU–LIFSHITZ EQUATION

A. The equation

The Landau–Lifshitz equation

$$\partial_t \vec{S}(x,t) = \vec{S}(x,t)_{xx} \times \vec{S}(x,t) - J\vec{S}(x,t) \times \vec{S}(x,t)$$

is a classical equation for nonlinear spin waves in a ferromagnet. Here, J_l $(l=1,2,3)$ are coupling constants, and $J=\mathrm{diag}(J_1,J_2,J_3)$.

The LLL equation is formulated[4] with an auxiliary real variable $S_{0n}(t)$ besides the three spin variables $S_{1n}(t)$, $S_{2n}(t)$, and $S_{3n}(t)$. The integer n is the index of a lattice site and unrestricted (i.e., the lattice is infinite). The four variables $(S_{0n}(t),S_{1n}(t),S_{2n}(t),S_{3n}(t))$ are required to obey the constraints

$$\kappa_0 = S_{1n}^2 + S_{2n}^3 + S_{3n}^2, \tag{1}$$

$$\kappa_1 = S_{0n}^2 - (J_1 S_{1n}^2 + J_2 S_{2n}^2 + J_3 S_{3n}^2), \tag{2}$$

where κ_0 and κ_1 are positive parameters, and J_1, J_2, and J_3 are coupling constants of two neighboring spins. We assume that

$$J_1 \leqslant J_2 \leqslant J_3, \quad \kappa_1 + J_3\kappa_0 \geqslant 0,$$

so that Eqs. (1) and (2) have a solution in $\mathbf{R}^4$. In the isotropic case $(J_1=J_2=J_3)$, the LLL equation reduces to the so called Heisenberg spin chain model.[12] We investigate two partially isotropic cases, easy-axis $(J_1=J_2<J_3)$ and easy-plane $(J_1<J_2=J_3)$.

We use the three functions of a complex parameter λ,

$$w_1(\lambda) = \rho/\mathrm{sn}(\lambda,k_0),$$

$$w_2(\lambda) = \rho\,\mathrm{dn}(\lambda,k_0)/\mathrm{sn}(\lambda,k_0),$$

$$w_3(\lambda) = \rho\,\mathrm{cn}(\lambda,k_0)/\mathrm{sn}(\lambda,k_0),$$

where sn, cn, and dn are Jacobi's elliptic functions, and k_0 is the modulus of elliptic functions $(0 \leqslant k_0 \leqslant 1)$. The constants ρ and k_0 are defined by the equations

$$\rho = \sqrt{J_3 - J_1}, \tag{3}$$

$$k_0 = \sqrt{\frac{J_2 - J_1}{J_3 - J_1}}. \tag{4}$$

Let λ_0 be a solution of

$$\kappa_1 + \kappa_0((w_\alpha(\lambda_0))^2 + J_\alpha) = 0. \tag{5}$$

We introduce the vector variables at lattice-site n,

$$\vec{S}_n(t) = (S_{1n}(t),S_{2n}(t),S_{3n}(t))^{\mathrm{T}},$$

$$\vec{T}_n(t) = \mathcal{W}(\lambda_0)\vec{S}_n(t),$$

where V^{T} is the transpose of the vector V, and $\mathcal{W}(\lambda) = \mathrm{diag}(w_1(\lambda),w_2(\lambda),w_3(\lambda))$. Here and below, t will be omitted. The LLL equation[4] is then written as follows:

$$\partial_t S_{0n}=2\det \mathcal{W}(\lambda_0)\left(\frac{\vec{T}_{n+1}}{h_{n+1}}+\frac{\vec{T}_{n-1}}{h_n}\right)\cdot\begin{pmatrix}\frac{1}{J_3^2}-\frac{1}{J_2^2} & & \\ & \frac{1}{J_1^2}-\frac{1}{J_3^2} & \\ & & \frac{1}{J_2^2}-\frac{1}{J_1^2}\end{pmatrix}\vec{T}_n, \tag{6}$$

$$\partial_t \vec{T}_n=2\det \mathcal{W}(\lambda_0)\left(\left(\frac{S_{0n+1}}{h_{n+1}}+\frac{S_{0n-1}}{h_n}\right)(\mathcal{W}^{-2}(\lambda_0)\vec{T}_n)\times\vec{T}_n-S_{0n}(\mathcal{W}^{-2}(\lambda_0)\vec{T}_n)\times\left(\frac{\vec{T}_{n+1}}{h_{n+1}}+\frac{\vec{T}_{n-1}}{h_n}\right)\right), \tag{7}$$

where "$\cdot$" and "$\times$" stand for the scalar and vector products, and

$$h_n=S_{0,n-1}S_{0,n}-\sum_{\alpha=1}^{3} w_\alpha^2(\lambda_0)S_{\alpha,n-1}S_{\alpha,n}.$$

In fact,

$$H=-\sum_{n-\infty}^{\infty}\log h_n$$

is the Hamiltonian of this system.[4] We assume that $h_n\neq 0$ because the situation where $h_n=0$ is physically nonsense.

B. Lax formalism

In order to write the LLL equation in the Lax formalism, we define $L_n(\lambda)$ and $M_n(\lambda)$ as follows:[4]

$$L_n(\lambda)=S_{0n}\mathbf{1}+i\sum_{l=1}^{3} w_l(\lambda)S_{ln}\sigma_l, \tag{8}$$

$$M_n(\lambda)=\frac{1}{h_n}\sum_{l=1}^{3}(w_l(\lambda-\lambda_0)\hat{M}_{ln}(\lambda_0)+w_l(\lambda+\lambda_0)\hat{M}_{ln}(-\lambda_0))\sigma_l. \tag{9}$$

Here

$$\hat{M}_{l_3,n}(\lambda)=iw_{l_3}(\lambda)(S_{0,n-1}S_{l_3,n}+S_{l_3,n-1}S_{0,n})-iw_{l_1}(\lambda)w_{l_2}(\lambda)(S_{l_1,n-1}S_{l_2,n}-S_{l_2,n-1}S_{l_1,n})$$

with (l_1,l_2,l_3) being a cyclic permutation of (1,2,3), and λ being a time-independent spectral parameter.

The LLL equation is then equivalent to the Lax equation

$$\partial_t L_n(\lambda)=M_{n+1}(\lambda)L_n(\lambda)-L_n(\lambda)M_n(\lambda) \tag{10}$$

of the linear equations

$$\Psi_{n+1}(\lambda)=L_n(\lambda)\Psi_n(\lambda), \tag{11}$$

$$\partial_t\Psi_n(\lambda)=M_n(\lambda)\Psi_n(\lambda). \tag{12}$$

Equation (10) is the so called compatibility condition of Eqs. (11) and (12). Namely Eqs. (11) and (12) have a nontrivial solution if and only if Eq. (10) is satisfied. Suppose that Eqs. (11) and (12) have a nontrivial solution. Then by calculating $\partial_t \Psi_{n+1}(\lambda)$ in two different ways as

$$\partial_t \Psi_{n+1}(\lambda) = (\partial_t L_n \lambda + L_n(\lambda) M_n(\lambda)) \Psi_n(\lambda)$$

and

$$\partial_t \Psi_{n+1}(\lambda) = M_{n+1}(\lambda) L_n(\lambda) \Psi_n(\lambda),$$

one obtains Eq. (10). The inverse is also true (though we do not need it in the subsequent consideration).

C. Trigonometric case

If k_0 equals zero, i.e., $J_1 = J_2 < J_3$, Jacobi's elliptic functions reduce to trigonometric functions. The L-matrix then takes the form

$$L_n(\lambda) = S_{0n}\mathbf{1} + i\frac{\rho}{\sin\lambda}(S_{1n}\sigma_1 + S_{2n}\sigma_2 + \cos\lambda S_{3n}\sigma_3), \tag{13}$$

and enjoys the symmetry properties

$$\sigma_3 L_n(\lambda)\sigma_3 = L_n(\lambda + \pi), \tag{14a}$$

$$\sigma_2 L_n(\lambda)\sigma_2 = (L_n(\lambda^*))^*, \tag{14b}$$

$$\lim_{y\to+\infty} \sigma_1 L_n(x+iy)\sigma_1 = \lim_{y\to+\infty} L_n(x-iy) \quad (x \in \mathbf{R}). \tag{14c}$$

Equations (14a) and (14c) stem from the double periodicity of the matrix elements of $L_n(\lambda)$ in the totally anisotropic case. Because of Eq. (14a), the diagonal elements of $L_n(\lambda)$ are periodic functions with period π; the off-diagonal elements of $L_n(\lambda)$ are antiperiodic functions with period π ($f(z+\pi) = -f(z)$). Equation (14b) implies that S_{ln} ($l = 0,1,2,3$) are real valued.

III. DRESSING METHOD

In this section, we construct solutions of the easy-axis partially isotropic ($k_0 = 0$) LLL equation. The construction is achieved by three steps. First, an analytic form of the dressing matrix is determined by its quasi-periodicity and its properties of the poles. The residues of the dressing matrix at the poles are free parameters. Second, a set of linear algebraic equations for the residues of the dressing matrix and its inverse matrix is derived and solved. Last, the (n,t) dependence of these residues is specified.

A. The first step

Let us consider the vacuum solution of the LLL equation,

$$\vec{S}_n = (0,0,\sqrt{\kappa_0})^{\mathrm{T}}.$$

The L- and M-matrices take the form

$$L^{(0)}(\lambda) = \sqrt{\kappa_1 + J_3\kappa_0}\mathbf{1} + \frac{i\sqrt{\kappa_0}\rho}{\tan\lambda}\sigma_3, \tag{15}$$

$$M^{(0)}(\lambda) = 2i\sqrt{\frac{\kappa_1 + J_3\kappa_0}{\kappa_0}}\frac{1}{1 + (1/\rho^2)[(\kappa_1 + J_1\kappa_0)/\kappa_0]\sin^2\lambda}\sigma_3. \tag{16}$$

An associated solution of the linear equations (11) and (12) is given by

$$\Phi_n(\lambda)=L^{(0)}(\lambda)^n \exp(M^{(0)}(\lambda)t). \tag{17}$$

The dressing methods seek a nontrivial solution by "dressing" this bare solution. We introduce $\Psi_n(\lambda)$ as

$$\Psi_n(\lambda)=W_n(\lambda)\Phi_n(\lambda). \tag{18}$$

We call $W_n(\lambda)$ the *dressing matrix*. The dressing matrix is determined such that $\Psi_n(\lambda)$ be a solution of the linear equations (11) and (12).

For Eq. (18) to be consistent with Eq. (11), we follow Mikhailov's idea[13] and require that $W_n(\lambda)$ satisfies the following three conditions parallel to Eqs. (14a)–(14c):

$$\sigma_3 W_n(\lambda)\sigma_3=W_n(\lambda+\pi), \tag{19a}$$

$$\sigma_2 W_n(\lambda)\sigma_2=(W_n(\lambda^*))^*, \tag{19b}$$

$$\sigma_1 W_n(i\infty)\sigma_1=W_n(-i\infty). \tag{19c}$$

See the remark at the end of this section. Furthermore, by Eqs. (11) and (12), $\det W_n(\lambda)$ is independent of n and t, thereby a function of only λ. Thus, without loss of generality, we can assume that

$$\lim_{y\to+\infty} \det W_n(iy)=1 \tag{20}$$

(see Appendix B).

To construct a soliton solution, we impose the following additional conditions:

(C-I) Each matrix element of $W_n(\lambda)$ is a meromorphic function of λ. The poles in the strip $D=\{\lambda|0\leqslant \mathrm{Re}\,\lambda<\pi\}$ are located at N mutually distinct nonreal numbers $\alpha_1,\ldots,\alpha_N$ and their complex conjugates $\alpha_1^*,\ldots,\alpha_N^*$. The α_j^*'s are written α_{N+j} in the following.

(C-II) There exists a y_0 (independent of $\mathrm{Re}\,\lambda$) such that each element of $W_n(\lambda)$ is bounded in the domain $|\mathrm{Im}\,\lambda|>y_0$.

(C-III) The residue matrices of $W_n(\lambda)$ at $\lambda=\alpha_j$ $(j=1,\ldots,2N)$ have rank 1.

Some comments are in order. Equation (19a) implies that the diagonal elements of $W_n(\lambda)$ are periodic functions with period π, and the off-diagonal elements are antiperiodic functions with period π. The condition C-II guarantees that the elements of $W_n(\lambda)$ are uniformly bounded in the limit $\mathrm{Im}\,\lambda\to\infty$. Equation (20) is a normalization condition; the condition at $\lambda=-i\infty$ follows from Eqs. (19c) and (20). Owing to the condition C-III, it is guaranteed that all the poles of $\det W_n(\lambda)$ at $\lambda=\alpha_j$ $(j=1,\ldots,2N)$ are simple. If the rank of the residue matrix at α_j is 2, then $\det W_n(\lambda)$ has a double pole at $\lambda=\alpha_j$; if the residue has rank 0, $W_n(\lambda)$ shall not have a pole at $\lambda=\alpha_j$. Under these conditions, the following results are deduced by complex analytic discussion (see Appendices A and B):

(1) $W_n(\lambda)$ can be written

$$W_n(\lambda)=d_{n0}\mathbf{1}+\sum_{j=1}^{2N}\left(\frac{d_{nj}\mathbf{1}+ic_{nj}\sigma_3}{\tan(\lambda-\alpha_j)}+\frac{ia_{nj}\sigma_1+ib_{nj}\sigma_2}{\sin(\lambda-\alpha_j)}\right). \tag{21}$$

Note that Eq. (21) takes the same form as the L-matrix has except for the coefficient of $\mathbf{1}$. The coefficients d_{nj} $(j=1,\ldots,2N)$ have to obey the relation

$$\sum_{j=1}^{2N} d_{nj}=0 \tag{22}$$

as a consequence of Eq. (19c).

(2) $\det W_n(\lambda)$ is a periodic function with period π, and has $2N$ simple poles at $\alpha_1,\ldots,\alpha_{2N}$ in D and the same number of zeros at $\beta_1,\ldots,\beta_{2N}$. Accordingly,

$$\det W_n(\lambda)=\frac{\Pi_{j=1}^{2N}\sin(\lambda-\beta_j)}{\Pi_{j=1}^{2N}\sin(\lambda-\alpha_j)}. \tag{23}$$

Moreover, $\beta_i\neq\alpha_j\,(\mathrm{mod}\,\pi)$. The restriction

$$\sum_{j=1}^{2N}\alpha_j=\sum_{j=1}^{2N}\beta_j\ \ (\mathrm{mod}\,2\pi) \tag{24}$$

follows from Eqs. (19c) and (20), and the inverse is also true.

(3) If the β_j's are mutually distinct, then $W_n^{-1}(\lambda)$ can be written

$$W_n^{-1}(\lambda)=\tilde{d}_{n0}\mathbf{1}+\sum_{j=1}^{2N}\left(\frac{\tilde{d}_{nj}\mathbf{1}+i\tilde{c}_{nj}\sigma_3}{\tan(\lambda-\beta_j)}+\frac{i\tilde{a}_{nj}\sigma_1+i\tilde{b}_{nj}\sigma_2}{\sin(\lambda-\beta_j)}\right), \tag{25}$$

which takes the same form as $W_n(\lambda)$.

B. The second step

Since the residues are rank 1 matrices, there exist column two-vectors $u_{nj},\tilde{u}_{nj}$ and row two-vectors $v_{nj},\tilde{v}_{nj}$ $(j=1,\ldots,2N)$ such that

$$d_{nj}\mathbf{1}+ia_{nj}\sigma_1+ib_{nj}\sigma_2+ic_{nj}\sigma_3=u_{nj}v_{nj},$$

$$\tilde{d}_{nj}\mathbf{1}+i\tilde{a}_{nj}\sigma_1+i\tilde{b}_{nj}\sigma_2+i\tilde{c}_{nj}\sigma_3=\tilde{u}_{nj}\tilde{v}_{nj}.$$

Moreover, since the residues of $W_n(\lambda)W_n^{-1}(\lambda)$ at $\lambda=\alpha_j,\beta_k$ $(1\leqslant j,k\leqslant 2N)$ have to vanish, we have the relations

$$u_{nj}v_{nj}W_n^{-1}(\alpha_j)=0, \tag{26a}$$

$$W_n(\beta_k)\tilde{u}_{nk}\tilde{v}_{nk}=0. \tag{26b}$$

We seek a nontrivial solution of these equations.

Let $u_{nj}^{(l)}$ and $\tilde{u}_{nj}^{(l)}$ ($v_{nj}^{(l)}$ and $\tilde{v}_{nj}^{(l)}$) be the lth components ($l=1,2$) of u_{nj} and $\tilde{u}_{nj}$ (v_{nj} and $\tilde{v}_{nj}$), respectively. $u_n^{(l)}$ and $\tilde{u}_n^{(l)}$ ($v_n^{(l)}$ and $\tilde{v}_n^{(l)}$) denote row (column) vectors whose jth components ($j=1,\ldots,2N$) are $u_{nj}^{(l)}$ and $\tilde{u}_{nj}^{(l)}$ ($v_{nj}^{(l)}$ and $\tilde{v}_{nj}^{(l)}$), respectively. With this notation, the foregoing equations can be rewritten

$$d_{n0}\tilde{u}_n^{(l)}+u_n^{(l)}X_n^{(l)}=0, \tag{27a}$$

$$\tilde{d}_{n0}v_n^{(l)}-X_n^{(l)}\tilde{v}_n^{(l)}=0, \tag{27b}$$

where $X_n^{(l)}(l=1,2)$ are $2N\times 2N$ matrices with the (j,k) elements

$$\{X_n^{(1)}\}_{j,k}=\frac{v_{nj}^{(1)}\tilde{u}_{nk}^{(1)}}{\tan(\beta_k-\alpha_j)}+\frac{v_{nj}^{(2)}\tilde{u}_{nk}^{(2)}}{\sin(\beta_k-\alpha_j)}, \tag{28a}$$

$$\{X_n^{(2)}\}_{j,k}=\frac{v_{nj}^{(1)}\tilde{u}_{nk}^{(1)}}{\sin(\beta_k-\alpha_j)}+\frac{v_{nj}^{(2)}\tilde{u}_{nk}^{(2)}}{\tan(\beta_k-\alpha_j)}. \tag{28b}$$

Here and later, we assume that $X_n^{(l)}$ are nonsingular matrices, so that $u_n^{(l)}$ and $\tilde{v}_n^{(l)}$ are uniquely determined by α_j's, β_j's, $v_{nj}^{(l)}$'s, and $\tilde{u}_{nj}^{(l)}$'s.

By Cramer's rule, we obtain the following expressions for the entries of $W_n(\lambda)$ and $W_n^{-1}(\lambda)$:

$$W_n(\lambda)=d_{n0}\begin{pmatrix}\dfrac{1}{|X_n^{(1)}|} & \\ & \dfrac{1}{|X_n^{(2)}|}\end{pmatrix}\begin{pmatrix}\begin{vmatrix}1 & \tilde{u}_n^{(1)}\\ T_n^{(1)}(\lambda) & X_n^{(1)}\end{vmatrix} & \begin{vmatrix}0 & \tilde{u}_n^{(1)}\\ S_n^{(2)}(\lambda) & X_n^{(1)}\end{vmatrix}\\ \begin{vmatrix}0 & \tilde{u}_n^{(2)}\\ S_n^{(1)}(\lambda) & X_n^{(2)}\end{vmatrix} & \begin{vmatrix}1 & \tilde{u}_n^{(2)}\\ T_n^{(2)}(\lambda) & X_n^{(2)}\end{vmatrix}\end{pmatrix}, \tag{29}$$

$$W_n^{-1}(\lambda)=-\tilde{d}_{n0}\begin{pmatrix}\begin{vmatrix}-1 & \tilde{T}_n^{(1)}(\lambda)\\ v_n^{(1)} & X_n^{(1)}\end{vmatrix} & \begin{vmatrix}0 & \tilde{S}_n^{(1)}(\lambda)\\ v_n^{(2)} & X_n^{(2)}\end{vmatrix}\\ \begin{vmatrix}0 & \tilde{S}_n^{(2)}(\lambda)\\ v_n^{(1)} & X_n^{(1)}\end{vmatrix} & \begin{vmatrix}-1 & \tilde{T}_n^{(2)}(\lambda)\\ v_n^{(2)} & X_n^{(2)}\end{vmatrix}\end{pmatrix}\begin{pmatrix}\dfrac{1}{|X_n^{(1)}|} & \\ & \dfrac{1}{|X_n^{(2)}|}\end{pmatrix}, \tag{30}$$

where $S_n^{(l)}$ and $T_n^{(l)}$ ($\tilde{S}_n^{(l)}$ and $\tilde{T}_n^{(l)}$) are column (row) $2N$-vectors with the jth components

$$\{S_n^{(l)}(\lambda)\}_j=\frac{v_{nj}^{(l)}}{\sin(\lambda-\alpha_j)},\quad \{T_n^{(l)}(\lambda)\}_j=\frac{v_{nj}^{(l)}}{\tan(\lambda-\alpha_j)}, \tag{31}$$

$$\{\tilde{S}_n^{(l)}(\lambda)\}_j=\frac{\tilde{u}_{nj}^{(l)}}{\sin(\lambda-\beta_j)},\quad \{\tilde{T}_n^{(l)}(\lambda)\}_j=\frac{\tilde{u}_{nj}^{(l)}}{\tan(\lambda-\beta_j)}. \tag{32}$$

The leading coefficients d_{n0} and $\tilde{d}_{n0}$ can be determined by the normalization condition (20). Since Eq. (20) implies that

$$\lim_{y\to+\infty}\det W_n(x\pm iy)=d_{n0}^2+\left(\sum_{j=1}^{2N}c_{nj}\right)^2=1,$$

combining this with the identity $W_n(\lambda)W_n^{-1}(\lambda)=\mathbf{1}$, we find that

$$d_{n0}=\pm\tilde{d}_{n0}=\frac{1}{\sqrt{1+(|{}_{v_n^{(l)}}{}^{0}_{X_n^{(l)}}{}^{\tilde{u}_n^{(l)}}|/|X_n^{(l)}|)^2}}, \tag{33}$$

where the denominator is invariant under the choice of the label $l=1,2$.

C. The last step

Let us now determine the (n,t) dependence of v_{nj} and $\tilde{u}_{nj}$.

Equations (11) and (12) yield the equations

$$W_{n+1}(\lambda)L^{(0)}(\lambda)W_n^{-1}(\lambda)=L_n(\lambda), \tag{34a}$$

$$\partial_t W_n(\lambda)W_n^{-1}(\lambda)+W_n(\lambda)M^{(0)}(\lambda)W_n^{-1}(\lambda)=M_n(\lambda) \tag{34b}$$

for $W_n(\lambda)$. Since the residues of the lhs at $\lambda=\alpha_j,\beta_k$ $(0\leqslant j,k\leqslant 2N)$ should vanish, one obtains the equations

$$u_{n+1j}v_{n+1j}L^{(0)}(\alpha_j)W_n^{-1}(\alpha_j)=0, \tag{35a}$$

$$W_{n+1}(\beta_k)L^{(0)}(\beta_k)\tilde{u}_{nk}\tilde{v}_{nk}=0, \tag{35b}$$

$$u_{nj}(\partial_t v_{nj}+v_{nj}M^{(0)}(\alpha_j))W_n^{-1}(\alpha_j)=0, \tag{35c}$$

$$W_n(\beta_k)(\partial_t\tilde{u}_{nk}-M^{(0)}(\beta_k)\tilde{u}_{nk})\tilde{v}_{nk}=0. \tag{35d}$$

A solution of Eqs. (35) is given by

$$v_{nj}(t)=v_{0j}L^{(0)}(-\alpha_j)^n\exp(-\mu(\alpha_j)\sigma_3 t), \tag{36a}$$

$$\tilde{u}_{nk}(t)=L^{(0)}(\beta_k)^n\exp(\mu(\beta_k)\sigma_3 t)\tilde{u}_{0k}, \tag{36b}$$

where v_{0j} and $\tilde{u}_{0k}$ $(j,k=1,\ldots,2N)$ are constant vectors and $\mu(\lambda)$ is the coefficient of σ_3 on the rhs of Eq. (16),

$$\mu(\lambda)=2i\sqrt{\frac{\kappa_1+J_3\kappa_0}{\kappa_0}}\frac{1}{1+(1/\rho^2)[(\kappa_1+J_1\kappa_0)/\kappa_0]\sin^2\lambda}. \tag{37}$$

Equation (19b) implies that

$$\sigma_2(u_{nj}v_{nj})^*\sigma_2=u_{nN+j}v_{nN+j},$$

$$\sigma_2(\tilde{u}_{nj}\tilde{v}_{nj})^*\sigma_2=\tilde{u}_{nN+j}\tilde{v}_{nN+j}.$$

These equations are satisfied if we choose the constant vectors v_{0j} and $\tilde{u}_{0j}$ $(j=N+1,\ldots,2N)$ as

$$v_{0N+j}=v_{0j}^*\sigma_2, \quad \tilde{u}_{0N+j}=\sigma_2\tilde{u}_{0j}^*.$$

We can thus determine the dressing matrix $W_n(\lambda)$ and its inverse matrix $W_n^{-1}(\lambda)$.

D. Spin variables

Evaluating the residues of both sides of Eq. (34a) at $\lambda=0$ gives

$$\sum_{l=1}^{3}S_{ln}\sigma_l=\sqrt{\kappa_0}W_{n+1}(0)\sigma_3W_n^{-1}(0), \tag{38}$$

which determines the spin variables (S_{1n},S_{2n},S_{3n}).

The auxiliary variable S_{0n} can be read off from the boundary values at $\lambda=\pm\infty$:

$$S_{0n}\mathbf{1}\pm S_{3n}\sigma_3=\frac{1}{\rho}W_{n+1}(\pm i\infty)L^{(0)}(\pm i\infty)W_n^{-1}(\pm i\infty).$$

E. Remarks

(1) We summarize the differences between the XXZ case and the isotropic case. The first difference is the number of the linear algebraic equations. We have encountered two different sets of linear algebraic equations—one for $X_n^{(1)}$ and the other for $X_n^{(2)}$. This is a new feature of the present setting. In the isotropic case, we have a single set of linear algebraic equations; this is consistent with the fact that both $X_n^{(1)}$ and $X_n^{(2)}$ tend to a matrix in the isotropic limit of the XXZ case. The second is the restriction of the positions of the poles, Eq. (24). In fact, this restriction is inherited from the corresponding property on zeros and poles of elliptic functions. In the isotropic limit, there is no such restriction because the spectral curve becomes rational.

(2) Equation (38) gives a $2N$-soliton solution in general. This solution is a nonlinear superposition of one-soliton solutions. In fact, one can find the one-soliton solutions associated with α_{j_0}

by setting $\tilde{u}^{(1)}_{nj_0}\tilde{u}^{(2)}_{nj_0}\neq 0$ and $\tilde{u}^{(1)}_{nk}\tilde{u}^{(2)}_{nk}=0$ $(k=1,\ldots,j_0-1,j_0+1,\ldots,N)$; one should set $v^{(1)}_{nj_0}v^{(2)}_{nj_0}\neq 0$ and $v^{(1)}_{nk}v^{(2)}_{nk}=0$ $(k=1,\ldots,j_0-1,j_0+1,\ldots,N)$ to obtain one-soliton solutions associated with β_{j_0}. In general, setting $\tilde{u}^{(1)}_{nj_0}\tilde{u}^{(2)}_{nj_0}=0$ annihilates the soliton associated with α_{j_0}, and setting $v^{(1)}_{nj_0}v^{(2)}_{nj_0}=0$ annihilates the soliton associated with β_{j_0}. Thus, one can obtain an M-soliton solution by setting an appropriate initial condition if $M\leqslant 2N$.

(3) It is easy to find an asymptotic form of the $2N$-soliton solution for N. Two one-soliton solutions associated with γ are obtained depending on either component $(l=1,2)$ of row (column) vector v_{nj_0} $(\tilde{u}_{nj_0})$ is set to be zero. The one for which the first component is set to be zero takes part in the asymptotic form as $t\to\pm\infty$ if $v_g(\gamma)\mathrm{Im}\,\gamma\gtrless 0$. The asymptotic form of the M-soliton solution as $|t|\to\infty$ is indeed a superposition of those one-soliton solutions associated with $\alpha_1,\ldots,\alpha_{2N}$ and $\beta_1,\ldots,\beta_{2N}$.

(4) Equation (19b) could be replaced by

$$W_n(\lambda)^{\dagger}=(W_n(\lambda^*))^{-1}. \tag{39}$$

For this construction to work, however, N has to be greater than one, and the distribution of poles of $W_n(\lambda)$ and $W_n^{-1}(\lambda)$ is required to obey the restrictions

$$\beta_j=\alpha_j^*, \quad \sum_{j=1}^{N}\alpha_j=\sum_{j=1}^{N}\beta_j. \tag{40}$$

IV. EASY-PLANE PARTIALLY ISOTROPIC CASE

In this section, we discuss the easy-plane partially isotropic case, i.e., $k_0=1$ $(J_1<J_2=J_3)$. We use the same notation as in Sec. III.

A. The first step

The L-matrix

$$L_n(\lambda)=S_{0n}\mathbf{1}+i\frac{\rho}{\sinh\lambda}(\cosh\lambda S_{1n}\sigma_1+S_{2n}\sigma_2+S_{3n}\sigma_3) \tag{41}$$

has the following symmetries:

$$\sigma_1 L_n(\lambda)\sigma_1=L_n(\lambda+i\pi), \tag{42a}$$

$$\sigma_2 L_n(\lambda)\sigma_2=(L_n(\lambda^*))^*, \tag{42b}$$

$$\lim_{x\to+\infty}\sigma_3 L_n(x+iy)\sigma_3=\lim_{x\to-\infty}L_n(x+iy). \tag{42c}$$

Under conditions similar to that in Sec. III A, the form of the dressing matrix $W_n(\lambda)$ is determined by the same discussion as in Appendix A:

$$W_n(\lambda)=d_{n0}\mathbf{1}+\sum_{j=1}^{2N}\left(\frac{d_{nj}\mathbf{1}+ia_{nj}\sigma_1}{\tanh(\lambda-\alpha_j)}+\frac{ib_{nj}\sigma_2+ic_{nj}\sigma_3}{\sinh(\lambda-\alpha_j)}\right), \tag{43}$$

$$W_n^{-1}(\lambda)=\tilde{d}_{n0}\mathbf{1}+\sum_{j=1}^{2N}\left(\frac{\tilde{d}_{nj}\mathbf{1}+i\tilde{a}_{nj}\sigma_1}{\tanh(\lambda-\beta_j)}+\frac{i\tilde{b}_{nj}\sigma_2+i\tilde{c}_{nj}\sigma_3}{\sinh(\lambda-\beta_j)}\right). \tag{44}$$

The restriction for the distribution of the poles and zeros is

$$\sum_{j=1}^{2N} \alpha_j = \sum_{j=1}^{2N} \beta_j \pmod{2\pi i}, \tag{45}$$

where $\alpha_{N+j}=\alpha_j^*$, and $\beta_{N+j}=\beta_j^*$ $(j=1,\ldots,N)$. In the following subsections, we construct a one-soliton solution by the same way as in Sec. III.

B. The second step

Because the residue of $W_n(\lambda)$ at $\lambda=\alpha_j$ is written by a column two-vector u_{nj} and a row two-vector v_{nj} as

$$\begin{pmatrix} d_{nj}+ic_{nj} & ia_{nj}+b_{nj} \\ ia_{nj}-b_{nj} & d_{nj}-ic_{nj} \end{pmatrix} = \begin{pmatrix} u_{nj}^{(1)}v_{nj}^{(1)} & u_{nj}^{(1)}v_{nj}^{(2)} \\ u_{nj}^{(2)}v_{nj}^{(1)} & u_{nj}^{(2)}v_{nj}^{(2)} \end{pmatrix},$$

the variables a_{nj}, b_{nj}, c_{nj}, and d_{nj} can be written in terms of the components of u_{nj} and v_{nj}:

$$d_{nj}=\tfrac{1}{2}(u_{nj}^{(1)}v_{nj}^{(1)}+u_{nj}^{(2)}v_{nj}^{(2)}), \tag{46a}$$

$$ia_{nj}=\tfrac{1}{2}(u_{nj}^{(1)}v_{nj}^{(2)}+u_{nj}^{(2)}v_{nj}^{(1)}), \tag{46b}$$

$$b_{nj}=\tfrac{1}{2}(u_{nj}^{(1)}v_{nj}^{(2)}-u_{nj}^{(2)}v_{nj}^{(1)}), \tag{46c}$$

$$ic_{nj}=\tfrac{1}{2}(u_{nj}^{(1)}v_{nj}^{(1)}-u_{nj}^{(2)}v_{nj}^{(2)}). \tag{46d}$$

The variables $\tilde{a}_{nj}$, $\tilde{b}_{nj}$, $\tilde{c}_{nj}$, and $\tilde{d}_{nj}$ have relations with $\tilde{u}_{nj}$ and $\tilde{v}_{nj}$ similar to Eqs. (46).

Since the residues of $W_n(\lambda)W_n^{-1}(\lambda)$ at $\alpha_1,\ldots,\alpha_{2N}$ and $\beta_1,\ldots,\beta_{2N}$ vanish, we have two algebraic relations:

$$v_{nj}W_n^{-1}(\alpha_j)=0,$$

$$W_n(\beta_k)\tilde{u}_{nk}=0.$$

These equations are rewritten as follows:

$$\tilde{d}_{n0}v_n^{(\pm)}-X_n^{(\pm)}\tilde{v}_n^{(\pm)}=0, \tag{47a}$$

$$d_{n0}\tilde{u}_n^{(\pm)}+u_n^{(\pm)}X_n^{(\pm)}=0, \tag{47b}$$

where $X_n^{(\pm)}$ are the $2N\times 2N$ matrices with the (j,k) elements

$$\{X_n^{(+)}\}_{jk}=\frac{v_{nj}^{(+)}\tilde{u}_{nk}^{(+)}}{\tanh(\beta_k-\alpha_j)}+\frac{v_{nj}^{(-)}\tilde{u}_{nk}^{(-)}}{\sinh(\beta_k-\alpha_j)}, \tag{48a}$$

$$\{X_n^{(-)}\}_{jk}=\frac{v_{nj}^{(+)}\tilde{u}_{nk}^{(+)}}{\sinh(\beta_k-\alpha_j)}+\frac{v_{nj}^{(-)}\tilde{u}_{nk}^{(-)}}{\tanh(\beta_k-\alpha_j)}. \tag{48b}$$

Here, we introduced $v_{nj}^{(\pm)}$ and $\tilde{u}_{nk}^{(\pm)}$ as

$$v_{nj}^{(\pm)}=\frac{1}{\sqrt{2}}(v_{nj}^{(1)}\pm v_{nj}^{(2)}), \quad \tilde{u}_{nj}^{(\pm)}=\frac{1}{\sqrt{2}}(\tilde{u}_{nj}^{(1)}\pm\tilde{u}_{nj}^{(2)}).$$

Note that Eqs. (47) have the same form as that of Eqs. (27).

One can solve the linear algebraic equations (47) by Cramer's rule. Therefore, the elements of $W_n(\lambda)$ are expressed in terms of $v_{nj}^{(\pm)}$, $\tilde{u}_{nj}^{(\pm)}$, α_j, and β_j $(j=1,\ldots,2N)$. The result is shown in Appendix C.

C. The last step

We now consider the (n,t) dependence of the vectors $v_{nj}^{(\pm)}$ and $\tilde{u}_{nj}^{(\pm)}$. The L- and M-matrices for the vacuum solution

$$\vec{S}_n=(0,0,\sqrt{\kappa_0})^{\mathrm{T}}$$

are

$$L^{(0)}(\lambda)=\sqrt{\kappa_1+J_3\kappa_0}\mathbf{1}+\frac{i\sqrt{\kappa_0}\rho}{\sinh\lambda}\sigma_3, \tag{49}$$

$$M^{(0)}(\lambda)=2i\sqrt{\frac{\kappa_1+J_3\kappa_0}{\kappa_0}}\frac{\cosh\lambda}{1+(1/\rho^2)[(\kappa_1+J_3\kappa_0)/\kappa_0]\sinh^2\lambda}\sigma_3. \tag{50}$$

The (n,t) dependence of the vectors $v_{nj}^{(\pm)}$ and $\tilde{u}_{nj}^{(\pm)}$ is determined by the linear system (35). A solution of the system is given by

$$v_{nj}=v_{0j}L^{(0)}(-\alpha_j)^n\exp(-\mu(\alpha_j)t\sigma_3), \tag{51}$$

$$\tilde{u}_{nk}=L^{(0)}(\beta_k)^n\exp(\mu(\beta_k)t\sigma_3)\tilde{u}_{0k}, \tag{52}$$

where $\mu(\lambda)$ is the coefficient of σ_3 on the rhs of Eq. (50). If we assume that $v_{0j}^{(1)}v_{0j}^{(2)}\neq 0$ and $\tilde{u}_{0j}^{(1)}\tilde{u}_{0j}^{(2)}\neq 0$, it follows from Eqs. (51) and (52) that

$$\frac{v_{nj}^{(+)}(t)}{v_{nj}^{(-)}(t)}=-\coth\left(\frac{1}{2}\xi(\alpha_j)n+\mu(\alpha_j)t+\delta_j\right), \tag{53}$$

$$\frac{\tilde{u}_{nj}^{(+)}(t)}{u_{nj}^{(-)}(t)}=-\coth\left(\frac{1}{2}\xi(\beta_j)n+\mu(\beta_j)t+\tilde{\delta}_j\right). \tag{54}$$

Here,

$$\delta_j=\frac{1}{2}\log\frac{v_{0j}^{(2)}}{v_{0j}^{(1)}},\quad \tilde{\delta}_j=\frac{1}{2}\log\frac{\tilde{u}_{0j}^{(1)}}{\tilde{u}_{0j}^{(2)}},$$

$$e^{\xi(\gamma)}=\frac{\sqrt{\kappa_1+\kappa_0J_3}+i\rho\sqrt{\kappa_0}/\sinh\gamma}{\sqrt{\kappa_1+\kappa_0J_3}-i\rho\sqrt{\kappa_0}/\sinh\gamma}.$$

One can see that the (n,t) dependence of $W_n(\lambda)$ is determined only by the ratios $v_{nj}^{(+)}/v_{nj}^{(-)}$ and $\tilde{u}_{nj}^{(+)}/\tilde{u}_{nj}^{(-)}$. Therefore, the multisoliton solution depends on n and t via the hyperbolic function $\coth(\frac{1}{2}\xi(\gamma)n+\mu(\gamma)l)$. Thus, the spin components do not oscillate in this case, as opposed to the easy-axis case where S_1 and S_2 oscillate. In other words, the soliton on the easy-plane spins has no carrier wave: The profiles of all spin components travel at the same velocity without changing their shape. On the other hand, the soliton on the easy-axis spins has a carrier wave and an envelope wave.

V. CONCLUSION

We constructed multisoliton solutions of the XXZ-LLL equation by a variant of the dressing method. Our method may be called a ''trigonometric dressing method,'' because the dressing matrix is a matrix valued trigonometric function of the spectral parameter λ. Remarkably, the dressing matrix has almost the same structure as the L-matrix. This is a natural consequence of the construction: The analytic properties of the L-matrix on the λ plane imply similar properties of the dressing matrix, which in turn determine the functional form of the dressing matrix uniquely. One can thus express the dressing matrix as a linear combination of trigonometric functions. The coefficients are then determined, just as in the ordinary dressing method, by a set of linear algebraic equations. We have, however, observed that these linear algebraic equations are slightly different from those of the ordinary dressing method based on a rational dressing matrix.

Let us also mention the issue of space–time discretization of the LL equation. A space–time discretized LL equation is proposed by Date *et al.*[14] They use the theory of τ-functions and free fermions. Nijhoff and Papageorgiou[15] presented another space–time discretization of the LL equation in the Lax formalism (along with a space–time discretized anisotropic principal chiral field model[16]). Since the latter two models have the same L-matrix as the lattice LL equation, our trigonometric dressing method and its ''elliptic'' version can be applied to these models as well. We discuss this issue in Ref. 17.

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APPENDIX A: THE FORM OF $W_n(\lambda)$

Let us express $W_n(\lambda)$ as a linear combination of the unit matrix $\mathbf{1}$ and the Pauli matrices σ_l $(l=1,2,3)$:

$$W_n(\lambda)=d_n(\lambda)\mathbf{1}+ia_n(\lambda)\sigma_1+ib_n(\lambda)\sigma_2+ic_n(\lambda)\sigma_3.$$

We first determine the functional form of $a_n(\lambda)$. Equation (19a) implies that $a_n(\lambda)$ is an antiperiodic function with period π. Because of the condition C-I in Sec. III A, $a_n(\lambda)$ has poles at $\lambda=\alpha_j+m\pi i$ $(m\in\mathbf{Z},\ \ j=1,\ldots,2N)$. Thus, $a_n(\lambda)$ acquires the form

$$a_n(\lambda)=\sum_{j=1}^{2N}\frac{a_{nj}}{\sin(\lambda-\alpha_j)}+f(\lambda),$$

where the a_{nj}'s are λ-independent numbers, and $f(\lambda)$ is an entire function of λ. We show that $f(\lambda)=0$. Because $f(\lambda)$ is an entire periodic function of λ, it is bounded on the simply connected domain $|\mathrm{Im}\,\lambda|\leqslant y_0$. On the other hand, owing to the condition C-II, f is uniformly bounded outside this domain. Thus, $f(\lambda)$ is a bounded entire function of λ, i.e., $f(\lambda)$ is a constant. Owing to the antiperiodicity, the constant equals zero. After all,

$$a_n(\lambda)=\sum_{j=1}^{2N}\frac{a_{nj}}{\sin(\lambda-\alpha_j)}.$$

The form of $d_n(\lambda)$ is determined in the same manner. Equation (19a) implies that $d_n(\lambda)$ is a periodic function with period π. Owing to the condition C-I, $d_n(\lambda)$ has poles at $\lambda=\alpha_j+m\pi i$ $(m\in\mathbf{Z},\ \ j=1,\ldots,2N)$. Thus, with an entire function of λ, one can write $d_n(\lambda)$ as follows:

$$d_n(\lambda)=\sum_{j=1}^{2N}\frac{d_{nj}}{\tan(\lambda-\alpha_j)}+(\text{entire function of }\lambda).$$

Because of the condition C-II, the entire function at the second term is bounded in the limit $\lambda \to \pm\infty$. Therefore the entire function equals a constant. Let d_{n0} be this constant. Then, we have obtained Eq. (21). The other two functions, $b_n(\lambda)$, $c_n(\lambda)$ can be determined also in the same way.

Because of Eq. (19c), the relation

$$d_{n0} - i\sum_{j=1}^{2N} d_{nj} = d_{n0} + i\sum_{j=1}^{2N} d_{jn}$$

holds, therefore we obtain Eq. (22).

APPENDIX B: DETERMINANT OF $W_n(\lambda)$

Since it follows from Eqs. (1), (2), (9), and (13) that

$$\det L_n(\lambda) = \det L^{(0)}(\lambda) = \kappa_1 + J_3\kappa_0 + \frac{\rho^2\kappa_0}{\tan^2\lambda}, \tag{B1}$$

$$\mathrm{tr}M_n(\lambda) = \mathrm{tr}M^{(0)}(\lambda) = 0, \tag{B2}$$

$\det W_n(\lambda)$ is a function of only λ.

Now, we calculate $\det W_n(\lambda)$ under the conditions in Sec. III A. Equation (19a) implies that $\det W_n(\lambda)$ is a periodic function with period π. Owing to the condition C-I, $\det W_n(\lambda)$ has simple poles at $\lambda = \alpha_j + m\pi i$ $(m \in \mathbf{Z},\ j = 1,\ldots,2N)$. With nonzero constants A_j $(j = 1,\ldots,2N)$, $\det W_n(\lambda)$ is written as

$$\det W_n(\lambda) = \sum_{j=1}^{2N} \frac{A_j}{\sin(\lambda - \alpha_j)} + (\text{entire function of } \lambda). \tag{B3}$$

Reduce Eq. (B3) to a common denominator and let β_j $(j = 1,\ldots,m)$ be the zeros on D of the numerator. Then

$$\det W_n(\lambda) = f(\lambda)\frac{\Pi_{j=1}^{m}\sin(\lambda - \beta_j)}{\Pi_{j=1}^{2N}\sin(\lambda - \alpha_j)},$$

where $f(\lambda)$ is an entire periodic function of λ without zeros. Then, $\beta_k \neq \alpha_j$ follows from the condition C-III. The integer m equals $2N$ because $\det W_n(iy)$ tends to a nonzero finite number in the limit $y \to +\infty$. As a consequence of Eq. (20), $f(\lambda)$ is identically equal to one, and the restriction Eq. (24) must be satisfied. At last, Eq. (23) is obtained. In the limit $\mathrm{Im}\,\lambda \to \pm\infty$, $\det W_n(\lambda)$ tends to one independently of $\mathrm{Re}\,\lambda$.

If Eq. (21) satisfies the conditions in Sec. III A and Eq. (24), then in the limit $\lambda \to \pm i\infty$,

$$W_n(\lambda) \to \left(d_{n0} \mp \sum_j d_{nj}\right)\mathbf{1} \pm \sum_j c_{nj}\sigma_3. \tag{B4}$$

Equations (B4), (19c), and (20) imply that

$$\left(d_{n0} \mp \sum_j d_{nj}\right)^2 - \left(\sum_j c_{nj}\right)^2 = 1,$$

which leads Eq. (22). With this result, one can conclude that soliton solutions can be constructed from the free parameters α_j's and β_j's if they satisfy Eq. (24).

APPENDIX C: THE ELEMENTS OF $W_n(\lambda)$ FOR THE EASY-PLANE CASE

Let $S_n^{(\pm)}$ and $T_n^{(\pm)}$ ($\tilde{S}_n^{(\pm)}$ and $\tilde{T}_n^{(\pm)}$) be column (row) $2N$-vectors with the jth component

$$\{S_n^{(\pm)}(\lambda)\}_j=\frac{v_{nj}^{(+)}}{\sinh(\lambda-\alpha_j)}\pm\frac{v_{nj}^{(-)}}{\tanh(\lambda-\alpha_j)}, \tag{C1}$$

$$\{T_n^{(\pm)}(\lambda)\}_j=\frac{v_{nj}^{(+)}}{\tanh(\lambda-\alpha_j)}\pm\frac{v_{nj}^{(-)}}{\sinh(\lambda-\alpha_j)}, \tag{C2}$$

$$\{\tilde{S}_n^{(\pm)}(\lambda)\}_j=\frac{\tilde{u}_{nj}^{(+)}}{\sinh(\lambda-\beta_j)}\pm\frac{\tilde{u}_{nj}^{(-)}}{\tanh(\lambda-\beta_j)}, \tag{C3}$$

$$\{\tilde{T}_n^{(\pm)}(\lambda)\}_j=\frac{\tilde{u}_{nj}^{(+)}}{\tanh(\lambda-\beta_j)}\pm\frac{\tilde{u}_{nj}^{(-)}}{\sinh(\lambda-\beta_j)}. \tag{C4}$$

(1) Matrix elements of $W_n(\lambda)$:

$$\{W_n(\lambda)\}_{11}=\frac{d_{n0}}{2|X_n^{(+)}|}\begin{vmatrix}1 & \tilde{u}_n^{(+)}\\ T_n^{(+)}(\lambda) & X_n^{(+)}\end{vmatrix}+\frac{d_{n0}}{2|X_n^{(-)}|}\begin{vmatrix}1 & \tilde{u}_n^{(-)}\\ S_n^{(+)}(\lambda) & X_n^{(-)}\end{vmatrix}, \tag{C5a}$$

$$\{W_n(\lambda)\}_{12}=\frac{d_{n0}}{2|X_n^{(+)}|}\begin{vmatrix}0 & \tilde{u}_n^{(+)}\\ T_n^{(-)}(\lambda) & X_n^{(+)}\end{vmatrix}+\frac{d_{n0}}{2|X_n^{(-)}|}\begin{vmatrix}0 & \tilde{u}_n^{(-)}\\ S_n^{(-)}(\lambda) & X_n^{(-)}\end{vmatrix}, \tag{C5b}$$

$$\{W_n(\lambda)\}_{21}=\frac{d_{n0}}{2|X_n^{(+)}|}\begin{vmatrix}0 & \tilde{u}_n^{(+)}\\ T_n^{(+)}(\lambda) & X_n^{(+)}\end{vmatrix}-\frac{d_{n0}}{2|X_n^{(-)}|}\begin{vmatrix}0 & \tilde{u}_n^{(-)}\\ S_n^{(+)}(\lambda) & X_n^{(-)}\end{vmatrix}, \tag{C5c}$$

$$\{W_n(\lambda)\}_{22}=\frac{d_{n0}}{2|X_n^{(+)}|}\begin{vmatrix}1 & \tilde{u}_n^{(+)}\\ T_n^{(-)}(\lambda) & X_n^{(+)}\end{vmatrix}-\frac{d_{n0}}{2|X_n^{(-)}|}\begin{vmatrix}-1 & \tilde{u}_n^{(-)}\\ S_n^{(-)}(\lambda) & X_n^{(-)}\end{vmatrix}. \tag{C5d}$$

(2) Matrix elements of $W_n^{-1}(\lambda)$:

$$\{W_n^{-1}(\lambda)\}_{11}=\frac{-\tilde{d}_{n0}}{2|X_n^{(+)}|}\begin{vmatrix}-1 & \tilde{T}_n^{(+)}(\lambda)\\ v_n^{(+)} & X_n^{(+)}\end{vmatrix}-\frac{\tilde{d}_{n0}}{2|X_n^{(-)}|}\begin{vmatrix}-1 & \tilde{S}_n^{(+)}(\lambda)\\ v_n^{(-)} & X_n^{(-)}\end{vmatrix}, \tag{C6a}$$

$$\{W_n^{-1}(\lambda)\}_{12}=\frac{-\tilde{d}_{n0}}{2|X_n^{(+)}|}\begin{vmatrix}0 & \tilde{T}_n^{(+)}(\lambda)\\ v_n^{(+)} & X_n^{(+)}\end{vmatrix}+\frac{\tilde{d}_{n0}}{2|X_n^{(-)}|}\begin{vmatrix}0 & \tilde{S}_n^{(+)}(\lambda)\\ v_n^{(-)} & X_n^{(-)}\end{vmatrix}, \tag{C6b}$$

$$\{W_n^{-1}(\lambda)\}_{21}=\frac{-\tilde{d}_{n0}}{2|X_n^{(+)}|}\begin{vmatrix}0 & \tilde{T}_n^{(-)}(\lambda)\\ v_n^{(+)} & X_n^{(+)}\end{vmatrix}-\frac{\tilde{d}_{n0}}{2|X_n^{(-)}|}\begin{vmatrix}0 & \tilde{S}_n^{(-)}(\lambda)\\ v_n^{(-)} & X_n^{(-)}\end{vmatrix}, \tag{C6c}$$

$$\{W_n^{-1}(\lambda)\}_{22}=\frac{-\tilde{d}_{n0}}{2|X_n^{(+)}|}\begin{vmatrix}-1 & \tilde{T}_n^{(-)}(\lambda)\\ v_n^{(+)} & X_n^{(+)}\end{vmatrix}+\frac{\tilde{d}_{n0}}{2|X_n^{(-)}|}\begin{vmatrix}1 & \tilde{S}_n^{(-)}(\lambda)\\ v_n^{(-)} & X_n^{(-)}\end{vmatrix}. \tag{C6d}$$

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Families of particular solutions to multidimensional partial differential equations

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Dressing methods are known as productive tools for construction of the particular solutions to the big class of nonlinear partial differential equations (PDEs) which are integrable by the inverse scattering technique. Recently the modification of the dressing method based on the system of algebraic equations has been suggested which allows us to find the families of particular solutions to certain types of nonintegrable (in classical sense) nonlinear PDEs. This modification represents PDEs as closure reductions of an appropriate differential-difference system. In this article we study the dressing procedure in more detail. Particularly, we consider different families of particular solutions available through the dressing method based on the algebraic system. We give two examples of the differential-difference systems and related PDEs and point to other possible generalizations of the dressing method. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1398337]

I. INTRODUCTION

Dressing method has been developed as a special technique for solving the nonlinear integrable partial differential equations (PDEs).[1–4] Many modifications of the dressing method have been found.[5–8] An important field of application of the dressing methods is the investigation of the $(n+1)$-dimensional $(n>2)$ integrable systems.[8–12]

Recently[13] the algebraic system of $N^{(c)}$ equations

$$L(\psi_m)\equiv\psi_m-\sum_{i=1}^{N^{(c)}}\psi_i\sum_{n=1}^{N^{(r)}}c_{in}R_{nm}=\eta_m,\quad m=1,...,N^{(c)}\ \text{or}$$
$$L(\psi)\equiv\psi-\psi\mathbf{CR}=\eta,\quad \psi=[\psi_1\cdots\psi_{N^{(c)}}],\quad \eta=[\eta_1\cdots\eta_{N^{(c)}}] \tag{1}$$

had been suggested as an auxiliary equation for construction of the particular solutions to the PDE of a certain types. In Eq. (1) we use constant $N^{(c)}\times N^{(r)}$ ($N^{(c)}\neq N^{(r)}$ in general) matrix $\mathbf{C}=\{c_{in}\}$ to provide the possibility to use rectangular (not only square) $N^{(r)}\times N^{(c)}$ matrix $\mathbf{R}=\{R_{nm}\}$. Although the algebraic system can be taken as a starting point for the following discussion, it is important to emphasize its relation with the classical dressing method. For simplicity we refer to the $\overline{\partial}$-problem,[5,6] since the above system of algebraic equations can be considered as the discrete version of this problem. In fact, the $\overline{\partial}$-problem represents the relation between solutions of the nonlinear PDE and solutions of the following linear integral equation:[14]

$$\psi(\lambda)-\int\psi(\nu)c(\nu,\mu)R(\mu,\lambda)d\mu\wedge d\overline{\mu}d\nu\wedge d\overline{\nu}=\eta(\lambda), \tag{2}$$

where R is a kernel of the integral operator and η is a normalization function. Parameters ν, μ, λ are complex. The additional parameters $\mathbf{x}=(x_1,\ldots,x_M)$ are introduced in the kernel R by the formulas

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$$\partial_i R(\mu,\lambda)=\sum_{k=1}^{N_i} f_k^{(i)}(\mu)g_k^{(i)}(\lambda), \quad i=1,...,M, \tag{3}$$

which are compatible provided

$$\partial_i \sum_{k=1}^{N_j} f_k^{(j)}(\mu)g_k^{(j)}(\lambda)=\partial_j \sum_{k=1}^{N_i} f_k^{(i)}(\mu)g_k^{(i)}(\lambda), \quad i,j=1,...,M. \tag{4}$$

The link to the particular system of nonlinear PDEs is produced by the special structure of the functions $f_k^{(j)}(\mu)$ and $g_k^{(j)}(\lambda)$. Parameters $\mathbf{x}$ are independent variables of this system.[5,6] Since the conditions (4) should be satisfied for all admitted values of the parameters μ and λ, there is no functional relations between functions $f_k^{(j)}(\mu)$ and $g_k^{(j)}(\lambda)$. This conclusion makes restrictions on the admitted form of the functions $f_k^{(j)}(\mu)$ and $g_k^{(j)}(\lambda)$. For this reason integral equation (2) is related only with completely integrable systems of nonlinear PDEs.

The situation becomes different if one considers the solution of Eq. (2) on the set of discrete points $\nu_i, \mu_n, \lambda_m\ (i,m=1,...,N^{(c)}, n=1,...,N^{(r)})$ on the complex planes of parameters ν, μ, λ and introduces matrices $\mathbf{C}$ and $\mathbf{R}$ with the entries

$$c_{in}\equiv c(\nu_i,\mu_n), \quad R_{nm}\equiv R(\mu_n,\lambda_m).$$

Then one gets the algebraic system (1) with the following discrete version of the equations (3) and (4)

$$\begin{gathered}\partial_i R_{nm}=\sum_{k=1}^{N_i} f_{nk}^{(i)}g_{km}^{(i)}, \quad n=1,...,N^{(r)}, \quad m=1,...,N^{(c)}, \quad i=1,...,M, \text{ or}\\ \partial_i \mathbf{R}=\sum_{k=1}^{N_i} \mathbf{f}^{(ik)}\mathbf{g}^{(ki)}, \quad \mathbf{f}^{(ik)}=[f_{1k}^{(i)}\cdots f_{N^{(r)}k}^{(i)}]^T, \quad \mathbf{g}^{(ki)}=[g_{k1}^{(i)}\cdots g_{kN^{(c)}}^{(i)}],\end{gathered} \tag{5}$$

$$\begin{gathered}\partial_i \sum_{k=1}^{N_j} f_{nk}^{(j)}g_{km}^{(j)}=\partial_j \sum_{k=1}^{N_i} f_{nk}^{(i)}g_{km}^{(i)}, \quad i,j=1,...,M, \text{ or}\\ \partial_i \sum_{k=1}^{N_j} \mathbf{f}^{(jk)}\mathbf{g}^{(kj)}=\partial_j \sum_{k=1}^{N_i} \mathbf{f}^{(ik)}\mathbf{g}^{(ki)}\end{gathered} \tag{6}$$

where

$$f_{nk}^{(j)}=f_k^{(j)}(\mu_n), \quad g_{km}^{(j)}=g_k^{(j)}(\lambda_m).$$

It turned out that the discrete version has a set of properties which makes it very adaptable in applications to different systems of nonlinear PDEs. The basic reason for this is the absence of complex continuous parameters in the equations (6), which become bilinear differential equations on the functions $f_{nk}^{(j)}$ and $g_{km}^{(j)}$ which are functions of parameters $\mathbf{x}$ only. In general the associated systems of nonlinear PDEs are not integrable, but integrable systems are situated among them.

One can recognize that the equations (1) and (2) can be combined into the following one:

$$\psi_m(\lambda)-\int d\mu\wedge d\bar{\mu}d\nu\wedge d\bar{\nu}\sum_{k=1}^{N^{(c)}} \psi_k(\nu)\sum_{n=1}^{N^{(r)}} c_{kn}(\nu,\mu)R_{nm}(\mu,\lambda;\mathbf{x})=\eta_m(\lambda), \quad m=1,...,N^{(c)}, \tag{7}$$

with

$$\partial_i R_{nm}(\mu,\lambda)=\sum_{k=1}^{N_i} f_{nk}^{(i)}(\mu)g_{km}^{(i)}(\lambda). \tag{8}$$

Equation (7) will not be discussed in this article.

For our purpose we require the following properties of the matrix $\mathbf{R}$:[13]

(1) The nonhomogeneous equation (1) has the unique solution, $\psi=[\psi_1\cdots\psi_{N^{(c)}}]$.
(2) The $\mathbf{x}$ dependence [$\mathbf{x}=(x_1,\ldots,x_M)$, M is dimension of $\mathbf{x}$-space] is introduced by the formulas (5).
(3) The equations (5) are compatible, i.e., the set of conditions (6) is held which is the system of PDEs imposed on the functions $f_{nk}^{(i)}$ and $g_{km}^{(i)}$.
(4) The set of self-consistent constraints is imposed on the functions $\mathbf{g}^{(ki)}$ in the form of the system of PDEs

$$\sum_{ik}\hat{L}_{ikm}^{(g)}\mathbf{g}^{(ki)}=0,\quad m=1,\ldots,P \tag{9}$$

(where $\hat{L}_{ikm}^{(g)}$ are scalar linear differential operators and $\mathbf{g}^{(ki)}$ is $1\times N^{(c)}$ row). These constraints should be consistent with the compatibility conditions (6). We will use operators $\hat{L}_{ikm}^{(g)}$ with constant coefficients for simplicity.

The consequence of the first requirement is the fact that homogeneous algebraic system with the same matrix $\mathbf{R}$ has only the trivial solution, i.e.,

$$L(\phi)=0\Leftrightarrow\phi\equiv 0. \tag{10}$$

Equations (1) and (5) produce the following system of algebraic equations (with the same matrix $\mathbf{R}$ and different right-hand sides) for the functions $\partial_j\psi$, $\partial_j^n\psi$ and $\Pi_{s=1}^M\partial_s^{n_s}\psi$:

$$L(\partial_j\psi)=\sum_{k=1}^{N_j} U_{\underbrace{0,\ldots,0}_{M}}^{(jk)}\mathbf{g}^{(jk)}+\partial_j\eta, \tag{11}$$

$$L(\partial_j^n\psi)=h_j,\quad h_j=\partial_j h_{j-1}+\sum_{k=1}^{N_j}\sum_{p=0}^{n}(-1)^p C_n^p\partial_j^{n-p}U_{\underbrace{0,\ldots,}_{j-1}\,p,\ldots,0}^{(jk)}\mathbf{g}^{(jk)}, \tag{12}$$

$$C_n^p=\frac{p!}{n!(n-p)!},$$

$$L\left(\prod_{s=1}^{M}\partial_s^{n_s}\psi\right)=h_{n_1\ldots n_M}, \tag{13}$$

$$h_{n_1\ldots n_M}=\partial_m h_{n_1\ldots(n_m-1)\ldots n_M}+\sum_{k=1}^{N_j}\left(\sum_{p_1=0}^{n_1}\cdots\sum_{p_m=0}^{n_m-1}\cdots\sum_{p_M=0}^{n_M}(-1)^{\Sigma_{i=1}^M p_i}\right.$$

$$\left.\times\left(\prod_{s=1,s\neq m}^{M}C_{n_s}^{p_s}\partial_s^{n_s-p_s}\right)C_{n_m-1}^{p_m}\partial_m^{n_m-p_m-1}U_{p_1,\ldots,p_M}^{(jk)}\mathbf{g}^{(jk)}\right),$$

where

$$U_{n_1\ldots n_M}^{(ik)}=\sum_{n=1}^{N^{(c)}}\psi_n\sum_{m=1}^{N^{(r)}}\left(\prod_{s=1}^{M}\partial_s^{n_s}\right)c_{nm}f_{mk}^{(i)}\equiv\psi\mathbf{C}\left(\prod_{s=1}^{M}\partial_s^{n_s}\right)\mathbf{f}^{(ik)},$$

$$i=1,\ldots,M,\quad k=1,\ldots,N_i. \tag{14}$$

Using these algebraic systems together with the original system (1) and applying the superposition principle for linear nonhomogeneous algebraic systems, one can provide $M^{(L)}$ differential operators $\hat{M}_j$ such that $L(\hat{M}_j\psi)=0$ or in accordance with Eq. (10)

$$\hat{M}_j\psi=0, \quad j=1,...,M^{(L)}, \quad M^{(L)}\geqslant 1. \tag{15}$$

One considers Eqs. (15) as the system of linear PDEs on the function ψ. In addition we require the independence of the operators $\hat{M}_k$, i.e., there is no nonzero set of differential operators $\hat{D}_j$, $j=1,...,M^{(L)}$, such that $\Sigma_{j=1}^{M^{(L)}}\hat{D}_j\hat{M}_j=0$.

The functions $U^{(ik)}_{n_1,...,n_M}$ defined by Eq. (14) are solutions of the appropriate system of differential-difference equations, which can be derived from the linear system (15) (where each equation is $1\times N^{(c)}$ row) by multiplying it by the $N^{(c)}\times 1$ vector

$$\mathbf{v}^{ik}_{n1...n_M}\equiv\mathbf{C}\left(\prod_{s=1}^{M}\partial_s^{n_s}\right)\mathbf{f}^{(ik)}. \tag{16}$$

Let $\mathbf{U}$ be the set of all matrices (14). Then the nonlinear system is the system of scalar equations of the general form

$$\hat{M}_j\psi\mathbf{v}^{ik}_{n1,...,n_M}\equiv\tilde{M}^{ikj}_{n_1,...,n_M}(\mathbf{U})=0, \quad j=1,...,M^{(L)}, \quad i=1,...,M, \quad k=1,...,N_i\,. \tag{17}$$

By construction the total number of discrete parameters equals the number of continuous parameters M in the system (17).

The system (17) represents the general system of differential-difference equations, which is related with the algebraic system (1). The system (17) is the system of pure PDEs if there are numbers $M^{(ikjs)}\geqslant 0$ $(s=1,...,M)$ such that the (sub)set of the equations (17) with subscripts

$$(n_1,\ldots,n_M)\leqslant(M^{(ikj1)},\ldots,M^{(ikjM)}), \quad j=1,...,M^{(L)}, \quad i=1,...,M, \quad k=1,...,N_i$$

(each entry on the left-hand side does not exceed the correspondent entry on the right-hand side) represents the complete system of PDEs.

Otherwise, the system of pure PDEs can be derived from the system (17) by imposing the reductions which introduce the relation among different discrete parameters n_j and reduce their number from M to $\tilde{M}<M$ in such a way that the (sub)system of the system (17) forms the complete system of pure nonlinear PDEs, i.e., the numbers $M^{(ikjs)}\geqslant 0$ $(s=1,...,\tilde{M})$ should exist such that the (sub)set of the equations (17) with subscripts

$$(n_1,\ldots,n_{\tilde{M}})\leqslant(M^{(ikj1)},\ldots,M^{(ikj\tilde{M})})$$

forms the complete system of pure PDEs. To clarify the general form of these reductions, note that each discrete parameter n_j is associated with the derivative $\partial_j\mathbf{f}^{(ik)}$. It means that one needs to impose the relations among the *derivatives* of the functions $\mathbf{f}^{(ik)}$. Then one gets the relations among the functions $U^{(ik)}_{n_1...n_M}$ with fixed superscripts (ik) and different subscripts $(n_1,\ldots,n_M)$ and, consequently, the relations among the discrete parameters. It means that the reductions of our interest have the general form

$$\sum_{in}\tilde{L}^{(f)}_{ikm}\mathbf{f}^{(ik)}=0, \quad m=1,...,P, \tag{18}$$

where $\hat{L}^{(f)}_{ikm}$ are the scalar linear differential operators (with constant coefficients for simplicity). Both systems (9) and (18) should be self-consistent and compatible with the system (6). It is

important to emphasize that the reductions which have the form of *algebraic* relations among different functions $\mathbf{f}^{(ik)}$ do not reduce the number of discrete parameters in the system.

The significant difference between integrable PDEs and ones considered in this article is that the integrable nonlinear systems have operator representation as the compatibility condition of the appropriate overdetermined linear system of equations with variable coefficients (zero curvature representation). The nonlinear PDEs under consideration are related with the systems of linear equations (15) as well, but correspondent operator representation for them has not been found yet.

In the next section (Sec. II) we develop the general approach for construction of the particular solutions for the systems of nonlinear PDEs, associated with the algebraic system (1). In Sec. III we consider the examples of the nonintegrable generalizations of the modified Kadomtsev–Petviashvili equation (mKP) with several families of particular solutions (some of them are given in Ref. 13). In Sec. IV we apply new dressing method to find the possible relations among different integrable hierarchies, for instance, between two different mKP hierarchies. Some generalizations of the dressing method based on the algebraic systems are discussed in Sec. V. We will mention about the algebraic system (1) with non-unit right-hand side, which serves, for example, the generalizations of the Kadomtsev–Petviashvili equation (KP) (see the Appendix). Conclusions are given in Sec. VI.

II. FAMILIES OF PARTICULAR SOLUTIONS

Next we discuss the available families of particular solutions to the nonlinear PDE related with the algebraic system (1). The main problem in construction of particular solutions is to satisfy the compatibility condition (6) together with constrains (9) and (18) for all pairs of variables $(x_i,x_j)\subset\mathbf{x}$. In general, for M-dimensional space one has to satisfy $(M-1)M/2$ conditions each represented by $N^{(r)}\times N^{(c)}$ equations. But under assumption that all products of the functions $f^{(i)}_{nk}g^{(i)}_{km}$ in (5) depend on complete set of variables, $\mathbf{x}$, the number of independent conditions becomes equal to $M-1$, i.e., the system (6) can be replaced, for instance, with the following one:

$$\partial_1\sum_{k=1}^{N_j}\mathbf{f}^{(jk)}\mathbf{g}^{(kj)}=\partial_j\sum_{k=1}^{N_1}\mathbf{f}^{(1k)}\mathbf{g}^{(k1)},\quad j=2,...,M. \tag{19}$$

We consider only such matrices $\mathbf{R}$ which give rise to the solution $\psi=[\psi_1,\dots,\psi_{N^{(c)}}]$ of the algebraic system (1) composed of linearly independent functions $\psi_m, m=1,...,N^{(c)}$:

$$\begin{aligned}&\text{functions } \psi_m\ (m=1,...,N^{(c)}) \text{ in the solution } \psi\\ &\quad=[\psi_1,\dots,\psi_{N^{(c)}}] \text{ of the system (1) are linearly independent.}\end{aligned} \tag{20}$$

The basic factor which defines the variety of the solutions is the allowed dimensions $N^{(r)}$ and $N^{(c)}$ of the matrix $\mathbf{R}$ in the algebraic system (1). Although the form of nonlinear PDEs does not depend on them, the admitted values of these dimensions are related essentially with the particular situation and are defined by both the equations (6) and the relations (9) and (18). In general, different families of particular solutions can be characterized by the four numbers, $N^{(r)}_{\min}$, $N^{(r)}_{\max}$, $N^{(c)}_{\min}$, $N^{(c)}_{\max}$, which represent the minimum and maximum possible values for the parameters $N^{(r)}$ and $N^{(c)}$, respectively, so that $N^{(r)}_{\min}\leqslant N^{(r)}\leqslant N^{(r)}_{\max}$ and $N^{(c)}_{\min}\leqslant N^{(c)}\leqslant N^{(c)}_{\max}$. For our convenience we combine all functions $\mathbf{f}^{(ik)}$ and $\mathbf{g}^{(ki)}$ related with each family in the manifolds $\mathbf{F}^i_{N^{(r)}_{\min}N^{(r)}_{\max}}$ and $\mathbf{G}^i_{N^{(c)}_{\min}N^{(c)}_{\max}}$, respectively. Note that condition (20) requires that parameters $N^{(r)}_{\min}$, $N^{(r)}_{\max}$, $N^{(c)}_{\min}$, $N^{(c)}_{\max}$ do not depend on i, $i=1,...,M-1$. We collect these two sets of manifolds in two general manifolds $\mathbf{F}=\cup_i\mathbf{F}^i_{N^{(r)}_{\min}N^{(r)}_{\max}}$ and $\mathbf{G}=\cup_i\mathbf{G}^i_{N^{(c)}_{\min}N^{(c)}_{\max}}$. Functions from these manifolds we call f- and g-functions, respectively.

We consider three steps of the investigation of the particular solutions, which can be applied to any nonlinear PDE, generated by the algebraic system (1). More detailed investigation can be

specifically performed for each particular system. Subscripts n and m run the values from 1 to $N^{(r)}$ and from 1 to $N^{(c)}$, respectively, in all formulas below, unless otherwise specified.

Step 1. *(Criterion for application of the dressing method.)* First of all, one needs to check if the compatibility conditions (19) can be satisfied at least for $N^{(r)}=N^{(c)}=1$. If this is possible, then the related system of nonlinear PDEs can be treated by the dressing method and one has at least a family of particular solutions for which f- and g-functions are collected in the manifolds $\mathbf{F}^i_{1,1}$ and $\mathbf{G}^i_{1,1}$.

After that we have to study the possibility to satisfy Eqs. (19) with $N^{(r)}>1$ and/or $N^{(c)}>1$. In general the system (19) is nonlinear and it is difficult to solve it. But one can separate the families of particular solutions for this system which can be received by ''splitting'' the equations (19) into the set of linear differential (or algebraic) equations on the f- and g-functions (or their Fourier amplitudes). We assume that all f- and g-functions depend on the whole set of variables $\mathbf{x}$. Due to the reductions (9) and (18) the equations (19) may involve the partial derivatives of f- and g-functions with respect to different sets of variables $\mathbf{x}_1$ and $\mathbf{x}_2$, respectively $(\mathbf{x}_1,\mathbf{x}_2\subseteq\mathbf{x})$. *Step 2* regards the situation when at least one of the sets $\mathbf{x}_1$ or $\mathbf{x}_2$ coincides with $\mathbf{x}$.

Step 2. Let us impose the set of reductions (9) and (18), assume that $\mathbf{x}_1\equiv\mathbf{x}$ (the case $\mathbf{x}_2\equiv\mathbf{x}$ can be considered in the analogous way, see Sec. III). Then the system (19) can be represented as the sum of the products:

$$\sum_{k=1}^{P_i} F^i_{nk}G^i_{km}=0,\quad i=1,...,M-1,$$

$$F^i_{nk}=F^i_k(f^{(j)}_{np},\quad j=1,...,M,\quad p=1,...,N_j), \tag{21}$$

$$G^i_{km}=G^i_k(g^{(j)}_{pm},\quad j=1,...,M,\quad p=1,...,N_j)$$

where we denote F^i_{nk} and G^i_{km} the linear combination of the functions $f^{(j)}_{np}$ and $g^{(j)}_{pm}$ $(j=1,...,M, p=1,...,N_j)$, respectively, and their derivatives in ith equation of the system (19). Let us put $N^{(r)}_{\min}=1$. To find $N^{(c)}_{\min}$ and $N^{(c)}_{\max}$, let us fix $n=1$ in the system (21):

$$\sum_{k=1}^{P_i} F^i_{1k}G^i_{km}=0,\quad i=1,...,M-1,\quad m=1,...,N^{(c)}, \tag{22}$$

and consider the last system as a system of equations on the functions $F^{(i)}_{1k}$.

Let us introduce several definitions. We call the set of functions $\{F^i_{nk},\ i$ is fixed, $k=1,...,G^{(g)}_i\}$ independent if for any permitted value of parameter n there is an appropriate set of functions $\tilde f_n\subset\{f^{(i)}_{nk}, i=1,...,M, k=1,...,N_i\}$ with the same length such that one can establish the uniquely invertible map $\{F^i_{nk}\}\leftrightarrow\tilde f_n$. Analogously, we call the set of functions $\{G^i_{km},\ i$ is fixed, $k=1,...,D^{(f)}_i\}$ linearly independent, if for any admitted value of parameter m there is an appropriate set of functions $\tilde g_m\subset\{g^{(i)}_{km}, i=1,...,M, k=1,...,N_i\}$ with the same length such that one can establish the uniquely invertible map $\{G^i_{km}\}\leftrightarrow\tilde g_m$. Let $D^{(g)}_i$ be the minimum number of independent functions F^i_k for each fixed i and $D^{(g)}=\min(D^{(g)}_i)$. One can always reenumerate functions F^i_k in such a way that functions F^i_k are independent for $k=1,...,D^{(g)}_i$. We impose two requirements:

(1) $D^{(g)}\geqslant M-1$, otherwise the succeeding consideration in the scopes of *Step 2* leads to the nonlinear equations on g-functions.
(2) All functions F^i_k with $k=1,...,D^{(g)}$ and $i=1,...,M-1$ are independent, i.e., one has $(M-1)D^{(g)}$ independent functions altogether.

Then for any number $\tilde D^{(g)}\leqslant D^{(g)}$ the system (22) with $m=1,...,\tilde D^{(g)}$ is the linear system on the functions F^i_k (or on f-functions), which can be resolved provided an appropriate choice of the arbitrary g-functions is made. In this way we have fixed $N^{(c)}_{\min}=N^{(c)}_{\max}=\tilde D^{(g)}$ in the system (21). Let

us denote $\tilde{D}_i^{(f)}$ the number of independent solutions of the equations (22) with $\tilde{D}^{(f)}=\min(\tilde{D}_i^{(f)})$. Then $N_{\min}^{(r)}=1$ and $N_{\max}^{(r)}=\tilde{D}^{(f)}$. So, *f*- and *g*-functions are combined in the manifolds $\mathbf{F}^i_{1\tilde{D}^{(f)}}$ and $\mathbf{G}^i_{\tilde{D}^{(g)}\tilde{D}^{(g)}}$ ($\tilde{D}^{(g)}=1,...,D^{(g)}$ and $\tilde{D}^{(f)}$ depends on $\tilde{D}^{(g)}$). The matrix $\mathbf{R}$ in the algebraic system (1) is represented by its elements $R_{nm}=\partial_i^{-1}\Sigma_{k=1}^{N_i} f_{nk}^{(i)} g_{km}^{(i)}$ with some fixed i and $\mathbf{f}^{(ik)}\in\mathbf{F}^i_{1\tilde{D}^{(f)}}, \mathbf{g}^{(ik)}\in\mathbf{G}^i_{\tilde{D}^{(g)}\tilde{D}^{(g)}}$. We emphasize that all *g*-functions are arbitrary functions of the set of variables $\mathbf{x}$ in the above formulas.

In the previous consideration we separated the part of the system (22) with $m\leqslant\tilde{D}^{(g)}$. Now let us consider the part of the system (22) with $m>\tilde{D}^{(g)}$. If we are able to provide $\tilde{N}$ equations in this system, which are compatible with the first part of the system and appropriate functions $g_{km}^{(i)}$ are linearly independent with functions $g_{km}^{(i)}$, $m\leqslant\tilde{D}^{(g)}$, then the parameter $N_{\max}^{(c)}$ will become equal to $\tilde{D}^{(g)}+\tilde{N}$. In fact, let us consider the subsystem of the system (22) with $m=1,...,\tilde{D}^{(g)}$ as an algebraic system, resolvable for the functions F_k^i ($i=1,...,M-1$, $k=1,...,P_i$). Let n run values from 1 to $\tilde{D}^{*(f)}\leqslant\tilde{D}^{(f)}$. Substitute the solution of this subsystem into the equations of the system (21) with $m>\tilde{D}^{(g)}$ and consider the resultant system as the set of identities for all $n=1,...,\tilde{D}^{*(f)}$. It leads to either the linear or nonlinear equations on *g*-functions. If $\tilde{N}$ is the number of solutions of this system linearly independent with *g*-functions fixed before, then $N_{\max}^{(c)}=\tilde{D}^{(g)}+\tilde{N}$. So, *g*-functions belong to the manifolds $\mathbf{G}^i_{\tilde{D}^{(g)}(\tilde{D}^{(g)}+\tilde{N})}$, with $\tilde{D}^{(g)}=1,...,D^{(g)}$, where $\tilde{N}$ depends on $\tilde{D}^{*(f)}$. *f*-functions belong to the manifolds $\mathbf{F}^i_{1\tilde{D}^{*(f)}}$.

Even if one of the sets $\mathbf{x}_1$ or $\mathbf{x}_2$ coincides with $\mathbf{x}$, it is not necessary that the system (19) be treated by the *Step 2*. It happens, for instance, if $D^{(g)}<M-1$. The solutions provided by the next step are available always if only the *criterion* is satisfied.

Step 3. Since the constrains (9) and (18) are given by the linear differential equations with constant coefficients, one can represent *f*- and *g*-functions in terms of Fourier integrals

$$f_{nk}^{(i)}=\int a_{nk}^{(i)}(\mathbf{k}_n)e^{\mathbf{k}_n\mathbf{x}_1+\tilde{\mathbf{k}}_n\tilde{\mathbf{x}}_1}\,d\mathbf{k}_n, \tag{23}$$

$$g_{km}^{(i)}=\int b_{km}^{(i)}(\omega_m)e^{\omega_m\mathbf{x}_2+\tilde{\omega}_m\tilde{\mathbf{x}}_2}\,d\omega_m, \tag{24}$$

$$\mathbf{k}_n=(k_{n1},\ldots,k_{n\,\dim(\mathbf{x}_1)}),\quad \tilde{\mathbf{k}}_n=(k_{n\,\dim(\mathbf{x}_1)+1},\ldots,k_{nM}), \tag{25}$$

$$\omega_m=(\omega_{m1},\ldots,\omega_{m\,\dim(\mathbf{x}_2)}),\quad \tilde{\omega}_m=(\omega_{m\,\dim(\mathbf{x}_2)+1},\ldots,\omega_{mM}),$$

$$d\omega_m=d\omega_{m1}\ldots d\omega_{m\,\dim(\mathbf{x}_2)},\quad d\mathbf{k}_n=dk_{n1}\ldots dk_{n\,\dim(\mathbf{x}_1)},$$

$$\mathbf{x}_i\cap\tilde{\mathbf{x}}_i=\varnothing,\quad \mathbf{x}_i\cup\tilde{\mathbf{x}}_i=\mathbf{x},$$

where $\tilde{\mathbf{k}}_n(\mathbf{k}_n)$ and $\tilde{\omega}_n(\omega_n)$ represent the dispersion relation for the linear differential equations (9) and (18). In order to satisfy the compatibility conditions (21) in the nonintegrable case, one needs to provide the possibility to establish the relations between spectral parameters $\mathbf{k}_n$ and ω_n. For this purpose one needs to replace at least one of the equations (23) or (24) by the finite Fourier series. Namely, the two following representations for *f*- and *g*-functions can be used (for the sake of simplicity we take the single Fourier harmonic instead of the finite series):

$$f_{nk}^{(i)}=a_{nk}^{(i)}e^{\mathbf{k}_n\mathbf{x}_1+\tilde{\mathbf{k}}_n\tilde{\mathbf{x}}_1},\quad g_{km}^{(i)}=\int b_{km}^{(i)}(\omega_m)e^{\omega_m\mathbf{x}_2+\tilde{\omega}_m\tilde{\mathbf{x}}_2}d\omega_m \tag{26}$$

and

$$f_{nk}^{(i)}=\int a_{nk}^{(i)}(\mathbf{k}_n)e^{\mathbf{k}_n\mathbf{x}_1+\tilde{\mathbf{k}}_n\tilde{\mathbf{x}}_1}\,d\mathbf{k}_n,\quad g_{km}^{(i)}=b_{km}^{(i)}e^{\omega_m\mathbf{x}_2+\tilde{\omega}_m\tilde{\mathbf{x}}_2}. \tag{27}$$

The examination of each of these representations is equivalent, so that we study only the first one.

The compatibility conditions (21) become the system of algebraic equations on the parameters $a_{nk}^{(i)}$, $k_{nj}, b_{km}^{(i)}$, w_{mj}:

$$\sum_{k=1}^{P_i} F_k^i(\mathbf{a}_n,\mathbf{k}_n)G_k^i(\mathbf{b}_m,\omega_m)=0,\quad i=1,...,M-1, \tag{28}$$

$$\mathbf{a}_n=(a_{nk}^{(i)},\quad i=1,...,M,\quad k=1,...,N_i), \tag{29}$$

$$\mathbf{b}_n=(b_{kn}^{(i)},\quad i=1,...,M,\quad k=1,...,N_i), \tag{30}$$

with $\mathbf{k}_n\neq\mathbf{k}_m$ and $\omega_n\neq\omega_m$ if $n\neq m$ in order to satisfy the requirement (20). This system admits following families of solutions:

(1) Let us keep independent continuous parameters ω_{mk} with different k $[k=1,...,\dim(\mathbf{x}_2)]$ and m in the representation (26). Assume $N_{\min}^{(r)}=N_{\min}^{(c)}=1$ and find out the appropriate values for $N_{\max}^{(r)}$ and $N_{\max}^{(c)}$. First of all let us fix $n=1$ in the above system, so that it can be written in the form

$$\sum_{k=1}^{P_i} F_k^i(\mathbf{a}_1,\mathbf{k}_1)G_k^i(\mathbf{b}_m,\omega_m)=0,\quad i=1,...,M-1. \tag{31}$$

Since parameters ω_{mk} are independent, the above equations represent the relations among parameters $b_{km}^{(i)}$. So, one has $M-1$ relations among these parameters for each particular value of the parameter m. This means that if the system (31) is consistent for some fixed m, then it is consistent for any m, i.e., $N_{\max}^{(c)}=\infty$ and the g-functions belong to the manifold $\mathbf{G}_{1\infty}^{(i)}$. Otherwise the system (31) is inconsistent. Assuming the consistence of the system (31), let us define $N_{\max}^{(r)}$. Suppose that $N_{\max}^{(r)}>1$ and consider two equations (28) with $n=1$ and $n=p\leqslant N^{(r)}$. Subtract one equation from another to get

$$\sum_{k=1}^{P_i} (F_k^i(\mathbf{a}_1,\mathbf{k}_1)-F_k^i(\mathbf{a}_p,\mathbf{k}_p))G_k^i(\mathbf{b}_m,\omega_m)=0,\quad i=1,...,M-1. \tag{32}$$

Since this equation should be satisfied for all admitted values of the parameter m, one gets the set of algebraic equations on parameters $\mathbf{a}_p^{(i)}$ and $\mathbf{k}_p$:

$$(F_k^i(\mathbf{a}_1,\mathbf{k}_1)-F_k^i(\mathbf{a}_p,\mathbf{k}_p))=0,\quad k=1,...,P_i,\quad i=1,...,M-1. \tag{33}$$

If set $(\mathbf{a}_p,\mathbf{k}_p), p=1,...,\tilde{n}+1$, represents solutions of this system with different spectral parameters (i.e., $\mathbf{k}_n\neq\mathbf{k}_p$ if $n\neq p$ for $n,p=1,...,\tilde{n}+1$), then $N_{\max}^{(r)}=\tilde{n}+1$ and f-functions belong to the manifolds $\mathbf{F}_{1(\tilde{n}+1)}^{(i)}$.

We assumed that parameters ω_{mk} with different k are independent in the formulas (31)–(33), which is not always possible [see Sec. III A, Eqs. (70)–(72)]. The following family of solutions is not based on this assumption.

(2) For this family of solutions we impose the additional relations among parameters ω_{mk} with different k. These relations can be established in the following way. Let us consider the system (31). For each particular m we select $\tilde{M}\leqslant M-1$ equations of these systems to impose the relations among $\tilde{m}_b$ parameters $b_{km}^{(i)}$ and $\tilde{m}\leqslant\dim(\mathbf{x}_2)$ parameters $\omega_{mk}(\tilde{m}_b+\tilde{m}=\tilde{M})$, i.e., split the complete system (31) into two subsystems,

$$\sum_{k=1}^{P_i} F_k^i(\mathbf{a}_1,\mathbf{k}_1)G_k^i(\mathbf{b}_m,\omega_m)=0, \quad i=1,...,\tilde{M}, \tag{34}$$

$$\sum_{k=1}^{P_i} F_k^i(\mathbf{a}_1,\mathbf{k}_1)G_k^i(\mathbf{b}_m,\omega_m)=0, \quad i=\tilde{M}+1,...,M-1, \tag{35}$$

and consider the first system as an algebraic system of equations for $\tilde{m}_b$ parameters $b_{km}^{(i)}$ and $\tilde{m}$ parameters ω_{mj}. This means that $N_{\min}^{(c)}=1$. If $\tilde{m}<\dim(\mathbf{x}_2)$ and the system (34) is resolvable for some particular m, then it is resolvable for arbitrary m with $(\dim(\mathbf{x}_2)-\tilde{m})$ arbitrary parameters ω_{mk} for each particular m, i.e., $N_{\max}^{(c)}$ is infinity, g-functions belong to the manifolds $\mathbf{G}_{1\infty}^{(i)}$, and the integral in (26) becomes $(\dim(\mathbf{x}_2)-\tilde{m})$-dimensional. If $\tilde{m}=\dim(\mathbf{x}_2)$, then there are no arbitrary parameters ω_{mk}, integration disappears from the Eq. (26), and the maximum dimension $N_{\max}^{(c)}$ is defined by the number m_0 of the solutions of the system (32) with different spectral parameters ω_m: $\omega_m\neq\omega_p$ if $m\neq p$ for all $m,p=1,...,m_0$. Consequently g-functions belong to the manifold $\mathbf{G}_{1m_0}^{(i)}$. Now we have to satisfy the system (35). First of all one needs to substitute the established relations among parameters $\mathbf{b}_m^{(i)}$ and ω_m into the system (35) to end up with the system of the form

$$\sum_{k=1}^{\tilde{P}_i} \tilde{F}_k^i(\mathbf{a}_1,\mathbf{k}_1)\tilde{G}_k^i(\mathbf{b}_m,\omega_m)=0, \quad i=\tilde{M}+1,...,M-1. \tag{36}$$

Considering this system as a set of identities for all admitted m one gets the following system of equations for parameters $\mathbf{a}_1$ and $\mathbf{k}_1$:

$$\tilde{F}_k^i(\mathbf{a}_1,\mathbf{k}_1)=0, \quad k=1,...,\tilde{P}_i, \quad i=\tilde{M}+1,...,M-1.$$

If this system is consistent, then the imposed relations among $b_{km}^{(j)}$ and ω_{mi} are allowed at least for $N_{\min}^{(r)}=1$.

To find $N_{\max}^{(r)}$ one has to assume that $N_{\max}^{(r)}>1$ in (28), substitute all found relations among parameters into the equations of the system (28) with $1<n\leqslant N_{\max}^{(r)}$, and consider them as identities for all m. One gets the system of algebraic equations on the parameters $\mathbf{a}_n$ and $\mathbf{k}_n$. The number of its solutions $\tilde{n}$ with different $\mathbf{k}_n$ ($\mathbf{k}_n\neq\mathbf{k}_p$ if $n\neq p$, $n,p=1,...\tilde{n}+1$) defines the maximum dimension $N_{\max}^{(r)}$: $N_{\max}^{(r)}=\tilde{n}+1$. So, f-functions belong to the manifolds $\mathbf{F}_{1,\tilde{n}+1}^{(i)}$.

(3) To establish the relations among parameters $b_{km}^{(i)}$ and ω_{mk} one can take the subsystem of n_0 equations out of the system (28) with $n=1,...,n_0$. The algorithm is exactly the same. One can establish $\tilde{M}$ relations among $\tilde{m}_b$ parameters $b_{km}^{(i)}$ and $\tilde{m}\leqslant\dim(\mathbf{x}_2)$ parameters ω_{mk} for each particular m ($\tilde{m}_b+\tilde{m}=\tilde{M}$). If the remaining $n_0(M-1)-\tilde{M}$ equations are compatible, one gets the relations among parameters $\mathbf{a}_{nk}^{(i)}$ and $\mathbf{k}_{nk}$ ($n=1,...,n_0$), which mean that $N_{\min}^{(r)}=n_0$. To find $N_{\max}^{(r)}$ one needs to assume that $N_{\max}^{(r)}>n_0$, substitute all found relations into the equation (28) with $n_0<n\leqslant N_{\max}^{(r)}$, consider them as identities for all m, and solve the appropriate system of algebraic equations on the parameters $\mathbf{a}_{nk}^{(i)}$ and $\mathbf{k}_{nk}$. If the set $(\mathbf{a}_p,\mathbf{k}_p)$, $p=1,...,\tilde{n}+n_0$, represents solutions of this system with different spectral parameters $\mathbf{k}_p$ (i.e., $\mathbf{k}_n\neq\mathbf{k}_p$ if $n\neq p$ and $n,p=1,...,\tilde{n}+n_0$), then $N_{\max}^{(r)}=\tilde{n}+n_0$ and f-functions are in the manifolds $\mathbf{F}_{n_0,\tilde{n}+n_0}^{(i)}$. g-functions belong to the manifolds $\mathbf{G}_{1\infty}^{(i)}$ or $\mathbf{G}_{1m_0}^{(i)}$ if $\tilde{m}=\dim(\mathbf{x}_2)$. In the last case m_0 is the number of solutions $(\mathbf{b}_m,\omega_m)$ to the system (28) ($n=1,...,n_0$, $i=1,...,\tilde{M}$) with different ω_m.

III. (3+1)-DIMENSIONAL GENERALIZATION OF mKP

In this section we use the algorithm described above to derive the $(3+1)$-dimensional nonintegrable generalization of mKP. We use $(3+1)$-dimensional equations to show how this algorithm works in multidimension, where the classical integrability theory is applicable only to special types of PDEs. There is no formal restriction on the dimension of PDEs, which can be

treated by the method considered in this article. One can construct $(2+1)$-dimensional nonintegrable generalizations of mKP which will involve different types of nonlinearity. Although the general nonlinear equations [see Eqs. (47) and (48)] are rather cumbersome, they admit a set of reductions which reduce the general system into the simpler equations like Eqs. (61)–(63),[13] which may be regarded as the simplest generalizations of mKP (64).

To start with, let us take $M=4$ (Ref. 13) and normalization $\eta_m=1$, $m=1,...,N^{(c)}$, in the system (1). Introduce $\mathbf{x}$-dependence by the set of equations (5)

$$\partial_1\mathbf{R}=\mathbf{f}^{(11)}\mathbf{g}^{(1)},\quad \partial_2\mathbf{R}=\mathbf{f}^{(21)}\mathbf{g}^{(2)},\quad \partial_3\mathbf{R}=\mathbf{f}^{(31)}\mathbf{g}^{(1)}+\mathbf{f}^{(32)}\partial_1\mathbf{g}^{(1)},$$

$$\partial_4\mathbf{R}=\mathbf{f}^{(41)}\mathbf{g}^{(2)}+\mathbf{f}^{(42)}\partial_2\mathbf{g}^{(2)}+\mathbf{f}^{(43)}\partial_2^2\mathbf{g}^{(2)}, \tag{37}$$

$$\mathbf{g}^{(i)}=[g_1^{(i)}\cdots g_{N^{(c)}}^{(i)}],\quad \mathbf{f}^{(ik)}=[f_{1k}^{(i)}\cdots f_{N^{(r)}k}^{(i)}]^T.$$

To construct the auxiliary linear system, let us write down the set of linear algebraic systems (11)–(13), which is generated by the original system (1) and Eqs. (37):

$$L(\partial_1\psi)=U_{0,0,0,0}^{(11)}\mathbf{g}^{(1)}, \tag{38}$$

$$L(\partial_1^2\psi)=(2\partial_1U_{0,0,0,0}^{(11)}-U_{1,0,0,0}^{(11)})\mathbf{g}^{(1)}+U_{0,0,0,0}^{(11)}\partial_1\mathbf{g}^{(1)}, \tag{39}$$

$$L(\partial_2\psi)=U_{0,0,0,0}^{(21)}\mathbf{g}^{(2)}, \tag{40}$$

$$L(\partial_2^2\psi)=(2\partial_2U_{0,0,0,0}^{(21)}-U_{0,1,0,0}^{(21)})\mathbf{g}^{(2)}+U_{0,0,0,0}^{(21)}\partial_2\mathbf{g}^{(2)}, \tag{41}$$

$$\begin{aligned}L(\partial_2^3\psi)=&(3\partial_2^2U_{0,0,0,0}^{(21)}-3\partial_2U_{0,1,0,0}^{(21)}+U_{0,2,0,0}^{(21)})\mathbf{g}^{(2)}\\&+(3\partial_2U_{0,0,0,0}^{(21)}-U_{0,1,0,0}^{(21)})\partial_2\mathbf{g}^{(2)}+U_{0,0,0,0}^{(21)}\partial_2^2\mathbf{g}^{(2)},\end{aligned} \tag{42}$$

$$L(\partial_3\psi)=U_{0,0,0,0}^{(31)}\mathbf{g}^{(1)}+U_{0,0,0,0}^{(32)}\partial_1\mathbf{g}^{(1)}, \tag{43}$$

$$L(\partial_4\psi)=U_{0,0,0,0}^{(41)}\mathbf{g}^{(2)}+U_{0,0,0,0}^{(42)}\partial_2\mathbf{g}^{(2)}+U_{0,0,0,0}^{(43)}\partial_2^2\mathbf{g}^{(2)}, \tag{44}$$

$$U_{n_1,n_2,n_3,n_4}^{(ik)}=\sum_{m=1}^{N^{(r)}}\psi_m\sum_{n=1}^{N^{(c)}}c_{mn}\partial_1^{n_1}\partial_2^{n_2}\partial_3^{n_3}\partial_4^{n_4}f_{nk}^{(i)}\equiv\psi\mathbf{C}\partial_1^{n_1}\partial_2^{n_2}\partial_3^{n_3}\partial_4^{n_4}\mathbf{f}^{(ik)}, \tag{45}$$

$$\psi=[\psi_1\ldots\psi_{N^{(c)}}].$$

Then the linear system (15) has the form

$$\begin{aligned}M_1\psi\equiv\partial_3\psi+V_1\partial_1^2\psi+V_2\partial_1\psi=0,\\M_2\psi\equiv\partial_4\psi+W_1\partial_2^3\psi+W_2\partial_2^2\psi+W_3\partial_2\psi=0\end{aligned} \tag{46}$$

with

$$V_1=-U_{0,0,0,0}^{(32)}/U_{0,0,0,0}^{(11)},\quad V_2=(-U_{0,0,0,0}^{(31)}-V_1(2\partial_1U_{0,0,0,0}^{(11)}-U_{1,0,0,0}^{(11)}))/U_{0,0,0,0}^{(11)},$$

$$W_1=-U_{0,0,0,0}^{(43)}/U_{0,0,0,0}^{(21)},\quad W_2=(-U_{0,0,0,0}^{(42)}-W_1(3\partial_2U_{0,0,0,0}^{(21)}-U_{0,1,0,0}^{(21)}))/U_{0,0,0,0}^{(21)},$$

$$W_3=(-U_{0,0,0,0}^{(41)}-W_1(3\partial_2^2U_{0,0,0,0}^{(21)}-3\partial_2U_{0,1,0,0}^{(21)}+U_{0,2,0,0}^{(21)})-W_2(2\partial_2U_{0,0,0,0}^{(21)}-U_{0,1,0,0}^{(21)}))/U_{0,0,0,0}^{(21)}.$$

In fact, one can check directly that $L(M_i\psi)=0$, $i=1,2$. Note that each of the equations (46) is a matrix $1\times N^{(c)}$ equation with scalar coefficients V_i and W_i. To get a nonlinear system let us

multiply them by the $N^{(c)}\times 1$ vector functions $\mathbf{C}\partial_1^{n_1}\partial_2^{n_2}\partial_3^{n_3}\partial_4^{n_4}\mathbf{f}^{(ij)}$ and use the definition of potentials $U^{(ik)}_{n1,n2,n3,n4}$ given by (45). One result is the following differential-difference system with four continuous and four discrete parameters:

$$\partial_3 U^{(ij)}_{n_1,n_2,n_3,n_4}-U^{(ij)}_{n_1,n_2,n_3+1,n_4}+V_1(\partial_1^2 U^{(ij)}_{n_1,n_2,n_3,n_4}-2\partial_1 U^{(ij)}_{n_1+1,n_2,n_3,n_4}+U^{(ij)}_{n_1+2,n_2,n_3,n_4})$$
$$+V_2(\partial_1 U^{(ij)}_{n_1,n_2,n_3,n_4}-U^{(ij)}_{n_1+1,n_2,n_3,n_4})=0, \tag{47}$$

$$\partial_4 U^{(ij)}_{n_1,n_2,n_3,n_4}-U^{(ij)}_{n_1,n_2,n_3,n_4+1}+W_1(\partial_2^3 U^{(ij)}_{n_1,n_2,n_3,n_4}-3\partial_2^2 U^{(ij)}_{n_1,n_2+1,n_3,n_4}+3\partial_2 U^{(ij)}_{n_1,n_2+2,n_3,n_4}$$
$$-U^{(ij)}_{n_1,n_2+3,n_3,n_4})+W_2(\partial_2^2 U^{(ij)}_{n_1,n_2,n_3,n_4}-2\partial_2 U^{(ij)}_{n_1,n_2+1,n_3,n_4}+U^{(ij)}_{n_1,n_2+2,n_3,n_4})$$
$$+W_3(\partial_2 U^{(ij)}_{n_1,n_2,n_3,n_4}-U^{(ij)}_{n_1,n_2+1,n_3,n_4})=0, \tag{48}$$

$$(ij)=(11),\ (21),\ (31),\ (32),\ (4p),\quad p=1,2,3.$$

This differential-difference system of equations is a general system generated by the algebraic system (1) with unit right-hand side and **x**-parameters introduced by the formulas (37).

Now let us impose reductions of the form (18) on the functions $f^{(j)}_{nk}$ to decrease the number of discrete parameters and reduce the system (47) and (48) to the complete system of pure PDEs. Below we consider the set of such reductions which eventually leads to mKP (64).

Reduction 1. Introduce the following relations among the functions $\mathbf{f}^{(ij)}$:

$$\partial_2\mathbf{f}^{(ij)}=\partial_1\mathbf{f}^{(ij)},\quad \partial_3\mathbf{f}^{(ij)}=-\partial_1^2\mathbf{f}^{(ij)},\quad \partial_4\mathbf{f}^{(ij)}=\partial_1^3\mathbf{f}^{(ij)}. \tag{49}$$

Appropriate relations among the functions $U^{(ij)}_{n_1,n_2,n_3,n_4}$ read

$$U^{(ij)}_{n_1,n_2,n_3,n_4}=(-1)^{n_3}U^{(ij)}_{n_1+n_2+2n_3+3n_4,0,0,0}\equiv(-1)^{n_3}U^{(ij)}_{n_1+n_2+2n_3+3n_4}. \tag{50}$$

Under this reduction the system (47) and (48) becomes of the form

$$\partial_3 U^{(ij)}_n+U^{(ij)}_{n+2}+V_1(\partial_1^2 U^{(ij)}_n-2\partial_1 U^{(ij)}_{n+1}+U^{(ij)}_{n+2})+V_2(\partial_1 U^{(ij)}_n-U^{(ij)}_{n+1})=0, \tag{51}$$

$$\partial_4 U^{(ij)}_n-U^{(ij)}_{n+3}+W_1(\partial_2^3 U^{(ij)}_n-3\partial_2^2 U^{(ij)}_{n+1}+3\partial_2 U^{(ij)}_{n+2}-U^{(ij)}_{n+3})+W_2(\partial_2^2 U^{(ij)}_n-2\partial_2 U^{(ij)}_{n+1}+U^{(ij)}_{n+2})$$
$$+W_3(\partial_2 U^{(ij)}_n-U^{(ij)}_{n+1})=0, \tag{52}$$

$$(ij)=(11),\ (21),\ (31),\ (32),\ (4p),\quad p=1,2,3,$$

where

$$V_1=-U^{(32)}_0/U^{(11)}_0,\quad V_2=(-U^{(31)}_0-V_1(2\partial_1 U^{(11)}_0-U^{(11)}_1))/U^{(11)}_0,$$

$$W_1=-U^{(43)}_0/U^{(21)}_0,\quad W_2=(-U^{(42)}_0-W_1(3\partial_2 U^{(21)}_0-U^{(21)}_1))/U^{(21)}_0,$$

$$W_3=(-U^{(41)}_0-W_1(3\partial_2^2 U^{(21)}_0-3\partial_2 U^{(21)}_1+U^{(21)}_2)-W_2(2\partial_2 U^{(21)}_0-U^{(21)}_1))/U^{(21)}_0.$$

The complete system of nonlinear PDEs is represented by the system (51) and (52) where index n runs the values 0, 1, 2 in Eq. (51) and 0, 1 in Eq. (52).

Reduction 2. Impose another reduction:

$$\mathbf{f}^{(11)}\equiv\mathbf{f}^{(1)},\quad \mathbf{f}^{(21)}\equiv\mathbf{f}^{(2)},\quad \mathbf{f}^{(31)}=-\partial_1\mathbf{f}^{(32)}\equiv-\partial_1\mathbf{f}^{(3)},$$
$$\mathbf{f}^{(41)}=\partial_1^2\mathbf{f}^{(43)}\equiv\partial_1^2\mathbf{f}^{(4)},\quad \mathbf{f}^{(42)}=-\partial_1\mathbf{f}^{(43)}\equiv-\partial_1\mathbf{f}^{(4)}, \tag{53}$$

or

$$U_n^{(11)} \equiv U_n^{(1)}, \quad U_n^{(21)} \equiv U_n^{(2)}, \quad U_n^{(31)} = -U_{n+1}^{(32)} \equiv -U_{n+1}^{(3)},$$
$$U_n^{(41)} = U_{n+2}^{(43)} \equiv U_{n+2}^{4}, \quad U_n^{(42)} = -U_{n+1}^{(43)} \equiv -U_{n+1}^{(4)}, \tag{54}$$

which reduces the system (51) and (52) into the following one:

$$\partial_3 U_n^{(i)} + U_{n+2}^{(j)} + V_1(\partial_1^2 U_n^{(i)} - 2\partial_1 U_{n+1}^{(i)} + U_{n+2}^{(i)}) + V_2(\partial_1 U_n^{(i)} - U_{n+1}^{(i)}) = 0, \tag{55}$$

$$\partial_4 U_n^{(i)} - U_{n+3}^{(i)} + W_1(\partial_2^3 U_n^{(i)} - 3\partial_2^2 U_{n+1}^{(i)} + 3\partial_2 U_{n+2}^{(i)} - U_{n+3}^{(i)}) + W_2(\partial_2^2 U_n^{(i)} - 2\partial_2 U_{n+1}^{(i)} + U_{n+2}^{(i)})$$
$$+ W_3(\partial_2 U_n^{(i)} - U_{n+1}^{(i)}) = 0, \quad i = 1,2,3,4, \tag{56}$$

where

$$V_1 = -U_0^{(3)}/U_0^{(1)}, \quad V_2 = (U_1^{(3)} - V_1(2\partial_1 U_0^{(1)} - U_1^{(1)}))/U_0^{(1)},$$
$$W_1 = -U_0^{(4)}/U_0^{(2)}, \quad W_2 = (U_1^{(4)} - W_1(3\partial_2 U_0^{(2)} - U_1^{(2)}))/U_0^{(2)},$$
$$W_3 = (-U_2^{(4)} - W_1(3\partial_2^2 U_0^{(2)} - 3\partial_2 U_1^{(2)} + U_2^{(2)}) - W_2(2\partial_2 U_0^{(2)} - U_1^{(2)}))/U_0^{(2)}.$$

The system (55) and (56) represents the complete system of nonlinear PDEs if index n runs the values 0, 1, 2 in Eq. (55) and 0, 1 in Eq. (56).

Reduction 3. Assume now

$$\mathbf{f}^{(3)} = \mathbf{f}^{(1)}, \quad \mathbf{f}^{(4)} = \mathbf{f}^{(2)}, \quad \text{or} \quad U_n^{(3)} = U_n^{(1)}, \quad U_n^{(4)} = U_n^{(2)}. \tag{57}$$

The system (55) and (56) becomes of the form

$$\partial_3 U_n^{(i)} - \partial_1^2 U_n^{(i)} + 2\partial_1 U_{n+1}^{(i)} + V_2(\partial_1 U_n^{(i)} - U_{n+1}^{(i)}) = 0, \tag{58}$$

$$\partial_4 U_n^{(i)} - \partial_2^3 U_n^{(i)} + 3\partial_2^2 U_{n+1}^{(i)} - 3\partial_2 U_{n+2}^{(i)} + W_2(\partial_2^2 U_n^{(i)} - 2\partial_2 U_{n+1}^{(i)} + U_{n+2}^{(i)}) + W_3(\partial_2 U_n^{(i)} - U_{n+1}^{(i)})$$
$$= 0, \quad i = 1,2, \tag{59}$$

where

$$V_2 = 2\partial_1 U_0^{(1)}/U_0^{(1)}, \quad W_2 = 3\partial_1 U_0^{(2)}/U_0^{(2)},$$
$$W_3 = (3\partial_2^2 U_0^{(2)} - 3\partial_2 U_1^{(2)} - W_2(2\partial_2 U_0^{(2)} - U_1^{(2)}))/U_0^{(2)}.$$

This system represents the complete system of PDEs if $n = 0,1$ in Eq. (58) and $n = 0$ in Eq. (59).

Reduction 4. The next possible reduction is

$$\mathbf{f}^{(1)} = \mathbf{f}^{(2)} = \mathbf{f} \quad \text{or} \quad U_n^{(1)} = U_n^{(2)} = U_n. \tag{60}$$

Then the system (58) and (59) becomes of the form

$$\partial_3 U_n - \partial_1^2 U_n + 2\partial_1 U_{n+1} + V_2(\partial_1 U_n - U_{n+1}) = 0, \tag{61}$$

$$\partial_4 U_n - \partial_2^3 U_n + 3\partial_2^2 U_{n+1} - 3\partial_2 U_{n+2} + W_2(\partial_2^2 U_n - 2\partial_2 U_{n+1} + U_{n+2}) + W_3(\partial_2 U_n - U_{n+1}) = 0, \tag{62}$$

where

$$V_2=2\partial_1 U_0/U_0,\quad W_2=3\partial_2 U_0/U_0,\quad W_3=(3\partial_2^2 U_0-3\partial_2 U_1-W_2(2\partial_2 U_0-U_1))/U_0.$$

This system[13] represents the complete system of PDEs if $n=0,1$ in Eq. (61) and $n=0$ in Eq. (62). It can be rewritten as

$$\begin{gathered}u_{x_3}-u_{x_1x_1}+2v_{x_1}+u_{x_1}^2=0,\quad v_{x_3}-v_{x_1x_1}+2w_{x_1}-2vv_{x_1}=0,\\ u_{x_4}-u_{x_2x_2x_2}+3v_{x_2x_2}-3w_{x_2}+3u_{x_2}u_{x_2x_2}-u_{x_2}^3-3u_{x_2}v_{x_2}+3vv_{x_2}=0,\end{gathered}\tag{63}$$

where $U_0=\exp u$, $U_1=vU_0$, and $U_2=wU_0$.

Reduction 5. Finally,[13] the reduction $\partial_2\equiv\partial_1$ reduces the $(3+1)$-dimensional system (63) into mKP:

$$\partial_4 v-1/4\ \partial_1^3 v+3/2\ v^2\partial_1 v+3/2\ \partial_1 v\,\partial_1^{-1}\partial_3 v-3/4\ \partial_1^{-1}\partial_3^2 v=0,\quad v=\partial_1 U_0/U_0.\tag{64}$$

In this way we have demonstrated that the general system (47) and (48) can be regarded as the differential-difference generalization of mKP with four continuous and four discrete parameters.

A. Construction of particular solutions

As we mentioned earlier, the main problem in construction of the particular solutions is the compatibility conditions (6) or (19). We start with the solutions to the general differential-difference system (47) and (48). The condition (19) is represented by the system of three equations:

$$\partial_2 f_m^{(1)}g_m^{(1)}+f_{n1}^{(1)}\partial_2 g_m^{(1)}-\partial_1 f_{n1}^{(2)}g_m^{(2)}-f_{n1}^{(2)}\partial_1 g_m^{(2)}=0,\tag{65}$$

$$(\partial_3 f_{n1}^{(1)}-\partial_1 f_{n1}^{(3)})g_m^{(1)}-(f_{n1}^{(3)}+\partial_1 f_{n2}^{(3)})\partial_1 g_m^{(1)}+f_{n1}^{(1)}\partial_3 g_m^{(1)}-f_{n2}^{(3)}\partial_1^2 g_m^{(1)}=0,\tag{66}$$

$$(\partial_4 f_{n1}^{(2)}-\partial_2 f_{n1}^{(4)})g_m^{(2)}-(f_{n1}^{(4)}+\partial_2 f_{n2}^{(4)})\partial_2 g_m^{(2)}-(f_{n2}^{(4)}+\partial_2 f_{n3}^{(4)})\partial_2^2 g_m^{(2)}+f_{n1}^{(2)}\partial_4 g_m^{(2)}-f_{n3}^{(4)}\partial_2^3 g_m^{(2)}=0,\tag{67}$$

so that one has $\mathbf{x}_1=\mathbf{x}_2=(x_1,x_2,x_3,x_4)$. This system can be considered as the linear system on the functions $f_{nk}^{(j)}$. It is not difficult to understand that this system is resolvable for $N^{(r)}=N^{(c)}=1$ (or $n=m=1$, *step* 1), when it can be treated as the system on the functions $f_{11}^{(j)}$, $j=2,3,4$. All other functions can be taken as arbitrary ones. It means that the whole nonlinear system (47) and (48) can be treated by the dressing method.

Let us fix $N_{\max}^{(c)}=1$ and show that the appropriate $N_{\max}^{(r)}=\infty$. In fact, for each particular n one can solve the system (65)–(67) for the functions $f_{n1}^{(j)}$, $j=2,3,4$. It means that f- and g-functions belong to the manifolds $\mathbf{F}_{1\infty}^{(i)}$ and $\mathbf{G}_{11}^{(i)}$ with arbitrary functions $g_1^{(i)}$ $(i=1,2)$, $f_{n1}^{(1)}$, $f_{n2}^{(j)}$ $(j=3,4)$, $f_{n3}^{(j)}$ $(j=4)$, $n=1,2,\ldots$.

Similarly, the system (65)–(67) is consistent for $N^{(c)}=2$ (*step 2*). In fact, in this case $g_m^{(j)}$ $(m=1,2)$ can be taken as arbitrary functions of $\mathbf{x}$. Then for each particular value of the parameter n the whole system is the linear system of six PDEs for seven functions $f_{nk}^{(j)}$, $(jk)=(1,1),(2,1),(3,1),(3,2),(4,1),(4,2),(4,3)$. One of these functions (say $f_{n1}^{(4)}$) can be arbitrary. So, each of the equations (65)–(67) is a PDE whose solution depends on the arbitrary functions $g_m^{(j)}$ $(m=1,2)$ and $f_{n1}^{(4)}$. This means that $N_{\max}^{(r)}=\infty$. From this we conclude that g-functions form manifolds $\mathbf{G}_{22}^{(i)}$, while f-functions form manifolds $\mathbf{F}_{1\infty}^{(i)}$.

The analysis of the case $N^{(c)}=3$ leads to the *nonlinear* four-dimensional PDE on f- and g-functions.

Let us consider the set of particular solutions in more detail, related with one of the representations (26) or (27) of the f- and g-functions (*step 3*). We take the representation (26), which reads in our case

$$f_{nm}^{(i)}=a_{nm}^{(i)}e^{-k_nx_1-k_nx_2-k_n^2x_3-k_n^3x_4}, \tag{68}$$

$$g_m^{(i)}=\int b_m^{(i)}(\omega_{m1},\omega_{m2},\omega_{m3},\omega_{m4})e^{\omega_{m1}x_1+\omega_{m2}x_2+\omega_{m3}x_3+\omega_{m4}x_4}\,d\omega_{m1}d\omega_{m2}d\omega_{m3}d\omega_{m4}. \tag{69}$$

This representation reduces the system (65)–(67) into the system of algebraic equations. Below we discuss particular solutions to the nonlinear PDEs (47) and (48) with *reductions 1–4*.

Consider the system (51) and (52) associated with *reduction 1*. The equations (65)–(67) become of the form

$$a_{n1}^{(1)}b_m^{(1)}(k_n-\omega_{m2})+a_{n1}^{(2)}b_m^{(2)}(\omega_{m1}-k_n)=0, \tag{70}$$

$$a_{n1}^{(1)}(k_n^2-\omega_{m3})+(a_{n1}^{(3)}+a_{n2}^{(3)}\omega_{m1})(\omega_{m1}-k_n)=0, \tag{71}$$

$$a_{n1}^{(2)}(k_n^3-\omega_{m4})+(a_{n1}^{(4)}+a_{n2}^{(4)}\omega_{m2}+a_{n3}^{(4)}\omega_{m2}^2)(\omega_{m2}-k_n)=0. \tag{72}$$

The following families of particular solutions are available:

(1) (*Criteria*). If $N^{(c)}=N^{(r)}=1$ in (70)–(72), the system is resolvable for $b_1^{(2)}$, ω_{13}, and ω_{14}, so that *f*- and *g*-functions belong to the manifolds $\mathbf{F}_{11}^{(i)}$ and $\mathbf{G}_{11}^{(i)}$, respectively, and (69) becomes of the form

$$g_1^{(i)}=\int b_1^{(i)}(\omega_{11},\omega_{12})e^{\omega_{11}x_1+\omega_{12}x_2+\omega_{13}x_3+\omega_{14}x_4}\,d\omega_{11}d\omega_{12}, \tag{73}$$

where ω_{13} and ω_{14} are functions of ω_{11} and ω_{12}.

(2) Let us take the system (70)–(72) with $n=1$ ($N_{\min}^{(r)}=1$) to fix relations among the parameters $b_m^{(j)}$ ($j=1,2$), ω_{mk} ($k=1,2,3,4$):

$$b_m^{(2)}=\frac{a_{11}^{(1)}b_m^{(1)}(k_1-\omega_{m2})}{a_{11}^{(2)}(k_1-\omega_{m1})}, \tag{74}$$

$$\omega_{m3}=(k_1^2a_{11}^{(1)}-k_1a_{11}^{(3)}+(a_{11}^{(3)}-k_1a_{12}^{(3)})\omega_{m1}+a_{12}^{(3)}\omega_{m1}^2)/a_{11}^{(1)}, \tag{75}$$

$$\omega_{m4}=(k_1^3a_{11}^{(2)}-k_1a_{11}^{(4)}+(a_{11}^{(4)}-k_1a_{12}^{(4)})\omega_{m2}+(a_{12}^{(4)}-k_1a_{13}^{(4)})\omega_{m2}^2+a_{13}^{(4)}\omega_{m2}^3)/a_{11}^{(2)}. \tag{76}$$

Here ω_{m1}, ω_{m2} are integration parameters in Fourier representation (73), which means that $N_{\min}^{(c)}=1$ and $N_{\max}^{(c)}=\infty$. One can check that the system (70)–(72) does not have solutions with different $\mathbf{k}_n\neq\mathbf{k}_1$, i.e., $N_{\max}^{(r)}=1$. So, *f*- and *g*-functions are collected in the manifolds $\mathbf{F}_{11}^{(i)}$ and $\mathbf{G}_{1\infty}^{(i)}$, respectively.

(3) Consider (70)–(72) with $n=1,2$ ($N_{\min}^{(r)}=2$) to express $b_m^{(2)}$, ω_{mj}, $j=1,2,3$, through ω_{m1} and $b_m^{(1)}$. Then along with (74)–(76) one has from the equation (70)

$$\omega_{m2}=\frac{k_1k_2(a_{21}^{(1)}a_{11}^{(2)}-a_{11}^{(1)}a_{21}^{(2)})+(q_1a_{11}^{(1)}a_{21}^{(2)}-q_2a_{21}^{(1)}a_{11}^{(2)})\omega_{m1}}{(q_1-\omega_{m1})a_{21}^{(1)}a_{11}^{(2)}-(q_2-\omega_{m1})a_{11}^{(1)}a_{21}^{(2)}}, \tag{77}$$

from the equation (71)

$$a_{12}^{(3)}=((k_1+k_2)a_{11}^{(1)}-a_{11}^{(3)})/k_2, \tag{78}$$

$$a_{22}^{(3)}=\frac{a_{21}^{(1)}}{a_{11}^{(1)}}a_{12}^{(3)}, \tag{79}$$

$$a_{21}^{(3)}=\frac{a_{21}^{(1)}}{k_2 a_{11}^{(1)}}((k_2^2-k_1^2)a_{11}^{(1)}+k_1 a_{11}^{(3)}), \tag{80}$$

and from the equation (72)

$$a_{13}^{(4)}=\frac{1}{k_2^2}(a_{11}^{(2)}(k_1^2+k_1k_2+k_2^2)-a_{11}^{(4)}-k_2 a_{12}^{(4)}), \tag{81}$$

$$a_{23}^{(4)}=a_{21}^{(2)}a_{13}^{(4)}/a_{11}^{(2)}, \tag{82}$$

$$a_{22}^{(4)}=(a_{21}^{(2)}a_{13}^{(4)}(k_2-k_1)+a_{21}^{(2)}a_{12}^{(4)})/a_{11}^{(2)}, \tag{83}$$

$$a_{21}^{(4)}=a_{21}^{(2)}(a_{11}^{(4)}+(k_2-k_1)a_{12}^{(4)}+a_{13}^{(4)}k_2(k_2-k_1))/a_{11}^{(2)}. \tag{84}$$

One can check that the system (70)–(72) together with formulas (74)–(84) has no solutions with $\mathbf{k}_n\neq\mathbf{k}_1,\mathbf{k}_2$. This means that $N_{\min}^{(r)}=N_{\max}^{(r)}=2$, $N_{\min}^{(c)}=1$, $N_{\max}^{(c)}=\infty$, *f*- and *g*-functions belong to the manifolds $\mathbf{F}_{22}^{(i)}$ and $\mathbf{G}_{1\infty}^{(i)}$, and ω_{m1} is an integration parameter in Fourier representation of *g*-functions:

$$g_m^{(i)}=\int b_m^{(i)}(\omega_{m1})e^{\omega_{m1}x_1+\omega_{m2}x_2+\omega_{m3}x_3+\omega_{m4}x_4}\,d\omega_{m1}. \tag{85}$$

(4) Consider Eqs. (70)–(72) with $n=1,2,3$ to fix the parameters $b_m^{(2)}$, ω_{mj}, $j=1,2,3,4$. One gets

$$\begin{aligned}\omega_{m1}=&(k_1k_2a_{31}^{(1)}(a_{21}^{(1)}a_{11}^{(2)}-a_{11}^{(1)}a_{21}^{(2)})+k_1k_3a_{21}^{(1)}(a_{11}^{(1)}a_{31}^{(2)}-a_{31}^{(1)}a_{11}^{(2)})+k_2k_3a_{11}^{(1)}(a_{31}^{(1)}a_{21}^{(2)}\\&-a_{21}^{(1)}a_{31}^{(2)}))(a_{21}^{(1)}a_{31}^{(1)}a_{11}^{(2)}(q_2-q_3)+a_{11}^{(1)}a_{31}^{(1)}a_{21}^{(2)}(q_3-q_1)+a_{11}^{(1)}a_{21}^{(1)}a_{31}^{(2)}(q_1-q_2))^{-1}\end{aligned} \tag{86}$$

along with (74)–(77). Then the equations (70)–(72) with $n>3$ admit an infinite number of solutions, parametrized, for example, by $a_{n1}^{(1)}$, k_n. The dimensions $N_{\min}^{(c)}=N_{\max}^{(c)}=1$, $N_{\min}^{(r)}=3$, $N_{\max}^{(r)}=\infty$ and integration in (85) disappears:

$$g_m^{(i)}=b_m^{(i)}e^{\omega_{m1}x_1+\omega_{m2}x_2+\omega_{m3}x_3+\omega_{m4}x_4}. \tag{87}$$

Here *f*- and *g*-functions belong to the manifolds $\mathbf{F}_{3\infty}^{(i)}$ and $\mathbf{G}_{11}^{(i)}$. In this case the representation (68) for *f*-functions can be replaced by the Fourier integral [see (27)].

Analogous families of particular solutions are available for the nonlinear systems (55) and (56), and (58) and (59) related to *reductions 2* and *3*, respectively (which mean appropriate reductions on the parameters $a_{nk}^{(i)}$).

Under *reduction 2* one has

$$\begin{gathered}a_{n1}^{(1)}=a_n^{(1)},\quad a_{n1}^{(2)}=a_n^{(2)},\quad a_{n1}^{(3)}=a_n^{(3)}k_n,\quad a_{n2}^{(3)}=a_n^{(3)},\\a_{n1}^{(4)}=a_n^{(4)}k_n^2,\quad a_{n2}^{(4)}=a_n^{(4)}k_n,\quad a_{n3}^{(4)}=a_n^{(4)}.\end{gathered} \tag{88}$$

The system (70)–(72) becomes of the form

$$a_n^{(1)}b_m^{(1)}(k_n-\omega_{m2})+a_n^{(2)}b_m^{(2)}(\omega_{m1}-k_n)=0, \tag{89}$$

$$a_n^{(1)}(k_n^2-\omega_{m3})+a_n^{(3)}(\omega_{m1}^2-k_n^2)=0, \tag{90}$$

$$a_n^{(2)}(k_n^3-\omega_{m4})+a_n^{(4)}(\omega_{m2}^3-k_n^3)=0. \tag{91}$$

Reduction 3 gives

$$a_n^{(3)}=a_n^{(1)}, \quad a_n^{(4)}=a_n^{(2)} \tag{92}$$

and one has

$$a_n^{(1)}b_m^{(1)}(k_n-\omega_{m2})+a_n^{(2)}b_m^{(2)}(\omega_{m1}-k_n)=0, \tag{93}$$

$$\omega_{m1}^2-\omega_{m3}=0, \quad \omega_{m2}^3-\omega_{m4}=0 \tag{94}$$

instead of Eqs. (89)–(91).

Reduction 4 ($a_n^{(1)}=a_n^{(2)}$) keeps Eq. (94) unchanged and reduces Eq. (93) into the following one:

$$b_m^{(1)}(k_n-\omega_{m2})+b_m^{(2)}(\omega_{m1}-k_n)=0, \tag{95}$$

which has been considered in Ref. 13. It admits the family of solutions with $N_{\min}^{(c)}=N_{\max}^{(c)}=1$, $N_{\min}^{(r)}=1$, $N_{\max}^{(r)}=\infty$, where ω_{m1}, ω_{m2} are integration variables in (69). *f*- and *g*-functions are collected in the manifolds $\mathbf{F}_{11}^{(i)}$ and $\mathbf{G}_{1\infty}^{(i)}$.

Finally, *reduction 5* assumes $b_m^{(1)}=b_m^{(2)}$, $\omega_{m1}=\omega_{m2}$ and reduces the system of nonlinear PDEs (63) into the completely integrable equation mKP (64).

IV. RELATION BETWEEN DIFFERENT INTEGRABLE HIERARCHIES

The dressing method based on the algebraic system (1) allows one to establish the relations between solutions of different integrable hierarchies. To demonstrate this let us consider two sets of parameters $\mathbf{x}=(x_1,\ldots)$ and $\mathbf{y}=(y_1,\ldots)$ which are independent variables in two different integrable hierarchies of nonlinear PDEs. These parameters are introduced by the system which is similar to the system (5):

$$\partial_{x_i}\mathbf{R}=\sum_{k=1}^{N_{x_i}}\mathbf{f}^{(x_i,k)}\mathbf{g}^{(k,x_i)}, \quad \partial_{y_i}\mathbf{R}=\sum_{k=1}^{N_{y_i}}\mathbf{f}^{(y_i,k)}\mathbf{g}^{(k,y_i)}, \tag{96}$$

$$\mathbf{f}^{z_i,k}=[f_{1k}^{(z_i)}\cdots f_{N^{(r)}k}^{(z_i)}]^T, \quad \mathbf{g}^{k,z_i}=[g_{k1}^{(z_i)}\cdots g_{kN^{(c)}}^{(z_i)}], \tag{97}$$

where z_i is either x_i or y_i. Since each of the equations (96) serves an integrable system, the compatibility conditions $(\partial_{x_ix_j}-\partial_{x_jx_i})\mathbf{R}=0$ and $(\partial_{y_iy_j}-\partial_{y_jy_i})\mathbf{R}=0$ are satisfied so that the only compatibility condition which should be considered is the following one [see note above the Eq. (19)]:

$$(\partial_{x_1y_1}-\partial_{y_1x_1})\mathbf{R}=0. \tag{98}$$

The equation (98) gives rise to the relations among *f*- and *g*-functions.

Let

$$M_n^{(1)}\psi=0, \quad M_m^{(2)}\psi=0, \quad n=1,..., \quad m=1,..., \quad \psi=[\psi_1\ldots\psi_{N^{(c)}}] \tag{99}$$

be the linear overdetermined systems related with two hierarchies pointed out earlier. The set of functions $\mathbf{U}^{(1)}=\{U_{n_{1\ldots}}^{(1ik)}=\psi\mathbf{C}(\Pi_s\partial_{x_s}^{n_s})\mathbf{f}^{(x_i,k)}\}$ satisfies the first hierarchy of nonlinear equations, while the set of functions $\mathbf{U}^{(2)}=\{U_{n_{1\ldots}}^{(2ik)}=\psi\mathbf{C}(\Pi_s\partial_{y_s}^{n_s})\mathbf{f}^{(y_i,k)}\}$ satisfies the second hierarchy of nonlinear equations. The relation between these two hierarchies is described by the nonlinear system on the ''mixed'' functions $\mathbf{U}=\{U_{n_{1\ldots}}^{(12ik)},U_{n_{1\ldots}}^{(21ik)}\}$, where

$$U^{(12ik)}_{n_1,\dots,m_1,\dots}=\psi\mathbf{C}\left(\prod_s \partial^{n_s}_{x_s}\right)\left(\prod_r \partial^{m_r}_{y_r}\right)\mathbf{f}^{(x_i,k)},\quad U^{(21ik)}_{n_1,\dots,m_1,\dots}=\psi\mathbf{C}\left(\prod_s \partial^{n_s}_{x_s}\right)\left(\prod_r \partial^{m_r}_{y_r}\right)\mathbf{f}^{(y_i,k)}.$$

As an example let us consider two different mKP hierarchies, associated with two different sets of independent variables: $\mathbf{x}=(x_1,\dots)$ and $\mathbf{y}=(y_1,\dots)$. The dependence on these variables is introduced by the following equations:

$$\partial_{x_1}\mathbf{R}=\mathbf{f}^{(1)}\mathbf{g}^{(1)},\quad \partial_{x_2}\mathbf{R}=\mathbf{f}^{(1)}\partial_{x_1}\mathbf{g}^{(1)}-\partial_{x_1}\mathbf{f}^{(1)}\mathbf{g}^{(1)}, \tag{100}$$

$$\partial_{x_3}\mathbf{R}=\mathbf{f}^{(1)}\partial^2_{x_1}\mathbf{g}^{(1)}-\partial_{x_1}\mathbf{f}^{(1)}\partial_{x_1}\mathbf{g}^{(1)}+\partial^2_{x_1}\mathbf{f}^{(1)}\mathbf{g}^{(1)}, \tag{101}$$

$$\partial_{y_1}\mathbf{R}=\mathbf{f}^{(2)}\mathbf{g}^{(2)},\quad \partial_{y_2}\mathbf{R}=\mathbf{f}^{(2)}\partial_{y_1}\mathbf{g}^{(2)}-\partial_{y_1}\mathbf{f}^{(2)}\mathbf{g}^{(2)}, \tag{102}$$

$$\partial_{y_3}\mathbf{R}=\mathbf{f}^{(2)}\partial^2_{y_1}\mathbf{g}^{(2)}-\partial_{y_1}\mathbf{f}^{(2)}\partial_{y_1}\mathbf{g}^{(2)}+\partial^2_{y_1}\mathbf{f}^{(2)}\mathbf{g}^{(2)}, \tag{103}$$

$$\partial_{x_j}\mathbf{g}^{(1)}=\partial^j_{x_1}\mathbf{g}^{(1)},\quad \partial_{x_j}\mathbf{f}^{(1)}=(-1)^j\partial^j_{x_1}\mathbf{f}^{(1)}, \tag{104}$$

$$\partial_{y_j}\mathbf{g}^{(2)}=\partial^j_{y_1}\mathbf{g}^{(2)},\quad \partial_{y_j}\mathbf{f}^{(2)}=(-1)^j\partial^j_{y_1}\mathbf{f}^{(2)}, \tag{105}$$

$$\mathbf{f}^{(i)}=[f^{(i)}_1\cdots f^{(i)}_{N^{(r)}}]^T,\quad \mathbf{g}^{(i)}=[g^{(i)}_1\cdots g^{(i)}_{N^{(c)}}],\quad i=1,2. \tag{106}$$

The compatibility condition (98) has the form

$$\partial_{y_1}(\mathbf{f}^{(1)}\mathbf{g}^{(1)})=\partial_{x_1}(\mathbf{f}^{(2)}\mathbf{g}^{(2)}). \tag{107}$$

The investigation of this condition is analogous to the investigation of the conditions (65)–(67). We do not represent it here. The linear system associated with parameters x_1,x_2,x_3 and y_1,y_2,y_3 follows:

$$\partial_{x_2}\psi-\partial^2_{x_1}\psi+V^{(1)}_1\partial_{x_1}\psi=0, \tag{108}$$

$$\partial_{x_3}\psi-\partial^3_{x_1}\psi+W^{(1)}_1\partial^2_{x_1}\psi+W^{(1)}_2\partial_{x_1}\psi=0, \tag{109}$$

$$\partial_{y_2}\psi-\partial^2_{y_1}\psi+V^{(2)}_1\partial_{y_1}\psi=0, \tag{110}$$

$$\partial_{y_3}\psi-\partial^3_{y_1}\psi+W^{(2)}_1\partial^2_{y_1}\psi+W^{(2)}_2\partial_{y_1}\psi=0, \tag{111}$$

where

$$V^{(1)}_1=2\partial_{x_1}U^{(1)}_{0,0}/U^{(1)}_{0,0},\quad W^{(1)}_1=3\partial_{x_1}U^{(1)}_{0,0}/U^{(1)}_{0,0}, \tag{112}$$

$$W^{(1)}_2=(3\partial^2_{x_1}U^{(1)}_{0,0}-3\partial_{x_1}U^{(1)}_{1,0}-W^{(1)}_1(2\partial_{x_1}U^{(1)}_{0,0,}-U^{(1)}_{1,0}))/U^{(1)}_{0,0} \tag{113}$$

$$V^{(2)}_1=2\partial_{y_1}U^{(2)}_{0,0}/U_{0,0},\quad W^{(2)}_1=3\partial_{y_1}U^{(2)}_{0,0}/U^{(2)}_{0,0}, \tag{114}$$

$$W^{(2)}_2=(3\partial^2_{y_1}U^{(2)}_{0,0}-3\partial_{y_1}U^{(2)}_{0,1}-W^{(2)}_1(2\partial_{y_1}U^{(2)}_{0,0}-U^{(2)}_{0,1}))/U^{(2)}_{0,0}, \tag{115}$$

$$U^{(j)}_{n,m}=\psi\mathbf{C}\partial^n_{x_1}\partial^m_{y_1}\mathbf{f}^{(j)},\quad j=1,2.$$

The system of nonlinear PDEs, which relates two hierarchies, results from the equations (108) and (110) if one multiplies them by the vectors $\mathbf{C}\partial_{x_1}^n\partial_{y_1}^m\mathbf{f}^{(i)}$ ($\mathbf{f}^{(i)}=[f_1^{(i)},\ldots,f_{N^{(r)}}^{(i)}]^T$, $i=1,2$):

$$\partial_{x_2}U_{n,m}^{(i)}-\partial_{x_1}^2U_{n,m}^{(i)}+2\partial_{x_1}U_{n+1,m}^{(i)}+V_1^{(1)}(\partial_{x_1}U_{n,m}^{(i)}-U_{n+1,m}^{(i)})=0,\quad n=0,\quad m=0,1, \tag{116}$$

$$\partial_{y_2}U_{n,m}^{(i)}-\partial_{y_1}^2U_{n,m}^{(i)}+2\partial_{y_1}U_{n,m+1}^{(i)}+V_1^{(2)}(\partial_{y_1}U_{n,m}^{(i)}-U_{n+1,m}^{(i)})=0,\quad n=0,1,\quad m=0. \tag{117}$$

Possible reductions are the following ones,

$$\mathbf{f}^{(1)}=\mathbf{f}^{(2)},\quad \text{or}\quad U_{n,m}^{(1)}=U_{n,m}^{(2)}, \tag{118}$$

and reductions which establish the relation between the discrete parameters n and m. For example, the reduction

$$\partial_{y_1}\mathbf{f}^{(i)}=\partial_{x_1}\mathbf{f}^{(i)} \tag{119}$$

eliminates one of the discrete parameters in the system (116) and (117).

V. POSSIBLE GENERALIZATIONS OF THE DRESSING METHOD

We give some remarks about two generalizations of the algorithm represented in this paper.

(1) Similarly to the $\bar{\partial}$-problem (2), which admits different normalization functions η,[6] the algebraic system (1) also admits different functions η on the right-hand side. For example, the algebraic system (1) can be replaced with the following one: $L(\psi^{(nm)})=\mathbf{g}^{(nm)}$. Generalization of KP is an example of the related system of nonlinear PDEs (see the Appendix).

(2) (Discrete version of the matrix $\bar{\partial}$-problem.[7]) Instead of the scalar system of $N^{(c)}$ equations (1), one can take matrix $K_1\times K_2$ algebraic system of $N^{(c)}$ equations (or tensor equation). In this case each entry of the matrices $\mathbf{C}$ and $\mathbf{R}$ is represented by $K_1\times K$ (K is an arbitrary integer) and $K\times K_2$ matrices, respectively, and the system (5) which introduces the independent variables $\mathbf{x}$ reads: $\partial_i\mathbf{R}_{nm}=\Sigma_{k=1}^{N_i}\mathbf{f}_{nk}^{(i)}\mathbf{g}_{km}^{(i)}$, $(n=1,\ldots,N^{(r)},\ m=1,\ldots,N^{(c)})$, where $\mathbf{f}_{nk}^{(i)}$ are $K\times K_1$ and $\mathbf{g}_{km}^{(i)}$ are $K_1\times K_2$ matrices for all possible values of the indexes i,k,n,m. All scalar equations of the previous sections become the $K_1\times K_2$ matrix equations. This generalization is beyond the scope of this article.

VI. CONCLUSIONS

The introduced modification of the dressing method is aimed at the construction of new classes of either integrable or nonintegrable equations together with families of particular solutions. The families of particular solutions are parametrized either by the arbitrary functions of independent variables or constant parameters. The maximum possible number of these arbitrary functions (or parameters) can be taken as the characteristic of the related nonlinear system. Another characteristic is the maximum possible dimensions $N^{(r)}$ and/or $N^{(c)}$ of the matrix $\mathbf{R}$ in the algebraic system (1). The introduced nonintegrable generalizations of the integrable systems of nonlinear PDEs can be applied in studies of the physical phenomena in systems with small parameters.

Another question which should be studied is the relation of this method with the Hirota method.[15–18] In both cases one relates the original nonlinear PDEs with the bilinear system of equations [Eqs. (6) in our case]. But in our case f- and g-functions are also subjected to the equations (9) and (18), which put additional restrictions on these functions.

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APPENDIX: GENERALIZATION OF KP

In this section we consider the example of the $(2+1)$-dimensional system of nonlinear PDEs, related with the first generalization of the dressing method, mentioned in Sec. V. Namely, let us consider the linear algebraic system of the form

$$L(\psi^{(p)})=\mathbf{g}^{(p)},\quad p=1,2,\quad \psi^{(p)}=[\psi_1^{(p)}\cdots\psi_{N^{(c)}}^{(p)}],\quad \mathbf{g}^{(p)}=[g_1^{(p)}\cdots g_{N^{(c)}}^{(p)}], \tag{A1}$$

with $M=3$. Introduce variables x_1,x_2,x_3 by the following formulas:

$$\begin{gathered}\partial_1\mathbf{R}=\mathbf{f}^{(11)}\mathbf{g}^{(1)},\quad \partial_2\mathbf{R}=\mathbf{f}^{(21)}\mathbf{g}^{(2)}+\mathbf{f}^{(22)}\partial_1\mathbf{g}^{(2)},\\ \partial_3\mathbf{R}=\mathbf{f}^{(31)}\mathbf{g}^{(3)}+\mathbf{f}^{(32)}\partial_1\mathbf{g}^{(3)}+\mathbf{f}^{(33)}\partial_1^2\mathbf{g}^{(3)},\quad \mathbf{f}^{(nk)}=[f_{1k}^{(n)}\cdots g_{N^{(r)}k}^{(n)}]^T.\end{gathered} \tag{A2}$$

The algebraic system (A1) and equations (A2) generate the following set of algebraic systems with different nonhomogeneous parts [compare with Eqs. (11)–(13)]:

$$L(\partial_1\psi^{(p)})=U_{0,0,0}^{(p11)}\mathbf{g}^{(1)}+\partial_1\mathbf{g}^{(p)}, \tag{A3}$$

$$L(\partial_1^2\psi^{(p)})=(2\partial_1U_{0,0,0}^{(p11)}-U_{1,0,0}^{(p11)})\mathbf{g}^{(1)}+U_{0,0,0}^{(p11)}\partial_1\mathbf{g}^{(1)}+\partial_1^2\mathbf{g}^{(p)}, \tag{A4}$$

$$\begin{aligned}L(\partial_1^3\psi^{(p)})=&(3\partial_1^2U_{0,0,0}^{(p11)}-3\partial_1U_{1,0,0}^{(p11)}+U_{2,0,0}^{(p11)})\mathbf{g}^{(1)}+(3\partial_1U_{0,0,0}^{(p11)}-U_{1,0,0}^{(p11)})\partial_1\mathbf{g}^{(1)}+U_{0,0,0}^{(p11)}\partial_1^2\mathbf{g}^{(1)}\\&+\partial_1^3\mathbf{g}^{(p)},\end{aligned} \tag{A5}$$

$$L(\partial_2\psi^{(p)})=U_{0,0,0}^{(p21)}\mathbf{g}^{(2)}+U_{0,0,0}^{(p22)}\partial_1\mathbf{g}^{(2)}+\partial_1^2\mathbf{g}^{(p)}, \tag{A6}$$

$$L(\partial_3\psi^{(p)})=U_{0,0,0}^{(p31)}\mathbf{g}^{(3)}+U_{0,0,0}^{(p32)}\partial_1\mathbf{g}^{(3)}+U_{0,0,0}^{(p33)}\partial_1^2\mathbf{g}^{(3)}+\partial_1^3\mathbf{g}^{(p)}, \tag{A7}$$

$$U_{n_1,n_2,n_3}^{pnk}=\psi^{(p)}\mathbf{C}\partial_1^{n_1}\partial_2^{n_2}\partial_3^{n_3}\mathbf{f}^{(nk)}. \tag{A8}$$

By using the set of systems (A1) and (A3)–(A7), one can construct the linear system (15) of PDEs on the functions $\psi^{(p)}$ which has the form

$$\partial_2\psi^{(p)}-\partial_1^2\psi^{(p)}+V_1^{(p)}\partial_1\psi^{(1)}+V_2^{(p)}\partial_1\psi^{(2)}+V_3^{(p)}\psi^{(1)}+V_4^{(p)}\psi^{(2)}=0, \tag{A9}$$

$$\partial_3\psi^{(p)}-\partial_1^3\psi^{(p)}+W_1^{(p)}\partial_1^2\psi^{(1)}+W_2^{(p)}\partial_1^2\psi^{(3)}+W_3^{(p)}\partial_1\psi^{(1)}+W_4^{(p)}\partial_1\psi^{(3)}+W_5^{(p)}\psi^{(1)}+W_6^{(p)}\psi^{(3)}=0, \tag{A10}$$

where V_i and W_i are related with functions $U_{n_1,n_2,n_3}^{(pij)}$ by the following formulas:

$$\begin{gathered}V_1^{(p)}-U_{0,0,0}^{(p11)}=0,\quad V_2^{(p)}+U_{0,0,0}^{(p22)}=0,\\ V_3^{(p)}-(2\partial_1U_{0,0,0}^{(p11)}-U_{1,0,0}^{(p11)})+V_1^{(p)}U_{0,0,0}^{(111)}+V_2^{(p)}U_{0,0,0}^{(211)}=0,\\ V_4^{(p)}+U_{0,0,0}^{(p21)}=0,\quad W_1^{(p)}-U_{0,0,0}^{(p11)}=0,\quad W_2^{(p)}+U_{0,0,0}^{(p33)}=0,\\ W_3^{(p)}-(3\partial_1U_{0,0,0}^{(p11)}-U_{1,0,0}^{(p11)})+W_1^{(p)}U_{0,0,0}^{(111)}+W_2^{(p)}U_{0,0,0}^{(311)}=0,\quad W_4^{(p)}+U_{0,0,0}^{(p32)}=0,\\ W_5^{(p)}-(3\partial_1^2U_{0,0,0}^{(p11)}-3\partial_1U_{0,0,0}^{(p11)}+U_{2,0,0}^{(p11)})+W_1^{(p)}(2\partial_1U_{0,0,0}^{(111)}-U_{1,0,0}^{(111)})+W_2^{(p)}(2\partial_1U_{0,0,0}^{(311)}-U_{1,0,0}^{(311)})\\ +W_3^{(p)}U_{0,0,0}^{(111)}+W_4^{(p)}U_{0,0,0}^{(311)}=0,\quad W_6^{(p)}+U_{0,0,0}^{(p31)}=0.\end{gathered} \tag{A11}$$

The appropriate nonlinear system on the functions $U^{pnk}_{n_1,n_2,n_3}$ (A8) can be received by multiplying each equation of the above linear system (A9) and (A10) (which are $1\times N^{(c)}$ matrix equations) by the $N^{(c)}\times 1$ vector $\mathbf{C}\partial_1^{n_1}\partial_2^{n_2}\partial_3^{n_3}\mathbf{f}^{(nk)}$. One obtains

$$\partial_2 U^{(pkn)}_{n_1,n_2,n_3}-U^{(pkn)}_{n_1,n_2+1,n_3}-\partial_1^2 U^{(pkn)}_{n_1,n_2,n_3}+2\partial_1 U^{(pkn)}_{n_1+1,n_2,n_3}-U^{(pkn)}_{n_1+2,n_2,n_3}+V_1^{(p)}(\partial_1 U^{(1kn)}_{n_1,n_2,n_3}-U^{(1kn)}_{n_1+1,n_2,n_3})+V_2^{(p)}(\partial_1 U^{(2kn)}_{n_1,n_2,n_3}-U^{(2kn)}_{n_1+1,n_2,n_3})+V_3^{(p)}U^{(1kn)}_{n_1,n_2,n_3}+V_4^{(p)}U^{(2kn)}_{n_1,n_2,n_3}=0, \tag{A12}$$

$$\partial_3 U^{(pkn)}_{n_1,n_2,n_3}-U^{(pkn)}_{n_1,n_2,n_3+1}-\partial_1^3 U^{(pkn)}_{n_1,n_2,n_3}+3\partial_1^2 U^{(pkn)}_{n_1+1,n_2,n_3}-3\partial_1 U^{(pkn)}_{n_1+2,n_2,n_3}+U^{(pkn)}_{n_1+3,n_2,n_3}+W_1^{(p)}\times(\partial_1^2 U^{(1kn)}_{n_1,n_2,n_3}-2\partial_1 U^{(1kn)}_{n_1+1,n_2,n_3}+U^{(1kn)}_{n_1+2,n_2,n_3})+W_2^{(p)}(\partial_1^2 U^{(3kn)}_{n_1,n_2,n_3}-2\partial_1 U^{(3kn)}_{n_1+1,n_2,n_3}+U^{(3kn)}_{n_1+2,n_2,n_3})+W_3^{(p)}(\partial_1 U^{(1kn)}_{n_1,n_2,n_3}-U^{(1kn)}_{n_1+1,n_2,n_3})+W_4^{(p)}(\partial_1 U^{(3kn)}_{n_1,n_2,n_3}-U^{(3kn)}_{n_1+1,n_2,n_3})+W_5^{(p)}U^{(1kn)}_{n_1,n_2,n_3}+W_6^{(p)}U^{(3kn)}_{n_1,n_2,n_3}=0, \tag{A13}$$

$$(pkn)=(p11),\ (p31),\ (p32),\ (p4s),\ p=1,2,\ s=1,2,3.$$

This differential-difference system involves three continuous and three discrete parameters. To reduce it to the system of pure nonlinear PDEs one needs to put some additional relations among functions $f^{(j)}_{nk}$. For example, consider the following *Reduction 1*:

$$\partial_2\mathbf{f}^{(jk)}=-\partial_1^2\mathbf{f}^{(jk)},\quad \partial_3\mathbf{f}^{(jk)}=\partial_1^3\mathbf{f}^{(jk)}, \tag{A14}$$

$$\mathbf{f}^{(21)}=-\partial_1\mathbf{f}^{(22)},\quad \mathbf{f}^{(32)}=-\partial_1\mathbf{f}^{(33)},\quad \mathbf{f}^{(31)}=\partial_1^2\mathbf{f}^{(33)}, \tag{A15}$$

or

$$U^{(pkn)}_{n_1,n_2,n_3}=(-1)^{n_2}U^{(pkn)}_{n_1+2n_2+3n_3,0,0}\equiv(-1)^{n_2}U^{(pkn)}_{n_1+2n_2+3n_3}, \tag{A16}$$

$$U_k^{(p11)}\equiv U_k^{(p1)},\quad U_k^{(p21)}=-U_{k+1}^{(p22)}\equiv -U_{k+1}^{(p2)}, \tag{A17}$$

$$U_k^{(p32)}=-U_{k+1}^{(p33)}\equiv -U_{k+1}^{(p3)},\quad U_k^{(p31)}=U_{k+2}^{(p33)}\equiv U_{k+2}^{(p3)}. \tag{A18}$$

Then the system [(A12),(A13)] becomes of the form

$$\partial_2 U_k^{pj}-\partial_1^2 U_k^{pj}+2\partial_1 U_{k+1}^{pj}+U_0^{(p1)}(\partial_1 U_k^{(1j)}-U_{k+1}^{(1j)})-U_0^{(p2)}(\partial_1 U_k^{(2j)}-U_{k+1}^{(2j)}) \tag{A19}$$

$$+(2\partial_1 U_0^{(p1)}-U_1^{(p1)}-U_0^{(p1)}U_0^{(11)}+U_0^{(p2)}U_0^{(21)})U_k^{(1j)}+U_1^{(p2)}U_k^{(2j)}=0,\quad k=0,1,$$

$$\partial_3 U_k^{(pj)}-(\partial_1^3 U_k^{(pj)}-3\partial_1^2 U_{k+1}^{(pj)}+3\partial_1 U_{k+2}^{(pj)})+W_1^{(p)}(\partial_1^2 U_k^{(1j)}-2\partial_1 U_{k+1}^{(1j)}+U_{k+2}^{(1j)})+W_2^{(p)}(\partial_1^2 U_k^{(3j)}-2\partial_1 U_{k+1}^{(3j)}+U_{k+2}^{(3j)}) \tag{A20}$$

$$+W_3^{(p)}(\partial_1 U_k^{(1j)}-U_{k+1}^{(1j)})+W_4^{(p)}(\partial_1 U_k^{(3j)}-U_{k+1}^{(3j)})+W_5^{(p)}U_k^{(1j)}+W_6^{(p)}U_k^{(3j)}=0,$$

$$p=1,2,\quad j=1,2,3,$$

$$W_1^{(p)}=U_0^{(p1)},\quad W_2^{(p)}=-U_0^{(p3)},$$

$$W_3^{(p)}=3\partial_1 U_0^{(p1)}-U_1^{(p1)}-U_0^{(p1)}U_0^{(11)}+U_0^{(p3)}U_0^{(31)},\quad W_4^{(p)}=U_1^{(p3)},$$

$$W_5^{(p)}=3\partial_1^2 U_0^{(p1)}-3\partial_1 U_1^{(p1)}+U_2^{(p1)}-U_0^{(p1)}(2\partial_1 U_0^{(11)}-U_1^{(11)})$$

$$+U_0^{(p3)}(2\partial_1 U_0^{(31)}-U_1^{(31)})-(3\partial_1 U_0^{(p1)}-U_1^{(p1)}-U_0^{(p1)}U_0^{(11)}$$
$$+U_0^{(p3)}U_0^{(31)})U_0^{(11)}-U_1^{(p3)}U_0^{(31)},\quad W_6^{(P)}=-U_2^{(p3)}.$$

Using another *Reduction 2*

$$\mathbf{f}^{(11)}=\mathbf{f}^{(22)}=\mathbf{f}^{(33)}\equiv\mathbf{f},\quad \mathbf{g}^{(11)}=\mathbf{g}^{(21)}=\mathbf{g}^{(31)}\equiv\mathbf{g},\quad \text{or } U_k^{(pj)}\equiv U_k \tag{A21}$$

one reduces the nonlinear system [(A19),(A20)] into KP on the function $u=\partial_1 U_0$:

$$u_{x_3}-\tfrac{1}{4}u_{x_1x_1x_1}+3uu_{x_1}-\tfrac{3}{4}\partial_{x_1}^{-1}u_{x_2x_2}=0. \tag{A22}$$

Different *Reduction 3*

$$\mathbf{f}^{(11)}=\mathbf{f}^{(33)}=-\mathbf{f}^{(22)}\equiv\mathbf{f},\quad \mathbf{g}^{(11)}=\mathbf{g}^{(21)}=\mathbf{g}^{(31)}\equiv\mathbf{g} \tag{A23}$$

reduces the nonlinear system [(A19),(A20)] into the following nonintegrable one

$$\partial_2 U_k-\partial_1^2 U_k+2\partial_1 U_{k+1}+2U_0(\partial_0 U_k-U_{k+1}) \tag{A24}$$

$$+2(\partial_1 U_0-U_1-U_0U_0)U_k=0,\quad k=0,1 \tag{A25}$$

$$\partial_3 U_0-\partial_1^3 U_0+3\partial_1^2 U_1-3\partial_1 U_2+3\partial_1 U_0(\partial_1 U_0-U_1)+3(\partial_1^2 U_0-\partial_1 U_1)U_0-3U_0U_0\partial_1 U_0=0.$$

One can demonstrate that the compatibility condition (6) can be satisfied (at least for $N^{(c)}=N^{(r)=1}$) for all nonlinear equations considered in the Appendix, i.e., the dressing method is applicable to them.

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Erratum: "Hyperbolic Kac–Moody algebra from intersecting *p*-branes" [J. Math. Phys. 40, 4072 (1999)]

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The list of changes is the following one.

(1) Astract, line 4: should be ''cosmological-type solution (in 11-dimensional model with two 4-forms)'' instead of ''cosmological solution to $D=11$ supergravity.''

(2) Section I. Third line from the end: should be ''in 11-dimensional model'' instead of ''in $D=11$ supergravity.''

(3) Section IV. Formula (4.8) with the surrounding sentence and two sentences after should be replaced by '' There exists an example of the solution with the A-matrix (4.1) for 11-dimensional model governed by the action

$$S=\int d^{11}z\sqrt{|g|}\left\{R[g]-\frac{1}{4!}(F^4)^2-\frac{1}{4!}(F^{4*})^2\right\}, \tag{4.8}$$

where $\mathrm{rank}\,F^4=\mathrm{rank}\,F^{4*}=4$. Here $\Delta=\{4,4*\}$. We consider a configuration with two magnetic 5-branes corresponding to the form F^4 and one electric 2-brane corresponding to the form F^{4*}. We denote $S=\{s_1,s_2,s_3\}$, $a_{s_1}=a_{s_3}=4$, $a_{s_2}=4*$ and $v_{s_1}=v_{s_3}=m$, $v_{s_2}=e$, where $d(I_{s_1})=d(I_{s_3})=6$ and $d(I_{s_2})=3$.''

(4) Formula (4.11) should be replaced by the following one:

$$F^4=\frac{dH}{dt}\{\nu_{s_1}\tau_3\wedge\tau_4\wedge\tau_5+\nu_{s_3}\tau_1\wedge\tau_5\},\quad F^{4*}=\frac{dH}{dt}\frac{\nu_{s_2}}{H^2}\,dt\wedge\tau_4\wedge\tau_5. \tag{4.11}$$

(5) Formula (4.14) with the surrounding sentence should be omitted.

(6) After the formula (4.17) should be inserted ''We remind that $D=11$ supergravity is governed by the action (in the bosonic sector)

$$S=\int d^{11}z\sqrt{|g|}\left\{R[g]-\frac{1}{4!}(F^4)^2\right\}+c\int A^3\wedge F^4\wedge F^4, \tag{4.17a}$$

where $c=\mathrm{const}$, $F^4=dA^3$.''

(7) At the end of Sec. IV should be inserted ''The solution (4.20)–(4.23) satisfies not only equations of motion for the truncated model (without the Chern–Simons term), but also the equations of motion for the 'total' model (4.17a), since the only modification related to 'Maxwell's' equations $d*F^4=\mathrm{const}\,F^4\wedge F^4$ is trivial due to $F^4\wedge F^4=0$ (since $\tau_i\wedge\tau_i=0$).''

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Scalar quantum field coupled to boundaries and to a background magnetic field

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The stationary states of a charged scalar quantum field interacting with a background consisting of both boundaries and a static magnetic field are investigated. Following the development of some general theory, the example of a uniform magnetic field perpendicular to two parallel Dirichlet boundaries is worked through in detail. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1413521]

I. INTRODUCTION

In this paper we investigate the stationary states of a charged scalar quantum field coupled to a static background magnetic field. The study of this problem began many years ago,[1–3] and of course substantial literature has come into existence (see, e.g., Refs. 4–13). Essentially all efforts have been directed toward uniform magnetic fields coupled to charged (spinor and scalar) quantum fields in free, infinite space. There seem to be very few calculations involving quantum fields which are modified by the presence of background objects (i.e., Casimir-type systems) as well as being coupled to background electromagnetic fields. One such study[14] presents a global calculation of the Casimir energy of a charged scalar field confined between parallel boundary planes, and acted on by a uniform magnetic field perpendicular to these planes.

One purpose of the present article is to begin the local investigation of such systems. We present a Schrödinger-picture analysis of a charged scalar field coupled to a general background described by a static potential $V(\mathbf{x})$, as well as to an arbitrary static magnetic field. Then we work through the detailed mathematics of a nontrivial problem with two parallel planar Dirichlet surfaces perpendicular to a uniform magnetic field.

As long as the background magnetic field is not time dependent one is free to assume the background electric field is exactly zero. Then the system has a stable vacuum. Magnetic fields deflect, but do not transfer energy to or from charged particles. No pairs are produced from the vacuum by magnetic fields. Therefore, stationary state methods can be used for an arbitrary arrangement of static boundaries and static background magnetic fields.

The problem of a charged scalar field coupled to a background electric field is far more complex because a sufficiently strong background electric field causes pair production from the vacuum. Consequently the vacuum is unstable and the system is never in equilibrium. Strictly speaking, stationary state methods are not adequate for describing such systems—at least not for following their time evolution. However, the Schrödinger picture provides a nonstationary framework within which one can attempt to deal with the highly nontrivial time evolution of such systems (see e.g., Ref. 15). In a separate paper we intend to pursue this direction of study.

II. CHARGED SCALAR FIELD IN A BACKGROUND MAGNETIC FIELD

A charged scalar field ϕ consists of two real scalar fields $\phi_{1,2}$. We shall write $\phi=(\phi_1+i\,\phi_2)/\sqrt{2}$, where the convenience of the factor $1/\sqrt{2}$ will become apparent later. Most books in

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QFT develop the theory of charged scalar fields in terms of the complex field ϕ. The complex field ϕ^* is treated as an independent variable, even though ϕ and ϕ^* satisfy the constraint $(\phi^*)_{cc} = \phi$, cc denoting complex conjugation. While this has certain notational advantages, one encounters notational ambiguities as well. Such ambiguities are eliminated by using the real variables $\phi_{1,2}$ as we shall do in all of our main calculations. However, it will be useful to employ the ϕ, ϕ^* notation as well, particularly when plane wave modes are to be used. Thus we shall change from one notation to the other as convenience dictates.

A. The field representation

The field representation belongs to the Schrödinger picture. One introduces at a specified time (say $t=0$) a complete set of eigenstates $\{|\phi\rangle\}$ of the scalar field operator $\hat{\phi}(\mathbf{x}) \equiv \hat{\phi}(\mathbf{x},0)$,

$$\hat{\phi}(\mathbf{x})|\phi\rangle = \phi(\mathbf{x})|\phi\rangle, \tag{II.1}$$

assuming δ-functional normalization

$$\langle \phi'|\phi\rangle = \delta[\phi' - \phi] = \prod_{\mathbf{x}} \delta(\phi'(\mathbf{x}) - \phi(\mathbf{x})), \tag{II.2}$$

where two-dimensional δ-functions appropriate for complex numbers are understood on the right-hand side.

Then an arbitrary field state $|\Psi(t)\rangle$ can be expressed as a functional integral,

$$|\Psi(t)\rangle = \int [d\phi]\Psi[\phi,t]|\phi\rangle, \tag{II.3}$$

where later more will be said about the functional integration measure. Here the wave functional $\Psi[\phi,t] = \langle\phi|\Psi(t)\rangle$ is the analog of the wave function in quantum mechanics. Specifically, $\Psi[\phi,t]$ is the probability amplitude that, with the field in state $|\Psi(t)\rangle$, a measurement of the field $\hat{\phi}$ everywhere in space at the time t will find the configuration $\phi(\mathbf{x})$.

Already in this statement an awkwardness of the complex variable ϕ has emerged. Not being real, ϕ is not observable; however, $\phi_{1,2}$ are, enabling ϕ to be constructed. Strictly speaking it would be preferable to introduce field configuration states $|\phi_1, \phi_2\rangle$ with

$$\hat{\phi}_{1,2}(\mathbf{x})\,|\phi_1, \phi_2\rangle = \phi_{1,2}(\mathbf{x})|\phi_1, \phi_2\rangle,$$

with δ-functional normalization and the wave functional

$$\Psi[\phi_1, \phi_2, t] = \langle \phi_1, \phi_2|\Psi(t)\rangle.$$

However, these differences are so slight that as a general notation (II.1)–(II.3) seems adequate.

Let us now couple the charged scalar field to a static background gauge potential $A^\mu(\mathbf{x}) = (0,\mathbf{A}(\mathbf{x}))$ representing an arbitrary static background magnetic field $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$ and vanishing electric field. The Lagrangian density of the system is

$$\mathcal{L} = (D_\mu \phi)^* D^\mu \phi - [m^2 + V(\mathbf{x})]\phi^* \phi, \tag{II.4}$$

where $D^\mu = \partial^\mu - iA^\mu$. Here and throughout this paper A^μ and the magnetic field $\mathbf{B}$ contain the electric charge e. In $\mathcal{L}$ the static potential $V(\mathbf{x}) \geqslant 0$ has been introduced to represent an arbitrary background force of nonelectromagnetic origin acting on the scalar field. The Hamiltonian density corresponding to $\mathcal{L}$ is

$$\mathcal{H} = |\partial_0 \phi|^2 + |\mathbf{D}\phi|^2 + [m^2 + V(\mathbf{x})]|\phi|^2. \tag{II.5}$$

Identifying in the field representation,

$$\Pi(\mathbf{x}) = \partial_0 \phi^*(\mathbf{x}) \to \hat{\Pi}(\mathbf{x}) = -i \frac{\delta}{\delta \phi(\mathbf{x})},$$

$$\Pi^*(\mathbf{x}) = \partial_0 \phi(\mathbf{x}) \to \hat{\Pi}^\dagger = -i \frac{\delta}{\delta \phi^*(\mathbf{x})},$$

and

$$\phi(\mathbf{x}) \to \hat{\phi}(\mathbf{x}) = \phi(\mathbf{x}),$$

the latter statement meaning that $\hat{\phi}(\mathbf{x})$ is simply a multiplicative operator, one obtains the Hamilton operator,

$$\mathbb{H} = \int d\mathbf{x} \left\{ -\frac{\delta^2}{\delta \phi^* \delta \phi} + \phi^* [-\mathbf{D}^2 + m^2 + V]\, \phi \right\}. \tag{II.6}$$

Here $|\mathbf{D}\phi|^2 = -\phi^* \mathbf{D}^2 \phi +$ divergence term is used and the divergence term is discarded. At the level of the Hamiltonian this is allowed, because the divergence term does not influence the equations of motion. However, at the level of densities [e.g., $T_{\mu\nu}(\mathbf{x})$] the same step is not allowed, as will be quite evident in the examples of Sec. III.

Now it is easy to separate $\mathbb{H}$ into a collection of harmonic oscillator (hereafter, HO) Hamiltonians. For this purpose we define a complete, orthonormal set of complex spatial modes $\{\varphi_n(\mathbf{x})\}$ and associated frequencies $\{\omega_n\}$ by the spectral equation,

$$[-\mathbf{D}^2 + V(\mathbf{x})]\varphi_n(\mathbf{x}) = \omega_n^2 \varphi_n(\mathbf{x}). \tag{II.7}$$

Because the operator on the left is Hermitian, the spectrum ω_n^2 on the right is real. Here we are introducing a formal discrete notation. The mode label n represents three sublabels in three spatial dimensions. At least one of these is continuous in infinite space. However, if we make space compact and finite, as we shall do in later calculations, then the notation here is completely appropriate.

Note also that the magnetic vector potential $\mathbf{A}(\mathbf{x})$ and the potential $V(\mathbf{x})$ make their principal contribution to the mathematics in Eq. (II.7). Both $\mathbf{A}(\mathbf{x})$ and $V(\mathbf{x})$ influence the spectral problem (II.7) in their separate ways, and thereby shape the spectral ingredients $\{\varphi_n\}$ and $\{\omega_n\}$ from which observable quantum functions will ultimately be constructed.

Now we expand an arbitrary complex field configuration $\phi(\mathbf{x})$ in terms of the complete set $\{\varphi_n(\mathbf{x})\}$,

$$\phi(\mathbf{x}) = \sum_n \tilde{\phi}_n \varphi_n(\mathbf{x}),$$

$$\tilde{\phi}_n = \int d\mathbf{x} \varphi_n^*(\mathbf{x}) \phi(\mathbf{x}), \tag{II.8}$$

$$\frac{\delta}{\delta \phi(\mathbf{x})} = \sum_n \varphi_n^*(\mathbf{x}) \frac{\partial}{\partial \tilde{\phi}_n},$$

where the variables $\tilde{\phi}_n$ are complex. For immediate use we write

$$\tilde{\phi}_n = (\tilde{\phi}_{1n} + i\tilde{\phi}_{2n})/\sqrt{2},$$

where $\tilde{\phi}_{1n}$, $\tilde{\phi}_{2n}$ are real. Because

$$\int d\mathbf{x}\, \phi^*(\mathbf{x})\phi(\mathbf{x}) = \sum_n \tilde{\phi}_n^* \tilde{\phi}_n = \frac{1}{2}\sum_n (\tilde{\phi}_{1n}^2 + \tilde{\phi}_{2n}^2), \tag{II.9}$$

$$\int d\mathbf{x} \frac{\delta^2}{\delta\phi^*(\mathbf{x})\,\delta\phi(\mathbf{x})} = \sum_n \frac{\partial^2}{\partial\tilde{\phi}_n^* \partial\tilde{\phi}_n} = \frac{1}{2}\sum_n \left(\frac{\partial^2}{\partial\tilde{\phi}_{1n}^2} + \frac{\partial^2}{\partial\tilde{\phi}_{2n}^2} \right), \tag{II.10}$$

the Hamiltonian (II.6) becomes a sum of elementary HO Hamiltonians,

$$\begin{aligned} \mathbb{H} &= \sum_n (\mathbb{H}_{1n} + \mathbb{H}_{2n}), \\ \mathbb{H}_{a\,n} &= \frac{1}{2}\left\{ -\frac{\partial^2}{\partial\tilde{\phi}_{an}^2} + [\omega_n^2 + m^2]\tilde{\phi}_{an}^2 \right\} \quad a = 1,2. \end{aligned} \tag{II.11}$$

Consequently the wave functional $\Psi[\phi,t]$ factorizes

$$\Psi[\phi,t] = \prod_n \psi_{1n}(\tilde{\phi}_{1n},t)\, \psi_{2n}(\tilde{\phi}_{2n},t), \tag{II.12}$$

and the field evolution problem

$$\mathbb{H}\Psi = i\,\partial_t \Psi \tag{II.13}$$

reduces to an infinite set of individual HO problems,

$$\mathbb{H}_{an}\psi_{an}(\tilde{\phi}_{an},t) = i\partial_t \psi_{an}(\tilde{\phi}_{an},t). \tag{II.14}$$

Here $-\infty < \tilde{\phi}_{an} < \infty$ is like a coordinate axis, and $\psi_{an}(\tilde{\phi}_{an},t)$ is a normalized solution of Eq. (II.14). The normalization requirement on ψ_{an} arises from the condition,

$$1 = \langle \Psi(t)|\Psi(t)\rangle = \int [d\phi]\,|\Psi[\phi,t]|^2 = \prod_n \int_{-\infty}^{\infty} \prod_{a=1,2} d\tilde{\phi}_{an} |\psi_{an}(\tilde{\phi}_{an},t)|^2. \tag{II.15}$$

Here we see in more detail what is meant by the functional integration measure. With Eqs. (II.11)–(II.14) we have reached a simple formulation of the time evolution problem $\mathbb{H}|\Psi(t)\rangle = i\partial_t|\Psi(t)\rangle$ of the quantum field in terms of solutions of the HO Eq. (II.14), using real field variables $\tilde{\phi}_{an}$ and complex spatial modes $\varphi_n(\mathbf{x})$ which satisfy Eq. (II.7). In fact, since one knows the solutions of the HO equation (II.14), we have solved the time evolution problem. There still remains the question of selecting, from all possible Hamiltonian eigenstates (II.12), the ones which are eigenstates of the charge operator. To address this problem we now specialize the discussion to stationary field states.

B. Stationary field states

The stationary solutions of the HO Schrödinger equation (II.14) are

$$\psi_{an}(\tilde{\phi}_{an},t) = e^{-i(p_{an}+(1/2))\,\epsilon_n t}\, \chi_{p_{an}}(\sqrt{\epsilon_n}\tilde{\phi}_{an}), \quad \epsilon_n^2 = \omega_n^2 + m^2, \quad p_{an} = 0,1,\ldots, \tag{II.16}$$

where (suppressing subscripts)

$$\chi_p(\sqrt{\epsilon}x)\equiv\left[\frac{1}{2^p p!}\sqrt{\frac{\epsilon}{\pi}}\right]^{1/2} e^{-(1/2)\epsilon x^2} H_p(\sqrt{\epsilon}x), \tag{II.17}$$

and $H_{an}\psi_{an}=(p_{an}+\frac{1}{2})\epsilon_n\psi_{an}$. The $H_p(z)$ are Hermite polynomials satisfying $H_p''-2zH_p'+2pH_p=0$. By inserting the stationary modes (II.16) into the wave functional (II.12) with an arbitrary integer p_{an} for each factor ψ_{an}, one obtains a complete orthonormal basis set of stationary wave functionals for the system, all of these being eigenstates of the Hamiltonian (II.11). Let us give this basis set the shorthand name

$$\Psi(\{p_{an}\})\equiv\text{functional (II.12) with } \psi_{an} \text{ as in Eq. (II.16).} \tag{II.18}$$

Then,

$$\mathbb{H}\Psi(\{p_{an}\})=E(\{p_{an}\})\Psi(\{p_{an}\}), \tag{II.19}$$

with energy eigenvalues

$$E(\{p_{an}\})=\sum_n (p_{1n}+p_{2n}+1)\epsilon_n. \tag{II.20}$$

However, the Hamiltonian eigenstates (II.18) are not eigenstates of the charge operator. To see this we recall that the current operator associated with the Lagrangian (II.4) is

$$j_\mu=\frac{\partial\mathcal{L}}{\partial A^\mu}=i\phi^* D_\mu\phi-i(D_\mu\phi)^*\phi. \tag{II.21}$$

This current density is conserved, $\partial^\mu j_\mu=0$, by virtue of the equation of motion,

$$(D_\mu D^\mu+m^2+V)\phi=0 \tag{II.22}$$

obtained from $\mathcal{L}$. The charge density is therefore

$$j_0=i[\Pi^*\phi^*-\Pi\phi]=\sum_{n,m}\varphi_n(\mathbf{x})\varphi_m^*(\mathbf{x})Q_{nm}, \tag{II.23}$$

where

$$Q_{nm}=\tilde{\phi}_m^*\frac{\partial}{\partial\tilde{\phi}_n^*}-\tilde{\phi}_n\frac{\partial}{\partial\tilde{\phi}_m}=\frac{1}{2}\left[\tilde{\phi}_{1m}\frac{\partial}{\partial\tilde{\phi}_{1n}}-\tilde{\phi}_{1n}\frac{\partial}{\partial\tilde{\phi}_{1m}}+(1\to 2)\right]$$
$$+\frac{i}{2}\left[\tilde{\phi}_{1m}\frac{\partial}{\partial\tilde{\phi}_{2n}}+\tilde{\phi}_{1n}\frac{\partial}{\partial\tilde{\phi}_{2m}}-(1\leftrightarrow 2)\right]. \tag{II.24}$$

The total charge operator is

$$Q=\int d\mathbf{x} j_0(\mathbf{x})=\sum_m Q_{mm}. \tag{II.25}$$

Acting on the wave functional (II.12) it gives

$$Q\,\Psi[\phi,t]=\sum_m Q_{mm}\prod_n \psi_{1n}\psi_{2n}=\sum_m Q_{mm}\psi_{1m}\psi_{2m}\prod_{n\neq m}\psi_{1n}\psi_{2n}, \tag{II.26}$$

where

$$
\begin{aligned}
i\,Q_{mm}\,\psi_{1m}\,\psi_{2m} &= \tilde{\phi}_{2m}\psi'_{1m}\,\psi_{2m} - \tilde{\phi}_{1m}\psi'_{2m}\,\psi_{1m} \\
&= \tilde{\phi}_{2m}\,\partial_{1m}H_{p_{1m}}(\sqrt{\epsilon_m}\tilde{\phi}_{1m})\,H_{p_{2m}}(\sqrt{\epsilon_m}\tilde{\phi}_{2m}) \\
&\quad - \tilde{\phi}_{1m}\,\partial_{2m}H_{p_{2m}}(\sqrt{\epsilon_m}\tilde{\phi}_{2m})\,H_{p_{1m}}(\sqrt{\epsilon_m}\tilde{\phi}_{1m}),
\end{aligned}
\tag{II.27}
$$

with the short-hand notation $\partial_{1m} := \partial/\partial\tilde{\phi}_{1m}$.

Clearly, the only way one can make Eq. (II.26) into an eigenvalue equation is to choose all the $p_{1,2m}=0$, in which case the right-hand side vanishes. This selects the vacuum functional $\Psi_0[\phi,t]$ consisting entirely of factors (II.16) with $p_{an}=0$ as the only wave functional in the basis set (II.18) having definite charge, namely, $Q=0$.

To identify simultaneous eigenstates of the Hamiltonian $\mathbb{H}=\Sigma_n\mathbb{H}_n$ [with $\mathbb{H}_n=\mathbb{H}_{1n}+\mathbb{H}_{2n}$ as in Eq. (II.11)] and the charge operator $Q=\Sigma_n Q_{nn}$ [with Q_{nn} as in Eq. (II.24)] we now focus our attention on the two-dimensional (2D) functional subspace $(\tilde{\phi}_{1n},\tilde{\phi}_{2n})$ associated with a single mode $\varphi_n(\mathbf{x})$. If we arbitrarily introduce a third axis $\tilde{\phi}_{3n}$ perpendicular to the plane $(\tilde{\phi}_{1n},\tilde{\phi}_{2n})$ for the purpose of constructing a fictitious 3D "mode subspace," then obviously

$$
-Q_{nn}=\frac{1}{i}\left(\tilde{\phi}_{1n}\frac{\partial}{\partial\tilde{\phi}_{2n}}-\tilde{\phi}_{2n}\frac{\partial}{\partial\tilde{\phi}_{1n}}\right)=L_{3n}
\tag{II.28}
$$

can be identified with the third component of the angular momentum operator in this subspace. Thus in each mode subspace separately, the task of finding simultaneous eigenstates of $\mathbb{H}$ and Q reduces to the task of identifying simultaneous eigenstates of $\mathbb{H}_n$ and $Q_{nn}=L_{3n}$. The latter is a solved problem in quantum mechanics (see, e.g., Ref. 16, p. 727). We now briefly sketch this solution using the usual coordinate language of quantum mechanics.

In the 2D harmonic oscillator problem, a complete set of normalized stationary eigenstates of $\mathbb{H}=\frac{1}{2}\{-\partial_x^2-\partial_y^2+[\omega^2+m^2](x^2+y^2)\}$ and L_3 is given by[16]

$$
\psi_{pq}=\frac{1}{\sqrt{M!N!}}(a_R^\dagger)^M(a_L^\dagger)^N\psi_{00}\,e^{-i(p+1)\beta^2 t},
\tag{II.29}
$$

where M, N are non-negative integers and $p=M+N$, $q=N-M$,

$$
a_{R,L}^\dagger=\frac{1}{2}\left[\beta(x\pm iy)-\frac{1}{\beta}(\partial_x\pm i\partial_y)\right]=\frac{1}{2}e^{\pm i\theta}\left[\beta r-\frac{1}{\beta}\frac{\partial}{\partial r}\mp\frac{i}{\beta r}\frac{\partial}{\partial\theta}\right],
\tag{II.30}
$$

with $\beta^4=\omega^2+m^2$ and $x=r\cos\theta, y=r\sin\theta$. The ground state is

$$
\psi_{00}=\frac{\beta}{\sqrt{\pi}}e^{-\beta^2r^2/2}\,e^{-i\beta^2 t}
$$

and $a_{R,L}\,\psi_{00}=0$. Because

$$
\mathbb{H}=[a_R^\dagger a_R+a_L^\dagger a_L+1]\,\beta^2
\tag{II.31}
$$

and

$$
L_z=a_R^\dagger a_R-a_L^\dagger a_L
\tag{II.32}
$$

while

$$
[a_R,a_R^\dagger]=[a_L,a_L^\dagger]=1
$$

with other commutators vanishing, one easily verifies

$$\mathbb{H}\psi_{pq}=(p+1)\beta^2\psi_{pq} \tag{II.33}$$

and with $Q:=-L_3$,

$$Q\psi_{pq}=-q\psi_{pq}. \tag{II.34}$$

Note that $-p\leqslant q\leqslant p$ in steps of $\Delta q=2$. Thus for $p=1$ we have states $\psi_{1,\pm 1}$, for $p=2$ the states $\psi_{2,\pm 2}$ and ψ_{20}, for $p=3$ the states $\psi_{3,\pm 3}$ and $\psi_{1,\pm 1}$, and so on. The following general formula can be given (for $N=p$, $M=0$ or $N=0$, $M=p$):

$$\psi_{p,\pm p}=e^{i(p+1)\beta^2 t}\frac{\beta}{\sqrt{\pi p!}}e^{\pm ip\theta}(\beta r)^p e^{-\beta^2 r^2/2}. \tag{II.35}$$

For $|q|<p$ it is more difficult to obtain general formulas. We note that for $N=M=1$,

$$\psi_{2,0}=e^{-i3\beta^2 t}\frac{\beta}{\sqrt{\pi}}[(\beta r)^2-1]e^{-\beta^2 r^2/2}, \tag{II.36}$$

and for $N=2$, $M=1$ or $N=1, M=2$,

$$\psi_{3,\pm 1}=e^{-i4\beta^2 t}e^{\pm i\theta}\frac{\beta^2}{\sqrt{2\pi}}r[(\beta r)^2-2]e^{-\beta^2 r^2/2}. \tag{II.37}$$

Returning to our QFT problem we can now replace the wave functional expression (II.12) by

$$\Psi(\{p_n,q_n\})=\prod_n \psi_{p_n q_n}(\tilde{\phi}_{1n},\tilde{\phi}_{2n},t) \tag{II.38}$$

with the correspondence $x\leftrightarrow\tilde{\phi}_{1n}$, $y\leftrightarrow\tilde{\phi}_{2n}$, $\beta\leftrightarrow\epsilon_n$ and $r_n^2=\tilde{\phi}_{1n}^2+\tilde{\phi}_{2n}^2$, $\theta_n=\arctan(\tilde{\phi}_{2n}/\tilde{\phi}_{1n})$. Clearly the functional (II.38) is a simultaneous eigenfunctional of $\mathbb{H}$ and Q with energy eigenvalue

$$E(\{p_n\})=\sum_n (p_n+1)\epsilon_n \tag{II.39}$$

and charge

$$Q=-\sum_n q_n. \tag{II.40}$$

Thus we are now in possession of a complete set of physical stationary wave functionals for the system, each with definite energy and charge, representing all possible stationary states with an arbitrary number of particles having arbitrary charge compatible with the particle number.

C. Field expectation values

One field expectation value of interest is that of the charge density operator,

$$\begin{aligned}
&\langle \Psi(\{p_n,q_n\})|j_0(\mathbf{x})|\Psi(\{p_n,q_n\})\rangle \\
&\quad=\int \prod_n d\tilde{\phi}_{1n} d\tilde{\phi}_{2n}\, \Psi^*(\{p_n,q_n\}) \sum_{l,m} \varphi_l \varphi_m^* Q_{lm} \Psi(\{p_n,q_n\}) \\
&\quad=\sum_{\substack{l,m \\ l\neq m}} \int d\tilde{\phi}_{1l} d\tilde{\phi}_{2l} d\tilde{\phi}_{1m} d\tilde{\phi}_{2m}\, \varphi_l \varphi_m^*\, \psi^*_{p_l q_l} \psi^*_{p_m q_m} Q_{lm}\, \psi_{p_l q_l} \psi_{p_m q_m} \\
&\qquad+\sum_m \int d\tilde{\phi}_{1m} d\tilde{\phi}_{2m}\, \varphi_m \varphi_m^*\, \psi^*_{p_m q_m} Q_{mm}\, \psi_{p_m q_m} = -\sum_m q_m |\varphi_m(\mathbf{x})|^2. \qquad \text{(II.41)}
\end{aligned}$$

Here in the second equality every term with $l\neq m$ contributes zero by symmetry arguments. For $l\neq m$, Q_{lm} is odd under $\tilde{\phi}_{jl}\to-\tilde{\phi}_{jl}$ $(j=1,2)$ while the remaining factors in the integrand (including the integration measure) are even under this replacement. Thus the area integrals over the upper and lower half of the $\tilde{\phi}_{1l}$–$\tilde{\phi}_{2l}$-plane cancel. However in those terms with $l=m$, the eigenvalue equation $Q_{mm}\,\psi_{p_m q_m}=-q_m\psi_{p_m q_m}$ eliminates Q_{mm}, leaving a trivial integration over normalized wave functions. For normalizable modes $\varphi_n(\mathbf{x})$, Eqs. (II.40) and (II.41) are in agreement. In Eq. (II.41) we see that the charge of a real particle in the mth mode is distributed (in general nonuniformly) throughout all the space occupied by the spatial mode $\varphi_m(\mathbf{x})$.

Formulas such as (II.41) are problematic in infinite space where one has to deal with nonnormalizable modes. For example, if the modes are plane waves $\varphi(\mathbf{x})\to(2\pi)^{-3/2}\exp(i\mathbf{k}\cdot\mathbf{x})$ with δ-function normalization, then in Eq. (II.41) there is a contribution $-q(2\pi)^{-3/2}$ to the density $\langle j_0(\mathbf{x})\rangle$ from each real excitation. Such a term in $\langle j_0(\mathbf{x})\rangle$ leads to infinite charge Q, and the discrete mode notation we are using fails. This difficulty is eliminated if one makes free boundaryless space compact, say by means of toroidal compactification,

$$\varphi(\mathbf{x})\to[L_1L_2L_3]^{-1/2}e^{i2\pi[x_1n_1/L_1+x_2n_2/L_2+x_3n_3/L_3]},$$

where the n_i run over all integers and the toroidal compactification lengths L_i are independent parameters. Then the contributions to the charge density $\langle j_0(\mathbf{x})\rangle$ from individual particle excitations are $-q/L_1L_2L_3$, and the corresponding contribution to Q is $-q$, as in Eq. (II.40).

Another important expectation value is that of the stress-energy-momentum tensor $T_{\mu\nu}$. For the scalar field theory in question the canonical, symmetric $T_{\mu\nu}$ is

$$T_{\mu\nu}=(D_\mu\phi)^*D_\nu\phi+(D_\nu\phi)^*D_\mu\phi-\eta_{\mu\nu}\mathcal{L}, \qquad \text{(II.42)}$$

where $\mathcal{L}$ is the Lagrange density (II.4). Using the equation of motion $[D^2+m^2+V(\mathbf{x})]\phi=0$ and the corresponding complex conjugate equation one finds

$$\partial^\mu T_{\mu\nu}=F_{\mu\nu}j^\mu+(\partial_\nu V)\phi^*\phi, \qquad \text{(II.43)}$$

where j_μ is the current density (II.21) and $F_{\mu\nu}=\partial_\mu A_\nu-\partial_\nu A_\mu$. Appropriately, $T_{\mu0}$ is conserved only if $F_{i0}=0$, i.e., if no background electric field is present. The static potential $V(\mathbf{x})$ does not influence the conservation of $T_{\mu0}$.

To calculate the expectation value $T_{\mu\nu}[\Psi]\equiv\langle\Psi|T_{\mu\nu}|\Psi\rangle$ for any field state $|\Psi\rangle$ of interest one needs certain basic matrix elements. One of these is

$$\langle\{p_n,q_n\}|\hat{\phi}^*(\mathbf{x})\hat{\phi}(\mathbf{y})|\{p_n,q_n\}\rangle=\int\prod_n\,[d\tilde{\phi}_{1n}\,d\tilde{\phi}_{2n}]|\psi_{p_nq_n}|^2\frac{1}{2}\sum_{c,d}\,\varphi_c^*(\mathbf{x})\varphi_d(\mathbf{y})$$
$$\times(\tilde{\phi}_{1c}-i\tilde{\phi}_{2c})(\tilde{\phi}_{1d}+i\tilde{\phi}_{2d})$$
$$=\sum_n\,A(p_nq_n)\,\varphi_n^*(\mathbf{x})\varphi_n(\mathbf{y}),\tag{II.44}$$

where

$$A(p_n,q_n)=\frac{1}{2}\int\,d\tilde{\phi}_{1n}\,d\tilde{\phi}_{2n}\,|\psi_{p_nq_n}|^2\,(\tilde{\phi}_{1n}^2+\tilde{\phi}_{2n}^2)=\frac{(p_n+1)}{2\epsilon_n}.\tag{II.45}$$

Symmetry arguments similar to those leading to the final equation in (II.41) yield the final equality in Eq. (II.42), and the second equality in Eq. (II.45) follows immediately from the virial theorem applied to the harmonic oscillator.

Another basic matrix element is

$$\langle\{p_n,q_n\}|\hat{\Pi}^*(\mathbf{x})\,\hat{\Pi}(\mathbf{y})|\{p_n,q_n\}\rangle=-\int\prod_n\,[d\tilde{\phi}_{1n}\,d\tilde{\phi}_{2n}]\,\Psi^*_{p_nq_n}\frac{1}{2}\sum_{c,d}\,\varphi_c(\mathbf{x})\varphi_d^*(\mathbf{y})$$
$$\times\left[\frac{\partial}{\partial\tilde{\phi}_{1c}}+i\frac{\partial}{\partial\tilde{\phi}_{2c}}\right]\left[\frac{\partial}{\partial\tilde{\phi}_{1d}}-i\frac{\partial}{\partial\tilde{\phi}_{2d}}\right]\Psi_{p_nq_n}$$
$$=\sum_n\,B(p_nq_n)\,\varphi_n(\mathbf{x})\,\varphi_n^*(\mathbf{y}),\tag{II.46}$$

where

$$B(p_n,q_n)=\frac{1}{2}\int\,d\tilde{\phi}_{1n}\,d\tilde{\phi}_{2n}\,\psi^*_{p_nq_n}\left[-\frac{\partial^2}{\partial\tilde{\phi}_{1n}^2}-\frac{\partial^2}{\partial\tilde{\phi}_{2n}^2}\right]\psi_{p_nq_n}=\tfrac{1}{2}(p_n+1)\,\epsilon_n\,.\tag{II.47}$$

Again symmetric area integration is used to reach the second equality in Eq. (II.46). We pause briefly to explain the two integrals (II.45) and (II.47).

According to the virial theorem of quantum mechanics one has, for any stationary state, the expectation value identity,

$$\langle|(\mathbf{r}\cdot\boldsymbol{\nabla})V|\rangle=\langle\mathbf{p}^2\rangle.\tag{II.48}$$

For the 2D harmonic oscillator problem with $V=(\epsilon^2/2)\,(x^2+y^2)$, Eq. (II.48) becomes $\langle V\rangle=\langle T\rangle=\langle\mathbf{p}^2/2\rangle$. Since $\langle T\rangle+\langle V\rangle=E$ it follows that $\langle V\rangle=\langle T\rangle=E/2$. Equations (II.45) and (II.47) express this latter result for the states $\psi_{p_nq_n}$.

Now it is easy to express the elements of $T_{\mu\nu}(\{p_n,q_n\})$ in mode-sum form,

$$T_{00}(\{p_nq_n\})=\langle\{p_n,q_n\}|2\Pi^\dagger\Pi-\mathcal{L}|\{p_n,q_n\}\rangle=\sum_n\,(p_n+1)\,\epsilon_n\,|\varphi_n(\mathbf{x})|^2-\mathcal{L}(\{p_n,q_n\}),\tag{II.49}$$

where

$$\mathcal{L}(\{p_n,q_n\}) = \langle \{p_n q_n\} | \Pi^\dagger \Pi - |\mathbf{D}\phi|^2 - (m^2+V)|\phi|^2 | \{p_n q_n\} \rangle$$
$$= \frac{1}{2}\sum_n \frac{1}{\epsilon_n}(p_n+1)\{[\epsilon_n^2 - m^2 - V]|\varphi_n|^2 - |\mathbf{D}\varphi_n|^2\}$$
$$= \frac{1}{2}\sum_n \frac{1}{\epsilon_n}(p_n+1)\{\varphi_n^*(-\mathbf{D}^2)\varphi_n - |\mathbf{D}\varphi_n|^2\}; \tag{II.50}$$

also

$$T_{ii}(\{p_n,q_n\}) = \langle \{p_n,q_n\} | 2\,(D_i\phi)^*(D_i\phi) + \mathcal{L} | \{p_n,q_n\} \rangle$$
$$= \sum_n \frac{p_n+1}{\epsilon_n}|D_i\varphi_n|^2 + \mathcal{L}(\{p_n,q_n\}), \quad i=1,2,3, \tag{II.51}$$

$$T_{ij}(\{p_n,q_n\}) = \sum_n \frac{p_n+1}{2\epsilon_n}\{(D_i\varphi_n)^* D_j\varphi_n + (D_j\varphi_n)^* D_i\varphi_n\} \quad i\neq j. \tag{II.52}$$

It is important to observe that

$$T_{\mu\nu}(\{p_n,q_n\}) = T_{\mu\nu}[\Psi_0] + \sum_n p_n T_{n\mu\nu}, \tag{II.53}$$

where $T_{n\mu\nu}$ represents the contribution from one real particle in the nth mode to $T_{\mu\nu}$. As long as $\Sigma_n p_n < \infty$ (i.e., the field state contains only a finite number of real particles) only the vacuum contribution $T_{\mu\nu}[\Psi_0]$ can be UV divergent. Thus only $T_{\mu\nu}[\Psi_0]$ needs renormalization.

III. EXAMPLES

The first example is that of a uniform magnetic field **B** in empty space (compactified appropriately so that the field modes are normalizable). This is hardly a new problem except that we are able to give $T_{\mu\nu}$ not only for the vacuum state Ψ_0, but also for all stationary excited field states $\Psi(\{p_n,q_n\})$. Then we observe that factorization enables one to introduce an arbitrary static potential V depending only on x^1, if we choose our coordinate system so that $\mathbf{B}=(B,0,0)$. Indeed, if one can solve the Casimir problem posed by a given background structure along, say, spatial direction x^1, then one can also solve this Casimir problem with added background magnetic field $\mathbf{B}=(B,0,0)$. As an example we present results for two parallel planar Dirichlet boundaries, with these planes perpendicular to the uniform magnetic field **B**.

A. Uniform magnetic field in empty space

To introduce a uniform background magnetic field $\mathbf{B}=(B,0,0)$ we choose the vector potential,

$$\mathbf{A}=(A^1,A^2,A^3)=(0,0,Bx^2). \tag{III.1}$$

Note that the spatial directions $x^{2,3}$ are treated differently by this gauge choice, and that x^2 plays a preferred role in what follows. Because we are going to keep x^2 noncompact, while x^3 will be compactified (see below), the usual gauge freedom displayed by

$$\mathbf{A}=(0,-\alpha x^3 B,\beta x^2 B), \tag{III.2}$$

with $\alpha+\beta=1$ is not available here. There are a number of things to be said about this. For example, the gauge transformation $\lambda=\alpha x^2 x^3 B$ linking the potentials (III.1) and (III.2) cannot be performed for compact x^3, because it introduces nonperiodic dependence on x^3 into the scalar field. Only if we make x^3 noncompact does this conflict disappear, and the gauge potential (III.2) then becomes available.

Alternatively, one can ask if the potential (III.2) is physically acceptable. The answer is—evidently not, as long as x^3 is compact, because (bosonic) physical functions should be periodic around x^3, and the potential (III.2) does not fulfill this criterion unless $\alpha=0$. The reader should also note that we are compactifying x^1 which further reduces the gauge invariance one usually associates with the uniform magnetic field **B**. In Sec. III D, we discuss the question of gauge invariance in somewhat more detail.

In empty space $V(\mathbf{x})$ vanishes. The label n in our general notation is replaced by (k_1,ν,k_3). The modes $\varphi_{k_1\nu k_3}$ are

$$\varphi_{k_1\nu k_3}(\mathbf{x})\to\frac{1}{\sqrt{L_1}}e^{ik_1x^1}\,\psi_{\nu k_3}(x^2)\,\frac{1}{\sqrt{L_3}}e^{ik_3x^3}, \tag{III.3}$$

where $k_{1,3}=2\pi n_{1,3}/L_{1,3}$ with $n_{1,3}$ running over all integers. In order to have normalizable modes we have compactified the x^1 and x^3 spatial directions. Then the mode Eq. (II.7) reduces to the 1D HO equation (as noted by Landau many years ago[17])

$$\left[-\partial_2^2+B^2\left(x^2+\frac{k_3}{B}\right)^2\right]\psi_{\nu k_3}(x^2)=2B\,(\nu+\tfrac{1}{2})\,\psi_{\nu k_3}(x^2), \tag{III.4}$$

whose complete orthonormal stationary solutions are (with $\nu=0,1,2,\ldots$)

$$\psi_{\nu k_3}(x^2)=\chi_\nu\left(\sqrt{B}\left(x^2+\frac{k_3}{B}\right)\right) \tag{III.5}$$

as specified by Eq. (II.17). In the general notation of Eq. (II.7) the eigenvalues ω_n^2 now become $k_1^2+2B(\nu+\frac{1}{2})$.

Setting all the excitation values $p_n=0$ in Eqs. (II.49)–(II.52) we obtain the vacuum stress tensor $T_{\mu\nu}[\Psi_0]$. Thus using various formulas from Appendix A we find

$$\begin{aligned}T_{00}[\Psi_0]+\mathcal{L}[\Psi_0]&=\frac{1}{L_1L_3}\sum_{n_1,n_3}\sum_{\nu}\,[2B(\nu+\tfrac{1}{2})+k_1^2+m^2]^{1/2}\,|\psi_{\nu k_3}(x^2)|^2\\&=-\int_0^\infty dt\,(4\pi t)^{-2}\,e^{-t\,m^2}\frac{B}{\sinh Bt}\,f_1(t)\,f_3(t|x^2),\end{aligned} \tag{III.6}$$

where

$$f_1(t)=1+2\sum_{n=1}^{\infty}\,e^{-n^2L_1^2/4t}, \tag{III.7}$$

$$f_3(t|x^2)=1+\sum_{n=1}^{\infty}\,e^{-n^2BL_3^2/4\tanh Bt}2\cos(nx^2BL_3); \tag{III.8}$$

and

$$\mathcal{L}[\Psi_0]=\int_0^\infty dte^{-tm^2}(4\pi t)^{-1}\,f_1(t)\frac{1}{L_3}\sum_{n_3}\,\sum_{\nu=0}^{\infty}\,e^{-2B(\nu+\frac{1}{2})t}\{-\psi_{\nu k_3}\psi''_{\nu k_3}-(\psi'_{\nu k_3})^2\} \tag{III.9}$$

$$=-(4\pi)^{-2}\int_0^\infty dt\,e^{-tm^2}t^{-1}f_1(t)\,\frac{B}{2\sinh Bt}\,\partial_2^2f_3, \tag{III.10}$$

where $\partial_2=\partial/\partial x^2$. Note that $\mathcal{L}[\Psi_0]$ is finite. Also

$$T_{11}[\Psi_0]-\mathcal{L}[\Psi_0]=\frac{1}{L_1L_3}\sum_{n_1,n_3}\sum_{\nu}\,[2B(\nu+\tfrac{1}{2})+k_1^2+m^2]^{-(1/2)}\,k_1^2|\psi_{\nu k_3}(x^2)|^2$$

$$=\int_0^\infty dt(4\pi t)^{-2}\,e^{-tm^2}\frac{B}{\sinh Bt}g_1(t)f_3(t|x^2), \tag{III.11}$$

where

$$g_1(t)=1+2\sum_{n=1}^{\infty}\left[1-\frac{n^2L_1^2}{2t}\right]e^{-n^2L_1^2/4t}; \tag{III.12}$$

$$T_{22}[\Psi_0]-\mathcal{L}[\Psi_0]=\frac{1}{L_1L_3}\sum_{n_1,n_3}\sum_{\nu}\,[2B(\nu+\tfrac{1}{2})+k_1^2+m^2]^{-(1/2)}|\psi'_{\nu k_3}(x^2)|^2$$

$$=\frac{1}{(4\pi)^2}\int_0^\infty dt\,e^{-t\,m^2}\,t^{-1}\frac{B^2\cosh Bt}{\sinh^2 Bt}f_1(t)$$

$$\times\left\{f_3(t|x^2)+\frac{\sinh Bt}{2B\cosh Bt}\partial_2^2 f_3(t|x^2)\right\}, \tag{III.13}$$

or more simply,

$$T_{22}[\Psi_0]=\left(\frac{B}{4\pi}\right)^2\int_0^\infty dt\,e^{-tm^2}\,t^{-1}\,f_1(t)\,\frac{\cosh Bt}{\sinh^2 Bt}f_3(t|x_2); \tag{III.14}$$

$$T_{33}[\Psi_0]-\mathcal{L}[\Psi_0]=\frac{1}{L_1L_3}\sum_{n_1,n_3}\sum_{\nu}\,[2B(\nu+\tfrac{1}{2})+k_1^2+m^2]^{-(1/2)}(k_3+Bx^2)^2|\psi_{\nu k_3}(x^2)|^2$$

$$=\frac{1}{(4\pi)^2}\int_0^\infty dt\,e^{-tm^2}t^{-1}\frac{B^2\cosh Bt}{\sinh^2 Bt}f_1(t)\left\{f_3(t|x^2)+\frac{\cosh Bt}{2B\sinh Bt}\partial_2^2 f_3(t|x^2)\right\}. \tag{III.15}$$

One readily verifies that $T_{ij}[\Psi_0]=0$ for $i\neq j$.

$T_{\mu\nu}[\Psi_0]$ of course requires renormalization. Because

$$\frac{B}{\sinh Bt}=\frac{1}{t}-\frac{B^2t}{6}+\frac{7B^4t^3}{360}-\cdots$$

$$\cosh Bt\left(\frac{B}{\sinh Bt}\right)^2=\frac{1}{t^2}+\frac{B^2}{6}-\frac{7B^4t^2}{120}+\cdots \tag{III.16}$$

one can easily regularize $T_{\mu\nu}[\Psi_0]$ by subtracting from $T_{\mu\nu}[\Psi_0]$ the divergent terms

$$T_{00}[\Psi_0]_{\rm div}=-T_{11}[\Psi_0]_{\rm div}=-\int_0^\infty dt(4\pi t)^{-2}\,e^{-tm^2}\left[\frac{1}{t}-\frac{B^2t}{6}\right], \tag{III.17}$$

$$T_{22}[\Psi_0]_{\rm div}=T_{33}[\Psi_0]_{\rm div}=\int_0^\infty dt\,\frac{1}{(4\pi)^2t}e^{-tm^2}\left[\frac{1}{t^2}+\frac{B^2}{6}\right]. \tag{III.18}$$

Thus we define

$$T_{\mu\nu}^{ren}\equiv T_{\mu\nu}[\Psi_0]-T_{\mu\nu}[\Psi_0]_{\rm div}. \tag{III.19}$$

Note that

$$T_{\mu\nu}[\Psi_0]_{\rm div} = T_{\mu\nu}[\Psi_0]_{B=0} + T^B_{\mu\nu} C,$$

where $T^B_{00} = -T^B_{11} = T^B_{22} = T^B_{33} = -B^2/8\pi$ is the classical stress tensor for the background magnetic field $\mathbf{B} = (B,0,0)$ and C is a divergent constant. This allows the absorption of the $O(B^2)$ terms in Eqs. (III.17), (III.18) into $T^B_{\mu\nu}$.

Returning to $T_{\mu\nu}(\{p_n, q_n\})$ for an excited field state, the renormalization procedure just described renormalizes all of these tensors as well, as long as the excitation numbers p_n decrease sufficiently rapidly with increasing n so that $T_{\mu\nu}(\{p_n, q_n\}) - T_{\mu\nu}[\Psi_0]$ is finite. The contribution of one real particle to T_{00} and to the charge density j_0 are $T_{n00} = \epsilon_n |\varphi_n|^2$ and $j_0 = -q_n |\varphi_n|^2$, where

$$|\varphi_n(\mathbf{x})|^2 = \frac{1}{L_1 L_3 2^\nu \nu!} \sqrt{\frac{B}{\pi}} e^{-B(x^2 + k_3/B)^2} [H_n(\sqrt{B}(x^2 + k_3/B))]^2.$$

To those unfamiliar with the Landau modes (III.3) this expression may look peculiar. $|\varphi_n(\mathbf{x})|^2$ represents (in quantum mechanical language) a layer of probability density uniformly distributed in the directions x^1 and x^3, centered at the plane $x^2 = -k_3/B$ and thinning exponentially away from this central plane. This probability layer with thickness $\Delta x^2 \approx 1/\sqrt{B}$ is as close as wave mechanics can come to reproducing the spiral classical trajectory of a charged particle in the uniform magnetic field $\mathbf{B} = (B,0,0)$. Circular motion in the $(x^2 x^3)$ plane is suggested in the modes Eq. (III.3) by the exponential decrease in probabilty amplitude away from $x^2 = -k_3/B$. At the same time, translation invariance along x^3 and along the magnetic field direction x^1 are built into the modes (III.3). The preferred role played by x^2 in Eq. (III.3) is merely a consequence of our gauge choice (III.1). If we were to choose other gauges we would rotate the ''probability layer'' in the $x^2 x^3$ plane about some axis parallel to the magnetic field. The x^1 dependence in Eq. (III.3) would be uneffected. In the example to follow similar comments can be made about the contribution of real particles to $T_{\mu\nu}$. Only the x^1 mode factors need to be modified. Thus we shall not say more about this in Secs. III B and III C.

What effect, exactly, does the background magnetic field **B** have on states of the quantum field? This question is rarely addressed—we know of no discussion in the literature—although surely many have thought about it. Quantum fluctuations of the charged scalar field $\hat{\phi}$ can be visualized in particle terms as electric dipoles. A dipole of vanishing size emerges from the fluctuating vacuum, grows to some maximum size, and shrinks again to nothing. In empty space with $\mathbf{B} = 0$ these dipoles have all possible orientations. In the presence of $\mathbf{B} \neq 0$ the dipoles oriented parallel to **B** are unaffected. However, dipoles oriented perpendicular to **B** are strongly effected. They change from linear dipole-like fluctuations to transient current loops. These transient current loops tend to be oriented such that their magnetic fields oppose **B**. Thus **B** modifies and significantly organizes the quantum fluctuations of the charged scalar field $\hat{\phi}$. The charged-particle vacuum responds like a diamagnetic material.

The factors $f_1(t)$ in $T_{00,22,33}$ and $g_1(t)$ in T_{11} resulting from the compactification of x^1 go smoothly to 1 in the limit $L_1 \to \infty$. More interesting is the factor $f_3(t|x^2)$ common to all nonzero components of $T_{\mu\nu}[\Psi_0]$. Surprisingly, perhaps, this factor is a Fourier cosine series in x^2 with period $\Delta x^2 = 2\pi/BL_3$ (as was mentioned elsewhere[13,18] in a related context). This periodic behavior in the *noncompact* coordinate x^2 is a consequence of both the background magnetic field and the compactification of the perpendicular direction x^3. In either of the limits $L_3 \to \infty$ or $B \to 0$ we see that $f_3(t|x^2) \to 1$. Evidently one is encountering here a physical quantum effect akin to the quantum Hall effect, with vacuum currents flowing around the compact x^3 direction. To verify this we compute the vacuum current density,

$$j_3[\Psi_0]=\langle\Psi_0|i\hat{\phi}^*(D_3\hat{\phi})-i(D_3\hat{\phi})^*\hat{\phi}|\Psi_0\rangle$$
$$=\frac{1}{L_1L_3}\sum_{n_1,n_3}\sum_{\nu}\left[k_1^2+2B(\nu+\tfrac{1}{2})+m^2\right]^{-1/2}(k_3+Bx^2)|\psi_{\nu k_3}|^2$$
$$=\int_0^\infty dt\,e^{-tm^2}(4\pi t)^{-1}f_1(t)\frac{B\cosh Bt}{4\pi\sinh^2 Bt}\partial_2 f_3, \tag{III.20}$$

which is indeed nonzero. However, the other components of the vacuum current vanish: $j_{1,2}[\Psi_0]=0$. In the limit $L_3\to\infty$ when $f_3\to 1$, the current density (III.20) vanishes exponentially. Clearly, vacuum currents around the compact direction x^3 are involved. Quantum fluctuations, visualized as vacuum pairs, can appear on one side of the x^3 circle and annihilate on the other side by traveling in opposite directions. Such vacuum currents are only possible for $L_3<\infty$. The perpendicular B field organizes these vacuum currents into a band structure periodic in x^2.

From the conservation formula (II.43) we see that

$$-\partial_2 T_{22}=F_{32}j^3=B\,j^3. \tag{III.21}$$

The formulas (III.14), (III.20) for T_{22} and j^3 obviously satisfy this relation.

B. Uniform magnetic field with parallel background force

The factorization in Eq. (III.3) (where the x^1 dependent mode factor is independent of $x^{2,3}$ and ν,k_3) enables one to introduce rather arbitrary background structure along x^1, without disturbing the rest of the calculation. Accordingly, in mode equation (II.7), we choose a potential of the form $V(\mathbf{x})=V(x^1)$ and replace the plane wave factors $\exp(ik_1x^1)/\sqrt{L_1}$ in Eq. (III.3) by unknown functions $u_p(x^1)$. Now the mode equation (II.7) reduces to

$$\left[-\frac{d^2}{dx^{1^2}}+V(x^1)\right]u_p(x^1)=\lambda_p^2\,u_p(x^1) \tag{III.22}$$

in addition to Eq. (III.4) which is uneffected by the introduction of $V(x^1)$. In our general notation $\omega_n^2\to\lambda_p^2+2B(n+1/2)$ with λ_p^2 replacing k_1^2. Equation (II.44) for the vacuum field state Ψ_0 becomes

$$\langle\Psi_0|\hat{\phi}^*(\mathbf{x})\hat{\phi}(\mathbf{y})|\Psi_0\rangle=\frac{1}{2\Gamma(s)}\int_0^\infty dt e^{-tm^2}t^{s-1}h(t|x^1,y^1)\sum_n e^{-tB(2n+1)}$$
$$\times\frac{1}{L_3}\sum_{n_3}e^{-ik_3(x^3-y^3)}\psi_{nk_3}(x^2)\psi_{nk_3}(y^2), \tag{III.23}$$

with $s=1/2$, where

$$h(t|x^1,y^1)=\sum_p e^{-t\lambda_p^2}u_p^*(x^1)u_p(y^1) \tag{III.24}$$

is the heat kernel associated with the spectral problem (III.22).

Similarly $\langle\Psi_0|\hat{\Pi}^*(\mathbf{x})\hat{\Pi}(\mathbf{y})|\Psi_0\rangle$ is given by the right-hand side of Eq. (III.23) with $s=-\frac{1}{2}$.

Now it is straighforward to evaluate the basic mode sums needed for $T_{\mu\nu}[\Psi_0]$ in terms of the still general heat kernel h,

$$\sum_n \epsilon_n|\varphi_n|^2=-\frac{2\sqrt{\pi}}{(4\pi)^2}\int_0^\infty dt\,e^{-tm^2}t^{-(3/2)}\frac{B}{\sinh Bt}h(t|x^1,x^1)f_3, \tag{III.25}$$

$$\sum_n \frac{1}{\epsilon_n}|D_1\varphi_n|^2=\frac{4\sqrt{\pi}}{(4\pi)^2}\int_0^\infty dt\, e^{-tm^2}t^{-(1/2)}\frac{B}{\sinh Bt}[\partial_{x^1}\partial_{y^1}h(t|x^1,y^1)]_{x^1=y^1}f_3, \quad \text{(III.26)}$$

$$\sum_n \frac{1}{\epsilon_n}|D_2\varphi_n|^2=\frac{2\sqrt{\pi}}{(4\pi)^2}\int_0^\infty dt\, e^{-tm^2}t^{-(1/2)}\frac{B^2\cosh Bt}{\sinh^2 Bt}h(t|x^1,x^1)\left\{f_3+\frac{\sinh Bt}{2B\cosh Bt}\partial_2^2 f_3\right\}, \quad \text{(III.27)}$$

$$\sum_n \frac{1}{\epsilon_n}|D_3\varphi_n|^2=\frac{2\sqrt{\pi}}{(4\pi)^2}\int_0^\infty dt\, e^{-tm^2}t^{-(1/2)}\frac{B^2\cosh Bt}{\sinh^2 Bt}h(t|x^1,x^1)\left\{f_3+\frac{\cosh Bt}{2B\sinh Bt}\partial_2^2 f_3\right\}, \quad \text{(III.28)}$$

$$\mathcal{L}=-\int_0^\infty dt\, e^{-tm^2}(4\pi t)^{-1/2}\frac{B}{4\pi\sinh Bt}\{(\partial_{y^1}^2+\partial_{x^1}\partial_{y^1})h(t|x^1,y^1)|_{x^1=y^1}f_3+h(t|x^1,x^1)\tfrac{1}{2}\partial_2^2 f_3\}, \quad \text{(III.29)}$$

where $f_3=f_3(t|x^2)$ is the function (III.8). Again we have used equations from the Appendix.

Note that in the limit $L_3\to\infty$ when $f_3\to 1$ the mode sums

$$\frac{1}{\epsilon_n}\sum_n |D_{2,3}\varphi_n|^2$$

become identical, insuring that $T_{22}[\Psi_0]=T_{33}[\Psi_0]$ for any background potential $V(x^1)$. However, $T_{22}[\Psi_0]\neq T_{33}[\Psi_0]$ for finite L_3.

One easily verifies

$$T_{22}=\int_0^\infty dt\, e^{-tm^2}(4\pi t)^{-1/2}\frac{B}{4\pi\sinh Bt}f_3\left\{h\,B\frac{\cosh Bt}{\sinh Bt}-(\partial_{y^1}^2+\partial_{x^1}\partial_{y^1})h|_{x^1=y^1}\right\}, \quad \text{(III.30)}$$

$$\begin{aligned}T_{12}&=\sum_n \frac{1}{2\epsilon_n}[(\partial_1\varphi_n)^*\partial_2\varphi_n+(\partial_2\varphi_n)^*\partial_1\varphi_n]\\&=\int_0^\infty dt e^{-tm^2}(4\pi t)^{-1/2}\frac{B}{8\pi\sinh Bt}(\partial_{x^1}+\partial_{y^1})h|_{x^1=y^1}\partial_2 f_3,\end{aligned} \quad \text{(III.31)}$$

$$\begin{aligned}T_{11}&=\sum_n \frac{1}{\epsilon_n}|\partial_1\varphi_n|^2+\mathcal{L}\\&=\int_0^\infty dt\, e^{-tm^2}(4\pi t)^{-1/2}\frac{B}{4\pi\sinh Bt}\left\{(\partial_{x^1}\partial_{y^1}-\partial_{y^1}^2)h\,f_3-\frac{1}{2}h\,\partial_2^2 f_3\right\}_{x^1=y^1},\end{aligned} \quad \text{(III.32)}$$

while $T_{23}=0$. Similarly $T_{13}=0$ if $\partial_{x^1}h=\partial_{y^1}h$ for $x^1=y^1$, as we do assume. For the vacuum currents we have

$$j^3=\int_0^\infty dt\, e^{-tm^2}(4\pi t)^{-1/2}h|_{x_1=y_1}\frac{B\cosh Bt}{4\pi\sinh^2 Bt}\partial_2 f_3, \quad \text{(III.33)}$$

while $j^2=0$, and $j^1=0$ under the same assumption that makes T_{13} vanish. The nontrivial parts of the conservation rule (II.43) are

$$-\partial_1 T_{11}-\partial_2 T_{21}=\partial_1 V\langle\phi^*\phi\rangle, \quad \text{(III.34)}$$

$$-\partial_1 T_{12}-\partial_2 T_{22}=F_{32}\,j^3. \tag{III.35}$$

One can verify that both relations are satisfied by our preceding quite specific and nontrivial results.

For brevity we do not discuss the renormalization of $T_{\mu\nu}[\Psi_0]$, other than to say that this is done essentially as in the free space example of Sec. III A. The vacuum current (III.33) does not need renormalization.

C. Uniform magnetic field perpendicular to two Dirichlet planes

Now let us consider the Casimir problem of parallel Dirichlet planes at $x^1=0$, L with a uniform background magnetic field perpendicular to them.

For $B=0$ the planes attract; how does $B\neq 0$ influence the Casimir force? Between the planes the mode factors $u_p(x^1)$ are

$$u_p(x^1)=\sqrt{\frac{2}{L}}\sin p\,\frac{\pi x^1}{L},\quad p=1,2,3,\ldots,\quad 0\leqslant x^1\leqslant L, \tag{III.36}$$

with eigenvalue $\lambda_p^2=(\pi p/L)^2$ in Eq. (III.22). Because of our compactification of coordinate x^1 in $0\leqslant x^1\leqslant L_1$ the region ''outside'' the planes has length L_1-L, where obviously we are assuming $L_1>L$. For the purpose of visualization one may as well assume that L_1 is substantially larger than L. Nonetheless our calculations will be exact. Outside the planes the mode factors $u_p(x^1)$ are

$$u_p(x^1)=\sqrt{\frac{2}{L_1-L}}\sin p\,\frac{\pi\,(x^1-L)}{L_1-L},\quad p=1,2,3,\ldots,\quad L\leqslant x^1\leqslant L_1. \tag{III.37}$$

In other words, we have exactly the same calculations to perform in the internal and external regions. Thus in the following we can concentrate on the internal region, and simply quote results from the external region when they are needed.

The heat kernel (III.24) for $u_p(x^1)$ in Eq. (III.36) is

$$h(t|x^1,y^1)=(4\pi t)^{-1/2}\sum_{n=-\infty}^{\infty}\left[e^{-(n\,2L+x^1-y^1)^2/4t}-e^{-(n\,2L+x^1+y^1)^2/4t}\right]. \tag{III.38}$$

Now all we have to do is substitute this h into the various formulas in the preceding subsection to obtain final expressions for $T_{\mu\nu}$ and j_μ. For brevity we concentrate on T_{11} and the Casimir force on the boundary planes.

In the integral (III.32) for T_{11} we have the integrand factor

$$(\partial_{x^1}\partial_{y^1}-\partial_{y^1}^2)\,h\big|_{x^1=y^1}=(4\pi t)^{-1/2}\sum_n\frac{1}{t}\left[1-\frac{2}{t}(nL)^2\right]e^{-n^2L^2/t}. \tag{III.39}$$

As expected, the part of T_{11} which survives the limit $L_3\to\infty$ is independent of x^1, in accordance with Eq. (III.34) above. For the internal region,

$$T_{11}=\int_0^\infty dt\,e^{-tm^2}(4\pi t)^{-1/2}\frac{B}{\sinh Bt}$$
$$\times\left\{\sum_{n=-\infty}^{\infty}\left[1-\frac{2}{t}(nL)^2\right]e^{-n^2L^2/t}f_3(t|x^2)-\frac{t}{2}h(t|x^1,x^1)\partial_2^2 f_3(t|x^2)\right\}. \tag{III.40}$$

The local force/area on the plane at $x^1=0$ is

$$F^1/A = \lim_{\epsilon\to 0}[T_{11}(x^1=-\epsilon)-T_{11}(x^1=\epsilon)]$$

$$= \frac{1}{(4\pi)^2}\int_0^\infty dt\, t^{-2}e^{-tm^2}\frac{B}{\sinh Bt}f_3(t|x^2)$$

$$\times 2\sum_{n=1}^{\infty}\left\{\left[\frac{2}{t}(nL)^2-1\right]e^{-(nL)^2/t}-\left[\frac{2}{t}(n\Delta L)^2-1\right]e^{-n^2\Delta L^2/t}\right\}, \qquad \text{(III.41)}$$

where $\Delta L = L_1 - L$. For $m=0$, $B=0$ and $L_1 \gg L$ this force/area reduces (as it should) to

$$\frac{F_1}{A} = 2\left[\frac{3}{(4\pi)^2 L^4}\zeta(4)\right], \qquad \text{(III.42)}$$

where the quantity in the bracket is the attractive Casimir force/area between parallel Dirichlet planes for a real massless scalar field. Looking at Eq. (III.41) we see that $B\neq 0$ weakens the Casimir force exponentially (relative to the $B=0$ case) by damping the $t\to\infty$ part of the integral. This was previously noticed in Ref. 14.

In Appendix B we compute the Casimir force/area (III.41) using the traditional method of the global Casimir energy. The answer obtained—Eq. (B10)—agrees with Eq. (III.41) except that f_3 is replaced by 1, i.e., the value of f_3 in the limit $L_3\to\infty$, which is also the average value of f_3 for finite L_3. The reason for this seems clear. A global calculation cannot see spatial dependence, such as the periodic x^2 dependence of $f_3(t|x^2)$.

The expected boundary divergences are present in $T_{\mu\nu}$ except for T_{11} where they cancel away. In general one can separate quantum functions like $T_{\mu\nu}(\mathbf{x})$ into "bulk field" (F) and "boundary" (B) terms: $T_{\mu\nu}=T^F_{\mu\nu}+T^B_{\mu\nu}$. The F terms require UV renormalization and are finite at boundaries. The B terms do *not* require UV renormalization and diverge as boundaries are approached. This structure is plainly evident in $T_{\mu\nu}[\Psi_0]$ above.

D. Gauge invariance

Something more should perhaps be said about the gauge invariance of the preceding calculations. We began with the background gauge potential $\mathbf{A}=(0,0,Bx^2)$ which led us to the set of empty-space Landau modes $\varphi_{k_1\nu k_3}(\mathbf{x})$ in Eq. (III.3). Individually, these modes represent a layer of stationary probability density, centered at $x^2=-k_3/B$ and uniform in the x^1 and x^3 directions. In this gauge, when the magnetic field $\mathbf{B}=(B,0,0)$ is turned on, each plane-wave mode of the $\mathbf{B}=0$ system (uniformly filling space, of course) shrinks down to the Landau mode selected by its momentum component k_3.

If x^3 is noncompact the Landau modes form a continuum along x^2 and there is no x^2 periodicity in $T_{\mu\nu}$ or in other local quantum functions. However, when $0\leqslant x^3\leqslant L_3$ is compact so that $k_3=n_3(2\pi/L_3)$ is discrete, the Landau modes become a discrete set of probability density layers centered at $x^2=-n_3(2\pi/BL_3)$. Because all local quantum functions such as $T_{\mu\nu}$ are constructed from these discrete modes, the periodicity along x^2 displayed by our local results seems mathematically understandable—even inevitable.

For $L_3=\infty$ the preferred role played by the coordinate x^2 in all of this is a consequence of our gauge choice. If we had chosen the gauge $\mathbf{A}=(0,-Bx^3,0)$ which leads to the same magnetic field $\mathbf{B}=(B,0,0)$, the spatial modes would be

$$\varphi_{k_1k_2\nu}(\mathbf{x}) = \frac{1}{\sqrt{L_1}}e^{ik_1x^1}\frac{1}{\sqrt{L_2}}e^{ik_2x^2}\,\psi_{\nu k_2}(x^3),$$

where the HO wave function satisfies

$$\left[-\partial_3^2+B^2\left(x^3-\frac{k_2}{B}\right)^2\right]\psi_{\nu k_2}(x_3)=2B\,(\nu+\tfrac{1}{2})\psi_{\nu k_2}(x_3). \tag{III.43}$$

Now the Landau modes are probability density layers arranged along the x^3 axis. Physically there is no difference between the two gauges, as must be the case. The only difference is a 90° coordinate rotation in the x^2x^3 plane, about the magnetic field direction. The orientation of the x^2x^3 plane about the field direction is completely arbitrary, of course.

As soon as coordinate x^3 is made compact, the minor gauge freedom just described disappears entirely. For this reason all the principal ($L_3<\infty$) calculations in this paper are gauge invariant. If x^2 is noncompact and x^3 is compact, rotations mixing these two coordinates are not possible. The gauge (III.1) is the only possible choice for introducing the background magnetic field $\mathbf{B}=(B,0,0)$. The more general potential (III.2) is not periodic in x^3 (for $\alpha>0$) and therefore is not acceptable. Equation (III.43) makes the same point in a different way. This HO Schrödinger equation is meaningless for a compact variable x^3. It only becomes meaningful when x^3 is made noncompact.

For noncompact x^2 and x^3 we can use the gauge potential (III.2). Then the mode equation (II.7) appears to be more complicated than before,

$$[-\partial_1^2-(\partial_2-i\alpha x^3B)^2-(\partial_3-i\beta x^2B)^2]\,\varphi_n=\omega_n^2\,\varphi_n\,. \tag{III.44}$$

However, the *ansatz*,

$$\varphi_n\rightarrow e^{i\alpha x^2x^3B}\,\varphi_{k_1\nu k_3}(\mathbf{x}) \tag{III.45}$$

with $\varphi_{k_1\nu k_3}(\mathbf{x})$ as in Eq. (III.3) reduces Eq. (III.44) to the HO equation (III.4), and the essential mathematics is unchanged. Equation (III.45) is just the appropriate gauge transform of the modes (III.3) of course.

IV. DISCUSSION

General theory has been developed for arbitrary (charged and uncharged) stationary states of a charged quantum scalar field $\hat{\phi}$ coupled to an arbitrary static background magnetic field $\mathbf{B}(\mathbf{x})$. An unusual feature of this general theory is the simultaneous coupling of $\hat{\phi}$ to $\mathbf{B}(\mathbf{x})$ and to a static background potential $V(\mathbf{x})$.

Although we have not discussed this aspect at all, it is a straightforward matter to extend the analysis in Secs. II and III to nonstationary states of the quantum field. For this one uses nonstationary solutions of the HO equation (II.14). We hope to say more about this elsewhere.

For explicit calculations we chose a uniform magnetic field $\mathbf{B}=(B,0,0)$ and considered (otherwise) empty space, and also space with two parallel Dirichlet planes perpendicular to $\mathbf{B}$. For both systems the exact vacuum stress tensor throughout space was calculated. In order to have normalizable modes we compactified a spatial direction (x^3) perpendicular to $\mathbf{B}$. We found that this compactification leads to the presence of a sustained current density j_3 in the vacuum.

In this paper we have only considered static magnetic fields $\mathbf{B}(\mathbf{x})$. Such a background field cannot transfer energy to/from real or virtual charged particles. Of course, neither can a time dependent magnetic field $\mathbf{B}(\mathbf{x},t)$, no matter how extreme the time dependence of $\mathbf{B}(\mathbf{x},t)$ may be. However, a time dependent $\mathbf{B}(\mathbf{x},t)$ cannot exist independently from the induced electric field $\mathbf{E}(\mathbf{x},t)$ prescribed by Maxwell's equations. In this way, the laws of classical electromagnetism dictate that $\mathbf{B}(\mathbf{x},t)$ also produces pairs from the vacuum—via the induced $\mathbf{E}(\mathbf{x},t)$ rather than directly.

Static background electric fields pose a much greater challenge than do static background magnetic fields. The reason, of course, is that background electric fields ongoingly transfer energy to/from charged (real and virtual) particles, and in particular cause pair production from the vacuum. Indeed, there do not exist stable, true stationary states of a charged quantum field in the

presence of any background electric field. An exact description of the states of the charged quantum field must necessarily be a nonstationary one. In subsequent work we intend to present a Schrödinger picture study of such systems.

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APPENDIX A: USEFUL FORMULAS

Here we collect and discuss formulas used in the examples in Sec. III. From the general Θ function identity,

$$\sum_{m=-\infty}^{\infty} e^{-x(m+g)^2} e^{2i\pi hm} = e^{-2\pi igh} \sqrt{\frac{\pi}{x}} \sum_{n=-\infty}^{\infty} e^{-\pi^2 (n+h)^2/x} e^{-2i\pi gn} \tag{A1}$$

we find for $k_1 = 2\pi n_1 / L_1$;

$$\frac{1}{L_1} \sum_{n_1=-\infty}^{\infty} e^{-tk_1^2} = (4\pi t)^{-1/2} f_1(t) \tag{A2}$$

with

$$f_1(t) \equiv \sum_{r=-\infty}^{\infty} e^{-r^2 L_1^2/4t} \tag{A3}$$

and

$$\frac{1}{L_1} \sum_{n_1=-\infty}^{\infty} k_1^2 e^{-tk_1^2} = \frac{1}{2t} (4\pi t)^{-1/2} g_1(t) \tag{A4}$$

with

$$g_1(t) \equiv \sum_{r=-\infty}^{\infty} [1 - r^2 L_1^2/2t] e^{-r^2 L_1^2/4t}. \tag{A5}$$

For $k_3 = 2\pi n_3 / L_3$ we have

$$\frac{1}{L_3} \sum_{n_3=-\infty}^{\infty} e^{-B(x^2 + k_3/B)^2 \tanh Bt} = \left[\frac{B}{4\pi \tanh Bt} \right]^{1/2} f_3(t|x^2), \tag{A6}$$

where

$$f_3(t|x^2) \equiv 1 + \sum_{r=1}^{\infty} e^{-r^2 B L_3^2/4 \tanh Bt} 2 \cos(r x^2 B L_3). \tag{A7}$$

Applying $\partial_2 = \partial / \partial x^2$ yields

$$\frac{1}{L_3} \sum_{n_3} (k_3 + Bx^2) e^{-B(x^2 + k_3/B)^2 \tanh Bt} = -\frac{1}{2} \left[\frac{B}{4\pi} \right]^{1/2} (\tanh Bt)^{-3/2} \partial_2 f_3, \tag{A8}$$

which vanishes exponentially as $L_3 \to \infty$, and

$$2B\tanh Bt\,\frac{1}{L_3}\sum_{n_3}\left(x^2+\frac{k_3}{B}\right)^2 e^{-B(x^2+(k_3/B))^2\tanh Bt}=\left[\frac{B}{4\pi\tanh Bt}\right]^{1/2}\left\{f_3+\frac{\cosh Bt}{2B\sinh Bt}\partial_2^2 f_3\right\}. \tag{A9}$$

The stationary HO wave function $\psi_{\nu k_3}(x^2)=\varphi_\nu(\sqrt{B}(x^2+k_3/B))$ is given by Eq. (II.17). It is normalized to one and satisfies

$$\frac{1}{L_3}\sum_{n_3}\sum_{\nu=0}^{\infty} e^{-Bt(2\nu+1)}\,|\psi_{\nu k_3}(x^2)|^2=\frac{B}{4\pi\sinh Bt}\,f_3(t|x^2), \tag{A10}$$

$$\frac{1}{L_3}\sum_{n_3}\sum_{\nu=0}^{\infty} e^{-Bt(2\nu+1)}\,|\psi'_{\nu k_3}(x^2)|^2=\frac{1}{8\pi}B^2\frac{\cosh Bt}{\sinh^2 Bt}\left\{f_3(t|x^2)+\frac{\sinh Bt}{2B\cosh Bt}\partial_2^2 f_3(t|x^2)\right\}, \tag{A11}$$

$$\frac{1}{L_3}\sum_{n_3}\sum_{\nu=0}^{\infty} e^{-Bt(2\nu+1)}\left(x^2+\frac{k_3}{B}\right)^2|\psi_{\nu k_3}(x^2)|^2=\frac{1}{8\pi}\frac{\cosh Bt}{\sinh^2 Bt}\left\{f_3(t|x^2)+\frac{\cosh Bt}{2B\sinh Bt}\partial_2^2 f_3(t|x^2)\right\}, \tag{A12}$$

$$\frac{1}{L_3}\sum_{n_3}\sum_{\nu=0}^{\infty} e^{-Bt(2\nu+1)}\,\psi_{\nu k_3}\psi''_{\nu k_3}=\frac{B^2\cosh Bt}{8\pi\sinh^2 Bt}\left\{-f_3+\frac{\sinh Bt}{2B\cosh Bt}\partial_2^2 f_3\right\}, \tag{A13}$$

$$\frac{1}{L_3}\sum_{n_3}\sum_{\nu=0}^{\infty} e^{-Bt(2\nu+1)}\,\psi_{\nu k_3}\psi'_{\nu k_3}=\frac{B}{8\pi\sinh Bt}\,\partial_2 f_3. \tag{A14}$$

The easiest derivation of Eqs. (A10)–(A14) is via the formula (Ref. 19, p. 194)

$$\sum_{n=0}^{\infty} e^{-tB(2n+1)}\psi_{nk_3}(x^2)\psi_{nk_3}(y^2)=\left[\frac{B}{2\pi\sinh 2Bt}\right]^{1/2} e^{-(1/2)B(x^2-y^2)^2\coth 2Bt}\times e^{-B(x^2+(k_3/B))(y^2+(k_3/B))\tanh Bt}. \tag{A15}$$

APPENDIX B: GLOBAL CASIMIR ENERGY

Here we summarize the global Casimir energy calculations for the examples in Sec. III. In these calculations the basic problem is to compute the mode sum,

$$E[\Psi_0]=E=\sum_n \epsilon_n=V\frac{B}{2\pi}\sum_{p,\nu}\left[\lambda_p^2+2B\left(\nu+\frac{1}{2}\right)+m^2\right]^{1/2} \tag{B1}$$

representing the unrenormalized vacuum energy. Here, as in Sec. III B, the frequencies ω_n are given by $[\lambda_p^2+2B(\nu+\frac{1}{4})]^{1/2}$ with the x^1 axis spectrum λ_p^2 defined by Eq. (III.22).

In the global sum (B1) V represents the (relevant) volume of space, and Σ_p has dimension $(\text{length})^{-1}$ like $\int dk_1$. Then E is an energy and E/V is an average energy density. Familiar manipulations enable one to rewrite Eq. (B1) in the form,

$$E=-V\int_0^\infty dt(4\pi t)^{-3/2}h_1(t)\,e^{-tm^2}\frac{B}{\sinh Bt}, \tag{B2}$$

where $h_1(t)=\Sigma_p\exp(-t\lambda_p^2)$ is the global version of the local 1D heat kernel (III.24).

1. Free infinite space

For noncompact $-\infty<x^1<\infty$ we have $\lambda_p^2\to k_1^2$ with $-\infty<k_1<\infty$ and $\Sigma_p\to(2\pi)^{-1}\int dk_1$, so that $h_1(t)=(4\pi t)^{-1/2}$. Thus

$$E=-V\int_0^\infty dt(4\pi t)^{-2}\,e^{-tm^2}\frac{B}{\sinh Bt} \tag{B3}$$

which reduces for $B\to 0$ to the usual (divergent) vacuum energy expression for infinite free space. This justifies the normalization $(B/2\pi)\,\Sigma_\nu$ of the HO sum in Eq. (B1) and establishes the correspondence,

$$\frac{B}{2\pi}\sum_\nu \leftrightarrow\frac{1}{2\pi}\int dk_2dk_3. \tag{B4}$$

Because

$$\frac{B}{\sinh Bt}=\frac{1}{t}-B^2\frac{t}{6}+B^4\frac{7}{360}t^3+\cdots$$

we see that the vacuum energy shift $E-E(B=0)$ associated with the magnetic field is still logarithmically divergent. The logarithmic divergence is proportional to B^2 and can therefore be absorbed into the energy of the background B field, leaving the finite Casimir energy density,

$$E_{\rm Cas}/V=-\int_0^\infty dt\,(4\pi t)^{-2}\,e^{-tm^2}\left[\frac{B}{\sinh Bt}-\frac{1}{t}+B^2\frac{t}{6}\right]. \tag{B5}$$

2. Free cylindrical space

For compact $0\leqslant x^1\leqslant L_1$, we have the spectrum $\lambda_p^2\to(n_1 2\pi/L_1)^2$ with $n_1=0,\pm1,\ldots$ and $\Sigma_p\to(L_1)^{-1}\Sigma_n$. Thus $h_1(t)=(4\pi t)^{-1}f_1(t)$ with $f_1(t)$ given by Eq. (A3), and

$$E(L_1)_{\rm free}=-A\,L_1\int_0^\infty dt\,(4\pi t)^{-2}\,e^{-tm^2}\frac{B}{\sinh Bt}f_1(t), \tag{B6}$$

where $V=A\,L_1$ and A is the area of the (x^2x^3) cross section of space. The Casimir energy contained within Eq. (B6) is defined exactly as in Eq. (B5).

3. Dirichlet planes at $x^1=0$ and L

Now let us insert parallel Dirichlet planes at $x^1=0$ and $x^1=L$. Between these planes $(0\leqslant x^1\leqslant L)$ we have discrete $k_1=n_1(\pi/L)$ with $n_1=1,2,3,\ldots$ and

$$h_1(t)=\frac{1}{L}\sum_{n_1=1}^\infty e^{-t(n_1\pi/L)^2}=-\frac{1}{2L}+(4\pi t)^{-1/2}\sum_{r=-\infty}^\infty e^{-r^2L^2/t}. \tag{B7}$$

The (unrenormalized) vacuum energy between the planes is, from Eq. (B2),

$$E(L)=-A\int_0^\infty dt\,(4\pi t)^{-3/2}\,e^{-tm^2}\frac{B}{\sinh Bt}\left\{-\frac{1}{2}+(4\pi t)^{-1/2}L\sum_{r=-\infty}^\infty e^{-r^2L^2/t}\right\}. \tag{B8}$$

To find the vacuum energy outside the planes (i.e., in $L\leqslant x_1\leqslant L_1$) we simply have to replace $L\to L_1-L$. Thus an obvious first attempt at defining the Casimir energy of the system is

$$\Delta E(L,L_1)\equiv E(L)+E(L_1-L)-E(L_1)_{\text{free}}$$
$$=-A\int_0^\infty dt(4\pi t)^{-2}e^{-tm^2}\frac{B}{\sinh Bt}\Bigg\{-(4\pi t)^{1/2}+2L\sum_{r=1}^{\infty}e^{-r^2L^2/t}$$
$$+2(L_1-L)\sum_{r=1}^{\infty}e^{-r^2(L_1-L)^2/t}-2L_1\sum_{r=1}^{\infty}e^{-r^2L_1^2/4t}\Bigg\}, \tag{B9}$$

where as expected the most singular terms have cancelled away. The only remaining singular term is the one $\{-(4\pi t)^{1/2}+\cdots\}$ in the curly bracket. Since this term is independent of L and L_1 we simply discard it in Eq. (B9). The finite remaining energy is then, as far as variations of boundary position L are concerned, the global Casimir energy of the system.

The Casimir force/area exerted by the distorted quantum field vacuum on the Dirichlet boundaries,

$$F(L,L_1)/A=\frac{d}{dL}\Delta E(L,L_1)/A$$
$$=-\int_0^\infty dt(4\pi t)^{-2}e^{-tm^2}\frac{B}{\sinh Bt}\sum_{r=1}^{\infty}\Bigg\{2[e^{-r^2L^2/t}-e^{-r^2(L_1-L)^2/t}]$$
$$-\frac{4}{t}r^2[L^2e^{-r^2L^2/t}-(L_1-L)^2e^{-r^2(L_1-L)^2/t}]\Bigg\} \tag{B10}$$

depends on plane separation L and on the x^1 circumference L_1. This force/area vanishes for $L_1=2L$ as it should, because the planes are then the same distance apart in either direction around the x^1 circle (unstable equilibrium). In the limit $L_1\to\infty$ one obtains F/A without finite (spatial) size effects. The two Dirichlet planes experience a mutually attractive Casimir force, weakened by the effects of (i) finite mass m and (ii) the background magnetic field. We recover the familiar Casimir force,

$$F(L,\infty)/A\big|_{m=B=0}=2\left[\frac{3\zeta(4)}{(4\pi)^2L^4}\right] \tag{B11}$$

for $m=B=0$ by performing a simple calculation using the analytic continuation formula

$$\int_0^\infty dt\,t^{s-1}e^{-r^2L^2/t}=(rL)^{2s}\Gamma(-s).$$

This leads to the Casimir energy,

$$\Delta E(L,\infty)\big|_{m=B=0}=2\left[-\frac{A\zeta(4)}{(4\pi)^2L^3}\right], \tag{B12}$$

and differentiation then yields Eq. (B11).

Equations (B11) and (B12) are, correctly, twice the Casimir force and energy of a *real* $m=0$ scalar field confined between parallel Dirichlet planes.

It is important to notice that, because of the lack of explicit dependence on k_3 in the spectrum summed over in Eq. (B1), these global calculations cannot be sensitive to the compactification of x^3. In other words, they are necessarily $L_3=\infty$ calculations. As we see in Sec. III by comparison with local calculations, this expectation is in fact correct.

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On the continuum limit of fermionic topological charge in lattice gauge theory

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It is proved that the fermionic topological charge of SU(N) lattice gauge fields on the four-torus, given in terms of a spectral flow of the Hermitian Wilson–Dirac operator or, equivalently, as the index of the overlap Dirac operator, reduces to the continuum topological charge in the classical continuum limit when the parameter m_0 is in the physical region $0<m_0<2$. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1415087]

I. INTRODUCTION

Let T^4 denote the Euclidean four-torus with fixed edge length L and fundamental domain $[0,L]^4 \subset \mathbf{R}^4$. A gauge potential on an SU(N) bundle over T^4 can be viewed as an su(N)-valued gauge field $A_\mu(x)$ on $\mathbf{R}^4$ satisfying

$$A_\mu(x+Le_\nu)=\Omega(x,\nu)A_\mu(x)\Omega(x,\nu)^{-1}+\Omega(x,\nu)\partial_\mu\Omega(x,\nu)^{-1}, \tag{1.1}$$

where e_ν is the unit vector in the positive ν-direction and $\Omega(x,\nu)$, $\nu=1,2,3,4$, are the SU(N)-valued monodromy fields which specify the principal SU(N) bundle over T^4. These also satisfy a cocycle condition which ensures that $A_\mu(x+Le_\nu+Le_\rho)$ is unambiguous and that Eq. (2.4) in this work is consistent. It is always possible to make a gauge transformation so that $\Omega(x,\nu)=1$ for $\nu=1,2,3$ and $\Omega(x,4)$ is periodic in x_1,x_2,x_3. Then for fixed x_4 $\Omega(x,4)$ determines a map $T^3 \to \mathrm{SU(N)}$. The degree of this map [which is independent of x_4 since $\Omega(x,4)$ depends smoothly on x_4] equals the Pontryargin number of the SU(N) bundle over T^4. The Pontryargin number of the bundle is encoded in the gauge field as its topological charge:

$$Q=\frac{-1}{8\pi^2}\int_{T^4}\mathrm{tr}(F\wedge F)=\frac{-1}{32\pi^2}\int d^4x\,\epsilon_{\mu\nu\rho\sigma}\mathrm{tr}(F_{\mu\nu}(x)F_{\rho\sigma}(x)). \tag{1.2}$$

The sections $\psi(x)$ in the standard spinor bundle over T^4 twisted by the SU(N) bundle can be viewed as spinor fields on $\mathbf{R}^4$ satisfying

$$\psi(x+Le_\nu)=\Omega(x,\nu)\psi(x). \tag{1.3}$$

The Dirac operator $\not{D}^A=\gamma^\mu(\partial_\mu+A_\mu)$ acts on these, and the Index Theorem[1] gives

$$Q=\mathrm{index}\not{D}^A. \tag{1.4}$$

The index$\not{D}^A$ is equal to the spectral flow of the Hermitian operator $-\gamma_5(i\not{D}^A-m)$ as m increases from any negative to any positive value [note that eigenvalues can only cross the origin at $m=0$ since $(\gamma_5(i\not{D}-m))^2=\not{D}^2+m^2$.]

The spectral flow description of Q motivates a fermionic definition of topological charge Q_{lat} in lattice gauge theory,[2–4] which has been extensively studied numerically in its various guises;

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see, e.g., Refs. 2 and 4–11. The purpose of this article is to analytically prove that Q_{lat} reduces to Q in the classical continuum limit. (This result was announced in Ref. 12 although the argument we give here is simpler and more direct than the one sketched there.)

II. STATEMENT OF THE MAIN RESULT

Put a hyper-cubic lattice on $\mathbf{R}^4$ with sites $a\mathbf{Z}^4$. We consider only the lattice spacings a for which L/a is a whole number. Furthermore, we restrict to lattice spacings with the property $a_1\mathbf{Z}^4 \subset a_2\mathbf{Z}^4$ for $a_2 < a_1$. This implies that if $x \in \mathbf{R}^4$ is a lattice site in the lattice with spacing a, then it is also a lattice site in all the other lattices with spacing $a' < a$. In the following, in statements concerning $a \to 0$ limits (in particular Proposition 2 to follow) the variable x always denotes such a point in $\mathbf{R}^4$; it is fixed in $\mathbf{R}^4$ and does not change as we go from one lattice to another.

The lattice transcript of A,

$$U_\mu(x) = T \exp\left(\int_0^1 a A_\mu(x + t a e_\mu) dt \right) \tag{2.1}$$

($T = t-$ ordering), satisfies

$$U_\mu(x + L e_\nu) = \Omega(x,\nu) U_\mu(x) \Omega(x + a e_\mu, \nu)^{-1}. \tag{2.2}$$

Given such a lattice, let $\mathcal{C}$ denote the infinite-dimensional complex vectorspace of lattice spinor fields $\psi(x)$ (i.e., functions on the lattice sites taking values in $\mathbf{C}^4 \otimes \mathbf{C}^N$) and define the inner product

$$\langle \psi_1, \psi_2 \rangle = a^4 \sum_{x \in a\mathbf{Z}^4} \psi_1(x)^* \psi_2(x), \tag{2.3}$$

where a contraction of spinor and color indices is implied. Let $\mathcal{H} \subset \mathcal{C}$ denote the Hilbert space of spinor fields with $\|\psi\| < \infty$ and let $\mathcal{C}_L \subset \mathcal{C}$ denote the finite-dimensional subspace of spinor fields satisfying the lattice version of (1.3):

$$\psi(x + L e_\nu) = \Omega(x,\nu) \psi(x), \quad \forall x \in a\mathbf{Z}^4. \tag{2.4}$$

The fields $\psi \in \mathcal{C}_L$ are determined by their restriction to $\mathcal{F}_L :=$ the set of lattice sites contained in $[0,L)^4 \subset \mathbf{R}^4$. We define an inner product in $\mathcal{C}_L$ by

$$\langle \psi_1, \psi_2 \rangle_L = a^4 \sum_{x \in \mathcal{F}_L} \psi_1(x)^* \psi_2(x). \tag{2.5}$$

The covariant forward (backward) finite difference operators $(1/a)\,\nabla_\mu^+$ ($(1/a)\,\nabla_\mu^-$) are defined on $\mathcal{C}$ by

$$\nabla_\mu^+ \psi(x) = U_\mu(x) \psi(x + a e_\mu) - \psi(x), \tag{2.6}$$

$$\nabla_\mu^- \psi(x) = \psi(x) - U_\mu(x - a e_\mu)^{-1} \psi(x - a e_\mu). \tag{2.7}$$

These are bounded ($\|\nabla_\mu^\pm\| \leqslant 2$) and therefore map $\mathcal{H}$ to $\mathcal{H}$. They also preserve (2.4) and therefore map $\mathcal{C}_L$ to $\mathcal{C}_L$. Note that

$$(\nabla_\mu^\pm)^* = -\nabla_\mu^\mp \tag{2.8}$$

on $\mathcal{H}$ and $\mathcal{C}_L$. The lattice version of $i\not{\partial}^A$ is the Wilson–Dirac operator:

$$D_w = i\frac{1}{a}\nabla\!\!\!/ + \frac{r}{2}a\left(\frac{1}{a^2}\Delta\right), \quad r>0, \tag{2.9}$$

where $(1/a)\,\nabla\!\!\!/ = \Sigma_\mu \gamma^\mu \frac{1}{2}(\nabla_\mu^+ + \nabla_\mu^-)$ is the naive lattice Dirac operator and $(1/a^2)\,\Delta = (1/a^2)\,\Sigma_\mu(\nabla_\mu^- + \nabla_\mu^+) = (1/a^2)\,\Sigma_\mu(\nabla_\mu^+)^*\nabla_\mu^+ = (1/a^2)\,\Sigma_\mu(\nabla_\mu^-)^*\nabla_\mu^-$ is the lattice Laplace operator. We are following the mathmatical convention where the γ^μ's are anti-Hermitian [this explains the factor i in $i(1/a)\,\nabla\!\!\!/$ in (2.9) which is not usually present in the physics literature where the γ^μ's are Hermitian]. Then $\nabla\!\!\!/$ is Hermitian due to (2.8) and Δ is Hermitian and positive. [The Wilson term, i.e., the second term in (2.9), which formally vanishes in the $a\to 0$ limit, is included to avoid the fermion doubling problem: a degeneracy of the nullspace of $\nabla\!\!\!/$ which is a lattice artifact unrelated to the continuum theory.[13,14]] The lattice version of $\gamma_5(i\partial\!\!\!/ - m)$ is the Hermitian operator $(1/a)\,H_m$:

$$\frac{1}{a}H_m = \gamma_5\left(D_w - \frac{rm}{a}\right), \tag{2.10}$$

$$H_m = \gamma_5(i\nabla\!\!\!/ + r(\tfrac{1}{2}\Delta - m)). \tag{2.11}$$

It can be shown that the spectrum of H_m is symmetric and without zero for all $m<0$. Hence the spectral flow of $-H_m$ as m increases from any negative value to some positive value m_0 is equal to half the spectral asymmetry of $-H_{m_0}$.[3,4] This suggests the following fermionic definition of the topological charge of the lattice gauge field $U_\mu(x)$:

$$Q_{\rm lat} = Q_{m_0} := -\frac{1}{2}{\rm Tr}\left(\frac{H_{m_0}}{|H_{m_0}|}\right), \tag{2.12}$$

where H_{m_0} is acting on $\mathcal{C}_L$. The spectral flow of H_m was first studied numerically in Ref. 2. The definition (2.12) arose in the overlap formulation of chiral gauge theory on the lattice.[3,4] Q_{m_0} also arises as an index: $Q_{m_0} = {\rm index}(D_{m_0}) := {\rm Tr}(\gamma_5|_{\ker D_{m_0}})$ where $D = (1/a)\,(1+\gamma_5\,(H/|H|))$ is the overlap Dirac operator.[15]

Unlike in the continuum case, the spectral flow of $-H_m$ depends on the final value $m_0>0$ of m. Numerical studies have shown that for reasonably smooth lattice gauge fields, e.g., when $U_\mu(x)$ is the lattice transcript of a smooth continuum gauge field and the lattice is reasonably fine, the eigenvalue crossings of $-H_m$ are localized around $m=0,2,4,6,8$.[2,8] Furthermore, when the lattice gauge field is the lattice transcript of a continuum field the spectral flow due to crossings close to $m=0$ was found to reproduce the continuum topological charge Q. In this article we complement the previous numerical studies with the following analytical result:

Theorem: In the above setting, where $U_\mu(x)$ is the lattice transcript (2.1) and $m_0 \notin \{0,2,4,6,8\}$, there exists an $a_0>0$ [depending on $A_\mu(x)$ and m_0] such that

$$Q_{m_0} = I(m_0)Q \quad \text{for all lattice spacings } a<a_0, \tag{2.13}$$

where

$$I(m_0) = \begin{array}{|c|c|c|c|c|} \hline 0<m_0<2 & 2<m_0<4 & 4<m_0<6 & 6<m_0<8 & m_0 \notin [0,8] \\ \hline 1 & -3 & 3 & -1 & 0 \\ \hline \end{array} \tag{2.14}$$

Remarks: (i) The dependence on m_0 in (2.13) and (2.14) coincides with that found in the above-mentioned numerical studies with smooth lattice gauge fields. (ii) The definition (2.12) of

Q_{m_0} is only meaningful when H_{m_0} does not have zero-modes. In the present case this is guaranteed when $m_0 \notin \{0,2,4,6,8\}$ and a is sufficiently small. Indeed, it is known that when $\|1-U(p)\|<\epsilon$ for all lattice plaquettes p, where $U(p)$ is the product of the link variables $U_\mu(x)$ around p, then there is a lower bound $H^2_{m_0}>b$, depending only on ϵ and m_0, such that for fixed $m_0 \notin \{0,2,4,6,8\} b>0$ when ϵ is sufficiently small. This bound was established in Ref. 16 (and improved in Ref. 17) for the case where $0<m_0<2$ and can be generalized to arbitrary $m_0 \notin \{0,2,4,6,8\}$.[18] In the present case, where $U_\mu(x)$ is the lattice transcript (2.1), we have

$$1-U(p_{x,\mu\nu})=a^2F_{\mu\nu}(x)+O(a^3)(x) \tag{2.15}$$

leading to

$$\|1-U(p)\|\sim O(a^2). \tag{2.16}$$

Hence the above-mentioned lower bound $H^2_{m_0}>b>0$ holds for all sufficiently small a. Here and in the following $O(a^p)(x)$ denotes a function on the lattice sites $x\in\mathcal{F}_L$ such that the operator norm of $O(a^p)(x)$, considered as a multiplication operator on $\mathcal{C}$, satisfies $\|O(a^p)(x)\|\leqslant a^pK$ for all $x\in\mathcal{F}_L$ where K is a constant independent of a and x. [In (2.15) $O(a^p)(x)$ takes values in the space of linear maps on $\mathbf{C}^N$; sometimes $O(a^p)(x)$ will just be a $\mathbf{C}$-valued function of x, in which case we have $|O(a^p)(x)|\leqslant a^pK$.] We discuss the derivation of (2.15) and (2.16), and other bounds used in the following, in the appendix. In general, to conclude (2.16) from (2.15) we need the $O(a^3)(x)$ term to satisfy $\|O(a^3)(x)\|\leqslant a^3K$ for all $x\in a\mathbf{Z}^4$. For general gauge field $A_\mu(x)$ on $\mathbf{R}^4$ this holds when $\|A_\mu(x)\|$ and $\|\partial_\mu A_\nu(x)\|$ are bounded on $\mathbf{R}^4$ (cf. the Appendix). In the present case the condition (1.1) generally results in divergence of $A_\mu(x)$ at infinity (for topologically nontrivial field). Nevertheless we still have (2.16) in this case: it is a consequence of (2.2) [note that $\|U_\mu(x)\|=1$ since $U_\mu(x)$ is unitary] and the fact that the $O(a^3)(x)$ term satisfies $\|O(a^3)(x)\|\leqslant a^3K$ when x is restricted to be in the fundamental domain $\mathcal{F}_L$.

III. PROOF OF THE THEOREM

The strategy for proving the theorem is to express Q_{m_0} as the sum of a density,

$$Q_{m_0}=a^4\sum_{x\in\mathcal{F}_L} q_L(x), \tag{3.1}$$

and show that

$$q_L(x)=I(m_0)q^A(x)+O(a)(x) \quad (x\in\mathcal{F}_L), \tag{3.2}$$

where

$$q^A(x)=\frac{-1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\mathrm{tr}F_{\mu\nu}(x)F_{\rho\sigma}(x). \tag{3.3}$$

Then $\lim_{a\to 0}Q_{m_0}=I(m_0)Q$, and since Q_{m_0} is integer it follows that Q_{m_0} must coincide with $I(m_0)Q$ for small nonzero a as stated in the theorem.

To specify the density $q_L(x)$ in (3.1) we introduce the following definitions. We decompose $\mathcal{C}=\mathcal{C}^{sc}\otimes(\mathbf{C}^4\otimes\mathbf{C}^N)$, $\mathcal{H}=\mathcal{H}^{sc}\otimes(\mathbf{C}^4\otimes\mathbf{C}^N)$ where $\mathcal{C}^{sc}$, $\mathcal{H}^{sc}$ denote the corresponding spaces of scalar lattice fields. $\mathcal{H}^{sc}$ has the orthonormal basis $\{\delta_x/a^2\}_{x\in a\mathbf{Z}^4}$ where $\delta_x(y)=\delta_{xy}$. For linear operator $\mathcal{O}_\mathcal{H}$ on $\mathcal{H}$ we define $\mathcal{O}_\mathcal{H}(x,y)=(1/a^4)\langle(\delta_x/a^2),\mathcal{O}_\mathcal{H}(\delta_y/a^2)\rangle$; this is a linear operator on $\mathbf{C}^4\otimes\mathbf{C}^N$ satisfying

$$\mathcal{O}_\mathcal{H}\psi(x)=a^4\sum_{y\in a\mathbf{Z}^4}\mathcal{O}_\mathcal{H}(x,y)\psi(y) \quad \forall\,\psi\in\mathcal{H}. \tag{3.4}$$

There is also an obvious decomposition $\mathcal{C}_L = \mathcal{C}_L^{sc} \otimes (\mathbf{C}^4 \otimes \mathbf{C}^N)$ with $\mathcal{C}_L^{sc}$ having the basis $\{\phi_x\}_{x \in \mathcal{F}_L}$ where $\phi_x(y) = (1/a^2)\,\delta_{xy}$ for $y \in \mathcal{F}_L$ and is extended to $a\mathbf{Z}^4$ in accordance with (2.4):

$$\phi_x(y+Ln) = \frac{1}{a^2}\Omega^{(n)}(x)\,\delta_{xy}, \quad \Omega^{(n)}(x) = \prod_\nu \Omega(x,\nu)^{n_\nu}, \quad n \in \mathbf{Z}^4. \tag{3.5}$$

For linear operator $\mathcal{O}_L$ on $\mathcal{C}_L$ we define $\mathcal{O}_L(x,y) = (1/a^4)\langle \phi_x, \mathcal{O}_L \phi_y \rangle_L$ for $x,y \in \mathcal{F}_L$; this is a linear operator on $\mathbf{C}^4 \otimes \mathbf{C}^N$ satisfying

$$\mathcal{O}_L\psi(x) = a^4 \sum_{y \in \mathcal{F}_L} \mathcal{O}_L(x,y)\,\psi(y) \quad \forall\ \psi \in \mathcal{C}_L, \quad x \in \mathcal{F}_L. \tag{3.6}$$

The Cauchy–Schwarz inequality gives $\|\mathcal{O}_{\mathcal{H}}(x,y)\| \leqslant (1/a^4)\,\|\mathcal{O}_{\mathcal{H}}\|$ and $\|\mathcal{O}_L(x,y)\| \leqslant (1/a^4)\,\|\mathcal{O}_L\|_L$.

The definition (2.12) of Q_{m_0} can now be rewritten as (3.1) with

$$q_L(x) = -\frac{1}{2}\mathrm{tr}\left(\frac{H}{\sqrt{H^2}}\right)_L (x,x), \tag{3.7}$$

where $H = H_{m_0}$ and the trace is over spinor and color indices (i.e., over $\mathbf{C}^4 \otimes \mathbf{C}^N$). The strategy for deriving (3.2) and (3.3) is now to relate $q_L(x)$ to $q_{\mathcal{H}}(x)$, defined by replacing $(H/\sqrt{H^2})_L$ by $(H/\sqrt{H^2})_{\mathcal{H}}$ in (3.7). (The latter is defined via the spectral theory for bounded operators on Hilbert space.) This approach was suggested to me by Martin Lüscher.[19] The point is that (3.2) and (3.3) are relatively easy to derive for $q_{\mathcal{H}}(x)$; in fact, this has essentially already been done in previous works.[20–23] One potentially problematic aspect with regards to these previous calculations is that in the present case $A_\mu(x)$ can diverge for $|x| \to \infty$. However, we will get around this by exploiting the locality property of $(H/\sqrt{H^2})_{\mathcal{H}}$,[16] which will allow us to replace $A_\mu(x)$ by a gauge field which vanishes outside a bounded region of $\mathbf{R}^4$.

The relation between $q_L(x)$ and $q_{\mathcal{H}}(x)$ is as follows:

Proposition 1:

$$\left(\frac{H}{\sqrt{H^2}}\right)_L (x,y) = \sum_{n \in \mathbf{Z}^4} \left(\frac{H}{\sqrt{H^2}}\right)_{\mathcal{H}} (x,y+Ln)\Omega^{(n)}(y) \quad (x,y \in \mathcal{F}_L), \tag{3.8}$$

where $\Omega^{(n)}(x)$ is defined in (3.5). In particular, setting $y = x$ and substituting in (3.7) we get

$$q_L(x) = q_{\mathcal{H}}(x) - \frac{1}{2}\sum_{n \in \mathbf{Z}^4 - \{0\}} \mathrm{tr}\left(\frac{H}{\sqrt{H^2}}\right)_{\mathcal{H}} (x,x+Ln)\,\Omega^{(n)}(x). \tag{3.9}$$

Proof: We begin by deriving a relation between $\mathcal{O}_L(x,y)$ and $\mathcal{O}_{\mathcal{H}}(x,y)$ for bounded operators $\mathcal{O}$ on $\mathcal{C}$ which leave $\mathcal{C}_L$ invariant. The proposition will then follow by exploiting the fact that $(H/\sqrt{H^2})_L$ and $(H/\sqrt{H^2})_{\mathcal{H}}$ can be simultaneously approximated by such operators. The approximation part is necessary since $H/\sqrt{H^2}$ is not a well-defined operator on the whole of $\mathcal{C}$; the technicalities are related to the fact that $\mathcal{C}_L \not\subset \mathcal{H}$, i.e., elements in $\mathcal{C}_L$ can have infinite norm.

Let $\mathcal{O}$ be a bounded operator on $\mathcal{C}$ which maps $\mathcal{C}_L$ to itself. Then it follows from the above definitions and (3.5) that, for $x,y \in \mathcal{F}_L$,

$$\mathcal{O}_L(x,y)=\frac{1}{a^4}\langle\phi_x,\mathcal{O}\phi_y\rangle_L$$

$$=\sum_{z\in\mathcal{F}_L}\phi_x(z)(\mathcal{O}\phi_y)(z)$$

$$=\frac{1}{a^2}(\mathcal{O}\phi_y)(x)=a^2\sum_{z\in a\mathbf{Z}^4}\mathcal{O}_{\mathcal{H}}(x,z)\,\phi_y(z)$$

$$=\sum_{n\in\mathbf{Z}^4}\mathcal{O}_{\mathcal{H}}(x,y+Ln)\,\Omega^{(n)}(y). \tag{3.10}$$

We now exploit the fact[16] that $1/\sqrt{H^2}$ has a power series expansion $\kappa\Sigma_{k=0}^{\infty}t^kP_k(H^2)$ norm-convergent to $(1/\sqrt{H^2})_L$ and $(1/\sqrt{H^2})_{\mathcal{H}}$ on $\mathcal{C}_L$ and $\mathcal{H}$, respectively. $P_k(\cdot)$ is a Legendre polynomial of order k; $\|P_k(H^2)\|\leqslant 1$; $t=e^{-\theta}$; and the constants $\kappa,\theta>0$ depend only on the (strictly positive) lower and upper bounds on H^2.[16] [We are assuming that a is sufficiently small so that H^2 has a lower bound $b>0$ cf. remark (ii) above]. Set

$$P^{(N)}:=H\left(\kappa\sum_{k=0}^{N}t^kP_k(H^2)\right).$$

For arbitrary finite N this is a bounded operator on $\mathcal{C}$ which maps $\mathcal{C}_L$ to itself. In light of (3.10), to prove the proposition it suffices to show that $(H/\sqrt{H^2})_L(x,y)-P_L^{(N)}(x,y)$ and $\Sigma_{n\in\mathbf{Z}^4}[(H/\sqrt{H^2})_{\mathcal{H}}(x,y+Ln)-P_{\mathcal{H}}^{(N)}(x,y+Ln)]\Omega^{(n)}(y)$ both vanish in the $N\to\infty$ limit. The former is obvious. To show the latter it suffices to show that $\Sigma_{n\in\mathbf{Z}^4}\Sigma_{k=N+1}^{\infty}t^k\|P_k(x,y+Ln)\|$ vanishes in the $N\to 0$ limit. (We have set $P_k(x,z)=[P_k(H^2)](x,z)$.) For simplicity we show this for $y=x$ [the relevant case for (3.9)]; the argument in the general case is a straightforward generalization. Since $P_k(H^2)$ is of order k in H^2, and H couples only nearest neighbor sites, we have $P_k(x,x+Ln)=0$ when $(L/a)\,\Sigma_\mu|n_\mu|>2k$. Since $\|P_k(x,z)\|\leqslant(1/a^4)\,\|P_k(H^2)\|\leqslant a^4$ it follows that

$$\sum_{n\in\mathbf{Z}^4}\sum_{k=N+1}^{\infty}t^k\|P_k(x,x+Ln)\|\leqslant\frac{1}{a^4}t^N\left(\sum_{n\in\mathbf{Z}^4,L/2a\,\Sigma_\mu|n_\mu|\leqslant N}\sum_{k=1}^{\infty}t^k\right)$$

$$+\frac{1}{a^4}\left(\sum_{n\in\mathbf{Z}^4,1/2a\,\Sigma_\mu|n_\mu|>N}t^{((L/2a)\,\Sigma_\mu|n_\mu|)}\sum_{k=1}^{\infty}t^k\right). \tag{3.11}$$

The first sum over n vanishes as N^4t^N for $N\to\infty$, while the second clearly vanishes for $N\to\infty$ since it is convergent for finite N. This completes the proof of the proposition.

We now derive a small a bound on the second term in (3.9). The facts that $P_k(x,x+Ln)=0$ for $(L/a)\,\Sigma_\mu|n_\mu|>2k$ and $\|P_k(H^2)\|\leqslant 1$ imply the following locality property of $(1/\sqrt{H^2})_{\mathcal{H}}$:[16]

$$\left\|\left(\frac{1}{\sqrt{H^2}}\right)_{\mathcal{H}}(x,x+Ln)\right\|\leqslant\left\|\kappa\sum_{k\geqslant(L/2a)\Sigma_\mu|n_\mu|}t^kP_k(x,y)\right\|$$

$$\leqslant\kappa\,t^{((L/2a)\Sigma_\mu|n_\mu|)}\sum_{k=0}^{\infty}t^k\frac{1}{a^4}=\tilde{\kappa}\frac{1}{a^4}\exp\left(-\theta\frac{L}{2a}\sum_\mu|n_\mu|\right), \tag{3.12}$$

where $\tilde{\kappa}:=\kappa/(1-e^{-\theta})$. For sufficiently small a this gives

$$\left\| \sum_{n\in\mathbf{Z}^4-\{0\}} \left(\frac{1}{\sqrt{H^2}}\right)_{\mathcal{H}}(x,x+Ln) \right\| \leqslant \sum_{n\in\mathbf{Z}^4-\{0\}} \frac{\tilde{\kappa}}{a^4}\prod_{\mu} \exp\left(-\theta\frac{L}{2a}|n_\mu|\right)$$

$$\leqslant \frac{\tilde{\kappa}}{a^4}\prod_{\mu}\left[2\int_{1/2}^{\infty}\exp\left(-\theta\frac{L}{2a}t_\mu\right)dt_\mu\right] = \tilde{\kappa}\left(\frac{4}{\theta L}\right)^4 \exp\left(-\frac{\theta L}{a}\right). \tag{3.13}$$

The second inequality follows from the fact that $\int_{1/2}^{\infty}\exp(-(\theta L/2a)\,t)\,dt \geqslant \exp(-(\theta L/2a))$ for sufficiently small a. It now follows from (3.9) that $q_L(x)=q_{\mathcal{H}}(x)+O(e^{-\rho/a})$ for sufficiently small a. (This had already been noted by M. Lüscher in the Abelian case in Ref. 24 although the derivation was not provided there.)

To prove the theorem it now suffices to show (3.2) and (3.3) for $q_{\mathcal{H}}(x)$ instead of $q_L(x)$, i.e., to show

$$q_{\mathcal{H}}(x)=I(m_0)q^A(x)+O(a)(x) \quad \text{for } x\in\mathcal{F}_L\,. \tag{3.14}$$

To simplify the derivation we exploit the fact that $q_{\mathcal{H}}(x)$ is local in the gauge field.[16] Because of this it suffices to show (3.14) in the case where $A_\mu(x)$ is replaced by another SU(N) gauge field $\tilde{A}_\mu(x)$ on $\mathbf{R}^4$ with $\tilde{A}_\mu(x)=A_\mu(x)$ in a neighborhood of $[0,L]^4$ and $\tilde{A}_\mu(x)=0$ outside a bounded region of $\mathbf{R}^4$. Specifically, we can take $\tilde{A}_\mu(x)=\lambda(x)A_\mu(x)$ where $\lambda(x)$ is a smooth function on $\mathbf{R}^4$ equal to 1 on $[-d,L+d]^4$ $(d>0)$ and vanishing outside a bounded region. To see this, let H and $\tilde{H}$ denote the operators defined by (2.11) with lattice gauge fields U and $\tilde{U}$ being the lattice transcripts [defined by (2.1)] of A and $\tilde{A}$, respectively. Then, for small a, just as for H^2 we have $\tilde{H}^2>b>0$ and an expansion $(1/\sqrt{\tilde{H}^2})_{\mathcal{H}}=\kappa\Sigma_{k=0}^{\infty}t^k\tilde{P}_k$ where $\tilde{P}_k=P_k(\tilde{H}^2)$. Since H and $\tilde{H}$ only couple nearest neighbor sites, $P_k(H^2)$ and $P_k(\tilde{H}^2)$ can only couple a lattice site in $[0,L]^4$ to another lattice site in $[0,L]^4$ via a site outside of $[-d,L+d]^4$ if $k\geqslant 2(d/2a)$. Therefore, $P_k(x,y)=\tilde{P}_k(x,y)$ for $x,y\in\mathcal{F}_L$ when $k<d/a$, and we find by an analogous argument to the one leading to (3.12) that, for $x,y\in\mathcal{F}_L$,

$$\left\| \left(\frac{1}{\sqrt{H^2}}\right)_{\mathcal{H}}(x,y) - \left(\frac{1}{\sqrt{\tilde{H}^2}}\right)_{\mathcal{H}}(x,y) \right\| \leqslant \kappa\sum_{k\geqslant d/a}^{\infty} t^k \|P_k(x,y)-\tilde{P}_k(x,y)\| \leqslant \frac{2\tilde{\kappa}}{a^4}e^{-\theta d/a}. \tag{3.15}$$

This together with the ultra-locality of H and $\tilde{H}$ implies

$$q_{\mathcal{H}}(x)=\tilde{q}_{\mathcal{H}}(x)+O\left(\frac{1}{a^4}e^{-\rho/a}\right)(x) \quad \text{for } x\in\mathcal{F}_L \tag{3.16}$$

In light of this, the theorem now follows from (a special case of) the following:

Proposition 2: Let $A_\mu(x)$ be a general smooth SU(N) gauge field on $\mathbf{R}^4$ with the property that $\|A_\mu(x)\|$, $\|\partial_\nu A_\mu(x)\|$, and $\|\partial_\sigma\partial_\nu A_\mu(x)\|$ are all bounded. Let $H=H_{m_0}$ be defined as in (2.11) with the lattice gauge field being the lattice transcript (2.1) of $A_\mu(x)$. Then $q_{\mathcal{H}}(x) = -\frac{1}{2}\mathrm{tr}(H/\sqrt{H^2})_{\mathcal{H}}(x,x)$ satisfies $q_{\mathcal{H}}(x)=I(m_0)q^A(x)+O(a)(x)$ for all $x\in a\mathbf{Z}^4$, where $\|O(a)(x)\|\leqslant aK$ for some constant K independent of x and small a.

Clearly the gauge field $\tilde{A}_\mu(x)$ introduced above satisfies the conditions of the proposition (since it vanishes outside a bounded region). Combining the proposition with (3.16) then gives (3.14), proving the theorem.

To prove Proposition 2 we use an integral representation to expand $1/\sqrt{H^2}$ as a power series following Refs. 12 and 21. (This gives a more explicit power series expansion than the expansion in Legendre polynomials[16] discussed earlier.) Henceforth all operators are assumed to be acting on

$\mathcal{H}$ and we drop the subscript "$\mathcal{H}$" in the notation. Also, from now on $O(a^p)(x)$ denotes a term with $\|O(a^p)(x)\| \leqslant a^p K$ for all $x \in a\mathbf{Z}^4$ (not just for $x \in \mathcal{F}_L$). We first decompose

$$H^2 = L - V, \tag{3.17}$$

where

$$L = -\nabla^2 + r^2(\tfrac{1}{2}\Delta - m_0)^2, \tag{3.18}$$

$$V = = ir\,\tfrac{1}{2}\gamma_\mu V_\mu - \tfrac{1}{4}[\gamma_\mu, \gamma_\nu] V_{\mu\nu}, \tag{3.19}$$

with

$$V_\mu = \frac{1}{2}\left[(\nabla_\mu^+ + \nabla_\mu^-), \sum_\nu (\nabla_\nu^- - \nabla_\nu^+)\right], \tag{3.20}$$

$$V_{\mu\nu} = \tfrac{1}{4}[(\nabla_\mu^+ + \nabla_\mu^-), (\nabla_\nu^+ + \nabla_\nu^-)]. \tag{3.21}$$

As pointed out in Ref. 16, the norms of the commutators of the $\nabla_\mu^\pm$'s are bounded by $\max_p \|1 - U(p)\|$. The bound (2.16) on $\|1 - U(p)\|$ is valid when the conditions of Proposition 2 are satisfied (cf. the Appendix), hence

$$\|V\| \sim O(a^2). \tag{3.22}$$

It follows that for small a we have $\|V\| < b/2$ where b is the lower bound on H^2 mentioned earlier in remark (ii). This in turn implies the lower bound $L > b/2 > 0$ for the positive operator L in (3.18). Thus for sufficiently small a the operator L is invertible, $\|L^{-1}\| \cdot \|V\| < 1$, and we can make the expansion

$$\frac{H}{\sqrt{H^2}} = H\int_{-\infty}^{\infty} \frac{d\sigma}{\pi} \frac{1}{H^2 + \sigma^2} = H\int_{-\infty}^{\infty} \frac{d\sigma}{\pi} \left(\frac{1}{1 - (L + \sigma^2)^{-1} V}\right)\left(\frac{1}{L + \sigma^2}\right) = \int_{-\infty}^{\infty} \frac{d\sigma}{\pi} \sum_{k=0}^{\infty} H(G_\sigma V)^k G_\sigma, \tag{3.23}$$

where $G_\sigma := (L + \sigma^2)^{-1}$. Note that the γ-matrices in (3.17) are all contained in V. Since the trace of γ_5 times a product of less than four γ-matrices vanishes, the $k = 0$ and $k = 1$ terms in (3.23) give vanishing contribution to $q_{\mathcal{H}}(x)$. On the other hand, the terms with $k \geqslant 3$ satisfy the following bound:

$$\begin{aligned}\left\| \int_{-\infty}^{\infty} \frac{d\sigma}{\pi} \sum_{k=3}^{\infty} [H(G_\sigma V)^k G_\sigma](x,x) \right\| &\leqslant \frac{1}{a^4}\|H\| \int_{-\infty}^{\infty} \frac{d\sigma}{\pi} \sum_{k=3}^{\infty} \|G_\sigma\|^{k+1} \|V\|^k \\ &\leqslant a^2 K^3 \|H\| \left[\int_{-\infty}^{\infty} \frac{d\sigma}{\pi} \frac{1}{(b/2 + \sigma^2)^4}\right] \sum_{k=0}^{\infty} \left(\frac{2}{b} a^2 K\right)^k,\end{aligned} \tag{3.24}$$

where we have used (3.22) and the bounds $G_\sigma < (b/2 + \sigma^2)^{-1} \leqslant 2/b$. This is $O(a^2)$ since the integral and sum are finite and remain so in the $a \to 0$ limit. Hence only the $k = 2$ term in (3.23) contributes in the $a \to 0$ limit:

$$q_{\mathcal{H}}(x) = q_{\mathcal{H}}^{(2)}(x) + O(a^2)(x), \tag{3.25}$$

where

$$q^{(2)}_{\mathcal{H}}(x) = -\frac{1}{2}\int_{-\infty}^{\infty}\frac{d\sigma}{\pi}\,\mathrm{tr}[HG_\sigma VG_\sigma VG_\sigma](x,x). \tag{3.26}$$

For lattice operators $\mathcal{O}$ which are polynomials in $\nabla^{\pm}_{\mu}$ we denote by $\mathcal{O}^{(0)}$ the operator obtained by setting $U=1$ in (2.6) and (2.7). Standard arguments give (cf. the Appendix) $\|H-H^{(0)}\| \sim O(a)$ and $\|L-L^{(0)}\|\sim O(a)$. The latter implies $\|G_\sigma - G^{(0)}_\sigma\|\sim O(a)$; this follows from $G_\sigma - G^{(0)}_\sigma = G^{(0)}_\sigma(L^{(0)}-L)G_\sigma$ since G_σ and $G^{(0)}_\sigma$ are bounded from above by $2/b$ when a is sufficiently small. This allows us to replace H and G_σ by $H^{(0)}$ and $G^{(0)}_\sigma$ in (3.26) at the expense of an $O(a)(x)$ term. Furthermore, we have $\|[L^{(0)},V]\|\sim O(a^3)$ (cf. the Appendix). This leads to $\|[G^{(0)}_\sigma,V]\|\sim O(a^3)$ as follows: The bound $\|\nabla^{\pm}_{\mu}\|\leqslant 2$ and triangle inequalities lead to an a-independent upper bound $L<c$ which allows us to expand

$$G_\sigma = \left(\frac{1}{c+\sigma^2}\right)\left(\frac{1}{1-(c-L)/(c+\sigma)}\right) = \frac{1}{c+\sigma^2}\sum_{m=0}^{\infty}\left(\frac{c-L}{c+\sigma^2}\right)^m.$$

Now, since

$$\|[(c-L^{(0)})^m,V]\|\leqslant m\|[L^0,V]\|\cdot\|c-L\|^{m-1}\leqslant m(a^3K)(c-b/2)^{m-1},$$

we get

$$\|[G^{(0)}_\sigma,V]\|\leqslant \frac{a^3K}{c^2}\sum_{m=0}^{\infty}(m+1)\left(\frac{c-b/2}{c}\right)^m,$$

and this is $\sim O(a^3)$ since the sum converges (since $0<b/2<c$). Taking this into account in (3.26), it follows from (3.25) that

$$\begin{aligned} q_{\mathcal{H}}(x) &= -\frac{1}{2}\int_{-\infty}^{\infty}\frac{d\sigma}{\pi}\,\mathrm{tr}[H^{(0)}V^2(G^{(0)}_\sigma)^3](x,x)+O(a)(x)\\ &= -\frac{1}{2}\mathrm{tr}\left[H^{(0)}V^2\int_{-\infty}^{\infty}\frac{d\sigma}{\pi}\,\frac{1}{(L^{(0)}+\sigma^2)^3}\right](x,x)+O(a)(x)\\ &= \frac{-3}{16}\mathrm{tr}[H^{(0)}V^2(L^{(0)})^{-5/2}](x,x)+O(a)(x). \end{aligned} \tag{3.27}$$

Evaluating the trace over spinor indices we find [with $\nabla_\mu = \frac{1}{2}(\nabla^+_\mu+\nabla^-_\mu)$]

$$\begin{aligned} q_{\mathcal{H}}(x) = \frac{-3r}{16}\epsilon_{\mu\nu\rho\sigma}\mathrm{tr}\left[\left(-\nabla^{(0)}_\mu(V_\nu V_{\rho\sigma}+V_{\nu\rho}V_\sigma)+\left(\frac{1}{2}\Delta^{(0)}-m_0\right)V_{\mu\nu}V_{\rho\sigma}\right)(L^{(0)})^{-5/2}\right](x,x)\\ +O(a)(x), \end{aligned} \tag{3.28}$$

where V_μ and $V_{\mu\nu}$ are given by (3.20) and (3.21). Calculations give (cf. the Appendix)

$$[\nabla^{\pm}_\mu,\nabla^{\pm}_\nu]\psi(x) = (a^2F_{\mu\nu}(x)+O(a^3)(x))\psi(x\pm ae_\mu\pm ae_\nu), \tag{3.29}$$

$$[\nabla^{\pm}_\mu,\nabla^{\mp}_\nu]\psi(x) = (a^2F_{\mu\nu}(x)+O(a^3)(x))\psi(x\pm ae_\mu\mp ae_\nu). \tag{3.30}$$

These determine the relevant contributions of V_μ and $V_{\mu\nu}$ in (3.28).

We now exploit the fact that there is a Fourier transformation on $\mathcal{H}^{sc}$ (=the space of scalar lattice fields with $\|\phi\|^2=\Sigma_{x\in a\mathbf{Z}^4}|\phi(x)|^2<\infty$); in particular, δ_x has the Fourier expansion

$$\delta_x = \int_{-\pi}^{\pi} \frac{d^4k}{(2\pi)^4} e^{-ikx/a} \phi_k , \tag{3.31}$$

where $\phi_k(y) := e^{iky/a}$. For a general operator $\mathcal{O}$ this leads to

$$\mathcal{O}_{\mathcal{H}}(x,x) = \frac{1}{a^4} \left\langle \frac{\delta_x}{a^2}, \mathcal{O} \frac{\delta_x}{a^2} \right\rangle = \frac{1}{a^4} \int_{-\pi}^{\pi} \frac{d^4k}{(2\pi)^4} e^{-ikx/a} \frac{1}{a^4} \langle \delta_x, \mathcal{O}\phi_k \rangle$$

$$= \frac{1}{a^4} \int_{-\pi}^{\pi} \frac{d^4k}{(2\pi)^4} e^{-ikx/a} (\mathcal{O}\phi_k)(x). \tag{3.32}$$

In the case where

$$\mathcal{O} = \epsilon_{\mu\nu\rho\sigma} (-\nabla_\mu^{(0)} (V_\nu V_{\rho\sigma} + V_{\nu\rho} V_\sigma) + (\tfrac{1}{2}\Delta^{(0)} - m_0) V_{\mu\nu} V_{\rho\sigma}) (L^{(0)})^{-5/2}, \tag{3.33}$$

a calculation using (3.20) and (3.21) with (3.29) and (3.30) gives

$$(\mathcal{O}\phi_k)(x) = 32\pi^2 a^4 \lambda(k;r,m_0) (q^A(x) + O(a)(x)) \phi_k(x), \tag{3.34}$$

where

$$\lambda(k;r,m_0) = \frac{\Pi_\nu \cos k_\nu (-m_0 + \Sigma_\mu (1 - \cos k_\mu) - \Sigma_\mu (\sin^2 k_\mu / \cos k_\mu))}{[\Sigma_\mu \sin^2 k_\mu + r^2 (-m_0 + \Sigma_\mu (1 - \cos k_\mu))^2]^{5/2}}. \tag{3.35}$$

It follows from (3.28) and (3.32) that

$$q_{\mathcal{H}}(x) = I(r,m_0) q^A(x) + O(a)(x), \tag{3.36}$$

where

$$I(r,m_0) = \frac{-3r}{8\pi^2} \int_{-\pi}^{\pi} d^4k \, \lambda(k;r,m_0). \tag{3.37}$$

This integral was evaluated earlier in Refs. 21 and 23. It was found to be independent of $r > 0$ and a locally constant function of m_0 with values given by (2.14). This completes the proof of Proposition 2.

Remark: It is straightforward to generalize the results of this paper to SU(N) gauge fields on the $2n$-torus for arbitrary $n \geqslant 2$ and to U(1) gauge fields on the two-torus.

Finally, following the suggestion of a referee, we emphasize that a key point in this work is that it is the topological charge (i.e., the integrated Chern character) rather than the topological density that is shown to have the correct continuum limit. In this respect the treatment differs from all earlier treatments which are essentially limited to small (hence topologically trivial) fields.

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APPENDIX

In this Appendix we recall, for completeness, certain standard facts concerning the lattice transcript of a smooth continuum gauge field on $\mathbf{R}^4$ which lead to the bounds used in this article. The lattice transcript (2.1) can be written as

$$U_\mu(x)=\sum_{n=0}^{\infty} a^n \int_{0\leqslant t_1\leqslant\cdots\leqslant t_n\leqslant 1} dt_n\cdots dt_1\, A_\mu(x,t_n)\cdots A_\mu(x,t_1), \tag{A1}$$

where $A_\mu(x,t)=A_\mu(x+(1-t)ae_\mu)$. When A is bounded, i.e., $\|A_\mu(x)\|\leqslant K$ for all x,μ, we have

$$\Big\|\sum_{n=p}^{\infty} a^n \int_{0\leqslant t_1\leqslant\cdots\leqslant t_n\leqslant 1} dt_n\cdots dt_1\, A_\mu(x,t_n)\cdots A_\mu(x,t_1)\Big\|\leqslant\sum_{n=p}^{\infty} a^n \frac{1}{n!}K^n\leqslant a^pK^pe^{aK}\sim O(a^p). \tag{A2}$$

Therefore, to derive the $O(a^p)$ and $O(a^p)(x)$ bounds used in the text it suffices to consider only a finite number of terms in the expansion (A1) (typically just the first few terms). An immediate consequence of (A2) with $p=1$ is the following: If A is bounded, then for any operator $P=P(\nabla_\mu^{\pm})$ which is a polynomial in the covariant finite difference operators (2.6) and (2.7) we have

$$\|P-P^{(0)}\|\sim O(a).$$

The bounds $\|H-H^{(0)}\|\sim O(a)$ and $\|L-L^{(0)}\|\sim O(a)$ are particular examples of this. If we furthermore assume that the first order partial derivatives of A are bounded, i.e., $\|\partial_\mu A_\nu(x)\|\leqslant K$ for all x,μ,ν, we have

$$\|[\nabla_\mu^{\pm(0)},U_\nu]\|\sim O(a). \tag{A3}$$

To see this, note that

$$\begin{aligned}[\nabla_\mu^{+(0)},U_\nu]\psi(x)&=(U_\nu(x+ae_\mu)-U_\nu(x))\,\psi(x+ae_\mu)\\&=\left(a\int_{0\leqslant t\leqslant 1} dt(A_\nu(x+ae_\mu,t)-A_\nu(x,t))+O(a^2)\right)\psi(x+ae_\mu).\end{aligned} \tag{A4}$$

By the middle-value theorem,

$$A_\nu(x+ae_\mu,t)-A_\nu(x,t)=\partial_\mu A_\nu(x+sae_\mu,t)$$

for some $s\in[0,1]$. Since $\|\partial_\mu A_\nu\|$ is bounded (A3) now follows from (A4). The bound (A3) has the following easy generalization: Let $P=P(\nabla_\mu^{\pm})$ be a polynomial of degree k in the $\nabla_\mu^{\pm}$'s; then, if all the partial derivatives of A of order $\leqslant k$ are bounded, we have

$$\|[P^{(0)},U_\nu]\|\sim O(a). \tag{A5}$$

Moreover, with the same boundedness assumptions on $A_\mu(x)$ and $\partial_\mu A_\nu(x)$, straightforward calculations using the middle-value theorem give

$$1-U(p_{x,\mu,\nu})=a^2F_{\mu\nu}(x)+O(a^3)(x). \tag{A6}$$

Noting that[16]

$$[\nabla_\mu^{+},\nabla_\nu^{+}]\psi(x)=(1-U(p_{x,\mu\nu}))U_\mu(x)U_\nu(x+ae_\mu)\,\psi(x+ae_\mu+ae_\nu) \tag{A7}$$

and similar formulas for the other commutators, a straightforward refinement of the arguments leading to (A5) and (A6) shows

$$\|[P^{(0)},[\nabla_\mu^{\pm},\nabla_\nu^{\pm}]]\|\sim O(a^3),\quad \|[P^{(0)},[\nabla_\mu^{\pm},\nabla_\nu^{\mp}]]\|\sim O(a^3). \tag{A8}$$

The requirement for this is that A and all its partial derivatives up to order r be bounded, where $r=\min\{k,2\}$. Since V is a linear combination of commutators of the $\nabla_\mu^{\pm}$'s we have, in particular,

$\|[L^{(0)},V]\| \sim O(a^3)$ when A and its partial derivatives up to order 2 are bounded. Finally, we remark that (3.29) and (3.30) follow from combining (A7) and the corresponding formulas for the other commutators with (A6).

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Some navigation rules for D-brane monodromy

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We explore some aspects of monodromies of D-branes in the Kähler moduli space of Calabi–Yau compactifications. Here a D-brane is viewed as an object of the derived category of coherent sheaves. We compute all the interesting monodromies in some nontrivial examples and link our work to recent results and conjectures concerning helices and mutations. We note some particular properties of the 0-brane. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1409963]

I. INTRODUCTION

There has been something of an evolution in our ideas about how a D-brane should be considered. For the purposes of this article we are interested only in the even-dimensional branes in a type II string (so-called ''B-branes''). The sequence of ideas has progressed roughly as follows

(1) A D-brane is something on which an open string may end.
(2) A D-brane is a U(N) gauge theory living on a subspace with scalar fields spanning the normal bundle.
(3) A D-brane should be viewed as coming from K-theory.[1,2]
(4) A D-brane should be viewed as an object of the derived category of coherent sheaves[3,4] (see also Ref. 5). (In this article the derived category will always be bounded at both ends.)

We could also add that for nontrivial H field a D-brane should be viewed as an object of the derived category of sheaves of modules over an Azumaya algebra.[6] We will assume H is trivial and so view D-branes as an object of the derived category of coherent sheaves. We will consider our target space to be a Calabi–Yau threefold X and we denote the derived category in question as $\mathbf{D}(X)$. For the purposes of this article we ignore any issues concerning the stability of D-branes. Our D-branes, which are objects of $\mathbf{D}(X)$, were called ''topological D-branes'' in Ref. 4 where issues of stability were discussed.

The reason that $\mathbf{D}(X)$ is ''better'' than K-theory is that it contains so much more information. For example *any* 0-brane on X corresponds to the same single element of K-theory whereas the object of $\mathbf{D}(X)$ corresponding to a 0-brane knows *where* this point is. That is, K-theory measures the charge of the D-brane but $\mathbf{D}(X)$ tells us more and possibly all we could wish to know about a particular D-brane.

As well as being knowledgeable about D-branes, $\mathbf{D}(X)$ is also very knowledgeable about X itself. This should not be too surprising as if we know about all the 0-branes on X, then we know about all the points on X and so we should know about X itself. Indeed, for a very large class of algebraic varieties it was shown by Bondal and Orlov[7] that X is completely determined, as an algebraic variety, by $\mathbf{D}(X)$. While this process does not quite work for Calabi–Yau varieties it is easy to speculate that adding such data as the spectrum of central charges while in a ''Calabi–Yau phase'' may provide the missing information. This would allow the target space to be constructed only given worldsheet information. Clearly, therefore, the derived category should be of great *physical* as well as mathematical interest.

An interesting question, also studied in Ref. 7, concerns in how many ways one may associate a derived category to a fixed X. An ''autoequivalence'' of a derived category is a map from the category to itself preserving all the intrinsic algebraic structure associated to the category. Such a

map need not preserve D-branes themselves. For example, an object representing a 2-brane may become something which more resembles a 4-brane under such a transformation. In terms of string theory, these autoequivalences can arise from monodromy in the moduli space of the complexified Kähler form as first observed by Kontsevich.[3] Indeed, the fact that this monodromy action on $\mathbf{D}(X)$ can be understood at all is one the appealing aspects of the derived category. It was suggested in Ref. 8 that the derived category should play a role in the heterotic string for similar reasons.

Since many interesting questions about $\mathbf{D}(X)$ are associated to these monodromies, the purpose of this article is to explore some of the aspects of these monodromies. The analysis of monodromies when the moduli space of complexified Kähler forms has only one complex dimension is pretty easy as we review in Sec. 3. Most of the interesting properties of monodromy do not appear until we explore higher-dimensional moduli spaces. We do this in the later sections.

One should note that many of these problems can be, and have been, performed using the method of solving the Picard–Fuchs equations and using analytic continuation (see Refs. 9–13, etc.). These methods have been used in the context of D-branes in such papers as Refs. 14–17. Instead we will use the language of derived categories where, we believe, the structure is much simpler to understand. In this way, computation of the monodromy is extremely easy (at least on the cohomology classes) and does not require the aid of a computer. Note that we are not being at all original in using the derived category—computations along these lines have been done in Refs. 18–21, for example. Our work differs from the latter only in the way we probe more deeply into the moduli space addressing such questions as monodromy around Landau–Ginzburg points in multi-parameter examples. Monodromy using the derived category approach has also been studied recently in papers such as Ref. 22.

Some interesting papers (Refs. 23–25) have appeared recently which compute the finite monodromy associated to orbifold theories by using the method of ''helices and mutations of exceptional sheaves.'' One of the motivations of this article was to better understand this construction in the language of the derived category. We discuss the connection (and differences) in Sec. IV. We also study the case of reducible exceptional divisors in Sec. VI B, which appears, at least at first sight, to lie somewhat outside the method of helices.

At least in the context of Batyrev-type Calabi–Yau varieties associated to toric geometry,[26] it seems possible to rigorously classify all types of monodromy. Indeed Horja[20] has achieved this in the neighborhood of the large radius limit. Rather than attempt such a classification we will simply go through some examples which appear to demonstrate most of the interesting things which can happen.

Our analysis is closely tied to the ''phase picture'' [27,28] of the moduli space. One has various limit points in the moduli space, each of which lies in the center of some phase. There are naturally embedded $\mathbb{P}^1$'s in the moduli space which connect adjacent limit points. We are concerned with monodromy within, or almost within, such $\mathbb{P}^1$'s. Most of the ''interesting'' questions one could ask about monodromy appear to be contained in this structure.

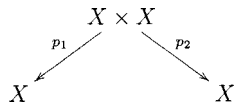
In Sec. V we exhaustively study a two-parameter example obtaining all interesting monodromies associated to this model. In Sec. VI we study some aspects of another couple of examples which exhibit some properties not seen in Sec. V.

Because of the prominent rôle played by the 0-brane in the construction of Bondal and Orlov, we discuss some of its properties under monodromies in Sec. VII.

II. AUTOEQUIVALENCES AND THE FOURIER–MUKAI TRANSFORM

In this section we will quickly review the language we use for the derived category. See Refs. 29 and 30 for more information about the derived category itself and Refs. 19 and 31 for more on some of the notation used later in this work.

Douglas[4] has argued that the even-dimensional D-branes on a Calabi–Yau X should be associated with objects in the derived category of coherent sheaves on X. The morphisms in this category are associated to open strings. Given a particular object $\mathscr{K}$ of $\mathbf{D}(X\times X)$ we associate projections



(1)

and the Fourier–Mukai transform[32,33]

$$T_{\mathscr{K}}(\mathscr{F}) = \mathbf{R}p_{2*}(\mathscr{K} \overset{L}{\otimes} p_1^*\mathscr{F}), \tag{2}$$

for any object $\mathscr{F}$ of $\mathbf{D}(X)$.

If $\mathscr{K}$ is chosen carefully (see Refs. 7 and 34 for details), then the Fourier–Mukai transform will be an "autoequivalence" of $\mathbf{D}(X)$. Namely, it maps $\mathbf{D}(X)$ back to itself while preserving the important algebraic structure associated to the "distinguished triangles." What this means for us is that the physics should remain invariant under such a transformation.

There are two cases of such $\mathscr{K}$'s which are of particular interest which will be denoted $\mathscr{K}^B$ and $\mathscr{K}^K$. First let L be a line bundle (or invertible sheaf) over X and let $j: X \to X \times X$ be the diagonal embedding. Then let $\mathscr{K}_L^B$ (where the superscript B stands for "B-field" for reasons to become clear) be the object of $\mathbf{D}(X \times X)$ given by

$$\cdots \to 0 \to j_* L \to 0 \to \cdots, \tag{3}$$

such that the nontrivial term is at the zeroth position.

Now consider the object of $\mathbf{D}(X)$ given by a sheaf at zeroth position:

$$\cdots \to 0 \to \mathcal{F} \to 0 \to \cdots. \tag{4}$$

If we apply to (4) the Fourier–Mukai transform associated to $\mathscr{K}_L^B$, we obtain

$$\cdots \to 0 \to \mathcal{F} \otimes L \to \cdots. \tag{5}$$

To relate this to string theory, let $\mathcal{F}$ be a sheaf supported over some subspace of X. That is, we have a D-brane wrapping this subspace. All we have done by applying this transform is to change the field strength of the U(1) gauge bundle over the D-brane. Gauge invariance forces the combination $F - B$ to be appear in the action of the D-brane. The above transformation must therefore be equivalent to $B \mapsto B + L$. [Note that we use L to denote the line bundle, the associated divisor class, and the dual two-form $c_1(L)$.]Thus we may assert (as was also done in Ref. 20) that *the transformations associated to $\mathscr{K}_L^B$ are those of a B-field shift $B \mapsto B + L$.*

Another transformation of interest is that of Seidel and Thomas[19] given by

$$\mathscr{K}_{\mathscr{E}}^K = \mathrm{Cone}\{\mathscr{E}^\vee \boxtimes \mathscr{E} \to j_* \mathcal{O}_x\}, \tag{6}$$

where $\mathcal{O}_X$ is the structure sheaf of X. The superscript K stands for "Kontsevich" who was the first to use this kind of transformation in the context of string theory.[18] Here the notation $A \boxtimes B$ is short for $p_1^* A \otimes p_2^* B$. The object $\mathscr{E}$ is any object of $\mathbf{D}(X)$ which satisfies the sphericity conditions given in Ref. 19. We refer to Ref. 30 for a nice description of the cone construction.

Now the associated Fourier–Mukai transform simplifies to the following:[19]

$$T_{\mathscr{K}_g^K}(\mathscr{F}) = \mathrm{Cone}\{\mathrm{Hom}(\mathscr{E}, \mathscr{F}) \otimes \mathscr{E} \overset{f}{\to} \mathscr{F}\}, \tag{7}$$

where f is the obvious evaluation map.

It is worth pointing out a subtle but potentially important point. The cone construction is not a particularly well-defined functor in the context of the derived category. We refer to Sec. 1.4 of Chap. 5 of Ref. 29 for a discussion of the problems. By writing the transformation in the form (7) we potentially expose ourselves to such ambiguities. One should always bear in mind, however,

that the transformation exists as a Fourier–Mukai transform (2) which yields a perfectly well-defined functor from $\mathbf{D}(X)$ to itself. In particular, the cone appearing in (6) is only defining $\mathscr{K}_{\mathscr{E}}^{K}$ as an object and no functorial properties of the cone are required there.

It is difficult to understand the physical meaning of the transformation associated to $\mathscr{K}_{\mathscr{E}}^{K}$ working directly in the derived category. Instead we take Chern characters to see the effect on cohomology. From (7) one deduces that[19]

$$ch(T_{\mathscr{K}_{g}^{K}(\mathscr{E})}(\mathscr{F}))=ch(\mathscr{F})-\langle\mathscr{E},\mathscr{F}\rangle ch(\mathscr{E}), \tag{8}$$

where

$$\langle\mathscr{E},\mathscr{F}\rangle=\sum_{i}(-1)^{i}\dim\ \mathrm{Hom}^{i}(\mathscr{E},\mathscr{F})=\int_{X}^{i}ch(\mathscr{E}^{\vee})ch(\mathscr{F})td(\mathscr{T}_{X}), \tag{9}$$

and $\mathscr{T}_X$ is the tangent sheaf of X.

Now it is generally believed that the (skew-symmetric) inner product $\langle\mathscr{E},\mathscr{F}\rangle$ on X is equal to the (equally skew-symmetric) intersection form for three-cycles on the mirror Y.[14,35,36] According to this analogy, the transformation (8) is nothing more than a Picard–Lefschetz transformation that one would associate to monodromy around a vanishing three-sphere in Y.[19,36] Because of this it seems natural to expect this kind of transformation to be associated to monodromy in the moduli space of complex structures around some parts of the discriminant locus.

III. A ONE-PARAMETER CASE

In this section we will review a computation apparently first done by Kontsevich.[18]

We consider the case where X is the quintic hypersurface in $\mathbb{P}^4$. As is very well known[9] the moduli space of complexified Kähler forms can be taken to be $\mathbb{P}^1$ with three interesting point. These point are as follows:

P_0: The Gepner point. Metrically it lies at an orbifold point $\mathbb{C}/\mathbb{Z}_5$.

P_1: The ''conifold point.'' The mirror of X acquires a conifold singularity. The conformal field theory associated to X is singular.

P_∞: The large radius limit. This point is an infinite distance away from the above two points.

Let H denote the homology class of the four-cycle given by the hyperplane section of the quintic threefold. We will also use H to denote its Poincaré dual which generates $H^2(X,\mathbb{Z})$. We then have

$$td(\mathscr{T}_X)=\frac{(H/1-e^{-H})^5}{(5H/(1-e^{-5H}))},=1+\frac{5}{6}H^2, \tag{10}$$

and

$$\int_X H^3=5. \tag{11}$$

The monodromy around P_0 is expected to be of order 5 because of the $\mathbb{Z}_5$ quantum symmetry of the Gepner model. The monodromy around P_∞ is known to correspond to $B\mapsto B+H$. In other words, we expect it to be given by the transformation $\mathscr{K}^{B}_{\mathcal{O}(H)}$. We will denote this by $\mathscr{K}^{B}_{H}$ for short.

Kontsevich conjectured that the monodromy around P_1 is given by the Fourier–Mukai transform $\mathscr{K}^{K}_{\mathscr{E}}$ of the previous section where $\mathscr{E}$ is given by the structure sheaf $\mathcal{O}_X$. We denote this $\mathscr{K}^{K}_{0}$ for short. We will return to this conjecture in a more precise form in Sec. V.

It follows from the topology of a sphere with three punctures that the product of the monodromy around P_∞ and the monodromy around P_1 should equal the monodromy around P_0 and hence should be of order 5. (Note that we are required to take the loops around P_1 and P_∞ in the

''same direction'' in order for their product to be a loop around P_0. Throughout this article we will have orientation problems such as this. We will not concern ourselves at all with such details. In all the examples we do, we simply find the right combination which gives the expected results.) We may verify that this is consistent with the Chern character of any starting D-brane.

Let us start with $\mathscr{F}$ given by $\mathcal{O}_X$ and apply the desired sequence of monodromy transformations. From (8) we obtain the following:

$$\begin{aligned} ch(\mathscr{F}) &= 1, \\ ch(\mathscr{K}_H^B \mathscr{F}) &= e^H, \\ ch(\mathscr{K}_0^K K_H^B \mathscr{F}) &= e^H - 5, \\ ch(\mathscr{K}_H^B \mathscr{K}_0^K \mathscr{K}_H^B \mathscr{F}) &= e^{2H} - 5e^H, \\ &\vdots \\ ch((\mathscr{K}_0^K \mathscr{K}_H^B)^5 \mathscr{F}) &= 1 + (e^H - 1)^5 = 1, \end{aligned} \tag{12}$$

as $H^4 = 0$ in X. This is therefore consistent.

It would be interesting to check that $(\mathscr{K}_0^K \mathscr{K}_H^B)^5$ gives the identity transform when applied directly to $\mathbf{D}(X)$ rather than just applied to cohomology. We will not attempt this here.

Note that it is easy to apply the same method to other one-parameter examples as listed in Ref. 37, for example.

IV. HELICES AND MUTATIONS

The purpose of this section is to briefly point out similarities and differences between the above computation for the quintic and the notion of helices and exceptional sheaves. The reader who is not directly interested in such things can skip this section.

It is easiest to describe mutations and helices directly in the derived category. See Ref. 38, for example, for more information. Let us consider the space $V = \mathbb{P}^4$ and let H denote the hyperplane class. Now consider the exceptional collection of sheaves $\{\mathcal{O}, \mathcal{O}(H)\}$. We may use a mutation to pull $\mathcal{O}(H)$ to the left through $\mathcal{O}$. Let $\mathscr{E}(H)$ denote the resulting object in $\mathbf{D}(\mathbb{P}^4)$. One can compute $ch(\mathscr{E}(H)) = e^H - 5$.

Similarly we may begin with the set $\{\mathcal{O}, \mathcal{O}(H), \mathcal{O}(2H)\}$ and pull $\mathcal{O}(2H)$ through $\mathcal{O}(H)$ and $\mathcal{O}$ to obtain $\mathscr{E}(2H)$, etc. The result of such mutations appears remarkably similar to the monodromy transformations we considered in the previous section. Indeed one obtains

$$ch(\mathscr{E}(nH)) = ch((\mathscr{K}_0^K \mathscr{K}_H^B)^n \mathscr{F}), \quad \text{for} \quad = 0,...,4. \tag{13}$$

This correspondence fails for $n = 5$, however. In this case we have $ch(\mathscr{E}(5H)) = 0$. This disagreement should come as no surprise. The language of mutations of helices can be recast in the form of the Fourier–Mukai transforms of Sec. II. The key point, however, is that the algebraic variety in question is the ambient $\mathbb{P}^4$ itself rather than the Calabi–Yau hypersurface X. Indeed exceptional sheaves cannot exist on X.

A Fourier–Mukai transformation does *not* yield an autoequivalence of $\mathbf{D}(\mathbb{P}^4)$ as it fails the canonical class constraint of Ref. 34. That is why the fifth application of the supposed monodromy transformation can kill the object in $\mathbf{D}(\mathbb{P}^4)$.

The language of mutations of helices was used in Refs. 23–25 successfully to obtain monodromies because Eq. (13) holds true. Note, however, that the procedure of going from $\mathscr{E}(nH)$ to $\mathscr{E}((n+1)H)$ cannot generally be identified with monodromy around the Gepner point because of the more general failure of this relation.

V. A TWO-PARAMETER CASE

The structure of monodromies becomes considerably more interesting when one starts to look at moduli spaces of more than one dimension. In this case, the ''discriminant locus'' of bad conformal field theories is a subvariety of the moduli space with dimension one or more.

We wish to see if the Fourier–Mukai transforms considered earlier can also be applied in these more complicated situations. Note that this problem has been studied by Horja[20] and by Seidel and Thomas.[19] Horja gave extensive results for monodromy loops which are ''close'' to the large radius limit in some sense. We will be interested in relations obtained by venturing further into the moduli space. The Fourier–Mukai transforms we will consider follow closely the construction by Seidel and Thomas.[19] Reference 39 has appeared very recently which shows that these methods are essentially a special case of Horja's construction.

Our goal in this section will be to obtain a similar result to Sec. III in a two-parameter example. Namely, can we find a sequence of monodromies which give a loop around some point which looks like a Gepner point, and hence has finite order?

Because the moduli space is two-dimensional there is no notion of ''monodromy around a point.'' Given a complex curve in our moduli space we can define a monodromy. We will use two notions extensively later in the text and we wish to emphasize the difference here to avoid confusion. We will often refer to monodromy *around* a curve for a loop in the two-dimensional moduli space which lies external to the curve. We will also refer to the completely different notion of monodromy *within* the curve around a specific point. The words ''around'' and ''within'' will always have the above meaning.

Our example is where X is a blown-up hypersurface of degree 18 in the weighted projected space $\mathbb{P}^4_{9,6,1,1,1}$. This space was studied extensively in Ref. 12 and analyzed in relation to D-branes in Ref. 17. The two generators of $H^2(X,\mathbb{Z})$ (and their Poincaré dual divisors) will be called H and L consistent with Ref. 12. If we put homogeneous coordinates $[z_1,\ldots,z_5]$ on $\mathbb{P}^4_{9,6,1,1,1}$, then the divisor class of $z_1=0$ is given by $3H$, the class of $z_2=0$ is given by $2H$. The class of $z_3=0$ or $z_4=0$ or $z_5=0$ (after the blow-up) is given by L. This weighted projective space has a curve of singularities which intersects the hypersurface at one point. Locally this point looks like the orbifold $\mathbb{C}^3/\mathbb{Z}_3$. We blow this up to produce an exceptional divisor $E\simeq\mathbb{P}^2$. In terms of homology classes, $E=H-3L$.

The remaining topological information required for X is as follows. H^2, HL, L^2 live in $H_2(X)$ or $H^4(X)$ subject to the constraint $H(H-3L)=0$. $H_0(X)$ or $H^6(X)$ has a single generator we denote p, and $H^3=9p$, $H^2L=3p$, $HL^2=p$, $L^3=0$. Obviously any monomial of degree 4 or higher in H or L vanishes. Finally,

$$td(\mathcal{T}_x)=1+\tfrac{1}{2}L^2+\tfrac{1}{4}HL. \tag{14}$$

The mirror, Y, of X has defining equation

$$a_0z_1z_2z_3z_4z_5+a_1z_1^2+a_1z_1^2+a_2z_3^{18}+a_4z_3^{18}+a_4z_4^{18}+a_6z_3^6z_4^6z_5^6. \tag{15}$$

The ''algebraic'' coordinates on the moduli space are then given by

$$x=\frac{a_1^3a_2^2a_6}{a_0^6},\quad y=\frac{a_3a_4a_5}{a_6^3}. \tag{16}$$

We may then define the discriminant as an expression in x and y which vanishes when Y becomes singular. If the data can be presented torically as in this case, then Sec. 3.5 of Ref. 40 gives a nice efficient way of computing this discriminant. In our example, the discriminant factorizes into two parts:

$$\Delta_0 = 6^{12}x^3y + (432x-1)^3,$$
$$\Delta_1 = 27y + 1. \tag{17}$$

We want to picture the moduli space in two different ways. First we use the ''phase'' description of Refs. 27 and 28. See also Sec. 3 of Ref. 41. We project the discriminant into $\mathbb{R}^2$ by plotting $-\log|y|$ against $-\log|x|$. We show the result in Fig. 1. The result is that the two-plane is divided into four ''phases.'' We chose our algebraic coordinates (16) so that the Calabi–Yau phase appears in the positive quadrant. The limit point of this phase is the large radius limit. The positive quadrant may also be viewed as the Kähler cone of X where the class H gives the horizontal direction and L gives the vertical direction.

The other phases are pictured as follows. There is an orbifold phase whose limit point has the orbifold singularity $\mathbb{C}^3/\mathbb{Z}_3$ but the Calabi–Yau has infinite volume. There is a $\mathbb{P}^2$ phase where X collapses onto a $\mathbb{P}^2$. This can happen as X is an elliptic fibration over $\mathbb{P}^2$. In the limit, this elliptic fiber has zero area and the $\mathbb{P}^2$ has infinite volume. Finally, we have a Landau–Ginzburg phase with the Gepner point as the limit point.

The other way of drawing the moduli space is as a complex surface. The phase picture in Fig. 1, i.e., the *secondary fan* of X, is viewed as the fan of a toric variety $\mathscr{M}$ as described in Ref. 28. The coordinates x and y are then naturally coordinates over a patch of the moduli space $\mathscr{M}$. (This is identified by associating the dual of the cone in the positive quadrant with Spec $\mathbb{C}[x,y]$.) In this case $\mathscr{M}$ is a surface with two quotient singularities. The discriminant is a divisor in $\mathscr{M}$.

We sketch $\mathscr{M}$ in Fig. 2 by drawing complex dimensions as real. Our limit points appear as dots in the diagram. We draw the curves $C_1,\ldots,C_4$ as the $\mathbb{P}^1$'s joining adjacent phase limits. Torically these curves are associated to the lines in Fig. 1 which separate the phases. Figure 2 also shows how the discriminant intersects these curves. Note that Δ_0 and Δ_1 are themselves smooth curves in $\mathscr{M}$. The extra circles around the LG and orbifold point denote the fact that both of these points lie at a quotient singularity of the form $\mathbb{C}^2/\mathbb{Z}_3$ in $\mathscr{M}$.

If we followed the analysis of Ref. 12 we would now blow-up $\mathscr{M}$ so that it was smooth and that the intersections of the discriminant with the curves C_i were transverse. This requires several blow-ups. Rather than do this, we find it easier to work directly in $\mathscr{M}$.

We would now like to take each of the curves $C_1,\ldots,C_4$ in turn and do a similar computation to that of Sec. III *within* that curve (or nearly so) to check our monodromy predictions. Note that each curve C_i has three special points on it—the two limit points and a third point where the

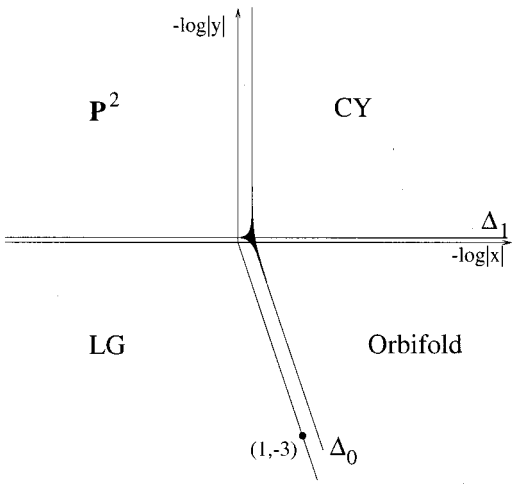


FIG. 1. The four phases of the two-parameter example.

discriminant hits the curve in some way. Thus, just as in Sec. III, we will show that the product of the monodromy around one of the limit points and around the discriminant is equal to the monodromy around the other limit point.

A. C_1

Let us fix a basepoint near the large Calabi–Yau limit point. Because we have identified the cone of this phase with the Kähler cone of X we immediately know the monodromies around C_1 and C_2. Each must be a shift in the B-field. To be precise, a loop around C_1 will correspond to $B \mapsto B+L$ and hence corresponds to $\mathscr{K}_L^B$. Similarly a loop around C_2 is given by $\mathscr{K}_H^B$.

Since C_1 and C_2 intersect transversely, the monodromy around the Calabi–Yau point within C_1 corresponds to going around C_2 and is thus given by $\mathscr{K}_H^B$. In other words $ch(\mathscr{F}) \mapsto e^H ch(\mathscr{F})$.

What about the monodromy within C_1 around the point in the middle where the discriminant hits? A method for computing this was presented in Ref. 20 but we will proceed a little differently. First we need to decide how to go around a generic part of Δ_0. Note that Δ_0 is the irreducible component of the discriminant corresponding to the appearance of singularities in (15) for *nonzero* $z_1,\ldots,z_5$. This was dubbed the "*A*-discriminant" in.[42] (Perhaps rather confusingly, Ref. 42 uses the term "principal *A*-determinant" for the full discriminant $\Delta_0\Delta_1$. Even more confusingly, Δ_0 has sometimes been called the "principal component" of the discriminant.[20]) We will call it the "*primary*" component of the discriminant. One could also define this as the component which is computed by finding solutions to Eqs. (3.45) of Ref. 40. We then state the following conjecture which appears to be due to Horja, Kontsevich, and Morrison in some form or another.[18,20,43]

Conjecture 1: For a suitable choice of basepoint near the Calabi–Yau limit point, a loop around the primary component of the discriminant is given by $\mathscr{K}_0^K = \mathscr{K}_{\mathscr{E}}^K$, *with* $\mathscr{E} = \mathcal{O}_X$.

This is certainly consistent with Sec. III where the primary component was the entire discriminant.

Assuming this conjecture to be true, we still have a complication that makes the computation a little less straightforward. Namely, C_1 does not intersect Δ_0 transversely but rather intersects it tangentially with multiplicity 3. This means that we cannot say that the monodromy within C_1 around the discriminant is given by Conjecture 1.

To proceed with the computation we can put a small three-sphere S^3 around the intersection of Δ_0 and C_1. Since Δ_0 and C_1 are both smooth, it follows that $L_1 = S^3 \cap C_1$ and $L_2 = S^3 \cap \Delta_0$ are both unknotted circles. Because of the tangential intersection, these circles are linked three times. We may remove a point of S^3 and imagine the link in $\mathbb{R}^3$. We show this in Fig. 3.

Next we need to describe $\pi_1(S^3 - (L_1 \cup L_2))$. To do this we use the Wirtinger presentation (see Ref. 44, for example). Imaging fixing a basepoint above the sheet of paper. The arrow a in

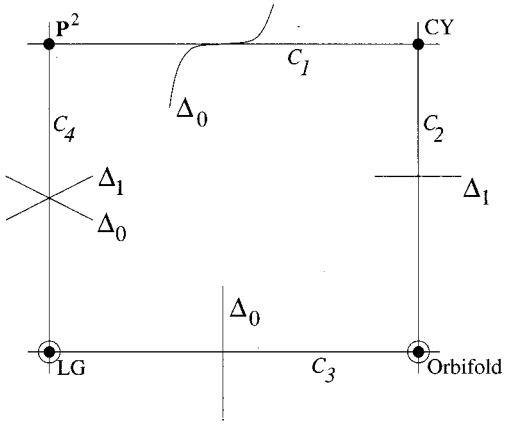


FIG. 2. The moduli space $\mathscr{M}$.

Fig. 3 then represents the element of π_1 looping under the left circle in the direction indicated by the arrow. Similarly, we define b for the right circle. We then have further elements e_i as shown in the figure. Crossing relations then determine

$$\begin{aligned} e_1 &= b^{-1}ab, \\ e_2 &= b^{-1}a^{-1}bab, \\ e_3 &= b^{-1}a^{-1}b^{-1}abab, \\ e_4 &= b^{-1}a^{-1}b^{-1}a^{-1}babab, \\ e_5 &= b^{-1}a^{-1}b^{-1}a^{-1}b^{-1}ababab, \end{aligned} \tag{18}$$

but clearly $e_5 = a$ which yields the relation

$$ababab = bababa. \tag{19}$$

(Our order convention is that ab represents the path b followed by the path a.) Indeed $\pi_1(S^3 - (L_1 \cup L_2))$ is given by the group on two generators (a,b) subject to the single relation (19).

Deform the path within C_1 around the discriminant point a little so that it lies outside C_1. This is the path around which we wish to compute the monodromy. This is the (clockwise) path which follows closely the circle $S^3 \cap C_1$. Such a path is homotopic to $e_1 e_3 e_5 = b^{-2}ababa$. But a is nothing more than a generic loop around Δ_0 and so is given by $\mathscr{K}_0^K$, and similarly b is given by $\mathscr{K}_L^B$. Therefore we claim that monodromy around the discriminant point within C_1 is given by $(\mathscr{K}_L^B)^{-2}\mathscr{K}_0^K\mathscr{K}_L^B\mathscr{K}_0^K\mathscr{K}_L^B\mathscr{K}_0^K$.

Let Q_1 denote the monodromy within $\mathbb{C}_1$ around the $\mathbb{P}^2$ limit point. As this is equal to the combined monodromy around the discriminant point and the Calabi–Yau limit point, we have $Q_1 = \mathscr{K}_H^B(\mathscr{K}_L^B)^{-2}\mathscr{K}_0^K\mathscr{K}_L^B\mathscr{K}_0^K\mathscr{K}_L^B\mathscr{K}_0^K$.

Passing from the Calabi–Yau limit point to the $\mathbb{P}^2$ limit point represents collapsing a large radius elliptic fiber to a Landau–Ginzburg orbifold theory in a manner very similar to the collapse

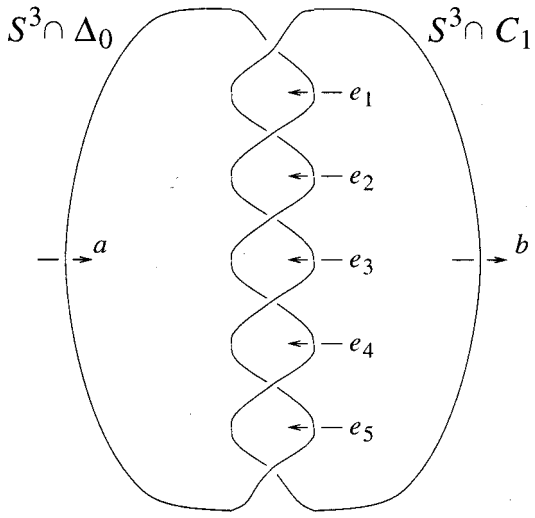


FIG. 3. The triply linked circles.

of the quintic in Sec. III. This Landau–Ginzburg theory is a $\mathbb{Z}_6$-orbifold and thus has a $\mathbb{Z}_6$ quantum symmetry. It should therefore follow that $Q_1^6=1$ in complete analogy with the Landau–Ginzburg point in Sec. III. This is a highly nontrivial check of our picture:

$$\begin{aligned} ch(\mathcal{O}_X)&=1,\\ ch(Q_1\mathcal{O}_X)&=e^H-3e^{H-L}+3e^{H-2L},\\ ch(Q_1^2\mathcal{O}_X)&=e^{2H}-3e^{2H-L}+3e^{2H-2L}-e^H,\\ &\vdots\\ ch(Q_1^6\mathcal{O}_X)&=e^{6H}-3e^{6H-L}+3e^{6H-2L}-e^{5H}-e^{4H}+3e^{4H-L}-3e^{4H-2L}\\ &\quad+3e^{3H-L}-3e^{3H-2L}+e^{2H}+e^H-3e^{H-L}+3e^{H-2L}=1. \end{aligned} \tag{20}$$

B. C_2

So far we have only used $\mathscr{E}=\mathcal{O}_X$ in the Fourier–Mukai transform $\mathscr{K}_{\mathscr{E}}^K$. In this section we use a less trivial choice. The curve C_2 represents the process of blowing-up the $\mathbb{C}^3/\mathbb{Z}_3$ singularity while keeping the rest of the Calabi–Yau at infinite volume. We will attempt to ''localize'' the computations to around the exceptional divisor $E\cong\mathbb{P}^2$.

Let us consider the general case of an irreducible exceptional divisor E in a Calabi–Yau space X of arbitrary dimension. Let the normal bundle be denoted by N. Let us assume that the zero locus of a generic section of $N^\vee$ gives an irreducible variety $W\subset E$ of complex dimension two less than X. W is automatically Calabi–Yau. In our example, W would be a cubic curve in $\mathbb{P}^2$. We therefore have two inclusions

$$i:E\hookrightarrow X,\quad j:W\hookrightarrow E. \tag{21}$$

Now consider two objects $\mathscr{E},\mathscr{F}\in\mathbf{D}(E)$ associated to sheaves on E. In terms of our inner product on X we may apply the Grothendieck–Riemann–Roch theorem to yield the following localization:

$$\begin{aligned} \langle i_*\mathscr{E},i_*\mathscr{F}\rangle_X&=\int_x (ch(i_*\mathscr{E}))^\vee ch(i_*\mathscr{F})td\left(\mathscr{T}_X=\int_E\right)(ch(i_*\mathscr{E}))^\vee ch(\mathscr{F})td(\mathscr{T}_E)\\ &=\int_W (ch(j^*\mathscr{E}))^\vee ch(j^*\mathscr{F})\frac{td(\mathscr{T}_E)}{td(N^\vee)}\\ &=\int_W (ch(j^*\mathscr{E}))^\vee ch(j^*\mathscr{F})td(\mathscr{T}_W)=\langle j^*\mathscr{E},j^*\mathscr{F}\rangle_W. \end{aligned} \tag{22}$$

Therefore, we may compute the inner product between objects of $\mathbf{D}(X)$ which are i_* of something in $\mathbf{D}(E)$ purely in terms of the local geometry of the blow-up.

We may now apply Conjecture 1 to W. In our example W is an elliptic curve and has only one deformation of complexified Kähler form. The discriminant is then a point and therefore primary with respect to W. The associated Fourier–Mukai transform for monodromy is then given by $\mathscr{K}_{\mathscr{E}}^K$ for $\mathscr{E}=\mathcal{O}_W=j^*\mathcal{O}_E$. This naturally motivates the following.

Conjecture 2: The monodromy around a component of the discriminant associated with an irreducible divisor E collapsing to a point is given by $\mathscr{K}_{\mathscr{E}}^K$ for $\mathscr{E}=i_*\mathcal{O}_E$, *where i is the inclusion map*.

Note that $i_*\mathcal{O}_E$ is the structure sheaf of E extended by zero over the rest of X. It can thus be denoted by $\mathcal{O}_E$ itself.

In our example we therefore associate Δ_1 with $\mathscr{K}^K_{\mathscr{E}}$ for $\mathscr{E}=\mathcal{O}_E$ where the class of E is given by $H-3L$. Let us use $\mathscr{K}^K_1$ to denote this transform. Another application of Grothendieck–Riemann–Roch quickly yields

$$ch(\mathcal{O}_E)=1-e^{3L-H}, \tag{23}$$

[and so $ch(\mathcal{O}_E^\vee)=1-e^{H-3L}$].

We are now in a position to compute all the monodromies for C_2. Around the Calabi–Yau limit we have $\mathscr{K}^B_L$. The component Δ_1 hits C_2 transversely and so the monodromy around the discriminant point is given by $\mathscr{K}^K_1$.

Let us use $Q_2=\mathscr{K}^K_1\mathscr{K}^B_L$ to refer to monodromy around the orbifold limit point. A $\mathbb{C}^3/\mathbb{Z}_3$ orbifold has a $\mathbb{Z}_3$ quantum symmetry, so one might naïvely guess that $Q_2^3=1$. Instead we find

$$\begin{aligned} ch(\mathcal{O}_X)&=1,\\ ch(Q_2\mathcal{O}_X)&=e^L,\\ ch(Q_2^2\mathcal{O}_X)&=e^{2L},\\ ch(Q_2^3\mathcal{O}_X)&=e^H. \end{aligned} \tag{24}$$

This suggests the relation $Q_2^3=\mathscr{K}^B_H$. To see why this is so, let us examine more carefully the geometry of the moduli space near the orbifold limit point. As mentioned earlier, this point is actually locally the singularity $\mathbb{C}^2/\mathbb{Z}_3$. We may therefore surround this limit point, not by a sphere, but by a *lens space* $M=S^3/\mathbb{Z}_3$. Now C_2 and C_3 are both smooth curves and therefore they intersect M in unknotted circles.

Consider the free $\mathbb{Z}_3$ quotient map $q:S^3\to M$. The intersection of C_2 and C_3 with M both lift to single circles in S^3 under q^{-1}. These circles are linked once and so π_1 of the complement of these circles in S^3 is the Abelian product $\mathbb{Z}\times\mathbb{Z}$. Let G denote π_1 of the complement of C_2 and C_3 in M. Since q is a normal cover we have

$$1\to\mathbb{Z}\times\mathbb{Z}\to G\to\mathbb{Z}_3\to 1. \tag{25}$$

A more detailed analysis of the geometry shows that $G\cong\mathbb{Z}\times\mathbb{Z}$ where there is a particular element $g_{\text{orb}}\in G$ which cannot be lifted to a loop in S^3 but such that g_{orb}^3 lifts to a loop in S^3 which loops around both C_2 and C_3.

To understand the monodromy we need to deform the loop "inside" C_2 around the orbifold point a little so that it does not intersect C_2 or C_3. There is no unique way to do this. The homotopy class of such a deformation is given by g_{orb} times an arbitrary number of windings *around* C_2. One might argue that the most natural lift is to reduce this extra winding around C_2 and say that the desired loop is simply given by g_{orb}.

Identifying Q_2 with g_{orb} it should then follow that the monodromy Q_2^3 is given by a loop around C_2 followed by a loop around C_3. We see that $Q_2^3=\mathscr{K}^B_H$ is entirely consistent with this so long as *the monodromy around C_3 is trivial*. We also see that our natural deformation of the loop within C_2 is the correct one.

We have therefore understood the monodromy in (24) and argued that the monodromy around C_3 is trivial.

For a true localization to the orbifold point we may put $H=0$. This has the effect of sending that component of the Kähler form of to infinity. Thus the target space looks like a resolution of $\mathbb{C}^3/\mathbb{Z}_3$. In this case the monodromy around the orbifold point really is of order 3. This fact was also determined directly using the Picard–Fuchs system in Ref. 15. Note also that any object of $\mathbf{D}(X)$ which can be written as i_* of something in $\mathbf{D}(E)$ is brought back to itself exactly after looping three times around the orbifold point.

C. C_3

Consider first the loop around the orbifold point within C_3. In order to understand the monodromy we need again to deform this loop a little as in Sec. V B. It turns out that the simplest deformation of this loop is homotopic to the same class g_{orb} as shown earlier. Figure 2 certainly makes this statement counterintuitive! At first sight it looks like a loop within C_2 is like a loop around C_3 and a loop within C_3 looks like a loop around C_2 and these are certainly not equal. It is the quotient singularity which stops this argument from working. Both the loop within C_2 and the loop within C_3 must deform to elements of G which map to the same element of $\mathbb{Z}_3$ in (25). The most natural deformation of these two loops actually makes the loops homotopic.

Therefore, monodromy around the orbifold point within C_3 is given by $Q_2=\mathscr{K}_1^K\mathscr{K}_L^B$. The loop around the discriminant point within C_3 is easy. Since Δ_0 intersects C_3 transversely, the monodromy is given by $\mathscr{K}_0$. The monodromy around the LG point is then given by

$$Q_3=\mathscr{K}_0^K\mathscr{K}_1^K\mathscr{K}_L^B. \tag{26}$$

What properties should we expect for Q_3? The geometry around the LG point is very similar (up to orientation questions) to the geometry around the orbifold point. In particular one may show that the loop corresponding to Q_3 is such that its third power is homotopic to a loop around C_3 and C_4. Now we know that a loop around C_3 induces no monodromy from Sec. V B. The fact that C_4 intersects C_1 transversely at a smooth point in $\mathscr{M}$ tells us that the loop around C_4 is given by Q_1 from Sec. V A. Thus Q_3^3 should have the same properties as Q_1. We saw in Sec. V A that Q_1 was of order 6. *It follows that Q_3 is of order 18.*

We may confirm this explicitly, e.g.,

$$\begin{aligned}
ch(\mathcal{O}_X)&=1,\\
ch(Q_3\mathcal{O}_X)&=e^L-3,\\
ch(Q_3^2\mathcal{O}_X)&=e^{2L}-3e^L+3,\\
ch(Q_3^3\mathcal{O}_X)&=e^H-3e^{2L}+3e^L-1,\\
ch(Q_3^4\mathcal{O}_X)&=e^{H+L}-3e^H+3e^{2L}-e^L,\\
ch(Q_3^5\mathcal{O})&=e^{H+2L}-3e^{H+L}+3e^{H+L}+e^H-e^{2L},\\
ch(Q_3^6\mathcal{O}_X)&=e^{2H}-3e^{H+2L}+3e^{H+L}-e^H-1,\\
ch(Q_3^7\mathcal{O}_X)&=e^{2H+L}-3e^{2H}+3e^{H2L}-e^{H+L}-e^L+3,\\
&\vdots\\
ch(Q_3^{18}\mathcal{O}_X)&=e^{6H}-3e^{5H+2L}+3e^{5H+L}-e^{5H}-e^{4H}+3e^{3H+2L}-3e^{3H+L}\\
&\quad+3e^{2H+2L}-3e^{2H+L}+e^{2H}+e^H-3e^{2L}+3e^L=1.
\end{aligned} \tag{27}$$

Comparing closely (20) and (27) we see that Q_3^3 is not quite the same thing as Q_1, although their effect is very similar. As we have described the loops corresponding to these transformations, they actually differ by a change in basepoint and so Q_1 and Q_3^3 are only equivalent up to conjugation.

The sequence of transformations given in (27) is identical to the sequence predicted by Refs. 23–25 in the language of helices and mutations. There one begins with a sequence of exceptional sheaves on $\mathbb{P}^4_{\{9,6,1,1,1\}}$ of the form $\{\mathcal{O},\mathcal{O}(L),\mathcal{O}(2L),\mathcal{O}(H),\mathcal{O}(H+L),\mathcal{O}(H+2L),\mathcal{O}(2H),\ldots,\mathcal{O}(5H+2L)\}$. One then mutates all the bundles to the left to reverse their order, giving a sequence of objects whose Chern characters are exactly given by (27). It is not hard to see why this is so.

Roughly speaking the transformation $Q_3=\mathscr{K}_0^K\mathscr{K}_1^K\mathscr{K}_L^B$ may be described as follows. $\mathscr{K}_L^B$ takes the sheaf $\mathcal{O}(nL)$ to $\mathcal{O}((n+1)L)$. Next $\mathscr{K}_1^K$ leaves $\mathcal{O}(mH+L)$ or $\mathcal{O}(mH+2L)$ invariant but takes $\mathcal{O}(mH+3L)$ to $\mathcal{O}((m+1)H)$. Finally $\mathscr{K}_0^K$ is a "left mutation" just as it was for the quintic in Sec. IV.

This gives a natural explanation for the funny "jump" seen in the required sequence of exceptional sheaves from $\mathcal{O}(mH+2L)$ to $\mathcal{O}((m+1)H)$. It is effectively caused by the action of $\mathscr{K}_1^K$. Note again the following shortcoming of the method of using sheaves on $\mathbb{P}^4_{\{9,6,1,1,1\}}$. If we extend this process by adding $\mathcal{O}(6H)$ to the above sequence of sheaves, then the 18th transformation of $\mathcal{O}$ would have Chern character equal to 0 rather than 1. Again this is because the corresponding Fourier–Mukai transform on $\mathbb{P}^4_{\{9,6,1,1,1\}}$ is not invertible.

D. C_4

Finally we do the monodromy computation within C_4. This actually yields nothing new. Let Q_4 be the monodromy given by the loop within C_4 around the LG point. Because the LG point is an orbifold point, one can show that this loop (or at least a small deformation of it) is the same as the loop within C_3 around the LG point for reasons essentially identical to the discussion in Sec. V B. This immediately implies $Q_4=Q_3$.

Indeed monodromy around the $\mathbb{P}^2$ point within C_4 is given by $\mathscr{K}_L^B$; and monodromy around the discriminant point requires loops around both Δ_1 and Δ_0 as seen in Fig. 2. Thus we see $Q_4=\mathscr{K}_0^K\mathscr{K}_1^K\mathscr{K}_L^B$ consistent with the above paragraph.

Consider trying to generalize the results of this example. One can show that the specific structure of the monodromy seen in this example depends mainly on the fact that X is a fibration. For example, we could consider a more complicated example with three Kähler moduli such as the resolved hypersurface of degree 24 in $\mathbb{P}^4_{\{1,1,2,8,12\}}$. This is an elliptic fibration over a Hirzebruch surface which itself is a $\mathbb{P}^1$-fibration over $\mathbb{P}^1$. In this example one has a curve in the moduli space which is the analog of C_4 above. It connects the Landau–Ginzburg phase with the $\mathbb{P}^1$ phase. Monodromy around the LG point can then be shown to be of a form $\mathscr{K}_0^K\mathscr{K}_1^K\mathscr{K}_2^K\mathscr{K}_L^B$. This will then reproduce the results of Sec. 9.3 of Ref. 25, for example. Note, however, that the fibration structure is essential here.

VI. OTHER EXAMPLES

The example of Sec. 5 demonstrated many features of monodromy, but there are many other important possibilities which did not appear. In this section we discuss some examples which do exhibit these effects.

A. Surfaces shrinking to curves

All the monodromies around components of the discriminant have been given by a Fourier–Mukai transform of the form (6) studied by Seidel and Thomas. Here we discuss an example that falls outside this class.

Let us consider the resolved hypersurface X of degree 8 in $\mathbb{P}^4_{\{2,2,2,1,1\}}$. We refer to Ref. 11 for extensive details of this model. The space X can be thought of as a K3-fibration over $\mathbb{P}_1$ or as the resolution of a singular space with a curve of singularities of the form $\mathbb{C}^2/\mathbb{Z}_2$. This model has the same moduli space as that of Sec. 5 except for the following aspects:

(i) The $\mathbb{P}^2$ phase is renamed a $\mathbb{P}^1$ phase as this is the base of the fibration.
(ii) The LG and orbifold limit points are now at orbifold points locally of the form $\mathbb{C}^2/\mathbb{Z}_2$.
(iii) The Δ_0 component of the discriminant now intersects C_1 at a point of multiplicity two rather than three.

When we compute the monodromies around the discriminant the real difference appears when we consider Δ_1. Let E be the exceptional divisor in X coming from the resolution of the curve of

singularities. E is a product of a genus 3 curve Z and $\Gamma \cong \mathbb{P}^1$. We associate Δ_1 with the collapse of E down to Z. The discussion in Sec. V B concerned an exceptional divisor contracting to a *point* and so cannot be applied to monodromy around Δ_1.

The computation of the monodromy on Chern characters was computed in Ref. 45. The result may be rephrased as follows. For a divisor E collapsing to a curve Z of genus g, monodromy around Δ_1 is given by

$$ch(\mathscr{F}) \mapsto ch(\mathscr{F}) - \langle \mathcal{O}_E + (1-g)\mathcal{O}_\Gamma, \mathscr{F} \rangle ch(\mathcal{O}_\Gamma) + \langle \mathcal{O}_\Gamma, \mathscr{F} \rangle ch(\mathcal{O}_E), \tag{28}$$

where $\Gamma \cong \mathbb{P}^1$ is the inverse image of a point for the blow-down.

The Fourier–Mukai transform given by (6) is incompatible with (28). A more general form which is consistent is given by Horja in Refs. 20 and 39. [I thank P. Horja for confirming that his construction is consistent with (28).] We refer to these references for more details.

Given the form of the monodromy (28) it is easy to reproduce all the corresponding results of Sec. V for this example.

B. A reducible exceptional divisor

One might have gotten the impression from the localization argument in Sec. V B that we can understand the monodromy associated to an orbifold singularity by studying the little Calabi–Yau W living inside the exceptional divisor E. Indeed this argument shows that the analysis we did in Sec. V for a Calabi-Yau threefold would also apply locally to a Calabi–Yau fivefold which has a $\mathbb{Z}_{18}$ orbifold singularity given by the action

$$(z_1, z_2, z_3, z_4, z_5) \mapsto (\alpha^9 z_1, \alpha^6 z_2, \alpha z_3, \alpha z_4, \alpha z_5), \tag{29}$$

where $\alpha = \exp(2\pi i/18)$. This is because the resolved $\mathbb{P}^4_{\{9,6,1,1,1\}}$ is the exceptional divisor for this five-dimensional orbifold.

While this is useful in some circumstances, it does not mean that any orbifold analysis can be reduced to a Calabi–Yau computation in lower dimensions. The problem is that the exceptional divisor for an orbifold singularity may be *reducible*. Indeed one generically expects an exceptional divisor be to reducible. In this case the notion of the Calabi–Yau ''inside'' the exceptional divisor makes no sense.

At least in the context of toric cases we can make some general statements about the difference between a reducible and irreducible exceptional divisor. The impression one might have been left with from the above examples is that each particular exceptional divisor E is associated with its own component Δ_E of the discriminant divisor. In this case one then associates monodromy around Δ_E with a process involving the collapse of E.

In the Batyrev[26] way of describing Calabi–Yau n-folds, one has a set of points, $\mathcal{A}$, lying in a hyperplane in $\mathbb{R}^{n+2}$. Vectors from the origin to these points generate the one-dimensional edges of a fan. By the usual algorithm in toric geometry this fan gives the canonical line bundle over some $(n+1)$-dimensional variety V. X is then the ''little Calabi–Yau'' living inside V.

Let Q be the convex hull of $\mathcal{A}$. One can show (see Chap. 10 of Ref. 42) that the irreducible components of the discriminant are determined by faces of Q of various dimensions. For a nontrivial component we require at least $k+2$ points in a k-dimensional face.

If each face of Q has at most one point in its interior, then each divisor associated to this interior point gets its own component of the discriminant. This was the case for the examples studied earlier and was the case for all the examples studied in Refs. 23–25. It is precisely when we have a reducible exceptional divisor that this fails.

We will consider an example of this. For a change we will use a K3 surface rather than a Calabi–Yau threefold. The results generalize easily to the threefold case.

Consider the surface X of degree 12 in $\mathbb{P}^3_{\{4,3,3,2\}}$. This has $\mathbb{C}^2/\mathbb{Z}_2$ singularities at three points and $\mathbb{C}^2/\mathbb{Z}_3$ singularities at four points. Each $\mathbb{Z}_2$ singularity is resolved by a single $\mathbb{P}^1$ and each $\mathbb{Z}_3$ singularity is resolved by a sum of two $\mathbb{P}^1$'s intersecting at a point. The fact that the K3 is

TABLE I. The point-set $\mathcal{A}$ for the K3 example.

a_0	0	0	0	1	$-2H$
a_1	0	0	1	1	B
a_2	1	0	0	1	C
a_3	1	2	0	1	C
a_4	-3	-3	-2	1	$-H+A$
a_5	-2	-2	-1	1	$2H-2A+B$
a_6	-1	-1	0	1	$A-2B$
a_7	1	1	0	1	$H-2C$

embedded in the given ambient space ties the blow-ups of the points of similar type together. There are, in fact, only four Kähler degrees of freedom—the overall size of the initial weighted projective space, one blow-up of all the $\mathbb{Z}_2$ fixed points, and two blow-ups for all the $\mathbb{Z}_3$ fixed points.

We list the coordinates of the points $\mathcal{A}$ in Table I. We also show the divisor classes in terms of a basis (H,A,B,C) associated to these vectors. These divisor classes restrict to form a partial basis of $H_2(X)=H^2(X)$. We then demand that the Kähler form of X lies in the span of these generators. This basis has been chosen so that the resulting slice of the Kähler cone is the positive orthant.

We will only concern ourselves with monodromies associated to the $\mathbb{Z}_3$ blow-ups. To do this we only consider variations in the A and B components of the Kähler form. The two divisor classes of interest are those associated to a_5 and a_6 having classes $2H-2A+B$ and $A-2B$, respectively. These each intersect X in four copies of $\mathbb{P}^1$. Each $\mathbb{P}^1$ from one set intersects one member from the other set of $\mathbb{P}^1$'s in one point. Together these form the resolutions of the four $\mathbb{Z}_3$ fixed points. Note that the set $\{a_4,a_5,a_6,a_1\}$ lies on a straight line.

Let us fix algebraic coordinates

$$x=\frac{a_4a_6}{a_5^2},\quad y=\frac{a_1a_5}{a_6^2}. \tag{30}$$

In terms of these, the component of the discriminant associated with the line $\{a_4,a_5,a_6,a_1\}$ is

$$\Delta_1=27x^2y^2-18xy-1+4x+4y. \tag{31}$$

There are two other components of the discriminant—the primary component and one associated to the three $\mathbb{Z}_2$ fixed points. Δ_1 is the part intrinsically associated to the $\mathbb{C}^2/\mathbb{Z}_3$ resolution.

The discriminant (31) divides the $(-\log x,-\log y)$ into four phases as shown in Fig. 4. One has the resolved phase, the $\mathbb{Z}_3$ orbifold phase, and two phases where one of the pair of $\mathbb{P}^1$'s has been blown up to partially resolve the $\mathbb{Z}_3$ fixed point to something that looks locally like a $\mathbb{Z}_2$ fixed point. We will call the latter two phases $\mathbb{Z}_2^{(A)}$ and $\mathbb{Z}_2^{(B)}$ since they are associated to blowing down using the A or B component of the Kähler form, respectively.

Note again that there is only a *single* irreducible component, Δ_1, of the divisor associated to this picture. The same component of the discriminant is responsible for blowing down either of the $\mathbb{P}^1$'s.

Now, of course, the moduli space is really four-dimensional. We want to think of Fig. 4 as representing a slice of the moduli space, where the H and C components of the Kähler form have been taken to infinity. Equivalently, think of Fig. 4 as the toric fan of a two-dimensional subspace of the moduli space associated to this limit.

Let $\mathcal{O}_{a_5}$ be the sum of the four structure sheaves of the $\mathbb{P}^1$'s associated to a_5. Similarly $\mathcal{O}_{a_6}$ is supported only over the four $\mathbb{P}^1$'s associated to a_6. Now consider the $\mathbb{P}^1$ in the moduli space connecting the large radius limit to the $\mathbb{Z}_2^{(A)}$ limit point where the $\mathbb{P}^1$'s associated to a_5 are blown

down. Let us denote this by C_A. We know the monodromy around the large radius limit within C_A multiplies the Chern characters by e^A. Since Δ_1 hits C_A transversely we expect that monodromy around the discriminant point is given by $\mathscr{K}^K_{\mathcal{O}_{a_5}}$ which induces

$$ch(\mathscr{F}) \mapsto ch(\mathscr{F}) - \tfrac{1}{4}\langle \mathcal{O}_{a_5}, \mathscr{F}\rangle \mathcal{O}_{a_5}, \tag{32}$$

where the factor 1/4 appears because $\mathcal{O}_{a_5}$ is associated to *four* irreducible divisors. [It is not hard to convince yourself that such a factor is necessary to get the monodromies to come out correctly. It would be nice to explain this factor more completely. Presumably this is similar to a asking for a better understanding of (28).]

The $\mathbb{Z}_2^{(A)}$ limit point is associated to a $\mathbb{Z}_2$ orbifold point and so we expect going twice around this point gives something simple. One can show that applying $\mathscr{K}^K_{\mathcal{O}_{a_5}} \mathscr{K}^B_A$ twice induces multiplication by exp $(2H+B)$ on the Chern characters. This should be viewed in the same way as in Sec. V B.

What about the curve C_B which connects the large radius limit to the $\mathbb{Z}_2^{(B)}$ limit point? In this case the discriminant point induces monodromy given by $\mathscr{K}^K_{\mathcal{O}_{a_6}}$ which induces

$$ch(\mathscr{F}) \mapsto ch(\mathscr{F}) - \tfrac{1}{4}\langle \mathcal{O}_{a_6}, \mathscr{F}\rangle \mathcal{O}_{a_6}. \tag{33}$$

One can then show that applying $\mathscr{K}^K_{\mathcal{O}_{a_6}} \mathscr{K}^B_B$ twice induces multiplication by exp(A) on the Chern characters.

This is all very well except that $\mathscr{K}^K_{\mathcal{O}_{a_5}}$ and $\mathscr{K}^K_{\mathcal{O}_{a_6}}$ are both monodromies around the *same* component of the discriminant. The reason they are different is that if we fix a base point near the large radius limit, then the loop around Δ_1 inside C_A is not homotopic to the loop around Δ_1 inside C_B. This can happen because Δ_1 itself is not smooth. It has a cusp at the point $(x,y) = (1/3,1/3)$. If we draw an S^3 around this cusp, then we obtain a trefoil knot in the intersection. It is well known that, for a fixed basepoint, loops around different parts of this knot are not homotopic to each other. This allows for the difference between $\mathscr{K}^K_{\mathcal{O}_{a_5}}$ and $\mathscr{K}^K_{\mathcal{O}_{a_6}}$. Note that this is the very same cusp as the one studied by Argyres and Douglas.[46]

Finally, let us see how to compute the effect of monodromy going three times around the $\mathbb{Z}_3$ limit point. Let C_{A2} be the curve connecting the $\mathbb{Z}_2^{(A)}$ limit point to the $\mathbb{Z}_3$ limit point. The monodromy within C_{A2} around the $\mathbb{Z}_2^{(A)}$ limit point is identical to the monodromy within C_A around the $\mathbb{Z}_2^{(A)}$ limit point for the reasons given in Sec. V C. The Δ_1 component of the discrimi-

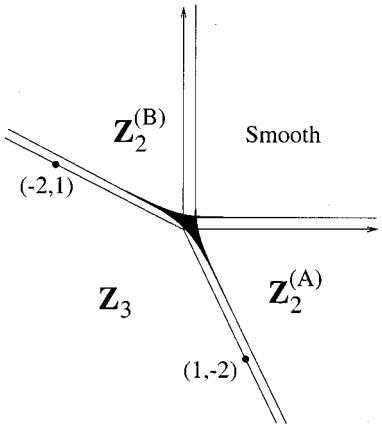


FIG. 4. The $\mathbb{C}^2/\mathbb{Z}_3$ resolution phase space.

nant intersects C_{A2} transversely. Since this is associated with collapsing the divisor associated to a_6, we will assume that monodromy around this discriminant point is given by $\mathscr{K}^K_{\mathcal{O}_{a_6}}$. *We therefore claim that monodromy with C_A around the $\mathbb{Z}_3$ limit point is given by* $\mathscr{K}^K_{\mathcal{O}_{a_6}}\mathscr{K}^K_{\mathcal{O}_{a_5}}\mathscr{K}^B_A$.

We may check that this cubes to something nice. Indeed the effect on the Chern characters implies that

$$\langle \mathscr{K}^K_{\mathcal{O}_{a_6}}, \mathscr{K}^K_{\mathcal{O}_{a_5}}\mathscr{K}^B_A\rangle^3 = (\mathscr{K}^B_H)^4. \tag{34}$$

One can show that this is consistent with the global geometry of the moduli space and so our monodromies all have the expected properties.

VII. DISCUSSION OF THE 0-BRANE

We have given various rules for how to compute the effect of monodromy on the Chern character of a D-brane. In this last section we will discuss the consequences for a 0-brane.

The 0-brane is of particular interest as it is the basic object used in the construction of Bondal and Orlov[7] to build the target space from the derived category. The fact that the 0-brane can transform into something else under monodromy is one reason why the Bondal and Orlov construction is ambiguous for a Calabi–Yau space.

Note again that the following results could have been guessed using the Picard–Fuchs differential equations. In that language the 0-brane often appears as a constant solution to the differential equations.[41] The derived category provides a much simpler picture, however.

For a Calabi–Yau threefold X, let P be an object in $\mathbf{D}(X)$ which corresponds to a 0-brane. This immediately implies that $ch(P)=p$, where $p\in H^6(X)$ is Poincaré dual to a point. Under monodromy about Δ_0 we have

$$p\mapsto p+\int_X p\wedge td(X) = p+1. \tag{35}$$

That is, the 0-brane always picks up a 6-brane charge upon an orbit around Δ_0.

Now consider the other monodromies in this article. They all involve taking the structure sheaf $\mathcal{O}_E$ of some collapsing cycle E and computing $\langle \mathcal{O}_{E,P}\rangle$. If E is of dimension less than 6, then this inner product is always zero. Thus the 0-brane undergoes no monodromy about these kinds of components in the discriminant.

We therefore make the following conjecture.

Conjecture 3: The 0-brane undergoes monodromy if and only if we circle the primary component, Δ_0, of the discriminant.

If we begin in a large-radius smooth Calabi–Yau phase, which other phases may we visit without crossing a wall in the phase diagram which contains Δ_0? In other words, over what area of the phase diagram can we fix a choice of 0-brane without worrying about monodromy? The answer consists of the so-called ''geometric phases'' or ''partially enlarged Kähler moduli space'' of Ref. 28.

The phases correspond to triangulations of Batyrev's reflexive polytope.[26,28] The statement that a phase is geometric corresponds to every simplex in the triangulation having the unique point in the interior of the polytope as a vertex.

Comparing to the example in Sec. V, for example, the geometric phases consist of the Calabi–Yau phase and the orbifold phase where we have a three complex dimensional picture of the target space. Indeed, these phases are separated only by Δ_1 around which the 0-brane has no monodromy.

The geometric phases consist of those reached from the Calabi–Yau phase only by blowing down subspaces. If one reduces the overall dimension of the target space, then one must cross a wall containing Δ_0. There are also exotic ''exoflop'' transitions[28] where part of the target space

remains three-dimensional but a lower-dimensional part grows out of the side of the target space. These exoflops also involve crossing a Δ_0 boundary and are not considered geometric.

Proving the statement about these phases is an application of the combinatorics discussed in Chap. 11 of Ref. 42. There is an object η_T which is a function on the cones of the secondary fan. If η_T changes as you pass to a neighboring cone, then the wall contained Δ_0. It is easy to show that η_T changes as you pass from a geometric phase to a nongeometric phase. This result is essentially contained in corollary 4.5 of Chap. 11 of Ref. 42. It is a more tedious exercise to show that passing between geometric phases of threefolds keeps η_T constant.

This result appears to agree nicely with the Bondal and Orlov construction. We may consistently tie the derived category to a target space interpretation so long as we confine ourselves to geometric phases. Once we leave these phases, then the 0-brane undergoes monodromy and we acquire an ambiguity in the way we construct the target space.

Finally, we should note that there can still be an ambiguity in what exactly is called a 0-brane in the geometric phases. If there are two or more smooth phases related by flops, then each phase has its own 0-branes. The exact way these branes are related to each other was given by Bridgeland.[47]

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Multidimensional phase space and sunset diagrams

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We derive expressions for the phase space of a particle of momentum p decaying into N particles, that are valid for any number of dimensions. These are the imaginary parts of so-called ''sunset'' diagrams, which we also obtain. The results are given as a series of hypergeometric functions, which terminate for odd dimensions and are also well suited for deriving the threshold behavior. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1416887]

I. INTRODUCTION

With so much attention focused on the properties of branes embedded in higher dimensions, it is of interest to examine the way in which the phase space changes as the space–time is enlarged, since this is what primarily determines the statistical properties of multiparticle systems; only when amplitudes are accentuated or suppressed along certain directions in space is there a pronounced effect on the phase space. This paper is devoted to the topic of multidimensional phase space. We assume that extra dimensions are spatial—though one may envisage that timelike coordinates can be handled by Euclidean continuation—and that all particles propagate into the bulk. Not only that, we suppose that the space–time is flat so that we can neglect topological aspects. If conditions arise that constrain the particles to some subspace, then one may obtain the reduced phase space by altering the number $D-1$ of spatial dimensions rather trivially; or else if topological effects become important we may be able to sum over discrete modes along flat directions. Thus in almost every respect we are simply investigating the dimensional continuation of standard four-dimensional expressions for the decay of a system carrying momentum p into *any number* N of particles.

There has been much early work in this area,[1] but it is mostly in the context of four dimensions (or lower) and has often been confined to few particles (like two, three, or four). The most pertinent recent results in this connection are those of Groote *et al.*[2] and of Davydychev and Smirnov[3] because they are the most general. Our own results apply to any value of N and D and are also singularly well suited for deriving threshold expansions as $\sqrt{p^2}\to(m_1+m_2+\cdots+m_N)$. Because phase space ρ is nothing but the imaginary part of the ''sunset diagram'' for $p\to p_1+p_2+\cdots p_N$, our procedure will be to start with this sort of diagram and then obtain ρ_N from its discontinuity in p^2 as we cross the threshold. (Pseudothreshold singularities of these diagrams exist, too, but are not relevant for physical phase space.)

In Sec. II, we give the most convenient Feynman parametric description of the general diagram for any dimension $D=2\ell$ and show how one may readily derive the leading threshold behavior by expanding about the minimum of the combined denominator; although one may in principle derive the next to leading behavior by this method, and so on, we do not pursue this parametric approach any further, as there is a much better way of handling the problem, which is described in the following sections. First, in Sec. III, we derive some special cases of the results (small N) by making use of phase space recurrence methods[1] and next show how they may more easily be found by Fourier transformation of the propagator products in Sec. IV. This is our cue for tackling the most general situation, but because the form of our expressions makes it tricky to take

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the massless limit of any individual particle we specifically suppose that M of the particles are massless and $N-M$ are massive. Our results, stated in Sec. V, are given as a series of hypergeometric terms having the form (hereafter F stands for the usual ${}_2F_1$ function)

$$\rho_N \propto \sum_{j=M(3/2-\ell)+2N(\ell-1)-\ell+1/2} \mathrm{d}_j (p^2-\sigma^2)^j F(a,b;c;1-p^2/\sigma^2),$$

where σ is the sum of the masses. An agreeable property of this expansion is that it terminates for odd D and is tailored for deriving the threshold behavior.

II. FEYNMAN PARAMETRIC FORM

In 2ℓ dimensions, sunset diagrams with N internal lines, produce integrals of the type[4]

$$I_N(p;\{\nu\}) = i\left(\prod_{i=1}^{N} \int \frac{i\Gamma(\nu_i)}{(p_i^2-m_i^2)^{\nu_i}} \bar{\mathrm{d}}^{2\ell} p_i\right) \bar{\delta}^{2\ell}\left(p-\sum_i p_i\right). \tag{1}$$

We have included a gamma function in each numerator since the propagator powers usually arise via momentum or mass derivatives of the case $\nu=1$, and it simplifies the subsequent expressions. By attaching a Feynman parameter α to each internal line, one may combine denominators in the standard fashion and integrate over the internal momenta to establish[5] that

$$I_N(p;\{\nu\}) = \frac{(-1)^N}{(-4\pi)^{(N-1)\ell}} \left(\prod_{i=1}^{N} \int_0^1 \frac{\mathrm{d}\alpha_i}{\alpha_i^{\nu_i-\ell+1}}\right) \frac{\Gamma(\Sigma_i \nu_i + \ell - N\ell)\,\delta(1-\Sigma_i \alpha_i)}{[p^2-\Sigma_i (m_i^2/\alpha_i)]^{\Sigma_i \nu_i + \ell - N\ell}}, \tag{2}$$

but it is easier to prove the result by induction in fact. Suppose that (2) is true for N; the case $N+1$ represents a further convolution:

$$I_{N+1}(p;\{\nu\}) = i\int \bar{\mathrm{d}}^{2\ell} k\, I_N(k;\{\nu\})\Gamma(\nu_{N+1})/[(k+p)^2-m_{N+1}^2]^{\nu_{N+1}}$$

so introduce an extra Feynman parameter β. Combining the new denominator with (2) and integrating over intermediate loop momentum k, one remains with

$$I_{N+1}(p) = \frac{(-1)^{N+1}}{(-4\pi)^{N\ell}} \left(\prod_{i=1}^{N} \int_0^1 \frac{\mathrm{d}\alpha_i}{\alpha_i^{\nu_i-\ell+1}}\right) \times \int_0^1 d\beta \frac{\Gamma(\Sigma_{i=1}^{N+1} \nu_i - N\ell)\,\delta(1-\Sigma_i \alpha_i)(1-\beta)^{\nu_{N+1}-1}\beta^{\ell-\nu_{N+1}-1}}{[p^2(1-\beta)-\Sigma_i (m_i^2/\alpha_i)-m_{N+1}^2(1-\beta)/\beta]^{\Sigma_i \nu_i - N\ell + \nu_{N+1}}}.$$

Now all one need do is rescale $\alpha_i = \beta_i/(1-\beta)$ for $i=1$ to N and call $\beta \equiv \beta_{N+1}$. A final relabeling of $\beta \to \alpha$ reproduces (2) for $N \to N+1$. Since we know the result (2) is correct for $N=2$—it is very familiar to graphologists as the simplest self-energy calculation—we have thereby proved the result inductively for any N.

The singularities of $I_N(p)$ in p^2 will arise when p^2 equals the combination $M^2(\alpha) \equiv \Sigma_{i=1}^N (m_i^2/\alpha_i)$, so let us examine the behavior of $M^2(\alpha)$ in the region of integration $0 \leqslant \alpha_i \leqslant 1$, subject to the condition $\Sigma_i \alpha_i = 1$. For definiteness, we shall assume for the rest of this section that all masses are nonzero. By introducing a Lagrangian multiplier for the last constraint, it is easy to see that $M^2(\alpha)$ is minimized in the physical region when the Feynman parameters equal $\alpha_{i0} \equiv m_i/\Sigma_{j=1}^N m_j \equiv m_i/\sigma$, whereupon $M^2(\alpha_0) = (\Sigma_{j=1}^N m_j)^2 = \sigma^2$. Other values of α_i are possible (by reversing one or other of the signs of α_{i0}) but they correspond to pseudothresholds and lie

outside the integration region. It is then clear that the magnitude of $I_N(p)$ will be dominated by α_i values in the vicinity of α_{i0}, so it is sensible to expand about these minima if we want to determine the leading behavior near threshold.

This procedure can be developed systematically (see the Appendix for the example $N=2$ with $\nu_1=\nu_2=1$) but as there is an alternative and preferable way of tackling the problem, which we defer to the following sections, here we shall simply extract the leading threshold behavior, because this can be done rather quickly and painlessly. Begin with (2) and note that

$$M^2(\alpha)=\sigma^2+\sum_i\ (\alpha_i-\alpha_{i0})^2\sigma^3/m_i-\sum_i\ (\alpha_i-\alpha_{i0})^3\sigma^4/m_i^2+\cdots.$$

One sees that for $1-p^2/\sigma^2\equiv\Delta^2$ small the integral is dominated by values of α near the minimum α_0. Therefore write $\alpha_i=\alpha_{i0}+\Delta\xi_i$, so that the denominator of (2) reads

$$-\Delta^2\sigma^2\left[1+\sigma\sum_i\ \xi_i^2/m_i-\Delta\sigma^2\sum_i\ \xi_i^3/m_i^2+O(\Delta^2)\right].$$

Since the integrals in α can be made to run between 0 and ∞, because of the delta-function constraint, the integral over ξ_i runs from $-m_i/\sigma\Delta$ to ∞. So, in the limit as $\Delta\to0$, we can take ξ_i to run from $-\infty$ to ∞ [the correction to the integral is exponentially small as $\exp(-1/\Delta^2)$] and expand the product of the α_i about the minimum. Assuming all masses are nonzero (see later sections for a relaxation of this condition) we are thereby led to the leading behavior,

$$I_N(p,\{\nu\})=c_{N\ell}\Delta^{(N-1)(2\ell+1)-2\Sigma_i\,\nu_i}\left(\prod_i\ m_i^{\ell-\nu_i-1}\right)\Big/\ (4\pi)^{\ell(N-1)}\sigma^{(2-N)\ell-N+\Sigma_i\,\nu_i},\qquad(3)$$

where

$$c_{N\ell}\simeq\left(\prod_i\ \int\ \mathrm{d}\xi_i\right)(-1)^{N-\Sigma_i\,\nu_i}\frac{\delta(\Sigma_i\,\xi_i)\Gamma(\Sigma_i\,\nu_i-(N-1)\ell)}{[1+\sigma\Sigma_i\xi_i^2/m_i]^{\Sigma_i\nu_i-(N-1)\ell}}.$$

If one now represents the delta function and the denominator by integrals, the coefficient $c_{N\ell}$ can be explicitly evaluated as follows:

$$\begin{aligned}c_{N\ell}=&\frac{1}{2\pi}\left(\prod_i\ \int\ \mathrm{d}\xi_i\right)\int_{-\infty}^{\infty}\mathrm{d}k\int_0^{\infty}\mathrm{d}\alpha\ \alpha^{\Sigma_i\,\nu_i-1-(N-1)\ell}\,e^{-\alpha-k^2/4\alpha}\\&\times(-1)^{N-\Sigma_i\,\nu_i}\prod_i\ \exp\left[-\frac{\alpha\sigma}{m_i}\left(\xi_i-\frac{ikm_i}{2\alpha\sigma}\right)^2\right]\\=&(-1)^{N-\Sigma_i\,\nu_i}\varpi^{1/2}\pi^{(N-1)/2}\sigma^{-N/2}\Gamma\left(\sum_i\ \nu_i-(\ell+1/2)(N-1)\right),\varpi\equiv\prod_i\ m_i.\end{aligned}$$

So, all told, the leading threshold behavior is dominated by

$$\begin{aligned}I_N(p,\{\nu\})=&(-1)^{N-\Sigma_i\nu_i}\frac{\pi^{(N-1)/2}}{(4\pi)^{(N-1)\ell}}\,\frac{\Gamma(\Sigma_i\,\nu_i-(N-1)(l+1/2))\Pi_i m_i^{\ell-\nu_i-1/2}}{\sigma^{(2-N)\ell-N/2+\Sigma_i\nu_i}}\\&\times\Delta^{(N-1)(2\ell+1)-2\Sigma_i\nu_i}.\end{aligned}\qquad(4)$$

The case of greatest interest is $\nu_i=1$, all i, when (4) reduces to

$$I_N(p)=\frac{\pi^{(N+1)/2}}{(4\pi)^{(N-1)\ell}}\,\frac{\Gamma((N-1)/2-\ell(N-1))}{\varpi^{3/2-\ell}\sigma^{N/2+\ell(2-N)}}(1-p^2/\sigma^2)^{\ell(N-1)-(N+1)/2}.\qquad(5)$$

We may then continue this expression above threshold ($p^2 \geqslant \sigma^2$), in order to obtain the behavior of the N-body phase space as the discontinuity:

$$\rho_N(p) = 2\Im I_N(p) \simeq \frac{\pi^{(N+1)/2}}{(4\pi)^{(N-1)\ell}} \frac{\varpi^{\ell-3/2}}{\sigma^{N/2+\ell(2-N)}} \frac{(p^2/\sigma^2-1)^{\ell(N-1)-(N+1)/2}}{\Gamma((N-1)(\ell-1/2))}. \tag{6}$$

This result agrees with the answer obtained by Davydychev and Smirnov[3] and reduces to the well-known four-dimensional behavior found by Hagedorn and Almgren,[1] when we set $\ell=2$, namely

$$\rho_N(p) \sim Q^{(3N-5)/2},$$

where $Q=\sqrt{p^2}-\sigma$ is the energy release. However (6) supplies the answer in any dimension with the appropriate coefficient.

III. EXACT RESULTS

We now consider phase space in general and derive some precise results for any ℓ, N as they arise from recurrence relations between phase space expressions for smaller N and not necessarily around threshold. Begin with the definition of the N-body phase space integral,

$$\rho_N(p) \equiv \rho_{p\to 1+2+\cdots N} \equiv \prod_i \left(\int \overline{\mathrm{d}^2}^{\ell} p_i \theta(p_i) \overline{\delta}(p_i^2 - m_i^2) \right) \overline{\delta^2}^{\ell} \left(p - \sum_{i=1}^{N} p_i \right). \tag{7}$$

The measures $\mathrm{d}^{2\ell-1}\vec{p} = |\vec{p}|^{2\ell-2}\mathrm{d}|\vec{p}|.(\sin\theta)^{2\ell-3}\mathrm{d}\theta.2\pi^{\ell-1}/\Gamma(\ell-1) = |\vec{p}|^{2\ell-2}\mathrm{d}|\vec{p}|.2\pi^{\ell-1/2}/\Gamma(\ell-1/2)$, come in useful if one were able to integrate over angles. Thus the two-body result is readily evaluated in this way to be

$$\rho_2(p) = \frac{\pi(4\pi)^{1/2-\ell} q^{2\ell-3}}{\Gamma(\ell-1/2)\sqrt{p^2}},$$

where q is the center of mass spatial momentum, so that $\sqrt{q^2+m_1^2}+\sqrt{q^2+m_2^2}=\sqrt{p^2}$. Tidying up, the result can be expressed covariantly as

$$\rho_{p\to 1+2} = \frac{\pi^{1-\ell}\Gamma(\ell-1)\lambda^{2\ell-3}}{2^{2\ell-1}(p^2)^{\ell-1}\Gamma(2\ell-2)}, \quad \lambda \equiv \sqrt{p^4+m_1^4+m_2^4-2m_1^2m_2^2-2p^2m_1^2-2p^2m_2^2}. \tag{8}$$

The three-body phase space can also be evaluated by brute force methods and reduced to a triangular integral over three Mandelstam variables:

$$\rho_{p\to 1+2+3} = \frac{2\pi(p^2)^{1-\ell}}{(4\pi)^{2\ell}\Gamma(2\ell-2)} \int\int\int \mathrm{d}s\,\mathrm{d}t\,\mathrm{d}u\ \delta(s+t+u-m_1^2-m_2^2-m_3^3-p^2) \times [\Phi(s,t,u)]^{\ell-2}\theta(\Phi),$$

where $\Phi(s,t,u)$ is the Kibble[6] cubic (simply a Gram determinant),

$$\begin{aligned}\Phi(s,t,u) &\equiv stu - s(m_2^2m_3^2+p^2m_1^2) - t(m_3^2m_1^2+p^2m_2^2) - u(m_1^2m_2^2+p^2m_3^2) \\ &\quad + 2(m_1^2m_2^2m_3^2+p^2m_1^2m_2^2+p^2m_2^2m_3^2+p^2m_3^2m_1^2) \\ &= -p^2\lambda^2(|\vec{p}_1|^2,|\vec{p}_2|^2,|\vec{p}_3|^2).\end{aligned}$$

By changing variables to s and $t-u$, one integration may be performed and the problem reduced to the single integral,[7]

$$\rho_{p\to 1+2+3}=\frac{(32\pi)^{2-2\ell}}{(\Gamma(\ell-1/2))^2(p^2)^{\ell-1}}\int_{(m_1+m_2)^2}^{(\sqrt{p^2}-m_3)^2} s^{1-\ell}\mathcal{D}^{\ell-3/2}\,\mathrm{d}s, \tag{9}$$

where $\mathcal{D}=[s-(m_3+\sqrt{p^2})^2][s-(m_3-\sqrt{p^2})^2][s-(m_1+m_2)^2][s-(m_1-m_2)^2]$. When we are in four dimensions ($\ell=2$) the integral is nothing but the area within the Dalitz plot but its evaluation for arbitrary masses is easier said than done, because (9) is an elliptic function in general! However in three dimensions the integration over the region becomes possible because it can be converted into

$$\rho_3(p)\to\frac{1}{32\pi\sqrt{p^2}}\int_{(m_1+m_2)^2}^{(\sqrt{p^2}-m_3)^2}\frac{\mathrm{d}s}{\sqrt{s}}=\frac{1}{16\pi}\left(1-\frac{m_1+m_2+m_3}{\sqrt{p^2}}\right).$$

In fact the three-body phase space integration is tractable for all odd D dimensions, because one remains with a polynomial in half-integral powers of s which is readily handled.[8] Two other cases are amenable to an exact treatment in terms of "elementary" functions for any ℓ and $N=3$, namely (i) two masses are set to zero, or (ii) one mass vanishes and the two other masses are equal. In case (i) put $m_2=m_3=0,\ m_1=m$ so $\mathcal{D}\to(s-p^2)^2(s-m^2)^2$ whereupon the three-body phase space reads

$$\rho_3(p)\to\frac{\pi^{1-2\ell}(p^2/m^2-1)^{4\ell-5}[\Gamma(\ell-1)]^2}{2^{4\ell-1}(m^2)^{3-2\ell}\Gamma(4\ell-4)}F\left(3\ell-3,\ 2\ell-2;4\ell-4;1-\frac{p^2}{m^2}\right)\theta(p^2-m^2),$$

while in case (ii) put $m_3=0,\ m_1=m_2=m$ so that $\mathcal{D}\to s(s-p^2)^2(s-4m^2)$ and

$$\rho_3(p)\to\frac{\pi^{3/2-2\ell}\Gamma(\ell-1)(p^2-4m^2)^{3\ell-7/2}}{2^{6\ell-3}\Gamma(3\ell-5/2)(p^2)^{\ell-1}m}F\left(\frac{1}{2},\ell-\frac{1}{2},\ 3\ell-\frac{5}{2};1-\frac{p^2}{4m^2}\right)\theta(p^2-4m^2).$$

Of course we can also proceed to the limit $m\to 0$ in either case. Any other set of masses produces "elliptic" results[1,7] for even D or integral ℓ.

A more systematic way of arriving at Lorentz invariant answers, without resorting to integrations over spatial momenta in the standard approach and interpreting them covariantly, is to apply Almgren's method. In that method one partitions the set of outgoing particles into subsets (call them A,B, etc.) and obtains ρ via mass integration convolutions; for instance the three-body result (9) can be construed as

$$\rho_{p\to 1+2+3}=\int \rho_{p\to A+3}\rho_{A\to 1+2}\overline{\mathrm{d}}m_A^2,$$

where s is interpreted as the intermediate m_A^2. More generally, one may evaluate the N-body phase space through the double integral

$$\rho_{p\to 1+2+\cdots+j+(j+1)\cdots+N}=\int \rho_{p\to A+B}\rho_{A\to 1+2+\cdots j}\rho_{B\to(j+1)+\cdots+N}\overline{\mathrm{d}}m_A^2\,\overline{\mathrm{d}}m_B^2. \tag{10}$$

Although this is quite a satisfactory numerical way of calculating ρ, it does not shed a great deal of analytical light on the nature of the problem; but it does serve as a nice check of analytical results obtained in a different manner, which we will now exhibit.

IV. COORDINATE SPACE METHOD

The sunset diagram having all $\nu=1$ is nothing but the 2ℓ-dimensional Fourier transform of the product of N causal functions:

$$I_N(p) = -i \int \mathrm{d}^{2\ell} x \exp(ip.x) \prod_{i=1}^{N} [i\Delta_c(x|m_i)], \tag{11}$$

and the phase space integral is simply given by

$$\rho_{p\to 1+2+\cdots+N} = 2\Im I_N(p),$$

which is nonvanishing for $p^2 \geqslant (m_1+m_2+\cdots+m_N)^2$. Of course (11) is easier stated than done except in the simplest cases (like $N=2$ or 3) because the causal function is a Bessel function in general,[9]

$$i\Delta_c(x|m) = \frac{1}{(2\pi)^\ell} \left(\frac{m}{r}\right)^{\ell-1} K_{\ell-1}(mr), \quad r \equiv \sqrt{-x^2+i\epsilon}.$$

In the massless limit, when $m\to 0$, the sunset diagram reduces to a ''superpropagator'' with integer index since

$$i\Delta_c(x|0) \equiv iD_c(x) = \Gamma(\ell-1)/4\pi^\ell r^{2\ell-2}.$$

However, as noted and indeed emphasized by Berends *et al.*[10] and by Groote *et al.*,[2] one can make considerable progress using coordinate space methods in the odd-dimensional massive cases, because the Bessel function reduces to an exponential times a polynomial.

Let us begin systematically by considering the most trivial case *when all intermediate masses vanish.* Carrying out the angular integration in (11), the sunset integral reduces to

$$I_N(p) \to -(2\pi)^\ell q^{1-\ell} \int_0^\infty \mathrm{d}r\, r^\ell J_{\ell-1}(qr) \left[\frac{\Gamma(\ell-1)}{4\pi^\ell r^{2\ell-2}}\right]^N, \quad q^2 \equiv -p^2, \tag{12}$$

which can be evaluated straightforwardly.[11] Thus one finds that

$$\lim_{m_i\to 0} I_N(p) = -(4\pi)^{\ell(1-N)} \frac{[\Gamma(\ell-1)]^N \Gamma(\ell+N-N\ell)}{\Gamma(N\ell-N)} (-p^2-i\epsilon)^{N\ell-\ell-N}, \tag{13}$$

so the massless phase space integral reduces, in 2ℓ dimensions, to[12]

$$\lim_{m_i\to 0} \rho_N(p) = 2\Im I_N(p) = \frac{(4\pi)^{1+\ell-N\ell} [\Gamma(\ell-1)]^N}{2\Gamma(N\ell-N)\Gamma((N-1)(\ell-1))} (p^2)^{N\ell-\ell-N} \theta(p^2). \tag{14}$$

Both (13) and (14) are exact, too. One may readily check that the cases $N=1,2,3$ produce the correct answers, by taking appropriate limits of earliers results. Also it is very instructive to check that the Almgren recurrence formulas, such as (10), are properly obeyed, not only in their momentum dependence, but in their multiplicative coefficients.

Now it turns out that the integral of two Bessel functions with an exponential can also be handled.[11] Therefore one can improve on above and calculate analytically the sunset integral for one particle massive (m) and the remaining N-1 particles massless. In those circumstances one is led to[13]

$$I_N(p)=-\left(\frac{q}{m}\right)^{1-\ell}\int_0^\infty \mathrm{d}r\, r^{2(N-1)(1-\ell)+1}J_{\ell-1}(qr)K_{\ell-1}(mr).\left(\frac{\Gamma(\ell-1)}{4\pi^\ell}\right)^{N-1}$$

$$=-\frac{[\Gamma(\ell-1)]^{N-1}\Gamma(\ell+N-N\ell)\Gamma(N-N\ell+2\ell-1)}{2^{2\ell(N-1)}\pi^{\ell(N-1)}(m^2)^{N+\ell-N\ell}\Gamma(\ell)}$$

$$\times F\left(\ell+N-N\ell,N-N\ell+2\ell-1;\ell;\frac{p^2}{m^2}\right). \tag{15}$$

Noting that in respect of the variable z the hypergeometric function $F(a,b;c;z)$ for real a,b,c has a branch point at $z=1$ and that the discontinuity across the cut (which runs to $+\infty$) is

$$\Im F(a,b;c;z)=-\frac{\pi\Gamma(c)(z-1)^{c-a-b}\theta(z-1)}{\Gamma(a)\Gamma(b)\Gamma(1-a-b+c)}F(c-a,c-b;c-a-b+1;1-z), \tag{16}$$

we deduce the phase space result,

$$\rho_N(p)=\frac{\pi^{1-\ell(N-1)}[\Gamma(\ell-1)]^{N-1}(p^2-m^2)^{2N\ell-2\ell-2N+1}\theta(p^2-m^2)}{2^{2\ell(N-1)-1}(m^2)^{N\ell-N-\ell+1}\Gamma(2(N-1)(\ell-1))}$$

$$\times F\left(N(\ell-1),(N-1)(\ell-1);2(N-1)(\ell-1);1-\frac{p^2}{m^2}\right). \tag{17}$$

The pair of expressions (16) and (17) are precise as well. Contrast (17) with the expression found by Beneke and Smirnov[14] for a one-loop vertex diagram with two massive and one massless particle. By taking the limit $m\to 0$ of (16) and (17) and suitably maneuvering the hypergeometric function[15] one can show that they collapse into (13) and (14). Additionally we may deduce the particular cases $N=2,3$ previously by direct substitution; for instance, in four dimensions ($\ell=2$), one gets

$$\rho_N(p)=\frac{2\pi(p^2-m^2)^{2N-3}}{(16\pi^2)^{N-1}(m^2)^{N-1}\Gamma(2N-2)}F\left(N,N-1;2(N-1);1-\frac{p^2}{m^2}\right)\theta(p^2-m^2),$$

so the three-body phase space with a single massive particle ($p^2\geqslant m^2$) brings in a logarithmic function:

$$\rho_3(p)=\frac{(p^2-m^2)^3}{768\pi^3m^4}F\left(3,2;4;1-\frac{p^2}{m^2}\right)=\frac{m^4}{256\pi^3p^2}\left[\left(\frac{p^4}{m^4}-1\right)-2\frac{p^2}{m^2}\ln\left(\frac{p^2}{m^2}\right)\right].$$

V. HYPERGEOMETRIC EXPANSIONS

As soon as we have at least two massive particles, we come across integrals involving products of three Bessel functions with different arguments and a power of r. This is not given in the standard texts,[16] though it is surely some generalization of a hypergeometric function for we definitely know how to evaluate the $N=2$ case directly in momentum space; but for larger N it would seem that the coordinate space method stalls. Only when $p=0$, which corresponds to a vacuum "watermelon diagram," can the integrations sometimes be carried out.[17] However, we will now present a method which is still suitable for handling the general problem and which works wonderfully well in odd-dimensional spaces. It relies on the observation that the modified Bessel function possesses an asymptotic representation ($\mu\equiv 4\nu^2$),

$$K_\nu(z)\sim\sqrt{\frac{\pi}{2z}}e^{-z}\left[1+\frac{\mu-1}{8z}+\frac{(\mu-1)(\mu-9)}{2!(8z)^2}+\frac{(\mu-1)(\mu-9)(\mu-25)}{3!(8z)^3}+\cdots\right]$$

that *terminates for ν or ℓ half-integral*, corresponding to D odd. Even for integral ℓ or even dimensions, we shall see that it provides a very nice threshold expansion in terms of hypergeometric functions.[18] To show how this works, assume first that all the intermediate particles are massive. Since

$$i\Delta_c(x|m)=\frac{1}{(2\pi)^{\ell}}\left(\frac{m}{r}\right)^{\ell-1}\sqrt{\frac{\pi}{2mr}}e^{-mr}\sum_{j=0}^{\infty}\frac{\Gamma(\ell+j-1/2)}{j!\Gamma(\ell-j-1/2)}(2mr)^{-j}, \tag{18}$$

the product of causal Green functions produces the series

$$\prod_{j=1}^{N} i\Delta_c(x|m_j)=\left(\frac{\pi^{1/2-\ell}}{2^{\ell+1/2}r^{\ell-1/2}}\right)^N\prod_{j=1}^{N} m_j^{\ell-3/2}.e^{-r\Sigma_j m_j}\left[1+\frac{(2\ell-1)(2\ell-3)}{8r}\sum_{j=1}^{N}\frac{1}{m_j}+\cdots\right].$$

The leading (and in 3D the only) term of the right-hand side above yields the leading behavior of the sunset diagram,

$$\begin{aligned}I_N^0(p)&=-\frac{(2\pi)^{\ell-N\ell+N/2}}{q^{\ell-1}\varpi^{3/2-\ell}}\int_0^{\infty}\mathrm{d}r\, r^{\ell-N\ell+N/2}e^{-r\sigma}J_{\ell-1}(qr)\\&=-\frac{2^{1-N\ell-N/2}\pi^{\ell-N\ell+N/2}\Gamma((2-N)\ell+N/2)}{\Gamma(\ell)\sigma^{(2-N)\ell+N/2}\varpi^{3/2-\ell}}\\&\quad\times F\left(\frac{2\ell-N\ell+N/2}{2},\frac{2\ell-N\ell+N/2+1}{2};\ell;\frac{p^2}{\sigma^2}\right),\end{aligned} \tag{19}$$

where $\varpi\equiv\Pi_i m_i$, $\sigma\equiv\Sigma_i m_i$. The imaginary part then produces the leading contribution to the phase space integral,

$$\begin{aligned}\rho_N^0(p)&=\frac{2^{2\ell(1-N)+1}\pi^{\ell(1-N)+(N+1)/2}(p^2-\sigma^2)^{\ell(N-1)-(N+1)/2}}{\varpi^{3/2-\ell}\sigma^{N\ell-1-N/2}\Gamma(\ell(N-1)-(N+1)/2)}\theta(p^2-\sigma^2)\\&\quad\times F\left(\frac{N\ell-N/2}{2},\frac{N\ell-1-N/2}{2};\ell(N-1)-\frac{N-1}{2};1-\frac{p^2}{\sigma^2}\right).\end{aligned} \tag{20}$$

It should be noted that expressions (19) and (20) represent the *complete* results for three dimensions (3D), when they reduce, respectively, to

$$I_N(p)\to-\frac{\pi^{3/2-N}\Gamma(3-N)}{2^{2N-2}\sigma^{3-N}\sqrt{\pi}}F\left(\frac{3-N}{2},\frac{4-N}{2};\frac{3}{2};\frac{p^2}{\sigma^2}\right)$$

and

$$\rho_N(p)\to\frac{\pi^{2-N}(p^2-\sigma^2)^{N-2}}{2^{3N-4}\sigma^{N-1}\Gamma(N-1)}F\left(\frac{N}{2},\frac{N-1}{2};N-1;1-\frac{p^2}{\sigma^2}\right)=\frac{\pi(\sqrt{p^2}-\sigma)^{N-2}\theta(p^2-\sigma^2)}{(4\pi)^{N-1}\Gamma(N-1)\sqrt{p^2}}.$$

The singularity in $I_N(p)$ for integer $N\geqslant 3$ is a reflection of the fact that there exist subdivergences in such multiloop 3D integrals, which must be regulated, e.g., using dimensional continuation, as in (19).

Nonleading behaviors (for values of $\ell\neq 3/2$) of I_N and ρ_N can be found from expansion (18); for instance to the next order we encounter the terms,

$$I_N^1(p)=\frac{(2\ell-1)(2\ell-3)\pi^{\ell((1-N)+N/2)}\Gamma(2\ell-1-N\ell+N/2)}{2^{2+N\ell+N/2}\varpi^{3/2-\ell}\sigma^{\ell(2-N)+N/2-1}\Gamma(\ell)\mu}$$
$$\times F\left(\frac{2\ell-N\ell+N/2-1}{2},\frac{2\ell-N\ell+N/2}{2};\ell;\frac{p^2}{\sigma^2}\right), \tag{21}$$

$$\rho_N^1(p)=\frac{(2\ell-1)(2\ell-3)\pi^{\ell(1-N)+(N+1)/2}(p^2-\sigma^2)^{\ell(N-1)+(1-N)/2}}{2^{2\ell(N-1)+3}\varpi^{3/2-\ell}\sigma^{N(\ell-1/2)}\mu\Gamma(\ell(N-1)+(3-N)/2)}\theta(p^2-\sigma^2)$$
$$\times F\left(\frac{N\ell+1-N/2}{2},\frac{N\ell-N/2}{2};\ell(N-1)+\frac{3-N}{2};1-\frac{p^2}{\sigma^2}\right), \tag{22}$$

where $1/\mu\equiv\Sigma_j 1/m_j$; and so on for higher I_N^k,ρ_N^k. The method is entirely systematic and one may proceed to as high an order k as needed. Observe that the resulting series is a sort of threshold expansion because the powers of $(p^2-\sigma^2)$ which multiply $F(a,b;c;1-p^2/\sigma^2)$ keep on increasing as we raise k while the denominators are associated with sums of the type $\Sigma_j(1/m_j)^k$.

However these expansions are deficient in one respect: it is very tricky to consider the limit as one or several masses vanishes, because the approximation (18) is fairly useless for massless propagators; in that case we should be using directly $iD_c(x)\propto r^{2-2\ell}$, rather than the asymptotic expansion (18). Finally then we will consider the case where M of the N particles are massive while the remaining $N-M$ are massless; this covers essentially all cases of interest. The sunset integral is given *ab initio* by

$$I_N(p)=-\frac{(2\pi)^\ell}{q^{\ell-1}}\int_0^\infty \mathrm{d}r\, r^\ell J_{\ell-1}(qr)\left(\frac{\Gamma(\ell-1)}{4\pi^\ell r^{2\ell-2}}\right)^{N-M}\left(\frac{(\pi r)^{1/2-\ell}}{2^{\ell+1/2}}\right)^M e^{-r\sigma}\varpi^{\ell-3/2}$$
$$\times\left[1+\frac{(2\ell-1)(2\ell-3)}{8r\mu}+\cdots\right], \tag{23}$$

where the symbols now refer simply to the massive intermediate particles; therefore $\varpi\equiv\Pi_{j=1}^M m_j$, $\sigma\equiv\Sigma_{j=1}^M m_j$, $1/\mu\equiv\Sigma_{j=1}^M(1/m_j)$. The integrals in (23) are readily performed and the leading term of the full answer is

$$I_N^0(p)$$
$$=-\frac{2^{2(M-N)+1-M\ell-M/2}\pi^{\ell(1-N)+M/2}[\Gamma(\ell-1)]^{N-M}\Gamma(\ell(2-M)+(M-N)(2\ell-2)+M/2)}{\varpi^{3/2-\ell}\sigma^{\ell(2-M)+(M-N)(2\ell-2)+M/2}\Gamma(\ell)}$$
$$\times F\left(\frac{\ell(2-M)+M/2}{2}+(M-N)(\ell-1),\frac{\ell(2-M)+1+M/2}{2}+(M-N)(\ell-1);\ell;\frac{p^2}{\sigma^2}\right). \tag{24}$$

Taking its discontinuity, the leading phase space behavior is [$c\equiv M(3/2-\ell)+2N(\ell-1)-\ell+1/2$ and $p^2\geqslant\sigma^2$ in the following],

$$\rho_N^0(p)=\frac{2^{2\ell(1-N)+1}\pi^{\ell(1-N)+(M+1)/2}[\Gamma(\ell-1)]^{N-M}(p^2-\sigma^2)^{M(3/2-\ell)+2N(\ell-1)-(\ell+1/2)}}{\varpi^{3/2-\ell}\sigma^{M(7/2-3\ell)+2(M+N)(\ell-1)-1}\Gamma(c)}$$
$$\times F\left((\ell-1)(N-M)+\frac{M(2\ell-1)}{4},(\ell-1)(N-M)+\frac{M(2\ell-1)}{4}-\frac{1}{2};c;1-\frac{p^2}{\sigma^2}\right). \tag{25}$$

All the previous cases fall out of (24) and (25) by making the relevant substitutions for M and ℓ. Of course one may also derive nonleading terms I_N^k, ρ_N^k in exactly the same way as before and they correspond to higher order threshold corrections. Again, these corrections entrain higher powers of $(p^2-\sigma^2)$ and terminate for half-integral ℓ.

VI. CONCLUSIONS

Before we can comprehend the statistical effects of phase space on brane physics, it is vital to understand phase space in flat D-dimensional space–time for any number of particles, with arbitrary masses. This paper has been devoted to that subject and we have arrived at results for $\rho_N(p)$ and $I_N(p)$ that have culminated in formulas (14), (23), (24), and (25). These comprise the high-energy and low-energy characteristics and at any energy in-between. We believe that these analytical expressions are as compact as one can make them and will turn out to be practically useful. Otherwise one will be obliged to resort to numerical methods.

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APPENDIX: AT THE THRESHOLD OF A SUNSET

In this appendix we show explicitly how the threshold expansion can be carried out in momentum space via Feynman parameters. We illustrate the case $N=2$ for any dimension 2ℓ to keep the algebra simple, when the sunset integral is just

$$I_2(p)=\frac{\Gamma(2-\ell)}{(-4\pi)^\ell}\int_0^1 d\alpha_1\int_0^1 d\alpha_2\frac{\delta(\alpha_1+\alpha_2-1)}{[p^2\alpha_1\alpha_2-m_1^2\alpha_2-m_2^2\alpha_1]^{2-\ell}}.$$

Never mind the fact that I_2 can be expressed as a linear combination of two hypergeometric functions ($a=\ell-1,\ b=2-\ell,\ c=\ell$) with arguments $1/2[(m_1^2-m_2^2\pm p^2)/\lambda+1]$ or that it can be accorded an exact geometrical interpretation;[19] our purpose here is to show how one may arrive at a systematic threshold expansion, by expanding about the minimum of the denominator, regarded as a function of α. Thus change variables to

$$\alpha_i=\frac{m_i}{m_1+m_2}+\Delta\rho_i,\quad p^2\equiv(m_1+m_2)^2[1-\Delta^2].$$

The delta-function constraint on α corresponds to $\rho_1=-\rho_2\equiv\rho$, whereupon the sunset integral reduces to

$$I_2(p)=\frac{\Gamma(2-\ell)}{(4\pi)^\ell}\Delta^{2\ell-3}\int_{-m_1/[(m_1+m_2)\Delta]}^{m_2/[(m_1+m_2)\Delta]}\frac{d\rho}{[m_1m_2+\rho^2(m_1+m_2)^2(1-\Delta^2)-\Delta\rho(m_1^2-m_2^2)]^{2-\ell}}.$$

The leading behavior is found by setting $\Delta=0$ in the denominator of the integrand and extending the limits to $\pm\infty$. Since

$$\int_0^\infty\frac{d\rho}{[m_1m_2+\rho^2(m_1+m_2)^2]^{2-\ell}}=\frac{(m_1m_2)^{\ell-3/2}}{2(m_1+m_2)}\int_0^\infty\frac{dv\,v^{-1/2}}{(1+v)^{2-\ell}}=\frac{(m_1m_2)^{\ell-3/2}}{2(m_1+m_2)}\frac{\sqrt{\pi}\Gamma(3/2-\ell)}{\Gamma(2-\ell)},$$

it follows that

$$I_2^0(p)=\frac{(m_1m_2\Delta^2)^{\ell-3/2}\sqrt{\pi}}{(4\pi)^{\ell}(m_1+m_2)}\Gamma(3/2-\ell).$$

However we are keen to obtain all the nonleading terms and this can be accomplished by rewriting the sunset integral as

$$I_2(p)=\frac{\Gamma(2-\ell)(m_1m_2\Delta^2)^{\ell-3/2}}{(4\pi)^{\ell}\sqrt{p^2}}\int_{u_-}^{u_+}\mathrm{d}u[1+u^2-u\,\eta]^{\ell-2},$$

where the new integration variable is $u=\rho\sqrt{p^2/m_1m_2}$, the limits are

$$u_+=\frac{m_2}{(m_1+m_2)\Delta}\sqrt{\frac{p^2}{m_1m_2}}$$

and

$$u_-=-\frac{m_1}{(m_1+m_2)\Delta}\sqrt{\frac{p^2}{m_1m_2}},$$

and the new expansion variable is

$$\eta\equiv\frac{\Delta(m_1^2-m_2^2)}{\sqrt{p^2m_1m_2}}.$$

The series in η reads

$$I_2(p)=\frac{(m_1m_2\Delta^2)^{\ell-3/2}}{(4\pi)^{\ell}\sqrt{p^2}}\sum_{n=0}^{\infty}\frac{\Gamma(2+n-\ell)}{n!}\eta^nU_n,\quad U_n\equiv\int_{u_-}^{u_+}\mathrm{d}u\,(1+u^2)^{\ell-2-n}u^n.$$

In evaluating the coefficients U_n, we make use of the fact that the limits are large and we should distinguish between the cases of n even and n odd. For n even, we split the integral into

$$\begin{aligned}U_n&=\left(2\int_0^{\infty}-\int_{|u_-|}^{\infty}-\int_{|u_+|}^{\infty}\right)\mathrm{d}u\,u^n(1+u^2)^{\ell-2-n}\\&=\frac{\Gamma((n+1)/2)\Gamma((3+n)/2-\ell)}{\Gamma(2+n-\ell)}-\left(\int_{|u_-|}^{\infty}+\int_{|u_+|}^{\infty}\right)\mathrm{d}u\,u^{2\ell-4-n}(1+1/u^2)^{\ell-2-n},\end{aligned}$$

where we may expand the latter two integrals in powers of $1/u^2$—which provides a further subexpansion in powers of Δ. Thus we get

$$\begin{aligned}\Gamma(2+n-\ell)U_n=\Gamma(n+1/2)\Gamma((3+n)/2-\ell)+\sum_{k=0}^{\infty}\frac{(-)^k\Gamma(2+n+k-\ell)}{k!(2\ell-3-n-2k)}\\\times[|u_+|^{2\ell-3-n-2k}+|u_-|^{2\ell-3-n-2k}].\end{aligned}$$

On the other hand, the case of odd n can be treated directly by expanding the integrand below in powers of $1/v$:

$$U_n=\frac{1}{2}\int_{u_-^2}^{u_+^2}\mathrm{d}v\,v^{\ell-(5+n)/2}(1+1/v)^{\ell-2-n}$$

so

$$\Gamma(2+n-\ell)U_n=\sum_{k=0}^{\infty}\frac{(-)^k\Gamma(2+n+k-\ell)}{k!(2\ell-3-n-2k)}[|u_+|^{2\ell-3-n-2k}-|u_-|^{2\ell-3-n-2k}].$$

Again one encounters a subseries in Δ. (The two series make up the "$h-h$" and "$p-p$" contributions of Ref. 3 at one stroke.) In short we see that the sunset integral, and of necessity its imaginary part, can be systematically expanded as a series in Δ which is proportional to the Q value of the reaction by appropriately handling the Feynman parametric representation. It is possible to treat the sunset diagram with N intermediate particles in a similar way, but the method becomes rather unwieldy, which is why we turned to coordinate space methods in Secs. IV and V.[20,21]

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Generalized Weyl–Wigner map and Vey quantum mechanics

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The Weyl–Wigner map yields the entire structure of Moyal quantum mechanics directly from the standard operator formulation. The covariant generalization of Moyal theory, also known as Vey quantum mechanics, was presented in the literature many years ago. However, a derivation of the formalism directly from standard operator quantum mechanics, clarifying the relation between the two formulations, is still missing. In this article we present a covariant generalization of the Weyl order prescription and of the Weyl–Wigner map and use them to derive Vey quantum mechanics directly from the standard operator formulation. The procedure displays some interesting features: it yields all the key ingredients and provides a more straightforward interpretation of the Vey theory including a direct implementation of unitary operator transformations as phase space coordinate transformations in the Vey idiom. These features are illustrated through a simple example. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1415086]

I. INTRODUCTION

The Weyl–Wigner map[1,2] yields the Moyal formulation of quantum mechanics,[3–8] alternative to the more conventional standard operator[9–12] and path integral formulations. The main features of Moyal quantum mechanics are that it is formulated in terms of phase space functions and the dynamics is based on a deformation of the Poisson bracket, named the Moyal bracket.[3,13–15] This formulation of quantum mechanics has been receiving increased attention namely in the context of the fields of the semiclassical limit of quantum mechanics,[5,14–19] quantum chaos,[20,21] hybrid dynamics[22,23] and also in M-theory.[24–26]

The Weyl–Wigner isomorphism between operators and phase space functions (symbols) provides the entire structure of Moyal quantum mechanics directly from the standard operator formulation. Let us choose a set of fundamental operators $(\hat{q}_i,\hat{p}_i)$ and the corresponding set of canonical variables $(q_i,p_i), i=1,...,N$, for an arbitrary N dimensional dynamical system. The Weyl–Wigner map $W_{(q,p)}:\hat{\mathcal{A}}\rightarrow\mathcal{A}(T^*M)$ attributes to a given operator $\hat{A}$ in the quantum algebra $\hat{\mathcal{A}}$ a unique element of the algebra of functions over the phase space T^*M:

$$W_{(q,p)}(\hat{A})=\int d^N\vec{y}\,e^{-i\vec{p}\cdot\vec{y}}\left\langle \vec{q}-\frac{\hbar}{2}\vec{y}\left|\hat{A}\right|\vec{q}+\frac{\hbar}{2}\vec{y}\right\rangle, \tag{1}$$

where we used the compact notation:

$$\vec{y}\equiv(y_1,\ldots,y_N);\;\; d^N\vec{y}\equiv dy_1\cdots dy_N;\;\; \vec{p}\equiv(p_1,\ldots,p_N)\;\; \vec{q}\equiv(q_1,\ldots,q_N),$$

and the subscript (q,p) means that the corresponding object (the Weyl–Wigner map in this case) is defined in the variables $(\vec{q},\vec{p})$. This specification seems redundant now but is important for the sequel. The Weyl–Wigner map is bijective and unequivocal. Moreover, it is an isomorphism

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between the quantum $(\hat{\mathcal{A}},\cdot,[,])$ and the "classical" $(\mathcal{A},*,[,]_M)$ algebras. The quantum algebra $\hat{\mathcal{A}}$ is based on the operator product $\cdot$ and the quantum commutator $[,]$, whereas the classical algebraic structures are the "star" product $*$ and the Moyal bracket $[,]_M$. The Weyl–Wigner map is a morphism in the sense that

$$\begin{aligned} &W_{(q,p)}(\hat{A}\cdot\hat{B})=W_{(q,p)}(\hat{A})*_{(q,p)}W_{(q,p)}(\hat{B}),\\ &W_{(q,p)}\left(\frac{1}{i\hbar}[\hat{A},\hat{B}]\right)=[W_{(q,p)}(\hat{A}),W_{(q,p)}(\hat{B})]_{M_{(q,p)}},\quad \forall\hat{A},\hat{B}\in\hat{\mathcal{A}}, \end{aligned} \tag{2}$$

and it yields the functional structure of the star product and Moyal bracket:

$$A*_{(q,p)}B=Ae^{(i\hbar/2)\hat{\mathcal{J}}_{(q,p)}}B,\quad [A,B]_{M_{(q,p)}}=\frac{2}{\hbar}A\sin\left(\frac{\hbar}{2}\hat{\mathcal{J}}_{(q,p)}\right)B,\quad A,B\in\mathcal{A}, \tag{3}$$

where $\hat{\mathcal{J}}_{(q,p)}$ is the "*Poisson*" operator:

$$\hat{\mathcal{J}}_{(q,p)}\equiv\sum_{i=1}^{N}\left(\frac{\overleftarrow{\partial}}{\partial q_i}\frac{\vec{\partial}}{\partial p_i}-\frac{\overleftarrow{\partial}}{\partial p_i}\frac{\vec{\partial}}{\partial q_i}\right),$$

the derivatives $\overleftarrow{\partial}$ and $\vec{\partial}$ acting on A and B, respectively. Alternatively, $\hat{\mathcal{J}}_{(q,p)}$ can be written as $\hat{\mathcal{J}}_{(q,p)}=\overleftarrow{\partial}_k J^{kl}_{(q,p)}\vec{\partial}_l$, where $J^{kl}_{(q,p)}$ is the klth element of the symplectic matrix in the variables $(\vec{q},\vec{p})$:

$$J_{(q,p)}=\begin{pmatrix}0_{N\times N} & -1_{N\times N}\\ 1_{N\times N} & 0_{N\times N}\end{pmatrix}. \tag{4}$$

We introduced the compact notation, $O^k=p_k, k=1,\ldots,N$; $O^k=q_{k-N}, k=N+1,\ldots,2N$; $\partial/\partial O_k=\partial_k$, and sum over repeated indices is understood.

From Eq. (3) it is trivial to obtain the following expansion in powers of $\hbar$:

$$A*_{(q,p)}B=A\cdot B+\frac{i\hbar}{2}A\overleftarrow{\partial}_k J^{kl}_{(q,p)}\vec{\partial}_l B+\frac{1}{2}\left(\frac{i\hbar}{2}\right)^2 A\overleftarrow{\partial}_k\overleftarrow{\partial}_s J^{kl}_{(q,p)}J^{sn}_{(q,p)}\vec{\partial}_l\vec{\partial}_n B+\cdots. \tag{5}$$

The Weyl–Wigner transform of the density matrix operator is the Wigner distribution function,[2] $f_W(\vec{q},\vec{p};t)=(1/2\Pi\hbar)W_{(q,p)}(|\psi(t)\rangle\langle\psi(t)|)$, which is the fundamental mathematical object of Moyal quantum mechanics. Its time evolution is given by the dynamical equation

$$\dot{f}_W(\vec{q},\vec{p};t)=[H(\vec{q},\vec{p}),f_W(\vec{q},\vec{p};t)]_{M_{(q,p)}},\quad H=W_{(q,p)}(\hat{H}), \tag{6}$$

where $\hat{H}$ is the quantum Hamiltonian. We see that the mathematical structure of Moyal quantum mechanics is very similar to that of classical statistical mechanics. However, these similarities should not be taken too seriously. The procedure by which physical relevant information is obtained is a lot more elaborate. In classical statistical mechanics the fundamental predictions are the probabilities for finding the system in an arbitrary configuration $(\vec{q}_0,\vec{p}_0)$, which are given by the values of a true probability distribution function $\rho(\vec{q}=\vec{q}_0,\vec{p}=\vec{p}_0)$.

On the contrary, in Moyal quantum mechanics the value of $f_W(\vec{q}=\vec{q}_0,\vec{p}=\vec{p}_0)$ cannot be given such straightforward interpretation, given the fact that $f_W(\vec{q},\vec{p})$ might take on negative values. The fundamental physical predictions of Moyal quantum mechanics are obtained through a procedure analogous to that of standard operator quantum mechanics. Given a general observable $A(\vec{q},\vec{p})$ we should solve the star-genvalue equation,[8,27,28]

$$A(\vec{q},\vec{p})*_{(q,p)}g^n_a(\vec{q},\vec{p})=ag^n_a(\vec{q},\vec{p}), \tag{7}$$

where n is a degeneracy index, to obtain the probability for a measurement of A at the time t yielding the value a:

$$P(A(\vec{q},\vec{p};t)=a)=\sum_n \int d^N\vec{q}\int d^N\vec{p}\,g_a^n(\vec{q},\vec{p})f_W(\vec{q},\vec{p};t), \tag{8}$$

where we assumed that the degeneracy index is discrete. If this is not the case, then the sum in n is replaced by a (set of) integral(s) in n. For the fundamental observables q_i and p_i, $i=1,...,N$, Eq. (8) reduces to a more ''classical type'' result:

$$\begin{aligned} P(q_i(t)=q_0)&=\int d^N\vec{q}\int d^N\vec{p}\,f_W(\vec{q},\vec{p};t)\,\delta(q_i-q_0);\\ P(p_i(t)=p_0)&=\int d^N\vec{q}\int d^N\vec{p}\,f_W(\vec{q},\vec{p};t)\,\delta(p_i-p_0), \end{aligned} \tag{9}$$

the same happening to the average value of $A(\vec{q},\vec{p})$:

$$\langle A(\vec{q},\vec{p};t)\rangle=\int d^N\vec{q}\int d^N\vec{p}\,A(\vec{q},\vec{p})f_W(\vec{q},\vec{p};t). \tag{10}$$

An important subject in any dynamical theory is the study of its invariances. Just like standard operator quantum mechanics the Moyal formulation is invariant under the action of general unitary transformations and, contrary to what happens in classical mechanics, is not invariant under the action of a significant set of coordinate transformations. In fact, most unitary operator transformations are not implemented as phase space coordinate transformations in the Moyal idiom.

Many years ago Vey[29] presented a generalization of the star product that renders Moyal quantum mechanics fully invariant under phase space coordinate transformations. The original motivation was not to enlarge the invariance properties of Moyal quantum mechanics, but to derive the general form of the Poisson algebra deformations for curved phase spaces. Vey's original developments have been used in investigations aiming at two major directions: First, to provide a consistent classical interpretation of Moyal dynamics,[14,15] and second, in more mathematically oriented research, to generalize the Moyal–Weyl–Wigner quantization procedure to nonflat phase space manifolds. In Refs. 14 and 15 the problem of constructing an associative star product in a general sympletic manifold was considered. The question of existence of such a product was completely solved in Ref. 30. The same problem for Poisson–Lie groups was consider in Ref. 31. In Refs. 32–34 an alternative construction of star products for a general sympletic manifold was proposed. This construction is given in pure geometrical terms and is thus quite an appealing framework to study the invariance properties of phase space quantum mechanics. In Ref. 33 the action of unitary transformations is implemented, in geometrical terms, as sympletic morphisms of the phase space manifold.

To our knowledge, however, a complete study of the relation between Vey covariant quantum mechanics and standard operator quantum mechanics casting Vey theory at the same level of completeness as Moyal quantum mechanics has not yet been presented. Take, for instance, the Weyl–Wigner map. Although trivial, the covariant generalization of this map is still missing in the literature.

In this article we emphasize the relation between standard operator quantum mechanics and Moyal quantum mechanics and attempt to derive the Vey formulation in a similar fashion. There are two main virtues in this approach: first, it clarifies the relation between the standard operator and Vey quantum mechanics (providing, for instance, a new point of view for the analysis of the invariance properties of covariant phase space quantum mechanics). Second, it yields a (previously missing) covariant generalization of some key ingredients of phase space quantum mechanics, such as the Weyl–Wigner map, the Weyl order prescription, the average and the marginal probability distribution functionals and the star-genvalue equation.

This article is organized as follows: in Sec. II we start by reviewing some well known properties concerning the action of canonical and coordinate transformations in the Moyal formalism. We then present (Sec. III) a covariant generalization of the Weyl–Wigner map. The new map makes it possible to implement a general unitary transformation of standard operator quantum mechanics as a coordinate transformation in the Moyal idiom. In Sec. IV we use the new map to derive the covariant star product and, as a by-product, the dynamical structure of Vey quantum mechanics. In Sec. V we present a summary of the structure of covariant quantum mechanics, including the generalizations of the star-genvalue equation, the average value and the probability functionals. Finally, in Sec. VI some of the features of the formalism are illustrated through a simple example.

Before proceeding let us make an important remark: from the outset we shall restrict our attention to the simpler case of dynamical systems displaying a phase space with the structure of a flat manifold.

II. CANONICAL AND COORDINATE TRANSFORMATIONS

In classical mechanics all canonical transformations are phase space coordinate transformations. Their action is of the form (we shall take the passive point of view)

$$T:T^*M\rightarrow T^*M;(\vec{q},\vec{p})\rightarrow(\vec{q}=\vec{q}(\vec{Q},\vec{P}),\vec{p}=\vec{p}(\vec{Q},\vec{P})), \tag{11}$$

where $(\vec{Q},\vec{P})$ and $(\vec{q},\vec{p})$ are two sets of canonical variables. T yields a transformation of a general observable given by

$$T:A(\vec{q},\vec{p})\rightarrow A'(\vec{Q},\vec{P})=A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})), \tag{12}$$

and for two general observables $A'(\vec{Q},\vec{P})=T\{A(\vec{q},\vec{p})\}$ and $B'(\vec{Q},\vec{P})=T\{B(\vec{q},\vec{p})\}$ we have

$$\{A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})),B(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))\}_{(q,p)}=\{A'(\vec{Q},\vec{P}),B'(\vec{Q},\vec{P})\}_{(Q,P)}, \tag{13}$$

and thus the Hamiltonian equations of motion in the variables $(\vec{q},\vec{p})$ and $(\vec{Q},\vec{P})$ are fully equivalent: they yield identical mathematical solutions and thus identical physical predictions.

This picture does not translate to Moyal quantum mechanics. To see this explicitly let us go back to standard operator quantum mechanics and consider, to make it simpler, the unitary transformation:

$$\hat{\vec{q}}\equiv\hat{\vec{q}}(\hat{\vec{Q}},\hat{\vec{P}})=\hat{U}\hat{\vec{Q}}\hat{U}^{-1},\quad \hat{\vec{p}}\equiv\hat{\vec{p}}(\hat{\vec{Q}},\hat{\vec{P}})=\hat{U}\hat{\vec{P}}\hat{U}^{-1},\quad \hat{A}(\hat{\vec{q}},\hat{\vec{p}})\equiv\hat{U}\hat{A}(\hat{\vec{Q}},\hat{\vec{P}})\hat{U}^{-1}=\hat{A}'(\hat{\vec{Q}},\hat{\vec{P}}). \tag{14}$$

The two sets of fundamental variables provide two Weyl-Wigner maps:

$$\begin{aligned} W_{(Q,P)}(\hat{A})&=\int d^N\vec{Y}e^{-i\vec{P}\cdot\vec{Y}}\left\langle \vec{Q}-\frac{\hbar}{2}\vec{Y}\middle|\hat{A}\middle|\vec{Q}+\frac{\hbar}{2}\vec{Y}\right\rangle,\\ W_{(q,p)}(\hat{A})&=\int d^N\vec{y}e^{-i\vec{p}\cdot\vec{y}}\left\langle \vec{q}-\frac{\hbar}{2}\vec{y}\middle|\hat{A}\middle|\vec{q}+\frac{\hbar}{2}\vec{y}\right\rangle, \end{aligned} \tag{15}$$

from which we can derive the action of unitary transformations in the Moyal formalism. The fundamental variables transform trivially,

$$T:(\vec{q},\vec{p})\rightarrow(\vec{q}=W_{(Q,P)}(\hat{\vec{q}}(\hat{\vec{Q}},\hat{\vec{P}}))=\vec{q}(\vec{Q},\vec{P}),\vec{p}=W_{(Q,P)}(\hat{\vec{p}}(\hat{\vec{Q}},\hat{\vec{P}}))=\vec{p}(\vec{Q},\vec{P})), \tag{16}$$

and a general observable transforms as

$$
\begin{aligned}
T{:}A(\vec{q},\vec{p}) &= W_{(q,p)}(\hat{A}(\hat{\vec{q}},\hat{\vec{p}})) \rightarrow A'(\vec{Q},\vec{P}) \\
&= W_{(Q,P)}(\hat{A}'(\hat{\vec{Q}},\hat{\vec{P}})) \\
&= U(\vec{Q},\vec{P}) *_{(Q,P)} A(\vec{Q},\vec{P}) *_{(Q,P)} U^{-1}(\vec{Q},\vec{P}),
\end{aligned} \tag{17}
$$

which, in general, does not correspond to the action of a coordinate transformation (except if T is linear) since

$$
A'(\vec{Q},\vec{P}) \neq A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})), \tag{18}
$$

even though the transformation is canonical. For two general observables $A(\vec{q},\vec{p})$ and $B(\vec{q},\vec{p})$ we have

$$
[A'(\vec{Q},\vec{P}),B'(\vec{Q},\vec{P})]_{M_{(Q,P)}} = T([A(\vec{q},\vec{p}),B(\vec{q},\vec{p})]_{M_{(q,p)}}), \tag{19}
$$

and thus the Moyal dynamical equations in the variables $(\vec{Q},\vec{P})$ and $(\vec{q},\vec{p})$,

$$
\dot{A}(\vec{q},\vec{p};t) = [A(\vec{q},\vec{p};t),H(\vec{q},\vec{p})]_{M_{(q,p)}} \quad \text{and} \quad \dot{A}'(\vec{Q},\vec{P};t) = [A'(\vec{Q},\vec{P};t),H'(\vec{Q},\vec{P})]_{M_{(Q,P)}}, \tag{20}
$$

yield two mathematical solutions, related by

$$
A(t) = F(\vec{q},\vec{p},t) \quad \text{and} \quad A'(t) = F'(\vec{Q},\vec{P},t) = U *_{(Q,P)} F(\vec{Q},\vec{P},t) *_{(Q,P)} U^{-1}, \tag{21}
$$

which, in general, are not the same phase space function: $F'(\vec{Q},\vec{P},t) \neq F(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}),t)$, albeit providing the same physical predictions: Eqs. (8)–(10). We see that no physical meaning can be attached to a single value of the observable A since this value is dependent of the particular representation chosen. Take, for instance, the Wigner distribution function that may be positive defined in one representation and become negative under a unitary transformation.

On the other hand, most coordinate transformations act noncanonically in the Moyal formalism (the exceptions, once again, are linear transformations): consider the transformation T in Eq. (16) and the two general phase space functions $G(\vec{q},\vec{p})$ and $F(\vec{q},\vec{p})$. In general we have

$$
\begin{aligned}
&[G(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})),F(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))]_{M_{(q,p)}} \\
&\quad \neq [G(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})),F(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))]_{M_{(Q,P)}},
\end{aligned} \tag{22}
$$

which is a consequence of the fact that the star product (sometimes expressed in terms of the symmetric bracket[13]) is also not invariant under a general coordinate transformation:

$$
\begin{aligned}
&G(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})) *_{(q,p)} F(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})) \\
&\quad \neq G(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})) *_{(Q,P)} F(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})).
\end{aligned} \tag{23}
$$

These features of the Weyl-Wigner map and consequently of the star product are well known and have been extensively studied in the past (see, for instance Refs. 14 and 15). Namely, it was proved that the set of observables invariant under general unitary transformations is the set of first order polynomials in the fundamental variables and the coordinate transformations that preserve the Moyal star product are the linear transformations. These properties restrict the validity of the deformation quantization procedure to those phase space manifolds where a global Darboux chart can be naturally defined and thus completely exclude the possibility of extending this quantization procedure to nonflat phase space manifolds. In this context they motivated the original developments by Vey[29] and subsequently by Bayen *et al.*,[14,15] aiming at producing a more robust, coor-

dinate invariant formulation of the deformed structures. This work culminated with the results of Fedosov[33,34] where a pure geometrical implementation of the star product was proposed.

Our analysis of the next sections differs in the approach but not in the final goals. Instead of working directly in the context of Wigner quantum mechanics (like in the previous references) we focus on the relation between standard operator and phase space quantum mechanics. From the analysis leading to Eq. (18) and Eqs. (22) and (23) we see that the behavior of Moyal quantum mechanics under the action of canonical and coordinate transformations can be seen as a consequence of the definition of the Weyl–Wigner map (15). This motivates the purpose of the next section where we will present a generalization of the Weyl–Wigner map and use it to prove that unitary operator transformations can be implemented as coordinate transformations in the Moyal formalism. Furthermore, we will see in Sec. IV that the new map provides a derivation of Vey covariant quantum mechanics directly from standard operator quantum mechanics.

III. GENERALIZED WEYL–WIGNER MAP

We start by introducing a new Weyl–Wigner map in the variables $(\vec{Q},\vec{P})$ (which are not required to be canonical) that copies the Weyl–Wigner map in the variables $(\vec{q},\vec{p})$:

Definition: Generalized Weyl–Wigner map: Let $W_{(q,p)}$ be the standard Weyl–Wigner map [in the variables $(\vec{q},\vec{p})$] from the algebra of linear operators $\hat{\mathcal{A}}(\mathcal{H})$ acting on the physical Hilbert space $\mathcal{H}$ to the algebra of observables in the phase space T^*M. For the variables $(\vec{Q},\vec{P})$, assumed in one-to-one correspondence with the canonical variables $(\vec{q},\vec{p})$, we define a new *generalized* Weyl–Wigner map:

$$W'_{(Q,P)}:\hat{\mathcal{A}}(\mathcal{H})\rightarrow\mathcal{A}(T^*M);\quad W'_{(Q,P)}(\hat{A})=W_{(q,p)}(\hat{A}),\quad \forall\hat{A}\in\hat{\mathcal{A}}(\mathcal{H})\,. \tag{24}$$

For each new choice of the canonical variables $(\vec{q},\vec{p})$ we obtain a new Weyl–Wigner map in the variables $(\vec{Q},\vec{P})$. If the transformation from $(\vec{q},\vec{p})$ to $(\vec{Q},\vec{P})$ is a polynomial of first degree, then $W'_{(Q,P)}=W_{(Q,P)}$. Otherwise the two maps differ.

The aim of this section is to obtain the explicit expression for $W'_{(Q,P)}$. We start by deriving the generalizations of the Weyl order and Weyl symbol prescriptions.

A generic dynamical operator $\hat{A}$ can be cast in a fully symmetrized form according to Weyl's prescription:

$$\hat{A}_{W(q,p)}=\hat{A}(\hat{\vec{q}},\hat{\vec{p}})=\int d^N\vec{x}d^N\vec{y}\,\alpha(\vec{x},\vec{y})e^{i\vec{x}\cdot\hat{\vec{q}}+i\vec{y}\cdot\hat{\vec{p}}}, \tag{25}$$

where the subscript $W(q,p)$ means that $\hat{A}$ is displayed as a fully symmetrized functional of the variables $(\hat{\vec{q}},\hat{\vec{p}})$, and $\vec{x}\cdot\hat{\vec{q}}+\vec{y}\cdot\hat{\vec{p}}\equiv\Sigma_{j=1}^{N}(x_j\hat{q}_j+y_j\hat{p}_j)$. If $\hat{A}$ is Hermitian, then the numerical (usually singular) function $\alpha(\vec{x},\vec{y})$ is subject to the constraint $\alpha^*(\vec{x},\vec{y})=\alpha(-\vec{x},-\vec{y})$. The Weyl symbol, $W_{(q,p)}(\hat{A})$, associated with the operator $\hat{A}$ in Eq. (25) is the c-function of $2N$ phase space variables $(\vec{q},\vec{p})$ given by

$$A(\vec{q},\vec{p})\equiv W_{(q,p)}[\hat{A}(\hat{\vec{q}},\hat{\vec{p}})]=\int d^N\vec{x}d^N\vec{y}\,\alpha(\vec{x},\vec{y})e^{i\vec{x}\cdot\vec{q}+i\vec{y}\cdot\vec{p}}. \tag{26}$$

Let now $(\hat{\vec{Q}},\hat{\vec{P}})$ be another complete set of variables in one-to-one correspondence with $(\hat{\vec{q}},\hat{\vec{p}})$ and let us display the variables $(\hat{\vec{q}},\hat{\vec{p}})$ in a completely symmetrized order in the basis $(\hat{\vec{Q}},\hat{\vec{P}})$, i.e.,

$$\hat{\vec{q}}\equiv\int d^N\vec{z}d^N\vec{w}\,\rho_q(\vec{z},\vec{w})e^{i\vec{z}\cdot\hat{\vec{Q}}+i\vec{w}\cdot\hat{\vec{P}}}, \tag{27}$$

$$\hat{\vec{p}} \equiv \int d^N\vec{x}\, d^N\vec{y}\, \rho_p(\vec{x},\vec{y})\, e^{i\vec{x}\cdot\hat{\vec{Q}}+i\vec{y}\cdot\hat{\vec{P}}}.$$

The new variables are not necessarily canonical: in general, $[\hat{Q}_i,\hat{P}_j]\neq i\hbar\,\delta_{ij}$. The $(\vec{Q},\vec{P})$-Weyl symbols associated with (27) are

$$\begin{aligned}\vec{q} &\equiv W_{(Q,P)}(\hat{\vec{q}}) = \int d^N\vec{z}\, d^N\vec{w}\, \rho_q(\vec{z},\vec{w})\, e^{i\vec{z}\cdot\vec{Q}+i\vec{w}\cdot\vec{P}},\\ \vec{p} &\equiv W_{(Q,P)}(\hat{\vec{p}}) = \int d^N\vec{x}\, d^N\vec{y}\, \rho_p(\vec{x},\vec{y})\, e^{i\vec{x}\cdot\vec{Q}+i\vec{y}\cdot\vec{P}}.\end{aligned} \tag{28}$$

Let us now consider again the operator $\hat{A}$ given by Eq. (25). In the $(\hat{\vec{Q}},\hat{\vec{P}})$ representation $\hat{A}$ is written as $\hat{A}=\hat{A}(\hat{\vec{q}}(\hat{\vec{Q}},\hat{\vec{P}}),\hat{\vec{p}}(\hat{\vec{Q}},\hat{\vec{P}}))=\hat{A}'(\hat{\vec{Q}},\hat{\vec{P}})$ and the explicit functional form of $\hat{A}'$ is given by the *generalized Weyl prescription*:

$$\hat{A}_{W'(Q,P)}=\hat{A}'(\hat{\vec{Q}},\hat{\vec{P}}) = \int d^N\vec{x}\, d^N\vec{y}\, \alpha(\vec{x},\vec{y})\, e^{i\vec{x}\cdot\hat{\vec{q}}(\hat{\vec{Q}},\hat{\vec{P}})+i\vec{y}\cdot\hat{\vec{p}}(\hat{\vec{Q}},\hat{\vec{P}})}, \tag{29}$$

where $\hat{\vec{q}}(\hat{\vec{Q}},\hat{\vec{P}})$ and $\hat{\vec{p}}(\hat{\vec{Q}},\hat{\vec{P}})$ are given (in a fully symmetrized order) by Eq. (27) and the subscript $W'(Q,P)$ means that $\hat{A}$ is displayed as a functional of the variables $(\hat{\vec{Q}},\hat{\vec{P}})$ in a fully symmetrized order in the variables $(\hat{\vec{q}},\hat{\vec{p}})$. Notice that the numerical function $\alpha(\vec{x},\vec{y})$ is the same as in Eq. (25). The standard $(\vec{q},\vec{p})$-Weyl symbol associated with $\hat{A}$ is given by Eq. (26) and thus, using the definition (24), it is straightfoward to conclude that the generalized Weyl symbol associated with $\hat{A}$ is given by

$$A'(\vec{Q},\vec{P}) \equiv W'_{(Q,P)}[\hat{A}'(\hat{\vec{Q}},\hat{\vec{P}})] = \int d^N\vec{x}\, d^N\vec{y}\, \alpha(\vec{x},\vec{y})\, e^{i\vec{x}\cdot\vec{q}(\vec{Q},\vec{P})+i\vec{y}\cdot\vec{p}(\vec{Q},\vec{P})}, \tag{30}$$

and one immediately realizes that $A'(\vec{Q},\vec{P})=A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))$ as it should.

Finally, we want to derive the covariant generalization of the Weyl–Wigner map given by Eq. (1). We start by rewriting $W_{(q,p)}$ as follows:

$$A(\vec{q},\vec{p}) = W_{(q,p)}(\hat{A}) = \int d^N\vec{x} \int d^N\vec{y}\, e^{-i\vec{p}\cdot\vec{y}}\, \delta(\vec{x}-\vec{q})\, F(\vec{x},\vec{y}), \tag{31}$$

where $F(\vec{x},\vec{y})=\langle \vec{x}-\frac{\hbar}{2}\vec{y}|\hat{A}|\vec{x}+\frac{\hbar}{2}\vec{y}\rangle$ and $|\vec{x}\pm\frac{\hbar}{2}\vec{y}\rangle$ are eigenstates of $\hat{\vec{q}}$. The function $F(\vec{x},\vec{y})$ is invariant under change of representation:

$$F(\vec{x},\vec{y}) = \left\langle \vec{x}-\frac{\hbar}{2}\vec{y}\right|\hat{A}(\hat{\vec{q}},\hat{\vec{p}})\left|\vec{x}+\frac{\hbar}{2}\vec{y}\right\rangle = \left\langle \vec{x}-\frac{\hbar}{2}\vec{y}\right|_Q \hat{A}(\hat{\vec{q}}(\hat{\vec{Q}},\hat{\vec{P}}),\hat{\vec{p}}(\hat{\vec{Q}},\hat{\vec{P}}))\left|\vec{x}+\frac{\hbar}{2}\vec{y}\right\rangle_Q, \tag{32}$$

where the subscript "Q" makes it explicit that the eigenstates of $\hat{\vec{q}}$ are displayed in the $\hat{\vec{Q}}$ representation. Furthermore, it is trivial to realize that

$$A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})) = \int d^N\vec{x} \int d^N\vec{y}\, e^{-i\vec{p}(\vec{Q},\vec{P})\cdot\vec{y}}\, \delta(\vec{x}-\vec{q}(\vec{Q},\vec{P}))\, F(\vec{x},\vec{y}), \tag{33}$$

and thus we get the explicit expression for the covariant Weyl–Wigner map:

$$W'_{(Q,P)}(\hat{A})=\int d^N\vec{x}\int d^N\vec{y}e^{-i\vec{p}(\vec{Q},\vec{P})\cdot\vec{y}}\delta(\vec{x}-\vec{q}(\vec{Q},\vec{P}))\left\langle \vec{x}-\frac{\hbar}{2}\vec{y}\right|_Q\hat{A}\left|\vec{x}+\frac{\hbar}{2}\vec{y}\right\rangle_Q \tag{34}$$

satisfying definition (24).

To illustrate the features of the new map let us consider the unitary transformation (14). The generalized map yields a different phase space version of this transformation. The analog of Eq. (17) is given by

$$T{:}A(\vec{q},\vec{p})=W_{(q,p)}(\hat{A}(\hat{\vec{q}},\hat{\vec{p}}))\rightarrow A'(\vec{Q},\vec{P})=W'_{(Q,P)}(\hat{A}'(\hat{\vec{Q}},\hat{\vec{P}})), \tag{35}$$

and we get

$$\begin{aligned}W'_{(Q,P)}(\hat{A}'(\hat{\vec{Q}},\hat{\vec{P}}))&=W'_{(Q,P)}(\hat{U}\hat{A}(\hat{\vec{Q}},\hat{\vec{P}})\hat{U}^{-1})\\&=\int d^N\vec{x}\int d^N\vec{y}e^{-i\vec{p}(\vec{Q},\vec{P})\cdot\vec{y}}\delta(\vec{x}-\vec{q}(\vec{Q},\vec{P}))\\&\quad\times\left\langle \vec{x}-\frac{\hbar}{2}\vec{y}\right|\hat{U}^{-1}(\hat{U}\hat{A}(\hat{\vec{Q}},\hat{\vec{P}})\hat{U}^{-1})\hat{U}\left|\vec{x}+\frac{\hbar}{2}\vec{y}\right\rangle\\&=A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P})),\end{aligned} \tag{36}$$

where $\vec{q}(\vec{Q},\vec{P})$ and $\vec{p}(\vec{Q},\vec{P})$ are given by Eq. (16) and $|\vec{x}\pm\frac{\hbar}{2}\vec{y}\rangle$ are eigenstates of $\hat{\vec{Q}}$ and thus $\hat{U}|\vec{x}\pm\frac{\hbar}{2}\vec{y}\rangle$ are eigenstates of $\hat{\vec{q}}$, displayed in the $\hat{\vec{Q}}$ representation, and with associated eigenvalues $\vec{x}\pm\frac{\hbar}{2}\vec{y}$. As expected, the previous result means that the unitary transformation is mapped by the generalized Weyl–Wigner map to a phase space coordinate transformation.

IV. COVARIANT STAR PRODUCT

The new Weyl–Wigner map yields a new star product through the definition

$$W'_{(Q,P)}(\hat{A}\cdot\hat{B})=W'_{(Q,P)}(\hat{A})*'_{(Q,P)}W'_{(Q,P)}(\hat{B});\quad \forall\hat{A},\hat{B}\in\hat{\mathcal{A}}(\mathcal{H}), \tag{37}$$

and one immediately recognizes that the new product satisfies

$$W'_{(Q,P)}(\hat{A})*'_{(Q,P)}W'_{(Q,P)}(\hat{B})=W'_{(Q,P)}(\hat{A}\hat{B})=W_{(q,p)}(\hat{A}\hat{B})=W_{(q,p)}(\hat{A})*_{(q,p)}W_{(q,p)}(\hat{B}). \tag{38}$$

If $W_{(q,p)}(\hat{A})=A(\vec{q},\vec{p})$, then $W'_{(Q,P)}(\hat{A})=A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))=A'(\vec{Q},\vec{P})$ and thus

$$A'(\vec{Q},\vec{P})*'_{(Q,P)}B'(\vec{Q},\vec{P})=A(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))*_{(q,p)}B(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))\quad \forall A,B\in\mathcal{A}(T^*M). \tag{39}$$

The former result immediately implies that the new product is also a noncommutative, associative product for the algebra of functions over the classical phase space. Moreover, using the new product we can define a new bracket (named generalized Moyal bracket) alternative to the standard Moyal bracket:

$$[A,B]_{M'_{(Q,P)}}=\frac{1}{i\hbar}(A*'_{(Q,P)}B-B*'_{(Q,P)}A). \tag{40}$$

It follows from Eq. (39) that this is also a Lie bracket.

Neither the new star product nor the new Moyal bracket display the same functional structure as the standard ones $*_{(Q,P)}$ and $[,]_{M_{(Q,P)}}$. The aim of the rest of this section is to derive the explicit form of the new product and in the sequel of the new bracket from the generalized Weyl–Wigner map. Let us start by introducing the notation:

$$\hat{O}^k=\hat{p}_k, \quad k=1,\ldots,N; \quad \hat{O}'^k=\hat{P}_k, \quad k=1,\ldots,N;$$

$$\hat{O}^k=\hat{q}_{k-N}, \quad k=N+1,\ldots,2N; \quad \hat{O}'^k=\hat{Q}_{k-N}, \quad k=N+1,\ldots,2N;$$

and the symbols $O^k\equiv W_{(q,p)}(\hat{O}^k)$, $O'^k\equiv W_{(Q,P)}(\hat{O}'^k)$. Consider the two following operators displayed in the generalized Weyl order (sum over repeated indices is understood):

$$\begin{aligned}\hat{A}_{W'(Q,P)}&=\hat{A}'(\hat{\vec{Q}},\hat{\vec{P}})=\int d^{2N}\vec{a}\,\alpha(\vec{a})e^{ia_k\hat{O}^k(\hat{O}'^s)},\\ \hat{B}_{W'(Q,P)}&=\hat{B}'(\hat{\vec{Q}},\hat{\vec{P}})=\int d^{2N}\vec{b}\,\beta(\vec{b})e^{ib_l\hat{O}^l(\hat{O}'^r)},\end{aligned} \tag{41}$$

where $\vec{a}=(a_1,\ldots,a_{2N})$, $\vec{b}=(b_1,\ldots,b_{2N})$. Let us then calculate $W'_{(Q,P)}(\hat{A}\cdot\hat{B})$ explicitly and express the result in terms of the symbols $A'(\vec{Q},\vec{P})=W'_{(Q,P)}(\hat{A})$ and $B'(\vec{Q},\vec{P})=W'_{(Q,P)}(\hat{B})$:

$$\begin{aligned}W'_{(Q,P)}(\hat{A}\cdot\hat{B})&=\int d^{2N}\vec{a}d^{2N}\vec{b}\,\alpha(\vec{a})\beta(\vec{b})W'_{(Q,P)}\{e^{ia_k\hat{O}^k(\hat{O}'^s)}\cdot e^{ib_l\hat{O}^l(\hat{O}'^r)}\}\\ &=\int d^{2N}\vec{a}d^{2N}\vec{b}\,\alpha(\vec{a})\beta(\vec{b})W_{(q,p)}\{e^{ia_k\hat{O}^k(O'^s)}\cdot e^{ib_l\hat{O}^l(O'^r)}\}\\ &=\int d^{2N}\vec{a}d^{2N}\vec{b}\,\alpha(\vec{a})\beta(\vec{b})[e^{ia_kO^k(O'^s)}]*_{(q,p)}[e^{ib_lO^l(O'^r)}].\end{aligned} \tag{42}$$

Using the explicit expression of the $(\vec{q},\vec{p})$ star product in Eq. (5), we obtain the following expansion in powers of $\hbar$:

$$W'_{(Q,P)}(\hat{A}\cdot\hat{B})=\sum_{k=0}^{\infty}\frac{1}{k!}\left(\frac{i\hbar}{2}\right)^k\int d^{2N}\vec{a}d^{2N}\vec{b}\,\alpha(\vec{a})\beta(\vec{b})[e^{ia_tO^t(O'^s)}]\hat{\mathcal{J}}_k[e^{ib_lO^l(O'^r)}], \tag{43}$$

where

$$\hat{\mathcal{J}}_k=\overleftarrow{\partial}_{i_1}\cdots\overleftarrow{\partial}_{i_k}J^{i_1j_1}_{(q,p)}\cdots J^{i_kj_k}_{(q,p)}\vec{\partial}_{j_1}\cdots\vec{\partial}_{j_k}. \tag{44}$$

At this point we recall that the phase space is assumed to have the structure of a flat manifold and introduce the $2N\times 2N$ "Euclidean" metric,

$$(g_{ij})=\begin{pmatrix}\alpha 1_{N\times N} & 0_{N\times N}\\ 0_{N\times N} & \beta 1_{N\times N}\end{pmatrix}, \tag{45}$$

and the associated covariant derivative ∇_i,

$$\begin{aligned}\nabla_iA&=\partial_iA,\\ \nabla_i\nabla_jA&=\partial_i\partial_jA-\Gamma^k_{ij}\partial_kA, \quad i,j,k=1,\ldots,2N,\end{aligned} \tag{46}$$

where the Christoffel symbols Γ^k_{ij} are fully determined by the metric:

$$\Gamma^{i}_{jk}=\tfrac{1}{2}g^{il}(\partial_k g_{lj}+\partial_j g_{lk}-\partial_l g_{jk}),\quad i,j,k=1,\ldots,2N. \tag{47}$$

Obviously, in the coordinates $(\vec{q},\vec{p})$ we have $\Gamma^{i}_{jk}=0$, $\forall i,j,k=1,\ldots,2N$ and thus $\nabla_i=\partial_i$. (α and β are arbitrary constants introduced to ensure the correct dimensions.)

Under the general coordinate transformation $O^i\to O^i(O'^s)$ $(i=1,\ldots,2N)$ the symplectic matrix and the covariant derivative transform according to

$$J'^{ij}_{(Q,P)}=\frac{\partial O'^{i}}{\partial O^{k}}\frac{\partial O'^{j}}{\partial O^{l}}J^{kl}_{(q,p)}=\{O'^{i},O'^{j}\}_{(q,p)}=O'^{i}\hat{\mathcal{J}}_{(q,p)}O'^{j}, \tag{48}$$

$$\Gamma'^{i}_{jk}=\Gamma^{m}_{bc}\frac{\partial O'^{i}}{\partial O^{m}}\frac{\partial O^{b}}{\partial O'^{j}}\frac{\partial O^{c}}{\partial O'^{k}}+\frac{\partial O'^{i}}{\partial O^{b}}\frac{\partial^2 O^{b}}{\partial O'^{j}\partial O'^{k}}=\frac{\partial O'^{i}}{\partial O^{b}}\frac{\partial^2 O^{b}}{\partial O'^{j}\partial O'^{k}}. \tag{49}$$

Moreover, the terms $[e^{ia_tO^t(O'^s)}]\hat{\mathcal{J}}_k[e^{ib_lO^l(O'^r)}]$ are scalars and thus are left invariant:

$$\begin{aligned}&[e^{ia_tO^t(O'^s)}]\overleftarrow{\partial}_{i_1}\cdots\ \overleftarrow{\partial}_{i_k}J^{i_1j_1}_{(q,p)}\ \cdots\ J^{i_kj_k}_{(q,p)}\vec{\partial}_{j_1}\cdots\ \vec{\partial}_{j_k}[e^{ib_lO^l(O'^r)}]\\&\quad=[e^{ia_tO^t(O'^s)}]\overleftarrow{\nabla}'_{i_1}\cdots\ \overleftarrow{\nabla}'_{i_k}J'^{i_1j_1}_{(Q,P)}\ \cdots\ J'^{i_kj_k}_{(Q,P)}\vec{\nabla}'_{j_1}\ \cdots\ \vec{\nabla}'_{j_k}[e^{ib_lO^l(O'^r)}],\end{aligned} \tag{50}$$

where the new covariant derivative ∇' is given by

$$\begin{aligned}&\nabla'_iA=\partial'_iA,\\&\nabla'_i\nabla'_jA=\partial'_i\partial'_jA-\Gamma'^{k}_{ij}\partial'_kA,\quad \partial'_i=\partial/\partial O'^{i};\quad i,j,k=1,\ldots,2N.\end{aligned} \tag{51}$$

Substituting the result (50) in Eq. (43) and taking into account (41), it is trivial to obtain $W'_{(Q,P)}(\hat{A}\cdot\hat{B})=W'_{(Q,P)}(\hat{A})*'_{(Q,P)}W'_{(Q,P)}(\hat{B})$ where the new star product is given by

$$A'(\vec{Q},\vec{P})*'_{(Q,P)}B'(\vec{Q},\vec{P})=A'(\vec{Q},\vec{P})e^{(i\hbar/2)\,\overleftarrow{\nabla}'_iJ'^{ij}_{(Q,P)}\vec{\nabla}'_j}B'(\vec{Q},\vec{P}), \tag{52}$$

and we recovered the covariant formulation of the star product first introduced by Vey.[29] The covariant formulation ensured the invariant nature of the numerical value for the star-product of two observables in any coordinate system. However, in general, the functional form of the product is altered under an arbitrary coordinate transformation.

We should point out that our construction of the covariant star product being based upon a sympletic and a metric structure over the phase space manifold slightly differs from the construction of Bayen *et al.*, Fedosov and others, where the covariant star product is built upon a sympletic structure w and a Poisson connection ∇, satisfying $\nabla w=0$. This difference, however, is only apparent since our metric uniquely determines the Poisson connection and vice versa.

Finally, we can easily obtain the functional form of the new bracket: $[A',B']_{M'_{(Q,P)}}=(1/i\hbar)\,W'_{(Q,P)}([\hat{A},\hat{B}])$:

$$[A'(\vec{Q},\vec{P}),B'(\vec{Q},\vec{P})]_{M'_{(Q,P)}}=\frac{2}{\hbar}A'(\vec{Q},\vec{P})\sin\left(\frac{\hbar}{2}\overleftarrow{\nabla}'_iJ'^{ij}_{(Q,P)}\vec{\nabla}'_j\right)B'(\vec{Q},\vec{P}), \tag{53}$$

and if $(\vec{Q},\vec{P})$ is a set of canonical variables this is equally a deformation of the Poisson bracket:

$$[A',B']_{M'_{(Q,P)}}\equiv\frac{1}{i\hbar}(A'*'_{(Q,P)}B'-B'*'_{(Q,P)}A')=\{A',B'\}_{(Q,P)}+O(\hbar^2). \tag{54}$$

V. COVARIANT VEY QUANTUM MECHANICS AND DISCUSSION

The covariant formulation of Moyal quantum mechanics lives on the classical phase space T^*M with the structure of the tangent bundle of the configuration space, where a symplectic structure J^{ij} and a metric structure g_{ij} (or alternatively a Poisson connection) can be naturally defined.

The fundamental mathematical objects of the theory are the Wigner distribution function $f'_W(\vec{Q},\vec{P};t)$ and the observables $A'(\vec{Q},\vec{P})$. They all are scalar functions over (T^*M,J^{ij},g_{ij}), and are related with the mathematical objects of standard operator quantum mechanics through the generalized Weyl–Wigner map: $f'_W(\vec{Q},\vec{P};t)=(1/2\pi\hbar)\,W'_{(Q,P)}(|\psi(t)\rangle\langle\psi(t)|)$ and $A'(\vec{Q},\vec{P};t)=W'_{(Q,P)}(\hat{A})$. The time evolution of the Wigner function is given by the dynamical equation:

$$\dot{f}'_W=[H',f'_W]_{M'_{(Q,P)}}, \tag{55}$$

which transforms covariantly under arbitrary phase space difeomorphisms yielding, in any coordinates, identical mathematical solutions and thus identical physical predictions.

Finally, the covariant form of Eqs. (7) and (8) yield the physical relevant predictions. The Moyal star-genvalue equation can be obtained, through the Weyl–Wigner map, from the standard operator eigenvalue equation: $\hat{A}|\psi_a^n\rangle\langle\psi_a^n|=a|\psi_a^n\rangle\langle\psi_a^n|$ (where n is the degeneracy index). We follow the same procedure but use the generalized Weyl–Wigner map and obtain

$$A'(\vec{Q},\vec{P})*'_{(Q,P)}g_a'^n(\vec{Q},\vec{P})=ag_a'^n(\vec{Q},\vec{P}). \tag{56}$$

It is trivial to check that $g_a'^n(\vec{Q},\vec{P})=g_a^n(\vec{q}(\vec{Q},\vec{P}),\vec{p}(\vec{Q},\vec{P}))$ where $g_a^n(\vec{q},\vec{p})$ is the solution of the original star-genvalue equation. Futhermore, the probabilistic functionals are just the coordinate transform of the original ones:

$$P(A'(\vec{Q},\vec{P};t)=a)=\sum_n\int d^N\vec{Q}\int d^N\vec{P}(\det J'^{ij}_{(Q,P)})^{-1/2}g_a'^n(\vec{Q},\vec{P})f'_W(\vec{Q},\vec{P};t), \tag{57}$$

and finally the average value prediction is also trivially covariantized:

$$\langle A'(\vec{Q},\vec{P};t)\rangle=\int d^N\vec{Q}\int d^N\vec{P}(\det J'^{ij}_{(Q,P)})^{-1/2}A'(\vec{Q},\vec{P})f'_W(\vec{Q},\vec{P};t). \tag{58}$$

The covariant formulation of phase space quantum mechanics is a familiar field of mathematical physics. The invariance properties of the theory are well studied even for the case of nonflat sympletic manifolds. The main point of this work was not to derive these results once again but to focus on the relation between standard operator quantum mechanics and phase space quantum mechanics. Such a relation given by the generalized Weyl–Wigner map provided a new point of departure to derive the covariant generalization of phase space quantum mechanics and clarifies the nature of the invariance properties of the theory.

Let us then summarize our results: we presented an original generalized (covariant) formulation of the Weyl-order operator prescription and of the Weyl–Wigner map yielding the entire structure of Vey quantum mechanics directly from standard operator quantum mechanics. All key ingredients of the theory were derived in this fashion, thus casting Vey quantum mechanics at the same level of completeness as Moyal quantum mechanics. Furthermore, we studied the action of standard operator transformations in the Moyal formalism and concluded that through the generalized Weyl–Wigner map these transformations can be implemented as phase space coordinate transformations in the Moyal idiom. It is now easy to realize that the group of ''canonical'' transformations of Vey quantum mechanics (those that preserve the bracket structure) is the subgroup of the symplectic transformations which are also isometries, i.e., the coordinate transformations $O^i\rightarrow O^i(O'^s)$ such that

$$J'^{ij}_{(Q,P)}=\frac{\partial O'^{i}}{\partial O^{k}}\frac{\partial O'^{j}}{\partial O^{l}}J^{kl}_{(q,p)}=J^{ij}_{(q,p)},$$
$$\Gamma'^{i}_{jk}=\frac{\partial O'^{i}}{\partial O^{b}}\frac{\partial^{2}O^{b}}{\partial O'^{j}\partial O'^{k}}=0, \tag{59}$$

and notice that in the limit $\hbar\to 0$ the requirement on the isometry character of the canonical transformations disappears, as it should, and we recover the standard sympletic group of classical mechanics.

Finally, let us make a small remark concerning possible future applications of the generalized Weyl–Wigner map. Recently there has been a considerable interest in developing a fully classical interpretation for Moyal dynamics.[14,15,19] This is a difficult task for several reasons of which the most important are that Moyal dynamics is nonlocal and there is no general criterion to understand what is meant by ''classical.'' Very recently, however, the authors presented a proposal for a classicality criterion and proved that it is fully compatible with the Weyl–Wigner map.[18,19] One of the problems that was left unsolved was how to understand the highly nonclassical behavior of an allegedly Moyal classical dynamics, under the action of canonical transformations. This problem has been previously considered in Refs. 14 and 15 using an approach based on a privileged set of observables.

We may now expect that if the results of Ref. 19 (concerning the compatibility between the classicality criteria and the Weyl–Wigner map) turn out to be extendable to the covariant Weyl–Wigner map, then they will most likely open the path for a consistent classical interpretation of the action of canonical transformations in Moyal dynamics. This will be the subject of a future work.[35]

VI. EXAMPLE

To illustrate some of the features of the formalism let us consider the system of two interacting particles described by the Hamiltonian

$$\hat{H}=\frac{\hat{p}^{2}}{2M}+\frac{\hat{y}^{2}}{2m}+k\hat{q}\hat{y}^{2}, \tag{60}$$

where $(\hat{q},\hat{p})$ are the fundamental variables of the particle of mass M, $(\hat{x},\hat{y})$ are the ones of the particle of mass m and k is a coupling constant.

A. Standard description in the original variables

In the Heisenberg picture the time evolution of the former system is given by

$$\hat{q}(t)=\hat{q}+\frac{\hat{p}}{M}t-\frac{k}{2M}\hat{y}^{2}t^{2},$$
$$\hat{p}(t)=\hat{p}-k\hat{y}^{2}t,$$
$$\hat{x}(t)=\hat{x}+\left\{\frac{\hat{y}}{m}+2k\hat{q}\hat{y}\right\}t+\frac{k}{M}\hat{p}\hat{y}t^{2}-\frac{k^{2}}{3M}\hat{y}^{3}t^{3}, \tag{61}$$
$$\hat{y}(t)=\hat{y}.$$

The standard Weyl–Wigner transform yields the Moyal description of the system. The Hamiltonian is trivially obtained,

$$H=W_{(q,x,p,y)}(\hat{H})=\frac{p^{2}}{2M}+\frac{y^{2}}{2m}+kqy^{2}, \tag{62}$$

and the Moyal time evolution of the system is given by the dynamical equations

$$\dot{A}=[A,H]_{M_{(q,x,p,y)}}, \tag{63}$$

which yield the following solutions (to make it simpler let us concentrate on the dynamics of the particle of mass M):

$$\begin{aligned} q(t)&=q(0)+\frac{p(0)}{M}t-\frac{k}{2M}y(0)^2t^2,\\ p(t)&=p(0)-ky(0)^2t. \end{aligned} \tag{64}$$

Notice that the same predictions can be obtained by applying the Weyl–Wigner map to the solutions (61).

B. Canonical transformation and the standard description in the new variables

Let us now consider the canonical transformation:

$$\begin{aligned} \hat{q}&=\hat{q},\quad \hat{x}=\ln\hat{Q},\\ \hat{p}&=\hat{p},\quad \hat{y}=\tfrac{1}{2}(\hat{Q}\hat{P}+\hat{P}\hat{Q}). \end{aligned} \tag{65}$$

In the new variables $\hat{H}$ takes the form

$$\hat{H}=\frac{\hat{p}^2}{2M}+\frac{(\hat{Q}\hat{P}+\hat{P}\hat{Q})^2}{8m}+\frac{k}{4}\hat{q}(\hat{Q}\hat{P}+\hat{P}\hat{Q})^2, \tag{66}$$

and it yields the Heisenberg picture time evolution (still just for the particle of mass M):

$$\begin{aligned} \hat{q}(t)&=\hat{q}+\frac{\hat{p}}{M}t-\frac{k}{8M}(\hat{Q}\hat{P}+\hat{P}\hat{Q})^2t^2\\ \hat{p}(t)&=\hat{p}-\frac{k}{4}(\hat{Q}\hat{P}+\hat{P}\hat{Q})^2t \end{aligned} \tag{67}$$

To obtain the Moyal formulation of the system in the variables (q,Q,p,P) the first step is to use the standard Weyl–Wigner map to get the phase space representation of the transformation (65):

$$\begin{aligned} q&=W_{(q,Q,p,P)}(\hat{q})=q,\quad x=W_{(q,Q,p,P)}(\hat{x}(\hat{Q},\hat{P}))=\ln Q,\\ p&=W_{(q,Q,p,P)}(\hat{p})=p,\quad y=W_{(q,Q,p,P)}(\hat{y}(\hat{Q},\hat{P}))=QP. \end{aligned} \tag{68}$$

We then express the Hamiltonian using the standard Weyl order prescription:

$$\hat{H}_{W(q,Q,p,P)}=\frac{\hat{p}^2}{2M}+\frac{(\hat{P}^2\hat{Q}^2)_S}{2m}+k\hat{q}(\hat{Q}^2\hat{P}^2)_S+\frac{k}{4}\hbar^2\hat{q}+\frac{\hbar^2}{8m}, \tag{69}$$

where we used the fact that $\frac{1}{4}(\hat{Q}\hat{P}+\hat{P}\hat{Q})^2_{W(q,Q,p,P)}=(\hat{P}^2\hat{Q}^2)_S+\hbar^2/4$ (the subscripted "S" standing for the full symmetrization of the operator), and so $\frac{1}{4}(\hat{Q}\hat{P}+\hat{P}\hat{Q})^2$ can be expressed in the standard Weyl order [Eq. (25)] by making $\alpha(a,b,c,d)=\delta(a)\delta(b)\{\delta''(c)\delta''(d)+\hbar/4\delta(c)\delta(d)\}$, where a, b, c, d are the integration variables associated to the fundamental operatores $\hat{q},\hat{p},\hat{Q},\hat{P}$, respectively. The standard Weyl–Wigner transform of $\hat{H}$ is thus

$$H = W_{(q,Q,p,P)}(\hat{H}) = \frac{p^2}{2M} + \frac{P^2Q^2}{2m} + kqQ^2P^2 + \frac{k}{4}\hbar^2 q + \frac{\hbar^2}{8m}. \tag{70}$$

Finally, the Moyal dynamical equations in the variables (q,Q,p,P) yield

$$q(t) = q(0) + \frac{p(0)}{M}t - \frac{k}{2M}Q(0)^2P(0)^2t^2 - \frac{k\hbar^2}{8M}t^2$$

$$p(t) = p(0) - kQ(0)^2P(0)^2t - \frac{k\hbar^2}{4}t^2. \tag{71}$$

Notice that equivalent results can be obtained by applying the Weyl–Wigner transform to the time evolution operator equations (67). Furthermore, we realize that the transformation (65) does not act as a coordinate transformation in the Moyal formalism. Taking, for instance, the Hamiltonian, we have $H(q,p,x(Q,P),y(Q,P)) \neq W_{(q,Q,p,P)}(\hat{H})$, the left-hand side being given by Eq. (62) and the right-hand side by Eq. (70). Consequently, the two phase space orbits [Eqs. (64) and (71)] are not the coordinate transformation of each other.

C. Covariant formulation

Finally, let us use the generalized Weyl–Wigner map. In the generalized Weyl order prescription Eq. (29), we make $\alpha(a,b,c,d) = -\delta(a)\delta(b)\delta(c)\delta''(d)$, where, this time, a,b,c,d are the integration variables associated to the fundamental operators $\hat{q},\hat{p},\hat{x}(\hat{Q},\hat{P}),\hat{y}(\hat{Q},\hat{P})$, and we obtain

$$\tfrac{1}{4}(\hat{Q}\hat{P}+\hat{P}\hat{Q})^2_{W'(q,Q,p,P)} = \tfrac{1}{4}(\hat{Q}\hat{P}\hat{Q}\hat{P} + \hat{Q}\hat{P}^2\hat{Q} + \hat{P}\hat{Q}^2\hat{P} + \hat{P}\hat{Q}\hat{P}\hat{Q}), \tag{72}$$

and thus

$$H'(q,Q,p,P) = W'_{(q,Q,p,P)}(\hat{H}) = \frac{p^2}{2M} + \frac{Q^2P^2}{2m} + kqQ^2P^2, \tag{73}$$

which, as expected, is the coordinate transformation of the observable H given by Eq. (62). The new star product and the new bracket are given by Eqs. (52) and (53), respectively, where $J'^{ij}_{(Q,P)} = J^{ij}_{(q,p)}$ and the covariant derivatives are associated to the Christoffel symbols:

$$\Gamma'^{1}_{11} = -1/Q; \quad \Gamma'^{2}_{11} = P/Q^2; \quad \Gamma'^{2}_{12} = \Gamma'^{2}_{21} = 1/Q, \tag{74}$$

all the others being zero (we used the notation: $O^1 = x$; $O^2 = y$; $O'^1 = Q$; $O'^2 = P$; $O'^3 = O^3 = q$; $O'^4 = O^4 = p$). Notice that using the new product we can go back and obtain the Hamiltonian H' through a slightly different procedure, by making

$$\begin{aligned} &W'_{(q,Q,p,P)}\{\tfrac{1}{2}(\hat{Q}\hat{P}+\hat{P}\hat{Q})\tfrac{1}{2}(\hat{Q}\hat{P}+\hat{P}\hat{Q})\} \\ &\quad = W'_{(q,Q,p,P)}\{\tfrac{1}{2}(\hat{Q}\hat{P}+\hat{P}\hat{Q})\} *'_{(q,Q,p,P)} W'_{(q,Q,p,P)}\{\tfrac{1}{2}(\hat{Q}\hat{P}+\hat{P}\hat{Q})\} \\ &\quad = QP *'_{(q,Q,p,P)} QP = Q^2P^2, \end{aligned} \tag{75}$$

where in the last step we used the explicit expression for the new star product (52) and (74). It is now easy to check that the generalized Moyal dynamical equations, $\dot{O}'^i = [O'^i, H']_{M'_{(q,Q,p,P)}}$, yield solutions that are just the coordinate transformation of the original ones (64). Equivalent results can obviously be obtained by applying the generalized Weyl–Wigner map to the operator time evolution equations (67).

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Spherically symmetric solutions of the sixth order SU(*N*) Skyrme models

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Following the construction described by Ioannidou *et al.* [J. Math. Phys. **40**, 6353 (1999)], we use the rational map ansatz to construct analytically some topologically nontrivial solutions of the generalized SU(3) Skyrme model defined by adding a sixth order term to the usual Lagrangian. These solutions are radially symmetric and some of them can be interpreted as bound states of Skyrmions. The same ansatz is used to construct low-energy configuration of the SU(N) Skyrme model.
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I. INTRODUCTION

The Skyrme model[1] is widely accepted as an effective theory to describe the low-energy properties of nucleons. It was indeed shown[2–4] that in the large N_c limit, the Skyrme model is the low-energy limit of QCD. The classical static solutions of the model describe the bound states of nucleons and every configuration is characterized by a topological charge which, following Skyrme's idea, is interpreted as the baryon charge.

The Skyrme model can be used to predict the properties of the nucleons within 10% to 20%.[3,4] To improve these phenomenological predictions various extensions of the model have been proposed mostly by adding higher order terms[5–8] or extra fields[9] to the Lagrangian.

The study of the classical solutions of the Skyrme model has been done mostly using numerical methods, but recently Houghton *et al.*[10] showed that the classical solutions of the SU(2) model can be well approximated by using an ansatz that involves the harmonic maps from S^2 to S^2. The harmonic map describes the angular distribution of the solution while a profile function describes its radial distribution. This construction was later generalized[11] for the SU(N) model using harmonic maps from S^2 to CP^{N-1}. Moreover, it was shown that using a further generalization of this ansatz one can construct exact spherically symmetric solutions of the SU(N) Skyrme model.

The same method was also used in Ref. 12 to construct solutions of another SU(N) fourth order Skyrme model. In this article, we use the same generalized ansatz to construct solutions of the sixth order SU(3) Skyrme model and low-energy configurations of the SU(N) models defined in Ref. 13.

II. THE SIXTH ORDER SKYRME MODEL

The Skyrme model is described by an SU(N) valued field $U(\vec{x},t)$ which, to ensure finiteness of the energy, is required to satisfy the boundary condition $U\rightarrow I$ as $|\vec{x}|\rightarrow\infty$, where I is the unit matrix. This boundary condition implies that the three dimensional Euclidean space on which the model is defined can be compactified into S^3 and, as a result, the Skyrme field U corresponds to mappings from S^3 into SU(N). As $\pi_3(\mathrm{SU}(N))=Z$ each configuration is characterized by its winding number, or topological charge, which can be obtained explicitly by evaluating the expression

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$$B=\frac{1}{24\pi^2}\int_{R^3} d\vec{x}^3 \varepsilon^{ijk}\, Tr(R_i R_j R_k), \tag{1}$$

where $R_\mu=(\partial_\mu U)U^{-1}$ is the right chiral current. Skyrme's idea was to interpret the winding number associated with these topologically nontrivial mappings as the baryon charge.

The generalized sixth order Skyrme model is defined by the Lagrangian

$$E=-\frac{1}{12\pi^2}\int d\vec{x}^3\left(\frac{1}{2}TrR_i^2+\frac{1-\lambda}{16}Tr[R_i,R_j]^2+\frac{1}{96}\lambda Tr[R_i,R_j][R_j,R_k][R_k,R_i]\right), \tag{2}$$

where this parametrization of the model is chosen such that $\lambda\in[0,1]$ is a mixing parameter between the Skyrme term and the sixth order term: when $\lambda=0$ the model reduces to the usual pure Skyrme model while for $\lambda=1$ the Skyrme term vanishes and the model reduces to what we refer to in what follows as the pure Sk6 model.

The Euler–Lagrange equations derived from (2) for the static solutions are given by

$$\partial_i(R_i-\tfrac{1}{4}(1-\lambda)[R_j,[R_j,R_i]]-\tfrac{1}{16}\lambda[R_j,[R_j,R_k][R_k,R_i]])=0, \tag{3}$$

and the following inequality holds for every configuration:

$$E\geqslant\sqrt{1-\lambda}B. \tag{4}$$

The multi-Skyrmion solutions of the SU(2) Skyrme model have been studied in Ref. 13 where it was shown that they have the same symmetry as the pure Skyrme model. It was also shown that the harmonic map ansatz gives a good approximation to the solutions.

In the next section we describe the harmonic map ansatz. In the third section we prove that due to a constraint coming from the sixth order term, the multi-projector harmonic map ansatz provides exact solutions only for the SU(3) generalized model. We then show that one can nevertheless use the ansatz to construct low-energy configurations of the SU(N) models. In the fourth section we look at these configurations for the SU(4) model, while in the last section we look at some special ansatz for the SU(N) model.

III. HARMONIC MAP ANSATZ

The rational map ansatz, introduced by Houghton *et al.*,[10] is a generalization of the hedgehog ansatz found by Skyrme,[1] to approximate multi-Skyrmion solution of the SU(2) model. The ansatz was later generalized by Ioannidou *et al.*[14] to approximate solutions of the SU(N) Skyrme model using harmonic maps from S^2 into CP^{N-1}. This generalized ansatz is given by

$$U(r,\theta,\varphi)=e^{2if(r)(P(\theta,\varphi)-I/N)}=e^{-2if(r)/N}(I+(e^{2if(r)}-1)P(\theta,\varphi)), \tag{5}$$

where r,θ and φ are the usual polar coordinates. The profile function $f(r)$ must satisfy the boundary conditions $f(0)=\pi$ and $\lim_{r\to\infty}f(r)=0$ and $P(\theta,\varphi)$ is a projector in C^N which must be a harmonic map from S^2 into CP^{N-1} or equivalently a classical solution of the two dimensional CP^{N-1} σ model. These solutions are well known[15,16] and to construct them it is convenient to introduce the complex coordinate $\xi=\tan(\theta/2)e^{i\varphi}$ which corresponds to the stereographic projection of the unit sphere onto the complex plane.

In these coordinates, P must satisfy the equation

$$P\frac{\partial P}{\partial\xi}=0, \tag{6}$$

and the solutions of that equation are given by any projector of the form

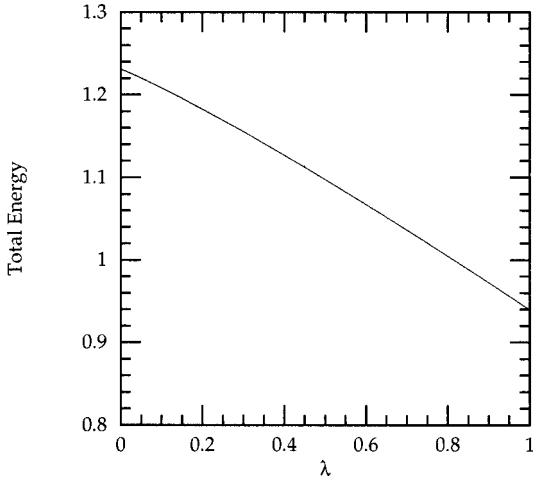

FIG. 1. Total energy of the 1 Skyrmion solution.

$$P(f)=\frac{h\otimes h^{\dagger}}{|h|^2}, \tag{7}$$

where $h\in C^N$ is holomorphic

$$\frac{\partial h}{\partial \bar{\xi}}=0. \tag{8}$$

The topological charge for the ansatz (5), with the prescribed boundary conditions for $f(r)$, is given by the winding number of the $S^2\to CP^{N-1}$. This winding number is itself given by the degree of the harmonic function h[15,16] which must then be a rational function of ξ.

To approximate a solution, one plugs the ansatz (5) into the energy (2) and notices that if P satisfies (6), the integration over the polar angles and the radius decouple. One then has to minimize the integral over the polar angles of an expression which depends only on P. Taking for P the most general harmonic map of the desired degree, one then has to find the parameters of the general map which minimize that integral. Having done this, the profile function f is obtained by solving the Euler Lagrange equation derived from the effective energy.

A special case of this construction is the so-called hedgehog ansatz for the SU(2) model corresponding to one Skyrmion. In this case, we have $h=(1,\xi)^t$ and after inserting (7) into (2) the energy reduces to

$$E=\frac{1}{3\pi}\int dr\left(f_r^2 r^2+2\sin^2 f\,(1+(1-\lambda)f_r^2)+(1-\lambda)\frac{\sin^4 f}{r^2}+\lambda\frac{\sin^4 f}{r^2}f_r^2\right), \tag{9}$$

and the equation for f is given by

$$f_{rr}\left(1+2\,(1-\lambda)\frac{\sin^2 f}{r^2}+\lambda\frac{\sin^4 f}{r^4}\right)+\frac{2}{r}f_r\left(1-\lambda\frac{\sin^4 f}{r^4}\right)$$
$$+\frac{\sin 2g}{r^2}\left((1-\lambda)f_r^2-1+\frac{\sin^2 f}{r^2}(\lambda f_r^2-1+\lambda)\right)=0. \tag{10}$$

This actually corresponds to an exact solution of the model and it is radially symmetric. In Fig. 1 we present the λ dependence of the energy and in Fig. 2 we show the profile function f and the energy density for the pure Skyrme model, $\lambda=0$, and the pure Sk6 model, $\lambda=1$.

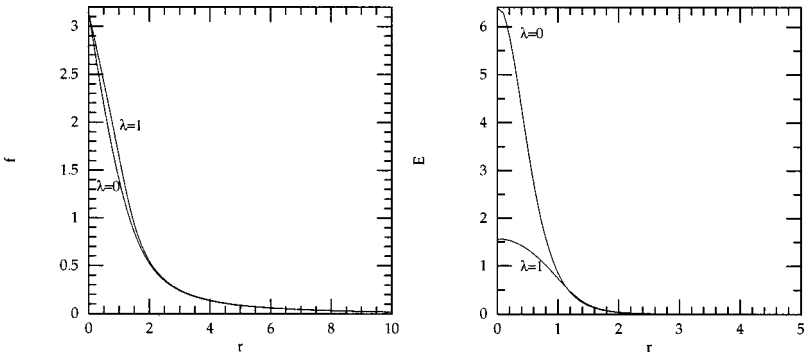

FIG. 2. Function profile f and energy density for the 1 Skyrmion solution of the pure Skyrme model, $\lambda=0$, and the pure Sk6 model, $\lambda=1$.

IV. SPHERICALLY SYMMETRIC SOLUTIONS FOR THE SU(N) MODEL

In this section we will follow the construction described in Ref. 14, to attempt to construct solutions of the extended SU(N) Skyrme model using a generalization of the harmonic map ansatz (5).

To build the new ansatz we need to introduce an operator P_+ which acts on any complex vector $u\in C^N$ and is defined as

$$P_+u=\partial_\xi u-u\,\frac{u^\dagger\,\partial_\xi u}{|u|^2}. \tag{11}$$

Taking a holomorphic vector $h(\xi)$ we then define $P_0^+h=h$ and by induction $V_k=P_+^k h=P_+(P_+^{k-1}h)$. These N vectors are mutually orthogonal[16] and so the corresponding projectors

$$P_k=P(P_+^k h)=\frac{P_+^k h(P_+^k h)^\dagger}{|P_+^k h|^2}\quad k=0,\ldots,N-1, \tag{12}$$

satisfy the orthogonality relations

$$\begin{aligned} P_kP_j&=\delta_{ij}P_k\,,\\ \sum_{k=0}^{N-1}P_k&=1, \end{aligned} \tag{13}$$

as well as other properties discussed in detail in Ref. 14.

The generalized harmonic map ansatz is then defined as

$$\begin{aligned} U&=\exp\left\{ig_0\left(P_0-\frac{I}{N}\right)+ig_1\left(P_1-\frac{I}{N}\right)-\ldots+ig_{N-2}\left(P_{N-2}-\frac{I}{N}\right)\right\}\\ &=e^{-ig_0/N}(I+A_0P_0)\,e^{-ig_1/N}(I+A_1P_1)\cdots e^{-ig_{N-2}/N}(I+A_{N-2}P_{N-2}), \end{aligned} \tag{14}$$

where $g_k(r)$ are $N-1$ profile functions and $A_k=e^{ig_k}-1$. Moreover, for the ansatz to be well defined, the profile functions $g_k(r)$ must be a multiple of 2π at the origin and at infinity.

To proceed with our construction, it is convenient to rewrite the Euler–Lagrange equations of the model (3) using the usual spherical coordinates

$$\partial_r\left\{r^2R_r+\frac{1-\lambda}{4}\left(A_{\theta r\theta}+\frac{1}{\sin^2\theta}A_{\varphi r\varphi}\right)+\frac{1}{16}\lambda\left[\frac{1}{\sin^2\theta}(B_{\theta\theta\varphi r\varphi}+B_{\varphi\varphi\theta r\theta})\right]\right\}$$
$$+\frac{1}{\sin\theta}\partial_\theta\left\{\sin\theta\left[R_\theta+\frac{1-\lambda}{4}\left(A_{r\theta r}+\frac{1}{r^2\sin^2\theta}A_{\varphi\theta\varphi}\right)\right]+\frac{\lambda}{16r^2\sin^2\theta}(B_{rr\varphi\theta\varphi}+B_{\varphi\varphi r\theta r})\right\}$$
$$+\frac{1}{\sin^2\theta}\partial_\varphi\left\{R_\varphi+\frac{1-\lambda}{4}\left(A_{r\varphi r}+\frac{1}{r^2}A_{\theta\varphi\theta}\right)+\frac{\lambda}{16r^2}(B_{rr\theta\varphi\theta}+B_{\theta\theta r\varphi r})\right\}=0, \tag{15}$$

where $A_{jij}\equiv[R_j,[R_i,R_j]]$ and $B_{jjkik}\equiv[R_j,[R_j,R_k][R_i,R_k]]$. It is fairly easy to show that

$$R_r=i\sum_{j=0}^{N-2}\dot g_j\left(P_j-\frac{I}{N}\right), \tag{16}$$

where $\dot g_j$ is the derivative of $g_j(r)$ with respect to r. Using the complex coordinates ξ and $\bar\xi$ introduced before we have

$$R_\xi=\sum_{i=1}^{N-1}[e^{i(g_i-g_{i-1})}-1]\frac{V_iV_{i-1}^\dagger}{|V_{i-1}|^2}, \tag{17}$$

and the derivatives with respect to θ and φ are given by

$$\partial_\theta=\frac{1+|\xi|^2}{2\sqrt{|\xi|^2}}(\xi\partial_\xi+\bar\xi\partial_{\bar\xi}),\quad \partial_\varphi=i(\xi\partial_\xi-\bar\xi\partial_{\bar\xi}). \tag{18}$$

Substituting the above into Eqs. (15) we get

$$\partial_r\left[r^2R_r+(1-\lambda)\frac{(1+|\xi|^2)^2}{8}(A_{\bar\xi r\xi}+A_{\xi r\bar\xi})\right]+\frac{(1+|\xi|^2)^2}{2}((R_{\bar\xi})_\xi+(R_\xi)_{\bar\xi})$$
$$+(1-\lambda)\frac{(1+|\xi|^2)^3}{8r^2}(\xi A_{\xi\xi\bar\xi}-\bar\xi A_{\bar\xi\xi\bar\xi})+(1-\lambda)\frac{(1+|\xi|^2)^4}{16r^2}([A_{\xi\xi\bar\xi}]_{\bar\xi}-[A_{\bar\xi\xi\bar\xi}]_\xi)$$
$$+(1-\lambda)\frac{(1+|\xi|^2)^2}{8}([A_{r\bar\xi r}]_\xi+[A_{r\xi r}]_{\bar\xi})+\frac{\lambda}{16}\left\{\partial_r\left[\frac{(1+|\xi|^2)^4}{4}(B_{\bar\xi\xi\bar\xi r\bar\xi}-B_{\xi\xi\bar\xi r\bar\xi})\right]\right.$$
$$+\frac{(1+|\xi|^2)^2}{4r^2}(\partial_{\bar\xi}[(1+|\xi|^2)^2B_{rr\xi\xi\bar\xi}]-\partial_\xi[(1+|\xi|^2)^2B_{rr\bar\xi\xi\bar\xi}])$$
$$+\frac{(1+|\xi|^2)^2}{2|\xi|^2r^2}\left(\xi\partial_\xi\left[\frac{(1+|\xi|^2)^2}{4|\xi|^2}(-\xi\xi\xi B_{\xi\xi r\xi r})\right]+\bar\xi\partial_{\bar\xi}\left[\frac{(1+|\xi|^2)^2}{4|\xi|^2}(-\overline{\xi\xi\xi}B_{\overline{\xi\xi r}\bar\xi r})\right]\right)$$
$$+\frac{(1+|\xi|^2)^2}{8r^2}(\partial_\xi[(1+|\xi|^2)^2(B_{\xi\bar\xi r\bar\xi r}+B_{\bar\xi\xi r\bar\xi r}-B_{\overline{\xi\xi}r\xi r})]+\partial_{\bar\xi}[(1+|\xi|^2)^2$$
$$\left.\times(-B_{\xi\xi r\bar\xi r}+B_{\xi\bar\xi r\xi r}+B_{\bar\xi\xi r\xi r})]\right)\Bigg\}=0. \tag{19}$$

In Ref. 14 it is shown that if one takes the special holomorphic vector

$$V_0=h=(h_0,h_1,\ldots,h_{N-1})^t, \tag{20}$$

where

$$h_k = \xi^k \sqrt{C_k^{N-1}} \tag{21}$$

and C_k^{N-1} denotes the binomial coefficients, then the terms in (19) coming from the usual Skyrme model, i.e., all the terms except the ones proportional to $\lambda/16$, are all proportional to $P_i - P_{i-1}$ and $P_i - I/N$. Using (13) one can get rid of the projector P_{N-1} and (19) will then be the sum of the $N-1$ terms $P_i - I/N$ for $i=0,\ldots,N-2$, with coefficients that depend only on r. This implies that the equations for the Skyrme model reduce to $N-1$ ordinary differential equations for the profile functions g_i and their solutions, if they exist, will provide us with exact solutions of the SU(N) Skyrme model.

In what follows we will show that the angular dependence of the terms proportional to λ in (19), i.e., the terms coming from the sixth order term, is also coming exclusively from the projectors $P_i - I/N$ or $P_i - P_{i-1}$, but that we have to impose an extra constraint on the profile functions g_i.

We start by noting that

$$[R_\xi, R_{\bar\xi}] = -\sum_{i=1}^{N-1} a_i^2 \frac{|V_i|^2}{|V_{i-1}|^2}\left(\frac{V_i V_i^\dagger}{|V_i|^2} - \frac{V_{i-1}V_{i-1}^\dagger}{|V_{i-1}|^2}\right), \tag{22}$$

$$[R_r, R_\xi] = i\sum_{i=1}^{N-1} (\dot g_i a_i - \dot g_{i-1} a_i)\frac{V_i V_{i-1}^\dagger}{|V_{i-1}|^2} = \sum_{i=1}^{N-1} K_i \frac{V_i V_{i-1}^\dagger}{|V_{i-1}|^2}, \tag{23}$$

$$[R_r, R_{\bar\xi}] = i\sum_{i=1}^{N-1} (\dot g_i a_i - \dot g_{i-1} a_i)\frac{V_{i-1} V_i^\dagger}{|V_{i-1}|^2} = \sum_{i=1}^{N-1} K_i \frac{V_{i-1} V_i^\dagger}{|V_{i-1}|^2}, \tag{24}$$

where $a_i = e^{i(g_i - g_{i-1})} - 1$. It is then straightforward to check that

$$B_{\bar\xi\bar\xi\bar\xi r\xi} - B_{\xi\bar\xi\bar\xi r\bar\xi} = \sum_{i=1}^{N-1}\left(b_i \frac{|V_{i-1}|^2}{|V_{i-2}|^2}\frac{|V_i|^2}{|V_{i-1}|^2} + c_i \frac{|V_i|^4}{|V_{i-1}|^4} + d_i \frac{|V_{i+1}|^2}{|V_i|^2}\frac{|V_i|^2}{|V_{i-1}|^2}\right)(P_i - P_{i-1}), \tag{25}$$

where b_i, c_i and d_i are functions of g_k only. However, as shown in Ref. 14, if V_0 is given by (20) and (21), then $|V_i|^2/|V_{i-1}|^2 \propto (1+|\xi|^2)^{-2}$ and thus

$$\frac{(1+|\xi|^2)^4}{4}(B_{\bar\xi\bar\xi\bar\xi r\xi} - B_{\xi\bar\xi\bar\xi r\bar\xi}) \propto (P_i - P_{i-1}). \tag{26}$$

Furthermore, we have

$$B_{r r \xi\bar\xi\bar\xi} = i\sum_{i=1}^{N-1}\left(e_i \frac{|V_i|^2}{|V_{i-1}|^2} + s_i \frac{|V_{i-1}|^2}{|V_{i-2}|^2}\right)\frac{V_i V_{i-1}^\dagger}{|V_{i-1}|^2} \tag{27}$$

with $e_i = e(g_i)$ and $s_i = s(g_i)$. But in Eq. (19) this term appears as

$$\partial_{\bar\xi}[(1+|\xi|^2)^2 B_{r r \xi\bar\xi\bar\xi}] = 2\bar\xi(1+|\xi|^2) B_{r r \xi\bar\xi\bar\xi} + (1+|\xi|^2)^2 \partial_{\bar\xi}(B_{r r \xi\bar\xi\bar\xi}). \tag{28}$$

Since $\partial_{\bar\xi}|V_i|^2/|V_{i-1}|^2 \propto -2\bar\xi(1+|\xi|^2)^{-3}$ the only parts of (28) that are nonzero are the ones that involve the derivatives of $V_i V_{i-1}^\dagger/|V_{i-1}|^2$ with respect to $\bar\xi$. Since it can be shown that the latter are proportional to $\Sigma_{i-1}^{N-1} C_i (1+|\xi|^2)^{-2}(P_i - P_{i-1})$ where $C_i = C(g_i)$, then one sees that the term that involves $B_{r r \xi\bar\xi\bar\xi}$ in (19) is proportional to $(P_i - P_{i-1})$.

Using similar arguments, it is easy to check that the terms involving $B_{r r \bar\xi\bar\xi\bar\xi}$, $B_{\xi\bar\xi r\bar\xi r}$, $B_{\bar\xi\xi r\bar\xi r}$, $B_{\bar\xi\bar\xi r\xi r}$, $B_{\xi\xi r\bar\xi r}$, $B_{\xi\bar\xi r\xi r}$ and $B_{\bar\xi\xi r\xi r}$ factorize in the same way.

There are a few terms in (19) which we still have to consider. They involve the expressions

$$B_{\xi\,\xi\,r\,\xi\,r}=\sum_{i=3}^{N-1}\,(a_iK_{i-1}K_{i-2}-a_{i-2}K_iK_{i-1})\,\frac{V_iV_{i-3}^{\dagger}}{|V_{i-3}|^2}, \tag{29}$$

$$B_{\overline{\xi}\,\xi\,r\,\overline{\xi}\,r}=\sum_{i=3}^{N-1}\,(a_iK_{i-1}K_{i-2}-a_{i-2}K_iK_{i-1}).\,\frac{V_{i-3}V_i^{\dagger}}{|V_{i-3}|^2}\,, \tag{30}$$

where $K_i=i(\dot{g}_ia_i-\dot{g}_{i-1}a_i)$. It is clear that these terms will always give a $\xi,\overline{\xi}$ dependence besides the projectors P_i and, hence, if we want (19) to reduce to $N-1$ equations that involve only the profile functions g_i, then we have to make sure that (29) and (30) vanish i.e., we must impose the conditions

$$a_iK_{i-1}K_{i-2}-a_{i-2}K_iK_{i-1}=0\;\;\Leftrightarrow\;\;\dot{g}_{i-2}-\dot{g}_{i-3}=\dot{g}_i-\dot{g}_{i-2}\,. \tag{31}$$

This last constraint, which is a result of the addition of the sixth order term, implies that we can only consider two profile functions g_0 and g_1 and that we should thus have only two equations. Unfortunately we have $N-1$ equations which are not compatible with each other. From this we see that the ansatz (5) will provide exact solutions of the generalized Skyrme model for the SU(2) and the SU(3) model only. For larger values of N, the ansatz will nevertheless give some low-energy radially symmetric configurations. The SU(2) case is nothing but the usual hedgehog ansatz and we will focus on the solutions of the SU(3) model in the next section.

In order to derive the equations for the profile functions, it is convenient to write the energy density of the model in terms of $(\xi,\overline{\xi})$:

$$\begin{aligned}E=-\frac{i}{12\pi^2}\int r^2dr\,d\xi d\overline{\xi}\,Tr\left(\frac{1}{(1+|\xi|^2)^2}R_r^2+\frac{1}{r^2}|R_\xi|^2+\frac{1-\lambda}{4r^2}[R_r,R_\xi][R_r,R_{\overline{\xi}}]\right.\\ \left.-(1-\lambda)\,\frac{(1+|\xi|^2)^2}{16r^4}[R_{\overline{\xi}},R_\xi]^2+\lambda\,\frac{(1+|\xi|^2)^2}{64r^4}[[R_r,R_{\overline{\xi}}],[R_r,R_\xi]][R_\xi,R_{\overline{\xi}}]\right).\end{aligned} \tag{32}$$

Defining

$$\begin{aligned}F_i&=g_i-g_{i+1}\quad\text{for}\quad i=0,\ldots,N-3,\\ F_{N-2}&=g_{N-2},\end{aligned} \tag{33}$$

as well as $W_i=(|V_i|^2/|V_{i-1}|^2)\,(1-\cos(F))$ and $W_{N-1}=(|V_{N-1}|^2/|V_{N-2}|^2)\,(1-\cos(g))$, the terms in the above expression can be rewritten as

$$Tr\,R_r^2=\frac{1}{N}\left(\sum_{i=0}^{N-2}\,\dot{g}_i\right)^2-\sum_{i=0}^{N-2}\,\dot{g}_i^2\,, \tag{34}$$

$$Tr|R_\xi|^2=-2\sum_{i=1}^{N-1}\,W_i\,, \tag{35}$$

$$Tr[R_r,R_\xi][R_r,R_{\overline{\xi}}]=-2\sum_{k=1}^{N-1}\,W_k\dot{F}_{k-1}^2\,, \tag{36}$$

$$Tr[R_{\overline{\xi}},R_\xi]^2=4\left(\,W_1^2+\sum_{i=1}^{N-2}\,(W_i-W_{i+1})^2+W_{N-1}^2\right), \tag{37}$$

$$Tr[[R_r,R_{\bar{\xi}}],[R_r,R_\xi][R_\xi,R_{\bar{\xi}}]]=4\left(\dot{F}_0^2W_1^2+\sum_{i=1}^{N-2}(\dot{F}_{i-1}W_i-\dot{F}_iW_{i+1})^2+\dot{F}_{N-2}^2W_{N-1}^2\right). \quad (38)$$

In Ref. 14 it was shown that

$$\frac{|V_k|^2}{|V_{k-1}|^2}=k(N-k)(1+|\xi|^2)^{-2}, \quad (39)$$

and from this we see that all the terms in (32) are proportional to $(1+|\xi|^2)^{-2}$ and that after integrating out the angular dependence the energy reduces to

$$\begin{aligned}E=\frac{1}{6\pi}\int r^2dr\Bigg\{&-\frac{1}{N}\left(\sum_{i=0}^{N-2}\dot{g}_i\right)^2+\sum_{i=0}^{N-2}\dot{g}_i^2+\frac{2}{r^2}\sum_{k=1}^{N-1}Z_k+\frac{(1-\lambda)}{2r^2}\sum_{k=1}^{N-1}(\dot{g}_k-\dot{g}_{k-1})^2Z_k\\&+\frac{(1-\lambda)}{4r^4}\left(Z_1^2+\sum_{k=1}^{N-2}(Z_k-Z_{k+1})^2+Z_{N-1}^2\right)\\&+\frac{\lambda}{16r^4}\left(\dot{F}_0^2Z_1^2+\sum_{k=1}^{N-2}(\dot{F}_{k-1}Z_k-\dot{F}_kZ_{k+1})^2+\dot{F}_{N-2}^2Z_{N-1}^2\right)\Bigg\}, \quad (40)\end{aligned}$$

where $Z_k=k(N-k)(1-\cos(F_{k-1}))$.

In Ref. 14 the fields F_i defined by (33) were used, and very special solutions were obtained by taking $F_0=F_1=\cdots=F_{N-2}$. It was observed that when $F_i(0)=2\pi$ and $F_i(\infty)=0$ this solution of the SU(N) pure Skyrme model has a topological charge $B=(N/6)(N^2-1)$ and has an energy equal exactly to $(N/6)(N^2-1)$ times the energy of the single Skyrmion solutions. It is easy to show that, if one uses the same ansatz for the sixth order Skyrme model, the profile $f=F_0/2$ satisfies the hedgehog profile equation (10) and the energy of the configuration is given by $E(\lambda)=4E_0(\lambda)$ where $E_0(\lambda)$ is the energy of the hedgehog solution for the generalized model. These configurations are not exact solutions, except for the SU(3) model.

To consider the most general ansatz, one can derive from (40) the following equations for the profile functions F_l, $l=0,...,(N-2)$:

$$\begin{aligned}&-\frac{2(l+1)}{N}\sum_{i=0}^{N-2}(i+1)\ddot{F}_i+2\sum_{k=0}^{l}\sum_{i=k}^{N-2}\ddot{F}_i+\frac{(1-\lambda)}{r^2}\ddot{F}_l(l+1)(N-l-1)(1-\cos F_l)\\&+\frac{2}{r}\left(-\frac{2(l+1)}{N}\sum_{i=0}^{N-2}(i+1)\dot{F}_i+2\sum_{k=0}^{l}\left(\sum_{i=k}^{N-2}\dot{F}_i\right)\right)+\frac{(1-\lambda)}{2r^2}\dot{F}_l^2(l+1)(N-l-1)\sin F_l\\&-\frac{2}{r^2}(l+1)(N-l-1)\sin F_l-\frac{(1-\lambda)}{r^4}(l+1)^2(N-l-1)^2(1-\cos F_l)\sin F_l\\&+\frac{(1-\lambda)}{2r^4}(l+1)(N-l-1)\sin F_l[l(N-l)(1-\cos F_{l-1})+(l+2)(N-l-2)(1-\cos F_{l+1})]\\&+\frac{\lambda}{8r^4}\{2\ddot{F}_l(l+1)^2(N-l-1)^2(1-\cos F_l)^2-\ddot{F}_{l-1}l(l+1)(N-l)(N-l-1)(1-\cos F_{l-1})\\&\times(1-\cos F_l)-\ddot{F}_{l+1}(l+1)(l+2)(N-l-1)(N-l-2)(1-\cos F_l)(1-\cos F_{l+1})\}\\&+\frac{-\lambda}{4r^5}\{2\dot{F}_l(l+1)^2(N-l-1)^2(1-\cos F_l)^2-\dot{F}_{l-1}l(l+1)(N-l)(N-l-1)(1-\cos F_{l-1})\\&\times(1-\cos F_l)-\dot{F}_{l+1}(l+1)(l+2)(N-l-1)(N-l-2)(1-\cos F_l)(1-\cos F_{l+1})\}\\&+\frac{\lambda}{8r^4}\{2\dot{F}_l^2(l+1)^2(N-l-1)^2(1-\cos F_l)\sin F_l-\dot{F}_{l-1}^2l(l+1)(N-l)(N-l-1)\sin F_{l-1}\\&\times(1-\cos F_l)-\dot{F}_{l+1}^2(l+1)(l+2)(N-l-1)(N-l-2)(1-\cos F_l)\sin F_{l+1}\}=0. \quad (41)\end{aligned}$$

When $N=3$, the solution of the two equations lead to exact solutions of the model, while for larger values of N, the ansatz (14) corresponds to low-energy configurations.

We would like to point out at this stage that as proved in Ref. 14, the topological charge for the configuration (14) is given by

$$B=\sum_{i=0}^{N-2}\mathcal{D}_k(F_i-\sin F_i)_{r=0}^{r=\infty}, \tag{42}$$

where

$$\mathcal{D}_k=-i\frac{1}{4\pi^2}\int\frac{|P_+^{k+1}h|^2}{|P_+^k h|^2}d\xi d\bar{\xi} \tag{43}$$

takes integer values given by the degree in ξ of the wedge product[16] of h and its derivatives

$$\mathcal{D}_k=\frac{1}{2\pi}\deg(h^{(k)}),\quad h^{(k)}=h\wedge\partial_+ h\wedge\cdots\wedge\partial_+^k h,\quad k=0,\ldots,N-1. \tag{44}$$

Each configuration is thus characterized by the boundary conditions for the profile function F_i and we can without loss of generality impose the condition $\lim_{r\to\infty}F_i(r)=0$. For the configuration to be well-defined at the origin we must also impose a condition of the type

$$F_i(0)=n_i 2\pi, \tag{45}$$

where $n_i\in N$.

V. RADIALLY SYMMETRIC SU(3) SOLUTIONS

To describe the solution of the SU(3) model, we use the profile $F=F_0$ and $g=F_1$ and the energy (40) simplifies to

$$\begin{aligned}E=\frac{1}{6\pi}\int r^2dr\Big\{&\frac{2}{3}(\dot{g}^2+\dot{F}^2+\dot{g}\,\dot{F})+\frac{1}{r^2}((1-\cos F)((1-\lambda)\dot{F}^2+4)+(1-\cos g)\\&\times((1-\lambda)\dot{g}^2+4))+(1-\lambda)\frac{2}{r^4}((1-\cos F)^2-(1-\cos F)(1-\cos g)+(1-\cos g)^2)\\&+\frac{\lambda}{2r^4}(\dot{F}^2(1-\cos F)^2+\dot{g}^2(1-\cos g)^2-(1-\cos F)(1-\cos g)\dot{g}\dot{F})\Big\}.\end{aligned} \tag{46}$$

The equations for the profile function F and g are then given by

$$\begin{aligned}&g_{rr}+\frac{1}{2}F_{rr}+\frac{F_r}{r}+2\frac{g_r}{r}+\frac{3}{2r^2}\left((1-\lambda)(1-\cos g)g_{rr}+\frac{1}{2}\sin g((1-\lambda)g_r^2-4)\right)\\&+\frac{1}{2}\sin g((1-\lambda)g_r^2-4)+(1-\lambda)\frac{3}{2r^4}((1-\cos F)-2(1-\cos g))\sin(g)+\frac{3\lambda}{8r^4}(1-\cos g)\\&\times\left(2\left(\sin g g_r^2+(1-\cos g)\left(g_{rr}-2\frac{g_r}{r}\right)\right)-\sin F F_r^2-(1-\cos F)\left(F_{rr}-2\frac{Fr}{r}\right)\right)=0,\end{aligned} \tag{47}$$

TABLE I. Topological charge and energy of the hedgehog SU(2) solution.

SU(2)		Energy	
n_g	B	$E(0)$	$E(1)$
1	1	1.2315	0.9395

$$F_{rr}+\frac{1}{2}g_{rr}+2\frac{F_r}{r}+\frac{g_r}{r}+\frac{3}{4r^2}(\sin F((1-\lambda)F_r^2-4)+2(1-\lambda)(1-\cos F)F_{rr})$$
$$-(1-\lambda)\frac{3}{2r^4}(2(1-\cos F)-(1-\cos g))\sin F+\frac{3\lambda}{8r^4}(1-\cos F)$$
$$\times\left(12\left(\sin F\,F_r^2+(1-\cos F)\left(F_{rr}-2\frac{F_r}{r}\right)\right)-\sin g\,g_r^2-(1-\cos g)\left(g_{rr}-2\frac{g_r}{r}\right)\right)=0. \tag{48}$$

The topological charge of the solution now reads

$$B=\frac{1}{\pi}((F-\sin F)|_{r=0}^{r=\infty}+(g-\sin(g))|_{r=0}^{r=\infty}) \tag{49}$$

and, if we take the boundary conditions

$$F(0)=n_F 2\pi,$$
$$g(0)=n_g 2\pi, \tag{50}$$

where n_F and n_g are integers, we have $B=2(n_f+n_g)$. When n_F and n_g are of opposite signs, we can interpret the solutions as a mixture of Skyrmions and anti-Skyrmions.

In Table I, we give the energy of the hedgehog solution ($B=1$) for the SU(2) model. This solution is an embedded solution of any SU(N) model and it is the solution with the lowest energy. We thus use it as the reference energy for all the other solutions.

In Table II we present the properties of the different solutions for the SU(3) models. The first two columns specify the boundary condition of the solution, and the third column gives the topological charge of that solution. In columns 4 and 5 we give the energy of the solutions for the pure Skyrme model and the pure Sk6 model while columns 6 and 7 give the corresponding relative energy per Skyrmion, that is, the energy divided by the energy of the single Skyrmion and the total number of Skyrmions. For the solutions corresponding to the superposition of Skyrmions and anti-Skyrmion, we define the total number of Skyrmions as the total number of Skyrmions and anti-Skyrmions. Notice that the cases $n_g=0, n_F=1$ and $n_g=1, n_F=0$ correspond to the same solution modulo an internal rotation.

In Fig. 3, we present the energy of the three different types of solution as a function of λ.

TABLE II. Topological charge and energy of some SU(3) solutions.

SU(3)			Total energy		Relative energy	
n_F	n_g	B	$E(0)$	$E(1)$	$E_B(0)/(\lvert B\rvert E_1(0))$	$E_B(1)/(\lvert B\rvert E_1(1))$
1	1	4	4.928	3.758	1	1
1	0	2	2.377	1.819	0.965	0.968
0	1	2	2.377	1.819	0.965	0.968
1	−1	2-2	3.862	3.191	0.784	0.849

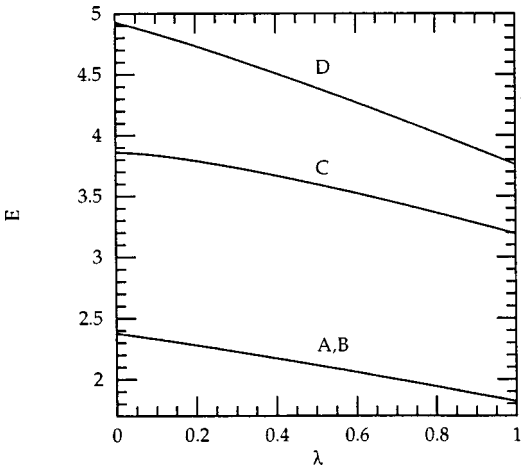

FIG. 3. Energy of the SU(3) solution for the boundary conditions (a) $n_F=0, n_g=1$, (b) $n_F=1, n_g=0$, (c) $n_F=1, n_g=-1$, (d) $n_F=1, n_g=1$.

VI. LOW-ENERGY SU(4) CONFIGURATIONS

As was shown in the last two sections, the ansatz (14) provides an exact solution of the sixth order model only for the SU(3) model, or when $\lambda=0$, that is for the usual Skyrme model. For the SU(N) model with $N\geqslant 4$, the ansatz still produces low-energy configurations. In particular, when λ is small, we can expect the ansatz to be very close to an exact solution. In this section we look at some configurations of the SU(4) model. For this model, we have three profile functions F_0, F_1 and F_2 and the energy for the general ansatz (14) is explicitly given by

$$
\begin{aligned}
E=\frac{1}{6\pi}\int r^2 dr\Bigg\{&\frac{1}{4}(3\dot{F}_0^2+4\dot{F}_1^2+3\dot{F}_2^2+4\dot{F}_0\dot{F}_1+4\dot{F}_1\dot{F}_2+2\dot{F}_0\dot{F}_2)+\frac{2}{r^2}[3(1-\cos F_0)\\
&+4(1-\cos F_1)+3(1-\cos F_2)]+(1-\lambda)\Bigg\{\frac{1}{2r^2}[3\dot{F}_0^2(1-\cos F_0)+4\dot{F}_1^2(1-\cos F_1)\\
&+3\dot{F}_2^2(1-\cos F_2)]+\frac{1}{2r^4}\{9\,(1-\cos F_0)^2+16\,(1-\cos F_1)^2+9\,(1-\cos F_2)^2\\
&-12(1-\cos F_0)(1-\cos F_1)-12(1-\cos F_1)(1-\cos F_2)\}\Bigg\}+\frac{\lambda}{8r^4}\{9\dot{F}_0^2(1-\cos F_0)^2\\
&+16\dot{F}_1^2(1-\cos F_1)^2+9\dot{F}_2^2(1-\cos F_2)^2-12F_0F_1(1-\cos F_0)(1-\cos F_1)\\
&-12F_1F_2(1-\cos F_1)(1-\cos F_2)\}\Bigg\}
\end{aligned}
\tag{51}
$$

from which we can derive the following equations:

$$
\begin{aligned}
&\left(\frac{3\lambda(1-\cos F_0)^2}{2r^4}+\frac{2(1-\lambda)(1-\cos F_0)}{r^2}+1\right)\ddot{F}_0+\left(\frac{2}{3}-\frac{\lambda(1-\cos F_0)(1-\cos F_1)}{r^4}\right)\ddot{F}_1+\frac{1}{3}\ddot{F}_2\\
&-\frac{4\sin F_0}{r^2}+\frac{6\,\dot{F}_0+4\dot{F}_1+2\dot{F}_2}{3r}+\frac{(1-\lambda)\dot{F}_0^2\sin F_0}{r^2}+(1-\lambda)\frac{\sin F_0}{r^4}(4(1-\cos F_1)\\
&-6(1-\cos F_0))+\lambda\frac{(1-\cos F_0)}{r^4}\left(\frac{3}{2}\dot{F}_0^2\sin F_0-\dot{F}_1^2\sin F_1\right)-\lambda\frac{(1-\cos F_0)}{r^5}(3\dot{F}_0(1-\cos F_0)\\
&-2\,\dot{F}_1(1-\cos F_1))=0,
\end{aligned}
\tag{52}
$$

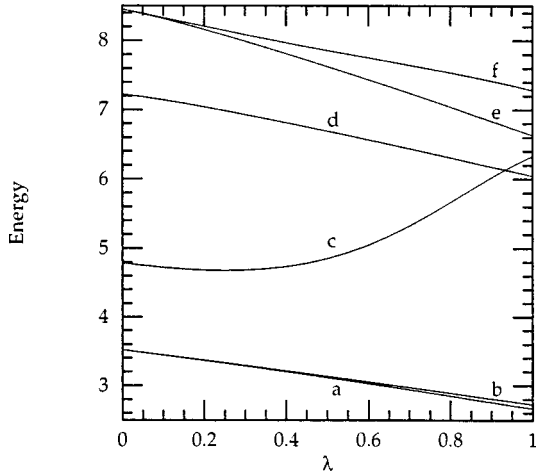

FIG. 4. Energy density of the Su(4) multi-projector ansatz (a) $n_0=0$, $n_1=0$, $n_2=1$; (b) $n_0=1$, $n_1=0$, $n_2=0$; (c) $n_0=0$, $n_1=1$, $n_2=0$; (d) $n_0=1$, $n_1=0$, $n_2=1$; (e) $n_0=1$, $n_1=1$, $n_2=0$; and (f) $n_0=0$, $n_1=1$, $n_2=1$.

$$\left(\frac{1}{2}-\frac{3\lambda(1-\cos F_0)(1-\cos F_1)}{4r^4}\right)\ddot{F}_0+\left(1+\frac{2\lambda(1-\cos F_1)^2}{r^4}+\frac{2(1-\lambda)(1-\cos F_1)}{r^2}\right)\ddot{F}_1$$
$$+\left(\frac{1}{2}-\frac{3\lambda(1-\cos F_1)(1-\cos F_2)}{4r^4}\right)\ddot{F}_2+\frac{(1-\lambda)\dot{F}_1^2\sin F_1}{r^2}+\frac{\dot{F}_0+2\dot{F}_1+\dot{F}_2}{r}-4\frac{\sin F_1}{r^2}$$
$$+(1-\lambda)\frac{\sin F_1}{r^4}(3(1-\cos F_0)+3(1-\cos F_2)-8(1-\cos F_1))-\frac{\lambda}{r^5}(1-\cos F_1)$$
$$\times\left(4\dot{F}_1(1-\cos F_1)-\frac{3}{2}\dot{F}_0(1-\cos F_0)-\frac{3}{2}\dot{F}_2(1-\cos F_2)\right)+\frac{\lambda}{r^4}(1-\cos F_1)$$
$$\times\left(2\dot{F}_1^2\sin F_1-\frac{3}{4}\dot{F}_0^2\sin F_0-\frac{3}{4}\dot{F}_2^2\sin F_2\right)=0, \tag{53}$$

and

$$\left(\frac{2}{3}-\frac{\lambda(1-\cos F_1)(1-\cos F_2)}{r^4}\right)\ddot{F}_1+\left(\frac{3\lambda(1-\cos F_2)^2}{2r^4}+\frac{2(1-\lambda)(1-\cos F_2)}{r^2}+1\right)\ddot{F}_2$$
$$+\frac{1}{3}\ddot{F}_0+\frac{2\dot{F}_0+4\dot{F}_1+6\dot{F}_2}{3r}-4\frac{\sin F_2}{r^2}+\frac{(1-\lambda)\dot{F}_2^2\sin F_2}{r^2}+(1-\lambda)\frac{\sin F_2}{r^4}(4(1-F_1)$$
$$-6(1-F_2))-\lambda\frac{(1-\cos F_2)}{r^5}(3\dot{F}_2(1-\cos F_2)-2\dot{F}_1(1-\cos F_1))$$
$$+\lambda\frac{(1-\cos F_2)}{r^4}\left(\frac{3}{2}\dot{F}_2^2\sin F_2-\dot{F}_1^2\sin F_1\right)=0. \tag{54}$$

Describing the boundary condition for the profile functions as before, $F_i(0)=n_i 2\pi$, the topological charge is given by

$$B=3n_0+4n_1+3n_2. \tag{55}$$

TABLE III. Topological charge and energy of some SU(4) configurations.

SU(4)				Total energy		Relative energy	
n_0	n_1	n_2	B	$E(0)$	$E(1)$	$E_B(0)/(\lvert B\rvert E_1(0))$	$E_B(1)/(\lvert B\rvert E_1(1))$
0	0	1	3	3.517 39	2.666 53	0.952 10	0.945 98
1	0	0	3	3.517 39	2.729 15	0.952 10	0.968 19
0	1	0	4	4.788 07	6.333 22	0.972 04	1.685 07
1	0	1	6	7.224 64	6.046 04	0.977 80	1.072 44
1	1	0	7	8.452 19	6.629 98	0.980 52	1.008 02
0	1	1	7	8.452 19	7.280 58	0.980 52	1.106 94
1	1	1	10	12.311	9.396 05	1	1

In Table III we present the energy values of various types of configurations when $\lambda=0$ and $\lambda=1$. We notice that when $\lambda=0$, the solutions are symmetric under the exchange $f_0\leftrightarrow f_2$, but that the sixth order term breaks the symmetry. This results in a difference of energy between the configuration with $n_0=0, n_1=0, n_2=1$ and $n_0=1, n_1=0, n_2=0$ as well as between the configurations with $n_0=1, n_1=1, n_2=0$ and $n_0=0, n_1=1, n_2=1$. In Fig. 4, we present the curve for the energy of the configurations as a function of λ.

VII. SU(N) LOW-ENERGY CONFIGURATION

After inserting the ansatz (5) in the full equation for the SU(N) model, we found that we had only two independent profile functions g_0 and g_1 and that the ansatz would only provide solutions for the SU(3) model. One can nevertheless use the SU(N) ansatz to compute low-energy configurations. For example, if we consider the reduced ansatz defined by (5) together with the constraint $\dot{g}_{i-2}-\dot{g}_{i-3}=\dot{g}_i-\dot{g}_{i-2}$ and define the profiles $F=g_0-g_1$ and $g=g_{N-2}$ we can minimize the energy (40) and solve the equations for F and g for various boundary conditions. We found that to get configurations corresponding to a bound state, i.e., a configuration with an energy per Skyrmion smaller than the energy of the hedgehog solution, we must take $n_F=0$ and $n_g=1$. The energies that we found are given in Table IV.

In Figs. 5 and 6 we present the profile and the energy density for different values of N and for $\lambda=0.5$. It shows that the energy density has the shape of a hollow sphere of radius $r=0.7\sqrt{N}$. The profile g has the same shape for all values of N but is shifted to the right as N increases. The profile F, on the other hand, is also shifted as the shell radius increases, but its amplitude decreases like $1/N^2$. Note that in Fig. 6, the profiles for $N=100$ and $N=200$ have been multiplied by 100 to make them visible. For other values of λ the graphics look very much the same except that the shell radius and width are slightly different, but the conclusions remain the same.

Figure 6(b) suggests to simplify the ansatz further for large N by taking $F(r)=0$. This implies that $g_i=g\ \forall i$ and the multi-projector ansatz (5) becomes

$$U=\exp(-ig(P_{N-1}-I/N)), \tag{56}$$

where P_{N-1} can also be written as

TABLE IV. Topological charge and energy for the reduced ansatz with $n_F=0$ and $n_g=1$.

		Total energy		Relative energy	
Model	B	$E(0)$	$E(1)$	$E_B(0)/(\lvert B\rvert E_1(0))$	$E_B(1)/(\lvert B\rvert E_1(1))$
SU(3)	2	2.377	1.819	0.965	0.968
SU(4)	3	3.624	2.759	0.981	0.979
SU(5)	4	4.811	3.632	0.977	0.966
SU(6)	5	6.015	4.518	0.977	0.962

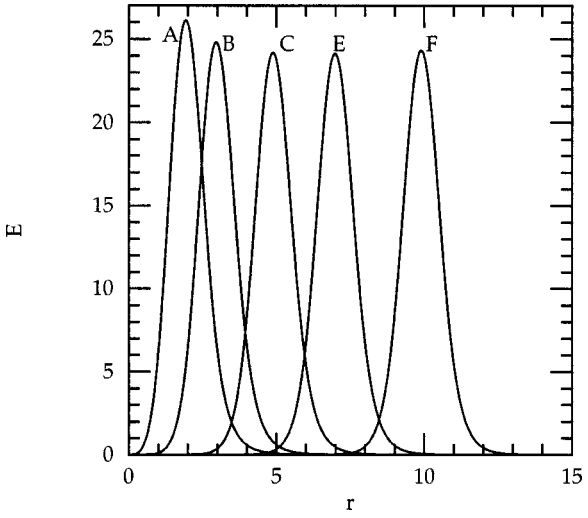

FIG. 5. Energy density of the multi-projector solution with $n_F=0$, $n_g=1$, $\lambda=0.5$. (a) $N=10$, (b) $N=20$, (c) $N=50$, (d) $N=100$, and (e) $n=200$.

$$P_{N-1}=\frac{\tilde{h}\tilde{h}^{\dagger}}{|\tilde{h}|^2}, \tag{57}$$

where $\tilde{h}$ is equal, up to a unitary rotation, to the complex conjugate of the holomorphic vector V_0 defined in (20) and (21): $\tilde{h}=A\overline{V_0}$ for some $A\in \mathrm{SU}(N)$ with $\partial_{\xi}A=\partial_{\bar{\xi}}A=0$. This is shown by using the fact that P_{N-1} is an antiholomorphic projector[16] and that solving (39) recursively we have

$$|V_k|^2=\frac{k!(N-1)!}{(N-1-k)!}|1+|\xi|^2|^{N-1-2k} \tag{58}$$

and so $|V_{N-1}|^2=(N-1)!^2|1+|\xi|^2|^{1-N}$. Knowing that up to an overall coefficient $|V_{N-1}|^2$ is a polynomial in $\bar{\xi}$ of degree $N-1$, we can conclude that up to a unitary iso-rotation, V_{N-1} is equal to the complex conjugate of V_0.

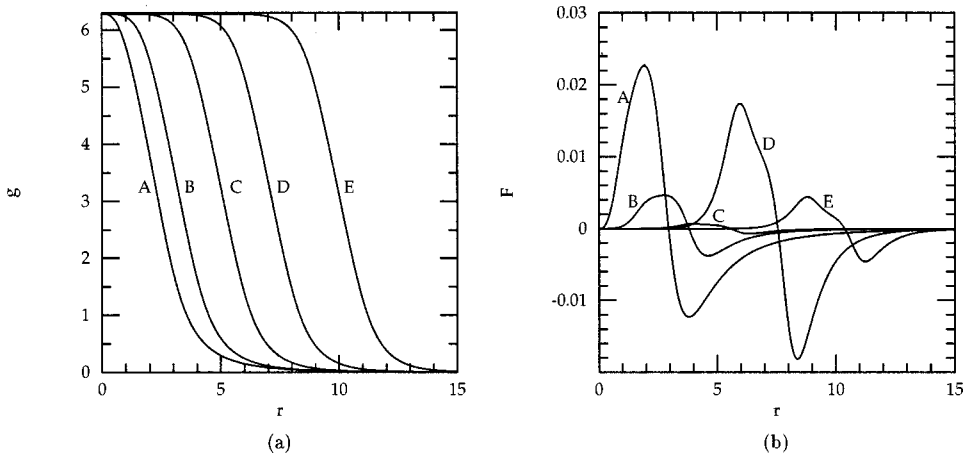

FIG. 6. Profile (a) g and (b) F of the multi-projector solution with $n_F=0$, $n_g=1$, $\lambda=0.5$. (a) F for $N=10$, (b) F for $N=20$, (c) F for $N=50$, (d) $100\times F$ for $N=100$, and (e) $100\times F$ for $N=200$.

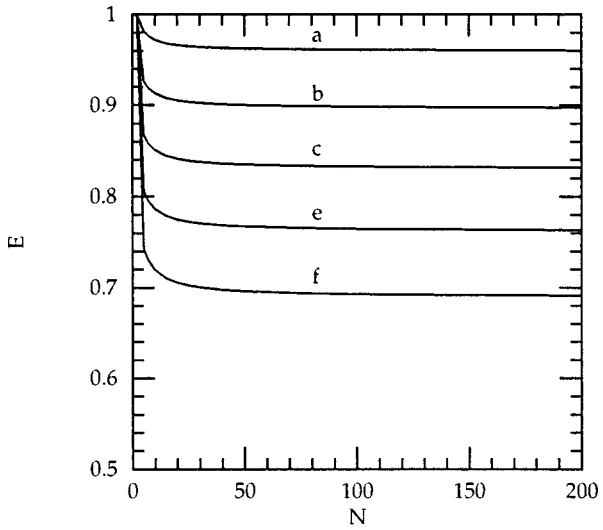

FIG. 7. Energy $E/(E_{B=1}(N-1))$ for the SU(N), configuration (56) for (a) $\lambda=0$, (b) $\lambda=0.25$, (c) $\lambda=0.5$, (d) $\lambda=0.75$, and (e) $\lambda=1$.

The topological charge of the antiholomorphic projector P_{N-1} is equal to $1-N$ and as the profile function is $-g$, the baryon number for this configuration is $N-1$. The ansatz (56) is not a solution, but its energy

$$E=\frac{1}{6\pi}\int r^2 dr\left\{\frac{N-1}{N}\dot{g}^2+\frac{1}{2r^2}+(N-1)(1-\cos g)((1-\lambda)\dot{g}^2+4)\right.$$
$$\left.+\frac{1}{2r^4}(N-1)^2(1-\cos g)^2\left((1-\lambda)+\frac{\lambda}{4r^4}\dot{g}^2\right)\right\}, \tag{59}$$

can easily be computed by solving the equation

$$2g_{rr}+4\frac{g_r}{r}+\frac{N}{r^2}\left((1-\lambda)(1-\cos g)g_{rr}+\frac{1}{2}\sin g((1-\lambda)g_r^2-4)\right)+\frac{\lambda}{4r^4}N(N-1)(1-\cos g)$$
$$\times\left(\sin g g_r^2+(1-\cos g)\left(g_{rr}-2\frac{g_r}{r}\right)\right)=0. \tag{60}$$

In Fig. 7, we present the relative energy, $E(\lambda)/(E_{B=1}(\lambda)(N-1))$, of this configuration as a function of N for different values of λ. We see that this configuration corresponds to a bound state of Skyrmions and that the energy per Skyrmion decreases with N. The energy of this configuration corresponds to an upper bound for the energy of the $B=N-1$ radially symmetric solution of the SU(N) model and these configurations correspond to bound states of Skyrmions for all values of N and all values of λ. As every SU(p) solution can be trivially embedded in an SU(q) solution when $p\leqslant q$ we can claim that for every $B<N$ the SU(N) model has a radially symmetric solution of charge B corresponding to a bound state. With the exception of the hedgehog solutions, these solutions are expected to be unstable when the radial symmetry is broken as their energies are larger than the known SU(2) solutions.[13]

VIII. CONCLUSIONS

In this article we have shown how to construct some radially symmetric solutions of the SU(3) sixth order Skyrme model. The construction is similar to the one used for the pure Skyrme model in Ref. 14 except that, because of an extra constraint, the construction only works for the SU(3)

model. The same ansatz can nevertheless be used to compute low-energy configurations of the SU(N) model. In particular we showed that for every N there is a radially symmetric solution of charge $B<N$ which corresponds to a bound state of Skyrmions.

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Gradient corrections for semiclassical theories of atoms in strong magnetic fields

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This paper is divided into two parts. In the first one the von Weizsäcker term is introduced to the magnetic Thomas–Fermi theory and the resulting MTFW functional is mathematically analyzed. In particular, it is shown that the von Weizsäcker term produces the Scott correction up to magnetic fields of order $B \ll Z^2$, in accordance with a result of Ivrii on the quantum mechanical ground state energy. The second part is dedicated to gradient corrections for semiclassical theories of atoms restricted to electrons in the lowest Landau band. We consider modifications of the Thomas–Fermi theory for strong magnetic fields (STF), i.e., for $B \ll Z^3$. The main modification consists in replacing the integration over the variables perpendicular to the field by an expansion in angular momentum eigenfunctions in the lowest Landau band. This leads to a functional (DSTF) depending on a sequence of one-dimensional densities. For a one-dimensional Fermi gas the analogue of a Weizsäcker correction has a negative sign and we discuss the corresponding modification of the DSTF functional. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In this paper we study gradient correction terms for semiclassical theories describing the ground state energies of heavy atoms in strong homogeneous magnetic fields. Such an atom, with N electrons of charge $-e$ and mass m_e and nuclear charge Ze is described by the nonrelativistic Pauli Hamiltonian

$$H_N = \sum_{1 \leqslant j \leqslant N} \left\{ ((-i\nabla^{(j)} + \mathbf{A}(x_j)) \cdot \sigma^j)^2 - \frac{Z}{|x_j|} \right\} + \sum_{1 \leqslant i < j \leqslant N} \frac{1}{|x_i - x_j|}, \tag{I.1}$$

acting on the Hilbertspace $\wedge_{1 \leqslant j \leqslant N} L^2(\mathbb{R}^3, \mathbb{C}^2)$ of electron wave functions. The units are chosen such that $\hbar = 2m_e = e = 1$. The magnetic field is $\mathbf{B} = (0,0,B)$, with vector potential $\mathbf{A} = \frac{1}{2}B \times (-x_2, x_1, 0)$, where B is the magnitude of the field in units of $B_0 = m_e^2 e^3 c/\hbar^3 = 2.35 \times 10^9$ G, the field strength for which the cyclotron radius $l_B = (\hbar c/(eB))^{1/2}$ is equal to the Bohr radius $a_0 = \hbar^2/(m_e e^2)$. The ground state energy is

$$E^{\mathrm{Q}}(N,Z,B) = \inf\{(\psi, H_N \psi) : \psi \in \text{domain } H_N, (\psi,\psi) = 1\}. \tag{I.2}$$

In Ref. 1 Lieb, Solovej, and Yngvason approximated (1.2) by means of the MTF (magnetic Thomas–Fermi) functional

$$\mathcal{E}^{\mathrm{MTF}}[\rho] = \int \tau_B(\rho) - \int V\rho + D(\rho,\rho), \tag{I.3}$$

where $V(x) = Z/|x|$ and $D(\rho,\rho) = \frac{1}{2}(\rho, |x|^{-1} * \rho)$. The magnetic energy density τ_B is, by definition, the Legendre transform of the pressure P_B, i.e.,

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$$\tau_B(t)=\sup_{w\geqslant 0}[tw-P_B(w)], \tag{I.4}$$

with

$$P_B(w)=\frac{B}{3\pi^2}\left(w^{3/2}-2\sum_{i=1}^{\infty}|2iB-w|_{-}^{3/2}\right). \tag{I.5}$$

The corresponding energy

$$E^{\mathrm{MTF}}(N,Z,B)=\inf\left\{\mathcal{E}^{\mathrm{MTF}}[\rho]\,\middle|\,\rho\geqslant 0,\rho\in D^{\mathrm{MTF}},\int\rho\leqslant N\right\} \tag{I.6}$$

was proved by Lieb, Solovej, and Yngvason to be asymptotically exact, as shown in the following Theorem:

Theorem I.1 (**Ref. 1, Theorem 5.1**)**:** *If $Z\to\infty$ with N/Z fixed and $B/Z^3\to 0$, then*

$$E^{\mathrm{Q}}(N,Z,B)/E^{\mathrm{MTF}}(N,Z,B)\to 1.$$

In the limit $B\to\infty$ the function τ_B is the kinetic energy describing particles confined to the lowest Landau band, i.e.,

$$\tau_\infty(t)=\frac{4\pi^4}{3}t^3/B^2,$$

which results in the STF (strong Thomas–Fermi) functional

$$\mathcal{E}^{\mathrm{STF}}[\rho]=\frac{4\pi^4}{3B^2}\int\rho^3-\int V\rho+D(\rho,\rho). \tag{I.7}$$

The corresponding energy E^{STF} is quantum mechanically exact in the limit $Z\to\infty$ for $Z^{4/3}\ll B\ll Z^3$ (Ref. 1, Proposition 4.16), which emphasizes the fact (Ref. 2, Theorem 1.2) that for $B\gg Z^{4/3}$ the electrons are to leading order confined to the lowest Landau band.

A. Corrections to the leading order of the full Hamiltonian (I.1)

The best result to date concerning corrections to the leading order of (I.2) is presented by Victor Ivrii in Ref. 3, Theorem 0.2:

Theorem I.2 (**Ref. 3, Theorem 0.2**)**:** *Let $B\leqslant Z^3$ and $N\sim Z$, then*

$$|E^{Q}(N,Z,B)-E^{\mathrm{MTF}}(N,Z,B)-\tfrac{1}{4}Z^2|\leqslant R_1+R_2, \tag{I.8}$$

with

$$R_1=CZ^{4/3}(N+B)^{1/3},\quad R_2=CZ^{3/5}B^{4/5}. \tag{I.9}$$

Recall the order of the energy, $E^{Q}\sim Z^{7/3}[1+B/Z^{4/3}]^{2/5}$.

We make a few comments concerning Ivrii's proof. Let

$$H_{\mathbf{A}}=[(-i\nabla+\mathbf{A}(x))\cdot\sigma]^2 \tag{I.10}$$

denote the free Pauli Hamiltonian and

$$\phi^{\mathrm{MTF}}=Z|\mathbf{x}|^{-1}-\rho^{\mathrm{MTF}}*|\mathbf{x}|^{-1} \tag{I.11}$$

the self-consistent magnetic TF potential. The main part of the estimate (I.8) is given by the difference between

$$\mathrm{Tr}[H_{\mathbf{A}}-\phi^{\mathrm{MTF}}+\mu]_-, \tag{I.12}$$

the sum of all negative eigenvalues of the operator $H_{\mathbf{A}}-\phi^{\mathrm{MTF}}+\mu$, and its semiclassical approximation

$$\int P_B(\phi^{\mathrm{MTF}}-\mu). \tag{I.13}$$

For those who are familiar with microlocal analysis we should remark that Ivrii does not really consider ϕ^{MTF} but a smooth mollification, which we also denote with ϕ^{MTF} for simplicity. In order to derive accurate estimates of

$$\left|\mathrm{Tr}[H_{\mathbf{A}}-\phi^{\mathrm{MTF}}+\mu]_- - \int P_B(\phi^{\mathrm{MTF}}-\mu)\right|, \tag{I.14}$$

Ivrii essentially divides the domain into two main zones, for $B\geqslant Z^{4/3}$, namely

$$\chi_1=\{\mathbf{x}|0\leqslant|\mathbf{x}|\leqslant B/Z\} \text{ and } \chi_2=\{\mathbf{x}|B/Z\leqslant|\mathbf{x}|\leqslant r_S=Z^{1/5}B^{-2/5}\}. \tag{I.15}$$

A corresponding partition of unity is given by two functions φ_1 and φ_2, with $\varphi_1+\varphi_2=1$ on $\chi_1\cup\chi_2$ and φ_i essentially supported in χ_i. Using scaling arguments and semiclassical spectral asymptotics Ivrii treats each zone separately. In the inner zone χ_1, where all Landau levels are taken into account and the MTF potential is very similar to the usual TF potential, he gets

$$\chi_1:\left|\mathrm{Tr}(\varphi_1[H_{\mathbf{A}}-\phi^{\mathrm{MTF}}+\mu]_-)-\int \varphi_1 P_B(\phi^{\mathrm{MTF}}-\mu)-\frac{1}{4}Z^2\right|\leqslant R_1. \tag{I.16}$$

We see that in χ_1 the Scott correction is recovered. Moreover, we should note that the machinery of semiclassical spectral asymptotics can only be applied to χ_1 under the condition $Z/B\gg 1/Z$, which means that (I.16) is only valid for $B\leqslant Z^{2-\delta}$, with arbitrary $\delta>0$. For $B\geqslant Z^2$ a semiclassical approximation is no longer possible and the terms (I.12) and (I.13) have to be estimated separately. Since R_2 overcomes Z^2 for $B\geqslant Z^{7/4}$, we should point out that the Scott correction in (I.8) only provides the next to leading order for $B\ll Z^{7/4}$, but in the domain χ_1 it nevertheless makes sense up to $B\ll Z^2$ according to (I.16).

In the outer zone χ_2 only the lowest Landau band is occupied, which implies that in this region the MTF energy is represented by the STF energy corresponding to the functional (I.7). In χ_2 Ivrii derives the estimate

$$\chi_2:\left|\mathrm{Tr}(\varphi_2[H_{\mathbf{A}}-\phi^{\mathrm{MTF}}+\mu]_-)-\int \varphi_2 P_B(\phi^{\mathrm{MTF}}-\mu)\right|\leqslant R_2, \tag{I.17}$$

where the main contribution of (I.17) really stems from the edge of the STF atom $r_S \sim Z^{1/5}B^{-2/5}$.

For low magnetic fields ($B\leqslant Z$) V. Ivrii even improves (I.8) and recovers Dirac and Schwinger corrections as well.

Theorem I.3 (**Ref. 3, Theorem 0.3**)**:** *If $B\leqslant Z$ then*

$$\left|E^{\mathrm{QM}}(N,Z,B)-E^{\mathrm{MTF}}(N,Z,B)-\frac{1}{4}Z^2+c_{\mathrm{DS}}\int(\rho^{\mathrm{TF}})^{4/3}\right|\leqslant CN^{5/3}((1+B)/N)^{\delta} \tag{I.18}$$

holds with some $\delta>0$ and an appropriate parameter c_{DS}.

The von Weizsäcker term introduced to MTF. The von Weizsäcker correction term was successfully introduced to the TF theory in the sense that it reproduces the Scott correction (rigorously proven in Refs. 4 and 5), i.e.,

$$E^{\mathrm{TFW}}=E^{\mathrm{TF}}+O(Z^2)+o(Z^2). \tag{I.19}$$

In addition to the Z^2 correction, the TFW theory remedies some defects of the TF theory: The corresponding TFW density is finite at the nuclei, binding of atoms occurs and negative ions are stable, furthermore the density has exponential fall off at infinity, at least for neutral atoms and molecules.

In the limit $B\to 0$ the function τ_B is the kinetic energy density in zero magnetic field, i.e.,

$$\tau_0(t)=\tfrac{3}{5}(3\pi^2)^{2/3}t^{5/3}.$$

Since for small values of B the introduction of the von Weizsäcker term to the MTF functional is justified, we will further check up to which values of B this definition makes sense. We get the functional

$$\mathcal{E}^{\mathrm{MTFW}}[\rho]=A\int|\nabla\rho^{1/2}|^2+\int\tau_B(\rho)-\int V\rho+D(\rho,\rho), \tag{I.20}$$

with a suitably chosen parameter A. The functional (I.20) can be treated analogously to the usual TFW functional in Ref. 6. So we will just sketch the proofs of the main propositions.

It turns out that for $B\ll Z^2$ the von Weizsäcker term still produces the Scott correction, but makes no longer sense for higher magnetic fields. We will derive the following Theorem:

Theorem I.4: *For all B,Z and N/Z fixed*

$$|E^{\mathrm{MTFW}}-E^{\mathrm{MTF}}-O(Z^2)|\leqslant CB^{4/5}Z^{3/5}+o(Z^2). \tag{I.21}$$

Remark: The estimate (I.21) is clearly useful if $B\leqslant Z^{7/4}$. Theorem I.4 will be proved in Sec. II B.

The Scott correction, just like in TFW theory, comes from distances of order $1/Z$ near the nucleus, whereas the bound $CB^{4/5}Z^{3/5}$ comes from the edge of the MTF atom and dominates the Scott correction for $B\geqslant Z^{7/4}$. Moreover, (I.21) is in accordance with Theorem I.2, which justifies *a posteriori* the introduction of the von Weizsäcker term to the MTF functional.

B. Physics in the lowest Landau band

The quantum mechanical ground state energy of particles confined to the lowest Landau band is given by

$$E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B)=\inf_{\|\psi\|_2=1}(\psi,\Pi_0^N H_N\Pi_0^N\psi), \tag{I.22}$$

where Π_0 represents the projector on the lowest Landau band, given by the kernel

$$\Pi_0(x,x')=\frac{B}{2\pi}\exp\left\{\frac{i}{2}(x_\perp\times x'_\perp)\cdot\mathbf{B}-\frac{1}{4}(x_\perp-x'_\perp)^2B\right\}\delta(x_3-x'_3)P_\downarrow, \tag{I.23}$$

where $P_\downarrow$ denotes the projection onto the spin down component, and Π_0^N denotes the Nth tensorial power of Π_0. The leading order of E^Q_{conf}, as $B,Z\to\infty$ with $B\ll Z^3$, is given by E^{STF}, the ground state energy of the functional (I.7). In a companion work we show what is expected by Ivrii's Theorem I.2,

$$|E^Q_{\mathrm{conf}}-E^{\mathrm{STF}}|\leqslant CB^{4/5}Z^{3/5}. \tag{I.24}$$

As we have argued previously the main contribution to the estimate (I.24) comes from the edge of the STF atom, $r_S \sim Z^{1/5}B^{-2/5}$. Recall the order of E^{STF}, $E^{\mathrm{STF}}[N,Z,B] = Z^3(B/Z^3)^{2/5}E^{\mathrm{STF}}[N/Z,1,1]$, so that the estimate is only of interest for $B \ll Z^3$.

As a better approximation to E^Q_{conf}, valid also for $B \geqslant Z^3$, Lieb, Solovej, and Yngvason suggested a density matrix functional defined as

$$\mathcal{E}^{\mathrm{DM}}[\Gamma] = \int_{\mathbb{R}^2} \mathrm{Tr}_{L^2(\mathbb{R})}[-\partial_3^2 \Gamma_{x_\perp}]\mathrm{d}x_\perp - Z\int |x|^{-1}\rho_\Gamma(x) + D(\rho_\Gamma,\rho_\Gamma).$$

Its variable is an operator valued function

$$\Gamma : x_\perp \to \Gamma_{x_\perp},$$

where $\Gamma_{x_\perp}$ is an integral operator on $L^2(\mathbb{R})$, given by a kernel $\Gamma_{x_\perp}(x_3,y_3)$ and satisfying

$$0 \leqslant \Gamma_{x_\perp} \leqslant (B/2\pi)I \tag{I.25}$$

as an operator on $L^2(\mathbb{R})$. The energy

$$E^{\mathrm{DM}}(N,Z,B) = \inf\left\{ \mathcal{E}^{\mathrm{DM}}[\Gamma] \,\middle|\, \Gamma \ \text{satisfies (I.25)} \ \text{and} \ \int \rho_\Gamma \leqslant N \right\}$$

turns out to be asymptotically exact for magnetic fields in the following precise sense:

Theorem I.5 [Ref. 2, Theorems 5.1 and 7.1 and Eqs. (7.3) and (8.5)]: *For some constants, C_λ and C'_λ, we have*

$$R_U \geqslant E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B) - E^{\mathrm{DM}}(N,Z,B) \geqslant -R_L, \tag{I.26}$$

with

$$R_L = C_\lambda \min\{Z^{17/15}B^{2/5}, Z^{8/3}[1+(\ln(B/Z^3))^2]\} \tag{I.27}$$

and

$$R_U = C'_\lambda \min\{Z^{5/3}B^{1/3}, Z^{8/3}[1+\ln(Z)+(\ln(B/Z^3))^2]^{5/6}\}.$$

We remark that the STF energy is the natural semiclassical approximation of the DM energy. More precisely, the DM energy can be written as

$$\frac{B}{2\pi}\int \mathrm{d}\mathbf{x}_\perp \, \mathrm{Tr}_{L^2(\mathbb{R})}[-\partial_z^2 - \phi^{\mathrm{DM}}_{x_\perp} - \mu^{\mathrm{DM}}]_- + \mu^{\mathrm{DM}}N - D(\rho^{\mathrm{DM}},\rho^{\mathrm{DM}}), \tag{I.28}$$

whereas the STF energy is given by the corresponding semiclassical expression

$$\frac{B}{2\pi}\int \mathrm{d}\mathbf{x}_\perp \int\int \mathbf{d}p \, \mathbf{d}z [p^2 - \phi^{\mathrm{STF}}_{\mathbf{x}_\perp} - \mu^{\mathrm{STF}}]_- + \mu^{\mathrm{STF}}N - D(\rho^{\mathrm{STF}},\rho^{\mathrm{STF}}). \tag{I.29}$$

With the decomposition $L^2(\mathbb{R}^3,\mathrm{d}\mathbf{x};\mathbb{C}^2) = L^2(\mathbb{R}^2,\mathrm{d}\mathbf{x}_\perp)\otimes L^2(\mathbb{R},\mathrm{d}z)\otimes\mathbb{C}^2$ the projector Π_0 can be written as

$$\Pi_0 = \sum_{m\geqslant 0} |\phi_m\rangle\langle\phi_m| \otimes 1 \otimes P_\downarrow, \tag{I.30}$$

where ϕ_m denotes the function in the lowest Landau band with angular momentum $-m \leqslant 0$, i.e., using polar coordinates (r,φ),

$$\phi_m(\mathbf{x}_\perp) = \sqrt{\frac{B}{2\pi}} \frac{1}{\sqrt{m!}} \left(\frac{Br^2}{2}\right)^{m/2} e^{-im\varphi} e^{-Br^2/4}. \tag{I.31}$$

Using this and $H_{\mathbf{A}}\Phi_m = 0$, we can write

$$\Pi_0 H_{\mathbf{A}} \Pi_0 = \sum_{m \geqslant 0} |\phi_m\rangle\langle\phi_m| \otimes (-\partial_z^2) \otimes P_\downarrow . \tag{I.32}$$

Based on this decomposition the author and R. Seiringer introduced in Ref. 7 a natural modification of the DM functional called *discrete density matrix functional* (DDM)

$$\mathcal{E}^{\mathrm{DDM}}_{B,Z}[\Gamma] = \sum_{m \in \mathbb{N}_0} \left(\mathrm{Tr}[-\partial_z^2 \Gamma_m] - Z \int V_m(z) \rho_m(z) \mathrm{d}z \right) + \widetilde{D}(\rho,\rho), \tag{I.33}$$

where

$$\widetilde{D}(\rho,\rho) = \frac{1}{2} \sum_{m,n} \int V_{m,n}(z-z') \rho_m(z) \rho_n(z') \mathrm{d}z \, \mathrm{d}z', \tag{I.34}$$

and the potentials V_m and $V_{m,n}$ are given by

$$\begin{aligned} V_m(z) &= \int \frac{1}{|\mathbf{x}|} |\phi_m(\mathbf{x}_\perp)|^2 \, \mathrm{d}\mathbf{x}_\perp , \\ V_{m,n}(z-z') &= \int \frac{|\phi_m(\mathbf{x}_\perp)|^2 |\phi_n(\mathbf{x}'_\perp)|^2}{|\mathbf{x}-\mathbf{x}'|} \mathrm{d}\mathbf{x}_\perp \, \mathrm{d}\mathbf{x}'_\perp . \end{aligned} \tag{I.35}$$

Here Γ is a sequence of fermionic density matrices acting on $L^2(\mathbb{R}, \mathrm{d}z)$,

$$\Gamma = (\Gamma_m)_{m \in \mathbb{N}_0}, \tag{I.36}$$

with corresponding densities $\rho = (\rho_m)_m$, $\rho_m(z) = \Gamma_m(z,z)$. Note that $\mathcal{E}^{\mathrm{DDM}}_{B,Z}$ depends on B via the potentials V_m and $V_{m,n}$. The corresponding energy is given by

$$E^{\mathrm{DDM}}(N,Z,B) = \inf \left\{ \mathcal{E}^{\mathrm{DDM}}_{B,Z}[\Gamma] \,\middle|\, \sum_m \mathrm{Tr}[\Gamma_m] \leqslant N \right\}. \tag{I.37}$$

It is shown in Ref. 7 that E^{DDM} correctly reproduces the confined ground state energy E^Q_{conf} apart from errors due to the indirect part of the Coulomb interaction energy:

Theorem I.6 (Ref. 7, Theorem 1.2): *For some constant c_λ depending only on $\lambda = N/Z$,*

$$0 \geqslant E^{\mathrm{Q}}_{\mathrm{conf}}(N,Z,B) - E^{\mathrm{DDM}}(N,Z,B) \geqslant -R_L , \tag{I.38}$$

with

$$R_L = c_\lambda \min\{Z^{17/15} B^{2/5}, Z^{8/3}(1 + [\ln(B/Z^3)]^2)\}. \tag{I.39}$$

Since the functional (I.33) can also be seen as a reduced Hartree–Fock functional, in the sense of Ref. 8, it does not surprise that the upper bound in (I.38) is an improvement to (I.26), the relation between E^{DDM} and E^Q_{conf}. In addition to better estimates, the DDM theory remedies the defect of the DM theory having a sharply cut ground state density supported in the set $\{\mathbf{x} \,|\, |\mathbf{x}| \leqslant \sqrt{2N/B}\}$, for the respective three-dimensional DDM density,

$$\rho^{\mathrm{DDM}}(\mathbf{x})=\sum_m \rho_m^{\mathrm{DDM}}(z)\phi_m^2(x_\perp), \tag{I.40}$$

has exponential fall off at infinity. Furthermore, since the DDM energy describes E^Q_{conf} correctly apart from errors due to the indirect part of the Coulomb interaction energy, the DDM energy could give rise to even recover the exchange term, by means of an improved lower bound on the two-body Coulomb repulsion for particles in the lowest Landau band. For the exchange energy is anticipated to be of order $\ln(B/Z^{4/3})Z^{7/5}B^{1/5}$ for $B\ll Z^3$, which in Ref. 9 by the author (C. H.) and R. Seiringer is conjectured to be given by the term

$$c\sum_i \ln\left(\frac{B^{1/2}\int\rho_i^{\mathrm{DDM}}}{\int(\rho_i^{\mathrm{DDM}})^2}\right)\int(\rho_i^{\mathrm{DDM}})^2. \tag{I.41}$$

This would lead to the relation

$$E^Q_{\mathrm{conf}}=E^{\mathrm{DDM}}-c\sum_i \ln\left(\frac{B^{1/2}\int\rho_i^{\mathrm{DDM}}}{\int(\rho_i^{\mathrm{DDM}})^2}\right)\int(\rho_i^{\mathrm{DDM}})^2+o(\ln(B/Z^{4/3})Z^{7/5}B^{1/5}), \tag{I.42}$$

with c appropriately chosen.

We have stated previously that the STF functional is the natural semiclassical approximation of the DM functional. Hence, we can ask for the natural semiclassical approximation of the DDM functional, of which the answer is given by the so-called DSTF functional

$$\mathcal{E}^{\mathrm{DSTF}}[\rho]=\sum_{m\in\mathbb{N}_0}\left(\kappa\int\rho_m^3(z)-Z\int V_m(z)\rho_m(z)\mathrm{d}z\right)+\tilde{D}(\rho,\rho), \tag{I.43}$$

where ρ is a sequence of one-dimensional densities, $\rho=(\rho_m)_{m\in\mathbb{N}_0}$, $\kappa=\pi^2/3$, and the respective DSTF energy is defined as

$$E^{\mathrm{DSTF}}(N,Z,B)=\inf\left\{\mathcal{E}^{\mathrm{DSTF}}[\rho]\,\middle|\,\sum_m\int\rho_m\leqslant N\right\}. \tag{I.44}$$

In Section III B 2 we will argue that the DSTF functional is even the natural semiclassical approximation of the ground state energy E^Q_{conf} itself.

C. Gradient corrections for semiclassical lowest Landau band theories

1. The Tomishima–Shinjo correction term

For higher magnetic fields, where only the lowest Landau band has to be taken into account, Tomishima and Shinjo[10] obtained the gradient correction term

$$\epsilon^{\mathrm{TS}}[\rho]=\frac{2\pi^4}{B^3}\rho(\nabla_\perp\rho)^2-\frac{1}{3}(\nabla_\parallel\rho^{1/2})^2, \tag{I.45}$$

i.e.,

$$\mathcal{E}^{\mathrm{TS}}[\rho]=\frac{2\pi^4}{B^3}\int\rho(\nabla_\perp\rho)^2-\frac{1}{3}\int(\nabla_\parallel\rho^{1/2})^2+\mathcal{E}^{\mathrm{STF}}[\rho], \tag{I.46}$$

by perturbation expansion of the canonical density matrix. In 1995 the authors of Ref. 11 recovered the TS theory within the framework of current density functional theory. Since (I.46) has a negative gradient correction along the magnetic field the TS functional is no longer bounded from

below. Hence the corresponding energy cannot, as usual, be defined by minimizing over a suitable domain of definition, but only through the solutions of the corresponding Euler–Lagrange equation under the restriction $\int \rho = N$, i.e.,

$$\frac{4\pi^4}{B^2}\rho^2 - \frac{\pi^4}{B^3}[(\nabla_\perp \rho)^2 + 2\rho\Delta_\perp \rho] - \frac{1}{12\rho}\left[\frac{1}{2\rho}(\nabla_\parallel \rho)^2 - \Delta_\parallel \rho\right] = V - \rho * \frac{1}{|x|} - \mu(N). \tag{I.47}$$

A direct attack on this complicated equation does not look promising, but a rough estimate of the corrections to STF can be obtained by inserting the density

$$\rho(r) = \begin{cases} \rho^{\mathrm{STF}}(B^{-1/2}) & \text{for } r \leqslant B^{-1/2}, \\ \rho^{\mathrm{STF}}(r) & \text{for } r \geqslant B^{-1/2}, \end{cases} \tag{I.48}$$

into (I.46). The negative gradient term gives a correction $-O(B^{4/5}Z^{3/5})$ coming from the edge of the STF atom. From (I.24) we know that

$$|E^Q_{\mathrm{conf}} - E^{\mathrm{STF}}| \leqslant CB^{4/5}Z^{3/5}, \tag{I.49}$$

where the main contribution also stems from $r_S \sim Z^{1/5}B^{-2/5}$, the edge of the STF atom.

On the other hand the positive gradient correction orthogonal to the magnetic field in (I.46) produces a correction $O(B^{1/4}Z^{3/2})$ at a distance of order $B^{-1/2}$ from the nucleus. This part of the correction can also be obtained from an *isotropic Tomishima functional*, defined as

$$\mathcal{E}^{\mathrm{IT}}[\rho] = \mathcal{E}^{\mathrm{STF}}[\rho] + \frac{2\pi^4}{B^3}\int \rho(\nabla\rho)^2. \tag{I.50}$$

The functional (I.50) has all the good properties of the usual TF theories, such as convexity and boundedness from below. The study of this functional, which we do in detail in Sec. III A, should help us to get a deeper understanding of the nature of the positive correction term in (I.46). For the ground state energy of (I.50) we will derive the following theorem.

Theorem I.7: *For all B, Z and N/Z fixed*

$$E^{\mathrm{IT}}(N,Z,B) - E^{\mathrm{STF}}(N,Z,B) = O(B^{1/4}Z^{3/2}) + o(B^{1/4}Z^{3/2}). \tag{I.51}$$

Furthermore we will argue in Sec. III A that the $\rho(\nabla\rho)^2$ term remedies the defect of the STF theory that the full Coulomb potential is used although the particles in the lowest Landau band do not see the full singularity, since they are smeared over a region of radius $B^{-1/2}$. In contrast to TFW theory, where the maximal number N_c of electrons that can be bound is strictly larger than Z, it will as a slight surprise turn out that in IT theory $N_c = Z$, just like in the STF theory itself. Also, the radius of atoms in IT theory is finite, as in STF theory. These features confirm that the $\rho(\nabla\rho)^2$ term essentially only effects the density close to the nucleus.

2. Gradient correction for the discrete STF theory

As discussed previously, the gradient term $\sim\rho(\nabla_\perp\rho)^2$ in (I.46) produces essentially a smearing of the Coulomb singularities over a distance of the radius $B^{-1/2}$. The same effect was obtained by replacing STF by DSTF.

Thus, it appears natural to look for a negative gradient term that has an analogous effect in DSTF as the negative gradient term in (I.46) has in STF theory, i.e., provides corrections at the edge of the atom.

The DSTF theory is effectively a theory of coupled one-dimensional problems. Analogous arguments as lead to the von Weizsäcker term for a three-dimensional Fermi gas give for a one-dimensional Fermi gas a gradient correction—$\frac{1}{3}(\nabla\rho^{1/2})^2$, cf. Ref. 12. Hence we suggest the definition of a *discrete von Weizsäcker* functional:

$$\mathcal{E}^{\mathrm{DW}}[\rho]=\sum_{m\in\mathbb{N}_0}\left(-\frac{1}{3}\int|\partial_z\sqrt{\rho_m(z)}|^2+\kappa\int\rho_m^3(z)-Z\int V_m(z)\rho_m(z)\right)+\tilde{D}(\rho,\rho). \quad \text{(I.52)}$$

By denoting $\sqrt{\rho_m}=\psi_m$ we arrive, at under the restriction $\Sigma_m\int\psi_m^2=N$, the corresponding TF equation

$$(1/3)\partial_z^2\psi_n(z)+3\kappa\psi_n^5(z)=[\varphi_n(z)-\mu(N)]\psi_n(z), \quad \forall n\in\mathbb{N}_0, \quad \text{(I.53)}$$

with

$$\varphi_n(z)=ZV_n(z)-\sum_m\int\psi_m^2(z')V_{m,n}(z-z')\mathrm{d}z'.$$

These coupled equations are probably somewhat easier to deal with than (I.47).

If we reduce (I.52) to the angular momentum channel $m=0$ and drop the Coulomb repulsion term, we get the one-dimensional functional

$$\mathcal{E}^{\mathrm{1DW}}[\rho]=-\frac{1}{3}\int|\partial_z\sqrt{\rho(z)}|^2+\kappa\int\rho^3(z)-Z\int V_0(z)\rho(z). \quad \text{(I.54)}$$

This simplified functional will be studied in Sec. III C 2. In particular, we shall show that the negative gradient term reproduces the right QM correction to the energy without the gradient term.

II. THE MAGNETIC TFW THEORY

A. Mathematical analysis of the MTFW functional

In this section we are going to mathematically analyze the MTFW functional

$$\mathcal{E}^{\mathrm{MTFW}}[\rho]=A\int|\nabla\rho^{1/2}|^2+\int\tau_B(\rho)-\int V\rho+D(\rho,\rho). \quad \text{(II.1)}$$

Since the mathematical propositions do not depend on the parameter A, we let A be 1 in this section. The most important features of $\tau_B(t)$ which will be used in our calculations are (compare Ref. 1, Lemma 4.1):

$$\tau_B'(t)\leqslant\kappa_1 t^{2/3}, \quad \tau_B(t)\leqslant\tfrac{3}{5}\kappa_1 t^{5/3}, \quad \text{(II.2)}$$

with $\kappa_1=(4\pi^2)^{2/3}$.

Since the MTFW functional does not differ very much from the functional in Ref. 6, where the authors used a kinetic energy density $\tau(\rho)=(1/p)\rho^p$, our procedure in analyzing (I.20) will be in analogy to their work. We are thus concerned with the minimizing problem

$$\mathrm{Min}\left\{\mathcal{E}^{\mathrm{MTFW}}[\rho]\,|\,\rho\geqslant 0,\rho\in L^1\cap L^{5/3}_{\mathrm{loc}},\nabla\rho^{1/2}\in L^2 \quad \text{and} \quad \int\rho=N\right\}, \quad \text{(II.3)}$$

where N is a positive constant, which physically is the total charge number. Our main result is the following:

Theorem II.1: *There is a critical number* $0<N_c<\infty$, *so that*

(1) if $N\leqslant N_c$ *(II.3) has a unique minimizer,*
(2) if $N>N_c$ *(II.3) has no minimizer,*
(3) $N_c>Z$.

Similar to Ref. 6 we first examine the problem

$$\mathrm{Min}\{\mathcal{E}^{\mathrm{MTFW}}[\rho]|\rho\in D\} \tag{II.4}$$

with

$$D=\{\rho|\rho\geqslant 0,\tau_B(\rho)<\infty,\rho\in L^3,\nabla\rho^{1/2}\in L^2,D(\rho,\rho)<\infty\} \tag{II.5}$$

and prove the existence of a unique minimizer ρ_0. Since D contains the domain of (II.3) we have to show $\rho_0\in L^1(\mathbb{R}^3)$ in order to guarantee $N_c<\infty$. Furthermore we will derive $N_c>Z$, which shows that this theory allows negative ions. The proofs will be based on the Euler–Lagrange equation for $\psi=\sqrt{\rho_0}$.

First we consider some basic properties of (II.1).

Lemma II.2: For D defined in (II.5) we have

$$D\subset\{\rho|\rho\geqslant 0,\rho\in L^3\cap L^{5/3}_{\mathrm{loc}},\nabla\rho^{1/2}\in L^2,D(\rho,\rho)<\infty\}\equiv\overline{D}. \tag{II.6}$$

Proof: According to Ref. 1 (4.19) one gets for all $\Omega\subset\mathbb{R}^3$,

$$\int_\Omega\rho(x)^{5/3}\mathrm{d}x\leqslant\frac{1}{\kappa_3}\int_{\Omega_1}\tau_B(\rho(x))\mathrm{d}x+C\ \mathrm{Vol}(\Omega_2)<\infty$$

with $\Omega=\Omega_1\cup\Omega_2$.

Proposition II.3: The absolute minimum of $\mathcal{E}^{\mathrm{MTFW}}[\rho]$ is achieved for a unique $\rho_0\in D$.

Proof (cf. Ref. 6, Lemmas 2–5): Recall that, by definition (I.4), $\tau_B(t)$ is strictly convex, hence $\mathcal{E}^{\mathrm{MTFW}}[\rho]$ is strictly convex.

Let ρ_n be a minimizing sequence. There exists a constant C such that

$$\|\rho_n\|_3\leqslant C,\int\tau_B(\rho_n)\leqslant C,\|\nabla\rho_n^{1/2}\|_2\leqslant C,D(\rho_n,\rho_n)\leqslant C.$$

By the Banach–Alaoglu theorem we can extract a subsequence, still denoted as ρ_n, with

$$\rho_n\rightharpoonup\rho_0\quad\text{weakly in } L^3, \tag{II.7}$$

$$\nabla\rho_n^{1/2}\rightharpoonup\nabla\rho_0^{1/2}\quad\text{weakly in } L^2. \tag{II.8}$$

Since by use of Hölder's inequality $\|\rho_n^{1/2}\|_{H^1(\Omega)}\leqslant C(\Omega)$ and $H^1(\Omega)$ is relatively compact in $L^2(\Omega)$, if Ω is a bounded smooth domain, $\rho_n^{1/2}$ has a subsequence converging in $L^2(\Omega)$. Using Cantor's diagonal trick on a sequence of increasing Ω's we arrive at

$$\rho_n^{1/2}\to\rho_0^{1/2}\quad\text{a.e.} \tag{II.9}$$

By Fatou's Lemma we get

$$\liminf\int\tau_B(\rho_n)\geqslant\int\tau_B(\rho_0)\ \text{ and }\ \liminf D(\rho_n,\rho_n)\geqslant D(\rho_0,\rho_0).$$

Since L^p norms are weakly lower semicontinuous,

$$\liminf\int|\nabla\rho_n^{1/2}|^2\geqslant\int|\nabla\rho_0^{1/2}|^2.$$

Moreover, one can show, in analogy to Proposition III.3, that

$$\int V\rho_n\to\int V\rho_0,$$

so we altogether arrive at

$$\liminf \mathcal{E}^{\mathrm{MTFW}}[\rho_n] \geqslant \mathcal{E}^{\mathrm{MTFW}}[\rho_0]. \tag{II.10}$$

The uniqueness follows from the strict convexity of $\mathcal{E}^{\mathrm{MTFW}}[\rho]$. □

For the minimizing ρ_0 we now can derive an Euler–Lagrange equation. Denote $\psi = \sqrt{\rho_0}$.

Proposition II.4: The minimizing $\psi^2 = \rho_0$ satisfies

$$-\Delta\psi + \tau_B'(\psi^2)\psi = \varphi\psi, \tag{II.11}$$

in the sense of distributions, with $\varphi = V - \psi^2 * 1/|x|$.

Proof (cf. Ref. 6 Lemma 6): Note that $\psi^2 \in D$ implies $\varphi\psi, \tau_B'(\psi^2)\psi \in L^1_{\mathrm{loc}}$, which gives (II.11) a meaning in the sense of distributions. Consider the set

$$\tilde{D} \equiv \{\zeta | \zeta \in L^6 \cap L^{10/3}_{\mathrm{loc}}, \nabla\zeta \in L^2 \text{ and } D(\zeta^2, \zeta^2) < \infty\}. \tag{II.12}$$

If $\zeta \in \tilde{D}$ then $\rho = \zeta^2 \in D$ and

$$\mathcal{E}^{\mathrm{MTFW}}[\rho] = \int |\nabla\zeta|^2 + \int \tau_B(\zeta^2) - \int V\zeta^2 + D(\zeta^2, \zeta^2) \equiv \phi(\zeta).$$

We find $\phi(\psi) \leqslant \phi(\zeta)$ for all $\zeta \in \tilde{D}$. Let $\eta \in C_0^\infty$. Using the fact that $(\mathrm{d}/\mathrm{d}t)\,\phi(\psi + t\eta)|_{t=0} = 0$, we easily arrive at

$$-\int \psi\Delta\eta + \int \tau_B'(\psi^2)\psi\eta = \int \varphi\psi\eta. \tag{II.13}$$

□

Starting from Eq. (II.11) we can now step by step gain several properties for ψ.

Lemma II.5: ψ is continuous on $\mathbb{R}^3$, more precisely $\psi \in C^{0,\alpha}_{\mathrm{loc}}$ for all $\alpha \leqslant 1$.

Proof (cf. Ref. 6, Lemma 7): Since (II.11) yields $-\Delta\psi \leqslant \varphi\psi$, with $\varphi\psi \in L^{2-\delta}_{\mathrm{loc}}$, one gets $\psi \in L^\infty_{\mathrm{loc}}$ (e.g., by applying a result of Stampaccia in Ref. 13). Again using (II.11) the proposition follows by means of standard elliptic regularity theory (see Ref. 14, Theorem 10.2). □

Proposition II.6: $\psi \in L^2(\mathbb{R}^3)$.

Proof (cf. Ref. 6, Lemma 8): Assume, by contradiction, $\int \psi^2 = \infty$. Then we can choose an r, such that

$$\int_{|x| \leqslant r} \psi^2(x) \geqslant Z + 2\delta,$$

for some $\delta > 0$. Therefore

$$\psi^2 * |x|^{-1} \geqslant \int_{|x| \leqslant r} \psi^2(x)(|x| + |y|)^{-1}\,\mathrm{d}y \geqslant (Z + 2\delta)/(|x| + r),$$

which gives us

$$\varphi(x) = V(x) - \psi^2 * |x|^{-1} \leqslant \frac{Z}{|x| - r} - \frac{Z + 2\delta}{|x| + r},$$

with $|x| > r$. Thus there exists an $r_1 > r$, such that for $|x| > r_1$,

$$\varphi(x) \leqslant -\delta|x|^{-1}. \tag{II.14}$$

From (II.11) we get

$$-\Delta\psi+\delta|x|^{-1}\psi\leqslant 0 \tag{II.15}$$

for $|x|>r_1$. Now we choose a comparison density

$$\tilde{\psi}(x)=Me^{-2(\delta|x|)^{1/2}},$$

which satisfies

$$-\Delta\tilde{\psi}+\delta|x|^{-1}\tilde{\psi}\geqslant 0. \tag{II.16}$$

Hence by (II.15) and (II.16)

$$-\Delta(\psi-\tilde{\psi})+\delta|x|^{-1}(\psi-\tilde{\psi})\leqslant 0$$

for $|x|\geqslant r_1$. We fix M such that

$$\psi(r_1)\leqslant\tilde{\psi}(r_1).$$

If $\psi\to 0$ for $|x|\to\infty$, we immediately get

$$\psi\leqslant\tilde{\psi}\quad\text{for}\quad|x|>r_1 \tag{II.17}$$

from the maximum principle. The fact that $\int\tilde{\psi}^2<\infty$ and $\psi\in L^\infty_{\mathrm{loc}}$ contradicts our assumption. Unfortunately, we only know that $\psi\to\infty$ as $|x|\to\infty$ in a weak sense, namely $\psi\in L^6$, so the authors in Ref. 6 used a variant of Stampaccia's method to verify the statement of the Lemma, which also works in our case. □

Mimicking the proof of Ref. 6, Lemma 10 and using the fact that $\tau_B'(\psi^2)\psi-\varphi\psi$ is continuous but not differentiable we get

Lemma II.7: $\psi>0$ *everywhere and* $\psi\in C^2$, *except at* $x=0$.

Using (II.2) in the proof of Ref. 6, Lemma 11 and afterwards following the proof of Lemma 13 we additionally get

Proposition II.8: $N_c=\int\psi^2>Z$.

Before concluding the proof of Theorem II.1, we need a final lemma, which is the equivalent to Ref. 6, Lemma 14.

Lemma II.9: For every $N>0$ *we have* $\inf\{\mathcal{E}^{\mathrm{MTFW}}[\rho]\,|\,\rho\in\overline{D}\text{ and }\int\rho=N\}=\inf\{\mathcal{E}^{\mathrm{MTFW}}[\rho]\,|\,\rho\in\overline{D}\text{ and }\int\rho\leqslant N\}$.

Proof of Theorem II.1: For every N we set

$$E(N)\equiv\inf\left\{\mathcal{E}^{\mathrm{MTFW}}[\rho]\,\middle|\,\rho\in\overline{D}\text{ and }\int\rho\leqslant N\right\}.$$

Obviously $E(N)$ is nonincreasing and convex. The same proof as in Proposition II.3 shows that there exists a $\rho_N\in\overline{D}$ with $\int\rho_N\leqslant N$ and

$$\mathcal{E}^{\mathrm{MTFW}}[\rho_N]=E(N).$$

With $N_c=\int\psi^2$ it is clear that $E(N)$ is constant for $N>N_c: E(N)=E(N_c)$, while $E(N)$ is strictly decreasing on the interval $[0,N_c]$. For $N\leqslant N_c: \int\rho_N=N$, which implies that (II.3) has a unique solution. On the other hand we deduce from Lemma II.9 that for $N>N_c$ (II.3) has no solution, which concludes the proof of Theorem II.1. □

After having guaranteed the existence of a minimizing density ρ_N for (II.3), we can derive an Euler–Lagrange equation under the variational restriction $\int\rho=N$.

Proposition II.10: Denote $\psi=\rho_N^{1/2}$, *with* ρ_N *the minimizing density for*

$$\inf\left\{ \mathcal{E}^{\mathrm{MTFW}}[\rho] \middle| \rho \in \overline{D}, \int \rho = N \right\}$$

under the restriction $N \leqslant N_c$. *Then we have*

$$-\Delta\psi + \tau_B'(\psi^2)\psi - \varphi\psi = \mu(N)\psi, \tag{II.18}$$

where

$$\mu(N) = \frac{\mathrm{d}}{\mathrm{d}N} E(N). \tag{II.19}$$

Proof: The derivation of (II.18) works analogously to (II.11) apart from the difference that μ is the Lagrange parameter for the restriction $\int \rho = N$. We can infer

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathcal{E}^{\mathrm{MTFW}}[t\rho + (1-t)\rho_N]\Big|_{t=0} = \mu(N) \int (\rho_N - \rho), \tag{II.20}$$

which implies by means of convexity of the functional

$$\mathcal{E}^{\mathrm{MTFW}}[\rho_N] - \mathcal{E}^{\mathrm{MTFW}}[\rho] \geqslant \mu(N) \int (\rho_N - \rho),$$

or equivalently for every N',

$$E(N) - E(N') \geqslant \mu(N)(N - N'). \tag{II.21}$$

On the other hand we derive from (II.20)

$$\mathcal{E}^{\mathrm{MTFW}}[t\rho + (1-t)\rho_N] - \mathcal{E}^{\mathrm{MTFW}}[\rho_N] = t\mu(N) \int (\rho_N - \rho) + o(t),$$

which yields with $\rho = 2\rho_N$ and $\rho = 1/2\rho_N$, respectively,

$$E(N \pm tN) - E(N) \leqslant \pm \mu(N) tN + o(t). \tag{II.22}$$

Hence (II.21) and (II.22) together imply (II.19). □

Next we take a look at the behavior at infinity of the minimizing densities ρ_N. At least for $N < N_c$ one gets exponential decay.

Proposition II.11: (a) Let $\mu < 0$, *which is equivalent to* $N < N_c$, *then for every* $\delta > 0$, *with* $\mu < -\delta$, *there exists a constant* M, *such that, for the corresponding minimizer* $\psi = \rho_N^{1/2}$,

$$\psi \leqslant M e^{-\delta^{1/2}|x|}. \tag{II.23}$$

(b) Let $N = N_c$, *then for every* $\delta < N_c - Z$ *there is a constant* M, *such that*

$$\psi \leqslant M e^{-2(\delta|x|)^{1/2}}. \tag{II.24}$$

Proof: Note that we have not yet shown that $\psi \to 0$ as $|x| \to \infty$ in a strong sense, for we only know $\psi \in L^2$. From Eq. (II.18) we derive $-\Delta\psi \leqslant V\psi$, which implies $(-\Delta + I)\psi \leqslant (V + I)\psi$. Since we know $(V+I)\psi \in L^2$, recall that $(V+I) \in L^2 + L^\infty$ and $\psi \in L^2 \cap L^\infty$, we conclude from

$$\psi \leqslant (-\Delta + I)^{-1}[(V + I)\psi], \tag{II.25}$$

that $\psi \to 0$ at infinity, e.g., from the well-known fact (Ref. 15, Lemma II.25) that the convolution $f * g$ of two functions $f \in L^p, g \in L^g$, with $1/p + 1/q = 1$, goes to 0 at infinity.

(a) (See Ref. 16, Theorem 7.24.) Let $\delta<-\mu$. From (II.18) we get

$$(-\Delta+\delta)\psi=[-\tau_B'(\psi^2)+\varphi+\mu+\delta]\psi \tag{II.26}$$

and

$$\psi=(-\Delta+\delta)^{-1}[-\tau_B'(\psi^2)+\varphi+\mu+\delta]\psi. \tag{II.27}$$

Since $V,\psi\to 0$ as $|x|\to\infty$, there is an r_1, such that $[-\tau_B'(\psi^2)+\varphi+\mu+\delta]<0$ for $|x|>r_1$. This implies

$$\psi(x)\leqslant\int_{|y|\leqslant r_1}(4\pi|x-y|)^{-1}e^{-\delta^{1/2}|x-y|}([-\tau_B'(\psi^2)+\varphi+\mu+\delta]\psi)(y)\mathrm{d}y<\infty, \tag{II.28}$$

and (II.23) with

$$M=\sup_x e^{\delta^{1/2}r_1}\int_{|y|\leqslant r_1}(4\pi|x-y|)^{-1}([-\tau_B'(\psi^2)+\varphi+\mu+\delta]\psi)(y)\mathrm{d}y. \tag{II.29}$$

(b) This follows directly from (II.17) and the fact that $\psi\to 0$ as $|x|\to\infty$. □

We state a final proposition concerning the behavior of the chemical potential at $N=0$ (which is $-\infty$ in the usual TF theory), because of the simple and illuminating proof.

Proposition II.12: Let $e_0=-\frac{1}{4}Z^2$ be the smallest eigenvalue of the Schrödinger operator $-\Delta-Z/|x|$. Then

$$\mu(0)=\frac{\mathrm{d}}{\mathrm{d}N}E(N)_{N=0}=e_0. \tag{II.30}$$

Proof (cf. Ref. 6, Lemma 15): Let $\varphi(x)$ be the normalized eigenvector of $-\Delta-Z/|x|$ belonging to the lowest eigenvalue $e_0=-\frac{1}{4}Z^2$ and let $\rho_N=N\varphi(x)^2$. Then

$$\begin{aligned}E(N)\leqslant\mathcal{E}^{\mathrm{MTFW}}[\rho_N]&=\int|\nabla\rho_N^{1/2}|^2-\int V\rho_N+\int\tau_B(\rho_N)+D(\rho_N,\rho_N)\\&=N[(\varphi,-\Delta\varphi)-Z(\varphi,|x|^{-1}\varphi)]\\&\quad+\int\tau_B(\rho_N)+D(\rho_N,\rho_N)\leqslant Ne_0+C_1N^{5/3}+C_2N^2.\end{aligned}$$

On the other hand we have

$$E(N)\geqslant\inf_{\int\rho=N}\left\{\int|\nabla\rho^{1/2}|^2-\int V\rho\right\}=N\inf\ \mathrm{spec}\{-\Delta-Z|x|^{-1}\}=Ne_0,$$

which altogether implies

$$\lim_{N\to+0}\frac{E(N)}{N}=e_0.$$

Taking into account that $E(0)=0$ this is equivalent to (II.30). □

B. The Scott correction

If one takes a look at Lieb's proof[16] that in the usual TF theory without magnetic fields the von Weizsäcker term produces the Scott correction, one realizes that the main correction comes from distances of order Z^{-1} from the nucleus. It is thus reasonable to guess that in the MTF theory the

von Weizsäcker term produces the Scott correction as long as ρ^{MTF}, the density corresponding to the MTF energy (1.6), is well approximated by the usual TF density ρ^{TF} up to distances of order Z^{-1} from the nucleus. This condition is equivalent to the demand that $\tau_B'(\rho)$ is proportional to $\rho^{2/3}$ for $r\sim Z^{-1}$ and this is the case for $B\ll Z^2$. In other words, for $B\ll Z^2$ the von Weizsäcker term produces a Z^2 correction at the distance of order Z^{-1} from the nucleus. At the edge of the MTF atom, the radius is known[1] to be proportional to $Z^{1/5}B^{-2/5}$ and the lowest Landau band is occupied, which leads to $\tau_B'(\rho^{\mathrm{MTF}})=4\pi^4B^{-2}(\rho^{\mathrm{MTF}})^2$ in the outer region. Hence, one computes very easily, by using ρ^{MTF} as comparison density, that the correction coming from the edge of the atom is of order $B^{4/5}Z^{3/5}$.

Proof of Theorem I.4: First of all notice that there is an r_B, such that for $r\geqslant r_B$ the density ρ^{MTF} corresponds to the lowest Landau band, i.e.,

$$\tau_B'(\rho^{\mathrm{MTF}}(r))=\frac{4\pi^4}{B^2}(\rho^{\mathrm{MTF}}(r))^2 \quad \text{for} \quad r\geqslant r_B, \tag{II.31}$$

and for $r\leqslant r_B$ we have

$$\kappa_3(\rho^{\mathrm{MTF}}(r))^{2/3}\leqslant \tau_B'(\rho^{\mathrm{MTF}}(r))\leqslant \kappa_1(\rho^{\mathrm{MTF}}(r))^{2/3}, \tag{II.32}$$

with $\kappa_3=0.83(3\pi^2)^{2/3}$, which we get from Ref. 1, Lemma 4.1. Using (II.31) and (II.32) one realizes that if one fixes any $\varepsilon>0$ with $B\leqslant Z^{2-\varepsilon}$ there is a $\delta>0$ such that $r_B\geqslant Z^{\delta-1}$.

First we treat the case $B\leqslant Z^{7/4}$.

Lower bound: We know from Sec. II A that there exists a ρ_0 satisfying

$$E^{\mathrm{MTFW}}=\mathcal{E}^{\mathrm{MTFW}}[\rho_0]=\int \tau_B(\rho_0)+\int |\nabla\rho_0^{1/2}|^2-\int V\rho_0+D(\rho_0,\rho_0). \tag{II.33}$$

Denote $Z|x|^{-1}=V=\tilde{V}+H$, with

$$H=Z/r-Z^2/b \quad \text{for } r<b/Z \quad \text{and } 0 \quad \text{otherwise},$$

$$\tilde{V}=Z^2/b \quad \text{for } r<b/Z \quad \text{and } Z/r \quad \text{otherwise}.$$

Now let us rewrite the energy functional in the following way:

$$\mathcal{E}^{\mathrm{MTFW}}[\rho_0]=\int \tau_B(\rho_0)-\int \rho_0^{1/2}\Delta\rho_0^{1/2}-\int \rho_0^{1/2}\tilde{V}\rho_0^{1/2}-\int H\rho_0+D(\rho_0,\rho_0).$$

Observe that $-\Delta-H\geqslant \inf_\rho\{(\nabla\rho^{1/2},\nabla\rho^{1/2})-(\rho^{1/2},H\rho^{1/2})\}$, which by using Sobolev's inequality can be bounded from below by

$$-\Delta-H\geqslant \inf_\rho\{\|\rho\|_3^3-\|\rho\|_3\|H\|_{3/2}\}.$$

Since $\|H\|_{3/2}\sim b$ we can guarantee $-\Delta-H\geqslant 0$ with b small enough. Choosing such a b we derive

$$E^{\mathrm{MTFW}}\geqslant \mathcal{E}^{\mathrm{MTF}}[\rho_0,\tilde{V}]\geqslant E^{\mathrm{MTF}}[\tilde{V}]=\int \tau_B(\tilde{\rho})-\int \tilde{\rho}\tilde{V}+D(\tilde{\rho},\tilde{\rho})\geqslant E^{\mathrm{MTF}}[V]+\int H\tilde{\rho}.$$

The density $\tilde{\rho}$ minimizes $\mathcal{E}^{\mathrm{MTF}}[\rho,\tilde{V}]$ and therefore fulfills the TF equation:

$$\tau_B'(\tilde{\rho})=\tilde{V}-\tilde{\rho}*|x|^{-1}.$$

From Ref. 1, Lemma 4.1 we know that (II.32) is valid for all t with $t \geqslant (1/\sqrt{2}\pi^2)\, B^{3/2}$. So it is easy to see that $\tilde{\rho}$ fulfills (II.32) at least for $r \leqslant 1/Z$ and $B \leqslant Z^2$. Therefore we get that $\int H\tilde{\rho} = O(Z^2)$ for $B \leqslant Z^2$, which yields

$$E^{\mathrm{MTFW}} \geqslant E^{\mathrm{MTF}} + O(Z^2). \tag{II.34}$$

Upper bound: In order to get an upper bound we use a variational density ρ in the following way:

$$\rho(r) = \begin{cases} \overline{\rho}^{\mathrm{TF}}(Z^{-1}) & \text{for } r < Z^{-1} \\ \overline{\rho}^{\mathrm{TF}}(r) & \text{for } Z^{-1} \leqslant r \leqslant r_B \\ \rho^{\mathrm{MTF}}(r) & \text{for } r \geqslant r_B, \end{cases} \tag{II.35}$$

where $\overline{\rho}^{\mathrm{TF}}$ indicates that in the surrounding of $r = 1/Z$ we use the usual TF density ρ^{TF}. Only in the region $r_1 \leqslant r \leqslant r_B$, with $r_1 \geqslant 1/Z^{1-\delta}$, we eventually have to modify ρ^{TF}, such that

$$|E^{\mathrm{MTF}} - \mathcal{E}^{\mathrm{MTF}}[\rho]| \leqslant O(Z^2). \tag{II.36}$$

In fact we can construct ρ by following the way of Ref. 3, and taking a (at least C^2) modification W of the effective potential ϕ^{MTF} and defining $4\pi\overline{\rho}^{\mathrm{TF}} = \Delta(W - Z|x|^{-1})$. We set $W = \phi^{\mathrm{TF}}$ for $r \leqslant r_1$. This radius r_1 is given by the maximum value of $\overline{r}$ such that

$$\int_{1/Z \leqslant |x| \leqslant \overline{r}} |\nabla(\phi^{\mathrm{TF}} - \phi^{\mathrm{MTF}})|^2 \leqslant o(Z^2), \tag{II.37}$$

since[3] (0.55) tells us that

$$|E^{\mathrm{MTF}} - \mathcal{E}^{\mathrm{MTF}}[\rho]| = O(Z^2) + C \int_{1/Z \leqslant |x| \leqslant r_B} |\nabla(W - \phi^{\mathrm{MTF}})|^2. \tag{II.38}$$

For $B \ll Z^2$, r_1 can be guaranteed to be $\gg 1/Z$ (see Ref. 3, Proposition 1.6).

By this construction we are sure that the gradient term produces a Z^2-correction at the radius $r \sim 1/Z$. For larger r we just have to choose W such that the oscillations are not too large. For $r \geqslant r_B$ let W be equal to ϕ^{MTF} which is even C^∞ as long as $\phi^{\mathrm{MTF}} > 0$. Between r_1 and r_B we just have to construct W such that

$$\int_{1/Z \leqslant |x| \leqslant r_B} |\nabla(W - \phi^{\mathrm{MTF}})|^2 \leqslant o(Z^2) \tag{II.39}$$

under the condition that W is at least $\in C^2$ (but only $\notin C^3$ on a finite set of surfaces $r = |x|$) and

$$\int_{r_1 \leqslant |x| \leqslant r_B} |\nabla(\Delta W)^{1/2}|^2 \leqslant o(Z^2), \tag{II.40}$$

which is arrived by smoothing ϕ^{MTF}. So ρ is at least continuous and we get

$$\int_{r \leqslant r_B} |\nabla \rho^{1/2}|^2 = O(Z^2), \tag{II.41}$$

$$\int_{r \geqslant r_B} |\nabla \rho^{1/2}|^2 = O(B^{4/5} Z^{3/5}). \tag{II.42}$$

For $B \leqslant Z^{7/4}$ this leads to

$$E^{\mathrm{MTFW}} \leqslant E^{\mathrm{MTF}} + O(Z^2).$$

In the case $B \geqslant Z^{7/4}$ the correction from the edge of the atom overcomes the Scott correction and using a similar variational density as in (II.35) (recall that for $B \sim Z^2$, $r_B \sim 1/Z$) we get the simple estimate

$$0 \leqslant E^{\mathrm{MTFW}} - E^{\mathrm{MTF}} \leqslant O(B^{4/5} Z^{3/5}). \tag{II.43}$$

□

III. GRADIENT CORRECTIONS FOR STF-TYPE THEORIES

A. The functional (I.50)

The starting point in this section is the functional

$$\mathcal{E}^{\mathrm{IT}}[\rho] = \frac{1}{B^2}\int \rho^3 + \frac{1}{B^3}\int (\nabla \rho^{3/2})^2 - \int V\rho + D(\rho,\rho), \tag{III.1}$$

with V and $D(\rho,\rho)$ defined as in (I.3). Compared to (I.50) we rewrite

$$\frac{1}{B^3}\int \rho(\nabla\rho)^2 = \frac{4}{9B^3}\int (\nabla \rho^{3/2})^2,$$

and for simplicity forget about the numerical constant, which does not affect any mathematical statements. The corresponding energy is defined as

$$E(N,Z,B) = \inf\left\{ \mathcal{E}^{\mathrm{IT}}[\rho] \,\middle|\, \rho \in \tilde{D}, \int \rho \leqslant N \right\}, \tag{III.2}$$

where the domain $\tilde{D}$ is given by

$$\tilde{D} = \{\rho \,|\, \rho \geqslant 0, \rho \in L^1 \cap L^3, \nabla \rho^{3/2} \in L^2\}.$$

In analogy to Sec. II we first consider the problem

$$\mathrm{Min}\{\mathcal{E}^{\mathrm{IT}}[\rho] \,|\, \rho \in D\}, \tag{III.3}$$

with

$$D = \{\rho \,|\, \rho \geqslant 0, \rho \in L^3, \nabla \rho^{3/2} \in L^2, D(\rho,\rho) < \infty\} \tag{III.4}$$

and show that the minimum is achieved for a unique ρ_0. By means of the corresponding Euler–Lagrange equation we shall deduce that ρ_0 is in $L^1(\mathbb{R}^3)$, more precisely $\int \rho_0 = Z$.

First of all, we collect some properties of (III.1).

Lemma III.1: There are positive constants α, C, so that

$$\mathcal{E}^{\mathrm{IT}}[\rho] \geqslant \alpha\left(\|\rho\|_3 + \int \tau_B(\rho) + \|\nabla \rho^{3/2}\|_2^2 + D(\rho,\rho) \right) - C, \tag{III.5}$$

Proof: This is a consequence of Lemma 2 in Ref. 6, which tells us that for every $\varepsilon > 0$ there exists a constant C_ε so that

$$\int V\rho \leqslant \varepsilon \|\rho\|_3 + C_\varepsilon D(\rho,\rho)^{1/2}$$

for every $\rho \geqslant 0$. □

Lemma III.2: $\mathcal{E}^{\mathrm{IT}}[\rho]$ is strictly convex in ρ.

Proof: This follows immediately from the strict convexity of $(\nabla\rho^{3/2})^2$ and $\mathcal{E}^{\mathrm{STF}}$. □

By means of these Lemmas we can prove the existence of a unique minimizer in $\tilde{D}$.

Proposition III.3: The minimum of $\mathcal{E}^{\mathrm{IT}}[\rho]$ is achieved by a unique $\rho_0 \in \tilde{D}$.

Proof: The proof is similar to that of Proposition II.3. Let ρ_n be a minimizing sequence. By Lemma III.1 we have

$$\|\rho_n\|_3^3 \leqslant C, \quad \|\nabla\rho_n^{3/2}\|_2^2 \leqslant C, \quad D(\rho_n,\rho_n) \leqslant C. \tag{III.6}$$

With Banach–Alaoglu theorem we therefore extract a subsequence, still denoted by ρ_n, such that

$$\rho_n \rightharpoonup \rho_0 \quad \text{weakly in } L^3, \tag{III.7}$$

$$\nabla\rho_n^{3/2} \rightharpoonup \nabla\rho_0^{3/2} \quad \text{weakly} \quad \text{in } L^2. \tag{III.8}$$

Actually (III.6) implies $\nabla\rho_n^{3/2} \rightharpoonup f$ weakly in L^2, for a function $f \in L^2$. But for $\varphi \in C_c^\infty$ we conclude with (III.7)

$$\int f\varphi = \lim_{n\to\infty} \int \nabla\rho_n^{3/2}\varphi = -\lim_{n\to\infty} \int \rho_n^{3/2}\nabla\varphi = -\int \rho_0^{3/2}\nabla\varphi = \int \nabla\rho_0^{3/2}\varphi. \tag{III.9}$$

Furthermore $\rho_n^{3/2}$ is bounded in H^1, which implies that there exists a further subsequence, again denoted as ρ_n, with

$$\rho_n^{3/2} \to \rho_0^{3/2} \quad \text{a.e.}$$

[This relies on the fact that for a smooth bounded domain Ω, $H^1(\Omega)$ is relatively compact in $L^2(\Omega)$.] Hence, using Fatou's Lemma we get

$$\liminf D(\rho_n,\rho_n) \geqslant D(\rho_0,\rho_0),$$

and by the weak lower semicontinuity of L^p-norms we deduce

$$\liminf \int (\nabla\rho_n^{3/2})^2 \geqslant \int (\nabla\rho_0^{3/2})^2,$$

$$\liminf \int \rho_n^3 \geqslant \int \rho_0^3.$$

In order to prove $\int V\rho_n \to \int V\rho_0$, we decompose $V = V_1 + V_2$ such that both functions are in C^∞. With $V_1 \in L^{3/2}$, (III.7) implies

$$\int V_1\rho_n \to \int V_1\rho_0.$$

On the other hand V_2 fulfills

$$\int V_2\rho_n = \int V_2[-\Delta(\rho_N * |x|^{-1})] = \int (-\Delta V_2)(\rho_n * |x|^{-1}),$$

which converges to

$$\int (-\Delta V_2)(\rho_0 * |x|^{-1}) = \int V_2\rho_0$$

for $-\Delta V_2 \in L^{6/5}$ and $\|\rho_n * |x|^{-1}\|_6$ is bounded. [Note that the boundedness of $\|\rho_n * |x|^{-1}\|_6$ together with (III.7) imply that $\rho_n * |x|^{-1} \rightharpoonup \rho_0 * |x|^{-1}$ weakly in L^6.]

Thus

$$\liminf \mathcal{E}^{\mathrm{IT}}[\rho_n] \geqslant \mathcal{E}^{\mathrm{IT}}[\rho_0].$$

The uniqueness is an immediate consequence of the strict convexity of the functional. □

For this minimizing ρ_0 we can derive an Euler–Lagrange equation.

Proposition III.4: The minimizing $\psi = \rho_0^{3/2}$ satisfies

$$(-\Delta + B)\psi = \frac{B^3}{3}\varphi\psi^{-1/3}, \tag{III.10}$$

with $\varphi = V - \psi^{2/3} * 1/|x|$, in the sense of distributions, on the set where $\psi > 0$.

Proof: The uniqueness of the minimum, the spherical symmetry of the functional (III.1), and the fact that $\psi \in H^1$ imply the continuity of ψ away from the origin. With $\varphi \in L^2_{\mathrm{loc}}$ Eq. (III.10) has a meaning in the sense of distributions on the domain $\{x | \psi(x) > 0\}$. Consider the set

$$\overline{D} = \{\eta | \eta \in H^1, D(\eta^{2/3}, \eta^{2/3}) < \infty\}.$$

If $\eta \in \overline{D}$, then $\rho = (\eta^2)^{1/3} \in D$ and

$$\mathcal{E}^{\mathrm{IT}}[\rho] = \frac{1}{B^2}\int \eta^2 + \frac{1}{B^3}\int (\nabla\eta)^2 - \int V\eta^{2/3} + D(\eta^{2/3}, \eta^{2/3}) \equiv \phi(\eta).$$

For all $\eta \in \overline{D}$ we find $\phi(\psi) \leqslant \phi(\eta)$.

Let $\xi \in C_0^\infty$, then using $(\mathrm{d}/\mathrm{d}t)\,\phi(\psi + t\xi)|_{t=0} = 0$ we infer

$$-\int \psi\Delta\xi + B\int \psi\xi = \frac{B^3}{3}\int \varphi\psi^{-1/3}\xi.$$

□

Proposition III.5: ψ is bounded and ψ is in C^∞ away from the origin and possible points with $\psi(x) = 0$.

Proof: Denote

$$\Omega_\epsilon = \{x | \psi(x) \geqslant \epsilon\}.$$

On this domain we have

$$(-\Delta + B)\psi = f,$$

with $f \in L^2_{\mathrm{loc}}$, since $\varphi \in L^2_{\mathrm{loc}}$. So we conclude from standard elliptic arguments (e.g., [LL] Sec. 10 that ψ is bounded, hence continuous everywhere. From

$$\Delta\varphi = 4\pi(\psi^{2/3}(x) - Z\delta(x))$$

we get the two times differentiability of φ away from the origin and as long as $\psi > 0$. By means of (III.10) and a standard bootstrap argument we conclude $\psi \in C^\infty$. □

Theorem III.6: $\int \psi^{2/3} = Z$.

Proof: Suppose by contradiction $\int \psi^{2/3} = \lambda \neq Z$. We do not assume λ to be finite. Then, as in (II.14), we get that there is some r_1 and an $\epsilon > 0$, such that

$$|\varphi(x)| \geqslant \epsilon/r = \epsilon/|x|, \tag{III.11}$$

for $|x| \geqslant r_1$. [Actually (III.11) follows for $\lambda > Z$. For $\lambda < Z$ we use Newton's theorem.]

We know $\psi \in L^2$ and $\psi(x) = \psi(|x|) = \psi(r)$. Therefore, let us choose $\mathcal{M} = \{r | \psi(r) \leqslant M/r^{3/2}\} \subset \mathbb{R}$ for an arbitrary but fixed $M > 0$. This leads to

$$\infty > \int_{\mathbb{R}^3} |\psi(x)|^2 dx = 4\pi \int_{\mathcal{M}} |\psi(r)|^2 r^2 dr + 4\pi \int_{\mathcal{M}' = \mathbb{R} \setminus \mathcal{M}} |\psi(r)|^2 r^2 dr$$

$$\geqslant 4\pi \int_{\mathcal{M}} |\psi(r)|^2 r^2 dr + 4\pi M^2 \int_{\mathcal{M}'} 1/r dr. \tag{III.12}$$

Consequently $\int_{\mathcal{M}'} 1/r dr < \infty$ and $\int_{\mathcal{M}} 1/r dr = \infty$.

Next we take an auxiliary function $\nu(r) = 1/(1+r^2)$, which is obviously in $H^1(\mathbb{R}^3)$, multiply (III.10) by $\nu(|x|)$ and integrate over $\mathbb{R}^3$. We get

$$\int \nabla \psi \cdot \nabla \nu + B \int \psi \nu = \frac{B^3}{3} \int \varphi \psi^{-1/3} \nu. \tag{III.13}$$

It is a well known fact that φ changes sign at most once. So, either $\varphi(r) > \epsilon/r$ and the right side of (III.13) reads

$$\int_{\mathbb{R}^3} \varphi \psi^{-1/3} \nu \geqslant \epsilon M^{-1/3} \int_{\mathcal{M}} \nu(r) r^{-1/2} r^2 dr = \infty, \tag{III.14}$$

or $\varphi(r) \geqslant -\epsilon/r$ for $r \leqslant r_1$, then

$$\int_{\mathbb{R}^3} \varphi \psi^{-1/3} \nu \leqslant \text{const.} - \epsilon M^{-1/3} \int_{\mathcal{M} \cap |x| \geqslant r_1} \nu(r) r^{-1/2} r^2 dr = -\infty. \tag{III.15}$$

Both cases are a contradition to ψ and $\nu \in H^1$. □

Remark III.7: Theorem III.6 is interesting, since gradient corrections usually give rise to binding of additional electrons. The reason that this is not the case in III.6 relies on the negative exponent of ψ on the right-hand side of (III.10). This fact forces the potential φ to fall off much faster than $O(1/r)$.

Since we only consider atoms with a point nucleus, we get the following remark for the minimizing ρ_0.

Proposition III.8: ρ_0 is a symmetric nonincreasing function of $|\mathbf{x}|$.

Proof: As we have already argued, the symmetry of ρ_0 follows from the symmetry of the functional and the uniqueness of ρ_0.

Denote ρ_0^* the nonincreasing rearrangement of ρ_0. (For a definition see, e.g., Ref. 14, Sec. 3.3.) From the fact that $\int \rho_0 \leqslant Z$ and Ref. 16, Theorem 2.12 we get $\mathcal{E}^{\text{STF}}[\rho_0^*] \leqslant \mathcal{E}^{\text{STF}}[\rho_0]$.[14] Lemma 7.17 implies

$$\int |\nabla (\rho_0^{3/2})^*|^2 \leqslant \int |\nabla (\rho_0^{3/2})|^2 \tag{III.16}$$

and again from Ref. 14, 3.3 (v) we get $(\rho_0^{3/2})^* = (\rho_0^*)^{3/2}$, which proves the statement. □

Proposition III.9: ψ has compact support.

Proof: Inserting $\Delta \varphi = \psi^{2/3}$ into (III.10) yields the following equation for the potential, away from the origin:

$$(\Delta \varphi)^{1/2} [\Delta (\Delta \varphi)^{3/2}] = (\Delta \varphi)^2 - \varphi, \tag{III.17}$$

where we replaced the constants by one. Since φ is spherical symmetric we can use the ansatz $\varphi = (1/r)\chi(r)$ and obtain by (III.17) the following fourth-order equation:

$$2\left[\frac{1}{r^4}\chi''^2-\frac{2}{r^3}\chi''\chi'''+\frac{1}{r^2}\chi'''^2\right]^2+\left[\frac{1}{r}\chi''\right]^2\left[\frac{1}{r}\chi''''\right]^2+\left[\frac{1}{r^4}\chi''^2-\frac{2}{r^3}\chi''\chi'''+\frac{1}{r^2}\chi'''^2\right]\left[\frac{1}{r}\chi''\right]\left[\frac{1}{r}\chi''''\right]$$
$$=\frac{4}{9}\left[\frac{1}{r^2}\chi^2-\frac{2}{r^3}\chi\chi''^2+\left(\frac{1}{r}\chi''\right)^4\right]. \tag{III.18}$$

We can see that in the surrounding of each point $r_0>0$ there exists a local solution

$$\chi=a_6(r-r_0)^6+O((r-r_0)^7),$$

with $a_6=(\text{const})r_0^2$. Since $\chi\equiv 0$ is also a solution of (III.18), every composed function

$$\chi=a_6(r-r_0)^6+O((r-r_0)^7) \quad \text{for } r\leqslant r_0, \quad \chi\equiv 0 \quad \text{for } r>r_0$$

is a local solution around r_0.

Away from 0 the solutions can be uniquely continued up to $r=0$. Hence, there exists a solution χ and a $r_1>0$, such that $\chi(0)=Z$ and $\operatorname{supp}\chi=[0,r_1]$.

Repeating the argument of Ref. 16, Theorem 2.6, one can show that a solution of (III.10), with $\psi\in H^1$ and $\int\psi^{2/3}<\infty$, $(\psi^2)^{1/3}$ uniquely determines the minimum of the functional (III.1). Therefore $\chi(r)$ uniquely determines the self-consistent potential $\phi=\chi/r$, which implies that $\psi=\rho_0^{3/2}=(\Delta\phi)^{3/2}$ has compact support, too. □

Remark III.10: The preceding three propositions are equivalent to those for the STF theory. This confirms that the $\rho(\nabla\rho)^2$ term only amounts to changes close to the nucleus.

By the convexity of the functional (III.1) one easily derives the following properties for the energy $E^{\mathrm{IT}}(N,Z,B)$:

Proposition III.11: $E^{\mathrm{IT}}(N,Z,B)$ is convex as a function of N and strictly monoton decreasing on the interval $[0,Z]$. For $N>Z$ we get $E^{\mathrm{IT}}(N,Z,B)=E^{\mathrm{IT}}(Z,Z,B)$.

Next we prove Theorem I.7.

Proof of Theorem I.7: Upper bound: We use the comparison density $\overline{\rho}$, with

$$\overline{\rho}(r)=\begin{cases}\rho^{\mathrm{STF}}(l_B) & \text{for } r\leqslant l_B=B^{-1/2}\\ \rho^{\mathrm{STF}}(r) & \text{otherwise}\end{cases} \tag{III.19}$$

and immediately get

$$E^{\mathrm{IT}}\leqslant E^{\mathrm{STF}}+O(Z^{3/2}B^{1/4}).$$

Lower bound: Let ρ be the minimizer of the energy (III.2), for given B,Z,N. We can rewrite

$$E^{\mathrm{IT}}=\mathcal{E}^{\mathrm{IT}}[\rho]=\frac{\kappa}{B^2}\int\rho^3+\frac{1}{B^3}\int|\nabla\rho^{3/2}|^2-\int\tilde{H}\rho-\int\tilde{V}\rho+D(\rho,\rho),$$

where $\tilde{H}=Z/r-B^{1/2}Z/b$ for $r\leqslant bl_B$ and 0 otherwise, $\tilde{V}=B^{1/2}Z/b$ for $r\leqslant bl_B$ and Z/r otherwise. Looking at the term

$$\frac{1}{B^3}\int|\nabla\rho^{3/2}|^2-\int\tilde{H}\rho,$$

we infer by means of the Sobolev inequality the estimate

$$\frac{1}{B^3}\int|\nabla\rho^{3/2}|^2-\int\tilde{H}\rho\geqslant\frac{4}{9B^3}\|\rho\|_9^3-\|\tilde{H}\|_{9/8}\|\rho\|_9. \tag{III.20}$$

Since $\|\tilde{H}\|_{9/8}\sim b^{15/9}$ we can choose b such that (III.20)>0. Hence

$$E^{\mathrm{IT}} \geqslant \frac{\kappa}{B^2}\int \rho^3 - \int \tilde{V}\rho + D(\rho,\rho) \geqslant E^{\mathrm{STF}}[\tilde{V}] = \mathcal{E}^{\mathrm{STF}}[\tilde{V},\tilde{\rho}] \geqslant E^{\mathrm{STF}} + \int \tilde{\rho}\tilde{H}.$$

Since $\int \tilde{\rho}\tilde{H} = O(Z^{3/2}B^{1/4})$ we prove the proposition. □

We see that the main contribution of the correction (1.50) comes from the radius $l_B = B^{-1/2}$, in other words the gradient correction repairs the infinity of the STF density at a distance $B^{-1/2}$ from the nucleus. This infinity stems from the fact that in the STF theory the full $|x|^{-1}$ potential is involved, although particles in the lowest Landau band, which are smeared over a radius of at least $B^{-1/2}$, never see the full Coulomb singularity.

Moreover, the Tomishima–Shinjo correction (1.46) orthogonal to the magnetic field remedies the singularity of the Coulomb potential in a similar way as the isotropic gradient term. We will see that the same effect, as caused by (III.1) and (1.46), is also naturally obtained by using the DSTF functional.

B. A discrete von Weizsäcker functional

1. The DSTF functional

First of all we are going to collect some information about the DSTF functional (which is rigorously proved in a companion work). The DSTF functional

$$\mathcal{E}^{\mathrm{DSTF}}[\rho] = \sum_{m\in\mathbb{N}_0}\left(\kappa\int \rho_m^3(z) - \int V_m(z)\rho_m(z)\mathrm{d}z\right) + \tilde{D}(\rho,\rho), \tag{III.21}$$

with V_n and $V_{m,n}$ as in (I.35), is defined on the domain

$$D = \left\{\rho \,\middle|\, \sum_m \int \rho_m^3 < \infty, \sum_m \int \rho_m < \infty, \tilde{D}(\rho,\rho) < \infty\right\} \tag{III.22}$$

with corresponding energy

$$E^{\mathrm{DSTF}}(N,Z,B) = \inf\left\{\mathcal{E}^{\mathrm{DSTF}}[\rho] \,\middle|\, \rho\in D \text{ and } \sum_m \int \rho_m \leqslant N\right\}. \tag{III.23}$$

Following the considerations of Ref. 1 one can easily see that (III.21) is convex and bounded from below on $D^N = \{\rho | \rho \in D, \Sigma_m \int \rho_m \leqslant N\}$ and derive the following Theorem:

Theorem III.12: *With $N \leqslant Z$ fixed there exists a unique minimizer ρ^N for $\mathcal{E}^{\mathrm{DSTF}}$, under the restriction $\Sigma_m \int \rho_m \leqslant N$,* i.e., *$E^{\mathrm{DSTF}}(N,Z,B) = \mathcal{E}^{\mathrm{DSTF}}[\rho^N]$. Moreover, ρ^N satisfies $\Sigma_m \int \rho_m^N = N$.*

Furthermore each minimizer ρ^N obeys the coupled TF equations

$$3\kappa(\rho_m^N(z))^2 = \left[ZV_m(z) - \sum_n \int V_{m,n}(z-z')\rho_n^N(z') + \mu(N)\right]_+ \forall (m\in\mathbb{N}_0), \tag{III.24}$$

where $\mu(N)$ is the Lagrange parameter belonging to the restriction $\Sigma_m \int \rho_m = N$ and $[\ ]_+$, with $[t]_+ = t$ for $t \geqslant 0$ and $[t]_+ = 0$ otherwise, corresponds to the fact that the functional is only varied over positive functions, i.e., $\rho_n \geqslant 0 \forall n \in \mathbb{N}_0$.

By means of the notation

$$ZV_m(z) - \sum_n \int V_{m,n}(z-z')\rho_n^N(z') + \mu(N) = \varphi_{\mathrm{eff}}^{(m)}(z) \tag{III.25}$$

and inserting in the TF equation we can rewrite the energy $E^{\mathrm{DSTF}}(N,Z,B) = \mathcal{E}^{\mathrm{DSTF}}[\rho^N]$ as

$$E^{\mathrm{DSTF}}(N,Z,B)=\sum_m \int\int [p^2-\varphi_{\mathrm{eff}}^{(m)}(z)]_- \frac{\mathrm{d}p\,\mathrm{d}z}{2\pi}+N\mu-\tilde{D}(\rho^N,\rho^N). \tag{III.26}$$

2. Semiclassical approximation of E^Q_{conf}

First of all we want to state a useful theorem concerning the sum of the negative eigenvalues of the one-particle operator $\Pi_0[H_A+\varphi]\Pi_0$, where $H_A=((-i\nabla+\mathbf{A}(x))\cdot\sigma)^2$ and φ is an axially symmetric potential $\varphi(r,z)$ with $r=|\mathbf{x}_\perp|$.

Theorem III.13: *Let $\varphi=\varphi(r,z)$ be axially symmetric. Then one can write the trace of the negative part of the operator $\Pi_0[H_A+\varphi]\Pi_0$ as the sum of one-dimensional traces,* i.e.,

$$\mathrm{Tr}[\Pi_0[H_A+\varphi]\Pi_0]_-=\sum_{m\in\mathbb{N}_0}\mathrm{Tr}_{L^2(\mathbb{R})}[-\partial_z^2+\varphi^{(m)}(z)]_-, \tag{III.27}$$

with

$$\varphi^{(m)}(z)=\int \varphi(x)|\phi_m(\mathbf{x}_\perp)|^2\mathrm{d}\mathbf{x}_\perp. \tag{III.28}$$

Proof: Let L_z denote the angular momentum operator parallel to the magnetic field. Since $\varphi=\varphi(r,z)$, we have

$$[\Pi_0[H_A+\varphi]\Pi_0,L_z]=0, \tag{III.29}$$

which implies that the eigenvectors of the operator $\Pi_0[H_A+\varphi]\Pi_0$ are of the form $|m,i\rangle=\phi_m(\mathbf{x}_\perp)f_m^i(z)$.

Hence we can write the sum of the negative eigenvalues as

$$\begin{aligned}\mathrm{Tr}[\Pi_0[H_A+\varphi]\Pi_0]_-&=\sum_{m,i}\langle m,i|[\Pi_0[H_A+\varphi]\Pi_0]|m,i\rangle\\&=\sum_m\left(\sum_i (f_m^i,[-\partial_z^2+\varphi^{(m)}(z)]f_m^i)\right),\end{aligned} \tag{III.30}$$

showing that the f_m^i's are the eigenvectors of the one-dimensional operator $-\partial_z^2+\varphi^{(m)}(z)$.

Proposition III.14: Let N,Z,B be fixed. Then

$$E^Q_{\mathrm{conf}}(N,Z,B)\leqslant E^{\mathrm{DSTF}}(N,Z,B)+R_1+R_2+R_3, \tag{III.31}$$

$$E^Q_{\mathrm{conf}}(N,Z,B)\geqslant E^{\mathrm{DSTF}}(N,Z,B)-R_1-C\int\rho_\psi^{4/3}, \tag{III.32}$$

with

$$R_1=\left|\sum_{m\in\mathbb{N}_0}\left(\mathrm{Tr}_{L^2(\mathbb{R})}[-\partial_z^2-\varphi_{\mathrm{eff}}^{(m)}(z)]_- -\int\int[p^2-\varphi_{\mathrm{eff}}^{(m)}(z)]_-\frac{\mathrm{d}p\,\mathrm{d}z}{2\pi}\right)\right|, \tag{III.33}$$

$$R_2=D(\rho_\psi-\tilde{\rho},\rho_\psi-\tilde{\rho}), \tag{III.34}$$

$$R_3=\sum_{\lambda_N<\lambda_i<\mu(N)}|(\lambda_i-\mu(N))|, \tag{III.35}$$

where λ_i and $\tilde{\rho}$ are defined in the proof.

Proof: Upper bound: First of all we note that for any Slater determinant ψ and fixed integer N we get

$$E^Q_{\mathrm{conf}} \leqslant (\psi, \Pi_0^N H_N \Pi_0^N \psi) \leqslant \sum_{i=1}^{N} (\psi, \Pi_0^N [H_A(\mathbf{x}_i) - Z|\mathbf{x}_i|^{-1}] \Pi_0^N \psi) + D(\rho_\psi, \rho_\psi), \qquad \text{(III.36)}$$

with

$$\rho_\psi(\mathbf{x}) = N \sum_{s^i} \int |\psi(\mathbf{x}, x_2, .., x_N; s^1, .., s^N)|^2 \mathrm{d}x_2 \ldots \mathrm{d}x_N .$$

If we set $\tilde{\rho}(\mathbf{x}) = \Sigma_m |\phi_m(\mathbf{x}_\perp)|^2 \rho_m^N(z)$, add and subtract $\tilde{\rho} * |\mathbf{x}|^{-1} - \mu(N)$ in the scalar product, and use $\psi = (1/\sqrt{N!})\, \phi_1 \wedge \cdots \wedge \phi_N$, where ϕ_i is the eigenvector corresponding to the ith lowest eigenvalue λ_i of the one-particle operator

$$\Pi_0 (H_A - Z|\mathbf{x}|^{-1} + \tilde{\rho} * |\mathbf{x}|^{-1} - \mu(N)) \Pi_0 , \qquad \text{(III.37)}$$

as comparison wave function, (III.36) reads

$$E^Q_{\mathrm{conf}} \leqslant \mathrm{Tr}[\Pi_0 (H_A - Z|\mathbf{x}|^{-1} + \tilde{\rho} * |\mathbf{x}|^{-1} - \mu(N)) \Pi_0]_- - 2D(\rho_\psi, \tilde{\rho}) + D(\rho_\psi, \rho_\psi) + N\mu(N)$$
$$+ \sum_{\lambda_N < \lambda_i < \mu(N)} |(\lambda_i - \mu(N))|. \qquad \text{(III.38)}$$

Applying Theorem III.13 and (III.26) to the above-mentioned inequality, we finally arrive at the upper bound (III.36).

Lower bound: Let ψ denote the minimizer of (I.22), i.e., $\psi = \psi_{\mathrm{conf}}$. So after again adding and subtracting $\tilde{\rho} * |\mathbf{x}|^{-1} - \mu(N)$ and using the Lieb–Oxford inequality,[17] we can write the lower bound on E^Q_{conf} as follows:

$$\begin{aligned} E^Q_{\mathrm{conf}} = (\psi, \Pi_0^N H_N \Pi_0^N) &\geqslant \sum_{i=1}^{N} (\psi, \Pi_0^N [H_A(\mathbf{x}_i) - Z|\mathbf{x}_i|^{-1} + \tilde{\rho}^* |\mathbf{x}_i|^{-1} - \mu(N)] \Pi_0^N \psi) + D(\rho_\psi, \rho_\psi) \\ &\quad + N\mu(N) - 2D(\rho_\psi, \tilde{\rho}) - C \int \rho_\psi^{4/3} \\ &\geqslant \mathrm{Tr}[\Pi_0 (H_A - Z|\mathbf{x}|^{-1} + \tilde{\rho} * |\mathbf{x}|^{-1} - \mu(N)) \Pi_0]_- + N\mu \\ &\quad - D(\tilde{\rho}, \tilde{\rho}) - C \int \rho_\psi^{4/3} . \end{aligned} \qquad \text{(III.39)}$$

Using (III.26) we arrive at (III.32).

Remark III.15: Due to (III.31) and (III.32) the main contribution to the difference between E^Q_{conf} and E^{DSTF} is given by

$$R_1 = \left| \sum_{m \in \mathbb{N}_0} \left(\mathrm{Tr}_{L^2(\mathbb{R})}[-\partial_z^2 - \varphi_{\mathrm{eff}}^{(m)}(z)]_- - \int \int [p^2 - \varphi_{\mathrm{eff}}^{(m)}(z)]_- \frac{\mathrm{d}p\mathrm{d}z}{2\pi} \right) \right|, \qquad \text{(III.40)}$$

which, by definition, shows that E^{DSTF} is the natural semiclassical approximation of E^Q_{conf}.

As a corollary, e.g., by following the way of Ref. 1 and using coherent states and the above-mentioned estimates, or simply by estimating the difference between E^{DSTF} and E^{STF} one gets

Corollary III.16: If $Z \to \infty$ with N/Z fixed and $B/Z^3 \to 0$, then $E^Q_{\mathrm{conf}}(N,Z,B)/E^{\mathrm{DSTF}}(N,Z,B) \to 1$.

The DSTF theory is equivalent to a three-dimensional functional using *modified* Coulomb potentials,

$$V_\chi(\mathbf{x})=\sum_n \chi^n(\mathbf{x}_\perp)V_n(z) \tag{III.41}$$

replacing the attractive Coulomb potential and

$$\sum_{m,n} V_{n,m}(z-z')\chi_n(\mathbf{x}_\perp)\chi_m(\mathbf{x}'_\perp) \tag{III.42}$$

replacing the Coulomb repulsion, with

$$\chi^n(\mathbf{x}_\perp)=\begin{cases}1 & \text{for } \sqrt{(2n)/B}\leqslant|x_\perp|\leqslant\sqrt{2(n+1)/B}\\ 0 & \text{otherwise.}\end{cases} \tag{III.43}$$

For example, for the respective minimizing density of a resulting MSTF functional, we have $\rho^{\mathrm{MSTF}}(\mathbf{x})=(B/2\pi)\,\Sigma_m\rho_m^{\mathrm{DSTF}}(z)\chi_m(x_\perp)$ as well as $E^{\mathrm{MSTF}}=E^{\mathrm{DSTF}}$ for the energy.

Since $V_\chi(0)\sim B^{1/2}$, $V_\chi(\mathbf{x})$ can be regarded as a cutoff Coulomb potential

$$\overline{V}(\mathbf{x})=\begin{cases}B^{1/2} & \text{for } |\mathbf{x}|\leqslant B^{-1/2},\\ |\mathbf{x}|^{-1} & \text{for } |\mathbf{x}|\geqslant B^{-1/2}.\end{cases} \tag{III.44}$$

Hence, it is obvious that the main contribution to the difference $E^{\mathrm{DSTF}}-E^{\mathrm{STF}}$ stems from the Coulomb potential in the region $r\leqslant B^{-1/2}$, given by the term

$$B\int_{0\leqslant r\leqslant B^{-1/2}}|\phi^{\mathrm{STF}}|^{3/2}=O(B^{1/4}Z^{3/2}), \tag{III.45}$$

which leads to the relation

$$E^{\mathrm{DSTF}}(N,Z,B)-E^{\mathrm{STF}}(N,Z,B)=O(B^{1/4}Z^{3/2}). \tag{III.46}$$

The comparison with Theorem I.7 shows that the DSTF theory has the same effect as the introduction of the gradient correction in (I.50) as well as in (I.46).

C. The discrete von Weizsäcker functional

The variable of the DSTF functional is given by a sum of one-dimensional densities, emphasizing the character of lowest Landau band particles, whose positions orthogonal to the magnetic field are ''frozen'' and they therefore only move parallel to the magnetic field. Now taking into account the result (see, e.g., Shao[12]) that the first-order correction to the semiclassical description of the one-dimensional free Fermi gas is given by $-(1/3)\int(\partial_z\sqrt{\rho(z)})^2$, we are motivated to propose the already mentioned *discrete von Weizsäcker functional*

$$\mathcal{E}^{\mathrm{DW}}[\rho]=\sum_{m\in\mathbb{N}_0}\left(-\frac{1}{3}\int|\partial_z\sqrt{\rho_m(z)}|^2+\kappa\int\rho_m^3(z)-Z\int V_m(z)\rho_m(z)\right)+\widetilde{D}(\rho,\rho). \tag{III.47}$$

Since the von Weizsäcker term appears with negative sign, (III.47) has the same defects as the Tomishima–Shinjo functional (I.46), i.e. it is not bounded from below and not convex. Precisely these two features (boundedness and convexity) of the semiclassical TF functionals, as well the (M)TFW functional, provided not only the existence of a minimizer but the existence of a solution of the corresponding TF equation.

As a way out of this problem we can define the energy corresponding to (III.47) by means of stationary solutions ρ^N, whose variational derivative vanishes under the restriction $\Sigma_m \int \rho_m = N$ and $\rho \geqslant 0$. In order to avoid the assumption of positivity we concentrate on real functions ψ, with $\psi^2 = \rho$ and consider the functional

$$\mathcal{E}[\psi] = \sum_{m \in \mathbb{N}_0} \left(-\frac{1}{3} \int |\partial_z \psi_m(z)|^2 + \kappa \int \psi_m^6(z) - Z \int V_m(z) \psi_m^2(z) \right) + \tilde{D}(\psi^2, \psi^2). \quad \text{(III.48)}$$

Let

$$D = \left\{ \psi \middle| \sum_m \int \psi_m^2 < \infty, \sum \int \psi_m^6 < \infty, \quad \text{and} \quad \sum_m \int (\partial_z \psi_m)^2 < \infty \right\} \quad \text{(III.49)}$$

be the domain of (III.48). The question for stationary points in D, under the restriction $\Sigma_m \int \psi_m^2 = N$, is equivalent to the existence of a Lagrange parameter $\mu(N)$ and a ψ^N, so that

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\mathcal{E}[\psi^N + t\eta] + \mu(N) \int (\psi^N + t\eta)^2 \right) \Big|_{t=0} = 0, \quad \text{(III.50)}$$

for each $\eta \in D$. (III.50) yields the Euler–Lagrange equation, denoting $\psi^N = \psi$,

$$(1/3) \partial_z^2 \psi_m(z) + 3\kappa \psi_m^5(z) = [\varphi_{\text{eff}}^{(m)}(z) - \mu(N)] \psi_m(z) \quad \forall m \in \mathbb{N}_0. \quad \text{(III.51)}$$

Starting from (III.48), (III.51) *a priori* only exists in the sense of distributions, but if there is a solution for (III.48) then one can conclude that it is even in $C^\infty(\mathbb{R}\backslash\{0\})$. If there is a solution ψ^N for $N \in [0, N_c]$, with $N_c \geqslant Z$, then we can define the corresponding energy by

$$E^{\text{DW}}(N, Z, B) = \mathcal{E}[\psi^N] = \mathcal{E}^{\text{DW}}[(\psi^N)^2]. \quad \text{(III.52)}$$

1. Recovering the exchange term

Now we even go a step further. Following the reflections of Sec. I C 1 concerning the magnitude of the negative von Weizsäcker term we guess that $\mathcal{E}^{\text{DW}}$ is equivalent to the DDM functional (1.33) for $B \ll Z^3$. Hence looking at (I.42) we suggest another functional,

$$\mathcal{E}^{\text{DWHF}}[\rho] = \sum_{m \in \mathbb{N}_0} \left(-(1/3) \int \left| \partial_z \sqrt{\rho_m(z)} \right|^2 + \kappa \int \rho_m^3(z) - Z \int V_m(z) \rho_m(z) \right.$$
$$\left. - c \ln \left(\frac{B^{1/2} \int \rho_m}{\int \rho_m^2} \right) \int \rho_m^2 \right) + \tilde{D}(\rho, \rho), \quad \text{(III.53)}$$

where we recover the exchange energy, which could be compared with the Thomas–Fermi–Dirac–von Weizsäcker functional[16] in the $B = 0$ case.

2. The one-dimensional DW functional

In this section we study a toy model obtained by reducing (I.52) to a one-dimensional functional and dropping the Coulomb repulsion, which leads to the functional

$$\mathcal{E}^{\text{1DW}}[\rho] = -\frac{1}{3} \int |\partial_z \sqrt{\rho(z)}|^2 + \kappa \int \rho^3(z) - Z \int V_0(z) \rho(z). \quad \text{(III.54)}$$

First of all we consider the corresponding TF functional

$$\mathcal{E}_{B,Z}^{\text{1D}}[\rho] = \kappa \int \rho^3(z) - Z \int V_0(z) \rho(z), \quad \text{(III.55)}$$

for which we easily get the following lemma:

Lemma III.17: $\mathcal{E}^{1D}_{B,Z}[\rho]$, *with* $\rho \in L^3(\mathbb{R})$, *is bounded from below, and there exists a unique minimizing density* $\rho_0 \in L^3$, *with* $\mathcal{E}^{1D}_{B,Z}[\rho_0]=E^{1D}(Z,B)$.

Proof: Since $\int V_0\rho \leqslant \|V_0\|_{3/2}\|\rho\|_3$, we get

$$\mathcal{E}^{1D}_{B,Z}[\rho] \geqslant \|\rho\|_3^3 - \|V_0\|_{3/2}\|\rho\|_3. \tag{III.56}$$

Minimizing over $\|\rho\|_3$, we get the first part of the lemma. The proof of second part works analogously to Proposition III.3. □

For the minimizing density ρ_0 we get the simple TF equation

$$3\kappa\rho_0^2(z)=ZV_0(z). \tag{III.57}$$

By the definition (I.35) one easily sees the relation

$$V_0(z)\equiv V_0^B(z)=B^{1/2}V_0^1(B^{1/2}z), \tag{III.58}$$

which implies an interesting scaling relation for the energy $E^{1D}(Z,B)$:

Lemma III.18:

$$E^{1D}(Z,B)=Z^{3/2}B^{1/4}E^{1D}(1,1). \tag{III.59}$$

Proof: Using the scaling relation (III.58) and defining

$$\rho(z)=B^{1/4}Z^{1/2}\overline{\rho}(B^{1/2}z), \tag{III.60}$$

we get

$$\mathcal{E}^{1D}_{B,Z}[\rho]=B^{1/4}Z^{3/2}\mathcal{E}^{1D}_{1,1}[\overline{\rho}]. \tag{III.61}$$

□

In the next Theorem we point out that for $B \ll Z^2$, the energy (III.59) is the semiclassical approximation of $\mathrm{Tr}[-\partial_z^2 - ZV_0(z)]_-$, the sum of all negative eigenvalues of $-\partial_z^2 - ZV_0(z)$.

Theorem III.19: *Let* $B \leqslant Z^2$ *and* $\psi \in C_0^\infty(B(0,B^{-1/2}))$. *Then*

$$\mathrm{Tr}(\psi[-\partial_z^2 - ZV_0(z)]_-)=Z^{3/2}B^{1/4}\int\int \frac{dz\,dp}{2\pi}\psi[p^2-V_0^1(z)]_- - O(B^{3/4}Z^{1/2}), \tag{III.62}$$

and there is a constant C, *such that*

$$\left|\mathrm{Tr}[-\partial_z^2 - ZV_0(z)]_- - Z^{3/2}B^{1/4}E^{1D}(1,1)\right| \leqslant CB^{3/4}Z^{1/2}. \tag{III.63}$$

Proof: Let us rewrite

$$-\partial_z^2 - ZV_0^B(z)=B^{1/2}Z[-(B^{1/2}Z)^{-1}\partial_z^2 - V_0^1(B^{1/2}z)] \tag{III.64}$$

and define the unitary operator

$$(U(l)\psi)(z)=l^{1/2}\psi(lz). \tag{III.65}$$

With $l=B^{-1/2}$ and the fact that unitary transformations do not change traces we derive

$$\mathrm{Tr}[-\partial_z^2 - ZV_0^B(z)]_- = B^{1/2}Z\,\mathrm{Tr}[-h^2\partial_z^2 - V_0^1(z)]_-, \tag{III.66}$$

where

$$h=B^{1/4}Z^{-1/2}. \tag{III.67}$$

So we have the self-adjoint Schrödinger operator

$$H=-h^2\partial_z^2-V_0^1(z), \tag{III.68}$$

and its symbol

$$h(z,p)=p^2-V_0^1(z). \tag{III.69}$$

Using the relation

$$|\partial^\nu V_0^1(z)|\leqslant C^\nu \quad \text{on } B(0,2)=\{z||z|<2\} \tag{III.70}$$

and by means of some cutoff function $\psi\in C_0^\infty$,[18] Theorem 6.1 yields

$$\mathrm{Tr}(\psi(z)[-h^2\partial_z^2-V_0^1(z)]_-)=h^{-1}\int\int\frac{\mathrm{d}p\,\mathrm{d}z}{2\pi}\psi(z)[p^2-V_0^1(z)]_--O(h), \tag{III.71}$$

which together with (III.66) and (III.67) immediately implies (III.62). Recall, that by $[t]_-=t$ for $t\leqslant 0$ and 0 otherwise.

In order to tackle the outer zone $\{z|1\leqslant|z|\leqslant\infty\}$, we note that the potential fulfills

$$|\partial^\nu V_0^1(z)|\leqslant C^\nu|z|^{-\nu} \quad \text{for } |z|\geqslant 1. \tag{III.72}$$

So by definition of the scaling functions $l(z)=|z|$ and $f(z)=1$, we can use[18] Theorem 7.1, which states that with a cutoff function $\psi\in C^\infty(B(1,\infty))$, we get

$$\left|\mathrm{Tr}(\psi[-h^2\partial_z^2-V_0^1(z)]_-)-h^{-1}\int\int\frac{\mathrm{d}p\,\mathrm{d}z}{2\pi}\psi[p^2-V_0^1(z)]_-\right|\leqslant h\int_1^\infty \mathrm{d}z\, l^{-2}\leqslant h. \tag{III.73}$$

Combining (III.71) and (III.73) together with (III.66) and (III.67) completes the proof of Theorem III.19.

Turning back to the functional (III.54), we recall that the corresponding energy has to be defined by means of the solution of the TF equation

$$\partial_z^2\psi(z)+3\kappa\psi^5(z)-ZV_0^B(z)\psi(z)=0. \tag{III.74}$$

Introducing the scaling relations

$$\psi(z)=B^{1/8}Z^{1/4}\varphi(zB^{1/2}), \quad z\to zB^{1/2}, \tag{III.75}$$

(III.74) can be written as

$$\frac{B^{1/2}}{Z}\partial_z^2\varphi(z)+3\kappa\varphi^5(z)-V_0^1(z)=0. \tag{III.76}$$

We set $\varepsilon\equiv B^{1/2}/Z\ll 1$ and make the ansatz $\varphi=\varphi_0+\varepsilon\varphi_1$ to get an approximate solution of (III.76). Rescaling and inserting into (III.54) yields

$$E^{1\mathrm{DW}}=\mathcal{E}^{1\mathrm{DW}}[\psi^2]=Z^{3/2}B^{1/4}E^{1\mathrm{D}}(1,1)-O(B^{3/4}Z^{1/2}), \tag{III.77}$$

which is in accordance with (III.62) and justifies *a posteriori* the introduction of the negative von Weizsäcker term in (I.52) and (III.54).

IV. SOME CONCLUDING REMARKS

Throughout this paper we have studied, among others, two functionals, the MTFW, which represents an approximation to the full quantum mechanical energy E^Q, and the DW functional, which should approximate the ground state energy E^Q_{conf} of particles in the lowest Landau band. Now we can ask for the magnitude of B, for which the use of DW becomes more reasonable than MTFW. This question is connected with the estimation of

$$|E^Q(N,Z,B)-E^Q_{\mathrm{conf}}(N,Z,B)|. \tag{IV.1}$$

For $B\ll Z^3$ this can be compared with the difference of the corresponding semiclassical approximations

$$\left| B\int \phi^{\mathrm{MTF}}(x)|_+^{3/2}\,\mathrm{d}x+2B\sum_{i\geqslant 1}\int |\phi^{\mathrm{MTF}}(x)-2iB|_+^{3/2}\mathrm{d}x-B\int |\phi^{\mathrm{STF}}(x)|_+^{3/2}\mathrm{d}x\right|$$

$$\leqslant C\int |Z|x|^{-1}-2B|_+^{3/2}\mathrm{d}x\leqslant CZ^3/B^{1/2}. \tag{IV.2}$$

From the preceding sections we guess, on the one hand,

$$|E^{\mathrm{DW}}-E^Q_{\mathrm{conf}}|\leqslant o(B^{4/5}Z^{3/5}), \tag{IV.3}$$

and on the other hand we know

$$|E^{\mathrm{MTFW}}-E^Q|\leqslant O(Z^2)+O(B^{4/5}Z^{3/5}). \tag{IV.4}$$

Hence, one might expect the DW theory to give the better description of the quantum mechanical energy, if $Z^3/B^{1/2}\leqslant B^{4/5}Z^{3/5}$, or, in other words, $B\geqslant Z^{24/13}$.

Summing up, we suggest to use MTFW theory for $B\leqslant Z^{24/13}$ and DW for $Z^{24/13}\leqslant B\ll Z^3$.

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Upper bounds on the density of states of single Landau levels broadened by Gaussian random potentials

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We study a nonrelativistic charged particle on the Euclidean plane $\mathbb{R}^2$ subject to a perpendicular constant magnetic field and an $\mathbb{R}^2$-homogeneous random potential in the approximation that the corresponding random Landau Hamiltonian on the Hilbert space $L^2(\mathbb{R}^2)$ is restricted to the eigenspace of a single but arbitrary Landau level. For a wide class of $\mathbb{R}^2$-homogeneous Gaussian random potentials we rigorously prove that the associated restricted integrated density of states is absolutely continuous with respect to the Lebesgue measure. We construct explicit upper bounds on the resulting derivative, the restricted density of states. As a consequence, any given energy is seen to be almost surely not an eigenvalue of the restricted random Landau Hamiltonian. © *2001 American Institute of Physics.*
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I. INTRODUCTION

In recent decades considerable attention has been paid to the physics of quasi-two-dimensional electronic structures.[1–5] Some of the occurring phenomena, like the integer quantum Hall effect,[6] are believed to be microscopically explainable in terms of a Fermi gas of noninteracting electrically charged particles in two dimensions subject to a perpendicular constant magnetic field and a static random potential. For these phenomena it should therefore be sufficient to study a single nonrelativistic spinless particle on the Euclidean plane $\mathbb{R}^2$ modeled by the *random Landau Hamiltonian*, which is informally given by

$$H(V^{(\omega)}) := H(0) + V^{(\omega)}. \tag{1}$$

As a random Schrödinger operator it acts on the Hilbert space $L^2(\mathbb{R}^2)$ of Lebesgue square-integrable complex-valued functions on the plane $\mathbb{R}^2$. For any realization $\omega \in \Omega$ of the randomness the potential $V^{(\omega)}$ mimics the disorder present in a real sample. Throughout, we will assume

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that V is homogeneous on the average with respect to Euclidean translations of $\mathbb{R}^2$. The unperturbed part in (1) is the *Landau Hamiltonian*. It represents the kinetic energy of the particle and is informally given (in the symmetric gauge) by the differential expression

$$H(0) := \frac{1}{2}\left[\left(i\frac{\partial}{\partial x_1} - \frac{B}{2}x_2\right)^2 + \left(i\frac{\partial}{\partial x_2} + \frac{B}{2}x_1\right)^2\right] = \frac{B}{2}\sum_{l=0}^{\infty}(2l+1)P_l, \tag{2}$$

in physical units where the mass and the charge of the particle, and Planck's constant divided by 2π are all equal to one. Moreover, $B>0$ denotes the strength of the magnetic field and $i=\sqrt{-1}$ stands for the imaginary unit. The second equality in (2) is the spectral resolution of $H(0)$. It dates back to Fock[7] and Landau.[8] The energy eigenvalue $(l+1/2)B$ is called the lth *Landau level* and the corresponding orthogonal eigenprojection P_l is an integral operator with continuous complex-valued kernel (in other words: position representation)

$$P_l(x,y) := \frac{B}{2\pi}\exp\left[i\frac{B}{2}(x_2y_1 - x_1y_2) - \frac{B}{4}|x-y|^2\right]L_l^{(0)}\left(\frac{B}{2}|x-y|^2\right). \tag{3}$$

Here and in the following, $|x-y|^2 := (x_1-y_1)^2+(x_2-y_2)^2$ denotes the square of the Euclidean distance between the points $x=(x_1,x_2)\in\mathbb{R}^2$ and $y=(y_1,y_2)\in\mathbb{R}^2$. Moreover, $L_l^{(k)}(\xi) := \Sigma_{j=0}^{l}(-1)^j\binom{l+k}{l-j}\xi^j/j!$, with $\xi\geqslant 0$ and $k\in\mathbb{N}_0-l := \{-l,-l+1,-l+2,...\}$, is a generalized Laguerre polynomial, see Sec. 8.97 in Ref. 9. The diagonal $P_l(x,x)=B/2\pi$ is naturally interpreted as the degeneracy per area of the lth Landau level.

A quantity of basic interest in the study of the random Landau Hamiltonian (1) is its *integrated density of states* $\nu(]-\infty,E[)$ as a function of the energy $E\in\mathbb{R}$. The underlying positive Borel measure ν on the real line $\mathbb{R}$ is called the *density-of-states measure* of $H(V)$. If the random potential is not only $\mathbb{R}^2$-homogeneous but also *isotropic*, that is, if all finite-dimensional distributions associated with the probability measure $\mathbb{P}$ on Ω, which governs the randomness, are invariant also under in-plane rotations (with respect to the origin), the density-of-states measure ν can be decomposed according to

$$\nu = \frac{B}{2\pi}\sum_{l=0}^{\infty}\hat{\nu}_l, \quad \hat{\nu}_l(I) := \frac{2\pi}{B}\mathbb{E}[(P_l\chi_I(H(V))P_l)(x,x)], \quad I\in\mathcal{B}(\mathbb{R}), \tag{4}$$

see Refs. 10, 11, and references therein. Here $\mathbb{E}$ denotes the expectation induced by $\mathbb{P}$ and $\chi_I(H(V^{(\omega)}))$ is the spectral projection operator of $H(V^{(\omega)})$ associated with the energy regime $I\in\mathcal{B}(\mathbb{R})$. The contribution $\hat{\nu}_l$ related to the *Landau-level index* l is a probability measure on the Borel sets $\mathcal{B}(\mathbb{R})$ in the real line $\mathbb{R}$. It is actually independent of $x\in\mathbb{R}^2$ due to the homogeneity of V.

In the limit of a strong magnetic field, the spacing B between successive Landau levels approaches infinity and the magnetic length $B^{-1/2}$ tends to zero. Therefore, the effect of so-called level mixing should be negligible if either the strength of the random potential V, typically given by the square root of its single-site variance $\mathbb{E}[V(0)^2]-(\mathbb{E}[V(0)])^2$, is small compared to the level spacing or if the (smallest) correlation length of V is much larger than the magnetic length. In both cases $\hat{\nu}_l(I)$ should be well approximated by $2\pi\mathbb{E}[(P_l\chi_I(P_lH(V)P_l)P_l)(x,x)]/B$. Indeed, this approximation is exact[12] if V is a spatially constant random potential $x\mapsto V^{(\omega)}(0)$. Since the first part of the lth *restricted random Landau Hamiltonian*, $P_lH(V)P_l=(l+1/2)BP_l+P_lVP_l$, causes only a shift in the energy, one may equivalently study the probability measure

$$\nu_l(I) := \frac{2\pi}{B}\mathbb{E}[(P_l\chi_I(P_lVP_l)P_l)(x,x)], \quad I\in\mathcal{B}(\mathbb{R}). \tag{5}$$

We call it the lth *restricted density-of-states measure* and its distribution function $E\mapsto\nu_l(]-\infty,E[)$ the lth *restricted integrated density of states*. Again, they are independent of $x\in\mathbb{R}^2$ due

to the homogeneity of V. From the physical point of view most interesting is the restriction to the *lowest* Landau level, corresponding to $l=0$. If the magnetic field is strong enough, all particles may be accommodated in the lowest level without conflicting with Pauli's exclusion principle, since the degeneracy (per area) $B/2\pi$ increases with B. Up to the energy shift $B/2$, the measure $B\nu_0/2\pi$ should then be a good approximation to ν, since the effects of higher Landau levels are negligible if B is large compared to the strength of the random potential, see Proposition 1 in Ref. 13 in case of a Gaussian random potential.

Neglecting effects of level mixing by only dealing with the sequence of restricted operators $(P_lVP_l)_{l\in\mathbb{N}_0}$ is a simplifying approximation which is often made. The interest in these operators relates to the existence of pure-point components in their spectra[14–17] and, what is simpler, to properties of their restricted density-of-states measures (ν_l). The aim of the present paper is to supply conditions under which ν_l is absolutely continuous with respect to the Lebesgue measure. Actually, in the physics literature this differentiability of the restricted integrated density of states $\nu_l(]-\infty,E[)$ with respect to E is usually taken for granted so that one deals from the outset with its derivative, the lth *restricted density of states*

$$E\mapsto w_l(E):=\frac{\mathrm{d}\nu_l(]-\infty,E[)}{\mathrm{d}E}=\frac{\nu_l(\mathrm{d}E)}{\mathrm{d}E}, \tag{6}$$

see, e.g., Refs. 1–6, 10, 12, 18–25. Due to the involved averaging, the disorder is indeed often believed to broaden each Landau level to a *Landau band* in such a way that the resulting restricted integrated density of states is sufficiently smooth. Example 1 in the following, however, which is taken from Ref. 12, illustrates that this belief is wrong without further assumptions. It even shows that for any given $l\geqslant 1$ it may happen that there is no broadening at all so that the operator P_lVP_l is zero almost surely (although V is nonzero) and hence ν_l is singular. For the formulation of the example we need some preparation. Without losing generality, we will always assume that the homogeneous (but not necessarily isotropic) random potential V has zero mean, $\mathbb{E}[V(0)]=0$. The *variance* σ_l^2 of ν_l is then given by[12]

$$\sigma_l^2:=\int_{\mathbb{R}}\nu_l(\mathrm{d}E)E^2=\frac{2\pi}{B}\,\mathbb{E}[(P_lVP_l)^2(0,0)]=\frac{2\pi}{B}\,(P_lCP_l)(0,0)\leqslant C(0), \tag{7}$$

where $x\mapsto C(x):=\mathbb{E}[V(x)V(0)]$ is the *covariance function* of V. When sandwiched between two projections, C is understood as a (bounded) multiplication operator acting on $L^2(\mathbb{R}^2)$. The standard deviation $\sigma_l:=\sqrt{\sigma_l^2}$ may physically be interpreted as the width of the lth Landau band. We note that the width σ_0 of the lowest Landau band is always strictly positive, provided that the covariance function is continuous and obeys $C(0)>0$. This follows from the formula $\sigma_l^2=\int_{\mathbb{R}^2}\widetilde{C}(\mathrm{d}^2k)\exp(-|k|^2/2B)[L_l^{(0)}(|k|^2/2B)]^2$. Here the so-called *spectral measure* $\widetilde{C}$ which, according to the Bochner–Khintchine theorem (Theorem IX.9 in Ref. 26), is the unique finite positive (and even) Borel measure on $\mathbb{R}^2$ yielding the Fourier representation $C(x)=\int_{\mathbb{R}^2}\widetilde{C}(\mathrm{d}^2k)\exp(ik\cdot x)$ where $k\cdot x:=k_1x_1+k_2x_2$ denotes the standard scalar product on $\mathbb{R}^2$.

Example 1: If V possesses the oscillating covariance function $C(x)=C(0)J_0(\sqrt{2}|x|/\tau)$, where $\tau>0$ and J_0 is the Bessel function of order zero,[9] then

$$\sigma_l^2=C(0)\exp\left(-\frac{1}{B\tau^2}\right)\left[L_l^{(0)}\left(\frac{1}{B\tau^2}\right)\right]^2. \tag{8}$$

Choosing the squared length ratio $1/(B\tau^2)$ equal to a zero of $L_l^{(0)}$, which exists if $l\geqslant 1$, one achieves that $\sigma_l^2=0$. Chebyshev's inequality then implies that ν_l is Dirac's point measure at the origin, informally $w_l(E)=\delta(E)$. Therefore, $P_lV^{(\omega)}P_l=0$ for $\mathbb{P}$-almost all $\omega\in\Omega$.

In the present paper we provide conditions under which exotic situations as in Example 1 cannot occur. More precisely, we prove that (6) indeed defines w_l as a bounded probability density for a wide class of *Gaussian* random potentials, see Theorems 1 and 2 in the following. Moreover,

we construct explicit upper bounds on w_l for these potentials. As an implication, we prove that for any $B>0$ and the class of Gaussian random potentials considered, any given energy $E\in\mathbb{R}$ is almost surely not an eigenvalue of the operator P_lVP_l. In particular, these Gaussian random potentials completely lift the infinite degeneracy of the Landau-level energy (here shifted to zero) for any strength of the magnetic field. This stands in contrast to situations with random point impurities considered in Refs. 19, 16, 27, 28, 17.

The present paper was partially motivated by results of Ref. 29 where the (unrestricted) density-of-states measure ν of the random Landau Hamiltonian is proven to be absolutely continuous with a locally bounded density for a certain class of random potentials (including the Gaussian ones considered in Theorem 1) and where any given energy $E\in\mathbb{R}$ is shown to be almost surely not an eigenvalue of $H(V)$. While absolute continuity of ν immediately implies by (4) that of $\hat{\nu}_l$ for all $l\in\mathbb{N}_0$ (for isotropic V), in itself it does not imply that of ν_l.

II. THE DENSITY OF STATES OF A SINGLE BROADENED LANDAU LEVEL

A. The restricted random Landau Hamiltonian and its integrated density of states

Let $\|F\|:=\sup\{|\langle\varphi,F\varphi\rangle|:\varphi\in L^2(\mathbb{R}^2),\langle\varphi,\varphi\rangle=1\}<\infty$ denote the (uniform) norm of a self-adjoint bounded operator F acting on the Hilbert space $L^2(\mathbb{R}^2)$. The restriction P_lFP_l of F to the eigenspace $P_lL^2(\mathbb{R}^2)\subset L^2(\mathbb{R}^2)$ corresponding to the lth Landau level is an integral operator with kernel $(x,y)\mapsto(P_lFP_l)(x,y):=B\langle\psi_{l,x},F\psi_{l,y}\rangle/2\pi$ which is jointly continuous thanks to the continuity of the usual scalar product $\langle\cdot,\cdot\rangle$ on $L^2(\mathbb{R}^2)$ and the strong continuity of the mapping $\mathbb{R}^2\ni x\mapsto\psi_{l,x}\in P_lL^2(\mathbb{R}^2)$. Here, the two-parameter family of normalized, complex-valued functions ("coherent states") is defined by

$$y\mapsto\psi_{l,x}(y):=\sqrt{\frac{2\pi}{B}}P_l(y,x),\quad x\in\mathbb{R}^2,\quad\langle\psi_{l,x}\psi_{l,x}\rangle=1. \tag{9}$$

Let $(\Omega,\mathcal{A},\mathbb{P})$ be a complete probability space. By a *random potential* we mean a random field $V:\Omega\times\mathbb{R}^2\to\mathbb{R},(\omega,x)\mapsto V^{(\omega)}(x)$ which is jointly measurable with respect to the sigma-algebra $\mathcal{A}$ of event sets in Ω and the sigma-algebra $\mathcal{B}(\mathbb{R}^2)$ of Borel sets in the Euclidean plane $\mathbb{R}^2$.

The next proposition provides conditions under which the (in general unbounded) integral operator P_lVP_l, the (shifted) lth *restricted random Landau Hamiltonian*, is almost surely essentially self-adjoint on the Schwartz space $\mathcal{S}(\mathbb{R}^2)$ of arbitrarily often differentiable complex-valued functions on $\mathbb{R}^2$ with rapid decrease (Definition on p. 133 in Ref. 26).

Proposition 1: Let V be an $\mathbb{R}^2$-homogeneous random potential and assume there exists a constant $M<\infty$ such that $\mathbb{E}[|V(0)|^{2k}]\leqslant(2k)!M^{2k}$ for all $k\in\mathbb{N}$. Then for all $l\in\mathbb{N}_0$ it holds:

(1) *The restricted operator $P_lV^{(\omega)}P_l$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^2)$ for all ω in some subset $\Omega_0\in\mathcal{A}$ of Ω with full probability, $\mathbb{P}(\Omega_0)=1$.*

(2) *The mapping $\Omega_0\ni\omega\mapsto P_lV^{(\omega)}P_l$ is measurable in the sense of Definition V.1.3 in Ref. 30.*

(3) *The restricted density-of-states measure ν_l, defined in* (5)*, is a probability measure on the sigma-algebra $\mathcal{B}(\mathbb{R})$ of Borel sets in the real line. Moreover, the following (weak) operator identity holds*

$$\mathbb{E}[P_l\chi_I(P_lVP_l)P_l]=\nu_l(I)P_l,\quad I\in\mathcal{B}(\mathbb{R}). \tag{10}$$

Remark: As far as we know, the operator identity (10) for general $\mathbb{R}^2$-homogeneous V and general $l\in\mathbb{N}_0$ was first shown in Ref. 20, see also Ref. 24.

Proof of Proposition 1: (1) The assumed limitation on the growth of the even moments $\mathbb{E}[|V(0)|^{2k}]$ as a criterion for the almost-sure essential self-adjointness of P_lVP_l is taken from the proof of Theorem 2.1 in Ref. 14, which is based on Nelson's analytic-vector theorem (Theorem X.39 in Ref. 31), see also Ref. 32.

(2) By truncating the large fluctuations of the random potential we construct a sequence of restricted random operators $(P_lV_n^{(\omega)}P_l)_{n\in\mathbb{N}}$, where $V_n^{(\omega)}(x):=V^{(\omega)}(x)\Theta(n-|V^{(\omega)}(x)|)$ is bounded and measurable for all n. Here $\Theta:=\chi_{]0,\infty[}$ denotes Heaviside's unit-step function. For $\mathbb{P}$-almost all

$\omega\in\Omega$ we have the strong convergence $P_l V_n^{(\omega)} P_l\varphi \to P_l V^{(\omega)} P_l\varphi$ as $n\to\infty$ for all $\varphi\in\mathcal{S}(\mathbb{R}^2)$. Consequently, Theorem VIII.25 in Ref. 26 implies that the sequence converges toward $P_l V^{(\omega)} P_l$ in the strong resolvent sense implying that the latter operator is also measurable thanks to Proposition V.1.4 in Ref. 30.

(3) Since $0\leqslant\langle\psi_{l,x},\chi_I(P_l V^{(\omega)}P_l)\psi_{l,x}\rangle\leqslant\langle\psi_{l,x},\chi_{\mathbb{R}}(P_l V^{(\omega)}P_l)\psi_{l,x}\rangle=1$ for all $x\in\mathbb{R}^2$, all $I\in\mathcal{B}(\mathbb{R})$, and $\mathbb{P}$-almost all $\omega\in\Omega$, the right-hand side of (5) indeed defines a probability measure on $\mathcal{B}(\mathbb{R})$. For the proof of (10) we introduce the family of *magnetic translation operators* $\{T_x\}_{x\in\mathbb{R}^2}$ which are unitary on $L^2(\mathbb{R}^2)$ and defined by

$$(T_x\varphi)(y):=\exp\left[i\frac{B}{2}(x_1y_2-x_2y_1)\right]\varphi(y-x),\quad \varphi\in L^2(\mathbb{R}^2). \tag{11}$$

They constitute an irreducible representation of the Heisenberg–Weyl group on $P_l L^2(\mathbb{R}^2)$.[20] Since V is $\mathbb{R}^2$-homogeneous, it follows that

$$T_x^{\dagger}\mathbb{E}[P_l\chi_I(P_l V P_l)P_l]T_x=\mathbb{E}[P_l\chi_I(P_l V P_l)P_l] \tag{12}$$

for all $x\in\mathbb{R}^2$ and all $I\in\mathcal{B}(\mathbb{R})$. A suitable variant of Schur's lemma (Proposition 4 of § 3, Chap. 5 in Ref. 33) then gives the claimed result. □

In Theorems 1 and 2, we will assume that V is a Gaussian random potential in the sense of

Definition 1: A Gaussian random potential is a Gaussian[34,35] random field V which is $\mathbb{R}^2$-homogeneous, has zero mean, $\mathbb{E}[V(0)]=0$, and is characterized by a covariance function $\mathbb{R}^2\ni x\mapsto C(x):=\mathbb{E}[V(x)V(0)]$ which is continuous at the origin where it obeys $0<C(0)<\infty$.

Remarks: (1) Our continuity requirement for the covariance function C of a Gaussian random potential implies that C is uniformly continuous and bounded by $C(0)$. Consequently, there exists a separable version of V which is jointly measurable, see Theorem 3.2.2 in Ref. 36. When speaking about a Gaussian random potential, we will tacitly assume that only this version is dealt with.

(2) A Gaussian random potential fulfills the assumption of Proposition 1 with $M=\sqrt{C(0)}$ by the usual ''Gaussian combinatorics'' to be found, for example, in Lemma 5.3.1 in Ref. 34.

B. Existence and boundedness of the restricted density of states

Wegner estimates[37] have turned out to be an efficient tool for proving the absolute continuity of density-of-states measures for certain random operators and for deriving upper bounds on their respective Lebesgue densities. One method to derive estimates of this genre uses *one-parameter spectral averaging*. It provides upper bounds on the averaged spectral projections of a self-adjoint operator which is perturbed by a bounded positive operator with fluctuating coupling strength. The abstract version of such an averaging, which we will use, is due to Combes and Hislop.[38] It is rephrased as

Lemma 1: Let K, L, and M be three self-adjoint operators acting on a Hilbert space $\mathcal{H}$ with scalar product $\langle\cdot,\cdot\rangle$. Moreover, let K and M be bounded such that $\kappa:=\inf_{K\varphi\neq 0}\langle\varphi,M\varphi\rangle/\langle\varphi,K^2\varphi\rangle>0$ is strictly positive. Finally, let $g\in L^{\infty}(\mathbb{R})$ be a Lebesgue-essentially bounded function on the real line, $\|g\|_{\infty}:=\operatorname{ess\,sup}_{\xi\in\mathbb{R}}|g(\xi)|<\infty$. Then the inequality

$$\int_{\mathbb{R}}\mathrm{d}\xi|g(\xi)|\langle\varphi,K\chi_I(L+\xi M)K\varphi\rangle\leqslant|I|\frac{\|g\|_{\infty}}{\kappa}\langle\varphi,\varphi\rangle \tag{13}$$

holds for all $\varphi\in\mathcal{H}$ and all $I\in\mathcal{B}(\mathbb{R})$.

Proof: See Corollary 4.2 in Ref. 38 and Lemma 3.1 in Ref. 29. □

If one focuses only on the absolute continuity of the measure ν_l without aspiring after sharp upper bounds on the resulting Lebesgue density, a straightforward application of Lemma 1 yields the following:

Theorem 1: *Let V be a Gaussian random potential in the sense of Definition 1. Suppose that there exists a finite signed Borel measure μ on $\mathbb{R}^2$ such that the covariance function C of V obeys*

$$0 \leqslant C_\mu(x) := \int_{\mathbb{R}^2} \mu(\mathrm{d}^2 y) C(x-y) < \infty, \quad \int_{\mathbb{R}^2} \mu(\mathrm{d}^2 y) C_\mu(y) = 1 \tag{14}$$

*for all $x \in \mathbb{R}^2$. Then the l*th *restricted density-of-states measure ν_l is absolutely continuous with respect to the Lebesgue measure and the resulting Lebesgue probability density w_l, the restricted density of states, is uniformly bounded according to*

$$w_l(E) := \frac{\nu_l(\mathrm{d}E)}{\mathrm{d}E} \leqslant \frac{1}{\sqrt{2\pi}\|P_l C_\mu P_l\|} \tag{15}$$

for Lebesgue-almost all energies $E \in \mathbb{R}$. Moreover, any given $E \in \mathbb{R}$ is not an eigenvalue of $P_l V^{(\omega)} P_l$ for $\mathbb{P}$-almost all $\omega \in \Omega$.

Remarks: (1) The second equality in (14) is just a convenient normalization of μ. The measure μ allows one to optimize the upper bound in (15) (see Example 2) as well as to apply Theorem 1 to Gaussian random potentials with certain covariance functions C, also taking on negative values. One such example is $C(x) = C(0)\exp[-|x|^2/(2\tau^2)][1-7|x|^2/(16\tau^2) + |x|^4/(32\tau^4)]$ with arbitrary length scale $\tau > 0$. This may be seen by choosing the Gaussian measure $\mu(\mathrm{d}^2 x) = \mathrm{d}^2 x N \times \exp[-|x|^2/(8\tau^2)]$ with a suitable normalization factor $N > 0$. Of course, for the oscillating covariance function of Example 1 no μ exists yielding the positivity condition (14).

(2) We note that $0 < \langle \psi_{l,0}, C_\mu \psi_{l,0} \rangle \leqslant \|P_l C_\mu P_l\| < \infty$. The first (strict) inequality follows from the assumptions on C in Definition 1, Eq. (14), and the explicit form (9) of $\psi_{l,0}$.

Proof of Theorem 1: The proof consists of two parts. In the first part, we use the fact that the Gaussian random potential V admits a one-parameter decomposition into a standard Gaussian random variable λ and a nonhomogeneous zero-mean Gaussian random field U which are defined by

$$\lambda^{(\omega)} := \int_{\mathbb{R}^2} \mu(\mathrm{d}^d y) V^{(\omega)}(y), \quad U^{(\omega)}(x) := V^{(\omega)}(x) - \lambda^{(\omega)} C_\mu(x). \tag{16}$$

The positive bounded function C_μ is defined in (14). Since $\mathbb{E}[\lambda U(x)] = 0$ for all $x \in \mathbb{R}^2$, λ and U are stochastically independent. We now multiply both sides of (10) from the left and right by $K := (P_l C_\mu P_l)^{1/2}$ and take the quantum-mechanical expectation with respect to an arbitrary nonzero $\varphi \in P_l L^2(\mathbb{R}^2)$ to obtain

$$\begin{aligned} \nu_l(I)\langle \varphi, K^2 \varphi \rangle &= \mathbb{E}[\langle \varphi, K \chi_I(P_l V P_l) K \varphi \rangle] \\ &= \mathbb{E}\left[\int_{\mathbb{R}} \mathrm{d}\xi \frac{e^{-\xi^2/2}}{\sqrt{2\pi}} \langle \varphi, K \chi_I(P_l U P_l + \xi K^2) K \varphi \rangle \right] \\ &\leqslant |I| \frac{\langle \varphi, \varphi \rangle}{\sqrt{2\pi}}. \end{aligned} \tag{17}$$

For the second equality we used the one-parameter decomposition (16) and the stochastic independence of λ and U. The Lebesgue integral in (17), which constitutes a partial averaging, is then bounded with the help of (13) uniformly in ω. The absolute continuity of ν_l with respect to the Lebesgue measure is now a consequence of (17) and the Radón–Nikodým theorem. Minimizing the upper bound on $\nu_l(I)$, coming from (17), with respect to $\varphi \in P_l L^2(\mathbb{R}^2)$ yields the claimed inequality (15).

In the second part, we note that (10) implies the equivalence: ν_l has no pure points, that is, $\nu_l(\{E\}) = 0$ for all $E \in \mathbb{R}$, if and only if $\mathbb{E}[\langle \varphi, \chi_{\{E\}}(P_l V P_l)\varphi \rangle] = 0$ for all $E \in \mathbb{R}$ and all $\varphi \in P_l L^2(\mathbb{R}^2)$. Given an orthonormal basis $\{\varphi_k\}_{k \in \mathbb{N}}$ in $P_l L^2(\mathbb{R}^2)$, there hence exists for every k

$\in\mathbb{N}$ some $\Omega_k\in\mathcal{A}$ with $\mathbb{P}(\Omega_k)=1$ such that $\langle\varphi_k,\chi_{\{E\}}(P_lV^{(\omega)}P_l)\varphi_k\rangle=0$ for all $\omega\in\Omega_k$. As a consequence, $\chi_{\{E\}}(P_lV^{(\omega)}P_l)=0$ for all $\omega\in\cap_{k\in\mathbb{N}}\Omega_k$, hence $\mathbb{P}$-almost all $\omega\in\Omega$. □

Remarks: (1) If the spectral measure $\tilde{C}$ has a (positive) Lebesgue density, C admits the representation $C(x)=\int_{\mathbb{R}^2}\mathrm{d}^2y\,\gamma(x+y)\,\gamma(y)$ with some $\gamma\in L^2(\mathbb{R}^2)$. If furthermore there exists some $f\in L^2(\mathbb{R}^2)$ with $\langle f,f\rangle=1$ such that $0\leqslant u(x):=\int_{\mathbb{R}^2}\mathrm{d}^2y f(x+y)\,\gamma(y)<\infty$ and $u\neq 0$, one may replace C_μ in (15) by u to obtain another upper bound on w_l for the given Gaussian random potential V. Roughly speaking, the idea is to write V as $V^{(\omega)}(x)=\int_{\mathbb{R}^2}\mathrm{d}^2y\,\gamma(x+y)W^{(\omega)}(y)$, where W is the standard delta-correlated (generalized) Gaussian random field on $\mathbb{R}^2$ informally characterized by $\mathbb{E}[W(x)]=0$ and $\mathbb{E}[W(x)W(y)]=\delta(x-y)$. The Gaussian random potential V hence admits a one-parameter decomposition into the standard Gaussian random variable $\lambda^{(\omega)}:=\int_{\mathbb{R}^2}\mathrm{d}^2y f(y)W^{(\omega)}(y)$ and the nonhomogeneous Gaussian random field $U^{(\omega)}(x):=V^{(\omega)}(x)-\lambda^{(\omega)}u(x)$, which is stochastically independent of λ.

(2) The essential ingredients of the above-given proof are the operator identity (10) and the fact that the (not necessarily Gaussian) random potential admits a one-parameter decomposition[39,29] $V^{(\omega)}(x)=U^{(\omega)}(x)+\lambda^{(\omega)}u(x)$ into a positive function u, a random field U, and a random variable λ whose conditional probability measure with respect to the sub-sigma-algebra generated by the family of random variables $\{U(x)\}_{x\in\mathbb{R}^2}$ has a bounded Lebesgue density ρ. Following the lines of reasoning of the above-given proof, the restricted density of states may then be shown to be bounded according to

$$w_l(E)=\frac{\nu_l(\mathrm{d}E)}{\mathrm{d}E}\leqslant\frac{\|\rho\|_\infty}{\|P_luP_l\|} \tag{18}$$

for Lebesgue-almost all $E\in\mathbb{R}$. Moreover, any given $E\in\mathbb{R}$ is not an eigenvalue of $P_lV^{(\omega)}P_l$ for $\mathbb{P}$-almost all $\omega\in\Omega$.

(3) The energy-independent estimate (15) is rather rough, because one expects $w_l(E)$ to fall off to zero for energies E approaching the edges $\pm\infty$ (if $\sigma_l^2>0$) of the almost-sure spectrum of P_lVP_l. More precisely, in the present case of a Gaussian random potential V it follows from arguments in Ref. 12 that the leading asymptotic behavior of the restricted integrated density of states for $|E|\to\infty$ is Gaussian according to

$$\lim_{E\to-\infty}\frac{\ln\nu_l(]-\infty,E[)}{E^2}=\lim_{E\to\infty}\frac{\ln\nu_l(]E,\infty[)}{E^2}=-\frac{1}{2\Gamma_l^2}, \tag{19}$$

where the *decay energy* Γ_l is the solution of the maximization problem

$$\Gamma_l^2:=\sup_{\substack{\varphi\in P_lL^2(\mathbb{R}^2)\\ \langle\varphi,\varphi\rangle=1}}\gamma^2(\varphi),\quad \gamma^2(\varphi):=\mathbb{E}[\langle\varphi,V\varphi\rangle^2]=\int_{\mathbb{R}^2}\mathrm{d}^2x\int_{\mathbb{R}^2}\mathrm{d}^2y|\varphi(x)|^2|\varphi(y)|^2C(x-y). \tag{20}$$

We recall from Ref. 12 the inequalities $\sigma_l^4/C(0)\leqslant\Gamma_l^2\leqslant\sigma_l^2$.

Gaussian random potentials with positive covariance functions nicely illustrate Theorem 1.

Example 2: If $0\leqslant C(x)<\infty$ for all $x\in\mathbb{R}^2$, the optimal μ in (15) belongs to the class of positive measures of the form $\mu(\mathrm{d}^2x)\,\gamma(\varphi)=\mathrm{d}^2x|\varphi(x)|^2$ with $\varphi\in P_lL^2(\mathbb{R}^2)$, $\langle\varphi,\varphi\rangle=1$, and $\gamma(\varphi)$ as defined in (20). Optimizing with respect to φ yields

$$w_l(E)\leqslant\frac{1}{\sqrt{2\pi\Gamma_l^2}}, \tag{21}$$

where Γ_l is the decay energy of the restricted integrated density of states. In particular, for the Gaussian covariance function $C(x)=\alpha^2\exp[-|x|^2/(2\tau^2)]/(2\pi\tau^2)$ with correlation length $\tau>0$ and single-site variance $C(0)=\alpha^2/(2\pi\tau^2)>0$, one has explicitly[12]

$$\Gamma_l^2=\gamma^2(\varphi_{l,-l})=\frac{\alpha^2}{2\pi\tau^2}\left(\frac{B\tau^2}{B\tau^2+2}\right)^{l+1}\mathrm{P}_l\left(\frac{(B\tau^2+1)^2+1}{(B\tau^2+1)^2-1}\right), \tag{22}$$

where the maximizer $\varphi_{l,-l}$ is given in (31) and $\mathrm{P}_l(\xi):=(1/l!2^l)(\mathrm{d}^l/\mathrm{d}\xi^l)(\xi^2-1)^l$ is the lth Legendre polynomial.[9]

Remarks: (1) That the class of measures referred to in Example 2 contains indeed the optimal one, derives from the Fourier representation

$$\langle\varphi,C_\mu\varphi\rangle=\int_{\mathbb{R}^2}\tilde{C}(\mathrm{d}^2k)\left(\int_{\mathbb{R}^2}\mathrm{d}^2x|\varphi(x)|^2e^{ik\cdot x}\right)\left(\int_{\mathbb{R}^2}\mu(\mathrm{d}^2y)e^{-ik\cdot y}\right) \tag{23}$$

valid for all $\varphi\in\mathrm{L}^2(\mathbb{R}^2)$. Since $\tilde{C}$ is positive, the claim follows from (23) with the help of the Cauchy–Schwarz inequality and the positivity of C.

(2) In the physics literature one often considers the limit of a *delta-correlated* Gaussian random potential informally characterized by $C(x)=\alpha^2\delta(x)$ with some $\alpha>0$. It emerges from the Gaussian random potential with the Gaussian covariance function given between (21) and (22) in the limit $\tau\downarrow 0$. In this limit (22) reduces to $\Gamma_l^2=(\alpha^2B/4\pi)(2l)!/(l!2^l)^2$ and the variance of ν_l becomes, by (7), independent of the Landau-level index, $\sigma_l^2=\sigma_0^2=\alpha^2B/(2\pi)$. Remarkably, in this limit explicit expressions for w_0 and w_l, in the additional high Landau-level limit $l\to\infty$, are available. The first result is due to Wegner[18] and reads

$$w_0(E)=\frac{2}{\pi^{3/2}\sigma_0}\frac{\exp(\eta^2)}{1+[2\pi^{-1/2}\int_0^\eta\mathrm{d}\xi\exp(\xi^2)]^2},\quad \eta:=\frac{E}{\sigma_0}, \tag{24}$$

also see Refs. 19, 20, 13. Of course, when specializing the bound in (21), it is consistent with (24) because $2<\pi$. As for the second result, it is known[21,22] that w_l approaches for $l\to\infty$ a semi-elliptic probability density,

$$\lim_{l\to\infty}w_l(E)=\frac{1}{2\pi\sigma_0}\Theta(4-\eta^2)\sqrt{4-\eta^2},\quad \eta=\frac{E}{\sigma_0}. \tag{25}$$

Unfortunately, in the delta-correlated limit the bound in (21) diverges asymptotically like $l^{1/4}/(\pi^{1/4}\sigma_0)$ as $l\to\infty$.

(3) Different from (25), for the above-mentioned Gaussian covariance function with a strictly positive correlation length $\tau>0$, the high Landau-level limit (informally) reads $\lim_{l\to\infty}w_l(E)=\delta(E)$. This follows from Chebyshey's inequality and the fact that the Landau-level broadening vanishes in this limit if $\tau>0$: $\lim_{l\to\infty}\sigma_l^2=0$.[12] In agreement with that, the bound in (21) diverges in this case, as may be seen either from $0\leqslant\Gamma_l^2\leqslant\sigma_l^2$, valid[12] for any covariance function, or directly from (22).

(4) The existence of a bounded w_0 in the delta-correlated limit of a Gaussian random potential stands in contrast to situations with random point impurities, $V^{(\omega)}(x)=\Sigma_j\lambda_j^{(\omega)}\delta(x-p_j^{(\omega)})$. To our knowledge, the following four cases have been considered so far:

(a) the *impurity positions* $p_j\in\mathbb{R}^2$ randomly located according to Poisson's distribution and the *coupling strengths* $\lambda_j\in\mathbb{R}$ nonrandom, strictly positive, and all equal.[19,28]
(b) $p_j\in\mathbb{R}^2$ randomly located according to Poisson's distribution and $\lambda_j\in\mathbb{R}$ independently identically distributed[19] according to a probability measure whose support is a compact interval containing the origin.[27]
(c) $p_j\in\mathbb{Z}^2$ nonrandom and $\lambda_j\in\mathbb{R}$ independently, identically distributed according to a bounded probability density whose support is a compact interval containing the origin.[16]
(d) $p_j=j+d_j$ with $j\in\mathbb{Z}^2$ nonrandom and the *displacements* $d_j\in\mathbb{R}^2$ independently, identically distributed according to a bounded probability density with support contained in the unit square $]-1/2,1/2[^2\subset\mathbb{R}^2$. Moreover, $\lambda_j\in\mathbb{R}$ as in the previous case.[17]

In any of these cases, it has been shown that $P_0V^{(\omega)}P_0$ has an infinitely degenerate eigenvalue at zero energy for $\mathbb{P}$-almost all $\omega\in\Omega$, if the magnetic-field strength B is sufficiently large.

C. Gaussian upper bound on the restricted density of states

As already pointed out, the estimate (15) is rather rough, because it does not depend on the energy. Fortunately, under an additional isotropy assumption and with more effort one may construct an energy-dependent estimate.

Theorem 2: *Suppose the situation of Theorem 1 and that the there-defined convolution C_μ is spherically symmetric (with respect to the origin). Then the l*th *restricted density of states w_l is bounded by a Gaussian in the sense that*

$$w_l(E)\leqslant \frac{1}{\sqrt{2\pi}\langle\psi_{l,0},C_\mu\psi_{l,0}\rangle}\exp\left(-\frac{E^2}{2C(0)}\right) \tag{26}$$

for Lebesgue-almost all energies $E\in\mathbb{R}$. [*Here $\psi_{l,0}$ is defined in (9).*]

Remarks: (1) Equality holds in (26) [and (27) in the following] with $\langle\psi_{l,0},C_\mu\psi_{l,0}\rangle=\sqrt{C(0)}=\sigma_l=\Gamma_l$ for the simple extreme case of a spatially constant Gaussian random potential V, that is, if $C(x)=C(0)$ for all $x\in\mathbb{R}^2$. Of course, V is not ergodic in this case. For a lucid discussion of ergodicity and related notions in the theory of random (Schrödinger) operators, see Ref. 40.

(2) In view of (19), we conjecture the true leading decay of $w_l(E)=\mathrm{d}\nu_l(]-\infty,E[)/\mathrm{d}E$ for $|E|\to\infty$ to be Gaussian with decay energy Γ_l. This energy is strictly smaller than $\sqrt{C(0)}$, if not $C(x)=C(0)$ for all $x\in\mathbb{R}^2$.

(3) Using $\exp(-E^2/2C(0))\leqslant 1$ in (26), one obtains an energy-independent estimate which in general is weaker than (15) because $\langle\psi_{l,0},C_\mu\psi_{l,0}\rangle\leqslant\|P_lC_\mu P_l\|$. In particular this is true in the delta-correlated limit in which the energy dependence of the bound in (26) disappears anyway.

Gaussian random potentials with positive, spherically symmetric covariance functions illustrate Theorem 2.

Example 3: For a positive covariance function $0\leqslant C(x)<\infty$, which is additionally spherically symmetric, the prefactor of the Gaussian in (26) is minimized by taking $\mu(\mathrm{d}^2x)\,\gamma(\psi_{l,0})=\mathrm{d}^2x|\psi_{l,0}(x)|^2$ so that $\langle\psi_{l,0},C_\mu\psi_{l,0}\rangle=\gamma(\psi_{l,0})$. By the Fourier representation (23) and Jensen's inequality, with $\widetilde{C}/C(0)$ as the underlying Borel probability measure on $\mathbb{R}^2$, one finds that $\gamma^2(\psi_{l,0})\geqslant\sigma_l^4/C(0)$. Therefore, the estimate (26) may be weakened to the following more explicit one:

$$w_l(E)\leqslant\frac{C(0)}{\sigma_l^2}\,\frac{1}{\sqrt{2\pi C(0)}}\exp\left(-\frac{E^2}{2C(0)}\right), \tag{27}$$

where σ_l^2 is the variance of ν_l, see (7). Alternatively, (27) may be obtained directly from (26) by choosing $\mu(\mathrm{d}^2x)\sqrt{C(0)}=\mathrm{d}^2x\,\delta(x)$ so that $C_\mu(x)=C(x)/\sqrt{C(0)}$.

Remark: For the Gaussian covariance function $C(x)=C(0)\exp[-|x|^2/(2\tau^2)]$, it is known[23,12] that $\gamma^2(\psi_{0,0})=\Gamma_0^2=C(0)B\tau^2/(B\tau^2+2)$, also see (22). Theorem 2 together with the minimizing result mentioned in Example 3 therefore gives the estimate

$$w_0(E)\leqslant\sqrt{\frac{B\tau^2+2}{B\tau^2}}\,\frac{1}{\sqrt{2\pi C(0)}}\exp\left(-\frac{E^2}{2C(0)}\right) \tag{28}$$

for the restricted density of states of the lowest Landau band. In this setting w_0 has been approximately constructed using a continued-fraction approach.[25] In accordance with the first remark below (26), a comparison with this approximation supports the fact that the estimates (28), (27), and (26) are the sharper, the longer the distance is over which the fluctuations of the Gaussian random potential are significantly correlated, more precisely, the larger the squared length ratio $B\tau^2$ is.

III. PROOF OF THE GAUSSIAN UPPER BOUND

The proof of Theorem 2 requires two major ingredients, an approximation result (Proposition 2) and a Wegner-type of estimate (Proposition 3). We defer the details and proofs of these results to Secs. III B and III C. Taking these results for granted, the arguments for the validity of Theorem 2 are as follows.

Proof of Theorem 2: Since the restricted density-of-states measure is even for a (zero-mean) Gaussian random potential, that is, $\nu_l(I)=\nu_l(-I)$ for all $I\in\mathcal{B}(\mathbb{R})$, and since we already know from Theorem 1 that the density of states w_l exists and is bounded by a constant which does not exceed the prefactor of the Gaussian in (26), it is sufficient to consider ν_l on the strictly negative half-line $]-\infty,0[$.

We now use Proposition 2 to show that a suitably defined sequence of probability measures $(\nu_{l,n})_{n\in\mathbb{N}}$ [see (45)] converges weakly to ν_l as $n\to\infty$. Given $E_1<E_2\leqslant 0$, we introduce the open interval $I:=]E_1,E_2[$. Then we have

$$\nu_l(I)\leqslant\liminf_{n\to\infty}\nu_{l,n}(I), \tag{29}$$

by the portmanteau theorem (Theorem 30.10 in Ref. 41). We now use Proposition 3 to estimate the prelimit expression and obtain

$$\nu_l(I)\leqslant\frac{|I|}{\sqrt{2\pi}\langle\psi_{l,0},C_\mu\psi_{l,0}\rangle}\exp\left(\beta E+\frac{\beta^2}{2}C(0)\right), \tag{30}$$

for all $E\in[E_2,0]$ and all $\beta\geqslant 0$. Choosing $\beta=-E/C(0)\geqslant 0$ gives the claimed upper bound on w_l for $E<0$. □

Before we proceed with the proofs of the approximation result and the Wegner-type of estimate, which were needed in the above-given proof, we collect some preparations in the following.

A. Angular-momentum eigenfunctions

The functions

$$x\mapsto\varphi_{l,k}(x):=\sqrt{\frac{l!}{(l+k)!}}\left[\sqrt{\frac{B}{2}}(x_1+ix_2)\right]^k L_l^{(k)}\left(\frac{B|x|^2}{2}\right)\sqrt{\frac{B}{2\pi}}\exp\left(-\frac{B|x|^2}{4}\right) \tag{31}$$

constitute[7] with $k\in\{-l,-l+1,...\}$ an orthonormal basis in the lth Landau-level eigenspace $P_lL^2(\mathbb{R}^2)$. In fact, $\varphi_{l,k}$ is an *eigenfunction of the (perpendicular component of the canonical) angular-momentum* operator $L_3:=i(x_2\partial/\partial x_1-x_1\partial/\partial x_2)$ corresponding to the eigenvalue k, that is, $L_3\varphi_{l,k}=k\varphi_{l,k}$.

Lemma 2: Let $u:\mathbb{R}^2\to[0,\infty[$ be a measurable, positive, bounded, and spherically symmetric function. Then the operator inequality

$$P_lu_xP_l\geqslant\langle\psi_{l,0},u\psi_{l,0}\rangle\psi_{l,x}\langle\psi_{l,x},\cdot\rangle \tag{32}$$

holds for all $x\in\mathbb{R}^2$. Here the function $u_x(\cdot):=u(\cdot-x)$ is the x-translate of u and $\psi_{l,x}\langle\psi_{l,x},\cdot\rangle$ denotes the orthogonal projection operator onto the one-dimensional subspace spanned by $\psi_{l,x}$, see (9).

Proof: Since the function u is spherically symmetric, the operator P_luP_l is diagonal in the angular-momentum basis such that

$$P_luP_l=\sum_{k=-l}^{\infty}\langle\varphi_{l,k},u\varphi_{l,k}\rangle\varphi_{l,k}\langle\varphi_{l,k},\cdot\rangle\geqslant\langle\varphi_{l,0},u\varphi_{l,0}\rangle\varphi_{l,0}\langle\varphi_{l,0},\cdot\rangle. \tag{33}$$

The shifted operator $P_l u_x P_l = T_x P_l u P_l T_x^\dagger$ results from the left-hand side of (33) by a unitary transformation with the magnetic translation T_x, see (11). The proof is hence completed by observing that $\varphi_{l,0} = \psi_{l,0}$ and $\psi_{l,x} = T_x \psi_{l,0}$. □

Subsequently, we will consider the n-dimensional subspaces $P_{l,n} L^2(\mathbb{R}^2) \subset P_l L^2(\mathbb{R}^2)$ spanned by the first n angular-momentum eigenfunctions. The orthogonal projection $P_{l,n}$ is therefore defined by

$$P_{l,n} := \sum_{k=-l}^{n-l-1} \varphi_{l,k} \langle \varphi_{l,k}, \cdot \rangle, \quad n \in \mathbb{N}. \tag{34}$$

The completeness of $\{\varphi_{l,k}\}$ in $P_l L^2(\mathbb{R}^2)$ implies the strong-limit relation $s\text{-}\lim_{n\to\infty} P_{l,n} = P_l$ on $L^2(\mathbb{R}^2)$. The projections $P_{l,n}$ are integral operators with (continuous) kernels $P_{l,n}(x,y)$, whose diagonals are given by $P_{l,n}(x,x) = B G_{l,n}(B|x|^2/2)/2\pi \leqslant B/2\pi$. Here the function

$$G_{l,n}(\xi) := e^{-\xi} \sum_{k=-l}^{n-l-1} \frac{l!}{(k+l)!} \xi^k (L_l^{(k)}(\xi))^2, \quad \xi \geqslant 0, \quad n \in \mathbb{N}, \tag{35}$$

is approximately one and approximately zero for ξ smaller and larger than $n - 1/2$, respectively. Moreover, the length of the interval on which its values differ significantly from one and zero does not depend on n, also see the remark after the following

Lemma 3: Let $G_{l,n}$ be defined by (35). Then the following scaling-limit relation holds

$$\lim_{n\to\infty} G_{l,n}(n\xi) = \begin{cases} 1 & \text{if} \quad 0 < \xi < 1 \\ 0 & \text{if} \quad 1 < \xi < \infty \end{cases}. \tag{36}$$

Moreover, for every $l \in \mathbb{N}_0$ there exist an $N_l \in \mathbb{N}$ and a real $A_l > 0$, such that $0 \leqslant G_{l,n}(n\xi) \leqslant A_l e^{-\xi}$ for all $\xi \geqslant 0$ and all $n \geqslant N_l$.

Remark: With more effort one may even prove that for every $l \in \mathbb{N}_0$ there exists some polynomial $\zeta \mapsto \mathrm{Pol}(\zeta, l)$ of maximal degree $2l+1$ such that

$$0 \leqslant G_{l,n}((\sqrt{n-1/2} + \zeta)^2) \leqslant e^{-\zeta^2} \mathrm{Pol}(\zeta, l) \tag{37}$$

for all $n \in \mathbb{N}$ and all $\zeta \geqslant 0$. Moreover,

$$1 - e^{-\zeta^2} \mathrm{Pol}(-\zeta, l) \leqslant G_{l,n}((\sqrt{n-1/2} - \zeta)^2) \leqslant 1 \tag{38}$$

for all $n \in \mathbb{N} + l$ and all $0 \leqslant \zeta \leqslant \sqrt{n-1/2}$.

Proof of Lemma 3: The proof is based on the following recurrence relation:

$$G_{l,n}(\xi) - G_{l-1,n}(\xi) = -e^{-\xi} \frac{(l-1)!}{(n-1)!} \xi^{n-l} L_{l-1}^{(n-1)}(\xi) L_l^{(n-l)}(\xi) =: D_{l,n}(\xi) \tag{39}$$

for all $l \geqslant 1$. It follows from the fact that $D_{l,n}$ may be written as a telescope sum according to

$$D_{l,n}(\xi) = e^{-\xi} \sum_{k=-l+1}^{n-l} \frac{(l-1)!}{(k+l-1)!} \xi^k \left[\frac{k+l-1}{\xi} L_{l-1}^{(k-1)}(\xi) L_l^{(k-1)}(\xi) - L_{l-1}^{(k)}(\xi) L_l^{(k)}(\xi) \right]. \tag{40}$$

Equation 8.971(4) in Ref. 9 may be written as $(k+l-1) L_{l-1}^{(k-1)}(\xi) = \xi L_{l-1}^{(k)}(\xi) + l L_l^{(k-1)}(\xi)$. Using this together with Eq. 8.971(5) in Ref. 9, the difference in the square brackets in (40) is seen to be equal to $(L_l^{(k-1)}(\xi))^2 l/\xi - (L_{l-1}^{(k)}(\xi))^2$. Splitting the sum into two parts yields (39). The proof of (36) then follows by mathematical induction on $l \in \mathbb{N}_0$. In case $l = 0$ we write

$$G_{0,n}(\xi)=e^{-\xi}\sum_{k=0}^{n-1}\frac{\xi^k}{k!}=:e^{-\xi}e_n(\xi)-e^{-\xi}\frac{\xi^n}{n!} \tag{41}$$

in terms of the incomplete exponential function e_n (Eq. 6.5.11 in Ref. 42). By Stirling's estimate $n!\geqslant\sqrt{2\pi n}n^n e^{-n}$ for the factorial (Eq. 6.1.38 in Ref. 42) and the elementary inequality $\xi-1-\ln\xi\geqslant 0$, the second term on the right-hand side of (41) vanishes in the scaling limit (36) such that the claim reduces to the content of Eq. 6.5.34 in Ref. 42 for $l=0$. For the induction clause, we use the following exponential, hence rough, growth limitation for Laguerre polynomials:

$$|L_l^{(k)}(\xi)|=\left|\sum_{j=0}^{l}(-1)^j\binom{l+k}{l-j}\frac{\xi^j}{j!}\right|\leqslant\sum_{j=0}^{l}(l+k)^{l-j}\frac{\xi^j}{j!}\leqslant(l+k)^l e^{\xi/(l+k)} \tag{42}$$

which is valid for $k\geqslant 1-l$ and obtained by bounding the binomial coefficients. Using again Stirling's estimate, this yields the inequality

$$|D_{l,n}(n\xi)|\leqslant(l-1)!e^{3\xi}\left(\frac{n}{\xi}\right)^l e^{-(\xi-1-\ln\xi)n} \tag{43}$$

for all $l\geqslant 1$ and all $n\geqslant 2$. Since $\xi-1-\ln\xi>0$ for all $\xi\neq 1$, we have $\lim_{n\to\infty}D_{l,n}(n\xi)=0$ and hence $\lim_{n\to\infty}G_{l,n}(n\xi)=\lim_{n\to\infty}G_{l-1,n}(n\xi)$ for all $\xi\neq 1$, which completes the proof of (36).

For a proof of the exponential bound $0\leqslant G_{l,n}(n\xi)\leqslant A_l e^{-\xi}$ with some $A_l>0$ and n large enough, we first recall that

$$0\leqslant G_{l,n}(\xi)\leqslant G_{l,\infty}(\xi)=1 \tag{44}$$

for all $\xi\geqslant 0$, $l\in\mathbb{N}_0$, and $n\in\mathbb{N}$. Using $n^k\leqslant(n-1)^k e$ for $0\leqslant k\leqslant n-1$ in (41), one obtains $G_{0,n}(n\xi)\leqslant e^{1-\xi}$ for all $\xi\geqslant 0$. The claimed exponential bound for all $l\in\mathbb{N}_0$ then follows from (43) and (39). □

B. Approximating sequence of probability measures on the real line

Employing the $n\times n$ random Hermitian matrices $P_{l,n}V^{(\omega)}P_{l,n}$, we define a sequence $(\nu_{l,n})_{n\in\mathbb{N}}$ of probability measures by

$$\nu_{l,n}(I):=\frac{1}{n}\mathbb{E}\{\mathrm{Tr}[P_{l,n}\chi_I(P_{l,n}VP_{l,n})P_{l,n}]\},\quad I\in\mathcal{B}(\mathbb{R}). \tag{45}$$

Here the trace $\mathrm{Tr}[P_{l,n}\chi_I(P_{l,n}V^{(\omega)}P_{l,n})P_{l,n}]$ is equal to the (random) number of eigenvalues (counting multiplicity) of $P_{l,n}V^{(\omega)}P_{l,n}$ in the Borel set I. For rather general random potentials the sequence $(\nu_{l,n})$ approximates the restricted density-of-states measure ν_l. This is the first ingredient of the proof of Theorem 2.

Proposition 2: Let V be an $\mathbb{R}^2$-homogeneous random potential with $\mathbb{E}\{|V(0)|\}<\infty$. Moreover, assume that $P_lV^{(\omega)}P_l$ and $P_{l,n}V^{(\omega)}P_{l,n}$ for all $n\in\mathbb{N}$ are self-adjoint on $L^2(\mathbb{R}^2)$ for $\mathbb{P}$-almost all $\omega\in\Omega$. Then

$$\nu_l=\lim_{n\to\infty}\nu_{l,n} \tag{46}$$

in the sense of weak convergence of finite measures.

Remark: The assumptions of the proposition are fulfilled for a Gaussian random potential in the sense of Definition 1, because P_lVP_l is almost surely essentially self-adjoint on $\mathcal{S}(\mathbb{R}^2)$ by Proposition 1. Moreover, the random matrix operator $P_{l,n}VP_{l,n}$ is almost surely self-adjoint for all $n\in\mathbb{N}$ because of the almost-sure finiteness $|\langle\varphi_{l,j},V\varphi_{l,k}\rangle|<\infty$ for all $j,k\in\mathbb{N}_0-l$.

Proof of Proposition 2: The claimed weak convergence of (finite) measures is equivalent to pointwise convergence of their Stieltjes transforms, that is,

$$\lim_{n\to\infty}\int_{\mathbb{R}}\frac{\nu_{l,n}(\mathrm{d}E)}{E-z}=\int_{\mathbb{R}}\frac{\nu_l(\mathrm{d}E)}{E-z} \tag{47}$$

for all $z\in\mathbb{C}\backslash\mathbb{R}$, see, for example, Proposition 4.9 in Ref. 43. The spectral theorem and (10) show that the latter convergence follows from

$$\lim_{n\to\infty}\frac{1}{n}\mathbb{E}\{|\mathrm{Tr}[P_{l,n}((P_{l,n}VP_{l,n}-z)^{-1}-(P_lVP_l-z)^{-1})P_{l,n}]|\}=0. \tag{48}$$

As a self-adjoint operator of finite rank, $P_{l,n}V^{(\omega)}P_{l,n}$ is defined on the whole space $L^2(\mathbb{R}^2)$ for $\mathbb{P}$-almost all $\omega\in\Omega$, so that we may use the (second) resolvent equation.[44] Together with the fact that $(P_{l,n}V^{(\omega)}P_{l,n}-z)^{-1}$ and $P_{l,n}$ commute with each other, the absolute value of the trace in (48) is hence seen to be equal to

$$\begin{aligned}&|\mathrm{Tr}[P_{l,n}(P_{l,n}V^{(\omega)}P_{l,n}-z)^{-1}P_{l,n}V^{(\omega)}(P_l-P_{l,n})(P_lV^{(\omega)}P_l-z)^{-1}P_{l,n}]|\\&\quad\leqslant\|(P_{l,n}V^{(\omega)}P_{l,n}-z)^{-1}\|\|(P_lV^{(\omega)}P_l-z)^{-1}\|\|P_{l,n}V^{(\omega)}(P_l-P_{l,n})\|_1\\&\quad\leqslant|\mathrm{Im}\,z|^{-2}\|P_{l,n}V^{(\omega)}(P_l-P_{l,n})\|_1.\end{aligned} \tag{49}$$

Here we employed Hölder's inequality for the trace norm $\|A\|_1:=\mathrm{Tr}(A^\dagger A)^{1/2}$ and $\mathrm{Im}\,z$ denotes the imaginary part of z. The trace norm in (49) is in turn estimated as follows:

$$\begin{aligned}\|P_{l,n}V^{(\omega)}(P_l-P_{l,n})\|_1&=\left\|\frac{B}{2\pi}\int_{\mathbb{R}^2}\mathrm{d}^2x\,V^{(\omega)}(x)\,\psi_{l,x,n}\langle\psi_{l,x}-\psi_{l,x,n},\cdot\rangle\right\|_1\\&\leqslant\frac{B}{2\pi}\int_{\mathbb{R}^2}\mathrm{d}^2x|V^{(\omega)}(x)|\|\psi_{l,x,n}\langle\psi_{l,x}-\psi_{l,x,n},\cdot\rangle\|_1\\&=\int_{\mathbb{R}^2}\mathrm{d}^2x|V^{(\omega)}(x)|\sqrt{P_{l,n}(x,x)[P_l(x,x)-P_{l,n}(x,x)]},\end{aligned} \tag{50}$$

where we introduced the sequence of two-parameter families of complex-valued functions

$$y\mapsto\psi_{l,x,n}(y):=(P_{l,n}\psi_{l,x})(y),\quad x\in\mathbb{R}^2. \tag{51}$$

Note that these functions are not normalized, $\langle\psi_{l,x,n},\psi_{l,x,n}\rangle=2\pi P_{l,n}(x,x)/B=G_{l,n}(B|x|^2/2)\leqslant 1$. Combining (49) and (50), using Fubini's theorem and the homogeneity of the random potential, the left-hand side of (48) is seen to be bounded from above by

$$\begin{aligned}&\lim_{n\to\infty}\frac{\mathbb{E}[|V(0)|]}{n|\mathrm{Im}\,z|^2}\int_{\mathbb{R}^2}\mathrm{d}^2x\sqrt{P_{l,n}(x,x)[P_l(x,x)-P_{l,n}(x,x)]}\\&\quad=\frac{\mathbb{E}[|V(0)|]}{|\mathrm{Im}\,z|^2}\lim_{n\to\infty}\int_0^\infty\mathrm{d}\xi\sqrt{G_{l,n}(n\xi)[1-G_{l,n}(n\xi)]}=0.\end{aligned} \tag{52}$$

Here we employed the definition of $G_{l,n}$ [see the text above (35)], performed the angular integration, changed variables $n\xi:=B|x|^2/2$ in the remaining integral, and used Lemma 3 and the dominated-convergence theorem. □

C. A Wegner-type of estimate

The second ingredient for the proof of Theorem 2 is the following:

Proposition 3: In the situation of Theorem 2 let $E_1<E_2\leqslant E\leqslant 0$ *and put* $I:=]E_1,E_2[$. *Then*

$$\nu_{l,n}(I)\leqslant\left(\frac{|I|}{\sqrt{2\pi}\langle\psi_{l,0},C_\mu\psi_{l,0}\rangle}+s_{l,n}\right)\exp\left(\beta E+\frac{\beta^2}{2}C(0)\right),\tag{53}$$

for all $\beta\geqslant 0$. *Here* $s_{l,n}:=\int_1^\infty \mathrm{d}\xi\, G_{l,n}(n\xi)$ *converges to zero as* $n\to\infty$.

Proof: By the definition of $\nu_{l,n}$ and the spectral theorem one has

$$\nu_{l,n}(I)\leqslant\frac{e^{\beta E}}{n}\,\mathbb{E}\{\mathrm{Tr}[P_{l,n}e^{-\beta P_{l,n}VP_{l,n}}\chi_I(P_{l,n}VP_{l,n})P_{l,n}]\}.\tag{54}$$

We evaluate the trace in an orthonormal eigenbasis of $P_{l,n}V^{(\omega)}P_{l,n}$ and apply the Jensen–Peierls inequality[45] to bound the probabilistic expectation in (54) from above by

$$\begin{aligned}&\mathbb{E}\{\mathrm{Tr}[P_{l,n}e^{-\beta V}P_{l,n}\chi_I(P_{l,n}VP_{l,n})P_{l,n}]\}\\&\quad=\frac{B}{2\pi}\int_{\mathbb{R}^2}\mathrm{d}^2x\,\mathbb{E}\{e^{-\beta V(0)}\langle\psi_{l,x,n},\chi_I(P_{l,n}V(\cdot-x)P_{l,n})\psi_{l,x,n}\rangle\},\end{aligned}\tag{55}$$

where we used Fubini's theorem and the $\mathbb{R}^2$-homogeneity of V. The Lebesgue integral in (55) over the plane may be split into two parts with domains of integration inside and outside a disk centered at the origin and with radius $\sqrt{2n/B}$.

To estimate the inner part, we use the one-parameter decomposition (16) of the Gaussian random potential V. Since U and λ are stochastically independent, we may estimate the conditional expectation of the integrand in (55) relative to the sub-sigma-algebra generated by $\{U(y)\}_{y\in\mathbb{R}^2}$ with the help of Lemma 1. Taking there $g(\xi)=\exp(-\beta\xi C_\mu(0)-\xi^2/2)/\sqrt{2\pi}$, $K=\psi_{l,x,n}\langle\psi_{l,x,n},\cdot\rangle/\langle\psi_{l,x,n},\psi_{l,x,n}\rangle$, and $M=P_{l,n}C_\mu(\cdot-x)P_{l,n}\geqslant\langle\psi_{l,0},C_\mu\psi_{l,0}\rangle\langle\psi_{l,x,n},\psi_{l,x,n}\rangle K^2$, where the last inequality follows from Lemma 2 and the positivity as well as the spherical symmetry of C_μ, we obtain an ω- and x-independent bound according to

$$\begin{aligned}&\int_{\mathbb{R}}\mathrm{d}\xi\,\frac{e^{-\xi^2/2}}{\sqrt{2\pi}}\,e^{-\beta\xi C_\mu(0)}\langle\psi_{l,x,n},\chi_I(P_{l,n}U^{(\omega)}(\cdot-x)P_{l,n}+\xi P_{l,n}C_\mu(\cdot-x)P_{l,n})\psi_{l,x,n}\rangle\\&\quad\leqslant\frac{|I|}{\sqrt{2\pi}\langle\psi_{l,0},C_\mu\psi_{l,0}\rangle}\exp\left(\frac{\beta^2}{2}(C_\mu(0))^2\right).\end{aligned}\tag{56}$$

Using $\mathbb{E}[\exp(-\beta U(0))]=\exp(\beta^2(C(0)-(C_\mu(0))^2)/2)$, the inner part of the integral in (55), may hence be estimated as follows:

$$\begin{aligned}&\int_{|x|^2\leqslant 2n/B}\mathrm{d}^2x\,\mathbb{E}\{e^{-\beta V(0)}\langle\psi_{l,x,n},\chi_I(P_{l,n}V(\cdot-x)P_{l,n})\psi_{l,x,n}\rangle\}\\&\quad\leqslant\frac{2\pi n}{B}\,\frac{|I|}{\sqrt{2\pi}\langle\psi_{l,0},C_\mu\psi_{l,0}\rangle}\exp\left(\frac{\beta^2}{2}C(0)\right).\end{aligned}\tag{57}$$

This gives the first part of the claimed inequality (53).

To complete the proof, we estimate the outer part of the integral in (55) as follows:

$$\int_{|x|^2\geqslant 2n/B} \mathrm{d}^2x\,\mathbb{E}\{e^{-\beta V(0)}\langle \psi_{l,x,n}, \chi_I(P_{l,n}V(\cdot - x)P_{l,n})\psi_{l,x,n}\rangle\}$$

$$\leqslant \mathbb{E}\{e^{-\beta V(0)}\}\int_{|x|^2\geqslant 2n/B} \mathrm{d}^2x\langle \psi_{l,x,n}, \psi_{l,x,n}\rangle = \frac{2\pi n}{B}\,\mathbb{E}\{e^{-\beta V(0)}\}\int_1^\infty \mathrm{d}\xi G_{l,n}(n\xi). \quad (58)$$

Here we employed (51) and changed variables $n\xi := B|x|^2/2$ to obtain the last equality. Thanks to Lemma 3, the last integral in (58), and hence $s_{l,n}$, converges to zero as $n\to\infty$ by the dominated-convergence theorem. □

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Investigation of the relativistic equivalent Hamiltonian in the *LS* coupling scheme

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Armstrong's method of relativistic description of atoms in *LS* coupling using the equivalent operator is developed. Its form in terms of standard unit operators acting within a space of one shell is obtained. The interpretation of separate terms of equivalent Breit operator is investigated in a general case of nonequivalent electrons. The relativistic Dirac–Fock equations for the level and term in *LS* coupling are derived. The equivalent operator is applied to obtain the averages of relativistic operators too. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1415429]

I. INTRODUCTION

Relativistic effects become rather important for heavy atoms, however, even within the $5f^N$ open electronic shell in actinidies the coupling remains closer to *LS* than to the *jj* scheme.[1] There are two ways to perform calculations in the relativistic *LS* coupling: to transform relativistic wave functions from *jj* to *LS* coupling[2,3] or to use a relativistic equivalent operator.[4–6] The transformation matrices from *jj* to *LS* coupling have rather complex form, because such transformation requires one not only to change the coupling of moments, but also to separate all equivalent electrons by fractional parentage coefficients of one scheme and then to join them by the corresponding coefficients of the other scheme or to use the recurrence relations.[7] This method was implemented in the computer code.[8] However, the other method proposed in Ref. 4 and elaborated in Refs. 5 and 6 also deserves attention: the introduction of an equivalent operator which can be evaluated with respect to nonrelativistic wave functions to produce the same result as obtained by evaluating the relativistic Hamiltonian with respect to relativistic wave functions. Such operator was obtained in Ref. 5 for the Breit equation using the summation rules for $3nj$ symbols and later by the more effective method of second quantization in Ref. 6. Advantages of this method are a simplicity of the calculation of matrix elements in the appropriate nonrelativistic scheme as well as the possibility to have additional insight into the properties of various parts of the Hamiltonian and in this way to introduce some approximations. The mixing of various relativistic configurations arising from the same nonrelativistic configuration is taken into account automatically by this method.

The aim of this work is to express the equivalent operator in terms of standard operators acting within the space of one shell and to consider the asymptotic of its terms in a general case (Sec. II) as well as to apply this operator to obtain the Dirac–Fock equations in *LS* coupling (Sec. III) and averages of relativistic operators (Sec. IV).

II. EXPRESSIONS FOR THE EQUIVALENT OPERATOR

We will consider the relativistic Dirac–Breit Hamiltonian:

$$H^{\mathrm{rel}} = H_{\alpha_1} + H_{\alpha_2} + H_\beta + H_\gamma + H_\delta, \tag{1}$$

where

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$$H_{\alpha_1}=\sum_i\ ((\alpha_i\,\mathbf{p}_i)+(\beta_i-1)\,mc^2),$$

$$H_{\alpha_2}=-\sum_i\ \frac{Ze^2}{r_i},\quad H_\beta=\sum_{i<j}\frac{e^2}{r_{ij}},\tag{2}$$

$$H_\gamma=-\frac{e^2}{2}\sum_{i<j}\frac{(\alpha_i\cdot\alpha_j)}{r_{ij}},\quad H_\delta=-\frac{e^2}{2}\sum_{i<j}\frac{(\alpha_i\cdot\mathbf{r}_{ij})(\alpha_j\cdot\mathbf{r}_{ij})}{r_{ij}^3}.$$

Here the usual notations are employed. The rest mass of electrons is excluded from (1) in order to have the Hamiltonian corresponding to its nonrelativistic analogue.

The way to obtain the equivalent operator O_i corresponding to the relativistic operator H_i as stated in Ref. 5 is as follows. The one-electron (H_1) and two-electron (H_2) relativistic operators are presented in the second quantization form:

$$H_1=\sum_{\substack{n_1l_1j_1m_1\\ n_2l_2j_2m_2}} q_{m_1}^{(j_1)+}(n_1l_1j_1m_1|h_1|n_2l_2j_2m_2)q_{m_2}^{(j_2)},\tag{3}$$

$$H_2=\sum_{\{n_il_ij_im_i\}} q_{m_1}^{(j_1)+}q_{m_2}^{(j_2)+}(n_1l_1j_1m_1n_2l_2j_2m_2|h_2|n_3l_3j_3m_3n_4l_4j_4m_4)q_{m_4}^{(j_4)}q_{m_3}^{(j_3)},\tag{4}$$

where $q_m^{(j)+}$ is a creation operator producing the one-electron state $|nljm)$ and $q_m^{(j)}$ is an annihilation operator destroying such a state; $\{n_il_ij_im_i\}$ means all sets with $i=1-4$. Expressions (3) and (4) also contain one- and two-electron matrix elements with respect to non-antisymmetrized wave functions. The relativistic single-electron state has the form:

$$|nljm)=\begin{pmatrix}|nljm\rangle\\ i|n\overline{l}jm\rangle\end{pmatrix},\tag{5}$$

where $\overline{l}=l\pm1$ as $j=l\pm\frac{1}{2}$. $|nljm\rangle$ can be treated as a nonrelativistic state[6] (relativistic states are indicated by a rounded ket and the nonrelativistic ones by an angular ket). Operators $q_m^{(j)+}$ and $\tilde{q}_m^{(j)}=(-1)^{j-m}q_{-m}^{(j)}$ are transformed like the components of a spherical tensor of rank j.

According to (5) the relativistic operators $q^{(j)+}$ and $\tilde{q}^{(j)}$ of creation or annihilation of electron can be expressed in terms of nonrelativistic operators $a^{(j)+}$ and $\tilde{a}^{(j)}$, and the latter can be transformed into the ls coupling scheme using Clebsch–Gordan coefficients:

$$a_m^{(j)+}=\sum_{m_lm_s}\begin{bmatrix}l & s & j\\ m_l & m_s & m\end{bmatrix}a_{m_lm_s}^{(ls)+},\quad \tilde{a}_m^{(j)}=\sum_{m_lm_s}\begin{bmatrix}l & s & j\\ m_l & m_s & m\end{bmatrix}\tilde{a}_{m_lm_s}^{(ls)}.\tag{6}$$

It is useful to introduce the standard operator $W^{(k_1k_2k)}$ with the orbital rank k_1, spin rank k_2, and total rank k. In the second quantization form of coupled operators a^+ and $\tilde{a}$ the operator $W^{(k_1k_2k)}$ is represented

$$W^{(k_1k_2k)}=-[k_1,k_2]^{-1/2}\sum_{n_1l_1n_2l_2}[a^{(l_1s)+}\times\tilde{a}^{(l_2s)}]^{(k_1k_2k)}\langle n_1l_1s\|w^{(k_1k_2)}(n_1l_1,n_2l_2)\|n_2l_2s\rangle,\tag{7}$$

where $[k_1,k_2]$ means $(2k_1+1)(2k_2+1)$. The reduced matrix element of the one-electron operator (7) is defined

$$\langle n_\alpha l_\alpha s\|w^{(k_1k_2)}(n_1l_1,n_2l_2)\|n_\beta l_\beta s\rangle=[k_1,k_2]^{1/2}\delta(n_1,n_\alpha)\,\delta(l_1,l_\alpha)\,\delta(n_\beta,n_2)\,\delta(l_\beta,l_2).\tag{8}$$

Then

$$W^{(k_1k_2k)}=-\sum_{n_1l_1n_2l_2}[a^{(l_1s)+}\times\tilde{a}^{(l_2s)}]^{(k_1k_2k)}=\sum_{n_1l_1n_2l_2}W^{(k_1k_2k)}(n_1l_1,n_2l_2). \tag{9}$$

At $n_1l_1\equiv n_2l_2$ the operator

$$W^{(k_1k_2k)}(n_1l_1,n_2l_2)\equiv W^{(k_1k_2k)}(n_1l_1) \tag{10}$$

is obtained. It is acting in the space of $n_1l_1^{N_1}$ shell and equals to the sum of one-electron operators $\Sigma_{i=1}^{N_1}w_i(n_1l_1)$.

Application of the Wigner–Eckart theorem to the matrix elements in (3) and (4), coupling of a^+, $\tilde{a}$ operators, and summation of all Clebsch–Gordan coefficients over the projections of moments result in the expressions for the equivalent operators O_1 and O_2.

Contrary to the suggestion given in Ref. 5 the derivation of an equivalent operator does not amount to ignoring the coupling of small components of the wave function. The corresponding terms with the operators $a^{(ls)+}_{m_lm_s}$ and $\tilde{a}^{(ls)}_{m_lm_s}$ vanish when considering the interaction within the particular shells [due to the presence of δ functions in (8)]. Thus these terms can be omitted without making any additional approximations.

The expressions for various one-electron equivalent operators were given in Refs. 4–6, and 9. Its general form for the Hamiltonian with total rank equal to 0 is

$$O_1=\sum_{jkn_1l_1n_2l_2}(-1)^{l_2+1/2+j+k}[j,k]^{1/2}\begin{Bmatrix} l_1 & 1/2 & j \\ 1/2 & l_2 & k \end{Bmatrix}(n_1l_1j\|h_1\|n_2l_2j)W^{(kk0)}(n_1l_1,n_2l_2). \tag{11}$$

This expression is valid not only for a single configuration, but also for configuration interaction approximation.

In the case of two-electron Hamiltonian of the general type

$$H_2=\sum_{i<j}\sum_k(g_i^{(k)}\cdot g_j^{(k)}), \tag{12}$$

where k is a rank with respect to the total momentum, the corresponding equivalent operator obtains the following expression:

$$\begin{aligned} O_2=&\frac{1}{2}\sum_{k\atop\{n_il_ij_i\}}[k]^{-1}(n_1l_1j_1n_2l_2j_2\|g_1^{(k)}g_2^{(k)}\|n_3l_3j_3n_4l_4j_4)\\ &\times\Bigg\{\sum_{k_1K_1k_2K_2}[k_1,K_1,k_2,K_2,j_1,j_2,j_3,j_4]^{1/2}\begin{Bmatrix} l_1 & l_3 & k_1 \\ 1/2 & 1/2 & K_1 \\ j_1 & j_3 & k \end{Bmatrix}\begin{Bmatrix} l_2 & l_4 & k_2 \\ 1/2 & 1/2 & K_2 \\ j_2 & j_4 & k \end{Bmatrix}\\ &\times(W^{(k_1K_1k)}(n_1l_1,n_3l_3)\cdot W^{(k_2K_2k)}(n_2l_2,n_4l_4))-\delta(n_2,n_3)\delta(l_2,l_3)\delta(j_2,j_3)\delta(j_1,j_4)\\ &\times\sum_{k_1}(-1)^{k_1+l_1+j_3+1/2}[k][k_1]^{1/2}\begin{Bmatrix} 1/2 & 1/2 & k_1 \\ l_1 & l_4 & j_1 \end{Bmatrix}W^{(k_1k_10)}(n_1l_1,n_4l_4)\Bigg\}. \end{aligned} \tag{13}$$

The second term appears from the transposition of operators $a^{(l_2s)+}$ and $\tilde{a}^{(l_3s)}$. Equation (13) was derived in Ref. 6, but the function $\delta(j_1,j_4)$ was omitted in its second term.

Expression (13) is applicable in the configuration interaction as well as in the single-configuration approximations. For the latter case it is more convenient to use the single shell reduced matrix elements of operator $W^{(k_1k_2k)}(nl)$ (10) as standard quantities for the calculation of

matrix elements. Consequently, in single-configuration approximation Eq. (13) is useful only for the interaction within a shell of equivalent electrons. The direct and the exchange interactions between $n_1 l_1^{N_1}$ and $n_2 l_2^{N_2}$ shells are described by the following equivalent operators:

$$O_2^d = \sum_{\substack{k k_1 K_1 k_2 K_2 \\ j_1 j_2 j_3 j_4}} [k]^{-1} [k_1, K_1, k_2, K_2, j_1, j_2, j_3, j_4]^{1/2} (n_1 l_1 j_1 n_2 l_2 j_2 \| g_1^{(k)} g_2^{(k)} \| n_1 l_1 j_3 n_2 l_2 j_4) \times \begin{Bmatrix} l_1 & l_1 & k_1 \\ 1/2 & 1/2 & K_1 \\ j_1 & j_3 & k \end{Bmatrix} \begin{Bmatrix} l_2 & l_2 & k_2 \\ 1/2 & 1/2 & K_2 \\ j_2 & j_4 & k \end{Bmatrix} (W^{(k_1 K_1 k)}(n_1 l_1) \cdot W^{(k_2 K_2 k)}(n_2 l_2)), \tag{14}$$

$$O_2^{\mathrm{ex}} = \sum_{\substack{\kappa k k_1 K_1 k_2 K_2 \\ j_1 j_2 j_3 j_4}} (-1)^{k+\kappa} [k_1, K_1, k_2, K_2, j_1, j_2, j_3, j_4]^{1/2} (n_1 l_1 j_1 n_2 l_2 j_2 \| g_1^{(k)} g_2^{(k)} \| n_2 l_2 j_4 n_1 l_1 j_3) \times \begin{Bmatrix} l_1 & l_1 & k_1 \\ 1/2 & 1/2 & K_1 \\ j_1 & j_3 & \kappa \end{Bmatrix} \begin{Bmatrix} l_2 & l_2 & k_2 \\ 1/2 & 1/2 & K_2 \\ j_2 & j_4 & \kappa \end{Bmatrix} \begin{Bmatrix} j_1 & j_3 & \kappa \\ j_2 & j_4 & k \end{Bmatrix} (W^{(k_1 K_1 \kappa)}(n_1 l_1) \cdot W^{(k_2 K_2 \kappa)}(n_2 l_2)). \tag{15}$$

The ranks of operators in the orbital and spin spaces can be joined into the common ranks:

$$(W^{(k_1 K_1 k)} \cdot W^{(k_2 K_2 k)}) = \sum_u [k][u]^{1/2} (-1)^{k_2 + K_1 + u} \begin{Bmatrix} k_1 & K_1 & k \\ K_2 & k_2 & u \end{Bmatrix} [W^{(k_1 K_1)} \times W^{(k_2 K_2)}]^{(uu0)}. \tag{16}$$

The equivalent operators O_β, O_γ, and O_δ are obtained in a simple way from (13) to (15) while substituting the corresponding formulas for the reduced matrix elements given in Refs. 6 and 10 into these equations.

For O_β:

$$(n_1 l_1 j_1 n_2 l_2 j_2 \| g_1^{(k)} g_2^{(k)} \| n_3 l_3 j_3 n_4 l_4 j_4)_\beta = e^2 \int\int (n_1 l_1 j_1 \| h_1^{(k)} \| n_3 l_3 j_3) \times (n_2 l_2 j_2 \| h_2^{(k)} \| n_4 l_4 j_4) \frac{r_<^k}{r_>^{k+1}} \mathrm{d}r_1 \mathrm{d}r_2 \tag{17}$$

with

$$(n_1 l_1 j_1 \| h^{(k)} \| n_3 l_3 j_3) = (-1)^{l_1 + l_3 - j_3 + 1/2} [j_1, j_3]^{1/2} \begin{pmatrix} j_1 & k & j_3 \\ -1/2 & 0 & 1/2 \end{pmatrix} \times [\Delta(l_1 l_3 k) P_1 P_3 + \Delta(\bar{l}_1 \bar{l}_3 k) Q_1 Q_3], \tag{18}$$

where P and Q are, respectively, the large and small components of radial wave function and $\Delta(l_1 l_3 k)$ means the condition that the parameters l_1, l_3, and k form a triangle and their sum is even. $P_i \equiv P_{n_i l_i j_i}(r)$; $Q_i \equiv Q_{n_i \bar{l}_i j_i}(r)$.

For O_γ:

$$(n_1l_1j_1n_2l_2j_2\|g_1^{(k)}g_2^{(k)}\|n_3l_3j_3n_4l_4j_4)_\gamma$$
$$=\frac{e^2}{2}\sum_t\int\int(-1)^{k+t}\frac{r_<^t}{r_>^{t+1}}(n_1l_1j_1\|[C_1^{(t)}\times\alpha_1^{(1)}]^{(k)}\|n_3l_3j_3)$$
$$\times(n_2l_2j_2\|[C_2^{(t)}\times\alpha_2^{(1)}]^{(k)}\|n_4l_4j_4)\mathrm{d}r_1\mathrm{d}r_2 \tag{19}$$

with

$$(n_1l_1j_1\|[C^{(t)}\times\alpha^{(1)}]^{(k)}\|n_3l_3j_3)$$
$$=i[k,j_1,j_3]^{1/2}(-1)^{l_1+l_3+j_1+j_3+k}\Bigg\{(-1)^{l_1+1}\sqrt{2}\begin{pmatrix}1&t&k\\-1&0&1\end{pmatrix}\begin{pmatrix}j_1&j_3&k\\-1/2&-1/2&1\end{pmatrix}$$
$$\times[\Delta(l_1\bar{l}_3t)P_1Q_3+\Delta(\bar{l}_1l_3t)Q_1P_3]+(-1)^{j_3+1/2+t}\begin{pmatrix}1&t&k\\0&0&0\end{pmatrix}\begin{pmatrix}j_1&j_3&k\\-1/2&1/2&0\end{pmatrix}$$
$$\times[\Delta(l_1\bar{l}_3t)P_1Q_3-\Delta(\bar{l}_1l_3t)Q_1P_3]\Bigg\}. \tag{20}$$

For O_δ:

$$(n_1l_1j_1n_2l_2j_2\|g_1^{(k)}g_2^{(k)}\|n_3l_3j_3n_4l_4j_4)_\delta$$
$$=\frac{e^2}{6}\sum_t\int\int(n_1l_1j_1\|[C_1^{(t)}\times\alpha_1^{(1)}]^{(k)}\|n_3l_3j_3)(n_2l_2j_2\|[C_2^{(t)}\times\alpha_2^{(1)}]^{(k)}\|n_4l_4j_4)$$
$$\times(-1)^{k+t}\frac{r_<^t}{r_>^{t+1}}\mathrm{d}r_1\mathrm{d}r_2+\frac{5e^2}{2}\sum_{tpq}F(tqp)\begin{Bmatrix}1&1&2\\q&p&k\end{Bmatrix}$$
$$\times\int_0^\infty\mathrm{d}r_2\Bigg[\int_0^{r_2}\mathrm{d}r_1\frac{r_1^t}{r_2^{t+1}}(n_1l_1j_1\|[C_1^{(q)}\times\alpha_1^{(1)}]^{(k)}\|n_3l_3j_3)(n_2l_2j_2\|[C_2^{(p)}\times\alpha_2^{(1)}]^{(k)}\|n_4l_4j_4)$$
$$+\int_{r_2}^\infty\mathrm{d}r_1\frac{r_2^t}{r_1^{t+1}}(n_1l_1j_1\|[C_1^{(p)}\times\alpha_1^{(1)}]^{(k)}\|n_3l_3j_3)(n_2l_2j_2\|[C_2^{(q)}\times\alpha_2^{(1)}]^{(k)}\|n_4l_4j_4)\Bigg] \tag{21}$$

with

$$F(tqp)=\begin{cases}\left[\dfrac{8t(t+1)(2t+1)}{15(2t-1)(2t+3)}\right]^{1/2}, & \text{if } q=p=t,\\ -\left[\dfrac{t(t-1)(2t-3)(2t+1)}{5(2t-1)}\right]^{1/2}, & \text{if } q=t-2,\ p=t,\\ \left[\dfrac{(t+1)(t+2)(2t+1)(2t+5)}{5(2t+3)}\right]^{1/2}, & \text{if } q=t,\ p=t+2.\end{cases} \tag{22}$$

In Ref. 6 the multiplier t was written instead of $t+1$ for $F(t\,t\,t+2)$.

It was shown in Ref. 5, that various terms of operators O_α, O_β, O_γ, and O_δ asymptotically turn into the operators of relativistic corrections in the Breit–Pauli approximation. For such identification the small component of relativistic wave function is expressed by the large component. After some transformations of radial integrals only the terms of the lowest order (up to α^2) are retained. In Ref. 5 such identification was accomplished for the equivalent electrons.

TABLE I. Correspondence of the terms of equivalent operators to the nonrelativistic and Breit–Pauli interaction operators.

Equivalent operator	Ranks k	Ranks k	Breit–Pauli interaction operator
O_{α_1}	0	0	Kinetic energy and mass correction
	1	1	Does not give contribution of order α^0, α^2
O_{α_2}	0	0	$-Ze^2/r$, Darwin and mass correction
	1	1	Spin–orbit

Equivalent operator	Ranks k_1	Ranks K_1	Ranks k_2	Ranks K_2	Breit–Pauli interaction operator
O_β	k	0	k	0	e^2/r_{12}, Darwin and mass correction
	k	0	k	1	Spin–other–orbit
	k	1	k	0	Spin–other–orbit
	k	0	$k-1$	1	Spin–other–orbit
	k	0	$k+1$	1	Spin–other–orbit
	$k-1$	1	k	0	Spin–other–orbit
	$k+1$	1	k	0	Spin–other–orbit
	k	1	k	1	Does not give contribution of order α^2
	$k-1$	1	$k-1$	1	Does not give contribution of order α^2
	$k-1$	1	$k+1$	1	Does not give contribution of order α^2
	$k+1$	1	$k-1$	1	Does not give contribution of order α^2
	$k+1$	1	$k+1$	1	Does not give contribution of order α^2
O_γ, O_δ	$k-1$	1	$k+1$	1	Spin–spin
	$k+1$	1	$k-1$	1	Spin–spin
	k	0	k	0	orbit–orbit
	k	0	k	1	Spin–other–orbit
	k	1	k	0	Spin–other–orbit
	k	0	$k-1$	1	Spin–other–orbit
	k	0	$k+1$	1	Spin–other–orbit
	$k-1$	1	k	0	Spin–other–orbit
	$k+1$	1	k	0	Spin–other–orbit
	$k-1$	1	$k-1$	1	Spin–spin–contact (at $u=0$) or
	k	1	k	1	does not give contribution
	$k+1$	1	$k+1$	1	of order α^2 (at $u \geqslant 1$)

It follows from the second quantization form for operator H_2 (4) that for such investigation in a general case it is sufficient to obtain the asymptotic relations for the two-electron matrix elements. Their expressions for various Breit–Pauli operators in the case of nonequivalent electrons were presented in Refs. 11–13. The final results are presented in Table I. They mainly correspond to the identification given in Ref. 5 but some restrictions for the ranks of operators are removed in a general case. The additional terms for the nonequivalent operators appear: the terms of O_β, O_γ, and O_δ with the ranks $k_1=k_2=k$, $K_1=1$, $K_2=0$ corresponding to the spin-other-orbit interaction as well as the terms of O_β with $k_1=k_2=k$, $K_1=K_2=1$, which do not give contribution of order α^2. The terms of O_γ and O_δ corresponding to spin–spin and spin–spin–contact interactions also give the additional operator, whose matrix elements vanish in the general case (direct and exchange parts of the matrix element cancel each other).

Some terms of the equivalent operators give the contributions to various Breit–Pauli operators: the terms of O_{α_2} with $k=0$ and of O_β with $k_1=k_2=k$, $K_1=K_2=0$ containing large components of orbitals turn into the operators of Coulomb interaction $-Ze^2/r$ and e^2/r_{12}. On the other hand, the same terms of these operators with small components of orbitals turn into the Darwin and mass corrections. The term of O_{α_1} with the rank $k=0$ in order α^0 gives the operator of kinetic energy and in order α^2 gives contribution to the mass correction; the part of this operator with the rank $k=1$ vanishes in the Breit–Pauli approximation. The part of the equivalent

operators O_γ and O_δ with orbital ranks $k_1=k_2$ equal to k, $k\pm1$ and spin ranks $K_1=K_2=1$ turns at $u=0$ into the operator of spin–spin–contact interaction but at $u=1,2$ does not give contribution of order α^2.

The terms of O_γ and O_δ corresponding to spin–spin and spin–spin–contact interactions also give some additional operators, whose matrix elements vanish in a general case.

The expressions for matrix elements of equivalent operators are obtained by applying the formulas presented in Refs. 14 and 15.

III. RELATIVISTIC DIRAC–FOCK EQUATIONS FOR A LEVEL AND TERM IN *LS* COUPLING

For some excited configurations, especially those with the collapsing electron, a dependence of the radial orbitals on the many-electron state can become rather strong. Then it is necessary to solve the term-dependent equations instead of the usual ones for the average energy.

If a coupling scheme within the electronic shell for rather heavy atoms remains closer to LS than to jj coupling, the relativistic equations for the LS state have to be solved.

The relativistic equations for the LS state can be obtained using the expression for the matrix element of the equivalent operator as a functional. We will take into account only the main terms of the equivalent relativistic Hamiltonian O_{α_1}, O_{α_2}, and O_β. Let us present the matrix elements of operators $O_{\alpha_1}+O_{\alpha_2}$, and O_β in the following form:

$$\langle K\gamma|O_{\alpha_1}+O_{\alpha_2}|K\gamma\rangle=\sum_{lj}\ \alpha_j(l^N\gamma)I(lj), \tag{23}$$

$$\begin{aligned}\langle K\gamma|O_\beta|K\gamma\rangle=&\sum_{ljj'}\ \sum_k\ \varphi_{kjj'}(l^N\gamma)F^k(lj,lj')+\sum_{ljj'(j\neq j')}\ \sum_k\ \gamma_{kjj'}(l^N\gamma)G^k(lj,lj')\\&+\frac{1}{2}\sum_{ll'(l\neq l')jj'}\ \sum_k\ [\varphi_{kjj'}(l^Nl'^{N'}\gamma)F^k(lj,l'j')+\gamma_{kjj'}(l^Nl'^{N'}\gamma)G^k(lj,l'j')],\end{aligned} \tag{24}$$

where I, F^k, and G^k are the relativistic radial integrals[8] and α_k, φ_k, and γ_k are the coefficients at these integrals.

The Dirac–Fock equations in LS coupling are then presented:

$$\begin{aligned}\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\kappa}{r}\right)P_{nlj}(r)=&\frac{1}{c}[2c^2-\varepsilon_{nlj}-Y_{nlj}(r)]\,Q_{n\bar{l}j}(r)-X^P_{nlj}(r)\\&-\frac{1}{c}\sum_{n'l'j'(\neq nlj)}\ \delta(\kappa,\kappa')\,\varepsilon_{nlj,n'l'j'}\,Q_{n'\bar{l}'j'}(r),\\\left(\frac{\mathrm{d}}{\mathrm{d}r}-\frac{\kappa}{r}\right)Q_{n\bar{l}j}(r)=&\frac{1}{c}[\varepsilon_{nlj}+Y_{nlj}(r)]\,P_{nlj}(r)+X^Q_{n\bar{l}j}(r)\\&+\frac{1}{c}\sum_{n'l'j'(\neq nlj)}\ \delta(\kappa,\kappa')\varepsilon_{nlj,n'l'j'}\,P_{n'l'j'}(r),\end{aligned} \tag{25}$$

where the direct and exchange potentials are given by

$$Y_{nlj}(r)=\frac{1}{r}\Bigg\{-Z+\alpha_j(l^N\gamma)^{-1}\sum_{j'k}\ \varphi_{kjj'}(l^N\gamma)\,[1+\delta(j,j')]\,[Y^k_{nlj',nlj'}(r)+Y^k_{n\bar{l}j',n\bar{l}j'}(r)]$$

$$+\alpha_j(l^N\gamma)^{-1}\sum_{n'l'(\neq nl)}\ \sum_{j'k}\ \varphi_{kjj'}(l^N l'^{N'}\gamma)[Y^k_{n'l'j',n'l'j'}(r)+Y^k_{n'\bar{l}'j',n'\bar{l}'j'}(r)]\Bigg\}, \tag{26}$$

$$X^P_{nlj}(r)=\frac{1}{cr}\,\alpha_j(l^N\gamma)^{-1}\Bigg\{\sum_{j'(\neq j)}\ \sum_k\ \gamma_{kjj'}(l^N\gamma)\,[Y^k_{nlj,nlj'}(r)+Y^k_{n\bar{l}j,n\bar{l}j'}(r)]\,Q_{n\bar{l}j'}(r)$$

$$+\sum_{l'\neq l}\ \sum_{kj'}\ \gamma_{kjj'}(l^N l'^{N'}\gamma)\,[Y^k_{nlj,n'l'j'}(r)+Y^k_{n\bar{l}j,n'\bar{l}'j'}(r)]\,Q_{n'\bar{l}'j'}(r)\Bigg\}, \tag{27}$$

$$X^Q_{nlj}(r)=\frac{1}{cr}\,\alpha_j(l^N\gamma)^{-1}\Bigg\{\sum_{j'(\neq j)}\ \sum_k\ \gamma_{kjj'}(l^N\gamma)\,Y^k_{n\bar{l}j,n\bar{l}j'}(r)\,P_{nlj'}(r)$$

$$+\sum_{n'l'(\neq nl)}\ \sum_{kj'}\ \gamma_{kjj'}(l^N l'^{N'}\gamma)\,Y^k_{nlj,n'\bar{l}'j'}(r)\,P_{n'l'j'}(r)\Bigg\}. \tag{28}$$

In (26)–(28) the integral function Y^k is defined:

$$Y^k_{nlj,n'l'j'}(r)=r^{-k}\int_0^r r_1^k\,P_{nlj}(r_1)\,P_{n'l'j'}(r_1)\,\mathrm{d}r_1+r^{k+1}\int_r^\infty r_1^{-k-1}\,P_{nlj}(r_1)\,P_{n'l'j'}(r_1)\,\mathrm{d}r_1. \tag{29}$$

When in its notation the quantum number l is replaced by $\bar{l}$, the radial function $Q_{n\bar{l}j}(r)$ is used instead of $P_{nlj}(r)$. The quantum number κ is defined:

$$\kappa=\begin{cases} l & \text{for } j=l-1/2\\ -l-1 & \text{for } j=l+1/2.\end{cases} \tag{30}$$

The potentials (26)–(28) correspond to the equations for the LSJ level. If we like to obtain the equations for the LS term, it is necessary to take into account only the term with the rank $k=0$ in α_{kj} and to leave only the terms with $K_1=K_2=0$ in $\varphi_{kjj'}$, $\gamma_{kjj'}$.

IV. THE AVERAGES OF THE RELATIVISTIC OPERATORS

The expressions for the equivalent operator in terms of standard operators enable us to obtain the average values of various parts of Hamiltonian in a simple way.

The average values of the operators $(W^{(k_1K_1k)}\cdot W^{(k_2K_2k)})$ and $W^{(kk0)}$ have the expressions:

$$\frac{1}{g(l^N)}\sum_{\gamma LSJ}[J]\langle nl^N\gamma LSJ|(W^{(k_1K_1k)}(nl)\cdot W^{(k_2K_2k)}(nl))|nl^N\gamma LSJ\rangle$$

$$=\frac{N(N-1)}{(4l+1)(2l+1)}\,\delta(k_1,k_2)\,\delta(K_1,K_2)[[l]\,\delta(k_1,0)\,\delta(K_1,0)+2l\,(-1)^{k_1+K_1+k}[k]], \tag{31}$$

$$\frac{1}{g(l^N)}\sum_{\gamma LSJ}[J]\langle nl^N\gamma LSJ|W^{(kk0)}(nl)|nl^N\gamma LSJ\rangle=\frac{N(N-1)}{2}\sqrt{\frac{2}{2l+1}}\,\delta(k,0), \tag{32}$$

$$\frac{1}{g(l_1^{N_1}l_2^{N_2})}\sum_{\gamma LSJ}[J]\langle n_1 l_1^{N_1} n_2 l_2^{N_2}\gamma LSJ|(W^{(k_1K_1k)}(n_1l_1)\cdot W^{(k_2K_2k)}(n_2l_2))|n_1 l_1^{N_1} n_2 l_2^{N_2}\gamma LSJ\rangle$$

$$=\frac{N_1N_2}{2[l_1,l_2]^{1/2}}\delta(k,0)\,\delta(k_1,0)\,\delta(k_2,0)\,\delta(K_1,0)\,\delta(K_2,0), \tag{33}$$

where $g(l^N)$ and $g(l_1^{N_1}l_2^{N_2})$ are the statistical weights of configurations.

The substitution of (31)–(33) into the averages of the equivalent operator O_2 and summation over the ranks give the following results:

$$\frac{1}{g(l^N)}\sum_{\gamma LSJ}[J]\langle nl^N\gamma LSJ|O_2|nl^N\gamma LSJ\rangle$$

$$=\frac{N(N-1)}{2(4l+1)(4l+2)}\Bigg[\sum_{k(>0)j_1j_2}(-1)^{j_1+j_2}(nlj_1nlj_2\|g_1^{(k)}g_2^{(k)}\|nlj_2nlj_1)$$

$$+\sum_{j_1j_2}[j_1,j_2]^{1/2}(nlj_1nlj_2\|g_1^{(0)}g_2^{(0)}\|nlj_1nlj_2)\Bigg], \tag{34}$$

$$\frac{1}{g(l_1^{N_1}l_2^{N_2})}\sum_{\gamma LSJ}[J]\langle n_1 l_1^{N_1} n_2 l_2^{N_2}\gamma LSJ|O_2^d|n_1 l_1^{N_1} n_2 l_2^{N_2}\gamma LSJ\rangle$$

$$=\frac{N_1N_2}{(4l_1+2)(4l_2+2)}\sum_{j_1j_2}[j_1,j_2]^{1/2}(n_1l_1j_1n_2l_2j_2\|g_1^{(0)}g_2^{(0)}\|n_1l_1j_1n_2l_2j_2), \tag{35}$$

$$\frac{1}{g(l_1^{N_1}l_2^{N_2})}\sum_{\gamma LSJ}[J]\langle n_1 l_1^{N_1} n_2 l_2^{N_2}\gamma LSJ|O_2^{\mathrm{ex}}|n_1 l_1^{N_1} n_2 l_2^{N_2}\gamma LSJ\rangle$$

$$=\frac{N_1N_2}{(4l_1+2)(4l_2+2)}\sum_{kj_1j_2}(-1)^{j_1+j_2}(n_1l_1j_1n_2l_2j_2\|g_1^{(k)}g_2^{(k)}\|n_2l_2j_2n_1l_1j_1). \tag{36}$$

The average energy of interactions described by the operators H_β, H_γ, and H_δ is obtained substituting in (34)–(36) the corresponding formulas for the reduced matrix elements.

Only the spherical terms with $k=0$ give the contribution to the average of the direct part of the interaction between electronic shells. However, such term vanishes for O_γ and O_δ operators due to the properties of the reduced matrix element (20). Thus the average of the corresponding interaction energy has only the exchange part.

The obtained averages are equivalent to the averages for a complex of relativistic configurations arising from the same nonrelativistic configuration.

V. CONCLUSIONS

The equivalent relativistic operator produces the same result in the nonrelativistic LS scheme as obtained by evaluating the relativistic Hamiltonian with respect to relativistic wave functions, any additional simplifications are not needed. The mixing of relativistic configurations arising from the same nonrelativistic configuration is taken into account. This method has several advantages in comparison with a rather complicated transformation from jj to LS coupling: (i) all parts of the equivalent Hamiltonian are expressed in terms of the same scalar product of standard operators and their matrix elements can be evaluated in the more simple nonrelativistic scheme; (ii) the insight into the structure of equivalent operator gives the possibility to make some approximations (for example, to omit small terms having no analogue in the Breit–Pauli Hamiltonian or corresponding to a weak spin–spin interaction).

The form of the equivalent operator useful for practical calculations is obtained. It is implemented in a general computer code. The Dirac–Fock equations for a level and term in LS coupling are derived, they can be useful for the description of excited configurations, especially with a collapsing electron as well as for the calculation of the binding energies and system differences.

The correspondence between the equivalent relativistic and Breit–Pauli operators gives the possibility to obtain the general relations between the nonrelativistic and relativistic radial integrals.

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Some exact results for mid-band and zero band-gap states of associated Lamé potentials

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Applying certain known theorems about one-dimensional periodic potentials, we show that the energy spectrum of the associated Lamé potentials, $a(a+1)m\,\mathrm{sn}^2(x,m)+b(b+1)m\,\mathrm{cn}^2(x,m)/\mathrm{dn}^2(x,m)$, consists of a finite number of bound bands followed by a continuum band when both a and b take integer values. Further, if a and b are unequal integers, we show that there must exist some zero band-gap states, i.e., doubly degenerate states with the same number of nodes. More generally, in case a and b are not integers, but either $a+b$ or $a-b$ is an integer $(a\neq b)$, we again show that several of the band-gaps vanish due to degeneracy of states with the same number of nodes. Finally, when either a or b is an integer and the other takes a half-integral value, we obtain exact analytic solutions for several mid-band states. © *2001 American Institute of Physics.*
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I. INTRODUCTION

The energy spectrum of electrons on a lattice is of central importance in condensed matter physics. In particular, the knowledge of the existence and locations of band edges and band-gaps determines many physical properties. Unfortunately, even in one dimension, there are very few analytically solvable periodic potential problems in quantum mechanics. The Lamé potential,

$$V(x)=a(a+1)m\,\mathrm{sn}^2(x,m),\quad a=1,2,3,\ldots, \tag{1}$$

is well-known to be exactly solvable. Here $\mathrm{sn}(x,m)$ is a Jacobi elliptic function of real elliptic modulus parameter m $(0\leqslant m\leqslant 1)$ with period $4K(m)$. For simplicity, from now onward, we will not explicitly display the modulus parameter m as an argument of Jacobi elliptic functions.[1]

Recently, we have vastly extended[2] the list of known solvable potentials by exploiting two different directions. First, we have shown that the supersymmetric partners of the Lamé potential constitute a wide class of new exactly solvable periodic potentials, which are distinctly different from the Lamé potential of Eq. (1) (for $a>1$), even though they have the same energy band structure. Second, we have shown[2] that the associated Lamé potentials,[3]

$$V(x)=pm\,\mathrm{sn}^2 x+qm\,\frac{\mathrm{cn}^2 x}{\mathrm{dn}^2 x},\quad p\equiv a(a+1),\quad q\equiv b(b+1) \tag{2}$$

(which constitute a much richer class of periodic potentials) and their supersymmetric partners yield many additional solvable and quasi-exactly solvable (QES) periodic problems provided $a+b$ and/or $a-b$ is an integer. Here, like $\mathrm{sn}\,x$, the Jacobi elliptic functions $\mathrm{cn}\,x$ and $\mathrm{dn}\,x$ also have the same modulus parameter m which, for notational convenience, is not explicitly displayed.

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Without any loss of generality, we shall always consider associated Lamé potentials with $p \geqslant q$.[2] All associated Lamé potentials have a period $2K(m)$, but the special case $p=q$ has a period $K(m)$.

There are several issues which were not addressed in our previous paper,[2] hereafter simply referred to as I. For example, in the case of the Lamé potential (1), it is well known that there are a ($|a+1|$) bound bands followed by a continuum band when a is a positive (negative) integer.[4] What about the associated Lamé case, especially when both a and b are integers? In particular, for these cases, are there only a finite number of bound bands followed by a continuum band? What happens if a and b are not integers but either $a+b$ or $a-b$ are integers? Furthermore, for the Lamé potential, when a takes half-integral values (say $a=n+1/2, \quad n=0,1,2,\ldots$), then $(n+1)$ doubly-degenerate solutions are known[3,4] for the mid-band states (i.e., states with period $8K$). Can one also analytically obtain the mid-band states for the associated Lamé potentials?

Our purpose in this paper is to address the issues raised above. In particular, using certain known theorems about periodic problems in one dimension, we show that even in the associated Lamé case, there are only a finite number of bound bands followed by a continuum band in case both a and b are integers. Further, as long as a and b (and hence p,q) are unequal integers, then we also show that some of the band-gaps (either of period $2K$ or $4K$) disappear. On the other hand, if a,b are not integers but either $a+b$ or $a-b$ is an integer ($a \neq b$), then in general there are an infinite number of bands out of which, but for the lowest few, all other band gaps of either period $2K$ or $4K$ vanish. Finally, when a is a half integer and b is an integer, we obtain several exact mid-band states (i.e., states of period $8K$).

The plan of this paper is as follows. In Sec. II we describe some known theorems about the number of band-gaps in a periodic potential in one dimension. Using these theorems, we show that if a and b are integers such that $p>q>0$, then the associated Lamé potential has also only a bound bands followed by a continuum band. Further, if $a-b$ is an even (odd) integer, then there are b doubly-degenerate band edges of period $4K$ $(2K)$ (i.e., in these cases the corresponding band-gaps are zero). Unfortunately, we are unable to obtain energy eigenstates for any of these $2b$ states. However, we do obtain exact expressions for the remaining $2a+1$ band edges. In particular, if $a-b$ is an even (odd) integer, then one can obtain the energy eigenvalues and eigenfunctions for the $a+b+1$ $(a-b)$ states of period $2K$ and $a-b$ $(a+b+1)$ states of period $4K$. In Sec. III we discuss the case when both a,b are half-integral and such that $p>q>0$. In this case we show that if $a-b$ is an even (odd) integer, one can obtain exact eigenvalues and eigenfunctions for the $b+1/2$ doubly-degenerate states of period $4K$ $(2K)$ (i.e., in these cases, the corresponding band gaps are zero) as well as $a-b$ nondegenerate states of the same period. Unfortunately, in this case one is not able to obtain any eigenstates of period $2K$ $(4K)$. In Sec. IV we consider the case when a is half-integral ($a=k+1/2$) and b is an integer ($b=s, \quad s=0,1,2,\ldots,N, \quad k=N-s$) and show that for every possible value of s, one can obtain exact, doubly-degenerate, $k+1$ mid-band states of period $8K$. Finally, in the last section we summarize the results obtained in this paper and point out some open problems.

II. a,b INTEGRAL AND FINITE NUMBER OF BOUND BANDS

Consider the Schrödinger equation for the associated Lamé potential specified in Eq. (2) for the usual case of a particle of mass 1/2 using units with $\hbar=1$:

$$-\frac{d^2\psi(x)}{dx^2}+\left[a(a+1)m\,\mathrm{sn}^2(x)+b(b+1)m\,\frac{\mathrm{cn}^2 x}{\mathrm{dn}^2 x}\right]\psi(x)=E\psi(x). \tag{3}$$

Following the procedure described in I, we substitute

$$\psi(x)=[\mathrm{dn}\,x]^{-b}y(x), \tag{4}$$

yielding

$$y''(x)+2bm\frac{\mathrm{sn}\,x\,\mathrm{cn}\,x}{\mathrm{dn}\,x}y'(x)+[\lambda-(a+b)(a+1-b)m\,\mathrm{sn}^2\,x]y(x)=0. \tag{5}$$

On further substituting $\mathrm{sn}\,x\equiv\sin t, y(x)\equiv z(t)$, it is easily shown that $z(t)$ satisfies Ince's equation,

$$(1+A\cos 2t)z''(t)+B\sin 2tz'(t)+(C+D\cos 2t)z(t)=0, \tag{6}$$

where

$$A=\frac{m}{2-m},\quad B=\frac{(2b-1)m}{2-m},\quad C=\frac{\lambda-(a+b)(a+1-b)m}{2-m},$$

$$D=\frac{(a+1-b)(a+b)m}{2-m},\quad \lambda=E-mb^2. \tag{7}$$

Now several exact results for Ince's equation are known in the literature. In particular, it is known that the system satisfying Ince's equation (6) has *at most* $j+1$ band-gaps of period $\pi[2\pi]$ in case the polynomial $Q(\mu)[Q^*(\mu)]$ has non-negative integral roots, the highest of which is j.[5] Here the quadratic polynomials $Q(\mu)$ and $Q^*(\mu)$ are given by

$$Q(\mu)=2A\mu^2-B\mu-\frac{D}{2},\quad Q^*(\mu)=2A\left(\mu-\frac{1}{2}\right)^2-B\left(\mu-\frac{1}{2}\right)-\frac{D}{2}. \tag{8}$$

On the other hand, if $Q(\mu)[Q^*(\mu)]$ has negative integral roots, the smallest of which is $-j_0-1$, then the system satisfying Ince's equation (6) has *at most* j_0+1 band-gaps of period $\pi[2\pi]$. It must be noted here that in the notation of Ref. 5, the lowest band-gap of period π *always* exists and is from $E=-\infty$ to $E=E_0$, when E_0 denotes the energy of the lower edge of the lowest energy band.

Using these theorems it is easily shown[3] that the Lamé potential (1) has a ($|a+1|$) bound bands followed by a continuum band in case a is a positive (negative) integer.

Let us now apply these results to the associated Lamé potential (2). We might add here that the period $\pi[2\pi]$ for Ince's equation corresponds to period $2K(m)[4K(m)]$ in the associated Lamé case (note $\mathrm{sn}\,x\equiv\sin t$). On using the expressions for A,B,C,D as given in Eq. (7) it is easily shown that the roots of $Q(\mu)$ are at

$$\mu_1=\frac{a+b}{2},\quad \mu_2=\frac{b-a-1}{2}, \tag{9}$$

while the roots of $Q^*(\mu)$ are at

$$\mu_1^*=\frac{a+b+1}{2},\quad \mu_2^*=\frac{b-a}{2}. \tag{10}$$

These roots are integral if and only if $a+b$ and/or $a-b$ take integer values. In this section we consider the case when both a and b are integral while in the next section we consider the other possibilities.

When both a and b take integer values then it follows from Eqs. (9) and (10) that either the roots μ_1 and μ_2^* or the roots μ_2 and μ_1^* are integral. In particular, it both a and b or odd or even then the roots μ_1 and μ_2^* are integral while if one of them is odd and the other even then μ_2 and μ_1^* are integral. Thus in both cases, there are only a finite number of band-gaps of period π and 2π [and hence of periods $2K$ and $4K$ for the associated Lamé potential (2)]. Hence it follows that when both a and b take integer values, then there are only a finite number of bound bands followed by a continuous band.

In fact, as we show now, these theorems when supplemented with the exact results obtained in I (see Table III of I) tell us quite a lot about the nature of band structure in these cases. We consider the two cases of $a-b$ being odd or even integer separately.

(i) $a-b=$ odd integer

From Eq. (9) it then follows that there are at most an $(a-b+1)/2$ number of band-gaps of period $2K$. An examination of the few explicit cases confirms the fact that there are indeed so many band-gaps (and not less) of period $2K$. This implies that in this case there are only $a-b$ number of nondegenerate states of period $2K$. Quite remarkably, all these $a-b$ states are QES states. In particular, the solution for these states can be obtained from Table III of I in case $p=a(a+1)$ while $q=[a-(a-b-1)][a-(a-b)]$.

On the other hand, from Eq. (10), it follows that in case $a-b$ is an odd integer, then there are at most an $(a+b+3)/2$ number of band-gaps of period $4K$. However, specific examples show that there are in fact only an $(a+b+1)/2$ number of band-gaps. This also follows from Eq. (10) in case we take $a>0$ but instead of b take $-b-1$ (note that q is invariant under $b\rightarrow -b-1$). We see that μ_2^* has an integral root at $-(a+b+1)/2$ and hence there are at most an $(a+b+1)/2$ number of band-gaps, i.e., $a+b+1$ number of nondegenerate states of period $4K$. Again all these are QES states, the solution for which is obtained from Table III of I in case $p=a(a+1)$, $q=[a-(a+b)][a-(a+b+1)]$.

Thus we see that when $a-b$ is an odd integer then there are $(a+b+1)/2$ band-gaps of period $4K$ but only $(a-b+1)/2$ band-gaps of period $2K$ and the corresponding band edges are known in principle from Table III of I. However, since the band edge wavefunctions arranged in order of increasing energy are of period $2K,4K,4K,2K,2K,\ldots$, hence it follows that in this case there must also be b band-gaps of period $2K$ which must be of zero width, i.e., there must be b doubly degenerate states of period $2K$. Unfortunately, so far, we have not been able to obtain either the eigenvalues or the eigenfunctions of even one of these states. Thus in this case there are in all a bound bands followed by a continuum band out of which the top b bound bands are a bit unusual in that both of their band edges have period $4K$ and two degenerate states of period $2K$ lie inside each of these bound bands.

As an illustration, consider the case of $p=12$, $q=6$, i.e., $a=3$, $b=2$. From the above discussion it follows that there must be 1 QES band edge of period $2K$ which is the ground state. Using Table III of I, it is easily seen that the eigenvalue and the eigenfunction of this state is

$$\psi_0=\mathrm{dn}^3 x, \quad E_0=9m. \tag{11}$$

In addition, there must be 6 nondegenerate QES band edges of period $4K$ and the eigenvalues and eigenfunctions for these six states are easily obtained. In particular, it is easily shown that three of the eigenstates have the form

$$\psi_{1,6,9}=\frac{\mathrm{cn}\, x}{\mathrm{dn}^2 x}[A+B\,\mathrm{sn}^2 x+D\,\mathrm{sn}^4 x], \tag{12}$$

and the corresponding three eigenvalues $E_{1,6,9}$ satisfy the cubic equation

$$\lambda^3-4(8-m)\lambda^2+48(4+m)\lambda-576m=0, \quad E=\lambda+1+4m. \tag{13}$$

The other three eigenstates have the form

$$\psi_{2,5,10}=\frac{\mathrm{sn}\, x}{\mathrm{dn}^2 x}[A+B\,\mathrm{sn}^2 x+D\,\mathrm{sn}^4 x], \tag{14}$$

and the corresponding three eigenvalues $E_{2,5,10}$ satisfy the cubic equation

$$\lambda^3-8(4+m)\lambda^2+48(4+7m)\lambda-576m(3+m)=0, \quad E=\lambda+1+m. \tag{15}$$

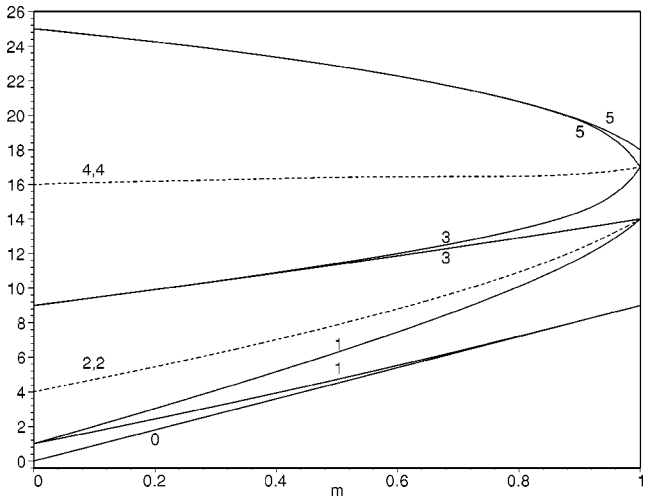

FIG. 1. Band edge energies for the associated Lamé potential (12,6) as a function of the elliptic modulus parameter m. The band edges are labeled by the number of wave function nodes in the interval $2K(m)$. Note that the band gap between the two states with 2 nodes as well as with four nodes is zero, that is $E_3=E_4$ and $E_7=E_8$. The energy eigenvalues of these degenerate states have been calculated numerically and are shown by dotted lines.

In view of the oscillation theorem, it is then clear that there must be a pair of doubly-degenerate states $(\psi_{3,4})$ and $(\psi_{7,8})$ of period $2K$ whose energy must go to 4(14) and 16(17), respectively, as $m\to 0(1)$. Thus whereas four states $\psi_{2,3,4,5}$ must merge at $E=14$ as $m\to 1$ the other four states $\psi_{6,7,8,9}$ must merge at $E=17$ as $m\to 1$. Thus, as shown in Fig. 1, in this case there are three bound bands followed by a continuum band. The two upper-most bound bands have both of their band edges of period $4K$ and in between are the pair of doubly-degenerate states $\psi_{3,4}$ and $\psi_{7,8}$ of period $2K$ whose energy eigenvalues and eigenfunctions are not known analytically. We have therefore computed these energy eigenvalues numerically and these are shown by the dotted lines in the figure.

As another illustration, consider the case of $p=6,q=2$, i.e., $a=2,b=1$. From the above discussion it follows that in this case there must be 1 QES band edge of period $2K$ and 4 QES band edges of period $4K$ and interestingly enough the eigenvalues and eigenfunctions for these five states were already given in the Table IV of I. Further, as stated in I, two states of period $2K$ must also be present but so far we are unable to obtain these states analytically. However, what was not clear at that time was that the two states of period $2K$ must be degenerate and whose energy goes to 4 (7) as $m\to 0(1)$ so that as $m\to 1$, four of the states $\psi_{2,3,4,5}$ must merge at $E=7$. Besides, it was also not clear then that in this case there are only two bound bands followed by a continuum band and that the upper band is a bit unusual in that both of its band edges are of period $4K$ and inside the band there are two degenerate states of period $2K$.

(ii) $a-b=$ even integer

From Eq. (9), it follows that in this case there are at most $(a+b+2)/2$ band-gaps of period $2K$. Explicit examples confirm that this is indeed so. Hence, in this case one has an $a+b+1$ number of nondegenerate states. Quite remarkably, all these are QES states for which a solution can be obtained from Table III of I when $p=a(a+1)$, $q=[a-(a+b)][a-(a+b+1)]$.

On the other hand, from Eq. (10), it follows that there are at most $(a-b)/2$ band-gaps of period $4K$ and hence $a-b$ number of nondegenerate states of period $4K$. Specific examples confirm the expectation. These are all QES states which can be obtained from Table III of I in case $p=a(a+1)$, $q=[a-(a-b)][a-(a-b-1)]$.

Thus when $a-b$ is an even integer (with both an a,b integer), then there are $(a+b+2)/2$ band gaps of period $2K$ but only $(a-b)/2$ band gaps of period $4K$ and in principle the corresponding band edges are all analytically known from Table III of I. In view of the fact that the band edge wave functions in increasing order of energy are of period $2K,4K,4K,2K,2K,\ldots,$ it

then follows that in this case, too, there must be b zero band-gaps of period $4K$, i.e., there must be b doubly-degenerate states of period $4K$. Unfortunately, so far, we have not been able to obtain an analytic solution for even one of these $(2b)$ states. Thus in this case also there are in all a bound bands followed by a continuum band out of which the top b bound bands are again a bit unusual in that both of their band edges are of period $2K$ and two degenerate states of period $4K$ lie inside each of these bound bands.

As an illustration, consider the case of $p=12$, $q=2$, i.e., $a=3$, $b=1$. As described in I, this potential is oscillatory for $m<\frac{5}{6}$, but has interesting structure coming from secondary extrema for $m>\frac{5}{6}$. From the above discussion it follows that the (12,2) potential must have 2 nondegenerate QES states of period $4K$. Using Table III of I, it is easily seen that the eigenvalues and the eigenfunctions of these states is given by

$$\psi_1=\mathrm{cn}\,x\,\mathrm{dn}^2\,x,\quad E_1=1+4m, \tag{16}$$

$$\psi_2=\mathrm{sn}\,x\,\mathrm{dn}^2\,x,\quad E_2=1+9m. \tag{17}$$

In addition there must be 5 nondegenerate states of period $2K$ whose eigenvalues and eigenfunctions are easily obtained from Table III of I. In particular, the eigenvalues and the eigenfunctions of two of the states are

$$\psi_{8,3}=\frac{\mathrm{sn}\,x\,\mathrm{cn}\,x}{\mathrm{dn}\,x}[5m\,\mathrm{sn}^2\,x-3-m\pm\delta_7],\quad E_{8,3}=10+2m\pm2\,\delta_7, \tag{18}$$

where $\delta_7=\sqrt{9-9m+m^2}$. On the other hand, the remaining three eigenstates have the form

$$\psi_{0,4,7}=\frac{1}{\mathrm{dn}\,x}[A+B\,\mathrm{sn}^2\,x+D\,\mathrm{sn}^4\,x], \tag{19}$$

and the three corresponding eigenvalues $E_{0,4,7}$ satisfy the cubic equation [see Eqs. (39) and (40) of I]

$$\lambda^3-4(2m+5)\lambda^2+16(4+11m)\lambda-192m(2+m)=0,\quad E=\lambda+m. \tag{20}$$

In view of the oscillation theorem, it is then clear that there must also be two degenerate states $(\psi_{5,6})$ of period $4K$ whose energy tends to 9(13) as $m\to0(1)$ so that the four states $\psi_{4,5,6,7}$ must merge at $E=13$ as $m\to1$. Thus, as shown in Fig. 2, in this case, there are three bound bands followed by a continuum band. Further, the upper-most bound band has both of its band edges of period $2K$ and in between are the two degenerate states of period $4K$ whose energy eigenvalue and eigenfunctions are not known analytically. We have computed the degenerate energy eigenvalue numerically and it is shown by a dotted line in Fig. 2.

What happens if $a=b$ with both being an integer? In this case the associated Lamé potential has period $K(m)$ rather than $2K(m)$ and hence the results from Ince's equation are not directly applicable. However, as has been shown in I for $a=b=1,2$ (and also explicitly verified for $a=b=3,4$), in this case there are a bound bands followed by a continuum band and $2a+1$ band edges all of which are in principle explicitly known from Table III of I. Further, in this case, there are no band gaps of zero width.

III. a,b HALF-INTEGRAL AND INFINITE NUMBER OF BAND-GAPS OF ZERO WIDTH

Let us now specialize to the case when both a and b are half-integral such that $p>q>0$. From Eqs. (9) and (10) it is clear that in this case either the roots μ_1 and μ_2 or μ_1^* and μ_2^* are integral but not both. In particular, if $a-b$ is an odd integer, then both the roots μ_1 and μ_2 are integral while μ_1^* and μ_2^* are not integral while if $a-b$ is an even integer, then the roots μ_1^* and μ_2^* are integral while μ_1 and μ_2 are not integral. Thus it follows that unlike the integral a,b case, here

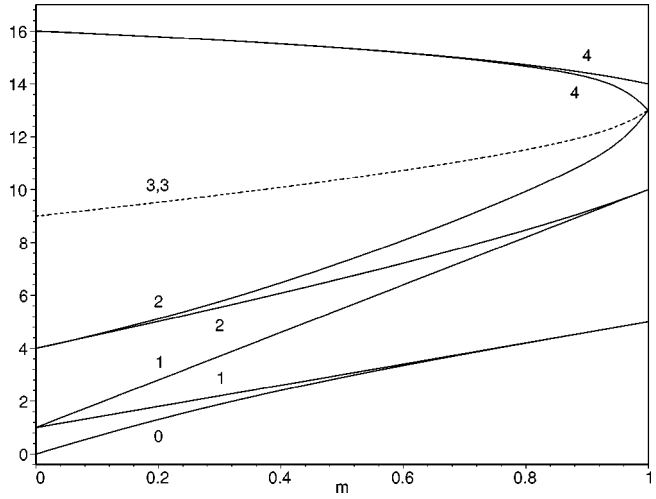

FIG. 2. Band edge energies for the associated Lamé potential (12,2) as a function of the elliptic modulus parameter m. The band edges are labeled by the number of wave function nodes in the interval $2K(m)$. Note that the band gap between the two states with 3 nodes is zero. The energy eigenvalue $E_5=E_6$ of these degenerate states has been calculated numerically and is shown by a dotted line.

one will in general have an infinite number of bands but only a finite number of band-gaps of either period $2K$ or $4K$ depending on whether $a-b$ is an odd or an even integer. As before, let us discuss the two cases separately.

(i) $a-b=$ odd integer

From Eqs. (9) and (10) it follows that in this case both μ_1 and μ_2 are integral while μ_1^* and μ_2^* are half-integral. Thus in this case there will be infinite number of band-gaps of period $4K$ but *at most* $(a+b+2)/2$ band gaps of period $2K$. However, a study of several explicit examples show that there are in fact only an $(a-b+1)/2$ number of band-gaps of period $2K$ and hence there are only an $a-b$ number of nondegenerate states of period $2K$ and all these are QES states. However, using Table III of I it is easily shown that in this case there are in fact $a+b+1$ QES states of period $2K$. This then implies that the remaining $2b+1$ QES states must correspond to doubly-degenerate eigenstates of period $2K$, i.e., in this case there are $b+1/2$ doubly degenerate QES states of period $2K$, each of which is lying inside a band. It is interesting to note that whereas when both a and b are integers, then one does not have an analytic expression for even one doubly degenerate state, when both a,b are half-integral, energy eigenvalues and eigenfunctions are known in principle from Table III of I for $b+1/2$ doubly-degenerate QES states.

Summarizing, when $a-b$ is an odd integer, then there are infinite number of bands out of which except for the lowest $a-b$ bands, the rest are rather unusual in that both of their band edges have period $4K$ and two degenerate states of period $2K$ reside inside each of these bands.

As an illustration, consider the case of $p=15/4, q=3/4$, i.e., $a=3/2$, $b=1/2$. From the above discussion, it follows that in this case one must have one nondegenerate and one doubly-degenerate QES state of period $2K$. Using Table III of I it is easily seen that the eigenvalue and the eigenfunction for the nondegenerate state is given by

$$\psi_0=\mathrm{dn}^{3/2}x, \quad E_0=\frac{9m}{4}, \tag{21}$$

while the energy eigenvalue and the corresponding two degenerate eigenfunctions are given by

$$\psi_3=\frac{\mathrm{sn}\,x\,\mathrm{cn}\,x}{\mathrm{dn}^{1/2}x}, \quad \psi_4=\frac{[2\,\mathrm{sn}^2x-1]}{\mathrm{dn}^{1/2}x}, \quad E_{3,4}=4+\frac{m}{4}. \tag{22}$$

Note that in this case, out of the infinite number of bands, except for the lowest band, all other bands have both of their band edges of period $4K$.

Another case, already discussed in I (see Table VII) is when $p=63/4, q=3/4$, i.e., $a=7/2$, $b=1/2$. As shown there, in this case one has three nondegenerate QES states of period $2K$ and one doubly-degenerate level of the same period. Further, in this case, but for the lowest three bands, all other bands have both of their band edges of period $4K$.

(ii) $a-b=$ even integer

From Eqs. (9) and (10) it follows that in this case both μ_1^* and μ_2^* are integral while μ_1 and μ_2 are half-integral. Hence, in this case there will be infinite number of band-gaps of period $2K$ but *at most* an $(a+b+1)/2$ number of band-gaps of period $4K$. However, a study of several explicit examples reveals that in this case there are only an $(a-b)/2$ number of band gaps and hence an $a-b$ number of nondegenerate QES states of period $4K$. However, using Table III of I it is easily shown that in this case there are in fact an $a+b+1$ number of QES states of period $4K$. This implies that in addition to the $a-b$ nondegenerate QES states, there must also be $2b+1$ QES degenerate states of period $4K$, i.e., in this case also there are $b+1/2$ doubly-degenerate QES states of period $4K$, each of which is lying inside a band.

Thus, in this case too, there are an infinite number of bands out of which except for the lowest $a-b$ bands, the rest are rather unusual in that both of their band edges are of period $2K$ and two degenerate states of period $4K$ reside inside each of these bands.

As an illustration, consider the case of $p=35/4, q=3/4$, i.e., $a=5/2, b=1/2$. In view of the above discussion, we expect two nondegenerate and one doubly-degenerate QES states of period $4K$. Using Table III of I it is easily shown that the energy eigenstates for the two nondegenerate states are

$$\psi_1=\mathrm{cn}\,x\,\mathrm{dn}^{3/2}x, \quad E_1=1+\frac{9m}{4}, \tag{23}$$

$$\psi_2=\mathrm{sn}\,x\,\mathrm{dn}^{3/2}x, \quad E_2=1+\frac{25m}{4}, \tag{24}$$

while for the two degenerate states one has

$$\psi_5=\frac{\mathrm{cn}\,x(4\,\mathrm{sn}^2x-1)}{\mathrm{dn}^{1/2}x}, \quad \psi_6=\frac{\mathrm{sn}\,x\,(4\,\mathrm{sn}^2x-3)}{\mathrm{dn}^{1/2}x}, \quad E_{5,6}=9+\frac{m}{4}. \tag{25}$$

Thus, in this case (out of the infinite number of bands) except for the two lowest bands, all other bands are a bit unusual in that both of their band edge eigenfunctions are of period $2K$.

We thus have seen that for half-integral a,b with $a>b$, one has $a-b$ nondegenerate and $b+1/2$ doubly-degenerate QES states of period $2K$ or $4K$ depending on whether $a-b$ is an odd or an even integer. Thus for $b=1/2,3/2,\ldots(a>b)$, we expect $1,2,\ldots$, doubly-degenerate QES states. We now show that the energy eigenvalues of these doubly-degenerate states can be easily obtained analytically in case $b=1/2$ or $3/2$ and a being an arbitrary half-integer (with $a>b$). In particular, if we start with the ansatz

$$y_1(x)=\sum_{k=0}^{N+1} A_k\,\mathrm{sn}^{2k}x, \tag{26}$$

then on substituting it in the associated Lamé equation (5) and equating coefficient of terms with $\mathrm{sn}^{2N+4}x$ and $\mathrm{sn}^{2N+2}x$ we find that in case $a=2N+3/2, b=1/2$ then the corresponding energy eigenvalue is

$$E=(2N+2)^2+m/4, \quad N=0,1,2,\ldots. \tag{27}$$

In fact E as given by Eq. (27) is also the energy eigenvalue in case we start with the ansatz

$$y_2(x)=\sum_{k=0}^{N} A_k \,\mathrm{sn}^{2k+1} x \,\mathrm{cn}\, x, \tag{28}$$

and substitute it in Eq. (5). As expected, the results given in Eq. (22) agree with these given above in case $N=0$ while for $N=1$ our results agree with those given in Table VII of I.

Similarly, it is easily shown that in case $a=2N+5/2,\ b=1/2$ then the degenerate eigenvalue and the corresponding eigenfunctions are

$$E=(2N+3)^2+m/4, N=0,1,2,\ldots, \tag{29}$$

$$y_1(x)=\sum_{k=0}^{N+1} A_k \,\mathrm{sn}^{2k+1} x, \quad y_2(x)=\sum_{k=0}^{N+1} B_k \,\mathrm{cn}\, x \,\mathrm{sn}^{2k} x. \tag{30}$$

For the special case of $N=0$, our results agree with those given in Eq. (25).

On the other hand, for $b=3/2$ and $a=2N+5/2$, the two degenerate energy eigenvalues are

$$E=4N^2+12N+10+\frac{5m}{4}\pm\sqrt{(4N+6)^2-(4N+6)^2m+m^2}, \quad N=0,1,2,\ldots, \tag{31}$$

while the corresponding eigenfunctions are of the form

$$y_1(x)=\sum_{k=0}^{N+2} A_k \,\mathrm{sn}^{2k} x, \quad y_2(x)=\sum_{k=0}^{N+1} B_k \,\mathrm{cn}\, x \,\mathrm{sn}^{2k+1} x. \tag{32}$$

However, for $b=3/2$ and $a=2N+7/2$, the two degenerate energy eigenvalues are

$$E=4N^2+16N+17+\frac{5m}{4}\pm\sqrt{16(N+2)^2-16(N+2)^2m+m^2}, \quad N=0,1,2,\ldots, \tag{33}$$

while the corresponding degenerate eigenfunctions are of the form

$$y_1(x)=\sum_{k=0}^{N+2} A_k \,\mathrm{sn}\, x^{2k+1}, \quad y_2(x)=\sum_{k=0}^{N+2} B_k \,\mathrm{cn}\, x \,\mathrm{sn}^{2k} x. \tag{34}$$

It is worth adding that in case $b=-1/2(a>b)$, one obtains $a+1/2$ nondegenerate QES states of period $2K(4K)$ depending on if $a+1/2$ is an odd or an even integer. Note that when $b=-1/2$ then $q=-1/4$ while $p>0$. As an illustration, consider $a=5/2,\ b=-1/2$, i.e., $p=35/4,\ q=-1/4$. In this case we have 3 QES states of period $2K$ whose energy eigenvalues and eigenfunctions are easily obtained from Table III of I when $q=(a-2)(a-3)$ and of course $p=a(a+1)$.

Finally, let us discuss the case when a,b are neither integral nor half-integral but are such that either $a+b$ or $a-b$ is an integer. It is easily seen from Eqs. (9) and (10) that if either $a+b=2N$ or $a-b=2N+1$ then there are at most $N+1$ band-gaps of period $2K$ while if $a-b=2N$ or $a+b=2N-1$ then there are at most N band-gaps of period $4K$. Further, from Table III of I we find that when either $a+b=2N$ or $a-b=2N+1$ then there are precisely $2N+1$ QES states of period $2K$ while if $a+b=2N-1$ or $a-b=2N$ then there are precisely $2N$ QES states of period $4K$ and all these are nondegenerate states.

IV. MID-BAND STATES

For the Lamé potential, the majority of results are for integral a (and hence p). However, for half-integral values of a, analytic expressions for $a+1/2$ mid-band states (of period $8K$) have been obtained.[4] In particular, it is known that if $a=2N+1/2$, there are $2N+1$ mid-band states of the form ($N=0,1,2,\ldots$)

$$\psi(x)=\sqrt{\mathrm{dn}\,x+\mathrm{cn}\,x}\,u(x), \tag{35}$$

where

$$u(x)=\sum_{k=0}^{N} A_k\,\mathrm{sn}^{2k}x+\sum_{k=0}^{N-1} B_k\,\mathrm{cn}\,x\,\mathrm{dn}\,x\,\mathrm{sn}^{2k}x, \tag{36}$$

while if $a=2N+3/2$, then there are $2N+2$ states of the form (35) but where ($N=0,1,2,\ldots$)

$$u(x)=\mathrm{dn}\,x\sum_{k=0}^{N} A_k\,\mathrm{sn}^{2k}x+\mathrm{cn}\,x\sum_{k=0}^{N} B_k\,\mathrm{sn}^{2k}x. \tag{37}$$

Further, since the Lamé equation is invariant under $x\to x+2K(m)$, it follows that in each case one obtains another solution with the *same* energy by changing $\mathrm{cn}\,x$ to $-\mathrm{cn}\,x$.

In this section we show that the associated Lamé potential (2) also has a similar form of mid-band solutions (of period $8K$) in case a is half-integral while b takes integral values. In particular, if $a=k+1/2, b=s$ while $k=2N$ with N,k,s being non-negative integers, then for a given k, one obtains $k+1$ doubly-degenerate solutions for every possible (non-negative integral) value of s. Further, in this case too, all solutions are also doubly degenerate since the associated Lamé equation is invariant under $\mathrm{cn}\,x\to-\mathrm{cn}\,x$.

We begin by substituting the ansatz

$$y(x)=\sqrt{\mathrm{dn}\,x+\mathrm{cn}\,x}\,z(x), \tag{38}$$

into Eq. (5). We find that $z(x)$ satisfies the equation

$$\begin{aligned}\mathrm{sn}\,x\,\mathrm{dn}\,x\,z''(x)+[2bm\,\mathrm{sn}^2x\,\mathrm{cn}\,x-\mathrm{dn}\,x+\mathrm{cn}\,x\,\mathrm{dn}^2x]z'(x)+[\lambda_1\,\mathrm{sn}\,x\,\mathrm{dn}\,x-rm\,\mathrm{sn}^3x\,\mathrm{dn}\,x\\ -bm\,\mathrm{cn}\,x\,\mathrm{sn}\,x+bm\,\mathrm{cn}^2x\,\mathrm{sn}\,x\,\mathrm{dn}\,x]z(x)=0,\end{aligned} \tag{39}$$

where

$$\lambda_1=\lambda-\frac{1+m}{4},\quad r=(a+1-b)(a+b)-3/4. \tag{40}$$

Not surprisingly, $z(x)=\mathrm{const}$ is a solution with energy $E=(1+m)/4$ (note $E=\lambda+mb^2$) provided $b=0$ and $a=1/2$, i.e., $p=3/4$, $q=0$. Following the discussion given above, we try the ansatz (37) with $N=0$, i.e.,

$$z(x)=A\,\mathrm{dn}\,x+B\,\mathrm{cn}\,x, \tag{41}$$

in Eq. (39). It is easily shown that there are two possible solutions in this case.

(i) $b=0$, $a=3/2$:

$$\psi(x)=[\mathrm{dn}\,x-(1-m\pm\sqrt{1-m+m^2})\,\mathrm{cn}\,x]\,\sqrt{\mathrm{dn}\,x+\mathrm{cn}\,x},\quad E=\tfrac{5}{4}(1+m)\pm\sqrt{1-m+m^2}. \tag{42}$$

(ii) $b=1$, $a=1/2$:

$$\psi(x)=\left[1-\frac{2\,\mathrm{cn}\,x}{\mathrm{dn}\,x}\right]\sqrt{\mathrm{dn}\,x+\mathrm{cn}\,x}, \quad E=\frac{9+m}{4}. \tag{43}$$

Several comments are in order at this stage.

(1) On making use of the fact that as $m\to 0$, $\mathrm{dn}\,x\to 1$ while $\mathrm{cn}\,x\to\cos x$ it is easily shown that in case $b=0$, $a=3/2$, the two solutions go over to $\cos(x/2)$ and $\cos(3x/2)$ with energies 1/4 and 9/4, respectively. On the other hand, as $m\to 1$, the two states go over to the ground and excited states of the potential $V=15/4\tanh^2 x$ with eigenvalues 3/2 and 7/2, respectively.
(2) On the other hand, as $m\to 0$ the solution with $b=1$ and $a=1/2$ goes over to $\cos(3x/2)$ with energy 9/4 while as $m\to 1$, it goes over to the ground state of the potential $V=3/4\tanh^2 x+2$ with energy eigenvalue 5/2.
(3) Degenerate solutions are obtained in all these cases by changing $\mathrm{cn}\,x$ to $-\mathrm{cn}\,x$, and as $m\to 0$ these go over to $\sin(x/2)$ or $\sin(3x/2)$ as the case may be.

One can now immediately generalize to the general ansatz (37) and show that for a given N, if $a=k+1/2$ and $b=s$ with $k=2N+1-s$ ($N=0,1,2,\ldots$) then $k+1$ doubly-degenerate eigenvalues and eigenfunctions can be obtained for every possible non-negative s. For example, let us consider the ansatz (37) with $N=1$, i.e.,

$$z(x)=\mathrm{dn}\,x\,[A_0+A_1\,\mathrm{sn}^2 x]+\mathrm{cn}\,x\,[B_0+B_1\,\mathrm{sn}^2 x]. \tag{44}$$

After substituting this ansatz in Eq. (39) and performing lengthy algebraic manipulations, it is easily shown that there are four possible solutions in this case.

(i) $b=0$, $a=7/2$

As is well known,[4] in this case $\lambda_1=E-(1+m)/4$ satisfies a quartic equation,

$$\lambda_1^4-20(1+m)\lambda_1^3+18(6+19m+6m^2)\lambda_1^2-36(4+39m+39m^2+4m^3)\lambda_1+135m(8+23m+8m^2)=0, \tag{45}$$

all of whose roots are real and that as $m\to 0$ the solutions go over to $\cos(x/2)$, $\cos(3x/2)$, $\cos(5x/2)$, $\cos(7x/2)$ with energies 1/4, 9/4, 25/4 and 49/4, respectively.

(ii) $b=1$, $a=5/2$

In this case λ_1 can be shown to satisfy the cubic equation [note $E=\lambda_1+(1+m)/4+mb^2$]

$$\lambda_1^3-(5m+14)\lambda_1^2+(24+88m-m^2)\lambda_1+5m^3-98m^2-96m=0, \tag{46}$$

whose all three roots are real for any $m(0\leqslant m\leqslant 1)$. As $m\to 0$, we find that the solutions go over to $\cos(x/2)$, $\cos(3x/2)$, $\cos(7x/2)$ with energies 1/4, 9/4, 49/4, respectively.

(iii) $b=2$, $a=3/2$

In this case there are two solutions with the corresponding energies being

$$E=\frac{29+5m}{4}\pm\sqrt{25-25m+m^2}. \tag{47}$$

Note that as $m\to 0$ the two energies go over to 9/4 and 49/4 and the corresponding solutions go over to $\cos(3x/2)$ and $\cos(7x/2)$, respectively.

(iv) $b=3$, $a=1/2$

In this case there is only one solution given by

$$\psi=\left(\mathrm{dn}\,x\left[1-\frac{(4-m)}{3}\,\mathrm{sn}^2 x\right]-\frac{4}{3}\,\mathrm{cn}\,x\,[1-(2-m)\,\mathrm{sn}^2 x]\right)\sqrt{\mathrm{dn}\,x+\mathrm{cn}\,x}, \quad E=\frac{49+m}{4}. \tag{48}$$

It is easily checked that as $m \to 0$ the solution goes over to $\cos(7x/2)$ and the corresponding energy is 49/4.

On the other hand if $a = k + 1/2, b = s$ and $k = 2N - s$ ($N = 0,1,2,\ldots$) then we start with the ansatz (36) and obtain $k+1$ (doubly-degenerate) eigenvalues and eigenfunctions for every possible non-negative s. For $N = 0$, the only possibility is of course $a = 1/2$, $b = 0$ and in this case the solution is already well known.[4] For $N = 1$ we start with the ansatz,

$$z(x) = A_0 + A_1 \,\mathrm{sn}^2 x + B_0 \,\mathrm{cn}\, x \,\mathrm{dn}\, x. \tag{49}$$

On substituting this ansatz in Eq. (39), after lengthy but straightforward algebraic manipulations, we find the following three solutions.

(i) $b = 0$, $a = 5/2$

As is well known,[4] in this case $\lambda_1 = E - (1+m)/4$ satisfies a cubic equation,

$$\lambda_1^3 - 8(1+m)\lambda_1^2 + 4(3+13m+3m^2)\lambda_1 - 48m(1+m) = 0, \tag{50}$$

all of whose roots are real and as $m \to 0$, the solutions go over to $\cos(x/2), \cos(3x/2), \cos(5x/2)$ with energies $1/4, 9/4$ and $25/4$, respectively.

(ii) $b = 1$, $a = 3/2$

In this case there are two solutions with the corresponding energies being

$$E = \frac{13+5m}{4} \pm \sqrt{9 - 9m + m^2}. \tag{51}$$

Note that as $m \to 0$ the energies go over to $1/4$ and $25/4$ while the corresponding solutions go over to $cos(x/2)$ and $\cos(5x/2)$, respectively.

(iii) $b = 2$, $a = 1/2$

In this case there is only one solution:

$$\psi = \sqrt{\mathrm{dn}\, x + \mathrm{cn}\, x}\left[1 - \frac{(4-m)}{3}\,\mathrm{sn}^2 x - \frac{2}{3}\,\mathrm{cn}\, x \,\mathrm{dn}\, x\right], \quad E = \frac{25+m}{4}. \tag{52}$$

As $m \to 0$ the solution goes over to $\cos(5x/2)$ with energy $25/4$.

Before closing this section it is worth pointing out that the mid-band states have already been obtained in I in case $a = b = N + 1/2 (N = 0,1,2,\ldots)$. In particular, it may be noted that when $a = b$, then the associated Lamé potential has period K rather than $2K$ and hence the band edges will be of period K and $2K$ while the mid-band states will be of period $4K$. Now if one looks at the Table III of I then one notices that if $a = b = N + 1/2$, then there are $N+1$ doubly-degenerate QES states of period $4K$ which are obtained in principle from Table III of I in case $a = N + 1/2$ and $q = [a - (N+1)][a - (N+2)]$. For example, for $N = 0$, i.e., for $p = q = 3/4$, the doubly-degenerate mid-band states are

$$\psi_1 = \frac{\mathrm{cn}\, x}{\sqrt{\mathrm{dn}\, x}}, \; \psi_2 = \frac{\mathrm{sn}\, x}{\sqrt{\mathrm{dn}\, x}}, \quad E = 1 + \frac{m}{4}. \tag{53}$$

On the other hand, for $N = 1$ the pair of doubly-degenerate mid-band states are

$$\psi_1 = \frac{\mathrm{cn}\, x(4 - m - 2\mathrm{sn}^2 x)}{\mathrm{dn}^{3/2} x}, \; \psi_2 = \frac{\mathrm{sn}\, x(4 - 2\mathrm{sn}^2 x)}{\mathrm{dn}^{3/2} x}, \quad E = 1 + \frac{9m}{4}, \tag{54}$$

$$\psi_1 = \frac{\mathrm{cn}\, x \,\mathrm{sn}^2 x}{\mathrm{dn}^{3/2} x}, \; \psi_2 = \frac{\mathrm{sn}\, x(2\mathrm{sn}^2 x - 1)}{\mathrm{dn}^{3/2} x}, \quad E = 9 + \frac{m}{4}. \tag{55}$$

V. CONCLUSION AND OPEN PROBLEMS

In this paper we have clarified several issues regarding the associated Lamé potential. In particular, we have shown that when both a,b are integers then just like Lamé, the associated Lamé potential is also a finite band problem. The only difference from the Lamé case arises when $a \neq b$—in that case one has some bands with both band edges of the same period. We have also seen that when both a,b take half-integral but unequal values then one has a genuine QES problem and band edges of either period $2K$ or $4K$ are known, but not both. We have also shown that in this case, but for the few low lying bands, all other bands have both of their band edges of the same period ($2K$ or $4K$). Finally, when a is a half-integer and b is an integer, we can obtain several mid-band states.

It would be nice if one could (i) say something concrete about the band structure when a,b are neither integral or half-integral; (ii) derive dispersion relations for at least some of the finite band associated Lamé problems; (iii) obtain the band edges of the associated Lamé problem algebraically, analogous to the Lamé potential. We hope to address some of these issues in the near future.

[1] For the properties of Jacobi elliptic functions, see, for example, I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic, 1980). The modulus parameter m is often called k^2 in the mathematics literature. The related complementary quantity $(1-m)$ is often called k'^2.

[2] A. Khare and U. Sukhatme, J. Math. Phys. **40**, 5473 (1999); hereafter, we will refer to this paper as I.

[3] W. Magnus and S. Winkler, *Hill's Equation* (Wiley, New York, 1966).

[4] F. M. Arscott, *Periodic Differential Equations* (Pergamon, Oxford, 1981); E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, Cambridge, 1980).

[5] See, for example, W. Magnus and S. Winkler, *Hill's Equation* (Wiley, New York, 1966), Chap. 7.

Hofstadter butterfly as quantum phase diagram

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The Hofstadter butterfly is viewed as a quantum phase diagram with infinitely many phases, labeled by their (integer) Hall conductance, and a fractal structure. We describe various properties of this phase diagram: We establish Gibbs phase rules; count the number of components of each phase, and characterize the set of multiple phase coexistence. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Azbel[1] recognized that the spectral properties of two-dimensional, periodic, quantum systems have sensitive dependence on the magnetic flux through a unit cell. A simple model conceived by Peierls and put to the eponymous Harper as a thesis problem, gained popularity with D. Hofstadter's Ph.D. thesis,[2] where a wonderful diagram, reminiscent of a fractal butterfly, provided a source of inspiration and a tool for spectral analysis.[3–9]

The Hofstadter butterfly can also be viewed as the quantum (zero temperature) phase diagram for the integer quantum Hall effect. It is a fractal phase diagram with infinitely many phases.[10,11] The diagram leads to certain natural questions: Count the number of components of a given phase; classify which phases coexist and where. It also leads to the general question: What form does the Gibbs phase rule[12,13] take for quantum phase transitions.

Fractal phase diagrams and/or infinitely many phases appear in dynamical systems.[14,15] In classical lattice systems fractal phase diagrams[12,16,17,13] are commonly viewed as a pathology due to either long range interactions, or, as is the case for spin glasses, loss of translation invariance. The Hofstadter model, when viewed as a statistical mechanical model, is both short range and translation invariant in a natural way. But, it is quantum and the translation group is noncommutative. It suggests that the fractal phase diagram may be more common in quantum phase transitions than in classical phase transitions.

II. THE HOFSTADTER MODEL

The model conceived by Peierls has two versions. For the sake of concreteness we shall focus here on the tight binding version. On the lattice $\mathbb{Z}^2$, define magnetic shifts

$$(U\psi)(n,m)=\psi(n-1,m), \quad (V(\Phi)\psi)(n,m)=e^{2\pi i n\Phi}\psi(n,m-1) \quad n,m\in\mathbb{Z}. \tag{1}$$

$2\pi\Phi$ is the magnetic flux through a unit cell. The Hofstadter model is

$$H(\Phi,a,b)=a(U+U^*)+b(V(\Phi)+V^*(\Phi)), \tag{2}$$

where $a,b>0$ are ''hopping'' amplitudes. $a=b$ is called the self-dual case[18] and we shall focus on that case in the following. We set $H(\Phi)=H(\Phi,1,1)$.

U and V, and therefore also $H(\Phi)$, commute with the (dual) magnetic translations $\mathcal{U}$ and $\mathcal{V}$,

$$(\mathcal{U}\psi)(n,m)=\psi(n,m-1) \quad (\mathcal{V}\psi)(n,m)=e^{2\pi i\Phi m}\psi(n-1,m). \tag{3}$$

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This makes $H(\Phi)$ translation invariant in a natural way. The group of magnetic translations[19] is noncommutative:

$$U^*V^*UV=\mathcal{U}\mathcal{V}\mathcal{U}^*\mathcal{V}^*=e^{-2\pi i\Phi}. \tag{4}$$

The one-particle representation of the Hofstadter model, Eq. (2), is natural for spectral studies. In the context of statistical mechanics the second quantized representation of the model is also instructive because it makes it clear that the model has short range, in fact, only on site and nearest neighbors, interactions. The fractal features of the phase diagram are, therefore, not a consequence of long range forces, as in some classical statistical mechanics models. The second quantized form is

$$\mathcal{H}(\Phi,\mu)=\sum\ e^{i\gamma(nm;n'm')}a^\dagger_{nm}a_{n'm'}+\mu\sum\ a^\dagger_{nm}a_{nm}, \tag{5}$$

where

$$e^{i\gamma(mn;m'n')}=\begin{cases}1, & n-n'=\pm 1,\ m=m'\\ e^{\pm 2\pi i n\Phi}, & m-m'=\pm 1,\ n=n'\\ 0 & \text{otherwise.}\end{cases} \tag{6}$$

μ is the chemical potential and $a^\dagger,a$ are the usual Fermionic operators.

Let us recall a few elementary features of the spectrum:

$$S(H(\Phi))=-S(H(\Phi))=-S(H(1-\Phi)). \tag{7}$$

The first is a consequence of $\mathbb{Z}^2$ being bipartite, and the second is a consequence of time reversal. Together, they imply a fourfold symmetry, manifest in the Hofstadter butterfly.

The electronic density, $\rho(\Phi,\mu)$ (=integrated density of state), is

$$\rho(\Phi,\mu)=\langle 0|\,\theta(\mu-H(\Phi))|0\rangle, \tag{8}$$

where $|0\rangle$ is Kroneker delta at the origin. $0\leqslant\rho(\Phi,\mu)\leqslant 1$ is an increasing function of μ. θ is the usual step function.

The gaps in the spectrum are labeled by an integer, k, which is a solution of[20,3]

$$\Phi\, k=\rho \bmod 1. \tag{9}$$

k is the Hall conductance. We picked the letter k because it is naturally associated with an integer, and it is also the first letter in von Klitzing's name. By Eqs. (9) and (7),

$$k(\mu,\Phi)=-k(\mu,1-\Phi)=-k(-\mu,\Phi), \tag{10}$$

which implies a fourfold (anti) symmetry of the butterfly.

We shall assume that the Ten Martini conjecture[21] holds. Namely, that for all irrational Φ's, all the gaps are open, so Eq. (9) has ρ in an open gap for all $k\in\mathbb{Z}$.

Figure 1 shows the Hofstadter butterfly, color coded according to the Hall conductance. Zero Hall conductance is left blank. The gross features of the diagram are associated with small integers where the color coding is faithful.

The colored picture emphasizes the gaps while the standard Hofstadter butterfly emphasizes the spectrum. The colored figure is prettier and displays the regular aspects of the diagram: Gaps are better behaved than spectra. The colored diagram is also more faithful to certain spectral characteristics. For example, the spectrum is a small set (in fact, one of zero Lebesgue measure), something that is manifest in the colored diagram, but is less obvious from the usual Hofstadter butterfly which plots the spectrum.

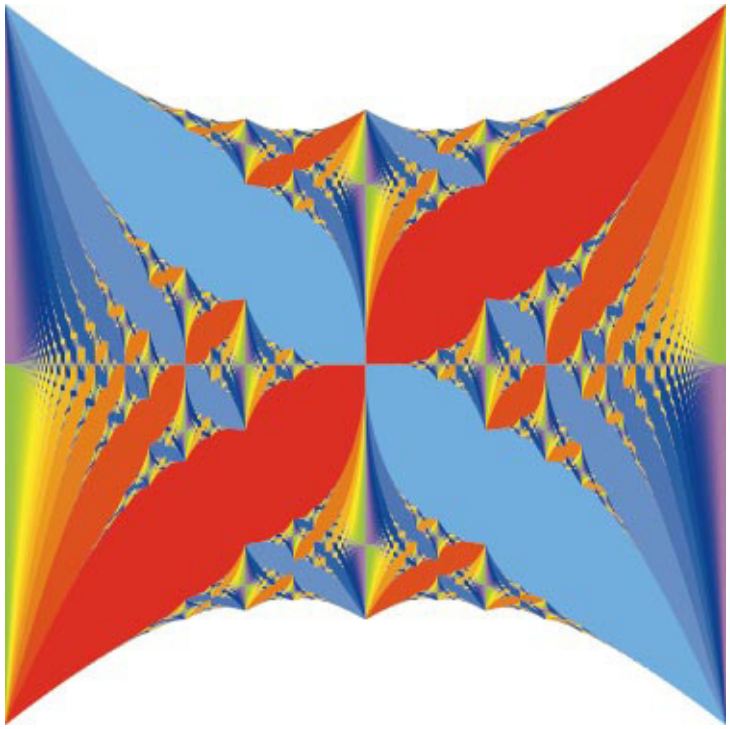

FIG. 1. (Color.) Hofstadter colored butterfly.

We also broke with tradition in that the colored Hofstadter butterfly is rotated by 90°: In Fig. 1 the horizontal axis is Φ and the vertical axis is the energy, or $S(H(\Phi))$. The reason we chose to do so is that this way emphasizes the fact that phase boundaries are functions (of Φ).

We denote by $P(k)$ the kth phase. Formally,

$$P(k)=\{\Phi,\mu|\Phi k=\rho(\Phi,\mu)\bmod 1,\mu\notin S(H(\Phi))\}. \tag{11}$$

$P(k)$ is an open set in the (Φ,μ) plane, with a finite number of components. For example, $P(1)$ is two of the four big wings of the butterfly. We call $P(k)$ a *pure phase* and denote its number of components $|P(k)|$. The closure of the pure phase is denoted $\overline{P(k)}$ and the phase boundary is $\partial P(k)$. We call $\cup_k \partial P(k)$ the total boundary.

III. COUNTING COMPONENTS

The kth pure phase is made of several components. The $k=0$ phase (blank) has two components. For $k\neq 0$ the number of components is

$$|P(k)|=\sum_{j=1}^{2|k|}\phi(j)=12\frac{k^2}{\pi^2}+O(k\log k), \tag{12}$$

where $\phi(j)$ is Euler (totient) function. Recall that $\phi(j)$ counts the number of integers, up to j (and including 1), that are prime to j: $\phi(1)=1$, $\phi(2)=1$, $\phi(3)=2$ etc.

To prove Eq. (12) note first that from Eq. (9)

$$k(\rho,\Phi)=k(\rho',\Phi)\Rightarrow\rho=\rho'. \tag{13}$$

Hence, a given color would appear *at most* once on any vertical line of fixed Φ.

When $\Phi = p/q$ with $\gcd(p,q)=1$ [$\gcd(p,q)$ is the greatest common divisor of p and q], the spectrum of the Hofstadter model has q finite bands and $q-1$ gaps which are all open intervals (except when q is even the central gap is closed). We then number the gaps by their natural order $1,\ldots,q-1$. The semi-infinite interval below the spectrum is, formally, the 0th gap, and the semi-infinite interval above the spectrum as the qth gap. Equation (9), for the jth gap, can be written as

$$p\,k = j \bmod q. \tag{14}$$

Given p,q, and j the equation has a unique solution for each open gap such that $|k|<q/2$. In particular, once q has been fixed, the Hall conductance takes all (nonzero) integer values, from $-\lfloor q/2 \rfloor$ to $\lfloor q/2 \rfloor$, and each value appears once. For even q, the central gap is closed and formally can be assigned a value of $\pm q/2$.

The number of components of the kth phase is the same as the number of flux values, $\Phi_{\diagup}$, which accommodate the wing tips, minus one. The kth wing tips are located at those values of Φ where the kth color is absent (the kth color *is* present in any small neighborhood of those values of Φ, because this neighborhood contains fractions with arbitrary large q's). Given $k\neq 0$, it must appear once on a horizontal interval with $\Phi = p/q$ provided $q/2>|k|$. The tips of a wing with a given color must, therefore, be located at those values of Φ which do not admit k as solution of Eq. (14) for any ρ. In other words, the wing tips lie at those values of Φ where q is too small to accommodate $|k|$. This is the finite set, a Farey sequence,

$$F_{2|k|}=\left\{\frac{p}{q}\middle| 0\leqslant p\leqslant q, \gcd(p,q)=1, q\leqslant 2|k|\right\}=\bigcup_{q=1}^{2|k|}\left\{\frac{p}{q}\middle| 0<p\leqslant q, \gcd(p,q)=1\right\}\bigcup\{0\}. \tag{15}$$

Let $|F|$ be the number of elements in F. Then from (15),

$$|P(k)|=|F_{2|k|}|-1=\sum_{q=1}^{2|k|}\phi(q) \tag{16}$$

essentially from the definition of the Euler function.

The asymptotic expansion for the sum in Eq. (12) is taken from Ref. 22.

IV. PURE PHASES AND PHASE BOUNDARIES

In thermodynamics and statistical mechanics, Gibbs phase rule is a statement about the structure of pure phases and their boundaries. A weak form of the Gibbs phase rule says that pure phases are a set of full measure; two phases coexist, generically, on a set of Hausdorff co-dimension one, etc.[12] This is the form that one gets if one considers general convex functions for thermodynamic potentials. The number of coexisting phases is related to the dimension of tangent planes, and the Gibbs phase rule is a consequence of theorems about convex functions. There is a stronger form of the rule[13] which posits, in addition, that the sets are (locally) manifolds. This form is a consequence of additional regularity of the thermodynamic potentials.

Gibbs phase rule is a consequence of the convexity of thermodynamic potentials and so is ultimately based on the second law of thermodynamics. It has nothing to say about the zero temperature phase diagram of quantum phase transitions in general,[23] and the Hofstadter model in particular (because the entropy vanishes identically). A question that arises is then what form might Gibbs phase rule take for quantum phase transition. The Hofstadter model restricts what could and what could not be true in general. As we shall see, the phase diagram of the Hofstadter model turns out to satisfy only a weak form of the Gibbs phase rules.

Figure 1 suggests that the set of unique phase is a set of full measure and that the phase boundaries, though fractal, are not too wild. More precisely, we have the following.

Gibbs-like phase rule: The phase diagram of the self-dual Hofstadter model is such that pure phases, labeled by their Hall conductances, are full measure; phase boundaries are not manifolds—they are nowhere differentiable—but they are almost so in the sense that their Hausdorff co-dimension is integral, in fact:

$$\dim_H(\partial P(k))=1. \tag{17}$$

Since the number of phases is countable the total phase boundary $\cup_m(\partial P(m))$ *is a set of Hausdorff dimension one as well. Finally, infinitely many phases coexist on a countable set, and therefore a set of Hausdorff dimension zero.*

The first part of the Gibbs-like phase rule is an easy consequence of a result of Last,[6] which states that $|S(H(\Phi))|=0$ for a set of Φ of full measure. That phase boundaries are nowhere differentiable follows from results of Wilkinson,[9] Rammal, and Helffer and Sjöstrand,[5] who showed that the phase boundaries $\partial P(k)$ possess distinct left and right tangent at every rational Φ. That the Hausdorff dimension of the boundary is one follows from results of Bellissard,[24] who showed that away from the wings tips, $\partial P(k)$ can be represented by functions of Φ that are *uniformly* Lipshitz. By standard results,[25] it then follows that the Hausdorff dimension is one. The set of infinite phase coexistence is analyzed in the following.

V. COEXISTENCE

In Ref. 15 the term lakes of Wada was used to describe dynamical systems with the property that any point on the boundary of the one basin of attraction is also on the boundary of all other basins. We shall say that a system is almost Wada of order m if every circle that contains two pure phases contains m pure phases.

The Hofstadter butterfly is almost Wada of infinite order. This is seen from the figure, and can also be shown to follow from Eq. (9).

We say that the two pure phases, $P(m)$, $P(n)$, coexist on

$$C(m,n)=\partial P(m)\cap\partial P(n). \tag{18}$$

No two phase coexists for any irrational flux. This is easily seen from Eq. (9): For irrational Φ the electron density ρ takes a dense set of values in the gaps. Therefore, any two phases, $P(m)$ and $P(n)$, are separated by infinitely many other phases. It follows that the set of phase coexistence is a countable set, and so of zero Hausdorff dimension.

The following result gives a complete characterization of phase coexistence:

Proposition: Consider a point $x\in\partial P(k)$ *with* $\Phi(x)=p/q$ *with* $\gcd(p,q)=1$. *Then* $x\in\partial P(k+\ell q)$ *for all* $\ell\in\mathbb{Z}$. *Moreover* $x\notin\partial P(k')$ *if* $k'\neq k+\ell q$ *for each* $\ell\in\mathbb{Z}$

Proof: Since $\gcd(p,q)=1$ the equation

$$pa-qb=1 \tag{19}$$

has a solution with integer a and b (where a is nonunique mod q). Let $p_n/q_n=(np-b)/(nq-a)$ with $n\in\mathbb{Z}$. Then

$$p_nq-q_np=1. \tag{20}$$

From Eq. (14) it follows that each band at p_n/q_n carries Hall conductance $q\ (\mathrm{mod}\, q_n)$.

Now consider a point x on the right boundary of $P(k)$. We shall first show that x is also on the left boundary of $P(k+q)$. Since $P(k+q)$ has a finite set of wing tips, Eq. (15), when n is large enough, the gap with label (=Hall conductance) $k+q$ at flux p_n/q_n must be open, and must remain open for all large n. By a bound of Last and Wilkinson[26] for the total width of the spectrum at p_n/q_n, each band is small and hence

$$\mathrm{dist}(P(k),P(k+q))<\frac{24}{q_n}. \tag{21}$$

Taking $n\to\infty$ we see that $x\in\partial P(k+q)$ as claimed.

By considering the next band we shall now show that x also lies on the boundary of $P(k+2q)$. Now, $P(k+2q)$ at p_n/q_n is separated from $P(k)$ by two bands and a gap. The bands are small by the Last–Wilkinson bound. The gap is also small by the Hölder continuity of the spectrum:

$$|\mathrm{gap}|<18\sqrt{\frac{p_n}{q_n}-\frac{p}{q}}=\frac{18}{\sqrt{qq_n}} \tag{22}$$

and from this

$$\mathrm{dist}(P(k),P(k+2q))<\frac{24}{q_n}+\frac{18}{\sqrt{qq_n}}. \tag{23}$$

Taking the limit $n\to\infty$ yields the result. The argument can be repeated for any $P(k+\ell q)$ with ℓ finite and positive. Negative values $P(k-\ell q)$ are obtained by letting $n\to-\infty$ in the above-mentioned argument.

For the left boundary point of $P(k)$, $n\to\infty$ will give $P(k-\ell q)$ and $n\to-\infty$ will give $P(k+\ell q)$. This formula applies also to the phase $k=0$, with its right boundary being the leftmost point of the spectrum and vice-versa. The Hall conductance for the middle gap with even q (which is closed) is formally $\pm q/2$, so it is common to phases $P(\pm q/2+\ell' q)$ which is the same as $P(q/2+\ell q)$ for $\ell,\ell'\in\mathbb{Z}$.

The second part of the proposition follows from the equality

$$\bigcup_{k\leqslant|\frac{q}{2}|}\bigcup_{\ell\in\mathbb{Z}}P(k+\ell q)=\bigcup_{k\in\mathbb{Z}}P(k)$$

and the fact that for fixed Φ, each Hall conductance k can appear only once.

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Coherent state path integral for the Bloch particle

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We construct a coherent state path integral formalism for the one-dimensional Bloch particle within the single band model. The transition amplitude between two coherent states is a sum of transition amplitudes with different winding numbers on the two-dimensional phase space which has the same topology as that of the cylinder. Appearance of the winding number is due to the periodicity of the quasimomentum of the Bloch particle. Our formalism is successfully applied to a semiclassical motion of the Bloch particle under a uniform electric field. The wave packet exhibits not only the Bloch oscillation but also a similar breathing to the one for the squeezed state of a harmonic oscillator. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1416489]

I. INTRODUCTION

The path integral formalism[1] of quantum mechanics uses classical paths to evaluate a quantum-mechanical transition amplitude. This is an advantage of the formalism over other formulations of quantum mechanics because intuitive arguments are available on solving separate problems in quantum mechanics. The path integral formalism is particularly useful when a physics in a semiclassical regime is considered. In quantum mechanics, dynamical variables are usually quantized and can be mutually incommutable. On the other hand, in the classical mechanics, they are continuous and are mutually commutable. The path integral formalism fully exploits these properties of the classical mechanics. A typical example is the coherent state path integral formalism[2,3] for the quantum spin system.[4]

Meanwhile, the motion of a single electron in a crystal lattice is successfully treated by the single band model,[5] in which the relevant Hilbert space is restricted to the subspace associated with a particular band. We may call such an electron a Bloch particle (electron).[6] We shall consider, for simplicity, the one-dimensional (1D) Bloch particle. On account of the restricted Hilbert space, the position and the momentum of the Bloch particle have important differences from those of the conventional particle: (i) the position is quantized in unit of the lattice spacing a and (ii) the momentum is not a true momentum but a quasimomentum which has a periodicity with the period $2\pi\hbar/a$. The two points, (i) and (ii), are closely related to each other because the position and the quasimomentum are canonically conjugate to each other. They prevent us from directly applying the path integral formalism for the conventional particle to quantum mechanics of the Bloch particle. If there ever exists a consistent path integral formalism for the Bloch particle, the position of the Bloch particle must be treated as a continuous variable in the formulation.

The purpose of this paper is to present a coherent state path integral formalism for the Bloch particle. The theory will be applied to the transition amplitude of the coherent state of the Bloch particle under a uniform electric field, and famous Bloch oscillations[6,7] will be reproduced.

The paper is organized as follows. In Sec. II we construct the coherent state for the Bloch particle. This is given in the Wannier representation. In Sec. III we compute matrix elements of the

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kinetic energy and the potential energy for the coherent states by use of the Poisson summation formula. In Sec. IV we construct the coherent state path integral formalism for the Bloch particle. In Sec. V, we evaluate the transition amplitude for the Bloch particle under a uniform electric field on the basis of the stationary-action approximation. In Sec. VI we conclude this paper with a summary and a discussion.

II. COHERENT STATE OF BLOCH PARTICLE

The Wannier states, $|n\rangle, n \in \mathbf{Z}$, form an orthonormal complete set of the Hilbert space of the Bloch particle:

$$\sum_{n=-\infty}^{\infty} |n\rangle\langle n| = 1. \tag{1}$$

The position operator, $\hat{x}$, is diagonal in the Wannier representation:

$$\hat{x} = \sum_{n=-\infty}^{\infty} |n\rangle x_n \langle n|, \quad x_n := na, \tag{2}$$

while the translation operator is off-diagonal:

$$\hat{T} = \sum_{n=-\infty}^{\infty} |n+1\rangle\langle n|, \tag{3}$$

or, equivalently, $\hat{T}|n\rangle = |n+1\rangle$. Then, $\hat{x}$ and $\hat{T}$ satisfy the commutation:

$$[\hat{x}, \hat{T}] = a\hat{T}, \tag{4}$$

in which the quantization of $\hat{x}$ is built in. The quasimomentum operator $\hat{p}$ is ill-defined but is related to the well-defined operator $\hat{T}$ by

$$\hat{T} = \exp\left(-\frac{i}{\hbar} a\hat{p}\right). \tag{5}$$

The translation operator $\hat{T}$, which is unitary, is diagonal in the Bloch representation which is based on the Bloch state (the momentum state), $|p\rangle$. That is,

$$\hat{T}|p\rangle = \exp\left(-\frac{i}{\hbar} ap\right)|p\rangle. \tag{6}$$

The Bloch state is specified by its wave function, $\langle n|p\rangle = \sqrt{a/(2\pi\hbar)}\exp(inap/\hbar)$. It is periodic: $|p + 2\pi\hbar/a\rangle = |p\rangle$, so that p is a variable on a circle (or, equivalently, the Brillouin zone) whose radius is equal to $\hbar/a$. It is unnormalizable but two different Bloch states are mutually orthogonal. The completeness of Bloch states is represented as

$$\int_{\mathrm{Bz}} \mathrm{d}p\, |p\rangle\langle p| = 1, \tag{7}$$

where the symbol Bz stands for the Brillouin zone.

It is convenient to introduce the angular variable, $\phi := ap/\hbar$, which is the dimensionless quasimomentum. It is a variable on the unit circle, S^1. Its operator version, $\hat{\phi}$, is related to $\hat{T}$ by

$$\hat{T} = \exp(-i\hat{\phi}). \tag{8}$$

Since ϕ has a different scale from that of p, we shall change the normalization for $|p\rangle$ to obtain $|\phi\rangle := \sqrt{\hbar/a}\,|p\rangle$ or, equivalently, $\langle n|\phi\rangle = \exp(in\phi)/\sqrt{2\pi}$. Hence, we may write

$$|\phi\rangle = \frac{1}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} e^{in\phi}|n\rangle, \tag{9}$$

$$\oint \mathrm{d}\phi\, |\phi\rangle\langle\phi| = 1. \tag{10}$$

Our path integral formalism for the Bloch particle will be established through an extension of the coherent state path integral formalism for the conventional particle.[3] In the latter formalism, we use coherent states, in each of which the position and the momentum are specified within the restriction imposed by the Heisenberg uncertainty principle. Therefore, the coherent state is a minimal packet and is an eigenstate of the non-Hermitian operator: $\hat{z} := \kappa\hat{x} + i\lambda\hat{p}$, where κ and λ are positive parameters characterizing the coherent state. Since $[\hat{z},\hat{z}^\dagger] = \kappa\lambda/2$, $\hat{z}$ is an unnormalized annihilation operator of a harmonic oscillator, and we assume that κ and λ are chosen so that $\hat{z}$ is dimensionless. Different coherent states are different eigenstates: $\hat{z}|z\rangle = z|z\rangle$, where $z := \kappa x + i\lambda p$ is a complex parameter specifying the coherent state. The position and the momentum of the coherent state are not sharply defined but their mean values are given by x and p, respectively, while their spreads by

$$\delta x = \sqrt{\frac{\hbar\lambda}{2\kappa}}, \quad \delta p = \sqrt{\frac{\hbar\kappa}{2\lambda}}, \tag{11}$$

which satisfy $\delta x\,\delta p = \hbar/2$. Note that the ratio κ/λ is more important than the two separate parameters themselves. The complex z plane is isomorphic to the two-dimensional phase space (x,p), and z can be treated as a complex dynamical variable in the coherent state path integral formalism.

We shall return to the case of the Bloch particle. A drawback for the case is that $\hat{p}$ is ill defined. To circumvent it, we set $\lambda = a/\hbar$ and introduce a new non-Hermitian operator by the formal equation, $\hat{A} := \exp(-\hat{z})$, which is well defined because

$$\hat{z} = \kappa\hat{x} + i\hat{\phi}. \tag{12}$$

The formal expression for $\hat{A}$ can be transformed with a standard procedure of the operator algebra into the exact one:

$$\hat{A} = \exp\left[-\kappa\left(\hat{x} - \frac{a}{2}\right)\right]\hat{T}. \tag{13}$$

The coherent state, $|z\rangle$, of the Bloch particle is an eigenstate of $\hat{A}$:

$$\hat{A}|z\rangle = e^{-z}|z\rangle, \quad z := \kappa x + i\phi. \tag{14}$$

It is of a vital importance in a later argument that the phase space for the complex dynamical variable z is the cylinder $\Gamma := \mathbf{R}\otimes S^1$ or, equivalently, the fundamental strip, $\Sigma := -\pi < \Im z \leqslant \pi$, on the complex z plane. Remember that Γ as well as S^1 is not simply connected.

If the coherent state is normalized appropriately, it is given in the Wannier representation as

$$|z\rangle = \sum_{n=-\infty}^{\infty} C_n(z)|n\rangle, \tag{15}$$

$$C_n(z) := \langle n|z\rangle = N\exp\left[-\frac{\kappa}{2a}(x_n - x)^2 + in\phi\right], \quad N = \left(\frac{\kappa a}{\pi}\right)^{1/4}. \tag{16}$$

Thus, the coherent state is of a wave packet, whose spread is equal to $\delta x := \sqrt{a/(2\kappa)}$.

The Bloch representation for the coherent state is readily obtained from this equation together with (9):

$$\langle \phi' | z \rangle = \sum_{n=-\infty}^{\infty} \frac{N}{\sqrt{2\pi}} \exp\left[-\frac{\kappa}{2a}(x_n - x)^2 + in(\phi - \phi') \right], \tag{17}$$

which can be rewritten with the Poisson summation formula into

$$\langle \phi' | z \rangle = \sum_{m=-\infty}^{\infty} N' \exp\left[-\frac{1}{2\kappa a}(\phi' - \phi_m)^2 - i\frac{x}{a}(\phi' - \phi_m) \right], \quad N' := (\pi\kappa a)^{-1/4} \tag{18}$$

with $\phi_m := \phi + 2\pi m$, where m is an integral variable to be called the *winding number*. The coherent state has a form of a wave packet in the momentum space as well, and its spread is equal to $\delta\phi := \sqrt{\kappa a/2}$, which is consistently related to δx by the Heisenberg uncertainty equality.

Although the left-hand side of (18) is periodic on the variable ϕ', each summand on the rhs (right-hand side) is not. Hence, the variable ϕ' should be regarded in the rhs as a variable on $\mathbf{R}$, which is simply connected and is the universally covering space for S^1. A similar situation will be realized in other infinite series of periodic functions to appear.

The inner product between different coherent states can be calculated in the Wannier representation as

$$\langle z | z' \rangle = N^2 \sum_{n=-\infty}^{\infty} \exp\left[-\kappa a n^2 + n(z^* + z') - \frac{\kappa}{2a}(x^2 + x'^2) \right], \tag{19}$$

which is transformed with the Poisson summation formula into

$$\langle z | z' \rangle = \sum_{m=-\infty}^{\infty} \exp\left[\frac{i}{\hbar}\mathcal{S}_c(z, z'_m) \right], \quad z'_m := z' + 2\pi m, \tag{20}$$

where

$$\frac{i}{\hbar}\mathcal{S}_c(\zeta, \zeta') = \frac{1}{8\kappa a}[2(\zeta^* + \zeta')^2 - (\zeta^* + \zeta)^2 - (\zeta'^* + \zeta')^2]. \tag{21}$$

Note that $\mathcal{S}_c(z, z'_m)$ depends on m because $\mathcal{S}_c(z, \zeta)$ is periodic on neither of the two variables. In particular, we obtain

$$\langle z | z \rangle = \sum_{m=-\infty}^{\infty} \exp\left[-\frac{\pi^2}{\kappa a} m^2 + i\frac{\pi x}{a} m \right] \tag{22}$$

$$= \vartheta_3\left(\frac{\pi x}{2a} \middle| \frac{i\pi}{\kappa a} \right), \tag{23}$$

where $\vartheta_3(z|\tau)$ is the θ-function[8] defined by

$$\vartheta_3(z|\tau) := \sum_{n=-\infty}^{\infty} e^{in^2\pi\tau + i2\pi nz}, \quad \Im\tau > 0. \tag{24}$$

Hence, the coherent state $|z\rangle$ is not normalized to unity. In fact, the right-hand sides of (17)–(20) are all represented with the third θ-function, ϑ_3, but with different arguments. The transformation combining the two expressions for $\langle\phi'|z\rangle$ or $\langle z|z'\rangle$ is the famous Jacobi's imaginary-number transformation for the θ-function.

We can consider $C_n^*(z)=\langle z|n\rangle$ to be the wave function of the Wannier state $|n\rangle$ in the coherent-state representation. The wave functions of Wannier states are orthonormal in the sense represented as

$$\int C_n(z)C_{n'}^*(z)\mathrm{d}\mu(z)=\delta_{n,n'}, \quad \mathrm{d}\mu(z):=\frac{\mathrm{d}x\,\mathrm{d}\phi}{2\pi a}, \tag{25}$$

where the integral must be performed over the entire phase space. The coherent states form an overcomplete set but we can derive from this result the following resolution of unit:

$$\int \mathrm{d}\mu(z)\,|z\rangle\langle z|=1. \tag{26}$$

This is a basic result for the construction of the coherent state path integral formalism.

The above-presented discussions show that the coherent state of the Bloch particle has similar properties to those of the coherent state of the conventional particle. The former coherent state tends asymptotically to the latter in the quasicontinuous limit, $a\kappa\ll 1$, where the spread of the packet in the real space is much larger than a, the lattice spacing.

It is important in a later discussion that, for a given ϕ', the summation on the rhs of (18) is dominated by a single term if $a\kappa\ll 1$, so that the interference among terms with different winding numbers vanishes then. Before closing this section, we should add a few articles on other representations for the state of the Bloch particle. The one is the "kq-representation" by Zak.[9] The other one is the "Gaussian representation" by Zeiner *et al.*[10]

III. MATRIX ELEMENTS

In order to construct the coherent state path integral formalism, we need to compute the matrix elements of the Hamiltonian, $\hat{H}$, for the coherent states. We assume that $\hat{H}$ is written as

$$\hat{H}=\hat{\mathcal{V}}+\hat{\mathcal{G}}, \tag{27}$$

where $\hat{\mathcal{V}}$ and $\hat{\mathcal{G}}$ are the kinetic energy and the potential energy, respectively, and are commutable with $\hat{T}$ and $\hat{x}$, respectively.

We begin our calculation with $\hat{\mathcal{G}}$. We assume it to be represented with an analytic function $g(\zeta)$ as $\hat{\mathcal{G}}=g(\hat{x})$. Its matrix element for coherent states is calculated in the Wannier representation as

$$\langle z|\hat{\mathcal{G}}|z'\rangle=N^2\sum_{n=-\infty}^{\infty} g(na)\exp\left[-\kappa a n^2+n(z^*+z')-\frac{\kappa}{2a}(x^2+x'^2)\right], \tag{28}$$

which is transformed by use of the Poisson summation formula into

$$\langle z|\hat{\mathcal{G}}|z'\rangle=\sum_{m=-\infty}^{\infty} \exp\left[\frac{i}{\hbar}\mathcal{S}_c(z,z'_m)\right]G(z^*,z'_m), \tag{29}$$

where

$$G(\zeta,\zeta')=\left(\frac{\kappa a}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}\mathrm{d}t\,e^{-\kappa t^2/a}g\left(t+\frac{\zeta+\zeta'}{2\kappa}\right). \tag{30}$$

Meanwhile, the Bloch state $|\phi\rangle$ is an eigenstate of $\hat{\mathcal{V}}$, which is commutable with $\hat{T}$. The eigenvalue $W(\phi)$ is a periodic function: $W(\phi+2\pi)=W(\phi)$. Let us write the Fourier expansion of $W(\phi)$ as

$$W(\phi)=\sum_{l=-\infty}^{\infty} V_l e^{-il\phi}, \quad V_{-l}=V_l^* . \tag{31}$$

If the potential term is absent, the eigen-energy is specified by ϕ as $E=W(\phi)$, which is nothing but the dispersion relation for the Bloch particle. A simplest expression for $W(\phi)$ is

$$W(\phi)=-V\cos\phi. \tag{32}$$

The relevant bandwidth is $2V$ provided that $V>0$.

For (31), we obtain

$$\hat{\mathcal{V}}=\sum_{l=-\infty}^{\infty} V_l \hat{T}^l. \tag{33}$$

The matrix elements of $\hat{T}^l$ for coherent states can be calculated by a similar procedure to the one for $\hat{\mathcal{G}}$:

$$\begin{aligned}\langle z|\hat{T}^l|z'\rangle &= N^2 \sum_{n=-\infty}^{\infty} \exp\left[-\kappa a n^2+n(z^*+z'+l\kappa a)-lz'-\frac{\kappa}{2a}(x^2+x'^2)-\frac{\kappa a}{2}l^2\right] \\ &= \sum_{m=-\infty}^{\infty} \exp\left[\frac{i}{\hbar}\mathcal{S}_c(z,z'_m)+\frac{l}{2}(z^*-z'_m)-\frac{\kappa a}{4}l^2\right].\end{aligned} \tag{34}$$

Thus,

$$\langle z|\hat{\mathcal{V}}|z'\rangle=\sum_{m=-\infty}^{\infty} \exp\left[\frac{i}{\hbar}\mathcal{S}_c(z,z'_m)\right]W(z^*,z'_m), \tag{35}$$

where

$$W(\zeta,\zeta')=\sum_{m=-\infty}^{\infty} e^{-\kappa a l^2/4}V_l e^{l(\zeta-\zeta')/2}. \tag{36}$$

From (27), (29), and (35), we obtain

$$\langle z|\hat{\mathcal{H}}|z'\rangle=\sum_{l=-\infty}^{\infty} \exp\left[\frac{i}{\hbar}\mathcal{S}_c(z,z'_m)\right]H(z^*,z'_m) \tag{37}$$

with

$$H(\zeta,\zeta'):=W(\zeta,\zeta')+G(\zeta,\zeta'). \tag{38}$$

IV. COHERENT STATE PATH INTEGRAL FORMALISM

Now, we can construct a coherent state path integral formalism for the Bloch particle. We write the transition amplitude between the initial state $|z_I\rangle$ and the final state $|z_F\rangle$ as

$$\mathcal{K}(z_F,z_I;T):=\langle z_F|\exp(-iT\hat{H}/\hbar)|z_I\rangle. \tag{39}$$

We slice the time interval into N identical pieces of length $\epsilon := T/N$, and write $\exp(-iT\hat{H}/\hbar) = [\exp(-i\hat{H}\epsilon/\hbar)]^N$. Inserting the resolution of unit, (26), into the relevant site associated with each discrete time yields

$$\mathcal{K}(z_F, z_I; T) = \lim_{N\to\infty} \int \prod_{j=1}^{N-1} \mathrm{d}\mu(z_j) \prod_{j=1}^{N} \langle z_j | e^{-i\epsilon\hat{H}/\hbar} | z_{j-1} \rangle \tag{40}$$

with $z_0 := z_I$ and $z_N := z_F$. The transition amplitude $\langle z|\exp(-i\epsilon\hat{H}/\hbar)|z'\rangle$ can be rewritten to the order ϵ as

$$\begin{aligned} \langle z | e^{-i\epsilon\hat{H}/\hbar} | z' \rangle &\simeq \langle z | (1 - i\epsilon\hat{H}/\hbar) | z' \rangle \\ &= \langle z | z' \rangle - \frac{i\epsilon}{\hbar} \langle z | \hat{H} | z' \rangle. \end{aligned} \tag{41}$$

Using (20) and (37), we can rewrite this equality to the order ϵ as

$$\langle z | e^{-i\epsilon\hat{H}/\hbar} | z' \rangle \simeq \sum_{m=-\infty}^{\infty} \exp\left[\frac{i}{\hbar} \mathcal{S}(z, z'_m) \right], \tag{42}$$

with

$$\mathcal{S}(\zeta, \zeta') := \mathcal{S}_c(\zeta, \zeta') - \epsilon H(\zeta, \zeta'). \tag{43}$$

Using (42), we can change (40) to obtain

$$\mathcal{K}(z_F, z_I; T) = \lim_{N\to\infty} \int \prod_{j=1}^{N-1} \mathrm{d}\mu(z_j) \prod_{j=1}^{N} \sum_{m_j=-\infty}^{\infty} \exp\left[\frac{i}{\hbar} \mathcal{S}(z_j, z_{j-1} + 2\pi i m_j) \right]. \tag{44}$$

Since $H(\zeta, \zeta')$ is composed of two terms, $W(\zeta, \zeta')$ and $G(\zeta, \zeta')$, $\mathcal{S}(\zeta, \zeta')$ has three terms. From (21), (30), and (36), we see that $\mathcal{S}(z_j, z_{j-1} + 2\pi i m_j)$ depends on m_j through the two forms:

$$z_j^* + z_{j-1} + 2\pi i m_j, \quad z_j^* - z_{j-1} - 2\pi i m_j. \tag{45}$$

We can rewrite (44) into a more convenient form if we employ a procedure in a textbook,[4] in which the authors discuss the Feynman kernel in a periodic system. We begin with changing the integer variables, m_j's, into others, m'_j's, by

$$m_j = m'_j - m'_{j-1}, \quad m'_0 = 0, \quad j = 1,2,\ldots,N. \tag{46}$$

Then, the sum on m_j's is transformed to that on m'_j's. We next change ϕ_j into

$$\phi_j = \phi'_j + 2\pi m'_j, \quad j = 1,2,\ldots,N-1. \tag{47}$$

Then, two quantities in (45) are transformed to

$$z_j'^* + z'_{j-1}, \quad z_j'^* - z'_{j-1} - 4\pi i m'_j, \tag{48}$$

respectively, where $z'_j := \kappa x_j + i\phi'_j$. Since z_j is a variable on the fundamental strip Σ, z'_j is a variable on the shifted strip, $\Sigma - 2\pi i m'_j$. From the considerations made up to this point, we can conclude that the integration on ϕ_j's in (44) is transformed as

$$\prod_{j=1}^{N}\sum_{m_j=-\infty}^{\infty}\prod_{j=1}^{N-1}\int_{-\pi}^{\pi}\mathrm{d}\phi_j=\sum_{m'_N=-\infty}^{\infty}\prod_{j=1}^{N-1}\int_{-\infty}^{\infty}\mathrm{d}\phi'_j\,, \tag{49}$$

where the quantity $\mathcal{S}(z_j,z_{j-1}+2\pi i m_j)$ included in the summand of (44) must be replaced simultaneously by $\mathcal{S}(z'_j,z'_{j-1})$. Note that the term $-4\pi i m'_j$ in the second quantity of (48) does not effect the summand because of the form of (36). Thus, we arrive at the final expression for the transition amplitude:

$$\mathcal{K}(z_F,z_I;T):=\sum_{m=-\infty}^{\infty}\mathcal{L}(z_F^m,z_I;T),\quad z_F^m:=z_F+i2\pi m \tag{50}$$

with

$$\mathcal{L}(z_F^m,z_I;T)=\lim_{N\to\infty}\prod_{j=1}^{N-1}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{\mathrm{d}x_j}{a}\frac{\mathrm{d}\phi_j}{2\pi}\exp\left(\frac{i}{\hbar}\mathcal{S}[\mathbf{z}^*,\mathbf{z}]\right), \tag{51}$$

where the action $\mathcal{S}[\mathbf{z}^*,\mathbf{z}]$ is a ''functional'' of the path $\mathbf{z}:=(z_0,z_1,\ldots,z_N)$ with $z_N:=z_F^m$, and is given by

$$\mathcal{S}[\mathbf{z}^*,\mathbf{z}]=\sum_{j=1}^{N}\mathcal{S}(z_j,z_{j-1}). \tag{52}$$

It is important to notice here that the phase space for the path $\mathbf{z}$ is the complex plane $\mathbf{C}$, which is the universally covering space for the cylinder Γ. The transition amplitude has been represented as a sum of transition amplitudes each of which is associated with the final state $z_F^m=z_F+i2\pi m$ with a specified m. Note that $z_F^m=\kappa x_F+i\phi_F^m$ with $\phi_F^m:=\phi_F+2\pi m$. Although $|z_F^m\rangle$ and $|z_F\rangle$ are an identical state of the Bloch particle, one needs to distinguish them and sum over the relevant paths in the path integral formula. This is derived from the fact that Γ is not simply connected.[11]

We shall rewrite the expression for $\mathcal{S}[\mathbf{z}^*,\mathbf{z}]$ into a more tractable form. It is composed of the canonical term and the dynamical term:

$$\mathcal{S}[\mathbf{z}^*,\mathbf{z}]=\mathcal{S}_c[\mathbf{z}^*,\mathbf{z}]+\mathcal{S}_d[\mathbf{z}^*,\mathbf{z}], \tag{53}$$

$$\mathcal{S}_c[\mathbf{z}^*,\mathbf{z}]:=\sum_{j=1}^{N}\mathcal{S}_c(z_j,z_{j-1}), \tag{54}$$

$$\mathcal{S}_d[\mathbf{z}^*,\mathbf{z}]:=-\sum_{j=1}^{N}\epsilon H(z_j,z_{j-1}). \tag{55}$$

We introduce here a new quantity by

$$\frac{i}{\hbar}\mathcal{S}_c(z_j,z_{j-1})=P(z_j)-P(z_{j-1})+\frac{i}{\hbar}\tilde{\mathcal{S}}_c(z_j,z_{j-1}) \tag{56}$$

with

$$P(z):=\frac{1}{8\kappa a}\{(z^*)^2-z^2\}. \tag{57}$$

Then, we may write

$$\frac{i}{\hbar}\mathcal{S}_c[\mathbf{z}^*,\mathbf{z}]=P(z_F^m)-P(z_I)+\frac{i}{\hbar}\tilde{\mathcal{S}}_c[\mathbf{z}^*,\mathbf{z}], \tag{58}$$

$$\frac{i}{\hbar}\tilde{\mathcal{S}}_c[\mathbf{z}^*,\mathbf{z}]:=\sum_{j=1}^{N}\left(-\frac{1}{4\kappa a}\right)\{z_j^*(z_j-z_{j-1})-(z_j^*-z_{j-1}^*)z_{j-1}\}, \tag{59}$$

where the summand is just an explicit form for $(i/\hbar)\tilde{\mathcal{S}}_c(z_j,z_{j-1})$. The first two terms on the rhs of (58) are purely imaginary, so that they may be called gauge terms because they give rise to a phase factor of (51). The phase factors affect the interference among different terms in (50).

Equation (59) reduces in the continuum-time limit to the functional:

$$\frac{i}{\hbar}\tilde{\mathcal{S}}_c[z^*,z]=-\frac{1}{4\kappa a}\int_0^T \mathrm{d}t\left\{z^*(t)\frac{\mathrm{d}z(t)}{\mathrm{d}t}-\frac{\mathrm{d}z^*(t)}{\mathrm{d}t}z(t)\right\}. \tag{60}$$

However, we should emphasize the necessity of the discrete-time formalism of the coherent state path integral in order to obtain a correct result for the transition amplitude.[12] Thus, Eq. (60) is usable only for the evaluation of the stationary action. We should mention, finally, that the discrete-time formalism of the coherent state path integral can be consistently formulated because $\tilde{\mathcal{S}}_c[\mathbf{z}^*,\mathbf{z}]$ and $\mathcal{S}_d[\mathbf{z}^*,\mathbf{z}]$ are holonomic functions of two sets of complex variables $\mathbf{z}$ and $\mathbf{z}^*$, where the two sets are regarded to be independent variables.[12]

V. APPLICATION TO THE BLOCH OSCILLATION

As an application of the present formalism, we consider the time evolution of the coherent state of the Bloch particle under a uniform electric field F. As a consequence of the boundedness of the energy band, the Bloch particle exhibits the so-called Bloch oscillation.[6,7] If the simplest dispersion (32) is adopted, the Hamiltonian assumes

$$\hat{H}=-V\cos\hat{\phi}-F\hat{x}, \tag{61}$$

whose matrix element is

$$H(z_j^*,z_{j-1})=-Ve^{-\kappa a/4}\cosh\left(\frac{z_j^*-z_{j-1}}{2}\right)-\frac{F}{2\kappa}(z_j^*+z_{j-1}). \tag{62}$$

To evaluate the transition amplitude, we employ the stationary-action approximation, which is justified for a semiclassical motion.

We consider here the classical motion of the Bloch particle. The equation of motion is

$$\frac{\mathrm{d}x}{\mathrm{d}t}=\frac{aV}{\hbar}\sin\phi, \tag{63}$$

$$\frac{\mathrm{d}\phi}{\mathrm{d}t}=\omega \tag{64}$$

with

$$\omega:=\frac{Fa}{\hbar}. \tag{65}$$

The solution for the initial condition, $x(0)=x_I$ and $\phi(0)=\phi_I$, is given by

$$x=x_{\mathrm{cl}}(t):=x_I+L_{\mathrm{cl}}[\cos\phi_I-\cos(\omega t+\phi_I)], \tag{66}$$

$$\phi = \phi_{\rm cl}(t) := \phi_I + \omega t, \tag{67}$$

where $L_{\rm cl} := V/F$ is the so-called localization length. This solution shows the Bloch oscillation with the angular frequency ω.

Thus, the condition for the motion to be semiclassical is given by $L_{\rm cl} \gg \delta x \simeq \sqrt{a/\kappa} \gg a$.

A. Stationary action

The primary task is to find the stationary point, namely, stationary action path of the action $\mathcal{S}[\mathbf{z}^*,\mathbf{z}]$ or, equivalently, $\tilde{\mathcal{S}}[\mathbf{z}^*,\mathbf{z}]$. We will execute it by a similar procedure to the one presented in Ref. 10. The equation of motion for the stationary action path is obtained by differentiating the action:

$$\left.\frac{\partial \tilde{\mathcal{S}}[\mathbf{z}^*,\mathbf{z}]}{\partial z_j^*}\right|_s = \left.\frac{\partial \tilde{\mathcal{S}}[\mathbf{z}^*,\mathbf{z}]}{\partial z_j}\right|_s = 0, \quad j = 1,2,\ldots,N-1. \tag{68}$$

For the stationary action path $\{\mathbf{z}^s,\overline{\mathbf{z}^s}\}$, we are allowed to take the continuous-time limit,[12] so that

$$\frac{{\rm d}z^s(t)}{{\rm d}t} = i\omega + i\Omega \sinh\left(\frac{\overline{z}^s(t) - z^s(t)}{2}\right), \tag{69}$$

$$\frac{{\rm d}\overline{z}^s(t)}{{\rm d}t} = -i\omega + i\Omega \sinh\left(\frac{\overline{z}^s(t) - z^s(t)}{2}\right) \tag{70}$$

with

$$\omega := \frac{Fa}{\hbar}, \quad \Omega := \frac{\kappa a}{\hbar} V e^{-\kappa a/4}. \tag{71}$$

These equations must be solved under the following boundary conditions:[12]

$$z^s(0) = z_I, \quad \overline{z}^s(T) = z_F^m{}^*. \tag{72}$$

It should be noted that $z^s(t)$ and $\overline{z}^s(t)$ are not necessary complex conjugate to each other.[12]

From (70) we obtain

$$\tfrac{1}{2}(z^s(t) - \overline{z}^s(t)) = i(\omega t + \phi_0), \tag{73}$$

where ϕ_0 is a complex constant. Inserting this into the rhs of (70), we can solve for $z^s(t)$ and $\overline{z}^s(t)$ to obtain

$$z^s(t) = z^s(t,\phi_0) := z_I + i\omega t - \frac{\Omega}{\omega}[\cos(\omega t + \phi_0) - \cos\phi_0], \tag{74}$$

$$\overline{z}^s(t) = \overline{z}^s(t,\phi_0) := z_F^m{}^* - i\omega(t-T) - \frac{\Omega}{\omega}[\cos(\omega t + \phi_0) - \cos(\omega T + \phi_0)], \tag{75}$$

where the integration constants are fixed by the boundary conditions (72). This solution is consistent to (73) only if ϕ_0 satisfies

$$D(\phi_0) := z_F^m{}^* - z^s(T,\phi_0) + 2i(\omega T + \phi_0) = 0, \tag{76}$$

where use has been made of $\overline{z}^s(T,\phi_0) = z_F^m{}^*$.

The following two quantities are introduced here for a convenience of later arguments:

$$\tilde{\Omega}(t) := \frac{\Omega}{2}\cos(\omega t + \phi_0), \tag{77}$$

$$Z(t,\phi_0) := \int_0^t dt' \tilde{\Omega}(t') = \frac{\Omega}{2\omega}[\sin(\omega t + \phi_0) - \sin\phi_0]. \tag{78}$$

Alternatively, we may write

$$Z(t,\phi_0) = \frac{1}{2}\frac{\partial z^s(t,\phi_0)}{\partial \phi_0}. \tag{79}$$

The stationary action, $\mathcal{S}_m^s := \mathcal{S}[\overline{\mathbf{z}}^s, \mathbf{z}^s]$, can be obtained by substituting (74) and (75) into the action (53) with (55), (58), and (60):

$$\frac{i}{\hbar}\mathcal{S}_m^s = -\frac{i}{2a}\{x_F\phi_F^m - x_I\phi_I\} - \frac{1}{4\kappa a}\Bigg[|z_F^m|^2 + |z_I|^2 - 2z_F^{m*}z_I - (z_F^{m*} - z_I + i\omega T + 2i\phi_0)^2$$
$$- 2i\omega T\left(z_F^{m*} + z_I + i\frac{\omega T}{2}\right) - 8iZ(T,\phi_0)\Bigg]. \tag{80}$$

B. Semiclassical stationary action

Let $z_{sc}(t) := z^s(t,\phi_I)$. Then $z(t) := z_{sc}(t)$ and $\overline{z}(t) := z_{sc}^*(t)$ satisfy the equation of motion (70) with the initial condition, $z(0) = z_I$ and $\overline{z}(0) = z_I^*$. More explicitly,

$$z_{sc}(t) = \kappa x_{sc}(t) + i\phi_{sc}(t), \tag{81}$$

$$x_{sc}(t) = x_I + L[\cos\phi_I - \cos(\omega t + \phi_I)], \tag{82}$$

$$\phi_{sc}(t) = \phi_I + \omega t \tag{83}$$

with

$$L := \frac{\Omega}{\omega\kappa} = \frac{V}{F}e^{-\kappa a/4}. \tag{84}$$

The solution (81) is the semiclassical solution, which tends to the classical solution (67) in the limit $\kappa a \to 0$ because $L = L_{cl}\exp(-\kappa a/4)$.

Let $\Delta z := z_F^m - z_{sc}(T)$. Then

$$\Delta z = \kappa\Delta x + i\Delta\phi, \tag{85}$$

$$\Delta x = x_F - x_{sc}(T), \tag{86}$$

$$\Delta\phi = \phi_F^m - \phi_{sc}(T). \tag{87}$$

The condition for the semiclassical solution to satisfy the boundary conditions (72) is given by $\Delta z = 0$ for an integer m. If this condition is satisfied, the solution of Eq. (76) is given by $\phi_0 = \phi_I$.

It will be shown later on that under the semiclassical condition, we can assume $|\Delta z|^2 = (\kappa\Delta x)^2 + (\Delta\phi)^2 \ll 1$. Then, we are allowed to solve Eq. (76) for ϕ_0 to the first order on Δz. We set $\phi_0 := \phi_I + \delta\phi$, and expand $D(\phi_0)$ to the first order on $\delta\phi$ to obtain

$$D(\phi_0) \simeq \Delta z^* + 2(i - Z(T,\phi_I))\,\delta\phi, \tag{88}$$

where use has been made of $D(\phi_I)=\Delta z^*$ and (79). Therefore, we obtain

$$\phi_0 \simeq \phi_I + \frac{i\Delta z^*}{2\{1+iZ(T,\phi_I)\}}. \tag{89}$$

In the similar way, let $\tilde{z}_{sc}(t) := z^s(t-T,\phi_F^m)$ and $\Delta\tilde{z} := \Delta\tilde{z}_{sc}(0)-z_I$. Then, under the semiclassical condition, $|\Delta\tilde{z}|^2 \ll 1$, we can obtain the correspondence with $\delta\phi$ as

$$\delta\tilde{\phi} := \frac{i\Delta\tilde{z}}{2\{1+iZ(T,\phi_F^m-\omega T)\}}. \tag{90}$$

We should remark here that the following equality holds to the zeroth order on $\Delta\phi$:

$$Z(T,\phi_I) \simeq Z(T,\phi_F^m-\omega T) \simeq \frac{\Omega}{\omega}\cos\left(\frac{\phi_F^m+\phi_I}{2}\right)\sin\frac{\omega T}{2} =: C(T), \tag{91}$$

which is symmetrical with respect to ϕ_I and ϕ_F^m. Hence, we set

$$\phi_0 = \frac{\phi_F^m+\phi_I-\omega T}{2} + \frac{i\kappa\Delta\overline{x}}{2\{1+iC(T)\}}, \tag{92}$$

$$\Delta\overline{x} := x_F - x_I + L\left[\cos\left(\frac{\phi_F^m+\phi_I+\omega T}{2}\right) - \cos\left(\frac{\phi_F^m+\phi_I-\omega T}{2}\right)\right], \tag{93}$$

and substituting (92) into (80) and (105), we find the following semiclassical stationary action:

$$\frac{i}{\hbar}\mathcal{S}_m^s = -\frac{\kappa}{4a}\frac{(\Delta\overline{x})^2}{1+iC(T)} - \frac{1}{4\kappa a}(\Delta\phi)^2 - \frac{i}{2a}(x_F+x_I)\Delta\phi + \frac{2i}{\kappa a}C(T). \tag{94}$$

C. Fluctuation

We introduce the fluctuation variables through

$$z_j = z_j^s + \zeta_j, \quad z_j^* = \overline{z_j^s} + \zeta_j^*, \quad j=1,2,\ldots,N-1. \tag{95}$$

Substituting (95) into the action $\mathcal{S}[\overline{\mathbf{z}},\mathbf{z}]$, and expanding the result up to the second order in the fluctuation, we obtain

$$\mathcal{S}[\overline{\mathbf{z}^s}+\zeta^*,\mathbf{z}^s+\zeta] \simeq \mathcal{S}_m^s + \mathcal{S}_m^2[\zeta^*,\zeta], \tag{96}$$

where $\mathcal{S}_m^2[\zeta^*,\zeta]$ is a quadratic form on the fluctuation variables. Therefore, the contribution of the fluctuation to the action is represented as a factor of

$$\mathcal{F}_m(T) := \lim_{N\to\infty}\int_{-\infty}^{\infty}\prod_{j=1}^{N-1}\frac{\mathrm{d}(\Re\zeta_j)\mathrm{d}(\Im\zeta_j)}{2\kappa a}\exp\left(\frac{i}{\hbar}\mathcal{S}_m^2[\zeta^*,\zeta]\right), \tag{97}$$

which is a multidimensional Gaussian integral. The leading contribution to $(i/\hbar)\mathcal{S}_m^2[\zeta^*,\zeta]$ is written as $-\Sigma_j\zeta_j^*\zeta_j/(2\kappa a)$, and the fluctuation of ζ is of the order $\sqrt{\kappa a}$, which is small when $\kappa a \ll 1$.

There exists a standard procedure to evaluate $\mathcal{F}_m(T)$.[13,14] To evaluate the Gaussian integral is reduced to a calculation of the determinant of a symmetric matrix associated with the quadratic form. Since the matrix is tridiagonal its determinant is given as the last term of coupled three-term recursion relations. In the limit of $\epsilon\to 0$, they reduce to a set of coupled first-order differential equations:

$$\frac{\mathrm{d}M(t)}{\mathrm{d}t} = -\tilde{\Omega}(t)M'(t), \tag{98}$$

$$\frac{\mathrm{d}M'(t)}{\mathrm{d}t} = -\tilde{\Omega}(t)\{M(t)+2iM'(t)\} \tag{99}$$

with the initial condition

$$M(0)=1, \tag{100}$$

$$M'(0)=0. \tag{101}$$

The differential equations are readily solved to obtain

$$M(t)=e^{-iZ(t)}[1+iZ(t)], \tag{102}$$

$$M'(t)=-Z(t)\,e^{-iZ(t)} \tag{103}$$

with $Z(t):=Z(t,\phi_0)$. Hence,

$$\mathcal{F}_m(T)=[M(T)]^{-1/2} \tag{104}$$

$$=\frac{e^{iC(T)/2}}{\sqrt{1+iC(T)}}, \tag{105}$$

where we have used the semiclassical expression, $C(T)\simeq Z(T,\phi_I)$.

D. Transition amplitude

The transition amplitude in the semiclassical approximation is given by

$$\mathcal{K}(z_F,z_I;T)\simeq\sum_{m=-\infty}^{\infty}\mathcal{L}^s(z_F^m,z_I;T), \tag{106}$$

$$\mathcal{L}^s(z_F^m,z_I;T):=\mathcal{F}_m(T)\,e^{iS^s_m/\hbar}, \tag{107}$$

$$\mathcal{F}_m(T)=\frac{1}{\sqrt{1+iC(T)}}. \tag{108}$$

It follows that

$$|\mathcal{L}^s(z_F^m,z_I;T)|^2=\frac{1}{\sqrt{1+(C(T))^2}}\exp\left[-\frac{\kappa}{2a}\frac{(\Delta\overline{x})^2}{1+(C(T))^2}-\frac{1}{2\kappa a}(\Delta\phi)^2\right] \tag{109}$$

or, equivalently,

$$|\mathcal{L}^s(z_F^m,z_I;T)|^2=\frac{1}{\sqrt{1+(C(T))^2}}\exp\left[-\frac{\kappa}{2a}\frac{(x_F-\overline{x}_{\mathrm{sc}}(T))^2}{1+(C(T))^2}-\frac{1}{2\kappa a}(\phi_F^m-\phi_{\mathrm{sc}}(T))^2\right], \tag{110}$$

$$\overline{x}_{\mathrm{sc}}(T):=x_I+2L\sin\left(\frac{\phi_F^m+\phi_I}{2}\right)\sin\frac{\omega T}{2}. \tag{111}$$

For given x_F and ϕ_F, the summation on the rhs of (106) is dominated by a single term because we have assumed that $a\kappa \ll 1$. Therefore, the interference among terms with different winding numbers vanishes then. Since $\phi_{sc}(T)$ changes linearly with T, the leading term in (106) changes discontinuously with T. It follows from (110) that, for a given initial condition (x_I, ϕ_I), the wave packet centroid in the extended phase space, $x_F - \phi_F$, exhibits the Bloch oscillations along the position axis. While, the time dependence of the spreads of the wave packet in the phase space is given by

$$\delta x(T) = \sqrt{\frac{2a}{\kappa}\{1 + (C(T))^2\}}, \quad \delta\phi = \sqrt{2\kappa a} \tag{112}$$

along the momentum and the position axes, respectively. The maximum value of $\delta x(T)$ is equal to $\sqrt{(2a/\kappa)\{1+(C(T))^2\}}$, so that our assumption $|\Delta z|^2 \ll 1$ has been justified under the semiclassical condition.

The expressions for $\delta x(0)$ and $\delta\phi$ are larger by the factor $\sqrt{2}$ than those for the relevant coherent states. This is because $\langle z_F^m | z_I \rangle$ is a sort of the convolution of the two coherent states. The time dependence of the spread of the wave packet along the position axis is periodic by (112) with (91). This breathing behavior is similar to the behavior of the squeezed state of the harmonic oscillator.[15]

Our solution remains correct in the zero-field limit, $F = 0$, where the Bloch particle exhibits a ballistic motion: $x_{sc}(T) = x_I + v_I T$, $\phi_{sc}(T) = \phi_I$, and $C(T) = (\Omega T/2)\cos\phi_I$ with $v_I := (aV/\hbar)\sin\phi_I$ being the group velocity. The spread of the wave packet, $\delta x(T)$, increases monotonously with T because of the dispersion of the phase velocity.

VI. SUMMARY AND DISCUSSION

We have succeeded in properly defining the coherent states for the Bloch particle. Using them, we have constructed a coherent state path integral formalism for the Bloch particle. The transition amplitude involves contribution from paths with different winding numbers associated with the quasimomentum. The theory has been successfully applied to the semiclassical motion of the Bloch particle under a uniform electric field, and the famous Bloch oscillation has been reproduced.

If one of two dynamical variables which are canonically conjugate to each other is continuous but periodic, the other is discrete and unbounded on both the positive and the negative sides of its value. The converse of this statement is also true. The second example in addition to the Bloch particle is the rigid rotator, where the rotation angle, ϕ, is continuous but the angular-momentum, L_z, is discrete. That is, the roles of the position and the momentum are reversed from the case of the Bloch particle. Therefore, the roles of the kinetic energy and the potential energy are reversed as well. The periodic potential energy $W(\phi)$ stands for the hindering potential, and can assume various forms depending on the physical condition for the rigid rotator. On the contrary, the kinetic energy is restricted to the form $(L_z)^2/(2I)$ with I being the moment of inertia. The third example is the order parameter of a mesoscopic superconductor or the BEC of an ultracold gas, where the phase of the order parameter, ϕ, is continuous but the number of the condensate, N, is discrete. Anyway, the coherent state path integral formalism established in the present paper can be applied to other systems than the Bloch particle.

It is our hope that the path integral formalism will help to achieve solving more complicated problems for the Bloch particle or other systems. In fact, the authors have found recently equivalence of the quantum dynamics of a domain wall in a quasi-one-dimensional mesoscopic ferromagnet to that of the Bloch particle. This subject is discussed in a separate paper.[16]

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Möbius structure of the spectral space of Schrödinger operators with point interaction

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The Schrödinger operator with point interaction in one dimension has a U(2) family of self-adjoint extensions. We study the spectrum of the operator and show that (i) the spectrum is uniquely determined by the eigenvalues of the matrix $U \in \mathrm{U}(2)$ that characterizes the extension, and that (ii) the space of distinct spectra is given by the orbifold $T^2/\mathbb{Z}_2$ which is a Möbius strip with boundary. We employ a parametrization of U(2) that admits a direct physical interpretation and furnishes a coherent framework to realize the spectral duality and anholonomy recently found. This allows us to find that (iii) physically distinct point interactions form a three-parameter quotient space of the U(2) family. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1415432]

I. INTRODUCTION

Quantum mechanical motion of a particle subject to a point interaction on a line $\mathbb{R}$ is described by the free Schrödinger (the Laplacian) operator,

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \tag{1}$$

with one point perturbation. This is implemented by deleting a point, say $x=0$ on the line, and thereby considering the family Ω of self-adjoint operators H defined on proper domains in the Hilbert space $\mathcal{H}=L^2(\mathbb{R}\backslash\{0\})$. The theory of self-adjoint extensions then dictates that the family Ω is given by the group U(2), which covers all allowable distinct point interactions.[1] Studies show that the spectrum of the operator H consists of the essential spectrum $[0,\infty)$ together with a discrete spectrum having at most two levels of bound states[2] (see also Refs. 3 and 4, and references therein). Symmetries such as parity or time reversal are used to classify the family $\Omega \simeq \mathrm{U}(2)$ in terms of their invariant subfamilies.[5]

Recently, we have examined the spectral properties of this simple system and found a number of interesting features which are usually ascribed to more complex systems. These features include duality in the spectra under strong versus weak coupling exchange,[6,7] anholonomy both in the phase of states (the Berry phase) and in levels under a cycle in Ω,[8,9] and the double degeneracy

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which leads to supersymmetry.[10] Meanwhile, a similar study has been made on a circle S^1 with point interaction,[11] where it is shown that the spectrum of H does not depend on the entire U(2) parameters as one naïvely expects.

The aim of the present paper is to furnish a comprehensive picture of the spectral structure of the entire family of the Schrödinger operators H on a line $\mathbb{R}$ as well as on an interval $[l,-l]$ (under some innocuous boundary conditions) with the point $x=0$ removed. Our main results are given in three theorems. Theorem 1 states that the spectrum is uniquely determined by the eigenvalues of the U(2) matrix which characterizes the point interaction, and Theorem 2 shows that, for the case of the interval, the space Σ consisting of all distinct spectra is given by a Möbius strip with boundary, while for the case of the line Σ is a subspace of it. The key observation to reach these statements is that the set of su(2) parity transformations on the operator H which preserve the spectrum[7,10] can be generalized in order to narrow the dependence from U(2) down to its subspace. We also provide a generalization in symmetry transformations in order to associate a pertinent invariant subfamily to any point interaction in Ω. In our treatment emerges a natural parametrization of Ω which admits a direct physical interpretation and furnishes a framework to describe the above-mentioned features in a coherent manner. As part of the physical interpretation given as Theorem 3, we find a one-parameter gauge equivalence within Ω and conclude that physically distinct point interactions form a three-parameter quotient space of Ω.

II. SPECTRAL STRUCTURE

Let us first recall the description of the U(2) family of self-adjoint operators H[7] (see also Ref. 12). The domain of such a self-adjoint operator H is a subspace of $\mathcal{H}$ specified by a boundary condition at the missing point $x=0$ on the line. Let φ be a state in the domain, and consider the two-component boundary vectors

$$\Phi := \begin{pmatrix} \varphi(0_+) \\ \varphi(0_-) \end{pmatrix}, \quad \Phi' := \begin{pmatrix} \varphi'(0_+) \\ -\varphi'(0_-) \end{pmatrix}, \tag{2}$$

where 0_+ and 0_- denote the limits at $x=0$ from the right and the left, respectively. We require φ and its derivative φ' to be absolutely continuous on $\mathbb{R}\backslash\{0\}$ (see Ref. 12). In terms of a matrix $U\in \mathrm{U}(2)$ the boundary condition is then given as

$$(U-I)\Phi + iL_0(U+I)\Phi' = 0, \tag{3}$$

with some constant $L_0\neq 0$ of length dimension, where I denotes the unit matrix in U(2). We note that the self-adjointness of H is equivalent to the requirement of (global) probability conservation, and that the constant L_0 adds no extra freedom to that given by U.[10] To indicate the U(2)-dependence of the operator H, we use the notation H_U.

We now begin our discussion of the spectral structure of the family Ω of the operators H_U by providing the following

Definition 1: A unitary transformation $\mathcal{X}:\mathcal{H}\to\mathcal{H}$ is called *a generalized symmetry* of the family Ω if, for any $U\in \mathrm{U}(2)$,

$$\mathcal{X}^{-1}H_U\mathcal{X} = H_{U_{\mathcal{X}}}, \tag{4}$$

for some $U_{\mathcal{X}}\in \mathrm{U}(2)$.

We note that condition (4) embodies two requirements: first, the domain of H_U is mapped into the domain of $H_{U_{\mathcal{X}}}$, and second, $\mathcal{X}^{-1}H_U\mathcal{X}$ acts on this new domain as the differential operator (1). Note also that the two operators H_U and $H_{U_{\mathcal{X}}}$ share the same spectrum.

The following lemmas will be useful in proving Theorem 1.

Lemma 1: The operators $\mathcal{P}_j$ $(j=1,2,3)$ *defined as*

$$(\mathcal{P}_1\varphi)(x) := \varphi(-x),$$

$$(\mathcal{P}_2\varphi)(x) := i[\Theta(-x)-\Theta(x)]\varphi(-x), \tag{5}$$

$$(\mathcal{P}_3\varphi)(x) := [\Theta(x)-\Theta(-x)]\varphi(x)$$

(where Θ denotes the Heaviside step function) are generalized symmetries. Further, they are parity-type operators (i.e., $\mathcal{P}_j^2=\mathrm{id}_{\mathcal{H}}$, $P_j\neq\pm\mathrm{id}_{\mathcal{H}}$) and satisfy the su(2) *commutation relations $[\mathcal{P}_j,\mathcal{P}_k]=2i\Sigma_{l=1}^{3}\epsilon_{jkl}\mathcal{P}_l$ and the anticommutation relations $\{\mathcal{P}_j,\mathcal{P}_k\}=2\delta_{jk}\,\mathrm{id}_{\mathcal{H}}$.*

Proof: It is straightforward to check that these operators are unitary and parity type, fulfilling the stated commutation and anticommutation relations. To show that they are generalized symmetries, let us observe that, under a $\mathcal{P}_j$, the boundary vectors (2) change as $\Phi\mapsto\sigma_j\Phi$ and $\Phi'\mapsto\sigma_j\Phi'$, where σ_j's denote the Pauli matrices. In the boundary condition (3), this change can be absorbed by the change in the matrix U as

$$U\mapsto U_{\mathcal{P}_j} := \sigma_j\, U\, \sigma_j\,. \tag{6}$$

This implies that a $\mathcal{P}_j$ maps the domain of an H_U to the domain of $H_{U_{\mathcal{P}_j}}$ with $U_{\mathcal{P}_j}$ given in (6) (clearly, $\mathcal{P}_j$'s preserve the smoothness properties mentioned in Ref. 1, too). It is also easy to see that $\mathcal{P}_jH_U\mathcal{P}_j$ remains the differential operator (1) on this new domain, since, under any of the transformations (5), φ acquires merely an overall complex phase factor that is constant on both $\mathbb{R}_+$ and $\mathbb{R}_-$. Q.E.D.

The three transformations defined previously are not the only parity-type generalized symmetries. Indeed, operators given by the linear combinations of the three,

$$\mathcal{P} := \sum_{j=1}^{3} c_j\,\mathcal{P}_j \quad \text{with} \quad c_j\in\mathbb{R}, \quad \sum_{j=1}^{3} c_j^2=1, \tag{7}$$

are all generalized symmetries and fulfill the parity property $\mathcal{P}^2=\mathrm{id}_{\mathcal{H}}$, where now the induced transformation on U reads

$$U\mapsto U_{\mathcal{P}}=\sigma U\sigma, \quad \sigma := \sum_{j=1}^{3} c_j\,\sigma_j\,. \tag{8}$$

We therefore arrive at

Lemma 2: For any su(2) *element σ normalized as $\sigma^2=I$, and for any $U\in\mathrm{U}(2)$, H_U and $H_{\sigma U\sigma}$ share an identical spectrum.*

Using Lemma 2, we now show

Theorem 1: *The spectrum of the Schrödinger operator H_U is uniquely determined by the eigenvalues of the matrix U.*

Proof: Let $e^{i\theta_+}$ and $e^{i\theta_-}$ with $\theta_\pm\in[0,2\pi)$ be the two eigenvalues of the unitary matrix U. These eigenvalues arise in the matrix,

$$D=\begin{pmatrix} e^{i\theta_+} & 0 \\ 0 & e^{i\theta_-} \end{pmatrix}, \tag{9}$$

which appears when one diagonalizes

$$U=V^{-1}DV, \tag{10}$$

with an appropriate $V\in\mathrm{SU}(2)$. To proceed, let us set

$$D=e^{i\xi}e^{i\rho\sigma_3}, \quad \xi=\frac{\theta_++\theta_-}{2}, \quad \rho=\frac{\theta_+-\theta_-}{2}, \tag{11}$$

to rewrite (10) as

$$U = e^{i\xi} e^{i\rho\, V^{-1}\sigma_3 V}. \tag{12}$$

Note that $V^{-1}\sigma_3 V$ in the exponent is just an element of su(2) obtained by the rotation of σ_3 with respect to an axis determined by V. Note also that, since $\sigma = (1/i)\, e^{(\pi/2)\, i\sigma} = \sigma^{-1}$, the product $\sigma\sigma_3\sigma$ is an element of su(2) obtained by the rotation of σ_3 with respect to σ by the angle π. This implies that, to a given V, one can always find some σ such that $V^{-1}\sigma_3 V = \sigma\sigma_3\sigma$ holds. With such σ we now have

$$U = e^{i\xi} e^{i\rho\, \sigma\sigma_3\sigma} = \sigma\, D\, \sigma. \tag{13}$$

Lemma 2 then ensures that the spectrum of H_U coincides with the spectrum of H_D. Q.E.D.

From this theorem we obtain

Corollary 1: A point interaction characterized by U possesses the isospectral subfamily

$$\Omega(D) := \{H_{V^{-1}DV} | V \in \mathrm{SU}(2)\}, \tag{14}$$

where D is the diagonal eigenvalue matrix in the decomposition (10) of U. The isospectral subspace $\Omega(D)$ *is homeomorphic to the coadjoint orbit of* SU(2) *passing through the element* $e^{i\rho\sigma_3}$, *and hence* $\Omega(D) \simeq S^2$ *except for the case* $D = e^{i\theta}\cdot I$ $(\theta \in [0, 2\pi))$ *for which* $\Omega(D)$ *consists of D alone*.

We mention that the exceptional cases $(\theta = \theta_+ = \theta_-)$ occur at

$$U = e^{i\theta}\cdot I, \quad \theta \in [0, 2\pi), \tag{15}$$

which form what we call the *self-dual subfamily* $\Omega_{\mathrm{SD}} \simeq \mathrm{U}(1)$ in the entire set of point interactions $\Omega \simeq \mathrm{U}(2)$ (see also Proposition 3 and the remark which follows).

Clearly, the two eigenvalues of U appearing in D are interchangeable, and this is realized for $\Omega(D)$ by setting, e.g., $V \mapsto i\sigma_2 V$. Thus, if we write $D = D(\theta_+, \theta_-)$ for the diagonal matrix D in (9), we have

Corollary 2: The two isospectral subfamilies associated with $D(\theta_+, \theta_-)$ *and* $D(\theta_-, \theta_+)$ *are identical,*

$$\Omega(D(\theta_+, \theta_-)) = \Omega(D(\theta_-, \theta_+)), \tag{16}$$

and hence the spectrum occurring at $D(\theta_+, \theta_-)$ *and that occurring at* $D(\theta_-, \theta_+)$ *are the same.*

The above-discussed spectral feature is seen in the discrete spectrum, but it is largely obscured because the spectrum consists mostly of the continuous spectrum $[0, \infty)$. However, the structure becomes manifest if one considers, instead of a line, a box (interval) on which the entire spectrum becomes discrete. This can be done by imposing a boundary condition at both ends of the box in such a way that it does not affect the consequences of the operations of $\mathcal{P}$ in (7). Specifically, if we let the interval $[-l, l]$ be the box where the point interaction is placed at $x = 0$, then we seek boundary conditions at $x = \pm l$ which remain invariant under any of the transformations induced by $\mathcal{P}$. These are given by

Proposition 1: The boundary conditions at $x = \pm l$ *which are left unchanged under any of the transformations induced by* $\mathcal{P}$ *(and hence provide a domain for H so that the entire discrete spectrum exhibits the spectral structure manifestly) are*

$$\varphi(l) + L\varphi'(l) = 0, \quad \varphi(-l) - L\varphi'(-l) = 0, \tag{17}$$

where $L \in (-\infty, \infty) \cup \{\infty\}$ *is an arbitrary parameter.*

Proof: The operator H remains self-adjoint if the boundary condition at $x = \pm l$ ensures the probability conservation, and this is exactly the demand we used to obtain the boundary condition

(3) at $x=0$. (More precisely, one needs to require further that the probability current vanish at the both ends, but this will be seen to be satisfied at the end.) This suggests that, if we use the boundary vectors similar to (2),

$$\Psi := \begin{pmatrix} \varphi(l) \\ \varphi(-l) \end{pmatrix}, \quad \Psi' := \begin{pmatrix} \varphi'(l) \\ -\varphi'(-l) \end{pmatrix}, \tag{18}$$

the boundary conditions at the ends can be given analogously as

$$(\tilde{U}-I)\Psi + iL_0(\tilde{U}+I)\Psi' = 0, \tag{19}$$

in terms of a matrix $\tilde{U}\in \mathrm{U}(2)$ characterizing the two ends. The transformation of the operator $\mathcal{P}$ on the boundary vectors (18) is the same as before, and hence it induces the same action $\tilde{U}\mapsto \tilde{U}_{\mathcal{P}}=\sigma\,\tilde{U}\,\sigma$ on the matrix $\tilde{U}$. Thus, the required boundary condition must satisfy $\sigma\,\tilde{U}\,\sigma = \tilde{U}$, that is, we find $\tilde{U}=e^{i\theta\cdot I}$ for $\theta\in[0,2\pi)$. Putting $L=L_0\cot(\theta/2)$ we obtain the statement. Q.E.D.

We remark that both the Dirichlet condition $\varphi(l)=\varphi(-l)=0$ and the Neumann condition $\varphi'(l)=\varphi'(-l)=0$ are of the type (17).

If we now introduce the space of distinct spectra, $\Sigma := \{\mathrm{Spec}(H_U) \,|\, U\in \mathrm{U}(2)\}$, then from the foregoing argument we find that Σ is a subspace of the torus $T^2=S^1\times S^1=\{(\theta_+,\theta_-)\}$ subject to the identification $(\theta_+,\theta_-)\equiv(\theta_-,\theta_+)$. The quotient space obtained by the identification is the orbifold $T^2/\mathbb{Z}_2$, which is the domain of the triangle shown in Fig. 1. The elementary observation in Fig. 1 leads to

Theorem 2: *The spectral space Σ of point interactions is a subspace of the orbifold $T^2/\mathbb{Z}_2$ which is homeomorphic to a Möbius strip with boundary. In particular, for the box $[l,-l]$ the spectral space Σ is the entire $T^2/\mathbb{Z}_2$.*

Proof: The first half is already shown (see Fig. 1). To show the second half, we observe that for an isospectral subfamily $\Omega(D)$ the spectrum is determined by the boundary condition (3) for $U=D$, which splits into

$$\varphi(0_+)+L_+\varphi'(0_+)=0, \quad \varphi(0_-)-L_-\,\varphi'(0_-)=0, \tag{20}$$

where we have used

$$L_\pm := L_0 \cot\frac{\theta_\pm}{2}. \tag{21}$$

Then for the box $[l,-l]$ the problem boils down to determining the spectrum of the operator in two separate boxes, $[-l,0_-)$ and $(0_+,l]$, under the combined boundary conditions, (17) and (20). For the interval $(0_+,l]$, for instance, the positive spectrum $E=\hbar^2k^2/(2m)$ is determined by the condition, $\tan kl = k(L-L_+)/(1+k^2LL_+)$, which admits a distinct set of solutions for different L_+ under fixed L. It thus follows that to each pair (L_+,L_-) or (θ_+,θ_-) modulo the exchange $\theta_+\leftrightarrow\theta_-$ there arises a distinct spectrum. Q.E.D.

We have seen that the product form (10) for the matrix U furnishes a useful parametrization for the point interaction in one dimension, where the spectral property resides solely in the diagonal part D. The adjoint part V, on the other hand, may be used to provide a parity transformation pertinent to the point interaction as follows.

Proposition 2: To a point interaction specified by U there is a parity operator $\mathcal{P}$ of the form (7) whose action leaves U invariant. The operator $\mathcal{P}$ is unique (up to the sign) except when $U\in\Omega_{\mathrm{SD}}$ for which $\mathcal{P}$ is arbitrary.

Proof: Consider the su(2) element σ in (8) given by

$$\sigma=\sigma(V):=V^{-1}\sigma_3 V, \tag{22}$$

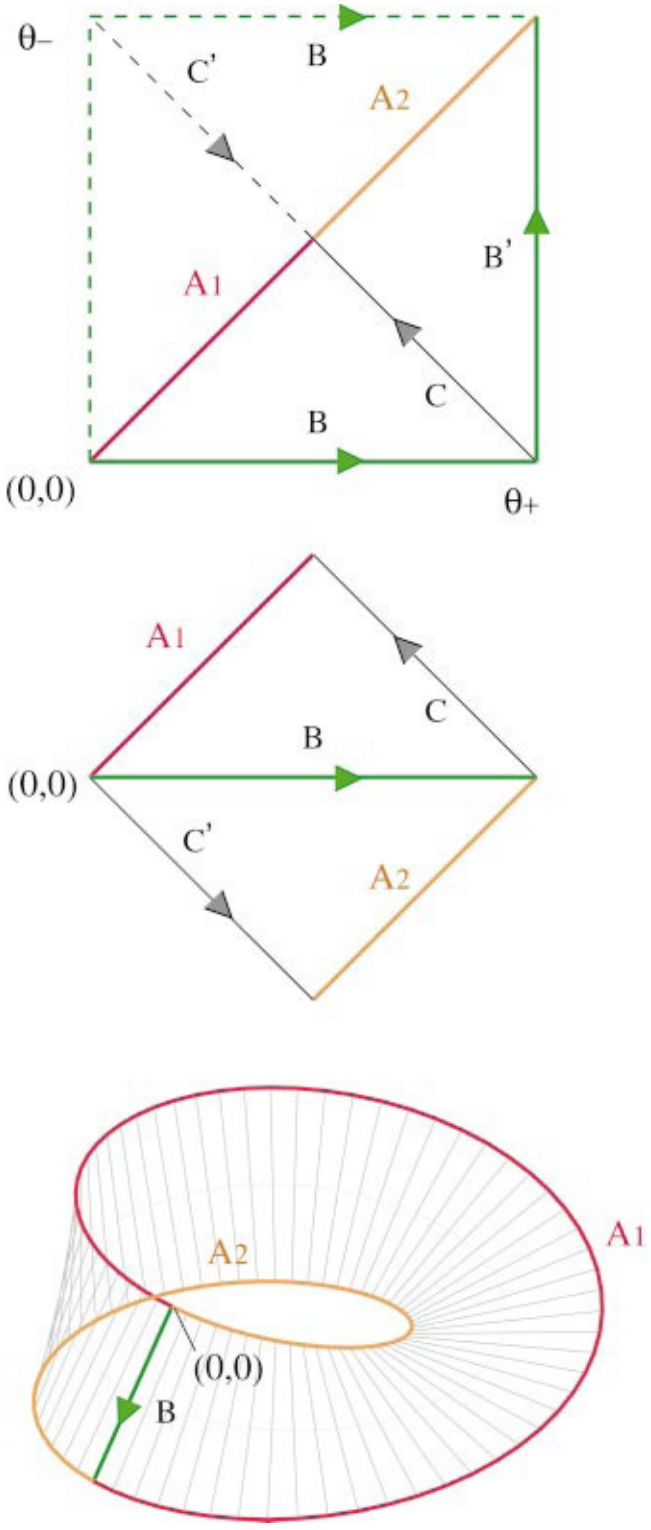

FIG. 1. (Color.) At the top, the spectral space Σ is the triangle surrounded by edges A_1+A_2, B and B'. We divide this triangle into two subtriangles $B-C-A_1$ and $B'-C-A_2$. Since the latter subtriangle is spectrally identical to its dual image $B-C'-A_2$, Σ can be represented by the square $A_1-C'-A_2-C$ in the middle figure. When the two spectrally identical edges C and C' are stitched together with the right orientation, we obtain the Möbius strip with boundary A_1-A_2 representing the self-dual subfamily Ω_{SD} (the bottom figure).

where V is the SU(2) matrix appearing in (10) for the the diagonalization of the matrix $U \notin \Omega_{\mathrm{SD}}$. Note that in (10) the matrix V is determined only up to the left action $e^{i\chi\sigma_3}V$, but this ambiguity does not affect in specifying σ in (22). We now expand $\sigma(V)$ in the su(2) basis as $\sigma(V) = \Sigma_{j=1}^{3} c_j(V)\,\sigma_j$ and define the corresponding parity operator,

$$\mathcal{P}(V) := \sum_{j=1}^{3} c_j(V)\,\mathcal{P}_j\,. \tag{23}$$

We then see at once that, under the transformation induced by $\mathcal{P}(V)$, the matrix U is left invariant, $\sigma(V)\,U\,\sigma(V) = U$. The parity $-\mathcal{P}(V)$ corresponding to $-\sigma(V)$ also leaves U invariant. For $U \in \Omega_{\mathrm{SD}}$, it is obvious that any σ, and hence any $\mathcal{P}$ in (7) leaves U invariant. Q.E.D.

The content of Proposition 2 may equally be stated as

Proposition 2′: The Schrödinger operator H_U commutes with a parity operator $\mathcal{P}$ given by (7), $[H_U, \mathcal{P}] = 0$, where for $U \notin \Omega_{\mathrm{SD}}$ the operator $\mathcal{P}$ is uniquely determined as $\mathcal{P} = \mathcal{P}(V)$ (up to sign) in (23), while for $U \in \Omega_{\mathrm{SD}}$ it is arbitrary.

We note that, for an H_U and the parity operator $\mathcal{P}$ commuting with it, the Hilbert space $\mathcal{H}$ can be decomposed into two orthogonal closed linear subspaces, $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$, where $\mathcal{H}_+$ and $\mathcal{H}_-$ are the eigenspaces of $\mathcal{P}$ corresponding to the eigenvalues 1 and -1, respectively. The nondegenerate eigenfunctions of H_U belong to either $\mathcal{H}_+$ or $\mathcal{H}_-$. For doubly degenerate eigenvalues, the eigenfunctions can be chosen such that one belongs to $\mathcal{H}_+$ and the other to $\mathcal{H}_-$. Note that, since the eigenvalue equation is a second-order differential equation on both half lines, the eigenvalues of H_U are at most doubly degenerate. Namely, these degenerate solutions contain two free constants each, and the boundary condition (3) reduces this four-parameter freedom to a two-parameter one. These statements are valid for the non-normalizable eigenfunctions (scattering states) of H_U, too, in the rigged Hilbert space sense [note that the definition (5), and correspondingly the definition of $\mathcal{P}(V)$, can be extended to any $\mathbb{R}\backslash\{0\} \to \mathbb{C}$ function in a natural way, which involves the natural extension of $\mathcal{H}_+$ and $\mathcal{H}_-$].

A distinguished family of generalized symmetries which interchange the subspaces $\mathcal{H}_+$ and $\mathcal{H}_-$ exist, that is,

Proposition 3: For an H_U and the associated parity operator $\mathcal{P}$ commuting with it, there exists a U(1) *family of generalized symmetries $\mathcal{D}$ such that each $\mathcal{D}$ maps $\mathcal{H}_+$ to $\mathcal{H}_-$ and vice versa, and satisfies $(U_{\mathcal{D}})_{\mathcal{D}} = U$.*

Proof: Consider the generalized symmetries $\mathcal{D}$ corresponding to the U(1) family of su(2) elements,

$$\sigma_{\mathcal{D}} := V^{-1}\,\tilde{\sigma}(\phi)\,V, \tag{24}$$

where we have defined $\tilde{\sigma}(\phi) = \cos\phi\,\sigma_1 + \sin\phi\,\sigma_2$ for $\phi \in [0, 2\pi)$, and introduced $\mathcal{D} := \Sigma_{j=1}^{3} c_j' \mathcal{P}_j$ using the expansion $\sigma_{\mathcal{D}} = \Sigma_{j=1}^{3} c_j' \sigma_j$ of $\sigma_{\mathcal{D}}$. On $U = V^{-1} D(\theta_+, \theta_-)\,V$ these $\mathcal{D}$ induce

$$U \mapsto U_{\mathcal{D}} = \sigma_{\mathcal{D}}\,U\,\sigma_{\mathcal{D}} = V^{-1}\,\tilde{\sigma}(\phi)\,D(\theta_+, \theta_-)\,\tilde{\sigma}(\phi)V = V^{-1} D(\theta_-, \theta_+)V, \tag{25}$$

and hence implement the interchange $\theta_+ \leftrightarrow \theta_-$. From this $(U_{\mathcal{D}})_{\mathcal{D}} = U$ is clear. To prove that a $\mathcal{D}$ maps any eigenfunction of $\mathcal{P}$ to another one with opposite eigenvalue, we show that $\{\mathcal{P}, \mathcal{D}\} = 0$. Indeed, from $\{\mathcal{P}_j, \mathcal{P}_k\} = \mathrm{Tr}(\sigma_j \sigma_k)\mathrm{id}_{\mathcal{H}}$ and (23) it follows that

$$\{\mathcal{P}, \mathcal{D}\} = \mathrm{Tr}\left(\sum_{j=1}^{3} c_j \sigma_j \sum_{k=1}^{3} c_k' \sigma_k \right) \mathrm{id}_{\mathcal{H}} = \mathrm{Tr}(\sigma \sigma_{\mathcal{D}})\mathrm{id}_{\mathcal{H}} = \mathrm{Tr}(\sigma_3 \tilde{\sigma}(\phi))\mathrm{id}_{\mathcal{H}} = 0. \tag{26}$$

Q.E.D.

Hence, in the light of these properties, $\mathcal{D}$ may be called *duality transformation*. The duality found in Refs. 7 and 10 is a special case of $\mathcal{D}$.

The role of the point interaction and the parity operator in Proposition 2 can be reversed to obtain

Proposition 4: To a parity operator $\mathcal{P}$ given in (7) there is a subfamily of point interactions which are left invariant under $\mathcal{P}$. For any $\mathcal{P}$ the subfamily $\Omega_{\mathcal{P}}$ is homeomorphic to a torus T^2.

Proof: The subfamily $\Omega_{\mathcal{P}}$ is given by

$$\Omega_{\mathcal{P}} := \{\, U \in \mathrm{U}(2) \,|\, \sigma U \sigma = U \,\}, \tag{27}$$

where σ is determined from $\mathcal{P}$ by (8). The matrices U belonging to $\Omega_{\mathcal{P}}$ are then found to be of the form,

$$U = e^{i\xi} e^{i\rho\sigma}, \quad \xi \in [0,\pi), \quad \rho \in [0,2\pi), \tag{28}$$

which is homeomorphic to a torus T^2 for any $\mathcal{P}$. Q.E.D.

For instance, if we choose $\mathcal{P}=\mathcal{P}_1$, the subfamily $\Omega_{\mathcal{P}_1}$ is just the set of parity invariant (left–right symmetric) point interactions in the usual sense of the word. If, on the other hand, we choose $\mathcal{P}=\mathcal{P}_3$, then the resultant subfamily $\Omega_{\mathcal{P}_3}$ becomes the so-called separated subfamily where no probability flow through the gap $x=0$ is allowed. One may also choose for $\mathcal{P}$ the one $\mathcal{P}(V)$ that corresponds to a specific U. The invariant subfamily $\Omega_{\mathcal{P}(V)}$ then contains U by construction, and becomes a subfamily pertinent to the point interaction characterized by U. One then finds from Propositions 3 and 4 that $\Omega_{\mathcal{P}(V)} \simeq T^2$ except when $U \in \Omega_{\mathrm{SD}}$ for which $\Omega_{\mathcal{P}(V)}$ coincides with the entire family $\Omega \simeq \mathrm{U}(2)$.[13]

The self-dual subfamily Ω_{SD} has also the following distinguished characteristics:

Proposition 5: For any point interaction belonging to Ω_{SD} (i.e., $U \in \Omega_{\mathrm{SD}}$), *all eigenvalues of H_U (including the generalized ones) are doubly degenerate.*

Proof: For any $U \in \Omega_{\mathrm{SD}}$, we have from Proposition 2′ that $[H_U, \mathcal{P}_j]=0$ for $j=1, 2, 3$. This implies that, on any eigenspace of H_U, a representation of su(2) formed by $\{\mathcal{P}_j\}_{j=1,2,3}$ is given. Since an eigenfunction of, say, $\mathcal{P}_1$ cannot be an eigenfunction of $\mathcal{P}_2$, the eigenspaces of H_U must be doubly degenerate. This argument is valid for the generalized eigenvalues (scattering state energies) and the corresponding eigenspaces as well. Q.E.D.

The double degeneracy implies that the system with point interaction belonging to Ω_{SD} may be regarded as supersymmetric. As shown in Ref. 10, this is in fact the case for $U=-I$, where the energy of the two bound states vanishes yielding an $N=2$ Witten model with a "good SUSY."[14] Generically, however, the ground state energy of the system is nonvanishing and the system is not supersymmetric even though it admits a formally supersymmetric reformulation for any U of Ω_{SD}. The obstacle for being supersymmetric is the fact that the presumed supercharges are not self-adjoint unless $U=-I$.

We have learned that the spectrum of the operator H_U is determined by the two parameters in D in the decomposition $U=V^{-1}DV$, and that, in particular, for the box the space Σ of the spectra is given by a Möbius strip. One can proceed further and assign more general physical meaning to the parameters in the matrix U. To see this we first rewrite the boundary condition (3) using the decomposition as

$$V\Phi + \begin{pmatrix} L_+ & 0 \\ 0 & L_- \end{pmatrix} V\Phi' = 0, \tag{29}$$

with $L_\pm$ given in (21). We further parametrize V by the Euler angles (with the first factor $e^{i\chi\sigma_3}$ which does not affect U being dropped),

$$V = e^{i(\mu/2)\sigma_2} e^{i(\nu/2)\sigma_3}, \quad \mu \in [0,\pi], \quad \nu \in [0,2\pi), \tag{30}$$

and thereby present

$$\{(L_+, L_-, \mu, \nu) \,|\, L_\pm \in (-\infty,\infty) \cup \{\infty\},\ \mu \in [0,\pi],\ \nu \in [0,2\pi)\}, \tag{31}$$

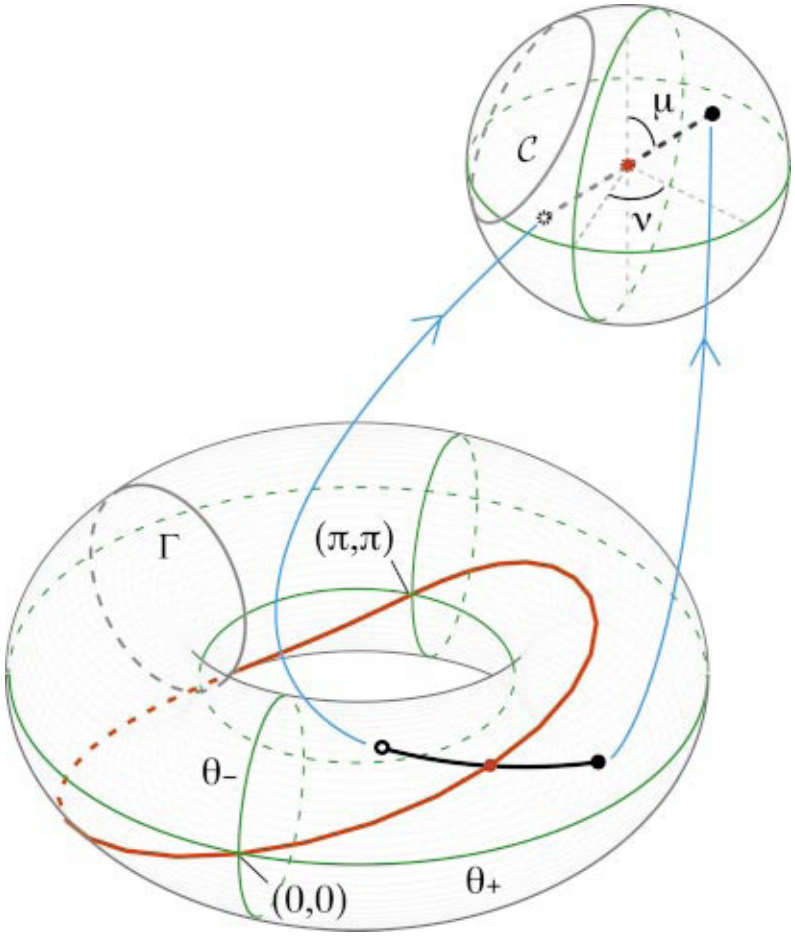

FIG. 2. (Color.) The parameter space $\{(\theta_+,\theta_-,\mu,\nu)\}$ is a product of the spectral torus T^2 specified by the angles (θ_+,θ_-) and the isospectral sphere S^2 specified by the angles (μ,ν) with radius $\rho=(\theta_+-\theta_-)/2$ (cf. Corollary 1) which collapses to a point for the self-dual case $\theta_+=\theta_-$. A cyclic path $\mathcal{C}$ on the sphere yields a phase anholonomy (the Berry phase) proportional to the area enclosed by $\mathcal{C}$ due to the degeneracy present at the center of the sphere. A cyclic path Γ on the torus, on the other hand, yields a level anholonomy (level shifts) if Γ is homotopically nontrivial. A generic cycle is a combination of the two, and hence yields an anholonomy in both phase and level. The parametrization shown here provides a double covering of the entire family $\Omega\simeq\mathrm{U}(2)$, where the two antipodal points on the spheres equidistant from the self-dual line $\theta_+=\theta_-$ are identified. This identification determines the spectral space Σ to be given by $T^2/\mathbb{Z}_2$ which is a Möbius strip with boundary.

as a basic set for the parametrization of the point interactions on a line. On account of the double specification of the eigenvalues of U, the set (31) is in a two-to-one correspondence to U, providing a double covering[15] of the whole family $\Omega\simeq\mathrm{U}(2)$ (see Fig. 2). We then have

Theorem 3: *The parameters in the set* (31) *possess the following physical properties:*

(i) The two parameters $L_\pm$ furnish two independent length scales to the point interaction.

(ii) The angle ν is physically irrelevant (unobservable).

(iii) The angle μ measures the extent of mixture of states between the positive and negative half lines.

Proof: (i) is evident because in the boundary condition (29) $L_\pm$ are the only parameters with length dimension. To show (ii), we observe from (30) and (29) that the angle ν can be absorbed by introducing the new vectors $e^{i\nu\sigma_3/2}\Phi$ and $e^{i\nu\sigma_3/2}\Phi'$ which arise if we replace $\varphi(0_\pm)\mapsto e^{\pm i\nu/2}\varphi(0_\pm)$ and $\varphi'(0_\pm)\mapsto e^{\pm i\nu/2}\varphi'(0_\pm)$. This is implemented by the U(1) phase transformation (gauge transformation) on the state,

$$\varphi(x)\mapsto e^{(i/\hbar)\,\vartheta(x)}\varphi(x),\quad \vartheta(x):=\frac{\nu}{2}[\Theta(x)-\Theta(-x)]\hbar. \tag{32}$$

Since the phase shift $\vartheta(x)$ is constant over $\mathbb{R}\backslash\{0\}$, and since the phase gap (which occurs at the missing point $x=0$) cannot be observed on a line,[16] the transformed state is equivalent to the original state in quantum theory, that is, the angle ν is irrelevant physically. Finally, (iii) is also evident in the boundary condition (29) because the factor $e^{i(\mu/2)\,\sigma_2}$ mixes the two rows of the boundary vectors by rotation according to the angle μ. Q.E.D.

An important point to be noted here is that the existence of the one-parameter gauge equivalence within Ω implies that point interactions which are distinct physically—not just on the spectral basis—form a three-parameter quotient space of Ω.

The properties stated in Theorem 3 can be seen explicitly in the solutions of the Schrödinger equation under the operator H_U being the Hamiltonian. For instance, the bound states allowed under H_U on the line are given by

$$\varphi_\kappa(x)=\begin{cases} A_\kappa^- e^{\kappa x}, & x<0 \\ B_\kappa^+ e^{-\kappa x}, & x>0 \end{cases}, \tag{33}$$

where κ determines the bound state energy $E_{\text{bound}}=-\hbar^2\kappa^2/(2m)$, and the constants A_κ^- and B_κ^+ are subject to the normalization condition $|A_\kappa^-|^2+|B_\kappa^+|^2=2\kappa$. A nonvanishing solution is then ensured if

$$\kappa=\frac{1}{L_+}\quad\text{or}\quad\kappa=\frac{1}{L_-}, \tag{34}$$

which shows that there exist two bound states if $L_+>0$ and $L_->0$, and one if $L_+L_-<0$, and none if $L_+<0$ and $L_-<0$. The parameters $L_\pm$ thus give (in case they are positive) the scales of the trapped particle. In terms of (30) the coefficients are found to be

$$\begin{pmatrix} B_\kappa^+ \\ A_\kappa^- \end{pmatrix}=\sqrt{\frac{2}{L_+}}\begin{pmatrix} e^{-2i\nu}\cos\dfrac{\mu}{2} \\ \sin\dfrac{\mu}{2} \end{pmatrix},\quad \begin{pmatrix} B_\kappa^+ \\ A_\kappa^- \end{pmatrix}=\sqrt{\frac{2}{L_-}}\begin{pmatrix} -e^{-2i\nu}\sin\dfrac{\mu}{2} \\ \cos\dfrac{\mu}{2} \end{pmatrix}, \tag{35}$$

for $\kappa=1/L_+$ and $1/L_-$, respectively. Note that the relative phase factor $e^{-2i\nu}$ attached to the coefficients of the states on the positive half line can be removed by (32). Similarly, the scattering states for the particle (with velocity $v=\hbar k/m$) incident, say, from the positive side,

$$\varphi_k^{(+)}(x)=\frac{1}{\sqrt{2\pi}}\begin{cases} t_k^{(+)}e^{-ikx}, & x<0 \\ e^{-ikx}+r_k^{(+)}e^{ikx}, & x>0 \end{cases}, \tag{36}$$

have the reflection and transmission coefficients

$$\begin{pmatrix} r_k^{(+)} \\ t_k^{(+)} \end{pmatrix}=-\frac{1}{(1+ikL_+)(1+ikL_-)}\begin{pmatrix} 1+k^2L_+L_--ik(L_+-L_-)\cos\mu \\ -ik(L_+-L_-)\sin\mu\, e^{i\nu} \end{pmatrix}. \tag{37}$$

We observe that, in accordance with the interpretation, the factor $e^{i\nu}$ is simply the phase which is acquired by the transmitted wave when the incoming wave passes the point $x=0$. We can also see that, unlike ν, each of the other three parameters plays an independent and physical role in the eigenstates of H_U.

Finally, let us illustrate the basic structure of the U(2) family by considering a generic point interaction specified by U in the U(2) parameter space which is shown in Fig. 2 as a product of a torus representing (θ_+,θ_-) and a sphere with radius ρ [see (13) and Corollary 1] representing

(μ,ν). On this torus, two point interactions connected by the duality transformation (25) are represented by two equidistant points from the self-dual loop, $\theta_+=\theta_-$. The double covering of the parametrization implies that the two spheres attached to these dual points are actually the same, with antipodal points on the two spheres identified. Under a cyclic process on the sphere one can expect a phase anholonomy (the Berry phase) to arise, since the spectrum becomes degenerated at the center $\theta_+=\theta_-$ which belongs to Ω_{SD} (see Proposition 5). One can also expect a level shift if the cycle is homotopically nontrivial on the torus (see, e.g., Ref. 17). The anholonomy both in phase and level has indeed been observed[10] for cycles passing through $U=\sigma_3$, that is, $(\theta_+,\theta_-)=(\pi,0)$ and $(\mu,\nu)=(0,0)$. We note that this point $U=\sigma_3$ is rather special because it has the invariant parity $\mathcal{P}(V=I)=\mathcal{P}_3$ and hence its invariant subfamily is just the separated subfamily $\Omega_{\mathcal{P}_3}$. Further, its isospectral subfamily $\Omega(D=\sigma_3)$ is (the continuous part of) the scale invariant subfamily Ω_W (Ref. 5) in view of the fact[10] that such U satisfies the condition for scale invariance, $\det(U\pm I)=\det(\sigma_3\pm I)=0$. We stress, however, that the anholonomy in phase and/or level is a generic phenomenon observed for any cyclic process in the parameter space $\Omega\simeq\mathrm{U}(2)$.

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Asymptotics for the condensate multivortex solutions in the self-dual Chern–Simons CP(1) model

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In this paper we study the asymptotics for the condensate multivortex solutions in the self-dual Chern–Simons CP(1) model. When the breaking parameter s belongs to $(-\frac{1}{2},\frac{1}{2})$, we show that for any sequence of multivortex solutions which lies between suitable super- and subsolutions with respect to the Chern–Simons coupling constant κ, we can find a subsequence which converges to a constant depending only on s as κ goes to zero. Also we investigate the locally uniform convergence speed. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1409962]

I. INTRODUCTION

The CP(1) model which is equivalent to the $O(3)$ sigma model is a basic model in field theory. Though this model is useful as a toy model for the instantons in non-Abelian Yang–Mills theories, it is scale invariant and yields instantons of arbitrary size. This makes the model unsuitable as a model for real particles and there have been many attempts to break the scale invariance. Among them, one of the most elegant ways is to introduce a gauge field which incorporates the kinetic term. Gauging a theory is useful to obtain the finite energy solitons. Schroers[1] proposed a gauged model by introducing a U(1) gauge field whose dynamics is governed by a Maxwell term. On the other hand, Ghosh and Ghosh[2] proposed a gauged $O(3)$ sigma model with the gauge field dynamics governed solely by a Chern–Simons term. In Ref. 3 the authors generalized the gauged CP(1) case to the gauged CP(N) models with the kinetic term governed by a Chern–Simons term. These models yield to a Bogomol'nyi limit or self-dual equations which are easy to analyze mathematically compared to full second-order Euler–Lagrange equation. We note that the Bogomol'nyi limit in superconductivity plays an important role as it permits one to distinguish between the type of superconductors.[4]

In this paper, we consider the Chern–Simons CP(1) model where the gauge field dynamics is solely governed by the Chern–Simons term. Multiple existence of solutions is already studied in our previous paper[5] and we will concentrate on the asymptotics for the solutions.

The organization of this paper is as follows. In Sec. II, we briefly introduce the Chern–Simons CP(1) model, formulate its mathematical settings, and recall previous results. In Sec. III, we study the asymptotics for multivortex solutions with the breaking parameter s belonging to $(-\frac{1}{2},\frac{1}{2})$. We show that for any sequence of multivortex solutions which lies between suitable super- and subsolutions with respect to the Chern–Simons coupling constant κ constructed in Ref. 5, we can find a subsequence which converges to a constant depending only on s as κ goes to zero. Also we study the locally uniform convergence speed.

We remark that Tarantello[6] studied the asymptotic behavior of solutions of the Chern–Simons–Higgs model in a doubly periodic domain. Han[7] applied the arguments in Ref. 8 to the above-mentioned model and obtained some interior estimates. Their studies were the main motivation for our work here.

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II. THE CHERN–SIMONS CP(1) MODEL

In this section we briefly introduce the Chern–Simons CP(1) model. After reducing the self-dual equations to semilinear elliptic partial differential equations, we recall the corresponding existence theorem (see Ref. 5).

The CP(1) model consists of two complex scalar fields z_1, z_2 in $\mathbb{R}^2$. Denoting $\mathbf{z}=(z_1,z_2)$, the model requires that $|\mathbf{z}|^2=z_1\overline{z_1}+z_2\overline{z_2}=1$ and $\mathbf{z}$ is equivalent to the overall phase rotations.

The Lagrangian for the self-dual Chern–Simons CP(1) model is

$$\mathcal{L}=\frac{\kappa}{2}\epsilon^{\mu\nu\rho}A_\mu\partial_\nu A_\rho+|\nabla_\mu\mathbf{z}|^2-V(\mathbf{z}),$$

where $\epsilon^{\mu\nu\rho}$ is the totally skew-symmetric tensor with $\epsilon^{012}=1$, $R=\mathrm{diag}(\frac{1}{2},-\frac{1}{2})$, $A_\mu R$ is the matrix valued gauge field, $V(\mathbf{z})$ is a potential term which will be fixed later, and the "covariant derivatives" ∇_μ and D_μ are defined as follows:

$$\nabla_\mu\mathbf{z}=D_\mu\mathbf{z}-(\overline{\mathbf{z}}D_\mu\mathbf{z})\mathbf{z},\quad D_\mu\mathbf{z}=\partial_\mu\mathbf{z}-iA_\mu R\mathbf{z}.$$

The Gauss law constraint obtained from the variation of A_0 is given by

$$\kappa F_{12}=i\{\nabla_0\overline{\mathbf{z}}[R\mathbf{z}-\mathbf{z}(\overline{\mathbf{z}}R\mathbf{z})]-\overline{\nabla_0\overline{\mathbf{z}}[R\mathbf{z}-\mathbf{z}(\overline{\mathbf{z}}R\mathbf{z})]}\},\tag{1}$$

where $F_{12}=\partial_1A_2-\partial_2A_1$. The theory possesses the following conserved topological current:

$$K^\mu=-i\epsilon^{\mu\nu\rho}\partial_\nu(\overline{\mathbf{z}}D_\rho\mathbf{z})$$

and a conserved global $U(1)$ current for the generator R,

$$J^\mu=i\{\nabla^\mu\overline{\mathbf{z}}[R\mathbf{z}-\mathbf{z}(\overline{\mathbf{z}}R\mathbf{z})]-\overline{\nabla^\mu\overline{\mathbf{z}}[R\mathbf{z}-\mathbf{z}(\overline{\mathbf{z}}R\mathbf{z})]}\}.$$

If we choose the potential as given by

$$V(\mathbf{z})=\frac{1}{\kappa^2}|[R\mathbf{z}-\mathbf{z}(\overline{\mathbf{z}}R\mathbf{z})](\overline{\mathbf{z}}R\mathbf{z})-s[R\mathbf{z}-\mathbf{z}(\overline{\mathbf{z}}R\mathbf{z})]|^2,$$

where s is a free real parameter, then we can find that the field configurations saturating the energy bound satisfy the Gauss law constraint (1) and the self-dual equations,

$$(\nabla_1\pm i\nabla_2)\mathbf{z}=0,$$

$$\nabla_0\mathbf{z}\pm\frac{i}{\kappa}\{[R\mathbf{z}-\mathbf{z}(\overline{\mathbf{z}}R\mathbf{z})](\overline{\mathbf{z}}R\mathbf{z})-s[R\mathbf{z}-\mathbf{z}(\overline{\mathbf{z}}R\mathbf{z})]\}=0.$$

Indeed, the energy functional E can be expressed as follows:

$$\begin{aligned}E&=\int \mathrm{d}^2x\{|\nabla_0\mathbf{z}|^2+|\nabla_1\mathbf{z}|^2+|\nabla_2\mathbf{z}|^2+V(\mathbf{z})\}\\&=\int \mathrm{d}^2x\{|(\nabla_1\pm i\nabla_2)\mathbf{z}|^2+|\nabla_0\mathbf{z}\pm\frac{i}{\kappa}\{[R\mathbf{z}-\mathbf{z}(\overline{\mathbf{z}}R\mathbf{z})]\\&\quad\times(\overline{\mathbf{z}}R\mathbf{z})-s[R\mathbf{z}-\mathbf{z}(\overline{\mathbf{z}}R\mathbf{z})]\}|^2\}\pm\int \mathrm{d}^2x\left(K_0+\frac{s}{\kappa}J_0\right)\\&\geqslant\pm\int \mathrm{d}^2x\left(K_0+\frac{s}{\kappa}J_0\right)\equiv T,\end{aligned}$$

and we will compute the generalized topological charge T later.

By elementary computations, from the above-mentioned self-dual equations, we obtain that, away from the zeroes of z_1 and z_2, there hold

$$\begin{cases} z_2\overline{\partial}z_1 - z_1\overline{\partial}z_2 = iz_1z_2(A_1+iA_2), \\ F_{12} = \mp\dfrac{\lambda}{2}|z_1|^2|z_2|^2(|z_1|^2-|z_2|^2-2s), \end{cases} \tag{2}$$

where $\overline{\partial}=(\partial_1+i\partial_2)/2$ and $\lambda=2/\kappa^2$.

We choose the upper signs and consider a doubly periodic boundary conditions due to 't Hooft.[9] First we note that the Lagrangian $\mathcal{L}$ is invariant under the following gauge transformations:

$$\mathbf{z}(x)\mapsto e^{i\theta(x)}\mathbf{z}(x), \quad A_0(x)\mapsto A_0(x), \quad A_j(x)\mapsto A_j(x)+\partial_j\theta(x),$$

where θ is a real-valued function and $j=1,2$. We set the doubly periodic region Ω by

$$\Omega=\{x=(x_1,x_2)\in\mathbb{R}^2 | x=t_1a^1+t_2a^2, 0<t_1,t_2<1\},$$

where a^1 and a^2 are linearly independent vectors in $\mathbb{R}^2$, and define $\Gamma^k=\{x\in\mathbb{R}^2|x=t_ka^k, 0<t_k<1\}$ for $k=1,2$. Then the boundary $\partial\Omega$ can be written as

$$\partial\Omega=\Gamma^1\cup\Gamma^2\cup\{a^1+\Gamma^2\}\cup\{a^2+\Gamma^1\}\cup\{O,a^1,a^2,a^1+a^2\}.$$

Here we impose the following doubly periodic boundary condition:

$$\exp(i\theta_k(x+a^k))\mathbf{z}(x+a^k)=\exp(i\theta_k(x))\mathbf{z}(x),$$

$$A_0(x+a^k)=A_0(x),$$

$$(A_j+\partial_j\theta_k)(x+a^k)=(A_j+\partial_j\theta_k)(x),$$

where $x\in\Gamma^1\cup\Gamma^2-\Gamma^k$ for $k=1,2$ and θ_1,θ_2 are real-valued smooth functions defined in a neighborhood of $\Gamma^2\cup\{a^1+\Gamma^2\}$, $\Gamma^1\cup\{a^2+\Gamma^1\}$, respectively.

If we denote by q_k's the zeroes of z_1 for $k=1,\ldots,m$ and p_l's the zeroes of z_2 for $l=1,\ldots,n$ counted with multiplicity, then we can calculate the magnetic flux Φ and the energy E as follows:

$$\Phi=\int_\Omega F_{12}\,dx=\int_{\partial\Omega}A_j\,dx^j=-\int_{\partial\Omega}\partial_j\theta_k\,dx^j=2\pi(m-n),$$

$$E=T=\int_\Omega K_0+\frac{s}{\kappa}J_0=\int_\Omega\partial_2(A_1R\mathbf{z})-\partial_1(A_2R\mathbf{z})+sF_{12}=2\pi((m+n)+s(m-n)).$$

On the other hand, setting $u=\ln|z_1/z_2|^2$ and following the argument of Taubes,[10] we reduce the self-dual equations (2) to

$$\Delta u=(1-2s)\lambda\frac{e^u}{(1+e^u)^3}\left(e^u-\frac{1+2s}{1-2s}\right)+4\pi\sum_{k=1}^{m}\delta_{q_k}-4\pi\sum_{l=1}^{n}\delta_{p_l} \quad \text{in } \Omega. \tag{3}$$

Conversely, if u is given, then we can recover $(\mathbf{z},A)$ using the relations

$$\frac{z_1}{z_2}=e^{u/2+i\Theta}, \quad \frac{A_1+iA_2}{2}=-i\partial\ln\frac{z_1}{z_2},$$

where $\Theta=\Sigma_{k=1}^m\arg(z-q_k)-\Sigma_{l=1}^n\arg(z-p_l)$.

It is convenient to introduce a reference function w as the unique solution of

$$\Delta w = -\frac{4\pi(m-n)}{|\Omega|} + 4\pi\sum_{k=1}^{m}\delta_{q_k} - 4\pi\sum_{l=1}^{n}\delta_{p_l}, \quad \int_\Omega w = 0. \tag{4}$$

Setting $u_\lambda = w + v_\lambda$, from (3) we have

$$\Delta v_\lambda = (1-2s)\lambda\frac{e^{w+v_\lambda}}{(1+e^{w+v_\lambda})^3}\left(e^{w+v_\lambda} - \frac{1+2s}{1-2s}\right) + \frac{4\pi(m-n)}{|\Omega|} \tag{5}$$

and the constraint obtained by integrating over Ω,

$$(1-2s)\lambda\int_\Omega \frac{e^{w+v_\lambda}}{(1+e^{w+v_\lambda})^3}\left(e^{w+v_\lambda} - \frac{1+2s}{1-2s}\right) = -4\pi(m-n).$$

Furthermore we can derive the associated functional I_λ as

$$I_\lambda(v) = \frac{1}{2}\|\nabla v\|_{L^2}^2 + \lambda\int_\Omega \frac{s-(2-s)e^{w+v}}{(1+e^{w+v})^2} + \frac{4\pi(m-n)}{|\Omega|}\int_\Omega v. \tag{6}$$

Let ϵ be a sufficiently small positive number so that the $(m+n)$ balls with center p_l's or q_k's of radius 2ϵ are mutually disjoint and $8\pi(m+n)\epsilon^2 < |\Omega|$. We define a smooth function g^+ with $-1 \leqslant g^+ \leqslant 0$ by

$$g^+(x) = \begin{cases} -1, & x \in \cup_{l=1}^n B(p_l, \epsilon) \\ 0, & x \in \Omega \setminus \cup_{l=1}^n B(p_l, 2\epsilon), \end{cases}$$

and let v^+ be a solution of

$$\Delta v^+ = \frac{4\pi m}{|\Omega|} + \frac{1}{\epsilon^2}g^+ - \frac{1}{\epsilon^2|\Omega|}\int_\Omega g^+ - 4\pi\sum_{k=1}^{m}\delta_{q_k}.$$

Since v^+ can be determined up to constant, we may assume that

$$w + v^+ \geqslant \ln\frac{2+\sqrt{4s^2+3}}{1-2s} \quad \text{in } \Omega.$$

Replacing -1, p_l, m with 1, q_k and n, respectively, in the definitions of g^+ and v^+, we obtain g^- and v^- analogously. Also we may assume that

$$w + v^- \leqslant \ln\frac{1+2s}{2+\sqrt{4s^2+3}} \quad \text{in } \Omega.$$

We note that v^+ and v^- are super- and subsolutions of (5), respectively. Finally we state the existence theorem.[5]

Theorem 1: *Let $-\frac{1}{2} < s < \frac{1}{2}$ and v^+ and v^- be defined as above. Then there exists λ_0 such that for all $\lambda \geqslant \lambda_0$, there exists a multivortex solution v_λ which is a local minimizer of I_λ and satisfies $v^- < v_\lambda < v^+$. Moreover, if $m \neq n$, then there exists another multivortex solution $\tilde{v}_\lambda$ which is a critical point of I_λ.*

III. ASYMPTOTICS

In this section, we will prove the following theorem:

Theorem 2: *Let $-\frac{1}{2} < s < \frac{1}{2}$ and v_λ be a solution which lies between v^- and v^+. Then for any $r_0 > 0$, there exists a constant $C = C(r_0)$ such that*

$$|v_\lambda(q_k)| \leqslant C\lambda^{r_0}, \quad |v_\lambda(p_l)| \leqslant C\lambda^{r_0}.$$

Moreover, there exists a subsequence $\{v_{\lambda_j}\}$ *such that* $u_{\lambda_j} = w + v_{\lambda_j}$ *satisfies*
(i) $(1-2s)\lambda_j e^{u_{\lambda_j}}(e^{u_{\lambda_j}} - (1+2s)/(1-2s))/(1+e^{u_{\lambda_j}})^3 \to -4\pi\Sigma_{k=1}^{m}\delta_{q_k} + 4\pi\Sigma_{l=1}^{n}\delta_{p_l}$ *in the sense of measure as* $\lambda_j \to \infty$,
(ii) $\|u_{\lambda_j} - \ln(1+2s)/(1-2s)\|_{W^{1,r}(\Omega)} \to 0$ *for* $1 < r < 2$ *as* $\lambda_j \to \infty$,
(iii) $\|u_{\lambda_j} - \ln(1+2s)/(1-2s)\|_{L^\infty(K)} \leqslant C(K)/\lambda_j$ *for* $K \subset\subset \Omega \setminus \cup_{l=1}^{n}\{p_l\} \cup_{k=1}^{m}\{q_k\}$.

The proof of the theorem consists of several lemmas and we begin by constructing upper and lower bounds. This lemma plays a key role.

Lemma 1: Let v_λ *be a solution of* (5) *which lies between* v^- *and* v^+. *For* $u_\lambda = w + v_\lambda$, *there exist* $\mathfrak{U}^-$, $\mathfrak{U}_\lambda^-$, $\mathfrak{U}^+$, $\mathfrak{U}_\lambda^+$ *such that* $\mathfrak{U}^-$ *and* $\mathfrak{U}^+$ *are independent of* λ *and the following inequalities hold for sufficiently large* λ:

$$\mathfrak{U}^- < \mathfrak{U}_\lambda^- < \ln\frac{1+2s}{1-2s} < \mathfrak{U}_\lambda^+ < \mathfrak{U}^+, \quad \mathfrak{U}_\lambda^- < u_\lambda < \mathfrak{U}_\lambda^+. \tag{7}$$

Moreover, $\mathfrak{U}_\lambda^-$ *and* $\mathfrak{U}_\lambda^+$ *satisfies*

$$\Delta\mathfrak{U}_\lambda^- = (1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{\mathfrak{U}_\lambda^-} - \frac{1+2s}{1-2s}\right) + 4\pi\sum_{k=1}^{m}\delta_{q_k} \quad \text{in } \Omega, \tag{8}$$

$$\Delta\mathfrak{U}_\lambda^+ = (1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{\mathfrak{U}_\lambda^+} - \frac{1+2s}{1-2s}\right) - 4\pi\sum_{l=1}^{n}\delta_{p_l} \quad \text{in } \Omega. \tag{9}$$

Proof: Let g be a smooth function with $0 \leqslant g \leqslant 1$ satisfying

$$g(x) = \begin{cases} 1, & x \in \cup_{l=1}^{n} B(p_l, \epsilon) \cup_{k=1}^{m} B(q_k, \epsilon) \\ 0, & x \in \Omega \setminus \cup_{l=1}^{n} B(p_l, 2\epsilon) \cup_{k=1}^{m} B(q_k, 2\epsilon). \end{cases}$$

We define $\mathfrak{U}^-$ as a solution of

$$\Delta\mathfrak{U}^- = -\frac{4\pi m}{|\Omega|} + 4\pi\sum_{k=1}^{m}\delta_{q_\lambda} + \frac{1}{\epsilon^2}g - \frac{1}{\epsilon^2|\Omega|}\int_\Omega g.$$

Since $\mathfrak{U}^-$ can be determined up to constant, we may assume that

$$\mathfrak{U}^- \leqslant \ln\frac{1+2s}{1-2s} - 1.$$

Similarly, we define $\mathfrak{U}^+ \geqslant \ln(1+2s)/(1-2s) + 1$ as a solution of

$$\Delta\mathfrak{U}^+ = \frac{4\pi n}{|\Omega|} - 4\pi\sum_{l=1}^{n}\delta_{p_l} - \frac{1}{\epsilon^2}g + \frac{1}{\epsilon^2|\Omega|}\int_\Omega g.$$

If $x \in \cup_{l=1}^{n} B(p_l, \epsilon) \cup_{k=1}^{m} B(q_k, \epsilon)$, then

$$\Delta\mathfrak{U}^- \geqslant -\frac{4\pi m}{|\Omega|}+4\pi\sum_{k=1}^{m}\delta_{q_k}+\frac{1}{\epsilon^2}-\frac{4\pi(m+n)}{|\Omega|}$$

$$\geqslant \frac{1}{\epsilon^2}-\frac{8\pi(m+n)}{|\Omega|}+4\pi\sum_{k=1}^{m}\delta_{q_k}$$

$$\geqslant (1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{\mathfrak{U}^-}-\frac{1+2s}{1-2s}\right)+4\pi\sum_{k=1}^{m}\delta_{q_k}.$$

We define two constants u_*^+, u_*^- which are independent of λ as

$$u_*^+\equiv\sup\{w+v^+|x\in\Omega\backslash\bigcup_{l=1}^{n}B(p_l,\epsilon)\}<\infty,$$

$$u_*^-\equiv\inf\{w+v^-|x\in\Omega\backslash\bigcup_{k=1}^{m}B(q_k,\epsilon)\}>-\infty.$$

If $x\in\Omega\backslash\cup_{l=1}^{n}B(p_l,\epsilon)\cup_{k=1}^{m}B(q_k,\epsilon)$, then

$$\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\geqslant c_*=\min\left\{\frac{e^{u_*^+}}{(1+e^{u_*^+})^3},\frac{e^{u_*^-}}{(1+e^{u_*^-})^3}\right\}>0$$

and

$$\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\geqslant\lambda c_*\to\infty \quad \text{as} \quad \lambda\to\infty.$$

Thus

$$\Delta\mathfrak{U}^- \geqslant -\frac{4\pi m}{|\Omega|}+4\pi\sum_{k=1}^{m}\delta_{q_k}-\frac{4\pi(m+n)}{|\Omega|}$$

$$\geqslant 4\pi\sum_{k=1}^{m}\delta_{q_k}-\frac{8\pi(m+n)}{|\Omega|}$$

$$\geqslant 4\pi\sum_{k=1}^{m}\delta_{q_k}-\frac{1}{\epsilon^2}$$

$$\geqslant (1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{\mathfrak{U}^-}-\frac{1+2s}{1-2s}\right)+4\pi\sum_{k=1}^{m}\delta_{q_k}$$

for $\lambda>e/(e-1)(1+2s)c_*\epsilon^2$. This shows that $\mathfrak{U}^-$ is a subsolution of (8) which is less than $\ln(1+2s)/(1-2s)$. Since $\ln(1+2s)/(1-2s)$ is a supersolution, the standard iteration method implies the existence of a solution $\mathfrak{U}_\lambda^-$ of (8).

Similarly, we can check that $\mathfrak{U}^+$ and $\ln(1+2s)/(1-2s)$ are super- and subsolutions of (9), respectively. Since $\ln(1+2s)/(1-2s)\leqslant\mathfrak{U}^+$, we obtain the existence of a solution $\mathfrak{U}_\lambda^+$ of (9). Finally, the maximum principle implies the desired inequality (7) and this completes the proof. Q.E.D.

Remark 1: Integrating (8) *over* Ω, *we obtain*

$$(1-2s)\int_\Omega\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{\mathfrak{U}_\lambda^-}-\frac{1+2s}{1-2s}\right)=-\frac{4\pi m}{\lambda}\to 0 \quad \text{as} \quad \lambda\to\infty.$$

Since $\mathfrak{U}^- < \mathfrak{U}_\lambda^- \leqslant \ln(1+2s)/(1-2s)$, *we can find a subsequence* $\{\lambda_j\}$ *such that*

$$\mathfrak{U}_{\lambda_j}^- \to \ln\frac{1+2s}{1-2s} \quad \text{a.e. as } \lambda_j \to \infty.$$

Similarly, we may assume that $\mathfrak{U}_{\lambda_j}^+ \to \ln(1+2s)/(1-2s)$ *almost everywhere as* $\lambda_j \to \infty$. *Then by lemma 1, we have*

$$u_{\lambda_j} \to \ln\frac{1+2s}{1-2s} \quad \text{a.e. as } \lambda_j \to \infty.$$

Lemma 2: Let v_λ *be as in Lemma 1. Then for any* $r_0 > 0$, *there exists a constant* $C = C(r_0)$ *such that*

$$\|v_\lambda\|_{L^\infty(\Omega)} \leqslant C\lambda^{r_0}.$$

In particular,

$$|v_\lambda(q_k)| \leqslant C\lambda^{r_0}, \quad |v_\lambda(p_l)| \leqslant C\lambda^{r_0}.$$

Proof: We may assume that $0 < r_0 < \frac{1}{2}$. Observing that the absolute value of the first term on the right-hand side of (5) is less than λ, if $r > 1$ then we have

$$\begin{aligned}
\|\Delta v_\lambda\|_{L^r(\Omega)}^r &= \int_\Omega \left| (1-2s)\lambda \frac{e^{w+v_\lambda}}{(1+e^{w+v_\lambda})^3}\left(e^{w+v_\lambda} - \frac{1+2s}{1-2s}\right) + \frac{4\pi(m-n)}{|\Omega|}\right|^r \\
&\leqslant 2^{r-1}\left[\lambda^{r-1}\int_\Omega (1-2s)\lambda \frac{e^{w+v_\lambda}}{(1+e^{w+v_\lambda})^3}\left| e^{w+v_\lambda} - \frac{1+2s}{1-2s}\right| + \left(\frac{4\pi|m-n|}{|\Omega|}\right)^r\right] \\
&\leqslant C\left[1 + \lambda^{r-1}\int_\Omega (1-2s)\lambda \frac{e^{w+v_\lambda}}{(1+e^{w+v_\lambda})^3}\left((e^{u_\lambda} - e^{\mathfrak{U}_\lambda^-}) + \left(\frac{1+2s}{1-2s} - e^{\mathfrak{U}_\lambda^-}\right)\right)\right] \\
&\leqslant C[1 + 4\pi(m+n)\lambda^{r-1}] \leqslant C\lambda^{r-1}.
\end{aligned}$$

We use the interpolation type inequality and Lemma 1 to obtain

$$\|v_\lambda\|_{L^\infty(\Omega)} \leqslant C\|v_\lambda\|_{L^1(\Omega)}^{(r-1)/(2r-1)}\|D^2 v_\lambda\|_{L^r(\Omega)}^{r/(2r-1)} \leqslant C\|\Delta v_\lambda\|_{L^r(\Omega)}^{r/(2r-1)} \leqslant C\lambda^{(r-1)/(2r-1)}.$$

Then for $r = (r_0-1)/(2r_0-1)$, we get the desired result. Q.E.D.

Modifying Tarantello's argument,[6] we have the following weak convergence results.

Lemma 3: Let $\{u_\lambda\}$ *be any sequence of solutions as in Lemma 1. Then there exists a subsequence* $\{\lambda_j\}$ *such that, as* $\lambda_j \to \infty$,
(i) $(1-2s)\lambda_j e^{u_{\lambda_j}}(e^{u_{\lambda_j}} - (1+2s)/(1-2s))/(1+e^{u_{\lambda_j}})^3 \to -4\pi\Sigma_{k=1}^m \delta_{q_k} + 4\pi\Sigma_{l=1}^n \delta_{p_l}$ *in the sense of measure,*
(ii) $u_{\lambda_j} \to \ln(1+2s)/(1-2s)$ *in* $W^{1,r}(\Omega)$, $1 < r < 2$.

Proof: We rewrite $u_\lambda - \ln(1+2s)/(1-2s)$ as a difference of two non-negative terms,

$$u_\lambda - \ln\frac{1+2s}{1-2s} = (u_\lambda - \mathfrak{U}_\lambda^-) - \left(\ln\frac{1+2s}{1-2s} - \mathfrak{U}_\lambda^-\right).$$

Subtracting (8) from (3), we have

$$\Delta(u_\lambda - \mathfrak{U}_\lambda^-) = (1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}(e^{u_\lambda} - e^{\mathfrak{U}_\lambda^-}) - 4\pi\sum_{l=1}^n \delta_{p_l} \equiv J_\lambda - 4\pi\sum_{l=1}^n \delta_{p_l}.$$

Since $J_\lambda \geqslant 0$ and $\|J_\lambda\|_{L^1(\Omega)} = 4\pi n$, there exist a subsequence $\{\lambda_j\}$ and a measure η such that $J_{\lambda_j} \to \eta$ in the sense of measure. By Lemma 1 we may assume that $\mathfrak{U}^{\pm}_{\lambda_j} \to \ln(1+2s)/(1-2s)$ as λ_j goes to infinity. Multiplying a smooth function φ, integrating over Ω, and taking the limit, we have

$$\int_\Omega \varphi J_{\lambda_j} \to 4\pi \sum_{l=1}^{n} \varphi(p_l) \quad \text{as} \quad \lambda_j \to \infty,$$

and thus $\eta = 4\pi \Sigma_{l=1}^{n} \delta_{p_l}$. Similarly,

$$(1-2s)\lambda_j \frac{e^{u_{\lambda_j}}}{(1+e^{u_{\lambda_j}})^3} \left(\frac{1+2s}{1-2s} - e^{\mathfrak{U}^-_{\lambda_j}} \right) \to 4\pi \sum_{k=1}^{m} \delta_{q_k}$$

in the sense of measure and (i) is proved.

Let w_1 be the unique solution of

$$\Delta w_1 = \frac{4\pi n}{|\Omega|} - 4\pi \sum_{l=1}^{n} \delta_{p_l}, \quad \int_\Omega w_1 = 0$$

and $u_{\lambda_j} - \mathfrak{U}^-_{\lambda_j} = w_1 + \mathcal{U}_{\lambda_j}$. Then $\mathcal{U}_{\lambda_j}$ satisfies

$$\Delta \mathcal{U}_{\lambda_j} = (1-2s)\lambda_j \frac{e^{u_{\lambda_j}}}{(1+e^{u_{\lambda_j}})^3} (e^{u_{\lambda_j}} - e^{\mathfrak{U}^-_{\lambda_j}}) - \frac{4\pi n}{|\Omega|}.$$

For any fixed $1 < r < 2$ and $r' = r/(r-1) > 2$,

$$\|\nabla(u_{\lambda_j} - \mathfrak{U}^-_{\lambda_j})\|^r_{L^r(\Omega)} = \int_\Omega |\nabla(w_1 + \mathcal{U}_{\lambda_j})|^r = \int_\Omega \nabla(w_1 + \mathcal{U}_{\lambda_j}) \nabla \varphi,$$

where φ is a unique solution of

$$\begin{cases} \Delta \varphi = \operatorname{div}[|\nabla(w_1 + \mathcal{U}_{\lambda_j})|^{r-2} \nabla(w_1 + \mathcal{U}_{\lambda_j})] & \text{in } \Omega \\ \int_\Omega \varphi = 0. \end{cases}$$

Using Calderon–Zygmund inequality, we have

$$\|\nabla \varphi\|_{L^{r'}(\Omega)} \leqslant C(r) \|\nabla(w_1 + \mathcal{U}_{\lambda_j})\|^{r-1}_{L^r(\Omega)}$$

and then

$$\begin{aligned} \|\nabla(w_1 + \mathcal{U}_{\lambda_j})\|_{L^r(\Omega)} = \frac{\int_\Omega \nabla(w_1 + \mathcal{U}_{\lambda_\varphi}) \nabla \varphi}{\|\nabla(w_1 + \mathcal{U}_{\lambda_j})\|^{r-1}_{L^r(\Omega)}} &\leqslant C(r) \int_\Omega \nabla(w_1 + \mathcal{U}_{\lambda_j}) \nabla \left(\frac{\varphi}{\|\nabla \varphi\|_{L^{r'}(\Omega)}} \right) \\ &\leqslant C(r) \int_\Omega \nabla(w_1 + \mathcal{U}_{\lambda_j}) \nabla \varphi_{\lambda_j}. \end{aligned} \tag{10}$$

Here φ_{λ_j} is defined by

$$\int_\Omega \nabla(w_1 + \mathcal{U}_{\lambda_j}) \nabla \varphi_{\lambda_j} = \sup \left\{ \int_\Omega \nabla(w_1 + \mathcal{U}_{\lambda_j}) \nabla \varphi \,\middle|\, \|\varphi\|_{W^{1,r'}(\Omega)} = 1, \int_\Omega \varphi = 0 \right\}.$$

Noting that $\|\varphi_{\lambda_j}\|_{W^{1,r'}(\Omega)}=1$ and $\int_\Omega \varphi_{\lambda_j}=0$, we can find $\varphi_0 \in W^{1,r'}(\Omega)$ and weakly convergent subsequence $\{\varphi_{\lambda_j}\}$, still we use the same notation, such that $\varphi_{\lambda_j}\to\varphi_0$ in $L^\infty(\Omega)$. From (10) we have

$$\begin{aligned}\frac{1}{C(r)}\|\nabla(w_1+\mathcal{U}_{\lambda_j})\|_{L^r(\Omega)} &\leqslant \int_\Omega \nabla(w_1+\mathcal{U}_{\lambda_j})\nabla\varphi_{\lambda_j}\\ &= \int_\Omega \nabla w_1\nabla\varphi_{\lambda_j}+\int_\Omega \nabla\mathcal{U}_{\lambda_j}\nabla(\varphi_{\lambda_j}-\varphi_0)+\int_\Omega \nabla\mathcal{U}_{\lambda_j}\nabla\varphi_0\\ &= -\int_\Omega \Delta w_1\varphi_{\lambda_j}-\int_\Omega \Delta\mathcal{U}_{\lambda_j}(\varphi_{\lambda_j}-\varphi_0)+\int_\Omega \nabla\mathcal{U}_{\lambda_j}\nabla\varphi_0\\ &\leqslant 4\pi\sum_{l=1}^n \varphi_{\lambda_j}(p_l)+4\pi n\|\varphi_{\lambda_j}-\varphi_0\|_{L^\infty(\Omega)}-4\pi\sum_{l=1}^n \varphi_0(p_l)+o(1).\end{aligned}$$

Here we used (i) in the last inequality. Since $\varphi_{\lambda_j}\to\varphi_0$ in $L^\infty(\Omega)$, we have that $\|\nabla(w_1+\mathcal{U}_{\lambda_j})\|_{L^r(\Omega)}\to 0$ as $\lambda_j\to\infty$. Finally, using dominated convergence theorem, $w_1+\mathcal{U}_{\lambda_j}\to 0$ in $L^r(\Omega)$ and $u_{\lambda_j}-\mathfrak{U}^-_{\lambda_j}\to 0$ in $W^{1,r}(\Omega)$.

Similarly, $\mathfrak{U}^-_{\lambda_j}-\ln(1+2s)/(1-2s)\to 0$ in $W^{1,r}(\Omega)$ and thus (ii) holds. Q.E.D.

Remark 2: From (i), for any compact subset K of $\Omega\backslash\cup_{l=1}^n\{p_l\}\cup_{k=1}^m\{q_k\}$,

$$\int_K (1-2s)\lambda_j\frac{e^{u_{\lambda_j}}}{(1+e^{u_{\lambda_j}})^3}\left(e^{u_{\lambda_j}}-\frac{1+2s}{1-2s}\right)\to 0 \quad \text{as } \lambda_j\to\infty.$$

Next, we investigate the locally uniform convergence. The arguments of the proof are due to Refs. 8 and 7.

Lemma 4: Let $\{u_\lambda\}$ *be as in Lemma 1. For any compact subset* $K\subset\Omega\backslash\cup_{l=1}^n\{p_l\}\cup_{k=1}^m\{q_k\}$, *there exists a subsequence* $\{u_{\lambda_j}\}$ *such that* $u_{\lambda_j}\to\ln(1+2s)/(1-2s)$ *uniformly on K as* $\lambda_j\to\infty$.

Proof: Let K and K' be compact subsets of Ω with $K\subset\subset K'\subset\subset\Omega\backslash\cup_{l=1}^n\{p_l\}\cup_{k=1}^m\{q_k\}$. Since $\mathfrak{U}^-_\lambda<u_\lambda<\mathfrak{U}^+_\lambda$ by Lemma 1, it suffices to show that $\mathfrak{U}^\pm_\lambda\to\ln(1+2s)/(1-2s)$ uniformly on K.

First consider the case $\mathfrak{U}^-_\lambda$. Let w_2 be the unique solution of

$$\Delta w_2=-\frac{4\pi m}{|\Omega|}+4\pi\sum_{k=1}^m \delta_{q_k},\quad \int_\Omega w_2=0. \tag{11}$$

If we set $\mathfrak{U}^-_\lambda=w_2+\mathcal{V}^-_\lambda$, then $\mathcal{V}^-_\lambda$ satisfies

$$\Delta\mathcal{V}^-_\lambda=(1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{w_2+\mathcal{V}^-_\lambda}-\frac{1+2s}{1-2s}\right)+\frac{4\pi m}{|\Omega|}. \tag{12}$$

Using Lemma 1 and interpolation type inequality (see, e.g., Ref. 8), we have

$$\|\nabla\mathcal{V}^-_\lambda\|^2_{L^\infty(K)}\leqslant C\left(\|\Delta\mathcal{V}^-_\lambda\|_{L^\infty(K')}\|\mathcal{V}^-_\lambda\|_{L^\infty(K')}+\frac{1}{\operatorname{dist}(K,\partial K')}\|\mathcal{V}^-_\lambda\|^2_{L^\infty(K')}\right)\leqslant C(K')\lambda.$$

Now suppose that $\|\mathfrak{U}^-_\lambda-\ln(1+2s)/(1-2s)\|_{L^\infty(K)}\nrightarrow 0$. Then there exists $\tilde\epsilon>0$ such that $\|\mathfrak{U}^-_{\lambda_j}-\ln(1+2s)/(1-2s)\|_{L^\infty(K)}>\tilde\epsilon$ for some subsequence $\{\lambda_j\}$. For $|x_j-x|<\operatorname{dist}(K,\partial K')$, we observe that

$$\left|\left(\mathfrak{U}_{\lambda_j}^- - \ln\frac{1+2s}{1-2s}\right)(x_j) - \left(\mathfrak{U}_{\lambda_j}^- - \ln\frac{1+2s}{1-2s}\right)(x)\right| \leqslant |w_2(x_j)-w_2(x)| + |\mathcal{V}_{\lambda_j}^-(x_j)-\mathcal{V}_{\lambda_j}^-(x)|$$
$$\leqslant \|\nabla w_2\|_{L^\infty(K')}|x_j-x| + \|\nabla \mathcal{V}_{\lambda_j}^-\|_{L^\infty(K')}|x_j-x|$$
$$\leqslant \sqrt{C(K')\lambda_j}|x_j-x|.$$

If we choose $x_j \in K$ so that $(\mathfrak{U}_{\lambda_j}^- - \ln(1+2s)/(1-2s))(x_j) < -\tilde{\epsilon}$, then

$$\left(\mathfrak{U}_{\lambda_j}^- - \ln\frac{1+2s}{1-2s}\right)(x) < -\frac{\tilde{\epsilon}}{2}$$

for $x \in B(x_j, r_j) \subset K'$ where $r_j \equiv \min\{\mathrm{dist}(K, \partial K'), \tilde{\epsilon}/2\sqrt{C(K')\lambda_j}\}$. Then for sufficiently large λ_j, we have $r_j = \tilde{\epsilon}/2\sqrt{C(K')\lambda_j}$ and

$$\int_{K'} (1-2s)\lambda_j \frac{e^{u_{\lambda_j}}}{(1+e^{u_{\lambda_j}})^3}\left(e^{\mathfrak{U}_{\lambda_j}^-} - \frac{1+2s}{1-2s}\right)$$
$$\leqslant (1-2s)\inf_{K'}\frac{e^{\mathfrak{U}^-}}{(1+e^{\mathfrak{U}^-})^3}\int_{K'}\lambda_j\left(e^{\mathfrak{U}_{\lambda_j}^-} - \frac{1+2s}{1-2s}\right)$$
$$\leqslant (1-2s)\inf_{K'}\frac{e^{\mathfrak{U}^-}}{(1+e^{\mathfrak{U}^-})^3}\inf_{K'} e^{\mathfrak{U}^-}\int_{B(x_j,r_j)}\lambda_j\left(\mathfrak{U}_{\lambda_j}^- - \ln\frac{1+2s}{1-2s}\right)$$
$$\leqslant -\frac{\tilde{\epsilon}}{2}(1-2s)\inf_{K'}\frac{e^{\mathfrak{U}^-}}{(1+e^{\mathfrak{U}^-})^3}\inf_{K'} e^{\mathfrak{U}^-}\lambda_j\pi\left(\frac{\tilde{\epsilon}}{2\sqrt{C(K')\lambda_j}}\right)^2$$
$$\leqslant -\frac{(1-2s)\pi\tilde{\epsilon}^3}{8C(K')}\inf_{K'}\frac{e^{\mathfrak{U}^-}}{(1+e^{\mathfrak{U}^-})^3}\inf_{K'} e^{\mathfrak{U}^-}.$$

On the other hand, as in the proof of Lemma 3(i), we have

$$\int_{K'}(1-2s)\lambda_j\frac{e^{u_{\lambda_j}}}{(1+e^{u_{\lambda_j}})^3}\left(e^{\mathfrak{U}_{\lambda_j}^-} - \frac{1+2s}{1-2s}\right) \to 0 \quad \text{as } \lambda_j \to \infty.$$

This is a contradiction and we obtain the uniform convergence.

The case for $\mathfrak{U}_\lambda^+$ is similar and we omit the details. Q.E.D.

To study the convergence speed, we need the following lemmas.

Lemma 5: Let $\{u_\lambda\}$ be as in Lemma 1. For any compact subset $K \subset\subset \Omega\backslash\cup_{l=1}^n\{p_l\}\cup_{k=1}^m\{q_k\}$, there exists a subsequence $\{u_{\lambda_j}\}$ such that

$$\int_K |\nabla u_{\lambda_j}|^2 \leqslant 2\int_K\left|\nabla\left(\mathfrak{U}_{\lambda_j}^- - \ln\frac{1+2s}{1-2s}\right)\right|^2 + |\nabla(u_{\lambda_j} - \mathfrak{U}_{\lambda_j}^-)|^2 \to 0 \quad \text{as } \lambda_j \to \infty.$$

Proof: Fix $K\subset\subset K'\subset\subset\Omega\backslash\cup_{l=1}^{n}\{p_l\}\cup_{k=1}^{m}\{q_k\}$ and let ζ be a smooth function with $0\leqslant\zeta\leqslant 1$, $\zeta\equiv 1$ on K and supp $\zeta\subset K'$. Multiplying $(\mathfrak{U}_\lambda^- - \ln(1+2s)/(1-2s))\zeta$ to (8) and integrating over Ω, we have

$$\begin{aligned}0&\leqslant\int_{K'}\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{\mathfrak{U}_\lambda^-}-\frac{1+2s}{1-2s}\right)\left(\mathfrak{U}_\lambda^- - \ln\frac{1+2s}{1-2s}\right)\zeta\\&=\int_{K'}\left(\mathfrak{U}_\lambda^- - \ln\frac{1+2s}{1-2s}\right)\zeta\Delta\left(\mathfrak{U}_\lambda^- - \ln\frac{1+2s}{1-2s}\right)\\&=-\int_{K'}\nabla\left[\left(\mathfrak{U}_\lambda^- - \ln\frac{1+2s}{1-2s}\right)\zeta\right]\nabla\left(\mathfrak{U}_\lambda^- - \ln\frac{1+2s}{1-2s}\right).\end{aligned}$$

By Lemma 3(ii), if $1<r<2$ then there exists a subsequence $\{\lambda_j\}$ such that

$$\begin{aligned}\int_K\left|\nabla\left(\mathfrak{U}_{\lambda_j}^- - \ln\frac{1+2s}{1-2s}\right)\right|^2&\leqslant\int_{K'}\left|\nabla\left(\mathfrak{U}_{\lambda_j}^- - \ln\frac{1+2s}{1-2s}\right)\right|^2\zeta\\&\leqslant-\int_{K'}\left(\mathfrak{U}_{\lambda_j}^- - \ln\frac{1+2s}{1-2s}\right)\nabla\left(\mathfrak{U}_{\lambda_j}^- - \ln\frac{1+2s}{1-2s}\right)\nabla\zeta\\&\leqslant\left\|\mathfrak{U}_{\lambda_j}^- - \ln\frac{1+2s}{1-2s}\right\|_{L^\infty(K')}\left\|\nabla\left(\mathfrak{U}_{\lambda_j}^- - \ln\frac{1+2s}{1-2s}\right)\right\|_{L^r(K')}\|\nabla\zeta\|_{L^{r'}(K')}\to 0.\end{aligned}$$

Similarly, we obtain that $\int_K|\nabla(u_{\lambda_j}-\mathfrak{U}_{\lambda_j}^-)|^2\to 0$ as $\lambda_j\to\infty$. Q.E.D.

Lemma 6: *Let* $\{\mathfrak{U}_\lambda^\pm\}$ *be as in Lemma 1. For any compact subset* $K\subset\subset\Omega\backslash\cup_{l=1}^{n}\{p_l\}\cup_{k=1}^{m}\{q_k\}$, *there exist a subsequence* $\{\mathfrak{U}_{\lambda_j}^\pm\}$ *and a constant* $C=C(K)$ *such that*

$$\|\mathfrak{U}_{\lambda_j}^\pm\|_{W^{2,2}(K)}\leqslant C.$$

Proof: Fix $K\subset\subset K'\subset\subset\Omega\backslash\cup_{l=1}^{n}\{p_l\}\cup_{k=1}^{m}\{q_k\}$. For any $\tilde{\epsilon}>0$, we can choose $r_1<\mathrm{dist}(K,\partial K')$ sufficiently small so that $\int_{B(x,r_1)}|\nabla w_2|^2\leqslant\tilde{\epsilon}/4$ where w_2 is defined in (11) and $x\in K$. If we fix $x_0\in K$, then by Lemma 5, there exists a subsequence $\{\lambda_j\}$, still we denote $\{\lambda\}$ for simplicity, such that

$$\int_{B(x_0,r_1)}|\nabla\mathcal{V}_\lambda^-|^2\leqslant 2\int_{B(x_0,r_1)}|\nabla w_2|^2+|\nabla\mathfrak{U}_\lambda^-|^2\leqslant\tilde{\epsilon}$$

for sufficiently large λ. For $r_2<r_1/2$, we define a smooth function ζ with $0\leqslant\zeta\leqslant 1$, $\zeta\equiv 1$ on $B(x_0,r_2)$ and supp $\zeta\subset B(x_0,2r_2)$.

We now recall the identity

$$\Delta|\nabla\mathcal{V}_\lambda^-|^2=2|D^2\mathcal{V}_\lambda^-|^2+2\nabla\mathcal{V}_\lambda^-\nabla(\Delta\mathcal{V}_\lambda^-).$$

From this identity and (12) we have that, for $x\in K'$,

$$
\begin{aligned}
|D^2\mathcal{V}_\lambda^-|^2 &= \frac{1}{2}\Delta|\nabla\mathcal{V}_\lambda^-|^2 - \nabla\mathcal{V}_\lambda^-\nabla(\Delta\mathcal{V}_\lambda^-) \\
&= \frac{1}{2}\Delta|\nabla\mathcal{V}_\lambda^-|^2 - (1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{w_2+\mathcal{V}_\lambda^-} - \frac{1+2s}{1-2s}\right)\nabla\mathcal{V}_\lambda^-\nabla u_\lambda \\
&\quad -(1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}e^{w_2+\mathcal{V}_\lambda^-}\nabla\mathcal{V}_\lambda^-\nabla(w_2+\mathcal{V}_\lambda^-) \\
&\quad +3(1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{w_2+\mathcal{V}_\lambda^-} - \frac{1+2s}{1-2s}\right)\frac{e^{u_\lambda}}{1+e^{u_\lambda}}\nabla\mathcal{V}_\lambda^-\nabla u_\lambda \\
&\leqslant \frac{1}{2}\Delta|\nabla\mathcal{V}_\lambda^-|^2 - \nabla\mathcal{V}_\lambda^-\nabla u_\lambda\left(\Delta\mathcal{V}_\lambda^- - \frac{4\pi m}{|\Omega|}\right) \\
&\quad +(1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}e^{w_2+\mathcal{V}_\lambda^-}\nabla w_2\nabla(w_2+\mathcal{V}_\lambda^-) \\
&\quad +3\left(\Delta\mathcal{V}_\lambda^- - \frac{4\pi m}{|\Omega|}\right)\frac{e^{u_\lambda}}{1+e^{u_\lambda}}\nabla\mathcal{V}_\lambda^-\nabla u_\lambda \\
&\leqslant \frac{1}{2}\Delta|\nabla\mathcal{V}_\lambda^-|^2 + C(|\nabla\mathcal{V}_\lambda^-|^4 + |\nabla v_\lambda|^4 + 1) \\
&\quad +\frac{1}{2}|\Delta\mathcal{V}_\lambda^-|^2 + (1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}e^{w_2+\mathcal{V}_\lambda^-}\nabla w_2\nabla(w_2+\mathcal{V}_\lambda^-),
\end{aligned}
$$

where we used Young's inequality in the last inequality. Thus

$$
|D^2\mathcal{V}_\lambda^-|^2 \leqslant \Delta|\nabla\mathcal{V}_\lambda^-|^2 + C(1+|\nabla v_\lambda|^4 + |\nabla\mathcal{V}_\lambda^-|^4) + (1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\nabla\left(e^{w_2+\mathcal{V}_\lambda^-} - \frac{1+2s}{1-2s}\right)\nabla w_2.
$$

Multiplying ζ^2 and integrating over Ω, we obtain

$$
\begin{aligned}
\int_\Omega |D^2\mathcal{V}_\lambda^-|^2\zeta^2 &\leqslant C\left(1 + \int_\Omega |\nabla\mathcal{V}_\lambda^-|^2\Delta\zeta^2 + \int_\Omega |\nabla v_\lambda|^4\zeta^2 + \int_\Omega |\nabla\mathcal{V}_\lambda^-|^4\zeta^2\right) \\
&\quad + \int_\Omega (1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\nabla\left(e^{w_2+\mathcal{V}_\lambda^-} - \frac{1+2s}{1-2s}\right)\nabla w_2\zeta^2 \\
&\leqslant C\left(1 + \int_\Omega |\nabla\mathcal{V}_\lambda^-|^2\Delta\zeta^2 + \int_\Omega |\nabla v_\lambda|^4\zeta^2 + \int_\Omega |\nabla\mathcal{V}_\lambda^-|^4\zeta^2\right),
\end{aligned}
$$

where we used Lemma 5 and the following estimate in the last inequality:

$$
\begin{aligned}
&(1-2s)\lambda\int_\Omega \frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\nabla\left(e^{w_2+\mathcal{V}_\lambda^-}-\frac{1+2s}{1-2s}\right)\nabla w_2\zeta^2\\
&\quad=-(1-2s)\lambda\int_\Omega \frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{w_2+\mathcal{V}_\lambda^-}-\frac{1+2s}{1-2s}\right)\nabla(\nabla w_2\zeta^2)\\
&\qquad-(1-2s)\lambda\int_\Omega \frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{w_2+\mathcal{V}_\lambda^-}-\frac{1+2s}{1-2s}\right)\frac{1-2e^{u_\lambda}}{1+e^{u_\lambda}}\nabla u_\lambda\nabla w_2\zeta^2\leqslant o(1)\\
&\qquad+\int_\Omega\left(\Delta\mathcal{V}_\lambda^- -\frac{4\pi m}{|\Omega|}\right)\zeta\frac{1-2e^{u_\lambda}}{1+e^{u_\lambda}}\nabla u_\lambda\nabla w_2\zeta\\
&\quad\leqslant o(1)+\int_\Omega|\Delta\mathcal{V}_\lambda^-\zeta||\nabla u_\lambda\nabla w_2\zeta|+\int_\Omega\frac{4\pi m}{|\Omega|}|\nabla u_\lambda\nabla w_2\zeta^2|\\
&\quad\leqslant\frac{1}{2}\int_\Omega|\Delta\mathcal{V}_\lambda^-|^2\zeta^2+C\int_{K'}|\nabla u_\lambda|^2+o(1)\leqslant\frac{1}{2}\int_\Omega|D^2\mathcal{V}_\lambda^-|^2\zeta^2+C.
\end{aligned}
$$

Similarly,

$$
\int_\Omega|D^2v_\lambda|^2\zeta^2\leqslant C\left(1+\int_\Omega|\nabla v_\lambda|^2\Delta\zeta^2+\int_\Omega|\nabla v_\lambda|^4\zeta^2\right).
$$

Again by Lemma 5 and the imbedding $W^{1,1}(\Omega)\hookrightarrow L^2(\Omega)$ applied to $|\nabla v_\lambda|^2\zeta$, we obtain

$$
\begin{aligned}
\int_\Omega|D^2v_\lambda|^2\zeta^2+|D^2\mathcal{V}_\lambda^-|^2\zeta^2&\leqslant C\left(1+\int_\Omega|\nabla v_\lambda|^4\zeta^2+|\nabla\mathcal{V}_\lambda^-|^4\zeta^2\right)\\
&\leqslant C\left(1+\int_\Omega\zeta|\nabla v_\lambda||D^2v_\lambda|+\int_\Omega\zeta|\nabla\mathcal{V}_\lambda^-||D^2\mathcal{V}_\lambda^-|\right)^2\\
&\leqslant C+\frac{1}{2}\left(\int_\Omega|D^2v_\lambda|^2\zeta^2+|D^2\mathcal{V}_\lambda^-|^2\zeta^2\right).
\end{aligned}
$$

Hence

$$
\int_{B(x_0,r_1)}|D^2v_\lambda|^2+|D^2\mathcal{V}_\lambda^-|^2\leqslant C.
$$

Since $x_0\in K$ is arbitrary and K is compact, we have $\|\mathfrak{U}_\lambda^-\|_{W^{2,2}(K)}\leqslant C$.

The other part is similar and we omit the details. Q.E.D.

Finally, we study the locally uniform convergence speed and this, combined with previous lemmas, completes the proof of Theorem 2.

Lemma 7: Let $\{u_\lambda\}$ *be as in Lemma 1. For* $K\subset\subset\Omega\backslash\cup_{l=1}^n\{p_l\}\cup_{k=1}^m\{q_k\}$, *there exist a subsequence* $\{\lambda_j\}$ *and a constant* $C=C(K)$ *such that*

$$
\left|u_{\lambda_j}-\ln\frac{1+2s}{1-2s}\right|\leqslant\frac{C}{\lambda_j}\quad in\,K.
$$

Proof: Since $\mathfrak{U}_\lambda^-<u_\lambda<\mathfrak{U}_\lambda^+$ by Lemma 1, it suffices to show $0\leqslant\ln(1+2s)/(1-2s)-\mathfrak{U}_\lambda^-\leqslant C/\lambda$. The other part is similar. Fix $K\subset\subset K'\subset\subset\Omega\backslash\cup_{l=1}^n\{p_l\}\cup_{k=1}^m\{q_k\}$. By Lemma 4, we may assume that $\mathfrak{U}_\lambda^-\geqslant\ln(1+2s)/2(1-2s)$ on K'. For any fixed $x_0\in K$ and $r_1=\frac{1}{2}\mathrm{dist}(K,\partial K')$, let ζ be a smooth function with $0\leqslant\zeta\leqslant1$, $\zeta\equiv1$ in $B(x_0,r_1)$ and $\zeta\equiv0$ outside $B(x_0,2r_1)$. Then

$$\Delta\left[\zeta^2\left(e^{\mathfrak{U}_\lambda^-}-\frac{1+2s}{1-2s}\right)\right]=\nabla\left[2\zeta\nabla\zeta\left(e^{\mathfrak{U}_\lambda^-}-\frac{1+2s}{1-2s}\right)+\zeta^2 e^{\mathfrak{U}_\lambda^-}\nabla\mathfrak{U}_\lambda^-\right]$$

$$=2\zeta\Delta\zeta\left(e^{\mathfrak{U}_\lambda^-}-\frac{1+2s}{1-2s}\right)+2|\nabla\zeta|^2\left(e^{\mathfrak{U}_\lambda^-}-\frac{1+2s}{1-2s}\right)$$

$$+2\nabla\zeta^2\nabla\mathfrak{U}_\lambda^- e^{\mathfrak{U}_\lambda^-}+\zeta^2\Delta\left(e^{\mathfrak{U}_\lambda^-}-\frac{1+2s}{1-2s}\right)$$

$$\leqslant 2\zeta|\Delta\zeta|\left(\frac{1+2s}{1-2s}-e^{\mathfrak{U}_\lambda^-}\right)+2|\nabla\zeta^2||\nabla\mathfrak{U}_\lambda^-|e^{\mathfrak{U}_\lambda^-}+\zeta^2 e^{\mathfrak{U}_\lambda^-}|\nabla\mathfrak{U}_\lambda^-|^2+\zeta^2 e^{\mathfrak{U}_\lambda^-}\Delta\mathfrak{U}_\lambda^-$$

$$\leqslant 2\zeta|\Delta\zeta|\left(\frac{1+2s}{1-2s}-e^{\mathfrak{U}_\lambda^-}\right)+2\frac{1+2s}{1-2s}|\nabla\zeta^2||\nabla\mathfrak{U}_\lambda^-|+\zeta^2 e^{\mathfrak{U}_\lambda^-}|\nabla\mathfrak{U}_\lambda^-|^2$$

$$+\zeta^2 e^{\mathfrak{U}_\lambda^-}(1-2s)\lambda\frac{e^{u_\lambda}}{(1+e^{u_\lambda})^3}\left(e^{\mathfrak{U}_\lambda^-}-\frac{1+2s}{1-2s}\right)$$

$$\leqslant 2\zeta|\Delta\zeta|\left(\frac{1+2s}{1-2s}-e^{\mathfrak{U}_\lambda^-}\right)+2\frac{1+2s}{1-2s}|\nabla\zeta^2||\nabla\mathfrak{U}_\lambda^-|+\zeta^2 e^{\mathfrak{U}_\lambda^-}|\nabla\mathfrak{U}_\lambda^-|^2$$

$$+C\lambda\zeta^2\left(e^{\mathfrak{U}_\lambda^-}-\frac{1+2s}{1-2s}\right).$$

If we set

$$\xi=\lambda\zeta^2\left(\frac{1+2s}{1-2s}-e^{\mathfrak{U}_\lambda^-}\right),$$

then

$$-\frac{1}{\lambda}\Delta\xi+C\xi\leqslant 2\zeta|\Delta\zeta|\left(\frac{1+2s}{1-2s}-e^{\mathfrak{U}_\lambda^-}\right)+2\frac{1+2s}{1-2s}|\nabla\zeta^2||\nabla\mathfrak{U}_\lambda^-|+\zeta^2 e^{\mathfrak{U}_\lambda^-}|\nabla\mathfrak{U}_\lambda^-|^2.$$

Using Young's inequality, we have

$$-\frac{1}{\lambda}\Delta\xi+C\xi\leqslant C(1+|\nabla\mathfrak{U}_\lambda^-|^2).$$

Multiplying $\xi^{r'-1}$ for $r'>2$ and integrating by parts, we obtain

$$\frac{r'-1}{\lambda}\int_\Omega\xi^{r'-2}|\nabla\xi|^2+C\int_\Omega\xi^{r'}\leqslant C\int_\Omega(1+|\nabla\mathfrak{U}_\lambda^-|^2)\xi^{r'-1}$$

$$\leqslant C\left[\int_{B(x_0,2r_1)}(1+|\nabla\mathfrak{U}_\lambda^-|^2)^{r'}\right]^{1/r'}\left(\int_{B(x_0,2r_1)}\xi^{r'}\right)^{(r'-1)/r'}$$

$$\leqslant C\left[1+\left(\int_{K'}|\nabla\mathfrak{U}_\lambda^-|^{2r'}\right)^{1/r'}\right]\|\xi\|^{r'-1}_{L^{r'}(B(x_0,2r_1))}.$$

By Lemma 6 there exists s subsequence $\{\lambda_j\}$ such that

$$\|\xi\|_{L^{r'}(B(x_0,2r_1))} \leqslant C\left[1+\left(\int_{K'}|\nabla \mathfrak{U}_{\lambda_j}^-|^{2r'}\right)^{1/r'}\right] \leqslant C.$$

Applying this to (12), we get $\|\mathcal{V}_{\lambda_j}^-\|_{W^{2,r'}(K)} \leqslant C$ for $r'>2$, and $\|\nabla \mathcal{V}_{\lambda_j}^-\|_{L^\infty(K)} \leqslant C$. Since the maximum of ξ occurs at an interior point of K', say $\tilde{x}_j$,

$$\begin{aligned}
0 &\leqslant \sup_{K\cap B(x_0,r_1)} \lambda\left(\frac{1+2s}{1-2s} - e^{\mathfrak{U}_{\lambda_j}^-}\right) \\
&= \sup_{K\cap B(x_0,r_1)} \xi \\
&\leqslant \sup_{B(x_0,2r_1)} \xi \\
&\leqslant -\frac{1}{\lambda}\Delta\xi(\tilde{x}_j) + C\xi(\tilde{x}_j) \\
&\leqslant C(1+\sup_{K'}\nabla|\mathfrak{U}_{\lambda_j}^-|^2) \leqslant C.
\end{aligned}$$

Hence

$$\sup_{K\cap B(x_0,r_1)} \lambda\left(\frac{1+2s}{1-2s} - e^{\mathfrak{U}_{\lambda_j}^-}\right) \leqslant C.$$

Since $x_0 \in K$ is arbitrary and $\mathfrak{U}^- < \mathfrak{U}_{\lambda_j}^- < \ln(1+2s)/(1-2s)$, we have

$$\left\| \ln\frac{1+2s}{1-2s} - \mathfrak{U}_{\lambda_j}^- \right\|_{L^\infty(K)} \leqslant \frac{C}{\lambda_j}.$$

Q.E.D.

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Partition asymptotics from one-dimensional quantum entropy and energy currents

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We give an alternative method to that of Hardy–Ramanujan–Rademacher to derive the leading exponential term in the asymptotic approximation to the partition function $p(n,a)$, defined as the number of decompositions of a positive integer n into integer summands, with each summand appearing at most a times in a given decomposition. The derivation involves mapping to an equivalent physical problem concerning the quantum entropy and energy currents of particles flowing in a one-dimensional (1D) channel connecting thermal reservoirs, and which obey Gentile's intermediate statistics with statistical parameter a. The method is also applied to partitions associated with Haldane's fractional exclusion statistics. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1416195]

A classic result in the theory of partitions is the Hardy–Ramanujan–Rademacher formula for the unrestricted partition function $p(n,\infty)$, wherein the latter, combinatoric quantity is represented as a power series whose terms involve elementary functions of n.[1–3] This series yields the following asymptotic approximation:

$$p(n,\infty)\sim \frac{1}{4\sqrt{3}n}e^{\pi\sqrt{2/3}\sqrt{n}}. \tag{1}$$

A series representing $p(n,1)$, the number of decompositions of n into distinct summands, has also been derived (see, e.g., Sec. 24.2.2 of Ref. 4), yielding the asymptotic approximation

$$p(n,1)\sim \frac{1}{4(3^{1/4})n^{3/4}}e^{\pi\sqrt{1/3}\sqrt{n}}. \tag{2}$$

And more recently,[5] Hagis used the Hardy–Ramanujan–Rademacher method to derive a power series representation of $p(n,a)$ for arbitrary $a=1,2,...$, yielding the asymptotic approximation

$$p(n,a)\sim \frac{\sqrt{12}a^{1/4}}{(1+a)^{3/4}(24n)^{3/4}}e^{\pi\sqrt{2a/[3(1+a)]}\sqrt{n}}, \tag{3}$$

where $n\gg a$. As an example, for $a=4$ the number of partitions of $n=1000$ to five significant figures is 2.4544×10^{28}, while approximation (3) gives 2.4527×10^{28}, accurate to within 0.1%.

In the present work, we give an alternative and more direct derivation of the asymptotic approximation to $\ln p(n,a)$ which, from Eq. (3), is

$$\ln p(n,a)\sim \pi\sqrt{\frac{2a}{3(1+a)}}\cdot\sqrt{n}. \tag{4}$$

The derivation begins by considering a one-dimensional (1D) quantum channel which supports particles obeying Gentile's intermediate statistics[6] characterized by statistical parameter a, the

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maximum occupation number of particles in a single particle state, with $a=1$ describing fermions and $a=\infty$ bosons. The left end of the channel is connected to a particle source and the right end to a particle sink. The channel is dispersionless so that particle packets with different mean energies have the same velocity c and hence transmission time $\tau=L/c$, where L is the channel length. Imposing periodic boundary conditions on the channel length, the single-particle energies are $\epsilon_j=hf_j=hj/\tau$, $j=1,2,...$, where h is Planck's constant. The total energy E_n of a given Fock state is $E_n=\Sigma_j \epsilon_j n_j=nh/\tau$, where $n=\Sigma_{j=1}^{\infty} jn_j$, and $n_j \leqslant a$ is the occupation number of, say, the right-propagating mode j.

We now suppose that the source emits a finite number of particles with fixed total energy E_n. The maximum possible entropy of this collection of right-propagating particles subject to the fixed energy constraint is $S(n,a)=k_B \ln p(n,a)$. Thus, the problem to determine the asymptotic approximation to $\ln p(n,a)$ is equivalent to determining the asymptotic approximation to the entropy $S(n,a)$ of the just-described physical system. (see Sec. 4 of Ref. 7, where the same setup restricted to bosons was considered in the problem to determine the optimum capacity for classical information transmission down a quantum channel.)

The crucial next step is to consider a slightly different setup, in which the particle source and sink are replaced by two thermal reservoirs described by grand canonical ensembles, with the chemical potentials of the left and right reservoirs satisfying $\mu_L=\mu_R=0$, the temperature of the right reservoir $T_R=0$, and the temperature T_L of the left reservoir chosen such that the thermal-averaged energy current flowing in the channel satisfies $\overline{\dot{E}}(T_L,a)=E_n/\tau$. (Note that the chemical potentials are set to zero since there is no constraint on the thermal-averaged particle number.) With this choice, the thermal-averaged, channel entropy current $\overline{\dot{S}}(T_L,a)$ coincides with $S(n,a)/\tau$ in the thermodynamic limit E_n(equivalently n)$\rightarrow\infty$.

The advantage with using the latter, grand canonical ensemble description as opposed to the former, microcanonical ensemble description is the greater ease with which the energy and entropy currents can be calculated. The starting formula for the single channel energy current is

$$\overline{\dot{E}}(T,a)=\sum_{j=1}^{\infty} \epsilon_j[\overline{n}_a(\epsilon_j)/L]c, \tag{5}$$

where we have dropped the subscript on T_L, and where $\overline{n}_a(\epsilon)$ is the intermediate statistics thermal-averaged occupation number of the right-moving state with energy ϵ:[6]

$$\overline{n}_a(\epsilon)=\frac{1}{e^{\beta\epsilon}-1}-+\frac{a+1}{e^{\beta\epsilon(a+1)}-1}. \tag{6}$$

In the limit $L\rightarrow\infty$ (equivalently $\tau\rightarrow\infty$), we can replace the sum with an integral over j and, changing integration variables $j\rightarrow\epsilon=(h/\tau)j=(hc/L)j$, we have [c.f. Eq. (13) of Ref. 8]:

$$\overline{\dot{E}}(T,a)=\frac{1}{h}\int_0^{\infty} \mathrm{d}\epsilon\, \epsilon \overline{n}_a(\epsilon). \tag{7}$$

A formula for entropy current can be derived as follows. First note that the thermal-averaged occupation energy $\overline{\epsilon}=\epsilon\overline{n}_a(\epsilon)$ and the entropy $\overline{s}$ for a given mode with energy ϵ are related through the first law: $\mathrm{d}\overline{s}/\mathrm{d}T=(1/T)\mathrm{d}\overline{\epsilon}/\mathrm{d}T$. Integrating with respect to temperature and then summing over the right propagating channel modes, we obtain

$$\overline{\dot{S}}(T,a)=\frac{k_B}{h}\int_0^{\infty} \mathrm{d}\epsilon\, \epsilon \int_0^{\beta} \mathrm{d}\beta' \beta' \frac{\partial \overline{n}_a}{\partial \beta'}. \tag{8}$$

The integrals are straightforwardly carried out by noting from (6) that the thermal-averaged occupation energy $\overline{\epsilon}=\epsilon\overline{n}_a(\epsilon)$ of level ϵ for statistical parameter a is just the difference in the

thermal-averaged occupation energies of levels ϵ and $\epsilon(a+1)$ for bosons. Thus, we require only the integrals for the bosonic case: $\overleftarrow{E}(T,\infty)=\pi^2(k_BT)^2/(6h)$ and $\overleftarrow{S}(T,\infty)=\pi^2k_B^2T/(3h)$, giving

$$\overleftarrow{E}(T,a)=\left(1-\frac{1}{1+a}\right)\frac{\pi^2(k_BT)^2}{6h} \tag{9}$$

and

$$\overleftarrow{S}(T,a)=\left(1-\frac{1}{1+a}\right)\frac{\pi^2k_B^2T}{3h}. \tag{10}$$

Comparing powers of T appearing in Eqs. (9) and (10), and recalling that $\overleftarrow{E}(T,a)=E_n/\tau$ and $\overleftarrow{S}(T,a)\sim S(n,a)/\tau$, we learn immediately that $\ln p(n,a)\sim C(a)\sqrt{n}$, where the n-independent factor $C(a)$ is given by

$$C(a)=\frac{\sqrt{h}\overleftarrow{S}(T,a)}{k_B\sqrt{\overleftarrow{E}(T,a)}}. \tag{11}$$

Substituting in the expressions (9) and (10) for $\overleftarrow{E}$ and $\overleftarrow{S}$, respectively, we finally obtain $C(a)=\pi\sqrt{2a/[3(1+a)]}$, in agreement with Eq. (4).

We will now carry out the same steps as above for particles obeying Haldane's fractional exclusion statistics[9] to derive the asymptotic approximation to the logarithm of yet another type of partition function, $\tilde{p}(n,g)$, which also interpolates between the unrestricted and distinct partition functions [Eqs. (1) and (2), respectively]. Following the usual conventions, the statistics parameter is denoted by $g=1/a$ (so that $g=0$ describes bosons and $g=1$ fermions). Partitions associated with exclusion statistics are subject to additional constraints as compared with partitions associated with intermediate statistics (see the following).

The energy and entropy currents for particles obeying exclusion statistics are[10,11]

$$\overleftarrow{E}(T,g)=\frac{(k_BT)^2}{h}\int_0^\infty dx\, x\overline{n_g}(x) \tag{12}$$

and

$$\overleftarrow{S}(T,g)=-\frac{k_B^2T}{h}\int_0^\infty dx\{\overline{n_g}\ln\overline{n_g}+(1-g\overline{n_g})\ln(1-g\overline{n_g})-[1+(1-g)\overline{n_g}]\ln[1+(1-g)\overline{n_g}]\}, \tag{13}$$

where $x=\beta\epsilon$ and the thermal-averaged occupation number is[12]

$$\overline{n_g}(x)=[w(x)+g]^{-1}, \tag{14}$$

with the function $w(x)$ given by the implicit equation

$$w(x)^g[1+w(x)]^{1-g}=e^x. \tag{15}$$

Again, comparing powers of T appearing in Eqs. (12) and (13), we learn immediately that $\ln\tilde{p}(n,g)\sim\tilde{C}(g)\sqrt{n}$, where the n-independent factor $\tilde{C}(g)$ is given in terms of $\overleftarrow{E}$ and $\overleftarrow{S}$ as in Eq. (11). Substituting in the expressions for $\overleftarrow{E}$ and $\overleftarrow{S}$ and performing a change of variables from x to w,[10] Eq. (11) becomes after some algebra

$$\tilde{C}(g)=\frac{s(g)}{\sqrt{e(g)}}, \tag{16}$$

where

$$e(g)=\int_{w_g(0)}^{\infty} dw\,\frac{1}{w(1+w)}[(1-g)\ln(1+w)+g\ln w] \tag{17}$$

and

$$s(g)=\int_{w_g(0)}^{\infty} dw[\ln(1+w)/w-\ln w/(w+1)]. \tag{18}$$

Using the identity $s(g)=2e(g)$, Eq. (16) can be further simplified to

$$\tilde{C}(g)=\sqrt{2s(g)}. \tag{19}$$

Let us now describe some of the properties and consequences of result (19). Integral (18) can be rewritten in terms of dilogarithms[13] and only for certain choices of lower integration limit do closed-form solutions exist. For example, from (15) we have $w_{g=0}(0)=0$ and $w_{g=1}(0)=1$ and solving the respective integrals, we obtain $s(0)=\pi^2/3$ and $s(1)=\pi^2/6$. Substituting these values into (19), we indeed obtain the arguments of the exponentials in the asymptotic approximations to the unrestricted and distinct partition functions, Eqs. (1) and (2), respectively. It is tempting to speculate that closed-form solutions to the integral $s(g)$ exist only for $g=0$, 1/2, 1/3, 1/4, and 1 in the interval [0, 1], since it is only for these rational values that Eq. (15) can be solved analytically for the lower integration limit $w_g(0)$. For $g=1/2$, we have $w_{1/2}(0)=(-1+\sqrt{5})/2$ and $s(1/2)=\pi^2/5$, so that

$$\ln\tilde{p}(n,1/2)\sim\pi\sqrt{2/5}\cdot\sqrt{n}. \tag{20}$$

Note that $\tilde{C}_{g=1/2}(=\pi\sqrt{2/5})<C_{a=2}(=2\pi/3)$, signaling the fact that $\tilde{p}(n,g)<p(n,a=1/g)$ for $0<g<1$, a consequence of additional constraints on the allowed partitions associated with Haldane's statistics. These constraints are discussed in Ref. 14. The above-mentioned, closed-form solutions for $g=0$, $g=1/2$, and 1 were obtained by solving the integral $s(g)$ numerically and then noting that the result when divided by π^2 was rational. This method does not work for the $g=1/3$, 1/4 cases, however, owing to the complicated form of the lower limits $w_{1/3}(0)$ and $w_{1/4}(0)$ (they are roots of third and fourth degree polynomial equations, respectively). A more sophisticated method is required in order to determine whether or not closed-form solutions exist for these latter two cases.

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"Single ring theorem" and the disk-annulus phase transition

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Recently, an analytic method was developed to study in the large N limit non-Hermitian random matrices that are drawn from a large class of circularly symmetric non-Gaussian probability distributions, thus extending the existing Gaussian non-Hermitian literature. One obtains an explicit algebraic equation for the integrated density of eigenvalues from which the Green's function and averaged density of eigenvalues could be calculated in a simple manner. Thus, that formalism may be thought of as the non-Hermitian analog of the method due to Brézin, Itzykson, Parisi, and Zuber for analyzing Hermitian non-Gaussian random matrices. A somewhat surprising result is the so called "single ring" theorem, namely, that the domain of the eigenvalue distribution in the complex plane is either a disk or an annulus. In this article we extend previous results and provide simple new explicit expressions for the radii of the eigenvalue distribution and for the value of the eigenvalue density at the edges of the eigenvalue distribution of the non-Hermitian matrix in terms of moments of the eigenvalue distribution of the associated Hermitian matrix. We then present several numerical verifications of the previously obtained analytic results for the quartic ensemble and its phase transition from a disk shaped eigenvalue distribution to an annular distribution. Finally, we demonstrate numerically the "single ring" theorem for the sextic potential, namely, the potential of lowest degree for which the "single ring" theorem has nontrivial consequences. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1412599]

I. INTRODUCTION

There has been considerable interest in random non-Hermitian matrices in recent years. Possible applications range over several areas of physics.[1–4] For some recent reviews see Ref. 5. One difficulty is that the eigenvalues of non-Hermitian matrices invade the complex plane, and, consequently, various methods developed over the years to deal with random Hermitian matrices are no longer applicable, as these methods typically all involve exploiting the powerful constraints of analytic function theory. (See in particular the paper by Brézin, Itzykson, Parisi, and Zuber.[6]) In Ref. 3, two of us proposed a "method of Hermitization," whereby a problem involving random non-Hermitian matrices can be reduced to a problem involving random Hermitian matrices, to which various standard methods (such as the diagrammatic method,[7] or the "renormalization group" method[8–11]) can be applied. An idea similar to the "method of Hermitization" was expressed independently in Ref. 2.

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To our knowledge, the literature on random non-Hermitian matrices[1,2] has focused exclusively on Gaussian randomness. For instance, it has been known for over 30 years, from the work of Ginibre,[12] that for the Gaussian probability distribution $P(\phi)=(1/Z)\exp(-N\mathrm{tr}\phi^\dagger\phi)$ (here, as in the rest of this article, ϕ denotes an $N\times N$ complex random matrix with the limit $N\to\infty$ understood), the density of eigenvalues of ϕ is uniformly distributed over a disk of radius 1 in the complex plane.

Analytic determination of the density of eigenvalues of a non-Gaussian probability distribution of the form

$$P(\phi)=\frac{1}{Z}e^{-N\mathrm{tr}V(\phi^\dagger\phi)}, \tag{1.1}$$

where V is an arbitrary polynomial of its argument, was given for the first time in Ref. 4. Based on the method of Hermitization, it was shown in Ref. 4 that by a simple trick, the desired density of eigenvalues could be obtained with a minimal amount of work, by judiciously exploiting the existing literature on random Hermitian matrices.

Due to the symmetry of $P(\phi)$ under the transformation $\phi\to e^{i\alpha}\phi$, the density of eigenvalues is obviously rotational invariant. It was shown in Ref. 4 that the class of probability distributions of the form (1.1) exhibits a universal behavior in the sense that whatever the polynomial V was, the shape of the eigenvalue distribution in the complex plane was always either a disk or an annulus. This result was referred to in Ref. 4 as the "single ring theorem."

In a certain sense, the formalism developed in Ref. 4 may be thought of as the analog of the work of Brézin *et al.* for random Hermitian matrices;[6] they showed how the density of eigenvalues of Hermitian matrices φ taken from the probability distribution $P(\varphi)=(1/Z)\exp[-N\mathrm{tr}V(\varphi)]$ with V an arbitrary polynomial can be determined, and not just for the Gaussian case studied by Wigner and others,[13] in which $V=(\frac{1}{2})\mathrm{tr}\varphi^2$. An important simplifying feature of the analysis in Ref. 6 is that $P(\varphi)$ depends only on the eigenvalues of φ, and not on the unitary matrix that diagonalizes it. In contrast, the probability distribution (1.1) for non-Hermitian matrices depends explicitly on the GL(N) matrix S used to diagonalize $\phi=S^{-1}\Lambda S$, and S does not decouple. Remarkably, however, for the Gaussian $P(\phi)$, Ginibre[12] managed to integrate over S explicitly and derived an explicit expression for the probability distribution of the eigenvalues of ϕ. Unfortunately, it is not clear how to integrate over S and derive the expression for the eigenvalue probability distribution for non-Gaussian distributions of the form (1.1). In Ref. 4 this difficulty was circumvented by using the method of Hermitization.

As an explicit example, the case $V(\phi^\dagger\phi)=2m^2\phi^\dagger\phi+g(\phi^\dagger\phi)^2$ was studied in detail in Ref. 4. As should perhaps be expected in advance, the following behavior in the parameter space $m^2,g>0$ was found: for m^2 positive, the eigenvalue distribution was disklike (and nonuniform), generalizing Ginibre's work, but as $m^2\equiv-\mu^2$ was made more and more negative, a phase transition at the critical value

$$\mu_c^2=\sqrt{2g}$$

occurred, after which the disk fragmented into an annulus. The density of eigenvalues was calculated in Ref. 4 in detail.

The article is organized as follows: In Sec. II we summarize the "method of hermitization."[3] We present (without derivation) the general algorithm for finding the density of eigenvalues associated with (1.1) which was developed in Ref. 4, and also add some new insight into the mechanism behind the "single ring" theorem. We then formulate a novel simple criterion on the couplings in $V(\phi^\dagger\phi)$ to decide whether the shape of the eigenvalue distribution is a disk or an annulus. Finally, we discuss some generic features of the disk-annulus phase transition. In particular, we prove that the Green's function associated with the Hermitian matrix $\phi^\dagger\phi$ (which plays an important role in the "Hermitization algorithm" just mentioned) is continuous through the disk-annulus phase transition.

In Sec. III we provide simple new expressions for the outer radius R_{out} and for the inner radius R_{in} (in the annular phase) of the eigenvalue distribution of the non-Hermitian matrix ϕ, and for the corresponding boundary values $\rho(R_{\text{out}})$ and $\rho(R_{\text{in}})$ of its eigenvalue density, in terms of the moments

$$\langle \sigma^k \rangle = \int d\sigma \sigma^k \tilde{\rho}(\sigma) \quad (k=0,\pm 1,\ldots)$$

of the eigenvalue distribution $\tilde{\rho}(\sigma)$ of the Hermitian matrix $\phi^\dagger \phi$. Thus, we find that

$$R_{\text{out}}^2 = \langle \sigma \rangle,$$

and

$$\rho(R_{\text{out}}) = \frac{2R_{\text{out}}^2}{\langle \sigma^2 \rangle - \langle \sigma \rangle^2}.$$

We see that R_{out}^2 is simply the average of σ, and the density $\rho(R_{\text{out}})$ is inversely proportional to the variance of σ.

Similarly, we find that in the annular phase,

$$\frac{1}{R_{\text{in}}^2} = \left\langle \frac{1}{\sigma} \right\rangle$$

and

$$\rho(R_{\text{in}}) = \frac{2R_{\text{in}}^{-6}}{\langle \sigma^{-2} \rangle - \langle \sigma^{-1} \rangle^2}.$$

Thus, R_{in}^{-2} is simply the σ^{-1} moment of $\tilde{\rho}(\sigma)$, and the density $\rho(R_{\text{out}})$ is inversely proportional to the variance of σ^{-1}.

In Sec. IV we verify that the explicit analytic expressions in Ref. 4 concerning the quartic ensemble $V(\phi^\dagger \phi) = 2m^2 \phi^\dagger \phi + g(\phi^\dagger \phi)^2$ are consistent with the results of Sec. III. We also compare these analytic predictions with results of Monte Carlo simulations of the quartic ensemble for various values of m^2 and g. The numerical results we obtained for the eigenvalue distribution in the disk phase and in the annular phase, as well as some quantitative features of the disk-annulus transition, are in good agreement with the analytic predictions in Ref. 4.

The ''single ring theorem'' may seem surprising at first sight. Our explanation of why the single ring theorem is not that surprising rests upon the simple argument that fragmentation of the eigenvalue distribution of $\phi^\dagger \phi$ into several disjoint segments does not necessarily imply that the eigenvalues of ϕ trace out annuli obtained, loosely speaking, by revolving the segments of the eigenvalue distribution of $\phi^\dagger \phi$ into the complex plane (see the discussion in Sec. II). In Sec. V we carry a numerical check of the ''single ring'' theorem for the sextic potential $V(\phi^\dagger \phi) = m^2 \phi^\dagger \phi + (\lambda/2)(\phi^\dagger \phi)^2 + (g/3)(\phi^\dagger \phi)^3$, which is the potential of lowest degree for which the eigenvalues of $\phi^\dagger \phi$ may split into more than a single segment (in this case, two segments at the most). We generated numerically an ensemble in which the spectrum of $\phi^\dagger \phi$ is split into two separated segments, yet we found that the spectrum of ϕ is a disk, and not a configuration of a disk encircled by a concentric annulus, as one would perhaps naively expect by rotating the two-segment spectrum of $\phi^\dagger \phi$ in the complex plane.

In the Appendix we briefly review the multi-cut phase structure of matrix ensembles with generic $V(\phi^\dagger \phi)$, and then specialize to the phase structure of the sextic potential ensemble.

II. THE METHOD OF HERMITIZATION AND NON-GAUSSIAN ENSEMBLES

Here we very briefly summarize the "method of Hermitization" [3,4] in the form of an algorithm, followed by a general discussion of the phase structure of the eigenvalue distribution.

Let us first introduce some notations and definitions. The averaged density of eigenvalues

$$\rho(x,y)=\left\langle \frac{1}{N}\sum_i \delta(x-\mathrm{Re}\,\lambda_i)\,\delta(y-\mathrm{Im}\,\lambda_i)\right\rangle \tag{2.1}$$

of the non-Hermitian matrix ϕ may be determined from the the Green's function associated with ϕ, namely,

$$G(z,z^*)=\left\langle \frac{1}{N}\mathrm{tr}\,\frac{1}{z-\phi}\right\rangle=\int d^2x'\,\frac{\rho(x',y')}{z-z'}, \tag{2.2}$$

in terms of which[14]

$$\rho(x,y)=\frac{1}{\pi}\partial^*\,G(z,z^*). \tag{2.3}$$

The probability distributions (1.1) studied in this article are invariant under $\phi\to e^{i\alpha}\phi$, rendering

$$\rho(x,y)\equiv\rho(r)/2\pi \tag{2.4}$$

circularly invariant. Rotational invariance thus leads to a simpler form of the defining formula (2.2) for $G(z,z^*)$ which reads

$$\gamma(r)\equiv zG(z,z^*)=\int_0^r r'dr'\,\rho(r'), \tag{2.5}$$

and thus

$$\rho(r)=\frac{1}{r}\,\frac{d\gamma}{dr}. \tag{2.6}$$

Clearly, the quantity $\gamma(r)$, which can be thought of as the integrated eigenvalue density, is a positive monotonically increasing function, which satisfies the obvious "sum-rules"

$$\gamma(0)=0 \quad \text{and} \quad \gamma(\infty)=1. \tag{2.7}$$

In particular, observe that the first condition in (2.7) insures that no $\delta(x)\,\delta(y)$ spike arises in $\rho(x,y)$ when calculating it from (2.3) with $G(z,z^*)$ given by (2.5), as it should be.

It was shown in Ref. 4 that by applying a simple trick, the desired Green's function of a non-Hermitian random matrix ϕ could be obtained with a minimal amount of work, by judiciously exploiting the existing literature on random Hermitian matrices. The algorithm, according to Ref. 4, for finding the Green's function and the averaged eigenvalue density of a non-Hermitian random matrix ϕ drawn from a non-Gaussian ensemble $P(\phi)=(1/Z)e^{-N\mathrm{tr}V(\phi^\dagger\phi)}$ [Eq. (1.1)] is as follows:

Start with the Green's function

$$F(w)=\left\langle \frac{1}{N}\mathrm{tr}_{(N)}\frac{1}{w-\phi^\dagger\phi}\right\rangle\equiv\int_0^\infty\frac{\tilde\rho(\sigma)d\sigma}{w-\sigma}, \tag{2.8}$$

where

$$\tilde{\rho}(\mu)=\frac{1}{N}\langle \mathrm{tr}_{(N)}\,\delta(\mu-\phi^\dagger\phi)\rangle \tag{2.9}$$

is the averaged eigenvalue density of $\phi^\dagger\phi$. [Of course, $F(w)$ is already known in the literature on chiral and rectangular block random Hermitian matrices for the Gaussian distribution,[11,15–17] as well as for non-Gaussian probability distributions of the form (1.1) with an arbitrary polynomial potential $V(\phi^\dagger\phi)$.[18–20]] Then, the desired equation for $\gamma(r)\equiv zG(z,z^*)$ is

$$\gamma\left[r^2F\left(\frac{\gamma r^2}{\gamma-1}\right)-\gamma+1\right]=0. \tag{2.10}$$

Thus, given F one can solve for $\gamma(r)$ using this master equation.

Equation (2.10) is an algebraic equation for $\gamma(r)$ and thus may have several r dependent solutions. In constructing the actual $\gamma(r)$ one may have to match these solutions smoothly into a single function which increases monotonically from $\gamma(0)=0$ to $\gamma(\infty)=1$. An explicit nontrivial example of such a procedure is the construction of $\gamma(r)$ in the disk phase of the quartic ensemble.[4]

A remarkable property of (2.10) is that it has only two r-independent solutions: $\gamma=0$ and $\gamma=1$.[4] Since the actual $\gamma(r)$ increases monotonically from $\gamma(0)=0$ to $\gamma(\infty)=1$, we immediately conclude from this observation that there can be no more than a single void in the eigenvalue distribution. Thus, in the class of models governed by $P(\phi)=(1/Z)\,e^{-N\mathrm{tr}V(\phi^\dagger\phi)}$ [Eq. (1.1)], the shape of the eigenvalue distribution is either a disk or an annulus, whatever polynomial the potential $V(\phi^\dagger\phi)$ is. This result is the ''single ring theorem'' of Ref. 4.

The ''single ring theorem'' may appear counter-intuitive at first sight. Indeed, consider a potential $V(\phi^\dagger\phi)$ with several wells or minima. For deep enough wells, we expect the eigenvalues of $\phi^\dagger\phi$ to ''fall into the wells.'' Thus, one might suppose that the eigenvalue distribution of ϕ to be bounded by a set of concentric circles of radii $0\leqslant r_1<r_2<\cdots<r_{n_{\max}}$, separating annular regions on which $\rho(r)>0$ from voids (annuli in which $\rho(r)=0$.) *A priori*, it is natural to assume that the maximal number of such circular boundaries should grow with the degree of V, because V may then have many deep minima. Remarkably, however, according to the ''single ring theorem'' the number of these boundaries is two at the most.

To reconcile this conclusion with the *a priori* expectation just mentioned, note that while the eigenvalues of the Hermitian matrix $\phi^\dagger\phi$ may split into several disjoint segments along the positive real axis, this does not necessarily constrain the eigenvalues of ϕ itself to condense into annuli. Indeed, the Hermitian matrix $\phi^\dagger\phi$ can always be diagonalized $\phi^\dagger\phi=U^\dagger\Lambda^2U$ by a unitary matrix U, with $\Lambda^2=\mathrm{diag}(\lambda_1^2,\lambda_2^2,...,\lambda_N^2)$, where the λ_i are all real. This implies that $\phi=V^\dagger\Lambda U$, with V a unitary matrix as well. Thus, the complex eigenvalues of ϕ are given by the roots of $\det(z-\Lambda W)=0$, with $W=UV^\dagger$. Evidently, as W ranges over $U(N)$ (which is what we expect to happen in the generic case), the eigenvalues of ΛW could be smeared (in the sense that they would not span narrow annuli around the circles $|z|=|\lambda_i|$.)

The last argument in favor of the ''single ring theorem'' clearly breaks down when W fails to range over $U(N)$, which occurs when the unitary matrices U and V are correlated. For example, ϕ may be such that $W=UV^\dagger$ is block diagonal, with the upper diagonal block being a $K\times K$ unitary diagonal matrix $\mathrm{diag}(e^{i\omega_1},...,e^{i\omega_K})$ (and with K a finite fraction of N). In the extreme case $K=N$, in which W is completely diagonal, $W\equiv e^{i\omega}=\mathrm{diag}(e^{i\omega_1},...,e^{i\omega_N})$, we see that $\phi=U^\dagger e^{i\omega}\Lambda U$ is a *normal* matrix (i.e., $[\phi,\phi^\dagger]=0$), with eigenvalues $\mathrm{diag}(e^{i\omega_1}\lambda_1,...,e^{i\omega_N}\lambda_N)$. Thus, normal matrices, or partially normal matrices (i.e., the case $K<N$), evade the ''single ring'' theorem: if the first K eigenvalues $\lambda_1^2,\lambda_2^2,\ldots,\lambda_K^2$ of $\phi^\dagger\phi$ split into several disjoint segments along the positive real axis, the corresponding eigenvalues of ϕ will split into concentric annuli in the complex plane obtained by revolving those λ-segments.

As a concrete demonstration of the latter qualitative discussion consider (1.1) with ϕ a normal matrix. According to the previous paragraph, we may diagonalize our normal matrix as ϕ

$=U^{\dagger}ZU$ with complex eigenvalues $Z=\mathrm{diag}(z_1,...,z_N)$, and U a unitary matrix. Thus, ϕ may be considered as a Hermitian matrix whose eigenvalues were continued into the complex plane. Thus, the partition function associated with (1.1) for ϕ normal,[21]

$$Z=\int \prod_{k=1}^{N} d^2z_k \prod_{i<j} |z_i-z_j|^2 \exp -N\sum_i V(|z_i|^2), \tag{2.11}$$

is a trivial generalization of the partition function of Hermitian matrices, where the complex eigenvalues form a two dimensional Dyson gas. It is expressed purely in terms of the complex eigenvalues z_i, contrary to ensembles of complex matrices (1.1) with a generic potential V. [With the exception, of course, of Ginibre's ensemble $V\sim\phi^{\dagger}\phi$,[12] for which the diagonalizing $GL(N)$ matrix can be integrated out explicitly, yielding (2.11).] Clearly, if $V(|z|^2)$ had several well separated and deep minima, the z_i would fall into them, and in principle produce an arbitrary number of eigenvalue rings, depending on V. Thus, normal matrices evade the single ring theorem.

Normal, or partially normal matrices, are, of course, extremely rare in the ensembles of non-Hermitian matrices, studied in this article, and do not affect the "single ring" behavior of the bulk of matrices in the ensemble.

We end this section by showing how simple features of $F(w)$ indicate whether the domain of the eigenvalue distribution is a disk or an annulus. As is well known,[11,19,20] for V a polynomial of degree p, the Green's function $F(w)$ is given by

$$F(w)=\tfrac{1}{2}V'(w)-P(w)\sqrt{(w-a)(w-b)}, \tag{2.12}$$

where

$$P(w)=\sum_{k=-1}^{p-2} c_k w^k. \tag{2.13}$$

(Here we assume for simplicity that the eigenvalues of $\phi^{\dagger}\phi$ condense into a single segment $[a,b]$. Discussion of condensation of $\phi^{\dagger}\phi$ eigenvalues into more segments appears in the Appendix.) The real constants $0\leqslant a<b$ and c_k are then determined completely by the requirement that $F(w)\to 1/w$ as w tends to infinity, and by the condition that $F(w)$ has at most an integrable singularity as $w\to 0$. Thus, if $a>0$, inevitably $c_{-1}=0$. However, if $a=0$, then c_{-1} will be determined by the asymptotic behavior for w large.

According to the "single ring" theorem,[4] the eigenvalue distribution of ϕ is either a disk or an annulus. The behavior of $F(w)$ as $w\sim 0$ turns out to be an indicator as to which phase of the two the system is in, as we now show:

A. Disk phase

In the disk phase we expect that $\rho(0)>0$, as in Ginibre's case. Thus, from (2.6) $\rho(r)=(1/r)(d\gamma/dr)\equiv 2(d\gamma/dr^2)$ and from the first sum rule $\gamma(0)=0$ in (2.7) we conclude that

$$\gamma(r)\sim \tfrac{1}{2}\rho(0)r^2 \tag{2.14}$$

near $r=0$. Therefore, for r small, (2.10) yields

$$F\left(-\frac{\rho(0)r^4}{2}+\cdots\right)\sim -\frac{1}{r^2}, \tag{2.15}$$

namely, $F(w)\sim 1/\sqrt{w}$ for $w\sim 0$, as we could have anticipated from Ginibre's case.[22] This means that in the disk phase we must set $a=0$ in (2.12). Consequently, in the disk phase c_{-1} does not vanish. We can do even better: paying attention to the coefficients in (2.12) and (2.13) (with $a=0$) we immediately obtain from (2.15) that

$$c_{-1}=\sqrt{\frac{\rho(0)}{2b}}. \tag{2.16}$$

B. Annular phase

In the annular phase $\gamma(r)$ must clearly vanish identically in the inner void of the annulus. Thus, (2.10) implies that $F(w)$ cannot have a pole at $w=0$, and therefore from (2.12) we must have $c_{-1}\sqrt{ab}=0$. Thus, the annulus must arise for $c_{-1}=0$ (the other possible solution $a=0$, $c_{-1}\neq 0$ leads to a disk configuration with $\gamma=0$ only at $r=0$, as we just discussed.)

Thus, to summarize, in the disk phase F has the form

$$F_{\text{disk}}(w)=\frac{1}{2}V'(w)-\left(\sqrt{\frac{\rho(0)}{2b}}w^{-1}+c_0+c_1 w+\cdots+c_{p-2}w^{p-2}\right)\sqrt{w(w-b)}, \tag{2.17}$$

while in the annular phase it has the form

$$F_{\text{annulus}}(w)=\tfrac{1}{2}V'(w)-(c_0+c_1 w+\cdots+c_{p-2}w^{p-2})\sqrt{(w-a)(w-b)}. \tag{2.18}$$

Having determined $F(w)$ in this way, i.e., having determined the various unknown parameters in (2.17) or in (2.18), we substitute it into (2.10) and find $G(z,z^*)$. We can thus calculate the density of eigenvalues $\rho(r)$ explicitly for an arbitrary V.

We now turn to the disk-annulus phase transition. An important feature of this transition is that $F(w)$ is continuous through it. To see this we argue as follows: By tuning the couplings in V, we can induce a phase transition from the disk phase into the annular phase, or vice versa. Note, of course, that we can parametrize any point in the disk phase either by the set of couplings in V or by the set of parameters $\{c_{-1},c_0,\ldots,c_{p-2};b\}$ in (2.17). The "coordinate transformation" between these two sets of parameters is encoded in the asymptotic behavior of $F(w)$. Similarly, we can parametrize any point in the annular phase either by the set of couplings in V or by the set of parameters $\{c_0,c_1,\ldots,c_{p-2};a,b\}$ in (2.18). Due to the one-to-one relation (in a given phase, once we have established it is the stable one) between the couplings in V and the parameters in $F(w)-\frac{1}{2}V'(w)$ [namely, the c_n's and the locations of the branch points of $F(w)$], we can describe the disk-annulus transition in terms of the latter parameters (instead of the couplings in V). Clearly, the transition point is reached from the disk phase when $\rho(0)=0$, that is, when c_{-1} in (2.17) vanishes:

$$c_{-1}^{\text{crit}}=0. \tag{2.19}$$

Similarly, the transition point is reached from the annular phase when the lower branch point a in (2.18) vanishes. Thus, e.g., in a transition from the disk phase into the annular phase, $F_{\text{disk}}(w)$ in (2.17) would cross-over continuously into $F_{\text{annulus}}(w)$ in (2.18) through a critical form

$$F_{\text{crit}}(w)=\tfrac{1}{2}V'_{\text{crit}}(w)-(c_0^{\text{crit}}+c_1^{\text{crit}}w+\cdots+c_{p-2}^{\text{crit}}w^{p-2})\sqrt{w(w-b^{\text{crit}})}. \tag{2.20}$$

The continuity of $F(w)$ through the transition was demonstrated explicitly in Ref. 4 for the quartic ensemble $V(\phi^\dagger\phi)=2m^2\phi^\dagger\phi+g(\phi^\dagger\phi)^2$ (see also Sec. IV).

This discussion obviously generalizes to cases when $F(w)$ has multiple cuts, which correspond to condensation of the eigenvalues of $\phi^\dagger\phi$ into many segments. If $w=0$ is a branch point of $F(w)$, that is, if the lowest cut extends to the origin, we are in the disk phase,

$$F_{\text{disk}}(w)=\tfrac{1}{2}V'(w)-(c_{-1}w^{-1}+c_0+c_1 w+\cdots+c_{p-2}w^{p-2})\sqrt{w(w-b_1)\cdots(w-b_n)}, \tag{2.21}$$

with $0<b_1<\cdots<b_n$. The relation (2.16) then generalizes to

$$c_{-1}=\sqrt{\frac{\rho(0)}{2(-1)^{n+1}\Pi_{k=1}^{n}b_k}}. \tag{2.22}$$

Since c_{-1} must be real we conclude that such a configuration exists only for n odd.

If the lowest branch point in $F(w)$ is positive, we are in the annular phase with

$$F_{\text{annulus}}(w)=\tfrac{1}{2}V'(w)-(c_0+c_1 w+\cdots+c_{p-2}w^{p-2})\sqrt{(w-a)(w-b_1)\cdots(w-b_n)}. \tag{2.23}$$

The phase transition would occur when the couplings in $V(\phi^\dagger\phi)$ are tuned such that $F_{\text{disk}}(w)$ and $F_{\text{annulus}}(w)$ match continuously, as was described in the previous paragraph.

III. BOUNDARIES AND BOUNDARY VALUES

Remarkably, with a minimal amount of effort, and based on the mere definition of $F(w)$ [Eq. (2.8), which we repeat here for convenience],

$$F(w)=\left\langle \frac{1}{N}\,\mathrm{tr}_{(N)}\frac{1}{w-\phi^\dagger\phi}\right\rangle \equiv \int_0^\infty \frac{\tilde{\rho}(\sigma)d\sigma}{w-\sigma}, \tag{3.1}$$

we are able to derive simple expressions for the location of the boundaries of the eigenvalue distribution and also for the boundary values of $\rho(r)$ in terms of the moments of $\tilde{\rho}(\sigma)$, which, we remind the reader, is the density of eigenvalues for a Hermitian matrix problem.

To this end it is useful to rewrite our master formula (2.10) for $\gamma(r)$ as

$$wF(w)=\gamma \tag{3.2}$$

with

$$w=\frac{\gamma r^2}{\gamma-1}. \tag{3.3}$$

We start with the outer edge $r=R_{\text{out}}$ (either in the disk phase or in the annular phase.) Near the outer edge $\gamma\to 1-$, and thus $w\to-\infty$. We therefore expand $F(w)$ in powers of $1/w$ and obtain from (3.1)–(3.3)

$$\frac{\langle\sigma\rangle}{r^2}+\frac{\gamma-1}{\gamma r^4}\langle\sigma^2\rangle+\frac{(\gamma-1)^2}{\gamma^2 r^6}\langle\sigma^3\rangle+\cdots=\gamma, \tag{3.4}$$

where

$$\langle\sigma^k\rangle=\int_0^\infty \tilde{\rho}(\sigma)\sigma^k d\sigma \tag{3.5}$$

are the moments of $\tilde{\rho}(\sigma)$ (which is of course normalized to 1). For the class of models we are interested in here, all the moments $\langle\sigma^k\rangle$, $k\geqslant 0$ are clearly finite. [$\tilde{\rho}(\sigma)\equiv(1/\pi)\mathrm{Im}\,F(\sigma-i\epsilon)$ is supported along a finite segment (or segments), and its singularity at $\sigma=0$ is no worse than $\sigma^{-1/2}$.] Thus, at the outer edge $r=R_{\text{out}}$ [where of course $\gamma(R_{\text{out}})=1$], all terms with $\langle\sigma^k\rangle$, $k\geqslant 2$, drop out of (3.4) and we obtain

$$R_{\text{out}}^2=\langle\sigma\rangle. \tag{3.6}$$

Namely, R_{out}^2 is simply the first moment of $\tilde{\rho}(\sigma)$.

We now calculate the boundary value $\rho(R_{\text{out}})$. Approaching R_{out} from the inside, we substitute $\gamma=1-f$ and $r^2=R_{\text{out}}^2(1-\delta)$ (with $f,\delta\ll 1$) in (3.4). After some work we obtain $f=\langle\sigma\rangle^2/[\langle\sigma^2\rangle-\langle\sigma\rangle^2]\,\delta+\mathcal{O}(\delta^2)$, namely,

$$\gamma=1-\frac{\langle\sigma\rangle^2}{\langle\sigma^2\rangle-\langle\sigma\rangle^2}\,\delta+\mathcal{O}(\delta^2). \tag{3.7}$$

Thus, from $\rho(r)=2(d\gamma/dr^2)$ [Eq. (2.6)] and (3.6) we find

$$\rho(R_{\text{out}})=\frac{2R_{\text{out}}^2}{\langle\sigma^2\rangle-\langle\sigma\rangle^2}. \tag{3.8}$$

The density $\rho(R_{\text{out}})$ is inversely proportional to the variance of σ!

For the $\tilde{\rho}(\sigma)$ under consideration here, $\langle\sigma^2\rangle$, and consequently $\rho(R_{\text{out}})$, are always finite. Outside the boundary $\rho(r)$ vanishes identically, of course, and, thus, $\rho(r)$ always "falls off a cliff" at the boundary, for all probability distributions of the form (1.1) with V polynomial. It would be thus interesting to study circularly invariant matrix ensembles $P(\phi^\dagger\phi)$ such that the eigenvalue distribution $\tilde{\rho}(\sigma)$ of $\phi^\dagger\phi$ has a finite $\langle\sigma\rangle$ but an infinite $\langle\sigma^2\rangle$. Then $\rho(R_{\text{out}})$ would vanish. This would naturally raise the question whether in such situations, $\rho(r)$ behaves universally near the edge [that is, if near the edge it vanishes like $(R_{\text{out}}-r)^\epsilon$ with ϵ being some universal exponent]. We do not pursue this question further in this article.

We now turn to the annular phase, and focus on the inner edge $r=R_{\text{in}}$ of the annulus. According to the discussion at the end of Sec. II [see Eq. (2.18) and the discussion preceding it], $a>0$ in (2.12), and thus $F(w)$ is analytic in the domain $|w|<a$. Expanding (3.1) in powers of w, we obtain from (3.2)

$$\frac{1-\gamma}{r^2}-\left\langle\frac{1}{\sigma}\right\rangle=w\left\langle\frac{1}{\sigma^2}\right\rangle+w^2\left\langle\frac{1}{\sigma^3}\right\rangle+\cdots. \tag{3.9}$$

A little above the inner radius, into the annulus, clearly $\gamma\to 0$ and $w\to 0-$ in (3.3). Thus, setting $w=0$ in (3.9) we obtain

$$\frac{1}{R_{\text{in}}^2}=\left\langle\frac{1}{\sigma}\right\rangle. \tag{3.10}$$

R_{in}^{-2} is simply the σ^{-1} moment of $\tilde{\rho}(\sigma)$.

We can now calculate the boundary value $\rho(R_{\text{in}})$. Near the inner edge we parametrize $r^2=R_{\text{in}}^2(1+\delta)$ with $\delta\ll 1$ (and of course, $\gamma\ll 1$ to begin with). Since $\tilde{\rho}(\sigma)$ obviously vanishes for $\sigma<a$, all moments $\langle\sigma^{-k}\rangle$ in (3.9) are finite. Thus, dropping all terms with $\langle\sigma^{-k}\rangle$, $k\geqslant 3$, in (3.9), we obtain after some work

$$\gamma=R_{\text{in}}^{-4}\frac{\delta}{\langle\sigma^{-2}\rangle-\langle\sigma^{-1}\rangle^2}+\mathcal{O}(\delta^2). \tag{3.11}$$

It then follows from (2.6) and (3.10) that

$$\rho(R_{\text{in}})=\frac{2R_{\text{in}}^{-6}}{\langle\sigma^{-2}\rangle-\langle\sigma^{-1}\rangle^2}. \tag{3.12}$$

The density $\rho(R_{\text{out}})$ is inversely proportional to the variance of σ^{-1}.

From (2.12) [or (2.18)] we learn that in the annular phase $\tilde{\rho}_{\text{annulus}}(\sigma)\equiv(1/\pi)\text{Im}F(\sigma-i\epsilon)$ $=\text{polynomial}(\sigma)\sqrt{(\sigma-a)(b-\sigma)}$, $0<a<\sigma<b$ (and vanishes elsewhere.) Thus, $\langle 1/\sigma^k\rangle$ $\equiv\int_a^b(\tilde{\rho}(\sigma)/\sigma^k)d\sigma$, $k=1,2$, are finite. Therefore, $\rho_{\text{annulus}}(r)$ jumps from zero (in the inner void of

the annulus) to a finite value at the inner edge $R_{\rm in}$. Note, however, that when $a\to 0$, that is, in the annular to disk transition, $\langle 1/\sigma\rangle$ remains finite, but $\langle 1/\sigma^2\rangle$ diverges like $1/\sqrt{a}$. [For a particular example, see Eq. (4.18).] Thus, from (3.10) we see that $R_{\rm inner}(a=0)$, the *critical* inner radius, is finite. The annulus starts up with a finite inner radius. Also, in this limit, we see from (3.12) that $\rho(R_{\rm in})$ vanishes like $\sqrt{a}$. As we approach the annulus-disk transition, the discontinuity in $\rho(r)$ at the (finite) inner edge disappears.

We saw at the end of Sec. II [see Eqs. (2.17)–(2.20)] that $F(w)$ is continuous through the disk-annulus phase transition. Thus, our master formula $wF(w)=\gamma$ to determine $\gamma(r)$ [Eq. (3.2)] is also continuous through the transition. Consequently, $\rho(r)=(1/r)(d\gamma/dr)$ must remain continuous through the disk-annulus transition, and has (at the transition) the universal behavior described in the previous paragraph.

IV. PHASE TRANSITIONS IN THE QUARTIC ENSEMBLE

The disk-annulus transition in the quartic ensemble

$$V(\phi^\dagger\phi)=2m^2\phi^\dagger\phi+g(\phi^\dagger\phi)^2 \tag{4.1}$$

was studied in detail in Ref. 4. The annular eigenvalue distribution $\rho_{\rm annular}(r)$ and the disk eigenvalue distribution $\rho_{\rm disk}(r)$ for this ensemble were calculated explicitly in Ref. 4. According to the expressions given in Ref. 4, as the critical point is approached from the annular phase, $\rho_{\rm annular}(r)$ behaves precisely as described in the paragraph following Eq. (3.12) at the end of the previous section [see also Eq. (4.13), at $\mu=\mu_c$.] Also according to Ref. 4, as the critical point is approached from the disk phase, $\rho_{\rm disk}(r)$ gets completely depleted inside a region of radius $R_{\rm in}(\mu_c)$ [remaining continuous at $r=R_{\rm in}(\mu_c)$]. [See Eq. (4.20).] Thus, $\rho(r)$ for the quartic ensemble is continuous through the disk-annulus transition.

In this section we verify the expressions (3.6), (3.8), (3.10) and (3.12) for $R_{\rm out}$, $\rho(R_{\rm out})$, $R_{\rm in}$ and $\rho(R_{\rm in})$ for the quartic ensemble (4.1) against the explicit expressions for these quantities given in Ref. 4, and also provide ample numerical results concerning the disk phase, the annular phase, and the transition between them, in support of the analytical results. In what follows we have omitted many technical details that can be found in Ref. 4.

A. The disk phase

For $m^2>-\sqrt{2g}$ the density of eigenvalues is a disk. According to Ref. 4 we have

$$F(w)=m^2+gw-\left(\frac{c}{w}+g\right)\sqrt{w(w-b)} \tag{4.2}$$

with

$$c=\frac{2m^2+\sqrt{m^4+6g}}{3}\quad\text{and}\quad b=\frac{-2m^2+2\sqrt{m^4+6g}}{3g}. \tag{4.3}$$

According to Eqs. (5.8) and (5.9) in Ref. 4, the eigenvalue density in this phase is

$$\rho_{\rm disk}(r)=2m^2+4gr^2+2\left[\,\mathrm{sgn}\left(\frac{b}{4}-r^2\right)\right]\frac{bc^2-(m^2+2gr^2)[1+2(m^2r^2+gr^4)]}{\sqrt{[1+2(m^2r^2+gr^4)]^2-4bc^2r^2}} \tag{4.4}$$

inside a disk of radius $R_{\rm out}$, where

$$R_{\rm out}^2=\frac{bc^2-2m^2}{2g}=\frac{(m^4+6g)^{3/2}-m^2(m^4+9g)}{27g^2}. \tag{4.5}$$

Thus, from (4.4) and (4.5) we have[23]

$$\rho_{\rm disk}(R_{\rm out})=\frac{4g(bc^2-2m^2)}{2g-bc^2(bc^2-2m^2)}=\frac{4gR_{\rm out}^2}{1-2R_{\rm out}^2(gR_{\rm out}^2+m^2)}. \tag{4.6}$$

These results should be compared with the predictions of Sec. III. From (4.2) we can read-off the density of eigenvalues $\tilde{\rho}(\sigma)=(1/\pi)\mathrm{Im}\,F(\sigma-i\epsilon)$ of $\phi^\dagger\phi$ as

$$\tilde{\rho}(\sigma)=\frac{1}{\pi}\left(\frac{c}{\sigma}+g\right)\sqrt{\sigma(b-\sigma)} \tag{4.7}$$

for $0\leqslant\sigma\leqslant b$, and zero elsewhere. We can readily check that (4.7) is properly normalized to 1.

The first two moments of (4.7) are

$$\langle\sigma\rangle=\frac{1}{2}\left(\frac{b}{2}\right)^2\left(c+\frac{gb}{2}\right)=\frac{(m^4+6g)^{3/2}-m^2(m^4+9g)}{27g^2}, \tag{4.8}$$

and

$$\langle\sigma^2\rangle=\frac{1}{8}\left(\frac{b}{2}\right)^4\left(\frac{8c}{b}+5g\right)=\frac{27g^2+18gm^4+2m^8-2m^2(6g+m^4)^{3/2}}{54g^3}. \tag{4.9}$$

Thus,

$$\begin{aligned}\langle\sigma^2\rangle-\langle\sigma\rangle^2&=-\frac{b^3}{256}[4bc^2+bg(b^2g-10)+4c(b^2g-4)]\\&=\frac{297g^3+108g^2m^4-18gm^8-4m^{12}-2m^2(9g-2m^4)(6g+m^4)^{3/2}}{1458g^4}.\end{aligned} \tag{4.10}$$

Comparing (4.5) and (4.8) we immediately verify (3.6), $R_{\rm out}^2=\langle\sigma\rangle$. After some additional work, using (4.10) and (4.5) in (3.8), we can see that (3.8), namely, that $\rho(R_{\rm out})=2R_{\rm out}^2/(\langle\sigma^2\rangle-\langle\sigma\rangle^2)$, coincides with (4.6).

1. Numerical results for the disk phase

We have generated numerically random matrix ensembles corresponding to the quartic potential (4.1) in the disk phase, for $m^2=1$ fixed and for various values of the coupling g (and for various sizes of matrices), and measured $\rho_{\rm disk}(r)$ for these realizations.

The generation of the matrices was done by a standard Metropolis Monte Carlo approach. A random change had been suggested in the real and imaginary parts of one of the elements of ϕ and then the change in $V(\phi)$ was evaluated. This ''move'' was accepted unconditionally if V was decreased, and with probability $p=e^{-\Delta V}$ if V was increased. General theorems on Monte Carlo then guaranteed that the resulting probability distribution of ϕ was the desired one. After the matrices were generated, their eigenvalues were determined with a standard solver from the LAPACK library. We tuned the size of the suggested changes in ϕ so that the acceptance rate was about one-half, and monitored the equilibration and autocorrelation times to ensure our starting configuration had evolved properly and error bars were accurate. In particular, the local changes in ϕ made the matrices correlated over some number of random changes, however, local changes also allowed one to employ various tricks to evaluate the change in V rapidly.

In Fig. 1 we display our numerical results for $\rho_{\rm disk}(r)$ for 128×128 dimensional matrices, and compare them to the analytical large-N result (4.4) of Ref. 4. [As a trivial check of our numerical code, we also included in this figure the results for the Gaussian (Ginibre) ensemble.] Evidently, the agreement between the numerical and the analytical results is good. Note the finite-N effects near the edge of the disk.

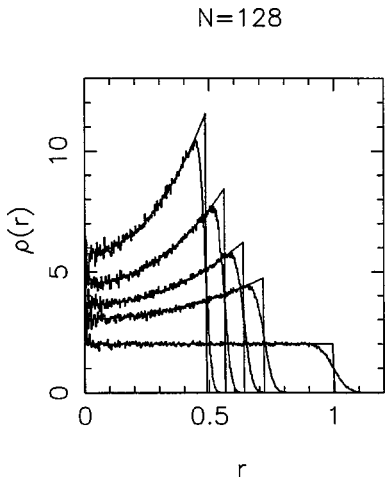

FIG. 1. Comparison between Monte Carlo measurements of the density of eigenvalues $\rho(r)$ of matrices ϕ of size 128×128, taken from the quartic ensemble $V(\phi^\dagger\phi)=2m^2\phi^\dagger\phi+g(\phi^\dagger\phi)^2$ with $m^2=0.5$ (disk phase) and for $g=0$, 0.5, 1, 2, 4 (g increases from bottom to top), compared to the analytical results of Ref. 4 (solid lines). At $g=0$ we obtain Ginibre's Gaussian ensemble with $V=\phi^\dagger\phi$, with its unit disk of eigenvalues.

B. The annular phase

For $m^2<-\sqrt{2g}$, the stable eigenvalue distribution is annular. For convenience, let us switch notations according to $m^2=-\mu^2$, and also write $\mu_c^2=\sqrt{2g}$.

According to Ref. 4 we have

$$F(w)=m^2+gw-g\sqrt{(w-a)(w-b)} \tag{4.11}$$

with

$$a=\frac{\mu^2}{g}-\sqrt{\frac{2}{g}} \quad \text{and} \quad b=\frac{\mu^2}{g}+\sqrt{\frac{2}{g}}. \tag{4.12}$$

We see that $a=(2/\mu_c^4)(\mu^2-\mu_c^2)$ which is positive for $\mu^2>\mu_c^2$, as it should be, by definition.

According to Eqs. (5.16)–(5.19) in Ref. 4, the eigenvalue density in this phase is

$$\rho_{\text{annulus}}(r)=8g\left(r^2-\frac{\mu^2}{2g}\right)=8g\left(r^2-\frac{\mu^2}{\mu_c^4}\right) \tag{4.13}$$

inside an annulus $R_{\text{in}}\leqslant r\leqslant R_{\text{out}}$, where

$$R_{\text{in}}^2=\frac{\mu^2+\sqrt{\mu^4-2g}}{2g}=\frac{\mu^2+\sqrt{\mu^4-\mu_c^4}}{\mu_c^4} \tag{4.14}$$

and

$$R_{\text{out}}^2=\frac{\mu^2}{g}=\frac{2\mu^2}{\mu_c^4}. \tag{4.15}$$

Thus, we see immediately that

$$\begin{aligned}\rho(R_{\text{in}})&=4\sqrt{\mu^4-\mu_c^4}\\ \rho(R_{\text{out}})&=4\mu^2.\end{aligned} \tag{4.16}$$

Note that $\rho(R_{\rm in})=0$ at $\mu=\mu_c$, as expected. Also note that the critical annulus has a finite inner radius: $R^2_{\rm in}(\mu_c)=1/\mu_c^2>0$.

We now compare these results with the predictions of Sec. III. From (4.11) we read-off the density of eigenvalues of $\phi^\dagger\phi$:

$$\tilde{\rho}(\sigma)=\frac{g}{\pi}\sqrt{(\sigma-a)(b-\sigma)} \tag{4.17}$$

for $a\leqslant\sigma\leqslant b$, and zero elsewhere. We can check that (4.17) is properly normalized to 1.

The relevant moments of (4.17) are

$$\begin{aligned}
\langle\sigma\rangle&=\frac{g}{2}\left(\frac{a+b}{2}\right)\left(\frac{b-a}{2}\right)^2=\frac{\mu^2}{g},\\
\langle\sigma^2\rangle&=\frac{g}{2}\left(\frac{b-a}{2}\right)^4\left[\left(\frac{b+a}{b-a}\right)^2+\frac{1}{4}\right]=\frac{\mu^4}{g^2}+\frac{1}{2g},\\
\left\langle\frac{1}{\sigma}\right\rangle&=\frac{g}{2}(\sqrt{b}-\sqrt{a})^2=\mu^2-\sqrt{\mu^4-2g}\\
\left\langle\frac{1}{\sigma^2}\right\rangle&=\frac{g}{2}\frac{(\sqrt{b}-\sqrt{a})^2}{\sqrt{ab}}=g\,\frac{\mu^2-\sqrt{\mu^4-2g}}{\sqrt{\mu^4-2g}}.
\end{aligned} \tag{4.18}$$

Comparing (4.14), (4.15) and the first and third equations in (4.18), we verify (3.6) and (3.10) straightforwardly.

Further, we find from (4.18) that

$$\begin{aligned}
\langle\sigma^2\rangle-\langle\sigma\rangle^2&=\frac{1}{2g}\\
\left\langle\frac{1}{\sigma^2}\right\rangle-\left\langle\frac{1}{\sigma}\right\rangle^2&=g-2\mu^4+\mu^2\frac{2\mu^4-3g}{\sqrt{\mu^4-2g}}.
\end{aligned} \tag{4.19}$$

Thus, comparing with (4.16) we find that

$$\frac{2R_{\rm out}^2}{\langle\sigma^2\rangle-\langle\sigma\rangle^2}=4\mu^2=\rho(R_{\rm out})$$

and

$$\frac{2R_{\rm in}^{-6}}{\langle\sigma^{-2}\rangle-\langle\sigma^{-1}\rangle^2}=4\sqrt{\mu^4-\mu_c^4}=\rho(R_{\rm in}),$$

and verify (3.8) and (3.12) for the annular phase.

1. Numerical results for the annular phase

In Figs. 2(a)–2(c) we display our numerical results for $\rho_{\rm annulus}(r)$ for matrices of various sizes, and compare them to the analytical large-N result (4.13) of Ref. 4. In these figures we hold $\mu^2=0.5$ fixed, and increase g from 0.025 to 0.1. (Here we have $\mu^2=0.5=\mu_c^2/2\sqrt{2g}$. Thus increasing g as indicated in the text brings us closer to the disk-annulus phase transition.)

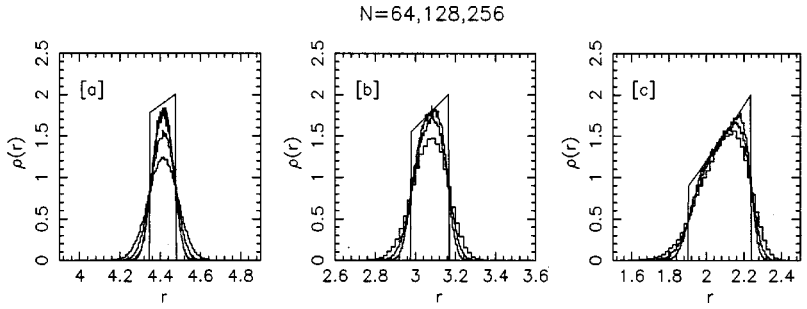

FIG. 2. Results of Monte Carlo measurements of the density of eigenvalues $\rho(r)$ of matrices ϕ of sizes corresponding to $N=64$, 128 and 256, taken from the quartic ensemble with $m^2=-\mu^2=-0.5$ (annular phase) for various values of the quartic coupling: $g=0.025$ in (a), $g=0.05$ in (b) and $g=0.1$ in (c). These are compared to the analytical results of Ref. 4 (solid lines). As N increases, the numerical results converge monotonically to the analytical results.

C. The disk-annulus phase transition

The phase boundary separating the disk phase and the annular phase in the m^2-g plane is the curve $m^2=-\sqrt{2g}$.

Consider approaching this boundary from within the disk phase by setting $m^2=-\sqrt{2g}+\delta$, with δ positive and small. Then, using (4.3), we find to first order in δ that $c=\delta/2$ and $b=2\sqrt{(2/g)}-\delta/g$. In particular, at the phase boundary itself $c=0$, in accordance with (2.19) and (2.20). It was shown in Ref. 4 that as one approaches the critical point $m^2=-\sqrt{2g}$ from the disk phase, the density of eigenvalues of ϕ approches the particularly simple critical configuration

$$\rho_{\mathrm{crit}}(r)=\begin{cases} 0, & r^2<1/\sqrt{2g} \\ 8g\left(r^2-\dfrac{1}{\sqrt{2g}}\right), & 1/\sqrt{2g}<r^2<\sqrt{2/g}. \end{cases} \tag{4.20}$$

Thus, as we decrease δ to zero, $\rho_{\mathrm{disk}}(r)$ [Eq. (4.4)] becomes increasingly depleted inside the disk $r^2<b(\delta)/4$, reaching complete depletion at $\delta=0$, at which point the disk breaks into an annulus. We also note that at the phase boundary (4.2) reads

$$F(w)=-\sqrt{2g}+gw-g\sqrt{w\left(w-2\sqrt{\frac{2}{g}}\right)}. \tag{4.21}$$

Consider now approaching the phase boundary $m^2=-\sqrt{2g}$ from within the annular phase. Thus, we set $\mu^2=\sqrt{2g}+\delta$, with δ positive and small. Then, since all the expressions in (4.12) are linear in μ^2, we find that $a=\delta/g$ and $b=2\sqrt{(2/g)}+\delta/g$. In particular, at the phase boundary itself $a=0$, and $b=1/\sqrt{2g}$. Therefore, at the phase boundary (4.11) reads

$$F(w)=-\sqrt{2g}+gw-g\sqrt{w\left(w-2\sqrt{\frac{2}{g}}\right)},$$

which coincides with (4.21). Thus, $F(w)$ (and consequently, the eigenvalue density of $\phi^\dagger\phi$) is also continuous at the transition, in accordance with (2.20).

Note from (4.14) and (4.15) that at the transition $R_{\mathrm{in}}^2=1/\mu_c^2=1/\sqrt{2g}$ is *finite*, and coincides with the radius (squared) of the depleted region in the disk configuration (4.20). Right at the transition, the disk breaks into an annulus with a finite hole! Note also that $R_{\mathrm{out}}^2=2/\mu_c^2=\sqrt{2/g}$, which coincides with the disk's R_{out}^2 at the phase boundary. Thus, at the phase boundary $\mu^2=\mu_c^2$ (4.13) coincides with (4.20), namely, $\rho(r)$ is continuous at the transition from the disk phase to the annular phase.

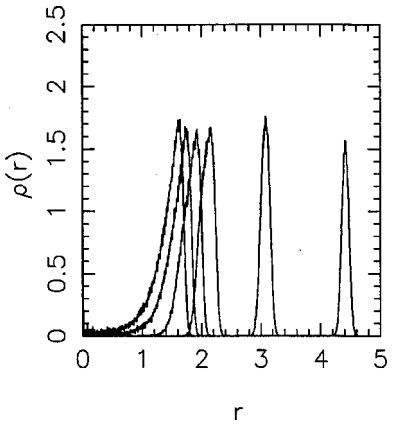

FIG. 3. Monte Carlo measurements of the density of eigenvalues $\rho(r)$ of matrices ϕ of size 128×128, taken from the quartic ensemble with $\mu^2=0.5$ and for $g=0.025$, 0.05, 0.1, 0.125, 0.15 and 0.175 (g increases from right to left). The first three profiles on the right (corresponding to the three lowest values of g) evidently belong to the annular phase. The fourth density profile from the right is the critical one (corresponding to $g_c=0.125$). Finally, the last two profiles (which correspond to the two higher values of g) belong to the disk configuration.

1. Numerical simulation of the disk-annulus phase transition

We have measured the density of eigenvalues $\rho(r)$ of matrices ϕ of size 128×128, taken from the the quartic ensemble with $\mu^2=0.5$ and for $g=0.025$, 0.05, 0.1, 0.125, 0.15 and 0.175. The results are displayed in Fig. 3.

For these values of g, we start in the annular phase at the lowest value of g. For our set of parameters we have $\mu^2=0.5=\mu_c^2/2\sqrt{2g}$. Thus, increasing g (while keeping μ^2 fixed at 0.5) brings us closer to the disk-annulus phase transition, which occurs (at large N) at $g_c=0.125$. Increasing g beyond that, puts us into the disk phase.

The first three profiles on the right in Fig. 3 belong to the annular phase. Their behavior is consistent with our discussion in Sec. IV B of the annular phase. Indeed, as g increases towards the transition point at $g_c=0.125$, these three graphs exhibit the expected decrease of $R_{\rm in}^2=(\mu^2+\sqrt{\mu^4-\mu_c^4})/\mu_c^4$ [Eq. (4.14), with $\mu_c^2=\sqrt{2g}$] and the decrease of $R_{\rm out}^2=2\mu^2/\mu_c^4$ [Eq. (4.15)].

The critical density profile, corresponding to $g_c=0.125$, is the fourth profile (from the right). For our choice of parameters, the theoretical boundary radii of the critical annulus, i.e., at $g=0.125$, are $R_{\rm in}^{\rm crit}=1/\mu_c=\sqrt{2}$ and $R_{\rm out}^{\rm crit}=\sqrt{2}/\mu_c=2$. These boundary values fit nicely with the features of the critical profile in Fig/ 3.

Finally, the last two profiles in Fig. 3 have pronounced tails extending to $r=0$ and thus belong to the disk phase.

V. PHASE TRANSITIONS IN THE SIXTH ORDER POTENTIAL AND THE "SINGLE RING" THEOREM

The sextic potential

$$V(\phi^\dagger\phi)=m^2\phi^\dagger\phi+\frac{\lambda}{2}(\phi^\dagger\phi)^2+\frac{g}{3}(\phi^\dagger\phi)^3 \tag{5.1}$$

is the potential of lowest degree in (1.1) for which the eigenvalues of $\phi^\dagger\phi$ may split into more then a single segment. In fact, it is easy to see that there can be at most two eigenvalue segments in the spectrum of $\phi^\dagger\phi$.

The qualitative features of the support of the eigenvalue density associated with (5.1) can be deduced by moving the cubic $V(x)=m^2x+(\lambda/2)x^2+(g/3)x^3$ around in the plane (i.e., by varying its couplings, fixing, say $g=1$), and concentrating on $x\geqslant0$. It is obvious from such considerations that there are three qualitatively different phases in the spectrum of $\phi^\dagger\phi$. In two of the

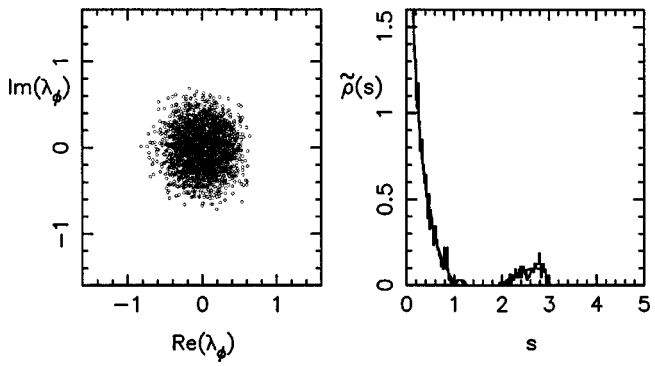

FIG. 4. Scatter plot of the eigenvalues of matrices ϕ of size 32×32, taken from (5.1) with $m^2=7.372$, $\lambda=-6.116$ and $g=1.372$ (left), and the corresponding density of eigenvalues $\tilde{\rho}(s)$ of $\phi^\dagger\phi$ (right). The solid line on the right is the analytical curve corresponding to (A22). The support of $\tilde{\rho}(s)$ is split into the two segments $\{0\leqslant s\leqslant a=1\}\cup\{b=2\leqslant s\leqslant c=3\}$, while the support of $\rho(r)$ on the left is manifestly a disk.

phases the eigenvalues s_i of $\phi^\dagger\phi$ live in a single segment. In one of these single segment phases, the segment includes the origin $(0\leqslant s\leqslant a)$, but in the other it does not $(0<a\leqslant s\leqslant b)$. Following the general discussion in the last part of Sec. II, we would expect that the spectrum of ϕ itself is a disk in the first case, and an annulus in the second case.

In the third phase of $\phi^\dagger\phi$, there are two segments, one of which hits the origin ($\{0\leqslant s\leqslant a\}\cup\{b\leqslant s\leqslant c\}$). (There is no two-segment phase of $\phi^\dagger\phi$ which does not include the origin.) Thus, according to the discussion in the last part of Sec. II, the non-Hermitian matrix ϕ is expected to be in the disk phase in this case (rather than having its eigenvalue fill in a disk surrounded by a concentric annulus), in accordance with the "single ring" theorem.

In this short section we limit our discussion to the two-segment phase of $\phi^\dagger\phi$. [A rather detailed sketch of the analytical conditions that determine the whole phase structure of the sextic ensemble (5.1) is given in the Appendix.] Our purpose here is to demonstrate numerically the "single ring" Theorem for the eigenvalue distribution of matrices ϕ taken from the sextic ensemble (5.1). To this end, we have to identify points well within the phase in which the eigenvalues of $\phi^\dagger\phi$ split into two segments.

We used the formalism of the Appendix to choose two ensembles in the two-segment phase of $\phi^\dagger\phi$, for which we verified that the eigenvalues of ϕ formed a disk. The results for these ensembles are displayed in Figs. 4 and 5.

Figure 4 shows the scatter plot of the eigenvalues of ϕ together with the density of eigenvalues $\tilde{\rho}(s)$ of $\phi^\dagger\phi$ for (5.1) with couplings $m^2=7.372$, $\lambda=-6.116$ and $g=1.372$. As can be seen on the right part of Fig. 4, for these couplings, the eigenvalues of $\phi^\dagger\phi$ live in two separated

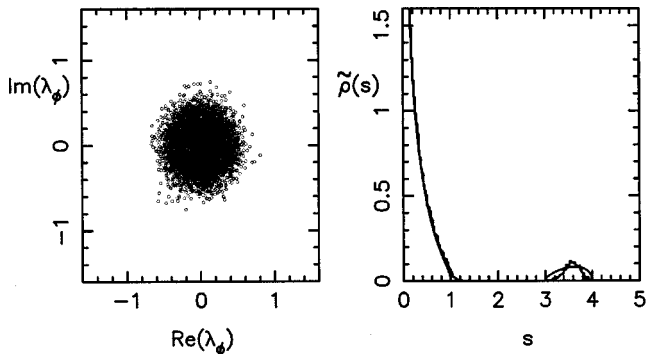

FIG. 5. Similar to Fig. 4, but with $m^2=6.403$, $\lambda=4.184$ and $g=0.713$. The support of $\tilde{\rho}(s)$ is split into the two segments $\{0\leqslant s\leqslant a=1\}\cup\{b=3\leqslant s\leqslant c=4\}$, while the support of $\rho(r)$ on the left remains a disk.

segments: $\{0\leqslant s\leqslant a=1\}\cup\{b=2\leqslant s\leqslant c=3\}$. The solid line there is the large N theoretical curve, which was plotted according to the analysis we have described in the Appendix [see the discussion following (A20)]. Evidently, the spectrum of ϕ is a disk, despite the split support of $\tilde{\rho}(s)$, in accordance with the ''single ring'' Theorem.

Figure 5 is similar to Fig. 4, but for (5.1) with couplings $m^2=6.403$, $\lambda=4.184$ and $g=0.713$, for which the eigenvalues of $\phi^\dagger\phi$ live in the segments $\{0\leqslant s\leqslant a=1\}\cup\{b=3\leqslant s\leqslant c=4\}$. The spectrum of ϕ remains a disk, even though the two segments of the support of $\tilde{\rho}(s)$ are more separated than in Fig. 4.

ACKNOWLEDGMENTS

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APPENDIX: THE PHASE DIAGRAM OF A GENERIC $V(\phi^\dagger\phi)$

In this Appendix we briefly review the necessary theoretical aspects of multi-cut phases of $\phi^\dagger\phi$. The first part of our discussion will apply for a generic polynomial $V(\phi^\dagger\phi)$. Then, in the second part of the Appendix, we will specialize to the sextic potential (5.1).

The following discussion is an adaptation and application of the ideas of Ref. 24 to non-Hermitian matrices. For a more detailed discussion of Hermitian and non-Hermitian random matrix ensembles with multi-cut eigenvalue distributions, see Ref. 25. [As a side remark, we mention at this point the recent interest in the surprising nonuniversal large distance behavior of the (smoothed) connected two-point function[26] in matrix models with multi-cut eigenvalue distributions.]

For practical reasons, we eliminate some (or all) of the couplings in $V(\phi^\dagger\phi)$ in terms of the end-points of the segments containing the eigenvalue distribution of $\phi^\dagger\phi$, and use the latter as (part of) the coordinates in the phase diagram. In this way we can find rather easily which couplings in $V(\phi^\dagger\phi)$ are needed to generate an eigenvalue distribution of $\phi^\dagger\phi$ with a prescribed set of support segments.

1. A generic potential $V(\phi^\dagger\phi)$

The saddle-point equation governing the Dyson gas of eigenvalues of $\phi^\dagger\phi$ is[19,20]

$$\mathrm{Re}\,F(s-i\epsilon)=\tfrac{1}{2}V'(s). \tag{A1}$$

By definition [see Eq. (2.8)]

$$F(w)=\frac{1}{N}\left\langle \mathrm{tr}_{(N)}\frac{1}{w-\phi^\dagger\phi}\right\rangle=\frac{1}{N}\sum_{i=1}^{N}\left\langle\frac{1}{w-s_i}\right\rangle \tag{A2}$$

(where s_i are the eigenvalues of $\phi^\dagger\phi$). Thus, as usual,

$$F(s-i\epsilon)=\mathrm{P.P.}\frac{1}{N}\sum_{j=1}^{N}\left\langle\frac{1}{s-s_j}\right\rangle+i\pi\tilde{\rho}(s), \tag{A3}$$

where $\tilde{\rho}(s)$ is the density of eigenvalues of $\phi^\dagger\phi$.

In order to study multi-cut configurations of $\tilde{\rho}(s)$, we also need the auxiliary function[24]

$$G(s)=\int_{a_1>0}^{s}d\mu(V'(\mu)-2F(\mu-i\epsilon)). \tag{A4}$$

In the last equation a_1 is the lowest branch point of $F(w)$. Thus, from (A3) and (A1), we see that for s real and in the support of eigenvalues,

$$G(s) = -2\pi i \int_{a_1}^{s} \tilde{\rho}(\mu) d\mu \tag{A5}$$

is pure imaginary. $-\mathrm{Im}\, G(s) = 2\pi\tilde{\rho}(s)$ is then positive and monotonically increasing (and reaches 2π when s hits the largest branch point).

Stability of multi-cut distributions. How do we know that a given distribution of eigenvalues is stable against migration of eigenvalues from one place to another? To answer this question, consider the Dyson gas energy functional

$$S_{\mathrm{eff}}[\tilde{\rho}] = \int_{s\geqslant 0} \tilde{\rho}(s) V(s) ds - \frac{1}{2} \int_{s,\mu\geqslant 0} \tilde{\rho}(s)\tilde{\rho}(\mu) \log(s-\mu)^2 \, ds d\mu. \tag{A6}$$

A general variation of (A6) under $\tilde{\rho}(s) \to \tilde{\rho}(s) + \delta\tilde{\rho}(s)$ is

$$\delta S_{\mathrm{eff}}[\tilde{\rho}] = \int_{s\geqslant 0} V(s)\, \delta\tilde{\rho}(s) ds - \int_{s,\mu\geqslant 0} \tilde{\rho}(\mu) \log(s-\mu)^2 \delta\tilde{\rho}(s) ds d\mu. \tag{A7}$$

Moving an eigenvalue from s_i to s_f corresponds to $\delta\tilde{\rho}(s) = (1/N)[\,\delta(s-s_f) - \delta(s-s_i)\,]$. Thus, from (A7) and (A4) (and after some work) we can show that such a move costs

$$\Delta S_{\mathrm{eff}}[\tilde{\rho}] = \frac{1}{N}[G(s_f) - G(s_i)] \tag{A8}$$

in energy.[24] Such a rearrangement of eigenvalues costs energy only if

$$\mathrm{Re}\, \Delta S_{\mathrm{eff}}[\tilde{\rho}] > 0\,, \tag{A9}$$

and therefore (A9) is the stability condition against such a rearrangement. Thus, a multi-cut $F(w)$, where the eigenvalues coalesce into n segments

$$[a_1, a_2] \cup [a_3, a_4] \cup \cdots \cup [a_{2n-1}, a_{2n}],$$

would be stable against migration of eigenvalues between neighboring cuts if and only if (A9) would hold for all neighboring pairs of cuts, and in both directions. Since $G(s)$ is real on the segments on the real axis that connect the cuts, this stability condition means

$$G(a_3) = G(a_2), \quad G(a_5) = G(a_4), \quad \ldots, \quad G(a_{2n-1}) = G(a_{2n-2}). \tag{A10}$$

In addition, of course, $\mathrm{Re}\, G(s) < 0$ cannot happen anywhere for $s \geqslant 0$. The $n-1$ equations (A10) comprise the desired stability condition for such an eigenvalue distribution. In addition to these conditions, we have to make sure that along the cuts themselves $-\mathrm{Im}\, G(s) > 0$, which is just the condition that $\tilde{\rho}(s)$ be positive.

The $n-1$ equations (A10), together with the obvious analytic properties of $F(w)$ and its asymptotic behavior

$$F(w) \sim \frac{1}{w} \tag{A11}$$

as $w \to \infty$, determine $F(w)$ uniquely. Indeed, as is well known, for a generic $V(\phi^\dagger\phi)$, in view of (A1) and (A11) (and as we discussed at the end of Sec. II), $F(w)$ (with n cuts) must be of the form

$$F(w)=\frac{1}{2}V'(w)-P(w)\sqrt{\prod_{l=1}^{2n}(w-a_l)}, \tag{A12}$$

where

$$P(w)=\frac{c_{-1}}{w}+\sum_{l=0}^{\deg V-n-1}c_l w^l. \tag{A13}$$

Here $a_1<a_2\cdots<a_{2n}$ and $c_{-1}\neq 0$ only if $a_1=0$ (see Sec. II). If $a_1>0$, then $c_{-1}=0$, and thus in such a case, there are $2n(a's)+(\deg V-n)(c's)=n+\deg V$ independent parameters in the expression (A12) for $F(w)$. On the other hand, there are $\deg V+1$ conditions from the asymptotic behavior (A11) plus additional $n-1$ conditions from (A10), which comprise a total of $\deg V+n$ conditions, equal to the number of unknown parameters. This balance remains if c_{-1} appears in the game as an unknown parameter, because then $a_1=0$, so that the number of parameters does not change. Finally, we have to remember to impose the positivity constraint

$$\tilde{\rho}(x)=\frac{1}{\pi}\mathrm{Im}\,F(x-i\epsilon)\geqslant 0, \tag{A14}$$

which translates into a set of inequalities among the a's and c's.

A convenient local parametrization of the phase diagram. Recall, that the phases of $\phi^\dagger\phi$ are specified by the number of segments in the support of $\tilde{\rho}(s)$, i.e., the number of cuts in $F(w)$ (and whether these cuts have $w=0$ as a branch point or not.) Thus, instead of the usual description of the phase structure in terms of the deg$V$ couplings in $V(\phi^\dagger\phi)$, our strategy is to use deg$V$ parameters out of the $2n$ branch-points $a_1,\ldots a_{,2n}$ of $F(w)$ and the deg$P$ coefficients c_k (with the total number deg$V$ first saturated by the a's in ascending order), which we refer to as "*phase coordinates,*" to express (in a given phase) the couplings appearing in $V(\phi^\dagger\phi)$ [such as m^2,λ and g in (5.1)], as well the as the c_k's and a_k's complementary to the phase coordinate parameter set. (See our discussion of the sextic potential in the next subsection for concrete examples of this parametrization.)

We have to be careful in giving the expressions for, say, the couplings of V, in terms of the phase coordinates. This because for a given configuration of $F(w)$, the equations from which we are to eliminate the couplings of V [such as the triad m^2,λ and g in (5.1)] as functions of the phase coordinates may have several solutions (in other words, the couplings in V are generally multivalued functions of the phase coordinates in a given phase). Thus, in a given phase, we must of course choose the parametrization of couplings in V which yields the minimal $S_{\mathrm{eff}}[\tilde{\rho}]$ appropriate for that phase.

This alternative parametrization is more convenient for our purposes in Sec. V. Indeed, once we are successful in expressing the couplings in V as functions of the phase coordinates, it will be very easy for us to tune the couplings in $V(\phi^\dagger\phi)$ to a generic point in a given phase and also to approach the phase boundaries in a controlled manner. In particular, phase transitions appear here, for example, when branch points collide and become equal (at some common real positive value a). This process removes two a's and thus closes one cut $(n\to n-1)$ but adds an additional term to $P(w)$. The number of unknown parameters drops by 1, but so does the number of stability conditions (A10). In the other direction, we can obviously reach the same coexistence point, by tuning the parameters of $P(w)$ to a point where it develops a linear factor $(w-a)=\sqrt{(w-a)^2}$ (with $a\geqslant 0$). Obviously, when these alternative phase coordinates approach a point on the coexistence surface from two different sides of the phase transition, the respective sets of couplings of V, expressed as sets of functions of the two phase coordinate patches, coincide. Thus, they lead to the same $S_{\mathrm{eff}}[\tilde{\rho}]$, which means that such a point is indeed a point on the phase boundary.

2. Results for the sextic potential

From (A12) and (5.1), the general form of $F(w)$ is

$$F(w)=\tfrac{1}{2}(m^2+\lambda w+gw^2)-P(w)\sqrt{\text{polynomial}}. \tag{A15}$$

a. Single cut, disk phase

Here

$$F(w)=\frac{1}{2}(m^2+\lambda w+gw^2)-\left(\frac{s}{w}+t+uw\right)\sqrt{w(w-a)}. \tag{A16}$$

There is a single cut, so (A10) is trivial in this case, and (A14) holds manifestly. We need only impose (A11). In the end, we find

$$\begin{aligned} u&=\frac{16-8as-2a^2t}{a^3},\\ g&=2u\\ \lambda&=2t-au=\frac{4a^2t+8as-16}{a^2},\\ m^2&=2s-at-\frac{a^2u}{4}=\frac{8as-a^2t-8}{2a}. \end{aligned} \tag{A17}$$

The phase coordinates are a, t and s.

b. Single cut, annular phase

We have

$$F(w)=\tfrac{1}{2}(m^2+\lambda w+gw^2)-(t+uw)\sqrt{(w-a)(w-b)}. \tag{A18}$$

Here $0<a<b$. Again, there is a single cut, so (A10) is trivial in this case too, and also (A14) holds manifestly. We need only impose (A11). In the end, we find

$$\begin{aligned} u&=\frac{16-2t(a-b)^2}{(a+b)(a-b)^2},\\ g&=2u,\\ \lambda&=2t-u(a+b)=4t-\frac{16}{(a-b)^2},\\ m^2&=-\frac{(a-b)^2}{4}u-t(a+b)=-\frac{4}{a+b}-t\frac{a^2+6ab+b^2}{2(a+b)}. \end{aligned} \tag{A19}$$

The phase coordinates are a, b and t.

c. Two cuts, disk phase

We have

$$F(w)=\frac{1}{2}(m^2+\lambda w+gw^2)-\left(\frac{s}{w}+t\right)\sqrt{w(w-a)(w-b)(w-c)}. \tag{A20}$$

Here $0<a<b<c$. Note that in this case we can trade the three couplings m^2, λ and g for the three branch points a, b and c. In this case there are two cuts, so for the first time (A10) is not trivial. We first impose (A11). We find

$$\begin{aligned} s &= \frac{8}{a^2+b^2+c^2-2(ab+ac+bc)} \\ &\quad -\frac{1}{2}\frac{a^3+b^3+c^3-a^2(b+c)-b^2(a+c)-c^2(a+b)+2abc}{a^2+b^2+c^2-2(ab+ac+bc)}t, \\ g &= 2t, \\ \lambda &= 2s-t(a+b+c), \\ m^2 &= -(a+b+c)s-\frac{a^2+b^2+c^2-2(ab+ac+bc)}{4}t. \end{aligned} \tag{A21}$$

We have yet to impose (A10), which is why t was not eliminated yet. Before doing that, we impose (A14). Our conventions are always to take each cut from the appropriate branch point to the left on the real axis. Thus, after some work, we find from (A20)

$$\pi\tilde{\rho}(x)=\operatorname{Im}F(x-i\epsilon)=\begin{cases} -\left(\dfrac{s}{x}+t\right)\sqrt{x(a-x)(b-x)(c-x)}, & 0<x<a, \\ +\left(\dfrac{s}{x}+t\right)\sqrt{x(x-a)(x-b)(c-x)}, & b<x<c, \\ 0 \quad \text{otherwise.} \end{cases} \tag{A22}$$

We have to impose (A14) on (A22). This means

$$\frac{s}{x}+t<0 \quad \text{for} \quad 0<x<a,$$

$$\frac{s}{x}+t>0 \quad \text{for} \quad b<x<c.$$

Thus, we must have

$$t>0 \quad \text{and} \quad -bt\leqslant s\leqslant -at<0, \tag{A23}$$

where s is given in (A21). (It is straightforward to check that these inequalities hold for the ensembles corresponding to Figs. 4 and 5 in Sec. V.) We are now ready to impose (A10). Here it simply means $G(a)=G(b)$, namely,

$$\int_a^b\left(\frac{s}{x}+t\right)\sqrt{x(x-a)(b-x)(c-x)}\,dx=0. \tag{A24}$$

Note from (A23) that $-b<s/t<-a$, and thus the factor multiplying the square root in (A24) flips its sign in the integration domain, so that the integral on the lhs of (A24) may vanish. The latter equation may be expressed in terms of the elliptic integrals

$$I(a,b,c)=\int_a^b \sqrt{x(x-a)(x-b)(x-c)}\,dx,$$
$$J(a,b,c)=\int_a^b \sqrt{x(x-a)(x-b)(x-c)}\,\frac{dx}{x}. \tag{A25}$$

Following the usual procedure, we may express I and J in terms of complete elliptic integrals in a straightforward manner. (We do not bother to write these expressions here, since for our purposes in Sec. V we evaluated I and J numerically.)

Finally, substituting these expressions in (A24) we obtain

$$s(t,a,b,c)J(a,b,c)+tI(a,b,c)=0, \tag{A26}$$

which we solve for t (recall from (A21) that s is merely linear in t, and also that $t>0$, in view of (A23).) Once $t(a,b,c)$ is known, we can go back to (A21) and evaluate $m^2(a,b,c)$, $\lambda(a,b,c)$ and $g(a,b,c)$ explicitly. Our phase coordinates in this case are thus a, b and c.

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[14] We use the following notational conventions: for $z=x+iy$ we define $\partial \equiv \partial/\partial z = \frac{1}{2}(\partial/\partial x - i\,\partial/\partial y)$ so that $\partial z = 1$. Similarly, we define $\partial^* \equiv \partial/\partial z^* = \frac{1}{2}(\partial/\partial x + i\,\partial/\partial y)$, so that $\partial^* z^* = 1$ and also $\partial^*(1/z) = \pi\delta^{(2)}(z)$. Finally, we denote $|z| = r$.

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Dynamical systems embedded into Lie algebras

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I. INTRODUCTION

This article deals with the problem of extracting information of a three-dimensional dynamical system **X**, when **X** is embedded into a Lie algebra of 3-D vectorfields.

This approach is interesting since up to now, as we explain later in this work, the only case considered has been that in which the generators of the Lie algebra are **X** and a certain number of symmetries or pseudosymmetries of **X**. Such restriction is dropped in this article.

Let us explain this in more detail.

It is well known[1] that when a vectorfield **X** (v.f. in what follows) admits a symmetry vector, that is, a v.f. **S** satisfying

$$\mathcal{L}_{\mathbf{S}}(\mathbf{X})=0, \tag{1}$$

$\mathcal{L}_{\mathbf{S}}$ standing for the Lie derivative along the streamlines of **S**, useful consequences on the local and global structure of **X** can be obtained: existence of local and global first integrals, limit cycles of **X**,[2] etc.

Remember that (1) implies that the flow of the v.f. **S** acts on the set of solutions of the differential equations

$$\frac{d\mathbf{x}}{dt}=\mathbf{X}(\mathbf{x}). \tag{2}$$

In other words, the local flow of **S** transforms a solution of (2) into another solution of Eq. (2).

Sometimes the pair of v.f. $(\mathbf{X},\mathbf{S})$ does not satisfy Eq. (1) but the equations

$$\mathcal{L}_{\mathbf{S}}(\mathbf{X})=\lambda(\mathbf{x})\mathbf{X}, \tag{3}$$

$\lambda(\mathbf{x})$ being a function. In this case **S** is called a pseudosymmetry of **X**. The geometrical meaning of Eq. (3) is that the local flow of **S** conserves *not* the solutions of (2) but the trajectories on which these solutions lie (a trajectory of **X** is just an unparametrized solution of **X**).

Interesting geometric information on the trajectories of **X** when (3) holds can be found in Ref. 2.

Motivated by Eqs. (1) and (3) we consider in this article that **X** (a $\mathbb{R}^3$ v.f. from now on) is one of the generators of a Lie algebra $A_{2,2}$ of dimension two or $A_{3,3}$ of dimension three. That is,

$$[\mathbf{X},\mathbf{S}_1]=a_0\mathbf{X}+a_1\mathbf{S}_1,$$

$$a_0, a_1 \in \mathbb{R}, \tag{4}$$

$$\text{rank}(\mathbf{X}, \mathbf{S}_1) = 2 \quad \text{for any } \mathbf{x} \in \mathbb{R}^3,$$

in the first case, and

$$\begin{gathered} [\mathbf{X}, \mathbf{S}_1] = a_0 \mathbf{X} + a_1 \mathbf{S}_1 + a_2 \mathbf{S}_2, \\ [\mathbf{X}, \mathbf{S}_2] = b_0 \mathbf{X} + b_1 \mathbf{S}_1 + b_2 \mathbf{S}_2, \\ [\mathbf{S}_1, \mathbf{S}_2] = c_0 \mathbf{X} + c_1 \mathbf{S}_1 + c_2 \mathbf{S}_2, \\ a_i, b_i, c_i \in \mathbb{R}, \\ \text{rank}(\mathbf{X}, \mathbf{S}_1, \mathbf{S}_2) = 3 \quad \text{for any } \mathbf{x} \in \mathbb{R}^3, \end{gathered} \tag{5}$$

in the case of an algebra of type $A_{3,3}$.

Note that [,] stands for the Lie bracket of v.f. and $A_{i,j}$ $(i \geqslant j)$ stands for a Lie algebra with i generators (including $\mathbf{X}$) and rank $(\mathbf{X}, \mathbf{S}_1, .., \mathbf{S}_{i-1}) = j$.

We shall say that $\mathbf{X}$ belongs to a certain Lie algebra if $\mathbf{X}$ is one of its generators. For example, $\mathbf{X}$ belongs to the Lie algebras $A_{2,2}$ and $A_{3,3}$ defined by Eqs. (4) and (5).

Note that the case of pseudosymmetries corresponds to $a_1 = 0$ in Eq. (4) and $a_1 = a_2 = b_1 = b_2 = 0$ in Eq. (5).

We shall prove in what follows that when a dynamical system $\mathbf{X}$ belongs to a Lie algebra this information can be useful in order to get qualitative information on the orbits of $\mathbf{X}$.

This article is organized this way. Lie algebras of type $A_{2,2}$ are briefly considered in Sec. II, where their influence on $\mathbf{X}$ is studied. The structure constants of $A_{3,3}$ algebras are reduced to a finite number of canonical forms in Sec. III. The case of a v.f. $\mathbf{X}$ embedded into an $A_{3,3}$ Lie algebra is studied in Sec. IV. Illustrative examples are given in Sec. V, and some open problems are discussed in Sec. VI.

We end this section by motivating our study with some considerations of the significance and applicability of the idea of embedding a v.f. $\mathbf{X}$ into a Lie algebra.

We shall refer to the illustrative example of $A_{2,2}$ algebras [that is, algebras with two generators and rank equal 2: see Eq. (4)]. For these algebras Eq. (4) can be interpreted in two ways:

(i) as the structure equation of a Lie transformation (local) group G acting on $\mathbb{R}^3$ of generators $\mathbf{X}$ and $\mathbf{S}$, or
(ii) as the equations defining an involutive distribution[3,4] generated by $\mathbf{X}$ and $\mathbf{S}$.

The fact that a_0 and a_1 in Eq. (4) are real numbers instead of functions of $\mathbf{x} = (x_1, x_2, x_3)$ is a useful piece of information that should be taken into account.
Therefore the philosophy of this article is the following:

(i) get $\mathbf{X}$ (if you can, via computer packages, etc.) be embedded into the algebras $A_{r,3}(r \geqslant 3)$ or $A_{r,2}(r \geqslant 2)$ of some Lie transformation group G. We shall speak immediately about the difficulties of this process.
(ii) apply the techniques of this article in order to get information on some structures of $\mathbf{X}$, as first integrals, invariant sets, existence of partitions of $\mathbb{R}^3$ invariant under $\mathbf{X}$, integrability via quadratures, etc.

The most difficult point is, of course, the finding of the concrete embedding of $\mathbf{X}$. In fact it may even happen that (for structural reasons connected with the orbit structure of $\mathbf{X}$, strange or complicated limit behavior of the orbits when $t \to +\infty$) the embedding process will be a failure because it does not exist at all. For example, by topological reasons it is *impossible* to get an embedding of $\mathbf{X}$ into an algebra of type $A_{3,2}$ or $A_{2,2}$ if $\mathbf{X}$ is a dynamical system with an orbit which is an asymptotic "limit cycle" (orbit of type S^1 acting as limit set of neighboring orbits). Nevertheless, the dynamical system $\mathbf{X}$ could be embedded into an algebra of type $A_{3,3}$.

However, we have *not* been able to find analytical conditions, geometric structures, etc. such that if **X** satisfies them, then **X** cannot be embedded into an algebra of type $A_{3,3}$. Upto today open problems are to decide

(i) whether or not a given v.f. **X** can be embedded into a finite dimensional Lie algebra, and
(ii) whether or not a given v.f. **X** can be embedded into an algebra of type $A_{n,3}(n\geqslant 3)$, where n is a fixed natural number.

In general, the problem of studying the relation between the geometry of the orbits of **X** and the type of algebra into which **X** can or cannot be embedded seems to be a very difficult one.

In conclussion, this article could be of interest to people working in differential equations, dynamical systems, etc., and to all those normally handling symmetry techniques in differential equations since we offer here a certain generalization of them yielding, under some conditions, first integrals, invariant sets, integrability via quadratures, foliations of $\mathbb{R}^3$ invariant under **X**, etc.

II. $\mathbb{R}^3$ DYNAMICAL SYSTEMS EMBEDDED INTO A LIE ALGEBRA $A_{2,2}$

Let us now develop some consequences of the fact that our dynamical system **X** is embedded into a Lie algebra of type $A_{2,2}$, that is,

$$[\mathbf{X},\mathbf{S}_1]=a_0\mathbf{X}+a_1\mathbf{S}_1,$$
$$a_0,a_1\in\mathbb{R}, \tag{6}$$
$$\operatorname{rank}(\mathbf{X},\mathbf{S}_1)=2.$$

We shall now obtain from Eq. (6) consequences of several kinds concerning the orbit structure of **X**. Most of these results fail when the real constants a_0 and a_1 of (6) are substituted by real functions $a(\mathbf{x})$ and $b(\mathbf{x})$, $\mathbf{x}\in\mathbb{R}^3$. Therefore, most of these results cannot be obtained when **X** is embedded into a two-dimensional foliation instead of being embedded into a $A_{2,2}$ algebra.

From now on all the functions v.f.'s, and differential forms of this article are assumed to be analytic (C^w). See Refs. 3–5 for the theory and applications of differential forms.

A. First integrals of X

We obtain now first integrals of **X** via the construction of exact one-forms. The reader can have a look at this method when $a_0=a_1=0$ in Ref. 3.

Our assumptions are the following:
X belongs to a $A_{2,2}$ Lie algebra [see Eq. (6)] and

$$\operatorname{Div}\mathbf{X}=-a_1,\ \operatorname{Div}\mathbf{S}_1=a_0, \tag{7}$$

a_0 and a_1 being the real numbers of Eq. (6) and Div **Y** standing for

$$\operatorname{Div}\mathbf{Y}=\frac{\partial Y_1}{\partial x_1}+\frac{\partial Y_2}{\partial x_2}+\frac{\partial Y_3}{\partial x_3},$$
$$\mathbf{Y}=Y_1\partial_1+Y_2\partial_2+Y_3\partial_3. \tag{8}$$

$\operatorname{Div}\mathbf{Y}$ can be alternatively defined by $\mathcal{L}_Y\Omega_3=\operatorname{Div}\mathbf{Y}\cdot\Omega_3$, Ω_3 being the standard volume form $dx_1\wedge dx_2\wedge dx_3$ of $\mathbb{R}^3$.

Under these hypotheses the one-form w_1 defined by

$$w_1=i_{\mathbf{x}}i_{\mathbf{s}_1}\Omega_3 \tag{9}$$

is exact ($dw_1=0$) and we can write

$$w_1 = dI, \tag{10}$$

and since $i_x w_1 = 0$ we can write

$$\mathcal{L}_{\mathbf{x}}(I) = 0. \tag{11}$$

Therefore I is a global first integral of $\mathbf{X}$.

Note that I can never become a trivial constant, as this would imply $w_1 = 0$ (identically), getting a contradiction with the rank condition appearing in Eq. (6).

B. Independent first integrals

Let us now assume that I_1, I_2 are two independent first integrals of $\mathbf{S_1}$; this situation often appears in physics[6] as $\mathbf{S_1}$ usually is a v.f. easier to handle than $\mathbf{X}$ (isometries of $\mathbb{R}^3$ considered as Euclidean space, linear or affine v.f. and so on). Under this assumption let us see that the integration of $\mathbf{X}$ can be simplified.

Under these conditions Eq. (6) implies

$$-\mathcal{L}_{\mathbf{S_1}}\mathcal{L}_{\mathbf{X}}(I_i) = a_0 \mathcal{L}_{\mathbf{X}}(I_i), \quad i = 1,2, \tag{12}$$

and when $a_0 = 0$ we get

$$\mathcal{L}_{\mathbf{X}}(I_i) = \varphi_i(I_1, I_2), \tag{13}$$

that is, $\mathbf{X}$ projects to the $\mathbb{R}^3$ v.f.

$$\mathbf{X}_2 = \varphi_1(I_1, I_2)\partial_{I_1} + \varphi_2(I_1, I_2)\partial_{I_2}, \tag{14}$$

that is

$$\begin{aligned} \frac{dI_1}{dt} &= \varphi_1(I_1, I_2), \\ \frac{dI_2}{dt} &= \varphi_2(I_1, I_2). \end{aligned} \tag{15}$$

Therefore, the integration of $\mathbf{X}$ has been simplified.

We now summarize the results of this section: We have seen that it is, in general, impossible to get geometric information on the trajectories of the $\mathbb{R}^3$ v.f. $\mathbf{X}$ just by knowing that $\mathbf{X}$ belongs to a certain Lie algebra of v.f. More information concerning the v.f. of the Lie algebra is needed: see, for example, the requirements in (7).

A similar observation can be made in relation to the study of the pseudosymmetries of $\mathbf{X}$ [see Eq. (3)]. Namely, pseudosymmetries, *per se*, are insufficient in order to get first integrals and other geometric structures related to the trajectories of $\mathbf{X}$.

What is new in this section is the fact that we have shown the possibility of getting global geometric information on the trajectories of $\mathbf{X}$ when *no* pseudosymmetries are known but we have discovered that our dynamical system $\mathbf{X}$ is a generator of an $A_{2,2}$ algebra of vectorfields.

For brevity reasons we shall not study in the following sections algebras of type $A_{3,2}$, but just algebras of type $A_{3,3}$.

III. CLASSIFICATION OF $A_{3,3}$ ALGEBRAS

A classification list of the $A_{3,3}$ algebras is given now. The proof shall not be given and will be sent on request. As we can see the classification contains 18 different types. Note that the non-

written brackets between $\mathbf{X}$, $\mathbf{S_1}$ and $\mathbf{S_2}$ vanish and have been omitted. Nevertheless, all brackets have been written in the algebra of type number one (for esthetic reasons).

Any $A_{3,3}$ algebra can be obtained from those appearing in the list by means of linear combinations of type

$$\begin{aligned}
\mathbf{X}^* &= \alpha_0 \mathbf{X}, \\
\mathbf{S}_1^* &= \beta_0 \mathbf{X} + \beta_1 \mathbf{S}_1 + \beta_2 \mathbf{S}_2, \\
\mathbf{S}_2^* &= \gamma_0 \mathbf{X} + \gamma_1 \mathbf{S}_1 + \gamma_2 \mathbf{S}_2, \\
&\alpha_0, \beta_0, \gamma_0 \in \mathbb{R} \quad \alpha_0 \neq 0, \\
&\beta_1 \gamma_2 - \gamma_1 \beta_2 \neq 0.
\end{aligned} \tag{16}$$

These linear combinations arise as the generator $\mathbf{X}$ (representing the dynamical system) must be isolated in all the algebraic manipulations; otherwise a generator $\mathbf{X}^*$ could be obtained mixing the dynamics of $\mathbf{X}$ with the dynamics of the v.f. $\mathbf{S_1}$ and $\mathbf{S_2}$. Therefore, the orbit structure of $\mathbf{X}$ would be unrelated to the orbit structure of $\mathbf{X}^*$.

The 18 types of $A_{3,3}$ algebras are

(1) $[\mathbf{X},\mathbf{S_i}]=0$, $[\mathbf{S_1},\mathbf{S_2}]=0$, $i=1,2$;
(2) $[\mathbf{X},\mathbf{S_1}]=\mathbf{X}$;
(3) $[\mathbf{S_1},\mathbf{S_2}]=\mathbf{X}$;
(4) $[\mathbf{X},\mathbf{S_1}]=\mathbf{S_1}$;
(5) $[\mathbf{X},\mathbf{S_2}]=\mathbf{S_1}$, $[\mathbf{S_1},\mathbf{S_2}]=\alpha\mathbf{S_1}$, $\alpha\in\mathbb{R}$;
(6) $[\mathbf{S_1},\mathbf{S_2}]=\mathbf{S_1}$;
(7) $[\mathbf{X},\mathbf{S_2}]=\mathbf{X}$, $[\mathbf{S_1},\mathbf{S_2}]=\mathbf{X}+\alpha\mathbf{S_1}$, $\alpha\in\mathbb{R}\backslash\{0\}$;
(8) $[\mathbf{X},\mathbf{S_2}]=\mathbf{X}+\mathbf{S_1}$, $[\mathbf{S_1},\mathbf{S_2}]=\mathbf{X}$;
(9) $[\mathbf{X},\mathbf{S_2}]=\mathbf{S_1}$, $[\mathbf{S_1},\mathbf{S_2}]=-\mathbf{X}$;
(10) $[\mathbf{X},\mathbf{S_2}]=\mathbf{S_1}$, $[\mathbf{S_1},\mathbf{S_2}]=\mathbf{X}$;
(11) $[\mathbf{X},\mathbf{S_1}]=\mathbf{S_1}$, $[\mathbf{X},\mathbf{S_2}]=\alpha\mathbf{S_2}$, $\alpha\in\mathbb{R}\backslash\{0\}$;
(12) $[\mathbf{X},\mathbf{S_1}]=\mathbf{S_1}$, $[\mathbf{X},\mathbf{S_2}]=\mathbf{S_1}+\mathbf{S_2}$;
(13) $[\mathbf{X},\mathbf{S_1}]=\alpha\mathbf{S_1}+\mathbf{S_2}$, $[\mathbf{X},\mathbf{S_2}]=-\mathbf{S_1}+\alpha\mathbf{S_2}$, $\alpha\in\mathbb{R}\backslash\{0\}$;
(14) $[\mathbf{X},\mathbf{S_1}]=\mathbf{X}$, $[\mathbf{X},\mathbf{S_2}]=\mathbf{S_1}$, $[\mathbf{S_1},\mathbf{S_2}]=\mathbf{X}+\mathbf{S_2}$;
(15) $[\mathbf{X},\mathbf{S_1}]=\mathbf{S_2}$, $[\mathbf{X},\mathbf{S_2}]=-\mathbf{S_1}$, $[\mathbf{S_1},\mathbf{S_2}]=\mathbf{X}$;
(16) $[\mathbf{X},\mathbf{S_1}]=\mathbf{S_2}$, $[\mathbf{X},\mathbf{S_2}]=\mathbf{S_1}$, $[\mathbf{S_1},\mathbf{S_2}]=\mathbf{X}$;
(17) $[\mathbf{X},\mathbf{S_1}]=-\mathbf{S_1}-\mathbf{S_2}$, $[\mathbf{X},\mathbf{S_2}]=\mathbf{S_2}$, $[\mathbf{S_1},\mathbf{S_2}]=\mathbf{X}$; and
(18) $[\mathbf{X},\mathbf{S_1}]=-\mathbf{S_1}+\mathbf{S_2}$, $[\mathbf{X},\mathbf{S_2}]=\mathbf{S_2}$, $[\mathbf{S_1},\mathbf{S_2}]=\mathbf{X}$.

IV. INVARIANT SETS AND FIRST INTEGRALS WHEN THE DYNAMICAL SYSTEM IS EMBEDDED INTO AN $A_{3,3}$ ALGEBRA

We now show that it is possible to get first integrals, invariant sets and foliations invariant under $\mathbf{X}$ when $\mathbf{X}$ belongs to an $A_{3,3}$ algebra. Reduction of $\mathbf{X}$ to a two-dimensional v.f. is also possible (see Sec. IV C).

A. Global results

We get in this paragraph global results on $\mathbf{X}$ assuming that

$$\mathcal{L}_{\mathbf{X}} w_i = f(\mathbf{x}) w_i, \tag{17}$$

w_i being a C^∞ differential form of degree i ($i=1,2,3$).

Define the functions Δ_i via

$$\Delta_1 = i_{\mathbf{X}} i_{\mathbf{S}_1} i_{\mathbf{S}_2} w_3, \tag{18}$$

$$\Delta_2 = i_{\mathbf{X}} i_{\mathbf{S}_j} w_2, \quad j=1,2, \tag{19}$$

$$\Delta_3 = i_{\mathbf{S}_1} i_{\mathbf{S}_2} w_2, \tag{20}$$

$$\Delta_4 = i_{\mathbf{X}} w_1, \tag{21}$$

$$\Delta_5 = i_{\mathbf{S}_j} w_1, \quad j=1,2. \tag{22}$$

We then get under standard manipulations[4]

$$\mathcal{L}_{\mathbf{X}}(\Delta_i) = (f(\mathbf{x})+K)\Delta_i, \quad K \in \mathbb{R}, \tag{23}$$

where the real number K depends on the constants a_i, b_i, c_i $(i=0,1,2)$ defining the $A_{3,3}$ algebra [see Eq. (5)].

Now, Eq. (23) implies the following.

(i) When the set $\{\Delta_i=0\}$ is a differential manifold ($\nabla(\Delta_i)\neq \mathbf{0}$ for any $P\in\{\Delta_i=0\}$), then the set $\{\Delta_i=0\}$ is invariant under $\mathbf{X}$. See Example 1 in Sec. V.

(ii) When $f+K$ is a function of Δ_i (in particular when $f+K$ is a constant real number), then the sets $\{\Delta_i=\text{const}\}$ form a two-foliation invariant under $\mathbf{X}$.

(iii) When $f(\mathbf{x})$ is a trivial constant function and $f+K$ is equal to zero, then the function Δ_i is a global first integral of $\mathbf{X}$.

These results give useful information on the orbits of $\mathbf{X}$ and they have been obtained without problems in spite of the fact that $\mathbf{S_1}$ and $\mathbf{S_2}$ are, in general, not pseudosymmetries of $\mathbf{X}$.

See the examples on these results at the end of the article.

Note that the techniques of this section can be applied to *any* of the canonical algebras of the list in Sec. III.

B. Subalgebras

We now assume that our $A_{3,3}$ algebra contains two $A_{2,2}$ subalgebras satisfying

$$\begin{aligned} [\mathbf{X},\mathbf{S_1}] &= a\mathbf{X}+b\mathbf{S_1}, \\ [\mathbf{S_2},\mathbf{X}] &= a'\mathbf{X}+b'\mathbf{S_1}, \\ [\mathbf{S_2},\mathbf{S_1}] &= a''\mathbf{X}+b''\mathbf{S_1}, \\ a,a',a'',b,b',b'' &\in \mathbb{R}, \end{aligned} \tag{24}$$

or

$$\begin{aligned} [\mathbf{S}_1^*,\mathbf{S}_2^*] &= c\mathbf{S}_1^*+d\mathbf{S}_2^*, \\ [\mathbf{X},\mathbf{S}_1^*] &= c'\mathbf{S}_1^*+d'\mathbf{S}_2^*, \\ [\mathbf{X},\mathbf{S}_2^*] &= c''\mathbf{S}_1^*+d''\mathbf{S}_2^*, \\ c,c',c'',d,d',d'' &\in \mathbb{R}, \end{aligned} \tag{25}$$

or both [i.e., $A_{3,3}$ might contain a subalgebra satisfying Eq. (24) and another two-dimensional subalgebra satisfying Eq. (25)]. Note that $\{\mathbf{X},\mathbf{S_1}\}$ in the case of Eq. (24) and $\{\mathbf{S_1^*},\mathbf{S_2^*}\}$ in the case of Eq. (25) are ideals of dimension two of $A_{3,3}$.[7]

First of all, notice that we can apply the techniques of Sec. II to the pair $(\mathbf{X},\mathbf{S_1})$ of Eq. (24).

Note that Eqs. (24) are fulfilled by the algebras 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 and 13 and Eqs. (25) are satisfied by the algebras 1, 4, 5, 6, 11, and 12.

On the other hand, algebras 13–18 satisfy neither Eqs. (24) nor Eqs. (25). The reader will have no difficulty in checking all these points.

We give now the geometric meaning of Eqs. (24) and (25). Calling $\mathcal{F}_2$ and $\mathcal{F}_2^*$ the two-foliations associated with the pairs $(\mathbf{X},\mathbf{S_1})$ and $(\mathbf{S_1^*},\mathbf{S_2^*})$, Eqs. (24) and (25) can be rewritten in the form

$$\mathcal{L}_{\mathbf{S_2}}(\mathcal{F}_2)\subset\mathcal{F}_2, \tag{26}$$

and

$$\mathcal{L}_{\mathbf{X}}(\mathcal{F}_2^*)\subset\mathcal{F}_2^*. \tag{27}$$

Accordingly, $\mathcal{F}_2$ and $\mathcal{F}_2^*$ can be locally integrated via the well known formulas[8]

$$\Delta^{-1}\cdot(i_{\mathbf{X}}i_{\mathbf{S_1}}\Omega_3)=dI,$$

$$\Omega_3=dx_1\wedge dx_2\wedge dx_3, \tag{28}$$

$$\Delta=i_{\mathbf{X}}i_{\mathbf{S_1}}i_{\mathbf{S_2}}\Omega_3,$$

and

$$\Delta^{-1}\cdot(i_{\mathbf{S_1^*}}i_{\mathbf{S_2^*}}\Omega_3)=dI^*, \tag{29}$$

I and I^* satisfying

$$\mathcal{L}_{\mathbf{X}}(I)=0 \tag{30}$$

and

$$\mathcal{L}_{\mathbf{X}}(I^*)=f(I^*) \tag{31}$$

for a certain function f.

The function I is, of course, a local integral of $\mathbf{X}$ and it globalizes to a $\mathbb{R}^3$ first integral of $\mathbf{X}$ when the function Δ of Eq. (28) never vanishes.

On the other hand, the geometrical meaning of Eq. (31) is that the local flow of $\mathbf{X}$ acts on the level sets of I^*. When the function f of (31) never vanishes, $\mathbf{X}$ is free from closed trajectories. If $f(I_0^*)=0$, then closed trajectories of $\mathbf{X}$ might appear on the level set $I^*=I_0^*$.

Note that I and I^* are genuine functions, not reducing to constant functions, since in an $A_{3.3}$ algebra the ranks of the pairs $(\mathbf{X},\mathbf{S})$ and $(\mathbf{S_1^*},\mathbf{S_2^*})$ cannot be lower than 2.

C. Results

We now get several results on the orbits of the dynamical system $\mathbf{X}$ assuming that a pair of first integrals common to $\mathbf{S_1}$ and $\mathbf{S_2}$ are known. For brevity's sake, the case of only a first integral I common to $\mathbf{S_1}$ and $\mathbf{S_2}$ shall not be studied.

See Ref. 6 for a similar use of a pair of first integrals of a symmetry of a $\mathbb{R}^3$ dynamical system related to the Bessel, Poisson–Boltzmann, Emden–Fowler and Fermi–Thomas equations. This

approach can be justified since in most of the applications the v.f. $\mathbf{S_i}$ are simple v.f.; often they are affine, or even linear v.f., and therefore the finding of their first integrals is, in general, not difficult.

Consider that

$$\mathcal{L}_{\mathbf{S_i}}(I_j)=0, \quad i,j=1,2 \tag{32}$$

that is I_1, I_2 are independent first integrals common to $\mathbf{S_1}, \mathbf{S_2}$. We then get via Eq. (5) ($c_0 \neq 0$)

$$\mathcal{L}_{\mathbf{X}}(I_i)=\varphi_i(I_1,I_2) \quad i=1,2. \tag{33}$$

Therefore $\mathbf{X}$ can be written in the form

$$\mathbf{X}=\varphi_1(x,y)\partial_1+\varphi_2(x,y)\partial_2. \tag{34}$$

Accordingly, $\mathbf{X}$ has been reduced to a $\mathbb{R}^2$ v.f.

V. EXAMPLES

Examples 1: Consider the conformal v.f.[4]

$$\mathbf{X}=(x_1^2-x_2^2-x_3^2)\partial_1+(2x_1x_2)\partial_2+(2x_1x_3)\partial_3 \tag{35}$$

and the v.f.

$$\begin{aligned}\mathbf{S}_1&=x_3\partial_2-x_2\partial_3,\\ \mathbf{S}_2&=x_1\partial_1+x_2\partial_2+x_3\partial_3,\end{aligned} \tag{36}$$

with commutation relations

$$[\mathbf{X},\mathbf{S_1}]=\mathbf{0}, \quad [\mathbf{X},\mathbf{S_2}]=-\mathbf{X}, \quad [\mathbf{S_1},\mathbf{S_2}]=\mathbf{0}. \tag{37}$$

By application of the results obtained in Secs. IV A and IV B we get

$$\Delta_1=i_{\mathbf{X}}i_{\mathbf{S_1}}i_{\mathbf{S_2}}(dx_1\wedge dx_2\wedge dx_3)=(x_2^2+x_3^2)(-x_1^2-x_2^2-x_3^2). \tag{38}$$

On the other hand,

$$\mathcal{L}_{\mathbf{X}}(\Delta_1)=6x_1\cdot\Delta_1. \tag{39}$$

Therefore, the set $\Delta_1=0$ is invariant under $\mathbf{X}$. Note that the set $\Delta_1=0$ is just the x_1-axis.

Let us now get a local first integral of $\mathbf{X}$ by application of the methods of Sec. IV B. In fact, computing $i_{\mathbf{X}}i_{\mathbf{S_1}}(dx_1\wedge dx_2\wedge dx_3)/\Delta_1$ we get the differential form

$$\frac{w_1}{\Delta_1}=\frac{2x_1dx_1}{-x_1^2-x_2^2-x_3^2}+\frac{(-x_2dx_2-x_3dx_3)(x_1^2-x_2^2-x_3^2)}{(x_2^2+x_3^2)(-x_1^2-x_2^2-x_3^2)}, \tag{40}$$

which is locally exact ($w_1/\Delta_1=dI$). Upon integration we get the local first integral I that can be reduced to

$$I'=\frac{x_2^2+x_3^2}{x_1^2+x_2^2+x_3^2}. \tag{41}$$

Example 2: Consider now the family of v.f.

$$\mathbf{X}=F(x_3)(x_1^2+x_2^2)^n x_1\partial_1+F(x_3)(x_1^2+x_2^2)^n x_2\partial_2+G(x_3)(x_1^2+x_2^2)^n\partial_3, \quad n=1,2,3,..., \tag{42}$$

where F and G are analytic and G vanishes on the set $Z(Z\subset\mathbb{R})$.

Let $\mathbf{S_i}$ $(i=1,2)$ be the v.f.

$$\begin{aligned}\mathbf{S_1}&=x_1\partial_1+x_2\partial_2,\\ \mathbf{S_2}&=x_2\partial_1-x_1\partial_2.\end{aligned} \tag{43}$$

The three v.f. $\mathbf{X},\mathbf{S_1},\mathbf{S_2}$ form a commutative algebra. By applying to them the techniques of Secs. IV A and IV B we get the invariant set

$$\Delta_1=G(x_3)(x_1^2+x_2^2)^{n+1}=0, \tag{44}$$

that is, the invariant sets

$$\begin{aligned}x_1^2+x_2^2&=0,\\ x_3&=z, \quad z\in Z.\end{aligned} \tag{45}$$

On the other hand, we can also write

$$\frac{w_1}{\Delta_1}=dI, \tag{46}$$

w_1 standing for the one-form

$$w_1=i_{\mathbf{x}}i_{\mathbf{s_2}}(dx_1\wedge dx_2\wedge dx_3). \tag{47}$$

We get in this way

$$I=\frac{1}{2}L(x_1^2+x_2^2)-\int\frac{F(x_3)}{G(x_3)}dx_3, \tag{48}$$

L standing for Neperian logarithm, that is, a local first integral of $\mathbf{X}$.

Example 3: We now give an example related to Sec. II B.

Let $H_i(x_1,x_2,x_3)$ be homogeneous polynomials of degrees d_1 and d_2. Define $\mathbf{X}$ and $\mathbf{S}$ viahe equations

$$\begin{aligned}\mathbf{X}&=\nabla H_1\wedge\nabla H_2+a_0(x_1\partial_1+x_2\partial_2+x_3\partial_3),\\ \mathbf{S}&=\nabla H_1\wedge\nabla H_2,\\ a_0&\in\mathbb{R}, \quad \nabla=\text{gradient operator}.\end{aligned} \tag{49}$$

The reader will check that

$$[\mathbf{X},\mathbf{S}]=b\mathbf{S}, \quad b\in\mathbb{R}. \tag{50}$$

Therefore the pair $(\mathbf{X},\mathbf{S})$ forms an $A_{2,2}$ algebra.

Since H_1 and H_2 are first integrals of $\mathbf{S}$, we get from (50)

$$\begin{aligned}\mathcal{L}_{\mathbf{x}}(H_1)&=\varphi_1(H_1,H_2),\\ \mathcal{L}_{\mathbf{x}}(H_2)&=\varphi_2(H_1,H_2),\end{aligned} \tag{51}$$

that is, **X** projects to the $\mathbb{R}^2$ v.f.

$$\varphi_1 \partial_{H_1} + \varphi_2 \partial_{H_2}. \tag{52}$$

Note that the v.f. **X** of (49) is not trivial, as it is *not* a homogeneous v.f.

Note also that any first integral $I(H_1, H_2)$ of the reduced differential equations (51) is a first integral of **X**.

Example 4: The considerations of Example 3 can be extended to nonhomogeneous functions in this way.

Let H_1 and H_2 be nonhomogeneous polynomials that can be transformed into homogeneous ones via a transformation of type

$$\begin{gathered} x_1 \to x_1^a, \\ x_2 \to x_2^b, \\ x_3 \to x_3^c, \\ a, b, c \in \mathbb{R}^+. \end{gathered} \tag{53}$$

For example, the pairs

$$H_1 = x_2 x_3, \quad H_2 = x_1^2 + x_2^2 + x_3$$

and

$$H_1 = x_2^2 + x_3^2, \quad H_2 = x_1^2 - x_3$$

become homogeneous under the transformations

$$x_1 \to x_1, \quad x_2 \to x_2, \quad x_3 \to {}^2_3$$

and

$$x_1 \to x_1 \quad x_2 \to {}^2_2, \quad x_3 \to x_3^2.$$

Under these circumstances the v.f. defined by

$$\begin{gathered} \mathbf{X} = \nabla H_1 \wedge \nabla H_2 + a_0 (x_1 \partial_1 + x_2 \partial_2 + x_3 \partial_3), \\ \mathbf{S} = \nabla H_1 \wedge \nabla H_2, \end{gathered} \tag{54}$$

commutes as in Eq. (50). Therefore, the conclusions in Example 3 are valid for the v.f. of Eq. (54). For example, the Lorenz dynamical system[9]

$$\mathbf{X}_L = \sigma(x_2 - x_1)\partial_1 + (-x_1 x_3 + r x_1 - x_2)\partial_2 + (x_1 x_2 - b x_3)\partial_3, \quad \sigma, r, b \in \mathbb{R}, \tag{55}$$

for the following particular values of the parameters,

$$\sigma = \tfrac{1}{2}, \quad r = 0, \quad b = 1,$$

forms an $A_{2,2}$ algebra, of the type discussed in this example, with the v.f.

$$\mathbf{S} = \nabla(x_2^2 + x_3^2) \wedge \nabla(x_1^2 - x_3) \tag{56}$$

as the reader can check.

Example 5: We end this section with a list of second order differential equations appearing in Physics (see in Ref. 6) admitting a symmetry vector **S** to which the methods of this article can be applied (see Sec. II B).

(5.1) $x^2y_{,xx}+xy_{,x}+x^2y=0$:

$$\text{Associated } \mathbf{X}\text{:}\mathbf{X}=\frac{-xu-x^2y}{x^2}\partial_u+u\partial_y+\partial_x \quad u=y_{,x}.$$

$$\text{Symmetry vector: } \mathbf{S}=y\partial_y+u\partial_u.$$

$$\text{Commutation relation: } [\mathbf{X},\mathbf{S}]=\mathbf{0}.$$

$$\text{First integrals of } \mathbf{S}\text{: } I_1=x, \quad I_2=u/y.$$

(5.2) $y_{,xx}+y_{,x}/x=e^y$.

$$\text{Associated } \mathbf{X}\text{: } \mathbf{X}=\left(e^y-\frac{u}{x}\right)\partial_u+u\partial_y+\partial_x, \quad u=y_{,x}.$$

$$\text{Symmetry vector: } \mathbf{X}=x\partial_x-2\partial_y-u\partial_u.$$

$$\text{Commutation relation: } [\mathbf{X},\mathbf{S}]=\mathbf{X}.$$

$$\text{First integrals of } \mathbf{S}\text{: } I_1=x^2e^y, \quad I_2=xu.$$

(5.3) $y_{,xx}+(2/x)y_{,x}+y^n=0$.

$$\text{Associated } \mathbf{X}\text{: } \mathbf{X}=\left(-y^n-\frac{2u}{x}\right)\partial_u+u\partial_y+\partial_x \quad u=y_{,x}.$$

$$\text{Symmetry vector: } \mathbf{S}=x\partial_x+\frac{2y}{1-n}\partial_y+\frac{1+n}{1-n}u\partial_u.$$

$$\text{Commutation relation: } [\mathbf{X},\mathbf{S}]=\mathbf{X}.$$

$$\text{First integrals of } \mathbf{S}\text{: } I_1=x^2y^{n-1}, \quad I_2=x^{n+1}u^{n-1}.$$

(5.4) $y_{,xx}=x^{-1/2}y^{3/2}$.

$$\text{Associated } \mathbf{X}\text{: } \mathbf{X}=(x^{-1/2}y^{3/2})\partial_u+u\partial_y+\partial_x, \quad u=y_{,x}.$$

$$\text{Symmetry vector: } \mathbf{S}=x\partial_x-3y\partial_y-4u\partial_u.$$

$$\text{Commutation relation: } [\mathbf{X},\mathbf{S}]=\mathbf{X}.$$

$$\text{First integrals of } \mathbf{S}\text{: } I_1=x^3y, \quad I_2=x^4u.$$

VI. FINAL REMARKS

We have seen that when a $\mathbb{R}^3$ dynamical system **X** lies inside an $A_{2,2}$, $A_{3,2}$ or $A_{3,3}$ algebra useful information on its trajectories can be obtained from this piece of information.

What happens when **X** can be embedded into a Lie algebra $A_{n,3}$ when $n>3$? Note that now the canonical forms of Sec. III are harder to obtain. On the other hand, $A_{n,3}$ might contain ideals I containing **X** of lower dimension n', reducing the problem to an algebra $A_{n',3}$ of lower dimension. If no ideal of this type can be found, we can always apply the techniques of Sec. IV A.

Considering only contractions of $\mathbf{X}$ and $\mathbf{S_i}$ with differential forms of type w_3, we can get in this way a whole set of functions Δ_{ij}:

$$\Delta_{ij}=i_X i_{S_i} i_{S_j} w_3, \quad i,j=1,...,n-1, \tag{57}$$

leading to the sets

$$\Delta_{ij}(x_1,x_2,x_3)=0 \tag{58}$$

that are invariant under $\mathbf{X}$ [at least near the points P on which (58) defines a differential manifold, that is $\nabla(\Delta_{ij})(P)\neq 0$].

Therefore, when n is high we can get, via Eq. (58), a collection of more and more sets invariant under $\mathbf{X}$.

An open problem is to study if the number N of invariant sets in (58) is bounded or not when n increases and whether or not these invariant sets accumulate (when N is unbounded). Does the topology of the trajectories of $\mathbf{X}$ ''feel'' that $\mathbf{X}$ is included in an $A_{n,3}$ algebra (without proper ideals) when n is large?

Another open problem meriting a separate study is this one: Assume that $\mathbf{X}$ is included among the generators of an $A_{\infty,3}$ algebra where $A_{\infty,3}$ is an infinite Lie algebra, free from finite or infinite proper ideals containing $\mathbf{X}$. Let us call them *simple* ∞-algebras.

Equation (57) can now be written in the form

$$\Delta_{ij}=i_X i_{S_i} i_{S_j} w_3, \tag{59}$$

and, therefore, invariant sets of $\mathbf{X}$ can be obtained this way.

The question arises again of classifying topologically the v.f. $\mathbf{X}$ that can be included in a simple $A_{\infty,3}$ algebra.

A final question is this one: can a dynamical system $\mathbf{X}$ embedded into a Lie algebra $A_{n,2}$, $A_{n,3}$ or $A_{\infty,2}$, $A_{\infty,3}$ possess a strange attractor?[9]

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Nonintegrable reductions of the self-dual Yang–Mills equations in a metric of plane wave type

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Symmetry reductions of the self-dual Yang–Mills equations for SL(2,C) bundles with the background metric $ds^2=2\,du\,dv-dx^2+f^2(u)dy^2$ are considered. One of the field components in the reduced equations can be cast into Jordan normal form after gauge transformations. The reduced equations for the two possible normal forms are equivalent, respectively, to certain generalizations of the Korteweg–de Vries (KdV) equation and the nonlinear Schrödinger (NLS) equation. It is shown that the generalized KdV and NLS equations fail the Painlevé test except when the metric is flat. The generalized KdV equation is transformed to a simple form in the case when $f(u)=u^a$ and it is shown that one may obtain either the KdV equation or the cylindrical KdV equation by this method only when the metric is flat. [DOI: 10.1063/1.1412466]

I. INTRODUCTION

The self-dual Yang–Mills (SDYM) equations for bundles defined over flat spacetime play a unifying role in the theory of integrable systems. This is because many well-known integrable equations may be obtained as symmetry reductions of these equations (Ref. 1, Ref. 9). The twistor description of solutions of the SDYM equations in flat spacetime (Ref. 10) then leads to a twistor description of the reduced equations.

Our aim in this paper is to study reductions of the SDYM equations for bundles defined over an open subset U of R^4 with the metric

$$ds^2=2\,du\,dv-dx^2+f^2(u)dy^2, \tag{1}$$

where u, v, x, y are coordinates on U and f is a smooth function.

Before proceeding further, we would like to mention that metrics of the type (1) with the Lorentzian signature (obtained by changing the sign of the middle term) arise in the study of plane waves in general relativity. The geodesic and curvature properties of these metrics (e.g., the fact that they are conformally Einstein) are given in Ref. 5. For our purposes, it is enough to note that the metric (1) is flat if and only if f is a linear function of u. We will now explain our motivation for studying the problem.

In Ref. 11, Ward presented an integral formula for the general solution of the wave equation in a plane wave spacetime. This formula was subsequently generalized by Mason (Ref. 7) to show how it is that Maxwell's equation satisfies a kind of Huygen's principle in plane wave spacetimes. We were therefore interested in studying solutions of the SDYM equations in these spacetimes. As a first step, we decided to study reductions of the SDYM equations with the background metric (1) along the lines of Ref. 8.

Somewhat to our surprise, the generalized Korteweg–de Vries (KdV) and nonlinear Schrödinger (NLS) equations which resulted from the reduction procedure both failed the Painlevé PDE test (Ref. 12) formulated for these equations in Refs. 2 and 4, respectively, except in the case when the metric (1) is flat.

The plan for our paper is as follows. In Sec. II, we will derive the SDYM equations for an SL(2,C) bundle with the background metric (1). The metric possesses a large group of symme-

tries. We impose two of these symmetries, one timelike and the other null, on the bundle and, after a choice of gauge, we obtain the reduced SDYM equations in a form suitable for use in the later sections.

One of the components of the connection in the reduced SDYM equation may, after gauge transformations, be cast into Jordan normal form. The reduced equations corresponding to one choice of the normal form leads to a generalized KdV equation. This reduction is discussed in Sec. III where we also prove the nonintegrability of the generalized KdV equation. It has been known for some time that there is a formal relation between solutions of the KdV equation and solutions of the so-called cylindrical KdV equation (Refs. 3 and 6). In Sec. IV, we set $f(u)=u^a$ in the metric (1) and give a direct proof that the generalized KdV equation from Sec. III can be reduced either to the KdV equation or to the cylindrical KdV equation in exactly two cases, namely, $a=0,1$. These values of a correspond to the cases when the metric (1) is flat.

The second choice of the normal form mentioned above leads us to the generalized NLS equation in Sec. V. Once again, we show that this equation is nonintegrable except in the flat case. We note that it may very well be possible to obtain the cylindrical NLS equation by following the method described in Sec. IV but we have not done this ourselves.

We end this introduction by observing that in the case of the generalized KdV equation all quantities may be interpreted as being real and hence the gauge group is $\mathrm{SL}(2,R)$. The gauge group for the generalized NLS equation is SU(1,1).

II. THE REDUCED SDYM EQUATIONS

In this section, we will derive the reduced self-dual Yang–Mills equations for an $\mathrm{SL}(2,C)$ bundle E defined over U with the metric (1).

We begin by recalling that a connection on E is a linear differential operator D that maps sections of E to 1-forms with values in E. In a local trivialization, we may write D as

$$D=D_a\,dx^a, \tag{2}$$

where

$$D_a=\partial_a-\Phi_a\,. \tag{3}$$

In this expression ∂_a denotes the partial derivative with respect to the coordinate x^a and Φ_a belongs to the Lie algebra of $\mathrm{SL}(2,C)$ $(a=1,2,3,4)$.

The curvature of the connection D is a 2-form F with values in the Lie algebra of $\mathrm{SL}(2,C)$. It is given by

$$F=F_{ab}=[D_a,D_b]=\partial_a\Phi_b-\partial_b\Phi_a+[\Phi_a,\Phi_b], \tag{4}$$

where the brackets denote the appropriate commutator in each case.

Next, let g^{ab} denote the inverse of the matrix g_{ab} associated with the metric (1) and let Δ denote square root of the determinant of g_{ab}. Also, let ϵ_{abcd} denote the totally skew Levi–Civita tensor density. The connection D is said to be a solution of the SDYM equations if

$$F_{ab}=\tfrac{1}{2}\Delta\,\epsilon_{abcd}g^{ce}g^{df}F_{ef}\,. \tag{5}$$

We now choose an orientation by setting $\epsilon_{uvxy}=1$. Then it is easy to see that the SDYM equations for the metric (1) are as follows:

$$[D_x,D_y]=-f[D_u,D_v], \tag{6}$$

$$[D_u,D_y]=-f[D_u,D_x], \tag{7}$$

and

$$[D_v, D_y] = f[D_v, D_x]. \tag{8}$$

(We have suppressed the argument of f for the sake of convenience.)

Next, we know that the vectors $\partial/\partial x$ and $\partial/\partial v$ are Killing vectors for the metric (1). We now impose these symmetries on the bundle, i.e., we assume that the field components are independent of x and v. We also let

$$D_y = \partial_y - A, \quad D_v = \partial_v - B, \tag{9}$$

$$D_u = \partial_u - C, \quad D_x = \partial_x - D, \tag{10}$$

where A, B, C, and D belong to the Lie algebra of SL(2,C). Then the SDYM equations reduce to the following three equations:

$$\partial_y D + [D,A] = -f(-\partial_u B + [C,B]), \tag{11}$$

$$-\partial_u A + \partial_y C + [C,A] = -f(-\partial_u D + [C,D]), \tag{12}$$

and

$$\partial_y B + [B,A] = f[B,D]. \tag{13}$$

Finally, we impose the gauge condition

$$A = fD. \tag{14}$$

The equation (13) now reduces to

$$\partial_y B = 0. \tag{15}$$

Hence, B is a function of u alone. Using gauge transformations involving only u, we may reduce B to one of the following constant normal forms:

$$B = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \quad \text{or} \quad B = \kappa \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{16}$$

where κ is a real or complex constant.

The equation (11) now reduces to

$$\partial_y D = -f[C,B] \tag{17}$$

and Eq. (12) reduces to

$$-f'D - 2f\partial_u D + \partial_y C + 2f[C,D] = 0, \tag{18}$$

where the prime denotes differentiation with respect to u.

We will use the two normal forms for B in Secs. III and V, respectively, in order to reduce the SDYM equations to the generalized KdV and Schrödinger equations, respectively.

III. REDUCTION TO THE GENERALIZED KdV EQUATION

We will begin this section by showing that if the field component B has the normal form

$$B = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \tag{19}$$

then the equations (17) and (18) are equivalent to a generalized (variable coefficient) KdV equation. In order to do this, we assume that $\mathrm{tr}(BD)\neq 0$ and set

$$C=\begin{bmatrix} p & s \\ r & -p \end{bmatrix}, \quad D=\begin{bmatrix} q & 1 \\ h & -q \end{bmatrix}. \tag{20}$$

Then after some simplification, the equation (17) implies the following relations between h,p,q,s:

$$q_y=-fs, \quad h_y=2fp. \tag{21}$$

Hence, we must have

$$C=\begin{bmatrix} \dfrac{h_y}{2f} & -\dfrac{q_y}{f} \\ r & -\dfrac{h_y}{2f} \end{bmatrix}. \tag{22}$$

Finally, we consider the equation (18). If we substitute the matrices D and C from above into this equation, then a rather tedious calculation simplifies this equation to

$$\begin{bmatrix} -f'q-2fq_u+\dfrac{h_{yy}}{2f}-2hq_y-2fr & -f'-\dfrac{q_{yy}}{f}+2h_y+4qq_y \\ -f'h-2fh_u+r_y+4fqr-2hh_y & f'q+2fq_u-\dfrac{h_{yy}}{2f}+2fr+2hq_y \end{bmatrix}=0, \tag{23}$$

where the 0 on the right-hand side stands for the zero matrix of order 2. Using the equation given by (1, 2) entries on both sides, we see that h may be taken to be

$$h=\tfrac{1}{2}\left(f'y+\frac{q_y}{f}-2q^2\right). \tag{24}$$

Next, using the equation given by the (1,1) entries and the expression for h from (24) we see that r is given by the expression

$$r=-\frac{f'}{2f}q-q_u+\frac{q_{yyy}}{8f^3}-\frac{q_y^2}{f^2}-\frac{qq_{yy}}{2f^2}-\frac{f'yq_y}{2f}+\frac{q^2q_y}{f}. \tag{25}$$

Finally, if we substitute the expressions for h and r in the equation given by the (2,1) entries, we see that the function q must satisfy the equation

$$-[ff']'y-2q_{uy}-\frac{f'q_y}{f}-\frac{f'yq_{yy}}{f}+\frac{q_{yyyy}}{8f^3}-\frac{3q_yq_{yy}}{f^2}=0. \tag{26}$$

We now relabel the coordinates u and y as t and x, respectively. The equation (26) then reads

$$-[ff']'x-2q_{tx}-\frac{f'q_x}{f}-\frac{f'xq_{xx}}{f}+\frac{q_{xxxx}}{8f^3}-\frac{3q_xq_{xx}}{f^2}=0. \tag{27}$$

Next, let $q_x=u$. Then the function u must satisfy the generalized (variable coefficient) KdV equation

$$-[ff']'x-2u_t-\frac{f'u}{f}-\frac{f'xu_x}{f}+\frac{u_{xxx}}{8f^3}-\frac{3uu_x}{f^2}=0. \tag{28}$$

Now, according to Brugarino (Ref. 2), the KdV equation with nonuniformities, given by

$$u_t + a(t)u + (b(x,t)u)_x + c(t)uu_x + d(t)u_{xxx} + e(x,t) = 0 \tag{29}$$

has the Painlevé property if its coefficients satisfy the following compatibility condition:

$$b_t + (a - L(c))b + bb_x + db_{xxx} = 2ah + hL\left(\frac{d}{c^2}\right) + h' + ce + x\left[2a^2 + aL\left(\frac{d^3}{c^4}\right) + a' + L\left(\frac{d}{c}\right)L\left(\frac{d}{c^2}\right) + \frac{d}{dt}L\left(\frac{d}{c}\right)\right], \tag{30}$$

where L denotes the logarithmic derivative and $h(t)$ is an arbitrary function of t.

In order to apply this criterion, we first write the equation (28) as

$$\frac{[ff']'x}{2} + u_t + \left(\frac{f'xu}{2f}\right)_x - \frac{u_{xxx}}{16f^3} + \frac{3uu_x}{2f^2} = 0. \tag{31}$$

Then on comparison with the equation (29) we see that

$$a = 0, \quad b = \frac{f'x}{2f}, \quad c = \frac{3}{2f^2}, \quad d = -\frac{1}{16f^3}, \quad e = \frac{[ff']'x}{2}. \tag{32}$$

Using these expressions, the condition (30) reduces to

$$\frac{3f''x}{4f} = h\left(\frac{f'}{f}\right) + h'. \tag{33}$$

Clearly, we can find a suitable h if and only if $f'' = 0$, i.e., if and only if the metric is flat. Hence the generalized KdV equation (28) fails the Painlevé test in nonflat spacetimes.

IV. REDUCTION TO KdV/CYLINDRICAL KdV

We would now like to study the equation (28) in the special case when $f(t) = t^a$, where a is a fixed real number. We begin by transforming the dependent variable u as follows:

$$u \to t^{-(a+3\beta)/2}u + \beta t^{2a-1}x. \tag{34}$$

Here β is one of the (necessarily real) solutions of the quadratic equation

$$a(2a-1) + 2\beta(3a-1) + 3\beta^2 = 0. \tag{35}$$

After some simplification, the PDE (28) reduces to

$$u_t + \frac{a+3\beta}{2}t^{-1}xu_x - \frac{1}{16}t^{-3a}u_{xxx} + \frac{3}{2}t^{-5a+3\beta/2}uu_x = 0. \tag{36}$$

In order to eliminate the term in xu_x, we apply the coordinate transformation

$$x' = t^{-(a+3\beta)/2}x, \quad t' = t \tag{37}$$

and then we rename the variables x' and t' as x and t, respectively. The equation (36) transforms to

$$u_t - \tfrac{1}{16}t^{-(9a+9\beta)/2}u_{xxx} + \tfrac{3}{2}t^{-(3a+3\beta)}uu_x = 0. \tag{38}$$

Next we transform u as follows:

$$u \to t^{-(3a+3\beta)/2} u. \tag{39}$$

Then we get the equation

$$-\frac{3a+3\beta}{2} t^{9a+9\beta-2} 2u + t^{9a+9\beta} 2u_t - \frac{1}{16} u_{xxx} + \frac{3}{2} u u_x = 0. \tag{40}$$

The last two terms in this equation are the same as the dissipative and nonlinear terms in the KdV equation (for a particular choice of coefficients).

Next, consider the transformation

$$t' = t^{-(9a+9\beta-2)/2} \tag{41}$$

and rename t' as t. The equation (40) reduces to

$$-\frac{3}{2}(a+\beta)\frac{u}{t} - \frac{9a+9\beta-2}{2} u_t - \frac{u_{xxx}}{16} + \frac{3}{2} u u_x = 0. \tag{42}$$

We now observe that if $a+\beta=0$ (i.e., $\beta=-a$) then this equation is the KdV equation (for a particular choice of coefficients). Further, on substituting $\beta=-a$ in (35) we see that $a=0,1$. Thus, the equation (28) can be reduced to the KdV equation by this method only if the metric (1) is flat.

We now wish to study the possibility of choosing a and β such that the equation (42) reduces to the cylindrical KdV equation, which is given by

$$w_t - 6 w w_x + w_{xxx} + \frac{w}{2t} = 0. \tag{43}$$

Let

$$u = \alpha w, \quad t = \gamma t', \quad x' = \delta x \tag{44}$$

in (42) and rename the variables t' and x' as t and x, respectively. Then (42) transforms to

$$-\frac{3a+3\beta}{2}\frac{\alpha}{\gamma}\frac{w}{t} - \frac{9a+9\beta-2}{2}\frac{\alpha}{\gamma} w_t - \frac{\alpha\delta^3}{16} w_{xxx} + \frac{3}{2}\alpha^2 \delta w w_x = 0. \tag{45}$$

Comparing this equation with (43), we see that we must have

$$-\frac{3a+3\beta}{2}\frac{\alpha}{\gamma} = \frac{1}{2}, \quad -\frac{9a+9\beta-2}{2}\frac{\alpha}{\gamma} = 1, \tag{46}$$

$$\alpha\delta^3 = -16, \quad \alpha^2\delta = 4. \tag{47}$$

The last two equations yield real values for α and δ as required. It is also easy to see that the first pair of equations are consistent if and only if $a+\beta=\frac{2}{3}$. Substitution of this condition in (35) again yields $a=0,1$. To summarize, we have exhibited a procedure which reduces (28) either to the KdV equation or to the cylindrical KdV equation precisely in the cases when the metric (1) is flat.

We end this section by noting that for a general value of the exponent a in the function f, the above procedure yields the equation

$$w_t - 6 w w_x + w_{xxx} + \frac{\epsilon}{t} w = 0. \tag{48}$$

It can be shown (Ref. 1) that the ODE arising from a scaling similarity solution of this equation has a movable logarithmic branch point except if $\epsilon = 0, \frac{1}{2}$, i.e., when the equation is either the KdV or the cylindrical KdV equation. Hence the Painlevé ODE test predicts that the equation (48) is nonintegrable if $\epsilon \neq 0, \frac{1}{2}$.

V. REDUCTION TO GENERALIZED NLS

We now consider the reduced SDYM equations in the case when the field component B has the normal form

$$B = \kappa \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{49}$$

We begin by making the following ansatz for the components D and C:

$$D = \begin{bmatrix} 0 & \psi \\ -\tilde{\psi} & 0 \end{bmatrix}, \quad C = \begin{bmatrix} p & q \\ r & -p \end{bmatrix}. \tag{50}$$

Then the equation (17) reduces to

$$\begin{bmatrix} 0 & \psi_y \\ -\tilde{\psi}_y & 0 \end{bmatrix} = -f\kappa \begin{bmatrix} 0 & -2q \\ 2r & 0 \end{bmatrix}. \tag{51}$$

Thus, we must have

$$q = \frac{\psi_y}{2f\kappa}, \quad r = \frac{\tilde{\psi}_y}{2f\kappa}, \tag{52}$$

i.e.,

$$C = \begin{bmatrix} p & \dfrac{\psi_y}{2f\kappa} \\ \dfrac{\tilde{\psi}_y}{2f\kappa} & -p \end{bmatrix}. \tag{53}$$

We now substitute D and C into (18) to obtain the following equation after some calculation:

$$\begin{bmatrix} p_y & -f'\psi - 2f\psi_u + \dfrac{\psi_{yy}}{2f\kappa} \\ f'\tilde{\psi} + 2f\tilde{\psi}_u - \dfrac{\tilde{\psi}_{yy}}{2f\kappa} & -p_y \end{bmatrix} + \begin{bmatrix} -\dfrac{(\psi\tilde{\psi})_y}{\kappa} & 4fp\psi \\ 4fp\tilde{\psi} & \dfrac{(\psi\tilde{\psi})_y}{\kappa} \end{bmatrix} = 0. \tag{54}$$

Using the equation given by the (1,1) entries on both sides of (54), we see that we may take

$$p = \frac{\psi\tilde{\psi}}{\kappa}. \tag{55}$$

If we set $\kappa = i/2$ and $\tilde{\psi} = -\overline{\psi}$ (where $\overline{\psi}$ denotes the complex conjugate of ψ), then

$$p = 2i|\psi|^2. \tag{56}$$

We now substitute this expression for p in the equation given by the (1, 2) entries on both sides of (54) to get

$$-ff'\psi-2f^2\psi_u-i\psi_{yy}+8if^2|\psi|^2\psi=0. \tag{57}$$

This is a generalized (variable coefficient) NLS equation.

We now wish to reduce this equation to a form which is suitable for application of the Painlevé PDE test. We begin by transforming the dependent variable ψ as follows:

$$\psi\rightarrow\frac{\psi}{f}. \tag{58}$$

Then (57) reduces to

$$ff'\psi-2f^2\psi_u-i\psi_{yy}+8i|\psi|^2\psi=0. \tag{59}$$

Next, let

$$t=\int\frac{1}{2f^2(u)}du. \tag{60}$$

Then (59) transforms to

$$\frac{if_t\psi}{2f}-i\psi_t+\psi_{yy}+8|\psi|^2\psi=0. \tag{61}$$

Finally, if we apply the transformation

$$\psi\rightarrow-2\psi,\quad y'=4y,\quad t'=16t, \tag{62}$$

and rename t' as t and y' as x, then we get the required form of the generalized NLS equation:

$$-\frac{if_t}{2f}\psi+i\psi_t+\psi_{xx}-2|\psi|^2\psi=0. \tag{63}$$

Now, according to Clarkson (Ref. 4), the generalized nonlinear Schrödinger equation

$$i\psi_t+\psi_{xx}-2|\psi|^2\psi=a(x,t)\psi+b(x,t) \tag{64}$$

passes the Painlevé PDE test if and only if

$$a(x,t)=x^2\left(\frac{1}{2}\frac{d\beta}{dt}-\beta^2\right)+i\beta(t)+x\alpha_1(t)+\alpha_0(t) \tag{65}$$

and

$$b(x,t)\equiv0. \tag{66}$$

In our case, $\alpha_1(t)=\alpha_0(t)=b(x,t)\equiv0$ and $\beta(t)=f_t/2f$. Also since there is no quadratic term in x [in $a(x,t)$] we must have

$$\frac{1}{2}\frac{d\beta}{dt}-\beta^2=0, \tag{67}$$

i.e.,

$$\beta = -\frac{1}{2(t-t_0)} \tag{68}$$

which is easily seen to imply that

$$f = ku + l, \tag{69}$$

where k and l are constants.

We conclude that the generalized NLS equation (63) passes the Painlevé PDE test if and only if the metric (1) is flat.

VI. DISCUSSION

As mentioned by us in the introduction, the SDYM equations in flat space and the twistor description of these equations have deep connections with the theory of integrable systems. However, as the results in our paper indicate, the situation appears to be quite different when we study these equations in a (conformally) curved spacetime. Since our results were obtained for a specific class of metrics, it may be of interest to study reductions of the SDYM equations in other curved spacetimes.

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A family of integrable nonlinear equations of hyperbolic type

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A new system of integrable nonlinear equations of hyperbolic type, obtained by a two-dimensional reduction of the anti-self-dual Yang–Mills equations, is presented. It represents a generalization of the Ernst–Weyl equation of General Relativity related to colliding neutrino and gravitational waves, as well as of the fourth order equation of Schwarzian type related to the KdV hierarchies, which was introduced by Nijhoff, Hone, and Joshi recently. An auto-Bäcklund transformation of the new system is constructed, leading to a superposition principle remarkably similar to the one connecting four solutions of the KdV equation. At the level of the Ernst–Weyl equation, this Bäcklund transformation and the associated superposition principle yield directly a generalization of the single and double Harrison transformations of the Ernst equation, respectively. The very method of construction also allows for revealing, in an essentially algorithmic fashion, other integrability features of the main subsystems, such as their reduction to the Painlevé transcendents. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1416488]

I. INTRODUCTION

The main relationship between the anti-self-dual Yang–Mills equations (ASDYM) and integrable systems of partial differential equations (PDEs) stems from the fact that most well-known integrable systems arise as reductions of the ASDYM equations, or higher-dimensional generalizations of them, by imposing appropriate symmetry conditions.[1] We adopt that saying a system of equations is integrable means that the equations under consideration can be linearized directly, or they can be expressed as consistency conditions for the solution of a linear overdetermined system of PDEs of a certain type (Lax pair).

Of particular interest are the two-dimensional reductions, which are constructed using specific two-dimensional subgroups of the full group of conformal isometries of the four-dimensional complex Minkowski space. A prime example of this kind of reduction is provided by the Ernst equation of General Relativity, which forms the basis of stationary axisymmetric, cylindrical or plane symmetric solutions of the Einstein equations.[2–8] A comprehensive review of two-dimensional reductions of the ASDYM equations is presented in Ref. 8, where a general class of a two-dimensional group of conformal transformations, not necessarily translations, is considered. In all of the above reductions to the Ernst equation, at least one of the two conformal Killing vectors (CKVs) has a nontrivial lift to the twistor space and the formulation is adapted to the Yang matrix J.

In the present paper we consider, instead, a two-dimensional reduction of the ASDYM equations based on a pair of commuting CKVs which are left rotations and leave the α-planes through the origin invariant. It leads to a quite general system of integrable equations of hyperbolic type in two independent variables, which represents a generalization not only of the Ernst–Weyl equation for coupled gravitational and neutrino waves in General Relativity, but of the fourth order equation

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of Schwarzian type introduced by Nijhoff, Hone, and Joshi[9] recently, which is related to the KdV hierarchy.

More specifically, our reduction scheme uses **GL**$(2,\mathbb{C})$ as the gauge group and connection potentials that are matrices of unit rank. The general background, as well as the specific features, of the reduction process are presented in Sec. II. In the same section we present the end result of the reduction. It consists of a system of equations which, written in an invariant form, reads as follows:

$$\mathrm{d}\,(P+R)-*\mathrm{d}\,(P-R)=\frac{P-R}{\rho}\,((P-R)*\mathrm{d}U-\mathrm{d}\beta), \tag{1a}$$

$$\rho\mathrm{d}*\mathrm{d}U-\mathrm{d}\beta\wedge\mathrm{d}U=(P-R)\mathrm{d}U\wedge*\mathrm{d}U, \tag{1b}$$

$$\mathrm{d}*\mathrm{d}\rho=0,\quad \mathrm{d}*\mathrm{d}\beta=0. \tag{1c}$$

The complex functions U, P, R depend on the real coordinates u, v. The functions ρ, β are arbitrary real and complex solutions of the wave equation, respectively. The operator $*$ is a two-dimensional Hodge duality operator acting on one-forms as

$$*\mathrm{d}u=\mathrm{d}u,\quad *\mathrm{d}v=-\mathrm{d}v. \tag{1d}$$

The above system of equations can also be considered as the compatibility or integrability condition of a linear pair of equations parametrized by a complex parameter. This Lax pair of equations is presented in Sec. III, where it is shown that it can be derived algorithmically from the Lax pair of the ASDYM equations. In the same section we derive an auto-Bäcklund transformation of system (1), using the above Lax pair and the standard Gauss decomposition of **GL**$(2,\mathbb{C})$.

The restrictions

$$\rho=\tfrac{1}{2}(v-u),\quad \mathrm{d}\beta=n\,\mathrm{d}u+m\,\mathrm{d}v,\quad n,m\ \text{complex parameters}, \tag{2}$$

of the functions ρ and β, reduce system (1) to a potential form of the fourth order equation of Schwarzian type introduced recently by Nijhoff *et al.*,[9] which was called a regular partial differential equation (RPDE) by the above authors. Its importance stems from the fact that it is directly associated with the KdV hierarchies. The exact relation of the system (1) to the RPDE, as well as to the well-known Euler–Poisson–Darboux equation, is the object of Sec. IV. In the same section, we present a new family of fourth order equations which contains the RPDE among its members.

Imposing appropriate conditions on the variables P, R and β, on the other hand, turns the system (1) into the Ernst–Weyl equation,

$$\mathcal{R}e(E)(\mathrm{d}(\rho*\mathrm{d}E)-\mathrm{i}\,\mathrm{d}a\wedge\mathrm{d}E)=\rho\,\mathrm{d}E\wedge*\mathrm{d}E, \tag{3}$$

for colliding neutrino waves accompanied by gravitational waves.[10] The Ernst equation for colliding pure gravitational waves in a flat background is also obtained in this way, by applying further restrictions on β. The Neugebauer–Kramer involution arises naturally from the conditions imposed on system (1) and defines a map connecting the real components of two Ernst–Weyl equations.

The relation of system (1) to the Ernst and Ernst–Weyl equations is described in full detail in Sec. V. Section VI, on the other hand, is devoted to another integrability feature of the Ernst–Weyl and RPDE subsystems of the system (1), namely their reduction to Painlevé transcendents. More specifically, in Sec. VI we show how the relation between the Ernst–Weyl and the RPDE equations, established by their being members of the same system (1), facilitates the construction of group invariant solutions of the former based on the Painlevé transcendents from similar kinds of solutions of the latter equation.

The final section of the paper consists of the Perspectives, where an overall evaluation of the results obtained in the main body of the paper is presented, along with the description of various avenues for expanding the above results.

II. REDUCTION OF THE ASDYM EQUATIONS

In this section we present the first main result of this paper. It consists of the new integrable system given by (32), which is derived by a specific two-dimensional reduction of the ASDYM equations.

In order to make the presentation of our result self-contained, we first summarize in Sec. II A the general framework of the ASDYM equations. Then, in Sec. II B, we give the details of the reduction scheme that leads to the new integrable system of equations mentioned above.

A. General considerations

Throughout this section we shall follow the notation and conventions of Refs. 8, 11. Let $M=\mathbb{CM}$ denote the four-dimensional complex Minkowski spacetime and G a Lie group, called the gauge group, and $\mathfrak{g}$ the corresponding Lie algebra. In the finite-dimensional case G can be taken to be $\mathbf{GL}(N,\mathbb{C})$.

Let $P(M,G)$ be a principal bundle, $\{U_i\}$ an open covering of M and s_i a local section defined on each U_i. The Lie algebra valued one-form $\omega\in\mathfrak{g}\otimes T^*P$, called the connection one-form, and the two-form $\Omega\in\mathfrak{g}\otimes\Omega^2(P)$, called the curvature two-form, satisfy the Cartan structure equation,

$$\Omega=\mathrm{d}_P\omega+\omega\wedge\omega,$$

where d_P is the exterior derivative on P. The $\mathfrak{g}$-valued one-form (gauge potential) Φ_i is defined locally as the pull-back $\Phi_i=s_i^*\omega$ of the connection one-form ω and the $\mathfrak{g}$-valued two-form F_i, also called curvature two-form or (Yang–Mills) field strength, is defined by $\mathrm{F}_i=s_i^*\Omega$. If s, s' are local sections over U such that $s'(p)=s(p)g(p)$, $p\in U$, $g\in G$ then the corresponding local one-forms Φ and Φ' are related by

$$\Phi'=g^{-1}\Phi g+g^{-1}\,\mathrm{d}g, \tag{4}$$

where d is the exterior derivative on M. The potentials Φ and Φ' are said to be related through a gauge transformation and they are regarded as being equivalent. From the Cartan structure equation it follows that the curvature F can be expressed in terms of the gauge potential Φ as

$$\mathrm{F}=\mathrm{d}\Phi+\Phi\wedge\Phi. \tag{5}$$

Under gauge transformations (4) the local two-forms F and F′ are related by

$$\mathrm{F}'=g^{-1}\mathrm{F}g.$$

In double null coordinates $x^a=(w,z,\tilde{w},\tilde{z})$ the metric on $\mathbb{CM}$ is given by

$$\mathrm{d}s^2=2(\mathrm{d}z\,\mathrm{d}\tilde{z}-\mathrm{d}w\,\mathrm{d}\tilde{w}). \tag{6}$$

In this coordinate system the gauge potential Φ may be written as

$$\Phi=\Phi_w\,\mathrm{d}w+\Phi_z\,\mathrm{d}z+\Phi_{\tilde{w}}\,\mathrm{d}\tilde{w}+\Phi_{\tilde{z}}\,\mathrm{d}\tilde{z}, \tag{7}$$

where the components are $\mathfrak{g}$-valued functions. Φ is said to be anti-self-dual iff F is Hodge anti-self-dual with respect to the metric (6), i.e.,

$$\mathrm{F}=-*\mathrm{F}. \tag{8}$$

Choosing an orientation, condition (8) is equivalent to the ASDYM equations,

$$\partial_z \Phi_w - \partial_w \Phi_z + [\Phi_z, \Phi_w] = 0, \tag{9a}$$

$$\partial_{\tilde{z}} \Phi_{\tilde{w}} - \partial_{\tilde{w}} \Phi_{\tilde{z}} + [\Phi_{\tilde{z}}, \Phi_{\tilde{w}}] = 0, \tag{9b}$$

$$\partial_z \Phi_{\tilde{z}} - \partial_{\tilde{z}} \Phi_z - \partial_w \Phi_{\tilde{w}} + \partial_{\tilde{w}} \Phi_w + [\Phi_z, \Phi_{\tilde{z}}] - [\Phi_w, \Phi_{\tilde{w}}] = 0. \tag{9c}$$

These equations are the integrability conditions of the overdetermined linear system (Lax pair),[12,13]

$$(\partial_w + \Phi_w - \zeta(\partial_{\tilde{z}} + \Phi_{\tilde{z}}))\Psi = 0, \tag{10a}$$

$$(\partial_z + \Phi_z - \zeta(\partial_{\tilde{w}} + \Phi_{\tilde{w}}))\Psi = 0, \tag{10b}$$

where $\Psi(x^a;\zeta)$ is a G-valued function of the spacetime coordinates and the spectral parameter ζ.

B. The reduced equations

For a two-dimensional reduction of the ASDYM equations, one first chooses a two-dimensional subgroup H of the full group of conformal isometries of the Minkowski space. Then, one can reduce the number of the dependent variables by imposing algebraic constraints on the components of Φ, in a way which is consistent with the equations.

A general class of two-dimensional reductions is considered in Ref. 8 where H is generated by two conformal Killing vectors:

$$X = a\partial_w + b\partial_z + \tilde{a}\partial_{\tilde{w}} + \tilde{b}\partial_{\tilde{z}}, \quad Y = c\partial_w + d\partial_z + \tilde{c}\partial_{\tilde{w}} + \tilde{d}\partial_{\tilde{z}}, \tag{11}$$

where a, b, c, d and $\tilde{a}$, $\tilde{b}$, $\tilde{c}$, $\tilde{d}$ depend only on w, z and $\tilde{w}$, $\tilde{z}$, respectively. Both of the quadruples $\{X, Y, \partial_w, \partial_z\}$ and $\{X, Y, \partial_{\tilde{w}}, \partial_{\tilde{z}}\}$ should be linearly independent and the reduced metric on the orbits of H should be nondegenerate. These conditions assure a compatible reduction.

The most straightforward reduction of this form arises when the corresponding algebra $\mathfrak{h}$ is *Abelian*. We assume that this is the case and we further limit the choices of the components of X and Y by demanding that X and Y leave invariant the α-planes through the origin (the meaning of this requirement will become clear later) and are not a combination of translations. It turns out that these requirements are satisfied only by the commuting null CKVs,

$$X = w\partial_w + \tilde{z}\partial_{\tilde{z}}, \quad Y = z\partial_z + \tilde{w}\partial_{\tilde{w}}. \tag{12}$$

The invariant spacetime coordinates on the orbits of the two-dimensional group of conformal transformations generated by X, Y are arbitrary functions of the fractions $w/\tilde{z}$, $z/\tilde{w}$. Without loss of generality we choose the coordinates of the space of orbits S to be

$$u = \frac{w}{\tilde{z}}, \quad v = \frac{z}{\tilde{w}}, \tag{13}$$

and restrict ourselves to the ultrahyperbolic slice of $\mathbb{CM}$ where the spacetime coordinates are real. The metric induced on S is conformal to two-dimensional Minkowski spacetime in null coordinates, i.e.,

$$\mathrm{d}s^2 = \frac{2}{v-u}\,\mathrm{d}u\,\mathrm{d}v. \tag{14}$$

The invariance conditions of the potential Φ with respect to the algebra generated by X, Y are

$$\mathcal{L}_X \Phi = \mathcal{L}_Y \Phi = 0, \tag{15}$$

where $\mathcal{L}_X$ denotes the Lie derivative along X. Under these conditions, one can write the components of the gauge potential Φ in the form

$$\Phi_w=\frac{1}{w}A(u,v),\quad \Phi_z=\frac{1}{z}B(u,v),\quad \Phi_{\tilde{w}}=\frac{1}{\tilde{w}}\tilde{A}(u,v),\quad \Phi_{\tilde{z}}=\frac{1}{\tilde{z}}\tilde{B}(u,v). \tag{16}$$

We choose to work with the invariant gauge where $\tilde{A}$ and $\tilde{B}$ become the Higgs fields of X and Y, respectively. This means that $\tilde{A}$ and $\tilde{B}$ are contractions of the invariant gauge potential Φ with the vector fields X and Y, respectively, i.e., $\tilde{A}=X\lrcorner\Phi$, $\tilde{B}=Y\lrcorner\Phi$. In this gauge one can put $A=B=0$, whereupon the ASDYM equations (9) become

$$v\tilde{B}_{,v}-u\tilde{A}_{,u}+[\tilde{B},\tilde{A}]=0, \tag{17a}$$

$$\tilde{B}_{,v}-\tilde{A}_{,u}=0. \tag{17b}$$

Equation (17b) implies the existence of a matrix function $K(u,v)$ such that

$$\tilde{B}=K_{,u},\quad \tilde{A}=K_{,v}, \tag{18}$$

and hence Eq. (17a) becomes

$$(v-u)K_{,u\,v}+[K_{,u},K_{,v}]=0. \tag{19}$$

The remaining gauge freedom is $\tilde{A}\to g^{-1}\tilde{A}g$ and $\tilde{B}\to g^{-1}\tilde{B}g$ or, equivalently, $K\to g^{-1}Kg+c$ where g, c constant matrices.

Alternatively, one can look at (17a) as a sufficient condition of the existence of the matrix function J such that

$$\tilde{A}=-vJ^{-1}J_{,v},\quad \tilde{B}=-uJ^{-1}J_{,u}. \tag{20}$$

Then (17b) takes the following form:

$$(uJ^{-1}J_{,u})_{,v}-(vJ^{-1}J_{,v})_{,u}=0. \tag{21}$$

Introducing the functions ρ, σ by

$$\rho=\tfrac{1}{2}(v-u),\quad \sigma=\tfrac{1}{2}(v+u), \tag{22}$$

one can now write Eq. (19) in an invariant form, namely

$$\rho\,\mathrm{d}{*}\mathrm{d}K-\mathrm{d}K\wedge\mathrm{d}K=0. \tag{23}$$

In a similar fashion Eq. (21) takes the coordinate free form,

$$\mathrm{d}(\rho J^{-1}{*}\mathrm{d}J)=\mathrm{d}(\sigma J^{-1}\,\mathrm{d}J). \tag{24}$$

From the way the coordinates (u,v) were introduced one sees that a more general coordinate system is obtained via the coordinate transformation

$$u\to f(u),\quad v\to g(v), \tag{25}$$

i.e., by relabeling the null coordinates (u,v). Within this more general setting it follows that

$$\rho=\tfrac{1}{2}(g(v)-f(u)),\quad \sigma=\tfrac{1}{2}(g(v)+f(u)), \tag{26}$$

and the functions ρ, σ may be invariantly defined as conjugate solutions of the wave equation $d*d\rho=0$.

Now, Eq. (17) imply that

$$\partial_u(\mathrm{tr}\,\tilde{A}^k)=\partial_v(\mathrm{tr}\,\tilde{B}^k)=0, \text{ where } k=1,2,...,N-1. \tag{27}$$

Hence

$$\mathrm{tr}\,\tilde{A}^k=m_k(v), \quad \mathrm{tr}\,\tilde{B}^k=n_k(u). \tag{28}$$

To reduce the number of the dependent variables we restrict to the case where $N=2$ and $\tilde{A},\tilde{B}$ are matrix functions with

$$\mathrm{rank}\,\tilde{A}=\mathrm{rank}\,\tilde{B}=1. \tag{29}$$

With these algebraic constraints, $\tilde{A}$, $\tilde{B}$ may be written as

$$\tilde{A}=\begin{pmatrix} m(v)-RQ & Q \\ R(m(v)-RQ) & RQ \end{pmatrix}, \quad \tilde{B}=\begin{pmatrix} n(u)-PS & S \\ P(n(u)-PS) & PS \end{pmatrix}, \tag{30}$$

where P, Q, R, S are complex functions of (u,v). Inserting $\tilde{A}$ and $\tilde{B}$ given by (30) into the matrix equation (17b), one finds that the upper right element gives

$$Q_{,u}=S_{,v}, \tag{31}$$

which implies the existence of a function U such that $Q=U_{,v}$ and $S=U_{,u}$. In virtue of these relations, Eq. (17a) yields the following system of PDEs:

$$(g(v)-f(u))P_{,v}=(R-P)(m(v)+(P-R)U_{,v}), \tag{32a}$$

$$(g(v)-f(u))R_{,u}=(R-P)(n(u)-(P-R)U_{,u}), \tag{32b}$$

$$(g(v)-f(u))U_{,uv}=m(v)U_{,u}-n(u)U_{,v}+2(P-R)U_{,u}U_{,v}. \tag{32c}$$

This system will be denoted by

$$\Sigma(u,v,U,P,R;m(v),n(u))=0 \tag{33}$$

in the following. We close this section by pointing out that the remaining equation of system (17), namely Eq. (17b), is trivially satisfied when (33) holds.

III. THE REDUCED LAX PAIR AND AN AUTO-BÄCKLUND TRANSFORMATION

Linear (Lax pairs) and nonlinear (Bäcklund transformations) deformation problems are invaluable techniques for generating solutions of integrable equations. As a matter of fact these problems are so interrelated that one can in general derive Bäcklund transformations from the corresponding Lax pair (see, for example, Refs. 14, 15).

Most of the well-known integrable equations in two independent variables, such as the KdV and the sine-Gordon equations, admit a Lax pair of the form

$$d\Psi=\Omega\Psi, \tag{34}$$

where Ψ belongs in $\mathbf{SL}(2,\mathbb{R})$ and Ω is a $\mathfrak{sl}(2,\mathbb{R})$-valued one form. The associated equation arises from the integrability condition $d\Omega=\Omega\wedge\Omega$ and the particular way the independent and dependent variables enter into Ω. Using the Iwasawa decomposition of $\mathbf{SL}(2,\mathbb{R})$ for Ψ, one may construct a Bäcklund transformation associated with the given PDE.[15]

The system $\Sigma=0$ also admits a Lax pair of the form (34). It can be derived algorithmically from the Lax pair (10) of the ASDYM equations by applying the invariance conditions[16]

$$\mathcal{L}_X\Psi=\mathcal{L}_Y\Psi=0. \tag{35}$$

These conditions imply that Ψ depends only on the invariant coordinates u, v and the spectral parameter ζ. Taking into account (16) and putting $A=B=0$, we find that Eqs. (10) reduce to

$$\Psi_{,u}=\frac{1}{f(u)-\lambda}\tilde{B}\Psi, \tag{36a}$$

$$\Psi_{,v}=\frac{1}{g(v)-\lambda}\tilde{A}\Psi, \tag{36b}$$

where we have set $\lambda=-\zeta^{-1}$. It is now easily verified that the integrability condition $\Psi_{,uv}=\Psi_{,vu}$ leads to $\Sigma=0$. This means that Eqs. (36) constitute a Lax pair for the system $\Sigma=0$.

At this point it is worth noting that using (18) and (26), the Lax pair (36) may be written in an invariant form as

$$(\sigma-\lambda-\rho*)\mathrm{d}\Psi=\mathrm{d}K\,\Psi, \tag{37a}$$

where

$$(\sigma-\lambda-\rho*)^{-1}=\frac{(\sigma-\lambda+\rho*)}{(\sigma-\lambda)^2-\rho^2}. \tag{37b}$$

We point out that the linear system (37), or equivalently (36), includes the Lax pair used by Hauser and Ernst in solving the initial value problem for colliding plane gravitational waves.[17]

We are now ready to construct a Bäcklund transformation of the system $\Sigma=0$, using the Lax pair (36). To this end, we generalize the technique employed in the case where $\Psi\in\mathbf{SL}(2,\mathbb{R})$ by considering the Gauss decomposition of $\mathbf{GL}(2,\mathbb{C})$.[18] It allows us to write the spectral potential Ψ in the form

$$\Psi=L^{-1}T, \tag{38}$$

where T is an upper triangular matrix and L is a lower triangular one of the form

$$L=\begin{pmatrix}1 & 0\\ -\tilde{U} & 1\end{pmatrix}. \tag{39}$$

Substituting (38) into the Lax pair (36) we obtain the following linear system for the matrix function T:

$$T_{,u}T^{-1}=L_{,u}L^{-1}+\frac{1}{f(u)-\lambda}L\tilde{B}L^{-1}, \tag{40a}$$

$$T_{,v}T^{-1}=L_{,v}L^{-1}+\frac{1}{g(v)-\lambda}L\tilde{A}L^{-1}. \tag{40b}$$

The lower left elements of the the above system lead to the following Riccati system for the function $\tilde{U}$:

$$\tilde{U}_{,u}=\frac{P-\tilde{U}}{f(u)-\lambda}(n(u)-(P-\tilde{U})U_{,u}), \tag{41a}$$

$$\tilde{U}_{,v}=\frac{R-\tilde{U}}{g(v)-\lambda}(m(v)-(R-\tilde{U})U_{,v}). \tag{41b}$$

The integrability condition of (41) is satisfied if the system $\Sigma=0$ holds. In other words, (41) defines a Bäcklund map for the system $\Sigma=0$. Using such a map, one may construct an auto-Bäcklund transformation for the system under consideration in a manner presented in Ref. 14.

More specifically, solving Eqs. (41) for the derivatives of U we obtain

$$U_{,u}=\frac{1}{P-\tilde{U}}\left(n(u)-\frac{f(u)-\lambda}{P-\tilde{U}}\tilde{U}_{,u}\right), \tag{42a}$$

$$U_{,v}=\frac{1}{R-\tilde{U}}\left(m(v)-\frac{g(v)-\lambda}{R-\tilde{U}}\tilde{U}_{,v}\right). \tag{42b}$$

When Eqs. (32a), (32b) and (42) are satisfied, the integrability condition $U_{,uv}=U_{,vu}$ implies that $\tilde{U}$ satisfies the following equation:

$$(f(u)-g(v))\tilde{U}_{,uv}=n(u)\tilde{U}_{,v}-m(v)\tilde{U}_{,u}+2\left(\frac{f(u)-\lambda}{\tilde{U}-P}-\frac{g(v)-\lambda}{\tilde{U}-R}\right)\tilde{U}_{,u}\tilde{U}_{,v}. \tag{43}$$

If not stated otherwise, we will assume that $P\neq R$ in what follows. The particular case $P=R$ will be considered separately in the next section.

Equation (43) takes the form

$$(f(u)-g(v))\tilde{U}_{,uv}=n(u)\tilde{U}_{,v}-m(v)\tilde{U}_{,u}-2(\tilde{P}-\tilde{R})\tilde{U}_{,u}\tilde{U}_{,v}, \tag{44}$$

by introducing

$$\tilde{P}=W-\frac{f(u)-\lambda}{\tilde{U}-P},\quad \tilde{R}=W-\frac{g(v)-\lambda}{\tilde{U}-R}, \tag{45}$$

where $W=W(u,v)$ is an auxiliary function. Equation (44) is none other than Eq. (32c) with (U,P,R) replaced by $(\tilde{U},\tilde{P},\tilde{R})$. It suffices to determine W in such a way that the functions $(\tilde{U},\tilde{P},\tilde{R})$, defined by (41) and (45), satisfy $\Sigma(u,v,\tilde{U},\tilde{P},\tilde{R})=0$ whenever $\Sigma(u,v,U,P,R)=0$ holds. This requirement and the differential consequences of (45) result in

$$W=U, \tag{46}$$

up to a nonsignificant constant of integration. In conclusion, we have established the following.

Proposition 1: The algebro-differential system,

$$\tilde{U}_{,u}=\frac{P-\tilde{U}}{f(u)-\lambda}(n(u)-(P-\tilde{U})U_{,u}), \tag{47a}$$

$$\tilde{U}_{,v}=\frac{R-\tilde{U}}{g(v)-\lambda}(m(v)-(R-\tilde{U})U_{,v}), \tag{47b}$$

$$(\tilde{U}-P)(U-\tilde{P})=f(u)-\lambda, \tag{48}$$

$$(\tilde{U}-R)(U-\tilde{R})=g(v)-\lambda, \tag{49}$$

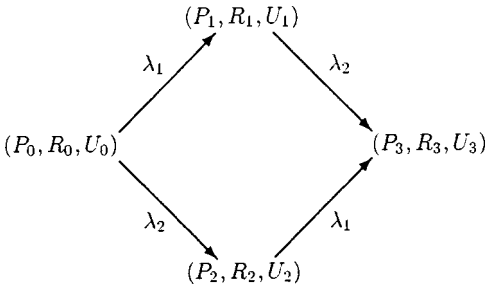

FIG. 1. Bianchi commuting diagram.

constitutes an auto-Bäcklund transformation for the system $\Sigma=0$.

By purely algebraic procedures Proposition 1 leads to the following permutability theorem.

Permutability theorem: *Let* (U_i,P_i,R_i), $i=1,2$, *be a solution of the system (32a)–(32c), generated by means of the Bäcklund transformation (47)–(49) from a known solution* (U_0,P_0,R_0) *via the Bäcklund parameters* λ_1 *and* λ_2, *respectively. Then there exists a new solution* (U_3,P_3,R_3) *which is given by*

$$(U_3-U_0)(U_2-U_1)=\lambda_2-\lambda_1, \tag{50a}$$

$$(P_3-P_0)(P_2-P_1)=\lambda_2-\lambda_1, \tag{50b}$$

$$(R_3-R_0)(R_2-R_1)=\lambda_2-\lambda_1, \tag{50c}$$

where (U_3,P_3,R_3) *is constructed according to* Fig. 1.

IV. NEW AND OLD EQUATIONS RELATED TO THE SYSTEM Σ

Many physically interesting integrable equations arise from the system $\Sigma=0$ by imposing further algebraic constraints on the independent and the dependent variables. This is illustrated in the following sections in terms of a new family of fourth order equations, which represents a generalization of the RPDE introduced by Nijhoff *et al.*[9] recently, the RPDE itself and the well-known Euler–Poisson–Darboux equation. The Ernst–Weyl equation is also contained in the system $\Sigma=0$ and is presented thoroughly in the next section.

A. The generalized RPDE

The system $\Sigma=0$ leads to a fourth order PDE for the function U solely in the following manner. First, one may solve Eq. (32c) for the difference $P-R$ to obtain

$$P-R=\mathcal{A}[U]:=\frac{1}{2}\left(2\rho\frac{U_{,uv}}{U_{,u}U_{,v}}+\frac{n(u)}{U_{,u}}-\frac{m(v)}{U_{,v}}\right), \tag{51}$$

where ρ is given by (26). Taking the partial derivative of both sides of (51) with respect to u and using Eq. (32b), we arrive at an expression for $P_{,u}$ involving the derivatives of U only. The latter expression and (32a) form a linear first order system for P which takes the following form:

$$P_{,u}=-\frac{\mathcal{A}}{2\rho}(n(u)-\mathcal{A}U_{,u})+\partial_u\mathcal{A},$$

$$P_{,v}=-\frac{\mathcal{A}}{2\rho}(m(v)+\mathcal{A}U_{,v}).$$

The compatibility condition $P_{,uv}=P_{,vu}$ leads to the equation

$$\partial_u\left(\partial_v\mathcal{A}+\frac{\mathcal{A}^2}{\rho}U_{,v}+m(v)\frac{\mathcal{A}}{\rho}\right)+\partial_v\left(\partial_u\mathcal{A}+\frac{\mathcal{A}^2}{\rho}U_{,u}-n(u)\frac{\mathcal{A}}{\rho}\right)=0. \tag{52}$$

This equation, when written out explicitly, reads as

$$\begin{aligned}U_{,uuvv}=&U_{,uuv}\left(-\frac{\rho_{,v}}{\rho}+\frac{U_{,vv}}{U_{,v}}+\frac{U_{,uv}}{U_{,u}}\right)+U_{,uvv}\left(-\frac{\rho_{,u}}{\rho}+\frac{U_{,uu}}{U_{,u}}+\frac{U_{,uv}}{U_{,v}}\right)-U_{,uu}U_{,vv}\frac{U_{,uv}}{U_{,u}U_{,v}}\\&+U_{,uu}\left(\frac{n(u)^2}{4\rho^2}\frac{U_{,v}^2}{U_{,u}^2}+\frac{\rho_{,v}}{\rho}\frac{U_{,uv}}{U_{,u}}-\frac{U_{,uv}^2}{U_{,u}^2}\right)+U_{,vv}\left(\frac{m(v)^2}{4\rho^2}\frac{U_{,u}^2}{U_{,v}^2}+\frac{\rho_{,u}}{\rho}\frac{U_{,uv}}{U_{,v}}-\frac{U_{,uv}^2}{U_{,v}^2}\right)\\&-\frac{n(u)^2}{8\rho^3}\frac{U_{,v}}{U_{,u}}(\rho_{,v}U_{,u}-\rho_{,u}U_{,v}+2\rho U_{,uv})+\frac{m(v)^2}{8\rho^3}\frac{U_{,u}}{U_{,v}}(\rho_{,v}U_{,u}-\rho_{,u}U_{,v}-2\rho U_{,uv})\\&+\frac{1}{2\rho}U_{,uv}^2\left(\frac{\rho_{,u}}{U_{,u}}+\frac{\rho_{,v}}{U_{,v}}\right)-\frac{n(u)n'(u)}{4\rho^2}\frac{U_{,v}^2}{U_{,u}}-\frac{m(v)m'(v)}{4\rho^2}\frac{U_{,u}^2}{U_{,v}}.\end{aligned} \tag{53}$$

This is a new integrable equation which generalizes the RPDE, as it will be clear from the following section. It will be referred to as the generalized RPDE (GRPDE). In order to clarify its relation to the system $\Sigma=0$, we first introduce a shorthand notation whereby Eq. (53) is written in the form

$$\mathcal{R}(u,v,U;m(v),n(u))=0. \tag{54}$$

In a manner to be explained shortly, one is led to similar equations for the functions P, R, starting from the system $\Sigma=0$. More specifically, these functions satisfy the fourth order equations

$$\mathcal{R}(u,v,P;m(v),n(u)-2\rho_{,u})=0, \tag{55}$$

and

$$\mathcal{R}(u,v,R;m(v)+2\rho_{,v},n(u))=0, \tag{56}$$

respectively. Thus, it becomes clear that the system $\Sigma=0$ represents an involution of a triad of GRPDEs. The members of this triad differ only by specific changes in the parameter functions $m(v)$ and $n(u)$.

Returning to the derivation of Eqs. (55), (56), let us first note that one may eliminate the derivatives of U from the system $\Sigma=0$ by solving (32a) and (32b) for $U_{,v}$ and $U_{,u}$, respectively. Using compatibility conditions and (32c), one then ends up with the following system for P, R:

$$P_{,uv}=\frac{2}{P-R}P_{,u}P_{,v}+\frac{m(v)}{2\rho}P_{,u}+\frac{n(u)-2\rho_{,u}}{2\rho}P_{,v}, \tag{57a}$$

$$R_{,uv}=\frac{2}{R-P}R_{,u}R_{,v}-\frac{m(v)+2\rho_{,v}}{2\rho}R_{,u}-\frac{n(u)}{2\rho}R_{,v}. \tag{57b}$$

It is now a matter of straightforward, but lengthy, calculations to decouple the above system and arrive to Eqs. (55), (56) for P and R, respectively.

At this point, it is worth noting that Eqs. (57) may be combined to yield[19]

$$(\rho SS_{,u})_{,v}+(\rho SS_{,v})_{,u}+\tau_{,u}S_{,v}+\tau_{,v}S_{,u}=0, \tag{58}$$

where

$$\tau:=\sigma+\beta, \tag{59a}$$

and S is a 2×2 matrix defined by

$$S=\frac{1}{R-P}\begin{pmatrix} P+R & -2 \\ 2PR & -(P+R)\end{pmatrix}. \tag{59b}$$

The matrix equation (58) represents a complexified hyperbolic version of the stationary Loewner–Konopelchenko–Rogers (LKR) system[20] proposed by Schief[21] as a 2×2 real matrix representation of the Ernst–Weyl equation in stationary, axisymmetric spacetimes. It should be pointed out that LKR systems have proven to be a repository of mathematically and physically interesting integrable equations in $2+1$-dimensions, including a $2+1$-dimensional Ernst-type equation, introduced by Schief recently.[22]

B. The RPDE

By choosing

$$f(u)=u, \quad g(v)=v \tag{60a}$$

and

$$m(v)=m, \quad n(u)=n, \tag{60b}$$

where n, m are complex parameters, Eq. (53) becomes

$$\begin{aligned} U_{,uuvv}=&U_{,uuv}\left(\frac{1}{u-v}+\frac{U_{,vv}}{U_{,v}}+\frac{U_{,uv}}{U_{,u}}\right)+U_{,uvv}\left(\frac{1}{v-u}+\frac{U_{,uu}}{U_{,u}}+\frac{U_{,uv}}{U_{,v}}\right)-U_{,uu}U_{,vv}\frac{U_{,uv}}{U_{,u}U_{,v}} \\ &+U_{,uu}\left(\frac{n^2}{(u-v)^2}\frac{U_{,v}^2}{U_{,u}^2}-\frac{1}{u-v}\frac{U_{,uv}}{U_{,u}}-\frac{U_{,uv}^2}{U_{,u}^2}\right)+U_{,vv}\left(\frac{m^2}{(u-v)^2}\frac{U_{,u}^2}{U_{,v}^2}+\frac{1}{u-v}\frac{U_{,uv}}{U_{,v}}-\frac{U_{,uv}^2}{U_{,v}^2}\right) \\ &+\frac{n^2}{2(u-v)^3}\frac{U_{,v}}{U_{,u}}(U_{,u}+U_{,v}+2(v-u)U_{,uv})-\frac{m^2}{2(u-v)^3}\frac{U_{,u}}{U_{,v}}(U_{,u}+U_{,v}+2(u-v)U_{,uv}) \\ &+\frac{1}{2(u-v)}U_{,uv}^2\left(\frac{1}{U_{,u}}-\frac{1}{U_{,v}}\right), \end{aligned} \tag{61}$$

which is the RPDE introduced by Nijhoff *et al.*[9] recently. Its importance stems from the fact that it is a generating equation for the whole hierarchy of the KdV equation. We presented several aspects of the integrability of the RPDE in Ref. 23.

C. The EPD equation

By choosing

$$P=R, \tag{62}$$

and referring to Eqs. (32a), (32b), we find that

$$P=c, \quad c \ \text{constant}. \tag{63}$$

Without loss of generality we set $c=0$. This can be achieved by performing a gauge transformation on $\tilde{A}$, $\tilde{B}$ by $g=\left(\begin{smallmatrix}1 & 0\\ -c & 1\end{smallmatrix}\right)$, whereupon one obtains equivalent Higgs fields with $P=R=0$. Within this setting, the system $\Sigma=0$ reduces to a single linear, second order PDE for U,

$$U_{,uv}=\frac{1}{f(u)-g(v)}(n(u)U_{,v}-m(v)U_{,u}), \tag{64}$$

which is known as the *Euler–Poisson–Darboux* (EPD) equation. From this point of view, the EPD equation may be considered as a linearization of the system $\Sigma=0$.

The substitution $\psi=\tilde{U}^{-1}$ transforms the Riccati equations (41) into the linear system,

$$\psi_{,u}=\frac{n(u)}{f(u)-\lambda}\psi+\frac{U_{,u}}{f(u)-\lambda}, \tag{65a}$$

$$\psi_{,v}=\frac{m(v)}{g(v)-\lambda}\psi+\frac{U_{,v}}{g(v)-\lambda}. \tag{65b}$$

It can be easily verified that the integrability condition $U_{,uv}=U_{,vu}$ and the system (65) lead to

$$\psi_{,uv}=\frac{1}{f(u)-g(v)}(n(u)\psi_{,v}-m(v)\psi_{,u}). \tag{66}$$

A comparison of this with Eq. (64) shows that the system (65) represents an auto-Bäcklund transformation for the EPD equation. The linearity of the same system in ψ indicates that it is also a Lax pair for the EPD equation.

Restricting $U(u,v),m(v),n(u)$ to be real functions of their arguments and choosing

$$n(u)=-\tfrac{1}{2}f'(u),\quad m(v)=-\tfrac{1}{2}g'(v),$$

Eq. (64) becomes

$$2U_{,uv}+\frac{\rho_{,u}}{\rho}U_{,v}+\frac{\rho_{,v}}{\rho}U_{,u}=0,\quad \rho=\frac{1}{2}(g(v)-f(u)). \tag{67}$$

This particular form of the EPD equation governs the collision of two plane gravitational waves with *collinear polarization*[24] in the context of Einstein's General Relativity. The reduced Lax pair (65) becomes the Lax pair used in Ref. 25 for solving the corresponding initial value problem.

V. REDUCTION TO THE ERNST–WEYL EQUATION

One of the most extensively studied problems in General Relativity is the collision of two plane gravitational waves. The Ernst–Weyl equation describes the collision of neutrino waves accompanied by gravitational waves.[10] The latter equation, which reduces to the famous Ernst equation when the neutrino fields vanish everywhere, arises naturally by applying appropriate reality conditions to the system $\Sigma=0$. Our reduction scheme unifies many aspects of the integrability of the Ernst equation like the Hauser–Ernst Lax pair, Neugebauer–Kramer involution, and the Harrison Bäcklund transformation and gives analogous generalizations for the Ernst–Weyl equation.

A. The reality conditions

The system $\Sigma=0$ may be written in the following invariant form:

$$\mathrm{d}(P+R)-*\mathrm{d}(P-R)=\frac{P-R}{\rho}((P-R)*\mathrm{d}U-\mathrm{d}\beta), \tag{68a}$$

$$\rho\mathrm{d}*\mathrm{d}U-\mathrm{d}\beta\wedge\mathrm{d}U=(P-R)\mathrm{d}U\wedge*\mathrm{d}U, \tag{68b}$$

where

$$\rho=\tfrac{1}{2}(g(v)-f(u))\quad\text{and}\quad \mathrm{d}\beta=n(u)\mathrm{d}u+m(v)\mathrm{d}v. \tag{69}$$

Here, we have used the Poincaré lemma to express the one-form $n(u)\mathrm{d}u+m(v)\mathrm{d}v$ as the exterior derivative of a scalar complex function β.

Let us now impose the reality condition,

$$P=-R^{\star}, \tag{70}$$

on (68) with $\star$ denoting complex conjugation. Furthermore, in order to make contact with the notation employed in General Relativity,[26] let us introduce the complex potentials $E,\mathcal{E}$ by

$$\mathcal{E}=\mathcal{F}+\mathrm{i}\chi=P, \quad E=F+\mathrm{i}\omega=U, \tag{71}$$

where $\mathrm{i}=\sqrt{-1}$ and $\mathcal{F}$, F and χ, ω are the real and imaginary parts, respectively, of $\mathcal{E}$, E. In the same fashion, we split the one-form $\mathrm{d}\beta$ into real and imaginary part by setting

$$\mathrm{d}\beta=\mathrm{d}\delta+\mathrm{i}\mathrm{d}a, \tag{72}$$

where a, δ are real solutions of the wave equation. Inserting these into Eq. (68a), the system separates into a real and an imaginary part:

$$\mathrm{d}\mathcal{F}=\frac{\mathcal{F}}{\rho}*\mathrm{d}\delta-\frac{2\mathcal{F}^2}{\rho}\mathrm{d}F \tag{73a}$$

and

$$\mathrm{d}\,\chi=\frac{2\mathcal{F}^2}{\rho}*\mathrm{d}\,\omega-\frac{\mathcal{F}}{\rho}\mathrm{d}a, \tag{73b}$$

respectively. Equation (68b) on the other hand becomes

$$\rho\mathrm{d}*\mathrm{d}E-\mathrm{d}\beta\wedge\mathrm{d}E=2\mathcal{F}\mathrm{d}E\wedge*\mathrm{d}E. \tag{74}$$

The integrability condition $\mathrm{d}^2\mathcal{F}=0$ of Eq. (73a) yields

$$2\mathcal{F}(\mathrm{d}\rho-*\mathrm{d}\delta)\wedge\mathrm{d}F=\mathrm{d}\rho\wedge*\mathrm{d}\delta, \tag{75}$$

which is satisfied for general real functions $\mathcal{F},F$ of (u,v) if

$$\mathrm{d}\delta=*\mathrm{d}\rho=-\mathrm{d}\sigma. \tag{76}$$

Consequently,

$$\mathrm{d}\beta=*\mathrm{d}\rho+\mathrm{i}\mathrm{d}a. \tag{77}$$

Then, Eq. (73a) can be integrated to give

$$\mathcal{F}F=\frac{\rho}{2}, \tag{78}$$

by setting the integration constant equal to zero. The integrability condition of Eq. (73b) is satisfied when Eqs. (74), (77) and (78) hold. In view of (77) and (78), Eq. (74) becomes

$$\mathcal{R}e(E)(\mathrm{d}(\rho*\mathrm{d}E)-\mathrm{i}\ \mathrm{d}a\wedge\mathrm{d}E)=\rho\,\mathrm{d}E\wedge*\mathrm{d}E. \tag{79}$$

Equivalently we may apply the reality condition (70) to the system (57). This condition is compatible with the system for general function $\mathcal{E}$ of (u,v) when (77) holds. In this case, the system (57) reduces to the following single second order PDE for $\mathcal{E}$:

$$\mathcal{R}e(\mathcal{E})(\mathrm{d}(\rho*\mathrm{d}\mathcal{E})+\mathrm{i}*\mathrm{d}a\wedge\mathrm{d}\mathcal{E})=\rho\,\mathrm{d}\mathcal{E}\wedge*\mathrm{d}\mathcal{E}. \tag{80}$$

Hence, the above considerations lead to the following.
Proposition 2: The conditions

$$P=-R^{\star} \tag{81a}$$

and

$$m(v)=-\rho_{,v}+\mathrm{i}\,a_{,v}, \quad n(u)=\rho_{,u}+\mathrm{i}\,a_{,u} \tag{81b}$$

reduce the system (68) and equivalently the system (57) to

$$\mathcal{R}e(E)(\mathrm{d}(\rho*\mathrm{d}E)-\mathrm{i}\,\mathrm{d}a\wedge\mathrm{d}E)=\rho\,\mathrm{d}E\wedge*\mathrm{d}E, \tag{82}$$

$$\mathcal{R}e(\mathcal{E})(\mathrm{d}(\rho*\mathrm{d}\mathcal{E})+\mathrm{i}*\mathrm{d}a\wedge\mathrm{d}\mathcal{E})=\rho\,\mathrm{d}\mathcal{E}\wedge*\mathrm{d}\mathcal{E}, \tag{83}$$

respectively, where E and $\mathcal{E}$ are related through the involution

$$\mathcal{F}F=\frac{\rho}{2}, \quad \mathrm{d}\chi=\frac{2\mathcal{F}^2}{\rho}*\mathrm{d}\omega-\frac{\mathcal{F}}{\rho}\mathrm{d}a. \tag{84}$$

- When $\mathrm{d}a=0$, Eq. (82) becomes the Ernst equation for colliding plane pure gravitational waves in a flat background. The map given by (84) which connects two solutions $(E,\mathcal{E})$ of the Ernst equation, is known as the *Neugebauer–Kramer involution*.[27]
- When $\mathrm{d}a\neq 0$, Eq. (82) is the Ernst–Weyl equation for colliding plane neutrino waves accompanied by gravitational waves. The form of the function a is specified by the initial profile of the neutrino waves on the null hypersurfaces $u=0$, $v=0$. After solving Eq. (82) for E, the neutrino fields and the metric components can be found by quadrature. It should be mentioned here that, in the present case, the spacetime metric is not of the block diagonal form and the two Killing vectors characterizing the plane symmetry of the spacetime are not surface-forming. The map given by (84), connecting solutions of the two different Ernst–Weyl equations (82) and (83), may be viewed as a *generalization of the Neugebauer–Kramer involution.*

The considerations in Sec. IV indicate that the solutions $(E,\mathcal{E})$ of the Ernst–Weyl equations (82), (83) also satisfy

$$\mathcal{R}(u,v,E;-\rho_{,v}+\mathrm{i}\,a_{,v},\rho_{,u}+\mathrm{i}\,a_{,u})=0 \tag{85a}$$

and

$$\mathcal{R}(u,v,\mathcal{E};-\rho_{,v}+\mathrm{i}\,a_{,v},-\rho_{,u}+\mathrm{i}\,a_{,u})=0, \tag{85b}$$

respectively. Thus, the solution space of the Ernst–Weyl equation is imbedded into the solution space of Eq. (53) for the specific choices of $m(v),n(u)$ given by (81b).

B. Reduction of the auto-Bäcklund transformation

Finding exact solutions of Einstein's field equations is quite a difficult task. This is mainly due to the nonlinearity of the field equations. Another reason is that the solutions should respect various types of boundary (side) conditions. In stationary axisymmetric spacetimes for example, the corresponding metric should be asymptotically flat. For colliding wave solutions, on the other hand, the metric must satisfy appropriate junction conditions across the wavefront surfaces. There-

fore, solution generating techniques, such as the inverse scattering transform and Bäcklund transformations, become invaluable methods in finding exact solutions or determining global properties of the field equations (for a survey of results see Ref. 28).

In this section we show how the auto-Bäcklund transformation (47)–(49) of the system $\Sigma=0$ can be reduced to a Bäcklund transformation for the Ernst–Weyl equation. Moreover, we establish the relation of this reduction to the well-known Harrison Bäcklund transformation[29] for the Ernst equation.

To this end, let us first denote by $\mathcal{D}$ the solution space of the system $\Sigma=0$ and by $\mathcal{D}_E\subset\mathcal{D}$ the corresponding space of the Ernst–Weyl equation. Then, the auto-Bäcklund transformation B, defined by (47)–(49), may be viewed as a symmetry transformation in $\mathcal{D}$. In order to construct the reduced Bäcklund transformation for the Ernst–Weyl equation we require $B(\mathcal{D}_E)\subset\mathcal{D}_E$. This requirement implies that the new functions should satisfy the system $\Sigma=0$ *and* conditions (81). Following the notation of the previous section, we shall denote in what follows $\tilde{P}$ by $\tilde{\mathcal{E}}$ and $\tilde{U}$ by $\tilde{E}$.

Under the above conditions the auto-Bäcklund transformation (47)–(49) takes the following form:

$$\tilde{E}_{,u}=\frac{\mathcal{E}-\tilde{E}}{f(u)-\lambda}(\rho_{,u}+\mathrm{i}\,a_{,u}-(\mathcal{E}-\tilde{E})E_{,u}), \tag{86a}$$

$$\tilde{E}_{,v}=\frac{\mathcal{E}^{\star}+\tilde{E}}{g(v)-\lambda}(\rho_{,v}-\mathrm{i}\,a_{,v}-(\mathcal{E}^{\star}+\tilde{E})E_{,v}), \tag{86b}$$

$$(\tilde{E}-\mathcal{E})(E-\tilde{\mathcal{E}})=f(u)-\lambda, \tag{87a}$$

$$(\tilde{E}+\mathcal{E}^{\star})(E+\tilde{\mathcal{E}}^{\star})=g(v)-\lambda. \tag{87b}$$

One can now easily verify the following fact. Starting with a pair of potentials $(E,\mathcal{E})$ related as in (84), then the system (86), (87) delivers a new pair of potentials $(\tilde{E},\tilde{\mathcal{E}})$ which satisfy the same relation.

In order to establish the connection of the above Bäcklund transformation to the one proposed by Harrison, let us first note that in terms of $(E,\mathcal{E})$ the first of Eqs. (84) reads as

$$(E+E^{\star})(\mathcal{E}+\mathcal{E}^{\star})=2\rho. \tag{88}$$

Then, combining (87a), (87b) and (88) one finds that

$$\left|\frac{\tilde{\mathcal{E}}+E^{\star}}{\tilde{\mathcal{E}}-E}\right|^2=\gamma, \tag{89}$$

where $|\,|$ stands for the modulus of a complex number and γ is defined by

$$\gamma:=\frac{g(v)-\lambda}{f(u)-\lambda}. \tag{90}$$

Introducing the function α via

$$\alpha:=\frac{\tilde{\mathcal{E}}+E^{\star}}{\tilde{\mathcal{E}}-E}, \tag{91}$$

we can write Eq. (89) as

$$\alpha\,\alpha^{\star}=\gamma, \tag{92}$$

and Eqs. (87), (91) as

$$\widetilde{E}=\frac{\gamma-\alpha}{\gamma-1}\mathcal{E}+\frac{1-\alpha}{\gamma-1}\mathcal{E}^{\star}, \tag{93a}$$

$$\widetilde{\mathcal{E}}=\frac{\alpha}{\alpha-1}E+\frac{1}{\alpha-1}E^{\star}, \tag{93b}$$

respectively. Finally, Eqs. (86) take the following form:

$$\alpha_{,u}=\alpha(\alpha-1)\frac{E_{,u}}{E+E^{\star}}+(\alpha-\gamma)\frac{E^{\star}_{,u}}{E+E^{\star}}+\frac{\alpha}{2}(\gamma-1)\frac{\rho_{,u}-\mathrm{i}\,a_{,u}}{\rho}, \tag{94a}$$

$$\alpha_{,v}=(\alpha-1)\frac{E^{\star}_{,v}}{E+E^{\star}}+\frac{\alpha}{\gamma}(\alpha-\gamma)\frac{E_{,v}}{E+E^{\star}}+\frac{\alpha}{2\gamma}(\gamma-1)\frac{\rho_{,v}-\mathrm{i}\,a_{,v}}{\rho}. \tag{94b}$$

The converse also holds. More specifically, let us suppose that a pair of potentials $(E,\mathcal{E})$ satisfying Eqs. (82), (84) is given. Then, the members of the Ricatti system (94) for the auxiliary function $\alpha(u,v)$ are compatible and can be integrated to yield a solution which satisfies the condition (92). Moreover, Eqs. (93) deliver a new pair of potentials $(\widetilde{E},\widetilde{\mathcal{E}})$ which *also* satisfy the generalized version of the Neugebauer–Kramer involution. The system (92)–(94) constitutes a generalization of the *single Harrison transformation* for the Ernst equation, to which it reduces when $\mathrm{d}a=0$. We would like to point out that the above novel construction is purely algebraic and yields *explicit* expressions for the new potentials. As far as we are aware only implicit expressions for the new potentials occur in the literature. Let it also be noted that if one considers each member of the pair $(E,\mathcal{E})$ separately, then the relations (92)–(94b) must be viewed as an auto- or hetero-Bäcklund transformation, depending on whether $\mathrm{d}a$ equals 0 or not, respectively. This follows from the fact that E and $\mathcal{E}$ satisfy Eqs. (82) and (83), respectively, which are identical or different depending on whether $\mathrm{d}a$ vanishes or not.

Returning to the considerations of the paragraph preceding the last one, we note that one has to apply the transformation (92)–(94) twice in order to decouple the new potentials. This can be achieved by using the superposition principle (50) in the form resulting by applying the reality conditions. This form is given by

$$E_3=E_0+\frac{\lambda_2-\lambda_1}{E_2-E_1}, \tag{95a}$$

$$\mathcal{E}_3=\mathcal{E}_0+\frac{\lambda_2-\lambda_1}{\mathcal{E}_2-\mathcal{E}_1}. \tag{95b}$$

The potentials $E_i,\mathcal{E}_i$, $i=1,2$, appearing in these relations are determined by

$$E_i=\frac{\gamma_i-\alpha_i}{\gamma_i-1}\mathcal{E}_0+\frac{1-\alpha_i}{\gamma_i-1}\mathcal{E}_0^{\star},$$

$$\mathcal{E}_i=\frac{\alpha_i}{\alpha_i-1}E_0+\frac{1}{\alpha_i-1}E_0^{\star}.$$

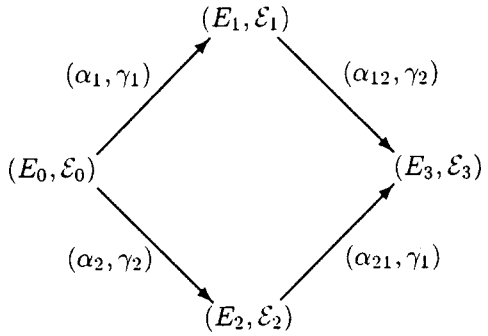

FIG. 2. Commuting diagram for the Harrison transformation.

Here, the γ_i's are defined by (92) with λ replaced by λ_i and the α_i's are obtained from the system (94) by replacing γ by γ_i. Using these expressions, Eqs. (95) reads as

$$E_3=E_0+\frac{(\gamma_2-\gamma_1)(E_0+E_0^\star)}{\gamma_1-\gamma_2-(1-\gamma_2)\alpha_1+(1-\gamma_1)\alpha_2}, \tag{96a}$$

$$\mathcal{E}_3=\mathcal{E}_0-\frac{\gamma_2-\gamma_1}{\alpha_2-\alpha_1}\frac{(1-\alpha_1)(1-\alpha_2)}{(1-\gamma_1)(1-\gamma_2)}(\mathcal{E}_0+\mathcal{E}_0^\star). \tag{96b}$$

Equations (96) represent the double Harrison transformation and are valid for both cases, $da=0$ and $da\neq 0$.

In the Bianchi commuting diagram given in Fig. 2 one can focus on the auxiliary functions α_i's instead of the potentials $(E_i,\mathcal{E}_i)$. Then the superposition principle is expressed by the following relations among the α's:

$$\frac{\alpha_{12}}{\alpha_{21}}=\frac{\alpha_2}{\alpha_1}, \tag{97}$$

where

$$\alpha_{12}=\frac{1}{\alpha_1}\frac{\alpha_1\alpha_2(\gamma_2-\gamma_1)+\alpha_1\gamma_2(\gamma_1-1)+\alpha_2\gamma_1(1-\gamma_2)}{\gamma_1-\gamma_2+\alpha_1(\gamma_2-1)+\alpha_2(1-\gamma_1)}. \tag{98}$$

VI. REDUCTIONS TO THE PAINLEVÉ TRANSCENDENTS

Similarity reductions of the Ernst equation to Painlevé transcendents have been of particular interest for a long time. More recently Schief[21] has shown that the Ernst–Weyl equation for stationary axially symmetric spacetimes [the elliptic analog of Eq. (82)] admits similarity reductions to Painlevé III, V, and VI. His reduction procedure to Painlevé III and V is based on solving the system of ordinary differential equations (ODEs) resulting from the application of the invariance conditions. For the reduction to Painlevé VI, however, the author resorts to a different approach, based on a matrix formulation of the Ernst–Weyl equation, motivated by the Loewner system. In this section, we present a reduction of the hyperbolic Ernst–Weyl equation (82) by a method which exploits the relation of the latter equation to the RPDE and the straightforward manner in which the symmetry group of the RPDE leads to Painlevé's transcendents.

As we have shown,[23] the RPDE admits straightforward similarity reductions to Painlevé III, V, and VI in full form. This was done by considering the invariant solutions under the optimal system of one-dimensional subalgebras of the Lie point symmetries of the RPDE. The link between the RPDE and the Ernst–Weyl equation is the system $\Sigma=0$. Specifically, in Sec. IV, it was shown that the RPDE may be given in involutive form by system (32) with the choices

$$f(u)=u, \quad g(v)=v, \quad m(v)=m, \quad n(u)=n. \tag{99}$$

Within the above setting, the Ernst–Weyl equation arises from the system $\Sigma=0$ by requiring that

$$P=-R^{\star}, \quad m=-\tfrac{1}{2}+\mathrm{i}a_1, \quad n=-\tfrac{1}{2}+\mathrm{i}a_2, \tag{100}$$

where a_1, a_2 are real constants.

On the basis of the above connection, we shall search for invariant solutions of the Ernst–Weyl equation that follow from imposing conditions (100) on corresponding invariant solutions of the RPDE. As we shall immediately show, this can best be achieved by first prolonging the symmetries of the RPDE to symmetries of the system $\Sigma=0$. For illustration purposes, we shall restrict our presentation to invariant solutions that are related to the full Painlevé V and VI cases, only. To make the presentation self-contained, we first summarize briefly the Lie point symmetries of the RPDE.

The Lie point symmetry group of the RPDE consists of transformations leaving the dependent variables unaffected (base transformations) and transformations acting on the dependent variables only (vertical transformations). The base transformations act on $(u,v)\in\mathbb{R}^2$ by

$$(u,v)\rightarrow(\lambda u+\epsilon,\lambda v+\epsilon), \quad \lambda\in\mathbb{R}^{+}, \ \epsilon\in\mathbb{R}, \tag{101}$$

and the generators are given by the vector fields

$$\partial_u+\partial_v, \quad u\partial_u+v\partial_v. \tag{102}$$

The group of vertical transformations is the most general group of transformations acting locally effectively on a one-dimensional complex manifold and is given by

$$U\rightarrow\frac{aU+b}{cU+d}, \quad \begin{pmatrix} a & b \\ c & d \end{pmatrix}\in\mathbf{SL}(2,\mathbb{C}). \tag{103}$$

The corresponding generators are the vector fields

$$\partial_U, \quad U\partial_U, \quad U^2\partial_U. \tag{104}$$

A. Reduction to Painlevé V

The group invariant solutions of the RPDE under the symmetry generator,

$$\partial_u+\partial_v+2\mu U\partial_U, \tag{105}$$

have the form

$$U(u,v)=S(y)\exp(\mu(u+v)), \quad y=u-v. \tag{106}$$

The prolongation of the vector field (105) in the P and R directions which yields a symmetry of the system $\Sigma=0$ reads as

$$\partial_u+\partial_v+2\mu U\partial_U-2\mu(P\partial_P+R\partial_R). \tag{107}$$

This implies that the invariant form of the functions P and R is

$$P(u,v)=p(y)\exp(-\mu(u+v)), \quad R(u,v)=r(y)\exp(-\mu(u+v)), \tag{108}$$

respectively. Inserting (106), (108) into the system $\Sigma=0$ we get the following system of ODEs:

$$(S'-\mu S)(p-r)^2-m(p-r)-y(p'+\mu p)=0, \tag{109a}$$

$$(S'+\mu S)(p-r)^2-n(p-r)+y(r'-\mu r)=0, \tag{109b}$$

$$yS''+2(p-r)S'^2-(m+n)S'-2\mu^2(p-r)S^2-\mu(m-n+\mu y)S=0. \tag{109c}$$

By a simple differentiation and elimination process applied to system (109), one ends up with a fourth order ODE for the function S, which can be integrated once leading to

$$y^2S(S'^2-\mu^2S^2)S'''-y^2SS'S''^2+y(-yS'^3+SS'^2+3\mu^2yS^2S'-\mu^2S^3)S''-yS'^4+\mu(m^2-n^2+\mu y)S^2S'^2+\mu^2[2(m^2+n^2)-\mu^2y^2]S^3S'+\mu^3(m^2-n^2)S^4-lyS'^2-\mu^2S^2)^2=0, \tag{110}$$

where l is the constant of integration. For later use, we note that, using system (109), the above first integral can be written in the following remarkably simple form:

$$2y\frac{(pr)'}{(p-r)^2}+(m-n)\frac{p+r}{p-r}+1+l=0. \tag{111}$$

Setting

$$\frac{S'(y)}{S(y)}=\mu\frac{1+G(y)}{1-G(y)}, \tag{112}$$

Eq. (110) becomes

$$\mathcal{P}_V\left(G,y;\frac{n^2}{2},-\frac{m^2}{2},2\mu l,-2\mu^2\right)=0. \tag{113}$$

Here $\mathcal{P}_V(G,y;\alpha,\beta,\gamma,\delta)=0$, with α, β, γ and δ arbitrary complex parameters, stands for the full Painlevé V equation, i.e.,

$$-G''+\left(\frac{1}{2G}+\frac{1}{G-1}\right)G'^2-\frac{1}{y}G'+\alpha\frac{G(G-1)^2}{y^2}+\beta\frac{(G-1)^2}{y^2G}+\gamma\frac{G}{y}+\delta\frac{G(G+1)}{G-1}=0. \tag{114}$$

Having determined S in the manner described above, one can return to system (109) to find the following explicit expressions for the functions p, r:

$$p(y)=\frac{yG'+nG^2-(l+2n+1-2\mu y)G+l+n+1}{4\mu S(1-G)}, \tag{115a}$$

$$r(y)=\frac{yG'-(l+m+1)G^2+(l+2m+1+2\mu y)G-m}{4\mu SG(1-G)}. \tag{115b}$$

At this point it is worth noting that using Eqs. (112), (113) and (115), one can easily verify that the functions W, V defined by

$$\frac{p'(y)}{p(y)}=\mu\frac{W(y)+1}{W(y)-1},\quad \frac{r'(y)}{r(y)}=\mu\frac{V(y)+1}{V(y)-1}, \tag{116}$$

satisfy

$$\mathcal{P}_V\left(W,y;\frac{(n+1)^2}{2},-\frac{m^2}{2},2\mu(l+1),-2\mu^2\right)=0, \tag{117a}$$

$$\mathcal{P}_V\left(V,y;\frac{n^2}{2},-\frac{(m+1)^2}{2},2\mu(l+1),-2\mu^2\right)=0, \tag{117b}$$

respectively. Thus, one may consider Eqs. (115) as Bäcklund transformations among the Painlevé V equations (113), (117).

Restricting our considerations to solutions of the Ernst–Weyl equation, we need to take conditions (100) into account. Under these conditions, Eqs. (108) imply that

$$p=-r^\star, \quad \mu=\mu^\star, \tag{118a}$$

while (111) yields

$$l=l^\star. \tag{118b}$$

Hence, the corresponding similarity solutions of the Ernst–Weyl equation (82) are determined by the potential

$$E=S(y)\exp(\mu(u+v)), \quad y=u-v, \tag{119}$$

where S is given by Eq. (112). In the latter, G represents a solution of the Painlevé equation (113), with

$$n=-\tfrac{1}{2}+\mathrm{i}a_1, \quad m=-\tfrac{1}{2}+\mathrm{i}a_2, \quad l=l^\star, \quad \mu=\mu^\star. \tag{120}$$

The analogous similarity solutions of the Ernst–Weyl equation (83) are specified by the potential

$$\mathcal{E}=p(y)\exp(-\mu(u+v)), \quad y=u-v, \tag{121}$$

where p is determined by the first of Eqs. (116). In the latter, W stands for a solution of the Painlevé equation (117a), with n, m, l, and μ satisfying the conditions (120) above.

B. Reduction to Painlevé VI

In a similar manner one may construct solutions of the Ernst–Weyl equation from the Painlevé VI transcendents, i.e., solutions of the ODE,

$$\begin{aligned}-G''+\frac{1}{2}\left(\frac{1}{G}+\frac{1}{G-1}+\frac{1}{G-y}\right)G'^2-\left(\frac{1}{y}+\frac{1}{y-1}+\frac{1}{G-y}\right)G'\\ +\frac{G(G-1)(G-y)}{y^2(y-1)^2}\left(\alpha+\beta\frac{y}{G^2}+\gamma\frac{y-1}{(G-1)^2}+\delta\frac{y(y-1)}{(G-y)^2}\right)=0,\end{aligned} \tag{122}$$

where α, β, γ, and δ arbitrary complex parameters, which will be denoted by $\mathcal{P}_{VI}(G,y;\alpha,\beta,\gamma,\delta)=0$ in the following.

The solutions of the RPDE which are invariant under the symmetry generated by the vector field

$$u\partial_u+v\partial_v+2\mu U\partial_U, \tag{123}$$

have the form

$$U(u,v)=S(y)(uv)^\mu, \quad y=u/v. \tag{124}$$

The prolongation of the vector field (123) in the P, R directions leading to a symmetry of system $\Sigma=0$ reads as

$$u\partial_u+v\partial_v+2\mu U\partial_U+(1-2\mu)(P\partial_P+R\partial_R). \tag{125}$$

This implies that the invariant form of the functions P and R is

$$P(u,v)=p(y)(uv)^{-\mu+1/2},\quad R(u,v)=r(y)(uv)^{-\mu+1/2}, \tag{126}$$

respectively. Inserting (124), (126) into the system $\Sigma=0$ we obtain the following system of ODEs:

$$y^{1/2}(\mu S-yS')(p-r)^2+(m+(\mu-\tfrac{1}{2})(y-1))p-mr+(y-1)yp'=0, \tag{127a}$$

$$y^{1/2}(\mu S+yS')(p-r)^2+(ny-(\mu-\tfrac{1}{2})(y-1))r-nyp+(y-1)yr'=0, \tag{127b}$$

$$(1-y)y^2S''+2y^{1/2}(p-r)(\mu^2S^2-y^2S'^2)+y(m+(n-1)y+1)S'+\mu(m-ny+\mu(y-1))S=0. \tag{127c}$$

Through a lengthy but straightforward process of differentiation and elimination one ends up with a fourth order ODE for the function S. The latter may be integrated once leading to a third order equation which is omitted because of its length. We note, however, that this first integral can be written in the following simple form by using system (127):

$$(1-2\mu)\frac{y^2-1}{(p-r)^2}(pr)'-2y\frac{(y-1)^2}{(p-r)^2}p'r'+\frac{(2\mu-1)^2}{2(p-r)^2}\left(p^2+r^2-\frac{1+y^2}{y}pr\right)$$

$$+(m-n)(1-2\mu)\frac{p+r}{p-r}+\frac{1}{2}(m-n)^2=l,\quad l\ \text{constant}. \tag{128}$$

Substituting

$$\frac{S'(y)}{S(y)}=\frac{\mu}{y}\frac{y+G(y)}{y-G(y)} \tag{129}$$

into the omitted third order ODE for S, we find that G satisfies the full Painlevé equation,

$$\mathcal{P}_{VI}\left(G,y;\frac{n^2}{2},-\frac{m^2}{2},l,\frac{1-4\mu^2}{2}\right)=0. \tag{130}$$

Once S is determined by solving the differential equations (129), (130), one can find the functions p, r algebraically using system (127). The explicit expressions for these functions are given by

$$p(y)=\frac{y^2(y-1)^2G'^2+\Gamma G^2(G-1)G'+A_i(y,m,n)G^i}{8\,\mu\,(2\mu-1)\,y^{1/2}(y-G)\,(G-1)\,G\,S}, \tag{131a}$$

$$r(y)=\frac{y^2(y-1)^2G'^2+\Gamma yG(G-1)G'+B_i(y,m,n)G^i}{8\,\mu\,(2\mu-1)\,y^{1/2}(y-G)\,(G-1)\,G\,S}, \tag{131b}$$

where summation over the repeated index $i=0,\ldots,4$ is understood and the coefficients A_i, B_i and Γ are given by

$$A_0(y,m,n)=-m^2y^2,$$

$$A_1(y,m,n)=y[(m^2-2l+(n-2\mu+1)^2)y+2m^2],$$

$$A_2(y,m,n)=-(n-2\mu+1)^2y^2-2(m^2-2l+(n-2\mu+1)^2)y+(1-2\mu)^2-m^2,$$

$$A_3(y,m,n)=2(n-2\mu+1)^2y+m^2+2n^2-2l-(n+2\mu-1)^2,$$

$$A_4(y,m,n)=-n(n-4\mu+2),$$

$$B_i(y,m,n)=y^2A_{4-i}(y^{-1},n,m),\quad i=0,\ldots,4,$$

$$\Gamma=2(2\mu-1)y(y-1).$$

As in the previous case, one may use Eqs. (129), (130) and (131) to verify that the functions W, V defined by

$$\frac{p'(y)}{p(y)}=\frac{1-2\mu}{2y}\frac{y+W(y)}{y-W(y)},\quad \frac{r'(y)}{r(y)}=\frac{1-2\mu}{2y}\frac{y+V(y)}{y-V(y)},\tag{132}$$

satisfy

$$\mathcal{P}_{VI}\left(W,y;\frac{(n+1)^2}{2},-\frac{m^2}{2},l,2\mu(1-\mu)\right)=0,\tag{133a}$$

$$\mathcal{P}_{VI}\left(V,y;\frac{n^2}{2},-\frac{(m+1)^2}{2},l,2\mu(1-\mu)\right)=0,\tag{133b}$$

respectively. Hence, one may view Eqs. (131) as defining Bäcklund transformations among the Painlevé VI equations (130) and (133).

Taking into account conditions (100), one is restricted to solutions of the Ernst–Weyl equation. Equations (126) imply that

$$p=-r^\star,\quad \mu=\mu^\star,\tag{134}$$

while Eq. (128) gives

$$l=l^\star.\tag{135}$$

Hence the invariant solutions of the Ernst–Weyl equation (82) are of the form

$$E=S(y)(uv)^\mu,\quad y=u/v,\tag{136}$$

where S is given by integrating (129) and G satisfies (130) with

$$n=-\tfrac{1}{2}+\mathrm{i}a_1,\quad m=-\tfrac{1}{2}+\mathrm{i}a_2,\quad l=l^\star,\quad \mu=\mu^\star.\tag{137}$$

Last, the similarity solutions of the Ernst–Weyl equation (83) have the form

$$\mathcal{E}=p(y)(uv)^{-\mu+1/2},\quad y=u/v,\tag{138}$$

where p is given by integrating the first equation of (132) and W satisfies (133a) with n, m, l, and μ given by (137).

VII. PERSPECTIVES

We presented a two-dimensional reduction of the ASDYM equations which leads to a novel system of integrable equations. This system incorporates the well-known Ernst–Weyl equation, as well as a significant generalization of the fourth order hyperbolic equation proposed by Nijhoff *et al.*[9] recently as the generating PDE for the KdV hierarchy. We have also constructed a Lax pair

and an auto-Bäcklund transformation for the above system and similarity solutions based on the Painlevé V and VI transcendents. Our reduction scheme unifies many aspects of integrability of the Ernst equation, like the Ernst–Hauser deformation problem, the Neugebauer–Kramer involution, the single and double-Harrison Bäcklund transformations, and gives analogous generalizations to the Ernst–Weyl equation. All these aspects follow algorithmically from the new system and the associated Lax pair, by imposing purely algebraic and compatibility conditions. Moreover, our reduction scheme allows for an easier construction of solutions to the Ernst–Weyl equation related to Painlevé transcendents by Lie group techniques. Using the reduction scheme presented in this paper and higher-dimensional gauge groups than $\mathbf{GL}(2,\mathbb{C})$, one should obtain integrable systems which incorporate the Ernst–Maxwell–Weyl equations, or even more general integrable equations describing the interaction of the gravitational field with other sources.[30,31]

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Kaluza's theory in generalized coordinates

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Maxwell's equations can be obtained in generalized coordinates by considering the electromagnetic field as an external agent. The work presented here shows how to obtain the electrodynamics for a charged particle in generalized coordinates eliminating the concept of external force. Based on Kaluza's formalism, the one presented here extends the 5×5 metric into a 6×6 space–time giving enough room to include magnetic monopoles in a very natural way. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1412463]

I. INTRODUCTION

Over 70 years ago, T. Kaluza developed a theory unifying electromagnetism and gravitation by working in a five-dimensional manifold.[1,2] In his work, influences of an electrical charge in space are treated as sources of curvature in a similar way as mass does in Einstein's theory of general relativity. With this formalism, Maxwell's equations can be obtained in Cartesian coordinates in a rather simple way. In generalized coordinates, only four out of eight (three for each rotational and one for each divergence) Maxwell equations can be recovered correctly–those with sources. The problem resides in the asymmetrical way in which each pair of equations, with and without sources, are obtained *if Kaluza's formalism is applied*. The equations with sources are obtained by means of the field equation, while the homogeneous ones have to be deduced from an identity which yields incorrect results unless the metric is Cartesian. A more conventional method for obtaining Maxwell equations consists in using Bianchi's identities.[3] Although it yields correct results using any metric, the electromagnetic field is treated as an external ''source'' by including it in the stress tensor. Kaluza's method, and consequently the one presented here, have the advantage of considering charge as a space curvature, thus following the tenets of general relativity.

In this work we propose an alternative method for treating charge and mass as curvature sources. This method is not only consistent with Kaluza's but also represents a generalization of it, by considering his 5×5 metric included in a larger one. A larger space also has enough room to establish a generalized theory in which magnetic monopoles can be introduced in a very natural way.

This paper is divided as follows. Section II contains a brief summary of Kaluza's theory without specifying any metric, as presented in his original article. In Sec. III, through a simplified example, the cause for the incorrectness of the inhomogeneous equations is explored. Section IV proposes an alternative to the theory, making a symmetrical generalization of the metric used before as a way of obtaining Maxwell equations using only Einstein's field equation. Section V goes deeper into the interpretation of the 6×6 space–time and finally in Sec. VI we discuss the implications of this formalism.

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II. KALUZA'S THEORY

Kaluza's formalism generates Maxwell's equations as well as the equations of motion for charged particles by working with a 5×5 metric defined as

$$g_{\mu\nu}=\begin{bmatrix} g_{11} & g_{12} & g_{13} & g_{14} & A_1 \\ g_{21} & g_{22} & g_{23} & g_{24} & A_2 \\ g_{31} & g_{32} & g_{33} & g_{34} & A_3 \\ g_{41} & g_{42} & g_{43} & g_{44} & \dfrac{1}{c}\phi \\ A_1 & A_2 & A_3 & \dfrac{1}{c}\phi & g_{55} \end{bmatrix}. \tag{1}$$

The 4×4 metric consisting of $g_{\mu\nu}$ elements with subscripts running from 1 to 4 has to be a solution of Einstein's equations, while the fifth column and row contain the four-vector electromagnetic potential A_ν, the first three components being the ones of the usual potential vector and the fourth the scalar potential ϕ. The fifth element g_{55} is undefined in Kaluza's article, but, as this extra dimension is considered as a spatial type one, g_{55} can be set equal to a constant taken to be equal to one in the case of a Minkowski metric.

The position and velocity vectors to consider in this formalism are defined as follows:

$$x^\nu=\begin{bmatrix} x^1 \\ x^2 \\ x^3 \\ ct \\ x^5 \end{bmatrix}, \tag{2}$$

$$v^\nu=\begin{bmatrix} v^1 \\ v^2 \\ v^3 \\ c \\ \dfrac{q}{m} \end{bmatrix}. \tag{3}$$

The fact that the time derivative of the fifth position coordinate is taken to be equal to the charge–mass ratio arises from comparing the equation of motion for a charged particle moving under Lorentz's force

$$\frac{\mathrm{d}^2x^\alpha}{\mathrm{d}t^2}=\frac{q}{m}\left[\varepsilon^\alpha_{\beta\gamma}\frac{\mathrm{d}x^\beta}{\mathrm{d}t}B^\gamma+E^\gamma\right] \tag{4}$$

with the one obtained by restricting the particle to move through a geodesic in this space namely,

$$\frac{\mathrm{d}^2x^\alpha}{\mathrm{d}s^2}+\Gamma^\alpha_{\mu\nu}\frac{\mathrm{d}x^\mu}{\mathrm{d}s}\frac{\mathrm{d}x^\nu}{\mathrm{d}s}=0. \tag{5}$$

Indeed Eq. (4) may be obtained from Eq. (5) only if $v^5=q/m$. An extra condition must be taken into account in order to recover electrodynamics within this framework. Such condition is usually referred to as the cylindrical condition,[1] namely

$$\frac{\partial}{\partial x^5}=0 \tag{6}$$

makes any derivative with respect to the fifth component equal to zero. The only justification for this restriction is that it leads to the correct Maxwell's equations.

The structural similarity between curls and Christoffel symbols, $\Gamma^{\alpha}_{\mu\nu}$, suggests a proportionality between the latter and the components of the electromagnetic field.[1] These symbols, taking $g^{ij}=\delta^{ij}$ (latin indices run from 1 to 3), are computed as follows:

$$\Gamma^{\alpha}_{\mu\nu}=\frac{1}{2}g^{\alpha\lambda}\left(\frac{\partial g_{\mu\lambda}}{\partial x^{\nu}}+\frac{\partial g_{\nu\lambda}}{\partial x^{\mu}}-\frac{\partial g_{\mu\nu}}{\partial x^{\lambda}}\right), \tag{7}$$

$$\Gamma^{\alpha}_{\mu 5}=\Gamma^{\alpha}_{5\mu}=\frac{1}{2}\,g^{\alpha\lambda}\left(\frac{\partial g_{5\lambda}}{\partial x^{\mu}}-\frac{\partial g_{\mu 5}}{\partial x^{\lambda}}\right)=F^{\alpha}_{\mu}, \tag{8}$$

where F^{α}_{μ}, the elements of the field tensor, are defined as

$$F^{\alpha}_{\mu}=\begin{bmatrix} 0 & B_z & -B_y & -\frac{1}{c}E_x \\ -B_z & 0 & B_x & -\frac{1}{c}E_y \\ B_y & -B_x & 0 & -\frac{1}{c}E_z \\ \frac{1}{c}E_x & \frac{1}{c}E_y & \frac{1}{c}E_z & 0 \end{bmatrix}. \tag{9}$$

In this scheme, Maxwell's inhomogeneous equations may be obtained through Einstein's field equation

$$G^{\alpha\beta}=\kappa T^{\alpha\beta} \tag{10}$$

since the energy momentum tensor $T^{\alpha\beta}$ now has a fifth column and row containing the electric current

$$T^{\alpha 5}=T^{5\alpha}=\rho_0 v^{\alpha} v^{5}=\begin{bmatrix} \rho_0 v^1 \frac{q}{m} \\ \rho_0 v^2 \frac{q}{m} \\ \rho_0 v^3 \frac{q}{m} \\ \rho_0 c \frac{q}{m} \\ \rho_0 \frac{q^2}{m^2} \end{bmatrix}=J^{\alpha} \tag{11}$$

and K is the coupling constant. The homogeneous equations can be derived, as suggested by Kaluza, from the identity

$$F^{\lambda\alpha,\beta}+F^{\alpha\beta,\lambda}+F^{\beta\lambda,\alpha}=0, \tag{12}$$

which arises from applying the cylindrical condition [Eq. (6)], to the identity

$$(\Gamma^{\alpha}_{\beta\lambda}+\Gamma^{\beta}_{\lambda\alpha}+\Gamma^{\lambda}_{\alpha\beta})_{,\mu}=\Gamma^{\alpha,\beta}_{\mu\lambda}+\Gamma^{\beta,\lambda}_{\mu\alpha}+\Gamma^{\lambda,\alpha}_{\mu\beta} \tag{13}$$

taking $\mu=5$.

In Cartesian coordinates this mechanism yields the complete set of Maxwell's equations. However, if one works in generalized coordinates, Eq. (13) does not correspond to the correct sourceless electromagnetic equations, a fact which will be shown in Sec. III. A strong objection can be primarily made to Eq. (13). Christoffel symbols by themselves are not tensors and, although some combinations of them are, Eq. (13) is not tensorial, in contrast with Eq. (10) which has tensors in both sides.

Summarizing, the theory has its weak point in the way sourceless equations are obtained. On the other hand, the mechanism by which inhomogeneous equations are derived, Einstein's field equation, is irrefutable and far more elegant.

III. FIVE DIMENSIONS AND GENERALIZED COORDINATES

In this section we give the necessary arguments to circumvent the objection raised in Sec. II regarding the derivation of Maxwell's sourceless equations following Kaluza's procedure. To do so and for the sake of simplicity we shall take as an example a Minkowski space with spherical symmetry. The covariant and contravariant metric tensors are thus given by

$$g_{\mu\nu}=\begin{bmatrix} 1 & 0 & 0 & 0 & A_1 \\ 0 & r^2 & 0 & 0 & r^2A_2 \\ 0 & 0 & r^2\sin^2\theta & 0 & r^2\sin^2\theta A_3 \\ 0 & 0 & 0 & -1 & -\frac{1}{c}\phi \\ A_1 & r^2A_2 & r^2\sin^2\theta A_3 & -\frac{1}{c}\phi & 1 \end{bmatrix}, \tag{14}$$

$$g^{\mu\nu}=\begin{bmatrix} 1 & 0 & 0 & 0 & -A_1 \\ 0 & \frac{1}{r^2} & 0 & 0 & -A_2 \\ 0 & 0 & \frac{1}{r^2\sin^2\theta} & 0 & -A_3 \\ 0 & 0 & 0 & -1 & \frac{1}{c}\phi \\ -A_1 & -A_2 & -A_3 & \frac{1}{c}\phi & 1 \end{bmatrix}. \tag{15}$$

In this metric, which is similar to the one used in Kaluza's article, the two metric tensors are inverse discarding quadratic terms. This means that (14) is the inverse of (15) only if second-order terms are eliminated. This approximation seems to be correct since it was also used in Kaluza's article with a Cartesian metric. Geometric coefficients must be added to the components of the electromagnetic potential which simply implies working in physical coordinates in order to obtain geometric terms and coefficients in the equations. If A^{ten}_{ν} are tensorial components of a vector, its physical components are computed as follows

$$A^{\text{phys}}_{\nu}=\sqrt{g_{\nu\nu}}A^{\text{ten}}_{\nu}. \tag{16}$$

It has to be pointed out that with these metric coefficients g^{ij}, permutations of indices in the Christoffel symbols of Eq. (13) do not *only* yield a change in sign as with a Cartesian metric in which $g^{ij}=\delta^{ij}$ with i and j running from 1 to 3, but also metric coefficients relate these permutations. Moreover,

$$\Gamma^{\alpha}_{\beta 5}=-\frac{g^{\alpha\alpha}}{g^{\beta\beta}}\Gamma^{\beta}_{\alpha 5} \tag{17}$$

gives a relation between permutations of indices in Christoffel symbols which makes Eq. (13) dependent on the value given to the indices unless the metric is Cartesian, resulting in more than four incorrect equations since each permutation of indices leads to an equation with different coefficients.

To clarify these statements let us take, for example, the third component of

$$\varepsilon^{\nu\beta\gamma}\left(\frac{\partial E_{\beta}}{\partial x^{\gamma}}-\frac{\partial E_{\gamma}}{\partial x^{\beta}}\right)=-\frac{1}{c}\frac{\partial B^{\nu}}{\partial t}. \tag{18}$$

In the space we are working in, both sides of Eq. (18) in terms of electromagnetic potentials should read

$$-\frac{2}{r\sin\theta}\frac{\partial A_2}{\partial t}-\frac{1}{\sin\theta}\frac{\partial^2 A_2}{\partial t\partial r}-\frac{1}{r^2\sin\theta}\frac{\partial^2 A_1}{\partial t\partial\theta}, \tag{19}$$

while Eq. (13), taking $\alpha=4$, $\beta=2$, $\lambda=1$, and $\mu=5$, turns out to be

$$-r\frac{\partial A_2}{\partial t}-\frac{1}{cr^3}\frac{\partial\phi}{\partial\theta}+\frac{\partial^2 A_1}{\partial\theta\partial t}+\frac{1}{2}(1-r^2)\frac{\partial^2 A_2}{\partial r\partial t}+\frac{1}{2c}\left(1+\frac{1}{r^2}\right)\frac{\partial^2\phi}{\partial r\partial\theta}=0, \tag{20}$$

which can be written as

$$\frac{1}{2r}\frac{\partial^2 A_2}{\partial r\partial t}-\frac{1}{cr^4}\frac{\partial\phi}{\partial\theta}+\frac{1}{2cr}\left(1+\frac{1}{r^2}\right)\frac{\partial^2\phi}{\partial r\partial\theta}=\frac{\partial A_2}{\partial t}+\frac{r}{2}\frac{\partial^2 A_2}{\partial r\partial t}-\frac{1}{2r}\frac{\partial^2 A_1}{\partial\theta\partial t}. \tag{21}$$

Equation (21) is obviously wrong. In Eq. (18), no derivatives of the scalar potential should appear since its right-hand side is a time derivative of **B** which is only in terms of the vector potential. The left-hand side contains the rotational of the gradient of ϕ which is equal to zero. Similar results are obtained by changing the indices for the rest of the equations. These equations are derived in Appendix A.

On the other hand, the inhomogeneous Maxwell equations are correctly recovered using Einstein's field equation as was mentioned. This induces us to reformulate the theory in order to be able to obtain electromagnetic equations, within Kaluza's formalism, based *only* on Einstein's field equation without having to invoke the cylindrical condition to work on the geometrical identity given by Eq. (13).

IV. KALUZA'S FORMALISM IN SIX DIMENSIONS

The alternative presented here for Kaluza's formalism is based on a 6×6 metric. This space–time can thus be considered as an extension of Kaluza's case. To proceed we define the following metric tensors with components accounting for spherical symmetry namely

$$g_{\mu\nu}=\begin{bmatrix} 1 & 0 & 0 & 0 & A_1 & Z_1 \\ 0 & r^2 & 0 & 0 & r^2A_2 & r^2Z_2 \\ 0 & 0 & r^2\sin^2\theta & 0 & r^2\sin^2\theta A_3 & r^2\sin^2\theta Z_3 \\ 0 & 0 & 0 & -1 & -\frac{1}{c}\phi & -\frac{1}{c}\eta \\ A_1 & r^2A_2 & r^2\sin^2\theta A_3 & \frac{1}{c}\phi & 1 & g_{56} \\ Z_1 & r^2Z_2 & r^2\sin^2\theta Z_3 & -\frac{1}{c}\eta & g_{65} & 1 \end{bmatrix}, \tag{22}$$

$$g^{\mu\nu}=\begin{bmatrix} 1 & 0 & 0 & 0 & -A_1 & -Z_1 \\ 0 & \frac{1}{r^2} & 0 & 0 & -A_2 & -Z_2 \\ 0 & 0 & \frac{1}{r^2\sin^2\theta} & 0 & -A_3 & -Z_3 \\ 0 & 0 & 0 & -1 & \frac{1}{c}\phi & \frac{1}{c}\eta \\ -A_1 & -A_2 & -A_3 & \frac{1}{c}\phi & 1 & g_{56} \\ -Z_1 & -Z_2 & -Z_3 & \frac{1}{c}\eta & g_{65} & 1 \end{bmatrix}. \tag{23}$$

The structure of these tensors is proposed to maintain symmetry between the fifth and sixth dimensions. The quantities Z_n and η are left unspecified for the time being but will be interpreted later when the role that each one plays in the equations becomes clear. Also $g_{56}=g_{65}$ is left unsettled but it has to be proposed as time independent in order to recover the conventional definitions for the fields (see Appendix B). The position and velocity vectors are proposed, just following Kaluza, as follows:

$$x^\nu=\begin{bmatrix} r \\ \theta \\ \varphi \\ ct \\ x^5 \\ x^6 \end{bmatrix}, \tag{24}$$

$$v^\nu=\begin{bmatrix} v^1 \\ v^2 \\ v^3 \\ c \\ \frac{q}{m} \\ \frac{dx^6}{dt} \end{bmatrix}. \tag{25}$$

The equation of motion to be considered in this formalism is that of a particle under the influence of a generalized Lorentz's force, namely

$$\frac{\mathrm{d}^2x^\alpha}{\mathrm{d}t^2}=\frac{q}{m}\left[\varepsilon^{\alpha}_{\beta\gamma}\frac{\partial x^\beta}{\partial t}B^\gamma+E^\alpha\right]+\frac{g}{m}\left[\varepsilon^{\alpha}_{\beta\gamma}\frac{\partial x^\beta}{\partial t}E^\gamma-B^\alpha\right]. \tag{26}$$

This space is a more general one and has enough room to work in a generalized scheme as will soon be shown. Here g stands for the magnetic charge. The Christoffel symbols that appear in the equation of a geodesic [Eq. (5)] in this space are to be compared with the coefficients of velocity components and charge in Eq. (26).

On the other hand, with the proposed metric Christoffel symbols can also be computed from definition (7). The symbols to be proportional to the electromagnetic field components are shown here as they arise directly by introducing the elements of the metric tensors (22) and (23) in definition (7). These symbols, in terms of potentials, become

$$\Gamma^\mu_{\beta 5}=g^{\mu\alpha}(A_{\beta,\alpha}-A_{\alpha,\beta}+Z_\alpha g_{56,\beta}), \tag{27}$$

$$\Gamma^\mu_{\beta 6}=g^{\mu\alpha}(Z_{\beta,\alpha}-Z_{\alpha,\beta}+A_\alpha g_{56,\beta}). \tag{28}$$

Comparing the symbols obtained from the geodesic and Eq. (26) with the ones obtained directly from their definition, expressions for electric and magnetic fields arise. Since we now have two sets of Christoffel symbols, there are two expressions for each field (see Appendix B),

$$E^\nu=-\frac{\partial\phi}{\partial x^\nu}-\frac{\partial A_\nu}{\partial t}, \tag{29}$$

$$E^\nu=\varepsilon^{\nu\beta\gamma}\left(\frac{\partial Z_\beta}{\partial x^\gamma}-\frac{\partial Z_\gamma}{\partial x^\beta}\right)+M^\nu, \tag{30}$$

$$B^\nu=-\frac{\partial\eta}{\partial x^\nu}-\frac{\partial Z_\nu}{\partial t}, \tag{31}$$

$$B^\nu=\varepsilon^{\nu\beta\gamma}\left(\frac{\partial A_\beta}{\partial x^\gamma}-\frac{\partial A_\gamma}{\partial x^\beta}\right)+Q^\nu, \tag{32}$$

where the vectors M^ν and Q^ν are defined as

$$M^\nu=\begin{bmatrix} Z_2\dfrac{\partial g_{56}}{\partial x^3} \\ Z_3\dfrac{\partial g_{56}}{\partial x^1} \\ Z_1\dfrac{\partial g_{56}}{\partial x^2} \end{bmatrix}, \quad Q^\nu=\begin{bmatrix} A_2\dfrac{\partial g_{56}}{\partial x^3} \\ A_3\dfrac{\partial g_{56}}{\partial x^1} \\ A_1\dfrac{\partial g_{56}}{\partial x^2} \end{bmatrix}. \tag{33}$$

These vectors are irrotational and since curls are solenoidal vectors, expressions (30) and (32) are in accordance with a generalized Helmolhtz theorem for tensors.[4] The duality in Faraday's tensor has been previously exhibited[4] as based in this theorem but dual expressions for the fields are now introduced. Vectorial fields can always be decomposed as a sum of a solenoidal vector field and an irrotational one which validates expressions (30) and (32). Thus two sets of symmetrical expressions for the fields are obtained—one of these sets being the expressions of the decomposition mentioned in the previous line. The implications of Eqs. (29)–(32) will be discussed in Sec. V.

Within this framework, the complete set of Maxwell equations can be derived (Appendix C). The inhomogeneous equations are obtained in the same way as in Sec. III. The new quantity Q^{ν} is irrotational and does not affect the structure of $\varepsilon^{\nu\beta\gamma}((\partial B_{\beta}/\partial x^{\gamma})-(\partial B_{\gamma}/\partial x^{\beta}))$ while the other equation with sources is identically obtained provided the same definition for E is used. The sourceless equations are obtained once again by means of Einstein's field equation

$$R^{6\beta}=\kappa T^{6\beta}, \tag{34}$$

since the energy momentum tensor now has one additional column and row

$$T^{6\beta}=T^{6\beta\alpha}=\rho_0 v^{\beta}v^{6}=\begin{bmatrix} \rho_0 v^{1}\dfrac{\mathrm{d}x^{6}}{\mathrm{d}t} \\ \rho_0 v^{2}\dfrac{\mathrm{d}x^{6}}{\mathrm{d}t} \\ \rho_0 v^{3}\dfrac{\mathrm{d}x^{6}}{\mathrm{d}t} \\ \rho_0 c\dfrac{\mathrm{d}x^{6}}{\mathrm{d}t} \\ \rho_0\left(\dfrac{\mathrm{d}x^{6}}{\mathrm{d}t}\right)^{2} \end{bmatrix}=K^{\beta}. \tag{35}$$

In Appendix C it is proved that Eq. (34) leads to the four missing Maxwell equations with some extra terms that make the complete set of equations symmetric. This new terms will be interpreted in Sec. V.

Thus, the purpose of this section is accomplished. The mechanism for obtaining both homogeneous and inhomogeneous equations is the same. This makes the theory completely symmetric and the cylindrical condition not so fundamental for the recovery of Maxwell's equations.

V. IMPLICATIONS OF THE SIXTH DIMENSION

In Kaluza's theory, the fifth dimension is associated with electric charge. As electric charge generates curvature in space, it becomes intuitive that the sixth dimension is a curvature source similar to it. The complete set of equations (the equation of motion and Maxwell relations) as is obtained in this formalism is given by

$$\frac{\mathrm{d}^2x^{\alpha}}{\mathrm{d}t^2}=\frac{q}{m}\left[\varepsilon^{\alpha}_{\beta\gamma}\frac{\mathrm{d}x^{\beta}}{\mathrm{d}t}B^{\gamma}+E^{\alpha}\right]+\frac{g}{m}\left[\varepsilon^{\alpha}_{\beta\gamma}\frac{\mathrm{d}x^{\beta}}{\mathrm{d}t}E^{\gamma}-B^{\alpha}\right], \tag{36}$$

$$\nabla\times\mathbf{E}=-\frac{1}{c}\frac{\partial\mathbf{B}}{\partial t}-\mathbf{K}, \tag{37}$$

$$\nabla\times\mathbf{B}=\frac{\partial\mathbf{E}}{\partial t}+\mu_0\mathbf{J}, \tag{38}$$

$$\nabla\cdot\mathbf{E}=\frac{\rho}{\varepsilon_0}\frac{q}{m}, \tag{39}$$

$$\nabla \cdot \mathbf{B} = \mu_0 \rho \frac{g}{m}. \tag{40}$$

This finally confirms that the sixth dimension is associated with a magnetic charge g. Equations (37) and (40) show the presence of magnetic charge and it's associated magnetic current **K**. These equations are completely symmetric as the new definitions (29)–(32) for electric and magnetic fields result in this formalism. The new potentials Z_α and η can be interpreted as electromagnetic potentials. Z_α plays the role of an electric vector potential and η a scalar magnetic potential. Both appear in these definitions but do not affect the behavior of charged particles since they do not introduce extra effects in the equations. The magnetic charge and current terms in the equations arise exclusively from the extra column in the energy–momentum tensor $T^{6\beta}$. To recover the equations without these extra terms, it is sufficient to make the magnetic charge equal to zero, $dx^6/dt = 0$, just as was done with the fifth component of the position vector to recover the equations of motion for a particle without electrical charge.

Also, from the combination of Eqs. (29)–(32) and Maxwell's equations one can easily obtain four wave equations for potentials, provided a Lorentz's gauge for the new four vector potential is considered. In the procedure, continuity relations for electric and magnetic charge are obtained.

The role of the vectors M^ν and Q^ν [Eq. (33)] becomes clear by taking a closer look at definitions (30) and (32). In these expressions, the fields are decomposed as a curl plus a vector which is irrotational. In order to obtain both Maxwell equations that feature charge density as a source, one has to calculate the divergence of both fields. In the procedure, the divergence of the rotational term vanishes since curls are solenoidal vectors leaving alone the divergence of M^ν and Q^ν, which should then be proportional to the charge densities. If these vectors do not appear in the definitions, the result would be solenoidal magnetic and *electric* fields meaning that neither magnetic *nor electric* charges exist. The spatial derivatives of the metric elements $g_{56} = g_{65}$ appear in M^ν and Q^ν which makes its value fundamental since if it is proposed as a constant, these vectors would be equal to zero with the consequences mentioned before.

VI. CONCLUSIONS

Many decades ago Kaluza proposed a way to unify electromagnetic and gravitational theories. His formalism, although very useful and elegant, shows a weak point in the way a pair of Maxwell's equations are obtained. Moreover, this mechanism does not give correct results when working in generalized coordinates, which are necessary to get the correct physics of most systems.

The alternative presented here is a similar formalism which consists in working in a larger space–time. The new extra dimension makes it possible to use Einstein's field equation twice and all the equations can be correctly recovered. Even in the absence of this curvature source, the extra dimension remains necessary.

In addition to leading to the complete and correct set of Maxwell equations, this formalism allows the introduction of magnetic charge in a very elegant and natural way. The metric and ensuing procedure are proposed based only on a symmetrical way of treating electric and magnetic fields. As a result, magnetic charge effects arise in the theory in the same way as electric effects do. Also, following the same procedure as in conventional electromagnetism, wave equations for potentials in the presence of magnetic charge can be obtained without having to introduce any singularity in space, as done in other works.[5]

Some approximations have been made in order to verify the equations that emerge from the classical treatment of electromagnetism. First of all, the metric used neglects quadratic terms. These terms may introduce additional measurable effects. In Kaluza's work, the basic hypothesis of a small electric charge–mass ratio has to be considered. In the formalism presented here a similar assumption has to be made about the magnetic charge–mass ratio. This is of course a mere conjecture since no magnetic monopoles have yet been detected.

The correct set of equations in generalized coordinates can also be obtained using Bianchi's identities. We consider the formalism presented here more elegant since charges and electromagnetic potentials are included in the geometrical description of space–time and no external forces or fields have to be introduced. Electromagnetic effects are consequences of space configuration. Kaluza's theory has been found to be very useful for the formulation of magnetohydrodynamics equations in the context of irreversible process thermodynamics[6] and in the development of gauge theories[2] so that we consider fundamental the reformulation of the theory in generalized coordinates to treat problems with different spatial symmetries.

APPENDIX A

Sourceless Maxwell's equations in vectorial notation read:

$$\nabla \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}, \tag{A1}$$

$$\nabla \cdot \mathbf{B} = 0. \tag{A2}$$

To write Eq. (A1) in terms of potentials, first we express the vector potential A_ν and the gradient of the scalar potential ϕ in physical coordinates:

$$A_\nu^{\text{phys}} = \begin{bmatrix} A_1 \\ rA_2 \\ r\sin\theta A_3 \end{bmatrix}, \tag{A3}$$

$$\nabla \phi^{\text{phys}} = \begin{bmatrix} \dfrac{\partial \phi}{\partial r} \\ \dfrac{1}{r}\dfrac{\partial \phi}{\partial \theta} \\ \dfrac{1}{r\sin\theta}\dfrac{\partial \phi}{\partial \varphi} \end{bmatrix}. \tag{A4}$$

The electric field is then

$$E^\nu = \begin{bmatrix} -\dfrac{\partial A_1}{\partial t} - \dfrac{\partial \phi}{\partial r} \\ -\dfrac{\partial (rA_2)}{\partial t} - \dfrac{1}{r}\dfrac{\partial \phi}{\partial \theta} \\ -\dfrac{\partial (r\sin\theta A_3)}{\partial t} - \dfrac{\partial \phi}{\partial \varphi} \end{bmatrix}. \tag{A5}$$

To calculate the curl of **E**, the following determinant has to be expanded:

$$\nabla \times \mathbf{E} = \frac{1}{r^2 \sin\theta} \begin{vmatrix} \vec{r} & r\vec{\theta} & r\sin\theta\vec{\varphi} \\ \dfrac{\partial}{\partial r} & \dfrac{\partial}{\partial \theta} & \dfrac{\partial}{\partial \varphi} \\ E^1 & rE^2 & r\sin\theta E^3 \end{vmatrix}. \tag{A6}$$

The third component of the $\nabla \times \mathbf{E}$ is then

$$\frac{r\sin\theta}{r^2\sin\theta}\left[\frac{\partial}{\partial r}\left(r\left(-\frac{\partial(rA_2)}{\partial t}-\frac{1}{r}\frac{\partial\phi}{\partial\theta}\right)\right)-\frac{\partial}{\partial\theta}\left(-\frac{\partial A_1}{\partial t}-\frac{\partial\phi}{\partial r}\right)\right]\vec{\varphi}. \tag{A7}$$

After some algebra Eq. (A7) reduces to

$$-2\frac{\partial A_2}{\partial t}-r\frac{\partial^2 A_2}{\partial t\partial r}+\frac{1}{r}\frac{\partial^2 A_1}{\partial t\partial\theta}. \tag{A8}$$

Equation (A8) has to be divided by $\sqrt{g_{33}}$ to return the expression to its tensorial components which finally results in Eq. (19). Note that in Eq. (A8) the scalar potential does not appear, which agrees with the property of the gradient being irrotational.

On the other hand, the left-hand side of Eq. (13), with $\alpha=4$, $\beta=2$, $\lambda=1$, and $\mu=5$ should be equal to zero because of the cylindrical condition [Eq. (6)]:

$$(\Gamma^4_{21}+\Gamma^2_{14}+\Gamma^1_{42})_{,5}=0, \tag{A9}$$

which means

$$\Gamma^{4,2}_{51}+\Gamma^{2,1}_{54}+\Gamma^{1,4}_{52}=0. \tag{A10}$$

The Christoffel symbols involved in Eq. (A9) are computed as follows:

$$\Gamma^4_{51}=\frac{1}{2}g^{44}\left(\frac{\partial g_{54}}{\partial x^1}+\frac{\partial g_{14}}{\partial x^5}-\frac{\partial g_{51}}{\partial x^4}\right)=\frac{1}{2c}\frac{\partial A_1}{\partial t}+\frac{1}{2c}\frac{\partial\phi}{\partial r}, \tag{A11}$$

$$\Gamma^2_{54}=\frac{1}{2}g^{22}\left(\frac{\partial g_{52}}{\partial x^4}+\frac{\partial g_{42}}{\partial x^5}-\frac{\partial g_{54}}{\partial x^2}\right)=\frac{1}{2cr^2}\frac{\partial(r^2A_2)}{\partial t}+\frac{1}{2cr^2}\frac{\partial\phi}{\partial\theta}, \tag{A12}$$

$$\Gamma^1_{52}=\frac{1}{2}g^{11}\left(\frac{\partial g_{51}}{\partial x^2}+\frac{\partial g_{21}}{\partial x^5}-\frac{\partial g_{52}}{\partial x^1}\right)=\frac{1}{2}\frac{\partial A_1}{\partial\theta}-r^2\frac{\partial A_2}{\partial r}-2rA_2. \tag{A13}$$

Introducing the previous results in Eq. (A10) we obtain an incorrect expression for Eq. (A1), namely

$$-\frac{r}{c}\frac{\partial A_2}{\partial t}-\frac{1}{2cr^3}\frac{\partial\phi}{\partial\theta}+\frac{1}{c}\frac{\partial^2 A_1}{\partial\theta\partial t}+\frac{1}{2c}(1-r^2)\frac{\partial^2 A_2}{\partial r\partial t}+\frac{1}{2c}\left(1+\frac{1}{r^2}\right)\frac{\partial^2\phi}{\partial r\partial\theta}=0. \tag{A14}$$

APPENDIX B

The equation for the geodesic is

$$\frac{d^2x^\alpha}{ds^2}+\Gamma^\alpha_{\mu\nu}\frac{dx^\mu}{ds}\frac{dx^\nu}{ds}=0. \tag{B1}$$

In the six-dimensional space proposed the first of the three equations in the geodesic turns out as follows:

$$\frac{d^2r}{dt^2}+\Gamma^1_{5\nu}\frac{q}{m}\frac{dx^\nu}{ds}+\Gamma^1_{6\nu}\frac{g}{m}\frac{dx^\nu}{ds}=0, \tag{B2}$$

which after expanding the sums over ν reads

$$\frac{d^2r}{dt^2}+\Gamma^1_{51}\frac{q}{m}\frac{dx^1}{ds}+\Gamma^1_{52}\frac{q}{m}\frac{dx^2}{ds}+\Gamma^1_{53}\frac{q}{m}\frac{dx^3}{ds}+\Gamma^1_{54}\frac{q}{m}\frac{dx^4}{ds}+\Gamma^1_{61}\frac{g}{m}\frac{dx^1}{ds}+\Gamma^1_{62}\frac{g}{m}\frac{dx^2}{ds}+\Gamma^1_{63}\frac{g}{m}\frac{dx^3}{ds}$$
$$+\Gamma^1_{64}\frac{g}{m}\frac{dx^4}{ds}=0. \tag{B3}$$

On the other hand, the first component of the equation of motion under a generalized Lorentz's [Eq. (26)] force is

$$\frac{d^2r}{dt^2}=\frac{q}{m}\frac{dx^2}{dt}B_3-\frac{q}{m}\frac{dx^3}{dt}B_2+\frac{q}{m}E_1+\frac{g}{m}\frac{dx^2}{dt}E_3-\frac{g}{m}\frac{dx^3}{dt}E_2-\frac{g}{m}B_1. \tag{B4}$$

Then the relationship between the Christoffel symbols and the components of the electromagnetic field should be, for Eq. (B4),

$$\Gamma^1_{51}=0, \tag{B5}$$

$$\Gamma^1_{52}=B_3, \tag{B6}$$

$$\Gamma^1_{53}=-B_2, \tag{B7}$$

$$\Gamma^1_{54}=\frac{1}{c}E_1, \tag{B8}$$

and

$$\Gamma^1_{61}=0, \tag{B9}$$

$$\Gamma^1_{62}=E_3, \tag{B10}$$

$$\Gamma^1_{63}=-E_2, \tag{B11}$$

$$\Gamma^1_{64}=-\frac{1}{c}B_1. \tag{B12}$$

Calculating the symbols Γ^1_{52} and Γ^1_{64} directly from the definition (7) we have

$$\Gamma^1_{52}=\frac{1}{2}g^{11}\left(\frac{\partial g_{51}}{\partial x^2}-\frac{\partial g_{52}}{\partial x^1}\right)+\frac{1}{2}g^{16}\frac{\partial g_{56}}{\partial x^2}=\frac{1}{2}\left(\frac{\partial A_1}{\partial x^2}-\frac{\partial A_2}{\partial x^1}\right)+\frac{1}{2}Z_1\frac{\partial g_{56}}{\partial x^2}=B_3, \tag{B13}$$

$$\Gamma^1_{64}=\frac{1}{2}g^{11}\left(\frac{\partial g_{61}}{\partial x^4}-\frac{\partial g_{64}}{\partial x^1}\right)+\frac{1}{2}g^{15}\frac{\partial g_{56}}{\partial x^4}=\frac{1}{2}\left(\frac{\partial Z_1}{\partial x^4}+\frac{1}{c}\frac{\partial \eta}{\partial x^1}\right)=-\frac{1}{c}B_1. \tag{B14}$$

In Eq. (B14) the quantity g_{56} is supposed as time independent in order to recover the conventional definition of the magnetic field. Equations (B13) and (B14) exhibit how the magnetic field can be represented in two different ways [Eqs. (32) and (31)]. Similar results, now verifying Eqs. (29) and (30), are obtained by computing Γ^1_{54} and Γ^1_{62} from definition (7) namely,

$$\Gamma^1_{54}=\frac{1}{2}g^{11}\left(\frac{\partial g_{51}}{\partial x^4}-\frac{\partial g_{54}}{\partial x^1}\right)+\frac{1}{2}g^{16}\frac{\partial g_{56}}{\partial x^4}=\frac{1}{2}\left(\frac{\partial A_1}{\partial x^4}+\frac{1}{c}\frac{\partial \phi}{\partial x^1}\right)=\frac{1}{c}E_1, \tag{B15}$$

$$\Gamma^1_{62}=\frac{1}{2}g^{11}\left(\frac{\partial g_{61}}{\partial x^2}-\frac{\partial g_{62}}{\partial x^1}\right)+\frac{1}{2}g^{15}\frac{\partial g_{65}}{\partial x^2}=\frac{1}{2}\left(\frac{\partial Z_1}{\partial x^2}-\frac{\partial Z_2}{\partial x^1}\right)+\frac{1}{2}A_1\frac{\partial g_{65}}{\partial x^2}=E_3. \tag{B16}$$

APPENDIX C

In this appendix it is shown how the complete set of correct Maxwell's equations is obtained only by means of Einstein's equation. In the first part, equations with sources are obtained. This procedure can be carried out in a 5×5 space–time giving the same results, since the Christoffel symbols required for the following operations are the ones with one index equal to 5.

Einstein's field equation relates Ricci's tensor with the mass–energy tensor. If we assume the curvature scalar to be zero, the field equation turns out as follows:

$$R_{\mu\nu}=\kappa T_{\mu\nu}, \tag{C1}$$

where Ricci's tensor is defined as[7]

$$R_{\mu\nu}=\Gamma^{n}_{\mu\nu,n}+\Gamma^{n}_{mn}\Gamma^{m}_{\mu\nu}-\Gamma^{n}_{\mu m}\Gamma^{m}_{\nu n}. \tag{C2}$$

In order to obtain the inhomogeneous equations, let us take $\mu=5$ and let ν run from 1 to 4,

$$R_{51}=\frac{\cot\theta}{r}A_2+\frac{1}{2}\frac{\partial^2A_1}{\partial t^2}+\frac{1}{r}\frac{\partial A_3}{\partial\varphi}-\frac{\csc^2\theta}{r^2}\frac{\partial^2A_1}{\partial\varphi^2}-\frac{\cot\theta}{2r^2}\frac{\partial A_1}{\partial\theta}+\frac{1}{r}\frac{\partial A_2}{\partial\theta}$$
$$-\frac{1}{2r^2}\frac{\partial^2A_1}{\partial\theta^2}+\frac{\cot\theta}{2}\frac{\partial A_2}{\partial r}+\frac{1}{2c}\frac{\partial^2\phi}{\partial r\partial t}+\frac{1}{2}\frac{\partial^2A_3}{\partial r\partial\varphi}+\frac{1}{2}\frac{\partial^2A_2}{\partial r\partial\theta}, \tag{C3}$$

$$R_{52}=-A_2+\frac{r^2}{2}\frac{\partial^2A_2}{\partial t^2}+\cot\theta\frac{\partial A_3}{\partial\varphi}-\frac{\csc^2\theta}{2}\frac{\partial^2A_2}{\partial\varphi^2}+\frac{1}{2c}\frac{\partial^2\phi}{\partial\theta\partial t}$$
$$+\frac{1}{2}\frac{\partial^2A_3}{\partial\theta\partial\varphi}-2r\frac{\partial A_2}{\partial r}+\frac{1}{2}\frac{\partial^2A_1}{\partial r\partial\theta}-\frac{r^2}{2}\frac{\partial^2A_2}{\partial r^2}, \tag{C4}$$

$$R_{53}=\frac{r^2}{2}\sin^2\theta\frac{\partial^2A_3}{\partial t^2}-\frac{\cot\theta}{2}\frac{\partial A_2}{\partial\varphi}+\frac{1}{2c}\frac{\partial^2\phi}{\partial\varphi\partial t}-\frac{3}{2}\cos\theta\sin\theta\frac{\partial A_3}{\partial\theta}+\frac{1}{2}\frac{\partial^2A_2}{\partial\theta\partial\varphi}$$
$$-\frac{1}{2}\sin^2\theta\frac{\partial^2A_3}{\partial\theta^2}-2r\sin^2\theta\frac{\partial A_3}{\partial r}+\frac{1}{2}\frac{\partial^2A_1}{\partial r\partial\varphi}-\frac{r^2}{2}\sin^2\theta\frac{\partial^2A_3}{\partial r^2}, \tag{C5}$$

$$R_{54}=\frac{1}{2r}\frac{\partial A_1}{\partial t}+\frac{\cot\theta}{2}\frac{\partial A_2}{\partial t}+\frac{1}{2}\frac{\partial^2A_3}{\partial\varphi\partial t}+\frac{\csc^2\theta}{2cr^2}\frac{\partial^2\phi}{\partial\varphi^2}+\frac{\cot\theta}{2cr^2}\frac{\partial\phi}{\partial\theta}+\frac{1}{2}\frac{\partial^2A_2}{\partial\theta\partial t}$$
$$+\frac{1}{2cr^2}\frac{\partial^2\phi}{\partial\theta^2}+\frac{1}{2cr}\frac{\partial\phi}{\partial r}+\frac{1}{2}\frac{\partial^2A_1}{\partial r\partial t}+\frac{1}{2c}\frac{\partial^2\phi}{\partial r^2}. \tag{C6}$$

If each one of these equations is equaled with its corresponding element of the energy–momentum tensor $T_{\mu5}$ [Eq. (11)], Maxwell's equations with sources are correctly recovered.

To obtain the homogeneous equations, the sixth row of Ricci's tensor has to be calculated. The procedure is exactly the same as the one to obtain the inhomogeneous equations and the results are

$$R_{61}=\frac{\cot\theta}{r}Z_2+\frac{1}{2}\frac{\partial^2Z_1}{\partial t^2}+\frac{1}{r}\frac{\partial Z_3}{\partial\varphi}-\frac{\csc^2\theta}{r^2}\frac{\partial^2Z_1}{\partial\varphi^2}-\frac{\cot\theta}{2r^2}\frac{\partial Z_1}{\partial\theta}+\frac{1}{r}\frac{\partial Z_2}{\partial\theta}$$
$$-\frac{1}{2r^2}\frac{\partial^2Z_1}{\partial\theta^2}+\frac{\cot\theta}{2}\frac{\partial Z_2}{\partial r}+\frac{1}{2c}\frac{\partial^2\eta}{\partial r\partial t}+\frac{1}{2}\frac{\partial^2Z_3}{\partial r\partial\varphi}+\frac{1}{2}\frac{\partial^2Z_2}{\partial r\partial\theta}, \tag{C7}$$

$$R_{62}=-Z_2+\frac{r^2}{2}\frac{\partial_2^2 Z}{\partial t^2}+\cot\theta\frac{\partial Z_3}{\partial\varphi}-\frac{\csc^2\theta}{2}\frac{\partial^2 Z_2}{\partial\varphi^2}+\frac{1}{2c}\frac{\partial^2\eta}{\partial\theta\partial t}$$
$$+\frac{1}{2}\frac{\partial_3^2 Z}{\partial\theta\partial\varphi}-2r\frac{\partial Z_2}{\partial r}+\frac{1}{2}\frac{\partial_1^2 Z}{\partial r\partial\theta}-\frac{r^2}{2}\frac{\partial_2^2 Z}{\partial r^2}, \tag{C8}$$

$$R_{63}=\frac{r^2}{2}\sin^2\theta\frac{\partial^2 Z_3}{\partial t^2}-\frac{\cot\theta}{2}\frac{\partial Z_2}{\partial\varphi}+\frac{1}{2c}\frac{\partial^2\eta}{\partial\varphi\partial t}-\frac{3}{2}\cos\theta\sin\theta\frac{\partial Z_3}{\partial\theta}+\frac{1}{2}\frac{\partial^2 Z_2}{\partial\theta\partial\varphi}$$
$$-\frac{1}{2}\sin^2\theta\frac{\partial^2 Z_3}{\partial\theta^2}-2r\sin^2\theta\frac{\partial Z_3}{\partial r}+\frac{1}{2}\frac{\partial^2 Z_1}{\partial r\partial\varphi}-\frac{r^2}{2}\sin^2\theta\frac{\partial^2 Z_3}{\partial r^2}, \tag{C9}$$

$$R_{64}=\frac{1}{2r}\frac{\partial Z_1}{\partial t}+\frac{\cot\theta}{2}\frac{\partial Z_2}{\partial t}+\frac{1}{2}\frac{\partial^2 Z_3}{\partial\varphi\partial t}+\frac{\csc^2\theta}{2cr^2}\frac{\partial^2\eta}{\partial\varphi^2}+\frac{\cot\theta}{2cr^2}\frac{\partial\eta}{\partial\theta}+\frac{1}{2}\frac{\partial^2 Z_2}{\partial\theta\partial t}$$
$$+\frac{1}{2cr^2}\frac{\partial^2\eta}{\partial\theta^2}+\frac{1}{2cr}\frac{\partial\eta}{\partial r}+\frac{1}{2}\frac{\partial^2 Z_1}{\partial r\partial t}+\frac{1}{2c}\frac{\partial^2\eta}{\partial r^2}. \tag{C10}$$

If we introduce expressions (30) and (31) as definitions for **E** and **B** respectively, and set each of the previous equations [(C7) to (C10)] equal to its corresponding element in the energy–momentum tensor $T_{\mu 6}$, Eqs. (37) and (40) are obtained. For example, to prove Eq. (C9) corresponds to the third component of Eq. (37) we will calculate the third component or the curl of the electric field using the alternative expression in Eq. (30). First, the vector potential Z_β has to be expressed in its physical components as follows:

$$Z_\nu^{\text{phys}}=\begin{bmatrix} Z_1 \\ rZ_2 \\ r\sin\theta Z_3 \end{bmatrix}. \tag{C11}$$

The curl of Z_ν^{phys} is calculated by expanding following the determinant:

$$\nabla\times\mathbf{Z}=\frac{1}{r^2\sin\theta}\begin{vmatrix} \vec{r} & r\vec{\theta} & r\sin\theta\vec{\varphi} \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial\theta} & \frac{\partial}{\partial\varphi} \\ Z_1 & r(rZ_2) & r\sin\theta(r\sin\theta Z_3) \end{vmatrix}$$
$$=\frac{1}{r^2\sin\theta}\begin{bmatrix} r^2\frac{\partial\sin^2\theta Z_3}{\partial\theta}-r^2\frac{\partial Z_2}{\partial\varphi} \\ r\left(\frac{\partial Z_1}{\partial\varphi}-\sin^2\theta\frac{\partial r^2 Z_3}{\partial r}\right) \\ r\sin\theta\left(\frac{\partial r^2 Z_2}{\partial r}-\frac{\partial Z_1}{\partial\theta}\right) \end{bmatrix}$$
$$=\begin{bmatrix} \sin\theta\frac{\partial Z_3}{\partial\theta}+2\cos\theta Z_3-\csc\theta\frac{\partial Z_2}{\partial\varphi} \\ \frac{1}{r\sin\theta}\frac{\partial Z_1}{\partial\varphi}-r\sin\theta\frac{\partial Z_3}{\partial r}-2\sin\theta Z_3 \\ r\frac{\partial Z_2}{\partial r}+2Z_2-\frac{1}{r}\frac{\partial Z_1}{\partial\theta} \end{bmatrix}. \tag{C12}$$

Since M^ν is irrotational, $\nabla\times\mathbf{E}=\nabla\times(\nabla\times\mathbf{Z})$, which is calculated as follows:

$$\nabla\times\mathbf{E}=\frac{1}{r^2\sin\theta}\begin{vmatrix}\vec{r} & r\vec{\theta} & r\sin\theta\vec{\varphi}\\ \dfrac{\partial}{\partial r} & \dfrac{\partial}{\partial\theta} & \dfrac{\partial}{\partial\varphi}\\ [\nabla\times\mathbf{Z}]^1 & r[\nabla\times\mathbf{Z}]^2 & r\sin\theta[\nabla\times\mathbf{Z}]^3\end{vmatrix}. \tag{C13}$$

The third component of the last equation reads

$$\frac{1}{r}\left[\frac{\partial}{\partial r}\left(r\left(\frac{1}{r\sin\theta}\frac{\partial Z_1}{\partial\varphi}-r\sin\theta\frac{\partial Z_3}{\partial r}-2\sin\theta Z_3\right)\right)-\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Z_3}{\partial\theta}+2\cos\theta Z_3-\csc\theta\frac{\partial Z_2}{\partial\varphi}\right)\right], \tag{C14}$$

which after some algebraic manipulation turns out as follows:

$$\frac{1}{r\sin\theta}\frac{\partial^2 Z_1}{\partial r\partial\varphi}-r\sin\theta\frac{\partial^2 Z_3}{\partial r^2}-4\sin\theta\frac{\partial Z_3}{\partial r}-\frac{\sin\theta}{r}\frac{\partial^2 Z_3}{\partial\theta^2}$$
$$-\frac{3\cos\theta}{r}\frac{\partial Z_3}{\partial\theta}-\frac{\cos\theta}{r\sin^2\theta}\frac{\partial Z_2}{\partial\varphi}+\frac{\csc\theta}{r}\frac{\partial^2 Z_2}{\partial\theta\partial\varphi}. \tag{C15}$$

Expression (C15) is the third physical component of the curl of the electric field. To obtain the third component of Eq. (37), also $-(1/c)(\partial\mathbf{B}/\partial t)-\mathbf{K}$ has to be in physical components which implies multiplying by $r\sin\theta$. Then, to make it clear that Eq. (C15) corresponds to (37) it has to be expressed in the following way:

$$\frac{1}{r\sin\theta}\left(\frac{\partial^2 Z_1}{\partial r\partial\varphi}-r^2\sin^2\theta\frac{\partial^2 Z_3}{\partial r^2}-4r\sin^2\theta\frac{\partial Z_3}{\partial r}-\sin^2\theta\frac{\partial^2 Z_3}{\partial\theta^2}\right.$$
$$\left.-\frac{3}{2}\sin 2\theta\frac{\partial Z_3}{\partial\theta}-\frac{\cos\theta}{\sin\theta}\frac{\partial Z_2}{\partial\varphi}+\frac{\partial^2 Z_2}{\partial\theta\partial\varphi}\right). \tag{C16}$$

This finally proves that Eqs. (C7)–(C10) correspond to the missing Maxwell's equations (37) and (40). These equations include magnetic sources.

It is important to point out, once again, that to obtain Maxwell's equations without magnetic sources it is sufficient to make $dx^6/dt=0$ which implies $T_{\mu 6}=0$.

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Electromagnetic propagators in hyperbolic Robertson–Walker cosmologies

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Green functions (retarded, advanced, Feynman and Dyson propagators) are calculated for the electromagnetic field in Robertson–Walker cosmologies with hyperbolic 3-manifolds as spacelike slices. The starting point is the Proca equation, i.e., the Maxwell field with a finite photon mass for infrared regularization, in a static cosmology with simply connected hyperbolic 3-sections. The time and space components of the resolvent kernel are scalar and vectorial point-pair invariants, respectively, and this symmetry allows for an explicit evaluation in the spectral representation. It is found that the quantum propagators have a logarithmic infrared singularity, which drops out in the zero curvature limit. Retarded and advanced Green functions remain well defined in the limit of zero photon mass, and they admit a simple generalization, by conformal scaling, to expanding 3-spaces. In cosmologies with multiply connected hyperbolic 3-manifolds as spacelike sections, the four enumerated propagators are constructed by means of Poincaré series. The spectral decomposition of the Green functions is given in terms of Eisenstein series for a certain class of open hyperbolic 3-spaces, including those with Schottky covering groups corresponding to solid handle-bodies as spacelike slices. [DOI: 10.1063/1.1413522]

I. INTRODUCTION

This is a study of vectorial Green functions in hyperbolic Robertson–Walker (RW) cosmology. I will keep the introduction short, given the length of the paper, and given that it is a very technical paper too. No applications are discussed; the usefulness of Green functions in cosmology is documented in two standard reviews,[1,2] which mainly focus on quantum field theory, and my motivation to write this paper is time-symmetric wave propagation in the cosmological absorber theory of Wheeler and Feynman,[3,4] which, however, will not be addressed here. Electromagnetic Green functions in RW cosmologies with hyperbolic 3-sections have not been studied so far. There do exist a great many investigations on vector equations in Riemannian spaces, but they are either of a general nature, and hence not really explicit, or approximate, cf. the reviews cited above. I also note that the spaces considered in this paper are not asymptotically flat, and the high symmetry of the hyperbolic 3-space together with the conformal coupling of the electromagnetic field to the background geometry makes it possible to avoid the Riemann curvature tensor. Green functions for scalar fields on hyperbolic spaces, that is, the resolvent kernel of the Laplace–Beltrami operator, have been exhaustively studied[5–10] (as far as one can go without specifying the covering group), but not so the resolvent kernels of vector operators, though, in two dimensions, there were attempts also in this regard.[7,8]

In Sec. II, the Proca equation is discussed (including spectral resolution and differential equations for the resolvent kernel) in a static RW cosmology with simply connected hyperbolic 3-sections. This equation is tantamount to electrodynamics with a finite photon mass,[11] but the mass parameter is regarded in this paper as a mere technical regularization of the Feynman and

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Dyson propagators, which turn out to be infrared divergent, a curvature effect. In Sec. III, the longitudinal time component (a scalar point-pair invariant) of the resolvent kernel is calculated, as well as the time component G_{00} of the real-space Green function, obtained by a Fourier transform. As in Minkowski space, the retarded and advanced Green functions and the two quantum propagators are defined by the choice of the integration path in the Fourier transform of the resolvent kernel.

In Sec. IV, the spatial resolvent kernel, a vectorial point-pair invariant, is calculated, and in Sec. V we study its Fourier transform, that is, the space components G_{ij} of the Green function on the 4-manifold. (The space–time mixing components G_{i0} vanish for symmetry reasons.) Explicit expressions for all four real-space propagators are given, and their infrared behavior and the Minkowski space limit (curvature radius of the 3-space to infinity) is explained. At the end of Sec. V, the time scaling of the two classical propagators (with zero photon mass) is discussed in RW cosmologies with arbitrary expansion factor.

In Sec. VI, we study Green functions on open, multiply connected hyperbolic manifolds (geometrically finite, without cusps) by periodizing the propagators calculated in the previous sections with the covering group. We focus on manifolds with $\delta(\Lambda)<1$ [$\delta(\Lambda)$: Hausdorff dimension of the limit set of the covering group], so that the Green functions can be defined by Poincaré series without the use of analytic continuation. There are three appendices, all dealing with the calculation of matrix elements, which are reduced to convolutions of Poisson kernels and Feynman integrals. The orthogonality and completeness relations, and the various spectral measures used in Secs. III and IV are calculated there. The paper is more or less self-contained, the notation is mainly that of Ref. 5, which is also the approach to hyperbolic Green functions followed here.

II. THE PROCA EQUATION IN A STATIC RW COSMOLOGY WITH NEGATIVELY CURVED 3-SECTIONS

We consider a static RW line element, $ds^2=-d\tau^2+d\sigma^2$, where $d\sigma^2$ is the line element of hyperbolic space, corresponding to the metric $\gamma_{ij}=t^{-2}\delta_{ij}$ in the Poincaré half-space model H^3 [with Cartesian coordinates (z, t), $t>0$, $z:=z_1+iz_2$], or to $\gamma_{ij}=4(1-|\mathbf{x}|^2)^{-2}\delta_{ij}$ in the ball model $B^3(|\mathbf{x}|<1)$, cf. Ref. 12. The field equations read

$$F^{\alpha\beta}{}_{;\beta}+\mu^2A^\alpha=j^\alpha, \tag{2.1}$$

where $F_{\alpha\beta}=A_{\beta,\alpha}-A_{\alpha,\beta}$, and we have included a photon mass μ for the infrared regularization of quantum propagators. We find in H^3, with $x^i=(z_1,z_2,t)$,

$$F_0{}^\beta{}_{;\beta}\equiv-t^2A_{0,n,n}+tA_{0,3}-tA_{3,0}+t^2A_{n,n,0}, \tag{2.2}$$

$$F_i{}^\beta{}_{;\beta}\equiv A_{i,0,0}-t^2A_{i,n,n}+tA_{3,i}-tA_{i,3}-A_{0,0,i}+t^2A_{n,n,i}. \tag{2.3}$$

[Greek indices run from 0 to 3, Latin ones from 1 to 3, unless explicitly stated otherwise. Whenever a Latin subscript is attached twice to the same vector, ordinary summation is implied, e.g., in (2.2) and (2.3), summation over n.] In (2.1), we could substitute $F^{\alpha\beta}{}_{;\beta}\equiv-A^{\alpha;\beta}{}_{;\beta}+R^\alpha{}_\beta A^\beta+A^\beta{}_{;\beta}{}^{,\alpha}$, but it is better to avoid Christoffel symbols and the Ricci tensor.

The Lorentz condition, $A^\alpha{}_{;\alpha}=0$, is a consequence of (2.1) and current conservation, and we find, by differentiation,

$$\begin{gathered}-A_{0,0}+t^2A_{n,n}-tA_3=0,\ \ A_{0,0,0}-t^2A_{n,n,0}+tA_{3,0}=0,\\ A_{0,0,i}-t^2A_{n,n,i}+tA_{3,i}-2t\delta_{3i}A_{n,n}+\delta_{3i}A_3=0.\end{gathered} \tag{2.4}$$

Using (2.4), we write the field Eqs. (2.1)–(2.3) as

$$A_{0,0,0}-\Delta_{H^3}A_0+\mu^2A_0=j_0,\ \ \Delta_{H^3}:=t^2\Delta_{E^3}-t\partial/\partial t, \tag{2.5}$$

$$A_{i,0,0}-\Delta_{H^3}A_i-2t(A_{i,3}-A_{3,i})-2t\,\delta_{3i}A_{n,n}+\delta_{3i}A_3+\mu^2A_i=j_i\,, \tag{2.6}$$

where Δ_{H^3}, is the scalar Laplace–Beltrami operator of H^3, and Δ_{E^3} is the Euclidean Laplace operator in Cartesian coordinates $x^i=(z_1,z_2,t)$. In this way we obtain separate equations for the space and time components of A_α.

Analogously to (2.2) and (2.3), we find in the ball model B^3,

$$F_0{}^{\beta}{}_{;\beta}\equiv-(1/4)(1-|\mathbf{x}|^2)^2(A_{0,n,n}-A_{n,n,0})+(1/2)(1-|\mathbf{x}|^2)x^n(A_{n,0}-A_{0,n}), \tag{2.7}$$

$$F_i{}^{\beta}{}_{;\beta}\equiv A_{i,0,0}-A_{0,0,i}-(1/4)(1-|\mathbf{x}|^2)^2(A_{i,n,n}-A_{n,n,i})-(1/2)(1-|\mathbf{x}|^2)x^n(A_{n,i}-A_{i,n}). \tag{2.8}$$

The Lorentz condition reads as

$$-A_{0,0}+(1/2)(1-|\mathbf{x}|^2)x^nA_n+(1/4)(1-|\mathbf{x}|^2)^2A_{n,n}=0, \tag{2.9}$$

to be differentiated with respect to space and time variables as in (2.4), and the separated field equations are

$$A_{0,0,0}-\Delta_{B^3}A_0+\mu^2A_0=j_0\,, \tag{2.10}$$

$$A_{i,0,0}-\Delta_{B^3}A_i+(1/2)(1-|\mathbf{x}|^2)(2x^n(A_{i,n}-A_{n,i})-A_i+2x_iA_{n,n})+x_ix^nA_n+\mu^2A_i=j_i\,, \tag{2.11}$$

$$\Delta_{B^3}:=\frac{(1-|\mathbf{x}|^2)^2}{4}\left(\Delta_{E^3}+\frac{2}{1-|\mathbf{x}|^2}x_n\frac{\partial}{\partial x_n}\right). \tag{2.12}$$

In H^3, a set of transversal modes propagating along the t-semiaxis is readily found, Eqs. (2.4)–(2.6) (with $j_\mu=0$) are solved by

$$A_1=t^{is}e^{-i\omega\tau},\ \ A_0=A_2=A_3=0,\ \ \omega^2=s^2+\mu^2, \tag{2.13}$$

and the same with A_1 and A_2 interchanged. The longitudinal modes traveling along the t-semiaxis read

$$A_3=t^{is}e^{-i\omega\tau},\ \ A_1=A_2=0,\ \ A_0=-i(1-is)\omega^{-1}tA_3\,,\ \ \omega^2=s^2+1+\mu^2. \tag{2.14}$$

The time component A_0 is inferred from the Lorentz condition in (2.4), and one should also stress that the dispersion relation is different from the transversal modes.

A complete set of eigenfunctions can be generated by applying certain symmetry transformations of H^3 [Möbius transformations $\alpha_\xi(z)=(z-\xi)^{-1}$, lifted into H^3, cf. Ref. 12] to the plane waves (2.13) and (2.14). The dispersion relations remain unaltered, and we find, with $A_\mu=(A_0,\mathbf{A})$ and $i=1,2$, cf. Ref. 13,

$$\begin{gathered}A_0^{T_i}=0,\ \ \mathbf{A}^{T_i}(z,t;\xi,s)=\mathbf{a}^{T_i}(z,t;\xi,s)e^{-i\omega\tau},\\ A_0^L(z,t;\xi,s)=-i\omega^{-1}(1-is)P^{1+is}(z,t;\xi)e^{-i\omega\tau},\end{gathered} \tag{2.15}$$

$$\begin{gathered}\mathbf{A}^L(z,t;\xi,s)=\mathbf{a}^L(z,t;\xi,s)e^{-i\omega\tau},\\ \mathbf{a}^L(z,t;\xi,s):=\frac{P^{2+is}(z,t;\xi)}{t^2}\begin{pmatrix}-2t(z_1-\xi_1)\\ -2t(z_2-\xi_2)\\ |z-\xi|^2-t^2\end{pmatrix},\ \ P(z,t;\xi):=\frac{t}{|z-\xi|^2+t^2},\end{gathered} \tag{2.16}$$

$$\mathbf{a}^{T_1}(z,t;\xi,s) := \frac{P^{2+is}(z,t;\xi)}{t^2}\begin{pmatrix} -(z_1-\xi_1)^2+(z_2-\xi_2)^2+t^2 \\ -2(z_1-\xi_1)(z_2-\xi_2) \\ -2t(z_1-\xi_1)\end{pmatrix},$$
$$\mathbf{a}^{T_2}(z,t;\xi,s) := \frac{P^{2+is}(z,t;\xi)}{t^2}\begin{pmatrix} -2(z_1-\xi_1)(z_2-\xi_2) \\ -(z_2-\xi_2)^2+(z_1-\xi_1)^2+t^2 \\ -2t(z_2-\xi_2)\end{pmatrix}. \tag{2.17}$$

[$z := (z_1,z_2)$, $\xi := (\xi_1,\xi_2)$; it is useful to use complex notation as at the beginning of this section.] We have chosen the normalization $\mathbf{a}^{T_i}(z,t;\xi,s)\cdot\mathbf{a}^{T_i}(z,t;\xi,-s)=(P/t)^2$, and the same for the longitudinal component, and these vectors form an orthogonal triad; the $\mathbf{a}^{T_{1,2}}$ generate the tangent planes of the horospheres[12] $P(z,t;\xi)=\text{const.}$, and $\mathbf{a}^L$ is proportional to the gradient of P.

The main part of this paper is based on the representation,

$$\mathbf{a}^L = \frac{1}{1+is}\begin{pmatrix} \dfrac{\partial P^{1+is}}{\partial z_1} \\ \dfrac{\partial P^{1+is}}{\partial z_2} \\ \dfrac{\partial P^{1+is}}{\partial t}\end{pmatrix},\quad \mathbf{a}^{T_1} = \frac{1}{1+is}\begin{pmatrix} \dfrac{-1}{4is}D_{12}P^{is}+(1+is)P^{2+is} \\ \dfrac{-1}{2is}\dfrac{\partial^2 P^{is}}{\partial z_1\partial z_2} \\ \dfrac{\partial P^{1+is}}{\partial z_1}\end{pmatrix},$$
$$\mathbf{a}^{T_2} = \frac{1}{1+is}\begin{pmatrix} \dfrac{-1}{2is}\dfrac{\partial^2 P^{is}}{\partial z_1\partial z_2} \\ \dfrac{-1}{4is}D_{21}P^{is}+(1+is)P^{2+is} \\ \dfrac{\partial P^{1+is}}{\partial z_2}\end{pmatrix},\quad D_{ij} := \frac{\partial^2}{\partial z_i^2}-\frac{\partial^2}{\partial z_j^2}, \tag{2.18}$$

and we will assume the identity,

$$\frac{\partial P^{1+is}}{\partial t} = (1+is)P^{2+is}\left(\frac{1}{tP}-2\right) \tag{2.19}$$

substituted into the third component of $\mathbf{a}^L$, so that no t-derivatives appear in the eigenvectors. The z_i-derivatives in (2.18) may also be replaced by ξ_i-derivatives, via the substitution $\partial/\partial z_i \to -\partial/\partial\xi_i$. When performing integrations over eigenfunctions, we will pull the differential operators in front of the integral signs, so that we are left with convolutions of Poisson kernels, which can be calculated by Feynman parametrization; this is the purpose of (2.18).

Finally, the eigenvectors (2.17) can be written as

$$(\mathbf{a}^L(z,t;\xi,s))^t = (0,0,1)[\alpha'_\xi(z,t)]P^{is}(z,t;\xi),$$
$$(\mathbf{a}^{T_1})^t = (1,0,0)[\alpha'_\xi]P^{is},\quad (\mathbf{a}^{T_2})^t = (0,-1,0)[\alpha'_\xi]P^{is}, \tag{2.20}$$

where $[\alpha'_\xi]$ denotes the Jacobian of the Möbius transformation $\alpha_\xi(z)=(z-\xi)^{-1}$ lifted into the half-space. The superscript t denotes transposition of the row-vectors (2.17), and ordinary matrix multiplication is assumed on the right-hand side of these equations. In Ref. 13, we derived

$$(\mathbf{a}^L(\gamma(z,t);\xi,s))^t[\gamma'(z,t)] = |\gamma^{-1\prime}\xi|^{is}(0,0,|\gamma^{-1\prime}\xi|)[\alpha'_{\gamma^{-1}\xi}(z,t)]P^{is}(z,t;\gamma^{-1}\xi),$$
$$(\mathbf{a}^{T_1}(\gamma;\xi,s))^t[\gamma'] = |\gamma^{-1\prime}\xi|^{is}(\mathrm{Re}(\gamma^{-1\prime}\xi),-\mathrm{Im}(\gamma^{-1\prime}\xi),0)[\alpha'_{\gamma^{-1}\xi}(z,t)]P^{is}(z,t;\gamma^{-1}\xi), \tag{2.21}$$

$$(\mathbf{a}^{T_2}(\gamma;\xi,s))^t[\gamma']=|\gamma^{-1\prime}\xi|^{is}(-\mathrm{Im}(\gamma^{-1\prime}\xi),-\mathrm{Re}(\gamma^{-1\prime}\xi),0)[\alpha'_{\gamma^{-1}\xi}(z,t)]P^{is}(z,t;\gamma^{-1}\xi),$$

where $\gamma^{-1}\xi$ is the Möbius transformation γ^{-1} acting in the complex plane, and $\gamma^{-1\prime}\xi$ denotes its ξ-derivative. Introducing a circulary polarized basis for the transversal components,

$$\sqrt{2}\mathbf{a}^{T_L}:=\mathbf{a}^{T_1}+i\mathbf{a}^{T_2},\quad \sqrt{2}\mathbf{a}^{T_R}:=\mathbf{a}^{T_1}-i\mathbf{a}^{T_2},$$
$$\mathbf{a}^{T_L}\overline{\mathbf{a}^{T_L}}+\mathbf{a}^{T_R}\overline{\mathbf{a}^{T_R}}=\mathbf{a}^{T_1}\overline{\mathbf{a}^{T_1}}+\mathbf{a}^{T_2}\overline{\mathbf{a}^{T_2}}, \tag{2.22}$$

we find

$$[\gamma'(z,t)]^t\mathbf{a}^L(\gamma(z,t);\xi,s)=|\gamma^{-1\prime}\xi|^{1+is}\mathbf{a}^L(z,t;\gamma^{-1}\xi,s),$$
$$[\gamma']^t\mathbf{a}^{T_L}(\gamma;\xi)=|\gamma^{-1\prime}\xi|^{is}\overline{\gamma^{-1\prime}\xi}\mathbf{a}^{T_L}(\gamma^{-1}\xi), \tag{2.23}$$
$$[\gamma']^t\mathbf{a}^{T_R}(\gamma;\xi)=|\gamma^{-1\prime}\xi|^{is}\gamma^{-1\prime}\xi\mathbf{a}^{T_R}(\gamma^{-1}\xi),$$

with $[\gamma']^t\mathbf{a}:=\mathbf{a}_i[\gamma']_{ij}$. ($T_{L,R}$ stands for left and right transversal polarization, respectively.) As for the time component of the longitudinal modes in (2.16), we use[5,6]

$$P^{1+is}(\gamma(z,t);\xi)=|\gamma^{-1\prime}\xi|^{1+is}P^{1+is}(z,t;\gamma^{-1}\xi), \tag{2.24}$$

which is the scalar analog to (2.23). These symmetries are crucial in constructing the eigenfunctions of (2.5) and (2.6) on multiply connected manifolds, as well as the spectral representation of the resolvent, cf. Sec. VI.

Next we derive the differential equations for the propagators of the Proca Eq. (2.1). We start with a bivector $G_{\alpha\alpha'}(x,x')$ on the 4-manifold; primed indices refer to the primed variable, and we define $F^G_{\alpha\alpha'\beta}(x,x'):=G_{\beta\alpha';\alpha}-G_{\alpha\alpha';\beta}$, which is evidently a second rank skew tensor with respect to x, and a vector with respect to x'. The covariant differentiations may be replaced by ordinary ones, as usual in $F_{\alpha\beta}$. Likewise, in the divergence $F^{G\ \ \beta}_{\alpha\alpha'\ ;\beta}$, the primed index and the primed variable are regarded as dummy parameters in the differentiation procedure. Green functions are defined as solutions of

$$F^{G\ \ \beta}_{\alpha\alpha'\ ;\beta}+\mu^2G_{\alpha\alpha'}=(-g)^{-1/2}\delta(x-x')g_{\alpha\alpha'}, \tag{2.25}$$

$(-g)^{-1/2}\delta$ denotes the Dirac function on the 4-manifold. The variable in the metric and the determinant on the right-hand side may be x or x', given the support of the δ-function. Clearly, $G_{\alpha\alpha'}(x,x')$ is an inverting kernel, since

$$A_\alpha=\int G_{\alpha\alpha'}(x,x')j^{\alpha'}(x')\sqrt{-g(x')}dx' \tag{2.26}$$

solves the field Eq. (2.1) according to

$$F_{\alpha\ \ ;\beta}^{\ \ \beta}+\mu^2A_\alpha=\int(F^{G\ \ \beta}_{\alpha\alpha'\ ;\beta}+\mu^2G_{\alpha\alpha'})j^{\alpha'}(x')\sqrt{-g(x')}dx'=j_\alpha. \tag{2.27}$$

We consider, formally, the Fourier transform

$$G_{\alpha\alpha'}(\tau;\mathbf{x},\mathbf{x}')=(2\pi)^{-1}\int_{-\infty}^{+\infty}d\omega e^{-i\omega\tau}\hat{G}_{\alpha\alpha'}(\omega;\mathbf{x},\mathbf{x}'), \tag{2.28}$$

and find, with (2.10) and (2.11),

$$-\Delta_{B^3}\hat{G}_{00}(\omega;\mathbf{x},\mathbf{y})+(\mu^2-\omega^2)\hat{G}_{00}=-(1/8)(1-|\mathbf{y}|^2)^3\delta(\mathbf{x}-\mathbf{y}), \tag{2.29}$$

$$-\Delta_{B^3}\hat{G}_{ij}(\omega;\mathbf{x},\mathbf{y})+(1/2)(1-|\mathbf{x}|^2)(2x^n(\hat{G}_{ij,n}-\hat{G}_{nj,i})-\hat{G}_{ij}+2x_i\hat{G}_{nj,n})+x_ix^n\hat{G}_{nj}$$
$$+(\mu^2-\omega^2)\hat{G}_{ij}=(1/2)(1-|\mathbf{y}|^2)\,\delta(\mathbf{x}-\mathbf{y}). \tag{2.30}$$

We have here slightly changed notation, writing $\mathbf{y}$ instead of $\mathbf{x}'$, and all differentiations are with respect to the variable $\mathbf{x}$. In (2.28), we write as a shortcut τ instead of $\tau-\tau'$. $\hat{G}_{00}$ and $\hat{G}_{ij}$ are scalar and vectorial point-pair invariants on the 3-space, respectively, cf. Ref. 13, and (6.3) and (6.4). (The first index always refers to $\mathbf{x}$ and the second to $\mathbf{y}$.) To achieve the symmetry $\hat{G}_{\mu\nu}(\omega;\mathbf{x},\mathbf{y})=\hat{G}_{\nu\mu}(\omega;\mathbf{y},\mathbf{x})$, we put the space–time mixing components to zero, that is $\hat{G}_{0j}$ and $\hat{G}_{i0}$, which satisfy the homogeneous Eqs. (2.29) and (2.30), respectively. Equations analogous to (2.29) and (2.30) hold in the half-space model H^3,

$$-\Delta_{H^3}\hat{G}_{00}(\omega;z,t;z_0,t_0)+(\mu^2-\omega^2)\hat{G}_{00}=-t^3\delta(t-t_0)\,\delta(z-z_0), \tag{2.31}$$

$$-\Delta_{H^3}\hat{G}_{ij}(\omega;z,t;z_0,t_0)-2t(\hat{G}_{ij,3}-\hat{G}_{3j,i})-2t\,\delta_{3i}\hat{G}_{nj,n}+\delta_{3i}\hat{G}_{3j}+(\mu^2-\omega^2)\hat{G}_{ij}$$
$$=t\,\delta(t-t_0)\,\delta(z-z_0). \tag{2.32}$$

[t is the coordinate in the half-space H^3 orthogonal to the complex plane; cosmic time is denoted by τ.] In Secs. III and IV, we will solve (2.31) and (2.32), respectively, and figure out the boundary conditions, in terms of pole coefficient and decay at infinity. In Secs. II and V, we will discuss the Fourier transform (2.28), specify the integration paths encircling the singularities of the resolvent, and calculate the propagators, i.e., the general solution of Eq. (2.25).

III. THE SCALAR TIME COMPONENT OF THE GREEN FUNCTION

The differential equations for the time-time component $\hat{G}_{00}$ of the resolvent kernel only involve the Laplace–Beltrami operator (2.29) or (2.31), and accordingly $\hat{G}_{00}$ transforms as a scalar under spatial coordinate transformations. We put $\mathbf{y}=0$ in (2.29), define $\lambda:=\mu^2-\omega^2$ as spectral parameter, and look for spherically symmetric solutions $\psi(\lambda,r)$ of $(-\Delta_{B^3}+\lambda)\psi(\lambda,r)=0$ or

$$\frac{-(1-r^2)^2}{4}\left[\psi''+2\left(\frac{1}{r}+\frac{r}{1-r^2}\right)\psi'\right]+\lambda\psi=0. \tag{3.1}$$

Two independent solutions of (3.1) are

$$\psi_{\pm}(\lambda,r)=(1-r^2)^{1+\sqrt{1+\lambda}}r^{-1}((1+r)^{-2\sqrt{1+\lambda}}\pm(1-r)^{-2\sqrt{1+\lambda}}), \tag{3.2}$$

and we assume $\mathrm{Re}\,\sqrt{1+\lambda}>0$. Since $\hat{G}_{00}(\omega;\mathbf{x},\mathbf{0})$ is spherically symmetric, it is a linear combination of the two solutions (3.2). As for boundary conditions, in the limit $r\to 0$, the asymptotic solution of Eq. (2.29) is $\hat{G}_{00}(\omega;r,\mathbf{0})\sim -1/(8\pi r)$, which follows from the Poisson equation $\Delta_{E^3}r^{-1}=-4\pi\delta(\mathbf{x})$. The second integration constant is chosen in a way that $\hat{G}_{00}(\omega;\mathbf{x},\mathbf{0})$ decays as fast as possible at infinity, that is, for $r\to 1$. Accordingly,

$$\hat{G}_{00}(\omega;\mathbf{x},\mathbf{0})=-\frac{1}{8\pi r}(1-r^2)^{1+\sqrt{1+\lambda}}(1+r)^{-2\sqrt{1+\lambda}}. \tag{3.3}$$

The Green function with pole at $\mathbf{y}$ is obtained by the substitution[5]

$$\mathbf{x}\to T_{\mathbf{y}}\mathbf{x}:=\frac{(1-|\mathbf{y}|^2)\mathbf{x}-(1-2\mathbf{x}\cdot\mathbf{y}+|\mathbf{x}|^2)\mathbf{y}}{1-2\mathbf{x}\cdot\mathbf{y}+|\mathbf{x}|^2|\mathbf{y}|^2}. \tag{3.4}$$

$T_{\mathbf{y}}$ is a Möbius transformation in B^3 that maps an arbitrary point $\mathbf{y}$ into the origin. In fact, $\hat{G}_{00}(\omega;T_{\mathbf{y}}\mathbf{x},\mathbf{0})$ is a solution of (2.29), denoted in the following by $\hat{G}_{00}(\omega;\mathbf{x},\mathbf{y})$, because (2.29) is invariant with respect to the symmetry group of B^3. The absolute value of (3.4) relates to the point-pair invariant[5,12] $L(\mathbf{x},\mathbf{y})$ as

$$|T_{\mathbf{y}}\mathbf{x}|=\sqrt{\frac{L(\mathbf{x},\mathbf{y})}{1+L(\mathbf{x},\mathbf{y})}},\quad L(\mathbf{x},\mathbf{y}):=\frac{|\mathbf{x}-\mathbf{y}|^2}{(1-|\mathbf{x}|^2)(1-|\mathbf{y}|^2)}. \tag{3.5}$$

By substituting $r=|T_{\mathbf{y}}\mathbf{x}|$ into (3.3), we find the Green function with pole at $\mathbf{y}$, cf. Refs. 5, 6, and 10,

$$\hat{G}_{00}(\omega;\mathbf{x},\mathbf{y})=-\frac{1}{8\pi}\frac{1}{\sqrt{L(1+L)}}\rho_+^{-\sqrt{1+\lambda}}(L)=-\frac{1}{4\pi}\frac{e^{-\sqrt{1+\lambda}d}}{\sinh d}, \tag{3.6}$$

$$\rho_\pm(L):=1+2L\pm 2\sqrt{L(L+1)},\quad \rho_+=1/\rho_-,\quad d:=\log\rho_+(L), \tag{3.7}$$

with $\lambda=\mu^2-\omega^2$ and $\mathrm{Re}\,\sqrt{1+\lambda}>0$. We have here also introduced the hyperbolic distance function $d(\mathbf{x},\mathbf{y})$ in B^3, and we will frequently make use of the identities,

$$(1/2)(\rho_++\rho_-)=\cosh d=1+2L, \tag{3.8}$$

$$(1/2)(\rho_+-\rho_-)=\sinh d=2\sqrt{L(L+1)}, \tag{3.9}$$

$$e^{-d}=\rho_-=\frac{1-\sqrt{L/(1+L)}}{1+\sqrt{L/(1+L)}}. \tag{3.10}$$

The Green function $\hat{G}_{00}(\omega;z,t;z_0,t_0)$ in the half-space model H^3, cf. (2.31), is obtained by the substitution,

$$L(\mathbf{x},\mathbf{y})\to L(z,t;z_0,t_0):=\frac{|z-z_0|^2+(t-t_0)^2}{4tt_0} \tag{3.11}$$

in (3.6) and (3.7). This follows from the isometry[12] $H^3\leftrightarrow B^3$,

$$x^i=(|z|^2+(1+t)^2)^{-1}(2z_1,2z_2,|z|^2+t^2-1), \tag{3.12}$$

with $z=z_1+iz_2$. The identities (3.6)–(3.10) also hold in H^3, with the distance function $d(z,t;z_0,t_0)$ defined by the third equation in (3.7).

Next we compile the spectral representation[6,10] of $\hat{G}_{00}(\omega;z,t;z_0,t_0)$,

$$\begin{aligned}\hat{G}_{00}(\omega;z,t;z_0,t_0)&=-\int_{R^2\times R^+}d\sigma(\xi,s)\frac{P^{1+is}(z,t;\xi)P^{1-is}(z_0,t_0;\xi)}{s^2+1+\lambda}\\&=-\frac{1}{2\pi^3}\int_0^\infty\frac{k(s,d)}{s^2+1+\lambda}s^2ds,\end{aligned} \tag{3.13}$$

$$k(s,d):=\int_{R^2}P^{1+is}(z,t;\xi)P^{1-is}(z_0,t_0;\xi)d\xi=\frac{\pi}{2}\frac{\sin(s\log\rho_+(L))}{s\sqrt{L(1+L)}}=\pi\frac{\sin(sd)}{s\sinh(d)}, \tag{3.14}$$

with $\lambda(\omega)=\mu^2-\omega^2$. The spectral measure, $d\sigma(\xi,s)$, is defined in (A13) (with the convergence factor dropped). Equation (3.13) readily follows from the completeness relation (A14), in conjunction with $-\Delta_{H^3}P^{1+is}=(s^2+1)P^{1+is}$, cf. (B12), and (2.31). The integral in (3.14) is calcu-

lated in (A7), and $\rho_{\pm}(L)$ is defined in (3.7). As $\hat{G}_{00}$ depends on the space variables only via the point-pair invariant L or the distance function d, we will write $\hat{G}_{00}(\omega,d)$; in this way we get model independent formulas, i.e., independent of the coordinate representation H^3, B^3, or any other.

Next we turn to the time dependent Green functions. The retarded Green function is denoted by G^{+}_{00}, the advanced one by G^{-}_{00}, the Feynman propagator by G^{+}_{F00}, and the Dyson propagator by $G_{\overline{F}00}$; they can be defined by certain contour integrations, and we use the conventions, though not quite the notation, of Ref. 14. The propagators relate to $\hat{G}_{00}(\omega,d)$ in (3.6) via (2.28),

$$G^{\pm}_{(F)00}(\tau,d) = -\frac{1}{8\pi^2}\int_{-\infty}^{+\infty} d\omega e^{-i\omega\tau}\frac{\exp(-\sqrt{1+\lambda^{\pm}_{(F)}(\omega)}d)}{\sinh d}, \tag{3.15}$$

$$\lambda^{\pm}(\omega) := \mu^2 - (\omega^2 \pm 2i\varepsilon\omega), \quad \lambda^{\pm}_{F}(\omega) := \mu^2 - (\omega^2 \pm i\varepsilon). \tag{3.16}$$

The ε-terms indicate the path of integration for the respective propagators. We find, via (3.13) and (3.14),

$$G^{\pm}_{(F)00}(\tau,d) = -\frac{1}{4\pi^4}\int_0^{\infty} I^{\pm}_{(F)}(s,\tau)k(s,d)s^2 ds,$$

$$I^{\pm}_{(F)}(s,\tau) := \int_{-\infty}^{+\infty} g^{\pm}_{(F)}(s,\omega)\exp(-i\omega\tau)d\omega, \tag{3.17}$$

$$g^{\pm}(s,\omega) := (\omega_0^2 - \omega^2 \mp 2i\varepsilon\omega)^{-1}, \quad g^{\pm}_{F}(s,\omega) := (\omega_0^2 - \omega^2 \mp i\varepsilon)^{-1},$$

with $\omega_0(s) := \sqrt{s^2+1+\mu^2}$, and $\omega_0 > 0$. A standard integration[14] gives

$$I^{\pm}(s,\tau) = \mp \pi i \omega_0^{-1}(e^{i\omega_0\tau} - e^{-i\omega_0\tau})\theta(\pm\tau), \quad I^{\pm}_{F}(s,\tau) = \pm\pi i\omega_0^{-1}e^{\mp i\omega_0|\tau|}. \tag{3.18}$$

Defining

$$\tilde{G}_{00}(\tau,d) := -\frac{1}{4\pi^4}\int_0^{\infty}\tilde{I}(s,\tau,\varepsilon)k(s,d)s^2 ds, \quad \tilde{I}(s,\tau,\varepsilon) := \omega_0^{-1}e^{-(i\tau+\varepsilon)\omega_0}, \tag{3.19}$$

we may write the propagators as linear combinations of $\tilde{G}_{00}(\pm\tau,d)$,

$$G^{\pm}_{00}(\tau,d) = \pm\pi i\,\theta(\pm\tau)(\tilde{G}_{00}(\tau,d) - \tilde{G}_{00}(-\tau,d)), \quad G^{\pm}_{F00}(\tau,d) = \pm\pi i\tilde{G}_{00}(\pm|\tau|,d). \tag{3.20}$$

The integral in (3.19) is likewise standard,[15] and we find

$$\tilde{G}_{00}(\tau;L) = -\frac{d}{4\pi^3}\frac{\Delta(\tau,d)}{\sinh d},$$
$$\Delta(\tau,d) := \frac{\sqrt{\mu^2+1}K_1(\sqrt{\mu^2+1}\sqrt{d^2-\tau^2+2i\tau\varepsilon})}{\sqrt{d^2-\tau^2+2i\tau\varepsilon}}. \tag{3.21}$$

Next we separate the pole part of $\Delta(\tau,d)$, and then perform the limit $\varepsilon\to 0$. We note[15]

$$K_1(\pm ix) = -(\pi/2)(J_1(x) \mp iN_1(x)), \quad x>0, \tag{3.22}$$

$$K_1(z) = z^{-1} + O(z\log z), \quad J_1(z) = z/2 + O(z^3),$$

$$N_1(z) = -(2/\pi)z^{-1} + O(z\log z). \tag{3.23}$$

Hence,

$$\Delta(\tau,d)=\frac{1}{d^2-\tau^2+2i\varepsilon\tau}-\frac{1}{d^2-\tau^2}+\hat{\delta}_K+\frac{\pi}{2}(\hat{\delta}_N+i\varepsilon(\tau)\hat{\delta}_J), \tag{3.24}$$

$$\hat{\delta}_K:=\theta(d^2-\tau^2)\sqrt{\mu^2+1}\frac{K_1(\sqrt{\mu^2+1}\sqrt{d^2-\tau^2})}{\sqrt{d^2-\tau^2}}, \tag{3.25}$$

$$\hat{\delta}_{J,N}:=\theta(\tau^2-d^2)\sqrt{\mu^2+1}\frac{(J_1,N_1)(\sqrt{\mu^2+1}\sqrt{\tau^2-d^2})}{\sqrt{\tau^2-d^2}}, \tag{3.26}$$

where $\varepsilon(\tau):=\mathrm{sign}(\tau)$ (not to be confused with the ε-regularization). The distributions (3.21) and (3.24) are identical. The second term in (3.24) is a principal value, and we arrive, by making use of the second formula in (A10), at

$$\Delta(\tau,d)=-i\pi\delta(d^2-\tau^2)\varepsilon(\tau)+\hat{\delta}_K+(\pi/2)(\hat{\delta}_N+i\varepsilon(\tau)\hat{\delta}_J). \tag{3.27}$$

Piecing together the above formulas, we find the retarded/advanced Green functions and the Feynman/Dyson propagators as

$$G^{\pm}_{00}(\tau,d)=-\frac{1}{2\pi}\frac{d\,\theta(\pm\tau)}{\sinh d}\left(\delta(d^2-\tau^2)-\frac{1}{2}\hat{\delta}_J\right), \tag{3.28}$$

$$G^{\pm}_{F00}(\tau,d)=-\frac{1}{4\pi}\frac{d}{\sinh d}\left(\delta(d^2-\tau^2)-\frac{1}{2}\hat{\delta}_J\pm\frac{i}{2}\left(\hat{\delta}_N+\frac{2}{\pi}\hat{\delta}_K\right)\right). \tag{3.29}$$

In the limit of vanishing photon mass, the classical propagators read

$$G^{\pm}_{00}(\tau,d;\mu=0)=-\frac{1}{2\pi}\frac{c^2}{R^2}\frac{d\,\theta(\pm\tau)}{\sinh(d/R)}\times\left(R\,\delta(d^2-c^2\tau^2)-\frac{1}{2}\frac{\theta(c^2\tau^2-d^2)}{\sqrt{c^2\tau^2-d^2}}J_1(R^{-1}\sqrt{c^2\tau^2-d^2})\right); \tag{3.30}$$

we have here restored the natural units, R is the curvature radius of the 3-space. The limit $\mu\to 0$ can also be carried out in (3.29), but the spatial components of the quantum propagators get singular, see after (5.18).

Remark: In (2.1), (2.26), and (2.27), the restoration of the units requires the substitution $j^\alpha\to c^{-1}j^\alpha$, and, for nonvanishing photon mass, $\mu:=mc/\hbar$. Moreover, $j^0=:\rho$ is the charge density of dimension $\sqrt{\hbar c}/R^3$. The components of the static RW-metric read in natural units $g_{00}=-c^2$ and $g_{ij}=(R/t)^2\delta_{ij}$, or $g_{ij}=4(1-|\mathbf{x}|^2/R^2)^{-2}\delta_{ij}$, $|\mathbf{x}|<R$. Dimensionally, $j^k\sim cj^0$, $A^k\sim cA^0\sim\sqrt{\hbar c}/R$, and $G_{00}\sim c^2G_{ij}\sim c^2/R^2$.

In the ball model B^3, the Minkowski space limit of (3.21) is recovered for $R\to\infty$. To this end, we restore the units in (3.21), analogously to (3.30). For $R\to\infty$, $d\sigma^2_{B^3}\sim 4d\mathbf{x}^2$, so that $d\sim 2|\mathbf{x}-\mathbf{y}|$, and the asymptotic limit of the point-pair invariant (3.5) is $\sqrt{L}\sim R^{-1}|\mathbf{x}-\mathbf{y}|$. Also, $\mu^2+1=(mc/\hbar)^2+R^{-2}$, see the Remark above. A rescaling of the space coordinates, $\mathbf{x}\to\mathbf{x}/2$, then gives

$$\tilde{G}_{00}(\tau,d;R\to\infty)\sim-\frac{\mu}{4\pi^3}\frac{K_1(\mu\sqrt{|\mathbf{x}-\mathbf{y}|^2-\tau^2+2i\tau\varepsilon})}{\sqrt{|\mathbf{x}-\mathbf{y}|^2-\tau^2+2i\tau\varepsilon}}. \tag{3.31}$$

Inserting this into (3.28) and (3.29), we recover of course the Minkowski results.[14]

Remark: The Green functions $G^{\pm}_{(F)00}(\tau,d)$ also happen to be the propagators of the minimally coupled Klein–Gordon equation, solving

$$(\Box-\mu^2)G^{\pm}_{(F)00}(\tau,d(\mathbf{x},\mathbf{y}))=c^{-1}\delta_{B^3}(\mathbf{x},\mathbf{y})\,\delta(\tau), \tag{3.32}$$

with the d'Alembertian $\Box=-\partial^2/\partial\tau^2+\Delta_{B^3}$. [The dimension of $G^{\pm}_{(F)00}$ is here $1/R^2$, so that we have to divide the right-hand side of (3.30) by c^2.] We may also couple the scalar field to the Ricci scalar, via the wave operator $\Box-\mu^2-\xi\hat{R}$. As the background geometry is static, the Ricci scalar is constant, $\hat{R}=-6$, cf. (5.28). Obviously, $G^{\pm}_{(F)00}(\tau,d)$ also applies to this case, with a redefinition of the mass parameter, as long as $\mu^2+\xi\hat{R}+1\geqslant 0$. Conformal coupling is achieved for $\mu=0$ and $\xi=1/6$. We will return to the conformally coupled Klein–Gordon equation, when we discuss electromagnetic propagators in an expanding background geometry, at the end of Sec. V.

IV. THE SPATIAL RESOLVENT KERNEL

The transversal and longitudinal components of the spatial resolvent kernel, $\hat{R}_{ij}:=\hat{R}^T_{ij}+\hat{R}^L_{ij}$, of the Proca equation are defined by

$$\hat{R}^T_{ij}(z,t;z',t';\lambda):=\int_{R^2\times R^+}\sum_{k=1,2}\mathbf{a}^{T_k}_i(z,t;\xi,s)\overline{\mathbf{a}^{T_k}_j(z',t';\xi,s)}\frac{d\sigma^T(\xi,s)}{s^2+\lambda}, \tag{4.1}$$

$$\hat{R}^L_{ij}(z,t;z',t';\lambda):=\int_{R^2\times R^+}\mathbf{a}^L_i(z,t;\xi,s)\overline{\mathbf{a}^L_j(z',t';\xi,s)}\frac{d\sigma^L(\xi,s)}{s^2+1+\lambda}. \tag{4.2}$$

The eigenvectors $\mathbf{a}^{T_{1,2},L}$ are listed in (2.18) and (2.19). In the spectral measures $d\sigma^{T,L}$, cf. (B13), the ε-regularizator can be dropped, as the integrals (4.1) and (4.2) are already convergent, unlike those in the completeness relation (B14). (As in Sec. III, we write the resolvent kernel with a roof, to distinguish it from its Fourier transform, when studying time-dependent Green functions on the 4-manifold in Sec. V.) If we put $\lambda=\mu^2-\omega^2$, then $\hat{R}_{ij}$ formally satisfies Eq. (2.32), which is an immediate consequence of the completeness relation (B.14). The vectorial space component of the (time independent) Green function of the Proca equation is thus

$$\hat{G}_{ij}(\omega;z,t;z_0,t_0)=\hat{R}_{ij}(z,t;z_0,t_0;\lambda=\mu^2-\omega^2). \tag{4.3}$$

The time dependent Green function on the 4-manifold is then obtained by means of the Fourier transform (2.28), studied in Sec. V. The purpose of this section is to find an explicit formula for the kernel (4.3). A complex spectral parameter λ is needed to define the integration paths in (2.28), which in turn define the propagators, cf. (3.17). In the following we assume Re $\sqrt{\lambda}>0$, as well as Re $\sqrt{\lambda+1}>0$.

At first we calculate the kernels (4.1) and (4.2) for $z=z'=0$, and then restore these variables by a symmetry argument. To this end we need the matrix elements

$$C^{T_k}_{ij}(t,t';s):=\int_{R^2}\mathbf{a}^{T_k}_i(0,t;\xi,s)\overline{\mathbf{a}^{T_k}_j(0,t';\xi,s)}d\xi,\quad C^T_{ij}:=C^{T_1}_{ij}+C^{T_2}_{ij},\quad C^L_{ij}:=\int_{R^2}\mathbf{a}^L_i\overline{\mathbf{a}^L_j}d\xi, \tag{4.4}$$

calculated in Appendix C. The nonvanishing matrix elements of the kernels (at $z=z'=0$) read, for $\beta=t'/t>1$,

$$\hat{R}^T_{11}(0,t;0,t';\lambda)=\int_0^\infty C^T_{11}(t,t';s)\,\frac{s^2+1}{s^2+\lambda}\,\frac{ds}{2\pi^3}=\frac{\beta}{2\pi(\beta^2-1)^3\lambda}\,\frac{1}{tt'}(4\beta^2(\beta^{-\sqrt{\lambda}}-1)$$
$$+(\beta^4-1)\sqrt{\lambda}\beta^{-\sqrt{\lambda}}+(\beta^2-1)^2\lambda\beta^{-\sqrt{\lambda}}), \tag{4.5}$$

$$\hat{R}^L_{11}=\int_0^\infty C^L_{11}(s)\,\frac{s^2}{s^2+1+\lambda}\,\frac{ds}{2\pi^3}=\frac{\beta^2}{\pi(\beta^2-1)^3\lambda}\,\frac{1}{tt'}$$
$$\times(2\beta-(\beta^2+1)\beta^{-\sqrt{1+\lambda}}-(\beta^2-1)\sqrt{1+\lambda}\beta^{-\sqrt{1+\lambda}}), \tag{4.6}$$

$$\hat{R}_{11}:=\hat{R}^T_{11}+\hat{R}^L_{11}=\frac{\beta}{2\pi(\beta^2-1)^3\lambda}\,\frac{1}{tt'}(4\beta^{2-\sqrt{\lambda}}+(\beta^4-1)\sqrt{\lambda}\beta^{-\sqrt{\lambda}}+(\beta^2-1)^2\lambda\beta^{-\sqrt{\lambda}}$$
$$-2\beta(\beta^2+1)\beta^{-\sqrt{1+\lambda}}-2\beta(\beta^2-1)\sqrt{1+\lambda}\beta^{-\sqrt{1+\lambda}}), \tag{4.7}$$

$$\hat{R}^{(T,L)}_{22}=\hat{R}^{(T,L)}_{11}, \tag{4.8}$$

$$\hat{R}^T_{33}:=\int_0^\infty C^T_{33}(s)\,\frac{s^2+1}{s^2+\lambda}\,\frac{ds}{2\pi^3}=\frac{2\beta^2}{\pi(\beta^2-1)^3\lambda}\,\frac{1}{tt'}$$
$$\times((\beta^2+1)(1-\beta^{-\sqrt{\lambda}})-(\beta^2-1)\sqrt{\lambda}\beta^{-\sqrt{\lambda}}), \tag{4.9}$$

$$\hat{R}^L_{33}:=\int_0^\infty C^L_{33}(s)\,\frac{s^2}{s^2+1+\lambda}\,\frac{ds}{2\pi^3}=\frac{\beta}{2\pi(\beta^2-1)^3\lambda}\,\frac{1}{tt'}(-4\beta(\beta^2+1)+(\beta^2-1)^2\lambda\beta^{-\sqrt{1+\lambda}}$$
$$+2(\beta^4-1)\sqrt{1+\lambda}\beta^{-\sqrt{1+\lambda}}+2(\beta^2+1)^2\beta^{-\sqrt{1+\lambda}}), \tag{4.10}$$

$$\hat{R}_{33}:=\hat{R}^T_{33}+\hat{R}^L_{33}=\frac{\beta}{2\pi(\beta^2-1)^3\lambda}\,\frac{1}{tt'}(-4(\beta^2+1)\beta^{1-\sqrt{\lambda}}-4(\beta^2-1)\sqrt{\lambda}\beta^{1-\sqrt{\lambda}}$$
$$+(\beta^2-1)^2\lambda\beta^{-\sqrt{1+\lambda}}+2(\beta^4-1)\sqrt{1+\lambda}\beta^{-\sqrt{1+\lambda}}+2(\beta^2+1)^2\beta^{-\sqrt{1+\lambda}}). \tag{4.11}$$

Replacing on the right-hand side of Eqs. (4.5)–(4.11) β by $1/\beta$, we obtain the kernels for $\beta=t'/t<1$. If we put $t'=1$, and $t=1-2r$, and calculate the leading order of $\hat{R}_{11}$ and $\hat{R}_{33}$ for $r\to 0$, we find $\hat{R}_{11}\sim\hat{R}_{33}\sim 1/(8\pi r)$, and $\hat{R}^L_{11}\sim 1/(16\pi r)$.

Next we will restore the z and z'-variables, assumed zero in (4.5)–(4.11). This can be done by symmetry, of course. The goal is to find the Green function $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{x}')$ with pole at $\mathbf{x}'$ in the Poincaré ball B^3, cf. (2.30). [We will frequently switch between the ball (B^3) and half-space (H^3) models of hyperbolic geometry, cf. Sec. II, and we will indicate that by a superscript.] $\hat{G}^{B^3}_{ij}$ transforms as a bivector, $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{x}')dx^i dx'^j$; we map B^3 onto H^3 via the isometry (3.12), and use the same transformation for the primed coordinates x'^i and (z',t'), so that $\mathbf{x}'=0$ is mapped onto $(z'=0,\ t'=1)$. In the B^3-model, the Green function with pole at the origin is spherically symmetric, $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{0})=f(\omega;|\mathbf{x}|)\,\delta_{ij}+g(\omega;|\mathbf{x}|)x_i x_j$. We map $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{x}')dx^i dx'^j$ into H^3, and then consider the special coordinate values $\mathbf{x}'=0$, $x^{1,2}=0$, $x^3=(t-1)(t+1)^{-1}$, $z=z'=0$, $t'=1$, with arbitrary $t>0$. [From now on we also put $t'=1$ in the components (4.5)–(4.11) of the resolvent kernel $\hat{R}_{ij}$, in particular $\beta=1/t$.] At these special coordinate values, the result of this transformation is $\hat{R}_{11}dz_1dz'_1+\hat{R}_{22}dz_2dz'_2+\hat{R}_{33}dtdt'$. [If $t>1$, we have to replace β by $1/\beta$ in (4.5)–(4.11), as mentioned above.] Moreover,

$$dx^i dx'^i=(1+t)^{-2}(dz_k dz'_k+dtdt'),\quad x^i x^j dx^i dx'^j=\frac{(t-1)^2}{(t+1)^4}dtdt'. \tag{4.12}$$

(We do not distinguish between x^i and x_i; the i and j-summations are from 1 to 3, the k-summation is from 1 to 2. Also note, that x^j in the second formula is not primed.) Accordingly, we may identify

$$f(\omega;|\mathbf{x}|)=(1+t)^2\hat{R}_{11},\quad g(\omega;|\mathbf{x}|)=\frac{(1+t)^4}{(1-t)^2}(\hat{R}_{33}-\hat{R}_{11}), \tag{4.13}$$

where $t=(1-|\mathbf{x}|)(1+|\mathbf{x}|)^{-1}$ if $t<1$, and $t=(1-|\mathbf{x}|)^{-1}(1+|\mathbf{x}|)$ if $t>1$. In this way we have determined the Green function $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{0})$ in B^3, with pole at the origin.

Remarks: We have put $t'=1$ in $\hat{R}_{ij}$ for the t-dependence of $t\hat{R}_{ij}$ to be solely via $\beta=1/t$. Equations (4.5)–(4.11) only hold for $\beta>1$, so that we have to choose $t=(1-|\mathbf{x}|)(1+|\mathbf{x}|)^{-1}$, if we use (4.7) and (4.11) in (4.13). As consistency check, the same result is obtained for $f(\omega;|\mathbf{x}|)$ and $g(\omega;|\mathbf{x}|)$, if we insert into (4.13) $\hat{R}_{ij}$ calculated for $\beta<1$ as indicated after (4.11). Then we have to identify $t=(1-|\mathbf{x}|)^{-1}(1+|\mathbf{x}|)$. As pointed out in (4.3), the spectral variable in $\hat{R}_{ij}$ relates to the frequency as $\lambda=\mu^2-\omega^2$.

Next we calculate, by a further symmetry argument, the Green function $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y})$ in B^3 with pole at an arbitrary point $\mathbf{y}$. We write for the moment $\hat{\mathbf{x}}$ instead of $\mathbf{x}$, so that $\hat{G}^{B^3}_{ij}(\omega;\hat{\mathbf{x}},\mathbf{0})=f(\omega;|\hat{\mathbf{x}}|)\delta_{ij}+g(\omega;|\hat{\mathbf{x}}|)\hat{x}_i\hat{x}_j$, which is to be regarded as a vector field depending on a dummy index j, solving the vector Eq. (2.30). Whenever we apply a Möbius transformation (i.e., a symmetry transformation of hyperbolic space) to this vector field, it will still solve the invariant Eq. (2.30). We consider the Möbius transformation (3.4), $\hat{\mathbf{x}}=T_{\mathbf{y}}\mathbf{x}$. The components of this transformation can be written in terms of the point-pair invariant $L(\mathbf{x},\mathbf{y})$, cf. (3.5),

$$\frac{\hat{x}_j}{1-|\mathbf{y}|^2}=-\frac{1}{2}\frac{1}{1+L}\frac{\partial L(\mathbf{x},\mathbf{y})}{\partial y_j}, \tag{4.14}$$

and the Jacobian, $\hat{x}_{j,i}:=\partial\hat{x}_j/\partial x_i$, reads as

$$\frac{\hat{x}_{j,i}}{1-|\mathbf{y}|^2}=\frac{1}{2}\frac{1}{(1+L)^2}\left(\frac{\partial L}{\partial x_i}\frac{\partial L}{\partial y_j}-(1+L)\frac{\partial^2 L}{\partial x_i\partial y_j}\right). \tag{4.15}$$

By means of the identities,

$$|\hat{\mathbf{x}}|^2=\frac{L}{1+L}=\frac{|\mathbf{x}-\mathbf{y}|^2}{1-2\mathbf{x}\cdot\mathbf{y}+|\mathbf{x}|^2|\mathbf{y}|^2}, \tag{4.16}$$

$$\frac{1}{1+L}\frac{\partial L}{\partial y_i}\frac{\partial L}{\partial y_i}=\frac{4}{(1-|\mathbf{y}|^2)^2}L, \tag{4.17}$$

we readily find

$$\frac{\hat{x}_k\hat{x}_{k,i}\hat{x}_j}{1-|\mathbf{y}|^2}=-\frac{1}{4}\frac{1}{(1+L)^3}\frac{\partial L}{\partial x_i}\frac{\partial L}{\partial y_j}. \tag{4.18}$$

[Summation over i in (4.17) and k in (4.18) is implied.] Applying the transformation $\hat{\mathbf{x}}=T_{\mathbf{y}}\mathbf{x}$ to $\hat{G}^{B^3}_{ij}(\omega;\hat{\mathbf{x}},\mathbf{0})d\hat{x}_i$, we find

$$\hat{G}^{B^3}_{ij}(\omega;\hat{\mathbf{x}},\mathbf{0})d\hat{x}_i=(1-|\mathbf{y}|^2)\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y})dx_i, \tag{4.19}$$

$$\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y}):=f(\omega;|\hat{\mathbf{x}}|)\frac{\hat{x}_{j,i}}{1-|\mathbf{y}|^2}+g(\omega;|\hat{\mathbf{x}}|)\frac{\hat{x}_k\hat{x}_{k,i}\hat{x}_j}{1-|\mathbf{y}|^2}, \tag{4.20}$$

and more explicitly, by inserting (4.16), (4.15), and (4.18),

$$\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y})=\rho_-\hat{R}_{11}\left(\frac{(1+2L)}{L(L+1)}L_{,i}L_{,j}-2L_{,i,j}\right)-\rho_-\hat{R}_{33}\frac{1}{L(L+1)}L_{,i}L_{,j}, \tag{4.21}$$

with $\rho_-=1+2L-2\sqrt{L(L+1)}$ as defined in (3.7). The index i denotes differentiation with respect to x_i, the index j means differentiation with respect to y_j, and $\hat{R}_{11}$ and $\hat{R}_{33}$ are defined in (4.7) and (4.11), with $t'=1$ and $t=1/\beta=\rho_-=\sqrt{\rho_-/\rho_+}$. Note that $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y})$ solely depends on the point-pair invariant $L(\mathbf{x},\mathbf{y})$ and the spectral parameter $\lambda=\mu^2-\omega^2$ (via $\hat{R}_{11}$ and $\hat{R}_{33}$). In the definition (4.20), we have also used a normalization factor $(1-|\mathbf{y}|^2)^{-1}$, to achieve the symmetry $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y})=\hat{G}^{B^3}_{ji}(\omega;\mathbf{y},\mathbf{x})$. By construction, $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y})$ satisfies the vector Eq. (2.30), with the vector index i corresponding to the argument $\mathbf{x}$. $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y})dx_i dy_j$ transforms as a bivector under arbitrary coordinate transformations $\mathbf{x}=h(\mathbf{x}')$, $\mathbf{y}=h(\mathbf{y}')$, and $L(\mathbf{x},\mathbf{y})$ is of course a biscalar. So it is clear how to map $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y})$ into the H^3-model; we just have to replace in (4.21) $L(\mathbf{x},\mathbf{y})$ by the H^3-point-pair invariant (3.11). [The biscalars $L(\mathbf{x},\mathbf{y})$ and $L(z,t;z',t')$ relate via the isometry (3.12).]

We also have to check that $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y})$ has the right pole. We find in the B^3-model, from (4.21) and the discussion following (4.11),

$$\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y})\sim\frac{1}{2\pi}\frac{1}{1-|\mathbf{y}|^2}\frac{1}{|\mathbf{x}-\mathbf{y}|}\delta_{ij}, \tag{4.22}$$

which solves

$$-\frac{1}{4}(1-|\mathbf{x}|^2)^2\Delta_{E^3}\hat{G}^{B^3}_{ij}=\gamma_{ij}\frac{1}{\sqrt{\gamma}}\delta(\mathbf{x}-\mathbf{y}), \tag{4.23}$$

where $\gamma_{ij}=4(1-|\mathbf{x}|^2)^{-2}\delta_{ij}$ is the B^3-metric and γ is its determinant. In fact, Eq. (2.30) boils down to (4.23) in leading asymptotic order.

We rewrite $\hat{G}^{B^3}_{ij}(\omega;\mathbf{x},\mathbf{y})$ in terms of the hyperbolic distance function $d(\mathbf{x},\mathbf{y})$, cf. (3.8)–(3.10). As in (4.21), the indices i and j denote differentiation with respect to the first and second argument, respectively. By differentiating Eq. (3.8), we readily find

$$d_{,i}d_{,j}\sinh^2 d=4L_{,i}L_{,j},\quad d_{,i}d_{,j}\cosh d+d_{,i,j}\sinh d=2L_{,i,j}. \tag{4.24}$$

We may now write, instead of (4.21),

$$\hat{G}_{ij}(\omega;\mathbf{x},\mathbf{y})=-e^{-d}(\hat{R}_{11}\sinh d\,d_{,i,j}+\hat{R}_{33}d_{,i}d_{,j}), \tag{4.25}$$

and in (4.7) and (4.11) we put $t'=1$ and $t=1/\beta=e^{-d}$, so that

$$\hat{R}_{11}=\frac{e^d}{4\pi\lambda\sinh^3 d}(e^{-\sqrt{\lambda}d}(1+\lambda\sinh^2 d+\sqrt{\lambda}\sinh d\cosh d)-e^{-\sqrt{1+\lambda}d}(\cosh d+\sqrt{1+\lambda}\sinh d)). \tag{4.26}$$

$$\hat{R}_{33}=\frac{-e^d}{2\pi\lambda\sinh^3 d}(e^{-\sqrt{\lambda}d}(\cosh d+\sqrt{\lambda}\sinh d)-e^{-\sqrt{1+\lambda}d}(\cosh^2 d+(\lambda/2)\sinh^2 d + \sqrt{1+\lambda}\sinh d\cosh d)), \tag{4.27}$$

with $\mathrm{Re}\,\sqrt{\lambda}>0$, and $\mathrm{Re}\,\sqrt{\lambda+1}>0$. The Green function $\hat{G}_{ij}(\omega;\mathbf{x},\mathbf{y})$, explicitly defined by (4.25)–(4.27) depends on the space arguments only via the hyperbolic distance function $d(\mathbf{x},\mathbf{y})$. We have dropped the B^3-superscript, as Eqs. (4.25)–(4.27) are valid in every model of hyperbolic geom-

etry, e.g., in the half-space model H^3, where $d(\mathbf{x},\mathbf{y})$ is to be replaced by the H^3-distance function $d(z,t;z_0,t_0)$, defined by (3.10) and (3.11). As special case, we note the Green function (4.25) with pole at $\mathbf{y}=0$ in the B^3-model,

$$\hat{G}^{B^3}_{ij}(\omega;|\mathbf{x}|,\mathbf{0})=\frac{4\hat{R}_{11}}{(1+r)^2}\,\delta_{ij}+\frac{4(\hat{R}_{33}-\hat{R}_{11})}{(1+r)^2}\,\frac{x_i x_j}{r^2}, \tag{4.28}$$

where $\hat{R}_{11}$ and $\hat{R}_{33}$ are defined by (4.26) and (4.27) and the substitutions

$$\sinh d=\frac{2r}{1-r^2},\quad \cosh d=\frac{1+r^2}{1-r^2},\quad e^d=\frac{1+r}{1-r}, \tag{4.29}$$

cf. (3.5) and (3.8)–(3.10).

Finally we give a direct proof of the completeness relation (B14), which is a good consistency check for the rather lengthy calculations in this section and Appendix C. We start with (4.25), but use for $\hat{R}_{11}$ and $\hat{R}_{33}$ the integral representations in (4.1) and (4.2), with the $(s^2+\lambda)^{-1}$ and $(s^2+1+\lambda)^{-1}$ factors dropped. Instead, we include into these integrals the convergence factor $e^{-\varepsilon s}$ that appears in the spectral measures (B13). In short, by replacing in (4.25) $\hat{R}_{ij}$ by

$$\hat{S}_{ij}:=\frac{1}{2\pi^3}\int_0^\infty ds e^{-\varepsilon s}((s^2+1)C^T_{ij}(s)+s^2C^L_{ij}(s)), \tag{4.30}$$

cf. (4.4) and (C.8), we may write the completeness relation (B14) as

$$-e^{-d}(\hat{S}_{11}\sinh d\, d_{,i,j}+\hat{S}_{33}d_{,i}d_{,j})=\gamma_{ij}\gamma^{-1/2}\delta(\mathbf{x}-\mathbf{y}). \tag{4.31}$$

It is here understood, that the substitutions $t'=1$ and $t=1/\beta=e^{-d}$, as indicated after (4.25), are carried out in the $C^{T,L}_{ij}$-coefficients. It is not difficult to verify (4.31). The various s-integrations in $\hat{S}_{11}$ and $\hat{S}_{33}$ are all standard in the limit $\varepsilon\to 0$. [We put $\varepsilon=0$ whenever the integrals over the individual trigonometric functions in the $C^{T,L}_{ij}$-coefficients converge without regularization, cf. (C8).] We find, with $d\sim 2\sqrt{L}$ for $\mathbf{x}\to\mathbf{y}$,

$$\hat{S}_{11}=4\pi\frac{\beta^2\log\beta}{\beta^2-1}\,\frac{\varepsilon}{(\varepsilon^2+\log^2\beta)^2}=\frac{1}{\pi^2}\,\frac{\varepsilon}{(\varepsilon^2+4L)^2}, \tag{4.32}$$

which is an ε-representation of the δ-function, $\gamma^{-1/2}\delta(\mathbf{x}-\mathbf{y})$, in hyperbolic space, cf. (A16). Moreover, at $\mathbf{x}=\mathbf{y}$,

$$L_{,i,j}=\frac{-2}{(1-|\mathbf{y}|^2)^2}\,\delta_{ij}+O(x_ix_j),\quad L_{,i}L_{,j}=O(x_ix_j), \tag{4.33}$$

and it is easy to check, that the $O(x_ix_j)$-terms entering in (4.31) via (4.24) do not give a contribution for $\varepsilon\to 0$, which proves (4.31) and hence the completeness relation (B14).

V. TIME DEPENDENT GREEN FUNCTIONS

In this section we focus on the Fourier integral (2.28) for the spatial component of the Green function, calculated in (4.25)–(4.27). The time component of the Green function has already been Fourier transformed in Sec. III, cf. (3.15)–(3.30), and a similar procedure is applied in this section to the spatial Fourier component (4.25). The integration paths in (2.28) are specified by substituting for λ in (4.25) one of the four ε-regularizations $\lambda^{\pm}_{(F)}(\omega)$ defined in (3.16). $\lambda^{\pm}$ refers to

retarded (+) and advanced Green functions, and $\lambda_F^{\pm}$ to Feynman (+) and Dyson propagators. Also note that we assumed in the derivation of (4.25) Re $\sqrt{\lambda}>0$, and Re $\sqrt{\lambda+1}>0$. We write the matrix elements (4.26) and (4.27) as

$$\hat R_{11}(\lambda,d)=\frac{e^d}{4\pi\sinh^3 d}\bigg(-\int_0^d\frac{e^{-\sqrt{\lambda}x}}{\sqrt{\lambda}}dx+\frac{e^{-\sqrt{\lambda}d}}{\sqrt{\lambda}}\sinh d\cosh d+e^{-\sqrt{\lambda}d}\sinh^2 d \\ +\int_0^d e^{-\sqrt{1+\lambda}x}\sinh x\,dx\bigg), \tag{5.1}$$

$$\hat R_{33}(\lambda,d)=\frac{e^d}{2\pi\sinh^3 d}\bigg(\cosh d\int_0^d\frac{e^{-\sqrt{\lambda}x}}{\sqrt{\lambda}}dx-\frac{e^{-\sqrt{\lambda}d}}{\sqrt{\lambda}}\sinh d-\cosh d\int_0^d e^{-\sqrt{1+\lambda}x}\sinh x\,dx \\ +\frac{1}{2}e^{-\sqrt{1+\lambda}d}\sinh^2 d\bigg), \tag{5.2}$$

and substitute

$$\frac{e^{-\sqrt{\lambda}d}}{\sqrt{\lambda}}=\frac{2}{\pi}\int_0^\infty\frac{\cos(sd)}{s^2+\lambda}ds,\quad e^{-\sqrt{\lambda}d}=\frac{2}{\pi}\int_0^\infty\frac{s\sin(sd)}{s^2+\lambda}ds, \tag{5.3}$$

and the same with $\lambda\to\lambda+1$, and $d\to x$. (We do not interchange the s and d-integrations here.) Next we define,

$$R^{\pm}_{(F)ij}(\tau,d):=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega e^{-i\omega\tau}\hat R_{ij}(\lambda^{\pm}_{(F)}(\omega),d), \tag{5.4}$$

so that retarded and advanced Green functions and Feynman and Dyson propagators read, according to (4.25),

$$G^{\pm}_{(F)ij}(\tau;\mathbf{x},\mathbf{y}):=-e^{-d}(R^{\pm}_{(F)11}(\tau,d)\sinh d\,d_{,i,j}+R^{\pm}_{(F)33}(\tau,d)d_{,i}d_{,j}). \tag{5.5}$$

This complements the time component $G^{\pm}_{(F)00}(\tau,d)$ in (3.15). To evaluate (5.4), we interchange s and ω-integrations. The ω-integration can be carried out as in (3.17) and (3.18), and we arrive at

$$R^{\pm}_{(F)11}(\tau,d)=\frac{e^d}{4\pi\sinh^3 d}\bigg(-\int_0^d S^{\pm}_{0(F)}(\tau,x;\mu)dx+S^{\pm}_{0(F)}(\tau,d;\mu)\sinh d\cosh d \\ +S^{\pm}_{1(F)}(\tau,d;\mu)\sinh^2 d+\int_0^d S^{\pm}_{1(F)}(\tau,x;\sqrt{1+\mu^2})\sinh x\,dx\bigg), \tag{5.6}$$

$$R^{\pm}_{(F)33}(\tau,d)=\frac{e^d}{2\pi\sinh^3 d}\bigg(\cosh d\int_0^d S^{\pm}_{0(F)}(\tau,x;\mu)dx-S^{\pm}_{0(F)}(\tau,d;\mu)\sinh d \\ -\cosh d\int_0^d S^{\pm}_{1(F)}(\tau,x;\sqrt{1+\mu^2})\sinh x\,dx+\frac{1}{2}S^{\pm}_{1(F)}(\tau,d;\sqrt{1+\mu^2})\sinh^2 d\bigg). \tag{5.7}$$

Here, $S^{\pm}_{i(F)}(\tau,d;\mu)$ and $S^{\pm}_{i(F)}(\tau,d;\sqrt{1+\mu^2})$ are defined by

$$S^{\pm}_{0(F)}(\tau,d;\mu):=\frac{1}{\pi^2}\int_0^\infty\cos(sd)I^{\pm}_{(F)}(\omega_0,\tau)ds,$$

$$S^{\pm}_{1(F)}(\tau,d;\mu) := \frac{1}{\pi^2}\int_0^\infty s\,\sin(sd) I^{\pm}_{(F)}(\omega_0,\tau)\,ds, \tag{5.8}$$

$$I^{\pm}(\omega_0,\tau) := \mp \pi i \omega_0^{-1}(e^{i\omega_0\tau} - e^{-i\omega_0\tau})\,\theta(\pm\tau),\quad I^{\pm}_F(\omega_0,\tau) := \pm \pi i \omega_0^{-1} e^{\mp i\omega_0|\tau|},$$

with $\omega_0 := \sqrt{s^2+\mu^2}$, and $\mathrm{Re}\,\omega_0 > 0$. Sometimes we will write ω_0^T for ω_0, the frequency of the transversal modes; the longitudinal frequency relates to the spectral parameter via $\omega_0^L := \sqrt{s^2+1+\mu^2}$, $\mathrm{Re}\,\omega_0^L > 0$. Evidently, $S^{\pm}_{i(F)}(\tau,d;\sqrt{1+\mu^2})$ is obtained by replacing in (5.8) ω_0 by ω_0^L. The terms in (5.6) and (5.7) depending on $S^{\pm}_{i(F)}(\tau,d;\mu)$ stem from the transversal modes in the spectral resolution, cf. the derivation of (4.26) and (4.27), whereas the terms containing $S^{\pm}_{i(F)}(\tau,d;\sqrt{1+\mu^2})$ are generated by the longitudinal modes. Clearly, $S_1 = -\partial S_0/\partial d$. The coefficients (5.8) are calculated via an integral representation of modified Bessel functions,[15] quite analogously to the scalar case (3.19) and (3.20),

$$S^{\pm}_i(\tau,d;\mu) = \pm \pi i(\tilde{S}_i(\tau,d;\mu) - \tilde{S}_i(-\tau,d;\mu))\,\theta(\pm\tau), \tag{5.9}$$

$$S^{\pm}_{iF}(\tau,d;\mu) = \pm \pi i \tilde{S}_i(\pm|\tau|,d;\mu), \tag{5.10}$$

where we have defined

$$\tilde{S}_0(\tau,d;\mu) := \frac{1}{\pi^2}\int_0^\infty \cos(sd)\tilde{I}(\omega_0,\tau)\,ds = \frac{1}{\pi^2} K_0(\mu\sqrt{d^2+(i\tau+\varepsilon)^2}), \tag{5.11}$$

$$\tilde{S}_1(\tau,d;\mu) := \frac{1}{\pi^2}\int_0^\infty s\,\sin(sd)\tilde{I}(\omega_0,\tau)\,ds = \frac{\mu d}{\pi^2}\,\frac{K_1(\mu\sqrt{d^2+(i\tau+\varepsilon)^2})}{\sqrt{d^2+(i\tau+\varepsilon)^2}}, \tag{5.12}$$

with $\tilde{I}(\omega_0,\tau) := \omega_0^{-1} e^{-(i\tau+\varepsilon)\omega_0}$, and the same with $\mu \to \sqrt{1+\mu^2}$. Performing the limit $\varepsilon \to 0$, cf. (3.21)–(3.27), we find

$$\begin{aligned}\tilde{S}_0(\tau,d;\mu) = {} & \frac{1}{\pi^2}\,\theta(d^2-\tau^2) K_0(\mu\sqrt{d^2-\tau^2}) - \frac{1}{2\pi}\,\theta(\tau^2-d^2) \\ & \times (N_0(\mu\sqrt{\tau^2-d^2}) + i\varepsilon(\tau) J_0(\mu\sqrt{\tau^2-d^2})),\end{aligned} \tag{5.13}$$

$$\begin{aligned}\tilde{S}_1(\tau,d;\mu) = {} & -\frac{i}{\pi} d\,\varepsilon(\tau)\,\delta(d^2-\tau^2) + \frac{\mu d}{\pi^2}\,\frac{\theta(d^2-\tau^2)}{\sqrt{d^2-\tau^2}} K_1(\mu\sqrt{d^2-\tau^2}) \\ & + \frac{\mu d}{2\pi}\,\frac{\theta(\tau^2-d^2)}{\sqrt{\tau^2-d^2}} (N_1(\mu\sqrt{\tau^2-d^2}) + i\varepsilon(\tau) J_1(\mu\sqrt{\tau^2-d^2})),\end{aligned} \tag{5.14}$$

and the $\tilde{S}_i(\tau,d;\sqrt{1+\mu^2})$ are obtained by the substitution $\mu \to \sqrt{1+\mu^2}$, of course; $\varepsilon(\tau)$ is the sign function. In the calculation of (5.13) and (5.14), we used the second and third formula in (A10), as well as (3.22) and (3.23), and[15]

$$K_0(\pm ix) = -(\pi/2)(N_0(x) \pm i J_0(x)),\quad x > 0, \tag{5.15}$$

$$\begin{aligned}K_0(z) &= -\gamma - \log(z/2) + O(z^2\log z),\quad J_0(z) = 1 + O(z^2), \\ N_0(z) &= (2/\pi)(\gamma + \log(z/2)) + O(z^2\log z).\end{aligned} \tag{5.16}$$

The integrals in (5.6) and (5.7) are calculated via (5.9) and (5.10), by making use of (5.13) and (5.14),

$$\int_0^d \tilde{S}_0(\tau,x;\mu)dx=\frac{1}{\pi^2}\,\theta(d^2-\tau^2)\int_0^{\sqrt{d^2-\tau^2}}\frac{K_0(\mu y)ydy}{\sqrt{\tau^2+y^2}}-\frac{1}{2\pi}\bigg(\theta(\tau^2-d^2)\int_{\sqrt{\tau^2-d^2}}^{|\tau|}$$
$$+\theta(d^2-\tau^2)\int_0^{|\tau|}\bigg)(N_0(\mu y)+i\varepsilon(\tau)J_0(\mu y))\,\frac{ydy}{\sqrt{\tau^2-y^2}}, \tag{5.17}$$

$$\int_0^d \tilde{S}_1(\tau,x;\sqrt{1+\mu^2})\sinh x\,dx=-\frac{i}{2\pi}\,\theta(d^2-\tau^2)\varepsilon(\tau)\sinh|\tau|+\frac{\sqrt{\mu^2+1}}{\pi^2}\,\theta(d^2-\tau^2)$$
$$\times\int_0^{\sqrt{d^2-\tau^2}}K_1(\sqrt{\mu^2+1}y)\sinh\sqrt{\tau^2+y^2}dy+\frac{\sqrt{\mu^2+1}}{2\pi}$$
$$\times\bigg(\theta(\tau^2-d^2)\int_{\sqrt{\tau^2-d^2}}^{|\tau|}+\theta(d^2-\tau^2)\int_0^{|\tau|}\bigg)(N_1(\sqrt{\mu^2+1}y)$$
$$+i\varepsilon(\tau)J_1(\sqrt{\mu^2+1}y))\sinh\sqrt{\tau^2-y^2}dy. \tag{5.18}$$

In the $\theta(d^2-\tau^2)$-terms, there are singularities in K_1 and N_1 for $y\to 0$, cf. (3.23), which, however, cancel each other. As a consistency check, we note $\int_0^d\tilde{S}_1^T(\tau,x)dx=\tilde{S}_0^T(\tau,0)-\tilde{S}_0^T(\tau,d)$, which can readily be verified by $(J_0',N_0',K_0')(z)=-(J_1,N_1,K_1)(z)$. The integrals in (5.17) and (5.18) are of indefinite type and cannot be further evaluated in closed form, but this representation is sufficiently explicit to reveal the singularity and asymptotic structure and in particular the support of the propagators. The most surprising feature is perhaps, that the Feynman and Dyson propagators defined by (5.10) have an infrared singularity for $\mu\to 0$. Hence, for the electromagnetic field, these propagators are ill-defined by the standard contour integration, unless one uses some kind of infrared regularization such as a finite photon mass. This is an effect of the space curvature; if one approximates in (5.6) and (5.7), in the limit of large curvature radius, $\cosh d\sim 1$, and $\sinh d\sim d$, then the $\log\mu$ singularities stemming from N_0 and K_0 cancel each other. (Throughout the calculations, we have put the curvature radius of the 3-space equal to one, but it can readily be restored by dimensional considerations, see below.) In retarded and advanced Green functions, cf. (5.9), the $\log\mu$-singularities cancel without performing this curvature limit. It would be interesting to investigate whether the infrared divergence of the quantum propagators can affect the emission probability of soft photons.[16] If so, one could possibly draw inferences on the curvature sign.

Making use of (5.13), (5.14), (5.17), and (5.18), we readily find

$$S_0^{\pm}(\tau,d;\mu)=\theta(\pm\tau)\,\theta(\tau^2-d^2)J_0(\mu\sqrt{\tau^2-d^2}),$$
$$S_1^{\pm}(\tau,d;\mu)=2d\,\theta(\pm\tau)\,\delta(d^2-\tau^2)-\mu d\,\theta(\pm\tau)\,\frac{\theta(\tau^2-d^2)}{\sqrt{\tau^2-d^2}}J_1(\mu\sqrt{\tau^2-d^2}), \tag{5.19}$$

$$\int_0^d S_0^{\pm}(\tau,x;\mu)dx=\theta(\pm\tau)\bigg(\theta(\tau^2-d^2)\int_{\sqrt{\tau^2-d^2}}^{|\tau|}+\theta(d^2-\tau^2)\int_0^{|\tau|}\bigg)J_0(\mu y)\,\frac{ydy}{\sqrt{\tau^2-y^2}}, \tag{5.20}$$

$$\int_0^d S_1^{\pm}(\tau,x;\sqrt{1+\mu^2})\sinh x\,dx$$
$$=\theta(\pm\tau)\,\theta(d^2-\tau^2)\sinh|\tau|-\sqrt{\mu^2+1}\,\theta(\pm\tau)$$
$$\times\bigg(\theta(\tau^2-d^2)\int_{\sqrt{\tau^2-d^2}}^{|\tau|}+\theta(d^2-\tau^2)\int_0^{|\tau|}\bigg)J_1(\sqrt{\mu^2+1}y)\sinh\sqrt{\tau^2-y^2}dy,$$

and the $S_i^{\pm}(\tau,d;\sqrt{1+\mu^2})$ are obtained by the substitution $\mu\to\sqrt{1+\mu^2}$. The retarded and advanced Green functions $G_{ij}^{\pm}(\tau;\mathbf{x},\mathbf{y})$ of a massive vector field are thus given by (5.5)–(5.7), with (5.19) and (5.20) inserted. The analogous coefficients for the Feynman propagator read as

$$S_{0F}^{+}(\tau,d;\mu)=\frac{i}{\pi}\,\theta(d^2-\tau^2)K_0(\mu\sqrt{d^2-\tau^2})+\frac{1}{2}\,\theta(\tau^2-d^2)(J_0(\mu\sqrt{\tau^2-d^2})-iN_0(\mu\sqrt{\tau^2-d^2})),$$

$$\begin{aligned}S_{1F}^{+}(\tau,d;\mu)&=d\,\delta(d^2-\tau^2)+\frac{i\mu d}{\pi}\,\frac{\theta(d^2-\tau^2)}{\sqrt{d^2-\tau^2}}K_1(\mu\sqrt{d^2-\tau^2})\\&\quad-\frac{\mu d}{2}\,\frac{\theta(\tau^2-d^2)}{\sqrt{\tau^2-d^2}}(J_1(\mu\sqrt{\tau^2-d^2})-iN_1(\mu\sqrt{\tau^2-d^2})),\end{aligned}\tag{5.21}$$

$$\begin{aligned}\int_0^d S_{0F}^{+}(\tau,x;\mu)dx&=\frac{i}{\pi}\,\theta(d^2-\tau^2)\int_0^{\sqrt{d^2-\tau^2}}\frac{K_0(\mu y)y\,dy}{\sqrt{\tau^2+y^2}}+\frac{1}{2}\Bigg(\theta(\tau^2-d^2)\int_{\sqrt{\tau^2-d^2}}^{|\tau|}+\theta(d^2-\tau^2)\\&\quad\times\int_0^{|\tau|}\Bigg)(J_0(\mu y)-iN_0(\mu y))\,\frac{y\,dy}{\sqrt{\tau^2-y^2}},\end{aligned}\tag{5.22}$$

$$\begin{aligned}\int_0^d S_{1F}^{+}(\tau,x;\sqrt{1+\mu^2})\sinh x\,dx&=\frac{1}{2}\,\theta(d^2-\tau^2)\sinh|\tau|+\frac{i}{\pi}\sqrt{\mu^2+1}\,\theta(d^2-\tau^2)\\&\quad\times\int_0^{\sqrt{d^2-\tau^2}}K_1(\sqrt{\mu^2+1}y)\sinh\sqrt{\tau^2+y^2}\,dy-\frac{1}{2}\sqrt{\mu^2+1}\\&\quad\times\Bigg(\theta(\tau^2-d^2)\int_{\sqrt{\tau^2-d^2}}^{|\tau|}+\theta(d^2-\tau^2)\int_0^{|\tau|}\Bigg)(J_1(\sqrt{\mu^2+1}y)\\&\quad-iN_1(\sqrt{\mu^2+1}y))\sinh\sqrt{\tau^2-y^2}\,dy.\end{aligned}$$

The coefficients for the Dyson propagator are obtained by complex conjugation, $S_{iF}^{-}(\tau,d;\mu)=\overline{S_{iF}^{+}(\tau,d;\mu)}$.

In the retarded and advanced propagators, the limit $\mu\to 0$ can be performed, and we find

$$\begin{aligned}G_{ij}^{\pm}(\tau;\mathbf{x},\mathbf{y};\mu=0)&=-e^{-d/R}(R_{11}^{\pm}(\tau,d;\mu=0)\sinh(d/R)Rd_{,i,j}\\&\quad+R_{33}^{\pm}(\tau,d;\mu=0)d_{,i}d_{,j}),\end{aligned}\tag{5.23}$$

with the matrix elements, cf. (5.19) and (5.20),

$$\begin{aligned}R_{11}^{\pm}(\tau,d;\mu=0)&=\frac{e^{d/R}\theta(\pm\tau)}{4\pi R^2\sinh^3(d/R)}\Bigg[2dR\sinh^2\Big(\frac{d}{R}\Big)\delta(d^2-c^2\tau^2)+\theta(c^2\tau^2-d^2)\\&\quad\times\Bigg(-\frac{d}{R}+\sinh\frac{d}{R}\cosh\frac{d}{R}-\frac{1}{R}\int_{\sqrt{c^2\tau^2-d^2}}^{c|\tau|}J_1(y/R)\sinh(R^{-1}\sqrt{c^2\tau^2-y^2})dy\Bigg)\\&\quad+\theta(d^2-c^2\tau^2)\Bigg(-\frac{c|\tau|}{R}+\sinh\frac{c|\tau|}{R}\\&\quad-\frac{1}{R}\int_0^{c|\tau|}J_1(y/R)\sinh(R^{-1}\sqrt{c^2\tau^2-y^2})dy\Bigg)\Bigg],\end{aligned}\tag{5.24}$$

$$R^{\pm}_{33}(\tau,d;\mu=0)=\frac{e^{d/R}\theta(\pm\tau)}{2\pi R^2\sinh^3(d/R)}\Bigg[dR\sinh^2\!\left(\frac{d}{R}\right)\delta(d^2-c^2\tau^2)+\theta(c^2\tau^2-d^2)$$
$$\times\Bigg(\frac{d}{R}\cosh\frac{d}{R}-\sinh\frac{d}{R}-\frac{d}{2}\sinh^2\!\left(\frac{d}{R}\right)\frac{J_1(R^{-1}\sqrt{c^2\tau^2-d^2})}{\sqrt{c^2\tau^2-d^2}}$$
$$+\cosh\!\left(\frac{d}{R}\right)\frac{1}{R}\int_{\sqrt{c^2\tau^2-d^2}}^{c|\tau|}J_1(y/R)\sinh(R^{-1}\sqrt{c^2\tau^2-y^2})\,dy\Bigg)+\theta(d^2-c^2\tau^2)$$
$$\times\cosh\frac{d}{R}\left(\frac{c|\tau|}{R}-\sinh\frac{c|\tau|}{R}+\frac{1}{R}\int_0^{c|\tau|}J_1(y/R)\sinh(R^{-1}\sqrt{c^2\tau^2-y^2})\,dy\right)\Bigg]. \tag{5.25}$$

We have here restored the natural units, the curvature radius R of the 3-space, and c. [The exponentials drop out, of course, we just have them included to be consistent with the previous notation, and they are also convenient when considering the $d\to\infty$ asymptotics, see after (6.14).] In the B^3-model, we recover for $R\to\infty$ the Green functions in Minkowski space, cf. the discussion preceding (3.31). In fact, $dd_{,i,j}+d_{,i}d_{,j}\sim-4\delta_{ij}$, so that (5.23) boils down to

$$G^{\pm}_{ij}(\tau;\mathbf{x},\mathbf{y};\mu=0,\ R\to\infty)\sim\frac{1}{2\pi}4\delta_{ij}\theta(\pm\tau)\delta(4|\mathbf{x}-\mathbf{y}|^2-c^2\tau^2), \tag{5.26}$$

supported only at the light cone. By a rescaling of the space coordinates, one can get rid of the two factors of 4. One can sometimes switch from negative to positive curvature just by analtyic continuation in the curvature radius, and it would be interesting to check in how far this persists here.

Up to now we considered a static RW cosmology [expansion factor $a(\tau)=1$]; the retarded and advanced electromagnetic Green functions as defined by (3.30) and (5.23) remain valid, with minor modifications, in a general RW cosmology, $ds^2=-d\tau^2+a^2(\tau)d\sigma^2$. In the spectral elementary waves (2.15) and (2.16), we have to substitute $\tau\to\int_{\tau_0}^{\tau}a^{-1}(\tau)d\tau$ into the exponentials, so that the frequencies of the transversal and longitudinal waves scale as $|s|a^{-1}(\tau)$ and $\sqrt{s^2+1}a^{-1}(\tau)$, respectively. In addition, the longitudinal time component A^L_0 in (2.16) has to be rescaled by a factor $a^{-1}(\tau)$. In the Green functions (3.30) and (5.23), we have to perform the same substitution for the time variable, and then to scale $G^{\pm}_{00}$ by a factor $(a(\tau)a(\tau_0))^{-1}$. These modifications only apply to the massless case, $\mu=0$, as a consequence of the conformal coupling of the electromagnetic field. If the rest mass is finite, a time separation of (2.4)–(2.6) is still possible, so that the time independent part of the spectral problem, in particular the resolvent kernel calculated in Secs. III and IV, also applies to a RW cosmology with arbitrary expansion factor without modifications. However, the time dependence of the eigenfunctions is then not any more exponential as in (2.15) and (2.16), and has to be calculated from scratch, and the integral transform (2.28) relating the time dependent Green functions to the resolvent kernel must be modified accordingly. In a Milne universe with linear expansion factor, $a(\tau)=(c/R)\tau$, it should be possible to obtain quite explicit formulas for the massive propagators.[17]

Remark: The time component $G^{\pm}_{00(F)}(\mu^2=-1)$, if scaled in the indicated way with the expansion factor, also defines the propagators of the conformally coupled Klein–Gordon equation, as discussed at the end of Sec. III. The limit $\mu^2\to-1$ can easily be carried out in (3.25) and (3.26). By a standard scaling argument[2] applied to (3.32), we find

$$(\Box-\hat{R}/6)G^{\pm}_{00(F)}(\tau,d;\mu^2=-1)=a^{-3}(\tau)\delta_{B^3}(\mathbf{x},\mathbf{y})\delta(\tau), \tag{5.27}$$

where $\Box$ is the d'Alembertian of the RW-line element, and

$$\hat{R} := 6\left(\frac{-1}{a^2} + \frac{\ddot{a}}{a} + \frac{\dot{a}^2}{a^2}\right) \tag{5.28}$$

is the Ricci scalar. The spectral elementary waves, solving $(\Box - \hat{R}/6)\psi = 0$, read

$$\psi = a^{-1}(\tau)\exp\left(\pm is\int a^{-1}(\tau)d\tau\right)P^{1+is}, \tag{5.29}$$

with the Poisson kernel P as defined in (2.17).

VI. GREEN FUNCTIONS IN RW COSMOLOGIES WITH MULTIPLY CONNECTED HYPERBOLIC 3-SPACE

We start with the time independent Green functions $\hat{G}_{00}(\omega;\mathbf{x},\mathbf{y})$, cf. (3.6) and $\hat{G}_{ij}(\omega;\mathbf{x},\mathbf{y})$, cf. (4.25). For λ, we substitute $\lambda^{\pm}_{(F)}(\omega)$ as in (3.16) and write accordingly, in the B^3-model, $\hat{G}^{\pm}_{(F)00}(\omega;\mathbf{x},\mathbf{y})$ and $\hat{G}^{\pm}_{(F)ij}(\omega;\mathbf{x},\mathbf{y})$, as at the beginning of Sec. V. We will switch between the B^3 and H^3-models whenever convenient; in the H^3-model, we write $\hat{G}^{\pm}_{(F)\alpha\beta}(\omega;z,t;z_0,t_0)$. Green functions on multiply connected hyperbolic manifolds can formally be obtained by periodizing B^3 or H^3-Green functions with the covering group Γ,

$$\hat{G}^{\Gamma\pm}_{(F)00}(\omega;\mathbf{x},\mathbf{y}) := \sum_{\gamma\in\Gamma}\hat{G}^{\pm}_{(F)00}(\omega;\gamma\mathbf{x},\mathbf{y}), \tag{6.1}$$

$$\hat{G}^{\Gamma\pm}_{(F)ij}(\omega;\mathbf{x},\mathbf{y}) := \sum_{\gamma\in\Gamma}\hat{G}^{\pm}_{(F)kj}(\omega;\gamma\mathbf{x},\mathbf{y})[\gamma'\mathbf{x}]_{ki}; \tag{6.2}$$

the scalar case (6.1) is well documented.[6,9,10,18] The Jacobian $[\gamma'\mathbf{x}]$ in (6.2) is readily calculated by making use of the representation[5] $\gamma(\mathbf{x}) = kT_{\gamma^{-1}(\mathbf{0})}\mathbf{x}$, with a constant matrix $k\in\mathrm{SO}(3)$; the Jacobian of $T_{\mathbf{y}}\mathbf{x}$ is given in (4.15).

The hard part is of course to show that the series (6.1) and (6.2) converge, see after (6.11). We restrict this investigation to hyperbolic manifolds that admit a finitely sided fundamental polyhedron without parabolic cusp singularities. The covering group Γ is a Kleinian group,[19–24] a discrete subgroup of $\mathrm{SL}(2,C)/\{\pm id\}$ acting via 3D Möbius transformations in B^3 or H^3. Γ is finitely generated, and does not contain parabolic (or elliptic) elements. As for the Hausdorff dimension δ of the limit set of Γ, the manifold is open if $0\leqslant\delta<2$, so that the fundamental polyhedron has faces on the boundary of H^3; it is compact if $\delta=2$, in this case the fundamental polyhedron does not touch the boundary. The domain defined by the polyhedral faces on the boundary is denoted by f; it is a fundamental domain of Γ acting via Möbius (i.e., linear fractional) transformations in the complex plane. Examples for open hyperbolic manifolds are solid handle-bodies with Schottky covering groups;[19] the limit sets of these groups are Cantor sets with $0<\delta<1$. Another class of open hyperbolic manifolds are thickened Riemann surfaces, hollow handle bodies, with (quasi-) Fuchsian[20] covering groups, whose limit sets are closed Jordan curves with Hausdorff dimensions $1\leqslant\delta<2$. As mentioned, the faces of the fundamental polyhedron corresponding to the surfaces of these 3D handle bodies lie on the boundary at infinity of hyperbolic space, i.e., in the complex plane, if we use the H^3-model, and so these manifolds are open. In the following only manifolds with $0\leqslant\delta<1$ are considered, to assure the convergence of the series (6.1) and (6.2).

The periodization in (6.1) and (6.2) may as well be with respect to $\mathbf{y}$, because $\hat{G}^{\pm}_{(F)00}$ and $\hat{G}^{\pm}_{(F)ij}$ are scalar and vectorial point-pair invariants, respectively,

$$\hat{G}^{\pm}_{(F)00}(\omega;\gamma\mathbf{x},\gamma\mathbf{y}) = \hat{G}^{\pm}_{(F)00}(\omega;\mathbf{x},\mathbf{y}), \tag{6.3}$$

$$\hat{G}^{\pm}_{(F)ij}(\omega;\gamma\mathbf{x},\gamma\mathbf{y})[\gamma'\mathbf{x}]_{im}[\gamma'\mathbf{y}]_{jn}=\hat{G}^{\pm}_{(F)mn}(\omega;\mathbf{x},\mathbf{y}),$$
$$\hat{G}^{\pm}_{(F)kn}(\omega;\gamma\mathbf{x},\mathbf{y})[\gamma'\mathbf{x}]_{km}=\hat{G}^{\pm}_{(F)mk}(\omega;\mathbf{x},\gamma^{-1}\mathbf{y})[\gamma^{-1\prime}\mathbf{y}]_{kn}. \tag{6.4}$$

These symmetries hold for every Möbius transformation in B^3, unrelated to the covering group Γ, because $\hat{G}^{\pm}_{(F)00}$ and $\hat{G}^{\pm}_{(F)ij}$ are functions of the scalar point-pair invariant $L(\mathbf{x},\mathbf{y})$, and the vectorial invariants $\partial L/\partial x_i \partial L/\partial y_j$ and $\partial^2 L/\partial x_i \partial y_j$. The periodization (6.1) and (6.2) may be replaced by a Γ-periodization with respect to $\mathbf{y}$ (and j). To see this, we replace in (6.3) and (6.4) $\mathbf{x}$ by $\gamma^{-1}\mathbf{x}$, and because the summation in (6.1) and (6.2) is over the whole group, we may replace there γ by γ^{-1}. By a similar reasoning, (6.3) and (6.4) still holds for the periodized functions (6.1) and (6.2), provided $\gamma\in\Gamma$.

The spectral representation of $\hat{G}^{\Gamma\pm}_{(F)\alpha\beta}$ is readily derived in the half-space model H^3. Starting with the scalar time component, we define the Eisenstein series[6,9,10]

$$E(z,t;\xi,1+is):=\sum_{\gamma\in\Gamma} P^{1+is}(\gamma(z,t);\xi)=\sum_{\gamma\in\Gamma}|\gamma'\xi|^{1+is}P^{1+is}(z,t;\gamma\xi), \tag{6.5}$$

where we used the symmetry (2.24), which also implies

$$E(\gamma(z,t);\xi,1+is)=E(z,t;\xi,1+is),\quad |\gamma'\xi|^{1+is}E(z,t;\gamma\xi,1+is)=E(z,t;\xi,1+is), \tag{6.6}$$

for $\gamma\in\Gamma$. In the first equation in (2.16), we substitute the series (6.5) for P^{1+is}, which amounts to periodizing the H^3-eigenfunctions with respect to the hyperbolic lattice. The series (6.5) converges for the indicated covering groups (with $\delta<1$), see after (6.11). It is easy to see, that the orthogonality and completeness relations (A12) and (A14) remain valid for $E(z,t;\xi,1\pm is)$ with some obvious modifications; apart from replacing $P^{1\pm is}$ by $E(z,t;\xi,1\pm is)$, the domain of integration (H^3) in (A12) has to be restricted to a fundamental polyhedron F of the covering group, and in (A14) the domain of integration ($R^2\times R^+$) is restricted to $f\times R^+$, where f is a fundamental domain of Γ in the complex plane. [The formal procedures to show this, and to derive (6.7) and (6.10) below, are quite similar to those indicated in (6.24) and (6.25).] It should be stressed, that these statements are only safe for the specified covering groups. For example, the series (6.5) diverges for covering groups as defined after (6.2) with $\delta\geqslant 1$, and analytic continuation is needed to define it for real s. This is not only a technicality, because bound states emerge in addition to the continuous spectrum,[6] and the set (6.5) is not complete.

If $\delta<1$, the completeness relation (A14) holds with the indicated modifications, and we may write, analogously to (3.13),

$$\hat{G}^{\Gamma\pm}_{(F)00}(\omega;z,t;z_0,t_0)=-\int_{f\times R^+} d\sigma(\xi,s)\,\frac{E(z,t;\xi,1+is)E(z_0,t_0;\xi,1-is)}{s^2+1+\lambda^{\pm}_{(F)}(\omega)}, \tag{6.7}$$

with the spectral measure defined in (A13). The formal identity of (6.7) with (6.1) can be easily shown by means of the completeness relation and the spectral representation (3.13) in the covering space, along the lines of (6.24) and (6.25).

The spatial component of the resolvent kernel admits a similar representation. The vectorial analog to (6.5) reads as[13]

$$\mathbf{a}_j^{\Gamma T_L}(z,t;\xi,s):=\sum_{\gamma\in\Gamma}\mathbf{a}_i^{T_L}(\gamma(z,t);\xi,s)[\gamma'(z,t)]_{ij}=\sum_{\gamma\in\Gamma}|\gamma'\xi|^{is}\overline{\gamma'\xi}\,\mathbf{a}_j^{T_L}(z,t;\gamma\xi,s),$$
$$\mathbf{a}_j^{\Gamma T_R}(z,t;\xi,s):=\sum_{\gamma\in\Gamma}|\gamma'\xi|^{is}\gamma'\xi\,\mathbf{a}_j^{T_R}(z,t;\gamma\xi,s), \tag{6.8}$$
$$\mathbf{a}_j^{\Gamma L}(z,t;\xi,s):=\sum_{\gamma\in\Gamma}|\gamma'\xi|^{1+is}\mathbf{a}_j^{L}(z,t;\gamma\xi,s),$$

with the invariance property, cf. (6.6),

$$\mathbf{a}_i^{\Gamma T_L}(\gamma(z,t);\xi,s)[\gamma'(z,t)]_{ij}=\mathbf{a}_j^{\Gamma T_L}(z,t;\xi,s)=|\gamma'\xi|^{is}\overline{\gamma'\xi}\mathbf{a}_j^{\Gamma T_L}(z,t;\gamma\xi,s), \tag{6.9}$$

and analogous relations hold for the right circular and longitudinal polarizations. These Eisenstein series are obtained by periodizing the circularly polarized transversal vectors $\mathbf{a}_j^{T_{L,R}}$ as defined in (2.22), and the longitudinal vector $\mathbf{a}_j^L$ in (2.20). The symmetries (2.23) have been invoked in (6.8) and (6.9). Again, for the indicated covering groups (with $\delta<1$), these series converge for real s, see the discussion following (6.11). The spatial components of the eigenfunctions in (2.15) and (2.16) get periodized (and circularly polarized) by replacing there $\mathbf{a}_j^{T_k,L}$ by (6.8), and then they solve again the Γ-invariant Eq. (2.6). The vectors in (6.8) are orthogonal, cf. (B4)–(B6), and the completeness relation (B14) stays valid with the substitutions $\mathbf{a}^{T_k,L}\to\mathbf{a}^{\Gamma T_{L,R},L}$ and the above-mentioned restriction of the domain of integration to a fundamental domain. Accordingly, the spectral resolution of the matrix elements (4.1) and (4.2) reads

$$\begin{aligned}\hat{R}_{ij}^{\Gamma T}(z,t;z_0,t_0;\lambda)&:=\int_{f\times R^+}\sum_{k=L,R}\mathbf{a}_i^{\Gamma T_k}(z,t;\xi,s)\overline{\mathbf{a}_j^{\Gamma T_k}(z_0,t_0;\xi,s)}\frac{d\sigma^T(\xi,s)}{s^2+\lambda},\\ \hat{R}_{ij}^{\Gamma L}(z,t;z_0,t_0;\lambda)&:=\int_{f\times R^+}\mathbf{a}_i^{\Gamma L}(z,t;\xi,s)\overline{\mathbf{a}_j^{\Gamma L}(z_0,t_0;\xi,s)}\frac{d\sigma^L(\xi,s)}{s^2+1+\lambda},\end{aligned} \tag{6.10}$$

and the spectral representation of the periodized spatial Green function is thus found as

$$\hat{G}_{(F)ij}^{\Gamma\pm}(\omega;z,t;z_0,t_0)=\hat{R}_{ij}^{\Gamma T}(z,t;z_0,t_0;\lambda_{(F)}^{\pm}(\omega))+\hat{R}_{ij}^{\Gamma L}(z,t;z_0,t_0;\lambda_{(F)}^{\pm}(\omega)). \tag{6.11}$$

[The k-summation in $\hat{R}_{ij}^{\Gamma T}$ is over left and right circular polarizations, which may as well be replaced by linearly polarized states, according to (2.22).] The spectral measures in (6.10) remain as defined in (B13), but the domain of the ξ-integration is restricted to a fundamental domain f in the complex plane.

The Poisson kernel $P(z,t;\gamma\xi)$ as well as the components of the vectors $\mathbf{a}^{T_{L,R},L}(z,t;\gamma\xi,s)$ are bounded for $\gamma\in\Gamma$, and hence the convergence abscissa of the Eisenstein series (6.5) and (6.8) coincides with that of the Poincaré series $\Sigma_{\gamma\in\Gamma}|\gamma'\xi|^{1+is}$. (The limit set is the set of accumulation points of the orbit $\gamma\xi$, by the way.) As for the covering groups indicated after (6.2), this series is known to converge only for $\mathrm{Re}(1+is)>\delta$, cf. Ref. 6.

To obtain the convergence behavior of the Poincaré series (6.1) and (6.2), we need an estimate on $\hat{G}_{(F)\alpha\beta}^{\pm}(\omega;\mathbf{x},\mathbf{y})$ [defined by (3.6) and (4.25)] for $d\to\infty$, which means for $|\mathbf{x}|\to1$, and $\mathbf{y}$ fixed, or vice versa. For the time component, this is easily settled, $\hat{G}_{00}(\omega;\mathbf{x},\mathbf{y})=O(\exp(-(1+\tilde{\varepsilon})d(\mathbf{x},\mathbf{y})))$, with $\tilde{\varepsilon}:=\mathrm{Re}\,\sqrt{1+\lambda}$, cf. (3.6). When calculating the real space Green functions (3.15), the limit $\tilde{\varepsilon}\to0$ is attained.

Next we turn to the $d\to\infty$ asymptotics of the space component and the Jacobian in (6.2). In the B^3-model, we can readily calculate $(\log L)_{,i,j}$, cf. (3.5), in the limit $|\mathbf{x}|\to1$,

$$\frac{L_{,i,j}}{L}-\frac{L_{,i}L_{,j}}{L^2}\sim\frac{-4}{1-2\mathbf{xy}+\mathbf{y}^2}\left(\frac{1}{2}\,\delta_{ij}-\frac{(x_i-y_i)(x_j-y_j)}{1-2\mathbf{xy}+\mathbf{y}^2}\right). \tag{6.12}$$

[As in (4.21), i means differentiation with respect to x_i, and j with respect to y_j.] Likewise, for $|\mathbf{x}|\to1$,

$$\frac{L_{,i}L_{,j}}{L^2}\sim\frac{4x_i(2y_j(1-\mathbf{xy})-x_j(1-\mathbf{y}^2))}{(1-\mathbf{x}^2)(1-\mathbf{y}^2)(1-2\mathbf{xy}+\mathbf{y}^2)}. \tag{6.13}$$

Moreover, we find from (4.24), for $L\to\infty$,

$$d_{,i}d_{,j}\sim L_{,i}L_{,j}/L^2=O(L),$$
$$\sinh(d)d_{,i,j}\sim 2L_{,i,j}-2\frac{L_{,i}L_{,j}}{L}+\frac{L_{,i}L_{,j}}{L^2}=O(L), \tag{6.14}$$

Clearly, $L\sim e^d/4$, so that $e^{-d}d_{,i}d_{,j}=O(1)$, as well as $e^{-d}\sinh(d)d_{,i,j}=O(1)$, for $d\to\infty$. Accordingly, $\hat{R}_{11}=O(e^{-\sqrt{\lambda}d})$, and $\hat{R}_{33}=O(e^{-\sqrt{1+\lambda}d})$, cf. (4.26) and (4.27), and hence the asymptotics of the Green function (4.25) is evident, $\hat{G}_{ij}(\omega;\mathbf{x},\mathbf{y})=O(\exp(-\tilde{\varepsilon}d(\mathbf{x},\mathbf{y})))$, with $\tilde{\varepsilon}:=\min(\mathrm{Re}\,\sqrt{\lambda},\mathrm{Re}\,\sqrt{1+\lambda})>0$. In the integration procedures for the time dependent Green functions, cf. (5.4) and (3.16), the limit $\tilde{\varepsilon}\to 0$ is again reached. In (6.2), the estimate for $\hat{G}_{ij}$ has still to be multiplied with the estimate for the Jacobian $[\gamma'\mathbf{x}]$.

As for the Jacobian $\hat{x}_{j,i}$ of $T_{\mathbf{y}}\mathbf{x}$, cf. (4.15), we find, for fixed $\mathbf{x}$ and $|\mathbf{y}|\to 1$, $\hat{x}_{j,i}=O(1-|\mathbf{y}|)$. We write $\gamma(\mathbf{x})=kT_{\gamma^{-1}(\mathbf{0})}\mathbf{x}$, with an orthogonal matrix k, as pointed out after (6.2). We thus obtain, for $|\gamma^{-1}(\mathbf{0})|\to 1$, the estimate $[\gamma'\mathbf{x}]_{mn}=O(1-|\gamma^{-1}\mathbf{0}|)$. Using $L(\mathbf{0},\gamma(\mathbf{y}))=L(\gamma^{-1}(\mathbf{0}),\mathbf{y})$, we find $[\gamma'\mathbf{x}]_{mn}=O(1-|\gamma\mathbf{y}|)$, for $|\gamma\mathbf{y}|\to 1$, with fixed $\mathbf{x}$ and $\mathbf{y}$, for every Kleinian group, and so we may write $[\gamma'\mathbf{x}]_{mn}=O(\exp(-d(\mathbf{y},\gamma\mathbf{x})))=O(\exp(-d(\gamma\mathbf{y},\mathbf{x})))$. (The geometric reasoning underlying such estimates, also with regard to uniformity in fundamental domains, is explained in Ref. 5.) We conclude, that the convergence of the series (6.1) and (6.2) is decided by the convergence of $\Sigma_{\gamma\in\Gamma}\exp(-d(\gamma\mathbf{x},\mathbf{y}))$, uniformly in $\lambda=\lambda^{\pm}_{(F)}(\varepsilon,\omega)$, for real ω and $\varepsilon\to 0$. The Poincaré series $\Sigma_{\gamma\in\Gamma}\exp(-\alpha d(\gamma\mathbf{x},\mathbf{y}))$ and $\Sigma_{\gamma\in\Gamma}|\gamma'\xi|^{\alpha}$ have the same abscissa of convergence. Accordingly, in the case of the covering groups specified after (6.2), we can use the series (6.1) and (6.2) only if $\delta<1$, which also happens to be the criterion for the convergence of the Eisenstein series (6.5) and (6.8).

The time-dependent Green function on the 4-manifold is defined as the Fourier transform of (6.1) and (6.2), cf. (2.28), (3.15), and (5.4),

$$G^{\Gamma\pm}_{(F)\alpha\beta}(\tau;\mathbf{x},\mathbf{y})=(2\pi)^{-1}\int_{-\infty}^{+\infty}d\omega e^{-i\omega\tau}\hat{G}^{\Gamma\pm}_{(F)\alpha\beta}(\omega;\mathbf{x},\mathbf{y}). \tag{6.15}$$

By formally interchanging summation and integration, we find

$$G^{\Gamma\pm}_{(F)00}(\tau;\mathbf{x},\mathbf{y})=\sum_{\gamma\in\Gamma}G^{\pm}_{(F)00}(\tau;\gamma\mathbf{x},\mathbf{y}), \tag{6.16}$$

$$G^{\Gamma\pm}_{(F)ij}(\tau;\mathbf{x},\mathbf{y})=\sum_{\gamma\in\Gamma}G^{\pm}_{(F)kj}(\tau;\gamma\mathbf{x},\mathbf{y})[\gamma'\mathbf{x}]_{ki}, \tag{6.17}$$

which means periodization of the real space Green functions defined in (3.28), (3.29), and (5.5)–(5.7). The convergence of the series (6.16) and (6.17) can be estimated as above, $G^{\pm}_{(F)00}(\tau;\mathbf{x},\mathbf{y})=O(e^{-d})$, uniformly in τ, for $|\mathbf{x}|\to 1$ and fixed $\mathbf{y}$, which follows from (3.28), (3.29), the asymptotics of the Bessel functions there, and (A10). Likewise, $G^{\pm}_{(F)ij}(\tau;\mathbf{x},\mathbf{y})=O(1)$, which follows from (5.5)–(5.7) and (5.19)–(5.22). The Jacobian in (6.17) is $O(e^{-d})$, so that we end up, like above, with $\Sigma_{\gamma\in\Gamma}e^{-d}$, as series determining the convergence of (6.16) and (6.17). Hence, for geometrically finite covering groups, without parabolic and elliptic elements, and with $\delta<1$, the propagators on the hyperbolic manifold are obtained by periodizing the corresponding Green functions in the covering space. Clearly, the symmetry (6.3) and (6.4) also applies to $G^{\Gamma\pm}_{(F)\alpha\beta}(\tau;\mathbf{x},\mathbf{y})$, for $\gamma\in\Gamma$.

Finally we point out a method to obtain wave solutions on the multiply connected manifold, that does not make explicit use of the periodized Green functions. This is not only useful for $\delta\geqslant 1$, when the above series fail to converge, but also if $\delta<1$, because the series $\Sigma_{\gamma\in\Gamma}|\gamma'\xi|^{\alpha}$ is not known for its rapid convergence.[21] Wave fields satisfying the field Eqs. (2.1) on the multiply connected 4-manifold are obtained as

$$A^{\Gamma}_{\alpha}(\tau,\mathbf{x})=\int_{F\times R} G^{\Gamma}_{\alpha\alpha'}(\tau-\tau';\mathbf{x},\mathbf{x}')j^{\Gamma\alpha'}(\tau',\mathbf{x}')dV_{B^3}d\tau' \tag{6.18}$$

analogously to (2.26). The spatial integration is over a fundamental polyhedron F, and $G^{\Gamma}_{\alpha\alpha'}$ denotes a linear combination of the propagators $G^{\Gamma\pm}_{(F)\alpha\beta}$, with coefficients adding up to unity, so that $G^{\Gamma}_{\alpha\alpha'}$ solves (2.25). The current is periodic with respect to the covering group,

$$j^{\Gamma 0}(\tau,\gamma\mathbf{x})=j^{\Gamma 0}(\tau,\mathbf{x}),\ \ [\gamma'\mathbf{x}]^{-1ik}j^{\Gamma k}(\tau,\gamma\mathbf{x})=j^{\Gamma i}(\tau,\mathbf{x}), \tag{6.19}$$

and so is the resulting vector potential,

$$A^{\Gamma}_{0}(\tau,\gamma\mathbf{x})=A^{\Gamma}_{0}(\tau,\mathbf{x}),\ \ A^{\Gamma}_{k}(\tau,\gamma\mathbf{x})[\gamma'\mathbf{x}]_{ki}=A^{\Gamma}_{i}(\tau,\mathbf{x}), \tag{6.20}$$

as $G^{\Gamma}_{\alpha\alpha'}$ admits the symmetries stated in (6.3) and (6.4) for $\gamma\in\Gamma$. The current density $j^{\Gamma\alpha}(\tau,\mathbf{x})$ is usually obtained by periodizing a density $j^{\alpha}(\tau,\mathbf{x})$ in B^3 or H^3,

$$j^{\Gamma 0}(\tau,\mathbf{x})=\sum_{\gamma\in\Gamma} j^{0}(\tau,\gamma\mathbf{x}),\ \ j^{\Gamma i}(\tau,\mathbf{x})=\sum_{\gamma\in\Gamma}[\gamma'\mathbf{x}]^{-1ik}j^{k}(\tau,\gamma\mathbf{x}). \tag{6.21}$$

Alternatively to (6.18), we may periodize the wave field

$$A_{\alpha}(\tau,\mathbf{x})=\int_{B^3\times R} G_{\alpha\alpha'}(\tau-\tau';\mathbf{x},\mathbf{x}')j^{\alpha'}(\tau',\mathbf{x}')dV_{B^3}d\tau', \tag{6.22}$$

where $G_{\alpha\alpha'}$ is again a linear combination of the propagators $G^{\pm}_{(F)\alpha\beta}$ in the covering space, so that

$$A^{\Gamma}_{0}(\tau,\mathbf{x})=\sum_{\gamma\in\Gamma} A_0(\tau,\gamma\mathbf{x}),\quad A^{\Gamma}_{i}(\tau,\mathbf{x})=\sum_{\gamma\in\Gamma} A_k(\tau,\gamma\mathbf{x})[\gamma'\mathbf{x}]_{ki}\,. \tag{6.23}$$

This periodization is formally equivalent to (6.18), by way of (6.21), (6.16), and (6.17),

$$\sum_{\gamma\in\Gamma} A_0(\tau,\gamma\mathbf{x})=\sum_{\gamma\in\Gamma}\sum_{\beta\in\Gamma}\int_{F\times R} G_{00}(\tau-\tau';\beta^{-1}\gamma\mathbf{x},\mathbf{x}')j^{0}(\tau',\beta\mathbf{x}')dV_{B^3}(\mathbf{x}')d\tau', \tag{6.24}$$

$$\begin{aligned}\sum_{\gamma\in\Gamma} A_k(\tau,\gamma\mathbf{x})[\gamma'\mathbf{x}]_{ki}=&\sum_{\gamma\in\Gamma}\sum_{\beta\in\Gamma}\int_{F\times R} G_{ab}(\tau-\tau';\beta^{-1}\gamma\mathbf{x},\mathbf{x}')\\ &\times[\beta^{-1\prime}(\gamma\mathbf{x})]_{ak}[\gamma'\mathbf{x}]_{ki}[\beta^{-1\prime}(\beta\mathbf{x}')]_{bm}j^{m}(\tau',\beta\mathbf{x}')dV_{B^3}(\mathbf{x}')d\tau'.\end{aligned} \tag{6.25}$$

Here we at first used $B^3=\cup_{\beta\in\Gamma}\beta(F)$, and then the invariance of the hyperbolic volume element, $dV_{B^3}(\beta\mathbf{x})=dV_{B^3}(\mathbf{x})$, as well as the point-pair invariance (6.3) and (6.4). The first two Jacobians in (6.25) can be replaced by $[(\beta^{-1}\gamma)'\mathbf{x}']_{ai}$, and the third by $[\beta'\mathbf{x}']^{-1bm}$. (As for Jacobians in Poincaré series, we do not distinguish between sub- and superscripts and avoid mixed indices; the summation convention applies whenever two indices are equal.) Next we pull the $\gamma\in\Gamma$ summation under the integral sign. As this summation is over the whole group Γ, we may drop the β^{-1} in $G_{\alpha\beta}$ and in the Jacobian, and obtain in this way $G^{\Gamma}_{\alpha\alpha'}$. The periodized current $j^{\Gamma\alpha}$ is finally recovered by pulling the $\beta\in\Gamma$ summation under the integral sign. In (6.23), no explicit use is made of the Green functions (6.16) and (6.17) on the 4-manifold.

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APPENDIX A: ORTHOGONALITY, COMPLETENESS, AND THE RESOLVENT KERNEL FOR THE LONGITUDINAL TIME COMPONENT

We calculate the resolvent kernel (3.14), and the spectral measure for the time component of the eigenvectors (2.16). The results obtained in this appendix are not new, and a more detailed account on the spectral theory of the hyperbolic Laplace–Beltrami operator, without explicit use of distributions, can be found in Refs. 9 and 10. I include this appendix, because the scalar Green function happens to be the time component of the electromagnetic propagators, and the integral (A1) is also a prerequisite for the calculation of the spatial resolvent kernel in Appendix B.

The key convolution of H^3-spectral theory is

$$C_{\alpha,\beta}(z_1,t_1;z_2,t_2)=\int_{R^2}(|z_1-\xi|^2+t_1^2)^{-\alpha}(|z_2-\xi|^2+t_2^2)^{-\beta}d\xi, \tag{A1}$$

with $z_i\in R^2$, and $t_i>0$. The exponents are complex numbers, and the convergence properties of this integral will turn out in the course of the calculation. We shift the integration variable, and use a Feynman parametrization for both factors, $x^{-\gamma}=\Gamma^{-1}(\gamma)\int_0^\infty s^{\gamma-1}e^{-xs}ds$. Then the ξ-integration gets Gaussian, and we obtain

$$C_{\alpha,\beta}=\frac{\pi}{\Gamma(\alpha)\Gamma(\beta)}\int_0^\infty\int_0^\infty ds_1ds_2\frac{s_1^{\alpha-1}s_2^{\beta-1}}{s_1+s_2}\exp\left(-\frac{|z_1-z_2|^2s_1s_2}{s_1+s_2}-s_1t_1^2-s_2t_2^2\right). \tag{A2}$$

Next we perform the transformation $s_1=us$, $s_2=(1-u)s$, $0\leqslant s\leqslant\infty$, $0\leqslant u\leqslant 1$, with the Jacobian $s=s_1+s_2$. The s-integration is trivial, and we are left with

$$C_{\alpha,\beta}=\pi\Gamma(\alpha+\beta-1)\Gamma^{-1}(\alpha)\Gamma^{-1}(\beta)\int_0^1 duu^{\alpha-1}(1-u)^{\beta-1}(|z_1-z_2|^2u(1-u)+ut_1^2+(1-u)t_2^2)^{1-(\alpha+\beta)}. \tag{A3}$$

We may write, by means of the transformation $y=(t_1/t_2)u(1-u)^{-1}$,

$$\begin{aligned}C_{\alpha,\beta}t_1^\alpha t_2^\beta&=\int_{R^2}P^\alpha(z_1,t_1;\xi)P^\beta(z_2,t_2;\xi)d\xi\\&=\frac{\pi\Gamma(\alpha+\beta-1)}{\Gamma(\alpha)\Gamma(\beta)}t_2^{2-\alpha-\beta}\int_0^\infty\frac{dyy^{\alpha-1}(1+(t_2/t_1)y)^{\alpha+\beta-2}}{(1+2(1+2L)y+y^2)^{\alpha+\beta-1}},\end{aligned} \tag{A4}$$

with the H^3-Poisson kernel and the Selberg point-pair invariant,

$$P(z,t;\xi):=\frac{t}{|z-\xi|^2+t^2},\quad L(z_1,t_1;z_2,t_2):=\frac{|z_1-z_2|^2+(t_1-t_2)^2}{4t_1t_2}, \tag{A5}$$

respectively. We specify $\alpha+\beta=2$, and writing L for $L(z_1,t_1;z_2,t_2)$, we find

$$C_{\alpha,2-\alpha}t_1^\alpha t_2^{2-\alpha}=\frac{\pi}{4}\frac{1}{1-\alpha}\frac{\rho_+^{1-\alpha}-\rho_-^{1-\alpha}}{\sqrt{L(1+L)}}, \tag{A6}$$

with $\rho_\pm:=1+2L\pm2\sqrt{L(L+1)}$, cf. (3.7). Finally, we put $\alpha=1+is$, and obtain the kernel (3.14) as

$$k(s,d) := C_{1+is,1-is} t_1^{1+is} t_2^{1-is} = \pi \frac{\sin(sd)}{s \sinh(d)}, \tag{A7}$$

with the hyperbolic distance function $d = \log \rho_+(L)$.

The scalar orthogonality relation for the longitudinal time component in (2.16) can be derived from

$$\begin{aligned} \tilde{\delta}(\xi,\xi';\alpha,\beta;\varepsilon) &= \int_0^\infty dt C_{\alpha,\beta}(\xi,t;\xi',t) t^{\alpha+\beta-3+\varepsilon} \\ &= \frac{\pi}{2} \frac{\Gamma(\alpha+\beta-1)}{\Gamma(\alpha)\Gamma(\beta)} |\xi-\xi'|^{\varepsilon-\alpha-\beta} \\ &\quad \times B\left(\frac{\alpha-\beta+\varepsilon}{2}, \frac{\beta-\alpha+\varepsilon}{2}\right) B\left(\frac{\alpha+\beta-2+\varepsilon}{2}, \frac{\alpha+\beta-\varepsilon}{2}\right). \end{aligned} \tag{A8}$$

We used here the representation (A3) and interchanged integrations. We put $\alpha = 1+is$, $\beta = 1-it$, and write

$$\delta(\xi,\xi';s,t) := \tilde{\delta}(\xi,\xi';1+is,1-it;\varepsilon) = \frac{\pi}{s^2} |\xi-\xi'|^{\varepsilon-2+i(t-s)} \frac{i\varepsilon}{t-s+i\varepsilon}, \tag{A9}$$

where we have dropped higher orders in ε. $\delta(\xi,\xi';s,t)$ is a distribution concentrated at $\xi=\xi'$, $t=s$. Next we note two ε-representations of the Dirac δ-function, as well as two other well known formulas frequently used in this paper, cf. Ref. 25,

$$\delta(x) = \frac{1}{\pi} \frac{\varepsilon}{x^2+\varepsilon^2}, \quad \mp \pi i \delta(x) = \frac{1}{x \pm i\varepsilon} - P\frac{1}{x}, \quad \pm \pi i \theta(-x) = \log(x \pm i\varepsilon) - \log|x|,$$

$$\delta(d^2-\tau^2) = (2d)^{-1}(\delta(d-\tau) + \delta(d+\tau)). \tag{A10}$$

By integrating over a test function in $R^2 \times R^+$, and making use of the first formula in (A10), one can easily show that

$$\delta(\xi,\xi';s,t) = 2\pi^3 s^{-2} \delta(\xi-\xi') \delta(s-t). \tag{A11}$$

$\delta(\xi-\xi')$ is the Dirac function in R^2. The orthogonality relation for the time component of the vectors (2.16), which satisfy the homogeneous scalar Eq. (2.5), now follows from (A1), (A8), (A9), and (A11),

$$\int_{H^3} dV_{H^3} P^{1+is}(z,t;\xi) P^{1-it}(z,t;\xi') = 2\pi^3 s^{-2} \delta(\xi-\xi') \delta(s-t). \tag{A12}$$

The H^3-volume element is $dV_{H^3} = t^{-3} dt dz_1 dz_2$. Accordingly, we find the spectral measure

$$d\sigma(\xi,s) := (2\pi^3)^{-1} s^2 e^{-\varepsilon s} d\xi ds \tag{A13}$$

on $R^2 \times R^+$. A convergence factor $e^{-\varepsilon s}$ is included to obtain an ε-representation of the δ-function via the completeness relation; a principal value as regularization is likewise possible.[10] The eigenfunctions P^{1+is} satisfy $-\Delta_{H^3} P^{1+is} = (s^2+1) P^{1+is}$.

Once the spectral measure is found, one can write down the completeness relation,

$$\int_{R^2 \times R^+} d\sigma(\xi,s) P^{1+is}(z,t;\xi) P^{1-is}(z_0,t_0;\xi) = \delta_{H^3}(z,t;z_0,t_0), \tag{A14}$$

or, more explicitly,

$$\delta(L,\varepsilon):=(2\pi^3)^{-1}\int_0^\infty k(s,d(L))e^{-\varepsilon s}s^2ds=\frac{1}{2\pi^2}\,\frac{\log\rho_+}{\sqrt{L(1+L)}}\,\frac{\varepsilon}{(\log^2\rho_++\varepsilon^2)^2}. \tag{A15}$$

If we expand in $\sqrt{L}$ and drop terms vanishing for $\varepsilon\to 0$, we find an ε-representation of the δ-function in hyperbolic space,

$$\delta(L(z,t;z_0,t_0),\varepsilon)=\frac{1}{\pi^2}\,\frac{\varepsilon}{(\varepsilon^2+4L)^2}=\delta_{H^3}(z,t;z_0,t_0), \tag{A16}$$

with L as in (A5). This can easily be checked by integration with a test function, preferably in the B^3-model; $\delta_{B^3}(\mathbf{x};\mathbf{x}_0)$ is obtained by replacing in (A16) $L(z,t;z_0,t_0)$ by the B^3-invariant $L(\mathbf{x},\mathbf{x}_0)$ as defined in (3.5). We may of course assume $\mathbf{x}_0=0$, because L is invariant with respect to the symmetry group of B^3, which includes the transformations (3.4), and then use polar coordinates and a Taylor expansion of the test function $f(\mathbf{x})$ in $\int_{B^3}dV_{B^3}f(\mathbf{x})\delta_{B^3}(\mathbf{x};\mathbf{x}_0)=f(\mathbf{x}_0)$; the B^3-volume element is $dV_{B^3}=8(1-|\mathbf{x}|^2)^{-3}d^3\mathbf{x}$.

APPENDIX B: TRANSVERSAL AND LONGITUDINAL SPECTRAL MEASURES FOR THE SPATIAL COMPONENT OF THE PROCA EQUATION

To calculate the space component of the resolvent kernel, we need the spectral measure in the completeness relation for the eigenvectors $\mathbf{a}^{T_{1,2},L}$, cf. (2.18) and (2.19), which can be extracted from the orthogonality relation derived in this appendix. The basic integral in this relation was already calculated in (A8),

$$\int_{H^3}P^\alpha(z,t;\xi)P^\beta(z,t;\xi')dzt^\gamma dt=\frac{\pi}{2}\,\frac{|\xi-\xi'|^{3-\alpha-\beta+\gamma}}{\Gamma(\alpha)\Gamma(\beta)\Gamma(3+\gamma)}\Gamma\left(\frac{\alpha-\beta+\gamma+3}{2}\right)\Gamma\left(\frac{3-\alpha+\beta+\gamma}{2}\right)$$
$$\times\Gamma\left(\frac{\alpha+\beta+\gamma+1}{2}\right)\Gamma\left(\frac{\alpha+\beta-\gamma-3}{2}\right), \tag{B1}$$

with the Poisson kernel P as defined in (A5) and arbitrary complex numbers α, β, and γ. (At this point there is no need to discuss convergence, though this is not hard to do; H^3 means here of course $R^2\times R^+$.) The orthogonality relation can be derived by differentiating this formula with respect to $\xi:=(\xi_1,\xi_2)$ and $\xi':=(\xi_1',\xi_2')$. Defining $e:=\varepsilon+i(s'-s)$, we find in leading asymptotic order, for $s'\to s$ and $\varepsilon\to 0$,

$$\int_{H^3}P^{is}(z,t;\xi)P^{-is'}(z,t;\xi')dzt^{-1+\varepsilon}dt\sim\frac{2\pi s^2}{e\overline{e}(1+e/2)}|\xi-\xi'|^{2+e},$$

$$\int_{H^3}P^{1+is}P^{1-is'}dzt^{-1+\varepsilon}dt\sim-\frac{\pi}{e}|\xi-\xi'|^e,$$

$$\int_{H^3}P^{2+is}P^{2-is'}dzt^{-1+\varepsilon}dt\sim\frac{\pi}{2(s^2+1)}(1+\overline{e}/2)|\xi-\xi'|^{-2+e}, \tag{B2}$$

$$\int_{H^3}P^{2+is}P^{-is'}dzt^{-1+\varepsilon}dt=\int P^{is}P^{2-is'}dzt^{-1+\varepsilon}dt\sim-\frac{\pi}{e}|\xi-\xi'|^e,$$

which readily follows from (B1), by expanding the Γ-functions.

In the eigenvectors (2.18), we may replace the z-differentiations by ξ-differentiations, $\partial/\partial z_i\to-\partial/\partial\xi_i$. [Note that in this appendix $z=(z_1,z_2)$, whereas in Appendix A the z_i are themselves complex.] We define $D_{ij}:=\partial^2/\partial\xi_i^2-\partial^2/\partial\xi_j^2$, and analogously D'_{ij} for ξ', so that

$$
\begin{aligned}
&D_{12}D'_{12}|\xi-\xi'|^{2+e}=(e+2)e[4(e-1)|\xi-\xi'|^{e-2}+((\xi_1-\xi'_1)^2\\
&\quad-(\xi_2-\xi'_2)^2)^2(e-2)(e-4)|\xi-\xi'|^{e-6}],\\
&\frac{\partial^4}{\partial\xi_1\partial\xi_2\partial\xi'_1\partial\xi'_2}|\xi-\xi'|^{2+e}=(e+2)e((e-1)|\xi-\xi'|^{e-2}+(\xi_1-\xi'_1)^2\\
&\qquad\times(\xi_2-\xi'_2)^2(e-2)(e-4)|\xi-\xi'|^{e-6}),\\
&D_{12}|\xi-\xi'|^e=D'_{12}|\xi-\xi'|^e=e(e-2)((\xi_1-\xi'_1)^2-(\xi_2-\xi'_2)^2)|\xi-\xi'|^{e-4},\\
&\frac{\partial^2}{\partial\xi_1\partial\xi'_1}|\xi-\xi'|^e=-e|\xi-\xi'|^{e-2}-e(e-2)(\xi_1-\xi'_1)^2|\xi-\xi'|^{e-4}.
\end{aligned}
\tag{B3}
$$

We thus find, by combining (2.18), (B2), and (B3),

$$
\begin{aligned}
&\int_{H^3}\mathbf{a}^{T_1}(s,\xi)\cdot\overline{\mathbf{a}^{T_1}(s',\xi')}dzt^{-1+\varepsilon}dt\\
&\quad=\frac{1}{(1+is)(1-is')}\left(\frac{1}{16ss'}D_{12}P^{is}(\xi)D'_{12}P^{-is'}(\xi')+(1+is)\right.\\
&\qquad\times(1-is')P^{2+is}(\xi)P^{2-is'}(\xi')+\frac{1+is}{4is'}P^{2+is}(\xi)D'_{12}P^{-is'}(\xi')\\
&\qquad-\frac{1-is'}{4is}P^{2-is'}(\xi')D_{12}P^{is}(\xi)+\frac{1}{4ss'}\frac{\partial^2}{\partial\xi_1\partial\xi_2}P^{is}(\xi)\frac{\partial^2}{\partial\xi'_1\partial\xi'_2}P^{-is'}(\xi')\\
&\qquad\left.+\frac{\partial}{\partial\xi_1}P^{1+is}(\xi)\frac{\partial}{\partial\xi'_1}P^{1-is'}(\xi')\right)\\
&\quad=\frac{\pi}{(s^2+1)}\frac{\varepsilon}{\bar{e}}|\xi-\xi'|^{e-2}=\int\mathbf{a}^{T_2}\cdot\overline{\mathbf{a}^{T_2}}dzt^{-1+\varepsilon}dt.
\end{aligned}
\tag{B4}
$$

We dropped here the (z,t)-arguments in the eigenfunctions and Poisson kernels. The t^{-1}-factor in the integral derives from the hyperbolic metric $\gamma_{ij}=t^{-2}\delta_{ij}$, via $\gamma^{ij}a_ia_j\sqrt{\gamma}$, and the ε-regularization is used to obtain an ε-representation of the δ-functions in the orthogonality relation. In fact, by integrating over a test function, one can readily show that

$$
(\varepsilon/\bar{e})|\xi-\xi'|^{e-2}=2\pi^2\delta(\xi-\xi')\delta(s-s'),
\tag{B5}
$$

with $\bar{e}:=\varepsilon-i(s'-s)$. Similarly, for the longitudinal vectors in (2.18),

$$
\begin{aligned}
&\int_{H^3}\mathbf{a}^{L}(s,\xi)\cdot\overline{\mathbf{a}^{L}(s',\xi')}dzt^{-1+\varepsilon}dt\\
&\quad=\frac{1}{(1+is)(1-is')}\left(\frac{\partial}{\partial\xi_1}P^{1+is}(\xi)\frac{\partial}{\partial\xi'_1}P^{1-is'}(\xi')+\frac{\partial}{\partial\xi_2}P^{1+is}(\xi)\frac{\partial}{\partial\xi'_2}P^{1-is'}(\xi')\right)\\
&\qquad+\frac{1}{t^2}P^{1+is}(\xi)P^{1-is'}(\xi')+4P^{2+is}(\xi)P^{2-is'}(\xi')-\frac{2}{t}P^{1+is}(\xi)P^{2-is'}(\xi')\\
&\qquad-\frac{2}{t}P^{2+is}(\xi)P^{1-is'}(\xi')=\frac{\pi}{s^2}\frac{\varepsilon}{\bar{e}}|\xi-\xi'|^{e-2}.
\end{aligned}
\tag{B6}
$$

Here we used (B2), (B3), and in addition,

$$\int_{H^3} P^{1+is}P^{1-is'}dzt^{-3+\varepsilon}dt\sim\frac{\pi\varepsilon}{\overline{es}s'}|\xi-\xi'|^{e-2},$$

$$\int_{H^3} P^{1+is}P^{2-is'}dzt^{-2+\varepsilon}dt\sim\frac{\pi}{2}\frac{\varepsilon}{(1-is')is'}|\xi-\xi'|^{e-2}, \tag{B7}$$

$$\int_{H^3} P^{2+is}P^{1-is'}dzt^{-2+\varepsilon}dt\sim-\frac{\pi}{2}\frac{\varepsilon}{(1+is)is}|\xi-\xi'|^{e-2},$$

which follows from (B1) for $s'\to s$ and $\varepsilon\to 0$. Equations (B4) and (B6), with (B5) substituted, constitute the orthogonality relations for the vector fields (2.18), if complemented by $\mathbf{a}^{Ti}(z,t;\xi,s)\cdot\mathbf{a}^{L}(z,t;\xi',s')\equiv 0$. The orthogonality of the longitudinal and transversal subspaces can readily be checked via (2.17), or via (2.18) and (2.19) and the following identities for the Poisson kernel,

$$\frac{\partial^2 P^\alpha}{\partial z_1\partial z_2}=\frac{\alpha}{1+\alpha}\frac{1}{P^{2+\alpha}}\frac{\partial P^{1+\alpha}}{\partial z_1}\frac{\partial P^{1+\alpha}}{\partial z_2}, \tag{B8}$$

$$D_{ij}P^\alpha=\frac{\alpha}{1+\alpha}\frac{1}{P^{2+\alpha}}\left(\left(\frac{\partial P^{1+\alpha}}{\partial z_i}\right)^2-\left(\frac{\partial P^{1+\alpha}}{\partial z_j}\right)^2\right), \tag{B9}$$

$$\left(\frac{\partial P^{1+\alpha}}{\partial z_1}\right)^2+\left(\frac{\partial P^{1+\alpha}}{\partial z_2}\right)^2=4(1+\alpha)^2P^{4+2\alpha}\left(\frac{1}{tP}-1\right), \tag{B10}$$

$$\frac{\partial P^{1+\alpha}}{\partial t}\frac{\partial P^{1+\beta}}{\partial t}+\frac{\partial P^{1+\alpha}}{\partial z_i}\frac{\partial P^{1+\beta}}{\partial z_i}=(1+\alpha)(1+\beta)\frac{P^{2+\alpha+\beta}}{t^2}, \tag{B11}$$

$$-\Delta_{H^3}P^\alpha(z,t;\xi)=\alpha(2-\alpha)P^\alpha(z,t;\xi). \tag{B12}$$

α and β are complex constants; the Laplace–Beltrami operator Δ_{H^3} is defined in (2.5), and the D_{ij} are defined either with z_i-derivatives as in (2.18) or with ξ_i-derivatives as after (B2); summation over i is implied in (B11).

The spectral measures for the transversal and longitudinal components can be read off from (B4)–(B6),

$$d\sigma^T(\xi,s):=\frac{s^2+1}{2\pi^3}e^{-\varepsilon s}d\xi ds,\quad d\sigma^L(\xi,s):=\frac{s^2}{2\pi^3}e^{-\varepsilon s}d\xi ds, \tag{B13}$$

the domain of integration is $R^2\times R^+$. As in (A13), we have included a convergence factor $e^{-\varepsilon s}$ needed in the completeness relation,

$$\int_{R^2\times R^+}\sum_{k=1,2}\mathbf{a}_i^{T_k}(z,t;\xi,s)\overline{\mathbf{a}_j^{T_k}(z',t';\xi,s)}d\sigma^T(\xi,s)$$
$$+\int_{R^2\times R^+}\mathbf{a}_i^{L}(z,t;\xi,s)\overline{\mathbf{a}_j^{L}(z',t';\xi,s)}d\sigma^L(\xi,s)=\gamma_{ij}\delta_{H^3}(z,t;z',t'), \tag{B14}$$

where δ_{H^3} denotes the δ-function in H^3, as defined in (A16). A check of this relation, by explicit calculation of the integrals, is given at the end of Sec. IV.

APPENDIX C: MATRIX ELEMENTS APPEARING IN THE SPATIAL RESOLVENT KERNEL

We will calculate the matrix elements (4.4), that is $C_{ij}^{T_k}:=\int_{R^2}\mathbf{a}_i^{T_k}\overline{\mathbf{a}_j^{T_k}}d\xi$, $C_{ij}^{T}:=C_{ij}^{T_1}+C_{ij}^{T_2}$, and $C_{ij}^{L}:=\int_{R^2}\mathbf{a}_i^{L}\overline{\mathbf{a}_j^{L}}d\xi$, with eigenfunctions as defined in (2.18) and (2.19), at $z=z'=0$. We consider, at first for arbitrary z and z', cf. (A4),

$$K(a,b;L;t,t'):=\int_{R^2}P^a(z,t;\xi)P^b(z',t';\xi)d\xi$$
$$=\frac{\pi\Gamma(a+b-1)}{\Gamma(a)\Gamma(b)}t'^{2-a-b}\int_0^\infty\frac{dyy^{a-1}(1+(t'/t)y)^{a+b-2}}{(1+2(1+2L)y+y^2)^{a+b-1}},\tag{C1}$$

with the H^3-point-pair invariant $L(z,t;z',t')$ as in (3.11), and define

$$K(a,b):=K(a,b;L;t,t')\big|_{z=z'=0},\quad K'(a,b):=\partial K(a,b;L;t,t')/\partial L\big|_{z=z'=0},\tag{C2}$$

and analogously $K''(a,b)$, where a and b are arbitrary complex numbers, so that the integrals converge. It is understood that the L-differentiation is carried out before the y-integration in (C1), to take care of the poles of $\Gamma(a+b-1)$. In the following, we put $\beta:=t'/t$, so that, at $z=z'=0$, $1+2(1+2L)y+y^2=(1+\beta y)(1+\beta^{-1}y)$. We also introduce the shortcuts $L_{,i}=\partial L/\partial z_i\big|_{z=z'=0}$ and $L_{,i'}=\partial L/\partial z_i'\big|_{z=z'=0}$, with $z=:(z_1,z_2)$ and $z'=:(z_1',z_2')$, and analogously for higher order derivatives. Evidently, $z_{1,2}$-derivatives of $K(a,b;L;t,t')$ at $z=z'=0$ are obtained via $\partial K/\partial z_i=:K_{,i}=K'(a,b)L_{,i}$, etc. We will only use $z_{1,2}$ and $z_{1,2}'$-derivatives, always at $z=z'=0$; t and t'-derivatives are not needed in the following. The only nonvanishing derivatives of L are $L_{,i,j}=(2tt')^{-1}\delta_{ij}$, $L_{,i,j'}=-(2tt')^{-1}\delta_{ij'}$, and $L_{,i',j'}=(2tt')^{-1}\delta_{i'j'}$. Accordingly, the only nonvanishing $z_{1,2}$-derivatives of $K(a,b;L;t,t')$ at $z=z'=0$ are, up to the fourth order

$$K_{,1,1}(a,b)=K_{,2,2}=(2tt')^{-1}K'(a,b),$$
$$K_{,1,1,2,2}=(2tt')^{-2}K''(a,b),\quad K_{,1,1,1,1}=K_{,2,2,2,2}=3K_{,1,1,2,2}.\tag{C3}$$

The indicated indices may of course be permuted. An index may also be replaced by the same primed index; in this case a minus sign has to be added on the right-hand side, e.g., $K_{,1,1',2,2}=-K_{,1,1,2,2}$, $K_{,1,1',2',2}=K_{,1,1,2,2}$, etc., since $\partial/\partial z_i=-\partial/\partial z_i'$ when applied to L.

With these preparations, the matrix elements (4.4) can be readily calculated. We use the representation (2.18), (2.19) for the eigenfunctions, interchange differentiations, and integrations, and do some bookkeeping by means of (C1)–(C3). In this way we find the nonvanishing matrix elements as

$$C_{11}^{T_1}=\frac{1}{16s^2(s^2+1)}\frac{K''(0,0)}{t^2t'^2}+K(2,2),$$
$$C_{22}^{T_1}=\frac{1}{16s^2(s^2+1)}\frac{K''(0,0)}{t^2t'^2},\quad C_{33}^{T_1}=\frac{-1}{2(s^2+1)}\frac{K'(1,1)}{tt'},$$
$$C_{11}^{T_2}=C_{22}^{T_1},\quad C_{22}^{T_2}=C_{11}^{T_1},\quad C_{11}^{L}=C_{22}^{L}=C_{33}^{T_2}=C_{33}^{T_1},\tag{C4}$$
$$C_{33}^{L}=\frac{K(1,1)}{tt'}+4K(2,2)-2\frac{K(1,2)}{t}-2\frac{K(2,1)}{t'}.$$

Next we define

$$\kappa(l,m,n;s):=\int_0^\infty\frac{dyy^{l+is}}{(1+\beta y)^m(1+\beta^{-1}y)^n},\tag{C5}$$

with $\beta:=t'/t$, so that

$$K(1,1)=\pi\frac{\kappa(0,1,1;s)}{\Gamma(1+is)\Gamma(1-is)},\quad K(1,2)=\frac{1}{t'}\frac{\pi\kappa(0,1,2;s)}{\Gamma(1+is)\Gamma(2-is)},$$

$$K(2,1)=\frac{1}{t'}\frac{\pi\kappa(1,1,2;s)}{\Gamma(2+is)\Gamma(1-is)},\quad K(2,2)=\frac{1}{t'^2}\frac{2\pi\kappa(1,1,3;s)}{\Gamma(2+is)\Gamma(2-is)},\tag{C6}$$

$$K'(1,1)=\frac{-4\pi\kappa(1,2,2;s)}{\Gamma(1+is)\Gamma(1-is)},\quad K''(0,0)=t'^2\frac{16\pi\kappa(1,3,1;s)}{\Gamma(is)\Gamma(-is)}.$$

As a consistency check, we note the symmetry

$$K(2,2;\beta\to\beta^{-1})=\frac{K''(0,0;\beta)}{8t'^4s^2(s^2+1)}.$$

The integrals (C6) are elementary,

$$K(1,1)=\frac{\pi}{is}\frac{\beta}{\beta^2-1}(\beta^{is}-\beta^{-is}),$$

$$K(1,2)=\frac{\pi}{is(1-is)}\frac{\beta}{(\beta^2-1)^2}\frac{1}{t'}(\beta^{2+is}-\beta^{2-is}-is\beta^{is}(\beta^2-1)),$$

$$K(2,1)=-\frac{\pi}{is(1+is)}\frac{\beta^2}{(\beta^2-1)^2}\frac{1}{t'}(\beta^{is}-\beta^{-is}-is\beta^{is}(\beta^2-1)),$$

$$K(2,2)=-\frac{2\pi}{(s^2+1)}\frac{\beta^4}{(\beta^2-1)^3}\frac{1}{t'^2}\frac{\beta^{is}-\beta^{-is}}{is}+\frac{\pi}{(s^2+1)}\frac{\beta^{2+is}}{(\beta^2-1)^2}\frac{1}{t'^2}((\beta^2+1)-is(\beta^2-1)),\tag{C7}$$

$$K'(1,1)=-4\pi\frac{\beta^2(\beta^2+1)}{(\beta^2-1)^3}\frac{\beta^{is}-\beta^{-is}}{is}+\frac{4\pi\beta^2}{(\beta^2-1)^2}(\beta^{is}+\beta^{-is}),$$

$$K''(0,0)=\frac{16\pi\beta^2}{(\beta^2-1)^3}t'^2is(\beta^{is}-\beta^{-is})+\frac{8\pi s^2\beta^{-is}}{(\beta^2-1)^2}t'^2((\beta^2+1)+is(\beta^2-1)).$$

Collecting terms, we obtain the nonvanishing matrix elements $C_{ij}^{T,L}$ in (4.4) as

$$C_{11}^T=C_{22}^T=\frac{\pi\beta}{(\beta^2-1)^3(s^2+1)}\frac{1}{tt'}$$
$$\times\left(-4\beta^2\frac{\beta^{is}-\beta^{-is}}{is}+(\beta^4-1)(\beta^{is}+\beta^{-is})-(\beta^2-1)^2is(\beta^{is}-\beta^{-is})\right),$$

$$C_{33}^T=C_{11}^L=C_{22}^L=\frac{2\pi\beta^2}{(\beta^2-1)^3(s^2+1)}\frac{1}{tt'}\left((\beta^2+1)\frac{\beta^{is}-\beta^{-is}}{is}-(\beta^2-1)(\beta^{is}+\beta^{-is})\right),\tag{C8}$$

$$C_{33}^L=\frac{\pi\beta}{(\beta^2-1)^3(s^2+1)}\frac{1}{tt'}$$
$$\times\left(-(\beta^4+6\beta^2+1)\frac{\beta^{is}-\beta^{-is}}{is}-(\beta^2-1)^2is(\beta^{is}-\beta^{-is})+2(\beta^4-1)(\beta^{is}+\beta^{-is})\right).$$

What remains is to substitute (C8) into the resolvent kernel (4.1) and (4.2), and to perform the *s*-integrations, which are likewise elementary, cf. (4.5)–(4.11).

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Combinatorial identities for binary necklaces from exact ray-splitting trace formulas

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Based on an exact trace formula for a one-dimensional ray-splitting system, we derive novel combinatorial identities for cyclic binary sequences (Pólya necklaces).
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I. INTRODUCTION

Wave propagation in systems with sharp interfaces is a fundamental problem in the natural sciences and engineering. Well-known examples include light waves impinging on a water–air interface or sound waves propagating in layered media.[1] All these systems have one feature in common: The splitting of the incident wave into reflected and transmitted components. In the geometrical optics limit of small wave lengths, incident, reflected, and transmitted waves are described by rays. The rays are split at the interface; hence the name ''ray-splitting systems'' [2] for the whole class of wave systems with sharp interfaces. Ray-splitting systems have recently attracted attention in the context of acoustic, quantum, and electromagnetic wave chaos.[2–10] It was shown that the mere presence of a ray-splitting boundary can drive an otherwise regular system into chaos.[2–4] It was also shown that ray-splitting systems produce corrections to the Weyl formula[11,12] for the average density of states that can be computed analytically.[5,6] The most conspicuous consequence of ray splitting is the existence of non-Newtonian periodic orbits in a ray-splitting system that contribute substantially to the fluctuating part of the level density.[3,4,7–9] The existence of non-Newtonian orbits in a dielectric-loaded Bunimovich ray-splitting stadium was demonstrated experimentally.[7–9] In addition it has been shown recently that exact trace formulas exist for a class of one-dimensional ray-splitting systems.[9,10] These formulas were derived using results from quantum graph theory.[13,14] Considering the two-point correlation function of the spectra of special quantum graphs, Schanz and Smilansky were able to derive novel combinatorial identities.[15] This was possible by deriving the two-point correlation function in two independent ways, (i) directly using input from the quantum spectrum and (ii) using the exactness of the trace formula. Motivated by the methods of Kottos, Schanz, and Smilansky[13–15] we show that novel combinatorial identities for binary Pólya necklaces[16,17] are obtained directly by comparing the spectral density of analytically solvable quantum graphs with their exact periodic orbit expansion.

The plan of this paper is as follows: In Sec. II we present our model system, a one-dimensional ray-splitting system, whose spectrum can be obtained analytically. We present an exact periodic-orbit expansion of its level density expressed as a generalized Fourier sum over binary Pólya necklaces. In Sec. III we outline our method for obtaining exact combinatorial identities for binary necklaces derived from analytically solvable cases of the one-dimensional ray-splitting system. In Sec. IV we present two worked examples that yield two infinite sets of combinatorial identities. In Sec. V we discuss our results and conclude the paper.

II. SPECTRUM

Denote by E_n the spectrum of the one-dimensional scaled Schrödinger equation

$$-\psi''(x)+V_\lambda(E,x)\psi(x)=E\psi(x), \tag{1}$$

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where

$$V_\lambda(E,x)=\begin{cases}0, & \text{for } 0<x\leqslant a\\ \lambda E, & \text{for } a<x<1,\\ \infty, & \text{for } x\notin(0,1)\end{cases} \tag{2}$$

and $\psi(x)\equiv 0$ for $x\notin(0,1)$. Scaling potentials of the form (2) arise naturally in many ray-splitting systems, for instance in dielectric-loaded cavities.[5,7–9] In this paper we concentrate on the case $E>V_\lambda(E,x)$ for all x. Then, without restriction of generality, the scaling constant λ can be assumed to satisfy $0\leqslant\lambda<1$. Define $E=k^2$, then the spectrum of (1) is determined by

$$\sin[k(\sigma_L+\sigma_R)]-r\sin[k(\sigma_L-\sigma_R)]=0, \tag{3}$$

where $\sigma_L=a$, $\sigma_R=\eta(1-a)$, $\eta=\sqrt{1-\lambda}$, and $r=(1-\eta)/(1+\eta)$ is the reflection coefficient. For the derivations below it is useful to define the transmission coefficient $t=\sqrt{1-r^2}$. Therefore, the reflection and transmission coefficients satisfy the relation

$$r^2+t^2=1. \tag{4}$$

Since in this paper we focus on the case $0\leqslant\lambda<1$, both r and t are real and positive and range between 0 and 1. Possible quantum phases incurred at reflection or transmission events are treated explicitly and separately [see, e.g., (6) below]. They are not included in r or t.

We now discuss an alternative method of solving the quantum dynamics in the potential (2). This method is based on coding the periodic orbits with the help of symbol strings. We denote a bounce off $x=0$ by the letter $\mathcal{L}$ and a bounce off $x=1$ by the letter $\mathcal{R}$. Words formed with these two letters code for periodic orbits in (2). The word $\mathcal{L}$, for instance, codes for the non-Newtonian orbit that bounces between $x=0$ and $x=a$ (above-barrier reflection orbit). The word $\mathcal{LR}$ codes for the (Newtonian) orbit that bounces between $x=0$ and $x=1$. Since a periodic orbit represented by the word w cycles through the letters of w without a well-defined beginning or end, two words w and w' are equivalent in our context, and code for the same periodic orbit, if they are of the same length (i.e., they consist of the same number of symbols) and their respective symbol sequences are identical up to cyclic permutations. Sequences of objects that are identical up to cyclic permutations are called (Pólya) necklaces.[16,17] If the number of objects they consist of is two, they are called binary necklaces. Apparently, therefore, the periodic orbits of (2) can be coded with the help of binary necklaces over the symbols $\mathcal{L}$ and $\mathcal{R}$. It is remarkable that for (2) every Newtonian or non-Newtonian periodic orbit can be mapped one-to-one onto a binary necklace. In other words, "pruning" is not necessary for the binary necklaces relevant for (2). Every binary necklace defines a possible periodic orbit of (2) and vice versa.

Given two letters, for instance $\mathcal{L}$ and $\mathcal{R}$, we can form 2^ℓ words of length ℓ. But, in general, many of these words will be cyclically equivalent, and correspond to the same necklace. So, how many necklaces of length ℓ are there? This question is answered by the following formula. There are exactly[17]

$$N(\ell)=\frac{1}{\ell}\sum_{n|\ell}\phi(n)2^{\ell/n}, \tag{5}$$

binary necklaces of length ℓ, where the symbol "$n|\ell$" denotes "n is a divisor of ℓ," and $\phi(n)$ is Euler's totient function defined as the number of positive integers smaller than n and relatively prime to n with $\phi(1)=1$ as a useful convention. Thus the first four totients are given by $\phi(1)=1$, $\phi(2)=1$, $\phi(3)=2$, and $\phi(4)=2$. We illustrate (5) with two examples for $\ell=1$ and $\ell=2$. There are two necklaces for $\ell=1$, $\mathcal{L}$ and $\mathcal{R}$. Applying (5) to this problem, we verify $N(1)=\phi(1)\times 2=2$. There are three necklaces of length 2, $\mathcal{LL}$, $\mathcal{LR}$, and $\mathcal{RR}$; again verified by (5), $N(2)=[\phi(1)\times 4+\phi(2)\times 2]/2=3$.

Given a binary necklace w, we define the following integer-valued functions on w: $n_{\mathcal{R}}(w)$ counts the number of $\mathcal{R}$s in w, $n_{\mathcal{L}}(w)$ counts the number of $\mathcal{L}$s, $n(w)=n_{\mathcal{L}}(w)+n_{\mathcal{R}}(w)$, $\chi(w)$ is the sum of $n(w)$ and the number of $\mathcal{R}$-pairs in w, $\alpha(w)$ counts all occurrences of $\mathcal{R}$-pairs or $\mathcal{L}$-pairs, $\beta(w)$ counts all occurrences of $\mathcal{RL}$ or $\mathcal{LR}$ and $\gamma(w)$ is defined as $\gamma(w)=2n_{\mathcal{L}}(w)+n_{\mathcal{R}}(w)$. Note that the counting of $\mathcal{R}$-pairs, $\mathcal{L}$-pairs, $\mathcal{LR}$- or $\mathcal{RL}$-combinations is to be understood cyclically, i.e., for example, $\alpha(\mathcal{R})=1$ and $\beta(\mathcal{LR})=2$. Next we define the set W_p of prime necklaces as the ones that cannot be written as a periodic concatenation of substrings. As shown recently,[10] there exists an exact periodic orbit expansion for the spectral density of (1) in terms of prime binary necklaces

$$\rho(k)=\overline{\rho}+\frac{1}{2\pi}\sum_{w\in W_p} S_w \sum_{\substack{\nu=-\infty \\ \nu\neq 0}}^{\infty} [(-1)^{\chi(w)} r^{\alpha(w)} t^{\beta(w)}]^{|\nu|} e^{i\nu S_w k}, \quad k>0, \tag{6}$$

where

$$S_w=2[n_{\mathcal{R}}(w)\sigma_R+n_{\mathcal{L}}(w)\sigma_L], \tag{7}$$

is the action of the primitive periodic orbit coded by the prime binary necklace w and $\overline{\rho}=(\sigma_L+\sigma_R)/\pi$ is the average level density.

III. METHOD

For special values of the parameters of the potential well (2) it is possible to solve (3) analytically, thus obtaining directly the density of states $\rho(k)$. Equating the explicit expression for $\rho(k)$ with the necklace expansion (6), one obtains combinatorial identities for binary necklaces. An illustrative example is the case $a=1$, for which the spectral density of (1) is given by

$$\rho(k)=\sum_{m=-\infty}^{\infty}\delta(k-\pi m). \tag{8}$$

In this case there exists only one primitive necklace, $\mathcal{LR}$, and the necklace expansion of (6) yields

$$\rho(k)=\frac{1}{\pi}\sum_{\nu=-\infty}^{\infty} e^{2i\nu k}. \tag{9}$$

Equating (8) and (9) yields the well-known Poisson formula.

A comment is in order here. For every finite a the necklace expansion (6) involves an infinite sum over prime periodic necklaces. At $a=1$ this sum collapses to a single term. One may ask the question how this singular limit arises. The answer is the following. For every finite a the actions of the right-hand lobes of the periodic orbits of (6) is finite. At $a=1$, these actions are zero. Consequently, all necklaces that represent *different* prime periodic orbits for $a\neq 1$ become *repetitions* of the Newtonian periodic orbit $\mathcal{LR}$ at $a=1$. This is the reason for the existence of only a single prime periodic orbit ($\mathcal{LR}$) at $a=1$.

Apart from trivial and well-known identities such as (8) and (9) above, (6) is a rich source of new and nontrivial combinatorial identities for binary necklaces. Specific examples are discussed in Sec. III. Here we outline the general method.

Equation (3) can be written as

$$\sin(\omega_1 k)-r\sin(\omega_2 k)=0, \tag{10}$$

where $\omega_1=\sigma_L+\sigma_R$ and $\omega_2=\sigma_L-\sigma_R$. A negative ω_2 corresponds to a mirror reflection of $V_\lambda(E,x)$ with respect to $x=1/2$. Thus, because of $\sigma_L,\sigma_R\geqslant 0$, and without loss of generality, we may assume $\omega_1\geqslant\omega_2\geqslant 0$.

In case ω_1 and ω_2 are rationally related, i.e., $\omega_1/\omega_2=p/q$, $p\geqslant q\in\mathbf{N}$ and p,q relatively prime, (10) is reduced to the algebraic equation

$$\sin(p\omega k)-r\sin(q\omega k)=0, \tag{11}$$

where $\omega_1=p\omega$ and $\omega_2=q\omega$. Using the formula

$$\sin(nx)=\sin(x)U_{n-1}(\cos(x)), \tag{12}$$

where $U_{n-1}(x)$ is the Chebyshev polynomial of the second kind, one obtains

$$\sin(\omega k)[U_{p-1}(\cos\omega k)-rU_{q-1}(\cos\omega k)]=0. \tag{13}$$

It follows immediately from (13) that in the case of rationally related ω_1 and ω_2 there always exists a sequence of roots $k_n^{(0)}=\pi n/\omega$. The remaining roots are determined by

$$U_{p-1}(x)-rU_{q-1}(x)=0, \tag{14}$$

where $x=\cos(\omega k)$. Since every root x_j of (14) gives rise to a periodic sequence of eigenvalues, $\cos(\omega k_n^{(j)})=x_j$, $j=1,2,\ldots,p-1$, together with the sequence $k_n^{(0)}$ the spectrum of (10) consists of p (possibly degenerate) periodic sequences of roots. Whenever (14) can be solved analytically, the density of states

$$\rho(k)=\sum_{j=0}^{p-1}\sum_{n=-\infty}^{\infty}\delta(k-k_n^{(j)}), \tag{15}$$

is known explicitly and together with (6) leads to a host of combinatorial identities for binary necklaces. Two examples are presented in the following section.

IV. COMBINATORIAL IDENTITIES

Example 1: For $\sigma_L=\sigma_R$ equation (3) becomes

$$\sin(2ka)=0, \tag{16}$$

with the solutions $k_n=\pi n/(2a)$. Note that there is no r-dependence in (16). The density of states is given by

$$\rho(k)=\sum_{n=-\infty}^{\infty}\delta\left(k-\frac{\pi n}{2a}\right)=\frac{2a}{\pi}\sum_{m=-\infty}^{\infty}e^{4imak}. \tag{17}$$

According to (7) and due to $\sigma_L=\sigma_R$, S_w depends only on the binary length of w and is given by $S_w=2an(w)$. Thus the sum (6) can be written as

$$\rho(k)=\frac{2a}{\pi}+\frac{a}{\pi}\sum_{\substack{m=-\infty\\ m\neq 0}}^{\infty}\sum_{w\cdot\nu\in W_{|m|}}n(w)[(-1)^{\chi(w)}r^{\alpha(w)}t^{\beta(w)}]^{\nu}e^{2imka}, \tag{18}$$

where W_n denotes the set of all length-n binary necklaces w, w is the shortest primitive code-piece *in* w and ν is the number of its repetitions in w. Comparing the series (17) and (18), we see that odd-length and even-length binary necklaces satisfy the sum rules

$$\sum_{w\cdot\nu\in W_{2m-1}}n(w)[(-1)^{\chi(w)}r^{\alpha(w)}t^{\beta(w)}]^{\nu}=0,\quad m=1,2,\ldots \tag{19}$$

and

TABLE I. List of the three cyclically nonequivalent binary necklaces of length 2 together with their primitives (w) and repetition indices (ν). Some properties of the primitives, such as their lengths (n), number of $\mathcal{R}$ or $\mathcal{L}$ pairs (α), number of transmissions (β), their weighted lengths (γ) and their phases (χ) are also listed.

j	w_j	w_j	ν_j	$n(w_j)$	$\alpha(w_j)$	$\beta(w_j)$	$\gamma(w_j)$	$\chi(w_j)$
1	$\mathcal{LL}$	$\mathcal{L}$	2	1	1	0	2	1
2	$\mathcal{LR}$	$\mathcal{LR}$	1	2	0	2	3	2
3	$\mathcal{RR}$	$\mathcal{R}$	2	1	1	0	1	2

$$\frac{1}{2}\sum_{w\cdot\nu\in W_{2m}} n(w)[(-1)^{\chi(w)}r^{\alpha(w)}t^{\beta(w)}]^{\nu}=1,\quad m=1,2,\ldots\ . \tag{20}$$

At first glance it may seem surprising that (20) is a constant for all r. The solution lies in the relation (4). When properly ordered according to powers of r and t, it turns out that (i) individual terms in (20) are of the form $r^{2p}t^{2q}$, where $p+q=m$ and (ii) the coefficients in front of the term $r^{2p}t^{2q}$ in (20) turn out to be binomial coefficients. Thus, for given m, the left-hand side of (20) reduces to $(r^2+t^2)^m$, which, according to (4) is equal to 1 for any choice of r. This explains why the seemingly variable left-hand side of (20) is nevertheless a constant. Thus we obtain from (20) the following infinite set of combinatorial identities for even-length binary necklaces:

$$\frac{1}{2}\sum_{w\cdot\nu\in W_{2m}} n(w)(-1)^{\nu\cdot\chi(w)}\delta_{\nu\cdot\alpha(w)/2,s}=\binom{m}{s},\quad s=0,\ldots,m,\quad m=1,2,\ldots, \tag{21}$$

where $\delta_{i,j}$ is the Kronecker symbol.

In order to illustrate (21) let us first focus on the case $m=1$. According to (5) there are exactly three cyclically nonequivalent necklaces of binary length 2 given by $\mathrm{w}_1=\mathcal{LL}$, $\mathrm{w}_2=\mathcal{LR}$, $\mathrm{w}_3=\mathcal{RR}$. The necklaces w_1 and w_3 are not primitive. The necklace w_1 is a twofold repetition of the primitive necklace $w_1=\mathcal{L}$. Thus $\nu_1=2$. An analogous consideration for w_3 yields $w_3=\mathcal{R}$ and $\nu_3=2$. The necklace w_2 is primitive. Therefore, $w_2=\mathrm{w}_2=\mathcal{LR}$ and $\nu_2=1$. The three necklaces w_j, $j=1,2,3$, are listed in Table I. Also listed are their primitives w_j, the repetition indices ν_j, and the values of the functions $n(w_j)$, $\alpha(w_j)$, $\beta(w_j)$, $\gamma(w_j)$, and $\chi(w_j)$.

We are now ready to check (21). For $m=1$ we have two choices for s: $s=0$ and $s=1$. For $s=0$ we have to scan the three words w_j, $j=1,2,3$, for $\nu_j\alpha(w_j)/2=s=0$. According to the entries in Table I, only w_2 qualifies and the sum on the left-hand side of (21) reduces to the single term

$$\frac{1}{2}n(w_2)(-1)^{\nu_2\chi(w_2)}=1=\binom{1}{0}. \tag{22}$$

This shows that (21) is indeed true for the simplest case $m=1$, $s=0$. For the case $m=1$, $s=1$ we have to check Table I for occurrences with $\nu_j\alpha(w_j)/2=1$. This is fulfilled for the necklaces w_1 and w_3. We obtain

$$\frac{1}{2}[n(w_1)(-1)^{\nu_1\chi(w_1)}+n(w_3)(-1)^{\nu_3\chi(w_3)}]=1=\binom{1}{1}. \tag{23}$$

This shows that (21) also works for $m=1$, $s=1$.

Testing (21) for $m=2$ involves finding all nonequivalent necklaces of binary length 4. According to (5) there are exactly six. All six necklaces are listed in Table II together with their properties. For $m=2$ we have three possibilities for s: $s=0,1,2$. For $s=0$ we have to check Table II for necklaces that fulfill $\nu_j\alpha(w_j)/2=0$. Only w_4 qualifies. We obtain $n(w_4)/2=1$, which equals $\binom{2}{0}$, the binomial coefficient on the right-hand side of (21). For $s=1$ we have to check for $\nu_j\alpha(w_j)/2=1$. We find three candidates: w_2, w_3, and w_5. This time we have to be careful when summing the three terms on the left-hand side of (21), since $\nu_3\chi(w_3)=5$. Therefore, the second

TABLE II. List of the six cyclically nonequivalent binary necklaces of length 4. The meaning of the columns is the same as in Table I.

j	w_j	w_j	ν_j	$n(w_j)$	$\alpha(w_j)$	$\beta(w_j)$	$\gamma(w_j)$	$\chi(w_j)$
1	$\mathcal{LLLL}$	$\mathcal{L}$	4	1	1	0	2	1
2	$\mathcal{LLLR}$	$\mathcal{LLLR}$	1	4	2	2	7	4
3	$\mathcal{LLRR}$	$\mathcal{LLRR}$	1	4	2	2	6	5
4	$\mathcal{LRLR}$	$\mathcal{LR}$	2	2	0	2	3	2
5	$\mathcal{LRRR}$	$\mathcal{LRRR}$	1	4	2	2	5	6
6	$\mathcal{RRRR}$	$\mathcal{R}$	4	1	1	0	1	2

term in (21) contributes with a minus sign. We obtain $[n(w_2)-n(w_3)+n(w_5)]/2=2$, which equals $\binom{2}{1}$, the corresponding binomial coefficient on the right-hand side of (21). Two necklaces, w_1 and w_6, contribute in the case $s=2$ and again satisfy (21).

Example 2: Suppose now that $\sigma_L=2\sigma_R$. In this case (3) becomes

$$\sin(ka/2)[4\cos^2(ka/2)-r-1]=0. \tag{24}$$

This equation has three sets of solutions

$$k_n^{(j)}=\frac{2j}{a}\arccos(\varphi)+\frac{2\pi n}{a},\quad j=-1,0,1, \tag{25}$$

where $\varphi=\sqrt{1+r}/2$. The density of states is

$$\begin{aligned}\rho(k)&=\sum_{j=-1}^{1}\sum_{m=-\infty}^{\infty}\delta\left(k+\frac{2j}{a}\arccos(\varphi)-\frac{2\pi m}{a}\right)\\&=\frac{a}{2\pi}\sum_{j=-1}^{1}\sum_{n=-\infty}^{\infty}e^{in[ak+2j\,\arccos(\varphi)]}\\&=\frac{a}{2\pi}\sum_{n=-\infty}^{\infty}e^{inak}[2T_{2n}(\varphi)+1],\end{aligned} \tag{26}$$

where $T_n(x)\equiv\cos(n\arccos x)$ are the Chebyshev polynomials of the first kind.[18] Equating (26) order-by-order with the necklace expansion (6) we obtain the sum rules

$$\begin{aligned}&\sum_{w\in W_p}\sum_{\nu=1}^{\infty}\gamma(w)[(-1)^{\chi(w)}r^{\alpha(w)}(1-r^2)^{\beta(w)/2}]^{\nu}\delta_{\nu\gamma(w),m}\\&\quad=1+\sum_{j=0}^{m}\frac{2m(-1)^j}{2m-j}\binom{2m-j}{j}(1+r)^{m-j},\quad m=1,2,\ldots\ .\end{aligned} \tag{27}$$

We used formula 22:6:1 of Ref. 18 for the Chebyshev polynomials in (26).

Ordering (27) according to powers of r, (27) can be reformulated as a combinatorial theorem on the set of binary necklaces, in which $\mathcal{L}$ beads weigh twice as much as $\mathcal{R}$ beads:

$$\begin{aligned}&\sum_{w\in W_p,C}\gamma(w)(-1)^{[2m\chi(w)+s\gamma(w)-m\alpha(w)]/[2\gamma(w)]}\binom{\dfrac{m\beta(w)}{2\gamma(w)}}{\dfrac{s\gamma(w)-m\alpha(w)}{2\gamma(w)}}\\&\quad=\delta_{s,0}+\sum_{j=0}^{m-s}\frac{2m(-1)^j}{2m-j}\binom{2m-j}{j}\binom{m-j}{s},\quad s=0,1,\ldots m,\quad m=1,2,\ldots\ .\end{aligned} \tag{28}$$

The condition C in the sum (28) is $C=\gamma(w)\,|\,m\wedge s-m\alpha(w)/\gamma(w)$ even. The sum on the left-hand side of (28) may be empty. In this case the sum is defined to be zero.

Let us check (28) with the help of a few examples. First we focus on the case $m=1$, $s=0$. In order to fulfill the first part of the condition C in (28) we need $\gamma=1$. This, in turn, requires to find a necklace with $n_{\mathcal{L}}=0$ and $n_{\mathcal{R}}=1$. There is just one such necklace, namely $\mathcal{R}$. But it does not fulfill the second part of C. Therefore, the sum on the left-hand side of (28) is empty, and the left-hand side is zero. The right-hand side adds up to $1+1-2=0$ and confirms (28) for this special case. For $s=1$ we find again that $\mathcal{R}$ is the only choice for w. But this time the second part of C is fulfilled and the left-hand side of (28) is

$$\gamma(\mathcal{R})(-1)^{[2\chi(\mathcal{R})+\gamma(\mathcal{R})-\alpha(\mathcal{R})]/[2\gamma(\mathcal{R})]}\begin{pmatrix}\beta(\mathcal{R})/[2\gamma(\mathcal{R})]\\ [\gamma(\mathcal{R})-\alpha(\mathcal{R})]/[2\gamma(\mathcal{R})]\end{pmatrix}=1. \tag{29}$$

We used $\alpha(\mathcal{R})=1$, $\beta(\mathcal{R})=0$, $\gamma(\mathcal{R})=1$, and $\chi(\mathcal{R})=2$. For $m=1$, $s=1$ the right-hand side of (28) consists of just one term, which turns out to be 1 as well. Thus we checked that (28) works for $m=1$. With the help of Tables I and II, other special cases may be checked as well.

V. DISCUSSION AND CONCLUSIONS

The work presented here is closely related to the theory of quantum graphs.[13–15] While the quantum graphs considered by Kottos, Schanz, and Smilansky[13–15] correspond to the case of zero potential on the bonds and delta potentials on the vertices, the step potentials considered in this paper correspond to constant potentials on the bonds and potential steps at the vertices. Thus, although the methods employed in this paper are essentially those used previously by Kottos, Schanz, and Smilansky, we obtain a different class of combinatorial identities that apply to cyclic binary codes (Pólya necklaces). Another difference concerns the derivation of identities. While Kottos, Schanz, and Smilansky use a route that involves two-point correlation functions, we show that novel combinatorial identities can be obtained directly from the periodic orbit expansions of explicitly solvable cases. These minor differences notwithstanding the central idea for generating entirely new classes of combinatorial identities is the same: Combinatorial identities can be obtained whenever a quantum system admits of (i) an explicit analytical solution and (ii) an exact periodic orbit expansion.

In addition to the two examples presented above, there exist many other cases in which (14) can be reduced to a low-order polynomial that can be solved by elementary means. Examples are the cases $p=3$, $q=2$ or $p=5$, $q=3$. Both cases can be treated in complete analogy to Example 2 above, and result in novel sum rules and combinatorial identities.

Recently we proved[10] that exact trace formulas exist for one-dimensional square wells with an arbitrary number of potential steps inside. Following the methods outlined above, our results can be generalized immediately to obtain novel combinatorial identities for necklaces with more than two types of beads.

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Democratic supersymmetry

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We present generalizations of N-extended supersymmetry algebras in four dimensions, using Lorentz covariance and invariance under permutation of the N supercharges as selection criteria. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Recent developments in string theory have revealed the need to study generalizations of supersymmetry which lie beyond the realm of existing classifications of space–time supersymmetry algebras. Space–time supersymmetry algebras are $\mathbb{Z}_2$-graded super Lie algebras $\mathfrak{g}=\mathfrak{g}_0\oplus\mathfrak{g}_1$ having even $\mathfrak{g}_0$ and odd $\mathfrak{g}_1$ subspaces, where the even part $\mathfrak{g}_0=\langle M\rangle\oplus\langle P\rangle\oplus\mathfrak{h}$ includes the generators of spacetime Lorentz transformations M, translations P, and a subspace of additional ''internal symmetries'' $\mathfrak{h}$. The usual relation between spin and statistics implies that generators of $\mathfrak{g}_1$ transform as half-integer spin representations under the Lorentz transformations. Traditional classifications of spacetime supersymmetries were based on assumptions arising from the additional requirement that the supersymmetries act on either S-matrix elements[1] or on some physical Hilbert space of particle states.[2] In particular these restrict the maximum spin of the generators to be one and require the internal symmetries to be ''central'' in the sense that they commute with all other generators. Moreover, in four dimensional space–time, the realization of these algebras on physical states restricts finite dimensional representations to contain fields of spin less than or equal to two and the maximal number N of independent supercharges in $\mathfrak{g}_1$ to eight.

There are several instances in which spacetime supersymmetries and representations more general than those allowed in traditional settings occur. In M-theory, for instance, the internal symmetries $\mathfrak{h}$ do not commute with the Lorentz generators (see e.g., Ref. 3). In N-extended super self-dual theories in four dimensional Euclidean space, finite dimensional representations containing fields of spin higher than two do occur and there are consistent theories for any choice of N.[4] In $N=2$ string theory,[5] the absence of the usual relation between spin and statistics gives rise to a realization of a purely even variant of supersymmetry[6] on an infinite dimensional space of string states. There are indications that this statistics-twisted version of supersymmetry is related to an $N\to\infty$ extension of the super Poincaré algebra, which has a realization on an $N=\infty$ self-dual Yang–Mills supermultiplet.[4] These examples show that there seems to be room for the study of more general superalgebras containing the (N-extended) super Poincaré algebra or the super de Sitter algebra as a subalgebra or as a contraction. The work of Fradkin and Vasiliev (e.g., Ref. 7) on higher spin superalgebras on anti de Sitter space is also noteworthy in this respect. The present paper is a further contribution in this direction.

In a series of recent papers[8] we recently developed an approach to the study of generalized super-Poincaré algebras containing generators having spins higher than one. We showed that, contrary to common belief, such superalgebras indeed exist and are realizable in terms of vector

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fields on generalized superspaces having coordinates of higher spin which commute or anticommute in accordance with their statistics. We constructed numerous examples of generalized superalgebras with generators having spins up to two.

In the present paper, we address ourselves to another type of generalization, concerning the question of higher multiplicities of certain representations in the superalgebra. Theories with N supercharges are of special interest. In these, there does not seem to be any principle which distinguishes some of the supercharges from the others and field theories containing such supercharges are usually taken to be invariant under permutation of the supercharges. In this paper, we impose this permutation invariance at the level of the superalgebra, introducing what we will call *democratic superalgebras*. Our purpose here is not a complete classification of possibilities; rather, we aim to show that under the imposition of *democracy*, even in the widely familiar four-dimensional case, an investigation of super Jacobi identities yields some potentially interesting democratic spacetime superalgebras which lie beyond known classifications. The main novel feature which arises in our approach is that the algebra of Lorentz scalars $\mathfrak{h}$ generated by the superderivations is no longer either Abelian or in the center of $\mathfrak{g}$. Although democracy implies the Coleman–Mandula requirement[9] that the scalars commute with (even) translations, they possibly rotate spinor derivations among themselves.

II. DEMOCRATIC SUPERALGEBRAS

A. Four-dimensional space–time supersymmetry

Since our aim is to generalize traditional discussions and since our considerations are purely algebraic, we restrict ourselves to the general complex setting. The question of the appropriate real form depends in any case on the signature of the space–time on which the superalgebra is to be realized; and this depends on the specific context of the application. We consider the Lorentz group to be SO(4,$\mathbb{C}$), with complex generators $M_{\alpha\beta}, M_{\dot\alpha\dot\beta}$, where there is of course no conjugation between dotted and undotted spinor indices.

We shall consider $\mathbb{Z}_2$-graded N-extended complex supersymmetry algebras of the form $\mathfrak{g} = \mathfrak{g}_0 \oplus \mathfrak{g}_1$, with even part

$$\mathfrak{g}_0 = \langle M_{\alpha\beta}, M_{\dot\alpha\dot\beta}, \nabla_{\alpha\dot\alpha} \rangle \oplus \mathfrak{h}, \tag{1}$$

where $\nabla_{\alpha\dot\alpha}$ denotes the derivative vector fields generating translations, and $\mathfrak{h}$ is the subspace of internal symmetries,

$$\mathfrak{h} = \left\langle Y^i, Z^{ij} = -Z^{ji};\ \sum_i Y^i = 0,\ \sum_i Z^{ij} = 0,\ i,j = 1,\ldots,N \right\rangle, \tag{2}$$

spanned by a set of Lorentz scalar generators, $(N-1)$ Y's and $(N-1)(N-2)/2$ Z's.

The odd subspace $\mathfrak{g}_1$ is spanned by N copies of the two types of spinor representations of so(4,$\mathbb{C}$), namely, the $2N$ fermionic operators $\nabla^i_\alpha, \nabla^i_{\dot\alpha}$ $(i = 1,\ldots,N)$, which together with the bosonic vectorial operator $\nabla_{\alpha\dot\beta}$, form the set of superderivations acting on an N-extended superspace. We denote the vector space of superderivations,

$$\mathcal{D} = \langle \nabla_{\alpha\dot\beta}, \nabla^i_\alpha, \nabla^i_{\dot\alpha} \rangle = \mathcal{D}_0 \oplus \mathcal{D}_1,$$

where the even and odd parts are spanned by the vector and spinor derivations, respectively. The vector space $\mathcal{D}$ may be extended to include vector fields having higher spins on the lines of the consideration in Ref. 8. For simplicity, however, we restrict ourselves here, to the consideration of operators having spin less than or equal to one.

We shall assume that all the elements in $\mathfrak{g}$ have commutation or anticommutation relations in agreement with their statistics and with covariance under the Lorentz transformations with generators $M_{\alpha\beta}$, $M_{\dot\alpha\dot\beta}$, $\alpha, \beta, \dot\alpha, \dot\beta = 1,2$ satisfying

$$
\begin{aligned}
&[M_{\alpha\beta},M_{\gamma\delta}]=\epsilon_{\beta\gamma}M_{\alpha\delta}+\epsilon_{\alpha\gamma}M_{\beta\delta}+\epsilon_{\beta\delta}M_{\alpha\gamma}+\epsilon_{\alpha\delta}M_{\beta\gamma},\\
&[M_{\dot\alpha\dot\beta},M_{\dot\gamma\dot\delta}]=\epsilon_{\dot\beta\dot\gamma}M_{\dot\alpha\dot\delta}+\epsilon_{\dot\alpha\dot\gamma}M_{\dot\beta\dot\delta}+\epsilon_{\dot\beta\dot\delta}M_{\dot\alpha\dot\gamma}+\epsilon_{\dot\alpha\dot\delta}M_{\dot\beta\dot\gamma},\\
&[M_{\alpha\beta},M_{\dot\gamma\dot\delta}]=0.
\end{aligned}
\tag{3}
$$

Lorentz covariance, in particular, determines all commutators of the basic operators with the M, namely,

$$
\begin{aligned}
&[M_{\alpha\beta},\nabla^i_\gamma]=\epsilon_{\alpha\gamma}\nabla^i_\beta+\epsilon_{\beta\gamma}\nabla^i_\alpha,\ [M_{\alpha\beta},\nabla^i_{\dot\gamma}]=0,\ [M_{\alpha\beta},Y_i]=0,\ [M_{\alpha\beta},Z^{ij}]=0,\\
&[M_{\dot\alpha\dot\beta},\nabla^i_{\dot\gamma}]=\epsilon_{\dot\alpha\dot\gamma}\nabla^i_{\dot\beta}+\epsilon_{\dot\beta\dot\gamma}\nabla^i_{\dot\alpha},\ [M_{\dot\alpha\dot\beta},\nabla^i_\gamma]=0,\ [M_{\dot\alpha\dot\beta},Y_i]=0,\ [M_{\dot\alpha\dot\beta},Z^{ij}]=0.
\end{aligned}
\tag{4}
$$

Given these commutation rules, all Jacobi identities involving at least two M's are automatically satisfied. Lorentz covariance also yields restrictions on the (anti)commutators of any two elements of $\mathfrak{g}$. These guarantee that the Jacobi identities involving at least one M are also automatically satisfied.

The spinor derivations $\nabla^i_\alpha,\nabla^i_{\dot\alpha}$ are taken to transform under some group of automorphisms T of the superalgebra $\mathfrak{g}$,

$$
T\nabla^i_\alpha T^{-1}=U^i_j\nabla^j_\alpha,\ \ T\nabla^i_{\dot\alpha}T^{-1}=V^i_j\nabla^j_{\dot\alpha},
\tag{5}
$$

where the matrices U,V are representations of the group element T. In this paper, we make particular use of discrete transformations, taking U and V to be permutation matrices on the index i. When the automorphism group is continuous, the action of the group can be expressed in the form of commutation relations with the generators of the group: for instance, the scalar generators Y or Z which appear in (32)–(37).

We shall also allow the possibility of generating scalars by anticommuting spinor derivations, e.g., $\{\nabla^i_\alpha,\nabla^j_\beta\}\sim\epsilon_{\alpha\beta}Z^{ij}$. Traditionally,[1] such Lorentz scalars are always taken to be central with respect to $\mathcal{D}$. In our approach we do not *a priori* restrict the Lorentz scalars to be central. In fact they rotate the spinor derivations $\nabla^i_\alpha,\nabla^i_{\dot\alpha}$ just as the automorphisms (5). This is the main source of our novel examples of spacetime supersymmetries.

B. Democracy

1. Permutation invariants

We shall impose what we call democracy: we require the supercommutation relations to be invariant under the combined permutations of the i-indices of ∇^i_α and of $\nabla^i_{\dot\alpha}$. The group generating democracy S_N is the diagonal group of two groups of permutations acting independently on the two sets of spinors, with permutation matrices $U=V$ in (5).

The Clebsch–Gordon coefficients of the democratic group may be described as follows. The permutation invariant coupling among p $(p>1)$ i type indices can be associated to Young-type diagrams. Given a Young diagram with p $(p>0)$ boxes denoted $[m]=[m_1,m_2,\ldots,m_p]$, with m_j boxes in the jth row $(\Sigma_j m_j=p, m_{i+1}\leqslant m_i)$, we associate with it a p-index tensor $\theta^{i_1i_2\cdots i_p}_{[m_1m_2\cdots m_p]}$ defined by

$$
\theta^{\overbrace{i_1\ldots i_{m_1}}^{m_1}\overbrace{j_1\ldots j_{m_2}}^{m_2}\overbrace{k_1\ldots k_{m_3}}^{m_3}\cdots}_{[m_1m_2\ldots m_p]}=1 \quad \text{if } i_1=\ldots=i_{m_1},\ j_1=\ldots=j_{m_2},\ k_1=\ldots=k_{m_3},\ldots=0 \quad \text{otherwise.}
\tag{6}
$$

Note that these tensors clearly do not have the standard Young diagram symmetries. From these θ tensors, by permuting indices, all the invariant tensors of the permutation group can be constructed. For a Young-type diagram with p boxes, if n_l is the number of rows having length $m_k = l$, the number of independent invariant tensors is given by $p!/(\Pi_k m_k! \Pi_l n_l!)$.

Some of these tensors have a simple interpretation in terms of the familiar Kronecker tensor δ^{ij}. In particular,

$$\theta^{ij}_{[2]} = \delta^{ij}, \quad \theta^{ijkl}_{[22]} = \delta^{ij}\delta^{kl}, \quad \theta^{ijklmn}_{[222]} = \delta^{ij}\delta^{kl}\delta^{mn}, \tag{7}$$

correspond to the invariant tensors of so(N). These are special cases of the identities,

$$\theta^{i_1\cdots i_{m_1} i_{m_1+1}\cdots i_{m_1+m_2}\cdots}_{[m_1 m_2 m_3\cdots]} = \theta^{i_1\cdots i_{m_1}}_{[m_1]}\theta^{i_{m_1+1}\cdots i_{m_1+m_2}}_{[m_2]}\theta^{\cdots}_{[m3]}\cdots. \tag{8}$$

One further useful identity (with summation over repeated indices assumed) is

$$\theta^{i}_{[1]}\theta^{ijk\cdots}_{[m]} = \theta^{jk\cdots}_{[m-1]}, \tag{9}$$

which is valid for all $m>0$ if we define

$$\theta_{[0]} := N. \tag{10}$$

2. Trace conditions

We note that the tensor $\theta^{i}_{[1]}$ can be used to decompose tensors into their permutation irreducible parts. In particular, a vector V^i has two irreducible components given by the scalar projection S,

$$S = \theta^{j}_{[1]} V^j \tag{11}$$

and its complementary piece, of dimension $N-1$,

$$Y^j = V^i - \frac{1}{N}\theta^{i}_{[1]} S. \tag{12}$$

Similarly, a general antisymmetric tensor T^{ij} can be decomposed under the permutation group into two irreducible pieces. A piece of the form Y^j is obtained by the projection

$$Y^j = \theta^{i}_{[1]} T^{ij}, \tag{13}$$

which satisfies

$$\theta^{j}_{[1]} Y^j = 0. \tag{14}$$

The other irreducible piece Z^{ij}, of dimension $(N-1)(N-2)/2$, can be defined by

$$Z^{ij} = T^{ij} - \frac{1}{N}(\theta^{i}_{[1]} Y^j - \theta^{j}_{[1]} Y^i) \tag{15}$$

and satisfies

$$\theta^{i}_{[1]} Z^{ij} = 0. \tag{16}$$

We will generically call conditions imposed on the structure constants which guarantee the irreducibility of the relevant tensors *trace conditions*. The tensors Y in (12) and Z in (15) will be called *trace-free*.

Since the Y^k and the Z^{kl} need to satisfy the trace-free conditions (16) and (14), it is convenient to use some partially trace-free combinations of the invariant θ-tensors with certain symmetries,

$$
\begin{aligned}
t^{ij}_{[2]} &:= \theta^{ij}_{[2]} - \frac{1}{N}\theta^{ij}_{[11]}, \\
t^{ijk}_{[21]} &:= \theta^{ijk}_{[21]} - \frac{1}{N}\theta^{ijk}_{[111]}, \\
t^{ijk}_{[3]} &:= \theta^{ijk}_{[3]} - \frac{1}{N}(\theta^{kji}_{[21]} + \theta^{ijk}_{[21]} + \theta^{ikj}_{[21]}), \\
t^{ijkl}_{[22]} &:= \theta^{ijkl}_{[22]} - \theta^{kjil}_{[22]} - \frac{1}{N}(\theta^{ijkl}_{[211]} - \theta^{kjil}_{[211]} - \theta^{ilkj}_{[211]} + \theta^{klij}_{[211]}),
\end{aligned}
\tag{17}
$$

$$
\begin{aligned}
t^{ijklm}_{[32]} &:= \theta^{jklim}_{[32]} - \theta^{ikljm}_{[32]} - \theta^{jkmil}_{[32]} + \theta^{ikmjl}_{[32]} - \frac{1}{N}(\theta^{jklim}_{[311]} - \theta^{ikljm}_{[311]} - \theta^{jkmil}_{[311]} + \theta^{ikmjl}_{[311]}) \\
&\quad + \frac{1}{N}(\theta^{jmilk}_{[221]} - \theta^{imjlk}_{[221]} + \theta^{jkilm}_{[221]} - \theta^{ikjlm}_{[221]} - \theta^{jkiml}_{[221]} + \theta^{ikjml}_{[221]} - \theta^{lkimj}_{[221]} + \theta^{lkjmi}_{[221]} + \theta^{mkilj}_{[221]} \\
&\quad - \theta^{mkjli}_{[221]}) - \frac{3}{N^2}(\theta^{jmkil}_{[2111]} - \theta^{imkjl}_{[2111]} - \theta^{jlkim}_{[2111]} + \theta^{ilkjm}_{[2111]}),
\end{aligned}
$$

$$
\begin{aligned}
t^{jkmiln}_{[222]} &:= \theta^{jkmiln}_{[222]} - \theta^{ikmjln}_{[222]} - \theta^{jlmikn}_{[222]} + \theta^{ilmjkn}_{[222]} - \theta^{jknilm}_{[222]} + \theta^{iknjlm}_{[222]} + \theta^{jlnikm}_{[222]} - \theta^{ilnjkm}_{[222]} - \frac{1}{N}(\theta^{jkmiln}_{[2211]} \\
&\quad - \theta^{ikmjln}_{[2211]} - \theta^{jlmikn}_{[2211]} + \theta^{ilmjkn}_{[2211]} - \theta^{jknilm}_{[2211]} + \theta^{iknjlm}_{[2211]} + \theta^{jlnikm}_{[2211]} - \theta^{ilnjkm}_{[2211]} - \theta^{limkjn}_{[2211]} + \theta^{kimljn}_{[2211]} \\
&\quad + \theta^{ljmkin}_{[2211]} - \theta^{kjmlin}_{[2211]} + \theta^{linkjm}_{[2211]} - \theta^{kinljm}_{[2211]} - \theta^{ljnkim}_{[2211]} + \theta^{kjnlim}_{[2211]} + \theta^{jmknil}_{[2211]} - \theta^{imknjl}_{[2211]} - \theta^{jmlnik}_{[2211]} \\
&\quad + \theta^{imlnjk}_{[2211]} - \theta^{jnkmil}_{[2211]} + \theta^{inkmjl}_{[2211]} + \theta^{jnlmik}_{[2211]} - \theta^{inlmjk}_{[2211]}).
\end{aligned}
$$

These satisfy the useful identities,

$$t^{jnim}_{[22]} + t^{jmin}_{[22]} \equiv 0, \tag{18}$$

$$t^{jkmiln}_{[222]} + t^{jmnilm}_{[222]} \equiv 0, \tag{19}$$

$$t^{ij}_{[2]} t^{km}_{[2]} - t^{kj}_{[2]} t^{im}_{[2]} - \tfrac{1}{2} t^{knip}_{[22]} t^{pjnm}_{[22]} \equiv 0, \tag{20}$$

$$t^{minl}_{[22]} t^{lqjp}_{[22]} - t^{mjnl}_{[22]} t^{lqip}_{[22]} + \tfrac{1}{2} t^{ikjl}_{[22]} t^{mkpnlq}_{[222]} \equiv 0, \tag{21}$$

$$t^{ijk}_{[3]} t^{knm}_{[3]} - t^{njk}_{[3]} t^{kim}_{[3]} + \frac{1}{2N} t^{npiq}_{[22]} t^{qjpm}_{[22]} \equiv 0, \tag{22}$$

$$t^{kmin}_{[22]} t^{njmp}_{[22]} + t^{kmjn}_{[22]} t^{minp}_{[22]} + t^{imjn}_{[22]} t^{nkmp}_{[22]} \equiv 0, \tag{23}$$

$$t^{qimpjn}_{[222]} t^{nkrmls}_{[222]} + t^{qkmpln}_{[222]} t^{jmrins}_{[222]} + t^{jkmiln}_{[222]} t^{qmspnr}_{[222]} \equiv 0. \tag{24}$$

C. The supercommutators of the superderivations

Using the invariant θ and t tensors, the most general permutation invariant and Lorentz covariant supercommutation relations of the superderivations may be expressed,

$$\{\nabla^i_\alpha,\nabla^j_{\dot\alpha}\}=(a_2 t^{ij}_{[2]}+a_{11}\theta^{ij}_{[11]})\nabla_{\alpha\dot\alpha}, \tag{25}$$

$$\{\nabla^i_\alpha,\nabla^j_\beta\}=(b_2 t^{ij}_{[2]}+b_{11}\theta^{ij}_{[11]})M_{\alpha\beta}+\epsilon_{\alpha\beta}b_{21}(t^{ikj}_{[21]}-t^{jki}_{[21]})Y^k+\epsilon_{\alpha\beta}b_{22}t^{ikjl}_{[22]}Z^{kl}, \tag{26}$$

$$\{\nabla^i_{\dot\alpha},\nabla^j_{\dot\beta}\}=(\overline{b}_2 t^{ij}_{[2]}+\overline{b}_{11}\theta^{ij}_{[11]})M_{\dot\alpha\dot\beta}+\epsilon_{\dot\alpha\dot\beta}\overline{b}_{21}(t^{ikj}_{[21]}-t^{jki}_{[21]})Y^k+\epsilon_{\dot\alpha\dot\beta}\overline{b}_{22}t^{ikjl}_{[22]}Z^{kl}, \tag{27}$$

$$[\nabla^i_\alpha,\nabla_{\beta\dot\beta}]=\epsilon_{\alpha\beta}(c_2 t^{ij}_{[2]}+c_{11}\theta^{ij}_{[11]})\nabla^j_{\dot\beta}, \tag{28}$$

$$[\nabla^i_{\dot\alpha},\nabla_{\beta\dot\beta}]=\epsilon_{\dot\alpha\dot\beta}(\overline{c}_2 t^{ij}_{[2]}+\overline{c}_{11}\theta^{ij}_{[11]})\nabla^j_\beta, \tag{29}$$

$$[\nabla_{\alpha\dot\alpha},\nabla_{\beta\dot\beta}]=r(\epsilon_{\alpha\beta}M_{\dot\alpha\dot\beta}+\epsilon_{\dot\alpha\dot\beta}M_{\alpha\beta}). \tag{30}$$

Comments:

(a) The equations involving Y^i and $Z^{ij}=-Z^{ji}$ on the right-hand side have been written so as to exhibit manifestly the irreducibility of these operators. In particular, use of the partially trace-free invariant tensors as coefficients automatically yields Y^i satisfying (14) and Z^{ij} satisfying (16), since using these tensors guarantees that the relevant term vanishes when one replaces Z^{kl} by $\theta^k_{[1]}V^l$ and independently Y^k by $\theta^k S$.

(b) For the ∇^i_α and the $\nabla^i_{\dot\alpha}$, we have not separated the permutation-irreducible tensors explicitly. However, the tensors t from (17) have been chosen to correspond to the decomposition into the irreducible pieces.

(c) That the two terms on the right-hand side of (30) always have the same coefficient, can be easily deduced from the Jacobi identity for three $\nabla_{\alpha\dot\alpha}$'s. The parameter r distinguishes the two main classes of supersymmetry algebras we shall consider: The contraction to the $r=0$ case corresponds to the *algebras of super-Poincaré type* and for $r\neq 0$ we obtain *algebras of the super de Sitter type*. We shall not consider algebras of superconformal type, which have a second element transforming as a Lorentz vector, the generator of conformal transformations.

(d) The right-hand sides involve the most general Lorentz covariant terms. This guarantees that Jacobi identities involving one M are automatically satisfied.

(e) The fifteen complex parameters $\{a_2,a_{11}\}$, $\{b_2,b_{11},b_{21},b_{22}\}$, $\{\overline{b}_2,\overline{b}_{11},\overline{b}_{21},\overline{b}_{22}\}$, $\{c_2,c_{11}\}$, $\{\overline{c}_2,\overline{c}_{11}\}$, and $\{r\}$ are *a priori* independent. They are to be chosen so as to satisfy the super Jacobi identities, which we shall consider in the next section.

D. The action of $\mathfrak{h}$ on the superderivations

The most general commutation relations of the Lorentz scalar operators Y and Z with the superderivations compatible with Lorentz and permutation covariance, e.g.,

$$[Y^i,\nabla^j_\alpha]=(d_3\theta^{ijk}_{[3]}+d^a_{21}\theta^{ijk}_{[21]}+d^b_{21}\theta^{ikj}_{[21]}+d^c_{21}\theta^{kji}_{[21]}+d_{111}\theta^{ijk}_{[111]})\nabla^k_\alpha, \tag{31}$$

on imposition of the trace conditions, yield the following eight-parameter set of relations involving the partially trace-free tensors (17):

$$[Y^i,\nabla^j_\alpha]=(d_3 t^{ijk}_{[3]}+d^a_{21}t^{ijk}_{[21]}+d^b_{21}t^{ikj}_{[21]})\nabla^k_\alpha, \tag{32}$$

$$[Y^i,\nabla^j_{\dot\alpha}]=(\overline{d}_3 t^{ijk}_{[3]}+\overline{d}^a_{21}t^{ijk}_{[21]}+\overline{d}^b_{21}t^{ikj}_{[21]})\nabla^k_{\dot\alpha}, \tag{33}$$

$$[Y^i,\nabla_{\alpha\dot\alpha}]=0, \tag{34}$$

$$[Z^{ij},\nabla^k_\alpha]=f_{22}t^{jkil}_{[22]}\nabla^l_\alpha, \tag{35}$$

$$[Z^{ij},\nabla^{k}_{\dot\alpha}]=\overline{f}_{22}t^{jkil}_{[22]}\nabla^{l}_{\dot\alpha}, \tag{36}$$

$$[Z^{ij},\nabla_{\alpha\dot\alpha}]=0. \tag{37}$$

We note that the Coleman–Mandula-type relation, $[\mathfrak{h},\mathcal{D}_0]=0$, is an immediate consequence of the trace conditions. However, the internal symmetry can still act nontrivially on the odd derivations.

E. The commutators in $\mathfrak{h}$

The subalgebra of the Y's and Z's has the Lorentz and permutation covariant form satisfying the trace-conditions,

$$[Y^{i},Y^{j}]=g_{22}t^{imjn}_{[22]}Z^{mn}, \tag{38}$$

$$[Z^{ij},Y^{k}]=h_{22}t^{jkil}_{[22]}Y^{l}+h_{32}t^{jklim}_{[32]}Z^{lm}, \tag{39}$$

$$[Z^{ij},Z^{kl}]=k_{222}t^{jkmiln}_{[222]}Z^{mn}. \tag{40}$$

In fact the Jacobi identities always imply that $h_{32}=0$ (see below). This reduces the number of parameters to three, which are constrained by the Jacobi identities.

III. DEMOCRATIC LIE ALGEBRAS $\mathfrak{g}$

The *a priori* Lorentz covariant commutators of our N-extended democratic algebras must satisfy super Jacobi identities which guarantee that the products of the underlying operators are associative. We shall now consider the constraints imposed on the parameters in (25)–(30), (32)–(37), (38)–(40) by the super Jacobi identities. Let us first recall that, by construction, all the Jacobi identities involving at least one M are automatically satisfied. We begin with the subalgebra $\mathfrak{h}$.

A. Democratic Lie algebras $\mathfrak{h}$

To find all possible S_N democratic algebras containing the $N(N-1)/2$ generators Y and Z, the Jacobi identities for (38)–(40) need to be satisfied. These yield the following four conditions on the four parameters g_{22}, h_{22}, h_{32}, k_{222}:

$$\begin{aligned} &h_{32}h_{22}=h_{32}k_{222}=0,\\ &h_{22}(h_{22}-2k_{222})=0,\\ &Ng_{22}(h_{22}-2k_{222})-2h_{32}^{2}=0. \end{aligned} \tag{41}$$

They generally imply that $h_{32}=0$, leaving the conditions

$$h_{22}(h_{22}-2k_{222})=0,\quad g_{22}(h_{22}-2k_{222})=0. \tag{42}$$

These equations lead to a classification in five distinct categories:
(**1a**) Abelian $\mathfrak{h}$: all the scalar operators commute

$$g_{22}=h_{22}=k_{222}=0 \tag{43}$$

and the Y and Z can still be renormalized freely.
(**1b**) The Z's commute, they commute with the Y's but the commutators of the Y's generate the Z's. By renormalization of the Z's or the Y's, we find

$$g_{22}=1,\quad h_{22}=k_{222}=0. \tag{44}$$

(**2**) The Z's form an so$(N-1)$ algebra, with $N-1$ commuting Y's which moreover are so$(N-1)$ scalars, i.e., do not transform under the Z. Using the normalization freedom, we may write

$$g_{22}=h_{22}=0, \quad k_{222}=1. \tag{45}$$

(**3a**) The inhomogeneous so$(N-1)$ case. By normalization of the Z's, the parameters can be brought to

$$g_{22}=0, \quad h_{22}=2, \quad k_{222}=1. \tag{46}$$

The Y's behave as a vector under so$(N-1)$ and commute. They behave as momenta with respect to so$(N-1)$ and hence this corresponds to an inhomogeneous so$(N-1)$ algebra. The normalizations of the Y's can still be adjusted freely.

(**3b**) The so(N) case. We clearly have as many Y and Z operators as there are generators of so(N), which is indeed a particular democratic Lie algebra $\mathfrak{h}$. In this case, by suitable renormalizations of the Y's and the Z's, the parameters can be brought to their so(N) values, which we normalize as

$$g_{22}=1, \quad h_{22}=2, \quad k_{222}=1. \tag{47}$$

That these values correspond to so(N) can be seen as follows. The commutation relations of the $N(N-1)/2$ generators $M^{ij}=M^{ji}$ of so(N) are usually written as,

$$[M^{ij},M^{kl}]=\theta^{jk}_{[2]}M^{il}-\theta^{ik}_{[2]}M^{jl}-\theta^{jl}_{[2]}M^{ik}+\theta^{il}_{[2]}M^{jk}.$$

Defining projections

$$V^j=\theta^k_{[1]}M^{kj}, \quad T^{jk}=M^{jk}-\frac{1}{N}(\theta^j_{[1]}V^k\theta^k_{[1]}V^j), \tag{48}$$

we obtain that the subset of the T operators alone form a democratic so$(N-1)$ subalgebra [with $(N-1)(N-2)/2$ independent operators] of the so(N) algebra. The $N-1$ independent V operators transform as a vector under the so$(N-1)$ subalgebra. The V and the T satisfy precisely the commutation relations (38)–(40) satisfied by Y and Z, respectively, with

$$g_{22}=-\frac{N}{2}, \quad h_{22}=1, \quad k_{222}=\frac{1}{2}. \tag{49}$$

Since there are possible arbitrary democratic rescalings of V with respect to Y and of T with respect to Z, the algebra of the Y's and the Z's corresponds to an so(N) algebra provided (47) holds.

B. Supersymmetry algebras $\mathfrak{g}$

The full discussion for the rest of the super Jacobi identities is rather intricate. We discuss the full set of solutions in the Appendix, discussing the main features here.

We have chosen to discuss the general solution of the Jacobi identities in terms of two criteria:

(1) The first criterion is related to the appearance of the term $\theta^{ij}_{[2]}\nabla_{\alpha\dot\alpha}$ in the anticommutators of ∇^i_α with $\nabla^j_{\dot\alpha}$ (parameter a_2) and of the Y's in the anticommutator of two ∇_a's (parameter b_{21}) or of two $\nabla_{\dot\alpha}$'s (parameter $\overline{b_{21}}$).
(2) The second criterion reveals the structure of the algebra $\mathfrak{h}$ of the Lorentz scalar elements as discussed in the preceding section.

We use the values of the parameters a_2, b_{21}, and $\overline{b_{21}}$ as the basis of our classification. It follows from (25), (26) and (27) that, if any of these three parameters is nonzero, it may be

renormalized to one by rescaling the three superderivations democratically. Hence, using also the fact that we have a natural symmetry under the interchange of the dotted and undotted operators, we are led to six independent classes of superalgebras:

$$\begin{aligned}
&\text{Class A:}\ \ a_2=1,\ \ b_{21}=1,\ \ \overline{b}_{21}=1,\\
&\text{Class B:}\ \ a_2=1,\ \ b_{21}=1,\ \ \overline{b}_{21}=0,\\
&\text{Class C:}\ \ a_2=0,\ \ b_{21}=1,\ \ \overline{b}_{21}=1,\\
&\text{Class D:}\ \ a_2=1,\ \ b_{21}=0,\ \ \overline{b}_{21}=0,\\
&\text{Class E:}\ \ a_2=0,\ \ b_{21}=1,\ \ \overline{b}_{21}=0,\\
&\text{Class F:}\ \ a_2=0,\ \ b_{21}=0,\ \ \overline{b}_{21}=0,
\end{aligned} \tag{50}$$

which we discuss in detail in the Appendix. Classes *B* and *E* are *chiral*, not having the mirror symmetry under the chirality interchanges between dotted and undotted indices ($\alpha\leftrightarrow\dot{\alpha},\ldots$) and between the parameters $c\leftrightarrow\overline{c},\ldots$ (for existing unbarred-barred pairs). The two further classes,

$$\begin{aligned}
&\text{Class B}':\ \ a_2=1,\ \ b_{21}=0,\ \ \overline{b}_{21}=1,\\
&\text{Class E}':\ \ a_2=0,\ \ b_{21}=0,\ \ \overline{b}_{21}=1,
\end{aligned} \tag{51}$$

can clearly be obtained trivially from the *B* and *E* classes by performing the above chirality exchanges; and we do not explicitly discuss these.

Within the above classes, the discussion is subdivided according to the values of k_{222} and h_{22}, corresponding to the division in Sec. III A,

$$\begin{aligned}
&\text{Case 1:}\ \ k_{222}=0,\ \ h_{22}=0,\\
&\text{Case 2:}\ \ k_{222}=1,\ \ h_{22}=0,\\
&\text{Case 3:}\ \ k_{222}=1,\ \ h_{22}=2.
\end{aligned} \tag{52}$$

C. Some solutions of the super Jacobi identities

In this section, we discuss the main noteworthy features revealed by our approach. Let us consider Case A3 from the Appendix:

$$\{\nabla^i_\alpha,\nabla^j_{\dot\alpha}\}=(t^{ij}_{[2]}+a_{11}\theta^{ij}_{[11]})\nabla_{\alpha\dot\alpha}, \tag{53}$$

$$\{\nabla^i_\alpha,\nabla^j_\beta\}=4(b_{22}t^{ij}_{[2]}+a_{11}\overline{b}_{22}\theta^{ij}_{[11]})M_{\alpha\beta}+\epsilon_{\alpha\beta}((t^{ikj}_{[21]}-t^{jki}_{[21]})Y^k+b_{22}t^{ikjl}_{[22]}Z^{kl}), \tag{54}$$

$$\{\nabla^i_{\dot\alpha},\nabla^j_{\dot\beta}\}=4(\overline{b}_{22}t^{ij}_{[2]}+a_{11}b_{22}\theta^{ij}_{[11]})M_{\dot\alpha\dot\beta}+\epsilon_{\dot\alpha\dot\beta}((t^{ikj}_{[21]}-t^{jki}_{[21]})Y^k+\overline{b}_{22}t^{ikjl}_{[22]}Z^{kl}), \tag{55}$$

$$[\nabla^i_\alpha,\nabla_{\beta\dot\beta}]=4\epsilon_{\alpha\beta}\left(b_{22}t^{ij}_{[2]}+\frac{\overline{b}_{22}}{N}\theta^{ij}_{[11]}\right)\nabla^j_{\dot\beta}, \tag{56}$$

$$[\nabla^i_{\dot\alpha},\nabla_{\beta\dot\beta}]=4\epsilon_{\dot\alpha\dot\beta}\left(\overline{b}_{22}t^{ij}_{[2]}+\frac{b_{22}}{N}\theta^{ij}_{[11]}\right)\nabla^j_{\beta}, \tag{57}$$

$$[\nabla_{\alpha\dot\alpha},\nabla_{\beta\dot\beta}]=16b_{22}\overline{b}_{22}(\epsilon_{\alpha\beta}M_{\dot\alpha\dot\beta}+\epsilon_{\dot\alpha\dot\beta}M_{\alpha\beta}), \tag{58}$$

$$[Y^i,\nabla_{\alpha\dot\alpha}]=0, \tag{59}$$

$$[Z^{ij},\nabla_{\alpha\dot\alpha}]=0, \tag{60}$$

$$[Y^i,\nabla^j_\alpha]=4\left(\overline{b}_{22}a_{11}t^{ikj}_{[21]}-\frac{b_{22}}{N}t^{ijk}_{[21]}\right)\nabla^k_\alpha, \tag{61}$$

$$[Y^i,\nabla^j_{\dot\alpha}]=4\left(b_{22}a_{11}t^{ikj}_{[21]}-\frac{\overline{b}_{22}}{N}t^{ijk}_{[21]}\right)\nabla^k_{\dot\alpha}, \tag{62}$$

$$[Z^{ij},\nabla^k_\alpha]=2t^{jkil}_{[22]}\nabla^l_\alpha, \tag{63}$$

$$[Z^{ij},\nabla^k_{\dot\alpha}]=2t^{jkil}_{[22]}\nabla^l_{\dot\alpha}, \tag{64}$$

$$[Y^i,Y^j]=-4a_{11}b_{22}\overline{b}_{22}t^{imjn}_{[22]}Z^{mn}, \tag{65}$$

$$[Z^{ij},Y^k]=2t^{jkil}_{[22]}Y^l, \tag{66}$$

$$[Z^{ij},Z^{kl}]=t^{jkmiln}_{[222]}Z^{mn}. \tag{67}$$

The main unusual features displayed by this algebra are:

(1) Nontrivial action of the subalgebra $\mathfrak{h}$ on the vector space of superderivations $\mathcal{D}$;
(2) Non-Abelian subalgebra of the Lorentz scalar generators;
(3) Occurrence of the a_{11} term in (53).

The above example is of super de Sitter-type. A chiral super Poincaré-type example, also displaying these interesting features, is given by Case B3:

$$\{\nabla^i_\alpha,\nabla^j_{\dot\alpha}\}=(t^{ij}_{[2]}+a_{11}\theta^{ij}_{[11]})\nabla_{\alpha\dot\alpha}, \tag{68}$$

$$\{\nabla^i_\alpha,\nabla^j_\beta\}=(4b_{22}t^{ij}_{[2]}+Nc_{11}a_{11}\theta^{ij}_{[11]})M_{\alpha\beta}+\epsilon_{\alpha\beta}((t^{ikj}_{[21]}-t^{jki}_{[21]})Y^k+b_{22}t^{ikjl}_{[22]}Z^{kl}), \tag{69}$$

$$\{\nabla^i_{\dot\alpha},\nabla^j_{\dot\beta}\}=0, \tag{70}$$

$$[\nabla^i_\alpha,\nabla_{\beta\dot\beta}]=\epsilon_{\alpha\beta}(4b_{22}t^{ij}_{[2]}+c_{11}\theta^{ij}_{[11]})\nabla^j_{\dot\beta}, \tag{71}$$

$$[\nabla^i_{\dot\alpha},\nabla_{\beta\dot\beta}]=0, \tag{72}$$

$$[\nabla_{\alpha\dot\alpha},\nabla_{\beta\dot\beta}]=0, \tag{73}$$

$$[Y^i,\nabla_{\alpha\dot\alpha}]=0, \tag{74}$$

$$[Z^{ij},\nabla_{\alpha\dot\alpha}]=0, \tag{75}$$

$$[Y^i,\nabla^j_\alpha]=\left(-\frac{4}{N}b_{22}t^{ijk}_{[21]}+Na_{11}c_{11}t^{ikj}_{[21]}\right)\nabla^k_\alpha, \tag{76}$$

$$[Y^i,\nabla^j_{\dot\alpha}]=(-c_{11}t^{ijk}_{[21]}+4a_{11}b_{22}t^{ikj}_{[21]})\nabla^k_{\dot\alpha}, \tag{77}$$

$$[Z^{ij},\nabla^k_\alpha]=2t^{jkil}_{[22]}\nabla^l_\alpha, \tag{78}$$

$$[Z^{ij},\nabla^k_{\dot\alpha}]=2t^{jkil}_{[22]}\nabla^l_{\dot\alpha}, \tag{79}$$

$$[Y^i,Y^j]=-Na_{11}c_{11}b_{22}t^{imjn}_{[22]}Z^{mn}, \tag{80}$$

$$[Z^{ij},Y^k]=2t^{jkil}_{[22]}Y^l, \tag{81}$$

$$[Z^{ij},Z^{kl}]=t^{jkmiln}_{[222]}Z^{mn}. \tag{82}$$

IV. CONCLUSION

The inclusion of multiplicities in our program,[8] extending in a Lorentz covariant way the algebra of coordinates and derivatives, has been shown to exhibit interesting new features and a rather rich structure of solutions for the super Jacobi identities. In order to obtain explicit solutions, we have chosen to restrict ourselves in this article to a set of operators of spin less than or equal to one and to impose *democracy*. Within these restricted hypotheses, we have been able to classify fully the allowed superalgebras of derivations and superderivations. Apart from the well-known examples,[1,2] new and potentially interesting cases have been uncovered.

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APPENDIX

With classes (A–F) defined in (50) and subcases (1–3) defined by (52) the full classification of the democratic supersymmetry algebras is given below.

1. Class A

Imposing the super Jacobi identities together with the class A constraints, $a_2=1$, $b_{21}=1$, $\overline{b_{21}}=1$, yields the relations,

$$\{\nabla^i_\alpha,\nabla^j_{\dot\alpha}\}=(t^{ij}_{[2]}+a_{11}\theta^{ij}_{[11]})\nabla_{\alpha\dot\alpha}, \tag{A1}$$

$$\{\nabla^i_\alpha,\nabla^j_\beta\}=4k_{222}(b_{22}t^{ij}_{[2]}+a_{11}\overline{b}_{22}\theta^{ij}_{[11]})M_{\alpha\beta}+\epsilon_{\alpha\beta}((t^{ikj}_{[21]}-t^{jki}_{[21]})Y^k+b_{22}t^{ikjl}_{[22]}Z^{kl}), \tag{A2}$$

$$\{\nabla^i_{\dot\alpha},\nabla^j_{\dot\beta}\}=4k_{222}(\overline{b}_{22}t^{ij}_{[2]}+a_{11}b_{22}\theta^{ij}_{[11]})M_{\dot\alpha\dot\beta}+\epsilon_{\dot\alpha\dot\beta}((t^{ikj}_{[21]}-t^{jki}_{[21]})Y^k+\overline{b}_{22}t^{ikjl}_{[22]}Z^{kl}), \tag{A3}$$

$$[\nabla^i_\alpha,\nabla_{\beta\dot\beta}]=4\epsilon_{\alpha\beta}k_{222}\left(b_{22}t^{ij}_{[2]}+\frac{\overline{b}_{22}}{N}\theta^{ij}_{[11]}\right)\nabla^j_{\dot\beta}, \tag{A4}$$

$$[\nabla^i_{\dot\alpha},\nabla_{\beta\dot\beta}]=4\epsilon_{\dot\alpha\dot\beta}k_{222}\left(\overline{b}_{22}t^{ij}_{[2]}+\frac{b_{22}}{N}\theta^{ij}_{[11]}\right)\nabla^j_\beta, \tag{A5}$$

$$[\nabla_{\alpha\dot\alpha},\nabla_{\beta\dot\beta}]=16b_{22}\overline{b}_{22}k^2_{222}(\epsilon_{\alpha\beta}M_{\dot\alpha\dot\beta}+\epsilon_{\dot\alpha\dot\beta}M_{\alpha\beta}), \tag{A6}$$

$$[Y^i,\nabla_{\alpha\dot\alpha}]=0, \tag{A7}$$

$$[Z^{ij},\nabla_{\alpha\dot\alpha}]=0, \tag{A8}$$

$$[Y^i,\nabla^j_\alpha]=4k_{222}\left(\overline{b}_{22}a_{11}t^{ikj}_{[21]}-\frac{b_{22}}{N}t^{ijk}_{[21]}\right)\nabla^k_\alpha, \tag{A9}$$

$$[Y^i,\nabla^j_{\dot\alpha}]=4k_{222}\left(b_{22}a_{11}t^{ikj}_{[21]}-\frac{\overline{b}_{22}}{N}t^{ijk}_{[21]}\right)\nabla^k_{\dot\alpha}, \tag{A10}$$

$$[Z^{ij},\nabla^k_\alpha]=h_{22}t^{jkil}_{[22]}\nabla^l_\alpha, \tag{A11}$$

$$[Z^{ij},\nabla^k_{\dot\alpha}]=h_{22}t^{jkil}_{[22]}\nabla^l_{\dot\alpha}, \tag{A12}$$

$$[Y^i,Y^j]=-4a_{11}b_{22}\overline{b}_{22}k_{222}t^{imjn}_{[22]}Z^{mn}, \tag{A13}$$

$$[Z^{ij},Y^k]=h_{22}t^{jkil}_{[22]}Y^l, \tag{A14}$$

$$[Z^{ij},Z^{kl}]=k_{222}t^{jkmiln}_{[222]}Z^{mn}, \tag{A15}$$

with the space of class A superalgebras defined by solutions of the system of quadratic equations,

$$\begin{aligned} &b_{22}(2k_{222}-h_{22})=0,\\ &\overline{b}_{22}(2k_{222}-h_{22})=0,\\ &h_{22}(2k_{222}-h_{22})=0. \end{aligned} \tag{A16}$$

We find three subcases [see (52)]

Case A1: Since $h_{22}=k_{222}=0$, the parameters a_{11}, b_{22}, and $\overline{b}_{22}$ are free. This includes the standard super Poincaré algebra with Abelian algebra $\mathfrak{h}$ of central charges.

Case A2: Here a_{11} is free, $k_{222}=1$ and all other parameters are zero. There is an so$(N-1)$ subalgebra [see (45)] of the Z's which decouples.

Case A3: This is a much less trivial case (see Sec. III C) and the full so(N) algebra (49) is included in the algebra. The independent parameters are a_{11}, b_{22}, $\overline{b}_{22}$ while $h_{22}=2$, $k_{222}=1$.

2. Class B

This class is *chiral* of super Poincaré-type: $a_2=1$, $b_{21}=1$, $\overline{b}_{21}=0$. It has relations

$$\{\nabla^i_\alpha,\nabla^j_{\dot\alpha}\}=(t^{ij}_{[2]}+a_{11}\theta^{ij}_{[11]})\nabla_{\alpha\dot\alpha}, \tag{B1}$$

$$\{\nabla^i_\alpha,\nabla^j_\beta\}=(4b_{22}k_{222}t^{ij}_{[2]}+Nc_{11}a_{11}\theta^{ij}_{[11]})M_{\alpha\beta}+\epsilon_{\alpha\beta}((t^{ikj}_{[21]}-t^{jki}_{[21]})Y^k+b_{22}t^{ikjl}_{[22]}Z^{kl}), \tag{B2}$$

$$\{\nabla^i_{\dot\alpha},\nabla^j_{\dot\beta}\}=\epsilon_{\dot\alpha\dot\beta}\overline{b}_{22}t^{ikjl}_{[22]}Z^{kl}, \tag{B3}$$

$$[\nabla^i_\alpha,\nabla_{\beta\dot\beta}]=\epsilon_{\alpha\beta}(4b_{22}k_{222}t^{ij}_{[2]}+c_{11}\theta^{ij}_{[11]})\nabla^j_{\dot\beta}, \tag{B4}$$

$$[\nabla^i_{\dot\alpha},\nabla_{\beta\dot\beta}]=0, \tag{B5}$$

$$[\nabla_{\alpha\dot\alpha},\nabla_{\beta\dot\beta}]=0, \tag{B6}$$

$$[Y^i,\nabla_{\alpha\dot\alpha}]=0, \tag{B7}$$

$$[Z^{ij},\nabla_{\alpha\dot\alpha}]=0, \tag{B8}$$

$$[Y^i,\nabla^j_\alpha]=\left(-\frac{4}{N}b_{22}k_{222}t^{ijk}_{[21]}+Na_{11}c_{11}t^{ikj}_{[21]}\right)\nabla^k_\alpha, \tag{B9}$$

$$[Y^i,\nabla^j_{\dot\alpha}]=(-c_{11}t^{ijk}_{[21]}+4a_{11}b_{22}k_{222}t^{ikj}_{[21]})\nabla^k_{\dot\alpha}, \tag{B10}$$

$$[Z^{ij},\nabla^k_\alpha]=h_{22}t^{jkil}_{[22]}\nabla^l_\alpha, \tag{B11}$$

$$[Z^{ij},\nabla^k_{\dot\alpha}]=h_{22}t^{jkil}_{[22]}\nabla^l_{\dot\alpha}, \tag{B12}$$

$$[Y^i,Y^j]=-Na_{11}c_{11}b_{22}t^{imjn}_{[22]}Z^{mn}, \tag{B13}$$

$$[Z^{ij},Y^k]=h_{22}t^{jkil}_{[22]}Y^l, \tag{B14}$$

$$[Z^{ij},Z^{kl}]=k_{222}t^{jkmiln}_{[222]}Z^{mn}. \tag{B15}$$

Here the parameters are constrained by the system of equations,

$$\begin{aligned}&\overline{b}_{22}h_{22}=\overline{b}_{22}k_{222}=0,\\ &b_{22}(2k_{222}-h_{22})=0,\\ &h_{22}(2k_{222}-h_{22})=0,\end{aligned} \tag{B16}$$

defining the space of class B superalgebras. They are all of chiral super Poincaré-type. There are three subcases of solutions [see (52)]:

Case B1: The parameters a_{11}, b_{22}, $\overline{b}_{22}$, and c_{11} are free, $h_{22}=k_{222}=0$. The Z's are central, not the Y's.

Case B2: The parameters a_{11}, and c_{11} are free, $k_{222}=1$ and the remaining are zero. The subalgebra $\mathfrak{h}$ contains the so$(N-1)$ of the Z's which decouples. The subalgebra of the Y's is Abelian.

Case B3: The parameters a_{11}, b_{22}, and c_{11} are free, $h_{22}=2$, $k_{222}=1$, $\overline{b}_{22}=0$ (see Sec. III C).

3. Class C

This class contains super algebras of the de Sitter-type. They allow contractions to super Poincaré-type algebras by setting c_2 and/or $\overline{c}_2$ to zero. The relations $a_2=0$, $b_{21}=1$, $\overline{b}_{21}=1$ yield the superbrackets,

$$\{\nabla^i_\alpha,\nabla^j_{\dot\alpha}\}=a_{11}\theta^{ij}_{[11]}\nabla_{\alpha\dot\alpha}, \tag{C1}$$

$$\{\nabla^i_\alpha,\nabla^j_\beta\}=a_{11}\overline{c}_2\theta^{ij}_{[11]}M_{\alpha\beta}+\epsilon_{\alpha\beta}((t^{ikj}_{[21]}-t^{jki}_{[21]})Y^k+b_{22}t^{ikjl}_{[22]}Z^{kl}), \tag{C2}$$

$$\{\nabla^i_{\dot\alpha},\nabla^j_{\dot\beta}\}=a_{11}c_2\theta^{ij}_{[11]}M_{\dot\alpha\dot\beta}+\epsilon_{\dot\alpha\dot\beta}((t^{ikj}_{[21]}-t^{jki}_{[21]})Y^k+\overline{b}_{22}t^{ikjl}_{[22]}Z^{kl}), \tag{C3}$$

$$[\nabla^i_\alpha,\nabla_{\beta\dot\beta}]=\epsilon_{\alpha\beta}\left(c_2t^{ij}_{[2]}+\frac{\overline{c}_2}{N}\theta^{ij}_{[11]}\right)\nabla^j_{\dot\beta}, \tag{C4}$$

$$[\nabla^i_{\dot\alpha},\nabla_{\beta\dot\beta}]=\epsilon_{\dot\alpha\dot\beta}\left(\overline{c}_2t^{ij}_{[2]}+\frac{c_2}{N}\theta^{ij}_{[11]}\right)\nabla^j_\beta, \tag{C5}$$

$$[\nabla_{\alpha\dot\alpha},\nabla_{\beta\dot\beta}]=c_2\overline{c}_2(\epsilon_{\alpha\beta}M_{\dot\alpha\dot\beta}+\epsilon_{\dot\alpha\dot\beta}M_{\alpha\beta}), \tag{C6}$$

$$[Y^i,\nabla_{\alpha\dot\alpha}]=0, \tag{C7}$$

$$[Z^{ij},\nabla_{\alpha\dot{\alpha}}]=0, \tag{C8}$$

$$[Y^i,\nabla^j_\alpha]=a_{11}\overline{c}_2 t^{ikj}_{[21]}\nabla^k_\alpha, \tag{C9}$$

$$[Y^i,\nabla^j_{\dot{\alpha}}]=a_{11}c_2 t^{ikj}_{[21]}\nabla^k_{\dot{\alpha}}, \tag{C10}$$

$$[Z^{ij},\nabla^k_\alpha]=h_{22}t^{jkil}_{[22]}\nabla^l_\alpha, \tag{C11}$$

$$[Z^{ij},\nabla^k_{\dot{\alpha}}]=h_{22}t^{jkil}_{[22]}\nabla^l_{\dot{\alpha}}, \tag{C12}$$

$$[Y^i,Y^j]=-a_{11}b_{22}\overline{c}_2 t^{imjn}_{[22]}Z^{mn}, \tag{C13}$$

$$[Z^{ij},Y^k]=h_{22}t^{jkil}_{[22]}Y^l, \tag{C14}$$

$$[Z^{ij},Z^{kl}]=k_{222}t^{jkmiln}_{[222]}Z^{mn}. \tag{C15}$$

Here the parameters are constrained by the system of equations

$$\begin{gathered}\overline{b}_{22}c_2-b_{22}\overline{c}_2=0,\\ b_{22}h_{22}=b_{22}k_{222}=0,\\ \overline{b}_{22}h_{22}=\overline{b}_{22}k_{222}=0,\\ a_{11}\overline{c}_2 b_{22}(2k_{222}-h_{22})=0,\\ h_{22}(2k_{222}-h_{22})=0.\end{gathered} \tag{C16}$$

We find three subcases [see (52)]:

Case C1: We have $h_{22}=k_{222}=0$ while a_{11} is free and b_{22}, $\overline{b}_{22}$, c_2, $\overline{c}_2$, are constrained by the condition

$$\overline{b}_{22}c_2=b_{22}\overline{c}_2. \tag{C17}$$

The Z's are central charges.

Case C2: The parameters a_{11}, c_2, $\overline{c}_2$ are free, $k_{222}=1$ and the remaining are zero. The subalgebra $\mathrm{so}(N-1)\subset\mathfrak{h}$ of the Z's decouples.

Case C3: The parameters a_{11}, c_2, $\overline{c}_2$ are free, $h_{22}=2$, $k_{222}=1$, and $b_{22}=\overline{b}_{22}=0$.

4. Class D

This has $a_2=1$, $b_{21}=0$, $\overline{b}_{21}=0$, yielding

$$\{\nabla^i_\alpha,\nabla^j_{\dot{\alpha}}\}=(t^{ij}_{[2]}+a_{11}\theta^{ij}_{[11]})\nabla_{\alpha\dot{\alpha}}, \tag{D1}$$

$$\{\nabla^i_\alpha,\nabla^j_\beta\}=\epsilon_{\alpha\beta}b_{22}t^{ikjl}_{[22]}Z^{kl}, \tag{D2}$$

$$\{\nabla^i_{\dot{\alpha}},\nabla^j_{\dot{\beta}}\}=\epsilon_{\dot{\alpha}\dot{\beta}}\overline{b}_{22}t^{ikjl}_{[22]}Z^{kl}, \tag{D3}$$

$$[\nabla^i_\alpha,\nabla_{\beta\dot{\beta}}]=0, \tag{D4}$$

$$[\nabla^i_{\dot{\alpha}},\nabla_{\beta\dot{\beta}}]=0, \tag{D5}$$

$$[\nabla_{\alpha\dot{\alpha}},\nabla_{\beta\dot{\beta}}]=0, \tag{D6}$$

$$[Y^i,\nabla_{\alpha\dot{\alpha}}]=0, \tag{D7}$$

$$[Z^{ij},\nabla_{\alpha\dot{\alpha}}]=0, \tag{D8}$$

$$[Y^i,\nabla^j_\alpha]=(d_3 t^{ijk}_{[3]}+d^a_{21}t^{ijk}_{[21]}-N\overline{d}^a_{21}a_{11}t^{ikj}_{[21]})\nabla^k_\alpha, \tag{D9}$$

$$[Y^i,\nabla^j_{\dot{\alpha}}]=(-d_3 t^{ijk}_{[3]}+\overline{d}^a_{21}t^{ijk}_{[21]}-Na_{11}d^a_{21}t^{ikj}_{[21]})\nabla^k_{\dot{\alpha}}, \tag{D10}$$

$$[Z^{ij},\nabla^k_\alpha]=f_{22}t^{jkil}_{[22]}\nabla^l_\alpha, \tag{D11}$$

$$[Z^{ij},\nabla^k_{\dot{\alpha}}]=f_{22}t^{jkil}_{[22]}\nabla^l_{\dot{\alpha}}, \tag{D12}$$

$$[Y^i,Y^j]=g_{22}t^{imjn}_{[22]}Z^{mn}, \tag{D13}$$

$$[Z^{ij},Y^k]=h_{22}t^{jkil}_{[22]}Y^l, \tag{D14}$$

$$[Z^{ij},Z^{kl}]=k_{222}t^{jkmiln}_{[222]}Z^{mn}. \tag{D15}$$

The remaining parameters must satisfy the 18 equations,

$$d_3b_{22}=0,\ d_3\overline{b}_{22}=0,\ d_3f_{22}=0,\ d_3h_{22}=0, \tag{D16}$$

$$b_{22}f_{22}=0,\ b_{22}h_{22}=0,\ b_{22}k_{222}=0,\ b_{22}a_{11}\overline{d}^a_{21}=0, \tag{D17}$$

$$\overline{b}_{22}f_{22}=0,\ \overline{b}_{22}h_{22}=0,\ \overline{b}_{22}k_{222}=0,\ \overline{b}_{22}a_{11}d^a_{21}=0, \tag{D18}$$

$$h_{22}(h_{22}-2k_{222})=0,\ g_{22}(h_{22}-2k_{222})=0,\ f_{22}(f_{22}-2k_{222})=0, \tag{D19}$$

$$d^a_{21}(f_{22}-h_{22})=0,\ \overline{d}^a_{21}(f_{22}-h_{22})=0,\ d_3^2+2Nf_{22}g_{22}+N^3a_{11}d^a_{21}\overline{d}^a_{21}=0. \tag{D20}$$

We find seven essentially different subcases [see (52)]:

Case D1a: The parameter g_{22} is free while $h_{22}=k_{222}=b_{22}=\overline{b}_{22}=f_{22}=0$ and a_{11}, d_3, d^a_{21}, $\overline{d}^a_{21}$, satisfy the condition

$$a_{11}d^a_{21}\overline{d}^a_{21}+\frac{d_3^2}{N^3}=0. \tag{D21}$$

Case D1b: The parameters $b_{22}\neq 0$, d^a_{21} and g_{22} are free, a_{11} and $\overline{d}^a_{21}$ are constrained by

$$\overline{d}^a_{21}a_{11}=0 \tag{D22}$$

and the remaining parameters are zero.

Case D1c: The parameters $b_{22}\neq 0$, $\overline{b}_{22}\neq 0$, g_{22} are free, a_{11}, d^a_{21}, $\overline{d}^a_{21}$ satisfy the conditions

$$d^a_{21}a_{11}=0,\quad \overline{d}^a_{21}a_{11}=0, \tag{D23}$$

and the remaining parameters are zero.

Case D2a: Here $k_{222}=1$, the parameters a_{11}, d_3, d^a_{21}, $\overline{d}^a_{21}$ satisfy the condition (D21) and the remaining parameters are zero.

Case D2b: All the parameters are zero except $k_{222}=1$, $f_{22}=2$ and a_{11} which is free.

Case D3a: All the other parameters are zero except $k_{222}=1$, $h_{22}=2$ and a_{11}, g_{22} which are free.

Case D3b: All the parameters are zero except $k_{222}=1$, $h_{22}=2$, $f_{22}=2$ and g_{22}, a_{11}, d^a_{21}, $\overline{d}^a_{21}$ satisfy

$$4g_{22}+N^2a_{11}d^a_{21}\overline{d}^a_{21}=0.$$

5. Class E

Imposing $a_2=0$, $b_{21}=1$, $\overline{b}_{21}=0$, we obtain the chiral superalgebra,

$$\{\nabla^i_\alpha,\nabla^j_{\dot\alpha}\}=a_{11}\theta^{ij}_{[11]}\nabla_{\alpha\dot\alpha}, \tag{E1}$$

$$\{\nabla^i_\alpha,\nabla^j_\beta\}=Na_{11}c_{11}\theta^{ij}_{[11]}M_{\alpha\beta}+\epsilon_{\alpha\beta}((t^{ikj}_{[21]}-t^{jki}_{[21]})Y^k+b_{22}t^{ikjl}_{[22]}Z^{kl}), \tag{E2}$$

$$\{\nabla^i_{\dot\alpha},\nabla^j_{\dot\beta}\}=\epsilon_{\dot\alpha\dot\beta}\overline{b}_{22}t^{ikjl}_{[22]}Z^{kl}, \tag{E3}$$

$$[\nabla^i_\alpha,\nabla_{\beta\dot\beta}]=\epsilon_{\alpha\beta}(c_2t^{ij}_{[2]}+c_{11}\theta^{ij}_{[11]})\nabla^j_{\dot\beta}, \tag{E4}$$

$$[\nabla^i_{\dot\alpha},\nabla_{\beta\dot\beta}]=0, \tag{E5}$$

$$[\nabla_{\alpha\dot\alpha},\nabla_{\beta\dot\beta}]=0, \tag{E6}$$

$$[Y^i,\nabla_{\alpha\dot\alpha}]=0, \tag{E7}$$

$$[Z^{ij},\nabla_{\alpha\dot\alpha}]=0, \tag{E8}$$

$$[Y^i,\nabla^j_\alpha]=Na_{11}c_{11}t^{ikj}_{[21]}\nabla^k_\alpha, \tag{E9}$$

$$[Y^i,\nabla^j_{\dot\alpha}]=a_{11}c_2t^{ikj}_{[21]}\nabla^k_{\dot\alpha}, \tag{E10}$$

$$[Z^{ij},\nabla^k_\alpha]=h_{22}t^{jkil}_{[22]}\nabla^l_\alpha, \tag{E11}$$

$$[Z^{ij},\nabla^k_{\dot\alpha}]=\overline{f}_{22}t^{jkil}_{[22]}\nabla^l_{\dot\alpha}, \tag{E12}$$

$$[Y^i,Y^j]=-Na_{11}c_{11}b_{22}t^{imjn}_{[22]}Z^{mn}, \tag{E13}$$

$$[Z^{ij},Y^k]=h_{22}t^{jkil}_{[22]}Y^l, \tag{E14}$$

$$[Z^{ij},Z^{kl}]=k_{222}t^{jkmiln}_{[222]}Z^{mn}. \tag{E15}$$

Here a_{11} and c_{11} are free and the remaining parameters satisfy the constraints,

$$b_{22}\overline{f}_{22}=b_{22}h_{22}=b_{22}k_{222}=0, \tag{E16}$$

$$\overline{b}_{22}c_2=\overline{b}_{22}\overline{f}_{22}=\overline{b}_{22}h_{22}=\overline{b}_{22}k_{222}=0, \tag{E17}$$

$$h_{22}(h_{22}-2k_{222})=\overline{f}_{22}(\overline{f}_{22}-2k_{222})=c_2(\overline{f}_{22}-h_{22})=0. \tag{E18}$$

We find six essentially different subcases:

Case E1a: The parameters $h_{22}=k_{222}=\overline{f}_{22}=c_2=0$, and a_{11}, b_{22}, $\overline{b}_{22}$, c_{11} are free.

Case E1b: The parameters $h_{22}=k_{222}=\overline{f}_{22}=\overline{b}_{22}=0$, and a_{11}, b_{22}, c_2, c_{11} are free.

Case E2a: Here $k_{222}=1$, a_{11}, c_{11}, and c_2 are free and the remaining parameters are zero.
Case E2b: Here $k_{222}=1$, $\overline{f}_{22}=2$, a_{11}, c_{11} are free and the remaining parameters are zero.
Case E3a: Here $k_{222}=1$, $h_{22}=2$, a_{11}, c_{11} are free and the remaining parameters are zero.
Case E3b: Here $k_{222}=1$, $h_{22}=2$, $\overline{f}_{22}=2$, a_{11}, c_{11}, c_2 are free and the remaining parameters are zero.

6. Class F

Class F has the following basic relations, $a_2=0$, $b_{21}=0$, $\overline{b}_{21}=0$, which yield the superalgebra

$$\{\nabla^i_\alpha,\nabla^j_{\dot\alpha}\}=a_{11}\theta^{ij}_{[11]}\nabla_{\alpha\dot\alpha}, \tag{F1}$$

$$\{\nabla^i_\alpha,\nabla^j_\beta\}=\epsilon_{\alpha\beta}b_{22}t^{ikjl}_{[22]}Z^{kl}, \tag{F2}$$

$$\{\nabla^i_{\dot\alpha},\nabla^j_{\dot\beta}\}=\epsilon_{\dot\alpha\dot\beta}\overline{b}_{22}t^{ikjl}_{[22]}Z^{kl}, \tag{F3}$$

$$[\nabla^i_\alpha,\nabla_{\beta\dot\beta}]=\epsilon_{\alpha\beta}(c_2t^{ij}_{[2]}+c_{11}\theta^{ij}_{[11]})\nabla^j_{\dot\beta}, \tag{F4}$$

$$[\nabla^i_{\dot\alpha},\nabla_{\beta\dot\beta}]=\epsilon_{\dot\alpha\dot\beta}(\overline{c}_2t^{ij}_{[2]}+\overline{c}_{11}\theta^{ij}_{[11]})\nabla^j_\beta, \tag{F5}$$

$$[\nabla_{\alpha\dot\alpha},\nabla_{\beta\dot\beta}]=c_2\overline{c}_2(\epsilon_{\alpha\beta}M_{\dot\alpha\dot\beta}+\epsilon_{\dot\alpha\dot\beta}M_{\alpha\beta}), \tag{F6}$$

$$[Y^i,\nabla_{\alpha\dot\alpha}]=0, \tag{F7}$$

$$[Z^{ij},\nabla_{\alpha\dot\alpha}]=0, \tag{F8}$$

$$[Y^i,\nabla^j_\alpha]=(d_3t^{ijk}_{[3]}+d^a_{21}t^{ijk}_{[21]}+d^b_{21}t^{ikj}_{[21]})\nabla^k_\alpha, \tag{F9}$$

$$[Y^i,\nabla^j_{\dot\alpha}]=(\overline{d}_3t^{ijk}_{[3]}+\overline{d}^a_{21}t^{ijk}_{[21]}+\overline{d}^b_{21}t^{ikj}_{[21]})\nabla^k_{\dot\alpha}, \tag{F10}$$

$$[Z^{ij},\nabla^k_\alpha]=f_{22}t^{jkil}_{[22]}\nabla^l_\alpha, \tag{F11}$$

$$[Z^{ij},\nabla^k_{\dot\alpha}]=\overline{f}_{22}t^{jkil}_{[22]}\nabla^l_{\dot\alpha}, \tag{F12}$$

$$[Y^i,Y^j]=g_{22}t^{imjn}_{[22]}Z^{mn}, \tag{F13}$$

$$[Z^{ij},Y^k]=h_{22}t^{jkil}_{[22]}Y^l, \tag{F14}$$

$$[Z^{ij},Z^{kl}]=k_{222}t^{jkmiln}_{[222]}Z^{mn}. \tag{F15}$$

For $k_{222}=h_{22}=0$, i.e., case F1, we will limit ourselves to giving the conditions which have to be fulfilled. In the cases F2, F3 where $k_{222}=1$, we give a more precise discussion. There are many subcases which we have classified as follows:

$$\begin{aligned}&\text{subcase a: } a_{11}\neq 0,\\ &\text{subcase b: } a_{11}=0,\ f_{22}=0,\ \overline{f}_{22}=0,\\ &\text{subcase c: } a_{11}=0,\ f_{22}=2,\ \overline{f}_{22}=0,\\ &\text{subcase d: } a_{11}=0,\ f_{22}=2,\ \overline{f}_{22}=2.\end{aligned} \tag{F16}$$

With this in mind, we find nine essentially different subcases.

Case F1: With $h_{22}=k_{222}=0$, which implies $f_{22}=\overline{f}_{22}=0$, the 20 conditions to be fulfilled are

$$\begin{gathered}
b_{22}d^b_{21}=0, \quad b_{22}d_3=0,\\
\overline{b}_{22}\overline{d}^b_{21}=0, \ \overline{b}_{22}\overline{d}_3=0,\\
a_{11}c_2=0, \ a_{11}c_{11}=0,\\
a_{11}\overline{c}_2=0, \ a_{11}\overline{c}_{11}=0,\\
a_{11}d^a_{21}=0, \ a_{11}\overline{d}^a_{21}=0,\\
c_2\overline{c}_2-N^2c_{11}\overline{c}_{11}=0, \ \overline{b}_{22}c_2-b_{22}\overline{c}_2=0,\\
c_2(\overline{d}_3-d_3)=0, \ \overline{c}_2(\overline{d}_3-d_3)=0,\\
c_2\overline{d}^a_{21}-Nc_{11}d^a_{21}=0, \ \overline{c}_2\overline{d}^b_{21}-N\overline{c}_{11}d^b_{21}=0,\\
c_2d^b_{21}-Nc_{11}\overline{d}^b_{21}=0, \ \overline{c}_2d^a_{21}-N\overline{c}_{11}\overline{d}^a_{21}=0,\\
d_3^2-N^2d^a_{21}d^b_{21}=0, \ \overline{d}_3^2-N^2\overline{d}^a_{21}\overline{d}^b_{21}=0.
\end{gathered} \tag{F17}$$

This leads to a rather long, easy but uninteresting discussion which we will not give.

Case F2a: Here $k_{222}=1$, $a_{11}\neq 0$, d^b_{21}, $\overline{d}^b_{21}$, f_{22}, and $\overline{f}_{22}$ satisfy the following conditions:

$$\begin{gathered}
f_{22}(f_{22}-2)=0, \quad \overline{f}_{22}(\overline{f}_{22}-2)=0,\\
f_{22}d^b_{21}=0, \quad \overline{f}_{22}\overline{d}^b_{21}=0,
\end{gathered} \tag{F18}$$

and the remaining parameters are zero.

Case F2b: Here $k_{222}=1$, c_2, c_{11}, $\overline{c}_2$, $\overline{c}_{11}$, d^a_{21}, d^b_{21}, d_3, $\overline{d}^a_{21}$, $\overline{d}^b_{21}$, $\overline{d}_3$ satisfy the conditions,

$$\begin{gathered}
c_2\overline{c}_2-N^2c_{11}\overline{c}_{11}=0,\\
c_2(\overline{d}_3-d_3)=0, \ \overline{c}_2(\overline{d}_3-d_3)=0,\\
c_2\overline{d}^a_{21}-Nc_{11}d^a_{21}=0, \ \overline{c}_2\overline{d}^b_{21}-N\overline{c}_{11}d^b_{21}=0,\\
c_2d^b_{21}-Nc_{11}\overline{d}^b_{21}=0, \ \overline{c}_2d^a_{21}-N\overline{c}_{11}\overline{d}^a_{21}=0,\\
d_3^2-N^2d^a_{21}d^b_{21}=0, \ \overline{d}_3^2-N^2\overline{d}^a_{21}\overline{d}^b_{21}=0,
\end{gathered} \tag{F19}$$

and the remaining parameters are zero.

Case F2c: All the parameters are zero except $k_{222}=1$, $f_{22}=2$ and c_{11}, $\overline{c}_{11}$, $\overline{d}_3$, $\overline{d}^a_{21}$, and $\overline{d}^b_{21}$ which satisfy

$$\begin{gathered}
c_{11}\overline{c}_{11}=0, \ \overline{d}_3^2-N^2\overline{d}^a_{21}\overline{d}^b_{21}=0,\\
c_{11}\overline{d}^b_{21}=0, \ \overline{c}_{11}\overline{d}^a_{21}=0.
\end{gathered} \tag{F20}$$

Case F2d: All the parameters are zero except $k_{222}=1$, $f_{22}=\overline{f}_{22}=2$ and c_2, c_{11}, $\overline{c}_2$, $\overline{c}_{11}$ which satisfy the condition,

$$c_2\bar{c}_2 - N^2 c_{11}\bar{c}_{11} = 0. \tag{F21}$$

Case F3a: All the parameters are zero except $k_{222}=1$, $h_{22}=2$, $a_{11}\neq 0$, and d^b_{21}, $\bar{d}^b_{21}$, f_{22}, $\bar{f}_{22}$, and g_{22} which satisfy the conditions,

$$\begin{gathered} f_{22}(f_{22}-2)=0,\ \ \bar{f}_{22}(\bar{f}_{22}-2)=0, \\ d^b_{21}(f_{22}-2)=0,\ \ \bar{d}^b_{21}(\bar{f}_{22}-2)=0, \\ f_{22}g_{22}=0,\ \ \bar{f}_{22}g_{22}=0. \end{gathered} \tag{F22}$$

Case F3b: All the parameters are zero except for $k_{222}=1$, $h_{22}=2$, g_{22}, and c_2, c_{11}, $\bar{c}_2$, and $\bar{c}_{11}$ which satisfy the condition,

$$c_2\bar{c}_2 - N^2 c_{11}\bar{c}_{11} = 0. \tag{F23}$$

Case F3c: All the parameters are zero except $k_{222}=1$, $h_{22}=2$, $f_{22}=2$, and c_{11}, $\bar{c}_{11}$, d^a_{21}, and d^b_{21} which satisfy the conditions,

$$c_{11}\bar{c}_{11}=0, \quad c_{11}d^a_{21}=0, \quad \bar{c}_{11}d^b_{21}=0, \tag{F24}$$

and the dependent parameter,

$$g_{22}=\frac{N}{4}d^a_{21}d^b_{21}. \tag{F25}$$

Case F3d: All the parameters are zero except for $k_{222}=1$, $h_{22}=2$, $f_{22}=\bar{f}_{22}=2$, and c_{11}, c_2, $\bar{c}_{11}$, $\bar{c}_2$, d^a_{21}, d^b_{21} $\bar{d}^a_{21}$, and $\bar{d}^b_{21}$ which satisfy the conditions,

$$\begin{gathered} c_2\bar{d}^a_{21} - N c_{11} d^a_{21} = 0,\ \ \bar{c}_2\bar{d}^b_{21} - N\bar{c}_{11}d^b_{21} = 0, \\ c_2 d^b_{21} - N c_{11}\bar{d}^b_{21} = 0,\ \ \bar{c}_2 d^a_{21} - N\bar{c}_{11}\bar{d}^a_{21} = 0, \\ c_2\bar{c}_2 - N^2 c_{11}\bar{c}_{11} = 0,\ \ d^a_{21}d^b_{21} - \bar{d}^a_{21}\bar{d}^b_{21} = 0, \end{gathered} \tag{F26}$$

and the dependent parameter,

$$g_{22}=\frac{N}{4}d^a_{21}d^b_{21}. \tag{F27}$$

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Sums of spherical waves for lattices, layers, and lines

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We consider the connections between sums of spherical wave functions over lattices, layers, and lines. The differences between sums over lattices and those over a doubly periodic constituent layer are expressed in terms of series with exponential convergence. Correspondingly, sums over the layer can be regarded as composed of a sum over a central line, and another sum over displaced lines exhibiting exponential convergence. We exhibit formulas which can be used to calculate accurately and efficiently sums of spherical waves over lattices, layers, and lines, which in turn may be used to construct quasiperiodic Green's functions for the Helmholtz equation, of use in scattering problems for layers and lines of spheres, and for finding the Bloch modes of lattices of spheres. We illustrate the numerical accuracy of our expressions. © *2001 American Institute of Physics.*
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I. INTRODUCTION

We discuss here sums of spherical waves, solutions of the Helmholtz equation which arise naturally in scattering problems for systems of spheres. The systems on which we focus are periodic collections, with the spheres arranged either along a line, or in doubly periodic fashion in a plane, or in triply periodic fashion in a lattice. If the sums over the basis of spherical waves can be evaluated accurately and efficiently, then they can be used to construct quasiperiodic Green's functions, of use in integral equation treatments of wave scattering problems.[1] The conventional basis used for the calculation of such Green's functions is of course plane waves, but for systems composed of spherical scatterers, the natural basis to employ is composed of spherical waves, and its use delivers advantages of rapidity of convergence, and accuracy in the implementation of boundary conditions, particularly important in cases of high contrast between the media between and within the spheres.[2]

For the case of the Schrödinger equation, sums of spherical waves over lattices arise in the well-known Korringa–Kohn–Rostoker (KKR) method for calculation of Bloch functions,[3–5] where they are referred to as matrix elements. However, their lineage predates the KKR formulation, as they were perhaps first introduced by Appel,[6] and were considered in an important paper by Rayleigh,[7] which has motivated much of our work utilizing them. We have established[8] convenient formulas which may be used to calculate quasiperiodic sums of spherical waves over arbitrary lattices of spheres. Such sums are useful in finding Bloch modes in lattices, e.g., in calculating their photonic band structures.[9,10]

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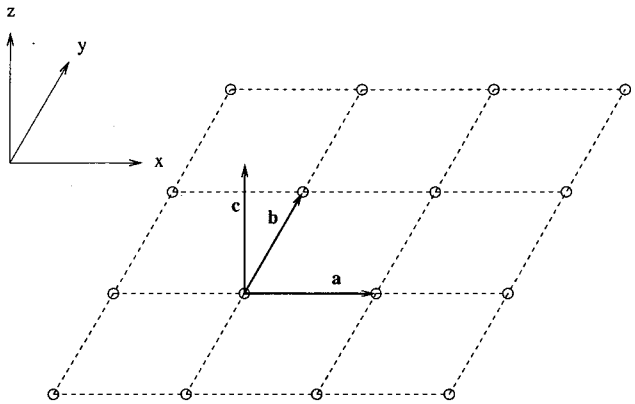

FIG. 1. A general array in the Oxy plane, characterized by (not necessarily orthogonal) basis vectors **a** and **b**, is made into a lattice using a third basis vector **c** along the Oz axis.

An important structure in three dimensions is the doubly periodic monolayer of spheres.[11] If sums of spherical waves over this structure can be calculated, and from them the quasiperiodic Green's functions, then efficient formulations can be constructed for the scattering by monolayers. These may be used in what Stefanou, Karathanos, and Modinos[10] call ''layer KKR methods,'' and enable the investigation of problems of wave localization by three-dimensional random systems, and of homogenization in them. We have carried out such investigations[11,12] of two-dimensional systems using sums over cylindrical wave functions.

Here we will investigate quasiperiodic sums of spherical wave functions over singly periodic, doubly periodic, and triply periodic sets of points. We will use Fourier methods, which have recently been employed by a number of groups,[13–17] and which enable convenient linkages to be established between wave functions summed over periodic sets, and constituent sets of lower dimension. As we have stressed,[11,12,17] these linkages are important in enabling a deeper understanding of the Bloch theorem, when applied to bases of functions other than plane waves. They also have computational advantages, in that the sums over lower dimension, when added to exponentially convergent series, generate those over a higher dimension.

We will begin by considering the sums of spherical waves over lattices. We will break up such sums into those over a central monolayer, and monolayers lying in positive and negative half spaces. The latter will be reduced to rapidly evaluable and quickly convergent series. We will next consider the central monolayer, and regard it as being composed of a set of displaced lines. Once again, we will obtain sums over the central line, and lines in the positive and negative half planes, with the latter being able to be simply and efficiently evaluated.

II. LATTICE AND LAYER SUMS

We consider the lattice shown in Fig. 1. It is characterized by basis vectors for a layer $\mathbf{a}=(a,0,0)$ and $\mathbf{b}=(b_x,b_y,0)$, with the third basis vector being taken to lie along the Oz axis: $\mathbf{c}=(0,0,c)$, with $c>0$. The general lattice vector is specified by a triplet of integers $p=(p_a,p_b,p_c)$:

$$\mathbf{R}_p=p_a\mathbf{a}+p_b\mathbf{b}+p_c\mathbf{c}=\mathbf{R}_{\mathbf{p}\perp}+p_c\mathbf{c}, \tag{1}$$

where we will introduce a unit vector to characterize direction: $\mathbf{R}_p=R_p\hat{\mathbf{R}}_p$. The lattice sums for the Helmholtz equation depend on a scalar parameter, k—the wave number, and a vector parameter, $\mathbf{k}_0$—the Bloch vector or quasiperiodicity vector. The sum of order n,m for the lattice is defined in terms of a superposition of the appropriately phased (n,m)th order solution of the Helmholtz equation, evaluated at the nodes of the lattice:

$$S_{nm}^{L}=\sum_{p\neq(0,0,0)} h_n^{(1)}(kR_p)Y_{nm}(\hat{\mathbf{R}}_p)\exp(i\mathbf{k}_0\cdot\mathbf{R_p}), \tag{2}$$

where $h_n^{(1)}$ represents the spherical Bessel function of the third kind (the Hankel function),[18] and multiplies the spherical harmonic angular function Y_{nm}. Note that the lattice point at the origin is excluded from the sum, and this distinguishes the central layer $p_c=0$ from those in the positive and negative half spaces $\mathbf{R}_p^+$ with $p_c>0$ and $\mathbf{R}_p^-$ with $p_c<0$.

In previous work,[11,12,17] we have established expressions from which the lattice sums may be evaluated:

$$S_{nm}^{L}=S_{nm}^{Lj}+iS_{nm}^{Ly}=-1/\sqrt{4\pi}\,\delta_{n,0}\delta_{m,0}+iS_{nm}^{Ly}, \tag{3}$$

where, using an asterisk to denote conjugation,

$$\begin{aligned}(-1)^m S_{n,-m}^{Ly} j_{n+q}(k\xi)=&-1/\sqrt{4\pi}\,\delta_{n,0}\delta_{m,0}[y_q(k\xi)+w_q(k\xi)]\\&-\frac{4\pi}{kV}i^n\sum_h\left(\frac{k}{Q_h}\right)^q\frac{j_{n+q}(Q_h\xi)}{Q_h^2-k^2}Y_{nm}^*(\hat{\mathbf{Q}}_h).\end{aligned} \tag{4}$$

Here, q is an arbitrary positive integer, representing the order of summation acceleration, while ξ is an arbitrary length, bounded from above by the shortest length of any integral combination of **a**, **b**, and **c**, and V is the volume of the unit cell. Also, $\mathbf{Q}_h$ denotes the general element of the space of reciprocal lattice vectors $\mathbf{K_h}$ translated by the quasiperiodicity vector $\mathbf{k}_0$, with its magnitude being Q_h and its direction being characterized by the unit vector $\hat{\mathbf{Q}}_h$. The function w_q removes the divergent part at the origin of the spherical Bessel function y_q:[19]

$$w_q(\xi)=\frac{1}{2\sqrt{\pi}}\sum_{p=0}^{q-1}\frac{\Gamma(q-p+1/2)}{p!}\left(\frac{2}{k\xi}\right)^{q-2p+1}. \tag{5}$$

These expressions give the S_{nm}^{L} as sums over a triplet of integers in reciprocal space.

We will now relate the lattice sums to those over the central layer, and the positive and negative half spaces:

$$S_{nm}^{L}=S_{nm}^{\mathrm{ML}}+S_{nm}^{L+}+S_{nm}^{L-}. \tag{6}$$

The monolayer term is the focus of interest in Eq. (6) and we will seek to establish simple expressions for the positive $(p_c>0)$ and negative $(p_c<0)$ half space sums.

Our basic tool will be Fourier transform expressions for spherical waves given by Wittmann.[19] These expressions contain a preferred coordinate z, and if $z>0$:

$$h_n^{(1)}(kr)Y_{nm}(\hat{\mathbf{r}})=\frac{1}{2\pi i^n}\int Y_{nm}(\hat{\mathbf{k}})\exp(i\mathbf{k}\cdot\mathbf{r})\frac{d\mathbf{K}}{\gamma k}. \tag{7}$$

Here the integral is from minus infinity to infinity in the two components K_x and K_y of the vector **K**, while γ is a function of K_x and K_y:

$$\gamma=\sqrt{k^2-K^2}, \tag{8}$$

with the square root being taken to be positive imaginary if $K>k$. The corresponding expression for $z<0$ is

$$h_n^{(1)}(kr)Y_{nm}(\hat{\mathbf{r}})=\frac{1}{2\pi(-i)^n}\int Y_{nm}(\hat{\mathbf{k}})\exp(-i\mathbf{k}\cdot\mathbf{r})\frac{d\mathbf{K}}{\gamma k}. \tag{9}$$

Convenient expressions for evaluating the Y_{nm} are

$$Y_{nm}(\hat{\mathbf{k}}) = (-1)^m K_{nm}(k_x/k + ik_y/k)^m P_n^{(m)}(k_z/k), \tag{10}$$

for positive m, and

$$Y_{n,-m}(\hat{\mathbf{k}}) = K_{nm}(k_x/k - ik_y/k)^m P_n^{(m)}(k_z/k), \tag{11}$$

where

$$K_{nm} = \sqrt{\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}}. \tag{12}$$

The function $P_n^{(m)}$ is defined to be the mth derivative of the nth Legendre polynomial:

$$P_n^{(m)}(x) = \frac{\mathrm{d}^m}{\mathrm{d}x^m} P_n(x). \tag{13}$$

Note that $P_n^{(m)}$ differs from the associated Legendre function in the absence of a prefactor involving a power of the square root function. Expressions (10)–(13) are well adapted to our purpose here since they pose no problems with branch cuts for evanescent orders (k_z imaginary).

We use these expressions now to evaluate S_{nm}^{L+}, assuming $m>0$. Writing $\mathbf{k}_0 = \mathbf{k}_{0\perp} + k_{0z}\hat{\mathbf{z}}$,

$$S_{nm}^{L+} = \sum_{p_c=1}^{\infty} \exp(ik_{0z}p_c c)\frac{K_{nm}(-1)^m}{2\pi i^n}\int \frac{\mathrm{d}\mathbf{K}}{\gamma k}\left(\frac{k_x + ik_y}{k}\right)^m P_n^{(m)}(\gamma/k)$$

$$\times \exp(i\gamma p_c c)\sum_{\mathbf{R}_{p\perp}} \exp[i(\mathbf{K}+\mathbf{k}_{0\perp})\cdot\mathbf{R}_{p\perp}]. \tag{14}$$

If $\mathbf{Q}_{h\perp}$ denotes the set of integer combinations of the two reciprocal lattice basis vectors lying in the xy plane, and $\mathcal{A}$ denotes the area of the unit cell in that plane, we have

$$\sum_{\mathbf{R}_{p\perp}} \exp[i(\mathbf{K}+\mathbf{k}_{0\perp})\cdot\mathbf{R}_{p\perp}] = \frac{4\pi^2}{\mathcal{A}}\sum_{\mathbf{Q}_{h\perp}} \delta(\mathbf{K}+\mathbf{k}_{0\perp}-\mathbf{Q}_{h\perp}). \tag{15}$$

Let us define

$$\mathbf{Q}_{h\perp}^{-} = -\mathbf{k}_{0\perp} + \mathbf{Q}_{h\perp} = Q_{hx}^{-}\hat{\mathbf{x}} + Q_{hy}^{-}\hat{\mathbf{y}}, \tag{16}$$

so that

$$S_{nm}^{L+} = \frac{2\pi K_{nm}(-1)^m}{\mathcal{A} i^n}\sum_{p_c=1}^{\infty}\sum_{\mathbf{Q}_{h\perp}^{-}} \frac{\exp[i(k_{0z}+\gamma)p_c c]}{\gamma k}\left(\frac{Q_{hx}^{-} + iQ_{hy}^{-}}{k}\right)^m P_n^{(m)}(\gamma/k). \tag{17}$$

We stress that factors involving γ cannot be moved outside the sum over $\mathbf{Q}_{h\perp}^{-}$, since γ depends implicitly on the transverse reciprocal lattice vector. Note that the individual terms in the sum over p_c have physical interest: They would be needed if one wished to evaluate the Green's function due to a quasiperiodic set of spherical wave sources in a plane, with the field point being shifted along the z axis from the source plane.

The final step in the evaluation for the positive half space is to sum the geometrical progression in Eq. (17):

TABLE I. Convergence of the series in (18), for $n=1$, with the truncation order $p_{\max}$, for the data: $k_{0x}=0.37$, $k_{0y}=0.79$, $k_{0z}=0.48$, $k=2\pi/7.69$, $a_x=1.00$, $b_x=0.65$, $b_y=0.81$, $c_z=0.94$, $q=4$.

	$m=-1$	$m=0$	$m=+1$
2–10	$3.88\times10^{-7}-i\,1.21\times10^{-7}$	$-4.97\times10^{-7}+i\,1.03\times10^{-6}$	$-1.45\times10^{-7}-i\,3.80\times10^{-7}$
5–10	$1.78\times10^{-14}-i\,7.11\times10^{-15}$	$-2.31\times10^{-14}+i\,4.93\times10^{-14}$	$-3.55\times10^{-15}-i\,2.13\times10^{-14}$
10+	$18.5309+i\,2.002\,73$	$8.756\,54-i\,3.034\,16$	$13.4095-i\,12.9531$
10−	$-13.4095-i\,12.9531$	$8.756\,54+i\,3.034\,16$	$-18.5309+i\,2.002\,73$
S^L	$9.499\,23-i\,20.4461$	$17.5131+i\,0.$	$-9.499\,23-i\,20.4461$
S^{ML}	$4.377\,86-i9.495\,68$	$-3.82\times10^{-7}-i\,3.11\times10^{-15}$	$-4.377\,86-i\,9.495\,68$

$$S_{nm}^{L+}=\frac{-2\pi K_{nm}(-1)^m}{\mathcal{A}i^n}\sum_{\mathbf{Q}_{h\perp}^-}\frac{1}{\gamma k}\left(\frac{Q_{hx}^-+iQ_{hy}^-}{k}\right)^m\frac{1}{1-\exp[-i(k_{0z}+\gamma)c]}P_n^{(m)}(\gamma/k). \tag{18}$$

The evaluation for the negative half space proceeds along similar lines, bearing in mind the differences between Eqs. (7) and (9). The result is

$$S_{nm}^{L-}=\frac{-2\pi K_{nm}(-1)^m}{\mathcal{A}(-i)^n}\sum_{\mathbf{Q}_{h\perp}^+}\frac{1}{\gamma k}\left(\frac{Q_{hx}^++iQ_{hy}^+}{k}\right)^m\frac{1}{1-\exp[-i(-k_{0z}+\gamma)c]}P_n^{(m)}(\gamma/k), \tag{19}$$

where

$$\mathbf{Q}_{h\perp}^+=\mathbf{k}_{0\perp}+\mathbf{Q}_{h\perp}=Q_{hx}^+\hat{\mathbf{x}}+Q_{hy}^+\hat{\mathbf{y}}. \tag{20}$$

Given these results, it is possible to employ Eq. (6) in two ways: to proceed from the two-dimensional sum S_{nm}^{ML} via these exponential correction terms to the three-dimensional sum S_{nm}^L, or to proceed by subtraction in the opposite direction. Here we follow the latter course, since we have the aim of providing results to validate the expressions for the monolayer sums derived in Sec. III.

In Table I, we give numerical values illustrating the rapid convergence of the sum in Eq. (18). For the data chosen, summation between -10 and 10 along both axes in reciprocal space is entirely adequate, and so the rows labeled $2-10$ and $5-10$ give the differences arising for summation between -2 and 2 and -10 and 10 (which are of order 10^{-6}), and between -5 and 5 and -10 and 10 (which are of order 10^{-14}). The next two rows give the values of $S_{1,m}^{L+}$ and $S_{1,m}^{L-}$. The last two rows give the values of $S_{1,m}^L$ from Eqs. (3) and (4), and of $S_{1,m}^{\mathrm{ML}}$ from Eq. (6). Note that in Eq. (6), the lattice sums S^L depend on k_z, while the monolayer sums do not.

III. LAYER AND LINE SUMS

Let us now proceed to construct the monolayer sums by regarding them as made up of the addition of sums along lines. It is convenient to choose these lines to be parallel to the Ox axis, and to preserve exponential convergence by having the lines displaced along the Oz axis. What this means is that the coordinates we use in this section are in fact rotated coordinates $Ox'y'z'$ relative to those of Sec. II. This rotation of course affects the monolayer sum values, and we will discuss the necessary corrections in Sec. IV.

The analog to Eq. (6) here is

$$S_{nm}^{\mathrm{ML}}=S_{nm}^C+S_{nm}^{\mathrm{ML}+}+S_{nm}^{\mathrm{ML}-}, \tag{21}$$

where the terms on the right-hand side correspond to the central chain ($z=0$) and to the contributions from $z>0$ and $z<0$, respectively.

We start with the central chain, along which $x=pa\hat{\mathbf{x}}$, $y=z=0$. Hence, this sum depends only on k_{0x}:

$$S_{nm}^{C}=\sum_{p\neq 0} h_n^{(1)}(k|p|a)Y_{nm}(\mathrm{sign}(p),0,0)\exp(ik_{0x}pa). \tag{22}$$

Using the normal expression for the spherical harmonic function,[18] we find

$$S_{nm}^{C}=K_{nm}P_n^m(0)\sum_{p=1}^{\infty} h_n^{(1)}(kpa)[\exp(ik_{0x}pa)+(-1)^m\exp(-ik_{0x}pa)]. \tag{23}$$

Here $P_n^m(0)$ denotes the normal associated Legendre function, evaluated at the origin, an analytic quantity.[18]

We replace the function $h_n^{(1)}$ by an integral using Eq. (7):

$$h_n^{(1)}(kpa)Y_{n0}(0,0,1)=h_n^{(1)}(kpa)\sqrt{\frac{2n+1}{4\pi}}P_n(1)=\frac{1}{2\pi i^n}\int Y_{n0}(\hat{\mathbf{k}})\frac{\exp(i\gamma pa)}{\gamma k}\mathrm{d}\mathbf{K}. \tag{24}$$

The sums over p are geometric progressions, which lead to

$$S_{nm}^{C}=\frac{-1}{2\pi i^n}\sqrt{\frac{(n-m)!}{(n+m)!}}P_n^m(0) \times\int\frac{Y_{n0}(\hat{\mathbf{k}})\mathrm{d}\mathbf{K}}{\gamma k}\left\{\frac{1}{1-\exp[-i(\gamma+k_{0x})a]}+\frac{(-1)^m}{1-\exp[-i(\gamma-k_{0x})a]}\right\}. \tag{25}$$

We can express Y_{n0} simply:

$$Y_{n0}(\hat{\mathbf{k}})=\sqrt{\frac{(2n+1)}{4\pi}}P_n(\gamma/k), \tag{26}$$

and evaluate the integral over $\mathbf{K}$ using polar coordinates to arrive at

$$S_{nm}^{C}=\frac{-K_{nm}P_n^m(0)}{i^n}\int_0^{\infty}\frac{KP_n(\gamma/k)\mathrm{d}K}{\gamma k}\left\{\frac{1}{1-\exp[-i(\gamma+k_{0x})a]}+\frac{(-1)^m}{1-\exp[-i(\gamma-k_{0x})a]}\right\}. \tag{27}$$

This gives the sum over the central line as an exponentially convergent integral. The integrand can have singularities at points corresponding to Wood anomalies, where diffracted orders pass off,[1] but these can be eliminated by rotating the contour by 45° below the real K axis.[15]

In Fig. 2 we compare the result of direct summation over progressively larger regions with the result of numerical integration of Eq. (27). Direct summation yields a result which oscillates with a slowly decreasing amplitude, but it is clear that the analytic result lies at the centroid of the oscillations.

We continue with the evaluation of sums over the positive half plane:

$$S_{nm}^{\mathrm{ML}+}=\sum_{\mathbf{R}_p^+} h_n^{(1)}(kR_p^+)Y_{nm}(\hat{\mathbf{R}}_p^+)\exp(i\mathbf{k}_0\cdot\mathbf{R}_p^+), \tag{28}$$

where $\mathbf{R}_p^+=p_a\mathbf{a}+p_c\mathbf{c}$, and where $\mathbf{c}=c_x\hat{\mathbf{x}}+c_z\hat{\mathbf{z}}$. Hence, using the integral expressions for the spherical wave functions:

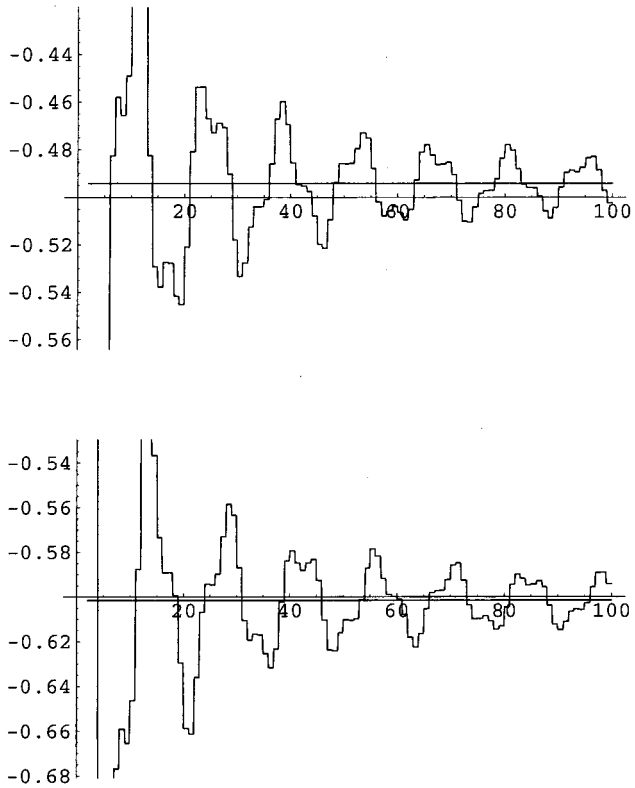

FIG. 2. A comparison of direct summation of S_{11}^{C} as a function of the size of the summation region with the result of Eq. (27) (horizontal line) for the real (top) and imaginary (bottom) parts. The data are: $k_{0x}=0.37$, $k_{0z}=-0.79$, $k=2\pi/7.69$, $a_x=1.00$, $c_x=-0.65$, $c_z=0.81$.

$$S_{nm}^{\mathrm{ML}+}=\sum_{p_{\mathbf{c}}=1}^{\infty}\exp[ip_c(c_xk_{0x}+c_zk_{0z})]\times\frac{1}{2\pi i^n}\int\frac{Y_{nm}(\hat{\mathbf{k}})\,\mathrm{d}\mathbf{K}}{\gamma k}$$
$$\times\exp[ip_c(c_xk_x+c_z\gamma)]\sum_{p_a=-\infty}^{\infty}\exp[ip_aa(k_x+k_{0x})]. \tag{29}$$

The sum over p_a gives rise to a sum of delta functions corresponding to $k_x=-k_q$, with q ranging over all integral values, and $k_q=k_{0x}+2\pi q/a$. We are left with a sum over q replacing the integral over k_x, and we combine the integrands from positive and negative k_y values, to give

$$S_{nm}^{\mathrm{ML}+}=\frac{1}{i^na}\sum_{q=-\infty}^{\infty}\int_0^{\infty}\frac{K_{nm}\mathrm{d}k_y}{\gamma k}P_n^{(m)}(\gamma/k)\times\left[\left(\frac{k_q-ik_y}{k}\right)^m+\left(\frac{k_q+ik_y}{k}\right)^m\right]$$
$$\times\sum_{p_c=1}^{\infty}\exp\{ip_c[c_x(k_{0x}-k_q)+c_z(k_{0z}+\gamma)]\}. \tag{30}$$

The summand here gives the contribution to the monolayer sum from a single line in $p_c>0$. Summing the geometrical progression over all such lines, we find

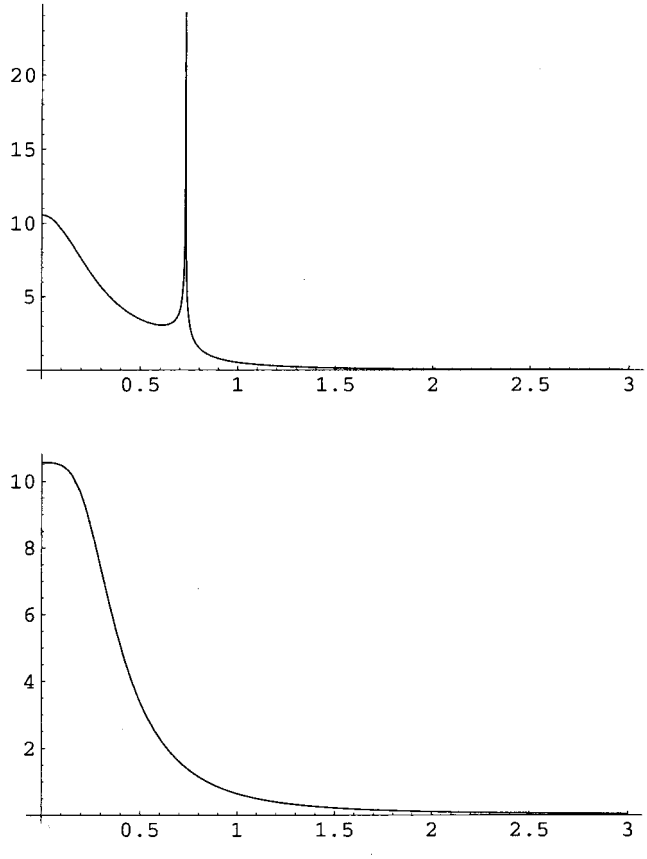

FIG. 3. Plots of the unshifted (top) and shifted (bottom) integrands in Eq. (31) for $n=1,m=1$ and for the data of Fig. 2.

$$S_{nm}^{\mathrm{ML}+}=\frac{-K_{nm}}{i^n a}\sum_{q=-\infty}^{\infty}\int_0^{\infty}\frac{\mathrm{d}k_y}{\gamma k}P_n^{(m)}(\gamma/k)$$
$$\times\left[\left(\frac{k_q-ik_y}{k}\right)^m+\left(\frac{k_q+ik_y}{k}\right)^m\right]\frac{1}{1-\exp-i[c_x(k_{0x}-k_q)+c_z(k_{0z}+\gamma)]}. \tag{31}$$

Once again, this contains an integral which should be evaluated over a line oriented at 45° below the real K axis. A comparison of the integrand in Eq. (31) plotted along the real axis and the line at $-45°$ is given in Fig. 3. Note how the integrable singularity evident in the former is smoothed out in the latter. For the case shown, the summation in Eq. (31) was carried out over q between -5 and 5, with this being entirely adequate for graphical accuracy.

A similar treatment may be applied to evaluate the lower half plane contribution:

$$S_{nm}^{\mathrm{ML}-}=\frac{-(-1)^m K_{nm}}{(-i)^n a}\sum_{q=-\infty}^{\infty}\int_0^{\infty}\frac{\mathrm{d}k_y}{\gamma k}P_n^{(m)}(\gamma/k)$$
$$\times\left[\left(\frac{k_q-ik_y}{k}\right)^m+\left(\frac{k_q+ik_y}{k}\right)^m\right]\frac{1}{1-\exp-i[c_x(-k_{0x}+k_q)+c_z(-k_{0z}+\gamma)]}. \tag{32}$$

IV. LATTICE SUMS AND ROTATIONS

We have described two different methods of arriving at the monolayer sums: working down from three-dimensional sums, and putting together one-dimensional sums. In order to verify that

TABLE II. Monolayer sums from Eq. (6), S_{nm}^{ML6}, after rotation using Eq. (35), S'^{ML6}_{nm}, and from Eq. (21), S_{nm}^{ML21}.

n,m	S_{nm}^{ML6}	S'^{ML6}_{nm}	S_{nm}^{ML21}
0,0	$-0.282\,095-i\,7.300\,57$	$-0.282\,095-i\,7.300\,57$	$-0.282\,095-i\,7.300\,57$
1,−1	$4.377\,86-i\,9.495\,68$	$4.377\,86+i\,2.70\times10^{-7}$	$4.377\,85+i\,4.7\times10^{-12}$
1,0	$-3.82\times10^{-7}-i\,3.11\times10^{-15}$	$-13.4289-i\,2.22\times10^{-15}$	$-13.4290+i\,2.1\times10^{-12}$
1,1	$-4.377\,86-i\,9.495\,68$	$-4.377\,86+i\,2.70\times10^{-7}$	$-4.377\,85+i\,4.7\times10^{-12}$
2,−2	$10.9071-i\,7.051\,39$	$-3.70\times10^{-9}-i\,8.444\,55$	$+1.2\times10^{-10}-i\,8.444\,74$
2,−1	$-1.5\times10^{-8}-i\,3.7\times10^{-9}$	$1.5\times10^{-8}-i\,10.9071$	$-3.4\times10^{-11}+i\,10.9081$
2,0	$0.+i\,8.032\,45$	$3.6\times10^{-15}+4.619\,93$	$2.4\times10^{-10}+i\,4.6183$
2,1	$-1.5\times10^{-8}+i\,3.7\times10^{-9}$	$1.5\times10^{-8}+i\,10.9071$	$3.4\times10^{-11}+i\,10.9081$
2,2	$-10.9071-i\,7.051\,39$	$3.70\times10^{-9}-i\,8.444\,55$	$-1.2\times10^{-10}-i\,8.444\,74$

the two methods agree, we need take into account that the axes used in Secs. II and III are rotated with respect to each other. The effect of rotations on the S_{nm}^{ML} is, from their definition, just the same as their effect on the spherical harmonic functions Y_{nm}. We follow the discussion of Rose[20] concerning the rotational properties of Y_{nm}.

We characterize the rotation by Euler angles α, β, and η. We call the axes of Sec. II the original set, and those of Sec. III the rotated or primed set. Then our transformation equations are

$$x=x',\quad z=y',\quad y=-z', \tag{33}$$

so that the Euler angles of interest are

$$\alpha=-\pi/2,\quad \beta=\pi/2,\quad \eta=\pi/2. \tag{34}$$

Under a rotation, then, S_{lm} is transformed into

$$S'_{lm}=\sum_{m'} D^{l}_{m'm}(\alpha,\beta,\eta)S_{lm'}, \tag{35}$$

where, if $m'\geqslant m$,

$$D^{l}_{m'm}(\alpha,\beta,\eta)=\exp(-im'\alpha)d^{l}_{m'm}(\beta)\exp(-im\eta), \tag{36}$$

and

$$d^{l}_{m'm}(\beta)=\sqrt{(l+m)!(l-m)!(l+m')!(l-m')!}\times\sum_{p}(-1)^{p}\frac{(\cos\beta/2)^{2l+m-m'-2p}(-\sin\beta/2)^{m'-m+2p}}{(l-m'-p)!(l+m-p)!(l+m'-m)!p!}. \tag{37}$$

For $m'<m$, we use

$$d^{l}_{m'm}(\beta)=(-1)^{m'-m}d^{l}_{mm'}(\beta). \tag{38}$$

In Table II we show the application of Eq. (35) to rotate the monolayer sums from the coordinate system of Sec. II to that of Sec. III. The results show good agreement between the two methods for evaluating the sums: subtractively, using the lattice sums as the starting point, and additively, building on the chain sums. The small differences between the two methods grow with order of sums, and reflect the fact that calculations were carried out in MATHEMATICA, with integration points and summation terms being limited because of computation time restrictions. Note the differing symmetry properties between the sums S^{ML} and S'^{ML}, arising because of the differences between the Legendre functions for angles of 0° and 90°.

V. AN ANALYTIC RESULT FOR MONOLAYER SUMS

The monolayer sums may be divided into two parts: one associated with functions j_n, which are finite at the origin, and the other with functions y_n, which are singular at the origin. We will now show that the former may be evaluated analytically.

We consider

$$\mathcal{J}_{nm}^{\mathrm{ML}}=\sum_{\mathbf{R}_p\neq(0,0)} j_n(kR_p)Y_{nm}(\hat{\mathbf{R}}_p)\exp(i\mathbf{k}_0\cdot\mathbf{R_p}), \tag{39}$$

or, adding and subtracting a term from the origin,

$$\mathcal{J}_{nm}^{\mathrm{ML}}=-\frac{1}{\sqrt{4\pi}}\delta_{n,0}\delta_{m,0}+\sum_{\mathbf{R}_p}\frac{1}{4\pi i^n}\int Y_{nm}(\hat{\mathbf{k}})d\hat{\mathbf{k}}\exp[i(\mathbf{k}_0+\mathbf{k})\cdot\mathbf{R}_p]. \tag{40}$$

We take the sum over $\mathbf{R}_p$ inside the integral, and recognize that the exponential term generates a delta function, whose argument requires that the part of $\mathbf{k}_0+\mathbf{k}$ in the monolayer plane, or $\mathbf{k}_{0\perp}+\mathbf{k}_\perp$, matches a reciprocal lattice vector $\mathbf{Q}_h$. Denoting by $\mathcal{A}$ the area of the unit cell in the array, we obtain

$$\mathcal{J}_{nm}^{\mathrm{ML}}=-\frac{1}{\sqrt{4\pi}}\delta_{n,0}\delta_{m,0}+\frac{\pi}{\mathcal{A}i^n}\sum_{\mathbf{Q}_h}\int Y_{nm}(\hat{\mathbf{k}})\mathrm{d}\hat{\mathbf{k}}\delta[(\mathbf{k}_{0\perp}+\mathbf{k}_\perp)-\mathbf{Q}_h]. \tag{41}$$

Now, $\mathbf{Q}_{h\perp}^{-}=-\mathbf{k}_{0\perp}+\mathbf{Q}_h$, and $\mathbf{K}_\perp$ can equal $\mathbf{Q}_{h\perp}^{-}$ only if $h\in\Omega$, the set of propagating orders which can be diffracted by the monolayer. The final steps in the argument are to recognize that to a given $\mathbf{Q}_{h\perp}^{-}$ there are two three-dimensional wave vectors $(\mathbf{Q}_{h\perp}^{-},Q_{h\|})$ and $(\mathbf{Q}_{h\perp}^{-},-Q_{h\|})$, with associated unit vectors $\hat{\mathbf{Q}}_{h\perp}^{-+}$ and $\hat{\mathbf{Q}}_{h\perp}^{--}$, and to evaluate the Jacobian corresponding to the change of integration vector from $\hat{\mathbf{k}}$ to its part in the monolayer plane. The result is

$$\mathcal{J}_{nm}^{\mathrm{ML}}=-\frac{1}{\sqrt{4\pi}}\delta_{n,0}\delta_{m,0}+\frac{\pi}{k\mathcal{A}i^n}\sum_{h\in\Omega}[Y_{nm}(\hat{Q}_{h\perp}^{-+})+Y_{nm}(\hat{Q}_{h\perp}^{--})]/Q_{h\|}^{-}. \tag{42}$$

We validate this result with numerical evidence given in Fig. 4. This shows that $\mathcal{J}^{\mathrm{ML}}$ is an oscillating function of the size of the summation region in real space, but that Eq. (42) accurately predicts the center line of the oscillations.

VI. THE MONOLAYER GREEN'S FUNCTION

We now present the expression which may be used to evaluate the Green's function G_{ML}, given the monolayer sums. G_{ML} satisfies

$$(\nabla^2+k^2)G_{\mathrm{ML}}(\mathbf{r})=-\sum_p \delta(\mathbf{r}-\mathbf{R}_{p\perp})e^{i\mathbf{k_0}\cdot\mathbf{R}_{p\perp}}. \tag{43}$$

The solution may be expressed in terms of spherical Hankel functions[2]

$$G_{\mathrm{ML}}(\mathbf{r})=\frac{ik}{4\pi}\sum_p h_0^{(1)}(k|\mathbf{r}-\mathbf{R}_{p\perp}|)e^{i\mathbf{k_0}\cdot\mathbf{R}_{p\perp}}. \tag{44}$$

The term for $\mathbf{R}_{p\perp}=0$ is separated from the sum, with all other terms being expanded using the addition theorem for spherical waves.[2] The result is

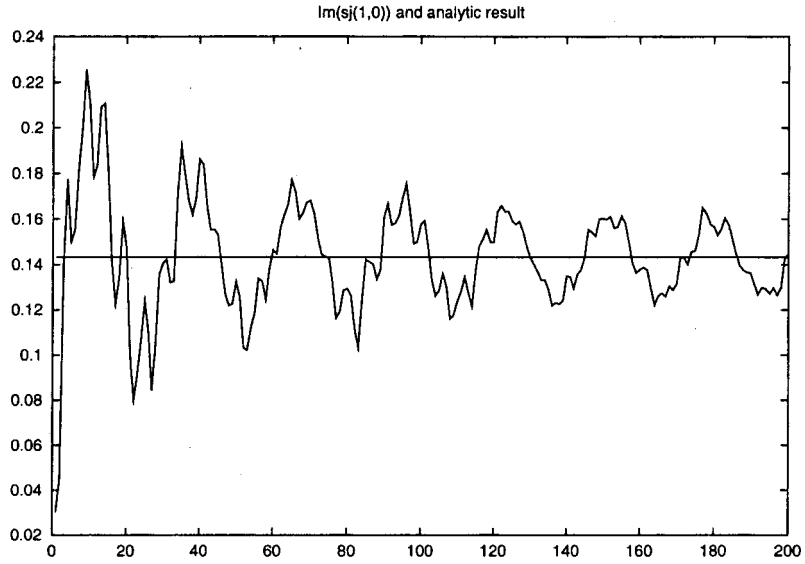

FIG. 4. A comparison of direct summation of $\mathrm{Im}(\mathcal{J}_{11}^{\mathrm{ML}})$ as a function of the size of the summation region with the result of Eq. (39) (horizontal line). The data are: $k=2\pi/0.69$, angles of incidence in polar form: $\theta=23°$, $\psi=37.18°$, $a_x=1.00$, $c_x=0.65$, $c_z=0.81$.

$$G_{\mathrm{ML}}(\mathbf{r})=\frac{ik}{4\pi}h_0^{(1)}(kr)+ik\sum_{n,m}(-1)^m S_{n,-m}^{\mathrm{ML}} j_l(kr)Y_{n,m}(\theta,\phi), \tag{45}$$

with θ, ϕ denoting the polar angles of $\mathbf{r}$.

The expression (45) converges like a geometric series whose radius of convergence is the smaller of a and b. If this is not sufficient to cover the unit parallelogram, then the origin of coordinates may be moved to another array point, with the monolayer sums being rephased appropriately.

VII. CONCLUSIONS

We have explored the connections between sums of spherical waves over lines, layers, and lattices. These connections are of interest numerically, in permitting the efficient and accurate construction of Green's functions for the fundamental alignments of spherical particles. They are also of interest theoretically, since they permit the construction of multipole Bloch methods, for example, to go from the scattering matrix of a sheet of spheres to the Bloch modes of a corresponding lattice of spheres. We will explore their applications in future studies of localization and homogenization in layered sphere systems.

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A note on the generalized fractal dimensions of a probability measure

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We prove the following result on the generalized fractal dimensions $D_q^{\pm}$ of a probability measure μ on $\mathbb{R}^n$. Let g be a complex-valued measurable function on $\mathbb{R}^n$ satisfying the following conditions: (1) g is rapidly decreasing at infinity, (2) g is continuous and nonvanishing at (at least) one point, (3) $\int g \neq 0$. Define the partition function $\Lambda_a(\mu,q)=a^{n(q-1)}\|g_a * \mu\|_q^q$, where $g_a(x)=a^{-n}g(a^{-1}x)$ and $*$ is the convolution in $\mathbb{R}^n$. Then for all $q>1$ we have $D_q^{\pm}=1/(q-1)\lim_{r\to 0}\,^{\sup}_{\inf} \times[\log \Lambda_a\mu(r,q)/\log r]$. © *2001 American Institute of Physics.*
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I. INTRODUCTION

Since the apparition of the fractal formalism in the late 1970s, there has been a huge amount of literature devoted to the different definitions of the fractal dimensions of probability measures (see, e.g., Refs. 1 and 2 for reviews). Roughly speaking, there are two types of fractal dimensions: the pointwise dimensions, which give essentially the local Hölder exponents of the measure, and the global ones, which can be seen as regularity indices in a scale of Besov spaces. Both families of dimensions are related to one another by the so-called multifractal formalism. The global dimensions were originally introduced by Renyi[3] and rediscovered by Hentschel and Procaccia in their seminal paper;[4] they are a generalization of the usual fractal dimension or capacity, and are therefore called ''generalized fractal dimensions.'' They are obtained by a box-counting algorithm, which amounts to partitioning the space in elementary cells and suming up powers of the individual contributions to the measure into what is called a partition function. There are several variants of this definition, according to the kind of covering that is chosen (grids, balls, redundant, nonredundant, etc.) and the kind of partition function (discrete or continuous). First used in the context of chaos and dynamical systems, the generalized fractal dimensions have regained interest in the framework of quantum diffusion in the presence of fractal spectra. After the pioonering work of Guarneri[5] many relations were established between the diffusive behavior of quantum wave packets and the generalized fractal dimensions (see, e.g., Refs. 6–9 for some recent results).

In order to simplify the numerous definitions and unify the results arising in dimension theory, it is important to find equivalences between the different approaches. This has been the aim of some recent works (e.g., Refs. 10–12, 2). In this short note we show that the generalized fractal dimensions can be obtained by replacing the boxes by arbitrary rapidly decaying complex-valued functions in the partition function, provided only these functions have nonzero mean.

II. THE GENERALIZED FRACTAL DIMENSIONS

Let μ be a probability Borel measure on $\mathbb{R}^n$ and consider a partition of the space in a grid of cubes $\mathcal{Q}(x_j,r)$ of center x_j and side $2r$. For $q \geqslant 0$, form the following partition function:

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$$\Lambda_1\mu(r,q)=\sum_j \mu(\mathcal{Q}(x_j,r))^q. \tag{2.1}$$

The so-called Rényi dimensions $D_q^{\pm}$ (Ref. 4) of the measure μ are defined as the limiting exponents of the last function as $r\to 0$, precisely:

$$D_q^{\pm}=\frac{\tau_q^{\pm}}{q-1}, \quad q\neq 1 \tag{2.2}$$

with

$$\tau_q^{\pm}=\lim_{r\to 0} \begin{matrix}\sup\\ \inf\end{matrix} \frac{\log \Lambda_1\mu(r,q)}{\log r}. \tag{2.3}$$

This normalization recasts the dimensions on the unit interval, $0\leqslant D_q^{\pm}\leqslant 1$, at least for $q>1$ (see Ref. 12 for a detailed discussion). Note that (2.2) is not defined for $q=1$. Hentschel and Proccacia[4] have shown heuristically the existence of the limit $q\to 1$, thereby defining $D_1^{\pm}$ by continuity. A rigorous analysis[12] however, shows that $D_q^{\pm}$ are only left- and right-continuous about $q=1$, with a possible discontinuity. The dimension $D_0^{\pm}$ is the usual fractal dimension or capacity. The dimension $D_2^{\pm}$ is known as the correlation dimension. A continuous version[4,10] of the partition function (2.1) is

$$\Lambda_2\mu(r,q)=\int_{\mathbb{R}^n}\mu(\mathcal{B}(x,r))^{q-1}\,\mathrm{d}\mu(x), \tag{2.4}$$

where $\mathcal{B}(x,r)$ is the ball of center x and radius r. The corresponding limiting exponents, defined after (2.2) and (2.3), are called *generalized fractal dimensions*. Note that the integration is performed against the measure μ, which is possibly singular. A more tractable definition consists in integrating versus the Lebesgue measure, by formally replacing $\mathrm{d}\mu(x)$ by the absolutely continuous measure $r^{-n}\mu(\mathcal{B}(x,r))$:

$$\Lambda_3\mu(r,q)=r^{-n}\int_{\mathbb{R}^n}\mu(\mathcal{B}(x,r))^q\mathrm{d}x. \tag{2.5}$$

Although more convenient, this formula seems to be less popular in the literature. The equivalence of definitions (2.1) and (2.4) has been shown in Ref. 13 for $q>1$ (also rewritten in Ref. 2, p. 184), and the equivalence of (2.1) and (2.5) follows by an obvious adaptation of the proof. The equivalence for $0<q<1$ has been proved more recently.[12] We thus have, for all $q>0 (q\neq 1)$, three equivalent definitions of the generalized fractal dimensions:

$$D_q^{\pm}=\frac{1}{q-1}\lim_{r\to 0} \begin{matrix}\sup\\ \inf\end{matrix} \frac{\log \Lambda_{j\mu}(r,q)}{\log r}, \quad j=1,2,3. \tag{2.6}$$

III. MAIN RESULT

As we are going to show, the balls or boxes used to define the partition functions $\Lambda_j\mu$ can be replaced by arbitrary measurable functions, provided the latter are rapidly decreasing. This is very natural for non-negative functions, which can be seen as smooth cutoff functions, but less obvious for complex or signed functions. For any measurable complex-valued function g on $\mathbb{R}^n$ denote by $g_a(x)=a^{-n}g(a^{-1}x)$, $a>0$, its dilated version and define the partition function

$$\Lambda_a(\mu,q)=a^{n(q-1)}\|g_a*\mu\|_q^q=a^{n(q-1)}\int \mathrm{d}b|g_a*\mu(b)|^q,$$

where the asterisk $(*)$ stands for the convolution:

$$g_a*\mu(b)=\int g_a(b-x)\mathrm{d}\mu(x),$$

We start by recalling a useful rule of computation for the limiting exponents. A proof of this result can be found in Ref. 14, for example.

Lemma 3.1: Let s be a non-negative measurable function. Then

$$\liminf_{t\to 0}\frac{\log s(t)}{\log t}=\sup\{\gamma: st(t)\leqslant O(t^{\gamma}),\ t\to 0\},$$

$$\limsup_{t\to 0}\frac{\log s(t)}{\log t}=\inf\{\gamma: t^{\gamma}\leqslant O(s(t)),\ t\to 0\}.$$

Next we consider the case of non-negative functions.

Lemma 3.2: Let g be a non-negative measurable function g on $\mathbb{R}^n$ which is continuous and nonvanishing at (at least) one point and rapidly decreasing at infinity. Then for all $q>1$ we have

$$D_q^{\pm}=\frac{1}{q-1}\lim_{r\to 0}\ \sup_{\inf}\ \frac{\log \Lambda_a\mu(r,q)}{\log r}. \tag{3.1}$$

Proof: First note that we do not change the limit (3.1) on replacing g by a translated and rescaled version $\lambda g(\alpha t-\beta)$. Since g remains positive in some neighborhood of, say, t_0, we can rescale g in such a way that $ch\leqslant g\leqslant Ch$, where h is some non-negative function with $h(t)=1$ for $t\in[-1,1]$ and c,C are two positive constants. Hence it suffices to prove the lemma for such a function h. Let $\epsilon>0$. For all $a>0$ small enough and $b\in\mathbb{R}$ we have

$$\begin{aligned}|h_a*\mu(b)|&=\int h_a(t)\mathrm{d}\mu(b-t)\\ &\geqslant\int_{|t|\leqslant a^{1+\epsilon}} h_a(t)\mathrm{d}\mu(b-t)\\ &\geqslant a^{-n}\min_{|t|\leqslant a^{\epsilon}}\{h(t)\}\mu(\mathcal{B}(b,a^{1+\epsilon}))\\ &\geqslant a^{-n}\mu(\mathcal{B}(b,a^{1+\epsilon})).\end{aligned}$$

Integrating over b this yields to

$$\|h_a*\mu\|_q^q\geqslant a^{(1-q)n+\epsilon n}\Lambda_3\mu(a^{1+\epsilon},q). \tag{3.2}$$

The reverse estimation is more touchy. For all $\epsilon>0$ we have

$$\begin{aligned}|h_a*\mu(b)|&\leqslant\int_{|t|\leqslant a^{1-\epsilon}}|h_a(t)|\mathrm{d}\mu(b-t)+\int_{|t|>a^{1-\epsilon}}|h_a(t)|\mathrm{d}\mu(b-t)\\ &\leqslant a^{-n}\|g\|_{\infty}\mu(\mathcal{B}(b,a^{1-\epsilon}))+\int_{|t|>a^{1-\epsilon}}|h_a(t)|\mathrm{d}\mu(b-t)\end{aligned}$$

and thus

$$\|h_a*\mu\|_q^q\leqslant C_q a^{(1-q)n-\epsilon n}\Lambda_3\mu(a^{1-\epsilon},q)+C_q\int \mathrm{d}b\left(\int_{|b-t|>a^{1-\epsilon}} h_a(b-t)\mathrm{d}\mu(t)\right)^q \tag{3.3}$$

for some constant C_q. We have to show that the contribution of the second term is negligible. By Jensen's inequality, we have for all $q>1$,

$$\left(\int_{|t|>a^{1-\epsilon}} h_a(t)\mathrm{d}\mu(b-t)\right)^q \leqslant \left(\int_{|b-t|>a^{1-\epsilon}} \mathrm{d}\mu(t)\right)^{q-1} \int_{|b-t|>a^{1-\epsilon}} h_a^q(b-t)\mathrm{d}\mu(t).$$

Thus, calling $I(a)$ the second term on the right-hand side of (3.3), we have

$$\begin{aligned} I(a) &\leqslant C_q \int \mathrm{d}b \int_{|t|>a^{1-\epsilon}} h_a^q(t)\mathrm{d}\mu(b-t) \\ &= C_q \int_{|t|>a^{1-\epsilon}} h_a^q(t) \int \mathrm{d}\mu(b-t) = C_q a^{(1-q)n} \int_{|t|>a^{-\epsilon}} g^q(t), \end{aligned}$$

where we use the finiteness of μ to exchange the integrals. Now since g is rapidly decreasing at infinity, the tails of its integrals also and thus $I(a)\leqslant O(a^\infty), a\to 0$. Since (3.2) and (3.3) hold for arbitrarily small ϵ, the conclusion follows from Lemma 3.1. □

Note: A proof of this result in the case $0<q<1$ has been given in Ref. 12, Theorem A.1.

We now can state the main result:

Theorem 3.3: *Let g be a complex-valued measurable function on $\mathbb{R}^n$ satisfying the following conditions:*

(1) g is rapidly decreasing at infinity,
(2) g is continuous and nonvanishing at (at least) one point,
(3) $\int g \neq 0$.

Then for all $q>1$ we have

$$D_q^{\pm} = \frac{1}{q-1} \lim_{r\to 0} \begin{matrix}\sup \\ \inf\end{matrix} \frac{\log \Lambda_a \mu(r,q)}{\log r}. \tag{3.4}$$

This will be an easy consequence of the following lemma.

Lemma 3.4: Let g be a rapidly decreasing complex-valued measurable function such that $\int g \neq 0$. Then there exists a non-negative function ϕ in $\mathcal{S}(\mathbb{R}^n)$ (the Schwartz space of infinitely differentiable rapidly decreasing functions) and a complex-valued function $\psi \in \mathcal{S}(\mathbb{R}^n)$ such that $\phi = g^* \psi$.

Proof: Let $\hat{g}$ be the notation for the Fourier transform of a L^1 function g:

$$\hat{g}(k) = \int e^{-ikx} g(x)\mathrm{d}x.$$

Without restriction we may suppose $|\int g| = |\hat{g}(0)| = 1$. Since $\hat{g}$ is a continuous function, we can find some neighborhood $V = B(0,\epsilon)$ about the origin in which $|\hat{g}|>1/2$ on V. Now take a smaller neighborhood $V' = B(0,\epsilon/2)$ and some nonzero $h \in C_0^\infty(\mathbb{R}^n)$ with support in V'. Define ϕ by its Fourier transform: $\hat{\phi} = h * \tilde{h}$, where $\tilde{h}(x) = \overline{h}(-x)$ and $\overline{h}$ is the complex conjugate of h. Then support $(\hat{\phi}) \subset V$ and $\phi = |\hat{h}|^2$ is a non-negative function in $\mathcal{S}(\mathbb{R}^n)$. It remains to construct ψ. This can be done by setting $\hat{\psi} = \hat{\phi}/\hat{g}$ on V, $\hat{\psi} = 0$ elsewhere. The two functions then satisfy $\phi = g * \psi$ and ψ is in $\mathcal{S}(\mathbb{R}^n)$ for $\hat{\psi}$ is in $C_0^\infty(\mathbb{R}^n)$. □

Proof (of Theorem 3.3): Take two functions ϕ and ψ as in Lemma 3.4. Then for all $q>1$, we have by Young's inequality:

$$\|\mu * \phi_a\|_q = \|(\mu * g_a) * \psi_a\|_q \leqslant \|\mu * g_a\|_q \|\psi\|_1.$$

On the other hand,

$$\|\mu * g_a\|_q \leqslant \|\mu * |g_a|\|_q .$$

Both functions ϕ and $|g|$ fulfill the hypothesis of Lemma 3.2. The partition functions $a^{n(q-1)}\|\mu * \phi_a\|_q$ and $a^{n(q-1)}\|\mu * |g_a|\|_q$ therefore satisfy (2.6), and since they "sandwich" $\Lambda_a(\mu,q)$, the conclusion follows. □

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Filtered random variables, bialgebras, and convolutions

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We introduce the *filtered *-bialgebra* which is a multivariate generalization of the unital *-bialgebra $\mathbf{C}\langle X,X',P\rangle$ of polynomials in noncommuting variables $X=X^*$, $X'^*=X'$ and a projection $P=P^*=P^2$, endowed with the coproduct $\Delta(X)=X\otimes 1+1\otimes X$, $\Delta(X')=X'\otimes P+P\otimes X'$, with P being group-like. We study the associated convolutions, random walks and *filtered random variables*. The GNS representations of the limit states lead to *filtered fundamental operators* which are the CCR fundamental operators on the multiple symmetric Fock space $\Gamma(\mathcal{H})$ over $\mathcal{H}=L^2(\mathbf{R}^+,\mathcal{G})$, where $\mathcal{G}$ is a separable Hilbert space, multiplied by appropriate projections. The importance of filtered random variables and fundamental operators stems from the fact that by addition and strong limits one obtains from them the main types of noncommutative random variables and fundamental operators, respectively, regardless of the type of noncommutative independence. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1412465]

I. INTRODUCTION

In this work we introduce and study basic noncommutative random variables, from which the main types of noncommutative random variables can be constructed regardless of the notion of independence.

The basic idea of introducing filtered random variables is pretty straightforward and has its origin in the definition of the convolution of measures and the associated states. Let $\mathbf{C}[X]$ be the unital *-algebra of polynomials in $X^*=X$, with the coproduct

$$\Delta(X)=X\otimes 1+1\otimes X. \tag{1.1}$$

If ϕ, ψ are states on $\mathbf{C}[X]$, then

$$\phi\star_c\psi=\phi\otimes\psi\circ\Delta$$

gives the convolution of states corresponding to the classical convolution of measures.

In order to define a quantum deformation of this simple model, we replace the unit in the coproduct (1.1) by a projection P to get

$$\Delta(X')=X'\otimes P+P\otimes X',\quad \Delta(P)=P\otimes P. \tag{1.2}$$

Then, for given state ϕ on $\mathbf{C}[X']$, we define its noncommutative extension $\tilde{\phi}$ to $\mathbf{C}\langle X',P\rangle$, which is the free product $\mathbf{C}[X']*\mathbf{C}[P]$ with identified units, by

$$\tilde{\phi}(P^{\alpha}Y^{n_1}PY^{n_2}P\cdots Y^{n_k}P^{\beta})=\phi(Y^{n_1})\phi(Y^{n_2})\cdots\phi(Y^{n_k}),$$

where $\alpha,\beta\in\{0,1\}$ and $n_1,\ldots,n_k\in\mathbf{N}$, called the Boolean extension.[1] The convolution

$$\tilde{\phi}\uplus\tilde{\psi}=\tilde{\phi}\otimes\tilde{\psi}\circ\Delta,$$

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where Δ is given by (1.2), gives a quantum analog of the classical convolution of states, called the Boolean convolution. Note that by introducing P, which plays a similar role to the q-commuting operators in q-deformed Hopf *-algebras[2,3] and *-bialgebras,[4] we can deal with tensor coproducts (for a different formalism, see Ref. 5). The same holds for the m-free and free products of states.

This new convolution is very important since its generalization to the multivariate case, when restricted to suitable *-bialgebras, gives also m-free and free convolutions.[1,6] In the multivariate case we study the unital *-algebra $\hat{\mathcal{B}}$ over $\mathbf{C}$ generated by $X_k(\sigma)$, $P(\sigma)$ $k\in\mathbf{N}$, $\sigma\in\mathcal{P}(\mathbf{N})$, where $\mathcal{P}(\mathbf{N})$ is the power set of $\mathbf{N}$, with the involution given by $X_k(\sigma)=X_k^*(\sigma)$, $P(\sigma)^*=P(\sigma)$, and subject to the relations

$$P(\sigma)P(\tau)=P(\sigma\cap\tau),\quad P(\varnothing)=1,$$

$$P(\sigma)X_k(\tau)=X_k(\tau)P(\sigma)\quad \text{iff}\ \ k\in\sigma,$$

i.e., $P(\sigma)$'s are projections which ''partially commute'' with the variables $X_k(\sigma)$. When equipped with the coproduct and the counit

$$\hat{\Delta}(X_k(\sigma))=X_k(\sigma)\otimes P(\sigma)+P(\sigma)\otimes X_k(\sigma),$$

$$\hat{\Delta}(P(\sigma))=P(\sigma)\otimes P(\sigma),\quad \hat{\epsilon}(X_k(\sigma))=0,\quad \hat{\epsilon}(P(\sigma))=1,$$

the algebra $\hat{\mathcal{B}}$ becomes a unital *-bialgebra called *filtered *-bialgebra*. Therefore, we are in the position to study random walks[7] and stochastic processes over *-bialgebras.[4,8]

We take a suitable state $\hat{\phi}$ on $\hat{\mathcal{B}}$, which is obtained by lifting the tensor product state $\tilde{\phi}^{\otimes\infty}$ on $\otimes_{k=1}^{\infty}\mathbf{C}\langle Y_k,P_k\rangle$ to $\hat{\mathcal{B}}$ through the mapping which sends each $X_k(\sigma)$ onto Y_k and $P(\sigma)$ onto the tensor product of P_k's with $k\in\sigma$, where $Y_k^*=Y_k$ and P_k a projection. The state $\hat{\phi}$ is our noncommutative, ''filtered'' analog of the classical product measure (σ's play the role of filters due to ''partial commutations'').

The corresponding convolution central limit theorem (or discrete random walk), which plays the role of a noncommutative analog of the classical multivariate central limit theorem, gives, under the usual normalization, pointwise convergence of the Nth convolution power

$$\hat{\phi}^{\star N}=\hat{\phi}^{\otimes N}\circ\hat{\Delta}^{N-1},$$

where $\hat{\Delta}^{N-1}$ is the $N-1$th iteration of the coproduct $\hat{\Delta}$.

The summands produced by iterating the coproduct are called *filtered random variables* and can be viewed as quantum analogs of independent *random vectors*. It is important to note that by taking suitable linear combinations (strongly convergent series on the GNS pre-Hilbert space) of filtered random variables we obtain m-free (free) random variables. Thus all three basic notions of quantum independence in the axiomatic theory[9,10] (tensor, free, and Boolean) are covered by this scheme.

By considering random walks with continuous time, or stochastic processes over the filtered *-bialgebra, we obtain in the limit the vacuum expectation state in the multiple symmetric Fock space $\Gamma(\mathcal{H})$, where

$$\mathcal{H}=L^2(\mathbf{R}^+)\otimes\mathcal{G}$$

and $\mathcal{G}$ is a separable Hilbert space called the multiplicity space. The GNS representation leads to *filtered fundamental operators* which are the CCR fundamental operators on $\Gamma(L^2(\mathbf{R}^+)\otimes\mathcal{G})$, multiplied by projections $P^{(\sigma)}$, is the second quantization of the canonical projection onto subspaces of $L^2(\mathbf{R}^+)\otimes\mathcal{G}$ built from the modes (called *colors*) which belong to the set σ.

Fundamental operators associated with different notions of independence can be expressed in terms of the filtered ones. In particular, one can define bounded extensions to $\Gamma(L^2(\mathbf{R}^+)\otimes\mathcal{G})$ of

m-free creation and annihilation operators[11] as strongly convergent series of filtered creation and annihilation operators, respectively. This formalism enables us not only to embed the free (or, full) Fock space over $L^2(\mathbf{R}^+)$ in $\Gamma(\mathcal{H})$, but also decompose $\Gamma(\mathcal{H})$ into an orthogonal sum of subspaces which are isomorphic to the free Fock space.

The corresponding *filtered stochastic calculus* is developed in Ref. 12 and it is, in fact, a generalization of the Hudson–Parthasarathy calculus[13] (see also Ref. 14) on multiple symmetric Fock spaces[15] and includes a new version of the free calculus, originally developed for the Cuntz algebra,[16] as well as gives calculi for the hierarchy of *m*-free Brownian motions.[6] In that context, see also Refs. 17 and 18.

In Sec. II we introduce the filtered *-bialgebra which sets the framework for a unified approach to noncommutative probability. This leads to filtered random variables, which are introduced in the more general setting of unital *-algebras in Sec. III. Their combinatorics and the recurrence relation for the product state is given in Sec. IV. Convolution limit theorems are proved in Sec. V. In Sec. VI we introduce the filtered fundamental operators. These are used for the GNS construction of the limit of a sequence of random walks on the filtered *-bialgebra in Sec. VII. In Sec. VIII we determine the combinatorics of general filtered white noises. In Sec. IX we study in more detail extensions of the *m*-free and free creation and annihilation operators to all of $\Gamma(\mathcal{H})$. A free Fock space decomposition of $\Gamma(\mathcal{H})$ is established.

We denote all scalar products by $\langle .,. \rangle$ and identify operators and their ampliations if no confusion arises.

II. FILTERED BIALGEBRA AND CONVOLUTION

In this section we discuss the bialgebra in our construction and the associated convolution. For general background on this, we refer the reader to Refs. 4 and 7.

For simplicity, consider first the unital *-algebra $\mathbf{C}[X]$ of polynomials in the variable $X = X^*$ endowed with the coproduct

$$\Delta : \mathbf{C}[X] \to \mathbf{C}[X] \otimes \mathbf{C}[X]$$

given by

$$\Delta(X) = X \otimes 1 + 1 \otimes X \tag{2.1}$$

and the counit $\epsilon : \mathbf{C}[X] \to \mathbf{C}$ given by $\epsilon(X) = 0$. This coproduct leads to the *classical convolution* of measures and thus classical convolution of states.

Namely, if ϕ, ψ are states on $\mathbf{C}[X]$ associated with measures μ, ν on the real line, i.e.,

$$\phi(X^n) = \int_{\mathbf{R}} x^n \, \mathrm{d}\mu(x), \quad \psi(X^n) = \int_{\mathbf{R}} x^n \, \mathrm{d}\nu(x),$$

then the convolution of states

$$\phi \star_c \psi = \phi \otimes \psi \circ \Delta$$

corresponds to the classical convolution of measures $\mu \star_c \nu$ in the sense that

$$\phi \star_c \psi(X^n) = m_n(\mu \star_c \nu),$$

where $m_n(\mu \star_c \nu)$ is the nth moment of the measure $\mu \star_c \nu$.

The coproduct is a convenient tool to produce independent random variables.[7] Namely, by applying successive iterations of Δ to X, we obtain

$$\Delta^{N-1}(X) = \sum_{k=1}^{N} j_{l,N}(X),$$

where $\Delta^N := (\mathrm{id}\otimes\Delta^{N-1})\circ\Delta$ for $N>1$ with $\Delta^1=\Delta$, and the summands

$$j_{l,N}(X)=1^{\otimes(l-1)}\otimes X\otimes 1^{\otimes(N-l)},\quad 1\leqslant l\leqslant N,$$

can be viewed as independent random variables with respect to the state $\phi^{\otimes N}$.

The so-called *Boolean convolution* can be obtained by considering the unital*-algebra of polynomials in two noncommuting self-adjoint variables $\mathbf{C}\langle X',P\rangle$, where P is a projection, with the coproduct

$$\Delta:\mathbf{C}\langle X',P\rangle\to\mathbf{C}\langle X',P\rangle\otimes\mathbf{C}\langle X',P\rangle,$$

given by

$$\Delta(X')=X'\otimes P+P\otimes X',\quad \Delta(P)=P\otimes P, \tag{2.2}$$

and the counit $\epsilon(X')=0$, $\epsilon(P)=1$. It can be shown that this coproduct gives the Boolean convolution of states and thus the Boolean convolution of measures.[19] This follows from the hierarchy of freeness construction,[1] but a direct proof will be presented in the following.

Definition 2.1: If ϕ is a state on $\mathbf{C}[Y]$, where $Y^*=Y$, then its *Boolean extension* is the state on $\mathbf{C}\langle Y,P\rangle$, where P is a projection, given by the linear extension of

$$\tilde{\phi}(P^{\alpha}Y^{n_1}PY^{n_2}P\cdots Y^{n_k}P^{\beta})=\phi(Y^{n_1})\phi(Y^{n_2})\cdots\phi(Y^{n_k}), \tag{2.3}$$

where $\alpha,\beta\in\{0,1\}$ and $n_1,\ldots,n_k\in\mathbf{N}$, with $\tilde{\phi}(P)=1$. If ϕ is a state on the unital *-algebra $\mathcal{A}$, then its Boolean extension $\tilde{\phi}$ to the free product $\tilde{\mathcal{A}}=\mathcal{A}*\mathbf{C}[P]$ (units identified) is defined in an analogous way.

The Boolean extension of a state is a state since it is obtained as the Boolean product of the state ϕ on $\mathbf{C}[Y]$ and the unital *-homomorphism h on $\mathbf{C}[P]$ given by $h(P)=h(1)=1$.

In order to have a unified model for both convolutions it is now enough to incorporate both coproducts (2.1) and (2.2) into one scheme. This is done as follows. The unital *-algebra $\mathcal{B}=\mathbf{C}\langle X,X',P\rangle$ where $X=X^*$, $X'=X'^*$ and P is a projection, endowed with the coproduct $\Delta:\mathcal{B}\to\mathcal{B}\otimes\mathcal{B}$ and counit $\epsilon:\mathcal{B}\to\mathbf{C}$ given by

$$\Delta(X)=X\otimes 1+1\otimes X,\quad \Delta(X')=X'\otimes P+P\otimes X',$$

$$\Delta(P)=P\otimes P,\quad \epsilon(X)=\epsilon(X')=0,\quad \epsilon(P)=1$$

(in other words, X is primitive, X' is P-primitive, and P is group-like), becomes a unital *-bialgebra. Both classical and Boolean convolutions are recovered from $(\mathcal{B},\Delta,\epsilon)$, as we show in the following.

Proposition 2.2: Let $\eta:\mathcal{B}\to\mathbf{C}\langle Y,P\rangle$, where $Y=Y^*$ and $P^2=P=P^*$, be the linear and multiplicative extension of

$$\eta(X)=\eta(X')=Y,\quad \eta(P)=P,\quad \eta(1)=1$$

and, for states ϕ, ψ on $\mathbf{C}[Y]$, let $\phi_0=\tilde{\phi}\circ\eta$, $\psi_0=\tilde{\psi}\circ\eta$ with the convolution

$$\phi_0\star\psi_0=\phi_0\otimes\psi_0\circ\Delta, \tag{2.4}$$

where Δ is the coproduct for $\mathcal{B}$. Then the restrictions of $\phi_0\star\psi_0$ to $\mathbf{C}[X]$ and $\mathbf{C}[X']$, respectively, agree with $\phi\star_c\psi$ and $\phi\uplus\psi$, respectively.

Proof: Recall[19] that the Boolean convolution of states ϕ, ψ on $\mathbf{C}[X]$ and $\mathbf{C}[X']$, respectively, is defined to be the state $\phi\uplus\psi$ on $\mathbf{C}[Y]$ given by the linear extension of $\phi\uplus\psi(Y^n)=\phi*^B\psi((X+X')^n)$, where $\phi*^B\psi$ is the Boolean product of states on the free product $\mathbf{C}[X]*\mathbf{C}[X']$.

Note that ϕ_0 and ψ_0 are states since η is a unital *-homomorphism. That the restriction of the convolution (2.4) to $\mathbf{C}[X]$ gives classical convolution is obvious. In turn, the statement concerning the Boolean convolution follows from the fact that the subalgebras $\mathbf{C}[Y]\otimes P, P\otimes\mathbf{C}[Y]$ of $\mathbf{C}\langle Y,P\rangle\otimes\mathbf{C}\langle Y,P\rangle$ are Boolean independent with respect to the state $\tilde{\phi}\otimes\tilde{\psi}$. This fact can be easily seen from the following calculation:

$$\tilde{\phi}\otimes\tilde{\psi}(Y^{k_1}\otimes P)(P\otimes Y^{n_2})(Y^{k_2}\otimes P)(P\otimes Y^{n_2})\cdots)=\hat{\phi}\,(Y^{k_1}PY^{k_2}P\cdots)\hat{\psi}\,(PY^{n_1}PY^{n_2}\cdots)$$
$$=\phi(Y^{k_1})\psi(Y^{n_1})\phi(Y^{k_2})\psi(Y^{n_2})\cdots.$$

A more general setting of the Boolean product of states was given in Ref. 1. □

The quadruple $(\mathcal{B},\Delta,\epsilon,\phi_0)$ can be called the *random walk* (we follow Majid[7] in this terminology) on the *pair of quantum planes*. Note that on the quantum probability space level we may also study the pair $(\mathbf{C}\langle Y,P\rangle,\tilde{\phi})$, which corresponds to (polynomial functions on) a *pair of quantum real lines*.

Let us consider now the multivariate generalization of the *-bialgebra $\mathcal{B}$. In classical probability, the multivariate case in an algebraic formulation would be reached if we considered the unital *-algebra $\mathbf{C}[X_k;k\in\mathbf{N}]$ of polynomials in commuting variables $(X_k)_{k\in\mathbf{N}}$, with the classical coproduct

$$\Delta(X_k)=X_k\otimes 1+1\otimes X_k \tag{2.5}$$

and the counit $\epsilon(X_k)=0$.

Let us now define a quantum analog of this multivariate *-bialgebra, of which the bialgebra $\mathcal{B}$ is the ''one-dimensional'' version. Thus, introduce the unital *-algebra

$$\hat{\mathcal{B}}=\mathbf{C}\langle X_k(\sigma),P(\sigma);\ k\in\mathbf{N},\sigma\in\mathcal{P}(\mathbf{N})\rangle/J,$$

where $X_k(\sigma)=X_k^*(\sigma)$, $P(\sigma)^*=P(\sigma)$, $\mathcal{P}(\mathbf{N})$ is the power set of $\mathbf{N}$ and J is the two-sided ideal generated by the relations

$$P(\sigma)P(\sigma')=P(\sigma\cap\sigma'),\quad P(\varnothing)=1, \tag{2.6}$$

$$P(\sigma)X_k(\tau)=X_k(\tau)P(\sigma)\quad \text{iff}\ \ k\in\sigma, \tag{2.7}$$

i.e., the projection associated with the set σ (we call σ a *filter*) ''filters through'' the variables $X_k(\sigma)$ if the index $k\in\sigma$.

Proposition 2.3: The algebra $\hat{\mathcal{B}}$, equipped with the coproduct $\hat{\Delta}:\hat{\mathcal{B}}\to\hat{\mathcal{B}}\otimes\hat{\mathcal{B}}$ and the counit $\hat{\epsilon}:\hat{\mathcal{B}}\to\mathbf{C}$ given by

$$\hat{\Delta}(X_k(\sigma))=X_k(\sigma)\otimes P(\sigma)+P(\sigma)\otimes X_k(\sigma), \tag{2.8}$$

$$\hat{\Delta}(P(\sigma))=P(\sigma)\otimes P(\sigma),\quad \hat{\epsilon}(X_k(\sigma))=0,\quad \hat{\epsilon}(P(\sigma))=1 \tag{2.9}$$

*for all k and σ, is a unital *-bialgebra called filtered *-bialgebra.*

Proof: The coproduct and the counit preserve relations (2.6) and (2.7). □

By iterating this coproduct, called *filtered coproduct*, we obtain the sum

$$\hat{\Delta}^{N-1}(X_k(\sigma))=\sum_{l=1}^{N}\hat{j}_{l,N}(X_k(\sigma)) \tag{2.10}$$

of $P(\sigma)$-deformed random variables

$$\hat{j}_{l,N}(X_k(\sigma))=P(\sigma)^{\otimes l-1}\otimes X_k(\sigma)\otimes P(\sigma)^{\otimes(N-l)}, \tag{2.11}$$

where $\sigma \in \mathcal{P}(\mathbf{N})$, $k \in \mathbf{N}$, $1 \leqslant l \leqslant N$, $N \in \mathbf{N}$.

When we go over from quantum groups to quantum probability spaces, we identify $X_k(\sigma)$'s for all different σ and fixed k, as we did by using the map η in the "one-dimensional" case of Proposition 2.2. This is done in order to include different notions of independence in one scheme. For that purpose, we consider the mapping

$$\hat{\eta}: \ \hat{\mathcal{B}} \to \bigotimes_{k=1}^{\infty} \mathbf{C}\langle Y_k, P_k \rangle \tag{2.12}$$

given by the linear and multiplicative extension of

$$\hat{\eta}(P(\sigma)) = P_1^{r_1} \otimes P_2^{r_2} \otimes \cdots \otimes P_k^{r_k} \otimes \cdots, \tag{2.13}$$

$$\hat{\eta}(X_k(\sigma)) = 1_1 \otimes 1_2 \otimes \cdots \otimes 1_{k-1} \otimes Y_k \otimes 1_{k+1} \otimes \cdots, \tag{2.14}$$

where $\mathbf{C}\langle Y_k, P_k \rangle$ is the kth copy of $\mathbf{C}\langle Y, P \rangle$ and $r_k = 0$ if $k \in \sigma$, whereas $r_k = 1$ if $k \notin \sigma$. The infinite tensor product is taken with respect to the set $\{1_k, P_k, k \in \mathbf{N}\}$ (see Ref. 11 for the formal definition).

It can be seen that η is a unital *-homomorphism. Therefore, for a given state ϕ on $\mathbf{C}[Y]$, the functional

$$\hat{\phi} = \tilde{\phi}^{\otimes \infty} \circ \hat{\eta}, \tag{2.15}$$

is a state on $\hat{\mathcal{B}}$. It plays the role of a noncommutative analog of a vector state in classical probability. A generalization to vector states corresponding to products of different measures is immediate. It is enough to take

$$\hat{\phi} = \bigotimes_{k=1}^{\infty} \tilde{\phi}_k \circ \hat{\eta}, \tag{2.16}$$

where ϕ_k is a state on $\mathbf{C}[Y_k]$, $k \in \mathbf{N}$.

When we take (2.15) [or, (2.16)], the quadruple $(\hat{\mathcal{B}}, \hat{\Delta}, \hat{\epsilon}, \hat{\phi})$ will give our stationary *filtered random walk*, using the terminology of Majid,[7] which carries two structures, that of the unital *-bialgebra and that of the quantum probability space. The corresponding convolution of states

$$\hat{\phi} \star \hat{\psi} = \hat{\phi} \otimes \hat{\psi} \circ \hat{\Delta} \tag{2.17}$$

(or, products of states) will be called the *filtered convolution*. One of the main motivations to study the filtered *-bialgebras, convolutions, random walks, and stochastic processes comes from the following result (cf. Ref. 1).

Proposition 2.4: If $\hat{\phi}$ *and* $\hat{\psi}$ *are of the form* (2.16) *and* i *is the unital* *-*homomorphism*

$$i: \mathbf{C}\langle X_k, k \in \mathbf{N} \rangle \to \hat{\mathcal{B}}, \quad i(X_k) = X_k(\mathbf{N}),$$

then $\hat{\phi} \star \hat{\psi} \circ i$ *agrees with the classical convolution of products of states. If* $\hat{\phi}$ *and* $\hat{\psi}$ *are of the form* (2.15) *and* $i^{(m)}$ *denotes the unital* *-*homomorphism*

$$i^{(m)}: \mathbf{C}[X] \to \hat{\mathcal{B}}, \quad i^{(m)}(X) = \sum_{k=1}^{m} (X_k(k) - X_k(k-1))$$

where $X_k(p) = X_k(\{1, \ldots, p-1\})$, *then* $\hat{\phi} \star \hat{\psi} \circ i^{(m)}$ *agrees with the additive m-free convolution of states* $\phi \star_m \psi$ *on* $\mathbf{C}[X]$, $1 \leqslant m < \infty$. *The pointwise limit* $\lim_{m \to \infty} \hat{\phi} \star \hat{\psi} \circ i^{(m)}$ *agrees with the free convolution.*

Proof: The statement concerning the classical convolution of products of states is obvious since $P(\mathbf{N})=1$. In turn, the second part of the proposition is nontrivial and follows from the construction of *m*-free product states and the associated *-bialgebras (see Ref. 1, Sec. 5, where we also refer the reader for the definition of the *m*-free convolution). □

Since $\mathbf{C}\langle Y,P\rangle$ can be viewed as a *quantum pair of real lines*, on the quantum probability space level we can interpret our object of interest as (polynomial functions on) the product of infinitely many quantum pairs of real lines, which is our noncommutative analog of $\mathbf{R}^{\infty}$. On the bialgebra level, we have a bigger object since every variable X_k admits a family of different convolutions.

III. FILTERED RANDOM VARIABLES

In this section we introduce filtered random variables which are our noncommutative analogs of independent random vectors in the general setting of arbitrary unital *-algebras.

In analogy to the classical case, we obtain them by iterating the coproduct $\hat{\Delta}$ as in (2.10). Then, we embed $\hat{j}_{l,N}(X_k(\sigma))$ into $\hat{\mathcal{B}}^{\infty}$ to get

$$P(\sigma)^{\otimes(l-1)}\otimes X_k(\sigma)\otimes P(\sigma)^{\otimes\infty} \tag{3.1}$$

and generalize these to the arbitrary unital *-algebras. In order to do that, write (3.1) as the product

$$(1^{\otimes(l-1)}\otimes X_k(\sigma)\otimes 1^{\otimes\infty})(P(\sigma)^{\otimes(l-1)}\otimes 1\otimes P(\sigma)^{\otimes\infty})$$

of an ampliation of $X_k(\sigma)$ into $\hat{\mathcal{B}}^{\otimes\infty}$ and a projection indexed by σ. This shows that the definitions given in the following are a natural generalization of those of Sec. II.

Let $(\mathcal{A}_l)_{l\in L}$ be a family of unital *-algebras with units 1_l and let $(\phi_l)_{l\in L}$ be the corresponding family of states. Consider a noncommutative probability space $(\hat{\mathcal{A}}_1,\hat{\Phi}_1)$, where

$$\hat{\mathcal{A}}_1=\bigotimes_{l\in L}\hat{\mathcal{A}}_l^{\otimes\infty},\quad \hat{\Phi}_1=\bigotimes_{l\in L}\hat{\phi}_l^{\otimes\infty},$$

and $\tilde{\mathcal{A}}_l=\mathcal{A}_l*\mathbf{C}[P_l]$ is the free product with identified units, P_l being a projection, whereas $\tilde{\phi}$ is the Boolean extension of ϕ (Definition 2.1). The infinite tensor products are understood as in Ref. 11, with the canonical involution. This noncommutative probability space will be called the *multiple probability space* associated with the considered family of probability spaces since each of them appears infinitely many times in the considered tensor products. We will refer to those copies as *colors*. Roughly speaking, $\tilde{\mathcal{A}}_l^{\otimes\infty}$ and $\tilde{\phi}_l^{\otimes\infty}$ correspond to $\otimes_{k=1}^{\infty}\mathbf{C}\langle Y_k,P_k\rangle$ and $\tilde{\phi}^{\otimes\infty}$ for each $l\in L$, respectively, of Sec. II.

If $(\mathcal{H}_l,\pi_l,\Omega_l)$ is the GNS triple for the pair $(\mathcal{A}_l,\phi_l)$, then $(\mathcal{H}_l,\tilde{\pi}_l,\Omega_l)$ is the GNS triple for $(\tilde{\mathcal{A}}_l,\tilde{\phi}_l)$, $l\in L$, where $\tilde{\pi}_l$ agrees with π_l on $\mathcal{A}_l$ and $\tilde{\pi}_l(P_l)$ is the projection onto the cyclic vector Ω_l. For convenience, we can identify $x\in\mathcal{A}_l$ with $\pi_l(x)$, P_l with P_{Ω_l} and ϕ_l with the expectation state $\langle\Omega_l,.\Omega_l\rangle$ (see Ref. 11).

Guided by (3.1), from projections P_m we construct projections $\mathbf{P}(l,\sigma)$ to be elementary tensors in $\hat{\mathcal{A}}_1$ with components

$$\mathbf{P}(l,\sigma)_{m,k}=\begin{cases}P_m & \text{if } m\neq l \text{ and } k\notin\sigma\\ 1_m & \text{otherwise,}\end{cases}$$

where $\sigma\in\mathcal{P}(\mathbf{N})$ and $l\in L$. In the case when $\sigma=\{1,...,r-1\}$, we will write $\mathbf{P}(l,r)=\mathbf{P}(l,\sigma)$.

Definition 3.1: By *filtered random variables* we will understand elements of $\hat{\mathcal{A}}_1$ which are of the form

$$\mathbf{XP}, \tag{3.2}$$

where $\mathbf{X}=\mathbf{X}(l,k)$ is the (l,k)th ampliation of $x\in\mathcal{A}_l$ into $\hat{\mathcal{A}}_l$ and $\mathbf{P}=\mathbf{P}(l,\sigma)$, where $l\in L$, $k\in\mathbf{N}$, $\sigma\in\mathcal{P}(\mathbf{N})$. In particular, the unit $\mathbf{1}=\otimes_{l\in L}1_l^{\otimes\infty}$ is a filtered random variable.

If $L=\mathbf{N}$, filtered random variables can be represented as infinite matrices. Assume that k numbers the rows and l numbers the columns. For instance, for $x\in\mathcal{A}_2$, $\mathbf{X}=\mathbf{X}(2,3)$, and $\mathbf{P}=\mathbf{P}(2,4)$ we have

$$\mathbf{XP}=\begin{pmatrix} 1_1 & 1_2 & 1_3 & \cdots \\ 1_1 & 1_2 & 1_3 & \cdots \\ 1_1 & x & 1_3 & \cdots \\ P_1 & 1_2 & P_3 & \cdots \\ P_1 & 1_2 & P_3 & \cdots \\ . & . & . & \cdots \end{pmatrix}.$$

Note that if $L=\mathbf{N}$, multiplication of filtered random variables corresponds to Schur's multiplication of matrices.

Definition 3.2: Let $\tilde{\mathcal{A}}$ be the unital *-subalgebra of $\hat{\mathcal{A}}_1$ generated by all filtered random variables and let $\hat{\Phi}=\hat{\Phi}_1|\hat{\mathcal{A}}$. The noncommutative probability space $(\hat{\mathcal{A}},\hat{\Phi})$ will be called the *filtered probability space* associated with $(\mathcal{A}_l,\phi_l)_{l\in L}$ and the state $\hat{\phi}$ will be called the *filtered product* of $(\phi_l)_{l\in L}$. The unital *-subalagebras of $\hat{\mathcal{A}}$,

$$\hat{\mathcal{A}}_l=\langle\mathbf{XP}|\mathbf{X}=\mathbf{X}(l,k),\mathbf{P}=\mathbf{P}(l,\sigma),x\in\mathcal{A}_l,k\in\mathbf{N},\ \sigma\in\mathcal{P}(\mathbf{H})\rangle,\quad l\in L,$$

will be called *filtered with respect* to $\hat{\Phi}$.

Example 1: Let $*_{l\in L}\mathcal{A}_l$ denote the free product of $(\mathcal{A}_l)_{l\in L}$ with nonidentified units. Fix $k\in\mathbf{N}$, $\sigma\in\mathcal{P}(\mathbf{N})$ and define a *-homomorphism

$$j^{(k,\sigma)}:\quad *_{l\in L}\mathcal{A}_l\to\hat{\mathcal{A}}$$

as the linear extension of

$$j^{(k,\sigma)}(x_1\cdots x_n)=\mathbf{X}_1(l_1,k)\mathbf{P}(l_1,\sigma)\cdots\mathbf{X}_n(l_n,k)\mathbf{P}(l_n,\sigma)$$

for $x_i\in\mathcal{A}_{l_i}$, $l_1\neq l_2\neq\cdots\neq l_n$. Let us define the mapping

$$i:\quad *_{l\in L}\mathcal{A}_l\to\bigotimes_{l\in L}\mathcal{A}_l$$

as the linear extension of

$$i(x_1\cdots x_n)=i_{l_1}(x_1)\cdots i_{l_n}(x_n),$$

where i_l are canonical *-homomorphic embeddings of $\mathcal{A}_l$ into $\bigotimes_{l\in L}\mathcal{A}_l$. Then,

$$\hat{\Phi}\circ j^{(k,\sigma)}=\begin{cases}\otimes_{l\in L}\phi_l\circ i & \text{if } k\in\sigma\\ *^B_{l\in L}\phi_l & \text{if } k\notin\sigma\end{cases}$$

where $*^B_{l\in L}\phi_l$ denotes the Boolean (or, one-free) product of states $(\phi_l)_{l\in L}$ on $*_{l\in L}\mathcal{A}_l$. In other words, for fixed k, σ, the set $\{\mathbf{X}(l,k)\mathbf{P}(l,\sigma):l\in L\}$ is a family of tensor independent r.v. if $k\in\sigma$ and Boolean independent r.v. if $k\notin\sigma$ (see Ref. 1).

Example 2: As we showed in Ref. 1, the Boolean product is just the first-order approximation of the free product of states in free probability.[20] Higher order approximations given by the

modified hierarchy of m-free products[11] (the case with nonidentified units of the usual hierarchy of freeness[1]) can also be obtained from the filtered product. Namely, let $m \in \mathbf{N}$, and define

$$\overline{j^{(m)}}: \quad *_{l\in L}\mathcal{A}_l \to \hat{\mathcal{A}}$$

as the linear extension of

$$\overline{j^{(m)}}(x_1 \cdots x_n) = \overline{j_{l_1}^{(m)}}(x_1) \cdots \overline{j_{l_n}^{(m)}}(x_n),$$

where $x_i \in \mathcal{A}_{l_i}$, $l_1 \neq l_2 \neq \cdots \neq l_n$, and

$$\overline{j_l^{(m)}}(x) = \sum_{k=1}^{m} \mathbf{X}(l,k)(\mathbf{P}(l,k) - \mathbf{P}(l,k-1)) \tag{3.3}$$

for $x \in \mathcal{A}_l$. Then

$$\hat{\Phi} \circ \overline{j^{(m)}} = *_{l\in L}^{(m)} \phi_l,$$

where $*_{l\in L}^{(m)} \phi_l$ denotes the modified m-free product of states. If $m=\infty$, the series given by the representation of (3.3) converges strongly on the GNS pre-Hilbert space (see Ref. 11). Moreover,

$$\overline{j_l^{(\infty)}}(\mathbf{1}_l) = \mathbf{1}, \quad l \in L$$

and thus $\hat{\Phi} \circ \overline{j^{(\infty)}}$ is well defined on the free product of $\mathcal{A}_l$, $l \in L$, with identified units and agrees on it with the free product of states (for details, see Ref. 11). Thus, the variables $\overline{j_l^{(m)}}(x)$, $x \in \mathcal{A}_l$, $l \in L$, are m-free random variables for $m \in \mathbf{N}$ and free random variables if $m=\infty$.

IV. COMBINATORICS

Let us now introduce a new class of partitions which is crucial to the combinatorics of filtered random variables.

Definition 4.1: Let $\vec{k}=(k_1,\ldots,k_n)$ and $\vec{\sigma}=(\sigma_1,\ldots,\sigma_n)$ be color and filter tuples of natural numbers and sets of natural numbers, respectively. A partition $R=\{R_1,\ldots,R_q\}$ of the set $\{1,...,n\}$ will be called $(\vec{k},\vec{\sigma})$-*adapted* if and only if it satisfies the conditions

(A1) $\forall 1 \leqslant q \leqslant n \forall i,j \in R_q, \quad k_i = k_j$

(A2) If $i<m<j$, where $i,j \in R_q$ and $m \notin R_q$, then $k_i = k_j \in \sigma_m$.

The collection of all $(\vec{k},\vec{\sigma})$-adapted partitions (pair partitions) will be denoted by $\mathcal{P}_n(\vec{k},\vec{\sigma})$ ($\mathcal{P}_n^{\text{pair}}(\vec{k},\vec{\sigma})$). The partitions of $\{1,\ldots,n\}$ which are not $(\vec{k},\vec{\sigma})$-adapted will be called $(\vec{k},\vec{\sigma})$-*nonadapted*.

In other words, $\mathcal{P}_n(\vec{k},\vec{\sigma})$ is the subset of all partitions $\mathcal{P}_n$ of $\{1,...,n\}$ which are adapted to the tuples $\vec{k}$ and $\vec{\sigma}$ in the following sense: (A1) colors corresponding to the elements of the same block have to match, (A2) between the elements of a given block there are no filters associated with other blocks which separate them. In particular, if $k_i=k$, $\sigma_i=\sigma$ for all $1 \leqslant i \leqslant n$, then the two extreme cases are given by

$$\mathcal{P}_n(\vec{k},\vec{\sigma}) = \begin{cases} \mathcal{P}_n & \text{if } k \in \sigma \\ \mathcal{P}_n^{\text{int}} & \text{if } k \notin \sigma, \end{cases}$$

where $\mathcal{P}_n^{\text{int}}$ denotes the interval partitions of $\{1,\ldots,n\}$. In turn, if $\sigma_i = \mathbf{N}$ for all $i=1,...,n$, then

$$\mathcal{P}_n(\vec{k},\vec{\sigma}) = \mathcal{P}_n(\vec{k}),$$

where $\mathcal{P}_n(\vec{k})$ denotes all partitions R of the set $\{1,\ldots,n\}$ such that $k_i=k_j$ iff i,j belong to the same block of R (this corresponds to the classical multivariate case).

Definition 4.2: If R is $(\vec{k},\vec{\sigma})$-nonadapted, then the unique coarsest subpartition of R which is $(\vec{k},\vec{\sigma})$-adapted will be denoted by $R(\vec{k},\vec{\sigma})$.

Examples: Consider the partition

$$R=\{\{1,3,5\},\{2,4\}\}$$

of {1, ..., 5} and let the color tuple be given by $\vec{k}=(1,1,2,1,1)$. Then R is not $(\vec{k},\vec{\sigma})$-adapted for any $\vec{\sigma}$ since it does not satisfy (A1). If we take now the filter tuple $\vec{\sigma}=(\sigma_1,\ldots,\sigma_5)$ given by $\sigma_i=\{1,\ldots,r_i-1\}$, with $r_1=r_3=r_5=1$, $r_2=r_4=2$, then

$$R(\vec{k},\vec{\sigma})=\{\{1\},\{2\},\{3\},\{4\},\{5\}\}.$$

In turn, if we take $\vec{\tau}=(\tau_1,\ldots,\tau_5)$, where $\tau_i=\{1,\ldots,s_i-1\}$ and $s_1=s_5=1$ and $s_2=s_3=s_4=2$, then

$$R(\vec{k},\vec{\tau})=\{\{1,5\},\{2,4\},\{3\}\}.$$

We will see that partitions which are not $(\vec{k},\vec{\sigma})$-adapted are less important since they do not survive in the limit theorems. Therefore, there is an analogy with the crossing and noncrossing partitions in free probability, the $(\vec{k},\vec{\sigma})$-adapted playing a similar role to noncrossing partitions, whereas the non-$(\vec{k},\vec{\sigma})$-adapted behave like crossing partitions.

Let us give a recurrence formula for moments of filtered random variables, or ''filtered moments.'' It is convenient to introduce the following notions.

Definition 4.3: Given a tuple of pairs $((l_1,k_1),\ldots(l_n,k_n))$, we will say that (l_j,k_j) is a *singleton* if $(l_j,k_j)\neq(l_i,k_i)$ for all $i\neq j$. If $(l_i,k_i)=(l_j,k_j)$ for $i<j$ such that there is no $i<r<j$ for which $(l_r,k_r)=(l_i,k_i)$ and there exists $i<m<j$ such that $l_m\neq l_i$ and $k_i\notin\sigma_m$, then we will say that the filter σ_m *separates* (l_i,k_i) and (l_j,k_j).

Proposition 4.4: Let $\mathbf{X}_i:=\mathbf{X}(l_i,k_i)$, $\mathbf{P}_i:=\mathbf{P}(l_i,\sigma_i)$, $1\leqslant i\leqslant n$, *where* $x_i\in\mathcal{A}_{l_i}$, $l_i\in L$, $k_i\in\mathbf{N}$, $\sigma_i\in\mathcal{P}(\mathbf{N})$, *with* $n\in\mathbf{N}$, *and* $(l_1,k_1)\neq(l_2,k_2)\neq\ldots\neq(l_n,k_n)$. *Then*

$$\hat{\Phi}(\mathbf{X}_1\mathbf{P}_1\mathbf{X}_2\mathbf{P}_2\cdots\mathbf{X}_n\mathbf{P}_n)=\hat{\Phi}(\mathbf{X}_1\mathbf{P}_1)\hat{\Phi}(\mathbf{X}_2\mathbf{P}_2\cdots\mathbf{X}_n\mathbf{P}_n)$$

if (l_1,k_1) *is a singleton, or if there exists a filter* σ_m *which separates* (l_1,k_1) *and* (l_r,k_r), *where* r *is the first index for which* $(l_1,k_1)=(l_r,k_r)$, *and otherwise*

$$\hat{\Phi}(\mathbf{X}_1\mathbf{P}_1\mathbf{X}_2\mathbf{P}_2\cdots\mathbf{X}_n\mathbf{P}_n)=\hat{\Phi}(\mathbf{X}_2\mathbf{P}_2\cdots\mathbf{X}_1\mathbf{X}_r\mathbf{P}_r\cdots\mathbf{X}_n\mathbf{P}_n).$$

Proof: These formulas follow from the definition of filtered random variables. □

Proposition 4.5: Under the assumptions of Proposition 4.4,

$$\hat{\Phi}(\mathbf{X}_1\mathbf{P}_1\cdots\mathbf{X}_n\mathbf{P}_n)=\hat{\Phi}(\mathbf{X}_{B_1})\cdots\hat{\Phi}(\mathbf{X}_{B_r})=\phi_{l(B_1)}(x_{B_1})\cdots\phi_{l(B_r)}(x_{B_r}),$$

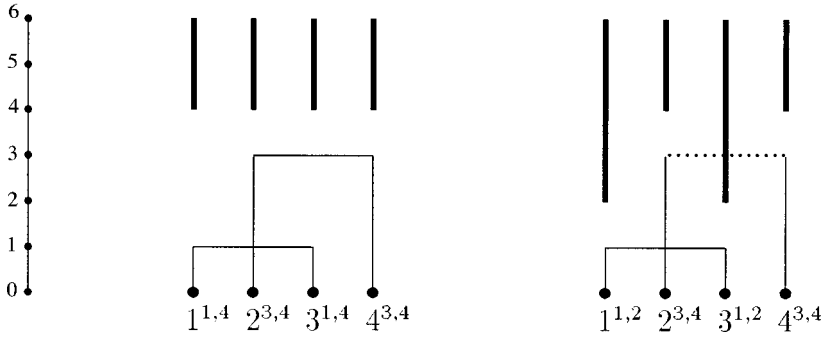
where R *is the partition associated with the tuple* $(l_1,\ldots,l_n)$, $B_1,\ldots,B_r$ *are the blocks of* $R(\vec{k},\vec{\sigma})$, $\mathbf{X}_B=\Pi_{j\in B}\mathbf{X}_j$ *and* $x_B=\Pi_{j\in B}x_j$ *are products taken in the natural order, and* $l(B)$ *is the index* $l\in L$ *associated with block* B.

Proof: This is a straightforward consequence of Proposition 4.4 and the fact that if $j_1,\ldots,j_r$ are elements of the same block $B\in R(\vec{k},\vec{\sigma})$, then

$$\hat{\Phi}(\mathbf{X}_{j_1}\mathbf{P}_{j_1}\cdots\mathbf{X}_{j_r}\mathbf{P}_{j_r})=\hat{\Phi}(\mathbf{X}_{j_1}\cdots\mathbf{X}_{j_r})=\phi_{l(B)}(x_{j_1}\cdots x_{j_r}).$$

(Definition 4.2 is crucial here.) □

Example: Let $L=\mathbf{N}$ and take $x_1,x_3\in\mathcal{A}_1$ and $x_2,x_4\in\mathcal{A}_2$. Then the partition $R=\{\{1,3\},\{2,4\}\}$ is associated with the tuple $(l_1,l_2,l_3,l_4)=(1,2,1,2)$. Let us consider two cases of color and filter tuples: (i) $\vec{k}=(1,3,1,3)$, $\vec{\sigma}=(4,4,4,4)$ and (ii) $\vec{m}=(1,3,1,3)$, $\vec{\tau}=(2,4,2,4)$. Then the corresponding "filtered moments" can be obtained by refinement of R and represented in terms of diagrams. By $p^{k,r}$ we understand the number p associated with color k and filter $\{1,...,r-1\}$.



In the diagrams, thick lines represent complements of filters, thin vertical lines represent the color (if the color is k, then their height is equal to k units on the axis shown), thin horizontal lines show connections between numbers which form a block, and the dotted line in the second diagram shows a connection (between 1 and 3) which is not realized (the filter $\tau_3=\{1\}$ "blocks" connections between colors $\geqslant 2$). The corresponding moments are given by

$$\text{(i)}\quad \phi_1(x_1x_3)\phi_2(x_2x_4),\quad \text{(ii)}\quad \phi_1(x_1x_3)\phi_2(x_2)\phi_2(x_4),$$

respectively. This simple example shows how a filter may kill certain connections in the "classical" partition R—this is the effect of "quantum" (filtered) independence.

V. CONVOLUTION LIMIT THEOREMS

In this section we will prove the central limit theorem and Poisson's limit theorem for filtered convolutions of states on the bialgebra $\hat{\mathcal{B}}$. We choose the convolution formulation for clarity of exposition, but the general case, based on the filtered product of states, is done in an analogous fashion.

The combinatorics of filtered convolution powers

$$\hat{\phi}^{\star N}=\hat{\phi}^{\otimes N}\circ\hat{\Delta}^{N-1},$$

where $N\in\mathbf{N}$, is given by Lemma 5.1. To a large extent we follow our approach for the convolution powers of q-deformed states on $U_q(su(2))$ given in Ref. 2.

Lemma 5.1: Let $\vec{k}=(k_1,\ldots,k_n)$, $\vec{\sigma}=(\sigma_1,\ldots,\sigma_n)$, *where* $k_i\in\mathbf{N}$, $\sigma_i\in\mathcal{P}(\mathbf{N})$, $1\leqslant i\leqslant n$, *and let* $N\in\mathbf{N}$. *Then*

$$\hat{\phi}^{\star N}(X_{k_1}(\sigma_1)\cdots X_{k_n}(\sigma_n))=\sum_{p=1}^{n}(N)_p\sum_{R=\{R_1,\ldots,R_p\}\in\mathcal{P}_n}\prod_{B\in R(\vec{k},\vec{\sigma})}\hat{\phi}(X_B),\tag{5.1}$$

where $(N)_p=N(N-1)\cdots(N-p+1)$ *and* $X_B=\pi_{i\in B}X_{k_i}(\sigma_i)$ *for the block* B *of the partition* $R(\vec{k},\vec{\sigma})$, *with the product taken in the natural order*.

Proof: Denote $X_1=X_{k_1}(\sigma_1),\ldots,X_n=X_{k_n}(\sigma_n)$. Using the notation of (2.11), we have

$$\hat{\phi}^{\star N}(X_1\cdots X_n)=\sum_{l_1,\ldots l_n=1}^{n}\hat{\phi}^{\otimes N}(\hat{j}_{l_1,N}(X_1)\cdots\hat{j}_{l_n,N}(X_n))$$

and

$$\hat{j}_{l_1,N}(X_1)\cdots\hat{j}_{l_n,N}(X_n)=\prod_{m=1}^{n} P(\sigma_m)^{\otimes(l_m-1)}\otimes X_m\otimes P(\sigma_m)^{\otimes(N-l_m)}.$$

The tuple $(l_1,\ldots,l_n)$ defines a partition R of the set $\{1,\ldots,n\}$ in the usual way. Namely, if $\{l_1,\ldots,l_n\}=\{k_1,\ldots,k_r\}$, where k_j's are all different, then $R_j=\{i:l_i=k_j\}$. Thus, from (2.15) we get

$$\hat{\phi}^{\otimes N}(\hat{j}_{l_1,N}(X_1)\cdots\hat{j}_{l_n,N}(X_n))=\prod_{i=1}^{r}\hat{\phi}(\xi_i^R(X_1\cdots X_n))$$

where ξ_i^R is a multiplicative extension of the mapping

$$\xi_i^R(X_p)=\begin{cases}P(\sigma_p) & \text{if } p\notin R_i\\ X_p & \text{if } p\in R_i\,.\end{cases}$$

Now, if $1\leqslant r\leqslant n$, then for each partition R consisting of r blocks, there are $(N)_r$ tuples $(l_1,\ldots,l_n)$ which give the same contribution $\Pi_i^r\hat{\phi}(\xi_i^R(X_1\cdots X_n))$ (the same combinatorial argument is presented in Ref. 2 in more detail). Thus

$$\hat{\phi}^{\star N}(X_1\cdots X_n)=\sum_{r=1}^{n}(N)_p\sum_{R=\{R_1,\ldots,R_p\}}\prod_{i=1}^{r}\hat{\phi}(\xi_{i=1}^R(X_1\cdots X_n)).$$

Finally, note that

$$\prod_{j=1}^{r}\hat{\phi}(\xi_i^R(X_1\cdots X_n))=\hat{\phi}(X_{B_1})\cdots\hat{\phi}(X_{B_r}),$$

where $B_1,\ldots,B_r$ are blocks of the partition $R(\vec{k},\vec{\sigma})$ since every block R_j of R splits up into subblocks for which all k_i's are the same and are not separated by any filters due to the way $\tilde{\phi}$ separates words. It is also worth noting that $\hat{\phi}(X_B)=\phi(X^{\#B})$ where # stands for the number of elements. □

In order to state the central limit theorem, let us introduce the gradation on $\hat{\mathcal{B}}$ given by $d(X_k(\sigma))=1$ and $d(P(\sigma))=0$ for all k and σ. Then, for $N\in\mathbf{N}$, define

$$D_{1/\sqrt{N}}(W)=\frac{1}{N^{d(W)/2}}W,$$

where W is a word in $\hat{\mathcal{B}}$ and $d(W)$ is its degree.

Corollary 5.2: Consider a family of states ϕ_N on $\mathbf{C}[Y]$, where $N\in\mathbf{N}$ and suppose that the limits

$$\lim_{N\to\infty}\phi_N(Y^k)=Q(k)$$

exist and are finite for all $k\in\mathbf{N}$. Then

$$\lim_{N\to\infty}\hat{\phi}_N^{\star N}(X_{k_1}(\sigma_1)\cdots X_{k_n}(\sigma_n))=\sum_{R\in\mathcal{P}_n(\vec{k},\vec{\sigma})}\prod_{B\in R}Q(\#B),\tag{5.2}$$

where $\#B$ is the number of elements in the block B.

Proof: It is an immediate consequence of Lemma 5.1 since if $R \in \mathcal{P}_n \backslash \mathcal{P}_n(\vec{k},\vec{\sigma})$, then the number of blocks in $R(\vec{k},\vec{\sigma})$ is strictly greater than the number of blocks in R which makes the contribution from R disappear as $N \to \infty$. □

Theorem 5.3 (central limit theorem): *Let* $k_i \in \mathbf{N}$, $\sigma_i \in \mathcal{P}(\mathbf{N})$, $i=1,\ldots,n$. *Suppose that* $\hat{\phi}(X_{k_i}(\sigma_i))=0$ *and* $\hat{\phi}(X_{k_i}^2(\sigma_i))=1$ *for* $i=1,...,n$. *If n is even, then*

$$\lim_{N\to\infty} \hat{\phi}^{\star N} \circ D_{1/\sqrt{N}}(X_{k_1}(\sigma_1)\cdots X_{k_n}(\sigma_n)) = |\mathcal{P}_n^{\mathrm{pair}}(\vec{k},\vec{\sigma})| \tag{5.3}$$

and, if n is odd, the limit vanishes.

Proof: It is enough to use Lemma 5.1 and notice that if there is a singleton in R, then there is no contribution from such a partition to the right-hand side of (5.1). In turn, if there are no singletons, then $(N)_p/N^{n/2} \to 0$ unless $2p=n$. That means that in the limit only pair-partitions may give a nonzero contribution. However, note that those pair partitions which are not $(\vec{k},\vec{\sigma})$-adapted give zero since in that case the number of blocks of $R(\vec{k},\vec{\sigma})$ is strictly greater than the number of blocks of R and $\Pi_{B\in R(\vec{k},\vec{\sigma})}\hat{\phi}(X_B)=0$ by the mean zero assumption.

Example 1: Note that if $\sigma_i=\mathbf{N}$ for all $1\leqslant i\leqslant n$ and all n, we obtain $|\mathcal{P}_n^{\mathrm{pair}}(\vec{k})|$ on the right-hand side of (5.3) which gives the moments of the classical multivariate Gaussian law.

Example 2: Here we give some one-dimensional examples. If $k_i=k$ and $\sigma_i=\sigma$ for $1\leqslant i\leqslant n$ and all n, then we obtain the Gaussian law if $k\in\sigma$ and the one-free (or, Boolean) central limit law corresponding to the discrete measure $\mu^{(1)}=1/2(\delta_{-1}+\delta_1)$ if $k\notin\sigma$. In turn, if we take

$$\Delta^{(m)} = \hat{\Delta} \circ \overline{j^{(m)}}, \tag{5.4}$$

where $\overline{j^{(m)}}$ is given by (3.3), we obtain the m-free coproduct defined in Ref. 1, for which the convolution powers tend to the m-free central limit laws and approximate pointwise the Wigner semicircle law for $m=\infty$. For details, see Ref. 6.

Theorem 5.4 (Poisson's limit theorem): *Under the assumptions of Corollary 5.2, suppose that* $Q(k)=\lambda$ *for all* $k\in\mathbf{N}$, *where* $\lambda>0$. *Then*

$$\lim_{N\to\infty} \hat{\phi}_N^{\star N}(X_{k_1}(\sigma_1)\cdots X_{k_n}(\sigma_n)) = \sum_{R\in\mathcal{P}_n(\vec{k},\vec{\sigma})} \lambda^{b(R)} \tag{5.5}$$

where $b(R)$ *is the number of blocks of R.*

Proof: It is an immediate consequence of Corollary 5.2. □

Example 1: Let us first give some one-dimensional examples. Again, if $k_i=k$ and $\sigma_i=\sigma$ for $1\leqslant i\leqslant n<\infty$, then we obtain the classical Poisson law for $k\in\sigma$ and the one-free (or Boolean) Poisson law for $k\notin\sigma$ corresponding to the discrete measure $\mu_\lambda^{(1)}=1/(1+\lambda)(\delta_0+\lambda\delta_{1+\lambda})$. Considering linear combinations of sample sums as in the preceeding example, we obtain the m-free Poisson laws for $m\in\mathbf{N}$ and the free Poisson law[21] for $m=\infty$ (see Ref. 6).

Example 2: If we take $\hat{\phi}$ given by (2.16), i.e., corresponding to the product of measures, then we can generalize Lemma 5.1 and Corollary 5.2 to the effect that if $\lim_{N\to\infty}\phi_{s,N}(Y^k)=\lambda_s$ where $\lambda_s>0$, $s\in\mathbf{N}$, then the right-hand side of (5.5) takes the form

$$\sum_{R\in\mathcal{P}_n(\vec{k},\vec{\sigma})} \lambda_{s_1}\lambda_{s_2}\cdots\lambda_{s_p},$$

where $s_1,\ldots,s_p$ correspond to the blocks $B_1,\ldots,B_p$ of the partition $R(\vec{k},\vec{\sigma})$ and denote their colors [which are the same within one block by (A1) of Definition 4.1]. These moments are the moments of the multivariate classical Poisson law.

VI. FILTERED FUNDAMENTAL OPERATORS

In this section we recall basic facts concerning multiple symmetric Fock spaces over $\mathcal{K}\equiv L^2(\mathbf{R}^+)$, which will be the underlying space for the filtered fundamental processes.

Let $\mathcal{G}$ be a separable Hilbert space with a countably infinite fixed orthonormal basis $(e_n)_{n\in\mathbf{N}}$. It is called the *multiplicity space*. By a *multiple symmetric Fock space* over $\mathcal{K}$ we understand the symmetric Fock space over $\mathcal{H}=L^2(\mathbf{R}^+,\mathcal{G})\cong L^2(\mathbf{R}^+)\otimes\mathcal{G}\equiv\mathcal{K}\otimes\mathcal{G}$, namely

$$\Gamma(\mathcal{H})=\mathbf{C}\Omega\oplus\bigoplus_{n=1}^{\infty}\mathcal{H}^{\circ n}$$

where $\mathcal{H}^{\circ n}$ denotes the nth symmetric tensor power of $\mathcal{H}$ and Ω is the vacuum vector, with the scalar product given by $\langle\Omega,\Omega\rangle=1$, $\langle\Omega,u\rangle=0$ and

$$\langle u_1\circ\cdots\circ u_n,v_1\circ\cdots\circ v_m\rangle=\delta_{n,m}\frac{1}{n!}\sum_{\sigma\in\mathbf{S}_n}\langle u_1,v_{\sigma(1)}\rangle\cdots\langle u_n,v_{\sigma(n)}\rangle,$$

where

$$u_1\circ\cdots\circ u_n=\frac{1}{n!}\sum_{\sigma\in\mathbf{S}_n}u_{\sigma(1)}\otimes\cdots\otimes u_{\sigma(n)}$$

and $\mathbf{S}_n$ denotes the symmetric group of order n.

Denote by $\mathcal{H}^{(\sigma)}$ the linear subspace of $\mathcal{H}$ spanned by all $u\in\mathcal{H}$ of the form

$$u=\sum_{k\in\sigma}u^{(k)}\otimes e_k,$$

where $\sigma\in\mathcal{P}(\mathbf{N})$. In particular, we put $\mathcal{H}^{(\varnothing)}=\{0\}$. The set σ will be called a *filter* and the associated canonical projection will be denoted $\pi^{(\sigma)}:\mathcal{H}\to\mathcal{H}^{(\sigma)}$ with $v^{(\sigma)}=\pi^{(\sigma)}v$ for any $v\in\mathcal{H}$. Then let $P^{(\sigma)}:\Gamma(\mathcal{H})\to\Gamma(\mathcal{H}^{(\sigma)})$ be the second quantization of $\pi^{(\sigma)}$. Thus, if $\varepsilon(v)$ is an exponential vector in $\Gamma(\mathcal{H})$, i.e.,

$$\varepsilon(v)=\bigoplus_{n=0}^{\infty}\frac{1}{\sqrt{n!}}v^{\otimes n}$$

with $v^{\otimes 0}=\Omega$, we have $P^{(\sigma)}\varepsilon(u)=\varepsilon(u^{(\sigma)})$.

Of special importance will be subspaces $\mathcal{H}^{(r)}$ of $\mathcal{H}$ spanned by all $u\in\mathcal{H}$ of the form

$$u=\sum_{k=1}^{r-1}u^{(k)}\otimes e_k,$$

where $r>1$, i.e., here $\sigma=\{1,...,r-1\}$; we set $\mathcal{H}^{(1)}=\{0\}$. In $\Gamma(\mathcal{H})$, we will use the *finite particle domain* $\Gamma_0(\mathcal{H})$, i.e., the linear space generated by vectors of the form

$$v_1\circ v_2\circ\cdots\circ v_n,$$

where $v_1,\ldots,v_n\in\mathcal{H}$, $n\in\mathbf{N}$.

Since $\mathcal{H}$ can be viewed as a direct sum of infinitely many copies of $\mathcal{K}$ and we need some convenient terminology concerning the numbering of those copies, we will refer to them as *colors*. Thus, in the direct sum decomposition

$$\mathcal{H}=\bigoplus_{k\in\mathbf{N}}\mathcal{K}\otimes e_k$$

the kth summand will be associated with the kth color and we will say that nonzero vectors from that summand are of kth color. In addition, to the zero vector we assign the 0th color.

By *filtered creation and annihilation operators* we will understand operators given by

$$a^{(\sigma)*}(f\otimes e_k)=a^*(f\otimes e_k)P^{(\sigma)}, \tag{6.1}$$

$$a^{(\sigma)}(f\otimes e_k)=P^{(\sigma)}a(f\otimes e_k), \tag{6.2}$$

respectively, where $a^*(f\otimes e_k)$ and $a(f\otimes e_k)$ are the usual boson creation and annihilation operators.[14] Thus, filtered creation operators first "filter out particles of colors which are not in σ and then create a particle of given color," whereas the filtered annihilation operators "first annihilate a particle of a given color and then filter out particles of colors which are not in σ."

In addition, we define

$$a^{(k,\sigma)\circ}=a^{(k)\circ}P^{(\sigma\cup\{k\})} \tag{6.3}$$

and call *filtered number operators*. In an analogous fashion one can define exchange operators.

Proposition 6.1: The finite particle domain $\Gamma_0(\mathcal{H})$ is contained in the domains of filtered fundamental operators. Furthermore, the following relations hold:

$$a^{(\sigma)}(f\otimes e_k)(v_1\circ v_2\circ\cdots\circ v_n)=\frac{1}{\sqrt{n}}\sum_{j=1}^{n}\langle f,v_j^{(k)}\rangle v_1^{(\sigma)}\circ\cdots\circ\check{v}_j\circ\cdots\circ v_n^{(\sigma)},$$

$$a^{(\sigma)*}(f\otimes e_k)(v_1\circ v_2\circ\cdots\circ v_n)=\sqrt{n+1}(f\otimes e_k)\circ v_1^{(\sigma)}\circ\cdots\circ v_n^{(\sigma)},$$

$$a^{(k,\sigma)\circ}(v_1\circ v_2\circ\cdots\circ v_n)=\sum_{j=1}^{n}v_1^{(\sigma)}\circ\cdots(v_j^{(k)}\otimes e_k)\circ\cdots\circ v_n^{(\sigma)}$$

with $a^{(\sigma)}(f\otimes e_k)\Omega=0$, $a^{(\sigma)*}(f\otimes e_k)\Omega=f\otimes e_k$ *and* $a^{(k,\sigma)0}\Omega=0$, *where* $v_1,\ldots,v_n\in\mathcal{H}$, $k\in\mathbf{N}$, $\sigma\in\mathcal{P}(\mathbf{N}),n\in\mathbf{N}$.

Proof: The first statement follows from the definitions (6.1)–(6.3) and an analogous property of the canonical (CCR) operators and the fact that the projections $P^{(\sigma)}$ leave the finite particle domain invariant. Similarly, the relations follow immediately from the analogous formulas for the canonical (CCR) operators (we use Hudson–Parthasarathy's normalization). □

Lemma 6.2: Filtered creation and annihilation operators satisfy the following relations on the finite particle domain:

$$a^{(\sigma)}(f\otimes e_k)a^{(\tau)*}(g\otimes e_l)-a^{(\tau)*}(g\otimes e_l)a^{(\sigma)}(f\otimes e_k)P^{(\tau)}]_{\{l\in\sigma\}}=\delta_{k,l}\langle f,g\rangle P^{(\sigma\cap\tau)}$$

for any $k,\ l\in\mathbf{N},\ \sigma,\ \tau\in\mathcal{P}(\mathbf{N}),\ f,\ g\in\mathcal{K}$.

Proof: In the proof given below we understand that the equations hold on the finite particle domain, but it remains valid on the whole intersection of the domains of the considered filtered operators. Using canonical commutation relations (CCR) of the form

$$a(f\otimes e_k)a^*(g\otimes e_l)-a^*(g\otimes e_l)a(f\otimes e_k)=\delta_{k,l}\langle f,g\rangle,$$

we obtain

$$\begin{aligned}a^{(\sigma)}(f\otimes e_k)a^{(\tau)*}(g\otimes e_l)&=P^{(\sigma)}a(f\otimes e_k)a^*(g\otimes e_l)P^{(\tau)}\\&=P^{(\sigma)}a^*(g\otimes e_l)a(f\otimes e_k)P^{(\tau)}+\delta_{k,l}\langle f,g\rangle P^{(\sigma\cap\tau)}.\end{aligned}$$

Now, note that if $l\notin\sigma$, then

$$P^{(\sigma)}a^*(g\otimes e_l)a(f\otimes e_k)P^{(\tau)}=0$$

and we obtain

$$a^{(\sigma)}(f\otimes e_k)a^{(\tau)*}(g\otimes e_l)=\delta_{k,l}\langle f,g\rangle P^{(\sigma\cap\tau)}.$$

Consider now the case $l\in\sigma$. Then

$$\begin{aligned}&P^{(\sigma)}a^*(g\otimes e_l)a(f\otimes e_k)P^{(\tau)}-a^*(g\otimes e_l)P^{(\sigma\cap\tau)}a(f\otimes e_k)P^{(\tau)}\\&\quad=a^*(g\otimes e_l)(P^{(\sigma)}-P^{(\sigma\cap\tau)})a(f\otimes e_k)P^{(\tau)}\end{aligned}$$

since $P^{(\sigma)}$ commutes with $a^*(g\otimes e_l)$ for $l\in\sigma$. Note that if $\sigma\subseteq\tau$, then $P^{(\sigma)}=P^{(\sigma\cap\tau)}$ and thus the above expression vanishes. In turn, if $\tau\subseteq\sigma$, then $P^{(\sigma)}-P^{(\sigma\cap\tau)}=P^{(\sigma)}-P^{(\tau)}$. However,

$$P^{(\tau)}:\quad\Gamma(\mathcal{H})\to\Gamma(\mathcal{H}^{(\tau)}).$$

and $a(f\otimes e_k)$ leaves $\Gamma(\mathcal{H}^{(\tau)})$ invariant, hence when we apply $P^{(\sigma)}-P^{(\tau)}$, we can see that the above-mentioned expression also vanishes. Therefore, if $l\in\sigma$, we obtain

$$\begin{aligned}&a^{(\sigma)}(f\otimes e_k)a^{(\tau)*}(g\otimes e_l)-a^*(g\otimes e_l)P^{(\sigma\cap\tau)}a(f\otimes e_k)P^{(\tau)}\\&\quad=a^{(\sigma)}(f\otimes e_k)a^{(\tau)*}(g\otimes e_l)-a^{(\tau)*}(g\otimes e_l)a^{(\sigma)}(f\otimes e_k)P^{(\tau)}\\&\quad=\langle f,g\rangle\delta_{k,l}P^{(\sigma\cap r)}.\end{aligned}$$

Combining the two cases $l\in\sigma$ and $l\notin\sigma$ ends the proof. □

Let us finally define the fundamental processes associated with the filtered fundamental operators introduced in this section. They will appear in Secs. VII and VIII when finding GNS realizations of limit states. They will also serve as integrators in the filtered calculus developed in Ref. 12. Thus, in connection with (6.1)–(6.3), let

$$A_t^{(k,\sigma)*}=a^{(\sigma)*}(\chi_{[0,1]}\otimes e_k),\tag{6.4}$$

$$A_t^{(k,\sigma)}=a^{(\sigma)}(\chi_{[0,t]}\otimes e_k),\tag{6.5}$$

$$A_t^{(k,\sigma)^\circ}=\lambda(I_{[0,t]}\otimes|e_k\rangle\langle e_k|)P^{(\sigma\cup\{k\})},\tag{6.6}$$

$$A_t^{(0,\sigma)}=tP^{(\sigma)},\tag{6.7}$$

where $t\geqslant 0, k\in\mathbf{N},\sigma\in\mathcal{P}(\mathbf{N})$, $I_{[0,t]}$ denotes the operator of multiplication by the characteristic function $\chi_{[0,t]}$ on $L^2(\mathbf{R}^+)$, and $\lambda(H)$ denotes the differential second quantization of $H\in\mathcal{B}(\mathcal{H})$. The families of processes given by (6.4)–(6.7) will be called *filtered creation, annihilation, number*, and *time processes*, respectively. When speaking of all of them, we will call them *filtered fundamental processes*. By *filtered Brownian motion* we will understand the unital *-algebra generated by filtered creation and annihilation operators indexed by time intervals.[2]

VII. RANDOM WALK ON THE FILTERED BIALGEBRA

In this section we show that a limit of continuous-time random walks on the filtered *-bialgebra gives the filtered Brownian motion. This gives a multivariate Brownian motion on the multiple symmetric Fock space which satisfies the properties required by the axioms for white noise on *-bialgebras[1,4] and includes quantum Brownian motions for different types of independence. For the first quantum version of the Wiener process, see Ref. 22. We follow the notation used in Ref. 23 for the random walk on $U_q(su(2))$.

Instead of $\hat{\mathcal{B}}$, we choose to work with a slightly more general unital *-bialgebra $\hat{\mathcal{C}}$, also called filtered *-bialgebra, which is defined to be the unital *-algebra over $\mathbf{C}$ generated by $X_k(\sigma)$, $X_k^*(\sigma)$, and $P(\sigma)$, where $k\in\mathbf{N},\sigma\in\mathcal{P}(\mathbf{N})$ subject to relations (2.6) and (2.7), where $P(\sigma)$ is a

projection for each $\sigma \in \mathcal{P}(\mathbf{N})$ [this of course also means that $P(\sigma)$ commutes with $X_k^*(\tau)$ for $k \in \sigma$], with the coproduct in which $X_k(\sigma)$ and $X_k^*(\sigma)$ are both $P(\sigma)$-primitive and $P(\sigma)$ is group-like [cf. (2.8) and (2.9)].

Let $k \in \mathbf{N}, \sigma \in \mathcal{P}(\mathbf{N}), N \in \mathbf{N}$, and consider a sequence of continuous-time random walks on $\hat{\mathcal{C}}$ given by

$$\hat{\Delta}_{s,t}^N(X_k^\natural(\sigma)) = \sum_{l=N_s+1}^{N_t} P(\sigma)^{\otimes(l-1)} \otimes X_k^\natural(\sigma) \otimes P(\sigma)^{\otimes\infty}, \tag{7.1}$$

$$\hat{\Delta}_{s,t}^N(P(\sigma)) = 1^{\otimes N_s} \otimes P(\sigma)^{\otimes(N_t - N_s)} \otimes 1^{\otimes\infty}, \tag{7.2}$$

where $0 \leqslant s \leqslant t < \infty$, $N_t = E[tN]$, $E[x] = n$ for $n \leqslant x < n+1$, with $X_k^\natural(\sigma) \in \{X_k(\sigma), X_k^*(\sigma)\}$.

It is easy to check that for each pair (s, t) and natural number N, the mapping

$$\hat{\Delta}_{s,t}^N : \hat{\mathcal{C}} \to \hat{\mathcal{C}}^{\otimes\infty}$$

given by the linear and multiplicative extension of (7.1) and (7.2) is a unital *-homomorphism and the triple $(\hat{\mathcal{C}}^{\otimes\infty}, (\Delta_{s,t}^N)_{0 \leqslant s \leqslant t}, \hat{\phi}^{\otimes\infty})$ satisfies for each $N \in \mathbf{N}$ the properties required from a stochastic process over the bialgebra $\hat{\mathcal{C}}$ given in Ref. 8. In particular,

$$\hat{\Delta}_{s,t}^N \star \hat{\Delta}_{t,r}^N = \hat{\Delta}_{s,r}^N$$

for all $0 \leqslant s \leqslant t \leqslant r$, where $\hat{\Delta}_{s,t}^N \star \hat{\Delta}_{t,r}^N = M \circ (\hat{\Delta}_{s,t}^N \otimes \hat{\Delta}_{t,r}^N) \circ \hat{\Delta}$ with $M(a \otimes b) = ab$. For details on stochastic processes over *-bialgebras see Refs. 4 and 8.

In this *-bialgebra formulation, further preparations are similar to those which lead to the central limit theorem. Namely, for a given state ϕ on $\mathbf{C}\langle Y, Y^* \rangle$ we denote by $\tilde{\phi}$ its Boolean extension to $\mathbf{C}\langle Y, Y^*, P \rangle$, where P is a projection and we set $\hat{\phi} = \tilde{\phi}^{\otimes\infty} \circ \eta$, where

$$\eta : \hat{\mathcal{C}} \to \bigotimes_{k=1}^{\infty} \mathbf{C}\langle Y_k, Y_k^*, P_k \rangle$$

is defined by the *-multiplicative extension of formulas (2.13) and (2.14).

In the following we will study the limit of distributions of the mixed moments of (7.1) as $N \to \infty$ and find the GNS representation of the limit state. Let us remark that more general sample sums indexed by $f \in L_c^2(\mathbf{R}^+)$ can also be given and the proofs of this section will still hold.

Theorem 7.1: *Let* $Z_i = X_{k_i}(\sigma_i)$, $Z_i^* = X_{k_i}^*(\sigma_i)$, *where* $k_i \in \mathbf{N}, \sigma_i \in \mathcal{P}(\mathbf{N})$, $i = 1,...,n$. *Suppose that* $\hat{\Phi} = \hat{\Phi}^{\otimes\infty}$ *with* $\phi(Y) = 0$ *and the only nonvanishing second-order moment of* ϕ *is given by* $\phi(YY^*) = 1$. *Then*

$$\lim_{N \to \infty} N^{-n/2} \hat{\Phi}(\hat{\Delta}_{s_1,t_1}^N(Z_1^\natural) \cdots \hat{\Delta}_{s_n,t_n}^N(Z_n^\natural)) = \varphi(a^{(\sigma_1)^\natural}(v_1) \cdots a^{(\sigma_n)^\natural}(v_n)),$$

where $Z_i^\natural \in \{Z_i, Z_i^*\}$, $v_i = \chi_{[s_i,t_i]} \otimes e_{k_i}$, $i = 1,...,n$, *and* $\varphi(.) = \langle \Omega, .\Omega \rangle$ *is the vacuum expectation in* $\Gamma(\mathcal{H})$.

Proof: From the general invariance principle[24] and the combinatorics of the filtered central limit theorem it follows that for even $n = 2p$ we have

$$\mathrm{LHS} = \sum_{R \in \mathcal{P}_{2p}^{\mathrm{pair}}(\vec{k}, \vec{\sigma})} \delta(R) \prod_{m=1}^{p} \langle v_{\alpha(m)}, v_{\beta(m)} \rangle,$$

where the blocks of R consist of two-element sets $\{\alpha(i),\beta(i)\}$, with $\alpha(i)<\beta(i)$, $i=1,...,p$ and $\delta(R)=1$ if for the given partition R we have $Z^{\natural}_{\alpha(i)}=Z_{\alpha(i)}$ and $Z^{\natural}_{\beta(i)}=Z^{*}_{\beta(i)}$ and otherwise $\delta(R)=0$. It is clear that if n is odd, then LHS$=0$.

It is clear that RHS$=0$ if n is odd, too—it is enough to use the properties of creation and annihilation operators following from Proposition 6.1. Therefore assume that $n=2p$. Next, notice that in order that LHS$=$RHS it is enough to show the following claim:

$$\varphi(a_1^{\natural}\cdots a_n^{\natural})=\sum_{R\in\mathcal{P}_{2p}^{\mathrm{pair}}(\vec{k},\vec{\sigma})}\delta(R)\prod_{m=1}^{p}\langle v_{\alpha(m)},v_{\beta(m)}\rangle$$

where, for simplicity, we denote $a_j^{\natural}=a^{\sigma_j\natural}(v_j)$.

We begin with the simplest case, i.e.,

$$\varphi(a_1a_2^{*}\cdots a_{2p-1}a_{2p}^{*})=\langle v_1,v_2\rangle\langle v_3,v_4\rangle\cdots\langle v_{2p-1},v_{2p}\rangle=\sum_{R\in\mathcal{P}_{2p}^{\mathrm{pair}}(\vec{k},\vec{\sigma})}\delta(R)\prod_{m=1}^{p}\langle v_{\alpha(m)},v_{\beta(m)}\rangle,$$

the second expression being formally written as a sum since we have at most one partition contributing to it. This is the beginning of an induction procedure. Namely, it is enough to show that from the claim being true for all expectations of orders $\leqslant 2p-2$ and for $\varphi(a_1^{\natural}\cdots a_i^{*}a_{i+1}\cdots a_{2p}^{\natural})$ it follows that it also holds for the expectation of the form $\varphi(a_1^{\natural}\cdots a_{i+1}a_i^{*}\cdots a_{2p}^{\natural})$.

Suppose that $k_i\notin\sigma_{i+1}$. Then

$$\begin{aligned}\varphi(a_1^{\natural}\cdots a_{i+1}a_i^{*}\cdots a_{2p}^{\natural})&=\langle v_i,v_{i+1}\rangle\varphi(a_1^{\natural}\cdots P^{(\sigma_i\cap\sigma_{i+1})}\cdots a_{2p}^{\natural})\\&=\sum_{R\in\mathcal{P}_{2p}^{\mathrm{pair}}(\hat{k},\hat{\sigma}|i,i+1)}\delta(R)\prod_{m=1}^{p}\langle v_{\sigma(m)},v_{\beta(m)}\rangle,\end{aligned}$$

where $\mathcal{P}_n^{\mathrm{pair}}(\hat{k},\hat{\sigma}|i,i+1)$ denotes all $(\hat{k},\hat{\sigma})$-adapted pair partitions with

$$\hat{k}=(k_1,\ldots,k_{i+1},k_i,\ldots,k_n),\quad \hat{\sigma}=(\sigma_1,\ldots,\sigma_{i+1},\sigma_i,\ldots,\sigma_n)$$

in which $(i,i+1)$ forms a pairing. The first equality follows from filtered relations of Lemma 6.2, whereas the second–from the inductive assumption and the fact that if $k_i\notin\sigma_{i+1}$, then

$$\forall R\in\mathcal{P}_{2q}^{\mathrm{pair}}(\hat{k},\hat{\sigma})\exists R'\in\mathcal{P}_{2q-2}^{\mathrm{pair}}(\zeta_{i,i+1}(\vec{k},\vec{\sigma})):\quad R=R'\cup\{(i,i+1)\},$$

where $\zeta_{i,i+1}(\vec{k},\vec{\sigma})=(\tilde{k},\tilde{\sigma})$, with

$$\tilde{k}=(k_1,\ldots,k_{i-1},k_{i+2},..,k_n),\quad \tilde{\sigma}=(\sigma_1,\ldots,\sigma_{i-1},\zeta(\sigma_{i+2}),\ldots,\zeta(\sigma_n)),$$

and

$$\zeta(\sigma_l)=\begin{cases}\sigma_l\cap\sigma_i\cap\sigma_{i+1} & \text{if } (s,l) \text{ is a pairing for } s<i\\ \sigma_l & \text{otherwise,}\end{cases}$$

where $i+2\leqslant l\leqslant n$.

In turn, if $k_i\in\sigma_{i+1}$, then using Lemma 6.2 again, we obtain

$$\varphi(a_1^{\natural}\cdots a_{i+1}a_i^{*}\cdots a_{2p}^{\natural})=\langle v_{i+1},v_i\rangle\varphi(a_1^{\natural}\cdots P^{(\sigma_i\cap\sigma_{i+1})}\cdots a_{2p}^{\natural})+\varphi(a_1^{\natural}\cdots a_i^{*}a_{i+1}P^{(\sigma_i)}\cdots a_{2p}^{\natural}).$$

By the inductive assumption and similar arguments as above, the first term gives

$$\sum_{R\in\mathcal{P}_{2p}^{\mathrm{pair}}(\hat{k},\hat{\sigma}|i,i+1)}\delta(R)\prod_{m=1}^{p}\langle v_{\alpha(m)},v_{\beta(m)}\rangle,$$

whereas the second, a sum over all the remaining partitions from $\mathcal{P}_n^{\mathrm{pair}}(\hat{k},\hat{\sigma})$ [it is disjoint from the first since $(i,i+1)$ cannot form a pairing as in the associated creation-annihilation pair the annihilation operator follows the creation operator], namely

$$\sum_{R\in\mathcal{P}_{2p}^{\mathrm{pair}}(\hat{k},\hat{\sigma})\setminus\mathcal{P}_{2p}^{\mathrm{pair}}(\hat{k},\hat{\sigma}|i,i+1)}\delta(R)\prod_{m=1}^{p}\langle v_{\alpha(m)},v_{\beta(m)}\rangle$$

by the inductive assumption. Note that the projection $P^{(\sigma_i)}$, which follows the annihilation operator in the second term, ensures that the annihilation operator $a^{(\sigma_{i+1})}(v_{i+1})$ in the original expression cannot be paired off with any creation operator (standing to the right of this annihilation operator) of color $k\notin\sigma_i$.

Now adding those two expressions, we can see that the claim holds for

$$\varphi(a_1^{\natural}\cdots a_{i+1}a_i^{*}\cdots a_{2p}^{\natural}),$$

which finishes the proof. □

Example: If $k_i=k$, $\sigma_i=\sigma$ for $1\leqslant i\leqslant n$ and arbitrary n, then we obtain the CCR Brownian motion if $k\in\sigma$ and Boolean Brownian motion if $k\notin\sigma$. By taking linear combinations of sample sums corresponding to m-free (free) independent random variables, we obtain the m-free (free) Brownian motion.[6]

VIII. FILTERED WHITE NOISE

In this section we define the general notion of filtered white noise, determine its combinatorics, and study the example of filtered Poisson white noises. Our approach largely parallels that used by Speicher[21] for free white noise.

Definition 8.1: Let $\mathrm{Int}(\mathbf{R}^+)$ denote the intervals in $\mathbf{R}^+$. An s-dimensional *filtered white noise* consists of a unital *-algebra $\mathcal{C}$, a state ρ on $\mathcal{C}$, and a family of finitely additive mappings $\mathrm{Int}(\mathbf{R}^+)\to\mathcal{C}$,

$$I\to(c_I(k,\sigma;1),\ldots,c_I(k,\sigma;s)),\quad k\in\mathbf{N},\quad \sigma\in\mathcal{P}(\mathbf{N})$$

such that

(i) for any pairwise disjoint intervals $I(1),\ldots,I(n)$,

$$\rho(c_{I(l_1)}(k_1,\sigma_1;q_1)\cdots c_{I(l_n)}(k_n,\sigma_n;q_n))=\rho(c_{B_1})\cdots\rho(c_{B_r}),\tag{8.1}$$

where $B_1,\ldots,B_r$ are the blocks of $R(\vec{k},\vec{\sigma})$, with R being the partition associated with $(l_1,\ldots,l_n)$ and c_B denotes the product, taken in the natural order, of $c_{I(l_i)}(k_i,\sigma_i;q_i)$'s for $i\in B$,

(ii) the distribution $\rho_I=\rho|\mathcal{C}_I$ depends only on the Lebesgue measure of the interval I, where $\mathcal{C}_I$ denotes the unital *-algebra generated by $c_I(k,\sigma;q)$, $k\in\mathbf{N}$, $\sigma\in\mathcal{P}(\mathbf{N})$, and $1\leqslant q\leqslant s$.

Lemma 8.2: Let $(\mathcal{C},\rho,(c_I(k,\sigma;1),\ldots,c_I(k,\sigma;n))_{I\in\mathrm{Int}(\mathbf{R}^+),k\in\mathbf{N},\sigma\in\mathcal{P}(\mathbf{N})})$ *be as s-dimensional filtered white noise and let* $c_t(k,\sigma)=c_{[0,t)}(k,\sigma)$ *for* $k\in\mathbf{N}$, $\sigma\in\mathcal{P}(\mathbf{N})$. *Then*

$$\rho(c_t(k_1,\sigma_1;q_1)\cdots c_t(k_n;\sigma_n;q_n))=\sum_{R\in\mathcal{P}_n(\vec{k},\vec{\sigma})}\prod_{B\in R}Q_t(B),$$

where

$$Q_t(B)=Q_t(k,(\sigma_i)_{i\in B},(q_i)_{i\in B})=\lim_{N\to\infty}\rho(c_{t/N}(k,\sigma_{i(1)};q_{i(1)})\cdots c_{t/N}(k,\sigma_{i(r)};q_{i(s)}))$$

and $B=\{i(1),\ldots,i(m)\}$ *with* $i(1)<\cdots<i(m)$ *with* $k=k(B)=k_{i(j)}$ *for all* $i(j)\in B$.

Proof: By additivity of the filtered white noise, we can split up each $c_t^{(k,\sigma;q)}$ into a sum of N summands:

$$c_t(k,\sigma;q)=\sum_{l=1}^{N} c_{I(l)}(k,\sigma;q),$$

where $I(l)=[(l-1)t/N,lt/N)$. Moreover, the summands have the same distributions.

Now, note that from (8.1) it follows that we can use the same combinatorial argument as in Corollary 5.2 providing the limits

$$\begin{aligned}Q_t(B)&=\lim_{N\to\infty} N\rho(c_{I(l)}(k,\sigma_1;q_{i(1)})\cdots c_{I(l)}(k,\sigma_r;q_{i(r)}))\\&=\lim_{N\to\infty} N\rho(c_{I(1)}(k,\sigma_1;q_{i(1)})\cdots c_{I(1)}(k,\sigma_r;q_{i(r)}))\end{aligned}$$

exist for all l, $k\in\mathbf{N}$, $i_1,\ldots,i_r$, $1\leqslant r\leqslant n$, where $k=k(B)$ and the dependence of the limit on k, $\sigma_{i(1)},\ldots,\sigma_{i(r)}$ and $q_{i(1)},\ldots,q_{i(r)}$ is suppressed. Existence of such limits follows from an induction procedure which is analogous to that in the free case.[21] □

Example: A two-dimensional filtered Gaussian noise is obtained from $c_t(k,\sigma;1)=A_t^{(k,\sigma)}$, $c_t(k,\sigma;2)=A_t^{(k,\sigma)*}$, given by (6.4) and (6.5), for any $k\in\mathbf{N}$, $\sigma\in\mathcal{P}(\mathbf{N})$, $t\geqslant 0$ with $\rho=\varphi$, the vacuum expectation in $\Gamma(\mathcal{H})$. Then

$$\varphi(c_t(k_1,\sigma_1;q_1)\cdots c_t(k_n,\sigma_n;q_n))=\begin{cases}\Sigma_{R\in\mathcal{P}_n^{\mathrm{pair}}(\vec{k},\vec{\sigma})}\Pi_{B\in R}Q_t(B) & n \text{ even}\\ 0 & n \text{ odd},\end{cases}$$

where the generator Q_t does not depend on $k(B)$ and σ_i's and is given by

$$Q_t(B)=Q_t(i(1),i(2))=\begin{cases}t & \text{if } q_{i(1)}=1,\ q_{i(2)}=2\\ 0 & \text{otherwise.}\end{cases}$$

Note that the filtered Gaussian noise was obtained before as the GNS representation of the limit state of the invariance principle (in a slightly more general version).

In the following we will find the expectations of the filtered (multivariate) Poisson noise constructed from filtered fundamental processes given by (6.4)–(6.7), which is also a way to justify the correctness of our definition of filtered number operators (6.3).

Theorem 8.3: *For any* $k\in\mathbf{N}$, $\sigma\in\mathcal{P}(\mathbf{N})$, *and* $t\geqslant 0$, *let*

$$\Lambda_t^{(k,\sigma)}=A_t^{(k,\sigma)}+A_t^{(k,\sigma)*}+A_t^{(k,\sigma)\circ}+A_t^{(0,\sigma)} \tag{8.2}$$

and let φ *be the vacuum expectation state in* $\Gamma(\mathcal{H})$. *Then*

$$\varphi(\Lambda_t^{(k_1,\sigma_1)}\cdots\Lambda_t^{(k_n,\sigma_n)})=\sum_{R\in\mathcal{P}_n(\vec{k},\vec{\sigma})} t^{b(R)},$$

where, $k_1,\ldots,k_n\in\mathbf{N},\sigma_1,\ldots,\sigma_n\in\mathcal{P}(\mathbf{N})$, *and* $b(R)$ *is the number of blocks of* R.

Proof: First of all, notice that if $I(1),\ldots,I(r)$ are disjoint intervals in $\mathbf{R}^+$, then

$$\varphi(\Lambda_{I(l_r)}^{(k_1,\sigma_1)}\ldots\Lambda_{I(l_r)}^{(k_r,\sigma_r)})=\varphi(\Lambda_{B_1})\ldots\varphi(\Lambda_{B_r}),$$

where $\Lambda_{[s,t)}=\Lambda_t-\Lambda_s$ and $B_1,\ldots,B_r$ are the blocks of $R(\vec{k},\vec{\sigma})$, with R being the partition associated with the tuple $(l_1,\ldots,l_n)$. This fact follows from the continuous tensor product decomposition of $\Gamma(\mathcal{H})$ with respect to time and the fact that all summands of $\Lambda_{I(l)}^{(k,\sigma)}$ have the form $a(I(l))p(I(l),\sigma)$, where $p(I(l),\sigma)$ plays the role of $\mathbf{P}(l,\sigma)$ in (3.1), whereas $a(I(l))$ is an elementary tensor which has units at all sites associated with $I(m)$'s for $m\neq l$. Note that they are not filtered random variables in the sense of Definition 3.1, however (8.1) still holds. Moreover, the distribution $\phi_I=\phi|\mathcal{C}_I$, where $\mathcal{C}_I$ is the unital *-algebra generated by $\Lambda_I^{(k,\sigma)}$, $k\in\mathbf{N}$, $\sigma\in\mathcal{P}(\mathbf{N})$, depends only on the Lebesgue measure $\lambda(I)$ of I since every expectation is in fact a polynomial in the length of I. This can be seen by using Proposition 6.1.

In view of Lemma 8.2, it suffices to show that

$$\lim_{N\to\infty}\varphi(\Lambda_{t/N}^{(k,\sigma_1)}\cdots\Lambda_{t/N}^{(k,\sigma_n)})=t$$

for any $k\in\mathbf{N}$ and $\sigma_1,\ldots,\sigma_n\in\mathcal{P}(\mathbf{N})$.

Looking at the action of the fundamental filtered operators on the finite particle domain (Proposition 6.1), we can see that in the considered expectation each creation-annihilation pair as well as each time operator produce t, whereas each number operator produces an integer. Therefore, we obtain

$$\varphi(\Lambda_t^{(k,\sigma)})=\varphi(A_t^{(0,\sigma)})=t,$$

$$\varphi(\Lambda_t^{(k,\sigma_1)}\Lambda_t^{(k,\sigma_2)})=\varphi(A_t^{(k,\sigma_1)}A_t^{(k,\sigma_2)*})+o(t)$$

$$\varphi(\Lambda_t^{(k,\sigma_1)}\cdots\Lambda_t^{(k,\sigma_n)})=\varphi(A_t^{(k,\sigma_1)}A_t^{(k,\sigma_2)\circ}\cdots A_t^{(k,\sigma_{n-1})\circ}A_t^{(k,\sigma_n)*})+o(t)=t+o(t)$$

for $n>2$ and any $k\in\mathbf{N},\sigma_1,\ldots,\sigma_n\in\mathcal{P}(\mathbf{N})$. Hence

$$\lim_{N\to\infty}N\varphi(\Lambda_{t/N}^{(k,\sigma_1)}\cdots\Lambda_{t/N}^{(k,\sigma_n)})=t,$$

which enables us to use Lemma 8.4 and obtain the desired form of the expectation. □

The above theorem gives the combinatorics of the filtered Poisson noise, defined by (8.1). As it contains infinitely many colors and filters, this combinatorics involves multivariate expectations (when speaking of a one-dimensional noise we mean one "type" of operator, although it has infinitely many "copies"). It can be noted that if $k\in\sigma$, then $\Lambda_t^{(k,\sigma)}$ for fixed k and σ gives classical Poisson white noise and if $k\notin\sigma$, then $\Lambda_t^{(k,\sigma)}$ gives Boolean (or, one-free) Poisson white noise (cf. Theorem 5.4). Moreover, m-free and free Poisson white noises are obtained from linear combinations of the same type as in (3.3) and (5.4). In general, also on the level of white noise, filtered Gaussian and Poisson's white noises are also the building blocks of other Gaussian and Poisson's white noises since the latter can be obtained from the former by addition or strong limits.

IX. A FREE FOCK SPACE DECOMPOSITION OF $\Gamma(\mathcal{H})$

In this section we embed the free and m-free Fock spaces over $\mathcal{K}$, denoted by $\mathcal{F}(\mathcal{K})$, $\mathcal{F}^{(m)}(\mathcal{K})$, $m\in\mathbf{N}$, respectively, in the multiple symmetric Fock space $\Gamma(\mathcal{H})$, where $\mathcal{H}=\mathcal{K}\otimes\mathcal{G}$, and extend the m-free and free creation and annihilation operators to bounded operators on $\Gamma(\mathcal{H})$. We assume that $\mathcal{K}=L^2(\mathbf{R}_+)$.

Let us introduce the following linear combinations of filtered creation and annihilation operators, respectively:

$$l^{(m)*}(f)=\sum_{k=1}^{m}(a^{(k)*}(f\otimes e_k)-a^{(k-1)*}(f\otimes e_k)), \tag{9.1}$$

$$l^{(m)}(f)=\sum_{k=1}^{m}(a^{(k)}(f\otimes e_k)-a^{(k-1)}(f\otimes e_k)), \tag{9.2}$$

where $m\in\mathbf{N}$. We will call $l^{(m)*}(f)$, $l^{(m)}(f)$, the *extended m-free creation and annihilation operators*, respectively. In order to compare them with the *m*-free creation and annihilation operators $a^{(m)*}(f)$, $a^{(m)}(f)$ introduced in Ref. 6, let us recall the definition of the latter.

First, the *m-free Fock space* over κ is the truncation of order *m* of the free Fock space, namely

$$\mathcal{F}^{(m)}(\mathcal{K})=\mathbf{C}\omega_m\oplus\bigoplus_{k=1}^{m}\kappa^{\otimes k},$$

where ω_m is the vacuum unit vector, with the canonical scalar product. The *m-free creation operators* are then given by

$$a^{(m)*}(f):\mathcal{F}^{(m)}(\mathcal{K})\to\mathcal{F}^{(m)}(\mathcal{K}),$$

$$a^{(m)*}(f)f_1\otimes\cdots\otimes f_n=\begin{cases}f\otimes f_1\otimes\cdots\otimes f_n & \text{if } 1\leqslant n<m\\ 0 & \text{if } n=m\end{cases}$$

with $a^{(m)*}(f)\omega_m=f$ and the *m-free annihilation operators*

$$a^{(m)}(f):\mathcal{F}^{(m)}(\mathcal{K})\to\mathcal{F}^{(m)}(\mathcal{K}),$$

$$a^{(m)}(f)f_1\otimes\cdots\otimes f_n=\langle f,f_1\rangle f_2\otimes\cdots\otimes f_n$$

if $1\leqslant n\leqslant m$ and $a^{(m)}(f)\omega_m=0$. Note that $a^{(m)*}(f)$, $a^{(m)}(f)$ are bounded on $\mathcal{F}^{(m)}(\mathcal{K})$ since they are truncations of order *m* of free creation and annihilation operators $a^*(f)$, $a(f)$ on the free Fock space $\mathcal{F}(\mathcal{K})$, respectively. We will see in the following that $l^{(m)*}(f)$, $l^{(m)}(f)$ are bounded extensions of $a^{(m)*}(f)$, $a^{(m)}(f)$, $f\in\mathcal{K}$, respectively, to $\Gamma(\mathcal{H})$.

If we set $m=\infty$ in the formulas for extended *m*-free creation and annihilation operators, we obtain operators which we denote $l^*(f)$ and $l(f)$, respectively, which will be called *extened free creation and annihilation operators*. They, too, are bounded extensions of free creation and annihilation operators $a^*(f)$, $a(f)$, $f\in\mathcal{K}$, to all of $\Gamma(\mathcal{H})$, respectively.

Thus, we identify two notations: $l^{(\infty)*}(f)\equiv l^*(f)$, $l^{(\infty)}(f)\equiv l(f)$, $f\in\mathcal{K}$. In that context we will understand that $P^{(\infty)}\equiv I$. In general, in this section we will often assume for convenience that $m\in\mathbf{N}^*=\mathbf{N}\cup\{\infty\}$. However, certain results will be stated for $m=\infty$ separately in order to single out the free case.

Remark: On the finite particle domain $\Gamma_0(\mathcal{H})$, spanned by Ω and vectors of the form

$$(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})$$

where $f_1,\ldots,f_n\in\mathcal{K}$, $k_1\leqslant k_2\leqslant\cdots\leqslant k_n$, $n\in\mathbf{N}$, the series given by (9.1) and (9.2) for $m=\infty$ are strongly convergent since only a finite number of terms do not vanish when acting on vectors of finite "color support" and thus given well-defined operators with domains dense in $\Gamma(\mathcal{H})$. A similar feature was exhibited by the series representation of free random variables obtained from the construction of the hierarchy of freeness.[1,11] We will see in the following that they have bounded extensions to $\Gamma(\mathcal{H})$.

Let us first determine the action of *m*-free creation and annihilation operators on $\Gamma_0(\mathcal{H})$.

Proposition 9.1: Let $f,f_1,\ldots,f_n\in\mathcal{K}$ and $k_1\leqslant k_2\leqslant\cdots\leqslant k_n$, $m\in\mathbf{N}^*$. Then

$$l^{(m)*}(f)(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})=\mathbb{1}_{\{m\geqslant k_n+1\}}\sqrt{(n+1)}(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})\circ(f\otimes e_{k_n+1})$$

$$l^{(m)}(f)(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})=\mathbb{1}_{\{m\geqslant k_n\}}\frac{1}{\sqrt{n}}\langle f,f_n\rangle\delta_{k_n,k_{n-1}+1}(f_1\otimes e_{k_1})\circ\cdots\circ(f_{n-1}\otimes e_{k_{n-1}})$$

where we set $k_0=0$, *with the action on the vacuum vector given by* $l^{(m)*}(f)\Omega=f\otimes e_1$ *and* $l^{(m)}(f)\Omega=0$.

Proof: Note that

$$a^{(k)*}(f\otimes e_k)-a^{(k-1)*}(f\otimes e_k)=a^*(f\otimes e_k)P^{[k-1]},$$

$$a^{(k)}(f\otimes e_k)-a^{(k-1)}(f\otimes e_k)=P^{[k-1]}a(f\otimes e_k)$$

where

$$P^{[k-1]}(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})=\delta_{k-1,k_n}(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})$$

since $P^{[k-1]}=P^{(k)}-P^{(k-1)}$ and $k_j\leqslant k_n$ for all $j=1,...,n$. Thus,

$$\begin{aligned}l^{(m)*}(f)(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})&=\sum_{k=1}^{m}a^*(f\otimes e_k)P^{[k-1]}(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})\\&=\sum_{k=1}^{m}\delta_{k-1,k_n}a^*(f\otimes e_k)(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})\\&=\mathbb{1}_{\{m\geqslant k_n+1\}}\sqrt{n+1}(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})\circ(f\otimes e_{k_n+1}).\end{aligned}$$

The action of the annihilation operators is derived in a similar manner. □

Corollary 9.2: In particular, if $m=\infty$, *we obtain*

$$l^*(f)(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})=\sqrt{(n+1)}(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})\circ(f\otimes e_{k_n+1}),$$

$$l(f)(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})=\frac{1}{\sqrt{n}}\langle f,f_n\rangle\delta_{k_n,k_{n-1}+1}(f_1\otimes e_{k_1})\circ\cdots\circ(f_{n-1}\otimes e_{k_{n-1}})$$

with the action on the vacuum vector given by $l^*(f)\Omega=f\otimes e_1$ *and* $l(f)\Omega=0$.

Theorem 9.3: *For any* $m\in\mathbf{N}^*$ *and* $f,g\in\mathcal{K}$, *the operators* $l^{(m)*}(f)$ and $l^{(m)}(f)$ *have unique bounded extensions to* $\Gamma(\mathcal{H})$, *are adjoints of each other, and satisfy the following relation:*

$$l^{(m)}(g)l^{(m)*}(f)=\langle g,f\rangle P^{(m)}.$$

Proof: By Proposition 9.1 we have

$$l^{(m)}(f)l^{(m)*}(g)(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})=\mathbb{1}_{\{m\geqslant k_n+1\}}\langle f,g\rangle(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n}),$$

where $k_1\leqslant k_2\leqslant\cdots\leqslant k_n$, which proves that the relation holds on $\Gamma_0(\mathcal{H})$. It is also elementary to show that

$$\langle l^{(m)}(f)x,y\rangle=\langle x,l^{(m)*}(f)y\rangle$$

for $x,y\in\Gamma_0(\mathcal{H})$. Now, note that

$$\|l^{(m)*}(f)(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})\|^2=\mathbb{1}_{\{m\geqslant k_n+1\}}\|f\|^2\|f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})\|^2$$

hence $l^{(m)*}(f)$ has a unique bounded extension to $\Gamma(\mathcal{H})$ of norm $\|l^{(m)*}(f)\|=\|f\|$ and thus the annihilation operator $l^{(m)}(f)$ also has a unique bounded extension to $\Gamma(\mathcal{H})$ of norm $\|l^{(m)}(f)\| =\|f\|$. □

Acting with the m-free creation and annihilation operators on Ω, $m\in\mathbf{N}$, and taking the closure, we recover a subspace isomorphic to the m-free Fock space $\mathcal{F}^{(m)}(\mathcal{K})$. Thus, denote by $\tilde{\mathcal{F}}^{(m)}(\mathcal{K})$ the closure of the space $\tilde{\mathcal{F}}_0^{(m)}(\mathcal{K})$ spanned by Ω and vectors of the form

$$(f_n\otimes e_1)\circ\cdots\circ(f_1\otimes e_n)$$

where $f_1,\ldots,f_n\in\mathcal{K}$, $1\leqslant n\leqslant m$ if m is finite. Similarly, denote by $\tilde{\mathcal{F}}(\mathcal{K})$ the closure of $\tilde{\mathcal{F}}_0(\mathcal{K})$ spanned by vectors of the above form with arbitrary $n\in\mathbf{N}$. We obtain

$$\langle(f_n\otimes e_1)\circ\cdots\circ(f_1\otimes e_n)\rangle,(g_m\otimes e_1)\circ\cdots\circ(g_1\otimes e_m)\rangle=\delta_{n,m}\frac{1}{n!}\langle f_1,g_1\rangle\cdots\langle f_n,g_n\rangle$$

by the orthogonality of $e_1,\ldots,e_n$.

Corollary 9.4: The m-free Fock space $\mathcal{F}^{(m)}(\mathcal{K})$ is *is isomorphic to* $\tilde{\mathcal{F}}^{(m)}(\mathcal{K})$. *The free Fock space* $\mathcal{F}(\mathcal{K})$ *is isomorphic to* $\tilde{\mathcal{F}}(\mathcal{K})$.

Proof: The unitary isomorphism from $\mathcal{F}_0(\mathcal{K})$ to $\tilde{\mathcal{F}}_0(\mathcal{K})$ is given by

$$f_1\otimes\cdots\otimes f_n\rightarrow\sqrt{n!}(f_n\otimes e_1)\circ\cdots\circ(f_1\otimes e_n)$$

and thus extends uniquely to $\mathcal{F}(\mathcal{K})$ [its restrictions give the results for $\mathcal{F}^{(m)}(\mathcal{K})$]. □

Thus, for each $m\in\mathbf{N}$, we obtain the filtration

$$\tilde{\mathcal{F}}^{(1)}(\mathcal{K})<\cdots<\tilde{\mathcal{F}}^{(m)}(\mathcal{K})<\cdots<\tilde{\mathcal{F}}(\mathcal{K})$$

in which $\tilde{\mathcal{F}}^{(m)}(\mathcal{K})$ is an invariant subspace for the C^*-algebra

$$\mathcal{C}^{(m)}=C^*\langle\mathbf{1},l^{(m)*}(f)|f\in\mathcal{K}\rangle$$

and $\tilde{\mathcal{F}}(\mathcal{K})$ is an invariant subspace for the C^*-algebra

$$\mathcal{C}=C^*\langle\mathbf{1},l^*(f)|f\in\mathcal{K}\rangle.$$

Moreover, each $\tilde{\mathcal{F}}(\mathcal{K})$ is only one copy of the free Fock space in $\Gamma(\mathcal{K})$ and it turns out that one can decompose $\Gamma(\mathcal{H})$ into a countable direct sum of subspaces isomorphic to the free Fock space and invariant under $\mathcal{C}$. In the sequel we will concentrate on this decomposition, in other words on what is "between" $\tilde{\mathcal{F}}(\mathcal{K})$ and $\Gamma(\mathcal{H})$.

In order to determine this, we need to take a closer look at the kernel of the annihilation operators. Let $\{d_n\}_{n=1}^{\infty}$ be an orthonormal basis in $\mathcal{K}$. Note that the set consisting of Ω and vectors of the form

$$(d_{i_1}\otimes e_{k_1})\circ\cdots\circ(d_{i_n}\otimes e_{k_n}),$$

where $k_1\leqslant k_2\leqslant\cdots\leqslant k_n$ and $i_r\leqslant i_{r+1}$ whenever $k_{i_r}=k_{i_{r+1}}$, is an orthogonal basis in $\Gamma(\mathcal{H})$ (the ordering of indices is used for convenience, which is possible due to the fact that the product is symmetrized). Denote by $\hat{\mathcal{D}}$ the subset of this basis consisting of Ω and vectors of the above form for which $k_n\neq k_{n-1}+1$, i.e., the last two vectors are of identical colors or their colors differ by more than 1 if $n>1$, and the last color is not equal to 1 if $n=1$. By normalizing the vectors from $\hat{\mathcal{D}}$ we get

$$\mathcal{D}=\{x/\|x\|\ |x\in\hat{\mathcal{D}}\},$$

which is an orthonormal set. Let $\mathcal{D}^{(m)}=\mathcal{D}\cap\Gamma^{m+1)}$, where $\Gamma^{m+1)}=\Gamma(\mathcal{H}^{(m+1)})$. We understand that $\mathcal{D}^{(\infty)}=\mathcal{D}$.

Proposition 9.5: $\mathcal{D}^{(m)}\subseteq\ker l^{(m)}(f)$ *for any* $m\in\mathbf{N}^*$ *and* $f\in\mathcal{K}$.

Proof: This follows from Proposition 9.1 due to the presence of $\delta_{k_n,k_{n-1}+1}$ on the right-hand side of the formula for the annihilation operators. □

Proposition 9.6: Let $m\in\mathbf{N}^*$. *Then*

$$\sum_{s=1}^{\infty} l^{(m)*}(d_s)l^{(m)}(d_s)=I-P_{[\mathcal{D}^{(m)}]\oplus\Gamma^{(m}}$$

where $P_{[D^{(m)}]\otimes\Gamma^{(m}}$ *is the projection onto* $[D^{(m)}]\otimes\Gamma^{(m}$ *and* $\Gamma^{(m}=\Gamma(\mathcal{H}\ominus\mathcal{H}^{(m+1)})$. *In particular,*

$$\sum_{s=1}^{\infty} l^*(d_s)l(d_s)=I-P_{[\mathcal{D}]}$$

thus $\mathcal{C}\cong\mathcal{O}_\infty$, *where* $\mathcal{O}_\infty$ *is the Cuntz algebra.*

Proof: It can be seen from Theorem 9.3 that

$$l^{(m)*}(d_s)l^{(m)}(d_s)=Q_s,$$

where Q_s is the projection onto the subspace spanned by vectors of the form

$$(d_{s_1}\otimes e_{k_1})\circ\cdots\circ(d_{s_{n-1}}\otimes e_{k_{n-1}})\circ(d_s\otimes e_{k_n})$$

where $k_1\leqslant\cdots\leqslant k_{n-1}=k_n-1<k_n\leqslant m$ (cf. Ref. 25). These subspaces are pairwise orthogonal and span the orthogonal complement of $[\mathcal{D}^{(m)}]\oplus\Gamma^{(m}$, which proves the first formula. The second formula is just a special case when $m=\infty$ and, together with Theorem 9.3, it implies that the C^*-algebra generated by $l^*(f), f\in\mathcal{K}$, is isomorphic to the Cuntz algebra $\mathcal{O}_\infty$ since $\mathcal{K}$ is countably separable. □

Let us introduce the following notation on $\Gamma_0(\mathcal{H})$:

$$u\odot w=u_1\circ\cdots\circ u_r\circ w_1\circ\cdots\circ w_n$$

where $u=u_1\circ\cdots\circ u_r$, $w=w_1\circ\cdots\circ w_n$.

Proposition 9.7: If $x=x_1\circ\cdots\circ x_r$, $z=z_1\circ\cdots\circ z_r$, $u=u_1\circ\cdots\circ u_n$, $v=v_1\circ\cdots\circ v_n$, *where* $x_i,z_i\in\mathcal{H}_1$, $1\leqslant i\leqslant r$ *and* $z_j, v_j\in\mathcal{H}_2$, $1\leqslant j\leqslant n$, *and* $\mathcal{H}_1$, $\mathcal{H}_2$ *are two orthogonal subspaces of* $\mathcal{H}$, *then*

$$\langle x\odot u,z\odot v\rangle=\frac{r!n!}{(r+n)!}\langle x,z\rangle\langle u,v\rangle.$$

Proof: Using the orthogonality of $\mathcal{H}_1$ and $\mathcal{H}_2$ and the formula for the scalar product in $\Gamma(\mathcal{H})$, we obtain

$$\begin{aligned}\langle x\odot u,z\odot v\rangle&=\frac{1}{(r+n)!}\sum_{\sigma\in S_r}\sum_{\tau\in S_n}\langle x_1,z_{\sigma(1)}\rangle\cdots\langle x_r,z_{\sigma(r)}\rangle\langle u_1,v_{\tau(1)}\rangle\cdots\langle u_n,v_{\tau(n)}\rangle\\&=\frac{r!n!}{(r+n)!}\langle x,z\rangle\langle u,v\rangle.\end{aligned}$$

□

The C^*-algebra $\mathcal{C}$ is a C^*-subalgebra of $\mathcal{B}(\Gamma(\mathcal{H}))$. Denote the faithful representation of $\mathcal{C}$ on $\Gamma(\mathcal{H})$ by π. Since $[\mathcal{C}x]$ is for each $x\in\mathcal{D}$ a closed subspace of $\Gamma(\mathcal{H})$, which is invariant under each

operator A in $\mathcal{C}$, the mapping $A \to A|[\mathcal{C}x]$ is a cyclic representation of $\mathcal{C}$ on $[\mathcal{C}x]$ with cyclic vector x. Denote this representation by π_x. We will show in the following that π is a direct sum of cyclic representations π_x, $x \in \mathcal{D}$.

Theorem 9.8: *The multiple symmetric Fock space has the direct sum decomposition*

$$\Gamma(\mathcal{H}) = \bigoplus_{x \in \mathcal{D}} [\mathcal{C}x]$$

where $[\mathcal{C}x] \cong \mathcal{F}(\mathcal{K})$, *according to which*

$$\pi = \bigoplus_{x \in \mathcal{D}} \pi_x,$$

where $\pi_x \cong \rho$, *and* ρ *is the free Fock space representation of* $\mathcal{C}$.

Proof: If $x = \hat{x}/\|x\| \in \mathcal{D}$, where $\hat{x}$ is of the form

$$\hat{x} = (d_1 \otimes e_{k_1}) \circ \cdots \circ (d_{i_r} \otimes e_{k_r})$$

with $k_r = l$, then $[\mathcal{C}x]$ is the closed subspace of $\Gamma(\mathcal{H})$ spanned by vectors of the form

$$x \odot (f_n \otimes e_{l+1}) \circ \cdots \circ (f_1 \otimes e_{l+n})$$

where $f_1, \ldots, f_n \in \mathcal{K}$. Clearly, $[\mathcal{C}x]$ is invariant under $\mathcal{C}$. Let us show that for each $x \in \mathcal{D}$, $[\mathcal{C}x] \cong \mathcal{F}(\mathcal{K})$.

For that purpose, define the linear mapping

$$U_x : \mathcal{F}_0(\mathcal{K}) \to [\mathcal{C}x]$$

by

$$U_x(\omega) = x,$$

$$U_x(f_1 \otimes \cdots \otimes f_n) = \sqrt{\frac{(r+n)!}{r!}}\, x \odot (f_n \otimes e_{l+1}) \circ \cdots \circ (f_1 \otimes e_{l+n}).$$

An elementary computation shows that U_x is scalar-product preserving and therefore has a unique extension to $\mathcal{F}(\mathcal{K})$. It is not hard to see that $[\mathcal{C}x] \perp [\mathcal{C}x']$ for $x \neq x'$ and that $\Gamma(\mathcal{H})$ is a direct sum of $[\mathcal{C}x]$ for all $x \in \mathcal{D}$.

It remains to be shown that U_x intertwines between π_x and the free Fock space representation ρ of $\mathcal{C}$ on $\mathcal{F}(\mathcal{K})$. We have

$$\pi_x(l^*(f)) U_x(\omega) = \sqrt{r+1}\, x \odot (f \otimes e_{r+1}) = U_x(f) = U_x \rho(l^*(f))\omega$$

and

$$\pi_x(l^*(f)) U_x(f_1 \otimes \cdots \otimes f_n) = \sqrt{\frac{(r+n+1)!}{r!}} \times x \odot (f_n \otimes e_{l+1}) \circ \cdots \circ (f_1 \otimes e_{l+n}) \circ (f \otimes e_{l+n+1})$$

$$= U_x(f \otimes f_1 \otimes \cdots \otimes f_n) = U_x \rho(l^*(f))(f_1 \otimes \cdots \otimes f_n)$$

for any $f_1, \ldots, f_n, f \in \mathcal{K}, n \geq 1$. Similarly, $\pi_x(l(f)) U_x \Omega = l(f)x = 0 = U_x \rho(l(f))\Omega$ and

$$\pi_x(l(f)) U_x(f_1 \otimes \cdots \otimes f_n) = U_x \rho(l(f))(f_1 \otimes \cdots \otimes f_n).$$

Therefore $\pi_x(a) U_x = U_x \rho(a)$ also for any $a \in \mathcal{C}$. This finishes the proof. □

Let us finally define *extended m-free number operators*. Guided by the definitions of extended creation and annihilation operators, we set

$$l^{(m)\circ}=\sum_{k=1}^{m}(a^{(k,k)\circ}-a^{(k,k-1)\circ}),$$

where $m\in\mathbf{N}^*$ and $a^{(k,r)\circ}=a^{(k,\sigma)\circ}$ for $\sigma=\{1,...,r-1\}$ and $a^{(k,\sigma)\circ}$ is given by (6.3). Let us determine the action of extended number operators on the finite particle domain.

Proposition 9.9: Let $f_1,\ldots,f_n\in\mathcal{K}$, $k_1\leqslant\cdots\leqslant k_n$, $m\in\mathbf{N}^*$. *The finite particle domain* $\Gamma_0(\mathcal{H})$ *is contained in the domains of extended m-free number operators and*

$$l^{(m)\circ}(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n})=\begin{cases}N_{k_n}(f_1\otimes e_{k_1})\circ\cdots\circ(f_n\otimes e_{k_n}) & \text{if } k_j+1=k_n\leqslant m \text{ for } j<n\\ 0 & \text{otherwise,}\end{cases}$$

where $N_k=\#\{i|k_i=k\}$.

Proof: The proof is elementary and therefore will be omitted. □

In other words, $l^{(m)\circ}$ "counts" particles of the highest color k_n if that one is smaller or equal to m and the second highest color is equal to k_n-1. Otherwise, the extended free number operator gives zero. In particular, on $\tilde{\mathcal{F}}_0^{(m)}(\mathcal{K})$ we obtain

$$l^{(m)\circ}\Omega=0,$$

$$l^{(m)\circ}(f_1\otimes e_n)\circ\cdots\circ(f_n\otimes e_1)=(f_1\otimes e_n)\circ\cdots\circ(f_n\otimes e_1)$$

for $1\leqslant n\leqslant m$.

It can be seen that, contrary to the case of extended m-free creation and annihilation operators, the operators $l^{(m)\circ}$ are not bounded on $\Gamma(\mathcal{H})$. Clearly, they are bounded on $\tilde{\mathcal{F}}^{(m)}(\mathcal{H})$ and, in fact, it can be shown that they are bounded on $[Cx]$ for each $x\in\mathcal{D}$.

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Order-automorphisms of the set of bounded observables

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Let H be a complex Hilbert space and denote by $B_s(H)$ the set of all self-adjoint bounded linear operators on H. In this article we describe the form of all bijective maps (no linearity or continuity is assumed) on $B_s(H)$ which preserve the order $\leqslant$ in both directions. © *2001 American Institute of Physics.*
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I. INTRODUCTION AND STATEMENTS OF THE RESULTS

In the Hilbert space framework of quantum mechanics the bounded observables are represented by self-adjoint bounded linear operators. If H denotes the underlying Hilbert space, then these operators form the set $B_s(H)$ on which usually several operations and relations are considered. The automorphisms of $B_s(H)$ with respect to those operations and/or relations are, just as with any algebraic structure in mathematics, of remarkable importance.

First of all, $B_s(H)$ with the usual addition, scalar multiplication and Jordan product forms a Jordan algebra. It is a well-known result that the corresponding automorphisms of $B_s(H)$ are implemented by unitary or antiunitary operators of H (see, for example, Ref. 1, where the automorphisms of some other important structures appearing in the probabilistic aspects of quantum mechanics are also treated).

The aim of this article is to determine another class of automorphisms of $B_s(H)$. Namely, we equip the set $B_s(H)$ with the usual order among self-adjoint operators. That is, for any $A,B \in B_s(H)$, we write $A \leqslant B$ if $\langle Ax,x\rangle \leqslant \langle Bx,x\rangle$ holds for every $x \in H$. Alternatively, in the language of quantum mechanics, the bounded observable A is said to be less than or equal to the bounded observable B if the expected value of A in any state is less than or equal to the expected value of B in the same state. The relation $\leqslant$ is no doubt an important one among observables.

In what follows we determine all the automorphisms of $B_s(H)$ as a partially ordered set with the relation $\leqslant$ (this is done in the main result of the paper, Theorem 2) and also present some corollaries (Corollaries 3 and 4) that we believe have physical meaning.

We begin with the following proposition on which the proof of our main result rests. Let H be a complex Hilbert space and let $B(H)^+$ denote the cone of all positive operators on H (that is, the set of all $A \in B_s(H)$ for which $\langle Ax,x\rangle \geqslant 0$ holds for every $x \in H$). Our first result describes the form of all bijective maps on $B(H)^+$ which preserve the order $\leqslant$ in both directions.

Theorem 1: *Assume that* $\dim H > 1$. *Let* $\phi: B(H)^+ \to B(H)^+$ *be a bijective map with the property that*

$$A \leqslant B \Leftrightarrow \phi(A) \leqslant \phi(B)$$

holds whenever $A,B \in B(H)^+$. *Then there exists an invertible bounded either linear or conjugate-linear operator* $T: H \to H$ *such that* ϕ *is of the form*

$$\phi(A) = TAT^* \quad (A \in B(H)^+).$$

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After having proved this result, it will be easy to deduce the main result of the article that follows.

Theorem 2: *Suppose that* $\dim H>1$. *Let* $\phi:B_s(H)\to B_s(H)$ *be a bijective map with the property that*

$$A\leqslant B\Leftrightarrow \phi(A)\leqslant \phi(B)$$

holds whenever $A,B\in B_s(H)$. *Then there exists an operator* $X\in B_s(H)$ *and an invertible bounded either linear or conjugate-linear operator* $T:H\to H$ *such that* ϕ *is of the form*

$$\phi(A)=TAT^*+X \quad (A\in B_s(H)).$$

This result has some corollaries that seem worth mentioning. In the first one we determine the form of all bijective transformations on $B_s(H)$ which preserve the order and the commutativity in both directions (in quantum mechanics, instead of commutativity they usually use the word compatibility for this important concept).

Corollary 3: Assume that $\dim H>1$. *Let* $\phi:B_s(H)\to B_s(H)$ *be a bijective map which preserves the order and the commutativity in both directions. Then there is an either unitary or antiunitary operator* $U:H\to H$, *a positive scalar* λ, *and a real number* μ *such that* ϕ *is of the form*

$$\phi(A)=\lambda UAU^*+\mu I \quad (A\in B_s(H)).$$

The next corollary describes all the bijective maps on $B_s(H)$ which preserve the order and the complementarity in both directions (two observables are called complementary if the range of any nontrivial projection from the range of the spectral measure of the first observable has zero intersection with the range of any nontrivial projection from the range of the spectral measure of the second observable). Although this latter concept is in some sense opposite to compatibility, as it turns out below we still have the same form for ϕ as above.

Corollary 4: Suppose that $\dim H>1$. *Let* $\phi:B_s(H)\to B_s(H)$ *be a bijective map which preserves the order and the complementarity in both directions. Then there is an either unitary or antiunitary operator* $U:H\to H$, *a positive scalar* λ, *and a real number* μ *such that* ϕ *is of the form*

$$\phi(A)=\lambda UAU^*+\mu I \quad (A\in B_s(H)).$$

Finally, our last corollary characterizes those bijective maps on $B_s(H)$ which preserve the order and the orthogonality in both directions [two operators $A,B\in B_s(H)$ are called orthogonal if $AB=0$ which is just equivalent to the mutual orthogonality of the ranges of A and B].

Corollary 5: Assume that $\dim H>1$. *Let* $\phi:B_s(H)\to B_s(H)$ *be a bijective map which preserves the order and the orthogonality in both directions. Then there is an either unitary or antiunitary operator* $U:H\to H$, *and a positive scalar* λ *such that* ϕ *is of the form*

$$\phi(A)=\lambda UAU^* \quad (A\in B_s(H)).$$

Closing this section we note that all the above statements could be conversed, that is, if a map ϕ is of any of the above forms, then it necessarily preserves the corresponding properties.

II. PROOFS

This section is devoted to the proofs of our results. We begin with the following auxiliary results. If A is a bounded linear operator, then rng A denotes its range. The rank of A is, by definition, the algebraic dimension of rng A and it is denoted by rank A. For any $A\in B(H)^+$, $\sqrt{A}$ stands for the unique positive linear operator whose square is A.

Lemma 1: Let $A,B\in B(H)^+$ *be such that* rank $A=1$ *and* rank $B<\infty$. *We have* $\lambda A\leqslant B$ *for some positive scalar* λ *if and only if* $\operatorname{rng}A\subset\operatorname{rng}B$.

Proof: We recall the following nice result of Busch and Gudder (Ref. 2, Theorem 3): if $B\in B(H)^+$, $x\in H$, and P is the rank-1 projection projecting onto the subspace generated by x, then

we have $\lambda P \leqslant B$ for some positive scalar λ if and only if x is in the range of $\sqrt{B}$. As in our case B is a finite rank operator, it follows from the spectral theorem that $\mathrm{rng}\, B = \mathrm{rng}\, \sqrt{B}$. Since the positive rank-1 operators are exactly the positive scalar multiples of rank-1 projections, we obtain the assertion. □

Lemma 2: Let $A \in B(H)^+$ *and* $n \in \mathbb{N}$. *We have* rank $A > n+1$ *if and only if there are operators* $E,F \in B(H)^+$ *such that* $E,F \leqslant A$, rank $E = n$, rank $F > 1$ *and there is no* $G \in B(H)^+$ *of rank 1 with* $G \leqslant E,F$.

Proof: Suppose that rank $A > n+1$. We assert that there exists a finite rank operator $A' \in B(H)^+$ such that $A' \leqslant A$ and rank $A' > n+1$. In case A is of finite rank, this is trivial. If A is compact and not of finite rank, then by the spectral theorem of compact self-adjoint operators we can verify our claim very easily. Finally, if A is noncompact, then using the spectral theorem of self-adjoint operators and the properties of the spectral integral, we can find an infinite rank projection P on H and a positive scalar λ such that $\lambda P \leqslant A$ from which the existence of an appropriate operator A' follows.

Clearly, A' can be written as the sum of positive scalar multiples of pairwise orthogonal rank-1 projections. Let E be the sum of the first n terms in this sum and let F be the sum of the remaining part. It is easy to see that E,F have the required property. In fact, the nonexistence of G follows from Lemma 1.

To prove the converse, suppose that there are operators $E,F \in B(H)^+$ with the properties formulated in the lemma. It follows from the relation $E,F \leqslant A$ that E,F are of finite rank and $\mathrm{rng}\, E$, $\mathrm{rng}\, F \subset \mathrm{rng}\, A$. As there is no positive rank-1 operator G with $G \leqslant E,F$, by Lemma 1 we have $\mathrm{rng}\, E \cap \mathrm{rng}\, F = \{0\}$. So, rng A contains two subspaces with trivial intersection the sum of whose dimensions is greater than $n+1$. This shows that rank $A > n+1$, completing the proof of the lemma. □

Now, we are in a position to prove our first theorem.

Proof of Theorem 1: We first remark that our proof is based on a beautiful result of Rothaus (Ref. 3) concerning the automatic linearity of bijective maps between closed convex cones in normed spaces preserving order in both directions. In Ref. 3 conclusions of that kind were reached under some quite restrictive assumptions. In our present situation, that is, when the normed space in question is an operator algebra, those assumptions are fulfilled exactly when the underlying Hilbert space H is finite dimensional. Accordingly, the main point of our proof is to reduce the problem to the finite dimensional case. This is in fact what we are going to do next.

Clearly, $\phi(0) = 0$. We prove that ϕ preserves the rank of operators. In fact, we show that the assertion that

$$\text{rank } A = k \Leftrightarrow \text{rank}\, \phi(A) = k$$

$(k = 1,\ldots,n)$ holds for every $n \in \mathbb{N}$. To begin, as for the case $n = 1$, we remark that a nonzero operator $A \in B(H)^+$ is of rank 1 if and only if the operator interval $[0,A]$ is total under the partial ordering $\leqslant$, that is, every two elements of it are comparable. Suppose that our assertion is true for some $n \in \mathbb{N}$. We show that in that case it holds also for $n+1$. Let $A \in B(H)^+$ be of rank $n+1$. By our assumption of induction, it follows that the rank of $\phi(A)$ is at least $n+1$. Suppose that rank $\phi(A) > n+1$. Using Lemma 2 and the order preserving property of ϕ we obtain that rank $A > n+1$, which is a contradiction. Therefore, we have rank $\phi(A) = n+1$. Referring to the fact that ϕ^{-1} shares the same properties as ϕ, we obtain the desired assertion.

We now prove that if $A_1,\ldots,A_n \in B(H)^+$ are of rank 1, then their ranges are linearly independent if and only if the ranges of $\phi(A_1),\ldots,\phi(A_n)$ are, too. [A system of one-dimensional subspaces in H of n members is called linearly independent if they cannot be included in an $(n-1)$-dimensional subspace.] This statement is clear for $n = 1$. Suppose that it holds for n and prove that it then necessarily holds also for $n+1$. Let $A_1,\ldots,A_n,A_{n+1}$ be rank-1 operators with linearly independent ranges and assume that this is not the case with the ranges of $\phi(A_1),\ldots,\phi(A_n),\phi(A_{n+1})$. Then these ranges can be included in an at most n-dimensional subspace implying that there is a rank-n operator $B \in B(H)^+$ such that $\phi(A_1),\ldots,\phi(A_{n+1}) \leqslant B$. By

the rank-preserving property of ϕ we have a rank-n operator $A \in B(H)^+$ such that $A_1,\ldots A_n, A_{n+1} \leqslant A$. By Lemma 1 this implies that $\mathrm{rng}\, A_1,\ldots,\ \mathrm{rng}\, A_{n+1} \subset \mathrm{rng}\, A$ and it follows that the ranges of $A_1,\ldots,A_{n+1}$ can be included in an n-dimensional subspace of H which is a contradiction. This verifies our claim.

Fix rank-1 operators $A_1,\ldots,A_n \in B(H)^+$ with linearly independent ranges which generate the n-dimensional subspace H_n of H. Denote by H_n' the n-dimensional subspace of H generated by the ranges of $\phi(A_1),\ldots,\phi(A_n)$. We assert that an operator $T \in B(H)^+$ acts on H_n if and only if $\phi(T)$ acts on H_n'. (We say that an operator T acts on the closed subspace M of H if M is an invariant subspace of T and T is zero on the orthogonal complement of M.) This will follow from the following observation: the positive finite rank operator T acts on H_n if and only if for every rank-1 operator A for which the ranges of $A_1,\ldots,A_n,A$ are linearly independent we have $A \not\leqslant T$. To see this, suppose that T acts on H_n. If $A \leqslant T$, then we have $\mathrm{rng}\, A \subset \mathrm{rng}\, T \subset H_n$ implying that the ranges of $A_1,\ldots,A_n,A$ cannot be linearly independent. This gives us the necessity. As for the sufficiency, suppose that T does not act on H_n. Then there exists a unit vector x in the range of T which does not belong to H_n. On the other hand, as $x \in \mathrm{rng}\, T$, by Lemma 1 it follows that a positive scalar multiple of the rank-1 projection projecting onto the subspace generated by x is less than or equal to T. This gives us a rank-1 operator A for which the ranges of $A_1,\ldots,A_n,A$ are linearly independent and we have $A \leqslant T$. This proves our claim.

So, for any n-dimensional subspace H_n of H, there exists an n-dimensional subspace H_n' of H such that for every $T \in B(H)^+$, T acts on H_n if and only if $\phi(T)$ acts on H_n'. This gives rise to a bijective transformation ψ on the cone $M_n(\mathbb{C})^+$ of all positive $n \times n$ complex matrices which preserves the order in both direction. (Here positivity is used in the operator theoretical sense, so our concept of positivity is just the same as positive semidefiniteness in matrix theory.)

Since ϕ preserves the rank, it follows that ψ preserves the rank-n matrices in both directions. The set of all such matrices is just the interior of $M_n(\mathbb{C})^+$ in the real normed space of all $n \times n$ Hermitian matrices. Now, the result (Ref. 3, Proposition 2) of Rothaus on the linearity of order preserving maps can be applied and it gives us that ψ is linear on the set of all rank-n elements in $M_n(\mathbb{C})^+$. We show that ψ is linear on the whole set $M_n(\mathbb{C})^+$. Pick $A, B \in M_n(\mathbb{C})^+$. Then there are sequences $(A_k),(B_k)$ of rank-n elements in $M_n(\mathbb{C})^+$ which are monotone decreasing with respect to the order $\leqslant$ and $A_k \to A$, $B_k \to B$. It is clear that the equalities $A = \inf_k A_k$, $B = \inf_k B_k$ and $A + B = \inf_k (A_k + B_k)$ hold in the partially ordered set $M_n(\mathbb{C})^+$. By the order preserving property of ψ we obtain that $\psi(A) = \inf_k \psi(A_k)$, $\psi(B) = \inf_k \psi(B_k)$ and $\psi(A+B) = \inf_k \psi(A_k + B_k)$. The sequences $\psi(A_k)$, $\psi(B_k)$, $\psi(A_k + B_k)$ are monotone decreasing and bounded below. By Vigier's theorem (Ref. 5 4.1.1. Theorem) they necessarily converge (strongly) to their infima. Now, by the partial additivity property of ψ which has been obtained previously as a consequence of Rothaus's result, we have

$$\psi(A+B) = \lim_k \psi(A_k + B_k) = \lim_k \psi(A_k) + \lim_k \psi(B_k) = \psi(A) + \psi(B).$$

So, ψ is additive on $M_n(\mathbb{C})^+$ and one can prove in the same way that it is positive homogeneous as well. Since every pair of finite rank elements in $B(H)^+$ can be embedded into a matrix space $M_n(\mathbb{C})^+$, we deduce that ϕ is additive and positive homogeneous on the set of all finite rank elements in $B(H)^+$.

Since every finite sum $\Sigma_i \lambda_i P_i$, where the λ_i's are positive numbers and the P_i's are projections of not necessarily finite rank, is the strong limit of a monotone increasing net of finite rank elements in $B(H)^+$, one can prove in a very similar way to that shown earlier that ϕ is additive and positive homogeneous on the set of all such finite sums. Finally, using the fact that every operator in $B(H)^+$ is the norm limit of a monotone increasing sequence of operators of the form $\Sigma_i \lambda_i P_i$ (this follows from the spectral theorem), repeating the previously stated argument once again, we obtain that ϕ is additive and positive homogeneous.

Extend ϕ from $B(H)^+$ to $B(H)_s$ in the obvious way, that is, define $\tilde{\phi}(T) = \phi(A) - \phi(B)$ for every $T \in B_s(H)$ and $A, B \in B(H)^+$ for which $T = A - B$. It is easy to check that $\tilde{\phi}: B(H)_s$

$\to B(H)_s$ is a linear transformation which preserves the order in both directions. To see the less trivial part of this last assertion, suppose that $T \in B_s(H)$, $T=A-B$, $A,B \in B(H)^+$ are such that $0 \leqslant \tilde{\phi}(T)=\phi(A)-\phi(B)$. This implies that $\phi(B) \leqslant \phi(A)$ which yields $B \leqslant A$, that is, we have $0 \leqslant T$. The linear transformation $\tilde{\phi}$ is surjective since $B(H)^+$ is included in its range. Moreover, it is injective as well which follows from the fact that $\tilde{\phi}$ preserves the order in both directions. Now, if one further extends $\tilde{\phi}$ to a linear transformation on the algebra $B(H)$ of all bounded linear operators on H, one gets a linear bijection of the C^*-algebra $B(H)$ which preserves the order in both directions. Due to a well-known result of Kadison (Ref. 4, Corollary 5) every such transformation sending the identity to itself is a Jordan *-automorphism. Therefore, the linear transformation

$$A \mapsto \sqrt{\phi(I)}^{-1} \phi(A) \sqrt{\phi(I)}^{-1}$$

is a Jordan *-automorphism of $B(H)$. But these transformations of $B(H)$ are well known to be implemented by unitary-antiunitary operators (see, for example, Ref. 1). It is now easy to infer that ϕ is of the desired form. This completes the proof of the theorem. □

Our main result is now easy to prove.

Proof of Theorem 2: Let $X=\phi(0)$ and consider the transformation

$$\psi: A \mapsto \phi(A)-X.$$

Clearly, ψ is a bijection of $B_s(H)$ preserving the order in both directions. So, without loss of generality we can assume that $\phi(0)=0$. Now, restricting ϕ onto $B(H)^+$ we have a bijection of $B(H)^+$ which preserves the order in both directions. So, we can apply Theorem 1 and obtain that there exists an invertible bounded either linear or conjugate-linear operator $T: H \to H$ for which we have

$$\phi(A)=TAT^* \quad (A \in B(H)^+). \tag{1}$$

It remains to show that this equality holds also for every $A \in B_s(H)$. Let $B \in B_s(H)$ be arbitrary but fixed. Then there exists a constant $K \in \mathbb{R}$ such that $K \leqslant B$ (for example, one can choose $K=-\|B\|$). Consider the transformation

$$A \mapsto \phi(A+K)-\phi(K)$$

on $B(H)^+$. Just as above, this transformation is a bijective map on $B(H)^+$ which preserves the order in both directions. Therefore, there exists an invertible bounded either linear or conjugate-linear operator $S: H \to H$ such that

$$\phi(A+K)-\phi(K)=SAS^* \quad (A \in B(H)^+). \tag{2}$$

If $A \geqslant -K,0$, then by (1) we have

$$T(A+K)T^*-\phi(K)=SAS^*. \tag{3}$$

Considering this equality for another A' with $A' \geqslant -K,0$, we see that

$$T(A-A')T^*=S(A-A')S^*.$$

As the difference $A-A'$ can be an arbitrary self-adjoint operator, we obtain that $TCT^*=SCS^*$ holds for every $C \in B_s(H)$. It now follows from (3) that

$$T(A+K)T^*-\phi(K)=SAS^*=TAT^*,$$

where $A \in B_s(H)$, $A \geqslant -K,0$. This yields $\phi(K)=TKT^*=SKS^*$. We deduce from (2) that

$$\phi(A+K)=SAS^*+\phi(K)=TAT^*+TKT^*=T(A+K)T^*$$

holds for every $A\in B(H)^+$. Choosing $A=B-K\geqslant 0$, we have

$$\phi(B)=TBT^*.$$

This completes the proof. □

We now turn to the proofs of the corollaries.

Proof of Corollary 3: By Theorem 2 there is an invertible bounded either linear or conjugate-linear operator T on H such that

$$\phi(A)=TAT^*+\phi(0)\quad (A\in B_s(H)).$$

Since 0 is commuting with every $A\in B_s(H)$, the same is true for $\phi(0)$. This gives us that $\phi(0)$ is a scalar operator, that is, there is a $\mu\in\mathbb{R}$ such that $\phi(0)=\mu I$. Similarly, we have a constant $\lambda\in\mathbb{R}$ such that $TT^*=\phi(I)-\phi(0)=\lambda I$. It is trivial that λ is necessarily positive and then we obtain that the operator $T/\sqrt{\lambda}$ is either unitary or antiunitary. □

Proof of Corollary 4: It is easy to see that $A\in B_s(H)$ is complementary with every $B\in B_s(H)$ if and only if A is scalar. Hence, ϕ preserves the scalar operators and one can apply the argument in the proof of Corollary 4 to get the desired form of ϕ. □

In the proof of Corollary 5 we make use of the following notation. If $x,y\in H$, then $x\otimes y$ denotes the operator defined by $(x\otimes y)z=\langle z,y\rangle x$ $(z\in H)$.

Proof of Corollary 5: Since 0 is the only operator in $B_s(H)$ which is orthogonal to every operator, we infer that $\phi(0)=0$. By Theorem 2 we have an invertible bounded either linear or conjugate-linear operator T on H such that $\phi(A)=TAT^*$ holds for every $A\in B_s(H)$. Without serious loss of generality we can suppose that T is linear. It now follows that for every $A,B\in B_s(H)$ with $AB=0$ we have $\phi(A)\phi(B)=0$ which implies that $AT^*TB=0$. Choosing nonzero orthogonal vectors $x,y\in H$, for $A=x\otimes x$ and $B=y\otimes y$ we get $x\otimes Tx\cdot Ty\otimes y=0$ which yields $\langle T^*Tx,y\rangle=\langle Tx,Ty\rangle=0$. So, we have $\langle T^*Tx,y\rangle=0$ whenever $\langle x,y\rangle=0$. This clearly implies that for every $x\in H$ there is a scalar λ_x such that $T^*Tx=\lambda_x x$. In another expression, the operators T^*T and I are locally linearly dependent. It is a folk result (whose proof requires only elementary linear algebra) that in that case the operators T^*T and I are necessarily linearly dependent, that is, there exists a scalar $\lambda\in\mathbb{R}$ such that $T^*T=\lambda I$. Now, the proof can be completed as in the proof of Corollary 3. □

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An expansion of the hypergeometric function in Bessel functions

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An expansion of the hypergeometric function ${}_2F_1(a,b,c+1;-z^2/4ab)$ in Bessel functions of argument z is derived. This expansion can be used to obtain an asymptotic expansion of the hypergeometric function for large absolute values of a and b. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1415431]

I. INTRODUCTION AND SUMMARY

In a recent article[1] the authors derived the first terms of an asymptotic expansion of the hypergeometric function ${}_2F_1(a,b,c+1;-z^2/4ab)$ for large values of the parameters a and b, including second-order terms in $1/a$ and $1/b$, and involving Bessel functions $J_\nu(z)$ of orders c up to $c+4$ in integer steps. The result was obtained by a direct expansion of the a and b dependent coefficients in the power series definition of ${}_2F_1$. Going to higher orders would probably become very complicated. The resulting expansion was used in an analysis of the connection between the quantal and the semiclassical treatments of Coulomb excitation of atomic systems by passing charged particles.

In this note we show that the above-mentioned asymptotic expansion can be derived (in principle to arbitrary order) by rearranging a convergent expansion of the hypergeometric function in Bessel functions. This expansion is obtained by applying the standard integral representation of the gamma function to the factors $(a)_n=\Gamma(a+n)/\Gamma(a)$ and $(b)_n$ in the coefficients of the power series representation of the hypergeometric function. The expansion is

$$\frac{(z/2)^c}{\Gamma(c+1)}\,{}_2F_1(a,b,c+1;-z^2/4ab)=\sum_{\nu=0}^{\infty}\frac{1}{\nu!}\,{}_3F_0(-\nu,a,b;1/ab)(z/2)^\nu J_{c+\nu}(z), \tag{1}$$

where

$${}_3F_0(-\nu)={}_3F_0(-\nu,a,b;1/ab)=\sum_{n=0}^{\nu}\frac{(-\nu)_n}{n!}(a)_n(b)_n/(ab)^n \tag{2}$$

is a generalized hypergeometric polynomial. It is easily seen that ${}_3F_0(0)=1$, ${}_3F_0(-1)=0$, and that ${}_3F_0(-\nu)$ for $\nu\geqslant 2$ is a symmetric polynomial in $1/a$ and $1/b$ of degree $2(\nu-1)$ with constant term 0 and the two highest degree terms coming from the last term in the sum in (2):

$$(-1)^\nu[(\nu-1)!]^2[1/(ab)^{\nu-1}+\{1+1/2+\cdots+1/(\nu-1)\}(1/a^{\nu-1}b^{\nu-2}+1/a^{\nu-2}b^{\nu-1})]. \tag{3}$$

It is less trivial to find the degree and value of the first nonvanishing term. We do this by using a saddle point asymptotic estimate—a and b large—in the double integral representation of ${}_3F_0$. The result is different for even and odd ν:

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$$ {}_3F_0(-2\kappa)\approx\frac{\Gamma(2\kappa+1)}{2^\kappa\Gamma(\kappa+1)}(1/a+1/b)^\kappa, \tag{4}$$

$$ {}_3F_0(-2\kappa-1)\approx\frac{\Gamma(2\kappa+1)}{2^{\kappa-1}\Gamma(\kappa)}[(1/a^2+1/b^2)/3+1/ab)](1/a+1/b)^{\kappa-1}. \tag{5}$$

This means that in reordering (1) into an expansion (possibly only asymptotic) after increasing powers of $1/a$ and $1/b$ the nth order terms, of the form $1/a^{n-\mu}b^\mu+1/a^\mu b^{n-\mu}$, contain Bessel functions of orders $c+[(n+3)/2]$ up to $c+2n$ ($[m]$ denotes the integer part of m). As an example we give the expansion including third-order terms in $1/a$ and $1/b$ [see (18)].

The asymptotic behavior of the terms on the right-hand side of (1) as $\nu\to\infty$ turns out to be the same as the behavior of the terms in the power series expansion of the left-hand side. The series is thus convergent provided $|z^2/4ab|<1$, and under this condition (1) is a valid expansion for all (possibly complex) z, a, and b, as follows from standard theorems on integration of series term by term, and on analytic continuation of series of holomorphic functions. It should be pointed out that the series obtained for the asymptotics in $1/a$ and $1/b$ might be only asymptotic, since its derivation involves a rearrangement of the convergent series using an increasing number of terms.

Finally it should be remarked that (1) is an example of what is called a modified Neumann series expansion of a function in a series of Bessel functions.[2,3] This means that the coefficients ${}_3F_0$ can also be derived from the general formula expressing the coefficients of the Bessel function expansion in terms of the power series coefficients of the function that one expands [see, e.g., Ref. 3, p. 66, (18)–(20)]. This presupposes that one knows which function to expand, and thus the derivation given here leads in a more natural way to the expansion of ${}_2F_1$ with the argument $-z^2/4ab$. Anyhow, it is very likely that the expansion (1) is already given somewhere in the enormous literature on Bessel functions, although it does not seem to occur in any of the standard handbooks.

II. DERIVATION OF FORMULAS (1)–(5)

Let us first derive the expansion (1). We start from the power series expansion of the relevant hypergeometric function,:

$$ F\equiv{}_2F_1(a,b,c+1;-z^2/4ab)=\sum_{n=0}^{\infty}\frac{(a)_n(b)_n}{(c+1)_n n!}(-z^2/4ab)^n. \tag{6}$$

We assume of course the convergence condition $|z^2/4ab|<1$, and shall also assume a and b real and positive, sometimes even large and going to infinity. Establishing relation (1) under these conditions we can use analytic continuation of both sides to extend the validity to general a and b.

Introducing the standard gamma function integral representation in the factors $(a)_n$ and $(b)_n$ in (6), and making a variable change $s=ax$, thus

$$ (a)_n=\frac{1}{\Gamma(a)}\int_0^\infty \mathrm{d}s\, e^{-s}s^{a+n-1}=\frac{a^{a+n}}{\Gamma(a)}\int_0^\infty \mathrm{d}x\, e^{-ax}x^{a+n-1},\ \text{etc.}, \tag{7}$$

we can interchange summation and integration and perform the summation to get

$$ F=\frac{a^a b^b}{\Gamma(a)\Gamma(b)}\int\int \mathrm{d}x\,\mathrm{d}y e^{-a(x-\ln x)-b(y-\ln y)}(xy)^{-1}\,{}_0F_1(c+1;-xy\,z^2/4), \tag{8}$$

where

$$ {}_0F_1(c+1;-u^2/4)=\sum_{n=0}^{\infty}\frac{1}{(c+1)_n n!}(-u^2/4)^n=\frac{\Gamma(c+1)}{(u/2)^c}J_c(u). \tag{9}$$

This relation, added to the following ''asymptotic expansion'' argument, motivates the choice of expanding the original F function with the argument $-z^2/4ab$. The function $f(x)=x-\ln x$ in the exponent of (8) goes from $+\infty$ at $x=0$ through a minimum 1 at $x=1$ to $+\infty$ at $x=\infty$. So if we want to study the behavior of the integral for large a and b we should obviously expand around $x=y=1$, which is a two-dimensional saddle point if we extend x and y to complex variables. We have $f(x)=1+(x-1)^2/2-(x-1)^3/3+\cdots$, so an asymptotic estimate (to be performed later) should use the new variables $\xi=\sqrt{a}(x-1)$, $\eta=\sqrt{b}(y-1)$. But first we shall establish formula (1) by expanding the ${}_0F_1$ function around $-z^2/4$, putting $-xyz^2/4=-z^2/4-(xy-1)z^2/4$. From the power series expansion one easily derives for the nth derivative ${}_0F_1^{(n)}(c+1;x)={}_0F_1(c+n+1;x)/(c+1)_n$. The Taylor expansion of ${}_0F_1$ around $-z^2/4$ then gives, with Bessel functions on the right-hand side,

$$ {}_0F_1(c+1;-xy\,z^2/4)=\frac{\Gamma(c+1))}{(z/2)^c}\sum_{\nu=0}^{\infty}\frac{1}{\nu!}(1-xy)^{\nu}(z/2)^{\nu}J_{c+\nu}(z). \tag{10}$$

Introducing (10) in (8), interchanging integration and summation, expanding the factor $(1-xy)^{\nu}$ in each term, and performing the integrations, we finally get the formulas (1) and (2), where as an intermediate result we get for ${}_3F_0$ the integral representation

$$ {}_3F_0(-\nu,a,b;1/ab)=\frac{a^a b^b}{\Gamma(a)\,\Gamma(b)}\int\int \mathrm{d}x\mathrm{d}y e^{-a(x-\ln x)-b((y-\ln y)}(xy)^{-1}(1-xy)^{\nu}. \tag{11}$$

It may be noted that (10), written for the Bessel function on the left-hand side:

$$ J_c(\varsigma z)=\varsigma^c\sum_{\nu=0}^{\infty}\frac{(1-\varsigma^2)^{\nu}}{\nu!}(z/2)^{\nu}J_{c+\nu}(z), \tag{12}$$

is the multiplication theorem for the Bessel function.[4]

Before we derive the lowest order expressions (4) and (5) for ${}_3F_0(-\nu)$, we shall establish the convergence of the expansion (1) provided $|z^2/4ab|<1$. So we should evaluate the asymptotic behavior as $\nu\to\infty$ of the factors on the right-hand side of (1). For the Bessel function the first term in the series expansion dominates, $J_{c+\nu}(z)\approx(z/2)^{c+\nu}/\Gamma(c+\nu+1)$. To make the asymptotic estimate for ${}_3F_0(-\nu)$ we use the integral representation (11) and observe that for large ν the main contribution to the integral comes from large x and y, so we can put $(1-xy)^{\nu}=(-xy)^{\nu}(1-\nu/xy+\cdots)\approx(-xy)^{\nu}$. The double integral can then be simply computed and we get ${}_3F_0(-\nu)\approx(-1)^{\nu}(a)_{\nu}(b)_{\nu}/(ab)^{\nu}$, not surprisingly just the last term in the expansion (2) of ${}_3F_0(-\nu)$. Altogether we get

$$ \frac{1}{\nu!}{}_3F_0(-\nu)(z/2)^{\nu}J_{c+\nu}(z)\approx\frac{(z/2)^c}{\Gamma(c+1)}\frac{(a)_{\nu}(b)_{\nu}}{(c+1)_{\nu}\,\nu!}(-z^2/4ab)^{\nu}. \tag{13}$$

So the asymptotic behavior of the terms of the series on the right-hand side of (1) is the same as the terms in the series expansion of the function on the left-hand side. Using basic theorems on integration of convergent function series it is then easy to establish the validity of (1) under the condition $|z^2/4ab|<1$, and furthermore a and b real and positive. But using analytic continuation of the functions of a and b (and even c) on both sides, we can conclude the validity of (1) for all a, b, and z satisfying $|z^2/4ab|<1$.

Let us now study the polynomial ${}_3F_0(-\nu)$ in $1/a$ and $1/b$. The series (2) can be written

$$ {}_3F_0(-\nu)=\sum_{n=0}^{\nu}(-1)^n\binom{\nu}{n}K_n, \tag{14}$$

where

$$K_{n+1}=(1+n/a)(1+n/b)\,K_n, K_0=1 \tag{15}$$

can be used for recursive calculation of ${}_3F_0(-\nu)$. Going from n to $n+1$ increases the polynomial degree in K_n by two units, so the two highest degree terms in ${}_3F_0$ come from the coefficient K_ν and are easily shown to be of the form given in (3). That ${}_3F_0(-\nu)$ has constant term 0 for $\nu \geqslant 1$ follows from the fact that all K_n have constant term 1. To study the first nonvanishing term in the series expansion seems less useful; instead we study the first term in an asymptotic expansion of the integral representation (11). In the standard spirit of asymptotic estimate by expansion around the saddle point $x=y=1$ we introduce, as already mentioned, the variables $\xi=\sqrt{a}(x-1)$, $\eta=\sqrt{b}(y-1)$, extend the integrations in these variables from $-\infty$ to $+\infty$, and find the lowest order term that is even in both variables (since odd terms give zero contribution from symmetry). To keep track of orders we put $a=mu$, $b=mw$, where m is large. There is a difference between the cases even or odd ν, $=2\kappa$, or $2\kappa+1$; in the even case the whole contribution comes from the leading term in the expansion of $(xy-1)^\nu \approx (\xi/\sqrt{u}+\eta/\sqrt{w})^\nu/m^{\nu/2}$, but for the odd case the next term comes in, and we also have to expand the third degree terms in the exponent and the factor $1/xy$. Doing this we get the expression

$$(-1)^\nu {}_3F_0(-\nu)\approx\frac{(a/e)^a(b/e)^b}{\Gamma(a)\Gamma(b)\sqrt{ab}}\int\int \mathrm{d}\xi\,\mathrm{d}\eta e^{-\xi^2/2-\eta^2/2}[\ldots], \tag{16}$$

where

$$[\ldots]=\left[1-\frac{1}{\sqrt{m}}\left(\frac{1}{\sqrt{u}}(\xi-\xi^3/3)+\frac{1}{\sqrt{w}}(\eta-\eta^3/3)\right)\right]\frac{1}{m^{\nu/2}}\left[(\xi/\sqrt{u}+\eta/\sqrt{w})^\nu+\nu\frac{1}{\sqrt{m}}(\xi/\sqrt{u}+\eta/\sqrt{w})^{\nu-1}\xi\eta/\sqrt{uw}\right]. \tag{17}$$

Expanding to the relevant lowest integer order of $1/m$ and performing the elementary integrations we finally get the results (4) or (5).

Expansion of ${}_2F_1$ to order three in $1/a$ and $1/b$ involves values of ν from 0 to 6. Here only ${}_3F_0(-4)$ contributes with terms not covered by the results given in (3), (4), or (5), namely the next lowest degree terms. The final result is

$$\begin{aligned}\frac{(z/2)^c}{\Gamma(c+1)}{}_2F_1(a,b,c+1;-z^2/4ab)=J_c(z)+\frac{1}{2}(1/a+1/b)(z/2)^2J_{c+2}(z)+(1/a^2+1/b^2)&\left[-\frac{1}{3}(z/2)^3J_{c+3}(z)+\frac{1}{8}(z/2)^4J_{c+4}(z)\right]\\+1/ab&\left[\frac{1}{2}(z/2)^2J_{c+2}(z)-(z/2)^3J_{c+3}(z)+\frac{1}{4}(z/2)^4J_{c+4}(z)\right]\\+\quad(1/a^3+1/b^3)&\left[\frac{1}{4}(z/2)^4J_{c+4}(z)-\frac{1}{6}(z/2)^5J_{c+5}(z)\right.\\&\left.+\frac{1}{48}(z/2)^6J_{c+6}(z)\right]+(1/a^2b+1/ab^2)\left[-(z/2)^3J_{c+3}(z)\right.\end{aligned}$$

$$+\frac{7}{4}(z/2)^4 J_{c+4}(z)-\frac{2}{3}(z/2)^5 J_{c+5}(z)+\frac{1}{16}(z/2)^6 J_{c+6}(z)\Bigg]$$
$$+\cdots. \tag{18}$$

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Time domain radiation by scalar sources: Plane wave to multipole transform

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The radiation from a pulsed source distribution can be described by a spectrum of time-dependent plane waves or of spherical waves (multipoles). These two fundamental representations are based on the slant stack transform and on the time-dependent multipole moment, respectively. In this article, we present a direct transformation relating these two representations. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1407282]

I. INTRODUCTION

In recent years there is a growing interest in the generation, detection and processing of ultra-wideband short-pulse fields, with emphasis on application pertaining to local interrogation and sensing of the propagation environment or to source-synthesis of collimated short-pulse beam fields. (For further discussions and references the readers are referred to Ref. 1.) Because of the broad frequency band of these fields, the conventional use of frequency domain techniques is often less efficient and physically less transparent than a direct solution in the space–time domain where the fields are well localized. The fundamental time-dependent field representations, namely the Green's function integral, the plane-wave spectrum, and the spherical waves (multipoles) expansion, have been thoroughly investigated recently with emphasis on their causal properties.[1–3] (For completeness, field representations based on spectral expansion using pulsed-beam basis functions should also be mentioned. Their main advantages are the spectral compactness and the use of local propagators; for further references, see Ref. 1) The results have been used in various applications, pertaining to time-domain antenna analysis in the *radiation* zone[4–6] and in the *reactive* zone,[7,8] to inverse scattering[9–11] and inverse source[12] problems, and to fast algorithms for numerical solution of time-dependent scattering problems.[13–15]

In the present article we derive a direct transformation relating the time-domain plane-wave and spherical-wave representations. This is done in Sec. III following a review in Sec. II of these representations.

The prototype problem considered is the radiation of the scalar field $u(\mathbf{r},t)$ in a uniform medium with wave speed c, satisfying the time-dependent wave equation

$$\left(\nabla^2-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)u(\mathbf{r},t)=-q(\mathbf{r},t), \tag{1}$$

where $\mathbf{r}=(x,y,z)\in\mathbb{R}^3$ and $t\in\mathbb{R}$. It is assumed that the source distribution $q(\mathbf{r},t)$ is confined in a volume V bounded within a sphere of radius R_0 centered at the origins and within the time window $t\in(0,T)$. The solution to (1) may be expressed by the well-known Green's function integration. Here, however, the emphasis is on the time-dependent plane waves and multipole representations.

II. BACKGROUND

A. The slant stack transform and time-dependent plane wave representations

The slant stack transform (SST) of a scalar volume source $q(\mathbf{r},t)$ is defined as

$$\tilde{q}(\mathbf{s},\tau)=\int_V dV\,\delta(\tau+c^{-1}\mathbf{s}\cdot\mathbf{r})*q(\mathbf{r},\tau) \tag{2a}$$

$$=\int_V dV q(\mathbf{r},\tau+c^{-1}\mathbf{s}\cdot\mathbf{r}), \tag{2b}$$

where $\tau\in\mathbb{R}$, $\mathbf{s}\in\mathbb{R}^3$, and $*$ denotes a temporal convolution. From (2a), the SST is identified as a Radon projection of $q(\mathbf{r},t)$ in the 4D space $(\mathbf{r},t)$, while (2b) is obtained by performing the τ convolution. Alternatively, performing the spatial integration in (2a) first, the SST can be expressed as two cascaded operations [Ref. 1, Eqs. (3.11) and (3.12)]

$$\mathcal{P}_q(\hat{\mathbf{s}};\sigma,\tau)=\int d^2r\, q(\mathbf{r},\tau)|_{\hat{\mathbf{s}}\cdot\mathbf{r}=\sigma} \tag{3a}$$

$$\tilde{q}(\mathbf{s},\tau)=\int d\sigma\,\mathcal{P}_q(\hat{\mathbf{s}};\sigma,\tau+|\mathbf{s}|\sigma/c), \tag{3b}$$

where (3a) is a spatial Radon projection of $q(\mathbf{r},\tau)$ at planes normal to the spectral direction $\hat{\mathbf{s}}\equiv\mathbf{s}/|\mathbf{s}|$ (unit vectors are denoted by over circles), while in (3b) these projections are stacked with a progressive time delay $\mathbf{s}\cdot\mathbf{r}/c$ associated with a planar front that propagates along the $\mathbf{s}$ axis at the spectral speed $v(\mathbf{s})=c/|\mathbf{s}|$.

The SST extracts the time-dependent plane-wave information of the source, hence the field can be recovered as a superposition of the SST constituents $\tilde{q}(\mathbf{s},\tau)$ via the inverse SST [Ref. 1, Eqs. (3.10)]. One option, which applies both inside and outside the source region, is an integration in the entire 3D $\mathbf{s}$ domain [Ref. 1, Eq. (3.17)]. This involves SST constituents that propagate in all directions $\hat{\mathbf{s}}$ and in all spectral speeds $v(\mathbf{s})=c/|\mathbf{s}|$ [see (3b)].

Outside the source region, on the other hand, the full 3D spectral representation may be contracted to a 2D representation on the unit-sphere $|\mathbf{s}|=1$, involving only plane-wave constituents with wave speed c. There are two options for such formulations: In the **Weyl-type** representation, the field synthesis involves both *propagating* and *evanescent* spectra, identified by *real* and *complex* $\mathbf{s}$, respectively (with $|\mathbf{s}|=1$ in both cases). The incorporation of complex $\mathbf{s}$ requires an extension of the SST to complex time variables, an operation that is performed systematically via the analytic signal formulation [Ref. 1. Eqs. (4.13) and (4.14)]. The resulting integral representation is *strictly causal*, i.e., it vanishes prior to the wave arrival. The **Wittaker-type** representation, on the other hand, involves only the propagating part of the SST spectrum. It is valid only for $t>T$ after the source has turned off, while for $t<T$ it yields noncausal contributions [Ref. 1, Eqs. (7.13) and (7.14)] (see also Ref. 16). For $t>T$ it is given by

$$u(\mathbf{r},t)=\frac{-1}{8\pi^2}\partial_{ct}\int_{4\pi} d^2s\,\tilde{q}(\mathbf{s}\cdot t-c^{-1}\mathbf{s}\cdot\mathbf{r}), \tag{4}$$

where here and henceforth $\mathbf{s}$ is a unit vector whose Cartesian coordinates are given by $(\sin\alpha\cos\beta,\sin\alpha\sin\beta,\cos\alpha)$, i.e., $\int_{4\pi} d^2s=\int_0^{\pi}\sin\alpha\,d\alpha\int_{-\pi}^{\pi}d\beta$. Finally, it is noted that in the far radiation zone the field has the form

$$u(\mathbf{r},t)\sim(4\pi r)^{-1}\tilde{q}(\hat{\mathbf{r}},t-r/c), \tag{5}$$

where $r=|\mathbf{r}|$ and $\hat{\mathbf{r}}=\mathbf{r}/r$. Thus the time-dependent radiation pattern is determined by the SST constituent $\mathbf{s}=\hat{\mathbf{r}}$ in the $\mathbf{r}$ direction.

B. Spherical wave (multipoles) expansion

The spherical wave solutions of the *homogeneous* wave equation are given by[17]

$$\varphi_\nu(\mathbf{r},t)=(-1)^n 2\pi\frac{c}{r}[P_n(ct/r)p(ct/r)]Y_\nu(\mathring{\mathbf{r}}), \tag{6}$$

where $\mathring{\mathbf{r}}$ is a unit vector in the $\mathbf{r}$ direction, identified by the spherical angles (θ, ϕ), and $Y_\nu(\mathring{\mathbf{r}})$ are the *real* spherical harmonics defined, for the triple index $\nu=(n,m,s)$ with $s=1,2$, $n=0,1,...$, and $m=0,1,...n$, by

$$\begin{Bmatrix} Y_{n,m,1}(\mathring{\mathbf{r}}) \\ Y_{n,m,2}(\mathring{\mathbf{r}}) \end{Bmatrix} = y_{nm}P_n^m(\cos\theta)\begin{Bmatrix} \cos \\ \sin \end{Bmatrix} m\phi. \tag{7}$$

with $y_{nm}=\sqrt{\varepsilon_m(2n+1)/4\pi}\sqrt{(n-m)!/(n+m)!}$ and the Neumann symbol $\varepsilon_m=1$ or 2 for $m=0$ or $m>0$, respectively. P_n^m and $P_n^0=P_n$ are the associate Legendre functions and polynomials, respectively (Ref. 18, Chap. 8), and $p(x)$ is a rectangular pulse, $p(x)=1$ for $|x|\leqslant 1$ and 0 otherwise. The solutions in (6) may readily be verified by solving the time-dependent wave equation in spherical coordinates, and are the Fourier transform of the frequency domain solutions $4\pi\cdot(-i)^n j_n(kr)Y_\nu(\mathring{\mathbf{r}})$ where $j_n(kr)$ is the spherical Bessel function (Ref. 18, Chap. 10).

The spherical wave expansion of the Green's function is (see also Ref. 17)

$$g(\mathbf{r},\mathbf{r}',t)=\delta(t-c^{-1}|\mathbf{r}-\mathbf{r}'|)/4\pi|\mathbf{r}-\mathbf{r}'| \tag{8}$$

$$=\sum_\nu \varphi_\nu(\mathbf{r}_<,t)*\psi_\nu(\mathbf{r}_>,t), \tag{9}$$

where $(\mathbf{r}_<,\mathbf{r}_>)=(\mathbf{r}',\mathbf{r})$ or $(\mathbf{r},\mathbf{r}')$ if $r'\leqslant r$, respectively, and the spherical propagators are

$$\psi_\nu(\mathbf{r},t)=(4\pi r)^{-1}Y_\nu(\mathring{\mathbf{r}})\partial_t[P_n(ct/r)H(t-r/c)]. \tag{10}$$

H being the Heaviside function, $H(x)=0$ or 1 for $x\lessgtr 0$, respectively. ψ_ν are the inverse Fourier transforms of the frequency domain propagators $(4\pi)^{-1}i^{n+1}kh_n^{(1)}(kr)Y_\nu(\mathring{\mathbf{r}})$. The $n=0$, 1, 2 terms of $\partial_t[P_n(ct/r)H(t-r/c)]$ in (10) are, respectively, $\delta(t-r/c)$, $\delta(t-r/c)+(c/r)H(t-r/c)$, and $\delta(t-r/c)+3[(c/r)+(c/r)^2(t-r/c)]H(t-r/c)$.

Substituting (9) into the Green's function solution of (1), $u=\int_V d^3r'q[\mathbf{r}'\cdot t-|\mathbf{r}-\mathbf{r}'|/c]/4\pi|\mathbf{r}-\mathbf{r}'|$, we may express the radiated field for $r>R_0$ as

$$u(\mathbf{r},t)=\sum_\nu \psi_\nu(\mathbf{r},t)*q_\nu(t), \tag{11}$$

where the multipole moment $q_\nu(t)$ of the volume source $q(\mathbf{r},t)$ are given by

$$q_\nu(\tau)=\langle\varphi_\nu(\mathbf{r},t),q(\mathbf{r},t)\rangle=\int_V dV\,\varphi_\nu(\mathbf{r},t)*q(\mathbf{r},t). \tag{12a}$$

Performing the integral, they may also be calculated via [Ref. 2, Eq. (3.25)]

$$q_\nu(t)=2\pi\frac{1}{2^n n!}\int_V dV\,Y_\nu(\mathring{\mathbf{r}})(r/c)^n\partial_t^n\int_{-1}^1 d\eta\,(1-\eta^2)^n q(\mathbf{r},t+\eta r/c). \tag{12b}$$

Finally, noting that $\psi_\nu\to(4\pi r)^{-1}Y_\nu(\mathring{\mathbf{r}})\delta(t-r/c)$ for $r\to\infty$ we find for the far radiation field (Ref. 2, Sec. 3b)

$$u(\mathbf{r},t)\sim\frac{1}{4\pi r}\sum_{\nu}\ q_{\nu}(\tau)Y_{\nu}(\mathring{\mathbf{r}}),\tag{13}$$

which is an alternative to the SST result in (5).

III. NEW RESULTS: THE TIME-DEPENDENT PLANE-WAVE–MULTIPOLE TRANSFORM

The time-dependent plane wave kernel that propagate in the **s** direction can be expanded in terms of multipoles (spherical waves) as

$$\delta(t+c^{-1}\mathbf{s}\cdot\mathbf{r})=\sum_{\nu}\ Y_{\nu}(\mathbf{s})\varphi_{\nu}(\mathbf{r},t).\tag{14}$$

The inverse relation, namely the time-dependent plane wave expansion of a multipole field, has the form of a Whittaker's expansion [see (4)]:

$$\varphi_{\nu}(\mathbf{r},t)=\int_{4\pi}d^2s\ \delta(t+c^{-1}\mathbf{s}\cdot\mathbf{r})Y_{\nu}(\mathbf{s}).\tag{15}$$

Equations (14) and (15) form a transform pair relating plane waves and spherical waves

Proof: The proof of (14) is based on the frequency domain relation[19]

$$e^{ik\mathbf{s}\cdot\mathbf{r}}=4\pi\sum_{\nu}\ i^n j_n(kr)Y_{\nu}(\mathring{\mathbf{r}})Y_{\nu}(\mathbf{s}),\tag{16}$$

which is transformed to the time domain using $4\pi(-i)^n j_n(kr)Y_{\nu}(\mathring{\mathbf{r}})\Rightarrow\varphi_{\nu}(\mathbf{r},t)$, $e^{ik\mathbf{s}\cdot\mathbf{r}}\Rightarrow\delta(t-c^{-1}\mathbf{s}\cdot\mathbf{r})$ and $Y_{\nu}(-\mathbf{s})=(-)^n Y_{\nu}(\mathbf{s})$. To prove (15) we multiply both sides of (14) by $Y_{\nu'}(\mathbf{s})$ and utilize the orthogonality relation $\int_{4\pi}d^s Y_{\nu}(\mathbf{s})Y_{\nu'}(\mathbf{s})=\delta_{\nu,\nu'}$, where $\delta_{\nu,\nu'}$ is the Kronecker's delta.

A. Applications: The relation between the SST and the multiple expansion

The transform relations above can be used to derive direct transform relations between the time-dependent multipole functions and the SST of the source distribution. Indeed, inserting (14) into (2a), using the definition in (12a), we obtain a *spherical waves synthesis of the SST*

$$\tilde{q}(\mathbf{s},t)=\sum_{\nu}\ Y_{\nu}(\mathbf{s})q_{\nu}(t).\tag{17}$$

Alternatively, inserting (15) in (12a) results in the *SST expansion of the multipole moment*

$$q_{\nu}(t)=\int_{4\pi}d^2s\ \tilde{q}(\mathbf{s},t)Y_{\nu}(\mathbf{s}).\tag{18}$$

Thus, based on Eqs. (14) and (15), one may rederive much of the spherical wave expansion theory of Sec. II B as a projection of the plane-wave transform theory of Sec. II A. In particular, (17) and (18) comply with the equivalence of the time-dependent radiation patterns in (5) and (13).

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